

DAFTAR PUSTAKA

- Akamatsu, M., 2011, Importance of Physicochemical Properties for the Design of New Pesticides, *J. Agric. Food Chem.*, 59, 2909–2917.
- Asmara, A.P., Mudasir, dan Siswanta, D., 2012, Studi QSAR Senyawa Turunan Triazolopiperazin Amida Sebagai Inhibitor Enzim Dipeptidil Peptidase-IV (DPP IV) Menggunakan Metode Semiempirik AM1, *Berkala MIPA*, 23 (3), 288-296.
- Cramer, C.J., 2004, *Essentials of Computational Chemistry: Theories and Models*, Second Edition, John Wiley & Sons Ltd., New York.
- Fang, J., Huang, D., Zhao, W., Ge, H., Luo, H., dan Xu, J., 2011, A New Protocol for Predicting Novel GSK-3 β ATP Competitive Inhibitors, *J. Chem. Inf. Model.*, 51, 1431–1438.
- Geidl, S., Bouchal, T., Raček, T., Vařeková, R.S., Hejret, V., Křenek, A., Abagyan, R., dan Koča, J., 2015, High-Quality and Universal Empirical Atomic Charges for Chemoinformatics Applications, *J. Cheminform*, 7 (59), 1-10.
- Golbraikh, A. dan Tropsha, A., 2000, Predictive QSAR Modeling Based on Diversity Sampling of Experimental Datasets for the Training and Test Set Selection, *Mol. Divers.*, 5, 231–243.
- Grewal, B.K. dan Sobhia, M.E., 2012, Theoretical Investigation on Maleimide and its Indolyl Derivatives: Rational Drug Design Approach for PKC β II Inhibitors, *J. Mol. Struct.*, 1029, 35–44.
- Han, X., Zhu, X., Zhu, S., Wei, L., Hong, Z., Guo, L., Chen, H., Chi, B., Liu, Y., Feng, L., Ren, Y., dan Wan, J., 2016, A Rational Design, Synthesis, Biological Evaluation and Structure–Activity Relationship Study of Novel Inhibitors against Cyanobacterial Fructose-1,6-bisphosphate Aldolase, *J. Chem. Inf. Model.*, 56, 73–81.
- Huang, H., Xiao, X., Lin, F., Grossart, H., Nie, Z., Sun, L., Xu, C., dan Shi, J., 2016, Continuous-Release Beads of Natural Allelochemical for the Long-Term Control of Cyanobacterial Growth: Preparation, Release Dynamics and Inhibitory Effects, *Water Res.*, 95, 113-123.
- Ionescu, C., Geidl, S., Vařeková, R.S., dan Koča, J., 2013, Rapid Calculation of Accurate Atomic Charges for Proteins via the Electronegativity Equalization Method, *J. Chem. Inf. Model.*, 53, 2548–2558.
- Kubinyi, H., 1993, *QSAR: Hansch Analysis and Related Approaches*, VCH Verlagsgesellschaft, Weinheim.

- Leach, A.R., 2001, *Molecular Modelling: Principle and Application 2nd ed.*, Longman, Singapura.
- Liu, P. dan Long, W., 2009, Current Mathematical Methods Used in QSAR /QSPR Studies, *Int. J. Mol. Sci.*, 10, 1978–1998.
- Mankiewicz-Boczek, J., Karwaciak, I., Ratajewski, M., Gagala, I., Jurczak, T., Zalewski, M., dan Pulaski, L., 2015, Application of Cellular Biosensor for Detection of Atypical Toxic Bioactivity in Microcytin-Containing Cyanobacterial Extracts, *Aquat. Toxicol.*, 168, 1-10.
- Mazzatorta, P., Smiesko, M., Piparo, E.L., dan Benfenati, E., 2005, QSAR Model for Predicting Pesticide Aquatic Toxicity, *J. Chem. Inf. Model.*, 45, 1767-1774.
- Menegon, G., Shimizu, K., Farah, J.P.S., Dias, L.G., dan Chaimovich, H., 2002, Parameterization of the Electronegativity Equalization Method Based on the Charge Model 1, *Phys. Chem. Chem. Phys.*, 4, 5933–5936.
- Mishra, M., Mishra, V.K., Senger, P., Pathak, A.K., dan Kashaw, S.K., 2014, Exploring QSAR Studies on 4-Substituted Quinazoline Derivatives as Antimalarial Compounds for the Development of Predictive Models, *Med. Chem. Res.*, 23, 1397–1405.
- Motta, L.F. dan Almeida, W.P., 2011, Quantitative Structure-Activity Relationships (QSAR) of a Series of Ketone Derivatives as Anti-Candida Albicans, *Int. J. Drug Discov.*, 3 (2), 100–117.
- Muranaka, K., 2001, Anticancer Activity of Estradiol Derivatives: A Quantitative Structure-Activity Relationship Approach, *Asian J. Chem.*, 78, 1390–1393.
- Pranowo, H.D. dan Hetadi, A.K.R., 2011, *Pengantar Kimia Komputasi*, Lubuk Agung, Bandung.
- Rajneesh, Singh, S.P., Pathaka, J., dan Sinhaa, R.P., 2017, Cyanobacterial Factories for the Production of Green Energy and Value-Added Products: An Integrated Approach for Economic Viability, *Renew. Sustain. Energy Rev.*, 69, 578–595.
- Saavedra, L.M., Romanelli, G.P., Rozo, C.E, dan Duchowicz, P.R., 2018, The Quantitative Structure-Insecticidal Activity Relationships from Plant Derived Compounds against Chikungunya and Zika *Aedes aegypti* (Diptera: Culicidae) Vector, *Sci. Total Environ.*, 610–611, 937–943.
- Sardjoko, 1993, *Rancangan Obat*, Gadjah Mada University Press, Yogyakarta.

- Vařeková, R.S., Jiroušková, Z., Vaněk, J., Suchomel, Š., dan Koča, J., 2007, Electronegativity Equalization Method: Parameterization and Validation for Large Sets of Organic, Organohalogen and Organometal Molecule, *Int. J. Mol. Sci.*, 8, 572-582.
- Verma, R.P. dan Hansch, C., 2009, Camphothecins: A SAR/QSAR Study, *Chem. Rev.*, 109(1), 213-235.
- Wu, J., Wang, Y., dan Shen, Y., 2014, Molecular Docking and QSAR Analysis on Maleimide Derivatives Selective Inhibition against Human Monoglyceride Lipase Based on Various Modeling Methods and Conformations, *Chemom. Intell. Lab. Syst.*, 131, 22–30.
- Xiong, W., Tang, Y., Shao, C., Zhao, Y., Jin, B., Huang, T., Miao, Y., Shu, L., Ma, W., Xu, X., dan Tang, R., 2017, Prevention of Cyanobacterial Blooms Using Nanosilica: A Biomineralization-Inspired Strategy, *Environ. Sci. Technol.*, 51, 12717–12726.
- Young, D.C., 2001, *Computational Chemistry: A Practical Guide for Applying Technique to Real-World Problems*, John Wiley and Sons Inc., New York.
- Yousefinejad, S. dan Hemmateenejad, B., 2015, Chemometrics and Intelligent Laboratory Systems Chemometrics Tools in QSAR / QSPR Studies: A Historical Perspective, *Chemom. Intell. Lab. Syst.*, 149, 177–204.
- Zegura, B., Straser, A., dan Filipic, M., 2011, Genotoxicity and Potential Carcinogenicity of Cyanobacterial Toxins - a Review, *Mutat. Res.*, 727, 16-41.
- Živković, J.V., Trutić, N.V., Veselinović, J.B., Nikolić, G.M., dan Veselinović, A.M., 2015, Monte Carlo method Based QSAR Modeling Of Maleimide Derivatives as Glycogen Synthase Kinase-3 β Inhibitors, *Comput. Biol. Med.*, 64, 276–282.