

DAFTAR PUSTAKA

- Armoogum, S., & Li, X. (2019). Big Data Analytics and Deep Learning in Bioinformatics With Hadoop. In *Deep Learning and Parallel Computing Environment for Bioengineering Systems*. Elsevier Inc. <https://doi.org/10.1016/b978-0-12-816718-2.00009-9>
- Banerjee, A. K., & Ray, U. (2020). Mutation hot spots in Spike protein of COVID-19 virus: Mutation in spike protein. *Proceedings of the Indian National Science Academy*, 86(April). <https://doi.org/10.16943/ptinsa/2020/155490>
- Brini, E., Algaer, E. A., Ganguly, P., Li, C., Rodríguez-Ropero, F., & van der Vegt, N. F. A. (2013). Systematic coarse-graining methods for soft matter simulations – a review. *Soft Matter*, 9(7), 2108–2119. <https://doi.org/10.1039/C2SM27201F>
- Burley, S. K., Berman, H. M., Bhikadiya, C., Bi, C., Chen, L., Di Costanzo, L., Christie, C., Dalenberg, K., Duarte, J. M., Dutta, S., Feng, Z., Ghosh, S., Goodsell, D. S., Green, R. K., Guranović, V., Guzenko, D., Hudson, B. P., Kalro, T., Liang, Y., ... Zardecki, C. (2019). RCSB Protein Data Bank: Biological macromolecular structures enabling research and education in fundamental biology, biomedicine, biotechnology and energy. *Nucleic Acids Research*, 47(D1), D464–D474. <https://doi.org/10.1093/nar/gky1004>
- Camacho, C., Madden, T., Tao, T., Agarwala, R., & Morgulis, A. (2019). BLAST Command Line Applications User Manual. *Bethesda (MD): National Center for Biotechnology Information (US), MD*, 1–28. <https://www.ncbi.nlm.nih.gov/books/NBK279690/>
- Casalino, L., Gaieb, Z., Goldsmith, J. A., Hjorth, C. K., Dommer, A. C., Harbison, A. M., Fogarty, C. A., Barros, E. P., Taylor, B. C., McLellan, J. S., Fadda, E., & Amaro, R. E. (2020). Beyond Shielding: The Roles of Glycans in the SARS-CoV-2 Spike Protein. *ACS Central Science*. <https://doi.org/10.1021/acscentsci.0c01056>
- Chen, W. H., Hotez, P. J., & Bottazzi, M. E. (2020). Potential for developing a SARS-CoV receptor-binding domain (RBD) recombinant protein as a heterologous human vaccine against coronavirus infectious disease (COVID)-19. *Human Vaccines and Immunotherapeutics*, 00(00), 1–4. <https://doi.org/10.1080/21645515.2020.1740560>
- Darré, L., Machado, M. R., Brandner, A. F., González, H. C., Ferreira, S., & Pantano, S. (2015). SIRAH: A structurally unbiased coarse-grained force field for proteins with aqueous solvation and long-range electrostatics. *Journal of Chemical Theory and Computation*, 11(2), 723–739. <https://doi.org/10.1021/ct5007746>
- Elbe, S., & Buckland-Merrett, G. (2017). Data, disease and diplomacy: GISAID's innovative contribution to global health. *Global Challenges*, 1(1), 33–46. <https://doi.org/10.1002/gch2.1018>
- Fernández, A. (2020). Structural Impact of Mutation D614G in SARS-CoV-2 Spike Protein: Enhanced Infectivity and Therapeutic Opportunity. *ACS Medicinal Chemistry Letters*, 11(9), 1667–1670. <https://doi.org/10.1021/acsmchemlett.0c00410>
- Fiser, A., & Šali, A. (2003). MODELLER: Generation and Refinement of Homology-Based Protein Structure Models. *Methods in Enzymology*, 374, 461–491. [https://doi.org/10.1016/S0076-6879\(03\)74020-8](https://doi.org/10.1016/S0076-6879(03)74020-8)

- Gardy, J. L., & Loman, N. J. (2018). Towards a genomics-informed, real-time, global pathogen surveillance system. *Nature Reviews Genetics*, *19*(1), 9–20. <https://doi.org/10.1038/nrg.2017.88>
- Giri, R., Bhardwaj, T., Shegane, M., Gehi, B., Kumar, P., Gadhawe, K., Oldfield, C., & Uversky, V. (2020). *When Darkness Becomes a Ray of Light in the Dark Times: Understanding the COVID-19 via the Comparative Analysis of the Dark Proteomes of SARS-CoV-2, Human SARS and Bat SARS-Like Coronaviruses*. 1–63. <https://doi.org/10.1101/2020.03.13.990598>
- Go, I. (2021). *Peta Sebaran*. <https://covid19.go.id/peta-sebaran>
- Gralinski, L. E., & Menachery, V. D. (2020). Return of the coronavirus: 2019-nCoV. *Viruses*, *12*(2), 1–8. <https://doi.org/10.3390/v12020135>
- Heath, A. P., Kaviraki, L. E., & Clementi, C. (2007). From coarse-grain to all-atom: toward multiscale analysis of protein landscapes. *Proteins*, *68*(3), 646–661. <https://doi.org/10.1002/prot.21371>
- Hidayat, R., Aini, N., Ilmi, A. F. N., Azzahroh, F., & Giantini, A. (2020). Test, Trace, and Treatment Strategy to Control COVID-19 Infection Among Hospital Staff in a COVID-19 Referral Hospital in Indonesia. *Acta Medica Indonesiana*, *52*(3), 206–213.
- Hoffmann, M., Kleine-Weber, H., Schroeder, S., Krüger, N., Herrler, T., Erichsen, S., Schiergens, T. S., Herrler, G., Wu, N. H., Nitsche, A., Müller, M. A., Drosten, C., & Pöhlmann, S. (2020). SARS-CoV-2 Cell Entry Depends on ACE2 and TMPRSS2 and Is Blocked by a Clinically Proven Protease Inhibitor. *Cell*, *181*(2), 271–280.e8. <https://doi.org/10.1016/j.cell.2020.02.052>
- Jaimes, J. A., André, N. M., Chappie, J. S., Millet, J. K., & Whittaker, G. R. (2020). Phylogenetic Analysis and Structural Modeling of SARS-CoV-2 Spike Protein Reveals an Evolutionary Distinct and Proteolytically Sensitive Activation Loop. *Journal of Molecular Biology*, *432*(10), 3309–3325. <https://doi.org/10.1016/j.jmb.2020.04.009>
- Jiang, S., Christopher, H., & Lanying, D. (2020). Antibodies against SARS-CoV-2 and Other Human Coronaviruses. *Trends in Immunology*, *xx*(xx), 1–5. <https://doi.org/10.1016/j.it.2020.03.007>
- Kamerlin, S. C. L., Vicatos, S., Dryga, A., & Warshel, A. (2011). Coarse-grained (multiscale) simulations in studies of biophysical and chemical systems. *Annual Review of Physical Chemistry*, *62*, 41–64. <https://doi.org/10.1146/annurev-physchem-032210-103335>
- Karathanou, K., Lazaratos, M., Bertalan, É., Siemers, M., Buzar, K., Schertler, G. F. X., del Val, C., & Bondar, A. N. (2020). A graph-based approach identifies dynamic H-bond communication networks in spike protein S of SARS-CoV-2. *Journal of Structural Biology*, *212*(2), 107617. <https://doi.org/10.1016/j.jsb.2020.107617>
- Kirchdoerfer, R. N., Cottrell, C. A., Wang, N., Pallesen, J., Yassine, H. M., Turner, H. L., Corbett, K. S., Graham, B. S., McLellan, J. S., & Ward, A. B. (2016). Pre-fusion structure of a human coronavirus spike protein. *Nature*, *531*(7592), 118–121. <https://doi.org/10.1038/nature17200>
- Kmiecik, S., Gront, D., Kolinski, M., Wieteska, L., Dawid, A. E., & Kolinski, A. (2016). Coarse-Grained Protein Models and Their Applications. *Chemical Reviews*, *116*(14), 7898–7936. <https://doi.org/10.1021/acs.chemrev.6b00163>

- Korber, B., Fischer, W. M., Gnanakaran, S., Yoon, H., Theiler, J., Abfalterer, W., Hengartner, N., Giorgi, E. E., Bhattacharya, T., Foley, B., Hastie, K. M., Parker, M. D., Partridge, D. G., Evans, C. M., Freeman, T. M., de Silva, T. I., Angyal, A., Brown, R. L., Carrilero, L., ... Montefiori, D. C. (2020). Tracking Changes in SARS-CoV-2 Spike: Evidence that D614G Increases Infectivity of the COVID-19 Virus. *Cell*, 182(4), 812-827.e19. <https://doi.org/10.1016/j.cell.2020.06.043>
- Krane, D. E., & Raymer, M. L. (2002). *Fundamental concepts of bioinformatics*. Benjamin Cummings.
- Kumar, P., & Arya, A. (2019). Ramachandran plot - A simplified approach. *Pathfinder Research and Training Foundation, India, January*, 6. https://www.researchgate.net/publication/330158666_Ramachandran_plot-_A_simplified_approach
- Levitt, M., & Warshel, A. (1975). Computer simulation of protein folding. *Nature*, 253(5494), 694–698. <https://doi.org/10.1038/253694a0>
- Li, X., Geng, M., Peng, Y., Meng, L., & Lu, S. (2020). Molecular immune pathogenesis and diagnosis of COVID-19. *Journal of Pharmaceutical Analysis*, 19(xxxx), 1–7. <https://doi.org/10.1016/j.jpha.2020.03.001>
- Lorusso, A., Calistri, P., Petrini, A., Savini, G., & Decaro, N. (2020). Novel coronavirus (Sars-cov-2) epidemic: A veterinary perspective. *Veterinaria Italiana*, 56(1), 5–10. <https://doi.org/10.12834/VetIt.2173.11599.1>
- Lukitaningsih, E., Mustikawaty, A. A., & Sudarmanto, A. (2013). Homology Modeling dan Molecular Docking Senyawa Aktif dari Bengkoang (*Pachyrrhizus erosus*) sebagai Inhibitor Tirosinase pada Homo sapiens (Homology Modeling and Molecular Docking of Active Compounds from Bengkoang (*Pachyrrhizus erosus*) as Tyrosinase. *Jurnal Ilmu Kefarmasian Indonesia*, 11(2), 134–141.
- Machado, M. R., Barrera, E. E., Klein, F., Sónora, M., Silva, S., & Pantano, S. (2019). The SIRAH 2.0 Force Field: Altius, Fortius, Citius. *Journal of Chemical Theory and Computation*, 15(4), 2719–2733. <https://doi.org/10.1021/acs.jctc.9b00006>
- Madijagan, M., & Raj, S. S. (2019). Parallel Machine Learning and Deep Learning Approaches for Bioinformatics. In *Deep Learning and Parallel Computing Environment for Bioengineering Systems*. Elsevier Inc. <https://doi.org/10.1016/b978-0-12-816718-2.00022-1>
- Mousavizadeh, L., & Ghasemi, S. (2020). Genotype and phenotype of COVID-19 : Their roles in pathogenesis. *Journal of Microbiology, Immunology and Infection*, xxxx, 0–4. <https://doi.org/10.1016/j.jmii.2020.03.022>
- Müller, C., Schulte, F. W., Lange-grünweller, K., Obermann, W., Madhugiri, R., Pleschka, S., Ziebuhr, J., Hartmann, R. K., & Grünweller, A. (2018). Broad-spectrum antiviral activity of the eIF4A inhibitor silvestrol against corona- and picornaviruses. *Antiviral Research*, 150(October 2017), 123–129. <https://doi.org/10.1016/j.antiviral.2017.12.010>
- Omotuyi, I. O., Nash, O., Ajiboye, O. B., Iwegbulam, C. G., Oyinloye, B. E., Oyedeji, O. A., Kashim, Z. A., & Okaiyeto, K. (2020). Atomistic simulation reveals structural mechanisms underlying D614G spike glycoprotein-enhanced fitness in SARS-COV-2. *Journal of Computational Chemistry*, 41(24), 2158–2161. <https://doi.org/10.1002/jcc.26383>

- Oostenbrink, C., Villa, A., Mark, A. E., & Van Gunsteren, W. F. (2004). A biomolecular force field based on the free enthalpy of hydration and solvation: The GROMOS force-field parameter sets 53A5 and 53A6. *Journal of Computational Chemistry*, 25(13), 1656–1676. <https://doi.org/10.1002/jcc.20090>
- Ortiz-Prado, E., Simbaña-Rivera, K., Gómez- Barreno, L., Rubio-Neira, M., Guaman, L. P., Kyriakidis, N. C., Muslin, C., Jaramillo, A. M. G., Barba-Ostria, C., Cevallos-Robalino, D., Sanches-SanMiguel, H., Unigarro, L., Zalakeviciute, R., Gadian, N., & López-Cortés, A. (2020). Clinical, molecular, and epidemiological characterization of the SARS-CoV-2 virus and the Coronavirus Disease 2019 (COVID-19), a comprehensive literature review. *Diagnostic Microbiology and Infectious Disease*, 98(1). <https://doi.org/10.1016/j.diagmicrobio.2020.115094>
- Ou, J., Zhou, Z., Dai, R., Zhang, J., Lan, W., Zhao, S., Wu, J., Seto, D., Cui, L., Zhang, G., & Zhang, Q. (2020). Emergence of RBD mutations in circulating SARS-CoV-2 strains enhancing the structural stability and human ACE2 receptor affinity of the spike protein. *BioRxiv*, 2020.03.15.991844. <https://www.biorxiv.org/content/10.1101/2020.03.15.991844v4%0Ahttps://www.biorxiv.org/content/10.1101/2020.03.15.991844v4.abstract>
- Paraskevis, D., Kostaki, E. G., Magiorkinis, G., Panayiotakopoulos, G., Sourvinos, G., & Tsiodras, S. (2020). Full-genome evolutionary analysis of the novel corona virus (2019-nCoV) rejects the hypothesis of emergence as a result of a recent recombination event. *Infection, Genetics and Evolution*, 79(January), 104212. <https://doi.org/10.1016/j.meegid.2020.104212>
- Piana, S., Klepeis, J. L., & Shaw, D. E. (2014). Assessing the accuracy of physical models used in protein-folding simulations: Quantitative evidence from long molecular dynamics simulations. *Current Opinion in Structural Biology*, 24(1), 98–105. <https://doi.org/10.1016/j.sbi.2013.12.006>
- Pitman, M. R., & Menz, R. I. (2006). 2 - Methods for Protein Homology Modelling. In D. K. Arora, R. M. Berka, & G. B. T.-A. M. and B. Singh (Eds.), *Applied Mycology and Biotechnology* (Vol. 6, pp. 37–59). Elsevier. [https://doi.org/https://doi.org/10.1016/S1874-5334\(06\)80005-5](https://doi.org/https://doi.org/10.1016/S1874-5334(06)80005-5)
- Rothan, H. A., & Byrareddy, S. N. (2020). The epidemiology and pathogenesis of coronavirus disease (COVID-19) outbreak. *Journal of Autoimmunity*, 109(February), 102433. <https://doi.org/10.1016/j.jaut.2020.102433>
- Salomon-Ferrer, R., Götz, A. W., Poole, D., Le Grand, S., & Walker, R. C. (2013). Routine Microsecond Molecular Dynamics Simulations with AMBER on GPUs. 2. Explicit Solvent Particle Mesh Ewald. *Journal of Chemical Theory and Computation*, 9(9), 3878–3888. <https://doi.org/10.1021/ct400314y>
- Shang, J., Ye, G., Shi, K., Wan, Y., Luo, C., Aihara, H., Geng, Q., Auerbach, A., & Li, F. (2020). Structural basis of receptor recognition by SARS-CoV-2. *Nature*, 581(7807), 221–224. <https://doi.org/10.1038/s41586-020-2179-y>
- Shen, M., & Sali, A. (2006). Statistical potential for assessment and prediction of protein structures. *Protein Science*, 15(11), 2507–2524. <https://doi.org/10.1110/ps.062416606>
- Su, S., Wong, G., Shi, W., Liu, J., Lai, A. C. K., Zhou, J., Liu, W., Bi, Y., & Gao, G. F. (2016). Epidemiology, Genetic Recombination, and Pathogenesis of Coronaviruses.

Trends in Microbiology, 24(6), 490–502. <https://doi.org/10.1016/j.tim.2016.03.003>

- Takada, S. (2012). Coarse-grained molecular simulations of large biomolecules. *Current Opinion in Structural Biology*, 22(2), 130–137. <https://doi.org/10.1016/j.sbi.2012.01.010>
- Vanommeslaeghe, K., & Mackerell, A. D. (2015). CHARMM additive and polarizable force fields for biophysics and computer-aided drug design. *Biochimica et Biophysica Acta - General Subjects*, 1850(5), 861–871. <https://doi.org/10.1016/j.bbagen.2014.08.004>
- Vendruscolo, M., & Dobson, C. M. (2011). Protein dynamics: Moore's law in molecular biology. *Current Biology*, 21(2), R68–R70. <https://doi.org/10.1016/j.cub.2010.11.062>
- Walls C, A., Park, Y., Tortorici, M. A., Wall, A., Mcguire, A. T., Velesler, D., Walls, A. C., Park, Y., Tortorici, M. A., Wall, A., & Mcguire, A. T. (2020). Structure , Function , and Antigenicity of the SARS- Structure , Function , and Antigenicity of the SARS-CoV-2 Spike Glycoprotein. *Cell*, 1–12. <https://doi.org/10.1016/j.cell.2020.02.058>
- Wan, Y., Shang, J., Graham, R., Baric, R. S., & Li, F. (2020). Receptor Recognition by the Novel Coronavirus from Wuhan: an Analysis Based on Decade-Long Structural Studies of SARS Coronavirus. *Journal of Virology*, 94(7), 1–9. <https://doi.org/10.1128/jvi.00127-20>
- Wang, K., Chen, W., Zhou, Y., Lian, J., Zhang, Z., Du, P., Gong, L., Zhang, Y., Cui, H., Geng, J., Wang, B., Sun, X., & Wang, C. (2020). SARS-CoV-2 invades host cells via a novel route: CD147-spike protein. *BioRxiv, March*.
- Warshel, A., & Levitt, M. (1976). Theoretical studies of enzymic reactions: Dielectric, electrostatic and steric stabilization of the carbonium ion in the reaction of lysozyme. *Journal of Molecular Biology*, 103(2), 227–249. [https://doi.org/https://doi.org/10.1016/0022-2836\(76\)90311-9](https://doi.org/https://doi.org/10.1016/0022-2836(76)90311-9)
- Yang, Y., Xiao, Z., Ye, K., He, X., Sun, B., Qin, Z., Yu, J., Yao, J., Wu, Q., Bao, Z., & Zhao, W. (2020). SARS-CoV-2: characteristics and current advances in research. *Virology Journal*, 17(1), 1–17. <https://doi.org/10.1186/s12985-020-01369-z>
- Ye, Z. W., Yuan, S., Yuen, K. S., Fung, S. Y., Chan, C. P., & Jin, D. Y. (2020). Zoonotic origins of human coronaviruses. *International Journal of Biological Sciences*, 16(10), 1686–1697. <https://doi.org/10.7150/ijbs.45472>
- Zhang, Linlin, Lin, D., Sun, X., Curth, U., Drosten, C., Sauerhering, L., Becker, S., Rox, K., & Hilgenfeld, R. (2020). Crystal structure of SARS-CoV-2 main protease provides a basis for design of improved a-ketoamide inhibitors. *Science*, 368(6489), 409–412. <https://doi.org/10.1126/science.abb3405>
- Zhang, Lizhou, Jackson, C., Mou, H., Ojha, A., Rangarajan, E., Izard, T., Farzan, M., & Choe, H. (2020). The D614G mutation in the SARS-CoV-2 spike protein reduces S1 shedding and increases infectivity. *BioRxiv: The Preprint Server for Biology*. <https://doi.org/10.1101/2020.06.12.148726>