Robin Taylor

List of Publications by Year
in descending order

40 papers	25,247 citations	218677 26 h-index	302126 39 g-index
40 all docs	40 docs citations	40 times ranked	20518 citing authors

#	Article	IF	Citations
1	Mercury CSD 2.0â€“ new features for the visualization and investigation of crystal structures. Journal of Applied Crystallography, 2008, 41, 466-470.	4.5	7,887
2	Tables of bond lengths determined by X-ray and neutron diffraction. Part 1. Bond lengths in organic compounds. Journal of the Chemical Society Perkin Transactions II, 1987, , S1.	0.9	6,937
3	New software for searching the Cambridge Structural Database and visualizing crystal structures. Acta Crystallographica Section B: Structural Science, 2002, 58, 389-397.	1.8	2,791
4	Intermolecular Nonbonded Contact Distances in Organic Crystal Structures: Comparison with Distances Expected from van der Waals Radii. The Journal of Physical Chemistry, 1996, 100, 7384-7391.	2.9	1,372
5	Supplement. Tables of bond lengths determined by X-ray and neutron diffraction. Part 2. Organometallic compounds and co-ordination complexes of the d- and f-block metals. Journal of the Chemical Society Dalton Transactions, 1989, , S1.	1.1	1,165
6	Organic Fluorine Hardly Ever Accepts Hydrogen Bonds. Chemistry - A European Journal, 1997, 3, 89-98.	3.3	907
7	Retrieval of Crystallographically-Derived Molecular Geometry Information. Journal of Chemical Information and Computer Sciences, 2004, 44, 2133-2144.	2.8	842
8	The Nature and Geometry of Intermolecular Interactions between Halogens and Oxygen or Nitrogen. Journal of the American Chemical Society, 1996, 118, 3108-3116.	13.7	790
9	The packing density in proteins: standard radii and volumes 1 1Edited by J. M. Thornton. Journal of Molecular Biology, 1999, 290, 253-266.	4.2	482
10	Three-Dimensional Pharmacophore Methods in Drug Discovery. Journal of Medicinal Chemistry, 2010, 53, 539-558.	6.4	326
11	IsoStar: a library of information about nonbonded interactions. Journal of Computer-Aided Molecular Design, 1997, 11, 525-537.	2.9	289
12	SuperStar: A Knowledge-based Approach for Identifying Interaction Sites in Proteins. Journal of Molecular Biology, 1999, 289, 1093-1108.	4.2	207
13	Hydrogen bonding of carbonyl, ether, and ester oxygen atoms with alkanol hydroxyl groups. Journal of Computational Chemistry, 1997, 18, 757-774.	3.3	195
14	A Million Crystal Structures: The Whole Is Greater than the Sum of Its Parts. Chemical Reviews, 2019, 119, 9427-9477.	47.7	191
15	Simulation Analysis of Experimental Design Strategies for Screening Random Compounds as Potential New Drugs and Agrochemicals. Journal of Chemical Information and Computer Sciences, 1995, 35, 59-67.	2.8	130
16	It Isnâ€™t, It Is: The Câ€“HÂ·Â·Â·X (X = O, N, F, Cl) Interaction Really Is Significant in Crystal Packing. Crystal Growth and Design, 2016, 16, 4165-4168.	3.0	87
17	Life-science applications of the Cambridge Structural Database. Acta Crystallographica Section D: Biological Crystallography, 2002, 58, 879-888.	2.5	65
18	Which intermolecular interactions have a significant influence on crystal packing?. CrystEngComm, 2014, 16, 6852-6865.	2.6	63

#	Article	IF	Citations
19	The hydrogen bond between Nâ€”H or Oâ€”H and organic fluorine: favourable yes, competitive no. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2017, 73, 474-488.	1.1	49
20	Generation of multiple pharmacophore hypotheses using multiobjective optimisation techniques. Journal of Computer-Aided Molecular Design, 2004, 18, 665-682.	2.9	47
21	Knowledge-Based Conformer Generation Using the Cambridge Structural Database. Journal of Chemical Information and Modeling, 2018, 58, 615-629.	5.4	47
22	Molecular Interactions in Crystal Structures with Zâ€² > 1. Crystal Growth and Design, 2016, 16, 2988-3001.	3.0	43
23	How Significant Are Unusual Proteinâ€“Ligand Interactions? Insights from Database Mining. Journal of Medicinal Chemistry, 2019, 62, 10441-10455.	6.4	42
24	Validating and Understanding Ring Conformations Using Small Molecule Crystallographic Data. Journal of Chemical Information and Modeling, 2012, 52, 956-962.	5.4	40
25	Knowledge-Based Libraries for Predicting the Geometric Preferences of Druglike Molecules. Journal of Chemical Information and Modeling, 2014, 54, 2500-2514.	5.4	34
26	The Cambridge Structural Database in molecular graphics: techniques for the rapid identification of conformational minima. Journal of Molecular Graphics, 1986, 4, 123-131.	1.1	27
27	Incorporating partial matches within multiobjective pharmacophore identification. Journal of Computer-Aided Molecular Design, 2007, 20, 735-749.	2.9	24
28	Deducing chemical structure from crystallographically determined atomic coordinates. Acta Crystallographica Section B: Structural Science, 2011, 67, 333-349.	1.8	23
29	Multiobjective Optimization of Pharmacophore Hypotheses: Bias Toward Low-Energy Conformations. Journal of Chemical Information and Modeling, 2009, 49, 2761-2773.	5.4	20
30	Combined use of physicochemical data and small-molecule crystallographic contact propensities to predict interactions in protein binding sites. Organic and Biomolecular Chemistry, 2004, 2, 3238.	2.8	17
31	Intermolecular Interactions of Organic Fluorine Seen in Perspective. Crystal Growth and Design, 2022, 22, 1352-1364.	3.0	17
32	Identifying intermolecular atomâ‹¯atom interactions that are not just bonding but also competitive. CrystEngComm, 2020, 22, 7145-7151.	2.6	16
33	Short Nonbonded Contact Distances in Organic Molecules and Their Use as Atom-Clash Criteria in Conformer Validation and Searching. Journal of Chemical Information and Modeling, 2011, 51, 897-908.	5.4	15
34	Development and validation of an improved algorithm for overlaying flexible molecules. Journal of Computer-Aided Molecular Design, 2012, 26, 451-472.	2.9	15
35	Quantifying the symmetry preferences of intermolecular interactions in organic crystal structures. CrystEngComm, 2015, 17, 2651-2666.	2.6	14
36	Identification of Noncompetitive Proteinâ€“Ligand Interactions for Structural Optimization. Journal of Chemical Information and Modeling, 2020, 60, 6595-6611.	5.4	10

#	Article	IF	Citations
37	Directional Preferences of Intermolecular Contacts to Hydrophobic Groups. Acta Crystallographica Section D: Biological Crystallography, 1998, 54, 1183-1193.	2.5	9
38	Prior Likelihoods and Space-Group Preferences of Solvates. Crystal Growth and Design, 2021, 21, 1178-1189.	3.0	6
39	Progress in the Understanding of Traditional and Nontraditional Molecular Interactions. , 2017, , 67-100.		4
40	The need for a new generation of substructure searching software. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2021, 77, 676-682.	1.1	2