

DAFTAR PUSTAKA

- Abdel-Halim, H., Traini, D., Hibbs, D., Gaisford, S., and Young, P., 2011, Modelling of Molecular Phase Transitions in Pharmaceutical Inhalation Compounds: An In Silico Approach, *Eur. J. Pharm. Biopharm.*, 78, 83–9.
- Alexander, C., Andersson, H.S., Andersson, L.I., Ansell, R.J., Kirsch, N., Nicholls, I.A., O'Mahony, J., and Whitcombe, M.J., 2006, Molecular Imprinting Science and Technology: A Survey of The Literature for the Years Up to and Including 2003, *J. Mol. Recognit.*, 19,106-180.
- Arshandy, R., and Mosbach K., 1981, Synthesis of Substrate-Selective Polymers by Hostguest Polymerization, *Macromol. Chem.*, 182, 2, 687-692.
- Azenha, M., Szeftczyk, B., Loureiro, D., Kathirvel, P., Cordeiro, M. N. D. S., and Silva, A. F., 2013, Computational and Experimental Study of the Effect of PEG in the Preparation of Damascenone-Imprinted Xerogels, *Langmuir*, 29, 2024.
- Butler, A.R., and Wu, Y.L., 1992, Artemisinin (Qinghaosu): A New Type of Antimalarial Drug, *Chem. Soc. Rec*, 21, 85–90.
- Cheng, Y., Jiang, P., Lin S., Li Y., and Dong, X., 2014, An Imprinted Fluorescent Chemosensor Prepared Using Dansyl-modified β -Cyclodextrin as the Functional Monomer for Sensing of Cholesterol with Tailor-made Selectivity, *Sensor. Actuat. B-Chem.*, 193,838-843.
- Cleland, D., Olsson, G. D., Karlsson, B. C. G., Nicholls, I. A., and McCluskey, A., 2014, Molecular Dynamics Approaches to the Design and Synthesis of PCB Targeting Molecularly Imprinted Polymers: Interference to Monomer–Template Interactions in Imprinting of 1,2,3-trichlorobenzene, *Org. Biomol. Chem.*, 12, 844.
- Cormack, P.A.G., and Elorza, A.Z., 2004, Molecularly imprinted polymers: synthesis and characterization, *J. Chromatogr. B. Analyt. Technol. Biomed. Life Sci.*, 804,173-182.
- Danielsson, B., 2008, Artificial Receptors, *Adv. Biochem. Engin./Biotechnol.*, 109, 97-122.
- Dipojono, H.K., 2001, Simulasi Dinamika Molekul, *Prosiding Seminar Nasional Hamburan Neutron dan Sinar X ke 4*, 6 Juni 2001, Serpong.

- Dong, W., Yan, M., Zhang, M., Liu, Z., and Li Y., 2005, A Computational and Experimental Investigation of The Interaction between The Template Molecule and The Functional Monomer Used in The Molecularly Imprinted Polymer, *Anal. Chim. Acta.*, 542, 186-192.
- Dourado, E. M. de A., 2011, Computer Simulations of Adsorption and Molecular Recognition Phenomena in Molecular Imprinted Polymer, *Thesis*, School of Engineering UoE, Edinburgh.
- Gong, X.Y., Cao, X.J., 2011, Preparation of Molecularly Imprinted Polymers for Artemisinin Based on The Surfaces of Silica Gel, *J. Biotech.*, 153, 8-14.
- Haupt, K., Linares, A.V., Bompert, M., Bui, B.T.S., 2011, Molecularly Imprinted Polymers, *Top. Curr.Chem.*, 325, 1-28
- Jeffrey, G. A., and Saenger, W., 1991, *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.
- 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.
- Khan, M.S., Wate. P.S., and Krupadam R.J., 2012, Combinatorial Screening of Polymer Precursors for Preparation of Benzo[a]pyrene: An Ab Initio Computational Approach, *J. Mol. Model.*, 18, 1969-1981.
- 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.
- Kitchen, D., Decornez, H., Furr, J., dan Bajorath, J., 2004, Docking and Scoring in Virtual Screening for Drug Discovery: Methods and Application, *Nat. Rev.*, 4, 935-949.
- Klayman, D.L., 1985, Qinghaosu (Artemisinin) An Antimalarial Drug From China, *Sci.*, 228, 1049-1055.
- Krupadam, R. J., Patel, G. P., and Balasubramanian, R., 2012, Removal of Cyanotoxins from Surface Water Resources Using Reusable Molecularly Imprinted Polymer Adsorbents, *Environ. Sci. Pollut. Res.*, 19, 1841.
- Li, Y., and Wu, Y.L., 2003, An Over Four Millennium Story Behind Qinghaosu (Artemisinin)—A Fantastic Antimalarial Drug from A Traditional Chinese Herb, *Curr. Med. Chem.* 10, 2179-2230.

- Mahony J.O., Nolan K., Smyth M.R., and Mizaikoff B., 2005, Molecularly imprinted polymers - potential and challenges in analytical chemistry, *Anal. Chim. Acta*, 534, 31–39.
- 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.*, 11, 4797-810.
- Paul, W., Bedrov, D., and Smith, G. D., 2006, Glass Transition in 1,4-Polybutadiene: Mode-Coupling Theory Analysis of Molecular Dynamics Simulations Using a Chemically Realistic Model, *Phys. Rev. E Stat. Nonlinear Soft Matter Phys.*, 74, 021501
- Piletsky, S.A., and Whitcombe M.J., 2013, *Designing Receptor for the Next Generation of Biosensor*, Springer, London.
- Pople, J. A., and Beveridge, D. L., 1970, *Approximate Molecular Orbital Theory*, McGraw-Hill, New York.
- Pranowo, H. D., 2006, *Kimia Komputasi*, Pusat Kimia Komputasi Indonesia Austria, Jurusan Kimia FMIPA UGM, Yogyakarta.
- Pranowo H. D., 2009, Teknologi Informasi dalam mendukung Riset di Bidang Kimia, *Prosiding Seminar Nasional Kimia dan Pendidikan Kimia*, 18 Maret 2009, Surakarta.
- Riahi, S., Eynollahi, S., Ganjali, M.R., dan Norouzi, P., 2009, Computational Approach to Investigation of Template/Monomer Complex in Imprinted Polymers; Dinitrobenzene Sensor, *Int. J. Electrochem. Sci.*, 5, 509–516.
- Santos, C.B.R., Vieira, J.B., Formigosa, A.S., Costa, E.V.M., Pinheiro, M.T., Silva, J.O., Macedo, C.W.J., dan Carvalho, J.C.T., 2014, Validation of Computational Methods Applied in Molecular Modeling of Artemisinin with Antimalarial Activity, *J. Comput. Theor. Nanosci.*, 11(3), 1-9.
- 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.
- Sellergen, B., 2001, *Molecularly Imprinted Polymers: Man-Made Mimics of Antibodies and Their Applications in Analytical Chemistry*, Elsevier, Amsterdam.

- Spivak, D.A., 2005, Optimization, Evaluation, and Characterization of Molecularly Imprinted Polymers, *Adv. Drug. Deliv. Rev.*, 57, 1779-1794.
- Sreenivasan, K., 2001, The Effect of Polymerisation Methods on The Adsorption Capacity of HEMA Based Molecularly Imprinted Polymers. *Journal of Polymer Research-Taiwan*, 8, 197-200.
- Stewart, J. J. P., 1989, Optimization of Parameters for Semiempirical Methods 11. Applications, *J. Comput. Chem.*, 10, 221-264.
- Stewart, J. J. P., 2004, Comparison of The Accuracy of Semiempirical and Some DFT Methods for Predicting Heats of Formation, *J. Mol. Model.*, 10, 6-12.
- Tahir. I., Ahmad, M.N. dan Dahyar A., 2012, Penggunaan Metode Semiempirik PM3 Untuk Evaluasi Interaksi Allopurinol-Asam Metakrilat Untuk Sintesis Polimer Tercetak Molekul, *Chem. Prog.*, 1, 11-18.
- Vanjani, D., 2017, Rancangan Berbasis Komputer Untuk Polimer Tercetak Molekul Auksin Berdasarkan Simulasi Dinamika Molekul, *Skripsi*, Fakultas MIPA Universitas Gajah Mada, Yogyakarta.
- Vasapollo, G., Sole, R.D., Mergola, L., Lazzo, 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.
- 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.
- Wulff, G., dan Sarhan, A., 1972, The Use of Polymers with Enzyme-analogous Structures for The Resolution of Racemates, *Angew. Chem. Int. Ed.*, 11, 341–344.
- Wulff, G. dan Biffis, A., 2001, *Molecularly Imprinted Polymers: Man-Made Mimics of Antibodies and their Applications in Analytical Chemistry*, 23, 1st Ed., Elsevier, Amsterdam.
- Yao, J., Li, X., dan Qin, W., 2008, Computational Design and Synthesis of Molecularly Imprinted Polymers with High Selectivity for Removal of Aniline from Contaminated Water, *Anal. Chim. Acta*, 610, 282-288.
- Yan, H., and Row, K.H., 2006, Characteristic and Synthetic Approach of Molecularly Imprinted Polymer, *Int. J. Mol. Sci.*, 7, 155-178.
- Ye L, 2013, *Molecular Imprinting: Principles and Applications of Micro-and Nanostructure Polymers*, Pan Stanford Publishing, Singapore.
- Young, D.C., 2001, *Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems*, John Wiley & Sons, Inc., United State of America.