Yuan-Ping Pang

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/7582311/publications.pdf

Version: 2024-02-01

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	Polysaccharide elasticity governed by chairâ€“boat transitions of the glucopyranose ring. Nature, 1998, 396, 661-664.	27.8	436
2	Structure of acetylcholinesterase complexed with the nootropic alkaloid, (â€“)-huperzine A. Nature Structural and Molecular Biology, 1997, 4, 57-63.	8.2	373
3	ABCC9 mutations identified in human dilated cardiomyopathy disrupt catalytic KATP channel gating. Nature Genetics, 2004, 36, 382-387.	21.4	342
4	Highly Potent, Selective, and Low Cost Bis-tetrahydroaminacrine Inhibitors of Acetylcholinesterase. Journal of Biological Chemistry, 1996, 271, 23646-23649.	3.4	313
5	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
6	Novel Zinc Protein Molecular Dynamics Simulations: Steps Toward Antiangiogenesis for Cancer Treatment. Journal of Molecular Modeling, 1999, 5, 196-202.	1.8	163
7	Structure-based discovery of dengue virus protease inhibitors. Antiviral Research, 2009, 82, 110-114.	4.1	162
8	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
9	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
10	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
11	Re-engineering Butyrylcholinesterase as a Cocaine Hydrolase. Molecular Pharmacology, 2002, 62, 220-224.	2.3	131
12	Successful Virtual Screening of a Chemical Database for Farnesyltransferase Inhibitor Leads. Journal of Medicinal Chemistry, 2000, 43, 401-408.	6.4	130
13	Heterodimeric Tacrine-Based Acetylcholinesterase Inhibitors:â€‰Investigating Ligandâ^'Peripheral Site Interactions. Journal of Medicinal Chemistry, 1999, 42, 4225-4231.	6.4	123
14	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
15	Cholinergic and non-cholinergic functions of two acetylcholinesterase genes revealed by gene-silencing in Tribolium castaneum. Scientific Reports, 2012, 2, 288.	3.3	113
16	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
17	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
18	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

#	Article	IF	Citations
19	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
20	Rational Design of Alkylene-Linked Bis-Pyridiniumaldoximes as Improved Acetylcholinesterase Reactivators. Chemistry and Biology, 2003, 10, 491-502.	6.0	89
21	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
22	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
23	Cocaine Metabolism Accelerated by a Re-Engineered Human Butyrylcholinesterase. Journal of Pharmacology and Experimental Therapeutics, 2002, 302, 710-716.	2.5	85
24	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
25	Predicted Michaelis-Menten Complexes of Cocaine-Butyrylcholinesterase. Journal of Biological Chemistry, 2001, 276, 9330-9336.	3.4	81
26	Configurational Entropy in Proteinâ€"Peptide Binding:. Journal of Molecular Biology, 2009, 389, 315-335.	4.2	79
27	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
28	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
29	Physiological roles for butyrylcholinesterase: A BChE-ghrelin axis. Chemico-Biological Interactions, 2016, 259, 271-275.	4.0	75
30	Potent, easily synthesized huperzine A-tacrine hybrid acetylcholinesterase inhibitors. Bioorganic and Medicinal Chemistry Letters, 1999, 9, 2335-2338.	2.2	74
31	Parkin Regulates Mitosis and Genomic Stability through Cdc20/Cdh1. Molecular Cell, 2015, 60, 21-34.	9.7	74
32	Proposed Ligand Binding Site of the Transmembrane Receptor for Neurotensin(8â€"13). Journal of Biological Chemistry, 1996, 271, 15060-15068.	3.4	73
33	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
34	In vitro binding and CNS effects of novel neurotensin agonists that cross the bloodâ€"brain barrier. Neuropharmacology, 1999, 38, 1027-1034.	4.1	67
35	Evaluation of the BH3-only Protein Puma as a Direct Bak Activator. Journal of Biological Chemistry, 2014, 289, 89-99.	3.4	65
36	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

#	Article	IF	Citations
37	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
38	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
39	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
40	Regulation of error-prone translesion synthesis by Spartan/C1orf124. Nucleic Acids Research, 2013, 41, 1661-1668.	14.5	56
41	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
42	Zincâ€²s Exclusive Tetrahedral Coordination Governed by Its Electronic Structure. Journal of Molecular Modeling, 1999, 5, 134-140.	1.8	53
43	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
44	TREM2 interacts with TDP-43 and mediates microglial neuroprotection against TDP-43-related neurodegeneration. Nature Neuroscience, 2022, 25, 26-38.	14.8	52
45	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
46	Novel and Viable Acetylcholinesterase Target Site for Developing Effective and Environmentally Safe Insecticides. Current Drug Targets, 2012, 13, 471-482.	2.1	49
47	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
48	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
49	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
50	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
51	Proteomics shows Hsp70 does not bind peptide sequences indiscriminately in vivo. Experimental Cell Research, 2004, 297, 108-117.	2.6	45
52	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
53	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
54	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

#	Article	IF	Citations
55	Novel Acetylcholinesterase Target Site for Malaria Mosquito Control. PLoS ONE, 2006, 1, e58.	2.5	42
56	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
57	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
58	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
59	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
60	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
61	Bak Conformational Changes Induced by Ligand Binding: Insight into BH3 Domain Binding and Bak Homo-Oligomerization. Scientific Reports, 2012, 2, 257.	3.3	41
62	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
63	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
64	Selective and Irreversible Inhibitors of Aphid Acetylcholinesterases: Steps Toward Human-Safe Insecticides. PLoS ONE, 2009, 4, e4349.	2.5	38
65	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
66	Small Molecules Showing Significant Protection of Mice against Botulinum Neurotoxin Serotype A. PLoS ONE, 2010, 5, e10129.	2.5	37
67	FF12MC: A revised AMBER forcefield and new protein simulation protocol. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1490-1516.	2.6	37
68	CFAP45 deficiency causes situs abnormalities and asthenospermia by disrupting an axonemal adenine nucleotide homeostasis module. Nature Communications, 2020, 11, 5520.	12.8	36
69	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
70	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
71	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
72	Small-Molecule Inhibitor Leads of Ribosome-Inactivating Proteins Developed Using the Doorstop Approach. PLoS ONE, 2011, 6, e17883.	2.5	34

#	Article	IF	Citations
73	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
74	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
75	Preference of Small Molecules for Local Minimum Conformations when Binding to Proteins. PLoS ONE, 2007, 2, e820.	2.5	31
76	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
77	Characterization of an alternative BAK-binding site for BH3 peptides. Nature Communications, 2020, 11, 3301.	12.8	31
78	Species marker for developing novel and safe pesticides. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 197-199.	2.2	30
79	Selective and Irreversible Inhibitors of Mosquito Acetylcholinesterases for Controlling Malaria and Other Mosquito-Borne Diseases. PLoS ONE, 2009, 4, e6851.	2.5	30
80	Chemical Structure of Retro-2, a Compound That Protects Cells against Ribosome-Inactivating Proteins. Scientific Reports, 2012, 2, 631.	3.3	30
81	Novel Selective and Irreversible Mosquito Acetylcholinesterase Inhibitors for Controlling Malaria and Other Mosquito-Borne Diseases. Scientific Reports, 2013, 3, 1068.	3.3	29
82	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
83	Critical role of the FERM domain in Pyk2 stimulated glioma cell migration. Biochemical and Biophysical Research Communications, 2006, 349, 939-947.	2.1	28
84	Casp8p41 generated by HIV protease kills CD4 T cells through direct Bak activation. Journal of Cell Biology, 2014, 206, 867-876.	5.2	28
85	Enzymatic activation of pyruvate kinase increases cytosolic oxaloacetate to inhibit the Warburg effect. Nature Metabolism, 2021, 3, 954-968.	11.9	28
86	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
87	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
88	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
89	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
90	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

#	Article	IF	Citations
91	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
92	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
93	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
94	Insect Acetylcholinesterase as a Target for Effective and Environmentally Safe Insecticides. Advances in Insect Physiology, 2014, , 435-494.	2.7	21
95	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
96	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
97	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
98	Differential binding of Sin3 interacting repressor domains to the PAH2 domain of Sin3A. FEBS Letters, 2003, 548, 108-112.	2.8	19
99	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
100	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
101	Inhibition of NMDA-gated ion channels by bis(7)-tacrine: Whole-cell and single-channel studies. Neuropharmacology, 2008, 54, 1086-1094.	4.1	18
102	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
103	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
104	Novel dimeric bis(7)-tacrine proton-dependently inhibits NMDA-activated currents. Biochemical and Biophysical Research Communications, 2007, 361, 505-509.	2.1	17
105	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
106	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
107	How fast fast-folding proteins fold in silico. Biochemical and Biophysical Research Communications, 2017, 492, 135-139.	2.1	16
108	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

#	Article	IF	Citations
109	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
110	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
111	A selective smallâ€molecule inhibitor of câ€Jun Nâ€terminal kinase 1. FEBS Letters, 2009, 583, 2208-2212.	2.8	14
112	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
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	Nonbonded bivalence approach to cell-permeable molecules that target DNA sequences. Bioorganic and Medicinal Chemistry, 2004, 12, 3063-3068.	3.0	12
115	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
116	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
117	Convenient synthesis of a library of discrete hydroxamic acids using the hydroxythiophenol (Marshall) resin. Tetrahedron Letters, 2008, 49, 1103-1106.	1.4	11
118	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
119	Common Pharmacophore of Structurally Distinct Small-Molecule Inhibitors of Intracellular Retrograde Trafficking of Ribosome Inactivating Proteins. Scientific Reports, 2013, 3, 3397.	3.3	10
120	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
121	Normal-Mode-Analysisâ€“Monitored Energy Minimization Procedure for Generating Smallâ€“Molecule Bound Conformations. PLoS ONE, 2007, 2, e1025.	2.5	10
122	Inhibition by bis(7)-tacrine of native delayed rectifier and KV1.2 encoded potassium channels. Neuroscience Letters, 2007, 412, 108-113.	2.1	9
123	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
124	Synthesis and 2D NMR analysis of a cyclopropane containing analogue of huperzine A. Tetrahedron Letters, 1992, 33, 2653-2656.	1.4	8
125	Applications of free energy derivatives to analog design. Journal of Computer - Aided Molecular Design, 1995, 3, 106-122.	1.0	8
126	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

#	Article	IF	Citations
127	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
128	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
129	Remote Activation of a Latent Epitope in an Autoantigen Decoded With Simulated B-Factors. Frontiers in Immunology, 2019, 10, 2467.	4.8	7
130	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
131	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
132	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
133	Inhibition by bis(7)-tacrine of 5-HT-activated current in rat TG neurons. NeuroReport, 2004, 15, 1335-1338.	1.2	6
134	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
135	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
136	Supercomputing-based dimeric analog approach for drug optimization. Parallel Computing, 1998, 24, 1557-1566.	2.1	5
137	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
138	Mechanism of bis(7)-tacrine inhibition of GABA-activated current in cultured rat hippocampal neurons. Neuropharmacology, 2009, 57, 33-40.	4.1	5
139	Synthesis and Chemical Resolution of a Novel Class of Rigid 1-(1-Phenylcyclohexyl)-iperidine(PCP) Analogues. Synlett, 1990, 1990, 58-63.	1.8	4
140	Pyrrole-Based Partial Peptidic Mimic of Neurotensin (8-13): Design and Synthesis (Experimental) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 22	0.5	2
141	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
142	How the water-soluble hemicarcerand incarcerates guests at room temperature decoded with modular simulations. Communications Chemistry, 2021, 4, .	4.5	1
143	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
144	Cover Image, Volume 84, Issue 10. Proteins: Structure, Function and Bioinformatics, 2016, 84, C4-C4.	2.6	0

#	Article	IF	Citations
145	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
146	Poster reception---Optimizing EUDOC for the IBM eServer Blue Gene supercomputer. , 2006, , .		0
147	Frataxin degrading peptidase: A multifunctional regulator of mitochondrial energy production and iron balance. FASEB Journal, 2006, 20, A48.	0.5	0
148	The Impact of Structural Proteomics on Drug Design. , 2008, , 347-360.		0
149	One-Compound-Multi-Targets at Amyloid Î² Cascade Offered By Bis(7)-Cognitin, a Novel Anti-Alzheimerâ€™s Dimer. , 2010, , 165-183.		0
150	How neocarcerand Octacid4 self-assembles with guests into irreversible noncovalent complexes and what accelerates the assembly. Communications Chemistry, 2022, 5, .	4.5	0