

Irene Maffucci

List of Publications by Year in descending order

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Version: 2024-02-01

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	Biocatalytic Dynamic Kinetic Resolution for the Synthesis of Atropisomeric Biaryl N-oxide Lewis Base Catalysts. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 10755-10759.	13.8	87
2	Explicit Ligand Hydration Shells Improve the Correlation between MM-PB/GBSA Binding Energies and Experimental Activities. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2706-2717.	5.3	67
3	Improved Computation of Protein-Protein Relative Binding Energies with the Nwat-MMGBSA Method. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 1692-1704.	5.4	59
4	An Efficient Implementation of the Nwat-MMGBSA Method to Rescore Docking Results in Medium-Throughput Virtual Screenings. <i>Frontiers in Chemistry</i> , 2018, 6, 43.	3.6	56
5	In Silico Drug Repurposing for SARS-CoV-2 Main Proteinase and Spike Proteins. <i>Journal of Proteome Research</i> , 2020, 19, 4637-4648.	3.7	50
6	An Updated Test of AMBER Force Fields and Implicit Solvent Models in Predicting the Secondary Structure of Helical, β^2 -Hairpin, and Intrinsically Disordered Peptides. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 714-727.	5.3	38
7	A tendril perversion in a helical oligomer: trapping and characterizing a mobile screw-sense reversal. <i>Chemical Science</i> , 2017, 8, 3007-3018.	7.4	38
8	2-Amino-3-(phenylsulfanyl)norborene-2-carboxylate: An Appealing Scaffold for the Design of Rac1-Tiam1 Protein-Protein Interaction Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 2953-2962.	6.4	31
9	Molecularly Imprinted Polymer Nanogels for Protein Recognition: Direct Proof of Specific Binding Sites by Solution STD and WaterLOGSY NMR Spectroscopies. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 20849-20857.	13.8	29
10	Mechanism of Stabilization of Helix Secondary Structure by Constrained α -Tetrasubstituted β -Amino Acids. <i>Journal of Physical Chemistry B</i> , 2015, 119, 1350-1361.	2.6	25
11	Model peptides containing the 3-sulfanyl-norborene amino acid, a conformationally constrained cysteine analogue effective inducer of β -helix secondary structures. <i>RSC Advances</i> , 2015, 5, 32643-32656.	3.6	20
12	Thermal Adaptation of Enzymes: Impacts of Conformational Shifts on Catalytic Activation Energy and Optimum Temperature. <i>Chemistry - A European Journal</i> , 2020, 26, 10045-10056.	3.3	19
13	Origin of Helical Screw Sense Selectivity Induced by Chiral Constrained α -Tetrasubstituted β -Amino Acids in Aib-based Peptides. <i>Journal of Physical Chemistry B</i> , 2015, 119, 14003-14013.	2.6	18
14	Differences in thermal structural changes and melting between mesophilic and thermophilic dihydrofolate reductase enzymes. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 18361-18373.	2.8	18
15	Fluoro-Aryl Substituted β , β 2,3-Peptides in the Development of Foldameric Antiparallel β -Sheets: A Conformational Study. <i>Frontiers in Chemistry</i> , 2019, 7, 192.	3.6	16
16	Advances in the Treatment of Explicit Water Molecules in Docking and Binding Free Energy Calculations. <i>Current Medicinal Chemistry</i> , 2020, 26, 7598-7622.	2.4	11
17	Molecularly imprinted polymer nanogels targeting the HAV motif in cadherins inhibit cell-cell adhesion and migration. <i>Journal of Materials Chemistry B</i> , 2022, 10, 6688-6697.	5.8	9
18	Genetic background and immunological status influence B cell repertoire diversity in mice. <i>Scientific Reports</i> , 2019, 9, 14261.	3.3	7

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19	Molecularly Imprinted Polymer Nanogels for Protein Recognition: Direct Proof of Specific Binding Sites by Solution STD and WaterLOGSY NMR Spectroscopies. <i>Angewandte Chemie</i> , 2021, 133, 21017-21025.	2.0	3