Amedeo Caflisch

List of Publications by Year in Descending Order

101 papers	7,021 citations	47 h-index	83 g-index
101 ext. papers	7,584 ext. citations	7.2 avg, IF	6.14 L-index

#	Paper	IF	Citations
101	Proteostasis of Islet Amyloid Polypeptide: A Molecular Perspective of Risk Factors and Protective Strategies for Type II Diabetes. *Chemical Reviews*, **2021**, 121, 1845-1893	68.1	38
100	Simulation Studies of Amyloidogenic Polypeptides and Their Aggregates. *Chemical Reviews*, **2019**, 119, 6956-6993	68.1	74
99	In silico fragment-based drug design with SEED. *European Journal of Medicinal Chemistry*, **2018**, 156, 907-917	4.8	10
98	Disorder at the Tips of a Disease-Relevant Aβ42 Amyloid Fibril: A Molecular Dynamics Study. *Journal of Physical Chemistry B*, **2018**, 122, 11072-11082	3.4	13
97	Amyloid Fibril Elongation by Monomers Involves Disorder at the Tip. *Journal of Chemical Theory and Computation*, **2017**, 13, 5117-5130	6.4	23
96	Proteomic analyses identify ARH3 as a serine mono-ADP-ribosylhydrolase. *Nature Communications*, **2017**, 8, 2055	17.4	74
95	Weighted Distance Functions Improve Analysis of High-Dimensional Data: Application to Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2015**, 11, 5481-92	6.4	7
94	Molecular dynamics in drug design. *European Journal of Medicinal Chemistry*, **2015**, 91, 4-14	6.8	130
93	Evolutionary conserved Tyr169 stabilizes the β2-α2 loop of the prion protein. *Journal of the American Chemical Society*, **2015**, 137, 2948-57	16.4	29
92	Structured water molecules in the binding site of bromodomains can be displaced by cosolvent. *ChemMedChem*, **2014**, 9, 573-9	3.7	37
91	Does bromodomain flexibility influence histone recognition?. *FEBS Letters*, **2013**, 587, 2158-63	3.8	33
90	Carnosine inhibits Aβ(1-42) aggregation by perturbing the H-bond network in and around the central hydrophobic cluster. *ChemBioChem*, **2013**, 14, 583-92	3.8	61
89	Macrodomain-containing proteins are new mono-ADP-ribosylhydrolases. *Nature Structural and Molecular Biology*, **2013**, 20, 502-7	17.6	229
88	Methylations of tryptophan-modified naphthoquinone affect its inhibitory potential toward Aβ aggregation. *Journal of Physical Chemistry B*, **2013**, 117, 1780-9	3.4	15
87	New insights into the folding of a β-sheet miniprotein in a reduced space of collective hydrogen bond variables: application to a hydrodynamic analysis of the folding flow. *Journal of Physical Chemistry B*, **2013**, 117, 6092-105	3.4	23
86	How Does Darunavir Prevent HIV-1 Protease Dimerization?. *Journal of Chemical Theory and Computation*, **2012**, 8, 1786-94	6.4	16
85	Efficient Construction of Mesostate Networks from Molecular Dynamics Trajectories. *Journal of Chemical Theory and Computation*, **2012**, 8, 1108-20	6.4	38

84	Free Energy Guided Sampling. *Journal of Chemical Theory and Computation*, **2012**, 8, 2134-40	6.4	21
83	Optimization of designed armadillo repeat proteins by molecular dynamics simulations and NMR spectroscopy. *Protein Science*, **2012**, 21, 1298-314	6.3	28
82	Distribution of Reciprocal of Interatomic Distances: A Fast Structural Metric. *Journal of Chemical Theory and Computation*, **2012**, 8, 2930-7	6.4	35
81	Complexity in Protein Folding: Simulation Meets Experiment. *Current Physical Chemistry*, **2012**, 2, 4-11	0.5	2
80	Inhibition of interdomain motion in g-actin by the natural product latrunculin: a molecular dynamics study. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 1998-2008	4.2	6
79	Peptide binding to the PDZ3 domain by conformational selection. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 2562-72	4.2	13
78	Photocontrol of reversible amyloid formation with a minimal-design peptide. *Journal of Physical Chemistry B*, **2012**, 116, 8961-73	3.4	17
77	Phenylalanine assembly into toxic fibrils suggests amyloid etiology in phenylketonuria. *Nature Chemical Biology*, **2012**, 8, 701-6	11.7	266
76	Mechanisms and Kinetics of Amyloid Aggregation Investigated by a Phenomenological Coarse-Grained Model **2012**, 191-214		6
75	Fragment-Based Approaches in Virtual Screening. *Methods and Principles in Medicinal Chemistry*, **2011**, 467-489	0.4	2
74	Surfactant effects on amyloid aggregation kinetics. *Journal of Molecular Biology*, **2011**, 414, 303-12	6.5	20
73	Structural basis for inhibiting -amyloid oligomerization by a non-coded -breaker-substituted endomorphin analogue. *ACS Chemical Biology*, **2011**, 6, 1265-76	4.9	28
72	Wordom: a user-friendly program for the analysis of molecular structures, trajectories, and free energy surfaces. *Journal of Computational Chemistry*, **2011**, 32, 1183-94	3.5	187
71	Equilibrium distribution from distributed computing (simulations of protein folding). *Journal of Physical Chemistry B*, **2011**, 115, 6358-65	3.4	16
70	Delineation of folding pathways of a -sheet miniprotein. *Journal of Physical Chemistry B*, **2011**, 115, 13065-74	3.4	39
69	Dynamics in the active site of -secretase: a network analysis of atomistic simulations. *Biochemistry*, **2011**, 50, 9328-39	3.2	18
68	Disordered binding of small molecules to A(12-28). *Journal of Biological Chemistry*, **2011**, 286, 41578-41588	5.4	43
67	The free energy landscape of small molecule unbinding. *PLoS Computational Biology*, **2011**, 7, e1002002	5	78

66	PARP1 ADP-ribosylates lysine residues of the core histone tails. *Nucleic Acids Research*, **2010**, 38, 6350-62	20.1	192
65	Extracting physically intuitive reaction coordinates from transition networks of a beta-sheet miniprotein. *Journal of Physical Chemistry B*, **2010**, 114, 6979-89	3.4	20
64	Soluble Protofibrils as Metastable Intermediates in Simulations of Amyloid Fibril Degradation Induced by Lipid Vesicles. *Journal of Physical Chemistry Letters*, **2010**, 1, 471-474	6.4	20
63	Amyloid fibril polymorphism is under kinetic control. *Journal of the American Chemical Society*, **2010**, 132, 14960-70	16.4	106
62	Crowding Effects on Amyloid Aggregation Kinetics. *Journal of Physical Chemistry Letters*, **2010**, 1, 3027-3032	6.4	45
61	Micelle-like architecture of the monomer ensemble of Alzheimer's amyloid-β peptide in aqueous solution and its implications for Aβ aggregation. *Journal of Molecular Biology*, **2010**, 403, 148-165	6.5	66
60	Free energy surfaces from single-distance information. *Journal of Physical Chemistry B*, **2010**, 114, 15227-35	3.4	27
59	Library screening by fragment-based docking. *Journal of Molecular Recognition*, **2010**, 23, 183-93	2.6	23
58	Complete phenotypic recovery of an Alzheimer's disease model by a quinone-tryptophan hybrid aggregation inhibitor. *PLoS ONE*, **2010**, 5, e11101	3.7	113
57	9,10-Anthraquinone hinders beta-aggregation: how does a small molecule interfere with Abeta-peptide amyloid fibrillation?. *Protein Science*, **2009**, 18, 792-800	6.3	74
56	Bulky side chains and non-native salt bridges slow down the folding of a cross-linked helical peptide: a combined molecular dynamics and time-resolved infrared spectroscopy study. *Journal of Physical Chemistry B*, **2009**, 113, 4435-42	3.4	15
55	Amyloid aggregation on lipid bilayers and its impact on membrane permeability. *Journal of Molecular Biology*, **2009**, 387, 407-15	6.5	119
54	How does a simplified-sequence protein fold?. *Biophysical Journal*, **2009**, 97, 1737-46	2.9	18
53	One-dimensional barrier-preserving free-energy projections of a beta-sheet miniprotein: new insights into the folding process. *Journal of Physical Chemistry B*, **2008**, 112, 8701-14	3.4	75
52	Molecular Dynamics Simulations to Study Protein Folding and Unfolding **2008**, 1143		1
51	Alpha-Helix folding in the presence of structural constraints. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 9588-93	11.5	101
50	Multistep greedy algorithm identifies community structure in real-world and computer-generated networks. *Physical Review E*, **2008**, 78, 026112	2.4	43
49	Kinetic analysis of molecular dynamics simulations reveals changes in the denatured state and switch of folding pathways upon single-point mutation of a beta-sheet miniprotein. *Proteins: Structure, Function and Bioinformatics*, **2008**, 70, 1185-95	4.2	77

48	FACTS: Fast analytical continuum treatment of solvation. *Journal of Computational Chemistry*, **2008**, 29, 701-15	3.5	181
47	Computational analysis of the S. cerevisiae proteome reveals the function and cellular localization of the least and most amyloidogenic proteins. *Proteins: Structure, Function and Bioinformatics*, **2007**, 68, 273-8	4.2	20
46	Wordom: a program for efficient analysis of molecular dynamics simulations. *Bioinformatics*, **2007**, 23, 2625-7	7.2	227
45	Pathways and intermediates of amyloid fibril formation. *Journal of Molecular Biology*, **2007**, 374, 917-24	6.5	122
44	Estimation of folding probabilities and phi values from molecular dynamics simulations of reversible Peptide folding. *Methods in Molecular Biology*, **2007**, 350, 225-49	1.4	6
43	Network and graph analyses of folding free energy surfaces. *Current Opinion in Structural Biology*, **2006**, 16, 71-8	8.1	66
42	Automatic and efficient decomposition of two-dimensional structures of small molecules for fragment-based high-throughput docking. *Journal of Medicinal Chemistry*, **2006**, 49, 7384-92	8.3	78
41	Interpreting the aggregation kinetics of amyloid peptides. *Journal of Molecular Biology*, **2006**, 360, 882-92	6.5	222
40	Computational models for the prediction of polypeptide aggregation propensity. *Current Opinion in Chemical Biology*, **2006**, 10, 437-44	9.7	118
39	Organism complexity anti-correlates with proteomic beta-aggregation propensity. *Protein Science*, **2005**, 14, 2735-40	6.3	34
38	Prediction of aggregation rate and aggregation-prone segments in polypeptide sequences. *Protein Science*, **2005**, 14, 2723-34	6.3	181
37	Estimation of protein folding probability from equilibrium simulations. *Journal of Chemical Physics*, **2005**, 122, 184901	3.9	32
36	Local modularity measure for network clusterizations. *Physical Review E*, **2005**, 72, 056107	2.4	87
35	Phi-value analysis by molecular dynamics simulations of reversible folding. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 628-33	11.5	63
34	The role of aromaticity, exposed surface, and dipole moment in determining protein aggregation rates. *Protein Science*, **2004**, 13, 1939-41	6.3	145
33	The protein folding network. *Journal of Molecular Biology*, **2004**, 342, 299-306	6.5	322
32	Analysis of the distributed computing approach applied to the folding of a small beta peptide. *Proceedings of the National Academy of Sciences of the United States of America*, **2003**, 100, 8217-22	11.5	42
31	Folding for binding or binding for folding?. *Trends in Biotechnology*, **2003**, 21, 423-5	15.1	19

30	Efficient evaluation of the effective dielectric function of a macromolecule in aqueous solution. *Journal of Computational Chemistry*, **2003**, 24, 1936-49	3.5	9
29	Fast protein folding on downhill energy landscape. *Protein Science*, **2003**, 12, 1801-3	6.3	38
28	A sphere-based model for the electrostatics of globular proteins. *Journal of the American Chemical Society*, **2003**, 125, 4600-8	16.4	8
27	The role of side-chain interactions in the early steps of aggregation: Molecular dynamics simulations of an amyloid-forming peptide from the yeast prion Sup35. *Proceedings of the National Academy of Sciences of the United States of America*, **2003**, 100, 5154-9	11.5	242
26	Replica exchange molecular dynamics simulations of reversible folding. *Journal of Chemical Physics*, **2003**, 119, 4035-4042	3.9	92
25	Evaluation of a fast implicit solvent model for molecular dynamics simulations. *Proteins: Structure, Function and Bioinformatics*, **2002**, 46, 24-33	4.2	260
24	Weak temperature dependence of the free energy surface and folding pathways of structured peptides. *Proteins: Structure, Function and Bioinformatics*, **2002**, 47, 305-14	4.2	59
23	Molecular dynamics simulations of protein folding from the transition state. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 6719-24	11.5	112
22	Flexibility of the murine prion protein and its Asp178Asn mutant investigated by molecular dynamics simulations. *Journal of Molecular Graphics and Modelling*, **2001**, 20, 169-82	2.8	49
21	Native topology or specific interactions: what is more important for protein folding?. *Journal of Molecular Biology*, **2001**, 306, 837-50	6.5	56
20	Role of native topology investigated by multiple unfolding simulations of four SH3 domains. *Journal of Molecular Biology*, **2001**, 309, 285-98	6.5	52
19	Design of dimerization inhibitors of HIV-1 aspartic proteinase: a computer-based combinatorial approach. *Journal of Computer-Aided Molecular Design*, **2000**, 14, 161-79	4.2	22
18	Hydrophobicity maps and docking of molecular fragments with solvation. *Journal of Computer - Aided Molecular Design*, **2000**, 20, 145-169		7
17	Free Energy Surface of the Helical Peptide Y(MEARA)6. *Journal of Physical Chemistry B*, **2000**, 104, 10080-10086	3.4	56
16	Targeted Molecular Dynamics Simulations of Protein Unfolding. *Journal of Physical Chemistry B*, **2000**, 104, 4511-4518	3.4	40
15	Thermodynamics and Kinetics of Folding of Two Model Peptides Investigated by Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2000**, 104, 5000-5010	3.4	130
14	Hydrophobicity maps and docking of molecular fragments with solvation **2000**, 145-169		0
13	Structural details of urea binding to barnase: a molecular dynamics analysis. *Structure*, **1999**, 7, 477-88	5.2	109

12	Comment on the validation of continuum electrostatics models. *Journal of Computational Chemistry* , **1999**, 20, 1533-1536	3.5	16
11	Exhaustive docking of molecular fragments with electrostatic solvation. *Proteins: Structure, Function and Bioinformatics*, **1999**, 37, 88-105	4.2	148
10	Docking small ligands in flexible binding sites. *Journal of Computational Chemistry*, **1998**, 19, 21-37	3.5	112
9	Computer-Aided Design of Thrombin Inhibitors. *Physiology*, **1998**, 13, 182-189	9.8	3
8	Continuum Electrostatic Energies of Macromolecules in Aqueous Solutions. *Journal of Physical Chemistry A*, **1997**, 101, 8098-8106	2.8	124
7	Docking by Monte Carlo minimization with a solvation correction: Application to an FKBP Substrate complex. *Journal of Computational Chemistry*, **1997**, 18, 723-743	3.5	48
6	Computational combinatorial ligand design: application to human alpha-thrombin. *Journal of Computer-Aided Molecular Design*, **1996**, 10, 372-96	4.2	55
5	Acid and thermal denaturation of barnase investigated by molecular dynamics simulations. *Journal of Molecular Biology*, **1995**, 252, 672-708	6.5	160
4	Computational combinatorial chemistry for de novo ligand design: Review and assessment. *Journal of Computer - Aided Molecular Design*, **1995**, 3, 51-84		35
3	Multiple copy simultaneous search and construction of ligands in binding sites: application to inhibitors of HIV-1 aspartic proteinase. *Journal of Medicinal Chemistry*, **1993**, 36, 2142-67	8.3	195
2	Fast Analytical Continuum Treatments of Solvation209-232		4
1	Molecular Dynamics Simulations to Study Protein Folding and Unfolding1143-1169		5