

## DAFTAR PUSTAKA

1. Aizah S. Antioksidan Memperlambat Penuaan Dini Sel Manusia Siti Aizah Abstrak. Pros Semnas Hayati IV. 2020;182–5.
2. Situmorang N, Zulham Z. Malondialdehyde (Mda) (Zat Oksidan Yang Mempercepat Proses Penuaan). J Keperawatan Dan Fisioter. 2020;2(2):117–23.
3. Siswanto FM, Pangkahila A. the Balancing of Physical Fitness Increase the Activity of Endogenous Stem Cell for Anti-Aging. ISSN 2302-688X Sport Fit J. 2014;2(1):1–9.
4. Haerani A, Chaerunisa AY, Subranas A. Artikel Tinjauan: Antioksidan untuk kulit. Farmaka. 2018;16(2):135–51. Available from: <https://jurnal.unpad.ac.id/farmaka/article/view/17789>
5. Pandel R, Poljšak B, Godic A, Dahmane R. Skin Photoaging and the Role of Antioxidants in Its Prevention. ISRN Dermatol. 2013;2013:1–11.
6. Sanusi FE, Agung A, Sawitri S, Citra W, Sucipta W, Program P, et al. Hubungan Aktivitas Merokok Dengan Penuaan Dini Kulit Pada Kelompok Masyarakat Usia 20-40 Tahun Di Universitas Udayana (The Relationship Of Smoking Activities With The Early Aging Of The Skin In The Age Of 20-40 Years In Udayana University). J Bios Logos. 2020;10(1):34–40.
7. Dewiastuti M, Hasanah IF. Pengaruh Faktor-Faktor Risiko Penuaan Dini di Kulit pada Remaja Wanita Usia 18-21 Tahun. J Profesi Med J Kedokt dan Kesehat. 2017;10(1):21–5.
8. Clémént-Palmer M, Spiegelhalter D. Hormone replacement therapy and the risk of breast cancer: How much should women worry about it? Post Reprod Heal. 2019;25(4):175–8.
9. Wagner RD, Fakhro A, Cox JA, Izaddoost SA. Etiology, Prevention, and Management of Infectious Complications of Dermal Fillers. Semin Plast Surg. 2016;30(2):83–6.
10. Pleguezuelos-Beltrán P, Herráiz-Gil S, Martínez-Moreno D, Medraño-Fernandez I, León C, Guerrero-Aspizua S. Regenerative Cosmetics: Skin Tissue Engineering for Anti-Aging, Repair, and Hair Restoration. Cosmetics. 2024;11(4):1–17.
11. Kementrian Perdagangan Republik Indonesia. Indonesian Essential Oils. 2011;1:1–40.
12. Ulfa SW. Inventarisasi Keanekaragaman Tumbuhan Obat di Kecamatan Medan Tembung Kota Medan Propinsi Sumatera Utara. Best J (Biology Educ Sci Tecnol. 2021;4(1):123–32.
13. Hanifah NN. Profil Metabolit dan Aktivitas Antibakteri Serta Anti- Aging Minyak Atsiri Kunyit Bolai (*Zingiber purpureum Roscoe*). 2024.
14. Fitriyani, Zannah M, Nazarudin M. Sains Medisina. Lit Rev Kaji Potensi Interak Obat Antidiabetes Pada Pasien Diabetes Melitus Tipe 2 dengan Komplikasi Hipertens. 2024;2(3):93–8. Available from: <https://wpcpublisher.com/jurnal/index.php/sainsmedisina/article/view/356>
15. Padmasari PD, Astuti KW, Warditiani NK. Skrining Fitokimia Ekstrak Etanol 70% Rimpang Bangle. J Farm Udayana. 2013;2(4):1–7. Available

- from: <https://ojs.unud.ac.id/index.php/jfu/article/view/7395/5645>
16. Setyani RA, Tangke Arung E, Yanti Puspita Sari, Matematika dan Ilmu Pengetahuan Alam F. Skrining Fitokimia, Antioksidan dan Aktivitas Antibakteri Ekstrak Etanol Akar Segar Bangle (*Zingiber montanum*) Phytochemical Screening, Antioxidant and Antibacterial Activity of Ethanol Extract of Bangle Fresh Root (*Zingiber montanum*). J Ris Teknol Ind. 2021;15(2):415.
  17. Farage MA, Maibach H, Francisco S. Textbook of Aging Skin. Textb Aging Ski. 2016;(July 2015).
  18. Wulandari D. Pengaruh Minyak Atsiri Bangle (*Zingiber Purpureum Roxb.*) sebagai Antibakteri terhadap Kualitas Sabun Cair. J Agroindustri Halal. 2018;4(1):001–9.
  19. Maulina D, Hermina PK. Peran Mangiferin Sebagai Inhibitor Enzim Kolagenase Dan Elastase. Indonesian Journal of Health Science. 2021;1(1):4–9.
  20. Moringa K, Terhadap O, Natanael GI, Simorangkir GF, Parariski N, Putri M, et al. Potensi Antioksidan dan Anti-Elastase Ekstrak Daun. 2021;4(1):69–76.
  21. Raharjo FP, Nova G, Putri L, Rokhim DA. jurnal  $\beta$  eta kimia Potensi Body Scrub Berbahan Dasar Bekicot Dan Teh Sebagai Perawatan Kulit Berkelanjutan. 2024;4:95–101.
  22. Rauf A, Ninggi S, Nurdin H. Potensi Penghambatan Tirosinase Ekstrak Etanol Daun Tomat (*Lycopersicon esculentum* Mill, var. Pyriforme Alef.). 2016.
  23. Ivanovic M, Zivic A, Tachos N, Gois G, Filipovic N, Fotiadis DI. In-silico Research Platform in the Cloud - Performance and Scalability Analysis. BIBE 2021 - 21st IEEE Int Conf Bioinforma Bioeng Proc. 2021;
  24. Jannah Absn, Ramadanti K, Uyun K. Identifikasi Ciri Morfologi pada Lengkuas (*Alpinia galanga*) dan Bangle (*Zingiber purpureum*) di Desa Mesjid Priyayi, Kecamatan Kasemen, Kota Serang, Banten. Trop Biosci J Biol Sci. 2022;2(1):27–34.
  25. Windarsih G, Utami DW, Yuriah S. Morphological characteristics of zingiberaceae In Serang District, Banten, Indonesia. Biodiversitas. 2021;22(12):5507–29.
  26. Rahmah NA, Farmasi PS, Kesehatan FI. Nida Auliya Rahmah-Fikes. 2018.
  27. Hartanto, S. F dan SN. Studi Etnobotani Famili Zingiberaceae dalam Kehidupan Masyarakat Lokal di Kecamatan Pangean Kabupaten Kuantan Singingi, Riau. Biosaintifika. 2014;6(2):98–108.
  28. Han AR, Kim H, Piao D, Jung CH, Seo EK. Phytochemicals and bioactivities of zingiber cassumunar roxb. Molecules. 2021;26(8):1–16.
  29. Nishidono Y, Saifudin A, Tanaka K. Characterization of the Volatile Constituents of Plai (*Zingiber purpureum*) by Gas Chromatography–Mass Spectrometry. Molecules. 2024;29(6):1–14.
  30. Ardiyani M, Senjaya SK, Maruzy A, Widiyastuti Y, Sulistyaningsih LD, Susila. Genetic diversity of “Bangle” (*Zingiber montanum* (J.Koenig) Link ex A.Dietr.) inferred from sequence-related amplified polymorphism markers. Agric Nat Resour. 2021;55(1):105–12.
  31. Singh C, N M, N S, Chanu S. Ethnobotany, Phytochemistry and

- Pharmacology of *Zingiber cassumunar Roxb.* (Zingiberaceae). J Pharmacogn Phytochem. 2015;4(1):01–6. Available from: <https://www.phytojournal.com/archives/2015.v4.i1.535/ethnobotany-phytochemistry-and-pharmacology-of-zingiber-cassumunar-roxb-zingiberaceae>
32. Noviyanto F, Hodijah S, Yusransyah Y. Aktivitas Ekstrak Daun Bangle (*Zingiber purpureum roxb.*) Terhadap Pertumbuhan Bakteri *Pseudomonas aeruginosa*. J Syifa Sci Clin Res. 2020;2(1):31–8.
33. Musdja MY. Potential bangle (*Zingiber montanum* J.König) rhizome extract as a supplement to prevent and reduce symptoms of Covid-19. Saudi J Biol Sci. 2021;28(4):2245–53. Available from: <https://doi.org/10.1016/j.sjbs.2021.01.015>
34. Bachtiar KR, Susanti S, Mardianingrum R. Uji Aktivitas Antiinflamasi Senyawa Dalam Minyak Atsiri Rimpang Bangle (*Zingiber Purpureum Roxb*) Secara In Silico. J Pharmacopilum. 2021;4(1):36–43.
35. Adhila G, Nurkhasanah N, Sulistyani N. In Vitro Immunomodulatory Activity Test Of Bengle Rhizoma Extract (*Zingiber cassumunar Roxb.*): phagocytic Activity of Macrophages and Lymphocyte Proliferation In Mice. Pharmaciana. 2019;9(2):211.
36. Setyani AR, Arung ET, Sari YP. Skrining Fitokimia, Antioksidan dan Aktivitas Antibakteri Ekstrak Etanol Akar Segar Bangle (*Zingiber montanum*). J Ris Teknol Ind. 2021;15(2):415.
37. Siswantito F, Natasya A, Nugroho R, Listiarini Iskandar R, Sitanggang CO, Al-Qordhiyah Z, et al. Produksi Minyak Atsiri Melalui Ragam Metode Ekstraksi Dengan Berbahan Baku Jahe. Inov Tek Kim. 2023;8(3):178–84.
38. Lim S hua erin, Loh J yan, Lai K song. Antimicrobial and Immunomodulatory Activities. Molecules. 2022;27:3589–601.
39. Ebadi MT, Sefidkon F, Azizi M, Ahmadi N. Packaging methods and storage duration affect essential oil content and composition of lemon verbena (*Lippia citriodora Kunth.*). Food Sci Nutr. 2017;5(3):588–95.
40. Sarkic A, Stappen I. Essential Oils and Their Single Compounds In Cosmetics-A Critical Review. Cosmetics. 2018;5(1):1–21.
41. Mubarak K, Natsir H, Wahab AW, Satrimafitrah P. Analysis of α-Tokopherol (Vitamin E) Extracted from *Moringa* Leaves (*Moringa oleifera Lam*) Collected from Seashore and Highland Areas and Its Potencyl as Antioxidant. Kovalen. 2017;3(1):78–88.
42. Warsito MF, Untari F, Prasetyoputri A, Rachman F, Septiana E, Bayu A, et al. Antibacterial and Antioxidant Activities of Ginger Essential Oils. Microbiol Indones. 2022;15(4):1.
43. Mayangsari FD, Khotimah K, Asyalafia. Effect of Essential Oil Types on The Physical Characteristics and Consumer Preference Level of Antiaging Body Lotion that Contain NLC-Coenzyme Q10. J Kesehat dr Soebandi. 2023;11(2):147–52.
44. Fatmasari Afriyanti, Rani Rubiyanti NA. Sains Indonesiana: Jurnal Ilmiah Nusantara Vol.1, N. 2023;1(April):182–90.
45. Birru, Hilmi S. Article Review : Retinol In Cosmetics. J Pharm Sci. 2023;6(1):256–60.
46. Gragnani A, Cornick S Mac, Chominski V, Ribeiro de Noronha SM, Alves

- Corrêa de Noronha SA, Ferreira LM. Review of Major Theories of Skin Aging. *Adv Aging Res.* 2014;03(04):265–84.
47. Karim PL, Inda Astri Aryani, Nopriyati. Anatomy and Histologic of Intrinsic Aging Skin. *Biosci Med J Biomed Transl Res.* 2021;5(11):1165–77.
48. Gromkowska-Kępka KJ, Puścion-Jakubik A, Markiewicz-Żukowska R, Socha K. The Impact of Ultraviolet Radiation on Skin Photoaging — Review of In Vitro Studies. *J Cosmet Dermatol.* 2021;20(11):3427–31.
49. Flament F, Bazin R, Laquieze S, Rubert V, Simonpietri E, Piot B. Effect of the sun on visible clinical signs of aging in Caucasian skin. *Clin Cosmet Investig Dermatol.* 2013;6:221–32.
50. Kasolang S, Adlina WA, Rahman NA, Roseley NRN. Common skin disorders: A review. *J Tribol.* 2020;25(April):59–82.
51. Weihermann AC, Lorencini M, Brohem CA, de Carvalho CM. Elastin Structure and Its Involvement In Skin Photoageing. *Int J Cosmet Sci.* 2017;39(3):241–7.
52. Hsu YC, Fuchs E. Building and Maintaining the Skin. *Cold Spring Harb Perspect Biol.* 2022;14(7).
53. Krutmann J, Schalka S, Watson REB, Wei L, Morita A. Daily Photoprotection to Prevent Photoaging. *Photodermatol Photoimmunol Photomed.* 2021;37(6):482–9.
54. Mohiuddin AK. Skin Aging & Modern Age Anti-aging Strategies. *Glob J Med Res.* 2019;7(4):15–60.
55. Solway et al. Dieta e Dermatologia: O Papel de uma Dieta Integral à Base de Plantas na Prevenção e Reversão do Envelhecimento da Pele - Uma Revisão. *J Clin Aesthet Dermatol.* 2020;13(5):38–42.
56. Fitrianingsih S, Nafi'ah LN, Ismah K. Studi Literatur: Formulasi Krim Dari Bahan Alam Pada Aktivitas Antiaging. *Cendekia J Pharm.* 2022;6(2):318–25.
57. Juncan AM, Moisă DG, Santini A, Morgovan C, Rus LL, Vonica-țincu AL, et al. Advantages of Hyaluronic Acid and Its Combination With Other Bioactive Ingredients In Cosmeceuticals. *Molecules.* 2021;26(15):1–43.
58. Knaggs H, Lephart ED. Enhancing Skin Anti-Aging through Healthy Lifestyle Factors. *Cosmetics.* 2023;10(5).
59. Son D hye, Park W jin, Lee Y jae. Recent Advances in Anti-Aging Medicine. 2019;289–96.
60. Ayaz M, Sadiq A, Junaid M, Ullah F, Subhan F, Ahmed J. Neuroprotective and Anti-Aging Potentials of Essential Oils From Aromatic and Medicinal Plants. *Front Aging Neurosci.* 2017;9(MAY):1–16.
61. Nimse SB, Pal D. Free Radicals, Natural Antioxidants, and Their Reaction Mechanisms. *RSC Adv.* 2015;5(35):27986–8006.
62. Zuo X, Gu Y, Wang C, Zhang J, Zhang J, Wang G, et al. A Systematic Review of the Anti-Inflammatory and Immunomodulatory Properties of 16 Essential Oils of Herbs. *Evidence-based Complement Altern Med.* 2020;2020.
63. Avola R, Granata G, Geraci C, Napoli E, Graziano ACE, Cardile V. Oregano (*Origanum vulgare L.*) Essential Oil Provides Anti-Inflammatory Activity and Facilitates Wound Healing In A Human Keratinocytes Cell Model. *Food Chem Tol.* 2020;144(June):111586. Available from:

- <https://doi.org/10.1016/j.fct.2020.111586>
64. Guzmán E, Lucia A. Essential Oils and Their Individual Components In Cosmetic Products. *Cosmetics*. 2021;8(4):1–28.
65. Maddheshiya S, Ahmad A, Ahmad W, Zakir F, Aggarwal G. Essential Oils For the Treatment of Skin Anomalies: Scope And Potential. *South African J Bot.* 2022;151:187–97. Available from: <https://doi.org/10.1016/j.sajb.2021.12.034>
66. Choi JY, Fuerst R, Knapinska AM, Taylor AB, Smith L, Cao X, et al. Structure-Based Design and Synthesis Of Potent And Selective Matrix Metalloproteinase 13 Inhibitors. *J Med Chem.* 2017;60(13):5816–25.
67. Von Nussbaum F, Li VM, Meibom D, Anlauf S, Bechem M, Delbeck M, et al. Potent and Selective Human Neutrophil Elastase Inhibitors with Novel Equatorial Ring Topology: In vivo Efficacy of the Polar Pyrimidopyridazine BAY-8040 in a Pulmonary Arterial Hypertension Rat Model. *ChemMedChem.* 2016;11(2):199–206.
68. Chao KL, Muthukumar L, Herzberg O. Structure Of Human Hyaluronidase-1, A Hyaluronan Hydrolyzing Enzyme Involved In Tumor Growth and Angiogenesis. *Biochemistry*. 2007;46(23):6911–20.
69. Lai X, Wicher HJ, Soler-Lopez M, Dijkstra BW. Structure of Human Tyrosinase Related Protein 1 Reveals a Binuclear Zinc Active Site Important for Melanogenesis. *Angew Chemie - Int Ed.* 2017;56(33):9812–5.
70. Makatita FA, Wardhani R, Nuraini. Riset In Silico Dalam Pengembangan Sains di Bidang Pendidikan, Studi Kasus: Analisis Potensi Cendana Sebagai Agen Anti-Aging. *J ABDI.* 2020;2(1):59–67.
71. Mirza DM. Studi In Silico dan In Vitro Aktivitas Antineuroinflamasi Ekstrak Etanol 96% Daun Marsilea crenata C Presl. Skripsi. 2019;1–134.
72. Viceconti M, Henney A, Morley-Fletcher E. In Silico Clinical Trials: How Computer Simulation Will Transform the Biomedical Industry. *Int J Clin Trials.* 2016;3(2):37.
73. Pope DJ, Fryer R, Masouros SD. In Silico Models. *Blast Inj Sci Eng A Guid Clin Res Second Ed.* 2023;(January):279–84.
74. Agamah FE, Mazandu GK, Hassan R, Bope CD, Thomford NE, Ghansah A, et al. Computational/In Silico Methods In Drug Target and Lead Prediction. *Brief Bioinform.* 2020;21(5):1663–75.
75. Ledda M, Pluchino A, Ragusa M. Unraveling Evolutionary Dynamics : Insights from In Silico Experiments on Selective Mechanisms in Controlled Environments. 2023;1–28.
76. Fan J, Fu A, Zhang L. Progress in Molecular Docking. *Quant Biol.* 2019;7(2):83–9.
77. Zhu H. Big data and artificial intelligence modeling for drug discovery. *Annu Rev Pharmacol Tol.* 2020;60:573–89.
78. Nightingale S, Spiby H, Sheen K, Slade P. LJMU Research Online m. Tour Recreat Res. 2018;19. Available from: <http://researchonline.ljmu.ac.uk/id/eprint/8705/>
79. Jean-Quartier C, Jeanquartier F, Jurisica I, Holzinger A. In silico Cancer Research Towards 3R. *BMC Cancer.* 2018;18(1):1–12.
80. Methods C aided DD. Antibiotics. *Biotechnol Bioeng.* 1965;7(1):29–51.
81. Singh DB, Pathak RK. Bioinformatics: Methods and Applications.

- Bioinforma Methods Appl. 2021;1–488.
82. Wang X, Song K, Li L, Chen L. Structure-Based Drug Design Strategies and Challenges. *Curr Top Med Chem.* 2018;18(12):998–1006.
83. Sharma V, Wakode S, Kumar H. Structure- and Ligand-Based Drug Design: Concepts, Approaches, and Challenges. *Chemoinformatics Bioinforma Pharm Sci.* 2021;(August):27–53.
84. Ajjarapu SM, Tiwari A, Ramteke PW, Singh DB, Kumar S. Ligand-Based Drug Designing. *Bioinforma Methods Appl.* 2021;233–52.
85. Setiawan H, Irawan MI. Kajian Pendekatan Penempatan Ligand Pada Protein Menggunakan Algoritma Genetika. *J Sains dan Seni ITS.* 2017;6(2):2–6.
86. Pinzi L, Rastelli G. Metode Berbasis Struktur Bergantung Pada Informasi yang Diperoleh dari Pengetahuan Tentang Struktur 3D Target yang Menarik, dan Mereka Memungkinkan Database Peringkat Molekul Sesuai dengan Struktur dan Komplementaritas Elektronik Ligand Ke Target Tertentu. Igms Drug Discov InternatInPinzi, L, Rastelli, G (2019) Mol docking Shifting Parad J Mol Sci 20(18) <https://doi.org/103390/ijms20184331>ternational J Mol Sci. 2019;20(18):1–23.
87. Ferreira LG, Dos Santos RN, Oliva G, Andricopulo AD. Molecular Docking and Structure-Based Drug Design Strategies. Vol. 20, *Molecules.* 2015. 13384–13421 p.
88. Rudrapal M, Chetia D. Virtual Screening, Molecular Docking and QSAR Studies in Drug Discovery and Development Programme. *J Drug Deliv Ther.* 2020;10(4):225–33.
89. Spassov DS. Binding Affinity Determination in Drug Design: Insights from Lock and Key, Induced Fit, Conformational Selection, and Inhibitor Trapping Models. *Int J Mol Sci.* 2024;25(13).
90. Tripathi A, Bankaitis VA. Molecular Docking : From Lock and Key to. *J Mol Med Clin Appl.* 2017;2 (1):1–9. Available from: <http://dx.doi.org/10.16966/2575-0305.106>
91. Rožman K, Lešník S, Brus B, Hrast M, Sova M, Patin D, et al. Discovery of New Mura Inhibitors Using Induced-Fit Simulation and Docking. *Bioorganic Med Chem Lett.* 2017;27(4):944–9.
92. Raval K, Ganatra T. Basics, Types and Applications of Molecular Docking: A Review. *IP Int J Compr Adv Pharmacol.* 2022;7(1):12–6.
93. Yadava U. Search Algorithms and Scoring Methods In Protein-Ligand Docking. *Endocrinol Int J.* 2018;6(6):359–67.
94. Pagadala NS, Syed K, Tuszyński J. Software for Molecular Docking: A Review. *Biophys Rev.* 2017;9(2):91–102. Available from: <http://dx.doi.org/10.1007/s12551-016-0247-1>
95. Khamis MA, Gomaa W, Ahmed WF. Machine Learning In Computational Docking. *Artif Intell Med.* 2015;63(3):135–52. Available from: <http://dx.doi.org/10.1016/j.artmed.2015.02.002>
96. Butt SS, Badshah Y, Shabbir M, Rafiq M. Molecular Docking Using Chimera and Autodock Vina Software for Nonbioinformaticians. *JMIR Bioinforma Biotechnol.* 2020;1(1):1–25.
97. Solis-Vasquez L, Tillack AF, Santos-Martins D, Koch A, LeGrand S, Forli S. Benchmarking the Performance of Irregular Computations In Autodock-GPU Molecular Docking. *Parallel Comput.* 2022;109:1–39.

98. Nguyen NT, Nguyen TH, Pham TNH, Huy NT, Bay M Van, Pham MQ, et al. Autodock Vina Adopts More Accurate Binding Poses but Autodock4 Forms Better Binding Affinity. *J Chem Inf Model.* 2020;60(1):204–11.
99. Che X, Liu Q, Zhang L. An Accurate and Universal Protein-Small Molecule Batch Docking Solution Using Autodock Vina. *Results Eng.* 2023;19(May):101335. Available from: <https://doi.org/10.1016/j.rineng.2023.101335>
100. Ravindranath PA, Forli S, Goodsell DS, Olson AJ, Sanner MF. AutoDockFR: Advances in Protein-Ligand Docking with Explicitly Specified Binding Site Flexibility. *PLoS Comput Biol.* 2015;11(12):1–28.
101. Kaftallı J, Bernini A, Bonetti G, Cristoni S, Marceddu G, Bertelli M. MAGI-Dock: a PyMOL Companion to Autodock Vina. *Eur Rev Med Pharmacol Sci.* 2023;27:148–51.
102. David L, Thakkar A, Mercado R, Engkvist O. Molecular Representations In AI-Driven Drug Discovery: A Review and Practical Guide. *J Cheminform.* 2020;12(1):1–22. Available from: <https://doi.org/10.1186/s13321-020-00460-5>
103. Rayan B, Rayan A. Avogadro Program for Chemistry Education: To What Extent can Molecular Visualization and Three-dimensional Simulations Enhance Meaningful Chemistry Learning? *World J Chem Educ.* 2017;5(4):136–41.
104. Pawar SS, Rohane SH. Review on Discovery Studio: An important Tool for Molecular Docking. *Asian J Res Chem.* 2021;14(1):1–3.
105. Shaw M, Petzer A, Petzer JP, Cloete TT. The Pterin Binding Site of Dihydropteroate Synthase (DHPS): In Silico Screening and In Vitro Antibacterial Activity of Existing Drugs. *Results Chem.* 2023;5(November 2022).
106. Saudale FZ, Lerrick RI, Parikesit AA, Mariti F. Chemistry Teachers' Awareness, Understanding, and Confidence Toward Computational Tools for Molecular Visualization. *J Pendidik IPA Indones.* 2019;8(4):436–46.
107. Silva J, Marinho MM, Marinho ES. Comparative Study of Molecular Docking Between the Carotenoid Bixin and HIV Inhibitor Protease Indinavir. *Int J Recent Res Rev.* 2018;XI(2):18–25.
108. Romanov M. Technical automation of Windows platform testing. 2019;(October). Available from: <https://www.theseus.fi/handle/10024/261042>
109. Mvondo JGM, Matondo A, Mawete DT, Bambi SMN, Mbala BM, Lohohola PO. In Silico ADME/T Properties of Quinine Derivatives using SwissADME and pkCSM Webservers. *Int J Trop Dis Heal.* 2021;42(11):1–12.
110. Mathematics A. Studi Penambatan Molekul dan Simulasi Dinamika Molekuler Senyawa Turunan Flavonoid dari Ekstrak Batang Gandaria. 2016;1–23.
111. Nagy PI. Competing intramolecular vs. Intermolecular Hydrogen Bonds In Solution. Vol. 15, International Journal of Molecular Sciences. 2014. 19562–19633 p.
112. Simanjuntak AP, Roza D. Seminar Nasional Kimia Dan Pendidikan Kimia Iv. 2021;(Media Webblog, Motivasi Belajar, Hasil Belajar dan Ikatan Kimia):275–9.

113. Aziz A, Andrianto D, Safithri M. Penambatan Molekuler Senyawa Bioaktif Daun Wungu (*Graptophyllum Pictum* (L) Griff) sebagai Inhibitor Tirosinase. *Indones J Pharm Sci Technol.* 2022;9(2):94.
114. Res IJC, Potensi S, Tersubstitusi P, Tiosemikarbazone D, Kilo A La, Aman LO, et al. Sebagai Agen Antiameba Melalui Uji In Silico Study of Potential of 1-N-Substituted Pyrazoline Analogues of Thiosemicarbazones as Antiamoebic Agent using In Silico Screening. 2019;7(1):9–24.
115. Dappe YJ, Basanta MA, Flores F, Ortega J. Weak Chemical Interaction And Van Der Waals Forces Between Graphene Layers: A Combined Density Functional And Intermolecular Perturbation Theory Approach. *Phys Rev B - Condens Matter Mater Phys.* 2006;74(20).
116. Sahu VK, Khan AKR, Singh RK, Singh PP. Hydrophobic, Polar and Hydrogen Bonding Based Drug-Receptor Interaction of Tetrahydroimidazobenzodiazepinones. *Am J Immunol.* 2008;4(3):33–42.
117. Sun Q. The Hydrophobic Effects: Our Current Understanding. *Molecules.* 2022;27(20).
118. Rena SR, Nurhidayah N, Rustan R. Analisis Molecular Docking Senyawa Garcinia Mangostana L Sebagai Kandidat Anti SARS-CoV-2. *J Fis Unand.* 2022;11(1):82–8.
119. da Fonseca AM, Caluaco BJ, Madureira JMC, Cabongo SQ, Gaieta EM, Djata F, et al. Screening of Potential Inhibitors Targeting the Main Protease Structure of SARS-CoV-2 via Molecular Docking, and Approach with Molecular Dynamics, RMSD, RMSF, H-Bond, SASA and MMGBSA. *Mol Biotechnol.* 2023;(February 2024). Available from: <https://doi.org/10.1007/s12033-023-00831-x>
120. Endriyatno NC, Walid M. Studi In Silico Kandungan Senyawa Daun Sriyana (*Annona squamosa* L.) Terhadap Protein Dihydrofolate Reductase Pada *Mycobacterium tuberculosis*. *Pharmacon J Farm Indones.* 2022;19(1):87–98.
121. Muslikh FA, Kurniawati E, Ma’arif B, Zenmas SZ, Salmasfattah N, Dhafin AA, et al. ADMET Prediction of the Dominant Compound from Mangosteen (*Garcinia mangostana* L.) using pkCSM: A Computational Approach. *Int J Contemp Sci.* 2023;1(1):33–8.
122. Setiawan R. Isolasi Dan Karakterisasi Senyawa Penanda dari Ekstrak Rimpang Bangle (*Zingiber Cassumunar*) Isolation and Characterization of Marker Compound from Bangle Rhizome Extract (*Zingiber cassumunar*). 2022;
123. Devkota HP, Paudel KR, Hassan MM, Dirar AI, Das N, Adhikari-Devkota A, et al. Bioactive Compounds from Zingiber Montanum and Their Pharmacological Activities With Focus On Zerumbone. *Appl Sci.* 2021;11(21):1–24.
124. Masyita A, Mustika Sari R, Dwi Astuti A, Yasir B, Rahma Rumata N, Emran T Bin, et al. Terpenes and Terpenoids As Main Bioactive Compounds of Essential Oils, Their Roles In Human Health and Potential Application As Natural Food Preservatives. *Food Chem X.* 2022;13(January):100217. Available from: <https://doi.org/10.1016/j.fochx.2022.100217>

- 125 Karim BK, Tsamarah DF, Zahira A, et al. In-Silico Study of Active Compounds in Guava Leaves (*Psidium guajava L.*) as Candidates for Breast Anticancer Drugs. 2023;3(3):194-209.
- 126 Mahdiyah U. Pencarian Rongga Berpotensi Binding Site pada Protein dengan Menggunakan Support Vector Machine (SVM). J Math. and Its Appl. 2017;14(2):89-101.
127. Nauli T. Penentuan Sisi Aktif Selulase *Aspergillus Niger* dengan Docking Ligand. JKTI. 2014;16(2):94-100.
128. Mutiara YM, Wahjudi M, Kok T. Studi In Silico Potensi Piperine, Piperlongumine, dan Thymoquinone sebagai Obat Alzheimer. Indonesian Journal of Biotechnology and Biodiversity. 2022;6(3):77-87.
129. Aswad M, Christine L, Nursamsiar, Hardianti B. Studi Penambatan Molekul Senyawa-Senyawa Bioaktif dari Kulit Akar Murbei (*Morus Sp.*) terhadap Reseptor Tnf-A. MFF. 2019;23(3):85-100.
130. Lai X, Wicher HJ, Lopez MS, Dijkstra BW. Structure of Human Tyrosinase Related Protein 1 Reveals a Binuclear Zinc ActiveSite Important for Melanogenesis. Angewandte Chemical International Edition. 2017; 56:9812 –9815.
131. Benet LZ, Hosey CM, Ursu O, Oprea TI. BDDCS, the Rule of 5 and Drugability. Adv Drug Deliv Rev. 2016:89-98.
132. Lailiyah H, Lisdiana L. Uji Aktivitas Antibakteri Senyawa Aktif Temu Kunci (*Boesenbergia rotunda*) terhadap *Mycobacterium tuberculosis* secara In Silico. Lentera Bio. 2023;12(2):132-149.
133. Abdullah SS, Putra PP, Antasionasti I. Analisis Sifat Fisikokimia, Farmakokinetik dan Toksikologi pada Pericarpium Pala (*Myristica Fragrans*) secara Artificial Intelligence. Chem Prog. 2021;14(2):81-92.
134. Chen CP, Chen CC, Huang CW, Chang YC. Evaluating Molecular Properties Involved in Transport of Small Molecules in Stratum Corneum: A Quantitative Structure-Activity Relationship for Skin Permeability. Molecules. 2018;23(911):1-17.
135. Krihariyani D, Sasongkowati R, Haryanto E. Studi In Silico Sifat Farmakokinetik, Toksisitas, dan Aktivitas Imunomodulator Brazilein Kayu Secang terhadap Enzim 3-Chymotrypsin-Like Cysteine Protease Coronavirus. J of Indonesian Medical Laboratory and Science. 2020;1(1):76-90.
136. Buscher B, Laakso S, Mascher H. Bioanalysis for Plasma Protein Binding Studies in Drug Discovery and Drug Development: Views and Recommendations of The European Bioanalysis Forum. Bioanalysis. 2014;6(5):673-682.
137. Guttman Y, Kerem Z. Dietary Inhibitors of CYP3A4 Are Revealed Using Virtual Screening by Using a New Deep-Learning Classifier. J of Agricultural and Food Chemistry. 2022;70:2752-2761.
138. Andrade C. The Practical Importance of Half-Life in Psychopharmacology. Clinical and Practical Psychopharmacology. 2022;83(4):1-5.
139. European Medicines Agency. Guideline On The Need For Carcinogenicity Studies Of Pharmaceuticals. 1996.

140. Farabaugh CS, Doak S, Roy S, Elespuru R. In vitro Micronucleus Assay: Method for Assessment of Nanomaterials Using Cytochalasin B. *Frontiers in Toxicology*. 2023;1-5.
141. Patlewicz G, Aptula AO, Roberts DW, Uriarte E. Skin Sensitisation (Q)Sars/Expert Systems: From Past, Present to Future. European Commission Directorate-General Joint Research Centre Institute IHCP. 2007.
142. Holford N, Yim DS. Clearance. *Trans Clin Pharmacol*. 2015;23(2):42-45.

