

DAFTAR PUSTAKA

- Ahmadi, F., Rezaei, H., and Tahvilian, R., 2009, Computational-Aided Design of Molecularly Imprinted Polymer for Selective Extraction of Methadone From Plasma and Saliva and Determination by Gas Chromatography, *J. Chromatogr. A*, 1270, 9–19.
- Anderson, H.S., and Nicholls, I.A., 1997, Spectroscopic Evaluation of Molecular Imprinting Polymerization Systems, *Bioorg. Chem.*, 25, 203-211.
- Argaman, N., and Makov, G., 1999, Density Functional Theory: An Introduction, *Am. J. Phys.*, 68, 69079.
- Armunanto, R., 2004, Simulation of Ag⁺, Au⁺, Co²⁺ in Water, Liquid Ammonia and Water-Ammonia Mixture, *Dissertation*, Leopold-Franzens-Universität, Innsbruck.
- Arshady, A., and Mosbach, K., 1981, Synthesis of Substrate-Selective Polymers by Host-Guest Polymerization, *Macromol. Chem.*, 182, 687-692.
- Batra, D., and Shea, K.J., 2003, Combinatorial Method in Molecular Imprinting, *Current Opin. Chem. Biol.*, 7, 434-442.
- Case, D. A., Cheatham III, T. E., Darden, T., Gohlke, H., Luo, R., Merz Jr., K. M., Onufriev, A., Simmerling, X., Wang, B., and Woods, R. J., 2005, The AMBER Biomolecular Simulation Programs, *J. Comput. Chem.*, 26, 1668-1688.
- Chianella, I., Lotierzo, M., Piletsky, S.A., Tothill, I.E., Chen, B.N., Karim, K., and Turner, A.P.F., 2002, Rational Design of a Polymer for Microcystin LR Using a Computational Approach, *Anal. Chem.*, 74, 1288– 1293.
- Cornell, W.D., Cieplak, P., Bayly, C.I., Gould, I.R., Merz, K.M., Ferguson, D.M., Spellmeyer, D.C., Fox, T., Caldwell, J.W., and Kollman, P.A., 1995, A Second Generation Force Fields for the Simulation of Proteins, Nucleic Acids, and Organic Molecules, *J. Am. Chem. Soc.*, 117, 5179-5197.
- Cowen, T., Karim, K., and Piletsky, S., 2016, Computational Approaches in The Design of Synthesis Receptors - A Review, *Anal. Chim. Acta*, 936, 62-74.
- Danielsson, B., 2008, Artificial Receptors, *Adv. Biochem. Engin./Biotechnol.*, 109, 97-122.



- 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. de A., 2011, Computer Simulations of Adsorption and Molecular Recognition Phenomena in Molecular Imprinted Polymer, *Thesis*, School of Engineering UoE, Edinburgh.
- 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.
- Frenkel, D., and Smit, B., 2002, *Understanding Molecular Simulation: from Algorithms to Applications*, Academic Press, London.
- 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., Fox, D. J., 2009, *Gaussian 09: Revision A.02*, Gaussian Inc., Wallington CT.
- Gholivand, M. B., Torkashvand, M., and Malekzadeh, G., 2012, Fabrication of an Electrochemical Sensor Based on Computationally Designed Molecularly Imprinted Polymers for Determination of Cyanazine in Food Samples, *Anal. Chim. Acta*, 713, 36-44.
- He, C., Long, Y., Pan, J., Li, K., Liu, F., 2007, Application of Molecularly Imprinted Polymers to Solid-Phase Extraction of Analysis from Real Samples, *J. Biochem. Biophys. Methods*, 70, 133-150.



- Hinchliffe, A., 2003, *Molecular Modelling for Beginner*, John Wiley & Sons Ltd., Manchester.
- Hohenberg, P., and Kohn, W., 1964, Inhomogeneous Electron Gas, *Phys. Rev.*, 136, B 864-B 871
- 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.
- Jin, Y., and Kyung, H.R., 2005, Adsorption Isotherm of Ibuprofen on Molecular Imprinted Polymer, *Korean J. Chem. Eng.*, 22, 2, 264-267.
- Karim, K., Breton, F., Rouillon, R., Piletska, V., Guerreiro, E.A., Chianella, I., and Piletsky, S.A., 2007, How to Find Effective Functional Monomers for Effective Molecularly Imprinted Polymers, *Adv. Drug Deliv. Rev.* 57, 1795-1808.
- Karlsson, B. C. G., O'Mahony, J., Karlsson, J. G., Bengtsson, 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, 13297-13304.
- Kirsch, N., Alexander, C., Lubke, M., Whitcombe, M.J., and Vulfson, E.N., 2000, Enhancement of Selectivity of Imprinted Polymers via Post-Imprinting Modification of Recognition Sites, *Polym.*, 14, 5583-5590.
- Kohn, W., and Sham, L. J., 1965, Self-Consistent Equations Including Exchange and Correlation Effects, *Phys. Rev.*, 140, A 1133-A 1138.
- Kuzkin, V.A., 2014, On Angular Momentum Balance In Particle Systems with Periodic Boundary Conditions, *J. Appl. Math. and Mech.*, 95, 1290–1295
- Lin, S. T., and Hsieh, C. M., 2006, Efficient and Accurate Solvation Energy Calculation from Polarizable Continuum Models, *J. Chem. Phys.*, 125, 1-10.
- Martínez, J. M., and Martínez, L., Packing Optimization for Automated Generation of Complex System's Initial Configuration for Molecular Dynamics and Docking, 2003, *J. Comput. Chem.*, 24, 819-825.
- Molinelli, A., Janotta, M., and Mizaiakoff, B., 2005, *Molecularly Imprinted*



Polymers for Biomolecular Recognition (Protein Nanotechnology: Protocols, Instrumentation and Applications), Vol. 300, Humana Press, Ottawa.

- Nicholls, I. A., Karlsson, B. C. G., Olsson, G. D., and Rosengren, A. M., 2013, Computational Strategies for the Design and Study of Molecularly Imprinted Materials, *Ind. Eng. Chem. Res.*, 52, 13900–13909.
- 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, 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.
- Piacham, T., Isarankura-Na-Ayudhya, C., Prachayasittikul, V., 2015, Quercetin-Imprinted Polymer for Anthocyanin Extraction from Mangosteen Pericarp, *Materl. Sci. and Eng. C.*, 51, 127-131.
- Prasetyo, N., Tahir, I., Sudiono, S., and Setiaji, B., 2016, *Computational Studies on Prepolymerization of Selective Molecular Imprinted Polymer Based on Caffeine*, The 5th International Conference of the Indonesian Chemical Society, 30-31 Agustus 2016, Samarinda.
- Ramachandran, K. I., Deepa, G., and Namboori, K., 2008, *Computational Chemistry and Molecular Modeling*, Springer, Coimbatore.
- Riahi, S., Edriz-Tabriz, 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, 829-836.
- 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.
- Russo, N., Toscano, M., and Uccella, N., 2000, Semiempirical Molecular Modeling into Quercetin Reactive Sites: Structural, Conformational, and Electronic Features, *J. Agric. Food. Chem.*, 48, 3232-3237.



- Saputra, A., 2014, Aplikasi Metode DFT dan Simulasi Dinamika Molekular pada Kajian Interaksi Monomer Fungsional untuk Desain Polimer Tercetak R(+)-katinon, *Tesis*, Departemen Kimia FMIPA UGM, Yogyakarta.
- Sellergen, B., 2001, *Molecularly Imprinted Polymers: Man-Made Mimics of Antibodies and Their Applications in Analytical Chemistry*, Elsevier, Amsterdam.
- Sole, R. D., Lazzoi, M. R., Arnone, M., Sala, F. D., Cannoletta, D., and Vasapollo, G., 2009, Experimental and Computational Studies on NonCovalent Imprinted Microspheres as Recognition System for Nicotinamide Molecules, *Molec.*, 14, 7, 2632-2649.
- Sousa, F.S, Fernandes, P.A, and Ramos, M. J, 2007, General Performance of Density Functionals, *J. Phys. Chem. A.*, 111, 10439-10452.
- Spivak, D.A., 2005, Optimization, Evaluation, and Characterization of Molecularly Imprinted Polymers, *Adv. Drug. Deliv. Rev.*, 57, 1779-1794.
- 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.
- Sukir, 2011, Simulasi Dinamika Molekular Hibrida Mekanika Kuantum/Mekanika Molekular Ion Y^{2+} dalam Amoniak Cair dan Air, *Tesis*, Departemen Kimia FMIPA UGM, Yogyakarta.
- 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*, The 2nd International Malaysia-Ireland Joint Symposium on Engineering, Science and Business, 1160–1168.
- Tomasi, J., Mennucci, B., and Cammi, R., 2005, Quantum Mechanical Continuum Solvation Model, *Chem. Rev.*, 105, 2999-3093.
- Turner, N.W., Piletska, E.V., Karim, K., Whitcombe, M., Malecha, M., Magan, N., Baggiani, C., and Piletsky, S.A., 2004, Effect of the Solvent on Recognition Properties of Molecularly Imprinted Polymer Specific for Ochratoxin A, *Biosens. Bioelectron.* 20, 1060–1067.
- 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, 5909-5945.
- 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 β -Estradiol Imprinting by Computational Prediction and Spectroscopic Analysis, *Anal. Bioanal. Chem.*, 389, 423-431.
- Wiratama, A. D., 2016, Pemodelan Molekul Berdasarkan Metoda Perhitungan Semiempirik AM1 untuk Sintesis Polimer Tercetak Molekul Asam Kafeat, *Skripsi*, Departemen Kimia FMIPA UGM, Yogyakarta.
- Wulff, G. and Sarhan, A., 1972, Use of Polymers with Enzyme-Analogous Structures for the Resolution of Racemates. *Angew. Chem. Int. Edt.*, 11, 341.
- Yan, H., and Row, K.H., 2006, Characteristic and Synthetic Approach of Molecularly Imprinted Polymer, *Int. J. Mol. Sci.*, 7, 155-178.
- Yan, M., and Ramström, O., 2004, *Molecular Imprinted Materials; Science and Technology*, CRC Press, New York.