Nicolas ChÃ©ron

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/4354370/publications.pdf

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17	481	840776 11	888059 17
papers	citations	h-index	g-index

19	19	19	787
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Challenging 50 Years of Established Views on Ugi Reaction: A Theoretical Approach. Journal of Organic Chemistry, 2012, 77, 1361-1366.	3.2	111
2	A qualitative failure of B3LYP for textbook organic reactions. Physical Chemistry Chemical Physics, 2012, 14, 7170.	2.8	62
3	A valence bond view of isocyanides' electronic structure. New Journal of Chemistry, 2012, 36, 1137.	2.8	53
4	OpenGrowth: An Automated and Rational Algorithm for Finding New Protein Ligands. Journal of Medicinal Chemistry, 2016, 59, 4171-4188.	6.4	53
5	Evidences for the Key Role of Hydrogen Bonds in Nucleophilic Aromatic Substitution Reactions. Chemistry - A European Journal, 2011, 17, 14929-14934.	3.3	38
6	A Hybrid Knowledge-Based and Empirical Scoring Function for Proteinâ€“Ligand Interaction: SMoG2016. Journal of Chemical Information and Modeling, 2017, 57, 584-593.	5.4	29
7	Repurposing of rutin for the inhibition of norovirus replication. Archives of Virology, 2015, 160, 2353-2358.	2.1	21
8	Protein Preferential Solvation in Water:Glycerol Mixtures. Journal of Physical Chemistry B, 2020, 124, 1424-1437.	2.6	18
9	Dual targeting of higher-order DNA structures by azacryptands induces DNA junction-mediated DNA damage in cancer cells. Nucleic Acids Research, 2021, 49, 10275-10288.	14.5	15
10	Effect of sampling on BACE-1 ligands binding free energy predictions via MM-PBSA calculations. Journal of Computational Chemistry, 2017, 38, 1941-1951.	3.3	14
11	Substituent Effects in Ugiâ€“Smiles Reactions. Journal of Physical Chemistry A, 2013, 117, 8035-8042.	2.5	13
12	Evolutionary dynamics of viral escape under antibodies stress: A biophysical model. Protein Science, 2016, 25, 1332-1340.	7.6	12
13	A Density Functional Theory Study of the Nef-Isocyanide Reaction: Mechanism, Influence of Parameters and Scope. Journal of Physical Chemistry A, 2011, 115, 10106-10112.	2.5	11
14	Coupled Valence-Bond State Molecular Dynamics Description of an Enzyme-Catalyzed Reaction in a Non-Aqueous Organic Solvent. Journal of Physical Chemistry B, 2017, 121, 7027-7041.	2.6	11
15	How does microhydration impact on structure, spectroscopy and formation of disulfide radical anions? An ab initio investigation on dimethyldisulfide. Chemical Physics Letters, 2009, 481, 173-179.	2.6	8
16	Predicting New Ugiâ€“Smiles Couplings: A Combined Experimental and Theoretical Study. Chemistry - A European Journal, 2014, 20, 9094-9099.	3.3	6
17	Click-Chemistry-Based Biomimetic Ligands Efficiently Capture G-Quadruplexes In Vitro and Help Localize Them at DNA Damage Sites in Human Cells. Jacs Au, 2022, 2, 1588-1595.	7.9	6