

DAFTAR PUSTAKA

1. Perhimpunan Dokter Paru Indonesia. Tuberkulosis: Pedoman Diagnostik dan Penatalaksanaan di Indonesia. Revisi 2. Jakarta: Perhimpunan Dokter Paru Indonesia; 2021.
2. History of World TB Day | World TB Day | CDC [Internet]. 2024 [cited 2026 Feb 27]. Available from: <https://www.cdc.gov/world-tb-day/history/index.html>
3. Kasaeva Tereza, Ghebreyesus Tedros. Global report tuberculosis 2025. 2025;6–70.
4. Tim Penyusun SKI 2023. Survei Kesehatan Indonesia 2023. BADAN KEBIJAKAN PEMBANGUNAN KESEHATAN; 2023.
5. Quinn GA, Banat AM, Abdelhameed AM, Banat IM. Streptomyces from traditional medicine: sources of new innovations in antibiotic discovery. J Med Microbiol [Internet]. 2020 Aug 1;69(8):1040–8. Available from: <https://www.microbiologyresearch.org/content/journal/jmm/10.1099/jmm.0.001232>
6. Tuberculosis: Causes and How It Spreads | Tuberculosis (TB) | CDC [Internet]. [cited 2025 May 2]. Available from: <https://www.cdc.gov/tb/causes/index.html>
7. Global immunization efforts have saved at least 154 million lives over the past 50 years [Internet]. [cited 2026 Feb 1]. Available from: <https://www.who.int/news/item/24-04-2024-global-immunization-efforts-have-saved-at-least-154-million-lives-over-the-past-50-years>
8. Filardi ETM, Carbonell RCC, Pavan FR, Cerni FA, Pucca MB. One hundred years of BCG: the journey of tuberculosis vaccination in Brazil. Front Immunol [Internet]. 2025 [cited 2026 Feb 1];16:1655969. Available from: <https://pmc.ncbi.nlm.nih.gov/articles/PMC12518289/>
9. Starshinova A, Kudryavtsev I, Rubinstein A, Dovgalyuk I, Kulpina A, Churilov LP, et al. BCG vaccination: historical role, modern applications, and future perspectives in tuberculosis and beyond. Front Pediatr [Internet]. 2025 Jul 31;13. Available from: <https://www.frontiersin.org/articles/10.3389/fped.2025.1603732/full>
10. Okafor CN, Rewane A, Momodu II. Bacillus Calmette Guerin [Internet]. StatPearls. 2025. Available from: <http://www.ncbi.nlm.nih.gov/pubmed/12145732>
11. Moliva JI, Turner J, Torrelles JB. Immune Responses to Bacillus Calmette–Guérin Vaccination: Why Do They Fail to Protect against Mycobacterium tuberculosis? Front Immunol [Internet]. 2017 Apr 5;8. Available from: <http://journal.frontiersin.org/article/10.3389/fimmu.2017.00407/full>
12. Moliva JI, Turner J, Torrelles

- JB. Prospects in Mycobacterium bovis Bacille Calmette et Guérin (BCG) vaccine diversity and delivery: Why does BCG fail to protect against tuberculosis? *Vaccine* [Internet]. 2015 Sep;33(39):5035–41. Available from: <https://linkinghub.elsevier.com/retrieve/pii/S0264410X15011597>
13. Padda IS, Parmar M. COVID (SARS-CoV-2) Vaccine. *StatPearls* [Internet]. 2023 Jun 3 [cited 2026 Feb 1]; Available from: <https://www.ncbi.nlm.nih.gov/books/NBK567793/>
 14. Nilvebrant J, Rockberg J. An Introduction to Epitope Mapping. In 2018. p. 1–10. Available from: http://link.springer.com/10.1007/978-1-4939-7841-0_1
 15. Song X, Li Y, Wu H, Qiu HJ, Sun Y. T-Cell Epitope-Based Vaccines: A Promising Strategy for Prevention of Infectious Diseases. *Vaccines* [Internet]. 2024 Oct 17;12(10):1181. Available from: <https://www.mdpi.com/2076-393X/12/10/1181>
 16. Yun JS, Kim AR, Kim SM, Shin E, Ha SJ, Kim D, et al. In silico analysis for the development of multi-epitope vaccines against Mycobacterium tuberculosis. *Front Immunol* [Internet]. 2024 Nov 18;15. Available from: <https://www.frontiersin.org/articles/10.3389/fimmu.2024.1474346/full>
 17. Passos BBS, Araújo-Pereira M, Vinhaes CL, Amaral EP, Andrade BB. The role of ESAT-6 in tuberculosis immunopathology. *Front Immunol*. 2024;15(April):1–11.
 18. Valizadeh A, imani Fooladi AA, Sedighian H, Mahboobi M, Gholami Parizad E, Behzadi E, et al. Evaluating the Performance of PPE44, HSPX, ESAT-6 and CFP-10 Factors in Tuberculosis Subunit Vaccines. *Curr Microbiol* [Internet]. 2022 Sep 19;79(9):260. Available from: <https://link.springer.com/10.1007/s00284-022-02949-8>
 19. Tobin EH, Tristram D. Tuberculosis Overview. *StatPearls* [Internet]. 2024 Dec 22 [cited 2025 Apr 25]; Available from: <https://www.ncbi.nlm.nih.gov/books/NBK441916/>
 20. Adam T, Arinaminpathy N, Baddeley A, Bastard M, Boon S den, Falzon D, et al. WHO TUBERCULOSIS REPORT 2024. 2024.
 21. Swinkels HM, Jilani TN, Tobin EH. Tuberculosis Prevention, Control, and Elimination. *StatPearls* [Internet]. 2025 Jul 6 [cited 2025 Sep 16]; Available from: <https://www.ncbi.nlm.nih.gov/books/NBK513246/>
 22. About Active Tuberculosis Disease | Tuberculosis (TB) | CDC [Internet]. [cited 2026 Mar 6]. Available from: https://www-cdc-gov.translate.google.com/tb/about/active-tuberculosis-disease.html?_x_tr_sl=en&_x_tr_tl=id&_x_tr_hl=id&_x_tr_pto=sge
 23. Alsayed SSR, Gunosewoyo H. Tuberculosis: Pathogenesis, Current Treatment Regimens and New Drug Targets. *Int J Mol Sci* [Internet]. 2023 Mar 8;24(6):5202. Available from: <https://www.mdpi.com/1422-0067/24/6/5202>

24. Surendra K Sharma, editor. Textbook of tuberculosis and non tuberculous mycobacterial diseases. 3rd ed. New Delhi: Jaypee Brothers Medical Publishers; 2020.
25. Alderwick LJ, Harrison J, Lloyd GS, Birch HL. The Mycobacterial Cell Wall—Peptidoglycan and Arabinogalactan. *Cold Spring Harb Perspect Med* [Internet]. 2015 Aug;5(8):a021113. Available from: <http://perspectivesinmedicine.cshlp.org/lookup/doi/10.1101/cshperspect.a021113>
26. Jacobo-Delgado YM, Rodríguez-Carlos A, Serrano CJ, Rivas-Santiago B. Mycobacterium tuberculosis cell-wall and antimicrobial peptides: a mission impossible? *Front Immunol* [Internet]. 2023 May 17;14. Available from: <https://www.frontiersin.org/articles/10.3389/fimmu.2023.1194923/full>
27. Rahlwes KC, Dias BRS, Campos PC, Alvarez-Arguedas S, Shiloh MU. Pathogenicity and virulence of Mycobacterium tuberculosis. *Virulence* [Internet]. 2023 Dec 31;14(1). Available from: <https://www.tandfonline.com/doi/full/10.1080/21505594.2022.2150449>
28. Garde S, Chodisetti PK, Reddy M. Peptidoglycan: Structure, Synthesis, and Regulation. Slauch JM, editor. *EcoSal Plus* [Internet]. 2021 Dec 15;9(2). Available from: <https://journals.asm.org/doi/10.1128/ecosalplus.ESP-0010-2020>
29. Yang W, Yang B, Ramadan S, Huang X. Preactivation-based chemoselective glycosylations: A powerful strategy for oligosaccharide assembly. *Beilstein J Org Chem* [Internet]. 2017 Oct 9;13:2094–114. Available from: <https://www.beilstein-journals.org/bjoc/articles/13/207>
30. Back YW, Choi S, Choi HG, Shin KW, Son YJ, Paik TH, et al. Cell wall skeleton of Mycobacterium bovis BCG enhances the vaccine potential of antigen 85B against tuberculosis by inducing Th1 and Th17 responses. Chang YF, editor. *PLoS One* [Internet]. 2019 Mar 8;14(3):e0213536. Available from: <https://dx.plos.org/10.1371/journal.pone.0213536>
31. Qin L, Xu J, Chen J, Wang S, Zheng R, Cui Z, et al. Cell-autonomous targeting of arabinogalactan by host immune factors inhibits mycobacterial growth. *Elife* [Internet]. 2024;13(RP92737). Available from: <https://elifesciences.org/articles/92737>
32. Batt SM, Minnikin DE, Besra GS. The thick waxy coat of mycobacteria, a protective layer against antibiotics and the host's immune system. *Biochem J* [Internet]. 2020 May 29;477(10):1983–2006. Available from: <https://portlandpress.com/biochemj/article/477/10/1983/225087/The-thick-waxy-coat-of-mycobacteria-a-protective>
33. Nataraj V, Varela C, Javid A, Singh A, Besra GS, Bhatt A. Mycolic acids: deciphering and targeting the chilles' heel of the tubercle bacillus. *Mol Microbiol* [Internet]. 2015 Oct 30;98(1):7–16. Available from: <https://onlinelibrary.wiley.com/doi/10.1111/mmi.13101>

34. Wang H, Liu D, Zhou X. Effect of Mycolic Acids on Host Immunity and Lipid Metabolism. *Int J Mol Sci* [Internet]. 2023 Dec 28;25(1):396. Available from: <https://www.mdpi.com/1422-0067/25/1/396>
35. Quigley J, Hughitt VK, Velikovskiy CA, Mariuzza RA, El-Sayed NM, Briken V. The Cell Wall Lipid PDIM Contributes to Phagosomal Escape and Host Cell Exit of *Mycobacterium tuberculosis*. Kaufmann SHE, editor. *MBio* [Internet]. 2017 May 3;8(2). Available from: <https://journals.asm.org/doi/10.1128/mBio.00148-17>
36. Hayashi JM, Morita YS. Mycobacterial membrane domain, or a primordial organelle? *Yale J Biol Med* [Internet]. 2019; Available from: <https://pmc.ncbi.nlm.nih.gov/articles/PMC6747930/>
37. Pal R, Bisht MK, Mukhopadhyay S. Secretory proteins of *Mycobacterium tuberculosis* and their roles in modulation of host immune responses: focus on therapeutic targets. *FEBS J* [Internet]. 2022 Jul 7;289(14):4146–71. Available from: <https://febs.onlinelibrary.wiley.com/doi/10.1111/febs.16369>
38. Miller BK, Zulauf KE, Braunstein M. The Sec Pathways and Exportomes of *Mycobacterium tuberculosis*. Jacobs Jr. WR, McShane H, Mizrahi V, Orme IM, editors. *Microbiol Spectr* [Internet]. 2017 Mar 10;5(2). Available from: <https://journals.asm.org/doi/10.1128/microbiolspec.TBTB2-0013-2016>
39. Qiang L, Wang J, Zhang Y, Ge P, Chai Q, Li B, et al. *Mycobacterium tuberculosis* Mce2E suppresses the macrophage innate immune response and promotes epithelial cell proliferation. *Cell Mol Immunol* [Internet]. 2019 Apr 23;16(4):380–91. Available from: <https://www.nature.com/articles/s41423-018-0016-0>
40. Li J, Chai QY, Zhang Y, Li BX, Wang J, Qiu XB, et al. *Mycobacterium tuberculosis* Mce3E Suppresses Host Innate Immune Responses by Targeting ERK1/2 Signaling. *J Immunol* [Internet]. 2015 Apr 15;194(8):3756–67. Available from: <https://academic.oup.com/jimmunol/article/194/8/3756/7960856>
41. Karbalaee Zadeh Babaki M, Soleimanpour S, Rezaee SA. Antigen 85 complex as a powerful *Mycobacterium tuberculosis* immunogen: Biology, immune-pathogenicity, applications in diagnosis, and vaccine design. *Microb Pathog* [Internet]. 2017 Nov;112:20–9. Available from: <https://linkinghub.elsevier.com/retrieve/pii/S0882401017308008>
42. Palmer T, Berks BC. The twin-arginine translocation (Tat) protein export pathway. *Nat Rev Microbiol* [Internet]. 2012 Jul 11;10(7):483–96. Available from: <https://www.nature.com/articles/nrmicro2814>
43. Feltcher ME, Sullivan JT, Braunstein M. Protein Export Systems of *Mycobacterium Tuberculosis* : Novel Targets for Drug Development? *Future Microbiol* [Internet]. 2010 Oct 12;5(10):1581–97. Available from: <https://www.tandfonline.com/doi/full/10.2217/fmb.10.112>

44. Bunduc CM, Fahrenkamp D, Wald J, Ummels R, Bitter W, Houben ENG, et al. Structure and dynamics of a mycobacterial type VII secretion system. *Nature* [Internet]. 2021 May 20;593(7859):445–8. Available from: <https://www.nature.com/articles/s41586-021-03517-z>
45. Abdallah AM, Gey van Pittius NC, DiGiuseppe Champion PA, Cox J, Luirink J, Vandembroucke-Grauls CMJE, et al. Type VII secretion — mycobacteria show the way. *Nat Rev Microbiol* [Internet]. 2007 Nov;5(11):883–91. Available from: <https://www.nature.com/articles/nrmicro1773>
46. Wong KW. The Role of ESX-1 in Mycobacterium tuberculosis Pathogenesis. Jacobs Jr. WR, McShane H, Mizrahi V, Orme IM, editors. *Microbiol Spectr* [Internet]. 2017 May 19;5(3). Available from: <https://journals.asm.org/doi/10.1128/microbiolspec.TBTB2-0001-2015>
47. Welin A, Björnsdóttir H, Winther M, Christenson K, Oprea T, Karlsson A, et al. CFP-10 from Mycobacterium tuberculosis Selectively Activates Human Neutrophils through a Pertussis Toxin-Sensitive Chemotactic Receptor. McCormick BA, editor. *Infect Immun* [Internet]. 2015 Jan;83(1):205–13. Available from: <https://journals.asm.org/doi/10.1128/IAI.02493-14>
48. Anes E, Pires D, Mandal M, Azevedo-Pereira JM. ESAT-6 a Major Virulence Factor of Mycobacterium tuberculosis. *Biomolecules* [Internet]. 2023 Jun 9;13(6):968. Available from: <https://www.mdpi.com/2218-273X/13/6/968>
49. Volkman HE, Pozos TC, Zheng J, Davis JM, Rawls JF, Ramakrishnan L. Tuberculous Granuloma Induction via Interaction of a Bacterial Secreted Protein with Host Epithelium. *Science* (80-) [Internet]. 2010 Jan 22;327(5964):466–9. Available from: <https://www.science.org/doi/10.1126/science.1179663>
50. Kupz A, Zedler U, Stäber M, Perdomo C, Dorhoi A, Brosch R, et al. ESAT-6–dependent cytosolic pattern recognition drives noncognate tuberculosis control in vivo. *J Clin Invest* [Internet]. 2016 Apr 25;126(6):2109–22. Available from: <https://www.jci.org/articles/view/84978>
51. Peng X, Sun J. Mechanism of ESAT-6 membrane interaction and its roles in pathogenesis of Mycobacterium tuberculosis. *Toxicon* [Internet]. 2016 Jun;116:29–34. Available from: <https://linkinghub.elsevier.com/retrieve/pii/S0041010115301069>
52. Qian J, Chen R, Wang H, Zhang X. Role of the PE/PPE Family in Host–Pathogen Interactions and Prospects for Anti-Tuberculosis Vaccine and Diagnostic Tool Design. *Front Cell Infect Microbiol* [Internet]. 2020 Nov 26;10. Available from: <https://www.frontiersin.org/articles/10.3389/fcimb.2020.594288/full>
53. D’Souza C, Kishore U, Tsolaki AG. The PE-PPE Family of Mycobacterium tuberculosis: Proteins in Disguise. *Immunobiology* [Internet]. 2023

- Mar;228(2):152321. Available from:
<http://linkinghub.elsevier.com/retrieve/pii/S0171298522001474>
54. Sanyal P, Uppada J, Sinha S, Bhat Y, Khan S, Rajaram SV, et al. Sec and Tat mediated secretion safeguards Mycobacterium tuberculosis membrane homeostasis [Internet]. 2025. Available from:
<http://biorxiv.org/lookup/doi/10.1101/2025.09.04.674216>
 55. Amir M, Aqdas M, Nadeem S, Siddiqui KF, Khan N, Sheikh JA, et al. Diametric Role of the Latency-Associated Protein Acr1 of Mycobacterium tuberculosis in Modulating the Functionality of Pre- and Post-maturational Stages of Dendritic Cells. *Front Immunol* [Internet]. 2017 May 30;8. Available from:
<http://journal.frontiersin.org/article/10.3389/fimmu.2017.00624/full>
 56. Mubin N, Pahari S, Owais M, Zubair S. Mycobacterium tuberculosis host cell interaction: Role of latency associated protein Acr-1 in differential modulation of macrophages. Rottenberg ME, editor. *PLoS One* [Internet]. 2018 Nov 5;13(11):e0206459. Available from:
<https://dx.plos.org/10.1371/journal.pone.0206459>
 57. Chess B. Talaro's Foundation of Microbiology. 12th ed. McGrawHill; 2024.
 58. Cyster JG, Allen CDC. B Cell Responses: Cell Interaction Dynamics and Decisions. *Cell* [Internet]. 2019 Apr;177(3):524–40. Available from:
<https://linkinghub.elsevier.com/retrieve/pii/S0092867419302788>
 59. Althwaiqeb SA, Fakoya AO, Bordoni B. Histology, B-Cell Lymphocyte. *StatPearls* [Internet]. 2024 Oct 13 [cited 2026 Jan 27]; Available from:
<https://www.ncbi.nlm.nih.gov/books/NBK560905/>
 60. Nandi A, Shet A. Why vaccines matter: understanding the broader health, economic, and child development benefits of routine vaccination. *Hum Vaccin Immunother* [Internet]. 2020 Aug 2;16(8):1900–4. Available from:
<https://www.tandfonline.com/doi/full/10.1080/21645515.2019.1708669>
 61. Ginglen JG, Doyle MQ. Immunization. *StatPearls* [Internet]. 2023 Feb 7 [cited 2025 Aug 21]; Available from:
<https://www.ncbi.nlm.nih.gov/books/NBK459331/>
 62. Siegrist CA, Lambert PH. How Vaccines Work. In: *The Vaccine Book* [Internet]. Elsevier; 2016. p. 33–42. Available from:
<https://linkinghub.elsevier.com/retrieve/pii/B9780128021743000023>
 63. Fritschi N, Curtis N, Ritz N. Bacille Calmette Guérin (BCG) and new TB vaccines: Specific, cross-mycobacterial and off-target effects. *Paediatr Respir Rev* [Internet]. 2020 Nov;36:57–64. Available from:
<https://linkinghub.elsevier.com/retrieve/pii/S1526054220301202>
 64. Nieuwenhuizen NE, Kaufmann SHE. Next-Generation Vaccines Based on Bacille Calmette–Guérin. *Front Immunol* [Internet]. 2018 Feb 5;9. Available from: <http://journal.frontiersin.org/article/10.3389/fimmu.2018.00121/full>

65. Lawrence A. Bacillus Calmette-Guérin (BCG) Revaccination and Protection Against Tuberculosis: A Systematic Review. *Cureus* [Internet]. 2024 Mar 21; Available from: <https://www.cureus.com/articles/239876-bacillus-calmette-gurin-bcg-revaccination-and-protection-against-tuberculosis-a-systematic-review>
66. Wang M, Jiang S, Wang Y. Recent advances in the production of recombinant subunit vaccines in *Pichia pastoris*. *Bioengineered* [Internet]. 2016 Apr 8;7(3):155–65. Available from: <http://www.tandfonline.com/doi/full/10.1080/21655979.2016.1191707>
67. Nisa A, Pinto R, Britton WJ, Triccas JA, Counoupas C. Immunogenicity and Protective Efficacy of a Multi-Antigen Mycobacterium tuberculosis Subunit Vaccine in Mice. *Vaccines* [Internet]. 2024 Aug 30;12(9):997. Available from: <https://www.mdpi.com/2076-393X/12/9/997>
68. Ullah I, Bibi S, Ul Haq I, Safia, Ullah K, Ge L, et al. The Systematic Review and Meta-Analysis on the Immunogenicity and Safety of the Tuberculosis Subunit Vaccines M72/AS01E and MVA85A. *Front Immunol* [Internet]. 2020 Oct 8;11. Available from: <https://www.frontiersin.org/article/10.3389/fimmu.2020.01806/full>
69. Jenum S, Tonby K, Rueegg CS, Rühwald M, Kristiansen MP, Bang P, et al. A Phase I/II randomized trial of H56:IC31 vaccination and adjunctive cyclooxygenase-2-inhibitor treatment in tuberculosis patients. *Nat Commun* [Internet]. 2021 Nov 22;12(1):6774. Available from: <https://www.nature.com/articles/s41467-021-27029-6>
70. Woodworth JS, Cohen SB, Moguche AO, Plumlee CR, Agger EM, Urdahl KB, et al. Subunit vaccine H56/CAF01 induces a population of circulating CD4 T cells that traffic into the Mycobacterium tuberculosis-infected lung. *Mucosal Immunol* [Internet]. 2017 Mar;10(2):555–64. Available from: <https://linkinghub.elsevier.com/retrieve/pii/S1933021922006663>
71. Akurut E, Gavamukulya Y, Mulindwa J, Isiagi M, Galiwango R, Bbuye M, et al. Design of a multi-epitope vaccine against drug-resistant mycobacterium tuberculosis and mycobacterium bovis using reverse vaccinology. *Sci Rep* [Internet]. 2025 Jul 26;15(1):27298. Available from: <https://www.nature.com/articles/s41598-025-11768-3>
72. Chang Y, Hawkins BA, Du JJ, Groundwater PW, Hibbs DE, Lai F. A Guide to In Silico Drug Design. *Pharmaceutics* [Internet]. 2022 Dec 23;15(1):49. Available from: <https://www.mdpi.com/1999-4923/15/1/49>
73. Martinelli DD. In silico vaccine design: A tutorial in immunoinformatics. *Healthc Anal* [Internet]. 2022 Nov;2:100044. Available from: <https://linkinghub.elsevier.com/retrieve/pii/S2772442522000156>
74. Kardani K, Bolhassani A, Namvar A. An overview of in silico vaccine design against different pathogens and cancer. *Expert Rev Vaccines* [Internet]. 2020 Aug 2;19(8):699–726. Available from: <https://www.tandfonline.com/doi/full/10.1080/14760584.2020.1794832>

75. Doytchinova IA, Flower DR. VaxiJen: a server for prediction of protective antigens, tumour antigens and subunit vaccines. *BMC Bioinformatics* [Internet]. 2007 Dec 5;8(1):4. Available from: <https://bmcbioinformatics.biomedcentral.com/articles/10.1186/1471-2105-8-4>
76. Calis JJA, Maybeno M, Greenbaum JA, Weiskopf D, De Silva AD, Sette A, et al. Properties of MHC Class I Presented Peptides That Enhance Immunogenicity. Asquith B, editor. *PLoS Comput Biol* [Internet]. 2013 Oct 24;9(10):e1003266. Available from: <https://dx.plos.org/10.1371/journal.pcbi.1003266>
77. Garg VK, Avashthi H, Tiwari A, Jain PA, Ramkete PWR, Kayastha AM, et al. MFPPi – Multi FASTA ProtParam Interface. *Bioinformatics* [Internet]. 2016 Apr 10;12(2):74–7. Available from: <http://www.bioinformatics.net/012/97320630012074.htm>
78. Soltan MA, Behairy MY, Abdelkader MS, Albogami S, Fayad E, Eid RA, et al. In silico Designing of an Epitope-Based Vaccine Against Common E. coli Pathotypes. *Front Med* [Internet]. 2022 Mar 4;9. Available from: <https://www.frontiersin.org/articles/10.3389/fmed.2022.829467/full>
79. Agu PC, Afiukwa CA, Orji OU, Ezeh EM, Ofoke IH, Ogbu CO, et al. Molecular docking as a tool for the discovery of molecular targets of nutraceuticals in diseases management. *Sci Rep* [Internet]. 2023 Aug 17;13(1):13398. Available from: <https://www.nature.com/articles/s41598-023-40160-2>
80. Hollingsworth SA, Dror RO. Molecular Dynamics Simulation for All. *Neuron* [Internet]. 2018 Sep;99(6):1129–43. Available from: <https://linkinghub.elsevier.com/retrieve/pii/S0896627318306846>
81. Rapin N, Lund O, Bernaschi M, Castiglione F. Computational Immunology Meets Bioinformatics: The Use of Prediction Tools for Molecular Binding in the Simulation of the Immune System. Brusica V, editor. *PLoS One* [Internet]. 2010 Apr 16;5(4):e9862. Available from: <https://dx.plos.org/10.1371/journal.pone.0009862>
82. Paremskaia AI, Kogan AA, Murashkina A, Naumova DA, Satish A, Abramov IS, et al. Codon-optimization in gene therapy: promises, prospects and challenges. *Front Bioeng Biotechnol* [Internet]. 2024 Mar 28;12. Available from: <https://www.frontiersin.org/articles/10.3389/fbioe.2024.1371596/full>
83. Pourseif MM, Yousefpour M, Aminianfar M, Moghaddam G, Nematollahi A. A multi-method and structure-based in silico vaccine designing against *Echinococcus granulosus* through investigating enolase protein. *BioImpacts* [Internet]. 2019 Mar 8;9(3):131–44. Available from: <https://bi.tbzmed.ac.ir/Abstract/bi-19719>
84. Souod N, Madanchi H, Bahrami F, Pakzad SR, Shahcheraghi F, Ajdary S. In silico design and evaluation of a multiepitope vaccine against Bordetella

- pertussis: structural, immunological, and biological properties. *Genomics Inform* [Internet]. 2025 Jul 1;23(1):16. Available from: <https://genomicsinform.biomedcentral.com/articles/10.1186/s44342-025-00049-0>
85. Ruaro-Moreno M, Monterrubio-López GP, Reyes-Gastellou A, Castelán-Vega JA, Jiménez-Alberto A, Aparicio-Ozores G, et al. Design of a Multi-Epitope Vaccine against Tuberculosis from *Mycobacterium tuberculosis* PE_PGRS49 and PE_PGRS56 Proteins by Reverse Vaccinology. *Microorganisms* [Internet]. 2023 Jun 24;11(7):1647. Available from: <https://www.mdpi.com/2076-2607/11/7/1647>
 86. Sarker A, Rahman MM, Khatun C, Barai C, Roy N, Aziz MA, et al. In Silico design of a multi-epitope vaccine for Human Parechovirus: Integrating immunoinformatics and computational techniques. Moin AT, editor. *PLoS One* [Internet]. 2024 Dec 4;19(12):e0302120. Available from: <https://dx.plos.org/10.1371/journal.pone.0302120>
 87. Peng C, Tang F, Wang J, Cheng P, Wang L, Gong W. Immunoinformatic-Based Multi-Epitope Vaccine Design for Co-Infection of *Mycobacterium tuberculosis* and SARS-CoV-2. *J Pers Med* [Internet]. 2023 Jan 5;13(1):116. Available from: <https://www.mdpi.com/2075-4426/13/1/116>
 88. Lemkul JA. Introductory Tutorials for Simulating Protein Dynamics with GROMACS. *J Phys Chem B* [Internet]. 2024 Oct 3;128(39):9418–35. Available from: <https://pubs.acs.org/doi/10.1021/acs.jpcc.4c04901>
 89. Bibi S, Ullah I, Zhu B, Adnan M, Liaqat R, Kong WB, et al. In silico analysis of epitope-based vaccine candidate against tuberculosis using reverse vaccinology. *Sci Rep* [Internet]. 2021 Jan 13;11(1):1249. Available from: <https://www.nature.com/articles/s41598-020-80899-6>
 90. Kaabinejadian S, Barra C, Alvarez B, Yari H, Hildebrand WH, Nielsen M. Accurate MHC Motif Deconvolution of Immunopeptidomics Data Reveals a Significant Contribution of DRB3, 4 and 5 to the Total DR Immunopeptidome. *Front Immunol* [Internet]. 2022 Jan 26;13. Available from: <https://www.frontiersin.org/articles/10.3389/fimmu.2022.835454/full>
 91. Nilsson JB, Greenbaum J, Peters B, Nielsen M. NetMHCpan-4.2: improved prediction of CD8+ epitopes by use of transfer learning and structural features. *Front Immunol*. 2025;16.
 92. Saha S, Raghava GPS. Prediction of continuous B-cell epitopes in an antigen using recurrent neural network. *Proteins Struct Funct Bioinforma* [Internet]. 2006 Oct 7;65(1):40–8. Available from: <https://onlinelibrary.wiley.com/doi/10.1002/prot.21078>
 93. Seidler CA, Zeindl R, Fernández-Quintero ML, Tollinger M, Liedl KR. Allergenicity and Conformational Diversity of Allergens. *Allergies* [Internet]. 2024 Jan 11;4(1):1–16. Available from: <https://www.mdpi.com/2313-5786/4/1/1>

94. Dimitrov I, Bangov I, Flower DR, Doytchinova I. AllerTOP v.2—a server for in silico prediction of allergens. *J Mol Model* [Internet]. 2014 Jun;20(6):2278. Available from: <http://link.springer.com/10.1007/s00894-014-2278-5>
95. Zhang J, Tao A. Antigenicity, Immunogenicity, Allergenicity. In 2015. p. 175–86. Available from: http://link.springer.com/10.1007/978-94-017-7444-4_11
96. Gupta S, Kapoor P, Chaudhary K, Gautam A, Kumar R, Raghava GPS. In Silico Approach for Predicting Toxicity of Peptides and Proteins. Patterson RL, editor. *PLoS One* [Internet]. 2013 Sep 13;8(9):e73957. Available from: <https://dx.plos.org/10.1371/journal.pone.0073957>
97. Dhanda SK, Gupta S, Vir P, Raghava GPS. Prediction of IL4 Inducing Peptides. *Clin Dev Immunol* [Internet]. 2013;2013:1–9. Available from: <http://www.hindawi.com/journals/jir/2013/263952/>
98. Tau G, Rothman P. Biologic functions of the IFN- γ receptors. *Allergy* [Internet]. 2001 Dec 24;54(12):1233–51. Available from: <https://onlinelibrary.wiley.com/doi/10.1034/j.1398-9995.1999.00099.x>
99. Dhanda SK, Vir P, Raghava GP. Designing of interferon-gamma inducing MHC class-II binders. *Biol Direct* [Internet]. 2013 Dec 5;8(1):30. Available from: <https://biologydirect.biomedcentral.com/articles/10.1186/1745-6150-8-30>
100. Andongma BT, Huang Y, Chen F, Tang Q, Yang M, Chou SH, et al. In silico design of a promiscuous chimeric multi-epitope vaccine against *Mycobacterium tuberculosis*. *Comput Struct Biotechnol J* [Internet]. 2023;21:991–1004. Available from: <https://linkinghub.elsevier.com/retrieve/pii/S2001037023000181>
101. Carlson MA, Haddad BG, Weis AJ, Blackwood CS, Shelton CD, Wuertth ME, et al. Ribosomal protein L7/L12 is required for GTP ase translation factors EF-G , RF3 , and IF2 to bind in their GTP state to 70S ribosomes. *FEBS J* [Internet]. 2017 Jun 10;284(11):1631–43. Available from: <https://febs.onlinelibrary.wiley.com/doi/10.1111/febs.14067>
102. Bhattacharya K, Chanu NR, Jha SK, Khanal P, Paudel KR. In silico design and evaluation of a multiepitope vaccine targeting the nucleoprotein of Puumala orthohantavirus. *Proteins Struct Funct Bioinforma* [Internet]. 2024 Oct 14;92(10):1161–76. Available from: <https://onlinelibrary.wiley.com/doi/10.1002/prot.26703>
103. Sinha PR, Hegde SR, Mittal R, Jagat CC, Gowda U, Chandrashekhara R, et al. In Silico Development of a Multi-Epitope Subunit Vaccine against Bluetongue Virus in *Ovis aries* Using Immunoinformatics. *Pathogens* [Internet]. 2024 Oct 29;13(11):944. Available from: <https://www.mdpi.com/2076-0817/13/11/944>

104. Jiang F, Han Y, Liu Y, Xue Y, Cheng P, Xiao L, et al. A comprehensive approach to developing a multi-epitope vaccine against *Mycobacterium tuberculosis*: from in silico design to in vitro immunization evaluation. *Front Immunol* [Internet]. 2023 Nov 2;14. Available from: <https://www.frontiersin.org/articles/10.3389/fimmu.2023.1280299/full>
105. Gasteiger E, Hoogland C, Gattiker A, Duvaud S, Wilkins MR, Appel RD, et al. Protein Identification and Analysis Tools on the ExPASy Server. In: *The Proteomics Protocols Handbook* [Internet]. Totowa, NJ: Humana Press; 2005. p. 571–607. Available from: <http://link.springer.com/10.1385/1-59259-890-0:571>
106. Roy S, Maheshwari N, Chauhan R, Sen NK, Sharma A. Structure prediction and functional characterization of secondary metabolite proteins of *Ocimum*. *Bioinformatics* [Internet]. 2011 Jul 6;6(8):315–9. Available from: <http://www.bioinformatics.net/006/97320630006315.htm>
107. Rehman HM, Naz M, Ghous AG, Malik M, Ahmad S, Bashir H. Computational design and evaluation of a novel temporin 1CEa-IL24 fusion protein for anti-tumor potential. *Biomed Res Ther* [Internet]. 2025 Feb 28;12(2):7138–52. Available from: <http://bmrat.org/index.php/BMRAT/article/view/959>
108. Ramachandran GN, Ramakrishnan C, Sasisekharan V. Stereochemistry of polypeptide chain configurations. *J Mol Biol* [Internet]. 1963 Jul;7(1):95–9. Available from: <https://linkinghub.elsevier.com/retrieve/pii/S0022283663800236>
109. Kumar M, Rathore RS. RamPlot : a webserver to draw 2D, 3D and assorted Ramachandran (ϕ , ψ) maps. *J Appl Crystallogr* [Internet]. 2025 Apr 1;58(2):630–6. Available from: <https://journals.iucr.org/paper?S1600576725001669>
110. Huang YJ, Mao B, Aramini JM, Montelione GT. Assessment of template-based protein structure predictions in CASP10. *Proteins Struct Funct Bioinforma* [Internet]. 2014 Feb 25;82(S2):43–56. Available from: <https://onlinelibrary.wiley.com/doi/10.1002/prot.24488>
111. Heo L, Park H, Seok C. GalaxyRefine: protein structure refinement driven by side-chain repacking. *Nucleic Acids Res* [Internet]. 2013 Jul 1;41(W1):W384–8. Available from: <http://academic.oup.com/nar/article/41/W1/W384/1108398/GalaxyRefine-protein-structure-refinement-driven>
112. Kufareva I, Abagyan R. Methods of Protein Structure Comparison. In 2011. p. 231–57. Available from: https://link.springer.com/10.1007/978-1-61779-588-6_10
113. Davis IW, Leaver-Fay A, Chen VB, Block JN, Kapral GJ, Wang X, et al. MolProbity: all-atom contacts and structure validation for proteins and nucleic acids. *Nucleic Acids Res* [Internet]. 2007 May 8;35(Web Server):W375–83. Available from: <https://academic.oup.com/nar/article->

lookup/doi/10.1093/nar/gkm216

114. Yu M. Computational analysis on two putative mitochondrial protein-coding genes from the *Emydura subglobosa* genome: A functional annotation approach. Verma RK, editor. PLoS One [Internet]. 2022 Aug 18;17(8):e0268031. Available from: <https://dx.plos.org/10.1371/journal.pone.0268031>
115. Yan Y, Tao H, He J, Huang SY. The HDOCK server for integrated protein-protein docking. Nat Protoc [Internet]. 2020 May 8;15(5):1829–52. Available from: <https://www.nature.com/articles/s41596-020-0312-x>
116. Millan-Casarrubias EJ, García-Tejeda YV, González-De la Rosa CH, Ruiz-Mazón L, Hernández-Rodríguez YM, Cigarroa-Mayorga OE. Molecular Docking and Pharmacological In Silico Evaluation of Camptothecin and Related Ligands as Promising HER2-Targeted Therapies for Breast Cancer. Curr Issues Mol Biol [Internet]. 2025 Mar 15;47(3):193. Available from: <https://www.mdpi.com/1467-3045/47/3/193>
117. López-Blanco JR, Garzón JI, Chacón P. iMod: multipurpose normal mode analysis in internal coordinates. Bioinformatics [Internet]. 2011 Oct 15;27(20):2843–50. Available from: <https://academic.oup.com/bioinformatics/article/27/20/2843/202794>
118. Zaib S, Rana N, Areeba, Hussain N, Alrbyawi H, Dera AA, et al. Designing multi-epitope monkeypox virus-specific vaccine using immunoinformatics approach. J Infect Public Health [Internet]. 2023 Jan;16(1):107–16. Available from: <https://linkinghub.elsevier.com/retrieve/pii/S1876034122003409>
119. Santra D, Maiti S. Molecular dynamic simulation suggests stronger interaction of Omicron-spike with ACE2 than wild but weaker than Delta SARS-CoV-2 can be blocked by engineered S1-RBD fraction. Struct Chem [Internet]. 2022 Oct 4;33(5):1755–69. Available from: <https://link.springer.com/10.1007/s11224-022-02022-x>
120. Saba A Al, Adiba M, Saha P, Hosen MI, Chakraborty S, Nabi AHMN. An in-depth in silico and immunoinformatics approach for designing a potential multi-epitope construct for the effective development of vaccine to combat against SARS-CoV-2 encompassing variants of concern and interest. Comput Biol Med [Internet]. 2021 Sep;136:104703. Available from: <https://linkinghub.elsevier.com/retrieve/pii/S0010482521004972>
121. Singh P, Singh VK, Verma M. Molecular docking and dynamics simulation analyses of ibuprofen derivatives as potential anti-cancer agents targeting COX-2. Silico Res Biomed. 2025 Jan 1;1:100100.
122. Bagewadi ZK, Yunus Khan TM, Gangadharappa B, Kamalapurkar A, Mohamed Shamsudeen S, Yaraguppi DA. Molecular dynamics and simulation analysis against superoxide dismutase (SOD) target of *Micrococcus luteus* with secondary metabolites from *Bacillus licheniformis* recognized by genome mining approach. Saudi J Biol Sci. 2023 Sep

1;30(9):103753.

123. Grote A, Hiller K, Scheer M, Munch R, Nortemann B, Hempel DC, et al. JCat: a novel tool to adapt codon usage of a target gene to its potential expression host. *Nucleic Acids Res* [Internet]. 2005 Jul 1;33(Web Server):W526–31. Available from: <https://academic.oup.com/nar/article-lookup/doi/10.1093/nar/gki376>

