Massimiliano Meli

List of Publications by Year
in descending order

39	1,602	411340	355658
papers	citations	20 h-index	38 g-index

41	41	41	2757
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Recipes for Inducing Cold Denaturation in an Otherwise Stable Protein. Journal of the American Chemical Society, 2022, 144, 7198-7207.	6.6	2
2	Biocompatible graft copolymers from bacterial poly(Î³-glutamic acid) and poly(lactic acid). Polymer Chemistry, 2021, 12, 3784-3793.	1.9	18
3	Editorial: Computational Drug Discovery for Targeting of Protein-Protein Interfaces. Frontiers in Chemistry, 2021, 9, 670569.	1.8	1
4	Chemical Chaperones Modulate the Formation of Metabolite Assemblies. International Journal of Molecular Sciences, 2021, 22, 9172.	1.8	7
5	Revealing Escherichia coli type II l-asparaginase active site flexible loop in its open, ligand-free conformation. Scientific Reports, 2021, 11, 18885.	1.6	3
6	Simple Model of Protein Energetics To Identify Ab Initio Folding Transitions from All-Atom MD Simulations of Proteins. Journal of Chemical Theory and Computation, 2020, 16, 5960-5971.	2.3	9
7	The Answer Lies in the Energy: How Simple Atomistic Molecular Dynamics Simulations May Hold the Key to Epitope Prediction on the Fully Glycosylated SARS-CoV-2 Spike Protein. Journal of Physical Chemistry Letters, 2020, 11, 8084-8093.	2.1	39
8	Mechanisms of Metabolite Amyloid Formation: Computational Studies for Drug Design against Metabolic Disorders. ACS Medicinal Chemistry Letters, 2019, 10, 666-670.	1.3	7
9	How the Ligand-Induced Reorganization of Protein Internal Energies Is Coupled to Conformational Events. Journal of Chemical Theory and Computation, 2018, 14, 5992-6001.	2.3	10
10	Are Amyloid Fibrils RNA-Traps? A Molecular Dynamics Perspective. Frontiers in Molecular Biosciences, 2018, 5, 53.	1.6	4
11	A protease-resistant Escherichia coli asparaginase with outstanding stability and enhanced anti-leukaemic activity in vitro. Scientific Reports, 2017, 7, 14479.	1.6	42
12	Crystal Structure of the DFNKF Segment of Human Calcitonin Unveils Aromatic Interactions between Phenylalanines. Chemistry - A European Journal, 2017, 23, 2051-2058.	1.7	28
13	Novel PARP-1 Inhibitor Scaffolds Disclosed by a Dynamic Structure-Based Pharmacophore Approach. PLoS ONE, 2017, 12, e0170846.	1.1	15
14	DNA Polymerase Conformational Dynamics and the Role of Fidelity-Conferring Residues: Insights from Computational Simulations. Frontiers in Molecular Biosciences, 2016, 3, 20.	1.6	15
15	Investigating the Dynamic Aspects of Drug-Protein Recognition through a Combination of MD and NMR Analyses: Implications for the Development of Protein-Protein Interaction Inhibitors. PLoS ONE, 2014, 9, e97153.	1.1	11
16	The Five-To-Six-Coordination Transition of Ferric Human Serum Heme-Albumin Is Allosterically-Modulated by Ibuprofen and Warfarin: A Combined XAS and MD Study. PLoS ONE, 2014, 9, e104231.	1.1	27
17	A Hamiltonian Replica Exchange Molecular Dynamics (MD) Method for the Study of Folding, Based on the Analysis of the Stabilization Determinants of Proteins. International Journal of Molecular Sciences, 2013, 14, 12157-12169.	1.8	23
18	Pharmacological Enhancement of Î±-Glucosidase by the Allosteric Chaperone N-acetylcysteine. Molecular Therapy, 2012, 20, 2201-2211.	3.7	90

#	Article	IF	Citations
19	Characterization of the Aggregation Pathway for a 20-mer of GNNQQNY using Coarse-Grained and All-Atom Representations. Biophysical Journal, 2011, 100, 200a.	0.2	0
20	Dynamic Diagnosis of Familial Prion Diseases Supports the Î²2-Î±2 Loop as a Universal Interference Target. PLoS ONE, 2011, 6, e19093.	1.1	56
21	Effects of water miscible organic solvents on the activity and conformation of the baeyerâ€“villiger monooxygenases from Thermobifida fusca and Acinetobacter calcoaceticus: A comparative study. Biotechnology and Bioengineering, 2011, 108, 491-499.	1.7	44
22	A Multiscale Approach to Characterize the Early Aggregation Steps of the Amyloid-Forming Peptide GNNQQNY from the Yeast Prion Sup-35. PLoS Computational Biology, 2011, 7, e1002051.	1.5	80
23	The structural intolerance of the PrP Î±-fold for polar substitution of the helix-3 methionines. Cellular and Molecular Life Sciences, 2010, 67, 2825-2838.	2.4	16
24	Combined in Silico and Experimental Approach for Drug Design: The Binding Mode of Peptidic and Nonâ€Peptidic Inhibitors to Hsp90 Nâ€terminal Domain. Chemical Biology and Drug Design, 2010, 76, 382-391.	1.5	10
25	Molecular Simulations of Peptides: A Useful Tool for the Development of New Drugs and for the Study of Molecular Recognition. Methods in Molecular Biology, 2009, 570, 77-153.	0.4	8
26	Combinatorial drug design targeting multiple cancer signaling networks controlled by mitochondrial Hsp90. Journal of Clinical Investigation, 2009, 119, 454-464.	3.9	198
27	Methionine Sulfoxides on Prion Protein Helix-3 Switch on the Î±-Fold Destabilization Required for Conversion. PLoS ONE, 2009, 4, e4296.	1.1	53
28	Computational studies of the structure, dynamics and native content of amyloidâ€like fibrils of ribonuclease A. Proteins: Structure, Function and Bioinformatics, 2008, 70, 863-872.	1.5	19
29	Investigating the Mechanism of Peptide Aggregation: Insights from Mixed Monte Carlo-Molecular Dynamics Simulations. Biophysical Journal, 2008, 94, 4414-4426.	0.2	46
30	Understanding ligand-based modulation of the Hsp90 molecular chaperone dynamics at atomic resolution. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 7976-7981.	3.3	73
31	Molecular Dynamics Simulations of Proteins and Peptides: From Folding to Drug Design. Current Protein and Peptide Science, 2008, 9, 181-196.	0.7	26
32	Small-Molecule Targeting of Heat Shock Protein 90 Chaperone Function:Â Rational Identification of a New Anticancer Lead. Journal of Medicinal Chemistry, 2006, 49, 7721-7730.	2.9	88
33	Antileukemic Activity of Shepherdin and Molecular Diversity of Hsp90 Inhibitors. Journal of the National Cancer Institute, 2006, 98, 1068-1077.	3.0	85
34	A dynamic perspective on the molecular recognition of chitooligosaccharide ligands by hevein domains. Carbohydrate Research, 2005, 340, 1039-1049.	1.1	11
35	Rational design of shepherdin, a novel anticancer agent. Cancer Cell, 2005, 7, 457-468.	7.7	311
36	Structure elucidation and 3D solution conformation of the antibiotic enduracidin determined by NMR spectroscopy and molecular dynamics. Magnetic Resonance in Chemistry, 2005, 43, 603-610.	1.1	22

#	Article	IF	Citations
37	Folding and Mis-Folding of Peptides and Proteins: Insights from Molecular Simulations. Mini-Reviews in Medicinal Chemistry, 2005, 5, 353-359.	1.1	7
38	Toward the understanding of the structure and dynamics of proteinâ€“carbohydrate interactions: molecular dynamics studies of the complexes between hevein and oligosaccharidic ligands. Carbohydrate Research, 2004, 339, 985-994.	1.1	25
39	Synthesis, Structure and Conformation of Partially-Modified Retro- and Retro-InversoÏ^[NHCH(CF3)]Gly Peptides. Chemistry - A European Journal, 2003, 9, 4510-4522.	1.7	72