DAFTAR PUSTAKA

Abad-Zapatero, C., & Metz, J. T. (2005). Ligand Efficiency Indices as Guideposts for Drug Discovery. *Drug Discovery Today*, *10*(7), 464-469.

Abdelaziz, B., Leila, N., Sakina, H., Imene, D., Fatiha, M., & DjamelEddine, K. (2013). Theoretical Investigation Study Based on PM3MM and ONIOM2 Calculations of β-Cyclodextrin Complexes with diphenylamine. *Journal of Inclusion Phenomena and Macrocyclic Chemistry*, *77*(1), 455-462.

Accelrys Enterprise Platform. (2005). *Introduction to the Discovery Studio Visualizer*. California : Accelrys Software Inc.

Adnyana, I. M. M. (2017). Klasifikasi, Respon Morfologi dan Respon Biokimia terhadap Herbisida. *Skripsi*. Universitas Udayana (UNUD). Bali.

Adrien, A. (1982). *Advances in Heterocyclic Chemistry*. United Kingdom : Academic Press.

Ahluwalia, V. K., Nayal, L., Kalia, N., Bala, S., & Tehim, A. K. (1987). Synthesis and Antimicrobial Activity of Substituted 3, 4-Dihydro-2H-1-benzopyrans. *ChemInform*, *18*(43).

Ahmad-Hamdani, M. S., Owen, M. J., Yu, Q., & Powles, S. B. (2012). ACCase-Inhibiting Herbicide-Resistant *Avena spp*. Populations from the Western Australian Grain Belt. *Weed Technology*, *26*(1), 130-136.

Aktar, M. W., Paramasivam, M., Sengupta, D., Purkait, S., Ganguly, M., & Banerjee, S. (2009). Impact Assessment of Pesticide Residues in Fish of Ganga River Around Kolkata in West Bengal. *Environmental Monitoring and Assessment*, *157*, 97-104.

Alagarsamy, V., Vijayakumar, S., & Solomon, V. R. (2007). Synthesis of 2-mercapto-3-substituted-5, 6-dimethylthieno [2, 3-d] pyrimidin-4 (3H)-ones as New Analgesic, Anti-Inflammatory Agents. *Biomedicine & Pharmacotherapy*, *61*(5), 285-291.

Alexander, D. L., Tropsha, A., & Winkler, D. A. (2015). Beware of R 2: Simple, Unambiguous Sssessment of the Prediction Accuracy of QSAR and QSPR Models. *Journal of Chemical Information and Modeling*, *55*(7), 1316-1322.

Alrouji, M., Benjamin, L. S., Alhumaydhi, F. A., Al Abdulmonem, W., Baeesa, S. S., Rehan, M., Shahwan, M., Shamsi, A., & Akhtar, A. (2023). Unlocking Potential Inhibitors for Bruton's Tyrosine Kinase through In-Silico Drug Repurposing Dtrategies. *Scientific Reports*, *13*(1), 17684.

Arisman, M. B. (2009). *Buku Ajar Ilmu Gizi: Keracunan Makanan*. Jakarta : EGC.

Baber, J. C., Thompson, D. C., Cross, J. B., & Humblet, C. (2009). GARD: A Generally Applicable Replacement for RMSD. *Journal of Chemical Information and Modeling*, *49*(8), 1889-1900.

Baeyer, A. (1877). Ueber Regelmässigkeiten im Schmelzpunkt Homologer Verbindungen. *Berichte Der Deutschen Chemischen Gesellschaft*, *10*(2), 1286-1288.

Berman, H. M., Westbrook, J., Feng, Z., Gilliland, G., Bhat, T. N., Weissig, H., Shindyalov, I. M., & Bourne, P. E. (2000). The Protein Data Bank. *Nucleic Acids Research*, *28*(1), 235-242.

Bernardes, M. F. F., Pazin, M., Pereira, L. C., & Dorta, D. J. (2015). Impact of Pesticides on Environmental and Human Health. *Toxicology Studies-Cells, Drugs and Environment*, 195-233.

Bernstein, H. J. (2000). Recent Changes to RasMol, Recombining the Variants. *Trends in Biochemical Sciences*, *25*(9), 453-455.

Bishnoi, A., Singh, S., Tiwari, A. K., Srivastava, K., Raghuvir, R., & Tripathi, C. M. (2013). Synthesis, Characterization and Biological Activity of New Cyclization Products of 3-(4-substituted benzylidene)-2 H-pyrido [1, 2-a] pyrimidine 2, 4-(3 H)-diones. *Journal of Chemical Sciences*, *125*, 305-312.

Bourbeau, M. P., & Bartberger, M. D. (2015). Recent Advances in the Development of Acetyl-CoA Carboxylase (ACC) Inhibitors for the Treatment of Metabolic Disease: Miniperspective. *Journal of Medicinal Chemistry*, *58*(2), 525-536.

Brown, D. J.(1984). *Comprehensive Heterocyclic Chemistry, Vol. 14*. United Kingdom : Pergamon Press.

Bruice, P. Y. (2007). *Organic Chemistry 3rd Edition*. Singapore : Pearson Education.

Calis, U., & Koksal, M. (2001). CNS-active Drugs-Hypnotics-Psychotropics-Sedatives-Synthesis and Evaluation of Anticonvulsant Activities of Some New Arylhexahydropyrimidine-2, 4-diones. *Arzneimittelforschung*, *51*(7), 523-528.

Carvalho, F. P. (2017). Pesticides, Environment, and Food Safety. *Food and Energy Security*, *6*(2), 48-60.

Chaudhary, K. K., Mishra, N. (2016). A Review on Molecular Docking : Novel Tool for Drug Discovery. *JSM Chem*, 4(3), 1029.

Chen, L., Duan, Y., Wei, H., Ning, H., Bi, C., Zhao, Y., Qin, Y., & Li, Y. (2019). Acetyl-CoA Carboxylase (ACC) as a Therapeutic Target for Metabolic Syndrome and Recent Developments in ACC1/2 Inhibitors. *Expert Opinion on Investigational Drugs*, *28*(10), 917-930.

Chen, Q., Zhu, X. L., Jiang, L. L., Liu, Z. M., & Yang, G. F. (2008). Synthesis, Antifungal Activity and CoMFA Analysis of Novel 1, 2, 4-triazolo [1, 5-a] Pyrimidine Derivatives. *European Journal of Medicinal Chemistry*, *43*(3), 595-603.

Chen, X., Yang, X., Shen, Y., Hou, J., & Bao, X. (2018). Screening Phosphorylation Site Mutations in Yeast Acetyl-CoA Carboxylase using Malonyl-CoA Sensor to Improve Malonyl-CoA-Derived Product. *Frontiers in Microbiology*, *9*, 47.

Chen, Y., Elizondo-Noriega, A., Cantu, D. C., & Reilly, P. J. (2012). Structural classification of biotin carboxyl carrier proteins. *Biotechnology letters*, *34*, 1869-1875.

Cheng, X., Wang, S., Cui, D., & Li, B. (2015). The Synthesis and Herbicidal Activity of 5-(Substituted-phenyl)-4, 6-dioxo− 4, 5, 6, 7-tetrahydropyrazolo [3, 4-d] pyrimidines. *Journal of Heterocyclic Chemistry*, *52*(2), 607-610.

Chikunova, A., & Ubbink, M. (2022). The Roles of Highly Conserved, non-Catalytic Residues in Class A β-lactamases. *Protein Science*, *31*(6), e4328.

Cole, J.C., Nissink, J. W., & Taylor, O. (2005). Protein-Ligand Docking and Virtual Screening with GOLD. In J. Alvarez, & B. Shoichet, *Virtual Screening in Drug Discovery* (p. 398). Boca Raton : CRC Press.

De Freitas, R. F., & Schapira, M. (2017). A Systematic Analysis of Atomic Protein–Ligand Interactions in the PDB. *Medchemcomm*, *8*(10), 1970-1981.

DeLano, W. L., & S. Bromberg. (2004). *PyMOL User's Guide*. California : DeLano Scientific LLC.

Délye, C., Zhang, X. Q., Chalopin, C., Michel, S., & Powles, S. B. (2003). An Isoleucine Residue within the Carboxyl-Transferase Domain of Multidomain Acetyl-Coenzyme A Carboxylase is a Major Determinant of Sensitivity to Aryloxyphenoxypropionate but Not to Cyclohexanedione Inhibitors. *Plant Physiology*, *132*(3), 1716-1723.

Deng, X., Zheng, W., Jin, C., & Bai, L. (2020). Synthesis of Novel 6-aryloxy-4-chloro-2-phenylpyrimidines as Fungicides and Herbicide Safeners. *ACS Omega*, *5*(37), 23996-24004.

Dermawan, D., Sumirtanurdin, R., & Dewantisari, D. (2019). Simulasi Dinamika Molekular Reseptor Estrogen Alfa dengan Andrografolid sebagai Anti Kanker Payudara. *Indones. J. Pharm. Sci. Technol*, *6*(2).

Devine, M. D., & Shukla, A. (2000). Altered Target Sites as a Mechanism of Herbicide Resistance. *Crop protection*, *19*(8-10), 881-889.

Dewi, R. A. (2023). TENSOR ALJABAR-C* DAN APLIKASINYA PADA KOMPOSIT DUA SISTEM SPIN-1/2 DENGAN HAMILTONIAN SINUSOIDAL BERGANTUNG WAKTU. *Skripsi*. Universitas Pendidikan Indonesia.

Djojosumarto, P. (2008). *Panduan Lengkap Pestisida dan Aplikasinya*. Jakarta : PT Agromedia Pustaka.

Elderfield, R. C. (1957). *Heterocyclic Compounds, Vol. 6*. New York : John Wiley & Sons.

El-Hachem, N., Haibe-Kains, B., Khalil, A., Kobeissy, F. H., & Nemer, G. (2017). AutoDock and AutoDockTools for Protein-Ligand Docking: Beta-Site Amyloid Precursor Protein Cleaving Enzyme 1 (BACE1) as a Case Study. *Neuroproteomics: Methods and Protocols*, 391-403.

EL-Mahdy, K. M., El-Kazak, A. M., Abdel-Megid, M., Seada, M., & Farouk, O. (2013). Synthesis, Characterization and Biological Evaluation of Some New thieno [2, 3-d] Pyrimidine Derivatives. *Journal: Journal of Advances in Chemistry*, *5*(1).

Erdoğan, Ş., Safi, Z. S., Kaya, S., Işın, D. Ö., Guo, L., & Kaya, C. (2017). A Computational Study on Corrosion Inhibition Performances of Novel Quinoline Derivatives Against the Corrosion of Iron. *Journal of Molecular Structure*, *1134*, 751-761.

Fang, Z., Zheng, S., Chan, K. F., Yuan, W., Guo, Q., Wu, W., Lui, H. K., Lu, Y., Leung, Y. C., Chan, T. H., Wong, K. Y., & Sun, N. (2019). Design, Synthesis and Antibacterial Evaluation of 2, 4-disubstituted-6-thiophenyl-pyrimidines. *European Journal of Medicinal Chemistry*, *161*, 141-153.

Fenik, J., Tankiewicz, M., & Biziuk, M. (2011). Properties and Determination of Pesticides in Fruits and Vegetables. *TrAC Trends in Analytical Chemistry*, *30*(6), 814-826.

Ferreira, L. G., Dos Santos, R. N., Oliva, G., & Andricopulo, A. D. (2015). Molecular Docking and Structure-Based Drug Design Strategies. *Molecules*, 20(7), 13384-13421.

Finar I. L. (1975). *Organic Chemistry, Stereochemistry and the Chemistry of Natural Products, 5th Ed., Vol. 2*. London : Pearson Education.

Gerhardt, E. C., Rodrigues, T. E., Müller-Santos, M., Pedrosa, F. O., Souza, E. M., Forchhammer, K., & Huergo, L. F. (2015). The Bacterial Signal Transduction Protein GlnB Regulates the Committed Step in Fatty Acid Biosynthesis by Acting as a Dissociable Regulatory Subunit of Acetyl-CoA Carboxylase. *Molecular Microbiology*, *95*(6), 1025-1035.

Ghozali, I. (2016) *Aplikasi Analisis Multivariete Dengan Program IBM SPSS 23. Edisi 8*. Semarang: Badan Penerbit Universitas Diponegoro.

Gößnitzer, E., Feierl, G., & Wagner, U. (2002). Synthesis, Structure Investigations, and Antimicrobial Activity of Selected s-trans-6-aryl-4-isopropyl-2-{2-[(E)-1-phenylalkylidene]-(E)-hydrazino}-1, 4-dihydropyrimidine hydrochlorides. *European Journal of Pharmaceutical Sciences*, *15*(1), 49-61.

Gómez-Jeria, J.S., Robles-Navarro, A., Kpotin, G.A., Garrido-Sáez, N., Gatica-Díaz, N. 2020. Some Remarks About the Relationships Between the Common Skeleton Concept within the KlopmanPeradejordi-Gómez QSAR Method and the Weak Molecule-Site Interactions. *Chemistry Research Journal*, *5*(2): 32-52.

Gronwald, J. W. (1991). Lipid Biosynthesis Inhibitors. *Weed Science*, *39*(3), 435-449.

Hao, M. H., Haq, O., & Muegge, I. (2007). Torsion Angle Preference and Energetics of Small-Molecule Ligands Bound to Proteins. *Journal of Chemical Information and Modeling*, *47*(6), 2242-2252.

Harisna, A. H., Nurdiansyah, R., Syaifie, P. H., Nugroho, D. W., Saputro, K. E., Prakoso, C. D., Rochman, N. T., Maulana, N.N., Noviyanto, A., & Mardliyati, E. (2021). In Silico Investigation of Potential Inhibitors to Main Protease and Spike Protein of SARS-CoV-2 in Propolis. *Biochemistry and Biophysics Reports*, *26*, 100969.

Harriman, G., Greenwood, J., Bhat, S., Huang, X., Wang, R., Paul, D., Tong, K., Saha, A. K., Westlin, W.F., Kapeller, R., & Harwood Jr, H. J. (2016). Acetyl-CoA Carboxylase Inhibition by ND-630 Reduces Hepatic Steatosis, Improves Insulin Sensitivity, and Modulates Dyslipidemia in Rats. *Proceedings of the National Academy of Sciences*, *113*(13), E1796-E1805.

Hassal, K. A. (1982). *The Chemistry of Pesticides: Their Metabolism, Mode of Action and Uses in Crop Protection*. London (BG) : English Language Book Society/Macmillan.

Hassan, N. M., Alhossary, A. A., Mu, Y., & Kwoh, C. K. (2017). Protein-Ligand Blind Docking Using QuickVina-W with Inter-Process Spatio-Temporal Integration. *Scientific Reports*, *7*(1), 15451.

Hata, H., Tran, D. P., Sobeh, M. M., & Kitao, A. (2021). Binding Free Energy of Protein/Ligand Complexes Calculated Using Dissociation Parallel Cascade Selection Molecular Dynamics and Markov State Model. *Biophysics and Physicobiology*, *18*, 305-316.

Hayes, T. B., & Hansen, M. (2017). From Silent Spring to Silent Night: Agrochemicals and the Anthropocene. *Elem Sci Anth*, *5*, 57.

Hernández, A. F., Gil, F., Lacasaña, M., Rodríguez-Barranco, M., Tsatsakis, A. M., Requena, M., Parrón, T., & Alarcón, R. (2013). Pesticide Exposure and Genetic Variation in Xenobiotic-Metabolizing Enzymes Interact to Induce Biochemical Liver Damage. *Food and Chemical Toxicology*, *61*, 144-151.

Hogale, M. B., Dhore, N. P., Shelar, A. R., & Pawar, P. K. (1986). Synthesis and Biological Activity of Some Urethane Derivatives of Chalkones. *Orient. J. Chem.*, *2*(1), 55-57.

Hopkins, A. L., Groom, C. R., & Alex, A. (2004). Ligand Efficiency: a Useful Metric for Lead Selection. *Drug discovery today*, *9*(10), 430-431.

Howe, R. K., & Shelton, B. R. (1990). Spiroheterocycles from the Reaction of Nitrile Oxides with 3-methylenephthalimidines. *The Journal of Organic Chemistry*, *55*(15), 4603-4607.

Huerlimann, R., & Heimann, K. (2013). Comprehensive Guide to Acetyl-Carboxylases in Algae. *Critical Reviews in Biotechnology*, *33*(1), 49-65.

Huey, R., Morris, G. M., Olson, A. J., & Goodsell, D. S. (2007). A Semiempirical Free Energy Force Field with Charge-Based Desolvation. *Journal of Computational Chemistry*, *28*(6), 1145-1152.

Ishitsuka, H., Ninomiya, Y. T., Ohsawa, C., Fujiu, M., & Suhara, Y. (1982). Direct and Specific Inactivation of Rhinovirus by Chalcone Ro 09-0410. *Antimicrobial Agents and Chemotherapy*, *22*(4), 617-621.

Iwakami, S., Kamidate, Y., Yamaguchi, T., Ishizaka, M., Endo, M., Suda, H., Nagai, K., Sunohara, Y., Toki, S., Uchino, A., Tominaga, T., & Matsumoto, H. (2019). CYP 81A P450s are Involved in Concomitant Cross-Resistance to Acetolactate Synthase and Acetyl-CoA Carboxylase Herbicides in *Echinochloa phyllopogon*. *New Phytologist*, *221*(4), 2112-2122.

Jain, A. N. (1996). Scoring Noncovalent Protein-Ligand Interactions: a Continuous Differentiable Function Tuned to Compute Binding Affinities. *Journal of Computer-Aided Molecular Design*, *10*, 427-440.

Jain, A. N. (2000). Morphological Similarity: a 3D Molecular Similarity Method Correlated with Protein-Ligand Recognition. *Journal of Computer-Aided Molecular Design*, *14*, 199-213.

Jani, M.K., Shah, B.R., Undavia, N.K., & Trivedi, P.B. (1994). *Chem. Abstr*. 121, 35513.

Jensen, F. (2007). *Introduction to Computational Chemistr*y. Chichester : John Willey & Sons.

Johnson, E. J., & Colmer, A. R. (1955). The Effect of Herbicides on Soil Microorganisms: I. The Effect of 2, 4-Dichlorophenoxyacetic Acid on Some

Phases of the Nitrogen Metabolism of *Bacillus cereus*. *Applied Microbiology*, *3*(2), 123-126.

Jones, G., Willett, P., Glen, R. C., Leach, A. R., & Taylor, R. (1997). Development and Validation of a Genetic Algorithm for Flexible Docking. *Journal of Molecular Biology*, *267*(3), 727-748.

Josef, E. (1988). Synthesis and Herbicidal Activity of 2H-1, 2, 4-thiadiazole [2, 3-a] Pyrimidines. *HU Patent, A01N47/30*, *46839*, 12.

Joyard, J., Ferro, M., Masselon, C., Seigneurin-Berny, D., Salvi, D., Garin, J., & Rolland, N. (2010). Chloroplast Proteomics Highlights the Subcellular Compartmentation of Lipid Metabolism. *Progress in Lipid Research*, *49*(2), 128-158.

Keereetaweep, J., Liu, H., Zhai, Z., & Shanklin, J. (2018). Biotin Attachment Domain-Containing Proteins Irreversibly Inhibit Acetyl CoA Carboxylase. *Plant Physiology*, *177*(1), 208-215.

Kufareva, I., & Abagyan, R. (2012). Methods of Protein Structure Comparison. *Homology Modeling: Methods and Protocols*, 231-257.

Kumar, K., Woo, S. M., Siu, T., Cortopassi, W. A., Duarte, F., & Paton, R. S. (2018). Cation-π interactions in Protein-Ligand Binding: Theory and Data-Mining Reveal Different Roles for Lysine and Arginine. *Chemical Science*, *9*(10), 2655-2665.

Kumar, Ranjit. (2005). *Research Methodology : A Step-by-Step Guide for Beginners (2nd Ed.)*. Singapore : Pearson Education.

Kuragano, T., & Tanaka, Y. (2004). *Pyrimidine Derivatives and Herbicides Containing the Same* (U.S. Patent No. 10/416,013). U.S. Patent and Trademark Office.

Kustyawati, M. E. (2018). *Saccharomyces cerevisiae: Metabolit dan Agensia Modifikasi Pangan*. Yogyakarta : Graha Ilmu.

Laforest, M., Soufiane, B., Simard, M., Obeid, K., Page, E., and Nurse, R. E. (2017). Acetyl-CoA Carboxylase Overexpression in Herbicide-Resistant Large Crabgrass (*Digitaria sanguinalis*). *Pest. Manag. Sci*. 73, 2227–2235.

Lagoja, I. M. (2005). Pyrimidine as constituent of natural biologically active compounds. *Chemistry & Biodiversity*, *2*(1), 1-50.

Lancaster, Z. D., Norsworthy, J. K., and Scott, R. C. (2018). Sensitivity of Grass Crops to Low Rates of Quizalofop. *Weed. Technol*. 32, 1–5.

Lee, C. K., Cheong, H. K., Ryu, K. S., Lee, J. I., Lee, W., Jeon, Y. H., & Cheong, C. (2008). Biotinoyl domain of human acetyl-CoA carboxylase: Structural insights into the carboxyl transfer mechanism. *Proteins: Structure, Function, and Bioinformatics*, *72*(2), 613-624.

Lewar, E. G. (2011). *Computational CHemistru : Introduction to the Theory and Applications of Molecular Quantum Mechanics*. New York : Springer.

Li, K. J., Qu, R. Y., Liu, Y. C., Yang, J. F., Devendar, P., Chen, Q., Niu, C. W., Xi, Z., & Yang, G. F. (2018). Design, Synthesis, and Herbicidal Activity of pyrimidine–biphenyl Hybrids as Novel Acetohydroxyacid Synthase Inhibitors. *Journal of Agricultural and Food Chemistry*, *66*(15), 3773-3782.

Li, L., Zhou, C., Liu, M., Zhang, P., Zhang, N., Li, J., Li, T., Liu, X., Cheng, S., Li, Q., & Liu, A. (2019). Design, Synthesis, Insecticidal, and Acaricidal

Activities of Novel Pyrimidinamine Derivatives Containing a Biphenyl Ether. *Journal of Heterocyclic Chemistry*, *56*(12), 3206-3214.

Li, N., Wu, J. X., Ding, D., Cheng, J., Gao, N., & Chen, L. (2017). Structure of a Pancreatic ATP-Sensitive Potassium Channel. *Cell*, *168*(1), 101-110.

Li, X. B., Wang, S. Q., Xu, W. R., Wang, R. L., & Chou, K. C. (2011). Novel inhibitor design for hemagglutinin against H1N1 influenza virus by core hopping method. *PloS one*, *6*(11), e28111.

Lipinski, C. A. (2004). Lead-and drug-like compounds: the rule-of-five revolution. *Drug discovery today: Technologies*, *1*(4), 337-341.

Liu, X. H., Wang, Q., Sun, Z. H., Wedge, D. E., Becnel, J. J., Estep, A. S., Tan, C. X., & Weng, J. Q. (2017). Synthesis and Insecticidal Activity of Novel Pyrimidine Derivatives Containing Urea Pharmacophore Against *Aedes aegypti*. *Pest Management Science*, *73*(5), 953-959.

Ma, J., Xu, L., & Wang, S. (2002). A quick, simple, and accurate method of screening herbicide activity using green algae cell suspension cultures. *Weed science*, *50*(5), 555-559.

Male, Y. T. (2009). Studi Komputasi Senyawa Kompleks Transisi Spin Besi (II). *Disertasi*. Institut Teknologi Bandung : Bandung.

Mansourian, M., Fassihi, A., Saghaie, L., Madadkar-Sobhani, A., Mahnam, K., & Abbasi, M. (2015). QSAR and Docking Analysis of A 2B Adenosine Receptor Antagonists Based on Non-Xanthine Scaffold. *Medicinal Chemistry Research*, *24*, 394-407.

Mardawati, E., Filianty, F., & Marta, H. (2008). Kajian aktivitas antioksidan ekstrak kulit Manggis (Garcinia mangostana L) dalam rangka pemanfaatan limbah kulit manggis di Kecamatan Puspahiang Kabupaten Tasikmalaya. *TEKNOTAN*, *2*(3).

Marsun, I. F. (2014). Analisis Residu Pestisida pada Tomat Buah dan Tomat Sayur pada Pasar Swalayan di Kota Makassar Tahun 2014. *Skripsi*. Fakultas Ilmu Kesehatan.Universitas Islam Negeri Alauddin Makassar.

Mathew, J., Rao, A. S., & Rambhav, S. (1984). Propterol-an Antibacterial Agent from *Pterocarpus marsupium*. *Current Science, India*, *53*(11), 576-577.

Mccullough, P. E., Yu, J., Raymer, P. L., and Chen, Z. (2017). First Report of ACCase-Resistant Goosegrass (*Eleusine indica*) in the United States. *Weed. Sci*. 64, 399–408.

Mikael, J. P. (2013). *Ab Initio, Density Functional Theory, and Semi-Empirical Calculations*. New York : Springer.

Moreland, D. E. (1999). Biochemical mechanisms of action of herbicides and the impact of biotechnology on the development of herbicides. *Journal of Pesticide Science*, *24*(3), 299-307.

Morris, G. M., Huey, R., Lindstrom, W., Sanner, M. F., Belew, R. K., Goodsell, D.S., & Olson, A. J. (2009). AutoDock4 and AutoDockTools4: Automated Docking with Selective Receptor Flexibility. *Journal of Computational Chemistry*, *30*(16), 2785-2791.

Mudasir, M., Tahir, I., & Putri, I. P. A. M. (2003). Quantitative Structure and Activity Relationship Analysis of 1, 2, 4-Thiadiazoline Fungicides Based

on Molecular Structure Calculated by Am1 Method. *Indonesian Journal of Chemistry*, *3*(1), 39-47.

Muhammad, R. F., Adnani, B., Arviana, S. D., Violita, A. H., Khotimah, H., Kurniawan, S. N., ... & Rahayu, M. (2023). Bioinformatics Study of 7, 8-Dihydroxyflavone as a Neuroprotective Agent in Ischemic Stroke via TRKB Regulation and Glutaminase Inhibition. *MNJ (Malang Neurology Journal)*, *9*(2), 144-150.

Nazmatullaila, S. (2015). Analisis Residu Pestisida pada Tomat Menggunakan Metode Quechers dengan Perlakuan Sebelum dan Setelah di Cuci. *Skripsi*. Fakultas Kedokteran dan Ilmu Kesehatan. UIN Syarif Hidayatullah Jakarta.

Ninomiya, Y., Shimma, N., & Ishitsuka, H. (1990). Comparative Studies on the Antirhinovirus Activity and the Mode of Action of the Rhinovirus Capsid Binding Agents, Chalcone Amides. *Antiviral Research*, *13*(2), 61-74.

O'Boyle, N. M., Banck, M., James, C. A., Morley, C., Vandermeersch, T., & Hutchison, G. R. (2011). Open Babel : an Open Chemical Toolbox. *Journal of cheminformatics*, *3*(1), 1-14.

Odell, L. R., Abdel-Hamid, M. K., Hill, T. A., Chau, N., Young, K. A., Deane, F. M., Sakoff, J. A., Andersson, S., Daniel, J. A., Robinson, P. J., & McCluskey, A. (2017). Pyrimidine-Based Inhibitors of Dynamin I GTPase Activity: Competitive Inhibition at the Pleckstrin Homology Domain. *Journal of Medicinal Chemistry*, *60*(1), 349-361.

Oliveira Jr, R. D., Constantin, J., & Inoue, M. H. (2011). Biologia e Manejo de Plantas Daninhas. *Curitiba, PR: Omnipax*, 348.

Pivazyan, V. A., Ghazaryan, E. A., Shainova, R. S., Tamazyan, R. A., Ayvazyan, A. G., & Yengoyan, A. P. (2017). Synthesis and Growth Stimulant Properties of 2-Acetyl-3, 7-dimethyl-5H-thiazolo [3, 2-a] pyrimidin-5-one Derivatives. *Journal of Chemistry*, *2017*.

Powles, S. B. (2005). Molecular Bases for Sensitivity to Acetyl-Coenzyme A Carboxylase Inhibitors in Black-Grass. *Plant Physiol*. 137, 794–806.

Pranowo, H. D. (2003). *Pengantar Kimia Komputasi; Pusat Kimia Komputasi Indonesia-Austria*. Yogyakarta : Fakultas Matematika dan Ilmu Pengetahuan Alam Universitas Gajah Mada.

Pranowo, H. D. (2011). *Pengantar Kimia Komputasi (1st Ed.)*. Bandung : Penerbit Lubuk Agung.

Pratiwi, N. M. G., Saraswati, N. M. A., Dewi, N. M. I. F. P., & Tirta, L. P. P. (2021). Potensi Sinamaldehid sebagai Anti Hiperpigmentasi secara In Silico. *Jurnal Ilmiah Medicamento*, *7*(2), 95-101.

Radosevich, S. R., Holt, J. S., & Ghersa, C. M. (2007). *Wood Ecology : Implication for Management*. *Second Edition*. New Jersey : John Wiley & Sons, Inc.

Ramachandran, K. I., Gopakumar, D., & Namboori, K. (2008). *Computational Chemistry and Molecular Modeling*. India : Springer.

RCSB. 2014. About the PDB Archive and the RCSB PDB. Retrieved from Protein Data Bank: http://www.rcsb.org/pdb/static.do?p=general_information/about_pdb/index.html.

Repasky, M. P., Shelley, M., & Friesner, R. A. (2007). Flexible Ligand Docking with Glide. *Current Protocols in Bioinformatics*, *18*(1), 8-12.

Repasky, M. P., Chandrasekhar, J., & Jorgensen, W. L. (2002). PDDG/PM3 and PDDG/MNDO: Improved Semiempirical Methods. *Journal of computational chemistry*, *23*(16), 1601-1622.

Reynolds, C. H., Tounge, B. A., & Bembenek, S. D. (2008). Ligand Binding Efficiency: Trends, Physical Basis, and Implications. *Journal of Medicinal Chemistry*, *51*(8), 2432-2438.

Rifai, Eko Aditya. 2012. Penapisan In Silico Antmalaria dari Basis Data Tanaman Obat Indonesia Terhadap Targe Plasmepsin. *Skripsi*, Program Studi Farmasi, Fakultas Matematika dan Ilmu Pengetahuan Alam, Universitas Indonesia. Depok.

Saini, R. K., Malone, J., Gill, G., and Preston, C. (2017). Inheritance of Evolved Clethodim Resistance in *Lolium rigidum* Populations from Australia. *Pest. Manag. Sci*. 73, 1604–1610.

Sari, I. W., Junaidin, J., & Pratiwi, D. (2020). Studi Molecular Docking Senyawa Flavonoid Herba Kumis Kucing (Orthosiphon Stamineus B) pada Reseptor A-Glukosidase sebagai Antidiabetes Tipe 2. *Jurnal Farmagazine*, *7*(2), 54.

Saudale, F. Z., & Suatu, I. R. (2020). Pemodelan Homologi Komparatif FABP Belalang Kembara (Locusta migratoria) Dengan PHYRE2 dan Skrining Virtual Inhibitor Potensial. *Indonesian Journal of Chemical Research*, *7*(2), 127-140.

Sayle, R. A., & Milner-White, E. J. (1995). RASMOL : Biomolecular Graphics for All. *Trends in Biochemical Sciences*, *20*(9), 374-376.

Schultes, S., de Graaf, C., Haaksma, E. E., de Esch, I. J., Leurs, R., & Krämer, O. (2010). Ligand efficiency as a guide in fragment hit selection and optimization. *Drug Discovery Today: Technologies*, *7*(3), e157-e162.

Seeliger, D., & de Groot, B. L. (2010). Ligand Docking and Binding Site Analysis with PyMOL and Autodock/Vina. *Journal of Computer-Aided Molecular Design*, *24*(5), 417-422.

Shadidizaji, A., Cinisli, K. T., Warda, M., Cicek, B., & Hacimuftoglu, A. (2023). Virtual Insights into the Quercetin-Melampsora Lini-Derived Effector AvrM14 Interaction: An In silico Exploration of Plant Defense Mechanisms. *Physiological and Molecular Plant Pathology*, 102200.

Shamsi, A., Shahwan, M., Khan, M. S., Husain, F. M., Alhumaydhi, F. A., Aljohani, A. S., Rehman, M. T., Hassan, M. I., & Islam, A. (2021). Elucidating the Interaction of Human Ferritin with Quercetin and Naringenin: Implication of Natural Products in Neurodegenerative Diseases: Molecular Docking and Dynamics Simulation Insight. *ACS Omega*, *6*(11), 7922-7930.

Shankar, B., Jalapathi, P., Ramesh, M., Kumar, A. K., Ragavender, M., & Bharath, G. (2016). Synthesis, Antimicrobial Evaluation, and Docking Studies of Some Novel Benzofuran Based Analogues of Chalcone and 1, 4-benzodiazepine. *Russian Journal of General Chemistry*, *86*, 1711-1721.

Shen, Z. H., Sun, Z. H., Becnel, J. J., Estep, A., Wedge, D. E., Tan, C. X., Weng, J. Q., Han, L., & Liu, X. H. (2018). Synthesis and Mosquiticidal Activity of

Novel Hydrazone Containing Pyrimidine Derivatives Against Aedes aegypt. *Letters in Drug Design & Discovery*, *15*(9), 951-956.

Shityakov, S., & Förster, C. (2014). In Silico Predictive Model to Determine Vector-Mediated Transport Properties for the Blood–Brain Barrier Choline Transporter. *Advances and Applications in Bioinformatics and Chemistry*, 23-36.

Shukla, A., Nycholat, C., Mani, V. S., Richard, J. A., and Malaolm, D. D. (2004). Use of Resistant ACCase Mutants to Screen for Novel Inhibitors Against Resistant and Susceptible Forms of ACCase from Grass Weeds. *J. Agric. Food. Chem*. 52, 5144–5150.

Siswandono. (2016). *Kimia Medisinal Edisi Kedua*. Surabaya : Airlangga University Press.

Stewart, J. J. (2007). Optimization of Parameters for Semiempirical Methods V: Modification of NDDO Approximations and Application to 70 Elements. *Journal of Molecular Modeling*, *13*, 1173-1213.

Stiede, K., Miao, W., Blanchette, H. S., Beysen, C., Harriman, G., Harwood Jr, H. J., Kelley, H., Kapeller, R., Schmalbalch, T., & Westlin, W. F. (2017). Acetyl-Coenzyme A Carboxylase Inhibition Reduces de novo Lipogenesis in Overweight Male Subjects : A Randomized, Double-Blind, Crossover Study. *Hepatology*, *66*(2), 324-334.

Strassemeyer, J., Daehmlow, D., Dominic, A. R., Lorenz, S., & Golla, B. (2017). SYNOPS-WEB, an Online Tool for Environmental Risk Assessment to Evaluate Pesticide Strategies on Field Level. *Crop Protection*, *97*, 28-44.

Sweeney, A., Mulvaney, T., Maiorca, M., & Topf, M. (2023). ChemEM: Flexible Docking of Small Molecules in Cryo-EM Structures. *Journal of Medicinal Chemistry*, *67*(1), 199-212.

Sulistyo, B. (2002). Analisis Hubungan Kuantitatif StrukturAktivitas Seri Senyawa Analog Kurkumin sebagai Antioksidan Menggunakan Deskriptor Kimia Kuantum. *Skripsi*. Gadjah Mada University Press.

Talahatu, D. R., & Papilaya, P. M. (2015). Pemanfaatan Ekstrak Daun Cengkeh (*Syzygium aromaticum L*.) sebagai Herbisida Alami terhadap Pertumbuhan Gulma Rumput Teki (*Cyperus rotundus L*.). *Biopendix: Jurnal Biologi, Pendidikan dan Terapan, 1*(2), 160-170.

Tapiory, A. A., Pertiwi, K. O., Fadilla, K., Reyhanditya, D., & Fatchiyah, F. (2020). In-Silico Analysis of Methoxyl Pectin Compounds from Banana Peels as HMG-CoA Reductase Inhibitor Complexes. *Journal of Smart Bioprospecting and Technology*, *1*(2), *2686*-0805.

Tehranchian, P., Nandula, V., Jugulam, M., Putta, K., and Jasieniuk, M. (2017). Multiple Resistance to Glyphosate, Paraquat and ACCase-Inhibiting Herbicides in Italian Ryegrass Populations from California: Confirmation and Mechanisms of Resistance. *Pest. Manag. Sci*, *74*(4), 868–877.

Tomassetti, M., Garavaglia, B. S., Vranych, C. V., Gottig, N., Ottado, J., Gramajo, H., & Diacovich, L. (2018). 3-methylcrotonyl Coenzyme A (CoA) Carboxylase Complex is Involved in the Xanthomonas citri subsp. citri Lifestyle During Citrus Infection. *PLoS One*, *13*(6), e0198414.

Tong, L. (2013). Structure and Function of Biotin-Dependent Carboxylases. *Cellular and Molecular Life Sciences*, *70*(5), 863-891.

Triloknadh, S., Rao, C. V., Nagaraju, K., Krishna, N. H., Ramaiah, C. V., Rajendra, W., Trinath, D., & Suneetha, Y. (2018). Design, Synthesis, Neuroprotective, Antibacterial Activities and Docking Studies of Novel Thieno [2, 3-d] Pyrimidine-Alkyne Mannich Base and Oxadiazole Hybrids. *Bioorganic & Medicinal Chemistry Letters*, *28*(9), 1663-1669.

Trott, O., & Olson, A. J. (2010). AutoDock Vina : Improving the Dpeed and Accuracy of Docking with a New Scoring Function, Efficient Optimization, and Multithreading. *Journal of Computational Chemistry*, 31(2), 455-461.

Tucaliuc, R. B., Risca, I. M., Drochioiu, G., & Mangalagiu, I. (2008). Biological Effect of Some New Pyridazine Derivatives on Wheat in Germination Experiments. *Romanian Biotechnological Letters*, *13*(4), 3837-3842.

Van Bruggen, A. H., He, M. M., Shin, K., Mai, V., Jeong, K. C., Finckh, M. R., & Morris Jr, J. G. (2018). Environmental and Health Effects of the Herbicide Glyphosate. *Science of the Total Environment*, *616*, 255-268.

Venugopal, P. P., & Chakraborty, D. (2022). Molecular Mechanism of Inhibition of COVID-19 Main Protease by β-adrenoceptor Agonists and Adenosine Deaminase Inhibitors Using In Silico Methods. *Journal of Biomolecular Structure and Dynamics*, *40*(11), 5112-5127.

Vidal, R. A., & Merotto Jr., A. (2001). *Herbicidas Inibidores da PROTOX. In 'Herbicidologia'. (Eds R.A Vidal, A Merotto Jr)*. Porto Alegre : Evangraf.

Wan, H., Sjölinder, M., Schairer, H. U., & Leclerque, A. (2004). A New Dominant Selection Marker for Transformation of Pichia pastoris to Soraphen A Resistance. *Journal of Microbiological Methods*, *57*(1), 33-39.

Wang, Y. Y., Xu, F. Z., Zhu, Y. Y., Song, B., Luo, D., Yu, G., Chen, S., Xue, W., & Wu, J. (2018). Pyrazolo [3, 4-d] Pyrimidine Derivatives Containing a Schiff Base Moiety as Potential Antiviral Agents. *Bioorganic & Medicinal Chemistry Letters*, *28*(17), 2979-2984.

Wang, Y., Yu, W., Li, S., Guo, D., He, J., & Wang, Y. (2022). Acetyl-CoA Carboxylases and Diseases. *Frontiers in Oncology*, *12*, 836058.

Wati, W., Widodo, G. P., & Herowati, R. (2020). Prediction of Pharmacokinetics Parameter and Molecular Docking Study of Antidiabetic Compounds from Syzygium polyanthum and Syzygium cumini. *Jurnal Kimia Sains dan Aplikasi*, *23*(6), 189-195.

Windarti, I., & Widayana, I. G. E. (2015). Effect Paraquat Dichloride Herbicides Orally on the Stage of Esophagus Damage in Male Rats. *Juke Unila*, *5*(9), 9-12.

Wu, Y. Y., Zhao, F. Q., & Ju, X. H. (2014). A Comparison of the Accuracy of Semi-empirical PM3, PDDG and PM6 methods in Predicting Heats of Formation for Organic Compounds. *Journal of the Mexican Chemical Society*, *58*(2), 223-229.

Xiang, S., Callaghan, M. M., Watson, K. G., & Tong, L. (2009). A Different Mechanism for the Inhibition of the Carboxyltransferase Domain of Acetyl-Coenzyme A Carboxylase by Tepraloxydim. *Proceedings of the National Academy of Sciences*, *106*(49), 20723-20727.

Xu, X., Wang, J., & Yao, Q. (2015). Synthesis and Quantitative Structure–Activity Relationship (QSAR) Analysis of Some Novel oxadiazolo [3, 4-d] Pyrimidine Nucleosides Derivatives as Antiviral Agents. *Bioorganic & Medicinal Chemistry Letters*, *25*(2), 241-244.

Yang, X., Guschina, I. A., Hurst, S., Wood, S., Langford, M., Hawkes, T., & Harwood, J. L. (2010). The Action of Herbicides on Fatty Acid Biosynthesis and Elongation in Barley and Cucumber. *Pest Management Science*, *66*(7), 794-800.

Ye, F., Ma, P., Zhang, Y. Y., Li, P., Yang, F., & Fu, Y. (2018). Herbicidal Activity and Molecular Docking Atudy of Novel ACCase Inhibitors. *Frontiers in Plant Science*, 9, 1850.

Yengoyan, A. P., Hambardzumyan, E. N., Vorskanyan, A. S., & Shahbazyan, L. V. (2021). Synthesis of 4, 6-dimethylpyrimidine 2-thiosubstituted Derivatives and Their Preliminary Biological Evaluation. *Letters in Organic Chemistry*, *18*(4), 311-317.

Yonemura, S., Hirao, M., Doi, Y., Takahashi, N., Kondo, T., Tsukita, S., & Tsukita, S. (1998). Ezrin/radixin/moesin (ERM) Proteins Bind to a Positively Charged Amino Acid Cluster in the Juxta-Membrane Cytoplasmic Domain of CD44, CD43, and ICAM-2. *The Journal of Cell Biology*, *140*(4), 885-895.

Yuantari, M. C. (2011). Dampak Pestisida Organoklorin terhadap Kesehatan Manusia dan Lingkungan serta Penanggulangannya. In *Prosiding Seminar Nasional Peran Kesehatan Masyarakat dalam Pencapaian MDG's di Indonesia* (pp. 187-199).

Zhou, Y., Al-Jarf, R., Alavi, A., Nguyen, T.B., Rodrigues, C.H.M., Pires, D.E.V., & Ascher, D.B. (2022). kinCSM : Using Graph-Based Signatures to Predict Small Molecule CDK2 Inhibitors. *The Protein Society, 31*(11), 1-11.

Zagnitko, O., Jelenska, J., Tevzadze, G., Haselkorn, R., & Gornicki, P. (2001). An Isoleucine/Leucine Residue in the Carboxyltransferase Domain of Acetyl-CoA carboxylase is Critical for Interaction with Aryloxyphenoxypropionate and Cyclohexanedione Inhibitors. *Proceedings of the National Academy of Sciences*, *98*(12), 6617-6622.

Zhang, H., Tweel, B., & Tong, L. (2004). Molecular Basis for the Inhibition of the Carboxyltransferase Domain of Acetyl-Coenzyme-A Carboxylase by Haloxyfop and Diclofop. *Proceedings of the National Academy of Sciences*, *101*(16), 5910-5915.

Zhang, H., Yang, Z., Shen, Y., & Tong, L. (2003). Crystal Structure of the Carboxyltransferase Domain of Acetyl-Coenzyme A Carboxylase. *Science*, *299*(5615), 2064-2067.

Zhang, J., Peng, J. F., Bai, Y. B., Wang, P., Wang, T., Gao, J. M., & Zhang, Z. T. (2016). Synthesis of pyrazolo [1, 5-a] Pyrimidine Derivatives and Their Antifungal Activities Against Phytopathogenic Fungi in vitro. *Molecular Diversity*, *20*, 887-896.

Zhang, N., Huang, M. Z., Liu, A. P., Liu, M. H., Li, L. Z., Zhou, C. G., Ren, Y. G., Ou, X. M., Long, C. Y., Sun, J., Dan, M. M., & Lan, Z. L. (2020). Design, Synthesis, and Insecticidal/Acaricidal Evaluation of Novel Pyrimidinamine

Derivatives Containing Phenyloxazole Moiety. *Chemical Papers*, *74*, 963-970.

Zhao, Y., Li, J., Gu, H., Wei, D., Xu, Y. C., Fu, W., & Yu, Z. (2015). Conformational Preferences of π–π Stacking between Ligand and Protein, Analysis Derived from Crystal Structure Data Geometric Preference of π–π Interaction. *Interdisciplinary Sciences: Computational Life Sciences*, *7*, 211-220.

Zolman, J. F. (1993). *Biostatistics : Experimental Design and Statistical Inference*. USA : Oxford University Press.