

DAFTAR PUSTAKA

- Abdullah, S. S., Putra, P. P., Antasionasti, I., Rundengan, G., Suoth, E. J., Abdullah, R. P. I., & Abdullah, F. (2021). ANALISIS SIFAT FISIKOKIMIA, FARMAKOKINETIK DAN TOKSIKOLOGI PADA PERICARPIUM PALA (*Myristica fragrans*) SECARA ARTIFICIAL INTELLIGENCE. *Chemistry Progress*, 14(2), 81. <https://doi.org/10.35799/cp.14.2.2021.37112>
- Agrawal, P., Singh, H., Srivastava, H. K., Singh, S., Kishore, G., & Raghava, G. P. S. (2019). Benchmarking of different molecular docking methods for protein-peptide docking. *BMC Bioinformatics*, 19(Suppl 13). <https://doi.org/10.1186/s12859-018-2449-y>
- Akbar, N.A., Amin, S.,& Wulandari, W. T. (2022). STUDI IN SILICO SENYAWA YANG TERKANDUNG DALAM TANAMAN DAUN SIRIH MERAH (*Piper crocatum* RUITZ & PAV) SEBAGAI KANDIDAT ANTI SARS CoV-2. *Ejurnal Universitas Bth*, 2, 378–391. <https://repository.universitas-bth.ac.id/2246/> DAFTAR PUSTAKA.pdf
- Al-Rasheed, H. H., Al Alshaikh, M., Khaled, J. M., Alharbi, N. S., & El-Faham, A. (2016). Ultrasonic Irradiation: Synthesis, Characterization, and Preliminary Antimicrobial Activity of Novel Series of 4,6-Disubstituted-1,3,5-triazine Containing Hydrazone Derivatives. *Journal of Chemistry*, 2016. <https://doi.org/10.1155/2016/3464758>
- Alfanaar, R., Yunianti, Y., & Rismiarti, Z. (2017). Studi Kinetika Dan Isoterm Adsorpsi Besi(Iii) Pada Zeolit Alam Dengan Bantuan Gelombang Sonikasi. *EduChemia (Jurnal Kimia Dan Pendidikan)*, 2(1), 63. <https://doi.org/10.30870/educhemia.v2i1.1297>
- Anand, U., Dey, A., Chandel, A. K. S., Sanyal, R., Mishra, A., Pandey, D. K., De Falco, V., Upadhyay, A., Kandimalla, R., Chaudhary, A., Dhanjal, J. K., Dewanjee, S., Vallamkondu, J., & Pérez de la Lastra, J. M. (2023). Cancer chemotherapy and beyond: Current status, drug candidates, associated risks and progress in targeted therapeutics. *Genes and Diseases*, 10(4), 1367–1401. <https://doi.org/10.1016/j.gendis.2022.02.007>
- Arafa, W. A. A., Ghoneim, A. A., & Mourad, A. K. (2022). N-Naphthoyl Thiourea Derivatives: An Efficient Ultrasonic-Assisted Synthesis, Reaction, and In Vitro Anticancer Evaluations. *ACS Omega*, 7(7), 6210–6222. <https://doi.org/10.1021/acsomega.1c06718>
- Bare, Y., Sari, D. R., Rachmad, Y. T., Tiring, S. S. N. D., Rophi, A. H., & Nugraha, F. A. D. (2019). Prediction Potential Chlorogenic Acid As Inhibitor Ace (In Silico Study). *Bioscience*, 3(2), 197. <https://doi.org/10.24036/0201932105856-0-00>

- Barile, E., De, S. K., & Pellecchia, M. (2011). *3-Phosphoinositide-Dependent protein Kinase-1 (PDK1) inhibitor : Sebuah tinjauan dari literatur paten Abstrak Perkenalan. 1.*
- Baroroh, S.Si., M.Biotek., U., Muscifa, Z. S., Destiarani, W., Rohmatullah, F. G., & Yusuf, M. (2023). Molecular interaction analysis and visualization of protein-ligand docking using Biovia Discovery Studio Visualizer. *Indonesian Journal of Computational Biology (IJCB)*, 2(1), 22. <https://doi.org/10.24198/ijcb.v2i1.46322>
- Bele, A. A., & Khale., A. (2011). AN OVERVIEW ON THIN LAYER CHROMATOGRAPHY Archana A. Bele* and Anubha Khale H. K. College of Pharmacy, Jogeshwari (W), Mumbai, Maharashtra, India. *Journal of Pharmaceutical Sciences*, 2(2), 256–267.
- Burley, S. K., Berman, H. M., Bhikadiya, C., Bi, C., Chen, L., Di Costanzo, L., Christie, C., Duarte, J. M., Dutta, S., Feng, Z., Ghosh, S., Goodsell, D. S., Green, R. K., Guranovic, V., Guzenko, D., Hudson, B. P., Liang, Y., Lowe, R., Peisach, E., ... Ioannidis, Y. E. (2019). Protein Data Bank: The single global archive for 3D macromolecular structure data. *Nucleic Acids Research*, 47(D1), D520–D528. <https://doi.org/10.1093/nar/gky949>
- Casero, R. A., Murray Stewart, T., & Pegg, A. E. (2018). Polyamine metabolism and cancer: treatments, challenges and opportunities. *Nature Reviews Cancer*, 18(11), 681–695. <https://doi.org/10.1038/s41568-018-0050-3>
- Da Costa, C. H. C., Dantas Filho, F. F., & Gonçalves da Silva Cordeiro Moita, F. M. (2017). Marvinsketch E Kahoot Como Ferramentas No Ensino De Isomeria. *Holos*, 1, 31–43. <https://doi.org/10.15628/holos.2017.4733>
- Davis, A. M., Teague, S. J., & Kleywegt, G. J. (2003). Application and limitations of x-ray crystallographic data in structure-based ligand and drug design. *Angewandte Chemie - International Edition*, 42(24), 2718–2736. <https://doi.org/10.1002/anie.200200539>
- 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. *Methods in Molecular Biology*, 1598, 391–403. https://doi.org/10.1007/978-1-4939-6952-4_20
- Endriyatno, N. C., & Walid, M. (2022). Studi In Silico Kandungan Senyawa Daun Srikaya (*Annona squamosa L.*)Terhadap Protein Dihydrofolate Reductase Pada Mycobacterium tuberculosis. *Pharmacon: Jurnal Farmasi Indonesia*, 19(1), 87–98. <https://doi.org/10.23917/pharmacon.v19i1.18044>
- Fransiska, Angel Novia, et al. (2022). Review: Target Aksi Obat Terhadap Reseptor Dopamin. *Jurnal Pendidikan Dan Konseling*, 4(6), 8706–8716. <https://doi.org/10.32539/sjm.v2i2.57>

Guo, Y., Liu, C., Ye, R., & Duan, Q. (2020). applied sciences Advances on Water Quality Detection by. *Applied Sciences*, 10(3), 1–18.

Hermansyah, O., Salsabila, F. J., Pertwi, R., Versita, R., & Ikhsan, I. (2022). Studi in Silico Senyawa Tumbuhan Famili Asteraceae Sebagai Penghambat Enzim Xantin Oxidase. *Pharma Xplore Jurnal Ilmiah Farmasi*, 7(2), 70–79. <https://doi.org/10.36805/jpx.v7i2.2942>

Hollingsworth, S. A., & Karplus, P. A. (2010). A fresh look at the Ramachandran plot and the occurrence of standard structures in proteins. *Biomolecular Concepts*, 1(3–4), 271–283. <https://doi.org/10.1515/bmc.2010.022>

Imanudin, N., Kurniawan, M. F., & Rohmayanti, T. (2022). Potensi Senyawa Aktif Ekstrak Kayu Manis Padang (*Cinnamomum burmanii*) sebagai Inhibitor Enzim Aldose Reductase secara Molecular Docking. *JRST (Jurnal Riset Sains Dan Teknologi)*, 6(2), 171. <https://doi.org/10.30595/jrst.v6i2.14262>

Kalász, H., Báthori, M., & Valkó, K. L. (2020). Basis and pharmaceutical applications of thin-layer chromatography. In *Handbook of Analytical Separations* (Vol. 8). <https://doi.org/10.1016/B978-0-444-64070-3.00010-2>

Kelutur, F. J., Mustarichie, R., & Umar, A. K. (2020). Virtual Screening Kandungan Senyawa Kipas Laut (*Gorgonia mariae*) sebagai Anti-Asma. *ALCHEMY Jurnal Penelitian Kimia*, 16(2), 48. <https://doi.org/10.20961/alchemy.16.2.39965.48-59>

Kesuma, D., Siswandono, S., Purwanto, B. T., & Hardjono, S. (2018). Uji in silico Aktivitas Sitotoksik dan Toksisitas Senyawa Turunan N-(Benzoil)-N'-feniltiourea Sebagai Calon Obat Antikanker. *JPSCR : Journal of Pharmaceutical Science and Clinical Research*, 3(1), 1. <https://doi.org/10.20961/jpscr.v3i1.16266>

Khasanah, N. U., Wardani, G. A., & Mardianingrum, R. (2023). *Jurnal Kimia Sains dan Aplikasi 3-Phenylthiourea Cobalt (III) as Anticancer Candidate*. 26(7), 238–248.

Kumar, A., Singh, P., & Nanda, A. (2020). Hot stage microscopy and its applications in pharmaceutical characterization. *Applied Microscopy*, 50(1). <https://doi.org/10.1186/s42649-020-00032-9>

Levina, A., Fleming, K. D., Burke, J. E., & Leonard, T. A. (2022). Activation of the essential kinase PDK1 by phosphoinositide-driven trans-autophosphorylation. *Nature Communications*, 13(1), 1–16. <https://doi.org/10.1038/s41467-022-29368-4>

Lewandowska, A. M., Rudzki, M., Rudzki, S., Lewandowski, T., & Laskowska, B. (2019). Environmental risk factors for cancer - review paper. *Annals of Agricultural and Environmental Medicine*, 26(1), 1–7. <https://doi.org/10.26444/aaem/94299>

- Mardiana, M., & Ruswanto. (2019). Simulasi Dinamika Molekular Senyawa Pyridin Pada Protein 2XNB. *Research Gate*, 9(5), 1–15.
- Marselia, A., Wahdaningsih, S., & Nugraha, F. (2021). Analisis gugus fungsi dari ekstrak metanol kulit buah naga merah (*Hylocereus polyrhizus*) menggunakan FT-IR. *Jurnal Mahasiswa Farmasi Fakultas Kedokteran UNTAN*, 5(1), 1–5.
- Mohimani, H., Gurevich, A., Mikheenko, A., Garg, N., Nothias, L.-F., Ninomiya, A., Kentaro Takada, P. C. D., & Pevzner, P. A. (2017). Molecular Dynamics for all. *Physiology & Behavior*, 176(3), 139–148. <https://doi.org/10.1016/j.neuron.2018.08.011>
- Mohtar, K., Fatimawali, Rumondor, E. M., Datu, O. S., & Tallei, T. (2021). Studi In Silico Senyawa Eugenol Cengkeh (*Syzygium Aromaticum L.*) Terhadap Reseptor Er-?, Er-? dan Her-2 pada Kanker Payudara. *Pharmacon*, 10(3), 1001–1008.
- Mvondo, J. G. M., Matondo, A., Mawete, D. T., Bambi, S.-M. N., Mbala, B. M., & Lohohola, P. O. (2021). In Silico ADME/T Properties of Quinine Derivatives using SwissADME and pkCSM Webservers. *International Journal of TROPICAL DISEASE & Health*, August, 1–12. <https://doi.org/10.9734/ijtdh/2021/v42i1130492>
- Narmani, A., & Jafari, S. M. (2021). Chitosan-based nanodelivery systems for cancer therapy: Recent advances. *Carbohydrate Polymers*, 272(May), 118464. <https://doi.org/10.1016/j.carbpol.2021.118464>
- Novita Sari, I., Setiawan, T., Seock Kim, K., Toni Wijaya, Y., Won Cho, K., & Young Kwon, H. (2021). Metabolism and function of polyamines in cancer progression. *Cancer Letters*, 519(June), 91–104. <https://doi.org/10.1016/j.canlet.2021.06.020>
- Nowotarski, S. L., Woster, P. M., & Jr, R. A. C. (2014). *chemotherapy*. 1–28. <https://doi.org/10.1017/erm.2013.3>
- Pagarra, H. (2022). *SEKUNDER EKSTRAK ETANOL DAUN KAYU JAWA *Lannea coromandelica**. 5(September 2022), 161–168.
- Pires, D. E. V, Blundell, T. L., & Ascher, D. B. (n.d.). *pkCSM : predicting small-molecule pharmacokinetic properties using graph-based signatures*.
- Ploskonos, M. V., Syatkin, S. P., Neborak, E. V., Hilal, A., Sungrapova, K. Y., Sokuyev, R. I., Blagonravov, M. L., Korshunova, A. Y., & Terentyev, A. A. (2020). Polyamine analogues of propanediamine series inhibit prostate tumor cell growth and activate the polyamine catabolic pathway. *Anticancer Research*, 40(3), 1437–1441. <https://doi.org/10.21873/anticanres.14085>
- Prasetiawati, R., Suherman, M., Permana, B., & Rahmawati, R. (2021). Molecular Docking Study of Anthocyanidin Compounds Against Epidermal Growth Factor Receptor (EGFR) as Anti-Lung Cancer. *Indonesian Journal of*

- Pudjono, Suparjan, T. I. (2006). *Sintesis benzaldehid dan siklopentanon dengan variasi pelarut dehyde and cyclopentanone by solvent variation*. 17(1), 45–49.
- Purwanto, B. T. (2018). Sintesis senyawa n-(2-klorobenzoil)-n'-fenilurea dan uji aktivitas anti kanker terhadap sel hela (synthesis and anti cancer activity test against hela cells from n-(2-chlorobenzoyl)-n'-phenylurea). *Jurnal Ilmu Kefarmasian Indonesia*, 16(2), 159–165.
- Ronchetti, R., Moroni, G., Carotti, A., Gioiello, A., & Camaioni, E. (2021). Recent advances in urea- And thiourea-containing compounds: focus on innovative approaches in medicinal chemistry and organic synthesis. *RSC Medicinal Chemistry*, 12(7), 1046–1064. <https://doi.org/10.1039/d1md00058f>
- Ruswanto, R. (2015). Sintesis Dan Analisis Spektrum Senyawa 3-Benzoyl-1-Feniltiourea Serta Uji Interaksinya Pada Reseptor Kanker. *Jurnal Kesehatan Bakti Tunas Husada: Jurnal Ilmu-Ilmu Keprawatan, Analis Kesehatan Dan Farmasi*, 12(1), 177. <https://doi.org/10.36465/jkbth.v12i1.77>
- Ruswanto, R., Mardianingrum, R., Siswandono, S., & Kesuma, D. (2020). Reverse docking, molecular docking, absorption, distribution, and toxicity prediction of artemisinin as an anti-diabetic candidate. *Molekul*, 15(2), 88–96. <https://doi.org/10.20884/1.jm.2020.15.2.579>
- Ruswanto, R., Mardianingrum, R., & Yanuar, A. (2022). Computational Studies of Thiourea Derivatives as Anticancer Candidates through Inhibition of Sirtuin-1 (SIRT1). *Jurnal Kimia Sains Dan Aplikasi*, 25(3), 87–96. <https://doi.org/10.14710/jksa.25.3.87-96>
- Ruswanto, R., Miftah, A. M., Tjahjono, D. H., & Siswandono. (2021). In silico study of 1-benzoyl-3-methylthiourea derivatives activity as epidermal growth factor receptor (EGFR) tyrosine kinase inhibitor candidates. *Chemical Data Collections*, 34(36), 100741. <https://doi.org/10.1016/j.cdc.2021.100741>
- Ruswanto, R., Nofianti, T., Mardianingrum, R., Kesuma, D., & Siswandono. (2022). Design, molecular docking, and molecular dynamics of thiourea-iron (III) metal complexes as NUDT5 inhibitors for breast cancer treatment. *Heliyon*, 8(9). <https://doi.org/10.1016/j.heliyon.2022.e10694>
- Ruswanto, R., Nofianti, T., Mardianingrum, R., & Lestari, T. (2018). Desain dan Studi In Silico Senyawa Turunan Kuwanon-H sebagai Kandidat Obat Anti-HIV. *Jurnal Kimia VALENSI*, 4(1), 57–66. <https://doi.org/10.15408/jkv.v4i1.6867>
- Ruswanto, R., & Nugraha, A. (2015). Sintesis Senyawa 1-(4-Hephtilbenzoil-3-Metiltiourea) Dan Uji Sitotoksitas Terhadap Sel T47D Sebagai Kandidat Antikanker. *Jurnal Kesehatan Bakti Tunas Husada: Jurnal Ilmu-Ilmu*

Keperawatan, Analis Kesehatan Dan Farmasi, 14(1), 145.
<https://doi.org/10.36465/jkbth.v14i1.123>

Ruswanto, R., Sarwatiningsih, Y., Pratita, A. T. K., Indra, & Dewi, R. (2019). Synthesis and Characterization of Fe(III) Complex with N'- (3-Nitrobenzoyl)Isonicotinohydrazide as an Anti-tuberculosis Candidate. *Journal of Physics: Conference Series*, 1179(1). <https://doi.org/10.1088/1742-6596/1179/1/012136>

Ruswanto, R., Trisna Wulandari, W., Mardianingrum, R., & Cantika, I. (2021). Synthesis and virtual screening of bis-(4-(tert-butyl)-N-(methylcarbamothioyl) benzamide)-Iron (III) complex as an anticancer candidate. *Pharmaciana*, 11(1), 1. <https://doi.org/10.12928/pharmaciana.v11i1.17837>

Ruswanto, Siswandono, Richa, M., Tita, N., & Tresna, L. (2017). Molecular docking of 1-benzoyl-3-methylthiourea as anti cancer candidate and its absorption, distribution, and toxicity prediction. *Journal of Pharmaceutical Sciences and Research*, 9(5), 680–684.

Ruswanto, Trisna, W., Mardianingrum, R., & Nurlatifah, M. R. (2021). Sintesis, Karakterisasi dan Penambatan Molekul Bis-2-Chloro-N-(Methylcarbamothioyl)-Benzamide-Iron (III) Sebagai Kandidat Anti Kanker. *Prosiding Seminar Nasional Diseminasi Penelitian, September*, 17–27.

Salim, E. I., Wanibuchi, H., Morimura, K., Kim, S., Yano, Y., Yamamoto, S., & Fukushima, S. (2000). Inhibitory effects of 1,3-diaminopropane, an ornithine decarboxylase inhibitor, on rat two-stage urinary bladder carcinogenesis initiated by N-butyl-N-(4-hydroxybutyl)nitrosamine. *Carcinogenesis*, 21(2), 195–203. <https://doi.org/10.1093/carcin/21.2.195>

Sari, I. W., Junaidin, J., & Pratiwi, D. (2020). STUDI MOLECULAR DOCKING SENYAWA FLAVONOID HERBA KUMIS KUCING (Orthosiphon stamineus B.) PADA RESEPTOR α -GLUKOSIDASE SEBAGAI ANTIDIABETES TIPE 2. *Jurnal Farmagazine*, 7(2), 54. <https://doi.org/10.47653/farm.v7i2.194>

Siagian, J. I., Purnomo, H., & Sasmito, E. (2022). Studi In Silico Senyawa Dalam Teripang Sebagai Imunomodulator. *Journal of Pharmaceutical And Sciences*, 5(1), 33–41. <https://doi.org/10.36490/journal-jps.com.v5i1.99>

Song, Y., Cong, Y., Wang, B., & Zhang, N. (2020). Applications of Fourier transform infrared spectroscopy to pharmaceutical preparations. *Expert Opinion on Drug Delivery*, 17(4), 551–571. <https://doi.org/10.1080/17425247.2020.1737671>

Sovia, A. B., & Neva, M. (2017). Prediksi Mekanisme Kerja Obat Terhadap Reseptornya Secara in Silico(Studi pada Antibiotika Sefotaksim). *Research Report*, 0(0), 89–94. <http://research-report.umm.ac.id/index.php/research->

report/article/view/1367

- Srivastava, N., Garg, P., Srivastava, P., & Seth, P. K. (2021). A molecular dynamics simulation study of the ACE2 receptor with screened natural inhibitors to identify novel drug candidate against COVID-19. *PeerJ*, 9, 1–18. <https://doi.org/10.7717/peerj.11171>
- Stefaniu, A. (2019). Introductory Chapter: Molecular Docking and Molecular Dynamics Techniques to Achieve Rational Drug Design. *Molecular Docking and Molecular Dynamics*, 1–5. <https://doi.org/10.5772/intechopen.84200>
- Suryani, Y., Taupiqurohman, O., Rikani, A., & Paujiah, E. (2018). Insilico docking studies of daidzein compounds as selective estrogen receptor modulator (SERMS) breast cancer. *MATEC Web of Conferences*, 197, 1–5. <https://doi.org/10.1051/matecconf/201819703009>
- Tam, B., Sinha, S., & Wang, S. M. (2020). Combining Ramachandran plot and molecular dynamics simulation for structural-based variant classification: Using TP53 variants as model. *Computational and Structural Biotechnology Journal*, 18, 4033–4039. <https://doi.org/10.1016/j.csbj.2020.11.041>
- Tchounwou, P. B., Dasari, S., Noubissi, F. K., Ray, P., & Kumar, S. (2021). Advances in our understanding of the molecular mechanisms of action of cisplatin in cancer therapy. *Journal of Experimental Pharmacology*, 13, 303–328. <https://doi.org/10.2147/JEP.S267383>
- Tulloh, & Andriane, Y. (2022). Sediaan Nanopartikel Alginat Ekstrak Etanol Daun Sirsak (*Annona muricata Linn*) Memiliki Efek Antikanker pada Kultur Sel Kanker Paru (HTB183). *Jurnal Riset Kedokteran*, 1(2), 124–129. <https://doi.org/10.29313/jrk.v1i2.565>
- Wade, L. G. (2013). *Organic Chemistry*. Eighth Edition. Pearson Education. IL. pp. 70-71, 782, 960-962, 969, 970-971, 986, 997-1000.
- Wahdaningsih, S., Nugraha, F., Kurniawan, H., Marselia, A., & Sari, D. N. (2022). Identifikasi Gugus Fungsi Fraksi Etil Asetat dan Fraksi n-Heksan Hylocereus polyrhizus (F.A.C.Weber) Britton & Rose. *Jurnal Pharmascience*, 9(1), 113. <https://doi.org/10.20527/jps.v9i1.11192>
- Wang, M., Zhang, Y., Wang, R., Wang, Z., Yang, B., & Kuang, H. (2021). An Evolving Technology That Integrates Classical Methods Chromatography Bioautography. *Multidisciplinary Digital Publishing Institute (MDPI)*, 26, 1–21.
- Wang, R., & Wang, Y. (2021). Fourier transform infrared spectroscopy in oral cancer diagnosis. *International Journal of Molecular Sciences*, 22(3), 1–21. <https://doi.org/10.3390/ijms22031206>
- Yahya, E. B., & Alqadhi, A. M. (2021). Recent trends in cancer therapy: A review on the current state of gene delivery. *Life Sciences*, 269(December 2020),

119087. <https://doi.org/10.1016/j.lfs.2021.119087>

Yualanda, V. G., Sary, I. P., & Pangaribowo, D. A. (2018). Sintesis dan Uji Aktivitas Antibakteri Senyawa N-Fenil-3,4-Diklorobenzamida (Synthesis and Antibacterial Activity Assay of N-Phenyl-3,4-Dichlorobenzamide). *Pustaka Kesehatan*, 6(1), 5. <https://doi.org/10.19184/pk.v6i1.6610>