



## DAFTAR PUSTAKA

- Adiwinata, R, dan Nelwan, E.J., 2015, Snakebite In Indonesia, *Acta. Med. Indones.*, 47(4), 358-365.
- Alder, B.J., dan Wainright, T.E., 1957, Phase Transition for A Hard Sphere System, *J. Chem. Phys.*, 27, 1208-1209.
- Allen, M.P., dan Tildesley, D.J., 1987, *Computer Simulation of Liquids*, Oxford University Press, Oxford.
- Armunanto, R., 2004, Simulation of Ag<sup>+</sup>, Au<sup>+</sup>, Co<sup>2+</sup> in Water, Liquid Ammonia and Water-Ammonia Mixture, *Dissertation*, Leopold-Franzens-Universitat Innsbruck, Austria.
- Bisswanger, H., 2002, *Enzyme Kinetics: Principles and Methods*, Wiley-VCH; Weinheim, Germany.
- Born, M., dan von Karman, 1912, Uber Schwingungen in Raumgittern, *Physik*, 13, 297-309.
- Burke, J.E., dan Dennis, E.A., 2009, Phospholipase A<sub>2</sub> Structure or Function, Mechanism, and Signaling, *J. Lipid. Res.*, 50, S237-S242.
- Byrd, J., Vila, F., Takimoto, Y., dan Rehr, J., 2005, *Molecular Dynamics Simulations of Ca<sup>2+</sup> Hydration and The Optical Response of Clustered Water*, Institute for Nuclear Theory, University of Washington.
- Chang, C.C., Chuang, S.C., Lee, C.Y., dan Wei, J.W., 1972, Role of Cardiotoxin and Phospholipase A in the Blockade of Nerve Conduction and Depolarization of Skeletal Muscle Induced by Cobra Venom, *Br. J. Pharm.*, 44, 752-764.
- Chippaux, J.P., Williams, V.J, dan White, J., 1991, Snake Venom Variability: Methods of Study, Results, and Interpretation, *Toxicon.*, 29, 1279-1303.
- Dahanayake, J.N., Gautam, D.N., Verma, R., dan Mitchel, K.K.R., 2016, To Keep or Not to Keep? The Question of Crystallographic Waters for Enzyme Simulations in Organic Solvent, *Mol. Simmul.*, 42(12), 1001-1013.
- Drakenberg, T., 2002, Calcium-43 NMR of Calcium-Binding Proteins: Methods in Molecular Biology, *Methods. Mol. Biol.*, 173, 217-230.
- Ferenczi, M.A., Bershitsky, S.Y., Koubassova, N.A., Kopylova, G.V., Fernandez, M., Narayanan, T., dan Tsaturyan, A.K., 2014, Why Muscle is an Efficient Shock Absorber, *PLoS. One.*, 9(1), 1-6.



Fremont, D.H., Anderson, D.H., Wilson, I.A., Dennis, E.A, dan Xuong, N.H., 1992, Crystal Structure of Phospholipase A2 from India Cobra Reveals a Trimeric Association, *Proc. Natl. Acad. Sci.*, 90, 342-346.

Glusker, J.P., Katz, A.M.Y.K, dan Bock, C.W., 1999, Metal Ion in Biological System, *Rigaku J.*, 16(2), 8-17.

Gutierrez, J.M., Warrel, D.A., Williams, D.J., Jensen, S., Brown, N., Calvete, J.J., 2013, The Need for Full Integration of Snakebite Envenoming within a Global Strategy to Combat the Neglected Tropical Diseases: The Way Forward, *PLoS.Negl.Trop. Dis.*, 7(6), e2162.

Hage, K.E., Hedin, F., Gupta, P.K., Meuwly, M., dan Karplus, M., 2018, Valid Molecular Dynamic Simulation of Human Hemoglobin Require a Surprisingly Large Box Size, *eLife*, 7, e35560.

Harris, J.B., dan Davey, T.S., 2013, Secreted Phospholipases A<sub>2</sub> of Snake Venoms: Effects on the Peripheral Neuromuscular System with Comments on the Role of Phospholipases A<sub>2</sub> in Disorders of the CNS and Their Uses in Industry, *Toxins.*, 5(12), 2533-2571.

Ho, Y.-P., Yang, M.W., Chen, L.T., dan Yang, Y.C., 2007, Relative Calcium-Binding Strength of Amino Acids Determined Using the Kinetic Method, *Rapid. Commun. Mass Spectrom.*, 21, 1083-1089.

Jalilehvand, F., Spangberg, D., Lindqvist-Reis, P., Hermansson, K., Persson, I., Sandström, M., 2001, Hydration of the Calcium Ion. An EXAFS, Large-Angle X-ray Scattering, and Molecular Dynamics Simulation Study. *J. Am. Chem. Soc.*, 123, 431-441.

Janezic, D., dan Merzel, F., 1995, An Efficient Sympletic Integration Algorith for Molecular Dynamics Simulations, *J. Chem. Inf. Comput. Sci.*, 35, 321-326.

Jiao, D., 2006, Simulation of Ca<sup>2+</sup> and Mg<sup>2+</sup> Solvation Using Polarizable Atomic Multiple Potential, *J. Chem. Phys. B.*, 110(37), 18553-18559.

Kini, R.M., dan Evans, H.J., 1989, A Model to Explain the Pharmacological Effects of Snake Venom, *Toxicon.*, 27(6), 613-635.

Kitchen, D.B., Decomez, H., Furr, J.R., dan Bajorath, J., 2004, Docking and Scoring in Virtual Screening for Drug Discovery: Methods and Application, *Nat. Rev.Drug. Discov.*, 3(11), 935-949.

Kuo, I.Y., dan Ehrlich, B.E., 2015, Signaling in Muscle Contraction, *Cold Spring Harb.Perspect. Biol.*, 7, a006023.

Li, L., Darden, T.A., Freedman, S.J., Furie, B.C., Furie, B., Baleja, J.D., Smith, H., Hiskey, R.G., dan Pedersen, L.G., 1997, Refinement of the NMR Solution



Structure of the  $\gamma$ -Carboxyglutamic Acid Domain of Coagulation Factor IX Using Molecular Dynamics Simulation With Initial Ca<sup>2+</sup> Position Determined by A Genetic Algorithm, *Biochemistry*, 36, 2132-2138.

Mark, P. dan Nilsson, L., 2001, Structure and Dynamics of TIP3P, SPC, and SPC/E, Water Models at 298 K, *J. Phys. Chem. A.*, 105, 9954-9960.

Megyes, T., Grosz, T., Radnai, T., Bakó, I., dan Palinkas, G., 2004, Solvation of Calcium Ion in Polar Solvents: An X-ray Diffraction and Ab Initio Study, *J. Phys. Chem.*, 108, 7261-7271.

Menedez, C.A., Accordino, S.R., Gerbino, D.C., dan Appignanesi, G.A., 2016, Hydrogen Bond Dynamic Propensity Studies for Protein Binding and Drug Design, *Plos One*, 11(10), 1-12.

Ochiai, I.-E., 1991, Biomineralization: Principles and Applications in Bioinorganic Chemistry V, *J. Chem. Educ.*, 68(8), 627-630.

Oostenbrink, C., Villa, A., Mark, A.E., dan van Gunsteren, W.F., 2004, A Biomolecular Force Field Based on the Free Enthalpy of Hydration and Solvation: The GROMOS Force-Field Parameters Sets 53a5 and 53a6, *J. Comput. Chem.*, 25, 1656-1676.

Panagitou, E., 2015, The Linking Number in Systems with Periodic Boundary Conditions, *J. Comput. Phys.*, 300, 533-573.

Pearson, R.G., 1963, Hard and Soft Acids and Bases, *J. Am. Chem. Soc.*, 85, 3533-3539.

Penangsang, P., 2016, *Reptile Undercover: Mitos, Pasar, Komunitas, dan Mimpi Konservasi*, Pelangi Cendikia Insani, Depok.

Pranowo, H.D., dan Hetadi, A.K., 2011, *Pengantar Kimia Komputasi*, CV. LUBUK AGUNG, Bandung.

Roy, J., Charles, A., dan Laughton, 2010, Long-Timescale Molecular Dynamics Simulations of the Major Urinary Protein Provide Atomistic Interpretations of the Unusual Thermodynamics of Ligand Binding, *Biophysics J.*, 99(1), 218-226.

Scott, W.R.P., Hunenberger, P.H., Tironi, I.G., Mark, A.E., Billeter, S.R., Fennen, J., Torda, A.E., Huber, T., Kruger, P., dan van Gunsteren, W.F., 1999, The GROMOS Biomolecular Simulation Program Package, *J. Phys. Chem.*, 103, 3596-3607.

Settanni, G., dan Fersht, A.R., 2008, High Temperature Unfolding Simulations of the TRPZ1 Peptide, *Biophys J.*, 94(11), 4444-4453.



- Socher, E., dan Sticht, H., 2016, Mimicking Titration Experiments with MD Simulations: A Protocol for The Investigation of pH-dependent Effects on Proteins, *Scientific Reports*, 6(22523).
- Sousa, S.F., Coimbra, J.T.S., Fernandes, P.A., Marino, T., Ramos, M.J., dan Russo, N., 2015, Molecular Dynamics Analysis of FAAH Complexed with Anandamide, *Prog. in Theor. Chem.*, 29, 115-127.
- Steinbach, P.J., dan Brooks, B.R., 1994, New Spherical-Cutoff Methods for Long Range Forces in Macromolecular Simulations, *J. Comp. Chem.*, 15, 667-683.
- Tan, N. H., Wong, K. Y, dan Tan, C. H., 2017, Venomics of *Naja sputatrix*, the Javan Spitting Cobra: A Short Neurotoxin-driven Venom Needing Improved Antivenom Neutralization, *J. Proteom.*, 157, 18-32.
- Tang, N., dan Skibsted, L.H., 2016, Calcium Binding to Amino Acids and Small Glycine Peptides in Aqueous Solution: Toward Peptide Design for Better Calcium Bioavailability, *J Agric Food Chem.*, 64(21), 4376-4389.
- Tielman, D.P., dan Berendsen, J.C., 1996, Molecular Dynamics Simulations of A Fully Hydrated Dipalmitoylphosphatidylcholine Bilayer with Different Macroscopic Boundary Conditions and Parameters, *J. Chem. Phys.*, 105, 4871-4880.
- Tongraar, A., Liedl, K.R., dan Rode, B.M., 1997, Solvation of Ca<sup>2+</sup> in Water Studied by Born-Oppenheimer Ab Initio QM/MM Dynamics, *J. Phys. Chem.*, 101, 6299-6309.
- Utami, W., 2016, Reaktivitas Ion Kalsium (II) Dalam Amoniak Cair: Studi Simulasi Dinamika Molekuler Quantum Mechanical Charge Field (QMCF), *Disertasi*, Universitas Gadjah Mada, Yogyakarta.
- Uetz, P., Freed, P., dan Hosek, J., 2019, *The Reptile Database*, <http://www.reptile-database.org>, diakses 1 Mei 2019.
- van Buuren, A.R., 1993, A Molecular Dynamics Study of Decane/Water Interface, *J. Phys. Chem.*, 97(36), 9206-9212.
- Warrel, David., 2016, Guidelines For The Management of Snakebites: 2<sup>nd</sup> Edition, World Health Organization.
- Wittung, P.S., 2002, Role of Cofactors in Protein Folding, *Acc. Chem. Res.*, 35(4), 201-208.
- Yap, M. K. K., Tan, N. H., Sim, S. M., Fung, S. Y, dan Tan, C. H., 2014, Pharmacokinetics of *Naja sumatrana* (Equitorial Spitting Cobra) Venom



UNIVERSITAS  
GADJAH MADA

Studi Interaksi Ion Ca<sup>2+</sup> Pada Enzim Fosfolipase A2 1A (PLA21A) Dari Bisa Ular Kobra (Naja naja)

Melalui Kajian Simulasi Dinamika Molekul

THOMAS INDRA, Drs. Iqmal Tahir, M.Si; Dr.Sc. Aulia Sukma Hutama

...

Universitas Gadjah Mada, 2019 | Diunduh dari <http://etd.repository.ugm.ac.id/>

and Its Major Toxin in Experimentally Envenomed Rabbits, *PloS Negl. Trop. Dis.*, 8(6), 1-13.

Yelle, R.B., Park, N.S., dan Ichiye, T., 1995, Molecular Dynamics Simulations of Rubredoxin from *Clostridium pasteurianum*: Changes in Structure and Electrostatic Potential During Redox Reactions, *Protein*, 22, 154-167.