

DAFTAR PUSTAKA

- Achutha, A. S., Pushpa, V. L., & Manoj, K. B. (2020). Comparative molecular docking studies of phytochemicals as Jak2 inhibitors using Autodock and ArgusLab. *Materials Today: Proceedings*, xxxx. <https://doi.org/10.1016/j.matpr.2020.05.661>
- Amin, S. (2015). Hubungan Kuantitatif Struktur-Aktivitas Antibakteri Turunan Benzimidazol Menggunakan Metode Pm3. *Jurnal Kesehatan Bakti Tunas Husada: Jurnal Ilmu-Ilmu Keperawatan, Analis Kesehatan Dan Farmasi*, 12(1), 254. <https://doi.org/10.36465/jkbth.v12i1.86>
- Aprilliza AM, M. N., Anggraeny, Y. N., & Wina, E. (2021). The Role of Catechin Compounds and Its Derivates to Mitigate Methane Gas Production in the Rumen Fermentation. *Indonesian Bulletin of Animal and Veterinary Sciences*, 31(1), 13. <https://doi.org/10.14334/wartazoa.v31i1.2548>
- Arifin, B., & Ibrahim, S. (2018). Struktur, Bioaktivitas Dan Antioksidan Flavonoid. *Jurnal Zarah*, 6(1), 21–29. <https://doi.org/10.31629/zarah.v6i1.313>
- Astuti, A. D., & Mutiara, A. B. (2011). Simulasi dinamika molekuler protein dengan aplikasi gromacs. *Teknik Informatika Dan Industri*, 1(2), 1–9.
- Attia, G. H., Moemen, Y. S., Youns, M., Ibrahim, A. M., Abdou, R., & El Raey, M. A. (2021). Antiviral zinc oxide nanoparticles mediated by hesperidin and in silico comparison study between antiviral phenolics as anti-SARS-CoV-2. *Colloids and Surfaces B: Biointerfaces*, 203(March), 111724. <https://doi.org/10.1016/j.colsurfb.2021.111724>.
- Bachtiar, K. R., Susanti, S., Mardianingrum, R., & Tasikmalaya, U. P. (2021). *Uji aktivitas antiinflamasi senyawa dalam minyak atsiri rimpang bangle* (. 4(1), 36–43.
- Behar, A., Dennouni- Medjati, N., Harek, Y., Dali- Sahi, M., Belhadj, M., & Meziane, F. Z. (2020). Selenium overexposure induces insulin resistance: In silico study. *Diabetes and Metabolic Syndrome: Clinical Research and Reviews*, 14(6), 1651–1657. <https://doi.org/10.1016/j.dsx.2020.08.005>
- Cheng, T., Pan, Y., Hao, M., Wang, Y., & Bryant, S. H. (2014). PubChem applications in drug discovery: A bibliometric analysis. *Drug Discovery Today*, 19(11), 1751–1756. <https://doi.org/10.1016/j.drudis.2014.08.008>
- Du, A., Zheng, R., Disoma, C., Li, S., Chen, Z., Li, S., Liu, P., Zhou, Y., Shen, Y., Liu, S., Zhang, Y., Dong, Z., Yang, Q., Alsaadawe, M., Mo, L., Li, S., & Xia, Z. (2021). International Journal of Biological Macromolecules Epigallocatechin-3-gallate , an active ingredient of Traditional Chinese Medicines , inhibits the 3CLpro activity of SARS-CoV- 2. *International Journal of Biological Macromolecules*, 176, 1–12. <https://doi.org/10.1016/j.ijbiomac.2021.02.012>

- Fadhilah, Z. H., Perdana, F., & Syamsudin, R. A. M. R. (2021). Review: Telaah Kandungan Senyawa Katekin dan Epigalokatekin Galat (EGCG) sebagai Antioksidan pada Berbagai Jenis Teh. *Jurnal Pharmascience*, 8(1), 31. <https://doi.org/10.20527/jps.v8i1.9122>
- Febriantara, S., Ruslin, & Yamin. (2014). Studi In Silico Senyawa 2-amino-5-(3-(4-hydroxy-3,5-dimethoxy- benzoyl)guanidino)pentanoic acid dan Turunannya sebagai Inhibitor Phospodiesterase-5. *Majalah Farmasi, Sains, Dan Kesehatan*, 2(1), 22–26.
- Frengki, F., Putra, D. P., Wahyuni, F. S., Khambri, D., Vanda, H., & Sofia, V. (2020). Potential antiviral of catechins and their derivatives to inhibit sars-cov-2 receptors of m pro protein and spike glycoprotein in covid-19 through the in silico approach. *Jurnal Kedokteran Hewan - Indonesian Journal of Veterinary Sciences*, 14(3), 59–65. <https://doi.org/10.21157/j.ked.hewan.v14i3.16652>
- Frimayanti, N., Djohari, M., & Khusnah, A. N. (2021). *Molekular Docking Senyawa Analog Kalkon sebagai Inhibitor untuk Sel Kanker Paru-Paru A549 (Molecular Docking for Chalcone Analogue Compounds as Inhibitor for Lung Cancer A549)*. 19(1), 87–95.
- Hasmono, D., Klinik, M. F., Farmasi, F., Surabaya, U. A., Klinik, D. F., Farmasi, F., & Surabaya, U. A. (2021). *SCIENTIA Jurnal Farmasi dan Kesehatan*. 11(1), 62–70.
- Jain, A. S., Sushma, P., Dharmashkar, C., Beelagi, M. S., Prasad, S. K., Shivamallu, C., Prasad, A., Syed, A., Marraiki, N., & Prasad, K. S. (2021). In silico evaluation of flavonoids as effective antiviral agents on the spike glycoprotein of SARS-CoV-2. *Saudi Journal of Biological Sciences*, 28(1), 1040–1051. <https://doi.org/10.1016/j.sjbs.2020.11.049>
- 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>
- Khezri, M. R., Zolbanin, N. M., Ghasemnejad-berenji, M., & Jafari, R. (2021). Azithromycin: Immunomodulatory and antiviral properties for SARS-CoV-2 infection. *European Journal of Pharmacology*, 905(November 2020), 174191. <https://doi.org/10.1016/j.ejphar.2021.174191>
- Kim, S., Thiessen, P. A., Cheng, T., Yu, B., Shoemaker, B. A., Wang, J., Bolton, E. E., Wang, Y., & Bryant, S. H. (2016). Literature information in PubChem: Associations between PubChem records and scientific articles. *Journal of Cheminformatics*, 8(1), 1–15. <https://doi.org/10.1186/s13321-016-0142-6>
- Kurniatri, A. A., Sulistyaningrum, N., & Rustanti, L. (2019). Purifikasi katekin dari ekstrak gambir. *Media Litbangkes*, 29(2), 153–160.
- Liskova, A., Samec, M., Koklesova, L., Samuel, S. M., Zhai, K., Al-Ishaq, R. K., Abotaleb, M., Nosal, V., Kajo, K., Ashrafizadeh, M., Zarrabi, A., Brockmueller, A., Shakibaei, M., Sabaka, P., Mozos, I., Ullrich, D., Prosecky,

- R., La Rocca, G., Caprnda, M., ... Kubatka, P. (2021). Flavonoids against the SARS-CoV-2 induced inflammatory storm. *Biomedicine and Pharmacotherapy*, 138, 111430. <https://doi.org/10.1016/j.biopharm.2021.111430>
- McElfresh, G. W., & Deligkaris, C. (2018). A vibrational entropy term for DNA docking with autodock. *Computational Biology and Chemistry*, 74, 286–293. <https://doi.org/10.1016/j.combiolchem.2018.03.027>
- Mhatre, S., Gurav, N., Shah, M., & Patravale, V. (2021). Entry-inhibitory role of catechins against SARS-CoV-2 and its UK variant. *Computers in Biology and Medicine*, 135(June), 104560. <https://doi.org/10.1016/j.combiomed.2021.104560>
- Mouffouk, C., Mouffouk, S., Mouffouk, S., Hambaba, L., & Haba, H. (2021). Flavonols as potential antiviral drugs targeting SARS-CoV-2 proteases (3CLpro and PLpro), spike protein, RNA-dependent RNA polymerase (RdRp) and angiotensin-converting enzyme II receptor (ACE2). *European Journal of Pharmacology*, 891(November 2020), 1–11. <https://doi.org/10.1016/j.ejphar.2020.173759>
- Narko, T., Permana, B., Prasetiawati, R., Soni, D., & Khairiyah, F. (2017). Studi Penambatan Molekulsenyawa Dari Umbi Bawang Dayak (Eleutherine Palmifolia (L) Merr.) Sebagai Obat Antikanker Serviks. *Jurnal Ilmiah Farmako Bahari*, 8(2), 1–14. <https://journal.uniga.ac.id/index.php/JFB/article/view/643>
- Noviardi, H., & Fachrurrazie, F. (2015). Potensi Senyawa Bullatalisin Sebagai Inhibitor Protein Leukotrien a4 Hidrolase Pada Kanker Kolon Secara in Silico. *FITOFARMAKA: Jurnal Ilmiah Farmasi*, 5(2), 65–73. <https://doi.org/10.33751/jf.v5i2.410>
- Nursamsiar, Toding, A. T., & Awaluddin, A. (2016). Studi In Silico Senyawa Turunan Analog Kalkon dan Pirimidin sebagai Antiinflamasi: Prediksi Absorpsi, Distribusi, dan Toksisitas. *Pharmacy*, 13(01), 92–100.
- Onishi, S., Mori, T., Kanbara, H., Habe, T., & Ota, N. (2020). Green tea catechins adsorbed on the murine pharyngeal mucosa reduce influenza A virus infection. *Journal of Functional Foods*, 68(February), 103894. <https://doi.org/10.1016/j.jff.2020.103894>
- Pratama, R. (2020). Studi in Silico Potensi Senyawa Turunan Kortikosteroid Sebagai Obat Covid-19. *Jurnal Veteriner Nusantara*, 3(2), 176–185. <http://ejurnal.undana.ac.id/jvn/article/view/3429>
- Purwaniati, P.-. (2020). Molecular Docking Study on COVID-19 Drug Activity of N-(2-phenylethyl)methanesulfonamide Derivatives as Main Protease Inhibitor. *Ad-Dawaa' Journal of Pharmaceutical Sciences*, 3(1), 1–11. <https://doi.org/10.24252/djps.v3i1.13945>
- Rachmania, R. A., Zikriah, R., & Soultan, A. (2018). Studi In Silico Senyawa Alkaloid Herba Bakung Putih (Crinum Asiaticum L .) pada Penghambatan

- Enzim Siklooksigenase (COX) In Silico Study of Alkaloid Herba Bakung Putih (Crinum Asiaticum L .) on Inhibition of Cyclooxygenase Enzyme (COX). *Jurnal Kimia Valensi*, 4(2), 124–136.
- Rahman, F., Tabrez, S., Ali, R., Alqahtani, A. S., Ahmed, M. Z., & Rub, A. (2021). Molecular docking analysis of rutin reveals possible inhibition of SARS-CoV-2 vital proteins. *Journal of Traditional and Complementary Medicine*, 11(2), 173–179. <https://doi.org/10.1016/j.jtcme.2021.01.006>
- Rastini, M. B. O., Giantari, N. K. M., Adnyani, K. D., & Laksmiani, N. P. L. (2019). Molecular Docking Aktivitas Antikanker Dari Kuersetin Terhadap Kanker Payudara Secara in Silico. *Jurnal Kimia*, 180. <https://doi.org/10.24843/jchem.2019.v13.i02.p09>
- Ruswanto, R., Garna, I. M., Tuslinah, L., Mardianingrum, R., Lestari, T., & Nofianti, T. (2018). Kuersetin, Penghambat Uridin 5-Monofosfat Sintase Sebagai Kandidat Anti-kanker. *ALCHEMY Jurnal Penelitian Kimia*, 14(2), 236. <https://doi.org/10.20961/alchemy.14.2.14396.236-254>
- Ruswanto, R., Mardhiah, M., Mardianingrum, R., & Novitriani, K. (2015). Sintesis Dan Studi in Silico Senyawa 3-Nitro-N’-[Pyridin-4-Yl] Carbonyl]Benzohydrazide Sebagai Kandidat Antituberkulosis. *Chimica et Natura Acta*, 3(2). <https://doi.org/10.24198/cna.v3.n2.9183>
- 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>
- Sahlan, M., Irdiani, R., Flamandita, D., Aditama, R., Alfarraj, S., Javed Ansari, M., Cahya Khayrani, A., Kartika Pratami, D., & Lischer, K. (2020). Molecular Interaction Analysis of Sulawesi Propolis Compounds with SARS-CoV-2 Main Protease as Preliminary Study for COVID-19 Drug Discovery. *Journal of King Saud University Science*, 101234. <https://doi.org/10.1016/j.jksus.2020.101234>
- Saputri, K. E., Fakhmi, N., Kusumaningtyas, E., Priyatama, D., & Santoso, B. (2016). Docking Molekular Potensi Anti Diabetes Melitus Tipe 2 Turunan Zerumbon Sebagai Inhibitor Aldosa Reduktase Dengan Autodock-Vina. *Chimica et Natura Acta*, 4(1), 16. <https://doi.org/10.24198/cna.v4.n1.10443>
- Vinsentricia, A., Hami Seno, D. S., & Bintang, M. (2015). *In Silico* Analysis of *Curcuma longa* Against PCAF Histon Asetiltransferase. *Current Biochemistry*, 2(2), 52–62. <https://doi.org/10.29244/cb.2.2.52-62>
- Wadapurkar, R. M., Shilpa, M. D., Katti, A. K. S., & Sulochana, M. B. (2018). In silico drug design for *Staphylococcus aureus* and development of host-pathogen interaction network. *Informatics in Medicine Unlocked*, 10(September 2017), 58–70. <https://doi.org/10.1016/j.imu.2017.11.002>
- Wang, X., Yang, C., Sun, Y., Sui, X., Zhu, T., Wang, Q., Wang, S., Yang, J., Yang, W., Liu, F., Zhang, M., Wang, Y., & Luo, Y. (2021). A novel screening

strategy of anti-SARS-CoV-2 drugs via blocking interaction between Spike RBD and ACE2. *Environment International*, 147, 106361. <https://doi.org/10.1016/j.envint.2020.106361>

Westbrook, J. D., & Burley, S. K. (2019). How Structural Biologists and the Protein Data Bank Contributed to Recent FDA New Drug Approvals. *Structure*, 27(2), 211–217. <https://doi.org/10.1016/j.str.2018.11.007>