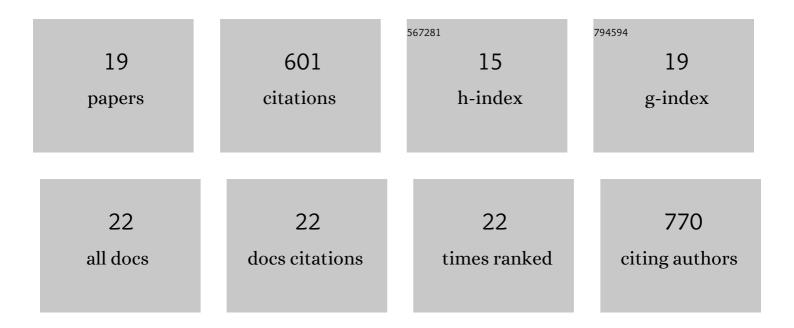
Irene Maffucci

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/4561476/publications.pdf Version: 2024-02-01



#	Article	IF	CITATIONS
1	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
2	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
3	Improved Computation of Protein–Protein Relative Binding Energies with the Nwat-MMGBSA Method. Journal of Chemical Information and Modeling, 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. Frontiers in Chemistry, 2018, 6, 43.	3.6	56
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	An Updated Test of AMBER Force Fields and Implicit Solvent Models in Predicting the Secondary Structure of Helical, β-Hairpin, and Intrinsically Disordered Peptides. Journal of Chemical Theory and Computation, 2016, 12, 714-727.	5.3	38
7	A tendril perversion in a helical oligomer: trapping and characterizing a mobile screw-sense reversal. Chemical Science, 2017, 8, 3007-3018.	7.4	38
8	2-Amino-3-(phenylsulfanyl)norbornane-2-carboxylate: An Appealing Scaffold for the Design of Rac1–Tiam1 Protein–Protein Interaction Inhibitors. Journal of Medicinal Chemistry, 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. Angewandte Chemie - International Edition, 2021, 60, 20849-20857.	13.8	29
10	Mechanism of Stabilization of Helix Secondary Structure by Constrained Cα-Tetrasubstituted α-Amino Acids. Journal of Physical Chemistry B, 2015, 119, 1350-1361.	2.6	25
11	Model peptides containing the 3-sulfanyl-norbornene amino acid, a conformationally constrained cysteine analogue effective inducer of 3 ₁₀ -helix secondary structures. RSC Advances, 2015, 5, 32643-32656.	3.6	20
12	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
13	Origin of Helical Screw Sense Selectivity Induced by Chiral Constrained Cα-Tetrasubstituted α-Amino Acids in Aib-based Peptides. Journal of Physical Chemistry B, 2015, 119, 14003-14013.	2.6	18
14	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
15	Fluoro-Aryl Substituted α,β2,3-Peptides in the Development of Foldameric Antiparallel β-Sheets: A Conformational Study. Frontiers in Chemistry, 2019, 7, 192.	3.6	16
16	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
17	Molecularly imprinted polymer nanogels targeting the HAV motif in cadherins inhibit cell–cell adhesion and migration. Journal of Materials Chemistry B, 2022, 10, 6688-6697.	5.8	9
18	Genetic background and immunological status influence B cell repertoire diversity in mice. Scientific Reports, 2019, 9, 14261.	3.3	7

#	Article	IF	CITATIONS
19	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