Colin R Groom

List of Publications by Year in Descending Order

32 papers	12,127 citations	19 h-index	37 g-index
37 ext. papers	13,716 ext. citations	7.9 avg, IF	6.95 L-index

#	Paper	IF	Citations
32	The Cambridge Structural Database (CSD) **2019**,		2
31	The use of small-molecule structures to complement protein-ligand crystal structures in drug discovery. *Acta Crystallographica Section D: Structural Biology*, **2017**, 73, 240-245	5.5	18
30	Using more than 801 296 small-molecule crystal structures to aid in protein structure refinement and analysis. *Acta Crystallographica Section D: Structural Biology*, **2017**, 73, 234-239	5.5	4
29	Report on the sixth blind test of organic crystal structure prediction methods. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2016**, 72, 439-59	1.8	338
28	Capturing neon - the first experimental structure of neon trapped within a metal-organic environment. *Chemical Communications*, **2016**, 52, 10048-51	5.8	8
27	Generation of crystal structures using known crystal structures as analogues. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2016**, 72, 530-41	1.8	14
26	Knowledge-Based Optimization of Molecular Geometries Using Crystal Structures. *Journal of Chemical Information and Modeling*, **2016**, 56, 652-61	6.1	11
25	Hydrogen bonding at C=Se acceptors in selenoureas, selenoamides and selones. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2016**, 72, 317-25	1.8	16
24	The Cambridge Structural Database. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, **2016**, 72, 171-9	1.8	5178
23	Data to knowledge: how to get meaning from your result. *IUCrJ*, **2015**, 2, 45-58	4.7	10
22	Small Molecule Crystal Structures in Drug Discovery. *NATO Science for Peace and Security Series A: Chemistry and Biology*, **2015**, 107-114	0.1	2
21	The Cambridge Structural Database in retrospect and prospect. *Angewandte Chemie - International Edition*, **2014**, 53, 662-71	16.4	912
20	A crystallographic perspective on sharing data and knowledge. *Journal of Computer-Aided Molecular Design*, **2014**, 28, 1015-22	4.2	24
19	Die Cambridge Structural Database: R□kblick und Vorausschau. *Angewandte Chemie*, **2014**, 126, 675-684	3.6	19
18	Evaluation of molecular crystal structures using Full Interaction Maps. *CrystEngComm*, **2013**, 15, 65-72	3.3	76
17	The good, the bad and the twisted: a survey of ligand geometry in protein crystal structures. *Journal of Computer-Aided Molecular Design*, **2012**, 26, 169-83	4.2	78
16	Up the Garden Path: A Chemical Trail through the Cambridge University Botanic Garden. *Journal of Chemical Education*, **2012**, 89, 1390-1394	2.4	7

15	Mining the Cambridge Structural Database for Bioisosteres **2012**, 75-101		5
14	The hydrogen bond environments of 1H-tetrazole and tetrazolate rings: the structural basis for tetrazole-carboxylic acid bioisosterism. *Journal of Chemical Information and Modeling*, **2012**, 52, 857-66	6.1	54
13	One in half a million: a solid form informatics study of a pharmaceutical crystal structure. *CrystEngComm*, **2012**, 14, 2391-2403	3.3	39
12	The Cambridge Structural Database: experimental three-dimensional information on small molecules is a vital resource for interdisciplinary research and learning. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2011**, 1, 368-376	7.9	19
11	Identification, classification and relative stability of tautomers in the cambridge structural database. *CrystEngComm*, **2011**, 13, 93-98	3.3	50
10	Atomic interactions and profile of small molecules disrupting protein-protein interfaces: the TIMBAL database. *Chemical Biology and Drug Design*, **2009**, 74, 457-67	2.9	132
9	Heteroaromatic rings of the future. *Journal of Medicinal Chemistry*, **2009**, 52, 2952-63	8.3	240
8	IRAK-4 inhibitors. Part II: a structure-based assessment of imidazo[1,2-a]pyridine binding. *Bioorganic and Medicinal Chemistry Letters*, **2008**, 18, 3291-5	2.9	41
7	Ligand efficiency: a useful metric for lead selection. *Drug Discovery Today*, **2004**, 9, 430-1	8.8	1500
6	Protein kinase drugs--optimism doesn₩ wait on facts. *Drug Discovery Today*, **2002**, 7, 801-2	8.8	14
5	The druggable genome. *Nature Reviews Drug Discovery*, **2002**, 1, 727-30	64.1	2427
4	Experimental and computational mapping of the binding surface of a crystalline protein. *Protein Engineering, Design and Selection*, **2001**, 14, 47-59	1.9	88
3	Locating interaction sites on proteins: The crystal structure of thermolysin soaked in 2% to 100% isopropanol **1999**, 37, 628-640		79
2	Three-dimensional structure of diferric bovine lactoferrin at 2.8 A resolution. *Journal of Molecular Biology*, **1997**, 274, 222-36	6.5	312
1	Pheromone binding to two rodent urinary proteins revealed by X-ray crystallography. *Nature*, **1992**, 360, 186-8	50.4	350