Optimizing cardio, hepato and phospholipidosis toxicity chemoinformatics and molecular modelling approach

SAR and QSAR in Environmental Research

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Citation Report

#	Article	IF	Citations
1	Design, synthesis, biological evaluation and in silico studies of novel 1,2,3-triazole linked benzoxazine-2,4-dione conjugates as potent antimicrobial, antioxidant and anti-inflammatory agents. Arabian Journal of Chemistry, 2022, 15, 104226.	4.9	15
2	Multifunctional Derivatives of Spiropyrrolidine Tethered Indeno-Quinoxaline Heterocyclic Hybrids as Potent Antimicrobial, Antioxidant and Antidiabetic Agents: Design, Synthesis, In Vitro and In Silico Approaches. Molecules, 2022, 27, 7248.	3.8	5
3	Design, synthesis and molecular docking and ADME studies of novel hydrazone derivatives for AChE inhibitory, BBB permeability and antioxidant effects. Journal of Biomolecular Structure and Dynamics, 2023, 41, 9022-9038.	3.5	12
4	Phytochemical Analysis, Antioxidant, and Antimicrobial Activities of Ducrosia flabellifolia: A Combined Experimental and Computational Approaches. Antioxidants, 2022, 11, 2174.	5.1	9
5	Evaluation of oxindole derivatives as a potential anticancer agent against breast carcinoma cells: In vitro, in silico, and molecular docking study. Toxicology in Vitro, 2023, 86, 105517.	2.4	15
6	Benzothiazole clubbed imidazolone derivatives: Synthesis, molecular docking, DFT studies, and antimicrobial studies. Current Computer-Aided Drug Design, 2022, 19, .	1.2	0
7	Antihypertensive activity of roasted cashew nut in mixed petroleum fractions-induced hypertension: An in vivo and in silico approaches. Heliyon, 2022, 8, e12339.	3.2	9
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9	Application of density functional theory (DFT) and response surface methodology (RSM) in drug discovery. , 2023, , 371-392.		3
11	Development of Isopropyl-Tailed Chalcones as a New Class of Selective MAO-B Inhibitors for the Treatment of Parkinsonâ€™s Disorder. ACS Omega, 2023, 8, 6908-6917.	3.5	15
12	Design and synthesis of some novel hybrid molecules based on 4-thiazolidinone bearing pyridine-pyrazole scaffolds: molecular docking and molecular dynamics simulations of its major constituent onto DNA gyrase inhibition. Molecular Diversity, 0, , .	3.9	4
13	Synthesis, Biological Evaluation, and Molecular Modeling Studies of New 1,3,4â€Thiadiazole Derivatives as Potent Antimicrobial Agents. Chemistry and Biodiversity, 2023, 20, .	2.1	8
14	Bioisosteric modification of Linezolid identified the potential M. tuberculosis protein synthesis inhibitors to overcome the myelosuppression and serotonergic toxicity associated with Linezolid in the treatment of the multi-drug resistance tuberculosis (MDR-TB). Journal of Biomolecular Structure and Dynamics, 2024, 42, 2111-2126.	3.5	6
15	In silico analysis to identify potential antitubercular molecules in Morus alba through virtual screening and molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2024, 42, 1924-1931.	3.5	4
16	A structural approach to investigate halogen substituted MAO-B inhibitors using QSAR modeling, molecular dynamics, and conceptual DFT analysis. Journal of Saudi Chemical Society, 2023, 27, 101675.	5.2	3
17	Molecular docking-based interaction studies on imidazo[1,2-a] pyridine ethers and squaramides as anti-tubercular agents. SAR and QSAR in Environmental Research, 2023, 34, 435-457.	2.2	1
18	Isoflavonoid and Furanochromone Natural Products as Potential DNA Gyrase Inhibitors: Computational, Spectral, and Antimycobacterial Studies. ACS Omega, 2023, 8, 16228-16240.	3.5	8
19	Antibacterial Potential of Trihydroxycyclohexa-2,4-Diene-1-Carboxylic Acid: Insight from DFT, Molecular Docking, and Molecular Dynamic Simulation. Polycyclic Aromatic Compounds, 0, , 1-24.	2.6	12

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20	A novel series of dipeptide derivatives containing indole-3-carboxylic acid conjugates as potential antimicrobial agents: the design, solid phase peptide synthesis, in vitro biological evaluation, and molecular docking study. RSC Advances, 2023, 13, 24250-24263.	3.6	2
21	Rhamnetin, a nutraceutical flavonoid arrests cell cycle progression of human ovarian cancer (SKOV3) cells by inhibiting the histone deacetylase 2 protein. Journal of Biomolecular Structure and Dynamics, 0, , 1-16.	3.5	0
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