Tuomo Laitinen

List of Publications by Year
in descending order

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71	1,689	257450	345221
papers	citations	24 h-index	36 g-index

80	80	80	2579
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Molecular dynamics studies on the thermostability of family 11 xylanases. Protein Engineering, Design and Selection, 2007, 20, 551-559.	2.1	109
2	Integrative and Personalized QSAR Analysis in Cancer by Kernelized Bayesian Matrix Factorization. Journal of Chemical Information and Modeling, 2014, 54, 2347-2359.	5.4	101
3	Covalent Binding of Three Epoxyalkyl Xylosides to the Active Site ofendo-1,4-Xylanase II fromTrichoderma reeseiâ€,â€¡. Biochemistry, 1996, 35, 9617-9624.	2.5	86
4	Piperazine and Piperidine Triazole Ureas as Ultrapotent and Highly Selective Inhibitors of Monoacylglycerol Lipase. Chemistry and Biology, 2013, 20, 379-390.	6.0	80
5	Assessment of mutation probabilities of KRAS G12 missense mutants and their long-timescale dynamics by atomistic molecular simulations and Markov state modeling. PLoS Computational Biology, 2018, 14, e1006458.	3.2	59
6	Chiral 1,3,4-Oxadiazol-2-ones as Highly Selective FAAH Inhibitors. Journal of Medicinal Chemistry, 2013, 56, 8484-8496.	6.4	54
7	SARSâ€CoVâ€2â€“host proteome interactions for antiviral drug discovery. Molecular Systems Biology, 2021, 17, e10396.	7.2	53
8	Identification and Optimization of 4â€Anilinoquinolines as Inhibitors of Cyclinâ€…G Associated Kinase. ChemMedChem, 2018, 13, 48-66.	3.2	51
9	Comparative and pharmacophore model for deacetylase SIRT1. Journal of Computer-Aided Molecular Design, 2006, 20, 589-599.	2.9	45
10	Use of comprehensive screening methods to detect selective human CAR activators. Biochemical Pharmacology, 2011, 82, 1994-2007.	4.4	38
11	New in Vitro Tools to Study Human Constitutive Androstane Receptor (CAR) Biology: Discovery and Comparison of Human CAR Inverse Agonists. Molecular Pharmaceutics, 2011, 8, 2424-2433.	4.6	37
12	Biochemical and Pharmacological Characterization of the Human Lymphocyte Antigen B-Associated Transcript 5 (BAT5/ABHD16A). PLoS ONE, 2014, 9, e109869.	2.5	35
13	Peptides and Pseudopeptides as SIRT6 Deacetylation Inhibitors. ACS Medicinal Chemistry Letters, 2012, 3, 969-974.	2.8	34
14	Robust Hydrolysis of Prostaglandin Glycerol Esters by Human Monoacylglycerol Lipase (MAGL). Molecular Pharmacology, 2014, 86, 522-535.	2.3	34
15	Design of a Cyclin G Associated Kinase (GAK)/Epidermal Growth Factor Receptor (EGFR) Inhibitor Set to Interrogate the Relationship of EGFR and GAK in Chordoma. Journal of Medicinal Chemistry, 2019, 62, 4772-4778.	6.4	34
16	Free energy simulations and MM-PBSA analyses on the affinity and specificity of steroid binding to antiestradiol antibody. Proteins: Structure, Function and Bioinformatics, 2004, 55, 34-43.	2.6	31
17	Identification of novel SIRT3 inhibitor scaffolds by virtual screening. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 2990-2995.	2.2	31
18	The Effects of Sequence Variation on Genome-wide NRF2 Bindingâ€”New Target Genes and Regulatory SNPs. Nucleic Acids Research, 2016, 44, 1760-1775.	14.5	30

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19	Comparative molecular field analysis and molecular dynamics studies of Î±/Î² hydrolase domain containing 6 (ABHD6) inhibitors. Journal of Molecular Modeling, 2015, 21, 250.	1.8	29
20	Optimization of 1,2,5â€Thiadiazole Carbamates as Potent and Selective ABHD6 Inhibitors. ChemMedChem, 2015, 10, 253-265.	3.2	29
21	Ab Initio Quantum Mechanical and Density Functional Theory Calculations on Nucleophile- and Nucleophile and Acid-Catalyzed Opening of an Epoxide Ring:Â A Model for the Covalent Binding of Epoxyalkyl Inhibitors to the Active Site of Glycosidases. Journal of Organic Chemistry, 1998, 63, 8157-8162.	3.2	27
22	Targeting an EGFR Water Network with 4â€Anilinoquin(az)oline Inhibitors for Chordoma. ChemMedChem, 2019, 14, 1693-1700.	3.2	27
23	Development of Pharmacophore Model for Indeno[1,2-b]indoles as Human Protein Kinase CK2 Inhibitors and Database Mining. Pharmaceuticals, 2017, 10, 8.	3.8	26
24	Synthesis and comparison of substituted 1,2,3-dithiazole and 1,2,3-thiaselenazole as inhibitors of the feline immunodeficiency virus (FIV) nucleocapsid protein as a model for HIV infection. Bioorganic and Medicinal Chemistry Letters, 2019, 29, 1765-1768.	2.2	25
25	Characterization of Polyesters Prepared from Three Different Phthalic Acid Isomers by CID-ESI-FT-ICR and PSD-MALDI-TOF Mass Spectrometry. Analytical Chemistry, 2002, 74, 4250-4258.	6.5	24
26	Discovery of Triterpenoids as Reversible Inhibitors of Î±/Î²-hydrolase Domain Containing 12 (ABHD12). PLoS ONE, 2014, 9, e98286.	2.5	24
27	Whole grain intake associated molecule 5-aminovaleric acid betaine decreases Î²-oxidation of fatty acids in mouse cardiomyocytes. Scientific Reports, 2018, 8, 13036.	3.3	24
28	Structure-function analysis indicates that sumoylation modulates DNA-binding activity of STAT1. BMC Biochemistry, 2012, 13, 20.	4.4	23
29	Loratadine analogues as MAGL inhibitors. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 1436-1442.	2.2	23
30	1,2,6-Thiadiazinones as Novel Narrow Spectrum Calcium/Calmodulin-Dependent Protein Kinase Kinase 2 (CaMKK2) Inhibitors. Molecules, 2018, 23, 1221.	3.8	23
31	Quinazoline-Based Antivirulence Compounds Selectively Target Salmonella PhoP/PhoQ Signal Transduction System. Antimicrobial Agents and Chemotherapy, 2019, 64, .	3.2	23
32	Piperazine and piperidine carboxamides and carbamates as inhibitors of fatty acid amide hydrolase (FAAH) and monoacylglycerol lipase (MAGL). Bioorganic and Medicinal Chemistry, 2014, 22, 6694-6705.	3.0	22
33	DPD-Inspired Discovery of Novel LsrK Kinase Inhibitors: An Opportunity To Fight Antimicrobial Resistance. Journal of Medicinal Chemistry, 2019, 62, 2720-2737.	6.4	21
34	Evaluation of Substituted 1,2,3â€Dithiazoles as Inhibitors of the Feline Immunodeficiency Virus (FIV) Nucleocapsid Protein via a Proposed Zinc Ejection Mechanism. ChemMedChem, 2016, 11, 2119-2126.	3.2	20
35	Potent and selective N-(4-sulfamoylphenyl)thiourea-based GPR55 agonists. European Journal of Medicinal Chemistry, 2016, 107, 119-132.	5.5	18
36	Design and Analysis of the 4â€Anilinoquin(az)oline Kinase Inhibition Profiles of GAK/SLK/STK10 Using Quantitative Structureâ€Activity Relationships. ChemMedChem, 2020, 15, 26-49.	3.2	18

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37	Evaluation of the antiviral efficacy of bis[1,2]dithiolo[1,4]thiazines and bis[1,2]dithiolopyrrole derivatives against the nucelocapsid protein of the Feline Immunodeficiency Virus (FIV) as a model for HIV infection. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 2640-2644.	2.2	17
38	In Vitro and in Silico Evaluation of Bikaverin as a Potent Inhibitor of Human Protein Kinase CK2. Molecules, 2019, 24, 1380.	3.8	17
39	PKMYT1: a forgotten member of the WEE1 family. Nature Reviews Drug Discovery, 2020, 19, 157-157.	46.4	17
40	Molecular Dynamics Simulations for Human CAR Inverse Agonists. Journal of Chemical Information and Modeling, 2012, 52, 457-464.	5.4	16
41	Mutation of Cys242 of Human Monoacylglycerol Lipase Disrupts Balanced Hydrolysis of 1- and 2-Monoacylglycerols and Selectively Impairs Inhibitor Potency. Molecular Pharmacology, 2014, 85, 510-519.	2.3	16
42	Novel fused tetrathiocines as antivirals that target the nucleocapsid zinc finger containing protein of the feline immunodeficiency virus (FIV) as a model of HIV infection. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 1352-1355.	2.2	16
43	Towards the Development of an In vivo Chemical Probe for Cyclin G Associated Kinase (GAK). Molecules, 2019, 24, 4016.	3.8	16
44	Discovery of novel cannabinoid receptor ligands by a virtual screening approach: Further development of 2,4,6-trisubstituted 1,3,5-triazines as CB2 agonists. European Journal of Pharmaceutical Sciences, 2013, 48, 9-20.	4.0	15
45	Chemoproteomic, biochemical and pharmacological approaches in the discovery of inhibitors targeting human Î±/Î²-hydrolase domain containing 11 (ABHD11). European Journal of Pharmaceutical Sciences, 2016, 93, 253-263.	4.0	12
46	Structureâ€Based Virtual Screening of LsrK Kinase Inhibitors to Target Quorum Sensing. ChemMedChem, 2018, 13, 2400-2407.	3.2	12
47	PIP5K1A: a potential target for cancers with KRAS or TP53 mutations. Nature Reviews Drug Discovery, 2020, 19, 436-436.	46.4	12
48	Recognition of reactive high-energy conformations by shape complementarity and specific enzymeâ€“substrate interactions in family 10 and 11 xylanases. Physical Chemistry Chemical Physics, 2004, 6, 5074-5080.	2.8	11
49	Design, synthesis, and biological evaluation of 2,4-dihydropyrano[2,3-c]pyrazole derivatives as autotaxin inhibitors. European Journal of Pharmaceutical Sciences, 2017, 107, 97-111.	4.0	11
50	Revisiting 1,3,4-Oxadiazol-2-ones: Utilization in the Development of ABHD6 Inhibitors. Bioorganic and Medicinal Chemistry, 2015, 23, 6335-6345.	3.0	10
51	Investigation of the Pentathiepin Functionality as an Inhibitor of Feline Immunodeficiency Virus (FIV) via a Potential Zinc Ejection Mechanism, as a Model for HIV Infection. ChemMedChem, 2019, 14, 454-461.	3.2	9
52	Targeting the Water Network in Cyclin Gâ€Associated Kinase (GAK) with 4â€Anilinoâ€quin(az)oline Inhibitors. ChemMedChem, 2020, 15, 1200-1215.	3.2	9
53	Docking-Based 3D-QSAR Studies for 1,3,4-oxadiazol-2-one Derivatives as FAAH Inhibitors. International Journal of Molecular Sciences, 2021, 22, 6108.	4.1	9
54	Inversion of the roles of the nucleophile and acid/base catalysts in the covalent binding of epoxyalkyl xyloside inhibitor to the catalytic glutamates of endo-1,4-Î²-xylanase (XYNII): a molecular dynamics study. Protein Engineering, Design and Selection, 2000, 13, 247-252.	2.1	8

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55	Antimicrobial and Antifungal Activity of Rare Substituted 1,2,3-Thiaselenazoles and Corresponding Matched Pair 1,2,3-Dithiazoles. Antibiotics, 2020, 9, 369.	3.7	8
56	MM-PBSA free energy analysis of endo-1,4-xylanase II (XynII)â€“substrate complexes: binding of the reactive sugar in a skew boat and chair conformation. Organic and Biomolecular Chemistry, 2003, 1, 3535-3540.	2.8	7
57	Time-Dependent Inhibition of CYP2C19 by Isoquinoline Alkaloids: In Vitro and In Silico Analysis. Drug Metabolism and Disposition, 2015, 43, 1891-1904.	3.3	7
58	Surface area, volume and shape descriptors as a novel tool for polymer lead design and discovery. European Journal of Pharmaceutical Sciences, 2017, 102, 188-195.	4.0	7
59	New Insights into 4-Anilinoquinazolines as Inhibitors of Cardiac Troponin Iâ€“Interacting Kinase (TNNi3K). Molecules, 2020, 25, 1697.	3.8	7
60	Novel epidithiodiketopiperazines as anti-viral zinc ejectors of the Feline Immunodeficiency Virus (FIV) nucleocapsid protein as a model for HIV infection. Bioorganic and Medicinal Chemistry, 2019, 27, 4174-4184.	3.0	6
61	Evaluation of FASN inhibitors by a versatile toolkit reveals differences in pharmacology between human and rodent FASN preparations and in antiproliferative efficacy in vitro vs. in situ in human cancer cells. European Journal of Pharmaceutical Sciences, 2020, 149, 105321.	4.0	6
62	Structural review of PPARÎ³ in complex with ligands: Cartesian- and dihedral angle principal component analyses of X-ray crystallographic data. Proteins: Structure, Function and Bioinformatics, 2017, 85, 1684-1698.	2.6	5
63	WaterMapâ€Guided Structureâ€Based Virtual Screening for Acetylcholinesterase Inhibitors. ChemMedChem, 2022, 17, .	3.2	5
64	Structural Characterization of LsrK as a Quorum Sensing Target and a Comparison between X-ray and Homology Models. Journal of Chemical Information and Modeling, 2021, 61, 1346-1353.	5.4	4
65	Synthesis and Evaluation of Novel 1,2,6-Thiadiazinone Kinase Inhibitors as Potent Inhibitors of Solid Tumors. Molecules, 2021, 26, 5911.	3.8	4
66	Synthesis and Biological Evaluation of Arylthiourea Derivatives with Antitubercular Activity. Letters in Drug Design and Discovery, 2013, 10, 640-650.	0.7	4
67	Exploration and Development of a Câ€“H-Activated Route to Access the [1,2]Dithiolo[4,3-b]indole-3(4H)-thione Core and Related Derivatives. Synlett, 2019, 30, 156-160.	1.8	3
68	WNK kinases: an untapped opportunity to modulate ion transport. Nature Reviews Drug Discovery, 2020, 19, 828-828.	46.4	2
69	Identification of 4â€anilinoâ€quin(az)oline as a cell active Protein Kinase Novel 3 (PKN3) inhibitor chemotype. ChemMedChem, 2022, , .	3.2	2
70	Synthesis and evaluation of 1,2,3-dithiazole inhibitors of the nucleocapsid protein of feline immunodeficiency virus (FIV) as a model for HIV infection. Bioorganic and Medicinal Chemistry, 2022, 68, 116834.	3.0	2
71	Identification of Key Amino Acids that Impact Organic Solute Transporter Î±/Î² (OSTÎ±/Î²). Molecular Pharmacology, 2021, 100, 599-608.	2.3	0