

## Documents

---

- 1) Karlberg, M., Kizhedath, A., Glassey, J.

**Model-Based Risk Assessment of mAb Developability**

(2022) *Springer Optimization and Its Applications*, 189, pp. 373-391.

- 2) Mahmoodi-Reihani, M., Abbasitabar, F., Zare-Shahabadi, V.

**In Silico Rational Design and Virtual Screening of Bioactive Peptides Based on QSAR I**

(2020) *ACS Omega*, 5 (11), pp. 5951-5958.

- 3) 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.

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

**Overlapping Clusters and Support Vector Machines Based Interval Type-2 Fuzzy System for Peptide Binding Affinity**

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

- 5) Karlberg, M., von Stosch, M., Glassey, J.

**Exploiting mAb structure characteristics for a directed QbD implementation in early product development**

(2018) *Critical Reviews in Biotechnology*, 38 (6), pp. 957-970.

- 6) Giles, J.B., Brill, D.A., Chavoya, A., Haworth, I.S.

**Algorithms for the prediction of peptides binding to Major Histocompatibility Complex**

(2018) *Advances in Chemistry Research*, 46, pp. 59-94.

7) Qian, Y., Liang, Y., Liu, W., Liang, G.

**Comprehensive comparison of twenty structural characterization scales applied as QS dodecapeptides derived from Bac2A against *P. aeruginosa***  
(2017) *Journal of Molecular Graphics and Modelling*, 71, pp. 88-95.

8) Sheikh, Q.M., Gatherer, D., Reche, P.A., Flower, D.R.

**Towards the knowledge-based design of universal influenza epitope ensemble vaccine**  
(2016) *Bioinformatics*, 32 (21), pp. 3233-3239.

9) He, Y., He, X.

**Molecular design and genetic optimization of antimicrobial peptides containing unnatural antibiotic-resistant bacterial infections**  
(2016) *Biopolymers*, pp. 746-756.

10) Davies, M.N., Flower, D.R.

**Towards an omic perspective on infectious disease and its therapy: Integrating immunology and vaccinomics**  
(2016) *OMICS: Biomedical Perspectives and Applications*, pp. 451-475.

11) Li, B., Zheng, X., Hu, C., Cao, Y.

**Human Papillomavirus Genome-Wide Identification of T-Cell Epitopes for Peptide Vaccines in Cervical Cancer: An Integration of Computational Analysis and Experimental Assay**  
(2015) *Journal of Computational Biology*, 22 (10), pp. 962-974.

12) Yousefinejad, S., Bagheri, M., Moosavi-Movahedi, A.A.

**Quantitative sequence-activity modeling of antimicrobial hexapeptides using a segmental strategy: An approach to describe and predict activities of peptide drugs containing L-proline**  
(2015) *Amino Acids*, 47 (1), pp. 125-134.

13) Dai, Z., Wang, L., Chen, Y., Wang, H., Bai, L., Yuan, Z.

**A pipeline for improved QSAR analysis of peptides: Physiochemical property parameter neighbor sample selection via semivariogram, and weighted SVR regression and prediction**  
(2014) *Amino Acids*, 46 (4), pp. 1105-1119.

14) Monzón-Argüello, C., Garcia De Leaniz, C., Gajardo, G., Consuegra, S.

**Eco-immunology of fish invasions: The role of MHC variation**

(2014) *Immunogenetics*, 66 (6), pp. 393-402.

15) Yuan, J., Pu, Y., Yin, L.

**Prediction of binding affinities of PCDDs, PCDFs and PCBs using docking-based Con Indices Analysis**

(2014) *Environmental Toxicology and Pharmacology*, 38 (1), pp. 1-7.

16) Ferguson, A.L., Falkowska, E., Walker, L.M., Seaman, M.S., Burton, D.R., Chakraborty, A.K.

**Computational prediction of broadly neutralizing HIV-1 antibody epitopes from neutra**

(2013) *PLoS ONE*, 8 (12), art. no. e80562, .

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

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

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

18) Juhász, A., Gell, G., Békés, F., Balázs, E.

**The epitopes in wheat proteins for defining toxic units relevant to human health**

(2012) *Functional and Integrative Genomics*, 12 (4), pp. 585-598.

19) Yousefinejad, S., Hemmateenejad, B., Mehdipour, A.R.

**New autocorrelation QTMS-based descriptors for use in QSAM of peptides**

(2012) *Journal of the Iranian Chemical Society*, 9 (4), pp. 569-577.

20) Hemmateenejad, B., Miri, R., Elyasi, M.

**A segmented principal component analysis-regression approach to QSAR study of pe**

(2012) *Journal of Theoretical Biology*, 305, pp. 37-44.

21) Roy, K., Mitra, I.

**Electrotopological state atom (E-State) index in drug design, QSAR, property predicti**

(2012) *Current Computer-Aided Drug Design*, 8 (2), pp. 135-158.

22) Cheng, Z., Zhang, Y., Zhou, C.

**QSAR models for phosphoramidate prodrugs of 2'-methylcytidine as inhibitors of hepatitis B virus replication**

(2011) *Chemical Biology and Drug Design*, 78 (6), pp. 948-959.

23) Sukumar, N., Das, S., Krein, M., Godawat, R., Vitol, I., Garde, S., Bennett, K.P., Breneman, J.

**Molecular Descriptors for Biological Systems**

(2011) *Computational Approaches in Cheminformatics and Bioinformatics*, pp. 107-143.

24) Cheng, Z., Zhang, Y., Fu, W.

**Predictive QSAR models of 3-acylamino-2-aminopropionic acid derivatives as partial agonists of the NMDA receptor**

(2011) *Medicinal Chemistry Research*, 20 (8), pp. 1235-1246.

25) Ren, Y., Chen, X., Feng, M., Wang, Q., Zhou, P.

**Gaussian process: A promising approach for the modeling and prediction of peptide binding affinities**

(2011) *Protein and Peptide Letters*, 18 (7), pp. 670-678.

26) Hemmateenejad, B., Yousefinejad, S., Mehdipour, A.R.

**Novel amino acids indices based on quantum topological molecular similarity and the analysis of peptides**

(2011) *Amino Acids*, 40 (4), pp. 1169-1183.

27) Gupta, S.K., Srivastava, M., Akhoun, B.A., Smita, S., Schmitz, U., Wolkenhauer, O., Vera, J.

**Identification of immunogenic consensus T-cell epitopes in globally distributed influenza A virus**

(2011) *Infection, Genetics and Evolution*, 11 (2), pp. 308-319.

28) Sirskyj, D., Diaz-Mitoma, F., Golshani, A., Kumar, A., Azizi, A.

**Innovative bioinformatic approaches for developing peptide-based vaccines against HIV-1**

(2011) *Immunology and Cell Biology*, 89 (1), pp. 81-89.

29) Bremel, R.D., Homan, E.J.

**An integrated approach to epitope analysis I: Dimensional reduction, visualization and using amino acid principal components and regression approaches**

(2010) *Immunome Research*, 6 (1), art. no. 7, .

30) Todeschini, R., Consonni, V.

**Molecular Descriptors for Chemoinformatics**

(2010) *Molecular Descriptors for Chemoinformatics*, 2, pp. 1-252.

31) 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.

32) Tong, J.C., Ren, E.C.

**Immunoinformatics: The way forward**

(2010) *Advances in Genetics Research*, 1, pp. 249-264.

33) Zhou, P., Chen, X., Wu, Y., Shang, Z.

**Gaussian process: An alternative approach for QSAM modeling of peptides**

(2010) *Amino Acids*, 38 (1), pp. 199-212.

34) Davies, M.N., Flower, D.R.

**Bridging the Pharmaceutical Shortfall: Informatics Approaches to the Discovery of Vaccines and Adjuvants**

(2009) *Pharmaceutical Data Mining: Approaches and Applications for Drug Discovery*, pp. 3

35) Ivanciuc, O.

**Machine learning quantitative structure-activity relationships (QSAR) for peptides binding to the amyloid-beta (A $\beta$ ) SH3 domain**

(2009) *Current Proteomics*, 6 (4), pp. 289-302.

36) Leong, M.K., Chen, Y.-M., Chen, T.-H.

**Prediction of human cytochrome P450 2B6-substrate interactions using hierarchical supi approach**

(2009) *Journal of Computational Chemistry*, 30 (12), pp. 1899-1909.

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

**Feature selection and classification employing hybrid ant colony optimization/random**

(2009) *Combinatorial Chemistry and High Throughput Screening*, 12 (5), pp. 507-513.

38) Lindström, A., Pettersson, F., Linusson, A.

**Quantitative protein descriptors for secondary structure characterization and protein**

(2009) *Chemometrics and Intelligent Laboratory Systems*, 95 (1), pp. 74-85.

39) Sukumar, N., Krein, M., Breneman, C.M.

**Bioinformatics and cheminformatics: Where do the twain meet?**

(2008) *Current Opinion in Drug Discovery and Development*, 11 (3), pp. 311-319.

40) 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.

41) 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 b variants**

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

42) Jacob, L., Vert, J.-P.

**Efficient peptide-MHC-I binding prediction for alleles with few known binders**

(2008) *Bioinformatics*, 24 (3), pp. 358-366.

43) Ivanciuc, O., Braun, W.

**Robust quantitative modeling of peptide binding affinities for MHC molecules using p**

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

44) Holm, L., Frech, K., Dzhabazov, B., Holmdahl, R., Kihlberg, J., Linusson, A.

**Quantitative structure-activity relationship of peptides binding to the class II major histocompatibility molecule Aq associated with autoimmune arthritis**

(2007) *Journal of Medicinal Chemistry*, 50 (9), pp. 2049-2059.

45) Davies, M.N., Flower, D.R.

**Harnessing bioinformatics to discover new vaccines**

(2007) *Drug Discovery Today*, 12 (9-10), pp. 389-395.

46) 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.

47) Antes, I., Siu, S.W.I., Lengauer, T.

**DynaPred: A structure and sequence based method for the prediction of MHC class I peptide binding and conformations**

(2006) *Bioinformatics*, 22 (14), pp. e16-e24.

48) Davies, M.N., Hattotuwegama, C.K., Moss, D.S., Drew, M.G.B., Flower, D.R.

**Statistical deconvolution of enthalpic energetic contributions to MHC-peptide binding**

(2006) *BMC Structural Biology*, 6, art. no. 5, 13 p.