F Javier Luque

List of Publications by Year
in descending order

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410 papers	19,297 citations	9786 73 h-index	20358 116 g-index
427 all docs	427 docs citations	427 times ranked	15870 citing authors

#	Article	IF	Citations
1	Perspective on "Electrostatic interactions of a solute with a continuum. A direct utilization of ab initio molecular potentials for the prevision of solvent effects". Theoretical Chemistry Accounts, 2000, 103, 343-345.	1.4	712
2	Theoretical Methods for the Description of the Solvent Effect in Biomolecular Systems. Chemical Reviews, 2000, 100, 4187-4226.	47.7	571
3	First Non-ATP Competitive Glycogen Synthase Kinase 3 Î² (GSK-3Î²) Inhibitors:Â Thiadiazolidinones (TDZD) as Potential Drugs for the Treatment of Alzheimer's Disease. Journal of Medicinal Chemistry, 2002, 45, 1292-1299.	6.4	421
4	Tautomerism and Protonation of Guanine and Cytosine. Implications in the Formation of Hydrogen-Bonded Complexes. Journal of the American Chemical Society, 1996, 118, 6811-6821.	13.7	318
5	MDpocket: open-source cavity detection and characterization on molecular dynamics trajectories. Bioinformatics, 2011, 27, 3276-3285.	4.1	265
6	Is polarization important in cation-Â interactions?. Proceedings of the National Academy of Sciences of the United States of America, 1998, 95, 5976-5980.	7.1	259
7	Toward Improved Description of DNA Backbone: Revisiting Epsilon and Zeta Torsion Force Field Parameters. Journal of Chemical Theory and Computation, 2013, 9, 2339-2354.	5.3	255
8	Dynamics of B-DNA on the Microsecond Time Scale. Journal of the American Chemical Society, 2007, 129, 14739-14745.	13.7	250
9	Hydrogen Bond versus Anti-Hydrogen Bond:â€‰ A Comparative Analysis Based on the Electron Density Topology. Journal of Physical Chemistry A, 1999, 103, 6394-6401.	2.5	223
10	Nature of Base Stacking: Reference Quantum-Chemical Stacking Energies in Ten Unique B-DNA Base-Pair Steps. Chemistry - A European Journal, 2006, 12, 2854-2865.	3.3	211
11	Design, Synthesis, and Biological Evaluation of Dual Binding Site Acetylcholinesterase Inhibitors:â€‰ New Disease-Modifying Agents for Alzheimer's Disease. Journal of Medicinal Chemistry, 2005, 48, 7223-7233.	6.4	203
12	Binding Site Detection and Druggability Index from First Principles. Journal of Medicinal Chemistry, 2009, 52, 2363-2371.	6.4	201
13	Synthesis, Biological Evaluation, and Molecular Modeling of Donepezil and N-[(5-(Benzyloxy)-1-methyl-1H-indol-2-yl)methyl]-N-methylprop-2-yn-1-amine Hybrids as New Multipotent Cholinesterase/Monoamine Oxidase Inhibitors for the Treatment of Alzheimerâ€™s Disease. Journal of Medicinal Chemistry, 2011, 54, 8251-8270.	6.4	198
14	Frontiers in Molecular Dynamics Simulations of DNA. Accounts of Chemical Research, 2012, 45, 196-205.	15.6	194
15	Correlated ab initio study of nucleic acid bases and their tautomers in the gas phase, in a microhydrated environment and in aqueous solution : Part 1. Cytosine. Physical Chemistry Chemical Physics, 2002, 4, 4192-4203.	2.8	187
16	Targeting Beta-Amyloid Pathogenesis Through Acetylcholinesterase Inhibitors. Current Pharmaceutical Design, 2006, 12, 4377-4387.	1.9	187
17	Novel Donepezil-Based Inhibitors of Acetyl- and Butyrylcholinesterase and Acetylcholinesterase-Induced Î²-Amyloid Aggregation. Journal of Medicinal Chemistry, 2008, 51, 3588-3598.	6.4	186
18	New Tacrineâ^'Huperzine A Hybrids (Huprines):â€‰ Highly Potent Tight-Binding Acetylcholinesterase Inhibitors of Interest for the Treatment of Alzheimer's Disease. Journal of Medicinal Chemistry, 2000, 43, 4657-4666.	6.4	185

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19	Shielded Hydrogen Bonds as Structural Determinants of Binding Kinetics: Application in Drug Design. Journal of the American Chemical Society, 2011, 133, 18903-18910.	13.7	178
20	SCRF calculation of the effect of water on the topology of the molecular electrostatic potential. The Journal of Physical Chemistry, 1993, 97, 9380-9384.	2.9	172
21	On the Performance of Continuum Solvation Methods. A Comment on â€œUniversal Approaches to Solvation Modelingâ€• Accounts of Chemical Research, 2009, 42, 489-492.	15.6	171
22	Pyrano[3,2-c]quinolineâ^'6-Chlorotacrine Hybrids as a Novel Family of Acetylcholinesterase- and Î²-Amyloid-Directed Anti-Alzheimer Compounds. Journal of Medicinal Chemistry, 2009, 52, 5365-5379.	6.4	164
23	Theoretical methods for the simulation of nucleic acids. Chemical Society Reviews, 2003, 32, 350-364.	38.1	150
24	Towards a molecular dynamics consensus view of B-DNA flexibility. Nucleic Acids Research, 2008, 36, 2379-2394.	14.5	147
25	Donepezilâ€“tacrine hybrid related derivatives as new dual binding site inhibitors of AChE. Bioorganic and Medicinal Chemistry, 2005, 13, 6588-6597.	3.0	145
26	Optimization of solute cavities and van der Waals parameters inab initio MST-SCRF calculations of neutral molecules. Journal of Computational Chemistry, 1994, 15, 446-454.	3.3	135
27	Synthesis of Enantiopuretrans-3,4-Disubstituted Piperidines. An Enantiodivergent Synthesis of (+)- and (â^')-Paroxetine. Journal of Organic Chemistry, 2000, 65, 3074-3084.	3.2	135
28	Tacripyrines, the First Tacrineâ^'Dihydropyridine Hybrids, as Multitarget-Directed Ligands for the Treatment of Alzheimerâ€™s Disease. Journal of Medicinal Chemistry, 2009, 52, 2724-2732.	6.4	134
29	Peripheral and Dual Binding Site Acetylcholinesterase Inhibitors: Implications in treatment of Alzheimers Disease. Mini-Reviews in Medicinal Chemistry, 2001, 1, 267-272.	2.4	134
30	Synthesis and Multitarget Biological Profiling of a Novel Family of Rhein Derivatives As Disease-Modifying Anti-Alzheimer Agents. Journal of Medicinal Chemistry, 2014, 57, 2549-2567.	6.4	132
31	3D Structure of Torpedo californica Acetylcholinesterase Complexed with Huprine X at 2.1 Ã... Resolution:â€‰ Kinetic and Molecular Dynamic Correlates[,]. Biochemistry, 2002, 41, 2970-2981.	2.5	126
32	Câ^'HÂ·Â·Â·O Contacts in the AdenineÂ·Â·Â·Uracil Watsonâ^'Crick and UracilÂ·Â·Â·Uracil Nucleic Acid Base Pairs:â€‰ Nonempirical ab Initio Study with Inclusion of Electron Correlation Effects. Journal of Physical Chemistry B, 2000, 104, 6286-6292.	2.6	125
33	Glycogen Synthase Kinase-3 (GSK-3) Inhibitory Activity and Structureâ€“Activity Relationship (SAR) Studies of the Manzamine Alkaloids. Potential for Alzheimerâ€™s Disease. Journal of Natural Products, 2007, 70, 1397-1405.	3.0	123
34	The Structure and Dynamics of DNA in the Gas Phase. Journal of the American Chemical Society, 2003, 125, 8007-8014.	13.7	121
35	Solvation in octanol: parametrization of the continuum MST model. Journal of Computational Chemistry, 2001, 22, 1180-1193.	3.3	120
36	Theoretical Study of Alkyl-Ï€ and Aryl-Ï€ Interactions. Reconciling Theory and Experiment. Journal of Organic Chemistry, 2002, 67, 7057-7065.	3.2	119

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37	The relative flexibility of B-DNA and A-RNA duplexes: database analysis. Nucleic Acids Research, 2004, 32, 6144-6151.	14.5	119
38	Induced dipole moment and atomic charges based on average electrostatic potentials in aqueous solution. Journal of Chemical Physics, 1993, 98, 2975-2982.	3.0	118
39	Solvent Effects in Chloroform Solution:Â Parametrization of the MST/SCRF Continuum Model. The Journal of Physical Chemistry, 1996, 100, 4269-4276.	2.9	116
40	On the use of AM1 and MNDO wave functions to compute accurate electrostatic charges. Journal of Computational Chemistry, 1990, 11, 909-923.	3.3	115
41	SAR and 3D-QSAR Studies on Thiadiazolidinone Derivatives:â€‰ Exploration of Structural Requirements for Glycogen Synthase Kinase 3 Inhibitors. Journal of Medicinal Chemistry, 2005, 48, 7103-7112.	6.4	114
42	Extension of MST/SCRF method to organic solvents:Ab initio and semiempirical parametrization for neutral solutes in CCl4. Journal of Computational Chemistry, 1996, 17, 806-820.	3.3	111
43	Cyclic nucleotide phosphodiesterases and their role in immunomodulatory responses: Advances in the development of specific phosphodiesterase inhibitors. Medicinal Research Reviews, 2005, 25, 229-244.	10.5	111
44	Theoretical Study of the Truncated Hemoglobin HbN:Â Exploring the Molecular Basis of the NO Detoxification Mechanism. Journal of the American Chemical Society, 2005, 127, 4433-4444.	13.7	111
45	On the potential role of the amino nitrogen atom as a hydrogen bond acceptor in macromolecules. Journal of Molecular Biology, 1998, 279, 1123-1136.	4.2	110
46	Comparative study of the molecular electrostatic potential obtained from different wavefunctions. Reliability of the semiempirical MNDO wavefunction. Journal of Computational Chemistry, 1990, 11, 416-430.	3.3	105
47	A Topological Analysis of Electron Density in Cationâ^'Ï€ Complexes. Journal of Physical Chemistry A, 1999, 103, 315-321.	2.5	103
48	Synthesis, in Vitro Pharmacology, and Molecular Modeling of Very Potent Tacrineâ^'Huperzine A Hybrids as Acetylcholinesterase Inhibitors of Potential Interest for the Treatment of Alzheimer's Disease. Journal of Medicinal Chemistry, 1999, 42, 3227-3242.	6.4	101
49	Essential Dynamics:â€‰ A Tool for Efficient Trajectory Compression and Management. Journal of Chemical Theory and Computation, 2006, 2, 251-258.	5.3	98
50	Merging Ligand-Based and Structure-Based Methods in Drug Discovery: An Overview of Combined Virtual Screening Approaches. Molecules, 2020, 25, 4723.	3.8	98
51	Novel cholinesterase inhibitors as future effective drugs for the treatment of Alzheimerâ€™s disease. Expert Opinion on Investigational Drugs, 2006, 15, 1-12.	4.1	97
52	Interactions of Hydrated Mg2+ Cation with Bases, Base Pairs, and Nucleotides. Electron Topology, Natural Bond Orbital, Electrostatic, and Vibrational Study. Journal of Physical Chemistry B, 2001, 105, 6051-6060.	2.6	95
53	Ligand-induced dynamical regulation of NO conversion in Mycobacterium tuberculosis truncated hemoglobin-N. Proteins: Structure, Function and Bioinformatics, 2006, 64, 457-464.	2.6	95
54	Development of optimized MST/SCRF methods for semiempirical calculations: The MNDO and PM3 Hamiltonians. Journal of Computational Chemistry, 1995, 16, 563-575.	3.3	94

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55	Relative Flexibility of DNA and RNA: a Molecular Dynamics Study. Journal of Molecular Biology, 2004, 343, 627-638.	4.2	94
56	Huprineâ€“Tacrine Heterodimers as Anti-Amyloidogenic Compounds of Potential Interest against Alzheimerâ€™s and Prion Diseases. Journal of Medicinal Chemistry, 2012, 55, 661-669.	6.4	90
57	Continuum solvation models: Dissecting the free energy of solvation. Physical Chemistry Chemical Physics, 2003, 5, 3827-3836.	2.8	89
58	An AM1-SCRF approach to the study of changes in molecular properties induced by solvent. The Journal of Physical Chemistry, 1993, 97, 4386-4391.	2.9	88
59	Molecular Mechanics in Biology: From Structure to Function, Taking Account of Solvation. Annual Review of Biophysics and Biomolecular Structure, 1994, 23, 847-863.	18.3	87
60	Classical molecular interaction potentials: Improved setup procedure in molecular dynamics simulations of proteins. Proteins: Structure, Function and Bioinformatics, 2001, 45, 428-437.	2.6	87
61	Synthesis, biological evaluation and molecular modelling of diversely functionalized heterocyclic derivatives as inhibitors of acetylcholinesterase/butyrylcholinesterase and modulators of Ca2+ channels and nicotinic receptors. Bioorganic and Medicinal Chemistry, 2004, 12, 2199-2218.	3.0	87
62	Electrostatic component of solvation: Comparison of SCRF continuum models. Journal of Computational Chemistry, 2003, 24, 284-297.	3.3	86
63	Protein Flexibility and Ligand Recognition: Challenges for Molecular Modeling. Current Topics in Medicinal Chemistry, 2011, 11, 192-210.	2.1	86
64	G-Quadruplexes Can Maintain Their Structure in the Gas Phase. Journal of the American Chemical Society, 2006, 128, 3608-3619.	13.7	85
65	Switching Reversibility to Irreversibility in Glycogen Synthase Kinase 3 Inhibitors: Clues for Specific Design of New Compounds. Journal of Medicinal Chemistry, 2011, 54, 4042-4056.	6.4	84
66	Polarization effects in generalized molecular interaction potential: New Hamiltonian for reactivity studies and mixed QM/MM calculations. Journal of Computational Chemistry, 1998, 19, 866-881.	3.3	83
67	Ab InitioStudy of Stacking Interactions in A- and B-DNA. Journal of Physical Chemistry B, 1997, 101, 3846-3853.	2.6	82
68	Toward accurate relative energy predictions of the bioactive conformation of drugs. Journal of Computational Chemistry, 2009, 30, 601-610.	3.3	82
69	Dimerization of Carboxylic Acids:â€‰ Reliability of Theoretical Calculations and the Effect of Solvent. Journal of Physical Chemistry B, 1998, 102, 2269-2276.	2.6	80
70	Theoretical Evaluation of Solvent Effects on the Conformational and Tautomeric Equilibria of 2-(2â€˜-Hydroxyphenyl)benzimidazole and on Its Absorption and Fluorescence Spectra. Journal of Physical Chemistry A, 1999, 103, 4525-4532.	2.5	79
71	Extension of the MST model to the IEF formalism: HF and B3LYP parametrizations. Computational and Theoretical Chemistry, 2005, 727, 29-40.	1.5	79
72	N-Benzylpiperidine derivatives of 1,2,4-thiadiazolidinone as new acetylcholinesterase inhibitors. European Journal of Medicinal Chemistry, 2000, 35, 913-922.	5.5	78

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73	Induction effects in metal cationâ€“benzene complexes. Physical Chemistry Chemical Physics, 2008, 10, 2616.	2.8	78
74	Effect of electron correlation on the electrostatic potential distribution of molecules. Journal of the American Chemical Society, 1991, 113, 5203-5211.	13.7	76
75	Salt bridge interactions: Stability of the ionic and neutral complexes in the gas phase, in solution, and in proteins. , 1998, 32, 67-79.		76
76	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
77	New tacrine-dihydropyridine hybrids that inhibit acetylcholinesterase, calcium entry, and exhibit neuroprotection properties. Bioorganic and Medicinal Chemistry, 2008, 16, 7759-7769.	3.0	75
78	Benzyl Derivatives of 2,1,3-Benzo- and Benzothieno[3,2-a]thiadiazine 2,2-Dioxides:â€‰ First Phosphodiesterase 7 Inhibitors. Journal of Medicinal Chemistry, 2000, 43, 683-689.	6.4	74
79	An optimized AM1/MST method for the MST-SCRF representation of solvated systems. Journal of Computational Chemistry, 1994, 15, 847-857.	3.3	73
80	Tautomerism of 1-Methyl Derivatives of Uracil, Thymine, and 5-Bromouracil. Is Tautomerism the Basis for the Mutagenicity of 5-Bromouridine?. Journal of Physical Chemistry B, 1998, 102, 5228-5233.	2.6	73
81	Theoretical Study of Azidoâ^'Tetrazole Isomerism:Â Effect of Solvent and Substituents and Mechanism of Isomerization. Journal of the American Chemical Society, 1998, 120, 4723-4731.	13.7	73
82	Tautomerism of Xanthine Oxidase Substrates Hypoxanthine and Allopurinol. Journal of Organic Chemistry, 1996, 61, 5964-5971.	3.2	71
83	Theoretical Study of Anion Binding to Calix[4]pyrrole:Â the Effects of Solvent, Fluorine Substitution, Cosolute, and Water Traces. Journal of the American Chemical Society, 2002, 124, 12796-12805.	13.7	71
84	Tacrine-based dual binding site acetylcholinesterase inhibitors as potential disease-modifying anti-Alzheimer drug candidates. Chemico-Biological Interactions, 2010, 187, 411-415.	4.0	71
85	Identification of Dihydrofuro[3,4-d]pyrimidine Derivatives as Novel HIV-1 Non-Nucleoside Reverse Transcriptase Inhibitors with Promising Antiviral Activities and Desirable Physicochemical Properties. Journal of Medicinal Chemistry, 2019, 62, 1484-1501.	6.4	70
86	Exploring the Size Limit of Templates for Inhibitors of the M2 Ion Channel of Influenza A Virus. Journal of Medicinal Chemistry, 2011, 54, 2646-2657.	6.4	69
87	Combined in Vitro Cell-Based/in Silico Screening of Naturally Occurring Flavonoids and Phenolic Compounds as Potential Anti-Alzheimer Drugs. Journal of Natural Products, 2017, 80, 278-289.	3.0	68
88	Dynamic undocking and the quasi-bound state as tools for drug discovery. Nature Chemistry, 2017, 9, 201-206.	13.6	68
89	Molecular Dynamics Simulations of PNAÂ·DNA and PNAÂ·RNA Duplexes in Aqueous Solution. Journal of the American Chemical Society, 2000, 122, 5997-6008.	13.7	67
90	Exploiting the Tolerant Region I of the Non-Nucleoside Reverse Transcriptase Inhibitor (NNRTI) Binding Pocket: Discovery of Potent Diarylpyrimidine-Typed HIV-1 NNRTIs against Wild-Type and E138K Mutant Virus with Significantly Improved Water Solubility and Favorable Safety Profiles. Journal of Medicinal Chemistry, 2019, 62, 2083-2098.	6.4	66

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91	Optimization of the cavity size for ab initio MST-SCRF calculations of monovalent ions. Chemical Physics, 1994, 182, 237-248.	1.9	65
92	Structure, Recognition Properties, and Flexibility of the DNAÂ·RNA Hybrid. Journal of the American Chemical Society, 2005, 127, 4910-4920.	13.7	64
93	Suitability of the PM3-derived molecular electrostatic potentials. Journal of Computational Chemistry, 1993, 14, 799-808.	3.3	62
94	A Microscopic Study of the Deoxyhemoglobin-Catalyzed Generation of Nitric Oxide from Nitrite Anion. Biochemistry, 2008, 47, 9793-9802.	2.5	62
95	The impact of monovalent ion force field model in nucleic acids simulations. Physical Chemistry Chemical Physics, 2009, 11, 10596.	2.8	62
96	Comparison of 6-31G*-based MST/SCRF and FEP evaluations of the free energies of hydration for small neutral molecules. Journal of Computational Chemistry, 1993, 14, 1498-1503.	3.3	61
97	Theoretical Methods for the Representation of Solvent. Journal of Molecular Modeling, 1996, 2, 1-15.	1.8	61
98	Electron density topological analysis of the Câ€“Hâ‹¯O anti-hydrogen bond in the fluoroformâ€“oxirane complex. Chemical Physics Letters, 1999, 310, 445-450.	2.6	61
99	Solvent effects on tautomerism equilibria in heterocycles. Theoretical Chemistry Accounts, 1997, 96, 105-113.	1.4	60
100	Assessing the Accuracy and Performance of Implicit Solvent Models for Drug Molecules: Conformational Ensemble Approaches. Journal of Physical Chemistry B, 2013, 117, 5950-5962.	2.6	60
101	Molecular Dynamics Simulations in Aqueous Solution of Triple Helices Containing d(GÂ·CÂ·C) Trios. Journal of the American Chemical Society, 1998, 120, 11226-11233.	13.7	59
102	Observation of Spontaneous Base Pair Breathing Events in the Molecular Dynamics Simulation of a Difluorotoluene-Containing DNA Oligonucleotide. Journal of the American Chemical Society, 1999, 121, 8653-8654.	13.7	59
103	Role of Pre-A Motif in Nitric Oxide Scavenging by Truncated Hemoglobin, HbN, of Mycobacterium tuberculosis. Journal of Biological Chemistry, 2009, 284, 14457-14468.	3.4	59
104	Nucleic Acid Triple Helices: Stability Effects of Nucleobase Modifications. Current Organic Chemistry, 2002, 6, 1333-1368.	1.6	59
105	Comparison of Different Three-site Interaction Potentials for Liquid Acetonitrile. Molecular Simulation, 2001, 26, 287-306.	2.0	58
106	Novel Levetiracetam Derivatives That Are Effective against the Alzheimer-like Phenotype in Mice: Synthesis, in Vitro, ex Vivo, and in Vivo Efficacy Studies. Journal of Medicinal Chemistry, 2015, 58, 6018-6032.	6.4	58
107	Non-ATP competitive glycogen synthase kinase 3Î² (GSK-3Î²) inhibitors: Study of structural requirements for thiadiazolidinone derivatives. Bioorganic and Medicinal Chemistry, 2008, 16, 495-510.	3.0	57
108	Evidence for a new binding mode to GSK-3: Allosteric regulation by the marine compound palinurin. European Journal of Medicinal Chemistry, 2013, 60, 479-489.	5.5	57

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109	Tetrahydrobenzo[h][1,6]naphthyridine-6-chlorotacrine hybrids as a new family of anti-Alzheimer agents targeting Î²-amyloid, tau, and cholinesterase pathologies. European Journal of Medicinal Chemistry, 2014, 84, 107-117.	5.5	57
110	Theoretical study of N-methylacetamide in vacuum and aqueous solution: implications for the peptide bond isomerization. Journal of Organic Chemistry, 1993, 58, 6397-6405.	3.2	56
111	Synthesis, Structural Analysis, and Biological Evaluation of Thioxoquinazoline Derivatives as Phosphodiesteraseâ€...7 Inhibitors. ChemMedChem, 2009, 4, 866-876.	3.2	56
112	Novel Huprine Derivatives with Inhibitory Activity toward Î²â€Amyloid Aggregation and Formation as Diseaseâ€Modifying Antiâ€Alzheimer Drug Candidates. ChemMedChem, 2010, 5, 1855-1870.	3.2	56
113	Role of Intramolecular Hydrogen Bonds in the Intermolecular Hydrogen Bonding of Carbohydrates. Journal of Physical Chemistry A, 1998, 102, 6690-6696.	2.5	54
114	Calibration of the Quantum/Classical Hamiltonian in Semiempirical QM/MM AM1 and PM3 Methods. Journal of Physical Chemistry A, 2000, 104, 10923-10931.	2.5	54
115	Conjugate Additions to Phenylglycinol-Derived Unsaturated Î´-Lactams. Enantioselective Synthesis of Uleine Alkaloids. Journal of Organic Chemistry, 2004, 69, 8681-8693.	3.2	53
116	Unique Tautomeric Properties of Isoguanine. Journal of the American Chemical Society, 2004, 126, 154-164.	13.7	53
117	Local Aromaticity in Natural Nucleobases and Their Size-Expanded Benzo-Fused Derivatives. Journal of Physical Chemistry A, 2006, 110, 12249-12258.	2.5	52
118	Geometrical and Electronic Structure Variability of the Sugarâ€"phosphate Backbone in Nucleic Acids. Journal of Physical Chemistry B, 2008, 112, 8188-8197.	2.6	52
119	Structural Determinants of the Multifunctional Profile of Dual Binding Site Acetylcholinesterase Inhibitors as Anti-Alzheimer Agents. Current Pharmaceutical Design, 2010, 16, 2818-2836.	1.9	51
120	Easily Accessible Polycyclic Amines that Inhibit the Wild-Type and Amantadine-Resistant Mutants of the M2 Channel of Influenza A Virus. Journal of Medicinal Chemistry, 2014, 57, 5738-5747.	6.4	51
121	Molecular interaction potential: A new tool for the theoretical study of molecular reactivity. Journal of Computational Chemistry, 1993, 14, 587-602.	3.3	50
122	New strategies to incorporate the solvent polarization in selfâ€consistent reaction field and freeâ€energy perturbation simulations. Journal of Chemical Physics, 1995, 103, 10183-10191.	3.0	49
123	Inhibitors of glycogen synthase kinase-3: future therapy for unmet medical needs?. Expert Opinion on Therapeutic Patents, 2002, 12, 1527-1536.	5.0	49
124	Theoretical Studies on the Inhibition Mechanism of Cyclooxygenase-2. Is There a Unique Recognition Site?. Journal of Medicinal Chemistry, 2003, 46, 1372-1382.	6.4	49
125	Dispersion and repulsion contributions to the solvation free energy: Comparison of quantum mechanical and classical approaches in the polarizable continuum model. Journal of Computational Chemistry, 2006, 27, 1769-1780.	3.3	49
126	Thienylhalomethylketones: Irreversible glycogen synthase kinase 3 inhibitors as useful pharmacological tools. Bioorganic and Medicinal Chemistry, 2009, 17, 6914-6925.	3.0	49

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127	Role of Heme Distortion on Oxygen Affinity in Heme Proteins: The Protoglobin Case. Journal of Physical Chemistry B, 2010, 114, 8536-8543.	2.6	49
128	A new strategy for the representation of environment effects in semi-empirical calculations based on Dewar's Hamiltonians. Chemical Physics Letters, 1992, 196, 27-36.	2.6	47
129	Structural determinants of ligand migration in Mycobacterium tuberculosis truncated hemoglobin O. Proteins: Structure, Function and Bioinformatics, 2008, 73, 372-379.	2.6	47
130	Reliability of the AM1 wavefunction to compute molecular electrostatic potentials. Chemical Physics Letters, 1990, 168, 269-275.	2.6	46
131	Ligand-induced changes in the binding sites of proteins. Bioinformatics, 2002, 18, 939-948.	4.1	46
132	Design and synthesis of N-benzylpiperidineâ€“purine derivatives as new dual inhibitors of acetyl- and butyrylcholinesterase. Bioorganic and Medicinal Chemistry, 2005, 13, 6795-6802.	3.0	46
133	Dynamical Regulation of Ligand Migration by a Gate-Opening Molecular Switch in Truncated Hemoglobin-N fromMycobacterium tuberculosis. Journal of the American Chemical Society, 2007, 129, 6782-6788.	13.7	46
134	Synthesis, in Vitro Pharmacology, and Molecular Modeling ofsyn-Huprines as Acetylcholinesterase Inhibitors. Journal of Medicinal Chemistry, 2001, 44, 4733-4736.	6.4	45
135	Exploration of Forbidden Povarov Processes as a Source of Unexpected Reactivity: A Multicomponent Mannichâ€“Ritter Transformation. Angewandte Chemie - International Edition, 2012, 51, 6874-6877.	13.8	45
136	MST Continuum Study of the Hydration Free Energies of Monovalent Ionic Species. Journal of Physical Chemistry B, 2005, 109, 3565-3574.	2.6	44
137	A practical procedure for the determination of electrostatic charges of large molecules. Journal of Computer-Aided Molecular Design, 1990, 4, 411-426.	2.9	43
138	Comparison of NDDO and quasi-ab initio approaches to compute semiempirical molecular electrostatic potentials. Journal of Computational Chemistry, 1994, 15, 12-22.	3.3	43
139	Theoretical Study of the Tautomerism and Protonation of 7-Aminopyrazolopyrimidine in the Gas Phase and in Aqueous Solution. Journal of the American Chemical Society, 1995, 117, 1378-1386.	13.7	43
140	Role of tautomerism of 2-azaadenine and 2-azahypoxanthine in substrate recognition by xanthine oxidase. Journal of Computer-Aided Molecular Design, 1997, 11, 153-162.	2.9	43
141	High pressure reveals structural determinants for globin hexacoordination: Neuroglobin and myoglobin cases. Proteins: Structure, Function and Bioinformatics, 2009, 75, 885-894.	2.6	43
142	The graphite deposit at Borrowdale (UK): A catastrophic mineralizing event associated with Ordovician magmatism. Geochimica Et Cosmochimica Acta, 2010, 74, 2429-2449.	3.9	43
143	Are the Hydrogen Bonds of RNA (Aâ‹…U) Stronger Than those of DNA (Aâ‹…T)? A Quantum Mechanics Study. Chemistry - A European Journal, 2005, 11, 5062-5066.	3.3	42
144	The polarization contribution to the free energy of hydration. Journal of Chemical Physics, 1995, 102, 6145-6152.	3.0	41

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145	Tautomerism of Neutral and Protonated 6-Thioguanine in the Gas Phase and in Aqueous Solution. An ab Initio Study. Journal of Organic Chemistry, 1995, 60, 969-976.	3.2	41
146	Theoretical Study of a New DNA Structure:â€‰ The Antiparallel Hoogsteen Duplex. Journal of the American Chemical Society, 2003, 125, 14603-14612.	13.7	41
147	Derivation of Distributed Models of Atomic Polarizability for Molecular Simulations. Journal of Chemical Theory and Computation, 2007, 3, 1901-1913.	5.3	41
148	Design, synthesis and multitarget biological profiling of second-generation anti-Alzheimer rheinâ€“huprine hybrids. Future Medicinal Chemistry, 2017, 9, 965-981.	2.3	40
149	Molecular Solvation Potential. A New Tool for the Quantum Mechanical Description of Hydration in Organic and Bioorganic Molecules. The Journal of Physical Chemistry, 1995, 99, 3084-3092.	2.9	39
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