

## DAFTAR PUSTAKA

- Albarelo, F., Pianura, E., Stefano, F.D., Cristofaro, M., Petrone, A., Marchioni, L., Palazzolo, C., Schinina, V., Nicastrì, E., Petrosillo, N., Campioni, P., Eskild, P., Zumla, A., Ippolito, G., 2020, 2019-Novel Coronavirus Severe Adult Respiratory Distress Syndrome in Two Cases in Italy: An Uncommon Radiological Presentation, *International Journal of Infectious Diseases*, 93, 192–197.
- Allinger, N.L., Schafer, L., Siam, K., Klimkowski, V.J., dan Alsenoy, C.V., 1985, The Effect of Electronegative Atoms on the Structures of Hydrocarbons. Ab Initio Calculations on Molecules Containing Fluorine or (Carbonyl) Oxygen, *Journal of Computational Chemistry*, 6(5), 331-342.
- An, F., Cao, X., Qu, H., dan Wang, S., 2015, Attenuation of Oxidative Stress of Erythrocytes by The Plant-Derived Flavonoids Vitexin and Apigenin, *Pharmazie*, 70, 724-732.
- An, F., Wang, S., Tian, Q., dan Zhu, D., 2015, Effects of Orientin and Vitexin from *Trollius chinensis* on The Growth and Apoptosis of Esophageal Cancer EC-109 Cells, *ONCOLOGY LETTERS*, 10, 2627-2633.
- Anderson, A.C., 2003, The Process of Structure-Based Drug Design, *Chemistry & Biology*, Vol. 10, 787–797.
- Aslam, M.S., Ahmad, M.S., dan Mamat, A.S., 2015, PHARMACOLOGICAL POTENTIAL OF VITEXIN, *Ind Res J Pharm & Sci.*, 2(2), 114-122.
- Barratt, E., Bingham, R.J., Warner, D.J., Laughton, C.A., Phillips, S.E.V., dan Homans, S.W., 2005, Van der Waals Interactions Dominate Ligand-Protein Association in a Protein Binding Site Occluded from Solvent Water, *J. Am. Chem. Soc.*, 127, 11827-11834.
- Brooks, W.H., Guida, W.C., dan Daniel, K.G., 2011, The Significance of Chirality in Drug Design and Development, *Curr Top Med Chem.*, 11(7): 760–770.
- Chen, G., Huang, K., Miao, M., Feng, B., dan Campanella, O.H., 2018, Molecular

- Dynamics Simulation for Mechanism Elucidation of Food Processing and Safety: State of the Art, *Comprehensive Reviews in Food Science and Food Safety*, 18, 243-263.
- Chen, X., Li, H., Tian, L., Li, Q., Luo, J., dan Zhang, Y., 2020, Analysis of the Physicochemical Properties of Acaricides Based on Lipinski's Rule of Five, *Journal of Computational Biology*, 27(0), 1-10.
- Cohen, A.J., Sanchez, P.M., dan Yang, W., 2012, Challenges for Density Functional Theory, *Chem. Rev.*, 112, 289–320.
- Daina, A., Blatter, M.C., Gerritsen, V.B., Palagi, P.M., Marek, D., Xenarios, I., Schwede, T., Michielin, O., dan Zoete, V., 2017, Drug Design Workshop: A Web-Based Educational Tool To Introduce Computer-Aided Drug Design to the General Public, *J. Chem. Educ.*, 94, 335–344.
- Davin, T.J., 2009, Computational Chemistry of Organometallic and Inorganic Species, *Disertasi*, Departemen Kimia Universitas Glasgow, United Kingdom.
- De Ruyck, J., Brysbaert, G., Blossey, R., dan Lensink, M.F., 2016, Molecular docking As A Popular Tool in Drug Design, An In Silico Travel, *Advances and Applications in Bioinformatics and Chemistry*, Vol. 9, 1-11.
- Dipojono, H.K., 2001, Simulasi Dinamika Molekul (Sebuah Pengantar), *Prosiding Seminar Nasional Hamburan Neutron dan Sinar X Ke 4*, Bandung, 1-12.
- Effenberger, M., Kronbichler, A., Shin, J.I., Mayer, G., Tilg, H., dan Perco, P., 2020, Association of the COVID-19 pandemic with Internet Search Volumes: A Google Trends™ Analysis, *International Journal of Infectious Diseases*, 95, 192–197.
- Erazua, E.A., dan Adeleke, B.B., 2019, DFT and Molecular Docking Investigation of Potential Anticancer Properties of some Flavonoids, *J. Pure App. Chem. Res.*, 8 (3), 225-231.
- Fitriani, I.N., dan Ansory, H.M., 2021, Molecular Docking Study of Nutmeg (*Myristica Fragrans*) Constituents as Anti-Skin Cancer Agents, *JKPK*, 6(1), 14-22.
- Gajjar, N.D., Dhameliya, T.M., dan Shah, G.B., 2021, In Search of RdRp and Mpro

- Inhibitors against SARS CoV-2: Molecular Docking, Molecular Dynamic Simulations and ADMET Analysis, *J. Molstruc*, 1239, 130488.
- Ganesan, K., dan Xu, B., 2017, Molecular Targets of Vitexin and IsoVitexin in Cancer Therapy: A Critical Review, *Ann. N.Y. Acad. Sci.*, 1401, 102–113.
- Garg, S., Anand, A., dan Roy, A., 2020, Molecular Docking Analysis of Selected Phytochemicals Against SARS-CoV-2 Mpro Receptor, *Vegetos*, 33, 766–781.
- Gosswami, B.M., 2011, Implementing Density Functional Theory (DFT) Methods on Many-core GPGPU Accelerators, *Thesis*, Stuttgart University, Stuttgart, Germany.
- Han, Z., Wei, X., Xu, C., Chiang, C., Zhang, Y., Wu, R., dan Ho, W., 2016, Imaging Van der Waals Interactions, *J. Phys. Chem. Lett.*, 7, 5205–5211.
- He, M., Min, J., Kong, W., He, X., Li, J., dan Peng, B., 2016, A Review on The Pharmacological Effects of Vitexin and IsoVitexin, *Fitoterapia*, 115, 74–85.
- Hollingsworth, S.A., dan Dror, R.O., Molecular Dynamics Simulation for All, *Neuron* 99, 1129-1143.
- Hospital, A., Goni, J.R., Orozco, M., dan Gelpi, J.L., 2015, Molecular Dynamics Simulations: Advances and Applications, *Advances and Applications in Bioinformatics and Chemistry*, 8, 37–47.
- Imam, S.S., dan Gilani, S.J., Computer Aided Drug Design: A Novel Loom To Drug Discovery, *Organic & Medicinal Chem IJ*, 1(4), 001-006.
- Jayakumar, R., Vadivel, R., dan Ananthi, N., 2018, Role of Chirality in Drugs, *Organic & Medicinal Chem IJ*, 5(3),1-6.
- Johnson, E.R., Mackie, I.A., dan DiLabio, G.A., 2009, Dispersion Interactions in Density-Functional Theory, *J. Phys. Org. Chem.*, 22, 1127–1135.
- Khan, S.L., Siddiqui, F.A., Jain, S.P., dan Sonwane, G.M., 2021, Discovery of Potential Inhibitors of SARS-CoV-2 (COVID-19) Main Protease (Mpro) from Nigella Sativa (Black Seed) by Molecular Docking Study, *Coronaviruses*, 2(3), 384-402.
- Nasution, D.A.D., Erlina, E., dan Muda, I., 2020, Dampak Pandemi COVID-19

- Terhadap Perekonomian Indonesia, *Jurnal Benefita*, 5(2), 212-224.
- Kufareva, I., dan Abagyan, R., 2012, Methods of Protein Structure Comparison, *Methods Mol Biol.*, 857, 231–257.
- Li. Y., Ma, S., Yang, Y., Ye, S., dan But, P.P., 2002, Antiviral Activities of Flavonoids and Organic Acid from *Trollius Chinensis* Bunge, *Journal of Ethnopharmacology*, 79, 365–368.
- Lipinski, C.A., Lombardo, F., Dominy, B.W., dan Feeney, P.J., 2019, Experimental and Computational Approaches to Estimate Solubility and Permeability in Drug Discovery and Development Q Settings, *Advanced Drug Delivery Reviews*, 46, 3 –26.
- Liu, X., Rezaee, E., Shan, H., Xu, J., Zhang, Y., Feng, Y., Dai, J., Chen, Z., Huang, W., dan Xu, Z., 2018, Dopant-Free Hole Transport Materials Based on Alkyl-Substituted Indacenodithiophene for Planar Perovskite Solar Cells, *Journal of Materials Chemistry C*, 1-17.
- Lu, S., Jiang, Y., Lu, J., Wu, T., Yu, Q., dan Zhu, W., 2010, Molecular Docking and Molecular Dynamics Simulation Studies of GPR40 Receptor–Agonist Interactions, *Journal of Molecular Graphics and Modelling*, 28, 766–774.
- Male, Y.T., Sutapa, I.P., dan Ranglalin, O.M., 2015, Computational Study Natural Color Essence (Dyes) as Active Material on Organic Solar Cell With Density Functional Theory (DFT), *Ind. J. Chem. Res.*, 2, 205 – 212.
- Marni, L.G., Emriadi, E., dan Syukri, S., dan Imelda, I., 2019, Mempelajari inhibisi korosi senyawa khellin dan visnagin pada atom besi menggunakan metode DFT (density functional theory), *Jurnal Litbang Industri*, 9(2), 111 – 118.
- Mazumdar, P., dan Coudhury, D., 2022, Study of the Alkyl- $\pi$  Interaction Between Methane and Few Substituted Pyrimidine Systems Using DFT, AIM and NBO Calculations, *Computational and Theoretical Chemistry*, 1208, 113560.
- McGibbon, R.T., Beauchamp, K.A., Harrigan, M.P., Klein, C., Swails, J.M., Hernandez, C.X., Schwantes, C.R., Wang, L.P., Lane, T.J, dan Pande, V.S., 2015, *Biophysical Journal*, 109(8), 1528–1532.

- Meng, X., Zhang, H., Mezei, M., dan Cui, M., 2011, Molecular Docking: A Powerful Approach for Structure-Based Drug Discovery, *Curr Comput Aided Drug*, 7(2), 146–157.
- Mourik, T.V., Michael, B., dan Gageot, M.P., 2014, Density Functional Theory Across Chemistry, Physics and Biology, *Phil. Trans. R. Soc. A 372: 20120488*, 1-5.
- Nadeem, M., Mumtaz, M.W., Danish, M., Rashid, U., Mukhtar, H., dan Irfan, A., 2020, Antidiabetic Functionality of Vitex Negundo L. Leaves Based on UHPLC-QTOF-MS/MS Based Bioactives Profiling and Molecular Docking Insights, *Industrial Crops & Products*, 152, 112445, 1-14.
- Neuman, R.C., 2013, *Organic Chemistry*, University of California, Riverside.
- Ninfali, P., Antonelli, A., Magnani, M., dan Scarpa, E.S., 2020, Antiviral Properties of Flavonoids and Delivery Strategies, *Nutrients*, 12, 2534, 1-19.
- Pan, H., Kou, P., Yang, J., Niu, L., Wan, N., Zhao, C., Liu, Z., Gu, C., dan Fu, Y., 2021, A Novel Approach for Efficient Extraction and Enrichment of Phytochemicals With CO<sub>2</sub>-Based Switchable-Solvent from Pigeon Pea Leaves, *Journal of Cleaner Production*, 284, 124629, 1-12.
- Panigrahi, S.K., dan Desiraju, G.R., 2007, Strong and Weak Hydrogen Bonds in the Protein–Ligand Interface, *PROTEINS: Structure, Function, and Bioinformatics*, 67, 128-141.
- Peng, Y., Gan, R., Li, H., Yang, M., McClements, D.J., Gao, R., dan Sun, Q., 2020, Absorption, Metabolism, and Bioactivity of Vitexin: Recent Advances in Understanding The Efficacy of An Important Nutraceutical, *Critical Reviews in Food Science and Nutrition*, 1-16.
- Pongajow, N.T., Juliandri, J., dan Hastiawan, I., 2013, Density Functional Teory Untuk Penentuan Geometri dan Karakteristik Ikatan dari Kompleks Ni(II)-Dibutilditiokarbamat dan Co(II)-Dibutilditiokarbamat, *Prosiding Seminar Nasional Sains dan Teknologi Nuklir PTNBR – BATAN Bandung*, 197-202.
- Putra, A.F.S., 2021, SIMULASI DINAMIKA MOLEKULUJI TARIK BAHAN

PADUAN NiTiAl, *Skripsi*, Program Studi Teknik Mesin Fakultas Teknik Universitas Muhammadiyah Ponorogo, Ponorogo.

- Rives, J.T., dan Jorgensen, W.L., 2008, Performance of B3LYP Density Functional Methods for a Large Set of Organic Molecules, *J. Chem. Theory Comput.*, 4, 297-306.
- Rudrapal, M., dan Chetia D., Virtual Screening, Molecular Docking and QSAR Studies in Drug Discovery and Development Programme, *Journal of Drug Delivery & Therapeutics*, 10(4), 225-233.
- Salentin, S., Haupt, V.J., Daminelli, S., dan Schroeder, M., 2014, Polypharmacology Rescored: Protein-ligand Interaction Profiles for Remote Binding Site Similarity Assessment, *Progress in Biophysics and Molecular Biology*, 116, 174-186.
- Sen, D.J., Nandi, K., dan Saha, D., 2021, Rule of Five: the Five Men Army to Cross the Blood Brain Barrier for Therapeutically Potent, *World Journal of Advance Healthcare Research*, 5(3), 206-211.
- Sicher, M., Mohr, S., dan Goedecker, S., 2011, Efficient Moves for Global Geometry Optimization Methods and Their Application to Binary Systems, *J. Chem. Phys.* 134, 044106.
- Singhal, T., 2020, A Review of Coronavirus Disease-2019 (COVID-19), *Indian J Pediatr*, 87(4), 281-286.
- Shaw, D.E., Deneroff, M.M., Dror, R.O., Kuskin, J.S., Larson, R.H., Salmon, J.K., Young, C., Batson, B., Bowers, K.J., Chao, J.C., Eastwood, M.P., Gagliardo, J., Grossman, J.P., Ho, C.R., Ierardi, D.J., Kolosscary, I., Klepeis, J.L., Layman, T., McLeavey, C., Moraes, M.A., Mueller, R., Priest, E.C., Shah, Y., Spengler, J., Theobald, M., Towles, B., dan Wang, S.C., 2008, Anton, a Special-Purpose Machine for Molecular Dynamics Simulation, *Communications of The Acm*, 51(7), 91-97.
- Su, H., Yao, S., Zhao, W., Zhang, Y., Liu, J., Shao, Q., Wang, Q., Li, M., Xie, H., Shang, W., Ke, C., Feng, L., Jiang, X., Shen, J., Xiao, G., Jiang, H., Zhang, L.,

- Ye, Y., dan Xu, Y., 2021, Identification of Pyrogallol as a Warhead in Design of Covalent Inhibitors for the SARS-CoV-2 3CL Protease, *Nature Communication*, 12:3623, 1-12.
- Susanna, D., 2020, When will the COVID-19 Pandemic in Indonesia End?, *National Public Health Journal*, 15(4), 160-162.
- Suvarna, B.S., 2011, Drug - Receptor Interactions, *Kathmandu Univ Med J*, 35(3), 203-207.
- Tallei, T.E., Tumilaar, S.G., Niode, N.J., Fatimawali, F., Kepel, B.J., Indroes, R., Effendi, Y., Sakib, S.A., dan Emran, T.L., 2020, Potential of Plant Bioactive Compounds as SARS-CoV-2 Main Protease (Mpro) and Spike (S) Glycoprotein Inhibitors: A Molecular Docking Study, *Scientifica*, 1-18.
- Tang, P., Zhang, Z., Niu, L., Gu, C., Zheng, W., Cui, H., dan Yuan, X., 2021, Fusarium Solani G6, a Novel Vitexin-Producing Endophytic Fungus: Characterization, Yield Improvement and Osteoblastic Proliferation Activity, *Biotechnol Lett*, 43, 1371–1383.
- Tijmstra, J., Bolsinova, M., Liaw, Y., Rutkowski, L., dan Rutkowski, D., 2019, Sensitivity of the RMSD for Detecting Item-Level Misfit in Low-Performing Countries, *Journal of Educational Measurement*, 12263, 1-18.
- Tiwari, G., dan Mohanty, D., 2013, An In Silico Analysis of the Binding Modes and Binding Affinities of Small Molecule Modulators of PDZ-Peptide Interactions, *PLOS ONE*, 8(8), 1-17.
- Wadood, A., Ahmed, N., Shah, L., Ahmad, A., Hassan, H., dan Shams, S., 2013, In-Silico Drug Design: An Approach Which Revolutionarised The Drug Discovery Process, *OA Drug Design & Delivery*, 1(1):3, 1-4.
- Williams, M.A., dan Daviter, T., 2013, *Protein-Ligand Interactions*, Humana Press, New York.
- Yahaya, M.A.F., Bakar, A.R.A., Stanslas, J., Nordin, N., Zainol, M., dan Mehat, M.Z., 2021, Insights from Molecular Docking and Molecular Dynamics on the Potential of Vitexin as an Antagonist Candidate Against Lipopolysaccharide

- (LPS) for Microglial Activation in Neuroinflammation, *BMC Biotechnology*, 21:38, 1-10.
- Yahaya, M.A.F., Bakar, A.R.A., Stanslas, J., Nordin, N., Zainol, M., dan Mehat, M.Z., 2021, Vitexin as a Potential Inhibitor for the Activation of Microglial Cells: Insights from Molecular Docking and Molecular Dynamics, *Research Square*, 1-25.
- Yasin, S.A., Azzahra, A., Ramadhan, N.E., dan Mylanda, V., 2020, Studi Penambatan Molekul dan Prediksi ADMET Senyawa Bioaktif Beberapa Jamu Indonesia Terhadap SARS-CoV-2 Main Protease (Mpro), *BIMFI*, 7(2), 24-41.
- Young, D.C., 2001, *Computational Chemistry: A Practical Guide for Applying Techniques to Real-World Problems*, A John Wiley & Sons, Inc., Publication, New York.
- Zev, S., Raz, K., Schwartz, R., Tarabeh, R., Gupta, P.K., dan Major, D.T., 2021, Benchmarking the Ability of Common Docking Programs to Correctly Reproduce and Score Binding Modes in SARS-CoV-2 Protease Mpro, *J. Chem. Inf. Model.*, 61, 2957–2966.
- Zheng, X., Ma, Z., dan Zhang, D., 2020, Synthesis of Imidazole-Based Medicinal Molecules Utilizing the van Leusen Imidazole Synthesis, *Pharmaceuticals*, 13, 37, 1-19.
- Zhou, S., dan Zhong, W., 2017, Drug Design and Discovery: Principles and Applications, *Molecules*, 22, 279, 1-6.
- Zhou, W., Yan, H., dan Hao, Q., 2012, Analysis of Surface Structures of Hydrogen Bonding in Protein–Ligand Interactions Using the Alpha Shape Model, *Chemical Physics Letters*, 545, 125–131.