

DAFTAR PUSTAKA

1. Torres A, Cilloniz C, Niederman MS, Menéndez R, Chalmers JD, Wunderink RG, dkk. Pneumonia. Nat Rev Dis Primers. 8 Desember 2021;7(1):25.
2. Jondle CN, Gupta K. Klebsiella pneumoniae infection of murine neutrophils impairs their efferocytic clearance by modulating cell death machinery. PLoS Pathog. 2018;14(10).
3. Tsereteli M, Sidamonidze K, Tsereteli D, Malania L, Vashakidze E. Epidemiology Of Carbapenem-Resistant Klebsiella Pneumoniae in Intensive Care Units of Multiprofile Hospitals in Tbilisi, Georgia. Georgian Med News. 2018;(280–281).
4. Esposito EP, Cervoni M, Bernardo M, Crivaro V, Cuccurullo S, Imperi F, dkk. Molecular epidemiology and virulence profiles of colistin-resistant Klebsiella pneumoniae blood isolates from the hospital agency “Ospedale dei Colli,” Naples, Italy. Front Microbiol. 2018;9(JUL).
5. Nguyen M, Brettin T, Long SW, Musser JM, Olsen RJ, Olson R, dkk. Developing an in silico minimum inhibitory concentration panel test for Klebsiella pneumonia. Sci Rep. 2018;8(1).
6. Cho J, Lee M, Skyler Cochrane C, Webster CG, Fenton BA, Zhao J, dkk. Structural basis of the UDP-diacylglicosamine pyrophosphohydrolase LpxH inhibition by sulfonyl piperazine antibiotics. Proc Natl Acad Sci U S A. 2020;117(8).
7. Daina A, Michelin O, Zoete V. SwissADME: A free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. Sci Rep. 2017;7.
8. Navien TN, Thevendran R, Hamdani HY, Tang TH, Citartan M. In silico molecular docking in DNA aptamer development. Vol. 180, Biochimie. 2021.
9. Huang SY, Grinter SZ, Zou X. Scoring functions and their evaluation methods for protein-ligand docking: Recent advances and future directions. Physical Chemistry Chemical Physics. 2010;12(40).
10. AD Puspita. Studi Hubungan Kuantitatif Struktur Aktivitas, Penelusuran Farmakofor, Virtual Skrining, Docking Molekul, Uji Toksisitas dan Profil Farmakokinetik Senyawa Turunan Kumarin-Kalkon-Urea Sebagai Agen Antikanker Pada Kanker Hati Secara In Silico. UIN Alauddin Makassar. 2018;
11. Myatt GJ, Ahlberg E, Akahori Y, Allen D, Amberg A, Anger LT, dkk. In silico toxicology protocols. Regulatory Toxicology and Pharmacology. 2018;96.

12. Viceconti M, Pappalardo F, Rodriguez B, Horner M, Bischoff J, Musuamba Tshinanu F. In silico trials: Verification, validation and uncertainty quantification of predictive models used in the regulatory evaluation of biomedical products. *Methods*. 2021;185.
13. Rim KT. In silico prediction of toxicity and its applications for chemicals at work. Vol. 12, *Toxicology and Environmental Health Sciences*. 2020.
14. Singh N, Chaput L, Villoutreix BO. Virtual screening web servers: Designing chemical probes and drug candidates in the cyberspace. Vol. 22, *Briefings in Bioinformatics*. Oxford University Press; 2021. hlm. 1790–818.
15. Gimeno A, Ojeda-Montes MJ, Tomás-Hernández S, Cereto-Massagué A, Beltrán-Debón R, Mulero M, dkk. The light and dark sides of virtual screening: What is there to know? Vol. 20, *International Journal of Molecular Sciences*. 2019.
16. Kimber TB, Chen Y, Volkamer A. Deep learning in virtual screening: Recent applications and developments. Vol. 22, *International Journal of Molecular Sciences*. MDPI; 2021.
17. Wilson GL, Lill MA. Integrating structure-based and ligand-based approaches for computational drug design. *Future Med Chem* [Internet]. 2011;3(6):735–50. Tersedia pada: <https://doi.org/10.4155/fmc.11.18>
18. Maia EHB, Assis LC, de Oliveira TA, da Silva AM, Taranto AG. Structure-Based Virtual Screening: From Classical to Artificial Intelligence. Vol. 8, *Frontiers in Chemistry*. 2020.
19. Fan J, Fu A, Zhang L. Progress in molecular docking. Vol. 7, *Quantitative Biology*. 2019.
20. Abraham DJ. Burger's Medicinal Chemistry and Drug Discovery. *Burger's Medicinal Chemistry and Drug Discovery*. 2003.
21. Gao H, Nishida J, Saito S, Kawabata J. Inhibitory effects of 5,6,7-trihydroxyflavones on tyrosinase. *Molecules*. 2007;12(1).
22. Pinzi L, Rastelli G. Molecular docking: Shifting paradigms in drug discovery. Vol. 20, *International Journal of Molecular Sciences*. 2019.
23. Waterer G. What is pneumonia? Vol. 17, *Breathe*. 2021.
24. Prina E, Ranzani OT, Torres A. Community-acquired pneumonia. Dalam: *The Lancet*. Lancet Publishing Group; 2015. hlm. 1097–108.
25. G BJ, M ML. Community-Acquired Pneumonia. *New England Journal of Medicine* [Internet]. 3 Juli 2024;333(24):1618–24. Tersedia pada: <https://doi.org/10.1056/NEJM199512143332408>

26. Warganegara E. Pneumonia Nosokomial (Hospital-acquired, Ventilator-associated, dan Health Care-associated Penumonia). Jurnal Kedokteran Universitas Lampung. 1 Oktober 2017;1(3):612–8.
27. Martin RM, Bachman MA. Colonization, infection, and the accessory genome of Klebsiella pneumoniae. Vol. 8, *Frontiers in Cellular and Infection Microbiology*. 2018.
28. Effah CY, Sun T, Liu S, Wu Y. Klebsiella pneumoniae: an increasing threat to public health. *Ann Clin Microbiol Antimicrob [Internet]*. 2020;19(1):1. Tersedia pada: <https://doi.org/10.1186/s12941-019-0343-8>
29. Zhu J, Wang T, Chen L, Du H. Virulence Factors in Hypervirulent Klebsiella pneumoniae. Vol. 12, *Frontiers in Microbiology*. 2021.
30. Abbaz T, Bendjeddou A, Villemin D. Structural and quantum chemical studies on aryl sulfonyl piperazine derivatives. *Journal of Drug Delivery and Therapeutics*. 2019;9(1-s).
31. Koes DR. The Pharmit backend: A computer systems approach to enabling interactive online drug discovery. *IBM J Res Dev*. 2018;62(6).
32. Sunseri J, Koes DR. Pharmit: interactive exploration of chemical space. *Nucleic Acids Res*. 2016;44(W1).
33. Wermuth CG, Ganellin CR, Lindberg P, Mitscher LA. Glossary of terms used in medicinal chemistry (IUPAC Recommendations 1998). 1998;70(5):1129–43. Tersedia pada: <https://doi.org/10.1351/pac199870051129>
34. Gao Q, Wang Y, Hou J, Yao Q, Zhang J. Multiple receptor-ligand based pharmacophore modeling and molecular docking to screen the selective inhibitors of matrix metalloproteinase-9 from natural products. *J Comput Aided Mol Des [Internet]*. 2017;31(7):625–41. Tersedia pada: <https://doi.org/10.1007/s10822-017-0028-3>
35. Bernstein FC, Koetzle TF, Williams GJB, Meyer EF, Brice MD, Rodgers JR, dkk. The protein data bank: A computer-based archival file for macromolecular structures. *J Mol Biol*. 25 Mei 1977;112(3):535–42.
36. Goodsell DS, Zardecki C, di Costanzo L, Duarte JM, Hudson BP, Persikova I, dkk. RCSB Protein Data Bank: Enabling biomedical research and drug discovery. Vol. 29, *Protein Science*. 2020.
37. Berman HM, Westbrook J, Feng Z, Gilliland G, Bhat TN, Weissig H, dkk. The Protein Data Bank. Vol. 28, *Nucleic Acids Research*. 2000.

38. 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 Health. 2021;
39. Jr. WF de A, Escola. Docking Screens for Drug Discovery. Vol. 2053, Methods in Molecular Biology. 2019.
40. McNutt AT, Francoeur P, Aggarwal R, Masuda T, Meli R, Ragoza M, dkk. GNINA 1.0: molecular docking with deep learning. J Cheminform. 1 Desember 2021;13(1).
41. Sunseri J, Koes DR. Virtual screening with gnina 1.0. Molecules. 1 Desember 2021;26(23).
42. Hanwell MD, Curtis DE, Lonie DC, Vandermeersch T, Zurek E, Hutchison GR. Avogadro: An advanced semantic chemical editor, visualization, and analysis platform. J Cheminform. Agustus 2012;4(8).
43. Johnston B. Google Colab | Educational & Classroom Technologies. [Internet]. [dikutip 3 November 2022]. Tersedia pada: <https://mcgrawect.princeton.edu/tool/google-colab/>
44. O'Boyle NM, Banck M, James CA, Morley C, Vandermeersch T, Hutchison GR. Open Babel: An Open chemical toolbox. J Cheminform. 2011;3(10).
45. Irwin JJ, Tang KG, Young J, Dandarchuluun C, Wong BR, Khurelbaatar M, dkk. ZINC20 - A Free Ultralarge-Scale Chemical Database for Ligand Discovery. J Chem Inf Model. 28 Desember 2020;60(12):6065–73.
46. Studio D. Dassault Systemes BIOVIA, Discovery Studio Modelling Environment, Release 4.5. Accelrys Software Inc. 2015;
47. Putra PP. Penambatan molekul dengan PLANTS dalam kimia medisinal. 1 ed. Banyumas: Wawasan Ilmu; 2023. 54–58 hlm.