Thomas Hamelryck

List of Publications by Citations

24 papers	2,836 citations	13 h-index	33 g-index
33 ext. papers	3,990 ext. citations	4.6 avg, IF	4.28 L-index

#	Paper	IF	Citations
24	Biopython: freely available Python tools for computational molecular biology and bioinformatics. *Bioinformatics*, **2009**, 25, 1422-3	7.2	2308
23	A generative, probabilistic model of local protein structure. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 8932-7	11.5	84
22	Sampling realistic protein conformations using local structural bias. *PLoS Computational Biology*, **2006**, 2, e131	5	66
21	Potentials of mean force for protein structure prediction vindicated, formalized and generalized. *PLoS ONE*, **2010**, 5, e13714	3.7	51
20	Inference of structure ensembles of flexible biomolecules from sparse, averaged data. *PLoS ONE*, **2013**, 8, e79439	3.7	41
19	Bayesian inference of protein ensembles from SAXS data. *Physical Chemistry Chemical Physics*, **2016** , 18, 5832-8	3.6	39
18	Probabilistic Determination of Native State Ensembles of Proteins. *Journal of Chemical Theory and Computation*, **2014**, 10, 3484-91	6.4	35
17	Beyond rotamers: a generative, probabilistic model of side chains in proteins. *BMC Bioinformatics*, **2010**, 11, 306	3.6	32
16	PHAISTOS: a framework for Markov chain Monte Carlo simulation and inference of protein structure. *Journal of Computational Chemistry*, **2013**, 34, 1697-705	3.5	31
15	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, 13852-7	11.5	26
14	Subtle Monte Carlo Updates in Dense Molecular Systems. *Journal of Chemical Theory and Computation*, **2012**, 8, 695-702	6.4	21
13	Protein structure validation and refinement using amide proton chemical shifts derived from quantum mechanics. *PLoS ONE*, **2013**, 8, e84123	3.7	20
12	Mixtures of concentrated multivariate sine distributions with applications to bioinformatics. *Journal of Applied Statistics*, **2012**, 39, 2475-2492	1	13
11	Probabilistic models and machine learning in structural bioinformatics. *Statistical Methods in Medical Research*, **2009**, 18, 505-26	2.3	13
10	Computational Redesign of Thioredoxin Is Hypersensitive toward Minor Conformational Changes in the Backbone Template. *Journal of Molecular Biology*, **2016**, 428, 4361-4377	6.5	13
9	A Generative Angular Model of Protein Structure Evolution. *Molecular Biology and Evolution*, **2017**, 34, 2085-2100	8.3	9
8	A community proposal to integrate structural bioinformatics activities in ELIXIR (3D-Bioinfo Community). *F1000Research*, **2020**, 9,	3.6	9

List of Publications

7	Bayesian inference of protein structure from chemical shift data. *PeerJ*, **2015**, 3, e861	3.1	8
6	Langevin diffusions on the torus: estimation and applications. *Statistics and Computing*, **2019**, 29, 1-22	1.8	5
5	MyPMFs: a simple tool for creating statistical potentials to assess protein structural models. *Biochimie*, **2018**, 151, 37-41	4.6	3
4	FragBuilder: an efficient Python library to setup quantum chemistry calculations on peptides models. *PeerJ*, **2014**, 2, e277	3.1	3
3	Proteins, physics and probability kinematics: a Bayesian formulation of the protein folding problem. *Wiley Series in Probability and Statistics*, **2015**, 356-376	1.3	2
2	GISA: using Gauss Integrals to identify rare conformations in protein structures. *PeerJ*, **2020**, 8, e9159	3.1	2
1	GISA: Using Gauss Integrals to identify rare conformations in protein structures		1