Andrew Leaver-Fay

List of Publications by Year in descending order

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#	Article	lF	CITATIONS
1	Comparative Analysis of Sulfoniumâ^'ï€, Ammoniumâ^'ï€, and Sulfurâ^'ï€ Interactions and Relevance to SAM-Dependent Methyltransferases. Journal of the American Chemical Society, 2022, 144, 2535-2545.	13.7	2
2	PyRosetta Jupyter Notebooks Teach Biomolecular Structure Prediction and Design. The Biophysicist, 2021, 2, 108-122.	0.3	8
3	Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks. Nature Communications, 2021, 12, 6947.	12.8	16
4	Better together: Elements of successful scientific software development in a distributed collaborative community. PLoS Computational Biology, 2020, 16, e1007507.	3.2	27
5	Macromolecular modeling and design in Rosetta: recent methods and frameworks. Nature Methods, 2020, 17, 665-680.	19.0	513
6	The Rosetta All-Atom Energy Function for Macromolecular Modeling and Design. Journal of Chemical Theory and Computation, 2017, 13, 3031-3048.	5.3	1,032
7	Foldit Standalone: a video game-derived protein structure manipulation interface using Rosetta. Bioinformatics, 2017, 33, 2765-2767.	4.1	77
8	A cyber-linked undergraduate research experience in computational biomolecular structure prediction and design. PLoS Computational Biology, 2017, 13, e1005837.	3.2	12
9	Computationally Designed Bispecific Antibodies using Negative State Repertoires. Structure, 2016, 24, 641-651.	3.3	54
10	SwiftLib: rapid degenerate-codon-library optimization through dynamic programming. Nucleic Acids Research, 2015, 43, e34-e34.	14.5	53
11	Combined Covalent-Electrostatic Model of Hydrogen Bonding Improves Structure Prediction with Rosetta. Journal of Chemical Theory and Computation, 2015, 11, 609-622.	5.3	204
12	Generation of bispecific IgG antibodies by structure-based design of an orthogonal Fab interface. Nature Biotechnology, 2014, 32, 191-198.	17.5	210
13	Scientific Benchmarks for Guiding Macromolecular Energy Function Improvement. Methods in Enzymology, 2013, 523, 109-143.	1.0	195
14	Rosetta3. Methods in Enzymology, 2011, 487, 545-574.	1.0	1,620
15	RosettaScripts: A Scripting Language Interface to the Rosetta Macromolecular Modeling Suite. PLoS ONE, 2011, 6, e20161.	2.5	506
16	A Generic Program for Multistate Protein Design. PLoS ONE, 2011, 6, e20937.	2.5	88