

DAFTAR PUSTAKA

- Abdurrahman, F., 2018, Pemodelan dan Simulasi untuk Rancangan Polimer Tercetak Molekul Brazilein, *Skripsi*, Departemen Kimia, Fakultas Matematika dan Ilmu Pengetahuan Alam, Universitas Gadjah Mada, Yogyakarta.
- Anonim, 2018, *Indonesia : Narkoba dalam Angka tahun 2017*.
- Armunanto, R., Schwenk, C.F., and Rode, B.M., 2003, Structure and dynamics of hydrated Ag(I): Ab Initio Quantum Mechanical-Molecular Mechanical Molecular Dynamics Simulation, *J. Phys. Chem. A*, 107(17), 3132–3138.
- Ayers, P.W., Banerjee, P., Burger, S.K., Carbo-Dorca, R., Cuevas-Saavedra, R., Fares, W., Ghosh, D. C., Heidar-Zadeh, F., Islam, N., Kaya, C., Kaya, S., Liu, Y., Miranda-Quintan, R. A., Mohammed, A. A. K., Nalewajski, R. F., Obot, I. B., Rabi, N., Safi, Z. S., and Saha, S. K., 2018, Conceptual Density Functional Theory and its Application in the Chemical Domain, Islam, N. and Kaya, S. (eds), *Apple Academic Press*, Inc.
- Bagayoko, D., 2016, Understanding density functional theory (DFT) and completing it in practice, *AIP Adv.*, 4, 1–12.
- Barone, V. and Cossi, M., 1998, Quantum Calculation of Molecular Energies and Energy Gradients in Solution by a Conductor Solvent Model, *J. Phys. Chem. A*, 102(97), 1995–2001.
- Barone, V., Cossi, M., and Tomasi, J., 1997, Geometry Optimization of Molecular Structures in Solution by the Polarizable Continuum Model, *J. Comput. Chem.*, 19(4), 404–417.
- Chen, J., 2018, The Development and Comparison of Molecular Dynamics Simulation and Monte Carlo Simulation, *IOP Conf. Ser. Earth Environ. Sci.*, 128.
- Cowen, T., Karim, K., and Piletsky, S., 2016, Computational Approaches in the Design of Synthetic Receptors – A Review, *Anal. Chim. Acta*, 936, 62–74.
- Diñeiro, Y., Menéndez, M.I., Blanco-López, M.C., Lobo-Castañón, M.J., Miranda-Ordieres, A.J., and Tuñón-Blanco, P., 2005, Computational approach to the rational design of molecularly imprinted polymers for voltammetric sensing of homovanillic acid, *Anal. Chem.*, 77(20), 6741–6746.
- 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(1), 117–124.

Ercanli, T. and Boyd, D.B., 2005, Evaluation of computational chemistry methods: Crystallographic and cheminformatics analysis of aminothiazole methoximes, *J. Chem. Inf. Model.*, 45(3), 591–601.

Fernandes, L. S., Homem-De-Mello, P., De Lima, E. C., and Honorio, K. M., 2015, Rational Design of Molecularly Imprinted Polymers for Recognition of Cannabinoids: A Structure-Property Relationship Study, *Eur. Polym. J.*, 71, 364–371.

Hackney, A.C., 2018, Narcotics,. In, *Doping, Performance Enhancing Drugs, and Hormones in Sport.*, pp. 91–101.

Harper, L., Powell, J., and Pijl, E.M., 2017, An Overview of Forensic Drug Testing Methods and their Suitability for Harm Reduction point-of-care Services, *Harm Reduct. J.*, 14(1), 1–13.

Hedman, F., 2006, Algorithms for Molecular Dynamics Simulations: Advancing the Computational Horizon, *Ph.D thesis*, Stockholms Universitet, Stockholm.

Hsin, J., Arkhipov, A., Yin, Y., Stone, J.E., and Schulten, K., 2008, Using VMD: An introductory tutorial, *Curr. Protoc. Bioinforma.*, 24(1), 5.7.1-5.7.48.

Huestis, M.A., 2007, Human Cannabinoid Pharmacokinetics, *Chem. Biodivers.*, 4, 1770–1804.

Jamieson, L.T.J., Baxter, G.S., and Murray, P.J., 2017, Identifying Suitable Detection Dogs, *Appl. Anim. Behav. Sci.*, 195, 1–7.

Janezic, D. and Merzel, F., 1995, An Efficient Symplectic Integration Algorithm for Molecular Dynamics Simulations, *J. Chem. Inf. Model.*, 35, 321–326.

Jeffrey, G.A. and Saenger, W., 1991, *Hydrogen Bonding in Biological Structures*, Springer-Verlag, New York.

Jezierski, T., Adamkiewicz, E., Walczak, M., Sobczyńska, M., Górecka-Bruzda, A., Ensminger, J., and Papet, E., 2014, Efficacy of Drug Detection by Fully-trained Police Dogs varies by Breed, Training Level, Type of Drug and Search Environment, *Forensic Sci. Int.*, 237, 112–118.

Karim, K., Cowen, T., Guerreiro, A., Piletska, E., Whitcombe, M.J., and Piletsky, S.A., 2017, A Protocol for the Computational Design of High Affinity

Molecularly Imprinted Polymer Synthetic Receptors, *Glob. J. Biotechnol. Biomater. Sci.*, 3, 1–7.

Karlsson, C.G., Mahony, J.O., 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, *Chart*, 9, 13297–13304.

Krishnan, H., Islam, K.M.S., Hamzah, Z., and Ahmad, M.N., 2017, Rational Computational Design for the Development of Andrographolide Molecularly Imprinted Polymer,. In, *AIP Conference Proceedings*. American Institute of Physics, pp. 1–7.

Kuzkin, V.A., 2014, On Angular Momentum Balance for Particle Systems with Periodic Boundary Conditions, *J. Appl. Math. Mech.*, 95, 1290–1295.

Lavrinenko, Y.S., Morozov, I. V., and Valuev, I.A., 2016, Reflecting Boundary Conditions for Classical and Quantum Molecular Dynamics Simulations of Nonideal Plasmas, *Contrib. to Plasma Phys.*, 56, 448–458.

Liu, S., Wang, L., and Mobley, D.L., 2015, Is Ring breaking feasible in relative binding free energy calculations ?, *J. Chem. Inf. Model.*, 55, 727–735.

Long, M.R.P. and Isborn, C.M., 2017, Combining Explicit Quantum Solvent with a Polarizable Continuum Model, *J. Phys. Chem. B*, 121, 10105–10117.

Mark, A.E., Malde, A.K., Zuo, L., Breeze, M., Stroet, M., Poger, D., Nair, P. C., and Oostenbrink, Chris., 2011, An Automated force field Topology Builder (ATB) and repository: Version 1.0, *J. Chem. Theory Comput.*, 7, 4026–4037.

Martins, N., Carreiro, E.P., Locati, A., Ramalho, J.P.P., Cabrita, M.J., Burke, A.J., and Garcia, R., 2015, Design and development of molecularly imprinted polymers for the selective extraction of deltamethrin in olive oil: An integrated computational-assisted approach, *J. Chromatogr. A*, 1409, 1–10.

Martins, S.A., Sousa, S.F., Joa, M., and Fernandes, P.A., 2014, Prediction of Solvation Free Energies with Thermodynamic Integration Using the General Amber Force Field, *J. Chem. Theory Comput.*, 10, 3570–3577.

Maxwell, J.C. and Brecht, Mary-Lynn., 2011, Methamphetamine: Here we go again ?, *Addict. Behav.*, 36(12), 1168–1173.

Mennucci, B., 2010, Continuum solvation models: What else can we learn from them ?, *J. Phys. Chem. Lett.*, 1(10), 1666–1674.

- Pitaloka, C. I. P., 2018, Rancangan Berbasis Komputter untuk Polimer Tercetak Molekul Kurkumin berdasarkan Simulasi Dinamika Molekular, *Skripsi*, Departemen Kimia Fakultas Matematika dan Ilmu Pengetahuan Alam Universitas Gadjah Mada, Yogyakarta.
- Puder, K.S., Kagan, D. V, and Morgan, J.P., 1988, Illicit Methamphetamine: Analysis, Synthesis, and Availability, *Am. J. Drug Alcohol Abus.*, 14(4), 463–473.
- Röck, F., Barsan, N., and Weimar, U., 2008, Electronic Nose: Current Status and Future Trends, *Chem. Rev.*, 108(2), 705–725.
- Roe, D.R. and Cheatham, T.E., 2013, PTRAJ and CPPTRAJ: Software for Processing and Analysis of Molecular Dynamics Trajectory Data, *J. Chem. Theory Comput.*, 9, 3084–3095.
- Shen, G. and Zhao, M., 2015, The Application of Molecularly Imprinted Polymers, *J. Mater. Sci. Chem. Eng.*, 3, 87–89.
- Skinner, H.F., 1990, Methamphetamine synthesis via hydriodic phosphorus reduction of ephedrine acid/red, *Forensic Sci. Int.*, 48, 123–134.
- Sommers, I. and Baskin, D., 2016, Methamphetamine Use and Violence, *J. Drug Issues*, 36(1), 77–96.
- Sousa, J.A., Silva, P.P., Machado, A.E.H., Reis, M.H.M., Romanielo, L.L., and Hori, C.E., 2013, Application of computational chemistry methods to obtain thermodynamic data for hydrogen production from Liquefied Petroleum Gas, *Brazilian J. Chem. Eng.*, 30(1), 83–93.
- Svenson, J., Zheng, N., and Nicholls, I.A., 2004, A molecularly imprinted polymer-based synthetic transaminase, *J. Am. Chem. Soc.*, 126(27), 8554–8560.
- Takano, Y. and Houk, K.N., 2005, Benchmarking the Conductor-like Polarizable Continuum Model (CPCM) for Aqueous Solvation Free Energies of Neutral and Ionic Organic Molecules, *J. Chem. Theory Comput.*, 1(1), 70–77.
- Tuckerman, M.E. dan Martyna, G.J., 2000, Understanding Modern Molecular Dynamics : Techniques and Applications, *J. Phys. Chem. B*, 104(2), 159–178.
- United Nations Office on Drugs and Crime, 2016, *Terminology and Information on Drugs: Third Edition*, United Nations Publication : New York.

- Urbano, F.J., Bisagno, V., and Garcia-Rill, E., 2017, Arousal and drug abuse, *Behav. Brain Res.*, 333, 276–281.
- Wang, J., Wolf, R. M., Caldwell, J.W., Kollman, P. A., dan Case, D. A., 2004, Development and Testing of a General Amber Force Field, *J. Comput. Chem.*, 25(9), 1157–1174.
- Wilson, A.D. and Baietto, M., 2009, Applications and advances in electronic-nose technologies, *Sensors*, 9, 5099–5148.
- Wu, X., Du, J., Li, M., Wu, L., Han, C., and Su, F., 2018, Recent advances in green reagents for molecularly imprinted polymers, *RSC Adv.*, 8(1), 311–327.
- Xiao, D., Jiang, Y., and Bi, Y., 2018, Molecularly imprinted polymers for the detection of illegal drugs and additives: a review, *Microchim. Acta*, 185(4), 1–20.
- Zhang, L., Chen, L., Zhang, H., Yang, Y., and Liu, X., 2017, Recognition of 5-fluorouracil by thermosensitive magnetic surface molecularly imprinted microspheres designed using a computational approach, *J. Appl. Polym. Sci.*, 45468, 1–9.
- Zhao, M., Chen, X., Zheng, H., Yan, H., and Zhang, H., 2014, Well-defined hydrophilic molecularly imprinted polymer microspheres for efficient molecular recognition in real biological samples by facile raft coupling chemistry, *Biomacromolecules*, 15, 1663–1675.
- Zhou, Y., Wang, S., Ji, J., Lou, H., and Fan, P., 2018, Hemp (*Cannabis sativa* L.) Seed Phenylpropionamides Composition and Effects on Memory Dysfunction and Biomarkers of Neuroinflammation Induced by Lipopolysaccharide in Mice, *ACS Omega*, 3, 15988–15995.