

Antoine Marion

List of Publications by Year in descending order

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papers

434
citations

759190

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docs citations

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times ranked

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citing authors

#	ARTICLE	IF	CITATIONS
1	The low spin - high spin equilibrium in the S2-state of the water oxidizing enzyme. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2018, 1859, 342-356.	1.0	77
2	Rationalization of the ρ Values of Alcohols and Thiols Using Atomic Charge Descriptors and Its Application to the Prediction of Amino Acid ρ 's. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 2200-2213.	5.4	58
3	Actin stabilizing compounds show specific biological effects due to their binding mode. <i>Scientific Reports</i> , 2019, 9, 9731.	3.3	30
4	Cyclization of RGD Peptides by Suzuki-Miyaura Cross-Coupling. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 7417-7430.	6.4	29
5	Glitoxin Biosynthesis: Structure, Mechanism, and Metal Promiscuity of Carboxypeptidase Glij. <i>ACS Chemical Biology</i> , 2017, 12, 1874-1882.	3.4	24
6	1,5-Disubstituted 1,2,3-Triazole-Containing Peptidotriazolamers: Design Principles for a Class of Versatile Peptidomimetics. <i>Chemistry - A European Journal</i> , 2018, 24, 953-961.	3.3	21
7	Water interactions with hydrophobic groups: Assessment and recalibration of semiempirical molecular orbital methods. <i>Journal of Chemical Physics</i> , 2014, 141, 034106.	3.0	16
8	Why Does Asn71 Deamidate Faster Than Asn15 in the Enzyme Triosephosphate Isomerase? Answers from Microsecond Molecular Dynamics Simulation and QM/MM Free Energy Calculations. <i>Biochemistry</i> , 2015, 54, 1429-1439.	2.5	16
9	DynaDom: structure-based prediction of T cell receptor inter-domain and T cell receptor-peptide-MHC (class I) association angles. <i>BMC Structural Biology</i> , 2018, 17, 2.	2.3	16
10	1,4-Disubstituted 1H-1,2,3-Triazole Containing Peptidotriazolamers: A New Class of Peptidomimetics With Interesting Foldamer Properties. <i>Frontiers in Chemistry</i> , 2019, 7, 155.	3.6	16
11	Simple Tyrosine Derivatives Act as Low Molecular Weight Organogelators. <i>Scientific Reports</i> , 2019, 9, 4893.	3.3	14
12	Sodium alginate-grafted submicrometer particles display enhanced reversible aggregation/disaggregation properties. <i>Carbohydrate Polymers</i> , 2018, 194, 61-68.	10.2	13
13	Predicting the bioactive conformations of macrocycles: a molecular dynamics-based docking procedure with DynaDock. <i>Journal of Molecular Modeling</i> , 2019, 25, 197.	1.8	13
14	Predictive modelling of the corrosion rate of carbon steel focusing on the effect of the precipitation of corrosion products. <i>Corrosion Engineering Science and Technology</i> , 2017, 52, 178-185.	1.4	11
15	Amber-Compatible Parametrization Procedure for Peptide-like Compounds: Application to 1,4- and 1,5-Substituted Triazole-Based Peptidomimetics. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 90-110.	5.4	11
16	Activity of Topotecan toward the DNA/Topoisomerase I Complex: A Theoretical Rationalization. <i>Biochemistry</i> , 2018, 57, 1542-1551.	2.5	10
17	Extended interaction networks with HCV protease NS3-4A substrates explain the lack of adaptive capability against protease inhibitors. <i>Journal of Biological Chemistry</i> , 2020, 295, 13862-13874.	3.4	10
18	Fullerene-Based Mimics of Biocatalysts Show Remarkable Activity and Modularity. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 45854-45863.	8.0	10

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19	Tuning the Biological Activity of RGD Peptides with Halotryptophans. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 586-601.	6.4	9
20	Ca ²⁺ binding induced sequential allosteric activation of sortase A: An example for ion-triggered conformational selection. <i>PLoS ONE</i> , 2018, 13, e0205057.	2.5	7
21	Peptide stapling by late-stage Suzuki–Miyaura cross-coupling. <i>Beilstein Journal of Organic Chemistry</i> , 2022, 18, 1-12.	2.2	5
22	Activity-Based Photosensitizers with Optimized Triplet State Characteristics Toward Cancer Cell Selective and Image Guided Photodynamic Therapy. <i>ACS Applied Bio Materials</i> , 2022, 5, 2754-2767.	4.6	5
23	Semi-Empirical Born–Oppenheimer Molecular Dynamics (SEBOMD) within the Amber Biomolecular Package. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 206-214.	5.4	4
24	Accurate Prediction of Protein-Ligand Binding by Combined Molecular Dynamics-Based Docking and QM/MM Methods. <i>Biophysical Journal</i> , 2018, 114, 42a.	0.5	2
25	Peptidotriazolamers Inhibit A β (1–42) Oligomerization and Cross a Blood–Brain Barrier Model. <i>ChemPlusChem</i> , 2021, 86, 840-851.	2.8	2
26	The Q41R mutation in the HCV-protease enhances the reactivity towards MAVS by suppressing non-reactive pathways. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 2126-2138.	2.8	1