Noel M O'boyle

List of Publications by Year
in descending order

26 papers	12,639 citations	361045 20 h-index	580395 25 g-index
27 all docs	27 docs citations	27 times ranked	16253 citing authors

#	Article	IF	Citations
1	Open Babel: An open chemical toolbox. Journal of Cheminformatics, 2011, 3, 33.	2.8	6,039
2	cclib: A library for packageâ€independent computational chemistry algorithms. Journal of Computational Chemistry, 2008, 29, 839-845.	1.5	4,766
3	Pybel: a Python wrapper for the OpenBabel cheminformatics toolkit. Chemistry Central Journal, 2008, 2, 5.	2.6	293
4	Random Forest Models To Predict Aqueous Solubility. Journal of Chemical Information and Modeling, 2007, 47, 150-158.	2.5	277
5	Confab - Systematic generation of diverse low-energy conformers. Journal of Cheminformatics, 2011, 3, 8.	2.8	211
6	Towards a Universal SMILES representation - A standard method to generate canonical SMILES based on the InChI. Journal of Cheminformatics, 2012, 4, 22.	2.8	179
7	Elucidating excited state electronic structure and intercomponent interactions in multicomponent and supramolecular systems. Chemical Society Reviews, 2005, 34, 641.	18.7	160
8	PYCHEM: a multivariate analysis package for python. Bioinformatics, 2006, 22, 2565-2566.	1.8	75
9	MACiE (Mechanism, Annotation and Classification in Enzymes): novel tools for searching catalytic mechanisms. Nucleic Acids Research, 2007, 35, D515-D520.	6.5	64
10	Open Data, Open Source and Open Standards in chemistry: The Blue Obelisk five years on. Journal of Cheminformatics, 2011, 3, 37.	2.8	63
11	Curcumin-induced degradation of PKCÎ´ is associated with enhanced dentate NCAM PSA expression and spatial learning in adult and aged Wistar rats. Biochemical Pharmacology, 2009, 77, 1254-1265.	2.0	62
12	Using Matched Molecular Series as a Predictive Tool To Optimize Biological Activity. Journal of Medicinal Chemistry, 2014, 57, 2704-2713.	2.9	50
13	MACiE: a database of enzyme reaction mechanisms. Bioinformatics, 2005, 21, 4315-4316.	1.8	47
14	Cinfony â€“ combining Open Source cheminformatics toolkits behind a common interface. Chemistry Central Journal, 2008, 2, 24.	2.6	43
15	Ground- and Excited-State Electronic Structure of an Emissive Pyrazine-Bridged Ruthenium(II) Dinuclear Complex. Journal of the American Chemical Society, 2005, 127, 1229-1241.	6.6	41
16	Using Reaction Mechanism to Measure Enzyme Similarity. Journal of Molecular Biology, 2007, 368, 1484-1499.	2.0	39
17	Testing Assumptions and Hypotheses for Rescoring Success in Proteinâ€'Ligand Docking. Journal of Chemical Information and Modeling, 2009, 49, 1871-1878.	2.5	31
18	Assessment of intercomponent interaction in phenylene bridged dinuclear ruthenium(ii) and osmium(ii) polypyridyl complexes. Dalton Transactions, 2004, , 3943.	1.6	28

#	Article	IF	Citations
19	Simultaneous feature selection and parameter optimisation using an artificial ant colony: case study of melting point prediction. Chemistry Central Journal, 2008, 2, 21.	2.6	26
20	Cheminformatics. Communications of the ACM, 2012, 55, 65-75.	3.3	21
21	Userscripts for the Life Sciences. BMC Bioinformatics, 2007, 8, 487.	1.2	14
22	A Density Functional Theory Study of the Electronic Properties of Os(II) and Os(III) Complexes Immobilized on Au(111). Inorganic Chemistry, 2007, 46, 117-124.	1.9	12
23	Using Buriedness To Improve Discrimination between Actives and Inactives in Docking. Journal of Chemical Information and Modeling, 2008, 48, 1269-1278.	2.5	10
24	Ground vs. excited state interaction in ruthenium-thienyl dyads: implications for through bond interactions in multicomponent systems. Journal of Molecular Structure, 2005, 735-736, 123-134.	1.8	7
25	Practical applications of matched series analysis: SAR transfer, binding mode suggestion and data point validation. Future Medicinal Chemistry, 2017, 9, 153-168.	1.1	4
26	Elucidating Excited State Electronic Structure and Intercomponent Interactions in Multicomponent and Supramolecular Systems. ChemInform, 2005, 36, no.	0.1	0