

DAFTAR PUSTAKA

- (1) finley, J. W.; Ah-Ng K; Korry H; Elizabeth H.J. Antioxidants in Foods: State of the Science Important to the Food Industry. *Journal of Agricultural Food Chemistry* 2011, 59, 6837–6846.
- (2) Pisoschi, A. M.; Pop, A. The Role of Antioxidants in the Chemistry of Oxidative Stress: A Review. *Med. Chem* 2015, 97, 55–74.
- (3) Juniarti, dan. *Analisis Senyawa Metabolit Sekunder Dari Ekstrak Metanol Daun Surian Yang Berpotensi Sebagai Antioksidan*; 2011; Vol. 15.
- (4) Wang A.; Yang L.; Peng, H. S.; Hui, Z. A Theoretical Study on the Antioxidant Activity of Uralenol and Neouralenol Scavenging Two Radicals, *Struct. Chem* 2018, 29, 1067–1075.
- (5) Dimitrić Marković, J. M.; Milenković, D.; Amić, D.; Popović-Bijelić, A.; Mojović, M.; Pašti, I. A.; Marković, Z. S. Energy Requirements of the Reactions of Kaempferol and Selected Radical Species In Different Media: Towards the Prediction of the Possible Radical Scavenging Mechanisms. *Struct Chem* 2014, 25 (6), 1795–1804.
- (6) Ren, J.; Lu, Y.; Qian, Y.; Chen, B.; Wu, T.; Ji, G. Recent Progress Regarding Kaempferol for the Treatment of Various Diseases (Review). *Exp Ther Med* 2019.
- (7) Subositi D; Kurnianingrum N; Mujahid R; Widiyastuti Y. Kaempferia Galanga L. a Medicinal Plant Used by Indonesian Ethnic Groups: Genetic Diversity Based on Inter-Simple Sequence Repeats (ISSR). *Agrivita*. 2020, 1, 45–52.
- (8) Singh, K.; Bhori, 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 Pharmaceutical Journal* 2018, 26 (2), 177–190.
- (9) Ponnam, D. K.; Srinivas, K. V. N.; Jonnala, K.; Kumar, T.; Savita, B.; Kakaraparthi, R. S. Phytochemical Investigation, Antioxidant, and Antifungal Activities of Rhizomes of *Euphorbia Fusiformis*. *Phcog J* 2014, 6 (4), 78–82.
- (10) 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.
- (11) Seeliger D; de Groot BL. Ligand Docking and Binding Site Analysis with PyMOL and Autodock/Vina. *J Comput Aided Mol Des* 2010, 24, 417–422.
- (12) 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, 66–78.
- (13) Devi K. P; Malar D. S; Nabavi S. F; Xiao J.; Nabavi S. M; Dadlia M. Kaempferol and Inflammation: From Chemistry to Medicine. *Pharmacol Ress* 2015, 1, 1–10.
- (14) Chiou, W. F.; Lee, C. H.; Liao, J. F.; Chen, C. C. 8-Prenylkaempferol Accelerates Osteoblast Maturation through Bone Morphogenetic Protein-2/P38 Pathway to Activate Runx2 Transcription. *Life Sci* 2011, 88 (7–8), 335–342.

- (15) Silalahi, M. Jamblang (*Syzygium Cumini* (L.) Dan Bioaktivitasnya. *Interest: Jurnal Ilmu Kesehatan* 2018, 7 (2). <https://doi.org/10.37341/interest.v7i2.20>.
- (16) Nguyen, V. S.; Shi, L.; Luan, F. Q.; Wang, Q. A. Synthesis of Kaempferide Mannich Base Derivatives and Their Antiproliferative Activity on Three Human Cancer Cell. *Acta Biochim Pol* 2015, 62 (3), 547–552.
- (17) Halliwell, B.; Guttendge, J. M. C. Free Radicals, Antioxidant in Biology and Medicine. *Oxford University Press* 2015, 5.
- (18) Mehta SK; Gowder SJT. Members of Antioxidant Machinery and 9. Their Functions. In Basic Principles and Clinical Significance of Oxidative Stress. . *In Tech* 2015.
- (19) Zheng, Y. Z.; Deng, G.; Liang, Q.; Chen, D. F.; Guo, R.; Lai, R. C. Antioxidant Activity of Quercetin and Its Glucosides from Propolis: A Theoretical Study. *Sci Rep* 2017, 7 (1).
- (20) Choi, Y. S.; Kang, W. D ; Kim, S. M ; Choi, Y. D ; Nam, J. H.; Park, C. S.; Choi, H. S. Human Papillomavirus L1 Capsid Protein and Human Papillomavirus Type 16 as Prognostic Markers in Cervical Intraepithelial Neoplasia 1. *International Journal of Gynecological Cancer* 2010, 20 (2), 288–293.
- (21) Kashyap, D.; Sharma, A.; Tuli, H. S.; Sak, K.; Punia, S.; Mukherjee, T. K. Kaempferol – A Dietary Anticancer Molecule with Multiple Mechanisms of Action: Recent Trends and Advancements. *Journal of Functional Foods*. Elsevier Ltd March 1, 2017, pp 203–219.
- (22) Male, Y. T.; Sutapa, I. W.; Pusung, Y. A. D. Prediksi Potensi Antikanker Senyawa Turunan Xanthon Menggunakan Hubungan Kuantitatif Struktur Dan Aktivitas (HKSA). *Chemistry Progress* 2018, 11, 1–6.
- (23) Raskov, H.; Orhan, A.; Christensen, J. P.; Gögenur, I. Cytotoxic CD8+ T Cells in Cancer and Cancer Immunotherapy. *British Journal of Cancer*. Springer Nature January 19, 2021, pp 359–367.
- (24) 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. *Journal of Applied Toxicology* 2021, 41 (7), 1038–1049.
- (25) Rajan, V. K.; Ragi, C.; Muraleedharan, K. A Computational Exploration into the Structure, Antioxidant Capacity, Toxicity and Drug-like Activity of the Anthocyanidin “Petunidin.” . 2019, 7, 1–9.
- (26) Ivanović, V.; Rančić, M.; Arsić, B.; Pavlović, A. *Lipinski's Rule of Five, Famous Extensions and Famous Exceptions*; Vol. 3.
- (27) Neidle, S. Design Principles for Quadruplex-Binding Small Molecules. In *Therapeutic Applications of Quadruplex Nucleic Acids*; Elsevier, 2012; pp 151–174.
- (28) Mandal, M.; Sarkar, M.; Khan, A.; Biswas, M.; Masi, A.; Rakwal, R.; Agrawal, G. K.; Srivastava, A.; Sarkar, A. Reactive Oxygen Species (ROS) and Reactive Nitrogen Species (RNS) in Plants– Maintenance of Structural Individuality and Functional Blend. *Advances in Redox Research* 2022, 5, 100039.

- (29) Squadrito, G. L.; Pryor, W. A. *Forum Oxidative Chemistry Of Nitric Oxide: The Roles Of Superoxide, Peroxynitrite, And Carbon Dioxide*; 1998; Vol. 25.
- (30) Halliwell, B. Reactive Oxygen Species (ROS), Oxygen Radicals and Antioxidants: Where Are We Now, Where Is the Field Going and Where Should We Go? *Biochemical and Biophysical Research Communications*. Elsevier B.V. December 10, 2022, pp 17–19.
- (31) Pauly, N.; Pucciariello, C.; Mandon, K.; Innocenti, G.; Jamet, A.; Baudouin, E.; Hérouart, D.; Frendo, P.; Puppo, A. Reactive Oxygen and Nitrogen Species and Glutathione: Key Players in the Legume-Rhizobium Symbiosis. In *Journal of Experimental Botany*; 2006; Vol. 57, pp 1769–1776.
- (32) Kashyap, D.; Sharma, A.; Tuli, H. S.; Sak, K.; Punia, S.; Mukherjee, T. K. Kaempferol – A Dietary Anticancer Molecule with Multiple Mechanisms of Action: Recent Trends and Advancements. *Journal of Functional Foods*. Elsevier Ltd March 1, 2017, pp 203–219.
- (33) Ortiz-Escarza, J. M.; Medina, M. E.; Trigo, A. On the Peroxyl Radical Scavenging Ability of β -Sitosterol in Lipid Media: A Theoretical Study. *J Phys Org Chem* 2021, 34 (1).
- (34) Imran, M.; Salehi, B.; Sharifi-Rad, J.; Gondal, T. A.; Saeed, F.; Imran, A.; Shahbaz, M.; Fokou, P. V. T.; Arshad, M. U.; Khan, H.; Guerreiro, S. G.; Martins, N.; Estevinho, L. M. Kaempferol: A Key Emphasis to Its Anticancer Potential. *Molecules*. MDPI AG 2019.
- (35) Liu, X.; Pan, X.; Wang, C.; Liu, H. Modulation of Reactive Oxygen Species to Enhance Sonodynamic Therapy. *Particuology* 2023, 75, 199–216.
- (36) Rosh R; Bloch I; Sklenar H; Shakked Z. Molecular Flexibility in Ab-Initio Drug Docking to DNA: Binding-Site and Binding-Mode Transitions in All-Atom Monte Carlo Simulations. *Nucl Acids Res* 2015, 33, 7048–7057.
- (37) Richa, K.; Karmaker, R.; Ao, T.; Longkumer, N.; Singha, B.; Singha, U. B. Rationale for Antioxidant Interaction Studies of 4-Bromo-1-Isothiocyanato-2-Methylbenzene – An Experimental and Computational Investigation. *Chem Phys Lett* 2020, 753.
- (38) 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.
- (39) Joyce, J. G.; Tung, J.-S.; Przysiecki, C. T.; Cook, J. C.; Lehman, E. D.; Sands, J. A.; Jansen, K. U.; Keller, P. M. The L1 Major Capsid Protein of Human Papillomavirus Type 11 Recombinant Virus-like Particles Interacts with Heparin and Cell-Surface Glycosaminoglycans on Human Keratinocytes*; 1999.
- (40) Boulebd, H. Structure-Activity Relationship of Antioxidant Prenylated (Iso)Flavonoid-Type Compounds: Quantum Chemistry and Molecular Docking Studies. *J Biomol Struct Dyn* 2021, 1–10.
- (41) Rajan VK; Hasna CK; Muraleedharan K. The Natural Food Colorant Peonidin from Cranberries as a Potential Radical Scavenger – a DFT Based Mechanistic Analysis. *Food Chem* 2018, 262, 184–190.

- (42) Orabi EA; Orabi MAA; Mahross MH; Abdel-Hakim M. Computational Investigation of the Structure and Antioxidant Activity of Some Pyrazole and Pyrazolone Derivatives. *J Saudi Chem Soc* 2018, 6 (22), 705–714.
- (43) Alov P; Tsakovska I; Pajeva I. Computational Studies of Free Radical-Scavenging Properties of Phenolic Compounds. *Curr Top Med Chem* 2014, 2 (15), 85–104.
- (44) Adole VA; More RA; Jagdale BS. 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, 109–115.
- (45) Richa K; Kamarker R; Ao T; Longkumer N; Singha B; Sinha UB. Rationale for Antioxidant Interaction Studies of 4-Bromo-1-Isothiocyanato-2-Methylbenzene – an Experimental and Computational Investigation. *Chem Phys Lett* 2020.
- (46) Richa, K. ; K. R. ; A. T. ; L. N. ; S. B. ; S. UB. Rationale for Antioxidant Interaction Studies of 4-Bromo 1 Isothiocyanato 2 Methylbenzene – An Experimental and Computational Investigation. *Chem Phys Lett* 2020, 753.
- (47) Hansch, C.; Leo, + A; Taft, R. W. *A Survey of Hammett Substituent Constants and Resonance and Field Parameters*; Vol. 97.
- (48) Murray, J. S.; Politzer, P. The Electrostatic Potential: An Overview. *Wiley Interdiscip Rev Comput Mol Sci* 2011, 1 (2), 153–163.
- (49) Sangeetha, T.; Sahana, R.; Mounica, P.; Elangovan, A.; Shanmugam, R.; Arivazhagan, G. Atoms in Molecules Theory, Electrostatic Potential Surface and Frontier Molecular Orbital Analyses on Water Multimers and Pyridine – Water Hydrogen Bonded Complexes. *Comput Theor Chem* 2023, 1219.
- (50) Murray, J. S.; Politzer, P. The Electrostatic Potential: An Overview. *Wiley Interdiscip Rev Comput Mol Sci* 2011, 1 (2), 153–163.
- (51) Schuster, I. I. Stereoelectronic Substituent Effects on Intramolecular H-Bonding in Crowded o-Anisic Acids. *Journal of the Chemical Society. Perkin Transactions 2* 2002, 2 (12), 1961–1966.
- (52) Safna Hussan, K. P.; Shahin Thayyil, M.; Rajan, V. K.; Muraleedharan, K. DFT Studies on Global Parameters, Antioxidant Mechanism and Molecular Docking of Amlodipine Besylate. *Comput Biol Chem* 2019, 80, 46–53.
- (53) Galano, A.; Tan, D. X.; Reiter, R. J. On the Free Radical Scavenging Activities of Melatonin's Metabolites, AFMK and AMK. *Journal of Pineal Research*. Blackwell Publishing Ltd 2013, pp 245–257. <https://doi.org/10.1111/jpi.12010>.
- (54) Raphael KL; Kraut JA. Assessing acid-base status in patients with ckd: does measurement of blood pH matter?. *Am J Kidney Dis*.
- (55) Goodwin, R. J. A.; Bunch, J.; McGinnity, D. F. Mass Spectrometry Imaging in Oncology Drug Discovery. In *Advances in Cancer Research*; Academic Press Inc., 2017; Vol. 134, pp 133–171.
- (56) Chen Y; Xiao H; Zheng J; Liang G. Structure-Thermodynamics-Antioxidant Activity Relationships of Selected Natural Phenolic Acids and Derivatives: An Experimental and Theoretical Evaluation. *PLoS One* 2015, 10 (3), 1–20.

- (57) Rachmania RA; Supandi; Larasati OA. In-Silico Analysis of Diterpenoid Lactobee Coumpounds of Bitter Herbs on Alpha-Glucosidase Receptor as Antidiabetic. *Pharmacy* 2019, 12 (2).
- (58) Wulandari, A.; Afrizal, A.; Emriadi, E.; Efdi, M.; Imelda. Studi Komputasi Terhadap Struktur, Sifat Antioksidan, Toksisitas Dan Skor Obat Dari Scopoletin Dan Turunannya. *Chempublish Journal* 2020, 5 (1), 77–92.
- (59) Goodwin, R. J. A.; Bunch, J.; McGinnity, D. F. Mass Spectrometry Imaging in Oncology Drug Discovery. In *Advances in Cancer Research*; Academic Press Inc., 2017; Vol. 134, pp 133–171.
- (60) Widia I; marline A; taufik R. Aspek Kimia Medisinal Senyawa Xanton Sebagai Anti Kanker. *Farmaka* 2018, 16, 213–221.
- (61) Syahputra G; Ambarsari L; T S. Simulasi Docking Kurkumin Enol, Bisdemetoksikurkumin Dan Analognya Sebagai Inhibitor Enzim12-Lipoksgenase. *Biofisika* 2020, 10 (1), 55–67.
- (62) Nusantoro, Y. R., Faqlan, A. Analisis Sifat Minus Obat, Prediksi ADMET, Dan Penambatan Molekular Isatinil-2-Aminobenzoilhidrazon Dan Kompleks Logam Transisi Co(II), Ni(II), Cu(II), Zn(II) Terhadap BCL2-XL. *Acta Kimia Indonesia* 2020, 5 (2), 114.
- (63) Pollastri, M. P. Overview on the Rule of Five. *Current Protocols in Pharmacology*. June 2010.
- (64) Da, J.; Xu, M.; Wang, Y.; Li, W.; Lu, M.; Wang, Z. Kaempferol Promotes Apoptosis While Inhibiting Cell Proliferation via Androgen-Dependent Pathway and Suppressing Vasculogenic Mimicry and Invasion in Prostate Cancer. *Analytical Cellular Pathology* 2019, 2019.
- (65) Kim, J. H.; Cho, I. S.; So, Y. K.; Kim, H. H.; Kim, Y. H. Kushenol A and 8-Prenylkaempferol, Tyrosinase Inhibitors, Derived from Sophora Flavescens. *J Enzyme Inhib Med Chem* 2018, 33 (M), 1048–1054.
- (66) El-Moneim, A.; Affy, M. R.; Fayed, S. A.; Shalaby, E. A.; El-Shemy, H. A. Syzygium Cumini (Pomposia) Active Principles Exhibit Potent Anticancer and Antioxidant Activities. *Afr J Pharm Pharmacol* 2011, 5 (7), 948–956.
- (67) Nguyen, V. S.; Shi, L.; Luan, F. Q.; Wang, Q. A. Synthesis of Kaempferide Mannich Base Derivatives and Their Antiproliferative Activity on Three Human Cancer Cell. *Acta Biochim Pol* 2015, 62 (3), 547–552.
- (68) Lin, R.; Yang, S.; Si, L.; Jia, Y.; Jian, W.; Yu, Q.; Wang, M. Kaempferol Exerts Anti-Proliferative Effects on Human Ovarian Cancer Cells by Inducing Apoptosis, G0/G1 Cell Cycle Arrest and Modulation of MEK/ERK and STAT3 Pathways. *JBUON* 2019, 24 (3), 975–981.
- (69) Abbasi, B. A.; Iqbal, J.; Zahra, S. A.; Shahbaz, A.; Kanwal, S.; Rabbani, A.; Mahmood, T. Bioinspired Synthesis and Activity Characterization of Iron Oxide Nanoparticles Made Using Rhamnus Triquetra Leaf Extract. *Mater Res Express* 2019, 6 (12).

- (70) Nguyen, V. S.; Shi, L.; Luan, F. Q.; Wang, Q. A. Synthesis of Kaempferide Mannich Base Derivatives and Their Antiproliferative Activity on Three Human Cancer Cell. *Acta Biochim Pol* 2015, 62 (3), 547–552.
- (71) Arputharaj, D. S.; Rajasekaran, M.; Nidhin, P. V. Sulfamethoxazole: Molecular Docking and Crystal Structure Prediction. *Results Chem* 2023, 5.
- (72) Asiamah, I.; Obiri, S. A.; Tamekloe, W.; Armah, F. A.; Borquaye, L. S. Applications of Molecular Docking in Natural Products-Based Drug Discovery. *Scientific African*. Elsevier B.V. July 1, 2023.
- (73) Forli S; Huey R; Pique ME; Sanner MF; DSG; Olson AJ. Computational Protein–Ligand Docking and Virtual Drug Screening with the Autodock Suite. *Polym J* 2016, 48 (7), 829–834.
- (74) Demir, S.; Turan, I.; Aliyazicioglu, R.; Yaman, S. O.; Aliyazicioglu, Y. Primula Vulgaris Extract Induces Cell Cycle Arrest and Apoptosis in Human Cervix Cancer Cells. *J Pharm Anal* 2018, 8 (5), 307–311.
- (75) Dong, D.; Zhu, Y.; Aili, Z.; Chen, Z.; Ding, J. Bioinformatics Analysis of HPV-68 E6 and E7 Oncoproteins for Designing a Therapeutic Epitope Vaccine against HPV Infection. *Infection, Genetics and Evolution* 2020, 81.

