Antoine Marion

List of Publications by Year
in descending order

26 papers	434 citations	759190 12 h-index	752679 20 g-index
29 all docs	29 docs citations	29 times ranked	705 citing authors

#	Article	IF	Citations
1	The Q41R mutation in the HCV-protease enhances the reactivity towards MAVS by suppressing non-reactive pathways. Physical Chemistry Chemical Physics, 2022, 24, 2126-2138.	2.8	1
2	Peptide stapling by late-stage Suzukiâ€“Miyaura cross-coupling. Beilstein Journal of Organic Chemistry, 2022, 18, 1-12.	2.2	5
3	Activity-Based Photosensitizers with Optimized Triplet State Characteristics Toward Cancer Cell Selective and Image Guided Photodynamic Therapy. ACS Applied Bio Materials, 2022, 5, 2754-2767.	4.6	5
4	Peptidotriazolamers Inhibit AÎ²(1â€“42) Oligomerization and Cross a Bloodâ€Brainâ€Barrier Model. ChemPlusChem, 2021, 86, 840-851.	2.8	2
5	Fullerene-Based Mimics of Biocatalysts Show Remarkable Activity and Modularity. ACS Applied Materials & Interfaces, 2021, 13, 45854-45863.	8.0	10
6	Tuning the Biological Activity of RGD Peptides with Halotryptophans. Journal of Medicinal Chemistry, 2021, 64, 586-601.	6.4	9
7	Extended interaction networks with HCV protease NS3-4A substrates explain the lack of adaptive capability against protease inhibitors. Journal of Biological Chemistry, 2020, 295, 13862-13874.	3.4	10
8	Actin stabilizing compounds show specific biological effects due to their binding mode. Scientific Reports, 2019, 9, 9731.	3.3	30
9	Cyclization of RGD Peptides by Suzukiâ€“Miyaura Cross-Coupling. Journal of Medicinal Chemistry, 2019, 62, 7417-7430.	6.4	29
10	Predicting the bioactive conformations of macrocycles: a molecular dynamics-based docking procedure with DynaDock. Journal of Molecular Modeling, 2019, 25, 197.	1.8	13
11	Simple Tyrosine Derivatives Act as Low Molecular Weight Organogelators. Scientific Reports, 2019, 9, 4893.	3.3	14
12	1,4-Disubstituted 1H-1,2,3-Triazole Containing Peptidotriazolamers: A New Class of Peptidomimetics With Interesting Foldamer Properties. Frontiers in Chemistry, 2019, 7, 155.	3.6	16
13	Semi-Empirical Bornâ€“Oppenheimer Molecular Dynamics (SEBOMD) within the Amber Biomolecular Package. Journal of Chemical Information and Modeling, 2019, 59, 206-214.	5.4	4
14	Activity of Topotecan toward the DNA/Topoisomerase I Complex: A Theoretical Rationalization. Biochemistry, 2018, 57, 1542-1551.	2.5	10
15	The low spin - high spin equilibrium in the S2-state of the water oxidizing enzyme. Biochimica Et Biophysica Acta - Bioenergetics, 2018, 1859, 342-356.	1.0	77
16	Accurate Prediction of Protein-Ligand Binding by Combined Molecular Dynamics-Based Docking and QM/MM Methods. Biophysical Journal, 2018, 114, 42a.	0.5	2
17	DynaDom: structure-based prediction of T cell receptor inter-domain and T cell receptor-peptide-MHC (class I) association angles. BMC Structural Biology, 2018, 17, 2.	2.3	16
18	Amber-Compatible Parametrization Procedure for Peptide-like Compounds: Application to 1,4- and 1,5-Substituted Triazole-Based Peptidomimetics. Journal of Chemical Information and Modeling, 2018, 58, 90-110.	5.4	11

#	Article	IF	Citations
19	1,5â€Disubstituted 1,2,3â€Triazoleâ€Containing Peptidotriazolamers: Design Principles for a Class of Versatile Peptidomimetics. Chemistry - A European Journal, 2018, 24, 953-961.	3.3	21
20	Ca2+ binding induced sequential allosteric activation of sortase A: An example for ion-triggered conformational selection. PLoS ONE, 2018, 13, e0205057.	2.5	7
21	Sodium alginate-grafted submicrometer particles display enhanced reversible aggregation/disaggregation properties. Carbohydrate Polymers, 2018, 194, 61-68.	10.2	13
22	Gliotoxin Biosynthesis: Structure, Mechanism, and Metal Promiscuity of Carboxypeptidase GliJ. ACS Chemical Biology, 2017, 12, 1874-1882.	3.4	24
23	Predictive modelling of the corrosion rate of carbon steel focusing on the effect of the precipitation of corrosion products. Corrosion Engineering Science and Technology, 2017, 52, 178-185.	1.4	11
24	Why Does Asn71 Deamidate Faster Than Asn15 in the Enzyme Triosephosphate Isomerase? Answers from Microsecond Molecular Dynamics Simulation and QM/MM Free Energy Calculations. Biochemistry, 2015, 54, 1429-1439.	2.5	16
25	Water interactions with hydrophobic groups: Assessment and recalibration of semiempirical molecular orbital methods. Journal of Chemical Physics, 2014, 141, 034106.	3.0	16
26	Rationalization of the pK_a Values of Alcohols and Thiols Using Atomic Charge Descriptors and Its Application to the Prediction of Amino Acid pK_aâ€™s. Journal of Chemical Information and Modeling, 2014, 54, 2200-2213.	5.4	58