

Juan Luis Pascual-Ahuir

List of Publications by Year in descending order

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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	GEPOL: An improved description of molecular surfaces. III. A new algorithm for the computation of a solvent-excluding surface. <i>Journal of Computational Chemistry</i> , 1994, 15, 1127-1138.	1.5	760
2	Electrostatic interaction of a solute with a continuum. Improved description of the cavity and of the surface cavity bound charge distribution.. <i>Journal of Computational Chemistry</i> , 1987, 8, 778-787.	1.5	351
3	Dispersion and repulsion contributions to the solvation energy: Refinements to a simple computational model in the continuum approximation. <i>Journal of Computational Chemistry</i> , 1991, 12, 784-791.	1.5	301
4	GEPOL: An improved description of molecular surfaces. I. Building the spherical surface set. <i>Journal of Computational Chemistry</i> , 1990, 11, 1047-1060.	1.5	243
5	GEPOL: An improved description of molecular surfaces II. Computing the molecular area and volume. <i>Journal of Computational Chemistry</i> , 1991, 12, 1077-1088.	1.5	237
6	Why is glycine a zwitterion in aqueous solution? A theoretical study of solvent stabilising factors. <i>Chemical Physics Letters</i> , 1996, 260, 21-26.	1.2	156
7	Molecular volumes and surfaces of biomacromolecules via GEPOL: A fast and efficient algorithm. <i>Journal of Molecular Graphics</i> , 1990, 8, 168-172.	1.7	98
8	Aminoacid zwitterions in solution: Geometric, energetic, and vibrational analysis using density functional theory-continuum model calculations. <i>Journal of Chemical Physics</i> , 1998, 109, 592-603.	1.2	87
9	Molecular surface area and hydrophobic effect. <i>Protein Engineering, Design and Selection</i> , 1992, 5, 715-716.	1.0	85
10	Neutral and Alkaline Hydrolyses of Model β -Lactam Antibiotics. An ab Initio Study of Water Catalysis. <i>Journal of the American Chemical Society</i> , 1998, 120, 2146-2155.	6.6	71
11	Ab Initio Calculations on Neutral and Alkaline Hydrolyses of β -Lactam Antibiotics. A Theoretical Study Including Solvent Effects. <i>Journal of Physical Chemistry B</i> , 1997, 101, 3581-3588.	1.2	56
12	Solubility of gases in water: Correlation between solubility and the number of water molecules in the first solvation shell. <i>Pure and Applied Chemistry</i> , 1998, 70, 1895-1904.	0.9	54
13	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. <i>Journal of the American Chemical Society</i> , 1993, 115, 2226-2230.	6.6	47
14	Continuum-uniform approach calculations of the solubility of hydrocarbons in water. <i>Chemical Physics Letters</i> , 1993, 203, 289-294.	1.2	43
15	Structural dynamics of calmodulin and troponin C. <i>Protein Engineering, Design and Selection</i> , 1991, 4, 625-637.	1.0	40
16	Can Hydrophobic Interactions Be Correctly Reproduced by the Continuum Models?. <i>The Journal of Physical Chemistry</i> , 1996, 100, 9955-9959.	2.9	32
17	Proton transfer between water molecules: a theoretical study of solvent effects using the continuum and the discrete-continuum models. <i>The Journal of Physical Chemistry</i> , 1993, 97, 11087-11091.	2.9	25
18	A theoretical study of solvent effects on the conformational equilibria of neutral glycine in aqueous solution. <i>Computational and Theoretical Chemistry</i> , 2003, 623, 203-210.	1.5	24

#	ARTICLE	IF	CITATIONS
19	Calmodulin structure and function: Implication of arginine in the compaction related to ligand binding. <i>Molecular Engineering</i> , 1991, 1, 231-247.	0.2	23
20	Evaluation of transfer free energies. <i>The Journal of Physical Chemistry</i> , 1994, 98, 377-379.	2.9	19
21	Modeling β -lactam interactions in aqueous solution through combined quantum mechanics-molecular mechanics methods. <i>Journal of Computational Chemistry</i> , 1999, 20, 1401-1411.	1.5	16
22	Calculation of the relative basicities of methylamines in solution. <i>Chemical Physics Letters</i> , 1990, 169, 297-300.	1.2	12
23	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. <i>The Journal of Physical Chemistry</i> , 1995, 99, 12525-12528.	2.9	12
24	Molecular surface calculations on organic compounds. <i>Computational and Theoretical Chemistry</i> , 1992, 254, 369-377.	1.5	11
25	Molecular dynamics simulation in aqueous solution of N-methylazetidinone as a model of β -lactam antibiotics. <i>Theoretical Chemistry Accounts</i> , 1999, 101, 336-342.	0.5	8
26	Analysis of a concerted mechanism in β -lactam enzymatic hydrolysis. A quantum mechanics/molecular mechanics study. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1999, , 1351-1356.	0.9	8
27	Reversibility and Diffusion in Mandelythiamin Decarboxylation. Searching Dynamical Effects in Decarboxylation Reactions. <i>Journal of the American Chemical Society</i> , 2012, 134, 10509-10514.	6.6	8
28	Correlation effects in proton transfer reactions in solution. <i>Computational and Theoretical Chemistry</i> , 1996, 371, 117-121.	1.5	6
29	The Solvent-Excluding Surface as a descriptor of ionic channels: Gramicidin-A. <i>Computational and Theoretical Chemistry</i> , 1998, 426, 331-338.	1.5	5
30	MO studies of the nature of the bifurcated hydrogen bond. Rotational barriers in cyclohexanol and 1,3-dioxan-5-ol. <i>Chemical Physics Letters</i> , 1984, 109, 468-470.	1.2	1