Pablo Campomanes

List of Publications by Year
in descending order

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52	1,268	361045 20	360668 35
papers	citations	h-index	g-index

56	56	56	2089
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Investigating the structural properties of hydrophobic solvent-rich lipid bilayers. Soft Matter, 2021, 17, 5329-5335.	1.2	8
2	Pre-existing bilayer stresses modulate triglyceride accumulation in the ER versus lipid droplets. ELife, 2021, 10, .	2.8	55
3	Protonation Equilibrium in the Active Site of the Photoactive Yellow Protein. Molecules, 2021, 26, 2025.	1.7	0
4	Recharging your fats: CHARMM36 parameters for neutral lipids triacylglycerol and diacylglycerol. Biophysical Reports, 2021, 1, 100034.	0.7	10
5	Accurate Estimation of Membrane Capacitance from Atomistic Molecular Dynamics Simulations of Zwitterionic Lipid Bilayers. Journal of Physical Chemistry B, 2020, 124, 8278-8286.	1.2	11
6	Local accumulation of diacylglycerol alters membrane properties nonlinearly due to its transbilayer activity. Communications Chemistry, 2019, 2, .	2.0	37
7	An Atomistic Look into Bio-inspired Nanoparticles and their Molecular Interactions with Cells. Chimia, 2019, 73, 78.	0.3	4
8	Molecular Simulations Integrated with Experiments Unravel the Key Factors of Lipid Selection in Fatty Acid Amide Hydrolase and Suggest A General Mechanism of Lipid-Processing in the Parent Enzymes. Biophysical Journal, 2016, 110, 202a-203a.	0.2	0
9	Structural Determinants for the Binding of Morphinan Agonists to the Î¼-Opioid Receptor. PLoS ONE, 2015, 10, e0135998.	1.1	20
10	Anandamide Hydrolysis in FAAH Reveals a Dual Strategy for Efficient Enzyme-Assisted Amide Bond Cleavage via Nitrogen Inversion. Journal of Physical Chemistry B, 2015, 119, 789-801.	1.2	36
11	The Molecular Mechanism of the Catalase-like Activity in Horseradish Peroxidase. Journal of the American Chemical Society, 2015, 137, 11170-11178.	6.6	86
12	Keys to Lipid Selection in Fatty Acid Amide Hydrolase Catalysis: Structural Flexibility, Gating Residues and Multiple Binding Pockets. PLoS Computational Biology, 2015, 11, e1004231.	1.5	31
13	Lessons from Nature: Computational Design of Biomimetic Compounds and Processes. Chimia, 2014, 68, 642.	0.3	4
14	Ligand substitutions between ruthenium–cymene compounds can control protein versus DNA targeting and anticancer activity. Nature Communications, 2014, 5, 3462.	5.8	257
15	Origin of the Spectral Shifts among the Early Intermediates of the Rhodopsin Photocycle. Journal of the American Chemical Society, 2014, 136, 3842-3851.	6.6	42
16	Generalized QM/MM Force Matching Approach Applied to the 11-cis Protonated Schiff Base Chromophore of Rhodopsin. Journal of Chemical Theory and Computation, 2014, 10, 412-422.	2.3	21
17	Assigning the EPR Fine Structure Parameters of the Mn(II) Centers in Bacillus subtilis Oxalate Decarboxylase by Site-Directed Mutagenesis and DFT/MM Calculations. Journal of the American Chemical Society, 2014, 136, 2313-2323.	6.6	17
18	Rhodopsin Absorption from First Principles: Bypassing Common Pitfalls. Journal of Chemical Theory and Computation, 2013, 9, 2441-2454.	2.3	81

#	Article	IF	Citations
19	Wagging the Tail: Essential Role of Substrate Flexibility in FAAH Catalysis. Journal of Chemical Theory and Computation, 2013, 9, 1202-1213.	2.3	24
20	Ion Binding and Internal Hydration in the Multidrug Resistance Secondary Active Transporter NorM Investigated by Molecular Dynamics Simulations. Biochemistry, 2012, 51, 1281-1287.	1.2	32
21	Mechanical (QM/MM) Simulations of Adiabatic and Nonadiabatic Ultrafast Phenomena. Chimia, 2011, 65, 330-333.	0.3	5
22	Studies of Glutathione Transferase P1â€1 Bound to a Platinum(IV)â€Based Anticancer Compound Reveal the Molecular Basis of Its Activation. Chemistry - A European Journal, 2011, 17, 7806-7816.	1.7	73
23	Pushing the Frontiers of First-Principles Based Computer Simulations of Chemical and Biological Systems. Chimia, 2011, 65, 667.	0.3	22
24	Heterogeneous reaction mechanisms of the reduction of nitric oxide on carbon surfaces: a theoretical analysis. Theoretical Chemistry Accounts, 2010, 127, 95-108.	0.5	21
25	Reactions of Alkynes with [RuCl(cyclopentadienyl)] Complexes: The Important First Steps. Chemistry - A European Journal, 2010, 16, 8400-8409.	1.7	50
26	Understanding Regioselective Cleavage in Peptide Hydrolysis by a Palladium(II) Aqua Complex: A Theoretical Point of View. Journal of Physical Chemistry B, 2010, 114, 8525-8535.	1.2	11
27	Reactivity of a rhenium hydroxoâ€“carbonyl complex toward carbon disulfide: insights from theory. Dalton Transactions, 2010, 39, 874-882.	1.6	6
28	On the Mechanism of Cyclization of 5-Hexenylchromate Intermediates in the Reactions of Fischer Carbene Complexes with a Lithium Enolate and Allylmagnesium Bromide. Journal of Organic Chemistry, 2009, 74, 7059-7066.	1.7	6
29	A Theoretical Study on the Reactivity of a Rhenium Hydroxoâ€Carbonyl Complex Towards Î²â€Lactams. European Journal of Inorganic Chemistry, 2008, 2008, 4547-4554.	1.0	1
30	Ring opening at N1â€“C2 bond of azetidin-2-ones by a molybdenum hydroxo-carbonyl complex: evidence from a computational study. Dalton Transactions, 2008, , 6427.	1.6	1
31	Structure, aromaticity, and bonding in subporphyrins: theoretical study of [14]tribenzosubporphine(1.1.1)hydroxyboron(III) and [14]subporphine(1.1.1)hydroxyboron(III) complexes. Journal of Porphyrins and Phthalocyanines, 2007, 11, 815-821.	0.4	8
32	Molecular magnetic properties of heteroporphyrins: a theoretical analysis. Physical Chemistry Chemical Physics, 2007, 9, 5644.	1.3	14
33	The Importance of a Conformational Equilibrium on the Reactivity of Molybdenum and Rhenium Hydroxoâ"Carbonyl Complexes toward Phenyl Acetate:â€‰ A Theoretical Investigation. Organometallics, 2007, 26, 5271-5277.	1.1	5
34	Synthesis of Cyclohexanol Derivatives by Zirconocene-Mediated Ring-Contraction Reactions of Seven-Membered Cyclic Enol Ethers. Angewandte Chemie - International Edition, 2007, 46, 2607-2609.	7.2	7
35	A theoretical study of the cleavage of the amide bond of formamide by attack of the hydroxyl ligand in [Mo(OH)(Î·3-C3H5)(CO)2(N2C2H4)] and [Re(OH)(CO)3(N2C2H4)] complexes. Computational and Theoretical Chemistry, 2007, 811, 241-247.	1.5	4
36	A Theoretical Proposal for the Synthesis of Carbapenems from 4-(2-Propynyl)azetidinones Promoted by [W(CO)5] as an Alternative to the Ag+-Assisted Process. Chemistry - A European Journal, 2006, 12, 7929-7934.	1.7	5

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37	Theoretical Studies on the Ring Opening of β-lactams: Processes in Solution and in Enzymatic Media. Current Organic Chemistry, 2006, 10, 805-821.	0.9	28
38	Resonance assisted hydrogen bonding and dynamic mechanism for crystal disorder in the enolic form of acetylacetone: a theoretical analysis. Computational and Theoretical Chemistry, 2005, 713, 59-63.	1.5	6
39	Stereodynamics of bond rotation in tertiary 1-naphthoic acid amides: A computational study. Journal of Computational Chemistry, 2005, 26, 365-373.	1.5	2
40	The Formation of Silylated Î²-Lactams from Silylketenes through Lewis Acid Promoted [2+2] Cycloaddition: A Combined Theoretical and Experimental Study. European Journal of Organic Chemistry, 2005, 2005, 2599-2606.	1.2	16
41	A Theoretical Analysis of the Coordination Modes of Cullwith Penicillins: Activation of the Î²-Lactam Cï£¿N Bond. ChemPhysChem, 2005, 6, 344-351.	1.0	2
42	[W(CO)5]-Catalyzedendo- orexo-Cycloisomerization Reactions of 1,1-Disubstituted 4-Pentyn-1-ols: Experimental and Theoretical Studies. Chemistry - A European Journal, 2005, 11, 5735-5741.	1.7	53
43	Solvent-Assisted New Reaction Pathways for the (THF)W(CO)5-Promotedendo-andexo-Cycloisomerization of 4-Pentyn-1-ol:Â A Theoretical Investigation. Journal of the American Chemical Society, 2005, 127, 944-952.	6.6	47
44	Synthesis of Î²-Lactams by Ag+-Induced Ring Expansion of 1-Hydroxycyclopropylamines:Â A Theoretical Analysis. Journal of Physical Chemistry A, 2005, 109, 7822-7831.	1.1	2
45	Mechanism of Cycloaddition Reactions between Ketene andN-Silyl-,N-Germyl-, andN-Stannylimines:Â A Theoretical Investigation. Journal of Physical Chemistry A, 2005, 109, 11022-11026.	1.1	9
46	Theoretical Study of Intramolecular SN2 Reactions of 3-Halogen or 3-Hydroxypropanamides To Obtain Î²-Lactams. Journal of Physical Chemistry A, 2004, 108, 11109-11115.	1.1	0
47	Theoretical Study of the Mechanism of the Formation of 3-Unsubstituted 4,4-Disubstituted Î²-Lactams by Silver-Induced Ring Expansion of Alkoxycyclopropylamines:Â A New Synthetic Route to 4-Alkoxycarbonyl-4-alkyl-2-azetidinones. Journal of Organic Chemistry, 2003, 68, 6685-6689.	1.7	13
48	Synthesis of Î²-Lactams from aN-Rhenaimine:Â Effect of the Transition Metal on the Energetic Profile of the Staudinger Reaction. Journal of the American Chemical Society, 2003, 125, 3706-3707.	6.6	38
49	A Theoretical Analysis of Enantiomerization in Aromatic Amides. Journal of Physical Chemistry A, 2002, 106, 2623-2628.	1.1	11
50	A Theoretical Study of the 2NCO + 2OH Reaction. Journal of Physical Chemistry A, 2001, 105, 229-237.	1.1	15
51	An ab initio study of the reaction of CH2F+ with acetylene. Computational and Theoretical Chemistry, 2001, 537, 193-198.	1.5	1
52	Theoretical Study of the Ionâ"Molecule Reaction of the Vinyl Cation with Ethane. Journal of Physical Chemistry A, 1999, 103, 5996-6002.	1.1	10