

## DAFTAR PUSTAKA

- Abdullah, S. S., Putra, P. P., Antasionasti, I., Suoth, E. J., Putri, R., & Abdullah, I. (2021). *ANALISIS SIFAT FISIKOKIMIA , FARMAKOKINETIK DAN TOKSIKOLOGI PADA PERICARPIUM PALA ( Myristica fragrans ) SECARA ARTIFICIAL INTELLIGENCE. 14(2).*
- Afriza, D., Suriyah, W. H., & A, I. S. J. (2018). In silico analysis of molecular interactions between the anti-apoptotic protein survivin and dentatin , nordentatin , and quercetin In silico analysis of molecular interactions between the anti-apoptotic protein survivin and dentatin , nordentatin , and. *In Silico Analysis Ofmolecular Interactions between the Anti- Apoptotic Protein Survivin and Dentatin, Nordentatin, and Quercetin.*
- Alfiani, D., Putri, M. P., & Widayanti, W. (2022). Literature Study: Obesitas sebagai Faktor Risiko pada Kanker Payudara Triple Negative. *Bandung Conference Series: Medical Science, 2(1).* <https://doi.org/10.29313/bcsms.v2i1.760>
- Anwar, C., & Laifa, F. (2018). Hubungan Informasi dan Umur dengan Kecemasan Ibu Kanker Payudara pada Tindakan Kemoterapi di Rumah Sakit Umum Daerah Zainoel Abidin. *Journal of Healthcare Technology and Medicine, 4(2), 185.* <https://doi.org/10.33143/jhtm.v4i2.208>
- Ashfaq, F., Barkat, M. A., Ahmad, T., Hassan, M. Z., Ahmad, R., Barkat, H., Idreesh Khan, M., Saad Alhodieb, F., Asiri, Y. I., & Siddiqui, S. (2023). Phytocompound screening, antioxidant activity and molecular docking studies of pomegranate seed: a preventive approach for SARS-CoV-2 pathogenesis. *Scientific Reports, 13(1), 1–21.* <https://doi.org/10.1038/s41598-023-43573-1>
- Az-zahra, F., Afidika, J., Diamantha, S. D. A., Rahmani, A. E., In, S., Senyawa, S., Piper, S., Asetilkolinesterase, E., & Alzheimer, P. (2022). *In Silico Study of Betel Leaves Compound ( Piper betle L .) as Acetylcholinesterase ( AChE ) Enzyme*

*Inhibitor in Alzheimer Disease*. 2(2), 44–58.

Bhaliya, J., & Shah, V. (2020). Identification of potent COVID-19 Main Protease (Mpro) inhibitors from Curcumin analogues by Molecular Docking Analysis. *International Journal of Advance Research, Ideas and Innovations in Technology*, 6(2), 664–672.

Chow, E., Rendleman, C. A., Bowers, K. J., Dror, R. O., Douglas, H., Gullingsrud, J., Sacerdoti, F. D., & Shaw, D. E. (2008). *Desmond Performance on a Cluster of Multicore Processors*. July, 1–14.

Endriyanto, N. C., & Santoso, B. (2020). Hasil Komputasi Vina untuk Kandungan Bawang Putih dan Adas Bintang Terhadap Protein Dehidrogenase Piruvat Mycobacterium tuberculosis. *University Research Colloquium*, 1(1), 366–372.

Fan, J., Fu, A., & Zhang, L. (2019). Progress in molecular docking. *Quantitative Biology*, 7(2), 83–89. <https://doi.org/10.1007/s40484-019-0172-y>

Firdiana, E. R. (2021). Delima (*Punica granatum* L.): salah satu koleksi Kebun Raya Purwodadi berpotensi obat. Prosiding Biologi Achieving the Sustainable Development Goals with Biodiversity in Confronting Climate Change; 2021 Nov 08; Makassar, Indonesia, *November*, 107–112.

Firnanda, F., Bimo Aksono Herupradoto, E., Rahmawati, K., Kurnijasanti, R., Sukmanadi, M., Hidajati, N., & Kedokteran Hewan Dasar, D. (2021). Uji Toksisitas Ekstrak Buah Delima Putih (*Punica granatum* L.) Dengan Metode Brine Shrimp Lethality Test Sebagai Kandidat Obat Antikanker Toxicity Testing Of White Pomegranate (*Punica granatum* L.) Fruit Extracts Using Brine Shrimp Lethality Test Method As A. *Journal of Basic Medical Veterinary Firnanda et Al. Desember 2021*, 10(2), 45–50. <https://e-journal.unair.ac.id/JBMV>

Gyebi, G. A., Ogunro, O. B., Adegunloye, A. P., & Ogunyemi, O. M. (2020). Potential inhibitors of coronavirus 3-chymotrypsin-like protease ( 3CL pro ): an in silico screening of alkaloids and terpenoids from African medicinal plants. *Journal of*

- Biomolecular Structure and Dynamics*, 0(0), 1–13.  
<https://doi.org/10.1080/07391102.2020.1764868>
- Harling van, V. N. (2019). Extract Free Radical Capture Activities Methanol Fruit Skins And Pomegranate Seeds (*Punica granatum*. L). *Sosced*, 2(2).
- Hollingsworth, S. A., & Dror, R. O. (2018). Review Molecular Dynamics Simulation for All. *Neuron*, 99(6), 1129–1143. <https://doi.org/10.1016/j.neuron.2018.08.011>
- Ivanović, V., Rančić, M., Arsić, B., & Pavlović, A. (2020). *Lipinski 's rule of five , famous extensions and famous exceptions Lipinski rule of five*. 3(1), 171–177.
- Jang, J. Y., Kim, D., & Im, E. (2024). *Therapeutic Potential of Pomegranate Extract for Women 's Reproductive Health and Breast Cancer*.
- Jessica, hermawan, A. (2021). *Molecular Docking Ligan ( Senyawa Antikanker ) dan Protein Reseptor*. September.
- Khan, S. L., Sonwane, G. M., Siddiqui, F. A., Jain, S. P., Kale, M. A., & Borkar, V. S. (2020). *Discovery of Naturally Occurring Flavonoids as Human Cytochrome P450 ( CYP3A4 ) Inhibitors with the Aid of Computational Chemistry*. 10(4), 58–69.
- Kim, S., Chen, J., Cheng, T., Gindulyte, A., He, J., He, S., Li, Q., Shoemaker, B. A., Thiessen, P. A., Yu, B., Zaslavsky, L., Zhang, J., & Bolton, E. E. (2019). PubChem 2019 update: Improved access to chemical data. *Nucleic Acids Research*, 47(D1), D1102–D1109. <https://doi.org/10.1093/nar/gky1033>
- Kim, S., Chen, J., Cheng, T., Gindulyte, A., He, J., He, S., Li, Q., Shoemaker, B. A., Thiessen, P. A., Yu, B., Zaslavsky, L., Zhang, J., & Bolton, E. E. (2021). PubChem in 2021: New data content and improved web interfaces. *Nucleic Acids Research*, 49(D1), D1388–D1395. <https://doi.org/10.1093/nar/gkaa971>
- Kumar, S., Sharma, P. P., Shankar, U., Kumar, D., Joshi, S. K., Pena, L., Durvasula, R., Kumar, A., Kempaiah, P., Poonam, & Rathi, B. (2020). Discovery of New

- Hydroxyethylamine Analogs against 3CLproProtein Target of SARS-CoV-2: Molecular Docking, Molecular Dynamics Simulation, and Structure-Activity Relationship Studies. *Journal of Chemical Information and Modeling*, 60(12), 5754–5770. <https://doi.org/10.1021/acs.jcim.0c00326>
- Mazumder, L., Hasan, R., Fatema, K., & Islam, Z. (2022). *Structural and Functional Annotation and Molecular Docking Analysis of a Hypothetical Protein from Neisseria gonorrhoeae : An In-Silico Approach*. 2022.
- Meli, R., & Biggin, P. C. (2020). spyrmsd : symmetry - corrected RMSD calculations in Python. *Journal of Cheminformatics*, 1–7. <https://doi.org/10.1186/s13321-020-00455-2>
- Mulyani, L., Lindayani, E., & Sukaesih, N. S. (2024). Systematic Literature Review : Risiko Penggunaan. *Jurnal Ners Universitas Pahlawan*, 8(2), 1959–1967.
- Muslikh, F. A., Tuah, U. H., & Kurniawati, E. (2023). *ADMET Prediction of the Dominant Compound from Mangosteen ( Garcinia mangostana L .) using pkCSM : A Computational Approach* *ADMET Prediction of the Dominant Compound from Mangosteen ( Garcinia mangostana L .) using pkCSM : A Computational Approach*. December. <https://doi.org/10.55927/ijcs.v1i1.7271>
- Numan, M., Anwer, S., Id, B., Rehman, M., Mustafa, G., & Sadia, B. (2021). *Phylogenetic analyses , protein modeling and active site prediction of two pathogenesis related ( PR2 and PR3 ) genes from bread wheat*. 1–16. <https://doi.org/10.1371/journal.pone.0257392>
- Nusantoro, Y. R., & Fadlan, A. (2020). Analisis Sifat Mirip Obat, Prediksi ADMET, dan Penambatan Molekular Isatinil-2-Aminobenzoilhidrazon dan kompleks logam transisi Co(II), Ni(II), Cu(II), Zn(II) Terhadap BCL2-XL. *Akta Kimia Indonesia*, 5(2), 114. <https://doi.org/10.12962/j25493736.v5i2.7881>
- Nusantoro, Y. R., & Fadlan, A. (2021). *THE EFFECT OF ENERGY MINIMIZATION ON THE MOLECULAR DOCKING OF ACETONE-BASED OXINDOLE*. 6(1),

69–77.

- Oktrinalida, A. M., Sahab, A., & Suryani, P. R. (2019). Kualitas Hidup Pasien Skizofrenia di Poliklinik Rawat Jalan Rumah Sakit Ernaldi Bahar Palembang. *Sriwijaya Journal of Medicine*, 2(2), 68–75. <https://doi.org/10.32539/sjm.v2i2.57>
- Owoloye, A. J., Ligali, F. C., Enejoh, O. A., Musa, A. Z., Aina, O., Id, E. T. I., & Id, K. M. O. (2022). *Molecular docking , simulation and binding free energy analysis of small molecules as Pf HT1 inhibitors.* 1–18. <https://doi.org/10.1371/journal.pone.0268269>
- PDB. (2024). *Protein Data Bank (PDB)*. <https://www.rcsb.org/pages/contactus>
- Pinzi, L., & Rastelli, G. (2019). *Molecular Docking : Shifting Paradigms in Drug Discovery.*
- Pokhrel, S. (2024). No TitleEAENH. *Αγαη*, 15(1), 37–48.
- Prasetio, N. F., Kepel, B. J., Bodhi, W., Fatimawali, ., Manampiring, A., & Budiarmo, F. (2021). Molecular Docking terhadap Senyawa Isoeleutherin dan Isoeleutherol sebagai Penghambat Pertumbuhan SARS-CoV-2. *Jurnal E-Biomedik*, 9(1), 101–106. <https://doi.org/10.35790/ebm.v9i1.31809>
- Pratama, F., Ruswanto, R., Nofianti, T., Tri, A., Pratita, K., & Daruwati, I. (2024). Radiolabeling and In-Silico Study of <sup>131</sup>I- ( 4-fluorobenzoyl-3-methylthiourea ) as Radiopharmaceuticals for Breast Cancer Theranostics. *Https://Journal.Uinjkt.Ac.Id/Index.Php/Valensi*, 18. <https://doi.org/10.15408/jkv.v10i1.34258>
- Purwaniati, P., & Roni, A. (2022). Molecular docking study and molecular dynamics simulation of spice metabolites against main protease enzymes and NSP3 macrodomain SARS CoV-2. *Pharmaciana*, 12(1), 1. <https://doi.org/10.12928/pharmaciana.v12i1.21501>
- Putra, P. P., Fauzana, A., & Lucida, H. (2020). *In Silico Analysis of Physical-Chemical*

*Properties , Target Potential , and Toxicology of Pure Compounds from Natural Products In Silico Analysis of Physical-Chemical Properties , Target Potential , and Toxicology of Pure Compounds from Natural Products Analisis Sifat Fisika-Kimia , Potensi Target dan Toksikologi Senyawa Isolat Murni dari Bahan Alam dengan Metode In Silico. October.* <https://doi.org/10.24198/ijpst.v7i3.26403>

- Rahmadi, M. A., Nasution, H., Mawar, L., & Sari, M. (2024). *Pengaruh Kecemasan Terhadap Kepatuhan Pengobatan Kanker Payudara Universitas Islam Negeri Syarif Hidayatullah Jakarta , Indonesia Universitas Negeri Padang , Indonesia Universitas Sumatera Utara , Indonesia Universitas Islam Negeri Sumatera Utara , Indone. 2(3).*
- Ratama, P. A. R. I. P., Sman, F. E. I., Adlan, D. A. N. A. R. I. F. F., Teknik, D., Teknologi, I., & Nopember, S. (2022). *MINYAK ATSIRI BUNGA MICHELIA ALBA SECARA IN SILICO. 9(1).*
- Reich, V., Majumdar, A., Müller, M., & Busch, S. (2022). *Comparison of molecular dynamics simulations of water with neutron and X-ray scattering experiments. 01015.*
- Renadi, S., Pratita, A. T. K., Mardianingrum, R., & Ruswanto, dan R. (2023). The Potency of Alkaloid Derivates as Anti-Breast Cancer Candidates: In Silico Study. *Jurnal Kimia Valensi, 9(1), 89–108.* <https://doi.org/10.15408/jkv.v9i1.31481>
- Ruswanto, Mardianingrum, R., & Yanuar, A. (2022). *Jurnal Kimia Sains dan Aplikasi Computational Studies of Thiourea Derivatives as Anticancer. 25(3), 87–96.*
- Ruswanto, Nofianti, T., Mardianingrum, R., Lestari, T., & Sepriliani, A. (2018). Desain dan Studi In Silico Senyawa Turunan Kuwanon-H sebagai Kandidat Obat Anti-HIV Design and In Silico Study of Kuwanon-H as Anti-HIV Drug Candidate. *Jurnal Penelitian Dan Pengembangan Ilmu Kimia, 4(1), 57–66.*
- Ruswanto, R., Mardianingrum, R., Nofianti, T., Fizriani, R., & Siswandono, S. (2023). Computational Study of Bis-(1-(Benzoyl)-3-Methyl Thiourea) Platinum (II)

- Complex Derivatives as Anticancer Candidates. *Advances and Applications in Bioinformatics and Chemistry*, 16(January), 15–36.  
<https://doi.org/10.2147/AABC.S392068>
- Ruswanto, R., Nofianti, T., Mardianingrum, R., & Kesuma, D. (2022). *Heliyon Design , molecular docking , and molecular dynamics of thiourea-iron ( III ) metal complexes as NUDT5 inhibitors for breast cancer treatment*. 8(September).  
<https://doi.org/10.1016/j.heliyon.2022.e10694>
- Saleem, H., Munir, S., Mumtaz, A., Ali, R., Maqbool, A., Malik, D., & Sideeq, M. A. (2019). Identification of Potent Inhibitors against Potential Drug Target for Schizophrenia Trough Virtual Screening Approach. *International Journal of Scientific and Research Publications (IJSRP)*, 9(6), p90119.  
<https://doi.org/10.29322/ijsrp.9.06.2019.p90119>
- Septian, A. D., Wardani, G. A., Mardianingrum, R., & Ruswanto, R. (2023). *The Virtual Screening of Flavonoid Derivatives on Progesterone , Estrogen , and HER-2 Receptor for Breast Cancer Treatment Candidate*. 9(May), 163–182.  
<https://doi.org/10.15408/jkv.v9i1.31482>
- Shaban, N. Z., Talaat, I. M., Elrashidy, F. H., Hegazy, A. Y., & Sultan, A. S. (2017). THERAPEUTIC ROLE OF PUNICA GRANATUM ( POMEGRANATE ) SEED OIL EXTRACT ON BONE TURNOVER AND RESORPTION INDUCED IN OVARECTOMIZED RATS. *The Journal of Nutrition, Health and Aging*, 21(10), 1299–1306. <https://doi.org/10.1007/s12603-017-0884-5>
- Sung, H., Ferlay, J., Siegel, R. L., Laversanne, M., Soerjomataram, I., Jemal, A., & Bray, F. (2021). Global Cancer Statistics 2020: GLOBOCAN Estimates of Incidence and Mortality Worldwide for 36 Cancers in 185 Countries. *CA: A Cancer Journal for Clinicians*, 71(3), 209–249.  
<https://doi.org/10.3322/caac.21660>
- Titin, S., & Ballo, A. (2019). Analisis Senyawa Polifenol Ekstrak Kulit Buah dan Biji Delima (*Punica granatum* L). *Jurnal Biotropikal Sains*, 16(1), 14–19.

- Ummah, M. S. (2019). American Society Of Clinical Oncology. *Sustainability (Switzerland)*, 11(1), 1–14.  
[http://scioteca.caf.com/bitstream/handle/123456789/1091/RED2017-Eng-8ene.pdf?sequence=12&isAllowed=y%0Ahttp://dx.doi.org/10.1016/j.regsciurbe.co.2008.06.005%0Ahttps://www.researchgate.net/publication/305320484\\_SISTEM\\_PEMBETUNGAN\\_TERPUSAT\\_STRATEGI\\_MELESTARI](http://scioteca.caf.com/bitstream/handle/123456789/1091/RED2017-Eng-8ene.pdf?sequence=12&isAllowed=y%0Ahttp://dx.doi.org/10.1016/j.regsciurbe.co.2008.06.005%0Ahttps://www.researchgate.net/publication/305320484_SISTEM_PEMBETUNGAN_TERPUSAT_STRATEGI_MELESTARI)
- Vieira, T. F., & Sousa, S. F. (2019). Comparing AutoDock and Vina in ligand/decoy discrimination for virtual screening. *Applied Sciences (Switzerland)*, 9(21).  
<https://doi.org/10.3390/app9214538>
- Vol, J. M., L, D. P., Dan, L. E., Islamisasi, P., Jawa, D. I., & Dan, B. (2022). *Jurnal Mediasi*. 1(2), 57–70.
- Warjianto, W., Soewoto, W., Alifianto, U., & Wujoso, H. (2020). Hubungan Reseptor Estrogen, Reseptor Progesteron dan Ekspresi Her-2/Neu Dengan Grading Histopatologi pada Pasien Kanker Payudara di RSUD dr. Moewardi Surakarta. *Smart Medical Journal*, 3(2), 96. <https://doi.org/10.13057/smj.v3i2.35228>
- Weni, M., Safithri, M., & Seno, D. S. H. (2020). *Molecular Docking of Active Compounds Piper crocatum on The Alpha- Glucosidase Enzyme as Antidiabetic Penambatan Molekuler Senyawa Aktif Daun Sirih Merah ( Piper Crocatum ) terhadap Enzim Alfa-Glukosidase sebagai Antidiabetes*. 7(2).
- Yeni, Y., & Rachmania, R. A. (2022). 1081 *The Prediction of Pharmacokinetic Properties of Compounds in Hemigraphis alternata ( Burm . F . ) T . Ander Leaves Using pkCSM*. 22(4), 1081–1089. <https://doi.org/10.22146/ijc.73117>
- Yunita Sari, A., & Febrina, E. (2023). Potensi Senyawa Aktif Tanaman Herbal untuk Pengobatan Kanker Payudara dengan Metode Penambatan Molekuler: Review Artikel. *Jurnal Farmasi Udayana*, 12(1), 23.  
<https://doi.org/10.24843/jfu.2023.v12.i01.p04>
- Yusuf, M., Hardianto, A., Muchtaridi, M., Nuwarda, R. F., Padjadjaran, U., & Java, W.

(2018). Introduction of Docking-Based Virtual Screening Work fl ow Using Desktop Personal Computer. In *Encyclopedia of Bioinformatics and Computational Biology*. Elsevier Ltd. <https://doi.org/10.1016/B978-0-12-809633-8.20277-X>