

DAFTAR PUSTAKA

- Abdelmonsef, A. H., Omar, M., Rashdan, H. R. M., Taha, M. M., & Abobakr, A. M. (2023). Design, synthetic approach, *in silico* molecular docking and antibacterial activity of quinazolin-2,4-dione hybrids bearing bioactive scaffolds. *RSC Advances*, 13(1), 292–308. <https://doi.org/10.1039/D2RA06527D>
- Abraham, M. J., Murtola, T., Schulz, R., Páll, S., Smith, J. C., Hess, B., & Lindahl, E. (2015). GROMACS: High performance molecular simulations through multi-level parallelism from laptops to supercomputers. *SoftwareX*, 1–2, 19–25. <https://doi.org/10.1016/j.softx.2015.06.001>
- Abramson, J., Adler, J., Dunger, J., Evans, R., Green, T., Pritzel, A., Ronneberger, O., Willmore, L., Ballard, A. J., Bambrick, J., Bodenstein, S. W., Evans, D. A., Hung, C.-C., O'Neill, M., Reiman, D., Tunyasuvunakool, K., Wu, Z., Žemgulytė, A., Arvaniti, E., ... Jumper, J. M. (2024). Accurate structure prediction of biomolecular interactions with AlphaFold 3. *Nature*, 630(8016), 493–500. <https://doi.org/10.1038/s41586-024-07487-w>
- Abreu, A. C., Saavedra, M. J., Simões, M., Abreu, A. C., Borges, A., & Chaves Simões, L. (2013). *Antibacterial activity of phenyl isothiocyanate on Escherichia coli and Staphylococcus aureus*. <https://www.researchgate.net/publication/230824736>
- Adcock, S. A., & McCammon, J. A. (2006). Molecular Dynamics: Survey of Methods for Simulating the Activity of Proteins. *Chemical Reviews*, 106(5), 1589–1615. <https://doi.org/10.1021/cr040426m>
- Agu, P. C., Afiukwa, C. A., Orji, O. U., Ezech, E. M., Ofoke, I. H., Ogbu, C. O., Ugwuja, E. I., & Aja, P. M. (2023). Molecular docking as a tool for the discovery of molecular targets of nutraceuticals in diseases management. *Scientific Reports*, 13(1), 13398. <https://doi.org/10.1038/s41598-023-40160-2>
- Ahmad, W., Ansari, M. A., Yusuf, M., Amir, M., Wahab, S., Alam, P., Alomary, M. N., Alhuwayri, A. A., Khan, M., Ali, A., Warsi, M. H., Ashraf, K., & Ali, M. (2022). Antibacterial, Anticandidal, and Antibiofilm Potential of Fenchone: In Vitro, Molecular Docking and In Silico/ADMET Study. *Plants*, 11(18), 2395. <https://doi.org/10.3390/plants11182395>
- Alattar, A., Alshaman, R., & Al-Gayyar, M. M. H. (2022). Therapeutic effects of sulforaphane in ulcerative colitis: effect on antioxidant activity, mitochondrial biogenesis and DNA polymerization. *Redox Report*, 27(1), 128–138. <https://doi.org/10.1080/13510002.2022.2092378>

- Alberts, B., Johnson, A., Lewis, J., Raff, M., Roberts, K., & Walter, P. (2002). Molecular biology of the cell. 4th edn. *Annals of Botany*, 1–1616. <https://www.ncbi.nlm.nih.gov/books/NBK26830/>
- Ali, A., Noor, I., Shaukat, M., Waheed, W., Akbar, K., Ji, Z., & Su, Z. (2025). Inhibition of Shiga Toxin 2 for E. coli O157 Control: An In-Silico Study on Natural and Synthetic Compounds. *Current Medicinal Chemistry*, 32. <https://doi.org/10.2174/0109298673363373250118144235>
- Allen, M. P., & Tildesley, D. J. (2017). *Computer Simulation of Liquids*. Oxford University PressOxford. <https://doi.org/10.1093/oso/9780198803195.001.0001>
- Ameen, F., Orfali, R., Mamidala, E., & Davella, R. (2023). *In silico* toxicity prediction, molecular docking studies and *in vitro* validation of antibacterial potential of alkaloids from *Eclipta alba* in designing of novel antimicrobial therapeutic strategies. *Biotechnology and Genetic Engineering Reviews*, 39(2), 760–774. <https://doi.org/10.1080/02648725.2022.2162264>
- Ameer, M. A., Wasey, A., & Salen, P. (2025). *Escherichia coli (e Coli 0157 H7)*.
- Amrulloh, L. S. W. F., Harmastuti, N., Prasetyo, A., & Herowati, R. (2023). Analysis of Molecular Docking and Dynamics Simulation of Mahogany (Swietenia macrophylla King) Compounds Against the PLpro Enzyme SARS-COV-2. *JURNAL FARMASI DAN ILMU KEFARMASIAN INDONESIA*, 10(3), 347–359. <https://doi.org/10.20473/jfiki.v10i32023.347-359>
- Apel, D., & Surette, M. G. (2008). Bringing order to a complex molecular machine: The assembly of the bacterial flagella. *Biochimica et Biophysica Acta (BBA) - Biomembranes*, 1778(9), 1851–1858. <https://doi.org/10.1016/j.bbamem.2007.07.005>
- Arora, N., Singh, V. K., Shah, K., & Pandey-Rai, S. (2012). Qualitative and Quantitative analysis of 3D predicted arachidonate 15-lipoxygenase-B (15-LOX-2) from Homo sapiens. *Bioinformation*, 8(12), 555–561. <https://doi.org/10.6026/97320630008555>
- Arunan, E., Desiraju, G. R., Klein, R. A., Sadlej, J., Scheiner, S., Alkorta, I., Clary, D. C., Crabtree, R. H., Dannenberg, J. J., Hobza, P., Kjaergaard, H. G., Legon, A. C., Mennucci, B., & Nesbitt, D. J. (2011). Definition of the hydrogen bond (IUPAC Recommendations 2011). *Pure and Applied Chemistry*, 83(8), 1637–1641. <https://doi.org/10.1351/PAC-REC-10-01-02>
- Arvidsson, I., Tontanahal, A., Johansson, K., Kristoffersson, A.-C., Kellnerová, S., Berger, M., Dobrindt, U., & Karpman, D. (2022). Apyrase decreases phage induction and Shiga toxin release from *E. coli* O157:H7 and has a protective

- effect during infection. *Gut Microbes*, 14(1).
<https://doi.org/10.1080/19490976.2022.2122667>
- Badar, M. S., Shamsi, S., Ahmed, J., & Alam, Md. A. (2022). *Molecular Dynamics Simulations: Concept, Methods, and Applications* (pp. 131–151).
https://doi.org/10.1007/978-3-030-94651-7_7
- Bagewadi, Z. K., Yunus Khan, T. M., Gangadharappa, B., Kamalapurkar, A., Mohamed Shamsudeen, S., & Yaraguppi, D. A. (2023). Molecular dynamics and simulation analysis against superoxide dismutase (SOD) target of *Micrococcus luteus* with secondary metabolites from *Bacillus licheniformis* recognized by genome mining approach. *Saudi Journal of Biological Sciences*, 30(9), 103753. <https://doi.org/10.1016/j.sjbs.2023.103753>
- Bartram, J., Baum, R., Coclanis, P., Gute, D., Kay, D., McFadyen, S., Pond, K., Robertson, W., & Rouse, M. (2015). *Routledge Handbook of Water and Health* (J. Bartram, Ed.). Routledge. <https://doi.org/10.4324/9781315693606>
- Berndsen, C. (2020). Analysis of protein structure using Molprobit. *Protocols.io*, 1–11. <https://www.protocols.io/view/analysis-of-protein-structure-using-molprobit-bgmaju2e.pdf>
- Bertoline, L. M. F., Lima, A. N., Krieger, J. E., & Teixeira, S. K. (2023). Before and after AlphaFold2: An overview of protein structure prediction. *Frontiers in Bioinformatics*, 3. <https://doi.org/10.3389/fbinf.2023.1120370>
- Bhattacharya, S., Dutta, A., Khanra, P. K., Gupta, N., Dutta, R., Tzvetkov, N. T., Milella, L., & Ponticelli, M. (2024). In silico exploration of 4(α -l-rhamnosyloxy)-benzyl isothiocyanate: A promising phytochemical-based drug discovery approach for combating multi-drug resistant *Staphylococcus aureus*. *Computers in Biology and Medicine*, 179, 108907. <https://doi.org/10.1016/j.combiomed.2024.108907>
- Burlingham, B. T., & Widlanski, T. S. (2003). An Intuitive Look at the Relationship of Ki and IC50: A More General Use for the Dixon Plot. *Journal of Chemical Education*, 80(2), 214. <https://doi.org/10.1021/ed080p214>
- Carugo, O. (2023). pLDDT Values in AlphaFold2 Protein Models Are Unrelated to Globular Protein Local Flexibility. *Crystals*, 13(11), 1560. <https://doi.org/10.3390/cryst13111560>
- Chen, V. B., Arendall, W. B., Headd, J. J., Keedy, D. A., Immormino, R. M., Kapral, G. J., Murray, L. W., Richardson, J. S., & Richardson, D. C. (2010). *MolProbity*: all-atom structure validation for macromolecular crystallography. *Acta Crystallographica Section D Biological Crystallography*, 66(1), 12–21. <https://doi.org/10.1107/S0907444909042073>

- Clarke, M. B., & Sperandio, V. (2005). Transcriptional regulation of *flhDC* by QseBC and σ 28 (FliA) in enterohaemorrhagic *Escherichia coli*. *Molecular Microbiology*, 57(6), 1734–1749. <https://doi.org/10.1111/j.1365-2958.2005.04792.x>
- Coscueta, E. R., Sousa, A. S., Reis, C. A., & Pintado, M. M. (2022). Phenylethyl Isothiocyanate: A Bioactive Agent for Gastrointestinal Health. *Molecules*, 27(3), 794. <https://doi.org/10.3390/molecules27030794>
- Csermely, P., Palotai, R., & Nussinov, R. (2010). Induced fit, conformational selection and independent dynamic segments: an extended view of binding events. *Trends in Biochemical Sciences*, 35(10), 539–546. <https://doi.org/10.1016/j.tibs.2010.04.009>
- Curtis, M. M., Russell, R., Moreira, C. G., Adebesein, A. M., Wang, C., Williams, N. S., Taussig, R., Stewart, D., Zimmermann, P., Lu, B., Prasad, R. N., Zhu, C., Rasko, D. A., Huntley, J. F., Falck, J. R., & Sperandio, V. (2014). QseC Inhibitors as an Antivirulence Approach for Gram-Negative Pathogens. *MBio*, 5(6). <https://doi.org/10.1128/mBio.02165-14>
- da Cruz Gouveia, M. A., Lins, M. T. C., & da Silva, G. A. P. (2020). Acute diarrhea with blood: diagnosis and drug treatment. *Jornal de Pediatria*, 96, 20–28. <https://doi.org/10.1016/j.jped.2019.08.006>
- Daina, A., Michielin, O., & Zoete, V. (2017). SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. *Scientific Reports*, 7(1), 42717. <https://doi.org/10.1038/srep42717>
- Darras, F. H., & Pang, Y.-P. (2017). On the use of the experimentally determined enzyme inhibition constant as a measure of absolute binding affinity. *Biochemical and Biophysical Research Communications*, 489(4), 451–454. <https://doi.org/10.1016/j.bbrc.2017.05.168>
- Della Sala, G., Teta, R., Esposito, G., & Costantino, V. (2019). The Chemical Language of Gram-Negative Bacteria. In *Quorum Sensing* (pp. 3–28). Elsevier. <https://doi.org/10.1016/B978-0-12-814905-8.00001-0>
- Deodhar, M., Al Rihani, S. B., Arwood, M. J., Darakjian, L., Dow, P., Turgeon, J., & Michaud, V. (2020). Mechanisms of CYP450 Inhibition: Understanding Drug-Drug Interactions Due to Mechanism-Based Inhibition in Clinical Practice. *Pharmaceutics*, 12(9), 846. <https://doi.org/10.3390/pharmaceutics12090846>
- Diniz, W. J. S., & Canduri, F. (2017). REVIEW-ARTICLE Bioinformatics: an overview and its applications. *Genetics and Molecular Research*, 16(1). <https://doi.org/10.4238/gmr16019645>

- Dunbrack, R. L., & Cohen, F. E. (1997). Bayesian statistical analysis of protein side-chain rotamer preferences. *Protein Science*, 6(8), 1661–1681. <https://doi.org/10.1002/pro.5560060807>
- El-Kattan, A., & Varm, M. (2012). Oral Absorption, Intestinal Metabolism and Human Oral Bioavailability. In *Topics on Drug Metabolism*. InTech. <https://doi.org/10.5772/31087>
- El-Mihoub, T. A., Hopgood, A. A., & Nolle, L. (2021). Self-adaptive learning for hybrid genetic algorithms. *Evolutionary Intelligence*, 14(4), 1565–1579. <https://doi.org/10.1007/s12065-020-00425-5>
- Emsley, P., & Cowtan, K. (2004). *Coot*: model-building tools for molecular graphics. *Acta Crystallographica Section D Biological Crystallography*, 60(12), 2126–2132. <https://doi.org/10.1107/S0907444904019158>
- Fatima, R., Nguyen, A. D., & Aziz, M. (2025). *Enterohemorrhagic Escherichia coli*.
- Fatriansyah, J. F., Boanerges, A. G., Kurnianto, S. R., Pradana, A. F., Fadilah, & Surip, S. N. (2022). Molecular Dynamics Simulation of Ligands from *Anredera cordifolia* (Binahong) to the Main Protease (Mpro) of SARS-CoV-2. *Journal of Tropical Medicine*, 2022, 1–13. <https://doi.org/10.1155/2022/1178228>
- Ferenczy, G. G., & Kellermayer, M. (2022). Contribution of hydrophobic interactions to protein mechanical stability. *Computational and Structural Biotechnology Journal*, 20, 1946–1956. <https://doi.org/10.1016/j.csbj.2022.04.025>
- Freestone, P. P., Haigh, R. D., & Lyte, M. (2007). Blockade of catecholamine-induced growth by adrenergic and dopaminergic receptor antagonists in *Escherichia coli* O157:H7, *Salmonella enterica* and *Yersinia enterocolitica*. *BMC Microbiology*, 7(1), 8. <https://doi.org/10.1186/1471-2180-7-8>
- Gambushe, S. M., Zishiri, O. T., & El Zowalaty, M. E. (2022). Review of *Escherichia coli* O157:H7 Prevalence, Pathogenicity, Heavy Metal and Antimicrobial Resistance, African Perspective. *Infection and Drug Resistance*, Volume 15, 4645–4673. <https://doi.org/10.2147/IDR.S365269>
- Gao, C., Desaphy, J., & Vieth, M. (2017). Are induced fit protein conformational changes caused by ligand-binding predictable? A molecular dynamics investigation. *Journal of Computational Chemistry*, 38(15), 1229–1237. <https://doi.org/10.1002/jcc.24714>

- Gelpi, J., Hospital, A., Goñi, R., & Orozco, M. (2015). Molecular dynamics simulations: advances and applications. *Advances and Applications in Bioinformatics and Chemistry*, 37. <https://doi.org/10.2147/AABC.S70333>
- Goldwater, P. N., & Bettelheim, K. A. (2012). Treatment of enterohemorrhagic *Escherichia coli* (EHEC) infection and hemolytic uremic syndrome (HUS). *BMC Medicine*, 10(1), 12. <https://doi.org/10.1186/1741-7015-10-12>
- Hadgraft, J., & Lane, M. E. (2005). Skin permeation: The years of enlightenment. *International Journal of Pharmaceutics*, 305(1–2), 2–12. <https://doi.org/10.1016/j.ijpharm.2005.07.014>
- Hadjittofis, E., Das, S. C., Zhang, G. G. Z., & Heng, J. Y. Y. (2017). Interfacial Phenomena. In *Developing Solid Oral Dosage Forms* (pp. 225–252). Elsevier. <https://doi.org/10.1016/B978-0-12-802447-8.00008-X>
- Hernandez, D. E., & Sintim, H. O. (2020). Quorum Sensing Autoinducer-3 Finally Yields to Structural Elucidation. *ACS Central Science*, 6(2), 93–96. <https://doi.org/10.1021/acscentsci.0c00033>
- 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>
- Hubbard, R. E., & Kamran Haider, M. (2010). Hydrogen Bonds in Proteins: Role and Strength. In *Encyclopedia of Life Sciences*. Wiley. <https://doi.org/10.1002/9780470015902.a0003011.pub2>
- Hughes, D. T., Clarke, M. B., Yamamoto, K., Rasko, D. A., & Sperandio, V. (2009). The QseC Adrenergic Signaling Cascade in Enterohemorrhagic *E. coli* (EHEC). *PLoS Pathogens*, 5(8), e1000553. <https://doi.org/10.1371/journal.ppat.1000553>
- Ivanova, L., & Karelson, M. (2022). The Impact of Software Used and the Type of Target Protein on Molecular Docking Accuracy. *Molecules*, 27(24), 9041. <https://doi.org/10.3390/molecules27249041>
- Izadi, S., & Onufriev, A. V. (2016). Accuracy limit of rigid 3-point water models. *The Journal of Chemical Physics*, 145(7). <https://doi.org/10.1063/1.4960175>
- Janczewski, Ł. (2022). Sulforaphane and Its Bifunctional Analogs: Synthesis and Biological Activity. *Molecules*, 27(5), 1750. <https://doi.org/10.3390/molecules27051750>
- Joseph, A., Cointe, A., Mariani Kurkdjian, P., Rafat, C., & Hertig, A. (2020). Shiga Toxin-Associated Hemolytic Uremic Syndrome: A Narrative Review. *Toxins*, 12(2), 67. <https://doi.org/10.3390/toxins12020067>

- Jumper, J., Evans, R., Pritzel, A., Green, T., Figurnov, M., Ronneberger, O., Tunyasuvunakool, K., Bates, R., Židek, A., Potapenko, A., Bridgland, A., Meyer, C., Kohl, S. A. A., Ballard, A. J., Cowie, A., Romera-Paredes, B., Nikolov, S., Jain, R., Adler, J., ... Hassabis, D. (2021). Highly accurate protein structure prediction with AlphaFold. *Nature*, 596(7873), 583–589. <https://doi.org/10.1038/s41586-021-03819-2>
- Jung, J., Kobayashi, C., & Sugita, Y. (2019). Optimal Temperature Evaluation in Molecular Dynamics Simulations with a Large Time Step. *Journal of Chemical Theory and Computation*, 15(1), 84–94. <https://doi.org/10.1021/acs.jctc.8b00874>
- Ke, Q., Gong, X., Liao, S., Duan, C., & Li, L. (2022). Effects of thermostats/barostats on physical properties of liquids by molecular dynamics simulations. *Journal of Molecular Liquids*, 365, 120116. <https://doi.org/10.1016/j.molliq.2022.120116>
- Kementerian Kesehatan Republik Indonesia. (2011, June 6). *Kemenkes Pantau Wabah E.coli*. <https://Nasional.Kompas.Com/Read/2011/06/06/11461474/Index.Html>.
- Kolodziejek, A. M., Minnich, S. A., & Hovde, C. J. (2022). Escherichia coli 0157:H7 virulence factors and the ruminant reservoir. *Current Opinion in Infectious Diseases*, 35(3), 205–214. <https://doi.org/10.1097/QCO.0000000000000834>
- Lee, J., & Kwon, H. (2015). *In vitro* metabolic conversion of the organic breakdown products of glucosinolate to goitrogenic thiocyanate anion. *Journal of the Science of Food and Agriculture*, 95(11), 2244–2251. <https://doi.org/10.1002/jsfa.6943>
- Lee, Y. M., Seon, M. R., Cho, H. J., Kim, J.-S., & Park, J. H. Y. (2009). Benzyl isothiocyanate exhibits anti-inflammatory effects in murine macrophages and in mouse skin. *Journal of Molecular Medicine*, 87(12), 1251–1261. <https://doi.org/10.1007/s00109-009-0532-6>
- Lemkul, J. (2019). From Proteins to Perturbed Hamiltonians: A Suite of Tutorials for the GROMACS-2018 Molecular Simulation Package [Article v1.0]. *Living Journal of Computational Molecular Science*, 1(1). <https://doi.org/10.33011/livecoms.1.1.5068>
- Lemkul, J. A. (2024). Introductory Tutorials for Simulating Protein Dynamics with GROMACS. *The Journal of Physical Chemistry B*, 128(39), 9418–9435. <https://doi.org/10.1021/acs.jpcb.4c04901>
- Lewis, D. F. V., Lake, B. G., & Dickins, M. (2007). Quantitative structure-activity relationships (QSARs) in inhibitors of various cytochromes P450: The

- importance of compound lipophilicity. *Journal of Enzyme Inhibition and Medicinal Chemistry*, 22(1), 1–6.
<https://doi.org/10.1080/14756360600952183>
- Lim, J. Y., Yoon, J., & Hovde, C. J. (2010). A brief overview of *Escherichia coli* O157:H7 and its plasmid O157. *Journal of Microbiology and Biotechnology*, 20(1), 5–14.
- Lin, P.-Y., Huang, S.-C., Chen, K.-L., Huang, Y.-C., Liao, C.-Y., Lin, G.-J., Lee, H., & Chen, P.-Y. (2025). Analysing protein complexes in plant science: insights and limitation with AlphaFold 3. *Botanical Studies*, 66(1), 14.
<https://doi.org/10.1186/s40529-025-00462-2>
- Lu, Y., Pang, X., & Yang, T. (2020). Microwave cooking increases sulforaphane level in broccoli. *Food Science & Nutrition*, 8(4), 2052–2058.
<https://doi.org/10.1002/fsn3.1493>
- Malau, N. D., & Azzahra, S. F. (2020). Molecular Docking Studies of Potential Quercetin 3,4'-dimethyl ether 7- α -L-Arabinofuranosyl-(1-6)-glucoside as Inhibitor antimalaria. *Journal of Physics: Conference Series*, 1428(1), 012057.
<https://doi.org/10.1088/1742-6596/1428/1/012057>
- Medarametla, P. (2020). *Identification and Design of New Antibacterial Agents Using Computational Approaches* [Publications of the University of Eastern Finland Dissertations in Health Sciences No 586]. Faculty of Health Sciences, University of Eastern Finland.
- Melchior, K., Salgaço, M. K., Sivieri, K., & Moreira, C. G. (2023). QseC sensor kinase modulates the human microbiota during enterohemorrhagic *Escherichia coli* O157:H7 infection in the Simulator of the Human Intestinal Microbial Ecosystem (SHIME®). *Brazilian Journal of Microbiology: [Publication of the Brazilian Society for Microbiology]*, 54(1), 1–14.
<https://doi.org/10.1007/s42770-022-00877-0>
- Mengistu, D. Y., & Mengesha, Y. (2023). New approaches for severity intervention and rapid diagnosis of enterohemorrhagic *Escherichia coli*: a review. *All Life*, 16(1). <https://doi.org/10.1080/26895293.2023.2218582>
- Mercer, D. G., & Rodriguez-Amaya, D. B. (2021). Reactions and interactions of some food additives. In *Chemical Changes During Processing and Storage of Foods* (pp. 579–635). Elsevier. <https://doi.org/10.1016/B978-0-12-817380-0.00012-9>
- Merz, P. T., & Shirts, M. R. (2018). Testing for physical validity in molecular simulations. *PLOS ONE*, 13(9), e0202764.
<https://doi.org/10.1371/journal.pone.0202764>

- Moreira, C. G., & Sperandio, V. (2016). *The Epinephrine/Norepinephrine /Autoinducer-3 Interkingdom Signaling System in Escherichia coli O157:H7* (pp. 247–261). https://doi.org/10.1007/978-3-319-20215-0_12
- Morris, G. M., Goodsell, D. S., Pique, M. E., Huey, R., Forli, S., Hart, W. E., Halliday, S., Belew, R., & Olson, A. J. (2017). *User Guide AutoDock Version 4.2 Updated for version 4.2.6 Automated Docking of Flexible Ligands to Flexible Receptors*. <http://autodock.scripps.edu/>
- Morris, K. F., Geoghegan, R. M., Palmer, E. E., George, M., & Fang, Y. (2020). Molecular dynamics simulation study of AG10 and tafamidis binding to the Val122Ile transthyretin variant. *Biochemistry and Biophysics Reports*, 21, 100721. <https://doi.org/10.1016/j.bbrep.2019.100721>
- Neudek, K., Kunz, T., Barth, H., & Schmidt, H. (2025). Excess A-subunits of Shiga toxin 2a are produced in enterohemorrhagic *Escherichia coli*. *Scientific Reports*, 15(1). <https://doi.org/10.1038/s41598-025-01342-2>
- Nicolau, G. O., Nigro Neto, C., Bezerra, F. J. L., Furlanetto, G., Passos, S. C., & Stahlschmidt, A. (2018). Vasodilator Agents in Pediatric Cardiac Surgery with Cardiopulmonary Bypass. *Journal of Cardiothoracic and Vascular Anesthesia*, 32(1), 412–422. <https://doi.org/10.1053/j.jvca.2017.07.007>
- Niu, L., Gao, M., Wen, S., Wang, F., Shangguan, H., Guo, Z., Zhang, R., & Ge, J. (2023). Effects of Catecholamine Stress Hormones Norepinephrine and Epinephrine on Growth, Antimicrobial Susceptibility, Biofilm Formation, and Gene Expressions of Enterotoxigenic *Escherichia coli*. *International Journal of Molecular Sciences*, 24(21), 15646. <https://doi.org/10.3390/ijms242115646>
- Odhiambo, D. O., Omosa, L. K., Njagi, E. C., Kithure, J. G., & Wekesa, E. N. (2025). In-silico pharmacokinetics ADME/Tox analysis of phytochemicals from genus *Dracaena* for their therapeutic potential. *Scientific African*, 29, e02796. <https://doi.org/10.1016/j.sciaf.2025.e02796>
- Ogura, Y., Mondal, S. I., Islam, M. R., Mako, T., Arisawa, K., Katsura, K., Ooka, T., Gotoh, Y., Murase, K., Ohnishi, M., & Hayashi, T. (2015). The Shiga toxin 2 production level in enterohemorrhagic *Escherichia coli* O157:H7 is correlated with the subtypes of toxin-encoding phage. *Scientific Reports*, 5(1), 16663. <https://doi.org/10.1038/srep16663>
- Ogura, Y., Seto, K., Morimoto, Y., Nakamura, K., Sato, M. P., Gotoh, Y., Itoh, T., Toyoda, A., Ohnishi, M., & Hayashi, T. (2018). Genomic Characterization of β -Glucuronidase–Positive *Escherichia coli* O157:H7 Producing Stx2a. *Emerging Infectious Diseases*, 24(12), 2219–2227. <https://doi.org/10.3201/eid2412.180404>

- Olayanju, J. B., Bozic, D., Naidoo, U., & Sadik, O. A. (2024). A Comparative Review of Key Isothiocyanates and Their Health Benefits. *Nutrients*, 16(6), 757. <https://doi.org/10.3390/nu16060757>
- OUABANE, M., TABTI, K., HAJJI, H., ELBOUHI, M., KHALDAN, A., ELKAMEL, K., SBAI, A., Aziz AJANA, M., SEKKATE, C., BOUACHRINE, M., & LAKHLIFI, T. (2023). Structure-odor relationship in pyrazines and derivatives: A physicochemical study using 3D-QSPR, HQSPR, Monte Carlo, molecular docking, ADME-Tox and molecular dynamics. *Arabian Journal of Chemistry*, 16(11), 105207. <https://doi.org/10.1016/j.arabjc.2023.105207>
- Pacheco, A. R., & Sperandio, V. (2012). Shiga toxin in enterohemorrhagic E.coli: regulation and novel anti-virulence strategies. *Frontiers in Cellular and Infection Microbiology*, 2. <https://doi.org/10.3389/fcimb.2012.00081>
- Palmer, T., & Bonner, P. L. (2011). The Structure of Proteins. In *Enzymes* (pp. 14–43). Elsevier. <https://doi.org/10.1533/9780857099921.1.14>
- Parker, C. T., Russell, R., Njoroge, J. W., Jimenez, A. G., Taussig, R., & Sperandio, V. (2017). Genetic and Mechanistic Analyses of the Periplasmic Domain of the Enterohemorrhagic Escherichia coli QseC Histidine Sensor Kinase. *Journal of Bacteriology*, 199(8). <https://doi.org/10.1128/JB.00861-16>
- Ramos, S., Silva, V., Dapkevicius, M. de L. E., Caniça, M., Tejedor-Junco, M. T., Igrejas, G., & Poeta, P. (2020). Escherichia coli as Commensal and Pathogenic Bacteria among Food-Producing Animals: Health Implications of Extended Spectrum β -Lactamase (ESBL) Production. *Animals*, 10(12), 2239. <https://doi.org/10.3390/ani10122239>
- Rashid, M. A., Khatib, F., & Sattar, A. (2015). *Protein preliminaries and structure prediction fundamentals for computer scientists*. <http://arxiv.org/abs/1510.02775>
- Rasko, D. A., Moreira, C. G., Li, D. R., Reading, N. C., Ritchie, J. M., Waldor, M. K., Williams, N., Taussig, R., Wei, S., Roth, M., Hughes, D. T., Huntley, J. F., Fina, M. W., Falck, J. R., & Sperandio, V. (2008). Targeting QseC Signaling and Virulence for Antibiotic Development. *Science*, 321(5892), 1078–1080. <https://doi.org/10.1126/science.1160354>
- Recio, R., Vengut-Climent, E., Borrego, L. G., Khair, N., & Fernández, I. (2017). *Biologically Active Isothiocyanates: Protecting Plants and Healing Humans* (pp. 167–242). <https://doi.org/10.1016/B978-0-444-63930-1.00006-5>
- Riyadi, P. H., Romadhon, Sari, I. D., Kurniasih, R. A., Agustini, T. W., Swastawati, F., Herawati, V. E., & Tanod, W. A. (2021). SwissADME predictions of pharmacokinetics and drug-likeness properties of small molecules present in

- Spirulina platensis*. *IOP Conference Series: Earth and Environmental Science*, 890(1), 012021. <https://doi.org/10.1088/1755-1315/890/1/012021>
- Robinson, S. W., Afzal, A. M., & Leader, D. P. (2014). Bioinformatics: Concepts, Methods, and Data. In *Handbook of Pharmacogenomics and Stratified Medicine* (pp. 259–287). Elsevier. <https://doi.org/10.1016/B978-0-12-386882-4.00013-X>
- Saeedi, P., Yazdanparast, M., Behzadi, E., Salmanian, A. H., Mousavi, S. L., Nazarian, S., & Amani, J. (2017). A review on strategies for decreasing *E. coli* O157:H7 risk in animals. *Microbial Pathogenesis*, 103, 186–195. <https://doi.org/10.1016/j.micpath.2017.01.001>
- Sangande, F., Julianti, E., & Tjahjono, D. H. (2020). Ligand-Based Pharmacophore Modeling, Molecular Docking, and Molecular Dynamic Studies of Dual Tyrosine Kinase Inhibitor of EGFR and VEGFR2. *International Journal of Molecular Sciences*, 21(20), 7779. <https://doi.org/10.3390/ijms21207779>
- Sanvictores, T., & Farci, F. (2022). *Biochemistry, Primary Protein Structure*. StatPearls Publishing. <https://www.ncbi.nlm.nih.gov/books/NBK564343/>
- Schake, P., Bolz, S. N., Linnemann, K., & Schroeder, M. (2025). PLIP 2025: introducing protein–protein interactions to the protein–ligand interaction profiler. *Nucleic Acids Research*, 53(W1), W463–W465. <https://doi.org/10.1093/nar/gkaf361>
- Schlick, Tamar. (2010). *Molecular modeling and simulation : an interdisciplinary guide*. Springer Science+Business Media, LLC. https://organical.org/modelacion/mm/Molecular_Modeling_and_Simulation__An_Interdisciplinary_Guide__Interdisciplinary_Applied_Mathematics_.pdf
- Shapovalov, M. V., & Dunbrack, R. L. (2011). A Smoothed Backbone-Dependent Rotamer Library for Proteins Derived from Adaptive Kernel Density Estimates and Regressions. *Structure*, 19(6), 844–858. <https://doi.org/10.1016/j.str.2011.03.019>
- 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>
- Soteras Gutiérrez, I., Lin, F.-Y., Vanommeslaeghe, K., Lemkul, J. A., Armacost, K. A., Brooks, C. L., & MacKerell, A. D. (2016). Parametrization of halogen bonds in the CHARMM general force field: Improved treatment of ligand–protein interactions. *Bioorganic & Medicinal Chemistry*, 24(20), 4812–4825. <https://doi.org/10.1016/j.bmc.2016.06.034>

- Sriramulu, D. K., Wu, S., & Lee, S.-G. (2020). Effect of ligand torsion number on the AutoDock mediated prediction of protein-ligand binding affinity. *Journal of Industrial and Engineering Chemistry*, 83, 359–365. <https://doi.org/10.1016/j.jiec.2019.12.009>
- Strzelecki, P., Karczewska, M., Szalewska-Pałasz, A., & Nowicki, D. (2025). Phytochemicals Controlling Enterohemorrhagic Escherichia coli (EHEC) Virulence—Current Knowledge of Their Mechanisms of Action. *International Journal of Molecular Sciences*, 26(1), 381. <https://doi.org/10.3390/ijms26010381>
- Sun, G., Yu, Z., Li, Q., Zhang, Y., Wang, M., Liu, Y., Liu, J., Liu, L., & Yu, X. (2023). Mechanism of Escherichia coli Lethality Caused by Overexpression of flhDC, the Flagellar Master Regulator Genes, as Revealed by Transcriptome Analysis. *International Journal of Molecular Sciences*, 24(18), 14058. <https://doi.org/10.3390/ijms241814058>
- Sung, S. (2015). Peptide folding driven by Van der Waals interactions. *Protein Science*, 24(9), 1383–1388. <https://doi.org/10.1002/pro.2710>
- Tarr, G. A. M., Stokowski, T., Shringi, S., Tarr, P. I., Freedman, S. B., Oltean, H. N., Rabinowitz, P. M., & Chui, L. (2019). Contribution and Interaction of Shiga Toxin Genes to Escherichia coli O157:H7 Virulence. *Toxins*, 11(10), 607. <https://doi.org/10.3390/toxins11100607>
- Torres, P. H. M., Sodero, A. C. R., Jofily, P., & Silva-Jr, F. P. (2019). Key Topics in Molecular Docking for Drug Design. *International Journal of Molecular Sciences*, 20(18), 4574. <https://doi.org/10.3390/ijms20184574>
- Udaondo, Z., Schilder, K. A., Blesa, A. R. M., Tena-Garitaonaindia, M., Mangana, J. C., & Daddaoua, A. (2025). Transcriptional Regulatory Systems in Pseudomonas: A Comparative Analysis of Helix-Turn-Helix Domains and Two-Component Signal Transduction Networks. *International Journal of Molecular Sciences*, 26(10), 4677. <https://doi.org/10.3390/ijms26104677>
- Volkamer, A., Kuhn, D., Grombacher, T., Rippmann, F., & Rarey, M. (2012). Combining Global and Local Measures for Structure-Based Druggability Predictions. *Journal of Chemical Information and Modeling*, 52(2), 360–372. <https://doi.org/10.1021/ci200454v>
- Volkamer, A., Kuhn, D., Rippmann, F., & Rarey, M. (2012). DoGSiteScorer: a web server for automatic binding site prediction, analysis and druggability assessment. *Bioinformatics*, 28(15), 2074–2075. <https://doi.org/10.1093/bioinformatics/bts310>
- Wacha, A. F., & Lemkul, J. A. (2023). charmm2gmX: An Automated Method to Port the CHARMM Additive Force Field to GROMACS. *Journal of Chemical*

Information and Modeling, 63(14), 4246–4252.
<https://doi.org/10.1021/acs.jcim.3c00860>

- Weigel, W. A., & Demuth, D. R. (2016). Qse <scp>BC</scp> , a two-component bacterial adrenergic receptor and global regulator of virulence in *Enterobacteriaceae* and *Pasteurellaceae*. *Molecular Oral Microbiology*, 31(5), 379–397. <https://doi.org/10.1111/omi.12138>
- Williams, C. J., Headd, J. J., Moriarty, N. W., Prisant, M. G., Videau, L. L., Deis, L. N., Verma, V., Keedy, D. A., Hintze, B. J., Chen, V. B., Jain, S., Lewis, S. M., Arendall, W. B., Snoeyink, J., Adams, P. D., Lovell, S. C., Richardson, J. S., & Richardson, D. C. (2018). MolProbity: More and better reference data for improved all-atom structure validation. *Protein Science : A Publication of the Protein Society*, 27(1), 293–315. <https://doi.org/10.1002/pro.3330>
- Williams, J. R., Rayburn, J. R., Cline, G. R., Sauterer, R., & Friedman, M. (2015). Effect of allyl isothiocyanate on developmental toxicity in exposed *Xenopus laevis* embryos. *Toxicology Reports*, 2, 222–227. <https://doi.org/10.1016/j.toxrep.2014.12.005>
- Wu, D., Baigalmaa, L., Yao, Y., Li, G., Su, M., Fan, L., & Morigen. (2021). The *Escherichia coli* QseB/QseC signaling is required for correct timing of replication initiation and cell motility. *Gene*, 773. <https://doi.org/10.1016/j.gene.2020.145374>
- Xie, W., Dickson, C., Kwiatkowski, W., & Choe, S. (2010). *Structure of the Cytoplasmic Segment of Histidine Kinase Receptor QseC, a Key Player in Bacterial Virulence* †. <http://www.rcsb.org/>
- Xie, X., Tu, J., You, H., & Hu, B. (2017). Design, synthesis, and biological evaluation of novel EF24 and EF31 analogs as potential IκB kinase β inhibitors for the treatment of pancreatic cancer. *Drug Design, Development and Therapy, Volume 11*, 1439–1451. <https://doi.org/10.2147/DDDT.S133172>
- Yang, J., Hediya, T. A., Chidambaram, S. B., Kaul-Ghanekar, R., & Sakharkar, M. K. (2024). Benzyl isothiocyanate as an alternative to antibiotics? a comparative in vivo study using *Pseudomonas aeruginosa* infection as a model. *PLOS ONE*, 19(5), e0303490. <https://doi.org/10.1371/journal.pone.0303490>
- Yang, Q., Zou, P., Cao, Z., Wang, Q., Fu, S., Xie, G., & Huang, J. (2021). QseC Inhibition as a Novel Antivirulence Strategy for the Prevention of Acute Hepatopancreatic Necrosis Disease (AHPND)-Causing *Vibrio parahaemolyticus*. *Frontiers in Cellular and Infection Microbiology*, 10. <https://doi.org/10.3389/fcimb.2020.594652>

- Zeng, R., Lv, C., Wang, C., & Zhao, G. (2021). Bionanomaterials based on protein self-assembly: Design and applications in biotechnology. *Biotechnology Advances*, 52, 107835. <https://doi.org/10.1016/j.biotechadv.2021.107835>
- Zhang, Y., & Skolnick, J. (2004). Scoring function for automated assessment of protein structure template quality. *Proteins: Structure, Function, and Bioinformatics*, 57(4), 702–710. <https://doi.org/10.1002/prot.20264>