

F Javier Luque

List of Publications by Year in descending order

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19,297
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9756

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427
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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". <i>Theoretical Chemistry Accounts</i> , 2000, 103, 343-345.	0.5	712
2	Theoretical Methods for the Description of the Solvent Effect in Biomolecular Systems. <i>Chemical Reviews</i> , 2000, 100, 4187-4226.	23.0	571
3	First Non-ATP Competitive Glycogen Synthase Kinase 3 β (GSK-3 β) Inhibitors: β -Thiadiazolidinones (TDZD) as Potential Drugs for the Treatment of Alzheimer's Disease. <i>Journal of Medicinal Chemistry</i> , 2002, 45, 1292-1299.	2.9	421
4	Tautomerism and Protonation of Guanine and Cytosine. Implications in the Formation of Hydrogen-Bonded Complexes. <i>Journal of the American Chemical Society</i> , 1996, 118, 6811-6821.	6.6	318
5	MDpocket: open-source cavity detection and characterization on molecular dynamics trajectories. <i>Bioinformatics</i> , 2011, 27, 3276-3285.	1.8	265
6	Is polarization important in cation- π interactions?. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 1998, 95, 5976-5980.	3.3	259
7	Toward Improved Description of DNA Backbone: Revisiting Epsilon and Zeta Torsion Force Field Parameters. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2339-2354.	2.3	255
8	Dynamics of B-DNA on the Microsecond Time Scale. <i>Journal of the American Chemical Society</i> , 2007, 129, 14739-14745.	6.6	250
9	Hydrogen Bond versus Anti-Hydrogen Bond: A Comparative Analysis Based on the Electron Density Topology. <i>Journal of Physical Chemistry A</i> , 1999, 103, 6394-6401.	1.1	223
10	Nature of Base Stacking: Reference Quantum-Chemical Stacking Energies in Ten Unique B-DNA Base-Pair Steps. <i>Chemistry - A European Journal</i> , 2006, 12, 2854-2865.	1.7	211
11	Design, Synthesis, and Biological Evaluation of Dual Binding Site Acetylcholinesterase Inhibitors: New Disease-Modifying Agents for Alzheimer's Disease. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 7223-7233.	2.9	203
12	Binding Site Detection and Druggability Index from First Principles. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 2363-2371.	2.9	201
13	Synthesis, Biological Evaluation, and Molecular Modeling of Donepezil and <i>N</i> -[(5-(Benzyloxy)-1-methyl-1 <i>H</i> -indol-2-yl)methyl]- <i>N</i> -methylprop-2-yn-1-amine Hybrids as New Multipotent Cholinesterase/Monoamine Oxidase Inhibitors for the Treatment of Alzheimer's Disease. <i>Journal of Medicinal Chemistry</i> , 2011, 54, 8251-8270.	2.9	198
14	Frontiers in Molecular Dynamics Simulations of DNA. <i>Accounts of Chemical Research</i> , 2012, 45, 196-205.	7.6	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. <i>Physical Chemistry Chemical Physics</i> , 2002, 4, 4192-4203.	1.3	187
16	Targeting Beta-Amyloid Pathogenesis Through Acetylcholinesterase Inhibitors. <i>Current Pharmaceutical Design</i> , 2006, 12, 4377-4387.	0.9	187
17	Novel Donepezil-Based Inhibitors of Acetyl- and Butyrylcholinesterase and Acetylcholinesterase-Induced β -Amyloid Aggregation. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 3588-3598.	2.9	186
18	New Tacrine-Huperzine A Hybrids (Huperzines): Highly Potent Tight-Binding Acetylcholinesterase Inhibitors of Interest for the Treatment of Alzheimer's Disease. <i>Journal of Medicinal Chemistry</i> , 2000, 43, 4657-4666.	2.9	185

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19	Shielded Hydrogen Bonds as Structural Determinants of Binding Kinetics: Application in Drug Design. <i>Journal of the American Chemical Society</i> , 2011, 133, 18903-18910.	6.6	178
20	SCRF calculation of the effect of water on the topology of the molecular electrostatic potential. <i>The Journal of Physical Chemistry</i> , 1993, 97, 9380-9384.	2.9	172
21	On the Performance of Continuum Solvation Methods. A Comment on "Universal Approaches to Solvation Modeling". <i>Accounts of Chemical Research</i> , 2009, 42, 489-492.	7.6	171
22	Pyrano[3,2- <i>c</i>]quinoline-6-Chlorotacrine Hybrids as a Novel Family of Acetylcholinesterase- and β -Amyloid-Directed Anti-Alzheimer Compounds. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 5365-5379.	2.9	164
23	Theoretical methods for the simulation of nucleic acids. <i>Chemical Society Reviews</i> , 2003, 32, 350-364.	18.7	150
24	Towards a molecular dynamics consensus view of B-DNA flexibility. <i>Nucleic Acids Research</i> , 2008, 36, 2379-2394.	6.5	147
25	Donepezil-tacrine hybrid related derivatives as new dual binding site inhibitors of AChE. <i>Bioorganic and Medicinal Chemistry</i> , 2005, 13, 6588-6597.	1.4	145
26	Optimization of solute cavities and van der Waals parameters in ab initio MST-SCRF calculations of neutral molecules. <i>Journal of Computational Chemistry</i> , 1994, 15, 446-454.	1.5	135
27	Synthesis of Enantiopure trans-3,4-Disubstituted Piperidines. An Enantiodivergent Synthesis of (+)- and (β)-Paroxetine. <i>Journal of Organic Chemistry</i> , 2000, 65, 3074-3084.	1.7	135
28	Tacripyrines, the First Tacrine-Dihydropyridine Hybrids, as Multitarget-Directed Ligands for the Treatment of Alzheimer's Disease. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 2724-2732.	2.9	134
29	Peripheral and Dual Binding Site Acetylcholinesterase Inhibitors: Implications in treatment of Alzheimer's Disease. <i>Mini-Reviews in Medicinal Chemistry</i> , 2001, 1, 267-272.	1.1	134
30	Synthesis and Multitarget Biological Profiling of a Novel Family of Rhein Derivatives As Disease-Modifying Anti-Alzheimer Agents. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 2549-2567.	2.9	132
31	3D Structure of <i>Torpedo californica</i> Acetylcholinesterase Complexed with Huprine X at 2.1 Å... Resolution: Kinetic and Molecular Dynamic Correlates. <i>Biochemistry</i> , 2002, 41, 2970-2981.	1.2	126
32	C-H...O Contacts in the Adenine-Uracil Watson-Crick and Uracil-Uracil Nucleic Acid Base Pairs: Nonempirical ab Initio Study with Inclusion of Electron Correlation Effects. <i>Journal of Physical Chemistry B</i> , 2000, 104, 6286-6292.	1.2	125
33	Glycogen Synthase Kinase-3 (GSK-3) Inhibitory Activity and Structure-Activity Relationship (SAR) Studies of the Manzamine Alkaloids. Potential for Alzheimer's Disease. <i>Journal of Natural Products</i> , 2007, 70, 1397-1405.	1.5	123
34	The Structure and Dynamics of DNA in the Gas Phase. <i>Journal of the American Chemical Society</i> , 2003, 125, 8007-8014.	6.6	121
35	Solvation in octanol: parametrization of the continuum MST model. <i>Journal of Computational Chemistry</i> , 2001, 22, 1180-1193.	1.5	120
36	Theoretical Study of Alkyl- π and Aryl- π Interactions. Reconciling Theory and Experiment. <i>Journal of Organic Chemistry</i> , 2002, 67, 7057-7065.	1.7	119

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37	The relative flexibility of B-DNA and A-RNA duplexes: database analysis. <i>Nucleic Acids Research</i> , 2004, 32, 6144-6151.	6.5	119
38	Induced dipole moment and atomic charges based on average electrostatic potentials in aqueous solution. <i>Journal of Chemical Physics</i> , 1993, 98, 2975-2982.	1.2	118
39	Solvent Effects in Chloroform Solution: Parametrization of the MST/SCRF Continuum Model. <i>The Journal of Physical Chemistry</i> , 1996, 100, 4269-4276.	2.9	116
40	On the use of AM1 and MNDO wave functions to compute accurate electrostatic charges. <i>Journal of Computational Chemistry</i> , 1990, 11, 909-923.	1.5	115
41	SAR and 3D-QSAR Studies on Thiadiazolidinone Derivatives: Exploration of Structural Requirements for Glycogen Synthase Kinase 3 Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 7103-7112.	2.9	114
42	Extension of MST/SCRF method to organic solvents: Ab initio and semiempirical parametrization for neutral solutes in CCl ₄ . <i>Journal of Computational Chemistry</i> , 1996, 17, 806-820.	1.5	111
43	Cyclic nucleotide phosphodiesterases and their role in immunomodulatory responses: Advances in the development of specific phosphodiesterase inhibitors. <i>Medicinal Research Reviews</i> , 2005, 25, 229-244.	5.0	111
44	Theoretical Study of the Truncated Hemoglobin HbN: Exploring the Molecular Basis of the NO Detoxification Mechanism. <i>Journal of the American Chemical Society</i> , 2005, 127, 4433-4444.	6.6	111
45	On the potential role of the amino nitrogen atom as a hydrogen bond acceptor in macromolecules. <i>Journal of Molecular Biology</i> , 1998, 279, 1123-1136.	2.0	110
46	Comparative study of the molecular electrostatic potential obtained from different wavefunctions. Reliability of the semiempirical MNDO wavefunction. <i>Journal of Computational Chemistry</i> , 1990, 11, 416-430.	1.5	105
47	A Topological Analysis of Electron Density in Cation-π Complexes. <i>Journal of Physical Chemistry A</i> , 1999, 103, 315-321.	1.1	103
48	Synthesis, in Vitro Pharmacology, and Molecular Modeling of Very Potent Tacrine-Huperzine A Hybrids as Acetylcholinesterase Inhibitors of Potential Interest for the Treatment of Alzheimer's Disease. <i>Journal of Medicinal Chemistry</i> , 1999, 42, 3227-3242.	2.9	101
49	Essential Dynamics: A Tool for Efficient Trajectory Compression and Management. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 251-258.	2.3	98
50	Merging Ligand-Based and Structure-Based Methods in Drug Discovery: An Overview of Combined Virtual Screening Approaches. <i>Molecules</i> , 2020, 25, 4723.	1.7	98
51	Novel cholinesterase inhibitors as future effective drugs for the treatment of Alzheimer's disease. <i>Expert Opinion on Investigational Drugs</i> , 2006, 15, 1-12.	1.9	97
52	Interactions of Hydrated Mg ²⁺ Cation with Bases, Base Pairs, and Nucleotides. <i>Electron Topology, Natural Bond Orbital, Electrostatic, and Vibrational Study. Journal of Physical Chemistry B</i> , 2001, 105, 6051-6060.	1.2	95
53	Ligand-induced dynamical regulation of NO conversion in Mycobacterium tuberculosis truncated hemoglobin-N. <i>Proteins: Structure, Function and Bioinformatics</i> , 2006, 64, 457-464.	1.5	95
54	Development of optimized MST/SCRF methods for semiempirical calculations: The MNDO and PM3 Hamiltonians. <i>Journal of Computational Chemistry</i> , 1995, 16, 563-575.	1.5	94

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55	Relative Flexibility of DNA and RNA: a Molecular Dynamics Study. <i>Journal of Molecular Biology</i> , 2004, 343, 627-638.	2.0	94
56	Huprineâ€“Tacrine Heterodimers as Anti-Amyloidogenic Compounds of Potential Interest against Alzheimerâ€™s and Prion Diseases. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 661-669.	2.9	90
57	Continuum solvation models: Dissecting the free energy of solvation. <i>Physical Chemistry Chemical Physics</i> , 2003, 5, 3827-3836.	1.3	89
58	An AM1-SCRF approach to the study of changes in molecular properties induced by solvent. <i>The Journal of Physical Chemistry</i> , 1993, 97, 4386-4391.	2.9	88
59	Molecular Mechanics in Biology: From Structure to Function, Taking Account of Solvation. <i>Annual Review of Biophysics and Biomolecular Structure</i> , 1994, 23, 847-863.	18.3	87
60	Classical molecular interaction potentials: Improved setup procedure in molecular dynamics simulations of proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2001, 45, 428-437.	1.5	87
61	Synthesis, biological evaluation and molecular modelling of diversely functionalized heterocyclic derivatives as inhibitors of acetylcholinesterase/butrylcholinesterase and modulators of Ca ²⁺ channels and nicotinic receptors. <i>Bioorganic and Medicinal Chemistry</i> , 2004, 12, 2199-2218.	1.4	87
62	Electrostatic component of solvation: Comparison of SCRF continuum models. <i>Journal of Computational Chemistry</i> , 2003, 24, 284-297.	1.5	86
63	Protein Flexibility and Ligand Recognition: Challenges for Molecular Modeling. <i>Current Topics in Medicinal Chemistry</i> , 2011, 11, 192-210.	1.0	86
64	G-Quadruplexes Can Maintain Their Structure in the Gas Phase. <i>Journal of the American Chemical Society</i> , 2006, 128, 3608-3619.	6.6	85
65	Switching Reversibility to Irreversibility in Glycogen Synthase Kinase 3 Inhibitors: Clues for Specific Design of New Compounds. <i>Journal of Medicinal Chemistry</i> , 2011, 54, 4042-4056.	2.9	84
66	Polarization effects in generalized molecular interaction potential: New Hamiltonian for reactivity studies and mixed QM/MM calculations. <i>Journal of Computational Chemistry</i> , 1998, 19, 866-881.	1.5	83
67	Ab Initio Study of Stacking Interactions in A- and B-DNA. <i>Journal of Physical Chemistry B</i> , 1997, 101, 3846-3853.	1.2	82
68	Toward accurate relative energy predictions of the bioactive conformation of drugs. <i>Journal of Computational Chemistry</i> , 2009, 30, 601-610.	1.5	82
69	Dimerization of Carboxylic Acids:â€” Reliability of Theoretical Calculations and the Effect of Solvent. <i>Journal of Physical Chemistry B</i> , 1998, 102, 2269-2276.	1.2	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. <i>Journal of Physical Chemistry A</i> , 1999, 103, 4525-4532.	1.1	79
71	Extension of the MST model to the IEF formalism: HF and B3LYP parametrizations. <i>Computational and Theoretical Chemistry</i> , 2005, 727, 29-40.	1.5	79
72	N-Benzylpiperidine derivatives of 1,2,4-thiadiazolidinone as new acetylcholinesterase inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2000, 35, 913-922.	2.6	78

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73	Induction effects in metal cation-benzene complexes. <i>Physical Chemistry Chemical Physics</i> , 2008, 10, 2616.	1.3	78
74	Effect of electron correlation on the electrostatic potential distribution of molecules. <i>Journal of the American Chemical Society</i> , 1991, 113, 5203-5211.	6.6	76
75	Salt bridge interactions: Stability of the ionic and neutral complexes in the gas phase, in solution, and in proteins. <i>J. Phys. Chem. B</i> , 1998, 32, 67-79.		76
76	5-Imino-1,2,4-Thiadiazoles: First Small Molecules As Substrate Competitive Inhibitors of Glycogen Synthase Kinase 3. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 1645-1661.	2.9	76
77	New tacrine-dihydropyridine hybrids that inhibit acetylcholinesterase, calcium entry, and exhibit neuroprotection properties. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 7759-7769.	1.4	75
78	Benzyl Derivatives of 2,1,3-Benzo- and Benzothieno[3,2-a]thiadiazine 2,2-Dioxides: First Phosphodiesterase 7 Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2000, 43, 683-689.	2.9	74
79	An optimized AM1/MST method for the MST-SCRF representation of solvated systems. <i>Journal of Computational Chemistry</i> , 1994, 15, 847-857.	1.5	73
80	Tautomerism of 1-Methyl Derivatives of Uracil, Thymine, and 5-Bromouracil. Is Tautomerism the Basis for the Mutagenicity of 5-Bromouridine?. <i>Journal of Physical Chemistry B</i> , 1998, 102, 5228-5233.	1.2	73
81	Theoretical Study of Azido-Tetrazole Isomerism: Effect of Solvent and Substituents and Mechanism of Isomerization. <i>Journal of the American Chemical Society</i> , 1998, 120, 4723-4731.	6.6	73
82	Tautomerism of Xanthine Oxidase Substrates Hypoxanthine and Allopurinol. <i>Journal of Organic Chemistry</i> , 1996, 61, 5964-5971.	1.7	71
83	Theoretical Study of Anion Binding to Calix[4]pyrrole: The Effects of Solvent, Fluorine Substitution, Cosolute, and Water Traces. <i>Journal of the American Chemical Society</i> , 2002, 124, 12796-12805.	6.6	71
84	Tacrine-based dual binding site acetylcholinesterase inhibitors as potential disease-modifying anti-Alzheimer drug candidates. <i>Chemico-Biological Interactions</i> , 2010, 187, 411-415.	1.7	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. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 1484-1501.	2.9	70
86	Exploring the Size Limit of Templates for Inhibitors of the M2 Ion Channel of Influenza A Virus. <i>Journal of Medicinal Chemistry</i> , 2011, 54, 2646-2657.	2.9	69
87	Combined in Vitro Cell-Based/in Silico Screening of Naturally Occurring Flavonoids and Phenolic Compounds as Potential Anti-Alzheimer Drugs. <i>Journal of Natural Products</i> , 2017, 80, 278-289.	1.5	68
88	Dynamic undocking and the quasi-bound state as tools for drug discovery. <i>Nature Chemistry</i> , 2017, 9, 201-206.	6.6	68
89	Molecular Dynamics Simulations of PNA-DNA and PNA-RNA Duplexes in Aqueous Solution. <i>Journal of the American Chemical Society</i> , 2000, 122, 5997-6008.	6.6	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. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 2083-2098.	2.9	66

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91	Optimization of the cavity size for ab initio MST-SCRF calculations of monovalent ions. <i>Chemical Physics</i> , 1994, 182, 237-248.	0.9	65
92	Structure, Recognition Properties, and Flexibility of the DNA-RNA Hybrid. <i>Journal of the American Chemical Society</i> , 2005, 127, 4910-4920.	6.6	64
93	Suitability of the PM3-derived molecular electrostatic potentials. <i>Journal of Computational Chemistry</i> , 1993, 14, 799-808.	1.5	62
94	A Microscopic Study of the Deoxyhemoglobin-Catalyzed Generation of Nitric Oxide from Nitrite Anion. <i>Biochemistry</i> , 2008, 47, 9793-9802.	1.2	62
95	The impact of monovalent ion force field model in nucleic acids simulations. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 10596.	1.3	62
96	Comparison of 6-31G*-based MST/SCRF and FEP evaluations of the free energies of hydration for small neutral molecules. <i>Journal of Computational Chemistry</i> , 1993, 14, 1498-1503.	1.5	61
97	Theoretical Methods for the Representation of Solvent. <i>Journal of Molecular Modeling</i> , 1996, 2, 1-15.	0.8	61
98	Electron density topological analysis of the C-H...O anti-hydrogen bond in the fluoroform-oxirane complex. <i>Chemical Physics Letters</i> , 1999, 310, 445-450.	1.2	61
99	Solvent effects on tautomerism equilibria in heterocycles. <i>Theoretical Chemistry Accounts</i> , 1997, 96, 105-113.	0.5	60
100	Assessing the Accuracy and Performance of Implicit Solvent Models for Drug Molecules: Conformational Ensemble Approaches. <i>Journal of Physical Chemistry B</i> , 2013, 117, 5950-5962.	1.2	60
101	Molecular Dynamics Simulations in Aqueous Solution of Triple Helices Containing d(G-C-C) Trios. <i>Journal of the American Chemical Society</i> , 1998, 120, 11226-11233.	6.6	59
102	Observation of Spontaneous Base Pair Breathing Events in the Molecular Dynamics Simulation of a Difluorotoluene-Containing DNA Oligonucleotide. <i>Journal of the American Chemical Society</i> , 1999, 121, 8653-8654.	6.6	59
103	Role of Pre-A Motif in Nitric Oxide Scavenging by Truncated Hemoglobin, HbN, of <i>Mycobacterium tuberculosis</i> . <i>Journal of Biological Chemistry</i> , 2009, 284, 14457-14468.	1.6	59
104	Nucleic Acid Triple Helices: Stability Effects of Nucleobase Modifications. <i>Current Organic Chemistry</i> , 2002, 6, 1333-1368.	0.9	59
105	Comparison of Different Three-site Interaction Potentials for Liquid Acetonitrile. <i>Molecular Simulation</i> , 2001, 26, 287-306.	0.9	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. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 6018-6032.	2.9	58
107	Non-ATP competitive glycogen synthase kinase 3 β (GSK-3 β) inhibitors: Study of structural requirements for thiadiazolidinone derivatives. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 495-510.	1.4	57
108	Evidence for a new binding mode to GSK-3: Allosteric regulation by the marine compound palinurin. <i>European Journal of Medicinal Chemistry</i> , 2013, 60, 479-489.	2.6	57

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109	Tetrahydrobenzo[h][1,6]naphthyridine-6-chlorotacrine hybrids as a new family of anti-Alzheimer agents targeting β -amyloid, tau, and cholinesterase pathologies. <i>European Journal of Medicinal Chemistry</i> , 2014, 84, 107-117.	2.6	57
110	Theoretical study of N-methylacetamide in vacuum and aqueous solution: implications for the peptide bond isomerization. <i>Journal of Organic Chemistry</i> , 1993, 58, 6397-6405.	1.7	56
111	Synthesis, Structural Analysis, and Biological Evaluation of Thioxoquinazoline Derivatives as Phosphodiesterase-7 Inhibitors. <i>ChemMedChem</i> , 2009, 4, 866-876.	1.6	56
112	Novel Huprine Derivatives with Inhibitory Activity toward β -Amyloid Aggregation and Formation as Disease-Modifying Anti-Alzheimer Drug Candidates. <i>ChemMedChem</i> , 2010, 5, 1855-1870.	1.6	56
113	Role of Intramolecular Hydrogen Bonds in the Intermolecular Hydrogen Bonding of Carbohydrates. <i>Journal of Physical Chemistry A</i> , 1998, 102, 6690-6696.	1.1	54
114	Calibration of the Quantum/Classical Hamiltonian in Semiempirical QM/MM AM1 and PM3 Methods. <i>Journal of Physical Chemistry A</i> , 2000, 104, 10923-10931.	1.1	54
115	Conjugate Additions to Phenylglycinol-Derived Unsaturated β -Lactams. Enantioselective Synthesis of Uleine Alkaloids. <i>Journal of Organic Chemistry</i> , 2004, 69, 8681-8693.	1.7	53
116	Unique Tautomeric Properties of Isoguanine. <i>Journal of the American Chemical Society</i> , 2004, 126, 154-164.	6.6	53
117	Local Aromaticity in Natural Nucleobases and Their Size-Expanded Benzo-Fused Derivatives. <i>Journal of Physical Chemistry A</i> , 2006, 110, 12249-12258.	1.1	52
118	Geometrical and Electronic Structure Variability of the Sugar-phosphate Backbone in Nucleic Acids. <i>Journal of Physical Chemistry B</i> , 2008, 112, 8188-8197.	1.2	52
119	Structural Determinants of the Multifunctional Profile of Dual Binding Site Acetylcholinesterase Inhibitors as Anti-Alzheimer Agents. <i>Current Pharmaceutical Design</i> , 2010, 16, 2818-2836.	0.9	51
120	Easily Accessible Polycyclic Amines that Inhibit the Wild-Type and Amantadine-Resistant Mutants of the M2 Channel of Influenza A Virus. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 5738-5747.	2.9	51
121	Molecular interaction potential: A new tool for the theoretical study of molecular reactivity. <i>Journal of Computational Chemistry</i> , 1993, 14, 587-602.	1.5	50
122	New strategies to incorporate the solvent polarization in self-consistent reaction field and free-energy perturbation simulations. <i>Journal of Chemical Physics</i> , 1995, 103, 10183-10191.	1.2	49
123	Inhibitors of glycogen synthase kinase-3: future therapy for unmet medical needs?. <i>Expert Opinion on Therapeutic Patents</i> , 2002, 12, 1527-1536.	2.4	49
124	Theoretical Studies on the Inhibition Mechanism of Cyclooxygenase-2. Is There a Unique Recognition Site?. <i>Journal of Medicinal Chemistry</i> , 2003, 46, 1372-1382.	2.9	49
125	Dispersion and repulsion contributions to the solvation free energy: Comparison of quantum mechanical and classical approaches in the polarizable continuum model. <i>Journal of Computational Chemistry</i> , 2006, 27, 1769-1780.	1.5	49
126	Thienylhalomethylketones: Irreversible glycogen synthase kinase 3 inhibitors as useful pharmacological tools. <i>Bioorganic and Medicinal Chemistry</i> , 2009, 17, 6914-6925.	1.4	49

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127	Role of Heme Distortion on Oxygen Affinity in Heme Proteins: The Protoglobin Case. <i>Journal of Physical Chemistry B</i> , 2010, 114, 8536-8543.	1.2	49
128	A new strategy for the representation of environment effects in semi-empirical calculations based on Dewar's Hamiltonians. <i>Chemical Physics Letters</i> , 1992, 196, 27-36.	1.2	47
129	Structural determinants of ligand migration in <i>Mycobacterium tuberculosis</i> truncated hemoglobin O. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 73, 372-379.	1.5	47
130	Reliability of the AM1 wavefunction to compute molecular electrostatic potentials. <i>Chemical Physics Letters</i> , 1990, 168, 269-275.	1.2	46
131	Ligand-induced changes in the binding sites of proteins. <i>Bioinformatics</i> , 2002, 18, 939-948.	1.8	46
132	Design and synthesis of N-benzylpiperidine-purine derivatives as new dual inhibitors of acetyl- and butyrylcholinesterase. <i>Bioorganic and Medicinal Chemistry</i> , 2005, 13, 6795-6802.	1.4	46
133	Dynamical Regulation of Ligand Migration by a Gate-Opening Molecular Switch in Truncated Hemoglobin-N from <i>Mycobacterium tuberculosis</i> . <i>Journal of the American Chemical Society</i> , 2007, 129, 6782-6788.	6.6	46
134	Synthesis, in Vitro Pharmacology, and Molecular Modeling of syn-Huprines as Acetylcholinesterase Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2001, 44, 4733-4736.	2.9	45
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