Andrej Perdih

List of Publications by Year
in descending order

61	1,433	331259	344852
papers	citations	21 h-index	36 g-index

62	62	62	1949
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Structure-Based Discovery of Substituted 4,5â€²-Bithiazoles as Novel DNA Gyrase Inhibitors. Journal of Medicinal Chemistry, 2012, 55, 6413-6426.	2.9	146
2	Recent Advances in the Synthesis of Unnatural Î±-Amino Acids. Current Organic Chemistry, 2007, 11, 801-832.	0.9	87
3	Discovery of novel benzene 1,3-dicarboxylic acid inhibitors of bacterial MurD and MurE ligases by structure-based virtual screening approach. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 2668-2673.	1.0	67
4	Binding free energy calculations of N-sulphonyl-glutamic acid inhibitors of MurD ligase. Journal of Molecular Modeling, 2009, 15, 983-996.	0.8	57
5	The Application of Freidinger Lactams and their Analogs in the Design of Conformationally Constrained Peptidomimetics. Current Medicinal Chemistry, 2006, 13, 1525-1556.	1.2	55
6	In silico discovery of 2-amino-4-(2,4-dihydroxyphenyl)thiazoles as novel inhibitors of DNA gyrase B. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 958-962.	1.0	54
7	Targeted molecular dynamics simulation studies of binding and conformational changes in E. coli MurD. Proteins: Structure, Function and Bioinformatics, 2007, 68, 243-254.	1.5	51
8	Recent Developments of DNA Poisons - Human DNA Topoisomerase IIα Inhibitors - as Anticancer Agents. Current Pharmaceutical Design, 2013, 19, 2474-2488.	0.9	49
9	Recent Advances in the Development of Catalytic Inhibitors of Human DNA Topoisomerase IIα As Novel Anticancer Agents. Current Medicinal Chemistry, 2013, 20, 694-709.	1.2	42
10	In silico discovery and biophysical evaluation of novel 5-(2-hydroxybenzylidene) rhodanine inhibitors of DNA gyrase B. Bioorganic and Medicinal Chemistry, 2012, 20, 2572-2580.	1.4	41
11	Flavonoids and cinnamic acid esters as inhibitors of fungal 17Î²-hydroxysteroid dehydrogenase: A synthesis, QSAR and modelling study. Bioorganic and Medicinal Chemistry, 2006, 14, 7404-7418.	1.4	40
12	Small Molecule Antagonists of Integrin Receptors. Current Medicinal Chemistry, 2010, 17, 2371-2392.	1.2	39
13	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.	1.4	34
14	Recent Advances in the Synthesis of Unnatural α-Amino Acids - An Updated Version. Current Organic Chemistry, 2011, 15, 3750-3799.	0.9	33
15	1,3â€Diamineâ€Derived Bifunctional Organocatalyst Prepared from Camphor. Advanced Synthesis and Catalysis, 2016, 358, 3786-3796.	2.1	32
16	Discovery of Monoâ€•and Disubstituted 1Hâ€Pyrazolo[3,4]pyrimidines and 9Hâ€Purines as Catalytic Inhibitors of Human DNA Topoisomeraseâ€…IIÎ±. ChemMedChem, 2015, 10, 345-359.	1.6	30
17	The CWB2 Cell Wall-Anchoring Module Is Revealed by the Crystal Structures of the Clostridium difficile Cell Wall Proteins Cwp8 and Cwp6. Structure, 2017, 25, 514-521.	1.6	29
18	Senescent cells as promising targets to tackle age-related diseases. Ageing Research Reviews, 2021, 66, 101251.	5.0	28

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19	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.	1.4	27
20	Combinatorially-generated library of 6-fluoroquinolone analogs as potential novel antitubercular agents: a chemometric and molecular modeling assessment. Journal of Molecular Modeling, 2012, 18, 1735-1753.	0.8	26
21	Molecular dynamics simulation and linear interaction energy study of d-Glu-based inhibitors of the MurD ligase. Journal of Computer-Aided Molecular Design, 2013, 27, 723-738.	1.3	25
22	Discovery and Characterization of 2,5-Substituted Benzoic Acid Dual Inhibitors of the Anti-apoptotic Mcl-1 and Bfl-1 Proteins. Journal of Medicinal Chemistry, 2020, 63, 2489-2510.	2.9	23
23	Development of a one-pot assay for screening and identification of Mur pathway inhibitors in Mycobacterium tuberculosis. Scientific Reports, 2016, 6, 35134.	1.6	22
24	Monocyclic 4-amino-6-(phenylamino)-1,3,5-triazines as inhibitors of human DNA topoisomerase IIÎ±. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 5762-5768.	1.0	21
25	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.	2.5	21
26	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.	1.3	21
27	Clusterâ€based molecular docking study for in silico identification of novel 6â€fluoroquinolones as potential inhibitors against Mycobacterium tuberculosis. Journal of Computational Chemistry, 2013, 34, 790-801.	1.5	20
28	In Silico Discovery of a Substituted 6-Methoxy-quinalidine with Leishmanicidal Activity in Leishmania infantum. Molecules, 2018, 23, 772.	1.7	20
29	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.	2.6	20
30	Discovery of the first inhibitors of bacterial enzyme d-aspartate ligase from Enterococcus faecium (Aslfm). European Journal of Medicinal Chemistry, 2013, 67, 208-220.	2.6	19
31	Substituted 4,5â€²-Bithiazoles as Catalytic Inhibitors of Human DNA Topoisomerase IIÎ±. Journal of Chemical Information and Modeling, 2020, 60, 3662-3678.	2.5	19
32	MurD ligase from E. coli: Tetrahedral intermediate formation study by hybrid quantum mechanical/molecular mechanical replica path method. Proteins: Structure, Function and Bioinformatics, 2009, 74, 744-759.	1.5	18
33	From carbohydrates to drug-like fragments: Rational development of novel Î±-amylase inhibitors. Bioorganic and Medicinal Chemistry, 2015, 23, 6725-6732.	1.4	18
34	Structural Analysis of a Peptide Fragment of Transmembrane Transporter Protein Bilitranslocase. PLoS ONE, 2012, 7, e38967.	1.1	17
35	The Participation of 2Hâ€Pyranâ€2â€ones in [4+2] Cycloadditions: An Experimental and Computational Study. European Journal of Organic Chemistry, 2010, 2010, 5870-5883.	1.2	16
36	Bioassays and In Silico Methods in the Identification of Human DNA Topoisomerase IIÎ± Inhibitors. Current Medicinal Chemistry, 2018, 25, 3286-3318.	1.2	15

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37	MurD ligase from Escherichia coli: C-terminal domain closing motion. Computational and Theoretical Chemistry, 2012, 979, 73-81.	1.1	14
38	A Water-Assisted Catalytic Mechanism in Glycoside Hydrolases Demonstrated on the Staphylococcus aureus Autolysin E. ACS Catalysis, 2018, 8, 4334-4345.	5.5	13
39	Discovery of Mcl-1 inhibitors from integrated high throughput and virtual screening. Scientific Reports, 2018, 8, 10210.	1.6	13
40	In Silico Discovery of Novel Potent Antioxidants on the Basis of Pulvinic Acid and Coumarine Derivatives and Their Experimental Evaluation. PLoS ONE, 2015, 10, e0140602.	1.1	12
41	Organocatalyzed Deracemization of Î”²â€Pyrrolinâ€4â€ones. Advanced Synthesis and Catalysis, 2017, 359, 2288-2296.	2.1	11
42	Design and synthesis of 3,5-substituted 1,2,4-oxadiazoles as catalytic inhibitors of human DNA topoisomerase IIÎ±. Bioorganic Chemistry, 2020, 99, 103828.	2.0	11
43	Distinct labelling of fusion events in rat lactotrophs by FM 1?43 and FM 4?64 is associated with conformational differences. Acta Physiologica, 2007, 191, 35-42.	1.8	9
44	3â€substitutedâ€1Hâ€indazoles as Catalytic Inhibitors of the Human DNA Topoisomerase IIÎ±. ChemistrySelect, 2017, 2, 480-488.	0.7	9
45	Evaluation of Firefly and Renilla Luciferase Inhibition in Reporter-Gene Assays: A Case of Isoflavonoids. International Journal of Molecular Sciences, 2021, 22, 6927.	1.8	8
46	Dynophore-Based Approach in Virtual Screening: A Case of Human DNA Topoisomerase IIÎ±. International Journal of Molecular Sciences, 2021, 22, 13474.	1.8	8
47	Domain sliding of two Staphylococcus aureus N-acetylglucosaminidases enables their substrate-binding prior to its catalysis. Communications Biology, 2020, 3, 178.	2.0	7
48	Structural elucidation of transmembrane transporter protein bilitranslocase: Conformational analysis of the second transmembrane region TM2 by molecular dynamics and NMR spectroscopy. Biochimica Et Biophysica Acta - Biomembranes, 2013, 1828, 2609-2619.	1.4	6
49	The in vitro protective effects of the three novel nanomolar reversible inhibitors of human cholinesterases against irreversible inhibition by organophosphorous chemical warfare agents. Chemico-Biological Interactions, 2019, 309, 108714.	1.7	6
50	Design, Synthesis and Evaluation of Fused Bicyclo[2.2.2]octene as a Potential Core Scaffold for the Non-Covalent Inhibitors of SARS-CoV-2 3CLpro Main Protease. Pharmaceuticals, 2022, 15, 539.	1.7	6
51	Discovery of (phenylureido)piperidinyl benzamides as prospective inhibitors of bacterial autolysin E from Staphylococcus aureus. Journal of Enzyme Inhibition and Medicinal Chemistry, 2018, 33, 1239-1247.	2.5	4
52	Structural Analysis and Dynamic Processes of the Transmembrane Segment Inside Different Micellar Environmentsâ€”Implications for the TM4 Fragment of the Bilitranslocase Protein. International Journal of Molecular Sciences, 2019, 20, 4172.	1.8	4
53	All-Atom Simulations Reveal a Key Interaction Network in the HLA-E/NKG2A/CD94 Immune Complex Fine-Tuned by the Nonameric Peptide. Journal of Chemical Information and Modeling, 2021, 61, 3593-3603.	2.5	4
54	Nonameric Peptide Orchestrates Signal Transduction in the Activating HLA-E/NKG2C/CD94 Immune Complex as Revealed by All-Atom Simulations. International Journal of Molecular Sciences, 2021, 22, 6670.	1.8	3

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55	Molecular recognition of acetylcholinesterase and its subnanomolar reversible inhibitor: a molecular simulations study. Journal of Biomolecular Structure and Dynamics, 2022, 40, 1671-1691.	2.0	2
56	3,5-Substituted Oxadiazoles as Catalytic Inhibitors of the Human Topoisomerase IIÎ± Molecular Motor. Proceedings (mdpi), 2019, 22, 78.	0.2	0
57	Potential modulating effect of the Ascaris suum nicotinic acetylcholine receptor (nAChR) by compounds GSK575594A, diazepam and flumazenil discovered by structure-based virtual screening approach. Molecular and Biochemical Parasitology, 2021, 242, 111350.	0.5	0
58	Abstract 1641: Structure-based design and development of pyrazolopyridine-based inhibitors of Mcl-1. , 2014, , .		0
59	Abstract 3658: Structure-guidedde novodesign of selective Mcl-1 Inhibitors: Synthesis, structural and biochemical characterization. , 2015, , .		0
60	Interdomain conformational flexibility of the peptidoglycan N-acetylglucosaminidases of Staphylococcus aureus. Acta Crystallographica Section A: Foundations and Advances, 2019, 75, e125-e125.	0.0	0
61	Abstract LB-226: Discovery of small molecule Mcl-1 and Bfl-1 inhibitors. , 2020, , .		0