

DAFTAR PUSTAKA

- Akbar, N.A., Amin, S., & Wulandari, W. T. (2022). Studi In Silico Senyawa yang Terkandung dalam Tanaman Daun Sirih Merah (*Piper crocatum* RUIZ & PAV) sebagai Kandidat Anti SARS CoV-2. *Ejurnal Universitas Bth*, 2, 378–391.
- Al-Mijalli, S. H., Mrabti, H. N., Elbouzidi, A., Ashmawy, N. S., Batbat, A., Abdallah, E. M., Laaboudi, W., Aladhadh, M., Alshabrm, F. M., Alnasser, S. M., Addi, M., & El Hachlafi, N. (2025). Thymus serpyllum L. Essential Oil: Phytochemistry and in Vitro and in Silico Screening of Its Antimicrobial, Antioxidant and Anti-Inflammatory Properties. *Phyton-International Journal of Experimental Botany*, 94(1), 209–227. <https://doi.org/10.32604/phyton.2025.060438>
- Alliod, C., Chemelle, J. A., Jacob, G., & Terreux, R. (2017). Ames Test Prediction on High Energy Molecules by On-The-Fly QSAR (OTF-QSAR). *Propellants, Explosives, Pyrotechnics*, 42(1), 24–35. <https://doi.org/10.1002/prep.201600155>
- Ambe, K., Nakamori, M., Tohno, R., Suzuki, K., Sasaki, T., Tohkin, M., & Yoshinari, K. (2024). Machine Learning-Based In Silico Prediction of the Inhibitory Activity of Chemical Substances Against Rat and Human Cytochrome P450s. *Chemical Research in Toxicology*. <https://doi.org/10.1021/acs.chemrestox.4c00168>
- Amin, A., Wunas, J., & Anin, Y. M. (2016). Uji Aktivitas Antioksidan Ekstrak Etanol Klika Faloak (*Sterculia quadrifida* R.Br) Dengan Metode DPPH (2,2-Diphenyl-1-Picrylhydrazyl). *Jurnal Fitofarmaka Indonesia*, 2(2), 111–114. <https://doi.org/10.33096/jffi.v2i2.180>
- Amsad, L. N., Liliyasi, L., Kadarohman, A., & Sardjono, R. E. (2023). *Connecting Students' Critical Thinking Skills with Conceptual Knowledge in Learning the Organic Compounds Stability by Using Marvin Sketch as a Tools to Adjust the Era of Society 5.0*. Atlantis Press SARL. https://doi.org/10.2991/978-2-38476-012-1_20
- Anastassios, Papageorgiou, Poudel, N., & Mattsson, J. (2021). Protein Structure Analysis and Validation with X-Ray Crystallography. *Methods in Molecular*

- Biology*, 2178, 377–402. https://doi.org/10.1007/978-1-0716-0775-6_25
- Anita Agustina S, Choiril HM, & Maylita ED. (2019). Analisa Kualitatif Asam Retinoat pada Sediaan Krim Malam di Pasar Klaten dengan Metode Kromatografi Lapis. *MOTORIK Jurnal Ilmu Kesehatan*, 14(2), 136–140. <https://doi.org/10.61902/motorik.v14i2.32>
- Aryanti, R., Perdana, F., & Syamsudin, R. A. M. R. (2021). Telaah Metode Pengujian Aktivitas Antioksidan pada Teh Hijau (*Camellia sinensis* (L.) Kuntze). *Jurnal Surya Medika*, 7(1), 15–24. <https://doi.org/10.33084/jsm.v7i1.2024>
- Aulifa, D. L., Al Shofwan, A. A., Megantara, S., Fakhri, T. M., & Budiman, A. (2024). Elucidation of *Molecular* Interactions Between Drug–Polymer in Amorphous Solid Dispersion by a Computational Approach Using *Molecular* Dynamics Simulations. *Advances and Applications in Bioinformatics and Chemistry*, 17(January), 1–19. <https://doi.org/10.2147/AABC.S441628>
- Ayodele, P. F., Bamigbade, A., Bamigbade, O. O., Adeniyi, I. A., Tachin, E. S., Seweje, A. J., & Farohunbi, S. T. (2023). Illustrated Procedure to Perform *Molecular Docking* Using PyRx and Biovia Discovery Studio Visualizer: A Case Study of 10kt With Atropine. *Progress in Drug Discovery & Biomedical Science*, 6(1), 1–31. <https://doi.org/10.36877/pddbs.a0000424>
- Baba, H., & Bunu, S. J. (2025). *Spectroscopic And Molecular Docking Analysis Of Phytoconstituent Isolated From Solenostemon Monostachyus As Potential Cyclooxygenase Enzymes Inhibitor*. 9(1), 1–6. <https://doi.org/http://dx.doi.org/10.22159/ijcr.2025v9i1.241>
- Bachtar, K. R., Susanti, S., & Mardianingrum, R. (2021). Uji Aktivitas Antiinflamasi Senyawa Dalam Minyak Atsiri Rimpang Bangle (*Zingiber purpureum* Roxb) Secara In Silico. *Journal of Pharmacopolium*, 4(1), 36–43. <https://doi.org/10.36465/jop.v4i1.719>
- Baroroh, 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>

- 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.
- Bintari, Y. R. (2018). Studi In Silico Potensi Ekstrak Lipida Tetraselmis chuii Sebagai Antioksidan. *Jurnal Ketahanan Pangan*, 2, 76–81. <https://pubchem.ncbi.nlm.nih.gov>
- Bitencourt-Ferreira, G., Veit-Acosta, M., & de Azevedo, W. F. (2019). Van der waals potential in protein complexes. *Methods in Molecular Biology*, 2053, 79–91. https://doi.org/10.1007/978-1-4939-9752-7_6
- Bordet, T., Berna, P., Abitbol, J. L., & Pruss, R. M. (2010). Olesoxime (TRO19622): A novel mitochondrial-targeted neuroprotective compound. *Pharmaceuticals*, 3(2), 345–368. <https://doi.org/10.3390/ph3020345>
- Brogi, S., Ramalho, T. C., Kuca, K., Medina-Franco, J. L., & Valko, M. (2020). Editorial: In silico Methods for Drug Design and Discovery. *Frontiers in Chemistry*, 8(August), 1–5. <https://doi.org/10.3389/fchem.2020.00612>
- Bulusu, G., & Desiraju, G. R. (2020). Strong and Weak Hydrogen Bonds in Protein–Ligand Recognition. *Journal of the Indian Institute of Science*, 100(1), 31–41. <https://doi.org/10.1007/s41745-019-00141-9>
- Candelario-Jalil, E., González-Falcón, A., García-Cabrera, M., Álvarez, D., Al-Dalain, S., Martínez, G., León, O. S., & Springer, J. E. (2003). Assessment of the relative contribution of COX-1 and COX-2 isoforms to ischemia-induced oxidative damage and neurodegeneration following transient global cerebral ischemia. *Journal of Neurochemistry*, 86(3), 545–555. <https://doi.org/10.1046/j.1471-4159.2003.01812.x>
- Celep, E., Charehsaz, M., Akyüz, S., Acar, E. T., & Yesilada, E. (2015). Effect of in vitro gastrointestinal digestion on the bioavailability of phenolic components and the antioxidant potentials of some Turkish fruit wines. *Food Research International*, 78, 209–215. <https://doi.org/10.1016/j.foodres.2015.10.009>
- Chen, D., Oezguen, N., Urvil, P., Ferguson, C., Dann, S. M., & Savidge, T. C. (2016). Regulation of protein-ligand binding affinity by hydrogen bond

- pairing. *Science Advances*, 2(3). <https://doi.org/10.1126/sciadv.1501240>
- Chen, S., Itoh, Y., Masuda, T., Shimizu, S., Zhao, J., Ma, J., Nakamura, S., Noguchi, H., Uosaki, K., & Aida, T. (2015). Subnanoscale hydrophobic modulation of salt bridges in aqueous media. *Science*, 348(6234), 555–559. <https://doi.org/10.1126/science.aaa7532>
- Chen, X., Li, H., Tian, L., Li, Q., Luo, J., & Zhang, Y. (2020). Analysis of the Physicochemical Properties of Acaricides Based on Lipinski's Rule of Five. *Journal of Computational Biology*, 27(9), 1397–1406. <https://doi.org/10.1089/cmb.2019.0323>
- Chow, E., Rendleman, C. A., Bowers, K. J., Dror, R. O., H, D., Gullingsrud, J., Sacerdoti, F. D., & Shaw, D. E. (2008). Desmond Performance on a Cluster of Multicore Processors. *Simulation*, July, 1–14.
- Colovos, C., & Yeates, T. O. (1993). Verification of protein structures: Patterns of nonbonded atomic interactions. *Protein Science*, 2(9), 1511–1519. <https://doi.org/10.1002/pro.5560020916>
- Dave, R. A., & Morris, M. E. (2016). Novel high/low solubility classification methods for new molecular entities. *International Journal of Pharmaceutics*, 511(1), 111–126. <https://doi.org/10.1016/j.ijpharm.2016.06.060>
- De Beer, T. A. P., Berka, K., Thornton, J. M., & Laskowski, R. A. (2014). PDBsum additions. *Nucleic Acids Research*, 42(D1), 292–296. <https://doi.org/10.1093/nar/gkt940>
- 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
- 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. [https://download.garuda.kemdikbud.go.id/article.php?article=3028608&val=27441&title=Hasil Komputasi Vina untuk Kandungan Bawang Putih dan Adas Bintang Terhadap Protein Dehidrogenase Piruvat Mycobacterium](https://download.garuda.kemdikbud.go.id/article.php?article=3028608&val=27441&title=Hasil%20Komputasi%20Vina%20untuk%20Kandungan%20Bawang%20Putih%20dan%20Adas%20Bintang%20Terhadap%20Protein%20Dehidrogenase%20Piruvat%20Mycobacterium)

tuberculosis

- Erari, P. (2022). Identifikasi Beberapa Jenis Ubi Jajar (*Ipomoea Batatas*, (L) Lamb) Di Disrtik Tigi Kabupaten Deiyai. *Jurnal FAPERTANAK : Jurnal Pertanian Dan Peternakan*, 7(2), 29–36. <https://uswim.e-journal.id/fapertanak/article/view/427>
- European Bioinformatics Institute. (2021). *CHEBI:18946 glucose*. ChEBI. <https://www.ebi.ac.uk/chebi/searchId.do?chebiId=18946>
- 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>
- Fatimatuzahro, D., Tyas, D. A., & Hidayat, S. (2019). Pemanfaatan Ekstrak Kulit Ubi Jalar Ungu (*Ipomea batatas* L.) sebagai Bahan Pewarna Alternatif untuk Pengamatan Mikroskopis *Paramecium* sp. dalam Pembelajaran Biologi. *Al-Hayat: Journal of Biology and Applied Biology*, 2(1), 1. <https://doi.org/10.21580/ah.v2i1.4641>
- Feng, Z., Westbrook, J. D., Sala, R., Smart, O. S., Bricogne, G., Matsubara, M., Yamada, I., Tsuchiya, S., Aoki-Kinoshita, K. F., Hoch, J. C., Kurisu, G., Velankar, S., Burley, S. K., & Young, J. Y. (2021). Enhanced validation of small-molecule ligands and carbohydrates in the Protein Data Bank. *Structure*, 29(4), 393-400.e1. <https://doi.org/10.1016/j.str.2021.02.004>
- Fidrianny, I., Suhendy, H., & Insanu, M. (2018). Correlation of phytochemical content with antioxidant potential of various sweet potato (*Ipomoea batatas*) in West Java, Indonesia. *Asian Pacific Journal of Tropical Biomedicine*, 7(1), 25–30. <https://doi.org/10.4103/2221-1691.221131>
- Ghaderi, S., Bozorgmehr, M. R., Tarahomjoo, S., Movahedi, A., Esmaelizad, M., & Noofeili, M. (2019). Comparing Structure and Conformation of Diphtheria Toxin With Its Non-toxic Mutant (E349K) at 300 K Using *Molecular Dynamics Simulations*. *Avicenna Journal of Clinical Microbiology and Infection*, 6(4), 111–117. <https://doi.org/10.34172/ajcmi.2019.20>
- Guedes, I. A., de Magalhães, C. S., & Dardenne, L. E. (2014). Receptor-ligand *molecular docking*. *Biophysical Reviews*, 6(1), 75–87. <https://doi.org/10.1007/s12551-013-0130-2>
- Guzik, T. J., & Harrison, D. G. (2006). Vascular NADPH *Oxidases* as drug targets

- for novel antioxidant strategies. *Drug Discovery Today*, 11(11–12), 524–533. <https://doi.org/10.1016/j.drudis.2006.04.003>
- Hacker, K., Maas, R., Kornhuber, J., Fromm, M. F., & Zolk, O. (2015). Substrate-dependent inhibition of the human organic cation transporter OCT2: A comparison of metformin with experimental substrates. *PLoS ONE*, 10(9), 1–16. <https://doi.org/10.1371/journal.pone.0136451>
- Hamadeh, A., Najjar, A., Troutman, J., & Edginton, A. (2023). Enhancement of Skin Permeability Prediction through PBPK Modeling, Bayesian Inference, and Experiment Design. *Pharmaceutics*, 15(12). <https://doi.org/10.3390/pharmaceutics15122667>
- Hanif, A. U., Lukis, P. A., & Fadlan, A. (2020). Pengaruh Minimisasi Energi MMFF94 dengan MarvinSketch dan Open Babel PyRx pada Penambatan Molekular Turunan Oksindola Tersubstitusi. *Alchemy*, 8(2), 33–40. <https://doi.org/10.18860/al.v8i2.10481>
- Hayati, M., Sabaruddin, Efendi, & Anhar, A. (2020). Morphological characteristics and yields of several sweet potato (*Ipomoea batatas* L.) tubers. *IOP Conference Series: Earth and Environmental Science*, 425(1). <https://doi.org/10.1088/1755-1315/425/1/012055>
- Higashino, H., Develin, C. F., Higashino, C., Lim, T. C.-H., Miezeiewski, B. J., Rawa, S. L., Strab, R. J., Patel, R., & Bhoopathy, S. (2024). Qualification of In Vitro Dissolution Absorption System 2 (IDAS2) with Caco-2 and MDCK Cell Monolayers: Dose Sensitivity Study Using BCS Class I and III Drugs. *Biological & Pharmaceutical Bulletin*, 47(6), 1123–1127.
- Hollingsworth, S. A., & Dror, R. O. (2018). *Molecular Dynamics Simulation for All. Neuron*, 99(6), 1129–1143. <https://doi.org/10.1016/j.neuron.2018.08.011>
- Ibrahim, Z. Y., Uzairu, A., Shallangwa, G. A., & Abechi, S. E. (2021). Pharmacokinetic predictions and *docking* studies of substituted aryl amine-based triazolopyrimidine designed inhibitors of Plasmodium falciparum dihydroorotate dehydrogenase (PfDHODH). *Future Journal of Pharmaceutical Sciences*, 7(1). <https://doi.org/10.1186/s43094-021-00288-2>
- Ivanović, V., Rančić, M., Arsić, B., & Pavlović, A. (2020). Lipinski's rule of five, famous extensions and famous exceptions. *Chemia Naissensis*, 3(1), 171–181.

<https://doi.org/10.46793/chemn3.1.171i>

- Jabir, N. R., Firoz, C. K., Baeesa, S. S., Ashraf, G. M., Akhtar, S., Kamal, W., Kamal, M. A., & Tabrez, S. (2015). Synopsis on the Linkage of Alzheimer's and Parkinson's Disease with Chronic Diseases. *CNS Neuroscience and Therapeutics*, 21(1), 1–7. <https://doi.org/10.1111/cns.12344>
- Jong, K., Grisanti, L., & Hassanali, A. (2017). Hydrogen Bond Networks and Hydrophobic Effects in the Amyloid β 30-35 Chain in Water: A Molecular Dynamics Study. *Journal of Chemical Information and Modeling*, 57(7), 1548–1562. <https://doi.org/10.1021/acs.jcim.7b00085>
- Josaphat, F., & Fadlan, A. (2023). Molecular Docking of Acetylacetone-Based Oxindole Against Indoleamine 2,3-Dioxygenase: Study of Energy Minimization. *Walisongo Journal of Chemistry*, 6(2), 149–157. <https://doi.org/10.21580/wjc.v6i2.17638>
- Kade, H., Yahdiana, H., & Supandi. (2019). Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS). In *PT. ISFI Penerbitan*. PT. ISFI Penerbitan. http://scioteca.caf.com/bitstream/handle/123456789/1091/RED2017-Eng-8ene.pdf?sequence=12&isAllowed=y%0Ahttp://dx.doi.org/10.1016/j.regsciurbeco.2008.06.005%0Ahttps://www.researchgate.net/publication/305320484_SISTEM_PEMBETUNGAN_TERPUSAT_STRATEGI_MELESTARI
- Kar, S., & Leszczynski, J. (2020). Open access in silico tools to predict the ADMET profiling of drug candidates. *Expert Opinion on Drug Discovery*, 15(12), 1473–1487. <https://doi.org/10.1080/17460441.2020.1798926>
- Karimi, P., Sanchooli, M., & Kiyanee-Ghaleno, M. (2021). Assessment of O–H...O and O–H...S intramolecular hydrogen bond energies in some substituted pyrimidines using quantum chemistry methods. *Journal of Molecular Graphics and Modelling*, 104, 107847. <https://doi.org/10.1016/j.jmgm.2021.107847>
- Khan, B., Ghous, T., Rasheed, A., Yasin, K. A., Ahmed, M. N., & Andleeb, S. (2016). Evaluation of anti-acetylcholinesterase activity and antioxidant potential of ricinine (a central nervous system stimulant) isolated from *Ricinus communis* L. *Journal of the Chemical Society of Pakistan*, 38(2), 326–332. <https://jcsp.org.pk/issueDetail.aspx?aid=4cfc5906-b67c-4c58->

bd4a-3fb90b4cea7d

- 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. *Indo Global Journal of Pharmaceutical Sciences*, 10(04), 58–69. <https://doi.org/10.35652/igjps.2020.10409>
- Khosravi, I., Sahihi, M., Rudbari, H. A., Borhan, G., & Chavoshpour-Natanzi, Z. (2017). The Interaction of a New Schiff Base Ligand with Human Serum Albumin: *Molecular Docking* and *Molecular Dynamics* Simulation Studies. *Journal of Macromolecular Science, Part B: Physics*, 56(9), 636–643. <https://doi.org/10.1080/00222348.2017.1356634>
- Kim, J. W., Yoo, I. D., & Kim, W. G. (2006). Free radical-scavenging δ -lactones from *Boletus calopus*. *Planta Medica*, 72(15), 1431–1432. <https://doi.org/10.1055/s-2006-951722>
- 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>
- Koduru, S., Jimoh, F., Grierson, D., & Afolayan, A. (2007). Antioxidant activity of two steroid alkaloids extracted from *Solanum aculeastrum*. *Journal of Pharmacology and Toxicology*, 2(2), 160–167. <https://doi.org/https://doi.org/10.3923/jpt.2007.160.167>
- Koneti, G., Ghosh, D., & Ramamurthi, N. (2017). Classification models for CaCo-2 permeability using chemical information and machine learning techniques: Scope and limitations. *Proceedings - 2017 IEEE International Conference on Bioinformatics and Biomedicine, BIBM 2017, 2017-Janua*, 2270–2271. <https://doi.org/10.1109/BIBM.2017.8218021>
- Korzekwa, K., & Nagar, S. (2017). Drug Distribution Part 2. Predicting Volume of Distribution from Plasma Protein Binding and Membrane Partitioning. *Pharmaceutical Research*, 34(3), 544–551. <https://doi.org/10.1007/s11095-016-2086-y>
- Kou, G., Wu, J., Liu, M., Lin, L., Xu, X., & Zhou, Z. (2019). Citrus tangeretin

- reduces the oxidative stress of the myocardium, with the potential for reducing fatigue onset and myocardial damage. *Journal of Functional Foods*, 54(November 2018), 249–253. <https://doi.org/10.1016/j.jff.2019.01.018>
- 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>
- Kurniawati, I. F., & Sutoyo, S. (2021). Review Artikel: Potensi Bunga Tanaman Sukun (*Artocarpus Altilis* [Park. I] Fosberg) Sebagai Bahan Antioksidan Alami. *Unesa Journal of Chemistry*, 10(1), 1–11. <https://doi.org/10.26740/ujc.v10n1.p1-11>
- Laveriano-Santos, E. P., López-Yerena, A., Jaime-Rodríguez, C., González-Coria, J., Lamuela-Raventós, R. M., Vallverdú-Queralt, A., Romanyà, J., & Pérez, M. (2022). Sweet Potato Is Not Simply an Abundant Food Crop: A Comprehensive Review of Its Phytochemical Constituents, Biological Activities, and the Effects of Processing †. *Antioxidants*, 11(9). <https://doi.org/10.3390/antiox11091648>
- Li, J., Fu, A., & Zhang, L. (2019). An Overview of Scoring Functions Used for Protein–Ligand Interactions in *Molecular Docking. Interdisciplinary Sciences – Computational Life Sciences*, 11(2), 320–328. <https://doi.org/10.1007/s12539-019-00327-w>
- Lipinski, C. A. (2004). Lead- and drug-like compounds: The rule-of-five revolution. *Drug Discovery Today: Technologies*, 1(4), 337–341. <https://doi.org/10.1016/j.ddtec.2004.11.007>
- Liu, T., Oprea, T., Ursu, O., Hasselgren, C., & Altman, R. B. (2016). Estimation of Maximum Recommended Therapeutic Dose Using Predicted Promiscuity and Potency. *Clinical and Translational Science*, 9(6), 311–320. <https://doi.org/10.1111/cts.12422>
- Liu, X., Shi, D., Zhou, S., Liu, H., Liu, H., & Yao, X. (2018). *Molecular dynamics simulations and novel drug discovery. Expert Opinion on Drug Discovery*,

- 13(1), 23–37. <https://doi.org/10.1080/17460441.2018.1403419>
- Liu, Z., Guo, F., Wang, Y., Li, C., Zhang, X., Li, H., Diao, L., Gu, J., Wang, W., Li, D., & He, F. (2016). BATMAN-TCM: A Bioinformatics Analysis Tool for *Molecular mechANism of Traditional Chinese Medicine*. *Scientific Reports*, 6(June 2015), 1–11. <https://doi.org/10.1038/srep21146>
- Maharani, A. I., Riskierdi, F., Febriani, I., Kaprian Alsyah Kurnia, Rahman, N. A., Ilahi, N. F., & Farma, S. A. (2021). Peran Antioksidan Alami Berbahan Dasar Pangan Lokal dalam Mencegah Efek Radikal Bebas. *Prosiding Seminar Nasional Bio*, 17(2), 171–178. <https://journal.unhas.ac.id/index.php/bioma>
- Maharani, P., Mulia, A. S., Wulandari, D., Veninda, H. R., & Pandapotan, F. A. (2023). Review: Plants As Candidates For Herbal Treatment Of Sle (Systemic Lupus Erythematosus). *Cerdika: Jurnal Ilmiah Indonesia*, 3(5), 458–468. <https://doi.org/10.59141/cerdika.v3i5.600>
- Makar, S., Saha, T., & Singh, S. K. (2019). Naphthalene, a versatile platform in medicinal chemistry: Sky-high perspective. *European Journal of Medicinal Chemistry*, 161, 252–276. <https://doi.org/10.1016/j.ejmech.2018.10.018>
- Malinda, D. (2024). *Uji Aktivitas Antioksidan Dan Flavonoid Total Beberapa Fraksi Tumbuhan Ubi Jalar (Ipomoea batatas L .) Varietas Ungu-Oranye*. Bakti Tunas Husada.
- Manurung, B. L., Monica, E., & Rollando, R. (2023). Formulasi Dan Evaluasi Antioksidan Daun Kelor Moringa Oleifer L Dalam Sediaan Serum Dengan Metode Senyawa Radikal Dpph. *Sainsbertek Jurnal Ilmiah Sains & Teknologi*, 3(2), 66–77. <https://doi.org/10.33479/sb.v3i2.233>
- Mardianingrum, R., Bachtiar, K. R., Susanti, S., Aas Nuraisah, A. N., & Ruswanto, R. (2021). Studi In Silico Senyawa 1,4-Naphthalenedione-2-Ethyl-3-Hydroxy sebagai Antiinflamasi dan Antikanker Payudara. *ALCHEMY Jurnal Penelitian Kimia*, 17(1), 83. <https://doi.org/10.20961/alchemy.17.1.43979.83-95>
- Mardianingrum, R., Endah, S. R. N., Suhardiana, E., Ruswanto, R., & Siswandono, S. (2021). *Docking and molecular dynamic study of isoniazid derivatives as anti-tuberculosis drug candidate*. *Chemical Data Collections*, 32, 100647. <https://doi.org/10.1016/j.cdc.2021.100647>
- Maryam, F., Taebe, B., & Toding, D. P. (2020). Pengukuran Parameter Spesifik

- Dan Non Spesifik Ekstrak Etanol Daun Matoa (*Pometia pinnata* J.R. & G.Forst). *Jurnal Mandala Pharmacon Indonesia*, 6(01), 1–12. <https://doi.org/10.35311/jmpi.v6i01.39>
- Maryam, S., Pratama, R., Effendi, N., & Naid, T. (2016). Analisis Aktivitas Antioksidan Ekstrak Etanolik Daun Yodium (*Jatropha multifida* L.) Dengan Metode Cupric Ion Reducing Antioxidant Capacity (CUPRAC). *Jurnal Fitofarmaka Indonesia*, 2(1), 90–93.
- Mayumi, K., Akazawa, T., Kanazu, T., Ohnishi, S., & Hasegawa, H. (2020). Successful Prediction of Human Pharmacokinetics After Oral Administration by Optimized Physiologically Based Pharmacokinetics Approach and Permeation Assay Using Human Induced Pluripotent Stem Cell–Derived Intestinal Epithelial Cells. *Journal of Pharmaceutical Sciences*, 109(4), 1605–1614. <https://doi.org/10.1016/j.xphs.2019.12.019>
- Mehta, S. K., & Gowder, S. J. T. (2015). Members of Antioxidant Machinery and Their Functions. *Basic Principles and Clinical Significance of Oxidative Stress*. <https://doi.org/10.5772/61884>
- Mitani, R., Tashiro, H., Arita, E., Ono, K., Haraguchi, M., Tokunaga, S., Sharmin, T., Aida, T. M., & Mishima, K. (2021). Extraction of nobiletin and tangeretin with antioxidant activity from peels of *Citrus poonensis* using liquid carbon dioxide and ethanol entrainer. *Separation Science and Technology (Philadelphia)*, 56(2), 290–300. <https://doi.org/10.1080/01496395.2020.1713813>
- Mu'nisa. (2022). *Antioksidan Pada Tanaman Dan Peranannya Terhadap Penyakit Degeneratif* (Agus Wijaya (ed.)). Brilian Internasional Surabaya.
- Nugroho, A. (2017). Buku Ajar: Teknologi Bahan Alam. In *Lambung Mangkurat University Press* (Issue November).
- Nur, S., Aswad, M., Yulianty, R., Burhan, A., Patabang, W. J. D., Fadri, A., & Nursamsiar, N. (2022). Profil Aktivitas Antioksidan dari Ekstrak Buah Kersen (*Muntingia calabura* L.) dengan Metode TAC dan CUPRAC. *JPSCR: Journal of Pharmaceutical Science and Clinical Research*, 7(1), 79. <https://doi.org/10.20961/jpscr.v7i1.56653>
- Ooi, S. F., Sukri, S. A. M., Zakaria, N. N. A., & Harith, Z. T. (2021). Carotenoids,

- phenolics and antioxidant properties of different sweet potatoes (*Ipomoea batatas*) varieties. *IOP Conference Series: Earth and Environmental Science*, 756(1). <https://doi.org/10.1088/1755-1315/756/1/012077>
- Oriola, A. O. (2024). Turmeric–Black Cumin Essential Oils and Their Capacity to Attenuate Free Radicals, Protein Denaturation, and Cancer Proliferation. *Molecules*, 29(15). <https://doi.org/10.3390/molecules29153523>
- Özyürek, M., Bektaşoğlu, B., Güçlü, K., Güngör, N., & Apak, R. (2008). Simultaneous total antioxidant capacity assay of lipophilic and hydrophilic antioxidants in the same acetone-water solution containing 2% methyl- β -cyclodextrin using the cupric reducing antioxidant capacity (CUPRAC) method. *Analytica Chimica Acta*, 630(1), 28–39. <https://doi.org/10.1016/j.aca.2008.09.057>
- Parasuraman, S., Rao, A., Balamurugan, S., Muralidharan, S., Jayaraj Kumar, K., & Vijayan, V. (2014). An Overview of Liquid Chromatography-Mass Spectroscopy Instrumentation. *Pharmaceutical Methods*, 5(2), 47–55. <https://doi.org/10.5530/phm.2014.2.2>
- Patel, H. M., Noolvi, M. N., Sharma, P., Jaiswal, V., Bansal, S., Lohan, S., Kumar, S. S., Abbot, V., Dhiman, S., & Bhardwaj, V. (2014). Quantitative structure-activity relationship (QSAR) studies as strategic approach in drug discovery. *Medicinal Chemistry Research*, 23(12), 4991–5007. <https://doi.org/10.1007/s00044-014-1072-3>
- Paulino, M., Alvareda, E., Iribarne, F., Miranda, P., Espinosa, V., Aguilera, S., & Pardo, H. (2016). Toward the understanding of the *molecular* basis for the inhibition of COX-1 and COX-2 by phenolic compounds present in Uruguayan propolis and grape pomace. *Journal of Biomolecular Structure and Dynamics*, 34(12), 2643–2657. <https://doi.org/10.1080/07391102.2015.1124808>
- Pérez-Torres, I., Manzano-Pech, L., Rubio-Ruíz, M. E., Soto, M. E., & Guarner-Lans, V. (2020). Nitrosative stress and its association with cardiometabolic disorders. *Molecules*, 25(11). <https://doi.org/10.3390/molecules25112555>
- Phaniendra, A., Jestadi, D. B., & Periyasamy, L. (2015). Free Radicals: Properties, Sources, Targets, and Their Implication in Various Diseases. *Indian Journal*

of Clinical Biochemistry, 30(1), 11–26. <https://doi.org/10.1007/s12291-014-0446-0>

- Pinzi, L., & Rastelli, G. (2019). *Molecular Docking: Shifting Paradigms in Drug Discovery*. *International Journal of Molecular Sciences*, 20(18), 1–23. <https://doi.org/10.3390/ijms20184331>
- Pires, D. E. V., Blundell, T. L., & Ascher, D. B. (2015). pkCSM: Predicting small-molecule pharmacokinetic and toxicity properties using graph-based signatures. *Journal of Medicinal Chemistry*, 58(9), 4066–4072. <https://doi.org/10.1021/acs.jmedchem.5b00104>
- Pisoschi, A. M., & Pop, A. (2015). The role of antioxidants in the chemistry of oxidative stress: A review. *European Journal of Medicinal Chemistry*, 97, 55–74. <https://doi.org/10.1016/j.ejmech.2015.04.040>
- Pisoschi, A. M., Pop, A., Iordache, F., Stanca, L., Predoi, G., & Serban, A. I. (2021). Oxidative stress mitigation by antioxidants - An overview on their chemistry and influences on health status. *European Journal of Medicinal Chemistry*, 209, 112891. <https://doi.org/10.1016/j.ejmech.2020.112891>
- Pizzino, G., Irrera, N., Cucinotta, M., Pallio, G., Mannino, F., Arcoraci, V., Squadrito, F., Altavilla, D., & Bitto, A. (2017). Oxidative Stress: Harms and Benefits for Human Health. *Oxidative Medicine and Cellular Longevity*, 2017. <https://doi.org/10.1155/2017/8416763>
- Precupas, A., & Ionescu, S. (2021). Exploring the interaction of 5,6-benzocoumarin-3-carboxylic acid with bovine serum albumin at the *molecular* level: A biophysical investigation using *molecular* dynamics. *Revue Roumaine de Chimie*, 66(1), 49–58. <https://doi.org/10.33224/rrch.2021.66.1.05>
- Prenzler, P. D., Ryan, D., & Robards, K. (2021). *Chapter 1. Introduction to Basic Principles of Antioxidant Activity* (Issue 28). <https://doi.org/10.1039/9781839165337-00001>
- Puspitasari, M. L., Wulansari, T. V., Widyaningsih, T. D., & Mahar, J. (2016). Aktivitas Antioksidan Suplemen Herbal Daun Sirsak (*Annona muricata* L .) Dan Kulit Manggis (*Garcinia mangostana* L .) : Kajian Pustaka. *Pangan Dan Agroindustri*, 4(1), 283–290.
- Putri, F. E., Diharmi, A., & Karnila, R. (2023). Identifikasi Senyawa Metabolit

- Sekunder Pada Rumput Laut Coklat (*Sargassum plagyophyllum*) Dengan Metode Fraksinasi. *Jurnal Teknologi Dan Industri Pertanian Indonesia*, 15(1), 40–46. <https://doi.org/10.17969/jtipi.v15i1.23318>
- Rahmani, S. P. (2024). *Uji Aktivitas Antioksidan Dan Inhibisi Xantin Oksidase Fraksi Beberapa Bagian Tumbuhan Ubi Jalar (Ipomoea batatas L.) Varietas Ungu-Oranye*. Bakti Tunas Husada.
- Rasul, H. O., Aziz, B. K., Morán, G. S., Mendoza-Huizar, L. H., Belhassan, A., Candia, L. G., Villada, W. C., & Sadasivam, K. (2023). a Computational Study of the Antioxidant Power of Eugenol Compared To Vitamin C. *Quimica Nova*, 46(9), 873–880. <https://doi.org/10.21577/0100-4042.20230073>
- 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>
- Riyanto, A., Aulia, M., Asni, N., Devi, S., Putri, E., & Dewi, M. (2024). *Eksplorasi Potensi Pigmen dalam Daun Pandan (Pandanus odoratissimus) melalui Kromatografi Kolom*. 2(1). <https://doi.org/10.52330/jpcet.v2i1.316>
- Roni, A., Kurnia, D., & Hafsyah, N. (2022). Penetapan Kadar Flavonoid Dan Aktivitas Antioksidan Pada Ekstrak Batang Brotowali (*Tinospora crispa* L.) Dengan Metode CUPRAC. *Jurnal Ilmiah Ibnu Sina (JIIS): Ilmu Farmasi Dan Kesehatan*, 7(1), 165–173. <https://doi.org/10.36387/jiis.v7i1.856>
- Rose, Y., Duarte, J. M., Lowe, R., Segura, J., Bi, C., Bhikadiya, C., Chen, L., Rose, A. S., Bittrich, S., Burley, S. K., & Westbrook, J. D. (2021). RCSB Protein Data Bank: Architectural Advances Towards Integrated Searching and Efficient Access to Macromolecular Structure Data from the PDB Archive. *Journal of Molecular Biology*, 433(11), 166704. <https://doi.org/10.1016/j.jmb.2020.11.003>
- Ruswanto, 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., 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; Vol 25, No 3 (2022): Volume 25 Issue 3 Year 2022DO - 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., Lestari, T., Septian, A. D., Firmansyah, A. P., & Mardianingrum, R. (2024). Potential Active Compounds of Propolis as Breast Anticancer Candidates: In Silico Study. *Jordan Journal of Biological Sciences*, 17(1), 153–161. <https://doi.org/10.54319/jjbs/170115>

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>

Safnowandi, S. (2022). Pemanfaatan Vitamin C Alami sebagai Antioksidan pada Tubuh Manusia. *Biocaster : Jurnal Kajian Biologi*, 2(1), 6–13. <https://doi.org/10.36312/bjkb.v2i1.43>

Salentin, S., Schreiber, S., Haupt, V. J., Adasme, M. F., & Schroeder, M. (2015). PLIP: Fully automated protein-ligand interaction profiler. *Nucleic Acids Research*, 43(W1), W443–W447. <https://doi.org/10.1093/nar/gkv315>

Sangavi, & Langeswaran. (2020). Anti-tumorigenic Efficacy of Tangeretin in Liver Cancer – An In Silico Approach. *Current Computer-Aided Drug Design*, 17(3), 337–343. <https://doi.org/10.2174/1573409916666200219120254>

Santos, C. M. M., Silva, A. M. S., Filipe, P., Santus, R., Patterson, L. K., Mazière, J. C., Cavaleiro, J. A. S., & Morlière, P. (2011). Structure-activity relationships in hydroxy-2,3-diaryl-xanthone antioxidants. Fast kinetics spectroscopy as a tool to evaluate the potential for antioxidant activity in biological systems.

- Organic and Biomolecular Chemistry*, 9(10), 3965–3974.
<https://doi.org/10.1039/c0ob00841a>
- Sari, A. N. (2016). Berbagai Tanaman Rempah Sebagai Sumber Antioksidan Alami. *Elkawanie*, 2(2), 203. <https://doi.org/10.22373/ekw.v2i2.2695>
- Schürmann, C., Rezende, F., Kruse, C., Yasar, Y., Löwe, O., Fork, C., Van De Sluis, B., Bremer, R., Weissmann, N., Shah, A. M., Jo, H., Brandes, R. P., & Schröder, K. (2015). The NADPH Oxidase Nox4 has anti-atherosclerotic functions. *European Heart Journal*, 36(48), 3447–3456.
<https://doi.org/10.1093/eurheartj/ehv460>
- Shaker, B., Ahmad, S., Lee, J., Jung, C., & Na, D. (2021). In silico methods and tools for drug discovery. *Computers in Biology and Medicine*, 137(July), 104851. <https://doi.org/10.1016/j.compbiomed.2021.104851>
- Siani, P., Frigerio, G., Donadoni, E., & Di Valentin, C. (2022). Modeling Zeta Potential for Nanoparticles in Solution: Water Flexibility Matters. *Journal of Physical Chemistry C*. <https://doi.org/10.1021/acs.jpcc.2c08988>
- Sluga, J., Venko, K., Drgan, V., & Novič, M. (2020). QSPR models for prediction of aqueous solubility: Exploring the potency of randic-type Indices. *Croatica Chemica Acta*, 93(4), 311–319. <https://doi.org/10.5562/CCA3776>
- Sobolev, O. V., Afonine, P. V., Moriarty, N. W., Hekkelman, M. L., Joosten, R. P., Perrakis, A., & Adams, P. D. (2020). A Global Ramachandran Score Identifies Protein Structures with Unlikely Stereochemistry. *Structure*, 28(11), 1249–1258.e2. <https://doi.org/10.1016/j.str.2020.08.005>
- Sorkun, M. C., Khetan, A., & Er, S. (2019). AqSolDB, a curated reference set of aqueous solubility and 2D descriptors for a diverse set of compounds. *Scientific Data*, 6(1), 1–8. <https://doi.org/10.1038/s41597-019-0151-1>
- Srinivas, U. S., Tan, B. W. Q., Vellayappan, B. A., & Jeyasekharan, A. D. (2019). ROS and the DNA damage response in cancer. *Redox Biology*, 25(October 2018), 101084. <https://doi.org/10.1016/j.redox.2018.101084>
- Su'aida, N., Mardiana, L., & Ramadhani, J. (2024). Studi in Silico Dan Prediksi Farmakokinetik Captopril- Herbal Untuk Potensi Terapi Kombinasi Antihipertensi. *Jurnal Farmasi Islam Kalimantan*, 1(1), 16–25.
<https://doi.org/10.31602/jfik.v1i1.15396>

- Su, J., Sun, T., Wang, Y., & Shen, Y. (2022). Conformational Dynamics of Glucagon-like Peptide-2 with Different Electric Field. *Polymer*, 14(2722). <https://doi.org/10.3390/polym14132722>
- Sulimov, A. V., Kutov, D. C., Katkova, E. V., & Sulimov, V. B. (2017). Combined Docking with Classical Force Field and Quantum Chemical Semiempirical Method PM7. *Advances in Bioinformatics*, 2017. <https://doi.org/10.1155/2017/7167691>
- Sumilah, Devy, N. F., & Hardiyanto. (2019). Karakterisasi Karakter Morfologi Daun dan Bunga Varietas Lokal Ubi Jalar (Ipomea batatas L .) Kabupaten Agam dan Solok , Provinsi Sumatra Barat. *Buletin Plasma Nutfah*, 25(2), 91–98.
- Suryadinata, A. N. (2018). Proses Inflamasi pada Penyakit Paru. *Amerta Nutrition UnAir*, 2(4), 317–324. [http://repository.ubaya.ac.id/34121/1/PengaruhRadikal Bebas Terhadap Proses Inflamasi pada Penyakit Paru.pdf](http://repository.ubaya.ac.id/34121/1/PengaruhRadikalBebasTerhadapProsesInflamasiPadaPenyakitParu.pdf)
- Suzuki, K., Shimizu, T., & Nakata, T. (1998). The cholesterol metabolite *Cholest-4-en-3-one* and its 3-oxo derivatives suppress body weight gain, body fat accumulation and serum lipid concentration in mice. *Bioorganic and Medicinal Chemistry Letters*, 8(16), 2133–2138. [https://doi.org/10.1016/S0960-894X\(98\)00362-X](https://doi.org/10.1016/S0960-894X(98)00362-X)
- 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>
- Tan, B. L., Norhaizan, M. E., Liew, W. P. P., & Rahman, H. S. (2018). Antioxidant and oxidative stress: A mutual interplay in age-related diseases. *Frontiers in Pharmacology*, 9(OCT), 1–28. <https://doi.org/10.3389/fphar.2018.01162>
- Tao, X., Huang, Y., Wang, C., Chen, F., Yang, L., Ling, L., Che, Z., & Chen, X. (2020). Recent developments in molecular docking technology applied in food science: a review. *International Journal of Food Science and Technology*, 55(1), 33–45. <https://doi.org/10.1111/ijfs.14325>
- Tjitraresmi, A., Moektiwardoyo, M., Susilawati, Y., Megantara, S., Shiono, Y., & Ruswanto, R. (2022). The Virtual Screening Of Secondary Metabolites Of

- Miana Leaves (*Plectranthus scutellarioides* (L) R. Br) Against Plasmodium Falciparum Lactate Dehydrogenase Enzyme (PfLDH). *Rasayan Journal of Chemistry*, 15(3), 2155–2164. <https://doi.org/10.31788/RJC.2022.1536963>
- Tu, M., Cheng, S., Lu, W., & Du, M. (2018). Advancement and prospects of bioinformatics analysis for studying bioactive peptides from food-derived protein: Sequence, structure, and functions. *TrAC - Trends in Analytical Chemistry*, 105, 7–17. <https://doi.org/10.1016/j.trac.2018.04.005>
- Valko, M., Jomova, K., Rhodes, C. J., Kuča, K., & Musílek, K. (2016). Redox- and non-redox-metal-induced formation of free radicals and their role in human disease. In *Archives of Toxicology* (Vol. 90, Issue 1). Springer Berlin Heidelberg. <https://doi.org/10.1007/s00204-015-1579-5>
- Vallianatou, T., Tsopelas, F., & Tsantili-Kakoulidou, A. (2022). Prediction Models for Brain Distribution of Drugs Based on Biomimetic Chromatographic Data. *Molecules*, 27(12), 1–22. <https://doi.org/10.3390/molecules27123668>
- Wang, S. (2016). Kandungan kimia dan efek kesehatan dari ubi jalar. 89, 90–116.
- Wang, X., Li, X., & Chen, D. (2011). Evaluation of antioxidant activity of isoferulic acid in vitro. *Natural Product Communications*, 6(9), 1285–1288. <https://doi.org/10.1177/1934578x1100600919>
- Wang, Y., Jin, R., Chen, J., Cao, J., Xiao, J., Li, X., & Sun, C. (2021). Tangeretin maintains antioxidant activity by reducing CUL3 mediated NRF2 ubiquitination. *Food Chemistry*, 365(June), 130470. <https://doi.org/10.1016/j.foodchem.2021.130470>
- Wu, K., Li, W., Song, J., & Li, T. (2015). Production, Purification, and Identification of *Cholest-4-en-3-one* Produced by Cholesterol Oxidase from *Rhodococcus* sp. in Aqueous/Organic Biphasic System . *Biochemistry Insights*, 8s1, BCI.S21580. <https://doi.org/10.4137/bci.s21580>
- Yeni, Y., & Rachmania, R. A. (2022). The Prediction of Pharmacokinetic Properties of Compounds in *Hemigraphis alternata* (Burm.F.) T. Ander Leaves Using pkCSM. *Indonesian Journal of Chemistry*, 22(4), 1081–1089. <https://doi.org/10.22146/ijc.73117>
- Yusuff, Omotosho, & Raji. (2023). Comparative Chains Dynamics Of Triosephosphate Isomerase Investigated By *Molecular Dynamics Simulation*.

- J. Chem Soc Nigeria*, 48(1), 146–153. <https://doi.org/10.46602/jcsn.v48i1.856>
- Zhang, D., Li, H., Wang, H., & Li, L. (2016). Docking accuracy enhanced by QM-derived protein charges. *Molecular Physics*, 114(20), 3015–3025. <https://doi.org/10.1080/00268976.2016.1213908>
- Zheleva-Dimitrova, D., Nedialkov, P., Girreser, U., & Kitanov, G. (2012). Benzophenones and flavonoids from *Hypericum maculatum* and their antioxidant activities. *Natural Product Research*, 26(17), 1576–1583. <https://doi.org/10.1080/14786419.2011.582468>
- Zhuang, Y., Wang, C., Wu, C., Ding, D., Zhao, F., Hu, C., Gong, W., Ding, G., Zhang, Y., Chen, L., Yang, G., Zhu, C., Zhang, A., Jia, Z., & Huang, S. (2018). Mitochondrial oxidative stress activates COX-2/mPGES-1/PGE2 cascade induced by albumin in renal proximal tubular cells. *Oncotarget*, 9(10), 9235–9245. <https://doi.org/10.18632/oncotarget.24187>