Juan Luis Pascual-Ahuir

List of Publications by Year
in descending order

30 papers	2,839 citations	393982 19 h-index	454577 30 g-index
30 all docs	30 docs citations	30 times ranked	2375 citing authors

#	Article	IF	Citations
1	Reversibility and Diffusion in Mandelythiamin Decarboxylation. Searching Dynamical Effects in Decarboxylation Reactions. Journal of the American Chemical Society, 2012, 134, 10509-10514.	6.6	8
2	A theoretical study of solvent effects on the conformational equilibria of neutral glycine in aqueous solution. Computational and Theoretical Chemistry, 2003, 623, 203-210.	1.5	24
3	Molecular dynamics simulation in aqueous solution of N -methylazetidinone as a model of Î² -lactam antibiotics. Theoretical Chemistry Accounts, 1999, 101, 336-342.	0.5	8
4	Modeling ?-lactam interactions in aqueous solution through combined quantum mechanics-molecular mechanics methods. Journal of Computational Chemistry, 1999, 20, 1401-1411.	1.5	16
5	Analysis of a concerted mechanism in Î²-lactam enzymatic hydrolysis. A quantum mechanics/molecular mechanics study. Journal of the Chemical Society Perkin Transactions II, 1999, , 1351-1356.	0.9	8
6	The Solvent-Excluding Surface as a descriptor of ionic channels: Gramicidin-A. Computational and Theoretical Chemistry, 1998, 426, 331-338.	1.5	5
7	Neutral and Alkaline Hydrolyses of Model Î²-Lactam Antibiotics. An ab Initio Study of Water Catalysis. Journal of the American Chemical Society, 1998, 120, 2146-2155.	6.6	71
8	Aminoacid zwitterions in solution: Geometric, energetic, and vibrational analysis using density functional theory-continuum model calculations. Journal of Chemical Physics, 1998, 109, 592-603.	1.2	87
9	Solubility of gases in water: Correlation between solubility and the number of water molecules in the first solvation shell. Pure and Applied Chemistry, 1998, 70, 1895-1904.	0.9	54
10	Ab Initio Calculations on Neutral and Alkaline Hydrolyses of Î²-Lactam Antibiotics. A Theoretical Study Including Solvent Effects. Journal of Physical Chemistry B, 1997, 101, 3581-3588.	1.2	56
11	Correlation effects in proton transfer reactions in solution. Computational and Theoretical Chemistry, 1996, 371, 117-121.	1.5	6
12	Why is glycine a zwitterion in aqueous solution? A theoretical study of solvent stabilising factors. Chemical Physics Letters, 1996, 260, 21-26.	1.2	156
13	Can Hydrophobic Interactions Be Correctly Reproduced by the Continuum Models?. The Journal of Physical Chemistry, 1996, 100, 9955-9959.	2.9	32
14	Solvent Effects on the Thermodynamics and Kinetics of the Proton Transfer between Hydronium Ion and Ammonia. A Theoretical Study Using the Continuum and the Discrete Models. The Journal of Physical Chemistry, 1995, 99, 12525-12528.	2.9	12
15	Evaluation of transfer free energies. The Journal of Physical Chemistry, 1994, 98, 377-379.	2.9	19
16	GEPOL: An improved description of molecular surfaces. III. A new algorithm for the computation of a solvent-excluding surface. Journal of Computational Chemistry, 1994, 15, 1127-1138.	1.5	760
17	Continuum-uniform approach calculations of the solubility of hydrocarbons in water. Chemical Physics Letters, 1993, 203, 289-294.	1.2	43
18	Theoretical study of the inversion of the alcohol acidity scale in aqueous solution. Toward an interpretation of the acid-base behavior of organic compounds in solution. Journal of the American Chemical Society, 1993, 115, 2226-2230.	6.6	47

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19	Proton transfer between water molecules: a theoretical study of solvent effects using the continuum and the discrete-continuum models. The Journal of Physical Chemistry, 1993, 97, 11087-11091.	2.9	25
20	Molecular surface area and hydrophobic effect. Protein Engineering, Design and Selection, 1992, 5, 715-716.	1.0	85
21	Molecular surface calculations on organic compounds. Computational and Theoretical Chemistry, 1992, 254, 369-377.	1.5	11
22	Dispersion and repulsion contributions to the solvation energy: Refinements to a simple computational model in the continuum approximation. Journal of Computational Chemistry, 1991, 12, 784-791.	1.5	301
23	GEPOL: An improved description of molecular surfaces II. Computing the molecular area and volume. Journal of Computational Chemistry, 1991, 12, 1077-1088.	1.5	237
24	Calmodulin structure and function: Implication of arginine in the compaction related to ligand binding. Molecular Engineering, 1991, 1, 231-247.	0.2	23
25	Structural dynamics of calmodulin and troponin C. Protein Engineering, Design and Selection, 1991, 4, 625-637.	1.0	40
26	GEPOL: An improved description of molecular surfaces. I. Building the spherical surface set. Journal of Computational Chemistry, 1990, 11, 1047-1060.	1.5	243
27	Calculation of the relative basicities of methylamines in solution. Chemical Physics Letters, 1990, 169, 297-300.	1.2	12
28	Molecular volumes and surfaces of biomacromolecules via GEPOL: A fast and efficient algorithm. Journal of Molecular Graphics, 1990, 8, 168-172.	1.7	98
29	Electrostatic interaction of a solute with a continuum. Improved description of the cavity and of the surface cavity bound charge distribution.. Journal of Computational Chemistry, 1987, 8, 778-787.	1.5	351
30	MO studies of the nature of the bifurcated hydrogen bond. Rotational barriers in cyclohexanol and 1,3-dioxan-5-ol. Chemical Physics Letters, 1984, 109, 468-470.	1.2	1