Andrew D Mesecar

List of Publications by Year
in descending order

145 papers	12,988 citations	22153 59 h-index	26613 107 g-index
156 all docs	156 docs citations	156 times ranked	16342 citing authors

#	Article	IF	Citations
1	The SARS-coronavirus papain-like protease: Structure, function and inhibition by designed antiviral compounds. Antiviral Research, 2015, 115, 21-38.	4.1	680
2	Discovery of SARS-CoV-2 antiviral drugs through large-scale compound repurposing. Nature, 2020, 586, 113-119.	27.8	672
3	The Papain-Like Protease of Severe Acute Respiratory Syndrome Coronavirus Has Deubiquitinating Activity. Journal of Virology, 2005, 79, 15189-15198.	3.4	482
4	Modifying specific cysteines of the electrophile-sensing human Keap1 protein is insufficient to disrupt binding to the Nrf2 domain Neh2. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 10070-10075.	7.1	420
5	A noncovalent class of papain-like protease/deubiquitinase inhibitors blocks SARS virus replication. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 16119-16124.	7.1	407
6	Severe acute respiratory syndrome coronavirus papain-like protease: Structure of a viral deubiquitinating enzyme. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 5717-5722.	7.1	356
7	Structural Basis for Tumor Pyruvate Kinase M2 Allosteric Regulation and Catalysis,. Biochemistry, 2005, 44, 9417-9429.	2.5	347
8	Severe Acute Respiratory Syndrome Coronavirus Papain-Like Protease Ubiquitin-Like Domain and Catalytic Domain Regulate Antagonism of IRF3 and NF-ÎºB Signaling. Journal of Virology, 2009, 83, 6689-6705.	3.4	325
9	Deubiquitinating and Interferon Antagonism Activities of Coronavirus Papain-Like Proteases. Journal of Virology, 2010, 84, 4619-4629.	3.4	267
10	Phosphorylation of Serine 256 Suppresses Transactivation by FKHR (FOXO1) by Multiple Mechanisms. Journal of Biological Chemistry, 2002, 277, 45276-45284.	3.4	265
11	Drug Development and Medicinal Chemistry Efforts toward SARSâ€Coronavirus and Covidâ€19 Therapeutics. ChemMedChem, 2020, 15, 907-932.	3.2	229
12	Modification of Keap1 Cysteine Residues by Sulforaphane. Chemical Research in Toxicology, 2011, 24, 515-521.	3.3	224
13	Preclinical characterization of an intravenous coronavirus 3CL protease inhibitor for the potential treatment of COVID19. Nature Communications, 2021, 12, 6055.	12.8	215
14	Orbital Steering in the Catalytic Power of Enzymes: Small Structural Changes with Large Catalytic Consequences. Science, 1997, 277, 202-206.	12.6	214
15	New Chemical Constituents ofEuphorbiaquinquecostataand Absolute Configuration Assignment by a Convenient Mosher Ester Procedure Carried Out in NMR Tubes. Journal of Natural Products, 2002, 65, 1278-1282.	3.0	208
16	Structural Basis for the Ubiquitin-Linkage Specificity and deISGylating Activity of SARS-CoV Papain-Like Protease. PLoS Pathogens, 2014, 10, e1004113.	4.7	199
17	MERS-CoV papain-like protease has deISGylating and deubiquitinating activities. Virology, 2014, 450-451, 64-70.	2.4	198
18	Black Cohosh Acts as a Mixed Competitive Ligand and Partial Agonist of the Serotonin Receptor. Journal of Agricultural and Food Chemistry, 2003, 51, 5661-5670.	5.2	185

#	Article	IF	Citations
19	Xanthohumol Isolated from Humulus lupulus Inhibits Menadione-Induced DNA Damage through Induction of Quinone Reductase. Chemical Research in Toxicology, 2005, 18, 1296-1305.	3.3	183
20	X-ray Structural and Biological Evaluation of a Series of Potent and Highly Selective Inhibitors of Human Coronavirus Papain-like Proteases. Journal of Medicinal Chemistry, 2014, 57, 2393-2412.	6.4	182
21	Discovery, Synthesis, And Structure-Based Optimization of a Series of N-(tert-Butyl)-2-(N-arylamido)-2-(pyridin-3-yl) Acetamides (ML188) as Potent Noncovalent Small Molecule Inhibitors of the Severe Acute Respiratory Syndrome Coronavirus (SARS-CoV) 3CL Protease. Journal of Medicinal Chemistry, 2013, 56, 534-546.	6.4	178
22	Silvestrol and Episilvestrol, Potential Anticancer Rocaglate Derivatives fromAglaia silvestris. Journal of Organic Chemistry, 2004, 69, 3350-3358.	3.2	175
23	Sites of alkylation of human Keap1 by natural chemoprevention agents. Journal of the American Society for Mass Spectrometry, 2007, 18, 2226-2232.	2.8	161
24	Evaluating the 3C-like protease activity of SARS-Coronavirus: Recommendations for standardized assays for drug discovery. Virus Research, 2008, 133, 63-73.	2.2	161
25	A new model for protein stereospecificity. Nature, 2000, 403, 614-615.	27.8	155
26	Pleiotropic mechanisms facilitated by resveratrol and its metabolites. Biochemical Journal, 2010, 429, 273-282.	3.7	154
27	Cul3-mediated Nrf2 ubiquitination and antioxidant response element (ARE) activation are dependent on the partial molar volume at position 151 of Keap1. Biochemical Journal, 2009, 422, 171-180.	3.7	141
28	Nidovirus papain-like proteases: Multifunctional enzymes with protease, deubiquitinating and deISGylating activities. Virus Research, 2014, 194, 184-190.	2.2	140
29	New Manzamine Alkaloids with Activity against Infectious and Tropical Parasitic Diseases from an Indonesian Sponge. Journal of Natural Products, 2003, 66, 823-828.	3.0	138
30	Ligand-induced Dimerization of Middle East Respiratory Syndrome (MERS) Coronavirus nsp5 Protease (3CLpro). Journal of Biological Chemistry, 2015, 290, 19403-19422.	3.4	134
31	Severe Acute Respiratory Syndrome Coronavirus Papain-like Novel Protease Inhibitors: Design, Synthesis, Proteinâ^'Ligand X-ray Structure and Biological Evaluation. Journal of Medicinal Chemistry, 2010, 53, 4968-4979.	6.4	129
32	A small moleculeÂcompound with an indole moiety inhibits the main protease of SARS-CoV-2 and blocks virus replication. Nature Communications, 2021, 12, 668.	12.8	126
33	Molecular mechanisms of natural products in chemoprevention: Induction of cytoprotective enzymes by Nrf2. Molecular Nutrition and Food Research, 2008, 52 Suppl 1, S84-94.	3.3	117
34	Catalytic Function and Substrate Specificity of the Papain-Like Protease Domain of nsp3 from the Middle East Respiratory Syndrome Coronavirus. Journal of Virology, 2014, 88, 12511-12527.	3.4	116
35	Design and Synthesis of Peptidomimetic Severe Acute Respiratory Syndrome Chymotrypsin-like Protease Inhibitors. Journal of Medicinal Chemistry, 2005, 48, 6767-6771.	6.4	114
36	respiratory syndrome coronavirus (SARS-CoV) 3CLpro inhibitors: Identification of ML300 and noncovalent nanomolar inhibitors with an induced-fit binding. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 6172-6177.	2.2	113

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37	Structure-Based Design, Synthesis, and Biological Evaluation of a Series of Novel and Reversible Inhibitors for the Severe Acute Respiratory Syndromeâ˜Coronavirus Papain-Like Protease. Journal of Medicinal Chemistry, 2009, 52, 5228-5240.	6.4	110
38	Isolation, Structure Elucidation, and Absolute Configuration of 26-Deoxyactein fromCimicifugaracemosaand Clarification of Nomenclature Associated with 27-Deoxyactein. Journal of Natural Products, 2002, 65, 601-605.	3.0	106
39	Isolation and characterization of bioactive principles of the leaves and stems of Physalis philadelphica. Tetrahedron, 2002, 58, 3453-3466.	1.9	101
40	Design, synthesis and antiviral efficacy of a series of potent chloropyridyl ester-derived SARS-CoV 3CLpro inhibitors. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 5684-5688.	2.2	99
41	Chimeric Exchange of Coronavirus nsp5 Proteases (3CLpro) Identifies Common and Divergent Regulatory Determinants of Protease Activity. Journal of Virology, 2013, 87, 12611-12618.	3.4	98
42	Structure-based design, synthesis, and biological evaluation of peptidomimetic SARS-CoV 3CLpro inhibitors. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 5876-5880.	2.2	94
43	New Sesquiterpenes fromLitseaverticillata. Journal of Natural Products, 2003, 66, 609-615.	3.0	92
44	Probing the structural requirements of non-electrophilic naphthalene-based Nrf2 activators. European Journal of Medicinal Chemistry, 2015, 103, 252-268.	5.5	88
45	Structural Insights into the Interaction of Coronavirus Papain-Like Proteases and Interferon-Stimulated Gene Product 15 from Different Species. Journal of Molecular Biology, 2017, 429, 1661-1683.	4.2	88
46	Proteolytic Processing and Deubiquitinating Activity of Papain-Like Proteases of Human Coronavirus NL63. Journal of Virology, 2007, 81, 6007-6018.	3.4	87
47	Prospective Type 1 and Type 2 Disulfides of Keap1 Protein. Chemical Research in Toxicology, 2008, 21, 2051-2060.	3.3	81
48	Kinetic, thermodynamic and X-ray structural insights into the interaction of melatonin and analogues with quinone reductase 2. Biochemical Journal, 2008, 413, 81-91.	3.7	81
49	Coronaviruses Resistant to a 3C-Like Protease Inhibitor Are Attenuated for Replication and Pathogenesis, Revealing a Low Genetic Barrier but High Fitness Cost of Resistance. Journal of Virology, 2014, 88, 11886-11898.	3.4	81
50	Design, synthesis, and biological evaluation of resveratrol analogues as aromatase and quinone reductase 2 inhibitors for chemoprevention of cancer. Bioorganic and Medicinal Chemistry, 2010, 18, 5352-5366.	3.0	79
51	Identification of the Highly Reactive Cysteine 151 in the Chemopreventive Agent-Sensor Keap1 Protein is Method-Dependent. Chemical Research in Toxicology, 2007, 20, 1878-1884.	3.3	75
52	Structure-Based and Random Mutagenesis Approaches Increase the Organophosphate-Degrading Activity of a Phosphotriesterase Homologue from Deinococcus radiodurans. Journal of Molecular Biology, 2009, 393, 36-57.	4.2	75
53	Synthesis of Casimiroin and Optimization of Its Quinone Reductase 2 and Aromatase Inhibitory Activities. Journal of Medicinal Chemistry, 2009, 52, 1873-1884.	6.4	74
54	Screening Natural Products for Inhibitors of Quinone Reductase-2 Using Ultrafiltration LCâ˜MS. Analytical Chemistry, 2011, 83, 1048-1052.	6.5	70

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55	Potential Cancer Chemopreventive Constituents of the Seeds ofDipteryxodorata(Tonka Bean). Journal of Natural Products, 2003, 66, 583-587.	3.0	69
56	Potential Chemopreventive Agents Based on the Structure of the Lead Compound 2-Bromo-1-hydroxyphenazine, Isolated from Streptomyces Species, Strain CNS284. Journal of Medicinal Chemistry, 2010, 53, 8688-8699.	6.4	69
57	Bioactive Constituents of the Seeds of Brucea javanica. Planta Medica, 2002, 68, 730-733.	1.3	67
58	Targeting zoonotic viruses: Structure-based inhibition of the 3C-like protease from bat coronavirus HKU4â€"The likely reservoir host to the human coronavirus that causes Middle East Respiratory Syndrome (MERS). Bioorganic and Medicinal Chemistry, 2015, 23, 6036-6048.	3.0	65
59	Structural basis for thermostability revealed through the identification and characterization of a highly thermostable phosphotriesterase-like lactonase from Geobacillus stearothermophilus. Archives of Biochemistry and Biophysics, 2009, 488, 109-120.	3.0	64
60	Structural Basis for the Inhibition of CRISPR-Cas12a by Anti-CRISPR Proteins. Cell Host and Microbe, 2019, 25, 815-826.e4.	11.0	63
61	Lamiridosins, Hepatitis C Virus Entry Inhibitors from Lamium album. Journal of Natural Products, 2009, 72, 2158-2162.	3.0	62
62	Activity-guided isolation of cytotoxic constituents from the bark of Aglaia crassinervia collected in Indonesia. Bioorganic and Medicinal Chemistry, 2006, 14, 960-972.	3.0	59
63	Absorption and subcellular localization of lycopene in human prostate cancer cells. Molecular Cancer Therapeutics, 2006, 5, 2879-2885.	4.1	57
64	Screening Method for the Discovery of Potential Cancer Chemoprevention Agents Based on Mass Spectrometric Detection of Alkylated Keap1. Analytical Chemistry, 2005, 77, 6407-6414.	6.5	56
65	A Mouse Model for Betacoronavirus Subgroup 2c Using a Bat Coronavirus Strain HKU5 Variant. MBio, 2014, 5, e00047-14.	4.1	55
66	Indole Chloropyridinyl Ester-Derived SARS-CoV-2 3CLpro Inhibitors: Enzyme Inhibition, Antiviral Efficacy, Structureâ€"Activity Relationship, and X-ray Structural Studies. Journal of Medicinal Chemistry, 2021, 64, 14702-14714.	6.4	55
67	Vitexlactam A, a novel labdane diterpene lactam from the fruits of Vitex agnus-castus. Tetrahedron Letters, 2002, 43, 5131-5134.	1.4	54
68	Resveratrol derivatives as promising chemopreventive agents with improved potency and selectivity. Molecular Nutrition and Food Research, 2011, 55, 1249-1265.	3.3	52
69	Structural and Functional Analysis of Two Glutamate Racemase Isozymes from Bacillus anthracis and Implications for Inhibitor Design. Journal of Molecular Biology, 2007, 371, 1219-1237.	4.2	50
70	Murine Coronavirus Ubiquitin-Like Domain Is Important for Papain-Like Protease Stability and Viral Pathogenesis. Journal of Virology, 2015, 89, 4907-4917.	3.4	50
71	Millisecond Laue structures of an enzymeâ€"product complex using photocaged substrate analogs. Nature Structural Biology, 1998, 5, 891-897.	9.7	49
72	Metal-Ion-Mediated Allosteric Triggering of Yeast Pyruvate Kinase. 1. A Multidimensional Kinetic Linked-Function Analysis. Biochemistry, 1997, 36, 6792-6802.	2.5	44

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73	Antimycobacterial Naphthopyrones fromSenna obliquaâŠ¥. Journal of Natural Products, 2004, 67, 225-227.	3.0	43
74	Development and validation of a yeast high-throughput screen for inhibitors of AÎ²42 oligomerization. DMM Disease Models and Mechanisms, 2011, 4, 822-831.	2.4	43
75	Decoupling deISGylating and deubiquitinating activities of the MERS virus papain-like protease. Antiviral Research, 2020, 174, 104661.	4.1	43
76	Metal-Ion-Mediated Allosteric Triggering of Yeast Pyruvate Kinase 2. A Multidimensional Thermodynamic Linked-Function Analysis. Biochemistry, 1997, 36, 6803-6813.	2.5	40
77	Design and Synthesis of Aryl Ether Inhibitors of the Bacillus Anthracis Enoylâ€ACP Reductase. ChemMedChem, 2008, 3, 1250-1268.	3.2	40
78	Constituents ofMusaÃ—paradisiacaCultivar with the Potential To Induce the Phase II Enzyme, Quinone Reductase. Journal of Agricultural and Food Chemistry, 2002, 50, 6330-6334.	5.2	39
79	Activity-Guided Isolation of Novel Norwithanolides from Deprea subtriflora with Potential Cancer Chemopreventive Activity. Journal of Organic Chemistry, 2003, 68, 2350-2361.	3.2	38
80	Structural and mutational studies of organophosphorus hydrolase reveal a cryptic and functional allosteric-binding site. Archives of Biochemistry and Biophysics, 2005, 442, 169-179.	3.0	38
81	Structural Basis for Catalysis of a Tetrameric Class IIa Fructose 1,6-Bisphosphate Aldolase from Mycobacterium tuberculosis. Journal of Molecular Biology, 2009, 386, 1038-1053.	4.2	38
82	Xâ€ray structural studies of quinone reductase 2 nanomolar range inhibitors. Protein Science, 2011, 20, 1182-1195.	7.6	38
83	New 3-O-Acyl Betulinic Acids fromStrychnos vanprukiiCraib. Journal of Natural Products, 2004, 67, 994-998.	3.0	36
84	Identification of a Glycogen Synthase Kinaseâ€3Î² Inhibitor that Attenuates Hyperactivity in CLOCK Mutant Mice. ChemMedChem, 2011, 6, 1593-1602.	3.2	36
85	Design, Synthesis, and Biological Evaluation of Potent Quinoline and Pyrroloquinoline Ammosamide Analogues as Inhibitors of Quinone Reductase 2. Journal of Medicinal Chemistry, 2012, 55, 367-377.	6.4	36
86	Progress in Anti-SARS Coronavirus Chemistry, Biology and Chemotherapy. Annual Reports in Medicinal Chemistry, 2006, 41, 183-196.	0.9	35
87	Bioactive Compounds from the Fern Lepisorus contortus. Journal of Natural Products, 2011, 74, 129-136.	3.0	34
88	X-ray Structural and Functional Studies of the Three Tandemly Linked Domains of Non-structural Protein 3 (nsp3) from Murine Hepatitis Virus Reveal Conserved Functions. Journal of Biological Chemistry, 2015, 290, 25293-25306.	3.4	34
89	Regioselective Covalent Modification of Hemoglobin in Search of Antisickling Agents. Journal of Medicinal Chemistry, 2003, 46, 936-953.	6.4	33
90	X-ray Structure and Enzymatic Activity Profile of a Core Papain-like Protease of MERS Coronavirus with utility for structure-based drug design. Scientific Reports, 2017, 7, 40292.	3.3	33

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91	Isolation and absolute stereochemistry of coussaric acid, a new bioactive triterpenoid from the stems of Coussarea brevicaulis. Phytochemistry, 2003, 64, 293-302.	2.9	32
92	Bacillus anthracis o-Succinylbenzoyl-CoA Synthetase: Reaction Kinetics and a Novel Inhibitor Mimicking Its Reaction Intermediate. Biochemistry, 2008, 47, 12434-12447.	2.5	32
93	Isolation and evaluation of kaempferol glycosides from the fern Neocheiropteris palmatopedata. Phytochemistry, 2010, 71, 641-647.	2.9	32
94	Synthesis of 3-(3-aryl-pyrrolidin-1-yl)-5-aryl-1,2,4-triazines that have antibacterial activity and also inhibit inorganic pyrophosphatase. Bioorganic and Medicinal Chemistry, 2014, 22, 406-418.	3.0	32
95	Conceptual design of a macromolecular neutron diffractometer (MaNDi) for the SNS. Journal of Applied Crystallography, 2005, 38, 964-974.	4.5	31
96	Bruguiesulfurol, A New Sulfur Compound fromBruguiera gymnorrhiza. Planta Medica, 2006, 72, 255-260.	1.3	31
97	Design and synthesis of 2-pyridones as novel inhibitors of the Bacillus anthracis enoyl-ACP reductase. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 3565-3569.	2.2	31
98	Miliusanes, A Class of Cytotoxic Agents fromMiliusa sinensis. Journal of Medicinal Chemistry, 2006, 49, 693-708.	6.4	30
99	Deubiquitinating Activity of the SARS-CoV Papain-Like Protease. Advances in Experimental Medicine and Biology, 2006, 581, 37-41.	1.6	30
100	Genetic interaction between yeast Saccharomyces cerevisiae release factors and the decoding region of 18 S rRNA. Journal of Molecular Biology, 2001, 305, 715-727.	4.2	28
101	Sites of Binding and Orientation in a Four-Location Model for Protein Stereospecificity. IUBMB Life, 2000, 49, 457-466.	3.4	27
102	Catechol Estrogen 4-Hydroxyequilenin Is a Substrate and an Inhibitor of Catechol-O-Methyltransferase. Chemical Research in Toxicology, 2003, 16, 668-675.	3.3	25
103	An ELISA method to measure inhibition of the COX enzymes. Nature Protocols, 2006, 1, 1915-1921.	12.0	25
104	Kinetic and Structural Characterization of a Heterohexamer 4-Oxalocrotonate Tautomerase from Chloroflexus aurantiacus J-10-fl: Implications for Functional and Structural Diversity in the Tautomerase Superfamily,. Biochemistry, 2010, 49, 5016-5027.	2.5	25
105	Synthesis of novel ÐœÐ¢3 receptor ligands via an unusual Knoevenagel condensation. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 7578-7581.	2.2	25
106	A 2.2â€…Ã… resolution structure of the USP7 catalytic domain in a new space group elaborates upon structural rearrangements resulting from ubiquitin binding. Acta Crystallographica Section F, Structural Biology Communications, 2014, 70, 283-287.	0.8	25
107	Kinetic, Thermodynamic, and Structural Insight into the Mechanism of Phosphopantetheine Adenylyltransferase from Mycobacterium tuberculosis. Journal of Molecular Biology, 2010, 404, 202-219.	4.2	24
108	Design, synthesis, biological and structural evaluation of functionalized resveratrol analogues as inhibitors of quinone reductase 2. Bioorganic and Medicinal Chemistry, 2013, 21, 6022-6037.	3.0	24

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109	Cholesterol Sulfonation Enzyme, SULT2B1b, Modulates AR and Cell Growth Properties in Prostate Cancer. Molecular Cancer Research, 2016, 14, 776-786.	3.4	24
110	Natural product leads for drug discovery: Isolation, synthesis and biological evaluation of 6-cyano-5-methoxyindolo[2,3-a]carbazole based ligands as antibacterial agents. Bioorganic and Medicinal Chemistry, 2009, 17, 7126-7130.	3.0	23
111	Enzyme Architecture: The Effect of Replacement and Deletion Mutations of Loop 6 on Catalysis by Triosephosphate Isomerase. Biochemistry, 2014, 53, 3486-3501.	2.5	23
112	Role of Lysine 240 in the Mechanism of Yeast Pyruvate Kinase Catalysis. Biochemistry, 1999, 38, 9137-9145.	2.5	22
113	Characterization of novel rad6/ubc2 ubiquitin-conjugating enzyme mutants in yeast. Current Genetics, 2000, 37, 221-233.	1.7	22
114	A Universal, Fully Automated High Throughput Screening Assay for Pyrophosphate and Phosphate Release from Enzymatic Reactions. Combinatorial Chemistry and High Throughput Screening, 2010, 13, 27-38.	1.1	21
115	Active Site Loop Dynamics of a Class IIa Fructose 1,6-Bisphosphate Aldolase from Mycobacterium tuberculosis. Biochemistry, 2013, 52, 912-925.	2.5	21
116	Computational modeling of the bat <scp>HKU4</scp> coronavirus <scp>3CL^{pro}</scp> inhibitors as a tool for the development of antivirals against the emerging <scp>M</scp>iddle <scp>E</scp>ast respiratory syndrome (<scp>MERS</scp>) coronavirus. Journal of Molecular Recognition, 2017, 30, e2644.	2.1	21
117	Structure-Guided Mutagenesis Alters Deubiquitinating Activity and Attenuates Pathogenesis of a Murine Coronavirus. Journal of Virology, 2020, 94, .	3.4	20
118	Screening for natural chemoprevention agents that modify human Keap1. Analytical Biochemistry, 2012, 421, 108-114.	2.4	19
119	X-ray structure and inhibition of the feline infectious peritonitis virus 3C-like protease: Structural implications for drug design. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 5072-5077.	2.2	19
120	An oxyanion-Hole selective serine protease inhibitor in complex with trypsin. Bioorganic and Medicinal Chemistry, 2002, 10, 41-46.	3.0	18
121	A Chimeric Virus-Mouse Model System for Evaluating the Function and Inhibition of Papain-Like Proteases of Emerging Coronaviruses. Journal of Virology, 2014, 88, 11825-11833.	3.4	18
122	Structure-based design, synthesis and biological evaluation of novel Î²-secretase inhibitors containing a pyrazole or thiazole moiety as the P3 ligand. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 668-672.	2.2	18
123	Mn ²⁺ coordinates Cap-0-RNA to align substrates for efficient 2â€²- O -methyl transfer by SARS-CoV-2 nsp16. Science Signaling, 2021, 14, .	3.6	17
124	Kinetic and X-Ray Structural Evidence for Negative Cooperativity in Substrate Binding to Nicotinate Mononucleotide Adenylyltransferase (NMAT) from Bacillus anthracis. Journal of Molecular Biology, 2009, 385, 867-888.	4.2	16
125	Development of an efficient E. coli expression and purification system for a catalytically active, human Cullin3â€“RINGBox1 protein complex and elucidation of its quaternary structure with Keap1. Biochemical and Biophysical Research Communications, 2010, 400, 471-475.	2.1	16
126	Desorption Electrospray Ionization Mass Spectrometry Assay for Labelâ€Free Characterization of SULT2B1b Enzyme Kinetics. ChemMedChem, 2022, 17, .	3.2	16

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127	Equine Catechol Estrogen 4-Hydroxyequilenin Is a More Potent Inhibitor of the Variant Form of Catechol-O-Methyltransferase. Chemical Research in Toxicology, 2004, 17, 512-520.	3.3	15
128	Design, synthesis, and X-ray structural studies of BACE-1 inhibitors containing substituted 2-oxopiperazines as P1â€²-P2â€² ligands. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 2432-2438.	2.2	14
129	Use of molecular modeling, docking, and 3D-QSAR studies for the determination of the binding mode of benzofuran-3-yl-(indol-3-yl)maleimides as GSK-3Î² inhibitors. Journal of Molecular Modeling, 2009, 15, 1463-1479.	1.8	13
130	X-Ray Structure and Inhibition of 3C-like Protease from Porcine Epidemic Diarrhea Virus. Scientific Reports, 2016, 6, 25961.	3.3	12
131	Design of potent and highly selective inhibitors for human Î²-secretase 2 (memapsin 1), a target for type 2 diabetes. Chemical Science, 2016, 7, 3117-3122.	7.4	11
132	Development of an Efficient Enzyme Production and Structure-Based Discovery Platform for BACE1 Inhibitors. Biochemistry, 2019, 58, 4424-4435.	2.5	10
133	Highly Selective and Potent Human Î²â€Secretaseâ€…2 (BACE2) Inhibitors against Typeâ€…2 Diabetes: Design, Synthesis, Xâ€ray Structure and Structureâ€“Activity Relationship Studies. ChemMedChem, 2019, 14, 545-560.	3.2	10
134	Viral destruction of cell surface receptors: Fig. 1.. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 8807-8808.	7.1	9
135	Chloropyridinyl Esters of Nonsteroidal Anti-Inflammatory Agents and Related Derivatives as Potent SARS-CoV-2 3CL Protease Inhibitors. Molecules, 2021, 26, 5782.	3.8	9
136	Design, synthesis, and evaluation of oxyanion-hole selective inhibitor substituents for the S1 subsite of factor Xa. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 5165-5170.	2.2	8
137	Steady-state kinetic studies reveal that the anti-cancer target Ubiquitin-Specific Protease 17 (USP17) is a highly efficient deubiquitinating enzyme. Archives of Biochemistry and Biophysics, 2016, 612, 35-45.	3.0	7
138	Cholesterol Sulfotransferase SULT2B1b Modulates Sensitivity to Death Receptor Ligand TNFÎ± in Castration-Resistant Prostate Cancer. Molecular Cancer Research, 2019, 17, 1253-1263.	3.4	7
139	The structures of T87I phosphono-CheY and T87I/Y106W phosphono-CheY help to explain their binding affinities to the FliM and CheZ peptides. Archives of Biochemistry and Biophysics, 2008, 479, 105-113.	3.0	6
140	A Structure-Based Discovery Platform for BACE2 and the Development of Selective BACE Inhibitors. ACS Chemical Neuroscience, 2021, 12, 581-588.	3.5	4
141	Design, synthesis, X-ray studies, and biological evaluation of novel BACE1 inhibitors with bicyclic isoxazoline carboxamides as the P3 ligand. Bioorganic and Medicinal Chemistry Letters, 2018, 28, 2605-2610.	2.2	3
142	Structural and mechanistic analysis oftrans-3-chloroacrylic acid dehalogenase activity. Acta Crystallographica Section D: Biological Crystallography, 2008, 64, 1277-1282.	2.5	2
143	Coronavirus Papain-like Peptidases. , 2013, , 2195-2199.		1
144	Design, Syntheis, and Evaluation of Oxyanion-Hole Selective Inhibitor Substituents for the S1 Subsite of Factor Xa.. ChemInform, 2005, 36, no.	0.0	0

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145	Abstract A58: Cul3â€mediated Nrf2 ubiquitination and ARE activation are dependent on the partial molar volume at position 151 of Keap1. , 2010, , .		0