Enrique Marcos

List of Publications by Year in descending order

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

#	Article	lF	Citations
1	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
2	Macromolecular modeling and design in Rosetta: recent methods and frameworks. Nature Methods, 2020, 17, 665-680.	9.0	513
3	De novo design of potent and selective mimics of IL-2 and IL-15. Nature, 2019, 565, 186-191.	13.7	362
4	De novo design of a non-local \hat{l}^2 -sheet protein with high stability and accuracy. Nature Structural and Molecular Biology, 2018, 25, 1028-1034.	3 . 6	101
5	De novo design of a fluorescence-activating β-barrel. Nature, 2018, 561, 485-491.	13.7	269
6	Essentials of <i>de novo</i> protein design: Methods and applications. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1374.	6.2	41
7	Principles for designing proteins with cavities formed by curved \hat{I}^2 sheets. Science, 2017, 355, 201-206.	6.0	117
8	Design of Hýckel–Möbius Topological Switches with High Nonlinear Optical Properties. Journal of Physical Chemistry C, 2017, 121, 19348-19357.	1.5	34
9	Effect of the Meso-Substituent in the Hückel-to-Möbius Topological Switches. Journal of Organic Chemistry, 2014, 79, 5036-5046.	1.7	27
10	Conformational Compression and Barrier Height Heterogeneity in the <i>N</i> -Acetylglutamate Kinase. Journal of Physical Chemistry B, 2013, 117, 14261-14272.	1.2	13
11	Dynamic Fingerprints of Protein Thermostability Revealed by Long Molecular Dynamics. Journal of Chemical Theory and Computation, 2012, 8, 1129-1142.	2.3	10
12	Theoretical Study of the Switching between Hýckel and Möbius Topologies for Expanded Porphyrins. Journal of Physical Chemistry C, 2012, 116, 24358-24366.	1.5	28
13	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
14	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
15	Pentacoordinated phosphorus revisited by highâ€level QM/MM calculations. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2405-2411.	1.5	17
16	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
17	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
18	Inductive and External Electric Field Effects in Pentacoordinated Phosphorus Compounds. Journal of Chemical Theory and Computation, 2008, 4, 49-63.	2.3	21