Colin A Smith

List of Publications by Citations

27 papers	16,325 citations	19 h-index	32 g-index
32 ext. papers	18,609 ext. citations	6.5 avg, IF	5.62 L-index

#	Paper	IF	Citations
27	Bioconductor: open software development for computational biology and bioinformatics. *Genome Biology*, **2004**, 5, R80	18.3	9148
26	XCMS: processing mass spectrometry data for metabolite profiling using nonlinear peak alignment, matching, and identification. *Analytical Chemistry*, **2006**, 78, 779-87	7.8	3048
25	METLIN: a metabolite mass spectral database. *Therapeutic Drug Monitoring*, **2005**, 27, 747-51	3.2	1623
24	ROSETTA3: an object-oriented software suite for the simulation and design of macromolecules. *Methods in Enzymology*, **2011**, 487, 545-74	1.7	1216
23	Solvent-dependent metabolite distribution, clustering, and protein extraction for serum profiling with mass spectrometry. *Analytical Chemistry*, **2006**, 78, 743-52	7.8	336
22	Backrub-like backbone simulation recapitulates natural protein conformational variability and improves mutant side-chain prediction. *Journal of Molecular Biology*, **2008**, 380, 742-56	6.5	232
21	RosettaBackrub--a web server for flexible backbone protein structure modeling and design. *Nucleic Acids Research*, **2010**, 38, W569-75	20.1	94
20	Structure-based prediction of the peptide sequence space recognized by natural and synthetic PDZ domains. *Journal of Molecular Biology*, **2010**, 402, 460-74	6.5	84
19	Predicting the tolerated sequences for proteins and protein interfaces using RosettaBackrub flexible backbone design. *PLoS ONE*, **2011**, 6, e20451	3.7	73
18	A simple model of backbone flexibility improves modeling of side-chain conformational variability. *Journal of Molecular Biology*, **2008**, 380, 757-74	6.5	60
17	A Web Resource for Standardized Benchmark Datasets, Metrics, and Rosetta Protocols for Macromolecular Modeling and Design. *PLoS ONE*, **2015**, 10, e0130433	3.7	58
16	Population shuffling of protein conformations. *Angewandte Chemie - International Edition*, **2015**, 54, 207-10	10.4	50
15	Allosteric switch regulates protein-protein binding through collective motion. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 3269-74	11.5	45
14	Discovery of novel inhibitors targeting enoyl-acyl carrier protein reductase in Plasmodium falciparum by structure-based virtual screening. *Biochemical and Biophysical Research Communications*, **2007**, 358, 686-91	3.4	38
13	Flexible backbone sampling methods to model and design protein alternative conformations. *Methods in Enzymology*, **2013**, 523, 61-85	1.7	36
12	Mechanistic Insights into Microsecond Time-Scale Motion of Solid Proteins Using Complementary N and H Relaxation Dispersion Techniques. *Journal of the American Chemical Society*, **2019**, 141, 858-869	16.4	28
11	Insights into the human CD59 complement binding interface toward engineering new therapeutics. *Journal of Biological Chemistry*, **2005**, 280, 34073-9	5.4	26

List of Publications

10	Phospholipid capture combined with non-linear chromatographic correction for improved serum metabolite profiling. *Metabolomics*, **2006**, 2, 145-154	4.7	24
9	New method for the assessment of all drug-like pockets across a structural genome. *Journal of Computational Biology*, **2008**, 15, 231-40	1.7	19
8	Recent advances in measuring the kinetics of biomolecules by NMR relaxation dispersion spectroscopy. *Archives of Biochemistry and Biophysics*, **2017**, 628, 81-91	4.1	19
7	ORIUM: optimized RDC-based Iterative and Unified Model-free analysis. *Journal of Biomolecular NMR*, **2014**, 58, 287-301	3	17
6	Metabolomics relative quantitation with mass spectrometry using chemical derivatization and isotope labeling. *Spectroscopy*, **2008**, 22, 327-343		15
5	Design of a phosphorylatable PDZ domain with peptide-specific affinity changes. *Structure*, **2013**, 21, 54-64	5.2	14
4	Personalised estimation of a womanɔs most fertile days. *European Journal of Contraception and Reproductive Health Care*, **2016**, 21, 323-8	1.8	13
3	Enhancing NMR derived ensembles with kinetics on multiple timescales. *Journal of Biomolecular NMR*, **2020**, 74, 27-43	3	5
2	Resolving overlapped signals with automated FitNMR analytical peak modeling. *Journal of Magnetic Resonance*, **2020**, 318, 106773	3	2
1	Free energy calculations of ALS-causing SOD1 mutants reveal common perturbations to stability and dynamics along the maturation pathway. *Protein Science*, **2021**, 30, 1804-1817	6.3	2