

## Documents

---

- 1) Cao, H., Peng, J., Zhou, Z., Yang, Z., Wang, L., Sun, Y., Wang, Y., Liang, Y.

**Investigation of the Binding Fraction of PFAS in Human Plasma and Underlying Mechanisms: A Machine Learning and Molecular Dynamics Simulation**

(2023) *Environmental Science and Technology*, 57 (46), pp. 17762-17773.

- 2) Komura, H., Watanabe, R., Mizuguchi, K.

**The Trends and Future Prospective of In Silico Models from the Viewpoint of ADME Evaluation**

(2023) *Pharmaceutics*, 15 (11), art. no. 2619, .

- 3) Jena, M., Mukadam, M., Telange, D., Dolas, R., Ramana, C.S.

**Nitrosamine Impurities: Assessing Concerns through Case Studies**

(2023) *Asian Journal of Chemistry*, 35 (4), pp. 794-804.

- 4) Tran, T.T.V., Tayara, H., Chong, K.T.

**Recent Studies of Artificial Intelligence on In Silico Drug Distribution Prediction**

(2023) *International Journal of Molecular Sciences*, 24 (3), art. no. 1815, .

- 5) Thomas, R., Tennant, R.E., Oliveira, A.A.F., Ponting, D.J.

**What Makes a Potent Nitrosamine? Statistical Validation of Expert-Derived Structure-Activity Relationships**

(2022) *Chemical Research in Toxicology*, 35 (11), pp. 1997-2013.

- 6) Fagerholm, U., Spjuth, O., Hellberg, S.

**The Impact of Reference Data Selection for the Prediction Accuracy of Intrinsic Hepatic Clearance**

(2022) *Journal of Pharmaceutical Sciences*, 111 (9), pp. 2645-2649.

7) Sharma, P., Ranjan, A., Gaur, A., Choudhary, S., Kumar, V., Singh, A.P.

**In-vitro plasma protein binding of marbofloxacin in sheep**

(2021) *Veterinary Practitioner*, 22 (1), pp. 140-142.

8) Mulpuru, V., Mishra, N.

**In Silico Prediction of Fraction Unbound in Human Plasma from Chemical Fingerprint Learning**

(2021) *ACS Omega*, 6 (10), pp. 6791-6797.

9) Fu, M., Zhu, Y., Wu, C., Hou, F., Guan, Y.

**Prediction of plasma protein binding rate based on machine learning [基于机器学习的药**

(2021) *Journal of China Pharmaceutical University*, 52 (6), pp. 699-706.

10) Fagerholm, U., Spjuth, O., Hellberg, S.

**Comparison between lab variability and in silico prediction errors for the unbound fraction in plasma**

(2021) *Xenobiotica*, 51 (10), pp. 1095-1100.

11) Yuan, Y., Chang, S., Zhang, Z., Li, Z., Li, S., Xie, P., Yau, W.-P., Lin, H., Cai, W., Zhang, Y., X

**A novel strategy for prediction of human plasma protein binding using machine learn**

(2020) *Chemometrics and Intelligent Laboratory Systems*, 199, art. no. 103962, .

12) Orozco, C.C., Atkinson, K., Ryu, S., Chang, G., Keefer, C., Lin, J., Riccardi, K., Mongillo, R.I., Kalgutkar, A.S., Litchfield, J., Scott, D., Di, L.

**Structural attributes influencing unbound tissue distribution**

(2020) *European Journal of Medicinal Chemistry*, 185, art. no. 111813, .

13) Toma, C., Gadaleta, D., Roncaglioni, A., Toropov, A., Toropova, A., Marzo, M., Benfenati, E.

**QSAR Development for Plasma Protein Binding: Influence of the Ionization State**

(2019) *Pharmaceutical Research*, 36 (2), art. no. 28, .

14) Watanabe, R., Esaki, T., Kawashima, H., Natsume-Kitatani, Y., Nagao, C., Ohashi, R., Mizug

**Predicting Fraction Unbound in Human Plasma from Chemical Structure: Improved A**

## Ranges

(2018) *Molecular Pharmaceutics*, 15 (11), pp. 5302-5311.

- 15) Deb, P.K., Al-Attraqchi, O., Prasad, M.R., Tekade, R.K.

**Protein and Tissue Binding: Implication on Pharmacokinetic Parameters. Implication Parameters.**

(2018) *Dosage Form Design Considerations: Volume I*, pp. 371-399.

- 16) Chandrasekaran, B., Abed, S.N., Al-Attraqchi, O., Kuche, K., Tekade, R.K.

**Computer-Aided Prediction of Pharmacokinetic (ADMET) Properties**

(2018) *Dosage Form Design Parameters*, 2, pp. 731-755.

- 17) Wang, N.-N., Deng, Z.-K., Huang, C., Dong, J., Zhu, M.-F., Yao, Z.-J., Chen, A.F., Lu, A.-P., I

**ADME properties evaluation in drug discovery: Prediction of plasma protein binding and consensus modeling**

(2017) *Chemometrics and Intelligent Laboratory Systems*, 170, pp. 84-95.

- 18) Alqahtani, S.

**In silico ADME-Tox modeling: progress and prospects**

(2017) *Expert Opinion on Drug Metabolism and Toxicology*, 13 (11), pp. 1147-1158.

- 19) Bech, E.M., Martos-Maldonado, M.C., Wismann, P., Sørensen, K.K., Van Witteloostuijn, SØ. Jelsing, J., Pedersen, SØ.L., Jensen, K.J.

**Peptide Half-Life Extension: Divalent, Small-Molecule Albumin Interactions Direct the Glucagon-Like Peptide 1 (GLP-1) Analogues**

(2017) *Journal of Medicinal Chemistry*, 60 (17), pp. 7434-7446.

- 20) Zhivkova, Z.

**Quantitative Structure – Pharmacokinetic Relationships for Plasma Clearance of Basic the Major Elimination Pathway**

(2017) *Journal of Pharmacy and Pharmaceutical Sciences*, 20, pp. 135-147.

- 21) Zhivkova, Z.

**Quantitative Structure – Pharmacokinetics Relationships for Plasma Protein Binding of B**  
(2017) *Journal of Pharmacy and Pharmaceutical Sciences*, 20, pp. 349-359.

- 22) Lu, J., Goldsmith, M.-R., Grulke, C.M., Chang, D.T., Brooks, R.D., Leonard, J.A., Phillips, M. Tornero-Velez, R., Johnson, J., Dary, C.C., Tan, Y.-M.

**Developing a Physiologically-Based Pharmacokinetic Model Knowledgebase in Support of Drug Development**

(2016) *PLoS Computational Biology*, 12 (2), art. no. e1004495, 22 p.

- 23) Basant, N., Gupta, S., Singh, K.P.

**Predicting binding affinities of diverse pharmaceutical chemicals to human serum proteins using different modelling approaches**

(2016) *SAR and QSAR in Environmental Research*, 27 (1), pp. 67-85.

- 24) Svennebring, A.

**The impact of plasma protein binding on toxic plasma drug concentration**

(2016) *International Journal of Computational Biology and Drug Design*, 9 (4), pp. 345-368.

- 25) Svennebring, A.M.

**Investigation of the prerequisites for the optimization of specific plasma protein binding and reduction of first-pass hepatic metabolism**

(2015) *Xenobiotica*, 45 (4), pp. 286-301.

- 26) Oliveira, T.B., Gobbo-Neto, L., Schmidt, T.J., Da Costa, F.B.

**Study of chromatographic retention of natural terpenoids by chemoinformatic tools**

(2015) *Journal of Chemical Information and Modeling*, 55 (1), pp. 26-38.

- 27) Zhivkova, Z.D.

**Studies on drug – human serum albumin binding: The current state of the matter**

(2015) *Current Pharmaceutical Design*, 21 (14), pp. 1817-1830.

- 28) Kharkar, P.S.

**In silico absorption, distribution metabolism and excretion**

(2013) *In Silico Drug Discovery and Design*, pp. 148-162.

ELSEVIER

Copyright © 2024 Elsevier B.V. All rights reserved. Scopus® is a re  
trademark of Elsevier B.V.