Stanislav Gobec

List of Publications by Year
in descending order

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Version: 2024-02-01

248 papers	7,223 citations	61984 43 h-index	98798 67 g-index

257 all docs	257 docs citations	257 times ranked	8232 citing authors

#	Article	IF	Citations
1	Nitroxoline and its derivatives are potent inhibitors of metallo-Î²-lactamases. European Journal of Medicinal Chemistry, 2022, 228, 113975.	5.5	6
2	Evaluation of novel cathepsin-X inhibitors in vitro and in vivo and their ability to improve cathepsin-B-directed antitumor therapy. Cellular and Molecular Life Sciences, 2022, 79, 34.	5.4	6
3	Indoles and 1-(3-(benzyloxy)benzyl)piperazines: Reversible and selective monoamine oxidase B inhibitors identified by screening an in-house compound library. Bioorganic Chemistry, 2022, 119, 105581.	4.1	2
4	Repurposing of 8â€Hydroxyquinolineâ€Based Butyrylcholinesterase and Cathepsin B Ligands as Potent Nonpeptidic Deoxyribonuclease I Inhibitors. ChemMedChem, 2022, 17, .	3.2	4
5	Upregulation of Cathepsin X in Glioblastoma: Interplay with Î³-Enolase and the Effects of Selective Cathepsin X Inhibitors. International Journal of Molecular Sciences, 2022, 23, 1784.	4.1	9
6	Redox active or thiol reactive? Optimization of rapid screens to identify less evident nuisance compounds. Drug Discovery Today, 2022, 27, 1733-1742.	6.4	12
7	ProBiS-Dock: A Hybrid Multitemplate Homology Flexible Docking Algorithm Enabled by Protein Binding Site Comparison. Journal of Chemical Information and Modeling, 2022, 62, 1573-1584.	5.4	4
8	From tryptophan-based amides to tertiary amines: Optimization of a butyrylcholinesterase inhibitor series. European Journal of Medicinal Chemistry, 2022, 234, 114248.	5.5	11
9	Synthesis of 3-Amino-4-substituted Monocyclic ÃŸ-Lactamsâ€”Important Structural Motifs in Medicinal Chemistry. International Journal of Molecular Sciences, 2022, 23, 360.	4.1	1
10	A Set of Experimentally Validated Decoys for the Human CC Chemokine Receptor 7 (CCR7) Obtained by Virtual Screening. Frontiers in Pharmacology, 2022, 13, 855653.	3.5	2
11	Towards discovery of inhibitors of the undecaprenyl-pyrophosphate phosphatase BacA by virtual high-throughput screening. Computational and Structural Biotechnology Journal, 2022, 20, 2360-2371.	4.1	3
12	Screening of Big Pharmaâ€™s Library against Various in-house Biological Targets. Molecules, 2022, 27, 4484.	3.8	0
13	Pyrimido[1,2-b]indazole derivatives: Selective inhibitors of human monoamine oxidase B with neuroprotective activity. European Journal of Medicinal Chemistry, 2021, 209, 112911.	5.5	23
14	Assessment of Tractable Cysteines for Covalent Targeting by Screening Covalent Fragments. ChemBioChem, 2021, 22, 743-753.	2.6	19
15	Indoleamine and tryptophan 2,3-dioxygenases as important future therapeutic targets. , 2021, 221, 107746.		34
16	Monocyclic betaâ€“lactams for therapeutic uses: a patent overview (2010â€“2020). Expert Opinion on Therapeutic Patents, 2021, 31, 247-266.	5.0	8
17	Synthesis and Biochemical Evaluation of Warhead-Decorated Psoralens as (Immuno)Proteasome Inhibitors. Molecules, 2021, 26, 356.	3.8	3
18	Longitudinal evaluation of a novel BChE PET tracer as an early in vivo biomarker in the brain of a mouse model for Alzheimer disease. Theranostics, 2021, 11, 6542-6559.	10.0	12

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19	Synthesis and Initial Characterization of a Reversible, Selective 18F-Labeled Radiotracer for Human Butyrylcholinesterase. Molecular Imaging and Biology, 2021, 23, 505-515.	2.6	4
20	Novel Selective IDO1 Inhibitors with Isoxazolo[5,4-d]pyrimidin-4(5H)-one Scaffold. Pharmaceuticals, 2021, 14, 265.	3.8	6
21	2â€™-Hydroxy-4â€™,5â€™-dimethyl-4-dimethylaminochalcone, a novel fluorescent flavonoid with capacity to detect aluminium in cells and modulate Alzheimerâ€™s disease targets. Journal of Photochemistry and Photobiology A: Chemistry, 2021, 409, 113137.	3.9	13
22	Nep1-like proteins as a target for plant pathogen control. PLoS Pathogens, 2021, 17, e1009477.	4.7	9
23	Mur ligases inhibitors with azastilbene scaffold: Expanding the structureâ€“activity relationship. Bioorganic and Medicinal Chemistry Letters, 2021, 40, 127966.	2.2	7
24	Discovery of multifunctional anti-Alzheimerâ€™s agents with a unique mechanism of action including inhibition of the enzyme butyrylcholinesterase and Î³-aminobutyric acid transporters. European Journal of Medicinal Chemistry, 2021, 218, 113397.	5.5	14
25	Discovery of selective fragment-sized immunoproteasome inhibitors. European Journal of Medicinal Chemistry, 2021, 219, 113455.	5.5	9
26	4-Phenethyl-1-Propargylpiperidine-Derived Dual Inhibitors of Butyrylcholinesterase and Monoamine Oxidase B. Molecules, 2021, 26, 4118.	3.8	5
27	Treatment of canine cognitive dysfunction with novel butyrylcholinesterase inhibitor. Scientific Reports, 2021, 11, 18098.	3.3	12
28	Discovery of 1-(phenylsulfonyl)-1H-indole-based multifunctional ligands targeting cholinesterases and 5-HT6 receptor with anti-aggregation properties against amyloid-beta and tau. European Journal of Medicinal Chemistry, 2021, 225, 113783.	5.5	11
29	Further hit optimization of 6-(trifluoromethyl)pyrimidin-2-amine based TLR8 modulators: Synthesis, biological evaluation and structureâ€“activity relationships. European Journal of Medicinal Chemistry, 2021, 225, 113809.	5.5	2
30	Development and crystallography-aided SAR studies of multifunctional BuChE inhibitors and 5-HT6R antagonists with Î²-amyloid anti-aggregation properties. European Journal of Medicinal Chemistry, 2021, 225, 113792.	5.5	13
31	WIDOCK: a reactive docking protocol for virtual screening of covalent inhibitors. Journal of Computer-Aided Molecular Design, 2021, 35, 223-244.	2.9	21
32	Catalytic Approach to Diverse Î±â€Aminoboronic Acid Derivatives by Iridiumâ€Catalyzed Hydrogenation of Trifluoroborateâ€iminiums. Advanced Synthesis and Catalysis, 2021, 363, 2396-2402.	4.3	3
33	Multitarget 2â€²-hydroxychalcones as potential drugs for the treatment of neurodegenerative disorders and their comorbidities. Neuropharmacology, 2021, 201, 108837.	4.1	6
34	Fragment-Sized and Bidentate (Immuno)Proteasome Inhibitors Derived from Cysteine and Threonine Targeting Warheads. Cells, 2021, 10, 3431.	4.1	6
35	Synthesis and Penicillinâ€binding Protein Inhibitory Assessment of Dipeptidic 4â€Phenylâ€Î²â€lactams from Î±â€Amino Acidâ€derived Imines. Chemistry - an Asian Journal, 2020, 15, 51-55.	3.3	3
36	Development of potent reversible selective inhibitors of butyrylcholinesterase as fluorescent probes. Journal of Enzyme Inhibition and Medicinal Chemistry, 2020, 35, 498-505.	5.2	16

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37	Stereoselective Activity of 1-Propargyl-4-styrylpiperidine-like Analogues That Can Discriminate between Monoamine Oxidase Isoforms A and B. Journal of Medicinal Chemistry, 2020, 63, 1361-1387.	6.4	33
38	1-Benzylpyrrolidine-3-amine-based BuChE inhibitors with anti-aggregating, antioxidant and metal-chelating properties as multifunctional agents against Alzheimerâ€™s disease. European Journal of Medicinal Chemistry, 2020, 187, 111916.	5.5	33
39	Structure-activity relationship study of tryptophan-based butyrylcholinesterase inhibitors. European Journal of Medicinal Chemistry, 2020, 208, 112766.	5.5	17
40	Recent Advances in the Synthesis of Acylboranes and Their Widening Applicability. ACS Omega, 2020, 5, 17868-17875.	3.5	22
41	Synthesis of Novel Nitroxoline Analogs with Potent Cathepsin B Exopeptidase Inhibitory Activity. ChemMedChem, 2020, 15, 2477-2490.	3.2	6
42	Bromo-Cyclobutenaminones as New Covalent UDP-N-Acetylglucosamine Enolpyruvyl Transferase (MurA) Inhibitors. Pharmaceuticals, 2020, 13, 362.	3.8	8
43	Structure-activity relationships of triazole-benzodioxine inhibitors of cathepsin X. European Journal of Medicinal Chemistry, 2020, 193, 112218.	5.5	4
44	Psoralen Derivatives as Inhibitors of Mycobacterium tuberculosis Proteasome. Molecules, 2020, 25, 1305.	3.8	6
45	8-Hydroxyquinoline-based anti-Alzheimer multimodal agents. Monatshefte FÃ¼r Chemie, 2020, 151, 1111-1120.	1.8	10
46	Efficient and Straightforward Syntheses of Two United States Pharmacopeia Sitagliptin Impurities: 3-Desamino-2,3-dehydrositagliptin and 3-Desamino-3,4-dehydrositagliptin. ACS Omega, 2020, 5, 5356-5364.	3.5	5
47	N-alkylpiperidine carbamates as potential anti-Alzheimerâ€™s agents. European Journal of Medicinal Chemistry, 2020, 197, 112282.	5.5	33
48	A Simple and Effective Synthesis of 3- and 4-((Phenylcarbamoyl)oxy)benzoic Acids. Acta Chimica Slovenica, 2020, 67, 940-948.	0.6	0
49	Discovery of Immunoproteasome Inhibitors Using Large-Scale Covalent Virtual Screening. Molecules, 2019, 24, 2590.	3.8	11
50	Synthesis and NMR spectroscopic assignment of chlorinated benzimidazole-2-thione derivatives. Tetrahedron Letters, 2019, 60, 151078.	1.4	5
51	Synthesis of Indolineâ€Based Benzhydroxamic Acids as Potential HDAC6 Inhibitors. ChemistrySelect, 2019, 4, 12308-12312.	1.5	1
52	Virtual screening approach and biochemical evaluation on MurB. Chemical Data Collections, 2019, 24, 100276.	2.3	2
53	Î±â€Unsaturated 3â€Aminoâ€1â€carboxymethylâ€Î²â€lactams as Bacterial PBP Inhibitors: Synthesis and Biochemical Assessment. Chemistry - A European Journal, 2019, 25, 16128-16140.	3.3	10
54	Organoruthenated Nitroxoline Derivatives Impair Tumor Cell Invasion through Inhibition of Cathepsin B Activity. Inorganic Chemistry, 2019, 58, 12334-12347.	4.0	28

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55	Kinetic mechanism of Enterococcus faecium d-aspartate ligase. Biochimie, 2019, 158, 217-223.	2.6	1
56	Selective Toll-like receptor 7 agonists with novel chromeno[3,4-d]imidazol-4(1H)-one and 2-(trifluoromethyl)quinoline/ quinazoline-4-amine scaffolds. European Journal of Medicinal Chemistry, 2019, 179, 109-122.	5.5	18
57	Synthesis of aminoboronic acid derivatives: an update on recent advances. Organic Chemistry Frontiers, 2019, 6, 2991-2998.	4.5	45
58	Evaluation of the published kinase inhibitor set to identify multiple inhibitors of bacterial ATP-dependent mur ligases. Journal of Enzyme Inhibition and Medicinal Chemistry, 2019, 34, 1010-1017.	5.2	12
59	Efficient synthesis and preliminary biological evaluations of trifluoromethylated imidazo[1,2-a]pyrimidines and benzimidazo[1,2-a]pyrimidines. New Journal of Chemistry, 2019, 43, 9961-9968.	2.8	13
60	Structure-guided optimization of 4,6-substituted-1,3,5-triazin-2(1H)-ones as catalytic inhibitors of human DNA topoisomerase IIÎ±. European Journal of Medicinal Chemistry, 2019, 175, 330-348.	5.5	20
61	Tryptophan-derived butyrylcholinesterase inhibitors as promising leads against Alzheimer's disease. Chemical Communications, 2019, 55, 3765-3768.	4.1	60
62	Chalcone derivatives: synthesis, inÂvitro and inÂvivo evaluation of their anti-anxiety, anti-depression and analgesic effects. Heliyon, 2019, 5, e01376.	3.2	41
63	Application of the N-Dibenzyl Protective Group in the Preparation of Î²-Lactam Pseudopeptides. Molecules, 2019, 24, 1261.	3.8	1
64	A focused structureâ€“activity relationship study of psoralen-based immunoproteasome inhibitors. MedChemComm, 2019, 10, 1958-1965.	3.4	9
65	Methylation of selenocysteine catalysed by thiopurine S-methyltransferase. Biochimica Et Biophysica Acta - General Subjects, 2019, 1863, 182-190.	2.4	13
66	Reaching toward underexplored targets in antibacterial drug design. Drug Development Research, 2019, 80, 6-10.	2.9	28
67	Biological Evaluation of 8-Hydroxyquinolines as Multi-Target Directed Ligands for Treating Alzheimerâ€™s Disease. Current Alzheimer Research, 2019, 16, 801-814.	1.4	5
68	Cathepsin B inhibitors: Further exploration of the nitroxoline core. Bioorganic and Medicinal Chemistry Letters, 2018, 28, 1239-1247.	2.2	23
69	Docking study with biological validation on bacterial enzyme MurD. Chemical Data Collections, 2018, 13-14, 139-155.	2.3	1
70	Novel Multitarget-Directed Ligands Aiming at Symptoms and Causes of Alzheimerâ€™s Disease. ACS Chemical Neuroscience, 2018, 9, 1195-1214.	3.5	44
71	Design, Synthesis, and Biological Evaluation of 1-Benzylamino-2-hydroxyalkyl Derivatives as New Potential Disease-Modifying Multifunctional Anti-Alzheimerâ€™s Agents. ACS Chemical Neuroscience, 2018, 9, 1074-1094.	3.5	47
72	In silico identification, synthesis and biological evaluation of novel tetrazole inhibitors of MurB. Chemical Biology and Drug Design, 2018, 91, 1101-1112.	3.2	10

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73	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
74	Antibacterial and Î²â€Lactamase Inhibitory Activity of Monocyclic Î²â€Lactams. Medicinal Research Reviews, 2018, 38, 426-503.	10.5	73
75	Heterocyclic electrophiles as new MurA inhibitors. Archiv Der Pharmazie, 2018, 351, e1800184.	4.1	22
76	A road map for prioritizing warheads for cysteine targeting covalent inhibitors. European Journal of Medicinal Chemistry, 2018, 160, 94-107.	5.5	80
77	Design, Synthesis, and Biological Evaluation of 2-(Benzylamino-2-Hydroxyalkyl)Isoindoline-1,3-Diones Derivatives as Potential Disease-Modifying Multifunctional Anti-Alzheimer Agents. Molecules, 2018, 23, 347.	3.8	27
78	Multi-target-directed ligands for treating Alzheimer's disease: Butyrylcholinesterase inhibitors displaying antioxidant and neuroprotective activities. European Journal of Medicinal Chemistry, 2018, 156, 598-617.	5.5	72
79	A patent review of immunoproteasome inhibitors. Expert Opinion on Therapeutic Patents, 2018, 28, 517-540.	5.0	21
80	In Silico Design and Enantioselective Synthesis of Functionalized Monocyclic 3â€Aminoâ€Îâ€carboxymethylâ€Î²â€lactams as Inhibitors of Penicillinâ€Binding Proteins of Resistant Bacteria. Chemistry - A European Journal, 2018, 24, 15254-15266.	3.3	13
81	Anthranilic Acid Inhibitors of Undecaprenyl Pyrophosphate Synthase (UppS), an Essential Enzyme for Bacterial Cell Wall Biosynthesis. Frontiers in Microbiology, 2018, 9, 3322.	3.5	8
82	Discovery of new MurA inhibitors using induced-fit simulation and docking. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 944-949.	2.2	24
83	Evaluation of US 2016/0115161 A1: isoindoline compounds and methods of their use. Expert Opinion on Therapeutic Patents, 2017, 27, 637-641.	5.0	3
84	Dual inhibitors of cholinesterases and monoamine oxidases for Alzheimerâ€™s disease. Future Medicinal Chemistry, 2017, 9, 811-832.	2.3	44
85	Synthesis and structureâ€“activity relationship study of novel quinazolinone-based inhibitors of MurA. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 3529-3533.	2.2	46
86	Identification and characterization of the novel reversible and selective cathepsin X inhibitors. Scientific Reports, 2017, 7, 11459.	3.3	15
87	Inhibition of D-Ala:D-Ala ligase through a phosphorylated form of the antibiotic D-cycloserine. Nature Communications, 2017, 8, 1939.	12.8	59
88	Identification of Conserved Water Sites in Protein Structures for Drug Design. Journal of Chemical Information and Modeling, 2017, 57, 3094-3103.	5.4	34
89	A new â€˜golden ageâ€™ for the antitubercular target InhA. Drug Discovery Today, 2017, 22, 492-502.	6.4	46
90	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

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91	N-Propargylpiperidines with naphthalene-2-carboxamide or naphthalene-2-sulfonamide moieties: Potential multifunctional anti-Alzheimerâ€™s agents. Bioorganic and Medicinal Chemistry, 2017, 25, 633-645.	3.0	49
92	BoBER: web interface to the base of bioisosterically exchangeable replacements. Journal of Cheminformatics, 2017, 9, 62.	6.1	12
93	Chlorocarbonylsulfenyl Chloride Cyclizations Towards Piperidin-3-yl-oxathiazol-2-ones as Potential Covalent Inhibitors of Threonine Proteases. Acta Chimica Slovenica, 2017, 64, 771-781.	0.6	4
94	Addition of 2-(ethylamino)acetonitrile group to nitroxoline results in significantly improved anti-tumor activity in vitro and in vivo. Oncotarget, 2017, 8, 59136-59147.	1.8	14
95	Synthesis, Molecular Modelling and Biological Evaluation of Novel Heterodimeric, Multiple Ligands Targeting Cholinesterases and Amyloid Beta. Molecules, 2016, 21, 410.	3.8	29
96	Synthesis and Biological Evaluation of Benzochromenopyrimidinones as Cholinesterase Inhibitors and Potent Antioxidant, Non-Hepatotoxic Agents for Alzheimerâ€™s Disease. Molecules, 2016, 21, 634.	3.8	22
97	Crystallographic Study of Peptidoglycan Biosynthesis Enzyme MurD: Domain Movement Revisited. PLoS ONE, 2016, 11, e0152075.	2.5	15
98	Discovery of Mycobacterium tuberculosis InhA Inhibitors by Binding Sites Comparison and Ligands Prediction. Journal of Medicinal Chemistry, 2016, 59, 11069-11078.	6.4	26
99	Development of an in-vivo active reversible butyrylcholinesterase inhibitor. Scientific Reports, 2016, 6, 39495.	3.3	105
100	Novel multi-target-directed ligands for Alzheimer's disease: Combining cholinesterase inhibitors and 5-HT 6 receptor antagonists. Design, synthesis and biological evaluation. European Journal of Medicinal Chemistry, 2016, 124, 63-81.	5.5	72
101	Clioquinolâ€“ruthenium complex impairs tumour cell invasion by inhibiting cathepsin B activity. Dalton Transactions, 2016, 45, 16913-16921.	3.3	33
102	Synthesis and Biological Assessment of Racemic Benzochromenopyrimidinimines as Antioxidant, Cholinesterase, and Aβ_{1–42} Aggregation Inhibitors for Alzheimer's Disease Therapy. ChemMedChem, 2016, 11, 1318-1327.	3.2	24
103	Nonpeptidic Selective Inhibitors of the Chymotrypsinâ€Like (β5â€‰i) Subunit of the Immunoproteasome. Angewandte Chemie - International Edition, 2016, 55, 5745-5748.	13.8	38
104	Synthesis and preliminary biological evaluations of (+)-isocampholenic acid-derived amides. Molecular Diversity, 2016, 20, 667-676.	3.9	3
105	New direct inhibitors of InhA with antimycobacterial activity based on a tetrahydropyran scaffold. European Journal of Medicinal Chemistry, 2016, 112, 252-257.	5.5	20
106	Unusual substrate specificity of the peptidoglycan MurE ligase from Erysipelothrix rhusiopathiae. Biochimie, 2016, 121, 209-218.	2.6	5
107	Inhibition of endopeptidase and exopeptidase activity of cathepsin B impairs extracellular matrix degradation and tumour invasion. Biological Chemistry, 2016, 397, 165-174.	2.5	29
108	Recent Advances in the Development of Undecaprenyl Pyrophosphate Synthase Inhibitors as Potential Antibacterials. Current Medicinal Chemistry, 2016, 23, 464-482.	2.4	12

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109	Synthesis and Biological Evaluation of N-Aryl-N'-(5-(2-hydroxybenzoyl) pyrimidin-2-yl)guanidines as Toll-Like Receptor 4 Antagonists. Medicinal Chemistry, 2016, 12, 742-750.	1.5	4
110	Multiple Ligands Targeting Cholinesterases and Î²â€Amyloid: Synthesis, Biological Evaluation of Heterodimeric Compounds with Benzylamine Pharmacophore. Archiv Der Pharmazie, 2015, 348, 556-563.	4.1	11
111	<scp>D</scp>â€Glucosamine in ironâ€catalysed crossâ€coupling reactions of Grignards with allylic and vinylic bromides: application to the synthesis of a key sitagliptin precursor. Applied Organometallic Chemistry, 2015, 29, 528-535.	3.5	18
112	Combined Liquid Chromatographyâ€“Tandem Mass Spectrometry Analysis of Progesterone Metabolites. PLoS ONE, 2015, 10, e0117984.	2.5	9
113	Isoindoline-1,3-dione derivatives targeting cholinesterases: Design, synthesis and biological evaluation of potential anti-Alzheimerâ€™s agents. Bioorganic and Medicinal Chemistry, 2015, 23, 1629-1637.	3.0	44
114	Development of multifunctional, heterodimeric isoindoline-1,3-dione derivatives as cholinesterase and Î²-amyloid aggregation inhibitors with neuroprotective properties. European Journal of Medicinal Chemistry, 2015, 92, 738-749.	5.5	60
115	4,6-Substituted-1,3,5-triazin-2(1H)-ones as monocyclic catalytic inhibitors of human DNA topoisomerase IIÎ± targeting the ATP binding site. Bioorganic and Medicinal Chemistry, 2015, 23, 4218-4229.	3.0	27
116	LiSiCA: A Software for Ligand-Based Virtual Screening and Its Application for the Discovery of Butyrylcholinesterase Inhibitors. Journal of Chemical Information and Modeling, 2015, 55, 1521-1528.	5.4	70
117	Cobalt-Catalyzed Cross-Coupling of Grignards with Allylic and Vinylic Bromides: Use of Sarcosine as a Natural Ligand. Journal of Organic Chemistry, 2015, 80, 7803-7809.	3.2	30
118	Structure-based development of nitroxoline derivatives as potential multifunctional anti-Alzheimer agents. Bioorganic and Medicinal Chemistry, 2015, 23, 4442-4452.	3.0	50
119	Benzoic acid derivatives with improved antifungal activity: Design, synthesis, structureâ€“activity relationship (SAR) and CYP53 docking studies. Bioorganic and Medicinal Chemistry, 2015, 23, 4264-4276.	3.0	17
120	Furan-based benzene mono- and dicarboxylic acid derivatives as multiple inhibitors of the bacterial Mur ligases (MurCâ€“MurF): experimental and computational characterization. Journal of Computer-Aided Molecular Design, 2015, 29, 541-560.	2.9	21
121	Synthesis of new N-benzylpiperidine derivatives as cholinesterase inhibitors with Î²-amyloid anti-aggregation properties and beneficial effects on memory in vivo. Bioorganic and Medicinal Chemistry, 2015, 23, 2445-2457.	3.0	42
122	Molecular dynamics to enhance structure-based virtual screening on cathepsin B. Journal of Computer-Aided Molecular Design, 2015, 29, 707-712.	2.9	19
123	New antagonists of toll-like receptor 7 discovered through 3D ligand-based virtual screening. Medicinal Chemistry Research, 2015, 24, 362-371.	2.4	15
124	Structureâ€“Activity Relationships of Novel Tryptamine-Based Inhibitors of Bacterial Transglycosylase. Journal of Medicinal Chemistry, 2015, 58, 9712-9721.	6.4	21
125	Design, Synthesis, and Evaluation of New Thiadiazole-Based Direct Inhibitors of Enoyl Acyl Carrier Protein Reductase (InhA) for the Treatment of Tuberculosis. Journal of Medicinal Chemistry, 2015, 58, 613-624.	6.4	58
126	Convenient syntheses of orthogonally protected aminocyclopentitols from aldopentoses. Tetrahedron Letters, 2015, 56, 529-531.	1.4	2

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127	Nitroxoline impairs tumor progression in vitro and in vivo by regulating cathepsin B activity. Oncotarget, 2015, 6, 19027-19042.	1.8	64
128	Inhibitors of the peptidoglycan biosynthesis enzymes MurA-F. Bioorganic Chemistry, 2014, 55, 2-15.	4.1	78
129	Straightforward synthesis of orthogonally protected piperidin-3-ylmethanamine and piperidin-4-ylmethanamine derivatives. Tetrahedron Letters, 2014, 55, 2037-2039.	1.4	14
130	Design, synthesis and evaluation of second generation MurF inhibitors based on a cyanothiophene scaffold. European Journal of Medicinal Chemistry, 2014, 73, 83-96.	5.5	25
131	Antifungal activity of cinnamic acid derivatives involves inhibition of benzoate 4-hydroxylase (CYP53). Journal of Applied Microbiology, 2014, 116, 955-966.	3.1	67
132	Inhibitor Design Strategy Based on an Enzyme Structural Flexibility: A Case of Bacterial MurD Ligase. Journal of Chemical Information and Modeling, 2014, 54, 1451-1466.	5.4	21
133	Structural characterization and biological evaluation of a clioquinolâ€“ruthenium complex with copper-independent antileukaemic activity. Dalton Transactions, 2014, 43, 9045-9051.	3.3	88
134	Discovery, Biological Evaluation, and Crystal Structure of a Novel Nanomolar Selective Butyrylcholinesterase Inhibitor. Journal of Medicinal Chemistry, 2014, 57, 8167-8179.	6.4	220
135	Endocrine Disruptomeâ€”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
136	Exploring the aryl esterase catalysis of paraoxonase-1 through solvent kinetic isotope effects and phosphonate-based isosteric analogues of the tetrahedral reaction intermediate. Biochimie, 2014, 106, 184-186.	2.6	5
137	A Simple Synthesis of Polyfunctionalized 4â€Aminopyrazolidinâ€3â€ones as â€˜Azaâ€deoxaâ€™ Analogs of ‹scp›D‹/scp›â€Cycloserine. Helvetica Chimica Acta, 2014, 97, 245-267.	1.6	3
138	Benzene-1,3-dicarboxylic acid 2,5-dimethylpyrrole derivatives as multiple inhibitors of bacterial Mur ligases (MurCâ€“MurF). Bioorganic and Medicinal Chemistry, 2014, 22, 4124-4134.	3.0	34
139	Discovery of Novel Small-Molecule Compounds with Selective Cytotoxicity for Burkittâ€™s Lymphoma Cells Using 3D Ligand-Based Virtual Screening. Molecules, 2014, 19, 19209-19219.	3.8	0
140	Novel toll-like receptor 4 (TLR4) antagonists identified by structure- and ligand-based virtual screening. European Journal of Medicinal Chemistry, 2013, 70, 393-399.	5.5	35
141	2,3-Diarylpropenoic acids as selective non-steroidal inhibitors of type-5 17Î²-hydroxysteroid dehydrogenase (AKR1C3). European Journal of Medicinal Chemistry, 2013, 62, 89-97.	5.5	10
142	New enzymatic assay for the AKR1C enzymes. Chemico-Biological Interactions, 2013, 202, 204-209.	4.0	4
143	Development of New Cathepsin B Inhibitors: Combining Bioisosteric Replacements and Structure-Based Design To Explore the Structureâ€“Activity Relationships of Nitroxoline Derivatives. Journal of Medicinal Chemistry, 2013, 56, 521-533.	6.4	56
144	Melanin is crucial for growth of the black yeast Hortaea werneckii in its natural hypersaline environment. Fungal Biology, 2013, 117, 368-379.	2.5	60

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145	Synthetic tripeptides as alternate substrates of murein peptide ligase (Mpl). Biochimie, 2013, 95, 1120-1126.	2.6	7
146	Synthesis of pyrazolo[1,2-a]pyrazole-based peptide mimetics. Tetrahedron, 2013, 69, 6648-6665.	1.9	15
147	Structureâ€“activity relationships of new cyanothiophene inhibitors ofÂthe essential peptidoglycan biosynthesis enzyme MurF. European Journal of Medicinal Chemistry, 2013, 66, 32-45.	5.5	62
148	Specificity Determinants for Lysine Incorporation in Staphylococcus aureus Peptidoglycan as Revealed by the Structure of a MurE Enzyme Ternary Complex. Journal of Biological Chemistry, 2013, 288, 33439-33448.	3.4	33
149	Crystallization and preliminary X-ray analysis of a UDP-MurNAc-tripeptide<scp>D</scp>-alanyl-<scp>D</scp>-alanine-adding enzyme (PaMurF) fromPseudomonas aeruginosa. Acta Crystallographica Section F: Structural Biology Communications, 2013, 69, 503-505.	0.7	3
150	MurD enzymes: some recent developments. Biomolecular Concepts, 2013, 4, 539-556.	2.2	28
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