# Iain H Moal

List of Publications by Year
in descending order

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|---|---|---|---|
| 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 | Updates to the Integrated Proteinâ€“Protein Interaction Benchmarks: Docking Benchmark Version 5 and Affinity Benchmark Version 2. Journal of Molecular Biology, 2015, 427, 3031-3041. | 4.2 | 348 |
| 2 | SwarmDock: a server for flexible proteinâ€“protein docking. Bioinformatics, 2013, 29, 807-809. | 4.1 | 259 |
| 3 | A structureâ€based benchmark for proteinâ€“protein binding affinity. Protein Science, 2011, 20, 482-491. | 7.6 | 252 |
| 4 | 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 |
| 5 | SKEMPI 2.0: an updated benchmark of changes in proteinâ€“protein binding energy, kinetics and thermodynamics upon mutation. Bioinformatics, 2019, 35, 462-469. | 4.1 | 191 |
| 6 | SwarmDock and the Use of Normal Modes in Protein-Protein Docking. International Journal of Molecular Sciences, 2010, 11, 3623-3648. | 4.1 | 154 |
| 7 | 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 |
| 8 | Community-Wide Assessment of Protein-Interface Modeling Suggests Improvements to Design Methodology. Journal of Molecular Biology, 2011, 414, 289-302. | 4.2 | 131 |
| 9 | Proteinâ€“protein binding affinity prediction on a diverse set of structures. Bioinformatics, 2011, 27, 3002-3009. | 4.1 | 103 |
| 10 | Blind prediction of homoâ€and heteroâ€protein complexes: The CASP13â€CAPRI experiment. Proteins: Structure, Function and Bioinformatics, 2019, 87, 1200-1221. | 2.6 | 99 |
| 11 | The scoring of poses in protein-protein docking: current capabilities and future directions. BMC Bioinformatics, 2013, 14, 286. | 2.6 | 98 |
| 12 | Scoring functions for proteinâ€“protein interactions. Current Opinion in Structural Biology, 2013, 23, 862-867. | 5.7 | 87 |
| 13 | 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 |
| 14 | An expanded benchmark for antibody-antigen docking and affinity prediction reveals insights into antibody recognition determinants. Structure, 2021, 29, 606-621.e5. | 3.3 | 65 |
| 15 | CCharPPI web server: computational characterization of proteinâ€“protein interactions from structure. Bioinformatics, 2015, 31, 123-125. | 4.1 | 61 |
| 16 | Detection and refinement of encounter complexes for proteinâ€“protein docking: Taking account of macromolecular crowding. Proteins: Structure, Function and Bioinformatics, 2010, 78, 3189-3196. | 2.6 | 59 |
| 17 | Blind prediction of interfacial water positions in CAPRI. Proteins: Structure, Function and Bioinformatics, 2014, 82, 620-632. | 2.6 | 50 |
| 18 | Kinetic Rate Constant Prediction Supports the Conformational Selection Mechanism of Protein Binding. PLoS Computational Biology, 2012, 8, e1002351. | 3.2 | 48 |

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|---|---|---|---|
| 19 | Intermolecular Contact Potentials for Proteinâ€“Protein Interactions Extracted from Binding Free Energy Changes upon Mutation. Journal of Chemical Theory and Computation, 2013, 9, 3715-3727. | 5.3 | 41 |
| 20 | IRaPPA: information retrieval based integration of biophysical models for protein assembly selection. Bioinformatics, 2017, 33, 1806-1813. | 4.1 | 36 |
| 21 | A Markovâ€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 |
| 22 | 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 |
| 23 | Expanding the frontiers of proteinâ€“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 |
| 24 | Flexible Protein-Protein Docking with SwarmDock. Methods in Molecular Biology, 2018, 1764, 413-428. | 0.9 | 20 |
| 25 | pyDock scoring for the new modeling challenges in docking: Proteinâ€“peptide, homoâ€multimers, and domainâ€“domain interactions. Proteins: Structure, Function and Bioinformatics, 2017, 85, 487-496. | 2.6 | 19 |
| 26 | A machine learning approach for ranking clusters of docked proteinâ€protein complexes by pairwise cluster comparison. Proteins: Structure, Function and Bioinformatics, 2017, 85, 528-543. | 2.6 | 18 |
| 27 | 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 |
| 28 | Inferring the microscopic surface energy of proteinâ€“protein interfaces from mutation data. Proteins: Structure, Function and Bioinformatics, 2015, 83, 640-650. | 2.6 | 13 |
| 29 | The structural basis for enhancerâ€dependent assembly and activation of the AAA transcriptional activator NorR. Molecular Microbiology, 2015, 95, 17-30. | 2.5 | 13 |
| 30 | A systematic analysis of scoring functions in rigidâ€body protein docking: The delicate balance between the predictive rate improvement and the risk of overtraining. Proteins: Structure, Function and Bioinformatics, 2017, 85, 1287-1297. | 2.6 | 12 |
| 31 | 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 |
| 32 | Modeling Structural Constraints on Protein Evolution via Side-Chain Conformational States. Molecular Biology and Evolution, 2019, 36, 2086-2103. | 8.9 | 10 |
| 33 | Comment on â€˜proteinâ€“protein binding affinity prediction from amino acid sequenceâ€™. Bioinformatics, 2015, 31, 614-615. | 4.1 | 8 |
| 34 | The Structural Determinants of Macrolide-Actin Binding: In Silico Insights. Biophysical Journal, 2007, 92, 3862-3867. | 0.5 | 6 |
| 35 | Modeling Protein Conformational Transition Pathways Using Collective Motions and the LASSO Method. Journal of Chemical Theory and Computation, 2017, 13, 1401-1410. | 5.3 | 2 |
| 36 | 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 |

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|---|---|---|---|
| 37 | A Guide for Proteinâ€“Protein Docking Using SwarmDock. Methods in Molecular Biology, 2020, 2165, 199-216. | 0.9 | 1 |