Irene Maffucci

List of Publications by Year
in descending order

19 papers	601 citations	567281 15 h-index	794594 19 g-index
22 all docs	22 docs citations	22 times ranked	770 citing authors

#	Article	IF	Citations
1	Molecularly imprinted polymer nanogels targeting the HAV motif in cadherins inhibit cellâ€“cell adhesion and migration. Journal of Materials Chemistry B, 2022, 10, 6688-6697.	5.8	9
2	Molecularly Imprinted Polymer Nanogels for Protein Recognition: Direct Proof of Specific Binding Sites by Solution STD and WaterLOGSY NMR Spectroscopies. Angewandte Chemie - International Edition, 2021, 60, 20849-20857.	13.8	29
3	Molecularly Imprinted Polymer Nanogels for Protein Recognition: Direct Proof of Specific Binding Sites by Solution STD and WaterLOGSY NMR Spectroscopies. Angewandte Chemie, 2021, 133, 21017-21025.	2.0	3
4	Differences in thermal structural changes and melting between mesophilic and thermophilic dihydrofolate reductase enzymes. Physical Chemistry Chemical Physics, 2020, 22, 18361-18373.	2.8	18
5	In Silico Drug Repurposing for SARS-CoV-2 Main Proteinase and Spike Proteins. Journal of Proteome Research, 2020, 19, 4637-4648.	3.7	50
6	Thermal Adaptation of Enzymes: Impacts of Conformational Shifts on Catalytic Activation Energy and Optimum Temperature. Chemistry - A European Journal, 2020, 26, 10045-10056.	3.3	19
7	Advances in the Treatment of Explicit Water Molecules in Docking and Binding Free Energy Calculations. Current Medicinal Chemistry, 2020, 26, 7598-7622.	2.4	11
8	Genetic background and immunological status influence B cell repertoire diversity in mice. Scientific Reports, 2019, 9, 14261.	3.3	7
9	Fluoro-Aryl Substituted Î±,Î²2,3-Peptides in the Development of Foldameric Antiparallel Î²-Sheets: A Conformational Study. Frontiers in Chemistry, 2019, 7, 192.	3.6	16
10	An Efficient Implementation of the Nwat-MMGBSA Method to Rescore Docking Results in Medium-Throughput Virtual Screenings. Frontiers in Chemistry, 2018, 6, 43.	3.6	56
11	A tendril perversion in a helical oligomer: trapping and characterizing a mobile screw-sense reversal. Chemical Science, 2017, 8, 3007-3018.	7.4	38
12	Biocatalytic Dynamic Kinetic Resolution for the Synthesis of Atropisomeric Biaryl Nâ€Oxide Lewis Base Catalysts. Angewandte Chemie - International Edition, 2016, 55, 10755-10759.	13.8	87
13	Improved Computation of Proteinâ€“Protein Relative Binding Energies with the Nwat-MMGBSA Method. Journal of Chemical Information and Modeling, 2016, 56, 1692-1704.	5.4	59
14	An Updated Test of AMBER Force Fields and Implicit Solvent Models in Predicting the Secondary Structure of Helical, Î²-Hairpin, and Intrinsically Disordered Peptides. Journal of Chemical Theory and Computation, 2016, 12, 714-727.	5.3	38
15	Model peptides containing the 3-sulfanyl-norbornene amino acid, a conformationally constrained cysteine analogue effective inducer of 3₁₀-helix secondary structures. RSC Advances, 2015, 5, 32643-32656.	3.6	20
16	Origin of Helical Screw Sense Selectivity Induced by Chiral Constrained CÎ±-Tetrasubstituted Î±-Amino Acids in Aib-based Peptides. Journal of Physical Chemistry B, 2015, 119, 14003-14013.	2.6	18
17	Mechanism of Stabilization of Helix Secondary Structure by Constrained CÎ±-Tetrasubstituted Î±-Amino Acids. Journal of Physical Chemistry B, 2015, 119, 1350-1361.	2.6	25
18	2-Amino-3-(phenylsulfanyl)norbornane-2-carboxylate: An Appealing Scaffold for the Design of Rac1â€“Tiam1 Proteinâ€“Protein Interaction Inhibitors. Journal of Medicinal Chemistry, 2014, 57, 2953-2962.	6.4	31

#	Article	IF	Citations
19	Explicit Ligand Hydration Shells Improve the Correlation between MM-PB/GBSA Binding Energies and Experimental Activities. Journal of Chemical Theory and Computation, 2013, 9, 2706-2717.	5.3	67