F Javier Luque

List of Publications by Year
in descending order

407 papers	19,297 citations	9775 73 h-index	20343 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
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