DAFTAR PUSTAKA

Adil Jamal, Aisha Nawaz, Amina Arif, & Muhammad Naveed Shahid. (2025). Phytochemical and pharmacological potential of Solanum nigrum: A concise review. *Acta Biologica Slovenica*, *3*, 142–160. https://doi.org/https://doi.org/10.14720/abs.68.3.20074

Alsedfy, M. Y., Ebnalwaled, A. A., Moustafa, M., & Said, A. H. (2024). Investigating the binding affinity, molecular dynamics, and ADMET properties of curcumin-IONPs as a mucoadhesive bioavailable oral treatment for iron deficiency anemia. *Scientific Reports*, *14*(1), 1–12. https://doi.org/10.1038/s41598-024-72577-8

Armenia, A., Hidayat, R., Meiliani, M., & Yuliandra, Y. (2019). Blood pressure lowering effect of scopoletin on oxidative stress-associated hypertensive rats. *Marmara Pharmaceutical Journal*, *23*(2), 249–258. https://doi.org/10.12991/jrp.2019.131

Attique, S. A., Hassan, M., Usman, M., Atif, R. M., Mahboob, S., Al-Ghanim, K. A., Bilal, M., & Nawaz, M. Z. (2019). A molecular docking approach to evaluate the pharmacological properties of natural and synthetic treatment candidates for use against hypertension. *International Journal of Environmental Research and Public Health*, *16*(6), 1–17. https://doi.org/10.3390/ijerph16060923

Balkrishna, A., Sharma, N., Srivastava, D., Kukreti, A., Srivastava, S., & Arya, V. (2024). Exploring the Safety, Efficacy, and Bioactivity of Herbal Medicines: Bridging Traditional Wisdom and Modern Science in Healthcare. *Future Integrative Medicine*, *3*(1), 35–49. https://doi.org/10.14218/fim.2023.00086

Banerjee, P., Kemmler, E., Dunkel, M., & Preissner, R. (2024). ProTox 3.0: A webserver for the prediction of toxicity of chemicals. *Nucleic Acids Research*, *52*(W1), W513–W520. https://doi.org/10.1093/nar/gkae303

Baroroh, S.Si., M.Biotek., 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

Bhagawan, W. S., Ekasari, W., & Agil, M. (2023). Ethnopharmacology of medicinal plants used by the Tenggerese community in Bromo Tengger Semeru National Park, Indonesia. *Biodiversitas*, *24*(10), 5464–5477. https://doi.org/10.13057/biodiv/d241028

Biswas, S. K., Banerjee, S., Baker, G. W., Kuo, C. Y., & Chowdhury, I. (2022).

The Mammary Gland: Basic Structure and Molecular Signaling during Development. *International Journal of Molecular Sciences*, *23*(7), 1–43. https://doi.org/10.3390/ijms23073883

Boyles, F., Deane, C. M., & Morris, G. M. (2020). Learning from the ligand: Using ligand-based features to improve binding affinity prediction. *Bioinformatics*, *36*(3), 758–764. https://doi.org/10.1093/bioinformatics/btz665

Brisken, C., & Scabia, V. (2020). Progesterone receptor signaling in the normal breast and its implications for cancer. *Journal of Molecular Endocrinology*, *65*(1), T81–T94. https://doi.org/10.1530/JME-20-0091

Buggiotti, L., Cheng, Z., Salavati, M., Wathes, C. D., Fahey, A., Crisà, A., Fouladi, A., Wylie, A., Vanlierde, A., Fogh, A., Santoro, A., Cromie, A., Van Laere, A. S., Pearn, A., Evertson, A., Laine, A., Bernardo, B. S., Moioli, B., Vanranst, B., … Chen, X. (2021). Comparison of the transcriptome in circulating leukocytes in early lactation between primiparous and multiparous cows provides evidence for age-related changes. *BMC Genomics*, *22*(1), 1–17. https://doi.org/10.1186/s12864-021-07977-5

Buriani, A., Fortinguerra, S., Sorrenti, V., Caudullo, G., & Carrara, M. (2020). Essential oil phytocomplex activity, a review with a focus on multivariate analysis for a network pharmacology-informed phytogenomic approach. *Molecules*, *25*(8), 1–15. https://doi.org/10.3390/molecules25081833

Chen, J. F., Wu, S. W., Shi, Z. M., Qu, Y. J., Ding, M. R., & Hu, B. (2023). Exploring the components and mechanism of Solanum nigrum L. for colon cancer treatment based on network pharmacology and molecular docking. *Frontiers in Oncology*, *13*, 1–14. https://doi.org/10.3389/fonc.2023.1111799

Chen, X., Dai, X., Liu, Y., Yang, Y., Yuan, L., He, X., & Gong, G. (2022). Solanum nigrum Linn.: An Insight into Current Research on Traditional Uses, Phytochemistry, and Pharmacology. *Frontiers in Pharmacology*, *13*, 1–32. https://doi.org/10.3389/fphar.2022.918071

Cragg, A., Levene, I., Darabi, S., & Willcox, M. (2025). Herbal galactagogues to improve breastmilk production and lactation in mothers of preterm babies: a systematic review of clinical trials. *European Journal of Clinical Nutrition*, 1–13. https://doi.org/10.1038/s41430-025-01679-x

Debik, J., Sangermani, M., Wang, F., Madssen, T. S., & Giskeødegård, G. F. (2022). Multivariate analysis of NMR-based metabolomic data. *NMR in Biomedicine*, *35*(2), 1–21. https://doi.org/10.1002/nbm.4638

Delbrouck, J. A., Desgagné, M., Comeau, C., Bouarab, K., Malouin, F., & Boudreault, P. L. (2023). The Therapeutic Value of Solanum Steroidal (Glyco)Alkaloids: A 10-Year Comprehensive Review. *Molecules*, *28*(13), 1–40. https://doi.org/10.3390/molecules28134957

Dong, Y., Hao, L., Fang, K., Han, X. xiao, Yu, H., Zhang, J. jun, Cai, L. jun, Fan, T., Zhang, W. da, Pang, K., Ma, W. ming, Wang, X. tao, & Han, C. hui. (2021). A network pharmacology perspective for deciphering potential mechanisms of action of Solanum nigrum L. in bladder cancer. *BMC Complementary Medicine and Therapies*, *21*(1), 1–14. https://doi.org/10.1186/s12906-021-03215-3

Elkhalifa, A. E. O., Banu, H., Khan, M. I., & Ashraf, S. A. (2023). Integrated Network Pharmacology, Molecular Docking, Molecular Simulation, and In Vitro Validation Revealed the Bioactive Components in Soy-Fermented Food Products and the Underlying Mechanistic Pathways in Lung Cancer. *Nutrients*, *15*(18), 1–32. https://doi.org/10.3390/nu15183949

Fadhil Pratama, M. R., Poerwono, H., & Siswodihardjo, S. (2021). Introducing a two-dimensional graph of docking score difference vs. similarity of ligand-receptor interactions. *Indonesian Journal of Biotechnology*, *26*(1), 54–60. https://doi.org/10.22146/IJBIOTECH.62194

Filimonov, D. A., Rudik, A. V., Dmitriev, A. V., & Poroikov, V. V. (2020). Computer-aided estimation of biological activity profiles of drug-like compounds taking into account their metabolism in human body. *International Journal of Molecular Sciences*, *21*(20), 1–13. https://doi.org/10.3390/ijms21207492

Gao, Z., Mi, R., Cheng, Z., Li, X., Zeng, H., Wu, G., Zhao, J., Zhang, W., & Ye, J. (2022). Integrated Metabolomics and Network Pharmacology Revealed Hong-Hua-Xiao-Yao Tablet's Effect of Mediating Hormone Synthesis in the Treatment of Mammary Gland Hyperplasia. *Frontiers in Pharmacology*, *13*, 1–16. https://doi.org/10.3389/fphar.2022.788019

García-Ortegón, M., Simm, G. N. C., Tripp, A. J., Hernández-Lobato, J. M., Bender, A., & Bacallado, S. (2022). DOCKSTRING: Easy Molecular Docking Yields Better Benchmarks for Ligand Design. *Journal of Chemical Information and Modeling*, *62*(15), 3486–3502. https://doi.org/10.1021/acs.jcim.1c01334

Gębarowska, E., Łyczko, J., Rdzanek, M., Wiatrak, B., Plaskowska, E., Gołębiowska, H., Kuźniarski, A., & Gębarowski, T. (2022). Evaluation of Antimicrobial and Chemopreventive Properties and Phytochemical Analysis of Solanum nigrum L. Aerial Parts and Root Extracts. *Applied Sciences (Switzerland)*, *12*(14), 1–19.

https://doi.org/10.3390/app12146845

Gorvin, C. M., Newey, P. J., & Thakker, R. V. (2023). Identification of prolactin receptor variants with diverse effects on receptor signalling. *Journal of Molecular Endocrinology*, *70*(3), 1–20. https://doi.org/10.1530/JME-22-0164

Goßen, J., Ribeiro, R. P., Bier, D., Neumaier, B., Carloni, P., Giorgetti, A., & Rossetti, G. (2023). AI-based identification of therapeutic agents targeting GPCRs: introducing ligand type classifiers and systems biology. *Chemical Science*, *14*(32), 8651–8661. https://doi.org/10.1039/d3sc02352d

Grzeskowiak, L. E., Wlodek, M. E., & Geddes, D. T. (2019). What evidence do we have for pharmaceutical galactagogues in the treatment of lactation insufficiency?—a narrative review. *Nutrients*, *11*(5), 1–21. https://doi.org/10.3390/nu11050974

Guo, H., Li, J., Wang, Y., Cao, X., Lv, X., Yang, Z., & Chen, Z. (2023). Progress in Research on Key Factors Regulating Lactation Initiation in the Mammary Glands of Dairy Cows. *Genes*, *14*(6), 1–11. https://doi.org/10.3390/genes14061163

Hannan, F. M., Elajnaf, T., Vandenberg, L. N., Kennedy, S. H., & Thakker, R. V. (2023). Hormonal regulation of mammary gland development and lactation. *Nature Reviews Endocrinology*, *19*, 46–61. https://doi.org/10.1038/s41574-022-00742-y

Hu, L., Luo, Y., Yang, J., & Cheng, C. (2025). Botanical Flavonoids: Efficacy, Absorption, Metabolism and Advanced Pharmaceutical Technology for Improving Bioavailability. *Molecules*, *30*, 1–35. https://doi.org/10.3390/molecules30051184

Huang, Y., Liu, Y., Yu, X. Y., & Zeng, T. Y. (2022). The rates and factors of perceived insufficient milk supply: A systematic review. *Maternal and Child Nutrition*, *18*, 1–13. https://doi.org/10.1111/mcn.13255

Idkowiak, J., Dehairs, J., Schwarzerová, J., Olešová, D., Truong, J. X. M., Kvasnička, A., Eftychiou, M., Cools, R., Spotbeen, X., Jirásko, R., Veseli, V., Giampà, M., de Laat, V., Butler, L. M., Weckwerth, W., Friedecký, D., Demeulemeester, J., Hron, K., Swinnen, J. V., & Holčapek, M. (2025). Best practices and tools in R and Python for statistical processing and visualization of lipidomics and metabolomics data. *Nature Communications* , *16*, 1–19. https://doi.org/10.1038/s41467-025-63751-1

Jena, M. K., Khan, F. B., Ali, S. A., Abdullah, A., Sharma, A. K., Yadav, V.,

Kancharla, S., Kolli, P., Mandadapu, G., Sahoo, A. K., Rath, P. K., Taneera, J., Kumar, S., Mohanty, A. K., Goh, K. W., Ming, L. C., & Ardianto, C. (2023a). Molecular complexity of mammary glands development: a review of lactogenic differentiation in epithelial cells. *Artificial Cells, Nanomedicine and Biotechnology*, *51*(1), 491–508. https://doi.org/10.1080/21691401.2023.2252872

Jena, M. K., Khan, F. B., Ali, S. A., Abdullah, A., Sharma, A. K., Yadav, V., Kancharla, S., Kolli, P., Mandadapu, G., Sahoo, A. K., Rath, P. K., Taneera, J., Kumar, S., Mohanty, A. K., Goh, K. W., Ming, L. C., & Ardianto, C. (2023b). Molecular complexity of mammary glands development: a review of lactogenic differentiation in epithelial cells. *Artificial Cells, Nanomedicine and Biotechnology*, *51*(1), 491–508. https://doi.org/10.1080/21691401.2023.2252872

Jin, X., Perrella, S. L., Lai, C. T., Taylor, N. L., & Geddes, D. T. (2024). Causes of Low Milk Supply: The Roles of Estrogens, Progesterone, and Related External Factors. *Advances in Nutrition*, *15*, 1–11. https://doi.org/10.1016/j.advnut.2023.10.002

Jung, T., & Cheon, C. (2024). Synergistic and Additive Effects of Herbal Medicines in Combination with Chemotherapeutics: A Scoping Review. *Integrative Cancer Therapies*, *23*, 1–13. https://doi.org/10.1177/15347354241259416

Jurowski, K., & Krośniak, A. (2024). Prediction of key toxicity endpoints of AP-238 a new psychoactive substance for clinical toxicology and forensic purposes using in silico methods. *Scientific Reports*, *14*, 1–14. https://doi.org/10.1038/s41598-024-79453-5

Kaunda, J. S., & Zhang, Y. J. (2019). The Genus Solanum: An Ethnopharmacological, Phytochemical and Biological Properties Review. In *Natural Products and Bioprospecting* (Vol. 9, Number 2, pp. 77–137). Springer. https://doi.org/10.1007/s13659-019-0201-6

Kelleher, S. L., Burkinshaw, S., & Kuyooro, S. E. (2024). Polyphenols and Lactation: Molecular Evidence to Support the Use of Botanical Galactagogues. *Molecular Nutrition and Food Research*, *68*, 1–16. https://doi.org/10.1002/mnfr.202300703

Khaiitova, M. (2023). Computer-aided evaluation of targets and biological activity spectra for new piperidine derivatives. *Journal of Clinical Medicine of Kazakhstan*, *20*(4), 60–67. https://doi.org/10.23950/jcmk/13541

Kim, S. Y., & Yi, D. Y. (2020). Components of human breast milk: From macronutrient to microbiome and microRNA. In *Clinical and*

Experimental Pediatrics (Vol. 63, Number 8, pp. 301–309). Korean Pediatric Society. https://doi.org/10.3345/cep.2020.00059

Kirsch, P., Kunadia, J., Shah, S., & Agrawal, N. (2022). Metabolic effects of prolactin and the role of dopamine agonists: A review. *Frontiers in Endocrinology*, *13*, 1–13. https://doi.org/10.3389/fendo.2022.1002320

Kiyama, R. (2022). Estrogenic flavonoids and their molecular mechanisms of action. *Journal of Nutritional Biochemistry*, *114*, 1–50. https://doi.org/10.1016/j.jnutbio.2022.109250

Kobayashi, K. (2023). Culture Models to Investigate Mechanisms of Milk Production and Blood-Milk Barrier in Mammary Epithelial Cells: a Review and a Protocol. *Journal of Mammary Gland Biology and Neoplasia*, *28*, 1–14. https://doi.org/10.1007/s10911-023-09536-y

Kobisi, A. N. A., Balah, M. A., & Hassan, A. R. (2024). Bioactivity of silverleaf nightshade (Solanum elaeagnifolium Cav.) berries parts against Galleria mellonella and Erwinia carotovora and LC-MS chemical profile of its potential extract. *Scientific Reports*, *14*(1), 1–11. https://doi.org/10.1038/s41598-024-68961-z

Kodra, D., Pousinis, P., Vorkas, P. A., Kademoglou, K., Liapikos, T., Pechlivanis, A., Virgiliou, C., Wilson, I. D., Gika, H., & Theodoridis, G. (2022). Is Current Practice Adhering to Guidelines Proposed for Metabolite Identification in LC-MS Untargeted Metabolomics? A Meta-Analysis of the Literature. *Journal of Proteome Research*, *21*, 590–598. https://doi.org/10.1021/acs.jproteome.1c00841

Kokić, B., Rakita, S., & Vujetić, J. (2024). Impact of Using Oilseed Industry Byproducts Rich in Linoleic and Alpha-Linolenic Acid in Ruminant Nutrition on Milk Production and Milk Fatty Acid Profile. *Animals*, *14*, 1–19. https://doi.org/10.3390/ani14040539

Kraus, V., Čižmárová, B., & Birková, A. (2025). When Your Body Tells You to Not Breastfeed—The Connivance of Oxytocin, Prolactin, and Dopamine. *International Journal of Molecular Sciences*, *26*, 1–25. https://doi.org/10.3390/ijms26125909

Lee, S. H., Yap, Y. H. Y., Lim, C. L., Woo, A. R. E., & Lin, V. C. L. (2022). Activation function 1 of progesterone receptor is required for mammary development and regulation of RANKL during pregnancy. *Scientific Reports*, *12*, 1–13. https://doi.org/10.1038/s41598-022-16289-x

Li, L., Yang, L., Yang, L., He, C., He, Y., Chen, L., Dong, Q., Zhang, H., Chen, S., & Li, P. (2023). Network pharmacology: a bright guiding light on the way to explore the personalized precise medication of traditional

Chinese medicine. *Chinese Medicine (United Kingdom)*, *18*, 1–19. https://doi.org/10.1186/s13020-023-00853-2

Li, P., Fang, X., Hao, G., Li, X., Cai, Y., Yan, Y., Zan, L., Yang, R., & Liu, B. (2023). Methionine Promotes Milk Protein Synthesis via the PI3K-mTOR Signaling Pathway in Human Mammary Epithelial Cells. *Metabolites*, *13*(11), 1–15. https://doi.org/10.3390/metabo13111149

Liao, C. C., Chien, C. H., Hsu, T. J., & Li, J. M. (2024). Advancing breastfeeding promotion: leveraging integrative natural galactagogues and unveiling their potential roles—Insights from a 19-year Taiwan nationwide registry to address lactation insufficiency in postpartum women. *Frontiers in Nutrition*, *11*, 1–18. https://doi.org/10.3389/fnut.2024.1293735

Lima, G. S., Lima, N. M., Roque, J. V., de Aguiar, D. V. A., Oliveira, J. V. A., dos Santos, G. F., Chaves, A. R., & Vaz, B. G. (2022). LC-HRMS/MS-Based Metabolomics Approaches Applied to the Detection of Antifungal Compounds and a Metabolic Dynamic Assessment of Orchidaceae. *Molecules*, *27*(22), 1–15. https://doi.org/10.3390/molecules27227937

Liu, J., Liu, J., Tong, X., Peng, W., Wei, S., Sun, T., Wang, Y., Zhang, B., & Li, W. (2021). Network pharmacology prediction and molecular docking-based strategy to discover the potential pharmacological mechanism of huai hua san against ulcerative colitis. *Drug Design, Development and Therapy*, *15*, 3255–3276. https://doi.org/10.2147/DDDT.S319786

Liu, Y., Zhen, H., Wu, X., Wang, J., Luo, Y., Hu, J., Liu, X., Li, S., Li, M., Shi, B., Ren, C., Gu, Y., & Hao, Z. (2024). Molecular Characteristics of JAK2 and Its Effect on the Milk Fat and Casein Synthesis of Ovine Mammary Epithelial Cells. *International Journal of Molecular Sciences*, *25*(7), 1–16. https://doi.org/10.3390/ijms25074027

Ma, X., Liu, H., Li, W., Chen, J., Cui, Z., Wang, Z., Hu, C., Ding, Y., & Zhu, H. (2024). Prolactin Modulates the Proliferation and Secretion of Goat Mammary Epithelial Cells via Regulating Sodium-Coupled Neutral Amino Acid Transporter 1 and 2. *Cells*, *13*(17), 1–19. https://doi.org/10.3390/cells13171461

Mantiniotou, M., Athanasiadis, V., Kalompatsios, D., Bozinou, E., Ntourtoglou, G., Dourtoglou, V. G., & Lalas, S. I. (2025). Atmospheric Room Temperature Plasma as a Green Pretreatment Strategy for Enhanced Phytochemical Extraction from Moringa oleifera Leaves. *Foods*, *14*(18), 1–26. https://doi.org/10.3390/foods14183233

Mayr, F., Möller, G., Garscha, U., Fischer, J., Castaño, P. R., Inderbinen, S. G., Temml, V., Waltenberger, B., Schwaiger, S., Hartmann, R. W., Gege,

C., Martens, S., Odermatt, A., Pandey, A. V., Werz, O., Adamski, J., Stuppner, H., & Schuster, D. (2020). Finding new molecular targets of familiar natural products using in silico target prediction. *International Journal of Molecular Sciences*, *21*(19), 1–18. https://doi.org/10.3390/ijms21197102

Mekky, A. E., Abdelaziz, A. E. M., Youssef, F. S., Elaskary, S. A., Shoun, A. A., Alwaleed, E. A., Gaber, M. A., Al-Askar, A. A., Alsamman, A. M., Yousef, A., AbdElgayed, G., Suef, R. A., Selim, M. A., Saied, E., & Khedr, M. (2024). Unravelling the Antimicrobial, Antibiofilm, Suppressing Fibronectin Binding Protein A (fnba) and cna Virulence Genes, Anti-Inflammatory and Antioxidant Potential of Biosynthesized Solanum lycopersicum Silver Nanoparticles. *Medicina (Lithuania)*, *60*, 1–31. https://doi.org/10.3390/medicina60030515

Meli, R., Morris, G. M., & Biggin, P. C. (2022). Scoring Functions for Protein-Ligand Binding Affinity Prediction Using Structure-based Deep Learning: A Review. *Frontiers in Bioinformatics*, *2*, 1–30. https://doi.org/10.3389/fbinf.2022.885983

Meng, X., Lyu, C., Ma, J., Zhang, X., Hu, C., Su, X., Ning, C., Xie, W., & Zhang, S. (2021). Metabolomics and Network Pharmacology-Based Investigation into the Mechanisms Underlying the Therapeutic Effect of a New Chinese Traditional Medicine (Cui Nai Ling) on Bromocriptine-Induced Hypogalactia. *Evidence-Based Complementary and Alternative Medicine*, *2021*, 1–17. https://doi.org/10.1155/2021/8857449

Mohammad Azhar Kamal, Hanadi M Baeissa, Israa J. Hakeem, Reem S Alazragi, Mohannad S. Hazzazi, Tahani Bakhsh, Akhmed Aslam, Bassem Refaat, Elshiekh B. Khidir, Kadhem Juma Alkhenaizi, & Qamre Alam. (2023). Insights from the molecular docking analysis of EGFR antagonists. *Bioinformation*, *19*(3), 260–265. https://doi.org/10.6026/97320630019260

Mohanty, M., & Mohanty, P. S. (2023). Molecular docking in organic, inorganic, and hybrid systems: a tutorial review. In *Monatshefte fur Chemie* (Vol. 154, Number 7, pp. 683–707). Springer. https://doi.org/10.1007/s00706-023-03076-1

Mswahili, M. E., & Jeong, Y. S. (2024). Transformer-based models for chemical SMILES representation: A comprehensive literature review. *Heliyon*, *10*(20), 1–18. https://doi.org/10.1016/j.heliyon.2024.e39038

Mukherjee, P. K., Banerjee, S., & Kar, A. (2021). Molecular combination networks in medicinal plants: understanding synergy by network pharmacology in Indian traditional medicine. In *Phytochemistry Reviews* (Vol. 20, Number 4, pp. 693–703). Springer Science and Business Media

B.V. https://doi.org/10.1007/s11101-020-09730-4

Muthuvel, A., Jothibas, M., & Manoharan, C. (2020). Effect of chemically synthesis compared to biosynthesized ZnO-NPs using Solanum nigrum leaf extract and their photocatalytic, antibacterial and in-vitro antioxidant activity. *Journal of Environmental Chemical Engineering*, *8*, 1–16. https://doi.org/10.1016/j.jece.2020.103705

Nemadodzi, L. E., Managa, G. M., & Nemukondeni, N. (2025). H NMR-Based Analysis to Determine the Metabolomics Profile of Solanum nigrum L. (Black Nightshade) Grown in Greenhouse Versus Open-Field Conditions. *Metabolites*, *15*(5), 1–17. https://doi.org/10.3390/metabo15050344

Neville, M. C. (2023). Lactation in the human. *Animal Frontiers*, *13*(3), 64–70. https://doi.org/10.1093/af/vfad021

Nicolas, S., Bois, B., Billet, K., Romanet, R., Bahut, F., Uhl, J., Schmitt-Kopplin, P., & Gougeon, R. D. (2024). High-Resolution Mass Spectrometry-Based Metabolomics for Increased Grape Juice Metabolite Coverage. *Foods*, *13*(1), 1–16. https://doi.org/10.3390/foods13010054

Niu, Y., Liu, M., Cui, S., Liu, K., Yang, M., Hu, X., Zheng, C., Wang, L., & Cao, J. (2025). Integrative Network Pharmacology and Multi-Omics Analysis Reveal Key Targets and Mechanisms of Saikosaponin B1 Against Acute Lung Injury. *Metabolites*, *15*(12), 1–24. https://doi.org/10.3390/metabo15120782

Pant, P., Pandey, S., & Dall'Acqua, S. (2021). The Influence of Environmental Conditions on Secondary Metabolites in Medicinal Plants: A Literature Review. *Chemistry and Biodiversity*, *18*(11), 1–14. https://doi.org/10.1002/cbdv.202100345

Peng, Y., Zhuang, K., & Huang, Y. (2024). Incidence and factors influencing delayed onset of lactation: a systematic review and meta-analysis. *International Breastfeeding Journal*, *19*(1), 1–15. https://doi.org/10.1186/s13006-024-00666-5

Purushotham, U. (2025). Enhanced Discussion on Reassessing Lipinski's Rule of Five in the Era of AI-Driven Drug Discovery. In *Advanced Pharmaceutical Bulletin* (Vol. 15, Number 3, pp. 474–476). Tabriz University of Medical Sciences. https://doi.org/10.34172/apb.025.45948

Queiroz, E. F., Guillarme, D., & Wolfender, J. L. (2024). Advanced high-resolution chromatographic strategies for efficient isolation of natural products from complex biological matrices: from metabolite profiling to pure chemical entities. *Phytochemistry Reviews*, *23*(5), 1415–1442.

https://doi.org/10.1007/s11101-024-09928-w

Rafi, M., Hayati, F., Umar, A. H., Septaningsih, D. A., & Rachmatiah, T. (2023). LC-HRMS-based metabolomics to evaluate the phytochemical profile and antioxidant capacity of Cosmos caudatus with different extraction methods and solvents. *Arabian Journal of Chemistry*, *16*(9), 1–9. https://doi.org/10.1016/j.arabjc.2023.105065

Rakusanova, S., & Cajka, T. (2024). Tips and tricks for LC–MS-based metabolomics and lipidomics analysis. *TrAC - Trends in Analytical Chemistry*, *180*, 1–18. https://doi.org/10.1016/j.trac.2024.117940

Ramadhani, N., Lukitaningsih, E., Rohman, A., & Nurrochmad, A. (2025). Simple Tool of Metabolomic Studies: TLC-Based Metabolite Profiling Peronema canescens Jack in Archipelago Indonesia. *Majalah Obat Tradisional*, *30*(3), 251–261. https://doi.org/10.22146/mot.95221

Rashidi, S., Yousefi, A. R., & Mastinu, A. (2024). Mycorrhizal Symbiosis Can Change the Composition of Secondary Metabolites in Fruits of Solanum nigrum L. *Chemistry and Biodiversity*, *21*(7), 1–6. https://doi.org/10.1002/cbdv.202400208

Rusidzé, M., Adlanmérini, M., Chantalat, E., Raymond-Letron, I., Cayre, S., Arnal, J. F., Deugnier, M. A., & Lenfant, F. (2021). Estrogen receptor-α signaling in post-natal mammary development and breast cancers. In *Cellular and Molecular Life Sciences* (Vol. 78, Number 15, pp. 5681–5705). Springer Science and Business Media Deutschland GmbH. https://doi.org/10.1007/s00018-021-03860-4

Sánchez, C., Franco, L., Regal, P., Lamas, A., Cepeda, A., & Fente, C. (2021). Breast milk: A source of functional compounds with potential application in nutrition and therapy. In *Nutrients* (Vol. 13, Number 3, pp. 1–34). MDPI AG. https://doi.org/10.3390/nu13031026

Shamsian, S., Sokouti, B., & Dastmalchi, S. (2024). Benchmarking different docking protocols for predicting the binding poses of ligands complexed with cyclooxygenase enzymes and screening chemical libraries. *BioImpacts*, *14*, 1–11. https://doi.org/10.34172/bi.2023.29955

Simbar, M., Nazarpour, S., Mojab, F., Kholosi Badr, F., Khorrami, M., Jafari Torkamani, Z., & Alavi-Majd, H. (2022). A Comparative Study on the Effects of "honey and Fenugreek" with "fenugreek" on the Breastfeeding Success: A Randomized Trial. *Evidence-Based Complementary and Alternative Medicine*, *2022*, 1–11. https://doi.org/10.1155/2022/6048280

Sindhu, R. K., Verma, R., Salgotra, T., Rahman, M. H., Shah, M., Akter, R., Murad, W., Mubin, S., Bibi, P., Qusti, S., Alshammari, E. M., Batiha, G.

E. S., Tomczyk, M., & Al-Kuraishy, H. M. (2021). Impacting the remedial potential of nano delivery-based flavonoids for breast cancer treatment. *Molecules*, *26*(17), 1–21. https://doi.org/10.3390/molecules26175163

Singh, S. P., Mukadam, S. S., & Bisht, A. (2024). An extensive investigation into the bioactive component of breast milk, lactation, and clinical application of Galactagogues: A review. *The Journal of Phytopharmacology*, *13*(2), 114–121. https://doi.org/10.31254/phyto.2024.13205

Suganya, J., Kumar, G. R., Radha, M., & Devi, S. M. (2022). A Computational approach in identifying the herbal compounds as Lactation inducer. *Research Journal of Pharmacy and Technology*, *15*(8), 3345–3350. https://doi.org/10.52711/0974-360X.2022.00559

Sukor, N. S. M., Zakri, Z. H. M., Rasol, N. E., & Salim, F. (2023). Annotation and Identification of Phytochemicals from Eleusine indica Using High-Performance Liquid Chromatography Tandem Mass Spectrometry: Databases-Driven Approach. *Molecules*, *28*(7), 1–27. https://doi.org/10.3390/molecules28073111

Sun, T., Quan, W., Peng, S., Yang, D., Liu, J., He, C., Chen, Y., Hu, B., & Tuo, Q. (2022). Network Pharmacology-Based Strategy Combined with Molecular Docking and in vitro Validation Study to Explore the Underlying Mechanism of Huo Luo Xiao Ling Dan in Treating Atherosclerosis. *Drug Design, Development and Therapy*, *16*, 1621–1645. https://doi.org/10.2147/DDDT.S357483

Suproborini, A., Soeprijadi, M., Laksana, D., & Yudiantoro, D. F. (2018). Etnobotani Tanaman Antipiretik Masyarakat Dusun Mesu Boto Jatiroto Wonogiri Jawa Tengah Ethnobotany Antipyretic Plants Peoples In Dusun Mesu Boto Jatiroto Wonogiri Central Java. *Journal of Pharmaceutical Science and Medical Research*, *1*, 2614–6118. https://doi.org/https://doi.org/10.25273/pharmed.v1i1.2274

Szyller, H., Antosz, K., Batko, J., Mytych, A., Dziedziak, M., Wrześniewska, M., Braksator, J., & Pytrus, T. (2024). Bioactive Components of Human Milk and Their Impact on Child's Health and Development, Literature Review. *Nutrients*, *16*(10), 1–28. https://doi.org/10.3390/nu16101487

Tafzi, F., Andarwulan, N., Edi Giriwono, P., & Dewi, F. N. (2024). Torbangun (Plectranthus amboinicus (Lour.) Spreng) Leaf Extract Upregulates Expression of Lactation-Related Genes in Human Mammary Epithelial Cells MCF-12A. *INDONESIAN FOOD SCIENCE AND TECHNOLOGY JOURNAL (IFSTJ)*, *8*(1), 52–59.

Tang, D., Chen, M., Huang, X., Zhang, G., Zeng, L., Zhang, G., Wu, S., & Wang, Y. (2023). SRplot: A free online platform for data visualization and graphing. *PLoS ONE*, *18*(11 October), 1–8. https://doi.org/10.1371/journal.pone.0294236

Thakur, M., Khedkar, R., Singh, K., & Sharma, V. (2023). Ethnopharmacology of Botanical Galactagogues and Comprehensive Analysis of Gaps Between Traditional and Scientific Evidence. *Current Research in Nutrition and Food Science*, *11*(2), 589–604. https://doi.org/10.12944/CRNFSJ.11.2.11

Theodoridis, G., Gika, H., Raftery, D., Goodacre, R., Plumb, R. S., & Wilson, I. D. (2023). Ensuring Fact-Based Metabolite Identification in Liquid Chromatography-Mass Spectrometry-Based Metabolomics. In *Analytical Chemistry* (Vol. 95, Number 8, pp. 3909–3916). American Chemical Society. https://doi.org/10.1021/acs.analchem.2c05192

Tian, M., Qi, Y., Zhang, X., Wu, Z., Chen, J., Chen, F., Guan, W., & Zhang, S. (2020). Regulation of the JAK2-STAT5 Pathway by Signaling Molecules in the Mammary Gland. *Frontiers in Cell and Developmental Biology*, *8*, 1–12. https://doi.org/10.3389/fcell.2020.604896

Wahab Khattak, F., Salamah Alhwaiti, Y., Ali, A., Faisal, M., & Siddiqi, M. H. (2021). Protein-Protein Interaction Analysis through Network Topology (Oral Cancer). *Journal of Healthcare Engineering*, *2021*, 1–9. https://doi.org/10.1155/2021/6623904

Wang, R., Tu, L., Pan, D., Gao, X., Du, L., Cai, Z., Wu, J., & Dang, Y. (2023). A Comparative Study of Binding Interactions between Proteins and Flavonoids in Angelica Keiskei: Stability, α-Glucosidase Inhibition and Interaction Mechanisms. *International Journal of Molecular Sciences*, *24*(7), 1–14. https://doi.org/10.3390/ijms24076582

Wang, R., Wang, X., & Ou, J. (2024). Network pharmacology-based approach reveals that Fructus mume exerts therapeutic effects against ulcerative colitis via the AGE/RAGE signaling pathway. *Arabian Journal of Chemistry*, *17*(2), 1–11. https://doi.org/10.1016/j.arabjc.2023.105534

Wang, T., Zhang, X., Liu, W., Ning, F., Hu, X., Qin, L., Cui, M., Yang, J., Lv, S., & Wang, Q. (2023). Identification of diagnostic molecules and potential traditional Chinese medicine components for Alzheimer's disease by single cell RNA sequencing combined with a systematic framework for network pharmacology. *Frontiers in Medicine*, *10*, 1–13. https://doi.org/10.3389/fmed.2023.1335512

Wang, X. rui, Cao, T. ting, Jia, C. M., Tian, X. mei, & Wang, Y. (2021). Quantitative prediction model for affinity of drug–target interactions

based on molecular vibrations and overall system of ligand-receptor. *BMC Bioinformatics*, *22*(1), 1–18. https://doi.org/10.1186/s12859-021-04389-w

Wang, Z., Zhang, T., Wang, B., & Li, S. (2025). TCM network pharmacology: new perspective integrating network target with artificial intelligence and multi-modal multi-omics technologies. *Chinese Journal of Natural Medicines*, *23*(11), 1425–1434. https://doi.org/10.1016/S1875-5364(25)60986-1

Wieser, N. V., Ghiboub, M., Verseijden, C., van Goudoever, J. B., Schoonderwoerd, A., de Meij, T. G. J., Niemarkt, H. J., Davids, M., Lefèvre, A., Emond, P., Derikx, J. P. M., Jonge, W. J. de, & Sovran, B. (2024). Exploring the Immunomodulatory Potential of Human Milk: Aryl Hydrocarbon Receptor Activation and Its Impact on Neonatal Gut Health. *Nutrients*, *16*(10), 1–18. https://doi.org/10.3390/nu16101531

Wu, N., Zhang, R., Peng, X., Fang, L., Chen, K., & Jestilä, J. S. (2024). Elucidation of protein-ligand interactions by multiple trajectory analysis methods. *Physical Chemistry Chemical Physics*, *26*(8), 6903–6915. https://doi.org/10.1039/d3cp03492e

Yan, L., Zhang, Z., Liu, Y., Ren, S., Zhu, Z., Wei, L., Feng, J., Duan, T., Sun, X., Xie, T., & Sui, X. (2022). Anticancer Activity of Erianin: Cancer-Specific Target Prediction Based on Network Pharmacology. *Frontiers in Molecular Biosciences*, *9*, 1–17. https://doi.org/10.3389/fmolb.2022.862932

Yang, L. J., Gao, S., Su, Z., Qin, X., & Li, Z. (2021). Identification of the constituents and the cancer-related targets of the fruit of Solanum nigrum based on molecular docking and network pharmacology. *Journal of Pharmaceutical and Biomedical Analysis*, *200*, 1–10. https://doi.org/10.1016/j.jpba.2021.114067

Yuan, J., Wu, Z., Wang, B., Fu, S., Te, R., Da, L., Wang, L., Qin, Q., & He, X. (2025). Research on the Changing Characteristics of Milk Composition and Serum Metabolites Across Various Lactation Periods in Xinggao Sheep. *Metabolites*, *15*(10), 1–19. https://doi.org/10.3390/metabo15100678

Zhang, K., Wang, K., Zhang, C., Teng, X., Li, D., & Chen, M. (2022). Exploring the potential mechanism of emetine against coronavirus disease 2019 combined with lung adenocarcinoma: bioinformatics and molecular simulation analyses. *BMC Cancer*, *22*(1), 1–18. https://doi.org/10.1186/s12885-022-09763-2

Zhao, Z. duo, Hu, C., Li, L., Zhang, J. qi, & Zhang, L. chao. (2024). Main

chemical constituents and mechanism of anti-tumor action of Solanum nigrum L. *Cancer Medicine*, *13*(16), 1–34. https://doi.org/10.1002/cam4.7314

Zhou, X., Ullah, A., Shi, L., Dou, M., Wang, C., Khan, M. Z., Wang, C., & Zhang, X. (2025). Molecular Regulatory Mechanisms of Mammary Gland Development: A Review. *Animals*, *15*(23), 1–23. https://doi.org/10.3390/ani15233480