Joel L Sussman

List of Publications by Year in Descending Order

223 papers	20,874 citations	74 h-index	142 g-index
234 ext. papers	22,420 ext. citations	7.7 avg, IF	6.2 L-index

#	Paper	IF	Citations
223	Torpedo californica acetylcholinesterase is stabilized by binding of a divalent metal ion to a novel and versatile 4D motif. *Protein Science*, **2021**, 30, 966-981	6.3	3
222	A practical guide to teaching with Proteopedia. *Biochemistry and Molecular Biology Education*, **2021**, 49, 707-719	1.3	1
221	IceBear: an intuitive and versatile web application for research-data tracking from crystallization experiment to PDB deposition. *Acta Crystallographica Section D: Structural Biology*, **2021**, 77, 151-163	5.5	3
220	A Second Look at the Crystal Structures of Acetylcholinesterase in Complex with Tacrine Derivatives Provides Insights Concerning Catalytic Intermediates and the Design of Specific Insecticides. *Molecules*, **2020**, 25,	4.8	5
219	Polyproline-rich peptides associated with Torpedo californica acetylcholinesterase tetramers. *Chemico-Biological Interactions*, **2020**, 319, 109007	5	1
218	A community proposal to integrate structural bioinformatics activities in ELIXIR (3D-Bioinfo Community). *F1000Research*, **2020**, 9,	3.6	9
217	Enzyme Evolution: An Epistatic Ratchet versus a Smooth Reversible Transition. *Molecular Biology and Evolution*, **2020**, 37, 1133-1147	8.3	15
216	Computational studies on cholinesterases: Strengthening our understanding of the integration of structure, dynamics and function. *Neuropharmacology*, **2020**, 179, 108265	5.5	5
215	The four-helix bundle in cholinesterase dimers: Structural and energetic determinants of stability. *Chemico-Biological Interactions*, **2019**, 309, 108699	5	2
214	Molecular dynamics simulations of the interaction of Mouse and Torpedo acetylcholinesterase with covalent inhibitors explain their differential reactivity: Implications for drug design. *Chemico-Biological Interactions*, **2019**, 310, 108715	5	7
213	Rivastigmine and metabolite analogues with putative Alzheimer□ disease-modifying properties in a Caenorhabditis elegans model. *Communications Chemistry*, **2019**, 2,	6.3	19
212	An intrinsically disordered proteins community for ELIXIR. *F1000Research*, **2019**, 8,	3.6	7
211	Design, biological evaluation and X-ray crystallography of nanomolar multifunctional ligands targeting simultaneously acetylcholinesterase and glycogen synthase kinase-3. *European Journal of Medicinal Chemistry*, **2019**, 168, 58-77	6.8	31
210	Novel multitarget-directed ligands targeting acetylcholinesterase and □receptors as lead compounds for treatment of Alzheimer's disease: Synthesis, evaluation, and structural characterization of their complexes with acetylcholinesterase. *European Journal of Medicinal Chemistry*, **2019**, 162, 234-248	6.8	28
209	Potent 3-Hydroxy-2-Pyridine Aldoxime Reactivators of Organophosphate-Inhibited Cholinesterases with Predicted Blood-Brain Barrier Penetration. *Chemistry - A European Journal*, **2018**, 24, 9675-9691	4.8	37
208	Comparing NMR and X-ray protein structure: Lindemann-like parameters and NMR disorder. *Journal of Biomolecular Structure and Dynamics*, **2018**, 36, 2331-2341	3.6	7
207	Structure-Based Optimization of Nonquaternary Reactivators of Acetylcholinesterase Inhibited by Organophosphorus Nerve Agents. *Journal of Medicinal Chemistry*, **2018**, 61, 7630-7639	8.3	30

206	Cryo-EM structure of the native butyrylcholinesterase tetramer reveals a dimer of dimers stabilized by a superhelical assembly. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 13270-13275	11.5	13
205	Overcoming an optimization plateau in the directed evolution of highly efficient nerve agent bioscavengers. *Protein Engineering, Design and Selection*, **2017**, 30, 333-345	1.9	41
204	Recent developments in structural studies on acetylcholinesterase. *Journal of Neurochemistry*, **2017** , 142 Suppl 2, 19-25	6	14
203	Computational Studies on Acetylcholinesterases. *Molecules*, **2017**, 22,	4.8	17
202	Automated Structure- and Sequence-Based Design of Proteins for High Bacterial Expression and Stability. *Molecular Cell*, **2016**, 63, 337-346	17.6	204
201	Single treatment of VX poisoned guinea pigs with the phosphotriesterase mutant C23AL: Intraosseous versus intravenous injection. *Toxicology Letters*, **2016**, 258, 198-206	4.4	21
200	Catalytic efficiencies of directly evolved phosphotriesterase variants with structurally different organophosphorus compounds in vitro. *Archives of Toxicology*, **2016**, 90, 2711-2724	5.8	35
199	The impact of crystallization conditions on structure-based drug design: A case study on the methylene blue/acetylcholinesterase complex. *Protein Science*, **2016**, 25, 1096-114	6.3	21
198	In vitro evaluation of the catalytic activity of paraoxonases and phosphotriesterases predicts the enzyme circulatory levels required for in vivo protection against organophosphate intoxications. *Chemico-Biological Interactions*, **2016**, 259, 252-256	5	15
197	Catalytic stimulation by restrained active-site floppiness--the case of high density lipoprotein-bound serum paraoxonase-1. *Journal of Molecular Biology*, **2015**, 427, 1359-1374	6.5	30
196	Post-exposure treatment of VX poisoned guinea pigs with the engineered phosphotriesterase mutant C23: a proof-of-concept study. *Toxicology Letters*, **2014**, 231, 45-54	4.4	34
195	pE-DB: a database of structural ensembles of intrinsically disordered and of unfolded proteins. *Nucleic Acids Research*, **2014**, 42, D326-35	20.1	159
194	Catalytic metal ion rearrangements underline promiscuity and evolvability of a metalloenzyme. *Journal of Molecular Biology*, **2013**, 425, 1028-38	6.5	52
193	The specific interaction of the photosensitizer methylene blue with acetylcholinesterase provides a model system for studying the molecular consequences of photodynamic therapy. *Chemico-Biological Interactions*, **2013**, 203, 63-6	5	3
192	What's in a name? Why these proteins are intrinsically disordered: Why these proteins are intrinsically disordered. *Intrinsically Disordered Proteins*, **2013**, 1, e24157		171
191	JSmol and the Next-Generation Web-Based Representation of 3D Molecular Structure as Applied to Proteopedia. *Israel Journal of Chemistry*, **2013**, 53, 207-216	3.4	169
190	Crystal structure of the enzyme acid glucosidase **2013**, 124-138		
189	Structure of recombinant human carboxylesterase 1 isolated from whole cabbage looper larvae. *Acta Crystallographica Section F: Structural Biology Communications*, **2012**, 68, 269-72		6

188	Computational redesign of a mononuclear zinc metalloenzyme for organophosphate hydrolysis. *Nature Chemical Biology*, **2012**, 8, 294-300	11.7	189
187	Catalytic versatility and backups in enzyme active sites: the case of serum paraoxonase 1. *Journal of Molecular Biology*, **2012**, 418, 181-96	6.5	122
186	Flexibility of the flap in the active site of BACE1 as revealed by crystal structures and molecular dynamics simulations. *Acta Crystallographica Section D: Biological Crystallography*, **2012**, 68, 13-25		70
185	Structural and functional characterization of the interaction of the photosensitizing probe methylene blue with Torpedo californica acetylcholinesterase. *Protein Science*, **2012**, 21, 1138-52	6.3	14
184	Acetylcholinesterase: substrate traffic and inhibition. *Biochemistry and Molecular Biology Education*, **2012**, 40, 144	1.3	
183	Backbone and side chain NMR assignments for the intrinsically disordered cytoplasmic domain of human neuroligin-3. *Biomolecular NMR Assignments*, **2012**, 6, 15-8	0.7	6
182	Evolved stereoselective hydrolases for broad-spectrum G-type nerve agent detoxification. *Chemistry and Biology*, **2012**, 19, 456-66		74
181	Proteopedia: Exciting Advances in the 3D Encyclopedia of Biomolecular Structure. *NATO Science for Peace and Security Series A: Chemistry and Biology*, **2012**, 149-161	0.1	
180	Expression of protein complexes using multiple Escherichia coli protein co-expression systems: a benchmarking study. *Journal of Structural Biology*, **2011**, 175, 159-70	3.4	34
179	Proteopedia: a status report on the collaborative, 3D web-encyclopedia of proteins and other biomolecules. *Journal of Structural Biology*, **2011**, 175, 244-52	3.4	42
178	In vitro detoxification of cyclosarin in human blood pre-incubated ex vivo with recombinant serum paraoxonases. *Toxicology Letters*, **2011**, 206, 24-8	4.4	15
177	Cyclodextrin-mediated crystallization of acid □glucosidase in complex with amphiphilic bicyclic nojirimycin analogues. *Organic and Biomolecular Chemistry*, **2011**, 9, 4160-7	3.9	30
176	Directed evolution of hydrolases for prevention of G-type nerve agent intoxication. *Nature Chemical Biology*, **2011**, 7, 120-5	11.7	156
175	Context-dependent resistance to proteolysis of intrinsically disordered proteins. *Protein Science*, **2011**, 20, 1285-97	6.3	56
174	Backdoor opening mechanism in acetylcholinesterase based on X-ray crystallography and molecular dynamics simulations. *Protein Science*, **2011**, 20, 1114-8	6.3	47
173	Comparison of a molecular dynamics model with the X-ray structure of the N370S acid-beta-glucosidase mutant that causes Gaucher disease. *Protein Engineering, Design and Selection*, **2011**, 24, 773-5	1.9	12
172	Structure of estradiol metal chelate and estrogen receptor complex: the basis for designing a new class of selective estrogen receptor modulators. *Journal of Medicinal Chemistry*, **2011**, 54, 3575-80	8.3	24
171	Long route or shortcut? A molecular dynamics study of traffic of thiocholine within the active-site gorge of acetylcholinesterase. *Biophysical Journal*, **2010**, 99, 4003-11	2.9	20

170	Molecular basis of reduced glucosylceramidase activity in the most common Gaucher disease mutant, N370S. *Journal of Biological Chemistry*, **2010**, 285, 42105-14	5.4	31
169	Characterization of gene-activated human acid-beta-glucosidase: crystal structure, glycan composition, and internalization into macrophages. *Glycobiology*, **2010**, 20, 24-32	5.8	97
168	Acetylcholinesterase: from 3D structure to function. *Chemico-Biological Interactions*, **2010**, 187, 10-22	5	420
167	Purification of Intrinsically Disordered Proteins **2010**, 695-704		3
166	Proteopedia: A collaborative, virtual 3D web-resource for protein and biomolecule structure and function. *Biochemistry and Molecular Biology Education*, **2010**, 38, 341-2	1.3	13
165	Design, expression and characterization of mutants of fasciculin optimized for interaction with its target, acetylcholinesterase. *Protein Engineering, Design and Selection*, **2009**, 22, 641-8	1.9	13
164	An encyclopedic effort to make 3D structures easier to understand. *Trends in Biochemical Sciences*, **2009**, 34, 100-1	10.3	9
163	6-Amino-6-deoxy-5,6-di-N-(N'-octyliminomethylidene)nojirimycin: synthesis, biological evaluation, and crystal structure in complex with acid beta-glucosidase. *ChemBioChem*, **2009**, 10, 1480-5	3.8	42
162	Assessment of disorder predictions in CASP8. *Proteins: Structure, Function and Bioinformatics*, **2009**, 77 Suppl 9, 210-6	4.2	93
161	Assessment of CASP8 structure predictions for template free targets. *Proteins: Structure, Function and Bioinformatics*, **2009**, 77 Suppl 9, 50-65	4.2	83
160	Amalgam, an axon guidance Drosophila adhesion protein belonging to the immunoglobulin superfamily: over-expression, purification and biophysical characterization. *Protein Expression and Purification*, **2009**, 63, 147-57	2	11
159	The quaternary structure of amalgam, a Drosophila neuronal adhesion protein, explains its dual adhesion properties. *Biophysical Journal*, **2009**, 97, 2316-26	2.9	7
158	Structural Studies on Acetylcholinesterase and Paraoxonase Directed Towards Development of Therapeutic Biomolecules for the Treatment of Degenerative Diseases and Protection Against Chemical Threat Agents. *NATO Science for Peace and Security Series A: Chemistry and Biology*, **2009**, 183-199	0.1	
157	Directed evolution of serum paraoxonase PON3 by family shuffling and ancestor/consensus mutagenesis, and its biochemical characterization. *Biochemistry*, **2009**, 48, 6644-54	3.2	35
156	The crystal structure of a complex of acetylcholinesterase with a bis-(-)-nor-meptazinol derivative reveals disruption of the catalytic triad. *Journal of Medicinal Chemistry*, **2009**, 52, 2543-9	8.3	22
155	Crystallographic snapshots of nonaged and aged conjugates of soman with acetylcholinesterase, and of a ternary complex of the aged conjugate with pralidoxime. *Journal of Medicinal Chemistry*, **2009**, 52, 7593-603	8.3	73
154	Tools to Make 3D Structural Data More Comprehensible: Emovie & Proteopedia. *NATO Science for Peace and Security Series A: Chemistry and Biology*, **2009**, 169-182	0.1	
153	Protein production and purification. *Nature Methods*, **2008**, 5, 135-46	21.6	655

152	Acetylcholinesterase: how is structure related to function?. *Chemico-Biological Interactions*, **2008**, 175, 3-10	5	137
151	Function and structure of inherently disordered proteins. *Current Opinion in Structural Biology*, **2008**, 18, 756-64	8.1	746
150	Biophysical characterization of the unstructured cytoplasmic domain of the human neuronal adhesion protein neuroligin 3. *Biophysical Journal*, **2008**, 95, 1928-44	2.9	34
149	Flexibility of aromatic residues in the active-site gorge of acetylcholinesterase: X-ray versus molecular dynamics. *Biophysical Journal*, **2008**, 95, 2500-11	2.9	84
148	Acid beta-glucosidase: insights from structural analysis and relevance to Gaucher disease therapy. *Biological Chemistry*, **2008**, 389, 1361-9	4.5	35
147	Proteopedia - a scientific 'wiki' bridging the rift between three-dimensional structure and function of biomacromolecules. *Genome Biology*, **2008**, 9, R121	18.3	85
146	Crystal structure of thioflavin T bound to the peripheral site of Torpedo californica acetylcholinesterase reveals how thioflavin T acts as a sensitive fluorescent reporter of ligand binding to the acylation site. *Journal of the American Chemical Society*, **2008**, 130, 7856-61	16.4	111
145	Shoot-and-Trap: use of specific x-ray damage to study structural protein dynamics by temperature-controlled cryo-crystallography. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 11742-7	11.5	49
144	Operational definition of intrinsically unstructured protein sequences based on susceptibility to the 20S proteasome. *Proteins: Structure, Function and Bioinformatics*, **2008**, 70, 1357-66	4.2	80
143	Control of the rate of evaporation in protein crystallization by the 'microbatch under oil' method. *Journal of Applied Crystallography*, **2008**, 41, 969-971	3.8	13
142	Structural disorder serves as a weak signal for intracellular protein degradation. *Proteins: Structure, Function and Bioinformatics*, **2008**, 71, 903-9	4.2	84
141	Crystal structure of YagE, a putative DHDPS-like protein from Escherichia coli K12. *Proteins: Structure, Function and Bioinformatics*, **2008**, 71, 2102-8	4.2	3
140	Induced-fit or preexisting equilibrium dynamics? Lessons from protein crystallography and MD simulations on acetylcholinesterase and implications for structure-based drug design. *Protein Science*, **2008**, 17, 601-5	6.3	48
139	Structural Genomics and Structural Proteomics: A Global Perspective **2008**, 505-537		
138	3-D structure of serum paraoxonase 1 sheds light on its activity, stability, solubility and crystallizability. *Arhiv Za Higijenu Rada I Toksikologiju*, **2007**, 58, 347-53	1.7	23
137	Use of a 'caged' analogue to study the traffic of choline within acetylcholinesterase by kinetic crystallography. *Acta Crystallographica Section D: Biological Crystallography*, **2007**, 63, 1115-28		38
136	RIKEN aids international structural genomics efforts. *Nature*, **2007**, 445, 21	50.4	14
135	Production of glucocerebrosidase with terminal mannose glycans for enzyme replacement therapy of Gaucher's disease using a plant cell system. *Plant Biotechnology Journal*, **2007**, 5, 579-90	11.6	317

134	eMovie: a storyboard-based tool for making molecular movies. *Trends in Biochemical Sciences*, **2007**, 32, 199-204	10.3	26
133	A server and database for dipole moments of proteins. *Nucleic Acids Research*, **2007**, 35, W512-21	20.1	146
132	Crystal structures of complexes of N-butyl- and N-nonyl-deoxynojirimycin bound to acid beta-glucosidase: insights into the mechanism of chemical chaperone action in Gaucher disease. *Journal of Biological Chemistry*, **2007**, 282, 29052-29058	5.4	102
131	An idea whose time has come. *Genome Biology*, **2007**, 8, 408	18.3	3
130	Shedding UV light on the phase problem. *Structure*, **2006**, 14, 629-30	5.2	1
129	Complexes of alkylene-linked tacrine dimers with Torpedo californica acetylcholinesterase: Binding of Bis5-tacrine produces a dramatic rearrangement in the active-site gorge. *Journal of Medicinal Chemistry*, **2006**, 49, 5491-500	8.3	170
128	The X-Ray Structure of Human Acid-beta-Glucosidase **2006**, 85-96		
127	Eukaryotic expression: developments for structural proteomics. *Acta Crystallographica Section D: Biological Crystallography*, **2006**, 62, 1114-24		67
126	Co-expression of protein complexes in prokaryotic and eukaryotic hosts: experimental procedures, database tracking and case studies. *Acta Crystallographica Section D: Biological Crystallography*, **2006**, 62, 1232-42		94
125	Structural comparison of differently glycosylated forms of acid-beta-glucosidase, the defective enzyme in Gaucher disease. *Acta Crystallographica Section D: Biological Crystallography*, **2006**, 62, 1458-65		38
124	Structural insights into substrate traffic and inhibition in acetylcholinesterase. *EMBO Journal*, **2006**, 25, 2746-56	13	140
123	Database and Comparative Identification of Prophages **2006**, 863-868		
122	Acetylcholinesterase: 'classical' and 'non-classical' functions and pharmacology. *Current Opinion in Pharmacology*, **2005**, 5, 293-302	5.1	362
121	Dynamic mechanism of E2020 binding to acetylcholinesterase: a steered molecular dynamics simulation. *Journal of Physical Chemistry B*, **2005**, 109, 23730-8	3.4	47
120	Crystal packing mediates enantioselective ligand recognition at the peripheral site of acetylcholinesterase. *Journal of the American Chemical Society*, **2005**, 127, 11029-36	16.4	40
119	The crystal structure of the complex of the anticancer prodrug 7-ethyl-10-[4-(1-piperidino)-1-piperidino]-carbonyloxycamptothecin (CPT-11) with Torpedo californica acetylcholinesterase provides a molecular explanation for its cholinergic action.	4.3	34
118	The 3D structure of the anticancer prodrug CPT-11 with Torpedo californica acetylcholinesterase rationalizes its inhibitory action on AChE and its hydrolysis by butyrylcholinesterase and carboxylesterase. *Chemico-Biological Interactions*, **2005**, 157-158, 153-7	5	11
117	Inhibition of acetylcholinesterase by the anticancer prodrug CPT-11. *Chemico-Biological Interactions* , **2005**, 157-158, 247-52	5	31

116	HalX: an open-source LIMS (Laboratory Information Management System) for small- to large-scale laboratories. *Acta Crystallographica Section D: Biological Crystallography*, **2005**, 61, 671-8		18
115	Three-dimensional structure determination of proteins related to human health in their functional context at The Israel Structural Proteomics Center (ISPC). This paper was presented at ICCBM10. *Acta Crystallographica Section D: Biological Crystallography*, **2005**, 61, 1364-72		4
114	Towards rationalization of crystallization screening for small- to medium-sized academic laboratories: the PACT/JCSG+ strategy. *Acta Crystallographica Section D: Biological Crystallography*, **2005**, 61, 1426-31		191
113	Analysis of genetic polymorphisms in acetylcholinesterase as reflected in different populations. *Current Alzheimer Research*, **2005**, 2, 207-18	3	12
112	FoldIndex: a simple tool to predict whether a given protein sequence is intrinsically unfolded. *Bioinformatics*, **2005**, 21, 3435-8	7.2	776
111	G protein-coupled receptors show unusual patterns of intrinsic unfolding. *Protein Engineering, Design and Selection*, **2005**, 18, 103-10	1.9	40
110	Three-dimensional structure of a halotolerant algal carbonic anhydrase predicts halotolerance of a mammalian homolog. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 7493-8	11.5	67
109	X-ray structure of human acid-beta-glucosidase covalently bound to conduritol-B-epoxide. Implications for Gaucher disease. *Journal of Biological Chemistry*, **2005**, 280, 23815-9	5.4	85
108	Molecular Determinants of Protein Halotolerance: Structural and Functional Studies of the Extremely Salt Tolerant Carbonic Anhydrases from Dunaliella salina **2005**, 503-515		
107	Natural protein engineering: a uniquely salt-tolerant, but not halophilic, alpha-type carbonic anhydrase from algae proliferating in low- to hyper-saline environments. *Protein Engineering, Design and Selection*, **2004**, 17, 191-200	1.9	25
106	The synaptic acetylcholinesterase tetramer assembles around a polyproline II helix. *EMBO Journal*, **2004**, 23, 4394-405	13	85
105	Structure and evolution of the serum paraoxonase family of detoxifying and anti-atherosclerotic enzymes. *Nature Structural and Molecular Biology*, **2004**, 11, 412-9	17.6	494
104	A paradigm for single nucleotide polymorphism analysis: the case of the acetylcholinesterase gene. *Human Mutation*, **2004**, 24, 408-16	4.7	20
103	Additivity of Cation–π Interactions: An ab Initio Computational Study on Cation–π–Cation Sandwich Complexes. *Journal of Physical Chemistry A*, **2004**, 108, 9400-9405	2.8	26
102	The complex of a bivalent derivative of galanthamine with torpedo acetylcholinesterase displays drastic deformation of the active-site gorge: implications for structure-based drug design. *Journal of the American Chemical Society*, **2004**, 126, 15405-11	16.4	106
101	Proteomic signatures: amino acid and oligopeptide compositions differentiate among phyla. *Proteins: Structure, Function and Bioinformatics*, **2004**, 54, 20-40	4.2	117
100	New directions in the treatment of Gaucher disease. *Trends in Pharmacological Sciences*, **2004**, 25, 147-51	13.2	91
99	Design and synthesis of peptides that bind alpha-bungarotoxin with high affinity and mimic the three-dimensional structure of the binding-site of acetylcholine receptor. *Biophysical Chemistry*, **2003**, 100, 293-305	3.5	23

98	Acetylcholinesterase: a multifaceted target for structure-based drug design of anticholinesterase agents for the treatment of Alzheimer's disease. *Journal of Molecular Neuroscience*, **2003**, 20, 369-83	3.3	85
97	The binding site of acetylcholine receptor: from synthetic peptides to solution and crystal structure. *Annals of the New York Academy of Sciences*, **2003**, 998, 93-100	6.5	18
96	Identification, cDNA cloning, expression, crystallization and preliminary X-ray analysis of an exceptionally halotolerant carbonic anhydrase from Dunaliella salina. *Acta Crystallographica Section D: Biological Crystallography*, **2003**, 59, 1084-6		8
95	The intracellular domain of the Drosophila cholinesterase-like neural adhesion protein, gliotactin, is natively unfolded. *Proteins: Structure, Function and Bioinformatics*, **2003**, 53, 758-67	4.2	52
94	X-ray structure of human acid-beta-glucosidase, the defective enzyme in Gaucher disease. *EMBO Reports*, **2003**, 4, 704-9	6.5	218
93	How does huperzine A enter and leave the binding gorge of acetylcholinesterase? Steered molecular dynamics simulations. *Journal of the American Chemical Society*, **2003**, 125, 11340-9	16.4	87
92	An unusual halotolerant alpha-type carbonic anhydrase from the alga Dunaliella salina functionally expressed in Escherichia coli. *Protein Expression and Purification*, **2003**, 28, 151-7	2	38
91	Acetylcholinesterase complexed with bivalent ligands related to huperzine a: experimental evidence for species-dependent protein-ligand complementarity. *Journal of the American Chemical Society*, **2003**, 125, 363-73	16.4	86
90	Structure of a complex of the potent and specific inhibitor BW284C51 with Torpedo californica acetylcholinesterase. *Acta Crystallographica Section D: Biological Crystallography*, **2002**, 58, 1765-71		34
89	Evidence for the formation of disulfide radicals in protein crystals upon X-ray irradiation. *Journal of Synchrotron Radiation*, **2002**, 9, 342-6	2.4	59
88	STRUCTURAL FEATURE OF AChE INHIBITOR HUPERZINE B IN NATURE AND IN THE BINDING SITE OF AChE: DENSITY FUNCTIONAL THEORY STUDY COMBINED WITH IR DETERMINATION. *Journal of Theoretical and Computational Chemistry*, **2002**, 01, 81-92	1.8	
87	The Relationship between Binding Models of TMA with Furan and Imidazole and the Molecular Electrostatic Potentials: DFT and MP2 Computational Studies. *Journal of Physical Chemistry A*, **2002**, 106, 157-164	2.8	14
86	A neutral molecule in a cation-binding site: specific binding of a PEG-SH to acetylcholinesterase from Torpedo californica. *Journal of Molecular Biology*, **2002**, 320, 721-5	6.5	39
85	Histochemical method for characterization of enzyme crystals: application to crystals of Torpedo californica acetylcholinesterase. *Acta Crystallographica Section D: Biological Crystallography*, **2001**, 57, 1348-50		1
84	Noncovalent interaction or chemical bonding between alkaline earth cations and benzene? A quantum chemistry study using MP2 and density-functional theory methods. *Chemical Physics Letters*, **2001**, 349, 113-122	2.5	47
83	Theoretical Insight into the Interactions of TMA-Benzene and TMA-Pyrrole with B3LYP Density-Functional Theory (DFT) and ab Initio Second Order Møller-Plesset Perturbation Theory (MP2) Calculations. *Journal of Physical Chemistry A*, **2001**, 105, 5431-5437	2.8	40
82	Quantum/Classical Mechanical Comparison of Cation-π Interactions between Tetramethylammonium and Benzene. *Journal of Physical Chemistry A*, **2001**, 105, 1326-1333	2.8	63
81	A structure-based design approach to the development of novel, reversible AChE inhibitors. *Journal of Medicinal Chemistry*, **2001**, 44, 3203-15	8.3	49

80	The binding site of acetylcholine receptor as visualized in the X-Ray structure of a complex between alpha-bungarotoxin and a mimotope peptide. *Neuron*, **2001**, 32, 265-75	13.9	110
79	Structural studies on vertebrate and invertebrate acetylcholinesterases and their complexes with functional ligands. *Drug Development Research*, **2000**, 50, 573-583	5.1	11
78	AutoDep: a web-based system for deposition and validation of macromolecular structural -information. *Acta Crystallographica Section D: Biological Crystallography*, **2000**, 56, 828-41		12
77	Structures of recombinant native and E202Q mutant human acetylcholinesterase complexed with the snake-venom toxin fasciculin-II. *Acta Crystallographica Section D: Biological Crystallography*, **2000**, 56, 1385-94		229
76	Apotheosis, not apocalypse: methods in protein crystallography. *Acta Crystallographica Section D: Biological Crystallography*, **2000**, 56, 1510-1		3
75	Three-dimensional structures of Drosophila melanogaster acetylcholinesterase and of its complexes with two potent inhibitors. *Protein Science*, **2000**, 9, 1063-72	6.3	246
74	Specific chemical and structural damage to proteins produced by synchrotron radiation. *Proceedings of the National Academy of Sciences of the United States of America*, **2000**, 97, 623-8	11.5	383
73	Active-site gorge and buried water molecules in crystal structures of acetylcholinesterase from Torpedo californica. *Journal of Molecular Biology*, **2000**, 296, 713-35	6.5	128
72	How Does Ammonium Interact with Aromatic Groups? A Density Functional Theory (DFT/B3LYP) Investigation. *Journal of Physical Chemistry A*, **2000**, 104, 9573-9580	2.8	64
71	A preliminary comparison of structural models for catalytic intermediates of acetylcholinesterase. *Chemico-Biological Interactions*, **1999**, 119-120, 43-52	5	25
70	Structure of acetylcholinesterase complexed with E2020 (Aricept): implications for the design of new anti-Alzheimer drugs. *Structure*, **1999**, 7, 297-307	5.2	571
69	Crystal structures of aged phosphonylated acetylcholinesterase: nerve agent reaction products at the atomic level. *Biochemistry*, **1999**, 38, 7032-9	3.2	248
68	Structure of acetylcholinesterase complexed with (-)-galanthamine at 2.3 A resolution. *FEBS Letters*, **1999**, 463, 321-6	3.8	220
67	A modular treatment of molecular traffic through the active site of cholinesterase. *Biophysical Journal*, **1999**, 77, 2430-50	2.9	46
66	Reaction Products of Acetylcholinesterase and VX Reveal a Mobile Histidine in the Catalytic Triad. *Journal of the American Chemical Society*, **1999**, 121, 9883-9884	16.4	142
65	Effect of mutations within the peripheral anionic site on the stability of acetylcholinesterase. *Molecular Pharmacology*, **1999**, 55, 982-92	4.3	36
64	Three-dimensional structure of a complex of E2020 with acetylcholinesterase from Torpedo californica. *Journal of Physiology (Paris)*, **1998**, 92, 191-4		75
63	Static Laue diffraction studies on acetylcholinesterase. *Acta Crystallographica Section D: Biological Crystallography*, **1998**, 54, 1359-66		26

62	Protein Data Bank (PDB): database of three-dimensional structural information of biological macromolecules. *Acta Crystallographica Section D: Biological Crystallography*, **1998**, 54, 1078-84		383
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