Diego Prada-Gracia

List of Publications by Year
in descending order

25 papers	629 citations	687363 13 h-index	642732 23 g-index
26 all docs	26 docs citations	26 times ranked	1153 citing authors

#	Article	IF	Citations
1	Exploring the Free Energy Landscape: From Dynamics to Networks and Back. PLoS Computational Biology, 2009, 5, e1000415.	3.2	114
2	Efficient Formalism for Large-ScaleAbÂInitioMolecular Dynamics based on Time-Dependent Density Functional Theory. Physical Review Letters, 2008, 101, 096403.	7.8	105
3	The quest for self-consistency in hydrogen bond definitions. Journal of Chemical Physics, 2013, 139, 084501.	3.0	63
4	Application of computational methods for anticancer drug discovery, design, and optimization. BoletÃn MÃ©dico Del Hospital Infantil De MÃ©xico, 2016, 73, 411-423.	0.3	51
5	Impact of Lipid Composition and Receptor Conformation on the Spatio-temporal Organization of Î¼-Opioid Receptors in a Multi-component Plasma Membrane Model. PLoS Computational Biology, 2016, 12, e1005240.	3.2	49
6	Molecular details of dimerization kinetics reveal negligible populations of transient Âμ-opioid receptor homodimers at physiological concentrations. Scientific Reports, 2018, 8, 7705.	3.3	36
7	Common conformational changes in flavodoxins induced by FMN and anion binding: The structure of Helicobacter pylori apoflavodoxin. Proteins: Structure, Function and Bioinformatics, 2007, 69, 581-594.	2.6	24
8	Structureâ€“dynamics relationship in coherent transport through disordered systems. Nature Communications, 2013, 4, 2296.	12.8	23
9	Towards a microscopic description of the free-energy landscape of water. Journal of Chemical Physics, 2012, 137, 144504.	3.0	18
10	Mesoscopic model for free-energy-landscape analysis of DNA sequences. Physical Review E, 2012, 86, 021908.	2.1	16
11	Accounting for the kinetics in order parameter analysis: Lessons from theoretical models and a disordered peptide. Journal of Chemical Physics, 2012, 137, 194101.	3.0	16
12	Consensus for the Fip35 folding mechanism?. Journal of Chemical Physics, 2013, 139, 035102.	3.0	16
13	Structure and dynamics of water in crowded environments slows down peptide conformational changes. Journal of Chemical Physics, 2014, 141, 045101.	3.0	15
14	Cloning and biochemical characterization of three glucoseâ€‘6â€‘phosphate dehydrogenase mutants presents in the Mexican population. International Journal of Biological Macromolecules, 2018, 119, 926-936.	7.5	13
15	Water Structure-Forming Capabilities Are Temperature Shifted for Different Models. Journal of Physical Chemistry B, 2012, 116, 7538-7543.	2.6	12
16	Expanding the Structural Diversity of DNA Methyltransferase Inhibitors. Pharmaceuticals, 2021, 14, 17.	3.8	12
17	Biochemical Characterization and Structural Modeling of Fused Glucose-6-Phosphate Dehydrogenase-Phosphogluconolactonase from Giardia lamblia. International Journal of Molecular Sciences, 2018, 19, 2518.	4.1	11
18	Live Attenuated Salmonella enterica Expressing and Releasing Cell-Permeable Bax BH3 Peptide Through the MisL Autotransporter System Elicits Antitumor Activity in a Murine Xenograft Model of Human B Non-hodgkin's Lymphoma. Frontiers in Immunology, 2019, 10, 2562.	4.8	11

#	Article	IF	Citations
19	A comparative analysis of clustering algorithms: O2 migration in truncated hemoglobin I from transition networks. Journal of Chemical Physics, 2015, 142, 025103.	3.0	10
20	Macro and nano scale modelling of waterâ€“water interactions at ambient and low temperature: relaxation and residence times. Physical Chemistry Chemical Physics, 2016, 18, 9377-9387.	2.8	5
21	Molecular dynamics of the histamine H3 membrane receptor reveals different mechanisms of GPCR signal transduction. Scientific Reports, 2020, 10, 16889.	3.3	4
22	Cell-Permeable Bak BH3 Peptide Induces Chemosensitization of Hematologic Malignant Cells. Journal of Oncology, 2020, 2020, 1-13.	1.3	3
23	New perspectives on the computational characterization of the kinetics of binding-unbinding in drug design: implications for novel therapies. BoletÃn MÃ©dico Del Hospital Infantil De MÃ©xico, 2016, 73, 424-431.	0.3	2
24	Analysis of Apoflavodoxin Folding Behavior with Elastic Network Models. AIP Conference Proceedings, 2006, , .	0.4	0
25	Kinetics of G Protein-Coupled Receptor Dimerization from Markov State Model Analysis of Coarse-Grained Simulations. Biophysical Journal, 2017, 112, 27a.	0.5	0