Tanja Schirmeister

List of Publications by Year
in descending order

181	5,839	76294	114418
papers	citations	40 h-index	63 g-index

196	196	196	6248
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Cysteine Proteases and Their Inhibitors. Chemical Reviews, 1997, 97, 133-172.	23.0	696
2	Development of Peptidomimetics with a Vinyl Sulfone Warhead as Irreversible Falcipain-2 Inhibitors. Journal of Medicinal Chemistry, 2008, 51, 988-996.	2.9	196
3	Biochemistry and Medicinal Chemistry of the Dengue Virus Protease. Chemical Reviews, 2014, 114, 11348-11381.	23.0	120
4	Prospective Evaluation of Free Energy Calculations for the Prioritization of Cathepsin L Inhibitors. Journal of Medicinal Chemistry, 2017, 60, 2485-2497.	2.9	110
5	Novel Dengue Virus NS2B/NS3 Protease Inhibitors. Antimicrobial Agents and Chemotherapy, 2015, 59, 1100-1109.	1.4	108
6	Flavonoids as noncompetitive inhibitors of Dengue virus NS2B-NS3 protease: Inhibition kinetics and docking studies. Bioorganic and Medicinal Chemistry, 2015, 23, 466-470.	1.4	105
7	Transcriptome and Functional Analysis of the Eukaryotic-Type Serine/Threonine Kinase PknB inStaphylococcus aureus. Journal of Bacteriology, 2009, 191, 4056-4069.	1.0	103
8	The Significance of Ionic Bonding in Sulfur Dioxide: Bond Orders from Xâ€ray Diffraction Data. Angewandte Chemie - International Edition, 2012, 51, 6776-6779.	7.2	99
9	Aziridine-2,3-dicarboxylate inhibitors targeting the major cysteine protease of Trypanosoma brucei as lead trypanocidal agents. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 2753-2757.	1.0	79
10	Inhibitors of Cysteine Proteases. Current Topics in Medicinal Chemistry, 2006, 6, 331-353.	1.0	79
11	Evidence for Substrate Binding-Induced Zwitterion Formation in the Catalytic Cys-His Dyad of the SARS-CoV Main Protease. Biochemistry, 2014, 53, 5930-5946.	1.2	78
12	Novel Peptidomimetics Containing a Vinyl Ester Moiety as Highly Potent and Selective Falcipain-2 Inhibitors. Journal of Medicinal Chemistry, 2009, 52, 2157-2160.	2.9	73
13	Quantum Chemical-Based Protocol for the Rational Design of Covalent Inhibitors. Journal of the American Chemical Society, 2016, 138, 8332-8335.	6.6	69
14	Antioxidant and Anti-Protease Activities of Diazepinomicin from the Sponge-Associated Micromonospora Strain RV115. Marine Drugs, 2012, 10, 2208-2221.	2.2	66
15	Metabolomics analysis and biological investigation of three Malvaceae plants. Phytochemical Analysis, 2020, 31, 204-214.	1.2	66
16	New Peptidic Cysteine Protease Inhibitors Derived from the Electrophilic Î±-Amino Acid Aziridine-2,3-dicarboxylic Acid. Journal of Medicinal Chemistry, 1999, 42, 560-572.	2.9	63
17	Allicin and derivates are cysteine protease inhibitors with antiparasitic activity. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 5541-5543.	1.0	61
18	Proline-Based Allosteric Inhibitors of Zika and Dengue Virus NS2B/NS3 Proteases. Journal of Medicinal Chemistry, 2019, 62, 11359-11382.	2.9	60

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19	On the Origin of the Stabilization of the Zwitterionic Resting State of Cysteine Proteases: A Theoretical Study. Journal of the American Chemical Society, 2008, 130, 8696-8705.	6.6	58
20	Theoretical Studies about the Influence of Different Ring Substituents on the Nucleophilic Ring Opening of Three-Membered Heterocycles and Possible Implications for the Mechanisms of Cysteine Protease Inhibitors. Journal of Organic Chemistry, 2005, 70, 233-237.	1.7	57
21	Aziridide-Based Inhibitors of Cathepsinâ€…L: Synthesis, Inhibition Activity, and Docking Studies. ChemMedChem, 2006, 1, 1126-1141.	1.6	56
22	Aziridine-2,3-Dicarboxylates, Peptidomimetic Cysteine Protease Inhibitors with Antileishmanial Activity. Antimicrobial Agents and Chemotherapy, 2006, 50, 2439-2447.	1.4	56
23	A New Lead for Nonpeptidic Active-Site-Directed Inhibitors of the Severe Acute Respiratory Syndrome Coronavirus Main Protease Discovered by a Combination of Screening and Docking Methodsâ€–. Journal of Medicinal Chemistry, 2005, 48, 6832-6842.	2.9	55
24	aziridinyl peptides as inhibitors of cysteine proteases: Effect of a free carboxylic acid function on inhibition. Bioorganic and Medicinal Chemistry, 2000, 8, 1281-1291.	1.4	53
25	Model Calculations about the Influence of Protic Environments on the Alkylation Step of Epoxide, Aziridine, and Thiirane Based Cysteine Protease Inhibitors. Journal of Physical Chemistry A, 2004, 108, 7691-7701.	1.1	53
26	Tuning and predicting biological affinity: aryl nitriles as cysteine protease inhibitors. Organic and Biomolecular Chemistry, 2012, 10, 5764.	1.5	49
27	Michael Acceptor Based Antiplasmodial and Antitrypanosomal Cysteine Protease Inhibitors with Unusual Amino Acids. Journal of Medicinal Chemistry, 2010, 53, 1951-1963.	2.9	48
28	A comparative study on the experimentally derived electron densities of three protease inhibitor model compounds. Organic and Biomolecular Chemistry, 2008, 6, 2295.	1.5	47
29	Development of Novel Peptidomimetics Containing a Vinyl Sulfone Moiety as Proteasome Inhibitors. ChemMedChem, 2011, 6, 1228-1237.	1.6	47
30	Development of Novel Peptide-Based Michael Acceptors Targeting Rhodesain and Falcipain-2 for the Treatment of Neglected Tropical Diseases (NTDs). Journal of Medicinal Chemistry, 2017, 60, 6911-6923.	2.9	46
31	Optimization of Triazine Nitriles as Rhodesain Inhibitors: Structureâ€“Activity Relationships, Bioisosteric Imidazopyridine Nitriles, and Xâ€ray Crystal Structure Analysis with Human Cathepsinâ€…L. ChemMedChem, 2013, 8, 967-975.	1.6	45
32	Nonpeptidic Vinyl and Allyl Phosphonates as Falcipainâ€2 Inhibitors. ChemMedChem, 2008, 3, 1030-1033.	1.6	44
33	An improved synthesis of aziridine-2,3-dicarboxylates via azido alcoholsâ€”epimerization studies. Tetrahedron: Asymmetry, 2003, 14, 3301-3312.	1.8	43
34	Screening of Protease Inhibitors as Antiplasmodial Agents. Part I: Aziridines and Epoxides. ChemMedChem, 2007, 2, 1214-1224.	1.6	43
35	Atomistic Insights into the Inhibition of Cysteine Proteases: First QM/MM Calculations Clarifying the Stereoselectivity of Epoxide-Based Inhibitors. Journal of Physical Chemistry B, 2008, 112, 11798-11808.	1.2	43
36	Atomistic Insights into the Inhibition of Cysteine Proteases:â€‰ First QM/MM Calculations Clarifying the Regiospecificity and the Inhibition Potency of Epoxide- and Aziridine-Based Inhibitors. Journal of Physical Chemistry B, 2008, 112, 5458-5469.	1.2	43

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37	Quantitative detection of C-deuterated drugs by CARS microscopy and Raman microspectroscopy. Analyst, The, 2011, 136, 3686.	1.7	43
38	Screening of electrophilic compounds yields an aziridinyl peptide as new active-site directed SARS-CoV main protease inhibitor. Bioorganic and Medicinal Chemistry Letters, 2005, 15, 5365-5369.	1.0	42
39	Dipeptidyl Nitroalkenes as Potent Reversible Inhibitors of Cysteine Proteases Rhodesain and Cruzain. ACS Medicinal Chemistry Letters, 2016, 7, 1073-1076.	1.3	42
40	Inhibition of the Cysteine Protease Human Cathepsinâ€…L by Triazine Nitriles: Amideâ‹…â‹…â‹…Heteroarene Ï€â€Stacking Interactions and Chalcogen Bonding in the S3 Pocket. ChemMedChem, 2017, 12, 257-270.	1.6	42
41	Benchmark Study for the Cysteineâ€“Histidine Proton Transfer Reaction in a Protein Environment: Gas Phase, COSMO, QM/MM Approaches. Journal of Chemical Theory and Computation, 2013, 9, 1765-1777.	2.3	41
42	Cysteine Protease Inhibitors Containing Small Rings. Mini-Reviews in Medicinal Chemistry, 2003, 3, 585-596.	1.1	40
43	2H-1,2,3-Triazole-Based Dipeptidyl Nitriles: Potent, Selective, and Trypanocidal Rhodesain Inhibitors by Structure-Based Design. Journal of Medicinal Chemistry, 2018, 61, 3370-3388.	2.9	40
44	Rational Design of Aziridine-Containing Cysteine Protease Inhibitors with Improved Potency: Studies on Inhibition Mechanism. ChemMedChem, 2006, 1, 1021-1028.	1.6	39
45	Aziridine-2,3-Dicarboxylate-Based Cysteine Cathepsin Inhibitors Induce Cell Death inLeishmania majorAssociated with Accumulation of Debris in Autophagy-Related Lysosome-Like Vacuoles. Antimicrobial Agents and Chemotherapy, 2010, 54, 5028-5041.	1.4	39
46	The Importance of the Active Site Histidine for the Activity of Epoxide- or Aziridine-Based Inhibitors of Cysteine Proteases. ChemMedChem, 2007, 2, 120-128.	1.6	37
47	Enzyme Kinetics and Hit Validation in Fluorimetric Protease Assays. Current Topics in Medicinal Chemistry, 2010, 10, 368-382.	1.0	37
48	Development of Rhodesain Inhibitors with a 3â€Bromoisoxazoline Warhead. ChemMedChem, 2013, 8, 2070-2076.	1.6	37
49	Lead Discovery of SARS-CoV-2 Main Protease Inhibitors through Covalent Docking-Based Virtual Screening. Journal of Chemical Information and Modeling, 2021, 61, 2062-2073.	2.5	37
50	Structureâ€Activity Relationships of Benzamides and Isoindolines Designed as SARSâ€CoV Protease Inhibitors Effective against SARSâ€CoVâ€2. ChemMedChem, 2021, 16, 340-354.	1.6	36
51	Tetracycline-Inducible Expression of Individual Secreted Aspartic Proteases in Candida albicans Allows Isoenzyme-Specific Inhibitor Screening. Antimicrobial Agents and Chemotherapy, 2008, 52, 146-156.	1.4	35
52	Fluorine Scan of Inhibitors of the Cysteine Protease Human Cathepsinâ€…L: Dipolar and Quadrupolar Effects in the Ï€â€Stacking of Fluorinated Phenyl Rings on Peptide Amide Bonds. ChemMedChem, 2016, 11, 1042-1047.	1.6	35
53	Synthesis of novel peptidomimetics as inhibitors of protozoan cysteine proteases falcipain-2 and rhodesain. European Journal of Medicinal Chemistry, 2010, 45, 3228-3233.	2.6	34
54	Anti-protease and Immunomodulatory Activities of Bacteria Associated with Caribbean Sponges. Marine Biotechnology, 2011, 13, 883-892.	1.1	34

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55	Development of peptidomimetic boronates as proteasome inhibitors. European Journal of Medicinal Chemistry, 2013, 64, 23-34.	2.6	34
56	Evaluation of dipeptide nitriles as inhibitors of rhodesain, a major cysteine protease of Trypanosoma brucei. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 45-50.	1.0	33
57	Mechanistic Study of the Reaction of Thiolâ€Containing Enzymes with Î±,Î²â€Unsaturated Carbonyl Substrates by Computation and Chemoassays. ChemMedChem, 2010, 5, 869-880.	1.6	32
58	Constrained peptidomimetics as antiplasmodial falcipain-2 inhibitors. Bioorganic and Medicinal Chemistry, 2010, 18, 4928-4938.	1.4	31
59	Cathepsin B in Antigen-Presenting Cells Controls Mediators of the Th1 Immune Response during Leishmania major Infection. PLoS Neglected Tropical Diseases, 2014, 8, e3194.	1.3	31
60	Natural products as inhibitors of recombinant cathepsin L of Leishmania mexicana. Experimental Parasitology, 2015, 156, 42-48.	0.5	31
61	Origin of the Reactivity Differences of Substituted Aziridines: CN vs CC Bond Breakages. Journal of Organic Chemistry, 2009, 74, 5244-5249.	1.7	30
62	Peptidomimetics containing a vinyl ketone warhead as falcipain-2 inhibitors. European Journal of Medicinal Chemistry, 2011, 46, 2058-2065.	2.6	30
63	Synthesis and Biological Evaluation of Papainâ€Family Cathepsinâ€…Lâ€Like Cysteine Protease Inhibitors Containing a 1,4â€Benzodiazepine Scaffold as Antiprotozoal Agents. ChemMedChem, 2014, 9, 1817-1825.	1.6	30
64	Potent and Selective Inhibition of Cysteine Proteases from Plasmodium falciparum and Trypanosoma brucei. ChemMedChem, 2011, 6, 273-278.	1.6	29
65	FINDUS: An Open-Source 3D Printable Liquid-Handling Workstation for Laboratory Automation in Life Sciences. SLAS Technology, 2020, 25, 190-199.	1.0	29
66	Î²-Lactam Derivatives as Enzyme Inhibitors: 1-Peptidyl Derivatives of 4-Phenylazetidin-2-one as Inhibitors of Elastase and Papain. Archiv Der Pharmazie, 2000, 333, 243-253.	2.1	28
67	Non-Peptidic Inhibitors of Cysteine Proteases. Mini-Reviews in Medicinal Chemistry, 2003, 3, 361-373.	1.1	28
68	Electron-Density Determination of Electrophilic Building Blocks as Model Compounds for Protease Inhibitors. European Journal of Organic Chemistry, 2007, 2007, 2759-2768.	1.2	28
69	Novel 2H-isoquinolin-3-ones as antiplasmodial falcipain-2 inhibitors. Bioorganic and Medicinal Chemistry, 2009, 17, 6505-6511.	1.4	28
70	Development of novel dipeptide-like rhodesain inhibitors containing the 3-bromoisoxazoline warhead in a constrained conformation. Bioorganic and Medicinal Chemistry, 2015, 23, 7053-7060.	1.4	28
71	Enzyme-catalyzed hydrolyses of E/Z-diastereotopic and E/Z-diastereomeric esters. Effect on selectivity by reaction media. Journal of Organic Chemistry, 1993, 58, 4819-4822.	1.7	27
72	Synthesis and Molecular Modeling Studies of Derivatives of a Highly Potent Peptidomimetic Vinyl Ester as Falcipainâ€2 Inhibitors. ChemMedChem, 2012, 7, 1594-1600.	1.6	27

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73	Optimization of peptidomimetic boronates bearing a P3 bicyclic scaffold as proteasome inhibitors. European Journal of Medicinal Chemistry, 2014, 83, 1-14.	2.6	27
74	Selected cytotoxic gold compounds cause significant inhibition of 20S proteasome catalytic activities. Journal of Inorganic Biochemistry, 2014, 141, 79-82.	1.5	27
75	Synthesis and biological evaluation of novel peptidomimetics as rhodesain inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 1184-1191.	2.5	27
76	Antiprotozoal and cysteine proteases inhibitory activity of dipeptidyl enoates. Bioorganic and Medicinal Chemistry, 2018, 26, 4624-4634.	1.4	27
77	Bis-Acridines as Lead Antiparasitic Agents: Structure-Activity Analysis of a Discrete Compound Library In Vitro. Antimicrobial Agents and Chemotherapy, 2007, 51, 2164-2172.	1.4	26
78	Repurposing a Library of Human Cathepsin L Ligands: Identification of Macrocyclic Lactams as Potent Rhodesain andTrypanosoma bruceiInhibitors. Journal of Medicinal Chemistry, 2018, 61, 3350-3369.	2.9	26
79	Novel Opportunities for Cathepsin S Inhibitors in Cancer Immunotherapy by Nanocarrier-Mediated Delivery. Cells, 2020, 9, 2021.	1.8	26
80	Synthesis and antiplasmodial activity of a cysteine protease-inhibiting biotinylated aziridine-2,3-dicarboxylate. Biological Chemistry, 2004, 385, 435-8.	1.2	25
81	Effect of protease inhibitors on exflagellation in Plasmodium falciparum. Molecular and Biochemical Parasitology, 2008, 158, 208-212.	0.5	25
82	Reactivity Differences between Î±,Î²-Unsaturated Carbonyls and Hydrazones Investigated by Experimental and Theoretical Electron Density and Electron Localizability Analyses. Journal of Physical Chemistry A, 2011, 115, 12715-12732.	1.1	25
83	Peptidomimetic nitriles as selective inhibitors for the malarial cysteine protease falcipain-2. MedChemComm, 2011, 2, 800.	3.5	25
84	Identification of a new series of amides as non-covalent proteasome inhibitors. European Journal of Medicinal Chemistry, 2014, 76, 1-9.	2.6	25
85	SAR of novel benzothiazoles targeting an allosteric pocket of DENV and ZIKV NS2B/NS3 proteases. Bioorganic and Medicinal Chemistry, 2021, 47, 116392.	1.4	25
86	Aziridine-2,3-dicarboxylic Acid Derivatives as Inhibitors of Papain. Archiv Der Pharmazie, 1996, 329, 239-244.	2.1	24
87	New Tetromycin Derivatives with Anti-Trypanosomal and Protease Inhibitory Activities. Marine Drugs, 2011, 9, 1682-1697.	2.2	24
88	Gold compounds as cysteine protease inhibitors: perspectives for pharmaceutical application as antiparasitic agents. BioMetals, 2017, 30, 313-320.	1.8	24
89	Asymmetric Disulfanylbenzamides as Irreversible and Selective Inhibitors of Staphylococcus aureus Sortase A. ChemMedChem, 2020, 15, 839-850.	1.6	24
90	Development of novel 1,4-benzodiazepine-based Michael acceptors as antitrypanosomal agents. Bioorganic and Medicinal Chemistry Letters, 2016, 26, 3453-3456.	1.0	23

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91	Targeting of the Leishmania mexicana cysteine protease CPB2.8Î”CTE by decorated fused benzo[b]thiophene scaffold. RSC Advances, 2016, 6, 30628-30635.	1.7	23
92	BANÎ”IT: Bâ€™â€Factor Analysis for Drug Design and Structural Biology. Molecular Informatics, 2021, 40, e2000144.	1.4	23
93	Effect of Electron-Withdrawing Substituents on the Epoxide Ring: An Experimental and Theoretical Electron Density Analysis of a Series of Epoxide Derivatives. Journal of Organic Chemistry, 2011, 76, 1305-1318.	1.7	22
94	Discovery of benzimidazoleâ€based Leishmania mexicana cysteine protease <scp>CPB</scp>2.8Î”<scp>CTE</scp> inhibitors as potential therapeutics for leishmaniasis. Chemical Biology and Drug Design, 2018, 92, 1585-1596.	1.5	22
95	Optimization Strategy of Novel Peptide-Based Michael Acceptors for the Treatment of Human African Trypanosomiasis. Journal of Medicinal Chemistry, 2019, 62, 10617-10629.	2.9	22
96	Rational Design of Improved Aziridine-Based Inhibitors of Cysteine Proteases. Journal of Physical Chemistry B, 2009, 113, 5282-5289.	1.2	21
97	Protocol for Rational Design of Covalently Interacting Inhibitors. ChemPhysChem, 2014, 15, 3226-3235.	1.0	21
98	Identification of noncovalent proteasome inhibitors with high selectivity for chymotrypsin-like activity by a multistep structure-based virtual screening. European Journal of Medicinal Chemistry, 2016, 121, 578-591.	2.6	21
99	Structureâ€“Function Evaluation of Imidazopyridine Derivatives Selective for Î´-Subunit-Containing Î³-Aminobutyric Acid Type A (GABAA) Receptors. Journal of Medicinal Chemistry, 2018, 61, 1951-1968.	2.9	21
100	Blocking effect of a biotinylated protease inhibitor on the egress of Plasmodium falciparum merozoites from infected red blood cells. Biological Chemistry, 2005, 386, 499-502.	1.2	20
101	A hyaluronic acidâ€“pentamidine bioconjugate as a macrophage mediated drug targeting delivery system for the treatment of leishmaniasis. RSC Advances, 2015, 5, 95545-95550.	1.7	20
102	Dipeptidyl Enoates As Potent Rhodesain Inhibitors That Display a Dual Mode of Action. ChemMedChem, 2015, 10, 1484-1487.	1.6	20
103	Taspase1: a 'misunderstood' protease with translational cancer relevance. Oncogene, 2016, 35, 3351-3364.	2.6	20
104	Fluorovinylsulfones and -Sulfonates as Potent Covalent Reversible Inhibitors of the Trypanosomal Cysteine Protease Rhodesain: Structureâ€“Activity Relationship, Inhibition Mechanism, Metabolism, and In Vivo Studies. Journal of Medicinal Chemistry, 2021, 64, 12322-12358.	2.9	20
105	Naphthoquinones as Covalent Reversible Inhibitors of Cysteine Proteasesâ€”Studies on Inhibition Mechanism and Kinetics. Molecules, 2020, 25, 2064.	1.7	20
106	Cisâ€Configured Aziridines Are New Pseudoâ€Irreversible Dualâ€Mode Inhibitors of Candida albicans Secreted Aspartic Proteaseâ€...2. ChemMedChem, 2008, 3, 302-315.	1.6	19
107	Selected gold compounds cause pronounced inhibition of Falcipain 2 and effectively block P. falciparum growth in vitro. Journal of Inorganic Biochemistry, 2011, 105, 1576-1579.	1.5	19
108	Vinyl sulfone building blocks in covalently reversible reactions with thiols. New Journal of Chemistry, 2015, 39, 5841-5853.	1.4	19

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109	Aziridineâ€2,2â€dicarboxylates: Synthesis, Reactions, and Photochromism. Liebigs Annalen, 1997, 1997, 1895-1899.	0.8	18
110	Synthesis of C3/C1-Substituted Tetrahydroisoquinolines. Molecules, 2015, 20, 14902-14914.	1.7	17
111	Bistacrine derivatives as new potent antimalarials. Bioorganic and Medicinal Chemistry, 2016, 24, 3636-3642.	1.4	17
112	Peptidyl Vinyl Ketone Irreversible Inhibitors of Rhodesain: Modifications of the P2 Fragment. ChemMedChem, 2020, 15, 1552-1561.	1.6	17
113	Identification of Plakortide E from the Caribbean Sponge Plakortis halichondroides as a Trypanocidal Protease Inhibitor using Bioactivity-Guided Fractionation. Marine Drugs, 2014, 12, 2614-2622.	2.2	16
114	Development of Novel Selective Peptidomimetics Containing a Boronic Acid Moiety, Targeting the 20S Proteasome as Anticancer Agents. ChemMedChem, 2014, 9, 1801-1816.	1.6	16
115	Structure of the Human TRPML2 Ion Channel Extracytosolic/Lumenal Domain. Structure, 2019, 27, 1246-1257.e5.	1.6	16
116	New Cysteine Protease Inhibitors: Electrophilic (Het)arenes and Unexpected Prodrug Identification for the Trypanosoma Protease Rhodesain. Molecules, 2020, 25, 1451.	1.7	16
117	Inhibition of cysteine proteases by peptides containing aziridine-2,3-dicarboxylic acid building blocks. , 1999, 51, 87-97.		15
118	(S)-Thiirancarboxylic acid as a reactive building block for a new class of cysteine protease inhibitors. Bioorganic and Medicinal Chemistry Letters, 2000, 10, 2647-2651.	1.0	15
119	On-Bead Screening of a Combinatorial Fumaric Acid Derived Peptide Library Yields Antiplasmodial Cysteine Protease Inhibitors with Unusual Peptide Sequences. Journal of Medicinal Chemistry, 2009, 52, 5662-5672.	2.9	15
120	Development of a New Antileishmanial Aziridine-2,3-Dicarboxylate-Based Inhibitor with High Selectivity for Parasite Cysteine Proteases. Antimicrobial Agents and Chemotherapy, 2016, 60, 797-805.	1.4	15
121	Anticancer study of heterobimetallic platinum(II)-ruthenium(II) and platinum(II)-rhodium(III) complexes with bridging dithiooxamide ligand. Journal of Organometallic Chemistry, 2019, 900, 120918.	0.8	15
122	Challenging Problems in Charge Density Determination: Polar Bonds and Influence of the Environment. Structure and Bonding, 2011, , 47-97.	1.0	14
123	New cisâ€Configured Aziridineâ€2â€carboxylates as Aspartic Acid Protease Inhibitors. ChemMedChem, 2011, 6, 141-152.	1.6	14
124	Cis autocatalytic cleavage of glycineâ€linked Zika virus NS2Bâ€NS3 protease constructs. FEBS Letters, 2019, 593, 2204-2213.	1.3	14
125	Conformational Dynamics of the Dengue Virus Protease Revealed by Fluorescence Correlation and Single-Molecule FRET Studies. Journal of Physical Chemistry B, 2021, 125, 6837-6846.	1.2	14
126	Drug combination studies of curcumin and genistein against rhodesain of Trypanosoma brucei rhodesiense. Natural Product Research, 2019, 33, 3577-3581.	1.0	13

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127	Conformation and Hydrogen Bonding Properties of an Aziridinyl Peptide:Â X-ray Structure Analysis, Raman Spectroscopy and Theoretical Investigations. Journal of Physical Chemistry A, 2004, 108, 11398-11408.	1.1	12
128	Development and validation of a separation method for the diastereomers and enantiomers of aziridine-type protease inhibitors. Electrophoresis, 2005, 26, 2313-2319.	1.3	12
129	Natural Product Repertoire of the Genus Amphimedon. Marine Drugs, 2019, 17, 19.	2.2	12
130	Investigation of the influence of chirality and halogen atoms on the anticancer activity of enantiopure palladium(<scp>ii</scp>) complexes derived from chiral amino-alcohol Schiff bases and 2-picolylamine. New Journal of Chemistry, 2022, 46, 6470-6483.	1.4	12
131	Can Experimental Electronâ€Density Studies be Used as a Tool to Predict Biologically Relevant Properties of Lowâ€Molecular Weight Enzyme Ligands?. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2013, 639, 1905-1921.	0.6	11
132	Structure, interdomain dynamics, and pH-dependent autoactivation of pro-rhodesain, the main lysosomal cysteine protease from African trypanosomes. Journal of Biological Chemistry, 2021, 296, 100565.	1.6	11
133	Interfering with Host Proteases in SARS-CoV-2 Entry as a Promising Therapeutic Strategy. Current Medicinal Chemistry, 2022, 29, 635-665.	1.2	11
134	Development of novel dipeptide nitriles as inhibitors of rhodesain of Trypanosoma brucei rhodesiense. European Journal of Medicinal Chemistry, 2022, 236, 114328.	2.6	11
135	Electrostatic complementarity in pseudoreceptor modeling based on drug molecule crystal structures: the case of loxistatin acid (E64c). New Journal of Chemistry, 2015, 39, 1628-1633.	1.4	10
136	Cytotoxicity of Endoperoxides from the Caribbean Sponge Plakortis halichondrioides towards Sensitive and Multidrug-Resistant Leukemia Cells: Acids vs. Esters Activity Evaluation. Marine Drugs, 2017, 15, 63.	2.2	10
137	Ensembleâ€based ADMEâ€“Tox profiling and virtual screening for the discovery of new inhibitors of the Leishmania mexicana cysteine protease CPB2.8Δ”CTE. Chemical Biology and Drug Design, 2018, 91, 597-604.	1.5	10
138	New aziridine-based inhibitors of cathepsin L-like cysteine proteases with selectivity for the Leishmania cysteine protease LmCPB2.8. European Journal of Medicinal Chemistry, 2018, 156, 587-597.	2.6	10
139	Antiproliferative Properties of a Few Auranofin-Related Gold(I) and Silver(I) Complexes in Leukemia Cells and their Interferences with the Ubiquitin Proteasome System. Molecules, 2020, 25, 4454.	1.7	10
140	Development of Novel Benzodiazepineâ€Based Peptidomimetics as Inhibitors of Rhodesain from Trypanosoma brucei rhodesiense. ChemMedChem, 2020, 15, 995-1001.	1.6	10
141	Similarities and Differences between Crystal and Enzyme Environmental Effects on the Electron Density of Drug Molecules. Chemistry - A European Journal, 2021, 27, 3407-3419.	1.7	10
142	Development of Antitrypanosomal and Antiplasmodial Nonpeptidic Cysteine Protease Inhibitors based on Nâ€Protectedâ€Guanidinoâ€Furan and â€Pyrrole Building Blocks. ChemMedChem, 2011, 6, 1581-1586.	1.6	9
143	Identification of the protease inhibitor miraziridine A in the Red sea sponge Theonella swinhoei. Pharmacognosy Research (discontinued), 2012, 4, 63.	0.3	9
144	Fly versus man: evolutionary impairment of nucleolar targeting affects the degradome of Drosophila's Taspase1. FASEB Journal, 2015, 29, 1973-1985.	0.2	9

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145	Synthesis, solution behaviour and potential anticancer activity of new trinuclear organometallic palladium(II) complex of {S}-1-phenylethyl dithiooxamide: Comparison with the trinuclear heterobimetallic platinum(II) analogue. Polyhedron, 2019, 164, 195-201.	1.0	9
146	Chemical biology and medicinal chemistry of RNA methyltransferases. Nucleic Acids Research, 2022, 50, 4216-4245.	6.5	9
147	Development of Urea-Bond-Containing Michael Acceptors as Antitrypanosomal Agents Targeting Rhodesain. ACS Medicinal Chemistry Letters, 2022, 13, 1083-1090.	1.3	9
148	Synthesis and Evaluation of Non-peptidic Cysteine Protease Inhibitors of P. falciparum Derived from Etacrynic Acid. Molecules, 2009, 14, 19-35.	1.7	8
149	Ruthenium(<scp>ii</scp>) and palladium(<scp>ii</scp>) homo- and heterobimetallic complexes: synthesis, crystal structures, theoretical calculations and biological studies. Dalton Transactions, 2019, 48, 15869-15887.	1.6	8
150	Drug Synergism: Studies of Combination of RK-52 and Curcumin against Rhodesain of Trypanosoma brucei rhodesiense. ACS Medicinal Chemistry Letters, 2020, 11, 806-810.	1.3	8
151	Development of Reduced Peptide Bond Pseudopeptide Michael Acceptors for the Treatment of Human African Trypanosomiasis. Molecules, 2022, 27, 3765.	1.7	8
152	Synthesis and Pharmacological Evaluation of [¹¹C]4-Methoxy-N-[2-(thiophen-2-yl)imidazo[1,2-a]pyridin-3-yl]benzamide as a Brain Penetrant PET Ligand Selective for the Î´-Subunit-Containing Î³-Aminobutyric Acid Type A Receptors. ACS Omega, 2019, 4, 8846-8851.	1.6	7
153	New non-peptidic Inhibitors of Papain Derived from Etacrynic Acid. Medicinal Chemistry, 2005, 1, 361-370.	0.7	7
154	Identification of novel small-molecular inhibitors of Staphylococcus aureus sortase A using hybrid virtual screening. Journal of Antibiotics, 2022, 75, 321-332.	1.0	7
155	Discovery of Inhibitors of DNA Methyltransferase 2, an Epitranscriptomic Modulator and Potential Target for Cancer Treatment. Journal of Medicinal Chemistry, 2022, 65, 9750-9788.	2.9	7
156	Anti-trypanosomal activities and structural chemical properties of selected compound classes. Parasitology Research, 2015, 114, 501-512.	0.6	6
157	Eliciting callus culture for production of hepatoprotective flavonoids and phenolics from Sequoia sempervirens (D. Don Endl). Natural Product Research, 2020, 34, 3125-3129.	1.0	6
158	Warhead Reactivity Limits the Speed of Inhibition of the Cysteine Protease Rhodesain. ACS Chemical Biology, 2021, 16, 661-670.	1.6	6
159	Structural Determinants for the Mode of Action of Imidazopyridine DS2 at Î´-Containing Î³-Aminobutyric Acid Type A Receptors. Journal of Medicinal Chemistry, 2021, 64, 4730-4743.	2.9	6
160	New peptidomimetic rhodesain inhibitors with improved selectivity towards human cathepsins. European Journal of Medicinal Chemistry, 2022, 238, 114460.	2.6	6
161	Comparison of the separation of aziridine isomers applyingheptakis(2,3-di-O-methyl-6-sulfato)Î²-CD andheptakis(2,3-di-O-acetyl-6-sulfato)Î²-CD in aqueous and nonaqueous systems. Electrophoresis, 2005, 26, 3897-3903.	1.3	5
162	Bistacrines as potential antitrypanosomal agents. Bioorganic and Medicinal Chemistry, 2017, 25, 4526-4531.	1.4	5

#	Article	IF	Citations
163	Identification of a potential allosteric site of Golgi Î±-mannosidase II using computer-aided drug design. PLoS ONE, 2019, 14, e0216132.	1.1	5
164	Metal Ions as Co-Inhibitors of Serine Proteases: A New Approach in the Search for Specific High-Affinity Ligands. Angewandte Chemie - International Edition, 1998, 37, 1830-1832.	7.2	4
165	Approaching an experimental electron density model of the biologically active trans â€epoxysuccinyl amide groupâ€"Substituent effects vs. crystal packing. Journal of Physical Organic Chemistry, 2017, 30, e3683.	0.9	4
166	Applicability of a singleâ€use bioreactor compared to a glass bioreactor for the fermentation of filamentous fungi and evaluation of the reproducibility of growth in pellet form. Engineering in Life Sciences, 2021, 21, 324-339.	2.0	4
167	E/Z Diastereoselective Enzymatic Hydrolysis of Esters and Diesters. Angewandte Chemie International Edition in English, 1993, 32, 572-574.	4.4	3
168	Inducible APOBEC3G-Vif Double Stable Cell Line as a High-Throughput Screening Platform To Identify Antiviral Compounds. Antimicrobial Agents and Chemotherapy, 2010, 54, 78-87.	1.4	3
169	Modular Solid-Phase Synthesis of Antiprotozoal Barnesin Derivatives. Organic Letters, 2020, 22, 3744-3748.	2.4	3
170	Nostotrebin 6 Related Cyclopentenediones and Î´-Lactones with Broad Activity Spectrum Isolated from the Cultivation Medium of the Cyanobacterium Nostoc sp. CBT1153. Journal of Natural Products, 2020, 83, 392-400.	1.5	3
171	The Medicinal Chemistry of Zika Virus. , 2021, , 233-295.		3
172	Synthesis, X-ray Structure Determination, and Comprehensive Photochemical Characterization of (Trifluoromethyl)diazirine-Containing TRPML1 Ligands. Journal of Organic Chemistry, 2021, 86, 6169-6183.	1.7	3
173	A low-cost 3D-printable differential scanning fluorometer for protein and RNA melting experiments. HardwareX, 2022, 11, e00256.	1.1	3
174	Identification, Characterization, and Synthesis of Natural Parasitic Cysteine Protease Inhibitors: Pentacitidins Are More Potent Falcitidin Analogues. ACS Chemical Biology, 2022, 17, 576-589.	1.6	3
175	Thiirancarboxamides as Inhibitors of Papain. Archiv Der Pharmazie, 2004, 337, 90-95.	2.1	2
176	Promising trypanocidal heterocyclic compounds of natural origin and their synthetic analogs. , 2019, , 165-217.		2
177	Evaluation of curcumin irreversibility. Natural Product Research, 2020, 34, 3159-3162.	1.0	2
178	GNPS-guided discovery of xylacremolide C and D, evaluation of their putative biosynthetic origin and bioactivity studies of xylacremolide A and B. RSC Advances, 2021, 11, 18748-18756.	1.7	2
179	2-Sulfonylpyrimidines as Privileged Warheads for the Development of S. aureus Sortase A Inhibitors. Frontiers in Molecular Biosciences, 2021, 8, 804970.	1.6	2
180	The discovery of novel antitrypanosomal 4-phenyl-6-(pyridin-3-yl)pyrimidines. European Journal of Medicinal Chemistry, 2021, 209, 112871.	2.6	1

#	Article	IF	Citations
181	Synthesis of peptides with aziridine-2,3-dicarboxylic acid as an Î²-amino acid equivalent building block. , 1999, , 634-636.		0