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- Anonim, 2021, *World malaria report 2021*.
- Anonim, 2020, *CDC's malaria program*.
- Belete, T.M., 2020, Recent progress in the development of new antimalarial drugs with novel targets, *Drug Des. Devel. Ther.*, 14, 3875–3889.
- Bilginer, S., Gul, H.I., Mete, E., Das, U., Sakagami, H., Umemura, N., and Dimmock, J.R., 2013, 1-(3-Aminomethyl-4-hydroxyphenyl)-3-pyridinyl-2-propen-1-ones: A novel group of tumour-selective cytotoxins, *Enzyme Inhib.*, 28(5), 974-980.
- Chakraborty, S., Alam, B., and Biswas, S., 2022, New insights of falcipain 2 structure from *Plasmodium falciparum* 3D7 strain, *Biochem. Biophys. Res. Commun.* 590, 145-151.
- Christensen, A.S., Kubar, T., Cui, Q., and Elstner, M., 2016 Semiempirical quantum mechanical methods for noncovalent interactions for chemical and biochemical applications, *Chem. Rev.*, 116(9), 5301-5337.
- Conrad, M.D., and Rosenthal, P.J., 2019, Antimalarial drug resistance in Africa: the calm before the storm?, *Lancet Infect. Dis.*, 19(10), 1-14.
- Daina, A., Michielin, O., and Zoete, V., 2017, SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules, *Sci. Rep.*, 7(1), 1-13.
- Das, M., and Manna, K., 2016, Chalcone scaffold in anticancer armamentarium: A molecular insight, *J. Toxicol.*, 2016(1), 1-14.
- Elkhalifa, D., Al-Hashimi, I., Moustafa, A.A., and Khalil, A., 2020, A comprehensive review on the antiviral activities of chalcones, *J. Drug Target.*, 29(4), 403-419.
- Ettari, R., Bova, F., Zappalà, M., Grasso, S., and Micale, N., 2009, Falcipain-2 inhibitors, *Med. Res. Rev.*, 30(1), 136-167.
- Ferreira, L.G., dos Santos, R. N., Oliva, G., and Andricopula, A.D., 2015, Molecular docking and structure-based drug design strategies, *Molecules*, 20(7), 13384-13421.
- Finch, A. and Pillans, P., 2014, P-glycoprotein and its role in drug-drug interactions, *Aust. Perscr.*, 37, 137-139.
- Flannery, L., Chatterjee, K., and Winzeler, A., 2013, Antimalarial drug discovery — approaches and progress towards new medicines, *Nat. Rev. Microbiol.*, 11(12), 849-862.

- Goldberg, D.E., 2005, Hemoglobin degradation, *Curr. Top. Microbiol. Immunol.* 295, 275-291.
- Guo, L., Yan, Z., Zheng, X., Hu, L., Yang, Y., and Wang, J., 2014, A comparison of various optimization algorithms of protein–ligand docking programs by fitness accuracy, *J. Mol. Model.*, 20(7), 2251-2261.
- Hogg, T., Nagarajan, K., Herzberg, S., Chen, L., Shen, X., Jiang, H., Wecke, M., Blohmke, C., Hilgenfeld, R., and Schmidt, C.L., 2006, Structural and functional characterization of falcipain-2, a hemoglobinase from the malarial parasite *Plasmodium falciparum*, *J. Biol. Chem.*, 281(35), 25425–25437.
- Husch, T., and Reiher, M., 2018, Comprehensive analysis of the neglect of diatomic differential overlap approximation, *J. Chem. Theory Comput.*, 14, 5169-5179.
- Huzinaga, S., 1985, Basis set for molecular calculations, *Comp. Phys. Rep.*, 279-340.
- Kerr, I.D., Lee, J.H., Pandey, K.C., Harrison, A., Sajid, M., Rosenthal, P.J., and Brinen, L.S., 2009, Structures of falcipain-2 and falcipain-3 found to small molecule inhibitors: implications for substrate specificity, *J. Med. Chem.*, 52(3), 852–857.
- Lipinski, C. A., Lombardo, F., Dominy, B. W., and Feeney, P. J., 2001, Experimental and computational approaches to estimate solubility and permeability in drug discovery and development settings, *Adv. Drug Delivery Reviews* 23 (1997) 3–25. 1. *Adv. Drug Deliv. Rev.* 46(1), 3–26
- Mahapatra, D. K., Bharti, S. K., and Asati, V., 2015, Chalcone scaffolds as anti-infective agents: structural and molecular target perspectives, *Eur. J. Med. Chem.*, 101, 496–524.
- Maier, A.G., Matuschewski, K., Zhang, M., and Rug, M., 2019, *Plasmodium falciparum*, *Trends Parasitol.*, 481-482.
- McDonnell, A.M. and Dang, C.H., 2013, Basic review of the cytochrome P450 system, *J. Adv. Pract. Oncol.* 4(4); 263-268.
- McMurry, J., 2008, *Organic Chemistry*, Thomson Brooks/Cole, Belmont.
- Mendenhall, W. M. dan Sincich, T.L., 2016, *Statistics for engineering and the sciences, sixth edition*, CRC Press, Boca Raton.
- Meng, X., Zhang, H., Mezei, M., and Cui, M., 2011, Molecular docking: A powerful approach for structure-based drug discovery, *Curr. Comput. Aided Drug Des.*, 7(2), 146-157.
- Milner, D.A., 2018, Malaria pathogenesis, *Cold Spring Harb. Perspect.*, 8(1), 1-12.

- Morris, G. M., Goodsell, D. S., Halliday, R. S., Huey, R., Hart, W. E., Belew, R. K., and Olson, A. J., 1998, Automated docking using a Lamarckian genetic algorithm and an empirical binding free energy function, *J. Comput. Chem.*, 19(14), 1639–1662.
- Morris, G., and Lim-Wibbly, M., 2008, *Molecular docking*, in Kukol, A. (ed), *Molecular modeling of proteins*, Humana Press, Totowa
- Morris, G. M., Huey, R., Lindstrom, W., Sanner, M. F., Belew, R. K., Goodsell, D. S., and Olson, A. J., 2009, AutoDock4 and AutoDockTools4: Automated docking with selective receptor flexibility, *J. Comput. Chem.*, 30(16), 2785–2791.
- Nagy, B., and Jensen, F., 2017, *Basis sets in quantum chemistry*. in Parrill, A.L., and Lipkowitz, K.B. (eds), *Reviews in computational chemistry*, Springer, Berlin.
- Pantsar, T. and Poso, A., 2018, Binding affinity via docking: fact and fiction, *Molecules*, 23(8): 1899.
- Patrick, G.L., 2020, *Antimalarial agents*, Elsevier, Amsterdam.
- Pinzi, L. dan Rastelli, G., 2019, Molecular docking: shifting paradigms in drug discovery, *Int. J. Mol. Sci.*, 20(18): 4331.
- Plowe, C.V., 2022, Malaria chemoprevention and drug resistance: a review of the literature and policy implications, *Malar. J.*, 21(1), 1-25.
- Rawat, A., Roy, M., Jyoti, A., Kaushik, S., Verma, K., and Srivastava, V. K., 2021, Cysteine proteases: Battling pathogenic parasitic protozoans with omnipresent enzymes. *Microbiol. Res.*, 249, 126784.
- Rimola, A., Ferrero, S., Germain, A., Corno, M., and Ugliengo, P., 2020, Computational surface modelling of ices and minerals of interstellar interest—insights and perspectives, *Minerals*, 11(1), 26.
- Rosenthal, P.J., 2020, Falcipain cysteine proteases of malaria parasites: An update, *Biochim. Biophys. Acta Proteins Proteom.*, 1868(10), 140475.
- Roy, K.K., 2017, Targeting the active sites of malarial proteases for antimalarial drug discovery: approaches, progress and challenges, *Int. J. Antimicrob. Agents*, 50(3), 287-302.
- Sabnis, Y.A., Desai, P.V., Rosenthal, P.J., and Avery, M.A., 2003, Probing the structure of falcipain-3, a cysteine protease from *Plasmodium falciparum*: Comparative protein modeling and docking studies, *Protein. Sci.*, 12(3): 501-509.

- Sahu, N.K., and Bari, S.B., 2011, Molecular modeling studies of some substituted chalcone derivatives as cysteine protease inhibitors, *Med. Chem. Res*, 21(11), 3835–3847.
- Sato, S., 2021, Plasmodium—a brief introduction to the parasites causing human malaria and their basic biology, *J. Physiol. Anthropol.*, 40(1), 1-13
- Sethi, A., Joshi, K., Sasikala, K., and Alvala, M., 2019, *Molecular docking in modern drug discovery: Principles and recent applications*, in Gaitonde, V., Karmakar, P., and Trivedi, A. (ed), *Drug discovery and development - new advances*, IntechOpen, London
- Shih, T., Liu, M., Li, C., and Kuo, C., 2018, Halo-substituted chalcones and azachalcones-inhibited, lipopolysaccharide-stimulated, pro-inflammatory responses through the TLR4-mediated pathway, *Molecule*, 23(3), 597-612
- Slater, A.F.G., 1993, Chloroquine: Mechanism of drug action and resistance in *Plasmodium falciparum*, *Pharmac. Ther.*, 57, 203-235.
- Smith, J. D., Rowe, J. A., Higgins, M. K., and Lavstsen, T., 2013, Malaria's deadly grip: cytoadhesion of *Plasmodium falciparum*-infected erythrocytes, *Cell. Microbiol.*, 15(12), 1976–1983.
- Teixeira, C., Gomes, J.R., and Gomes, P., 2011, Falcipains, *Plasmodium falciparum* cysteine proteases as key drug targets against malaria, *Curr. Med. Chem.*, 18(10), 1555–1572.
- Tekale, S., Mashele, S., Pooe, O., Thore, S., Kendrekar, P., and Pawar, R., 2020, *Biological role of chalcones in medicinal chemistry*. in Claborn, D., Bhattacharya, S., and Roy, S., *Vector-Borne diseases - recent developments in epidemiology and control*, IntechOpen, London
- Tse, E.G., Korsik, M., and Todd, M.H., 2019, The past, present and future of anti-malarial medicines, *Malar. J.*, 18(1), 1-21
- Turowska-Tyrk, I., Grzesniak, K., Trzop, E., and Zych, T., 2003, Monitoring structural transformation in crystals. Part 4. Monitoring structural changes in crystals of pyridine analogs of chalcone during [2+2] photodimerization and possibilities of the reaction in hydroxy derivatives. *J. Solid State Chem.*, 174(2), 459-465.
- Veber, D. F., Johnson, S. R., Cheng, H.Y., Smith, B. R., Ward, K. W., and Kopple, K. D., 2002, Molecular Properties That Influence the Oral Bioavailability of Drug Candidates, *J. Med. Chem.*, 45(12), 2615–2623.
- Wong, K. M., Tai, H. K., and Siu, S. W. I., 2020, GWOVina: A grey wolf optimization approach to rigid and flexible receptor docking. *Chem. Biol. Drug Des.*, 1-14

- Zhu, L., van der Pluijm, R., Kucharski, M., Nayak, S., Tripathi, J., White, N.J., Day, N.P.J., Faiz, A., Phyto, A.P., Amaratunga, C., Lek, D., Ashley, E.A., Nosten, F., Smithuis, F., Ginsburg, H., von Seidlein, L., Lin, K., Imwong, M., Chotivanich, K., Mayxay, M., Dhorda, M., Nguyen, H.C., Nguyen, T.N.T., Olivo Miotto, Newton, P.N., Jittamala, P., Tripura, R., Pukrittayakamee, S., Thomas J. Peto, T.J., Hien, T.T., Dondorp, A.M., and Bozdech, Z., 2022, Artemisinin resistance in the malaria parasite, *Plasmodium falciparum*, originates from its initial transcriptional response, *Commun. Biol.*, 5(274), 1-13.
- Zhuang, C., Zhang, W., Sheng, C., Zhang, W., Xing, C., and Miao, Z., 2017, Chalcone: A privileged structure in medicinal chemistry, *Chem. Rev.*, 117(12), 7762–7810.