



## REFERENCES

- Aghajani , J., Farnia, P., Farnia, P., Ghanavi, J., & Velayati, A. A., 2022, Molecular Dynamic Simulations and Molecular Docking as a Potential Way for Designed New Inhibitor Drug without Resistance, *Tanaffos*, 21(1), 1-14.
- Agraharam, G., Girigoswami, A., & Girigoswami, K., 2022, Myricetin: a Multifunctional Flavonol in Biomedicine, *Curr. Pharmaco. Rep.*, 8(1), 48–61.
- Ambarsari, L., Nur, N. A., Zanah, S. S. R., Kurniawanti, Dianhar, H., Warnasih, S., Rahayu, D. U. C., & Sugita, P., 2024, Molecular Docking of Biflavonoids from Genus Araucaria as Denv Ns5 Rna-Dependent Rna Polymerase Inhibitor using Yasara and Plants Programs, *Int J. Appl. Pharm.*, 291–299.
- Amin, Md. R., Yasmin, F., Anowar Hosen, M., Dey, S., Mahmud, S., Saleh, Md. A., Emran, T. B., Hasan, I., Fujii, Y., Yamada, M., Ozeki, Y., & Kawsar, S. M. A., 2021, Synthesis, Antimicrobial, Anticancer, PASS, Molecular Docking, Molecular Dynamic Simulations & Pharmacokinetic Predictions of Some Methyl β-D-Galactopyranoside Analogs, *Mol.*, 26(22).
- Badar, M. S., Shamsi, S., Ahmed, J., & Alam, Md. A., 2022, *Molecular Dynamics Simulations: Concept, Methods, and Applications*. In Rezaei, N., *Transdisciplinarity*, Springer Cham, Switzerland.
- Bruggemann, H., 2004, The Complete Genome Sequence of *Propionibacterium acnes*, a Commensal of Human Skin, *Sci.*, 305(5684), 671–673.
- Burkhart, C. G., 2024, Assessment of *Cutibacterium acnes*: Acne Biofilm, Comedones, and Future Treatments for Acne, *Open Dermatol. J.*, 18(1).
- Chen, K., Yang, C.-H., Li, T., Zouboulis, C. C., & Huang, Y.-C., 2019, Suppression of Propionibacterium acnes -stimulated proinflammatory cytokines by Chinese bayberry extracts and its active constituent myricetin in human sebocytes in vitro, *Phytoter. Res.*, 33(4), 1104–1113.
- Cornell, W. D., Cieplak, P., Bayly, C. I., Gould, I. R., Merz, K. M., Ferguson, D. M., Spellmeyer, D. C., Fox, T., Caldwell, J. W., & Kollman, P. A., 1995, A Second Generation Force Field for the Simulation of Proteins, Nucleic Acids, and Organic Molecules, *J. Am. Chem. Soc.*, 117(19), 5179–5197.
- Daud, N. H., Leow, T. C., Oslan, S. N., & Salleh, A. B., 2019, A Novel Mini Protein Design of Haloalkane Dehalogenase, *Mol. Biotechnol.*, 61(7), 477–488.
- Ferreira, L., dos Santos, R., Oliva, G., & Andricopulo, A., 2015, Molecular Docking and Structure-Based Drug Design Strategies, *Mol.*, 20(7).



- Genheden, S., Reymer, A., Saenz-Méndez, P., & Eriksson, L. A., 2017, *Chapter 1. Computational Chemistry and Molecular Modelling Basics*. In Martín-Santamaría, S., *Computational Tools for Chemical Biology*, RSC Publishing, Cambridge.
- Ghahremanian, S., Rashidi, M. M., Raeisi, K., & Toghraie, D., 2022, Molecular dynamics simulation approach for discovering potential inhibitors against SARS-CoV-2: A structural review. *J. Mol. Liq.*, 354, 118901.
- Hill, A. D., & Reilly, P. J., 2015, Scoring Functions for AutoDock. *Methods Mol. Biol.*, 1273, 467–474.
- Istyastono, E. P., 2023, *Simulasi dan Validasi Penambatan Molekul dengan Pugasan YASARA-Structure*, Sanata Dharma University Press, Yogyakarta.
- Kajjout, M., & Rolando, C., 2011, Regiospecific synthesis of quercetin O- $\beta$ -d-glucosylated and O- $\beta$ -d-glucuronidated isomers, *Tetrahedron*, 67(25), 4731–4741.
- Knapp, B., Frantal, S., Cibena, M., Schreiner, W., & Bauer, P., 2011, Is an Intuitive Convergence Definition of Molecular Dynamics Simulations Solely Based on the Root Mean Square Deviation Possible?, *J. Comput. Biol.*, 18(8), 997–1005.
- Kufareva, I., & Abagyan, R., 2012, Methods of Protein Structure Comparison, *Methods Mol. Biol.*, 857, 231–257.
- Kurokawa, I., Danby, F. W., Ju, Q., Wang, X., Xiang, L. F., Xia, L., Chen, W., Nagy, I., Picardo, M., Suh, D. H., Ganceviciene, R., Schagen, S., Tsatsou, F., & Zouboulis, C. C., 2009, New developments in our understanding of acne pathogenesis and treatment, *Exp. Dermatol.*, 18(10), 821–832.
- Lambrechts, I. A., Canha, M. N. de , & Lall, N., 2018, *Exploiting Medicinal Plants as Possible Treatments for Acne Vulgaris*, Elsevier, Amsterdam.
- Ma, E. Z., & Khachemoune, A., 2022, Flavonoids and their therapeutic applications in skin diseases, *Arch. Dermatol. Res.*
- Mayslich, C., Grange, P. A., & Dupin, N., 2021, *Cutibacterium acnes* as an Opportunistic Pathogen: An Update of Its Virulence-Associated Factors. *Microorganisms*, 9(2), 303.
- Michel, J., 2006, The Use of Free Energy Simulations as Scoring Functions, *Dissertation*, University of Southampton, Southampton.



- Nakatsuji, T., Liu, Y.-T., Huang, C.-P., Gallo, R. L., & Huang, C.-M., 2008, Vaccination Targeting a Surface Sialidase of *P. acnes*: Implication for New Treatment of Acne Vulgaris, *PLoS ONE*, 3(2), e1551.
- Nasri, H., Bahmani, M., Shahinfard, N., Moradi Nafchi, A., Saberianpour, S., & Rafieian Kopaei, M., 2015, Medicinal Plants for the Treatment of Acne Vulgaris: A Review of Recent Evidences, *Jundishapur J. Microbiol.*, 8(11).
- Owoloye, A., Ligali, F. C., Enejoh, O. A., Musa, A. Z., Aina, O. O., Idowu, E. T., & Oyebola, K., 2022, Molecular docking, simulation and binding free energy analysis of small molecules as PfHT1 inhibitors. *PLoS One*, 17(8), e0268269–e0268269.
- Pissurlenkar, R., Shaikh, M., Iyer, R., & Coutinho, E., 2009, Molecular Mechanics Force Fields and their Applications in Drug Design, *Anti-Infect. Agents Med. Chem.*, 8(2), 128–150.
- Purnama, A., Mardina, V., Puspita, K., Qanita, I., Rizki, D. R., Hasballah, K., Iqbal, M., & Sarong, M., 2021, Molecular docking of two cytotoxic compounds from Calotropis gigantea leaves against therapeutic molecular target of pancreatic cancer, *Narra J.*, 1(2).
- Roy, K., Kar, S., & Das, R. N., 2015, *Understanding the Basics of QSAR for Applications in Pharmaceutical Sciences and Risk Assessment*. Elsevier, Amsterdam.
- Rz̄esikowska, K., Kalinowska-Tluścik, J., & Krawczuk, A., 2022, Hierarchical analysis of the target-based scoring function modification for the example of selected class A GPCRs, *Phys. Chemi.*, 25(4), 3513–3520.
- Salo-Ahen, O. M. H., Alanko, I., Bhadane, R., Bonvin, A. M. J. J., Honorato, R. V., Hossain, S., Juffer, A. H., Kabedev, A., Lahtela-Kakkonen, M., Larsen, A. S., Lescrinier, E., Marimuthu, P., Mirza, M. U., Mustafa, G., Nunes-Alves, A., Pantsar, T., Saadabadi, A., Singaravelu, K., & Vanmeert, M., 2021, Molecular Dynamics Simulations in Drug Discovery and Pharmaceutical Development, *Processes*, 9(1), 71.
- Semwal, D., Semwal, R., Combrinck, S., & Viljoen, A., 2016, Myricetin: A Dietary Molecule with Diverse Biological Activities, *Nutrients*, 8(2), 90.
- Sharma, R., Kishore, N., Hussein, A., & Lall, N., 2013, Antibacterial and anti-inflammatory effects of Syzygium jambos L. (Alston) and isolated compounds on acne vulgaris, *BMC Complementary Altern. Med.*, 13(1).
- Shivalingaiah, Thoyojaksha, Chakith M R, S., Pradeep, S., Pallavi K. S., Kavana C. P., Navyashree B., Kumar, D. G., Girish M. S., Srinivasa, C., Kollur, S. P.,



- & Shivamallu, C., 2022, In-Silico Evaluation Of Anti-Acne Property Of Syzygium (S.) Aromaticum, *IJFANS Int. J. Food. Nutr. Sci.*, 11(3).
- Singh, A. P., Arya, H., Singh, V., Kumar, P., & Gautam, H. K., 2022, Identification of natural inhibitors to inhibit *C. acnes* lipase through docking and simulation studies, *J. Mol. Model.* 28(9).
- Tobiasz, A., Nowicka, D., & Szepietowski, J. C., 2022, Acne Vulgaris—Novel Treatment Options and Factors Affecting Therapy Adherence: A Narrative Review, *J. Clin. Med.*, 11(24), 7535.
- Tronina, T., Łužny, M., Dymarska, M., Urbaniak, M., Kozłowska, E., Piegza, M., Stępień, Ł., & Janeczko, T., 2023, Glycosylation of Quercetin by Selected Entomopathogenic Filamentous Fungi and Prediction of Its Products' Bioactivity, *Int. J. Mol. Sci.*, 24(14), 11857–11857.
- Ullah, S., Rahman, W., Ullah, F., Ullah, A., Jehan, R., Iqbal, M. N., Ali, I., & Gao Tianshun, 2023, Identification of lead compound screened from the natural products atlas to treat renal inflammasomes using molecular docking and dynamics simulation, *J. Biomol. Struct. Dyn.*, 42(9), 4851–4861.
- Vadalà, M., 2021, Alive and Inactivated *Cutibacterium Acnes*: Properties, Functions and Pathogenicity, *Clin. Immunol. Immunother.*, 7(2), 1–7.
- Vasam, M., Korutla, S., & Bohara, R. A., 2023, Acne vulgaris: A review of the pathophysiology, treatment, and recent nanotechnology based advances, *Biochem. Biophys. Rep.*, 36, 101578–101578.
- Venkatachalam, K. V., & Ettrich, R. H., 2021, Role of aspartic acid residues D87 and D89 in APS kinase domain of human 3'-phosphoadenosine 5'-phosphosulfate synthase 1 and 2b: A commonality with phosphatases/kinases. *Biochem. Biophys. Rep.*, 28, 101155–101155.
- Yang, J. H., Yoon, J. Y., Kwon, H. H., Min, S., Moon, J., & Suh, D. H., 2017, Seeking new acne treatment from natural products, devices and synthetic drug discovery, *Dermato-Endocrinol.*, 9(1), e1356520.
- Yu, A. C., Volkers, G., Jongkees, S. A., Worrall, L. J., Withers, S. G., & Strynadka, N. C., 2021, Crystal structure of the Propionibacterium acnes surface sialidase, a drug target for *P. acnes* associated diseases, *Glycobiology*, 32(2), 162–170.
- Yu, Y., Champer, J., & Kim, J., 2015, Analysis of the surface, secreted, and intracellular proteome of Propionibacterium acnes. *EuPA Open Proteomics*, 9, 1–7.