

REFERENCES

- Abraham, M. J., Murtola, T., Schulz, R., Páll, S., Smith, J. C., Hess, B. and Lindahl, E., 2015, Gromacs: High performance molecular simulations through multi-level parallelism from laptops to supercomputers, *SoftwareX*, 1–2, 19–25.
- Achaiah, N. C., Subbarajasetty, S. B. and Shetty, R. M., 2020, R O and R e of COVID-19: Can We Predict When the Pandemic Outbreak will be Contained?, *Indian J. Crit. Care Med.*, 24(11), 1125-1127.
- Ahamad, S., Kanipakam, H., Birla, S., Ali, Md. S. and Gupta, D., 2021, Screening Malaria-box compounds to identify potential inhibitors against SARS-CoV-2 M^{pro}, using molecular docking and dynamics simulation studies, *Eur. J. Pharm.*, 890, 173664.
- Al-Amer, R., Maneze, D., Everett, B., Montayre, J., Villarosa, A. R., Dwekat, E. and Salamonson, Y., 2022, COVID-19 vaccination intention in the first year of the pandemic: A systematic review, *J. Clin. Nurs.*, 31, 62–86.
- Al-Karmalawy, A. A., Dahab, M. A., Metwaly, A. M., Elhady, S. S., Elkaeed, E. B., Eissa, I.H. and Darwish, K.M., 2021, Molecular Docking and Dynamics Simulation Revealed the Potential Inhibitory Activity of ACEIs Against SARS-CoV-2 Targeting the hACE2 Receptor, *Front. Chem.*, 9(661230), 1-21.
- Anonymous, 2020, Coronavirus disease (COVID-2019) situation reports, *World Health Organisation*, <https://www.who.int/emergencies/diseases/novel-coronavirus-2019/situation-reports> (accessed 18 March 2022 at 09:46).
- Anonymous, 2021, Safety Data Sheet - Peltatoside ROTICHROM® HPLC, *Carl Roth*, GHS 1.0 en, 1-9.
- Anonymous, 2021, Safety Data Sheet - Rutin trihydrate ROTI®STAR Primary Standard, *Carl Roth*, GHS 1.1 en, 1-10.
- Benson, N. C. and Daggett, V., 2012, A Comparison of Multiscale Methods for the Analysis of Molecular Dynamics Simulations, *J. Phys. Chem. B.*, 116(29), 8722–8731.
- Berendsen, H. J. C., van der Spoel, D. and van Drunen, R., 1995, GROMACS: A message-passing parallel molecular dynamics implementation, *Comp. Phys. Com.*, 91(1–3), 43–56.
- BIOVIA, D. S., 2017, *Discovery Studio, 2017 R2 64-bit Client*, Dassault Systèmes, San Diego.
- Burki, T. K., 2022, The role of antiviral treatment in the COVID-19 pandemic, *The Lancet. Resp. med.*, e18.
- Casella, M., Rajnik, M., Aleem, A., Dulebohn, S. C. and Di Napoli, R., 2022,

Features, Evaluation, and Treatment of Coronavirus (COVID-19), Statpearls Publishing, Treasure Island.

- Daccache, C., Rizk, R., Dahham, J., Evers, S. M. A. A., Hiligsmann, M. and Karam, R., 2022, Economic evaluation guidelines in low-and middle-income countries: a systematic review, *Int. J. Tech. Assess. Health Care*, 38, 1–14.
- Das, S., Sarmah, S., Lyndem, S. and Roy, A. S., 2021, An investigation into the identification of potential inhibitors of SARS-CoV-2 main protease using molecular docking study, *J. Biomol. Struct. Dyn.*, 39(9), 3347–3357.
- De Souza, L. A., Tavares, W. M. G., Lopes, A. P. M., Soeiro, M. M. and De Almeida, W. B., 2017, Structural analysis of flavonoids in solution through DFT 1H NMR chemical shift calculations: Epigallocatechin, Kaempferol and Quercetin, *Chem. Phy. Let.*, 676, 46–52.
- Fan, J., Fu, A. and Zhang, L., 2019, REVIEW Progress in molecular docking, *Quant. Bio.*, 7(2), 83–89.
- Fehr, A. R. and Perlman, S., 2015, Chapter 1 Coronaviruses: An Overview of Their Replication and Pathogenesis, *Methods Mol. Bio.*, 1282, 1–23.
- Ferreira, J. C., Fadl, S., Villanueva, A. J. and Rabeh, W.M., 2021, Catalytic Dyad Residues His41 and Cys145 Impact the Catalytic Activity and Overall Conformational Fold of the Main SARS-CoV-2 Protease 3-Chymotrypsin-Like Protease, *Front. Chem.*, 9(692168), 1–11.
- Galindez, G., Matschinske, J., Rose, T. D., Sadegh, S., Salgado-Albarrán, M., Späth, J., Baumbach, J. and Pauling, J. K., 2021, Lessons from the COVID-19 pandemic for advancing computational drug repurposing strategies, *Nat. Comp. Sci.*, 1, 33–41.
- Gondokesumo, M. E., Budipramana, K. and Aini, S. Q., 2021, Study of Jamu as Indonesian Herbal Medicine for Covid-19 Treatment, *Adv. Health Sci. Res.*, 40(Iccscp).
- Goodsell, D. S. and Olson, A. J., 1990, Automated docking of substrates to proteins by simulated annealing, *Proteins*, 8(3), 195–202.
- Gordon, D. E., Jang, G. M., Bouhaddou, M., *et al.*, 2020, A SARS-CoV-2 protein interaction map reveals targets for drug repurposing, *Nature*, 583(7816), 459–468.
- Grief, S. N. and Loza, J. K., 2018, Guidelines for the Evaluation and Treatment of Pneumonia, *Prim. Care Clin. Off. Prac.*, 45(3), 485–503.
- Hu, B., Guo, H., Zhou, P. and Shi, Z., 2021, Characteristics of SARS-CoV-2 and COVID-19, *Nat. Rev. Microbio.*, 19, 141–154.

- Jamal, Q. M. S., Dhasmana, A., Lohani, M., Firdaus, S., Ansari, Md Y., Sahoo, G., Chandra, H., S., 2015, Binding pattern elucidation of NNK and NNAL cigarette smoke carcinogens with NER pathway enzymes: An onco-informatics study, *Asian Pac. J. Can. Prev.*, 16(13), 5311–5317.
- Khuroo, M. S., 2020, Chloroquine and hydroxychloroquine in coronavirus disease 2019 (COVID-19). Facts, fiction and the hype: a critical appraisal, *Int. J. Antimicro. Agents*, 56(3), 106101.
- Kim, C. H., 2021, Anti-SARS-CoV-2 Natural Products as Potentially Therapeutic Agents, *Front. Pharm.*, 12, 1–27.
- Law, W. Y., Asaruddin, M. R., Bhawani, S. A. and Mohamad, S., 2020, Pharmacophore modelling of vanillin derivatives, favipiravir, chloroquine, hydroxychloroquine, monolaurin and tetrodotoxin as M^{Pro} inhibitors of severe acute respiratory syndrome coronavirus-2 (SARS-CoV-2), *BMC Res. Notes*, 13(1), 1–8.
- Likic', V. A., Gooley, P. R., Speed, T. P. and Strehler, E. E., 2005, A statistical approach to the interpretation of molecular dynamics simulations of calmodulin equilibrium dynamics, *Protein Sci.*, 14(12), 2955–2963.
- Liu, Y., Gayle, A. A., Wilder-Smith, A. and Rocklöv, J., 2020, The reproductive number of COVID-19 is higher compared to SARS coronavirus, *J. Travel Med.*, 2020, 1–4.
- Marlina, S., Kusnanto, H. and Graber, M. A., 2022, Sharing Management of COVID-19 in America as well as Public Health Centers and Primary Clinics in Indonesia, *Indonesia Rev. Prim. Care Prac. Educ.*, 5(1), 2–6.
- Mengist, H. M., Dilnessa, T. and Jin, T., 2021, Structural Basis of Potential Inhibitors Targeting SARS-CoV-2 Main Protease, *Front. Chem.*, 9, 1–19.
- Mesecar, A. D., 2020, A taxonomically-driven approach to development of potent, broad-spectrum inhibitors of coronavirus main protease including SARS-CoV-2, COVID-19'.
- Moh Zaki, A., Van Boheemen, S., Bestebroer, T. M., Osterhaus, A. D. M. E. and Fouchier, R. A. M., 2012, Isolation of a Novel Coronavirus from a Man with Pneumonia in Saudi Arabia, *N. Engl. J. Med.*, 367, 1814–1834.
- Morris, G. M., Huey, R., Lindstrom, W., Sanner, M. F., Belew, R. K., Goodsell, D. S. and Olson, A., 2009, AutoDock4 and AutoDockTools4: Automated Docking with Selective Receptor Flexibility, *J. Comput. Chem.*, 30(16), 2785–2791.
- Murray, C. J. L., 2022, COVID-19 will continue but the end of the pandemic is near, *The Lancet*, 399(10323), 417–419.
- Ngwa, W., Kumar, R., Thompson, D., Lysterly, W., Moore, R. and Reid, T., 2020,

molecules Potential of Flavonoid-Inspired Phytomedicines against COVID-19, *Molecules*, 25(11), 2707.

Nielsen, A. B. and Holder, A. J., 2009, *Gauss View 5.0, User's Reference*, GAUSSIAN Inc., Pittsburgh.

Nuraida, D., Nuraida, D., Abdurrajak, Y., Amin, M. and Hastutik, U. S., 2017, Genetic variation analysis of superior cotton varieties of *Gossypium hirsutum* through microsatellite markers, *Int. J. Plant Bio.*, 8, 6996.

O'Boyle, N. M., Banck, M., James, C. A., Morley, C., Vandermeersch, T. and Hutchison, G. R., 2011, Open Babel, *J. Cheminfo.*, 3(33), 1–14.

Olivia, S., Gibson, J. and Nasrudin, R., 2020, Indonesia in the Time of Covid-19, *Bull. Indonesian Eco. Stud.*, 56(2), 143–174.

Orfali, G. C., Duarte, A. C., Bonadio, V., Martinez, N. P., de Araújo, M. E. M. B., Priviero, F. B. M., Carvalho, P. O. and Priolli, D. G., 2016, Review of anticancer mechanisms of isoquercitin World Journal of Clinical Oncology, *World J. Clin. Oncol.*, 7(2), 189–199.

Pant, S., Singh, M., Ravichandiran, V., Murty, U. S.N. and Srivastava, H. K., 2021, Peptide-like and small-molecule inhibitors against Covid-19, *J. Biomol. Struct. Dyn.*, 39(8), 1–10.

Peiris, J. S. M., Guan, Y. and Yuen, K. Y., 2004, Severe acute respiratory syndrome, *Nat. Med.*, 10(12), S88–S97.

Pettersen, E. F., Goddard, T. D., Huang, C. C., Couch, G. S., Greenblatt, D. M., Meng, E. C. and Ferrin, T. E., 2004, UCSF Chimera - A visualization system for exploratory research and analysis, *J. Comp. Chem.*, 25(13), 1605–1612.

Pundir, H., Joshi, T., Joshi, T., Sharma, P., Mathpal, S., Chandra, S. and Tamta, S., 2021, Using Chou's 5-steps rule to study pharmacophore-based virtual screening of SARS-CoV-2 M^{pro} inhibitors, *Mol. Div.*, 25, 1731–1744.

Pushpakom, S., Iorio, F., Eyers, P. A., Escott, K. J., Hopper, S., Wells, A., Doig, A., Williams, T., Latimer, J., McNamee, C., Norris, A., Sanseau, P., Cavalla, D. and Pirmohamed, M., 2018, Drug repurposing: Progress, challenges and recommendations, *Nat. Rev. Drug Dis.*, 18(1), 41–58.

Riou, J. and Althaus, C. L., 2020, Pattern of early human-to-human transmission of Wuhan 2019 novel coronavirus (2019-nCoV), December 2019 to January 2020, *Eurosurv.*, 25(4), 1–5.

Rossi, G. A., Sacco, O., Mancino, E., Cristiani, L. and Midulla, F., 2020, Differences and similarities between SARS-CoV and SARS-CoV-2: spike receptor-binding domain recognition and host cell infection with support of cellular serine proteases, *Infect.*, 48, 665–669.

- Rotshild, V., Hirsh-Racah, B., Miskin, I., Muszkat, M. and Matok, I., 2021, Comparing the clinical efficacy of COVID-19 vaccines: a systematic review and network meta-analysis, *Sci. Rep.*, 11, 22777.
- Saadat, S., Rawtani, D. and Hussain, C. M., 2020, Environmental perspective of COVID-19, *Sci. Tot. Env.*, 728, 138870.
- Sarkar, C., Jamaddar, S., Mondal, M., Khalipha, A. B. R., Islam, M. T. and Mubarak, M. S., 2021, Natural Products as Anti-COVID-19 Agents: An *In Silico* Study, *Bent. Sci. Pub.*, 2(5), 10–17.
- Sepay, N., Sekar, A., Halder, U. C., Alarifi, A. and Afzal, M., 2021, Anti-COVID-19 terpenoid from marine sources: A docking, admet and molecular dynamics study, *J. Mol. Struct.*, 1228, 129433.
- Shereen, M. A., Khan, S., Kazmi, A., Bashir, N. and Siddique, R., 2020, COVID-19 infection: Origin, transmission, and characteristics of human coronaviruses, *J. Adv. Res.*, 24, 91–98.
- Shi, J., Xiao, Y., Zhang, Y., Geng, D., Cong, D., Shi, K. X., Richard, I. and Knapp, J., 2021, Challenges of drug development during the COVID-19 pandemic: Key considerations for clinical trial designs, *Br. J. Clin. Pharmacol.*, 87, 2170–2185.
- Singh, T. U., Parida, S., Lingaraju, M. C., Kesavan, M., Kumar, D. and Singh, R. K., 2020, Drug repurposing approach to fight COVID-19, *Pharm. Rep.*, 72(6), 1479–1508.
- Singla, R. K., He, X., Chopra, H., Tsagkaris, C., Shen, L., Kamal, M. A. and Shen, B., 2021, Natural Products for the Prevention and Control of the COVID-19 Pandemic: Sustainable Bioresources, *Front. Pharm.*, 12, 1–37.
- Spinelli, A. and Pellino, G., 2020, COVID-19 pandemic: perspectives on an unfolding crisis, *BJS*, 107, 785-787.
- Stoddard, S. V., Stoddard, S. D., Oelkers, B. K., Fitts, K., Whalum, K., Whalum, K., Hemphill, A. D., Manikonda, J., Martinez, L. M., Riley, E. G., Roof, C. M., Sarwar, N., Thomas, D. M., Ulmer, E., Wallace, F. E., Pandey, P. and Roy, S., 2020, Optimization Rules for SARS-CoV-2 M^{pro} Antivirals: Ensemble Docking and Exploration of the Coronavirus Protease Active Site, *Viruses*, 12, 942.
- Tallei, T. E., Tumilaar, S. G., Niode, N. J., Fatimawali, Kepel., B. J., Idroes, R., Effendi, Y., Sakib, S. A. and Emran, T. B., 2020, Potential of Plant Bioactive Compounds as SARS-CoV-2 Main Protease (M^{pro}) and Spike (S) Glycoprotein Inhibitors: A Molecular Docking Study, *Scientifica*, 2020, 1-18.
- Tirado-Rives, J. and Jorgensen, W. L., 2008, Performance of B3LYP Density Functional Methods for a Large Set of Organic Molecules, *J. chem. theory*

comp., 4(2), 297–306.

- Ullah, A. and Ullah, K., 2021, Inhibition of SARS-CoV-2 3CL M^{pro} by Natural and Synthetic Inhibitors: Potential Implication for Vaccine Production Against COVID-19, *Front. Mol. Biosci.*, 8, 1–9.
- Umar, A. K., 2021, Flavonoid compounds of buah merah (*Pandanus conoideus* Lamk) as a potent SARS-CoV-2 main protease inhibitor: *in silico* approach, *Fut. J. Pharm. Sci.*, 7(1), 0–8.
- Vincent, M. J., Bergeron, E., Benjannet, S., Erickson, B. R., Rollin, P. E., Ksiazek, T. G., Seidah, N. G. and Nichol, S. T., 2005, Chloroquine is a potent inhibitor of SARS coronavirus infection and spread, *Vir. J.*, 2, 1–10.
- Wen, W., Chen, C., Tang, J., Wang, C., Zhou, M., Cheng, Y., Zhou, X., Wu, Q., Zhang, X., Feng, Z., Wang, M. and Mao, Q., 2022, Efficacy and safety of three new oral antiviral treatment (molnupiravir, fluvoxamine and Paxlovid) for COVID-19: a meta-analysis, *Ann. Med.*, 54(1), 516–523.
- Zhang, S., Krumberger, M., Morris, M. A., Parrocha, C. M. T., Kreutzer, A. G. and Nowick, J. S., 2021, Structure-based drug design of an inhibitor of the SARS-CoV-2 (COVID-19) main protease using free software: A tutorial for students and scientists, *Euro. J. Med. Chem.*, 218, 113390.
- Zhavoronkov, A., Zagribelnyy, B., Zhebrak, A., Aladinskiy, V., Terentiev, V., Vanhaelen, Q., Bezrukov, D. S., Polykovskiy, D., Shayakhmetov, R., Filimonov, A., Bishop, M., McCloskey, S., Leija, E., Bright, D., Funakawa, K., Lin, Y., Huang, S., Liao, H., Aliper, A. and Yan, I., 2020, Potential non-covalent SARS-CoV-2 3C-like protease inhibitors designed using generative deep learning approaches and reviewed by human medicinal chemist in virtual reality, *ChemRxiv*, 1–18.
- Zheng, J., 2020, SARS-CoV-2: an Emerging Coronavirus that Causes a Global Threat, *Int. J. Bio. Sci.*, 2020(10), 1678–1685.