Colin R Groom

List of Publications by Year
in descending order

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32 papers	15,284 citations	331259 21 h-index	395343 33 g-index
37 all docs	37 docs citations	37 times ranked	18496 citing authors

#	Article	IF	Citations
1	The Cambridge Structural Database (CSD). , 2019, , .		2
2	The use of small-molecule structures to complement proteinâ€“ligand crystal structures in drug discovery. Acta Crystallographica Section D: Structural Biology, 2017, 73, 240-245.	1.1	25
3	Using more than 801â€…296 small-molecule crystal structures to aid in protein structure refinement and analysis. Acta Crystallographica Section D: Structural Biology, 2017, 73, 234-239.	1.1	6
4	Hydrogen bonding at C=Se acceptors in selenoureas, selenoamides and selones. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 317-325.	0.5	23
5	The Cambridge Structural Database. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 171-179.	0.5	7,159
6	Report on the sixth blind test of organic crystal structure prediction methods. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 439-459.	0.5	445
7	Capturing neon â€“ the first experimental structure of neon trapped within a metalâ€“organic environment. Chemical Communications, 2016, 52, 10048-10051.	2.2	13
8	Generation of crystal structures using known crystal structures as analogues. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 530-541.	0.5	18
9	Knowledge-Based Optimization of Molecular Geometries Using Crystal Structures. Journal of Chemical Information and Modeling, 2016, 56, 652-661.	2.5	12
10	Data to knowledge: how to get meaning from your result. IUCrJ, 2015, 2, 45-58.	1.0	12
11	Small Molecule Crystal Structures in Drug Discovery. NATO Science for Peace and Security Series A: Chemistry and Biology, 2015, , 107-114.	0.5	2
12	The Cambridge Structural Database in Retrospect and Prospect. Angewandte Chemie - International Edition, 2014, 53, 662-671.	7.2	1,004
13	A crystallographic perspective on sharing data and knowledge. Journal of Computer-Aided Molecular Design, 2014, 28, 1015-1022.	1.3	27
14	Evaluation of molecular crystal structures using Full Interaction Maps. CrystEngComm, 2013, 15, 65-72.	1.3	109
15	Up the Garden Path: A Chemical Trail through the Cambridge University Botanic Garden. Journal of Chemical Education, 2012, 89, 1390-1394.	1.1	9
16	The Hydrogen Bond Environments of 1H-Tetrazole and Tetrazolate Rings: The Structural Basis for Tetrazoleâ€“Carboxylic Acid Bioisosterism. Journal of Chemical Information and Modeling, 2012, 52, 857-866.	2.5	65
17	One in half a million: a solid form informatics study of a pharmaceutical crystal structure. CrystEngComm, 2012, 14, 2391-2403.	1.3	42
18	The good, the bad and the twisted: a survey of ligand geometry in protein crystal structures. Journal of Computer-Aided Molecular Design, 2012, 26, 169-183.	1.3	92

#	Article	IF	Citations
19	Identification, classification and relative stability of tautomers in the cambridge structural database. CrystEngComm, 2011, 13, 93-98.	1.3	58
20	Data-Driven High-Throughput Prediction of the 3-D Structure of Small Molecules: Review and Progress. A Response from The Cambridge Crystallographic Data Centre. Journal of Chemical Information and Modeling, 2011, 51, 2787-2787.	2.5	8
21	The Cambridge Structural Database: experimental threeâ€dimensional information on small molecules is a vital resource for interdisciplinary research and learning. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 368-376.	6.2	22
22	Institutional Profile: Crystal structure information in drug discovery and development: current perspectives and new possibilities from the Cambridge Crystallographic Data Centre. Future Medicinal Chemistry, 2010, 2, 933-939.	1.1	5
23	Atomic Interactions and Profile of Small Molecules Disrupting Proteinâ€“Protein Interfaces: the TIMBAL Database. Chemical Biology and Drug Design, 2009, 74, 457-467.	1.5	144
24	Heteroaromatic Rings of the Future. Journal of Medicinal Chemistry, 2009, 52, 2952-2963.	2.9	286
25	IRAK-4 inhibitors. Part II: A structure-based assessment of imidazo[1,2-a]pyridine binding. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 3291-3295.	1.0	47
26	Ligand efficiency: a useful metric for lead selection. Drug Discovery Today, 2004, 9, 430-431.	3.2	1,687
27	Protein kinase drugs â€“ optimism doesn't wait on facts â–¾. Drug Discovery Today, 2002, 7, 801-802.	3.2	15
28	The druggable genome. Nature Reviews Drug Discovery, 2002, 1, 727-730.	21.5	2,918
29	Experimental and computational mapping of the binding surface of a crystalline protein. Protein Engineering, Design and Selection, 2001, 14, 47-59.	1.0	104
30	Locating interaction sites on proteins: The crystal structure of thermolysin soaked in 2% to 100% isopropanol. , 1999, 37, 628-640.		99
31	Three-dimensional structure of diferric bovine lactoferrin at 2.8 Ã... resolution. Journal of Molecular Biology, 1997, 274, 222-236.	2.0	361
32	Pheromone binding to two rodent urinary proteins revealed by X-ray crystallography. Nature, 1992, 360, 186-188.	13.7	374