Massimiliano Meli

List of Publications by Citations

37 papers	1,353 citations	19 h-index	36 g-index
41 ext. papers	1,471 ext. citations	5.8 avg, IF	4 L-index

#	Paper	IF	Citations
37	Rational design of shepherdin, a novel anticancer agent. *Cancer Cell*, **2005**, 7, 457-68	24.3	275
36	Combinatorial drug design targeting multiple cancer signaling networks controlled by mitochondrial Hsp90. *Journal of Clinical Investigation*, **2009**, 119, 454-64	15.9	168
35	Antileukemic activity of shepherdin and molecular diversity of hsp90 inhibitors. *Journal of the National Cancer Institute*, **2006**, 98, 1068-77	9.7	80
34	Small-molecule targeting of heat shock protein 90 chaperone function: rational identification of a new anticancer lead. *Journal of Medicinal Chemistry*, **2006**, 49, 7721-30	8.3	79
33	Pharmacological enhancement of □glucosidase by the allosteric chaperone N-acetylcysteine. *Molecular Therapy*, **2012**, 20, 2201-11	11.7	72
32	Synthesis, structure and conformation of partially-modified retro- and retro-inverso psi[NHCH(CF3)]Gly peptides. *Chemistry - A European Journal*, **2003**, 9, 4510-22	4.8	70
31	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	5	68
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, 7976-81	11.5	60
29	Dynamic diagnosis of familial prion diseases supports the □-□ loop as a universal interference target. *PLoS ONE*, **2011**, 6, e19093	3.7	51
28	Methionine sulfoxides on prion protein Helix-3 switch on the alpha-fold destabilization required for conversion. *PLoS ONE*, **2009**, 4, e4296	3.7	49
27	Investigating the mechanism of peptide aggregation: insights from mixed monte carlo-molecular dynamics simulations. *Biophysical Journal*, **2008**, 94, 4414-26	2.9	44
26	Effects of water miscible organic solvents on the activity and conformation of the Baeyer-Villiger monooxygenases from Thermobifida fusca and Acinetobacter calcoaceticus: a comparative study. *Biotechnology and Bioengineering*, **2011**, 108, 491-9	4.9	39
25	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	3.7	24
24	Molecular dynamics simulations of proteins and peptides: from folding to drug design. *Current Protein and Peptide Science*, **2008**, 9, 181-96	2.8	24
23	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	6.4	24
22	Toward the understanding of the structure and dynamics of protein-carbohydrate interactions: molecular dynamics studies of the complexes between hevein and oligosaccharidic ligands. *Carbohydrate Research*, **2004**, 339, 985-94	2.9	23
21	A protease-resistant Escherichia coli asparaginase with outstanding stability and enhanced anti-leukaemic activity in vitro. *Scientific Reports*, **2017**, 7, 14479	4.9	22

20	Crystal Structure of the DFNKF Segment of Human Calcitonin Unveils Aromatic Interactions between Phenylalanines. *Chemistry - A European Journal*, **2017**, 23, 2051-2058	4.8	22
19	Structure elucidation and 3D solution conformation of the antibiotic enduracidin determined by NMR spectroscopy and molecular dynamics. *Magnetic Resonance in Chemistry*, **2005**, 43, 603-10	2.1	19
18	Computational studies of the structure, dynamics and native content of amyloid-like fibrils of ribonuclease A. *Proteins: Structure, Function and Bioinformatics*, **2008**, 70, 863-72	4.2	18
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, 12157-69	6.3	17
16	The structural intolerance of the PrP alpha-fold for polar substitution of the helix-3 methionines. *Cellular and Molecular Life Sciences*, **2010**, 67, 2825-38	10.3	14
15	A dynamic perspective on the molecular recognition of chitooligosaccharide ligands by hevein domains. *Carbohydrate Research*, **2005**, 340, 1039-49	2.9	11
14	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	3.7	10
13	Combined in silico and experimental approach for drug design: the binding mode of peptidic and non-peptidic inhibitors to hsp90 N-terminal domain. *Chemical Biology and Drug Design*, **2010**, 76, 382-91	2.9	10
12	Novel PARP-1 Inhibitor Scaffolds Disclosed by a Dynamic Structure-Based Pharmacophore Approach. *PLoS ONE*, **2017**, 12, e0170846	3.7	10
11	DNA Polymerase Conformational Dynamics and the Role of Fidelity-Conferring Residues: Insights from Computational Simulations. *Frontiers in Molecular Biosciences*, **2016**, 3, 20	5.6	8
10	Folding and mis-folding of peptides and proteins: insights from molecular simulations. *Mini-Reviews in Medicinal Chemistry*, **2005**, 5, 353-9	3.2	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	6.4	7
8	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	1.4	6
7	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	6.4	6
6	Biocompatible graft copolymers from bacterial poly(Ɣglutamic acid) and poly(lactic acid). *Polymer Chemistry*, **2021**, 12, 3784-3793	4.9	6
5	Mechanisms of Metabolite Amyloid Formation: Computational Studies for Drug Design against Metabolic Disorders. *ACS Medicinal Chemistry Letters*, **2019**, 10, 666-670	4.3	4
4	Are Amyloid Fibrils RNA-Traps? A Molecular Dynamics Perspective. *Frontiers in Molecular Biosciences*, **2018**, 5, 53	5.6	3
3	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		1

2	Chemical Chaperones Modulate the Formation of Metabolite Assemblies. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	1
1	Revealing Escherichia coli type II L-asparaginase active site flexible loop in its open, ligand-free conformation. *Scientific Reports*, **2021**, 11, 18885	4.9	1