

Documents

- 1) Jade, D., Gupta, S., Mohan, S., Ponnambalam, S., Harrison, M., Bhatnagar, R.

Homology modelling and molecular simulation approach to prediction of B-cell and T-cell peptide vaccine against *Brucella abortus*

(2023) *Molecular Simulation*, 49 (5), pp. 441-452.

- 2) Möller, J., Bodenschatz, M., Sangal, V., Hofmann, J., Burkovski, A.

Multi-Omics of *Corynebacterium Pseudotuberculosis* 12CS0282 and an In Silico Reverse Immunology Approach Reveal Novel Vaccine and Drug Targets

(2022) *Proteomes*, 10 (4), art. no. 39, .

- 3) Goumari, M.M., Farhani, I., Nezafat, N., Mahmoodi, S.

Multi-epitope vaccines (MEVs), as a novel strategy against infectious diseases

(2020) *Current Proteomics*, 17 (5), pp. 354-364.

- 4) Akya, A., Farasat, A., Ghadiri, K., Rostamian, M.

Identification of HLA-I restricted epitopes in six vaccine candidates of *Leishmania tropica* using immunoinformatics and molecular dynamics simulation approaches

(2019) *Infection, Genetics and Evolution*, 75, art. no. 103953, .

- 5) Thurston, B.A., Ferguson, A.L.

Machine learning and molecular design of self-assembling -conjugated oligopeptides

(2018) *Molecular Simulation*, 44 (11), pp. 930-945.

- 6) Dikhit, M.R., Amit, A., Singh, A.K., Kumar, A., Mansuri, R., Sinha, S., Topno, R.K., Mishra, R., Sahoo, G.C., Ali, V., Bimal, S., Das, P.

Vaccine potential of HLA-A2 epitopes from *Leishmania* Cysteine Protease Type III (CPC)

(2017) *Parasite Immunology*, 39 (9), art. no. e12451, .

7) Lu, H., Tang, B., He, Y., Zhou, W., Qiu, J., Li, Y.

Identification of HLA-A1101-restricted cytotoxic T lymphocyte epitopes derived from e pathway substrate number 8

(2016) *Molecular Medicine Reports*, 14 (6), pp. 4999-5006.

8) Dikhit, M.R., Kumar, S., Vijaymahantesh, Sahoo, B.R., Mansuri, R., Amit, A., Yousuf Ansari, N P.

Computational elucidation of potential antigenic CTL epitopes in Ebola virus

(2015) *Infection, Genetics and Evolution*, 36, pp. 369-375.

9) 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 neutrali

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

10) Thangapandian, S., John, S., Son, M., Arulalapperumal, V., Lee, K.W.

Development of predictive quantitative structure-Activity relationship model and its a human leukotriene A4 hydrolase inhibitors

(2013) *Future Medicinal Chemistry*, 5 (1), pp. 27-40.

11) Hsu, S.-C., Chang, C.-P., Tsai, C.-Y., Hsieh, S.-H., Wu-Hsieh, B.A., Lo, Y.-S., Yang, J.-M.

Steric recognition of T-cell receptor contact residues is required to map mutant epitope programmes

(2012) *Immunology*, 136 (2), pp. 139-152.

12) Seyed, N., Zahedifard, F., Safaiyan, S., Gholami, E., Doustdari, F., Azadmanesh, K., Mirzaei Eslami far, A., Sharifi, I., Rafati, S.

In silico analysis of six known leishmania major antigens and in vitro evaluation of sp A2 restricted CD8 T cell response

(2011) *PLoS Neglected Tropical Diseases*, 5 (9), art. no. e1295, .

13) Joosten, S.A., Van Meijgaarden, K.E., Van Weeren, P.C., Kazi, F., Geluk, A., Savage, N.D.L. Hanekom, W.A., Klein, M.R., Ottenhoff, T.H.M.

Mycobacterium tuberculosis peptides presented by HLA-E molecules are targets for T

cytotoxic as well as regulatory activity

(2010) *PLoS Pathogens*, 6 (2), art. no. e1000782, .

14) 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.

15) Hansen, L., Lee, E.A., Hestir, K., Williams, L.T., Farrelly, D.

Controlling feature selection in random forests of decision trees using a genetic algorithm for MHC peptides

(2009) *Combinatorial Chemistry and High Throughput Screening*, 12 (5), pp. 514-519.

16) 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.

17) Vilar, S., Cozza, G., Moro, S.

Medicinal chemistry and the Molecular Operating Environment (MOE): Application of MOE to drug discovery

(2008) *Current Topics in Medicinal Chemistry*, 8 (18), pp. 1555-1572.

18) Vivona, S., Gardy, J.L., Ramachandran, S., Brinkman, F.S.L., Raghava, G.P.S., Flower, D.R.

Computer-aided biotechnology: from immuno-informatics to reverse vaccinology

(2008) *Trends in Biotechnology*, 26 (4), pp. 190-200.

19) 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: a molecular dynamics simulation study

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

20) von Herrath, M., Taylor, P.

Immunoinformatics: An overview of computational tools and techniques for understanding the immune response

(2007) *Expert Review of Clinical Immunology*, 3 (6), pp. 993-1002.

ELSEVIER

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