Ignacio Soteras

List of Publications by Year
in descending order

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24	1,040	471509 17	642732 23
papers	citations	h-index	g-index

26	26	26	1605
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Parametrization of halogen bonds in the CHARMM general force field: Improved treatment of ligandâ€“protein interactions. Bioorganic and Medicinal Chemistry, 2016, 24, 4812-4825.	3.0	168
2	Exploring the Binding Sites of Glycogen Synthase Kinase 3. Identification and Characterization of Allosteric Modulation Cavities. Journal of Medicinal Chemistry, 2011, 54, 8461-8470.	6.4	91
3	Continuum solvation models: Dissecting the free energy of solvation. Physical Chemistry Chemical Physics, 2003, 5, 3827-3836.	2.8	89
4	Extension of the MST model to the IEF formalism: HF and B3LYP parametrizations. Computational and Theoretical Chemistry, 2005, 727, 29-40.	1.5	79
5	Induction effects in metal cationâ€“benzene complexes. Physical Chemistry Chemical Physics, 2008, 10, 2616.	2.8	78
6	5-Imino-1,2,4-Thiadiazoles: First Small Molecules As Substrate Competitive Inhibitors of Glycogen Synthase Kinase 3. Journal of Medicinal Chemistry, 2012, 55, 1645-1661.	6.4	76
7	The impact of monovalent ion force field model in nucleic acids simulations. Physical Chemistry Chemical Physics, 2009, 11, 10596.	2.8	62
8	Effect of Phosphodiesterase 7 (PDE7) Inhibitors in Experimental Autoimmune Encephalomyelitis Mice. Discovery of a New Chemically Diverse Family of Compounds. Journal of Medicinal Chemistry, 2012, 55, 3274-3284.	6.4	52
9	MST Continuum Study of the Hydration Free Energies of Monovalent Ionic Species. Journal of Physical Chemistry B, 2005, 109, 3565-3574.	2.6	44
10	Derivation of Distributed Models of Atomic Polarizability for Molecular Simulations. Journal of Chemical Theory and Computation, 2007, 3, 1901-1913.	5.3	41
11	Modeling Induction Phenomena in Intermolecular Interactions with an Ab Initio Force Field. Journal of Chemical Theory and Computation, 2007, 3, 1914-1926.	5.3	34
12	Polarizable Intermolecular Potentials for Water and Benzene Interacting with Halide and Metal Ions. Journal of Chemical Theory and Computation, 2009, 5, 3022-3031.	5.3	34
13	The boronâ€“boron single bond in diborane(4) as a non-classical electron donor for hydrogen bonding. Physical Chemistry Chemical Physics, 2011, 13, 14026.	2.8	33
14	Boronâ€Based Dipolar Multicomponent Reactions: Simple Generation of Substituted Aziridines, Oxazolidines and Pyrrolidines. Chemistry - A European Journal, 2010, 16, 7904-7915.	3.3	27
15	Performance of the IEF-MST solvation continuum model in the SAMPL2 blind test prediction of hydration and tautomerization free energies. Journal of Computer-Aided Molecular Design, 2010, 24, 281-291.	2.9	24
16	Benzoderivatives of Nucleic Acid Bases as Modified DNA Building Blocksâ€. Journal of Physical Chemistry A, 2006, 110, 510-518.	2.5	21
17	Structural and energetic study of cationâ€“Ïâ€“cation interactions in proteins. Physical Chemistry Chemical Physics, 2017, 19, 9849-9861.	2.8	19
18	On the Origin of the Stereoselectivity in the Alkylation of Oxazolopiperidone Enolates. Journal of the American Chemical Society, 2006, 128, 6581-6588.	13.7	17

#	Article	IF	Citations
19	Performance of the IEF-MST Solvation Continuum Model in a Blind Test Prediction of Hydration Free Energies. Journal of Physical Chemistry B, 2009, 113, 9330-9334.	2.6	17
20	Structure-Directed Reversion in the Ï€-Facial Stereoselective Alkylation of Chiral Bicyclic Lactams. Journal of Organic Chemistry, 2008, 73, 7756-7763.	3.2	13
21	Group contributions to the solvation free energy from MST continuum calculations. Brazilian Journal of Physics, 2004, 34, 48-57.	1.4	7
22	Machine Learning applied to Wi-Fi fingerprinting: The experiences of the Ubiqum Challenge. , 2019, , .		6
23	Unraveling phosphodiesterase surfaces. Identification of phosphodiesterase 7 allosteric modulation cavities. European Journal of Medicinal Chemistry, 2013, 70, 781-788.	5.5	5
24	An ab initio strategy for handling induction phenomena in metal ion complexes. Molecular Physics, 2008, 106, 1685-1696.	1.7	3