

Giuseppina De Simone

List of Publications by Year in descending order

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158
papers

8,766
citations

47004

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163
all docs

163
docs citations

163
times ranked

6067
citing authors

#	ARTICLE	IF	CITATIONS
1	Multiple Binding Modes of Inhibitors to Carbonic Anhydrases: How to Design Specific Drugs Targeting 15 Different Isoforms?. <i>Chemical Reviews</i> , 2012, 112, 4421-4468.	47.7	1,056
2	Crystal structure of the catalytic domain of the tumor-associated human carbonic anhydrase IX. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 16233-16238.	7.1	451
3	Histone deacetylase and Cullin3-RING1 ubiquitin ligase interplay regulates Hedgehog signalling through Gli acetylation. <i>Nature Cell Biology</i> , 2010, 12, 132-142.	10.3	292
4	Biochemical Characterization of CA IX, One of the Most Active Carbonic Anhydrase Isozymes. <i>Journal of Biological Chemistry</i> , 2008, 283, 27799-27809.	3.4	258
5	Exploiting the hydrophobic and hydrophilic binding sites for designing carbonic anhydrase inhibitors. <i>Expert Opinion on Drug Discovery</i> , 2013, 8, 793-810.	5.0	229
6	Anticancer carbonic anhydrase inhibitors: a patent review (2008 - 2013). <i>Expert Opinion on Therapeutic Patents</i> , 2013, 23, 737-749.	5.0	226
7	Inhibition of carbonic anhydrase IX targets primary tumors, metastases, and cancer stem cells: Three for the price of one. <i>Medicinal Research Reviews</i> , 2018, 38, 1799-1836.	10.5	207
8	Carbonic Anhydrase Inhibitors: An X-ray and Molecular Modeling Study for the Interaction of a Fluorescent Antitumor Sulfonamide with Isozyme II and IX. <i>Journal of the American Chemical Society</i> , 2006, 128, 8329-8335.	13.7	200
9	(In)organic anions as carbonic anhydrase inhibitors. <i>Journal of Inorganic Biochemistry</i> , 2012, 111, 117-129.	3.5	186
10	Carbonic anhydrase inhibitors. Zonisamide is an effective inhibitor of the cytosolic isozyme II and mitochondrial isozyme V: solution and X-ray crystallographic studies. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2005, 15, 2315-2320.	2.2	176
11	Carbonic anhydrase IX: Biochemical and crystallographic characterization of a novel antitumor target. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2010, 1804, 404-409.	2.3	166
12	Carbonic anhydrase inhibitors as emerging drugs for the treatment of obesity. <i>Expert Opinion on Emerging Drugs</i> , 2008, 13, 383-392.	2.4	165
13	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. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 5721-5727.	6.4	157
14	Are Carbonic Anhydrase Inhibitors Suitable for Obtaining Antiobesity Drugs ?. <i>Current Pharmaceutical Design</i> , 2008, 14, 655-660.	1.9	150
15	The crystal structure of a hyper-thermophilic carboxylesterase from the archaeon <i>Archaeoglobus fulgidus</i> 1 Edited by R. Huber. <i>Journal of Molecular Biology</i> , 2001, 314, 507-518.	4.2	148
16	Insights into peptide nucleic acid (PNA) structural features: The crystal structure of a D-lysine-based chiral PNA-DNA duplex. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2003, 100, 12021-12026.	7.1	143
17	A snapshot of a transition state analogue of a novel thermophilic esterase belonging to the subfamily of mammalian hormone-sensitive lipase 1 Edited by D. Rees. <i>Journal of Molecular Biology</i> , 2000, 303, 761-771.	4.2	128
18	Carbonic Anhydrase Inhibitors Targeting Metabolism and Tumor Microenvironment. <i>Metabolites</i> , 2020, 10, 412.	2.9	116

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19	Out of the active site binding pocket for carbonic anhydrase inhibitors. <i>Chemical Communications</i> , 2015, 51, 302-305.	4.1	111
20	The zinc coordination pattern in the β -carbonic anhydrase from <i>Plasmodium falciparum</i> is different from all other carbonic anhydrase genetic families. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2015, 25, 1385-1389.	2.2	108
21	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. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2008, 18, 2267-2271.	2.2	104
22	Carbonic Anhydrase Inhibitors: Hypoxia-Activatable Sulfonamides Incorporating Disulfide Bonds that Target the Tumor-Associated Isoform IX. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 5544-5551.	6.4	100
23	Drug Design Studies of the Novel Antitumor Targets Carbonic Anhydrase IX and XII. <i>Current Medicinal Chemistry</i> , 2010, 17, 1516-1526.	2.4	100
24	Structural and inhibition insights into carbonic anhydrase CDCA1 from the marine diatom <i>Thalassiosira weissflogii</i> . <i>Biochimie</i> , 2012, 94, 1232-1241.	2.6	100
25	X-ray structure of the first 'extremo- β -carbonic anhydrase', a dimeric enzyme from the thermophilic bacterium <i>Sulfurihydrogenibium yellowstonense</i> YO3AOP1. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013, 69, 1150-1159.	2.5	100
26	2-Substituted Estradiol Bis-sulfamates, Multitargeted Antitumor Agents: Synthesis, In Vitro SAR, Protein Crystallography, and In Vivo Activity. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 7683-7696.	6.4	98
27	Crystal structure of human carbonic anhydrase XIII and its complex with the inhibitor acetazolamide. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 74, 164-175.	2.6	97
28	Dithiocarbamates are strong inhibitors of the beta-class fungal carbonic anhydrases from <i>Cryptococcus neoformans</i> , <i>Candida albicans</i> and <i>Candida glabrata</i> . <i>Bioorganic and Medicinal Chemistry Letters</i> , 2012, 22, 859-862.	2.2	97
29	Antiobesity Carbonic Anhydrase Inhibitors. <i>Current Topics in Medicinal Chemistry</i> , 2007, 7, 879-884.	2.1	95
30	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. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2006, 16, 437-442.	2.2	93
31	Crystal structure of the C183S/C217S mutant of human CA VII in complex with acetazolamide. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2010, 20, 5023-5026.	2.2	81
32	The proteoglycan region of the tumor-associated carbonic anhydrase isoform IX acts as an intrinsic buffer optimizing CO ₂ hydration at acidic pH values characteristic of solid tumors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2009, 19, 5825-5828.	2.2	79
33	Hypoxia-Targeting Carbonic Anhydrase IX Inhibitors by a New Series of Nitroimidazole-Sulfonamides/Sulfamides/Sulfamates. <i>Journal of Medicinal Chemistry</i> , 2013, 56, 8512-8520.	6.4	76
34	Recent Advances in Research on the Most Novel Carbonic Anhydrases, CA XIII and XV. <i>Current Pharmaceutical Design</i> , 2008, 14, 672-678.	1.9	72
35	Which Carbonic Anhydrases are Targeted by the Antiepileptic Sulfonamides and Sulfamates?. <i>Chemical Biology and Drug Design</i> , 2009, 74, 317-321.	3.2	72
36	Crystal structure of the most catalytically effective carbonic anhydrase enzyme known, SazCA from the thermophilic bacterium <i>Sulfurihydrogenibium azorense</i> . <i>Bioorganic and Medicinal Chemistry Letters</i> , 2015, 25, 2002-2006.	2.2	72

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37	Benzoxaborole as a new chemotype for carbonic anhydrase inhibition. <i>Chemical Communications</i> , 2016, 52, 11983-11986.	4.1	69
38	Thermostable Carbonic Anhydrases in Biotechnological Applications. <i>International Journal of Molecular Sciences</i> , 2015, 16, 15456-15480.	4.1	66
39	Hydroxamate represents a versatile zinc binding group for the development of new carbonic anhydrase inhibitors. <i>Chemical Communications</i> , 2012, 48, 8838.	4.1	63
40	High GADA titer increases the risk of insulin requirement in LADA patients: a 7-year follow-up (NIRAD) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	3.7	63
41	Cloning, expression and purification of the complete domain of the α -carbonic anhydrase from <i>Plasmodium falciparum</i> . <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2016, 31, 54-59.	5.2	59
42	Carbonic anhydrase VII is S-glutathionylated without loss of catalytic activity and affinity for sulfonamide inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2012, 22, 1560-1564.	2.2	53
43	Development of Potent Carbonic Anhydrase Inhibitors Incorporating Both Sulfonamide and Sulfamide Groups. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 6776-6783.	6.4	52
44	Structure-Activity Relationships of C-17 Cyano-Substituted Estratrienes as Anticancer Agents. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 1295-1308.	6.4	50
45	Carbonic anhydrase inhibitors: X-ray crystallographic studies for the binding of N-substituted benzenesulfonamides to human isoform II. <i>Chemical Communications</i> , 2011, 47, 11636.	4.1	50
46	Carbonic Anhydrase IX as a Target for Designing Novel Anticancer Drugs. <i>Current Medicinal Chemistry</i> , 2012, 19, 821-830.	2.4	50
47	Carbonic Anhydrase Inhibitors: Bioreductive Nitro-Containing Sulfonamides with Selectivity for Targeting the Tumor Associated Isoforms IX and XII. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 3230-3237.	6.4	49
48	Cadmium-Containing Carbonic Anhydrase CDCA1 in Marine Diatom <i>Thalassiosira weissflogii</i> . <i>Marine Drugs</i> , 2015, 13, 1688-1697.	4.6	48
49	Carbonic anhydrase inhibitors: Inhibition of human, bacterial, and archaeal isozymes with benzene-1,3-disulfonamides—Solution and crystallographic studies. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2007, 17, 4201-4207.	2.2	47
50	A Substrate-induced Switch in the Reaction Mechanism of a Thermophilic Esterase. <i>Journal of Biological Chemistry</i> , 2004, 279, 6815-6823.	3.4	45
51	The structural comparison between membrane-associated human carbonic anhydrases provides insights into drug design of selective inhibitors. <i>Biopolymers</i> , 2014, 101, 769-778.	2.4	44
52	Characterization of Carbonic Anhydrase IX Interactome Reveals Proteins Assisting Its Nuclear Localization in Hypoxic Cells. <i>Journal of Proteome Research</i> , 2013, 12, 282-292.	3.7	43
53	A Combined Crystallographic and Theoretical Study Explains the Capability of Carboxylic Acids to Adopt Multiple Binding Modes in the Active Site of Carbonic Anhydrases. <i>Chemistry - A European Journal</i> , 2016, 22, 97-100.	3.3	43
54	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. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2005, 15, 1937-1942.	2.2	40

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55	The first example of a significant active site conformational rearrangement in a carbonic anhydrase-inhibitor adduct: the carbonic anhydrase α -topiramate complex. <i>Organic and Biomolecular Chemistry</i> , 2010, 8, 3528.	2.8	40
56	Discovery of 1,1'-Biphenyl-4-sulfonamides as a New Class of Potent and Selective Carbonic Anhydrase XIV Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 8564-8572.	6.4	40
57	Probing Molecular Interactions between Human Carbonic Anhydrases (hCAs) and a Novel Class of Benzenesulfonamides. <i>Journal of Medicinal Chemistry</i> , 2017, 60, 4316-4326.	6.4	40
58	Anticancer steroid sulfatase inhibitors: synthesis of a potent fluorinated second-generation agent, <i>in vitro</i> and <i>in vivo</i> activities, molecular modeling, and protein crystallography. <i>Molecular Cancer Therapeutics</i> , 2008, 7, 2435-2444.	4.1	39
59	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. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2007, 17, 1726-1731.	2.2	38
60	Inhibition of the R1 fragment of the cadmium-containing α -class carbonic anhydrase from the diatom <i>Thalassiosira weissflogii</i> with anions. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2010, 20, 4745-4748.	2.2	38
61	Kinetic and anion inhibition studies of a β -carbonic anhydrase (FbiCA 1) from the C4 plant <i>Flaveria bidentis</i> . <i>Bioorganic and Medicinal Chemistry Letters</i> , 2013, 23, 1626-1630.	2.2	38
62	Molecular modeling study for the binding of zonisamide and topiramate to the human mitochondrial carbonic anhydrase isoform VA. <i>Bioorganic and Medicinal Chemistry</i> , 2007, 15, 4152-4158.	3.0	37
63	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. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2008, 18, 2669-2674.	2.2	35
64	Insights into the role of reactive sulfhydryl groups of Carbonic Anhydrase III and VII during oxidative damage. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2017, 32, 5-12.	5.2	35
65	Metal Ion Substitution in the Catalytic Site Greatly Affects the Binding of Sulfhydryl-Containing Compounds to Leucyl Aminopeptidase. <i>Biochemistry</i> , 2006, 45, 3226-3234.	2.5	34
66	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. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2006, 16, 6204-6208.	2.2	32
67	Recent Advances in Structural Studies of the Carbonic Anhydrase Family: The Crystal Structure of Human CA IX and CA XIII. <i>Current Pharmaceutical Design</i> , 2010, 16, 3246-3254.	1.9	32
68	Protective Role of Carbonic Anhydrases III and VII in Cellular Defense Mechanisms upon Redox Unbalance. <i>Oxidative Medicine and Cellular Longevity</i> , 2018, 2018, 1-9.	4.0	32
69	Functional and structural features of the oxyanion hole in a thermophilic esterase from <i>Alicyclobacillus acidocaldarius</i> . <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 71, 1721-1731.	2.6	31
70	Structural Analysis of BldR from <i>Sulfolobus solfataricus</i> Provides Insights into the Molecular Basis of Transcriptional Activation in Archaea by MarR Family Proteins. <i>Journal of Molecular Biology</i> , 2009, 388, 559-569.	4.2	31
71	Exploring structural properties of potent human carbonic anhydrase inhibitors bearing a 4-(cycloalkylamino-1-carbonyl)benzenesulfonamide moiety. <i>European Journal of Medicinal Chemistry</i> , 2019, 163, 443-452.	5.5	31
72	Human carbonic anhydrase VII protects cells from oxidative damage. <i>Biological Chemistry</i> , 2013, 394, 1343-1348.	2.5	30

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73	Multiple catalytically active thioredoxin folds: a winning strategy for many functions. <i>Cellular and Molecular Life Sciences</i> , 2010, 67, 3797-3814.	5.4	28
74	Carbonic anhydrase inhibitors: Crystallographic and solution binding studies for the interaction of a boron-containing aromatic sulfamide with mammalian isoforms Iâ€šXV. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2010, 20, 3601-3605.	2.2	27
75	Faox enzymes inhibited Maillard reaction development during storage both in protein glucose model system and low lactose UHT milk. <i>Amino Acids</i> , 2014, 46, 279-288.	2.7	27
76	The Crystal Structure of an EST2 Mutant Unveils Structural Insights on the H Group of the Carboxylesterase/Lipase Family. <i>Journal of Molecular Biology</i> , 2004, 343, 137-146.	4.2	26
77	Insights on a New PDI-like Family: Structural and Functional Analysis of a Protein Disulfide Oxidoreductase from the Bacterium <i>Aquifex aeolicus</i> . <i>Journal of Molecular Biology</i> , 2006, 356, 155-164.	4.2	26
78	X-ray crystallographic and kinetic investigations of 6-sulfamoyl-saccharin as a carbonic anhydrase inhibitor. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 4064-4069.	2.8	26
79	The anticonvulsant sulfamide JNJ-26990990 and its S,S-dioxide analog strongly inhibit carbonic anhydrases: solution and X-ray crystallographic studies. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 4853-4858.	2.8	26
80	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. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2018, 33, 151-157.	5.2	26
81	Insights into the binding mode of sulphamates and sulphamides to hCA II: crystallographic studies and binding free energy calculations. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2017, 32, 1002-1011.	5.2	26
82	Insights into the catalytic mechanism of the Bcp family: Functional and structural analysis of Bcp1 from <i>Sulfolobus solfataricus</i> . <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 76, 995-1006.	2.6	25
83	Are Carbonic Anhydrases Suitable Targets to Fight Protozoan Parasitic Diseases?. <i>Current Medicinal Chemistry</i> , 2019, 25, 5266-5278.	2.4	25
84	From natural to synthetic multisite thrombin inhibitors. , 1999, 51, 19-39.		24
85	C68 from the <i>Sulfolobus islandicus</i> plasmidâ€švirus pSSVx is a novel member of the AbrB-like transcription factor family. <i>Biochemical Journal</i> , 2011, 435, 157-166.	3.7	24
86	The Crystal Structure of a hCA VII Variant Provides Insights into the Molecular Determinants Responsible for Its Catalytic Behavior. <i>International Journal of Molecular Sciences</i> , 2018, 19, 1571.	4.1	23
87	Biochemical and Structural Insights into Carbonic Anhydrase XII/Fab6A10 Complex. <i>Journal of Molecular Biology</i> , 2019, 431, 4910-4921.	4.2	23
88	Carbonic Anhydrases: An Overview. , 2015, , 3-13.		22
89	A Novel Member of the Protein Disulfide Oxidoreductase Family from <i>Aeropyrum pernix</i> K1: Structure, Function and Electrostatics. <i>Journal of Molecular Biology</i> , 2006, 362, 743-752.	4.2	21
90	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. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 5990-5998.	6.4	21

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91	Crystal structure of an <i>S</i> -formylglutathione hydrolase from <i>Pseudoalteromonas haloplanktis</i> TAC125. <i>Biopolymers</i> , 2010, 93, 669-677.	2.4	21
92	Exploring the catalytic mechanism of the first dimeric Bcp: Functional, structural and docking analyses of Bcp4 from <i>Sulfolobus solfataricus</i> . <i>Biochimie</i> , 2010, 92, 1435-1444.	2.6	20
93	Biochemical, biophysical and molecular dynamics studies on the proteoglycan-like domain of carbonic anhydrase IX. <i>Cellular and Molecular Life Sciences</i> , 2018, 75, 3283-3296.	5.4	20
94	Catechols: a new class of carbonic anhydrase inhibitors. <i>Chemical Communications</i> , 2020, 56, 13033-13036.	4.1	20
95	Inhibition of carbonic anhydrases IX/XII by SLC-0111 boosts cisplatin effects in hampering head and neck squamous carcinoma cell growth and invasion. <i>Journal of Experimental and Clinical Cancer Research</i> , 2022, 41, 122.	8.6	20
96	Functionalized cyclodextrins: Synthesis and structural characterization of 6-deoxy-6-{4-[N-tert-butoxycarbonyl-2-aminoethyl]-imidazolyl}-cyclomaltoheptaose. <i>Supramolecular Chemistry</i> , 1996, 7, 47-54.	1.2	19
97	Biochemical characterization of the chloroplastic β -carbonic anhydrase from <i>Flaveria bidentis</i> (L.) Kuntze. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2014, 29, 500-504.	5.2	19
98	Inhibition of carbonic anhydrases by a substrate analog: benzyl carbamate directly coordinates the catalytic zinc ion mimicking bicarbonate binding. <i>Chemical Communications</i> , 2018, 54, 10312-10315.	4.1	19
99	Human carbonic anhydrases and post-translational modifications: a hidden world possibly affecting protein properties and functions. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2020, 35, 1450-1461.	5.2	19
100	Biochemical and structural characterisation of a protozoan beta-carbonic anhydrase from <i>Trichomonas vaginalis</i> . <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2020, 35, 1292-1299.	5.2	19
101	Human α -thrombin inhibition by the highly selective compounds N-ethoxycarbonyl-d-phe-pro- α -azalys p-nitrophenyl ester and N-carbobenzoxy-pro- α -azalys p-nitrophenyl ester: A kinetic, thermodynamic and x-ray crystallographic study. <i>Journal of Molecular Biology</i> , 1997, 269, 558-569.	4.2	17
102	Hirunorms are true hirudin mimetics. The crystal structure of human α -thrombin-hirunorm V complex. <i>Protein Science</i> , 1998, 7, 243-253.	7.6	17
103	Disclosing the Interaction of Carbonic Anhydrase IX with Cullin-Associated NEDD8-Dissociated Protein 1 by Molecular Modeling and Integrated Binding Measurements. <i>ACS Chemical Biology</i> , 2017, 12, 1460-1465.	3.4	17
104	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. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 5185-5200.	6.4	16
105	Probing the reactivity of nucleophile residues in human 2,3-diphosphoglycerate/deoxy-hemoglobin complex by aspecific chemical modifications. <i>FEBS Letters</i> , 1999, 452, 190-194.	2.8	15
106	Design, synthesis and characterization of a peptide able to bind proteins of the KCTD family: implications for KCTD cullin 3 recognition. <i>Journal of Peptide Science</i> , 2011, 17, 373-376.	1.4	15
107	Kinetic and X-ray crystallographic investigations of substituted 2-thio-6-oxo-1,6-dihydropyrimidine benzenesulfonamides acting as carbonic anhydrase inhibitors. <i>Bioorganic and Medicinal Chemistry</i> , 2016, 24, 3643-3648.	3.0	15
108	L-Histidinol Dehydrogenase as a New Target for Old Diseases. <i>Current Topics in Medicinal Chemistry</i> , 2016, 16, 2369-2378.	2.1	15

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109	Crystallization and preliminary X-ray diffraction studies of the carboxylesterase EST2 from <i>Alicyclobacillus acidocaldarius</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 1999, 55, 1348-1349.	2.5	14
110	The crystal structure of Afc-containing peptides. <i>Biopolymers</i> , 2000, 53, 150-160.	2.4	14
111	Design of Weakly Basic Thrombin Inhibitors Incorporating Novel P1 Binding Functions: A Molecular and X-ray Crystallographic Studies. <i>Biochemistry</i> , 2003, 42, 9013-9021.	2.5	14
112	Hydrophobic Substituents of the Phenylmethylsulfamide Moiety Can Be Used for the Development of New Selective Carbonic Anhydrase Inhibitors. <i>BioMed Research International</i> , 2014, 2014, 1-11.	1.9	14
113	A Novel Inhibitor of Carbonic Anhydrases Prevents Hypoxia-Induced TNBC Cell Plasticity. <i>International Journal of Molecular Sciences</i> , 2020, 21, 8405.	4.1	14
114	<i>Sulfolobus solfataricus</i> thiol redox puzzle: characterization of an atypical protein disulfide oxidoreductase. <i>Extremophiles</i> , 2014, 18, 219-228.	2.3	13
115	Carbonic Anhydrase Inhibitors: Binding of Indanesulfonamides to the Human Isoform. <i>ChemMedChem</i> , 2008, 3, 473-477.	3.2	11
116	The crystal structure of the thrombin-chirunorm IV complex reveals a novel specificity site recognition mode. <i>Protein Science</i> , 1999, 8, 91-95.	7.6	11
117	Hydroxylamine-O-sulfonamide is a versatile lead compound for the development of carbonic anhydrase inhibitors. <i>Chemical Communications</i> , 2015, 51, 11519-11522.	4.1	10
118	Inhibition of the newly discovered carbonic anhydrase from the protozoan pathogen <i>Trichomonas vaginalis</i> with inorganic anions and small molecules. <i>Journal of Inorganic Biochemistry</i> , 2020, 213, 111274.	3.5	10
119	Intrinsically disordered features of carbonic anhydrase IX proteoglycan-like domain. <i>Cellular and Molecular Life Sciences</i> , 2021, 78, 2059-2067.	5.4	10
120	Zeta-carbonic anhydrases show CS ₂ hydrolase activity: A new metabolic carbon acquisition pathway in diatoms?. <i>Computational and Structural Biotechnology Journal</i> , 2021, 19, 3427-3436.	4.1	10
121	Thermal-Stable Carbonic Anhydrases: A Structural Overview. <i>Sub-Cellular Biochemistry</i> , 2014, 75, 387-404.	2.4	9
122	Structural basis for the rational design of new anti-Brucella agents: The crystal structure of the C366S mutant of l-histidinol dehydrogenase from <i>Brucella suis</i> . <i>Biochimie</i> , 2014, 97, 114-120.	2.6	9
123	Human Carbonic Anhydrases: Catalytic Properties, Structural Features, and Tissue Distribution. , 2015, , 17-30.		9
124	Sultam based Carbonic Anhydrase VII inhibitors for the management of neuropathic pain. <i>European Journal of Medicinal Chemistry</i> , 2022, 227, 113956.	5.5	9
125	An Integrated Structural and Computational Study of the Thermostability of Two Thioredoxin Mutants from <i>Alicyclobacillus acidocaldarius</i> . <i>Journal of Bacteriology</i> , 2003, 185, 4285-4289.	2.2	8
126	Conformational studies of heterochiral peptides with diastereoisomeric residues: Crystal and molecular structures of linear dipeptides derived from leucine, isoleucine, and allo-isoleucine. <i>Biopolymers</i> , 1995, 36, 401-408.	2.4	7

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127	Exploration of the residues modulating the catalytic features of human carbonic anhydrase XIII by a site-specific mutagenesis approach. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2019, 34, 1506-1510.	5.2	7
128	The Amazing World of IDPs in Human Diseases. <i>Biomolecules</i> , 2021, 11, 333.	4.0	7
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