Jason C Cole

List of Publications by Year
in descending order

62 papers	10,260 citations	201674 27 h-index	110387 64 g-index
66 all docs	66 docs citations	66 times ranked	11876 citing authors

#	Article	IF	Citations
1	Intermolecular Interactions of Organic Fluorine Seen in Perspective. Crystal Growth and Design, 2022, 22, 1352-1364.	3.0	17
2	Fragment Hotspot Mapping to Identify Selectivity-Determining Regions between Related Proteins. Journal of Chemical Information and Modeling, 2022, 62, 284-294.	5.4	9
3	First global analysis of the GSK database of small molecule crystal structures. CrystEngComm, 2021, 23, 5430-5442.	2.6	4
4	Augmenting Structureâ€Based Design with Experimental Proteinâ€Ligand Interaction Data: Molecular Recognition, Interactive Visualization, and Rescoring. ChemMedChem, 2021, 16, 3428-3438.	3.2	4
5	Use of molecular docking computational tools in drug discovery. Progress in Medicinal Chemistry, 2021, 60, 273-343.	10.4	154
6	Prior Likelihoods and Space-Group Preferences of Solvates. Crystal Growth and Design, 2021, 21, 1178-1189.	3.0	6
7	Conformational Change in Molecular Crystals: Impact of Solvate Formation and Importance of Conformational Free Energies. Crystal Growth and Design, 2021, 21, 6924-6936.	3.0	9
8	Validation of a Field-Based Ligand Screener Using a Novel Benchmarking Data Set for Assessing 3D-Based Virtual Screening Methods. Journal of Chemical Information and Modeling, 2021, 61, 5841-5852.	5.4	1
9	Identification of Noncompetitive Proteinâ€“Ligand Interactions for Structural Optimization. Journal of Chemical Information and Modeling, 2020, 60, 6595-6611.	5.4	10
10	The impact of the Cambridge Structural Database and the small molecule crystal structures it contains: a bibliographic and literature study. CrystEngComm, 2020, 22, 7233-7241.	2.6	6
11	Hotspots API: A Python Package for the Detection of Small Molecule Binding Hotspots and Application to Structure-Based Drug Design. Journal of Chemical Information and Modeling, 2020, 60, 1911-1916.	5.4	15
12	Resolving alternative organic crystal structures using density functional theory and NMR chemical shifts. Chemical Science, 2020, 11, 2987-2992.	7.4	18
13	How Significant Are Unusual Proteinâ€“Ligand Interactions? Insights from Database Mining. Journal of Medicinal Chemistry, 2019, 62, 10441-10455.	6.4	42
14	New insights and innovation from a million crystal structures in the Cambridge Structural Database. Structural Dynamics, 2019, 6, 054301.	2.3	16
15	Knowledge-Based Conformer Generation Using the Cambridge Structural Database. Journal of Chemical Information and Modeling, 2018, 58, 615-629.	5.4	47
16	Mining the Cambridge Structural Database for Matched Molecular Crystal Structures: A Systematic Exploration of Isostructurality. Crystal Growth and Design, 2017, 17, 3192-3203.	3.0	15
17	Improved crystal structure solution from powder diffraction data by the use of conformational information. Journal of Applied Crystallography, 2017, 50, 1421-1427.	4.5	14
18	Improved performance of crystal structure solution from powder diffraction data through parameter tuning of a simulated annealing algorithm. Journal of Applied Crystallography, 2017, 50, 1411-1420.	4.5	20

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19	New active leads for tuberculosis booster drugs by structure-based drug discovery. Organic and Biomolecular Chemistry, 2017, 15, 10245-10255.	2.8	22
20	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.	2.3	25
21	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.	2.3	6
22	Molecular Interactions in Crystal Structures with Zâ€² > 1. Crystal Growth and Design, 2016, 16, 2988-3001.	3.0	43
23	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.	1.1	445
24	Generation of crystal structures using known crystal structures as analogues. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2016, 72, 530-541.	1.1	18
25	Knowledge-Based Optimization of Molecular Geometries Using Crystal Structures. Journal of Chemical Information and Modeling, 2016, 56, 652-661.	5.4	12
26	Interactive and Versatile Navigation of Structural Databases. Journal of Medicinal Chemistry, 2016, 59, 4257-4266.	6.4	26
27	Quantifying the symmetry preferences of intermolecular interactions in organic crystal structures. CrystEngComm, 2015, 17, 2651-2666.	2.6	14
28	Assessment of a Cambridge Structural Database-Driven Overlay Program. Journal of Chemical Information and Modeling, 2014, 54, 3091-3098.	5.4	11
29	Utilizing organic and organometallic structural data in powder diffraction. Powder Diffraction, 2014, 29, S19-S30.	0.2	7
30	Kernel Density Estimation Applied to Bond Length, Bond Angle, and Torsion Angle Distributions. Journal of Chemical Information and Modeling, 2014, 54, 1284-1288.	5.4	12
31	Knowledge-Based Libraries for Predicting the Geometric Preferences of Druglike Molecules. Journal of Chemical Information and Modeling, 2014, 54, 2500-2514.	5.4	34
32	Evaluation of molecular crystal structures using Full Interaction Maps. CrystEngComm, 2013, 15, 65-72.	2.6	109
33	Validating and Understanding Ring Conformations Using Small Molecule Crystallographic Data. Journal of Chemical Information and Modeling, 2012, 52, 956-962.	5.4	40
34	Potential and Limitations of Ensemble Docking. Journal of Chemical Information and Modeling, 2012, 52, 1262-1274.	5.4	149
35	Pose prediction and virtual screening performance of GOLD scoring functions in a standardized test. Journal of Computer-Aided Molecular Design, 2012, 26, 737-748.	2.9	138
36	Development and validation of an improved algorithm for overlaying flexible molecules. Journal of Computer-Aided Molecular Design, 2012, 26, 451-472.	2.9	15

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37	The Ensemble Performance Index: An Improved Measure for Assessing Ensemble Pose Prediction Performance. Journal of Chemical Information and Modeling, 2011, 51, 2915-2919.	5.4	6
38	An automated method for consistent helix assignment using turn information. Proteins: Structure, Function and Bioinformatics, 2011, 79, 1416-1426.	2.6	7
39	WebCSD: the online portal to the Cambridge Structural Database. Journal of Applied Crystallography, 2010, 43, 362-366.	4.5	125
40	GDASH: a grid-enabled program for structure solution from powder diffraction data. Journal of Applied Crystallography, 2009, 42, 356-359.	4.5	9
41	MDASH: a multi-core-enabled program for structure solution from powder diffraction data. Journal of Applied Crystallography, 2009, 42, 360-361.	4.5	12
42	Secbase: Database Module To Retrieve Secondary Structure Elements with Ligand Binding Motifs. Journal of Chemical Information and Modeling, 2009, 49, 2388-2402.	5.4	14
43	Testing Assumptions and Hypotheses for Rescoring Success in Proteinâ˜Ligand Docking. Journal of Chemical Information and Modeling, 2009, 49, 1871-1878.	5.4	31
44	DASH: a program for crystal structure determination from powder diffraction data. Journal of Applied Crystallography, 2006, 39, 910-915.	4.5	495
45	Proteinâ€šÃ„Ã¬Ligand Docking Virtual Screening with GOLD. Drug Discovery Series, 2005, , 379-415.	0.1	52
46	Comparing protein-ligand docking programs is difficult. Proteins: Structure, Function and Bioinformatics, 2005, 60, 325-332.	2.6	275
47	Modeling Water Molecules in Proteinâ˜Ligand Docking Using GOLD. Journal of Medicinal Chemistry, 2005, 48, 6504-6515.	6.4	354
48	Retrieval of Crystallographically-Derived Molecular Geometry Information. Journal of Chemical Information and Computer Sciences, 2004, 44, 2133-2144.	2.8	842
49	A database survey of molecular and crystallographic symmetry. Acta Crystallographica Section B: Structural Science, 2003, 59, 634-640.	1.8	65
50	Improved protein-ligand docking using GOLD. Proteins: Structure, Function and Bioinformatics, 2003, 52, 609-623.	2.6	2,417
51	Structure solution and refinement of tetracaine hydrochloride from X-ray powder diffraction data. New Journal of Chemistry, 2002, 26, 469-472.	2.8	47
52	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
53	CSDSymmetry: the definitive database of point-group and space-group symmetry relationships in small-molecule crystal structures. Acta Crystallographica Section B: Structural Science, 2002, 58, 640-646.	1.8	41
54	The use of restraints in Rietveld refinement of molecular compounds; a case study using the crystal structure determination of tryptamine free base. Acta Crystallographica Section B: Structural Science, 2002, 58, 835-840.	1.8	16

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55	A new test set for validating predictions of protein-ligand interaction. Proteins: Structure, Function and Bioinformatics, 2002, 49, 457-471.	2.6	416
56	Superstar: improved knowledge-based interaction fields for protein binding sites11Edited by R. Huber. Journal of Molecular Biology, 2001, 307, 841-859.	4.2	101
57	Superstar: comparison of CSD and PDB-based interaction fields as a basis for the prediction of protein-ligand interactions 1 1Edited by R. Huber. Journal of Molecular Biology, 2001, 312, 275-287.	4.2	40
58	Automatic detection of molecular symmetry in the Cambridge Structural Database. Acta Crystallographica Section B: Structural Science, 2001, 57, 88-94.	1.8	15
59	SuperStar: A Knowledge-based Approach for Identifying Interaction Sites in Proteins. Journal of Molecular Biology, 1999, 289, 1093-1108.	4.2	207
60	The Development and Application of Knowledge-Based Approaches to Molecular Design. , 1999, , 243-260.		0
61	Directional Preferences of Intermolecular Contacts to Hydrophobic Groups. Acta Crystallographica Section D: Biological Crystallography, 1998, 54, 1183-1193.	2.5	9
62	IsoStar: a library of information about nonbonded interactions. Journal of Computer-Aided Molecular Design, 1997, 11, 525-537.	2.9	289