Enrique Marcos

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/1790295/publications.pdf

Version: 2024-02-01

18 papers	1,678 citations	623188 14 h-index	839053 18 g-index
19 all docs	19 docs citations	19 times ranked	2507 citing authors

#	Article	IF	Citations
1	Macromolecular modeling and design in Rosetta: recent methods and frameworks. Nature Methods, 2020, 17, 665-680.	9.0	513
2	De novo design of potent and selective mimics of IL-2 and IL-15. Nature, 2019, 565, 186-191.	13.7	362
3	De novo design of a fluorescence-activating Î²-barrel. Nature, 2018, 561, 485-491.	13.7	269
4	Principles for designing proteins with cavities formed by curved Î² sheets. Science, 2017, 355, 201-206.	6.0	117
5	De novo design of a non-local Î²-sheet protein with high stability and accuracy. Nature Structural and Molecular Biology, 2018, 25, 1028-1034.	3.6	101
6	Changes in Dynamics upon Oligomerization Regulate Substrate Binding and Allostery in Amino Acid Kinase Family Members. PLoS Computational Biology, 2011, 7, e1002201.	1.5	49
7	On the Conservation of the Slow Conformational Dynamics within the Amino Acid Kinase Family: NAGK the Paradigm. PLoS Computational Biology, 2010, 6, e1000738.	1.5	41
8	Essentials of de novo protein design: Methods and applications. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1374.	6.2	41
9	Design of HÃ¼ckelâ€“MÃ¶bius Topological Switches with High Nonlinear Optical Properties. Journal of Physical Chemistry C, 2017, 121, 19348-19357.	1.5	34
10	Theoretical Study of the Switching between HÃ¼ckel and MÃ¶bius Topologies for Expanded Porphyrins. Journal of Physical Chemistry C, 2012, 116, 24358-24366.	1.5	28
11	Effect of the Meso-Substituent in the HÃ¼ckel-to-MÃ¶bius Topological Switches. Journal of Organic Chemistry, 2014, 79, 5036-5046.	1.7	27
12	Inductive and External Electric Field Effects in Pentacoordinated Phosphorus Compounds. Journal of Chemical Theory and Computation, 2008, 4, 49-63.	2.3	21
13	Pentacoordinated phosphorus revisited by highâ€level QM/MM calculations. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2405-2411.	1.5	17
14	Description of pentacoordinated phosphorus under an external electric field: which basis sets and semi-empirical methods are needed?. Physical Chemistry Chemical Physics, 2008, 10, 2442.	1.3	15
15	Conformational Compression and Barrier Height Heterogeneity in the N-Acetylglutamate Kinase. Journal of Physical Chemistry B, 2013, 117, 14261-14272.	1.2	13
16	Crowding Induces Differences in the Diffusion of Thermophilic and Mesophilic Proteins: A New Look at Neutron Scattering Results. Biophysical Journal, 2011, 101, 2782-2789.	0.2	12
17	Dynamic Fingerprints of Protein Thermostability Revealed by Long Molecular Dynamics. Journal of Chemical Theory and Computation, 2012, 8, 1129-1142.	2.3	10
18	An engineered protein-based submicromolar competitive inhibitor of the Staphylococcus aureus virulence factor aureolysin. Computational and Structural Biotechnology Journal, 2022, 20, 534-544.	1.9	5