Pablo Campomanes

List of Publications by Year
in descending order

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52	1,268	361413 20	361022 35
papers	citations	h-index	g-index

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

#	Article	IF	Citations
1	Ligand substitutions between rutheniumâ€“cymene compounds can control protein versus DNA targeting and anticancer activity. Nature Communications, 2014, 5, 3462.	12.8	257
2	The Molecular Mechanism of the Catalase-like Activity in Horseradish Peroxidase. Journal of the American Chemical Society, 2015, 137, 11170-11178.	13.7	86
3	Rhodopsin Absorption from First Principles: Bypassing Common Pitfalls. Journal of Chemical Theory and Computation, 2013, 9, 2441-2454.	5.3	81
4	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.	3.3	73
5	Pre-existing bilayer stresses modulate triglyceride accumulation in the ER versus lipid droplets. ELife, 2021, 10, .	6.0	55
6	[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.	3.3	53
7	Reactions of Alkynes with [RuCl(cyclopentadienyl)] Complexes: The Important First Steps. Chemistry - A European Journal, 2010, 16, 8400-8409.	3.3	50
8	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.	13.7	47
9	Origin of the Spectral Shifts among the Early Intermediates of the Rhodopsin Photocycle. Journal of the American Chemical Society, 2014, 136, 3842-3851.	13.7	42
10	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.	13.7	38
11	Local accumulation of diacylglycerol alters membrane properties nonlinearly due to its transbilayer activity. Communications Chemistry, 2019, 2, .	4.5	37
12	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.	2.6	36
13	Ion Binding and Internal Hydration in the Multidrug Resistance Secondary Active Transporter NorM Investigated by Molecular Dynamics Simulations. Biochemistry, 2012, 51, 1281-1287.	2.5	32
14	Keys to Lipid Selection in Fatty Acid Amide Hydrolase Catalysis: Structural Flexibility, Gating Residues and Multiple Binding Pockets. PLoS Computational Biology, 2015, 11, e1004231.	3.2	31
15	Theoretical Studies on the Ring Opening of β-lactams: Processes in Solution and in Enzymatic Media. Current Organic Chemistry, 2006, 10, 805-821.	1.6	28
16	Wagging the Tail: Essential Role of Substrate Flexibility in FAAH Catalysis. Journal of Chemical Theory and Computation, 2013, 9, 1202-1213.	5.3	24
17	Pushing the Frontiers of First-Principles Based Computer Simulations of Chemical and Biological Systems. Chimia, 2011, 65, 667.	0.6	22
18	Heterogeneous reaction mechanisms of the reduction of nitric oxide on carbon surfaces: a theoretical analysis. Theoretical Chemistry Accounts, 2010, 127, 95-108.	1.4	21

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19	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.	5.3	21
20	Structural Determinants for the Binding of Morphinan Agonists to the Î¼-Opioid Receptor. PLoS ONE, 2015, 10, e0135998.	2.5	20
21	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.	13.7	17
22	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.	2.4	16
23	A Theoretical Study of the 2NCO + 2OH Reaction. Journal of Physical Chemistry A, 2001, 105, 229-237.	2.5	15
24	Molecular magnetic properties of heteroporphyrins: a theoretical analysis. Physical Chemistry Chemical Physics, 2007, 9, 5644.	2.8	14
25	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.	3.2	13
26	A Theoretical Analysis of Enantiomerization in Aromatic Amides. Journal of Physical Chemistry A, 2002, 106, 2623-2628.	2.5	11
27	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.	2.6	11
28	Accurate Estimation of Membrane Capacitance from Atomistic Molecular Dynamics Simulations of Zwitterionic Lipid Bilayers. Journal of Physical Chemistry B, 2020, 124, 8278-8286.	2.6	11
29	Theoretical Study of the Ionâ^'Molecule Reaction of the Vinyl Cation with Ethane. Journal of Physical Chemistry A, 1999, 103, 5996-6002.	2.5	10
30	Recharging your fats: CHARMM36 parameters for neutral lipids triacylglycerol and diacylglycerol. Biophysical Reports, 2021, 1, 100034.	1.2	10
31	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.	2.5	9
32	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.	0.8	8
33	Investigating the structural properties of hydrophobic solvent-rich lipid bilayers. Soft Matter, 2021, 17, 5329-5335.	2.7	8
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.	13.8	7
35	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
36	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.	3.2	6

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37	Reactivity of a rhenium hydroxoâ€“carbonyl complex toward carbon disulfide: insights from theory. Dalton Transactions, 2010, 39, 874-882.	3.3	6
38	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.	3.3	5
39	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.	2.3	5
40	Mechanical (QM/MM) Simulations of Adiabatic and Nonadiabatic Ultrafast Phenomena. Chimia, 2011, 65, 330-333.	0.6	5
41	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
42	Lessons from Nature: Computational Design of Biomimetic Compounds and Processes. Chimia, 2014, 68, 642.	0.6	4
43	An Atomistic Look into Bio-inspired Nanoparticles and their Molecular Interactions with Cells. Chimia, 2019, 73, 78.	0.6	4
44	Stereodynamics of bond rotation in tertiary 1-naphthoic acid amides: A computational study. Journal of Computational Chemistry, 2005, 26, 365-373.	3.3	2
45	A Theoretical Analysis of the Coordination Modes of Cullwith Penicillins: Activation of the Î²-Lactam Cï£¿N Bond. ChemPhysChem, 2005, 6, 344-351.	2.1	2
46	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.	2.5	2
47	An ab initio study of the reaction of CH2F+ with acetylene. Computational and Theoretical Chemistry, 2001, 537, 193-198.	1.5	1
48	A Theoretical Study on the Reactivity of a Rhenium Hydroxoâ€Carbonyl Complex Towards Î²â€Lactams. European Journal of Inorganic Chemistry, 2008, 2008, 4547-4554.	2.0	1
49	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.	3.3	1
50	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.	2.5	0
51	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.	0.5	0
52	Protonation Equilibrium in the Active Site of the Photoactive Yellow Protein. Molecules, 2021, 26, 2025.	3.8	0