

## DAFTAR PUSTAKA

- Allen, M.P., and Tildesley, D.J., 2002, *Computer Simulation of Liquids*, Oxford University Press, Oxford.
- Ameer, K., Shahbaz, H.M., and Kwon, J., 2017, Green Extraction Methods for Polyphenols from Plant Matrices and Their Byproducts: A Review, *Compr. Rev. Food Sci. Food Saf.*, 16(2), 295-315.
- Amrullah, A., 2017, Simulasi Dinamika Molekular Untuk Rancangan Polimer Tercetak Molekul Senyawa Kuersetin, *Skripsi*, Departemen Kimia, Fakultas Matematika dan Ilmu Pengetahuan Alam, Universitas Gadjah Mada, Yogyakarta.
- Anderson, R.A., Ariffin, M.M., Cormack, P.A.G., and Miller, E.I., 2008, Comparison of Molecularly Imprinted Solid-Phase Extraction (MISPE) with Classical Solid-Phase Extraction (SPE) for the Detection of Benzodiazepines in Post-mortem Hair Samples, *Forensic. Sci. Int.*, 174, 40-46.
- Azwanida, N.N., 2015, A Review on the Extraction Methods Use in Medicinal Plants, Principle, Strength and Limitation, *Med. Aromat. Plants*, 4(3), 1-6.
- Batra, D., and Shea, K.J., 2003, Combinatorial Methods in Molecular Imprinting, *Curr. Opin. Chem. Biol.*, 7, 434-442.
- Beerueta, L.A., Gallo, B., and Vicente, F., 1995, A Review of Solid Phase Extraction: Basic Principles and New Developments, *Chromatographia*, 40(7), 474-483.
- Chianella, I., Lotierzo, M., Piletsky, S.A., Tothill, I.E., Chen, B., Karim, K., and Turner, A.P.F., 2002, Rational Design of a Polymer Specific for Microcystin-LR Using a Computational Approach, *Anal. Chem.*, 74(6), 1288-1293.
- Cowen, T., Karim, K., and Piletsky, S., 2016, Computational Approaches in The Design of Synthesis Receptors - A Review, *Anal. Chim. Acta*, 936, 62- 74.
- Cramer, C.J., 2004, *Essentials of Computational Chemistry: Theories and Models*, Second Edition, John Wiley & Sons Inc., West Sussex.
- Dethlefs, K.M. and Hobza, P., 2000, Non-covalent Interactions: A Challenge for Experimental and Theory, *Chem. Rev.*, 100, 143-167.
- Dogan, M., 2008, Solid-Phase Extraction Technique in Analytical Chemistry, *Hacettepe J. Biol. Chem.*, 36(3), 235-246.
- Dong, C., Li, X., Guo, Z., and Qi, J., 2009, Development of A Model for the Rational Design of Molecular Imprinted Polymer: Computational Approach for Combined Molecular Dynamics/Quantum Mechanics Calculations, *Anal. Chim. Acta.*, 647, 117-124.

- Dourado, E.M.A., 2011, Computer Simulations of Adsorption and Molecular Recognition Phenomena in Molecular Imprinted Polymer, *Thesis*, School of Engineering, University of Edinburgh, Edinburgh.
- Erturk, G., and Mattiasson, B., 2017, Molecular Imprinting Techniques Used for the Preparation of Biosensors, *Sensors*, 17(2), 288.
- Essmann, U., Perera, L., Berkowitz, M.L., Darden, T., Lee, H., and Pedersen, L.G.A., 1995, Smooth Particle Mesh Ewald Method, *J. Chem. Phys.*, 103, 8577-8593.
- Farrington, K., and Regan, F., 2007, Investigation of The Nature of MIP Recognition: The Development and Characterization of MIP for Ibuprofen, *Biosens. Bioelectron.*, 22, 1138-1146.
- Ferreiro-Gonzalez, M., Carrera, C., Ruiz-Rodríguez, A., Barbero, G.F., Ayuso, J., Palma, M., and Barroso, C.G., 2014, A New Solid-Phase Extraction for the Determination of Anthocyanins in Grapes, *Molecules*, 19(12), 21398-21410.
- Frisch, M. J., Trucks, G. W., Schlegel, H. B., Scuseria, G. E., Robb, M. A., Cheeseman, J. R., Scalmani, G., Barone, V., Mennucci, B., Petersson, G. A., Nakatsuji, H., Caricato, M., Li, X., Hratchian, H. P., Izmaylov, A. F., Bloino, J., Zheng, G., Sonnenberg, J. L., Hada, M., Ehara, M., Toyota, K., Fukuda, R., Hasegawa, J., Ishida, M., Nakajima, T., Honda, Y., Kitao, O., Nakai, H., Vreven, T., Montgomery Jr., J. A., Peralta, J. E., Ogliaro, F., Bearpark, M., Heyd, J. J., Brothers, E., Kudin, K. N., Staroverov, V. N., Kobayashi, R., Normand, J., Raghavachari, K., Rendell, A., Burant, J. C. Iyengar, S. S., Tomasi, J., Cossi, M., Rega, N., Millam, J. M., Klene, M., Knox, J. E., Cross, J. B., Bakken, V., Adamo, C., Jaramillo, J., Gomperts, R., Stratmann, R. E., Yazyev, O., Austin, A. J., Cammi, R., Pomelli, C., Ochterski, J. W., Martin, R. L., Morokuma, K., Zakrzewski, V. G., Voth, G. A., Salvador, P., Dannenberg, J. J., Dapprich, S., Daniels, A. D., Farkas, Ö., Foresman, J. B., Ortiz, J. V., Cioslowski, J., and Fox, D. J., 2009, *Gaussian 09: Revision A.02*, Gaussian Inc., Wallington CT.
- Handayani, S., Susidarti, R.A., Udin, Z., Meiyanto, E., and Jenie, R.I., 2016, Brazilein in Combination with Cisplatin Inhibit Proliferation and Migration on Highly Metastatic Cancer Cells, 4T1, *Indones. J. Biotechnol.*, 21(1), 38-47.
- He, C., Long, Y., Pan, J., Li, K., and Liu, F., 2007, Application of Molecularly Imprinted Polymers to Solid-Phase Extraction of Analytes from Real Samples, *J. Biochem. Biophys. Methods*, 70, 133-150.
- Hennion, M.C., 1999, Solid-Phase Extraction: Method Development, Sorbents, and Coupling with Liquid Chromatography, *J. Chromatogr. A*, 856, 3-54.
- Hsieh, C., Tsai, P., Chu, C., Chang, F., Chang, L., Wu, Y., and Lin, S., 2013, Brazilein Suppresses Migration and Invasion of MDA-MB-231 Breast Cancer Cells, *Chem. Biol. Interact.*, 204, 105-115.

- Huang, Y., and Zhu, Q., 2015, Computational Modeling and Theoretical Calculations on the Interactions between Spermidine and Functional Monomer (Methacrylic Acid) in a Molecularly Imprinted Polymer, *J. Chem.*, 216983, 1-9.
- Humphrey, W., Dalke, A., and Schulten, K., 1996, VMD: Visual Molecular Dynamics, *J. Mol. Graph.*, 14, 33-38.
- Jeffrey, G.A., and Saenger, W., *Hydrogen Bonding in Biological Structures*, Springer-Verlag, New York.
- Karlsson, B.C.G., O'Mahony, J., Karlsson, J.G., Bengtsson, H., Eriksson, L.A., and Nicholls, I.A., 2009, Structure and Dynamics of Monomer-Template Complexation: An Explanation for Molecularly Imprinted Polymer Recognition Site Heterogeneity, *J. Am. Chem. Soc.*, 131(37), 13297-13304.
- Khan, S., Bhatia, T., Trivedi, P., Satyanarayana, G.N.V., Mandrah, K., Saxena, P.N., Mudiam, M.K.R., and Roy, S.K., 2016, Selective Solid-Phase Extraction using Molecularly Imprinted Polymer as A Sorbent for the Analysis of Fenarimol in Food Samples, *Food Chem.*, 199, 870-875.
- Kohn, W., Becke, A.D., and Parr, R.G., 1996, Density Functional Theory of Electronic Structure, *J. Phys. Chem.*, 100, 12974-12980.
- Kong, Y., Wang, N., Ni, X., Yu, Q., Liu, H., Huang, W., and Xu, W., 2016, Molecular Dynamics Simulations of Molecularly Imprinted Polymer Approaches to the Preparation of Selective Materials to Remove Norfloxacin, *J. Appl. Polym. Sci.*, 133(1), 1-11.
- Kurniati, K., Prasetya, A., dan Winarni, W., 2012, Ekstraksi dan Uji Stabilitas Zat Warna Brazilein dari Kayu Secang (*Caesalpinia sappan* L.), *Indones. J. Chem. Sci.*, 1(1), 32-36.
- Laksmiani, N.L.P., Susidarti, R.A., and Meiyanto, E., 2015, Breazilein Increases the Sensitivity of Doxorubicin on MCF-7 Resistant Doxorubicin (MCF-7/DOX) Cells Through Inhibition of HER-2 Activation, *Int. J. Pharm. Pharm. Sci.*, 7(2), 525-528.
- Laksmiani, N.P.L., Meiyanto, E.D.Y., and Susidarti, R.A., 2017, Cytotoxic Activity of Brazilein Isolated from Secang (*Caesalpinia sappan* L.) against MCF7/DOX Cells by Inhibition of P-Glycoprotein, *Int. J. Pharm. Pharm. Sci.*, 9(12), 124-130.
- Lee, W., Chang, J., and Ju, S., 2010, Hydrogen-Bond Structure at the Interfaces between Water/Poly(methyl methacrylate), Water/Poly(methacrylic acid), and Water/ Poly(2-aminoethylmethacrylamide), *Langmuir*, 26(15), 12640-12647.
- Li, X., Wang, Y., Sun, Q., Xu, B., Yang, Z., and Wang, X., 2016, Molecularly Imprinted Dispersive Solid-Phase Extraction for the Determination of Triazine Herbicides in Grape Seeds by High-Performance Liquid Chromatography, *J. Chromatogr. Sci.*, 54(5), 871-877.

- Liang, C., Chan, L., Chou, T., Chiang, F., Yen, C., Chen, P., Ding, H., and Lin, R., 2013, Brazilein from *Caesalpinia sappan* L. Antioxidant Inhibits Adipocyte Differentiation and Induces Apoptosis through Caspase-3 Activity and Anthelmintic Activities against *Hymenolepis nana* dan *Anisakis simplex*, *J. Evid. Based. Complementary Altern. Med.*, 864892, 1-14.
- Lioe, H.N., Adawiyah, D.R., and Anggraeni, R., 2012, Isolation and Characterization of the Major Natural Dyestuff Component of Brazilwood (*Caesalpinia sappan* L.), *Int. Food Res. J.*, 19(2), 537-542.
- Luo, D., Zhaob, Z., Zhanga, L., Wang, Q., and Wang, J., 2014, On the Structure of Molecularly Imprinted Polymers by Modifying Charge on Functional Groups through Molecular Dynamics Simulations, *Mol. Simul.*, 40(6), 431-438.
- Manouchehri, F., Izadmanesh, Y., Aghae, E., and Ghasemi, J.B., 2016, Experimental, Computational and Chemometrics Studies of BSA-Vitamin B6 Interaction by UV-Vis, FT-IR, Fluorescence Spectroscopy, Molecular Dynamics Simulation and Hard-Soft Modeling Methods, *Bioorg. Chem.*, 68(13), 124-136.
- Martínez, J.M., and Martínez, L., 2003, Packing Optimization for Automated Generation of Complex System's Initial Configuration for Molecular Dynamics and Docking, *J. Comput. Chem.*, 24, 819-825.
- McQuarrie, D.A., 2000, *Statistical Mechanics*, University Science Books, Sausalito.
- Mladenova, E., Karadjova, I., and Tsalev, D.L., 2012, Solid-Phase Extraction in the Determination of Gold, Palladium, and Platinum, *J. Sep. Sci.*, 35(10), 1249-1265.
- Mozgawa, K., 2016, Interfacial Solvation Modelling with PCM, *Dissertation*, Department of Chemistry, Faculty of Science and Technology, The Arctic University of Norway, Tromsø.
- Nirmal, N.P., Rajput, M.S., Prasad, R.G.S.V., and Ahmad, M., 2015. Brazilin from *Caesalpinia sappan* Heartwood and Its Pharmacological Activities: A Review, *Asian Pac. J. Trop. Med.*, 8(6): 421-430.
- Oka, M., Kamisaka, H., Fukumura, T., and Hasegawa, T., 2015, DFT-Based Ab Initio MD Simulation of the Ionic Conduction in Doped ZrO<sub>2</sub> Systems Under Epitaxial Strain, *Phys. Chem. Chem. Phys.*, 17(43), 29057-29063.
- Olcer, Y.A., Demirkurt, M., Demirb, M.M., and Eroglu, A.E., 2017, Development of Molecularly Imprinted Polymers (MIPs) as A Solid-Phase Extraction (SPE) Sorbent for the Determination of Ibuprofen in Water, *RSC Adv.*, 7, 31441-31447.
- Pardeshi, S., Patrikar, R., Dhodapkar, R., and Kumar, A., 2012, Validation of Computational Approach to Study Monomer Selectivity toward the

- Template Gallic Acid for Rational Molecularly Imprinted Polymer Design, *J. Mol. Model.*, 18(11), 4797-4810.
- Petterson, E.F., Goddard, T.D., Huang, C.C., Couch, G.S., Greenblatt, D.M., Meng, E.C., and Ferrin, T.E., 2004, UCSF Chimera – a Visualization System for Exploratory Research and Analysis, *J. Comput. Chem.*, 25, 1605-1612.
- Pranowo, H.D., dan Hetadi, A.K.R., 2011, *Pengantar Kimia Komputasi*, Lubuk Agung, Bandung.
- Prasetyo, N., Tahir, I., Sudiono, S., and Setiaji, B., 2016, Computational Studies on Prepolymerization of Selective Molecular Imprinted Polymer Based on Caffeine, *Proceeding, The 5th International Conference of the Indonesian Chemical Society*, 30-31 Agustus 2016, Samarinda.
- Riahi, S., Edris-Tabrizi, F., Javanbakht, M., Ganjali, M.R., and Norouzi, P., 2009, A Computational Approach to Studying Monomer Selectivity towards the Template in An Imprinted Polymer, *J. Mol. Model.*, 15(7), 829-836.
- Rina, O., Ibrahim, S., Dharma, A., Afrizal, A., Utami, C., and Widodo, Y.R., 2017. Stabilities Natural Colorant of Sappan Wood (*Caesalpinia sappan L.*) for Food and Beverages in Various pH, Temperature, and Matrices of Food, *Int J Chemtech Res*, 10(1), 98-103.
- Roe., D.R., and Cheatham III, T.E., 2013, PTRAJ and CPPTRAJ: Software for Processing and Analysis of Molecular Dynamics Trajectory Data, *J. Chem. Theory Comput.*, 9, 3084-3095.
- Saputra, A., 2014, Aplikasi Metode DFT dan Simulasi Dinamika Molekular pada Kajian Interaksi Monomer Fungsional untuk Desain Polimer Tercetak R(+)-kationon, *Tesis*, Departemen Kimia, Fakultas Matematika dan Ilmu Pengetahuan Alam, Universitas Gadjah Mada, Yogyakarta.
- Saputra, A., Wijaya, K., Armunanto, R., Tania, L., and Tahir, I., 2017, Determination of Effective Functional Monomer and Solvent for R(+)-Cathinone Imprinted Polymer Using Density Functional Theory and Molecular Dynamics Simulation Approaches, *Indones. J. Chem.*, 17(3), 516 – 522.
- Sharma, B.I., and Thapa, R.K., 2016, Basic Concepts of Density Functional Theory: Electronic Structure Calculation, *Proceeding, The 24th Condensed Matter Days National Conference (CMDAYS2016)*, 29-31 Agustus 2016, Mizoram.
- Shome, M., and Mishra, N., 2016, Molecular Recognition of Carboxylic Acid and Carboxylates: A Review, *Indian J. Adv. Chem. Sci.*, 4(1), 56-67.
- Sole, R.F., Lazzoi, M.R., Arnone, M., Sala, F.D., Cannoletta, D., and Vasapollo, G., 2009, Experimental and Computational Studies on Non-Covalent Imprinted Microspheres as Recognition System for Nicotinamide Molecules, *Molecules*, 14, 2632-2649.

- Steffen, C., Thomas, K., Huniar, U., Hellweg, A., Rubner, O., and Schroer, A., 2010, Tmolex – A Graphical User Interface for TURBOMOLE, *J. Comput. Chem.*, 16, 2967-2970.
- Tahir, I., Ahmad, M.N., Islam, A.K.M.S., and Arbain, D., 2012, Molecular Modeling and Experimental Study on The Interaction Between Quercetin and Methacrylic Acid, *Proceeding, The 2nd International Malaysia-Ireland Joint Symposium on Engineering, Science and Business (IMiEJS 2012)*, Kangar.
- Turner, N.W., Piletskaa, E.V., Karima, K., Whitcombe, M., Malechaa, M., Magana, N., Baggianic, C., and Piletskya, S.A., 2004, Effect of the Solvent on Recognition Properties of Molecularly Imprinted Polymer Specific for Ochratoxin A, *Biosens. Bioelectron.*, 20, 1060–1067.
- Urraca, J.L., Carbajo, M.C., Torralvo, M.J., Gonzalez-Vazquez, J., Orellana, G., and Moreno-Bondi, M.C., 2008, Effect of the Templates and Functional Monomer on the Textural Properties of Molecularly Imprinted Polymer, *Biosens. Bioelectron.*, 24, 155–161.
- Utari, F.D., Sumirat, S., dan Djaeni, M., 2017, Produksi Antioksidan dari Ekstrak Kayu Secang (*Caesalpinia sappan* L.) Menggunakan Pengering Berkelembaban Rendah, *J. Apli. Tek. Pang.*, 6(3), 1-4.
- Vanjani, P., 2017, Rancangan Berbasis Komputer Untuk Polimer Tercetak Molekul Auksin Berdasarkan Simulasi Dinamika Molekul, *Skripsi*, Departemen Kimia, Fakultas Matematika dan Ilmu Pengetahuan Alam, Universitas Gadjah Mada, Yogyakarta.
- Vasapollo, G., Sole, R.D., Mergola, L., Lazzoi, M.R., Scardino, A., Scorrano, S., and Mele, G., 2011, Molecularly Imprinted Polymers: Present and Future Prospective, *Int. J. Mol. Sci.*, 12(9), 5908-5945.
- Vasconcelos, I., and Fernandes, C., 2017, Magnetic Solid-Phase Extraction for Determination of Drugs in Biological Matrices, *Trends Analyt. Chem.*, 89, 41-52.
- Wang, J., Wolf, R.M., Caldwell, J.W., Kollman, P.A., and Case, D.A., 2004, Development and Testing of a General AMBER Force Field, *J. Comput. Chem.*, 9, 1157-1174.
- Wei, S., Jakusch, M., and Mizaikoff, B., 2007, Investigating the mechanisms of 17 $\beta$ -Estradiol Imprinting by Computational Prediction and Spectroscopic Analysis, *Anal. Bioanal. Chem.*, 389, 423–431.
- Widayani, W., Wungu, T.D.K., Marsha, S.E., and Suprijadi, S., 2017, Study of Target Recognition of MAA-based Molecularly Imprinted Polymer (MIP) Using Density Functional Theory (DFT) Computation on the Interaction of Methacrylic Acid (MAA)-D-Glucose, *J. Polym. Biopolym. Phys. Chem.*, 5(1), 10-12.

- Wiratama, A.D., 2016, Pemodelan Molekul Berdasarkan Metoda Perhitungan Semiempirik AM1 untuk Sintesis Polimer Tercetak Molekul Asam Kafeat, *Skripsi*, Departemen Kimia, Fakultas Matematika dan Ilmu Pengetahuan Alam, Universitas Gadjah Mada, Yogyakarta.
- Wojnarowicz, A., Sharma, P.S., Sosnowska, M., Lisowski, W., Huynh, T.P., Pszona, M., Borowicz, P., D'Souza, F., and Kutnera, W., 2016, An Electropolymerized Molecularly Imprinted Polymer for Selective Carnosine Sensing with Impedimetric Capacity, *J. Mater. Chem. B*, 4(6), 1156-1165.
- Wungu, T.D.K., Marsha, S.E., Widayani, W., and Suprijadi, S., 2017, Density Functional Theory (DFT) Study of Molecularly Imprinted Polymer (MIP) Methacrylic Acid (MAA) with D-glucose, *Proceeding*, 2nd Materials Research Society of Indonesia Meeting, 24-26 Oktober 2016, Bandung.
- Yemis, F., Alkan, P., Yenigül, B., and Yenigül, M., 2013, Molecularly Imprinted Polymers and Their Synthesis by Different Methods, *Polym. Polym. Compos.*, 21(3), 145-150.
- Yi, L., Fang, R., and Chen, G., 2013, Molecularly Imprinted Solid-Phase Extraction in the Analysis of Agrochemicals, *J. Chromatogr. Sci.*, 51(7), 608-618.
- Zhao, S., Wang, X., Jiang, J., Chai, Y., Tian, Y., Feng, T., Ding, Y., Huang, J., Lei, F., Xing, D., and Du, L., 2014, Transport and Metabolism Behavior of Brazilein during Its Entrance into Neural Cells, *PLoS One*, 9(10), 1-11.
- Zwir-Ferenc, A., and Biziuk, M., 2006, Solid Phase Extraction Technique: Trends, Opportunities and Applications, *Polish J. Environ. Stud.*, 15(5), 677-690.