F Javier Luque

List of Publications by Year
in descending order

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407 papers	19,297 citations	9756 73 h-index	20307 116 g-index
427 all docs	427 docs citations	427 times ranked	15870 citing authors

#	Article	IF	Citations
1	Novel indolic AMPK modulators induce vasodilatation through activation of the AMPKâ€“eNOSâ€“NO pathway. Scientific Reports, 2022, 12, 4225.	1.6	2
2	Searching for effective antiviral small molecules against influenza A virus: A patent review. Expert Opinion on Therapeutic Patents, 2021, 31, 53-66.	2.4	11
3	HIVâ€1 Envelope Spike MPER: From a Vaccine Target to a New Druggable Pocket for Novel and Effective Fusion Inhibitors. ChemMedChem, 2021, 16, 105-107.	1.6	5
4	Azobioisosteres of Curcumin with Pronounced Activity against Amyloid Aggregation, Intracellular Oxidative Stress, and Neuroinflammation. Chemistry - A European Journal, 2021, 27, 6015-6027.	1.7	4
5	Evaluation of the Interactions between Human Serum Albumin (HSA) and Non-Steroidal Anti-Inflammatory (NSAIDs) Drugs by Multiwavelength Molecular Fluorescence, Structural and Computational Analysis. Pharmaceuticals, 2021, 14, 214.	1.7	18
6	New Trimethoprim-Like Molecules: Bacteriological Evaluation and Insights into Their Action. Antibiotics, 2021, 10, 709.	1.5	5
7	Prediction of n-octanol/water partition coefficients and acidity constants (pKa) in the SAMPL7 blind challenge with the IEFPCM-MST model. Journal of Computer-Aided Molecular Design, 2021, 35, 803-811.	1.3	10
8	Predicting the Relative Binding Affinity for Reversible Covalent Inhibitors by Free Energy Perturbation Calculations. Journal of Chemical Information and Modeling, 2021, 61, 4733-4744.	2.5	9
9	Structure-Based Design and Discovery of Pyridyl-Bearing Fused Bicyclic HIV-1 Inhibitors: Synthesis, Biological Characterization, and Molecular Modeling Studies. Journal of Medicinal Chemistry, 2021, 64, 13604-13621.	2.9	10
10	Holistic approach to anti-knock agents: A high-throughput screening of aniline-like compounds. Fuel, 2021, 305, 121518.	3.4	8
11	From virtual screening hits targeting a cryptic pocket in BACE-1 to a nontoxic brain permeable multitarget anti-Alzheimer lead with disease-modifying and cognition-enhancing effects. European Journal of Medicinal Chemistry, 2021, 225, 113779.	2.6	7
12	Structural basis of the selective activation of enzyme isoforms: Allosteric response to activators of Î²1- and Î²2-containing AMPK complexes. Computational and Structural Biotechnology Journal, 2021, 19, 3394-3406.	1.9	10
13	Elucidating the Activation Mechanism of AMPK by Direct Pan-Activator PF-739. Frontiers in Molecular Biosciences, 2021, 8, 760026.	1.6	1
14	From Acid Activation Mechanisms of Proton Conduction to Design of Inhibitors of the M2 Proton Channel of Influenza A Virus. Frontiers in Molecular Biosciences, 2021, 8, 796229.	1.6	6
15	Breakthroughs in Medicinal Chemistry: New Targets and Mechanisms, New Drugs, New Hopesâ€“6. Molecules, 2020, 25, 119.	1.7	8
16	Interplay between Ionization and Tautomerism in Bioactive Î²-Enamino Ester-Containing Cyclic Compounds: Study of Annulated 1,2,3,6-Tetrahydroazocine Derivatives. Journal of Physical Chemistry B, 2020, 124, 28-37.	1.2	3
17	Prediction of the n-octanol/water partition coefficients in the SAMPL6 blind challenge from MST continuum solvation calculations. Journal of Computer-Aided Molecular Design, 2020, 34, 443-451.	1.3	11
18	Centrally Active Multitarget Anti-Alzheimer Agents Derived from the Antioxidant Lead CR-6. Journal of Medicinal Chemistry, 2020, 63, 9360-9390.	2.9	25

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19	Merging Ligand-Based and Structure-Based Methods in Drug Discovery: An Overview of Combined Virtual Screening Approaches. Molecules, 2020, 25, 4723.	1.7	98
20	Structural and functional properties of Antarctic fish cytoglobins-1: Cold-reactivity in multi-ligand reactions. Computational and Structural Biotechnology Journal, 2020, 18, 2132-2144.	1.9	10
21	Assessing the Performance of Mixed Strategies To Combine Lipophilic Molecular Similarity and Docking in Virtual Screening. Journal of Chemical Information and Modeling, 2020, 60, 4231-4245.	2.5	6
22	Bicyclic Î±-Iminophosphonates as High Affinity Imidazoline I₂ Receptor Ligands for Alzheimerâ€™s Disease. Journal of Medicinal Chemistry, 2020, 63, 3610-3633.	2.9	17
23	N-benzyl 4,4-disubstituted piperidines as a potent class of influenza H1N1 virus inhibitors showing a novel mechanism of hemagglutinin fusion peptide interaction. European Journal of Medicinal Chemistry, 2020, 194, 112223.	2.6	11
24	Dioxygen Binding and Sensing Proteins. Antioxidants and Redox Signaling, 2020, 32, 1151-1154.	2.5	1
25	On the Binding of Congo Red to Amyloid Fibrils. Angewandte Chemie - International Edition, 2020, 59, 8104-8107.	7.2	36
26	Insights into the Effect of the Membrane Environment on the Three-dimensional Structure-function Relationship of Antimicrobial Peptides. Biophysical Journal, 2020, 118, 236a.	0.2	1
27	On the Binding of Congo Red to Amyloid Fibrils. Angewandte Chemie, 2020, 132, 8181-8184.	1.6	11
28	Breakthroughs in Medicinal Chemistry: New Targets and Mechanisms, New Drugs, New Hopesâ€“5. Molecules, 2019, 24, 2415.	1.7	5
29	Ligand Binding Rate Constants in Heme Proteins Using Markov State Models and Molecular Dynamics Simulations. ChemPhysChem, 2019, 20, 2451-2460.	1.0	1
30	Synthesis, In Vitro Profiling, and In Vivo Efficacy Studies of a New Family of Multitarget Anti-Alzheimer Compounds. Proceedings (mdpi), 2019, 22, .	0.2	0
31	Modulating Ligand Dissociation through Methyl Isomerism in Accessory Sites: Binding of Retinol to Cellular Carriers. Journal of Physical Chemistry Letters, 2019, 10, 7333-7339.	2.1	5
32	Understanding the Mechanism of Direct Activation of AMP-Kinase: Towards a Fine Allosteric Tuning of the Kinase Activity. Proceedings (mdpi), 2019, 22, .	0.2	0
33	Searching for Selective Scaffolds against Plasmodium falciparum Glucose-6-Phosphate Dehydrogenase 6-Phosphogluconolactonase. Proceedings (mdpi), 2019, 22, .	0.2	1
34	Biological Evaluation of a Mitochondrial Phosphoenolpyruvate Carboxykinase Inhibitor. Proceedings (mdpi), 2019, 22, 95.	0.2	0
35	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.	2.9	66
36	Lipophilicity in drug design: an overview of lipophilicity descriptors in 3D-QSAR studies. Future Medicinal Chemistry, 2019, 11, 1177-1193.	1.1	28

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37	Understanding the Mechanism of Direct Activation of AMP-Kinase: Toward a Fine Allosteric Tuning of the Kinase Activity. Journal of Chemical Information and Modeling, 2019, 59, 2859-2870.	2.5	10
38	Development of a Structure-Based, pH-Dependent Lipophilicity Scale of Amino Acids from Continuum Solvation Calculations. Journal of Physical Chemistry Letters, 2019, 10, 883-889.	2.1	20
39	4,4-Disubstituted N-benzylpiperidines: A Novel Class of Fusion Inhibitors of Influenza Virus H1N1 Targeting a New Binding Site in Hemagglutinin. Proceedings (mdpi), 2019, 22, .	0.2	0
40	Interaction of human hemoglobin and semi-hemoglobins with the Staphylococcus aureus hemophore IsdB: a kinetic and mechanistic insight. Scientific Reports, 2019, 9, 18629.	1.6	21
41	Breakthroughs in Medicinal Chemistry: New Targets and Mechanisms, New Drugs, New Hopesâ€“4. Molecules, 2019, 24, 130.	1.7	4
42	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.	2.9	70
43	Thermal Stability of Globins: Implications of Flexibility and Heme Coordination Studied by Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2019, 59, 441-452.	2.5	20
44	Generation and Reactions of an Octacyclic Hindered Pyramidalized Alkene. Journal of Organic Chemistry, 2018, 83, 5420-5430.	1.7	1
45	Computational Study of the Azaâ€Michael Addition of the Flavonoid (+)â€Taxifolin in the Inhibition of Î²â€Amyloid Fibril Aggregation. Chemistry - A European Journal, 2018, 24, 5813-5824.	1.7	11
46	First homology model of Plasmodium falciparum glucose-6-phosphate dehydrogenase: Discovery of selective substrate analog-based inhibitors as novel antimalarial agents. European Journal of Medicinal Chemistry, 2018, 146, 108-122.	2.6	9
47	Aniline-Based Inhibitors of Influenza H1N1 Virus Acting on Hemagglutinin-Mediated Fusion. Journal of Medicinal Chemistry, 2018, 61, 98-118.	2.9	31
48	Frontiers in Computational Chemistry for Drug Discovery. Molecules, 2018, 23, 2872.	1.7	5
49	Multiple Multicomponent Reactions: Unexplored Substrates, Selective Processes, and Versatile Chemotypes in Biomedicine. Chemistry - A European Journal, 2018, 24, 14513-14521.	1.7	31
50	Development and Validation of Molecular Overlays Derived from Three-Dimensional Hydrophobic Similarity with PharmScreen. Journal of Chemical Information and Modeling, 2018, 58, 1596-1609.	2.5	14
51	Determination of the protonation preferences of bilin pigments in cryptophyte antenna complexes. Physical Chemistry Chemical Physics, 2018, 20, 21404-21416.	1.3	11
52	Breakthroughs in Medicinal Chemistry: New Targets and Mechanisms, New Drugs, New Hopesâ€“2. Molecules, 2018, 23, 65.	1.7	2
53	Electrostatic Tuning of the Ligand Binding Mechanism by Glu27 in Nitrophorin 7. Scientific Reports, 2018, 8, 10855.	1.6	4
54	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.	1.5	68

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55	Tuning the local solvent composition at a drug carrier surface: the effect of dimethyl sulfoxide/water mixture on the photofunctional properties of hypericinâ€“Î²-lactoglobulin complexes. Journal of Materials Chemistry B, 2017, 5, 1633-1641.	2.9	16
56	Pharmacological tools based on imidazole scaffold proved the utility of PDE10A inhibitors for Parkinsonâ€™s disease. Future Medicinal Chemistry, 2017, 9, 731-748.	1.1	11
57	Origin of the Baseâ€Dependent Facial Selectivity in Annulation Reactions of Nazarovâ€Type Reagents with Unsaturated Indolo[2,3â€a]quinolizidine Lactams. European Journal of Organic Chemistry, 2017, 2017, 3969-3979.	1.2	5
58	Novel propanamides as fatty acid amide hydrolase inhibitors. European Journal of Medicinal Chemistry, 2017, 136, 523-542.	2.6	10
59	Structural and energetic study of cationâ€“Ïâ€“cation interactions in proteins. Physical Chemistry Chemical Physics, 2017, 19, 9849-9861.	1.3	19
60	Prediction of pH-Dependent Hydrophobic Profiles of Small Molecules from Miertusâ€“Scroccoâ€“Tomasi Continuum Solvation Calculations. Journal of Physical Chemistry B, 2017, 121, 9868-9880.	1.2	16
61	Enantioselective Synthesis of Spiro[indolizidine-1,3â€²-oxindoles]. Organic Letters, 2017, 19, 4050-4053.	2.4	9
62	Design, synthesis and inÂvivo study of novel pyrrolidine-based 11Î²-HSD1 inhibitors for age-related cognitive dysfunction. European Journal of Medicinal Chemistry, 2017, 139, 412-428.	2.6	12
63	Design, synthesis and multitarget biological profiling of second-generation anti-Alzheimer rheinâ€“huprine hybrids. Future Medicinal Chemistry, 2017, 9, 965-981.	1.1	40
64	Dynamic undocking and the quasi-bound state as tools for drug discovery. Nature Chemistry, 2017, 9, 201-206.	6.6	68
65	Breakthroughs in Medicinal Chemistry: New Targets and Mechanisms, New Drugs, New Hopes. Molecules, 2017, 22, 743.	1.7	3
66	Design of Potential Antimalarial Agents Based on a Homology Model of Plasmodium falciparum Glucose-6-Phosphate Dehydrogenase. Proceedings (mdpi), 2017, 1, 665.	0.2	0
67	Unveiling a novel transient druggable pocket in BACE-1 through molecular simulations: Conformational analysis and binding mode of multisite inhibitors. PLoS ONE, 2017, 12, e0177683.	1.1	17
68	Structural Plasticity in Globins. Advances in Protein Chemistry and Structural Biology, 2016, 105, 59-80.	1.0	5
69	Insertion of Isocyanides into Nâ”Si Bonds: Multicomponent Reactions with Azines Leading to Potent Antiparasitic Compounds. Angewandte Chemie - International Edition, 2016, 55, 8994-8998.	7.2	28
70	The Nâ€terminal preâ€A region of MycobacteriumÂtuberculosis 2/2HbN promotes <scp>NO</scp>â€dioxygenase activity. FEBS Journal, 2016, 283, 305-322.	2.2	10
71	Insertion of Isocyanides into Nâ”Si Bonds: Multicomponent Reactions with Azines Leading to Potent Antiparasitic Compounds. Angewandte Chemie, 2016, 128, 9140-9144.	1.6	7
72	Design, synthesis and biological evaluation of N-methyl-N-[(1,2,3-triazol-4-yl)alkyl]propargylamines as novel monoamine oxidase B inhibitors. Bioorganic and Medicinal Chemistry, 2016, 24, 4835-4854.	1.4	23

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73	Mechanism of the Pseudoirreversible Binding of Amantadine to the M2 Proton Channel. Journal of the American Chemical Society, 2016, 138, 15345-15358.	6.6	21
74	Application of the quantum mechanical IEF/PCM-MST hydrophobic descriptors to selectivity in ligand binding. Journal of Molecular Modeling, 2016, 22, 136.	0.8	3
75	Development and validation of hydrophobic molecular fields derived from the quantum mechanical IEF/PCMâ€MST solvation models in 3Dâ€QSAR. Journal of Computational Chemistry, 2016, 37, 1147-1162.	1.5	8
76	Effect of secondary anchor amino acid substitutions on the immunogenic properties of an HLA-A*0201-restricted T cell epitope derived from the Trypanosoma cruzi KMP-11 protein. Peptides, 2016, 78, 68-76.	1.2	7
77	Transferability and additivity of dihedral parameters in polarizable and nonpolarizable empirical force fields. Journal of Computational Chemistry, 2015, 36, 1874-1884.	1.5	15
78	Stereocontrolled Annulations of Indolo[2,3â€a]quinolizidineâ€Derived Lactams with a Silylated Nazarov Reagent: Access to Allo and Epiallo Yohimbineâ€Type Derivatives. Chemistry - A European Journal, 2015, 21, 13382-13389.	1.7	7
79	Short Access to Belt Compounds with Spatially Close Cï£¾C Bonds and Their Transannular Reactions. Chemistry - A European Journal, 2015, 21, 14036-14046.	1.7	2
80	Assessing the Suitability of the Multilevel Strategy for the Conformational Analysis of Small Ligands. Journal of Physical Chemistry B, 2015, 119, 1164-1172.	1.2	16
81	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.	2.9	58
82	Combined experimental and computational investigation of the absorption spectra of E- and Z -cinnamic acids in solution: The peculiarity of Z -cinnamics. Journal of Photochemistry and Photobiology B: Biology, 2015, 148, 128-135.	1.7	17
83	New polycyclic dual inhibitors of the wild type and the V27A mutant M2 channel of the influenza A virus with unexpected binding mode. European Journal of Medicinal Chemistry, 2015, 96, 318-329.	2.6	18
84	Easy access to (2-imidazolin-4-yl)phosphonates by a microwave assisted multicomponent reaction. Tetrahedron, 2015, 71, 2872-2881.	1.0	19
85	Novel 11Î²-HSD1 inhibitors: C-1 versus C-2 substitution and effect of the introduction of an oxygen atom in the adamantane scaffold. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 4250-4253.	1.0	3
86	Searching for novel applications of the benzohomoadamantane scaffold in medicinal chemistry: Synthesis of novel 11Î²-HSD1 inhibitors. Bioorganic and Medicinal Chemistry, 2015, 23, 7607-7617.	1.4	4
87	The complex of hypericin with Î²-lactoglobulin has antimicrobial activity with potential applications in dairy industry. Journal of Dairy Science, 2015, 98, 89-94.	1.4	36
88	Engineered chimeras reveal the structural basis of hexacoordination in globins: A case study of neuroglobin and myoglobin. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 169-177.	1.1	20
89	Structure and dynamics of the membrane attaching nitric oxide transporter nitrophorin 7. F1000Research, 2015, 4, 45.	0.8	7
90	Interaction of the N-(3-Methylpyridin-2-yl)amide Derivatives of Flurbiprofen and Ibuprofen with FAAH: Enantiomeric Selectivity and Binding Mode. PLoS ONE, 2015, 10, e0142711.	1.1	12

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91	Structural Model of the hUbA1-UbcH10 Quaternary Complex: In Silico and Experimental Analysis of the Protein-Protein Interactions between E1, E2 and Ubiquitin. PLoS ONE, 2014, 9, e112082.	1.1	7
92	Mechanistic Insight into the Enzymatic Reduction of Truncated Hemoglobin N of Mycobacterium tuberculosis. Journal of Biological Chemistry, 2014, 289, 21573-21583.	1.6	15
93	TuberQ: a Mycobacterium tuberculosis protein druggability database. Database: the Journal of Biological Databases and Curation, 2014, 2014, bau035-bau035.	1.4	35
94	Exploring the structural basis of the selective inhibition of monoamine oxidase A by dicarbonitrile aminoheterocycles: Role of Asn181 and Ile335 validated by spectroscopic and computational studies. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2014, 1844, 389-397.	1.1	16
95	The DNA-forming properties of 6-selenoguanine. Physical Chemistry Chemical Physics, 2014, 16, 1101-1110.	1.3	13
96	1,2,3,4-Tetrahydrobenzo[h][1,6]naphthyridines as a new family of potent peripheral-to-midgorge-site inhibitors of acetylcholinesterase: Synthesis, pharmacological evaluation and mechanistic studies. European Journal of Medicinal Chemistry, 2014, 73, 141-152.	2.6	39
97	Polythiazole linkers as functional rigid connectors: a new RGD cyclopeptide with enhanced integrin selectivity. Chemical Science, 2014, 5, 3929.	3.7	10
98	Shogaolâ€“huprine hybrids: Dual antioxidant and anticholinesterase agents with Î²-amyloid and tau anti-aggregating properties. Bioorganic and Medicinal Chemistry, 2014, 22, 5298-5307.	1.4	37
99	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.	2.6	57
100	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.	2.9	51
101	Molecular basis of the selective binding of MDMA enantiomers to the alpha4beta2 nicotinic receptor subtype: Synthesis, pharmacological evaluation and mechanistic studies. European Journal of Medicinal Chemistry, 2014, 81, 35-46.	2.6	11
102	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.	2.9	132
103	On the transferability of fractional contributions to the hydration free energy of amino acids. Highlights in Theoretical Chemistry, 2014, , 119-132.	0.0	0
104	On the transferability of fractional contributions to the hydration free energy of amino acids. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	2
105	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.	2.6	57
106	Toward Improved Description of DNA Backbone: Revisiting Epsilon and Zeta Torsion Force Field Parameters. Journal of Chemical Theory and Computation, 2013, 9, 2339-2354.	2.3	255
107	Evolution of a Multicomponent System: Computational and Mechanistic Studies on the Chemoâ€•and Stereoselectivity of a Divergent Process. Chemistry - A European Journal, 2013, 19, 13355-13361.	1.7	15
108	Dynamical Treatment of Charge Transfer through Duplex Nucleic Acids Containing Modified Adenines. ACS Nano, 2013, 7, 9396-9406.	7.3	8

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109	Kinetics and computational studies of ligand migration in nitrophorin 7 and its Î”1â€“3 mutant. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2013, 1834, 1711-1721.	1.1	10
110	Wild daffodils of the section Ganymedes from the Iberian Peninsula as a source of mesembrane alkaloids. Phytochemistry, 2013, 95, 384-393.	1.4	12
111	Ligand migration through hemeprotein cavities: insights from laser flash photolysis and molecular dynamics simulations. Physical Chemistry Chemical Physics, 2013, 15, 10686.	1.3	18
112	First diastereoselective [3 + 2] cycloaddition reaction of diethyl isocyanomethylphosphonate and maleimides. Organic and Biomolecular Chemistry, 2013, 11, 1640.	1.5	16
113	Comparative analysis of inner cavities and ligand migration in non-symbiotic AHb1 and AHb2. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2013, 1834, 1957-1967.	1.1	6
114	Assessing the Accuracy and Performance of Implicit Solvent Models for Drug Molecules: Conformational Ensemble Approaches. Journal of Physical Chemistry B, 2013, 117, 5950-5962.	1.2	60
115	CO Rebinding Kinetics and Molecular Dynamics Simulations Highlight Dynamic Regulation of Internal Cavities in Human Cytoglobin. PLoS ONE, 2013, 8, e49770.	1.1	28
116	Chapter 4. Molecular Dynamics: a Tool to Understand Nuclear Receptors. RSC Drug Discovery Series, 2012, , 60-83.	0.2	1
117	A Novel Approach for Deriving Force Field Torsion Angle Parameters Accounting for Conformation-Dependent Solvation Effects. Journal of Chemical Theory and Computation, 2012, 8, 3232-3242.	2.3	27
118	Frontiers in Molecular Dynamics Simulations of DNA. Accounts of Chemical Research, 2012, 45, 196-205.	7.6	194
119	Recognition of Ligands by Macromolecular Targets. RSC Drug Discovery Series, 2012, , 1-22.	0.2	1
120	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.	2.9	76
121	Huprineâ€“Tacrine Heterodimers as Anti-Amyloidogenic Compounds of Potential Interest against Alzheimerâ€™s and Prion Diseases. Journal of Medicinal Chemistry, 2012, 55, 661-669.	2.9	90
122	A Multilevel Strategy for the Exploration of the Conformational Flexibility of Small Molecules. Journal of Chemical Theory and Computation, 2012, 8, 1808-1819.	2.3	35
123	Role of PheE15 Gate in Ligand Entry and Nitric Oxide Detoxification Function of Mycobacterium tuberculosis Truncated Hemoglobin N. PLoS ONE, 2012, 7, e49291.	1.1	26
124	Binding Free Energy Calculation and Scoring in Small-Molecule Docking. RSC Drug Discovery Series, 2012, , 195-222.	0.2	5
125	Exploration of Forbidden Povarov Processes as a Source of Unexpected Reactivity: A Multicomponent Mannichâ€“Ritter Transformation. Angewandte Chemie - International Edition, 2012, 51, 6874-6877.	7.2	45
126	Molecular simulation methods in drug discovery: a prospective outlook. Journal of Computer-Aided Molecular Design, 2012, 26, 81-86.	1.3	17

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127	First asymmetric cascade reaction catalysed by chiral primary aminoalcohols. Organic and Biomolecular Chemistry, 2011, 9, 5079.	1.5	17
128	Ligand Migration in Methanosarcina acetivorans Protoglobin: Effects of Ligand Binding and Dimeric Assembly. Journal of Physical Chemistry B, 2011, 115, 13771-13780.	1.2	31
129	Histidine E7 Dynamics Modulates Ligand Exchange between Distal Pocket and Solvent in AHb1 from Arabidopsis thaliana. Journal of Physical Chemistry B, 2011, 115, 4138-4146.	1.2	20
130	Role of the Distal Hydrogen-Bonding Network in Regulating Oxygen Affinity in the Truncated Hemoglobin III fromCampylobacter jejuni. Biochemistry, 2011, 50, 3946-3956.	1.2	23
131	Structural, Dynamical, and Electronic Transport Properties of Modified DNA Duplexes Containing Size-Expanded Nucleobases. Journal of Physical Chemistry A, 2011, 115, 11344-11354.	1.1	16
132	Shielded Hydrogen Bonds as Structural Determinants of Binding Kinetics: Application in Drug Design. Journal of the American Chemical Society, 2011, 133, 18903-18910.	6.6	178
133	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.	2.9	198
134	Structural analysis in nonsymbiotic hemoglobins: What can we learn from inner cavities?. Plant Science, 2011, 181, 8-13.	1.7	14
135	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.	2.9	69
136	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.	2.9	84
137	Polarization effects in molecular interactions. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 844-854.	6.2	28
138	Oxygen binding to Arabidopsis thaliana AHb2 nonsymbiotic hemoglobin: evidence for a role in oxygen transport. IUBMB Life, 2011, 63, 355-362.	1.5	19
139	Enhanced reactivity of Lys182 explains the limited efficacy of biogenic amines in preventing the inactivation of glucose-6-phosphate dehydrogenase by methylglyoxal. Bioorganic and Medicinal Chemistry, 2011, 19, 1613-1622.	1.4	6
140	Protein dynamics: Experimental and computational approaches. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2011, 1814, 913-915.	1.1	1
141	Protein Flexibility and Ligand Recognition: Challenges for Molecular Modeling. Current Topics in Medicinal Chemistry, 2011, 11, 192-210.	1.0	86
142	MDpocket: open-source cavity detection and characterization on molecular dynamics trajectories. Bioinformatics, 2011, 27, 3276-3285.	1.8	265
143	Reactivity versus steric effects in fluorinated ketones as esterase inhibitors: a quantum mechanical and molecular dynamics study. Journal of Molecular Modeling, 2010, 16, 1753-1764.	0.8	9
144	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.	1.3	24

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145	Molecular modeling of class I and II alleles of the major histocompatibility complex in Salmo salar. Journal of Computer-Aided Molecular Design, 2010, 24, 1035-1051.	1.3	12
146	Tacrine-based dual binding site acetylcholinesterase inhibitors as potential disease-modifying anti-Alzheimer drug candidates. Chemico-Biological Interactions, 2010, 187, 411-415.	1.7	71
147	Novel Huprine Derivatives with Inhibitory Activity toward Î²â€Amyloid Aggregation and Formation as Diseaseâ€Modifying Antiâ€Alzheimer Drug Candidates. ChemMedChem, 2010, 5, 1855-1870.	1.6	56
148	Boronâ€Based Dipolar Multicomponent Reactions: Simple Generation of Substituted Aziridines, Oxazolidines and Pyrrolidines. Chemistry - A European Journal, 2010, 16, 7904-7915.	1.7	27
149	Unraveling the molecular basis for ligand binding in truncated hemoglobins: The trHbO Bacillus subtilis case. Proteins: Structure, Function and Bioinformatics, 2010, 78, 962-970.	1.5	36
150	Structural Determinants of the Multifunctional Profile of Dual Binding Site Acetylcholinesterase Inhibitors as Anti-Alzheimer Agents. Current Pharmaceutical Design, 2010, 16, 2818-2836.	0.9	51
151	Role of Heme Distortion on Oxygen Affinity in Heme Proteins: The Protoglobin Case. Journal of Physical Chemistry B, 2010, 114, 8536-8543.	1.2	49
152	The graphite deposit at Borrowdale (UK): A catastrophic mineralizing event associated with Ordovician magmatism. Geochimica Et Cosmochimica Acta, 2010, 74, 2429-2449.	1.6	43
153	Role of Pre-A Motif in Nitric Oxide Scavenging by Truncated Hemoglobin, HbN, of Mycobacterium tuberculosis. Journal of Biological Chemistry, 2009, 284, 14457-14468.	1.6	59
154	Exploring the Nitric Oxide Detoxification Mechanism of Mycobacterium tuberculosis Truncated Haemoglobin N. NATO Science for Peace and Security Series A: Chemistry and Biology, 2009, , 33-47.	0.5	6
155	Synthesis, Structural Analysis, and Biological Evaluation of Thioxoquinazoline Derivatives as Phosphodiesteraseâ€...7 Inhibitors. ChemMedChem, 2009, 4, 866-876.	1.6	56
156	Toward accurate relative energy predictions of the bioactive conformation of drugs. Journal of Computational Chemistry, 2009, 30, 601-610.	1.5	82
157	Solvation enthalpies of neutral solutes in water and octanol. Theoretical Chemistry Accounts, 2009, 123, 11-20.	0.5	7
158	High pressure reveals structural determinants for globin hexacoordination: Neuroglobin and myoglobin cases. Proteins: Structure, Function and Bioinformatics, 2009, 75, 885-894.	1.5	43
159	Thienylhalomethylketones: Irreversible glycogen synthase kinase 3 inhibitors as useful pharmacological tools. Bioorganic and Medicinal Chemistry, 2009, 17, 6914-6925.	1.4	49
160	On the Performance of Continuum Solvation Methods. A Comment on â€œUniversal Approaches to Solvation Modelingâ€. Accounts of Chemical Research, 2009, 42, 489-492.	7.6	171
161	Polarizable Intermolecular Potentials for Water and Benzene Interacting with Halide and Metal Ions. Journal of Chemical Theory and Computation, 2009, 5, 3022-3031.	2.3	34
162	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.	1.2	17

#	Article	IF	Citations
163	Ab initio Study of the Structural, Tautomeric, Pairing, and Electronic Properties of Seleno-Derivatives of Thymine. Journal of Physical Chemistry B, 2009, 113, 14465-14472.	1.2	15
164	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.	2.9	164
165	Binding Site Detection and Druggability Index from First Principles. Journal of Medicinal Chemistry, 2009, 52, 2363-2371.	2.9	201
166	Structural Plasticity and Functional Implications of Internal Cavities in Distal Mutants of Type 1 Non-Symbiotic Hemoglobin AHb1 fromArabidopsis thaliana. Journal of Physical Chemistry B, 2009, 113, 16028-16038.	1.2	20
167	The first enantioselective synthesis of palinurin. Chemical Communications, 2009, , 3252.	2.2	24
168	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.	2.9	134
169	Unique Tautomeric and Recognition Properties of Thioketothymines?. Journal of the American Chemical Society, 2009, 131, 12845-12853.	6.6	4
170	The impact of monovalent ion force field model in nucleic acids simulations. Physical Chemistry Chemical Physics, 2009, 11, 10596.	1.3	62
171	Structural determinants of ligand migration in Mycobacterium tuberculosis truncated hemoglobin O. Proteins: Structure, Function and Bioinformatics, 2008, 73, 372-379.	1.5	47
172	Towards a Tunable Tautomeric Switch in Azobenzene Biomimetics: Implications for the Binding Affinity of 2â€(4â€²â€Hydroxyphenylazo)benzoic Acid to Streptavidin. Chemistry - A European Journal, 2008, 14, 2277-2285.	1.7	26
173	Extension of the MST continuum solvation model to the RM1 semiempirical hamiltonian. Journal of Computational Chemistry, 2008, 29, 578-587.	1.5	17
174	CODES, a novel procedure for ligand-based virtual screening: PDE7 inhibitors as an application example. European Journal of Medicinal Chemistry, 2008, 43, 1349-1359.	2.6	33
175	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.	1.4	57
176	New tacrine-dihydropyridine hybrids that inhibit acetylcholinesterase, calcium entry, and exhibit neuroprotection properties. Bioorganic and Medicinal Chemistry, 2008, 16, 7759-7769.	1.4	75
177	Towards a molecular dynamics consensus view of B-DNA flexibility. Nucleic Acids Research, 2008, 36, 2379-2394.	6.5	147
178	Nitric Oxide Reactivity with Globins as Investigated Through Computer Simulation. Methods in Enzymology, 2008, 437, 477-498.	0.4	26
179	Ab Initio Study of Naphtho-Homologated DNA Bases. Journal of Physical Chemistry B, 2008, 112, 2179-2186.	1.2	23
180	Geometrical and Electronic Structure Variability of the Sugarâ^'phosphate Backbone in Nucleic Acids. Journal of Physical Chemistry B, 2008, 112, 8188-8197.	1.2	52

#	Article	IF	Citations
181	Novel Donepezil-Based Inhibitors of Acetyl- and Butyrylcholinesterase and Acetylcholinesterase-Induced Î²-Amyloid Aggregation. Journal of Medicinal Chemistry, 2008, 51, 3588-3598.	2.9	186
182	Induction effects in metal cationâ€“benzene complexes. Physical Chemistry Chemical Physics, 2008, 10, 2616.	1.3	78
183	A Microscopic Study of the Deoxyhemoglobin-Catalyzed Generation of Nitric Oxide from Nitrite Anion. Biochemistry, 2008, 47, 9793-9802.	1.2	62
184	Mechanism of Product Release in NO Detoxification from Mycobacterium tuberculosis Truncated Hemoglobin N. Journal of the American Chemical Society, 2008, 130, 1688-1693.	6.6	35
185	Structure-Directed Reversion in the Ï€-Facial Stereoselective Alkylation of Chiral Bicyclic Lactams. Journal of Organic Chemistry, 2008, 73, 7756-7763.	1.7	13
186	Theoretical Analysis of Antisense Duplexes:â€‰ Determinants of the RNase H Susceptibility. Journal of the American Chemical Society, 2008, 130, 3486-3496.	6.6	30
187	An ab initio strategy for handling induction phenomena in metal ion complexes. Molecular Physics, 2008, 106, 1685-1696.	0.8	3
188	Thermochemical Analysis of the Hydration of Neutral Solutes. Challenges and Advances in Computational Chemistry and Physics, 2008, , 103-113.	0.6	0
189	Dynamics of B-DNA on the Microsecond Time Scale. Journal of the American Chemical Society, 2007, 129, 14739-14745.	6.6	250
190	Derivation of Distributed Models of Atomic Polarizability for Molecular Simulations. Journal of Chemical Theory and Computation, 2007, 3, 1901-1913.	2.3	41
191	Modeling Induction Phenomena in Intermolecular Interactions with an Ab Initio Force Field. Journal of Chemical Theory and Computation, 2007, 3, 1914-1926.	2.3	34
192	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.	6.6	46
193	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.	1.5	123
194	Exploring the Dynamics of Calix[4]pyrrole: Effect of Solvent and Fluorine Substitution. Chemistry - A European Journal, 2007, 13, 1108-1116.	1.7	37
195	The Tautomerism of 5â€Aminoâ€3â€oxoâ€1,2,4â€thiadiazole: An Experimental and Theoretical Study. European Journal of Organic Chemistry, 2007, 2007, 5603-5608.	1.2	2
196	A hydrophobic similarity analysis of solvation effects on nucleic acid bases. Journal of Molecular Modeling, 2007, 13, 357-365.	0.8	8
197	Novel cholinesterase inhibitors as future effective drugs for the treatment of Alzheimerâ€™s disease. Expert Opinion on Investigational Drugs, 2006, 15, 1-12.	1.9	97
198	Essential Dynamics:â€‰ A Tool for Efficient Trajectory Compression and Management. Journal of Chemical Theory and Computation, 2006, 2, 251-258.	2.3	98

#	Article	IF	Citations
199	Local Aromaticity in Natural Nucleobases and Their Size-Expanded Benzo-Fused Derivatives. Journal of Physical Chemistry A, 2006, 110, 12249-12258.	1.1	52
200	Theoretical Study of the Hoogsteenâ€“Watson-Crick Junctions in DNA. Biophysical Journal, 2006, 90, 1000-1008.	0.2	17
201	Data Mining of Molecular Dynamics Trajectories of Nucleic Acids. Journal of Biomolecular Structure and Dynamics, 2006, 23, 447-455.	2.0	12
202	G-Quadruplexes Can Maintain Their Structure in the Gas Phase. Journal of the American Chemical Society, 2006, 128, 3608-3619.	6.6	85
203	Benzoderivatives of Nucleic Acid Bases as Modified DNA Building Blocksâ€. Journal of Physical Chemistry A, 2006, 110, 510-518.	1.1	21
204	On the Origin of the Stereoselectivity in the Alkylation of Oxazolopiperidone Enolates. Journal of the American Chemical Society, 2006, 128, 6581-6588.	6.6	17
205	Binding of 13-Amidohuprines to Acetylcholinesterase:Â Exploring the Ligand-Induced Conformational Change of the Gly117-Gly118 Peptide Bond in the Oxyanion Hole. Journal of Medicinal Chemistry, 2006, 49, 6833-6840.	2.9	19
206	Aromaticity-induced changes in electronic properties of size-expanded DNA bases: Case of xC. International Journal of Quantum Chemistry, 2006, 106, 2339-2346.	1.0	17
207	Ligand-induced dynamical regulation of NO conversion in Mycobacterium tuberculosis truncated hemoglobin-N. Proteins: Structure, Function and Bioinformatics, 2006, 64, 457-464.	1.5	95
208	A fast method for the determination of fractional contributions to solvation in proteins. Protein Science, 2006, 15, 2525-2533.	3.1	3
209	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.	1.7	211
210	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.	1.5	49
211	Targeting Beta-Amyloid Pathogenesis Through Acetylcholinesterase Inhibitors. Current Pharmaceutical Design, 2006, 12, 4377-4387.	0.9	187
212	Design and synthesis of N-benzylpiperidineâ€“purine derivatives as new dual inhibitors of acetyl- and butyrylcholinesterase. Bioorganic and Medicinal Chemistry, 2005, 13, 6795-6802.	1.4	46
213	Donepezilâ€“tacrine hybrid related derivatives as new dual binding site inhibitors of AChE. Bioorganic and Medicinal Chemistry, 2005, 13, 6588-6597.	1.4	145
214	Extension of the MST model to the IEF formalism: HF and B3LYP parametrizations. Computational and Theoretical Chemistry, 2005, 727, 29-40.	1.5	79
215	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.	2.9	114
216	Synthesis and Biological Evaluation of Tacrine-Thiadiazolidinone Hybrids as Dual Acetylcholinesterase Inhibitors. Archiv Der Pharmazie, 2005, 338, 18-23.	2.1	17

#	Article	IF	Citations
217	Cyclic nucleotide phosphodiesterases and their role in immunomodulatory responses: Advances in the development of specific phosphodiesterase inhibitors. Medicinal Research Reviews, 2005, 25, 229-244.	5.0	111
218	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.	1.7	42
219	Electrostatic exchange-correlation charge density in Be and Ne: quantal density functional theoretic analysis. Theoretical Chemistry Accounts, 2005, 114, 124-128.	0.5	1
220	Hydrophobic Molecular Similarity from MST Fractional Contributions to the Octanol/water Partition Coefficient. Journal of Computer-Aided Molecular Design, 2005, 19, 401-419.	1.3	9
221	First-order correlation-kinetic contribution to Kohn-Sham exchange charge density function in atoms, using quantal density functional theory approach. International Journal of Quantum Chemistry, 2005, 101, 231-238.	1.0	4
222	Role of stacking interactions in the binding sequence preferences of DNA bis-intercalators: insight from thermodynamic integration free energy simulations. Nucleic Acids Research, 2005, 33, 6214-6224.	6.5	34
223	Marine compounds for the therapeutic treatment of neurological disorders. Expert Opinion on Therapeutic Patents, 2005, 15, 1377-1386.	2.4	30
224	Structure, Recognition Properties, and Flexibility of the DNAÂ·RNA Hybrid. Journal of the American Chemical Society, 2005, 127, 4910-4920.	6.6	64
225	Nature of Minor-Groove Bindersâ”DNA Complexes in the Gas Phase. Journal of the American Chemical Society, 2005, 127, 11690-11698.	6.6	35
226	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.	6.6	111
227	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.	2.9	203
228	MST Continuum Study of the Hydration Free Energies of Monovalent Ionic Species. Journal of Physical Chemistry B, 2005, 109, 3565-3574.	1.2	44
229	Group contributions to the solvation free energy from MST continuum calculations. Brazilian Journal of Physics, 2004, 34, 48-57.	0.7	7
230	The relative flexibility of B-DNA and A-RNA duplexes: database analysis. Nucleic Acids Research, 2004, 32, 6144-6151.	6.5	119
231	Tautomeric conjugate acids of 2-aminopyrroles: effect of substituents, solvation and cosolute. Theoretical Chemistry Accounts, 2004, 111, 223-230.	0.5	3
232	Linear response theory: An alternative to PB and GB methods for the analysis of molecular dynamics trajectories?. Proteins: Structure, Function and Bioinformatics, 2004, 57, 458-467.	1.5	8
233	Partition of protein solvation into group contributions from molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2004, 58, 101-109.	1.5	8
234	Theoretical Methods for the Simulation of Nucleic Acids. ChemInform, 2004, 35, no.	0.1	0

#	Article	IF	Citations
235	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.	1.4	87
236	MST study of group contributions for alkane derivatives: effect of the charge normalization. Chemical Physics Letters, 2004, 384, 299-305.	1.2	6
237	Conjugate Additions to Phenylglycinol-Derived Unsaturated Î´-Lactams. Enantioselective Synthesis of Uleine Alkaloids. Journal of Organic Chemistry, 2004, 69, 8681-8693.	1.7	53
238	Modulation of Binding Strength in Several Classes of Active Site Inhibitors of Acetylcholinesterase Studied by Comparative Binding Energy Analysis. Journal of Medicinal Chemistry, 2004, 47, 4471-4482.	2.9	19
239	Relative Flexibility of DNA and RNA: a Molecular Dynamics Study. Journal of Molecular Biology, 2004, 343, 627-638.	2.0	94
240	Unique Tautomeric Properties of Isoguanine. Journal of the American Chemical Society, 2004, 126, 154-164.	6.6	53
241	Solute-Solvent Interactions from QM SCRF Methods. , 2004, , 475-495.		2
242	Molecular Modelling Approaches to the Design of Acetylcholinesterase Inhibitors: New Challenges for the Treatment of Alzheimers Disease. Current Pharmaceutical Design, 2004, 10, 3131-3140.	0.9	29
243	Electrostatic component of solvation: Comparison of SCRF continuum models. Journal of Computational Chemistry, 2003, 24, 284-297.	1.5	86
244	Transferability of fragmental contributions to the octanol/water partition coefficient: An NDDO-based MST study. Journal of Computational Chemistry, 2003, 24, 32-45.	1.5	11
245	Energy decomposition in molecular complexes: Implications for the treatment of polarization in molecular simulations. Journal of Computational Chemistry, 2003, 24, 1263-1275.	1.5	14
246	Continuum and discrete calculation of fractional contributions to solvation free energy. Journal of Computational Chemistry, 2003, 24, 1610-1623.	1.5	8
247	Molecular Dynamics Study of [2]Rotaxanes: Influence of Solvation and Cation on Co-conformation.. ChemInform, 2003, 34, no.	0.1	0
248	Theoretical Studies on the Inhibition Mechanism of Cyclooxygenase-2. Is There a Unique Recognition Site?. Journal of Medicinal Chemistry, 2003, 46, 1372-1382.	2.9	49
249	Continuum solvation models: Dissecting the free energy of solvation. Physical Chemistry Chemical Physics, 2003, 5, 3827-3836.	1.3	89
250	Perturbation Approach to Combined QM/MM Simulation of Soluteâ^'Solvent Interactions in Solution. Journal of Physical Chemistry B, 2003, 107, 1664-1671.	1.2	30
251	Molecular Dynamics Study of [2]Rotaxanes:Â Influence of Solvation and Cation on Co-conformation. Journal of Organic Chemistry, 2003, 68, 4663-4673.	1.7	24
252	Theoretical Study of a New DNA Structure:â€‰ The Antiparallel Hoogsteen Duplex. Journal of the American Chemical Society, 2003, 125, 14603-14612.	6.6	41

#	Article	IF	Citations
253	The Structure and Dynamics of DNA in the Gas Phase. Journal of the American Chemical Society, 2003, 125, 8007-8014.	6.6	121
254	Theoretical methods for the simulation of nucleic acids. Chemical Society Reviews, 2003, 32, 350-364.	18.7	150
255	Peripheral and dual binding site inhibitors of acetylcholinesterase as neurodegenerative disease modifying agents. Expert Opinion on Therapeutic Patents, 2003, 13, 1725-1732.	2.4	15
256	Prediction of Conformational Free Energy Differences of Solutes in Solutionâ¯ An MC-MST Study. Molecular Simulation, 2002, 28, 153-171.	0.9	5
257	Can Divalent Metal Cations Stabilize the Triplex Motif? Theoretical Study of the Interaction of the Hydrated Mg2+ Cation with the Gâ¯GÂ·C Triplet. Journal of Physical Chemistry B, 2002, 106, 8849-8857.	1.2	20
258	Rational Design of Reversible Acetylcholinesterase Inhibitors. Mini-Reviews in Medicinal Chemistry, 2002, 2, 27-36.	1.1	22
259	Ligand-induced changes in the binding sites of proteins. Bioinformatics, 2002, 18, 939-948.	1.8	46
260	Hoogsteen-Based Parallel-Stranded Duplexes of DNA. Effect of 8-Amino-purine Derivatives. Journal of the American Chemical Society, 2002, 124, 3133-3142.	6.6	38
261	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.	2.9	421
262	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.	6.6	71
263	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.	1.2	126
264	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.	1.3	187
265	Theoretical Study of Alkyl-Ï€ and Aryl-Ï€ Interactions. Reconciling Theory and Experiment. Journal of Organic Chemistry, 2002, 67, 7057-7065.	1.7	119
266	Inhibitors of glycogen synthase kinase-3: future therapy for unmet medical needs?. Expert Opinion on Therapeutic Patents, 2002, 12, 1527-1536.	2.4	49
267	Crystallographic, NMR and ab initio calculation studies of tautomerism among substituted dihydrothiazol-2-ylhydrazones. Perkin Transactions II RSC, 2002, , 1012-1016.	1.1	2
268	Hydrophobic similarity between molecules: A MST-based hydrophobic similarity index. Journal of Computational Chemistry, 2002, 23, 554-563.	1.5	18
269	Aminoimidazo[1,2-a]pyridines: regioselective synthesis of substituted imidazonaphthyridines, azacarbolines and cyclazines. Tetrahedron, 2002, 58, 295-307.	1.0	22
270	Fast estimation of hydrogen-bonding donor and acceptor propensities: a GMIPp study. Journal of Computer-Aided Molecular Design, 2002, 16, 569-583.	1.3	3

#	Article	IF	Citations
271	Nucleic Acid Triple Helices: Stability Effects of Nucleobase Modifications. Current Organic Chemistry, 2002, 6, 1333-1368.	0.9	59
272	3D structures of Acetylcholinesterase complexes with potential drugs for the treatment of Alzheimer's disease. Acta Crystallographica Section A: Foundations and Advances, 2002, 58, c138-c138.	0.3	0
273	Comparison of Different Three-site Interaction Potentials for Liquid Acetonitrile. Molecular Simulation, 2001, 26, 287-306.	0.9	58
274	Synthesis, in Vitro Pharmacology, and Molecular Modeling ofsyn-Huprines as Acetylcholinesterase Inhibitors. Journal of Medicinal Chemistry, 2001, 44, 4733-4736.	2.9	45
275	Theoretical Methods for the Description of the Solvent Effect in Biomolecular Systems. (Chem.) Tj ETQq1 1 0.784314 rgBT /Overlock 10	23.0	19
276	Aminoâ^'Imino Tautomerism in Derivatives of Cytosine:Â Effect on Hydrogen-Bonding and Stacking Properties. Journal of Physical Chemistry A, 2001, 105, 6575-6580.	1.1	34
277	Alternative Approaches for the Calculation of Induction Energies:Â Characterization, Effectiveness, and Pitfalls. Journal of Physical Chemistry A, 2001, 105, 11505-11514.	1.1	23
278	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.	1.2	95
279	Theoretical Studies of d(A:T)-Based Parallel-Stranded DNA Duplexes. Journal of the American Chemical Society, 2001, 123, 12018-12025.	6.6	33
280	How accurate can molecular dynamics/linear response and Poisson-Boltzmann/solvent accessible surface calculations be for predicting relative binding affinities? Acetylcholinesterase huprine inhibitors as a test case. Theoretical Chemistry Accounts, 2001, 106, 2-9.	0.5	25
281	Parallel-stranded hairpins containing 8-aminopurines. novel efficient probes for triple-helix formation. Bioorganic and Medicinal Chemistry Letters, 2001, 11, 1761-1763.	1.0	15
282	Classical molecular interaction potentials: Improved setup procedure in molecular dynamics simulations of proteins. Proteins: Structure, Function and Bioinformatics, 2001, 45, 428-437.	1.5	87
283	A theoretical investigation on the effect of remote amino groups in hydrogen bonding of nucleic acids. Biopolymers, 2001, 61, 52-60.	1.2	4
284	Solvation in octanol: parametrization of the continuum MST model. Journal of Computational Chemistry, 2001, 22, 1180-1193.	1.5	120
285	General Access to Tacamine and Vinca-Eburna Alkaloids through Tandem Non-Biomimetic Oxidation of Dihydropyridines/Zn-Mediated Radical Addition Processes â^' Unexpected Facial Selectivity of Flattened Cyclohexyl-Type Radicals. European Journal of Organic Chemistry, 2001, 2001, 3719.	1.2	31
286	The effect of amino groups on the stability of DNA duplexes and triplexes based on purines derived from inosine. Nucleic Acids Research, 2001, 29, 2522-2534.	6.5	33
287	Towards Improved Acetylcholinesterase Inhibitors: A Structural and Computational Approach. Mini-Reviews in Medicinal Chemistry, 2001, 1, 255-266.	1.1	24
288	Partitioning of Free Energies of Solvation into Fragment Contributions: Applications in Drug Design. Mathematical and Computational Chemistry, 2001, , 143-168.	0.3	8

#	Article	IF	Citations
289	Peripheral and Dual Binding Site Acetylcholinesterase Inhibitors: Implications in treatment of Alzheimers Disease. Mini-Reviews in Medicinal Chemistry, 2001, 1, 267-272.	1.1	134
290	Fast evaluation of induction energies: a second-order perturbation theory approach. Chemical Physics Letters, 2000, 332, 190-198.	1.2	10
291	N-Benzylpiperidine derivatives of 1,2,4-thiadiazolidinone as new acetylcholinesterase inhibitors. European Journal of Medicinal Chemistry, 2000, 35, 913-922.	2.6	78
292	Mixed QM/MM molecular electrostatic potentials. Journal of Computer-Aided Molecular Design, 2000, 14, 329-339.	1.3	9
293	Synthesis of Enantiopuretrans-3,4-Disubstituted Piperidines. An Enantiodivergent Synthesis of (+)- and (â^')-Paroxetine. Journal of Organic Chemistry, 2000, 65, 3074-3084.	1.7	135
294	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.	0.5	712
295	DNA-triplex stabilizing properties of 8-aminoguanine. Nucleic Acids Research, 2000, 28, 4531-4539.	6.5	36
296	Misincorporation of 2'-deoxyoxanosine into DNA: a molecular basis for NO-induced mutagenesis derived from theoretical calculations. Nucleic Acids Research, 2000, 28, 4873-4883.	6.5	15
297	Inhibition of tau phosphorylation: a new therapeutic strategy for the treatment of Alzheimerâ€™s disease and other neurodegenerative disorders. Expert Opinion on Therapeutic Patents, 2000, 10, 1519-1527.	2.4	39
298	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.	2.9	74
299	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.	2.9	185
300	Theoretical Methods for the Description of the Solvent Effect in Biomolecular Systems. Chemical Reviews, 2000, 100, 4187-4226.	23.0	571
301	Simplified descriptions of the topological distribution of hydrophilic/hydrophobic characteristics of molecules. Physical Chemistry Chemical Physics, 2000, 2, 4897-4905.	1.3	13
302	Molecular Dynamics Simulations of PNAÂ·DNA and PNAÂ·RNA Duplexes in Aqueous Solution. Journal of the American Chemical Society, 2000, 122, 5997-6008.	6.6	67
303	Molecular Dynamics Study of Oligonucleotides Containing Difluorotoluene. Journal of the American Chemical Society, 2000, 122, 6891-6899.	6.6	29
304	Calibration of the Quantum/Classical Hamiltonian in Semiempirical QM/MM AM1 and PM3 Methods. Journal of Physical Chemistry A, 2000, 104, 10923-10931.	1.1	54
305	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.	1.2	125
306	On the Use of SCRF Methods in Drug Design Studies. , 2000, , 129-134.		1

#	Article	IF	Citations
307	Can G-C Hoogsteen-wobble pairs contribute to the stability of d(G{middle dot}C-C) triplexes?. Nucleic Acids Research, 1999, 27, 2248-2255.	6.5	17
308	Nucleic Acid Bases in Solution. Theoretical and Computational Chemistry, 1999, 8, 119-166.	0.2	7
309	Cavitation contribution to the free energy of solvation.. Chemical Physics, 1999, 240, 253-264.	0.9	38
310	On the tautomerism of 2,1,3-benzothiadiazinone S,S-dioxide and related compounds. Tetrahedron, 1999, 55, 12405-12410.	1.0	12
311	Electron density topological analysis of the Câ€“Hâ‹¯O anti-hydrogen bond in the fluoroformâ€“oxirane complex. Chemical Physics Letters, 1999, 310, 445-450.	1.2	61
312	Fractional description of free energies of solvation. Journal of Computer-Aided Molecular Design, 1999, 13, 139-152.	1.3	33
313	Monte Carlo-MST: New strategy for representation of solvent configurational space in solution. Journal of Computational Chemistry, 1999, 20, 665-678.	1.5	15
314	Parametrization of the GMIPp for the study of stacking interactions. Journal of Computational Chemistry, 1999, 20, 937-946.	1.5	11
315	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.	1.1	223
316	Role of Sugar Re-Puckering in the Transition of A and B Forms of DNA in Solution. A Molecular Dynamics Study. Journal of Biomolecular Structure and Dynamics, 1999, 17, 89-99.	2.0	28
317	2-Aminopyrrole and simple 1-substituted 2-aminopyrroles: preparation and ab initio study on the effect of solvent on the aminoâ€“imino tautomeric equilibriumâ€Šâ€. Journal of the Chemical Society Perkin Transactions II, 1999, , 1433-1438.	0.9	18
318	Predicting Relative Binding Free Energies of Tacrineâˆ’Huperzine A Hybrids as Inhibitors of AcetylcholinesteraseÂ§. Journal of Medicinal Chemistry, 1999, 42, 5110-5119.	2.9	36
319	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.	1.1	79
320	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.	6.6	59
321	A Topological Analysis of Electron Density in Cationâˆ’Ï€ Complexes. Journal of Physical Chemistry A, 1999, 103, 315-321.	1.1	103
322	Dimerization of Formamide in Gas Phase and Solution. An Ab Initio MCâˆ’MST Study. Journal of Physical Chemistry A, 1999, 103, 6200-6208.	1.1	30
323	Synthesis, in Vitro Pharmacology, and Molecular Modeling of Very Potent Tacrineâˆ’Huperzine A Hybrids as Acetylcholinesterase Inhibitors of Potential Interest for the Treatment of Alzheimer's Disease. Journal of Medicinal Chemistry, 1999, 42, 3227-3242.	2.9	101
324	Interactions of Nucleic Acid Bases: The Role of Solvent. Computational Chemistry - Reviews of Current Trends, 1999, , 191-225.	0.4	2

#	Article	IF	Citations
325	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.	1.5	83
326	Salt bridge interactions: Stability of the ionic and neutral complexes in the gas phase, in solution, and in proteins. , 1998, 32, 67-79.		76
327	Triple helix stabilization properties of oligonucleotides containing 8-amino-2â€²-deoxyguanosine. Bioorganic and Medicinal Chemistry Letters, 1998, 8, 3011-3016.	1.0	11
328	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.	1.2	73
329	Azidoazomethineâ^'Tetrazole Isomerism in Solution:Â A Thermochemical Study. Journal of Organic Chemistry, 1998, 63, 2354-2356.	1.7	25
330	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.	6.6	59
331	A Priori Prediction of Substituent and Solvent Effects in the Basicity of Nitriles. Journal of Organic Chemistry, 1998, 63, 4947-4953.	1.7	27
332	Dimerization of Carboxylic Acids:â€‰ Reliability of Theoretical Calculations and the Effect of Solvent. Journal of Physical Chemistry B, 1998, 102, 2269-2276.	1.2	80
333	On the potential role of the amino nitrogen atom as a hydrogen bond acceptor in macromolecules. Journal of Molecular Biology, 1998, 279, 1123-1136.	2.0	110
334	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.	6.6	73
335	Role of Intramolecular Hydrogen Bonds in the Intermolecular Hydrogen Bonding of Carbohydrates. Journal of Physical Chemistry A, 1998, 102, 6690-6696.	1.1	54
336	Is polarization important in cation-Â interactions?. Proceedings of the National Academy of Sciences of the United States of America, 1998, 95, 5976-5980.	3.3	259
337	Response to â€œComment on â€˜New strategies to incorporate the solvent polarization in self-consistent reaction field and free-energy perturbation simulationsâ€™â€‰â€•[J. Chem. Phys. 107, 1291 (1997)]. Journal of Chemical Physics, 1997, 107, 1293-1294.	1.2	17
338	Semiclassical-Continuum Approach to the Electrostatic Free Energy of Solvation. Journal of Physical Chemistry B, 1997, 101, 5573-5582.	1.2	33
339	Ab InitioStudy of Stacking Interactions in A- and B-DNA. Journal of Physical Chemistry B, 1997, 101, 3846-3853.	1.2	82
340	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.	1.3	43
341	Solvent effects on tautomerism equilibria in heterocycles. Theoretical Chemistry Accounts, 1997, 96, 105-113.	0.5	60
342	Reliability of MEP and MEP-derived properties computed from DFT methods for molecules containing P, S and CL. Theoretical Chemistry Accounts, 1997, 98, 42-49.	0.5	25

#	Article	IF	Citations
343	Suitability of density functional methods for calculation of electrostatic properties. Journal of Computational Chemistry, 1997, 18, 980-991.	1.5	37
344	Helical preferences of alanine, glycine, and aminoisobutyric homopeptides. , 1997, 28, 83-93.		39
345	On the reaction mechanism of class Pi glutathione S-transferase. , 1997, 28, 530-542.		11
346	Generalized linear response approximation in discrete methods. Chemical Physics Letters, 1997, 265, 473-480.	1.2	20
347	Tautomerism of Xanthine Oxidase Substrates Hypoxanthine and Allopurinol. Journal of Organic Chemistry, 1996, 61, 5964-5971.	1.7	71
348	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.	6.6	318
349	Theoretical Methods for the Representation of Solvent. Journal of Molecular Modeling, 1996, 2, 1-15.	0.8	61
350	Theoretical representation of solvent effects in the study of biochemical systems. Computational and Theoretical Chemistry, 1996, 371, 269-278.	1.5	14
351	An ab initio SCRF continuum study of the Lewis acid complexation of esters. Computational and Theoretical Chemistry, 1996, 371, 123-132.	1.5	3
352	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.	1.5	111
353	Theoretical representation of solvation in biochemical systems: From discrete solute-solvent interactions to bulk solvation. International Journal of Quantum Chemistry, 1996, 60, 1179-1187.	1.0	3
354	Synthesis, chemical trapping and dimerization of tricyclo[3.3.0.03,7]oct-1(5)-ene, the consummate member of a series of pyramidalized alkenes. Tetrahedron Letters, 1996, 37, 8605-8608.	0.7	29
355	Theoretical determination of the solvation free energy in water and chloroform of the nucleic acid bases. Chemical Physics, 1996, 209, 19-29.	0.9	27
356	Tautomerism of xanthine and alloxanthine: A model for substrate recognition by xanthine oxidase. Journal of Computer-Aided Molecular Design, 1996, 10, 535-544.	1.3	29
357	Effect of Solvation on the Charge Distribution of a Series of Anionic, Neutral, and Cationic Species. A Quantum Molecular Similarity Study. The Journal of Physical Chemistry, 1996, 100, 606-610.	2.9	27
358	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
359	Molecular Dynamics Study of the Binding of Elsamicin A to DNA. FEBS Journal, 1995, 230, 555-566.	0.2	9
360	The effect of hydration on the molecular charge distribution of cations. An ab initio SCRF study. Chemical Physics Letters, 1995, 232, 509-517.	1.2	19

#	Article	IF	Citations
361	Development of optimized MST/SCRF methods for semiempirical calculations: The MNDO and PM3 Hamiltonians. Journal of Computational Chemistry, 1995, 16, 563-575.	1.5	94
362	Synthetic studies on indole alkaloids VIII. 1 Synthesis and reactivity of asymmetric 2-indolyi-4-methylenepiperidines. Tetrahedron, 1995, 51, 7527-7546.	1.0	5
363	Alkaloids from Crinum kirkii. Phytochemistry, 1995, 40, 1291-1293.	1.4	28
364	The polarization contribution to the free energy of hydration. Journal of Chemical Physics, 1995, 102, 6145-6152.	1.2	41
365	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.	1.2	49
366	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
367	Counterion Distribution around DNA Studied by Molecular Dynamics and Quantum Mechanical Simulations. The Journal of Physical Chemistry, 1995, 99, 11591-11599.	2.9	30
368	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.	6.6	43
369	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.	1.7	41
370	Effect of Solvent Polarization on Bimolecular Interactions. The Journal of Physical Chemistry, 1995, 99, 11344-11349.	2.9	8
371	Binding of Echinomycin to d(GCGC)2and d(CCGG)2: Distinct Stacking Interactions Dictate the Sequence-Dependent Formation of Hoogsteen Base Pairs. Journal of Biomolecular Structure and Dynamics, 1994, 12, 111-129.	2.0	17
372	Effect of solvation on the shapes, sizes, and anisotropies of polyatomic anions via molecular electrostatic potential topography: Anab initioselfâ€consistent reaction field approach. Journal of Chemical Physics, 1994, 100, 6718-6726.	1.2	33
373	Comparison of NDDO and quasi-ab initio approaches to compute semiempirical molecular electrostatic potentials. Journal of Computational Chemistry, 1994, 15, 12-22.	1.5	43
374	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.	1.5	135
375	An optimized AM1/MST method for the MST-SCRF representation of solvated systems. Journal of Computational Chemistry, 1994, 15, 847-857.	1.5	73
376	Optimization of the cavity size for ab initio MST-SCRF calculations of monovalent ions. Chemical Physics, 1994, 182, 237-248.	0.9	65
377	Multicentric charges for the accurate representation of electrostatic interactions in force-field calculations for small molecules. Chemical Physics, 1994, 189, 573-584.	0.9	15
378	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

#	Article	IF	Citations
379	DNA Sequence-Specific Reading by Echinomycin: Role of Hydrogen Bonding and Stacking Interactions. Journal of Medicinal Chemistry, 1994, 37, 1602-1609.	2.9	33
380	Self-consistent reaction field computation of the reactive characteristics of DNA bases in water. Biopolymers, 1993, 33, 1851-1869.	1.2	35
381	Molecular interaction potential: A new tool for the theoretical study of molecular reactivity. Journal of Computational Chemistry, 1993, 14, 587-602.	1.5	50
382	Suitability of the PM3-derived molecular electrostatic potentials. Journal of Computational Chemistry, 1993, 14, 799-808.	1.5	62
383	Ab initio study of bond stretching: Implications in force-field parametrization for molecular mechanics and dynamics. Journal of Computational Chemistry, 1993, 14, 881-894.	1.5	13
384	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.	1.5	61
385	A new scaling procedure to correct semiempirical MEP and MEP-derived properties. Journal of Computer-Aided Molecular Design, 1993, 7, 721-742.	1.3	25
386	Reactivity of planar and twisted amides in vacuum and aqueous environments: an ab initio MEP study. Journal of the Chemical Society Perkin Transactions II, 1993, , 683.	0.9	24
387	Theoretical study of N-methylacetamide in vacuum and aqueous solution: implications for the peptide bond isomerization. Journal of Organic Chemistry, 1993, 58, 6397-6405.	1.7	56
388	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
389	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
390	Induced dipole moment and atomic charges based on average electrostatic potentials in aqueous solution. Journal of Chemical Physics, 1993, 98, 2975-2982.	1.2	118
391	A practical approach to the computation of the electrostatic energy in large molecules. Computational and Theoretical Chemistry, 1992, 254, 31-42.	1.5	8
392	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.	1.2	47
393	Conformational Analysis of 2-Aryl-4-piperidones. Effect of the Indole Protective Phenylsulfonyl Group. Heterocycles, 1992, 34, 449.	0.4	3
394	Effect of electron correlation on the electrostatic potential distribution of molecules. Journal of the American Chemical Society, 1991, 113, 5203-5211.	6.6	76
395	A practical procedure for the determination of electrostatic charges of large molecules. Journal of Computer-Aided Molecular Design, 1990, 4, 411-426.	1.3	43
396	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.	1.5	105

#	Article	IF	Citations
397	On the use of AM1 and MNDO wave functions to compute accurate electrostatic charges. Journal of Computational Chemistry, 1990, 11, 909-923.	1.5	115
398	Reliability of the AM1 wavefunction to compute molecular electrostatic potentials. Chemical Physics Letters, 1990, 168, 269-275.	1.2	46
399	Ab initio study of the molecular activation mechanism of the histamine H2-receptor. Journal De Chimie Physique Et De Physico-Chimie Biologique, 1990, 87, 1569-1582.	0.2	1
400	On the use of mixed basis sets to compute accurate molecular electrostatic potentials. Chemical Physics Letters, 1989, 160, 305-310.	1.2	17
401	Structure-activity relationships of H2-receptor histamine antagonists based on quantum chemical methods. Progress in Clinical and Biological Research, 1989, 291, 373-6.	0.2	0
402	Relationships between the activity of some H2-receptor agonists of histamine and their ab initio molecular electrostatic potential (MEP) and electron density comparison coefficients. European Journal of Medicinal Chemistry, 1988, 23, 7-10.	2.6	30
403	POEMS: program for outliers elimination in multidimensional space. Bioinformatics, 1988, 4, 381-385.	1.8	2
404	TDZD's: Selective and ATP Noncompetitive Glycogen Synthase Kinase 3 Inhibitors. , 0, , 257-280.		2
405	Chemical Reactivity in the Ground and the Excited State. , 0, , 313-497.		1
406	Structure and dynamics of the membrane attaching nitric oxide transporter nitrophorin 7. F1000Research, 0, 4, 45.	0.8	13
407	Field-based virtual screening: New trends to increase the chemical diversity of your leads. , 0, , .		0