Barun Bhhatarai

List of Publications by Year
in descending order

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Version: 2024-02-01

26 papers	1,421 citations	430874 18 h-index	580821 25 g-index
27 all docs	27 docs citations	27 times ranked	2533 citing authors

#	Article	IF	Citations
1	Allosteric Inhibition of the IRE1Î± RNase Preserves Cell Viability and Function during Endoplasmic Reticulum Stress. Cell, 2014, 158, 534-548.	28.9	384
2	Divergent allosteric control of the IRE1Î± endoribonuclease using kinase inhibitors. Nature Chemical Biology, 2012, 8, 982-989.	8.0	175
3	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	6.0	120
4	Prediction of Aqueous Solubility, Vapor Pressure and Critical Micelle Concentration for Aquatic Partitioning of Perfluorinated Chemicals. Environmental Science & Technology, 2011, 45, 8120-8128.	10.0	112
5	Opportunities and challenges using artificial intelligence in ADME/Tox. Nature Materials, 2019, 18, 418-422.	27.5	69
6	The activities of drug inactive ingredients on biological targets. Science, 2020, 369, 403-413.	12.6	61
7	Novel Selective Allosteric and Bitopic Ligands for the S1P₃ Receptor. ACS Chemical Biology, 2012, 7, 1975-1983.	3.4	55
8	Alternative approaches for identifying acute systemic toxicity: Moving from research to regulatory testing. Toxicology in Vitro, 2017, 41, 245-259.	2.4	54
9	A sphingosine 1-phosphate receptor 2 selective allosteric agonist. Bioorganic and Medicinal Chemistry, 2013, 21, 5373-5382.	3.0	53
10	Evaluation of TOPKAT, Toxtree, and Derek Nexus in Silico Models for Ocular Irritation and Development of a Knowledge-Based Framework To Improve the Prediction of Severe Irritation. Chemical Research in Toxicology, 2016, 29, 810-822.	3.3	44
11	Per- and Polyfluoro Toxicity (LC₅₀ Inhalation) Study in Rat and Mouse Using QSAR Modeling. Chemical Research in Toxicology, 2010, 23, 528-539.	3.3	35
12	CADASTER QSPR Models for Predictions of Melting and Boiling Points of Perfluorinated Chemicals. Molecular Informatics, 2011, 30, 189-204.	2.5	32
13	Modelling physico-chemical properties of (benzo)triazoles, and screening for environmental partitioning. Water Research, 2011, 45, 1463-1471.	11.3	31
14	Oral LD50 toxicity modeling and prediction of per- and polyfluorinated chemicals on rat and mouse. Molecular Diversity, 2011, 15, 467-476.	3.9	29
15	Evaluation of OASIS QSAR Models Using ToxCastâ„¢ in Vitro Estrogen and Androgen Receptor Binding Data and Application in an Integrated Endocrine Screening Approach. Environmental Health Perspectives, 2016, 124, 1453-1461.	6.0	26
16	From SAR to comparative QSAR: role of hydrophobicity in the design of 4-hydroxy-5,6-dihydropyran-2-ones HIV-1 protease inhibitors. Bioorganic and Medicinal Chemistry, 2005, 13, 4078-4084.	3.0	25
17	GPCR ontology: development and application of a G protein-coupled receptor pharmacology knowledge framework. Bioinformatics, 2013, 29, 3211-3219.	4.1	24
18	A mechanistic study of 3-aminoindazole cyclic urea HIV-1 protease inhibitors using comparative QSAR. Bioorganic and Medicinal Chemistry, 2004, 12, 5819-5831.	3.0	22

#	Article	IF	Citations
19	Acute Toxicity Prediction in Multiple Species by Leveraging Mechanistic ToxCast Mitochondrial Inhibition Data and Simulation of Oral Bioavailability. Toxicological Sciences, 2015, 147, 386-396.	3.1	17
20	Performance evaluation of the GastroPlusTM software tool for prediction of the toxicokinetic parameters of chemicals. SAR and QSAR in Environmental Research, 2018, 29, 875-893.	2.2	12
21	Are Mechanistic and Statistical QSAR Approaches Really Different? MLR Studies on 158 Cycloalkylâ€Pyranones. Molecular Informatics, 2010, 29, 511-522.	2.5	11
22	The QSPR-THESAURUS: The Online Platform of the CADASTER Project. ATLA Alternatives To Laboratory Animals, 2014, 42, 13-24.	1.0	10
23	A QSAR Study of HIV Protease Inhibitors Using Theoretical Descriptors. Current Computer-Aided Drug Design, 2010, 6, 269-282.	1.2	8
24	Comparative QSAR as a Cheminformatics Tool in the Design of Dihydro- Pyranone Based HIV-1 Protease Inhibitors. Current Computer-Aided Drug Design, 2008, 4, 283-310.	1.2	6
25	QSAR and Molecular Modeling Studies of HIV Protease Inhibitors. , 0, , 181-271.		5
26	Possible allosteric interactions of monoindazole-substituted P2 cyclic urea analogues with wild-type and mutant HIV-1 protease. Journal of Computer-Aided Molecular Design, 2008, 22, 737-745.	2.9	1