

DAFTAR PUSTAKA

- Alder, B.J., Wainwright, T.E., 1957, Phase Transition for a Hard Sphere System, *J. Chem. Phys.*, 27, 1208-1209.
- Alker, A.P., Lim, P., Sem, R., Shah, N.K., Yi, P., Bouth, D.M., Tsuyuoka, R., Maguire, J.D., Fandeur, T., Arie, F., Wongsrichanalai, C., Meshnick, S.R., 2007, Pfm-dr1 and in vivo Resistance to Artesunate-Mefloquine in falciparum Malaria on The Cambodian Thai Border, *Am. J. Trop. Med. Hyg.*, 76, 641-647.
- Allen, M. P., and Tildesley, D. J., 1987, *Computer Simulation of Liquids*, Oxford University Press.
- Alonso, H., Andrey, A. B., and Jill, E. G., 2006, Combining *Docking* and Molecular Dynamic Simulations in Drug Design, *Wiley InterScience*, 26 (5), 531-568.
- Anderson LA, Harris A and Phillipson JD (1983) Production of Cytotoxic Canthin-6-one Alkaloids by *Ailanthus Altissima*. *Plant Cell Cultures. J. Nat. Products*, 46(3), 374-378.
- Angelina, M., Indah, D. D., Banjarnahor, S. D. S., Megawati, Tri, Y., Acute Toxicity of *Brucea javanica* Merrill Leaves Extract on Mice, *J. Trop. Life Science*, 2 (2), 10-15.
- Anonim, 2014, *WHO Malaria Report 2014, WHO Global Malaria Programme*, WHO Press, Switzerland.
- Arnou, B., Mongtigny, C., Morth, J.P., Nissen, P., Jaxel, C., Moller, J.V., Le Maire, M., 2011, The *Plasmodium falciparum* Ca²⁺ ATPase PfATP6: Intensive to Artemisinin, but A Potential Drug Target, *Biochem. Soc. Trans.*, 39, 823-831.
- Becker, O. M., MacKerell, A. D., Roux, B., and Watanabe, M., 2001, *Computational Biochemistry and Biophysics*, MerceL Dekker, Inc., New York.
- Bentum, K.B., Ayi, I., Suzuku, T., Otchere, J., Kumagai, T., Anyan, W.K., et al, 2011, *Plasmodium falciparum* Isolates from Southern Ghana Exhibit Polymorphisms in The SERCA Type PfATPase Though Sensitive to Artesunate in Vitro, *Malar. J.*, 10 (1), 187-190.
- Buehler, M.J., 2008, *Atomistic Modeling of Materials Failure*, Springer, New York.

- Buehler, M.J., Ackbarow, T., 2007, Fracture Mechanics of Protein Materials, *Materials Today*, 10, 46-58.
- Büyüköztürk, O., Markus, J.B., Denvid, L., Chakrapan, T., 2011, Structural Solution Using Molecular Dynamics: Fundamental and a Case Study of Epoxy-Silica Interface, *Internasional Journal of Solid and Structures*, 48, 2131-2140.
- Cox-Singh, J., Timothy, M.E.D., Kim, S.L., Sunita, S.G.S., Asmad, M., Shanmuga, R., Hasan, A.R., David, J.C., Balbir, S., 2008, *Plasmodium knowlesi* Malaria in Humans is Widely Distributed and Potentially Life Threatening, *Clin Infect Dis.*, 46 (2), 165-171.
- Elyzaar, I.R.F., Hay, S.I., and Baird, J.K., 2011, Malaria Distribution, Prevalence, Drug Resistance and Control in Indonesia, *Adv. Parasitol.*, 74 (41), 170-175.
- Foloppe, N., and Hubbard, R., 2006, Towards Predictive Ligand Design with Free Energy Based Computational Methods, *Curr. Med. Chem.*, 13, 3583-3608.
- Gardner, M.J., Hall, N., Fung, E., White, O., Berriman, M., Hyman, R.W., et.al., 2002, Genome Sequence of The Human Malaria Parasite *Plasmodium falciparum*, *Malar. J.*, 419 (6906), 498-511.
- Gillin, F.D., Reiner D.S., and Suffness, M., 1982, Bruseantin, a Potent Amoebicide from a Plant, *Brucea antidysenterica*, *Antimicrobial Agents and Chemotherapy*, 22 (2), 342-345.
- Gohlke, H., Kiel, C., Case, D. A., 2003, Insights into Protein – Protein Binding by Binding Free Energy Calculation and Free Energy Decomposition for the Ras – Raf and Ras – RalGDS Complexes, *J. Mol. Biol.*, 330, 891-913.
- Grallier, P., Deregnacourt, C., Florent, I., 2012, Advances in Antimalarial Drug Evaluation and New Targets for Antimalarials, *Malaria Parasites*, 321-350.
- Grimberg, B.T., Mehlotra, R.K., 2011, Expanding The Antimalarial Drug Arsenal, *Pharmaceuticals*, 4, 681-712.
- Hartshorn, M.J., Verdonk, M.L., Chessari, G., Brewerton, S.C.W., Mooij, T. M., Mortenson, P. N., and Murray, C. W., 2007, High Quality Test Set for The Validation of Protein-Ligand Docking Performance, *J. Med. Chem.*, 50, 726-741.
- Huang, S.Y., and Zou, X., 2010, Advances and Challenges in Protein-Ligand Docking, *Int. J. Mol. Sci.*, 11, 3016-3034.

- Huang, S.Y., and Grinter, S.Z., 2010, Scoring Functions and Their Evaluation Methods for Protein-Ligand Docking: Recent Advances and Future Directions, *Phys. Chem. Chem. Phys.*, 12, 12899-12908.
- Jelinek, T., Gabriele, P.H., Nikolai, M., Ole, W., Michael, W., Nadja, S., Martin, P.G., Frank, V.S., Joaquim, G., Hermann, L., Christoph, H., Michael, A., Gerd, B., Paul, M., Marco, S., Herwig, K., Saraiva, C., Jiri, B., Peter, K., Ida, G., and Juan, C., 2002, Molecular Surveillance of Drug Resistance Through Imported Isolates of *Plasmodium falciparum* in Europe, *Malar. J.*, 1, 11.
- Kaur, K., Jain, M., Kaur, T., and Jain, R., 2009, Antimalarials from Nature, *J. Bioorg. Med. Chem.*, 02, 50.
- Kimura, M., Yamaguchi, Y., Takada, S., Tanabe, K., 1993, Cloning of a Ca^{2+} -ATPase gene of *Plasmodium falciparum* and comparison with vertebrate Ca^{2+} -ATPases, *J. Cell Biol.*, 104, 1129–1136.
- Krishna, S., Møller, J.V., le Maire, M. and Jaxel, C., 2010, Purified E255L Mutant SERCA1a and Purified PfATP6 are Sensitive to SERCA Type Inhibitors but Insensitive to Artemisinins, *J. Biol. Chem.*, 285, 26406–26416.
- Kyle, R.A., Shampe, M.A., 1974, Discoverers of Quinine, *JAMA*, 229, 462.
- Ludwig, E.U., Webb, R.J., van Goethem, I.D.A., East, J.M., Lee, A.G., Kimura, M., O'Neill, P.M., Bray, P.G., Ward, S.A., and Krishna, S., Artemisinins Target the SERCA of *Plasmodium falciparum*, *Nature*, 424, UK.
- Mark, P., and Nilsson, L., 2001, Structure and Dynamics of TIP3P, SPC, and SPC/E, Water Models at 298 K, *J. Phys. Chem. A.*, 105, 9954-9960.
- Meller, J., 2001, *Molecular Dynamics, Encyclopedia of Life Sciences*, Cornell University Press, New York.
- Meng, X.Y., Zhang, H.X., Mezei, M., and Cui, M., 2011, Molecular Docking : A Powerful Approach for Structure Based Drug Discovery, *Curr. Comput. Aided Drug Des.*, 7, 146-157.
- Moncoq, K., Trieber, C. A., Young, H. S., 2007, The Molecular Basis for Cyclopiazonic Acid Inhibition of the Sarcoplasmic Reticulum Calcium Pump, *J. Biol. Chem.*, 282, 9748-9757.
- Muhammad, I., Samoylenko, V., 2007, Antimalarial Quassinoids: Past, Present and Future, *Expert Opin. Drug Discov.*, 2 (8), 1-20.
- Nurbaiti, S., 2009, Stabilitas Termal dan Pergerakan Dinamis Klenow-Like DNA Polimerase I ITB-1 Berdasarkan Simulasi Dinamika Molekul, *Disertasi Program Studi Kimia Institut Teknologi Bandung, Bandung*.

- Pan, L., Young, W. C., Hee, B. C., Tran, N. N., Djaja, D. D. S., and Douglas, K., 2009, Bioactivity Guided Isolation of Cytotoxic Constituents of *Brucea javanica* Collected in Vietnam, *Bioorg. Med. Chem.*, 17 (6), 2219-2224.
- Pranowo, H. D., dan Hetadi, A. K. R., 2010, *Pengantar Kimia Komputasi*, Lubuk Agung, Bandung.
- Rajabpour, A., Akizi, F.Y., Heyhat, M.M., and Gordiz, K., 2013, Molecular Dynamics Simulation of The Specific Heat Capacity of Water-Cu Nanofluids, *International Nano Letters*, 3, 58.
- Saxena, S., Neerja, P., Jain, D. C., and Bhakuni, S., 2003, Antimalarial Agents from Plants Sources, *Current Science*, 85 (9), 1314-1329.
- Sharma, N.K., Jha, K.K., Priyanka, 2010, Molecular Docking: Anoverview, *J. Adv. Sci. Res.*, 1, 67-72.
- Shen, J., Wenqian, Z., Hong, F., Roger, P., Weida, T., Huixiao, H., 2013, Homology Modeling, Molecular Docking, and Molecular Dynamics Simulations Elucidated α -Fetoprotein Binding Modes, *BMC Bioinformatics*, 14 (2), 57-70.
- Sousa, S.F., Fernandes, P.A., and Ramos, M.J., 2006, Protein-Ligand Docking: Current Status and Future Challenges, *Proteins Struct. Funct. Bioinform.*, 65, 15-26.
- Syamsudin, 2008, Penapisan Senyawa Antimalaria yang Berasal dari Tumbuhan, *Jurnal Ilmu Kefarmasian Indonesia*, 6 (2), 95-99.
- Tu, Y., 2011, The Discovery of Artemisinin (Qinghaosu) and Gifts from Chinese Medicine, *Nat. Med.*, 17, 1217-1220.
- Uline, M. J., and Corti, D. S., 2013, Molecular Dynamics at Constant Pressure: Allowing the System to Control Volume Fluctuations via a Shell Particle, *Entropy*, 15, 3941-3969.
- White, N.J., 2008, Plasmodium knowlesi: The Fifth Human Malaria Parasite, *Clin. Infect. Dis.*, 46, 172-173.
- Winger, M., Daniel, T., Riccardo, B., and Wilfred, F. G., 2009, *On Using a Too Large Integration Time Step in Molecular Dynamics Simulations of Coarse-Grained Molecular Models*, ETH, Switzerland.
- Yuriev, E., Agostino, M., and Ramsland, P.A., 2011, Challenges and Advances in Computational Docking 2009 in Review, *J. Mol. Recognit*, 24, 149-164.