Julien Michel

List of Publications by Year
in descending order

50 papers	2,735 citations	201674 27 h-index	189892 50 g-index
66 all docs	66 docs citations	66 times ranked	2794 citing authors

#	Article	IF	Citations
1	Energetics of Displacing Water Molecules from Protein Binding Sites: Consequences for Ligand Optimization. Journal of the American Chemical Society, 2009, 131, 15403-15411.	13.7	222
2	Prediction of proteinâ€“ligand binding affinity by free energy simulations: assumptions, pitfalls and expectations. Journal of Computer-Aided Molecular Design, 2010, 24, 639-658.	2.9	221
3	Prediction of the Water Content in Protein Binding Sites. Journal of Physical Chemistry B, 2009, 113, 13337-13346.	2.6	175
4	Best Practices for Alchemical Free Energy Calculations [Article v1.0]. Living Journal of Computational Molecular Science, 2020, 2, .	6.4	125
5	Assessment of Binding Affinity via Alchemical Free-Energy Calculations. Journal of Chemical Information and Modeling, 2020, 60, 3120-3130.	5.4	114
6	Biomolecular simulations: From dynamics and mechanisms to computational assays of biological activity. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1393.	14.6	110
7	Investigating Cryptic Binding Sites by Molecular Dynamics Simulations. Accounts of Chemical Research, 2020, 53, 654-661.	15.6	106
8	A Simple QM/MM Approach for Capturing Polarization Effects in Proteinâ^'Ligand Binding Free Energy Calculations. Journal of Physical Chemistry B, 2011, 115, 4911-4926.	2.6	97
9	Protein-Ligand Binding Affinity Predictions by Implicit Solvent Simulations:Â A Tool for Lead Optimization?. Journal of Medicinal Chemistry, 2006, 49, 7427-7439.	6.4	92
10	FESetup: Automating Setup for Alchemical Free Energy Simulations. Journal of Chemical Information and Modeling, 2015, 55, 2485-2490.	5.4	92
11	The SAMPL6 SAMPLing challenge: assessing the reliability and efficiency of binding free energy calculations. Journal of Computer-Aided Molecular Design, 2020, 34, 601-633.	2.9	86
12	Prediction of Partition Coefficients by Multiscale Hybrid Atomic-Level/Coarse-Grain Simulations. Journal of Physical Chemistry B, 2008, 112, 657-660.	2.6	82
13	Effects of Water Placement on Predictions of Binding Affinities for p38Î± MAP Kinase Inhibitors. Journal of Chemical Theory and Computation, 2010, 6, 3850-3856.	5.3	81
14	Rigorous Free Energy Calculations in Structureâ€Based Drug Design. Molecular Informatics, 2010, 29, 570-578.	2.5	71
15	Rapid decomposition and visualisation of proteinâ€“ligand binding free energies by residue and by water. Faraday Discussions, 2014, 169, 477-499.	3.2	71
16	In Silico Improvement of Î²³-Peptide Inhibitors of p53â€¢hDM2 and p53â€¢hDMX. Journal of the American Chemical Society, 2009, 131, 6356-6357.	13.7	68
17	Reproducibility of Free Energy Calculations across Different Molecular Simulation Software Packages. Journal of Chemical Theory and Computation, 2018, 14, 5567-5582.	5.3	66
18	The Impact of Small Molecule Binding on the Energy Landscape of the Intrinsically Disordered Protein C-Myc. PLoS ONE, 2012, 7, e41070.	2.5	61

#	Article	IF	Citations
19	Hit Identification and Binding Mode Predictions by Rigorous Free Energy Simulations. Journal of Medicinal Chemistry, 2008, 51, 6654-6664.	6.4	59
20	Prediction of Small Molecule Hydration Thermodynamics with Grid Cell Theory. Journal of Chemical Theory and Computation, 2014, 10, 35-48.	5.3	54
21	Current and emerging opportunities for molecular simulations in structure-based drug design. Physical Chemistry Chemical Physics, 2014, 16, 4465-4477.	2.8	45
22	Proteinâ˜Ligand Complexes:â€‰ Computation of the Relative Free Energy of Different Scaffolds and Binding Modes. Journal of Chemical Theory and Computation, 2007, 3, 1645-1655.	5.3	43
23	Metabolism and hydrophilicity of the polarised â€˜Janus faceâ€™ all-cis tetrafluorocyclohexyl ring, a candidate motif for drug discovery. Chemical Science, 2018, 9, 3023-3028.	7.4	41
24	Designing stapled peptides to inhibit <scp>proteinâ€protein</scp> interactions: An analysis of successes in a rapidly changing field. Peptide Science, 2021, 113, e24191.	1.8	38
25	Evaluation of Selected Classical Force Fields for Alchemical Binding Free Energy Calculations of Protein-Carbohydrate Complexes. Journal of Chemical Theory and Computation, 2015, 11, 3333-3345.	5.3	32
26	Blinded predictions of binding modes and energies of HSP90-Î± ligands for the 2015 D3R grand challenge. Bioorganic and Medicinal Chemistry, 2016, 24, 4890-4899.	3.0	32
27	Mechanisms of small-molecule binding to intrinsically disordered proteins. Biochemical Society Transactions, 2012, 40, 1004-1008.	3.4	31
28	Hybrid Alchemical Free Energy/Machine-Learning Methodology for the Computation of Hydration Free Energies. Journal of Chemical Information and Modeling, 2020, 60, 5331-5339.	5.4	31
29	Elucidation of Nonadditive Effects in Proteinâ€“Ligand Binding Energies: Thrombin as a Case Study. Journal of Physical Chemistry B, 2016, 120, 5340-5350.	2.6	30
30	Blinded predictions of host-guest standard free energies of binding in the SAMPL5 challenge. Journal of Computer-Aided Molecular Design, 2017, 31, 61-70.	2.9	29
31	Efficient Generalized Born Models for Monte Carlo Simulations. Journal of Chemical Theory and Computation, 2006, 2, 732-739.	5.3	27
32	BioSimSpace: An interoperable Python framework for biomolecular simulation. Journal of Open Source Software, 2019, 4, 1831.	4.6	26
33	A fluorogenic probe for granzyme B enables in-biopsy evaluation and screening of response to anticancer immunotherapies. Nature Communications, 2022, 13, 2366.	12.8	26
34	A Collective Variable for the Rapid Exploration of Protein Druggability. Journal of Chemical Theory and Computation, 2015, 11, 1292-1307.	5.3	22
35	Evaluation of Hostâ€“Guest Binding Thermodynamics of Model Cavities with Grid Cell Theory. Journal of Chemical Theory and Computation, 2014, 10, 4055-4068.	5.3	21
36	Elucidation of Ligand-Dependent Modulation of Disorder-Order Transitions in the Oncoprotein MDM2. PLoS Computational Biology, 2015, 11, e1004282.	3.2	19

#	Article	IF	Citations
37	Impact of domain knowledge on blinded predictions of binding energies by alchemical free energy calculations. Journal of Computer-Aided Molecular Design, 2018, 32, 199-210.	2.9	19
38	Allosteric effects in cyclophilin mutants may be explained by changes in nano-microsecond time scale motions. Communications Chemistry, 2019, 2, .	4.5	19
39	A computationally designed binding mode flip leads to a novel class of potent tri-vector cyclophilin inhibitors. Chemical Science, 2019, 10, 542-547.	7.4	17
40	Pushing the Limits of Detection of Weak Binding Using Fragment-Based Drug Discovery: Identification of New Cyclophilin Binders. Journal of Molecular Biology, 2017, 429, 2556-2570.	4.2	16
41	Dynamic design: manipulation of millisecond timescale motions on the energy landscape of cyclophilin A. Chemical Science, 2020, 11, 2670-2680.	7.4	16
42	Impact of Ser17 Phosphorylation on the Conformational Dynamics of the Oncoprotein MDM2. Biochemistry, 2016, 55, 2500-2509.	2.5	15
43	Blinded predictions of standard binding free energies: lessons learned from the SAMPL6 challenge. Journal of Computer-Aided Molecular Design, 2018, 32, 1047-1058.	2.9	15
44	Blinded predictions of distribution coefficients in the SAMPL5 challenge. Journal of Computer-Aided Molecular Design, 2016, 30, 1101-1114.	2.9	13
45	The parameterization and validation of generalized born models using the pairwise descreening approximation. Journal of Computational Chemistry, 2004, 25, 1760-1770.	3.3	11
46	Effect of set up protocols on the accuracy of alchemical free energy calculation over a set of ACK1 inhibitors. PLoS ONE, 2019, 14, e0213217.	2.5	11
47	Energetics of a protein disorderâ€“order transition in small molecule recognition. Chemical Science, 2022, 13, 5220-5229.	7.4	7
48	Combining Virtual Reality Visualization with Ensemble Molecular Dynamics to Study Complex Protein Conformational Changes. Journal of Chemical Information and Modeling, 2020, 60, 6344-6354.	5.4	6
49	Implementation of the QUBE Force Field in SOMD for High-Throughput Alchemical Free-Energy Calculations. Journal of Chemical Information and Modeling, 2021, 61, 2124-2130.	5.4	5
50	Best Practices for Alchemical Free Energy Calculations [Article v1.0]. Living Journal of Computational Molecular Science, 2019, 2, .	6.4	3