

## DAFTAR PUSTAKA

- Alberts, B., Johnson, A., Lewis, J., Raff, M., and Roberts, K., 2002, *Molecular Biology of the Cell*, 4th ed., *Garland Science*, New York.
- Allen, M.P., 2004, *Introduction to Molecular Dynamics Simulation*, John von Neumann Institute for Computing Publisher, Jülich, 1-5.
- Almog, N., 2010, Molecular Mechanism Underlying Tumor Dormancy, *Cancer Letters*, 294, 139-146.
- Bykov, V.J.N., Issaeva, N., Shilov, A., Hultcrantz, M., and Pugacheva, E., 2002, Restoration of the Tumor Suppressor Function to Mutant p53 by a Low-Molecular Weight Compound, *Nat. Med.*, 8, 282 – 288.
- Bykov, V.J., Issaeva, N., Zache, N., Shilov, A., and Hultcrantz, M., 2005, Reactivation of Mutant p53 and Induction of *Apoptosis* in Human Tumor Cells by Maleimide Analogs, *J. Biol. Chem.*, 280, 30384–30391.
- Cornell, W.D., Cieplak, P., Bayly, C.I., Gould, I.R., Merz, K.M., and 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.
- Cui, Q., Sulea, T., Schrag, J. D., Munger, C., Hung, M., Naïm, M., Cygler, M., and Purisima, E.O., 2008, Molecular Dynamics—Solvated Interaction Energy Studies of Protein–Protein Interactions: The MP1–p14 Scaffolding Complex, *J. Mol. Biol.*, 379, 787-802.
- Danielson, M.L., Desai, P.V., Mohutsky, M.A., Wrighton, S.A. and Lill, M.A., 2011, Potentially Increasing the Metabolic Stability of Drug Candidates via Computational Site of Metabolism Prediction by CYP2C9: The Utility of Incorporating Protein Flexibility via an Ensemble of Structures, *Eur. J. Med. Chem.*, 46, 3953–3963.
- Dastmalchi, S., Mivehroud, M.H., and Sokouti, B., 2016, *Methods and Algorithms For Molecular Docking-based Drug Design and Discovery*, IGI Global, Hershey, 8-9.
- Desheng, L., Jian, G., Yuanhua, C., Wei, C., Huai, Z., and Mingjuan, J., 2011, Molecular Dynamics Simulations and MM/GBSA Methods to Investigate Binding Mechanisms of Aminomethylpyrimidine Inhibitors with DPP-IV, *Bioorg. Med. Chem. Lett.*, 21, 6630-6635.

- 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, *Anal. Chim. Acta*, 647, 117–124.
- Giuliano M., Catalano A., Strizzi L., Vianale G., Capogrossi M., and Procopio A., 2000, Adenovirus-mediated Wild-type p53 Overexpression Reverts Tumourigenicity of Human Mesothelioma Cells, *Int. J. Mol. Med.*, 5, 591 – 596.
- Hadzi, D., Kidric, J., Koller, J., and Mavri, J., 1990, The Role of Hydrogen Bonding in Drug-Receptor Interactions, *J. Molec. Struct.*, 237, 139-150.
- Hainaut, P. and Hollstein, M., 2000, p53 and Human Cancer: The First Ten Thousand Mutations, *Adv. Cancer Res.*, 77, 81–137.
- Hanahan, D., and Weinberg, R.A., 2000, The Hallmarks of Cancer, *Cell*, 100, 57-70.
- Hayes, R., Imberti, S., Warr, G.G., and Atkin, R., 2013, The Nature of Hydrogen Bonding in Protic Ionic Liquids, *Angew. Chem.*, 125, 4721-4725.
- Jeffrey, G.A., 1997, *An Introduction to Hydrogen Bonding*, Oxford University Press, Oxford, 3-7.
- Joerger, A.C., Ang, H.C., Veprintsev, D.B., Blair, C.M., and Fersht, A. R., 2005, Structure of p53 Cancer Mutants and Mechanism or Rescue by Second-situs Suppressor Mutations, *J. Biol. Chem.*, 280(3), 16030.
- Kithcen, D.B., Decomez, H., Furr, J.R., and Bajorath, J., 2004, Docking and Scoring in Virtual Screening for Drug Discovery: Methods and Application, *Nat. Rev. Drug Discov.*, 3(11), 935-949.
- Konc, J., Lesnik, S., and Janezic, D., 2015, Modeling Enzyne-Ligand Binding in Drug Discovery, *J. Cheminform.*, 48(7), 1-8.
- Korb, O., Stützle, T., and Exner, T.E., 2006, PLANTS: Application of Ant Colony Optimization to Structure-based Drug Design, *Chem. Cent. J.*, 98, 247-258.
- Lahcen B., 2006, Anticancer Effect of Three Pyrazole Derivatives, *Pharmakon.*, 20, 124–130.
- Maliya, A., 2004, Perubahan Sel Menjadi Kanker dari Sudut Pandang Biologi Molekuler, *Infokes.*, 12, 34-46.

- Mark, P., and Nilsson, L., 2001, Structure and Dynamics of TIP3P, SPC, and SPC/E, Water Models at 298 K, *J. Phys. Chem. A.*, 105, 9954-9960.
- Maryam, A., Hojjat, S., Farshid, H., dan Massoud, A., 2015, Acticancer Activity and QSAR Study of Pyrazole Derivatives, *J. Mol. Graph.*, 61, 180-195.
- Masone, D., and Grosdidier, S., 2014, Collective Variable Driven Molecular Dynamics to Improve Protein-Protein Docking Scoring, *Comput. Biol. Chem.*, 49, 1-6.
- Meng, X.Y., Zhang, H.X., Mezei, M., and Cui, M., 2011, Molecular Docking: A Powerful Approach for Structure-based Drug Discovery, *Curr. Comput. Aided. Drug Des.*, 7(2), 146-157.
- Panaganto, E., 2015, The Linking Number in Systems with Periodic Boundary Conditions, *J. Comput. Phys.*, 300, 533–573.
- Purnomo, H., 2011, *Kimia Komputasi, Molecular Docking PLANTS, Penambatan Molekul PLANTS (Protein Ligand Ant System)*, Pustaka Pelajar, Yogyakarta.
- Sinha, R., Vidyarthi, A.S., and Shankaracharya, 2011, A Molecular Docking Study of Anticancer Drug Paclitaxel and Its Analogues, *Indian J. Biochem. Biophys.*, 48(2), 101-105.
- Sottriffer, C., 2014, *Strasbourg Summer School on Chemoinformatics*, University of Würzburg Press, Würzburg, 2-5.
- Sousa, S.F., Coimbra, J.T.S., Fernandes, P.A., Marino, T., Ramos, M.J., and Russo, N., 2015, Molecular Dynamics Analysis of FAAH Complexed with Anandamide, *Prog. Theor. Chem.*, 29, 115-127.
- Young, D.C., 2001, *Computational Chemistry: A Pratical Guide for Applying Techniques to Real-World Problems*, John Willey and Sons inc., New Jersey.