Thomas Hamelryck

List of Publications by Year
in descending order

22	4,768	567247 15	610883 24
papers	citations	h-index	g-index

33	33	33	8683
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Biopython: freely available Python tools for computational molecular biology and bioinformatics. Bioinformatics, 2009, 25, 1422-1423.	4.1	4,097
2	A generative, probabilistic model of local protein structure. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 8932-8937.	7.1	113
3	Sampling Realistic Protein Conformations Using Local Structural Bias. PLoS Computational Biology, 2006, 2, e131.	3.2	84
4	Potentials of Mean Force for Protein Structure Prediction Vindicated, Formalized and Generalized. PLoS ONE, 2010, 5, e13714.	2.5	64
5	Inference of Structure Ensembles of Flexible Biomolecules from Sparse, Averaged Data. PLoS ONE, 2013, 8, e79439.	2.5	50
6	Bayesian inference of protein ensembles from SAXS data. Physical Chemistry Chemical Physics, 2016, 18, 5832-5838.	2.8	49
7	Beyond rotamers: a generative, probabilistic model of side chains in proteins. BMC Bioinformatics, 2010, 11, 306.	2.6	40
8	Probabilistic Determination of Native State Ensembles of Proteins. Journal of Chemical Theory and Computation, 2014, 10, 3484-3491.	5.3	38
9	PHAISTOS: A framework for Markov chain Monte Carlo simulation and inference of protein structure. Journal of Computational Chemistry, 2013, 34, 1697-1705.	3.3	35
10	Equilibrium simulations of proteins using molecular fragment replacement and NMR chemical shifts. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 13852-13857.	7.1	33
11	Subtle Monte Carlo Updates in Dense Molecular Systems. Journal of Chemical Theory and Computation, 2012, 8, 695-702.	5.3	22
12	Protein Structure Validation and Refinement Using Amide Proton Chemical Shifts Derived from Quantum Mechanics. PLoS ONE, 2013, 8, e84123.	2.5	21
13	Computational Redesign of Thioredoxin Is Hypersensitive toward Minor Conformational Changes in the Backbone Template. Journal of Molecular Biology, 2016, 428, 4361-4377.	4.2	21
14	Mixtures of concentrated multivariate sine distributions with applications to bioinformatics. Journal of Applied Statistics, 2012, 39, 2475-2492.	1.3	17
15	Probabilistic models and machine learning in structural bioinformatics. Statistical Methods in Medical Research, 2009, 18, 505-526.	1.5	16
16	A Generative Angular Model of Protein Structure Evolution. Molecular Biology and Evolution, 2017, 34, 2085-2100.	8.9	13
17	A community proposal to integrate structural bioinformatics activities in ELIXIR (3D-Bioinfo) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf	E.6	12
18	Bayesian inference of protein structure from chemical shift data. PeerJ, 2015, 3, e861.	2.0	11

#	ARTICLE	IF	CITATIONS
19	Langevin diffusions on the torus: estimation and applications. Statistics and Computing, 2019, 29, 1-22.	1.5	9
20	GISA: using Gauss Integrals to identify rare conformations in protein structures. PeerJ, 2020, 8, e9159.	2.0	7
21	FragBuilder: an efficient Python library to setup quantum chemistry calculations on peptides models. PeerJ, 2014, 2, e277.	2.0	6
22	MyPMFs: a simple tool for creating statistical potentials to assess protein structural models. Biochimie, 2018, 151, 37-41.	2.6	4