

## Documents

- 1) Lopes-Ribeiro, Á., Araujo, F.P., Oliveira, P.D.M., Teixeira, L.D.A., Ferreira, G.M., Lourenço, A., Retes, H.M., Lopes, É.N., Versiani, A.F., Barbosa-Stancioli, E.F., da Fonseca, F.G., Martins-F Magalhães, V., Coelho-dos-Reis, J.G.A.

**In silico and in vitro arboviral MHC class I-restricted-epitope signatures reveal immune overlapping patterns**

(2022) *Frontiers in Immunology*, 13, art. no. 1035515, .

- 2) Zhou, P., Wen, L., Lin, J., Mei, L., Liu, Q., Shang, S., Li, J., Shu, J.

**Integrated unsupervised-supervised modeling and prediction of protein-peptide affinity**

(2022) *Briefings in Bioinformatics*, 23 (3), art. no. bbac097, .

- 3) Zhou, P., Liu, Q., Wu, T., Miao, Q., Shang, S., Wang, H., Chen, Z., Wang, S., Wang, H.

**Systematic Comparison and Comprehensive Evaluation of 80 Amino Acid Descriptors**

(2021) *Journal of Chemical Information and Modeling*, 61 (4), pp. 1718-1731.

- 4) Mei, S., Li, F., Leier, A., Marquez-Lago, T.T., Giam, K., Croft, N.P., Akutsu, T., Ian Smith, A., Li Song, J.

**A comprehensive review and performance evaluation of bioinformatics tools for HLA class II peptide prediction**

(2019) *Briefings in Bioinformatics*, 21 (4), pp. 1119-1135.

- 5) Li, Z., Miao, Q., Yan, F., Meng, Y., Zhou, P.

**Machine learning in quantitative protein-peptide affinity prediction: Implications for the**

(2019) *Current Drug Metabolism*, 20 (3), pp. 170-176.

- 6) Uslan, V., Seker, H., John, R.

**Overlapping Clusters and Support Vector Machines Based Interval Type-2 Fuzzy Systems**

## Peptide Binding Affinity

(2019) *IEEE Access*, 7, art. no. 8685099, pp. 49756-49764.

7) Kogay, R., Schönbach, C.

### Epitope predictions

(2018) *Encyclopedia of Bioinformatics and Computational Biology: ABC of Bioinformatics*, 1-3

8) Antunes, D.A., Abella, J.R., Devaurs, D., Rigo, M.M., Kavraki, L.E.

### Structure-based methods for binding mode and binding affinity prediction for peptide-

(2018) *Current Topics in Medicinal Chemistry*, 18 (26), pp. 2239-2255.

9) Wang, Y., Zhou, P., Lin, Y., Shu, M., Hu, Y., Xia, Q., Lin, Z.

### Quantitative prediction of class I MHC/epitope binding affinity using QSAR modeling and structural information

(2015) *Combinatorial Chemistry and High Throughput Screening*, 18 (1), pp. 75-82.

10) Aguilar-Bonavides, C., Sanchez-Arias, R., Lanzas, C.

### Accurate prediction of major histocompatibility complex class II epitopes by sparse representation minimization

(2014) *BioData Mining*, 7 (1), art. no. 23, .

11) Srivastava, A., Ghosh, S., Anantharaman, N., Jayaraman, V.K.

### Hybrid biogeography based simultaneous feature selection and MHC class I peptide binding support vector machines and random forests

(2013) *Journal of Immunological Methods*, 387 (1-2), pp. 284-292.

12) Liao, W.W.P., Arthur, J.W.

### Predicting peptide binding to Major Histocompatibility Complex molecules

(2011) *Autoimmunity Reviews*, 10 (8), pp. 469-473.

13) Hu, L., Ai, Z., Liu, P., Xiong, Q., Min, M., Lan, C., Wang, J., Fan, L., Chen, D.

### Predicting the binding affinity of epitope-peptides with HLA-A\*0201 by encoding atom information between receptor and ligands

(2010) *Chemical Biology and Drug Design*, 75 (6), pp. 597-606.

14) Demir-Kavuk, O., Riedesel, H., Knapp, E.-W.

**Exploring classification strategies with the CoEPrA 2006 contest**  
(2010) *Bioinformatics*, 26 (5), art. no. btq021, pp. 603-609.

15) Li, Y., Yang, Y., He, P., Yang, Q.

**QM/MM study of epitope peptides binding to HLA-A\*0201: The roles of anchor residues**  
(2009) *Chemical Biology and Drug Design*, 74 (6), pp. 611-618.

16) Lafuente, E.M., Reche, P.A.

**Prediction of MHC-peptide binding: A systematic and comprehensive overview**  
(2009) *Current Pharmaceutical Design*, 15 (28), pp. 3209-3220.

17) Patil, D., Raj, R., Shingade, P., Kulkarni, B., Jayaraman, V.K.

**Feature selection and classification employing hybrid ant colony optimization/random forest**  
(2009) *Combinatorial Chemistry and High Throughput Screening*, 12 (5), pp. 507-513.

18) Tian, F., Yang, L., Lv, F., Yang, Q., Zhou, P.

**In silico quantitative prediction of peptides binding affinity to human MHC molecule: A structure-activity relationship approach**  
(2009) *Amino Acids*, 36 (3), pp. 535-554.

19) Zhou, P., Chen, X., Shang, Z.

**Side-chain conformational space analysis (SCSA): A multi conformation-based QSAR prediction of protein-peptide binding affinities**  
(2009) *Journal of Computer-Aided Molecular Design*, 23 (3), pp. 129-141.

20) Tian, F., Lv, F., Zhou, P., Yang, Q., Jalbout, A.F.

**Toward prediction of binding affinities between the MHC protein and its peptide ligand: A structure-affinity relationship approach**  
(2008) *Protein and Peptide Letters*, 15 (10), pp. 1033-1043.

21) Zhou, P., Tian, F., Wu, Y., Li, Z., Shang, Z.

**Quantitative sequence-activity model (QSAM): Applying QSAR strategy to model and function of peptides, proteins and nucleic acids**

(2008) *Current Computer-Aided Drug Design*, 4 (4), pp. 311-321.

22) Verma, J., Khedkar, V.M., Prabhu, A.S., Khedkar, S.A., Malde, A.K., Coutinho, E.C.

**A comprehensive analysis of the thermodynamic events involved in ligand-receptor binding variants**

(2008) *Journal of Computer-Aided Molecular Design*, 22 (2), pp. 91-104.

23) Schiewe, A.J., Haworth, I.S.

**Structure-based prediction of MHC-peptide association: Algorithm comparison and validation design**

(2007) *Journal of Molecular Graphics and Modelling*, 26 (3), pp. 667-675.

24) Ivanciuc, O., Braun, W.

**Robust quantitative modeling of peptide binding affinities for MHC molecules using principal component analysis**

(2007) *Protein and Peptide Letters*, 14 (9), pp. 903-916.

25) Zhao, C., Zhang, H., Luan, F., Zhang, R., Liu, M., Hu, Z., Fan, B.

**QSAR method for prediction of protein-peptide binding affinity: Application to MHC class II**

(2007) *Journal of Molecular Graphics and Modelling*, 26 (1), pp. 246-254.

26) Pissurlenkar, R.R.S., Malde, A.K., Khedkar, S.A., Coutinho, E.C.

**Encoding type and position in peptide QSAR: Application to peptides binding to class II MHC**

(2007) *QSAR and Combinatorial Science*, 26 (2), pp. 189-203.

27) Flower, D., Timmis, J.

**In silico immunology**

(2007) *In Silico Immunology*, pp. 1-450.

28) Lundegaard, C., Lund, O., Keşmir, C., Brunak, S., Nielsen, M.

## **Modeling the adaptive immune system: Predictions and simulations**

(2007) *Bioinformatics*, 23 (24), pp. 3265-3275.

29) Zhou, P., Tian, F., Li, Z.

### **A structure-based, quantitative structure-activity relationship approach for predicting cytotoxic T lymphocyte epitopes**

(2007) *Chemical Biology and Drug Design*, 69 (1), pp. 56-67.

30) Dingfang, L., Wenchao, H.

### **A relevance vector machine based quantitative prediction method for mouse class I M**

(2006) *ICBPE 2006 - Proceedings of the 2006 International Conference on Biomedical and* no. 4155921, pp. 344-353.

31) Wan, J., Liu, W., Xu, Q., Ren, Y., Flower, D.R., Li, T.

### **SVRMHC prediction server for MHC-binding peptides**

(2006) *BMC Bioinformatics*, 7, art. no. 463, .

32) Bordner, A.J., Abagyan, R.

### **Ab initio prediction of peptide-MHC binding geometry for diverse class I MHC allotype**

(2006) *Proteins: Structure, Function and Genetics*, 63 (3), pp. 512-526.

33) Bui, H.-H., Schiewe, A.J., Von Grafenstein, H., Haworth, I.S.

### **Structural prediction of peptides binding to MHC class I molecules**

(2006) *Proteins: Structure, Function and Genetics*, 63 (1), pp. 43-52.

34) Liu, W., Meng, X., Xu, Q., Flower, D.R., Li, T.

### **Quantitative prediction of mouse class I MHC peptide binding affinity using support v (SVR) models**

(2006) *BMC Bioinformatics*, 7, art. no. 182, .

35) Desmet, J., Meersseman, G., Boutonnet, N., Pletinckx, J., De Clercq, K., Debulpaep, M., Br

### **Anchor profiles of HLA-specific peptides: Analysis by a novel affinity scoring method**

(2005) *Proteins: Structure, Function and Genetics*, 58 (1), pp. 53-69.

36) Lin, Z.-H., Hu, Y., Wu, Y.-Z.

**3D-QSAR study on the HLA-A\*0201 restricted CTL epitope**

(2004) *Acta Chimica Sinica*, 62 (18), pp. 1835-1840.

37) Zhihua, L., Wu, Y., Bo, Z., Ni, B., Li, W.

**Toward the quantitative prediction of T-cell epitopes: QSAR studies on peptides having Molecular HLA-A\*0201**

(2004) *Journal of Computational Biology*, 11 (4), pp. 683-694.

38) Lin, Z., Wu, Y., Wei, Y., Ni, B., Zhu, B., Wang, L.

**A rapid method for quantitative prediction of high affinity CTL epitopes: QSAR studies with the class I MHC molecular HLA-A\*0201**

(2003) *Letters in Peptide Science*, 10 (1), pp. 15-23.

39) Flower, D.R.

**Databases and data mining for computational vaccinology**

(2003) *Current Opinion in Drug Discovery and Development*, 6 (3), pp. 396-400.

40) Flower, D.R.

**Towards in silico prediction of immunogenic epitopes**

(2003) *Trends in Immunology*, 24 (12), pp. 667-674.