

**ЦИТИРАНИЯ**  
**на чл.-кор. проф. дбн Илга Константинова Пъжева**

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**В международни и чуждестранни списания и книги (в хронологичен ред):**

- 1. Pajeva, I.K., M. Wiese, H.-P.Cordes, J. K. Seydel. Membrane interactions of some catamphiphilic drugs and relation to their multidrug resistance reversing ability, *J. Cancer Res. Clin. Oncol.* 1996, 122 (1), 27-40.**

Цитирания: 94

1. Belhoussine R, Morjani H, Manfait M Effect of quinine on the multidrug resistance and intracellular distribution of THP-DOX in LR73 tumor cells: Comparative study with verapamil and S9788 by confocal laser microspectrofluorometry. *B CANCER* 84 (4): 343-349 APR 1997
2. Ecker G, Chiba P Recent developments in overcoming tumour cell multi-drug resistance. *EXPERT OPIN THER PAT* 7 (6): 589-599 JUN 1997
3. Morjani H, Millot JM, Belhoussine R, et al. Anthracycline subcellular distribution in human leukemic cells by microspectrofluorometry: Factors contributing to drug-induced cell death and reversal of multidrug resistance. *LEUKEMIA* 11 (7): 1170-1179 JUL 1997
4. Wattel E, Lepelley P Multidrug resistance in myelodysplastic syndromes: a potential role for reversion-inducing agents? *PATHOL BIOL* 45 (8): 637-642 OCT 1997
5. DeFlora S, Camoirano A, Cartiglia C, et al. Modulation of the potency of promutagens and direct acting mutagens in bacteria by inhibitors of the multidrug resistance mechanism. *MUTAGENESIS* 12 (6): 431-435 NOV 1997
6. Hanusovska E, Dovinova I, Tkac I, et al. Application of NMR spectroscopy in biochemical studies of tumor cells sensitive and resistant to anticancer drugs. *NEOPLASMA* 45 (4): 187-197 1998
7. Shimada H, Grutzner JB, Kozlowski JF, et al. Membrane conformations and their relation to cytotoxicity of asimicin and its analogues. *BIOCHEMISTRY-US* 37 (3): 854-866 JAN 20 1998
8. Alsenz J, Steffen H, Alex R Active apical secretory efflux of the HIV protease inhibitors saquinavir and zidovudine in Caco-2 cell monolayers. *PHARMACEUT RES* 15 (3): 423-428 MAR 1998
9. Wattel, E.; Solary, E.; Hecquet, B.; Caillot, D.; Ifrah, N.; Brion, A.; Mahe, B.; Milpied, N.; Janvier, M.; Guerci, A.; Rochant, H.; Cordonnier, C.; Dreyfus, F.; Buzyn, A.; Hoang-Ngoc, L.; Stoppa, A. M.; Gratecos, N.; Sadoun, A.; Stamatoulas, A.; Tilly, H.; Brice, P.; Maloisel, F.; Lioure, B.; Desablens, B.; Pignon, B.; Abgrall, J. P.; Leporrier, M.; Dupriez, B.; Guyotat, D.; Lepelley, P.; Fenaux, P. Quinine improves the results of intensive chemotherapy in myelodysplastic syndromes expressing P glycoprotein: results of a randomized study. *BRIT J HAEMATOL* 102 (4): 1015-1024 SEP 1998
10. Morjani H, Belhoussine R, Lahlil R, et al. Pirarubicin nuclear uptake does not correlate with its induced cell death effect during reversal of multidrug resistance by quinine in human K562 and CEM leukemic cells. *EUR J HAEMATOL* 61 (4): 240-249 OCT 1998
11. Preuner JG, Lehle K, Keyser A, et al. Development of severe adverse effects after discontinuing amiodarone therapy in human heart transplant recipients. *TRANSPLANT P* 30 (8): 3943-3944 DEC 1998
12. Liu KZ, Schultz CP, Johnston JB, et al. Infrared spectroscopic study of bryostatin 1-induced membrane alterations in a B-CLL cell line. *LEUKEMIA* 13 (8): 1273-1280 AUG 1999
13. Wattel, E.; Solary, E.; Hecquet, B.; Caillot, D.; Ifrah, N.; Brion, A.; Milpied, N.; Janvier, M.; Guerci, A.; Rochant, H.; Cordonnier, C.; Dreyfus, F.; Veil, A.; Hoang-Ngoc, L.; Stoppa, A. M.; Gratecos, N.; Sadoun, A.; Tilly, H.; Brice, P.; Lioure, B.; Desablens, B.; Pignon, B.; Abgrall, J. P.; Leporrier, M.; Dupriez, B.; Guyotat, D.; Lepelley, P.; Fenaux, P. Quinine improves results of intensive chemotherapy (IC) in myelodysplastic syndromes (MDS) expressing P-glycoprotein (Pgp) - Updated results of a randomized study In: *Drug Resistance in Leukemia and Lymphoma III (Advances in Experimental Medicine and Biology)*, G.J.L. Kaspers, R. Pieters, and A.J.P. Veerman (Eds.), Springer, 457, 35-46, 1999. (cit. p. 45)
14. Bermudez M, Martinez E, Mora M, et al. Molecular and physicochemical aspects of the interactions of the tuberculostatics ofloxacin and rifampicin with liposomal bilayers: a P-31-NMR and DSC study. *COLLOID SURFACE A* 158 (1-2): 59-66 NOV 10 1999
15. FU li wu, PAN Qi chao, HUANG Hong bing, et al. Influence of some potent modulators of multidrug resistance on cellular membrane fluidity and expression of P gp protein, Cancer Center, Sun Yat sen University of Medical Sciences, Guangzhou 510060, China, *CHINESE JOURNAL OF CANCER*, vol.18, No.3, 1999

16. Millot, J.-M.; Morjani, H.; Millot, C.; Belhoussine, R.; Sebillé, S.; Manfait, M. Incorporation of anthracyclines into tumor cells and pleiotropic resistance. *Dynamique de la Cellule Vivante* (1999), 333-347.
17. Holzgrabe, U., I. Wawer, B. Diehl (eds.) In: *NMR spectroscopy in Drug Development, Ligand-membrane interaction*, Chapter 11, Wiley-VCH, 1999, pp.175-230.(citation 93, p.230)
18. Ferte J Analysis of the tangled relationships between P-glycoprotein-mediated multidrug resistance and the lipid phase of the cell membrane . *EUR J BIOCHEM* 267 (2): 277-294 JAN 2000
19. Pallares-Trujillo J, Lopez-Soriano FJ, Argiles JM Lipids: A key role in multidrug resistance? (Review) *INT J ONCOL* 16 (4): 783-798 APR 2000
20. Castaing M, Brouant P, Loiseau A, et al. Membrane permeation by multidrug-resistance-modulators and non-modulators: Effects of hydrophobicity and electric charge *J PHARM PHARMACOL* 52 (3): 289-296 MAR 2000
21. Hianik T, Fajkus M, Tarus B, et al. The changes of capacitance relaxation of bilayer lipid membranes induced by chlorpromazine. *PHARMAZIE* 55 (7): 546-547 JUL 2000
22. Shibata N, Matsumura Y, Okamoto H, et al. Pharmacokinetic interactions between HIV-1 protease inhibitors in rats: Study on combinations of two kinds of HIV-1 protease inhibitors. *J PHARM PHARMACOL* 52 (10): 1239-1246 OCT 2000
23. Castaing M, Loiseau A, Dani M Thermal dependence of multidrug-resistant-modulator efficiency: A study in anionic liposomes. *J PHARM PHARMACOL* 52 (10): 1171-1178 OCT 2000
24. Ulrich Joerg Franke, Quantitative Analyse von Arzneistoff-Membran-Wechselwirkungen am Beispiel von Neuroleptika und Calcium-Kanal Blockern Dissertation, MLU Halle-Wittenberg, 2000.
25. Durandt C, 2000, *P-glikoproteien neutraliseringspotensiaal en weefsel verspreiding van tetramietel-piperidien derivate van klofasimien*, PhD thesis, University of Pretoria, Pretoria, <http://upetd.up.ac.za/thesis/available/etd-08302010-170400>
26. Dei, S.; Gualtieri, F.; Scapecchi, S.; Teodori, E.; Garnier-Suillerot, A. Mediators of classical multidrug resistance [MDR] and the medicinal chemistry of reversing drugs. *Recent Research Developments in Medicinal Chemistry* (2001), 1, 18-64.
27. Hendrich AB, Wesolowska O, Michalak K Trifluoperazine induces domain formation in zwitterionic phosphatidylcholine but not in charged phosphatidylglycerol bilayers. *BBA-BIOMEMBRANES* 1510 (1-2): 414-425 FEB 9 2001
28. Fruttero, R. NMR spectroscopy for the study of drug-phospholipid interactions. In: *Pharmacokinetic optimization in drug research*, B.Testa, H.Waterbeemd, G. Folkers, T. Guy (Eds.), Wiley-VCH, Zurich, 2002, pp.465-482.
29. DSC Lipids/Membrane Studies In: *Bibliography of Calorimetry Science Corporation*, 2001, p. 85, <http://huffy.bioeng.washington.edu/~hyre/docs/Cal-Refs.pdf>
30. Michalak K, Hendrich AB, Wesolowska O, Pola A. Compounds that modulate multidrug resistance in cancer cells, *CELL. BIOL. MOL. LETT.* Vol. 6, No. 2A, 2001, 362-368.
31. Castaing M, Loiseau A, Dani M, Designing multidrug-resistance modulators circumventing the reverse pH gradient in tumours. *J PHARM PHARMACOL* 53 (7): 1021-1028 JUL 2001
32. Lange K, Gartzke J Microvillar cell surface as a natural defense system against xenobiotics: a new interpretation of multidrug resistance. *AM J PHYSIOL-CELL PH* 281 (2): C369-C385 AUG 2001
33. Wesolowska O, Hendrich AB, Motohashi N, Michalak K Interaction of major phospholipids of erythrocyte membrane's inner leaflet (PS, PE) with phenothiazine methansulfonylamides. *CELL MOL BIOL LETT* 6(2), 232, 2001
34. Wesolowska O, Hendrich AB, Motohashi N, Michalak K Phenothiazine derivative causes phase separation in phosphatidylethanolamine model membranes. *CURR TOPICS BIOPHYS* 25(2): 71-73 2001
35. Arvelo F., Merentes E, *Biomodulation Farmacologia en Cancer. Revision (Farmacologia) ACTA CIANTIFFICA VENEZOLANA*, 52: 68-77, 2001
36. Avendano C, Menendez JC Inhibitors of multidrug resistance to antitumor agents (MDR) *CURR MED CHEM* 9 (2): 159-193 JAN 2002
37. Shibata N, Gao WH, Okamoto H, et al. In-vitro and in-vivo pharmacokinetic interactions of amprenavir, an HIV protease inhibitor with other current HIV protease inhibitors in rats. *J PHARM PHARMACOL* 54 (2): 221-229 FEB 2002
38. Wattel, E., P. Fenaux, E. Gamelin et al., Etude en phase I/II d'une réversion du phénotype de résistance multidrogue (mdr) par la quinine à posologie ajustée dans le traitement des syndromes myélodysplasiques (SMD) mdr+ par chimiothérapie intensive à base d'anthracyclines, GFM protocole 2, Groupes GFM et GOELAMS, 2002. [www.gfmgroup.org/pdf/protocole2.pdf](http://www.gfmgroup.org/pdf/protocole2.pdf)

39. Hendrich AB, Wesolowska O, Komorowska M, Motohashi N, Michalak K The alterations of lipid bilayer fluidity induced by newly synthesized phenothiazine derivative. *BIOPHYS CHEM* 98: 275-282 2002
40. Teodori E, Dei S, Scapecchi S, et al. The medicinal chemistry of multidrug resistance (MDR) reversing drugs. *FARMACO* 57 (5): 385-415 MAY 2002
41. Wesolowska, O., Molnar, J., Motohashi, N., Michalak, K. Inhibition of P-glycoprotein transport function by N-acylphenothiazines. *ANTICANCER RESEARCH*, 2002, Sept-Oct, 22 (5), 2863-2867.
42. Michalak K, Hendrich AB. Role of cell membrane lipids in multidrug resistance and its modulation. Review. *Postepy Biochem.* 2002; 48(3):208-19.
43. L Ziru, L Shengli, L Shaokai. Effects of microwave on human multidrug-resistant leukemic cell line K562/MDR *GUANGDONG MEDICAL JOURNAL* Vol.23 No.3 P.233-235, 2002
44. Castaing M, Loiseau A, Djoudi L. Effects of cholesterol on dye leakage induced by multidrug-resistance modulators from anionic liposomes. *EUR J PHARM SCI.* 2003 Jan;18(1):81-8.
45. Hendrich AB, Michalak K. Lipids as a target for drugs modulating multidrug resistance of cancer cells. *CURR DRUG TARGETS.* 2003 Jan;4 (1):23-30.
46. Castaing, M, Loiseau, A, Mulliert, G. Interactions between verapamil and neutral and acidic liposomes: effects of the ionic strength. *BIOCHIMICA ET BIOPHYSICA ACTA-BIOMEMBRANES* 2003, APR 1, 1611 (1-2) 107-114.
47. Hendrich AB, Wesolowska O, Motohashi N, Molnar J, Michalak K. New phenothiazine-type multidrug resistance modifiers: anti-MDR activity versus membrane perturbing potency. *BIOCHEM BIOPHYS RES COMMUN.* 2003 May 2;304(2):260-265.
48. Hendrich AB, Wesolowska O, Pola A, Motohashi N, Molnar J, Michalak K. Neither lipophilicity nor membrane-perturbing potency of phenothiazine maleates correlate with the ability to inhibit P-glycoprotein. *MOL MEMBR BIOL* 2003 20 (1) 53-60.
49. Bobrowska-Hägerstrand, M, A. Wróbel, L. Mrówczyńska, T. Söderström, H. Hägerstrand. Modulation of MRP1-like efflux activity in human erythrocytes caused by membrane perturbing agents. *MOL MEMBR BIOL* 2003 20 (3) 255-259.
50. Klopman G, Zhu H, Ecker G, Chiba, P. MCASE study of the multidrug resistance reversal activity of propafenone analogs. *J COMPUT AID MOL DES* 17 (5-6): 291-297 MAY-JUN 2003
51. Motohashi N, Kawase M, Molnar J, Ferenczy L, Wesolowska O, Hendrich AB, Bobrowska-Hägerstrand M, Hägerstrand H, Michalak K. Antimicrobial activity of N-acylphenothiazines and their influence on lipid model membranes and erythrocyte membranes. *ARZNEIMITTEL-FORSCH* 53 (8): 590-599 2003
52. Funao T, Oda Y, Tanaka K, Asada, A. The P-glycoprotein inhibitor quinidine decreases the threshold for bupivacaine-induced, but not lidocaine-induced, convulsions in rats. *CAN J ANAESTH* 50 (8): 805-811 OCT 2003
53. Zhang Jian Quan ; Liu Yong Jiang ; Gao Zhi Bin ; Huang Gui Lin. The Expression of MDR, its Clinical Significance and Exploration Related, *Journal of Nongken Medicine (Chinese journal of clinical oncology and rehabilitation)*, 2003, Vol.6; 435-440. cited as [18]
54. Georgette Plemper van Balen, Catherine a Marca Martinet, Giulia Caron, Géraldine Bouchard, Marianne Reist, Pierre-Alain Carrupt, Roberta Fruttero, Alberto Gasco, Bernard Testa, Liposome/water lipophilicity: Methods, information content, and pharmaceutical applications. *MED RES REV* 24 (3): 299-324 MAY 2004
55. Wesolowska O, Hendrich AB, Motohashi N, Kawase M, Dobryszycycki P, Ozyhar A, Michalak K. Presence of anionic phospholipids rules the membrane localization of phenothiazine type multidrug resistance modulator. *BIOPHYS CHEM* 109 (3): 399-412 JUN 1 2004
56. Avendano, C., J.C. Menedez. Recent Advances in Multidrug Resistance Modulators *MEDICINAL CHEMISTRY REVIEWS – ONLINE*, 2004, vol. 1, no. 4, pp. 419-444 (26).
57. Триндяк, Володимир Петрович. Особливості структурно-функціонального стану плазматичних мембран пухлинних клітин, резистентних до доксорубіцину [Текст] : дис. канд. біол. наук: 14.01.07 / Триндяк Володимир Петрович ; НАН України, Інститут експериментальної патології, онкології і радіобіології ім. П.С.Кавецького. - К., 2004 PhD
58. Zaheeruddin, Acridones as reversers of drug resistance in cancer cells and their anti-bacterial activities. PhD Thesis, Department of pharmaceutical chemistry, v. L. College of pharmacy, Raichur-584103, Rajiv Gandhi University of Health Sciences, Bangalore, Karnataka, 2005. PhD thesis <http://14.139.159.4:8080/jspui/handle/123456789/2076>
59. Raub, T.J. P-glycoprotein recognition of substrates and circumvention through rational drug design, *MOLECULAR PHARMACEUTICS*, 3 (1), 78-86, 2006.

60. Hendrich, A.B., Stańczak, K., Komorowska, M., Motohashi, N., Kawase, M., Michalak, K. A study on the perturbation of model lipid membranes by phenoxazines. *BIOORGANIC AND MEDICINAL CHEMISTRY* 14 (17), pp. 5948-5954, 2006.
61. Ortuño, J.A., Hernández, J., Sánchez-Pedreño, C. Ion-selective electrode for the determination of some multidrug resistance reversers. *SENSORS AND ACTUATORS, B: CHEMICAL* 119 (1), pp. 282-287, 2006
62. Michalak, K., O. Wesolowska, N. Motohashi, J. Molnar and A. B. Hendrich Interactions of Phenothiazines with Lipid Bilayer and their Role in Multidrug Resistance Reversal. *CURRENT DRUG TARGETS*, Volume 7, Number 9, 1095-1105, September 2006.
63. Ahmed, Osman. Reversal of multidrug resistance in cancer cells by different N10-substituted acridone derivatives. Dissertation, Rajiv Gandhi University of health sciences, Bangalore, Karnataka, Department of pharmaceutical chemistry, V.L. College of pharmacy, 2006, pp. 1-133.  
<http://14.139.159.4:8080/jspui/handle/123456789/2014>
64. Konstantin Chegaev, Loretta Lazzarato, Barbara Rolando, Elisabetta Marini, Gloria V. Lopez, Massimo Bertinaria, Antonella Di Stilo, Roberta Fruttero, Alberto Gasco: Amphiphilic NO-Donor Antioxidants. *CHEMMEDCHEM*, Volume 2, Issue 2, 2007. Pages 234-240.
65. Puay-Wah Phuan, Julie A. Zorn, Jiri Safar, Kurt Giles, Stanley B. Prusiner, Fred E. Cohen and Barnaby C. H. May: Discriminating between cellular and misfolded prion protein by using affinity to 9-aminoacridine compounds. *J Gen Virol* 88 (2007), 1392-1401.
66. Castaing, Madeleine; Loiseau, Alain; Cornish-Bowden, Athel. Synergy between verapamil and other multidrug-resistance modulators in model membranes. *J. Biosci.* 32(4), June 2007, 737-746.
67. Ortuno, J. A.; Gil, A.; Serna, C.; Molina, A. Voltammetry of some catamphiphilic drugs with solvent polymeric membrane ion sensors. *Journal of Electroanalytical Chemistry*, 2007, 605(2), 157-161.
68. Michalak, K., O. Wesolowska, N. Motohashi, A.B. Hendrich. The Role of the Membrane Actions of Phenothiazines and Flavonoids as Functional Modulators. *Topics in Heterocyclic Chemistry* (2007), 8 (Bioactive Heterocycles II), 223-302. (S. Egguchi, Ed.), Volume 8, Springer Berlin / Heidelberg, 2007, 223-302.
69. Li, Y., Zhang, H.-B., Huang, W.-l., Li, Y.-M. Design and synthesis of tetrahydroisoquinoline derivatives as potential multidrug resistance reversal agents in cancer. *Bioorganic and Medicinal Chemistry Letters* 18 (12), 2008, pp. 3652-3655.
70. Kars MD, Iseri OD, Gunduz U, Molnar J: Reversal of Multidrug Resistance by Synthetic and Natural Compounds in Drug-Resistant MCF-7 Cell Lines. *Chemotherapy* 2008; 54:194-200.
71. Wesolowska O, Hendrich AB, Lania-Pietrzak B, et al: Perturbation of the lipid phase of a membrane is not involved in the modulation of MRP1 transport activity by flavonoids *CELLULAR & MOLECULAR BIOLOGY LETTERS* 2008 Volume: 14 Issue: 2 Pages: 199-221.
72. Tripathi, Kishu; Kulshreshtha, Shobha. Membrane-active agents-II. *Oriental Journal of Chemistry* (2008), 24(2), 623-628.
73. Cordes: Webster's Quatations, Facts and Phrases. ICON Group Int. Inc., San Diego, California, 2008.
74. Lucio, M; Lima, JLFC; Reis, S. Drug-Membrane Interactions: Significance for Medicinal Chemistry. *CURRENT MEDICINAL CHEMISTRY* 17 (17): 1795-1809 JUN 2010.
75. Lucio, M.; Lima, J.L.F.C.; Reis, S. Drug-Membrane Interactions: Molecular Mechanisms Underlying Therapeutic and Toxic Effects of Drugs. In: *Ideas in Chemistry and Molecular Sciences: Where Chemistry Meets Life* (Bruno Pignataro, ed.), Wiley-VCH, 2010, pp. 191-214.
76. Peetla, C; Bhave, R; Vijayaraghavalu, S; Stine, A; Kooijman, E; Labhasetwar, V. Drug Resistance in Breast Cancer Cells: Biophysical Characterization of and Doxorubicin Interactions with Membrane Lipids. *MOLECULAR PHARMACEUTICS* 7 (6): 2334-2348 NOV-DEC 2010.
77. Wesolowska, O. Interaction of phenothiazines, stilbenes and flavonoids with multidrug resistance-associated transporters, P-glycoprotein and MRP1, *ACTA BIOCHIMICA POLONICA*, 58 (4):433-448; 2011.
78. Andreia Palmeira. Design, synthesis and evaluation of xanthone derivatives for dual activity: antitumor and P-glycoprotein inhibition. Thesis presented to the Faculdade de Farmácia, Universidade do Porto, Porto, 2011, pp. 1-402. <https://br.123dok.com/document/z31on7my-design-synthesis-and-evaluation-of-xanthone-derivatives-for-dual-activity-antitumor-and-p-glycoprotein-inhibition.html> PhD Thesis
79. Jaszczyszyn A, K Gasiorowski, P Swiatek, W Malinka, K. Cieolik-Boczula, J. Petrus, B. Czarnik-Matusiewicz. Chemical structure of phenothiazines and their biological activity. *PHARMACOLOGICAL REPORTS*, 2012, 64, 16-23.
80. Palmeira, A; Sousa, E; Vasconcelos, MH; Pinto, MM. Three Decades of P-gp Inhibitors: Skimming Through Several Generations and Scaffolds. *CURRENT MEDICINAL CHEMISTRY*, 19 (13):1946-2025; MAY 2012

81. Agnieszka Knopik-Skrocka, Józef Bielawski, Szymon Chowański, Paulina Walkowiak. Changes in erythrocyte membrane permeability induced by verapamil, chlorpromazine, and their combinations with amphotericin B. *BIOLOGICAL LETTERS*. Volume 48, Issue 2, Pages 225–241, ISSN (Online) 1734-7467, ISSN (Print) 1644-7700, DOI: 10.2478/v10120-011-0021-9, July 2012
82. Basu S, H Rastogi, VB Patel. Effect of Herbal Bioenhancers on Saquinavir in Human Caco-2 Cell Monolayers and Pharmacokinetics in Rats. *INTERNATIONAL JOURNAL OF MEDICINE AND PHARMACEUTICAL SCIENCES (IJPMS)* 10/2012 2(29):28-42.
83. B.D. Joshi, P. Tandon, S. Jain. Structure, MESP and HOMO-LUMO study of 10-Acetyl- 10H-phenothiazine 5-oxide using vibrational spectroscopy and quantum chemical methods. *BIBECHANA* 9, 38-49, 2013
84. Krystyna Michalak, Andrzej B. Hendrich, Olga Wesołowska, Andrzej Poła. Compounds that modulate multidrug resistance in cancer cells. *CELLULAR & MOLECULAR BIOLOGY LETTERS*, 2013, 6(2), 362-368.
85. Huang, D; Zhao, T; Xu, W; Yang, TL; Cremer, PS. Sensing Small Molecule Interactions with Lipid Membranes by Local pH Modulation. *ANALYTICAL CHEMISTRY*, 85 (21):10240-10248; 10.1021/ac401955t NOV 5 2013.
86. Kars MD, G Kars, U Gunduz. Paclitaxel Resistance in MCF-7/Pac Cell Line is Reversed Successfully by Saikosaponin A and Saikosaponin D. *INTERNATIONAL JOURNAL OF HEMATOLOGY AND ONCOLOGY*, 23 (4), 2013, 227-232.
87. Barroso, RP; Basso, LGM; Costa, AJ. Interactions of the antimalarial amodiaquine with lipid model membranes, *CHEMISTRY AND PHYSICS OF LIPIDS*, 186, 68-78; 10.1016/j.chemphyslip.2014.12.003 FEB 2015
88. Jabeen, I. In silico strategies to probe stereoselective interactions of multidrug resistant transporter P-glycoprotein. *Letters in Drug Design & Discovery*, 2016, 13 (8):824-832.
89. Liao, Z.-G.; Tang, T.; Guan, X.-J.; Dong, W.; Zhang, J.; Zhao, G.-W.; Yang, M.; Liang, X.-L. Improvement of Transmembrane Transport Mechanism Study of Imperatorin on P-Glycoprotein-Mediated Drug Transport. *MOLECULES*, 21 (12):10.3390/molecules21121606 DEC 2016.
90. Mishra, Ravinesh; Sareen, Swati; Sharma, Bhartendu; Goyal, Shubham; Kaur, Gurpreet; Bhardwaj, Sweta; A. Siddiqui, Anees; Husain, Asif; K. Singla, Rajeev; Rashid, Mohd; Kumar, Deepak; Sati, Bhawana; Shalmali, Nishtha; Kumar, Rajiv "Phenothiazines and Related Drugs as Multi Drug Resistance Reversal Agents in Cancer Chemotherapy Mediated by p-glycoprotein." *Current Cancer Therapy Reviews* 13 (1), 2017: 28-42.
91. Roney, M.S.I. & Park, SK. Antipsychotic dopamine receptor antagonists, cancer, and cancer stem cells. *ARCHIVES OF PHARMACAL RESEARCH*, 41 (4):384-408; 10.1007/s12272-018-1017-3 APR 2018. <https://doi.org/10.1007/s12272-018-1017-3>
92. Berrocal, M; Corbacho, I; Gutierrez-Merino, C; Mata, AM. Methylene blue activates the PMCA activity and cross-interacts with amyloid beta-peptide, blocking A beta-mediated PMCA inhibition. *NEUROPHARMACOLOGY*, 139 163-172; SEP 1 2018 <https://doi.org/10.1016/j.neuropharm.2018.07.012>
93. Venkatesan, K., Satyanarayana, V.S.V., Sivakumar, A., Ramamurthy, C., Thirunavukkarasu, C. Synthesis, spectral characterization and antitumor activity of phenothiazine derivatives. *JOURNAL OF HETEROCYCLIC CHEMISTRY* Volume: 57, Issue: 7, Pages: 2722-2728, JUL 2020 <https://doi.org/10.1002/jhet.3980>
94. Dalhoff A. Are antibacterial effects of non-antibiotic drugs random or purposeful because of a common evolutionary origin of bacterial and mammalian targets? *INFECTION*, 2020 Dec 15;1-21. doi: 10.1007/s15010-020-01547-9

**2. Pajeva, I.K., M.Wiese: QSAR and molecular modelling study of multidrug resistance modifiers, *Quant. Struct.-Act. Relat.* 1997, 16 (1), 1-10.**

Цитирания: 54

1. Hudson V.W., E. de Berry (Eds.). Alternatives to the use of live vertebrates in biomedical research and testing, NLM-NIH, Bethesda, USA, 1997, No.4, A Bibliography with Abstracts, p.111.
2. Kim K.H., G.Greco, E.Novellino, A critical review of recent CoMFA applications, In: *3D QSAR in Drug Design*, H.Kubinyi, G.Folkers, Y.Martin (Eds.) Vol. 3, 1998, Kluwer Academic Publishers, 257-315.
3. Kim: K.H., List of CoMFA references, 1997, In: *Perspectives in Drug Discovery and Design*, Volume 12-14, pp. 334 - 338
4. Tmej C, Chiba P, Huber M, et al. A combined Hansch/Free-Wilson approach as predictive tool in QSAR studies on propafenone-type modulators of multidrug resistance. *ARCH PHARM* 331 (7-8): 233-240 JUL-AUG 1998

5. Holzgrabe, U., I. Wawer, B. Diehl (eds.) In: *NMR spectroscopy in Drug Development, Ligand-membrane interaction*, Chapter 11, Wiley-VCH, 1999, pp.175-230.(citation 96, p.230)
6. Ferte J. Analysis of the tangled relationships between P-glycoprotein-mediated multidrug resistance and the lipid phase of the cell membrane. *EUR J BIOCHEM* 267 (2): 277-294 JAN 2000
7. Ekins, S., B.J.Ring, G.Bravi, J.H.Wikel, and S.A.Wrighton: Predicting drug-drug interactions in silico using pharmacophore: paradigm for the next millennium, pp. 271-300. In: *Pharmacophore Perception, Development, and Use in Drug Design (Iul Biotechnology Series)* by Osman F. Guner (Editor), 560 pages, International University Line (February 1, 2000).
8. Palyulin VA, Radchenko EV, Zefirov NS Molecular field topology analysis method in QSAR studies of organic compounds. *J CHEM INF COMP SCI* 40 (3): 659-667 MAY-JUN 2000
9. Ekins S, Waller CL, Swaan PW, et al. Progress in predicting human ADME parameters in silico *J PHARMACOL TOXICOL* 44 (1): 251-272 JUL-AUG 2000
10. Jarmo T. Alander, Indexed Bibliography of Genetic Algorithms in Chemistry and Physics, University of Vaasa, Department of Information Technology and Production Economics, Report, 2001, citation 1644.
11. Dei, S.; Gualtieri, F.; Scapecchi, S.; Teodori, E.; Garnier-Suillerot, A. Mediators of classical multidrug resistance [MDR] and the medicinal chemistry of reversing drugs. *Recent Research Developments in Medicinal Chemistry* (2001), 1 18-64.
12. Avendano C, Menendez JC Inhibitors of multidrug resistance to antitumor agents (MDR) *CURR MED CHEM* 9 (2): 159-193 JAN 2002
13. Sean Ekins, Richard B. Kim, Brenda F. Leake, Anne H. Dantzig, Erin G. Schuetz, Lu-Bin Lan, Kazuto Yasuda, Robert L. Shepard, Mark A. Winter, John D. Schuetz, James H. Wikel, and Steven A. Wrighton. Three-dimensional quantitative structure-activity relationships of inhibitors of P-glycoprotein. *MOL PHARMACOL* 61 (5): 964-973 MAY 2002
14. Kellen J.A. Reversal of multidrug resistance – Revisited, *Current Oncology*, 2002, 9(1), 13-19
15. Holik M, Halamek H Transformation of a free-Wilson matrix into Fourier coefficients *QUANT STRUCT-ACT REL* 20 (5-6): 422-428 APR 2002
16. Teodori E, Dei S, Scapecchi S, et al. The medicinal chemistry of multidrug resistance (MDR) reversing drugs. *FARMACO* 57 (5): 385-415 MAY 2002
17. Michalak K, Hendrich AB. Role of cell membrane lipids in multidrug resistance and its modulation. *Postepy Biochem.* 2002; 48(3):208-219.
18. Kellen JA. The reversal of multidrug resistance: an update. *J EXP THER ONCOL* 2003 3(1), 5-13.
19. Seydel, J. K. Drug-membrane interactions and pharmacodynamics. *Methods and Principles in Medicinal Chemistry* (2002), 15, 217-289.
20. Seydel, J. K. Analytical tools for the analysis and quantification of drug-membrane interactions. *Methods and Principles in Medicinal Chemistry* (2002), 15, 51-139.
21. Kellogg, Glen E.; Semus, Simon F. 3D QSAR in modern drug design. In: *Modern Methods in Drug Discovery*, A. Hillisch and R. Hilgenfeld (Eds.), Birkhauser Verlag, Basel, Boston, Berlin, pp. 223-242, 2003. citation p.240.
22. Hendrich AB, Wesolowska O, Motohashi N, Molnar J, Michalak K. New phenothiazine-type multidrug resistance modifiers: anti-MDR activity versus membrane perturbing potency. *Biochem Biophys Res Commun.* 2003 May 2;304(2):260-265.
23. Tsakovska IM. QSAR and 3D QSAR of Phenothiazine Type Multidrug Resistance Modulators in P388/ADR Cells. *BIOORG MED CHEM*, 2003, 11(13), 2889-2899.
24. Hendrich AB, Michalak K. Lipids as a target for drugs modulating multidrug resistance of cancer cells. *Curr Drug Targets.* 2003 Jan;4 (1):23-30.
25. Barbieri F, Alama A, Tasso B, Boido V, Bruzzo C, Sparatore F. Quinolizidinyl derivatives of iminodibenzyl and phenothiazine as multidrug resistance modulators in ovarian cancer cells. *INVEST NEW DRUG* 21 (4): 413-420 NOV 2003
26. Dearden JC, Al-Noobi A, Scott AC, Thomson SA. QSAR studies on P-glycoprotein-regulated multidrug resistance and on its reversal by phenothiazines. *SAR QSAR Environ Res.* 2003 Oct-Dec;14(5-6):447-54.
27. Degenhardt, Charles Raymond; Eickhoff, David Joseph: Substituted piperazine compounds optionally containing a quinolyl moiety for treating multidrug resistance, United States Patent 6693099, issued on February 17, 2004.
28. Ekins S, Swaan PW. Development of computational models for enzymes, transporters, channels, and receptors relevant to ADME/Tox. *REVIEWS IN COMPUTATIONAL CHEMISTRY* 20: 333-415 2004
29. Pleban K, Ecker GF. Inhibitors of P-glycoprotein - Lead identification and optimisation *MINI-REV MED CHEM* 5 (2): 153-163 FEB 2005
30. Zaheeruddin. Acridones as reversers of drug resistance in cancer cells and their anti-bacterial activities. Dissertation. Rajiv Gandhi University of health sciences, Bangalore, Karnataka, Department of

- pharmaceutical chemistry, V.L. College of pharmacy, 2005, pp. 1-118.  
<http://14.139.159.4:8080/jspui/handle/123456789/2076>
31. Michalak, K., O. Wesolowska, N. Motohashi, J. Molnar and A. B. Hendrich Interactions of Phenothiazines with Lipid Bilayer and their Role in Multidrug Resistance Reversal. *CURRENT DRUG TARGETS*, Volume 7, Number 9, 1095-1105, September 2006.
  32. Degenhardt, Charles Raymond / Eickhoff, David Joseph, Substituted heterocyclic compounds for treating multidrug resistance, *UNITED STATES PATENT* 7135483, Patent number 6376514, 14 Nov 2006.
  33. Labrie P, Maddaford SP, Fortin S, Rakhit S, Kotra LP, Gaudreault RC. A comparative molecular field analysis (CoMFA) and comparative molecular similarity indices analysis (CoMSIA) of anthranilamide derivatives that are multidrug resistance modulators. *J Med Chem.* 2006 Dec 28; 49(26):7646-60.
  34. Edafiogho, Ivan O.; Kombian, Samuel B.; Ananthalakshmi, Kethireddy V. V.; Salama, Noha N.; Eddington, Natalie D.; Wilson, Tiffany L.; Alexander, Mariano S.; Jackson, Patrice L.; Hanson, Clive D.; Scott, K. R. Enaminones: exploring additional therapeutic activities. *Journal of Pharmaceutical Sciences* (2007), 96(10), 2509-2531.
  35. Michalak, K., O.Wesołowska, N.Motohashi, A.B.Hendrich. The Role of the Membrane Actions of Phenothiazines and Flavonoids as Functional Modulators. In: *Topics in Heterocyclic Chemistry, Bioactive Heterocycles II*, (S. Egguchi, Ed.), Volume 8, Springer Berlin / Heidelberg, 2007, 223-302.
  36. Adenot M.: A Practical Approach to Computational Models of the Blood–Brain Barrier, In: *Handbook of Neurochemistry and Molecular Neurobiology Neural Membranes and Transport*. Abel Lajtha and Maarten E. A. Reith (eds.) Springer US, 2007, 109-150.
  37. Enrique Molina, Ernesto Estrada, Delvin Nodarse, Luis A. Torres, Humberto González, Eugenio Uriarte. Quantitative structure-antibacterial activity relationship modeling using a combination of piecewise linear regression-discriminant analysis (I): Quantum chemical, topographic, and topological descriptors. *INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY*, Volume 108, Issue 10, Pages 1856 – 1871, 2008.
  38. Matthias Schmidt, Marlen Teitge, Marianela E. Castillo, Tobias Brandt, Bodo Dobner, Andreas Langner: Synthesis and Biochemical Characterization of New Phenothiazines and Related Drugs as MDR Reversal Agents, *ARCHIV DER PHARMAZIE*, 2008, Vol. 341 (10), 624-638.
  39. Jarmo T. Alander. An Indexed Bibliography of Genetic Algorithms in Physical Sciences. Report Series No. 94-1-PHYS Copyright c 1994-2008, <ftp://site.ftp.uwasa.fi/directory/cs/report94-1/file/gaPHYSbib.pdf>
  40. Wu, JH; Li, X; Cheng, WD; Xie, QJ; Liu, YQ; Zhao, CY. Quantitative Structure Activity Relationship (QSAR) Approach to Multiple Drug Resistance (MDR) Modulators Based on Combined Hybrid System. *QSAR & COMBINATORIAL SCIENCE* 28 (9): 969-978 SEP 2009.
  41. Carbó-Dorca R, Besalú E, Mercado LD. Communications on quantum similarity, part 3: a geometric-quantum similarity molecular superposition algorithm. *J Comput Chem.* 2011 Mar;32(4):582-99.
  42. Huber, PC; Maruiama, CH; Almeida, WP. P-glycoprotein and multidrug resistance: structure-activity relationships of modulators. *QUIMICA NOVA* 33 (10): 2148-2154 2010.
  43. Jaszczyszyn A, K Gasiowski, P Swiatek, W Malinka, K. Cieoelik-Boczula, J. Petrus, B. Czarnik-Matuszewicz. Chemical structure of phenothiazines and their biological activity. *PHARMACOLOGICAL REPORTS*, 2012, 64, 16–23.
  44. B.D. Joshi, P. Tandon, S. Jain. Structure, MESP and HOMO-LUMO study of 10-Acetyl- 10H-phenothiazine 5-oxide using vibrational spectroscopy and quantum chemical methods. *BIBECHANA* 9, 38-49, 2013.
  45. Marie-Josée Fournier, Laetitia Coudert, Samia Mellaoui, Pauline Adjibade, Cristina Gareau, Marie-France Côté, Nahum Sonenberg, Réne C Gaudreault, Rachid Mazroui. Inactivation of the mTORC1-eIF4E Pathway alters Stress Granules Formation. *Mol Cell Biol.* 2013 Jun;33(11):2285-301. doi: 10.1128/MCB.01517-12. Epub 2013 Apr 1.
  46. Belaidi, S., Almi, Z., Bouzidi, D. Electronic structure and physical-chemistry properties relationship for phenothiazine derivatives by quantum chemical calculations. *JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE*, 11 (12):2481-2488; 10.1166/jctn.2014.3665 DEC 2014.
  47. Almi, Zineb; Belaidi, Salah; Melkemi, Nadjib; Boughdiri, Salima; Belkhir, Lotfi. Structure Activity Relationship and Quantitative Structure-Activity Relationships Modeling of Cyto-Toxicity of Phenothiazine Derivatives. *QUANTUM MATTER*, Volume 5, Number 1, February 2016, pp. 124-129.
  48. Almi Zineb. Etude qualitative et quantitative des relations structures-activités dans des hétérocycles à intérêt pharmaceutique. Thèses de Doctorat, University of Biskra, 2016, pp.1-83. <http://dspace.univ-biskra.dz:8080/jspui/handle/123456789/7423>
  49. Yonar, D., Sunnetcioglu, M.M. Effect of cis-(Z)-flupentixol on DPPC membranes in the presence and absence of cholesterol (2016) *Chemistry and Physics of Lipids*, 198, pp. 61-71.
  50. Jabeen, I. In silico strategies to probe stereoselective interactions of multidrug resistant transporter P-glycoprotein. *Letters in Drug Design and Discovery*, 2016, 13 (8), pp. 824-832.

51. M. Asif. Biological potential of phenothiazine derivatives and some new heterocycles based on phenothiazine moiety. *International Journal of Current Research in Applied Chemistry & Chemical Engineering*, Vol. 2, Issue 2, 2016, 39-57.
52. Mishra, Ravinesh; Sareen, Swati; Sharma, Bhartendu; Goyal, Shubham; Kaur, Gurpreet; Bhardwaj, Sweta; A. Siddiqui, Anees; Husain, Asif; K. Singla, Rajeev; Rashid, Mohd; Kumar, Deepak; Sati, Bhawana; Shalmali, Nishtha; Kumar, Rajiv "Phenothiazines and Related Drugs as Multi Drug Resistance Reversal Agents in Cancer Chemotherapy Mediated by p-glycoprotein." *Current Cancer Therapy Reviews* 13 (1), 2017: 28-42.
53. Berrocal, M; Corbacho, I; Gutierrez-Merino, C; Mata, AM. Methylene blue activates the PMCA activity and cross-interacts with amyloid beta-peptide, blocking A beta-mediated PMCA inhibition. *NEUROPHARMACOLOGY*, 139 163-172; 10.1016/j.neuropharm.2018.07.012 SEP 1 2018
54. Sroda-Pomianek, K; Michalak, K; Swiatek, P; Pola, A; Palko-Labuz, A; Wesolowska, O. Increased lipid peroxidation, apoptosis and selective cytotoxicity in colon cancer cell line LoVo and its doxorubicin-resistant subline LoVo/Dx in the presence of newly synthesized phenothiazine derivatives. *BIOMEDICINE & PHARMACOTHERAPY*, 106 624-636; 10.1016/j.biopha.2018.06.170 OCT 2018.

**3. Wiese, M., I.K.Pajeva: Molecular modeling study of the multidrug resistance modifiers cis- and trans-flupentixol, *Pharmazie* 1997, 52 (9), 679-685.**

Цитирания: 27

1. George A The design and molecular modeling of CNS drugs Review. *Current Opinion in Drug Discovery & Development* 1999, 2:286-292 (28 July 1999)
2. Keseru GM, Molnar L, Greiner I A neural network based virtual high throughput screening test for the prediction of CNS activity. *COMB CHEM HIGH T SCR* 3 (6): 535-543 DEC 2000
3. Castaing M, Brouant P, Loiseau A, et al. Membrane permeation by multidrug-resistance-modulators and non-modulators: Effects of hydrophobicity and electric charge *J PHARM PHARMACOL* 52 (3): 289-296 MAR 2000
4. Kellogg GE, Abraham DJ Hydrophobicity: is LogP(o/w) more than the sum of its parts? *EUR J MED CHEM* 35 (7-8): 651-661 JUL-AUG 2000
5. Dei, S.; Gualtieri, F.; Scapecchi, S.; Teodori, E.; Garnier-Suillerot, A. Mediators of classical multidrug resistance [MDR] and the medicinal chemistry of reversing drugs. *Recent Research Developments in Medicinal Chemistry* (2001), 1, 18-64.
6. Seydel, Joachim K. Drug-membrane interactions and pharmacodynamics. *Methods and Principles in Medicinal Chemistry* (2002), 15, 217-289.
7. Avendano C, Menendez JC Inhibitors of multidrug resistance to antitumor agents (MDR) *CURR MED CHEM* 9 (2): 159-193 JAN 2002
8. Kellen JA. Reversal of multidrug resistance—Revisited. *Current Oncology*, 2002, 9(1), 13-19
9. Zhang EY, Phelps MA, Cheng C, et al. Modeling of active transport systems. *ADV DRUG DELIVER REV* 54 (3): 329-354 MAR 31 2002
10. Teodori E, Dei S, Scapecchi S, et al. The medicinal chemistry of multidrug resistance (MDR) reversing drugs. *FARMACO* 57 (5): 385-415 MAY 2002
11. Kellen JA. The reversal of multidrug resistance: an update. *J EXP THER ONCOL* 2003 3(1), 5-13.
12. Swaan, Peter W., Abraham, Donald J. Drug Transport and Membrane Transport Proteins. In: Burger's Medicinal Chemistry and Drug Discovery. 2003, John Wiley & Sons, Inc., 1-52. <http://dx.doi.org/10.1002/0471266949.bmc027.pub2>.
13. Degenhardt, Charles Raymond; Eickhoff, David Joseph: Substituted piperazine compounds optionally containing a quinolyl moiety for treating multidrug resistance, United States Patent 6693099, issued on February 17, 2004.
14. Avendano, Carmen; Menendez, J. Carlos. Recent advances in multidrug resistance modulators. *Medicinal Chemistry Reviews-Online* (2004), 1(4), 419-444.
15. Zaheeruddin. Acridones as reversers of drug resistance in cancer cells and their anti-bacterial activities. Dissertation. Rajiv Gandhi University of health sciences, Bangalore, Karnataka, Department of pharmaceutical chemistry, V.L. College of pharmacy, 2005, pp. 1-118. <http://14.139.159.4:8080/jspui/handle/123456789/2076>
16. Y. Li, Y. Wang, L. Yang, S. Zhang, and C. Liu, Impact of Molecular Hydrophobic Field on Passive Diffusion, P–Glycoprotein Active Efflux, and P–Glycoprotein Modulation of Steroids, *Internet Electron. J. Mol. Des.* 2006, 5, 60–78, <http://www.biochempress.com>.
17. Ahmed, Osman. Reversal of multidrug resistance in cancer cells by different N10-substituted acridone derivatives. Dissertation, Rajiv Gandhi University of health sciences, Bangalore, Karnataka, Department of pharmaceutical chemistry, V.L. College of pharmacy, 2006, pp. 1-133. <http://14.139.159.4:8080/jspui/handle/123456789/2014>

18. Degenhardt, Charles Raymond, and David Joseph Eickhoff. "Substituted heterocyclic compounds for treating multidrug resistance." U.S. Patent No. 7,476,680. 13 Jan. 2009.
19. Swaan, Peter W. "Drug Transport and Membrane Transport Proteins." *Burger's Medicinal Chemistry and Drug Discovery* (2010).
20. Lübcke, Friederike. Arzneimittelinteraktionen über das P-Glykoprotein und verwandte Transportenzyme. PhD, Universität Regensburg, 2010. PhD
21. Andreia Palmeira. Design, synthesis and evaluation of xanthone derivatives for dual activity: antitumor and P-glycoprotein inhibition. Thesis presented to the Faculdade de Farmácia, Universidade do Porto, Porto, 2011, pp. 1-402. <https://br.123dok.com/document/z31on7my-design-synthesis-and-evaluation-of-xanthone-derivatives-for-dual-activity-antitumor-and-p-glycoprotein-inhibition.html> PhD Thesis
22. Palmeira, A; Sousa, E; Vasconcelos, MH; Pinto, MM. Three Decades of P-gp Inhibitors: Skimming Through Several Generations and Scaffolds. *CURRENT MEDICINAL CHEMISTRY*, 19 (13):1946-2025; MAY 2012
23. Palmeira, A; Sousa, E; Vasconcelos, MH; Pinto, M; Fernandes, MX. Structure and Ligand-based Design of P-glycoprotein Inhibitors: A Historical Perspective. *CURRENT PHARMACEUTICAL DESIGN*, 18 (27):4197-4214; SEP 2012
24. Jiwon Kim, Jin-Ho Song, Thioxanthenes, chlorprothixene and flupentixol inhibit proton currents in BV2 microglial cells, *EUROPEAN JOURNAL OF PHARMACOLOGY*, 779 31-37; 10.1016/j.ejphar.2016.03.009 MAY 15 2016.
25. Yonar, D; Sunnetcioglu, MM. Effect of cis-(Z)-flupentixol on DPPC membranes in the presence and absence of cholesterol, *CHEMISTRY AND PHYSICS OF LIPIDS*, 198 61-71; 10.1016/j.chemphyslip.2016.06.002 JUN 2016
26. Kim, J., Song, J.-H. Thioxanthenes, chlorprothixene and flupentixol inhibit proton currents in BV2 microglial cells (2016) *European Journal of Pharmacology*, 779, pp. 31-37.
27. Jabeen, I. In silico strategies to probe stereoselective interactions of multidrug resistant transporter P-glycoprotein. *Letters in Drug Design and Discovery*, 2016, 13 (8), pp. 824-832.

**4. Pajeva, I.K., M. Wiese: Molecular modeling of phenothiazines and related drugs as multidrug resistance modifiers: a comparative molecular field analysis, *J. Med. Chem.* 1998, 41, 1815-1826.**

Цитирания: 116

1. Debnath AK Three-dimensional quantitative structure-activity relationship study on cyclic urea derivatives as HIV-1 protease inhibitors: Application of comparative molecular field analysis. *J MED CHEM* 42 (2): 249-259 JAN 28 1999
2. Kellogg GE, Abraham DJ Development of empirical molecular interaction models that incorporate hydrophobicity and hydropathy. The HINT paradigm. *ANALYSIS* 27 (1): 19-23 JAN-FEB 1999
3. Teodori E, Dei S, Quidu P, et al. Design, synthesis, and in vitro activity of catamphiphilic reverters of multidrug resistance: Discovery of a selective, highly efficacious chemosensitizer with potency in the nanomolar range. *J MED CHEM* 42 (10): 1687-1697 MAY 20 1999
4. Ouyang XH, Kiselyov AS Novel synthesis of dibenzo[b,g]1,5-oxazocines. *TETRAHEDRON LETT* 40 (32): 5827-5830 AUG 6 1999
5. Ecker G, Huber M, Schmid D, et al. The importance of a nitrogen atom in modulators of multidrug resistance. *MOL PHARMACOL* 56 (4): 791-796 OCT 1999
6. Bergmann, R.; Brust, P.; Pietzsch, H.-J.; Scheunemann, M.; Seifert, S.; Johannsen, B. Evaluation of the in vitro and in vivo properties of a potential Tc-labelled inhibitor of the MDR gene product P-glycoprotein. *Wissenschaftlich-Technische Berichte - Forschungszentrum Rossendorf* (1999), (FZR-270), 62-67.
7. Anon. Classical QSAR. *Environmental science, toxicology. Quantitative Structure-Activity Relationships* (1999), 18(1), 69-82.
8. Shah A, Gaveriya H, Motohashi N, et al. 3,5-diacetyl-1,4-dihydropyridines: Synthesis and MDR reversal in tumor cells. *ANTICANCER RES* 20 (1A): 373-377 JAN-FEB 2000
9. Ekins, S., B.J.Ring, G.Bravi, J.H.Wikel, S.A.Wrighton: Predicting drug-drug interactions in silico using pharmacophore: paradigm for the next millennium, pp. 271-300. In: *Pharmacophore Perception, Development, and Use in Drug Design (Iul Biotechnology Series)* by Osman F. Guner (Editor), 560 pages, International University Line (February 1, 2000).
10. Ouyang XH, Chen ZD, Liu LB, et al. Novel and highly efficient synthesis of substituted dibenz[b,g]1,5-oxazocines. A direct comparison of the solution versus solid-phase approach *TETRAHEDRON* 56 (16): 2369-2377 APR 14 2000
11. Bergmann R, Brust P, Scheunemann M, Pietzsch HJ, Seifert S, Roux F, Johannsen B. Assessment of the in vitro and in vivo properties of a Tc-99m-labeled inhibitor of the multidrug resistant gene product P-glycoprotein *NUCL MED BIOL* 27 (2): 135-141 FEB 2000

12. Kawase M, Saito S, Motohashi N Chemistry and biological activity of new 3-benzazepines INT J ANTIMICROB AG 14 (3): 193-201 APR 2000
13. Kellogg GE, Abraham DJ Hydrophobicity: is LogP(o/w) more than the sum of its parts? EUR J MED CHEM 35 (7-8): 651-661 JUL-AUG 2000
14. Tripos Go. Discover, SYBYL: Supplemental technologies, HINT! quantitate and visualize non-covalent inreaction energies, Tripos Inc. USA, <http://www.tripos.com/sciTech/inSilicoDisc/strActRelationship/hint.html#references>
15. Bakken GA, Jurs PC Classification of multidrug-resistance reversal agents using structure-based descriptors and linear discriminant analysis. J MED CHEM 43 (23): 4534-4541 NOV 16 2000.
16. Dei, S.; Gualtieri, F.; Scapecchi, S.; Teodori, E.; Garnier-Suillerot, A. Mediators of classical multidrug resistance [MDR] and the medicinal chemistry of reversing drugs. Recent Research Developments in Medicinal Chemistry (2001), 1, 18-64.
17. Doytchinova I CoMFA-based comparison of two models of binding site on adenosine A(1) receptor J COMPUT AID MOL DES 15 (1): 29-39 JAN 2001
18. Ekins S, Waller CL, Swaan PW, et al. Progress in predicting human ADME parameters in silico J PHARMACOL TOXICOL 44 (1): 251-272 JUL-AUG 2000
19. Galatin PS, Abraham DJ QSAR: Hydropathic analysis of inhibitors of the p53-mdm2 interaction PROTEINS 45 (3): 169-175 NOV 15 2001
20. Avendano C, Menendez JC Inhibitors of multidrug resistance to antitumor agents (MDR) CURR MED CHEM 9 (2): 159-193 JAN 2002
21. Sean Ekins, Richard B. Kim, Brenda F. Leake, Anne H. Dantzig, Erin G. Schuetz, Lu-Bin Lan, Kazuto Yasuda, Robert L. Shepard, Mark A. Winter, John D. Schuetz, James H. Wikel, and Steven A. Wrighton. Three-dimensional quantitative structure-activity relationships of inhibitors of P-glycoprotein. MOL PHARMACOL 61 (5): 964-973 MAY 2002
22. Stouch TR, Gudmundsson A Progress in understanding the structure-activity relationships of P-glycoprotein. ADV DRUG DELIVER REV 54 (3): 315-328 MAR 31 2002
23. Zhang EY, Phelps MA, Cheng C, et al. Modeling of active transport systems. ADV DRUG DELIVER REV 54 (3): 329-354 MAR 31 2002
24. Teodori E, Dei S, Scapecchi S, et al. The medicinal chemistry of multidrug resistance (MDR) reversing drugs. FARMACO 57 (5): 385-415 MAY 2002
25. Palafox MA, Gil M, Nunez JL, et al. Study of phenothiazine and N-methyl phenothiazine by infrared, Raman, H-1-, and C-13-NMR spectroscopies. INT J QUANTUM CHEM 89 (3): 147-171 AUG 15 2002
26. Chiba P, Erker T, Galanski M, et al. Synthesis and multidrug-resistance modulating activity of a series of thienothiazines. ARCH PHARM 335 (5): 223-228 MAY 2002
27. Mi QW, Cui BL, Chavez D, et al. Characterization of tropane alkaloid aromatic esters that reverse the multidrug-resistance phenotype. ANTICANCER RES 22 (3): 1385-1397 MAY-JUN 2002
28. Doytchinova IA, Flower DR Physicochemical explanation of peptide binding to HLA-A\*0201 major histocompatibility complex: A three-dimensional quantitative structure-activity relationship study. PROTEINS 48 (3): 505-518 AUG 15 2002
29. Doytchinova IA, Flower DR Quantitative approaches to computational vaccinology IMMUNOL CELL BIOL 80 (3): 270-279 JUN 2002
30. Kawase, M., Motohashi, N. New multidrug resistance reversal agents. CURRENT DRUG TARGETS, 2003, Jan., 4 (1), 31-43.
31. Rebitzer S, Annibali D, Kopp S, Eder M, Langer T, Chiba P, Ecker GF, Noe CR. In silico screening with benzofurane- and benzopyrane-type MDR-modulators. FARMACO 2003 Mar; 58(3):185-91.
32. Tsakovska IM. QSAR and 3D QSAR of Phenothiazine Type Multidrug Resistance Modulators in P388/ADR Cells. BIOORG MED CHEM, 2003, 11(13), 2889-2899.
33. Wesolowska, O., Molnar, J., Motohashi, N., Michalak, K. Inhibition of P-glycoprotein transport function by N-acylphenothiazines. ANTICANCER RESEARCH, 2002, Sep-Oct, 22(5), 2863-2867.
34. Kellen JA Reversal of multidrug resistance – Revisited, Current Oncology, 2002, 9(1), 13-19
35. Dearden JC, Al-Noobi A, Scott AC, Thomson SA. QSAR studies on P-glycoprotein-regulated multidrug resistance and on its reversal by phenothiazines. SAR QSAR Environ Res. 2003 Oct-Dec;14(5-6):447-54.
36. Motohashi N, Kawase M, Molnar J, Ferenczy L, Wesolowska O, Hendrich AB, Bobrowska-Hägerstrand M, Hägerstrand H, Michalak K. Antimicrobial activity of N-acylphenothiazines and their influence on lipid model membranes and erythrocyte membranes. ARZNEIMITTEL-FORSCH 53 (8): 590-599 2003

37. Barbieri F, Alama A, Tasso B, Boido V, Bruzzo C, Sparatore F. Quinolizidinyl derivatives of iminodibenzyl and phenothiazine as multidrug resistance modulators in ovarian cancer cells. *INVEST NEW DRUG* 21 (4): 413-420 NOV 2003
38. G.E.Kellogg, S.F. Semus: 3D QSAR in modern drug discovery. In: *Modern Methods in Drug Discovery*, A. Hillisch and R. Hilgenfeld (Eds.), Birkhauser Verlag, Basel, Boston, Berlin, pp. 223-242, 2003. citation p. 240.
39. Degenhardt, Charles Raymond; Eickhoff, David Joseph: Substituted piperazine compounds optionally containing a quinolyl moiety for treating multidrug resistance , United States Patent 6693099, issued on February 17, 2004.
40. Lin, Ai J.; Guan, Jian; Kyle, Dennis E.; Milhous, Wilbur K.; Chemosensitizing agents against chloroquine resistant plasmodium falciparum and methods of making and using thereof , United States Patent 6800618, issued on October 5, 2004.
41. Ecker GF, Noe CR. In silico prediction models for blood-brain barrier permeation. *CURR MED CHEM* 11 (12): 1617-1628 JUN 2004
42. Ekins S, Swaan PW. Development of computational models for enzymes, transporters, channels, and receptors relevant to ADME/Tox. *REVIEWS IN COMPUTATIONAL CHEMISTRY* 20: 333-415 2004
43. Langer T, Eder M, Hoffmann RD, Chiba P, Ecker GF. Lead identification for modulators of multidrug resistance based on in silico screening with a pharmacophoric feature model *ARCH PHARM* 337 (6): 317-327 JUN 2004
44. Bender A, Glen RC. Molecular similarity: a key technique in molecular informatics. *Org Biomol Chem*. 2004 Nov 21;2(22):3204-18.
45. Antel, J., A Weber, C.A. Sotriffer, G. Klebe: Multiple binding modes observed in x-structures of carbonic anhydrase inhibitor complexes and other systems: consequences for structure based drug design, Chapter 3, In: *Carbonic Anhydrase: Its Inhibitors and Activators*, Editors: Claudiu T. Supuran, Andrea Scozzafava, Janet Conway, Taylor & Francis, 2004 (p. 50).
46. Fumiyoshi YAMASHITA and Mitsuru HASHIDA. In Silico Approaches for Predicting ADME Properties of Drugs. *DRUG METAB. PHARMACOKIN.* 19 (5): 327-338, 2004.
47. Kaiser, D.; Smiesko, M.; Kopp, S.; Chiba, P.; Ecker, G. F.: Interaction Field Based and Hologram Based QSAR Analysis of Propafenone-type Modulators of Multidrug Resistance, *Medicinal Chemistry*, Volume 1, Number 5, September 2005, pp. 431-444(14).
48. Roy, R. U.; Desai, K. R. Anticancer evaluation of azetidinone and thiazolidinone derivatives of quinolone. *International Journal of Chemical Sciences* (2005), 3(3), 529-536
49. Pleban K, Ecker GF. Inhibitors of P-glycoprotein - Lead identification and optimisation *MINI-REV MED CHEM* 5 (2): 153-163 FEB 2005
50. Cianchetta G, Singleton RW, Zhang M, Wildgoose M, Giesing D, Fravolini A, Cruciani G, Vaz RJ. A pharmaeophore hypothesis for P-glycoprotein substrate recognition using GRIND-based 3D-QSAR. *J MED CHEM* 48 (8): 2927-2935 APR 21 2005
51. Fratev F, Benfenati E. 3D-QSAR and molecular mechanics study for the differences in the azole activity against yeastlike and filamentous fungi and their relation to P450DM inhibition. 1. 3-substituted-4(3H)-quinazolinones. *JOURNAL OF CHEMICAL INFORMATION AND MODELING* 45 (3): 634-644 MAY-JUN 2005
52. Sun, HM. A naive bayes classifier for prediction of multidrug resistance reversal activity on the basis of atom typing. *J Med Chem*. 2005 Jun 16; 48(12):4031-9.
53. Edison J. Osorio, Sara M. Robledo, Gabriel J. Arango, Carlos E. Muskus *Leishmania*: papel de la glicoproteína P en la mediación de resistencia a medicamentos y estrategias de reversión, *Biomédica* 2005;25:242-60.
54. Zaheeruddin. Acridones as reversers of drug resistance in cancer cells and their anti-bacterial activities. Dissertation. Rajiv Gandhi University of health sciences, Bangalore, Karnataka, Department of pharmaceutical chemistry, V.L. College of pharmacy, 2005, pp. 1-118. <http://14.139.159.4:8080/jspui/handle/123456789/2076>
55. Bender, Andreas: Studies on molecular similarity, A thesis submitted for the degree of Doctor of Philosophy of the Darwin College, University of Cambridge on 11 November 2005. PhD
56. Zhou XF, Shao QX, Coburn RA, Morris ME Quantitative structure-activity relationship and quantitative structure-pharmacokinetics relationship of 1,4-dihydropyridines and pyridines as multidrug resistance modulators. *PHARMACEUTICAL RESEARCH* 22 (12): 1989-1996 DEC 2005
57. Srinivas E, Murthy JN, Rao AR., Sastry GN. Recent advances in molecular modeling and medicinal chemistry aspects of phospho-glycoprotein. *CURRENT DRUG METABOLISM* 7 (2): 205-217 FEB 2006

58. Osorio D., Edison J.; Montoya P., Guillermo L. and Arango A., Gabriel J. Productos Naturales Alcaloidales Con Actividad Antiprotozoaria. *Vitae* [online]. 2006, vol.13, n.1 [cited 2016-07-28], pp.61-84.
59. Vistoli, G.; Pedretti, A. Molecular fields to assess recognition forces and property spaces. *Comprehensive Medicinal Chemistry II* (2006), 5, 577-602.
60. Y. Li, Y. Wang, L. Yang, S. Zhang, and C. Liu, Impact of Molecular Hydrophobic Field on Passive Diffusion, P-Glycoprotein Active Efflux, and P-Glycoprotein Modulation of Steroids, *Internet Electron. J. Mol. Des.* 2006, 5, 60-78, <http://www.biochempress.com>.
61. Johnson SR, Zheng W. Recent Progress in the Computational Prediction of Aqueous Solubility and Absorption. *AAPS J.* 2006; 8(1): E27-40.
62. Koenig, G., G.F. Ecker: HYDRRA – a tool to implement hydrophobic moments in structure-activity relationship studies and molecular alignment, Proceedings of European School of Medicinal Chemistry (XXVI Advanced Course of Medicinal Chemistry and "E. Duranti" National Seminar for PhD Students), 2-7 July 2006, Urbino, Italy, p. 60-61. <http://www.uniurb.it/MedChem/dottorandir.pdf>
63. United States Patent 6800618: Chemosensitizing agents against chloroquine resistant plasmodium falciparum and methods of making and using thereof, <http://www.freepatentsonline.com/6800618.html>
64. Schmitt U, Abou El-Ela A, Guo LJ, Glavinas H, Krajcsi P, Baron JM, Tillmann C, Hiemke C, Langguth P, Hartter S. Cyclosporine a (CsA) affects the pharmacodynamics and pharmacokinetics of the atypical antipsychotic amisulpride probably via inhibition of P-glycoprotein (P-gp), *J. NEURAL TRANSMISSION*, 2006, 113 (7), 787-801.
65. Teodori, E., Dei, S., Martelli, C., Scapecchi, S., Gualtieri, F. The functions and structure of ABC transporters: Implications for the design of new inhibitors of Pgp and MRP1 to control multidrug resistance (MDR) *CURRENT DRUG TARGETS* 7 (7), pp. 893-909, 2006.
66. Michalak, K., O. Wesolowska, N. Motohashi, J. Molnar and A. B. Hendrich Interactions of Phenothiazines with Lipid Bilayer and their Role in Multidrug Resistance Reversal. *CURRENT DRUG TARGETS*, Volume 7, Number 9, 1095-1105, September 2006.
67. Degenhardt, Charles Raymond / Eickhoff, David Joseph, Substituted heterocyclic compounds for treating multidrug resistance, United States Patent 7135483, Patent number 6376514, 14 Nov 2006
68. Labrie P, Maddaford SP, Fortin S, Rakhit S, Kotra LP, Gaudreault RC. A comparative molecular field analysis (CoMFA) and comparative molecular similarity indices analysis (CoMSIA) of anthranilamide derivatives that are multidrug resistance modulators. *J Med Chem.* 2006 Dec 28; 49(26):7646-60.
69. Ahmed, Osman. Reversal of multidrug resistance in cancer cells by different N10-substituted acridone derivatives. **Dissertation**, Rajiv Gandhi University of health sciences, Bangalore, Karnataka, Department of pharmaceutical chemistry, V.L. College of pharmacy, 2006, pp. 1-133. <http://14.139.159.4:8080/jspui/handle/123456789/2014>
70. Kaiser, D., Terfloth, L., Kopp, S., Schulz, J., De Laet, R., Chiba, P., Ecker, G.F., Gasteiger, J.: Self-organizing maps for identification of new inhibitors of P-glycoprotein. *Journal of Medicinal Chemistry* 50 (7), pp. 1698-1702, 2007.
71. De Groot, MJ, DFV Lewis, S Modi: Molecular modeling and quantitative structure-activity relationship of substrates and inhibitors of drug metabolism enzymes, *In silico* models for interactions with transporters, Chapter 5.34, In: *Comprehensive Medicinal Chemistry II*, (Editors-in-Chief: John B Taylor and David J Triggle) Vol. 5: ADMET/Property based approaches, (Eds. B. Testa, H. Water-beemed), Part 4: *In silico* tools in ADMET, Elsevier: Oxford, 2007, 809-825.
72. Edafigho, Ivan O.; Kombian, Samuel B.; Ananthalakshmi, Kethireddy V. V.; Salama, Noha N.; Eddington, Natalie D.; Wilson, Tiffany L.; Alexander, Mariano S.; Jackson, Patrice L.; Hanson, Clive D.; Scott, K. R. Enaminones: exploring additional therapeutic activities. *Journal of Pharmaceutical Sciences* (2007), 96(10), 2509-2531.
73. Ruiz-Garcia, Ana; Bermejo, Marival; Moss, Aaron; Casabo, Vicente G. Pharmacokinetics in drug discovery. *JOURNAL OF PHARMACEUTICAL SCIENCES* (2007), Volume Date 2008, 97(2), 654-690.
74. Michalak, K., O. Wesolowska, N. Motohashi, A. B. Hendrich. The Role of the Membrane Actions of Phenothiazines and Flavonoids as Functional Modulators. In: *Topics in Heterocyclic Chemistry, Bioactive Heterocycles II*, (S. Egguchi, Ed.), Volume 8, Springer Berlin / Heidelberg, 2007, 223-302.
75. Konig G, Chiba P, Ecker GF: Hydrophobic moments as physicochemical descriptors in structure-activity relationship studies of P-glycoprotein inhibitors *MONATSHEFTE FUR CHEMIE* Volume: 139 Issue: 4 Pages: 401-405 Published: APR 2008.
76. Ecker, G.F., Stockner, T., Chiba, P. Computational models for prediction of interactions with ABC-transporters. *Drug Discovery Today* 13 (7-8), 2008, pp. 311-317.

77. Zhu, Xiao-Qing; Dai, Zhi; Yu, Ao; Wu, Shuai; Cheng, Jin-Pei. Driving Forces for the Mutual Conversions between Phenothiazines and Their Various Reaction Intermediates in Acetonitrile. *Journal of Physical Chemistry B* (2008), 112(37), 11694-11707.
78. Matthias Schmidt, Marlen Teitge, Marianela E. Castillo, Tobias Brandt, Bodo Dobner, Andreas Langner: Synthesis and Biochemical Characterization of New Phenothiazines and Related Drugs as MDR Reversal Agents, *ARCHIV DER PHARMAZIE*, 2008, Vol. 341 (10), 624-638.
79. Nicolle, E., Boumendjel, A., Macalou, S., Genoux, E., Ahmed-Belkacem, A., Carrupt, P.-A., Di Pietro, A. QSAR analysis and molecular modeling of ABCG2-specific inhibitors. *Advanced Drug Delivery Reviews* 61 (1), pp. 34-46, 2009.
80. de la Nuez, Ania; Rodriguez, Rolando. Current methodology for the assessment of ADME-Tox properties on drug candidate molecules. *BIOTECNOLOGIA APLICADA* (2008), 25(2), 97-110.
81. Osorio, Edison J.; Robledo, Sara M.; Bastida, Jaume. Alkaloids with antiprotozoal activity. *Alkaloids* (San Diego, CA, United States) (2008), 66 113-190.
82. Hepworth J.D., B.M. Heron. Thiopyrans and their Benzo Derivatives. In: *Comprehensive Heterocyclic Chemistry III*, Volume 7, 2008, Pages 727-954.
83. Aaron, J. J., M. D. Gaye Seye, S. Trajkovska, N. Motohashi: Bioactive Phenothiazines and Benzo[a]phenothiazines: Spectroscopic Studies, and Biological and Biomedical properties and Applications. In: *Bioactive Heterocycles VII: Flavonoids and Anthocyanins in Plants, and Latest Bioactive Heterocycles II, Volume 16 of Topics in Heterocyclic Chemistry Series*. Ed. N. Motohashi, Springer, 2009, 153-232.
84. Ecker, Gerhard F.; Chiba, Peter. QSAR studies on drug transporters involved in toxicology. *Computational Toxicology*, In: *Computational Toxicology: Risk Assessment for Pharmaceutical and Environmental Chemicals*. Sean Ekins (Ed.), Wiley, 2009, 295-314
85. Sarkar, A., Kellogg, G.E. Hydrophobicity - Shake flasks, protein folding and drug discovery. *Current Topics in Medicinal Chemistry*, Volume 10, Issue 1, January 2010, Pages 67-83.
86. Klepsch, F., G.F. Ecker. Impact of the Recent Mouse P-Glycoprotein Structure for Structure-Based Ligand Design. *MOLECULAR INFORMATICS*, 29, 4, 276-286, 2010.
87. Yi Fan, Rayomand Unwalla, Rajiah A. Denny, Li Di†, Edward H. Kerns, David J. Diller and Christine Humblet. Insights for Predicting Blood-Brain Barrier Penetration of CNS Targeted Molecules Using QSPR Approaches. *JOURNAL OF CHEMICAL INFORMATION AND MODELING* 50 (6): 1123-1133 JUN 2010.
88. Estrada, E; Molina, E; Nodarse, D; Uriarte, E. Structural Contributions of Substrates to their Binding to P-Glycoprotein. A TOPS-MODE Approach. *CURRENT PHARMACEUTICAL DESIGN* 16 (24): 2676-2709 2010.
89. Aurijit Sarkar. Development and applications of the hint forcefield in prediction of antibiotic efflux and virtual screening for antivirals. Dissertation. Virginia Commonwealth University, Richmond VA , August 2010.
90. Teodori, E.; Dei, S.; Martelli, C.; Scapecchi, S. N,N-bis(cyclohexanol)amine aryl esters: the discovery of a new class of highly potent inhibitors of transporter-dependent multidrug resistance (MDR). *CURRENT TOPICS IN MEDICINAL CHEMISTRY*, 2010, 10(17), 1715-1731.
91. Ekins S. Drug Transporter Pharmacophores. In: *Transporters as Drug Carriers: Structure, Function, Substrates*, Vol. 44, (eds G. Ecker and P. Chiba), Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany, 215-227, 2010.
92. Molnar L., G.M. Keseru. Recent Advances in ADME Predictions. In: *Solubility, Delivery and ADME Problems of Drugs and Drug-Candidates*, edited by Karoly Tihanyi, Monika Vastag, Bentham Science Publishers, Jan 1, 2011, 3-32
93. Andreia Palmeira. Design, synthesis and evaluation of xanthone derivatives for dual activity: antitumor and P-glycoprotein inhibition. Thesis presented to the Faculdade de Farmácia, Universidade do Porto, Porto, 2011, pp. 1-402. <https://br.123dok.com/document/z31on7my-design-synthesis-and-evaluation-of-xanthone-derivatives-for-dual-activity-antitumor-and-p-glycoprotein-inhibition.html> PhD Thesis
94. Zhang L., K.-C. Tsai, L. Du, H. Fang, M. Li, W. Xu. How to Generate Reliable and Predictive CoMFA Models. *CURRENT MEDICINAL CHEMISTRY* 18 (6): 923-930 FEB 2011.
95. Donmez, Y; Akhmetova, L; Iseri, OD; Kars, MD; Gunduz, U. Effect of MDR modulators verapamil and promethazine on gene expression levels of MDR1 and MRP1 in doxorubicin-resistant MCF-7 cells. *CANCER CHEMOTHERAPY AND PHARMACOLOGY* 67 (4): 823-828 APR 2011
96. Wesolowska, O. Interaction of phenothiazines, stilbenes and flavonoids with multidrug resistance-associated transporters, P-glycoprotein and MRP1, *ACTA BIOCHIMICA POLONICA*, 58 (4):433-448; 2011.

97. Jabeen, I. Combined Ligand- and Structure-based Studies on inhibitors of P-glycoprotein DISSERTATION, Dr.-Studium der Naturwissenschaften, University of Wien, Wien, 2011. othes.univie.ac.at/17980/1/2011-11-15\_0746423.pdf
98. Jabeen I, Pleban K, Rinner U, Chiba P, Ecker GF. Structure-activity relationships, ligand efficiency, and lipophilic efficiency profiles of benzophenone-type inhibitors of the multidrug transporter p-glycoprotein. *J MED CHEM.* 2012 Apr 12;55(7):3261-73.
99. Palmeira, A; Sousa, E; Vasconcelos, MH; Pinto, M; Fernandes, MX. Structure and Ligand-based Design of P-glycoprotein Inhibitors: A Historical Perspective. *CURRENT PHARMACEUTICAL DESIGN*, 18 (27):4197-4214; SEP 2012
100. Jabeen I, Wetwitayaklung P, Chiba P, Pastor M, Ecker GF. 2D- and 3D-QSAR studies of a series of benzopyranes and benzopyrano[3,4b][1,4]-oxazines as inhibitors of the multidrug transporter P-glycoprotein. *JOURNAL OF COMPUTER-AIDED MOLECULAR DESIGN*, 27 (2):161-171; 10.1007/s10822-013-9635-9 FEB 2013
101. Liu, HM; Ma, ZG; Wu, BJ. Structure-activity relationships and in silico models of P-glycoprotein (ABCB1) inhibitors. *XENOBIOTICA*, 43 (11):1018-1026; NOV 2013.
102. Jara GE, DMA Vera, AB Pierini. Binding of Modulators to Mouse and Human Multidrug Resistance P-glycoprotein. A Computational Study. *JOURNAL OF MOLECULAR GRAPHICS AND MODELLING*, 46, 2013, 10-21.
103. Tsubaki, M; Komai, M; Itoh, T; Imano, M; Sakamoto, K; Shimaoka, H; Takeda, T; Ogawa, N; Mashimo, K; Fujiwara, D; Mukai, J; Sakaguchi, K; Satou, T; Nishida, S. By inhibiting Src, verapamil and dasatinib overcome multidrug resistance via increased expression of Bim and decreased expressions of MDR1 and survivin in human multidrug-resistant myeloma cells, *LEUKEMIA RESEARCH*, 38 (1):121-130; 10.1016/j.leukres.2013.10.017 JAN 2014.
104. Zyta, J; Jaszczyszyn, A; Swiatek, P; Gasiorowski, K; Malinka, W. Synthesis, pro-apoptotic activity and 2D-QSAR studies of new analogues of fluphenazine. *ACTA POLONIAE PHARMACEUTICA*, 71 (1):49-58; JAN-FEB 2014
105. Belaidi, S., Almi, Z., Bouzidi, D. Electronic structure and physical-chemistry properties relationship for phenothiazine derivatives by quantum chemical calculations. *JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE*, 11 (12):2481-2488; 10.1166/jctn.2014.3665 DEC 2014.
106. Almi, Zineb; Belaidi, Salah; Melkemi, Nadjib; Boughdiri, Salima; Belkhiri, Lotfi. Structure Activity Relationship and Quantitative Structure-Activity Relationships Modeling of Cyto-Toxicity of Phenothiazine Derivatives. *QUANTUM MATTER*, Volume 5, Number 1, February 2016, pp. 124-129(6).
107. Almi Zineb. Etude qualitative et quantitative des relations structures-activités dans des hétérocycles à intérêt pharmaceutique. Thèses de Doctorat, University of Biskra, 2016, pp.1-83. <http://dspace.univ-biskra.dz:8080/jspui/handle/123456789/7423>
108. Balaji Ramachandran, Sabitha Kesavan, Thangarajan Rajkumar. Molecular modeling and docking of small molecule inhibitors against NEK2. *BIOINFORMATION* 12(2) 62-68 (2016).
109. Jabeen, I. In silico strategies to probe stereoselective interactions of multidrug resistant transporter P-glycoprotein. (2016) *Letters in Drug Design and Discovery*, 13 (8), pp. 824-832.
110. Wang, M., Fan, Q., Jiang, X. Transition-Metal-Free Diarylannulated Sulfide and Selenide Construction via Radical/Anion-Mediated Sulfur-Iodine and Selenium-Iodine Exchange *ORGANIC LETTERS*, 18 (21):5756-5759; 10.1021/acs.orglett.6b03078 NOV 4 2016.
111. Boukarai, Y., Khalil, F., Bouachrine, M. DFT-based QSAR Studies of cytotoxicity of phenothiazine derivatives as in vitro anti-cancer agents using the statistical analysis methods. *Der Pharma Chemica*, 2016, 8 (18), pp. 171-185.
112. Wang, M; Wei, JP; Fan, QL; Jiang, XF. Cu(II)-Catalyzed Sulfide Construction: Both Aryl Groups Utilization of Intermolecular and Intramolecular Diaryliodonium Salt. *CHEMICAL COMMUNICATIONS*, 53 (20):2918-2921; 10.1039/c6cc09201b MAR 11 2017
113. Prachayasittikul, V; Worachartcheewan, A; Toropova, AP; Toropov, AA; Schaduengrat, N; Prachayasittikul, V; Nantasenamat, C. Large-scale classification of P-glycoprotein inhibitors using SMILES-based descriptors. *SAR AND QSAR IN ENVIRONMENTAL RESEARCH*, 28 (1):1-16; 10.1080/1062936X.2016.1264468 2017.
114. Montanari, F; Zdrzil, B. How Open Data Shapes In Silico Transporter Modeling. *MOLECULES*, 22 (3):10.3390/molecules22030422 MAR 2017.
115. Mishra, Ravinesh; Sareen, Swati; Sharma, Bhartendu; Goyal, Shubham; Kaur, Gurpreet; Bhardwaj, Sweta; A. Siddiqui, Anees; Husain, Asif; K. Singla, Rajeev; Rashid, Mohd; Kumar, Deepak; Sati, Bhawana; Shalmali, Nishtha; Kumar, Rajiv. Phenothiazines and Related Drugs as Multi Drug Resistance

Reversal Agents in Cancer Chemotherapy Mediated by p-glycoprotein." *Current Cancer Therapy Reviews* 13 (1), 2017: 28-42.

116. Cao, B., Yang, S., Li, W., Chen, H., Chen, Y., Liu, Y., & Liu, B. (2018). GMZ-1 is a podophyllotoxin derivative that suppresses growth and induces apoptosis in adriamycin-resistant K562/A02 cells through modulation of MDR1 expression. *MOLECULAR MEDICINE REPORTS*, 17 (1):474-478; 10.3892/mmr.2017.7862 JAN 2018

**5. Pajeva, I.K., M.Wiese: A comparative molecular field analysis of propafenone-type modulators of cancer multidrug resistance, *Quant. Struct.-Act. Relat.* 1998, 17, 301-312.**

Цитирания: 39

1. Dove S, Buschauer A Improved alignment by weighted field fit in CoMFA of histamine H-2 receptor agonists imidazolylpropylguanidines. *QUANT STRUCT-ACT REL* 18 (4): 329-341 OCT 1999
2. Diudea M.V., Gutman, I., Lorentz, J. Fragmental property indices (Chapter 7), In: *Molecular Toplogy*, 1999, Nova, pp. 197-232 (citation 22).
3. Ekins, S., B.J.Ring, G.Bravi, J.H.Wikel, S.A.Wrighton: Predicting drug-drug interactions in silico using pharmacophore: paradigm for the next millennium, pp. 271-300. In: *Pharmacophore Perception, Development, and Use in Drug Design (Iul Biotechnology Series)* by Osman F. Guner (Editor), 560 pages, International University Line (February 1, 2000).
4. Kellogg GE, Abraham DJ Hydrophobicity: is LogP(o/w) more than the sum of its parts? *EUR J MED CHEM* 35 (7-8): 651-661 JUL-AUG 2000
5. Ekins S, Waller CL, Swaan PW, et al. Progress in predicting human ADME parameters in silico *J PHARMACOL TOXICOL* 44 (1): 251-272 JUL-AUG 2000
6. Minailiuc, Ovidiu M. and Mircea V. Diudea: TI-MTD model applications in molecular design, In: M. V. Diudea, Ed., *QSPR/QSAR Studies by Molecular Descriptors*. NOVA SCIENCE, Huntington, New York, 2001, pp. 363-388.
7. Mircea V. Diudea, Ivan Gutman, Lorentz Jantschi. *Molecular topology*, Nova Science Publishers, 2001, 332 pages.
8. Karelson, Mati: *Molecular Descriptors in QSAR/QSPR including CD-ROM*, Wiley-Interscience; Bk&CD-Rom edition, 2000, pp. 448 (citation p. 374).
9. van Veen HW, Higgins CF, Konings WN Molecular basis of multidrug transport by ATP-binding cassette transporters: A proposed two-cylinder engine model *J MOL MICROB BIOTECH* 3 (2): 185-192 APR 2001
10. Jantschi L, Metode Moderne in Studiul QSAR/QSPR (Chapter 6.7), In: *Microbiologie si Toxicologie, Studii Fitosanitare*, Nova, 2002, pp.1-186 (citation 62).
11. Jantschi L. (PhD Thesis), *Studii Fitosanitare*, Faculty of Agriculture, University of Agriculture and Veterinary Medicine, Cluj-Napoca, 2002, pp. 1-65 (citation 56). PhD
12. Van Veen HW, Higgins CF, Konings WN: Molecular basis of multidrug transport by ATP-binding cassette transporters: A proposed two-cylinder engine model, Chapter 8, In: *Microbial Multidrug Efflux*, Ian P. Paulsen and Kim Lewis (Eds.), Horison Sci. Press, 2002, 99-120.
13. Avendano C, Menendez JC Inhibitors of multidrug resistance to antitumor agents (MDR) *CURR MED CHEM* 9 (2): 159-193 JAN 2002
14. Sean Ekins, Richard B. Kim, Brenda F. Leake, Anne H. Dantzig, Erin G. Schuetz, Lu-Bin Lan, Kazuto Yasuda, Robert L. Shepard, Mark A. Winter, John D. Schuetz, James H. Wikel, and Steven A. Wrighton. Three-dimensional quantitative structure-activity relationships of inhibitors of P-glycoprotein. *MOL PHARMACOL* 61 (5): 964-973 MAY 2002
15. Stouch TR, Gudmundsson A Progress in understanding the structure-activity relationships of P-glycoprotein *ADV DRUG DELIVER REV* 54 (3): 315-328 MAR 31 2002.
16. Rebitzer S, Annibali D, Kopp S, Eder M, Langer T, Chiba P, Ecker GF, Noe CR. In silico screening with benzofurane- and benzopyrane-type MDR-modulators. *FARMACO* 2003 Mar; 58(3):185-91.
17. Pleban K, Hoffer C, Kopp S, Peer M, Chiba P, Ecker GF. Intramolecular Distribution of Hydrophobicity Influences Pharmacological Activity of Propafenone-type MDR Modulators. *Arch Pharm (Weinheim)*. 2004 Jun;337(6):328-34.
18. Langer T, Eder M, Hoffmann RD, Chiba P, Ecker GF. Lead identification for modulators of multidrug resistance based on in silico screening with a pharmacophoric feature model. *ARCH PHARM* 337 (6): 317-327 JUN 2004
19. Degenhardt, Charles Raymond; Eickhoff, David Joseph: Substituted piperazine compounds optionally containing a quinolyl moiety for treating multidrug resistance, United States Patent 6693099, issued on February 17, 2004.
20. Ecker GF, Chiba P. Development of modulators of multidrug resistance: A pharmacoinformatic approach. *PURE APPL CHEM* 76 (5): 997-1005 MAY 2004

21. Ekins S, Swaan PW. Development of computational models for enzymes, transporters, channels, and receptors relevant to ADME/Tox. *REVIEWS IN COMPUTATIONAL CHEMISTRY* 20: 333-415 2004
22. Pleban K, Ecker GF. Inhibitors of P-glycoprotein - Lead identification and optimisation. *MINI-REV MED CHEM* 5 (2): 153-163 FEB 2005
23. Kaiser, D.; Smiesko, M.; Kopp, S.; Chiba, P.; Ecker, G. F.: Interaction Field Based and Hologram Based QSAR Analysis of Propafenone-type Modulators of Multidrug Resistance, *Medicinal Chemistry, Volume 1, Number 5, September 2005*, pp. 431-444(14).
24. Lorentz JÄNTSCHI Molecular Descriptors Family on Structure Activity Relationships 1. Review of the Methodology Leonardo Electronic Journal of Practices and Technologies, Issue 6, January-June 2005 p. 76-98.
25. Degenhardt, Charles Raymond / Eickhoff, David Joseph, Substituted heterocyclic compounds for treating multidrug resistance, *UNITED STATES PATENT* 7135483, Patent number 6376514, 14 Nov 2006.
26. Labrie P, Maddaford SP, Fortin S, Rakhit S, Kotra LP, Gaudreault RC. A comparative molecular field analysis (CoMFA) and comparative molecular similarity indices analysis (CoMSIA) of anthranilamide derivatives that are multidrug resistance modulators. *J Med Chem.* 2006 Dec 28; 49(26):7646-60.
27. Kaiser, D., Terfloth, L., Kopp, S., Schulz, J., De Laet, R., Chiba, P., Ecker, G.F., Gasteiger, J. Self-organizing maps for identification of new inhibitors of P-glycoprotein. *Journal of Medicinal Chemistry* 50 (7), pp. 1698-1702, 2007.
28. Edafiogho, Ivan O.; Kombian, Samuel B.; Ananthalakshmi, Kethireddy V. V.; Salama, Noha N.; Eddington, Natalie D.; Wilson, Tiffany L.; Alexander, Mariano S.; Jackson, Patrice L.; Hanson, Clive D.; Scott, K. R. Enaminones: exploring additional therapeutic activities. *Journal of Pharmaceutical Sciences* (2007), 96(10), 2509-2531.
29. Mittal, R.R., McKinnon, R.A., Sorich, M.J. Effect of steric molecular field settings on CoMFA predictivity *Journal of Molecular Modeling* 14 (1), 2008, pp. 59-67.
30. Ecker, G.F., Stockner, T., Chiba, P. Computational models for prediction of interactions with ABC-transporters. *Drug Discovery Today* 13 (7-8), 2008, pp. 311-317.
31. Nilesh R. Tawari, Seema Bag, Mariam S. Degani. Pharmacophore mapping of a series of pyrrolopyrimidines, indolopyrimidines and their congeners as multidrug-resistance-associated protein (MRP1) modulators. *J Mol Model* (2008) 14:911-921.
32. Keay B.A., J.M. Hopkins and P.W. Dibble, 3.08 - Furans and their Benzo Derivatives: Applications, In *Comprehensive Heterocyclic Chemistry III*, edited by Alan R. Katritzky, Christopher A. Ramsden, Eric F.V. Scriven and Richard J.K. Taylor, Reference Module in Chemistry, Molecular Sciences and Chemical Engineering, from *Comprehensive Heterocyclic Chemistry III*, Volume 3, 2008, Pages 571-623, Elsevier, Oxford, ISBN 9780080449920, <http://dx.doi.org/10.1016/B978-008044992-0.00308-4>.
33. Nicolle, E., Boumendjel, A., Macalou, S., Genoux, E., Ahmed-Belkacem, A., Carrupt, P.-A., Di Pietro, A. QSAR analysis and molecular modeling of ABCG2-specific inhibitors. *Advanced Drug Delivery Reviews* 61 (1), pp. 34-46, 2009.
34. Zdrzil B, GF Ecker. Cancer Drug Resistance: Targets and Therapies. In: *Burger's Medicinal Chemistry - Drug Discovery and Development*, Editors: Rotella D, Abrahams D., September 2010 DOI: 10.1002/0471266949.bmc215
35. Ecker, Gerhard F.; Chiba, Peter. QSAR studies on drug transporters involved in toxicology. *Computational Toxicology*, In: *Computational Toxicology: Risk Assessment for Pharmaceutical and Environmental Chemicals*. Sean Ekins (Ed.), Wiley, 2009, 295-314.
36. Ekins S. Drug Transporter Pharmacophores. In: *Transporters as Drug Carriers: Structure, Function, Substrates*, Vol. 44, (eds G. Ecker and P. Chiba), Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany, 215-227, 2010.
37. Jabeen, I. Combined Ligand- and Structure-based Studies on inhibitors of P-glycoprotein DISSERTATION, Dr.-Studium der Naturwissenschaften, University of Wien, Wien, 2011. [othes.univie.ac.at/17980/1/2011-11-15\\_0746423.pdf](https://othes.univie.ac.at/17980/1/2011-11-15_0746423.pdf)
38. Jabeen I, Wetwitayaklung P, Chiba P, Pastor M, Ecker GF. 2D- and 3D-QSAR studies of a series of benzopyranes and benzopyrano[3,4b][1,4]-oxazines as inhibitors of the multidrug transporter P-glycoprotein. *JOURNAL OF COMPUTER-AIDED MOLECULAR DESIGN*, 27 (2):161-171; 10.1007/s10822-013-9635-9 FEB 2013
39. Ivkovic, BM; Nikolic, K; Ilic, BB; Zizak, ZS; Novakovic, RB; Cudina, OA; Vladimirov, SM. Phenylpropiophenone derivatives as potential anticancer agents: Synthesis, biological evaluation and quantitative structure-activity relationship study. *EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY*, 63c, 239-255; 10.1016/j.ejmech.2013.02.013 MAY 2013

**6. Naydenova Z.L., K. Grancharov, D. Alargov, E.Golovinsky, I. Stanoeva, L. Shalamanova, I.Pajeva: Inhibition of UDP-glucuronosyltransferase by 5'-O-amino acid and oligopeptide derivatives of uridine: structure-activity relationships, *Z. Naturforsch.* 1998, 53c, 173-181.**

Цитираня: 6

1. Radominska-Pandya A, Czernik PJ, Little JM, et al. Structural and functional studies of UDP-glucuronosyltransferases. *DRUG METAB REV* 31 (4): 817-899 1999
2. Ekins, S., B.J.Ring, G.Bravi, J.H.Wikel, S.A.Wrighton: Predicting drug-drug interactions in silico using pharmacophore: paradigm for the next millennium, pp. 271-300. In: *Pharmacophore Perception, Development, and Use in Drug Design (Iul Biotechnology Series)* by Osman F. Guner (Editor), 560 pages, International University Line (February 1, 2000).
3. Smith PA, Sorich MJ, McKinnon RA, Miners JO. Pharmacophore and Quantitative Structure-Activity Relationship Modeling: Complementary Approaches for the Rationalization and Prediction of UDP-Glucuronosyltransferase 1A4 Substrate Selectivity. *J MED CHEM* 2003 Apr 24;46(9):1617-26.
4. Smith PA, Sorich MJ, McKinnon RA, Miners JO. In silico insights: Chemical and structural characteristics associated with uridine diphosphate-glucuronosyltransferase substrate selectivity. *CLIN EXP PHARMACOL P* 30 (11): 836-840 NOV 2003
5. Smith PA, Sorich MJ, Low LSC, et al. Towards integrated ADME prediction: past, present and future directions for modelling metabolism by UDP-glucuronosyltransferases. *J MOL GRAPH MODEL* 22 (6): 507-517 JUL 2004
6. Ekins S, Swaan PW. Development of computational models for enzymes, transporters, channels, and receptors relevant to ADME/Tox. *REVIEWS IN COMPUTATIONAL CHEMISTRY* 20: 333-415 2004.

**7. Todorov, D.K., M.V. Ilarionova, K.B. Timcheva, I.K. Pajeva: Antitumor activity of a *Dionaea Muscipula* E.preparation Carnivora R new in vitro and in vivo on animal and human tumors, sensitive and resistant to antitumor drugs, *Biotechnol. & Biotechnol. Eq.* 1998, 12(2), 61-66.**

Цитираня: 4

1. Kukulczanka K., and J. Budzianowski: *Dionaea muscipula* Ellis (Venus Flytrap): In vitro cultures and in vitro production of secondary metabolites. In: *Medicinal and Aromatic Plants XII*, T. Nagata, Y. Ebizuka (Eds.), *Biotechnology in Agriculture and Forestry*, Vol. 51, Springer-Verlag, Berlin, Heidelberg, 2001, p. 50-74. (citation p. 73)
2. Helmut Keller: *Handbuch der ganzheitlichen Krebstherapie.: Eine 'Bibel' für Betroffene und Gefährdete.* BOD GmbH DE, 1999, pp.290. (citation p. 245).
3. Elena T. Contreras, Jennifer R. Hawley, Michael R. Lappin. Effects of Administration of Carnivora™ on Clinical Signs in Cats After Repeat Challenge with Feline Herpesvirus 1, *INTERNATIONAL JOURNAL OF APPLIED RESEARCH IN VETERINARY MEDICINE*, 14 (3):208-216; 2016.
4. Schlosser, A; Laurain-Mattar, D; Spina, R; Couic-Marinier, F. From plants to homeopathy, interest in carnivorous plants as therapeutics. *ACTUALITES PHARMACEUTIQUES*, 57 (579):54-57; 10.1016/j.actpha.2018.07.012 OCT 2018

**8. Атанасов, К., Л. Вайсберг, К.Гарсия, М.Даскалов, И.Пъжева, Р.Струб, А.Шенон, Й.Шоршич: Обобщени мрежи в биологията и медицината, *Списание на БАН* 1998, CX1, 1-2, 44-49.**

Цитираня: 1

1. Stefanova-Pavlova M., Andonov V., Tasseva V., Gateva, A., Stefanova, E. Generalized Nets in Medicine: An Example of Telemedicine for People with Diabetes. In: *Imprecision and Uncertainty in Information Representation and Processing*, Volume 332 of the series *Studies in Fuzziness and Soft Computing*, (Eds. P. Angelov, S. Sotirov), Springer International Publishing, pp. 327-357, 2016.

**9. Pajeva, I.K., M. Wiese: Interpretation of CoMFA results - a probe set study using hydrophobic fields, *Quant. Struct.-Act. Relat.* 1999, 18 (4), 369-379.**

Цитираня: 10

1. Martinez A, Gil C, Abasolo MI, Bruno AM Perez C, Prieto C, Otero J. Benzothiadiazine dioxide dibenzyl derivatives as potent human cytomegalovirus inhibitors: Synthesis and comparative molecular field analysis. *J MED CHEM* 43 (17): 3218-3225 AUG 24 2000.
2. Kellogg GE, Abraham DJ Hydrophobicity: is LogP(o/w) more than the sum of its parts? *EUR J MED CHEM* 35 (7-8): 651-661 JUL-AUG 2000
3. Wong MG, Tehan BG, Lloyd EJ Molecular mapping in the CNS. *CURR PHARM DESIGN* 8 (17): 1547-1570 2002
4. Tsakovska IM. QSAR and 3D QSAR of Phenothiazine Type Multidrug Resistance Modulators in P388/ADR Cells. *BIOORG MED CHEM*, 2003, 11(13), 2889-2899.

5. Sewell JC, Sear JW. Derivation of preliminary three-dimensional pharmacophoric maps for chemically diverse intravenous general anaesthetics. *BRIT J ANAESTH* 92 (1): 45-53 JAN 2004.
6. Lill, M., Dobler, M. RAPTOR: User guide, Biographics Laboratory 3R, Basel, Switzerland. <http://www.biograf.ch/PDFS/Raptor.pdf>
7. Lill MA, Vedani A, Dobler M. Raptor: Combining dual-shell representation, induced-fit simulation, and hydrophobicity scoring in receptor modeling: Application toward the simulation of structurally diverse ligand sets. *J MED CHEM* 47 (25): 6174-6186 DEC 2 2004.
8. Mittal, RR; McKinnon, RA; Sorich, MJ. The Effect of Molecular Fields, Lattice Spacing and Analysis Options on CoMFA Predictive Ability. *QSAR & COMBINATORIAL SCIENCE* 28 (6-7): 637-644 JUL 2009.
9. Zhang L., K.-C. Tsai, L. Du, H. Fang, M. Li, W. Xu. How to Generate Reliable and Predictive CoMFA Models. *CURRENT MEDICINAL CHEMISTRY* 18 (6): 923-930 FEB 2011.
10. Doucet JP, A. Panaye. In: *Three Dimensional QSAR. Applications in Pharmacology and Toxicology*. Chapter 1: Comparative Molecular Field Analysis. CRC Press 2011, 3–59. eBook ISBN: 978-1-4200-9116-8, DOI: 10.1201/b10419-3

**10. Todorov, D.K., M.V. Ilarionova, I.K.Pajeva: Effectiveness of a Dionaea Muscipula E.preparation Carnivora on antitumor drug-resistant tumour cells, *Compt. rend. Acad. bulg. Sci.* 2000, 53 (1), 129-132.**

Цитирания: 1

1. Schlauer J. Global carnivorous plant diversity a contribution from the carnivorous plant specialist group (cpsg) of the international union for the conservation of nature (iucn,ssc) CPN (Carnivora Plant Newsletter), 2000, 29(3):75-82.

**11. Pajeva, I.K., M. Wiese (2000): Comparative molecular field analysis of multidrug resistance modifiers, In: *Molecular Modeling and Prediction of Bioactivity*, K. Gundertofte and F.S. Jorgensen (Eds.), Kluwer Academic/Plenum Publishers, New York, 2000, pp. 414-416.**

Цитирания: 1

1. Stefan Balaz. Modeling Kinetics of Subcellular Disposition of Chemicals. *Chem Rev.* 2009, 109(5):1793-899.

**12. Pajeva, I.K., M. Wiese: Human P-glycoprotein pseudoreceptor modeling: 3D-QSAR study of thioxanthene type multidrug resistance modulators, *Quant. Str.-Act. Relat.* 2001, 20 (2), 130-138.**

Цитирания: 16

1. Chiba P, Erker T, Galanski M, et al. Synthesis and multidrug-resistance modulating activity of a series of thienothiazines. *ARCH PHARM* 335 (5): 223-228 MAY 2002
2. Lewis R.A. Computer-Aided Drug Design 2000-2001, Chapter 5 In: *Chemical Modelling: Applications and Theory*, Volume 2, Editor: A. Hinchliffe, The Royal Society of Chemistry, 2002, pp. 271-292.
3. Waterbeemd H, Grifford E. ADMET in silico modelling: towards prediction paradise? *NATURE REV DRUG DISCOV* 2: 192-204, 2003
4. Waterbeemd, H. and B. Johnes: Predicting oral absorption and bioavailability, Chapter 1, In: *Progress in Medicinal Chemistry*, Vol. 41, Editors: F.D.King, A.W.Oxford, Elsevier, 2003, pages 322, pp.1-60 (p. 58, citation 214).
5. Dickins, M., van de Waterbeemd, H., Simulation models for drug disposition and drug interactions. *DRUG DISCOVERY TODAY: BIOSILICO* 2 (1) 38-45, 2004.
6. Avendano, C., J.C. Menedez. Recent Advances in Multidrug Resistance Modulators. *MEDICINAL CHEMISTRY REVIEWS – ONLINE*, 2004, vol. 1, no. 4, pp. 419-444 (26).
7. Hilgeroth A, Molnar A, Molnar J, Voigt B. Correlation of calculated molecular orbital energies of some phenothiazine compounds with MDR reversal properties. *Eur J Med Chem.* 2006 Apr;41(4):548-551.
8. Tomblin G, Donnelly DJ, Holt JJ, You Y, Ye M, Gannon MK, Nygren CL, Detty MR.: Stimulation of P-glycoprotein ATPase by analogues of tetramethylrosamine: coupling of drug binding at the "R" site to the ATP hydrolysis transition state. *BIOCHEMISTRY.* 2006 Jul 4; 45(26): 8034-8047.
9. Arakawa, Masamoto; Hasegawa, Kiyoshi; Funatsu, Kimito. The recent trend in QSAR modeling - variable selection and 3D-QSAR methods. *Current Computer-Aided Drug Design* (2007), 3(4), 254-262.
10. Nilesh R. Tawari, Seema Bag, Mariam S. Degani. Pharmacophore mapping of a series of pyrrolopyrimidines, indolopyrimidines and their congeners as multidrug-resistance-associated protein (MRP1) modulators. *J Mol Model* (2008) 14:911–921.
11. Balaz, Stefan. Modeling Kinetics of Subcellular Disposition of Chemicals. *Chemical Reviews* (Washington, DC, United States) (2009), 109(5), 1793-1899.

12. Gannon MK, Holt JJ, Bennett SM, Wetzel BR, Loo TW, Bartlett MC, Clarke DM, Sawada GA, Higgins JW, Tomblin G, Raub TJ, Detty MR. Rhodamine Inhibitors of P-Glycoprotein: An Amide/Thioamide "Switch" for ATPase Activity, *J Med Chem.* 2009, 52 (10): 3328-3341.
13. Wu, JH; Li, X; Cheng, WD; Xie, QJ; Liu, YQ; Zhao, CY. Quantitative Structure Activity Relationship (QSAR) Approach to Multiple Drug Resistance (MDR) Modulators Based on Combined Hybrid System. *QSAR & COMBINATORIAL SCIENCE* 28 (9): 969-978 SEP 2009.
14. Estrada, E; Molina, E; Nodarse, D; Uriarte, E. Structural Contributions of Substrates to their Binding to P-Glycoprotein. A TOPS-MODE Approach. *CURRENT PHARMACEUTICAL DESIGN* 16 (24): 2676-2709 2010.
15. Wei, DD; Wang, JS; Kong, LY. Reversal Effects of Components from the Fruits of *Illicium simonsii* on Human Adriamycin-resistant MCF-7 and 5-Fluorouracil-resistant Bel7402 Cells. *PHYTOTHERAPY RESEARCH*, 26 (4):562-567; APR 2012.
16. Orchard, A; Schamerhorn, GA; Calitree, BD; Sawada, GA; Loo, TW; Bartlett, MC; Clarke, DM; Detty, MR. Thiorhodamines containing amide and thioamide functionality as inhibitors of the ATP-binding cassette drug transporter P-glycoprotein (ABCB1). *BIOORGANIC & MEDICINAL CHEMISTRY* (2012), 20(14), 4290-4302.

**13. Wiese, M., I.K. Pajeva: Structure-activity relationships of multidrug resistance reversers, *Curr. Med. Chem.* 2001, 8 (6), 685-713.**

Цитирания: 193

1. Wang EJ, Lew K, Barecki M, Casciano CN, Clement RP, Johnson WW. Quantitative distinctions of active site molecular recognition by P-glycoprotein and cytochrome P450 3A4 *CHEM RES TOXICOL* 14 (12): 1596-1603 DEC 2001
2. Cledera P, Caballero E, Sanchez JD, Avendano C, Ramos MT, Menendez JC. Microwave-assisted synthesis of pyrazino[2,1-*b*]quinazoline-3,6-diones, 5<sup>th</sup> Intnatl. Electronic Conf. on Synth. Org. Chem. (ESCOS-5), 1-30 Sept 2001. <http://www.mdpi.org/escos-5.htm>
3. Fricker G, Miller DS Relevance of multidrug resistance proteins for intestinal drug absorption in vitro and in vivo *PHARMACOL TOXICOL* 90 (1): 5-13 JAN 2002
4. Ecker GF, Csaszar E, Kopp S, Plagens B, Holzer W, Ernst W, Chiba P. Identification of ligand-binding regions of P-glycoprotein by activated-pharmacophore photoaffinity labeling and matrix-assisted laser desorption/ionization-time-of-flight mass spectrometry. *MOL PHARMACOL* 61 (3): 637-648 MAR 2002
5. Stouch TR, Gudmundsson A Progress in understanding the structure-activity relationships of P-glycoprotein *ADV DRUG DELIVER REV* 54 (3): 315-328 MAR 31 2002
6. Winkler D.A. The role of quantitative structure-activity relationships (QSAR) in biomolecular discovery, *BRIEFINGS IN BIOINFORMATICS*, March 2002, vol. 3, no. 1, pp. 73-86(14)6.
7. Hendrich AB, Wesolowska O, Komorowska M, Motohashi N, Michalak K The alterations of lipid bilayer fluidity induced by newly synthesized phenothiazine derivative. *BIOPHYS CHEM* 98: 275-282 2002
8. Salerno M, Przewloka T, Fokt I, Priebe W, Garnier-Suillerot A. Preferential efflux by P-glycoprotein, but not MRP1, of compounds containing a free electron donor amine. *BIOCHEM PHARMACOL* 63 (8): 1471-1479 APR 15 2002
9. Chiba P, Erker T, Galanski M, Hitzler, M., Ecker, G.F. Synthesis and multidrug-resistance modulating activity of a series of thienothiazines. *ARCH PHARM* 335 (5): 223-228 MAY 2002
10. Teodori E, Dei S, Scapecchi S., Gualtieri F. The medicinal chemistry of multidrug resistance (MDR) reversing drugs. *FARMACO* 57 (5): 385-415 MAY 2002
11. Lopez-Alvarado P, Garcia-Granda S, Alvarez-Rua C, et al. Controlled generation of three contiguous stereocentres in the Michael addition of 1-pyrrolidinocyclohexene to (E)-(1-methyl-2-oxoindolin-3-ylidene)acetophenone. *EUR J ORG CHEM* (10): 1702-1707 MAY 2002
12. Clark, DE, Grootenhuis, PDJ, Progress in computational methods for the prediction of ADMET properties. *CURRENT OPINION IN DRUG DISCOVERY & DEVELOPMENT*, 2002, MAY, 5(3), 382-390.
13. Boumendjel A, Beney C, Deka N, Mariotte AM, Lawson MA, Tromprier D, Baubichon-Cortay H, Di Pietro A. 4-hydroxy-6-methoxyaurones with high-affinity binding to cytosolic domain of P-glycoprotein. *CHEM PHARM BULL* 50 (6): 854-856 JUN 2002
14. Enokida H, Gotanda T, Oku S, Imazono Y, Kubo H, Hanada T, Suzuki S, Inomata K, Kishiye T, Tahara Y, Nishiyama K, Nakagawa M. Reversal of P-glycoprotein-mediated paclitaxel resistance by new synthetic isoprenoids in human bladder cancer cell line. *JPN J CANCER RES* 93 (9): 1037-1046 SEP 2002
15. Boumendjel A, Di Pietro A, Dumontet C, Barron D. Recent advances in the discovery of flavonoids and analogs with high-affinity binding to P-glycoprotein responsible for cancer cell multidrug resistance. *MED RES REV* 22 (5): 512-529 SEP 2002

16. Garrigues A, Loiseau N, Delaforge M, Ferté J, Garrigos M, André F, Orłowski S. Characterization of two pharmacophores on the multidrug transporter P-glycoprotein. *MOL PHARMACOL* 62 (6): 1288-1298 DEC 2002
17. Seydel, J.K. Drug-membrane interactions and pharmacodynamics (Chapter 5), In: *Drug-Membrane Interactions, Analysis, Drug Distribution, Modelling*, J.K.Seydel and M. Wiese (Eds.), Willey VCH Verlag GmbH, Weinheim, 2002, pp. 237-289.
18. BOTSTEIN, David / BROWN, Patrick, O. / PEROU, Chuck / ROSS, Douglas / RING, Brian / SEITZ, Rob / BSTP-TRANS PROTEIN AND RELATED REAGENTS AND METHODS OF USE THEREOF, Patent publication number WO0208261, Publication date: 2002-01-31
19. Tiligada E, Miligkos V, Delitheos A. Cross-talk between cellular stress, cell cycle and anticancer agents: mechanistic aspects. *CURR MED CHEM ANTI-CANC AGENTS*. 2002 Jul;2(4):553-66. Review.
20. Moffat, Kristin, Dissertation, University of Sheffield, UK, 2002 [dagda.shef.ac.uk/dissertations/2001-02/Internal/Moffat\\_Kirstin\\_MScChem.pdf](http://dagda.shef.ac.uk/dissertations/2001-02/Internal/Moffat_Kirstin_MScChem.pdf)
21. Kokosi J, Almási J, Podanyi B, Hermecz I. The multidrug resistance modulators heterocondensed quinazolones. *ACTA PHARM HUNG*. 2003;73(1):29-39.
22. van der Waterbeemd H, Grifford E. ADMET in silico modelling: towards prediction paradise? *NATURE REV DRUG DISCOV* 2: 192-204, 2003
23. Hadjeri M, Barbier M, Ronot X, Mariotte AM, Boumendjel A, Boutonnat J. Modulation of p-glycoprotein-mediated multidrug resistance by flavonoid derivatives and analogues. *J Med Chem*. 2003 May 22; 46(11):2125-31.
24. Sidorova, TA Solnzeva, TI, P-glycoprotein as constitutively active Pgp-ATPase *BIOLOGICHESKIE MEMBRANY*, 2003, MAY-JUN, 20 (3), 225-235.
25. Soenen, DR, Hwang, I, Hedrick, MP, Boger, DL, Multidrug resistance reversal activity of key ningalin analogues. *BIOORGANIC & MEDICINAL CHEMISTRY LETTERS*, 2003, MAY, 13 (10), 1777-1781.
26. Nakagawa, M., Enokida, H., Gotanda, T., Tachiwada, T., Imazono, Y., Kubo, H., Nishiyama, K., Kishiye, T. Taxol resistance and its reversal by synthetic isoprenoids in human bladder cancer cell line. *AKTUEL UROL* 34 (4): 250-252 JUL 2003
27. Merighi S, Mirandola P, Varani K, Gessi S, Capitani S, Leung E, Baraldi PG, Tabrizi MA, Borea PA. Pyrazolotriazolopyrimidine derivatives sensitize melanoma cells to the chemotherapeutic drugs: taxol and vindesine. *BIOCHEM PHARMACOL* 66 (5): 739-748 SEP 1 2003
28. Barbieri F, Alama A, Tasso B, Boido V, Bruzzo C, Sparatore F. Quinolizidinyl derivatives of iminodibenzyl and phenothiazine as multidrug resistance modulators in ovarian cancer cells. *INVEST NEW DRUG* 21 (4): 413-420 NOV 2003
29. Gilles Klopman; Hao Zhu; Gerhard Ecker; Peter Chiba. MCASE study of the multidrug resistance reversal activity of propafenone analogs. *JCAMD*, 17(5): 291-297; May 2003
30. Dearden, JC, Thomson SA, QSAR study of reversal of multidrug resistance by phenothiazines, *JPP*, 55 (supl.), 2003, 134, p. S-63.
31. Robert J., Jarry, C. Multidrug resistance reversal agents. *J MED CHEM*. 2003 Nov 6;46 (23):4805-17.
32. Dearden JC, Al-Noobi A, Scott AC, Thomson SA. QSAR studies on P-glycoprotein-regulated multidrug resistance and on its reversal by phenothiazines. *SAR QSAR Environ Res*. 2003 Oct-Dec;14(5-6):447-54.
33. Glavinas Hristos, Péter Krajcsi, Judit Cserepes, and Balázs Sarkadi THE ROLE OF ABC TRANSPORTERS IN DRUG RESISTANCE, METABOLISM, AND TOXICITY *SOLVO Biotechnology*, Szeged, Hungary <http://www.solvo.hu/custommade.html> (cit. 5)
34. Waterbeemd, H. and B. Johnes: Predicting oral absorption and bioavailability, Chapter 1, In: *Progress in Medicinal Chemistry*, Vol. 41, Editors: F.D.King, A.W.Oxford, Elsevier, 2003, pages 322, pp.1-60 (p. 58, citation 213).
35. Dickins, M., van de Waterbeemd, H., Simulation models for drug disposition and drug interactions. *DRUG DISCOVERY TODAY: BIOSILICO* 2 (1) 38-45, 2004
36. Valente C, Ferreira MJU, Abreu PM, et al. Pubescenes, jatrophone diterpenes, from *Euphorbia pubescens*, with multidrug resistance reversing activity on mouse lymphoma cells *PLANTA MED* 70 (1): 81-84 JAN 2004
37. Madureira AM, Ferreira MJU, Gyemant N., Ugocsai K, Ascenso JR, Abreu PM, Hohmann J, Molnár J. Rearranged jatrophone-type diterpenes from *Euphorbia* species. Evaluation of their effects on the reversal of multidrug resistance. *PLANTA MED* 70 (1): 45-49 JAN 2004
38. Hou TJ, Xu XJ. Recent development and application of virtual screening in drug discovery: An overview. *CURR PHARM DESIGN* 10 (9): 1011-1033 2004

39. Fu LW, Liang YJ, Deng LW, Ding Y, Chen L, Ye Y, Yang X, Pan Q. Characterization of tetrandrine, a potent inhibitor of P-glycoprotein-mediated multidrug resistance. *CANCER CHEMOTH PHARM* 53 (4): 349-356 APR 2004
40. Chiba P, Ecker GF. Inhibitors of ABC-type drug efflux pumps: an overview of the current patent situation. *EXPERT OPIN THER PAT* 14 (4): 499-508 APR 2004
41. Cledera P, Sanchez JD, Caballero E, et al. Solvent-free cyclocondensation of lactim ethers with anthranilic acid under microwave irradiation. *SYNLETT* (5): 803-806 APR 3 2004
42. Wesolowska O, Hendrich AB, Motohashi N, Kawase M, Dobryszycycki P, Ozyhar A, Michalak K. Presence of anionic phospholipids rules the membrane localization of phenothiazine type multidrug resistance modulator. *BIOPHYS CHEM* 109 (3): 399-412 JUN 1 2004
43. Madureira AM, Spengler G, Molnar A, Varga A, Molnár J, Abreu PM, Ferreira MJ. Effect of cycloartanes on reversal of multidrug resistance and apoptosis induction on mouse lymphoma cells. *ANTICANCER RES* 24 (2B): 859-864 MAR-APR 2004
44. Ecker GF, Noe CR. In silico prediction models for blood-brain barrier permeation. *CURR MED CHEM* 11 (12): 1617-1628 JUN 2004
45. Kalgutkar AS, Nguyen HT. Identification of an N-methyl-4-phenylpyridinium-like metabolite of the anti-diarrheal agent loperamide in human liver microsomes: Underlying reason(s) for the lack of neurotoxicity despite the bioactivation event. *DRUG METAB DISPOS* 32 (9): 943-952 SEP 2004
46. Madureira AM, Molnar A, Abreu PM, Molnár J, Ferreira MJ. A new sesquiterpene-coumarin ether and a new abietane diterpene and their effects as inhibitors of p-glycoprotein. *PLANTA MED* 70 (9): 828-833 SEP 2004
47. Prehm P, Schumacher U. Inhibition of hyaluronan export from human fibroblasts by inhibitors of multidrug resistance transporters. *BIOCHEM PHARMACOL* 68 (7): 1401-1410 OCT 1 2004
48. Levina VV, Drobchenko EA, Shabalina EV. A new human breast carcinoma cell line resistant to DNA-damaging drugs. *ATLA-ALTERN LAB ANIM* 32 (4): 391-399 OCT 2004
49. Tao HC, Hwang IK, Boger DL. Multidrug resistance reversal activity of permethyl ningalin B amide derivatives. *BIOORG MED CHEM LETT* 14 (24): 5979-5981 DEC 20 2004
50. Johnson, W.W. ABC Transporter Proteins and Cellular Drug Resistance: P-glycoprotein and Analogous Transporters, Chapter 8, In: *Cellular Drug Delivery: Principles and practice*, D. Robert Lu, Svein Oie (eds.), Humana Press, 2004, (p. 152, citation 70).
51. Anna Seelig, Ewa Landwojtowicz, Holger Fischer, Xiaochun Li Blatter: Towards understanding P-Glycoprotein Structure-Activity Relationships, In: *Drug Bioavailability*, Editors: Han van de Waterbeemd, Hans Lennernäs, Per Artursson, In Series: *Methods and Principles in Medicinal Chemistry*. Editors: Raimund Mannhold, Hugo Kubinyi, Gerd Folkers, 2004
52. Avendano C, Sanchez JD, Menendez JC. An efficient procedure for the deprotection of N-pivaloylindoles, carbazoles and beta-carbolines with LDA. *SYNLETT* (1): 107-110 JAN 5 2005
53. Dzierzbicka K, Kolodziejczyk AM. Anthracenedione analogues - Synthesis and biological activity. *POL J CHEM* 79 (1): 1-29 JAN 2005
54. Pleban K, Ecker GF. Inhibitors of P-glycoprotein - Lead identification and optimisation. *MINI-REV MED CHEM* 5 (2): 153-163 FEB 2005
55. Wang YH, Li Y, Yang SL, Yang L. An in silico approach for screening flavonoids as P-glycoprotein inhibitors based on a Bayesian-regularized neural network. *JOURNAL OF COMPUTER-AIDED MOLECULAR DESIGN* 19 (3): 137-147 MAR 2005
56. Wang YH, Li Y, Yang SL, Yang L. Classification of substrates and inhibitors of P-glycoprotein using unsupervised machine learning approach. *JOURNAL OF CHEMICAL INFORMATION AND MODELING* 45 (3): 750-757 MAY-JUN 2005
57. Sun HM. A naive bayes classifier for prediction of multidrug resistance reversal activity on the basis of atom typing. *JOURNAL OF MEDICINAL CHEMISTRY* 48 (12): 4031-4039 JUN 16 2005
58. Fujikawa M, Ano R, Nakao K, Shimizu R, Akamatsu M. Relationships between structure and high-throughput screening permeability of diverse drugs with artificial membranes: Application to prediction of Caco-2 cell permeability. *BIOORGANIC & MEDICINAL CHEMISTRY* 13 (15): 4721-4732 AUG 1 2005
59. Pleban K, Kaiser D, Kopp S, Peer M, Chiba P, Ecker GF. Targeting drug-efflux pumps - a pharmacoinformatic approach. *ACTA BIOCHIMICA POLONICA* 2005; 52(3): 737-40.
60. Boumendjel A, Baubichon-Cortay H, Trompier D, Perrotton T, Di Pietro A. Anticancer multidrug resistance mediated by MRP1: Recent advances in the discovery of reversal agents. *MEDICINAL RESEARCH REVIEWS* 25 (4): 453-472 JUL 2005.

61. Qian F, Ye CL, Wei DZ, Lu YH, Yang SL In vitro and in vivo reversal of cancer cell multidrug resistance by 2',4'-dihydroxy-6'-methoxy-3',5'-dimethylchalcone. *JOURNAL OF CHEMOTHERAPY* 17 (3): 309-314 JUN 2005
62. Walenzyk T, Carola C, Buchholz H, Konig B Chromone derivatives which bind to human hair. *TETRAHEDRON* 61 (31): 7366-7377 AUG 1 2005
63. Liu JF, Ye P, Zhang BL, Bi G, Sargent K, Yu LB, Yohannes D, Baldino CM Three-component one-pot total syntheses of gyantrypine, fumiquinazoline F, and fiscalin B promoted by microwave irradiation. *JOURNAL OF ORGANIC CHEMISTRY* 70 (16): 6339-6345 AUG 5 2005
64. Hamasaki A, Zimpleman JM, Hwang I, Boger DL Total synthesis of ningalin D. *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY* 127 (30): 10767-10770 AUG 3 2005
65. Loo TW, Clarke DM. Recent progress in understanding the mechanism of P-glycoprotein-mediated drug efflux. *JOURNAL OF MEMBRANE BIOLOGY* 206 (3): 173-185 AUG 2005
66. Breier A, Barancik M, Sulova Z, Uhrík B P-glycoprotein - Implications of metabolism of neoplastic cells and cancer therapy. *CURRENT CANCER DRUG TARGETS* 5 (6): 457-468 SEP 2005
67. Sulova Z, Orlicky J, Fiala R, Dovinova I, Uhrík B, Seres M, Gibalova L, Breier A Expression of P-glycoprotein in L1210 cells is linked with rise in sensitivity to Ca<sup>2+</sup>. *BIOCHEMICAL AND BIOPHYSICAL RESEARCH COMMUNICATIONS* 335 (3): 777-784 SEP 30 2005
68. Borowski E, Bontemps-Gracz MM, Piwkowska A Strategies for overcoming ABC-transporters-mediated multidrug resistance (MDR) of tumor cells. *ACTA BIOCHIMICA POLONICA* 52 (3): 609-627 2005
69. Kayalar, M. Synthesis of 1,2,3,5-tetrasubstituted pyrrole derivatives via 5-exo-dig type cyclization and stereoselective functionalisation of ferrogene derivatives, Thesis for the degree of Master of Science in Chemistry, METU, 2005 | PhD
70. Thomas Walenzyk, Synthesis and immobilisation of biologically active substances, Dissertation Zur Erlangung des Doktorgrades der Naturwissenschaften (Dr. rer. nat.) der naturwissenschaftlichen Fakultät IV – Chemie und Pharmazie – der Universität Regensburg, 2005 PhD
71. PREHM PETER (DE) MEANS AND METHODS FOR TREATING A DISEASE WHICH IS ASSOCIATED WITH AN EXCESS TRANSPORT OF HYALURONAN ACROSS A LIPID BILAYER, **Patent:** WO2005013947, 2005
72. Munoz Martinez, F.: Sesquiterpenos dihidro-beta-agarofuranos como revertiores naturales de la resistencia celulr a multiples faracos causada por la Glicoproteina-P MDR1 Humana, Thesis, Universidad de Granada, 2005. PhD
73. Ros, F., Gallego, P., Power, D., Sanz, J., Jiménez, I. Use of lactamide diastereoisomers to permit resolution of a racemic modulator of cancer drug resistance. *Journal of Chemical Research* (1), pp. 32-34, 2005.
74. Ionescu, S., Diaconu, C.C., Hillebrand, M. Theoretical study of some verapamil derivatives. *INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY* 106 (6), 1457-1464, 2006.
75. Vaclavikova R, Boumendjel A, Ehrlichova M, Kovar J, Gut I. Modulation of paclitaxel transport by flavonoid derivatives in human breast cancer cells. Is there a correlation between binding affinity to NBD of P-gp and modulation of transport? *BIOORG MED CHEM.* 2006;14(13):4519-25.
76. Li, Y., Wang, L. Yang, S. Zhang, and C. Liu, Impact of Molecular Hydrophobic Field on Passive Diffusion, P-Glycoprotein Active Efflux, and P-Glycoprotein Modulation of Steroids, *INTERNET ELECTRON. J. MOL. DES.* 2006, 5, 60–78. <http://www.biochempress.com>.
77. Luco, J.M., Marchevsky, E. QSAR studies on blood-brain barrier permeation. *CURRENT COMPUTER-AIDED DRUG DESIGN* 2 (1), pp. 31-55, 2006.
78. Teodori, E., Dei, S., Martelli, C., Scapecchi, S., Gualtieri, F. The functions and structure of ABC transporters: Implications for the design of new inhibitors of Pgp and MRP1 to control multidrug resistance (MDR). *CURRENT DRUG TARGETS* 7 (7), pp. 893-909, 2006.
79. Ortuño, J.A., Hernández, J., Sánchez-Pedreño, C. Ion-selective electrode for the determination of some multidrug resistance reversers. *SENSORS AND ACTUATORS, B: CHEMICAL* 119 (1), pp. 282-287, 2006
80. ZHENG Zhong-hua;; ZHANG Yi-zhong;; FANG Qing;; Development of Research on P-gp dynamics kinetics. *JOURNAL OF JILIN MEDICAL COLLEGE* Vol.27 No.2 P.108-113, 2006
81. Ferreira, M.-J.U., Duarte, N., Gyémánt, N., Radics, R., Cherepnev, G., Varga, A., Molnár, J. Interaction between doxorubicin and the resistance modifier stilbene on multidrug resistant mouse lymphoma and human breast cancer cells. *ANTICANCER RESEARCH*, 26 (5 A), 2006, 3541-3546.
82. Barancik, M., Bohacova, V., Sedlak, J., Sulova, Z., Breier, A. LY294,002, a specific inhibitor of PI3K/Akt kinase pathway, antagonizes P-glycoprotein-mediated multidrug resistance. *EUROPEAN JOURNAL OF PHARMACEUTICAL SCIENCES*, 29, 426-434, 2006.

83. Barthold Deiters: Untersuchungen zum Hyaluronan Export aus Chondrozyten bei arthrotischen Veränderungen, Inaugural-Dissertation zur Erlangung des Doktorgrades der Naturwissenschaften im Fachbereich Chemie und Pharmazie der Mathematisch-Naturwissenschaftlichen Fakultät der Westfälischen Wilhelms-Universität Münster, 2006. PhD thesis
84. Duarte, N., Varga, A., Cherepnev, G., Radics, R., Molnar, J., Ferreira, M.J.U.: Apoptosis induction and modulation of P-glycoprotein mediated multidrug resistance by new macrocyclic lathyrane-type diterpenoids. *Bioorganic & Medicinal Chemistry*, 15 (1), 546-554, 2007.
85. Sharom FJ. Shedding light on drug transport: structure and function of the P-glycoprotein multidrug transporter (ABCB1). *BIOCHEM CELL BIOL.* 2006 Dec;84(6):979-92.
86. Solazzo, M., O. Fantappiè, N. Lasagna, C. Sassoli, D. Nosi, R. Mazzanti: P-gp localization in mitochondria and its functional characterization in multiple drug-resistant cell lines. *Experimental Cell Research*, Volume 312, Issue 20, 10 December 2006, Pages 4070-4078.
87. Ecker, G., C.R.Noë. In silico prediction models for blood-brain permeation. In: *Blood-Brain Barriers: From Ontogeny to Artificial Interfaces*, R. Dermietzel, D. C. Spray, M. Nedergaard (Edts.), Vol.1, 2006, Wiley-VCH, 403-428. (ref. 41)
88. LI Yan, WANG Yong-hua, YANG Ling, ZHANG Shu-wei, LIU Chang-hou: Study of concerted mechanism between P-glycoprotein and cytochrome P4503A4 by 3D-pharmacophore modeling. *JOURNAL OF MOLECULAR SCIENCE*. 22 (4), 237-242, 2006.
89. Siarheyeva, Alena. Solid-state NMR investigations of the ATP binding cassette multidrug transporter LmrA. University, Diss., 2006--Frankfurt (Main) <http://deposit.d-nb.de/cgi-bin/dokserv?idn=981459951> PhD
90. McDevitt, C.A., Callaghan, R. How can we best use structural information on P-glycoprotein to design inhibitors? *Pharmacology and Therapeutics* 113 (2), 2007, 429-441.
91. Schmidt, M., Ungvári, J., Gloede, J., Dobner, B., Langner, A.: New 1,3-dioxolane and 1,3-dioxane derivatives as effective modulators to overcome multidrug resistance *Bioorganic and Medicinal Chemistry* 15 (6), pp. 2283-2297, 2007.
92. Pilar Cledera Crespo, Analogos de ardeemina derivados del sistema de pirazino[2-1-b]quinazolina-3,6-diona. Thesis Doctoral, Universidad Complutense de Madrid, Facultad de Farmacia, Madrid 2007. PhD
93. Zhou, C., Shen, P., Cheng, Y.: Quantitative study of the drug efflux kinetics from sensitive and MDR human breast cancer cells. *Biochimica et Biophysica Acta - General Subjects* 1770 (7), pp. 1011-1020, 2007.
94. Liu, J.-F.: Rapid syntheses of biologically active quinazolinone natural products using microwave technology. *Current Organic Synthesis* 4 (2), pp. 223-237, 2007.
95. Christine Müller. New approaches to the therapy of glioblastoma: investigations on RNA interference, kinesin Eg5 and ABCB1/ABCG2 inhibition, Dissertation, Universität Regensburg, 2007.
96. Egger, Michael; Li, Xuqin; Mueller, Christine; Bernhardt, Guenther; Buschauer, Armin; Koenig, Burkhard. Tariquidar analogues: synthesis by CuI-catalysed N/O-aryl coupling and inhibitory activity against the ABCB1 transporter. *European Journal of Organic Chemistry* (2007), (16), 2643-2649.
97. Ortuno, J. A.; Gil, A.; Serna, C.; Molina, A. Voltammetry of some catamphiphilic drugs with solvent polymeric membrane ion sensors. *Journal of Electroanalytical Chemistry* (2007), 605(2), 157-161.
98. Ponte-Sucre, A. Availability and applications of ATP-binding cassette (ABC) transporter blockers. *Applied Microbiology and Biotechnology* 76 (2), pp. 279-286, 2007.
99. Abraham, M. H.; Hersey, A. In silico models to predict brain uptake. *Comprehensive Medicinal Chemistry II* (2006), 5 745-766
100. Dykens, J. A. Redox enzymes. *Comprehensive Medicinal Chemistry II* (2006), 2, 1053-1087.
101. Sharom, Frances J. Allergic contact dermatitis from toluene-2,5-diamine in a cream dye for eyelashes and eyebrows-quantitative exposure assessment. *Drug Transporters* (2007), 223-262.
102. Reyes, C.P., Muñoz-Martínez, F., Torrecillas, I.R., Mendoza, C.R., Gamarro, F., Bazzocchi, I.L., Núñez, M.J., Pardo, L., Castanys, S., Campillo, M., Jiménez, I.A.: Biological evaluation, structure-activity relationships, and three-dimensional quantitative structure-activity relationship studies of dihydro- $\beta$ -agarofuran sesquiterpenes as modulators of P-glycoprotein-dependent, *Journal of Medicinal Chemistry*, Volume 50, Issue 20, 20 October 2007, Pages 4808-4817.
103. Liu, J., Cui, G., Zhao, M., Cui, C., Ju, J., Peng, S.: Dual-acting agents that possess reversing resistance and anticancer activities: Design, synthesis, MES-SA/Dx5 cell assay, and SAR of Benzyl 1,2,3,5,11,11a-hexahydro-3,3-dimethyl-1-oxo-6H-imidazo[3',4':1,2]pyridin[3,4-b]indol-2-substituted acetates. *Bioorganic and Medicinal Chemistry* 15 (24), 2007, pp. 7773-7788.
104. Pauwels, E.K.J., P. Erba, G. Mariani, C.M.F. Gomes Multidrug Resistance in Cancer: Its Mechanism and its Modulation. *Drug News Perspect.* 20(6), 2007, 371.

105. Cledera, Pilar; Sanchez, Juan Domingo; Caballero, Esmeralda; Yates, Tamara; Ramirez, Elena G.; Avendano, Carmen; Ramos, M. Teresa; Menendez, J. Carlos. Microwave-assisted, solvent-free synthesis of several quinazoline alkaloid frameworks. *Synthesis* (2007), (21), 3390-3398.
106. Ha, Sookhee N.; Hochman, Jerome; Sheridan, Robert P. Mini review on molecular modeling of P-glycoprotein (Pgp). *Current Topics in Medicinal Chemistry* (Sharjah, United Arab Emirates), 2007, 7(15), 1525-1529.
107. Liu, J., Cui, G., Zhao, M., Cui, C., Ju, J., Peng, S. Dual-acting agents that possess reversing resistance and anticancer activities: Design, synthesis, MES-SA/Dx5 cell assay, and SAR of Benzyl 1,2,3,5,11,11a-hexahydro-3,3-dimethyl-1-oxo-6H-imidazo[3',4':1,2]pyridin[3,4-b]indol-2-substituted acetates. *Bioorganic and Medicinal Chemistry* 15 (24), 2007, pp. 7773-7788.
108. Ecker, G.F., Stockner, T., Chiba, P. Computational models for prediction of interactions with ABC-transporters. *Drug Discovery Today* 13 (7-8), 2008, pp. 311-317.
109. Avendano, C. and J. Carlos Menendez: Drugs that modulate resistance to antitumor agents, Chapter 12, In: *Medicinal Chemistry of Anticancer Drugs*, Elsevier, 2008, 387-416.
110. WANG Jue-Qiong, CHEN Bao-An, CHENG Jian, XU Wen-Lin, SUN Xin-Chen. Comparison of Reversal Effects of 5-Bromotetrandrine and Tetrandrine on P-Glycoprotein-dependent Resistance to Adriamycin in Human Leukemia Cell Line K562/A02 *CHINESE JOURNAL OF CANCER*, 2008 Vol.27 No.5 P.491-495.
111. Coburger, Claudius; Wollmann, Jorg; Baumert, Christiane; Krug, Martin; Molnar, Josef; Lage, Hermann; Hilgeroth, Andreas. Novel Insight in Structure-Activity Relationship and Bioanalysis of P-Glycoprotein Targeting Highly Potent Tetrakis-hydroxymethyl Substituted 3,9-Diazatetraasteranes. *Journal of Medicinal Chemistry* (2008), 51(18), 5871-5874
112. Duarte N, Jardanhazy A, Molnar J, Andreas Hilgeroth A., Ferreira, M.-J. U. Synergistic interaction between p-glycoprotein modulators and epirubicin on resistant cancer cells, *BIOORGANIC & MEDICINAL CHEMISTRY*, 2008, 16 (20), 9323-9330.
113. Matthias Schmidt, Marlen Teitge, Marianela E. Castillo, Tobias Brandt, Bodo Dobner, Andreas Langner: Synthesis and Biochemical Characterization of New Phenothiazines and Related Drugs as MDR Reversal Agents, *ARCHIV DER PHARMAZIE*, 2008, Vol. 341 (10), 624-638.
114. Prasad VVSR, Rao JV, Giri RS, Sathish NK, Shanta Kumar SM, Mayur, YC. Chloro acridone derivatives as cytotoxic agents active on multidrug-resistant cell lines and their duplex DNA complex studies by electrospray ionization mass spectrometry *CHEMICO-BIOLOGICAL INTERACTIONS*, 2008, 176 (2-3), 212-219.
115. Colabufo, NA, F Berardi, MC Inglese and R. Perrone. Flavonoids as MDR modulating agents: SAR studies. In: *Multidrug Resistance: Biological and Pharmaceutical Advance in the Antitumour Treatment*, Editor: Nicola Antonio Colabufo, 2008: 171-201 ISBN: 978-81-308-0258-9.
116. Tobias Brandt. Untersuchung und charakterisierung von inhibitoren des p-glykoproteins zur überwindung der multidrug resistance. Dissertation. Naturwissenschaftlichen Fakultät I Biowissenschaften der Martin-Luther-Universität Halle-Wittenberg, 2008. <http://dx.doi.org/10.25673/2284> PhD
117. Ni NT, Li MY, Wang JF, et al. Inhibitors and Antagonists of Bacterial Quorum Sensing *MEDICINAL RESEARCH REVIEWS* Vol. 29(1), 65-124, JAN 2009.
118. Martelli C, Alderighi D, Coronello M, Dei S Frosini M Le Bozec B Manetti D Neri A Romanelli MN Salerno M Scapecchi S Mini E Sgaragli G Teodori E. N,N-bis(Cyclohexanol)amine Aryl Esters: A New Class of Highly Potent Transporter-Dependent Multidrug Resistance Inhibitors. *JOURNAL OF MEDICINAL CHEMISTRY*, 52, 3, 807-817, FEB 12 2009
119. Balaz, Stefan. Modeling Kinetics of Subcellular Disposition of Chemicals. *Chemical Reviews* (Washington, DC, United States) (2009), 109(5), 1793-1899.
120. Sun, L.-R., Cui, S.-X., Qu, X.-J. Overcoming multidrug resistance in cancer: An update on research of natural products. *Drugs Fut* 2009, 34(1): 53 ISSN 0377-8282 Copyright 2009 Prous Science CCC: 0377-8282.
121. Mayur, Y. C.; Peters, G. J.; Rajendra Prasad, V. V.S.; Lemos, C.; Sathish, N. K. Design of New Drug Molecules to be Used in Reversing Multidrug Resistance in Cancer Cells. *Current Cancer Drug Targets*, 9(3), 2009, pp. 298-306.
122. Tayyab A. Mansoor, Catia Ramalheite, Joseph Molnr, Silva Mulhovo and Maria Jos U. Ferreira. Tabernines A-C,  $\beta$ -Carbolines from the Leaves of *Tabernaemontana elegans*, *J. Nat. Prod.*, 2009 72(6), 1147-1150.
123. Jiao W, Dong W, Li Z, Deng M, Lu R. Lathyrane diterpenes from *Euphorbia lathyris* as modulators of multidrug resistance and their crystal structures. *Bioorg Med Chem*. 2009; 17(13):4786-92.

124. Ecker, Gerhard F.; Chiba, Peter. QSAR studies on drug transporters involved in toxicology. *Computational Toxicology*, In: *Computational Toxicology: Risk Assessment for Pharmaceutical and Environmental Chemicals*. Sean Ekins (Ed.), Wiley, 2009, 295-314.
125. Bogush, T., J. Robert. Multidrug Resistance Reversal in Solid Tumors. In: *ABC Transporters and Multidrug Resistance*, Editor(s): A. Boumendjel, J. Boutonnat, J. Robert, 2009 John Wiley & Sons, Inc., Chapter 12, 349-362.
126. Gatti, L.; Beretta, G. L.; Cossa, G.; Zunino, F.; Perego, P. ABC transporters as potential targets for modulation of drug resistance. *Mini-Reviews in Medicinal Chemistry* (2009), 9(9), 1102-1112.
127. Ponte-Sucre, A., M. Padron-Nieves, E. Diaz. ABC transporter blockers and reversal of drug resistance in microorganisms. In: *ABC transporters in microorganisms: Research, Innovation and Value as Targets against Drug Resistance*, Horizon Scientific Press, 2009, 177-195. ISBN: 978-1-904455-49-3 <http://saber.ucv.ve/123456789/1737>.
128. Akamatsu, M; Fujikawa, M; Nakao, K; Shimizu, R. In silico Prediction of Human Oral Absorption Based on QSAR Analyses of PAMPA Permeability. *CHEMISTRY & BIODIVERSITY* 6 (11): 1845-1866 2009.
129. Mensch, J., Oyarzabal, J., Mackie, C., Augustijns, P. In vivo, in vitro and in silico methods for small molecule transfer across the BBB *Journal of Pharmaceutical Sciences* 98 (12), pp. 4429-4468, 2009.
130. Duarte, N; Ramalheite, C; Varga, A; Molnar, J; Ferreira, MJU. Multidrug Resistance Modulation and Apoptosis Induction of Cancer Cells by Terpenic Compounds Isolated from Euphorbia Species. *ANTICANCER RESEARCH* 29 (11): 4467-4472 NOV 2009.
131. María Fabiana De Rosa. Multidrug Resistance Protein 1 (MDR1) And Glycosphingolipids Biosynthesis: Advantages for Therapeutics, Doctor of Philosophy, Department of Laboratory Medicine and Pathobiology, University of Toronto, 2009. PhD <https://space.library.utoronto.ca/handle/1807/19262>
132. Michael Egger. Inhibition of ABC Transporters Associated with Multidrug Resistance. Dissertation zur Erlangung des Doktorgrades der Naturwissenschaften (Dr. rer. nat.) an der naturwissenschaftlichen Fakultät IV - Chemie und Pharmazie - der Universität Regensburg, 2009. PhD thesis
133. Xiong, J. M. Taniguchi, Y. Kashiwada, M. Sekiya, T. Yamagishi and Y. Takaishi. Papyriferic acid derivatives as reversal agents of multidrug resistance in cancer cells *Bioorganic & Medicinal Chemistry*, Volume 18, Issue 8, 15 April 2010, Pages 2964-2975.
134. S. Apte. Selecting surfactants for the maximum inhibition of the activity of the multidrug resistance efflux pump transporter, P-glycoprotein: conceptual development. *Journal of Excipients and Food Chemicals*, Vol 1, No 3, 51-59 (2010).
135. Müller, H. The ABC transporter P-glycoprotein: Physiological and pathophysiological significance [Der ABC-transporter P-glykoprotein physiologische und pathophysiologische bedeutung] *PZ Prisma* Volume 17, Issue 2, 2010, Pages 93-102.
136. Hany Hassounah. Investigations on the phylogenetic diversity of urease producing bacteria in soil, the inhibition of urea active transportation and metabolizing in *Bacillus megaterium* DSM 90. Faculty of Natural Sciences (I) Life Sciences, Martin-Luther-University Halle-Wittenberg, Halle (Saale) 2010. PhD thesis
137. Krug, M; Voigt, B; Baumert, C; Lupken, R; Molnar, J; Hilgeroth, A. First biological evaluation of developed 3-benzyloxyfluorenes as novel class of MDR modulators. *EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY* 45 (6): 2683-2688 JUN 2010.
138. Coburger, C; Wollmann, J; Krug, M; Baumert, C; Seifert, M; Molnar, J; Lage, H; Hilgeroth, A. Novel structure-activity relationships and selectivity profiling of cage dimeric 1,4-dihydropyridines as multidrug resistance (MDR) modulators. *BIOORGANIC & MEDICINAL CHEMISTRY* 18 (14): 4983-4990 JUL 15 2010
139. Bao-an Chen, Xue-yun Shan, Chen Jian, Fei Wang, Jia-hua Ding, Gao Chong, Zhao Gang, Wang Xuemei, Wen-lin Hsu, Xia Guohua, Michael Schmitt. Study on reversal effect of nilotinib in combination with 5-BrTet on multidrug resistance of k562/a02 cell line. *CHINESE JOURNAL OF HEMATOLOGY*, 2010, 31(6). Doi: 10.3760/cma.j.issn.1253-2727.2010.06.006.
140. Docolomansky, P; Bohacova, V; Barancik, M; Breier, A. Why the xanthine derivatives are used to study of P-glycoprotein-mediated multidrug resistance in L1210/VCR line cells. *GENERAL PHYSIOLOGY AND BIOPHYSICS* 29 (3): 215-221 SEP 2010
141. Teodori, E.; Dei, S.; Martelli, C.; Scapecchi, S. N,N-bis(cyclohexanol)amine aryl esters: the discovery of a new class of highly potent inhibitors of transporter-dependent multidrug resistance (MDR). *CURRENT TOPICS IN MEDICINAL CHEMISTRY*, 2010, 10(17), 1715-1731.
142. Mahobia N. K., R. D. Patel, N.W. Sheikh, S. K. Singh, A. Mishra, R. Dhardubey. Validation Method Used In Quantitative Structure Activity Relationship. *DER PHARMA CHEMICA*, 2010, 2(5):260-271 <http://derpharmachemica.com/archive.html>

143. Prakash, A. S. Selecting surfactants for the maximum inhibition of the activity of the multidrug resistance efflux pump transporter, P-glycoprotein: conceptual development JOURNAL OF EXCIPIENTS AND FOOD CHEMICALS, Vol 1, No 3 (2010).
144. Huber, PC; Maruiama, CH; Almeida, WP. P-glycoprotein and multidrug resistance: structure-activity relationships of modulators. QUIMICA NOVA 33 (10): 2148-2154 2010.
145. Liu, J; Li, Y; Zhang, SW; Xiao, ZT; Ai, CZ. Studies of New Fused Benzazepine as Selective Dopamine D3 Receptor Antagonists Using 3D-QSAR, Molecular Docking and Molecular Dynamics. INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES 12 (2): 1196-1221 FEB 2011.
146. Giorgi, G; Maiti, S; Lopez-Alvarado, P; Menendez, JC. Synthesis of benzo- and naphtho-fused bicyclo[n.3.1]alkane frameworks with a bridgehead nitrogen function by palladium-catalyzed intramolecular alpha'-arylation of alpha-nitroketones. ORGANIC & BIOMOLECULAR CHEMISTRY 9 (8): 2722-2730 2011.
147. Di Ianni M., Talevi A., Eduardo A., Castro A.E., Bruno-Blanch L.E. Development of a highly specific ensemble of topological models for early identification of P-glycoprotein substrates. JOURNAL OF CHEMOMETRICS, 25(6), 313-322, 2011.
148. Robert, J. Reversal Of Cancer Multidrug Resistance: Expectations And Disappointments. BULLETIN DE L ACADEMIE VETERINAIRE DE FRANCE, 164 (3):271-274; JUL-SEP 2011.
149. HISTORY IN THE REVOLUTION OF QSAR: A REVIEW. PharmaTutor (Pharmacy Infopedia). <http://www.pharmatutor.org/articles/history-revolution-of-qsar-quantitative-structural-activity-relationship?page=0,2>
150. He, X., Cheng, Z., Nie, X., Li, K., Zhao, X., Chen, J. Effects of Norfloxacin on the phase I and II enzyme activities and mRNA expressions of CYP1A1 and P-gp of *Mugilogobius abei*. *Huanjing Kexue Xuebao/Acta Scientiae Circumstantiae* 31 (4) , pp. 846-853, 2011.
151. Jabeen, I. Combined Ligand- and Structure-based Studies on inhibitors of P-glycoprotein DISSERTATION, Dr.-Studium der Naturwissenschaften, University of Wien, Wien, 2011. [thes.univie.ac.at/17980/1/2011-11-15\\_0746423.pdf](https://thes.univie.ac.at/17980/1/2011-11-15_0746423.pdf)
152. Cátia Vicente Vieira. Compostos Bioativos Isolados de *Euphorbia boetica* Modulação da Glicoproteína-P. Mestrado em Química Farmacêutica e Terapêutica. UNIVERSIDADE DE LISBOA. FACULDADE DE FARMÁCIA. Lisboa, 2011. [www.ff.ul.pt/FCT/PTDC/QEQ.../Tese-Msci1.pdf](http://www.ff.ul.pt/FCT/PTDC/QEQ.../Tese-Msci1.pdf)
153. Yap, Wai Sum (2011) *Biologically active alkaloids from kopsia / Yap Wai Sum*. Masters thesis, Department Of Chemistry, Faculty of Science, University Malaya, 2011.
154. Andreia Palmeira. Design, synthesis and evaluation of xanthone derivatives for dual activity: antitumor and P-glycoprotein inhibition. Thesis presented to the Faculdade de Farmácia, Universidade do Porto, Porto, 2011, pp. 1-402. PhD Thesis <https://br.123dok.com/document/z31on7my-design-synthesis-and-evaluation-of-xanthone-derivatives-for-dual-activity-antitumor-and-p-glycoprotein-inhibition.html>
155. Ricardo José Ferreira, Maria José Umbelino Ferreira, and Daniel J. V. A. dos Santos. Insights on P-Glycoprotein's Efflux Mechanism obtained by Molecular Dynamics Simulations. JOURNAL OF CHEMICAL THEORY AND COMPUTATION, 8 (6):1853-1864; 10.1021/ct300083m JUN 2012.
156. Liu, Z; Li, Y; Ren, H; Zhang, SW; Wang, YH; Li, GH; Yang, L. Structure Requirements for 4-Aryl-4H-Chromenes as Apoptosis Inducers Using 3D QSAR Methods and Docking Studies. ASIAN JOURNAL OF CHEMISTRY, 24 (6):2450-2460; JUN 2012.
157. Xu, Y; Zhi, F; Xu, GM; Tang, XL; Lu, S; Wu, JH; Hu, YQ. Overcoming Multidrug Resistance in Vitro and in Vivo by a Novel P-glycoprotein Inhibitor 1416. BIOSCIENCE REPORTS, 32 (6):559-566; 10.1042/BSR20120020 DEC 2012.
158. Palmeira, A; Sousa, E; Vasconcelos, MH; Pinto, M; Fernandes, MX. Structure and Ligand-based Design of P-glycoprotein Inhibitors: A Historical Perspective. CURRENT PHARMACEUTICAL DESIGN, 18 (27):4197-4214; SEP 2012
159. MJU Ferreira, N Duarte, H Lage, J Molnár. Reversal of Multidrug Resistance by Macrocyclic and Polycyclic Diterpenoids from *Euphorbia* species. In: *Recent Progress in Medicinal Plants. Volume 32: Ethnomedicine and Therapeutic Validation*. Eds. J.N. Govil and Geetanjali Kaushik. 2012, 193-213.
160. Reis, M; Ferreira, RJ; Serly, J; Duarte, N; Madureira, AM; Santos, DJVA; Molnar, J; Ferreira, MJU. Colon Adenocarcinoma Multidrug Resistance Reverted by *Euphorbia* Diterpenes: Structure-Activity Relationships and Pharmacophore Modeling. ANTI-CANCER AGENTS IN MEDICINAL CHEMISTRY, 12 (9):1015-1024; NOV 2012.
161. Almeida, W., P. Huber, L. Kohn, J. de Carvalho. In vitro antiproliferative effect of  $\beta$ -phenylethylamine derivatives and doxorubicin combinations on MCF/ADR cell lines. MEDICINAL CHEMISTRY RESEARCH, February 2013, Volume 22, Issue 2, pp 548-557.

162. Chakraborty, A; Pan, S; Chattaraj, PK. Biological Activity and Toxicity: A Conceptual DFT Approach. In: APPLICATIONS OF DENSITY FUNCTIONAL THEORY TO BIOLOGICAL AND BIOINORGANIC CHEMISTRY (Editor(s): Putz MV; Mingos DMP), 2013, 150 143-179.
163. POŁA, A., MOSIĄDZ, D., Saczko, J., Modrzycka, T., & Michalak, K.. The Influence of Phenothiazine Derivatives on Intracellular Accumulation of Cationic Cyanine Dye DiOC<sub>6</sub>(3) in LoVo-DX. *CELLS ANTICANCER RES.* 33 (3) 857-863, 2013.
164. Jie Yang and Jie Chen. QSAR Analysis of Purine-Type and Propafenone-Type Substrates of P-Glycoprotein Targeting  $\beta$ -Amyloid Clearance, *Neurodegenerative Diseases*, Dr. Uday Kishore (Ed.), ISBN: 978-953-51-1088-0, InTech, DOI: 10.5772/54975.2013 Available from: <http://www.intechopen.com/books/neurodegenerative-diseases/qsar-analysis-of-purine-type-and-propafenone-type-substrates-of-p-glycoprotein-targeting-amyloid-cle>
165. Ferreira RJ, Maria-José U. Ferreira, and Daniel J. V. A. dos Santos. Molecular Docking Characterizes Substrate-Binding Sites and Efflux Modulation Mechanisms within P-Glycoprotein. *JOURNAL OF CHEMICAL INFORMATION AND MODELING*, 53 (7):1747-1760; 10.1021/ci400195v JUL 2013
166. Ferreira, RJ; Ferreira, MJU; dos Santos, DJVA. Assessing the Stabilization of P-Glycoprotein's Nucleotide-Binding Domains by the Linker, Using Molecular Dynamics. *MOLECULAR INFORMATICS*, 32 (5-6):529-540; SI 10.1002/minf.201200175 JUN 2013.
167. Zhu, T. , Chen, J. and Yang, J. (2013) Some substrates of P-glycoprotein targeting  $\beta$ -amyloid clearance by quantitative structure-activity relationship (QSAR)/membrane-interaction (MI)-QSAR analysis. *ADVANCES IN BIOSCIENCE AND BIOTECHNOLOGY*, 4, 872-895. doi: 10.4236/abb.2013.49116.
168. Breier, A; Gibalova, L; Seres, M; Barancik, M; Sulova, Z. New Insight into P-Glycoprotein as a Drug Target. *ANTI-CANCER AGENTS IN MEDICINAL CHEMISTRY*, 13 (1):159-170; JAN 2013.
169. Simon, S. Inhibitorischer Einfluss von Phospholipiden auf den Effluxtransporter P-Glykoprotein (Inhibitory influence of phospholipids on the efflux transporter P-glycoprotein). zur Erlangung der Doktorwürde der Fakultät für Chemie und Pharmazie der Albert-Ludwigs-Universität, Freiburg im Breisgau, Germany. PhD thesis <http://www.freidok.uni-freiburg.de/volltexte/8916/>
170. Rubelt MS. Enhancement of the Intestinal Epithelial Permeability of Peripherally Acting Opioid Analgesics by Chitosan. Dissertation. Mathematisch-Naturwissenschaftlichen Fakultät I der Humboldt-Universität zu Berlin. Oct 2013. PhD
171. L Lv, X Zhang, J Lv, Y Zhou, W Hu, P Yu, H Sun, Y Teng. Design, Synthesis and Biological Evaluation of the Novel Antitumor Agent 5-Bromobenzofuran-3(2H)-One and its Derivatives. *Proceedings of the 2012 International Conference on Applied Biotechnology (ICAB 2012). Lecture Notes in Electrical Engineering. Volume 250, 2014, pp 835-841.*
172. Singh, S; Prasad, NR; Kapoor, K; Chufan, EE; Patel, BA; Ambudkar, SV; Talele, TT. Design, Synthesis, and Biological Evaluation of (S)-Valine Thiazole-Derived Cyclic and Noncyclic Peptidomimetic Oligomers as Modulators of Human P-Glycoprotein (ABCB1). *CHEMBIOCHEM*, 15 (1):157-169; 10.1002/cbic.201300565 JAN 3 2014.
173. Vadlapatla, RK; Vadlapudi, AD; Pal, D; Mitra, AK. Mechanisms of Drug Resistance in Cancer Chemotherapy: Coordinated Role and Regulation of Efflux Transporters and Metabolizing Enzymes. *CURRENT PHARMACEUTICAL DESIGN*, 19 (40):7126-7140; DEC 2013.
174. Parveen, Z; Brunhofer, G; Jabeen, I; Erker, T; Chiba, P; Ecker, GF. Synthesis, biological evaluation and 3D-QSAR studies of new chalcone derivatives as inhibitors of human P-glycoprotein. *BIOORGANIC & MEDICINAL CHEMISTRY*, 22 (7):2311-2319; 10.1016/j.bmc.2014.02.005 APR 1 2014.
175. Ferreira, Maria-José U., Duarte, Noélia, Reis, Mariana, Madureira, Ana Margarida, Molnár, Joseph. Euphorbia and Momordica metabolites for overcoming multidrug resistance. *PHYTOCHEM REV*, *Phytochemistry Reviews*, 13 (4), pp. 915-935, 2014.
176. Szafraniec, MJ; Szczygiel, M; Urbanska, K; Fiedor, L. Determinants of the activity and substrate recognition of breast cancer resistance protein (ABCG2). *DRUG METABOLISM REVIEWS*, 46 (4):459-474; 10.3109/03602532.2014.942037 NOV 2014.
177. Vasas, A; Hohmann, J. Euphorbia Diterpenes: Isolation, Structure, Biological Activity, and Synthesis (2008-2012). *CHEMICAL REVIEWS*, 114 (17):8579-8612; 10.1021/cr400541j SEP 10 2014
178. Ferreira, R. J., Ferreira, M.-J. U. and dos Santos, D. J. V. A. Reversing cancer multidrug resistance: insights into the efflux by ABC transports from *in silico* studies. *WILEY INTERDISCIPLINARY REVIEWS-COMPUTATIONAL MOLECULAR SCIENCE*, 5 (1):27-55; 10.1002/wcms.1196 JAN-FEB 2015.
179. Vieira, C; Duarte, N; Reis, MA; Spengler, G; Madureira, AM; Molnar, J; Ferreira, MJU. Improving the MDR reversal activity of 6,17-epoxylathyrane diterpenes, *BIOORGANIC & MEDICINAL CHEMISTRY*, 22 (22):6392-6400; 10.1016/j.bmc.2014.09.041 NOV 15 2014

180. Rinner, U. Progress in the Preparation of Jatrophone Diterpenes. *EUROPEAN JOURNAL OF ORGANIC CHEMISTRY*, (15):3197-3219; 10.1002/ejoc.201403598 MAY 2015
181. Pan, S; Gupta, A; Roy, DR; Sharma, RK; Subramanian, V; Mitra, A; Chattaraj, PK. Application of Conceptual Density Functional Theory in Developing QSAR Models and their Usefulness in the Prediction of Biological Activity and Toxicity of Molecules. Chapter 6 In: *Chemometrics Applications and Research: QSAR in Medicinal Chemistry*. Edited by Mercader AG; Duchowicz PR; Sivakumar PM, Apple Academic Press 2016, 183–214.
182. de Mello, JC; Moraes, VWR; Watashi, CM; da Silva, DC; Cavalcanti, LP; Franco, MKKD; Yokaichiya, F; de Araujo, DR; Rodrigues, T. Enhancement of chlorpromazine antitumor activity by Pluronic F127/L81 nanostructured system against human multidrug resistant leukemia. *PHARMACOLOGICAL RESEARCH*, 111 102-112; 10.1016/j.phrs.2016.05.032 SEP 2016
183. Hussain, SA; Sulaiman, AA; Balch, C; Chauhan, H; Alhadidi, QM; Tiwari, AK. Natural Polyphenols in Cancer Chemoresistance. *NUTRITION AND CANCER-AN INTERNATIONAL JOURNAL*, 68 (6):879-891; 10.1080/01635581.2016.1192201 2016
184. I.N. Cruz, H.M. Coley, H.B. Kramer, T.K. Madhuri, N.A.M Safuwani, A.R. Angelino, M. Yang. Proteomics Analysis of Ovarian Cancer Cell Lines and Tissues Reveals Drug Resistance-associated Proteins. *CANCER GENOMICS & PROTEOMICS*, 14 (1):35-52; 10.21873/cgp.20017 JAN-FEB 2017
185. Paterna, A; Kincses, A; Spengler, G; Mulhovo, S; Molnar, J; Ferreira, MJU. Dregamine and tabernaemontanine derivatives as ABCB1 modulators on resistant cancer cells. *EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY*, 128 247-257; 10.1016/j.ejmech.2017.01.044 MAR 10 2017.
186. Gurusamy Mariappan, Anju Kumari: Virtual Screening and Its Applications in Drug Discovery Process, In: *Computer Applications in Drug Discovery and Development*. edited by Puratchikody, A., Prabu, S. Lakshmana, 2019. Chapter 5, 101-126, 2019 DOI: 10.4018/978-1-5225-7326-5.ch005
187. Tapojyoti Sanyal, Swapan Kumar Ghosh. Anti-cancer property of *Lenzites betulina* (L) Fr. on cervical cancer cell. lines and its anti-tumor effect on HeLa-implanted mice. bioRxiv 540567, 2019. <https://doi.org/10.1101/540567>
188. Mendoza-Macías C.L., Solorio-Alvarado C.R., Alonso-Castro A.J. Alba-Betancourt C., Deveze-Álvarez MA, Padilla-Vaca F, Reyes-Gualito A. Discovery of new effective *N*-alkyl-3,4-diarylmaleimides-based drugs for reversing the bacterial resistance to rhodamine 6G in *Bacillus subtilis*. *CHEMICAL PAPERS* Volume: 74 Issue: 5 Pages: 1429-1438 Published: MAY 2020. <https://doi.org/10.1007/s11696-019-00992-7>
189. Zhang-Xu He, Tao-Qian Zhao, Yun-Peng Gong, Xin Zhang, Li-Ying Ma, Hong-Min Liu, Pyrimidine: A promising scaffold for optimization to develop the inhibitors of ABC transporters. *EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY* Volume: 200, Article Number: UNSP 112458 Published: AUG 15 2020 <https://doi.org/10.1016/j.ejmech.2020.112458>
190. Svenningsen SW, Frederiksen RF, Council C, Ficker M, Leisner JJ, Christensen JB. Synthesis and Antimicrobial Properties of a Ciprofloxacin and PAMAM-dendrimer Conjugate. *MOLECULES* Volume: 25 Issue: 6 Article Number: 1389. Published 2020 Mar 18. doi:10.3390/molecules25061389
191. Fattahian, Maryam; Ghanadian, Mustafa; Ali, Zulfiqar; Khan, Ikhlas A. Jatrophone and rearranged jatrophone-type diterpenes: biogenesis, structure, isolation, biological activity and SARs (1984-2019). *PHYTOCHEMISTRY REVIEWS* Volume: 19 Issue: 2 Pages: 265-336. Published: APR 2020
192. Katarzyna Szczepańska, Annamária Kincses, Klaudia Vincze, Ewa Szymańska, Gniewomir Latacz, Kamil J. Kuder, Holger Stark, Gabriella Spengler, Jadwiga Handzlik, Katarzyna Kieć-Kononowicz. *N*-substituted piperazine derivatives as potential multitarget agents acting on histamine H3 receptor and cancer resistance proteins, *BIOORGANIC & MEDICINAL CHEMISTRY LETTERS*, 2020, 30(22), art. no. 127522. <https://doi.org/10.1016/j.bmcl.2020.127522>
193. Suree Jianmongkol. Overcoming P-Glycoprotein-Mediated Doxorubicin Resistance. In: *Overview of Doxorubicin - Clinical Use, Resistance, Side Effects, and Palliative Care*. Intechopen, Published: January 14th 2021. DOI: 10.5772/intechopen.95553

**14. Pajeva, I.K., M. Wiese. Multidrug resistance related drugs: estimation of hydrophobicity as a space directed molecular property, *Compt. rend. Acad. bulg. Sci.* 2001, Tome 54, 11, 81-84.**

Цитирания: 2

1. Pleban K, Ecker GF. Inhibitors of P-glycoprotein - Lead identification and optimisation *MINI-REV MED CHEM* 5 (2): 153-163 FEB 2005.
2. Gerhard König, Peter Chiba and Gerhard F. Ecker. Hydrophobic moments as physicochemical descriptors in structure-activity relationship studies of P-glycoprotein inhibitors. *Monatshefte für Chemie / Chemical Monthly* Volume 139, Number 4 / April, 2008.

**15. Lesigiarska I., I. Pajeva, S. Yanev. QSAR and 3D QSAR analysis of a series of xanthates as inhibitors and inactivators of cytochrome P-450 2B1, *Xenobiotica* 2002, 32 (16), 1063-1077.**

Цитирања: 15

1. de Groot MJ, Kirton SB, Sutcliffe MJ. In silico methods for predicting ligand binding determinants of cytochromes P450. *CURR TOP MED CHEM* 4 (16): 1803-1824 2004
2. Jalaie, Mehran; Rieco Arimoto; Eric Gifford; Sabine Schefzick; Chris Waller: Prediction of Drug Like Molecular Properties: Modeling Cytochrome P450 Interactions, Chapter 15, In: Chemoinformatics: Concepts, Methods, and Tools for Drug Discovery Editor: Jurgen Bajorath, Humana Press, 2004, pages 544 (p. 515).
3. Tiekink, ERT, J. Haiduc: Stereochemical aspects of metal xanthate complexes: molecular structures and supramolecular self-assembly, pp. 127-320. In: Progress in Inorganic Chemistry, Volume 54, by Kenneth D. Karlin, 535 pages, Wiley-Interscience (June 3, 2005) (citation p. 319).
4. Fontana E, Dansette PM, Poli SM Cytochrome P450 enzymes mechanism based inhibitors: Common sub-structures and reactivity. *CURRENT DRUG METABOLISM* 6 (5): 413-454 OCT 2005
5. Worth AP, Bassan A, Gallegos A, Netzeva TI, Patlewicz G, Pavan M, Tsakovska I, Vracko M. The Characterisation of (Quantitative) Structure-Activity Relationships: Preliminary Guidance, Chapter 5: Mechanistic relevance, EUR 21866 EN © European Communities, 2005, Printed in Italy, pp. 1-95.
6. Fontana, Elena : Les inhibiteurs "suicides" des Cytochromes P450: Etablissement d'une banque de données, mise au point d'un test de screening et études structures-activité concernant des substrats furaniques du CYP 3A4. Thèse, Université René Descartes - PARIS 5, UFR Biomédicale Ecole Doctorale du Medicament. Novembre 2005, PhD.
7. Chohan, K.K., Paine, S.W., Waters, N.J.: Quantitative structure activity relationships in drug metabolism. *Current Topics in Medicinal Chemistry* 6 (15), pp. 1569-1578, 2006.
8. GUIDANCE DOCUMENT ON THE VALIDATION OF (QUANTITATIVE) STRUCTURE-ACTIVITY RELATIONSHIP [(Q)SAR] MODELS, Environment Directorate, ORGANISATION FOR ECONOMIC CO-OPERATION AND DEVELOPMENT. OECD Environment Health and Safety Publications. Series on Testing and Assessment, No. 69, Paris, 2007.
9. Fox, T., Kriegl, J.M.: Chapter 5 Linear Quantitative Structure-Activity Relationships for the Interaction of Small Molecules with Human Cytochrome P450 Isoenzymes. *Annual Reports in Computational Chemistry* (David C. Spellmeyer and Ralph A. Wheeler, Eds.) Vol. 3, pp. 63-81, 2007.
10. Gleeson, M.P., Davis, A.M. Chohan, K.K., Paine, S.W., Boyer, S., Gavaghan, C.L., Arnby, C.H., Kankkonen, C., Albertson, N.: Generation of in-silico cytochrome P450 1A2, 2C9, 2C19, 2D6, and 3A4 inhibition QSAR models. *Journal of Computer-Aided Molecular Design*, Volume 21, Issue 10-11, October 2007, Pages 559-573.
11. Elton Zvinavashe The potential of computer-based quantitative structure activity approaches for predicting acute toxicity of chemicals. Thesis Wageningen University, Wageningen, The Netherlands (2008). PhD
12. Zvinavashe E, Murk AJ, Rietjens IMCM. Promises and Pitfalls of Quantitative Structure-Activity Relationship Approaches for Predicting Metabolism and Toxicity. *CHEMICAL RESEARCH IN TOXICOLOGY* Vol. 21 Issue: 12 Pages: 2229-2236, DEC 2008.
13. Sridhar J, Liu J, Foroozesh M, Stevens CL. Insights on cytochrome p450 enzymes and inhibitors obtained through QSAR studies. *MOLECULES*. 2012 Aug 3;17(8):9283-305.
14. Handa K, Nakagome I, Yamaotsu N, Gouda H, Hirono S. Three-Dimensional Quantitative Structure-Activity Relationship Analysis of Inhibitors of Human and Rat Cytochrome P4503A Enzymes. *DRUG METABOLISM AND PHARMACOKINETICS*, 28 (4):345-355; 10.2133/dmpk.DMPK-12-RG-133 AUG 25 2013.
15. Li, N; Chen, Y; Zhang, C; Zhou, W; Fu, MY; Chen, WL; Wang, S. Highly Sensitive Determination of Butyl Xanthate in Surface and Drinking Water by Headspace Gas Chromatography with Electron Capture Detector. *CHROMATOGRAPHIA*, 78 (19-20):1305-1310; 10.1007/s10337-015-2940-9 OCT 2015.

**16. Pajeva, I., M. Wiese, Pharmacophore model of drugs involved in P-glycoprotein multidrug resistance: explanation of structural variety (Hypothesis), *J. Med. Chem.* 2002, 45 (26), 5671-5686.**

Цитирања: 200

1. van der Waterbeemd H, Grifford E. ADMET in silico modelling: towards prediction paradise? *NATURE REV DRUG DISCOV* 2: 192-204, 2003.
2. Soenen, DR, Hwang, I, Hedrick, MP, Boger, DL. Multidrug resistance reversal activity of key ningalin analogues. *BIOORGANIC & MEDICINAL CHEMISTRY LETTERS*, 2003, MAY, 13 (10), 1777-1781.
3. Freir, DB, Costello, DA, Herron, CE. A Beta(25-35)-induced depression of long-term potentiation in area CA1 in vivo and in vitro is attenuated by verapamil. *JOURNAL OF NEUROPHYSIOLOGY*, 2003, JUN, 89(6), 3061-3069.

4. Varma, S. (Accelrys), Z. Hou (Intern), Elucidation of pharmacophore patterns for drugs that bind to P-glycoprotein, 2003, [www.accelrys.com/cases/pharmacophore-patterns.html](http://www.accelrys.com/cases/pharmacophore-patterns.html)
5. Engman, Helena, Intestinal Barriers to Oral Drug Absorption, Cytochrome P4503A and ABC-Transport Proteins, Dissertation for the PhD Degree, Faculty of Pharmacy, Acta Universitatis Upsalensis, Uppsala 2003. citation 90, p. 53. PhD
6. Robert J., Jarry, C. Multidrug resistance reversal agents. *J MED CHEM.* 2003 Nov 6;46 (23):4805-17.
7. Didziapetris R, Japertas P, Avdeef A, Petrauskas A. Classification analysis of P-glycoprotein substrate specificity. *J DRUG TARGET* 11 (7): 391-406 AUG 2003
8. Sam Au Yeung: CNS Pharmacokinetics of Diphenhydramine in Sheep. PhD Thesis. The University of British Columbia, July 2003. PhD [https://circle.ubc.ca/bitstream/2429/15107/1/ubc\\_2003-859770.pdf](https://circle.ubc.ca/bitstream/2429/15107/1/ubc_2003-859770.pdf)
9. Safa AR. Identification and characterization of the binding sites of P-glycoprotein for multidrug resistance-related drugs and modulators. *Curr Med Chem Anti-Canc Agents.* 2004 Jan;4(1):1-17.
10. Lorenc-Koci E, Wojcikowski J, Kot M, Haduch, A., Boksa, J., Daniel, W.A. Disposition of 1,2,3,4,- tetrahydroisoquinoline in the brain of male Wistar and Dark Agouti rats. *BRAIN RES* 996 (2): 168-179 JAN 23 2004
11. Hou TJ, Xu XJ. Recent development and application of virtual screening in drug discovery: An overview *CURR PHARM DESIGN* 10 (9): 1011-1033 2004
12. Ekins S. Predicting undesirable drug interactions with promiscuous proteins in silico *DRUG DISCOV TODAY* 9 (6): 276-285 MAR 15 2004
13. Chiba P, Ecker GF. Inhibitors of ABC-type drug efflux pumps: an overview of the current patent situation. *EXPERT OPIN THER PAT* 14 (4): 499-508 APR 2004
14. Langer T, Eder M, Hoffmann RD, Chiba P, Ecker GF. Lead identification for modulators of multidrug resistance based on in silico screening with a pharmacophoric feature model. *ARCH PHARM* 337 (6): 317-327 JUN 2004
15. Pirard B. Computational methods for the identification and optimisation of high quality leads. *COMB CHEM HIGH T SCR* 7 (4): 271-280 JUN 2004
16. Grant MA, Morelli XJ, Rigby AC. Conotoxins and structural biology: A prospective paradigm for drug discovery. *CURR PROTEIN PEPT SC* 5 (4): 235-248 AUG 2004
17. Szakacs G, Annereau JP, Lababidi S, Shankavaram U, Arciello A, Bussey KJ, Reinhold W, Guo Y, Kruh GD, Reimers M, Weinstein JN, Gottesman MM. Predicting drug sensitivity and resistance: Profiling ABC transporter genes in cancer cells. *CANCER CELL* 6 (2): 129-137 AUG 2004
18. Tao HC, Hwang IK, Boger DL. Multidrug resistance reversal activity of permethyl ningalin B amide derivatives. *BIOORG MED CHEM LETT* 14 (24): 5979-5981 DEC 20 2004
19. Riley RJ, Kenna JG. Cellular models for ADMET predictions and evaluation of drug-drug interactions. *CURR OPIN DRUG DISC* 7 (1): 86-99 JAN 2004
20. Mihalyi A, Gaspar R, Zalan Z, Lazar L, Fulop F, de Witte PA. Synthesis and multidrug resistance reversal activity of 1,2-disubstituted tetrahydroisoquinoline derivatives. *Anticancer Res.* 2004 May-Jun;24(3a):1631-1636.
21. Lewis R.A. Computer-Aided Drug Design 2001-2003, Chapter 2 In: *Chemical Modelling: Applications and Theory*, Volume 3, Editor: A. Hinchliffe, The Royal Society of Chemistry, 2004, pp. 45-68 (p. 66, citation 95).
22. Robert J. MS-209 (Schering) *Current Opinion in Investigational Drugs* 2004, 5:1340-1348.
23. Hersey, A., C. Luscombe, S. Modi: In silico transporter modelling and its application, In: *Pharmaceutical Profiling In Drug Discovery For Lead Selection* R.T. Borchardt, E.H. Kerns, C.A. Lipinski, D. Thakker, B. Wang (Eds.), AAPS Press, pp.53-61, 2004
24. Ekins S, Swaan PW. Development of computational models for enzymes, transporters, channels, and receptors relevant to ADME/Tox. *REVIEWS IN COMPUTATIONAL CHEMISTRY* 20: 333-415 2004
25. Elsinga. P. H., N. H. Hendrikse, J. Bart, A. van Waarde and W. Vaalburg. Positron Emission Tomography Studies on Binding of Central Nervous System Drugs and P-Glycoprotein Function in the Rodent Brain. *MOLECULAR IMAGING AND BIOLOGY* 7(1): 37-44 JAN 2005
26. Pleban K, Ecker GF. Inhibitors of P-glycoprotein - Lead identification and optimisation *MINI-REV MED CHEM* 5 (2): 153-163 FEB 2005
27. Masip I, Cortes N, Abad MJ, et al. Design and synthesis of an optimized positional scanning library of peptoids: identification of novel multidrug resistance reversal agents *BIOORGAN MED CHEM* 13 (6): 1923-1929 MAR 15 2005
28. Pleban K, Kaiser D, Kopp S, Peer M, Chiba P, Ecker GF. Targeting drug-efflux pumps - a pharmacoinformatic approach. *ACTA BIOCHIMICA POLONICA* 52 (3): 737-740 2005
29. Balakin, K.V., Ivanenkov, Y.A., Savchuk, N.P., Ivashchenko, A.A., Ekins, S. Comprehensive computational assessment of ADME properties using mapping techniques *Current Drug Discovery Technologies* 2 (2), pp. 99-113

30. Mahadevan, Daruka; Shirahatti, Nikhil: Strategies for Targeting the Multidrug Resistance-1 (MDR1)/P-gp Transporter in Human Malignancies, *CURRENT CANCER DRUG TARGETS* 5 (6): 445-455 SEP 2005
31. Ahcène Boumendjel, Hélène Baubichon-Cortay, Doriane Tromprier, Thomas Perrotton, Attilio Di Pietro: Anticancer multidrug resistance mediated by MRP1: Recent advances in the discovery of reversal agents, *MEDICINAL RESEARCH REVIEWS* 25 (4): 453-472 JUL 2005
32. Delisle, Robert K.; Lowrie, Jeffery F.; Hobbs, Doug W.; Diller, David J.: Computational ADME/Tox Modeling: Aiding Understanding and Enhancing Decision Making in Drug Design, *Current Computer - Aided Drug Design*, Volume 1, Number 4, October 2005, pp. 325-345(21).
33. Ecker GF In silico screening of promiscuous targets and antitargets. *CHIMICA OGGI-CHEMISTRY TODAY* 23 (3): 39-42 MAY-JUN 2005
34. Hamasaki A, Zimpleman JM, Hwang I, Boger DL Total synthesis of ningalin D. *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY* 127 (30): 10767-10770 AUG 3 2005
35. Cortes-Selva F, Jimenez IA, Munoz-Martinez F, Campillo M, Bazzocchi IL, Pardo L, Ravelo AG, Castanys S, Gamarro F Dihydro-beta-agarofuran sesquiterpenes: A new class of reversal agents of the multidrug resistance phenotype mediated by P-glycoprotein in the protozoan parasite Leishmania. *CURRENT PHARMACEUTICAL DESIGN* 11 (24): 3125-3139 2005
36. Breier A, Barancik M, Sulova Z, Uhrík B P-glycoprotein - Implications of metabolism of neoplastic cells and cancer therapy. *CURRENT CANCER DRUG TARGETS* 5 (6): 457-468 SEP 2005
37. Bera T, Lakshman K, Ghanteswari D, Pal S, Sudhakar D, Islam MN, Bhuyan NR, Das P Characterization of the redox components of transplasma membrane electron transport system from Leishmania donovani promastigotes *BIOCHIMICA ET BIOPHYSICA ACTA-GENERAL SUBJECTS* 1725 (3): 314-326 OCT 10 2005
38. Van Bambeke, Françoise: Antibiotic accumulation and efflux in eukaryotic cells : a journey at the frontier of pharmacokinetics and pharmacodynamics Dissertation, Université catholique de Louvain, Nov 2005
39. Cheng Chang In Silico Approaches for Studying Transporter and Receptor Structure-Activity Relationships, Dissertation, Graduate School of The Ohio State University, 2005.
40. Santosh G. Dixit. Interferon- $\gamma$  modulates intestinal p-glycoprotein: molecular mechanism and clinical implications. Dissertation, Division of Pharmaceutical Sciences of the College of Pharmacy, University of Cincinnati, 2005. PhD thesis
41. Muñoz Martínez, F.: Sesquiterpenos dihidro-beta-agarofuranos como reversiones naturales de la resistencia celular a múltiples fármacos causada por la Glicoproteína-P MDR1 Humana, Thesis, Universidad de Granada, 2005. PhD thesis
42. Ungvári, H. J. Synthese Potentieller Modulatoren Zur Überwindung Der Multidrug Resistance Dissertation. Mathematisch-Naturwissenschaftlich-Technischen Fakultät (mathematisch-naturwissenschaftlicher Bereich) der Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), 2005. PhD thesis
43. Popovic M, Caballero-Bleda M, Popovic N, Puelles L, van Groen T, Witter MP. Verapamil prevents, in a dose-dependent way, the loss of ChAT-immunoreactive neurons in the cerebral cortex following lesions of the rat nucleus basalis magnocellularis. *Exp Brain Res.* 2006 Apr;170(3):368-75.
44. Srinivas E, Murthy JN, Rao AR, Sastry GN. Recent advances in molecular modeling and medicinal chemistry aspects of phospho-glycoprotein. *CURRENT DRUG METABOLISM* 7 (2): 205-217 FEB 2006
45. Vandevuer, S., Van Bambeke, F., Tulkens, P.M., Prevost, M. Predicting the three-dimensional structure of human P-glycoprotein in absence of ATP by computational techniques embodying crosslinking data: Insight into the mechanism of ligand migration and binding sites. *Proteins Structure, Function and Genetics.* 2006; 63(3):466-478.
46. Li, Y., Wang, L. Yang, S. Zhang, C. Liu. Structural determinants of flavones interacting with the C-terminal nucleotide-binding domain as P-glycoprotein inhibitors. *Internet Electron. J. Mol. Des.* 5, 1-12, 2006. [www.biochempress.com](http://www.biochempress.com)
47. Crivori, P., B. Reinach, D. Pezzetta, I. Pogessi: Computational models for identifying potential P-glycoprotein substrates and inhibitors, *Molecular Pharmaceutics*, Vol. 3(1), 33-44, 2006.
48. Liederer BM, Fuchs T, Vander Velde D, Siahaan TJ, Borchardt RT. Effects of amino acid chirality and the chemical linker on the cell permeation characteristics of cyclic prodrugs of opioid peptides. *J Med Chem.* 2006 Feb 23;49(4):1261-70.
49. Ewa Gatlik-Landwojtowicz, Päivi Äänismaa, and Anna Seelig. Quantification and Characterization of P-Glycoprotein-Substrate Interactions. *Biochemistry*; 2006; 45(9) pp 3020 – 3032.
50. Raub, T.J. P-glycoprotein recognition of substrates and circumvention through rational drug design, *Molecular Pharmaceutics*, 3 (1), 78-86, 2006
51. Johnson SR, Zheng W. Recent Progress in the Computational Prediction of Aqueous Solubility and Absorption. *AAPS J.* 2006; 8(1): E27-40.

52. Kaur, G., M. Hollingshead, S. Holbeck, V. Schauer-Vukašinovi, R.F. Camalier, A. Doemling, S. Agarwal: Biological Evaluation of Tubulysin A: a Potential Anticancer and Antiangiogenic Natural Product. *Biochem J.* 2006, 396(2):235-42.
53. Omote, H., Al-Shawi MK. Interaction of transported drugs with the lipid bilayer and P-glycoprotein through a solvation exchange mechanism. *Biophys J.* 2006, 90(11):4046-59.
54. Manisha Iyer, Erica J Reschly, Matthew D Krasowski. Functional evolution of the pregnane X receptor. *Expert Opinion on Drug Metabolism & Toxicology*, 2006, Vol. 2, No. 3, Pages 381-397.
55. Qi, X. Stochastic models for prodrug targeting. 1. Diffusion of the efflux drug *Molecular Pharmaceutics* 2006 3 (2), pp. 187-195.
56. Tomblin G, Donnelly DJ, Holt JJ, You Y, Ye M, Gannon MK, Nygren CL, Detty MR.: Stimulation of P-glycoprotein ATPase by analogues of tetramethylrosamine: coupling of drug binding at the "R" site to the ATP hydrolysis transition state. *Biochemistry.* 2006 Jul 4; 45(26): 8034-8047.
57. Menniti FS, Faraci WS, Schmidt CJ. Phosphodiesterases in the CNS: targets for drug development. *Nat Rev Drug Discov.* 2006 Aug;5(8):660-70.
58. De Cerqueira Lima, P., Golbraikh, A., Oloff, S., Xiao, Y., Tropsha, A. Combinatorial QSAR modeling of P-glycoprotein substrates. *Journal of Chemical Information and Modeling* 46 (3), pp. 1245-1254, 2006.
59. Teodori, E., Dei, S., Martelli, C., Scapocchi, S., Gualtieri, F. The functions and structure of ABC transporters: Implications for the design of new inhibitors of Pgp and MRP1 to control multidrug resistance (MDR) *Current Drug Targets* 7 (7), pp. 893-909, 2006.
60. Fusi, F., Saponara, S., Valoti, M., Dragoni, S., D'Elia, P., Sgaragli, T., Alderighi, D., Sgaragli, G.: Cancer cell permeability-glycoprotein as a target of MDR reverters: Possible role of novel dihydropyridine derivatives. *Current Drug Targets* 7 (8), pp. 949-959, 2006.
61. Shen, X., Chen, G., Zhu, G., Fong, W.-F. ( $\pm$ )-3'-O, 4'-O-dicynamoyl-cis-khellactone, a derivative of ( $\pm$ )-prauerptorin A, reverses P-glycoprotein mediated multidrug resistance in cancer cells. *Bioorganic and Medicinal Chemistry*, 14 (21), 7138-7145, 2006
62. Keck, Cornelia M. Cyclosporine Nanosuspensions: Optimised Size Characterisation & Oral Formulations Inaugural-Dissertation, Fachbereich Biologie, Chemie, Pharmazie der Freien Universität Berlin, Berlin 2006. PhD thesis
63. Chang, C., P.W. Swaan: Computational modeling of Drug Disposition, In: *Computer Applications in Pharmaceutical Research and Development (Wiley Series in Drug Discovery and Development)* Sean Ekins and Binghe Wang (eds.), John Wiley&Sons, Inc., Hoboken, New Jersey, 495-512, 2006. (citation p. 511).
64. Mandola, C.: Nuovi inibitori della Multidrug Resistance (MDR): sintesi di derivati amminoalchilici ad elevata flessibilità molecolare Thesis, Università degli Studi di Firenze, 2005-06.. PhD thesis
65. Sharom FJ. Shedding light on drug transport: structure and function of the P-glycoprotein multidrug transporter (ABCB1). *Biochem Cell Biol.* 2006 Dec;84(6):979-92.
66. Iyer, M., Reschly, E.J., Krasowski, M.D. Functional evolution of the pregnane X receptor *Expert Opinion on Drug Metabolism and Toxicology* 2 (3), 2006, 381-397.
67. Schmidt, M., Ungvári, J., Gloede, J., Dobner, B., Langner, A.: New 1,3-dioxolane and 1,3-dioxane derivatives as effective modulators to overcome multidrug resistance *Bioorganic and Medicinal Chemistry* 15 (6), pp. 2283-2297, 2007.
68. Raub, T.J.: Defining structure-activity relationships for drug transporters. *AAPS Workshop on Drug Transport in ADME: From the Bench to the Bedside*, March 5-7 2007.
69. Kaiser, D., Terfloth, L., Kopp, S., Schulz, J., De Laet, R., Chiba, P., Ecker, G.F., Gasteiger, J.: Self-organizing maps for identification of new inhibitors of P-glycoprotein. *Journal of Medicinal Chemistry* 50 (7), pp. 1698-1702, 2007.
70. Zdrzil B, Kaiser D, Kopp S, et al. Similarity-based descriptors (SIBAR) as tool for QSAR studies on P-glycoprotein inhibitors: Influence of the reference set. *QSAR & COMBINATORIAL SCIENCE* 26 (5): 669-678 MAY 2007.
71. Pharmacophore for human ADME/Tox-related proteins, Chapter 14.4., In: *Pharmacophores and Pharmacophore Searches*, edited by Thierry Langer, Remy D. Hoffmann Published 2007, Wiley-VCH, 396 pages, ( p. 305).
72. Khedkar, Santosh A.; Malde, Alpeshkumar K.; Coutinho, Evans C.; Srivastava, Sudha. Pharmacophore modeling in drug discovery and development: an overview. *Medicinal Chemistry* (2007), 3(2), 187-197.
73. Huang, Jianping; Ma, Guangli; Muhammad, Ishtiaq; Cheng, Yiyu. Identifying P-Glycoprotein Substrates Using a Support Vector Machine Optimized by a Particle Swarm. *Journal of Chemical Information and Modeling* (2007).
74. Ekins, Sean; Embrechts, Mark J.; Breneman, Curt M.; Jim, Kam; Wery, Jean-Pierre. Novel applications of kernel-partial least squares to modeling a comprehensive array of properties for drug discovery. *Computational Toxicology* (2007), 403-432.

75. Pär Matsson, Gunilla Englund, Gustav Ahlin, Christel A. S. Bergström, Ulf Norinder, and Per Artursson: A Global Drug Inhibition Pattern for the Human ABC Transporter breast cancer resistance protein (ABCG2). *Journal of Pharmacology and Experimental Therapeutics* 323 (1), pp. 19-30, 2007.
76. Sharom, F. J. Allergic contact dermatitis from toluene-2,5-diamine in a cream dye for eyelashes and eyebrows-quantitative exposure assessment. *Drug Transporters* (2007), 223-262.
77. Egan, W.J. Computational Models for ADME In: *Annual Reports in Medicinal Chemistry* (Ed. J. Macor) Chapter 29, Volume 42, 2007, Pages 449-467.
78. Paer MATSSON: ATP-Binding Cassette EffluxTransporters and Passive Membrane Permeability in Drug Absorption and Disposition. *Digital Comprehensive Summaries of Uppsala Dissertationsfrom the Faculty of Pharmacy* 67, ACTA UNIVERSITATIS UPSALIENSIS UPPSALA, 2007. PhD
79. Ma GL, Zhao XP, Cheng YY Identification of P-gp substrates using a random forest method based on chemistry development kit descriptors *CHEMICAL JOURNAL OF CHINESE UNIVERSITIES-CHINESE* Volume: 28 Issue: 10 Pages: 1885-1888 Published: OCT 2007.
80. Sharom, F.J. ABC multidrug transporters: structure, function and role in chemoresistance. *Pharmacogenomics*, 2008, Vol. 9, No. 1, 105-127.
81. Tomblin, Gregory; Holt, Jason J.; Gannon, Michael K.; Donnelly, David J.; Wetzel, Bryan; Sawada, Geri A.; Raub, Thomas J.; Detty, Michael R. ATP Occlusion by P-Glycoprotein as a Surrogate Measure for Drug Coupling. *Biochemistry*, 2008, 47(10), 3294-3307.
82. Kim, In-Wha; Booth-Genthe, Catherine; Ambudkar, Suresh V. Relationship between drugs and functional activity of various mammalian P-glycoproteins (ABCB1). *Mini-Reviews in Medicinal Chemistry* (2008), 8(3), 193-200.
83. Srivastava S. Computational strategies to predict effect of P-Glycoprotein transporter efflux and minimize its impact on the penetration of drugs into the Central Nervous System (CNS) *CURRENT COMPUTER-AIDED DRUG DESIGN* Volume: 4 Issue: 1 Pages: 67-75. Published: MAR 2008
84. Yuan HY, Li X, Wu JF, et al. Strategies to overcome or circumvent P-glycoprotein mediated multidrug resistance *CURRENT MEDICINAL CHEMISTRY* Volume: 15 Issue: 5 Pages: 470-476 Published: FEB 2008.
85. Ecker, G.F., Stockner, T., Chiba, P. Computational models for prediction of interactions with ABC-transporters. *Drug Discovery Today* 13 (7-8), 2008, pp. 311-317.
86. Crivori, Crivori, P. Computational Models for P-Glycoprotein Substrates and Inhibitors. In: *Antitargets: Prediction and Prevention of Drug Side Effects* Book series: *Methods and Principles in Medicinal Chemistry* (Roy J. Vaz, Thomas Klabunde, Raimund Mannhold, Hugo Kubinyi, Gerd Folkers, Eds.), John Wiley & Sons Inc, 2008, 367-397.
87. OETTGEN, Peter, LIBERMANN, Towia, RIGBY, Alan Identification And Use Of Small Molecules To Modulate Pdef Transcription Factor Function And To Treat Pdef Transcription Factor Associated Diseases. Publication number: WO2008057555 Publication date: 2008-05-15
88. OETTGEN, Peter, LIBERMANN, Towia, RIGBY, Alan. Identification And Use Of Small Molecules To Modulate Ese L Transcription Factor Function And To Treat Ese-I Transcription Factor Associated Diseases. Patent publication number WO2008057556, Publication date: 2008-05-15.
89. OETTGEN, Peter, LIBERMANN, Towia, RIGBY, Alan. Identification And Use Of Small Molecules To Modulate Transcription Factor Function And To Treat Transcription Factor Associated Diseases. Patent publication number WO2008066672, 2008-06-05
90. Demel MA., R Schwaha, O Krämer, P Ettmayer, Eric EJ Haaksma, G F Ecker: In silico prediction of substrate properties for ABC-multidrug transporters, *Expert Opinion on Drug Metabolism & Toxicology*, September 2008, Vol. 4, No. 9, Pages 1167-1180.
91. Duarte N, Jardanhazy A, Molnar J, Andreas Hilgeroth A., Ferreira, M.-J. U. Synergistic interaction between p-glycoprotein modulators and epirubicine on resistant cancer cells, *BIOORGANIC & MEDICINAL CHEMISTRY*, 2008, 16 (20), 9323-9330.
92. Matthias Schmidt , Marlen Teitge, Marianela E. Castillo, Tobias Brandt, Bodo Dobner, Andreas Langner: Synthesis and Biochemical Characterization of New Phenothiazines and Related Drugs as MDR Reversal Agents, *ARCHIV DER PHARMAZIE*, 2008, Vol. 341 (10), 624-638.
93. Sawada GA., T. J. Raub, J. W. Higgins, N.K. Brennan, T. M. Moore, G. Tomblin, M.R. Detty. Chalcogenopyrylium dyes as inhibitors/modulators of P-glycoprotein in multidrug-resistant cells. *BIOORGANIC & MEDICINAL CHEMISTRY*, 2008, 16 (22), 9745-9756.
94. de la Nuez, Ania; Rodriguez, Rolando. Current methodology for the assessment of ADME-Tox properties on drug candidate molecules. *Biotechnologia Aplicada* (2008), 25(2), 97-110.
95. Duarte, N. Structural characterization and biological activities of terpenic and phenolic compounds isolated from *Euphorbia Lagascae* and *Euphorbia Tuckeyana*. Thesis. Department of Pharmacy, University of Lisboa, 2008. PhD

96. Tobias Brandt. Untersuchung und charakterisierung von inhibitoren des p-glykoproteins zur überwindung der multidrug resistance. Dissertation. Naturwissenschaftlichen Fakultät I Biowissenschaften der Martin-Luther-Universität Halle-Wittenberg, 2008. PhD
97. Boccard, J., Bajot, F., Di Pietro, A., Rudaz, S., Boumendjel, A., Nicolle, E., Carrupt, P.-A. A 3D linear solvation energy model to quantify the affinity of flavonoid derivatives toward P-glycoprotein. *European Journal of Pharmaceutical Sciences* 36 (2-3), pp. 254-264, 2009.
98. Nicolle, E., Boumendjel, A., Macalou, S., Genoux, E., Ahmed-Belkacem, A., Carrupt, P.-A., Di Pietro, A. QSAR analysis and molecular modeling of ABCG2-specific inhibitors. *Advanced Drug Delivery Reviews* 61 (1), pp. 34-46, 2009.
99. Seelig, Anna. Toward understanding P-glycoprotein structure-activity relationships. In: *Methods and Principles in Medicinal Chemistry* (2009), 40 (Drug Bioavailability), 497-519.
100. Balaz, Stefan. Modeling Kinetics of Subcellular Disposition of Chemicals. *Chemical Reviews* (Washington, DC, United States) (2009), 109(5), 1793-1899.
101. Nicolazzo JA, Katneni K Drug Transport Across the Blood-Brain Barrier and the Impact of Breast Cancer Resistance Protein (ABCG2) *CURRENT TOPICS IN MEDICINAL CHEMISTRY*, 9 (2), 130-147, 2009.
102. Gannon MK, Holt JJ, Bennett SM, Wetzel BR, Loo TW, Bartlett MC, Clarke DM, Sawada GA, Higgins JW, Tomblin G, Raub TJ, Detty MR. Rhodamine Inhibitors of P-Glycoprotein: An Amide/Thioamide "Switch" for ATPase Activity, *J Med Chem.* 2009, 52 (10): 3328-3341
103. Xing, Li; Hu, Yiding; Lai, Yurong. Advancement of Structure-Activity Relationship of Multidrug Resistance-Associated Protein 2 Interactions. *AAPS JOURNAL* 11 (3): 406-413 SEP 2009.
104. Mayur, Y. C.; Peters, G. J.; Rajendra Prasad, V. V.S.; Lemos, C.; Sathish, N. K. Design of New Drug Molecules to be Used in Reversing Multidrug Resistance in Cancer Cells. *Current Cancer Drug Targets*, 9(3), 2009, pp. 298-306.
105. Jain S, Abraham I, Carvalho P, Kuang YH, Shaala LA, Youssef DT, Avery MA, Chen ZS, El Sayed KA. Sipholane Triterpenoids: Chemistry, Reversal of ABCB1/P-Glycoprotein-Mediated Multidrug Resistance, and Pharmacophore Modeling. *J Nat Prod* (2009), 72(7), 1291-1298.
106. Pär Matsson, Jenny M. Pedersen, Ulf Norinder, Christel A. S. Bergström and Per Artursson. Identification of Novel Specific and General Inhibitors of the Three Major Human ATP-Binding Cassette Transporters P-gp, BCRP and MRP2 Among Registered Drugs, *Pharmaceutical Research*, 26(8), 1816-1831, 2009.
107. Eckford, PDW; Sharom, FJ ABC Efflux Pump-Based Resistance to Chemotherapy Drugs. *CHEMICAL REVIEWS* 109 (7): 2989-3011 JUL 2009
108. Gassel, M. J. Cramer, C. Kern, S. Noack, W. Streber. Lessons learned from target-based lead discovery. In: *Antiparasitic and Antibacterial Drug Discovery: From Molecular Targets to Drug Candidates*. Ed. P.M. Selzer, Wiley, 2009, 99-116.
109. Ecker, Gerhard F.; Chiba, Peter. QSAR studies on drug transporters involved in toxicology. *Computational Toxicology*, In: *Computational Toxicology: Risk Assessment for Pharmaceutical and Environmental Chemicals*. Sean Ekins (Ed.), Wiley, 2009, 295-314.
110. Sean Ekins, Mark J. Embrechts, Curt M. Breneman, Kam Jim, and Jean-Pierre Wery. Novel Applications of Kernel-Partial Least Squares to Modeling a Comprehensive Array of Properties for Drug Discovery In: *Computational Toxicology: Risk Assessment for Pharmaceutical and Environmental Chemicals*. Sean Ekins (Ed.), Wiley, 2009, 403-432.
111. Ponte-Sucre, A., M. Padron-Nieves, E. Diaz. ABC transporter blockers and reversal of drug resistance in microorganisms. In: *ABC transporters in microorganisms: Research, Innovation and Value as Targets against Drug Resistance*, Horizon Scientific Press, 2009, 177-195. ISBN: 978-1-904455-49-3 <http://saber.ucv.vt/123456789/1737>.
112. Demel, MA; Kramer, O; Etmayer, P; Haaksma, EEJ; Ecker, GE. Predicting Ligand Interactions with ABC Transporters in ADME, *CHEMISTRY & BIODIVERSITY* 6 (11): 1960-1969 2009.
113. Bryan J. Cole. Cost, effectiveness and developmental expression of multidrug transporters, Stanford University, *HOPKINS THESES* 3781 2010 C , pp. 252 (citation 35, p. 27). PhD thesis
114. Crowley, E., C.A. McDevitt, R. Callaghan. Generating Inhibitors of P-Glycoprotein: Where to, Now? In: *Multi-Drug Resistance in Cancer* (Ed. Jun Zhou), *Methods in Molecular Biology*, Volume 596, Humana Press, 2010, 405-432.
115. Li, Y; Yuan, H; Yang, K; Xu, W; Tang, W; Li, X. The Structure and Functions of P-Glycoprotein. *CURRENT MEDICINAL CHEMISTRY* 17 (8): 786-800 MAR 2010.
116. Xiong, J. M. Taniguchi, Y. Kashiwada, M. Sekiya, T. Yamagishi and Y. Takaishi. Papyriferic acid derivatives as reversal agents of multidrug resistance in cancer cells, *Bioorganic & Medicinal Chemistry*, Volume 18, Issue 8, 15 April 2010, Pages 2964-2975.
117. Egan, W. Predicting ADME in drug discovery. In: *Drug Design: Structure- and Ligand-Based Approaches* (Kenneth M. Merz, Dagmar Ringe, Charles H. Reynolds, eds.), Cambridge University Press, 2010, 137-150.

118. Estrada, E; Molina, E; Nodarse, D; Uriarte, E. Structural Contributions of Substrates to their Binding to P-Glycoprotein. A TOPS-MODE Approach. *CURRENT PHARMACEUTICAL DESIGN* 16 (24): 2676-2709 2010.
119. Docolomansky, P; Bohacova, V; Barancik, M; Breier, A. Why the xanthine derivatives are used to study of P-glycoprotein-mediated multidrug resistance in L1210/VCR line cells. *GENERAL PHYSIOLOGY AND BIOPHYSICS* 29 (3): 215-221 SEP 2010
120. Teodori, E.; Dei, S.; Martelli, C.; Scapecchi, S. N,Nn-bis(cyclohexanol)amine aryl esters: the discovery of a new class of highly potent inhibitors of transporter-dependent multidrug resistance (MDR). *CURRENT TOPICS IN MEDICINAL CHEMISTRY*, 2010, 10(17), 1715-1731.
121. Zhou, T; Shi, QA; Bastow, KF; Lee, KH. Antitumor Agents 286. Design, Synthesis, and Structure-Activity Relationships of 3 'R,4 ' R-Disubstituted-2 ' ,2 '-dimethyldihydropyrano[2,3-f]chromone (DSP) Analogues as Potent Chemosensitizers to Overcome Multidrug Resistance. *JOURNAL OF MEDICINAL CHEMISTRY* 53 (24): 8700-8708 DEC 23 2010
122. Patton JS, Brain JD, Davies LA, et al. The Particle has Landed-Characterizing the Fate of Inhaled Pharmaceuticals. *JOURNAL OF AEROSOL MEDICINE AND PULMONARY DRUG DELIVERY* 23 S71-S87 Suppl. 2 DEC 2010.
123. Ekins S. Drug Transporter Pharmacophores. In: Transporters as Drug Carriers: Structure, Function, Substrates, Vol. 44, (eds G. Ecker and P. Chiba), Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany, 215–227, 2010.DOI: 10.1002/9783527627424.ch8
124. Dowty, M. E., Messing, D. M., Lai, Y. and Kirkovsky, L. ADME, in ADMET for Medicinal Chemists: A Practical Guide (eds K. Tsaïoun and S. A. Kates), John Wiley & Sons, Inc., Hoboken, NJ, USA, 2011, 145-200.
125. Oettgen, Peter (Brookline, MA, US), Rigby, Alan C. (Newton, MA, US), Libermann, Towia (Newton, MA, US). Identification and use of small molecules to modulate transcription factor function and to treat transcription factor associated diseases. US Patent 20110071142, <http://www.freepatentsonline.com/y2011/0071142.html>
126. Gumbleton, M; Al-Jayyousi, G; Crandon-Lewis, A; Francombe, D; Kreitmeyr, K; Morris, CJ; Smith, MW. Spatial expression and functionality of drug transporters in the intact lung: Objectives for further research. *ADVANCED DRUG DELIVERY REVIEWS* 63 (1-2): 110-118 JAN-FEB 2011
127. Ferreira, R. J.,D. dos Santos, M. J. U. Ferreira, R. C. Guedes. Towards a better pharmacophore description of P-glycoprotein modulators, based on macrocyclic diterpenes from Euphorbia species. *JOURNAL OF CHEMICAL INFORMATION AND MODELING* 51 (6): 1315-1324 JUN 2011.
128. Wang, Z; Chen, YY; Liang, H; Bender, A; Glen, RC; Yan, AX. P-glycoprotein Substrate Models Using Support Vector Machines Based on a Comprehensive Dataset. *JOURNAL OF CHEMICAL INFORMATION AND MODELING* 51 (6): 1447-1456 JUN 2011.
129. Palmeira, A; Rodrigues, F; Sousa, E; Pinto, M; Vasconcelos, MH; Fernandes, MX. New Uses for Old Drugs: Pharmacophore-Based Screening for the Discovery of P-Glycoprotein Inhibitors. *CHEMICAL BIOLOGY & DRUG DESIGN* 78 (1): 57-72, 2011.
130. Ferreira R. J.; dos Santos D. J.; Ferreira M. U.; RC Guedes. Improved pharmacophore description of P-glycoprotein modulators *PLANTA MEDICA* Volume: 77 Issue: 12 Pages: 1442-1443 Published: AUG 2011
131. Darby, RAJ; Callaghan, R; McMahon, RM. P-glycoprotein Inhibition: The Past, the Present and the Future. *CURRENT DRUG METABOLISM*, 12 (8):722-731; OCT 2011
132. Telbisz A, Hegedüs C, Ozvegy-Laczka C, Goda K, Várady G, Takáts Z, Szabó E, Sorrentino BP, Váradi A, Sarkadi B. Antibody binding shift assay for rapid screening of drug interactions with the human ABCG2 multidrug transporter. *EUR J PHARM SCI.* 2012 Jan 23;45(1-2):101-109.
133. Kay, C. Introduction, In: ADMET for Medicinal Chemists: A Practical Guide (Katya Tsaïoun, Steven A. Kates, Eds)., John Wiley and Sons, 2011, 2-28.
134. Jabeen, I. Combined Ligand- and Structure-based Studies on inhibitors of P-glycoprotein *DISSERTATION*, Dr.-Studium der Naturwissenschaften, University of Wien, Wien, 2011. [othes.univie.ac.at/17980/1/2011-11-15\\_0746423.pdf](https://othes.univie.ac.at/17980/1/2011-11-15_0746423.pdf) PhDthesis
135. Ricardo Jose Diogo Gracio Ferreira. Vencendo a multi-resistência: Modelos computacionais da Glicoproteína-P. Mestrado em Química Farmacéutica e Terapêutica. UNIVERSIDADE DE LISBOA. FACULDADE DE FARMÁCIA. 2011. [www.ff.ul.pt/FCT/PTDC/QEQ.../Tese-Msci2.pdf](http://www.ff.ul.pt/FCT/PTDC/QEQ.../Tese-Msci2.pdf) PhDthesis
136. Cátia Vicente Vieira. Compostos Bioativos Isolados de Euphorbia boetica Modulação da Glicoproteína-P. Mestrado em Química Farmacéutica e Terapêutica. UNIVERSIDADE DE LISBOA. FACULDADE DE FARMÁCIA. Lisboa, 2011. **PhDthesis** [www.ff.ul.pt/FCT/PTDC/QEQ.../Tese-Msci1.pdf](http://www.ff.ul.pt/FCT/PTDC/QEQ.../Tese-Msci1.pdf)
137. Andreia Palmeira. Design, synthesis and evaluation of xanthone derivatives for dual activity: antitumor and P-glycoprotein inhibition. Thesis presented to the Faculdade de Farmácia, Universidade do Porto, Porto,

- 2011, pp. 1-402. PhD Thesis <https://br.123dok.com/document/z31on7my-design-synthesis-and-evaluation-of-xanthone-derivatives-for-dual-activity-antitumor-and-p-glycoprotein-inhibition.html>
138. Shen, X., Chen, G., Zhu, G., Cai, J., Wang, L., Hu, Y. and Fong, W.-F. 3'-O, 4'-O-aromatic acyl substituted 7,8-pyrano-coumarins: a new class of P-glycoprotein modulators. *J Pharm Pharmacol.* 2012 Jan; 64(1):90-100.
  139. Leong MK, Chen H-B, Shih Y-H (2012) Prediction of Promiscuous P-Glycoprotein Inhibition Using a Novel Machine Learning Scheme. *PLoS ONE* 7(3): e33829, 2012. doi:10.1371/journal.pone.0033829.
  140. Joung JY, H Kim, HM Kim, SK Ahn, KY Nam, KT No. Prediction Models of P-Glycoprotein Substrates Using Simple 2D and 3D Descriptors By a Recursive Partitioning Approach. *BULL. KOREAN CHEM. SOC.* 2012, Vol. 33, No. 4 1123-1127.
  141. Chen L, Li Y, Yu H, Zhang L, Hou T. Computational models for predicting substrates or inhibitors of P-glycoprotein. *DRUG DISCOVERY TODAY*, 17 (7-8):343-351; 10.1016/j.drudis.2011.11.003 APR 2012.
  142. Tsiklauri, L. K.; Hoyer, H.; Chkhikvadze, G. V.; Vachnadze, V. Yu.; Tsagareishvili, G. V.; Bakuridze, A. G.; Bernkop-Schnurch, A. Role of P-glycoproteins in the transepithelial transport of indoline alkaloids isolated from *Vinca herbacea*. *Pharmaceutical Chemistry Journal* (2012), 42(12), 693-695.
  143. Zhou, T., Emika Ohkoshi, Qian Shi, Kenneth F. Bastow, Kuo-Hsiung Lee, Anti-AIDS agents 89. Identification of DCX derivatives as anti-HIV and chemosensitizing dual function agents to overcome P-gp-mediated drug resistance for AIDS therapy, *Bioorganic&Medicinal Chemistry Letters*, Volume 22, Issue 9, 1 May 2012, Pages 3219-3222.
  144. Palmeira, A; Sousa, E; Vasconcelos, MH; Pinto, MM. Three Decades of P-gp Inhibitors: Skimming Through Several Generations and Scaffolds. *CURRENT MEDICINAL CHEMISTRY*, 19 (13):1946-2025; MAY 2012.
  145. Hung, HY; Ohkoshi, E; Goto, M; Bastow, KF; Nakagawa-Goto, K; Lee, KH. Antitumor Agents. 293. Nontoxic Dimethyl-4,4'-dimethoxy-5,6,5',6'-dimethylenedioxybiphenyl-2,2'-dicarboxylate (DDB) Analogues Chemosensitize Multidrug-Resistant Cancer Cells to Clinical Anticancer Drugs. *JOURNAL OF MEDICINAL CHEMISTRY*, 55 (11):5413-5424; 10.1021/jm300378k JUN 14 2012
  146. Shen, Xiaoling; Chen, Guangying; Zhu, Guoyuan; Cai, Jiazhong; Wang, Lu; Hu, Yingjie; Fong, Wang-Fun. 3'-O,4'-O-aromatic acyl substituted 7,8-pyrano-coumarins: a new class of P-glycoprotein modulators. *JOURNAL OF PHARMACY AND PHARMACOLOGY* (2012), 64(1), 90-100.
  147. Orchard, A; Schamerhorn, GA; Calitree, BD; Sawada, GA; Loo, TW; Bartlett, MC; Clarke, DM; Detty, MR. Thiorhodamines containing amide and thioamide functionality as inhibitors of the ATP-binding cassette drug transporter P-glycoprotein (ABCB1). *BIOORGANIC & MEDICINAL CHEMISTRY* (2012), 20(14), 4290-4302.
  148. Palmeira, A; Sousa, E; Vasconcelos, MH; Pinto, M; Fernandes, MX. Structure and Ligand-based Design of P-glycoprotein Inhibitors: A Historical Perspective. *CURRENT PHARMACEUTICAL DESIGN*, 18 (27):4197-4214; SEP 2012
  149. MJU Ferreira, N Duarte, H Lage, J Molnár. Reversal of Multidrug Resistance by Macrocyclic and Polycyclic Diterpenoids from *Euphorbia* species. In: *Recent Progress in Medicinal Plants. Volume 32: Ethnomedicine and Therapeutic Validation*. Eds. J.N. Govil and Geetanjali Kaushik. 2012, 193-213. ISBN: 1-933699-22-1
  150. Hung, HY; Ohkoshi, E; Goto, M; Nakagawa-Goto, K; Lee, KH. 1-(3,4,5-Trimethoxyphenyl)ethane-1,2-diyl esters, a novel compound class with potent chemoreversal activity, *BIOORGANIC & MEDICINAL CHEMISTRY LETTERS*, 22 (24):7726-7729; DEC 15 2012.
  151. Levatic, J; Curak, J; Kralj, M; Smuc, T; Osmak, M; Supek, F. Accurate Models for P-gp Drug Recognition Induced from a Cancer Cell Line Cytotoxicity Screen. *JOURNAL OF MEDICINAL CHEMISTRY* 56 (14), 5691-5708, 2013.
  152. Halder, AK; Saha, A; Jha, T. The Role of 3D Pharmacophore Mapping Based Virtual Screening for Identification of Novel Anticancer Agents: An Overview. *CURRENT TOPICS IN MEDICINAL CHEMISTRY*, 13 (9):1098-1126; MAY 2013.
  153. Ricardo J. Ferreira, Maria-José U. Ferreira, and Daniel J. V. A. dos Santos Molecular Docking Characterizes Substrate-Binding Sites and Efflux Modulation Mechanisms within P-Glycoprotein. *JOURNAL OF CHEMICAL INFORMATION AND MODELING*, 53 (7):1747-1760; 10.1021/ci400195v JUL 2013
  154. Xu, Y; Shen, Q; Liu, X; Lu, J; Li, S; Luo, C; Gong, L; Luo, X; Zheng, M; Jiang, H. Computational Models for Predicting Interactions with Membrane Transporters. *CURRENT MEDICINAL CHEMISTRY*, 20 (16):2118-2136; MAY 2013.
  155. Thai, KM; Ngo, TD; Tran, TD; Le, MT. Pharmacophore Modeling for Antitargets. *CURRENT TOPICS IN MEDICINAL CHEMISTRY*, 13 (9):1002-1014; MAY 2013.
  156. Zhang, DM; Li, YJ; Shu, C; Ruan, ZX; Chen, WM; Yiu, A; Peng, YH; Wang, J; Lan, P; Yao, Z; Fung, KP; Fu, LW; Chen, ZS; Ye, WC. Bipiperidinyl derivatives of 23-hydroxybetulinic acid reverse resistance of HepG2/ADM and MCF-7/ADR cells. *ANTI-CANCER DRUGS*, 24 (5):441-454; 10.1097/CAD.0b013e32835fcc77 JUN 2013.

157. Liu, JH; Wang, X; Liu, P; Deng, RX; Lei, M; Chen, WT; Hu, LH. 20(S)-Protopanaxadiol (PPD) analogues chemosensitize multidrug-resistant cancer cells to clinical anticancer drugs. *BIOORGANIC & MEDICINAL CHEMISTRY*, 21 (14):4279-4287; 10.1016/j.bmc.2013.04.067 JUL 15 2013.
158. Y Tajima, H Nakagawa, A Tamura, O Kadioglu, K Satake, Y Mitani, H Murase, LO Regasini, V da Silva Bolzani, T Ishikawa, G Fricker, T Efferth. Nitensidine A, a guanidine alkaloid from *Pterogyne nitens* is a novel substrate for human ABC transporter ABCB1. *PHYTOMEDICINE*, Oct 2013. <http://dx.doi.org/10.1016/j.phymed.2013.08.024>.
159. Xu, Y; Liu, X; Li, SS; Zhou, NN; Gong, LK; Luo, C; Luo, XM; Zheng, MY; Jiang, HL; Chen, KX. Combinatorial Pharmacophore Modeling of Organic Cation Transporter 2 (OCT2) Inhibitors: Insights into Multiple Inhibitory Mechanisms. *MOLECULAR PHARMACEUTICS*, 10 (12):4611-4619; 10.1021/mp400423g DEC 2013.
160. Vadlapatla, RK; Vadlapudi, AD; Pal, D; Mitra, AK. Mechanisms of Drug Resistance in Cancer Chemotherapy: Coordinated Role and Regulation of Efflux Transporters and Metabolizing Enzymes. *CURRENT PHARMACEUTICAL DESIGN*, 19 (40):7126-7140; DEC 2013.
161. Zyta, J; Jaszczyszyn, A; Swiatek, P; Gasiorowski, K; Malinka, W. Synthesis, pro-apoptotic activity and 2D-QSAR studies of new analogues of fluphenazine. *ACTA POLONIAE PHARMACEUTICA*, 71 (1):49-58; JAN-FEB 2014.
162. Menniti, F. S., Plath, N., Svenstrup, N. and Schmidt, C. J. Pharmacological Manipulation of Cyclic Nucleotide Phosphodiesterase Signaling for The Treatment of Neurological and Psychiatric Disorders In The Brain. In: *CYCLIC-NUCLEOTIDE PHOSPHODIESTERASES IN THE CENTRAL NERVOUS SYSTEM: FROM BIOLOGY TO DRUG DISCOVERY*, 77-114; 2014 doi: 10.1002/9781118836507.ch04
163. Parveen, Z; Brunhofer, G; Jabeen, I; Erker, T; Chiba, P; Ecker, GF. Synthesis, biological evaluation and 3D-QSAR studies of new chalcone derivatives as inhibitors of human P-glycoprotein. *BIOORGANIC & MEDICINAL CHEMISTRY*, 22 (7):2311-2319; 10.1016/j.bmc.2014.02.005 APR 1 2014.
164. Silva, R; Carmo, H; Viras-Boas, V; Barbosa, DJ; Palmeira, A; Sousa, E; Carvalho, F; Bastos, MDL; Remiao, F. Colchicine effect on P-glycoprotein expression and activity: In silico and in vitro studies, *CHEMICO-BIOLOGICAL INTERACTIONS*, 218 50-62; 10.1016/j.cbi.2014.04.009 JUL 25 2014
165. Shukla, S; Kouanda, A; Silvertson, L; Talele, TT; Ambudkar, SV. Pharmacophore modeling of nilotinib as an inhibitor of ABC drug transporters and BCR-ABL kinase using a 3D-QSAR approach. *MOLECULAR PHARMACEUTICS*, 11 (7):2313-2322; 2014.
166. Zhang N, Zhang Z, Wong IL, Wan S, Chow LM, Jiang T. 4,5-Di-substituted benzyl-imidazol-2-substituted amines as the structure template for the design and synthesis of reversal agents against P-gp-mediated multidrug resistance breast cancer cells. *Eur J Med Chem*. 2014 Jun 10;83C:74-83. doi: 10.1016/j.ejmech.2014.06.016.
167. Kumar V., P Taya, Neetu. 3D QSAR studies on pyrrolopyrimidines as selective P-glycoprotein antagonist. *INTERNATIONAL JOURNAL OF PHARMACY AND PHARMACEUTICAL SCIENCES*, 6 (8), 2014, 232-239.
168. El-Kattan A., Varma M.V., Lai YR. Transporters in Drug Discovery: In Silico Approaches. In: *Drug Transporters: Molecular Characterization and Role in Drug Disposition, Second Edition*. Edited by Guofeng You, Marilyn E. Morris, Binghe Wang.. © 2014 John Wiley & Sons, Inc. Published 2014 by John Wiley & Sons, Inc., 371-387. ISBN: 978-1-118-48993-2.
169. Slanina, J; Pachnikova, G; Carnecka, M; Koubikova, LP; Adamkova, L; Humpa, O; Smejkal, K; Slaninova, I. Identification of Key Structural Characteristics of Schisandra chinensis Lignans Involved in P-Glycoprotein Inhibition. *JOURNAL OF NATURAL PRODUCTS*, 77 (10):2255-2263; 10.1021/np500521v OCT 2014.
170. Vázquez RN, Camargo AB, Marchevsky EJ, Luco JM. Molecular factors influencing the affinity of flavonoid compounds on P-glycoprotein efflux transporter. *CURRENT COMPUTER-AIDED DRUG DESIGN*, 10 (3):250-258; 2014
171. Vázquez, R.N., Camargo, A.B., Marchevsky, E.J., Luco, J.M. Molecular factors influencing the affinity of flavonoid compounds on pglycoprotein efflux transporter (2014) *Current Computer-Aided Drug Design*, 10 (3), pp. 250-258.
172. LMM Jaramillo. Structural and functional study of efflux pumps involved in drug resistance. PhD thesis, Agricultural sciences. Université Claude Bernard - Lyon I, 2014. <https://tel.archives-ouvertes.fr/tel-00985593> PhD
173. Silva, R; Palmeira, A; Carmo, H; Barbosa, DJ; Gameiro, M; Gomes, A; Paiva, AM; Sousa, E; Pinto, M; Bastos, MD; Remiao, F. P-glycoprotein induction in Caco-2 cells by newly synthesized thioxanthenes prevents paraquat cytotoxicity. *ARCHIVES OF TOXICOLOGY*, 89 (10):1783-1800; 10.1007/s00204-014-1333-4 OCT 2015
174. Foudah, A.I., Sallam, A.A., El Sayed, K.A. Discovery and Computer-Aided Drug Design Studies of the Anticancer Marine Triterpene Sipholanos as Novel P-gp and Brk. In: *Handbook of Anticancer Drugs from*

- Marine Origin Modulators, Kim, Se-Kwon (ed), Springer International Publishing, 2015, 547-569.  
[http://dx.doi.org/10.1007/978-3-319-07145-9\\_26](http://dx.doi.org/10.1007/978-3-319-07145-9_26)
175. Erić, S., M. Kalinić. Računarski modeli za predviđanje transporta lekova posredovanog P-glikoproteinom. *ARCH. FARM* 2015, 65, 89-114.
  176. Li Z, Alisaraie L. Microtubules dual chemo and thermo-responsive depolymerization. *PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS*, 83 (5):970-981; 10.1002/prot.24793 MAY 2015
  177. Subhani, S; Jayaraman, A; Jamil, K. Homology modelling and molecular docking of MDR1 with chemotherapeutic agents in non-small cell lung cancer, *BIOMEDICINE & PHARMACOTHERAPY*, 71 37-45; 10.1016/j.biopha.2015.02.009 APR 2015.
  178. Chufan E.E., Sim H-M., Ambudkar S.V. Molecular Basis of the Polyspecificity of P-glycoprotein (ABCB1): Recent Biochemical and Structural Studies. Chapter 3, In: *ABC TRANSPORTERS AND CANCER*, 125 71-96; 10.1016/bs.acr.2014.10.003 2015.
  179. Mitra R., Coyle E.M., Callaghan R. Just How and Where Does P-glycoprotein Bind All Those Drugs? In: *ABC Transporters - 40 Years on*, Ed. A. M. George, Springer International Publishing, pp. 153-194, 2016. [http://dx.doi.org/10.1007/978-3-319-23476-2\\_8](http://dx.doi.org/10.1007/978-3-319-23476-2_8)
  180. Pan, X., Mei, H., Qu, S., Huang, S., Sun, J., Yang, L., Chen, H. Prediction and characterization of P-glycoprotein substrates potentially bound to different sites by emerging chemical pattern and hierarchical cluster analysis *INTERNATIONAL JOURNAL OF PHARMACEUTICS*, 502 (1-2):61-69; 10.1016/j.ijpharm.2016.02.022 APR 11 2016.
  181. Pomilio AB, SM Battista, AA Vitale. Antimicrobial and immunosuppressive activities of cyclopeptides as targets for medicinal chemistry. Chapter 8. In: *Chemometrics Applications and Research: QSAR in Medicinal Chemistry*, A. G. Mercader, P. R. Duchowicz, P. M. Sivakumar (Eds.) CRC Press, Mar 30, 2016, 253-298.
  182. Matsson, P; Doak, BC; Over, B; Kihlberg, J. Cell permeability beyond the rule of 5, *ADVANCED DRUG DELIVERY REVIEWS*, 101 42-61; 10.1016/j.addr.2016.03.013 JUN 1 2016.
  183. Price, Daniel F. 2015Examining the selectivity in the impact of pulmonary P-gp upon the absorption of its substrates using an IPML model with knockout mice. PhD Thesis, Cardiff University, 2015, pp.176
  184. Ngo, T.-D., Tran, T.-D., Le, M.-T., Thai, K.-M. Machine learning-, rule- and pharmacophore-based classification on the inhibition of P-glycoprotein and NorA (2016) *SAR AND QSAR IN ENVIRONMENTAL RESEARCH*, 27 (9):747-780; 10.1080/1062936X.2016.1233137 2016.
  185. Gherbovet, O; Alvarez, MCG; Bignon, J; Roussi, F. Original Vinca Derivatives: from P-Glycoprotein Substrates to P-Glycoprotein Inhibitors *Journal of Medicinal Chemistry*, *JOURNAL OF MEDICINAL CHEMISTRY*, 59 (23):10774-10780; 10.1021/acs.jmedchem.6b00525 DEC 8 2016
  186. Venkata Krishnan Ramaswamy, Pierpaolo Cacciotto, Giuliano Mallocci, Paolo Ruggerone, Attilio V. Vargiu. Multidrug Efflux Pumps and Their Inhibitors Characterized by Computational Modeling. In: *Efflux-Mediated Antimicrobial Resistance in Bacteria*. (Eds. Xian-Zhi Li, Christopher A. Elkins, Helen I. Zgurskaya), Springer International Publishing, Nov 2016, pp 797-831.
  187. Pomilio, AB; Battista, SM; Vitale, AA. ANTIMICROBIAL AND IMMUNOSUPPRESSIVE ACTIVITIES OF CYCLOPEPTIDES AS TARGETS FOR MEDICINAL CHEMISTRY. *CHEMOMETRICS APPLICATIONS AND RESEARCH: QSAR IN MEDICINAL CHEMISTRY* (Edited by: Mercader AG; Duchowicz PR; Sivakumar PM, 253-298; 2016.
  188. Popović N, Giménez de Béjar V, Caballero-Bleda M, Popović M. Verapamil Parameter- and Dose-Dependently Impairs Memory Consolidation in Open Field Habituation Task in Rats. *Frontiers in Pharmacology*. 2017;7:539. doi:10.3389/fphar.2016.00539.
  189. Varma, MV; Lai, YR; El-Kattan, AF. Molecular properties associated with transporter-mediated drug disposition. *ADVANCED DRUG DELIVERY REVIEWS*, 116 92-99; 10.1016/j.addr.2017.05.014 JUL 1 2017.
  190. Mishra, Ravinesh; Sareen, Swati; Sharma, Bhartendu; Goyal, Shubham; Kaur, Gurpreet; Bhardwaj, Sweta; A. Siddiqui, Anees; Husain, Asif; K. Singla, Rajeev; Rashid, Mohd; Kumar, Deepak; Sati, Bhawana; Shalmali, Nishtha; Kumar, Rajiv"Phenothiazines and Related Drugs as Multi Drug Resistance Reversal Agents in Cancer Chemotherapy Mediated by p-glycoprotein." *Current Cancer Therapy Reviews* 13 (1), 2017: 28-42.
  191. J. Kehler. Targeting Phosphodiesterases in the CNS. In book: *Reference Module in Chemistry, Molecular Sciences and Chemical Engineering*, 2017, DOI:10.1016/B978-0-12-409547-2.12445-X
  192. Mohammed Ahmed Fayyad. The Effect of Diltiazem on Propranolol Absorption Using in Situ Single Pass Intestinal Perfusion Technique in Rats, Thesis, Al-Azhar University–Gaza, Deanship of Postgraduate Studies, Faculty of Pharmacy, 2017, pp. 134.
  193. Singla D., Bishnoi R., Dhanda S.K., Asthana S. (2018) Drug Transporters as Therapeutic Targets: Computational Models, Challenges, and Future Perspective. In: Purohit H., Kalia V., More R. (eds) *Soft*

- Computing for Biological Systems. Springer, Singapore, 2018, pp 143-168. DOI: 10.1007/978-981-10-7455-4\_9
194. Zhang, Yuchen. Identification and Characterization of the Oligomerization and Structural Functional Relationship of Organic Anion Transporting Polypeptide 1B3. University of Kansas, Dissertation, 129 pages, 2018. PhD <http://dissertations.umi.com/ku:15566>
  195. Negi, B; Rawat, DS, Synthesis, Characterization, and Antimycobacterial Activity of Novel Thymol- Triazole Hybrids. INDIAN JOURNAL OF HETEROCYCLIC CHEMISTRY, 28 (1):113-123; JAN-MAR 2018.
  196. Qu, GW; Hou, SY; Qu, D; Tian, CL; Zhu, JC; Xue, LJ; Ju, CY; Zhang, C, Self-assembled micelles based on N-octyl-N'-phthalyl-O-phosphoryl chitosan derivative as an effective oral carrier of paclitaxel, CARBOHYDRATE POLYMERS, 207 428-439; 10.1016/j.carbpol.2018.11.099 MAR 1 2019
  197. G. Mariappan, A. Kumari: Virtual Screening and Its Applications in Drug Discovery Process, In: Computer Applications in Drug Discovery and Development. edited by Puratchikody, A., Prabu, S. Lakshmana, 2019. Chapter 5, 101-126, 2019. DOI: 10.4018/978-1-5225-7326-5.ch005
  198. Hinge, V.K., Roy, D. & Kovalenko, A. Prediction of P-glycoprotein inhibitors with machine learning classification models and 3D-RISM-KH theory based solvation energy descriptors. J Comput Aided Mol Des (2019) 33: 965. <https://doi.org/10.1007/s10822-019-00253-5>
  199. Gupta, Mayuri; Bogdanowicz, Thomas; Reed, Mark A.; Barden, Christopher J.; Weaver, Donald F. The Brain Exposure Efficiency (BEE) Score. ACS CHEMICAL NEUROSCIENCE Volume: 11 Issue: 2 Pages: 205-224 Published: JAN 15 2020 DOI: 10.1021/acscemneuro.9b00650
  200. Sharma S., Bhatia V. (2021) In Silico Modeling of Anticancer Drugs: Recent Advances. In: Nayak J., Favorskaya M.N., Jain S., Naik B., Mishra M. (eds) Advanced Machine Learning Approaches in Cancer Prognosis. Intelligent Systems Reference Library, vol 204, pp 275-296, Springer, Cham. [https://doi.org/10.1007/978-3-030-71975-3\\_10](https://doi.org/10.1007/978-3-030-71975-3_10)

**17. Tsakovska, I., I. Pajeva (2002): Molecular modeling of triazine type MDR modulators using CoMFA and CoMSIA approaches. SAR QSAR Environ. Res. 2002, 13(3-4), 487-498.**

Цитирания: 4

1. Jonathan A. Pachter, Viyyoor M. Girijavallabhan, Anil Saksena, Ronald J. Doll, Yi-Tsung Liu, Timothy J. Guzi: 17  $\beta$ -hydroxysteroid dehydrogenase type 3 inhibitors for the treatment of androgen dependent diseases. US Patent Issued 7,053,091 on May 30, 2006.
2. Guzi, Timothy J. ; Liu, Yi-Tsung ; Doll, Ronald J. ; Saksena, Anil ; Girijavallabhan, Viyyoor M.. 17 $\beta$ -hydroxysteroid dehydrogenase type 3 inhibitors for the treatment of androgen dependent diseases. UNITED STATES PATENT AND TRADEMARK OFFICE GRANTED PATENT, February 2009
3. Sarkar, A., Kellogg, G.E. Hydrophobicity - Shake flasks, protein folding and drug discovery. Current Topics in Medicinal Chemistry, Volume 10, Issue 1, January 2010, Pages 67-83.
4. Aurijit Sarkar. Development and applications of the HINT forcefield in prediction of antibiotic efflux and virtual screening for antivirals. Dissertation. Virginia Commonwealth University, Richmond VA , August 2010. PhD

**18. Tsakovska, I., M. Wiese, I.Pajeva. Molecular modeling of phenothiazines and structurally related multidrug resistance modulators: comparative study in human and animal tumor cell lines, Biotechnol. & Biotechnol. Eq. 2003, 17 (2), 163-169.**

Цитирания: 2

1. Sefedin Biljali, Paraskev Nedialkov, Dimitrina Zheleva-Dimitrova, Gerassim Kitanov, Denitsa Momekova and Georgi Momekov. Cytotoxic effects and multidrug resistance modulation by five benzophenones and a xanthone isolated from *Hypericum annulatum* Moris subsp. *annulatum*. BIOTECHNOL. & BIOTECHNOL. EQ. 2013, 27(1), 3561-3568.
2. Venkatesan, K., Satyanarayana, V.S.V., Sivakumar, A., Ramamurthy, C., Thirunavukkarasu, C. Synthesis, spectral characterization and antitumor activity of phenothiazine derivatives. Journal of Heterocyclic Chemistry, 2020, DOI: 10.1002/jhet.3980

**19. Pajeva, I.K., J.K. Seydel, D. K. Todorov. Interactions of the anticancer drugs doxorubicin and thaliblastine with model membranes and their relation to multidrug resistance, Biotechnol. & Biotechnol. Eq. 2004, 18 (1), 132-139.**

Цитирания: 1

1. Sefedin Biljali, Paraskev Nedialkov, Dimitrina Zheleva-Dimitrova, Gerassim Kitanov, Denitsa Momekova and Georgi Momekov. Cytotoxic effects and multidrug resistance modulation by five benzophenones and a xanthone isolated from *Hypericum annulatum* Moris subsp. *annulatum*. BIOTECHNOL. & BIOTECHNOL. EQ. 2013, 27(1), 3561-3568.

**20. Pajeva I., D.K. Todorov, J.K. Seydel. Membrane effects of the antitumor drugs doxorubicin and thaliblastine: comparison to multidrug resistance modulators verapamil and trans-flupentixol, *Eur. J. Pharm. Sci.* 2004, 21(2-3), 243-250.**

Цитирания: 25

1. Blagoi, Gabriela, Fluorescence Resonance Energy Transfer (FRET) Based Sensors for Bioanalysis. *University of New Orleans Theses and Dissertations*. Paper 171, 2004. <http://scholarworks.uno.edu/td/171>
2. Marian, Terez; Balkay, Laszlo; Tron, Lajos; Krasznai, Zoard T.; Szabo-Peli, Judit; Krasznai, Zoltan. Effects of miltefosine on membrane permeability and accumulation of [Tc-99m]-hexakis-2-methoxyisobutyl isonitrile, 2-[F-18] fluoro-2deoxy-D-glucose, daunorubicin and rhodamine123 in multidrug-resistant and sensitive cells. *EUR J PHARM SCI* 24 (5): 495-501 APR 2005
3. Marian, Terez; Balkay, Laszlo; Szabo, Gabor; Krasznai, Zoard T.; Hernadi, Zoltan; Galuska, Laszlo; Szabo-Peli, Judit; Esik, Olga; Tron, Lajos; Krasznai, Zoltan. Biphasic accumulation kinetics of [Tc-99m]-hexakis-2-methoxyisobutyl isonitrile in tumour cells and its modulation by lipophilic P-glycoprotein ligands. *EUROPEAN JOURNAL OF PHARMACEUTICAL SCIENCES* 25 (2-3): 201-209 JUN 2005
4. Krasznai ZT, Peli-Szabo J, Nemeth E, Balkay L, Szabo G, Goda K, Galuska L, Tron L, Major T, Hernadi Z. Paclitaxel modifies the accumulation of tumor-diagnostic tracers in different ways in P-glycoprotein-positive and negative cancer cells. *EUR J PHARM SCI*. 2006; 28(3):249-256.
5. Castaing M, Loiseau A and Cornish-Bowden A 2007 Synergy between verapamil and other multidrug - resistance modulators in model membranes; *J. Biosci.* 32(4), June 2007, 737-746.
6. Zoárd Krasznai. Multidrog rezisztenciát okozó P-glikoprotein kimutatása és funkciójának vizsgálata humán tumorból származó mintákban. University of Debrecen 2007, pp. 92. <https://dea.lib.unideb.hu/dea/handle/2437/3101> PhD
7. Alderden, Rebecca. The Distribution of Platinum Complexes in Biological Systems. <http://hdl.handle.net/2123/1419>, University of Sydney. School of Chemistry, Feb 2006. PhD thesis
8. Michalak, K., O.Wesołowska, N.Motohashi, A.B.Hendrich. The Role of the Membrane Actions of Phenothiazines and Flavonoids as Functional Modulators. In: *Topics in Heterocyclic Chemistry, Bioactive Heterocycles II*, (S. Egguchi, Ed.), Volume 8, Springer Berlin / Heidelberg, 2007, 223-302.
9. Mavromoustakos, T.M.: The Use of Differential Scanning Calorimetry in Study Drug-Membrane Interactions, Chapter 39, In: *Methods in Molecular Biology*, Vol. 400: *Methods in Membrane Lipids*, Ed. by A.M. Dopico, Humana Press Inc., 587-598.
10. D.Fan, S.-J. Kim, R. L. Langley, I. J. Fidler. Metastasis and Drug Resistance. In: *Drug Resistance In Cancer Cells*. Ed. Kapil Mehta, Springer New York, 2009, 21-52.
11. Peetla, C; Bhave, R; Vijayaraghavalu, S; Stine, A; Kooijman, E; Labhasetwar, V. Drug Resistance in Breast Cancer Cells: Biophysical Characterization of and Doxorubicin Interactions with Membrane Lipids. *MOLECULAR PHARMACEUTICS* 7 (6): 2334-2348 NOV-DEC 2010.
12. Effrosyni Gkikopoulou. Voies de signalisation cobalamine-dépendantes de l'expression du gène *MDR-1*. Une cible pharmacologique nouvelle pour la chimiothérapie? Ecole Doctorale *BIOSE*, Université de Lorraine, France, Dec 2012. PhD
13. Okan Tezcan. Metastatic behaviour of doxorubicin resistant MCF-7 breast cancer cells after vimentin silencing. The Graduate School of Natural and Applied Sciences of Middle East Technical University, Turkey. Jan 2013, 78 pages. PhD thesis
14. Gozde Unsoy. The synthesis and characterization of doxorubicin and bortezomib loaded magnetic nanoparticles for targeting tumor cells. Graduate school of natural and applied sciences of Middle East Technical University, September 2013, pp.1-128. <https://www.researchgate.net/publication/326843490> PhD
15. Marguerite, V; Gkikopoulou, E; Alberto, JM; Gueant, JL; Merten, M. Phospholipase D activation mediates cobalamin-induced downregulation of Multidrug Resistance-1 gene and increase in sensitivity to vinblastine in HepG2 cells, *INTERNATIONAL JOURNAL OF BIOCHEMISTRY & CELL BIOLOGY*, 45 (2):213-220; FEB 2013
16. Park, S; Jansen, RK; Park, S. Complete plastome sequence of *Thalictrum coreanum* (Ranunculaceae) and transfer of the *rpl32* gene to the nucleus in the ancestor of the subfamily *Thalictroideae*. *BMC PLANT BIOLOGY*, Volume 15, Issue 1, February 05, 2015, Article number 40.
17. Ferreira RJ, dos Santos DJ, Ferreira MJ. P-glycoprotein and membrane roles in multidrug resistance. *FUTURE MEDICINAL CHEMISTRY*, 7 (7):929-946; 10.4155/FMC.15.36 2015
18. Şen-Çağlar GP, Yalcin S, Gunduz U (2015) *Synthesis and Cytotoxicity of a TAT Peptide-Doxorubicin Conjugate for Breast Treatment*, *JOURNAL OF DRUG DESIGN AND RESEARCH* 2(1): 1007, 2015.
19. Ghimire B., Lee H., Choi G.E., Jeong M.J., Suh G.U., Lee C.H., Heo K., Son S.W.. Seed morphology of 12 taxa of the genus *Thalictrum* L. (Thalictroideae, Ranunculaceae) and its systematic implication. *Phytotaxa*, v. 283, n. 3, p. 271-285, Nov. 2016

20. M. Asif. Biological potential of phenothiazine derivatives and some new heterocycles based on phenothiazine moiety. *International Journal of Current Research in Applied Chemistry & Chemical Engineering*, Vol. 2, Issue 2, 2016, 39-57.
21. Tao, Y; Li, MQ; Auguste, DT. Pattern-based sensing of triple negative breast cancer cells with dual-ligand cofunctionalized gold nanoclusters. *BIOMATERIALS*, 116 21-33; 10.1016/j.biomaterials.2016.11.050 FEB 2017
22. Dong Chan Son, Minjung Joo, Kang-Hyup Lee, Jun-Soo Han, Kae Sun Chang, *Thalictrum acutifolium* (Hand.-Mazz.) B. Boivin: a new record to the flora of the Jeju-do, Korea, In *Journal of Asia-Pacific Biodiversity*, Volume 10, Issue 1, 2017, Pages 112-117.
23. Dong Chan Son, Beom Kyun Park, Kae Sun Chang, Kyung Choi, Chang Ho Shin, Cladistic analysis of the section *Adonanthe* under genus *Adonis* L. (Ranunculaceae) from East Asia, In: *Journal of Asia-Pacific Biodiversity*, Volume 10, Issue 2, 2017, Pages 232-236, ISSN 2287-884X, <https://doi.org/10.1016/j.japb.2017.02.002>.
24. Saleh ZA, SB Novir, E Balali. QUANTUM CHEMICAL INVESTIGATION OF trans- and cis-ISOMERS OF FLUPENTIXOL AS A NANO-DRUG. *Journal of Applied Spectroscopy*, 86 (6), 1007(1)-1007(10), 2019, <https://elibrary.ru/item.asp?id=41330822>.
25. Park JW, Hong S-p, Lee JH, Moon SH, Cho YS, Jung K-H, Jeeyun Lee, Kyung-Han Lee. <sup>99m</sup>Tc-MIBI uptake as a marker of mitochondrial membrane potential in cancer cells and effects of MDR1 and verapamil. *PLOS ONE* Volume: 15 Issue: 2 Article Number: e0228848 Published: FEB 12 2020. <https://doi.org/10.1371/journal.pone.0228848>

**21. Pajeva, I.K., C. Globisch, M. Wiese. Structure-Function Relationships of Multidrug Resistance P-glycoprotein, *J. Med. Chem.* 2004, 47 (10), 2523-2533.**

Цитирания: 77

1. Cianchetta G, Singleton RW, Zhang M, Wildgoose M, Giesing D, Fravolini A, Cruciani G, Vaz RJ. A pharmaeophore hypothesis for P-glycoprotein substrate recognition using GRIND-based 3D-QSAR. *J MED CHEM* 48 (8): 2927-2935 APR 21 2005
2. Prasad R, Kapoor K. Multidrug resistance in yeast *Candida*. In: *INTERNATIONAL REVIEW OF CYTOLOGY-A SURVEY OF CELL BIOLOGY* 242: 215-248, Ed. by Kwang W. Jeon, Academic Press (January 6, 2005) (citation p. 232)
3. Balakin, K.V., Ivanenkov, Y.A., Savchuk, N.P., Ivashchenko, A.A., Ekins, S. Comprehensive computational assessment of ADME properties using mapping techniques *Current Drug Discovery Technologies* 2 (2), pp. 99-113
4. Zhang ZY, Wong YN. Enzyme kinetics for clinically relevant CYP inhibition *CURRENT DRUG METABOLISM* 6 (3): 241-257 JUN 2005
5. Sun, HM. Predicting ADMET Properties by Projecting onto Chemical Space? Benefits and Pitfalls. *Current Computer - Aided Drug Design*, April 2005, vol. 1, no. 2, pp. 179-193(15)
6. Sun, HM. A naive bayes classifier for prediction of multidrug resistance reversal activity on the basis of atom typing. *J MED CHEM.* 2005 Jun 16;48(12):4031-9.
7. Boumendjel, A., Baubichon-Cortay, H., Trompier, D., Perrotton, T., Di Pietro, A. Anticancer multidrug resistance mediated by MRP1: Recent advances in the discovery of reversal agents. *MEDICINAL RESEARCH REVIEWS* 2005, 25 (4), pp. 453-472
8. Aleman C, Namba AM, Casanovas J. Acid-base and electronic structure-dependent properties of Hoechst 33342. *J BIOMOL STRUCT DYN.* 2005 Aug; 23(1):29-36.
9. Cortés-Selva, F., Jiménez, I.A., Muñoz-Martínez, F., Campillo, M., Bazzocchi, I.L., Pardo, L., Ravelo, A.G., Castanys, S., Gamarro, F. Dihydro- $\beta$ -agarofuran sesquiterpenes: A new class of reversal agents of the multidrug resistance phenotype mediated by P-glycoprotein in the protozoan parasite *Leishmania*. *CURRENT PHARMACEUTICAL DESIGN* 2005 11 (24), pp. 3125-3159.
10. Van Bambeke, Françoise: Antibiotic accumulation and efflux in eukaryotic cells : a journey at the frontier of pharmacokinetics and pharmacodynamics. Dissertation, Universite catolique de Louvaine, Nov 2005 PhD
11. Cheng Chang *IN SILICO* APPROACHES FOR STUDYING TRANSPORTER AND RECEPTOR STRUCTURE-ACTIVITY RELATIONSHIPS, DISSERTATION, Graduate School of The Ohio State University, 2005. PhD
12. Hui-Hsuan Tu .Dynamics, Conformational Transition and Drug Interactions of P-glycoprotein upon ATP Binding, Thesis, Graduate Institute of Pharmacy, National Taiwan University, July 2005. [http://etds.lib.ntu.edu.tw/etdservice/view\\_metadata?etdun=U0001-2107200514464000&query\\_field1=keyword&&query\\_word1=MD& PhD](http://etds.lib.ntu.edu.tw/etdservice/view_metadata?etdun=U0001-2107200514464000&query_field1=keyword&&query_word1=MD& PhD)
13. Ungvári, H. J. Synthese Potentieller Modulatoren Zur Überwindung Der Multidrug Resistance Dissertation. Mathematisch-Naturwissenschaftlich-Technischen Fakultät (mathematisch-naturwissenschaftlicher Bereich) der Martin-Luther-Universität Halle-Wittenberg, Halle (Saale), 2005 PhD

14. Takano, M., Yumoto, R., Murakami, T.: Expression and function of efflux drug transporters in the intestine. *PHARMACOLOGY & THERAPEUTICS* 109 (1-2): 137-161 JAN 2006
15. Vandevuer, S., Van Bambeke, F., Tulkens, P.M., Prevost, M. Predicting the three-dimensional structure of human P-glycoprotein in absence of ATP by computational techniques embodying crosslinking data: Insight into the mechanism of ligand migration and binding sites. *PROTEINS*. 2006; 63(3):466-78
16. Li, Y., Wang, L., Yang, S., Zhang, C., Liu. Structural determinants of flavones interacting with the C-terminal nucleotide-binding domain as P-glycoprotein inhibitors. *Internet Electron. J. Mol. Des.*, 5, 1-12, 2006. [www.biochempress.com](http://www.biochempress.com)
17. Srinivas E, Murthy JN, Rao ARR, Sastry GN. Recent advances in molecular modeling and medicinal chemistry aspects of phospho-glycoprotein. *CURRENT DRUG METABOLISM* 7 (2): 205-217 FEB 2006
18. Crivori, P., B. Reinach, D. Pezzetta, I. Pogessi. Computational models for identifying potential P-glycoprotein substrates and inhibitors. *Molecular Pharmaceutics*, Vol. 3(1), 33-44, 2006.
19. Xia, C., Xiao, G, Liu, N, Pimprale, S, Fox, L, Patten, CJ, Crespi, CL, Miwa, G, Gan, L-S Comparison of species differences of P-glycoproteins in beagle dog, rhesus monkey, and human using ATPase activity assays. *Molecular Pharmaceutics*, Vol. 3(1), 78-86, 2006.
20. Raub, T.J. P-glycoprotein recognition of substrates and circumvention through rational drug design, *Molecular Pharmaceutics*, 3 (1), 78-86, 2006.
21. Tomblin G, Donnelly DJ, Holt JJ, You Y, Ye M, Gannon MK, Nygren CL, Detty MR.: Stimulation of P-glycoprotein ATPase by analogues of tetramethylrosamine: coupling of drug binding at the "R" site to the ATP hydrolysis transition state. *BIOCHEMISTRY*. 2006 Jul 4; 45(26): 8034-8047.
22. Fusi, F., Saponara, S., Valoti, M., Dragoni, S., D'Elia, P., Sgaragli, T., Alderighi, D., Sgaragli, G.: Cancer cell permeability-glycoprotein as a target of MDR reverters: Possible role of novel dihydropyridine derivatives. *CURRENT DRUG TARGETS* 7 (8), pp. 949-959, 2006.
23. Balázs Sarkadi, László Homolya, Gergely Szakács and András Váradi: Human Multidrug Resistance ABCB and ABCG Transporters: Participation in a Chemoimmunity Defense System. *PHYSIOL. REV.* 86: 1179-1236, 2006
24. Teodori, E., Dei, S., Martelli, C., Scapecchi, S., Gualtieri, F. The functions and structure of ABC transporters: Implications for the design of new inhibitors of Pgp and MRP1 to control multidrug resistance (MDR). *CURRENT DRUG TARGETS* 7 (7), pp. 893-909, 2006.
25. Mandola, C.: Nuovi inibitori della Multidrug Resistance (MDR): sintesi di derivati amminoalchilici ad elevata flessibilità molecolare Thesis, Università degli Studi di Firenze, 2005-06. PhD
26. Labrie P, Maddaford SP, Fortin S, Rakhit S, Kotra LP, Gaudreault RC. A comparative molecular field analysis (CoMFA) and comparative molecular similarity indices analysis (CoMSIA) of anthranilamide derivatives that are multidrug resistance modulators. *J Med Chem*. 2006 Dec 28; 49(26):7646-60.
27. Oloo EO, Kandt C, O'mara ML, Tieleman DP. Computer simulations of ABC transporter components. *BIOCHEM CELL BIOL*. 2006 Dec; 84(6):900-11.
28. Turcotte, S., M. Demeule, A. Regina, C. Fournier, J. Jodoin, A. Moghrabi, R. Beliveau : The blood-brain barrier : roles of the multidrug resistance transporter P-glycoprotein, Vol. 2, Part V, In: *Blood-Brain Barriers: From Ontogeny to Artificial Interfaces*, R. Dermietzel, D. C. Spray, M. Nedergaard (Edts.), Published 2006, Wiley-VCH, 774 pages, p. 452 (ref. 38).
29. Fournier, Chantal: Etude de la p-glycoprotéine : effet des coumarins et du niveau d'interaction entre la p-gp et la cavéoline-1 sur les activités associées à la p-gp. Mémoire présenté comme exigence partielle de la maîtrise en chimie. Université du Québec à Montréal, Janvier 2007.
30. Schmidt, M., Ungvári, J., Gloede, J., Dobner, B., Langner, A.: New 1,3-dioxolane and 1,3-dioxane derivatives as effective modulators to overcome multidrug resistance *Bioorganic and Medicinal Chemistry* 15 (6), pp. 2283-2297, 2007.
31. Gangjee, Aleem; Yu, Jianming; Copper, Jean E.; Smith, Charles D. Discovery of Novel Antitumor Antimitotic Agents That Also Reverse Tumor Resistance. *Journal of Medicinal Chemistry* (2007), 50(14), 3290-3301.
32. Fabian Heisig, F. Synthese neuer, funktionalisierter BODIPY-Fluorophore zur Fluoreszenzmarkierung von Membranrezeptor-Liganden. Dissertation Zur Erlangung des Doktorgrades Dr. rer. nat. Der Mathematisch-Naturwissenschaftlichen Fakultät der Rheinischen Friedrich-Wilhelms-Universität Bonn, Bonn 2007 (citation 148). PhD
33. Tobias Brandt. Untersuchung und Charakterisierung von Inhibitoren des p-glykoproteins zur Überwindung der multidrug resistance. Dissertation. Naturwissenschaftlichen Fakultät I Biowissenschaften der Martin-Luther-Universität Halle-Wittenberg, 2008. PhD.
34. Li, X., Li, J.-P., Yuan, H.-Y., Gao, X., Qu, X.-J., Xu, W.-F., Tang, W. Recent advances in P-glycoprotein-mediated multidrug resistance reversal mechanisms. *Methods and Findings in Experimental and Clinical Pharmacology* 29 (9), pp. 607-617, 2008.

35. Bandyopadhyay, D., Agrafiotis, D.K. A self-organizing algorithm for molecular alignment and pharmacophore development *Journal of Computational Chemistry*. Volume 29, Issue 6, 30 April 2008, Pages 965-982.
36. Szakács, G., Váradi, A., Özvegy-Laczka, C., Sarkadi, B. The role of ABC transporters in drug absorption, distribution, metabolism, excretion and toxicity (ADME-Tox) *Drug Discovery Today* 13 (9-10), 2008, pp. 379-393.
37. Crivori, P. Computational Models for P-Glycoprotein Substrates and Inhibitors. In: *Antitargets: Prediction and Prevention of Drug Side Effects Book series: Methods and Principles in Medicinal Chemistry* (Roy J. Vaz, Thomas Klabunde, Raimund Mannhold, Hugo Kubinyi, Gerd Folkers, Eds.), John Wiley & Sons Inc, 2008, 367-397.
38. Matthias Schmidt, Marlen Teitge, Marianela E. Castillo, Tobias Brandt, Bodo Dobner, Andreas Langner: Synthesis and Biochemical Characterization of New Phenothiazines and Related Drugs as MDR Reversal Agents, *ARCHIV DER PHARMAZIE*, 2008, Vol. 341 (10), 624-638.
39. Gannon MK, Holt JJ, Bennett SM, Wetzel BR, Loo TW, Bartlett MC, Clarke DM, Sawada GA, Higgins JW, Tomblin G, Raub TJ, Detty MR. Rhodamine Inhibitors of P-Glycoprotein: An Amide/Thioamide "Switch" for ATPase Activity, *J Med Chem*. 2009, 52 (10): 3328-3341.
40. Balaz, Stefan. Modeling Kinetics of Subcellular Disposition of Chemicals. *Chemical Reviews* (Washington, DC, United States) (2009), 109(5), 1793-1899.
41. Pär Matsson, Jenny M. Pedersen, Ulf Norinder, Christel A. S. Bergström and Per Artursson. Identification of Novel Specific and General Inhibitors of the Three Major Human ATP-Binding Cassette Transporters P-gp, BCRP and MRP2 Among Registered Drugs, *Pharmaceutical Research*, 26(8), 1816-1831, 2009.
42. Hegedus, Csilla; Ozvegy-Laczka, Csilla; Szakacs, Gergely; Sarkadi, Balazs. Interaction of ABC multidrug transporters with anticancer protein kinase inhibitors: substrates and/or inhibitors? *Current Cancer Drug Targets*, (2009), 9(3), 252-272.
43. Ponte-Sucre, A., M. Padron-Nieves, E. Diaz. ABC transporter blockers and reversal of drug resistance in microorganisms. In: *ABC transporters in microorganisms: Research, Innovation and Value as Targets against Drug Resistance*, Horizon Scientific Press, 2009, 177-195. ISBN: 978-1-904455-49-3 <http://saber.ucv.ve/123456789/1737>.
44. Hu CQ, Xu DQ, Du WT, et al. Novel 4 beta-anilino-podophyllotoxin derivatives: design synthesis and biological evaluation as potent DNA-topoisomerase II poisons and anti-MDR agents *MOLECULAR BIOSYSTEMS* 6 2 410-420 2010.
45. Li, Y; Yuan, H; Yang, K; Xu, W; Tang, W; Li, X. The Structure and Functions of P-Glycoprotein. *CURRENT MEDICINAL CHEMISTRY* 17 (8): 786-800 MAR 2010.
46. Yan Li, Jezrael L. Revalde, Glen Reid, James W. Paxton. Interactions of dietary phytochemicals with ABC transporters: possible implications for drug disposition and multidrug resistance in cancer. *DRUG METABOLISM REVIEWS*, 42 (4), 590-611, 2010.
47. Palmeira, A; Rodrigues, F; Sousa, E; Pinto, M; Vasconcelos, MH; Fernandes, MX. Pharmacophore-based screening as a clue for the discovery of new P-gp inhibitors. In: *Advances in Bioinformatics: 4th International Workshop on Practical Applications of Computational Biology and Bioinformatics 2010 (IWPACBB 2010)* (Miguel P. Rocha, Florentino Fernández Riverola, Hagit Shatkay, Juan Manuel Corchado Rodríguez, eds.) Springer Science & Business Media, May 29, 2010, 175-180.
48. Teodori, E.; Dei, S.; Martelli, C.; Scapocchi, S. N,N-bis(cyclohexanol)amine aryl esters: the discovery of a new class of highly potent inhibitors of transporter-dependent multidrug resistance (MDR). *CURRENT TOPICS IN MEDICINAL CHEMISTRY*, 2010, 10(17), 1715-1731.
49. Ricardo Jose Diogo Gracio Ferreira. Vencendo a multi-resistência: Modelos computacionais da Glicoproteína-P. Mestrado em Química Farmacéutica e Terapêutica. UNIVERSIDADE DE LISBOA. FACULDADE DE FARMÁCIA. 2011. [www.ff.ul.pt/FCT/PTDC/QEQ.../Tese-Msci2.pdf](http://www.ff.ul.pt/FCT/PTDC/QEQ.../Tese-Msci2.pdf)
50. Andreia Palmeira. Design, synthesis and evaluation of xanthone derivatives for dual activity: antitumor and P-glycoprotein inhibition. Thesis presented to the Faculdade de Farmácia, Universidade do Porto, Porto, 2011, pp. 1-402. PhD <https://br.123dok.com/document/z31on7my-design-synthesis-and-evaluation-of-xanthone-derivatives-for-dual-activity-antitumor-and-p-glycoprotein-inhibition.html>
51. Shen, X., Chen, G., Zhu, G., Cai, J., Wang, L., Hu, Y., Fong, W.-F. 3'-O, 4'-O-aromatic acyl substituted 7,8-pyranocoumarins: A new class of P-glycoprotein modulators. *Journal of Pharmacy and Pharmacology* 64 (1), pp. 90-100, 2012.
52. Xie, H; Zeng, LL; Zeng, SG; Lu, X; Zhang, GC; Zhao, X; Cheng, N; Tu, ZC; Li, ZY; Xu, HJ; Yang, L; Zhang, XQ; Huang, M; Zhao, JL; Hu, WH, Novel pyrrolopyrimidine analogues as potent dipeptidyl peptidase IV inhibitors based on pharmacokinetic property-driven optimization, *EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY*, 52 205-212; 10.1016/j.ejmech.2012.03.015 JUN 2012
53. Chen L, Li Y, Yu H, Zhang L, Hou T. Computational models for predicting substrates or inhibitors of P-glycoprotein. *DRUG DISCOVERY TODAY*, 17 (7-8):343-351; 10.1016/j.drudis.2011.11.003 APR 2012.

54. John G. Wise. Catalytic Transitions in the Human MDR1 P-Glycoprotein Drug Binding Sites. *BIOCHEMISTRY*, 51 (25):5125-5141; 10.1021/bi300299z JUN 26 2012
55. Shen, Xiaoling; Chen, Guangying; Zhu, Guoyuan; Cai, Jiazhong; Wang, Lu; Hu, Yingjie; Fong, Wang-Fun. 3'-O,4'-O-aromatic acyl substituted 7,8-pyrano-coumarins: a new class of P-glycoprotein modulators. *JOURNAL OF PHARMACY AND PHARMACOLOGY* (2012), 64(1), 90-100.
56. Orchard, A; Schamerhorn, GA; Calitree, BD; Sawada, GA; Loo, TW; Bartlett, MC; Clarke, DM; Detty, MR. Thiorhodamines containing amide and thioamide functionality as inhibitors of the ATP-binding cassette drug transporter P-glycoprotein (ABCB1) *BIOORGANIC & MEDICINAL CHEMISTRY*, 20 (14):4290-4302; 10.1016/j.bmc.2012.05.075 JUL 15 2012
57. Palmeira, A; Sousa, E; Vasconcelos, MH; Pinto, M; Fernandes, MX. Structure and Ligand-based Design of P-glycoprotein Inhibitors: A Historical Perspective. *CURRENT PHARMACEUTICAL DESIGN*, 18 (27):4197-4214; SEP 2012
58. Ferreira, JAB; Sanchez-Coronilla, A; Togashi, DM; Ferreira, H; Ascenso, JR; Costa, SMB. Electrophilic Reactivity of Tetrabromorhodamine 123 is Bromine Induced: Convergent Interpretation through Complementary Molecular Descriptors. *JOURNAL OF PHYSICAL CHEMISTRY A*, 116 (48):11938-11945; 10.1021/jp307461m DEC 6 2012
59. Ricardo J. Ferreira, Maria-José U. Ferreira, and Daniel J. V. A. dos Santos Molecular Docking Characterizes Substrate-Binding Sites and Efflux Modulation Mechanisms within P-Glycoprotein. *JOURNAL OF CHEMICAL INFORMATION AND MODELING*, 53 (7):1747-1760; 10.1021/ci400195v JUL 2013.
60. Steiger, Scott. 4-Isoxazolyl-1,4-Dihydropyridines Bind The Multidrug-Resistance Transporter, The University of Montana Missoula, MT May 2013. PhD
61. Liu, HM; Ma, ZG; Wu, BJ. Structure-activity relationships and in silico models of P-glycoprotein (ABCB1) inhibitors. *XENOBIOTICA*, 43 (11):1018-1026; 10.3109/00498254.2013.791003 NOV 2013
62. Saneja, A; Khare, V; Alam, N; Dubey, RD; Gupta, PN. Advances in P-glycoprotein-based approaches for delivering anticancer drugs: pharmacokinetic perspective and clinical relevance. *EXPERT OPINION ON DRUG DELIVERY*, 11 (1):121-138; 10.1517/17425247.2014.865014 JAN 2014
63. Martinez L. Arnaud O., Henin E., Tao H., Chaptal V., Doshi R., Andrieu T., Dussurgey, S., Tod M., Pietro AD., Zhang Q., Chang, G., Falson P. Understanding Polyspecificity Within The Substrate-Binding Cavity Of The Human Multidrug Resistance P-Glycoprotein. *FEBS JOURNAL*, 281 (3):673-682; 10.1111/febs.12613 FEB 2014
64. Silva, R; Carmo, H; Viras-Boas, V; Barbosa, DJ; Palmeira, A; Sousa, E; Carvalho, F; Bastos, MDL; Remiao, F. Colchicine effect on P-glycoprotein expression and activity: In silico and in vitro studies, *CHEMICO-BIOLOGICAL INTERACTIONS*, 218 50-62; 10.1016/j.cbi.2014.04.009 JUL 25 2014.
65. LMM Jaramillo. Structural and functional study of efflux pumps involved in drug resistance. PhD thesis, Agricultural sciences. Université Claude Bernard - Lyon I, 2014. <https://tel.archives-ouvertes.fr/tel-00985593> PhD
66. Zyta, J; Jaszczyszyn, A; Swiatek, P; Gasiowski, K; Malinka, W. Synthesis, pro-apoptotic activity and 2D-QSAR studies of new analogues of fluphenazine. *ACTA POLONIAE PHARMACEUTICA*, 71 (1):49-58; JAN-FEB 2014.
67. Prajapati, R; Sangamwar, AT. Translocation mechanism of P-glycoprotein and conformational changes occurring at drug-binding site: Insights from multi-targeted molecular dynamics. *BIOCHIMICA ET BIOPHYSICA ACTA-BIOMEMBRANES*, 1838 (11):2882-2898; 10.1016/j.bbamem.2014.07.018 NOV 2014
68. Xu-Qin Li, Lin Wang, Yan Lei, Tao Hu, Fei-Long Zhang, Chi-Hin Cho, Kenneth K.W. To, Reversal of P-gp and BCRP-mediated MDR by tariquidar derivatives, *European Journal of Medicinal Chemistry*, Volume 101, 28 August 2015, Pages 560-572, ISSN 0223-5234, <http://dx.doi.org/10.1016/j.ejmech.2015.06.049>
69. Erić, S., Kalinić, M. Computational models for predicting drug transport mediated by P-glycoprotein [Računarski modeli za predviđanje transporta lekova posredovanog P-glikoproteinom]. (2015) *Arhiv za Farmaciju*, 65 (2), pp. 89-114
70. Sharrol Bachas, Bryan Kohrs, Herschel Wade. Charge is Major Determinant of Activation of the Ligand-Responsive Multidrug Resistance Gene Regulator, BmrR. *ChemMedChem*, 2016, 11 (10), 1038-1041.
71. Xu, BQ; Peng, B; Cai, BL; Wang, SS; Wang, XX; Lv, X. Facile and Selective Synthesis of Imidazobenzimidazoles via a Copper-Catalysed Domino Addition/ Cycloisomerisation/ Coupling Process. *ADVANCED SYNTHESIS & CATALYSIS*, 358 (4):653-660; 10.1002/adsc.201500455 FEB 18 2016.
72. Gunio, D; Froehlig, J; Pappas, K; Ferguson, U; Wade, H. Solution-Binding and Molecular Docking Approaches Combine to Provide an Expanded View of Multidrug Recognition in the MDR Gene Regulator BmrR. *JOURNAL OF CHEMICAL INFORMATION AND MODELING*, 56 (2):377-389; 10.1021/acs.jcim.5b00704 FEB 2016
73. Matsson, P; Doak, BC; Over, B; Kihlberg, J. Cell permeability beyond the rule of 5, *ADVANCED DRUG DELIVERY REVIEWS*, 101 42-61; 10.1016/j.addr.2016.03.013 JUN 1 2016.

74. P. Palestro, L. Gavernet, Discovering New Antiepileptic Drugs Addressing the Transporter Hypothesis of Refractory Epilepsy: Structure-Based Approximation. In: Antiepileptic Drug Discovery, Novel approaches, Humana Press Inc., 2016, pp 281-297.
75. Pimthon, J., R. Dechaanontasup, C. Ratanaphipop, C. Phromprasert. Homology modeling and substrate binding studies of human P-glycoprotein. *Pharm. Sci. Asia*, 44 (2), 96-107, 2017.
76. Ricardo J Ferreira. Reversing multidrug resistance (MDR) in cancer cells by targeting P-glycoprotein (P-gp)- Insights into the mechanism of MDR reversal from in silico P-gp modelling. Thesis for PhD, Oct 2017 PhD
77. Mollazadeh, S; Sahebkar, A; Hadizadeh, F; Behravan, J; Arabzadeh, S. Structural and functional aspects of P-glycoprotein and its inhibitors. *LIFE SCIENCES*, 214 118-123; 10.1016/j.lfs.2018.10.048 DEC 1 2018

**22. Lessigiarska, I., I. Pajeva, I., M.T.D. Cronin, A.P. Worth, 3D SAR and QSAR investigation of blood-brain barrier penetration of chemical compounds, *SAR QSAR Environ. Res.* 2005, 16(1-2), 79-91.**

Цитирания: 10

1. Claudia-Carolin Weber. Effekte von Johanniskrautextrakt und anderen Antidepressiva auf die Funktion und Expression von P-Glykoprotein sowie die Plasma-Hirn-Verteilung von Corticosteron, Dissertation, Fachbereich Chemische und Pharmazeutische Wissenschaften der Johann Wolfgang Goethe-Universität in Frankfurt am Main Frankfurt, 2005. PhD
2. Hitchcock, S.A., Pennington, L.D. Structure-brain exposure relationships *Journal of Medicinal Chemistry*, Volume 49, Issue 26, 28 December 2006, Pages 7559-7583.
3. Leonardo Grilli Torres and Tiago Luiz Moda: Database for Pharmacokinetic Properties - IFSC/USP. <http://miro.ifsc.usp.br/pkdb/index.php>
4. Fotaki, Nikoletta Pros and cons of methods used for the prediction of oral drug absorption *Expert Review of Clinical Pharmacology*, 2009, Vol. 2, No. 2, Pages 195-208.
5. Zhang, YH; Xia, ZN; Qin, LT; Liu, SS. Prediction of blood-brain partitioning: A model based on molecular electronegativity distance vector descriptors. *JOURNAL OF MOLECULAR GRAPHICS & MODELLING* 29 (2): 214-220 SEP 2010.
6. Tiago Luiz Moda. Pharmacokinetic Properties *In Silico* Modeling for New Chemical Entities Evaluation. Doctoral thesis, Institute of Physics of São Carlos, São Carlos, 2011. <http://www.teses.usp.br/teses/disponiveis/76/76132/tde-19102011-141448/en.php>
7. Hecht, D. Applications of machine learning and computational intelligence to drug discovery and development. *DRUG DEVELOPMENT RESEARCH* 72 (1): 53-65 Sp. Iss. SI FEB 2011.
8. Honorio, KM; Moda, TL; Andricopulo, AD. Pharmacokinetic Properties and In Silico ADME Modeling in Drug Discovery. *MEDICINAL CHEMISTRY*, 9 (2):163-176; MAR 2013.
9. Cattaneo A. G., R. Gornati, G. Bernardini, E. Sabbioni, L. Manzo, M. Di Gioacchino. Nanomedicine for the Brain and the Eye: Disease Management in Poorly Accessible Compartments of the Body, In *Handbook of Nanotoxicology, Nanomedicine and Stem Cell Use in Toxicology* (eds S. C. Sahu and D. A. Casciano), John Wiley & Sons, Ltd, Chichester, UK. Published Online : 18 APR 2014, Pages: 223-247. doi: 10.1002/9781118856017.ch13
10. Vilar, S; Sobarzo-Sanchez, E; Santana, L; Uriarte, E. Ligand and Structure-based Modeling of Passive Diffusion through the Blood-Brain Barrier. *CURRENT MEDICINAL CHEMISTRY*, 25 (9):1073-1089; 10.2174/0929867324666171106163742 2018

**23. Lessigiarska, I., A. Nankov, A. Bocheva, I. Pajeva, A. Bijev (2005): 3D-QSAR and preliminary evaluation of anti-inflammatory activity of series of N-pyrrolylcarboxylic acids, *Il Farmaco* 2005, 60(3), 209-218.**

Цитирания: 22

1. Argentieri, T.M., Butera, J.A. An overview of potassium channel activators for the treatment of overactive bladder: a survey of new structures 2000 – 2005. *Expert Opinion on Therapeutic Patents*, 2006, Vol. 16, No. 5, 573-585.
2. Singh, P., Mittal, A., Kaur, S., Kumar, S. 5-Substituted-2,3-diphenyltetrahydrofurans: A new class of moderately selective COX-2 inhibitors. *Bioorganic and Medicinal Chemistry* 14 (23), pp. 7910-7916, 2006.
3. Elmegeed, G.A., Baiuomy, A.R., Abdel-Salam, O.M.E.: Evaluation of the anti-inflammatory and antipociceptive activities of novel synthesized melatonin analogues, *European Journal of Medicinal Chemistry* 42 (10), 2007, pp. 1285-1292.
4. Головкин, Ю. С., Ивашкевич, О. А., Матулис, В. Э., & Гапоник, П. Н. Основные направления компьютерного моделирования биологической активности молекул. *Химические проблемы создания новых материалов и технологий* : сб. ст./под ред. О. А. Ивашкевича. - Минск, 2008. - Вып.3, 144-164.
5. Kim, Yongju; Kim, Jonghoon; Park, Seung Bum. Regioselective Synthesis of Tetrasubstituted Pyrroles by 1,3-Dipolar Cycloaddition and Spontaneous Decarboxylation. *Organic Letters* (2009), 11(1), 17-20.

6. Chakraborti, Asit K.; Garg, Sanjeev K.; Kumar, Raj; Motiwala, Hashim F.; Jadhavar, Pradeep S. Progress in COX-2 Inhibitors: A Journey So Far. *Current Medicinal Chemistry*, Volume 17, Number 15, May 2010, pp. 1563-1593.
  7. Mohamed MS, Kamel R, Fathallah SS. Synthesis of new pyrroles of potential anti-inflammatory activity. *ARCHIV DER PHARMAZIE*, 344 (12):830-839; DEC 2011
  8. Khalid M. H. Hilmy, Dalia H. Soliman, Esmat B. A. Shahin and Rakia Abd Alhameed. Synthesis and molecular modeling study of novel pyrrole Schiff Bases as anti-HSV-1 agents. *LIFE SCI J*, 2012;9(2):841-850 (ISSN:1097- 8135). <http://www.lifesciencesite.com>
  9. Kumar, I. Organocatalytic Mannich/cyclization/aromatization sequence: direct synthesis of substituted pyrrole-3-carboxaldehydes. *RSC ADVANCES*, 2012, 2 (24):8922-8925
  10. Mohamed MS, SS Fathallah. Pyrroles and Fused Pyrroles: Synthesis and Therapeutic Activities. *MINI-REVIEWS IN ORGANIC CHEMISTRY*, 01/2014; 11.
  11. Mohamed, M. S.; Ali, S. A.; Abdelaziz, D. H. A.; Fathallah, Samar S. Synthesis and Evaluation of Novel Pyrroles and Pyrrolopyrimidines as Anti-Hyperglycemic Agents," *BIOMED RESEARCH INTERNATIONAL*, Article ID 249780, 13 pages, 2014. doi:10.1155/2014/249780
  12. Shattat, G.F., Abuskeika, G.M., Al-Qirim, T.M., Huwaitat, R., El-Huneidi, W., Abu Khalaf, R., Al-Hiari, Y.M., Jasim, S.H., Hamadaneh, L. Novel pyrrole derivatives as potent lipid-lowering agents in Triton-WR-1339-induced hyperlipidemic rats.(2015) *LATIN AMERICAN JOURNAL OF PHARMACY*, 34 (6):1258-1264; 2015.
  13. Sarg, M., Koraa, M., Bayoumi, A. and Gilil, S. (2015) Synthesis of Pyrroles and Condensed Pyrroles as Anti-Inflammatory Agents with Multiple Activities and Their Molecular Docking Study. *Open Journal of Medicinal Chemistry*, 5, 49-96, 2015. doi: 10.4236/ojmc.2015.54005.
  14. Shattat, G.F. Hypotriglyceridemic and hypocholesterolemic effects of novel n-(9,10-dihydro-9,10-dioxoanthracen-1-yl)-1h-pyrrole-2-carboxamides in Triton WR-1339-induced hyperlipidemic rats. *INTERNATIONAL JOURNAL OF BIOLOGY, PHARMACY AND ALLIED SCIENCES*, 4 (12), 2015, 6712-6723. ISSN: 2277-4998
  15. Mir, N.A., Choudhary, S., Ramaraju, P., Singh, D., Kumar, I. Microwave assisted aminocatalyzed [3 + 2] annulation between  $\alpha$ -iminonitriles and succinaldehyde: Synthesis of pyrrole-3-methanols and related polycyclic ring systems (2016) *RSC Advances*, 6 (46), pp. 39741-39749
  16. Zlatanova HI, Vladimirova S P, Kostadinov ID, Delev DP, Kostadinova II. Experimental Evaluation of the Analgesic Activity of 2-(3-Diethylcarbamoyl-2-Methyl-5-Phenyl-Pyrrol-1-Yl)-3-Phenyl-Propionic Acid. *International Journal of Pharmaceutical and Clinical Research* 2016; 8(11): 1483-1488
  17. Fatahala, SS; Hasabelnaby, S; Goudah, A; Mahmoud, GI; Abd-El Hameed, RH. Pyrrole and Fused Pyrrole Compounds with Bioactivity against Inflammatory Mediators. *MOLECULES*, 22 (3):10.3390/molecules22030461 MAR 2017
  18. Fatahala, SS; Khedr, MA; Mohamed, MS. Synthesis and Structure Activity Relationship of Some Indole Derivatives as Potential Anti-inflammatory Agents. *ACTA CHIMICA SLOVENICA*, 64 (4):865-876; 10.17344/acsi.2017.3481 2017. ISSN 1580-3155.
  19. Tzankova, Diana, Lily Peikova, Stanislava Vladimirova, & Maya Georgieva. "Synthesis, druglikeness estimation and prediction of possible pharmacological effects of new pyrrole hydrazones." *Scripta Scientifica Pharmaceutica* [Online], 4.2 (2017): 35-41.
  20. Mahdieh Sharifian Anari, Farahnaz K. Behbahani. Four components synthesis of 1,2,3,4-tetrasubstituted pyrroles using iron (iii) phosphate as a green activator. *Lebanese Science Journal*, Vol. 18, No. 2, 2017, 219-225. <http://dx.doi.org/10.22453/LSJ-018.2.219-225>
  21. Al-Rashdi, AA; Naggar, AH; Farghaly, OAM; Khouda, MM; Shafter, MM. Potentiometric and Conductometric Determination of Metal Complexes of Tenoxicam in Different Dosage Forms. *INTERNATIONAL JOURNAL OF PHARMACEUTICAL AND PHYTOPHARMACOLOGICAL RESEARCH*, 8 (4):13-22; AUG 2018
  22. Vladimirova, S. In vivo Evaluation of the Anti-inflammatory Activity of 2-[3-Acetyl-5-(4-chloro-phenyl)-2-methyl-pyrrol-1-yl]-4-methylsulfanyl-butyric Acid. *Folia medica* Volume 60(2):95-98. February 2018
- 24. Bogdanova S., I. Pajeva, P. Nikolova, I. Tsakovska, B. Müller, Interactions of poly(vinylpyrrolidone) with ibuprofen and naproxen: experimental and modeling studies, *Pharmaceut. Res.* 2005, 22 (5), 806-815.**

Цитирания: 73

1. Laborde, B., Moine-Ledoux, V., Richard, T., Saucier, C., Dubourdieu, D., Monti, J.-P. PVPP-polyphenol complexes: A molecular approach. *JOURNAL OF AGRICULTURAL AND FOOD CHEMISTRY* 54 (12), pp. 4383-4389, 20AMMOS06.
2. Medek, Ales : Solid state NMR spectrometry, In: *Spectroscopy of Pharmaceutical Solids (Drugs and the Pharmaceutical Sciences)* Harry G. Brittain (ed.) Informa Healthcare, 413-558, 2006. (citation p.554)

3. ICA Mbonu. Predicting Intestinal Permeation of Drugs Through Neural Network Analysis Based on Five Molecular Descriptors, Thesis, Faculty of Pharmaceutical Sciences, University of Nigeria, Nsukka, 2006.
4. Teberekidis, V.I., Sigalas, M.P. Theoretical study of hydrogen bond interactions of felodipine with polyvinylpyrrolidone and polyethyleneglycol *Journal of Molecular Structure: THEOCHEM* 803 (1-3), 2007, 29-38.
5. Karavas, E., Georgarakis, E., Sigalas, M.P., Avgoustakis, K., Bikiaris, D. Investigation of the release mechanism of a sparingly water-soluble drug from solid dispersions in hydrophilic carriers based on physical state of drug, particle size distribution and drug-polymer interactions. *EUROPEAN JOURNAL OF PHARMACEUTICS AND BIOPHARMACEUTICS* 66 (3), pp. 334-347, 2007.
6. Gilpin, R. K.; Gilpin, C. S. *Pharmaceuticals and Related Drugs. Analytical Chemistry* (Washington, DC, United States) (2007), 79(12), 4275-4293.
7. Lu XU, San Ming LI, Hisakazu SUNADA: Preparation and Evaluation of Ibuprofen Solid Dispersion Systems with Kollidon Particles using a Pulse Combustion Dryer System, *Chem. Pharm. Bull* (Tokyo), 55 (11), 2007, pp. 1545-1550.
8. Vasconcelos, T., Sarmiento, B., Costa, P. : Solid dispersions as strategy to improve oral bioavailability of poor water soluble drugs *Drug Discovery Today* 12 (23-24), 2007, pp. 1068-1075.
9. Brudy, Jörg . Systematische Rezepturentwicklung für die Walzenkompaktierung Anhand binärer und ternärer Mischungen ausgewählter Komponenten Dissertation : Universität Heidelberg, Fakultät für Biowissenschaften, 2007 URN (NBN) : urn:nbn:de:bsz:16-opus-74844. PhD
10. Lima AAN, Sobrinho JLS, Correa RAC, Rolim Neto, PJ. Alternative Technologies to Improve Solubility of Poorly Water Soluble Drugs. *LATIN AMERICAN JOURNAL OF PHARMACY*, Volume: 27 Issue: 5 Pages: 789-797 Published: SEP-OCT 2008
11. El-Maradny, Hoda A. Preparation and characterization of different binary complexes of carvedilol using freeze-drying technique. *Alexandria Journal of Pharmaceutical Sciences*, 2008, 22(2), 85-93.
12. Lee JH, Ku J, Lee YH, Park JH, Kim DS, Kim W, Il Ahn S, Kim YT, Lee D, Yoo IS, Rhee JM, Lee HK, Khang G: Recent Advances of the Improvement of Bioavailability for Poorly Water Soluble Drugs by Solid Dispersions. *TISSUE ENGINEERING AND REGENERATIVE MEDICINE*, 2009, Volume: 6 Issue: 1-3 Pages: 43-51.
13. Aiping Zhu, Yingnan Pan, Sheng Dai, Fengjuan Li, Jian Shen. Preparation of N-Maleoylchitosan Nanocapsules for Loading and Sustained Release of Felodipine. *Biomacromolecules*, 10(7), 1997-2002, 2009.
14. Ivanov, Ivan T.; Tsokeva, Zhivka. Effect of chirality on PVP/drug interaction within binary physical mixtures of ibuprofen, ketoprofen, and naproxen: A DSC study. *Chirality* (2009), 21(8), 719-727.
15. Gashi Z, Censi R, Malaj L, Gobetto R, Mozzicafreddo M, Angeletti M, Masic A, Di Martino P. Differences in the interaction between aryl propionic acid derivatives and poly (vinylpyrrolidone) K30: A multi-methodological approach. *J Pharm Sci*. Volume 98 Issue 11, Pages 4216 - 4228.
16. Senna, M., Nakayama, S. Preparation and properties of nano-amorphous organic and inorganic particles via chemical and mechanochemical routes. *Journal of Alloys and Compounds* 483 (1-2), pp. 265-270, 2009.
17. Verma, Sudhir; Huey, Bryan D.; Burgess, Diane J. Scanning Probe Microscopy Method for Nanosuspension Stabilizer Selection. *LANGMUIR* 25 (21): 12481-12487 NOV 3 2009.
18. Elgindy, N; Elkhodairy, K; Molokhia, A; Elzoghby, A. Lyophilization monophase solution technique for improvement of the physicochemical properties of an anticancer drug, flutamide. *EUROPEAN JOURNAL OF PHARMACEUTICS AND BIOPHARMACEUTICS* 74 (2): 397-405 FEB 2010.
19. Paudel A., JVan Humbeeck, GV den Mooter. Theoretical and Experimental Investigation on the Solid Solubility and Miscibility of Naproxen in Polyvinylpyrrolidone. *Mol. Pharmaceutics*, DOI: 10.1021/mp100013p. Publication Date (Web): June 4, 2010
20. Patil, J. S.; Kadam, D. V.; Marapur, S. C.; Kamalapur, M. V. Inclusion complex system; a novel technique to improve the solubility and bioavailability of poorly soluble drugs: a review. *INTERNATIONAL JOURNAL OF PHARMACEUTICAL SCIENCES REVIEW AND RESEARCH* (2010), 2(2), 29-34.
21. Malaj, L., Censi, R., Mozzicafreddo, M., Pellegrino, L., Angeletti, M., Gobetto, R., Di Martino, P. Influence of relative humidity on the interaction between different aryl propionic acid derivatives and poly(vinylpyrrolidone) K30: Evaluation of the effect on drug bioavailability. *INTERNATIONAL JOURNAL OF PHARMACEUTICS* 398 (1-2): 61-72, 2010
22. Tajarobi, F; Abrahmsen-Alami, S; Larsson, A. Dissolution Rate Enhancement of Parabens in PEG Solid Dispersions and Its Influence on the Release from Hydrophilic Matrix Tablets. *JOURNAL OF PHARMACEUTICAL SCIENCES* 100 (1): 275-283 JAN 2011
23. Crupi, V; Guella, G; Majolino, D; Mancini, I; Paciaroni, A; Rossi, B; Venuti, V; Verrocchio, P; Viliani, G. Effect of the chiral discrimination on the vibrational properties of (R)-, (S)- and (R, S)-ibuprofen/methyl-beta-cyclodextrin inclusion complexes. *PHILOSOPHICAL MAGAZINE* 91 (13-15): 1776-1785 Sp. Iss. SI 2011.

24. Khan S., H. Batchelor, P. Hanson, Y. Perrie, A. R. Mohammed. Physicochemical characterisation, drug polymer dissolution and *in vitro* evaluation of phenacetin and phenylbutazone solid dispersions with polyethylene glycol 8000. J. PHARM. SCI., 2011. <http://dx.doi.org/10.1002/jps.22613>
25. Fink, J.K. Handbook of Engineering and Specialty Thermoplastics, Water Soluble Polymers, John Wiley & Sons, 2011, pp. 452.
26. Chieng, N; Rades, T; Aaltonen, J. An overview of recent studies on the analysis of pharmaceutical polymorphs. JOURNAL OF PHARMACEUTICAL AND BIOMEDICAL ANALYSIS 55 (4): 618-644 Sp. Iss. SI JUN 25 2011
27. Papadopoulos, AG; Sigalas, MP. Theoretical study of hydrogen bond interactions of fluvastatin with iota-carrageenan and lambda-carrageenan. JOURNAL OF MOLECULAR MODELING 17 (7): 1669-1678 JUL 2011
28. Yu, M., Sun, L., Li, W., Lan, Z., Li, B., Tan, L., Li, M., Yang, X. Investigation of structure and dissolution properties of a solid dispersion of lansoprazole in polyvinylpyrrolidone. JOURNAL OF MOLECULAR STRUCTURE, 1005 (1-3), 2011, pp. 70 – 77.
29. Paudel, A; Van den Mooter, G. Influence of Solvent Composition on the Miscibility and Physical Stability of Naproxen/PVP K 25 Solid Dispersions Prepared by Cosolvent Spray-Drying. PHARMACEUTICAL RESEARCH, 29 (1):251-270, JAN 2012.
30. Reddy, GVR; Vidyadhara, S; Anusha, C. Formulation and Evaluation of Simvastatin Fast Dissolving Tablets with Croscarmellose Sodium as Super Disintegrant. ASIAN JOURNAL OF CHEMISTRY, 24 (3):1082-1086; MAR 2012.
31. Purohit, Nirav S.; Patel, Jayvadan K. Preparation, characterization and dissolution studies of inclusion complexes of Escitalopram oxalate , JOURNAL OF PHARMACY RESEARCH (2012), 5(4), 2259-2263.
32. Niemczyk, A.I., Williams, A.C., Rawlinson-Malone, C.F., Hayes, W., Greenland, B.W., Chappell, D., Khutoryanskaya, O., Timmins, P Novel Polyvinylpyrrolidones To Improve Delivery of Poorly Water-Soluble Drugs: From Design to Synthesis and Evaluation. MOLECULAR PHARMACEUTICS, 2012 9 (8), 2237-2247.
33. V. Vinay Kumar, Kumara Swamy S, Thriveen Ch and Agaiah Goud B. Enhancement of Solubility and Physicochemical Characterization of Paliperidone Solid Dispersions JOURNAL OF ADVANCED PHARMACEUTICAL SCIENCES JAPS, Vol.2/ Issue.2/ 2012, 278-288.
34. Ouyang, DF. Investigating the Molecular Structures of Solid Dispersions by the Simulated Annealing Method, CHEMICAL PHYSICS LETTERS, 554, 177-184; DEC 3 2012.
35. Maver, U; Bele, M; Jamnik, J; Gaberscek, M; Planinsek, O. A fast and simple method for preparation of calcium carbonate-drug composites for fast drug release. MATERIALS RESEARCH BULLETIN, 48 (1):137-145; JAN 2013.
36. S. Paroha, R. Dhar Dubey, S. Mallick. Physicochemical interaction of naproxen with aluminium hydroxide and its effect on dissolution. FARMACIA, 2013, Vol. 61, 1, 103-115.
37. Crupi, V; Fontana, A; Giarola, M; Guella, G; Majolino, D; Mancini, I; Mariotto, G; Paciaroni, A; Rossi, B; Venuti, V. Cyclodextrin-Complexation Effects on the Low-Frequency Vibrational Dynamics of Ibuprofen by Combined Inelastic Light and Neutron Scattering Experiments. JOURNAL OF PHYSICAL CHEMISTRY B, 117 (14):3917-3926; 10.1021/jp400509r APR 11 2013
38. Mallick, S; Pradhan, SK. Characterization of Particle Packing and Drug Release Studies After Solvent Evaporation of Ibuprofen, Avicel, and Aerosil. PARTICULATE SCIENCE AND TECHNOLOGY, 31 (3):301-308; 10.1080/02726351.2012.732678 MAY 1 2013.
39. Oftadeh M., Mahani NM. Polymer drug interactions in thiadiazolylthioacetamide derivatives–linear dendritic copolymer nanoparticles: ONIOM approach. JOURNAL OF PHARMACEUTICAL INVESTIGATION, 43( 4), 2013, 323-331.
40. Crupi, V; Guella, G; Longeville, S; Majolino, D; Mancini, I; Paciaroni, A; Rossi, B; Venuti, V. Influence of Chirality on Vibrational and Relaxational Properties of (S)- and (R,S)-Ibuprofen/methyl- $\beta$ -cyclodextrin Inclusion Complexes: An INS and QENS Study. JOURNAL OF PHYSICAL CHEMISTRY B, 117 (39):11466-11472; 10.1021/jp403099a OCT 3 2013.
41. Kumar, S; Burgess, DJ. Wet milling induced physical and chemical instabilities of naproxen nano-crystalline suspensions. INTERNATIONAL JOURNAL OF PHARMACEUTICS, 466 (1-2):223-232; 10.1016/j.ijpharm.2014.03.021 MAY 15 2014
42. Paroha, S; Dubey, RD; Mallick, S. Interaction of naproxen with calcium carbonate: physicochemical characterization and in vitro drug release studies. QUIMICA NOVA, 37 (1):81-84; 2014
43. Kyeremateng, S. O., Pudlas, M. and Woehrle, G. H. (2014), A Fast and Reliable Empirical Approach for Estimating Solubility of Crystalline Drugs in Polymers for Hot-Melt Extrusion Formulations. JOURNAL OF PHARMACEUTICAL SCIENCES, 103 (9): 2847-2858.

44. Ilic-Stojanovic, SS; Nikolic, VD; Nikolic, LB; Zdravkovic, AS; Kapor, AJ; Popsavin, MM; Petrovic, SD. The improved photostability of naproxen in the inclusion complex with 2-hydroxypropyl-beta-cyclodextrin. *HEMIJSKA INDUSTRIJA*, 69 (4):361-370; JUL-AUG 2015.
45. Chan, SY; Chung, YY; Cheah, XZ; Tan, EYL; Quah, J. The characterization and dissolution performances of spray dried solid dispersion of ketoprofen in hydrophilic carriers, *ASIAN JOURNAL OF PHARMACEUTICAL SCIENCES*, 10 (5):372-385; 10.1016/j.ajps.2015.04.003 OCT 2015.
46. Raimi-Abraham, BT; Mahalingam, S; Davies, PJ; Edirisinghe, M; Craig, DQM. Development and Characterization of Amorphous Nanofiber Drug Dispersions Prepared Using Pressurized Gyration. *MOLECULAR PHARMACEUTICS*, 12 (11):3851-3861; 10.1021/acs.molpharmaceut.5b00127 NOV 2015.
47. Ke P., S. Qi, G. Sadowski, D. Ouyang. Solid Dispersion – a Pragmatic Method to Improve the Bioavailability of Poorly Soluble Drugs. In: *Computational Pharmaceutics: Application of Molecular Modeling in Drug Delivery* (Eds.:Defang Ouyang, Sean C. Smith), Wiley, 2015, 328 pages. ISBN: 1118573978, 9781118573976.
48. Maswadeh, H.M. Incompatibility study of ibuprofen in ternary interactive mixture by using differential scanning calorimetry *JOURNAL OF THERMAL ANALYSIS AND CALORIMETRY*, 123 (3):1963-1971; 10.1007/s10973-015-4773-z MAR 2016.
49. Concu, R; Cordeiro, MNDS. Molecular dynamics simulation study of the selectivity of a silica polymer for ibuprofen(2016) *INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES*, 17 (7):10.3390/ijms17071083 JUL 2016
50. Nadal, JM; Gomes, MLS; Borsato, DM; Almeida, MA; Barboza, FM; Zawadzki, SF; Farago, PV; Zanin, SMW. Spray-dried solid dispersions containing ferulic acid: comparative analysis of three carriers, in vitro dissolution, antioxidant potential and in vivo anti-platelet effect. *DRUG DEVELOPMENT AND INDUSTRIAL PHARMACY*, 42 (11):1813-1824; 10.3109/03639045.2016.1173055 2016
51. Cordeiro, T; Santos, AFM; Nunes, G; Cunha, G; Sotomayor, JC; Fonseca, IM; Danede, F; Dias, CJ; Cardoso, MM; Correia, NT; Viciosa, MT; Dionisio, M. Accessing the Physical State and Molecular Mobility of Naproxen Confined to Nanoporous Silica Matrixes. *The JOURNAL OF PHYSICAL CHEMISTRY C*, 120 (26):14390-14401; 10.1021/acs.jpcc.6b04078 JUL 7 2016
52. Chenevas-Paule, C; Wolff, HM; Ashton, M; Schubert, M; Dodou, K. Development of a Predictive Model for the Stabilizer Concentration Estimation in Microreservoir Transdermal Drug Delivery Systems Using Lipophilic Pressure-Sensitive Adhesives as Matrix/Carrier. *JOURNAL OF PHARMACEUTICAL SCIENCES*, 106 (5):1371-1383; 10.1016/j.xphs.2017.01.031 MAY 2017
53. Liu, X; Zhou, L; Zhang, F. Reactive Melt Extrusion To Improve the Dissolution Performance and Physical Stability of Naproxen Amorphous Solid Dispersions. *MOLECULAR PHARMACEUTICS*, 14 (3):658-673; 10.1021/acsmolpharmaceut.6b00960 MAR 2017
54. Al-Obaidi, H; Majumder, M; Bari, F. Amorphous and Crystalline Particulates: Challenges and Perspectives in Drug Delivery. *CURRENT PHARMACEUTICAL DESIGN*, 23 (3):350-361; 10.2174/1381612822666161107162109 2017
55. Hisham Al-Obaidi. Applications of Particulate Carriers in Drug Delivery: Challenges and Future Perspectives. *Current Pharmaceutical Design* 23(3):339-339, 2017. 10.2174/138161282303170221202749
56. Ziaee, A; Albadarin, AB; Padrela, L; Faucher, A; O'Reilly, E; Walker, G. Spray drying ternary amorphous solid dispersions of ibuprofen – An investigation into critical formulation and processing parameters. *EUROPEAN JOURNAL OF PHARMACEUTICS AND BIOPHARMACEUTICS*, 120 43-51; 10.1016/j.ejpb.2017.08.005 NOV 2017
57. Maswadeh H.. Incompatibility of Paracetamol with Pediatric Suspensions Containing Amoxicillin, Azithromycin and Cefuroxime Axetil. *Pharmacology & Pharmacy* 08 (11): 355-368, 2017
58. Xu Liu, Lin Zhou, Feng Zhang. Reactive Melt Extrusion To Improve the Dissolution Performance and Physical Stability of Naproxen Amorphous Solid Dispersions. *Molecular Pharmaceutics* 14(3), Jan 2017.
59. Maswadeh H. Concomitant oral administration of ibuprofen and some commonly used antibiotics for children: compatibility study using DSC and FTIR. *Acta Poloniae Pharmaceutica - Drug Research*, 74 (6), 1627-1636, 2017.
60. Sandeep Patnaik, Aditya Dileep Kurdekar, Lakshmi Adinarayana Avinash Chunduri, Chinnakoti Prathibha, Kamiseti Venkataramaniah, Naproxen-Gelucire Nanoformulations for Improved Solubility and Dissolution Rate of Poorly Water-Soluble Drug Naproxen, *Journal of Drug Design and Medicinal Chemistry*. Vol. 3, No. 6, 2017, pp. 77-85. doi: 10.11648/j.jddmc.20170306.11
61. Sandeep Patnaik, Aditya D. Kurdekar, L.A. Avinash Chunduri, C. Prathibha, V. Sai Vamsi Krishna, K. Venkataramaniah. Naproxen-Soluplus® Nano formulations for Enhanced Oral Bioavailability. *Int J Pharm* 2017; 7(4): 99-112.
62. Ojarinta, R; Saarinen, J; Strachan, CJ; Korhonen, O; Laitinen, R. Preparation and characterization of multi-component tablets containing co-amorphous salts: Combining multimodal non-linear optical imaging with

- established analytical methods. EUROPEAN JOURNAL OF PHARMACEUTICS AND BIOPHARMACEUTICS, 132 112-126; 10.1016/j.ejpb.2018.09.013 NOV 2018
63. Sandeep Patnaik, Aditya D Kurdekar<sup>2</sup>, LA Avinash Chunduri<sup>1</sup>, C Prathibha<sup>2</sup> and K Venkataramaniah. In Vitro Dissolution Studies on Naproxen-PVP Nanoformulations Show Enhanced Oral Bioavailability of Naproxen. International Journal of Medical Nano Research, 2018, 5 (1), 023. DOI: 10.23937/2378-3664/1410023
  64. Xiang, TX; Anderson, BD. Effects of Molecular Interactions on Miscibility and Mobility of Ibuprofen in Amorphous Solid Dispersions with Various Polymers. JOURNAL OF PHARMACEUTICAL SCIENCES, 108 (1):178-186; 10.1016/j.xphs.2018.10.052 JAN 2019
  65. NM Mahani. Quantum Chemical Study of Interaction of PLGA Polymeric Nanoparticles as Drug Delivery with Anti-Cancer Agents of Thiazoline - Int. J. New. Chem, Article 4, Volume 6, Issue 1, 2019, Page 34-42, 2019. DOI:10.22034/ijnc.2019.33281
  66. Marouene Bejaoui, Galai H., Amara A.B., Rhaïem H.B. Formation of Water Soluble and Stable Amorphous Ternary System: Ibuprofen/ $\beta$ -Cyclodextrin/PVP. *Glass Phys Chem* 45, 580–588 (2019). <https://doi.org/10.1134/S1087659619060130>
  67. Pereva, S., Nikolova, V., Sarafska, T., Angelova, S., Spassov, T., Dudev, T. Inclusion complexes of ibuprofen and  $\beta$ -cyclodextrin: Supramolecular structure and stability. *Journal of Molecular Structure*, Volume 1205, 5 April 2020, Article number 127575
  68. Tramis O., Fujioka A., Imanaka H., Ishida N., Imamura K. Spontaneous foaming during vacuum drying of polyvinylpyrrolidone- and sugar-alcohol mixtures and enhancement of water-dissolution of water insoluble drug. DRYING TECHNOLOGY , Early Access: SEP 2020. DOI: 10.1080/07373937.2020.1822863
  69. Zeng Y., Wang Y., Liang Z., Jiao Z. The study of chiral recognition on ibuprofen enantiomers by a fluorescent probe based on  $\beta$ -cyclodextrin modified ZnS:Mn quantum dots. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, 246, art. no. 119002, 2021.
  70. Ilić-Stojanović, S.; Nikolić, L.; Nikolić, V.; Petrović, S.; Oro, V.; Mitić, Ž.; Najman, S. Semi-Crystalline Copolymer Hydrogels as Smart Drug Carriers: In Vitro Thermo-Responsive Naproxen Release Study. PHARMACEUTICS, Volume: 13, Issue: 2, Article Number: 158, FEB 2021. <https://doi.org/10.3390/pharmaceutics13020158>
  71. Teófilo Vasconcelos, Fabíola Prezotti, Francisca Araújo, Carlos Lopes, Ana Loureiro, Sara Marques, Bruno Sarmento, Third-generation solid dispersion combining Soluplus and poloxamer 407 enhances the oral bioavailability of resveratrol, INTERNATIONAL JOURNAL OF PHARMACEUTICS, Volume 595, 2021, 120245, <https://doi.org/10.1016/j.ijpharm.2021.120245>.
  72. Marouene Bejaoui, Hanan Oueslati, Haykel Galai. Ternary Solid Dispersion Strategy for Solubility Enhancement of Poorly Soluble Drugs by Co-Milling Technique. In book: Chitin and Chitosan - Physicochemical Properties and Industrial Applications [Online First], IntechOpen. pp.1-14, February 2021. <https://doi.org/10.5772/intechopen.95518>.
  73. Shan, X.; Moghul, M.A.; Williams, A.C.; Khutoryanskiy, V.V. Mutual Effects of Hydrogen Bonding and Polymer Hydrophobicity on Ibuprofen Crystal Inhibition in Solid Dispersions with Poly(*N*-vinyl pyrrolidone) and Poly(2-oxazolines). *Pharmaceutics* 2021, 13, 659. <https://doi.org/10.3390/pharmaceutics13050659>

**25. Pajeva, I., C. Globisch, R. Fleischer, I. Tsakovska, M. Wiese. Molecular modeling of P-glycoprotein and related drugs, *Med. Chem. Res.* 2005, 14(2), 106-117.**

Цитирания: 10

1. Schmidt, M., Ungvári, J., Gloede, J., Dobner, B., Langner, A.: New 1,3-dioxolane and 1,3-dioxane derivatives as effective modulators to overcome multidrug resistance *Bioorganic and Medicinal Chemistry* 15 (6), pp. 2283-2297, 2007.
2. Cátia Beatriz Almeida Ramalheite. Search for bioactive compounds from medicinal plants used as antimalarials. PhD thesis, 2010, Repositório da Universidade de Lisboa, <http://hdl.handle.net/10451/2278>
3. Leong MK , Chen H-B , Shih Y-H. Prediction of Promiscuous P-Glycoprotein Inhibition Using a Novel Machine Learning Scheme. PLoS ONE 7(3): e33829. 2012 doi:10.1371/journal.pone.0033829.
4. Halder, AK; Saha, A; Jha, T. The Role of 3D Pharmacophore Mapping Based Virtual Screening for Identification of Novel Anticancer Agents: An Overview. CURRENT TOPICS IN MEDICINAL CHEMISTRY, 13 (9):1098-1126; MAY 2013.
5. Thai, KM; Ngo, TD; Tran, TD; Le, MT. Pharmacophore Modeling for Antitargets. CURRENT TOPICS IN MEDICINAL CHEMISTRY, 13 (9):1002-1014; MAY 2013.
6. Danoo Vitsupakorn. Drug-Drug interactions in the binding pocket of the P-Glycoprotein multidrug transporter, PhD thesis, 2014, The University of Guelph, <http://hdl.handle.net/10214/8398>
7. Воронина Е.И. Молекулярно-клеточные и патоморфологические особенности в злокачественных лимфомах при проявлении опухолевой прогрессии в условиях полихимиотерапии (экспериментально-

клиническое исследование). Diss. Новосибирский Государственный Медицинский Университет, пп128, 2014.

8. Pomilio AB, SM Battista, AA Vitale. Antimicrobial and immunosuppressive activities of cyclopeptides as targets for medicinal chemistry. Chapter 8. In: Chemometrics Applications and Research: QSAR in Medicinal Chemistry, A. G. Mercader, P. R. Duchowicz, P. M. Sivakumar (Eds.) CRC Press, Mar 30, 2016, 253-298.
9. Ngo, T.-D., Tran, T.-D., Le, M.-T., Thai, K.-M. Machine learning-, rule- and pharmacophore-based classification on the inhibition of P-glycoprotein and NorA (2016) SAR AND QSAR IN ENVIRONMENTAL RESEARCH, 27 (9):747-780; 10.1080/1062936X.2016.1233137 2016.
10. Pomilio, AB; Battista, SM; Vitale, AA. ANTIMICROBIAL AND IMMUNOSUPPRESSIVE ACTIVITIES OF CYCLOPEPTIDES AS TARGETS FOR MEDICINAL CHEMISTRY. CHEMOMETRICS APPLICATIONS AND RESEARCH: QSAR IN MEDICINAL CHEMISTRY (Edited by: Mercader AG; Duchowicz PR; Sivakumar PM, 253-298; 2016.

**26. Globisch, C, I.K. Pajeva, M. Wiese, Structure-Activity Relationships of a Series of Tariquidar Analogs as Multidrug Resistance Modulators, *Bioorg. Med. Chem.* 2006, 14(5), 1588-1598.**

Цитирания: 53

1. Tomblin G, Donnelly DJ, Holt JJ, You Y, Ye M, Gannon MK, Nygren CL, Detty MR.: Stimulation of P-glycoprotein ATPase by analogues of tetramethylrosamine: coupling of drug binding at the "R" site to the ATP hydrolysis transition state. *BIOCHEMISTRY*. 2006 Jul 4; 45(26): 8034-8047.
2. Stein, U.; Walther, W.: Reversal of ABC Transporter-Dependent Multidrug Resistance in Cancer: A Realistic Option? *Current Opinion. American Journal of Cancer*. 5(5):285-297, 2006.
3. Labrie P, Maddaford SP, Fortin S, Rakhit S, Kotra LP, Gaudreault RC. A comparative molecular field analysis (CoMFA) and comparative molecular similarity indices analysis (CoMSIA) of anthranilamide derivatives that are multidrug resistance modulators. *J MED CHEM*. 2006 Dec 28; 49(26):7646-60.
4. CHEN Ming-hui, LI Xun, YANG Kang-hui: Latest advancement in designing and evaluation of MDR inhibitors targeting P-glycoprotein. *Journal of International Oncology*, 2006 Vol.33 No.9, p.644-646.
5. Taft, C. A., C. H. T. de Paula da Silva: *Cancer and Aids: New Trends in Drug Design and Chemotherapy Current Computer - Aided Drug Design*, Volume 2, Number 3, September 2006, pp. 307-324.
6. Fortuné, Antoine : *Techniques de Modélisation Moléculaire Appliquées à l'Etude et à l'Optimisation de Molécules Immunogènes et de Modulateurs de la Chimiorésistance*. PhD Thesis (THESE pour obtenir le grade de DOCTEUR DE L'UNIVERSITE JOSEPH FOURIER, Discipline: SCIENCES DU MEDICAMENT), Université Joseph Fourier, Grenoble I, France, Décembre 2006. PhD
7. Schmidt, M., Ungvári, J., Gloede, J., Dobner, B., Langner, A.: New 1,3-dioxolane and 1,3-dioxane derivatives as effective modulators to overcome multidrug resistance *Bioorganic and Medicinal Chemistry* 15 (6), pp. 2283-2297, 2007.
8. Fox, E., Bates, S.: Tariquidar (XR9576): a P-glycoprotein drug efflux pump inhibitor *Expert Review of Anticancer Therapy*; April 2007, Vol. 7, No. 4, Pages 447-459.
9. Lai, Y., Xing, L., Poda, G.I., Hu, Y.: Structure-activity relationships for interaction with multidrug resistance protein 2 (ABCC2/MRP2): The role of torsion angle for a series of biphenyl-substituted heterocycles, *Drug Metabolism and Disposition* 35 (6), pp. 937-945, 2007.
10. Ecker, Gerhard F.; Chiba, Peter. QSAR studies on drug transporters involved in toxicology. *Computational Toxicology*, 295-314, 1 plate, 2007.
11. Ślisz, Magdalena : *Pochodne amfoterycyny B z zawadą przestrzenną – nowa grupa antymykotyków o niskiej toksyczności i aktywnych względem szczepów z opornością wielolekową. Badanie natury i mechanizmów ich właściwości fizykochemicznych i biologicznych*. Politechnical University Gdansk, 2007. PhD <http://www.wbss.pg.gda.pl/preview?from=60&show=phdthesis>
12. Li, X., Li, J.-P., Yuan, H.-Y., Gao, X., Qu, X.-J., Xu, W.-F., Tang, W. Recent advances in P-glycoprotein-mediated multidrug resistance reversal mechanisms. *Methods and Findings in Experimental and Clinical Pharmacology* 29 (9), pp. 607-617, 2008.
13. Nilesh R. Tawari, Seema Bag, Mariam S. Degani. Pharmacophore mapping of a series of pyrrolopyrimidines, indolopyrimidines and their congeners as multidrug-resistance-associated protein (MRP1) modulators. *J MOL MODEL* (2008) 14:911–921.
14. CHEN Hong-xiang, WU Zhi-hong, CHEN Rong-yi, TU Ya-ting, SHUAI Jun, ZHANG Li-xia. Effects of monoclonal antibody against MtrC on ciprofloxacin resistance level of *Neisseria gonorrhoeae*. *Chinese Journal of Dermatology*, 2008 Vol.41 No.2 P.80-83.
15. Patel Y, Gillet VJ, Howe T, Pastor J, Oyarzabal J, Willett P. Assessment of Additive/Nonadditive Effects in Structure-Activity Relationships: Implications for Iterative Drug Design. *JOURNAL OF MEDICINAL CHEMISTRY*, 2008, Vol. 51 (23), 7552-7562.

16. Balaz, S. Modeling Kinetics of Subcellular Disposition of Chemicals. *Chemical Reviews* (Washington, DC, United States) (2009), 109(5), 1793-1899.
17. Nicolle, E., Boumendjel, A., Macalou, S., Genoux, E., Ahmed-Belkacem, A., Carrupt, P.-A., Di Pietro, A. QSAR analysis and molecular modeling of ABCG2-specific inhibitors. *Advanced Drug Delivery Reviews* 61 (1), pp. 34-46, 2009.
18. Ecker, Gerhard F.; Chiba, Peter. QSAR studies on drug transporters involved in toxicology. *Computational Toxicology*, In: *Computational Toxicology: Risk Assessment for Pharmaceutical and Environmental Chemicals*. Sean Ekins (Ed.), Wiley, 2009, 295-314.
19. Wu, JH; Li, X; Cheng, WD; Xie, QJ; Liu, YQ; Zhao, CY. Quantitative Structure Activity Relationship (QSAR) Approach to Multiple Drug Resistance (MDR) Modulators Based on Combined Hybrid System. *QSAR & COMBINATORIAL SCIENCE* 28 (9): 969-978 SEP 2009.
20. Colabufo NA, Berardi F, Cantore M, Contino M, Inglese C, Niso M, Perrone R. Perspectives of P-Glycoprotein Modulating Agents in Oncology and Neurodegenerative Diseases: Pharmaceutical, Biological, and Diagnostic Potentials. *J MED CHEM.*, 53 (5): 1883-1897 MAR 11 2010
21. Ling Zhang, Shutao Ma. Efflux Pump Inhibitors: A Strategy to Combat P-Glycoprotein and the NorA Multidrug Resistance Pump. *ChemMedChem* 2010, 5 (6), 811-822.
22. Praveen M. Bahadduri, James E. Polli, Peter W. Swaan and Sean Ekins. Targeting Drug Transporters – Combining In Silico and In Vitro Approaches to Predict In Vivo. In: *Membrane Transporters in Drug Discovery and Development* (Qing Yan, ed.), *Methods in Molecular Biology*, Vol. 637, Humana Press, 2010, 65-103.
23. Docolomansky, P; Bohacova, V; Barancik, M; Breier, A. Why the xanthine derivatives are used to study of P-glycoprotein-mediated multidrug resistance in L1210/VCR line cells. *GENERAL PHYSIOLOGY AND BIOPHYSICS* 29 (3): 215-221 SEP 2010.
24. Ecker, G. F. QSAR Studies on ABC Transporter – How to Deal with Polyspecificity. In: *Transporters as Drug Carriers: Structure, Function, Substrates*, Vol. 44, (eds G. Ecker and P. Chiba), Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany, 195–214, 2010.
25. Rabal O., M. Urbano-Cuadrado, J. Oyarzabal. Computational medicinal chemistry in fragment-based drug discovery: what, how and when, *FUTURE MEDICINAL CHEMISTRY*, January 2011, Vol. 3, No. 1, Pages 95-134.
26. Gadhe C.G. , T. Madhavan, G. Kothandan, S.J. Cho. In Silico Quantitative Structure-Activity Relationship Studies on P-gp Modulators of Tetrahydroisoquinoline-Ethyl-Phenylamine Series. *BMC STRUCTURAL BIOLOGY* 11: Art. No. 5 JAN 26 2011.
27. Hajos, G; Jemnitz, K; Riedl, Z; Takacs, D; Veres, Z. Heterocyclic Compounds as MDR Modulators. *LETTERS IN DRUG DESIGN & DISCOVERY* 8 (2): 102-113 FEB 2011.
28. Jabeen, I. Combined Ligand- and Structure-based Studies on inhibitors of P-glycoprotein DISSERTATION, Dr.-Studium der Naturwissenschaften, University of Wien, Wien, 2011. othes.univie.ac.at/17980/1/2011-11-15\_0746423.pdf
29. Andreia Palmeira. Design, synthesis and evaluation of xanthone derivatives for dual activity: antitumor and P-glycoprotein inhibition. Thesis presented to the Faculdade de Farmácia, Universidade do Porto, Porto, 2011, pp. 1-402. PhD <https://br.123dok.com/document/z31on7my-design-synthesis-and-evaluation-of-xanthone-derivatives-for-dual-activity-antitumor-and-p-glycoprotein-inhibition.html>
30. Palmeira, A; Sousa, E; Vasconcelos, MH; Pinto, MM. Three Decades of P-gp Inhibitors: Skimming Through Several Generations and Scaffolds. *CURRENT MEDICINAL CHEMISTRY*, 19 (13):1946-2025; MAY 2012
31. Xia, CQ; Smith, PG. Drug Efflux Transporters and Multidrug Resistance in Acute Leukemia: Therapeutic Impact and Novel Approaches to Mediation *MOLECULAR PHARMACOLOGY*, 82 (6):1008-1021; DEC 2012.
32. Zhu Lilan. A Free-Wilson model of antioxidative activities for flavonoids compounds. *ACTA NUTRIMENTA SINICA*, 34 (4):392-394,399; 2012.
33. Devillers, J. Methods for building QSARs. *METHODS IN MOLECULAR BIOLOGY*, 930, 2013, 3-27.
34. Zhang, SL; Wei, YX; Li, Q; Sun, HP; Peng, H; You, QD. Pharmacophore-Based Drug Design and Biological Evaluation of Novel ABCB1 Inhibitors. *CHEMICAL BIOLOGY & DRUG DESIGN*, 81 (3):349-358; 10.1111/cbdd.12081 MAR 2013.
35. Madhavan, T., Gadhe, C., Kothandan, G., Cho, S. Enhancement of P-glycoprotein modulators of arylmethylamine-phenyl derivatives: an integrative modeling approach. *MEDICINAL CHEMISTRY RESEARCH*, 22 (5):2511-2523; 10.1007/s00044-012-0246-0 MAY 2013.
36. Patel NR, BS Pattni, AH Abouzeid, VP Torchilin. Nanopreparations to overcome multidrug resistance in cancer *ADVANCED DRUG DELIVERY REVIEWS*, 65 (13-14):1748-1762; 10.1016/j.addr.2013.08.004 NOV 30 2013.

37. Jara GE, DMA Vera, AB Pierini. Binding of Modulators to Mouse and Human Multidrug Resistance P-glycoprotein. A Computational Study. *JOURNAL OF MOLECULAR GRAPHICS AND MODELLING*, 46, 2013, 10-21.
38. Liu, HM; Ma, ZG; Wu, BJ. Structure-activity relationships and in silico models of P-glycoprotein (ABCB1) inhibitors. *XENOBIOTICA*, 43 (11):1018-1026; 10.3109/00498254.2013.791003 NOV 2013.
39. El-Kattan A., Varma M.V., Lai Y. Transporters in Drug Discovery: In Silico Approaches. In: *Drug Transporters: Molecular Characterization and Role in Drug Disposition, Second Edition*. Edited by Guofeng You, Marilyn E. Morris, Binghe Wang. © 2014 John Wiley & Sons, Inc. Published 2014 by John Wiley & Sons, Inc., 371-388. ISBN: 978-1-118-48993-2
40. Y Tajima, H Nakagawa, A Tamura, O Kadioglu, K Satake, Y Mitani, H Murase, LO Regasini, V da Silva Bolzani, T Ishikawa, G Fricker, T Efferth. Nitensidine A, a guanidine alkaloid from *Pterogyne nitens* is a novel substrate for human ABC transporter ABCB1. *PHYTOMEDICINE*, Oct 2013. <http://dx.doi.org/10.1016/j.phymed.2013.08.024>.
41. Merzendorfer, H. ABC Transporters and Their Role in Protecting Insects from Pesticides and Their Metabolites. *TARGET RECEPTORS IN THE CONTROL OF INSECT PESTS: In: Advances in Insect Physiology*, Editor(s): Cohen E, PT II, 46 1-72, 10.1016/B978-0-12-417010-0.00001-X 2014
42. M.M. Sprachman, AM. Laughney, RH. Kohler, and R Weissleder. In Vivo Imaging of Multidrug Resistance Using a Third Generation MDR1 Inhibitor. *BIOCONJUGATE CHEMISTRY*, 25 (6):1137-1142; 10.1021/bc500154c JUN 2014.
43. Hu Z, Zhou Z, Hu Y, Wu J, Li Y, Huang W (2015) HZ08 Reverse P-Glycoprotein Mediated Multidrug Resistance *In Vitro* and *In Vivo*. *PLOS ONE*, 10 (2):10.1371/journal.pone.0116886 FEB 17 2015
44. Xu-Qin Li, Lin Wang, Yan Lei, Tao Hu, Fei-Long Zhang, Chi-Hin Cho, Kenneth K.W. To, Reversal of P-gp and BCRP-mediated MDR by tariquidar derivatives, *European Journal of Medicinal Chemistry*, Volume 101, 28 August 2015, Pages 560-572, ISSN 0223-5234, <http://dx.doi.org/10.1016/j.ejmech.2015.06.049>
45. Shayanfar, S., Shayanfar, A., Ghandadi, M. Image-Based Analysis to Predict the Activity of Tariquidar Analogs as P-Glycoprotein Inhibitors: The Importance of External Validation. *Archiv der Pharmazie*, 349 (2), pp. 124-131, Feb 2016.
46. Prachayasittikul, V; Worachartcheewan, A; Toropova, AP; Toropov, AA; Schaduangrat, N; Prachayasittikul, V; Nantasenamat, C. Large-scale classification of P-glycoprotein inhibitors using SMILES-based descriptors. *SAR AND QSAR IN ENVIRONMENTAL RESEARCH*, 28 (1):1-16; 10.1080/1062936X.2016.1264468 2017.
47. Varma, MV; Lai, YR; El-Kattan, AF. Molecular properties associated with transporter-mediated drug disposition. *ADVANCED DRUG DELIVERY REVIEWS*, 116 92-99; 10.1016/j.addr.2017.05.014 JUL 1 2017.
48. Hano M, Tomášová L, Šereš M, Pavlíková L, Breier A, Sulová Z. Interplay between P-Glycoprotein Expression and Resistance to Endoplasmic Reticulum Stressors. *MOLECULES*, 23 (2):10.3390/molecules23020337 FEB 2018.
49. Mohammad, IS; He, W; Yin, LF. Understanding of human ATP binding cassette superfamily and novel multidrug resistance modulators to overcome MDR. *BIOMEDICINE & PHARMACOTHERAPY*, 100 335-348; 10.1016/j.biopha.2018.02.038 APR 2018
50. Hinge, V.K., Roy, D. & Kovalenko, A. Prediction of P-glycoprotein inhibitors with machine learning classification models and 3D-RISM-KH theory based solvation energy descriptors. *J Comput Aided Mol Des* (2019) 33: 965. <https://doi.org/10.1007/s10822-019-00253-5>
51. Robinson K and Tiriveedhi V. Perplexing Role of P-Glycoprotein in Tumor Microenvironment. *FRONTIERS IN ONCOLOGY* Volume: 10 Article Number: 265 Published: MAR 5 2020. doi: 10.3389/fonc.2020.00265
52. Tejinder Kaur, Divya Dhawal Bhandari Ray R, Kumar V. A review of BCRP inhibitors: An upcoming strategy for cancer treatment, *Ann Trop Med & Public Health*; 2020, 23(15), 231-550. <http://doi.org/10.36295/ASRO.2020.231550>
53. Yao, T., Wang, B., Ren, B., Qin, X., Li, T. Palladium-catalyzed Ugi-type reaction of 2-iodoanilines with isocyanides and carboxylic acids affording N-acyl anthranilamides. *CHEMICAL COMMUNICATIONS*, 2021, 57, 4247-4250. <https://doi.org/10.1039/D1CC01226F>

**27. Pinto-Bazurko M.M., I. Tsakovska, I. Pajeva. QSAR and 3D QSAR of inhibitors of the epidermal growth factor receptor, *Int. J. Quant. Chem.* 2006, 106 (3), 1432-1444.**

Цитирания: 7

1. Si Yan Liao, Li Qian, Jin Can Chen, Hai Liang Lu, Kang Cheng Zheng, 2D and 3D-QSAR studies on antiproliferative thiazolidine analogs, *INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY*, 108 (8), 1380-1390, 2008.

2. Deeb O, Clare BW. QSAR of aromatic substances: EGFR inhibitory activity of quinazoline analogues. *J Enzyme Inhib Med Chem.* 2008 Dec;23(6):763-75.
3. La Motta, C; Sartini, S; Tuccinardi, T; Nerini, E; Da Settimo, F; Martinelli, A. Computational Studies of Epidermal Growth Factor Receptor: Docking Reliability, Three-Dimensional Quantitative Structure-Activity Relationship Analysis, and Virtual Screening Studies. *JOURNAL OF MEDICINAL CHEMISTRY* 52 (4): 964-975 FEB 26 2009.
4. Liao SY, Qian L, Miao TF, et al. Theoretical Studies on QSAR and Mechanism of 2-Indolinone Derivatives as Tubulin Inhibitors. *INTERNATIONAL JOURNAL OF QUANTUM CHEMISTRY* Volume: 109 Issue: 5 Pages: 999-1008, 2009.
5. Pasha, Farhan Ahmad, Muhammad Muddassar, Anil Kumar Srivastava and Seung Joo Cho: In silico QSAR studies of anilinoquinolines as EGFR inhibitors, *J. MOL. MODEL.* 16 (2): 263-277 FEB 2010.
6. Neaz, MM; Muddassar, M; Pasha, FA; Cho, SJ. Structural studies of B-type Aurora kinase inhibitors using computational methods. *ACTA PHARMACOLOGICA SINICA* 31 (2): 244-258 FEB 2010.
7. Rabal O., M. Urbano-Cuadrado, J. Oyarzabal. Computational medicinal chemistry in fragment-based drug discovery: what, how and when, *FUTURE MEDICINAL CHEMISTRY* 3 (1): 95-134 JAN 2011.

**28. Tsakovska I., I. Pajeva, Phenothiazines and structurally related compounds as modulators of cancer multidrug resistance, c, 7, 1123-1134.**

Цитирања: 19

1. Michalak, K., O.Wesołowska, N.Motohashi, A.B.Hendrich. The Role of the Membrane Actions of Phenothiazines and Flavonoids as Functional Modulators. In: *Topics in Heterocyclic Chemistry, Bioactive Heterocycles II*, (S. Egguchi, Ed.), Volume 8, Springer Berlin / Heidelberg, 2007, 223-302.
2. Garrett, Sarah C.; Hodgson, Louis; Rybin, Andrew; Touchkine, Alexei; Hahn, Klaus M.; Lawrence, David S.; Bresnick, Anne R. A Biosensor of S100A4 Metastasis Factor Activation: Inhibitor Screening and Cellular Activation Dynamics. *Biochemistry* (2008), 47(3), 986-996.
3. Sabatini, Stefano; Kaatz, Glenn W.; Rossolini, Gian Maria; Brandini, David; Fravolini, Arnaldo. From Phenothiazine to 3-Phenyl-1,4-benzothiazine Derivatives as Inhibitors of the *Staphylococcus aureus* NorA Multidrug Efflux Pump. *Journal of Medicinal Chemistry, ACS ASAP*. CODEN: JMCMAR ISSN:0022-2623. AN 2008:779831 CAPLUS
4. Aaron, J.J., M. D. Gaye Seye, S. Trajkovska and N. Motohashi. Bioactive Phenothiazines and Benzo[ a ]phenothiazines: Spectroscopic Studies, and Biological and Biomedical Properties and Applications. In: *Topics in Heterocyclic Chemistry, Volume 15*, Editor: R. R. Gupta, Springer Berlin / Heidelberg, 2008, 253-280.
5. Yde, Christina W.; Clausen, Mathias P.; Bennetzen, Martin V.; Lykkesfeldt, Anne E.; Mouritsen, Ole G.; Guerra, Barbara, The antipsychotic drug chlorpromazine enhances the cytotoxic effect of tamoxifen in tamoxifen-sensitive and tamoxifen-resistant human breast cancer cells. *Anti-Cancer Drugs*, vol. 20 (8), 723-735, 2009.
6. Cieslik-Boczula, K; Szwed, J; Jaszczyszyn, A; Gasiorowski, K; Koll, A Interactions of Dihydrochloride Fluphenazine with DPPC Liposomes: ATR-IR and 31P NMR Studies *J. Phys. Chem. B*, 2009, 113 (47), pp 15495–15502.
7. Ponte-Sucre, A., M. Padron-Nieves, E. Diaz. ABC transporter blockers and reversal of drug resistance in microorganisms. In: *ABC transporters in microorganisms: Research, Innovation and Value as Targets against Drug Resistance*, Horizon Scientific Press, 2009, 177-195. ISBN: 978-1-904455-49-3 <http://saber.ucv.ve/123456789/1737>.
8. Hajos, G; Jemnitz, K; Riedl, Z; Takacs, D; Veres, Z. Heterocyclic Compounds as MDR Modulators. *LETTERS IN DRUG DESIGN & DISCOVERY* 8 (2): 102-113 FEB 2011.
9. Wesołowska, O. Interaction of phenothiazines, stilbenes and flavonoids with multidrug resistance-associated transporters, P-glycoprotein and MRP1, *ACTA BIOCHIMICA POLONICA*, 58 (4):433-448; 2011
10. YX Hu, Y Zhou, FM Wang, WW Zhang. catena-Poly[[[triacuacobalt(II)]- -10-methylphenothiazine-3,7-dicarboxylato] monohydrate]. *ACTA CRYSTALLOGRAPHICA SECTION E: Structure Reports online*, 68, 4, m402-m403, 2012.
11. J. Petrus, R. Petrus, B. Czarnik-Matusiewicz. Fluphenazine dihydrochloride dimethanol solvate. *ACTA CRYST.*, 2012, E68, o1004-o1005. [ doi:10.1107/S1600536812008707 ]
12. Zyta, J; Jaszczyszyn, A; Swiatek, P; Gasiorowski, K; Malinka, W. Synthesis, pro-apoptotic activity and 2D-QSAR studies of new analogues of fluphenazine. *ACTA POLONIAE PHARMACEUTICA*, 71 (1):49-58; JAN-FEB 2014.
13. Martinez, A., Gil, C. Chapter 9: Heterocycles containing nitrogen and sulfur as potent biologically active scaffolds. *PRIVILEGED SCAFFOLDS IN MEDICINAL CHEMISTRY: DESIGN, SYNTHESIS, EVALUATION*, 50 231-261; 2016.

14. de Mello, JC; Moraes, VWR; Watashi, CM; da Silva, DC; Cavalcanti, LP; Franco, MKKD; Yokaichiya, F; de Araujo, DR; Rodrigues, T. Enhancement of chlorpromazine antitumor activity by Pluronic F127/L81 nanostructured system against human multidrug resistant leukemia. *PHARMACOLOGICAL RESEARCH*, 111 102-112; 10.1016/j.phrs.2016.05.032 SEP 2016
15. Andrea Astolfi, Tommaso Felicetti, Nunzio Iraci, Giuseppe Manfroni, Serena Massari, Donatella Pietrella, Oriana Tabarrini, Glenn W. Kaatz, Maria L. Barreca, Stefano Sabatini, and Violetta Cecchetti. Pharmacophore-Based Repositioning of Approved Drugs as Novel Staphylococcus aureus NorA Efflux Pump Inhibitors. *JOURNAL OF MEDICINAL CHEMISTRY*, 60 (4):1598-1604; 10.1021/acs.jmedchem.6b01439 FEB 23 2017
16. Mishra R., Sareen S., Sharma B., Goyal S., Kaur G., Bhardwaj S., Siddiqui A.A., Husain A., Singla R.K., Rashid M., Kumar D., Sati B., Shalmali N., Kumar R. Phenothiazines and related drugs as multi drug resistance reversal agents in cancer chemotherapy mediated by p-glycoprotein. *Current Cancer Therapy Reviews*, 2017, **13** (1), pp.28-42.
17. Hsieh, YH; Chan, HL; Lin, CF; Liang, SHY; Lu, ML; McIntyre, RS; Lee, Y; Lin, TC; Chiu, WC; Chen, VCH. Antipsychotic use is inversely associated with gastric cancer risk: A nationwide population- based nested case- control study. *CANCER MEDICINE*, 8 (9):4484-4496; 10.1002/cam4.2329 AUG 2019
18. Szymanska M., Majerz I. Geometry and electron density of phenothiazines. *JOURNAL OF MOLECULAR STRUCTURE* Volume: 1200 Article Number: UNSP 127095, JAN 15 2020.
19. Luan, YP; Liu, JY; Gao, JJ; Wang, JH. The Design and Synthesis of Novel Phenothiazine Derivatives as Potential Cytotoxic Agents. *LETTERS IN DRUG DESIGN & DISCOVERY*, Volume: 17, Issue: 1, Pages: 57-67, 2020. DOI: 10.2174/1570180816666181115112236

**29. Wiese, M., I. Pajeva. Algorithms to predict affinity for transporters, In: *Virtual ADMET assessment in target selection and maturation*, Solvay Pharmaceuticals Conferences Series (Volume 6), B. Testa, L. Turski (Eds.), IOS Press, Amsterdam, 187-208, 2006.**

Цитирания: 2

1. Balaz, Stefan. Modeling Kinetics of Subcellular Disposition of Chemicals, *Chem Rev.* 2009, 109(5):1793-899.
2. Andrew G. Horti, Hayden T. Ravert, Yongjun Gao, Daniel P. Holt, William H. Bunnelle, Michael R. Schrimpf, Tao Li, Jianguo Ji, Heather Valentine, Ursula Scheffel, Hiroto Kuwabara, Dean F. Wong, Robert F. Dannals, Synthesis and evaluation of new radioligands [11C]A-833834 and [11C]A-752274 for positron-emission tomography of  $\alpha$ 7-nicotinic acetylcholine receptors, *NUCLEAR MEDICINE AND BIOLOGY*, 40 (3), 395-402, 2013.

**30. Tsakovska, I., Lessigiarska, I., Netzeva, T., Pajeva, I., Worth, A. Review of quantitative structure-activity relationships for acute mammalian toxicity. *Int. J. Bioautomation* 2006, 5, pp. 90.**

Цитирания: 1

1. Koleva, Y.K. Mechanistic predicting the acute toxicity of the Michael acceptors for rat Oxidation Communications, 2012, 35 (4), pp. 972-981.

**31. Wiese, M. & Pajeva, I. K. in *Comprehensive Medicinal Chemistry II* Vol. 5 (eds Testa, B. & Van De Waterbeemd, H.), Elsevier Science, New York, 2007, 767-794.**

Цитирания: 2

1. Sugano, K., M. Kansy, P. Artursson, A. Avdeef, S. Bendels, L. Di, G.F. Ecker, B. Faller, H. Fischer, G. Gerebtzoff, H. Lennernaes, F. Senne. Coexistence of passive and carrier-mediated processes in drug transport. *NATURE REVIEWS DRUG DISCOVERY* 9, 597-614 (AUGUST 2010).
2. Reference Module in Chemistry, Molecular Sciences and Chemical Engineering. Copyright © 2013 Elsevier Inc. ISBN: 978-0-12-409547-2

**32. Müller, H., W. Klinkhammer, C. Globisch, M. Kassack, I. Pajeva, M. Wiese. New functional assay of P-glycoprotein activity using Hoechst 33342. *Bioorg. Med. Chem.*, 2007, 15, 7470-7479.**

Цитирания: 27

1. Stanley LA., Horsburgh BC, Ross J, Scheer N, Wolf CR. Drug transporters: Gatekeepers controlling access of xenobiotics to the cellular interior. *Drug Metabolism Reviews* Vol. 41, No.1, 2009, 27-65.
2. Nicolle, E., Boumendjel, A., Macalou, S., Genoux, E., Ahmed-Belkacem, A., Carrupt, P.-A., Di Pietro, A. QSAR analysis and molecular modeling of ABCG2-specific inhibitors. *Advanced Drug Delivery Reviews* 61 (1), pp. 34-46, 2009.
3. Bartosiewicz, D; Krasowska, A. Inhibitors of ABC Transporters and Biophysical Methods to Study their Activity. *ZEITSCHRIFT FUR NATURFORSCHUNG SECTION C-A JOURNAL OF BIOSCIENCES* 64 (5-6): 454-458, 2009.

4. Jack Cook , Bo Feng , Katherine S Fenner , Sarah Kempshall , Ray Liu , Charles Rotter , Dennis A. Smith , Matthew D Troutman , Mohammed Ullah and Caroline Amy Lee. More efficient Drug Discovery: In Vitro Values of [I]/IC50 and [I2]/IC50 Determined for P-Glycoprotein which Allow the Exclusion of Drug Candidates from Clinical Digoxin Interaction Studies. *IVIVC Digoxin Critical Parameters Mol. Pharmaceutics*, 2010, 7 (2), pp. 398-411.
5. Puckett, CA; Ernst, RJ; Barton, JK. Exploring the cellular accumulation of metal complexes. *Dalton Trans.*, 2010, 39, 1159 – 1170.
6. De Souza, M.Q.V., T.V. Barros, E. Torrezan, A.L.M. Cavalcanti, R.C.B.Q. Figueiredo and L.F. Marques-Santos. Characterization of functional activity of ABCB1 and ABCC1 proteins in eggs and embryonic cells of the sea urchin *Echinometra lucunter*, *Bioscience Reports*, 2010, 30, 257–265.
7. Paul A. Lapchak & James M. McKim Jr. CeeTox™ Analysis of CNB-001 a Novel Curcumin-Based Neurotrophic/Neuroprotective Lead Compound to Treat Stroke: Comparison with NXY-059 and Radicut. *TRANSL. STROKE RES.* 2011 Mar;2(1):51-59.
8. Broccatelli, F; Carosati, E; Neri, A; Frosini, M; Goracci, L; Oprea, TI; Cruciani, G. A Novel Approach for Predicting P-Glycoprotein (ABCB1) Inhibition Using Molecular Interaction Fields. *JOURNAL OF MEDICINAL CHEMISTRY* 54 (6): 1740-1751 MAR 24 2011.
9. Christoph Schnabel. Synthese von Jatrophan-Diterpenen. Dissertation. Fakultät Chemie der Technischen Universität Dortmund, 2011, pp. 1-290. <https://eldorado.tu-dortmund.de/handle/2003/27728>
10. Sasaki, H; Kawano, R; Osaki, T; Kamiya, K; Takeuchi, S. Single-vesicle estimation of ATP-binding cassette transporters in microfluidic channels. *LAB ON A CHIP*, 12 (4):702-704; 10.1039/c2lc21058d , 2012.
11. Lapchak, Paul A. CeeTox Analysis to De-risk Drug Development: The Three Antioxidants (NXY-059, Radicut, and STAZN) . In: *Translational Stroke Research* (Editors: Lapchak, Paul A. , Zhang, John H ), Springer US, 639-656, 2012. ISBN: 978-1-4419-9530-8.
12. Tan, W; Cooley, J; Austin, F; Lu, SE; Pruett, SB; Smith, L. Nonclinical Toxicological Evaluation of Occidiofungin, a Unique Glycolipopeptide Antifungal. *INTERNATIONAL JOURNAL OF TOXICOLOGY*, 31 (4):326-336; 10.1177/1091581812445185 JUL-AUG 2012.
13. Changdev G. Gadhe, Seung Joo Cho. Flavonoids: An Emerging Lead in the P-glycoprotein Inhibition. *Journal of the Chosun Natural Science* 01/2012 5(2).
14. Cortes-Ciriano, I; Koutsoukas, A; Abian, O; Glen, RC; Velazquez-Campoy, A; Bender, A. Experimental Validation of In Silico Target Predictions on Synergistic Protein Targets. *MED. CHEM. COMMUN.*, 2012, *MEDCHEMCOMM*, 4 (1), 2013, 278-288.
15. Lemmen, J; Tozakidis, IEP; Galla, HJ. Pregnane X receptor upregulates ABC-transporter Abcg2 and Abcb1 at the blood-brain barrier. *BRAIN RESEARCH*, 1491 1-13; 10.1016/j.brainres.2012.10.060 JAN 23 2013.
16. Lemmen, J; Tozakidis, IEP; Bele, P; Galla, HJ. Constitutive androstane receptor upregulates Abcb1 and Abcg2 at the blood-brain barrier after CITCO activation. *BRAIN RESEARCH*, 1501 68-80; 10.1016/j.brainres.2013.01.025 MAR 21 2013.
17. Lapchak, P. Drug-Like Property Profiling of Novel Neuroprotective Compounds to Treat Acute Ischemic Stroke: Guidelines to Develop Pleiotropic Molecules. *TRANSLATIONAL STROKE RESEARCH*, 4 (3):328-342; 10.1007/s12975-012-0200-y JUN 2013.
18. Lapchak PA, Bombien R, Rajput PS (2013) J-147 a Novel Hydrazide Lead Compound to Treat Neurodegeneration: CeeTox™ Safety and Genotoxicity Analysis. *J NEUROL NEUROPHYSIOL* 4:158. doi: 10.4172/2155-9562.1000158 July 25, 2013.
19. Dalzell, AM; Mistry, P; Wright, J; Williams, FM; Brown, CDA. Characterization of multidrug transporter-mediated efflux of avermectins in human and mouse neuroblastoma cell lines, *TOXICOLOGY LETTERS*, 235 (3):189-198; 10.1016/j.toxlet.2015.04.005 JUN 15 2015.
20. Xu-Qin Li, Lin Wang, Yan Lei, Tao Hu, Fei-Long Zhang, Chi-Hin Cho, Kenneth K.W. To, Reversal of P-gp and BCRP-mediated MDR by tariquidar derivatives, *European Journal of Medicinal Chemistry*, Volume 101, 28 August 2015, Pages 560-572, ISSN 0223-5234, <http://dx.doi.org/10.1016/j.ejmech.2015.06.049>.
21. Cory, TJ; He, H; Winchester, LC; Kumar, S; Fletcher, CV. Alterations in P-Glycoprotein Expression and Function Between Macrophage Subsets al. *PHARMACEUTICAL RESEARCH*, 33 (11):2713-2721; 10.1007/s11095-016-1998-x NOV 2016
22. Zhai, W; Sun, Y; Jiang, M; Wang, M; Gasiewicz, TA; Zheng, J; Chang, C. Differential regulation of LncRNA-SARCC suppresses VHL-mutant RCC cell proliferation yet promotes VHL-normal RCC cell proliferation via modulating androgen receptor/HIF-2 alpha/C-MYC axis under hypoxia. *ONCOGENE*, 35 (37):4866-4880; 10.1038/onc.2016.19 SEP 15 2016

23. Westfall, DA; Krishnamoorthy, G; Wolloscheck, D; Sarkar, R; Zgurskaya, HI; Rybenkov, VV. Bifurcation kinetics of drug uptake by Gram-negative bacteria. PLOS ONE, 12 (9):10.1371/journal.pone.0184671 SEP 19 2017
24. Krishnamoorthy G, Leus IV, Weeks JW, Wolloscheck D, Rybenkov VV, Zgurskaya HI. 2017. Synergy between active efflux and outer membrane diffusion defines rules of antibiotic permeation into Gram-negative bacteria. MBIO, 8 (5):10.1128/mBio.01172-17 SEP-OCT 2017
25. Chin-Chuan Hung, Chien-Yu Chen, Yu-Chieh Wu, Chien-Fu Huang, Yu-Chun Huang, Ying-Chieh Chen, Chih-Shiang Chang, Synthesis and biological evaluation of thiophenylbenzofuran derivatives as potential P-glycoprotein inhibitors EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY Volume: 201, Article Number: 112422 Published: SEP 1 2020, <https://doi.org/10.1016/j.ejmech.2020.112422>. (<http://www.sciencedirect.com/science/article/pii/S0223523420303937>)
26. Joseph, M. M., Ramya, A. N., Vijayan, V. M., Nair, J. B., Bastian, B. T., Pillai, R. K., Therakathinal, S. T., Maiti, K. K., Targeted Theranostic Nano Vehicle Endorsed with Self- Destruction and Immunostimulatory Features to Circumvent Drug Resistance and Wipe- Out Tumor Reinitiating Cancer Stem Cells. SMALL 2020, 2003309. <https://doi.org/10.1002/sml.202003309>
27. Grigoreva T, Sagaidak A, Romanova A, Novikova D, Garabadzhiu A, Tribulovich V. Establishment of drug-resistant cell lines under the treatment with chemicals acting through different mechanisms, *Chemico-Biological Interactions*, 2021, 344, art. no. 109510, <https://doi.org/10.1016/j.cbi.2021.109510>
33. Kacprzyk, Janusz, M. Angelova, P. Vassilev, V. Tasseva, P. Tchesmedjiev, I. Pajeva, K. Atanassov. On the Modelling of Genetic Networks with Generalized Nets, In: “*Issues in intuitionistic fuzzy sets and generalized nets*” (K. Atanassov, J. Kacprzyk, M. Krawczak, E. Szmidi, eds.), Vol. 5, Warsaw school of information technology, Warsaw, 2007, 87-96.

Цитирания: 1

1. Kosev, K., Melo-Pinto, P., Roeva, O. Generalized net model of the lac operon in bacterium E. coli. *6th IEEE International Conference Intelligent Systems, Proceedings*, art. no. 6335224, pp. 237-241, 2012. doi: 10.1109/IS.2012.6335224

34. Globisch, C., I. Pajeva, M. Wiese. Identification of putative binding sites of P-glycoprotein based on its homology model. *ChemMedChem*. 2008, 3(2), 280-295.

Цитирания: 82

1. Loo, Tip W.; Clarke, David M. Mutational analysis of ABC proteins. *Archives of Biochemistry and Biophysics* (2008), 476(1), 51-64.
2. Velamakanni, Saroj; Yao, Yao; Gutmann, Daniel A. P.; van Veen, Hendrik W. Multidrug transport by the ABC transporter Sav1866 from Staphylococcus aureus. *Biochemistry* (2008), 47(35), 9300-9308.
3. Lima SAC, Cordeiro-Da-Silva A, de Castro B, Gameirol, P. Benzodiazepine-mediated structural changes in the multidrug transporter p-glycoprotein: An intrinsic fluorescence quenching analysis JOURNAL OF MEMBRANE BIOLOGY, 2008, Vol. 223 (3), 117-125.
4. Matthias Schmidt, Marlen Teitge, Marianela E. Castillo, Tobias Brandt, Bodo Dobner, Andreas Langner: Synthesis and Biochemical Characterization of New Phenothiazines and Related Drugs as MDR Reversal Agents, ARCHIV DER PHARMAZIE, 2008, Vol. 341 (10), 624-638.
5. Damien Monet. Identification de nouvelles voies d'inhibition ciblant les mouvements fonctionnels de protéines : application à la transition allostérique du récepteur nicotinique de l'acétylcholine. Sorbonne université, dans le cadre de École doctorale Complexité du vivant (Paris), en partenariat avec Institut Pasteur (Paris). Unité Bio-informatique structurale (laboratoire). Dec 2018. PhD <http://www.theses.fr/2018SORUS206>
6. Stockner, T., De Vries, S.J., Bonvin, A.M.J.J., Ecker, G.F., Chiba, P. Data-driven homology modelling of P-glycoprotein in the ATP-bound state indicates flexibility of the transmembrane domains. *FEBS Journal* 276 (4), pp. 964-972, 2009.
7. Martelli C, Alderighi D, Coronello M, Dei S, Frosini M, Le Bozec B, Manetti D, Neri A, Romanelli MN, Salerno M, Scapecchi S, Mini E, Sgaragli G, Teodori E. N,N-bis(Cyclohexanol)amine Aryl Esters: A New Class of Highly Potent Transporter-Dependent Multidrug Resistance Inhibitors. JOURNAL OF MEDICINAL CHEMISTRY, 52, 3, 807-817, FEB 12 2009.
8. Becker, J.-P., Depret, G., Van Bambeke, F., Tulkens, P.M., Prévost, M. Molecular models of human P-glycoprotein in two different catalytic states. *BMC Structural Biology*, Volume:9, no page given., 2009
9. Enquist, K., Fransson, M., Boekel, C., Bengtsson, I., Geiger, K., Lang, L., Pettersson, A., Johansson, S., von Heijne, G., Nilsson, I. Membrane-integration Characteristics of Two ABC Transporters, CFTR and P-glycoprotein. *Journal of Molecular Biology* Volume 387, Issue 5, 17 April 2009, Pages 1153-1164.

10. Baumert, Christiane; Hilgeroth, Andreas Recent advances in the development of P-gp inhibitors. *Anti-Cancer Agents in Medicinal Chemistry* (2009), 9(4), 415-436.
11. Sato, T; Kodan, A; Kimura, Y; Ueda, K; Nakatsu, T; Kato, H. Functional role of the linker region in purified human P-glycoprotein. *FEBS JOURNAL* 276 (13): 3504-3516 JUL 2009.
12. Loo TW, Bartlett MC, Clarke DM. Identification of Residues in the Drug Translocation Pathway of the Human Multidrug Resistance P-glycoprotein by Arginine Mutagenesis. *JOURNAL OF BIOLOGICAL CHEMISTRY* Volume: 284 Issue: 36 Pages: 24074-24087 Published: SEP 4 2009.
13. Demel, MA; Kramer, O; Etmayer, P; Haaksma, EEJ; Ecker, GE. Predicting Ligand Interactions with ABC Transporters in ADME, *CHEMISTRY & BIODIVERSITY* 6 (11): 1960-1969 2009.
14. Crowley, E., C.A. McDevitt, R. Callaghan. Generating Inhibitors of P-Glycoprotein: Where to, Now? In: Multi-Drug Resistance in Cancer (Ed. Jun Zhou), *Methods in Molecular Biology*, Volume 596, Humana Press, 2010, 405-432.
15. Martelli, Cecilia, Marcella Coronello, Silvia Dei, Dina Manetti, Francesca Orlandi, Serena Scapecchi, Maria Novella Romanelli, Milena Salerno, Enrico Mini and Elisabetta Teodori: Structure–Activity Relationships Studies in a Series of *N,N*-Bis(alkanol)amine Aryl Esters as P-Glycoprotein (Pgp) Dependent Multidrug Resistance (MDR) Inhibitors. *J. Med. Chem.*, 2010, 53 (4), pp. 1755–1762.
16. María Fabiana De Rosa. Multidrug Resistance Protein 1 (MDR1) And Glycosphingolipids Biosynthesis: Advantages for Therapeutics, Doctor of Philosophy, Department of Laboratory Medicine and Pathobiology, University of Toronto, 2009. <https://tspace.library.utoronto.ca/handle/1807/19262> PhD
17. Klepsch, F; Jabeen, I; Chiba, P; Ecker, GF. Pharmacoinformatic Approaches to Design Natural Product Type Ligands of ABC-Transporters. *CURRENT PHARMACEUTICAL DESIGN* 16 (15): 1742-1752 MAY 2010.
18. Klepsch, F., G.F. Ecker. Impact of the Recent Mouse P-Glycoprotein Structure for Structure-Based Ligand Design. *MOLECULAR INFORMATICS*, 29, 4, 276–286.
19. Tip W. Loo, M. Claire Bartlett and David M. Clarke. Human P-glycoprotein is active when the two halves are clamped together in the closed conformation. *BIOCHEMICAL AND BIOPHYSICAL RESEARCH COMMUNICATIONS* 395 (3): 436-440 MAY 7 2010.
20. Höcherl, Peter. New tariquidar-like ABCB1 modulators in cancer chemotherapy: Preclinical pharmacokinetic, pharmacodynamic investigations and computational studies. Universität Regensburg, 2010. PhD
21. Mahringer, A., S. Karamustafa, D. Klotz, S. Kahl, V. B. Konkimalla, Y. Wang, J. Wang, Hai-Yang Liu, H. Boechzelt, X. Hao, R. Bauer, G. Fricker, T. Efferth. Inhibition of P-glycoprotein at the Blood–Brain Barrier by Phytochemicals Derived from Traditional Chinese Medicine. *CANCER GENOMICS AND PROTEOMICS* July 1, 2010 vol. 7 no. 4, 191-205.
22. Teodori, E.; Dei, S.; Martelli, C.; Scapecchi, S. *N,N*-bis(cyclohexanol)amine aryl esters: the discovery of a new class of highly potent inhibitors of transporter-dependent multidrug resistance (MDR). *CURRENT TOPICS IN MEDICINAL CHEMISTRY*, 2010, 10(17), 1715-1731.
23. Klepsch, F; Stockner, T; Erker, T; Muller, M; Chiba, P; Ecker, GF. Using structural and mechanistic information to design novel inhibitors/ substrates of P-glycoprotein. *CURRENT TOPICS IN MEDICINAL CHEMISTRY* 10 (17): 1769-1774 DEC 2010
24. Martelli C, Dei S, Lambert C, Manetti D, Orlandi F, Romanelli MN, Scapecchi S, Salerno M, Teodori E. Inhibition of P-glycoprotein-mediated Multidrug Resistance (MDR) by *N,N*-bis(cyclohexanol)amine aryl esters: further restriction of molecular flexibility maintains high potency and efficacy. *BIOORG MED CHEM LETT*. 2011 Jan 1;21(1):106-9.
25. Loo TW., M.C Bartlett, DM Clarke The W232R Suppressor Mutation Promotes Maturation of a Truncation Mutant Lacking Both Nucleotide-Binding Domains and Restores Interdomain Assembly and Activity of P-glycoprotein Processing Mutants. *BIOCHEMISTRY* 50 (5): 672-685 FEB 8 2011.
26. Saponara S, Gorelli B, Tzankova V, Martelli C, Teodori E, Sgaragli G, Fusi F. The novel potent multidrug resistance inhibitors *N,N*-bis(cyclohexanol)amine aryl esters are devoid of vascular effects. *PHARMACOLOGY*. 2011;88(3-4):137-41.
27. Tarcsay, A; Keseru, GM. Homology modeling and binding site assessment of the human P-glycoprotein. *FUTURE MEDICINAL CHEMISTRY* 3 (3): 297-307 MAR 2011.
28. Klepsch F, Chiba P, Ecker GF, 2011 Exhaustive Sampling of Docking Poses Reveals Binding Hypotheses for Propafenone Type Inhibitors of P-Glycoprotein. *PLOS COMPUT BIOL* 7(5): Art. No. e1002036. May 2011.
29. Jabeen, I. Combined Ligand- and Structure-based Studies on inhibitors of P-glycoprotein DISSERTATION, Dr.-Studium der Naturwissenschaften, University of Wien, Wien, 2011. [othes.univie.ac.at/17980/1/2011-11-15\\_0746423.pdf](https://othes.univie.ac.at/17980/1/2011-11-15_0746423.pdf)

30. Andreia Palmeira. Design, synthesis and evaluation of xanthone derivatives for dual activity: antitumor and P-glycoprotein inhibition. Thesis presented to the Faculdade de Farmácia, Universidade do Porto, Porto, 2011, pp. 1-402. PhD <https://br.123dok.com/document/z31on7my-design-synthesis-and-evaluation-of-xanthone-derivatives-for-dual-activity-antitumor-and-p-glycoprotein-inhibition.html>
31. Mitra P., K. Audus, G. Williams, M. Yazdanian, D. Galinis. A comprehensive study demonstrating that p-glycoprotein function is directly affected by changes in pH: Implications for intestinal pH and effects on drug absorption. *J. PHARM. SCI.* 2011, <http://dx.doi.org/10.1002/jps.22596>
32. Mudra DR, Desino KE, Desai PV. In Silico, In Vitro and In Situ Models to Assess Interplay Between CYP3A and P-gp. *CURR DRUG METAB.* 2011 Oct 1;12(8):750-73
33. Eberini, I; Daniele, S; Parravicini, C; Sensi, C; Trincavelli, ML; Martini, C; Abbracchio, MP. In silico identification of new ligands for GPR17: a promising therapeutic target for neurodegenerative diseases. *JOURNAL OF COMPUTER-AIDED MOLECULAR DESIGN* 2011, 25 (8): 743-752.
34. Gyimesi, G; Ramachandran, S; Kota, P; Dokholyan, NV; Sarkadi, B; Hegedus, T. ATP hydrolysis at one of the two sites in ABC transporters initiates transport related conformational transitions, *BIOCHIMICA ET BIOPHYSICA ACTA-BIOMEMBRANES* 2011, 1808 (12): 2954-2964.
35. Stoll F, Göller AH, Hillisch A. Utility of protein structures in overcoming ADMET-related issues of drug-like compounds. *DRUG DISCOV TODAY*, 2011 Jun;16 (11-12):530-8
36. Neri, A; Frosini, M; Valoti, M; Cacace, MG; Teodori, E; Sgaragli, G. N,N-Bis(cyclohexanol)amine aryl esters inhibit P-glycoprotein as transport substrates. *BIOCHEMICAL PHARMACOLOGY* 2011, 82 (12): 1822-1831.
37. Loo, T.W., Bartlett, M.C., Shi, L., Clarke, D.M. Corrector-mediated rescue of misprocessed CFTR mutants can be reduced by the P-glycoprotein drug pump. *BIOCHEMICAL PHARMACOLOGY* 83 (3) , pp. 345-354, 2012.
38. Steglich, B., A Mahringer, Y Li, GH Posner, G Fricker. Inhibition of P-glycoprotein by two artemisinin derivatives. *NATURAL PRODUCTS AND BIOPROSPECTING*, 2012, 2 (2), 59-64
39. Chen L, Li Y, Yu H, Zhang L, Hou T. Computational models for predicting substrates or inhibitors of P-glycoprotein. *DRUG DISCOV TODAY*. 2012 Apr;17(7-8):343-51.
40. Ethan J. Speir. Modeling the human P-glycoprotein translocation mechanism using targeted molecular dynamics. An undergraduate thesis for the degree B.s. Biology with research option.. Georgia Institute of Technology, USA, May 2012. <https://smartech.gatech.edu/handle/1853/43770>
41. D.Jayasimha Rayalu, E.Maruthi Prasad., Elham Poorajabiabarghouei., K.Lakshmidevi. Homology Modeling And Flavonoid Binding Study Of P-Glycoprotein Domain. *INTERNATIONAL JOURNAL OF ADVANCES IN PHARMACY AND BIOLOGICAL SCIENCES (IJAPBS)*. Vol 2 , No. 1, 116-125, 2012. [www.ijapbsonline.org](http://www.ijapbsonline.org)
42. Leong MK , Chen H-B , Shih Y-H (2012) Prediction of Promiscuous P-Glycoprotein Inhibition Using a Novel Machine Learning Scheme. *PLOS ONE*, 7 (3):10.1371/journal.pone.0033829 MAR 16 2012
43. Tamas Hegedus, Gergely Gyimesi, Merse E. Gaspar, Kristof Z. Szalay, Rajeev Gangal, Peter Csermely. Potential application of network descriptions for understanding conformational changes and protonation states of ABC transporters. *QUANTITATIVE BIOLOGY* (2012), 1-34, arXiv:1206.0123v1 [q-bio.MN]<http://arxiv.org/abs/1206.0123v1>
44. Wise J.G. Catalytic Transitions in the Human MDR1 P-Glycoprotein Drug Binding Sites. *BIOCHEMISTRY*, 51 (25):5125-5141; 10.1021/bi300299z JUN 26 2012
45. Gyimesi G, Borsodi D, Sarankó H, Tordai H, Sarkadi B, Hegedüs T. ABCMdb: A database for comparative analysis of protein mutations in ABC transporters, and potential framework for a general application. *HUMAN MUTATION*, 33 (11):1547-1556; 10.1002/humu.22138 NOV 2012.
46. Loo TW, Bartlett MC, Detty MR, Clarke DM. The ATPase Activity of the P-glycoprotein Drug Pump is Highly Activated when the N-Terminal and Central Regions of the Nucleotide-Binding Domains are Linked Closely Together. *J BIOL CHEM.* 2012 Jun 14, *Chemistry*, 287, 26806-26816.
47. Eichhorn, T; Efferth, T. P-glycoprotein and its inhibition in tumors by phytochemicals derived from Chinese herbs. *JOURNAL OF ETHNOPHARMACOLOGY*, 141 (2):557-570; SI 10.1016/j.jep.2011.08.053 JUN 1 2012
48. Corradi, V; Singh, G; Tieleman, DP. The Human Transporter Associated with Antigen Processing molecular models to describe peptide binding competent states. *JOURNAL OF BIOLOGICAL CHEMISTRY*, 287 (33):28099-28111; 10.1074/jbc.M112.381251 AUG 10 2012.
49. Palmeira, A; Sousa, E; Vasconcelos, MH; Pinto, M; Fernandes, MX. Structure and Ligand-based Design of P-glycoprotein Inhibitors: A Historical Perspective. *CURRENT PHARMACEUTICAL DESIGN*, 18 (27):4197-4214; SEP 2012

50. Hulubei, V; Meikrantz, SB; Quincy, DA; Houle, T; McKenna, JI; Rogers, ME; Steiger, S; Natale, NR. 4-Isoxazolyl-1,4-dihydropyridines exhibit binding at the multidrug-resistance transporter, *BIOORGANIC & MEDICINAL CHEMISTRY*, 20 (22): 6613-6620; 10.1016/j.bmc.2012.09.022 NOV 15 2012.
51. F.Orlandi, M. Coronello, C. Bellucci, S. Dei, L. Guandalini, D. Manetti, C. Martelli, M. N. Romanelli, S. Scapecchi, M. Salerno, H. Menif, I. Bello, E. Mini, E. Teodori, New structure-activity relationship studies in a series of N,N-bis(cyclohexanol)amine aryl esters as potent reversers of P-glycoprotein-mediated Multidrug Resistance (MDR), *BIOORGANIC & MEDICINAL CHEMISTRY*, 2013 Jan 15;21(2):456-65.
52. Tarcsay Ákos. Számításos megközelítések a preklinikai. ADMET optimalizálásban. *Tézisfüzet*. Budapesti m\_szaki és gazdaságtudományi egyetem vegyészmérnöki és biomérnöki karoláh györgy doktori iskola. Richter Gedeon Nyrt. Felfedez\_ Kémiai Kutatólaboratórium, 2013.  
[www.omikk.bme.hu/collections/.../tezis\\_hun.pdf](http://www.omikk.bme.hu/collections/.../tezis_hun.pdf)
53. Chang S., Liu F. Molecular Simulations of ATP-Binding Cassette Transporters. *PROGRESS IN CHEMISTRY*, 25(07): 1208-1218, 2013.
54. Loo, TW; Clarke, DM. A Salt Bridge in Intracellular Loop 2 Is Essential for Folding of Human P-Glycoprotein. *BIOCHEMISTRY*, 52 (19):3194-3196; 10.1021/bi4400425k MAY 14 2013.
55. Xu, Y; Shen, Q; Liu, X; Lu, J; Li, S; Luo, C; Gong, L; Luo, X; Zheng, M; Jiang, H. Computational Models for Predicting Interactions with Membrane Transporters. *CURRENT MEDICINAL CHEMISTRY*, 20 (16):2118-2136; MAY 2013.
56. Liu, M; Hou, TJ; Feng, ZW; Li, YY. The flexibility of P-glycoprotein for its poly-specific drug binding from molecular dynamics simulations. *JOURNAL OF BIOMOLECULAR STRUCTURE & DYNAMICS*, 31 (6):612-629; JUN 1 2013.
57. Wen, PC; Verhalen, B; Wilkens, S; Mchaourab, HS; Tajkhorshid, E. On the Origin of Large Flexibility of P-glycoprotein in the Inward-facing State. *JOURNAL OF BIOLOGICAL CHEMISTRY*, 288 (26):19211-19220; 10.1074/jbc.M113.450114 JUN 28 2013.
58. Hegedus, T; Gyimesi, G; Gaspar, ME; Szalay, KZ; Gangal, R; Csermely, P. Potential Application of Network Descriptions for Understanding Conformational Changes and Protonation States of ABC Transporters. *CURRENT PHARMACEUTICAL DESIGN*, 19 (23):4155-4172; JUL 2013.
59. Loo, TW; Bartlett, MC; Clarke, DM. Human P-glycoprotein Contains a Greasy Ball-and-Socket Joint at the Second Transmission Interface. *JOURNAL OF BIOLOGICAL CHEMISTRY*, 288 (28):20326-20333; 10.1074/jbc.M113.484550 JUL 12 2013.
60. Kapoor K., H.M. Sim, S.V. Ambudkar. Multidrug resistance in cancer: a tale of ABC drug transporters. In: *Molecular Mechanisms of Tumor Cell Resistance to Chemotherapy*, Resistance to Targeted Anti-Cancer Therapeutics 1 (B. Bonavida (ed.), Springer Science+Business Media New York, 2013, pp.1-34.
61. Su, LL; Jenardhanan, P; Mruk, DD; Mathur, PP; Cheng, YH; Mok, KW; Bonanomi, M; Silvestrini, B; Cheng, CY. Role of P-Glycoprotein At The Blood-Testis Barrier On Adjudin Distribution In The Testis .A Revisit of Recent Data. *BIOLOGY AND REGULATION OF BLOOD-TISSUE BARRIERS*, 763 318-333; 2013
62. Loo, TW; Clarke, DM. Locking Intracellular Helices 2 and 3 Together Inactivates Human P-glycoprotein. *JOURNAL OF BIOLOGICAL CHEMISTRY*, 289 (1):229-236; 10.1074/jbc.M113.527804 JAN 3 2014.
63. Jara GE, DMA Vera, AB Pierini. Binding of Modulators to Mouse and Human Multidrug Resistance P-glycoprotein. A Computational Study. *JOURNAL OF MOLECULAR GRAPHICS AND MODELLING*, 46, 2013, 10-21.
64. TW Loo, DM Clarke. The Cystic Fibrosis V232D Mutation Inhibits CFTR Maturation by Disrupting a Hydrophobic Pocket Rather than Formation of Aberrant Interhelical Hydrogen Bonds. *BIOCHEMICAL PHARMACOLOGY*, 88 (1):46-57; 10.1016/j.bcp.2013.12.027 MAR 1 2014
65. Szabon-Watola, MI; Ulatowski, SV; George, KM; Hayes, CD; Steiger, SA; Natale, NR. Fluorescent probes of the isoxazole-dihydropyridine scaffold: MDR-1 binding and homology model. *BIOORGANIC & MEDICINAL CHEMISTRY LETTERS*, 24 (1):117-121; 10.1016/j.bmcl.2013.11.068 JAN 1 2014
66. Loo, TW; Clarke, DM. Identification of the Distance between the Homologous Halves of P-glycoprotein That Triggers the High/Low ATPase Activity Switch. *JOURNAL OF BIOLOGICAL CHEMISTRY*, 289 (12):8484-8492; 10.1074/jbc.M114.552075 MAR 21 2014.
67. Emmert, D; Campos, CR; Ward, D; Lu, PH; Namanja, HA; Bohn, K; Miller, DS; Sharom, FJ; Chmielewski, J; Hrycyna, CA. Reversible Dimers of the Atypical Antipsychotic Quetiapine Inhibit P-Glycoprotein-Mediated Efflux in Vitro with Increased Binding Affinity and in Situ at the Blood-Brain Barrier. *ACS CHEMICAL NEUROSCIENCE*, 5 (4):305-317; 10.1021/cn4002329 APR 2014.
68. Jani M, Ambrus C, Magnan R, Jakab KT, Beéry E, Zolnerciks JK, Krajcsi P. Structure and function of BCRP, a broad specificity transporter of xenobiotics and endobiotics. *ARCHIVES OF TOXICOLOGY*, 88 (6):1205-1248; 10.1007/s00204-014-1224-8 JUN 2014.

69. Zeino M., Saeed M.E.M., Kadioglu O., Efferth T. The ability of molecular docking to unravel the controversy and challenges related to P-glycoprotein—a well-known, yet poorly understood drug transporter. *INVESTIGATIONAL NEW DRUGS*, 2014 Apr 22. <http://dx.doi.org/10.1007/s10637-014-0098-1>
70. TW. Loo, DM. Clarke. Cysteines Introduced into Extracellular Loops 1 and 4 of Human P-glycoprotein that are Close Only in the Open Conformation Spontaneously Form a Disulfide Bond that Inhibits Drug Efflux and ATPase Activity. *J. BIOL. CHEM.* 2014, 289 (36), 24749 – 24758.
71. Loo, TW; Clarke, DM. Tariquidar inhibits P-glycoprotein drug efflux but activates ATPase activity by blocking transition to an open conformation, *BIOCHEMICAL PHARMACOLOGY*, 92 (4):558-566; 10.1016/j.bcp.2014.10.006 DEC 15 2014.
72. Erić, S., M. Kalinić. Computational models for predicting drug transport mediated by P-glycoprotein [Računarski modeli za predviđanje transporta lekova posredovanog P-glikoproteinom](2015) *Arhiv za Farmaciju*, 65 (2), pp. 89-114.
73. L Pan, SG Aller. Equilibrated Atomic Models of Outward-Facing P-glycoprotein and Effect of ATP Binding on Structural Dynamics. *Scientific Reports*, Article number: 7880. doi:10.1038/srep07880. Published 20 January 2015
74. Hegedus, C; Telbisz, A; Hegedus, T; Sarkadi, B; Ozvegy-Laczka, C. Lipid Regulation of the ABCB1 and ABCG2 Multidrug Transporters, *ABC TRANSPORTERS AND CANCER*, 125 97-137; 10.1016/bs.acr.2014.10.004 2015
75. Tip W. Loo, David M. Clarke, P-glycoprotein ATPase activity requires lipids to activate a switch at the first transmission interface, *BIOCHEMICAL AND BIOPHYSICAL RESEARCH COMMUNICATIONS*, 472 (2):379-383; 10.1016/j.bbrc.2016.02.124 APR 1 2016.
76. Loo, TW; Clarke, DM. Attachment of a ‘molecular spring’ restores drug-stimulated ATPase activity to P-glycoprotein lacking both Q loop glutamines, *BIOCHEMICAL AND BIOPHYSICAL RESEARCH COMMUNICATIONS*, 483 (1):366-370; 10.1016/j.bbrc.2016.12.137 JAN 29 2017
77. Szollosi D., Chiba P., Szakacs G., Stockner T., Hegedus T. Mechanism of drug transport by ABC multidrug proteins in structural perspectives. *AMINO ACIDS, PEPTIDES AND PROTEINS, VOL 41*, 41 152-187; 10.1039/9781782625377-00152 2017.
78. Miteva, M. A., Villoutreix, B. O. Computational Biology and Chemistry in MTi: Emphasis on the Prediction of Some ADMET Properties. *MOLECULAR INFORMATICS*, 36 (10):SI 10.1002/minf.201700008 OCT 2017
79. Ferreira, R. J., Bonito, C. A., Ferreira, M. J. U. and dos Santos, D. J.V.A. (2017), About P-glycoprotein: a new drugable domain is emerging from structural data. *WILEY INTERDISCIPLINARY REVIEWS-COMPUTATIONAL MOLECULAR SCIENCE*, 7 (5):10.1002/wcms.1316 SEP-OCT 2017.
80. Ricardo J Ferreira. Reversing multidrug resistance (MDR) in cancer cells by targeting P-glycoprotein (P-gp)- Insights into the mechanism of MDR reversal from in silico P-gp modelling. Thesis for PhD, Oct 2017  
PhD
81. RB Gharavi, HE Hassan. Genomics and Drug Transporters and Application in Drug Discovery, Delivery, and Development. In book: *Genomics-Driven Healthcare: Trends in Disease Prevention and Treatment*. Y. Pathak (ed.), Springer Nature Singapore Pte Ltd. 2018, 133-183. DOI: 10.1007/978-981-10-7506-3\_8
82. Monet D., Desdouts N., Nilges M., Blondel A. mkgriDf: Consistent identification of plausible binding sites despite the elusive nature of cavities and grooves in protein dynamics. *JOURNAL OF CHEMICAL INFORMATION AND MODELING*, 59 (8):3506-3518; 10.1021/acs.jcim.9b00103 AUG 2019

**35. Mueller, H., I. Pajeva, C. Globisch, M. Wiese. Functional assay and structure-activity relationships of new 3<sup>rd</sup> generation P-glycoprotein inhibitors. *Bioorg. Med. Chem.* 2008, 16, 2456-2470.**

Цитиранија: 40

1. Nicolle, E., Boumendjel, A., Macalou, S., Genoux, E., Ahmed-Belkacem, A., Carrupt, P.-A., Di Pietro, A. QSAR analysis and molecular modeling of ABCG2-specific inhibitors. *Advanced Drug Delivery Reviews* 61 (1), pp. 34-46, 2009.
2. Seeger, M.A., van Veen, H.W. Molecular basis of multidrug transport by ABC transporters *Biochimica et Biophysica Acta - Proteins and Proteomics* 1794 (5), pp. 725-737, 2009.
3. Dai CL, Liang YJ, Chen LM, Zhang X, Deng WJ, Su XD, Shi Z, Wu CP, Ashby CR Jr, Akiyama SI, Ambudkar SV, Chen ZS, Fu LW. Sensitization of ABCB1 overexpressing cells to chemotherapeutic agents by FG020326 via binding to ABCB1 and inhibiting its function. *BIOCHEM PHARMACOL.* 78 (4): 355-364, 2009.
4. Hammann, F; Gutmann, H; Jecklin, U; Maunz, A; Helma, C; Drewe, J. Development of Decision Tree Models for Substrates, Inhibitors, and Inducers of P-Glycoprotein, *CURRENT DRUG METABOLISM* 10 (4): 339-346 MAY 2009.

5. Balaz, Stefan. Modeling Kinetics of Subcellular Disposition of Chemicals. *Chemical Reviews* (Washington, DC, United States) (2009), 109(5), 1793-1899.
6. Bartosiewicz, D; Krasowska, A. Inhibitors of ABC Transporters and Biophysical Methods to Study their Activity. *ZEITSCHRIFT FUR NATURFORSCHUNG SECTION C-A JOURNAL OF BIOSCIENCES* 64 (5-6): 454-458, 2009.
7. Akamatsu, M; Fujikawa, M; Nakao, K; Shimizu, R. In silico Prediction of Human Oral Absorption Based on QSAR Analyses of PAMPA Permeability. *CHEMISTRY & BIODIVERSITY* 6 (11): 1845-1866 2009.
8. Ecker, G. F. QSAR Studies on ABC Transporter – How to Deal with Polyspecificity. In: *Transporters as Drug Carriers: Structure, Function, Substrates*, Vol. 44, (eds G. Ecker and P. Chiba), Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany, 195–214, 2010.
9. Ghavami G, Kazemali MR, Sardari S. Informatics of drug synergism in naturally occurring anticancer agents. *RECENT PAT ANTICANCER DRUG DISCOV.* 2011 Jan; 6(1):26-44.
10. Velingkar, VS; VD. Dandekar. Microwave-Assisted Synthesis and Evaluation of Substituted Aryl Propyl Acridone-4-Carboxamides as Potential Chemosensitizing Agents for Cancer. *LETTERS IN DRUG DESIGN AND DISCOVERY*, 2011, 8 (3), 2011 , pp. 268-275(8).
11. Gadhe C.G. , T. Madhavan, G. Kothandan, S.J. Cho. In Silico Quantitative Structure-Activity Relationship Studies on P-gp Modulators of Tetrahydroisoquinoline-Ethyl-Phenylamine Series. *BMC STRUCTURAL BIOLOGY* 11: Art. No. 5 JAN 26 2011.
12. Velingkar, V. S., V. D. Dandekar. Design, Synthesis and Evaluation of Substituted *N*-(3-Arylpropyl)-9,10-dihydro-9-oxoacridine-4-carboxamides as Potent MDR Reversal Agents in Cancer. *Chinese JOURNAL OF CHEMISTRY*, 28 MAR 2011, 29 (3), 504-509.
13. Broccatelli, F; Carosati, E; Neri, A; Frosini, M; Goracci, L; Oprea, TI; Cruciani, G. A Novel Approach for Predicting P-Glycoprotein (ABCB1) Inhibition Using Molecular Interaction Fields. *JOURNAL OF MEDICINAL CHEMISTRY* 54 (6): 1740-1751 MAR 24 2011
14. Di Ianni M., Talevi A., Eduardo A., Castro A.E., Bruno-Blanch L.E. Development of a highly specific ensemble of topological models for early identification of P-glycoprotein substrates. *JOURNAL OF CHEMOMETRICS*, 25(6), 313-322, 2011.
15. Puentes, CO; Hoehler, P; Kuhnle, M; Bauer, S; Burger, K; Bernhardt, G; Buschauer, A; Konig, B. Solid phase synthesis of tariquidar-related modulators of ABC transporters preferring breast cancer resistance protein (ABCG2). *BIOORGANIC & MEDICINAL CHEMISTRY LETTERS* 21 (12): 3654-3657 JUN 15 2011
16. Palmeira, A; Rodrigues, F; Sousa, E; Pinto, M; Vasconcelos, MH; Fernandes, MX. New Uses for Old Drugs: Pharmacophore-Based Screening for the Discovery of P-Glycoprotein Inhibitors. *CHEMICAL BIOLOGY & DRUG DESIGN* 78 (1): 57-72, 2011
17. Jabeen, I. Combined Ligand- and Structure-based Studies on inhibitors of P-glycoprotein *DISSERTATION*, Dr.-Studium der Naturwissenschaften, University of Wien, Wien, 2011. [othes.univie.ac.at/17980/1/2011-11-15\\_0746423.pdf](https://othes.univie.ac.at/17980/1/2011-11-15_0746423.pdf) PhD
18. Andreia Palmeira. Design, synthesis and evaluation of xanthone derivatives for dual activity: antitumor and P-glycoprotein inhibition. Thesis presented to the Faculdade de Farmácia, Universidade do Porto, Porto, 2011, pp. 1-402. PhD <https://br.123dok.com/document/z31on7my-design-synthesis-and-evaluation-of-xanthone-derivatives-for-dual-activity-antitumor-and-p-glycoprotein-inhibition.html>
19. Chen L, Li Y, Yu H, Zhang L, Hou T. Computational models for predicting substrates or inhibitors of P-glycoprotein. *DRUG DISCOVERY TODAY*, 17 (7-8):343-351; 10.1016/j.drudis.2011.11.003 APR 2012.
20. Cao, XF; Xu, SZ; Li, XG; Shen, XX; Zhang, QY; Li, JH; Chen, CS. N-Nitrourea Derivatives as Novel Potential Fungicides against *Rhizoctonia solani*: Synthesis, Antifungal Activities, and 3D-QSAR. *CHEMICAL BIOLOGY & DRUG DESIGN*, 80 (1):80-88; 10.1111/j.1747-0285.2012.01346.x JUL 2012
21. Gisela Caceres, Robert W Robey, Lubomir Sokol, Kathy L McGraw, Justine Clark, Nicholas Lawrence. HG-829 Is a Potent Noncompetitive Inhibitor of the ATP-Binding Cassette Multidrug Resistance Transporter ABCB1. *Cancer Research* 72(16):4204-13, July 2012.
22. Palmeira, A; Sousa, E; Vasconcelos, MH; Pinto, M; Fernandes, MX. Structure and Ligand-based Design of P-glycoprotein Inhibitors: A Historical Perspective. *CURRENT PHARMACEUTICAL DESIGN*, 18 (27):4197-4214; SEP 2012
23. Zhu, HR; Liu, ZL; Tang, LS; Liu, JH; Zhou, M; Xie, F; Wang, Z; Wang, YQ; Shen, SD; Hu, LH; Yu, L. Reversal of P-gp and MRP1-mediated multidrug resistance by H6, a gypenoside aglycon from *Gynostemma pentaphyllum*, in vincristine-resistant human oral cancer (KB/VCR) cells. *EUROPEAN JOURNAL OF PHARMACOLOGY*, 696 (1-3):43-53; DEC 5 2012.
24. Changdev G. Gadhe, Seung Joo Cho. Flavonoids: An Emerging Lead in the P-glycoprotein Inhibition. *Journal of the Chosun Natural Science* 01/2012 5(2).

25. Sun YL, Chen JJ, Kumar P, Chen K, Sodani K, Patel A, Chen YL, Chen SD, Jiang WQ, Chen ZS. Reversal of MRP7 (ABCC10)-Mediated Multidrug Resistance by Tariquidar. *PLOS ONE*, 8 (2):10.1371/journal.pone.0055576 FEB 5 2013.
26. Madhavan, T., Gadhe, C., Kothandan, G., Cho, S. Enhancement of P-glycoprotein modulators of arylmethylamine-phenyl derivatives: an integrative modeling approach. *MEDICINAL CHEMISTRY RESEARCH*, 22 (5):2511-2523; 10.1007/s00044-012-0246-0 MAY 2013.
27. Liu, HM; Ma, ZG; Wu, BJ. Structure-activity relationships and in silico models of P-glycoprotein (ABCB1) inhibitors. *XENOBIOTICA*, 43 (11):1018-1026; 10.3109/00498254.2013.791003 NOV 2013
28. Tan W, Mei H, Chao L, Liu T, Pan X, Shu M, Yang L. Combined QSAR and molecule docking studies on predicting P-glycoprotein inhibitors. *JOURNAL OF COMPUTER-AIDED MOLECULAR DESIGN*, 27 (12):1067-1073; 10.1007/s10822-013-9697-8 DEC 2013.
29. Guo, HQ; Zhang, GN; Wang, YJ; Zhang, YK; Sodani, K; Talele, TT; Ashby, CR; Chen, ZS.  $\beta$ -elemene, a compound derived from *Rhizoma zedoariae*, reverses multidrug resistance mediated by the ABCB1 transporter. *ONCOLOGY REPORTS*, 31 (2):858-866; 10.3892/or.2013.2870 FEB 2014.
30. Z Wang, L Yang, Y Xia, C Guo, L Kong. Icarin Enhances Cytotoxicity of Doxorubicin in Human Multidrug-Resistant Osteosarcoma Cells by Inhibition of ABCB1 and Down-Regulation of the PI3K/Akt Pathway. *BIOLOGICAL & PHARMACEUTICAL BULLETIN*, 38 (2):277-284; FEB 2015
31. Xu-Qin Li, Lin Wang, Yan Lei, Tao Hu, Fei-Long Zhang, Chi-Hin Cho, Kenneth K.W. To, Reversal of P-gp and BCRP-mediated MDR by tariquidar derivatives, *European Journal of Medicinal Chemistry*, Volume 101, 28 August 2015, Pages 560-572, ISSN 0223-5234, <http://dx.doi.org/10.1016/j.ejmech.2015.06.049>
32. Zhang, GN; Ashby, CR; Zhang, YK; Chen, ZS; Guo, HQ. The reversal of antineoplastic drug resistance in cancer cells by beta-elemene. *CHINESE JOURNAL OF CANCER*, 34 10.1186/s40880-015-0048-0 SEP 14 2015.
33. Prachayasittikul, V; Worachartcheewan, A; Toropova, AP; Toropov, AA; Schaduangrat, N; Prachayasittikul, V; Nantasenamat, C. Large-scale classification of P-glycoprotein inhibitors using SMILES-based descriptors. *SAR AND QSAR IN ENVIRONMENTAL RESEARCH*, 28 (1):1-16; 10.1080/1062936X.2016.1264468 2017.
34. Qiu, QQ; Liu, BM; Cui, J; Li, Z; Deng, X; Qiang, H; Li, JM; Liao, C; Zhang, B; Shi, W; Pan, MB; Huang, WL; Qian, H. Design, Synthesis, and Pharmacological Characterization of N-(4-(2-(6,7-Dimethoxy-3,4-dihydroisoquinolin-2(1H)yl)ethyl)phenyl)quinazolin-4-amine Derivatives: Novel Inhibitors Reversing P-Glycoprotein-Mediated Multidrug Resistance. *JOURNAL OF MEDICINAL CHEMISTRY*, 60 (8):3289-3302; 10.1021/acs.j.medchem.6b01787 APR 27 2017.
35. Montanari, F; Zdrzil, B. How Open Data Shapes In Silico Transporter Modeling. *MOLECULES*, 22 (3):10.3390/molecules22030422 MAR 2017.
36. Mollazadeh S., Shamsara J., Iman M., Hadizadeh F. Docking and QSAR studies of 1,4-dihydropyridine derivatives as anti-cancer agent. *RECENT PATENTS ON ANTI-CANCER DRUG DISCOVERY*, 12 (2):174-185; 10.2174/1574892812666170126162521 2017.
37. Singla D., Bishnoi R., Dhanda S.K., Asthana S. (2018) Drug Transporters as Therapeutic Targets: Computational Models, Challenges, and Future Perspective. In: Purohit H., Kalia V., More R. (eds) *Soft Computing for Biological Systems*. Springer, Singapore, 2018, pp 143-168. DOI: 10.1007/978-981-10-7455-4\_9
38. Qiu, QQ; Zhu, JL; Chen, QT; Jiang, ZQ; Xu, JT; Jiang, XT; Huang, WL; Liu, ZQ; Ye, J; Xu, XJ. Discovery of aromatic amides with triazole-core as potent reversal agents against P-glycoprotein-mediated multidrug resistance. *BIOORGANIC CHEMISTRY*, 90 SI 10.1016/j.bioorg.2019.103083 SEP 2019.
39. Hinge, V.K., Roy, D. & Kovalenko, A. Prediction of P-glycoprotein inhibitors with machine learning classification models and 3D-RISM-KH theory based solvation energy descriptors. *J Comput Aided Mol Des* (2019) 33: 965. <https://doi.org/10.1007/s10822-019-00253-5>
40. Joshua Silva, Sheraz Khoja, Liana Asatryan, Eunjoo Pacifici, Daryl L. Davies. A novel pharmacotherapy approach using P-glycoprotein (PGP/ABCB1) efflux inhibitor combined with ivermectin to reduce alcohol drinking and preference in mice, *Alcohol*, Volume 86, 2020, Pages 1-8, ISSN 0741-8329. <https://doi.org/10.1016/j.alcohol.2020.03.013>.

**36. Pencheva, T. D. Lagorce, I. Pajeva, B. O. Villoutreix, M.A. Miteva. AMMOS: Automated Molecular Mechanics Optimization tool for in silico Screening, *BMC Bioinformatics* 2008, 9, 438-452.**

Цитирания: 37

1. Skjevik A. A., K. Teigen, A. Martinez, Overview of Computational Methods Employed in Early-Stage Drug Discovery, *FUTURE MEDICINAL CHEMISTRY* 1 (1): 49-63 APR 2009.
2. Brylinski M., J. Skolnick. Q-Dock<sup>LHM</sup>: Low-resolution refinement for ligand comparative modeling. *Journal of Computational Chemistry*, 2010, 31, 5, 1093–11055.

3. Henzler, A.M., Rarey, M. In pursuit of fully flexible protein-ligand docking: modeling the bilateral mechanism of binding 2010, *MOLECULAR INFORMATICS* 29 (3), pp. 164-173.
4. Rolo-Naranjo A, Codorniu-Hernández E, Ferro N. Quantum chemical associations ligand-residue: their role to predict flavonoid binding sites in proteins. *J Chem Inf Model.* 2010 May 24; 50(5):924-33. doi: 10.1021/ci900358z.
5. Brylinski M, Skolnick J. Comprehensive Structural and Functional Characterization of the Human Kinome by Protein Structure Modeling and Ligand Virtual Screening. *JOURNAL OF CHEMICAL INFORMATION AND MODELING* 2010, 50, 10, 1839-1854.
6. O'Boyle N. M., M. Banck, C. A. James, C. Morley, T. Vandermeersch, G. R. Hutchison, Open Babel: An Open Chemical Toolbox, *JOURNAL OF CHEMINFORMATICS*, 3 10.1186/1758-2946-3-33 OCT 7 2011
7. Jäntschi L., Computer Assisted Geometry Optimization for *in silico* Modeling, *APPLIED MEDICAL INFORMATICS*, 2011, 29(3), 11-18.
8. Brylinski, M., Lee, S.Y., Zhou, H., Skolnick, J. The utility of geometrical and chemical restraint information extracted from predicted ligand-binding sites in protein structure refinement. *JOURNAL OF STRUCTURAL BIOLOGY* 2011, 173 (3), pp. 558-569.
9. Henzler, A. M. and Rarey. Protein Flexibility in Structure-Based Virtual Screening: From Models to Algorithms. In: *Virtual Screening: Principles, Challenges, and Practical Guidelines.*(ed C. Sotriffer), Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany, 2011, pp. 223-244. ISBN 978-3-527-32636-5. doi: 10.1002/9783527633326.ch8.
10. Cabrera, AC; Gil-Redondo, R; Perona, A; Gago, F; Morreale, A. VSDMIP 1.5: an automated structure- and ligand-based virtual screening platform with a PyMOL graphical user interface. *JOURNAL OF COMPUTER-AIDED MOLECULAR DESIGN* 2011, 25 (9): 813-824.
11. Jean-Paul Ebejer, Garrett M. Morris, and Charlotte M. Deane. Freely Available Conformer Generation Methods: How Good Are They? *JOURNAL OF CHEMICAL INFORMATION AND MODELING*, 52 (5):1146-1158; 10.1021/ci2004658 MAY 2012
12. S. Prasanth Kumar, Ravi G. Kapopara, Saumya K. Patel, Himanshu A. Pandya and Yogesh T. Jasrai. Conformational Ensemble of Digoxin and Digitoxin and its Interamolecular Energy in Torsional Space. *INTERNATIONAL JOURNAL OF PHARMACY AND BIOLOGICAL SCIENCES* (eISSN: 2230-7605), Volume 2, Issue 2, APRIL-JUNE, 2012, 57-66.
13. Cavasotto C.N. Binding Free Energy Calculation and Scoring in Small Molecule Docking, Chapter 8 In: *PHYSICO-CHEMICAL AND COMPUTATIONAL APPROACHES TO DRUG DISCOVERY* (Eds. Javier Luque, Xavier Barril, David E Thurston, David Rotella, David Fox), Royal Society of Chemistry, 2012, 23, 195-225. 10.1039/9781849735377-00195 2012.
14. Lexa, KW; Carlson, HA. Protein flexibility in docking and surface mapping. *QUARTERLY REVIEWS OF BIOPHYSICS*, 45 (3):301-343; AUG 2012.
15. Heinzerling, L; Klein, R; Rarey, M. Fast force field-based optimization of protein-ligand complexes with graphics processor. *JOURNAL OF COMPUTATIONAL CHEMISTRY*, 33 (32):2554-2565; DEC 15 2012.
16. Brylinski, M. Nonlinear Scoring Functions for Similarity-Based Ligand Docking and Binding Affinity Prediction. *JOURNAL OF CHEMICAL INFORMATION AND MODELING*, 53 (11):3097-3112; 10.1021/ci400510e NOV 2013.
17. F. Pereira de Souza, M.P. Sabbag, G. C. de Araujo, H. L.P. Cravo, T.P.S.Teixeira, D.E. Gomes, V.Fadel, M.A. Fossey. Interaction Model between HRSV G-Protein and Flavonoids. *INT. J. SCIENCES*, 2013, 2 (10), 12-19. <http://www.ijSciences.co>
18. Brylinski M., G. L. Waldrop. Computational Redesign of Bacterial Biotin Carboxylase Inhibitors Using Structure-Based Virtual Screening of Combinatorial Libraries. *MOLECULES*, 19 (4):4021-4045; 10.3390/molecules19044021 APR 2014
19. B. Wang, C. Buchman, L. Li, TD. Hurley, and SO. Meroueh. Enrichment of Chemical Libraries Docked to Protein Conformational Ensembles and Application to Aldehyde Dehydrogenase 2. *JOURNAL OF CHEMICAL INFORMATION AND MODELING*, 54(7), 2105-2116, 2014.
20. Thakur, R; Das, A; Sharma, V; Adhikari, C; Ghosh, KS; Chakraborty, A. Interaction of different prototropic species of an anticancer drug ellipticine with HSA and IgG proteins: multispectroscopic and molecular modeling studies. *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*, 17 (26):16937-16946; 10.1039/c4cp05734a 2015
21. Cozma C. Alina, Bolboacă D. Sorana, Jantschi Lorentz. Geometry optimization in water and vacuum: QPPR modeling on selenazole compounds, *Analele Universității din Oradea, Fascicula Protectia Mediului*, Vol. XXIV, 1-8, 2015.
22. М. М. Фізер, О. І. Фізер, О. Т. Девіняк, М.В. Сливка, В.Г. Лендел. Теоретичне дослідження 1,2,4-тризоліл-1-дитіокарбонної кислоти як аналога диклофенаку [Текст] // Науковий вісник Ужгородського університету : Серія: Хімія / редкол.: С.Ю. Чундак (голова), І.С. Барчій, С.М. Сухарев,

- В.Г. Лендел та ін. – Ужгород : «Видавництво УжНУ «Говерла», 2016. – Вип. 2 (36). – С. 53–56.  
<https://dspace.uzhnu.edu.ua/jspui/handle/lib/13771>
23. Fizer M.M., Fizer O.I., Devinyak O.T., Slivka M.V., Lendel V.G. SYNTHESIS AND THEORETICAL STUDY OF 2-[(5-AMINO-4-PHENYL-1,2,4-TRIAZOL-3-YL)SULFANYL]ACETOHYDRAZIDE AS AN ANALOGUE OF ISONIAZID. *Nauk. visn. Uzhgorod. univ., Ser. Him.*, 2016, № 1 (35), 62-67. УДК 547.792.1 : 547.792.6 : 615.332
  24. Wieder, M; Garon, A; Perricone, U; Boresch, S; Seidel, T; Almerico, AM; Langer, T. Common Hits Approach: Combining Pharmacophore Modeling and Molecular Dynamics Simulations. *JOURNAL OF CHEMICAL INFORMATION AND MODELING*, 57 (2):365-385; 10.1021/acs.jcim.6b00674 FEB 2017
  25. Friedrich, NO; Meyder, A; Kops, CD; Sommer, K; Flachsenberg, F; Rarey, M; Kirchmair, J. High-Quality Dataset of Protein-Bound Ligand Conformations and Its Application to Benchmarking Conformer Ensemble Generators. *JOURNAL OF CHEMICAL INFORMATION AND MODELING*, 57 (3):529-539; 10.1021/acs.jcim.6b00613 MAR 2017.
  26. Surendra Babu M., Santhosh Reddy K., Ghosh K.S., (...), Himasekar C.H., Mustafa S. Design, Synthesis, Single X-Ray Crystal Structure, DFT and Molecular Docking Studies of Novel Clip Type-Pyridyltetrazole Analogues, *Asian Journal of Chemistry*, 30(2), pp. 333-342, 2018.
  27. Garima Tanwar, Rituraj Purohit. Gain of native conformation of Aurora A S155R mutant by small molecules: TANWAR and PUROHIT, *JOURNAL OF CELLULAR BIOCHEMISTRY*, 120 (7):11104-11114; 10.1002/jcb.28387 JUL 2019
  28. Mazanetz, Michael P.; Goode, Charlotte H. F.; Chudyk, Ewa I. Ligand- and Structure-Based Drug Design and Optimization using KNIME. *Current Medicinal Chemistry*, <https://doi.org/10.2174/0929867326666190409141016> да се допълни
  29. Wang, X; Zhu, GH; Liang, WJ; Zhao, SQ; Yuan, B; Zhou, XH; Lu, LY; Xu, H. Design, Synthesis and Docking of Linear and Hairpin-Like Alpha Helix Mimetics Based on Alkoxyated Oligobenzamide. *CHEMISTRYSELECT*, 4 (21):6651-6655; 10.1002/slct.201900171 JUN 7 2019
  30. Sisco, N.J., Helsell, C.V.M. & Van Horn, W.D. Competitive Interactions between PIRT, the Cold Sensing Ion Channel TRPM8, and PIP<sub>2</sub> Suggest a Mechanism for Regulation. *SCIENTIFIC REPORTS*, 9 10.1038/s41598-019-49912-5 OCT 1 2019 doi:10.1038/s41598-019-49912-5
  31. Melanie Schneider. Chémoinformatique intégrative pour guider la conception des médicaments: application à la re-conception d'un inhibiteur clinique de kinase protéinique. *Agricultural sciences. Université Montpellier*, 2019. English. NNT : 2019MONTT057 <https://tel.archives-ouvertes.fr/tel-02485659> PhD
  32. Schneider M., Pons JL, Bourguet W., Labesse G. Towards accurate high-throughput ligand affinity prediction by exploiting structural ensembles, docking metrics and ligand similarity. *Bioinformatics* 36(1), 160-168, 2020. DOI: 10.1093/bioinformatics/btz538
  33. Laijun Song, Chunyu Zhu, Wenxin Zheng, Dan Lu, Hong Jiao, Rongbing Zhao, Zhonglei Bao, Computational systematic selectivity of the Fasalog inhibitors between ROCK-I and ROCK-II kinase isoforms in Alzheimer's disease. *COMPUTATIONAL BIOLOGY AND CHEMISTRY* Volume: 87 Article Number: 107314 Published: AUG 2020. <https://doi.org/10.1016/j.compbiolchem.2020.107314> <http://www.sciencedirect.com/science/article/pii/S1476927120305880>
  34. Kerem Terali, Buket Baddal, Hayrettin Ozan Gülcan. Prioritizing potential ACE2 inhibitors in the COVID-19 pandemic: insights from a molecular mechanics-assisted structure-based virtual screening experiment. *Journal of Molecular Graphics and Modelling*, 2020, 100:107697. <https://doi.org/10.1016/j.jm gm.2020.107697>
  35. Mazanetz, Michael P.; Goode, Charlotte H. F.; Chudyk, Ewa I. Ligand- and Structure-Based Drug Design and Optimization using KNIME. *CURRENT MEDICINAL CHEMISTRY*, Volume: 27, Issue: 38, Pages: 6458-6479, 2020. <https://doi.org/10.2174/0929867326666190409141016> *E-pub Ahead of Print*
  36. Dexian Li, Chunbo Li, Deguang Liu. Analyses of structural dynamics revealed flexible binding mechanism for the *Agrilus mali* odorant binding protein 8 towards plant volatiles. *Pest Management Science*, November 2020. <https://doi.org/10.1002/ps.6184>
  37. Divya Jhinharia, Aman Chandra Kaushik, Shakti Sahi, Chapter 3 - Advances in structure-based drug design, Editor(s): Navneet Sharma, Himanshu Ojha, Pawan Kumar Raghav, Ramesh k. Goyal, *Chemoinformatics and Bioinformatics in the Pharmaceutical Sciences*, Academic Press, 2021, Pages 55-103, ISBN 9780128217481, <https://doi.org/10.1016/B978-0-12-821748-1.00009-9>
- 37. Tsekova, D.S., E. Ts. Makakova, P. S. Alov, G. A. Gorneva, I. K. Pajeva, L. P. Tancheva, V. V. Petkov, A. R. Surleva, B. Escuder, J. F. Miravet, E. Katz. Structure-activity relationships of new L-valine derivatives with neuropharmacological effects. *Bulg. Chem. Commun.* 2009, 41(2), 133-138.**

Цитирания: 2

1. Eryilmaz, G., Ceylan, M. E., Unsalver, B. O., Gogcegoz, I., Ozilhan, S., & Saglam, E., P. 1. g. 074 Plasma concentrations of paroxetine among treatment responder inpatients at week one and before discharge. *EUROPEAN NEUROPSYCHOPHARMACOLOGY*, 23, 2013, S233-S234.
2. Pharande, S.G.; Rentería-Gómez, M.A.; Gámez-Montaño, R. Synthesis of Polyheterocyclic Dimers Containing Restricted and Constrained Peptidomimetics via IMCR-Based Domino/Double CuAAC Click Strategy. *Molecules* 2020, 25, 5246. <https://doi.org/10.3390/molecules25225246>

**38. Fratev, F., S.O. Jonsdottir, E. Mihaylova, I. Pajeva. Molecular basis of inactive B-RAF(WT) and B-RAF(V600E) ligand inhibition, selectivity and conformational stability: an *in silico* study. *Mol. Pharmaceutics* 2009, 6(1), 144-157.**

Цитирания: 15

1. Liu, H., X. Yao. Molecular Basis of the Interaction for an Essential Subunit PA–PB1 in Influenza Virus RNA Polymerase: Insights from Molecular Dynamics Simulation and Free Energy Calculation. *MOL. PHARMACEUTICS*, 7 (1): 75-85 JAN-FEB 2010.
2. Genheden S, Ryde U. How to Obtain Statistically Converged MM/GBSA Results *JOURNAL OF COMPUTATIONAL CHEMISTRY* Volume: 31 Issue: 4 Pages: 837-846 Published: MAR 2010.
3. Li, HF; Chen, YD; Rao, SS; Chen, XM; Liu, HC; Qin, JH; Tang, WF; Yue-Wang; Zhou, X; Lu, T. Recent Advances in the Research and Development of B-Raf Inhibitors. *CURRENT MEDICINAL CHEMISTRY* 17 (16): 1618-1634 JUN 2010.
4. Soderhjelm, P; Kongsted, J; Ryde, U. Ligand Affinities Estimated by Quantum Chemical Calculations. *JOURNAL OF CHEMICAL THEORY AND COMPUTATION* 6 (5): 1726-1737 MAY 2010.
5. Alzate-Morales JH, A. Vergara-Jaque, J. Caballero. Computational Study on the Interaction of N1 Substituted Pyrazole Derivatives with B-Raf Kinase: An Unusual Water Wire Hydrogen-Bond Network and Novel Interactions at the Entrance of the Active Site. *JOURNAL OF CHEMICAL INFORMATION AND MODELING* 50 (6): 1101-1112 JUN 2010.
6. Yang, Y; Qin, J; Liu, HX; Yao, XJ. Molecular Dynamics Simulation, Free Energy Calculation and Structure-Based 3D-QSAR Studies of B-RAF Kinase Inhibitors. *JOURNAL OF CHEMICAL INFORMATION AND MODELING* 51 (3): 680-692, MAR 2011
7. Caballero J, Alzate-Morales JH, Vergara-Jaque A. Investigation of the Differences in Activity between Hydroxycycloalkyl N1 Substituted Pyrazole Derivatives As Inhibitors of B-Raf Kinase by Using Docking, Molecular Dynamics, QM/MM, and Fragment-Based De Novo Design: Study of Binding Mode of Diastereomer Compounds. *J CHEM INF MODEL*. 2011 Nov 28;51(11):2920-31
8. Yani, YN; Chow, PS; Tan, RBH. Molecular Simulation Study of the Effect of Various Additives on Salbutamol Sulfate Crystal Habit. *MOLECULAR PHARMACEUTICS* Volume: 8 Issue: 5 Pages: 1910-1918, SEP-OCT 2011.
9. Xue W, Liu H, Yao X. Molecular mechanism of HIV-1 integrase-vDNA interactions and strand transfer inhibitor action: A molecular modeling perspective. *J COMPUT CHEM*. 2012 Feb 15;33(5):527-36.
10. Reva, B. Revealing selection in cancer using the predicted functional impact of cancer mutations. Application to nomination of cancer drivers. *BMC GENOMICS*, 14 (3): S8 doi: 10.1186/1471-2164-14-S3-S8 MAY 28 2013.
11. Li, Y; Han, CX; Wang, JH; Yang, YF; Zhang, JX; Zhang, SW; Yang, L Insight into the Structural Features of Pyrazolopyrimidine- and Pyrazolopyridine-based B-RafV600E Kinase Inhibitors by Computational Explorations. *CHEMICAL BIOLOGY & DRUG DESIGN*, 83 (6):643-655; 10.1111/cbdd.12276 JUN 2014
12. Marino, KA; Sutto, L; Gervasio, FL. The Effect of a Widespread Cancer-Causing Mutation on the Inactive to Active Dynamics of the B-Raf Kinase. *JOURNAL OF THE AMERICAN CHEMICAL SOCIETY*, 137 (16):5280-5283; 10.1021/jacs.5b01421 APR 29 2015.
13. Shallal, H. M., & Russu, W. A. (2017). Understanding the Molecular Basis of Tyrosine Kinase Intrinsic Promiscuity Toward Binding Type-I and Type-II Kinase Inhibitors. KIT versus INSR as a Case Study. *IJRDO Journal of Biological Science (ISSN: 2455-7676)*, 3(11), 01-25. Retrieved from <http://www.ijrdo.org/index.php/bs/article/view/1644>
14. Jordan, EJ; Patil, K; Suresh, K; Park, JH; Mosse, YP; Lemmon, MA; Radhakrishnan, R. Computational algorithms for in silico profiling of activating mutations in cancer, *CELLULAR AND MOLECULAR LIFE SCIENCES*, 76 (14):2663-2679; 10.1007/s00018-019-03097-2 JUL 2019
15. Keshav Patil, Earl Joseph Jordan, Jin H. Park, Krishna Suresh, Courtney M. Smith, Abigail A. Lemmon, Yaël P. Mossé, Mark A. Lemmon, Ravi Radhakrishnan. Computational studies of anaplastic lymphoma kinase mutations reveal common mechanisms of oncogenic activation. *PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA*, Volume 118, Issue: 10, Article Number: e2019132118, Published: MAR 9 2021. DOI: 10.1073/pnas.2019132118

39. Klinkhammer, W., H. Müller, C. Globisch, I.K. Pajeva, M. Wiese. Synthesis and biological evaluation of a small molecule library of 3rd generation multidrug resistance modulators, *Bioorg. Med. Chem.* 2009, 17, 2524–2535.

Цитирания: 33

1. Neuhaus, W; Stessl, M; Strizsik, E; Bennani-Baiti, B; Wirth, M; Toegel, S; Modha, M; Winkler, J; Gabor, F; Viernstein, H; Noe, CR. Blood-brain barrier cell line PBMEC/C1-2 possesses functionally active P-glycoprotein. *NEUROSCIENCE LETTERS* 469 (2): 224-228 JAN 22 2010.
2. Ling Zhang, Shutao Ma. Efflux Pump Inhibitors: A Strategy to Combat P-Glycoprotein and the NorA Multidrug Resistance Pump. *ChemMedChem* 2010, 5 (6), 811-822.
3. Dolle, Roland E.; Le Bourdonnec, Bertrand; Worm, Karin; Morales, Guillermo A.; Thomas, Craig J.; Zhang, Wei. Comprehensive Survey of Chemical Libraries for Drug Discovery and Chemical Biology: 2009. *JOURNAL OF COMBINATORIAL CHEMISTRY* 12 (6): 765-806 NOV-DEC 2010.
4. Gadhe C.G. , T. Madhavan, G. Kothandan, S.J. Cho. In Silico Quantitative Structure-Activity Relationship Studies on P-gp Modulators of Tetrahydroisoquinoline-Ethyl-Phenylamine Series. *BMC STRUCTURAL BIOLOGY* 11: Art. No. 5 JAN 26 2011.
5. Hajos, G; Jemnitz, K; Riedl, Z; Takacs, D; Veres, Z. Heterocyclic Compounds as MDR Modulators. *LETTERS IN DRUG DESIGN & DISCOVERY* 8 (2): 102-113 FEB 2011.
6. Zheng, MQ; Yang, YF; Zhao, M; Zhang, XY; Wu, JH; Chen, G; Peng, L; Wang, YJ; Peng, SQ. A Class of Novel *N*-Isoquinoline-3-carbonyl-L-amino Acid Benzylesters: Synthesis, Anti-tumor Evaluation and 3D QSAR Analysis. *EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY* 46 (5): 1672-1681, MAY 2011
7. Puentes, CO; Hoherl, P; Kuhnle, M; Bauer, S; Burger, K; Bernhardt, G; Buschauer, A; König, B. Solid phase synthesis of tariquidar-related modulators of ABC transporters preferring breast cancer resistance protein (ABCG2). *BIOORGANIC & MEDICINAL CHEMISTRY LETTERS* 21 (12): 3654-3657, JUN 15 2011
8. Zhao, QY; Li, J; Yan, XJ; Yuan, HZ; Qin, ZH; Fu, B. Synthesis and Fungicidal Activity of 1,3-Thiazoline Derivatives Bearing Nitrophenyl Group on the 2-Position. *JOURNAL OF HETEROCYCLIC CHEMISTRY* 48 (3): 729-732 MAY 2011
9. Zou, Z., Xiao-bu Lan, Hai Qian, Wen-long Huang, Yun-man Li, Synthesis and evaluation of furoxan-based nitric oxide-releasing derivatives of tetrahydroisoquinoline as anticancer and multidrug resistance reversal agents, *Bioorganic & Medicinal Chemistry Letters*, 2011, *BIOORGANIC & MEDICINAL CHEMISTRY LETTERS*, 21 (19), 5934-5938.
10. Jabeen, I. Combined Ligand- and Structure-based Studies on inhibitors of P-glycoprotein DISSERTATION, Dr.-Studium der Naturwissenschaften, University of Wien, Wien, 2011. [othes.univie.ac.at/17980/1/2011-11-15\\_0746423.pdf](https://othes.univie.ac.at/17980/1/2011-11-15_0746423.pdf) PhD
11. Melchior, DL; Sharom, FJ; Evers, R; Wright, GE; Chu, JW; Wright, SE; Chu, XY; Yabut, J. Determining P-glycoprotein-drug interactions: evaluation of reconstituted P-glycoprotein in a liposomal system and LLC-MDR1 polarized cell monolayers. *JOURNAL OF PHARMACOLOGICAL AND TOXICOLOGICAL METHODS*, 65 (2):64-74; 10.1016/j.vascn.2012.02.002 MAR-APR 2012.
12. Sun, Y.-L., Patel, A., Kumar, P., Chen, Z.-S. Role of ABC transporters in cancer chemotherapy *CHINESE JOURNAL OF CANCER* 31 (2) , pp. 51-57, 2012.
13. Abigail M Dalzell. The importance of efflux transporters in CNS exposure to avermectin insecticides: studies in human and mouse neuroblastoma cell lines. Epithelial Research Group Institute for Cell & Molecular Bioscience, Medical School Newcastle University, NE2 4HH UK, 2012 PhD
14. Lan, XB; Lin, HY; Tang, CL; Zhu, XY; Qian, H; Huang, WL; Li, YM. Evaluation of In-Vitro Multidrug Resistance Reversal Activities of HZ08 analogues with Improved Soluble Property. *LETTERS IN DRUG DESIGN & DISCOVERY*, 10 (1):56-60; JAN 2013.
15. Sun YL, Chen JJ, Kumar P, Chen K, Sodani K, Patel A, Chen YL, Chen SD, Jiang WQ, Chen ZS. Reversal of MRP7 (ABCC10)-Mediated Multidrug Resistance by Tariquidar. *PLOS ONE*, 8 (2):10.1371/journal.pone.0055576 FEB 5 2013.
16. Liu, BM; Qiu, QQ; Zhao, TX; Jiao, L; Hou, JY; Li, YM; Qian, H; Huang, WL. Discovery of Novel P-Glycoprotein-Mediated Multidrug Resistance Inhibitors Bearing Triazole Core via Click Chemistry. *CHEMICAL BIOLOGY & DRUG DESIGN*, 84 (2):182-191; 10.1111/cbdd.12301 AUG 2014
17. Kathawala, RJ; Wang, YJ; Ashby, CR; Chen, ZS. Recent advances regarding the role of ABC subfamily C member 10 (ABCC10) in the efflux of antitumor drugs. *CHINESE JOURNAL OF CANCER*, 33 (5):223-230; 10.5732/cjc.013.10122 MAY 2014
18. Kumar, R; Bahia, MS; Silakari, O. Synthesis, cytotoxic activity, and computational analysis of N10-substituted acridone analogs. *MEDICINAL CHEMISTRY RESEARCH, MEDICINAL CHEMISTRY RESEARCH*, 24 (3):921-933; 10.1007/s00044-014-1156-0 MAR 2015
19. De Ravel MR, Alameh G, Melikian M, Mahiout Z, Emptoz-Bonneton A, Matera EL, Lomberget T, Barret R, Rocheblave L, Walchshofer N, Beltran S, El Jawad L, Mappus E, Grenot C, Pugeat M, Dumontet C, Le

- Borgne M, Cuilleron CY. Synthesis of new steroidal inhibitors of P-glycoprotein-mediated multidrug resistance and biological evaluation on K562/R7 erythroleukemia cells. *JOURNAL OF MEDICINAL CHEMISTRY*, 58 (4):1832-1845; 10.1021/jm0501676v FEB 26 2015
20. Karthikeyan, S; Hoti, SL. Development of Fourth Generation ABC Inhibitors from Natural Products: A Novel Approach to Overcome Cancer Multidrug Resistance. *ANTI-CANCER AGENTS IN MEDICINAL CHEMISTRY*, 15 (5):605-615; 2015
  21. Xu-Qin Li, Lin Wang, Yan Lei, Tao Hu, Fei-Long Zhang, Chi-Hin Cho, Kenneth K.W. To, Reversal of P-gp and BCRP-mediated MDR by tariquidar derivatives, *European Journal of Medicinal Chemistry*, Volume 101, 28 August 2015, Pages 560-572, ISSN 0223-5234, <http://dx.doi.org/10.1016/j.ejmech.2015.06.049>
  22. Fardel, O., Le Vee, M., Jouan, E., Denizot, C., Parmentier, Y. Nature and uses of fluorescent dyes for drug transporter studies(2015) *EXPERT OPINION ON DRUG METABOLISM & TOXICOLOGY*, 11 (8):1233-1251; 10.1517/17425255.2015.1053462 AUG 2015
  23. Gao, F; Liu, HQ; Li, L; Guo, JP; Wang, YJ; Zhao, M; Peng, SQ. Design, synthesis, and testing of an isoquinoline-3-carboxylic-based novel anti-tumor lead. *BIOORGANIC & MEDICINAL CHEMISTRY LETTERS*, 25 (20):4434-4436; 10.1016/j.bmcl.2015.09.014 OCT 15 2015
  24. Spengler G, Ocsovszki I, Tönki ÁS, Saijo R, Watanabe G, Kawase M, Molnár J. Fluorinated  $\beta$ -Diketo Phosphorus Ylides Are Novel Inhibitors of the ABCB1 Efflux Pump of Cancer Cells. *ANTICANCER RESEARCH*, 35 (11):5915-5919; NOV 2015
  25. Shayanfar, S., Shayanfar, A., Ghandadi, M. Image-Based Analysis to Predict the Activity of Tariquidar Analogs as P-Glycoprotein Inhibitors: The Importance of External Validation. *Archiv der Pharmazie*, 349 (2), pp. 124-131, Feb 2016.
  26. Benmansour, F; Trist, I; Coutard, B; Decroly, E; Querat, G; Brancale, A; Barral, K. Discovery of novel dengue virus NS5 methyltransferase non-nucleoside inhibitors by fragment-based drug design, *EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY*, 125 865-880; 10.1016/j.ejmech.2016.10.007 JAN 5 2017.
  27. Qiu, QQ; Liu, BM; Cui, J; Li, Z; Deng, X; Qiang, H; Li, JM; Liao, C; Zhang, B; Shi, W; Pan, MB; Huang, WL; Qian, H. Design, Synthesis, and Pharmacological Characterization of N-(4-(2-(6,7-Dimethoxy-3,4-dihydroisoquinolin-2(1H)yl)ethyl)phenyl)quinazolin-4-amine Derivatives: Novel Inhibitors Reversing P-Glycoprotein-Mediated Multidrug Resistance. *JOURNAL OF MEDICINAL CHEMISTRY*, 60 (8):3289-3302; 10.1021/acs.j.medchem.6b01787 APR 27 2017.
  28. E. Teodori, S. Dei, G. Bartolucci, M. G. Perrone, D. Manetti, M. N. Romanelli, M. Contino, N. A. Colabufo. Structure- Activity Relationship Studies on 6, 7- Dimethoxy- 2- phenethyl- 1, 2, 3, 4-tetrahydroisoquinoline Derivatives as Multidrug Resistance (MDR) reversers. *CHEMMEDCHEM*, 12 (16):1369-1379; 10.1002/cmcd.201700239 AUG 22 2017.
  29. Mologni, L; Via, MD; Chilin, A; Palumbo, M; Marzaro, G. Discovery of (RET)-R-wt and (RET)-R-V804M Inhibitors: From Hit to Lead. *CHEMMEDCHEM*, 12 (16):1390-1398; SI 10.1002/cmcd.201700243 AUG 22 2017.
  30. Ghaleb, H; Li, HL; Kairuki, M; Qiu, QQ; Bi, XZ; Liu, CX; Liao, C; Li, JM; Hezam, K; Huang, WL; Qian, H. Design, synthesis and evaluation of a novel series of inhibitors reversing P-glycoprotein-mediated multidrug resistance. *CHEMICAL BIOLOGY & DRUG DESIGN*, 92 (3):1708-1716; 10.1111/cbdd.13338 SEP 2018
  31. Spengler, G; Kincses, A; Racz, B; Varga, B; Watanabe, G; Saijo, R; Sekiya, H; Tamai, E; Maki, J; Molnar, J; Kawase, M. Benzoxazole-based Zn(II) and Cu(II) Complexes Overcome Multidrug-resistance in Cancer. *ANTICANCER RESEARCH*, 38 (11):6181-6187; 10.21873/anticancer.12971 NOV 2018
  32. Ahmed R. Hamed, Nahla S. Abdel-Azim, Khaled A. Shams, Faiza M. Hammouda. Targeting multidrug resistance in cancer by natural chemosensitizers. *Bulletin of the National Research Centre*, 2019, 43:8 <https://doi.org/10.1186/s42269-019-0043-8>
  33. Turner AP., C. Alam, R. Bendayan. Efflux transporters in cancer resistance: molecular and functional characterization of P-glycoprotein. In: A. Sosnik, R. Bendayan. *Drug Efflux Pumps in Cancer Resistance Pathways: From Molecular Recognition and Characterization to Possible Inhibition Strategies in Chemotherapy*. Book Series: Cancer Sensitizing Agents for Chemotherapy Volume: 7 Pages: 1-30 Published: 2020. <https://doi.org/10.1016/B978-0-12-816434-1.00001-2>
- 40. Pajeva, I. K., C. Globisch, M. Wiese. Combined pharmacophore modeling, docking and 3D QSAR study of ABCB1 and ABCC1 transporter inhibitors. *ChemMedChem* 2009, 4 (11), 1883-1896.**
- Цитирания: 97
1. Klepsch, F; Jabeen, I; Chiba, P; Ecker, GF. Pharmacoinformatic Approaches to Design Natural Product Type Ligands of ABC-Transporters. *CURRENT PHARMACEUTICAL DESIGN* 16 (15): 1742-1752 MAY 2010.
  2. Klepsch, F., G.F. Ecker. Impact of the Recent Mouse P-Glycoprotein Structure for Structure-Based Ligand Design. *MOLECULAR INFORMATICS*, 29, 4, 276–286, APRIL 2010.
  3. Miteva, M.A., Guyon, F., Tufféry, P. Frog2: Efficient 3D conformation ensemble generator for small compounds. *NUCLEIC ACIDS RESEARCH* 38 (SUPPL. 2), art. no. gkq325, pp. W622-W627, 2010.

4. Klepsch, F; Stockner, T; Erker, T; Muller, M; Chiba, P; Ecker, GF. Using structural and mechanistic information to design novel inhibitors/ substrates of P-glycoprotein. *CURRENT TOPICS IN MEDICINAL CHEMISTRY* 10 (17): 1769-1774 DEC 2010
5. Zhao, Q., Li, Y., Peng, H. Structure basis of P-gp-ligands interaction and reversal of P-gp-mediated multidrug resistance. *JOURNAL OF INTERNATIONAL PHARMACEUTICAL RESEARCH*, 2011, 37 (6), pp. 439-445.
6. He, SM; Li, R; Kanwar, JR; Zhou, SF. Structural and Functional Properties of Human Multidrug Resistance Protein 1 (MRP1/ABCC1). *CURRENT MEDICINAL CHEMISTRY* 18 (3): 439-481 JAN 2011.
7. Tarcsay, A; Keseru, GM. Homology modeling and binding site assessment of the human P-glycoprotein. *FUTURE MEDICINAL CHEMISTRY* 3 (3): 297-307 MAR 2011.
8. Liu, Y., Hong, L., Yu, L.-S., Jiang, H.-D., Chen, J.-Z., Meng, Q., Chen, S.-Q., Zeng, S. The role of ADME evaluation in translation research of innovative drug. *YAOXUE XUEBAO*, 2011, 46 (1), pp. 19-29.
9. Stoll, F., A. H. Göller, A. Hillisch. Utility of protein structures in overcoming ADMET-related issues of drug-like compounds. *DRUG DISCOVERY TODAY* 16 (11-12): 530-538 JUN 2011.
10. Klepsch F, Chiba P, Ecker GF, 2011 Exhaustive Sampling of Docking Poses Reveals Binding Hypotheses for Propafenone Type Inhibitors of P-Glycoprotein. *PLOS COMPUT BIOL* 7(5): Art. No. e1002036. May 2011.
11. Ferreira, R. J.,D. dos Santos, M. J. U. Ferreira, R. C. Guedes. Towards a better pharmacophore description of P-glycoprotein modulators, based on macrocyclic diterpenes from Euphorbia species. *JOURNAL OF CHEMICAL INFORMATION AND MODELING* 51 (6): 1315-1324 JUN 2011.
12. Darby, R.A.J., Callaghan, R., McMahon, R. M. P-glycoprotein inhibition: The past, the present and the future. *CURRENT DRUG METABOLISM* 2011, 12 (8) , 722-731.
13. Wesolowska, O. Interaction of phenothiazines, stilbenes and flavonoids with multidrug resistance-associated transporters, P-glycoprotein and MRP1, *ACTA BIOCHIMICA POLONICA*, 58 (4):433-448; 2011.
14. Jabeen, I. Combined Ligand- and Structure-based Studies on inhibitors of P-glycoprotein DISSERTATION, Dr.-Studium der Naturwissenschaften, University of Wien, Wien, 2011. othes.univie.ac.at/17980/1/2011-11-15\_0746423.pdf PhD
15. Ricardo Jose Diogo Gracio Ferreira. Vencendo a multi-resistencia: Modelos computacionais da Glicoproteína-P. Mestrado em Química Farmacéutica e Terapêutica. UNIVERSIDADE DE LISBOA. FACULDADE DE FARMÁCIA. 2011. PhD [www.ff.ul.pt/FCT/PTDC/QEQ.../Tese-Msci2.pdf](http://www.ff.ul.pt/FCT/PTDC/QEQ.../Tese-Msci2.pdf)
16. Andreia Palmeira. Design, synthesis and evaluation of xanthone derivatives for dual activity: antitumor and P-glycoprotein inhibition. Thesis presented to the Faculdade de Farmácia, Universidade do Porto, Porto, 2011, pp. 1-402. PhD <https://br.123dok.com/document/z31on7my-design-synthesis-and-evaluation-of-xanthone-derivatives-for-dual-activity-antitumor-and-p-glycoprotein-inhibition.html>
17. Chen L, Li Y, Yu H, Zhang L, Hou T. Computational models for predicting substrates or inhibitors of P-glycoprotein. *DRUG DISCOV TODAY*. 2012 Apr;17(7-8):343-51.
18. Andreas Jurik, Freya Klepsch and Barbara Zdrazil. Modeling and Simulation of Membrane Transport Proteins. Chapter 18. In: *Medicinal Chemistry and Drug Design*, Edited by Deniz Ekinici, InTech, Published: May 16, 2012. DOI: 10.5772/2457
19. Ethan J. Speir. Modeling the human P-glycoprotein translocation mechanism using targeted molecular dynamics. An undergraduate thesis for the degree B.S. Biology with research option.. Georgia Institute of Technology, USA, May 2012. <https://smartechnology.gatech.edu/handle/1853/43770>
20. Hung, HY; Ohkoshi, E; Goto, M; Bastow, KF; Nakagawa-Goto, K; Lee, KH. Antitumor Agents. 293. Nontoxic Dimethyl-4,4'-dimethoxy-5,6,5',6'-dimethylenedioxybiphenyl-2,2'-dicarboxylate (DDB) Analogues Chemosensitize Multidrug-Resistant Cancer Cells to Clinical Anticancer Drugs. *JOURNAL OF MEDICINAL CHEMISTRY*, 55 (11):5413-5424; 10.1021/jm300378k JUN 14 2012.
21. Sodani, K; Tiwari, AK; Singh, S; Patel, A; Xiao, ZJ; Chen, JJ; Sun, YL; Talele, TT; Chen, ZS. GW583340 and GW2974, human EGFR and HER-2 inhibitors, reverse ABCG2-and ABCB1-mediated drug resistance. *BIOCHEMICAL PHARMACOLOGY*, 83 (12):1613-1622; 10.1016/j.bcp.2012.02.028 JUN 15 2012.
22. Mohd Razip Asaruddin, Habibah A Wahab, Normisah Mohamed and Md Abu Affan. Pharmacophore modelling, docking and biological evaluation of vanillin derivatives as neuraminidase inhibitors. *INT.J.A.PS.BMS* , APR-JUNE .2012, Vol.1(2), 95-104. [www.ijapsbs.com/admin/pdf\\_files/IJAPSB\\_1.2.3.pdf](http://www.ijapsbs.com/admin/pdf_files/IJAPSB_1.2.3.pdf)
23. Cheng, C; Liu, ZG; Zhang, H; Xie, JD; Chen, XG; Zhao, XQ; Wang, F; Liang, YJ; Chen, LK; Singh, S; Chen, JJ; Talele, TT; Chen, ZS; Zhong, FT; Fu, LW. Enhancing Chemosensitivity in ABCB1- and ABCG2-Overexpressing Cells and Cancer Stem-Like Cells by An Aurora Kinase Inhibitor CCT129202. *MOLECULAR PHARMACEUTICS*, 9 (7):1971-1982; 10.1021/mp2006714 JUL 2012.
24. Poongavanam, V., Haider, N., Ecker, G.F., Fingerprint-based in silico models for the prediction of P-glycoprotein substrates and inhibitors, *BIOORGANIC & MEDICINAL CHEMISTRY*, 20 (18):5388-5395; 10.1016/j.bmc.2012.03.045 SEP 15 2012.

25. Satpathy, R., Guru, R.K., Behera, R. Evaluation of anti-influenza activity of Curcumin derivatives by docking and pharmacophore modeling approach. *International Journal of PHARMACY AND PHARMACEUTICAL SCIENCES* 4 (SUPPL.1) , pp. 469-474, 2012.
26. Palmeira, A; Sousa, E; Vasconcelos, MH; Pinto, M; Fernandes, MX. Structure and Ligand-based Design of P-glycoprotein Inhibitors: A Historical Perspective. *CURRENT PHARMACEUTICAL DESIGN*, 18 (27):4197-4214; SEP 2012
27. H-Y. Hung, E. Ohkoshi, M. Goto, K. Nakagawa-Goto, K-H. Lee, 1-(3,4,5-Trimethoxyphenyl)ethane-1,2-diol esters, a novel compound class with potent chemoreversal activity, *BIOORGANIC & MEDICINAL CHEMISTRY LETTERS*, Volume 22, Issue 24, 15 December 2012, Pages 7726-7729, ISSN 0960-894X, 10.1016/j.bmcl.2012.09.096
28. Liu, KJ; He, JH; Su, XD; Sim, HM; Xie, JD; Chen, XG; Wang, F; Liang, YJ; Singh, S; Sodani, K; Talele, TT; Ambudkar, SV; Chen, ZS; Wu, HY; Fu, LW. Saracatinib (AZD0530) is a potent modulator of ABCB1-mediated multidrug resistance in vitro and in vivo, *INTERNATIONAL JOURNAL OF CANCER*, 132 (1):224-235; 10.1002/ijc.27649 JAN 1 2013.
29. F.Orlandi, M. Coronello, C. Bellucci, S. Dei, L. Guandalini, D. Manetti, C. Martelli, M. N. Romanelli, S. Scapecchi, M. Salerno, H. Menif, I. Bello, E. Mini, E. Teodori, New structure-activity relationship studies in a series of N,N-bis(cyclohexanol)amine aryl esters as potent reversers of P-glycoprotein-mediated Multidrug Resistance (MDR), *BIOORGANIC & MEDICINAL CHEMISTRY*, Volume 21, Issue 2, 15 January 2013, Pages 456-465.
30. Singh DB, Gupta, MK, Kesharwani RK, Misra K. Comparative docking and ADMET study of some curcumin derivatives and herbal congeners targeting  $\beta$ -amyloid. *NETWORK MODELING ANALYSIS IN HEALTH INFORMATICS AND BIOINFORMATICS*. 2013, 2 (1), 13-27.
31. He, D; Zhao, XQ; Chen, XG; Fang, Y; Singh, S; Talele, TT; Qiu, HJ; Liang, YJ; Wang, XK; Zhang, GQ; Chen, ZS; Fu, LW. BIRB796, the Inhibitor of p38 Mitogen-Activated Protein Kinase, Enhances the Efficacy of Chemotherapeutic Agents in ABCB1 Overexpression Cells. *PLOS ONE*, 8 (1), e54181, JAN 18 2013.
32. Singh, DB; Gupta, MK; Singh, DV; Singh, SK; Misra, K. Docking and in silico ADMET Studies of Noraristeromycin, Curcumin and Its Derivatives with Plasmodium falciparum SAH Hydrolase: A Molecular Drug Target against Malaria. *INTERDISCIPLINARY SCIENCES-COMPUTATIONAL LIFE SCIENCES*, 5 (1):1-12; 10.1007/s12539-013-0147-z MAR 2013.
33. RJ. Ferreira, M-JU. Ferreira, DJVA. dos Santos. Molecular Docking Characterizes Substrate-Binding Sites and Efflux Modulation Mechanisms within P-Glycoprotein. *JOURNAL OF CHEMICAL INFORMATION AND MODELING*, 53 (7):1747-1760; 10.1021/ci400195v JUL 2013.
34. Steiger, Scott. 4-Isoxazolyl-1,4-Dihydropyridines Bind The Multidrug-Resistance Transporter, The University of Montana Missoula, MT May 2013 PhD
35. Ferreira, RJ; Ferreira, MJU; dos Santos, DJVA. Assessing the Stabilization of P-Glycoprotein's Nucleotide-Binding Domains by the Linker, Using Molecular Dynamics. *MOLECULAR INFORMATICS*, 32 (5-6):529-540; SI 10.1002/minf.201200175 JUN 2013.
36. Liu, JH; Wang, X; Liu, P; Deng, RX; Lei, M; Chen, WT; Hu, LH. 20(S)-Protopanaxadiol (PPD) analogues chemosensitize multidrug-resistant cancer cells to clinical anticancer drugs. *BIOORGANIC & MEDICINAL CHEMISTRY*, 21 (14):4279-4287; 10.1016/j.bmc.2013.04.067 JUL 15 2013.
37. Liu, HM; Ma, ZG; Wu, BJ. Structure-activity relationships and in silico models of P-glycoprotein (ABCB1) inhibitors. *XENOBIOTICA*, 43 (11):1018-1026; 10.3109/00498254.2013.791003 NOV 2013
38. S. Kanaoka S., Y. Kimura, M. Fujikawa, Y. Nakagawa, K. Ueda, M. Akamatsu. Substrate recognition by P-glycoprotein efflux transporters: Structure-ATPase activity relationship of diverse chemicals and agrochemicals. *JOURNAL OF PESTICIDE SCIENCE*. 38, 2013, 112-122.
39. Chang, S-Y., Liu, F-F., Dong, X-Y., Sun, Y. Molecular insight into conformational transmission of human P-glycoprotein. *JOURNAL OF CHEMICAL PHYSICS*, 139 (22):10.1063/1.4832740 DEC 14 2013.
40. Tan W, Mei H, Chao L, Liu T, Pan X, Shu M, Yang L. Combined QSAR and molecule docking studies on predicting P-glycoprotein inhibitors. *JOURNAL OF COMPUTER-AIDED MOLECULAR DESIGN*, 27 (12):1067-1073; 10.1007/s10822-013-9697-8 DEC 2013.
41. Simon, S. Inhibitorischer Einfluss von Phospholipiden auf den Effluxtransporter P-Glykoprotein (Inhibitory influence of phospholipids on the efflux transporter P-glycoprotein). zur Erlangung der Doktorwürde der Fakultät für Chemie und Pharmazie der Albert-Ludwigs-Universität, Freiburg im Breisgau, Germany. 2014 PhD <http://www.freidok.uni-freiburg.de/volltexte/8916/>
42. Якушева Елена Николаевна, Щулькин Алексей Владимирович, Попова Наталья Михайловна, Черных Иван Владимирович, Титов Дмитрий Сергеевич. Структура, функции гликопротеина-P и его значение для рациональной фармакотерапии // *Обзоры по клинич. фармакол. и лек. терапии*. 2014. №2. Научная библиотека КиберЛенинка: <http://cyberleninka.ru/article/n/struktura-funktsii-glikoproteina-r-i-ego-znachenie-dlya-ratsionalnoy-farmakoterapii#ixzz4UiW4jJD8>

43. Singh, S; Prasad, NR; Kapoor, K; Chufan, EE; Patel, BA; Ambudkar, SV; Talele, TT. Design, Synthesis, and Biological Evaluation of (S)-Valine Thiazole-Derived Cyclic and Noncyclic Peptidomimetic Oligomers as Modulators of Human P-Glycoprotein (ABCB1). CHEMBIOCHEM, 15 (1):157-169; 10.1002/cbic.201300565 JAN 3 2014.
44. Villar VH, O Vögler, F Barceló, M Gómez-Florit, J. Martínez-Serra, A. Obrador-Hevia, J. Martín-Broto, V. Ruiz-Gutiérrez, R. Alemany. Oleonic and maslinic acid Sensitize soft tissue sarcoma Cells to Doxorubicin by inhibiting the multidrug resistance protein mrp-1, but not p-glycoprotein. JOURNAL OF NUTRITIONAL BIOCHEMISTRY, 25 (4):429-438; 10.1016/j.jnutbio.2013.12.003 APR 2014
45. Pinto M., D Digles, GF. Ecker. Computational models for predicting the interaction with ABC transporters. DRUG DISCOVERY TODAY: TECHNOLOGIES, 212, 2014, e69-e77
46. Romagnoli R, Baraldi PG, Salvador MK, Chayah M, Camacho ME, Prencipe F, Hamel E, Consolaro F, Basso G, Viola G. Design, synthesis and biological evaluation of arylcinnamide hybrid derivatives as novel anticancer agents. EUR J MED CHEM. 2014 Jun 23;81:394-407. doi: 10.1016/j.ejmech.2014.05.028. Epub 2014 May 10.
47. Singh, S; Prasad, NR; Chufan, EE; Patel, BA; Wang, YJ; Chen, ZS; Ambudkar, SV; Talele, TT. Design and Synthesis of Human ABCB1 (P-Glycoprotein) Inhibitors by Peptide Coupling of Diverse Chemical Scaffolds on Carboxyl and Amino Termini of (S)-Valine-Derived Thiazole Amino Acid. JOURNAL OF MEDICINAL CHEMISTRY, 57 (10):4058-4072; 10.1021/jm401966m MAY 22 2014
48. Shukla, S; Kouanda, A; Silverton, L; Talele, TT; Ambudkar, SV. Pharmacophore modeling of nilotinib as an inhibitor of ABC drug transporters and BCR-ABL kinase using a 3D-QSAR approach. MOLECULAR PHARMACEUTICS, 11 (7):2313-2322; 2014.
49. Wang, Y.-J., Zhang, Y.-K., Kathawala, R.J., Chen, Z.-S. Repositioning of Tyrosine Kinase Inhibitors as Antagonists of ATP-Binding Cassette Transporters in Anticancer Drug Resistance. CANCERS 2014, 6(4), 1925-1952; doi:10.3390/cancers6041925
50. Jezrael Lafuente Revalde. The inhibition of ABC transporters in cancer multidrug resistance heterocyclic heterocyclic cyclohexanone analogues of curcumin. PhD thesis, The University of Auckland, 2014. <http://researchspace.auckland.ac.nz> PhD
51. Tarcsay, Ákos, and György M. Keserü. "ADMET Prediction Based on Protein Structures." *Protein Modelling* 9783319099767 (G. Naray\_Szabo (ed.). Springer International Publishing, 2014. 287-322.
52. Clay A.T., Sharom F.J.. Multidrug Resistance Protein: P-Glycoprotein. In: *Drug Transporters: Molecular Characterization and Role in Drug Disposition*, Second Edition. Edited by Guofeng You and Marilyn E. Morris. © 2014 John Wiley & Sons, Inc. Published 2014 by John Wiley & Sons, Inc., 141-160. ISBN: 978-1-118-48993-2.
53. El-Kattan A., Varma M.V., Lai Y. Transporters in Drug Discovery: In Silico Approaches. In: *Drug Transporters: Molecular Characterization and Role in Drug Disposition, Second Edition*. Edited by Guofeng You, Marilyn E. Morris, Binghe Wang.. © 2014 John Wiley & Sons, Inc. Published 2014 by John Wiley & Sons, Inc., 371-388. ISBN: 978-1-118-48993-2
54. Erić, S., M. Kalinić. Računarski modeli za predviđanje transporta lekova posredovanog P-glikoproteinom. ARCH. FARM 2015, 65, 89-114.
55. Bisi, A; Gobbi, S; Merolle, L; Farruggia, G; Belluti, F; Rampa, A; Molnar, J; Malucelli, E; Cappadone, C. Design, synthesis and biological profile of new inhibitors of multidrug resistance associated proteins carrying a polycyclic scaffold. EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY, 92 471-480; 10.1016/j.ejmech.2015.01.004 MAR 6 2015
56. Subhani, S; Jayaraman, A; Jamil, K. Homology modelling and molecular docking of MDR1 with chemotherapeutic agents in non-small cell lung cancer, BIOMEDICINE & PHARMACOTHERAPY, 71 37-45; 10.1016/j.biopha.2015.02.009 APR 2015
57. Liu, J; Xu, M; Zhu, MY; Feng, Y. Chemoreversal Metabolites from the Endophytic Fungus *Penicillium citrinum* Isolated from a Mangrove *Avicennia marina*. NATURAL PRODUCT COMMUNICATIONS, 10 (7):1203-1205; JUL 2015
58. Zhang, Y.-K., Zhang, H., Zhang, G.-N., Wang, Y.-J., Kathawala, R.J., Si, R., Patel, B.A., Xu, J., Chen, Z.-S. Semi-synthetic ocotillol analogues as selective ABCB1-mediated drug resistance reversal agents ONCOTARGET, 6 (27):24277-24290; SEP 15 2015.
59. Lu JF, Pokharel D, Bebawy M. MRP1 and its role in anticancer drug resistance. DRUG METABOLISM REVIEWS, 47 (4):406-419; 10.3109/03602532.2015.1105253 OCT 2 2015.
60. Domicевичa L, Biggin PC. Homology modelling of human P-glycoprotein. Biochem Soc Trans. 2015 Oct 1;43(5):952-8. doi: 10.1042/BST20150125
61. Chufan E.E., Sim H.-M., Ambudkar S.V. Molecular Basis of the Polyspecificity of P-glycoprotein (ABCB1): Recent Biochemical and Structural Studies. Chapter 3, In: ABC TRANSPORTERS AND CANCER, 125 71-96; 10.1016/bs.acr.2014.10.003 2015.

62. Shukla, S.; Patel, A.; Ambudkar, S.V. Mechanistic and Pharmacological Insights into Modulation of ABC Drug Transporters by Tyrosine Kinase Inhibitors. In: ABC Transporters - 40 Years on, Ed. A. M. George, Springer International Publishing, pp. 227-272, 2016. [http://dx.doi.org/10.1007/978-3-319-23476-2\\_10](http://dx.doi.org/10.1007/978-3-319-23476-2_10)
63. Dana A. AlQudah, Malek A. Zihlif, Mutasem O. Taha, Ligand-based modeling of diverse aryalkylamines yields new potent P-glycoprotein inhibitors, *European Journal of Medicinal Chemistry*, Volume 110, 2016, Pages 204-223, <https://doi.org/10.1016/j.ejmech.2016.01.034>
64. AlQudah, DA; Zihlif, MA; Taha, MO. Ligand-Based Modeling of Diverse Aryalkylamines Yields New Potent P-Glycoprotein Inhibitors, *EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY*, 110 204-223; 10.1016/j.ejmech.2016.01.034 MAR 3 2016.
65. Malik, R; Bunkar, D; Choudhary, BS; Srivastava, S; Mehta, P; Sharma, M. High throughput virtual screening and in silico ADMET analysis for rapid and efficient identification of potential PAP248-286 aggregation inhibitors as anti-HIV agents, *JOURNAL OF MOLECULAR STRUCTURE*, 1122 239-246; 10.1016/j.molstruc.2016.05.086 OCT 15 2016.
66. Miyata, K; Nakagawa, Y; Kimura, Y; Ueda, K; Akamatsu, M. Structure–activity relationships of dibenzoylhydrazines for the inhibition of P-glycoprotein-mediated quinidine transport, *BIOORGANIC & MEDICINAL CHEMISTRY*, 24 (14):3184-3191; 10.1016/j.bmc.2016.05.039 JUL 15 2016
67. Trippier, Paul C. Selecting Good 'Drug-Like' Properties to Optimize Small Molecule Blood-Brain Barrier Penetration. *CURRENT MEDICINAL CHEMISTRY*, 23 (14):1392-1407; 2016
68. Jabeen, I. In silico strategies to probe stereoselective interactions of multidrug resistant transporter P-glycoprotein. (2016) *Letters in Drug Design and Discovery*, 13 (8), pp. 824-832.
69. Marcus, D; Mak, L. Methods and Resources for Transport Proteins in Bioinformatics and Cheminformatics. *DRUG TRANSPORTERS, VOL 2: RECENT ADVANCES AND EMERGING TECHNOLOGIES*, Edited by: Nicholls G; Youdim K. 195-226; 2016.
70. Ngo, T.-D., Tran, T.-D., Le, M.-T., Thai, K.-M. Machine learning-, rule- and pharmacophore-based classification on the inhibition of P-glycoprotein and NorA (2016) *SAR AND QSAR IN ENVIRONMENTAL RESEARCH*, 27 (9):747-780; 10.1080/1062936X.2016.1233137 2016
71. Sharifi M, Raevsky AV, Ghafourian T (2016) Effect of Molecular Structure, Substrate and Docking Scores on the Prediction of the Inhibition Constants of P-glycoprotein Inhibitors. *J Drug Metab Toxicol* 7:217. doi: 10.4172/2157-7609.1000217
72. Lorendeau, D; Dury, L; Nasr, R; Boumendjel, A; Teodori, E; Gutschow, M; Falson, P; Di Pietro, A; Baubichon-Cortay, H. MRP1-dependent collateral sensitivity of multidrug-resistant cancer cells: identifying selective modulators inducing cellular glutathione depletion. *CURRENT MEDICINAL CHEMISTRY*, 24 (12):1186-1213; 10.2174/0929867324666161118130238 2017
73. Miteva, M. A., Villoutreix, B. O. Computational Biology and Chemistry in MTi: Emphasis on the Prediction of Some ADMET Properties. *MOLECULAR INFORMATICS*, 36 (10):SI 10.1002/minf.201700008 OCT 2017
74. Mollazadeh S., Shamsara J., Iman M., Hadizadeh F. Docking and QSAR studies of 1,4-dihydropyridine derivatives as anti-cancer agent. *RECENT PATENTS ON ANTI-CANCER DRUG DISCOVERY*, 12 (2):174-185; 10.2174/1574892812666170126162521 2017.
75. Varma, MV; Lai, YR; El-Kattan, AF. Molecular properties associated with transporter-mediated drug disposition. *ADVANCED DRUG DELIVERY REVIEWS*, 116 92-99; 10.1016/j.addr.2017.05.014 JUL 1 2017.
76. Rasulev B. Recent developments in 3D QSAR and molecular docking studies of organic and nanostructures. *Handbook of Computational Chemistry*, 2017, pp. 2133-2161.
77. E. Kotsampasakou, S. Jain, D. Digles, GF. Ecker. Transporters in Hepatotoxicity. In: *Computational Toxicology: Risk Assessment for Chemicals*, First Edition. Edited by Sean Ekins.© 2018 JohnWiley & Sons, Inc., Chapter 5, 145-174. ISBN1119282578, 9781119282570
78. Patel, BA; Abel, B; Barbuti, AM; Velagapudi, UK; Chen, ZS; Ambudkar, SV; Talele, TT. Comprehensive Synthesis of Amino Acid-Derived Thiazole Peptidomimetic Analogues to Understand the Enigmatic Drug/Substrate-Binding Site of P-Glycoprotein. *JOURNAL OF MEDICINAL CHEMISTRY*, 61 (3):834-864; 10.1021/acs.jmedchem.7b01340 FEB 8 2018
79. Pradines B. P-Glycoprotein-Like Transporters in *Leishmania*: A Search for Reversal Agents. In: Ponte-Sucre A., Padrón-Nieves M. (eds) *Drug Resistance in Leishmania Parasites: Consequences, Molecular Mechanisms and Possible Treatments*, pp. 319-340, 2018. [https://doi.org/10.1007/978-3-319-74186-4\\_14](https://doi.org/10.1007/978-3-319-74186-4_14)
80. Jain, S; Grandits, M; Ecker, GF. Interspecies comparison of putative ligand binding sites of human, rat and mouse P-glycoprotein. *EUROPEAN JOURNAL OF PHARMACEUTICAL SCIENCES*, 122 134-143; 10.1016/j.ejps.2018.06.022 SEP 15 2018
81. Wang, B; Ma, LY; Wang, JQ; Lei, ZN; Gupta, P; Zhao, YD; Li, ZH; Liu, Y; Zhang, XH; Li, YN; Zhao, B; Chen, ZS; Liu, HM. Discovery of 5-Cyano-6-phenylpyrimidin Derivatives Containing an Acylurea Moiety as

- Orally Bioavailable Reversal Agents against P-Glycoprotein-Mediated Multidrug Resistance. *JOURNAL OF MEDICINAL CHEMISTRY*, 61 (14):5988-6001; 10.1021/acs.jmedchem.8b00335 JUL 26 2018.
82. Schlessinger, A; Welch, MA; van Vlijmen, H; Korzekwa, K; Swaan, PW; Matsson, P. Molecular Modeling of Drug-Transporter Interactions-An International Transporter Consortium Perspective. *CLINICAL PHARMACOLOGY & THERAPEUTICS*, 104 (5):818-835; 10.1002/cpt.1174 NOV 2018
  83. Mollazadeh, S; Sahebkar, A; Hadizadeh, F; Behravan, J; Arabzadeh, S. Structural and functional aspects of P-glycoprotein and its inhibitors. *LIFE SCIENCES*, 214 118-123; 10.1016/j.lfs.2018.10.048 DEC 1 2018
  84. E. Kotsampasakou, S. Jain, D. Digles, GF. Ecker. "Transporters in Hepatotoxicity. In: Computational Toxicology: Risk Assessment for Chemicals", First Edition. Edited by Sean Ekins.© 2018 JohnWiley & Sons, Inc., Chapter 5, 145-174. ISBN1119282578, 9781119282570
  85. Clerbaux, LA; Coecke, S; Lumen, A; Kliment, T; Worth, AP; Paini, A, Capturing the applicability of in vitro-in silico membrane transporter data in chemical risk assessment and biomedical research. *SCIENCE OF THE TOTAL ENVIRONMENT*, 645 97-108; 10.1016/j.scitotenv.2018.07.122 DEC 15 2018.
  86. Wen, Y; Zhao, RQ; Gupta, P; Fan, YF; Zhang, YK; Huang, ZG; Li, XH; Su, YG; Liao, LJ; Xie, YA; Yang, DH; Chen, ZS; Liang, G. The epigallocatechin gallate derivative Y-6 reverses drug resistance mediated by the ABCB1 transporter both in vitro and in vivo. *ACTA PHARMACEUTICA SINICA B*, 9 (2):316-323, 2019. ISSN 2211-3835, <https://doi.org/10.1016/j.apsb.2018.10.001>
  87. Zhang YT, Yu YQ, Yan XX, Wang WJ, Tian XT, Wang L, Zhu WL, Gong LK, Pan GY. Different structures of berberine and five other protoberberine alkaloids that affect P-glycoprotein-mediated efflux capacity. *ACTA PHARMACOLOGICA SINICA*, 40 (1):133-142; 10.1038/s41401-018-0183-7 JAN 2019
  88. Clerbaux, LA; Paini, A; Lumen, A; Osman-Ponchet, H; Worth, AP; Fardel, O. Membrane transporter data to support kinetically-informed chemical risk assessment using non-animal methods: Scientific and regulatory perspectives. *ENVIRONMENT INTERNATIONAL*, 126 659-671; 10.1016/j.envint.2019.03.003 MAY 2019
  89. Vilar, S; Sobarzo-Sanchez, E; Uriarte, E. In Silico Prediction of P-glycoprotein Binding: Insights from Molecular Docking Studies. *CURRENT MEDICINAL CHEMISTRY*, 26 (10):1746-1760; 10.2174/0929867325666171129121924 2019
  90. Hinge, V.K., Roy, D. & Kovalenko, A. Prediction of P-glycoprotein inhibitors with machine learning classification models and 3D-RISM-KH theory based solvation energy descriptors. *J Comput Aided Mol Des* (2019) 33: 965. <https://doi.org/10.1007/s10822-019-00253-5>
  91. Rasulev B. Ecotoxicological QSAR Modeling of Nanomaterials: Methods in 3D-QSARs and Combined Docking Studies for Carbon Nanostructures. In: Roy K. (eds) Ecotoxicological QSARs. Methods in Pharmacology and Toxicology. Humana, New York, NY, 2020, 215-233. DOI: 10.1007/978-1-0716-0150-1\_10
  92. Gupta, Mayuri; Bogdanowicz, Thomas; Reed, Mark A.; Barden, Christopher J.; Weaver, Donald F. The Brain Exposure Efficiency (BEE) Score. *ACS CHEMICAL NEUROSCIENCE* Volume: 11 Issue: 2 Pages: 205-224 Published: JAN 15 2020 DOI: 10.1021/acschemneuro.9b00650
  93. Turner AP., C. Alam, R. Bendayan. Efflux transporters in cancer resistance: molecular and functional characterization of P-glycoprotein. In: A. Sosnik, R. Bendayan. Drug Efflux Pumps in Cancer Resistance Pathways: From Molecular Recognition and Characterization to Possible Inhibition Strategies in Chemotherapy. Book Series: Cancer Sensitizing Agents for Chemotherapy Volume: 7 Pages: 1-30 Published: 2020. <https://doi.org/10.1016/B978-0-12-816434-1.00001-2>
  94. Yalcin, S. Molecular Docking, Drug Likeness, and ADMET Analyses of Passiflora Compounds as P-Glycoprotein (P-gp) Inhibitor for the Treatment of Cancer. *Curr Pharmacol Rep* (2020). <https://doi.org/10.1007/s40495-020-00241-6>
  95. Cao, Yuhong; Shi, Yiwei; Cai, Ying; Hong, Zhanying; Chai, Yifeng. The Effects of Traditional Chinese Medicine on P-Glycoprotein-Mediated Multidrug Resistance and Approaches for Studying the Herb-P-Glycoprotein Interactions. *DRUG METABOLISM AND DISPOSITION* Volume: 48 Issue: 10 Pages: 972-979 Published: OCT 1 2020. DOI: 10.1124/dmd.120.000050
  96. Paolo Governa. Identification and development of active principles from plant sources. Thesis for PhD Chemical and Pharmaceutical Sciences, University of Siena, February 2021. PhD
  97. Jarosław Sączewski, Joanna Fedorowicz. Three Heterocyclic Rings Fused (6-5-6), In book: Reference Module in Chemistry, Molecular Sciences and Chemical Engineering, Elsevier, 2020, ISBN 9780124095472, <https://doi.org/10.1016/B978-0-12-409547-2.14881-4>.

**41. Pajeva, I. K., C. Globisch, M. Wiese. Comparison of the inward- and outward-open homology models and ligand binding of human P-glycoprotein. *FEBS J.* 2009, 276 (23), 7016–7026.**

Цитирания: 39

1. Klepsch, F., G.F. Ecker. Impact of the Recent Mouse P-Glycoprotein Structure for Structure-Based Ligand Design. *MOLECULAR INFORMATICS*, 29, 4, 276–286, 2010.

2. Choong E., M. Dobrinás, P-A. Carrupt, CB Eap. The permeability P-glycoprotein: a focus on enantioselectivity and brain distribution EXPERT OPINION ON DRUG METABOLISM & TOXICOLOGY, 6 (8), pp. 953-965, 2010.
3. Klepsch, F; Stockner, T; Erker, T; Müller, M; Chiba, P; Ecker, GF. Using structural and mechanistic information to design novel inhibitors/ substrates of P-glycoprotein. CURRENT TOPICS IN MEDICINAL CHEMISTRY 10 (17): 1769-1774 DEC 2010.
4. Martelli C, Dei S, Lambert C, Manetti D, Orlandi F, Romanelli MN, Scapecchi S, Salerno M, Teodori E. Inhibition of P-glycoprotein-mediated Multidrug Resistance (MDR) by N,N-bis(cyclohexanol)amine aryl esters: further restriction of molecular flexibility maintains high potency and efficacy. BIOORG MED CHEM LETT. 2011 Jan 1;21(1):106-9.
5. Jabeen, I; Wetwitayaklung, P; Klepsch, F; Parveen, Z; Chiba, P; Ecker, GF. Probing the stereoselectivity of P-glycoprotein-synthesis, biological activity and ligand docking studies of a set of enantiopure benzopyrano[3,4-b][1,4]oxazines. CHEMICAL COMMUNICATIONS 47 (9): 2586-2588 2011.
6. Honorat, M.; Falson, P.; Terreux, R.; Di Pietro, A.; Dumontet, C.; Payen, L. Multidrug Resistance ABC Transporter Structure Predictions by Homology Modeling Approaches. CURRENT DRUG METABOLISM 12 (3): 268-277 MAR 2011.
7. Mohan CG Impact of Computational Structure-Based Predictive Toxicology in Drug Discovery COMBINATORIAL CHEMISTRY & HIGH THROUGHPUT SCREENING 14 5 417-426 JUN 2011.
8. Klepsch F, Chiba P, Ecker GF, 2011 Exhaustive Sampling of Docking Poses Reveals Binding Hypotheses for Propafenone Type Inhibitors of P-Glycoprotein. PLOS COMPUT BIOL 7(5): Art. No. e1002036. May 2011.
9. Mudra DR, Desino KE, Desai PV. In Silico, In Vitro and In Situ Models to Assess Interplay Between CYP3A and P-gp. CURR DRUG METAB. 2011 Oct 1;12(8):750-773.
10. Moroy G, Martiny VY, Vayer P, Villoutreix BO, Miteva MA. Toward in silico structure-based ADMET prediction in drug discovery. DRUG DISCOV TODAY, 17 (1-2), 44-55, 2012.
11. Jabeen, I. Combined Ligand- and Structure-based Studies on inhibitors of P-glycoprotein DISSERTATION, Dr.-Studium der Naturwissenschaften, University of Wien, Wien, 2011. othes.univie.ac.at/17980/1/2011-11-15\_0746423.pdf PhD
12. Andreia Palmeira. Design, synthesis and evaluation of xanthone derivatives for dual activity: antitumor and P-glycoprotein inhibition. Thesis presented to the Faculdade de Farmácia, Universidade do Porto, Porto, 2011, pp. 1-402. PhD <https://br.123dok.com/document/z31on7my-design-synthesis-and-evaluation-of-xanthone-derivatives-for-dual-activity-antitumor-and-p-glycoprotein-inhibition.html>
13. Bailly A, Yang H, Martinoia E, Geisler M, Murphy S. Plant lessons: exploring ABCB functionality through structural modeling, FRONTIERS IN PLANT SCIENCE, 2012, 2, DOI=10.3389/fpls.2011.00108
14. Wise JG. Catalytic Transitions in the Human MDR1 P-Glycoprotein Drug Binding Sites. BIOCHEMISTRY, 51 (25):5125-5141; 10.1021/bi300299z JUN 26 2012
15. Gokirmak, T; Campanale, JP; Shipp, LE; Moy, GW; Tao, HC; Hamdoun, A. Localization and Substrate Selectivity of Sea Urchin Multidrug (MDR) Efflux Transporters J. JOURNAL OF BIOLOGICAL CHEMISTRY, 287 (52):43876-43883, 2012.
16. JW Biesiada, S Sadhasivam, M Wagner, J Meller. From SNP Genotyping to Improved Pediatric Healthcare. PEDIATRIC BIOMEDICAL INFORMATICS. 2, 2012, 359-378.
17. Callaghan R., A.M. George and I.D. Kerr, 8.8 Molecular Aspects of the Translocation Process by ABC Proteins, In *Comprehensive Biophysics*, edited by Edward H. Egelman, Elsevier, Amsterdam, 2012, Pages 145-173, ISBN 9780080957180, <http://dx.doi.org/10.1016/B978-0-12-374920-8.00812-2>.
18. Simon, S. Inhibitorischer Einfluss von Phospholipiden auf den Effluxtransporter P-Glykoprotein (Inhibitory influence of phospholipids on the efflux transporter P-glycoprotein). zur Erlangung der Doktorwürde der Fakultät für Chemie und Pharmazie der Albert-Ludwigs-Universität, Freiburg im Breisgau, Germany. PhD <http://www.freidok.uni-freiburg.de/volltexte/8916/>
19. F.Orlandi, M. Coronello, C. Bellucci, S. Dei, L. Guandalini, D. Manetti, C. Martelli, M. N. Romanelli, S. Scapecchi, M. Salerno, H. Menif, I. Bello, E. Mini, E. Teodori, New structure-activity relationship studies in a series of N,N-bis(cyclohexanol)amine aryl esters as potent reversers of P-glycoprotein-mediated Multidrug Resistance (MDR), BIOORGANIC & MEDICINAL CHEMISTRY, Volume 21, Issue 2, 15 January 2013, Pages 456-465.
20. Prajapati, R; Singh, U; Patil, A; Khomane, KS; Bagul, P; Bansal, AK; Sangamwar, AT. In silico model for P-glycoprotein substrate prediction: insights from molecular dynamics and in vitro studies. JOURNAL OF COMPUTER-AIDED MOLECULAR DESIGN, 27 (4):347-363; 10.1007/s10822-013-9650-x APR 2013.
21. Honorat M, Terreux R, Falson P, Di Pietro A, Dumontet C, Payen L. Localization of putative binding sites for cyclic guanosine monophosphate and the anti-cancer drug 5-fluoro-2'-deoxyuridine-5'-monophosphate on ABCB11 in silico models. BMC STRUCT BIOL. 2013 May 6;13:7. doi: 10.1186/1472-6807-13-7.

22. Loo, TW; Clarke, DM. A Salt Bridge in Intracellular Loop 2 Is Essential for Folding of Human P-Glycoprotein. *BIOCHEMISTRY*, 52 (19):3194-3196; 10.1021/bi4400425k MAY 14 2013.
23. Wen, PC; Verhalen, B; Wilkens, S; Mchaourab, HS; Tajkhorshid, E. On the Origin of Large Flexibility of P-glycoprotein in the Inward-facing State. *JOURNAL OF BIOLOGICAL CHEMISTRY*, 288 (26):19211-19220; 10.1074/jbc.M113.450114 JUN 28 2013.
24. Chang, S-Y., Liu, F-F. Molecular simulations of ATP-Binding Cassette Transporters. *PROGRESS IN CHEMISTRY*, 25, 2013, 1208-1218.
25. Loo TW, Clarke DM. Drug Rescue Distinguishes between Different Structural Models of Human P-Glycoprotein. *BIOCHEMISTRY*, 52 (41):7167-7169; 10.1021/bi401269m OCT 15 2013
26. Chang, S-Y., Liu, F-F., Dong, X-Y., Sun, Y. Molecular insight into conformational transmission of human P-glycoprotein. *THE JOURNAL OF CHEMICAL PHYSICS*, 139, 225102, 2013. DOI:http://dx.doi.org/10.1063/1.4832740.
27. Dei S, Coronello M, Floriddia E, Bartolucci G, Bellucci C, Guandalini L, Manetti D, Romanelli MN, Salerno M, Bello I, Mini E, Teodori E. Multidrug resistance (MDR) reversers: High activity and efficacy in a series of asymmetrical N,N-bis(alkanol)amine aryl esters. *EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY* 87C: 2014 Sep 30 pg 398-412.
28. Clay A.T., Sharom F.J.. Multidrug Resistance Protein: P-Glycoprotein. In: *Drug Transporters: Molecular Characterization and Role in Drug Disposition*, Second Edition. Edited by Guofeng You and Marilyn E. Morris. © 2014 John Wiley & Sons, Inc. Published 2014 by John Wiley & Sons, Inc., 141-160. ISBN: 978-1-118-48993-2.
29. Erić, S., M. Kalinić. Računarski modeli za predviđanje transporta lekova posredovanog P-glikoproteinom. *ARCH. FARM* 2015, 65, 89-114.
30. Hegedus, C; Telbisz, A; Hegedus, T; Sarkadi, B; Ozvegy-Laczka, C. Lipid Regulation of the ABCB1 and ABCG2 Multidrug Transporters, *ABC TRANSPORTERS AND CANCER*, 125 97-137; 10.1016/bs.acr.2014.10.004 2015
31. Wang, F., Liu, Z., Wang, J., Tao, J., Gong, P., Bao, X., Zhao, Y., Wang, Y., The interaction of 4-thiazolidinone derivatives containing indolin-2-one moiety with P-glycoprotein studied using K562 cell lines, *EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY*, 101, Aug 2015, 126-132, ISSN 0223-5234, http://dx.doi.org/10.1016/j.ejmech.2015.06.002.
32. Zhou, XL; Wang, Y; Lee, WYW; Or, PMY; Wan, DCC; Kwan, YW; Yeung, JHK. Miltirone Is a Dual Inhibitor of P-Glycoprotein and Cell Growth in Doxorubicin-Resistant HepG2 Cells. *JOURNAL OF NATURAL PRODUCTS*, 78 (9): 2266-2275; 10.1021/acs.jnatprod.5b00516 SEP 2015
33. Domicевичa L, Biggin PC. Homology modelling of human P-glycoprotein. *Biochem Soc Trans.* 2015 Oct 1;43(5):952-8. doi: 10.1042/BST20150125
34. Jabeen, I. In silico strategies to probe stereoselective interactions of multidrug resistant transporter P-glycoprotein. (2016) *Letters in Drug Design and Discovery*, 13 (8), pp. 824-832.
35. HK Shin, YM Kang, KT No. Predicting ADME Properties of Chemicals. In: *Handbook of Computational Chemistry*, Editors: Jerzy Leszczynski, pp. 2265-2301, 2017. DOI: 10.1007/978-94-007-6169-8\_59-1
36. Laszlo, L; Sarkadi, B; Hegedus, T. Jump into a new fold-A homology based model for the ABCG2/BCRP multidrug transporter *PLOS ONE*, 11 (10):10.1371/journal.pone.0164426 OCT 14 2016.
37. Szollosi D., Chiba P., Szakacs G., Stockner T., Hegedus T. Mechanism of drug transport by ABC multidrug proteins in structural perspectives. *AMINO ACIDS, PEPTIDES AND PROTEINS*, VOL 41, 41 152-187; 10.1039/9781782625377-00152 2017.
38. Pan, LR; Aller, SG. Allosteric Role of Substrate Occupancy Toward the Alignment of P-glycoprotein Nucleotide Binding Domains. *SCIENTIFIC REPORTS*, 8 10.1038/s41598-018-32815-2 OCT 2 2018.
39. Lokeswari P. Tangella, Mahreen Arooj, Evelyne Deplazes, Elin S. Gray, Ricardo L. Mancera, Identification and characterisation of putative drug binding sites in human ATP-binding cassette B5 (ABCB5) transporter, *Computational and Structural Biotechnology Journal*, 2020, https://doi.org/10.1016/j.csbj.2020.12.042

**42. Pajeva I., Wiese M. Structure-activity relationships of tariquidar analogs as multidrug resistance modulators. *The AAPS Journal* 2009, 11, 435-444.**

Цитиранија: 35

1. Ramalhete, Cátia Beatriz Almeida. Search for bioactive compounds from medicinal plants used as antimalarials: the study of *Momordica balsamina* L. Tese de doutoramento, Farmácia (Química Farmacêutica e Terapêutica), Universidade de Lisboa, Faculdade de Farmácia, 2010. PhD
2. Kelly RJ, Draper D, Chen CC, Robey RW, Figg WD, Piekarz RL, Chen X, Gardner ER, Balis FM, Venkatesan AM, Steinberg SM, Fojo AT, Bates SE A Pharmacodynamic Study of Docetaxel in Combination with the P-glycoprotein Antagonist, Tariquidar (XR9576) in Patients with Lung, Ovarian, and Cervical Cancer. *CLINICAL CANCER RESEARCH* 17 (3): 569-580 FEB 1 2011.

3. Akhtar, N; Ahad, A; Khar, RK; Jaggi, M; Aqil, M; Iqbal, Z; Ahmad, FJ; Talegaonkar, S. The emerging role of P-glycoprotein inhibitors in drug delivery: a patent review. EXPERT OPINION ON THERAPEUTIC PATENTS 21 (4): 561-576 APR 2011
4. Kanintronkul, Y., R. Worayuthakarn, N. Thasana, P. Winayanuwattikun, K. Pattanapanyasat, R. Surarit, S. Ruchirawat, J. Svasti. Overcoming Multidrug Resistance in Human Lung Cancer with Novel Benzo[a]quinolizin-4-ones. ANTICANCER RES March 2011 31:921-927.
5. Ferreira, R. J., D. dos Santos, M. J. U. Ferreira, R. C. Guedes. Towards a better pharmacophore description of P-glycoprotein modulators, based on macrocyclic diterpenes from Euphorbia species. JOURNAL OF CHEMICAL INFORMATION AND MODELING 51 (6): 1315-1324 JUN 2011
6. Ricardo Jose Diogo Gracio Ferreira. Vencendo a multi-resistância: Modelos computacionais da Glicoproteína-P. Mestrado em Química Farmacéutica e Terapêutica. UNIVERSIDADE DE LISBOA. FACULDADE DE FARMÁCIA. 2011. PhD [www.ff.ul.pt/FCT/PTDC/QEQ.../Tese-Msci2.pdf](http://www.ff.ul.pt/FCT/PTDC/QEQ.../Tese-Msci2.pdf)
7. Jabeen, I. Combined Ligand- and Structure-based Studies on inhibitors of P-glycoprotein DISSERTATION, Dr.-Studium der Naturwissenschaften, University of Wien, Wien, 2011. [othes.univie.ac.at/17980/1/2011-11-15\\_0746423.pdf](https://othes.univie.ac.at/17980/1/2011-11-15_0746423.pdf) PhD
8. Andreia Palmeira. Design, synthesis and evaluation of xanthone derivatives for dual activity: antitumor and P-glycoprotein inhibition. Thesis presented to the Faculdade de Farmácia, Universidade do Porto, Porto, 2011, pp. 1-402. PhD <https://br.123dok.com/document/z31on7my-design-synthesis-and-evaluation-of-xanthone-derivatives-for-dual-activity-antitumor-and-p-glycoprotein-inhibition.html>
9. Campos-Arroyo, D., Martínez-Lazcano, J., Melendez-Zajgla, J. Probenecid is a chemosensitizer in cancer cell lines. CANCER CHEMOTHERAPY AND PHARMACOLOGY, 69 (2):495-504; 10.1007/s00280-011-1725-6 FEB 2012
10. Palmeira, A; Sousa, E; Vasconcelos, MH; Pinto, MM. Three Decades of P-gp Inhibitors: Skimming Through Several Generations and Scaffolds. CURRENT MEDICINAL CHEMISTRY, 19 (13):1946-2025; MAY 2012
11. Ricardo José Ferreira, Maria José Umbelino Ferreira, and Daniel J. V. A. dos Santos. Insights on P-Glycoprotein's Efflux Mechanism obtained by Molecular Dynamics Simulations. JOURNAL OF CHEMICAL THEORY AND COMPUTATION, 8 (6):1853-1864; 10.1021/ct300083m JUN 2012.
12. Thirumurthy Madhavan, Changdev G. gadhe, Gugan Kothandan, Seung Joo Cho.. Enhancement of P-glycoprotein modulators of arylmethylaminephenyl derivatives: an integrative modeling approach. Medicinal Chemistry Research, 2012; 22(5):2511-2523.
13. Orlandi F., M. Coronello, C. Bellucci, S. Dei, L. Guandalini, D. Manetti, C. Martelli, M. N. Romanelli, S. Scapecchi, M. Salerno, H. Menif, I. Bello, E. Mini, E. Teodori, New structure-activity relationship studies in a series of N,N-bis(cyclohexanol)amine aryl esters as potent reversers of P-glycoprotein-mediated Multidrug Resistance (MDR), BIOORGANIC & MEDICINAL CHEMISTRY, 2013 Jan 15;21(2):456-65.
14. J. Dickenson, F. Freeman, CL Mills, S. Sivasubramaniam, C. Thode MG. Darlison. *Molecular Pharmacology: From DNA to Drug Discovery*, Chapter 5: Transporter proteins, 129-173. John Wiley & Sons, 2012, p409. ISBN111845197X, 9781118451977 .
15. Sun YL, Chen JJ, Kumar P, Chen K, Sodani K, Patel A, Chen YL, Chen SD, Jiang WQ, Chen ZS. Reversal of MRP7 (ABCC10)-Mediated Multidrug Resistance by Tariquidar. PLOS ONE, 8 (2):10.1371/journal.pone.0055576 FEB 5 2013.
16. Liu, HM; Ma, ZG; Wu, BJ. Structure-activity relationships and in silico models of P-glycoprotein (ABCB1) inhibitors. XENOBIOTICA, 43 (11):1018-1026; 10.3109/00498254.2013.791003 NOV 2013.
17. Tambunan USF, H Pratomo, AA Parikesit. Modification of Kampmann A5 as Potential Fusion Inhibitor of Dengue Virus using Molecular Docking and Molecular Dynamics Approach. J. MED. SCI, 13 (8), 621-634, 2013.
18. Popeda, M; Pluciennik, E; Bednarek, AK. Proteins in cancer multidrug resistance. POSTĘPY HIGIENY I MEDYCYNY DOSWIADCZALNEJ, 68 616-632; MAY 20 2014. e-ISSN 1732-2693
19. Pati, ML., C Abate, M Contino, S Ferorelli, R Luisi, L. Carroccia, M. Niso, F. Berardi, Deconstruction of 6,7-dimethoxy-1,2,3,4-tetrahydroisoquinoline moiety to separate P-glycoprotein (P-gp) activity from  $\sigma_2$  receptor affinity in mixed P-gp/ $\sigma_2$  receptor agents, EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY, 89, 2015, 691-700.
20. Xu-Qin Li, Lin Wang, Yan Lei, Tao Hu, Fei-Long Zhang, Chi-Hin Cho, Kenneth K.W. To, Reversal of P-gp and BCRP-mediated MDR by tariquidar derivatives, European Journal of Medicinal Chemistry, Volume 101, 28 August 2015, Pages 560-572, ISSN 0223-5234.

21. Cui, HG; Zhang, AJ; Chen, MW; Liu, JJ. ABC Transporter Inhibitors in Reversing Multidrug Resistance to Chemotherapy. *CURRENT DRUG TARGETS*, 16 (12):1356-1371; 10.2174/1389450116666150330113506 2015
22. Kakarla P., M. Inupakutika, A. R. Devireddy, S. K. Gunda, T. M. Willmon, Ranjana KC , U. Shrestha, I. Ranaweera, A. J. Hernandez, S. Barr, M. F. Varela. 3D-QSAR and contour map analysis of tariquidar analogues as multidrug resistance protein-1 (MRP1) inhibitors. *International Journal of Pharmaceutical Sciences A.*, 2016, 11, 554-572. DOI: 10.13040/IJPSR.0975-8232.7(2).554-72
23. Shayanfar, S., Shayanfar, A., Ghandadi, M. Image-Based Analysis to Predict the Activity of Tariquidar Analogs as P-Glycoprotein Inhibitors: The Importance of External Validation. *Archiv der Pharmazie*, 349 (2), pp. 124-131, Feb 2016.
24. Wen Li, Han Zhang, Yehuda G. Assaraf, Kun Zhao, Xiaojun Xu, Jinbing Xie, Dong-Hua Yang, Zhe-Sheng Chen, Overcoming ABC transporter-mediated multidrug resistance: Molecular mechanisms and novel therapeutic drug strategies, *DRUG RESISTANCE UPDATES*, 27 14-29; 10.1016/j.drup.2016.05.001 JUL 2016
25. Miyata, K; Nakagawa, Y; Kimura, Y; Ueda, K; Akamatsu, M. Structure–activity relationships of dibenzoylhydrazines for the inhibition of P-glycoprotein-mediated quinidine transport, *BIOORGANIC & MEDICINAL CHEMISTRY*, 24 (14):3184-3191; 10.1016/j.bmc.2016.05.039 JUL 15 2016.
26. AC. Jaramillo, F. Al Saig, J. Cloos, G. Jansen, G J. Peters. How to overcome ATP-binding cassette drug efflux transporter-mediated drug resistance? *Cancer Drug Resist* v. 1, n. 1, p. 6-29, 2018. <https://cdrjournal.com/article/view/2440>
27. Karthika, C; Sureshkumar, R; Shivasaraun, UV; Vasanthi, C; Nethravathi, P. Plasma glycoprotein efflux induced Resistance: Implications, Mechanism, Inhibitors, and Novel Strategies to Overcome. *ASIAN JOURNAL OF PHARMACEUTICS*, 12 (4):261-271; OCT-DEC 2018
28. S Dei, L Braconi, MN Romanelli, E Teodori. Recent advances in the search of BCRP-and dual P-gp/BCRP-based multidrug resistance modulators. *Cancer Drug Resist* 2019;2:710-743. <http://dx.doi.org/10.20517/cdr.2019.31>
29. Dong Jinyun, Qin Zuodong, Zhang Wei-Dong, Cheng Gang, G. Assaraf Yehuda, R. Ashby Charles, Chen Zhe-Sheng, Cheng Xiang-Dong, Qin Jiang-Jiang, Medicinal Chemistry Strategies to Discover P-glycoprotein Inhibitors: An Update, *Drug Resistance Updates*, 2020,100681, ISSN 1368-7646, <https://doi.org/10.1016/j.drup.2020.100681>.
30. Chenmala Karthika, Raman Sureshkumar (June 3rd 2020). P-Glycoprotein Efflux Transporters and Its Resistance Its Inhibitors and Therapeutic Aspects [Online First], In book: Creatinine - A Comprehensive Update, IntechOpen, DOI: 10.5772/intechopen.90430. <https://www.intechopen.com/online-first/p-glycoprotein-efflux-transporters-and-its-resistance-its-inhibitors-and-therapeutic-aspects>
31. Robinson K., V. Tiriveedhi. Perplexing Role of P-Glycoprotein in Tumor Microenvironment. *Front. Oncol.*, 10, art. no. 265, 05 March 2020 <https://doi.org/10.3389/fonc.2020.00265>
32. Kopecka, J.; Godel, M.; Dei, S.; Giampietro, R.; Belisario, D.C.; Akman, M.; Contino, M.; Teodori, E.; Riganti, C. Insights into P-Glycoprotein Inhibitors: New Inducers of Immunogenic Cell Death. *Cells* **2020**, 9(4),1033; <https://doi.org/10.3390/cells9041033>.
33. Ray R, Kumar V. A review of BCRP inhibitors: An upcoming strategy for cancer treatment, *Ann Trop Med & Public Health*; 23(S15): SP231550; 2020. DOI: <http://doi.org/10.36295/ASRO.2020.231550>
34. Tuyelee Das, Utpal Anand, Swaroop Kumar Pandey, Charles R. Ashby, Yehuda G. Assaraf, Zhe-Sheng Chen, Abhijit Dey, Therapeutic strategies to overcome taxane resistance in cancer, *DRUG RESISTANCE UPDATES*, Volume: 55, Article Number: 100754, MAR 2021, <https://doi.org/10.1016/j.drup.2021.100754>
35. Smolinski, M.P., Uргаonkar, S., Pitzonka, L. Cutler, M. Lee, G., Suh, K.H., Lau, J.Y.N., Discovery of Encequidar, First-in-Class Intestine Specific P-glycoprotein Inhibitor. *JOURNAL OF MEDICINAL CHEMISTRY* Volume: 64 Issue: 7 Pages: 3677-3693 Published: APR 8 2021 <https://doi.org/10.1021/acs.jmedchem.0c01826>

**43. Pencheva T, O.S, Soumana, I. Pajeva , M.A. Miteva. Post-docking virtual screening of diverse binding pockets: Comparative study using DOCK, AMMOS, X-Score and FRED scoring functions. *Eur. J. Med. Chem.* 2010, 45, 2622–2628.**

Цитирания: 14

1. Korb O, Ten Brink T, Victor Paul Raj FR, Keil M, Exner TE. Are predefined decoy sets of ligand poses able to quantify scoring function accuracy? *JOURNAL OF COMPUTER-AIDED MOLECULAR DESIGN*, 26 (2):185-197; 10.1007/s10822-011-9539-5 FEB 2012
2. Cavasotto C.N. Binding Free Energy Calculation and Scoring in Small Molecule Docking, Chapter 8 In: *PHYSICO-CHEMICAL AND COMPUTATIONAL APPROACHES TO DRUG DISCOVERY* (Eds. Javier

- Luque, Xavier Barril, David E Thurston, David Rotella, David Fox), Royal Society of Chemistry, 2012, 23, 195-225. 10.1039/9781849735377-00195 2012.
3. Mantsyzov AB, G Bouvier, N Evrard-Todeschi, G Bertho. Contact-based ligand-clustering approach for the identification of active compounds in virtual screening. *ADV APPL BIOINFORM CHEM.* 2012; 5: 61–79. Published online 2012.
  4. Koseki, Y; Kinjo, T; Kobayashi, M; Aoki, S. Identification of novel antimycobacterial chemical agents through the in silico multi-conformational structure-based drug screening of a large-scale chemical library. *EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY*, 60 333-339; 10.1016/j.ejmech.2012.12.012 FEB 2013.
  5. Yuriev, E; Ramsland, PA. Latest developments in molecular docking: 2010-2011 in review. *JOURNAL OF MOLECULAR RECOGNITION*, 26 (5):215-239; 10.1002/jmr.2266 MAY 2013.
  6. Ding Z, L Kang, X Cao. Application of docking methods for metal chelate affinity precipitation of endo-glucanase using pH-response polymer. *COLLOIDS AND SURFACES B-BIOINTERFACES*, 113 412-420; 10.1016/j.colsurfb.2013.09.041 JAN 1 2014
  7. Koseki, Y; Aoki, S. Computational Medicinal Chemistry for Rational Drug Design: Identification of Novel Chemical Structures with Potential Anti-Tuberculosis Activity. *CURRENT TOPICS IN MEDICINAL CHEMISTRY*, 14 (1):176-188; JAN 2014
  8. Yan Li, Li Han, Zhihai Liu, and Renxiao Wang. Comparative Assessment of Scoring Functions on an Updated Benchmark: II. Evaluation Methods and General Results. *JOURNAL OF CHEMICAL INFORMATION AND MODELING*, 2014, 54 (6), pp 1717–1736. DOI: 10.1021/ci500081m Publication Date (Web): April 7, 2014
  9. Uddin, R., Saeed, K., An exhaustive yet simple virtual screening campaign against Sortase A from multiple drug resistant *Staphylococcus aureus*. *MOLECULAR BIOLOGY REPORTS*, 2014 May 6, 41(8), 5167-5175.
  10. Montesano, C., Sergi, M., Perez, G., Curini, R., Compagnone, D., Mascini, M. Bio-inspired solid phase extraction sorbent material for cocaine: A cross reactivity study. *TALANTA*, 2014, 130, pp. 382-387.
  11. Yin L, Zheng L, Xu L, Dong D, Han X, Qi Y, Zhao Y, Xu Y, Peng J. In-silico prediction of drug targets, biological activities, signal pathways and regulating networks of dioscin based on bioinformatics. *BMC Complement Altern Med.* 2015 Mar 5; **15** (1), art. no. 41. doi: 10.1186/s12906-015-0579-6.
  12. Ding, ZY; Li, SP; Cao, XJ. Microbial Transglutaminase Separation by pH-Responsive Affinity Precipitation with Crocein Orange G as the Ligand. *APPLIED BIOCHEMISTRY AND BIOTECHNOLOGY*, 177 (1):253-266; 10.1007/s12010-015-1742-8 SEP 2015
  13. Cao Y., Dai W., Miao Z. Evaluation of Protein–Ligand Docking by Cyscore. In: Gore M., Jagtap U. (eds) *Computational Drug Discovery and Design. Methods in Molecular Biology*, Humana Press, New York, NY, vol 1762. pp 233-243, 2018.
  14. Yunsheng Yuan. Mechanisms Inspired Targeting Peptides. Book Series: *Advances in Experimental Medicine and Biology*, Volume: 1248, Pages: 531-546 2020.
- 44. Pick, A., H. Müller, R. Mayer, B. Haenisch, I.K. Pajeva, M. Weight, H. Bönisch, C. E. Müller, M. Wiese. Structure-Activity Relationships of Flavonoids ss Inhibitors of Breast Cancer Resistance Protein (BCRP). *Bioorg. Med. Chem.* 2011, 19(6), 2090-2102.**

Цитирания: 153

1. Khan M.S., D. Halagowder, S. N. Devaraj. Methylated chrysin induces co-ordinated attenuation of the canonical Wnt and NF-kB signaling pathway and upregulates apoptotic gene expression in the early hepatocarcinogenesis rat model. *CHEM BIOL INTERACT.* 2011 Aug 15; 193(1), 12-21.
2. Catherine Anne Mowbray. In vitro systems to predict hepatotoxicity: models based on hepatocarcinoma cell lines. Thesis for the degree of Doctor of Philosophy. Newcastle University, Faculty of Medical Sciences, Institute of Cell and Molecular Biosciences, Epithelial Research Group, August 2011. PhD
3. Fei X, S Xie, S Hu, X Zeng, Y Zou, J Zhao, L Xiang, G Xu, X Zhou. Experimental observation on antihypertensive ability of total flavonoids from Jumi in spontaneously hypertensive rats. In: *Human Health and Biomedical Engineering (HHBE)*, International Conference, Jilin, 19-22 Aug 2011, pp. 912-915, 2011. Print ISBN: 978-1-61284-723-8.
4. Moreno-Sanz, G., B Barrera, A Guijarro, I d'Elia, J Andoni Otero, A I. Alvarez, T Bandiera, G Merino, D Piomelli, The ABC membrane transporter ABCG2 prevents access of FAAH inhibitor URB937 to the central nervous system. *PHARMACOLOGICAL RESEARCH*, 2011 Oct;64(4):359-63.
5. Xu GT, XW Wu, XM Zhou, SP Chen, SR Shen, Experimental Observation on Antiatherosclerosis Ability of Total Flavonoids from Jumi in Hyperlipidemia Rats. *APPLIED MECHANICS AND MATERIALS*, Vol. 140, 2011, 137-141

6. De Paula CAA, Coulson-Thomas VJ, Ferreira JG, Maza PK, Suzuki E, Nakahata AM, Nader HB, Sampaio MU, Oliva ML. EcTI, a plant proteinase inhibitor, decreases in vitro cell adhesion and invasion by inhibition of Src-FAK signaling pathways. *J BIOL CHEM.* 287 (1), 170-182, 2012.
7. Wu LX, Guo CX, Qu Q, Yu J, Chen WQ, Wang G, Fan L, Li Q, Zhang W, Zhou HH. Effects of natural products on the function of human organic anion transporting polypeptide 1B1. *XENOBIOTICA*, 42 (4):339-348; APR 2012
8. Valdameri, G; Genoux-Bastide, E; Peres, B; Gauthier, C; Guitton, J; Terreux, R; Winnischofer, SMB; Rocha, MEM; Boumendjel, A; Di Pietro, A. Substituted chromones as highly-potent nontoxic inhibitors, specific for the breast cancer resistance protein. *JOURNAL OF MEDICINAL CHEMISTRY*, 55 (2):966-970; JAN 26 2012.
9. Choi, EJ; Lee, JI; Kim, GH. Evaluation of the anticancer activities of thioflavanone and thioflavone in human breast cancer cell lines. *INTERNATIONAL JOURNAL OF MOLECULAR MEDICINE*, 29 (2):252-256; 10.3892/ijmm.2011.834 FEB 2012
10. Kruzlicova D,M. Danihelova, M. Veverka. Quantitative structure-antioxidant activity relationship of quercetin and its new synthesized derivatives. *NOVA BIOTECHNOLOGICA ET CHIMICA* 11-1 (2012), 37-44.
11. Chirumbolo, S. Plant phytochemicals as new potential drugs for immune disorders and cancer therapy: really a promising path?. *JOURNAL OF THE SCIENCE OF FOOD AND AGRICULTURE*, 92 (8):1573-1577; 10.1002/jsfa.5670 JUN 2012.
12. Speck-Planche A. V.V. Kleandrova, F. Luan, M.Natália D.S. Cordeiro, Chemoinformatics in anti-cancer chemotherapy: Multi-target QSAR model for the in silico discovery of anti-breast cancer agents, *EUROPEAN JOURNAL OF PHARMACEUTICAL SCIENCES*, 47 (1):273-279; 10.1016/j.ejps.2012.04.012 AUG 30 2012
13. Ebert, SP; Wetzel, B; Myette, RL; Conseil, G; Cole, SPC; Sawada, GA; Loo, TW; Bartlett, MC; Clarke, DM; Detty, MR. Chalcogenopyrylium Compounds as Modulators of the ATP-Binding Cassette Transporters P-glycoprotein (P-gp/ABCB1) and Multidrug Resistance Protein 1 (MRP1/ABCC1). *JOURNAL OF MEDICINAL CHEMISTRY*, 55 (10):4683-4699; 10.1021/jm3004398 MAY 24 2012
14. Li, Yan; Lu, Jun; Paxton, James W. The role of ABC and SLC transporters in the pharmacokinetics of dietary and herbal phytochemicals and their interactions with xenobiotics. *CURRENT DRUG METABOLISM* (2012), 13(5), 624-639.
15. Shih, TL; Hsiao, CA; Lin, ZY; Chen, YH. An Alternative Synthesis of 3',4'-Diaminoflavones to Evaluate Their Antioxidant Ability and Cell Apoptosis of Zebrafish Larvae. *MOLECULES*, 17 (7):8206-8216; 10.3390/molecules17078206 JUL 2012.
16. Valdameri, Glaucio. Avaliação da morte celular induzida por flavonas em células HepG2 e identificação de novos inibidores de ABCG2. Teses e Dissertações. Universidade Federal do Paraná, Brazil. Setor de Ciências Biológicas. Programa de Pós-Graduação em Bioquímica, August 2012. PhD
17. Mercader, AG; Pomilio, AB. (Iso)Flav(an)ones, Chalcones, Catechins, and Theaflavins as Anticarcinogens: Mechanisms, Anti-Multidrug Resistance and QSAR Studies. *CURRENT MEDICINAL CHEMISTRY*, 19 (25):4324-4347; SEP 2012
18. Kar, S; Roy, K. QSAR of phytochemicals for the design of better drugs. *EXPERT OPINION ON DRUG DISCOVERY*, 7 (10):877-902; 10.1517/17460441.2012.716420 OCT 2012.
19. Michalak, K; Wesolowska, O. Polyphenols Counteract Tumor Cell Chemoresistance Conferred by Multidrug Resistance Proteins. *ANTI-CANCER AGENTS IN MEDICINAL CHEMISTRY*, 12 (8):880-890; OCT 2012.
20. Dyrager, Christine. Design and Synthesis of Chalcone and Chromone Derivatives as Novel Anticancer Agents. Doctoral thesis. University of Gothenburg. Sweden . Faculty of Science, Department of Chemistry, 2012. PhD
21. Aspenström-Fagerlund, Bitte (2012). Dietary fatty acids increase the absorption of toxic substances and drugs by modifying different absorption pathways in the intestinal epithelium. Diss. (sammanfattning/summary) Uppsala : Sveriges lantbruksuniv., Acta Universitatis agriculturae Sueciae, 1652-6880 ; 2012:88 ISBN 978-91-576-7735-8 PhD
22. Jiang, W., Hu, M. Mutual interactions between flavonoids and enzymatic and transporter elements responsible for flavonoid disposition via phase II metabolic pathways. *RSC ADVANCES* 2 (21) , pp. 7948-7963, 2012.
23. Scotti, L; Mendonca, FJB; Moreira, DRM; da Silva, MS; Pitta, IR; Scotti, MT. SAR, QSAR and Docking of Anticancer Flavonoids and Variants: A Review. *CURRENT TOPICS IN MEDICINAL CHEMISTRY*, 12 (24):2785-2809; DEC 2012.

24. Sadeghi-Aliabadi H, Mosavi H, Mirian M, Kakhki S, Zarghi A. The Cytotoxic and Synergistic Effects of Flavonoid Derivatives on Doxorubicin Cytotoxicity in Hela, MDA-MB-231, and HT-29 Cancer Cells. *IJT*. 2012; 5 (15) :558-564.
25. Beretta, GL; Gatti, L; Perego, P; Zaffaroni, N. Camptothecin Resistance in Cancer: Insights into the Molecular Mechanisms of a DNA-Damaging Drug. *CURRENT MEDICINAL CHEMISTRY*, 20 (12):1541-1565; APR 2013
26. Tan KW, Y Li, JW Paxton, NP Birch, A Scheepens. Identification of novel dietary phytochemicals inhibiting the efflux transporter breast cancer resistance protein (BCRP/ABCG2). *FOOD CHEMISTRY*, volume 138, issue 4, 2267 – 2274, 2013.
27. Guo, R.-X., Li, L.-G., Huo, C.-H., Li, Z., Shi, Q.-W. Semisynthesis and structure-activity relationship of O-methylated derivatives of quercetin. *CHINESE TRADITIONAL AND HERBAL DRUGS*, 44 (3), pp. 359-369, 2013.
28. Ekinci, D; Karagoz, L; Ekinci, D; Senturk, M; Supuran, CT. Carbonic anhydrase inhibitors: in vitro inhibition of alpha isoforms (hCA I, hCA II, bCA III, hCA IV) by flavonoids. *JOURNAL OF ENZYME INHIBITION AND MEDICINAL CHEMISTRY*, 28 (2):283-288; 10.3109/14756366.2011.643303 APR 2013.
29. Pan, YM; Chothe, PP; Swaan, PW. Identification of Novel Breast Cancer Resistance Protein (BCRP) Inhibitors by Virtual Screening. *MOLECULAR PHARMACEUTICS*, 10 (4):1236-1248; 10.1021/mp300547h APR 2013.
30. Sedykh, A; Fourches, D; Duan, JM; Hucke, O; Garneau, M; Zhu, H; Bonneau, P; Tropsha, A. Human Intestinal Transporter Database: QSAR Modeling and Virtual Profiling of Drug Uptake, Efflux and Interactions. *PHARMACEUTICAL RESEARCH*, 30 (4):996-1007; 10.1007/s11095-012-0935-x APR 2013.
31. Gonzalez-Sarrias, A; Miguel, V; Merino, G; Lucas, R; Morales, JC; Tomas-Barberan, F; Alvarez, AI; Espin, JC. The Gut Microbiota Ellagic Acid-Derived Metabolite Urolithin A and Its Sulfate Conjugate Are Substrates for the Drug Efflux Transporter Breast Cancer Resistance Protein (ABCG2/BCRP). *JOURNAL OF AGRICULTURAL AND FOOD CHEMISTRY*, 61 (18):4352-4359; 10.1021/jf4007505 MAY 8 2013.
32. Xu, Y; Shen, Q; Liu, X; Lu, J; Li, S; Luo, C; Gong, L; Luo, X; Zheng, M; Jiang, H. Computational Models for Predicting Interactions with Membrane Transporters. *CURRENT MEDICINAL CHEMISTRY*, 20 (16):2118-2136; MAY 2013.
33. Stuurman, FE; Nuijen, B; Beijnen, JH; Schellens, JHM. Oral Anticancer Drugs: Mechanisms of Low Bioavailability and Strategies for Improvement. *CLINICAL PHARMACOKINETICS*, 52 (6):399-414; 10.1007/s40262-013-0040-2 JUN 2013.
34. Zhou, YX; Lu, N; Zhang, HW; Wei, LB; Tao, L; Dai, QS; Zhao, L; Lin, BQ; Ding, QL; Guo, QL. HQS-3, a newly synthesized flavonoid, possesses potent anti-tumor effect in vivo and in vitro, *EUROPEAN JOURNAL OF PHARMACEUTICAL SCIENCES*, 49 (4), 649-658. 16 July 2013. <http://dx.doi.org/10.1016/j.ejps.2013.04.016>.
35. Kapoor K., H.M. Sim, S.V. Ambudkar. Multidrug resistance in cancer: a tale of ABC drug transporters. In: *Molecular Mechanisms of Tumor Cell Resistance to Chemotherapy*, Resistance to Targeted Anti-Cancer Therapeutics 1 (B. Bonavida (ed.), Springer Science+Business Media New York, 2013, pp.1-34.
36. Yue, RC; Li, B; Shen, YH; Zeng, HW; Li, B; Yuan, H; He, YR; Shan, L; Zhang, WD. 6-C-Methyl Flavonoids Isolated from *Pinus densata* Inhibit the Proliferation and Promote the Apoptosis of the HL-60 Human Promyelocytic Leukaemia Cell Line. *PLANTA MEDICA*, 79 (12):1024-1030; 10.1055/s-0033-1350617 AUG 2013.
37. Kee Wee Tan. Studies on the Interactions between Breast Cancer Resistance Protein (BCRP/ABCG2) and Dietary Phytochemicals: Implications for Phytochemical Bioavailability. A thesis for the degree of doctor of philosophy in biological sciences the University of Auckland, 2013, pp.362 PhD
38. Derya Ekinci , Lutfi Karagoz , Deniz Ekinci , Murat Senturk , Claudiu T. Supuran Carbonic anhydrase inhibitors: in vitro inhibition of  $\alpha$  isoforms (hCA I, hCA II, bCA III, hCA IV) by flavonoids. *Journal of Enzyme Inhibition and Medicinal Chemistry*, Vol. 28, Iss. 2, 2013
39. Tang L., Y Li, WY Chen, S Zeng, LN Dong, XJ Peng, W. Jiang, M. Hu, ZQ Liu. Breast Cancer Resistance Protein-Mediated Efflux of Luteolin Glucuronides in HeLa Cells Overexpressing UDP-Glucuronosyltransferase 1A9. *PHARMACEUTICAL RESEARCH*, 31 (4):847-860; 10.1007/s11095-013-1207-0 APR 2014.
40. Vuppalapati, SVN; Xia, LK; Edayadulla, N; Lee, YR. Mild and efficient one-pot synthesis of diverse flavanone derivatives via an organocatalyzed Mannich-type reaction. *SYNTHESIS-STUTTGART*, 46 (4):465-474; 10.1055/s-0033-1340466 FEB 2014

41. Liu Y., X Song, J He, X Zheng, H Wu. Synthetic derivatives of chrysin and their biological activities. *MEDICINAL CHEMISTRY RESEARCH*, 23 (2):555-563; 10.1007/s00044-013-0711-4 FEB 2014.
42. Liu, X; Yang, DL; Liu, JJ; Xu, K; Wu, GH. Modeling of supercritical fluid extraction of flavonoids from *Calycopteris floribunda* leaves. *CHEMICAL PAPERS*, 68 (3):316-323; 10.2478/s11696-013-0451-4 MAR 2014.
43. Gupta, VK; Bhalla, Y; Jaitak, V. Impact of ABC transporters, glutathione conjugates in MDR and their modulation by flavonoids: an overview. *MEDICINAL CHEMISTRY RESEARCH*, 23 (1):1-15; 10.1007/s00044-013-0612-6 JAN 2014
44. Ding Y-L, Shih Y-H, Tsai F-Y, Leong MK. *In Silico* Prediction of Inhibition of Promiscuous Breast Cancer Resistance Protein (BCRP/ABCG2). *PLoS ONE* 9(3): e90689. 2014, doi:10.1371/journal.pone.0090689
45. Nebo, L., Varela, R.M., Molinillo, J.M.G., Sampaio, O.M., Severino, V.G.P., Cazal, C.M., Fernandes, M.F.D.G., Fernandes, J.B., Macías, F.A. Phytotoxicity of alkaloids, coumarins and flavonoids isolated from 11 species belonging to the Rutaceae and Meliaceae families, *PHYTOCHEMISTRY LETTERS*, 8 226-232; 10.1016/j.phytol.2014.02.010 MAY 2014
46. Lin Y, Liu HL, Fang J, Yu CH, Xiong YK, Yuan K. Anti-fatigue and vasoprotective effects of quercetin-3-O-gentiobiose on oxidative stress and vascular endothelial dysfunction induced by endurance swimming in rats. *FOOD AND CHEMICAL TOXICOLOGY*, 68 290-296; 10.1016/j.fct.2014.03.026 JUN 2014.
47. Barrera Cuesta, Borja. Interacción del antihelmíntico triclabendazol, el analgésico URB937 y sus derivados con transportadores de membrana dependientes de ATP. Facultad de Veterinaria, Universidad de Leon, Spain. 2014-02-13. PhD . <http://hdl.handle.net/10612/3262>
48. Montanari, F., Ecker, GF. BCRP Inhibition: from Data Collection to Ligand-Based Modeling. *MOLECULAR INFORMATICS*, 33 (5):322-331; 10.1002/minf.201400012 MAY 2014.
49. Pinto M., D Digles, GF. Ecker. Computational models for predicting the interaction with ABC transporters. *DRUG DISCOVERY TODAY: TECHNOLOGIES*, 12, 2014, e69-e77. <http://dx.doi.org/10.1016/j.ddtec.2014.03.007>
50. Xiao, JB; Muzashvili, TS; Georgiev, MI. Advances in the biotechnological glycosylation of valuable flavonoids, *BIOTECHNOLOGY ADVANCES*, 2014 Nov 1;32(6):1145-56. doi: 10.1016/j.biotechadv.2014.04.006. Epub 2014 Apr 26.
51. Khandelwal K, Gangwal RP, Singh U., Prajapati R., Damre MV, Sangamwar AT. Computational insights into the active site of human breast cancer resistance protein (BCRP/ABCG2): a similarity search approach. *MEDICINAL CHEMISTRY RESEARCH*, 23 (11):4657-4668; 10.1007/s00044-014-1035-8 NOV 2014
52. J Xiao, T Chen, H Cao. Flavonoid glycosylation and biological benefits. *BIO-TECHNOLOGY ADVANCES*, 2014 May 22. pii: S0734-9750(14)00092-5. doi: 10.1016/j.biotechadv.2014.05.004
53. Szafraniec, MJ; Szczygiel, M; Urbanska, K; Fiedor, L. Determinants of the activity and substrate recognition of breast cancer resistance protein (ABCG2). *DRUG METABOLISM REVIEWS*, 46 (4):459-474; 10.3109/03602532.2014.942037 NOV 2014
54. Isoda, H., Motojima, H., Onaga, S., Samet, I., Villareal, M.O., Han, J. Analysis of the erythroid differentiation effect of flavonoid apigenin on K562 human chronic leukemia cells (2014) *CHEMICO-BIOLOGICAL INTERACTIONS*, 220, pp. 269-277.
55. Tome S.M., A.M.S. Silva, C.M.M. Santos. Synthesis and Transformation of Halochromones. *CURRENT ORGANIC SYNTHESIS*, 11 (3), 317-341, 2014.
56. Videira, M., Reis, R.L., Brito, M.A. Deconstructing breast cancer cell biology and the mechanisms of multidrug resistance. *BIOCHIMICA ET BIOPHYSICA ACTA-REVIEWS ON CANCER*, 1846 (2):312-325; 10.1016/j.bbcan.2014.07.011 DEC 2014
57. Hamzeh-Mivehroud, M., Rahmani, S., Feizi, M.-A.H., Dastmalchi, S., Rashidi, M.-R. In Vitro and in Silico studies to explore structural features of flavonoids for aldehyde oxidase inhibition. *ARCHIV DER PHARMAZIE*, 347 (10), 2014, pp. 738-747.
58. Nikalje, APG; Shaikh, SI; Mulay, A; Khan, FAK; Sangshetti, JN; Shaikh, S. Ultrasound-Assisted Synthesis, Anticonvulsant Activity, and Docking Study of Indole-Appended Thiazolidin-4-ones. *ARCHIV DER PHARMAZIE*, 347 (10):756-767; 10.1002/ardp.201400148 OCT 2014.
59. Jezrael Lafuente Revalde. The inhibition of ABC transporters in cancer multidrug resistance by heterocyclic heterocyclic cyclohexanone analogues of curcumin. PhD thesis, The University of Auckland, 2014. <http://researchspace.auckland.ac.nz> PhD
60. Tawfik, Hanaa A., Ewies F. Ewies, and Wageeh S. El-Hamouly. Synthesis of chromones and their applications during the last ten years. *INTERNATIONAL JOURNAL OF RESEARCH IN PHARMACY AND CHEMISTRY (IJRPC)*, 2014, 4(4), 1046-1085.

61. Basseville, A; Robey, RW; Bahr, JC; Bates, SE. Breast Cancer Resistance Protein (BCRP) or ABCG2. In: *Drug Transporters: Molecular Characterization and Role in Drug Disposition*, Second Edition. Edited by Guofeng You and Marilyn E. Morris. © 2014 John Wiley & Sons, Inc. Published 2014 by John Wiley & Sons, Inc., 187-221. ISBN: 978-1-118-48993-2
62. Abdallah, H.M., Al-Abd, A.M., El-Dine, R.S., El-Halawany, A.M. P-glycoprotein inhibitors of natural origin as potential tumor chemo-sensitizers: A review, *JOURNAL OF ADVANCED RESEARCH*, 6(1), 45-62, 2015. ISSN 2090-1232.
63. Nebo L, Varela RM, Molinillo JM, Severino VG, Sarria AL, Cazal CM, Fernandes MF, Fernandes JB, Macías FA. Phytotoxicity of triterpenes and limonoids from the Rutaceae and Meliaceae.  $5\alpha,6\beta,8\alpha,12\alpha$ -Tetrahydro-28-norisotoonafolin--a potent phytotoxin from *Toona ciliata*. *Nat Prod Commun*. 2015 Jan;10(1):17-20.
64. Zhou, Y., Wei, L., Zhang, H., Dai, Q., Li, Z., Yu, B., Guo, Q., Lu, N., FV-429 induced apoptosis through ROS-mediated ERK2 nuclear translocation and p53 activation in gastric cancer cells. *JOURNAL OF CELLULAR BIOCHEMISTRY*, 116 (8):1624-1637; 10.1002/jcb.25118 AUG 2015
65. Bhaumik A., B. Ramu, Sk. Basheer, P. Das, J. Mastanaiah. Synthetic novel flavonoid derivatives act as potential antineoplastic agent. *International Journal of Medicine and Pharmaceutical Research*, 2015, 3 (2), 956-961.
66. Kaur M, Badhan RK. Phytoestrogens Modulate Breast Cancer Resistance Protein Expression and Function at the Blood-Cerebrospinal Fluid Barrier. *JOURNAL OF PHARMACY AND PHARMACEUTICAL SCIENCES*, 18 (2):132-154; 2015.
67. Gaudêncio, S.P., Pereira, F. Dereplication: Racing to speed up the natural products discovery process. *NATURAL PRODUCT REPORTS*, 32 (6):779-810; 10.1039/c4np00134f 2015
68. Belekar, Vilas; Lingineni, Karthik; Garg, Prabha. Classification of Breast Cancer Resistant Protein (BCRP) Inhibitors and Non-Inhibitors Using Machine Learning Approaches. *COMBINATORIAL CHEMISTRY & HIGH THROUGHPUT SCREENING* Volume: 18 Issue: 5 Pages: 476-485 Published: 2015
69. Gonzales, G.B., Smagge, G., Grootaert, C., Zotti, M., Raes, K., Camp, J.V. Flavonoid interactions during digestion, absorption, distribution and metabolism: A sequential structure-activity/property relationship-based approach in the study of bioavailability and bioactivity. *DRUG METABOLISM REVIEWS*, 47 (2):175-190; 10.3109/03602532.2014.1003649 2015
70. Ma, LP; Qin, YH; Shen, ZW; Bi, HC; Hu, HY; Huang, M; Zhou, H; Yu, LS; Jiang, HD; Zeng, S. Aristolochic acid I is a substrate of BCRP but not P-glycoprotein or MRP2, *JOURNAL OF ETHNOPHARMACOLOGY*, 172, 430-435; 10.1016/j.jep.2015.07.011 AUG 22 2015.
71. Bircsak, KM; Aleksunes, LM. Interaction of Isoflavones with the BCRP/ABCG2 Drug Transporter. *CURRENT DRUG METABOLISM*, 16 (2):124-140; 2015.
72. Arroyo-Acevedo, J., Chávez-Asmat, R.J., Anampa-Guzmán, A., Donaires, R., Ráez-González, J. Protective effect of piper aduncum capsule on DMBA-induced breast cancer in rats. *BREAST CANCER-BASIC AND CLINICAL RESEARCH*, 9 10.4137/BCBCR.S24420 2015
73. Wang, YL; Xing, J; Xu, Y; Zhou, NN; Peng, JL; Xiong, ZP; Liu, X; Luo, XM; Luo, C; Chen, KX; Zheng, MY; Jiang, HL. In silico ADME/T modelling for rational drug design. *QUARTERLY REVIEWS OF BIOPHYSICS*, 48 (4):488-515; NOV 2015
74. Rani N, Velan LP, Vijaykumar S, Arunachalam A.. An insight into the potentially old-wonder molecule—quercetin: the perspectives in foresee. *Chinese Journal of Integrative Medicine*, pp. 1-16. First online: 09 September 2015. <http://dx.doi.org/10.1007/s11655-015-2073-x>
75. Wang, S.-H., Chen, C.-H., Lo, C.-Y., Feng, J.-Z., Lin, H.-J., Chang, P.-Y., Yang, L.-L., Chen, L.-G., Liu, Y.-W., Kuo, C.-D., Wu, J.-Y. Synthesis and biological evaluation of novel 7-O-lipophilic substituted baicalein derivatives as potential anticancer agents(2015) *MEDCHEMCOMM*, 6 (10):1864-1873; 10.1039/c5md00163c 2015.
76. K Devika , Soma Acharjee , M Krishnaveni , Shibu Das. Synthesis, Characterization and Evaluation of In vivo Hepatoprotective Activity of Some Novel Flavonoid Derivatives. *Indo American Journal of Pharmacy*, 1(1), 15-21, 2015.
77. Di, L., Kerns, E.H. *Drug-Like Properties: Concepts, Structure Design and Methods from ADME to Toxicity Optimization*(2016) *Drug-Like Properties: Concepts, Structure Design and Methods from ADME to Toxicity Optimization*, pp. 1-560.
78. Wu, X; Ma, J; Ye, Y; Lin, G. Transporter modulation by Chinese herbal medicines and its mediated pharmacokinetic herb–drug interactions, *JOURNAL OF CHROMATOGRAPHY B-ANALYTICAL TECHNOLOGIES IN THE BIOMEDICAL AND LIFE SCIENCES*, Volume 1026, 24 August 2015, Pages 236-253, JUL 15 2016

79. Li, YQ; Yang, F; Wang, L; Cao, Z; Han, TJ; Duan, ZA; Li, Z; Zhao, WJ. Phosphoramidate protides of five flavones and their antiproliferative activity against HepG2 and L-O2 cell lines. EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY, 112 196-208; 10.1016/j.ejmech.2016.02.012 APR 13 2016.
80. Martínez-Pérez, C., Ward, C., Turnbull, A.K., Mullen, P., Cook, G., Meehan, J., Jarman, E.J., Thomson, P.I.T., Campbell, C.J., McPhail, D., J Harrison, D., P Langdon, S. Antitumour activity of the novel flavonoid Oncamex in preclinical breast cancer models. BRITISH JOURNAL OF CANCER, 114 (8):905-916; 10.1038/bjc.2016.6 APR 13 2016
81. Fang, YJ; Lu, YL; Zang, XX; Wu, T; Qi, XJ; Pan, SY; Xu, XY. 3D-QSAR and docking studies of flavonoids as potent Escherichia coli inhibitors. SCIENTIFIC REPORTS, 6, art. no. 23634, 2016.
82. Dai, YQ; Ma, T; Ge, M; Li, J; Huo, Q; Li, HM; Zhang, XY; Liu, H; Wu, CZ Enzymatic Synthesis of Novel Bavachinin Glucoside by UDP-glycosyltransferase JOURNAL OF THE CHINESE CHEMICAL SOCIETY, 63 (4):376-378; 10.1002/jccs.201500497 APR 2016
83. Shipra Kalra, Kanav Midha, Sarbjit Kaur. Purification of Quercetin by HPLC from green tea leaves and its application in cancer therapy. Indian Journal of Research in Pharmacy and Biotechnology, 4(2), 2016, 77.
84. Fei, GS; Fan, XF; Ma, HP; Fan, PC; Jia, ZP; Jing, LL. Synthesis of Glycosylated Chrysin Derivatives Via Ester Linkers. CHEMISTRY OF NATURAL COMPOUNDS, 52 (4):602-610; 10.1007/s10600-016-1721-5 JUL 2016
85. Ali, W.K., Ihoual, S., Abidli, N. Antioxidant and MDR reversal activity in resistant human ovarian cancer cells of methanolic extract from Ruta Montana located in the North of Algeria (2016) Der Pharma Chemica, 8 (12), pp. 215-223.
86. Lungare, S; Hallam, K; Badhan, RKS. Phytochemical-loaded mesoporous silica nanoparticles for nose-to-brain olfactory drug delivery, INTERNATIONAL JOURNAL OF PHARMACEUTICS, 513 (1-2):280-293; 10.1016/j.ijpharm.2016.09.042 NOV 20 2016
87. P Chakraborty, M Ramakrishnan. Role of P-glycoprotein in Chemotherapeutic Drug Resistance and Mechanisms of Pump Deactivation to Overcome MDR in Cancer Cells—A Critical. Frontiers in Biomedical Sciences, Vol. 1, No. 2, 2016, pp. 31-38.
88. Yu, J; Zhou, P; Asenso, J; Yang, XD; Wang, C; Wei, W. Advances in plant-based inhibitors of P-glycoprotein. JOURNAL OF ENZYME INHIBITION AND MEDICINAL CHEMISTRY, 31 (6):867-881; 10.3109/14756366.2016.1149476, 2016.
89. Noora Sjöstedt, Kira Holvikari, Päivi Tammela, and Heidi Kidron. Inhibition of BCRP and MRP2 by natural compounds and their derivatives. *Molecular Pharmaceutics* Just Accepted Manuscript DOI:10.1021/acs.molpharmaceut.6b00754
90. Zeng X, Shi J, Zhao M, Chen Q, Wang L, Jiang H, et al. (2016) Regioselective Glucuronidation of Diosmetin and Chrysoeriol by the Interplay of Glucuronidation and Transport in UGT1A9-Overexpressing HeLa Cells. PLOS ONE, 11 (11):10.1371/journal.pone.0166239 NOV 10 2016-
91. Andrade, PB; Grosso, C; Valentao, P; Bernardo, J. Flavonoids in Neurodegeneration: Limitations and Strategies to Cross CNS Barriers. CURRENT MEDICINAL CHEMISTRY, 23 (36):4151-4174; 10.2174/0929867323666160809094934 2016.
92. Kamlesh KN, Sivakumar T, Afroze A. Antimicrobial Activity of Flavone Analogues. J App Pharm 9:232. doi: 10.21065/1920-4159.1000232, 2016
93. Li, Y; Revalde, J; Paxton, JW. The effects of dietary and herbal phytochemicals on drug transporters, ADVANCED DRUG DELIVERY REVIEWS, 116 45-62; 10.1016/j.addr.2016.09.004 JUL 1 2017.
94. Pena-Solorzano, D; Stark, SA; Konig, B; Sierra, C; Ochoa-Puentes, C ABCG2/BCRP: Specific and Nonspecific Modulators. MEDICINAL RESEARCH REVIEWS, 37 (5):987-1050; 10.1002/med.21428 SEP 2017.
95. Kaur, M; Badhan, RKS. Phytochemical mediated-modulation of the expression and transporter function of breast cancer resistance protein at the blood-brain barrier: An in-vitro study, BRAIN RESEARCH, 1654 9-23; 10.1016/j.brainres.2016.10.020 A JAN 1 2017
96. Machado, NFL; Dominguez-Perles, R. Addressing Facts and Gaps in the Phenolics Chemistry of Winery By-Products. MOLECULES, 22 (2):10.3390/molecules22020286 FEB 2017.
97. Sjöstedt, N; Holvikari, K; Tammela, P; Kidron, H. Inhibition of Breast Cancer Resistance Protein and Multidrug Resistance Associated Protein 2 by Natural Compounds and Their Derivatives. MOLECULAR PHARMACEUTICS, 14 (1):135-146; 10.1021/acs.molpharmaceut.6b00754 JAN 2017
98. Dash, AK; Madhubabu, T; Yousuf, SK; Raina, S; Mukherjee, D. One-pot Mukaiyama type carbon-Ferrier rearrangement of glycals: Application in the synthesis of chromanone 3-C-glycosides. CARBOHYDRATE RESEARCH, 438 1-8; 10.1016/j.carres.2016.11.018 JAN 13 2017

99. Huang, JT; Cheng, YY; Lin, LC; Tsai, TH. Structural Pharmacokinetics of Polymethoxylated Flavones in Rat Plasma Using HPLC-MS/MS. *JOURNAL OF AGRICULTURAL AND FOOD CHEMISTRY*, 65 (11):2406-2413; 10.1021/acs.jafc.6b05390 MAR 22 2017
100. Xiao, JB. Dietary flavonoid aglycones and their glycosides: Which show better biological significance? *CRITICAL REVIEWS IN FOOD SCIENCE AND NUTRITION*, 57 (9):1874-1905; 10.1080/10408398.2015.1032400 2017
101. Marcus, D; Mak, L. Methods and Resources for Transport Proteins in Bioinformatics and Cheminformatics. *DRUG TRANSPORTERS, VOL 2: RECENT ADVANCES AND EMERGING TECHNOLOGIES*, Edited by: Nicholls G; Youdim K. 195-226; 2016.
102. Tangeti V.S., Vasundhara D., Satyanarayana K.V.V.V., Pavan Kumar K.S. Synthesis and antiproliferative activity of some dihydro-1 H-furo[2,3-c]pyrazole-Flavone hybrids. *Asian Journal of Chemistry*, 29 (7) pp. 1525-1532, 2017.
103. Dongare, P. 3D QSAR STUDIES OF FLAVONOID ANALOGUES FOR VASCULAR RELAXANT ACTIVITY IN CORONARY HEART DISEASES. *PHARMACOPHORE*, 8 (1):11-18; JAN 2017
104. Lingam, S. Expression and purification of the multidrug resistance protein P-glycoprotein and high-throughput assay development for drug discovery. A thesis submitted to the University of Manchester for the degree of Doctor of Philosophy in the Faculty of Biology, Medicine and Health, University of Manchester, 2017, pp.1-181. PhD [https://www.research.manchester.ac.uk/portal/files/61846201/FULL\\_TEXT.PDF](https://www.research.manchester.ac.uk/portal/files/61846201/FULL_TEXT.PDF)
105. Silva, Paulo Henrique da. "Estudos da interação da proteína adaptadora Grb2 (Growth Factor Receptor-Bound Protein 2) com os flavonoides morina e rutina." Thesis, Universidade Estadual Paulista "Júlio de Mesquita Filho", Brazil, (2017).
106. Shi, L; Zhang, YH; Wang, CF; Liu, HR; Wang, QA. Synthesis and Acetylcholinesterase Inhibitory Activity of Polymethoxyflavone Mannich Base Derivatives. *CHEMICAL RESEARCH IN CHINESE UNIVERSITIES*, 33 (4):594-597; 10.1007/s40242-017-6462-x AUG 2017
107. Naik, KK; Thangavel, S; Alam, A; Kumar, S. Flavone analogues as antimicrobial agents. *RECENT PATENTS ON INFLAMMATION & ALLERGY DRUG DISCOVERY*, 11 (1):53-63; 10.2174/1872213X11666170119094702 2017
108. El-Sherief, HA; Abu-Rahma, GEA; Shoman, ME; Beshr, EA; Abdel-baky, RM. Design and synthesis of new coumarin-chalcone/NO hybrids of potential biological activity. *MEDICINAL CHEMISTRY RESEARCH*, 26 (12):3077-3090; 10.1007/s00044-017-2004-9 DEC 2017
109. Simon L. In Vitro cytotoxicity and antioxidant evaluation of 7-amino-2-styrylchromone derivatives. *Asian Journal of Pharmaceutical and Clinical Research*, 2017, 10(11), pp. 152-156.
110. Ricardo J Ferreira. Reversing multidrug resistance (MDR) in cancer cells by targeting P-glycoprotein (P-gp)- Insights into the mechanism of MDR reversal from in silico P-gp modelling. Thesis, Oct 2017 PhD
111. Schwarz, Theresa. From propafenone to funitremorgin C – Probing Pgp/BCRP Inhibitor Selectivity. Dissertation, University of Vienna. Fakultät für Lebenswissenschaften 2017, pp. 1-173. PhD <https://othes.univie.ac.at/48806/>
112. Pomilio, AB; Mercader, AG. Natural Acylated Anthocyanins and Other Related Flavonoids: Structure Elucidation of Ipomoea cairica Compounds and QSAR Studies Including Multidrug Resistance, Editor(s): Atta-ur-Rahman, In *STUDIES IN NATURAL PRODUCTS CHEMISTRY, VOL 55*, 293-322; 10.1016/B978-0-444-64068-0.00009-7 2018, ISSN 1572-5995, ISBN 9780444640680
113. Wang, Z; Deng, XP; Xiong, SJ; Xiong, RD; Liu, J; Zou, L; Lei, XY; Cao, X; Xie, ZZ; Chen, YM; Liu, YM; Zheng, X; Tang, GT. Design, synthesis and biological evaluation of chrysin benzimidazole derivatives as potential anticancer agents. *NATURAL PRODUCT RESEARCH*, 32 (24):2900-2909; 10.1080/14786419.2017.1389940 DEC 17 2018
114. Sari, S. (Arilalkil)Azol Yapısında Yeni Oksim Ester Türevleri Üzerinde Çalışmalar: Sentez, Biyolojik Aktivite ve Moleküler Modelleme, Hacettepe University, Ankara, 2018. PhD <http://hdl.handle.net/11655/4204> <http://www.openaccess.hacettepe.edu.tr:8080/xmlui/handle/11655/4204>
115. Ferreira RJ, Baptista R, Moreno A, Madeira PG, Khonkarn R, Baubichon-Cortay H, Dos Santos DJ, Falson P, Ferreira MU. Optimizing the flavanone core toward new selective nitrogen-containing modulators of ABC transporters. *FUTURE MEDICINAL CHEMISTRY*, 10 (7):725-741; 10.4155/fmc-2017-0228 APR 2018.
116. Srivarangkul, P; Yuttithamnon, W; Suroengrit, A; Pankaew, S; Hengphasatporn, K; Rungrotmongkol, T; Phuwapraisirisan, P; Ruxrungham, K; Boonyasuppayakorn, S. A novel flavanone derivative inhibits dengue virus fusion and infectivity. *ANTIVIRAL RESEARCH*, 151 27-38; 10.1016/j.antiviral.2018.01.010 MAR 2018

117. Shakhdofa, MME; Mousa, HA; Labib, AA; Abd-El-All, AS; El-Beih, AA; Abdalla, MM. Synthesis and characterization of novel chromone Schiff base complexes as p53 activators. *APPLIED ORGANOMETALLIC CHEMISTRY*, 32 (6):10.1002/aoc.4345 JUN 2018
118. Romana Parveen, Tooba Naz Shamsi, Sumbul Afreen, Mudsser Azam, Tasneem Fatma, Qazi Mohd. Rizwanul Haque, Sadaf Fatima. Vigna unguiculata Trypsin Inhibitor: A Protein with Versatile Biological Applications. *Current Enzyme Inhibition*, 14 (1), 2018. DOI: 10.2174/1573408013666170619085504
119. Singla D., Bishnoi R., Dhanda S.K., Asthana S. (2018) Drug Transporters as Therapeutic Targets: Computational Models, Challenges, and Future Perspective. In: Purohit H., Kalia V., More R. (eds) *Soft Computing for Biological Systems*. Springer, Singapore, 2018, pp 143-168. DOI: 10.1007/978-981-10-7455-4\_9
120. Schlessinger, A; Welch, MA; van Vlijmen, H; Korzekwa, K; Swaan, PW; Matsson, P. Molecular Modeling of Drug-Transporter Interactions-An International Transporter Consortium Perspective. *CLINICAL PHARMACOLOGY & THERAPEUTICS*, 104 (5):818-835; 10.1002/cpt.1174 NOV 2018
121. Filho JAC. Endophytic Microbes as a Novel Source for Producing Anticancer Compounds as Multidrug Resistance Modulators. In: *Anticancer Plants: Natural Products and Biotechnological Implements*, M. S. Akhtar, M. K. Swamy (eds), Springer Nature Singapore Pte Ltd. 2018, 343-381. DOI: 10.1007/978-981-10-8064-7\_15
122. Tsunekawa, R; Katayama, K; Hanaya, K; Higashibayashi, S; Sugimoto, Y; Sugai, T. Synthesis of 5-Hydroxy-3',4',7-trimethoxyflavone and Related Compounds and Elucidation of Their Reversal Effects on BCRP/ABCG2-Mediated Anticancer Drug Resistance. *CHEMBIOCHEM*, 20 (2):210-220; SI 10.1002/cbic.201800431 JAN 18 2019
123. Rohman, MA; Baruah, P; Yesylevskyy, SO; Mitra, S. Specific solvent effect on the photophysical behavior of substituted chromones: A combined fluorescence, DFT and MD study. *CHEMICAL PHYSICS*, 517 67-79; 10.1016/j.chemphys.2018.09.042 JAN 24 2019
124. Li, Y; Li, YP; He, J; Liu, D; Zhang, QZ; Li, K; Zheng, X; Tang, GT; Guo, Y; Liu, YM. The Relationship between Pharmacological Properties and Structure-Activity of Chrysin Derivatives. *MINI-REVIEWS IN MEDICINAL CHEMISTRY*, 19 (7):555-568; 10.2174/1389557518666180424094821 2019
125. Sudhakaran, M; Sardesai, S; Doseff, AI. Flavonoids: New Frontier for Immuno-Regulation and Breast Cancer Control. *ANTIOXIDANTS*, 8 (4):10.3390/antiox8040103 APR 2019
126. Kaushik, S., Sanawar, R., Lekshmi, A., Chandrasekhar, L., Nair, M., Bhatnagar, S., Santhoshkumar, T.R. ER alpha selective chromone, isoxazolylchromones, induces ROS-mediated cell death without autophagy. *CHEMICAL BIOLOGY & DRUG DESIGN*, 94 (1):1352-1367; 10.1111/cbdd.13510 JUL 2019
127. S Dei, L Braconi, MN Romanelli, E Teodori. Recent advances in the search of BCRP-and dual P-gp/BCRP-based multidrug resistance modulators. *Cancer Drug Resist* 2019;2:[Online First] 2019 DOI: 10.20517/cdr.2019.31
128. Kumar, A; Jaitak, V. Natural products as multidrug resistance modulators in cancer. *EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY*, 176 268-291; 10.1016/j.ejmech.2019.05.027 AUG 15 2019.
129. Sidorov, P; Naulaerts, S; Arley-Bonnet, J; Pasquier, E; Ballester, PJ. Predicting Synergism of Cancer Drug Combinations Using NCI-ALMANAC Data. *FRONTIERS IN CHEMISTRY*, 7 10.3389/fchem.2019.00509 JUL 16 2019
130. Peixoto, JD; Neves, BJ; Vasconcelos, FG; Napolitano, HB; Barbalho, MGD; Silva, SDE; Rosseto, LP. Flavonoids from Brazilian Cerrado: Biosynthesis, Chemical and Biological Profile. *MOLECULES*, 24 (16):10.3390/molecules24162891 AUG 2019
131. Xiaoqing Fan, Jie Bai, Shengyu Zhao, Minwan Hu, Yanhong Sun, Baolian Wang, Ming Ji, Jing Jin, Xiaojian Wang, Jinping Hu, Yan Li,-Evaluation of inhibitory effects of flavonoids on breast cancer resistance protein (BCRP): From library screening to biological evaluation to structure-activity relationship,-*TOXICOLOGY IN VITRO* Volume: 61 Article Number: UNSP 104642 Published: DEC 2019.
132. Clarissa Feltrin, Cláudia Maria Oliveira Simões. Reviewing the mechanisms of natural product-drug interactions involving efflux transporters and metabolic enzymes, *Chemico-Biological Interactions*, Volume 314, 2019, 108825, ISSN 0009-2797. <https://doi.org/10.1016/j.cbi.2019.108825>
133. Yang, LZ; Liu, M. 3D-QSAR Model of Polybrominated Biphenyls Tri-effect Modified by Standard Deviation Standardization Method and Its Application in Environmental Friendly Molecular Modification. *CHEMICAL JOURNAL OF CHINESE UNIVERSITIES-CHINESE*, 2019, 40 (12), 2471-2479. doi: 10.7503/cjcu20190402
134. SIMON NJENGA WAIHENYA. Synthesis and characterization of sulfonated-flavonoid derivatives; a step towards improved solubility, lipophilicity and stability against oxidative degradation. *THESIS*, Graduate School of Binghamton University, State University of New York, 2019

135. Hsin-Ju Li, Nan-Lin Wu, Chi-Ming Pu, Chien-Yu Hsiao, Der-Chen Chang & Chi-Feng Hung. Chrysin alleviates imiquimod-induced psoriasis-like skin inflammation and reduces the release of CCL20 and antimicrobial peptides. *SCIENTIFIC REPORTS*, Volume: 10, Issue: 1, Article No: 2932 Published: FEB 19 2020. <https://doi.org/10.1038/s41598-020-60050-1>
136. Tuntiteerawit P., Jarukamjorn K., Porasuphatana S. The effect of green tea catechins on breast cancer resistance protein activity and intestinal efflux of aflatoxin B<sub>1</sub> via breast cancer resistance protein in Caco-2 cells. *Toxicological Research* 2020, in press. DOI: 10.1007/s43188-019-00032-2
137. Jiang, D., Lei, T., Wang, Z., Shen, C, Cao, D., Hou, T. ADMET evaluation in drug discovery. 20. Prediction of breast cancer resistance protein inhibition through machine learning. *JOURNAL OF CHEMINFORMATICS* Volume: 12 Issue: 1 Article Number: 16 Published: MAR 5 2020. <https://doi.org/10.1186/s13321-020-00421-y>
138. Chambers CS, Viktorová J, Řehořová K, et al. Defying Multidrug Resistance! Modulation of Related Transporters by Flavonoids and Flavonolignans. *J Agric Food Chem.* 2020; 68(7):1763- 1779. doi:10.1021/acs.jafc.9b00694
139. Song, Y.-K.; Yoon, J.-H.; Woo, J.K.; Kang, J.-H.; Lee, K.-R.; Oh, S.H.; Chung, S.-J.; Maeng, H.-J. Quercetin Is a Flavonoid Breast Cancer Resistance Protein Inhibitor with an Impact on the Oral Pharmacokinetics of Sulfasalazine in Rats. *PHARMACEUTICS*, Volume: 12 Issue: 5, Article Number: 397 Published: MAY 2020. DOI: 10.3390/pharmaceutics12050397
140. Zhang H., Zhao C., Na H. Enhanced biodegradation of phthalic acid esters' derivatives by plasticizer-degrading bacteria (*Burkholderia cepacia*, *archaeoglobus fulgidus*, *pseudomonas aeruginosa*) using a correction 3D-QSAR model. *INTERNATIONAL JOURNAL OF ENVIRONMENTAL RESEARCH AND PUBLIC HEALTH*, Volume: 17, Issue: 15, Article Number: 5299, AUG 2020 DOI:10.3390/ijerph17155299
141. Chauhan A., Langyan R. Study of photophysical behaviour of some Sm(III) complexes with 4-oxo-4H-1-benzopyran-3-carboxaldehyde and other N,N'-donor  $\pi$ -conjugated ligands. *JOURNAL OF CHEMICAL SCIENCES* Volume: 132 Issue: 1 Article Number: 95 Published: AUG 4 2020
142. M. F. Gonçalves, B.; S. P. Cardoso, D.; U. Ferreira, M.-J. Overcoming Multidrug Resistance: Flavonoid and Terpenoid Nitrogen-Containing Derivatives as ABC Transporter Modulators. *MOLECULES*, Volume: 25, Issue: 15, Article Number: 3364 Published: AUG 2020. DOI: 10.3390/molecules25153364
143. Archana Chauhan, Sheetal Lohra & Ritu Langyan (2020) Synthesis and characterization of three ternary samarium(III) complexes and their optical properties, *Spectroscopy Letters*, DOI: 10.1080/00387010.2020.1806081
144. Chauhan, A., Langyan, R. Preparation, characterization and luminescence behavior of some samarium complexes. *Rare Metals.* (2020). <https://doi.org/10.1007/s12598-020-01552-9>
145. Achut R. Shind, Dyanoba B. Muley. Synthesis, Characterization and Evaluation of Antioxidant and Antimicrobial activity of Spirochromones Derivatives, *Anti-Infective Agents* 2020; 18(4) . <https://doi.org/10.2174/2211352518666200117095346>
146. Han, Z., Chen, X., Li, G. *et al.* A novel 3D-QSAR model assisted by coefficient of variation method and its application in FQs' modification. *JOURNAL OF THE IRANIAN CHEMICAL SOCIETY*, **18**, 661–675 (2021). <https://doi.org/10.1007/s13738-020-02052-4>
147. Al-Amood H.K., Al-Shamsi H.F., Abbas H.H. Quantitative structure-activity relationships of some new beta amino-carbonyl compounds. *AIP Conference Proceedings*, 2290, art. no. 0029650, 2020 <https://doi.org/10.1063/5.0029650>
148. Bhowmik, S., Anand, P., Das, R. *et al.* Synthesis of new chrysin derivatives with substantial antibiofilm activity *MOLECULAR DIVERSITY* (2021). <https://doi.org/10.1007/s11030-020-10162-7>
149. Silva dos Santos Jéssica, Gonçalves Cirino João Pedro, de Oliveira Carvalho Patrícia, Ortega Manoela Marques. The Pharmacological Action of Kaempferol in Central Nervous System Diseases: A Review, *Frontiers in Pharmacology*, 11, 2021, 2143, <https://www.frontiersin.org/article/10.3389/fphar.2020.565700>
150. Yu-Ning Teng, Kun-I Lin, Yu-Chao Lin, Tran-Dinh Thang, Yu-Hsuan Lan, Chin-Chuan Hung, A novel flavonoid from *Fissistigma cupreonitens*, 5-hydroxy-7,8-dimethoxy-flavanone, competitively inhibited the efflux function of human P-glycoprotein and reversed cancer multi-drug resistance, *PHYTOMEDICINE*, Volume 85, 2021, 153528. <https://doi.org/10.1016/j.phymed.2021.153528>
151. Simon Waihenya, Pelin Şenel, Francis J. Osonga, Taner Erdoğan, Filiz Altay, Ayşegül Gölcü, Omowunmi A. Sadik. Mechanism of Interactions of dsDNA Binding with Apigenin and Its Sulfamate Derivatives Using Multispectroscopic, Voltammetric, and Molecular Docking Studies, *ACS Omega* 2021, Volume: 6 Issue: 8 Pages: 5124-5137, <https://doi.org/10.1021/acsomega.0c02612>
152. Ibrahim Luru Abdulai, Samuel Kojo Kwofie, Winfred Seth Gbewonyo, Daniel Boison, Joshua Buer Pupilampu, Michael Buenor Adinortey, "Multitargeted Effects of Vitexin and Isovitexin on Diabetes Mellitus

and Its Complications", *The Scientific World Journal*, vol. 2021, Article ID 6641128, 20 pages, 2021.  
<https://doi.org/10.1155/2021/6641128>

153. Borgo, J.; Laurella, L.C.; Martini, F.; Catalán, C.A.N.; Sülsen, V.P. *Stevia* Genus: hytochemistry and Biological Activities Update. *MOLECULES*, 26(9), Article Number: 2733, MAY 2021.  
<https://doi.org/10.3390/molecules26092733>

**45. Tsakovska, I., I. Pajeva, P. Alov, A. Worth. Recent advances in the molecular modelling of estrogen receptor-mediated toxicity. *Adv. Protein Chem. Struct. Biol.* 2011, 85, 217-251.**

Цитирания: 12

1. Jin, YX; Wang, LG; Fu, ZW. Oral exposure to atrazine modulates hormone synthesis and the transcription of steroidogenic genes in male peripubertal mice. *GENERAL AND COMPARATIVE ENDOCRINOLOGY*, 184 120-127; 10.1016/j.ygcen.2013.01.010 APR 1 2013.
2. Zhang, LY; Sedykh, A; Tripathi, A; Zhu, H; Afantitis, A; Mouchlis, VD; Melagraki, G; Rusyn, I; Tropsha, A. Identification of putative estrogen receptor-mediated endocrine disrupting chemicals using QSAR- and structure-based virtual screening approaches, *TOXICOLOGY AND APPLIED PHARMACOLOGY*, 272 (1):67-76; 10.1016/j.taap.2013.04.0.
3. Brogi S, P Papazafiri, V Roussis, A Tafi. 3D-QSAR using pharmacophore-based alignment and virtual screening for discovery of novel MCF-7 cell line inhibitors. *EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY, EUROPEAN JOURNAL OF MEDICINAL CHEMISTRY*, 67 344-351; 10.1016/j.ejmech.2013.06.048 SEP 2013
4. Przybylak KR, Schultz TW. Informing chemical categories through the development of adverse outcome pathways. In: *CHEMICAL TOXICOLOGY PREDICTION: CATEGORY FORMATION AND READ-ACROSS*. (by MTD Cronin, JC Madden, SJ Enoch, DW Roberts), 17, 44-71; 10.1039/9781849734400-00044 2013.
5. Enoch, S. J.; Przybylak, K. R.; Cronin, M. T. D. Category formation case studies. In: *CHEMICAL TOXICOLOGY PREDICTION: CATEGORY FORMATION AND READ-ACROSS*. (by MTD Cronin, JC Madden, SJ Enoch, DW Roberts), 17, 127-154; 10.1039/9781849734400-00127 2013
6. Teeguarden, J; Hanson-Drury, S; Fisher, JW; Doerge, DR. Are typical human serum BPA concentrations measurable and sufficient to be estrogenic in the general population. *FOOD AND CHEMICAL TOXICOLOGY*, 62 949-963; 10.1016/j.fct.2013.08.001 DEC 2013.
7. Politi, R., Rusyn, I., Tropsha, A. Prediction of binding affinity and efficacy of thyroid hormone receptor ligands using QSAR and structure-based modeling methods, *TOXICOLOGY AND APPLIED PHARMACOLOGY*, 2014, 280 (1), 177-189.
8. Alireza Nemat Rashtehroodi, Ghasem Ghasemi. QSAR investigation on benzimidazole derivatives in Trichomonosis disease. 2014, DOI: 10.24297/jbt.v4i3.4998
9. Todorov, M.P. Identification of endocrine disrupting chemicals by in silico methods. *Ecology & Safety*, Volume 9, 293-299, 2015.
10. Todorov, M. Evaluation of in silico approach for identification of estrogen receptor ligands from chemical inventories. *Industrial Technologies*, Vol. III (1), 2016, 87-93.
11. Ruiz, P; Sack, A; Wampole, M; Bobst, S; Vracko, M. Integration of in silico methods and computational systems biology to explore endocrine-disrupting chemical binding with nuclear hormone receptors. *CHEMOSPHERE*, 178, 99-109; 10.1016/j.chemosphere.2017.03.026 JUL 2017
12. Paul Awolade, Nosipho Cele, Oluwakemi Ebenezer, Nagaraju Kerru, Lalitha Gummidi, Liang Gu, Gabriella Palma, Mandeep Kaur and Parvesh Singh, Synthesis of 1H-1,2,3-Triazole-Linked Quinoline-Isatin Molecular Hybrids as Anti- Breast Cancer and Anti-Methicillin-Resistant Staphylococcus aureus (MRSA) Agents, Anti-Cancer Agents in Medicinal Chemistry. *ANTI-CANCER AGENTS IN MEDICINAL CHEMISTRY*, Volume: 21 Issue: 10 Pages: 1228-1239 Published: 2021.  
<https://doi.org/10.2174/1871520620666200929153138>

**46. Pajeva I., M. Wiese. Application of in Silico Methods to study ABC Transporters Involved in Multidrug Resistance. In : *In Silico Lead Discovery*, 2011, Ed. M. Miteva, Bentham Science, 2011, Vol. 1, 144-162. eISBN: 978-1-60805-142-7**

Цитирания: 2

1. Morooy G, Martiny VY, Vayer P, Villoutreix BO, Miteva MA. Toward in silico structure-based ADMET prediction in drug discovery. *DRUG DISCOV TODAY*, 2012 Jan; 17(1-2):44-55.
2. Ferreira, R. J., Ferreira, M.-J. U. and dos Santos, D. J. V. A. Reversing cancer multidrug resistance: insights into the efflux by ABC transports from in silico studies. *WIREs Comput Mol Sci*. 2014, doi: 10.1002/wcms.1196.

**47. Lessigiarska I., I. Pajeva, P. Prodanova, M. Georgieva, A. Bijev. Structure-activity relationships of pyrrole hydrazones as new anti-tuberculosis agents. Medicinal Chemistry 2012, 8 (3), 462-473.**

Цитирания: 7

1. Morjan, R.Y.; Mkdahm, A.M.; Abu-Awwad, F.M.; Helliwell, M.; Awadallah, A.M.; Gardiner, J.M. Synthesis, Structural Characterization, and Computational Study of Novel (E)-N'-(1-p-tolyloethylidene)furan-2-carbohydrazide, JOURNAL OF MOLECULAR STRUCTURE, 1051 345-353; 10.1016/j.molstruc.2013.08.008 NOV 5 2013.
2. Mironov, V.F., Buzykin, B.I., Garaev, R.S., Tatarinov, D.A., Kashapov, L.R., Chestnova, R.V., Nabiullin, V.N., Ilyasov, A.V., Zobova, V.V. Dimphosphone analogs: A pharmacological aspect(2014) Russian Chemical Bulletin, 63 (9), pp. 2114-2125.
3. Pedro Henrique de Azambuja Carvalho , Auri Rocha Duval , Fabio Renato Manzolli Leite , Fernanda Nedel , Wilson Cunico , Rafael Guerra Lund. 7-Chloroquinolin-4-yl)arylhydrazones: Candida albicans enzymatic repression and cytotoxicity evaluation, Part 2. JOURNAL OF ENZYME INHIBITION AND MEDICINAL CHEMISTRY, 31 (1):126-131; 10.3109/14756366.2015.1010527 JAN 2 2016
4. Desai V, Gawandi S. SYNTHESIS OF NEW 2, 4 – DINITRO PHENYL HYDRAZONE DERIVATIVES OF CHALCONES AND ITS BIOLOGICAL EVALUATION. IAJPR. 2016; 6(3): 4779-4786.
5. De Azambuja Carvalho, P.H., Duval, A.R., Manzolli Leite, F.R., Nedel, F., Cunico, W., Lund, R.G.(7-Chloroquinolin-4-yl)arylhydrazones: Candida albicans enzymatic repression and cytotoxicity evaluation, Part 2(2016) Journal of Enzyme Inhibition and Medicinal Chemistry, 31 (1), pp. 126-131.
6. Angelova, V.T.; Valcheva, V.; Vassilev, N.G.; Buyukliev, R.; Momekov, G.; Dimitrov, I.; Saso, L.; Djukic, M.; Shivachev, B. Antimycobacterial activity of novel hydrazide-hydrazone derivatives with 2H-chromene and coumarin scaffold. BIOORGANIC & MEDICINAL CHEMISTRY LETTERS, 27 (2):223-227. ISSN 0960-894X, <http://dx.doi.org/10.1016/j.bmcl.2016.11.071>, 2016.
7. Mkdahm A.M., Morjan R.Y., Raftery J., Awadallah A.M., Gardiner J.M., Synthesis, Structural Characterization, and Computational Study of New (E)-N'-(3,4-dimethoxybenzylidene)furan-2-carbohydrazide, ARABIAN JOURNAL OF CHEMISTRY, 13 (1), 3571-3584, 2020. DOI: 10.1016/j.arabjc.2018.12.008.

**48. Pencheva T., D. Lagorce, I. Pajeva, B. O. Villoutreix, M. A. Miteva. AMMOS Software: Method and Application, In: Computational Drug Discovery and Design. Baron, Riccardo (Ed.) Series: Methods Mol. Biol. 2012, 819, 127-141. ISBN 978-1-61779-464-3**

Цитирания: 3

1. Yuriev, E, Holien, J, Ramsland, PA (2015), Improvements, trends, and new ideas in molecular docking: 2012–2013 in review. J. Mol. Recognit., 2015, 28, 581–604. doi: 10.1002/jmr.2471.
2. Mueller C., A. Samoo, P.-M. Hammoudi, N. Klages, J. P. Kallio, I. Kursula, D. Soldati-Favre. Structural and Functional Dissection of Toxoplasma Gondii Armadillo Repeats Only Protein, Journal of Cell Science, 2016, 129(5), 1031-1045.
3. Azevedo, F.; Richardt, J.; Oliveira, M.; Araujo, I.; Oliveira, R.; Baptista, L.; Amorim, H. In Silico Screening and Analysis of Potential Inhibitors of Arylamine N-Acetyltransferases (NATs) from the Traditional Chinese Medicine: A Study Using Free Available Tools. Preprints 2017, 2017060132 (doi: 10.20944/preprints201706.0132.v1)

**49. Fratev, F., S. Osk Jonsdottir, S., I. Pajeva. Structural insight into the UNC-45-myosin complex. Proteins 2013, 7, 1212-1221.**

Цитирания: 10

1. LM Prabhu. Effect of mutations in DUNC-45 on its activity as a myosin chaperone, using Drosophila as a model. A Thesis. San Diego State University, 2013. **PhD**
2. Lee, C.F., Melkani, G.C., Bernstein, S.I. The UNC-45 Myosin Chaperone. From Worms to Flies to Vertebrates.(2014) International Review of Cell and Molecular Biology, 313, pp. 103-144.
3. Bujalowski, Paul J., P Nicholls, JM Barral, AF Oberhauser. Thermally-induced structural changes in an armadillo repeat protein suggest a novel thermosensor mechanism in a molecular chaperone, FEBS LETTERS, 589 (1):123-130; 10.1016/j.febslet.2014.11.034 JAN 2 2015.
4. W Ni, OO Odunuga. UCS Proteins: Chaperones for Myosin and Co-Chaperones for Hsp90. In: The Networking of Chaperones by Co-chaperones, GL Blatch, AL Edkins (eds.) Springer International Publishing, Switzerland Chapter 7, 133-152, 2015.
5. Mueller, C., Samoo, A., Hammoudi, P.-M., Klages, N., Kallio, J.P., Kursula, I., Soldati-Favre, D. Structural and functional dissection of Toxoplasma gondii armadillo repeats only protein (TgARO). (2016) Journal of Cell Science, 129 (5), pp. 1031-1045.
6. Rona J. Strawbridge. Angela Silveira, Marcel den Hoed,,Stefan Gustafsson,Jian'an Luan, Denis Rybin, José Dupuis, Ruifang Li-Gao, Maryam Kavousi, Abbas Dehghan, Kadri Haljas, Jari Lahti, Jesper R. Gädin,

- Alexandra Bäcklund, Ulf de Faire, Karl Gertow. Phillipe Giral, Anuj Goel, Steve E. Humphries, Sudhir Kurl, Claudia Langenberg, Lars L. Lannfelt, Lars Lind, Cecilia C.M. Lindgren, Elmo Mannarino, Dennis O. Mook-Kanamori, Andrew P. Morris, Renée de Mutsert, Rainer Rauramaa, Peter Saliba-Gustafsson, Bengt Sennblad, Andries J. Smit, Ann-Christine Syvänen. Elena Tremoli, Fabrizio Veglia, Björn Zethelius, Hanna M. Björck, Johan G. Eriksson, Albert Hofman, Oscar H. Franco, Hugh Watkins, J. Wouter Jukema, Jose C. Florez, Nicholas J. Wareham, James B. Meigs, Erik Ingelsson, Damiano Baldassarre, Anders Hamsten. Study group Identification of a novel proinsulin-associated SNP and demonstration that proinsulin is unlikely to be a causal factor in subclinical vascular remodelling using Mendelian randomisation, *Atherosclerosis*, 266, pp.196-204, 2017
7. Bujalowski, P. J., Nicholls, P., Garza, E. and Oberhauser, A. F. The central domain of UNC-45 chaperone inhibits the myosin power stroke. *FEBS Open Bio*. *FEBS Open Bio*, 2018, 8(1), pp. 41–48.
  8. Macalino, S.J.Y.; Basith, S.; Clavio, N.A.B.; Chang, H.; Kang, S.; Choi, S. Evolution of In Silico Strategies for Protein-Protein Interaction Drug Discovery. *Molecules* 2018, 23, 1963.
  9. Hormos Salimi Dafsari, Nur Mehpare Kocaturk, Hülya-Sevcan Daimagüler, Anna Brunn, Jörg Dötsch, Joachim Weis, Martina Deckert and Sebahattin Cirak. Bi-allelic mutations in *uncoordinated mutant number-45 myosin chaperone B* are a cause for congenital myopathy. *Acta Neuropathol commun* 7(1), art. no. 211. (2019) doi:10.1186/s40478-019-0869-1
  10. Ivana Gaziouva, Taylor Moncrief, Courtney J. Christian, Michael Villarreal, Simon Powell, Hubert Lee, Hiroshi Qadota, Mark A. White, Guy M. Benian, Andres F. Oberhauser, Mutational Analysis of the Structure and Function of the Chaperoning Domain of UNC-45B, *Biophysical Journal*, Volume 119, Issue 4, 2020, Pages 780-791, <https://doi.org/10.1016/j.bpj.2020.07.012>

**50. Pajeva, I., M. Hanl, M. Wiese. Protein contacts and ligand binding in the inward-facing model of human P-glycoprotein, *ChemMedChem* 2013, 8 (5), 748–762.**

Цитирания: 24

1. Karoor, K; Bhatnagar, J; Chufan, EE; Ambudkar, S. Mutations in Intracellular Loops 1 and 3 Lead To Misfolding of Human P-Glycoprotein (ABCB1) That Can Be Rescued By Cyclosporine A, Which Reduces its Association With Chaperone Hsp70. *JOURNAL OF BIOLOGICAL CHEMISTRY*, 288 (45):32622-32636; 10.1074/jbc.M113.498980 NOV 8 2013.
2. Loo, TW; Clarke, DM. Locking Intracellular Helices 2 and 3 Together Inactivates Human P-glycoprotein. *JOURNAL OF BIOLOGICAL CHEMISTRY*, 289 (1):229-236; 10.1074/jbc.M113.527804 JAN 3 2014.
3. Ferreira, R. J., Ferreira, M.-J. U. and dos Santos, D. J. V. A. Reversing cancer multidrug resistance: insights into the efflux by ABC transports from *in silico* studies. *WILEY INTERDISCIPLINARY REVIEWS-COMPUTATIONAL MOLECULAR SCIENCE*, 5 (1):27-55; 10.1002/wcms.1196 JAN-FEB 2015.
4. Chufan E.E., Sim H-M., Ambudkar S.V. Molecular Basis of the Polyspecificity of P-glycoprotein (ABCB1): Recent Biochemical and Structural Studies. Chapter 3, In: *ABC TRANSPORTERS AND CANCER*, 125 71-96; 10.1016/bs.acr.2014.10.003 2015.
5. Tip W Loo, David M Clarke. The Transmission Interfaces Contribute Asymmetrically to the Assembly and Activity of Human P-glycoprotein. *JOURNAL OF BIOLOGICAL CHEMISTRY*, 290 (27):16954-16963; 10.1074/jbc.M115.652602 JUL 3 2015.
6. Ferreira, RJ; Ferreira, MJU; dos Santos, DJVA. Do adsorbed drugs onto P-glycoprotein influence its efflux capability? *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*, 17 (34):22023-22034; 10.1039/c5cp03216d 2015.
7. Domicевичa L, Biggin PC. Homology modelling of human P-glycoprotein. *Biochem Soc Trans*. 2015 Oct 1;43(5):952-8. doi: 10.1042/BST20150125
8. Loo, TP., DM. Clarke. Mapping the Binding Site of the Inhibitor Tariquidar That Stabilizes the First Transmembrane Domain of P-glycoprotein, 2015, 290 (49), 29389-29401. doi:10.1074/jbc.M115.695171
9. Aggarwal, G., Prajapati, R., Tripathy, R. K., Bajaj, P., Iyengar, A. R. S., Sangamwar, A. T., Pande, A. H. Toward Understanding the Catalytic Mechanism of Human Paraoxonase 1: Site-Specific Mutagenesis at Position 192. *PLoS ONE*, 2016, 11(2), e0147999. <http://doi.org/10.1371/journal.pone.0147999>
10. Pan, X., Mei, H., Qu, S., Huang, S., Sun, J., Yang, L., Chen, H. Prediction and characterization of P-glycoprotein substrates potentially bound to different sites by emerging chemical pattern and hierarchical cluster analysis. *INTERNATIONAL JOURNAL OF PHARMACEUTICS*, 502 (1-2):61-69; 10.1016/j.ijpharm.2016.02.022 APR 11 2016.
11. Ferreira, R. J., Bonito, C. A., Ferreira, M. J. U. and dos Santos, D. J.V.A. (2017), About P-glycoprotein: a new drugable domain is emerging from structural data. *WILEY INTERDISCIPLINARY REVIEWS-COMPUTATIONAL MOLECULAR SCIENCE*, 7 (5):10.1002/wcms.1316 SEP-OCT 2017.
12. Tip W. Loo, David M. Clarke, A short cross-linker activates human P-glycoprotein missing a catalytic carboxylate, *BIOCHEMICAL PHARMACOLOGY*, 2017, 145, 27-33. <https://doi.org/10.1016/j.bcp.2017.08.014>.

13. Lingam, S. Expression and purification of the multidrug resistance protein P-glycoprotein and high-throughput assay development for drug discovery. A thesis submitted to the University of Manchester for the degree of Doctor of Philosophy in the Faculty of Biology, Medicine and Health, University of Manchester, 2017, pp.1-181. PhD [https://www.research.manchester.ac.uk/portal/files/61846201/FULL\\_TEXT.PDF](https://www.research.manchester.ac.uk/portal/files/61846201/FULL_TEXT.PDF)
14. Meng T., Lu B., Shao S., Yuan M., Liu X., Yuan H., Huang X., Hu F. Sequential therapy with redox-responsive glucolipid nanocarrier separately delivering siRNA and doxorubicin to overcome multidrug resistance, *International Journal of Pharmaceutics*, 534 (1-2), pp.368-377, 2017
15. Ricardo J Ferreira. Reversing multidrug resistance (MDR) in cancer cells by targeting P-glycoprotein (P-gp)- Insights into the mechanism of MDR reversal from in silico P-gp modelling. Thesis, Oct 2017 PhD
16. Schwarz, Theresa. From propafenone to fumitremorgin C – Probing Pgp/BCRP Inhibitor Selectivity. Dissertation, University of Vienna. Fakultät für Lebenswissenschaften 2017, pp. 1-173. PhD <https://othes.univie.ac.at/48806/>
17. Giovanni Bocci, Amélie Moreau, Philippe Vayer, Claire Denizot, Olivier Fardel, Yannick Parmentier. New insights in the in vitro characterisation and molecular modelling of the P-glycoprotein inhibitory promiscuity. *European Journal of Pharmaceutical Sciences*, 121, 2018, 85-94, 2018. ISSN 0928-0987, <https://doi.org/10.1016/j.ejps.2018.04.039>
18. Yue Zhang, Weikang Gong, Yan Wang, Yang Liu & Chunhua Li. Exploring movement and energy in human P-glycoprotein conformational rearrangement, *Journal of Biomolecular Structure and Dynamics*, 2018. <https://doi.org/10.1080/07391102.2018.1461133>
19. Tingting Meng, Guoxi Qiu, Yun Hong, Ming Yuan, Binbin Lu, Jie Wu, Hong Yuan, Fuqiang Hu, Effect of chitosan based glycolipid-like nanocarrier in prevention of developing acquired drug resistance in tri-cycle treatment of breast cancer, *INTERNATIONAL JOURNAL OF PHARMACEUTICS*, 555, 2019, 303-313. <https://doi.org/10.1016/j.ijpharm.2018.11.056>
20. Yuanqing Wei, Hongping Xia, Fen Zhang, Kan Wang, Peicheng Luo, Yafeng Wu, Songqin Liu. Theranostic Nanoprobes Mediated Simultaneous Monitoring and Inhibition of P-glycoprotein Potentiates Multidrug-Resistant Cancer Therapy. *Anal.*
21. Kaczor, A.; Nové, M.; Kincses, A.; Spengler, G.; Szymańska, E.; Latacz, G.; Handzlik, J. Search for ABCB1 Modulators Among 2-Amine-5-Arylideneimidazolones as a New Perspective to Overcome Cancer Multidrug Resistance. *Molecules* **2020**, 25, 2258. doi: 10.3390/molecules25092258
22. Wei X, Xu L, Jeddo SFA, Li K, Li X, Li J. MARK2 enhances cisplatin resistance via PI3K/AKT/NF-κB signaling pathway in osteosarcoma cells. *Am J Transl Res*. 2020; 12(5):1807- 1823. Published 2020 May 15.
23. Bonito, C.A., Ferreira, R.J., Ferreira, M.U. *et al.* Theoretical insights on helix repacking as the origin of P-glycoprotein promiscuity. *Scientific Reports*, **10**, 9823 (2020). <https://doi.org/10.1038/s41598-020-66587-5>
24. Katarzyna Szczepańska, Annamária Kincses, Klaudia Vincze, Ewa Szymańska, Gniewomir Latacz, Kamil J. Kuder, Holger Stark, Gabriella Spengler, Jadwiga Handzlik, Katarzyna Kieć-Kononowicz. N-substituted piperazine derivatives as potential multitarget agents acting on histamine H3 receptor and cancer resistance proteins, *Bioorganic & Medicinal Chemistry Letters*, 2020, 30(22), art. no. 127522, <https://doi.org/10.1016/j.bmcl.2020.127522>

**51. Pajeva, I., K. Sterz, K. Steggemann, F. Marighetti, M. Christlieb, M. Wiese. Interactions of the multidrug resistance modulators tariquidar and elacridar and their analogs with P-glycoprotein. *ChemMedChem* 2013, 8 (10), 1701–1713.**

Цитирания: 30

1. Martinez L. Arnaud O., Henin E., Tao H., Chaptal V., Doshi R., Andrieu T., Dussurgey, S., Tod M., Pietro AD., Zhang Q., Chang, G., Falson P. Understanding Polyspecificity Within The Substrate-Binding Cavity Of The Human Multidrug Resistance P-Glycoprotein. *FEBS JOURNAL*, 281 (3):673-682; 10.1111/febs.12613 FEB 2014.
2. Geng M., L. Wang, X. Chen, R. Cao, P. Li. The association between chemosensitivity and Pgp, GST-pi and Topo II expression in gastric cancer. *DIAGNOSTIC PATHOLOGY* 2013, 8:198. doi:10.1186/1746-1596-8-198.
3. Sprachman, M.M., Laughney, A.M., Kohler, R.H., Weissleder, R. In vivo imaging of multidrug resistance using a third generation mdr1 inhibitor. *BIOCONJUGATE CHEMISTRY*, 25 (6):1137-1142; 10.1021/bc500154c JUN 2014.
4. Loo, TW; Clarke, DM. Tariquidar inhibits P-glycoprotein drug efflux but activates ATPase activity by blocking transition to an open conformation, *BIOCHEMICAL PHARMACOLOGY*, 92 (4):558-566; 10.1016/j.bcp.2014.10.006 DEC 15 2014.
5. LMM Jaramillo. Structural and functional study of efflux pumps involved in drug resistance. PhD thesis, Agricultural sciences. Université Claude Bernard - Lyon I, 2014. <https://tel.archives-ouvertes.fr/tel-00985593> PhD

6. Ferreira, R. J., Ferreira, M.-J. U. and dos Santos, D. J. V. A. Reversing cancer multidrug resistance: insights into the efflux by ABC transports from *in silico* studies. *WILEY INTERDISCIPLINARY REVIEWS-COMPUTATIONAL MOLECULAR SCIENCE*, 5 (1):27-55; 10.1002/wcms.1196 JAN-FEB 2015.
7. Thai, KM; Huynh, NT; Ngo, TD; Mai, TT; Nguyen, TH; Tran, TD. Three- and four-class classification models for P-glycoprotein inhibitors using counter-propagation neural networks. *SAR AND QSAR IN ENVIRONMENTAL RESEARCH*, 26 (2):139-163; 10.1080/1062936X.2014.995701 FEB 1 2015
8. Chufan E.E., Sim H-M., Ambudkar S.V. Molecular Basis of the Polyspecificity of P-glycoprotein (ABCB1): Recent Biochemical and Structural Studies. Chapter 3, In: *ABC TRANSPORTERS AND CANCER*, 125 71-96; 10.1016/bs.acr.2014.10.003 2015.
9. Wong, ILK; Wang, BC; Yuan, J; Duan, LX; Liu, Z; Liu, T; Li, XM; Hu, XS; Zhang, XY; Jiang, T; Wan, SB; Chow, LMC. Potent and Nontoxic Chemosensitizer of P-Glycoprotein-Mediated Multidrug Resistance in Cancer: Synthesis and Evaluation of Methylated Epigallocatechin, Gallocatechin, and Dihydromyricetin Derivatives. *JOURNAL OF MEDICINAL CHEMISTRY*, 58 (11):4529-4549; 10.1021/acs.jmedchem.5b00085 JUN 11 2015
10. Follit, Courtney A., Brewer, Frances K., Wise, John G., Vogel, Pia D. In silico identified targeted inhibitors of P-glycoprotein overcome multidrug resistance in human cancer cells in culture. *Pharmacology Research & Perspectives*, 3(5), 2015, e00170, doi: 10.1002/prp2.170
11. Li, J., Ren, Z. Research progress of folate functionalized nanoparticles in diverting P-glycoprotein mediated drug efflux (2015) *Cancer Research and Clinic*, 2015, 27 (7), pp. 502-504.
12. Fox, E., Widemann, B.C., Pastakia, D., Chen, C.C., Yang, S.X., Cole, D., Balis, F.M. Pharmacokinetic and pharmacodynamic study of tariquidar (XR9576), a P-glycoprotein inhibitor, in combination with doxorubicin, vinorelbine, or docetaxel in children and adolescents with refractory solid tumors(2015) *Cancer Chemotherapy and Pharmacology*, 76 (6), pp. 1273-1283.
13. Domicевичa L, Biggin PC. Homology modelling of human P-glycoprotein. *Biochem Soc Trans.* 2015 Oct 1; 43(5):952-8. doi: 10.1042/BST20150125
14. Loo, TP., DM. Clarke. Mapping the Binding Site of the Inhibitor Tariquidar That Stabilizes the First Transmembrane Domain of P-glycoprotein, 2015, 290 (49), 29389-29401. doi:10.1074/jbc.M115.695171
15. Shayanfar, S., Shayanfar, A., Ghandadi, M. Image-Based Analysis to Predict the Activity of Tariquidar Analogs as P-Glycoprotein Inhibitors: The Importance of External Validation. *Archiv der Pharmazie*, 349 (2), pp. 124-131, Feb 2016.
16. Yang, J., Cheng, L.-F., Yang, S., Hu, Q., Zhang, J., Xu, L., Chen, D.-W. Reversal of breast cancer multidrug resistance in vitro by Doxorubicin and Elacridar co-delivery nanoparticle (2016) *Chinese Pharmaceutical Journal*, 51 (5), pp. 379-385.
17. Sung-Han Hsiao, Yu-Jen Lu, Yan-Qing Li, Yang-Hui Huang, Chia-Hung Hsieh, and Chung-Pu W. Osimertinib (AZD9291) Attenuates the Function of Multidrug Resistance-Linked ATP-Binding Cassette Transporter ABCB1 in Vitro. *Molecular Pharmaceutics* 2016 13 (6), 2117-2125
18. Cédric Orelle, Jean-Michel Jault. Structures and Transport Mechanisms of the ABC Efflux Pumps. In: *Efflux-Mediated Antimicrobial Resistance in Bacteria*. (Eds. Xian-Zhi Li, Christopher A. Elkins, Helen I. Zgurskaya), Springer International Publishing, 2016, pp 73-98. [http://link.springer.com/chapter/10.1007/978-3-319-39658-3\\_4](http://link.springer.com/chapter/10.1007/978-3-319-39658-3_4)
19. Li J, Liu Y, Zhang J, Yu X, Wang X, Zhao L. Effects of resveratrol on P-glycoprotein and cytochrome P450 3A in vitro and on pharmacokinetics of oral saquinavir in rats. *Drug Design, Development and Therapy*. 2016;10:3699-3706. doi:10.2147/DDDT.S118723.
20. Jenny L. Pokorny, Gaspar J. Kitange, Daniel J. Ma. Small-Molecule Inhibitors in Glioblastoma: Key Pathways and Resistance Mechanisms. *Resistance to Targeted Therapies Against Adult Brain Cancers*. In: *Resistance to Targeted Anti-Cancer Therapeutics* (Ed. Amanda Tivnan), Springer, pp. 145-174, 2016.
21. Xiaoqing Yi, Dan Zhao, Quan Zhang, Jiaqi Xu, Gongdao Yuan, Renxi Zhuo and Feng Li. Preparation of multilocation reduction-sensitive core crosslinked folate-PEG-coated micelles for rapid release of doxorubicin and tariquidar to overcome drug resistance, *Nanotechnology* 28.8 (2017): 085603.
22. Alam A., R. Küng, J. Kowal, R.A. McLeod, N. Tremp, E.V. Broude, I.B. Roninson, H. Stahlberg, K.P. Locher. Structure of a zosuquidar and UIC2-bound human-mouse chimeric ABCB1. *PNAS* 115(9), pp. E1973-E1982, 2018 <https://doi.org/10.1073/pnas.1717044115>
23. Chung-Pu Wu, Megumi Murakami, Sung-Han Hsiao, Te-Chun Liu, Ni Yeh, Yan-Qing Li, Tai-Ho Hung, Yu-Shan Wu, Suresh. V. Ambudkar, SIS3, a specific inhibitor of Smad3 reverses ABCB1- and ABCG2-mediated multidrug resistance in cancer cell lines, *Cancer Letters*, 433, 2018, 259-272.
24. Stanković T., A Podolski-Renić, J Dinić, M Pešić. Selective Anti-Cancer Drugs against Multi-drug Resistance (Chapter 4), In: *Frontiers in Anti-Cancer Drug Discovery* (Eds.:Atta-ur-Rahman, M. Iqbal Choudhary), Bentham Science Publishers, 2018, 9, 114-192. DOI: 10.2174/97816810870161180901

25. JuanXing, HuMei, ShuHengHuang, DuoZhang, XianChaoPan. An Energetically Favorable Ligand Entrance Gate of a Multidrug Transporter Revealed by Partial Nudged Elastic Band Simulations. *Computational and Structural Biotechnology Journal* Volume 17, 2019, Pages 319-323, 2019, DOI: 10.1016/j.csbj.2019.02.008
26. Nathalia B. D. Lima; Gerd B. Rocha; Ricardo O. Freire; Alfredo M. Simas. RM1 Semiempirical Model: Chemistry, Pharmaceutical Research, Molecular Biology and Materials Science. *Journal of the Brazilian Chemical Society*, 2019, DOI number: 10.21577/0103-5053.20180239
27. Yuanqing Wei, Hongping Xia, Fen Zhang, Kan Wang, Peicheng Luo, Yafeng Wu, Songqin Liu. Theranostic Nanoprobe Mediated Simultaneous Monitoring and Inhibition of P-Glycoprotein Potentiating Multidrug-Resistant Cancer Therapy. *Anal. Chem.* 2019, 91, 17, 11200-11208. <https://doi.org/10.1021/acs.analchem.9b02118>
28. Alexander A Titov, Mauro Niso, Modesto de Candia, Maxim S Kobzev, Alexey V Varlamov, Tatiana N Borisova, Leonid G Voskressensky, Nicola A Colabufo, Saverio Cellamare, Leonardo Pisani, Cosimo D Altomare. 3-benzazecine-based cyclic allene derivatives as highly potent P-glycoprotein inhibitors overcoming doxorubicin multidrug resistance. *Future Medicinal Chemistry* Vol. 11, No. 16, 2019. <https://doi.org/10.4155/fmc-2019-0037>
29. Cseke A, Schwarz T, Jain S, Decker S, Vogl K, Urban E, Ecker GF. Propafenone analogue with additional H-bond acceptor group shows increased inhibitory activity on P-glycoprotein. *Arch Pharm (Weinheim)*. 2020 Jan 9:e1900269. doi: 10.1002/ardp.201900269.
30. Xu Wu, Chun Yin, Jiang Ma, Stella Chai, Chunyuan Zhang, Sheng Yao, Onat Kadioglu, Thomas Efferth, Yang Ye, Kenneth Kin-Wah To, Ge Lin, Polyoxypregnanes as safe, potent and specific ABCB1-inhibitory pro-drugs to overcome multidrug resistance in cancer chemotherapy in vitro and in vivo, *Acta Pharmaceutica Sinica B*, 2021, <https://doi.org/10.1016/j.apsb.2020.12.021>. (<http://www.sciencedirect.com/science/article/pii/S2211383521000034>)

**52. Al Sharif M., P. Alov, M.T.D Cronin, E. Fioravanzo, I. Tsakovska, V. Vitcheva, A. Worth, C. Yang, I. Pajeva. Toward better understanding of liver steatosis MoA: Molecular modeling study of PPAR gamma receptor, *Toxicol. Lett.* 2013, 221, S85.**

Цитирания: 1

1. Sullivan, K. M.; Manuppello, J. R.; Willett, C. E. Building on a solid foundation: SAR and QSAR as a fundamental strategy to reduce animal testing. *SAR AND QSAR IN ENVIRONMENTAL RESEARCH*, 25 (5):357-365; SI 10.1080/1062936X.2014.907203 2014.

**53. Pencheva, T., Jereva, D., Miteva, M.A., Pajeva, I. Post-docking optimization and analysis of protein–ligand interactions of estrogen receptor alpha using AMMOS software. *Curr. Comput. Aided Drug Des.* 2013, 9, 83–94.**

Цитирания: 2

1. Garbutt, CC; Bangalore, PV; Kannar, P; Mukhtar, MS. Getting to the Edge: Protein dynamical networks as a new frontier in plant-microbe interactions. *FRONTIERS IN PLANT SCIENCE*, 5 10.3389/fpls.2014.00312 JUN 30 2014.
2. M. Catarro, J. Serrano, E.Cavalheiro, S. Ramos, A. O. Santos, S. Silvestre, P. Almeida, Novel 4-acetamide-2-alkylthio-N-acetanilides resembling nimesulide: Synthesis, cell viability evaluation and in silico studies, *Bioorganic & Medicinal Chemistry*, Volume 25, Issue 16, 2017, Pages 4304-4313, ISSN 0968-0896

**54. Al Sharif M., P. Alov, V. Vitcheva, I. Pajeva, I. Tsakovska. Modes-of-Action Related to Repeated Dose Toxicity: Tissue-Specific Biological Roles of PPAR gamma Ligand-Dependent Dysregulation in Nonalcoholic Fatty Liver Disease. *PPAR Res.* 2014, Article Number: 432647.**

Цитирания: 21

1. Claire L. Mellor, Fabian P. Steinmetz, Mark T. D. Cronin The identification of nuclear receptors associated with hepatic steatosis to develop and extend adverse outcome pathways. *Crit Rev Toxicol.* 2015 Oct 9:1-15.
2. Valérie Zuang, Bertrand Desprez, João Barroso, Suzanne Belz, Elisabet Berggren,, Camilla Bernasconi, Jos Bessems, Stephanie Bopp, Silvia Casati, Sandra Coecke, Raffaella Corvi, Coralie Dumont, Varvara Gouliarmou, Claudius Griesinger, Marlies Halder, Annett Janusch-Roi, Aude Kienzler, Brigitte Landesmann, Federica Madia, Anne Milcamps, Sharon Munn, Anna Price, Pilar Prieto, Michael Schäffer, Jutta Triebe, Clemens Wittwehr, Andrew Worth, Maurice Whelan. EURL ECVAM status report on the development, validation and regulatory acceptance of alternative methods and approaches, European Union, 2015, pp. 1-114. DOI: 10.2788/62058, ISBN: 978-92-79-51990-1.
3. Barbosa, A.M., Francisco, P.C., Motta, K., Chagas, T.R., dos Santos, C., Rafacho, A., Nunes, E.A. Fish oil supplementation attenuates changes in plasma lipids caused by dexamethasone treatment in rats

- (2016) APPLIED PHYSIOLOGY NUTRITION AND METABOLISM, 41 (4):382-390; 10.1139/apnm-2015-0487 APR 2016.
4. Nuño-Lámbarri N, Barbero-Becerra VJ, Uribe M, Chávez-Tapia NC. Mitochondrial Molecular Pathophysiology of Nonalcoholic Fatty Liver Disease: A Proteomics Approach. INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES, 17 (3):10.3390/ijms17030281 MAR 2016.
  5. Angrish, MM; Kaiser, JP; McQueen, CA; Chorley, BN. Tipping the balance: Hepatotoxicity and the 4 apical key events of hepatic steatosis. TOXICOLOGICAL SCIENCES, 150 (2):261-268; 10.1093/toxsci/kfw018 APR 2016
  6. Chikamoto, K; Misu, H; Takayama, H; Kikuchi, A; Ishii, K; Lan, F; Takata, N; Tajima-Shirasaki, N; Takeshita, Y; Tsugane, H; Kaneko, S; Matsugo, S; Takamura, T. Rapid response of the steatosis-sensing hepatokine LECT2 during diet-induced weight cycling in mice. BIOCHEMICAL AND BIOPHYSICAL RESEARCH COMMUNICATIONS, 478 (3):1310-1316; 10.1016/j.bbrc.2016.08.117 SEP 23 2016
  7. Tabish AM, Poels K, Byun H-M, et al. Changes in DNA Methylation in Mouse Lungs after a Single Intra-Tracheal Administration of Nanomaterials. Cao C, ed. PLoS ONE. 2017;12 (1): e0169886.
  8. Mostrag-Szlichtyng AS. Development of Knowledge Within a Chemical-Toxicological Database to Formulate Novel Computational Approaches for Predicting Repeated Dose Toxicity of Cosmetics-Related Compounds, Doctoral thesis, Liverpool John Moores University.2017. PhD <http://researchonline.ljmu.ac.uk/6798/1/2017mostrag-szlichtyngphd.pdf>
  9. Daniela Schuster. Pharmacophore Models for Toxicology Prediction. In: *Computational Toxicology: Risk Assessment for Chemicals*, First Edition. Edited by Sean Ekins. © 2018 John Wiley & Sons, Inc., Chapter 5, 121-144.
  10. Auger, F; Martin, F; Petrault, O; Samaillie, J; Hennebelle, T; Trabelsi, MS; Bailleul, F; Staels, B; Bordet, R; Duriez, P Risperidone-induced metabolic dysfunction is attenuated by *Curcuma longa* extract administration in mice. METABOLIC BRAIN DISEASE, 33 (1):63-77; 10.1007/s11011-017-0133-y FEB 2018
  11. Dong, QM; Kuefner, MS; Deng, X; Bridges, D; Park, EA; Elam, MB; Raghov, R. Sex-specific differences in hepatic steatosis in obese spontaneously hypertensive (SHROB) rats. BIOLOGY OF SEX DIFFERENCES, 9 10.1186/s13293-018-0202-x SEP 10 2018.
  12. YS Berezniysky, RV Duka. Characteristics of changes in lipid and carbohydrate metabolism indices in patients with morbid obesity before and after surgical treatment depending on the type of surgical intervention.- GASTROENTEROLOGY, 52 (1), 30-40. 2018 DOI: <https://doi.org/10.22141/2308-2097.52.1.2018.130777>
  13. Youness E.R., Aly H.F., El Nemr M. Role of apelin/monocyte chemoattractant protein-1, inflammatory, apoptotic markers in the regulation of patients with non-alcoholic fatty liver disease. *Asian Journal of Pharmaceutical and Clinical Research*, 11(8), pp. 138-142. DOI: 10.22159/ajpcr.2018.v11i8.25281.
  14. Hiart Navarro-Imaz, Yolanda Chico, Yuri Rueda, Olatz Fresnedo, Channeling of newly synthesized fatty acids to cholesterol esterification limits triglyceride synthesis in SND1-overexpressing hepatoma cells, *Biochimica et Biophysica Acta (BBA) - Molecular and Cell Biology of Lipids*, 1864 (2), 2019, 137-146, 2019.
  15. Perkins, EJ; Gayen, K; Shoemaker, JE; Antczak, P; Burgoon, L; Falciani, F; Gutsell, S; Hodges, G; Kienzler, A; Knappen, D; McBride, M; Willett, C; Doyle, FJ; Garcia-Reyero, N. Chemical Hazard Prediction and Hypothesis Testing Using Quantitative Adverse Outcome Pathways. ALTEX-ALTERNATIVES TO ANIMAL EXPERIMENTATION, 36 (1):91-102; 10.14573/altex.1808241 2019.
  16. Anna Palczewska, Simona Kovarich, Andrea Ciacci, Elena Fioravanzo, Arianna Bassan, Daniel Neagu, Ranking strategies to support toxicity prediction: A case study on potential LXR binders, *Computational Toxicology*, Volume 10, 2019, Pages 130-144, ISSN 2468-1113, <https://doi.org/10.1016/j.comtox.2019.01.004>
  17. Albhaisi, S. & Sanyal, A.J. Applying Non-Invasive Fibrosis Measurements in NAFLD/NASH: Progress to Date. *Pharm Med* (2019) 33: 451-463. <https://doi.org/10.1007/s40290-019-00305-z>
  18. Martínez Ferreras, Ángel. Effect of an experimental treatment with flavonoid quercetin on the development of steatosis, steatohepatitis, and hepatocarcinoma in in vivo and in vitro models of NAFLD, Instituto Universitario de Biomedicina, PhD Thesis, 2019 PhD
  19. Zhongyu Wang, Jingwen Chen, and Huixiao Hong. Applicability Domains Enhance Application of PPAR $\gamma$  Agonist Classifiers Trained by Drug-like Compounds to Environmental Chemicals. CHEMICAL RESEARCH IN TOXICOLOGY Volume: 33 Issue: 6 Pages: 1382-1388 Published: JUN 15 2020 DOI: 10.1021/acs.chemrestox.9b00498
  20. Chuan-Hai Li, Ya-Li Shi, Minjie Li, Liang-Hong Guo, Ya-Qi Cai. Receptor-Bound Perfluoroalkyl Carboxylic Acids Dictate Their Activity on Human and Mouse Peroxisome Proliferator-Activated Receptor  $\gamma$ . ENVIRONMENTAL SCIENCE & TECHNOLOGY Volume: 54 Issue: 15 Pages: 9529-9536 Published: AUG 4 2020 <https://doi.org/10.1021/acs.est.0c02386>

21. Zhongyu Wang, Jingwen Chen, Huixiao Hong. Developing QSAR Models with Defined Applicability Domains on PPAR $\gamma$  Binding Affinity Using Large Data Sets and Machine Learning Algorithms, *Environ. Sci. Technol.*, 2021, 55, 10, 6857–6866. <https://doi.org/10.1021/acs.est.0c07040>

**55. V.Y. Martiny, I. Pajeva, M. Wiese, A.M. Davis, M.A. Miteva** **Cheminformatic and Chemometric Approach to ADMET, First ed., Predictive ADMET: Integrative Approaches in Drug Discovery and Development. John Wiley & Sons, Inc. (2014), pp. 125-143**

Цитирания: 1

1. Dana A. AlQudah, Malek A. Zihlif, Mutasem O. Taha, Ligand-based modeling of diverse aryalkylamines yields new potent P-glycoprotein inhibitors, *European Journal of Medicinal Chemistry*, Volume 110, 2016, Pages 204-223, <https://doi.org/10.1016/j.ejmech.2016.01.034>

**56. Fratev F.; E. Mihaylova; I. Pajeva. Combination of genetic screen and molecular dynamics as a useful tool for identification of diseases-related mutations: ZASP PDZ domain G54S mutation case. *J. Chem. Inf. Model.* 2014, 54(5), 1524-1536.**

Цитирания: 9

1. Lopez-Ayala, J. M.; Ortiz-Genga, M.; Gomez-Milanes, I.; Lopez-Cuenca, D.; Ruiz-Espejo, F.; Sanchez-Munoz, J. J.; Oliva-Sandoval, M. J.; Monserrat, L.; Gimeno, J. R. A mutation in the Z-line Cypher/ZASP protein is associated with arrhythmogenic right ventricular cardiomyopathy. *CLINICAL GENETICS*, 88 ( 2 ) pp. 172 – 176, 2014. <http://dx.doi.org/10.1111/cge.12458>
2. Gao, N; Liang, T; Yuan, Y; Xiao, XC; Zhao, YH; Guo, YZ; Li, ML; Pu, XM. Exploring the mechanism of F282L mutation-caused constitutive activity of GPCR by a computational study. *PHYSICAL CHEMISTRY CHEMICAL PHYSICS*, 18 (42):29412-29422; 10.1039/c6cp03710k NOV 14 2016.
3. Muhammad Thoyib, C. Harsito, Suyitno Suyitno, Syamsul Hadi. Simple Procedure for Reducing Cratering Defect of Water-Based Paint Using Caesalpinia Sappan Dye. The 3rd Natural Pigment Conference for South-East Asia (NP-SEA), Malang, Aug. 2016, Citing conference paper.
4. Bang, M.-L. Animal Models of Congenital Cardiomyopathies Associated With Mutations in Z-Line Proteins. *JOURNAL OF CELLULAR PHYSIOLOGY*, 232 (1):38-52; 10.1002/jcp.25424 JAN 2017
5. Baoli Zhang, Xue Yang, Ning Feng, Hong Jiang. Progress of Genetics in Inherited Cardiomyopathies- Induced Heart Failure. In: *Heart Genomics*, edited by Hong Jiang, Ming Liu, Springer Nature Singapore Pte Ltd. 2018, pp. 293-332. DOI: 10.1007/978-981-13-1429-2\_11
6. Daday C., Mateyka L.M., Grater F., How ARVC-Related Mutations Destabilize Desmoplakin: An MD Study, *BIOPHYSICAL JOURNAL*, 116 (5):831-835; 10.1016/j.bpj.2019.01.023 MAR 5 2019
7. Grazioli, G; Martin, RW; Butts, CT. Comparative Exploratory Analysis of Intrinsically Disordered Protein Dynamics Using Machine Learning and Network Analytic Methods. *FRONTIERS IN MOLECULAR BIOSCIENCES*, 6 10.3389/fmolb.2019.00042 JUN 12 2019
8. Brodehl, A.; Ebbinghaus, H.; Deutsch, M.-A.; Gummert, J.; Gärtner, A.; Ratnavadivel, S.; Milting, H. Human Induced Pluripotent Stem-Cell-Derived Cardiomyocytes as Models for Genetic Cardiomyopathies. *Int. J. Mol. Sci.* **2019**, *20*, 4381.
9. Ting Zhao, Yuting Ma, Zuoquan Zhang, Jianzhong Xian, Xiaojing Geng, Feng Wang, Jiana Huang, Zhe Yang, Yi Luo, Yubi Lin. Young and early- onset dilated cardiomyopathy with malignant ventricular arrhythmia and sudden cardiac death induced by the heterozygous LDB3, MYH6, and SYNE1 missense mutations. *ANNALS OF NONINVASIVE ELECTROCARDIOLOGY*, 2021; 00:e12840. <https://doi.org/10.1111/anec.12840>

**57. Tsakovska I., M. Al Sharif, P. Alov, A. Diukendjieva, E. Fioravanzo, M.T.D. Cronin, I. K. Pajeva. Molecular modelling study of PPAR $\gamma$  receptor in relation to the mode of action / adverse outcome pathway framework for liver steatosis. *Int. J. Mol. Sci.* 2014, 15, 7651-7666.**

Цитирания: 23

1. Allen T. E. H., J.M. Goodman, S. Gutsell, and P. J. Russell. Defining Molecular Initiating Events in the Adverse Outcome Pathway Framework for Risk Assessment. *Chemical Research in Toxicology*, 2014 27 (12), 2100-2112
2. Zuang V., B. Desprez, J. Barroso, S. Belz, E. Berggren., C. Bernasconi, J. Bessems, S.e Bopp, S. Casati, S. Coecke, R. Corvi, C. Dumont, V. Gouliarmou, C. Griesinger, M. Halder, A. Janusch-Roi, A. Kienzler, B. Landesmann, F. Madia, A. Milcamps, S. Munn, A. Price, P. Prieto, M. Schäffer, J. Triebe, C. Wittwehr, A. Worth, M. Whelan.. EURL ECVAM status report on the development, validation and regulatory acceptance of alternative methods and approaches, European Union, 2015, pp. 1-114. DOI: 10.2788/62058, ISBN: 978-92-79-51990-1.
3. Hewitt, M., Przybylak, K. In silico models for hepatotoxicity IN SILICO METHODS FOR PREDICTING DRUG TOXICITY, 1425 201-236; 10.1007/978-1-4939-3609-0\_11 2016.

4. Allen, TEH; Liggi, S; Goodman, JM; Gutsell, S; Russell, PJ. Using Molecular Initiating Events To Generate 2D Structure–Activity Relationships for Toxicity Screening. *CHEMICAL RESEARCH IN TOXICOLOGY*, 29 (10):1611-1627; 10.1021/acs.chemrestox.6b00101 OCT 2016
5. Allen T.E.H., Goodman J.M., Gutsell S., Russell P.J. A History of the Molecular Initiating Event, *CHEMICAL RESEARCH IN TOXICOLOGY*, 29 (12):2060-2070, DEC 2016.
6. Lavallée-Bourget MH, Rôle de la phosphorylation sur tyrosine dans la régulation de l'activité de PPAR $\gamma$ , Thèses et mémoires, Université Laval, 2016 PhD  
<https://corpus.ulaval.ca/jspui/handle/20.500.11794/33285?locale=en>
7. Satarupa Acharjee Sengupta, Tapan K. Maity, Subir Samanta. Synthesis, Biological Screening and *in Silico* Studies of Chalcone Based Novel Phenyl Urea Derivatives as Potential Antihyperglycemics. *Journal of Pharmaceutical Research* Volume 16, Issue 3, Jul-Sep, 2017: 237-246.
8. Berggren E., White A., Ouedraogo G., Paini A., Richarz A.-N., Bois F.Y., Exner T., Leite S., Grunsven L.A.V., Worth A., Mahony C. Ab initio chemical safety assessment: A workflow based on exposure considerations and non-animal methods. *Computational Toxicology*, 4, pp.31-44, 2017.
9. Chemical Safety Assessment Workflow Based on Exposure Considerations and Non-Animal Methods, OECD Environment, Health and Safety Publications, Series on Testing and Assessment, No. 275, ENV/JM/MONO(2017) 27
10. Niklas Andersson, Maria Arena, Domenica Auteri, Stefania Barmaz, Elise Grignard, Aude Kienzler, Peter Lepper, Alfonso Maria Lostia, Sharon Munn, Juan Manuel Parra Morte, Francesca Pellizzato, Jose Tarazona, Andrea Terron, Sander Van der Linden. European Chemicals Agency ECHA; EFSA. Guidance for the identification of endocrine disruptors in the context of Regulations (EU) No 528/2012 and (EC) No 1107/2009. *EFSA JOURNAL*, 16 (6). <https://doi.org/10.2903/j.efsa.2018.5312> JUN 2018
11. Daniela Schuster. Pharmacophore Models for Toxicology Prediction. In: *Computational Toxicology: Risk Assessment for Chemicals*, First Edition. Edited by Sean Ekins. © 2018 JohnWiley & Sons, Inc., Chapter 5, 121-144.
12. Esaki, S; Nagasawa, T; Tanaka, H; Tominaga, A; Mikami, D; Usuki, S; Hamajima, H; Hanamatsu, H; Sakai, S; Hama, Y; Igarashi, Y; Kitagaki, H; Mitsutake, S. The fungal 9-methyl-sphingadiene is a novel ligand for both PPAR and GPR120. *JOURNAL OF FOOD BIOCHEMISTRY*, 42 (5):10.1111/jfbc.12624 OCT 2018.
13. Gim, HJ; Choi, YS; Li, H; Kim, YJ; Ryu, JH; Jeon, R. Identification of a Novel PPAR- Agonist through a Scaffold Tuning Approach. *INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES*, 19 (10):10.3390/ijms19103032 OCT 2018
14. Wang, J., Wang, B., Zhang, Y. Agonism activities of lyso-phosphatidylcholines (LPC) Ligands binding to peroxisome proliferator-activated receptor gamma (PPAR $\gamma$ ). *Journal of Biomolecular Structure and Dynamics*, 38:2, 398-409 Published: JAN 22 2020 DOI: 10.1080/07391102.2019.1577175
15. Thangavel N, Al Bratty M, Javed SA, Ahsan W, Alhazmi HA. Critical Insight into the Design of PPAR- $\gamma$  Agonists by Virtual Screening Techniques. *Curr Drug Discov Technol*. 2019; 16(1):82-90. doi: 10.2174/1570163815666180227164028.
16. Arnesen, H; Haj-Yasein, NN; Tungen, JE; Soedling, H; Matthews, J; Paulsen, SM; Nebb, HI; Sylte, I; Hansen, TV; Saether, T. Molecular modelling, synthesis, and biological evaluations of a 3,5-disubstituted isoxazole fatty acid analogue as a PPAR $\alpha$ -selective agonist, *BIOORGANIC & MEDICINAL CHEMISTRY*, 27 (18):4059-4068; 10.1016/j.bmc.2019.07.032 SEP 15 2019
17. Wedlake, A. J. (2019). Structure-based Predictions for Molecular Initiating Events (Doctoral thesis). <https://doi.org/10.17863/CAM.44741> PhD
18. Rodrigues RM, Kollipara L, Chaudhari U, Sachinidis A, Zahedi RP, Sickmann A, Kopp-Schneider A, Jiang X, Keun H, Hengstler J, Oorts M, Annaert P, Hoeben E, Gijbels E, De Kock J, Vanhaecke T, Rogiers V, Vinken M. Omics-based responses induced by bosentan in human hepatoma HepaRG cell cultures. *Arch Toxicol*. 2018 Jun;92(6):1939-1952.
19. Xiaobin Liu, Danhua Zheng, Yi Zhong, Zhaofan Xia, Heng Luo, and Zuquan Weng. Machine-Learning Prediction of Oral Drug-Induced Liver Injury (DILI) via Multiple Features and Endpoints. May 2020. *BioMed Research International*, 2020, Volume 2020 |Article ID 4795140 | 2314-6133.| <https://doi.org/10.1155/2020/4795140>
20. Zhongyu Wang, Jingwen Chen, and Huixiao Hong. Applicability Domains Enhance Application of PPAR $\gamma$  Agonist Classifiers Trained by Drug-like Compounds to Environmental Chemicals. *CHEMICAL RESEARCH IN TOXICOLOGY* Volume: 33 Issue: 6 Pages: 1382-1388 Published: JUN 15 2020 DOI: 10.1021/acs.chemrestox.9b00498
21. Hyun Soo Kim, Jun Hyuek Yang, Doo Seok Kang, Nam Gook Kee, Cheol Min Lee, Jong-Hyeon Jung, Yeon-Soon Ahn, Young Rok Seo. Suggestions for applications of toxicogenomic approaches in the adverse outcome pathway of 2,4-dinitrotoluene. *TOXICOLOGY AND ENVIRONMENTAL HEALTH SCIENCES*, June 2020, 12 (2), 109-118. DOI: 10.1007/s13530-020-00054-6

22. Timothy E. H. Allen, Mark D. Nelms, Stephen W. Edwards, Jonathan M. Goodman, Steve Gutsell, Paul J. Russell. In Silico Guidance for In Vitro Androgen and Glucocorticoid Receptor ToxCast Assays. ENVIRONMENTAL SCIENCE & TECHNOLOGY, Volume 54, Issue: 12, Pages: 7461-7470, Published: JUN 16 2020. <https://doi.org/10.1021/acs.est.0c01105>
23. David A. Dreier, John A. Bowden, Juan J. Aristizabal-Henao, Nancy D. Denslow, Christopher J. Martyniuk, Ecotoxicolipidomics: An emerging concept to understand chemical-metabolic relationships in comparative fish models, *Comparative Biochemistry and Physiology Part D: Genomics and Proteomics*, Volume 36, 2020, 100742, ISSN 1744-117X, <https://doi.org/10.1016/j.cbcd.2020.100742>

**58. Martiny V. Y., I. Pajeva, M. Wiese, A. M. Davis, M. A. Miteva. Chemoinformatic and Chemometric Approach to ADMET, First ed., In: Predictive ADMET: Integrative Approaches in Drug Discovery and Development 2014, John Wiley & Sons, Inc., pp. 125–143.**

Цитирания: 1

1. AlQudah, D.A., Zihlif, M.A., Taha, M.O. Ligand-based modeling of diverse aralkylamines yields new potent P-glycoprotein inhibitors. *European Journal of Medicinal Chemistry*, 2016, 110, pp. 204-223.

**59. Wiese M., I. Pajeva. HAGE, the helicase antigen as a biomarker for breast cancer prognosis (WO2013144616) (2014) Expert Opin. Ther. Pat. 2014, 24 (6) , pp. 723-725.**

Цитирания: 5

1. Vakrania, AK; Variya, BC; Patel, SS. Novel targets for paclitaxel nano formulations: Hopes and hypes in triple negative breast cancer (Review PHARMACOLOGICAL RESEARCH, 111 577-591; 10.1016/j.phrs.2016.07.023 SEP 2016
2. T Talwar. Biochemical Characterization of DDX43 (HAGE) Helicase. Thesis, Department of Biochemistry, University of Saskatchewan , Saskatoon, Canada, March, 2017.
3. Andrea MAHR, Toni Weinschenk, Oliver Schoor, Jens FRITSCH, Harpreet Singh. Novel peptides and combination of peptides for use in immunotherapy and methods for generating scaffolds for the use against pancreatic cancer and other cancers, US 20160368965 A1, 2017 (patent)
4. D. Nagarajan. Towards the development of HAGE -based vaccines for the treatment of patients with triple negative breast cancers. A thesis submitted in partial fulfilment of the requirements of Nottingham Trent University for Doctor of Philosophy, 2018 PhD
5. M Andrea, T Weinschenk, O Schoor, J Fritsche. H. Singh. Peptides and combination of peptides for use in immunotherapy and methods for generating scaffolds for the use against pancreatic cancer and other cancers. US Patent US10385109B2. 2019

**60. Alov P, I. Tsakovska. I. Pajeva. Computational studies of free radical-scavenging properties of phenolic compounds. Curr. Top. Med. Chem. 2015, 15, 85–104.**

Цитирания: 62

1. Goutzourelas, N., Stagos, D., Spanidis, Y., Liosi, M., Apostolou, A., Priftis, A., Haroutounian, S., Spandidos, D. A., Tsatsakis, A. M., Kouretas, D. Polyphenolic composition of grape stem extracts affects antioxidant activity in endothelial and muscle cells (2015) *Molecular Medicine Reports*, 12 (4), pp. 5846-5856.
2. Vakarelska-Popovska, M., Velkov, Z. Monohydroxy flavones. Part III: The mulliken analysis (2015) *Chemistry*, 24 (3), pp. 363-369.
3. Kandouli Chouaib, Emilie Ricquebourg, Mathieu Cassien, Anne Mercier, Pierre Stocker, Zineb Leulmi, Mechakra Aicha, Marcel Culcasi, Sylvia Pietri. In vitro and in vivo evaluation of the antioxidant, antidiabetic and cardioprotective activities from the aerial parts of *Anvillea radiata* (Coss. & Dur.) 15th International Conference on Oxidative Stress Reduction, Redox Homeostasis and Antioxidants, Paris, France. Ordinal: ISANH2015, June 2015
4. Hubert, J; Angelis, A; Aligiannis, N; Rosalia, M; Abedini, A; Bakiri, A; Reynaud, R; Nuzillard, JM; Gangloff, SC; Skaltsounis, AL; Renault, JH. In Vitro Dermo-Cosmetic Evaluation of Bark Extracts from Common Temperate Trees. *PLANTA MEDICA*, 82 (15):1351-1358; 10.1055/s-0042-110180 OCT 2016
5. Dzialo, M; Mierziak, J; Korzun, U; Preisner, M; Szopa, J; Kulma, A. The Potential of Plant Phenolics in Prevention and Therapy of Skin Disorders. *INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES*, 17 (2):10.3390/ijms17020160 FEB 2016
6. Elena Alvareda, Pablo A. Denis, Federico Iribarne, Margot Paulino, Bond dissociation energies and enthalpies of formation of flavonoids: A G4 and M06-2X investigation, *Computational and Theoretical Chemistry*, Volume 1091, 1 September 2016, Pages 18-23, ISSN 2210-271X, <http://dx.doi.org/10.1016/j.comptc.2016.06.021>.
7. Zhuravlev, AV; Zakharov, GA; Shchegolev, BF; Savvateeva-Popova, EV. Antioxidant Properties of Kynurenines: Density Functional Theory Calculations. *PLOS COMPUTATIONAL BIOLOGY*, 12 (11):10.1371/journal.pcbi.1005213 NOV 2016

8. N.Chornenka, Y. Rayetska, O. Savchuk, L.Ostapchenko. Biochemical changes in blood serum of rats with experimental burn disease and their correction with melanin. Taras Shevchenko National University of Kyiv, Kyiv, Ukraine, 2016, 44-48. УДК 616.329-001.37-053 ISSN 1728-3817.
9. I. M. Sytnik, M. V. Khaitovych, P. A. Chernovol. Antioxidant activity of angiotensin II inhibitors and metabotropic cardioprotectors under conditions in vitro and in silico. Фармакологія та лікарська токсикологія, № 2 (48), 2016, 80-85. УДК 615.224: 036.8: 612.08: 004.382
10. Peerannawar, S; Horton, W; Kokel, A; Torok, F; Torok, M; Torok, B. Theoretical and experimental analysis of the antioxidant features of diarylhydrazones. STRUCTURAL CHEMISTRY, 28 (2):391-402; SI 10.1007/s11224-016-0867-x APR 2017.
11. Kudanga T., Nemadziva B., Le Roes-Hill M. Laccase catalysis for the synthesis of bioactive compounds. APPLIED MICROBIOLOGY AND BIOTECHNOLOGY, 101 (1):13-33; 10.1007/s00253-016-7987-5 JAN 2017
12. Ben Ahmed, Z; Yousfi, M; Viaene, J; Dejaegher, B; Demeyer, K; Mangelings, D; Heyden, YV. Seasonal, gender and regional variations in total phenolic, flavonoid, and condensed tannins contents and in antioxidant properties from Pistacia atlantica ssp leaves. PHARMACEUTICAL BIOLOGY, 55 (1):1185-1194; 10.1080/13880209.2017.1291690 2017.
13. Machado, NFL; Dominguez-Perles, R. Addressing Facts and Gaps in the Phenolics Chemistry of Winery By-Products. MOLECULES, 22 (2):10.3390/molecules22020286 FEB 2017.
14. Cetin, MM; Hodson, RT; Hart, CR; Cordes, DB; Findlater, M; Casadonte, DJ; Cozzolino, AF; Mayer, MF. Characterization and photocatalytic behavior of 2,9-di(aryl)-1,10-phenanthroline copper(I) complexes. DALTON TRANSACTIONS, 46 (20):6553-6569; 10.1039/c7dt00400a MAY 28 2017.
15. Okayama Y., Harada M., Morita M., Mochizuki M., Inami K. Synthesis and radical scavenging activity of substituted Benzo [H] chromanols. HETEROCYCLES, 94 (5):865-878; 10.3987/COM-17-13671 MAY 1 2017
16. Kandouli, C; Cassien, M; Mercier, A; Delehedde, C; Ricquebourg, E; Stocker, P; Mekaouche, M; Leulmi, Z; Mechakra, A; Thetiot-Laurent, S; Culcasi, M; Pietri, S. Antidiabetic, antioxidant and anti inflammatory properties of water and n-butanol soluble extracts from Saharian Anvillea radiata in high-fat-diet fed mice, JOURNAL OF ETHNOPHARMACOLOGY, 207 251-267; 10.1016/j.jep.2017.06.042 JUL 31 2017.
17. Anjomshoa, S., Namazian, M. & Noorbala, M.R. Is curcumin a good scavenger of reactive oxygen species? A computational investigation. THEORETICAL CHEMISTRY ACCOUNTS, 136 (9):10.1007/s00214-017-2128-5 SEP 5 2017
18. N. Chornenka, K. Valetska, Ya. Rayetska, L.Ostapchenko, CORRECTION OF MELANIN PROTEOLYTIC ACTIVITY IN THE CONDITIONS OF MODELING ALKALI BURNS OF THE ESOPHAGUS. Bulletin of Taras Shevchenko National University of Kyiv. Series: Problems of Physiological Functions Regulation, vol. 22 (1), 53-57, 2017. DOI: 10.17721/2616\_6410.2017.22.53-57
19. R. Hajiboland, N. Moradtalab, Z. Eshaghi & J. Feizy: Effect of silicon supplementation on growth and metabolism of strawberry plants at three developmental stages, NEW ZEALAND JOURNAL OF CROP AND HORTICULTURAL SCIENCE, 46 (2):144-161; 10.1080/01140671.2017.1373680 2018
20. Fernández Moriano, C. Estudio con criterios filogenéticos del potencial neuroprotector de líquenes parmeliáceos: mecanismos de acción de sus metabolitos secundarios. UNIVERSIDAD COMPLUTENSE DE MADRID FACULTAD DE FARMACIA, Departamento de Biología Vegetal II, 2018 PhD <http://eprints.ucm.es/46016/1/T39498.pdf>
21. Jabeen, H; Saleemi, S; Razzaq, H; Yaqub, A; Shakoor, S; Qureshi, R. Investigating the scavenging of reactive oxygen species by antioxidants via theoretical and experimental methods, JOURNAL OF PHOTOCHEMISTRY AND PHOTOBIOLOGY B-BIOLOGY, 180 268-275; 10.1016/j.jphotobiol.2018.02.006 MAR 2018
22. Silva, M; Castellanos, L; Ottens, M. Capture and Purification of Polyphenols Using Functionalized Hydrophobic Resins. INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH, 57 (15):5359-5369; 10.1021/acs.iecr.7b05071 APR 18 2018
23. Hajiboland, R. Moradtalab, N. Aliasghar zad, N. Eshaghi, Z. Feizy, J. Silicon influences growth and mycorrhizal responsiveness in strawberry plants. Physiology and Molecular Biology of Plants. 24(6), 2018, DOI:10.1007/s12298-018-0533-4
24. Parvathy, U; Sivaraman, GK; Murthy, LN; Visnuvinayagam, S; Jeyakumari, A; Ravishankar, CN. Green coffee extract as a natural antioxidant in chill stored indian mackerel (Rastrelliger kanagurta) mince. INDIAN JOURNAL OF FISHERIES, 65 (1):86-95; 10.21077/ijf.2018.65.1.73739-14 2018.
25. Silva, M; Garcia, JC; Ottens, M. Polyphenol Liquid-Liquid Extraction Process Development Using NRTL-SAC. INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH, 57 (28):9210-9221; 10.1021/acs.iecr.8b00613 JUL 18 2018
26. Bettencourt, A; Castro, M; Silva, J; Fernandes, F; Coutinho, O; Sousa,

- MJ; Proenca, MF; Areias, F. New Nitrogen Compounds Coupled to Phenolic Units with Antioxidant and Antifungal Activities: Synthesis and Structure-Activity Relationship. *MOLECULES*, 23 (10):10.3390/molecules23102530 OCT 2018
27. Yunsheng Xue, Yunping Liu, Qingquan Luo, Han Wang, Ran Chen, Yin Liu, and Ya Li. Antiradical Activity and Mechanism of Coumarin–Chalcone Hybrids: Theoretical Insights. *The Journal of Physical Chemistry A* **2018** 122 (43), 8520-8529 DOI: 10.1021/acs.jpca.8b06787
  28. William Horton. Design and Assessment of Small Molecules as Free Radical Scavengers and Potential Multi-target Therapeutic Agents against Alzheimer's Disease, Diabetes and Cancer. University of Massachusetts, Boston, 2018, pp 263 PhD
  29. Nematziva B. Small laccases as catalysts for the synthesis of antioxidants. 2018 Submitted in fulfillment for the Master of Applied Science (Biotechnology) degree, Durban University of Technology, Durban, South Africa, 2018 <http://openscholar.dut.ac.za/handle/10321/3176>
  30. Elder, AS; Coupland, JN; Elias, RJ. Antioxidant activity of a winterized, acetonetic rye bran extract containing alkylresorcinols in oil-in-water emulsions. *FOOD CHEMISTRY*, 272 174-181; 10.1016/j.foodchem.2018.08.011 JAN 30 2019.
  31. Sana Khatri, Additiya Paramanya, Ahmad Ali. Phenolic Acids and Their Health-Promoting Activity: Phytochemistry and Molecular Aspects. In: Ozturk M., Hakeem K. (eds.) *Plant and Human Health*, Volume 2. Springer, 661-680, 2019. DOI: 10.1007/978-3-030-03344-6\_27
  32. Ahamed, TKS; Rajan, VK; Sabira, K; Muraleedharan, K. DFT and QTAIM based investigation on the structure and antioxidant behavior of lichen substances Atranorin, Evernic acid and DiffRACTAIC acid. *COMPUTATIONAL BIOLOGY AND CHEMISTRY*, 80 66-78; 10.1016/j.compbiolchem.2019.03.009 JUN 2019
  33. Varricchio, E; Coccia, E; Orso, G; Lombardi, V; Imperatore, R; Vito, P; Paolucci, M. Influence of polyphenols from olive mill wastewater on the gastrointestinal tract, alveolar macrophages and blood leukocytes of pigs. *ITALIAN JOURNAL OF ANIMAL SCIENCE*, 18 (1):574-586; 10.1080/1828051X.2018.1548911 JAN 2 2019
  34. Bettencourt, AP; Castro, M; Silva, JP; Fernandes, F; Coutinho, OP; Sousa, MJ; Proenca, MF; Areias, FM. Phenolic Imidazole Derivatives with Dual Antioxidant/Antifungal Activity: Synthesis and Structure-Activity Relationship. *MEDICINAL CHEMISTRY*, 15 (4):341-351; 10.2174/1573406414666181005143431 2019
  35. Coccia, E; Imperatore, R; Orso, G; Melck, D; Varricchio, E; Volpe, MG; Paolucci, M. Explants of *Oncorhynchus mykiss* intestine to detect bioactive molecules uptake and metabolic effects: Applications in aquaculture. *AQUACULTURE*, 506 193-204; <https://doi.org/10.1016/j.aquaculture.2019.03.041> MAY 15 2019
  36. Velkov Z., Traykov M., Trenchev I., Saso L., Tadjer A. Topology-Dependent Dissociation Mode of the O-H Bond in Monohydroxycoumarins. 2019. *JOURNAL OF PHYSICAL CHEMISTRY A*, 123 (24):5106-5113; 10.1021/acs.jpca.9b00535 JUN 20 2019. <https://doi.org/10.1021/acs.jpca.9b00535>
  37. Vilela, A; Pinto, T. Grape Infusions: The Flavor of Grapes and Health-Promoting Compounds in Your Tea Cup. *BEVERAGES*, 5 (3, 48. doi:10.3390/beverages5030048 SEP 2019
  38. Szymanowska, U; Baraniak, B. Antioxidant and Potentially Anti-Inflammatory Activity of Anthocyanin Fractions from Pomace Obtained from Enzymatically Treated Raspberries. *ANTIOXIDANTS*, 8 (8), art. No. 299. 10.3390/antiox8080299 AUG 2019.
  39. Olszowy M. What is responsible for antioxidant properties of polyphenolic compounds from plants? *PLANT PHYSIOLOGY AND BIOCHEMISTRY*, 144, 135-143, NOV 2019. DOI: 10.1016/j.plaphy.2019.09.039
  40. Benarfa, A; Gourine, N; Mahfoudi, R; Harrat, M; Yousfi, M. Effect of Seasonal and Regional Variations on Phenolic Compounds of *Deverra scoparia* (Flowers/Seeds) Methanolic Extract and the Evaluation of Its *in Vitro* Antioxidant Activity. *CHEMISTRY & BIODIVERSITY*, Volume 16, Issue 11, 17 September 2019, <https://doi.org/10.1002/cbdv.201900420>
  41. Ali, Soad A. and S. M. A. Bakr, Hepatoprotective Impact of Cinnamon Aqueous Extract. *Journal of Food and Dairy Sciences*, 10 (8) 249-255, 2019. DOI: 10.21608/jfds.2019.58136
  42. Aruwa, Christiana Eleojo. Characterisation of Opuntia phenolic extracts and enzymatic modification of selected compounds. Submitted in fulfillment of the requirements for the degree of Doctor of Philosophy (PhD): Biotechnology, Durban University of Technology, Durban, South Africa, 2019. <http://hdl.handle.net/10321/3355> PhD
  43. ІН Сьтник. Фармакологічне Обґрунтування Застосування N-Ацетилцистеїну Та Лозартану При Кардіальних Порушеннях Цукрового Діабету 1 Типу. Національний медичний університет імені О.О. Богомольця МОЗ України (м. Київ). Дисертації на здобуття наукового ступеня кандидата фармацевтичних наук, 2019. PhD <http://dspace.nuph.edu.ua/handle/123456789/19788>
  44. DA Hernandez, JG Rodriguez-Zavala, FJ Tenorio. DFT study of antioxidant molecules from traditional Japanese and Chinese teas: comparing allylic and phenolic antiradical activity. *STRUCTURAL CHEMISTRY* (2019). Volume: 31 Issue: 1 Pages: 359-369, 2020.

45. Rasha H Elsayed, Emadeldin M Kamel, Ayman M Mahmoud, Ashraf A El Bassuony, May Bin-Jumah, Al Mokhtar Lamsabhi, Sayed A Ahmed. Rumex dentatus L. phenolics ameliorate hyperglycemia by modulating hepatic key enzymes of carbohydrate metabolism, oxidative stress and PPAR $\gamma$  in diabetic rats. *FOOD CHEM TOXICOL.*, 2020 Apr;138:111202. doi: 10.1016/j.fct.2020.111202.
46. Anitha, S.; Krishnan, S.; Senthilkumar, K.; Sasirekha, V. Theoretical investigation on the structure and antioxidant activity of (+) catechin and (-) epicatechin - a comparative study. *Molecular Physics*, 118 (17), art. no. e1745917, 2020, DOI: 10.1080/00268976.2020.1745917
47. Adel Benarfa, Nadhir Gourine, Soumaya Hachani, Mohamed Harrat, Mohamed Yousfi. Optimization of ultrasound- assisted extraction of antioxidative phenolic compounds from *Deverra scoparia* Coss. & Durieu (flowers) using response surface methodology. *JOURNAL OF FOOD PROCESSING AND PRESERVATION* Article Number: e145142020. <https://doi.org/10.1111/jfpp.14514>
48. Belaya, N.I., Belyi, A.V. & Shcherbakov, I.N. Predictive Model of the Relationship of the Antiradical Activity and the Ionization Potential of Molecules and Ions of Flavonoids. *KINETICS AND CATALYSIS* Volume: 61 Issue: 3 Pages: 360-368 Published: MAY 2020. <https://doi.org/10.1134/S0023158420030040>
49. Otukile, Kgalaletso Precious, Reactions of phloroglucinols with radical species, a theoretical study in different media. MSc (Chemistry), North-West University (South Africa), 2020. <http://repository.nwu.ac.za/handle/10394/35099?show=full> PhD
50. NOGUEIRA, Kerolayne de Melo. Efeito Anti-Inflamatório, Antioxidante E Antipirético, Do Vanilato De Isopropila, Um Derivado Semissintetico Do Ácido Vanílico. Dissertação apresentada ao Programa de PósGraduação em iotecnologia da Universidade Federal do Piauí - UFPI, como requisito para obtenção do título de mestre em Biotecnologia. Área de concentração: Farmacologia Molecular aplicada a Biotecnologia, 2020. <https://repositorio.ufpi.br/xmlui/handle/123456789/2347> PhD
51. Xiaowei Zhang, Chunhui Liu, Wenhan Tian, Hui Zhang, Peirui Li, Jiahua Wang, Weiwei He. Theoretical and experimental investigation of the antioxidative activity of monascin. *FOOD & FUNCTION* Volume: 11 Issue: 7 Pages: 5915-5923 Published: JUL 1 2020. <http://dx.doi.org/10.1039/C9FO02410G>
52. Annisa Wulandari, Afrizal Afrizal, Emriadi Emriadi, Mai Efdi, Imelda. Studi komputasi terhadap struktur, sifat antioksidan, toksisitas dan skor obat dari scopoletin dan turunannya *Chempublish Journal*, Vol 5, No 1, (2020), 77-92. <https://doi.org/10.22437/chp.v5i1.9023>
53. Vazquez-Flores, A. A., Góngora-Pérez, O., Olivas-Orduña, I., Muñoz-Bernal, O. A., Osuna-Avila, P., Rodrigo-García, J., de la Rosa, L. A., & Alvarez-Parilla, E. (2020). Pytochemical profile and antioxidant activity of chiltepin chili (*Capsicum annum* var. *glabriusculum*), Sonora, Mexico. *Journal of Food Bioactives*, 11. <https://doi.org/10.31665/JFB.2020.11237>
54. Castelucci, A. C. L., de Toledo, N. M. V., Juliano, F. F., da Silva, P. P. M., & Spoto, M. H. F. (2020). Influence of processing on the phenolic compounds of feijoa pulp (*Feijoa sellowiana*). *Journal of Food Bioactives*, 11. <https://doi.org/10.31665/JFB.2020.11238>
55. Knez Hrnčič, M.; Cör, D.; Simonovska, J.; Knez, Ž.; Kavrakovski, Z.; Rafajlovska, V. Extraction Techniques and Analytical Methods for Characterization of Active Compounds in *Origanum* Species. *Molecules* **2020**, 25, 4735
56. Miguel A. Hernández-Valdepeña, Carmen G. Hernández-Valencia, Pablo Labra-Vázquez, Carmen Wachter, Gloria Díaz-Ruiz, Alfredo Vázquez, José Pedraza-Chaverri, Keiko Shirai, Alberto Rosas-Aburto, Eduardo Vivaldo-Lima, Eduardo Bárzana, Romina Rodríguez-Sonoja, Miquel Gimeno, Antioxidant and antimicrobial material by grafting of L-Arginine onto enzymatic poly(gallic acid), *MATERIALS SCIENCE & ENGINEERING C-MATERIALS FOR BIOLOGICAL APPLICATIONS*, Vol. 121, Article Number: 111650 FEB 2021, <https://doi.org/10.1016/j.msec.2020.111650>
57. Prafulla Madhukarrao Sable, Nusrat Bhuru Ali Sayyad. Synthesis and QSAR Studies of Novel Pyrazoline Derivatives as Antiproliferative Agent. *Indian Journal of Pharmaceutical Education and Research*, 54(3), pp. S610-S619, Jul-Sep, 2020. <https://doi.org/10.5530/ijper.54.3s.161>
58. Shyamalendu Nath, Kashyap J. Tamuli, Barnali Gogoi, Manobjyoti Bordoloi, Aparoop Das, Chandana C. Barua, Iswar C. Barua, Antioxidant properties, phenolic and mineral profiling, assessment of angiotensin I converting enzyme (ACE) inhibitory potential of *Elsholtzia communis* (Collett & Hemsl.) Diels from North East India, *EUROPEAN JOURNAL OF INTEGRATIVE MEDICINE* Volume: 40 Article Number: 101247 Published: DEC 2020, <https://doi.org/10.1016/j.eujim.2020.101247>
59. Kumar N., Gusain A., Kumar J., Singh R., Hota P.K. Anti-oxidation properties of 2-substituted furan derivatives: A mechanistic study. *Journal of Luminescence*, 230, art. no. 117725, 2021
60. Khairullina, V.; Safarova, I.; Sharipova, G.; Martynova, Y.; Gerchikov, A. QSAR Assessing the Efficiency of Antioxidants in the Termination of Radical-Chain Oxidation Processes of Organic Compounds. *MOLECULES*, Volume: 26, Issue: 2, Article Number: 421 Published: JAN 2021. DOI: 10.3390/molecules26020421

61. Kumar C. R. S., Jha A., Deepthi S, "DFT Studies of Distinct Anilines with p-Hydroxycinnamic Acids for Antioxidant Profile", *MEDICINAL CHEMISTRY*, Volume: 17, Issue: 1, Pages: 60-70. Published: 2021. <https://doi.org/10.2174/1573406416666200506085152>

**61. Fratev, F.; Tsakovska, I.; Sharif, M.; Mihaylova, E.; Pajeva, I. Structural and Dynamical Insights into PPAR $\gamma$  Antagonism: In Silico Study of the Ligand-Receptor Interactions of Non-Covalent Antagonists. *Int. J. Mol. Sci.* 2015, 16, 15405-15424.**

Цитирания: 8

1. Batista, MRB; Martinez, L. Conformational Diversity of the Helix 12 of the Ligand Binding Domain of PPAR $\gamma$  and Functional Implications. *JOURNAL OF PHYSICAL CHEMISTRY B*, 119 (50):15418-15429; 10.1021/acs.jpcc.5b09824 DEC 17 2015
2. Mellor, C.L., Steinmetz, F.P., Cronin, M.T.D. Using Molecular Initiating Events to Develop a Structural Alert Based Screening Workflow for Nuclear Receptor Ligands Associated with Hepatic Steatosis. *CHEMICAL RESEARCH IN TOXICOLOGY*, 29 (2):203-212; 10.1021/acs.chemrestox.5b00480 FEB 2016.
3. Chia, LL; Jantan, I; Chua, KH; Lem, KW; Rullah, K; Aluwi, MFM. Effects of Tocotrienols on Insulin Secretion-Associated Genes Expression of Rat Pancreatic Islets in a Dynamic Culture. *FRONTIERS IN PHARMACOLOGY*, 7 10.3389/fphar.2016.00291 AUG 30 2016
4. Routti, H., Lille-Langoy, R., Berg, M.K., Fink, T., Harju, M., Kristiansen, K., Rostkowski, P., Rusten, M., Sylte, I., Øygarden, L., Goksoyr, A. Environmental Chemicals Modulate Polar Bear (*Ursus maritimus*) Peroxisome Proliferator-Activated Receptor Gamma (PPARG) and Adipogenesis in Vitro (2016) *Environmental Science and Technology*, 50 (19), pp. 10708-10720.
5. Mottin, M; Souza, PCT; Ricci, CG; Skaf, MS. CHARMM Force Field Parameterization of Peroxisome Proliferator-Activated Receptor  $\gamma$  Ligands. *INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES*, 18 (1):10.3390/ijms18010015 JAN 2017.
6. Heli Routti, Bjørn Munro Jenssen, Sabrina Tartu. Ecotoxicologic Stress in Arctic Marine Mammals, With Particular Focus on Polar Bears. In: *Marine Mammal Ecotoxicology*, Maria Cristina Fossi, Cristina Pantì (eds.) Academic Press, Aug 6, 2018, pp.345-380.
7. Holli-Joi Sullivan, Xiaoyan Wang, Shaina Nogle, Siyan Liao, Chun Wu. To Probe Full and Partial Activation of Human Peroxisome Proliferator-Activated Receptors by Pan-Agonist Chiglitazar Using Molecular Dynamics Simulations, *PPAR RESEARCH* Volume: 2020 Article Number: 5314187 Published: APR 1 2020. <https://doi.org/10.1155/2020/5314187>
8. Kaupang A., Hansen T.V. The PPAR  $\Omega$  Pocket: Renewed Opportunities for Drug Development. *PPAR RESEARCH*, Vol. 2020, Article Number: 9657380. Published: JUL 1 2020. <https://doi.org/10.1155/2020/9657380>

**62. Vitcheva V, Mostrag-Szlichtyng A, Sacher O, Bienfait B, Schwab CH, Richarz AN, Tsakovska I, Al Sharif M, Pajeva I, Yang C. In vivo data mining and in silico metabolic profiling to predict diverse hepatotoxic phenotypes: Case study of piperonyl butoxide. *Toxicol. Lett.* 2015, 238(2): S173, 2015.**

Цитирания: 2

1. Berggren E, White A, Ouedraogo G, Paini A, Richarz AN, Bois FY, Exner T, Leite S, Grunsven LAV, Worth A, Mahony C. Ab initio chemical safety assessment: A workflow based on exposure considerations and non-animal methods. *Comput Toxicol.*, 2017, 4, 31-44
2. Chemical Safety Assessment Workflow Based on Exposure Considerations and Non-Animal Methods, OECD Environment, Health and Safety Publications, Series on Testing and Assessment, No. 275, ENV/JM/MONO(2017) 27

**63. P. Alov, M.T.D. Cronin, A. Diukendjieva, J.C. Madden, I. Pajeva, F.P. Steinmetz, I. Tsakovska, and C. Yang, In silico models for skin permeability and gastrointestinal absorption to facilitate extrapolation between oral and dermal administrations for repeated dose toxicity, SEURAT-1 5th Annual Meeting, Barcelona, Spain, 21–22 January 2015.**

Цитирания: 1

1. Eleftheriadou, D; Luetete, S; Kneuer, C. In silico prediction of dermal absorption of pesticides – an evaluation of selected models against results from in vitro testing. *SAR AND QSAR IN ENVIRONMENTAL RESEARCH*, 30 (8):561-585; 10.1080/1062936X.2019.1644533 AUG 3 2019

**64. Al Sharif M., I. Tsakovska, I. Pajeva, P. Alov, E. Fioravanzo, A. Bassan, S. Kovarich, C. Yang, A. Mostrag-Szlichtyng, V. Vitcheva, A. P. Worth, A. N. Richarz, M.T. D. Cronin. The Application of Molecular Modelling in the Safety Assessment of Chemicals: A Case Study on Ligand-Dependent PPAR $\gamma$  Dysregulation, *Toxicology* 2017, 392, 140-154.**

Цитирания: 15

1. Aytun Onay, Melih Onay, Osman Abul, Classification of nervous system withdrawn and approved drugs with ToxPrint features via machine learning strategies, *Computer Methods and Programs in Biomedicine*, Volume 142, April 2017, Pages 9-19.
  2. Berggren E., White A., Ouedraogo G., Paini A., Richarz A.-N., Bois F.Y., Exner T., Leite S., Grunsven L.A.V., Worth A., Mahony C. Ab initio chemical safety assessment: A workflow based on exposure considerations and non-animal methods. *Computational Toxicology*, 4, pp.31-44, 2017
  3. Chemical Safety Assessment Workflow Based on Exposure Considerations and Non-Animal Methods, OECD Environment, Health and Safety Publications, Series on Testing and Assessment, No. 275, ENV/JM/MONO(2017) 27
  4. Niklas Andersson, Maria Arena, Domenica Auteri, Stefania Barmaz, Elise Grignard, Aude Kienzler, Peter Lepper, Alfonso Maria Lostia, Sharon Munn, Juan Manuel Parra Morte, Francesca Pellizzato, Jose Tarazona, Andrea Terron, Sander Van der Linden. European Chemicals Agency ECHA; EFSA. Guidance for the identification of endocrine disruptors in the context of Regulations (EU) No 528/2012 and (EC) No 1107/2009. *EFSA JOURNAL*, 16 (6). <https://doi.org/10.2903/j.efsa.2018.5312> JUN 2018
  5. Daniela Schuster. Pharmacophore Models for Toxicology Prediction. In: *Computational Toxicology: Risk Assessment for Chemicals*, First Edition. Edited by Sean Ekins. © 2018 John Wiley & Sons, Inc., Chapter 5, 121-144.
  6. Jun Wang, Daniel R. Hallinger, Ashley S.Murr, Angela R.Buckalew, Ryan R.Lougee, Ann M.Richard, Susan C.Laws, Tammy E.Stoker. High-throughput screening and chemotype-enrichment analysis of ToxCast phase II chemicals evaluated for human sodium-iodide symporter (NIS) inhibition. *Environment International*, Volume 126, May 2019, Pages 377-386. DOI: 10.1016/j.envint.2019.02.024
  7. Lynch A.M., Eastmond D., Elhajouji A., (...), Schuler M., Tweats D. Targets and mechanisms of chemically induced aneuploidy. Part 1 of the report of the 2017 IWGT workgroup on assessing the risk of aneugens for carcinogenesis and hereditary diseases. *Mutation Research - Genetic Toxicology and Environmental Mutagenesis*. 2019, 847, 403025
  8. Wang, J., Wang, B., Zhang, Y. Agonism activities of lyso-phosphatidylcholines (LPC) Ligands binding to peroxisome proliferator-activated receptor gamma (PPAR $\gamma$ ) (2019) *Journal of Biomolecular Structure and Dynamics*. 2020 38:2, 398-409 DOI: 10.1080/07391102.2019.1577175
  9. Jeong J, Kim H, Choi J. In Silico Molecular Docking and In Vivo Validation with *Caenorhabditis elegans* to Discover Molecular Initiating Events in Adverse Outcome Pathway Framework: Case Study on Endocrine-Disrupting Chemicals with Estrogen and Androgen Receptors. *Int J Mol Sci*. 2019 Mar 10;20(5). pii: E1209. doi: 10.3390/ijms20051209.
  10. Ibrahim, I.T., Uzairu, A. & Sagagi, B. QSAR, molecular docking approach on the estrogenic activities of persistent organic pollutants using quantum chemical disruptors. *SN Appl. Sci.* (2019) 1: 1599. <https://doi.org/10.1007/s42452-019-1624-8>
  11. Krewski D., Andersen ME., Tyshenko MG., Krishnan K., Hartung T., Boekelheide K., Wambaugh JF., Jones D., Whelan M., Thomas R., Yauk C., Barton-Maclaren T., Cote I. Toxicity testing in the 21st century: progress in the past decade and future perspectives. *Arch Toxicol*. 2019. doi: 10.1007/s00204-019-02613-4.
  12. Hyun Soo Kim, Jun Hyuek Yang, Doo Seok Kang, Nam Gook Kee, Cheol Min Lee, Jong-Hyeon Jung, Yeon-Soon Ahn, Young Rok Seo. Suggestions for applications of toxicogenomic approaches in the adverse outcome pathway of 2,4-dinitrotoluene. *Toxicology and Environmental Health Sciences*, Apr 2020. DOI: 10.1007/s13530-020-00054-6 **въведено в Соникс**
  13. Legler, J.; Zalko, D.; Jourdan, F.; Jacobs, M.; Fromenty, B.; Balaguer, P.; Bourguet, W.; Munic Kos, V.; Nadal, A.; Beausoleil, C.; Cristobal, S.; Remy, S.; Ermler, S.; Margiotta-Casaluci, L.; Griffin, J.L.; Blumberg, B.; Chesné, C.; Hoffmann, S.; Andersson, P.L.; Kamstra, J.H., on behalf of the GOLIATH Consortium; The GOLIATH Project: Towards an Internationally Harmonised Approach for Testing Metabolism Disrupting Compounds. *Int. J. Mol. Sci.* 2020, 21, 3480. doi: 10.3390/ijms21103480
  14. Aljallal, M. Investigation of in Silico Modelling to Predict the Human Health Effects of Cosmetics Ingredients. Doctoral thesis, Liverpool John Moores University. 2020, PhD
  15. Krewski, D., Andersen, M.E., Tyshenko, M.G. *et al.* Toxicity testing in the 21st century: progress in the past decade and future perspectives. *Arch Toxicol* 94, 1–58 (2020). <https://doi.org/10.1007/s00204-019-02613-4>
- 65. Jereva, D., F. Fratev, I. Tsakovska, P. Alov, T. Pencheva, I. Pajeva. Molecular Dynamics Simulation of the Human Estrogen Receptor Alpha: Contribution to the Pharmacophore of the Agonists. *Math.Comput.Simul.* 2017, 133, 124-134. 10.1016/j.matcom.2015.07.003.**

Цитирания: 6

1. Ho Leung Ng, Simulations reveal increased fluctuations in estrogen receptor-alpha conformation upon antagonist binding, *Journal of Molecular Graphics and Modelling*, Volume 69, September 2016, Pages 72-77, ISSN 1093-3263, <http://dx.doi.org/10.1016/j.jmgm.2016.08.009>.

2. Eisold, A; Labudde, D. Detailed Analysis of 17-Estradiol-Aptamer Interactions: A Molecular Dynamics Simulation Study. *MOLECULES*, 23 (7): 1690, JUL 2018 <https://doi.org/10.3390/molecules23071690>
3. Aranthya H. Lima Costa, Washington S. Clemente, Jr., Katyanna S. Bezerra, José X. Lima Neto, Eudenilson L. Albuquerque, Umberto L. Fulco. Computational biochemical investigation of the binding energy interactions between an estrogen receptor and its agonists *New J. Chem.*, 2018,42, 19801-19810
4. C. Denise Okafor, Jennifer K. Colucci, and Eric A. Ortlund. Ligand-Induced Allosteric Effects Governing SR Signaling. *NUCLEAR RECEPTOR RESEARCH* Vol. 6 (2019), Article ID 101382, 16 pages [doi:10.32527/2019/101382](https://doi.org/10.32527/2019/101382)
5. Tejería, E., Giglio, J., Fernández, L., Rey, A. Development and evaluation of a <sup>99m</sup>Tc(V)-nitrido complex derived from estradiol for breast cancer imaging. *APPLIED RADIATION AND ISOTOPES*, Volume 154, 2019, Article number 108854
6. Laura Marroqui, Juan Martinez-Pinna, Manuel Castellano-Muñoz, Reinaldo S. dos Santos, Regla M. Medina-Gali, Sergi Soriano, Ivan Quesada, Jan-Ake Gustafsson, José A. Encinar, Angel Nadal. Bisphenol-S and Bisphenol-F alter mouse pancreatic  $\beta$ -cell ion channel expression and activity and insulin release through an estrogen receptor ER $\beta$  mediated pathway, *CHEMOSPHERE* Volume: 265 Article Number: 129051 Published: FEB 2021 <https://doi.org/10.1016/j.chemosphere.2020.129051>

**66. Labbe, C., T. Pencheva, D. Jereva, D. Desvillechabrol, J. Becot, B.O. Villoutreix, I. Pajeva, M. Miteva. AMMOS2: a web server for protein-ligand-water complexes refinement via molecular mechanics, *Nucleic Acids Res.* 2017, Volume 45, Issue W1, pp. W350–W355.**

Цитирания: 17

1. Minkiewicz P, Iwaniak A, Darewicz M. Annotation of Peptide Structures Using SMILES and Other Chemical Codes-Practical Solutions. *MOLECULES*, 22 (12):10.3390/molecules22122075 DEC 2017
2. Banach, M; Konieczny, L; Roterman, I. Why do antifreeze proteins require a solenoid?, In *BIOCHIMIE*, 144 74-84; 10.1016/j.biochi.2017.10.011 JAN 2018
3. Grande F, Rizzuti B, Occhiuzzi MA, Ioele G, Casacchia T, Gelmini F, Guzzi R, Garofalo A, Statti G. Identification by Molecular Docking of Homoisoflavones from *Leopoldia comosa* as Ligands of Estrogen Receptors. *MOLECULES*, 23 (4):10.3390/molecules23040894 APR 2018.
4. Soufan, O; Ba-alawi, W; Magana-Mora, A; Essack, M; Bajic, V. DPubChem: a web tool for QSAR modeling and high-throughput virtual screening. *SCIENTIFIC REPORTS*, 8 10.1038/s41598-018-27495-x JUN 14 2018.
5. Zhao, Yan; Jiao, Yingjie; Sun, Fengzhe; Liu, Xudong. Revisiting the molecular mechanism of acquired resistance to reversible tyrosine kinase inhibitors caused by EGFR gatekeeper T790M mutation in non-small-cell lung cancer. *MEDICINAL CHEMISTRY RESEARCH*, 27 (9):2160-2170; 10.1007/s00044-018-2224-7 SEP 2018
6. Liu, T; Wang, ZS; Guo, P; Ding, N. Electrostatic mechanism of V600E mutation-induced B-Raf constitutive activation in colorectal cancer: molecular implications for the selectivity difference between type-I and type-II inhibitors. *EUROPEAN BIOPHYSICS JOURNAL WITH BIOPHYSICS LETTERS*, 48 (1):73-82; 10.1007/s00249-018-1334-y JAN 2019
7. Anna Vangone, Joerg Schaarschmidt, Panagiotis Koukos, Cunliang Geng, Nevia Citro, Mikael E Trellet, Li C Xue, Alexandre M J J Bonvin, Large-scale prediction of binding affinity in protein–small ligand complexes: the PRODIGY-LIG web server, *Bioinformatics*, Volume 35, Issue 9, 1 May 2019, Pages 1585–1587, <https://doi.org/10.1093/bioinformatics/bty816>
8. Xu, Z; Chen, H; Fan, FJ; Shi, PJ; Tu, ML; Cheng, SZ; Wang, ZY; Du, M. Bone formation activity of an osteogenic dodecapeptide from blue mussels (*Mytilus edulis*). *FOOD & FUNCTION*, 10 (9):5616-5625; 10.1039/c9fo01201j SEP 1 2019
9. Adeshina Y; EJ. Deeds, J. Karanicolas. Machine learning classification can reduce false positives in structure-based virtual screening. *Proceedings of the National Academy of Sciences*, 2020 117 (31) 18477-18488; <https://doi.org/10.1073/pnas.2000585117>
10. Hui Wang, Zengjian Yang, Yanliang Liu. Systematic characterization of adenosine triphosphate response to lung cancer epidermal growth factor receptor missense mutations: A molecular insight into “generic” drug resistance mutations. *JOURNAL OF THE CHINESE CHEMICAL SOCIETY*, 2020. <https://doi.org/10.1002/jccs.201900435>
11. Zsidó, B.Z.; Hetényi, C. Molecular Structure, Binding Affinity, and Biological Activity in the Epigenome. *INTERNATIONAL JOURNAL OF MOLECULAR SCIENCES* Volume: 21 Issue: 11, Article Number: 4134 Published: JUN 2020. DOI: 10.3390/ijms21114134
12. Laijun Song, Chunyu Zhu, Wenxin Zheng, Dan Lu, Hong Jiao, Rongbing Zhao, Zhonglei Bao, Computational systematic selectivity of the Fasalog inhibitors between ROCK-I and ROCK-II kinase isoforms in Alzheimer’s disease, *Computational Biology and Chemistry*, Vol. 87, 2020, 107314,

- <https://doi.org/10.1016/j.compbiolchem.2020.107314>, ISSN 1476-9271, <http://www.sciencedirect.com/science/article/pii/S1476927120305880>)
13. Kerem Terali, Buket Baddal, Hayrettin Ozan Gülcan. Prioritizing potential ACE2 inhibitors in the COVID-19 pandemic: insights from a molecular mechanics-assisted structure-based virtual screening experiment. *JOURNAL OF MOLECULAR GRAPHICS & MODELLING* Volume: 100 Article Number: 107697 Published: NOV 2020. <https://doi.org/10.1016/j.jmngm.2020.107697>
  14. Patnala Ganga Raju Achary. Applications of Quantitative Structure-Activity Relationships (QSAR) based Virtual Screening in Drug Design: A Review”, *MINI-REVIEWS IN MEDICINAL CHEMISTRY* Volume: 20 Issue: 14 Pages: 1375-1388 Published: 2020. <https://doi.org/10.2174/1389557520666200429102334>
  15. Li, B., Zhang, L., Wang, K, Jie, Y. Substrate-Based Design of Human Farnesyltransferase Peptide-like Pain Antagonists. *INTERNATIONAL JOURNAL OF PEPTIDE RESEARCH AND THERAPEUTICS* (2021). <https://doi.org/10.1007/s10989-021-10169-0>
  16. Qifei Wang, Fei Chen, Peng Liu, Yushu Mu, Shibin Sun, Xulong Yuan, Pan Shang, Bo Ji, Scaffold-based Analysis of Nonpeptide Oncogenic FTase Inhibitors using Multiple Similarity Matching, Binding Affinity Scoring and Enzyme Inhibition Assay, *Journal of Molecular Graphics and Modelling*, 2021, 107898, <https://doi.org/10.1016/j.jmngm.2021.107898>.
  17. Siyu Zhu, Meixian Wu, Ziwei Huang, Jing An. Trends in application of advancing computational approaches in GPCR ligand discovery. *Experimental Biology and Medicine*, 246, 9, 1011-1024, 2021. <https://doi.org/10.1177/1535370221993422>

**67. Diukendjieva A., M. Al Sharif, P. Alov, T. Pencheva, I. Tsakovska, I. Pajeva. ADME/Tox Properties and Biochemical interactions of Silybin Congeners: In Silico Study. *Natural Product Communications*, 2017, 12 (2), 175-178.**

Цитирания: 2

1. Vrba, J.; Papoušková, B.; Kosina, P.; Lněničková, K.; Valentová, K.; Ulrichová, J. Identification of Human Sulfotransferases Active towards Silymarin Flavonolignans and Taxifolin. *Metabolites* **2020**, *10*, 329.
2. Borah, Pobitra; Hazarika, Sangeeta; Deka, Satyendra; Venugopala, Katharigatta N.; Nair, Anroop B.; Attimarad, Mahesh; Sreeharsha, Nagaraja; Mailavaram, Raghu Prasad. Application of Advanced Technologies in Natural Product Research: A Review with Special Emphasis on ADMET Profiling, Volume: 21, Issue10, Pages: 751-767. Published: 2020. <https://doi.org/10.2174/1389200221666200714144911>

**68. Al Sharif, M., Alov, P., Vitcheva, V., Diukendjieva, A., Mori, M., Botta, B., Tsakovska, I., Pajeva, I. Natural modulators of nonalcoholic fatty liver disease: Mode of action analysis and in silico ADME-Tox prediction. *Toxicol. Appl. Pharmacol.* 2017, 337, DOI:10.1016/j.taap.2017.10.013, 45-66.**

Цитирания: 7

1. Shiri F., S. Pirhadi, A. Rahmani. Identification of new potential HIV-1 reverse transcriptase inhibitors by QSAR modeling and structure-based virtual screening. *JOURNAL OF RECEPTORS AND SIGNAL TRANSDUCTION*, 38 (1):37-47; 2018 10.1080/10799893.2017.1414844
2. Feng WW, Kuang SY, Tu C, Ma ZJ, Pang JY, Wang YH, Zang QC, Liu TS, Zhao YL, Xiao XH, Wang JB. Natural products berberine and curcumin exhibited better ameliorative effects on rats with non-alcohol fatty liver disease than lovastatin. *Biomedicine and Pharmacotherapy*, 99, pp. 325-333, 2018
3. Martín Estrada-Valencia, Clara Herrera-Arozamena, Concepción Pérez, Dolores Viña, José A. Morales-García, Ana Pérez-Castillo, Eva Ramos, Alejandro Romero, Erik Laurini, Sabrina Priel & María Isabel Rodríguez-Franco (2019) New flavonoid – *N,N*-dibenzyl(*N*-methyl)amine hybrids: Multi-target-directed agents for Alzheimer’s disease endowed with neurogenic properties, *Journal of Enzyme Inhibition and Medicinal Chemistry*, 34:1, 712-727, DOI: 10.1080/14756366.2019.1581184
4. Junfeng Lu, Chen Chen, Xiaobing Deng, Marvin SH Mak, Zeyu Zhu, Xixin He, Jinhao Liang, Swetha K. Maddili, Karl W. K. Tsim, Yifan Han, Rongbiao Pi. Design, Synthesis, and Biological Evaluation of Novel Multifunctional Rolipram–Tranilast Hybrids As Potential Treatment for Traumatic Brain Injury. *ACS Chem. Neurosci.* 2020, 11, 15, 2348–2360. <https://doi.org/10.1021/acschemneuro.0c00339>
5. Borah, Pobitra; Hazarika, Sangeeta; Deka, Satyendra; Venugopala, Katharigatta N.; Nair, Anroop B.; Attimarad, Mahesh; Sreeharsha, Nagaraja; Mailavaram, Raghu Prasad. Application of Advanced Technologies in Natural Product Research: A Review with Special Emphasis on ADMET Profiling. *Current Drug Metabolism*, 21(10), pp. 751-767, 2020 <https://doi.org/10.2174/1389200221666200714144911>
6. Anna Więckowska, Natalia Szałaj, Izabella Góral, Adam Bucki, Gniewomir Latacz, Katarzyna Kiec-Kononowicz, Óscar. M. Bautista-Aguilera, Alejandro Romero, Eva Ramos, Javier Egea, Victor Farré Alíns, Águeda González-Rodríguez, Francisco López-Muñoz, Mourad Chioua, José Marco-Contelles. *In Vitro and In Silico* ADME-Tox Profiling and Safety Significance of Multifunctional Monoamine Oxidase Inhibitors Targeting Neurodegenerative Diseases. *ACS Chem. Neurosci.* 2020, 11, 22, 3793–3801.

<https://doi.org/10.1021/acscemneuro.0c00489> Hehai Huang, Yuan Jin, Chuanying Chen, Meiyao Feng, Qing Wang, Daochuan Li, Wen Chen, Xiumei Xing, Dianke Yu, Yongmei Xiao, A toxicity pathway-based approach for modeling the mode of action framework of lead-induced neurotoxicity, *Environmental Research*, Volume 199, 2021, 111328, <https://doi.org/10.1016/j.envres.2021.111328>

**69. Tsakovska I., I. Pajeva, M. Al Sharif, P. Alov, E. Fioravanzo, S. Kovarich, A. P. Worth, A. Richarz, C. Yang, A. Mostrag-Szlichtyng, M.T.D. Cronin. Quantitative structure-skin permeability relationships. Review Article, *Toxicology*, 2017, 387, 27-42.**

Цитирания: 43

1. Rosa, J; Suzuki, I; Kravicz, M; Caron, A; Pupo, AV; Praca, FG; Bentley, MVLB. Current Non-viral siRNA Delivery Systems as a Promising Treatment of Skin Diseases. *CURRENT PHARMACEUTICAL DESIGN*, 24 (23):2644-2663 2174/1381612824666180807120017 2018
2. Schenk, L; Rauma, M; Fransson, MN; Johanson, G. Percutaneous absorption of thirty-eight organic solvents in vitro using pig skin. *PLOS ONE*, 13 (10):10.1371/journal.pone.0205458 OCT 31 2018
3. Iqra Ahmad, Kevin B Ita, Matthew J Morra, Inna E Popova. Microneedle-assisted delivery of anti-migraine drugs across porcine skin: almotriptan malate and naratriptan hydrochloride. *Frontiers in Nanoscience and Nanotechnology*, 4(2): 1-7, 2018 doi: 10.15761/FNN.1000169
4. Kabbad, Kh. L'infection bactérienne chez le patient brûlé. PhD Thesis, 2018  
<http://ao.um5.ac.ma/xmlui/bitstream/handle/123456789/16980/M%20%20354%202018.pdf>
5. Sairi, Maryam. Prediction and Experimental Validation of the Char Yield of Crosslinked Polybenzoxazines. A thesis submitted to the Department of Chemistry in conformity with the requirement for the Degree of Doctor of Philosophy. Faculty of Engineering and Physical Sciences, University of Surrey, Guildford GU2 9PT, 2018. <https://core.ac.uk/reader/161936804> PhD
6. V Carrer Vives. Skin permeability methodologies for topical absorption prediction.  
<http://hdl.handle.net/2445/128151> 2018. PhD
7. Maciel Tabosa, Maria. Development and validation of a physiologically-based pharmacokinetic model for dermal absorption. Award date: 2019, Awarding institution: University of Bath, UK, PhD
8. Pecoraro, B; Tutone, M; Hoffman, E; Hutter, V; Almerico, AM; Traynor, M. Predicting Skin Permeability by Means of Computational Approaches: Reliability and Caveats in Pharmaceutical Studies. *JOURNAL OF CHEMICAL INFORMATION AND MODELING*, 59 (5):1759-1771; SI 10.1021/acs.jcim.8b00934 MAY 2019
9. Johannes A.H. Schwöbel, Andreas Klamt, Mechanistic skin penetration model by the COSMOperm method: Routes of permeation, vehicle effects and skin variations in the healthy and compromised skin, *Computational Toxicology*, Volume 11, 2019, Pages 50-64, ISSN 2468-1113, <https://doi.org/10.1016/j.comelacridartox.2019.02.004>
10. Anne J. Keurentjes, Howard I. Maibach, Percutaneous penetration of drugs applied in transdermal delivery systems: an in vivo based approach for evaluating computer generated penetration models, *Regulatory Toxicology and Pharmacology*, Volume 108, 2019, 104428, ISSN 0273-2300, <https://doi.org/10.1016/j.yrtph.2019.1044>
11. Eleftheriadou, D; Luette, S; Kneuer, C. In silico prediction of dermal absorption of pesticides – an evaluation of selected models against results from in vitro testing. *SAR AND QSAR IN ENVIRONMENTAL RESEARCH*, 30 (8):561-585; 10.1080/1062936X.2019.1644533 AUG 3 2019
12. Marcella Cipelli, Aline Ignacio, Niels Olsen Saraiva Camara. Infection: Immunological Barriers, In book: *eLS*, 2019, DOI: 10.1002/9780470015902.a0000940.pub3
13. Kumar M., Shanthi N., Mahato A.K. Pharmaceutical Drug Nanocrystals: Role in Dermal Delivery, *Nanoscience & Nanotechnology-Asia*, 9(3), pp. 300-310, 2019 **DOI** : 10.2174/2210681208666180516093855
14. Del Pezo Reyes, L. D., & Quimis Choez, S. P. (2019). Tesis. Recuperado a partir de <http://repositorio.ug.edu.ec/handle/redug/43582>.
15. Amézqueta S., X. Subirats, E. Fuguet, M. Rosés, C. Ràfols. Chapter 6 - Octanol-Water Partition Constant, Editor(s): Colin F. Poole, In *Handbooks in Separation Science, Liquid-Phase Extraction*, Elsevier, 2020, Pages 183-208, 2019
16. Etienne Bourgart. Métabolisme cutané et biomarqueurs d'exposition aux mélanges complexes d'hydrocarbures aromatiques polycycliques. *Médecine humaine et pathologie*. Université Grenoble Alpes, 2019. Français. (NNT : 2019GREAS026). <https://tel.archives-ouvertes.fr/tel-02503982>
17. Anne J. Keurentjes, Howard I. Maibach. Percutaneous penetration of drugs applied in transdermal delivery systems: an in vivo based approach for evaluating computer generated penetration models, *Regulatory Toxicology and Pharmacology*, Volume 108, 2019, 104428, ISSN 0273-2300, <https://doi.org/10.1016/j.yrtph.2019.104428>. (<http://www.sciencedirect.com/science/article/pii/S0273230019301928>)

18. Pin Dong, Viktor Nikolaev, Marius Kröger, Christian Zoschke, Maxim E. Darvin, Christian Witzel, Jürgen Lademann, Alexa Patzelt, Monika Schäfer-Korting, Martina C. Meinke, Barrier-disrupted skin: Quantitative analysis of tape and cyanoacrylate stripping efficiency by multiphoton tomography, *INTERNATIONAL JOURNAL OF PHARMACEUTICS*, Volume 574, 2020, art. no.118843, ISSN 0378-5173, <https://doi.org/10.1016/j.ijpharm.2019.118843>
19. Burli A., Law R.M., Rodriguez J., Maibach H.I. Organic compounds percutaneous penetration in vivo in man: Relationship to mathematical predictive model. *REGULATORY TOXICOLOGY AND PHARMACOLOGY* Volume: 112 Article Number: UNSP 104614 Published: APR 2020 <https://doi.org/10.1016/j.yrtph.2020.104614>
20. XueKe Lin, ZhenHua Wang, Ou Huilong, Mitragotri, Samir, Ming Chen. Correlations Between Skin Barrier Integrity and Delivery of Hydrophilic Molecules in the Presence of Penetration Enhancers. *PHARMACEUTICAL RESEARCH* Volume: 37 Issue: 6, Article Number: 100 Published: MAY 20 2020. <https://doi.org/10.1007/s11095-020-02800-4>
21. Alalaiwe, A., Lin, C.-F., Hsiao, C.-Y., Chen, E.-L., Lin, C.-Y., Lien, W.-C., Fang, J.-Y. Development of flavanone and its derivatives as topical agents against psoriasis: The prediction of therapeutic efficiency through skin permeation evaluation and cell-based assay (Article). *INTERNATIONAL JOURNAL OF PHARMACEUTICS* Volume: 581 Article Number: 119256 Published: MAY 15 2020. ISSN 0045-6535, <https://doi.org/10.1016/j.chemosphere.2020.126955>
22. Ching-Yi Cheng, Yin-Ku Lin, Shih-Chun Yang, Ahmed Alalaiwe, Chia-Jung Lin, Jia-You Fang, Chwan-Fwu Lin, Percutaneous absorption of resveratrol and its oligomers to relieve psoriasiform lesions: In silico, in vitro and in vivo evaluations, *INTERNATIONAL JOURNAL OF PHARMACEUTICS* Volume: 585 Article Number: 119507 Published: JUL 30 2020, <https://doi.org/10.1016/j.ijpharm.2020.119507>
23. Jebbawi, R., Oukhrib, A., Clement, E., Blanzat, M., Turrin, C. O., Caminade, A. M., Lacoste, E., Fruchon, S., & Poupot, R. An Anti-Inflammatory Poly(PhosphorHydrazone) Dendrimer Capped with AzaBisPhosphonate Groups to Treat Psoriasis. *BIOMOLECULES* Volume: 10 Issue: 6 Article Number: 949 Published: JUN 2020. <https://doi.org/10.3390/biom10060949>
24. Alalaiwe, Ahmed; Lin, Yin-Ku; Lin, Chih-Hung; Wang, Pei-Wen; Lin, Jie-Yu; Fang, Jia-You. The absorption of polycyclic aromatic hydrocarbons into the skin to elicit cutaneous inflammation: The establishment of structure-permeation and in silico-in vitro-in vivo relationships. *CHEMOSPHERE*, Volume: 255, Article Number: 126955 Published: SEP 2020
25. Hanumanth Srikanth Cheruvu, Xin Liu, Jeffrey E. Grice & Michael S. Roberts (2020) Modeling percutaneous absorption for successful drug discovery and development, *EXPERT OPINION ON DRUG DISCOVERY*, Jun 2020. <https://doi.org/10.1080/17460441.2020.1781085>
26. Daniel Sebastia-Saez, Adam Burbidge, Jan Engmann, Marco Ramaioli. New trends in mechanistic transdermal drug delivery modelling: Towards an accurate geometric description of the skin microstructure, *Computers & Chemical Engineering*, Volume 141, 2020, 106976. <https://doi.org/10.1016/j.compchemeng.2020.106976>
27. Khater Ahmed Saeed AL-Japairai, Syed Mahmood, Samah Hamed Almurisi, Jayarama Reddy Venugopal, Ayah Rebhi Hilles, Motia Azmana, Subashini Raman, Current trends in polymer microneedle for transdermal drug delivery, *INTERNATIONAL JOURNAL OF PHARMACEUTICS* Volume: 587 Article Number: 119673 Published: SEP 25 2020 <https://doi.org/10.1016/j.ijpharm.2020.119673>
28. Anayatollah Salimia, Eskandar Moghimipoura, Payam Koganic, Saeed Mohammad Soleymani. The Effect of Various Penetration Enhancers on the Octyl Methoxycinnamate Permeability: Mechanisms of Action Study. *Iranian Journal of Pharmaceutical Sciences*, 2020: 16 (2): 87-104. <https://doi.org/10.22034/ijps.2019.103550.1531>
29. Gopalakrishnan Venkatesan, Yuri Dancik, Arup Sinha, Hpone Myint Kyaw, Ramasamy Srinivas, Thomas L. Dawson, Mei Bigliardi, Paul Bigliardi, Giorgia Pastorin, Development of novel alternative hair dyes to hazardous para-phenylenediamine, *Journal of Hazardous Materials*, 2020, 402, art. no. 123712, <https://doi.org/10.1016/j.jhazmat.2020.123712>
30. Omaima N. Najib, Stewart B. Kirton, Gary P. Martin, Michelle J. Botha, Al-Sayed Sallam, Darragh Murnane. Multivariate Analytical Approaches to Identify Key Molecular Properties of Vehicles, Permeants and Membranes That Affect Permeation through Membranes. *PHARMACEUTICS* Volume: 12 Issue: 10 Article Number: 958 Published: OCT 2020; doi:10.3390/pharmaceutics12100958
31. Stepanov, D., Canipa, S. & Wolber, G. HuskinDB, a database for skin permeation of xenobiotics. *Sci Data* 7, art. no. 426 (2020). <https://doi.org/10.1038/s41597-020-00764-z>
32. Machado B.H.B., Frame J., Zhang J., Najlah M.. Comparative Study on the Outcome of Periorbital Wrinkles Treated with Laser-Assisted Delivery of Vitamin C or Vitamin C Plus Growth Factors: A Randomized, Double-blind, Clinical Trial. *AESTHETIC PLASTIC SURGERY*, 2020. <https://doi.org/10.1007/s00266-020-02057-7> вероятно ще е 2021

33. S. Amézqueta, X. Subirats, E. Fuguet, M. Rosés, C. Ràfols, Chapter 6 - Octanol-Water Partition Constant, Editor(s): Colin F. Poole, In *Handbooks in Separation Science, Liquid-Phase Extraction*, Elsevier, 2020, Pages 183-208, ISBN 9780128169117, <https://doi.org/10.1016/B978-0-12-816911-7.00006-2>
34. Jebbawi R., Fruchon S., Turrin C.-O., Blanzat M., Poupot R. Supramolecular and macromolecular matrix nanocarriers for drug delivery in inflammation-associated skin diseases. *PHARMACEUTICS*, 2020, 12(12), art. no. 1224, pp. 1-13. <https://doi.org/10.3390/pharmaceutics12121224>
35. Vasyuchenko, E.P.; Orekhov, P.S.; Armeev, G.A.; Bozdaganyan, M.E. CPE-DB: An Open Database of Chemical Penetration Enhancers. *PHARMACEUTICS* Volume 13, Issue 1 Article Number: 66 Published: JAN 2021. <https://doi.org/10.3390/pharmaceutics13010066>
36. Eva Abramov, Nissim Garti. Development of polymeric films embedded with liquid nanodomains, *JOURNAL OF COLLOID AND INTERFACE SCIENCE*, Volume 591, 2021, 363-372. <https://doi.org/10.1016/j.jcis.2021.02.032>
37. Salimi, A, Emam, M, Mohammad Soleymani, S. Increase adapalene delivery using chemical and herbal enhancers. *J Cosmet Dermatol*. 2021; 00: 1– 7. <https://doi.org/10.1111/jocd.13960>
38. Georgios N. Stamatias, Jalil Bensaci, Elea Greugny, Simarna Kaur, Hequn Wang, Maria Victoria Dizon, Michael J. Cork, Adam J. Friedman, Thierry Oddos. A predictive self-organizing multicellular computational model of infant skin permeability to topically applied substances, *Journal of Investigative Dermatology*, 2021, In Press, Journal Pre-proof. <https://doi.org/10.1016/j.jid.2021.02.012>
39. Neacsu, I.A.; Leau, S.-A.; Marin, S.; Holban, A.M.; Vasile, B.-S.; Nicoara, A.-I.; Ene, V.L.; Bleotu, C.; Albu Kaya, M.G.; Ficai, A. Collagen-Carboxymethylcellulose Biocomposite Wound-Dressings with Antimicrobial Activity. *MATERIALS*, Volume: 14, Issue: 5, Article Number: 1153, Published: MAR 2021. <https://doi.org/10.3390/ma14051153>
40. Momoko Kitaoka, Trung Cong Nguyen, Masahiro Goto. Water- in- oil microemulsions composed of monoolein enhanced the transdermal delivery of nicotinamide. *INTERNATIONAL JOURNAL OF COSMETIC SCIENCE*, Volume: 591 Pages: 363-372 Published: JUN 2021. <https://doi.org/10.1111/ics.12695>
41. Samanc, B., Yener F.G., Değim I.T. Enhancing Skin Penetration: The Role of Microneedles. *Fabad Journal of Pharmaceutical Sciences*, Volume 46, Issue 1, 2021, Pages 105-120.
42. Yasmine Grooten, Aleksandra Sych, Debby Mangelings, Yvan Vander Heyden, Comparison of in-silico modelling and reversed-phase liquid chromatographic retention on an octadecyl silica column to predict skin permeability of pharmaceutical and cosmetic compounds, *Journal of Pharmaceutical and Biomedical Analysis*, Volume 201, 2021, 114095. <https://doi.org/10.1016/j.jpba.2021.114095>
43. Kuznetsova, E.G., Kuryleva, O.M., Salomatina, L.A. Sevastianov, V. I. The Combined Use of Synthetic and Biological Test Systems in the Development of Transdermal Therapeutic Systems. *Inorg. Mater. Appl. Res.* **12**, 386–392 (2021). <https://doi.org/10.1134/S2075113321020295>

**70. Diukendjieva, A., P. Alov, I. Tsakovska, T. Pencheva, A. Richarz, V. Kren, M.T.D. Cronin, I. Pajeva. *In vitro* and *in silico* studies of the membrane permeability of natural flavonoids from *Silybum marianum* (L.) Gaertn. and their derivatives, *Phytomedicine*, 2019, 53, 79-85.**

Цитирания: 9

1. Cheng-Ting Chi, Ming-Han Lee, Ching Feng Weng, Max Leong. In Silico Prediction of PAMPA Effective Permeability Using a Two-QSAR Approach, *International Journal of Molecular Sciences* 20(13):3170, 2019. DOI: 10.3390/ijms20133170
2. Cui Q., Ma F., Tao J., Jiang, M., Bai G., Luo G. Efficacy evaluation of Qingyan formulation in a smoking environment and screening of anti-inflammatory compounds. *Biomedicine and Pharmacotherapy*, 2019, 118, art. no. 109315.
3. Joaquin Navarro del Hierro, Vieri Piazzini, Guillermo Reglero, Diana Martin and Maria Camilla Bergonzi. In Vitro Permeability of Saponins and Sapogenins from Seed Extracts by the Parallel Artificial Membrane Permeability Assay: Effect of in Vitro Gastrointestinal Digestion. *J. Agric. Food Chem.* 2020, 68, 5, 1297–1305.
4. Vrba, J.; Papoušková, B.; Kosina, P.; Lněničková, K.; Valentová, K.; Ulrichová, J. Identification of Human Sulfotransferases Active towards Silymarin Flavonolignans and Taxifolin. *Metabolites* **2020**, 10, 329.
5. Rivera-Mondragón, A., Peeters, L., Van, A.A., Breynaert, A., Caballero-George, C., Pieters, L., Hermans, N., Foubert, K. Simulated gastrointestinal biotransformation of chlorogenic acid, flavonoids, flavonolignans and triterpenoid saponins in cecropia obtusifolia leaf extract. *Planta Medica*. 2020. <https://doi.org/10.1055/a-1258-4383>
6. Roy, D., Dutta, D., Wishart, D.S. *et al.* Predicting PAMPA permeability using the 3D-RISM-KH theory: are we there yet?. *J Comput Aided Mol Des* (2021). <https://doi.org/10.1007/s10822-020-00364-4>
7. Valentyn Mohylyuk, Thomas Pauly, Oleksandr Dobrovolnyi, Nathan Scott, David S. Jones, Gavin P. Andrews, Effect of carrier type and Tween® 80 concentration on the release of silymarin from amorphous

solid dispersions, *Journal of Drug Delivery Science and Technology*, Volume 63, 2021, 102416, ISSN 1773-2247, <https://doi.org/10.1016/j.jddst.2021.102416> .

8. Brboric, J., Klisic, A., Kotur-Stevuljevic, J., Delogu, G., Gjorgieva Ackova, D., Kostic, K., Antonietta Dettori, M., Fabbri, D., Carta, P., and Saso, L. Natural and natural-like polyphenol compounds: in vitro antioxidant activity and potential for therapeutic application. *Archives of Medical Science*. 2021, <https://doi.org/10.5114/aoms/135379>
9. O.M. Losev, H.M. Voytenko, N.V. Kurdil, M.H. Povochnikov, A.A. Kalashnikov, L.L. Davtian, A.P. Hryenko, V.S. Mykhailov, O.A. Makarova, O.H. Lutsenko. Modeling of content of biologically active hepatoprotective substances in the composition of natural honey. *One Health and Nutrition Problems of Ukraine*, 2021, #1 (54). DOI: 10.33273/2663-9726-2021-54-1-34-40

**71. Diukendjieva A., I. Tsakovska, P. Alov, T. Pencheva, I. Pajeva, A. Worth, J. Madden, M.T.D. Cronin. Advances in the Prediction of Gastrointestinal Absorption: Quantitative Structure-Activity Relationship (QSAR) modelling of PAMPA Permeability. *Computational Toxicology*, 2019, 10, 51-59.**

Цитирания: 8

1. Renu Pratiwi, Veda Prachayasittikul, Supaluk Prachayasittikul, Chanin Nantasenamat. Rational design of novel sirtuin 1 activators via structure-activity insights from application of QSAR modeling, 2019. *EXCLI Journal*, 18, pp. 207-222.
2. Cheng-Ting Chi, Ming-Han Lee, Ching Feng Weng, Max Leong. In Silico Prediction of PAMPA Effective Permeability Using a Two-QSAR Approach, *International Journal of Molecular Sciences* 20(13):3170, 2019. DOI: 10.3390/ijms20133170
3. Johannes A.H. Schwöbel, Andreas Klamt, Mechanistic skin penetration model by the COSMOperm method: Routes of permeation, vehicle effects and skin variations in the healthy and compromised skin, *Computational Toxicology*, Volume 11, 2019, Pages 50-64, ISSN 2468-1113, <https://doi.org/10.1016/j.comtox.2019.02.004>.
4. Anne J. Keurentjes, Howard I. Maibach, Percutaneous penetration of drugs applied in transdermal delivery systems: an in vivo based approach for evaluating computer generated penetration models, *Regulatory Toxicology and Pharmacology*, Volume 108, 2019, 104428, ISSN 0273-2300, <https://doi.org/10.1016/j.yrtph.2019.1044>
5. Qingfang Xiang, Weijie Zhang, Qian Li, Jie Zhao, Weiwei Feng, Ting Zhao, Guanghua Mao, Yao Chen, Xiangyang Wu, Liuqing Yang, Guangying Chen. Investigation of the uptake and transport of polysaccharide from Se-enriched *Grifola frondosa* in Caco-2 cells model, *International Journal of Biological Macromolecules*, Volume 158, 2020, Pages 1330-1341, ISSN 0141-8130, <https://doi.org/10.1016/j.ijbiomac.2020.04.160>.
6. Aristote B Buya · Ana Beloqui · Patrick B Memvanga · Véronique Prémat. Self-Nano-Emulsifying Drug-Delivery Systems: From the Development to the Current Applications and Challenges in Oral Drug Delivery. *Pharmaceutics*, 12(12):1194, 2020. DOI:10.3390/pharmaceutics12121194
7. HONG, J., OUDDANE, B., HWANG, J., DAHMS, H. (2021). *In silico* assessment of human health risks caused by cyanotoxins from cyanobacteria. *BIOCELL*, 45(1), 65–77.
8. Hayat Elharafi, Naoual Elhamedani, Mouhi Eddine Hachim, Hajar Tebbaai, Karima Sadik, Firdaus El Hachadi, Aziz Aboulmouhajir. In silico exploration of bioavailability, druggability, toxicity alerts and biological activity of a large series of fatty acids, *Computational Toxicology*, Volume 17, 2021, 100153. <https://doi.org/10.1016/j.comtox.2021.100153>.

**72. Al Sharif M., P. Alov, A. Diukendjieva, V. Vitcheva; R. Simeonova, I. Krasteva, A. Shkondrov, I. Tsakovska, I. Pajeva. Molecular determinants of PPAR $\gamma$  partial agonism and related in silico / in vivo studies of natural saponins as potential type 2 diabetes modulators, *Food and Chemical Toxicology*, 2018, 112, 47-59.**

Цитирания: 3

1. Liwei Wu, Chuan-Yong Guo, Jianye Wu. Therapeutic potential of PPAR $\gamma$  natural agonists in liver diseases. *Journal of Cellular and Molecular Medicine*, February 2020. DOI:10.1111/jcmm.15028
2. Wang Y., Hu B., Feng S., Wang J., Zhang F. Target recognition and network pharmacology for revealing anti-diabetes mechanisms of natural product. 2020, *Journal of Computational Science*, 45, art. no. 101186. <https://doi.org/10.1016/j.jocs.2020.101186>
3. Zichen Luo, Weichen Xu, Ying Zhang, Liuqing Di, Jinjun Shan. A review of saponin intervention in metabolic syndrome suggests further study on intestinal microbiota, *Pharmacological Research*, Volume 160, 2020, art. no. 105088. <https://doi.org/10.1016/j.phrs.2020.105088>.

**73. Dinić J., A. Podolski-Renić, M. Jovanović, L. Musso, I. Tsakovska, I. Pajeva, S. Dallavalle, M. Pešić. Novel Heat Shock Protein 90 inhibitors suppress P-glycoprotein activity and overcome multidrug resistance in cancer cells. *International Journal of Molecular Sciences*, 2019, 20, 4575.**

Цитирања: 4

1. Dong Jinyun, Qin Zuodong, Zhang Wei-Dong, Cheng Gang, G. Assaraf Yehuda, R. Ashby Charles, Chen Zhe-Sheng, Cheng Xiang-Dong, Qin Jiang-Jiang. Medicinal Chemistry Strategies to Discover P-glycoprotein Inhibitors: An Update, Drug Resistance Updates, 2020, 100681, ISSN 1368-7646, <https://doi.org/10.1016/j.drug.2020.100681>
2. Małgorzata Anna Krawczyk, Agata Pospieszynska, Małgorzata Styczewska, Ewa Bien, Sambor Sawicki, Antonella Marino Gammazza, Alberto Fucarino, Magdalena Gorska-Ponikowska, Extracellular Chaperones as Novel Biomarkers of Overall Cancer Progression and Efficacy of Anticancer Therapy. *Applied Sciences*, 2020, 10 (17), art. no. 6009. <https://doi.org/10.3390/app10176009>
3. Xue Li, Yuanqi He, Liqun Wei, Jianzhong Zhang, Xiaoxiao Li, Weiwei Cui, Shihong Zhang, Physcion-8-O- $\beta$ -d-glucoside interferes with the nuclear factor- $\kappa$ B pathway and downregulates P-glycoprotein expression to reduce paclitaxel resistance in ovarian cancer cells, *Journal of Pharmacy and Pharmacology* 2021, 73(4):545-552. <https://doi.org/10.1093/jpp/rgaa025>
4. Yin L, Yang Y, Zhu W, Xian Y, Han Z, Huang H, Peng L, Zhang K and Zhao Y (2021) Heat Shock Protein 90 Triggers Multi-Drug Resistance of Ovarian Cancer via AKT/GSK3 $\beta$ / $\beta$ -Catenin Signaling. *Front. Oncol.* 11:620907. <https://doi.org/10.3389/fonc.2021.620907>

**74. Lagarde N., E. Goldwaser, T. Pencheva, D. Jereva, I. Pajeva, J. Rey, P. Tuffery, B.O. Villoutreix, M.A. Miteva. A free web-based protocol to assist structure-based virtual screening experiments. *International Journal of Molecular Sciences* (ISSN 1422-0067). Special Issue "Recent Advances in Virtual Screening" ("Molecular Biophysics" section), 2019, 20(18). pii: E4648.**

Цитирања: 8

1. Eduardo H. B. Maia · Lucas Rolim Medaglia · Alisson Marques da Silva · Alex G. Taranto. Molecular Architect: A User-Friendly Workflow for Virtual Screening. *ACS Omega* 2020, 5, 12, 6628–6640. <https://doi.org/10.1021/acsomega.9b04403>
2. Al-Khafaji ZM, Mahmood AB, Mahmood MB (2020). Inhibitors for Attachment Protein BabA of *Helicobacter pylori*. *World Journal of Microbiology*, 2020, 5(1): 146-154.
3. K. Terali, B. Baddal, H.O. Gülcan. Prioritizing potential ACE2 inhibitors in the COVID-19 pandemic: insights from a molecular mechanics-assisted structure-based virtual screening experiment. *Journal of Molecular Graphics and Modelling*, 2020, 100:107697. <https://doi.org/10.1016/j.jmgl.2020.107697>
4. Yuanyuan Jiang, Lanxin Liu, Morenci Manning, Madison Bonahoom, Aaron Lotvola and ZengQuan Yang. Structural analysis, virtual screening and molecular simulation to identify potential inhibitors targeting 2'-O-ribose methyltransferase of SARS-CoV-2 coronavirus. *Journal of Biomolecular Structure and Dynamics*. 2020 DOI: 10.1080/07391102.2020.1828172
5. Lee, E.J.; Shaikh, S.; Ahmad, K.; Ahmad, S.S.; Lim, J.H.; Park, S.; Yang, H.J.; Cho, W.-K.; Park, S.-J.; Lee, Y.-H.; Park, S.-Y.; Ma, J.-Y.; Choi, I. Isolation and Characterization of Compounds from *Glycyrrhiza uralensis* as Therapeutic Agents for the Muscle Disorders. *Int. J. Mol. Sci.* **2021**, 22, 876. <https://doi.org/10.3390/ijms22020876>
6. Gupta, R., Srivastava, D., Sahu, M., Tiwari, S., Ambasta, R.K., Kumar, P. Artificial intelligence to deep learning: machine intelligence approach for drug discovery. *Mol Divers* (2021). <https://doi.org/10.1007/s11030-021-10217-3>
7. Federico L.B., Barcelos M.P., Silva G.M., Francischini I.A.G., Taft C.A., da Silva C.H.T. Key Aspects for Achieving Hits by Virtual Screening Studies. In: La Porta F.A., Taft C.A. (eds) *Functional Properties of Advanced Engineering Materials and Biomolecules*. Engineering Materials. Springer, Cham, 2021. [https://doi.org/10.1007/978-3-030-62226-8\\_16](https://doi.org/10.1007/978-3-030-62226-8_16)
8. Shweta Kulshrestha, Tanmay Arora, Manisha Sengar, Navneet Sharma, Raman Chawla, Shereen Bajaj, Pawan Kumar Raghav, Chapter 6 - Advanced approaches and in silico tools of chemoinformatics in drug designing, Editor(s): Navneet Sharma, Himanshu Ojha, Pawan Kumar Raghav, Ramesh k. Goyal, *Chemoinformatics and Bioinformatics in the Pharmaceutical Sciences*, Academic Press, 2021, Pages 173-206, ISBN 9780128217481, <https://doi.org/10.1016/B978-0-12-821748-1.00006-3>

**75. Dallavalle S.; V. Dobričić; L. Lazzarato; E. Gazzano; M. Machucheroe, I. Pajeva; I. Tsakovska, N. Zidar; R. Fruttero. Improvement of Conventional Anti-Cancer Drugs as New Tools against Resistant Tumors, *Drug Resistance Update*, 2020, 50, 100682.**

Цитирања: 32

1. Kontar, S.; Imrichova, D.; Bertova, A.; Mackova, K.; Poturnayova, A.; Sulova, Z.; Breier, A. Cell Death Effects Induced by Sulforaphane and Allyl Isothiocyanate on P-Glycoprotein Positive and Negative Variants in L1210 Cells. *Molecules* **2020**, *25*, 2093.
2. Bukowski, K.; Kciuk, M.; Kontek, R. Mechanisms of Multidrug Resistance in Cancer Chemotherapy. *Int. J. Mol. Sci.* **2020**, *21*, 3233.
3. Yanshu Jia, Xiaoyue Wen, Yufeng Gong, Xuefeng Wang, Current scenario of indole derivatives with potential anti-drug-resistant cancer activity, *European Journal of Medicinal Chemistry*, Volume 200, 2020, 112359, ISSN 0223-5234, <https://doi.org/10.1016/j.ejmech.2020.112359>
4. Chu, Siwei & Stochaj, Ursula. Exploring near-infrared absorbing nanocarriers to overcome cancer drug resistance, *Cancer Drug Resist* 2020;3. <https://doi.org/10.20517/cdr.2020.20>.
5. Zhang, Zhe; Zhou, Li; Xie, Na; Nice, Edouard C.; Zhang, Tao; Cui, Yongping; Huang, Canhua. Overcoming cancer therapeutic bottleneck by drug repurposing. *Sig Transduct Target Ther* **5**, 113 (2020). <https://doi.org/10.1038/s41392-020-00213-8>
6. Pecyna, P.; Wargula, J.; Murias, M.; Kucinska, M. More than Resveratrol: New Insights into Stilbene-Based Compounds. *Biomolecules* 2020, *10*, 1111. <https://doi.org/10.3390/biom10081111>
7. Li, Huan-Ting; Zhu, Xiaoyong. Quinoline-based Compounds with Potential Activity against Drugresistant Cancers. *Current Topics in Medicinal Chemistry*, 2020, <https://doi.org/10.2174/1568026620666200618113957>
8. Xu, Dan ; Xu, Zhi. Indole Alkaloids with Potential Anticancer Activity. *Current Topics in Medicinal Chemistry*, Volume 20 , Issue 21 , 2020, pp. 1938-1949. <https://doi.org/10.2174/1568026620666200622150325>
9. Bowen Li, Jingwen Jiang, Yehuda G. Assaraf, Hengyi Xiao, Zhe-Sheng Chen, Canhua Huang. Surmounting Cancer Drug Resistance: New Insights from the perspective of N6-Methyladenosine RNA Modification, *Drug Resistance Updates*, 53, 2020, 100720, <https://doi.org/10.1016/j.drug.2020.100720>
10. Xue P., Chen Q., Ren X, Yang Y., Yang X., Liu D. A novel protoapigenone analog RY10-4 induces apoptosis of breast cancer cells by regulating mitochondrial Ca<sup>2+</sup> influx through the mitochondrial calcium uniporter. *Research Square*; 2020. <https://doi.org/10.21203/rs.3.rs-17058/v1>
11. Al Qathama Aljawharah, Ezuruike Udoamaka F., Mazzari Andre L. D. A., Yonbawi Ahmed, Chieli Elisabetta, Prieto Jose M. Effects of Selected Nigerian Medicinal Plants on the Viability, Mobility, and Multidrug-Resistant Mechanisms in Liver, Colon, and Skin Cancer Cell Lines, *Frontiers in Pharmacology*, VOL.11, 2020, art. no. 546439. <https://doi.org/10.3389/fphar.2020.546439>
12. Yao Q., Gu L., Su R., Chen B., Cao H. Efficacy and safety of combination PD-1/PD-L1 checkpoint inhibitors for malignant solid tumours: A systematic review. *Journal of Cellular and Molecular Medicine*.2020. <https://doi.org/10.1111/jcmm.15991>
13. Tamer El Malah, Randa E. Abdel Mageid, Hanem M. Awad and Hany F. Nour. Copper(i)-catalysed azide-alkyne cycloaddition and antiproliferative activity of mono- and bis-1,2,3-triazole derivatives. *New J. Chem.*, 2020, 44(42), pp. 18256-18263. <https://doi.org/10.1039/D0NJ04308G>
14. Shang C, Hou Y, Meng T, Shi M, Cui G. The Anticancer Activity of Indazole Compounds: A Mini Review. *Curr Top Med Chem*. 2020 Nov 24. doi:10.2174/1568026620999201124154231
15. Olga M. Tsivileva, Inna M. Uchaeva, Nikolay A. Yurasov. Biotesting of technologically important carboxy containing acridones with solid-state fungal culture. *AIMS Bioengineering*, Volume 8, Issue 1, 1–13, 2020. DOI: 10.3934/bioeng.2021001
16. Dong, Xingli, Bai, Xupeng, Ni, Jie, Zhang, Hao, Duan, Wei, Graham, Peter, Li, Yong. Exosomes and breast cancer drug resistance. *Cell Death Dis* **11**, 987 (2020). <https://doi.org/10.1038/s41419-020-03189->
17. Mine Isaoglu , Medine Güllüce , Mehmet Karadayı Plant-Derived Natural Products as Multidrug Resistance Modulators in Cancer Therapy, *Anatolian Journal of Biology*, 2020, Volume 1 , Issue 2, Pages 1 – 51. <https://dergipark.org.tr/tr/pub/ajbiol/issue/58508/844245>
18. Gangqiang Wang, Shaofa Sun, Bin Wu and Jikai Liu, Coumarins as Potential Anti-drug Resistant Cancer Agents: A Mini Review”, *Current Topics in Medicinal Chemistry* (2020) 20: 1. <https://doi.org/10.2174/1568026620999201113110041>
19. Anubhav Dubey, Deepanshi Tiwari, Yatendra Singh, Om Prakash, Pankaj Singh. Drug repurposing in Oncology: Opportunities and challenges. *International Journal of Allied Medical Sciences and Clinical Research*, 9(1), 68-87, 2021
20. Binghua Wang, Shuqi Liu, Wentao Huang, Mengxin Ma, Xiaoqian Chen, Wenxuan Zeng, Kaicheng Liang, Hongbo Wang, Yi Bi, Xiaopeng Li, Design, synthesis, and biological evaluation of hederagenin derivatives with improved aqueous solubility and tumor resistance reversal activity, *European Journal of Medicinal Chemistry*, Volume 211, 2021, 113107, ISSN 0223-5234, <https://doi.org/10.1016/j.ejmech.2020.113107>.

21. Luciana Mosca, Andrea Ilari, Francesco Fazi, Yehuda G. Assaraf, Gianni Colotti. Taxanes in cancer treatment: Activity, chemoresistance and its overcoming. *Drug Resistance Updates* Volume 54, January 2021, 100742.
22. Bo Han; Xiang-Hong He; Yan-Qing Liu; Gu He; Cheng Peng; Jun-Long Li. Asymmetric organocatalysis: an enabling technology for medicinal chemistry *Chemical Society Reviews* 2021, <https://doi.org/10.1039/d0cs00196a>
23. Gajda, E.; Grzanka, M.; Godlewska, M.; Gawel, D. The Role of miRNA-7 in the Biology of Cancer and Modulation of Drug Resistance. *Pharmaceuticals* **2021**, *14*, 149. <https://doi.org/10.3390/ph14020149>
24. Yin L, Yang Y, Zhu W, Xian Y, Han Z, Huang H, Peng L, Zhang K and Zhao Y (2021) Heat Shock Protein 90 Triggers Multi-Drug Resistance of Ovarian Cancer via AKT/GSK3 $\beta$ / $\beta$ -Catenin Signaling. *Front. Oncol.* **11**:620907. <https://doi.org/10.3389/fonc.2021.620907>
25. Maria A. Kolesnikova, Aleksandra V. Sen'kova, Tatiana I. Pospelova, Marina A. Zenkova. Drug responsiveness of leukemic cells detected in vitro at diagnosis correlates with therapy response and survival in patients with acute myeloid leukemia. *Cancer Reports*, e1362, 2021, <https://doi.org/10.1002/cnr2.1362>.
26. Briolay, T., Petithomme, T., Fouet, M., Nguyen-Pham, N., Blanquart, C., Boisgerault, N. Delivery of cancer therapies by synthetic and bio-inspired nanovectors. *Mol Cancer* **20**, 55, 2021. <https://doi.org/10.1186/s12943-021-01346-2>
27. Marques, S.M.; Šupolíková, L.; Molčanová, L.; Šmejkal, K.; Bednar, D.; Slaninová, I. Screening of Natural Compounds as P-Glycoprotein Inhibitors against Multidrug Resistance. *Biomedicines* **2021**, *9*, 357. <https://doi.org/10.3390/biomedicines9040357>
28. Mohammed Aarjane, Siham Slassi, Bouchra Tazi, Amina Amine, "Microwave-Assisted Regioselective Synthesis and 2D-NMR Studies of New 1,2,3-Triazole Compounds Derived from Acridone", *Journal of Chemistry*, vol. 2021, Article ID 5540173, 10 pages, 2021. <https://doi.org/10.1155/2021/5540173>
29. Szumilak, M.; Wiktorowska-Owczarek, A.; Stanczak, A. Hybrid Drugs—A Strategy for Overcoming Anticancer Drug Resistance? *Molecules* **2021**, *26*, 2601. <https://doi.org/10.3390/molecules26092601>
30. Feng, Lian-Shun. Development and Advances of Drugs for Cancer Theranostics – PART-III. *Current Topics in Medicinal Chemistry*, Volume 21, Number 5, 2021, 347 <https://doi.org/10.2174/156802662105210216122217>
31. Rahman, S.; Kumar, V.; Kumar, A.; Abdullah, T.S.; Rather, I.A.; Jan, A.T. Molecular Perspective of Nanoparticle Mediated Therapeutic Targeting in Breast Cancer: An Odyssey of Endoplasmic Reticulum Unfolded Protein Response (UPR<sup>ER</sup>) and Beyond. *Biomedicines* **2021**, *9*, 635. <https://doi.org/10.3390/biomedicines9060635>
32. Solomon Habtemariam, Berberine pharmacology and the gut microbiota: A hidden therapeutic link, *Pharmacological Research*, Volume 155, 2020, 104722, <https://doi.org/10.1016/j.phrs.2020.104722>

**76. Diukendjieva A., M. Zaharieva, M. Mori, P. Alov, I. Tsakovska, T. Pencheva, H. Najdenski, V. Kren, C. Felici, F. Bufalieri, L. Di Marcotullio, B. Botta, M. Botta, I. Pajeva. Dual Smo/BRAF inhibition by flavonolignans from *Silybum marianum*. *Antioxidants*, 2020, 9(5), 384, 13 pages.**

Цитирания: 4

1. Tomko, A.M.; Whynot, E.G.; Ellis, L.D.; Dupré, D.J. Anti-Cancer Potential of Cannabinoids, Terpenes, and Flavonoids Present in Cannabis. *Cancers* 2020, *12*, 1985. <https://doi.org/10.3390/cancers12071985>
2. Valentová, K. Cytoprotective Activity of Natural and Synthetic Antioxidants. *Antioxidants* 2020, *9*, 713. <https://doi.org/10.3390/antiox9080713>
3. Said, M.A.; Albohy, A.; Abdelrahman, M.A.; Ibrahim, H.S. Importance of glutamine 189 flexibility in SARS-CoV-2 main protease: Lesson learned from in silico virtual screening of ChEMBL database and molecular dynamics. *European Journal of Pharmaceutical Sciences* **2021**, *160*, 105744. <https://doi.org/10.1016/j.ejps.2021.105744>.
4. Gerasimova, E.; Gazizullina, E.; Radosteva, E.; Ivanova, A. Antioxidant and Antiradical Properties of Some Examples of Flavonoids and Coumarins—Potentiometric Studies. *Chemosensors* **2021**, *9*(5), 112. <https://doi.org/10.3390/chemosensors9050112>

**77. Dinić J., T. Efferth, A.T. García-Sosa, J. Grahovac, J. M. Padrón, I.Pajeva, F. Rizzolio, S. Saponara, G. Spengler, I. Tsakovska, Repurposing old drugs to fight multidrug resistant cancers, *Drug Resistance Updates*, Volume 52, 2020, 100713, ISSN 1368-7646, <https://doi.org/10.1016/j.drug.2020.100713>.**

Цитирания: 12

1. Harguindey, S.; Alfarouk, K.; Polo Orozco, J.; Fais, S.; Devesa, J. Towards an Integral Therapeutic Protocol for Breast Cancer Based upon the New H<sup>+</sup>-Centered Anticancer Paradigm of the Late Post-Warburg Era. *Int. J. Mol. Sci.* **2020**, *21*, 7475, pp. 1-39. <https://doi.org/10.3390/ijms21207475>

2. Cucchi D.G.J., Groen R.W.J., Janssen J.J.W.M., Cloos J. Ex vivo cultures and drug testing of primary acute myeloid leukemia samples: Current techniques and implications for experimental design and outcome. *Drug Resistance Updates*, 53, art. no. 100730, 2020. <https://doi.org/10.1016/j.drug.2020.100730>
3. Özenver, N., Abdelfatah, S., Klinger, A. *et al.* Identification and characterization of deschloro-chlorothricin obtained from a large natural product library targeting aurora A kinase in multiple myeloma. *Invest New Drugs* **39**, 348–361 (2021). <https://doi.org/10.1007/s10637-020-01012-2>
4. Vivarelli S., Candido S., Caruso G., Falzone L., Libra M. Patient-derived tumor organoids for drug repositioning in cancer care: A promising approach in the era of tailored treatment. *Cancers*, 12(12), art. no. 3636, pp. 1-22, 2020. DOI: 10.3390/cancers12123636
5. Wejdan A. Shroukh (2020). RISK MANAGEMENT OF THALIDOMIDE IN JORDAN: AN APPLICATION OF THE WORLD HEALTH ORGANIZATION'S HEALTH SYSTEMS FRAMEWORK. A thesis submitted to The University of Manchester for the degree of Doctor of Philosophy In the Faculty of Biology, Medicine and Health, 2020. <https://www.escholar.manchester.ac.uk/uk-ac-man-scw:326558> PhD
6. Hernández-Lemus Enrique, Martínez-García Mireya. Pathway-Based Drug-Repurposing Schemes in Cancer: The Role of Translational Bioinformatics. *Frontiers in Oncology*, 10, 2021, 2996. <https://www.frontiersin.org/article/10.3389/fonc.2020.605680>
7. Monk, B.C.; Keniya, M.V. Roles for Structural Biology in the Discovery of Drugs and Agrochemicals Targeting Sterol 14 $\alpha$ -Demethylases. *J. Fungi* **2021**, 7, 67. <https://doi.org/10.3390/jof7020067>
8. Migliore Rossella, Granata Giuseppe, Rivoli Andrea, Consoli Grazia Maria Letizia, Sgarlata Carmelo. Binding Affinity and Driving Forces for the Interaction of Calixarene-Based Micellar Aggregates With Model Antibiotics in Neutral Aqueous Solution. *Frontiers in Chemistry*, 8, 2021, 626467. <https://doi.org/10.3389/fchem.2020.626467> <https://www.frontiersin.org/article/10.3389/fchem.2020.626467>.
9. Martínez-Escobar Alejandro, Luna-Callejas Benjamín, Ramón-Gallegos Eva. CRISPR-dCas9-Based Artificial Transcription Factors to Improve Efficacy of Cancer Treatment With Drug Repurposing: Proposal for Future Research. *Frontiers in Oncology*, 10, 2021, 3348. DOI: 10.3389/fonc.2020.604948 <https://www.frontiersin.org/article/10.3389/fonc.2020.604948>
10. Gasmi, A., Peana, M., Arshad, M., Butnariu, M., Menzel, A., Björklund, G. Krebs cycle: activators, inhibitors and their roles in the modulation of carcinogenesis. *Arch Toxicol* (2021). <https://doi.org/10.1007/s00204-021-02974-9>
11. Rebelo, R.; Polónia, B.; Santos, L.L.; Vasconcelos, M.H.; Xavier, C.P.R. Drug Repurposing Opportunities in Pancreatic Ductal Adenocarcinoma. *Pharmaceuticals* **2021**, 14, 280. <https://doi.org/10.3390/ph14030280>
12. Tiliya Pun, N.; Jeong, C.-H. Statin as a Potential Chemotherapeutic Agent: Current Updates as a Monotherapy, Combination Therapy, and Treatment for Anti-Cancer Drug Resistance. *Pharmaceuticals* **2021**, 14(5), art. no. 470. <https://doi.org/10.3390/ph14050470>

#### **В български списания, книги и дисертации:**

##### **1. Pajeva, I.K., J.K.Seydel, and L.Bock (1994): Study of Interactions between phospholipids and amphiphilic drugs active in reversing multidrug resistance in tumour cells, *Jahresbericht 1993, Forschungsinstitut Borstel*, 138-142.**

1. Тодоров, Д.К., К.Тимчева, М.Иларионова, А.Дудов, Фармакологични подходи за преодоляване на множествената лекарствена резистентност при злокачествени тумори, *Онкологичен преглед*, III (2), 1996, 3-9. цитат [7]

##### **2. Todorov,D.K., I.K.Pajeva, W.J.Zeller, G.Chen, and J.K.Seydel (1994): Molecular mechanisms of overcoming MDR by the plant anti-tumor drug thaliblastine (TBL) at non-cytotoxic concentrations, achievable in the plasma of treated cancer patients, *Anti-Cancer Drugs*, 5, Suppl.1, 25.**

2. Дудов, А. Терапевтични стратегии при множествената лекарствена резистентност (MDR) на туморите, *Онкологос*, 3-4, 2001, 33-35

##### **3. Тодоров, Д.К., К. Тимчева, И.Пъжева (1995): Лекарствена резистентност при злокачествени тумори и подходи за преодоляването и, *Онкология*, 32 (3-4), 9-12.**

3. Цаковска, И., Зависимости между структура и активност на съединения, преодоляващи множествената лекарствена резистентност при тумори, *Онкологичен преглед*, VI, 4, 1999, 3-9. цитат 1

##### **4. Pajeva,I.K., D.K.Todorov (1995): Studies of Doxorubicin in model membranes: relation to the mechanism of action and multidrug resistance, *Compt. rend. Acad. bulg. Sci.*, Tome 48(11-12), 159-162.**

4. Тимчева, К., И. Трифонова, Е. Пиперкова, А. Дренска, Ю. Горанчева, М. Николова, Е. Начева, Преодоляване на множествената лекарствена резистентност с дилтиазем при болни карцином на млечната жлеза, *Онкологичен преглед*, VI, 1, 1999, 8-14. цитат [9]

**Pajeva, I.K., M.Wiese, H.-P.Cordes, and J.K.Seydel (1996): Membrane interactions of some catamphiphilic drugs and relation to their multidrug resistance reversing ability, *J. Cancer Res. Clin. Onc.*, 122 (1), 27-40.**

5. Тодоров, Д.К., К.Тимчева, М.Иларионова, А.Дудов, Фармакологични подходи за преодоляване на множествената лекарствена резистентност при злокачествени тумори, *Онкологичен преглед*, III(2), 1996, 3-9. цитат [8]
6. Цаковска, И., Зависимости между структура и активност на съединения, преодоляващи множествената лекарствена резистентност при тумори, *Онкологичен преглед*, VI, 4, 1999, 3-9. цитат 3
7. Дудов, А., М. Иларионова, Л. Хорват, Д. Тодоров, Фармакологичните модификатори на множествената лекарствена резистентност (MDR) в комплексното лечение на онкозаболяванията, *Онкологос*, 2001, 3-4, 29-32.
8. Дудов, А.П., Подходи за преодоляване на естествената лекарствена резистентност на злокачествените тумори, *Онкология и радиология*, 2002, 9 (4), 3-11.

**5. Тимчева, К., И.Пъжева, Д.К.Тодоров (1996): Лекарствена резистентност на туморите - същност, клинично значение, преодоляване, *Фармакотерапия*, 2 (2),15-20.**

9. Дудов, А. Терапевтични стратегии при множествената лекарствена резистентност (MDR) на туморите, *Онкологос*, 3-4, 2001, 33-35

**6. Pajeva, I.K., D.K.Todorov (1996): Study of Thaliblastine in model membranes: relation to mechanism of action and multidrug resistance, *Compt. rend. Acad. bulg. Sci.*, Tome 50(2), 137-140.**

10. Тимчева, К., И. Трифонова, Е. Пиперкова, А. Дренска, Ю. Горанчева, М. Николова, Е. Начева, Преодоляване на множествената лекарствена резистентност с дилтиазем при болни карцином на млечната жлеза, *Онкологичен преглед*, VI, 1, 1999, 8-14. Цитат [10]

**7. Timcheva, C., I.Pajeva, D.Todorov, E.Pipercova, I.Triphonova (1996): Calcium channel blocker diltiazem as MDR-modulator, *J. Balkan Union of Oncology*, 2, 31-35.**

11. Цаковска, И., Зависимости между структура и активност на съединения, преодоляващи множествената лекарствена резистентност при тумори, *Онкологичен преглед*, VI, 4, 1999, 3-9. цитат 5

**Pajeva, I.K., M.Wiese (1997): QSAR and molecular modelling study of multidrug resistance modifiers, *Quant. Struct.-Act. Relat.*, 16 (1), 1-10.**

12. Цаковска, И., Зависимости между структура и активност на съединения, преодоляващи множествената лекарствена ре-зистентност при тумори, *Онкологичен преглед*, VI, 4, 1999, 3-9. цитат 10
13. Дудов, А., М. Иларионова, Л. Хорват, Д. Тодоров, Фармакологичните модификатори на множествената лекарствена резистентност (МДР) в комплексното лечение на онкозаболяванията, *Онкологос*, 2001, 3-4, 29-32.

**Pajeva, I.K., M.Wiese(1998): Molecular modeling of phenothiazines and related drugs as multidrug resistance modifiers: a comparative molecular field analysis study, *J.Med. Chem*, 41, 1815-1826.**

14. Цаковска, И., Зависимости между структура и активност на съединения, преодоляващи множествената лекарствена резистентност при тумори, *Онкологичен преглед*, VI, 4, 1999, 3-9. цитат 11
15. Дудов, А., М. Иларионова, Л. Хорват, Д. Тодоров, Фармакологичните модификатори на множествената лекарствена резистентност (МДР) в комплексното лечение на онкозаболяванията, *Онкологос*, 2001, 3-4, 29-32.
16. Фратев, Ф. Нови подходи в описанието на връзката между биологична активност и лиганд-протеинни взаимодействия. Метод на локалните свързващи енергии (LBE) и интегриране на 3D-QSAR, Docking, LBE и GRID анализите", Дисертация «Доктор», София, 2007.
17. Дойчинова, И. А. In silico изследване на пептиди – епитопи на на Т-лимфоцитите. Дисертация „Доктор на науките”, София, 2008.

**8. Todorov D.K., I.K. Pajeva, J.K.Seydel (2000): Doxorubicin and Taliblastine: membrane effects and relation to multidrug resistance, NATO Advanced Research Workshop *Antibiotic Transport and Drug Resistance*, 6-9 Oct 2000, St. Constantine–Varna, Bulgaria, Abstracts, p. 34.**

18. Дудов, А. Терапевтични стратегии при множествената лекарствена резистентност (MDR) на туморите, *Онкологос*, 3-4, 2001, 33-35.

**9. Тимчева, К., И. Пъжева, Д. Годоров (2000): Лекарствена резистентност при злокачествени тумори – фундаментални и клинични аспекти, *Studia Oncologia*, I (1), 9-27.**

19. Дудов, А.П., Подходи за преодоляване на естествената лекарствена резистентност на злокачествените тумори, *Онкология и радиология*, 2002, 9 (4), 3-11.
20. Първанова, В. Анемия и хипоксия при лъчелечение на онкологично болни – подходи за преодоляване, *Онкология и радиология*, 2004, 11 (1), 8-16.

**Цитирания на статии от дисертацията “Доктор” 8 (в чужбина, 2 в Б-я)**

**In international journals and books:**

**10. Pajeva, I.K., Z.Ch.Lateva, and G.V.Dimitrov: BACOMP - Database of Bioactive Compounds for Structure-Activity Relationship, *Int. J. Bio-med. Comput.*, 1986, 18, 7- 24.**

1. Poroikov V.: Computer-aided predictions in research and development of pharmaceuticals, D.Sc. thesis in Pharmacology, 1995, National Research Center for Biologically Active Compounds, Staraya Kupavna, Moscow Region. Citation No. 367
2. Walker, J.: 25 years of workshops and publications related to QSARs for pollution prevention, toxicity, screening, risk assessment, and the world wide web, In: *Quantitative Structure-Activity Relationships for Pollution Prevention, Toxicity Screening, Risk Assessment, and Web Applications*. John D. Walker (Editor), SETAC Press, 2003, pp. 205-230. (citation p. 220)

**11. Pajeva, I.K., Z.Ch.Lateva, and G.V.Dimitrov: SAR Oriented Database Aids Selection of Compounds for Screening, In: *Pharmacochemistry Library, Vol. 10, QSAR in Drug Design and Toxicology*, D.Hadzi and B.Jerman-Blazic (Eds.), Elsevier, Amsterdam, 1987, 49-51.**

3. McFarland, J.W. and D.J.Gans: Linear Discriminant Analysis and Cluster Significance Analysis, In: C.Hansch, P.G.Sammes, and J.B.Taylor (Eds.), *Comprehensive Medicinal Chemistry*, Vol.4 (C.A.Ramsden (Ed.) Quantitative Drug Design), Pergamon Press, 1990, 667-689. цитат [34]
4. Kubinyi, H.: Quantitative Structure-Activity Relationships (QSAR) and Molecular Modelling in Cancer Research, *J.Cancer Res. Clin. Onc.*, 1990, 116, 522-537. цитат[351]

**12. Pajeva, I.K.: Antineoplastic Activity Prediction by means of a Statistical-Heuristic Technique, In: *Progress in Clinical and Biological Research, Vol. 291, QSAR: Quantitative Structure-Activity Relationships in Drug Design*, J.L.Fauchere (Ed.), Alan R. Liss, Inc., 1989, 209-212.**

5. Kubinyi, H.: Quantitative Structure-Activity Relationships (QSAR) and Molecular Modelling in Cancer Research, *J. Cancer Res. Clin. Onc.*, 1990, 116, 522-537. цитат[352]

**13. Pajeva, I. and E.Golovinsky: Substructural Analysis of Antineoplastic Drugs in respect of *in Vivo* Tumor Models, *Quant.Struct.-Act. Relat.*, 9, 1990, 216-222.**

6. Franke R., S. Dove, A. Gruska: Physicochemical properties and drug action, alternative QSAR methods, In: *Advanced Drug Design & Development: A Medicinal Chemistry Approach*, (Ellis Horwood Series in Pharmaceutical Technology) P.H. Kourounakis and E. Rekkas (Eds.), Prentis Hall, 1994, Chapter 4, p. 97. citation [231].
7. Frenkel., M. and K.N. Marsh: Spectral Data for Steroids (Trc Data Series), CRC, Texas, USA, 1994, pp.966. (citation p. 685).

**14. Pajeva, I., I. Manolov, and E.Golovinsky (1990) : Structure - Activity Relationship Investigation of Bis(2-Chloroethyl)-aminoethyl Esters of Some Carboxylic Acids, *Pharmazie*, 45, 361-363.**

8. Chinese authors: MEDICINE AND PHARMACY OF YUNNAN, 1998年 19 (4), 300-302.

**В България:**

**15. Пъжева, И.К.: Микрокомпютърна система за изследване и прогнозиране на зависимости химическа структура - противотуморна активност при туморни модели *in vivo*, Дисертация, София, 1989, 1-177.**

1. Начева, Р.Н.: QSAR-ориентирано изследване на химичната структура на някои серии биологично активни вещества, Дисертация, София, 1989.

2. Нецева, Т. И.: Влияние на полярността на средата в QSAR анализа на серии биологично-активни вещества. 3D-QSAR анализ. Дисертация, София, 2001.