# Amedeo Caflisch

## List of Publications by Citations



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|---|---|---|---|
| 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 | The protein folding network. *Journal of Molecular Biology*, **2004**, 342, 299-306 | 6.5 | 322 |
| 100 | Phenylalanine assembly into toxic fibrils suggests amyloid etiology in phenylketonuria. *Nature Chemical Biology*, **2012**, 8, 701-6 | 11.7 | 266 |
| 99 | Evaluation of a fast implicit solvent model for molecular dynamics simulations. *Proteins: Structure, Function and Bioinformatics*, **2002**, 46, 24-33 | 4.2 | 260 |
| 98 | 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 |
| 97 | Macrodomain-containing proteins are new mono-ADP-ribosylhydrolases. *Nature Structural and Molecular Biology*, **2013**, 20, 502-7 | 17.6 | 229 |
| 96 | Wordom: a program for efficient analysis of molecular dynamics simulations. *Bioinformatics*, **2007**, 23, 2625-7 | 7.2 | 227 |
| 95 | Interpreting the aggregation kinetics of amyloid peptides. *Journal of Molecular Biology*, **2006**, 360, 882-92 | 6.5 | 222 |
| 94 | 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 |
| 93 | PARP1 ADP-ribosylates lysine residues of the core histone tails. *Nucleic Acids Research*, **2010**, 38, 6350-62 | 10.1 | 192 |
| 92 | 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 |
| 91 | FACTS: Fast analytical continuum treatment of solvation. *Journal of Computational Chemistry*, **2008**, 29, 701-15 | 3.5 | 181 |
| 90 | Prediction of aggregation rate and aggregation-prone segments in polypeptide sequences. *Protein Science*, **2005**, 14, 2723-34 | 6.3 | 181 |
| 89 | Acid and thermal denaturation of barnase investigated by molecular dynamics simulations. *Journal of Molecular Biology*, **1995**, 252, 672-708 | 6.5 | 160 |
| 88 | Exhaustive docking of molecular fragments with electrostatic solvation. *Proteins: Structure, Function and Bioinformatics*, **1999**, 37, 88-105 | 4.2 | 148 |
| 87 | The role of aromaticity, exposed surface, and dipole moment in determining protein aggregation rates. *Protein Science*, **2004**, 13, 1939-41 | 6.3 | 145 |
| 86 | Molecular dynamics in drug design. *European Journal of Medicinal Chemistry*, **2015**, 91, 4-14 | 6.8 | 130 |
| 85 | 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 |

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| 84 | Continuum Electrostatic Energies of Macromolecules in Aqueous Solutions. *Journal of Physical Chemistry A*, **1997**, 101, 8098-8106 | 2.8 | 124 |
| 83 | Pathways and intermediates of amyloid fibril formation. *Journal of Molecular Biology*, **2007**, 374, 917-24 | 6.5 | 122 |
| 82 | Amyloid aggregation on lipid bilayers and its impact on membrane permeability. *Journal of Molecular Biology*, **2009**, 387, 407-15 | 6.5 | 119 |
| 81 | Computational models for the prediction of polypeptide aggregation propensity. *Current Opinion in Chemical Biology*, **2006**, 10, 437-44 | 9.7 | 118 |
| 80 | Complete phenotypic recovery of an Alzheimer\'s disease model by a quinone-tryptophan hybrid aggregation inhibitor. *PLoS ONE*, **2010**, 5, e11101 | 3.7 | 113 |
| 79 | Docking small ligands in flexible binding sites. *Journal of Computational Chemistry*, **1998**, 19, 21-37 | 3.5 | 112 |
| 78 | 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 |
| 77 | Structural details of urea binding to barnase: a molecular dynamics analysis. *Structure*, **1999**, 7, 477-88 | 5.2 | 109 |
| 76 | Amyloid fibril polymorphism is under kinetic control. *Journal of the American Chemical Society*, **2010**, 132, 14960-70 | 16.4 | 106 |
| 75 | 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 |
| 74 | Replica exchange molecular dynamics simulations of reversible folding. *Journal of Chemical Physics*, **2003**, 119, 4035-4042 | 3.9 | 92 |
| 73 | Local modularity measure for network clusterizations. *Physical Review E*, **2005**, 72, 056107 | 2.4 | 87 |
| 72 | The free energy landscape of small molecule unbinding. *PLoS Computational Biology*, **2011**, 7, e1002002 | 5 | 78 |
| 71 | 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 |
| 70 | 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 |
| 69 | 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 |
| 68 | Simulation Studies of Amyloidogenic Polypeptides and Their Aggregates. *Chemical Reviews*, **2019**, 119, 6956-6993 | 68.1 | 74 |
| 67 | Proteomic analyses identify ARH3 as a serine mono-ADP-ribosylhydrolase. *Nature Communications*, **2017**, 8, 2055 | 17.4 | 74 |

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| 66 | 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 |
| 65 | 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 |
| 64 | Network and graph analyses of folding free energy surfaces. *Current Opinion in Structural Biology*, **2006**, 16, 71-8 | 8.1 | 66 |
| 63 | 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 |
| 62 | 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 |
| 61 | 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 |
| 60 | Free Energy Surface of the Helical Peptide Y(MEARA)6. *Journal of Physical Chemistry B*, **2000**, 104, 10080-10086 | 3.4 | 56 |
| 59 | Native topology or specific interactions: what is more important for protein folding?. *Journal of Molecular Biology*, **2001**, 306, 837-50 | 6.5 | 56 |
| 58 | Computational combinatorial ligand design: application to human alpha-thrombin. *Journal of Computer-Aided Molecular Design*, **1996**, 10, 372-96 | 4.2 | 55 |
| 57 | Role of native topology investigated by multiple unfolding simulations of four SH3 domains. *Journal of Molecular Biology*, **2001**, 309, 285-98 | 6.5 | 52 |
| 56 | 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 |
| 55 | 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 |
| 54 | Crowding Effects on Amyloid Aggregation Kinetics. *Journal of Physical Chemistry Letters*, **2010**, 1, 3027-3032 | 6.4 | 45 |
| 53 | Disordered binding of small molecules to Aβ(12-28). *Journal of Biological Chemistry*, **2011**, 286, 41578-41588 | 3.4 | 43 |
| 52 | Multistep greedy algorithm identifies community structure in real-world and computer-generated networks. *Physical Review E*, **2008**, 78, 026112 | 2.4 | 43 |
| 51 | 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 |
| 50 | Targeted Molecular Dynamics Simulations of Protein Unfolding. *Journal of Physical Chemistry B*, **2000**, 104, 4511-4518 | 3.4 | 40 |
| 49 | Delineation of folding pathways of a β-sheet miniprotein. *Journal of Physical Chemistry B*, **2011**, 115, 13065-74 | 3.4 | 39 |

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| 48 | Efficient Construction of Mesostate Networks from Molecular Dynamics Trajectories. *Journal of Chemical Theory and Computation*, **2012**, 8, 1108-20 | 6.4 | 38 |
| 47 | Fast protein folding on downhill energy landscape. *Protein Science*, **2003**, 12, 1801-3 | 6.3 | 38 |
| 46 | 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 |
| 45 | Structured water molecules in the binding site of bromodomains can be displaced by cosolvent. *ChemMedChem*, **2014**, 9, 573-9 | 3.7 | 37 |
| 44 | Distribution of Reciprocal of Interatomic Distances: A Fast Structural Metric. *Journal of Chemical Theory and Computation*, **2012**, 8, 2930-7 | 6.4 | 35 |
| 43 | Computational combinatorial chemistry for de novo ligand design: Review and assessment. *Journal of Computer - Aided Molecular Design*, **1995**, 3, 51-84 | | 35 |
| 42 | Organism complexity anti-correlates with proteomic beta-aggregation propensity. *Protein Science*, **2005**, 14, 2735-40 | 6.3 | 34 |
| 41 | Does bromodomain flexibility influence histone recognition?. *FEBS Letters*, **2013**, 587, 2158-63 | 3.8 | 33 |
| 40 | Estimation of protein folding probability from equilibrium simulations. *Journal of Chemical Physics*, **2005**, 122, 184901 | 3.9 | 32 |
| 39 | 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 |
| 38 | Optimization of designed armadillo repeat proteins by molecular dynamics simulations and NMR spectroscopy. *Protein Science*, **2012**, 21, 1298-314 | 6.3 | 28 |
| 37 | Structural basis for inhibiting β-amyloid oligomerization by a non-coded β-breaker-substituted endomorphin analogue. *ACS Chemical Biology*, **2011**, 6, 1265-76 | 4.9 | 28 |
| 36 | Free energy surfaces from single-distance information. *Journal of Physical Chemistry B*, **2010**, 114, 15227-35 | 3.4 | 27 |
| 35 | Amyloid Fibril Elongation by Monomers Involves Disorder at the Tip. *Journal of Chemical Theory and Computation*, **2017**, 13, 5117-5130 | 6.4 | 23 |
| 34 | 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 |
| 33 | Library screening by fragment-based docking. *Journal of Molecular Recognition*, **2010**, 23, 183-93 | 2.6 | 23 |
| 32 | 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 |
| 31 | Free Energy Guided Sampling. *Journal of Chemical Theory and Computation*, **2012**, 8, 2134-40 | 6.4 | 21 |

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| 30 | Surfactant effects on amyloid aggregation kinetics. *Journal of Molecular Biology*, **2011**, 414, 303-12 | 6.5 | 20 |
| 29 | 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 |
| 28 | 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 |
| 27 | 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 |
| 26 | Folding for binding or binding for folding?. *Trends in Biotechnology*, **2003**, 21, 423-5 | 15.1 | 19 |
| 25 | Dynamics in the active site of □secretase: a network analysis of atomistic simulations. *Biochemistry*, **2011**, 50, 9328-39 | 3.2 | 18 |
| 24 | How does a simplified-sequence protein fold?. *Biophysical Journal*, **2009**, 97, 1737-46 | 2.9 | 18 |
| 23 | Photocontrol of reversible amyloid formation with a minimal-design peptide. *Journal of Physical Chemistry B*, **2012**, 116, 8961-73 | 3.4 | 17 |
| 22 | How Does Darunavir Prevent HIV-1 Protease Dimerization?. *Journal of Chemical Theory and Computation*, **2012**, 8, 1786-94 | 6.4 | 16 |
| 21 | Equilibrium distribution from distributed computing (simulations of protein folding). *Journal of Physical Chemistry B*, **2011**, 115, 6358-65 | 3.4 | 16 |
| 20 | Comment on the validation of continuum electrostatics models. *Journal of Computational Chemistry* , **1999**, 20, 1533-1536 | 3.5 | 16 |
| 19 | Methylations of tryptophan-modified naphthoquinone affect its inhibitory potential toward A□ aggregation. *Journal of Physical Chemistry B*, **2013**, 117, 1780-9 | 3.4 | 15 |
| 18 | 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 |
| 17 | Peptide binding to the PDZ3 domain by conformational selection. *Proteins: Structure, Function and Bioinformatics*, **2012**, 80, 2562-72 | 4.2 | 13 |
| 16 | Disorder at the Tips of a Disease-Relevant A□42 Amyloid Fibril: A Molecular Dynamics Study. *Journal of Physical Chemistry B*, **2018**, 122, 11072-11082 | 3.4 | 13 |
| 15 | In silico fragment-based drug design with SEED. *European Journal of Medicinal Chemistry*, **2018**, 156, 907-917 | 6.8 | 10 |
| 14 | Efficient evaluation of the effective dielectric function of a macromolecule in aqueous solution. *Journal of Computational Chemistry*, **2003**, 24, 1936-49 | 3.5 | 9 |
| 13 | A sphere-based model for the electrostatics of globular proteins. *Journal of the American Chemical Society*, **2003**, 125, 4600-8 | 16.4 | 8 |

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| 12 | 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 |
| 11 | Hydrophobicity maps and docking of molecular fragments with solvation. *Journal of Computer - Aided Molecular Design*, **2000**, 20, 145-169 | | 7 |
| 10 | 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 |
| 9 | 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 |
| 8 | Mechanisms and Kinetics of Amyloid Aggregation Investigated by a Phenomenological Coarse-Grained Model **2012**, 191-214 | | 6 |
| 7 | Molecular Dynamics Simulations to Study Protein Folding and Unfolding1143-1169 | | 5 |
| 6 | Fast Analytical Continuum Treatments of Solvation209-232 | | 4 |
| 5 | Computer-Aided Design of Thrombin Inhibitors. *Physiology*, **1998**, 13, 182-189 | 9.8 | 3 |
| 4 | Complexity in Protein Folding: Simulation Meets Experiment. *Current Physical Chemistry*, **2012**, 2, 4-11 | 0.5 | 2 |
| 3 | Fragment-Based Approaches in Virtual Screening. *Methods and Principles in Medicinal Chemistry*, **2011**, 467-489 | 0.4 | 2 |
| 2 | Molecular Dynamics Simulations to Study Protein Folding and Unfolding **2008**, 1143 | | 1 |
| 1 | Hydrophobicity maps and docking of molecular fragments with solvation **2000**, 145-169 | | 0 |