

DAFTAR PUSTAKA

1. World Health Organization. *Cancer* [Internet]. 2022 [cited 2024 Jan 16]. Available from: <https://www.who.int/news-room/fact-sheets/detail/cancer>
2. Singer S, Goerling U, Mehnert A. *PsychoOncology: Psychosocial Impact of Cancer*. 2018.
3. DiPiro JT, Yee GC, Posey LM, Hainer ST, Nolin TD, Ellingrod V. *Pharmacotherapy: A Pathophysiologic Approach*. 11th ed. McGraw-Hill; 2020.
4. Sung H, Ferlay J, Siegel RL, Laversanne M, Soerjomataram I, Jemal A, et al. Global Cancer Statistics 2020: GLOBOCAN Estimates of Incidence and Mortality Worldwide for 36 Cancers in 185 Countries. *CA Cancer J Clin*. 2021 May;71(3):209–49.
5. Mao Y, Yang D, He J, Krasna MJ. Epidemiology of Lung Cancer. Vol. 25, *Surgical Oncology Clinics of North America*. W.B. Saunders; 2016. p. 439–45.
6. Zhang Q, Liu J, Li R, Zhao R, Zhang M, Wei S, et al. A Network Pharmacology Approach to Investigate the Anticancer Mechanism and Potential Active Ingredients of *Rheum palmatum* L. Against Lung Cancer via Induction of Apoptosis. *Front Pharmacol*. 2020 Nov 4;11.
7. El-Kenawy AEM, Hassan SMA, Osman HEH. Mangosteen (*Garcinia mangostana* L.). In: *Nonvitamin and Nonmineral Nutritional Supplements*. Elsevier; 2018. p. 313–9.
8. Ansori ANM, Fadholly A, Hayaza S, Susilo RJK, Inayatillah B, Winarni D, et al. A Review on Medicinal Properties of Mangosteen (*Garcinia mangostana* L.). *Res J Pharm Technol*. 2020 Feb 1;13(2):974–82.
9. Zhang C, Yu G, Shen Y. The Naturally Occurring Xanthone α -mangostin Induces ROS-mediated Cytotoxicity in Non-small Scale Lung Cancer Cells. *Saudi J Biol Sci*. 2018 Sep 1;25(6):1090–5.
10. Shih YW, Chien ST, Chen PS, Lee JH, Wu SH, Yin L Te. α -Mangostin Suppresses Phorbol 12-myristate 13-acetate-induced MMP-2/MMP-9 Expressions via α v β 3 Integrin/FAK/ERK and NF- κ B Signaling Pathway in Human Lung Adenocarcinoma A549 Cells. *Cell Biochem Biophys*. 2010;58(1):31–44.
11. Kaomongkolgit R, Chaisomboon N, Pavasant P. Apoptotic Effect of Alpha-mangostin on Head and Neck Squamous Carcinoma Cells. *Arch Oral Biol*. 2011 May;56(5):483–90.
12. Seo KH, Ryu HW, Park MJ, Park KH, Kim JH, Lee MJ, et al. Mangosenone F, A Furanoxanthone from *Garciana mangostana*, Induces Reactive Oxygen Species-Mediated Apoptosis in Lung Cancer Cells and Decreases Xenograft Tumor Growth. *Phytotherapy Research*. 2015 Nov 1;29(11):1753–60.
13. Ku MJ, Kim JH, Lee J, Cho JY, Chun T, Lee SY. Maclurin Suppresses Migration and Invasion of Human Non-small-Sell Lung Cancer Cells via Anti-oxidative Activity and Inhibition of the Src/FAK–ERK– β -catenin Pathway. *Mol Cell Biochem*. 2015 Feb 10;402(1–2):243–52.
14. Sahrina Hasibuan L, Fariqi A, Prayitno L, Bangun MB. Integrasi data Protein-Protein Interactions dan Pathway untuk Menentukan Score pada

- pathway Menggunakan Analisis Graf. *KLIK: Kajian Ilmiah Informatika dan Komputer*. 2023 Jun;3(6):719–27.
15. Faroby MHZ AI, Fadhilah HN, Sembiring FH. Identifikasi Interaksi Protein-Protein Meningitis Menggunakan ClusterONE dan Analisis Jaringan. *Journal of Advances in Information and Industrial Technology*. 2022 May 31;4(1):17–28.
 16. Zhang YH, Zeng T, Chen L, Huang T, Cai YD. Determining Protein–protein Functional Associations by Functional Rules Based on Gene Ontology and KEGG Pathway. *Biochim Biophys Acta Proteins Proteom*. 2021 Jun 1;1869(6).
 17. Zhang R, Zhu X, Bai H, Ning K. Network Pharmacology Databases for Traditional Chinese Medicine: Review and Assessment. Vol. 10, *Frontiers in Pharmacology*. Frontiers Media S.A.; 2019. p. 1–14.
 18. Patil SA, Patil VS, Malgi AP, Hupparage VB, Mallapur SP, Naik RR. *Cananga odorata* (Ylang-Ylang) modulate pathways involved in cancer: Gene set enrichment and network pharmacology approach. *International Journal of Ayurvedic Medicine*. 2023;14(2):453–63.
 19. Nasution NH, Nasutin IW. *Induksi Kalus Manggis (Garcinia mangostana L.): Sebuah Teknik dalam Kultur Jaringan Tanaman*. NEM; 2022.
 20. Gull A, Nayik GA. *Antioxidants in Fruits: Properties and Health Benefits*. Springer Nature Singapore; 2020. 83–98 p.
 21. Bi C, Xu H, Yu J, Ding Z, Liu Z. Botanical Characteristics, Chemical Components, Biological Activity, and Potential Applications of Mangosteen. *PeerJ*. 2023;11.
 22. National Center for Biotechnology Information. PubChem Compound Summary for CID 7020, Xanthone [Internet]. [cited 2024 Jan 16]. Available from: <https://pubchem.ncbi.nlm.nih.gov/compound/Xanthone>
 23. Gul S, Aslam K, Pirzada Q, Rauf A, Khalil AA, Semwal P, et al. Xanthonenes: A Class of Heterocyclic Compounds with Anticancer Potential. *Curr Top Med Chem*. 2022 Sep 3;22(23):1930–49.
 24. Rizaldy D, Hartati R, Nadhifa T, Fidrianny I. Chemical Compounds and Pharmacological Activities of Mangosteen (*Garcinia mangostana* L.) - Updated Review. Vol. 12, *Biointerface Research in Applied Chemistry*. AMG Transcend Association; 2022. p. 2503–16.
 25. National Center for Biotechnology Information. PubChem Compound Summary for CID 3102, Benzophenone [Internet]. [cited 2024 Jan 16]. Available from: <https://pubchem.ncbi.nlm.nih.gov/compound/Benzophenone>
 26. National Center for Biotechnology Information. PubChem Compound Summary for CID 145858, Flavylum [Internet]. [cited 2024 Jan 16]. Available from: <https://pubchem.ncbi.nlm.nih.gov/compound/Flavylum>
 27. Ovalle-Magallanes B, Eugenio-Pérez D, Pedraza-Chaverri J. Medicinal Properties of Mangosteen (*Garcinia mangostana* L.): A Comprehensive Update. Vol. 109, *Food and Chemical Toxicology*. Elsevier Ltd; 2017. p. 102–22.
 28. Li S. *Network Pharmacology*. Li S, editor. Singapore: Springer Nature Singapore; 2021.

29. Indradi RB, Pitaloka DAE, Suryani. Network Pharmacology to Uncover Potential Anti-inflammatory and Immunomodulatory Constituents in *Curcuma longa* Rhizome as Complementary Treatment in COVID-19. *Pharmacia*. 2022;69(4):995–1003.
30. Li S, Hu Y, Zhou X. *Network Pharmacology and Traditional Medicine: Setting the New Standards by Combining In silico and Experimental Work*. Frontiers Media SA; 2022.
31. Koh GCKW, Porras P, Aranda B, Hermjakob H, Orchard SE. Analyzing Protein-protein Interaction Networks. *J Proteome Res*. 2012 Apr 6;11(4):2014–31.
32. Milroy LG, Grossmann TN, Hennig S, Brunsveld L, Ottmann C. Modulators of Protein-protein Interactions. Vol. 114, *Chemical Reviews*. American Chemical Society; 2014. p. 4695–748.
33. Safari-Alighiarloo N, Taghizadeh M, Rezaei-Tavirani M, Goliaei B, Peyvandi AA. Protein-protein Interaction Networks (PPI) and Complex diseases. Vol. 7, *Gastroenterol Hepatol Bed Bench*. 2014.
34. Rao VS, Srinivas K, Sujini GN, Kumar GNS. Protein-Protein Interaction Detection: Methods and Analysis. *Int J Proteomics*. 2014 Feb 17;2014:1–12.
35. Mabonga L, Kappo AP. Protein-protein Interaction Modulators: Advances, Successes and Remaining Challenges. Vol. 11, *Biophysical Reviews*. Springer Verlag; 2019. p. 559–81.
36. Xing S, Wallmeroth N, Berendzen KW, Grefen C. Techniques for the Analysis of Protein-protein Interactions in Vivo. *Plant Physiol*. 2016 Jun 1;171(2):727–58.
37. Higuero AP, Jubb H, Blundell TL. Protein-protein Interactions as Druggable Targets: Recent Technological Advances. Vol. 13, *Current Opinion in Pharmacology*. Elsevier Ltd; 2013. p. 791–6.
38. Suharini YS, Ramli M, Sulistyowati, Endang R.D. Pendekatan Teori Graf untuk Analisis Jaringan Interaksi Protein-Protein. *IPTEK*. 2023 Aug;7(2):1–7.
39. Chen L, Zhang YH, Wang SP, Zhang YH, Huang T, Cai YD. Prediction and Analysis of Essential Genes Using the Enrichments of Gene Ontology and KEGG Pathways. *PLoS One*. 2017 Sep 1;12(9):1–22.
40. Xing Z, Chu C, Chen L, Kong X. The Use of Gene Ontology Terms and KEGG Pathways for Analysis and Prediction of Oncogenes. *Biochim Biophys Acta Gen Subj*. 2016 Nov 1;1860(11):2725–34.
41. Du J, Li M, Yuan Z, Guo M, Song J, Xie X, et al. A Decision Analysis Model for KEGG Pathway Analysis. *BMC Bioinformatics*. 2016 Oct 6;17(1):1–12.
42. Kanehisa M, Furumichi M, Tanabe M, Sato Y, Morishima K. KEGG: New Perspectives on Genomes, Pathways, Diseases and Drugs. *Nucleic Acids Res*. 2017 Jan 1;45(D1):D353–61.
43. Du J, Yuan Z, Ma Z, Song J, Xie X, Chen Y. KEGG-PATH: Kyoto Encyclopedia of Genes and Genomes-Based Pathway Analysis Using a Path Analysis Model. *Mol Biosyst*. 2014;10(9):2441–7.
44. Kanehisa M, Sato Y, Kawashima M, Furumichi M, Tanabe M. KEGG as a Reference Resource for Gene and Protein Annotation. *Nucleic Acids Res*. 2016;44(D1):D457–62.

45. Kanehisa M, Sato Y, Furumichi M, Morishima K, Tanabe M. New Approach for Understanding Genome Variations in KEGG. *Nucleic Acids Res.* 2019 Jan 8;47(D1):D590–5.
46. Dalmer TRA, Clugston RD. Gene Ontology Enrichment Analysis of Congenital Diaphragmatic Hernia-Associated Genes. Vol. 85, *Pediatric Research.* Nature Publishing Group; 2019. p. 13–9.
47. Huntley RP, Sawford T, Mutowo-Meullenet P, Shypitsyna A, Bonilla C, Martin MJ, et al. The GOA Database: Gene Ontology Annotation Updates for 2015. *Nucleic Acids Res.* 2015 Jan 28;43(D1):D1057–63.
48. Blake JA, Christie KR, Dolan ME, Drabkin HJ, Hill DP, Ni L, et al. Gene Ontology Consortium: Going Forward. *Nucleic Acids Res.* 2015 Jan 28;43(D1):D1049–56.
49. Chen L, Zhang YH, Zheng M, Huang T, Cai YD. Identification of Compound–Protein Interactions Through the Analysis of Gene Ontology, KEGG Enrichment for Proteins and Molecular Fragments of Compounds. *Molecular Genetics and Genomics.* 2016 Dec 1;291(6):2065–79.
50. McNutt AT, Francoeur P, Aggarwal R, Masuda T, Meli R, Ragoza M, et al. GNINA 1.0: Molecular Docking with Deep Learning. *J Cheminform.* 2021 Dec 1;13(1).
51. Lecun Y, Bengio Y, Hinton G. Deep Learning. Vol. 521, *Nature.* Nature Publishing Group; 2015. p. 436–44.
52. Jiménez-Luna J, Cuzzolin A, Bolcato G, Sturlese M, Moro S. A Deep-Learning Approach toward Rational Molecular Docking Protocol Selection. *Molecules.* 2020 Jun 1;25(11).
53. Fauziah A, Fatharani A, Nurawaliah CM, Rivianto FA, Sakina IV, Rahmawati M, et al. Molecular Docking of Compound with Potential as Anti-breast Cancer: Literature Review. *Journal of Pharmaceutical and Sciences* [Internet]. 2023;6(2):416–27. Available from: <https://www.journal-jps.com>
54. Ciccotti G, Dellago C, Ferrario M, Hernández ER, Tuckerman ME. Molecular Simulations: Past, Present, and Future (A Topical Issue in EPJB). Vol. 95, *European Physical Journal B.* Springer Science and Business-Media Deutschland GmbH; 2022.
55. Alonso H, Bliznyuk AA, Gready JE. Combining Docking and Molecular Dynamic Simulations in Drug Design. Vol. 26, *Medicinal Research Reviews.* 2006. p. 531–68.
56. Refianti R, Mutiara AB, Astuti AD, Refianti R, Mutiara AB. Molecular Dynamics Simulation on Protein Using Gromacs [Internet]. Vol. 9, *Article in International Journal of Computer Science and Information Security.* 2011. Available from: <http://www.fftw.org>
57. Prayoga H, Yulianti Y, Riyanto A. Analisis Dinamika Molekul Protein Lysozyme Putih Telur Dengan Model Potensial Lennard-Jones Menggunakan Aplikasi Gromacs. Vol. 06, *Jurnal Teori dan Aplikasi Fisika.* 2018.
58. Martín-García F, Papaleo E, Gomez-Puertas P, Boomsma W, Lindorff-Larsen K. Comparing Molecular Dynamics Force Fields in the Essential Subspace. *PLoS One.* 2015 Mar 26;10(3).

59. Ponder JW, Case DA. *Force Fields for Protein Simulations*. Vol. 66. 2003. p. 27–85.
60. Mardiana M, Ruswanto. Simulasi Dinamika Molekular Senyawa Pyridin Pada Protein 2XNB Sebagai Antikanker Menggunakan Aplikasi Gromas. *ResearchGate* [Internet]. 2019;9(5):1–15. Available from: <https://www.researchgate.net/publication/335601273>
61. Wang J, Wolf RM, Caldwell JW, Kollman PA, Case DA. Development and Testing of a General Amber Force Field. *J Comput Chem*. 2004;25:1157–74.
62. Putra PP, Junaidin. *Simulasi Molecular Dynamics Protein-Ligand, Perhitungan MMPBSA dan MMGBSA Menggunakan Gromacs*. Maladan Y, editor. Malang: Future Science; 2022.
63. Lindahl E. Molecular Dynamics Simulations. *Methods in Molecular Biology*. 2015;1215:3–26.
64. Van Der Spoel D, Lindahl E, Hess B, Groenhof G, Mark AE, Berendsen HJC. GROMACS: Fast, Flexible, and Free. Vol. 26, *Journal of Computational Chemistry*. 2005. p. 1701–18.
65. Afendi FM, Okada T, Yamazaki M, Hirai-Morita A, Nakamura Y, Nakamura K, et al. KNAPSAcK family databases: Integrated Metabolite-plant Species Databases for Multifaceted Plant Research. *Plant Cell Physiol*. 2012 Feb;53(2).
66. U.S. Department of Agriculture. Dr. Duke's Phytochemical and Ethnobotanical Databases [Internet]. [cited 2024 Jan 17]. Available from: <https://phytochem.nal.usda.gov/phytochem/search>
67. Daina A, Michielin O, Zoete V. SwissADME: A Free Web Tool to Evaluate Pharmacokinetics, Drug-Likeness and Medicinal Chemistry Friendliness of Small Molecules. *Sci Rep*. 2017 Mar 3;7.
68. Benet LZ, Hosey CM, Ursu O, Oprea TI. BDDCS, the Rule of 5 and Drugability. Vol. 101, *Advanced Drug Delivery Reviews*. Elsevier B.V.; 2016. p. 89–98.
69. Wang X, Shen Y, Wang S, Li S, Zhang W, Liu X, et al. PharmMapper 2017 Update: A Web Server for Potential Drug Target Identification with A Comprehensive Target Pharmacophore Database. *Nucleic Acids Res*. 2017 Jul 3;45(W1):W356–60.
70. Daina A, Michielin O, Zoete V. SwissTargetPrediction: Updated Data and New Features for Efficient Prediction of Protein Targets of Small Molecules. *Nucleic Acids Res*. 2019 Jul 1;47(W1):W357–3664.
71. Liu Z, Guo F, Wang Y, Li C, Zhang X, Li H, et al. BATMAN-TCM: A Bioinformatics Analysis Tool for Molecular mechANism of Traditional Chinese Medicine. *Sci Rep*. 2016 Feb 16;6.
72. Szklarczyk D, Gable AL, Nastou KC, Lyon D, Kirsch R, Pyysalo S, et al. The STRING Database in 2021: Customizable Protein-protein Networks, and Functional Characterization of User-uploaded Gene/Measurement Sets. *Nucleic Acids Res*. 2021 Jan 8;49(D1):D605–12.
73. Shannon P, Markiel A, Ozier O, Baliga NS, Wang JT, Ramage D, et al. Cytoscape: A Software Environment for Integrated Models of Biomolecular Interaction Networks. *Genome Res*. 2003 Nov;13(11):2498–504.

74. Jiao X, Sherman BT, Huang DW, Stephens R, Baseler MW, Lane HC, et al. DAVID-WS: A stateful web service to facilitate gene/protein list analysis. *Bioinformatics*. 2012 Jul;28(13):1805–6.
75. Reimand J, Isserlin R, Voisin V, Kucera M, Tannus-Lopes C, Rostamianfar A, et al. Pathway enrichment analysis and visualization of omics data using g:Profiler, GSEA, Cytoscape and EnrichmentMap. *Nat Protoc*. 2019 Feb 1;14(2):482–517.
76. Tang D, Chen M, Huang X, Zhang G, Zeng L, Zhang G, et al. SRplot: A Free Online Platform for Data Visualization and Graphing. *PLoS One*. 2023 Nov 1;18(11 October).
77. Hanwell MD, Hutchison GR, Curtis DE, Lonie DC, Vandermeersch T, Zurek E. Avogadro: Free, Open Source, Cross-Platform Computer Program for Building Molecules and Visualizing Structure [Internet]. Vol. 4, *Journal of Cheminformatics*. 2012. Available from: <http://www.jcheminf.com/content/4/1/17>
78. Duan Y, Wu C, Chowdhury S, Lee MC, Xiong G, Zhang W, et al. A Point-Charge Force Field for Molecular Mechanics Simulations of Proteins Based on Condensed-Phase Quantum Mechanical Calculations. *J Comput Chem*. 2003;24(16):1999–2012.
79. Abraham MJ, Murtola T, Schulz R, Páll S, Smith JC, Hess B, et al. GROMACS: High Performance Molecular Simulations Through Multi-level Parallelism from Laptops to Supercomputers. *SoftwareX*. 2015;1–2:19–25.
80. Lipinski CA, Lombardo F, Dominy BW, Feeney PJ. Experimental and Computational Approaches to Estimate Solubility and Permeability in Drug Discovery and Development Settings. *Adv Drug Deliv Rev* [Internet]. 2001;46:3–26. Available from: www.elsevier.com/locate/drugdeliv
81. Nepusz T, Yu H, Paccanaro A. Detecting Overlapping Protein Complexes in Protein-protein Interaction Networks. *Nat Methods*. 2012 May;9(5):471–2.
82. Mou PK, Yang EJ, Shi C, Ren G, Tao S, Shim JS. Aurora Kinase A, A Synthetic Lethal Target for Precision Cancer medicine. Vol. 53, *Experimental and Molecular Medicine*. Springer Nature; 2021. p. 835–47.
83. Galetta D, Cortes-Dericks L. Promising Therapy in Lung Cancer: Spotlight on Aurora Kinases. Vol. 12, *Cancers*. MDPI AG; 2020. p. 1–15.
84. Blengini CS, Ibrahimian P, Vaskovicova M, Drutovic D, Solc P, Schindler K. Aurora Kinase A is Essential for Meiosis In Mouse Oocytes. *PLoS Genet*. 2021 Apr 26;17(4 April 2021).
85. Shah KN, Bhatt R, Rotow J, Rohrberg J, Olivas V, Wang VE, et al. Aurora Kinase A drives the Evolution of Resistance to Third-Generation EGFR Inhibitors in Lung Cancer. *Nat Med*. 2019 Jan 1;25(1):111–8.
86. Tagal V, Roth MG. Loss of Aurora Kinase Signaling Allows Lung Cancer Cells to Adopt Endoreplication and Form Polyploid Giant Cancer Cells That Resist Antimitotic Drugs. *Cancer Res*. 2021 Jan 15;81(2):400–13.
87. Xu X, Wang X, Xiao Z, Li Y, Wang Y. Two TPX2-dependent Switches Control the Activity of Aurora A. *PLoS One*. 2011;6(2).
88. Read RJ, Adams PD, Arendall WB, Brunger AT, Emsley P, Joosten RP, et al. A new generation of crystallographic validation tools for the Protein Data Bank. *Structure*. 2011 Oct 12;19(10):1395–412.

89. Yang H, Peisach E, Westbrook JD, Young J, Berman HM, Burley SK. DCC: A Swiss Army Knife for Structure Factor Analysis and Validation. *J Appl Crystallogr*. 2016;49:1081–4.
90. Chen VB, Arendall WB, Headd JJ, Keedy DA, Immormino RM, Kapral GJ, et al. MolProbity: All-atom Structure Validation for Macromolecular Crystallography. *Acta Crystallogr D Biol Crystallogr*. 2010;66(1):12–21.
91. Kleywegt GJ, Harris MR, Zou JY, Taylor TC, Wählby A, Jones TA. The Uppsala Electron-Density Server. *Acta Crystallogr D Biol Crystallogr*. 2004 Dec;60(12 Pt 1):2240–9.
92. Ragoza M, Hochuli J, Idrobo E, Sunseri J, Koes DR. Protein-Ligand Scoring with Convolutional Neural Networks. *J Chem Inf Model*. 2017 Apr 24;57(4):942–57.
93. Putra PP, Asnawi A, Hamdayuni F, Arfan, Aman LO. Pharmacoinformatics Analysis of *Morus macroura* for Drug Discovery and Development. *International Journal of Applied Pharmaceutics*. 2024 Feb 15;111–7.
94. Arwansyah, Ambarsari L, Sumaryada TI. Simulasi Docking Senyawa Kurkumin dan Analognya Sebagai Inhibitor Reseptor Androgen pada Kanker Prostat. *Current Biochemistry*. 2014;1(1):11–9.
95. Hochuli J, Helbling A, Skaist T, Ragoza M, Koes DR. Visualizing Convolutional Neural Network Protein-Ligand Scoring. *J Mol Graph Model*. 2018 Sep 1;84:96–108.
96. Suksamrarn S, Komutiban O, Ratananukul P, Chimnoi N, Lartpornmatulee N, Suksamrarn A. Cytotoxic Prenylated Xanthenes from the Young Fruit of *Garcinia mangostana*. *Chem Pharm Bull*. 2006;54(3):310–305.
97. Xu Z, Huang L, Chen XH, Zhu XF, Qian XJ, Feng GK, et al. Cytotoxic Prenylated Xanthenes from the Pericarps of *Garcinia mangostana*. *Molecules*. 2014 Feb;19(2):1820–7.
98. Hollingsworth SA, Dror RO. Molecular Dynamics Simulation for All. Vol. 99, *Neuron*. Cell Press; 2018. p. 1129–43.
99. Filipe HAL, Loura LMS. Molecular Dynamics Simulations: Advances and Applications. Vol. 27, *Molecules*. MDPI; 2022.
100. Liu X, Shi D, Zhou S, Liu H, Liu H, Yao X. Molecular Dynamics Simulations and Novel Drug Discovery. *Expert Opin Drug Discov*. 2018 Jan 2;13(1):23–37.
101. Waterhouse A, Bertoni M, Bienert S, Studer G, Tauriello G, Gumienny R, et al. SWISS-MODEL: Homology Modelling of Protein Structures and Complexes. *Nucleic Acids Res*. 2018 Jul 2;46(W1):W296–303.
102. Pearson WR. An Introduction to Sequence Similarity (‘Homology’) Searching. *Curr Protoc Bioinformatics*. 2013;(SUPPL.42).
103. Medina JS, Prosimiti R, Villarreal P, Delgado-Barrio G, Winter G, González B, et al. Molecular Dynamics Simulations of Rigid and Flexible Water Models: Temperature Dependence of Viscosity. *Chem Phys*. 2011 Sep 22;388(1–3):9–18.
104. Santos LHS, Ferreira RS, Caffarena ER. Integrating Molecular Docking and Molecular Dynamics Simulations. In: *Methods in Molecular Biology*. Humana Press Inc.; 2019. p. 13–34.

105. Gerrard JA, Domigan LJ. *Protein Nanotechnology: Protocols, Instrumentation, and Applications* [Internet]. 3rd ed. Auckland: Humana Press; 2020. Available from: <http://www.springer.com/series/7651>
106. Ghahremanian S, Rashidi MM, Raeisi K, Toghraie D. Molecular Dynamics Simulation Approach for Discovering Potential Inhibitors Against SARS-CoV-2: A Structural Review. Vol. 354, *Journal of Molecular Liquids*. Elsevier B.V.; 2022.
107. Carugo O, Pongor S. A Normalized Root-Mean-Square Distance for Comparing Protein Three-Dimensional Structures. *Protein Science*. 2001 Jul;10(7):1470–3.
108. Tripathi N, Goel B, Bhardwaj N, Sahu B, Kumar H, Jain SK. Virtual Screening and Molecular Simulation Study of Natural Products Database For Lead Identification of Novel Coronavirus Main Protease Inhibitors. *J Biomol Struct Dyn*. 2022;40(8):3655–67.
109. McIntyre PJ, Collins PM, Vrzal L, Birchall K, Arnold LH, Mpamhanga C, et al. Characterization of Three Druggable Hot-Spots in the Aurora-A/TPX2 Interaction Using Biochemical, Biophysical, and Fragment-Based Approaches. *ACS Chem Biol*. 2017 Nov 17;12(11):2906–14.

