David R Hall

List of Publications by Year
in descending order

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31 papers	5,640 citations	218677 26 h-index	434195 31 g-index
32 all docs	32 docs citations	32 times ranked	8265 citing authors

#	Article	IF	Citations
1	Interaction Energetics and Druggability of the Proteinâ€“Protein Interaction between Kelch-like ECH-Associated Protein 1 (KEAP1) and Nuclear Factor Erythroid 2 Like 2 (Nrf2). Biochemistry, 2020, 59, 563-581.	2.5	28
2	Kinase Atlas: Druggability Analysis of Potential Allosteric Sites in Kinases. Journal of Medicinal Chemistry, 2019, 62, 6512-6524.	6.4	52
3	Exploring the structural origins of cryptic sites on proteins. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E3416-E3425.	7.1	96
4	Proteinâ€“ligand docking using FFT based sampling: D3R case study. Journal of Computer-Aided Molecular Design, 2018, 32, 225-230.	2.9	9
5	The ClusPro web server for proteinâ€“protein docking. Nature Protocols, 2017, 12, 255-278.	12.0	1,959
6	New additions to the <scp>C</scp>lus<scp>P</scp>ro server motivated by <scp>CAPRI</scp>. Proteins: Structure, Function and Bioinformatics, 2017, 85, 435-444.	2.6	395
7	ClusPro-DC: Dimer Classification by the Cluspro Server for Proteinâ€“Protein Docking. Journal of Molecular Biology, 2017, 429, 372-381.	4.2	36
8	Prediction of homoprotein and heteroprotein complexes by protein docking and templateâ€based modeling: A CASPâ€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2016, 84, 323-348.	2.6	148
9	New Frontiers in Druggability. Journal of Medicinal Chemistry, 2015, 58, 9063-9088.	6.4	93
10	Ligand deconstruction: Why some fragment binding positions are conserved and others are not. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E2585-94.	7.1	61
11	The FTMap family of web servers for determining and characterizing ligand-binding hot spots of proteins. Nature Protocols, 2015, 10, 733-755.	12.0	496
12	Lessons from Hot Spot Analysis for Fragment-Based Drug Discovery. Trends in Pharmacological Sciences, 2015, 36, 724-736.	8.7	58
13	Computational solvent mapping in structure-based drug design. Future Medicinal Chemistry, 2015, 7, 337-353.	2.3	14
14	Stimulators of translation identified during a small molecule screening campaign. Analytical Biochemistry, 2014, 447, 6-14.	2.4	4
15	Encounter complexes and dimensionality reduction in proteinâ€“protein association. ELife, 2014, 3, e01370.	6.0	61
16	How good is automated protein docking?. Proteins: Structure, Function and Bioinformatics, 2013, 81, 2159-2166.	2.6	570
17	Sampling and scoring: A marriage made in heaven. Proteins: Structure, Function and Bioinformatics, 2013, 81, 1874-1884.	2.6	58
18	FTFlex: accounting for binding site flexibility to improve fragment-based identification of druggable hot spots. Bioinformatics, 2013, 29, 1218-1219.	4.1	30

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19	Community-wide evaluation of methods for predicting the effect of mutations on protein-protein interactions. Proteins: Structure, Function and Bioinformatics, 2013, 81, 1980-1987.	2.6	87
20	Application of asymmetric statistical potentials to antibodyâ€“protein docking. Bioinformatics, 2012, 28, 2608-2614.	4.1	156
21	Computational mapping reveals dramatic effect of Hoogsteen breathing on duplex DNA reactivity with formaldehyde. Nucleic Acids Research, 2012, 40, 7644-7652.	14.5	37
22	FTMAP: extended protein mapping with user-selected probe molecules. Nucleic Acids Research, 2012, 40, W271-W275.	14.5	130
23	Analysis of Protein Binding Sites by Computational Solvent Mapping. Methods in Molecular Biology, 2012, 819, 13-27.	0.9	19
24	Hot Spot Analysis for Driving the Development of Hits into Leads in Fragment-Based Drug Discovery. Journal of Chemical Information and Modeling, 2012, 52, 199-209.	5.4	52
25	Minimal ensembles of side chain conformers for modeling proteinâ€“protein interactions. Proteins: Structure, Function and Bioinformatics, 2012, 80, 591-601.	2.6	26
26	Relationship between Hot Spot Residues and Ligand Binding Hot Spots in Proteinâ€“Protein Interfaces. Journal of Chemical Information and Modeling, 2012, 52, 2236-2244.	5.4	99
27	FTSite: high accuracy detection of ligand binding sites on unbound protein structures. Bioinformatics, 2012, 28, 286-287.	4.1	189
28	Blocking eIF4E-eIF4G Interaction as a Strategy To Impair Coronavirus Replication. Journal of Virology, 2011, 85, 6381-6389.	3.4	93
29	Reversing chemoresistance by small molecule inhibition of the translation initiation complex eIF4F. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 1046-1051.	7.1	153
30	Structural conservation of druggable hot spots in proteinâ€“protein interfaces. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 13528-13533.	7.1	220
31	Achieving reliability and high accuracy in automated protein docking: Cluspro, PIPER, SDU, and stability analysis in CAPRI rounds 13â€“19. Proteins: Structure, Function and Bioinformatics, 2010, 78, 3124-3130.	2.6	211