

## DAFTAR PUSTAKA

- Acharya, C., Coop, A., Polli, J. E., & Mackerell, A. D. (2011). Recent advances in ligand-based drug design: Relevance and utility of the conformationally sampled pharmacophore approach. *Current Computer-Aided Drug Design*, 7(1), Article 1. <https://doi.org/10.2174/157340911793743547>
- 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), Article 1. <https://doi.org/10.1038/s41598-023-40160-2>
- Ahmad, R. S., Hussain, M. B., Sultan, M. T., Arshad, M. S., Waheed, M., Shariati, M. A., Plygun, S., & Hashempur, M. H. (2020). Biochemistry, Safety, Pharmacological Activities, and Clinical Applications of Turmeric: A Mechanistic Review. *Evidence-Based Complementary and Alternative Medicine: eCAM*, 2020, 7656919. <https://doi.org/10.1155/2020/7656919>
- Almazroo, O. A., Miah, M. K., & Venkataramanan, R. (2017). Drug Metabolism in the Liver. *Clinics in Liver Disease*, 21(1), Article 1. <https://doi.org/10.1016/j.cld.2016.08.001>
- Androutsopoulos, V. P., Tsatsakis, A. M., & Spandidos, D. A. (2009). Cytochrome P450 CYP1A1: Wider roles in cancer progression and prevention. *BMC Cancer*, 9(1), 187. <https://doi.org/10.1186/1471-2407-9-187>
- Aparoy, P., Reddy, K. K., & Reddanna, P. (2012). Structure and ligand based drug design strategies in the development of novel 5- LOX inhibitors. *Current Medicinal Chemistry*, 19(22), Article 22. <https://doi.org/10.2174/092986712801661112>
- Appiahopong, R., Commandeur, J., Vanvugtluessenburg, B., & Vermeulen, N. (2007). Inhibition of human recombinant cytochrome P450s by curcumin and curcumin decomposition products. *Toxicology*, 235(1–2), 83–91. <https://doi.org/10.1016/j.tox.2007.03.007>
- Bart, A. G., & Scott, E. E. (2018). Structures of human cytochrome P450 1A1 with bergamottin and erlotinib reveal active-site modifications for binding of diverse ligands. *Journal of Biological Chemistry*, 293(50), 19201–19210. <https://doi.org/10.1074/jbc.RA118.005588>
- Castro-Alvarez, A., Costa, A. M., & Vilarrasa, J. (2017). The Performance of Several Docking Programs at Reproducing Protein-Macrolide-Like Crystal Structures. *Molecules (Basel, Switzerland)*, 22(1), 136. <https://doi.org/10.3390/molecules22010136>

- Cheng, D., Li, W., Wang, L., Lin, T., Poiani, G., Wassef, A., Hudlikar, R., Ondar, P., Brunetti, L., & Kong, A.-N. (2019). Pharmacokinetics, Pharmacodynamics, and PKPD Modeling of Curcumin in Regulating Antioxidant and Epigenetic Gene Expression in Healthy Human Volunteers. *Molecular Pharmaceutics*, 16(5), Article 5. <https://doi.org/10.1021/acs.molpharmaceut.8b01246>
- Dei Cas, M., & Ghidoni, R. (2019). Dietary Curcumin: Correlation between Bioavailability and Health Potential. *Nutrients*, 11(9), Article 9. <https://doi.org/10.3390/nu11092147>
- Demchenko, A. P. (2023). Sensors Based on Peptides and Proteins as Recognition Units. In A. P. Demchenko, *Introduction to Fluorescence Sensing* (pp. 103–137). Springer International Publishing. [https://doi.org/10.1007/978-3-031-19089-6\\_4](https://doi.org/10.1007/978-3-031-19089-6_4)
- Ekins, S., Mestres, J., & Testa, B. (2007). In silico pharmacology for drug discovery: Methods for virtual ligand screening and profiling. *British Journal of Pharmacology*, 152(1), Article 1. <https://doi.org/10.1038/sj.bjp.0707305>
- Fanali, G., di Masi, A., Trezza, V., Marino, M., Fasano, M., & Ascenzi, P. (2012). Human serum albumin: From bench to bedside. *Molecular Aspects of Medicine*, 33(3), Article 3. <https://doi.org/10.1016/j.mam.2011.12.002>
- Foti, R. S., Rock, D. A., Han, X., Flowers, R. A., Wienkers, L. C., & Wahlstrom, J. L. (2012). Ligand-Based Design of a Potent and Selective Inhibitor of Cytochrome P450 2C19. *Journal of Medicinal Chemistry*, 55(3), 1205–1214. <https://doi.org/10.1021/jm201346g>
- Ghuman, J., Zunszain, P. A., Petitpas, I., Bhattacharya, A. A., Otagiri, M., & Curry, S. (2005). Structural Basis of the Drug-binding Specificity of Human Serum Albumin. *Journal of Molecular Biology*, 353(1), 38–52. <https://doi.org/10.1016/j.jmb.2005.07.075>
- Griffiths, S. K., & Campbell, J. P. (2015). Placental structure, function and drug transfer. *Continuing Education in Anaesthesia Critical Care & Pain*, 15(2), Article 2. <https://doi.org/10.1093/bjaceaccp/mku013>
- Haddad, Y., Adam, V., & Heger, Z. (2020). Ten quick tips for homology modeling of high-resolution protein 3D structures. *PLOS Computational Biology*, 16(4), e1007449. <https://doi.org/10.1371/journal.pcbi.1007449>
- Hewlings, S. J., & Kalman, D. S. (2017). Curcumin: A Review of Its Effects on Human Health. *Foods (Basel, Switzerland)*, 6(10), Article 10. <https://doi.org/10.3390/foods6100092>

- Hollingsworth, S. A., & Karplus, P. A. (2010). A fresh look at the Ramachandran plot and the occurrence of standard structures in proteins. *Biomolecular Concepts*, 1(3–4), 271–283. <https://doi.org/10.1515/BMC.2010.022>
- Hong, C.-C., Tang, B.-K., Hammond, G. L., Tritchler, D., Yaffe, M., & Boyd, N. F. (2004). Cytochrome P450 1A2 (CYP1A2) activity and risk factors for breast cancer: A cross-sectional study. *Breast Cancer Research*, 6(4), R352. <https://doi.org/10.1186/bcr798>
- Kar, T., Basak, P., Sen, S., Ghosh, R. K., & Bhattacharyya, M. (2017a). Analysis of curcumin interaction with human serum albumin using spectroscopic studies with molecular simulation. *Frontiers in Biology*, 12(3), 199–209. <https://doi.org/10.1007/s11515-017-1449-z>
- Kar, T., Basak, P., Sen, S., Ghosh, R. K., & Bhattacharyya, M. (2017b). Analysis of curcumin interaction with human serum albumin using spectroscopic studies with molecular simulation. *Frontiers in Biology*, 12(3), Article 3. <https://doi.org/10.1007/s11515-017-1449-z>
- Kotynia, A., Marciniak, A., Kamysz, W., Neubauer, D., & Krzyżak, E. (2023). Interaction of Positively Charged Oligopeptides with Blood Plasma Proteins. *International Journal of Molecular Sciences*, 24(3), Article 3. <https://doi.org/10.3390/ijms24032836>
- Li, J., Fu, A., & Zhang, L. (2019). An Overview of Scoring Functions Used for Protein-Ligand Interactions in Molecular Docking. *Interdisciplinary Sciences, Computational Life Sciences*, 11(2), Article 2. <https://doi.org/10.1007/s12539-019-00327-w>
- Lu, J., Shang, X., Zhong, W., Xu, Y., Shi, R., & Wang, X. (2020). New insights of CYP1A in endogenous metabolism: A focus on single nucleotide polymorphisms and diseases. *Acta Pharmaceutica Sinica. B*, 10(1), Article 1. <https://doi.org/10.1016/j.apsb.2019.11.016>
- Macalino, S. J. Y., Gosu, V., Hong, S., & Choi, S. (2015). Role of computer-aided drug design in modern drug discovery. *Archives of Pharmacal Research*, 38(9), Article 9. <https://doi.org/10.1007/s12272-015-0640-5>
- Marbun, P., Hakim, A. R., Sri Octa Ujiantari, N., Sulisty Ari Sudarmanto, B., & Endro Nugroho, A. (2023). In Silico Pharmacokinetics Study of 2,5-Dibenzylidenecyclopentanone Analogs as Mono-Ketone Versions of Curcumin. *BIO Web of Conferences*, 75, 04002. <https://doi.org/10.1051/bioconf/20237504002>
- Meng, X.-Y., Zhang, H.-X., Mezei, M., & Cui, M. (2011). Molecular docking: A powerful approach for structure-based drug discovery. *Current Computer-*

*Aided Drug Design*, 7(2), Article 2.  
<https://doi.org/10.2174/157340911795677602>

Mescher, M., & Haarmann-Stemmann, T. (2018). Modulation of CYP1A1 metabolism: From adverse health effects to chemoprevention and therapeutic options. *Pharmacology & Therapeutics*, 187, 71–87. <https://doi.org/10.1016/j.pharmthera.2018.02.012>

Mishra, S., & Palanivelu, K. (2008). The effect of curcumin (turmeric) on Alzheimer's disease: An overview. *Annals of Indian Academy of Neurology*, 11(1), 13. <https://doi.org/10.4103/0972-2327.40220>

Mishra, V., & Heath, R. J. (2021). Structural and Biochemical Features of Human Serum Albumin Essential for Eukaryotic Cell Culture. *International Journal of Molecular Sciences*, 22(16), 8411. <https://doi.org/10.3390/ijms22168411>

Naveja, J. J., & Vogt, M. (2021). Automatic Identification of Analogue Series from Large Compound Data Sets: Methods and Applications. *Molecules (Basel, Switzerland)*, 26(17), Article 17. <https://doi.org/10.3390/molecules26175291>

Onetto, A. J., & Sharif, S. (2024). Drug Distribution. In *StatPearls*. StatPearls Publishing. <http://www.ncbi.nlm.nih.gov/books/NBK567736/>

Pandey, A., Chaturvedi, M., Mishra, S., Kumar, P., Somvanshi, P., & Chaturvedi, R. (2020). Reductive metabolites of curcumin and their therapeutic effects. *Heliyon*, 6(11), Article 11. <https://doi.org/10.1016/j.heliyon.2020.e05469>

Pardridge, W. M. (2012). Drug transport across the blood-brain barrier. *Journal of Cerebral Blood Flow and Metabolism: Official Journal of the International Society of Cerebral Blood Flow and Metabolism*, 32(11), Article 11. <https://doi.org/10.1038/jcbfm.2012.126>

Priyadarsini, K. (2014). The Chemistry of Curcumin: From Extraction to Therapeutic Agent. *Molecules*, 19(12), Article 12. <https://doi.org/10.3390/molecules191220091>

Pudjono, S., & Irawati, T. (2006). Sintesis 2,5-dibenzilidinsiklopentanon dari benzaldehid dan siklopentanon dengan variasi pelarut. *Majalah Farmasi Indonesia*, 17(1), Article 1.

Rastelli, E. J., Sannino, S., Hart, D. J., Sharlow, E. R., Lazo, J. S., Brodsky, J. L., & Wipf, P. (2021). Synthesis and evaluation of bifunctional PTP4A3 phosphatase inhibitors activating the ER stress pathway. *Bioorganic & Medicinal Chemistry Letters*, 46, 128167. <https://doi.org/10.1016/j.bmcl.2021.128167>

- Rege, S. A., Arya, M., & Momin, S. A. (2019). Structure activity relationship of tautomers of curcumin: A review. *Ukrainian Food Journal*, 8(1), Article 1. <https://doi.org/10.24263/2304-974X-2019-8-1-6>
- Romano T. Kroemer. (2007). Structure-Based Drug Design: Docking and Scoring. *Current Protein & Peptide Science*, 8(4), Article 4. <https://doi.org/10.2174/138920307781369382>
- Sakurama, K., Kawai, A., Tuan Giam Chuang, V., Kanamori, Y., Osa, M., Taguchi, K., Seo, H., Maruyama, T., Imoto, S., Yamasaki, K., & Otagiri, M. (2018). Analysis of the Binding of Aripiprazole to Human Serum Albumin: The Importance of a Chloro-Group in the Chemical Structure. *ACS Omega*, 3(10), 13790–13797. <https://doi.org/10.1021/acsomega.8b02057>
- Sansen, S., Yano, J. K., Reynald, R. L., Schoch, G. A., Griffin, K. J., Stout, C. D., & Johnson, E. F. (2007). Adaptations for the Oxidation of Polycyclic Aromatic Hydrocarbons Exhibited by the Structure of Human P450 1A2. *Journal of Biological Chemistry*, 282(19), 14348–14355. <https://doi.org/10.1074/jbc.M611692200>
- Silverman, R. B., & Holladay, M. W. (2014). *The organic chemistry of drug design and drug action* (Third edition). Elsevier/AP, Academic Press, is an imprint of Elsevier.
- Sridhar, J., Goyal, N., Liu, J., & Foroozesh, M. (2017). Review of Ligand Specificity Factors for CYP1A Subfamily Enzymes from Molecular Modeling Studies Reported to-Date. *Molecules*, 22(7), 1143. <https://doi.org/10.3390/molecules22071143>
- Thorn, C. F., Aklillu, E., Klein, T. E., & Altman, R. B. (2012). PharmGKB summary: Very important pharmacogene information for CYP1A2. *Pharmacogenetics and Genomics*, 22(1), Article 1. <https://doi.org/10.1097/FPC.0b013e32834c6efd>
- Tossetta, G., Fantone, S., Giannubilo, S. R., & Marzioni, D. (2021). The Multifaced Actions of Curcumin in Pregnancy Outcome. *Antioxidants (Basel, Switzerland)*, 10(1), Article 1. <https://doi.org/10.3390/antiox10010126>
- Tran, T. T. V., Tayara, H., & Chong, K. T. (2023). Recent Studies of Artificial Intelligence on In Silico Drug Distribution Prediction. *International Journal of Molecular Sciences*, 24(3), Article 3. <https://doi.org/10.3390/ijms24031815>
- Ujiantari, N. S. O., Ham, S., Nagiri, C., Shihoya, W., Nureki, O., Hutchinson, D. S., & Schuster, D. (2022). Pharmacophore-guided Virtual Screening to Identify

New  $\beta_3$ -adrenergic Receptor Agonists. *Molecular Informatics*, 41(7), 2100223. <https://doi.org/10.1002/minf.202100223>

Walsh, A. A., Szklarz, G. D., & Scott, E. E. (2013). Human Cytochrome P450 1A1 Structure and Utility in Understanding Drug and Xenobiotic Metabolism. *Journal of Biological Chemistry*, 288(18), 12932–12943. <https://doi.org/10.1074/jbc.M113.452953>

Zanger, U. M., & Schwab, M. (2013). Cytochrome P450 enzymes in drug metabolism: Regulation of gene expression, enzyme activities, and impact of genetic variation. *Pharmacology & Therapeutics*, 138(1), Article 1. <https://doi.org/10.1016/j.pharmthera.2012.12.007>

Zhou, S.-F., Wang, B., Yang, L.-P., & Liu, J.-P. (2010). Structure, function, regulation and polymorphism and the clinical significance of human cytochrome P450 1A2. *Drug Metabolism Reviews*, 42(2), 268–354. <https://doi.org/10.3109/03602530903286476>