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	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
2	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
3	Senescent cells as promising targets to tackle age-related diseases. Ageing Research Reviews, 2021, 66, 101251.	5.0	28
4	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
5	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
6	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
7	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
8	Dynophore-Based Approach in Virtual Screening: A Case of Human DNA Topoisomerase IIÎ±. International Journal of Molecular Sciences, 2021, 22, 13474.	1.8	8
9	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
10	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
11	Domain sliding of two Staphylococcus aureus N-acetylglucosaminidases enables their substrate-binding prior to its catalysis. Communications Biology, 2020, 3, 178.	2.0	7
12	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
13	Abstract LB-226: Discovery of small molecule Mcl-1 and Bfl-1 inhibitors. , 2020, , .		0
14	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
15	3,5-Substituted Oxadiazoles as Catalytic Inhibitors of the Human Topoisomerase IIÎ± Molecular Motor. Proceedings (mdpi), 2019, 22, 78.	0.2	0
16	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
17	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
18	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

#	Article	IF	Citations
19	A Water-Assisted Catalytic Mechanism in Glycoside Hydrolases Demonstrated on the Staphylococcus aureus Autolysin E. ACS Catalysis, 2018, 8, 4334-4345.	5.5	13
20	Discovery of Mcl-1 inhibitors from integrated high throughput and virtual screening. Scientific Reports, 2018, 8, 10210.	1.6	13
21	In Silico Discovery of a Substituted 6-Methoxy-quinalidine with Leishmanicidal Activity in Leishmania infantum. Molecules, 2018, 23, 772.	1.7	20
22	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
23	Bioassays and In Silico Methods in the Identification of Human DNA Topoisomerase IIÎ± Inhibitors. Current Medicinal Chemistry, 2018, 25, 3286-3318.	1.2	15
24	3â€substitutedâ€1Hâ€indazoles as Catalytic Inhibitors of the Human DNA Topoisomerase IIÎ±. ChemistrySelect, 2017, 2, 480-488.	0.7	9
25	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
26	Organocatalyzed Deracemization of Î”²â€Pyrrolinâ€4â€ones. Advanced Synthesis and Catalysis, 2017, 359, 2288-2296.	2.1	11
27	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
28	1,3â€Diamineâ€Derived Bifunctional Organocatalyst Prepared from Camphor. Advanced Synthesis and Catalysis, 2016, 358, 3786-3796.	2.1	32
29	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
30	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
31	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
32	From carbohydrates to drug-like fragments: Rational development of novel Î±-amylase inhibitors. Bioorganic and Medicinal Chemistry, 2015, 23, 6725-6732.	1.4	18
33	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
34	Abstract 3658: Structure-guidedde novodesign of selective Mcl-1 Inhibitors: Synthesis, structural and biochemical characterization. , 2015, , .		0
35	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
36	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

#	Article	IF	Citations
37	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
38	Abstract 1641: Structure-based design and development of pyrazolopyridine-based inhibitors of Mcl-1. , 2014, , .		0
39	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
40	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
41	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
42	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
43	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
44	Recent Developments of DNA Poisons - Human DNA Topoisomerase IIα Inhibitors - as Anticancer Agents. Current Pharmaceutical Design, 2013, 19, 2474-2488.	0.9	49
45	MurD ligase from Escherichia coli: C-terminal domain closing motion. Computational and Theoretical Chemistry, 2012, 979, 73-81.	1.1	14
46	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
47	Structural Analysis of a Peptide Fragment of Transmembrane Transporter Protein Bilitranslocase. PLoS ONE, 2012, 7, e38967.	1.1	17
48	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
49	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
50	Recent Advances in the Synthesis of Unnatural α-Amino Acids - An Updated Version. Current Organic Chemistry, 2011, 15, 3750-3799.	0.9	33
51	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
52	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
53	Small Molecule Antagonists of Integrin Receptors. Current Medicinal Chemistry, 2010, 17, 2371-2392.	1.2	39
54	Binding free energy calculations of N-sulphonyl-glutamic acid inhibitors of MurD ligase. Journal of Molecular Modeling, 2009, 15, 983-996.	0.8	57

#	Article	IF	Citations
55	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
56	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
57	Recent Advances in the Synthesis of Unnatural Î±-Amino Acids. Current Organic Chemistry, 2007, 11, 801-832.	0.9	87
58	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
59	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
60	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
61	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