

DAFTAR PUSTAKA

- Adasme, M. F., Linnemann, K. L., Bolz, S. N., Kaiser, F., Salentin, S., Haupt, V. J., & Schroeder, M. (2021). PLIP 2021: Expanding the Scope of the Protein-ligand Interaction Profiler to DNA and RNA. *Nucleic Acids Research*, 49(W1): W530-W534.
- Adedotun, I. O., Abdul-Hammed, M., Hamzat, B. A., Adepoju, A. J., Akinboade, M. W., Afolabi, T. I. & Ismail, U. T. (2022). Molecular Docking, ADMET Analysis and Bioactivity Studies of Phytochemicals from *Phyllanthus niruri* as Potential Inhibitors of Hepatitis C Virus NS5B Polymerase. *Journal of the Indian Chemical Society*, 99(2): 100321.
- Aftab, H., Ullah, S., Khan, A., Al-Rashida, M., Islam, T., Dahlous, K. A., Mohammad, S., Kashtoh, H. & Shafiq, Z. (2024). Design, Synthesis, in Vitro and in Silico Studies of Novel Piperidine Derived Thiosemicarbazones as Inhibitors of Dihydrofolate Reductase. *Scientific Reports*, 14(1): 22645.
- 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.
- Ahamed, S. T., Roy, B., Basu, U., Dutta, S., Ghosh, A. N., Bandyopadhyay, B. & Giri, N. (2019). Genomic and Proteomic Characterizations of *Sfin-1*, a Novel Lytic Phage Infecting Multidrug-resistant *Shigella* spp. and *Escherichia coli* C. *Frontiers in Microbiology*, 10: 1876.
- Ahmed, J., Khan, M. H., Unnikrishnan, S. & Ramalingam, K. (2022). Acute Hepatopancreatic Necrosis Diseases (AHPND) as Challenging Threat in Shrimp. *Biointerface Research in Applied Chemistry*, 12(1): 978-991.
- Alanazi, S. (2025). Recent Advances in Liquid Chromatography–Mass Spectrometry (LC–MS) Applications in Biological and Applied Sciences. *Analytical Science Advances*, 6(1): e70024.
- Albelwi, F. F., Abdu Mansour, H. M., Elshatanofy, M. M., El Kilany, Y., Kandeel, K., Elwakil, B. H., Hagar, M., Aouad, M. R., Ashry, E. S. H. E., Rezki, N. & El Sawy, M. A. (2022). Design, Synthesis and Molecular Docking of Novel Acetophenone-1, 2, 3-Triazoles Containing Compounds as Potent Enoyl-Acyl Carrier Protein Reductase (InhA) Inhibitors. *Pharmaceuticals*, 15(7): 799.
- Allo, V. L., Rahmah, S. & Gunawan, R. (2023). Studi Molecular Docking Senyawa Turunan sebagai Inhibitor Glikoprotein Spike Sars-Cov2. *Akta Kimia Indonesia*, 8(2): 126-137.

- Alshehri, M. A., Asiri, S. A., Helmi, N., Baeissa, H. M., Hamadi, A., Alzahrani, A., Alghamdi, R. M., Rafeeq, M. M., Alharbi, Z. M., Kamal, M. A., & Kamal, M. A. (2024). Unrevealing the Multitargeted Potency of 3-1-BCMIYPPA Against Lung Cancer Structural Maintenance and Suppression Proteins through Pharmacokinetics, QM-DFT, and Multiscale MD Simulation Studies. *Plos One*, 19(6): e0303784.
- Anissa, R. K., Lisdiana, L. & Widyayanti, A. T. (2024). Optimasi Metode Nested PCR untuk Deteksi *Vibrio parahaemolyticus* AHPND pada Udang Vaname (*Litopenaeus vannamei*). *LenteraBio*, 13(1): 1-13.
- Arivo, D. & Sjahriani, T. (2019). Isolasi, Efektivitas, dan Karakterisasi Bakteriofag Litik *Salmonella Enterica* sebagai Biokontrol Penyakit Gastroenteritis. *Mandala Of Health*, 12(2): 169-182.
- Asma, S. T., Imre, K., Morar, A., Herman, V., Acaroz, U., Mukhtar, H., Arslan-Acaroz, D., Shah, A. R. A. & Gerlach, R. (2022). An Overview of Biofilm Formation-combating Strategies and Mechanisms of Action of Antibiofilm Agents. *Life*, 12(8): 1110.
- Astuty, E. & Angkejaya, O. W. (2022). Pelatihan Sterilisasi Alat dan Bahan Medis pada Anggota Tim Bantuan Medis Vertebrae Fakultas Kedokteran Universitas Pattimura. *Society: Jurnal Pengabdian Masyarakat*, 1(5): 284-290.
- Badan Pusat Statistik. (2024). *Produksi dan Nilai Produksi Perikanan Budidaya Menurut Provinsi dan Komoditas Utama, 2022*. Diakses 30 September 2024, dari <https://www.bps.go.id>.
- Barreto, C. A., Vitorino, J. N., Reis, P. B., Machuqueiro, M., & Moreira, I. S. (2024). p K a Calculations of GPCRs: Understanding Protonation States in Receptor Activation. *Journal of Chemical Information and Modeling*, 64(17): 6850-6856.
- Binbay, F. A., Rathod, D. C., George, A. A. P., & Imhof, D. (2023). Quality Assessment of Selected Protein Structures Derived from Homology Modeling and AlphaFold. *Pharmaceuticals*, 16(12): 1662.
- Boadi, N. O., Degbevi, M., Saah, S. A., Badu, M., Borquaye, L. S., & Kortei, N. K. (2021). Antimicrobial Properties of Metal Piperidine Dithiocarbamate Complexes Against *Staphylococcus aureus* and *Candida albicans*. *Scientific African*, 12: e00846.
- Bolcato, G., Heid, E., & Bostrom, J. (2022). On the Value of Using 3D Shape and Electrostatic Similarities in Deep Generative Methods. *Journal of Chemical Information and Modeling*, 62(6): 1388-1398.

- Bugnon, M., Rohrig, U. F., Goullieux, M., Perez, M. A., Daina, A., Michielin, O., & Zoete, V. (2024). SwissDock 2024: Major Enhancements for Small-molecule Docking with Attracting Cavities and AutoDock Vina. *Nucleic Acids Research*, 52(W1): W324-W332.
- Camens, S., Liu, S., Hon, K., Bouras, G. S., Psaltis, A. J., Wormald, P. J., & Vreugde, S. (2021). Preclinical Development of a Bacteriophage Cocktail for Treating Multidrug Resistant *Pseudomonas aeruginosa* Infections. *Microorganisms*, 9(09): 2001.
- Campbell, V. M., Chouljenko, A. & Hall, S. G. (2022). Depuration of Live Oysters to Reduce *Vibrio parahaemolyticus* and *Vibrio vulnificus*: A Review of Ecology and Processing Parameters. *Comprehensive Reviews in Food Science and Food Safety*, 21(4): 3480-3506.
- Chaves-Carballo, K., Lamoureux, G. V., Perez, A. L., Cruz, A. B., & Cechinel Filho, V. (2022). Novel One-pot Synthesis of a Library of 2-aryloxy-1, 4-naphthoquinone Derivatives. *RSC advances*, 12(29): 18507-18523.
- Che, X., Chai, S., Zhang, Z., & Zhang, L. (2022). Prediction of Ligand Binding Sites using Improved Blind Docking Method with a Machine Learning-Based Scoring Function. *Chemical Engineering Science*, 261: 117962.
- Chen, G., Seukep, A. J. & Guo, M. (2020). Recent Advances in Molecular Docking for the Research and Discovery of Potential Marine Drugs. *Marine Drugs*, 18(11): 545.
- Chen, W., He, H., Wang, J., Wang, J., & Chang, C. E. A. (2023). Uncovering Water Effects in Protein-ligand Recognition: Importance in the Second Hydration Shell and Binding Kinetics. *Physical Chemistry Chemical Physics*, 25(3): 2098-2109.
- Comajuncosa-Creus, A., Jorba, G., Barril, X., & Aloy, P. (2024). Comprehensive Detection and Characterization of Human Druggable Pockets through Binding Site Descriptors. *Nature Communications*, 15(1): 7917.
- Cornelissen, F. M., Markert, G., Deutsch, G., Antonara, M., Faaij, N., Bartelink, I., Noske, D., Vandertop, W. P., Bender, A. & Westerman, B. A. (2023). Explaining Blood-brain Barrier Permeability of Small Molecules by Integrated Analysis of Different Transport Mechanisms. *Journal of Medicinal Chemistry*, 66(11): 7253-7267.
- Dong, C. L., Wu, T., Dong, Y., Qu, Q. W., Chen, X. Y., & Li, Y. H. (2024). Exogenous Methionine Contributes to Reversing the Resistance of *Streptococcus suis* to Macrolides. *Microbiology Spectrum*, 12(2): e02803-23.

- Elafify, M., Chen, J., Abdelkhalek, A., Elsherbini, M., Al-Ashmawy, M., & Koseki, S. (2020). Combined D-Tryptophan Treatment and Temperature Stress Exert Antimicrobial Activity Against *Listeria monocytogenes* in Milk. *Journal of Food Protection*, 83(4): 644-650.
- Elafify, M., Sadoma, N. M., Abd El Aal, S. F., Bayoumi, M. A., & Ahmed Ismail, T. (2022). Occurrence and D-Tryptophan Application for Controlling the Growth of Multidrug-resistant Non-o157 Shiga Toxin-producing *Escherichia coli* in Dairy Products. *Animals*, 12(7): 922.
- Elvira, F. A., Sedas, V. T. P., Herrera, D. M., Castro, R. Q., Ros, R. M. O., Hernandez, K. L., Primo, A. F. & Elvira, K. R. (2020). Comparative Survival and the Cold-Induced Gene Expression of Pathogenic and Nonpathogenic *Vibrio parahaemolyticus* from Tropical Eastern Oysters During Cold Storage. *International Journal of Environmental Research and Public Health*, 17(6): 1836.
- Fan, J., Fu, A. & Zhang, L. (2019). Progress in Molecular Docking. *Quantitative Biology*, 7: 83-89.
- Fatmawati, Y., Sandrina, S., Aina, R. N. & Narulita, E. (2022). Molecular Docking Analysis of Seagrass (*Enhalus acoroides*) Phytochemical Compounds as an Antidiabetic. *Journal of Biological Research*, 95: 1224.
- Fikadu, A., Amankwah, S., Alemu, B., Alemu, Y., Naga, A., Tekle, E. & Kassa, T. (2024). Isolation and Phenotypic Characterization of Virulent Bacteriophages Against Multidrug-Resistant *Escherichia coli* and its Phage-Resistant Variant from Sewage Sources. *Infection and Drug Resistance*, 293-303.
- Flegel, T. W. (2019). A Future Vision for Disease Control in Shrimp Aquaculture. *Journal of the World Aquaculture Society*, 50(2): 249-266.
- Fondjo, S. E., Njoya, A. S., Tamokou, J. D. D., Doungmo, G., Ndjakou Lenta, B., Simon, P. F., Tsopmo, A. & Kuiate, J. R. (2022). Synthesis, Characterization and Antimicrobial Properties of Two Derivatives of Pyrrolidine-2, 5-dione Fused at Positions-3, 4 to a Dibenzobarrelene Backbone. *BMC chemistry*, 16(1): 8.
- Franswinsly, B., & Savira, M. (2023). Isolasi Bakteriofag dari Limbah Cair dengan Aktivitas Litik terhadap *Escherichia coli*. *Jurnal Kedokteran Syiah Kuala*, 23(1).
- Frimayanti, N., Lukman, A. & Nathania, L. (2021). Studi Molecular Docking Senyawa 1,5-benzothiazepine sebagai Inhibitor Dengue DEN-2 NS2B/NS3 Serine Protease. *Chempublish Journal*, 6(1): 54-62.

- Gagandeep, K. R., Narasingappa, R. B., & Vyas, G. V. (2024). Unveiling Mechanisms of Antimicrobial Peptide: Actions Beyond the Membranes Disruption. *Heliyon*, 10(19).
- Ghazali, T. M., Sitinjak, F. R. & Simanullang, W. (2020). Deskripsi dan Komposisi Kimia Daging dan Karapas Udang Rama-rama (*Thalassina anomala*). *Jurnal Perikanan dan Kelautan*, 25(2): 138-144.
- Giebultowicz, J., Kucharski, D., Nalecz-Jawecki, G., Skowronek, A., Strzelecka, A., Maciag, L., & Drzewicz, P. (2025). Factors Affecting Distribution of Pharmaceutically Active Compounds in Bottom Sediments of Odra River Estuary (SW Baltic Sea). *Molecules*, 30(19): 3935.
- Gluge, J., Escher, B. I., & Scheringer, M. (2023). How Error-prone Bioaccumulation Experiments Affect the Risk Assessment of Hydrophobic Chemicals and What Could be Improved. *Integrated Environmental Assessment and Management*, 19(3): 792-803.
- Gomez-Regalado, M. D. C., M., Martin, J., Santos, J. L., Aparicio, I., Alonso, E., & Zafra-Gomez, A. (2023). Bioaccumulation/bioconcentration of Pharmaceutical Active Compounds in Aquatic Organisms: Assessment and Factors Database. *Science of the Total Environment*, 861: 160638.
- Hahn, D. F., Bayly, C. I., Bobby, M. L., Macdonald, H. E. B., Chodera, J. D., Gapsys, V., Mey, A. S. J. S., Mobley, D. L., Benito, L. P., Schindler, C. E. M., Tresadern, G., & Warren, G. L. (2022). Best Practices for Constructing, Preparing, and Evaluating Protein-ligand Binding Affinity Benchmarks [Article v1. 0]. *Living journal of computational molecular science*, 4(1): 1497.
- Hetta, H. F., Sirag, N., Alsharif, S. M., Alharbi, A. A., Alkindy, T. T., Alkhamali, A., Albalawi, A. S., Ramadan, Y. S., Rashed, Z. I. & Alanazi, F. E. (2024). Antimicrobial Peptides: The Game-changer in the Epic Battle Against Multidrug-resistant Bacteria. *Pharmaceuticals*, 17(11): 1555.
- Hornberger, K. R., & Araujo, E. M. (2023). Physicochemical Property Determinants of Oral Absorption for PROTAC Protein Degraders. *Journal of Medicinal Chemistry*, 66(12): 8281-8287.
- Huyyirnah, H. & Fitriyani, F. (2020). Metode Penyimpanan Bakteri *Vibrio alginolitycus* dan *Vibrio harveyi* dalam Media TSB (*Tryptic Soy Broth*) Dan Gliserol. *Integrated Lab Journal*, 8(2): 91-101.
- Ismael, N. M., Azzam, M., Abdelmoteleb, M., & El-Shibiny, A. (2024). Phage vB_Ec_ZCEC14 to Treat Antibiotic-resistant *Escherichia coli* Isolated from Urinary Tract Infections. *Virology Journal*, 21(1): 44.

- Jakubec, D., Skoda, P., Krivak, R., Novotny, M., & Hoksza, D. (2022). PrankWeb 3: Accelerated Ligand-binding Site Predictions for Experimental and Modelled Protein Structures. *Nucleic Acids Research*, 50(W1): W593-W597.
- Jatmiko, Y. D., Purwanto, A. P., & Ardyati, T. (2018). Uji aktivitas bakteriofage litik dari limbah rumah tangga terhadap *Salmonella Typhi*. *Jurnal biodjati*, 3(2): 134-147.
- Javed, M. R., Salman, M., Tariq, A., Tawab, A., Zahoor, M. K., Naheed, S., Shahid, M., Ijaz, A. & Ali, H. (2022). The Antibacterial and Larvicidal Potential of Bis-(2-ethylhexyl) Phthalate from *Lactiplantibacillus plantarum*. *Molecules*, 27(21): 7220.
- Jitsuhiro, A., Maeda, T., Ogawa, A., Yamada, S., Konoeda, Y., Maruyama, H., Endo, F., Kitagawa, M., Tanimoto, K., Hotta, A. & Tsuji, T. (2024). Contact-killing Antibacterial Polystyrene Polymerized using a Quaternized Cationic Initiator. *ACS omega*, 9(8): 9803-9812.
- Kaddah, M. M., El Demellawy, M. A., & Talaat, W. (2025). Comprehensive Analytical Approaches: The Use of LC-MS and LC-MS in Modern Pharmaceutical and Biomedical Sciences. *Microchemical Journal*: 114780.
- Kajal, G., Sangita, A. & Rajan, W. (2021). Isolation and Study of Bacteriophage of Citrus Cancer Causing Bacterial Pathogen. *Journal of Life Sciences*, 9(2): 175-180.
- Kasman, L. M., & Porter, L. D. (2022). Bacteriophages. Diakses 07 Januari 2026, dari https://www.ncbi.nlm.nih.gov/books/NBK493185/?utm_source.
- Kattoub, R. G., Sliman, F., & Kousara, M. (2021). Development of Novel Benzimidazole Derivates as Potent and Selective Akt Kinase Inhibitors Using In-silico Approaches. *International Journal of Organic Chemistry*, 11(3): 106-127.
- Kementerian Kelautan dan Perikanan. (2023). *Indonesia Gandeng ADB untuk Tingkatkan Produksi Udang Nasional*. Diakses 30 September 2024, dari <https://www.kkp.go.id/djpb/indonesia-gandeng-adb-untuk-tingkatkan-produksi-udang-nasional65c2fe8b71111/detail.html>.
- Kementerian Kelautan dan Perikanan. (2023). *KKP Siap Berkolaborasi dengan K/L Lain Genjot Produksi Udang di 2024*. Diakses 30 September 2024, dari <https://kkp.go.id/news/news-detail/kkp-siap-berkolaborasi-dengan-kl-lain-genjot-produksi-udang-di-202465c1924c13a3e.html>.
- Kementerian Kelautan dan Perikanan. (2023). *Profil Pasar Udang*. Jakarta: Direktorat Jenderal Penguatan Daya Saing Produk Kelautan dan Perikanan.

- Khusnah, A., Satyantini, W. H. & Amin, M. (2023). Studi Perbandingan Histopatologi Udang Vaname yang Terinfeksi *Vibrio parahaemolyticus* dari Tiga Tambak Berbeda. *Jurnal Grouper*, 14(2): 144-151.
- Korlepara, D. B., Vasavi, C. S., Jeurkar, S., Pal, P. K., Roy, S., Mehta, S., Sharma, S., Kumar, V., Muvva, C., Sridharan, B., Garg, A., Modee, R., Bhati, A. P., Nayar, D., & Priyakumar, U. D. (2022). Plas-5k: Dataset of Protein-ligand Affinities from Molecular Dynamics for Machine Learning Applications. *Scientific Data*, 9(1): 548.
- Kralj, S., Jukic, M., & Bren, U. (2023). Molecular Filters in Medicinal Chemistry. *Encyclopedia*, 3(2): 501-511.
- Krivak, R., & Hoksza, D. (2018). P2Rank: Machine Learning Based Tool for Rapid and Accurate Prediction of Ligand Binding Sites from Protein Structure. *Journal of Cheminformatics*, 10(1): 39.
- Kumar, R., Ng, T. H. & Wang, H. C. (2020). Acute Hepatopancreatic Necrosis Disease in Penaeid Shrimp. *Reviews in Aquaculture*, 12(3): 1867-1880.
- Kumar, V., Roy, S., Behera, Bossier, P. & Das, B. K. (2021). Acute Hepatopancreatic Necrosis Disease (AHPND): Virulence, Pathogenesis and Mitigation Strategies in Shrimp Aquaculture. *Toxins*, 18(8).
- Kurniawan, I. H. (2023). *Pemeliharaan Larva Udang Vannamei (Litopenaeus vannamei) dengan genetika Berbeda di CV. Manunggal Rasa*. Skripsi, Teknologi Pembenihan Ikan, Politeknik Negeri Lampung, Lampung.
- Kusuma, J., Wahyudi, A., Abdullah, M. K., Hasan, A. Z., Asrowardi, I., & Tahir, M. (2025). Diversity of the Non-targeted Metabolomic Data Across Various Varieties of Cloves (*Syzygium* spp.). *Data in Brief*, 58: 111237.
- Li, H., Fu, S., Wang, Y., Yuan, X., Liu, L., Dong, H., Wang, Q. & Zhang, Z. (2021). Antimicrobial and Antitumor Activity of Peptidomimetics Synthesized from Amino Acids. *Bioorganic chemistry*, 106: 104506.
- Li, J., Liu, J., Fu, K., Qin, K., Wu, C., Yu, X., Zhou, S. & Zhou, L. (2020). Rapid Identification and Detection of *Vibrio parahaemolyticus* Via Different Types of Modus Operandi with LAMP Method in Vivo. *Annals of Microbiology*, 70: 1-15.
- Liang, S., Qi, Y., Yu, H., Sun, W., Raza, S. H. A., Alkhorayef, N., Alkhalil, S. S., Salama, E. E. A. & Zhang, L. (2023). Bacteriophage Therapy as an Application for Bacterial Infection in China. *Antibiotics*, 12(2): 417.
- Lingga, R. & Budiarti, S. (2023). Bacteriophage and its Potential Application in Wastewater Treatment. *Tropical Microbiome*, 1(1): 25-34.

- Liu, J., Zhang, K., Song, J., Wu, H., Hao, H., Bi, J., Hou, J. & Zhang, G. (2021). Bacteriostatic Effects of Benzyl Isothiocyanate on *Vibrio parahaemolyticus*: Transcriptomic Analysis and Morphological Verification. *BMC Biotechnology*, 21: 1-10.
- Liu, Y., Yang, X., Gan, J., Chen, S., Xiao, Z. X., & Cao, Y. (2022). CB-Dock2: Improved Protein-ligand Blind Docking by Integrating Cavity Detection, Docking and Homologous Template Fitting. *Nucleic acids research*, 50(W1): W159-W164.
- Liu, Y., Yu, Y., Li, S., Sun, M. & Li, F. (2023). Comparative Transcriptomic Analysis of Gill Reveals Genes Belonging to mTORC1 Signaling Pathway Associated with the Resistance Trait of Shrimp to VPAHPND. *Frontiers in Immunology*, 14: 1150628.
- Lubis, A. R. A. (2024). *Deteksi Molekuler Acute Hepatopancreatic Necrosis Disease (AHPND) pada Komoditas Udang Vannamei (Litopenaeus Vannamei) di Sumatera Utara*. Skripsi, Biologi, Universitas Sumatera Utara, Sumatera Utara.
- Lubkowska, B., Czajkowska, E., Stodolna, A., Sroczynski, M., Zylicz-Stachula, A., Sobolewski, I. & Skowron, P. M. (2023). A Novel Thermostable TP-84 Capsule Depolymerase: A Method for Rapid Polyethyleneimine Processing of a Bacteriophage-expressed Proteins. *Microbial Cell Factories*, 22(1): 80.
- Ma, S. B., Liu, L., Li, X., Xie, Y. H., Shi, X. P., & Wang, S. W. (2023). Virtual Screening-molecular Docking-activity Evaluation of *Ailanthus altissima* (Mill.) Swingle Bark in the Treatment of Ulcerative Colitis. *BMC Complementary Medicine and Therapies*, 23(1): 197.
- Ma, Z., Ajibade, A., & Zou, X. (2024). Docking Strategies for Predicting Protein-ligand Interactions and Their Application to Structure-based Drug Design. *Communications in Information and Systems*, 24(3): 199.
- Mardirossian, M., Sola, R., Beckert, B., Collis, D. W. P., Stasi, A. D., Armas, F., Hilpert, K., Wilson, D. N. & Scocchi, M. (2020). Proline-Rich Peptides with Improved Antimicrobial Activity against *E. coli*, *K. pneumoniae*, and *A. baumannii*. *ChemMedChem*, 14(24): 2025-2033.
- Margiotto, E., van der Lubbe, S. C., de Azevedo Santos, L., Paragi, G., Moro, S., Bickelhaupt, F. M., & Fonseca Guerra, C. (2020). Halogen Bonds in Ligand-protein Systems: Molecular Orbital Theory for Drug Design. *Journal of Chemical Information and Modeling*, 60(3): 1317-1328.
- Maruyama, H., Kishi, A., Konoeda, Y., Ito, H., & Tsuji, T. (2024). Antibacterial, Transparency, and Mechanical Properties of Cationic Radical Initiator Triggered Polystyrene Sheets Obtained by Thermal Blending. *Polymers*, 16(22): 3167.

- McGibbon, M., Money-Kyrle, S., Blay, V., & Houston, D. R. (2023). SCORCH: Improving Structure-based Virtual Screening with Machine Learning Classifiers, Data Augmentation, and Uncertainty Estimation. *Journal of Advanced Research*, 46: 135-147.
- McNutt, A. T., Bisiriyu, F., Song, S., Vyas, A., Hutchison, G. R., & Koes, D. R. (2023). Conformer Generation for Structure-based Drug Design: How Many and How Good?. *Journal of Chemical Information and Modeling*, 63(21): 6598-6607.
- McNutt, A. T., Francoeur, P., Aggarwal, R., Masuda, T., Meli, R., Ragoza, M., Sunseri, J., & Koes, D. R. (2021). GNINA 1.0: Molecular Docking with Deep Learning. *Journal of Cheminformatics*, 13(1): 43.
- Mobitz, H. (2024). Design Principles for Balancing Lipophilicity and Permeability in Beyond Rule of 5 Space. *ChemMedChem*, 19(5): e202300395.
- Moghimani, M., Noori, S. M. A., Afshari, A., & Hashemi, M. (2024). D-Tryptophan, an Eco-friendly Natural, Safe, and Healthy Compound with Antimicrobial Activity Against Food-borne Pathogens: A Systematic Review. *Food Science & Nutrition*, 12(5): 3068-3079.
- Moses, S., Aftalion, M., Mamroud, E., Rotem, S., & Steinberger-Levy, I. (2021). Reporter-Phage-Based Detection and Antibiotic Susceptibility Testing of *Yersinia pestis* for a Rapid Plague Outbreak Response. *Microorganisms*, 9(6): 1278.
- Mulyaningsih, S. N. (2022). *Perbandingan Efektivitas Ekstrak Akar, Batang, dan Daun Mangrove Rhizophora apiculata (Tomlinson, 1986) dalam Menghambat Vibrio parahaemolyticus Penyebab Penyakit Udang Vaname (Litopenaeus vannamei) (Boone, 1931)*. Skripsi, Budidaya Perairan, Universitas Lampung, Lampung.
- Nasser, A., Azizian, R., Tabasi, M., Khezerloo, J. K., Heravi, F. S., Kalani, M. T., Sadeghifard, N., Amini, R., Pakzad, I., Radmanesh A. & Jalilian, F. A. (2019). Specification of Bacteriophage Isolated Against Clinical Methicillin-resistant *Staphylococcus aureus*. *Osong Public Health and Research Perspectives*, 10(1): 20.
- Nasrolloh, A. (2022). *Pembesaran Udang Vaname (Litopenaeus vannamei) pada Fase Blind Feeding*. Tesis, Agrikultur, Politeknik Negeri Lampung, Lampung.
- Nendza, M., Kosfeld, V., & Schlechtriem, C. (2025). Consolidated Octanol/water Partition Coefficients: Combining Multiple Estimates from Different Methods to Reduce Uncertainties in Log K_{ow}. *Environmental Sciences Europe*, 37(1): 44.

- Ni, P., Wang, L., Deng, B., Jiu, S., Ma, C., Zhang, C., Almeida, A., Wang, D., Xu, W. & Wang, S. (2021). Characterization of a Lytic Bacteriophage Against *Pseudomonas syringae* pv. *actinidiae* and its Endolysin. *Viruses*, 13(4): 631.
- Nikolich, M. P. & Filippov, A. A. (2020). Bacteriophage Therapy: Developments and Directions. *Antibiotics*, 9(3): 135.
- Nugraha, A., Yustiati, A. & Andriani, Y. (2022). Pembesaran Udang Vannamei pada Berbagai Sistem Akuakultur: Telaah Pustaka. *Jurnal of Fish Nutrition*, 2(1): 26-36.
- Ononamadu, C. J., & Ibrahim, A. (2021). Molecular Docking and Prediction of ADME/Drug-likeness Properties of Potentially Active Antidiabetic Compounds Isolated from Aqueous-methanol Extracts of *Gymnema sylvestre* and *Combretum micranthum*. *BioTechnologia*, 102(1): 85.
- Paggi, J. M., Pandit, A., & Dror, R. O. (2024). The Art and Science of Molecular Docking. *Annual Review of Biochemistry*, 93(1): 389-410.
- Pazhani, G. P., Chowdhury, G. & Ramamurthy, T. (2021). Adaptations of *Vibrio parahaemolyticus* to Stress During Environmental Survival, Host Colonization, and Infection. *Frontiers in Microbiology*, 12: 737299.
- Peng, J., Qiu, S., Jia, F., Zhang, L., He, Y., Zhang, F., Sun, M., Deng, Y., Guo, Y., Xu, Z., Liang, X., Yan, W. & Wang, K. (2021). The Introduction of L-Phenylalanine Into Antimicrobial Peptide Protonectin Enhances the Selective Antibacterial Activity of its Derivative phe-Prt Against Gram-positive Bacteria. *Amino Acids*, 53(1): 23-32.
- Poyraz, S., Dondaş, H. A., Dondaş, N. Y., & Sansano, J. M. (2023). Recent Insights about Pyrrolidine Core Skeletons in Pharmacology. *Frontiers in Pharmacology*, 14: 1239658.
- Pratiwi, R. H. (2021). Virus Bakteri sebagai Terapi untuk Penyakit Infeksi. *Jurnal Pendidikan Biologi dan Sains*, 4(2): 193-204.
- Putri, A. N., Fakih, T. M. & Mulyanti, D. (2022). Uji Aktivitas In Silico Senyawa Turunan Flavonoid sebagai Antiviral (HIV). *Bandung Conference Series: Pharmacy*, 2(2): 1-4.
- Qodriyah, N. L., Meilina, L., & Jannah, M. (2025). Potensi Bakteriofag sebagai biokontrol Kasus Resistensi Antibiotik pada Budidaya Udang di Indonesia. *Journal of Food Industrial Technology*, 2(2), 60-67.
- Rajak, P., & Ganguly, A. (2023). The Ligand-docking Approach Explores the Binding Affinity of PFOS and PFOA for Major Endogenous Antioxidants: A Potential Mechanism to Fuel Oxidative Stress. *Sustainable Chemistry for the Environment*, 4: 100047.

- Ramadani, M. F., Salsabila, S., Ratna, M., Iskandar, A. S., Hajirah, R. N., Azani, S. A. & Putri, N. E. (2023). *Teknik Budidaya Udang Vaname Skala Super Intensif*. Makassar: Perpustakaan Universitas Negeri Makassar.
- Rivaldi, M., Frediansyah, A., Aziz, S. A. A., & Nugroho, A. P. (2025). Active Biomonitoring of Stream Ecosystems: Untargeted Metabolomic and Proteomic Responses and Free Radical Scavenging Activities in Mussels. *Ecotoxicology*, 1-19.
- Ruswahyuni, A. H. & Rudiyaniti, S. (2010). Aplication of Chitosan for Water Quality and Macrobenthic Fauna Rehabilitation in Vannamei Shrimps (*Litopenaeus Vannamei*) Ponds, North Coast of Semarang, Central Java-Indonesia. *Journal of Coastal Development*, 14(1): 1-10.
- Sabino, J., Hirten, R. P. & Colombel, J. F. (2020). Review Article: Bacteriophages in Gastroenterology from Biology to Clinical Applications. *Alimentary Pharmacology and Therapeutics*, 51(1): 53-63.
- Samir, S., El-Far, A., Okasha, H., Mahdy, R., Samir, F. & Nasr, S. (2022). Isolation and Characterization of Lytic Bacteriophages from Sewage at an Egyptian Tertiary Care Hospital Against Methicillin-Resistant *Staphylococcus aureus* Clinical Isolates. *Saudi Journal of Biological Sciences*, 29(5): 3097-3106.
- Sarkar, C., Abdalla, M., Mondal, M., Khalipha, A. B. R., & Ali, N. (2022). Ebselen Suitably Interacts with the Potential SARS-CoV-2 Targets: an in-silico Approach. *Journal of Biomolecular Structure and Dynamics*, 40(22): 12286-12301.
- Schoch, C. L., Ciufo, S., Domrachev, M., Hottton, C. L., Kannan, S., Khovanskaya, R., Leipe, D., Mcveigh, R., O'Neill, K., Robbertse, B., Sharma, S., Soussov, V., Sullivan, J. P., Sun, L., Turner, S. & Karsch-Mizrachi, I. (2020). NCBI Taxonomy: a Comprehensive Update on Curation, Resources and Tools. *The Journal of Biological Databases and Curation*, 1-21.
- Shamsian, S., Sokouti, B., & Dastmalchi, S. (2023). Benchmarking Different Docking Protocols for Predicting the Binding Poses of Ligands Complexed with Cyclooxygenase Enzymes and Screening Chemical Libraries. *BiolImpacts: BI*, 14(2): 29955.
- Sharma, L., Nagpal, R., Jackson, C. R., Patel, D. & Singh, P. (2021). Antibiotic-Resistant Bacteria and Gut Microbiome Communities Associated with Wild-Caught Shrimp from the United States Versus Imported Farm-Raised Retail Shrimp. *Scientific Reports*, 11(1): 3356.
- Shen, F., Wang, L., Chen, R., Li, W., Li, Y., Feng, Y., Lu, T., Caminati, W., Lesarri, A., & Feng, G. (2025). Unraveling the S-S $\cdots$ π Interactions in Furan-Disulfide Heterodimers: Insights from Microwave Spectroscopy and Ab

- initio Computations. *Physical Chemistry Chemical Physics*, 27(28): 20802-20809.
- Shutter, M. C., & Akhondi, H. (2023). Tetracycline. Diakses 07 Januari 2026, dari https://www.ncbi.nlm.nih.gov/sites/books/NBK549905/?utm_source.
- Smulek, W., & Kaczorek, E. (2022). Factors Influencing the Bioavailability of Organic Molecules to Bacterial Cells-a Mini-Review. *Molecules*, 27(19): 6579.
- Sobanska, A. W. (2022). Affinity of Compounds for Phosphatidylcholine-Based Immobilized Artificial Membrane-A Measure of Their Bioconcentration in Aquatic Organisms. *Membranes*, 12(11): 1130.
- Sofia, S. & Elviantari, A. (2024). Isolasi Bakteri pada Ekor Lobster Pasir (*Panilius homarus*) di Daerah Plampang, Sumbawa NTB. *SATONDA: Journal of Tropical Bioresources and Biotechnology*, 1(1): 13-16.
- Song, M., Hua, Y., Liu, Y., Xiao, X., Yu, H., & Deng, X. (2023). Design, Synthesis, and Antimicrobial Activity Evaluation of Ciprofloxacin-Indole Hybrids. *Molecules*, 28(17): 6325.
- Soto-Rodriguez, S. A., Lozano-Olvera, R., Ramos-Clamont Montfort, G., Zenteno, E., Sanchez-Salgado, J. L., Vibanco-Perez, N. & Aguilar Rendon, K. G. (2022). New Insights Into the Mechanism of Action of PirAB from *Vibrio Parahaemolyticus*. *Toxins*, 14(4): 243.
- Spasov, D. S. (2024). Binding Affinity Determination in Drug Design: Insights from Lock and Key, Induced Fit, Conformational Selection, and Inhibitor Trapping Models. *International Journal of Molecular Sciences*, 25(13): 7124.
- Sravika, N., Priya, S., Divya, N., Jyotsna, P. M. S., Anusha, P., Kudumula, N., & Bai, S. A. (2021). Swiss ADME Properties Screening of the Phytochemical Compounds Present in *Bauhinia acuminata*. *Journal of Pharmacognosy and Phytochem*, 10(4): 411-419.
- Sun, F., Liu, J., Tariq, A., Wang, Z., Wu, Y., & Li, L. (2023). Unraveling the Mechanism of Action of Cepharanthine for the Treatment of Novel Coronavirus Pneumonia (COVID-19) from the Perspectives of Systematic Pharmacology. *Arabian Journal of Chemistry*, 16(6): 104722.
- Sun, Q. (2022). The Hydrophobic Effects: Our Current Understanding. *Molecules*, 27(20): 7009.
- Supriadi, A., Ridhowati, S., Saputra, D., & Lestari, S. D. (2025). Untargeted Metabolomics Profiling for the Geographical Authentication of Traditional Pempek Using High-Resolution Orbitrap Mass Spectrometry. *Food Chemistry Advances*, 100914.

- Suryana, A., Asih, E. N. N. & Insafitri. (2023). Fenomena Infeksi Acute Hepatopancreatic Necrosis Disease pada Budidaya Udang Vaname di Kabupaten Bangkalan. *Journal of Marine Research*, 12(2): 212-220.
- Syamsuddin, H. S. A., Bimantara, A. & Susanti, D. (2023). Deteksi *Acute Hepatopancreatic Necrosis Disease* (AHPND) pada udang putih (*Litopenaeus vannamei*) dan air tambak dengan metode Nested PCR. *Prosiding Seminar Nasional Penelitian dan Pengabdian Kepada Masyarakat* (166-173). Yogyakarta: LPPM Universitas Aisyiyah Yogyakarta.
- Tan, C. W., Rukayadi, Y., Hasan, H., Abdul-Mutalib, N. A., Jambari, N. N., Hara, H., Thung, T. Y., Lee, E. & Radu, S. (2021). Isolation and Characterization of Six *Vibrio parahaemolyticus* Lytic Bacteriophages from Seafood Samples. *Front Microbiol* 12: 616548.
- Taylor, M., & Ho, J. (2023). MM/GBSA Prediction of Relative Binding Affinities of Carbonic Anhydrase Inhibitors: Effect of Atomic Charges and Comparison with Autodock4Zn. *Journal of Computer-Aided Molecular Design*, 37(4): 167-182.
- Tayyebi, A., Alshami, A. S., Rabiei, Z., Yu, X., Ismail, N., Talukder, M. J., & Power, J. (2023). Prediction of Organic Compound Aqueous Solubility using Machine Learning: a Comparison Study of Descriptor-based and Fingerprints-based Models. *Journal of Cheminformatics*, 15(1): 99.
- Telli, A. E. & Dogruer, Y. (2019). Discrimination of Viable and Dead *Vibrio parahaemolyticus* Subjected to Low Temperatures using Propidium Monoazide-Quantitative Loop Mediated Isothermal Amplification (PMA-qLAMP) and PMA-qPCR. *Microbial Pathogenesis*, 132: 109-116.
- Tian, F., Li, J., Hu, Y., Zhao, F., Ren, H., Pan, Q., Nazir, A., Li, F., & Tong, Y. (2022). Characterization and Complete Genome Sequence Analysis of a Newly Isolated phage Against *Vibrio parahaemolyticus* from Sick Shrimp in Qingdao, China. *PLoS One*, 17(5): e0266683.
- Tsugami, Y., Nii, T., & Isobe, N. (2023). Valine Treatment Enhances Antimicrobial Component Production in Mammary Epithelial Cells and the Milk of Lactating Goats without Influencing the Tight Junction Barrier. *Journal of Mammary Gland Biology and Neoplasia*, 28(1): 3.
- Turovika, Y. B. (2022). *Performa Pertumbuhan dan Kelulushidupan Udang Vaname (Litopenaeus vannamei) (Boone, 1931) yang Dipelihara pada Salinitas Berbeda*. Skripsi, Budidaya Perairan, Universitas Lampung, Lampung.
- Ugurlu, S. Y., McDonald, D., Lei, H., Jones, A. M., Li, S., Tong, H. Y., Butler, M. S., & He, S. (2024). Cobdock: an Accurate and Practical Machine Learning-

based Consensus Blind Docking Method. *Journal of Cheminformatics*, 16(1): 5.

- Ukonu, C. U. & Alagamba, E. A. (2023). In silico Anticancer Assessment of the Bioactive Compounds of *Afromomium Melengueta* on HER2 Protein Associated with Breast Cancer. *International Journal of Women in Technical Education and Employment*, 4(2): 1-15.
- Utami, D., Syahputra, R. & Widyaningsih, W. (2022). Studi Docking Molekular Aktivitas Panghambatan Enzim Tirosinase Ubi Jalar (*Ipomoea batatas* L. Lam). *Pharmacon: Jurnal Farmasi Indonesia*, 19(1): 21-34.
- Utges, J. S., & Barton, G. J. (2024). Comparative Evaluation of Methods for the Prediction of Protein-ligand Binding Sites. *Journal of Cheminformatics*, 16(1): 126.
- Vaishnav, N., Khare, N., Katariya, P. K. & Jha, A. K. (2020). To Study the Effect of Harmine Against DNMT1 for the Treatment of Cervical Cancer Through Molecular Docking Studies. *International Journal of Pharmacy and Biological Science*, 10(3): 125-132.
- Valdes-Pena, M. A., Ratchford, A., Nie, M., Schnabel, L. V., & Pierce, J. G. (2024). Pyrrolidine-2, 3-diones: Heterocyclic Scaffolds that Inhibit and Eradicate *S. aureus* Biofilms. *Chemical Communications*, 60(81): 11540-11543.
- Venturini, C., Petrovic Fabijan, A., Fajardo Lubian, A., Barbirz, S. & Iredell, J. (2022). Biological Foundations of Successful Bacteriophage Therapy. *EMBO Molecular Medicine*, 14(7): e12435.
- Verteramo, M. L., Ignjatovic, M. M., Kumar, R., Wernersson, S., Ekberg, V., Wallerstein, J., Carlstrom, G., Chadimova, V., Leffler, H., Zatterberg, F., Logan, D. T., Ryde, U., Akke, M., & Nilsson, U. J. (2024). Interplay of Halogen Bonding and Solvation in Protein-ligand Binding. *Isience*, 27(4): 109636.
- Vinod, S. M., Murugan Sreedevi, S., Krishnan, A., Ravichandran, K., Karthikeyan, P., Kotteswaran, B., & Rajendran, K. (2023). Complexity of the Role of Various Site-specific and Selective Sudlow Binding Site Drugs in the Energetics and Stability of the Acridinedione Dye-bovine Serum Albumin Complex: A Molecular Docking Approach. *ACS Omega*, 8(6): 5634-5654.
- Voitsitskyi, T., Bdzhola, V., Stratiichuk, R., Koleiev, I., Ostrovsky, Z., Vozniak, V., Khropachov, I., Henitsoi, P., Popryho, L., Zhytar, R., Yesylevskyy, S., Nafiiev, A., & Starosyla, S. (2024). Augmenting a Training Dataset of the Generative Diffusion Model for Molecular Docking with Artificial Binding Pockets. *RSC advances*, 14(2): 1341-1353.

- Vural, O., & Jololian, L. (2025). Machine Learning Approaches for Predicting Protein-ligand Binding Sites from Sequence Data. *Frontiers in Bioinformatics*, 5: 1520382.
- Wally, A. D., Pribadi, E. S., & Setyaningsih, S. (2021). Bakteriofag Spesifik *Escherichia coli* yang Diisolasi dari Berbagai Sumber Air di Bogor Tengah, Kota Bogor sebagai Antibiotika Alternatif. *Jurnal Biologi Udayana*, 25(2): 183-188.
- Wang, Y., Sun, K., Li, J., Guan, X., Zhang, O., Bagni, D., Zhang, Y., Carlson, H. A., & Head-Gordon, T. (2025). A Workflow to Create a High-quality Protein-Ligand Binding Dataset for Training, Validation, and Prediction Tasks. *Digital Discovery*, 4(5): 1209-1220.
- Welch, N. G., Li, W., Hossain, M. A., Separovic, F., O'Brien-Simpson, N. M. & Wade, J. D. (2020). (Re)Defining the Proline-Rich Antimicrobial Peptide Family and the Identification of Putative New Members. *Front Chem*, 8:607769.
- Wlodawer, A. (2017). Stereochemistry and Validation of Macromolecular Structures. *Protein Crystallography: Methods and Protocols*, 595-610.
- Wong, F., Krishnan, A., Zheng, E. J., Stärk, H., Manson, A. L., Earl, A. M., Jaakkola, T., & Collins, J. J. (2022). Benchmarking AlphaFold-enabled Molecular Docking Predictions for Antibiotic Discovery. *Molecular Systems Biology*, 18(9): e11081.
- Wu, K., Kwon, S. H., Zhou, X., Fuller, C., Wang, X., Vadgama, J., & Wu, Y. (2024). Overcoming Challenges in Small-molecule Drug Bioavailability: A Review of Key Factors and Approaches. *International Journal of Molecular Sciences*, 25(23): 13121.
- Wu, N., Zhang, R., Peng, X., Fang, L., Chen, K., & Jestila, J. S. (2024). Elucidation of Protein-ligand Interactions by Multiple Trajectory Analysis Methods. *Physical Chemistry Chemical Physics*, 26(8): 6903-6915.
- Wu, S., Ji, J., Sheng, L., Ye, Y., Zhang, Y., & Sun, X. (2024). Lysine and Valine Weaken Antibiotic Resistance in *Salmonella Typhimurium* Induced by Disinfectant Stress. *Journal of Hazardous Materials*, 480: 135858.
- Wu, Q., Peng, Z., Zhang, Y., & Yang, J. (2018). COACH-D: Improved Protein-ligand Binding Sites Prediction with Refined Ligand-binding Poses through Molecular Docking. *Nucleic Acids Research*, 46(W1): W438-W442.
- Xiao, Y., & Woods, R. J. (2023). Protein-ligand CH- π Interactions: Structural Informatics, Energy Function Development, and Docking Implementation. *Journal of Chemical Theory and Computation*, 19(16): 5503-5515.

- Xu, J. (2024). Recent Advances in π -Stacking Interaction-Controlled Asymmetric Synthesis. *Molecules*, 29(7): 1454.
- Yang, C., Chen, E. A., & Zhang, Y. (2022). Protein-ligand Docking in the Machine-Learning Era. *Molecules*, 27(14): 4568.
- 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: 594652.
- Yolanda, A. P. (2023). *Aplikasi Promix dengan Dosis Berbeda pada Pakan terhadap Performa Pertumbuhan dan Tingkat Kelangsungan Hidup Benih Udang Vaname Litopenaeus vannamei (Boone, 1931)*. Skripsi, Budidaya Perairan, Universitas Lampung, Lampung.
- Yoon, J. H., Bae, Y. M., Song, H., Lee, S., Moon, S. K., Oh, S. W. & Lee, S. Y. (2021). Development of Enhanced Selective Media for Detection of *Vibrio parahaemolyticus* in Oysters. *Food Science and Biotechnology*, 30: 475-485.
- Yuan, H., Hou, Y., Jiao, Y., Lu, X., & Liu, L. (2025). An Integrated Network Pharmacology, Molecular Docking, Molecular Dynamics Simulation, and Experimental Validation Study to Investigate the Potential Mechanism of Isoliquiritigenin in the Treatment of Ischemic Stroke. *Current Issues in Molecular Biology*, 47(8): 627.
- Zang, Z., Duncan, O. K., Sabonis, D., Shi, Y., Miraj, G., Fedorova, I., Le, S., Deng, J., Zhu, Y., Cai, Y., Zhang, C., Arya, G., Duerkop, B. A., Liang, H., Bondy-Denomy, J., Ve, T., Tamulaitiene, G., & Gerdt, J. P. (2025). Chemical Inhibition of a Bacterial Immune System 1. *bioRxiv*.
- Zheng, S. (2025). Navigating the Unstructured by Evaluating AlphaFold's Efficacy in Predicting Missing Residues and Structural Disorder in Proteins. *PloS one*, 20(3): e0313812.
- Zhu, L., Li, J., & Huan, W. (2023). Combating Drug-resistant Bacteria with Sulfonium Cationic Poly (Methionine). *RSC advances*, 13(39): 27608-27612.
- Zinke, M., Schroder, G. F. & Lange, A. (2022). Major Tail Proteins of Bacteriophages of the Order *Caudovirales*. *Journal of Biological Chemistry*, 298(1).