DAFTAR PUSTAKA

Alberts, B., Johnson, A., Lewis, J., Raff, M., Roberts, K., dan Walter, P., 2002. *Molecular Biology of the Cell, 4th Edition*, Garland Science, New York.

Allen, M.P. dan Tildesley, D.J., 1987, *Computer Simulation of Liquids*, Oxford University Press, Oxford.

Alonso, H., Bliznyunk, A.A., dan Gready, J.E., 2006, Combining Docking and Molecular Dynamic Simulations in Drug Design, *Med. Res. Rev.*, 5 (26), 531-568.

Armunanto, R., Schwenk, C.F., dan Rode, B.M., 2004, Gold(I) in Liquid Ammonia: Ab Initio QM/MM Molecular Dynamic Simulations*, J. Am. Chem. Soc*., 126, 9934.

Bai, L., dan Zhu, W., 2006, p53: Structure, Function and Therapeutic Applications, *J. Cancer Molecules*, 4(2), 141-153.

Batoulis, H., Schmidt, T. H., Weber, P., Schloetel, J. G., Kandt, C., dan Lang, T., 2016, Concentration Dependent Ion-Protein Interaction Patterns Underlying Protein Oligomerization Behaviours, *Scientific Reports*, 6, 2–10.

Baxevanis, A.D., dan Outlette, B.F., 2001, *Bioinformatics A Pratical Guide to the Analysis of Genes and Protein 2nd Edition*, Wiley Interscience, USA.

Becker, O. M., MacKerrel, A. D., Roux, B., dan Watanabe, M., 2001, *Computaional Biochemistry and Biophysics,* Mercel Dekker, Inc., New York.

Beg, Q., Kapoor, M., Mahajan, L., dan Hoondal, G., 2001, Microbial Xylanases and their Industrial Applications: a review, *Microbiol. Biotechnol.*. 56, 326-338.

Bernal-Uruchurtu, M.I., dan Ortega-Blake, I., 1995, A Refined Monte Carlo study of Mg^{2+} and Ca^{2+} Hydration. *J. Chem. Phys*, 4(103), 1588–1598.

Bourdon, J.C., Laurenzi, V.D., Melino, G., dan Lane, D., 2003, p53: 25 years of Reaserch and More Question to Answer , *Cell Death and Differentiation 10th Edition*, 397-399.

Bykov, V.J.N., Issaeva, N., Shilov, A., Hultcrantz, M., Pugacheva, E., Chumakov, P., Bergman, J., Wiman, K.G., dan Selivanova, G., 2002, Restoration of the Tumor Suppresor Function to Mutant p53 by A Low-Molecular Weight Compound, *Nat. Med.*, 3(8), 282 – 28.

Case, D.A., Betz, R.M., Botello-Smith, W., Cerutti, D.S., Cheatham, T.E., Darden, T.A., Duke, R.E., Giese, T.J., Gohlke, H., Goetz, A.W., Homeyer, N., Izadi, S., Janowski, P., Kaus, J., Kovalenko, A., Lee, T.S., LeGrand, S., Li, P., Lin, C., Luchko, T., Luo, R., Madej, B., Mermelstein, D., Merz, K.M., Monard, G., Nguyen, H., Nguyen, H.T., Omelyan, I., Onufriev, A., Roe, D.R., Roitberg, A., Sagui, C., Simmerling, C.L., Swails, J., Walker, R.C., Wang, J., Wolf, R.M., Wu, X., Xiao, L., York, D.M., dan Kollman, P.A., 2016, *AMBER 2016*, University of California, San Fransisco.

Cornell, W.D., Cieplak, P., Bayly, C.I., Gould, I.R., Merz, K.M., dan Ferguson, D.M., 1995, A Second Generation Force Field for the Simulation of Proteins, Nucleic Acids, and Organic Molecules, *J. Am. Chem. Soc.*, 117, 5179-5197.

De Courcy, B., Pedersen, L.G., Parisel, O., Gresh, N., Silvi, B., Pilmé, J., dan Piquemal, J.P., 2010, Understanding Selectivity of Hard and Soft Metal Cations within Biological Systems Using the Subvalence Concept. 1. Application to Blood Coagulation: Direct Cation-Protein Electronic Effects Versus Indirect Interactions Through Water Networks. *J. Chem. Theory Comput.*, 6(4), 1048–1063.

Dolmetsch, R.E., Lewis, R.S., Goodnow, C.C., dan Healy, J.I., 1997, Differential Activation of Transcription Factors Induced by Ca^{2+} Response Amplitude and Duration, *Nature,* 386, 855–858.

Falke, J.J., Drake, S.K.,Hazard, A.L., dan Peersen, O.B., 1994, *Molecular Tuning of Ion Binding to Calcium Signaling Proteins*, *Quarterly Revincs of Biophysics*, 27(3), Department of Chemistry and Biochemistry, University of Colorado, Boulder.

Friedman, R., 2011, Ions and The Protein Surface Revisited: Extensive Molecular Dynamics Simulations and Analysis of Protein Structures in Alkali-Chloride Solutions, *J. Phys. Chem. B.*, 115(29), 9213–9223.

Frenkel, D., dan Smit, B., 2002, *Understanding Molecular Simulation from Algoritms to Applications, 2nd Edition*, Academic Press, San Diego.

George, D.P., 2011, P53 How Crucial Is Its Role in Cancer?, *Int. J. Curr. Pharm. Res.*, 2(3), 19–25.

Haile, J.M., 1992, *Molecular Dynamics Simulation: Elementary Methods*, Wiley-Interscience, Clemson.

Hemmer, M.C., 2006, *Handbook of Vibrational Spectroscopy*, John Willey & Sons Inc., New Jersey.

Hitzenberger, M., dan Hofer, T.S., 2016, The Influence of Metal-Ion Binding on The Structure and Surface Composition of Sonic Hedgehog: A Combined Classical and Hybrid QM/MM MD Study, *Phys. Chem. Chem. Phys*., 32(18), 22254–22265.

Hofer, T.S., dan Van Gunsteren, W.F., 2012, Molecular BioSystems Exploring the Properties of Small Molecule Protein Binding via Molecular Simulations : The TRSH – p53 Core Domain Complex W, *Mol. Biosyst*., 2891–2900.

Humphrey, W., Dalke, A., dan Schulten, K., 1996, VMD: Visual Molecular Dynamics, *J. Mol. Graph*., 14, 33-38.

Jalilehvand, F., Spangberg, D., Lindqvist-Reis, P., Hermansson, K., Persson, I., dan 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.

Jeffrey, G.A. dan Saenger, W., 1991, *Hydrogen Bonding in Biological Structure*, Springer-Verlaig, Berlin.

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.

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 γ-Carboxyglutamic Acid Domain of Coagulation Factor IX Using Molecular Dynamics Simulation With Initial Ca^{2+} 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., Bako, 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.

Molinelli, A., 2004, *Molecularly Imprinted Polymers : Towards a Rational Understanding of Bio mimetic Materials*, Georgia Institute of Technology, Georgia.

Naor, M.M., Van Nostrand, K., Dellago, C., 2003, Car–Parrinello Molecular Dynamics Simulation of the Calcium Ion in Liquid Water, *Chem. Phys. Lett.*, 369, 159–164.

Pearson, R.G., 1995, Hard and Soft Acids and Bases, *J. Am. Chem. Soc*., 85, 3533-3539.

Pettersen, E.F., Goddard, T.D., Huang, C.C., Couch, G.S., Greenblatt, D.M., Meng, E.C., dan Ferrin, T.E., 2004, UCSF Chimera – A Visualization System for Exploratory Research and Analysis, *J. Comput. Chem*., 25, 1605-1612.

Pidcock, E., dan Moore, G. R., 2001, Structural Characteristics of Protein Binding Sites for Calcium and Lanthanide Ions, *Journal of Biological Inorganic Chemistry*, 6(5–6), 479–489.

Pranowo, H.D., dan Hetadi, A.K.R., 2010, *Pengantar Kimia Komputasi*, Lubuk Agung, Bandung.

Price, S.A., Wilson, L.M., 2006, *Patofisiologi Konsep Klinis Proses-Proses Penyakit Volume 2, Edisi 6,* EGC, Jakarta.

Rehder, D., 2008, *Introduction to Bioanorganic Chemistry*, University of Lund, Sweden.

Satoh, A., 2011, *Introduction to Practice of Molecular Simulation: Molecular Dynamics, Monte Carlo, Brownian Dynamics, Lattice Bolzmann and Dissipative Particle Dynamic,* Elsevier Insights, Amsterdam.

Schwenk, C.F., Loeffler, H.H., dan Rode, B.M., 2001, Dynamics of the Solvation Process of Ca^{2+} in Water, *Chem. Phys. Lett*., 349(1–2), 99–103.

Tongraar, A., Liedl, K.R., dan Rode, B.M., 1997, Solvation of Ca^{2+} 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), *Tesis*, Pascasarjana Kimia FMIPA Universitas Gadjah Mada, Yogyakarta.

Young, D.C., 2001, *Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems*, John Willey & Sons Inc., New Jersey

.