DAFTAR PUSTAKA

Anastassiadis, T. Duong-Ly, K. C., Deacon, S. W., Lafontant, A., Ma, H., Devarajan, K., Dunbrack, R. L., Jr, Wu, J., & Peterson, J. R. 2013, 'A Highly Selective Dual *Insulin Receptor* (IR)/*Insulin-Like Growth Factor 1 Receptor* (IGF-1R) Inhibitor Derived From An Extracellular Signal-Regulated Kinase (ERK) Inhibitor', *Journal of Biological Chemistry*, vol. 288, no. 39, pp. 28068–28077.

Arcidiacono, B., Iiritano, S., Nocera, A., Possidente, K., Nevolo, M. T., Ventura, V., Foti, D., Chiefari, E., & Brunetti, A. 2012, 'Insulin resistance and cancer risk: an overview of the pathogenetic mechanisms', *Experimental diabetes research*, vol. *2012*, 789174.

Arwansyah & Hasrianti. 2015, 'Simulasi Molecular Docking Senyawa Kurkumin dan Analognya sebagai Selective Androgen Receptor Modulators (SARMs) pada Kanker Prostat', *Dinamika*, vol. 5, no. 2, pp. 60-75.

Bacanli, M., Başaran, A. A., & Başaran, N. 2018, '*Galangin as a Plant Phenolic and Usage in Health and Disease. Polyphenols: Prevention and Treatment of Human Disease (Second Edition)*', US : Academic Press, pp. 433–438.

Bavi, R., Kumar, R., Choi, L., & Woo Lee, K. 2016, 'Exploration of novel inhibitors for Bruton's tyrosine kinase by 3D QSAR modeling and molecular dynamics simulation', *PloS one*, vol. 11, no. 1, p. e0147190.

Benet, L. Z., Hosey, C. M., Ursu, O., & Oprea, T. I. 2016, 'BDDCS, the Rule of 5 and drugability', *Advanced drug Delivery Reviews*, vol. 101, pp. 89–98.

Broomhead, N. K., & Soliman, M. E. 2017, 'Can we rely on computational predictions to correctly identify ligand binding sites on novel protein drug targets? Assessment of binding site prediction methods and a protocol for validation of predicted binding sites', *Cell biochemistry and biophysics*, vol. 75, no. 1, pp. 15-23.

Chang, H. F. & Yang, L. L. 2012, 'Gamma-Mangostin, A Micronutrient of Mangosteen Fruit, Induces Apoptosis in Human Colon Cancer Cells', *Molecules*, vol. 17, no. 7, pp. 8010–8021.

Ciemny, M., Kurcinski, M., Kamel, K., Kolinski, A., Alam, N., Schueler-Furman, O., & Kmiecik, S. 2018, 'Protein–peptide docking: opportunities and challenges', *Drug discovery today*, vol. *23*, no. 8, pp. 1530-1537.

Ciuleanu, T. E., Ahmed, S., Kim, J. H., Mezger, J., Park, K., Thomas, M., Chen, J., Poondru, S., VanTornout, J. M., Whitcomb, D., & Blackhall, F. 2017, 'Randomised Phase 2 Study Of Maintenance Linsitinib (OSI-906) In Combination With Erlotinib Compared With Placebo Plus Erlotinib After Platinum-Based Chemotherapy In Patients With Advanced Non-Small Cell

Lung Cancer', *British journal of cancer*, vol. 117, no. 6, pp. 757-766.

De Vivo, M., Masetti, M., Bottegoni, G., & Cavalli, A. 2016, 'Role of molecular dynamics and related methods in drug discovery', *Journal of medicinal chemistry*, vol. *59*, no. 9, pp. 4035-4061.

Doak, B. C., & Kihlberg, J. 2017, 'Drug discovery beyond the rule of 5-Opportunities and challenges', *Expert Opinion on Drug Discovery*, vol. 12, no. 2, pp. 115-119.

Eid, E. E. M., S Alanazi, A., Koosha, S., A Alrasheedy, A., Azam, F., M Taban, I., Khalilullah, H., Sadiq Al-Qubaisi, M., & A Alshawsh, M. 2019, 'Zerumbone Induces Apoptosis in Breast Cancer Cells by Targeting αvβ3 Integrin upon Co-Administration with TP5-iRGD Peptide', *Molecules*, vol. 24, no. 14, pp. 2554.

Ekowati, J., Hardjono, S., & Hamid, I. S. 2015, 'Ethyl p-methoxycinnamate from Kaempferia galanga inhibits angiogenesis through tyrosine kinase', *Universa Medicina*, vol. 34, no. 1, pp. 43-51.

Fadilla, D., Arifian, H., Rahmadani, A., Rusli, R. 2018, 'Kajian in silico senyawa turunan klorokalkon sebagai antikanker', *Proceeding of the 7th Mulawarman Pharmaceutical Conferences*, Fakultas Farmasi Universitas Mulawarman, Samarinda, pp. 45–50.

Ferreira, L.G., Santos, R.N., Olivia, G., Andricopulo, A.D. 2015, 'Molecular Docking and Structure-Based Drug Design Strategies', *Molecules*, vol. 20, pp. 13384-13421. Forli, S., Huey, R., Pique, M.E., Sanner, M., Goodsell, D.S., Olson, A.J. 2016, 'Computational protein-ligand docking and virtual drug screening with the AutoDock suite', *Nat Protoc*, vol. 11, no. 5, pp. 905–919.

Forli, S., Huey, R., Pique, M.E., Sanner, M.F., Goodsell, D.S. & Olson, A.J. 2016, 'Computational protein-ligand docking and virtual drug screening with the AutoDock suite', *Nature Protocols*, vol. 11, no. 5, pp. 905-919.

Frimayanti, N., Zamri, A., Eryanti, Y., Herfindo, N., & Azteria, V. 2021, 'Docking and Molecular Dynamic Simulations Study to Search Curcumin Analogue Compounds as Potential Inhibitor Against SARS-CoV-2: A Computational Approach', *Jurnal Kimia Sains dan Aplikasi*, vol. 24, no. 3, pp. 85-90.

Globocan, 2020, 'I*ndonesia : Incidence, Mortality and Prevalence by cancer site*', Diakses pada tanggal 12 Agustus 2022, URL : https://gco.iarc.fr/today/data/factsheets/populations/360-indonesia-fact-sheets.pdf.

Guo, M., Wang, X., Lu, X., Wang, H., & Brodelius, P. E. 2016, 'α-Mangostin Extraction From The Native Mangosteen (*Garcinia mangostana* L.) and the Binding Mechanisms of A-Mangostin to HSAorTRF', *PLoS ONE*, vol. 11,

no. 9, pp. 1–22.

Han, F., Xiao, Y., & Lee, I. S. 2021. 'Microbial transformation of galangin derivatives and cytotoxicity evaluation of their metabolites', *Catalysts*, vol. 11, no. 9, p. 1020.

Hati, J. 2014, 'Analisis Kestabilan Protein 1Gb1 Menggunakan Simulasi Dinamika Molekul', *Skripsi*, Departemen Fisika Institut Pertanian Bogor, Bogor.

Heliawati, L., Khatimah, H., Hermawati, E., & Syah, Y. M. 2020, 'Four Dammarane Triterpenes And Their Inhibitory Properties Against Eight Receptor Tyrosine Kinases', *Natural Product Sciences*, vol. 26, no. 4, pp. 345–350.

Hennek, J., Alves, J., Yao, E., Goueli, S. A., & Zegzouti, H. 2016, 'Bioluminescent kinase strips: A novel approach to targeted and flexible kinase inhibitor profiling', *Analytical Biochemistry*, vol. *495*, pp. 9-20.

Hevener, K. E., Zhao, W., Ball, D. M., Babaoglu, K., Qi, J., White, S. W., & Lee, R. E. 2009, 'Validation of Molecular Docking Programs for Virtual Screening Against Dihydropteroate Synthase', *Journal of chemical information and modeling*, vol. 49, no. 2, pp. 444–460.

Hollingsworth, S. A., & Dror, R. O. 2018, 'Molecular dynamics simulation for all;, *Neuron*, vol. 99, no. 6, pp. 1129-1143.

Hosseini, S. A., Zand, H., & Cheraghpour, M. 2019, The Influence Of Curcumin On The Downregulation Of MYC, Insulin And IGF-1 Receptors: A Possible Mechanism Underlying The Anti-Growth and Anti-Migration in Chemoresistant Colorectal Cancer Cells. *Medicina*, vol. 55, no. 4, p. 90.

Hua, H., Kong, Q., Yin, J., Zhang, J., & Jiang, Y. 2020, 'Insulin-like growth factor receptor signaling in tumorigenesis and drug resistance: a challenge for cancer therapy', *Journal of hematology & oncology*, vol. 13, no. 1, pp. 1-17.

Hubbard, S. R. 2013, 'The Insulin Receptor: Both A Prototypical and Atypical Receptor Tyrosine Kinase', *Cold Spring Harbor Perspectives in Biology*, vol. 5, no. 3, pp. 1–12.

Ikawati, Z., 2018., '*Farmakologi Molekuler Target Aksi Obat dan Mekanisme Molekulernya*.' Yogyakarta : Gadjah Mada University Press.

Istyastono, E., & Gani, M. 2021, 'Identification of Interactions of ABT-341 to Dipeptidyl Peptidase IV during Molecular Dynamics Simulations', *Jurnal Farmasi Galenika (Galenika Journal of Pharmacy)(e-Journal)*, vol. *7,* no. 2, pp. 91-98.

Imamura, R. M., Kumagai, K., Nakano, H., Okabe, T., Nagano, T., & Kojima, H. 2019, 'Inexpensive High-Throughput Screening of Kinase Inhibitors Using One-Step Enzyme-Coupled Fluorescence Assay for ADP Detection', *SLAS*

Discovery, vol. 24, no. 3, pp. 284–294.

Jaghoori, M. M., Bleijlevens, B., & Olabarriaga, S. D. 2016, '1001 Ways to run AutoDock Vina for virtual screening', *Journal of computer-aided molecular design*, vol. 30, no. 3, pp. 237-249.

Kilo, A. L., La, O. A., Ismail, S. & Jafar, L. K. 2019, 'Studi Potensi Pirazolin Tersubstitusi 1-N dari Tiosemikarbazon Sebagai Agen Antiamuba Melalui Uji *In Silico*. *Indonesian Journal Chemical Research*, vol. 7, no. 1, pp. 9−16.

Kim, J. S., Kim, E. S., Liu, D., Lee, J. J., Solis, L., Behrens, C., Lippman, S. M., Hong, W. K., Wistuba, I. I. & Lee, H. Y. 2012, 'Prognostic impact of insulin receptor expression on survival of patients with nonsmall cell lung cancer', *Cancer*, vol. 118, no. 9, pp. 2454-2465.

Komarudin, A. D. P., Purnama, M. F. G., Sari, A. Y., Izzati, A., Sahila, E. N. M. R., Hidayat, S., & Apriliya11, T. N. 2021, 'Studi In Silico Senyawa Tanaman Nerium oleander terhadap STAT-3 pada Kanker Payudara', *Jurnal Farmasi Udayana*, vol. 10, no. 2, pp. 149-155.

Lin, L. T., Wu, S. J., & Lin, C. C. 2013, 'The Anticancer Properties And Apoptosis-Inducing Mechanisms Of Cinnamaldehyde and The Herbal Prescription Huang-Lian-Jie-Du-Tang (Huáng Lián Jiě Dú Tang) in Human Hepatoma Cells', *Journal of Traditional and Complementary Medicine*, vol. 3, no. 4, pp. 227–233.

Liu, K., Watanabe, E., & Kokubo, H. 2017, 'Exploring the stability of ligand binding modes to proteins by molecular dynamics simulations', *Journal of computer-aided molecular design*, vol. 31, no. 2, pp. 201-211.

Liu, Y., An, T., Wan, D., Yu, B., Fan, Y., & Pei, X. 2020, 'Targets and Mechanism Used by Cinnamaldehyde, the Main Active Ingredient in Cinnamon, in the Treatment of Breast Cancer', *Frontiers in Pharmacology*, vol. 11, p. 582719.

Malaguarnera, R. & Belfiore, A. 2011, 'The insulin receptor: A new target for cancer therapy', *Frontiers in Endocrinology*, 2(DEC), pp. 1–16.

Martz, E., Sussman, J.L., Decatur, W., Hodis, E., Jiang, Y., & Prilusky, J. 2021, '*Resolution*', diakses pada 20 Agustus 2022, URL : https://proteopedia.org/wiki/index.php/Resolution#Determination_of_Resolution

Meng, X. Y., Zhang, H. X., Mezei, M., & Cui, M. 2011, 'Molecular Docking: A Powerful Approach for Structure-Based Drug Discovery. Current Computer-Aided Drug Design', *Current Computer Aided Drug Design*, vol. 7, no. 2, pp. 146–157.

Musfiroh, I., Muchtaridi, M., Muhtadi, A., Diantini, A., Hasanah, A. N., Udin, L. Z., Susilawati, Y., Mustarichie, R., Kartasasmita, R. E., & Ibrahim, S. 2013, 'Cytotoxicity Studies of Xanthorrhizol and its Mechanism Using Molecular

Docking Simulation and Pharmacophore Modelling', *Journal of Applied Pharmaceutical Science*, vol. 3, no. 6, pp. 7–15.

Nusantoro, Y. R. & Fadlan, A. 2021, 'The Effect of Energy Minimization on The Molecular Docking of Acetone-Based Oxindole Derivatives', *JKPK (Jurnal Kimia dan Pendidikan Kimia)*, vol. 6, no. 1, pp. 69-77.

Niveshika, Verma, E., Maurya, S. K., Mishra, R., & Mishra, A. K. 2017, 'The Combined Use of in silico, in vitro, and in vivo analyses to assess anti-cancerous potential of a bioactive compound from cyanobacterium Nostoc sp. MGL001', *Frontiers in pharmacology*, vol. 8, no. 873.

Oon, S. F., Nallappan, M., Tee, T. T., Shohaimi, S., Kassim, N. K., Sa'ariwijaya, M. S. F., & Cheah, Y. H. 2015, 'Xanthorrhizol: A review of Its Pharmacological Activities And Anticancer Properties', *Cancer Cell International*, vol. 15, no. 1, pp. 1–15.

Pantsar, T., & Poso, A. 2018, 'Binding affinity via docking: fact and fiction', *Molecules*, vol. 23, no. 8, p. 1899.

Patel, N. K., Jaiswal, G. and Bhutani, K. K. 2016, 'A Review On Biological Sources, Chemistry And Pharmacological Activities Of Pinostrobin', *Natural Product Research*, vol. 30, no. 18, pp. 2017–2027.

Patil, R. & Jain, V. 2021 'Andrographolide: A review of analytical methods', *Journal of Chromatographic Science*, vol. 59, no. 2, pp. 191–203.

Płowuszyńska, A., & Gliszczyńska, A. 2021, 'Recent Developments In Therapeutic And Nutraceutical Applications Of P-Methoxycinnamic Acid From Plant Origin', *Molecules*, vol. 26, no. 13.

Prasasty, V. D., Cindana, S., Ivan, F. X., Zahroh, H., & Sinaga, E. 2020, 'Structure-based discovery of novel inhibitors of Mycobacterium tuberculosis CYP121 from Indonesian natural products', *Computational Biology and Chemistry*, vol. 85, no. 107205.

Rahayu, Y. C. 2012, 'Potential of Mangosteen Xanthones as Anti-Oral Cancer Agents by Induction of Apoptosis Potensi', *Idj*, vol. 1, no. 2, pp. 34–41.

Ramírez, D., & Caballero, J. 2018, 'Is it reliable to take the molecular docking top scoring position as the best solution without considering available structural data?', *Molecules*, vol. 23, no. 5, p. 1038.

RCSB, 2021, '*Resolution*', diakses pada 20 Agustus 2022, URL : http://pdb101.rcsb.org/learn/guide-to-understanding-pdb-data/resolution

Sastry, G. M., Adzhigirey, M., Day, T., Annabhimoju, R. and Sherman, W. 2013, 'Protein and Ligand Preparation: Parameters, Protocols, and Influence on Virtual Screening Enrichments', *J. Comput. Aided Mol. Des.*, vol. 27, no. 3, pp. 221– 234.

Setiawan, T., Ambarsari, L., and Sumaryada, T. 2017, 'Anticancer Study of Wonogiri's Curcuma Xanthorrhiza roxb Ethanol Fraction as Jamu by Flexible Docking Methods', *International Journal of Hybrid Information Technology*', vol. 10, no. 1, pp. 277–288.

Shanak, S., Bassalat, N., Barghash, A., Kadan, S., Ardah, M., & Zaid, H. 2022, 'Drug Discovery of Plausible Lead Natural Compounds That Target the Insulin Signaling Pathway: Bioinformatics Approaches', *Evidence-Based Complementary and Alternative Medicine*, vol. *2022*.

Shivanika, C., Kumar, S. D., Ragunathan, V., Tiwari, P., A, S., & P, B. D. 2020, 'Molecular Docking, Validation, Dynamics Simulations, and Pharmacokinetic Prediction of Natural Compounds Against The SARS-CoV-2 Main-Protease', *Journal of Biomolecular Structure & Dynamics*, vol. 2020, pp. 1–27.

Suherlan, S., Rohayah, & Fakih, T. M. 2021, 'Uji Aktivitas Antikanker Payudara Senyawa Andrografolida dari Tumbuhan Sambiloto (*Andrographis paniculata* (Burm F) Ness.) Terhadap *Human Epidermal Growth Factor Receptor 2 (HER-2)* Secara *In Silico', Jurnal Ilmiah Farmasi Farmasyifa*, vol. 4, no. 2, pp. 39-50.

Susanti, N. M. P., NPL, L., PPP, D., & PYC, D. 2019, 'Molecular docking terpinen-4-ol pada protein IKK sebagai antiinflamasi pada aterosklerosis secara *in silico'*, *Jurnal Farmasi Udayana*, vol. 1*,* no. 8, pp. 44-49.

Tasbichaty, F. T. 2010, 'Analisis dimulasi dinamika molekuler kompleks 12-lipoksigenase dengan beberapa senyawa antiinflamasi golongan kurkumin hasil penambatan molekuler', *skripsi*, Departemen Farmasi Universitas Indonesia, Depok.

Tjahjono, D.H. & Hamzah, N. 2013, 'Studi hubungan kuantitatif struktur-aktivitas, fitur farmakofor, dan docking molekuler senyawa turunan pirazolo-[3,4-d]-pirimidin sebagai inhibitor mer tirosin kinase', *Acta Pharmaceutica Indonesia*, vol. 38, no. 1, pp. 1−10.

Tomeh, M. A., Hadianamrei, R. & Zhao, X. 2019, 'A Review Of Curcumin And Its Derivatives As Anticancer Agents', *International Journal of Molecular Sciences*, vol. 20, no. 5.

Umar, M. I., Iqbal, M. A., Ahamed, M. B. K., Altaf, R., Hassan, L. E. A., Haque, R. A., Majeed, A. M. S. A., & Asmawi, M. Z. 2018, 'Cytotoxic and Pro-Apoptotic Properties of Ethyl-P-Methoxycinnamate and Its Hydrophilic Derivative Potassium-P-Methoxycinnamate', *Chemistry Africa*, vol. 1, no. 1, pp. 87-95.

Vania, L., Widyananda, M. H., Kharisma, V. D., Ansori, A. N. M., Naw, S. W., Maksimiuk, N., Derkho, M., Denisenko, A., Sumantri, N. I., & Nugraha, A. P. 2021, 'Anticancer Activity Prediction Of Garcinia Mangostana L. Against

Her2-Positive Breast Cancer Through Inhibiting EGFR, HER2 And IGF1R Protein: A Bioinformatics Study', *Biochem. Cell Arch*, vol. 21, no 2, pp.3313-3321.

Winiwarter, S., Ridderström, M., Ungell, A. L., Andersson, T. B., & Zamora, I. 2007, 'Use of molecular descriptors for absorption, distribution, metabolism, and excretion predictions', *Comprehensive Medicinal Chemistry II*, vol. 4, pp. 531-554.

Wu, J., Chen, K., Zhang, F., Jin, J., Zhang, N., Li, D., Ying, L., Chen, W., Yu, H., Mao, W., & Su, D. 2017, 'Overcoming Linsitinib Intrinsic Resistance Through Inhibition Of Nuclear Factor-Kb Signaling In Esophageal Squamous Cell Carcinoma', *Cancer Medicine*, vol. 6, no. 6, pp. 1353–1361.

Yadav, I. S., Nandekar, P. P., Shrivastava, S., Sangamwar, A., Chaudhury, A., & Agarwal, S. M. 2014, 'Ensemble docking and molecular dynamics identify knoevenagel curcumin derivatives with potent anti-EGFR activity', *Gene*, vol. *539,* no. 1, pp. 82-90.

Yang, Y., Chong-Yin, S., Jing, X., Jia-He, D., Shui-Lian, H. Y. T. 2020, 'Identification of Potential Dipeptidyl Peptidase', *Molecules*, vol. 25, no. 189.

Yang, F. R., Li, S. Y., Hu, X. W., Li, X. R., & Li, H. J. 2022, 'Identifying the Antitumor Effects of Curcumin on Lung Adenocarcinoma Using Comprehensive Bioinformatics Analysis', *Drug Design, Development and Therapy*, vol. *16*, pp. 2365–2382

Zhang, R., Feng, X., Su, G., Mu, Z., Zhang, H., Zhao, Y., Jiao, S., Cao, L., Chen, S., Tu, P., & Chai, X. 2018, 'Bioactive Sesquiterpenoids from the Peeled Stems of *Syringa pinnatifolia*', *Journal of Natural Products*, vol. 81, no. 8, pp. 1711–1720.

Zhang, C., Yu, G., & Shen, Y. 2018, 'The naturally occurring xanthone α-mangostin induces ROS-mediated cytotoxicity in non-small scale lung cancer cells', *Saudi Journal of Biological Sciences*, vol. 25, no. 6, pp. 1090-1095.

Zhang, J., Li, C., Zhang, L., Heng, Y., Xu, T., Zhang, Y., Chen, X., Hoffman, R. M., & Jia, L. 2021, 'Andrographolide induces noxa-dependent apoptosis by transactivating ATF4 in human lung adenocarcinoma cells', *Frontiers in pharmacology*, vol. 12, pp. 680589.

Zubair, M. S., Maulana, S., & Mukaddas, A. 2020, 'Penambatan molekuler dan simulasi dinamika molekuler senyawa dari genus nigella terhadap penghambatan aktivitas enzim protease HIV-1', *Jurnal Farmasi Galenika (Galenika Journal of Pharmacy)(E-Journal)*, vol. 6, no. 1, pp. 132-140.