

DAFTAR PUSTAKA

- Abdel-Ilah, L., Veljović, E., Gurbeta, L., and Badnjević, A., 2017, Applications of QSAR Study in Drug Design, *IJERT*, 6(6), 582-587.
- Aisyarahma, S., 2018, Penggunaan Deskriptor Muatan Bersih Atom Hasil Perhitungan Metode Penyetaraan Elektronegativitas pada Analisis Hubungan Kuantitatif Struktur-Aktivitas Senyawa *Anticyanobacteria* Turunan Maleimida, *Skripsi*, Jurusan Kimia Fakultas Ilmu Pengetahuan Alam Universitas Gadjah Mada, Yogyakarta.
- Alfarouk, K.O., Shayoub, M.E., Muddathir, A.K., Elhassan, G.O., and Bashir, A.H., 2011, Evolution of Tumor Metabolism Might Reflect Carcinogenesis as Reverse Evolution Process (Dismantling of Multicellularity), *Cancers*, 3(3), 3002–3017.
- Alfarouk, K.O., Verduzco, D., Rauch, C., Muddathir, A.K., Adil, H.H., Elhassan, G.O., Ibrahim, M.E., David, J., Cardone, R.A., Reshkin, S.J., and Harguindey, S., 2014, Glycolysis, Tumor Metabolism, Cancer Growth and Dissemination. A New pH-Based Etiopathogenic Perspective and Therapeutic Approach to An Old Cancer Question, *Oncoscience*, 1(12), 777–802.
- Amanatie, Jumina, Mustofa, Hanafi, M., and Armunanto, R., 2010, QSAR Study of Xanthone Derivatives as Anti Plasmodial Agents, *Indo. J. Chem*, 10(3), 357-362.
- Armunanto, R., and Sudiono, S., 2004, Relation of Electronic Structures with Their Antimalarial Activities on Artemisinin Derivatives, *Indo. J. Chem.*, 4, 212- 217.
- Cancer Research UK, 2017, *General Cancer Information*, www.cancerresearchuk.org.
- Chaneton, B., and Gottlieb, E., 2012, PGAMgnam Style: A Glycolytic Switch Controls Biosynthesis, *Cancer Cell.*, 565-566.
- Cox, David, L., Nelson, Michael, M., 2005, *Lehninger Principles of Biochemistry*, 4th ed., W.H. Freeman, New York.
- Datar, P.A., Aher, S.B., Washimkar, M.H., and Auti, P.B., 2012, 2D QSAR of Novel 1,4-Dihydropyridine Derivative Blocking N-Type Calcium Channels, *J. Chem. Pharm. Res.*, 4(2), 1117-1122.

- Doichinova, I.A., Natcheva, R.N., and Mihailova, D.N., 1994, QSAR Studies of 8-Substituted Xanthines as Adenosine Receptor Antagonists, *Eur. J. Med. Chem.*, 29(2), 133-138.
- Durany, N., Joseph, J., Jimenez, O.M., Climent, F., Fernández, P.L., Rivera, F., and Carreras, J., 2000, Phosphoglycerate Mutase, 2, 3-Bisphosphoglycerate Phosphatase, Creatine Kinase and Enolase Activity and Isoenzymes in Breast Carcinoma. *Br. J. Cancer.*, 82, 20–27.
- El-Seedi, H.R., El-Barbary, M.A., El-Ghorab, D.M.H., Bohlin, L., Anna-Karin Borg-Karlson, Goransson, U., and Verpoorte, R., 2010 Recent Insights into the Biosynthesis and Biological Activities of Natural Xanthenes, *Curr. Med. Chem.*, 9(17), 854 – 901.
- Evans, M.J., Saghatelian, A., Sorensen, E.J., and Cravatt, B.F., 2005, Target discovery in small-molecule cell-based screens by in situ proteome reactivity profiling, *Nature Biotechnol.*, 23(10), 1303-1307.
- Ferreira, M.M.C., 2002, Multivariate QSAR, *J. Braz. Chem. Soc.*, 13(6), 742-753.
- Geidl, S., Bouchal, T., Raček, T., Vařeková, R.S., Hejret, V., Křenek, A., Abagyan, R., and Koča, J., 2015, High - Quality and Universal Empirical Atomic Charges for Chemoinformatics Applications, *J. Cheminform.*, 7 (59), 1-10.
- Hartono, 2011, *SPSS 16.0 : Analisis Data Statistika dan Penelitian*, Pustaka Pelajar, Yogyakarta.
- Hitosugi, T., Zhou, L., Elf, S., Fan, J., Kang, H., Seo, J.H., Shan, C., Dai, Q., Zhang, L., Xie, J., Gu, T., Jin, P., Alčević, M., LeRoy, G., Kang, Y., Sudderth, J.A., DeBerardinis, R.J., Luan, C., Chen, G.Z., Muller, S., Shin, D.M., Owonikoko, T.K., Lonial, S., Arellano, M.L., Khoury, H.J., Khuri, F.R., Lee, B.H., Ye, K., Boggon, T.J., Kang, K., He, C., and Chen, J., 2012, Phosphoglycerate Mutase 1 Coordinates Glycolysis and Biosynthesis to Promote Tumor Growth, *Cancer Cell*, 22, 585–600.
- Ionescu, C., Sehnal, D., Falginella, F.L., Pant, P., Pravda, L., Bouchal, T., Vařeková, R.S., Geidl, S., and Koča, J., 2015, AtomicChargeCalculator: Interactive Web-Based Calculation of Atomic Charges in Large Biomolecular Complexes and Drug-Like Molecules, *J. Cheminform.*, 7(50), 1-13.
- Iswanto, P., Chasani, M., Harjono, Tahir, I., Hanafi, M., and Delsy, E.V.Y., 2011, Novel Design of Calanone Derivatives as Anti-Leukimia Compounds Based on Quantitative Structure-Activity Relationship Analysis, *Indo. J. Chem.*, 11(1), 31-36.

- Johnson, R.A., and Wichern, D.W., 1992, *Applied Multivariate Statistical Analysis*, 18th ed., Prentice Hall, New Jersey.
- Kapetanovic I.M., 2011, *Drug Discovery and Development - Present and Future*, IntechOpen, USA.
- Khan, N., Afaq, F., Saleem, M., Ahmad, N., and Mukhtar, H., 2006, Targeting Multiple Signaling Pathways by Green Tea Polyphenol (-)-Epigallocatechin-3-Gallate, *Cancer Res.*, 66(5), 2500–2505.
- Kokpol, S.K., Hannongboa, S.V., Thongrit, N., Polman, S., Rode, B.,M.,and Schwendinger, M.G., 1988, Analysis of Structur Activity Relation for Primaquine Antimalarial Drugs by Quantum Pharmacological Approach, *Anal. Sci.*, 4, 565-568.
- Kolossov, E., and Stanforth, R., 2007, SAR and QSAR, *Environ. Res.*, 18, 89-100.
- Kruse, H., Goerigk, L., and Grimme, S., 2012, Why the Standar B3LYP/6-31* Model Chemistry Should Not Be Used in DFT Calculations of Molecular Thermochemistry: Understanding and Correcting the Problems, *J. Org. Chem.*, 77(23), 10824-10834.
- Kubinyi, H., 1993, *HKSA: Hansch Analysis and Related Approachs*, VCH Verlagsgesellschaft, Weinheim.
- Leach, A.R., 2001, *Molecular Modelling: Principle and Application*, 2nd ed., Longman, Singapura.
- Li, C., Xiao, Z.Q., Chen, Z., Zhang, X., Li, J., Wu, X., Li, X., Yi, H., Li, M., Zhu, G., and Liang, S., 2006, Proteome analysis of human lung squamous carcinoma, *Proteomics*, 6(2), 547–558.
- Liu, L., Wang, S., Zhang, Q., and Ding, Y., 2008, Identification of Potential Genes/Proteins Regulated by Tiam1 in Colorectal Cancer by Microarray Analysis and Proteome Analysis. *Cell Biol. Int.*, 32, 1215–1222.
- Liu, P., and Long, W., 2009, Current Mathematical Methods Used in QSAR/QSPR Studies, *Int. J. Mol. Sci.*, 10, 1978-1998.
- McNaught, A.D., and Wilkinson, A., 1997, *Compendium of Chemical Terminology (the "Gold Book")*, 2nd ed. Blackwell Scientific Publications, Oxford.

- Menegon, G., Shimizu, K., Farah, J.P.S., Dias, L.G., and Chaimovich, H., 2002, Parameterization of the Electronegativity Equalization Method Based on the Charge Model 1, *Phys. Chem. Chem. Phys.*, 4, 5933-5936.
- Nantasenamat, C., Isarankura-Na-Ayudhya, C., Naenna, T., and Prachayasittikul, V., 2009, A Practical Overview of Quantitative Structure-Activity Relationship., *EXCLI J.*, 8, 74-88.
- Narayanan, N.K., Narayanan, B.A., and Nixon D.W., 2004, Resveratrol-induced Cell Growth Inhibition and Apoptosis is Associated With Modulation of Phosphoglycerate Mutase B in Human Prostate Cancer Cells: Two-Dimensional Sodium Dodecyl Sulfate-Polyacrylamide Gel Electrophoresis and Mass Spectrometry Evaluation, *Cancer Detect Prev.*, 28, 443-452.
- Panda, S.S., Chand, M., Sakhuja, R., and Jain, S.C., 2013, Xanthone as Potential Antioxidants, *Curr. Med. Chem.*, 36(20), 4481 – 4507.
- Peter, S.C., Dhanja, J.K., Malik, V., Radhakrishnan, N., Jayakanthan, M., and Sundar, D., 2018, Quantitative Structure-Activity Relationship (QSAR): Modeling Approaches to Biological Applications, *Encyclopedia of Bioinformatics and Computational Biology*, 2, 661- 676.
- Pranowo, H.D., dan Hetadi, A.K.R., 2011, *Pengantar Kimia Komputasi*, Lubuk Agung, Bandung.
- Rode, B.M., Schwendinger M.G., Kokpol, S.U., Hanogboa S.V., and Polman S., 1989, Quantum Pharmacological Studies on Antimalarial Drugs, *J. Med. Chem.*, 1(15), 17-22.
- Roy, K., and Roy, P.P., 2009, Comparative Chemometric Modeling of Cytochrome 3A4 Inhibitory Activity of Structurally Diverse Compounds Using Stepwise MLR, FA-MLR, PLS, GFA, G/PLS and ANN Techniques, *Eur. J. Med. Chem.*, 44, 2913-2922.
- Roy, K., Kar, S., and Das, R.N., 2015, *Understanding the Basics of HKSA for Applications in Pharmaceutical Sciences and Risk Assessment*, Academic Press, India.
- Seydel, J.K., 1990, *Mild Career Training in Pharmacochemistry*, Summary Lecture Course HKSA, Fakultas Farmasi UGM, Yogyakarta.
- Siswandono dan Soekardjo, B., 2000, *Prinsip-prinsip Rancangan Obat*, Airlangga University Press, Surabaya.
- Van Damme, S., and Bultinck, P., 2007, A New Computer Program for QSAR-Analysis: ARTE-QSAR, *J. Comput. Chem.*, 28, 1924-1928.

- Vařeková, R.S., Jiroušková, Z., Vaněk, J., Suchomel, Š., dan Koča, J., 2007, Electronegativity Equalization Method: Parameterization and Validation for Large Sets of Organic, Organohalogene and Organometal Molecule, *Int. J. Mol. Sci.*, 8, 572-582.
- Veerasamy, R., Rajak, H., Jain, A., Sivadasan, S., Varghese, C.P., and Agrawal, R.K., 2011, Validation of HKSA Models - Strategies and Importance, *Int. J. Drug Des. Discov.*, 2, 511-519.
- Walker, J.D., Jaworska, J., Comber, M.H.I., Schultz, T.W., and Dearden, J.C., 2003, Guidelines for Developing and Using Quantitative Structure-Activity Relationships, *Environ. Toxicol. Chem.*, 22, 1653-1665.
- Wang, P., Jiang, L., Cao, Y., Zhang, X., Chen, B., Zhang, S., Huang, K., Ye, D., and Zhou, L., 2018, Xanthone Derivatives as Phosphoglycerate Mutase 1 Inhibitors: Design, Synthesis, and Biological Evaluation, *Bioorg. Med. Chem.*, 26(8), 1961-1970.
- Warburg, O., 1956, On the Origin of Cancer Cells, *Science* 123, 309-314.
- Wibowo, A.E., 2012, *Aplikasi Praktis SPSS dalam Penelitian*, Gava Media, Yogyakarta.
- Wirayanti, Setiawan A., dan Susanto, B., 2011, Studi Simulasi Tentang Penerapan Grafik Pengendalian Berdasarkan Analisis Komponen Utama (Principal Component Analysis), *Prosiding Matematika dan Pendidikan Karakter dalam Pembelajaran*, Yogyakarta.
- World Health Organization, 2018, *Cancer*, www.who.int.
- Yuliana, 2004, Analisis Hubungan Kuantitatif Struktur Elektronik dan Aktivitas Antimutagen Senyawa Turunan Benzalaseton Menggunakan Pendekatan Principal Component Regression, *Tesis*, Universitas Gadjah Mada, Yogyakarta.
- Young, D.C., 2001, *Computational Chemistry: A Practical Guide for Applying Technique to Real-World Problems*, John Wiley and Sons Inc., New York.