# Barun Bhhatarai

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/2446905/publications.pdf

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|---|---|---|---|
| 26 papers | 1,421 citations | 489802 18 h-index | 651938 25 g-index |
| 27 all docs | 27 docs citations | 27 times ranked | 2823 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | The activities of drug inactive ingredients on biological targets. Science, 2020, 369, 403-413. | 6.0 | 61 |
| 2 | CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002. | 2.8 | 120 |
| 3 | Opportunities and challenges using artificial intelligence in ADME/Tox. Nature Materials, 2019, 18, 418-422. | 13.3 | 69 |
| 4 | 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. | 1.0 | 12 |
| 5 | Alternative approaches for identifying acute systemic toxicity: Moving from research to regulatory testing. Toxicology in Vitro, 2017, 41, 245-259. | 1.1 | 54 |
| 6 | 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. | 2.8 | 26 |
| 7 | 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. | 1.7 | 44 |
| 8 | Acute Toxicity Prediction in Multiple Species by Leveraging Mechanistic ToxCast Mitochondrial Inhibition Data and Simulation of Oral Bioavailability. Toxicological Sciences, 2015, 147, 386-396. | 1.4 | 17 |
| 9 | The QSPR-THESAURUS: The Online Platform of the CADASTER Project. ATLA Alternatives To Laboratory Animals, 2014, 42, 13-24. | 0.7 | 10 |
| 10 | Allosteric Inhibition of the IRE1Î± RNase Preserves Cell Viability and Function during Endoplasmic Reticulum Stress. Cell, 2014, 158, 534-548. | 13.5 | 384 |
| 11 | A sphingosine 1-phosphate receptor 2 selective allosteric agonist. Bioorganic and Medicinal Chemistry, 2013, 21, 5373-5382. | 1.4 | 53 |
| 12 | GPCR ontology: development and application of a G protein-coupled receptor pharmacology knowledge framework. Bioinformatics, 2013, 29, 3211-3219. | 1.8 | 24 |
| 13 | Novel Selective Allosteric and Bitopic Ligands for the S1P<sub>3</sub> Receptor. ACS Chemical Biology, 2012, 7, 1975-1983. | 1.6 | 55 |
| 14 | Divergent allosteric control of the IRE1Î± endoribonuclease using kinase inhibitors. Nature Chemical Biology, 2012, 8, 982-989. | 3.9 | 175 |
| 15 | Prediction of Aqueous Solubility, Vapor Pressure and Critical Micelle Concentration for Aquatic Partitioning of Perfluorinated Chemicals. Environmental Science & Technology, 2011, 45, 8120-8128. | 4.6 | 112 |
| 16 | Modelling physico-chemical properties of (benzo)triazoles, and screening for environmental partitioning. Water Research, 2011, 45, 1463-1471. | 5.3 | 31 |
| 17 | Oral LD50 toxicity modeling and prediction of per- and polyfluorinated chemicals on rat and mouse. Molecular Diversity, 2011, 15, 467-476. | 2.1 | 29 |
| 18 | CADASTER QSPR Models for Predictions of Melting and Boiling Points of Perfluorinated Chemicals. Molecular Informatics, 2011, 30, 189-204. | 1.4 | 32 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Are Mechanistic and Statistical QSAR Approaches Really Different? MLR Studies on 158 Cycloalkylâ€Pyranones. Molecular Informatics, 2010, 29, 511-522. | 1.4 | 11 |
| 20 | Per- and Polyfluoro Toxicity (LC<sub>50</sub> Inhalation) Study in Rat and Mouse Using QSAR Modeling. Chemical Research in Toxicology, 2010, 23, 528-539. | 1.7 | 35 |
| 21 | A QSAR Study of HIV Protease Inhibitors Using Theoretical Descriptors. Current Computer-Aided Drug Design, 2010, 6, 269-282. | 0.8 | 8 |
| 22 | 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. | 1.3 | 1 |
| 23 | 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. | 0.8 | 6 |
| 24 | 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. | 1.4 | 25 |
| 25 | A mechanistic study of 3-aminoindazole cyclic urea HIV-1 protease inhibitors using comparative QSAR. Bioorganic and Medicinal Chemistry, 2004, 12, 5819-5831. | 1.4 | 22 |
| 26 | QSAR and Molecular Modeling Studies of HIV Protease Inhibitors. , 0, , 181-271. | | 5 |