David W Ritchie

List of Publications by Year
in descending order

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Version: 2024-02-01

60	4,097	159585	133252
papers	citations	30 h-index	59 g-index

64	64	64	5153
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	HexServer: an FFT-based protein docking server powered by graphics processors. Nucleic Acids Research, 2010, 38, W445-W449.	14.5	529
2	Protein docking using spherical polar Fourier correlations. Proteins: Structure, Function and Bioinformatics, 2000, 39, 178-194.	2.6	494
3	Ultra-fast FFT protein docking on graphics processors. Bioinformatics, 2010, 26, 2398-2405.	4.1	330
4	Recent Progress and Future Directions in Protein-Protein Docking. Current Protein and Peptide Science, 2008, 9, 1-15.	1.4	283
5	Docking essential dynamics eigenstructures. Proteins: Structure, Function and Bioinformatics, 2005, 60, 269-274.	2.6	221
6	Evaluation of protein docking predictions usingHex 3.1 in CAPRI rounds 1 and 2. Proteins: Structure, Function and Bioinformatics, 2003, 52, 98-106.	2.6	179
7	Accelerating and focusing proteinâ€“protein docking correlations using multi-dimensional rotational FFT generating functions. Bioinformatics, 2008, 24, 1865-1873.	4.1	175
8	Fast computation, rotation, and comparison of low resolution spherical harmonic molecular surfaces. Journal of Computational Chemistry, 1999, 20, 383-395.	3.3	161
9	Terminating eukaryote translation: Domain 1 of release factor eRF1 functions in stop codon recognition. Rna, 2000, 6, 1236-1247.	3.5	156
10	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
11	Comprehensive Comparison of Ligand-Based Virtual Screening Tools Against the DUD Data set Reveals Limitations of Current 3D Methods. Journal of Chemical Information and Modeling, 2010, 50, 2079-2093.	5.4	121
12	Blind prediction of homoâ€•and heteroâ€protein complexes: The CASP13â€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1200-1221.	2.6	99
13	Protein docking using caseâ€based reasoning. Proteins: Structure, Function and Bioinformatics, 2013, 81, 2150-2158.	2.6	98
14	PDB-wide identification of biological assemblies from conserved quaternary structure geometry. Nature Methods, 2018, 15, 67-72.	19.0	69
15	Comparison of Ligand-Based and Receptor-Based Virtual Screening of HIV Entry Inhibitors for the CXCR4 and CCR5 Receptors Using 3D Ligand Shape Matching and Ligandâ^'Receptor Docking. Journal of Chemical Information and Modeling, 2008, 48, 509-533.	5.4	67
16	Toward High Throughput 3D Virtual Screening Using Spherical Harmonic Surface Representations. Journal of Chemical Information and Modeling, 2007, 47, 1787-1796.	5.4	55
17	Flexible protein docking refinement using poseâ€dependent normal mode analysis. Proteins: Structure, Function and Bioinformatics, 2012, 80, 2262-2274.	2.6	52
18	Blind prediction of interfacial water positions in CAPRI. Proteins: Structure, Function and Bioinformatics, 2014, 82, 620-632.	2.6	50

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19	Unraveling the molecular architecture of a G protein-coupled receptor/Î²-arrestin/Erk module complex. Scientific Reports, 2015, 5, 10760.	3.3	50
20	Proteinâ€“protein docking by fast generalized Fourier transforms on 5D rotational manifolds. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E4286-93.	7.1	43
21	Spherical polar Fourier assembly of protein complexes with arbitrary point group symmetry. Journal of Applied Crystallography, 2016, 49, 158-167.	4.5	42
22	High-order analytic translation matrix elements for real-space six-dimensional polar Fourier correlations. Journal of Applied Crystallography, 2005, 38, 808-818.	4.5	39
23	Discovery of Novel HIV Entry Inhibitors for the CXCR4 Receptor by Prospective Virtual Screening. Journal of Chemical Information and Modeling, 2009, 49, 810-823.	5.4	39
24	Using Consensus-Shape Clustering To Identify Promiscuous Ligands and Protein Targets and To Choose the Right Query for Shape-Based Virtual Screening. Journal of Chemical Information and Modeling, 2011, 51, 1233-1248.	5.4	39
25	Fast protein structure alignment using Gaussian overlap scoring of backbone peptide fragment similarity. Bioinformatics, 2012, 28, 3274-3281.	4.1	38
26	Modeling the Structural Basis of Human CCR5 Chemokine Receptor Function:Â From Homology Model Building and Molecular Dynamics Validation to Agonist and Antagonist Docking. Journal of Chemical Information and Modeling, 2006, 46, 1223-1235.	5.4	36
27	Spatial clustering of protein binding sites for template based protein docking. Bioinformatics, 2011, 27, 2820-2827.	4.1	36
28	Clustering and Classifying Diverse HIV Entry Inhibitors Using a Novel Consensus Shape-Based Virtual Screening Approach: Further Evidence for Multiple Binding Sites within the CCR5 Extracellular Pocket. Journal of Chemical Information and Modeling, 2008, 48, 2146-2165.	5.4	34
29	KBDOCK 2013: a spatial classification of 3D protein domain family interactions. Nucleic Acids Research, 2014, 42, D389-D395.	14.5	31
30	Analysis of Fish IL-1β and Derived Peptide Sequences Indicates Conserved Structures with Species-Specific IL-1 Receptor Binding: Implications for Pharmacological Design. Current Pharmaceutical Design, 2004, 10, 3857-3871.	1.9	30
31	Detecting Drug Promiscuity Using Gaussian Ensemble Screening. Journal of Chemical Information and Modeling, 2012, 52, 1948-1961.	5.4	28
32	Recent Trends and Future Prospects in Computational GPCR Drug Discovery: From Virtual Screening to Polypharmacology. Current Topics in Medicinal Chemistry, 2013, 13, 1069-1097.	2.1	27
33	The CYP71AZ P450 Subfamily: A Driving Factor for the Diversification of Coumarin Biosynthesis in Apiaceous Plants. Frontiers in Plant Science, 2018, 9, 820.	3.6	24
34	GESSE: Predicting Drug Side Effects from Drugâ€“Target Relationships. Journal of Chemical Information and Modeling, 2015, 55, 1804-1823.	5.4	23
35	DockTrina: Docking triangular protein trimers. Proteins: Structure, Function and Bioinformatics, 2014, 82, 34-44.	2.6	20
36	Identification and characterisation of a novel immune-type receptor (NITR) gene cluster in the European sea bass, Dicentrarchus labrax, reveals recurrent gene expansion and diversification by positive selection. Immunogenetics, 2009, 61, 773-788.	2.4	18

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37	gEMfitter: A highly parallel FFT-based 3D density fitting tool with GPU texture memory acceleration. Journal of Structural Biology, 2013, 184, 348-354.	2.8	18
38	gEMpicker: a highly parallel GPU-accelerated particle picking tool for cryo-electron microscopy. BMC Structural Biology, 2013, 13, 25.	2.3	18
39	GES Polypharmacology Fingerprints: A Novel Approach for Drug Repositioning. Journal of Chemical Information and Modeling, 2014, 54, 720-734.	5.4	18
40	Biological Profiling of Antiâ€HIV Agents and Insight into CCR5 Antagonist Binding Using inâ€...silico Techniques. ChemMedChem, 2009, 4, 1153-1163.	3.2	17
41	PEPSI-Dock: a detailed data-driven proteinâ€“protein interaction potential accelerated by polar Fourier correlation. Bioinformatics, 2016, 32, i693-i701.	4.1	17
42	Recent Trends and Applications in 3D Virtual Screening. Combinatorial Chemistry and High Throughput Screening, 2012, 15, 749-769.	1.1	16
43	Identifying and characterizing promiscuous targets: Implications for virtual screening. Expert Opinion on Drug Discovery, 2012, 7, 1-17.	5.0	14
44	Exploring câ€Met kinase flexibility by sampling and clustering its conformational space. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1227-1238.	2.6	11
45	Calculating and scoring high quality multiple flexible protein structure alignments. Bioinformatics, 2016, 32, 2650-2658.	4.1	11
46	Using Spherical Harmonic Surface Property Representations for Ligandâ€Based Virtual Screening. Molecular Informatics, 2011, 30, 151-159.	2.5	10
47	PPIDomainMiner: Inferring domain-domain interactions from multiple sources of protein-protein interactions. PLoS Computational Biology, 2021, 17, e1008844.	3.2	10
48	EROS-DOCK: proteinâ€“protein docking using exhaustive branch-and-bound rotational search. Bioinformatics, 2019, 35, 5003-5010.	4.1	9
49	Protein docking using spherical polar Fourier correlations. Proteins: Structure, Function and Bioinformatics, 2000, 39, 178.	2.6	8
50	Representing and comparing protein folds and fold families using threeâ€dimensional shapeâ€density representations. Proteins: Structure, Function and Bioinformatics, 2012, 80, 530-545.	2.6	6
51	A Structure-Based Classification and Analysis of Protein Domain Family Binding Sites and Their Interactions. Biology, 2015, 4, 327-343.	2.8	5
52	Predicting drug polypharmacology using a novel surface property similarity-based approach. Journal of Cheminformatics, 2011, 3, .	6.1	4
53	Applying in silico tools to the discovery of novel CXCR4 inhibitors. Drug Development Research, 2011, 72, 95-111.	2.9	4
54	Classification and Exploration of 3D Protein Domain Interactions Using Kbdock. Methods in Molecular Biology, 2016, 1415, 91-105.	0.9	4

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55	Using Kendall-Ï„ Meta-Bagging to Improve Protein-Protein Docking Predictions. Lecture Notes in Computer Science, 2011, , 284-295.	1.3	4
56	Chapter 3. Modeling Proteinâ€“Protein Interactions by Rigid-body Docking. RSC Drug Discovery Series, 2012, , 56-86.	0.3	2
57	Modeling and minimizing CAPRI round 30 symmetrical protein complexes from CASPâ€11 structural models. Proteins: Structure, Function and Bioinformatics, 2017, 85, 463-469.	2.6	2
58	Using restraints in <scp>EROSâ€ĐOCK</scp> improves model quality in pairwise and multicomponent protein docking. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1121-1128.	2.6	2
59	Predicting Multi-Component Protein Assemblies Using an Ant Colony Approach. International Journal of Swarm Intelligence Research, 2012, 3, 19-31.	0.7	2
60	Protein docking using spherical polar Fourier correlations. , 2000, 39, 178.		1