References

[1] World Health Organization, *World malaria report 2021*. Geneva: World Health Organization, 2021. Accessed: Jun. 08, 2022. [Online]. Available: https://www.who.int/publications/i/item/9789240040496

[2] Talapko, Škrlec, Alebić, Jukić, and Včev, "Malaria: The Past and the Present," *Microorganisms*, vol. 7, no. 6, p. 179, Jun. 2019, doi: 10.3390/microorganisms7060179.

[3] E. Nizi *et al.*, "Peptidomimetic nitrile inhibitors of malarial protease falcipain-2 with high selectivity against human cathepsins," *Bioorganic & Medicinal Chemistry Letters*, vol. 28, no. 9, pp. 1540–1544, May 2018, doi: 10.1016/j.bmcl.2018.03.069.

[4] L. N. Alberca, S. R. Chuguransky, C. L. Álvarez, A. Talevi, and E. Salas-Sarduy, "In silico Guided Drug Repurposing: Discovery of New Competitive and Non-competitive Inhibitors of Falcipain-2," *Front. Chem.*, vol. 7, p. 534, Aug. 2019, doi: 10.3389/fchem.2019.00534.

[5] J. B. Ghasemi and F. Shiri, "Molecular docking and 3D-QSAR studies of falcipain inhibitors using CoMFA, CoMSIA, and Open3DQSAR," *Med Chem Res*, vol. 21, no. 10, pp. 2788–2806, Oct. 2012, doi: 10.1007/s00044-011-9803-1.

[6] T. Huang, G. Sun, L. Zhao, N. Zhang, R. Zhong, and Y. Peng, "Quantitative Structure-Activity Relationship (QSAR) Studies on the Toxic Effects of Nitroaromatic Compounds (NACs): A Systematic Review," *IJMS*, vol. 22, no. 16, p. 8557, Aug. 2021, doi: 10.3390/ijms22168557.

[7] Z. Shehu, A. Uzairu, and B. Sagagi, "Quantitative Structure Activity Relationship (QSAR) and Molecular Docking Study of Some Pyrrolones Antimalarial Agents against Plasmodium Falciparum," *Journal of the Turkish Chemical Society, Section A: Chemistry*, pp. 569–584, Mar. 2018, doi: 10.18596/jotcsa.346661.

[8] H. Hadni and M. Elhallaoui, "Molecular docking and QSAR studies for modeling the antimalarial activity of hybrids 4-anilinoquinoline-triazines derivatives with the wild-type and mutant receptor pf-DHFR," *Heliyon*, vol. 5, no. 8, p. e02357, Aug. 2019, doi: 10.1016/j.heliyon.2019.e02357.

[9] I. Kurniawan, M. S. Fareza, and P. Iswanto, "CoMFA, Molecular Docking and Molecular Dynamics Studies on Cycloguanil Analogues as Potent Antimalarial Agents," *Indones. J. Chem.*, vol. 21, no. 1, p. 66, Sep. 2020, doi: 10.22146/ijc.52388.

[10] I. Kurniawan, D. Tarwidi, and Jondri, "QSAR modeling of PTP1B inhibitor by using Genetic algorithm-Neural network methods," *J. Phys.: Conf. Ser.*, vol. 1192, p. 012059, Mar. 2019, doi: 10.1088/1742-6596/1192/1/012059.

[11] I. Kurniawan, M. Rosalinda, and N. Ikhsan, "Implementation of ensemble methods on QSAR Study of NS3 inhibitor activity as anti-dengue agent," *SAR and QSAR in Environmental Research*, vol. 31, no. 6, pp. 477–492, Jun. 2020, doi: 10.1080/1062936X.2020.1773534.

[12] H. F. Azmi, K. M. Lhaksmana, and I. Kurniawan, "QSAR Study of Fusidic Acid Derivative as Anti-Malaria Agents by using Artificial Neural Network-Genetic Algorithm," in *2020 8th International Conference on Information and Communication Technology (ICoICT)*, Yogyakarta, Indonesia, Jun. 2020, pp. 1–4. doi: 10.1109/ICoICT49345.2020.9166158.

[13] F. Rahman, K. M. Lhaksmana, and I. Kurniawan, "Implementation of Simulated Annealing-Support Vector Machine on QSAR Study of Fusidic Acid Derivatives as Anti-Malarial Agent," in *2020 6th International Conference on Interactive Digital Media (ICIDM)*, Bandung, Indonesia, Dec. 2020, pp. 1–4. doi: 10.1109/ICIDM51048.2020.9339632.

[14] I. Kurniawan, R. Wardhani, M. Rosalinda, and N. Ikhsan, "QSAR Study for Prediction of HIV-1 Protease Inhibitor Using the Gravitational Search Algorithm–Neural Network (GSA-NN) Methods," *LKJITI*, vol. 12, no. 2, p. 62, Jul. 2021, doi: 10.24843/LKJITI.2021.v12.i02.p01.

[15] M. Abdullahi, G. A. Shallangwa, and A. Uzairu, "In silico QSAR and molecular docking simulation of some novel aryl sulfonamide derivatives as inhibitors of H5N1 influenza A virus subtype," *Beni-Suef Univ J Basic Appl Sci*, vol. 9, no. 1, p. 2, Dec. 2020, doi: 10.1186/s43088-019-0023-y.

[16] Z. Wu *et al.*, "Do we need different machine learning algorithms for QSAR modeling? A comprehensive assessment of 16 machine learning algorithms on 14 QSAR data sets," *Briefings in Bioinformatics*, vol. 22, no. 4, p. bbaa321, Jul. 2021, doi: 10.1093/bib/bbaa321.

[17] M. Abdel-Basset, L. Abdel-Fatah, and A. K. Sangaiah, "Metaheuristic Algorithms: A Comprehensive Review," in *Computational Intelligence for Multimedia Big Data on the Cloud with Engineering Applications*, Elsevier, 2018, pp. 185–231. doi: 10.1016/B978-0-12-813314-9.00010-4.

[18] S. Mirjalili, "Genetic Algorithm," in *Evolutionary Algorithms and Neural Networks*, vol. 780, Cham: Springer International Publishing, 2019, pp. 43–55. doi: 10.1007/978-3-319-93025-1_4.

[19] A. Shmilovici, "Support Vector Machines," in *Data Mining and Knowledge Discovery Handbook*, O. Maimon and L. Rokach, Eds. Boston, MA: Springer US, 2009, pp. 231–247. doi: 10.1007/978-0-387-09823-4_12.

[20] M. Hussain, S. K. Wajid, A. Elzaart, and M. Berbar, "A Comparison of SVM Kernel Functions for Breast Cancer Detection," in *2011 Eighth International Conference Computer Graphics, Imaging and Visualization*, Singapore, Aug. 2011, pp. 145–150. doi: 10.1109/CGIV.2011.31.

[21] H. Hadni and M. Elhallaoui, "3D-QSAR, docking and ADMET properties of aurone analogues as antimalarial agents," *Heliyon*, vol. 6, no. 4, p. e03580, Apr. 2020, doi: 10.1016/j.heliyon.2020.e03580.

[22] A. Golbraikh and A. Tropsha, "Beware of q2!," *Journal of Molecular Graphics and Modelling*, vol. 20, no. 4, pp. 269–276, Jan. 2002, doi: 10.1016/S1093-3263(01)00123-1.

[23] P. K. Ojha, I. Mitra, R. N. Das, and K. Roy, "Further exploring rm2 metrics for validation of QSPR models," *Chemometrics and Intelligent Laboratory Systems*, vol. 107, no. 1, pp. 194–205, May 2011, doi: 10.1016/j.chemolab.2011.03.011.