Ross McGuire

List of Publications by Year
in descending order

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25 papers	1,490 citations	430442 18 h-index	642321 23 g-index
25 all docs	25 docs citations	25 times ranked	2172 citing authors

#	Article	IF	Citations
1	3Dâ€eâ€Chem: Structural Cheminformatics Workflows for Computerâ€Aided Drug Discovery. ChemMedChem, 2018, 13, 614-626.	1.6	17
2	3D-e-Chem-VM: Structural Cheminformatics Research Infrastructure in a Freely Available Virtual Machine. Journal of Chemical Information and Modeling, 2017, 57, 115-121.	2.5	21
3	Data-driven medicinal chemistry in the era of big data. Drug Discovery Today, 2014, 19, 859-868.	3.2	126
4	Discovery of Glycine Sulfonamides as Dual Inhibitors of sn-1-Diacylglycerol Lipase Î± and Î±/Î²-Hydrolase Domain 6. Journal of Medicinal Chemistry, 2014, 57, 6610-6622.	2.9	28
5	Development of an Activityâ€Based Probe and In Silico Design Reveal Highly Selective Inhibitors for Diacylglycerol Lipaseâ€Î± in Brain. Angewandte Chemie - International Edition, 2013, 52, 12081-12085.	7.2	73
6	CURRENT PROGRESS IN STRUCTURE-BASED RATIONAL DRUG DESIGN MARKS A NEW MINDSET IN DRUG DISCOVERY. Computational and Structural Biotechnology Journal, 2013, 5, e201302011.	1.9	173
7	From the protein's perspective: the benefits and challenges of protein structure-based pharmacophore modeling. MedChemComm, 2012, 3, 28-38.	3.5	81
8	X-ray Structures of Progesterone Receptor Ligand Binding Domain in Its Agonist State Reveal Differing Mechanisms for Mixed Profiles of 11Î²-Substituted Steroids. Journal of Biological Chemistry, 2012, 287, 20333-20343.	1.6	31
9	A Prospective Cross-Screening Study on G-Protein-Coupled Receptors: Lessons Learned in Virtual Compound Library Design. Journal of Medicinal Chemistry, 2012, 55, 5311-5325.	2.9	28
10	Drug design for ever, from hype to hope. Journal of Computer-Aided Molecular Design, 2012, 26, 137-150.	1.3	34
11	Org 214007-0: A Novel Non-Steroidal Selective Glucocorticoid Receptor Modulator with Full Anti-Inflammatory Properties and Improved Therapeutic Index. PLoS ONE, 2012, 7, e48385.	1.1	26
12	Structural Basis for Agonism and Antagonism for a Set of Chemically Related Progesterone Receptor Modulators. Journal of Biological Chemistry, 2011, 286, 35079-35086.	1.6	33
13	A molecular informatics view on best practice in multi-parameter compound optimization. Drug Discovery Today, 2011, 16, 555-568.	3.2	19
14	X-Ray Structures of the LXRÎ± LBD in Its Homodimeric Form and Implications for Heterodimer Signaling. Journal of Molecular Biology, 2010, 399, 120-132.	2.0	44
15	Derivation and Validation of Toxicophores for Mutagenicity Prediction. Journal of Medicinal Chemistry, 2005, 48, 312-320.	2.9	501
16	Î±-Amino Acid Phenolic Ester Derivatives:Â Novel Water-Soluble General Anesthetic Agents Which Allosterically Modulate GABAAReceptors. Journal of Medicinal Chemistry, 2001, 44, 3582-3591.	2.9	26
17	The First Potent and Selective Inhibitors of the Glycine Transporter Type 2. Journal of Medicinal Chemistry, 2001, 44, 2679-2682.	2.9	89
18	Design and Synthesis of a Maximally Diverse and Druglike Screening Library Using REM Resin Methodology. ACS Combinatorial Science, 2001, 3, 534-541.	3.3	19

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19	Conformationally Constrained Anesthetic Steroids That Modulate GABAA Receptors. Journal of Medicinal Chemistry, 2000, 43, 4118-4125.	2.9	42
20	Expert System Assisted Pharmacophore Identification. Journal of Chemical Information and Computer Sciences, 2000, 40, 347-353.	2.8	8
21	Non-depolarizing Neuromuscular Blocking Activity of Bisquaternary Amino Di- and Tripeptide Derivatives. Journal of Medicinal Chemistry, 2000, 43, 4822-4833.	2.9	7
22	Conformations of Anaesthetic Steroids: a1H and13C NMR Study of (2Î²,3Î±,5Î±)-2-[(2R)-Ethyl-4-morpholinyl]-3-hydroxypregnane-11,20-dione and(2Î²,3Î±,5Î±)-2-[(2S)-Ethyl-4-morpholinyl]-3-hydroxypregnane-11,20-dione.. , 1997, 35, 184-190.		6
23	A Molecular Chameleon:Â Chair and Twist-Boat Conformations of a 5,9-Methanobenzo[8]annulene. Journal of Organic Chemistry, 1996, 61, 5978-5981.	1.7	6
24	Principal Components Describing Biological Activities and Molecular Diversity of Heterocyclic Aromatic Ring Fragments. Journal of Medicinal Chemistry, 1996, 39, 4065-4072.	2.9	48
25	Determination of Absolute Stereochemistry of 2-Alkylmorpholines by a13C NMR Study of Steroid Derivatives. , 1996, 34, 59-62.		4