

Stanislav Gobec

List of Publications by Year in descending order

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248
papers

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citations

61984

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98798

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257
all docs

257
docs citations

257
times ranked

8232
citing authors

#	ARTICLE	IF	CITATIONS
1	Cytoplasmic steps of peptidoglycan biosynthesis. FEMS Microbiology Reviews, 2008, 32, 168-207.	8.6	583
2	Discovery, Biological Evaluation, and Crystal Structure of a Novel Nanomolar Selective Butyrylcholinesterase Inhibitor. Journal of Medicinal Chemistry, 2014, 57, 8167-8179.	6.4	220
3	Discovery of Novel 5-Benzylidenerhodanine and 5-Benzylidenethiazolidine-2,4-dione Inhibitors of MurD Ligase. Journal of Medicinal Chemistry, 2010, 53, 6584-6594.	6.4	115
4	Endocrine Disruptome—An Open Source Prediction Tool for Assessing Endocrine Disruption Potential through Nuclear Receptor Binding. Journal of Chemical Information and Modeling, 2014, 54, 1254-1267.	5.4	113
5	The Magic of Crystal Structure-Based Inhibitor Optimization: Development of a Butyrylcholinesterase Inhibitor with Picomolar Affinity and in Vivo Activity. Journal of Medicinal Chemistry, 2018, 61, 119-139.	6.4	112
6	Inhibitors of Cathepsin B. Current Medicinal Chemistry, 2006, 13, 2309-2327.	2.4	106
7	Development of an in-vivo active reversible butyrylcholinesterase inhibitor. Scientific Reports, 2016, 6, 39495.	3.3	105
8	False Positives in the Early Stages of Drug Discovery. Current Medicinal Chemistry, 2010, 17, 4231-4255.	2.4	96
9	Structural characterization and biological evaluation of a clioquinol—ruthenium complex with copper-independent antileukaemic activity. Dalton Transactions, 2014, 43, 9045-9051.	3.3	88
10	Novel Naphthalene-N-sulfonyl-glutamic Acid Derivatives as Inhibitors of MurD, a Key Peptidoglycan Biosynthesis Enzyme. Journal of Medicinal Chemistry, 2008, 51, 7486-7494.	6.4	86
11	Design, synthesis and biological evaluation of new phthalimide and saccharin derivatives with alicyclic amines targeting cholinesterases, beta-secretase and amyloid beta aggregation. European Journal of Medicinal Chemistry, 2017, 125, 676-695.	5.5	85
12	Structural and Functional Characterization of Enantiomeric Glutamic Acid Derivatives as Potential Transition State Analogue Inhibitors of MurD Ligase. Journal of Molecular Biology, 2007, 370, 107-115.	4.2	83
13	A road map for prioritizing warheads for cysteine targeting covalent inhibitors. European Journal of Medicinal Chemistry, 2018, 160, 94-107.	5.5	80
14	Inhibitors of 17 β -Hydroxysteroid Dehydrogenase Type 1. Current Medicinal Chemistry, 2008, 15, 137-150.	2.4	78
15	Inhibitors of the peptidoglycan biosynthesis enzymes MurA-F. Bioorganic Chemistry, 2014, 55, 2-15.	4.1	78
16	Novel Mechanism of Cathepsin B Inhibition by Antibiotic Nitroxoline and Related Compounds. ChemMedChem, 2011, 6, 1351-1356.	3.2	75
17	Antibacterial and β -Lactamase Inhibitory Activity of Monocyclic β -Lactams. Medicinal Research Reviews, 2018, 38, 426-503.	10.5	73
18	5-Benzylidenethiazolidinones as Multitarget Inhibitors of Bacterial Mur Ligases. ChemMedChem, 2010, 5, 286-295.	3.2	72

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19	Novel multi-target-directed ligands for Alzheimer's disease: Combining cholinesterase inhibitors and 5-HT ₆ receptor antagonists. Design, synthesis and biological evaluation. <i>European Journal of Medicinal Chemistry</i> , 2016, 124, 63-81.	5.5	72
20	Multi-target-directed ligands for treating Alzheimer's disease: Butyrylcholinesterase inhibitors displaying antioxidant and neuroprotective activities. <i>European Journal of Medicinal Chemistry</i> , 2018, 156, 598-617.	5.5	72
21	LiSiCA: A Software for Ligand-Based Virtual Screening and Its Application for the Discovery of Butyrylcholinesterase Inhibitors. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 1521-1528.	5.4	70
22	Discovery of novel benzene 1,3-dicarboxylic acid inhibitors of bacterial MurD and MurE ligases by structure-based virtual screening approach. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2009, 19, 2668-2673.	2.2	67
23	Antifungal activity of cinnamic acid derivatives involves inhibition of benzoate 4-hydroxylase (CYP53). <i>Journal of Applied Microbiology</i> , 2014, 116, 955-966.	3.1	67
24	Structure-Based Design of a New Series of D-Glutamic Acid Based Inhibitors of Bacterial UDP-N-acetylmuramoyl-L-alanine:D-glutamate Ligase (MurD). <i>Journal of Medicinal Chemistry</i> , 2011, 54, 4600-4610.	6.4	64
25	Nitroxoline impairs tumor progression in vitro and in vivo by regulating cathepsin B activity. <i>Oncotarget</i> , 2015, 6, 19027-19042.	1.8	64
26	Structure-activity relationships of new cyanothiophene inhibitors of the essential peptidoglycan biosynthesis enzyme MurF. <i>European Journal of Medicinal Chemistry</i> , 2013, 66, 32-45.	5.5	62
27	Synthesis and Biological Evaluation of (6- and 7-Phenyl) Coumarin Derivatives as Selective Nonsteroidal Inhibitors of 17 β -Hydroxysteroid Dehydrogenase Type 1. <i>Journal of Medicinal Chemistry</i> , 2011, 54, 248-261.	6.4	61
28	New 5-benzylidenethiazolidin-4-one inhibitors of bacterial MurD ligase: Design, synthesis, crystal structures, and biological evaluation. <i>European Journal of Medicinal Chemistry</i> , 2011, 46, 5512-5523.	5.5	61
29	Melanin is crucial for growth of the black yeast <i>Hortaea werneckii</i> in its natural hypersaline environment. <i>Fungal Biology</i> , 2013, 117, 368-379.	2.5	60
30	Development of multifunctional, heterodimeric isoindoline-1,3-dione derivatives as cholinesterase and β -amyloid aggregation inhibitors with neuroprotective properties. <i>European Journal of Medicinal Chemistry</i> , 2015, 92, 738-749.	5.5	60
31	Tryptophan-derived butyrylcholinesterase inhibitors as promising leads against Alzheimer's disease. <i>Chemical Communications</i> , 2019, 55, 3765-3768.	4.1	60
32	Inhibition of D-Ala:D-Ala ligase through a phosphorylated form of the antibiotic D-cycloserine. <i>Nature Communications</i> , 2017, 8, 1939.	12.8	59
33	Design, Synthesis, and Evaluation of New Thiadiazole-Based Direct Inhibitors of Enoyl Acyl Carrier Protein Reductase (InhA) for the Treatment of Tuberculosis. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 613-624.	6.4	58
34	Design, synthesis and structure-activity relationships of new phosphinate inhibitors of MurD. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2006, 16, 343-348.	2.2	57
35	Development of New Cathepsin B Inhibitors: Combining Bioisosteric Replacements and Structure-Based Design To Explore the Structure-Activity Relationships of Nitroxoline Derivatives. <i>Journal of Medicinal Chemistry</i> , 2013, 56, 521-533.	6.4	56
36	Discovery of new inhibitors of the bacterial peptidoglycan biosynthesis enzymes MurD and MurF by structure-based virtual screening. <i>Bioorganic and Medicinal Chemistry</i> , 2009, 17, 1884-1889.	3.0	54

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37	Second-generation sulfonamide inhibitors of d-glutamic acid-adding enzyme: Activity optimisation with conformationally rigid analogues of d-glutamic acid. <i>European Journal of Medicinal Chemistry</i> , 2011, 46, 2880-2894.	5.5	51
38	Structure-based development of nitroxoline derivatives as potential multifunctional anti-Alzheimer agents. <i>Bioorganic and Medicinal Chemistry</i> , 2015, 23, 4442-4452.	3.0	50
39	N-Propargylpiperidines with naphthalene-2-carboxamide or naphthalene-2-sulfonamide moieties: Potential multifunctional anti-Alzheimer's agents. <i>Bioorganic and Medicinal Chemistry</i> , 2017, 25, 633-645.	3.0	49
40	Flavonoids and cinnamic acid derivatives as inhibitors of 17 β -hydroxysteroid dehydrogenase type 1. <i>Molecular and Cellular Endocrinology</i> , 2009, 301, 229-234.	3.2	48
41	Biochemical Characterization and Physiological Properties of Escherichia coli UDP- N -Acetylmuramate: l -Alanyl- β - d -Glutamyl- meso - Diaminopimelate Ligase. <i>Journal of Bacteriology</i> , 2007, 189, 3987-3995.	2.2	47
42	Design, Synthesis, and Biological Evaluation of 1-Benzylamino-2-hydroxyalkyl Derivatives as New Potential Disease-Modifying Multifunctional Anti-Alzheimer's Agents. <i>ACS Chemical Neuroscience</i> , 2018, 9, 1074-1094.	3.5	47
43	Synthesis and structure-activity relationship study of novel quinazolinone-based inhibitors of MurA. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2017, 27, 3529-3533.	2.2	46
44	A new "golden age" for the antitubercular target InhA. <i>Drug Discovery Today</i> , 2017, 22, 492-502.	6.4	46
45	Nonsteroidal anti-inflammatory drugs and their analogues as inhibitors of aldo-keto reductase AKR1C3: New lead compounds for the development of anticancer agents. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2005, 15, 5170-5175.	2.2	45
46	Cinnamic acids as new inhibitors of 17 β -hydroxysteroid dehydrogenase type 5 (AKR1C3). <i>Molecular and Cellular Endocrinology</i> , 2006, 248, 233-235.	3.2	45
47	Dual Inhibitor of MurD and MurE Ligases from <i>Escherichia coli</i> and <i>Staphylococcus aureus</i> . <i>ACS Medicinal Chemistry Letters</i> , 2012, 3, 626-630.	2.8	45
48	Synthesis of aminoboronic acid derivatives: an update on recent advances. <i>Organic Chemistry Frontiers</i> , 2019, 6, 2991-2998.	4.5	45
49	Synthesis and biological evaluation of new glutamic acid-based inhibitors of MurD ligase. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2009, 19, 153-157.	2.2	44
50	Isoindoline-1,3-dione derivatives targeting cholinesterases: Design, synthesis and biological evaluation of potential anti-Alzheimer's agents. <i>Bioorganic and Medicinal Chemistry</i> , 2015, 23, 1629-1637.	3.0	44
51	Dual inhibitors of cholinesterases and monoamine oxidases for Alzheimer's disease. <i>Future Medicinal Chemistry</i> , 2017, 9, 811-832.	2.3	44
52	Novel Multitarget-Directed Ligands Aiming at Symptoms and Causes of Alzheimer's Disease. <i>ACS Chemical Neuroscience</i> , 2018, 9, 1195-1214.	3.5	44
53	Discovery of New Inhibitors of d-Alanine: d-Alanine Ligase by Structure-Based Virtual Screening. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 7442-7448.	6.4	43
54	A new approach towards peptid sulfonamides: synthesis of potential inhibitors of bacterial peptidoglycan biosynthesis enzymes MurD and MurE. <i>Tetrahedron</i> , 2006, 62, 10980-10988.	1.9	42

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55	Design, synthesis, biochemical evaluation and antimycobacterial action of phosphonate inhibitors of antigen 85C, a crucial enzyme involved in biosynthesis of the mycobacterial cell wall. <i>European Journal of Medicinal Chemistry</i> , 2007, 42, 54-63.	5.5	42
56	Synthesis of new N-benzylpiperidine derivatives as cholinesterase inhibitors with β -amyloid anti-aggregation properties and beneficial effects on memory in vivo. <i>Bioorganic and Medicinal Chemistry</i> , 2015, 23, 2445-2457.	3.0	42
57	Design and synthesis of new hydroxyethylamines as inhibitors of d-alanyl-d-lactate ligase (VanA) and d-alanyl-d-alanine ligase (DdlB). <i>Bioorganic and Medicinal Chemistry Letters</i> , 2009, 19, 1376-1379.	2.2	41
58	Chalcone derivatives: synthesis, in vitro and in vivo evaluation of their anti-anxiety, anti-depression and analgesic effects. <i>Heliyon</i> , 2019, 5, e01376.	3.2	41
59	Flavonoids and cinnamic acid esters as inhibitors of fungal 17 β -hydroxysteroid dehydrogenase: A synthesis, QSAR and modelling study. <i>Bioorganic and Medicinal Chemistry</i> , 2006, 14, 7404-7418.	3.0	40
60	Phosphorylated hydroxyethylamines as novel inhibitors of the bacterial cell wall biosynthesis enzymes MurC to MurF. <i>Bioorganic Chemistry</i> , 2009, 37, 217-222.	4.1	39
61	Phytoestrogens as inhibitors of the human progesterone metabolizing enzyme AKR1C1. <i>Molecular and Cellular Endocrinology</i> , 2006, 259, 30-42.	3.2	38
62	Nonpeptidic Selective Inhibitors of the Chymotrypsin-Like (β -5) Subunit of the Immunoproteasome. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 5745-5748.	13.8	38
63	Novel 2-thioxothiazolidin-4-one inhibitors of bacterial MurD ligase targeting d-Glu- and diphosphate-binding sites. <i>European Journal of Medicinal Chemistry</i> , 2011, 46, 3964-3975.	5.5	37
64	Diazenedicarboxamides as inhibitors of d-alanine-d-alanine ligase (Ddl). <i>Bioorganic and Medicinal Chemistry Letters</i> , 2007, 17, 2047-2054.	2.2	36
65	New Noncovalent Inhibitors of Penicillin-Binding Proteins from Penicillin-Resistant Bacteria. <i>PLoS ONE</i> , 2011, 6, e19418.	2.5	36
66	Phosphonate inhibitors of antigen 85C, a crucial enzyme involved in the biosynthesis of the <i>Mycobacterium tuberculosis</i> cell wall. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2004, 14, 3559-3562.	2.2	35
67	Novel toll-like receptor 4 (TLR4) antagonists identified by structure- and ligand-based virtual screening. <i>European Journal of Medicinal Chemistry</i> , 2013, 70, 393-399.	5.5	35
68	Design and Synthesis of Novel N-Benzylidenesulfonohydrazide Inhibitors of MurC and MurD as Potential Antibacterial Agents. <i>Molecules</i> , 2008, 13, 11-30.	3.8	34
69	Inhibitors of Aldo-Keto Reductases AKR1C1-AKR1C4. <i>Current Medicinal Chemistry</i> , 2011, 18, 2554-2565.	2.4	34
70	Benzene-1,3-dicarboxylic acid 2,5-dimethylpyrrole derivatives as multiple inhibitors of bacterial Mur ligases (MurC-MurF). <i>Bioorganic and Medicinal Chemistry</i> , 2014, 22, 4124-4134.	3.0	34
71	Identification of Conserved Water Sites in Protein Structures for Drug Design. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 3094-3103.	5.4	34
72	Indoleamine and tryptophan 2,3-dioxygenases as important future therapeutic targets. , 2021, 221, 107746.		34

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73	Specificity Determinants for Lysine Incorporation in Staphylococcus aureus Peptidoglycan as Revealed by the Structure of a MurE Enzyme Ternary Complex. <i>Journal of Biological Chemistry</i> , 2013, 288, 33439-33448.	3.4	33
74	Clioquinolâ€“ruthenium complex impairs tumour cell invasion by inhibiting cathepsin B activity. <i>Dalton Transactions</i> , 2016, 45, 16913-16921.	3.3	33
75	Stereoselective Activity of 1-Propargyl-4-styrylpiperidine-like Analogues That Can Discriminate between Monoamine Oxidase Isoforms A and B. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 1361-1387.	6.4	33
76	1-Benzylpyrrolidine-3-amine-based BuChE inhibitors with anti-aggregating, antioxidant and metal-chelating properties as multifunctional agents against Alzheimerâ€™s disease. <i>European Journal of Medicinal Chemistry</i> , 2020, 187, 111916.	5.5	33
77	N-alkylpiperidine carbamates as potential anti-Alzheimerâ€™s agents. <i>European Journal of Medicinal Chemistry</i> , 2020, 197, 112282.	5.5	33
78	Recent Advances in Design, Synthesis and Biological Activity of Aminoalkylsulfonates and Sulfonamidopeptides. <i>Current Medicinal Chemistry</i> , 2004, 11, 3263-3278.	2.4	32
79	Phosphinate Inhibitors of UDP-N-Acetylmuramoyl-L-Alanyl-D-Glutamate:L-Lysine Ligase (MurE). <i>Archiv Der Pharmazie</i> , 2007, 340, 127-134.	4.1	31
80	Synthesis and Biological Evaluation of <i>N</i> -Acylhydrazones as Inhibitors of MurC and MurD Ligases. <i>ChemMedChem</i> , 2008, 3, 1362-1370.	3.2	31
81	Synthesis of <i>N</i> -phthalimido \hat{I}^2 -aminoethanesulfonyl chlorides: the use of thionyl chloride for a simple and efficient synthesis of new peptidosulfonamide building blocks. <i>Tetrahedron Letters</i> , 2005, 46, 4069-4072.	1.4	30
82	Progestins as inhibitors of the human 20-ketosteroid reductases, AKR1C1 and AKR1C3. <i>Chemico-Biological Interactions</i> , 2011, 191, 227-233.	4.0	30
83	Cobalt-Catalyzed Cross-Coupling of Grignards with Allylic and Vinylic Bromides: Use of Sarcosine as a Natural Ligand. <i>Journal of Organic Chemistry</i> , 2015, 80, 7803-7809.	3.2	30
84	Development of screening assays and discovery of initial inhibitors of pneumococcal peptidoglycan deacetylase PgdA. <i>Biochemical Pharmacology</i> , 2011, 82, 43-52.	4.4	29
85	Synthesis, Molecular Modelling and Biological Evaluation of Novel Heterodimeric, Multiple Ligands Targeting Cholinesterases and Amyloid Beta. <i>Molecules</i> , 2016, 21, 410.	3.8	29
86	Inhibition of endopeptidase and exopeptidase activity of cathepsin B impairs extracellular matrix degradation and tumour invasion. <i>Biological Chemistry</i> , 2016, 397, 165-174.	2.5	29
87	Structure Guided Development of Potent Reversibly Binding Penicillin Binding Protein Inhibitors. <i>ACS Medicinal Chemistry Letters</i> , 2011, 2, 219-223.	2.8	28
88	MurD enzymes: some recent developments. <i>Biomolecular Concepts</i> , 2013, 4, 539-556.	2.2	28
89	Organoruthenated Nitroxoline Derivatives Impair Tumor Cell Invasion through Inhibition of Cathepsin B Activity. <i>Inorganic Chemistry</i> , 2019, 58, 12334-12347.	4.0	28
90	Reaching toward underexplored targets in antibacterial drug design. <i>Drug Development Research</i> , 2019, 80, 6-10.	2.9	28

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91	4,6-Substituted-1,3,5-triazin-2(1H)-ones as monocyclic catalytic inhibitors of human DNA topoisomerase III \pm targeting the ATP binding site. <i>Bioorganic and Medicinal Chemistry</i> , 2015, 23, 4218-4229.	3.0	27
92	Design, Synthesis, and Biological Evaluation of 2-(Benzylamino-2-Hydroxyalkyl)Isoindoline-1,3-Diones Derivatives as Potential Disease-Modifying Multifunctional Anti-Alzheimer Agents. <i>Molecules</i> , 2018, 23, 347.	3.8	27
93	New cyclopentane derivatives as inhibitors of steroid metabolizing enzymes AKR1C1 and AKR1C3. <i>European Journal of Medicinal Chemistry</i> , 2009, 44, 2563-2571.	5.5	26
94	Ellipticines and 9-acridinylamines as inhibitors of d-alanine:d-alanine ligase. <i>Bioorganic and Medicinal Chemistry</i> , 2011, 19, 5137-5146.	3.0	26
95	Discovery of <i>Mycobacterium tuberculosis</i> InhA Inhibitors by Binding Sites Comparison and Ligands Prediction. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 11069-11078.	6.4	26
96	Cinnamic acid esters as potent inhibitors of fungal 17 β -hydroxysteroid dehydrogenase—a model enzyme of the short-chain dehydrogenase/reductase superfamily. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2004, 14, 3933-3936.	2.2	25
97	Design, synthesis and evaluation of second generation MurF inhibitors based on a cyanothiophene scaffold. <i>European Journal of Medicinal Chemistry</i> , 2014, 73, 83-96.	5.5	25
98	Synthesis and Biological Assessment of Racemic Benzochromenopyrimidinimines as Antioxidant, Cholinesterase, and A β Aggregation Inhibitors for Alzheimer's Disease Therapy. <i>ChemMedChem</i> , 2016, 11, 1318-1327.	3.2	24
99	Discovery of new MurA inhibitors using induced-fit simulation and docking. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2017, 27, 944-949.	2.2	24
100	Synthesis of 1-C-linked diphosphate analogues of UDP-N-Ac-glucosamine and UDP-N-Ac-muramic acid. <i>Tetrahedron</i> , 2008, 64, 9093-9100.	1.9	23
101	Recent Advances in the Synthesis and Applications of Reduced Amide Pseudopeptides. <i>Current Medicinal Chemistry</i> , 2009, 16, 2289-2304.	2.4	23
102	Cathepsin B inhibitors: Further exploration of the nitroxoline core. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2018, 28, 1239-1247.	2.2	23
103	Pyrimido[1,2-b]indazole derivatives: Selective inhibitors of human monoamine oxidase B with neuroprotective activity. <i>European Journal of Medicinal Chemistry</i> , 2021, 209, 112911.	5.5	23
104	Synthesis and Biological Evaluation of Benzochromenopyrimidinones as Cholinesterase Inhibitors and Potent Antioxidant, Non-Hepatotoxic Agents for Alzheimer's Disease. <i>Molecules</i> , 2016, 21, 634.	3.8	22
105	Heterocyclic electrophiles as new MurA inhibitors. <i>Archiv Der Pharmazie</i> , 2018, 351, e1800184.	4.1	22
106	Recent Advances in the Synthesis of Acylboranes and Their Widening Applicability. <i>ACS Omega</i> , 2020, 5, 17868-17875.	3.5	22
107	Cinnamic Acid Derivatives Induce Cell Cycle Arrest in Carcinoma Cell Lines. <i>Medicinal Chemistry</i> , 2013, 9, 633-641.	1.5	22
108	6-Arylpyrido[2,3-d]pyrimidines as Novel ATP-Competitive Inhibitors of Bacterial D-Alanine:D-Alanine Ligase. <i>PLoS ONE</i> , 2012, 7, e39922.	2.5	21

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109	Inhibitor Design Strategy Based on an Enzyme Structural Flexibility: A Case of Bacterial MurD Ligase. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 1451-1466.	5.4	21
110	Furan-based benzene mono- and dicarboxylic acid derivatives as multiple inhibitors of the bacterial Mur ligases (MurC–MurF): experimental and computational characterization. <i>Journal of Computer-Aided Molecular Design</i> , 2015, 29, 541-560.	2.9	21
111	Structure–Activity Relationships of Novel Tryptamine-Based Inhibitors of Bacterial Transglycosylase. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 9712-9721.	6.4	21
112	A patent review of immunoproteasome inhibitors. <i>Expert Opinion on Therapeutic Patents</i> , 2018, 28, 517-540.	5.0	21
113	WIDOCK: a reactive docking protocol for virtual screening of covalent inhibitors. <i>Journal of Computer-Aided Molecular Design</i> , 2021, 35, 223-244.	2.9	21
114	Redox-Based Inactivation of Cysteine Cathepsins by Compounds Containing the 4-Aminophenol Moiety. <i>PLoS ONE</i> , 2011, 6, e27197.	2.5	20
115	Selective Inhibitors of Aldo-Keto Reductases AKR1C1 and AKR1C3 Discovered by Virtual Screening of a Fragment Library. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 7417-7424.	6.4	20
116	MurD enzymes from different bacteria: Evaluation of inhibitors. <i>Biochemical Pharmacology</i> , 2012, 84, 625-632.	4.4	20
117	New direct inhibitors of InhA with antimycobacterial activity based on a tetrahydropyran scaffold. <i>European Journal of Medicinal Chemistry</i> , 2016, 112, 252-257.	5.5	20
118	Structure-guided optimization of 4,6-substituted-1,3,5-triazin-2(1H)-ones as catalytic inhibitors of human DNA topoisomerase II–. <i>European Journal of Medicinal Chemistry</i> , 2019, 175, 330-348.	5.5	20
119	Cinnamates and cinnamamides inhibit fungal 17⁻-hydroxysteroid dehydrogenase. <i>Molecular and Cellular Endocrinology</i> , 2006, 248, 239-241.	3.2	19
120	Small molecule inhibitors of peptidoglycan synthesis targeting the lipid II precursor. <i>Biochemical Pharmacology</i> , 2011, 81, 1098-1105.	4.4	19
121	Cathepsin X cleavage of the ™ integrin regulates talin-binding and LFA-1 affinity in T cells. <i>Journal of Leukocyte Biology</i> , 2011, 90, 99-109.	3.3	19
122	Function of the <scp>d</scp>-Alanine:<scp>d</scp>-Alanine Ligase Lid Loop: A Molecular Modeling and Bioactivity Study. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 6849-6856.	6.4	19
123	Molecular dynamics to enhance structure-based virtual screening on cathepsin B. <i>Journal of Computer-Aided Molecular Design</i> , 2015, 29, 707-712.	2.9	19
124	Assessment of Tractable Cysteines for Covalent Targeting by Screening Covalent Fragments. <i>ChemBioChem</i> , 2021, 22, 743-753.	2.6	19
125	Novel inhibitors of ⁻-ketoacyl-ACP reductase from <i>Escherichia coli</i> . <i>Chemico-Biological Interactions</i> , 2009, 178, 310-316.	4.0	18
126	Trihydroxynaphthalene reductase of <i>Curvularia lunata</i> –A target for flavonoid action?. <i>Chemico-Biological Interactions</i> , 2009, 178, 259-267.	4.0	18

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127	Glucosamine in iron-catalysed cross-coupling reactions of Grignards with allylic and vinylic bromides: application to the synthesis of a key sitagliptin precursor. <i>Applied Organometallic Chemistry</i> , 2015, 29, 528-535.	3.5	18
128	Selective Toll-like receptor 7 agonists with novel chromeno[3,4-d]imidazol-4(1H)-one and 2-(trifluoromethyl)quinoline/quinazoline-4-amine scaffolds. <i>European Journal of Medicinal Chemistry</i> , 2019, 179, 109-122.	5.5	18
129	Synthesis of ethyl 3-(hydroxyphenoxy)benzyl butylphosphonates as potential antigen 85C inhibitors. <i>Tetrahedron</i> , 2007, 63, 10698-10708.	1.9	17
130	Derivatives of pyrimidine, phthalimide and anthranilic acid as inhibitors of human hydroxysteroid dehydrogenase AKR1C1. <i>Chemico-Biological Interactions</i> , 2009, 178, 158-164.	4.0	17
131	Benzoic acid derivatives with improved antifungal activity: Design, synthesis, structure-activity relationship (SAR) and CYP53 docking studies. <i>Bioorganic and Medicinal Chemistry</i> , 2015, 23, 4264-4276.	3.0	17
132	Structure-activity relationship study of tryptophan-based butyrylcholinesterase inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2020, 208, 112766.	5.5	17
133	Phytoestrogens as inhibitors of fungal 17 β -hydroxysteroid dehydrogenase. <i>Steroids</i> , 2005, 70, 694-703.	1.8	16
134	New lipophilic phthalimido- and 3-phenoxybenzyl sulfonates: Inhibition of antigen 85C mycolyltransferase activity and cytotoxicity. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2006, 21, 391-397.	5.2	16
135	A Novel Scalable Synthesis of Pramipexole. <i>Organic Process Research and Development</i> , 2010, 14, 1125-1129.	2.7	16
136	Discovery and kinetic evaluation of 6-substituted 4-benzylthio-1,3,5-triazin-2(1H)-ones as inhibitors of cathepsin B. <i>European Journal of Medicinal Chemistry</i> , 2011, 46, 4648-4656.	5.5	16
137	Virtual screening for potential inhibitors of bacterial MurC and MurD ligases. <i>Journal of Molecular Modeling</i> , 2012, 18, 1063-1072.	1.8	16
138	Development of potent reversible selective inhibitors of butyrylcholinesterase as fluorescent probes. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2020, 35, 498-505.	5.2	16
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