

Iain H Moal

List of Publications by Year in descending order

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Version: 2024-02-01

37
papers

2,791
citations

304743

22
h-index

330143

37
g-index

41
all docs

41
docs citations

41
times ranked

2764
citing authors

#	ARTICLE	IF	CITATIONS
1	An expanded benchmark for antibody-antigen docking and affinity prediction reveals insights into antibody recognition determinants. <i>Structure</i> , 2021, 29, 606-621.e5.	3.3	65
2	A Guide for Protein-Protein Docking Using SwarmDock. <i>Methods in Molecular Biology</i> , 2020, 2165, 199-216.	0.9	1
3	SKEMPI 2.0: an updated benchmark of changes in protein-protein binding energy, kinetics and thermodynamics upon mutation. <i>Bioinformatics</i> , 2019, 35, 462-469.	4.1	191
4	Blind prediction of homo- and hetero-protein complexes: The CASP13-CAPRI experiment. <i>Proteins: Structure, Function and Bioinformatics</i> , 2019, 87, 1200-1221.	2.6	99
5	Modeling Structural Constraints on Protein Evolution via Side-Chain Conformational States. <i>Molecular Biology and Evolution</i> , 2019, 36, 2086-2103.	8.9	10
6	Flexible Protein-Protein Docking with SwarmDock. <i>Methods in Molecular Biology</i> , 2018, 1764, 413-428.	0.9	20
7	Modeling Protein Conformational Transition Pathways Using Collective Motions and the LASSO Method. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1401-1410.	5.3	2
8	A systematic analysis of scoring functions in rigid-body protein docking: The delicate balance between the predictive rate improvement and the risk of overtraining. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017, 85, 1287-1297.	2.6	12
9	A machine learning approach for ranking clusters of docked protein-protein complexes by pairwise cluster comparison. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017, 85, 528-543.	2.6	18
10	pyDock scoring for the new modeling challenges in docking: Protein-peptide, homo-multimers, and domain-domain interactions. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017, 85, 487-496.	2.6	19
11	IRaPPA: information retrieval based integration of biophysical models for protein assembly selection. <i>Bioinformatics</i> , 2017, 33, 1806-1813.	4.1	36
12	Prediction of homoprotein and heteroprotein complexes by protein docking and template-based modeling: A CASP-CAPRI experiment. <i>Proteins: Structure, Function and Bioinformatics</i> , 2016, 84, 323-348.	2.6	148
13	Inferring the microscopic surface energy of protein-protein interfaces from mutation data. <i>Proteins: Structure, Function and Bioinformatics</i> , 2015, 83, 640-650.	2.6	13
14	The structural basis for enhancer-dependent assembly and activation of the AAA transcriptional activator NorR. <i>Molecular Microbiology</i> , 2015, 95, 17-30.	2.5	13
15	Updates to the Integrated Protein-Protein Interaction Benchmarks: Docking Benchmark Version 5 and Affinity Benchmark Version 2. <i>Journal of Molecular Biology</i> , 2015, 427, 3031-3041.	4.2	348
16	Comment on "protein-protein binding affinity prediction from amino acid sequence". <i>Bioinformatics</i> , 2015, 31, 614-615.	4.1	8
17	CCharPPI web server: computational characterization of protein-protein interactions from structure. <i>Bioinformatics</i> , 2015, 31, 123-125.	4.1	61
18	Blind prediction of interfacial water positions in CAPRI. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 620-632.	2.6	50

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19	Prediction of Kunitz ion channel effectors and protease inhibitors from the Ixodes ricinus sialome. Ticks and Tick-borne Diseases, 2014, 5, 947-950.	2.7	10
20	Expanding the frontiers of protein-protein modeling: From docking and scoring to binding affinity predictions and other challenges. Proteins: Structure, Function and Bioinformatics, 2013, 81, 2192-2200.	2.6	20
21	Scoring functions for protein-protein interactions. Current Opinion in Structural Biology, 2013, 23, 862-867.	5.7	87
22	SwarmDock: a server for flexible protein-protein docking. Bioinformatics, 2013, 29, 807-809.	4.1	259
23	Intermolecular Contact Potentials for Protein-Protein Interactions Extracted from Binding Free Energy Changes upon Mutation. Journal of Chemical Theory and Computation, 2013, 9, 3715-3727.	5.3	41
24	The scoring of poses in protein-protein docking: current capabilities and future directions. BMC Bioinformatics, 2013, 14, 286.	2.6	98
25	Characterizing Changes in the Rate of Protein-Protein Dissociation upon Interface Mutation Using Hotspot Energy and Organization. PLoS Computational Biology, 2013, 9, e1003216.	3.2	29
26	A Markov-chain model description of binding funnels to enhance the ranking of docked solutions. Proteins: Structure, Function and Bioinformatics, 2013, 81, 2143-2149.	2.6	32
27	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
28	SKEMPI: a Structural Kinetic and Energetic database of Mutant Protein Interactions and its use in empirical models. Bioinformatics, 2012, 28, 2600-2607.	4.1	237
29	Kinetic Rate Constant Prediction Supports the Conformational Selection Mechanism of Protein Binding. PLoS Computational Biology, 2012, 8, e1002351.	3.2	48
30	Community-Wide Assessment of Protein-Interface Modeling Suggests Improvements to Design Methodology. Journal of Molecular Biology, 2011, 414, 289-302.	4.2	131
31	A structure-based benchmark for protein-protein binding affinity. Protein Science, 2011, 20, 482-491.	7.6	252
32	Protein-protein binding affinity prediction on a diverse set of structures. Bioinformatics, 2011, 27, 3002-3009.	4.1	103
33	Bridging the gaps: atomic simulation of macromolecular environment brings together protein docking, interaction kinetics and the crowding effects. BMC Bioinformatics, 2010, 11, .	2.6	1
34	Detection and refinement of encounter complexes for protein-protein docking: Taking account of macromolecular crowding. Proteins: Structure, Function and Bioinformatics, 2010, 78, 3189-3196.	2.6	59
35	SwarmDock and the Use of Normal Modes in Protein-Protein Docking. International Journal of Molecular Sciences, 2010, 11, 3623-3648.	4.1	154
36	The Structural Determinants of Macrolide-Actin Binding: In Silico Insights. Biophysical Journal, 2007, 92, 3862-3867.	0.5	6

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37	Effects of ulapualide A and synthetic macrolide analogues on actin dynamics and gene regulation. Cellular and Molecular Life Sciences, 2007, 64, 487-497.	5.4	17