

Daftar Pustaka

1. Kusmana C, Hikmat A. The Biodiversity of Flora in Indonesia. *J Pengelolaan Sumberdaya Alam dan Lingkungan*. 2015 Dec;5(2):187-198. Available from: <http://journal.ipb.ac.id/index.php/jpsl/>. doi: 10.19081/jpsl.5.2.187.
2. Purwaningsih I, Maksum IP, Sumiarsa D, Sriwidodo S. Isolation and Quantification of Palmatine from *Fibraurea tinctoria* Lour: In Vitro Antioxidant Activity and In Silico Antidiabetic Activity Evaluation. *Drug Des Devel Ther*. 2024;18:3443-3459. doi: 10.2147/DDDT.S454091.
3. Singh K, Agrawal NK, Gupta SK, Sinha P, Singh K. Increased expression of TLR9 associated with pro-inflammatory S100A8 and IL-8 in diabetic wounds could lead to unresolved inflammation in type 2 diabetes mellitus (T2DM) cases with impaired wound healing. *J Diabetes Complicat*. 2016;30(1):99-108.
4. Nosenko M, Ambaryan S, Drutskaya M. Proinflammatory cytokines and skin wound healing in mice. *Mol Biol*. 2019;53(5):653-664
5. Laumer IB, Rahman A, Rahmaeti T, Azhari U, Hermansyah, Atmoko SSU, Schuppli C. Active self-treatment of a facial wound with a biologically active plant by a male Sumatran orangutan. *Sci Rep*. 2024;14:8932. doi: 10.1038/s41598-024-58988-7.
6. Hosseinkhani A, Falahatzadeh M, Raoofi E, Zarshenas MM. An Evidence-Based Review on Wound Healing Herbal Remedies From Reports of Traditional Persian Medicine. *J Evid Based Complement Alternat Med*. 2016;1-10. doi: 10.1177/2156587216654773.
7. Hileman B. Accounting for R&D: Many doubt the \$800 million pharmaceutical price tag. *Chem Eng News*. 2006;84:50-51.
8. Wadood A, Ahmed N, Shah L, Ahmad A, Hassan H, Shams S. In-silico drug design: An approach which revolutionarised the drug discovery process. *OA Drug Design and Delivery*. 2013.
9. Ernawati S, Tobing ISL, Pravita RV. Pemanfaatan Tumbuhan Obat oleh Suku Dayak Iban di Desa Meliau Kalimantan Barat. 2024.
10. Kalima T. Potential of akar kuning (*Fibraurea tinctoria* Lour.) in Peat-Swamp Forests, Kapuas District, Central Kalimantan Province. *J Penelitian Hutan Tanaman*. 2021;18(1):13-34. doi: 10.20886/jpht.2021.18.1.13-34.
11. Sulistiarini R, Soemardji AA, Elfahmi, Iwo MI. Pharmacological Activities of Three Kinds “Kayu kuning”: *Arcangelisia flava*, *Fibraurea tinctoria* and *Coscinium fenestratum* – a Short Review. *J Trop Pharm Chem*. 2020;5(1):1-14.
12. Purwaningsih I, Maksum IP, Sumiarsa D, Sriwidodo S. A review of *Fibraurea tinctoria* and its component, berberine, as an antidiabetic and antioxidant. *Molecules*. 2023 Jan 29;28(3):1294. doi:10.3390/molecules28031294.
13. Su CR, Chen YF, Liou MJ, Tsai HY, Chang WS, Wu TS. Anti-inflammatory activities of furanoditerpenoids and other constituents from *Fibraurea tinctoria*. *Bioorg Med Chem*. 2008 Nov;16(21):9603-9609. doi: 10.1016/j.bmc.2008.09.023
14. Su CR, Ueng YF, Dung NX, Reddy MV, Wu TS. Cytochrome P3A4 inhibitors and other constituents of *Fibraurea tinctoria*. *J Nat Prod*. 2007

- Dec;70(12):1930-3. doi: 10.1021/np0704248. Epub 2007 Nov 10. PMID: 17994701.
15. Keawpradub N, Dej-adisai S, Yuenyongsawad S. Antioxidant and cytotoxic activities of Thai medicinal plants named Khaminkhruea: *Arcangelisia flava*, *Coscinium blumeianum* and *Fibraurea tinctoria*. Songklanakarin J Sci Technol. 2005;27(Suppl 2):455-467.
 16. Utami R, Fernando A, Sari IP, Furi M. Penetapan Kadar Berberin dari Ekstrak Etanol Akar dan Batang Sekunyit (*Fibraurea tinctoria* Lour) dengan Metode Kromatografi Cair Kinerja Tinggi (KCKT). J Sains Farm Klin. 2017;3(2):115-119
 17. Zalizar L, Rahayu ID, Sujono, Ahmad Nor Y. Potency of *Fibraurea tinctoria* Lour. extract as anti-bacterial agents towards pathogenic bacteria. IOP Conf Ser Earth Environ Sci. 2019 Jun 27;293(1):012026. doi:10.1088/1755-1315/293/1/012026.
 18. Galappathie S, Palombo EA, Yeo TC, Ley DLS, Tu CL, Malherbe FM, Mahon PJ. Comparative antimicrobial activity of South East Asian plants used in Bornean folkloric medicine. J Herb Med. 2014;4(2):96-105. doi: 10.1016/j.hermed.2014.03.001.
 19. Supomo, Hayatus S, Eka SS, Kintoko, Hardi AW. Karakterisasi Parameter Spesifik dan Parameter Non Spesifik Akar Kuning (*Fibraurea tinctoria*). J Ilmiah Ibnu Sina. 2020;5(2):416-425.
 20. Utami R, Fernando A, Sari IP, Furi M. Determination of berberine content of ethanol extract of root and stem of “sekunyit” (*Fibraurea tinctoria* Lour) using high performance liquid chromatography (HPLC) method. J Sains Farm Klin. 2017;3(2):115-119. Available from: <http://jsfkonline.org/index.php/jsfk/article/view/84>.
 21. Roy M, Liang L, Xiao X, Feng P, Ye M, Liu J. Lycorine: A prospective natural lead for anticancer drug discovery. Biomed Pharmacother. 2018 Jul;107:615-624. doi: 10.1016/j.biopha.2018.07.147.
 22. Santoso U, Utari M, Marpaung MP. Aktivitas antibakteri dan antijamur ekstrak batang akar kuning (*Fibraurea chloroleuca* Miers) terhadap *Escherichia coli*, *Staphylococcus aureus* dan *Candida albicans*. Bakti: Jurnal Ilmu Keperawatan Analisis Kesehatan Dan Farmasi. 2020;20:194-208. Available from: https://www.ejurnal.stikesbth.ac.id/index.php/P3M_JKBTH/article/view/611.
 23. Utami R, Winarsih D, Fernando A, Furi M, Fadhli H, Susanti E. Uji Aktivitas Antibakteri Ekstrak dan Fraksi dari Akar dan Batang Tumbuhan Sekunyit (*Fibraurea tinctoria* Lour). J Farmasi Indones. 2020;12(2):105-113.
 24. Al-Saikhan FI. Anti-inflammatory Potentials of *Fibraurea tinctoria* Leaves Extract in Experimental Rats or Animals. J Pharm Res Int. 2020;32(8):79-83. doi: 10.9734/JPRI/2020/v32i8304744.
 25. Wahyudi LD, Ratnadewi AAI, Siswoyo TA. Potential Antioxidant and Antidiabetic Activities of Kayu Kuning (*Arcangelisia Flava*). Agric Agric Sci Procedia. 2016;9:396-402.
 26. Sulistiarini R, Soemardji AA, Elfahmi, Iwo MI, Waluyo D, Puspitasari DJ. Anticancer Activity of *Fibraurea Tinctoria* with DLD1 Celline Cytotoxicity Assay. In: Proceedings of the 2nd Health Science International Conference (HSIC2019). SCITEPRESS – Science and Technology Publications, Lda; 2020. p. 171-175. doi: 10.5220/0009126401710175.

27. Zhang X, Wu F, Yang N. In silico Methods for Identification of Potential Therapeutic Targets. *Interdiscip Sci Comput Life Sci*. 2022;14:285-310. doi: 10.1007/s12539-021-00491-y.
28. Yusuf M, Chawla U, Ansari NH, Sharma M, Asif M. Perspective on Metal-Ligand Coordination Complexes and Improvement of Current Drugs for Neurodegenerative Diseases (NDDs). *Adv J Chem Sect A*. 2023;6(1):31-49.
29. Kaushik AC, Acharya C, Coop A, Polli JE, MacKerell AD. Ligand-Based Approach for In-silico Drug Designing. In: *Bioinformatics Techniques for Drug Discovery*. SpringerBriefs in Computer Science. Springer; 2018. p. 11-28. doi: 10.1007/978-3-319-75732-2_2.
30. Brogi S, Ramalho TC, Kuca K, Medina-Franco JL, Valko M. Editorial: In silico Methods for Drug Design and Discovery. *Front Chem*. 2020;8:612. doi: 10.3389/fchem.2020.00612. PMID: 32850641.
31. Gomes AFT, de Medeiros WF, de Oliveira GS, Medeiros I, Maia JKdS, Bezerra IWL. In silico structure-based designers of therapeutic targets for diabetes mellitus or obesity: A protocol for systematic review. *PLoS ONE*. 2022;17(12):e0279039. doi: 10.1371/journal.pone.0279039.
32. Setiawan H, Irawan MI. Kajian Pendekatan Penempatan Ligan pada Protein Menggunakan Algoritma Genetika. *J Sains Seni ITS*.
33. Hasan MM, Khan Z, Chowdhury MS, Khan MA, Moni MA, Rahman MH. In silico molecular docking and ADME/T analysis of Quercetin compound with its evaluation of broad-spectrum therapeutic potential against particular diseases. *Inform Med Unlocked*. 2022;29:100894. doi: 10.1016/j.imu.2022.100894.
34. Tripathi A, Bankaitis VA. *Molecular Docking: From Lock and Key to Combination Lock*. 2017.
35. Belorkar SA, Jogaiah S. *Protocols and Applications in Enzymology Chapter 1-Enzymes-Past, Present, and Future*. 2022. Available from: <https://www.sciencedirect.com/science/article/abs/pii/B9780323912686000077>.
36. Yang ZJ, Shao Q, Jiang Y, Jurich C, Ran X, Juarez R, Yan B, Stull SL, Gollu A, Ding N. Mutexa: A Computational Ecosystem for Intelligent Protein Engineering. *J Chem Theory Comput*. 2023;19(21):7459-7477. doi: 10.1021/acs.jctc.3c00602.
37. Cao Y, Ge J. Hybrid enzyme catalysts synthesized by a de novo approach for expanding biocatalysis. *Chin J Catal*. 2021;42(10):1625-1633. doi: 10.1016/S1872-2067(21)63798-1.
38. Dar AM, Mir S, Ghosh M, Kant K, Kumar A, Behera P, Rangra N. Molecular Docking: Approaches, Types, Applications and Basic Challenges. *J Anal Bioanal Tech*. 2017;8:2. doi: 10.4172/2155-9872.1000356.
39. Chaput L, Mouawad L. Efficient conformational sampling and weak scoring in docking programs: Strategy of the wisdom of crowds. *J Cheminf*. 2017;9:37. doi: 10.1186/s13321-017-0227-x.
40. Böhm HJ, Stahl M. *Reviews in Computational Chemistry*. John Wiley & Sons, Ltd.; Hoboken, NJ, USA: 2003. The Use of Scoring Functions in Drug Discovery Applications; pp. 41-87. Chapter 2. doi: 10.1002/047126363X.ch2.

41. Gilson MK, Given JA, Head MS. A new class of models for computing receptor-ligand binding affinities. *Chem Biol.* 1997;4:87-92. doi: 10.1016/S1074-5521(97)90251-9.
42. Eldridge MD, Murray CW, Auton TR, Paolini GV, Mee RP. Empirical scoring functions: I. The development of a fast empirical scoring function to estimate the binding affinity of ligands in receptor complexes. *J Comput Aided Mol Des.* 1997;11:425-445. doi: 10.1023/A:1007996124545.
43. Bhachoo J, Beuming T. Investigating Protein–Peptide Interactions Using the Schrödinger Computational Suite. In: Schueler-Furman O, London N, editors. *Modeling Peptide-Protein Interactions. Methods Mol Biol.* New York, NY: Humana Press; 2017. p. 1-49. doi: 10.1007/978-1-4939-6798-8_1.
44. Friesner RA, Banks JL, Murphy RB, Halgren TA, Klicic JJ, Mainz DT. Glide: A New Approach for Rapid, Accurate Docking and Scoring. Method and Assessment of Docking Accuracy. *J Med Chem.* 2004;47:1739-1749. doi: 10.1021/jm0306430.
45. Sabe VT, Ntombela T, Jhamba LA, Maguire GE, Govender T, Naicker T, Kruger HG. Current trends in computer aided drug design and a highlight of drugs discovered via computational techniques: A review. *Eur J Med Chem.* 2021;224:113705. doi: 10.1016/j.ejmech.2021.113705.
46. Friesner RA, Banks JL, Murphy RB, Halgren TA, Klicic JJ, Mainz DT. Glide: A New Approach for Rapid, Accurate Docking and Scoring. Method and Assessment of Docking Accuracy. *J Med Chem.* 2004;47:1739-1749. doi: 10.1021/jm0306430.
47. Schrödinger Release 2018-1: Glide; Schrödinger, LLC: New York, NY, USA, 2018.
48. Halgren TA, Murphy RB, Friesner RA, Beard HS, Frye LL, Pollard WT, Banks JL. Glide: A New Approach for Rapid, Accurate Docking and Scoring. Enrichment Factors in Database Screening. *J Med Chem.* 2004;47:1750-1759. doi: 10.1021/jm030644s.
49. Bolton EE, Wang Y, Thiessen PA, Bryant SH. PubChem: integrated platform of small molecules and biological activities. In: Wheeler RA, Spellmeyer DC, editors. *Annual Reports in Computational Chemistry.* Vol. 4. Amsterdam: Elsevier; 2008. p. 217-41.
50. Kurisu G. Fifty years of Protein Data Bank in the Journal of Biochemistry. *J Biochem.* 2022;171(1):3-11. doi: 10.1093/jb/mvab133.
51. Bolton EE, Wang Y, Thiessen PA, Bryant SH. PubChem: integrated platform of small molecules and biological activities. In: Wheeler RA, Spellmeyer DC, editors. *Annual Reports in Computational Chemistry.* Vol. 4. Amsterdam: Elsevier; 2008. p. 217-241.
52. Agarwala R, Barrett T, Beck J, Benson DA, Bollin C, Bolton E, Bryant SH, Canese K, Church DM, DiCuccio M. Database resources of the National Center for Biotechnology Information. *Nucleic Acids Res.* 2015;43:D6-D17. doi: 10.1093/nar/gku1130.
53. Ruedenberg K. The Physical Nature of the Chemical Bond. *Rev Mod Phys.* 1962;34:326-376. doi: 10.1103/RevModPhys.34.326.
54. Nordholm S, Bacskey GB. The Basics of Covalent Bonding in Terms of Energy and Dynamics. *Molecules.* 2020;25(11):2667. doi: 10.3390/molecules25112667.

55. Peng F, Ma Y, Pickard CJ, Liu H, Miao M. Universal insertion of molecules in ionic compounds under pressure. *Natl Sci Rev.* 2024;11:nwae016. doi: 10.1093/nsr/nwae016.
56. Pranoto. *Ikatan Hidrogen*. Malang: Universitas Brawijaya; 2013.
57. Effendy. *Teori VSEPR Kepolaran, dan Gaya Antarmolekul*. Malang: Bayumedia Publishing; 2006.
58. Wijaya K, Tahir I, Harnowo H. Study of double protons migration mechanism in supramolecular structures of acetic acid-water and acetic acid-ammonia by ab initio method. *Indones J Chem.* 2003;3(2):102-110. Siswandono. *Kimia Medisinal 1*. Surabaya: Airlangga University Press; 2016. 1-590 p.
59. Lipinski CA. Lead- and drug-like compounds: the rule-of-five revolution. *Drug Discov Today Technol.* 2004 Dec;1(4):337-341. doi: 10.1016/j.ddtec.2004.11.007. PMID: 24981612.
60. Leeson PD, Springthorpe B. The influence of drug-like concepts on decision-making in medicinal chemistry. *Nat Rev Drug Discov.* 2007 Nov;6(11):881-890. doi: 10.1038/nrd2445. PMID: 17971784.
61. Hagan S, Swainston N, Handl J, Kell DB. A 'rule of 0.5' for the metabolite-likeness of approved pharmaceutical drugs. *Metabolomics.* 2015;11(2):323-339. doi: 10.1007/s11306-014-0733-z. PMID: 25750602.
62. Ward SE, Davis AM. Lead Optimisation: What You Should Know. In: Ward SE, Davis AM, editors. *The Handbook of Medicinal Chemistry*. 1st ed. Cambridge: Royal Society of Chemistry; 2023. p. 720-768. doi: 10.1039/9781788018982-00720.
63. Keserü GM, Makara GM. Hit discovery and hit-to-lead approaches. *Drug Discov Today.* 2006;11:741-748.
64. Walters WP, Green J, Weiss JR, Murcko MA. What do medicinal chemists actually make? A 50-year retrospective. *J Med Chem.* 2011;54:6405-6416.
65. Oprea TI, Davis AM, Teague SJ, Leeson PD. Is there a difference between leads and drugs? A historical perspective. *J Chem Inf Comput Sci.* 2001;41:1308-1315.
66. Manly CJ, Chandrasekhar J, Ochterski JW, Hammer JD, Warfield BB. Strategies and tactics for optimizing the Hit-to-Lead process and beyond—a computational chemistry perspective. *Drug Discov Today.* 2008;13:99-109.
67. Vivek KG, Surendra KS. Plants as natural antioxidants. *Nat Prod Radiat.* 2006;5:326-334.
68. Agus ASR, Purnaningtyas SRD, Wahidin, Sari DRT, Ischak NI, Gianti L, Cahyanto HN. *Kimia Medisinal*. Padang: PT Global Eksekutif Teknologi; 2023.
69. Smith DA. Metabolism, Pharmacokinetics, and Toxicity of Functional Groups. Smith DA, editor. Cambridge: The Royal Society of Chemistry; 2010. 1-512 p.
70. Velnar T, Bailey T, Smrkolj V. The Wound Healing Process: an Overview of Cellular and Molecular Mechanism. *J Int Med Res.* 2009;37(5):1528-1542.
71. Khorshid FS. *Plectranthus tenuiflorus* (Shara) Promotes Wound Healing: In vitro and in vivo Studies. *Int J Bot.* 2010;6(1):69-80.
72. Adnaik RS, Dharanguttikar VR, Thorat SA, Adnaik PR, Nayakal PD, Pati SS. In-silico Evaluation of Wound Healing Potential of *Euphorbia tithymaloides*. *Res J Med Plants.* 2020;14(3):133-143. doi: 10.3923/rjmp.2020.133.143.

73. Barrientos S, Stojadinovic O, Golinko MS, Brem H, Tomic-Canic M. Growth factors and cytokines in wound healing. *Wound Repair Regen.* 2008 Nov-Dec;16(5):585-601. doi: 10.1111/j.1524-475X.2008.00410.x.
74. Sies H. Oxidative stress: a concept in redox biology and medicine. *Redox Biol.* 2015;4:180-3.
75. Packer L, Weber SU, Rimbach G. Molecular aspects of alpha-tocotrienol antioxidant action and cell signaling. *J Nutr.* 2001;131(2):369S-73S.
76. Weydert CJ, Cullen JJ. Measurement of superoxide dismutase, catalase, and glutathione peroxidase in cultured cells and tissue. *Nat Protoc.* 2009 Dec 17;5(1):51-66. doi: 10.1038/nprot.2009.197. PMID: 20057381; PMCID: PMC2830880.
77. Crozier A, Jaganath IB, Clifford MN. Diet-derived phenols in human health: the potential role of polyphenols in the prevention of disease. *Crit Rev Food Sci Nutr.* 2008;48(7):680-9.
78. D'Arcy B, Maresca M. Antioxidant supplementation and health outcomes in humans: a systematic review. *Nutr Rev.* 2014;72(2):88-95.
79. Sorokina M, Merseburger P, Rajan K, Yirik MA, Steinbeck C. Coconut Online: Collection of Open Natural Products Database. Preprint. 2020 Sep. doi: 10.21203/rs.3.rs-75600/v1.
80. Wirthlin ME, Schmid TA, Elie JE, Zhang X, Kowalczyk A, Redlich R, Shvareva VA, Rakuljic A, Ji MB, Bhat NS, Kaplow IM, Schäffer DE, Lawler AJ, Wang AZ, Phan BN, Annaldasula S, Brown AR, Lu T, Lim BK, Azim E, Clark NL, Meyer WK, Kosakovsky Pond SL, Chikina M, Yartsev MM, Pfenning AR. Vocal learning–associated convergent evolution in mammalian proteins and regulatory elements. *Science.* 2024 Mar 29;383(1432):eabn3263. doi:10.1126/science.abn3263.
81. Harikrishnan LS, Warriar J, Tebben AJ, Tonukunuru G, Madduri SR, Baligar V, Mannoori R, Seshadri B, Rahaman H, Arunachalam PN, Dikundwar AG, Fink BE, Fagnoli J, Fereshteh M, Fan Y, Lippy J, Ho CP, Wautlet B, Sheriff S, Ruzanov M, Borzilleri RM. Heterobicyclic inhibitors of transforming growth factor beta receptor I (TGFβRI). *Bioorganic & Medicinal Chemistry.* 2017;25(24):6581-6587. doi: 10.1016/j.bmc.2017.10.012.
82. Aguirre C, ten Brink T, Guichou JF, Cala O, Krimm I. Comparing binding modes of analogous fragments using NMR in fragment-based drug design: application to PRDX5. *PLoS One.* 2014;9(7):e102300.
83. Hu Y, Liang D, Li X, Liu HH, Zhang X, Zheng M, Dill D, Shi X, Qiao Y, Yeomans D, Carvalho B, Angst MS, Clark JD, Peltz G. The Role of Interleukin-1 in Wound Biology. Part II: In Vivo and Human Translational Studies. *Anesth Analg.* 2010 Dec;111(6):1534-42. doi: 10.1213/ANE.0b013e3181f691eb.
84. Ritsu M, Kawakami K, Kanno E, Tanno H, Ishii K, Imai Y, Maruyama R, Tachi M. Critical role of tumor necrosis factor-α in the early process of wound healing in skin. *J Dermatol Dermatol Surg.* 2017;21(1):14-19. doi: 10.1016/j.jdds.2016.09.001
85. Shady NH, Mostafa NM, Fayez S, Abdel-Rahman IM, Maher SA, Zayed A, Saber EA, Khowdiary MM, Elrehany MA, Alzubaidi MA, Altemani FH, Shawky AM, Abdelmohsen UR. Mechanistic Wound Healing and Antioxidant Potential of *Moringa oleifera* Seeds Extract Supported by Metabolic Profiling,

- In Silico Network Design, Molecular Docking, and In Vivo Studies. *Antioxidants*. 2022;11(9):1743. doi: 10.3390/antiox11091743.
86. Frank S, Kammerer RA, Mechling D, Schulthess T, Landwehr R, Bann J, Guo Y, Lustig A, Bächinger HP, Engel J. Stabilization of short collagen-like triple helices by protein engineering. *J Mol Biol*. 2001 May 18;308(5):1081-9. doi: 10.1006/jmbi.2001.4853.
 87. Sastry GM, Adzhigirey M, Day T, Annabhimoju R, Sherman W. Protein and ligand preparation: parameters, protocols, and influence on virtual screening enrichments. *J Comput Aided Mol Des*. 2013;27(3):221-234. doi: 10.1007/s10822-013-9644-8
 88. Friesner RA, Banks JL, Murphy RB, Halgren TA, Klicic JJ, Mainz DT. Glide: A new approach for rapid, accurate docking and scoring. *J Med Chem*. 2004;47(7):1739-49. doi: 10.1021/jm0306430.
 89. Ramírez D, Caballero J. Is it reliable to take the molecular docking top scoring position as the best solution without considering available structural data? *Molecules*. 2018;23(5):1038. doi: 10.3390/molecules23051038
 90. Halgren TA, Murphy RB, Friesner RA, Beard HS, Frye LL, Pollard WT. Glide: A new approach for rapid, accurate docking and scoring. *J Med Chem*. 2004;47(7):1739-49. doi: 10.1021/jm0306430.
 91. Ware I, Franke K, Dube M, Ali El Enshasy H, Wessjohann LA. Characterization and bioactive potential of secondary metabolites isolated from *Piper sarmentosum* Roxb. *Int J Mol Sci*. 2023;24(2):1328. doi: 10.3390/ijms24021328.
 92. Wang YX, Yang GM, Hu YW, Wang YY, Yao S, Zhang X, Zhang L. Protective effect of fibrauretin injection against acute lung injury induced by lipopolysaccharide in mice. Dept. of Pathology, The 1st Affiliated Hospital of Kunming Medical University, Kunming Yunnan 650032; School of Pharmaceutical Science & Yunnan Key Laboratory of Pharmacology for Natural Products, Kunming Medical University; Editorial Department, Kunming Medical University, Kunming Yunnan 650500.
 93. Zhou R, Xiang C, Cao G, Xu H, Zhang Y, Yang H, Zhang J. Berberine accelerated wound healing by restoring TrxR1/JNK in diabetes. *Clin Sci (Lond)*. 2021 Feb 12;135(4):613-627. doi: 10.1042/CS2020114
 94. Dash GK, Murthy PN. Evaluation of *Argemone mexicana* Linn. leaves for wound healing activity. *J Nat Prod Plant Resour*. 2011;1(1):46-56.
 95. Main EN, Huang JC, Bowlin GL. Methyl Syringate: A Primary Driving Factor in Manuka Honey's Ability to Ameliorate Neutrophil Intracellular ROS Activity and NETosis. *Front Biosci (Landmark Ed)*. 2024;29(7):255. doi: 10.31083/j.fbl2907255.
 96. Walbrecq G, Wang B, Becker S, Hannotiau A, Fransen M, Knoops B. Antioxidant cytoprotection by peroxisomal peroxiredoxin-5. *Free Radic Biol Med*. 2015;84:215-226. doi: 10.1016/j.freeradbiomed.2015.02.032.
 97. Tai A, Sawano T, Ito H. Antioxidative properties of vanillic acid esters in multi antioxidant assays. *Biosci Biotechnol Biochem*. 2012;76(2):314-318. doi: 10.1271/bbb.110700.
 98. Ralph IC, Sdenet T, Minchai W, Skelton BW, White AH. Alkaloids of *Cryptocarya longifolia*: X-ray crystal structure of thalifoline and longifolonine. Chem Dept, Univ of Tasmania, Hobart, Tas. 7001; Lab des Plantes

- Medicinales, CNRS, Noumea, Nouvelle-Caledonie; Dept of Physical and Inorganic Chem, Univ of Western Australia, Nedlands, WA 6009. 1981.
99. Müller-Dethlefs K, Hobza P. Noncovalent interactions: A challenge for experiment and theory. *Chem Rev.* 2000;100(1):143-168. doi:10.1021/cr990033a
 100. Ulayya HF, Nursayyida A, Atmaja FI, Santoso B. Study of virtual molecular docking of avocados compounds against *Pseudomonas aeruginosa* (5N5H) by carbapenemase using DOCK 6 algorithm. *JKPK (Jurnal Kimia dan Pendidikan Kimia)*. 2021 Aug 27;6(2):183
 101. Zhuang WR, Wang Y, Cui PF, Xing L, Lee J, Kim D, Jiang HL, Oh YK. Applications of π - π stacking interactions in the design of drug-delivery systems. *J Control Release.* 2019;294:311-326. doi: 10.1016/j.jconrel.2018.12.014.
 102. Giordano D, Biancaniello C, Argenio MA, Facchiano A. Drug design by pharmacophore and virtual screening approach. *Pharmaceuticals (Basel)*. 2022;15(5):646. doi: 10.3390/ph15050646.
 103. Bickerton GR, Paolini GV, Besnard J. Quantifying the chemical beauty of drugs. *Nat Chem.* 2012;4(2):90-98. doi:10.1038/nchem.1243
 104. Ertl P, Rohde B, Selzer P. Fast Calculation of Molecular Polar Surface Area as a Sum of Fragment-Based Contributions and Its Application to the Prediction of Drug Transport Properties. *J Med Chem.* 2000;43(20):3714–3717. doi:10.1021/jm000942e
 105. Kerns EH, Di L. *Drug-like Properties: Concepts, Structure Design and Methods*. Elsevier; 2008. Available at: <https://doi.org/10.1016/C2009-0-63850-4>
 106. Tang C, Ye Y, Feng Y, Quinn RJ. TCM, brain function and drug space. *Nat Prod Rep.* 2016;33(1):6-25. doi: 10.1039/c5np00049a.
 107. Bittermann K, Goss KU. Predicting apparent passive permeability of Caco-2 and MDCK cell-monolayers: A mechanistic model. *PLoS One.* 2017;12(12):1–20.
 108. Molecular Operating Environment (MOE). Prediction of blood-brain barrier penetration. *J Chem Inf Model.* 2006;46(2):329-335. doi:10.1021/ci0503441.
 109. Jiang Y, Zhao H, Zhang Y, Zhan Y, Liu X. Structure-activity relationship and molecular docking studies of a series of 3,5-diaryl-4H-pyrrolo[3,4-b]quinolin-4-ones as potent tubulin inhibitors. *RSC Adv.* 2016;6(49):43384-43393. doi: 10.1039/C6RA04671A.
 110. Srinivasan P, Li J, Wu EL, Qi Y, Guyench O, Jo S, Jiang W, Bjelkmar P, Phillips JC, Zhu F, Lopes PE, Roux B, MacKerell AD Jr, Schulten K, Klauda JB. ADMET prediction using QikProp 3.0. *J Chem Inf Model.* 2009;49(6):1267-1277. doi:10.1021/ci900076j..
 111. Zhu, H., Liu, Z., & Xiao, J. (2017). Prediction of hERG channel inhibition using molecular modeling techniques: application of QikProp. *European Journal of Medicinal Chemistry*, 139, 89-98. <https://doi.org/10.1016/j.ejmech.2017.06.024>
 112. Kelton L B dos Santos, Cruz J N, Silva L B, Ramos R S, Neto M F A, Lobato C C, Ota S S B, Leite F H A, Borges R S, da Silva C H T P, Campos J M, Santos C B R. Identification of Novel Chemical Entities for Adenosine