

DAFTAR PUSTAKA

- Agrios, G., 1997, *Plant Pathology*, Fourth Edition, Academic Press, New York.
- Akamatsu, M., 2011, Importance of Physicochemical Properties for the Design of New Pesticides, *J. Agric. Food Chem.*, 59, 2909–2917.
- Bai, Y.B., Zhang, A.L., Tang, J.J., and Gao, J.M., 2013, Synthesis and Antifungal Activity of 2-Chloromethyl-1H-benzimidazole Derivatives against Phytopathogenic Fungi in Vitro, *J. Agric. Food Chem.*, 61, 2789-2795.
- Basavaraj, S., and Betageri, G.V., 2014, Can Formulation and Drug Delivery Reduce Attrition during Drug Discovery and Development-Review of Feasibility, Benefits and Challenges, *Acta Pharm. Sin. B.*, 4(1), 3-17.
- Bräse, S., Encinas, A., Keck, J., and Nising, C.F., 2009, Chemistry and Biology of Mycotoxins and Related Fungal Metabolites, *Chem. Rev.*, 109, 3903-3990.
- Cao, F.J., Yang, R., Lv, C., Ma, Q., Lei, M., Geng, H.L., and Zhou, L., 2015, Pseudocyanides of Sanguinarine and Chelerythrine and their series of Structurally Simple Analogues as New Anticancer Lead Compounds : Cytotoxic Activity, Structure-Activity Relationship and Apoptosis Induction, *Eur. J. Pharm. Sci.*, 67, 45-54.
- Charifson, P.S., 1997, *Practical Application of Computer-Aided Drug Design*, Marcel Dekker, Inc., New York.
- Cramer, C.J., 2004, *Essentials of Computational Chemistry: Theories and Models*, Second Edition, John Wiley & Sons Ltd., England.
- Devillers, J., 1996, *Neural Networks in QSAR and Drug Design*, Academic Press, London.
- Franke, R., 1984, *Theoretical Drug Design Methods*, Elsevier, New York.
- Free, S.M., and Wilson, J.W., 1964, A Mathematical Contribution to Structure-Activity Studies, *J. Med. Chem.*, 7, 395–399.
- Ban, T., and Fujita, T., 1969, Mathematical Approach to Structure-Activity Study of Sympathomimetic Amines, Norepinephrine-Uptake Inhibition, *J. Med. Chem.*, 12(3), 353–356.
- Becke, A. D., 1988, Density-functional exchange-energy approximation with correct asymptotic behaviour, *Phys. Rev. A*, 38, 3098-3100.
- Bryantsev, V. S., Diallo, M. S., van Duin, A. C. T., and Goddard III, W. A., 2009, Evaluation of B3LYP, X3LYP and M06-Class Density Functional for Predicting Binding Energies of Neutral, Protonated and Deprotonated Water Clusters, *J. Chem. Theory Comput.*, 5, 1016-1026
- Golbraikh, A., and Tropsha, A., 2002, Predictive QSAR Modeling Based on Diversity Sampling of Experimental Datasets for the Training and Test Set Selection, *J. Comput. Aid. Mol. Des.*, 16, 357-369.
- Golbraikh, A., and Tropsha, A.J., 2002, Beware of q^2 !, *J. Mol. Graph. Model*, 20, 269-276.
- Hartono, 2011, *SPSS 16.0 : Analisis Data Statistika dan Penelitian*, Pustaka Pelajar, Yogyakarta.
- Hmammouchi, R., Taghki, A.I., Larif, M., Adad, A., Abdellaoui, A., Bouachrine, M., and Lakhlifi, T., 2013, Combining DFT and QSAR Result for

- Predicting the Biological Activity of the Phenylsuccinimide Derivatives, *J. Chem. Pharm. Res.*, 5(10), 45-56.
- Hou, Z., Yang, R., Zhang, C., Zhu, L.F., Miao, F., Yang, X.J., and Zhou, L., 2013, 2-(Substitued phenyl)-3,4-dihydroisoquinolin-2-iums as Novel Antifungal Lead Compounds : Biological Evaluation and Structure-Activity Relationships, *Molecules*, 18, 10413-10424.
- Hussein, M.A., El-Sayed, W., and Tomader, A.R.G., 2007, Synthesis, Pesticidal Activity and Quantitative Structure-Activity Relationships of Aseries of N-(2-oxido-1,3,2-benzodioxaphosphol-2-yl) Amino Acid Ethyl or Diethyl Esters, *Aust. J. Basic & Appl. Sci.*, 1(4): 593-599.
- Jain, S.V., Ghate, M., Bhadoriya, K.S., Bari, S.B., Chaudhari, A., and Borse, J.S., 2012, 2D, 3D-QSAR and Docking Studies of 1,2,3-Thiadiazole Thioacetanilides Analogues as Potent HIV-1 Non-Nucleoside Reverse Transcriptase Inhibitors, *Org. and Med. Chem. Lett.* 2 : 22.
- Jensen, F., 2007, *Introduction to Computational Chemistry Second Edition*, John Wiley and Sons, England.
- Kapur, G.S., Ecker, A., and Meusinger, R., 2001, Establishing Quantitative Structure-Property Relationships (QSPR) of Diesel Samples by Proton-NMR & Multiple Linear Regression (MLR) analysis, *Energy & Fuel*, 15, 943-948.
- Karelson, M., Lobanov, V.S., and Katrizky, A.R., 1996, Quantum-Chemical Descriptors in QSAR/QSPR Studies, *Chem. Rev.*, 96, 1027-1043.
- Katrizky, A.R., Lobanov, V.S. and Karelson, M., 1996, Quantum-Chemical Descriptors in QSAR/QSPR Studies. *Chem. Rev.*, 96, 1027-1043.
- Kolossov, E., and Stanforth, R., 2007, SAR and QSAR, *Environ. Res.*, 18, 89-100.
- Kovačević, S.Z., Kuzmanović, S.O.P., Jevrić, L.R., and Kalajdzija, N.D., 2013, Neural Network Modelling of Antifungal Activity of A Series of Oxazole Derivates Based on in Silico Pharmacokinetic Parameters, *APTEFF*, 44, 1-321.
- Krane, B.D., Fagbule, M.O., Shamma, M., and Gözler, B., 1984, The Benzophenanthridine Alkaloids, *J. Nat. Prod.*, 47, 1-43.
- 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.*, Article in Press.
- Kubinyi, H., 1993, *QSAR: Hansch Analysis and Related Approaches*, VCH Verlagsgesellschaft, Weinhem.
- Kubinyi, H., Hamprecht, F.A., and Mietzner, T., 1998, Three-dimensional Quantitative Similarity-Activity Relationships (3D QsiAR) from SEAL Similarity Matrices, *J. Med. Chem.*, 41, 2553-2564.
- Kumar, A., Srivastava, A.K., Gangwar, S., Misra, N., Mondal, A., and Brahmachari, G., 2015, Combined Experimental (FT-IR, UV-Visible Spectra, NMR) and Theoretical Studies on the Molecular Structure, Vibrational Spectra, HOMO, LUMO, MESP Surfaces, Reactivity Descriptor and Molecular Docking of Phomarin, *J. Mol. Struct.*, 1096, 94-101.

- Lakshman, B., and Gupta, R.L., 2010, Fungitoxicity and QSAR of 4-amino-5-substituted aryl-3-mercapto-(4H)-1,2,4-triazoles, *Indian J. Chem.*, 49B, 1235-1242.
- Lee, C., Yang, W., and Parr, R. G., 1988, Development of Colle-Salvetti correlation energy formula into a functional of the electron density, *Pys. Rev. B.*, 37, 785-789.
- Lee, K.W., Kwon, S.Y., Hwang, S., Lee, J.U., and Kim, H., 1996, Quantitative Structure-Activity Relationship (QSAR) Study on C-7 Substituted Quinolone, *Bull. Korean Chem. Soc.*, 17, 147-152.
- Liu, H., Wang, J., Zhao, J., Lu, S., Wang, J., Jiang, W., Ma, Z., and Zhou, L., 2009, Isoquinoline Alkaloids from *Macleaya Cordata* Active Against Plant Microbial Pathogens. *Nat. Prod. Commun.*, 4, 1557-1560.
- Liu, P., and Long, W., 2009, Current Mathematical Methods Used in QSAR /QSPR Studies, *Int. J. Mol. Sci.*, 10, 1978-1998.
- Livingstone, D.J., Manallack, D.T., and Tetko, I.V., 1997, Data Modelling with Neural Networks: Advantages and Limitations, *J. Comput. Aided Mol.*, 135-142.
- Lučić, N., and Trinajstić, 1997, New Developments in QSPR/QSAR Modeling Based on Topological Indices, SAR QSAR, *Environ. Res.*, 7, 45-62.
- Ma, Y.N., Yang, X.J., Pan, L., Hou, Z., Geng, H.L., Song, X.P., Zhou, L., and Miao, F., 2013, Synthesis of 2-Aryl-3,4-dihydroisoquinolin-2-ium Bromides and Their in Vitro Acaricidal Activity against *Psoroptes cuniculi*, *Chem. Pharm. Bull.*, 61, 204.
- Mandlik, V., Bejugam P.R., and Singh, S., 2016, *Artificial Neural Network for Drug Design, Delivery and Disposition*, Elsevier.
- Mishra, M., Mishra, V.K., Senger, P., Pathak, A.K., and 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.
- Moretti, and Antonio, 2009, Taxonomy of *Fusarium* Genus: A Continuous Fight between Lumpers and Splitters, *Zbornik Matice srpske za prirodne nauke*, 117, 7-13.
- Motta, L.F., and Almeida, W.P., 2011, Quantitative Structure-Activity Relationships (QSAR) of a Series of Ketone Derivatives as Anti-Candida Albicans, *Int. J. Drug Discov.*, 3, 100-117.
- Mudasir., Tahir, I. dan Putri, I.P.A.M., 2003, Analisis Hubungan Kuantitatif Antara Struktur dan Aktivitas Fungisida Turunan 1,2,4-Thiadiazolin Berdasarkan Parameter Molekular Hasil Perhitungan Metoda AM1, *Indo. J. Chem.*, 3(1), 39-47.
- 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.
- Neter, J., Wasserman, W., and Kunter, M.H., 1985, *Applied Linear Statistical Models*, Irwin, Homewood, IL.
- O'Donnell, K., Sutton, D.A., Fothergill, A., McCarthy, D., Rinaldi, M.G., Brandt, M.E., Zhang, N., and Geiser, D.M., 2008. Molecular Phylogenetic

- Diversity, Multilocus Haplotype Nomenclature, and In Vitro Antifungal Resistance within the *Fusarium Solani* Species Complex. *J. Clin. Microbiol.*, 2477–2490.
- Ohno, K., 2004, *Quantum Chemistry*, Iwanami Publishing Company, Tokyo.
- Paliwal, S., Sharma, J., and Paliwal, S., 2012, Quantitative Structure Activity Relationship Analysis of Bisbenzofuran Cations as Antimalarial Agents Employing Multivariate Statistical Approach, *Indian J. Chem.*, 51, 617–630.
- Paula, Y.B., 2003, *Organic Chemistry*, Fourth Edition, Prentice-Hall : London.
- Pranowo, H.D., and Hetadi, A.K.R., 2011, *Pengantar Kimia Komputasi*, Lubuk Agung, Bandung.
- Quin, C., Trnka, J., Hay, A., Murphy, M. P., and Hartley, R. C., 2009, Synthesis of a mitochondria-targeted spin trap using a novel Parham-type cyclization, *Tetrahedron*, 65 (39), 8154-8160.
- Roy, K., and Paul, S., 2008, QSAR, *Comb. Sci.*, 28, 406-425.
- 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.
- Sachs, L., 1984, *Applied Statistics: A Handbook of Techniques*, Springer-Verlag, Berlird New York.
- Sahu, N.K., Sharma, M., Vishnukanth, M., and Kohli, D.V., 2014, QSAR Studies of Some Side Chain Modified 7-Chloro- 4-Aminoquinolines as Antimalarial Agents, *Arab. J. Chem.*, 7, 701–707.
- Sardjoko, 1993, *Rancangan Obat*, Gadjah Mada University Press, Yogyakarta.
- Savary, S., Teng, P.S., Willocquet, L., and Nutter, F.W.Jr., 2006, Quantification and Modeling of Crop Losses: A Review of Purposes, *Annu. Rev. Phytopathol.*, 44, 89-112.
- Shahane, S., Louafi, F., Moreau, J., Hurvois, J. P., Renaud, J. L., Van de Weghe, P., and Roisnel, T., 2008, Synthesis of Alkaloids of *Galipea officinalis* by Alkylation of an α -Amino Nitrile, *Eur. J. Org. Chem.*, 4622.
- Singh, J., Singh, S., Thakur, S., Lakhwani, M., Khadikar, P.V., Agrawal, V.K., and Supuranf, C.T., 2006, QSAR Study on Murine Recombinant Isozyme mCAXIII: Topological vs Structural Descriptors, *Arkivoc*, 14, 103–118.
- Šimánek, V., 1985, *Benzophenanthridine Alkaloids*. In *The Alkaloids*, Brossi, A., Ed., Academic Press: New York, NY, USA, 26, 185–240.
- Siswandono, Soekardjo, B., 1995, *Kimia Medisinal*, Airlangga University Press, Surabaya.
- Siswandono dan Soekarjo, B., 2000, *Prinsip-prinsip Rancangan Obat*, Airlangga University Press, Surabaya.
- Sudirman, 2009, Pengaruh Penggunaan Fungisida terhadap Perkecambahan Spora Fungi Mikoriza Arbuskula, *Tesis*, Universitas Sumatera Utara, Medan.
- Suvitha, A., Periandy, S., Boomadevi, S., and Govindarajan, M., 2014, Vibrational Frequency Analysis, FT-IR, FT-Raman, Ab Initio, HF and DFT Studies, NBO, HOMO-LUMO and Electronic Structure Calculations on Pycolinaldehyde Oxime, *Spectrochim. Acta - Part A Mol. Biomol. Spectrosc.*, 117, 216–224.

- Syahputra, A., Mudasir, Nuryono, Aziz A., and Tahir, I., 2014, QSAR Study of Insecticides of Phthalamide Derivates using Multiple Linear Regression and Artificial Neural Network Methods, *Indo. J. Chem.*, 14(1), 94-101.
- Szaleniec, M., Tadeusiewicz, and R., Witko, M., 2008, How to Select an Optimal Neural Model of Chemical Reactivity, *Neurocomputing*, 72, 241–256.
- Tetko, I.V., Tanchuk, V.Y., Chentsova, N.P., Antonenko, S.V., Poda, G.I., and Kukhar, V.P., 1994, HIV-1 Reverse Transcriptase Inhibitor Design using Artificial Neural Networks, *J. Med. Chem.* 37, 2520–2526.
- Tetko, I.V., Livingstone, D.J., and Luik, A.I., 1995, Neural Network Studies : Comparison of Overfitting and Overtraining, *J. Chem. Inf. Comput. Sci.*, 35, 826–833.
- Tetko, I.V., Villa, A.E.P., and Livingstone, D.J., 1996, Neural Network Studies : Variable selection, *J. Chem. Inf. Model.*, 36, 794–803.
- Veerasamy, R., Rajak, H., Jain, A., Sivadasan, S., Varghese, C.P., and Agrawal, R.K., 2011, Validation of QSAR Models - Strategies and Importance, *Int. J. Drug Des. Discov.*, 2, 511–519.
- Volk, W.A., and Wheeler, M.F., 1993, *Mikrobiologi Dasar, Edisi Kelima*, Jilid 1, Penerbit Erlangga, Jakarta.
- 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.
- Wedge, D.E., Camper, N.D., 2000, *Biologically Active Natural Products. In Agrochemicals and Pharmaceuticals*; Cutler, H.G., Cutler, S.J., Eds.; CRC Press: Boca Raton, FL, USA, 1–15.
- Wikel, J., and E. Dow, 1993, The Use of Neural Networks for Variable Selection in QSAR, *Bioorg. Med. Chem. Lett.*, 3, 645–651.
- Wudianto, R., 2007, *Petunjuk Penggunaan Pestida*, Penerbit Penebar Swadaya, Jakarta.
- Yang, R., Gao, Z.F., Zhao, J.Y., Li, W.B., Zhou, L., and Miao, F., 2015, New Class of 2-Aryl-6-chloro-3,4-dihydroisoquinolinium Salts as Potential Antifungal Agents for Plant Protection : Synthesis, Bioactivity and Structure-Activity Relationships, *J. Agric. Food Chem.*, 63, 1906.
- Yang, X.J., Miao, F., Yao, Y., Cao, F.J., Yang, R., Ma, Y.N., Qin, B.F., and Zhou, L., 2012, Invitro Antifungal Activity of Sanguinarine and Chelerythrine Derivates Againts Phytopathogenic Fungi, *Molecules*, 17, 13026.
- Yang, X., Yao, Y., Qin, Y., Hou, Z., Yang, R., Miao, F., and Zhou, L., 2013, Synthesis and in Vitro Antifungal Activities of New 2-Aryl-6,7-methylenedioxy-3,4-dihydroisoquinolin-2-ium Bromides, *Chem. Pharm. Bull.*, 61(7), 731.
- Yin, C., Liu, X., Guo, W., Lin, T., Wang, X., and Wang, L., 2002, Prediction and Application in QSPR of Aqueous Solubility of Sulfur-Containing Aromatic Esters using GA-Based MLR with Quantum Descriptors, *Water Res.*, 36, 2975–2982.
- Young, D.C., 2001, *Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problem*, Willey-Interscience, New York.

- Yousefinejad, S., and Hemmateenejad, B., 2015, Chemometrics and Intelligent Laboratory Systems Chemometrics Tools in QSAR / QSPR Studies : A Historical Perspective, *Chemom. Intell. Lab. Syst.*, 149, 177–204.
- Zhang, B.Y., Zheng, Z.L., Miao, F., Yang, X.J., Ma, X.H., and Zhou, L., 2013, Effects of 2-Aryl-3,4-dihydroisoquinolin-2-iums on Seed Germination and Seedling Growth, *J. Northwest A&F University (Nat. Sci. Ed.)*, 42, 169-174.
- Zheng, Z.L., Miao, F., Yang, X.J., and Zhou, L., 2015, Effects of 2-Aryl-3,4-dihydroisoquin-2-iums as Antifungal Agents on Plant Seed Germination and Seedling Growth, *J. Northwest A&F University (Nat. Sci. Ed.)*, 43, 116-122.
- Zhu, L.F., Hou, Z., Zhou, K., Tong, Z.B., Kuang, Q., Geng, H.L., Zhou, L., 2016, Synthesis, Bioactivity and Structure-Activity Relationships of New 2-aryl-8-OR-3,4-dihydroisoquinolin-2-iums Salts as Potential Antifungal Agents, *Bio. and Med. Chem. Let.*, 26, 2413.