

DAFTAR PUSTAKA

1. Lushchak, V. I.; Lushchak, O. Interplay between reactive oxygen and nitrogen species in living organisms. *Chem. Biol. Interact.* 2021, *349* (October), 109680.
2. Zamzuri, M. 'Ammar I. A.; Mansor, J.; Nurumal, S. R.; Jamhari, M. N.; Arifin, M. A.; Nawir, A. M. Herbal antioxidants as tertiary prevention against cardiovascular complications in type 2 diabetes mellitus: a systematic review. *J. Herb. Med.* 2023, *37* (December 2022), 100621.
3. Warraich, U. e. A.; Hussain, F.; Kayani, H. U. R. Aging - oxidative stress, antioxidants and computational modeling. *Heliyon* 2020, *6* (5), e04107.
4. Hu, Y.; Liang, P.; Wang, Z.; Jiang, C.; Zeng, Q.; Shen, C.; Wu, Y.; Liu, L.; Yi, Y.; Zhu, H.; Liu, Q. Explore the effect of the structure-activity relationship and dose-effect relationship on the antioxidant activity of licorice flavonoids. 2023, *1292* (May).
5. Phong, H. X.; Viet, N. T.; Quyen, N. T. N.; Van Thinh, P.; Trung, N. M.; Ngan, T. T. K. Phytochemical screening, total phenolic, flavonoid contents, and antioxidant activities of four spices commonly used in vietnamese traditional medicine. *Mater. Today Proc.* 2022, *56*, A1–A5.
6. Gupta, O.; Pradhan, T.; Chawla, G. An updated review on diverse range of biological activities of 1,2,4-triazole derivatives: insight into structure activity relationship. *J. Mol. Struct.* 2023, *1274*, 134487.
7. Pitucha, M.; Janeczko, M.; Klimek, K.; Fornal, E.; Wos, M.; Pachuta-Stec, A.; Ginalska, G.; Kaczor, A. A. 1,2,4-Triazolin-5-Thione derivatives with anticancer activity as CK1 γ kinase inhibitors. *Bioorg. Chem.* 2020, *99* (December 2019), 103806.
8. Addo, J. K.; Owusu-Ansah, E.; Dayie, N. T. K. D.; Cheseto, X.; Torto, B. Synthesis of 1,2,3-triazole-thymol derivatives as potential antimicrobial agents. *Heliyon* 2022, *8* (10), e10836.
9. Singh, K.; Bhor, M.; Kasu, Y. A.; Bhat, G.; Marar, T. Antioxidants as precision weapons in war against cancer chemotherapy induced toxicity – exploring the armoury of obscurity. *Saudi Pharm. J.* 2018, *26* (2), 177–190.
10. Purushothaman, A.; Teena Rose, K. S.; Jacob, J. M.; Varatharaj, R.; Shashikala, K.; Janardanan, D. Curcumin analogues with improved antioxidant properties: a theoretical exploration. *Food Chem.* 2022, *373* (PB), 131499.
11. Pansuriya, K.; Lalpara, J. N.; Hadiyal, S. D.; Dhaduk, B. B.; Dubal, G. G.

- Phenylboronic acid catalyzed synthesis of polysubstituted 1,4-dihydropyridine derivatives as promising antioxidant agents correlated with molecular docking. *Chem. Data Collect.* 2022, 42 (August), 100946.
12. Truong, D. H.; Nhung, N. T. A.; Dao, D. Q. Iron ions chelation-based antioxidant potential vs. pro-oxidant risk of ferulic acid: a DFT study in aqueous phase. *Comput. Theor. Chem.* 2020, 1185 (April), 112905.
 13. Rajan, V. K.; Ragi, C.; Muraleedharan, K. A computational exploration into the structure, antioxidant capacity, toxicity and drug-like activity of the anthocyanidin "Petunidin." *Heliyon* 2019, 5 (7), e02115.
 14. Shameera Ahamed, T. K.; Rajan, V. K.; Sabira, K.; Muraleedharan, K. DFT and QTAIM based investigation on the structure and antioxidant behavior of lichen substances atranorin, evernic acid and diffractaic acid. *Comput. Biol. Chem.* 2019, 80 (August 2018), 66–78.
 15. Venkata Ramana, P.; Rama Krishna, Y.; Chandra Mouli, K. Experimental (FT-IR, UV-Vis) spectroscopic analysis and molecular docking investigations of anti-cancer drugs Alkeran and Bicalutamide. *J. Mol. Struct.* 2022, 1270, 133984.
 16. Nazarbahjat, N.; Nordin, N.; Abdullah, Z.; Abdulla, M. A.; Yehye, W. A.; Nadiyah, S.; Halim, A.; Kee, C. H.; Ariffin, A. New thiosemicarbazides and 1,2,4-triazolethiones derived from 2-(Ethylsulfanyl) benzohydrazide as potent antioxidants. 2014, 11520–11537.
 17. Li, K.; Zhong, W.; Li, P.; Ren, J.; Jiang, K.; Wu, W. International journal of biological macromolecules recent advances in lignin antioxidant: antioxidant mechanism, evaluation methods, influence factors and various applications. *Int. J. Biol. Macromol.* 2023, 251 (April), 125992.
 18. Raskov, H.; Orhan, A.; Christensen, J. P.; Gögenur, I. Cytotoxic CD8+ T cells in cancer and cancer immunotherapy. *Br. J. Cancer* 2021, 124 (2), 359–367.
 19. Lim, S. K.; Yoo, J.; Kim, H.; Lim, Y. M.; Kim, W.; Shim, I.; Kim, H. R.; Kim, P.; Eom, I. chun. Prediction of acute inhalation toxicity using cytotoxicity data from human lung epithelial cell lines. *J. Appl. Toxicol.* 2021, 41 (7), 1038–1049.
 20. Al-Shehri, S. S. Reactive oxygen and nitrogen species and innate immune response. *Biochimie* 2021, 181, 52–64.
 21. Ren, L. kun; Yang, Y.; Ma, C. min; Fan, J.; Bian, X.; Liu, B. xiang; Wang, D. feng; Zhu, P. yu; Fu, Y.; Zhang, N. Identification and in silico analysis of novel antioxidant peptides in broken rice protein hydrolysate and its cytoprotective effect against H₂O₂-induced 2BS cell model. *Food Res. Int.* 2022, 162 (1).

22. Boyd, R. J. *Theoretical and Computational Chemistry*; Elsevier Inc., 2019.
23. He, L.; Bai, L.; Dionysiou, D. D.; Wei, Z.; Spinney, R.; Chu, C.; Lin, Z.; Xiao, R. Applications of computational chemistry, artificial intelligence, and machine learning in aquatic chemistry research. *Chem. Eng. J.* 2021, 426 (May), 131810.
24. Imelda, I.; Aziz, H.; Aziz, H.; Putri, H. Modifikasi struktur zat warna berbasis trifenilamin untuk meningkatkan kinerja Dye-Sensitized Solar Cells (DSSCs): metode komputasi. *J. Res. Educ. Chem.* 2022, 4 (1), 34.
25. Liu, Z.; Wang, P.; Chen, H.; Wold, E. A.; Tian, B.; Brasier, A. R.; Zhou, J. Drug Discovery targeting Bromodomain-Containing Protein 4. *J. Med. Chem.* 2017, 60 (11), 4533–4558. <https://doi.org/10.1021/acs.jmedchem.6b01761>.
26. Donati, B.; Lorenzini, E.; Ciarrocchi, A. BRD4 and cancer: going beyond transcriptional regulation. *Mol. Cancer* 2018, 17 (1), 1–13.
27. Choi, J. Y.; Podust, L. M.; Roush, W. R. Drug strategies targeting CYP51 in neglected tropical diseases. *Chem. Rev.* 2014, 114 (22), 11242–11271.
28. Podust, L. M.; Poulos, T. L.; Waterman, M. R. Crystal structure of cytochrome P450 14 α -sterol demethylase (CYP51) from *Mycobacterium Tuberculosis* in complex with azole inhibitors. *Proc. Natl. Acad. Sci. U. S. A.* 2001, 98 (6), 3068–3073.
29. Beytur, M.; Turhan Irak, Z.; Manap, S.; Yüksek, H. Synthesis, characterization and theoretical determination of corrosion inhibitor activities of some new 4,5-dihydro-1H-1,2,4-triazol-5-one derivatives. *Heliyon* 2019, 5 (6), e01809.
30. Hassan, B.; Shireen, A.; Muraleedharan, K.; Mujeeb, V. M. A. Virtual screening of molecular properties of chitosan and derivatives in search for druggable molecules. *Int. J. Biol. Macromol.* 2015, 74, 392–396.
31. El Rhabori, S.; El Aissouq, A.; Chtita, S.; Khalil, F. 3D-QSAR, molecular docking and ADMET studies of thioquinazolinone derivatives against breast cancer. *J. Indian Chem. Soc.* 2022, 99 (10), 100675.
32. P, A. L. Frontier molecular orbitals (FMO) and molecular electrostatic potential (MEP) surface of method. 2020, No. 2, 1333–1334.
33. Boulebd, H.; Carmena-Bargueño, M.; Pérez-Sánchez, H. Exploring the antioxidant properties of caffeoylquinic and feruloylquinic acids: a computational study on hydroperoxyl radical scavenging and xanthine oxidase inhibition. *Antioxidants* 2023, 12 (9).
34. Barreca, D. Mechanisms of plant antioxidants action. *Plants* 2021, 10 (1), 1–4.
35. Elharafi, H.; Elhamdani, N.; Hachim, M. E.; Tebbaai, H.; Sadik, K.; El Hachadi,

- F.; Aboulmouhajir, A. In silico exploration of bioavailability, druggability, toxicity alerts and biological activity of a large series of fatty acids. *Comput. Toxicol.* 2021, 17 (August 2020), 100153.
36. Adole, V. A.; More, R. A.; Jagdale, B. S.; Pawar, T. B.; Chobe, S. S.; Shinde, R. A.; Dhonnar, S. L.; Koli, P. B.; Patil, A. V.; Bukane, A. R.; Gacche, R. N. Microwave prompted solvent-free synthesis of new series of heterocyclic tagged 7-arylidene indanone hybrids and their computational, antifungal, antioxidant, and cytotoxicity study. *Bioorg. Chem.* 2021, 115 (August), 105259.
37. Belaya, N. I.; Belyi, A. V. Semi-empirical model for predicting phenol carboxylic acids antiradical activity. *ChemChemTech* 2019, 62 (7), 80–84.
38. Marković, Z. Study of the mechanisms of antioxidative action of different antioxidants. *J. Serbian Soc. Comput. Mech.* 2016, 10 (1), 135–150.
39. Govindammal, M.; Kannan, S.; Srinivasan, P.; Prasath, M. Heliyon quantum chemical calculations , spectroscopic studies and molecular docking investigations of the anti-cancer drug quercitrin with B-RAF inhibitor. *Heliyon* 2022, 8 (May), e09539.
40. Amić, A.; Marković, Z.; Dimitrić Marković, J. M.; Milenković, D.; Lučić, B. The role of guaiacyl moiety in free radical scavenging by 3,5-dihydroxy-4-methoxybenzyl alcohol: thermodynamics of 3H⁺/3e⁻ mechanisms. *Mol. Phys.* 2019, 117 (2), 207–217.
41. Manoj, K. M.; Nikolai, B.; Parashar, A.; Gideon, D. A.; Jacob, V. D.; Haarith, D.; Manekkathodi, A. Murburn Precepts for the Light Reaction of Oxygenic Photosynthesis. 2020, 2, 1–19.
42. Spiegel, M.; Kapusta, K.; Kołodziejczyk, W.; Saloni, J.; Zbikowska, B.; Hill, G. A.; Sroka, Z. Antioxidant activity of selected phenolic acids–ferric reducing antioxidant power assay and QSAR analysis of the structural features. *Molecules* 2020, 25 (13).
43. Zeiler, G. E.; Meyer, L. C. R. Blood acid-base status in impala (*Aepyceros Melampus*) immobilised and maintained under total intravenous anaesthesia using two different drug protocols. *BMC Vet. Res.* 2017, 13 (1), 1–10.
44. Zakrzewski, R.; Urbaniak, P.; Nowicki, A.; Tejchman, W. Chromatographic and computational studies of molecular lipophilicity and drug-likeness for few 2-thioxo-1,3-thiazolidin-4-one derivatives and their analogs. *J. Chromatogr. Sci.* 2018, 56 (8), 709–715.
45. Roy, K.; Kar, S.; Das, R. N. *Other Related Techniques*; 2015.

46. Amoras, M.; Fujishima, T.; Raulino, S.; Ramos, S.; Figueiredo, E.; Ferreira, B.; Lu, K.; Rosa, C.; Breno, C. An antioxidant potential , quantum-chemical and molecular docking study of the major chemical constituents present in the leaves of curatella americana linn.
47. Trac, L. N.; Schmidt, S. N.; Holmstrup, M.; Mayer, P. Headspace passive dosing of volatile hydrophobic organic chemicals from a lipid donor - linking their toxicity to well-defined exposure for an improved risk assessment. *Environ. Sci. Technol.* 2019.
48. Trusek-Holownia, A.; Latka, A. Polymeric carriers – the influence of body fluid compounds on a drug local release. *BIODEVICES 2018 - 11th Int. Conf. Biomed. Electron. Devices, Proceedings; Part 11th Int. Jt. Conf. Biomed. Eng. Syst. Technol. BIOSTEC 2018* 2018, 1 (Biostec), 241–246.
49. Fadilah, F.; Arsianti, A.; Yanuar, A.; Andrajati, R.; Paramita, R. I.; Purwaningsih, E. H. Structure activity relationship analysis of antioxidant activity of simple benzene carboxylic acids group, based on multiple linear regression. *Orient. J. Chem.* 2018, 34 (5), 2656–2660.
50. Velázquez-Libera, J. L.; Durán-Verdugo, F.; Valdés-Jiménez, A.; Valdés-Jiménez, A.; Núñez-Vivanco, G.; Caballero, J. LigRMSD: A web server for automatic structure matching and RMSD calculations among identical and similar compounds in protein-ligand docking. *Bioinformatics* 2020, 36 (9), 2912–2914.
51. Forli, S.; Huey, R.; Pique, M. E.; Sanner, M.; Goodsell, D. S.; Arthur, J. 00006565-201002000-00017. 2016, 11 (5), 905–919.
52. Surabaya, K.; Surabaya, K.; Kesehatan, D.; Surabaya, K.; Correlation, P.; Moment, P.; Mei, B.; Dbd, K.; Surabaya, K. 233837344. 2014.