Giuseppina De Simone

List of Publications by Year in Descending Order

155 papers	7,529 citations	45 h-index	83 g-index
163 ext. papers	8,098 ext. citations	5.6 avg, IF	5.92 L-index

#	Paper	IF	Citations
155	Interaction Studies between Carbonic Anhydrase and a Sulfonamide Inhibitor by Experimental and Theoretical Approaches. *ACS Medicinal Chemistry Letters*, **2022**, 13, 271-277	4.3	1
154	Sultam based Carbonic Anhydrase VII inhibitors for the management of neuropathic pain. *European Journal of Medicinal Chemistry*, **2022**, 227, 113956	6.8	1
153	Inhibition of carbonic anhydrases IX/XII by SLC-0111 boosts cisplatin effects in hampering head and neck squamous carcinoma cell growth and invasion.. *Journal of Experimental and Clinical Cancer Research*, **2022**, 41, 122	12.8	2
152	Beta-Carbonic Anhydrase 1 from Trichomonas Vaginalis as New Antiprotozoan Drug Target. *Topics in Medicinal Chemistry*, **2021**, 1	0.4	
151	Post-translational modifications in tumor-associated carbonic anhydrases. *Amino Acids*, **2021**,	3.5	5
150	Inhibition of the Ecarbonic anhydrase from the protozoan pathogen with sulphonamides. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2021**, 36, 329-334	5.6	3
149	Benzyl alcohol inhibits carbonic anhydrases by anchoring to the zinc coordinated water molecule. *Biochemical and Biophysical Research Communications*, **2021**, 548, 217-221	3.4	4
148	Intrinsically disordered features of carbonic anhydrase IX proteoglycan-like domain. *Cellular and Molecular Life Sciences*, **2021**, 78, 2059-2067	10.3	2
147	Zeta-carbonic anhydrases show CS hydrolase activity: A new metabolic carbon acquisition pathway in diatoms?. *Computational and Structural Biotechnology Journal*, **2021**, 19, 3427-3436	6.8	4
146	The crystal structures of 2-(4-benzhydrylpiperazin-1-yl)-N-(4-sulfamoylphenyl)acetamide in complex with human carbonic anhydrase II and VII provide insights into selective CA inhibitor development. *New Journal of Chemistry*, **2021**, 45, 147-152	3.6	1
145	Design, synthesis and biochemical evaluation of novel carbonic anhydrase inhibitors triggered by structural knowledge on hCA VII. *Bioorganic and Medicinal Chemistry*, **2021**, 44, 116279	3.4	0
144	Phenyl(thio)phosphon(amid)ate Benzenesulfonamides as Potent and Selective Inhibitors of Human Carbonic Anhydrases II and VII Counteract Allodynia in a Mouse Model of Oxaliplatin-Induced Neuropathy. *Journal of Medicinal Chemistry*, **2020**, 63, 5185-5200	8.3	6
143	2-Mercaptobenzoxazoles: a class of carbonic anhydrase inhibitors with a novel binding mode to the enzyme active site. *Chemical Communications*, **2020**, 56, 8297-8300	5.8	3
142	Biochemical and structural characterisation of a protozoan beta-carbonic anhydrase from. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2020**, 35, 1292-1299	5.6	18
141	Looking toward the Rim of the Active Site Cavity of Druggable Human Carbonic Anhydrase Isoforms. *ACS Medicinal Chemistry Letters*, **2020**, 11, 1000-1005	4.3	1
140	Inhibition of the newly discovered Ecarbonic anhydrase from the protozoan pathogen Trichomonas vaginalis with inorganic anions and small molecules. *Journal of Inorganic Biochemistry*, **2020**, 213, 111274	4.2	8
139	Human carbonic anhydrases and post-translational modifications: a hidden world possibly affecting protein properties and functions. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2020**, 35, 1450-1461	5.6	11

138	A Novel Inhibitor of Carbonic Anhydrases Prevents Hypoxia-Induced TNBC Cell Plasticity. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	5
137	Carbonic Anhydrase Inhibitors Targeting Metabolism and Tumor Microenvironment. *Metabolites*, **2020**, 10,	5.6	70
136	Catechols: a new class of carbonic anhydrase inhibitors. *Chemical Communications*, **2020**, 56, 13033-13036	5.8	13
135	Exploration of the residues modulating the catalytic features of human carbonic anhydrase XIII by a site-specific mutagenesis approach. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2019**, 34, 1506-1510	5.6	6
134	Carbonic anhydrases **2019**, 131-137		
133	Carbonic anhydrases **2019**, 19-54		1
132	and carbonic anhydrases **2019**, 139-148		
131	Biochemical and Structural Insights into Carbonic Anhydrase XII/Fab6A10 Complex. *Journal of Molecular Biology*, **2019**, 431, 4910-4921	6.5	13
130	Exploring benzoxaborole derivatives as carbonic anhydrase inhibitors: a structural and computational analysis reveals their conformational variability as a tool to increase enzyme selectivity. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2019**, 34, 1498-1505	5.6	5
129	Targeted treatment of anaerobic cancer. Patent evaluation of US2016279084 and US2017056350. *Expert Opinion on Therapeutic Patents*, **2019**, 29, 1-6	6.8	4
128	Exploring structural properties of potent human carbonic anhydrase inhibitors bearing a 4-(cycloalkylamino-1-carbonyl)benzenesulfonamide moiety. *European Journal of Medicinal Chemistry*, **2019**, 163, 443-452	6.8	16
127	Inhibition of carbonic anhydrase IX targets primary tumors, metastases, and cancer stem cells: Three for the price of one. *Medicinal Research Reviews*, **2018**, 38, 1799-1836	14.4	159
126	Biochemical, biophysical and molecular dynamics studies on the proteoglycan-like domain of carbonic anhydrase IX. *Cellular and Molecular Life Sciences*, **2018**, 75, 3283-3296	10.3	13
125	The Crystal Structure of a hCA VII Variant Provides Insights into the Molecular Determinants Responsible for Its Catalytic Behavior. *International Journal of Molecular Sciences*, **2018**, 19,	6.3	19
124	Inhibition of carbonic anhydrases by a substrate analog: benzyl carbamate directly coordinates the catalytic zinc ion mimicking bicarbonate binding. *Chemical Communications*, **2018**, 54, 10312-10315	5.8	14
123	Are Carbonic Anhydrases Suitable Targets to Fight Protozoan Parasitic Diseases?. *Current Medicinal Chemistry*, **2018**, 25, 5266-5278	4.3	18
122	Crystal structure of the human carbonic anhydrase II adduct with 1-(4-sulfamoylphenyl-ethyl)-2,4,6-triphenylpyridinium perchlorate, a membrane-impermeant, isoform selective inhibitor. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2018**, 33, 151-157	5.6	24
121	Protective Role of Carbonic Anhydrases III and VII in Cellular Defense Mechanisms upon Redox Unbalance. *Oxidative Medicine and Cellular Longevity*, **2018**, 2018, 2018306	6.7	19

120	Disclosing the Interaction of Carbonic Anhydrase IX with Cullin-Associated NEDD8-Dissociated Protein 1 by Molecular Modeling and Integrated Binding Measurements. *ACS Chemical Biology*, **2017**, 12, 1460-1465	4.9	13
119	Probing Molecular Interactions between Human Carbonic Anhydrases (hCAs) and a Novel Class of Benzenesulfonamides. *Journal of Medicinal Chemistry*, **2017**, 60, 4316-4326	8.3	30
118	Insights into the role of reactive sulfhydryl groups of Carbonic Anhydrase III and VII during oxidative damage. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2017**, 32, 5-12	5.6	26
117	Insights into the binding mode of sulphamates and sulphamides to hCA II: crystallographic studies and binding free energy calculations. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2017**, 32, 1002-1011	5.6	25
116	Cloning, expression and purification of the complete domain of the β-carbonic anhydrase from Plasmodium falciparum. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2016**, 31, 54-59	5.6	50
115	Kinetic and X-ray crystallographic investigations of substituted 2-thio-6-oxo-1,6-dihydropyrimidine-benzenesulfonamides acting as carbonic anhydrase inhibitors. *Bioorganic and Medicinal Chemistry*, **2016**, 24, 3643-8	3.4	12
114	L-Histidinol Dehydrogenase as a New Target for Old Diseases. *Current Topics in Medicinal Chemistry*, **2016**, 16, 2369-78	3	5
113	A Combined Crystallographic and Theoretical Study Explains the Capability of Carboxylic Acids to Adopt Multiple Binding Modes in the Active Site of Carbonic Anhydrases. *Chemistry - A European Journal*, **2016**, 22, 97-100	4.8	34
112	The anticonvulsant sulfamide JNJ-26990990 and its S,S-dioxide analog strongly inhibit carbonic anhydrases: solution and X-ray crystallographic studies. *Organic and Biomolecular Chemistry*, **2016**, 14, 4853-8	3.9	21
111	Benzoxaborole as a new chemotype for carbonic anhydrase inhibition. *Chemical Communications*, **2016**, 52, 11983-11986	5.8	60
110	X-ray crystallographic and kinetic investigations of 6-sulfamoyl-saccharin as a carbonic anhydrase inhibitor. *Organic and Biomolecular Chemistry*, **2015**, 13, 4064-9	3.9	18
109	Discovery of 1,1SBiphenyl-4-sulfonamides as a New Class of Potent and Selective Carbonic Anhydrase XIV Inhibitors. *Journal of Medicinal Chemistry*, **2015**, 58, 8564-72	8.3	34
108	Out of the active site binding pocket for carbonic anhydrase inhibitors. *Chemical Communications*, **2015**, 51, 302-5	5.8	96
107	Carbonic Anhydrase VII **2015**, 151-168		1
106	Carbonic Anhydrase II as Target for Drug Design **2015**, 51-90		2
105	Human Carbonic Anhydrases: Catalytic Properties, Structural Features, and Tissue Distribution **2015**, 17-30		5
104	Thermostable Carbonic Anhydrases in Biotechnological Applications. *International Journal of Molecular Sciences*, **2015**, 16, 15456-80	6.3	50
103	Cadmium-containing carbonic anhydrase CDCA1 in marine diatom Thalassiosira weissflogii. *Marine Drugs*, **2015**, 13, 1688-97	6	34

102	Hydroxylamine-O-sulfonamide is a versatile lead compound for the development of carbonic anhydrase inhibitors. *Chemical Communications*, **2015**, 51, 11519-22	5.8	9
101	The zinc coordination pattern in the Ecarbonic anhydrase from Plasmodium falciparum is different from all other carbonic anhydrase genetic families. *Bioorganic and Medicinal Chemistry Letters*, **2015**, 25, 1385-9	2.9	95
100	Crystal structure of the most catalytically effective carbonic anhydrase enzyme known, SazCA from the thermophilic bacterium Sulfurihydrogenibium azorense. *Bioorganic and Medicinal Chemistry Letters*, **2015**, 25, 2002-6	2.9	60
99	Carbonic Anhydrases: An Overview **2015**, 3-13		11
98	CDCA1 From Thalassiosira weissflogii as Representative Member of ECclass CAs: General Features and Biotechnological Applications **2015**, 351-359		
97	Sulfolobus solfataricus thiol redox puzzle: characterization of an atypical protein disulfide oxidoreductase. *Extremophiles*, **2014**, 18, 219-28	3	9
96	Biochemical characterization of the chloroplastic Ecarbonic anhydrase from Flaveria bidentis (L.) "Kuntze". *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2014**, 29, 500-4	5.6	16
95	Thermal-stable carbonic anhydrases: a structural overview. *Sub-Cellular Biochemistry*, **2014**, 75, 387-404	5.5	6
94	Hydrophobic substituents of the phenylmethylsulfamide moiety can be used for the development of new selective carbonic anhydrase inhibitors. *BioMed Research International*, **2014**, 2014, 523210	3	12
93	The structural comparison between membrane-associated human carbonic anhydrases provides insights into drug design of selective inhibitors. *Biopolymers*, **2014**, 101, 769-78	2.2	39
92	High GADA titer increases the risk of insulin requirement in LADA patients: a 7-year follow-up (NIRAD study 7). *European Journal of Endocrinology*, **2014**, 171, 697-704	6.5	45
91	Structural basis for the rational design of new anti-Brucella agents: the crystal structure of the C366S mutant of L-histidinol dehydrogenase from Brucella suis. *Biochimie*, **2014**, 97, 114-20	4.6	8
90	Faox enzymes inhibited Maillard reaction development during storage both in protein glucose model system and low lactose UHT milk. *Amino Acids*, **2014**, 46, 279-88	3.5	23
89	Amine, amino acid and oligopeptide carbonic anhydrase activators **2014**, 142-156		
88	Exploiting the hydrophobic and hydrophilic binding sites for designing carbonic anhydrase inhibitors. *Expert Opinion on Drug Discovery*, **2013**, 8, 793-810	6.2	215
87	Characterization of carbonic anhydrase IX interactome reveals proteins assisting its nuclear localization in hypoxic cells. *Journal of Proteome Research*, **2013**, 12, 282-92	5.6	37
86	Kinetic and anion inhibition studies of a Ecarbonic anhydrase (FbiCA 1) from the C4 plant Flaveria bidentis. *Bioorganic and Medicinal Chemistry Letters*, **2013**, 23, 1626-30	2.9	33
85	Anticancer carbonic anhydrase inhibitors: a patent review (2008 - 2013). *Expert Opinion on Therapeutic Patents*, **2013**, 23, 737-49	6.8	208

84	Hypoxia-targeting carbonic anhydrase IX inhibitors by a new series of nitroimidazole-sulfonamides/sulfamides/sulfamates. *Journal of Medicinal Chemistry*, **2013**, 56, 8512-20	8.3	68
83	Human carbonic anhydrase VII protects cells from oxidative damage. *Biological Chemistry*, **2013**, 394, 1343-8	4.5	29
82	X-ray structure of the first extremo-carbonic anhydrase, a dimeric enzyme from the thermophilic bacterium Sulfurihydrogenibium yellowstonense YO3AOP1. *Acta Crystallographica Section D: Biological Crystallography*, **2013**, 69, 1150-9		89
81	Dithiocarbamates are strong inhibitors of the beta-class fungal carbonic anhydrases from Cryptococcus neoformans, Candida albicans and Candida glabrata. *Bioorganic and Medicinal Chemistry Letters*, **2012**, 22, 859-62	2.9	89
80	Carbonic anhydrase VII is S-glutathionylated without loss of catalytic activity and affinity for sulfonamide inhibitors. *Bioorganic and Medicinal Chemistry Letters*, **2012**, 22, 1560-4	2.9	46
79	(In)organic anions as carbonic anhydrase inhibitors. *Journal of Inorganic Biochemistry*, **2012**, 111, 117-29	4.2	173
78	Structural and inhibition insights into carbonic anhydrase CDCA1 from the marine diatom Thalassiosira weissflogii. *Biochimie*, **2012**, 94, 1232-41	4.6	88
77	Development of potent carbonic anhydrase inhibitors incorporating both sulfonamide and sulfamide groups. *Journal of Medicinal Chemistry*, **2012**, 55, 6776-83	8.3	43
76	Multiple binding modes of inhibitors to carbonic anhydrases: how to design specific drugs targeting 15 different isoforms?. *Chemical Reviews*, **2012**, 112, 4421-68	68.1	889
75	Hydroxamate represents a versatile zinc binding group for the development of new carbonic anhydrase inhibitors. *Chemical Communications*, **2012**, 48, 8838-40	5.8	58
74	Carbonic anhydrase IX as a target for designing novel anticancer drugs. *Current Medicinal Chemistry*, **2012**, 19, 821-30	4.3	44
73	C68 from the Sulfolobus islandicus plasmid-virus pSSVx is a novel member of the AbrB-like transcription factor family. *Biochemical Journal*, **2011**, 435, 157-66	3.8	22
72	Design, synthesis and characterization of a peptide able to bind proteins of the KCTD family: implications for KCTD-cullin 3 recognition. *Journal of Peptide Science*, **2011**, 17, 373-6	2.1	14
71	Carbonic anhydrase inhibitors: X-ray crystallographic studies for the binding of N-substituted benzenesulfonamides to human isoform II. *Chemical Communications*, **2011**, 47, 11636-8	5.8	42
70	Histone deacetylase and Cullin3-REN(KCTD11) ubiquitin ligase interplay regulates Hedgehog signalling through Gli acetylation. *Nature Cell Biology*, **2010**, 12, 132-42	23.4	252
69	Drug design studies of the novel antitumor targets carbonic anhydrase IX and XII. *Current Medicinal Chemistry*, **2010**, 17, 1516-26	4.3	88
68	Exploring the catalytic mechanism of the first dimeric Bcp: Functional, structural and docking analyses of Bcp4 from Sulfolobus solfataricus. *Biochimie*, **2010**, 92, 1435-44	4.6	20
67	The first example of a significant active site conformational rearrangement in a carbonic anhydrase-inhibitor adduct: the carbonic anhydrase I-topiramate complex. *Organic and Biomolecular Chemistry*, **2010**, 8, 3528-33	3.9	34

66	Recent advances in structural studies of the carbonic anhydrase family: the crystal structure of human CA IX and CA XIII. *Current Pharmaceutical Design*, **2010**, 16, 3246-54	3.3	27
65	Multiple catalytically active thioredoxin folds: a winning strategy for many functions. *Cellular and Molecular Life Sciences*, **2010**, 67, 3797-814	10.3	24
64	Crystal structure of an S-formylglutathione hydrolase from Pseudoalteromonas haloplanktis TAC125. *Biopolymers*, **2010**, 93, 669-77	2.2	17
63	Carbonic anhydrase IX: Biochemical and crystallographic characterization of a novel antitumor target. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2010**, 1804, 404-9	4	151
62	Carbonic anhydrase inhibitors: crystallographic and solution binding studies for the interaction of a boron-containing aromatic sulfamide with mammalian isoforms I-XV. *Bioorganic and Medicinal Chemistry Letters*, **2010**, 20, 3601-5	2.9	25
61	Inhibition of the R1 fragment of the cadmium-containing zeta-class carbonic anhydrase from the diatom Thalassiosira weissflogii with anions. *Bioorganic and Medicinal Chemistry Letters*, **2010**, 20, 4745-8	2.9	35
60	Crystal structure of the C183S/C217S mutant of human CA VII in complex with acetazolamide. *Bioorganic and Medicinal Chemistry Letters*, **2010**, 20, 5023-6	2.9	73
59	Crystal structure of the catalytic domain of the tumor-associated human carbonic anhydrase IX. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 16233-8	11.5	399
58	Crystal structure of human carbonic anhydrase XIII and its complex with the inhibitor acetazolamide. *Proteins: Structure, Function and Bioinformatics*, **2009**, 74, 164-75	4.2	90
57	Insights into the catalytic mechanism of the Bcp family: functional and structural analysis of Bcp1 from Sulfolobus solfataricus. *Proteins: Structure, Function and Bioinformatics*, **2009**, 76, 995-1006	4.2	22
56	Which carbonic anhydrases are targeted by the antiepileptic sulfonamides and sulfamates?. *Chemical Biology and Drug Design*, **2009**, 74, 317-21	2.9	62
55	The proteoglycan region of the tumor-associated carbonic anhydrase isoform IX acts as anintrinsic buffer optimizing CO2 hydration at acidic pH values characteristic of solid tumors. *Bioorganic and Medicinal Chemistry Letters*, **2009**, 19, 5825-8	2.9	73
54	Structural analysis of BldR from Sulfolobus solfataricus provides insights into the molecular basis of transcriptional activation in Archaea by MarR family proteins. *Journal of Molecular Biology*, **2009**, 388, 559-69	6.5	29
53	Carbonic anhydrase inhibitors. Comparison of aliphatic sulfamate/bis-sulfamate adducts with isozymes II and IX as a platform for designing tight-binding, more isoform-selective inhibitors. *Journal of Medicinal Chemistry*, **2009**, 52, 5990-8	8.3	19
52	Biochemical characterization of CA IX, one of the most active carbonic anhydrase isozymes. *Journal of Biological Chemistry*, **2008**, 283, 27799-27809	5.4	224
51	Carbonic anhydrase inhibitors: bioreductive nitro-containing sulfonamides with selectivity for targeting the tumor associated isoforms IX and XII. *Journal of Medicinal Chemistry*, **2008**, 51, 3230-7	8.3	46
50	Structure-activity relationships of C-17 cyano-substituted estratrienes as anticancer agents. *Journal of Medicinal Chemistry*, **2008**, 51, 1295-308	8.3	47
49	Anticancer steroid sulfatase inhibitors: synthesis of a potent fluorinated second-generation agent, in vitro and in vivo activities, molecular modeling, and protein crystallography. *Molecular Cancer Therapeutics*, **2008**, 7, 2435-44	6.1	37

48	Recent advances in research on the most novel carbonic anhydrases, CA XIII and XV. *Current Pharmaceutical Design*, **2008**, 14, 672-8	3.3	64
47	Are carbonic anhydrase inhibitors suitable for obtaining antiobesity drugs?. *Current Pharmaceutical Design*, **2008**, 14, 655-60	3.3	137
46	Functional and structural features of the oxyanion hole in a thermophilic esterase from Alicyclobacillus acidocaldarius. *Proteins: Structure, Function and Bioinformatics*, **2008**, 71, 1721-31	4.2	26
45	Carbonic anhydrase inhibitors: binding of indanesulfonamides to the human isoform II. *ChemMedChem*, **2008**, 3, 473-7	3.7	10
44	Investigations of the esterase, phosphatase, and sulfatase activities of the cytosolic mammalian carbonic anhydrase isoforms I, II, and XIII with 4-nitrophenyl esters as substrates. *Bioorganic and Medicinal Chemistry Letters*, **2008**, 18, 2267-71	2.9	88
43	Carbonic anhydrase inhibitors: the X-ray crystal structure of ethoxzolamide complexed to human isoform II reveals the importance of thr200 and gln92 for obtaining tight-binding inhibitors. *Bioorganic and Medicinal Chemistry Letters*, **2008**, 18, 2669-74	2.9	30
42	Carbonic anhydrase inhibitors as emerging drugs for the treatment of obesity. *Expert Opinion on Emerging Drugs*, **2008**, 13, 383-92	3.7	139
41	Molecular modeling study for the binding of zonisamide and topiramate to the human mitochondrial carbonic anhydrase isoform VA. *Bioorganic and Medicinal Chemistry*, **2007**, 15, 4152-8	3.4	34
40	Carbonic anhydrase inhibitors: binding of an antiglaucoma glycosyl-sulfanilamide derivative to human isoform II and its consequences for the drug design of enzyme inhibitors incorporating sugar moieties. *Bioorganic and Medicinal Chemistry Letters*, **2007**, 17, 1726-31	2.9	35
39	Carbonic anhydrase inhibitors: inhibition of human, bacterial, and archaeal isozymes with benzene-1,3-disulfonamides--solution and crystallographic studies. *Bioorganic and Medicinal Chemistry Letters*, **2007**, 17, 4201-7	2.9	45
38	Antiobesity carbonic anhydrase inhibitors. *Current Topics in Medicinal Chemistry*, **2007**, 7, 879-84	3	82
37	Carbonic anhydrase inhibitors: Valdecoxib binds to a different active site region of the human isoform II as compared to the structurally related cyclooxygenase II "selective" inhibitor celecoxib. *Bioorganic and Medicinal Chemistry Letters*, **2006**, 16, 437-42	2.9	89
36	Carbonic anhydrase inhibitors: X-ray crystallographic studies for the binding of 5-amino-1,3,4-thiadiazole-2-sulfonamide and 5-(4-amino-3-chloro-5-fluorophenylsulfonamido)-1,3,4-thiadiazole-2-sulfonamide to human isoform II. *Bioorganic and Medicinal Chemistry Letters*, **2006**, 16, 6204-8	2.9	31
35	2-substituted estradiol bis-sulfamates, multitargeted antitumor agents: synthesis, in vitro SAR, protein crystallography, and in vivo activity. *Journal of Medicinal Chemistry*, **2006**, 49, 7683-96	8.3	91
34	Carbonic anhydrase inhibitors: Hypoxia-activatable sulfonamides incorporating disulfide bonds that target the tumor-associated isoform IX. *Journal of Medicinal Chemistry*, **2006**, 49, 5544-51	8.3	93
33	Carbonic anhydrase inhibitors: X-ray and molecular modeling study for the interaction of a fluorescent antitumor sulfonamide with isozyme II and IX. *Journal of the American Chemical Society*, **2006**, 128, 8329-35	16.4	186
32	Metal ion substitution in the catalytic site greatly affects the binding of sulfhydryl-containing compounds to leucyl aminopeptidase. *Biochemistry*, **2006**, 45, 3226-34	3.2	30
31	Insights on a new PDI-like family: structural and functional analysis of a protein disulfide oxidoreductase from the bacterium Aquifex aeolicus. *Journal of Molecular Biology*, **2006**, 356, 155-64	6.5	26

30	A novel member of the protein disulfide oxidoreductase family from Aeropyrum pernix K1: structure, function and electrostatics. *Journal of Molecular Biology*, **2006**, 362, 743-52	6.5	20
29	Carbonic anhydrase inhibitors: stacking with Phe131 determines active site binding region of inhibitors as exemplified by the X-ray crystal structure of a membrane-impermeant antitumor sulfonamide complexed with isozyme II. *Journal of Medicinal Chemistry*, **2005**, 48, 5721-7	8.3	150
28	Carbonic anhydrase inhibitors: X-ray crystal structure of a benzenesulfonamide strong CA II and CA IX inhibitor bearing a pentafluorophenylaminothioureido tail in complex with isozyme II. *Bioorganic and Medicinal Chemistry Letters*, **2005**, 15, 1937-42	2.9	38
27	Carbonic anhydrase inhibitors. Zonisamide is an effective inhibitor of the cytosolic isozyme II and mitochondrial isozyme V: solution and X-ray crystallographic studies. *Bioorganic and Medicinal Chemistry Letters*, **2005**, 15, 2315-20	2.9	166
26	Crystallization and preliminary X-ray diffraction studies of a protein disulfide oxidoreductase from Aeropyrum pernix K1. *Acta Crystallographica Section F: Structural Biology Communications*, **2005**, 61, 335-6		4
25	A substrate-induced switch in the reaction mechanism of a thermophilic esterase: kinetic evidences and structural basis. *Journal of Biological Chemistry*, **2004**, 279, 6815-23	5.4	37
24	Crystallization and preliminary X-ray diffraction studies of a protein disulfide oxidoreductase from Aquifex aeolicus. *Acta Crystallographica Section D: Biological Crystallography*, **2004**, 60, 2076-7		6
23	The crystal structure of an EST2 mutant unveils structural insights on the H group of the carboxylesterase/lipase family. *Journal of Molecular Biology*, **2004**, 343, 137-46	6.5	24
22	Design of weakly basic thrombin inhibitors incorporating novel P1 binding functions: molecular and X-ray crystallographic studies. *Biochemistry*, **2003**, 42, 9013-21	3.2	13
21	Crystallization and preliminary X-ray diffraction studies of Aes acetyl-esterase from Escherichia coli. *Acta Crystallographica Section D: Biological Crystallography*, **2003**, 59, 1846-8		2
20	An integrated structural and computational study of the thermostability of two thioredoxin mutants from Alicyclobacillus acidocaldarius. *Journal of Bacteriology*, **2003**, 185, 4285-9	3.5	8
19	Insights into peptide nucleic acid (PNA) structural features: the crystal structure of a D-lysine-based chiral PNA-DNA duplex. *Proceedings of the National Academy of Sciences of the United States of America*, **2003**, 100, 12021-6	11.5	134
18	Crystallization and preliminary X-ray diffraction studies of a D-lysine-based chiral PNA-DNA duplex. *Acta Crystallographica Section D: Biological Crystallography*, **2002**, 58, 553-5		4
17	The crystal structure of a hyper-thermophilic carboxylesterase from the archaeon Archaeoglobus fulgidus. *Journal of Molecular Biology*, **2001**, 314, 507-18	6.5	137
16	The crystal structure of Afc-containing peptides. *Biopolymers*, **2000**, 53, 150-60	2.2	12
15	A snapshot of a transition state analogue of a novel thermophilic esterase belonging to the subfamily of mammalian hormone-sensitive lipase. *Journal of Molecular Biology*, **2000**, 303, 761-71	6.5	117
14	The crystal structure of alpha-thrombin-hirunorm IV complex reveals a novel specificity site recognition mode. *Protein Science*, **1999**, 8, 91-5	6.3	6
13	Crystallization and preliminary X-ray diffraction studies of the carboxylesterase EST2 from Alicyclobacillus acidocaldarius. *Acta Crystallographica Section D: Biological Crystallography*, **1999**, 55, 1348-9		13

12	From natural to synthetic multisite thrombin inhibitors. *Biopolymers*, **1999**, 51, 19-39	2.2	20
11	Probing the reactivity of nucleophile residues in human 2,3-diphosphoglycerate/deoxy-hemoglobin complex by aspecific chemical modifications. *FEBS Letters*, **1999**, 452, 190-4	3.8	12
10	Hirunorms are true hirudin mimetics. The crystal structure of human alpha-thrombin-hirunorm V complex. *Protein Science*, **1998**, 7, 243-53	6.3	12
9	Human alpha-thrombin inhibition by the highly selective compounds N-ethoxycarbonyl-D-Phe-Pro-alpha-azaLys p-nitrophenyl ester and N-carbobenzoxy-Pro-alpha-azaLys p-nitrophenyl ester: a kinetic, thermodynamic and X-ray crystallographic study. *Journal of Molecular Biology*, **1997**, 269, 558-69	6.5	14
8	Functionalized cyclodextrins: Synthesis and structural characterization of 6-deoxy-6-{4-[N-tert-butoxycarbonyl-2-aminoethyl]-imidazolyl}-cyclomaltoheptaose. *Supramolecular Chemistry*, **1996**, 7, 47-54	1.8	15
7	Conformational studies of heterochiral peptides with diastereoisomeric residues: crystal and molecular structures of linear dipeptides derived from leucine, isoleucine, and allo-isoleucine. *Biopolymers*, **1995**, 36, 401-8	2.2	5
6	Comparative effects on blood pressure and regional hemodynamics of nicardipine and captopril. *Journal of Cardiovascular Pharmacology*, **1991**, 18, 807-12	3.1	4
5	Responses of serum insulin and blood pressure to cold and handgrip in obese patients. *International Journal of Cardiology*, **1991**, 32, 353-9	3.2	3
4	Cardiovascular response to adrenergic stimulation during treatment with tertatolol. A new non-cardioselective beta-blocking agent in primary hypertensive patients. *International Heart Journal*, **1991**, 32, 435-44		1
3	Advances in the Inhibitory and Structural Investigations on Carbonic Anhydrase Isozymes XIII and XV273-283		
2	X-Ray Crystallography of Carbonic Anhydrase Inhibitors and Its Importance in Drug Design138-66		10
1	Drug Design of Antiobesity Carbonic Anhydrase Inhibitors241-254		2