

## DAFTAR PUSTAKA

- Abd El-Raouf, O. M., El-Sayed, E. S. M., & Manie, M. F. (2015). Cinnamic Acid and Cinnamaldehyde Ameliorate Cisplatin-Induced Splenotoxicity in Rats. *Journal of Biochemical and Molecular Toxicology*, 29(9), 426–431.  
<https://doi.org/10.1002/jbt.21715>
- Ahmed, A. H., & Alkali, Y. I. (2019). In silico Pharmacokinetics and Molecular Docking Studies of Lead Compounds Derived from *Diospyros Mespiliformis*. *PharmaTutor*, 7(3), 31. <https://doi.org/10.29161/pt.v7.i3.2019.31>
- Akash, S., Abdelkrim, G., Bayil, I., Hosen, M. E., Mukerjee, N., Shater, A. F., Saleh, F. M., Albadrani, G. M., Al-Ghadi, M. Q., Abdel-Daim, M. M., & Tok, T. T. (2023). Antimalarial drug discovery against malaria parasites through haploine modification: An advanced computational approach. *Journal of Cellular and Molecular Medicine*, 27(20), 3168–3188.  
<https://doi.org/10.1111/jcmm.17940>
- Ali, F., Rather, B. A., Naeem, M., & Wang, W. (2024). Degree and distance based topological descriptors of power graphs of finite non-abelian groups. *Discrete Applied Mathematics*, 345, 62–76.  
<https://doi.org/10.1016/J.DAM.2023.11.038>
- Ambure, P., Aher, R. B., Gajewicz, A., Puzyn, T., & Roy, K. (2015). “NanoBRIDGES” software: Open access tools to perform QSAR and nano-QSAR modeling. *Chemometrics and Intelligent Laboratory Systems*, 147, 1–13. <https://doi.org/10.1016/J.CHEMOLAB.2015.07.007>
- Amengor, C. D. K., Biniyam, P. D., Brabbey, A. A., Kekessie, F. K., Zoiku, F. K., Hamidu, S., Gyan, P., & Abudey, B. M. (2024). N-Substituted Phenylhydrazone Kill the Ring Stage of *Plasmodium falciparum*. *BioMed Research International*, 2024. <https://doi.org/10.1155/2024/6697728>
- Aswad, M., Nugraha, R., Yulianty, R., Ismail, Evary, Y. M., Kasmiati, & Tachrim, Z. P. (2024). Potency of Bisindoles from *Caulerpa racemosa* in Handling Diabetes-Related Complications: In silico ADMET Properties and Molecular Docking Simulations. *Turkish Computational and Theoretical Chemistry*, 8(3), 99–107. <https://doi.org/10.33435/tcandtc.1055649>
- Belete, T. M. (2020). Recent Progress in the Development of New Antimalarial Drugs with Novel Targets. *Drug Design, Development and Therapy*, 3875–3889.



Bhatt, S. S., Podablah, Y., Shabbir, M., & Rafiq, M. (2020). Molecular Docking Using Autodock Vina Software for Nonbioinformaticians. *JMIR mHealth and UHealth* 2020;1(1):e14232  
<https://doi.org/10.2196/14232>

- Chandra, S., Roy, A., Jana, M., & Pahan, K. (2018). *Cinnamic acid activates PPAR $\alpha$  to stimulate Lysosomal biogenesis and lower Amyloid plaque pathology in an Alzheimer's disease mouse model.* <https://doi.org/10.1016/j.nbd.2018.12.007>
- Chen, F., Liu, H., Sun, H., Pan, P., Li, Y., Li, D., & Hou, T. (2016). Assessing the performance of the MM/PBSA and MM/GBSA methods. 6. Capability to predict protein-protein binding free energies and re-rank binding poses generated by protein-protein docking. *Physical Chemistry Chemical Physics*, 18(32), 22129–22139. <https://doi.org/10.1039/c6cp03670h>
- Dasmahapatra, U., Kumar, C. K., Das, S., Subramanian, P. T., Murali, P., Isaac, A. E., Ramanathan, K., Balamurali, M. M., & Chanda, K. (2022). In-silico molecular modelling, MM/GBSA binding free energy and molecular dynamics simulation study of novel pyrido fused imidazo[4,5-c]quinolines as potential anti-tumor agents. *Frontiers in Chemistry*, 10. <https://doi.org/10.3389/fchem.2022.991369>
- de Oliveira, D. B., & Gaudio, A. C. (2000). BuildQSAR: A New Computer Program for QSAR Analysis. *Quantitative Structure-Activity Relationships*, 19(6), 599–601. [https://doi.org/10.1002/1521-3838\(200012\)19:6<599::AID-QSAR599>3.0.CO;2-B](https://doi.org/10.1002/1521-3838(200012)19:6<599::AID-QSAR599>3.0.CO;2-B)
- Duay, S. S., Yap, R. C. Y., Gaitano, A. L., Santos, J. A. A., & Macalino, S. J. Y. (2023). Roles of Virtual Screening and Molecular Dynamics Simulations in Discovering and Understanding Antimalarial Drugs. In *International Journal of Molecular Sciences* (Vol. 24, Issue 11). Multidisciplinary Digital Publishing Institute (MDPI). <https://doi.org/10.3390/ijms24119289>
- Dwi, D. K., Sasongkowati, R., & Haryanto, E. (2020). Studi In Silico Sifat Farmakokinetik, Toksisitas, Dan Aktivitas Imunomodulator Brazilein Kayu Secang Terhadap Enzim 3-Chymotrypsin-Like Cysteine Protease Coronavirus. *Journal of Indonesian Medical Laboratory and Science (JoIMedLabS)*, 1(1), 76–85. <https://doi.org/10.53699/JOIMEDLABS.V1I1.14>
- Ezebue, F. C., & Uzochukwu, I. C. (2022). Drug repurposing for schistosomiasis: molecular docking and dynamics investigations. *Journal of Biomolecular Structure and Dynamics*, 40(3), 995–1009. <https://doi.org/10.1080/07391102.2020.1820382>
- Feng, L. S., Xu, Z., Chang, L., Li, C., Yan, X. F., Gao, C., Ding, C., Zhao, F., Shi, F., & Wu, X. (2020). Hybrid molecules with potential in vitro antiplasmodial and in vivo antimalarial activity against drug-resistant Plasmodium falciparum. In *search Reviews* (Vol. 40, Issue 3, pp. 931–971). John Wiley and Sons. <https://doi.org/10.1002/med.21643>
- Restianingsih, T., Yeny Sirait, F., & Regina, I. (2024). Analisis Docking In Silico Terhadap Bakteri Mycobacterium tuberculosis dengan Ekstrak Daunan Herbal Eukaliptus Lemon (*Corymbia citriodora*). [www.balesio.com](https://www.balesio.com)



*Neutron-Maxwell Journal of Physics.*  
<https://www.ejournal.unib.ac.id/index.php/nmj>

- Forli, S., Huey, R., Pique, M. E., Sanner, M. F., Goodsell, D. S., & Olson, A. J. (2016). Computational protein-ligand docking and virtual drug screening with the AutoDock suite. *Nature Protocols*, 11(5), 905. <https://doi.org/10.1038/NPROT.2016.051>
- Frimayanti, N., Yam, M. L., Lee, H. B., Othman, R., Zain, S. M., & Rahman, N. A. (2011). Validation of quantitative structure-activity relationship (QSAR) model for photosensitizer activity prediction. *International Journal of Molecular Sciences*, 12(12), 8626–8644. <https://doi.org/10.3390/ijms12128626>
- Genheden, S., & Ryde, U. (2015). The MM/PBSA and MM/GBSA methods to estimate ligand-binding affinities. *Expert Opinion on Drug Discovery*, 10(5), 449–461. <https://doi.org/10.1517/17460441.2015.1032936>
- Golbraikh, A., Shen, M., Xiao, Z., Xiao, Y.-D., Lee, K.-H., & Tropsha, A. (2003). Rational selection of training and test sets for the development of validated QSAR models. In *Journal of Computer-Aided Molecular Design* (Vol. 17).
- Guo, S., Zhen, Y., Zhu, Z., Zhou, G., & Zheng, X. (2019). Cinnamic acid rescues behavioral deficits in a mouse model of traumatic brain injury by targeting miR-455-3p/HDAC2. *Life Sciences*, 235. <https://doi.org/10.1016/j.lfs.2019.116819>
- Hanwell, M. D., Curtis, D. E., Lonie, D. C., Vandermeersch, T., Zurek, E., & Hutchison, G. R. (2012). SOFTWARE Open Access Avogadro: an advanced semantic chemical editor, visualization, and analysis platform. In *Journal of Cheminformatics* (Vol. 4). <http://www.jcheminf.com/content/4/1/17>
- Himangini, Pathak, D. P., Sharma, V., & Kumar, S. (2018). Designing novel inhibitors against falcipain-2 of Plasmodium falciparum. *Bioorganic and Medicinal Chemistry Letters*, 28(9), 1566–1569. <https://doi.org/10.1016/j.bmcl.2018.03.058>
- Irsal, R. A. P., Gholam, G. M., Firdaus, D. A., Liwanda, N., & Chairunisa, F. (2024). Molecular Docking and Dynamics of Xylocarpus granatum as A Potential Parkinson's Drug Targeting Multiple Enzymes. *Borneo Journal of Pharmacy*, 7(2), 161–171. <https://doi.org/10.33084/bjop.v7i2.6810>
- Jafar La Kilo, A. L. K. (2019). Kajian HKSA Antimalaria Senyawa Turunan QuinoloN4(1H)-imines Menggunakan Metode MLR-ANN. *Jambura Journal of Chemistry*, 1(1), 1–10. <https://doi.org/10.33959/jjc.v1i1.113>
- Ishak Chetia, & Mithun Rudrapal. (2019). Molecular Docking, Drug-liabilities and ADMET Prediction of Quinoline Imines for Antimalarial Activity. *Journal of Medicinal Chemistry and Drug Design*, 2(1). <https://doi.org/10.16966/2578-9589.113>



Optimized using  
trial version  
[www.balesio.com](http://www.balesio.com)

- Kaharudin, C. L., Afkauni, A. A., Pramudyansyah, A. Y., & Prasetyo, N. (2022). Penambatan Molekul dan Simulasi Dinamika Molekular Kandungan Minyak Kayu Manis dan Minyak Serai Dapur Sebagai Antibakteri Methicillin Resistant Staphylococcus aureus. *ALCHEMY Jurnal Penelitian Kimia*, 18(2), 140. <https://doi.org/10.20961/alchemy.18.2.54997.140-147>
- Kemenkes. (2022). *Report On Malaria Control Program In Indonesia Year 2021*.
- Kerr, I. D., Lee, J. H., Farady, C. J., Marion, R., Rickert, M., Sajid, M., Pandey, K. C., Caffrey, C. R., Legac, J., Hansell, E., Mckerrow, J. H., Craik, C. S., Rosenthal, P. J., & Brinen, L. S. (2009). Vinyl sulfones as antiparasitic agents and a structural basis for drug design. *Journal of Biological Chemistry*, 284(38), 25697–25703. <https://doi.org/10.1074/jbc.M109.014340>
- Kumari, M., Chandra, S., Tiwari, N., & Subbarao, N. (2016). 3D QSAR, pharmacophore and molecular docking studies of known inhibitors and designing of novel inhibitors for M18 aspartyl aminopeptidase of Plasmodium falciparum. *BMC Structural Biology*, 16(1), 1–11. <https://doi.org/10.1186/s12900-016-0063-7>
- Land, H., & Humble, M. S. (2018). YASARA: A tool to obtain structural guidance in biocatalytic investigations. In *Methods in Molecular Biology* (Vol. 1685, pp. 43–67). Humana Press Inc. [https://doi.org/10.1007/978-1-4939-7366-8\\_4](https://doi.org/10.1007/978-1-4939-7366-8_4)
- Lipinski, C. A. (2000). Drug-like properties and the causes of poor solubility and poor permeability. *Journal of Pharmacological and Toxicological Methods*, 44(1), 235–249. [https://doi.org/10.1016/S1056-8719\(00\)00107-6](https://doi.org/10.1016/S1056-8719(00)00107-6)
- Manhas, A., Kumar, S., & Jha, P. C. (2022). Identification of the natural compound inhibitors against Plasmodium falciparum plasmepsin-II via common feature based screening and molecular dynamics simulations. *Journal of Biomolecular Structure and Dynamics*, 40(1), 31–43. <https://doi.org/10.1080/07391102.2020.1806110>
- Mansaly, M., Cave, C., Cojean, S., Seck, R., Gassama, A., & Cavé, C. (2019). *Synthesis And Antimalarial Activity Of Cinnamic Acid Derivatives*. 6(2), 450–454. [www.ejbps.com](http://www.ejbps.com)
- Mark, P., & Nilsson, L. (2001). Structure and dynamics of the TIP3P, SPC, and SPC/E water models at 298 K. *Journal of Physical Chemistry A*, 105(43), 9954–9960. <https://doi.org/10.1021/jp003020w>
- McCarthy, C., & Vaughan, T. (2015). Micromechanical failure analysis of advanced materials. *Numerical Modelling of Failure in Advanced Composite* 9–409. <https://doi.org/10.1016/B978-0-08-100332-9.00014-1>
- Nessa, T., & Jin, T. (2021). Structural Basis of Potential Inhibitors RS-CoV-2 Main Protease. *Frontiers in Chemistry*, 9, 622898. <https://doi.org/10.3389/FCHEM.2021.622898>



- Mishra, M., Mishra, V. K., Senger, P., Pathak, A. K., & Kashaw, S. K. (2014). Exploring QSAR studies on 4-substituted quinazoline derivatives as antimalarial compounds for the development of predictive models. *Medicinal Chemistry Research*, 23(3), 1397–1405. <https://doi.org/10.1007/s00044-013-0744-8>
- Morris, G. M., Ruth, H., Lindstrom, W., Sanner, M. F., Belew, R. K., Goodsell, D. S., & Olson, A. J. (2009). Software news and updates AutoDock4 and AutoDockTools4: Automated docking with selective receptor flexibility. *Journal of Computational Chemistry*, 30(16), 2785–2791. <https://doi.org/10.1002/jcc.21256>
- Moulishankar, A., & Sundarajan, T. (2023). QSAR modeling, molecular docking, dynamic simulation and ADMET study of novel tetrahydronaphthalene derivatives as potent antitubercular agents. *Beni-Suef University Journal of Basic and Applied Sciences*, 12(1). <https://doi.org/10.1186/s43088-023-00451-z>
- Nasamu, A. S., Polino, A. J., Istvan, E. S., & Goldberg, D. E. (2020). Malaria parasite plasmepsins: More than just plain old degradative pepsins. *Journal of Biological Chemistry*, 295(25), 8425–8441. <https://doi.org/10.1074/jbc.REV120.009309>
- Neese, F., Wennmohs, F., Becker, U., & Riplinger, C. (2020). The ORCA quantum chemistry program package. *Journal of Chemical Physics*, 152(22). <https://doi.org/10.1063/5.0004608>
- Nitish Kumar, A. P. (2019). Cinnamic acid derivatives: An ERA. *The Pharma Innovation Journal*, 8(5), 580–595. [www.thepharmajournal.com](http://www.thepharmajournal.com)
- Nusantoro, Y. R., & Fadlan, A. (2020). Analisis Sifat Mirip Obat, Prediksi ADMET, dan Penambatan Molekular Isatinil-2-Aminobenzoilhidrazon dan kompleks logam transisi Co(II), Ni(II), Cu(II), Zn(II) Terhadap BCL2-XL. *Akta Kimia Indonesia*, 5(2), 114–126. <https://doi.org/10.12962/J25493736.V5I2.7881>
- Pasha, F. A., Neaz, M. M., Cho, S. J., Ansari, M., Mishra, S. K., & Tiwari, S. (2009). In Silico Quantitative Structure–Toxicity Relationship Study of Aromatic Nitro Compounds. *Chemical Biology & Drug Design*, 73(5), 537–544. <https://doi.org/10.1111/J.1747-0285.2009.00799.X>
- Patel, C. N., Kumar, S. P., Pandya, H. A., & Rawal, R. M. (2021). Identification of potential inhibitors of coronavirus hemagglutinin-esterase using molecular docking, molecular dynamics simulation and binding free energy calculation. *Journal of Pharmacy and Nanotechnology*, 25(1), 421–433. <https://doi.org/10.1007/s11030-020-00930-1>
- Malić, S., Fontinha, D., Prudêncio, M., Pessanha de Carvalho, L., Đurić, T., Vianello, R., Zorc, B., & Rajić, Z. (2020). Harmicines – cinnamic acid hybrids as novel antiplasmodial hits. *European Journal of Medicinal Chemistry*, 194, 112253. <https://doi.org/10.1016/j.ejmech.2020.112253>



Malić, S., Fontinha, D., Prudêncio, M., Pessanha de Carvalho, L., Đurić, T., Vianello, R., Zorc, B., & Rajić, Z. (2020). Harmicines – cinnamic acid hybrids as novel antiplasmodial hits. *European Journal of Medicinal Chemistry*, 194, 112253. <https://doi.org/10.1016/j.ejmech.2020.112253>

*Journal of Medicinal Chemistry*, 187, 111927.

<https://doi.org/10.1016/j.ejmech.2019.111927>

Pettersen, E. F., Goddard, T. D., Huang, C. C., Couch, G. S., Greenblatt, D. M., Meng, E. C., & Ferrin, T. E. (2004). UCSF Chimera - A visualization system for exploratory research and analysis. *Journal of Computational Chemistry*, 25(13), 1605–1612. <https://doi.org/10.1002/jcc.20084>

Pires, D. E. V., Blundell, T. L., & Ascher, D. B. (2015). pkCSM: Predicting small-molecule pharmacokinetic and toxicity properties using graph-based signatures. *Journal of Medicinal Chemistry*, 58(9), 4066–4072. <https://doi.org/10.1021/acs.jmedchem.5b00104>

Rajguru, T., Bora, D., & Modi, M. K. (2022). Identification of promising inhibitors for Plasmodium haemoglobinase Falcipain-2, using virtual screening, molecular docking, and MD Simulation. *Journal of Molecular Structure*, 1248. <https://doi.org/10.1016/j.molstruc.2021.131427>

Ramadhan, D. S. F., Rusli, R., & Fakih, T. M. (2023). Hubungan Kuantitatif Struktur-Aktivitas dan Desain Senyawa Novel Phenyl Benzimidazoles sebagai Penghambat Wnt/-Catenin untuk Terapi Pancreatic Ductal Adenocarcinoma. *Jurnal Sains Dan Kesehatan*, 5(5), 584–590. <https://doi.org/10.25026/jsk.v5i5.1713>

Ramadhani, F. A., Prastika, M. F., Fikriyah, N., Isnaeni, & Diyah, N. W. (2024). Molecular Docking of Flavonoids from Extract of Roselle (*Hibiscus sabdariffa* L.) Calyx on PBP2a as the Basis for Antibacterial Activity Against Methicillin Resistant *Staphylococcus aureus*. *Science and Technology Indonesia*, 9(2), 487–493. <https://doi.org/10.26554/sti.2024.9.2.487-493>

Rasyid, H., Purwono, B., Hofer, T. S., & Pranowo, H. D. (2019). Hydrogen bond stability of quinazoline derivatives compounds in complex against EGFR using molecular dynamics simulation. *Indonesian Journal of Chemistry*, 19(2), 461–469. <https://doi.org/10.22146/ijc.39567>

Rasyid, H., Soekamto, N. H., Firdausiah, S., Mardiyanti, R., Bahrun, B., Siswanto, S., Muhammad Aswad, M. A., Saputri, W. D., Suma, A. A. T., Syahrir, N. H., & Listyarini, R. V. (2023). Revealing the Potency of 1,3,5-Trisubstituted Pyrazoline as Antimalaria Through Combination of in Silico Studies. *Sains Malaysiana*, 52(10), 2855–2867. <https://doi.org/10.17576/jsm-2023-5210-10>

Rosenthal, P. J. (2020). Falcipain cysteine proteases of malaria parasites: An update. In *Biochimica et Biophysica Acta - Proteins and Proteomics* (Vol. 1869). Elsevier B.V. <https://doi.org/10.1016/j.bbapap.2020.140362>



ribigbe, B. A. (2020). Cinnamic acid derivatives and their antimalarial activity. *International Journal of Molecular Sciences*, 21(16), 1–36. <https://doi.org/10.3390/ijms21165712>

Salo-Ahen, O. M. H., Alanko, I., Bhadane, R., Alexandre, A. M., Honorato, R. V., Hossain, S., Juffer, A. H., Kabedev, A., Lahtela-Kakkonen, M., Larsen, A. S., Lescrinier, E., Marimuthu, P., Mirza, M. U., Mustafa, G., Nunes-Alves, A., Pantsar, T., Saadabadi, A., Singaravelu, K., & Vanmeert, M. (2021). Molecular dynamics simulations in drug discovery and pharmaceutical development. In *Processes* (Vol. 9, Issue 1, pp. 1–63). MDPI AG.  
<https://doi.org/10.3390/pr9010071>

Sivaramakrishnan, M., Kandaswamy, K., Natesan, S., Devarajan, R. D., Ramakrishnan, S. G., & Kothandan, R. (2020). Molecular docking and dynamics studies on plasmepsin V of malarial parasite Plasmodium vivax. *Informatics in Medicine Unlocked*, 19.  
<https://doi.org/10.1016/j.imu.2020.100331>

Thu, A. M., Phyto, A. P., Landier, J., Parker, D. M., & Nosten, F. H. (2017). Combating multidrug-resistant Plasmodium falciparum malaria. In *FEBS Journal* (Vol. 284, Issue 16, pp. 2569–2578). Blackwell Publishing Ltd.  
<https://doi.org/10.1111/febs.14127>

Wang, J., Wolf, R. M., Caldwell, J. W., Kollman, P. A., & Case, D. A. (2004). Development and Testing of a General Amber Force Field. In *J Comput Chem* (Vol. 25).

Wang, R., Yang, W., Fan, Y., Dehaen, W., Li, Y., Li, H., Wang, W., Zheng, Q., & Huai, Q. (2019). Design and synthesis of the novel oleanolic acid-cinnamic acid ester derivatives and glycyrrhetic acid-cinnamic acid ester derivatives with cytotoxic properties. *Bioorganic Chemistry*, 88.  
<https://doi.org/10.1016/j.bioorg.2019.102951>

World Health Organization. (2021). WHO Guidelines for malaria. *World Health Organization*, 5–65.

World Health Organization. (2022). *World malaria report 2022*.  
<https://www.who.int/teams/global-malaria-programme>

Yap, C. W. (2011). PaDEL-descriptor: An open source software to calculate molecular descriptors and fingerprints. *Journal of Computational Chemistry*, 32(7), 1466–1474. <https://doi.org/10.1002/jcc.21707>

Yellasubbaiah, N., & Velmurugan, V. (2023). QSAR modeling, molecular docking, and adme studies of novel 5-oxo-imidazoline derivatives as anti-breast cancer drug compounds against MCF-7 Cell Line. *Journal of Medicinal and Chemical Sciences*, 6(12), 3087–3112.  
<https://doi.org/10.26655/JMCHEMSCI.2023.12.24>



., & Ergün, S. (2018). Antimicrobial activity of trans-cinnamic monly used antibiotics against important fish pathogens and ic isolates. *Journal of Applied Microbiology*, 125(6), 1714–1727.  
<https://doi.org/10.1111/JAM.14097>