Yuan-Ping Pang

List of Publications by Year
in descending order

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150 papers	7,483 citations	47006 47 h-index	62596 80 g-index
170 all docs	170 docs citations	170 times ranked	7809 citing authors

#	Article	IF	Citations
1	How neocarcerand Octacid4 self-assembles with guests into irreversible noncovalent complexes and what accelerates the assembly. Communications Chemistry, 2022, 5, .	4.5	0
2	TREM2 interacts with TDP-43 and mediates microglial neuroprotection against TDP-43-related neurodegeneration. Nature Neuroscience, 2022, 25, 26-38.	14.8	52
3	How the water-soluble hemicarcerand incarcerates guests at room temperature decoded with modular simulations. Communications Chemistry, 2021, 4, .	4.5	1
4	Enzymatic activation of pyruvate kinase increases cytosolic oxaloacetate to inhibit the Warburg effect. Nature Metabolism, 2021, 3, 954-968.	11.9	28
5	CFAP45 deficiency causes situs abnormalities and asthenospermia by disrupting an axonemal adenine nucleotide homeostasis module. Nature Communications, 2020, 11, 5520.	12.8	36
6	Comment on â€œCysteine-Targeted Insecticides against A. gambiae Acetylcholinesterase Are Neither Selective nor Reversible Inhibitorsâ€• ACS Medicinal Chemistry Letters, 2020, 11, 1063-1064.	2.8	0
7	Characterization of an alternative BAK-binding site for BH3 peptides. Nature Communications, 2020, 11, 3301.	12.8	31
8	Remote Activation of a Latent Epitope in an Autoantigen Decoded With Simulated B-Factors. Frontiers in Immunology, 2019, 10, 2467.	4.8	7
9	Bis(propyl)-cognitin potentiates rehabilitation of treadmill exercise after a transient focal cerebral ischemia, possibly via inhibiting NMDA receptor and regulating VEGF expression. Neurochemistry International, 2019, 128, 143-153.	3.8	6
10	222.â€ƒPREFERENTIAL BINDING TO AN UNEXPECTED EPITOPE OF A CHIMERIC RECOMBINANT PROTEINASE 3 VARIANT BY ANTI-NEUTROPHIL CYTOPLASMIC ANTIBODIES. Rheumatology, 2019, 58, .	1.9	2
11	A pilot clinical trial testing topical resiquimod and a xenopeptide as immune adjuvants for a melanoma vaccine targeting MART-1. Melanoma Research, 2019, 29, 420-427.	1.2	10
12	Peptide-Binding Groove Contraction Linked to the Lack of T Cell Response: Using Complex Structure and Energy To Identify Neoantigens. ImmunoHorizons, 2018, 2, 216-225.	1.8	8
13	On the use of the experimentally determined enzyme inhibition constant as a measure of absolute binding affinity. Biochemical and Biophysical Research Communications, 2017, 489, 451-454.	2.1	15
14	How fast fast-folding proteins fold in silico. Biochemical and Biophysical Research Communications, 2017, 492, 135-139.	2.1	16
15	Use of multiple picosecond high-mass molecular dynamics simulations to predict crystallographic B-factors of folded globular proteins. Heliyon, 2016, 2, e00161.	3.2	21
16	FF12MC: A revised AMBER forcefield and new protein simulation protocol. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1490-1516.	2.6	37
17	Cover Image, Volume 84, Issue 10. Proteins: Structure, Function and Bioinformatics, 2016, 84, C4-C4.	2.6	0
18	Prime, Shock, and Kill: Priming CD4 T Cells from HIV Patients with a BCL-2 Antagonist before HIV Reactivation Reduces HIV Reservoir Size. Journal of Virology, 2016, 90, 4032-4048.	3.4	85

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19	Physiological roles for butyrylcholinesterase: A BChE-ghrelin axis. Chemico-Biological Interactions, 2016, 259, 271-275.	4.0	75
20	Protection against Î²-amyloid-induced synaptic and memory impairments via altering Î²-amyloid assembly by bis(heptyl)-cognitin. Scientific Reports, 2015, 5, 10256.	3.3	29
21	Low-mass molecular dynamics simulation for configurational sampling enhancement: More evidence and theoretical explanation. Biochemistry and Biophysics Reports, 2015, 4, 126-133.	1.3	24
22	Dimeric bis (heptyl)â€Cognitin Blocks Alzheimer's Î²â€Amyloid Neurotoxicity Via the Inhibition of AÎ² Fibrils Formation and Disaggregation of Preformed Fibrils. CNS Neuroscience and Therapeutics, 2015, 21, 953-961.	3.9	12
23	Use of 1â€“4 interaction scaling factors to control the conformational equilibrium between Î±-helix and Î²-strand. Biochemical and Biophysical Research Communications, 2015, 457, 183-186.	2.1	22
24	Plasma butyrylcholinesterase regulates ghrelin to control aggression. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 2251-2256.	7.1	96
25	At least 10% shorter Câ€“H bonds in cryogenic protein crystal structures than in current AMBER forcefields. Biochemical and Biophysical Research Communications, 2015, 458, 352-355.	2.1	14
26	Substantial Neuroprotective and Neurite Outgrowth-Promoting Activities by Bis(propyl)-cognitin via the Activation of Alpha7-nAChR, a Promising Anti-Alzheimerâ€™s Dimer. ACS Chemical Neuroscience, 2015, 6, 1536-1545.	3.5	24
27	Modulation of Mitochondrial Complex I Activity Averts Cognitive Decline in Multiple Animal Models of Familial Alzheimer's Disease. EBioMedicine, 2015, 2, 294-305.	6.1	87
28	Robust Neuritogenesisâ€Promoting Activity by Bis(heptyl)â€Cognitin Through the Activation of alpha7â€Nicotinic Acetylcholine Receptor/ERK Pathway. CNS Neuroscience and Therapeutics, 2015, 21, 520-529.	3.9	9
29	Parkin Regulates Mitosis and Genomic Stability through Cdc20/Cdh1. Molecular Cell, 2015, 60, 21-34.	9.7	74
30	Insect Acetylcholinesterase as a Target for Effective and Environmentally Safe Insecticides. Advances in Insect Physiology, 2014, , 435-494.	2.7	21
31	Evaluation of the BH3-only Protein Puma as a Direct Bak Activator. Journal of Biological Chemistry, 2014, 289, 89-99.	3.4	65
32	Low-mass molecular dynamics simulation: A simple and generic technique to enhance configurational sampling. Biochemical and Biophysical Research Communications, 2014, 452, 588-592.	2.1	18
33	Casp8p41 generated by HIV protease kills CD4 T cells through direct Bak activation. Journal of Cell Biology, 2014, 206, 867-876.	5.2	28
34	Substantial Neuroprotection Against <scp><scp>K</scp></scp>⁺ Deprivationâ€Induced Apoptosis in Primary Cerebellar Granule Neurons by Novel Dimer Bis(propyl)â€Cognitin Via the Activation of <scp>VEGFR</scp>â€2 Signaling Pathway. CNS Neuroscience and Therapeutics, 2013, 19, 764-772.	3.9	18
35	Common Pharmacophore of Structurally Distinct Small-Molecule Inhibitors of Intracellular Retrograde Trafficking of Ribosome Inactivating Proteins. Scientific Reports, 2013, 3, 3397.	3.3	10
36	Bis(propyl)-cognitin protects against glutamate-induced neuro-excitotoxicity via concurrent regulation of NO, MAPK/ERK and PI3-K/Akt/GSK3Î² pathways. Neurochemistry International, 2013, 62, 468-477.	3.8	42

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37	Regulation of error-prone translesion synthesis by Spartan/C1orf124. Nucleic Acids Research, 2013, 41, 1661-1668.	14.5	56
38	Novel Selective and Irreversible Mosquito Acetylcholinesterase Inhibitors for Controlling Malaria and Other Mosquito-Borne Diseases. Scientific Reports, 2013, 3, 1068.	3.3	29
39	Cholinergic and non-cholinergic functions of two acetylcholinesterase genes revealed by gene-silencing in Tribolium castaneum. Scientific Reports, 2012, 2, 288.	3.3	113
40	Activation of Transcription Factor MEF2D by Bis(3)-cognitin Protects Dopaminergic Neurons and Ameliorates Parkinsonian Motor Defects. Journal of Biological Chemistry, 2012, 287, 34246-34255.	3.4	38
41	Novel and Viable Acetylcholinesterase Target Site for Developing Effective and Environmentally Safe Insecticides. Current Drug Targets, 2012, 13, 471-482.	2.1	49
42	Bak Conformational Changes Induced by Ligand Binding: Insight into BH3 Domain Binding and Bak Homo-Oligomerization. Scientific Reports, 2012, 2, 257.	3.3	41
43	Chemical Structure of Retro-2, a Compound That Protects Cells against Ribosome-Inactivating Proteins. Scientific Reports, 2012, 2, 631.	3.3	30
44	Genome Organization, Phylogenies, Expression Patterns, and Three-Dimensional Protein Models of Two Acetylcholinesterase Genes from the Red Flour Beetle. PLoS ONE, 2012, 7, e32288.	2.5	36
45	Small-Molecule Inhibitor Leads of Ribosome-Inactivating Proteins Developed Using the Doorstop Approach. PLoS ONE, 2011, 6, e17883.	2.5	34
46	Transient binding of an activator BH3 domain to the Bak BH3-binding groove initiates Bak oligomerization. Journal of Cell Biology, 2011, 194, 39-48.	5.2	139
47	Crystal structures of oxime-bound fenamiphos-acetylcholinesterases: Reactivation involving flipping of the His447 ring to form a reactive Glu334â€“His447â€“oxime triad. Biochemical Pharmacology, 2010, 79, 507-515.	4.4	31
48	Kinetic analysis of interactions between alkylene-linked bis-pyridiniumaldoximes and human acetylcholinesterases inhibited by various organophosphorus compounds. Biochemical Pharmacology, 2010, 80, 941-946.	4.4	22
49	Insect-specific irreversible inhibitors of acetylcholinesterase in pests including the bed bug, the eastern yellowjacket, German and American cockroaches, and the confused flour beetle. Chemico-Biological Interactions, 2010, 187, 142-147.	4.0	15
50	Small Molecules Showing Significant Protection of Mice against Botulinum Neurotoxin Serotype A. PLoS ONE, 2010, 5, e10129.	2.5	37
51	Pathologically Activated Neuroprotection via Uncompetitive Blockade of N-Methyl-d-aspartate Receptors with Fast Off-rate by Novel Multifunctional Dimer Bis(propyl)-cognitin. Journal of Biological Chemistry, 2010, 285, 19947-19958.	3.4	32
52	One-Compound-Multi-Targets at Amyloid Î² Cascade Offered By Bis(7)-Cognitin, a Novel Anti-Alzheimerâ€™s Dimer. , 2010, , 165-183.		0
53	Selective and Irreversible Inhibitors of Aphid Acetylcholinesterases: Steps Toward Human-Safe Insecticides. PLoS ONE, 2009, 4, e4349.	2.5	38
54	Selective and Irreversible Inhibitors of Mosquito Acetylcholinesterases for Controlling Malaria and Other Mosquito-Borne Diseases. PLoS ONE, 2009, 4, e6851.	2.5	30

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55	Structure-based discovery of dengue virus protease inhibitors. Antiviral Research, 2009, 82, 110-114.	4.1	162
56	A selective smallâ€molecule inhibitor of câ€Jun Nâ€terminal kinase 1. FEBS Letters, 2009, 583, 2208-2212.	2.8	14
57	Promising multifunctional anti-Alzheimer's dimer bis(7)-Cognitin acting as an activator of protein kinase C regulates activities of Î±-secretase and BACE-1 concurrently. European Journal of Pharmacology, 2009, 623, 14-21.	3.5	24
58	Novel Anti-Alzheimer's Dimer Bis(7)-Cognitin: Cellular and Molecular Mechanisms of Neuroprotection Through Multiple Targets. Neurotherapeutics, 2009, 6, 187-201.	4.4	63
59	Mechanism of bis(7)-tacrine inhibition of GABA-activated current in cultured rat hippocampal neurons. Neuropharmacology, 2009, 57, 33-40.	4.1	5
60	Configurational Entropy in Proteinâ€“Peptide Binding:. Journal of Molecular Biology, 2009, 389, 315-335.	4.2	79
61	Structure of HI-6â€¢Sarin-Acetylcholinesterase Determined by X-Ray Crystallography and Molecular Dynamics Simulation: Reactivator Mechanism and Design. PLoS ONE, 2009, 4, e5957.	2.5	77
62	Potent New Small-Molecule Inhibitor of Botulinum Neurotoxin Serotype A Endopeptidase Developed by Synthesis-Based Computer-Aided Molecular Design. PLoS ONE, 2009, 4, e7730.	2.5	43
63	The physicochemical properties and the in vivo AChE inhibition of two potential anti-Alzheimer agents, bis(12)-hupyridone and bis(7)-tacrine. Journal of Pharmaceutical and Biomedical Analysis, 2008, 46, 75-81.	2.8	41
64	Convenient synthesis of a library of discrete hydroxamic acids using the hydroxythiophenol (Marshall) resin. Tetrahedron Letters, 2008, 49, 1103-1106.	1.4	11
65	Preclinical characterization of intestinal absorption and metabolism of promising anti-Alzheimer's dimer bis(7)-tacrine. International Journal of Pharmaceutics, 2008, 357, 85-94.	5.2	20
66	Bis(7)-tacrine, a promising anti-Alzheimer's dimer, affords dose- and time-dependent neuroprotection against transient focal cerebral ischemia. Neuroscience Letters, 2008, 439, 160-164.	2.1	26
67	Inhibition of NMDA-gated ion channels by bis(7)-tacrine: Whole-cell and single-channel studies. Neuropharmacology, 2008, 54, 1086-1094.	4.1	18
68	Promising anti-Alzheimerâ€™s dimer bis(7)-tacrine reduces Î²-amyloid generation by directly inhibiting BACE-1 activity. Biochemical and Biophysical Research Communications, 2008, 366, 631-636.	2.1	60
69	Bis(7)-tacrine prevents glutamate-induced excitotoxicity more potently than memantine by selectively inhibiting NMDA receptors. Biochemical and Biophysical Research Communications, 2008, 369, 1007-1011.	2.1	14
70	EUDOC on the IBM Blue Gene/L system: Accelerating the transfer of drug discoveries from laboratory to patient. IBM Journal of Research and Development, 2008, 52, 69-81.	3.1	6
71	The Impact of Structural Proteomics on Drug Design. , 2008, , 347-360.		0
72	Preference of Small Molecules for Local Minimum Conformations when Binding to Proteins. PLoS ONE, 2007, 2, e820.	2.5	31

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73	Cryptic proteolytic activity of dihydrolipoamide dehydrogenase. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 6158-6163.	7.1	107
74	Inhibition of Mitochondrial Respiration as a Source of Adaphostin-induced Reactive Oxygen Species and Cytotoxicity. Journal of Biological Chemistry, 2007, 282, 8860-8872.	3.4	64
75	Novel dimeric bis(7)-tacrine proton-dependently inhibits NMDA-activated currents. Biochemical and Biophysical Research Communications, 2007, 361, 505-509.	2.1	17
76	Inhibition by bis(7)-tacrine of native delayed rectifier and KV1.2 encoded potassium channels. Neuroscience Letters, 2007, 412, 108-113.	2.1	9
77	Species marker for developing novel and safe pesticides. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 197-199.	2.2	30
78	Development of a high performance liquid chromatography-tandem mass method for determination of bis(7)-tacrine, a promising anti-Alzheimer's dimer, in rat blood. Journal of Pharmaceutical and Biomedical Analysis, 2007, 44, 1133-1138.	2.8	5
79	In Silico Drug Discovery: Solving the â€œTarget-rich and Lead-poorâ€•Imbalance Using the Genome-to-drug-lead Paradigm. Clinical Pharmacology and Therapeutics, 2007, 81, 30-34.	4.7	19
80	Accurate Reproduction of 161 Small-Molecule Complex Crystal Structures using the EUDOC Program: Expanding the Use of EUDOC to Supramolecular Chemistry. PLoS ONE, 2007, 2, e531.	2.5	12
81	Computer-Aided Lead Optimization: Improved Small-Molecule Inhibitor of the Zinc Endopeptidase of Botulinum Neurotoxin Serotype A. PLoS ONE, 2007, 2, e761.	2.5	48
82	Normal-Mode-Analysisâ€“Monitored Energy Minimization Procedure for Generating Smallâ€“Molecule Bound Conformations. PLoS ONE, 2007, 2, e1025.	2.5	10
83	Complexes of Alkylene-Linked Tacrine Dimers withTorpedo californicaAcetylcholinesterase:Â Binding of Bis(5)-tacrine Produces a Dramatic Rearrangement in the Active-Site Gorge. Journal of Medicinal Chemistry, 2006, 49, 5491-5500.	6.4	186
84	Critical role of the FERM domain in Pyk2 stimulated glioma cell migration. Biochemical and Biophysical Research Communications, 2006, 349, 939-947.	2.1	28
85	Pyrrole-Based Partial Peptidic Mimic of Neurotensin (8-13): Design and Synthesis (Experimental) Tj ETQq1 1 0.784314 rgBT /Overlock 10	0.5	2
86	Novel Acetylcholinesterase Target Site for Malaria Mosquito Control. PLoS ONE, 2006, 1, e58.	2.5	42
87	From genome to drug lead: Identification of a small-molecule inhibitor of the SARS virus. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 830-833.	2.2	46
88	Serotype-selective, small-molecule inhibitors of the zinc endopeptidase of botulinum neurotoxin serotype A. Bioorganic and Medicinal Chemistry, 2006, 14, 395-408.	3.0	71
89	Bis-imidazoles as molecular probes for peripheral sites of the zinc endopeptidase of botulinum neurotoxin serotype A. Bioorganic and Medicinal Chemistry, 2006, 14, 3583-3591.	3.0	20
90	Crystal structures of acetylcholinesterase in complex with HI-6, Ortho-7 and obidoxime: Structural basis for differences in the ability to reactivate tabun conjugates. Biochemical Pharmacology, 2006, 72, 597-607.	4.4	119

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91	Poster reception---Optimizing EUDOC for the IBM eServer Blue Gene supercomputer. , 2006, , .		0
92	Frataxin degrading peptidase: A multifunctional regulator of mitochondrial energy production and iron balance. FASEB Journal, 2006, 20, A48.	0.5	0
93	Crystal Packing Mediates Enantioselective Ligand Recognition at the Peripheral Site of Acetylcholinesterase. Journal of the American Chemical Society, 2005, 127, 11029-11036.	13.7	44
94	ABCC9 mutations identified in human dilated cardiomyopathy disrupt catalytic KATP channel gating. Nature Genetics, 2004, 36, 382-387.	21.4	342
95	Three-dimensional model of a substrate-bound SARS chymotrypsin-like cysteine proteinase predicted by multiple molecular dynamics simulations: Catalytic efficiency regulated by substrate binding. Proteins: Structure, Function and Bioinformatics, 2004, 57, 747-757.	2.6	45
96	Nonbonded bivalence approach to cell-permeable molecules that target DNA sequences. Bioorganic and Medicinal Chemistry, 2004, 12, 3063-3068.	3.0	12
97	Improved Loading and Cleavage Methods for Solid-Phase Synthesis Using Chlorotrityl Resins:Â Synthesis and Testing of a Library of 144 Discrete Chemicals as Potential Farnesyltransferase Inhibitors. ACS Combinatorial Science, 2004, 6, 407-413.	3.3	16
98	Proteomics shows Hsp70 does not bind peptide sequences indiscriminately in vivo. Experimental Cell Research, 2004, 297, 108-117.	2.6	45
99	Inhibition by bis(7)-tacrine of 5-HT-activated current in rat TG neurons. NeuroReport, 2004, 15, 1335-1338.	1.2	6
100	Rational Design of Alkylene-Linked Bis-Pyridiniumaldoximes as Improved Acetylcholinesterase Reactivators. Chemistry and Biology, 2003, 10, 491-502.	6.0	89
101	Differential binding of Sin3 interacting repressor domains to the PAH2 domain of Sin3A. FEBS Letters, 2003, 548, 108-112.	2.8	19
102	Acetylcholinesterase Complexed with Bivalent Ligands Related to Huperzine A:Â Experimental Evidence for Species-Dependent Proteinâ"Ligand Complementarity. Journal of the American Chemical Society, 2003, 125, 363-373.	13.7	94
103	Cocaine Metabolism Accelerated by a Re-Engineered Human Butyrylcholinesterase. Journal of Pharmacology and Experimental Therapeutics, 2002, 302, 710-716.	2.5	85
104	Re-engineering Butyrylcholinesterase as a Cocaine Hydrolase. Molecular Pharmacology, 2002, 62, 220-224.	2.3	131
105	The antiangiogenic activity of cleaved high molecular weight kininogen is mediated through binding to endothelial cell tropomyosin. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 12224-12229.	7.1	54
106	Theoretical 3D Model of Histamine N-Methyltransferase: Insights into the Effects of a Genetic Polymorphism on Enzymatic Activity and Thermal Stability. Biochemical and Biophysical Research Communications, 2001, 287, 204-208.	2.1	24
107	Discovery of a new inhibitor lead of adenovirus proteinase: steps toward selective, irreversible inhibitors of cysteine proteinases. FEBS Letters, 2001, 502, 93-97.	2.8	34
108	Predicted Michaelis-Menten Complexes of Cocaine-Butyrylcholinesterase. Journal of Biological Chemistry, 2001, 276, 9330-9336.	3.4	81

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109	Effects of Bis(7)-Tacrine on Spontaneous Synaptic Activity and on the Nicotinic ACh Receptor of Torpedo Electric Organ. Journal of Neurophysiology, 2001, 86, 183-189.	1.8	18
110	Rabbit indolethylamine N -methyltransferase three-dimensional structure prediction: a model approach to bridge sequence to function in pharmacogenomic studies. Journal of Molecular Modeling, 2001, 7, 324-333.	1.8	8
111	Successful molecular dynamics simulation of two zinc complexes bridged by a hydroxide in phosphotriesterase using the cationic dummy atom method. Proteins: Structure, Function and Bioinformatics, 2001, 45, 183-189.	2.6	132
112	EUDOC: a computer program for identification of drug interaction sites in macromolecules and drug leads from chemical databases. Journal of Computational Chemistry, 2001, 22, 1750-1771.	3.3	101
113	Comparison of DFT, MÃllerâ€“Plesset, and coupled cluster calculations of the proton dissociation energies of imidazole and N -methylacetamide in the presence of zinc(II). Computational and Theoretical Chemistry, 2001, 545, 271-274.	1.5	13
114	Dimerization of an Inactive Fragment of Huperzine A Produces a Drug with Twice the Potency of the Natural Product. Angewandte Chemie - International Edition, 2000, 39, 1775-1777.	13.8	76
115	A single amino acid of the human and rat neurotensin receptors (subtype 1) determining the pharmacological profile of a species-selective neurotensin agonist. Biochemical Pharmacology, 2000, 60, 793-801.	4.4	7
116	Bis(7)-tacrine, a novel acetylcholinesterase inhibitor, reverses AF64A-induced deficits in navigational memory in rats. Neuroscience Letters, 2000, 282, 165-168.	2.1	44
117	Protection against ischemic injury in primary cultured astrocytes of mouse cerebral cortex by bis(7)-tacrine, a novel anti-Alzheimer's agent. Neuroscience Letters, 2000, 288, 95-98.	2.1	40
118	Corrigendum to 'Protection against ischemic injury in primary cultured mouse astrocytes by bis(7)-tacrine, a novel acetylcholinesterase inhibitor' [Neurosci. Lett. 288 (2000) 95â€“98]. Neuroscience Letters, 2000, 290, 84.	2.1	0
119	Bis(7)-tacrine, a promising anti-Alzheimer's agent, reduces hydrogen peroxide-induced injury in rat pheochromocytoma cells: comparison with tacrine. Neuroscience Letters, 2000, 290, 197-200.	2.1	63
120	Proton Dissociation Energies of Zinc-Coordinated Hydroxamic Acids and Their Relative Affinities for Zinc:Â Insight into Design of Inhibitors of Zinc-Containing Proteinases. Journal of Physical Chemistry B, 2000, 104, 6499-6504.	2.6	41
121	Successful Virtual Screening of a Chemical Database for Farnesyltransferase Inhibitor Leads. Journal of Medicinal Chemistry, 2000, 43, 401-408.	6.4	130
122	Zinc's Affect on Proton Transfer between Imidazole and Acetate Predicted by ab Initio Calculations. Journal of Physical Chemistry B, 2000, 104, 6662-6667.	2.6	32
123	Protonation States of the Chromophore of Denatured Green Fluorescent Proteins Predicted by ab Initio Calculations. Journal of the American Chemical Society, 2000, 122, 11411-11415.	13.7	47
124	Potent, easily synthesized huperzine A-tacrine hybrid acetylcholinesterase inhibitors. Bioorganic and Medicinal Chemistry Letters, 1999, 9, 2335-2338.	2.2	74
125	Evaluation of short-tether Bis-THA AChE inhibitors. A further test of the dual binding site hypothesis. Bioorganic and Medicinal Chemistry, 1999, 7, 351-357.	3.0	161
126	Dual-site binding of bivalent 4-aminopyridine- and 4-aminoquinoline-based AChE inhibitors: contribution of the hydrophobic alkylene tether to monomer and dimer affinities. Bioorganic and Medicinal Chemistry, 1999, 7, 2569-2575.	3.0	38

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127	Zincâ€²s Exclusive Tetrahedral Coordination Governed by Its Electronic Structure. Journal of Molecular Modeling, 1999, 5, 134-140.	1.8	53
128	Novel Zinc Protein Molecular Dynamics Simulations: Steps Toward Antiangiogenesis for Cancer Treatment. Journal of Molecular Modeling, 1999, 5, 196-202.	1.8	163
129	Models of Ternary Complexes for Nonpeptidic Farnesyltransferase Inhibitors: Insights into Structure-Based Screen and Design of Potential Anticancer Therapeutics. Journal of Molecular Modeling, 1999, 5, 203-217.	1.8	6
130	In vitro binding and CNS effects of novel neurotensin agonists that cross the bloodâ€“brain barrier. Neuropharmacology, 1999, 38, 1027-1034.	4.1	67
131	Novel Stable Configurations and Tautomers of the Neutral and Deprotonated Hydroxamic Acids Predicted from High-Level ab Initio Calculations. Journal of Physical Chemistry A, 1999, 103, 8346-8350.	2.5	34
132	Heterodimeric Tacrine-Based Acetylcholinesterase Inhibitors:â€‰ Investigating Ligandâ^'Peripheral Site Interactions. Journal of Medicinal Chemistry, 1999, 42, 4225-4231.	6.4	123
133	Ab Initio Calculations of Proton Dissociation Energies of Zinc Ligands:â€‰ Hypothesis of Imidazolate as Zinc Ligand in Proteins. Journal of Physical Chemistry B, 1999, 103, 8773-8779.	2.6	53
134	Computational and Experimental Studies of (2,2)-Bis(indol-1-yl-methyl)acetate Suggest the Importance of the Hydrophobic Effect in Aromatic Stacking Interactions. Journal of the American Chemical Society, 1999, 121, 1717-1725.	13.7	41
135	Polysaccharide elasticity governed by chairâ€“boat transitions of the glucopyranose ring. Nature, 1998, 396, 661-664.	27.8	436
136	Supercomputing-based dimeric analog approach for drug optimization. Parallel Computing, 1998, 24, 1557-1566.	2.1	5
137	Synthesis of alkylene linked bis-THA and alkylene linked benzyl-THA as highly potent and selective inhibitors and molecular probes of acetylcholinesterase. Journal of the Chemical Society Perkin Transactions 1, 1997, , 171-176.	0.9	24
138	Structure of acetylcholinesterase complexed with the nootropic alkaloid, (â€“)-huperzine A. Nature Structural and Molecular Biology, 1997, 4, 57-63.	8.2	373
139	Docking Studies on the Complexed and Uncomplexed FKBP12 Structures with Bound and Unbound Ligands: An Implication of a Conformational Selection Mechanism for Binding. Journal of Molecular Modeling, 1997, 3, 240-248.	1.8	6
140	Chimeric Rat/Human Neurotensin Receptors Localize a Region of the Receptor Sensitive to Binding of a Novel, Species-specific, Picomolar Affinity Peptide. Journal of Biological Chemistry, 1996, 271, 15054-15059.	3.4	16
141	Proposed Ligand Binding Site of the Transmembrane Receptor for Neurotensin(8â€“13). Journal of Biological Chemistry, 1996, 271, 15060-15068.	3.4	73
142	Highly Potent, Selective, and Low Cost Bis-tetrahydroaminacrine Inhibitors of Acetylcholinesterase. Journal of Biological Chemistry, 1996, 271, 23646-23649.	3.4	313
143	Applications of free energy derivatives to analog design. Journal of Computer - Aided Molecular Design, 1995, 3, 106-122.	1.0	8
144	Pharmacological and Biochemical Profiles of Unique Neurotensin 8-13 Analogs Exhibiting Species Selectivity, Stereoselectivity, and Superagonism. Journal of Biological Chemistry, 1995, 270, 18359-18366.	3.4	49

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145	Synthesis of partial nonpeptidic peptide mimetics as potential neurotensin agonists and antagonists. Journal of the Chemical Society Perkin Transactions 1, 1995, , 1615.	0.9	10
146	Prediction of the binding sites of huperzine A in acetylcholinesterase by docking studies. Journal of Computer-Aided Molecular Design, 1994, 8, 669-681.	2.9	88
147	Prediction of the binding site of 1-benzyl-4-[(5,6-dimethoxy-1-indanon-2-yl)methyl]piperidine in acetylcholinesterase by docking studies with the SYSDOC program. Journal of Computer-Aided Molecular Design, 1994, 8, 683-693.	2.9	41
148	Rational design of novel neurotensin mimetics: Discovery of a pharmacologically unprecedented agent exhibiting concentration-dependent dual effects as antagonist and full agonist. Journal of Computer-Aided Molecular Design, 1994, 8, 433-440.	2.9	6
149	Synthesis and 2D NMR analysis of a cyclopropane containing analogue of huperzine A. Tetrahedron Letters, 1992, 33, 2653-2656.	1.4	8
150	Synthesis and Chemical Resolution of a Novel Class of Rigid 1-(1-Phenylcyclohexyl)-iperidine(PCP) Analogues. Synlett, 1990, 1990, 58-63.	1.8	4