Antti T Poso

List of Publications by Year
in descending order

192 papers	5,577 citations	70961 41 h-index	133063 59 g-index
202 all docs	202 docs citations	202 times ranked	7108 citing authors

#	Article	IF	Citations
1	Binding Affinity via Docking: Fact and Fiction. Molecules, 2018, 23, 1899.	1.7	292
2	A MYCâ€“aurora kinase A protein complex represents an actionable drug target in p53-altered liver cancer. Nature Medicine, 2016, 22, 744-753.	15.2	207
3	Characterization of the Sulfhydryl-Sensitive Site in the Enzyme Responsible for Hydrolysis of 2-Arachidonoyl-Glycerol in Rat Cerebellar Membranes. Chemistry and Biology, 2005, 12, 649-656.	6.2	145
4	DeepCDA: deep cross-domain compoundâ€“protein affinity prediction through LSTM and convolutional neural networks. Bioinformatics, 2020, 36, 4633-4642.	1.8	110
5	An In Silico Approach to Discovering Novel Inhibitors of Human Sirtuin Type 2. Journal of Medicinal Chemistry, 2004, 47, 6292-6298.	2.9	105
6	Integrative and Personalized QSAR Analysis in Cancer by Kernelized Bayesian Matrix Factorization. Journal of Chemical Information and Modeling, 2014, 54, 2347-2359.	2.5	101
7	Prediction of human population responses to toxic compounds by a collaborative competition. Nature Biotechnology, 2015, 33, 933-940.	9.4	88
8	Discovery of Salermide-Related Sirtuin Inhibitors: Binding Mode Studies and Antiproliferative Effects in Cancer Cells Including Cancer Stem Cells. Journal of Medicinal Chemistry, 2012, 55, 10937-10947.	2.9	84
9	Development of a 3D Model for the Human Cannabinoid CB1 Receptor. Journal of Medicinal Chemistry, 2004, 47, 3048-3057.	2.9	83
10	Piperazine and Piperidine Triazole Ureas as Ultrapotent and Highly Selective Inhibitors of Monoacylglycerol Lipase. Chemistry and Biology, 2013, 20, 379-390.	6.2	80
11	Oxadiazole-carbonylaminothioureas as SIRT1 and SIRT2 Inhibitors. Journal of Medicinal Chemistry, 2008, 51, 4377-4380.	2.9	72
12	Virtual Screening of Novel CB2 Ligands Using a Comparative Model of the Human Cannabinoid CB2 Receptor. Journal of Medicinal Chemistry, 2005, 48, 7166-7171.	2.9	64
13	Predictive Three-Dimensional Quantitative Structureâ^'Activity Relationship of Cytochrome P450 1A2 Inhibitors. Journal of Medicinal Chemistry, 2005, 48, 3808-3815.	2.9	64
14	The Effect of Ligand-Based Tautomer and Protomer Prediction on Structure-Based Virtual Screening. Journal of Chemical Information and Modeling, 2009, 49, 2742-2748.	2.5	63
15	A rhodopsin-based model for melatonin recognition at its G protein-coupled receptor. European Journal of Pharmacology, 1996, 304, 173-183.	1.7	61
16	Targeting the cannabinoid CB2 receptor: modelling and structural determinants of CB2 selective ligands. British Journal of Pharmacology, 2008, 153, 335-346.	2.7	61
17	Targeting the Cannabinoid CB2 Receptor: Mutations, Modeling and Development of CB2 Selective Ligands. Current Medicinal Chemistry, 2005, 12, 1217-1237.	1.2	59
18	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.	1.5	59

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19	Fatty Acid Amide Hydrolase Inhibitors from Virtual Screening of the Endocannabinoid System. Journal of Medicinal Chemistry, 2006, 49, 4650-4656.	2.9	58
20	Synthesis and SAR Studies of 2-Oxoquinoline Derivatives as CB2 Receptor Inverse Agonists. Journal of Medicinal Chemistry, 2006, 49, 2022-2027.	2.9	57
21	N^{Ïµ}-Thioacetyl-Lysine-Containing Tri-, Tetra-, and Pentapeptides as SIRT1 and SIRT2 Inhibitors. Journal of Medicinal Chemistry, 2009, 52, 2153-2156.	2.9	56
22	Drug release from starch-acetate microparticles and films with and without incorporated Î±-amylase. Biomaterials, 2004, 25, 4355-4362.	5.7	55
23	Discovery of Boronic Acids as Novel and Potent Inhibitors of Fatty Acid Amide Hydrolase. Journal of Medicinal Chemistry, 2008, 51, 7057-7060.	2.9	54
24	Chiral 1,3,4-Oxadiazol-2-ones as Highly Selective FAAH Inhibitors. Journal of Medicinal Chemistry, 2013, 56, 8484-8496.	2.9	54
25	Transcription and Translation Inhibitors in Cancer Treatment. Frontiers in Chemistry, 2020, 8, 276.	1.8	54
26	SARSâ€CoVâ€2â€“host proteome interactions for antiviral drug discovery. Molecular Systems Biology, 2021, 17, e10396.	3.2	53
27	Dehydration of theophylline monohydrateâ€”a two step process. International Journal of Pharmaceutics, 1997, 158, 47-55.	2.6	52
28	Amino Acids Important for Ligand Specificity of the Human Constitutive Androstane Receptor. Journal of Biological Chemistry, 2005, 280, 5960-5971.	1.6	52
29	Discovering Inhibitors of Human Sirtuin Type 2:â€‰ Novel Structural Scaffolds. Journal of Medicinal Chemistry, 2006, 49, 7239-7241.	2.9	52
30	Quantitative Insight into the Design of Compounds Recognized by the <scp>L</scp>â€Type Amino Acid Transporterâ€…1 (LAT1). ChemMedChem, 2014, 9, 2699-2707.	1.6	52
31	Substrate-dependent, non-hyperbolic kinetics of pig brain prolyl oligopeptidase and its tight binding inhibition by JTP-4819. Biochemical Pharmacology, 2002, 64, 463-471.	2.0	51
32	Structureâ€Based Virtual Screening for Dopamine D₂ Receptor Ligands as Potential Antipsychotics. ChemMedChem, 2016, 11, 718-729.	1.6	51
33	Predicting plasticization efficiency from three-dimensional molecular structure of a polymer plasticizer. Pharmaceutical Research, 2001, 18, 1760-1766.	1.7	48
34	N-(3-(4-Hydroxyphenyl)-propenoyl)-amino acid tryptamides as SIRT2 inhibitors. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 2448-2451.	1.0	48
35	Quantitative Structureâ^'Activity Relationship Analysis of Inhibitors of the Nicotine Metabolizing CYP2A6 Enzyme. Journal of Medicinal Chemistry, 2005, 48, 440-449.	2.9	47
36	The feasibility of using acoustic emissions for monitoring of fluidized bed granulation. Chemometrics and Intelligent Laboratory Systems, 2009, 97, 75-81.	1.8	46

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37	Discovery of Small Molecules Targeting the Synergy of Cardiac Transcription Factors GATA4 and NKX2-5. Journal of Medicinal Chemistry, 2017, 60, 7781-7798.	2.9	46
38	Comparative and pharmacophore model for deacetylase SIRT1. Journal of Computer-Aided Molecular Design, 2006, 20, 589-599.	1.3	45
39	Screening of Various Hormoneâ€Sensitive Lipase Inhibitors as Endocannabinoidâ€Hydrolyzing Enzyme Inhibitors. ChemMedChem, 2009, 4, 1253-1259.	1.6	45
40	Structure-Based Design of Pseudopeptidic Inhibitors for SIRT1 and SIRT2. Journal of Medicinal Chemistry, 2011, 54, 6456-6468.	2.9	45
41	N,Nâ€˜-Bisbenzylidenebenzene-1,4-diamines andN,Nâ€˜-Bisbenzylidenenaphthalene-1,4-diamines as Sirtuin Type 2 (SIRT2) Inhibitors. Journal of Medicinal Chemistry, 2006, 49, 7907-7911.	2.9	44
42	An empirical and theoretical study on mechanisms of mutagenic activity of hydrazine compounds. Mutation Research - Fundamental and Molecular Mechanisms of Mutagenesis, 1995, 332, 63-71.	0.4	43
43	Deep Learning in Drug Target Interaction Prediction: Current and Future Perspectives. Current Medicinal Chemistry, 2021, 28, 2100-2113.	1.2	43
44	Identification of WIN55212-3 as a competitive neutral antagonist of the human cannabinoid CB2 receptor. British Journal of Pharmacology, 2005, 145, 636-645.	2.7	42
45	Critical Comparison of Virtual Screening Methods against the MUV Data Set. Journal of Chemical Information and Modeling, 2009, 49, 2168-2178.	2.5	42
46	Structureâ€“activity relationship study of compounds binding to large amino acid transporter 1 (LAT1) based on pharmacophore modeling and in situ rat brain perfusion. European Journal of Pharmaceutical Sciences, 2013, 48, 523-531.	1.9	42
47	New potent and selective cytochrome P450 2B6 (CYP2B6) inhibitors based on three-dimensional quantitative structure-activity relationship (3D-QSAR) analysis. British Journal of Pharmacology, 2007, 150, 932-942.	2.7	41
48	Sulfur analogues of polychlorinated dibenzoâ€Pâ€dioxins, dibenzofurans and diphenyl ethers as inducers of CYP1A1 in mouse hepatoma cell culture and structureâ€activity relationships. Environmental Toxicology and Chemistry, 1994, 13, 1543-1548.	2.2	39
49	BRUTUS:Â Optimization of a Grid-Based Similarity Function for Rigid-Body Molecular Superposition. 1. Alignment and Virtual Screening Applications. Journal of Medicinal Chemistry, 2005, 48, 4076-4086.	2.9	39
50	The pictetâ€spengler reaction and biogenic tryptamines: Formation of tetrahydroâ€Î²â€carbolines at physiological pH. Journal of Heterocyclic Chemistry, 1994, 31, 431-435.	1.4	38
51	Ligand Recognition by Drug-Activated Nuclear Receptors PXR and CAR: Structural, Site-Directed Mutagenesis and Molecular Modeling Studies. Mini-Reviews in Medicinal Chemistry, 2006, 6, 937-943.	1.1	38
52	A comparative molecular field analysis of cytochrome P450 2A5 and 2A6 inhibitors. Journal of Computer-Aided Molecular Design, 2001, 15, 195-202.	1.3	37
53	Comparing the Quality and Predictiveness between 3D QSAR Models Obtained from Manual and Automated Alignment. Journal of Chemical Information and Computer Sciences, 2004, 44, 807-816.	2.8	37
54	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.	2.3	37

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55	Deregulated hepsin protease activity confers oncogenicity by concomitantly augmenting HGF/MET signalling and disrupting epithelial cohesion. Oncogene, 2016, 35, 1832-1846.	2.6	37
56	Predictive value of comparative molecular field analysis modelling of naphthalene inhibition of human CYP2A6 and mouse CYP2A5 enzymes. Toxicology in Vitro, 2003, 17, 449-455.	1.1	35
57	Synthesis, in vitro and in vivo evaluation of 1,3,5-triazines as cannabinoid CB2 receptor agonists. European Journal of Pharmaceutical Sciences, 2015, 67, 85-96.	1.9	35
58	Small-Molecule Thioesters as SARS-CoV-2 Main Protease Inhibitors: Enzyme Inhibition, Structureâ€“Activity Relationships, Antiviral Activity, and X-ray Structure Determination. Journal of Medicinal Chemistry, 2022, 65, 9376-9395.	2.9	35
59	Insights into Ligand-Elicited Activation of Human Constitutive Androstane Receptor Based on Novel Agonists and Three-Dimensional Quantitative Structureâ^'Activity Relationship. Journal of Medicinal Chemistry, 2008, 51, 7181-7192.	2.9	34
60	Peptides and Pseudopeptides as SIRT6 Deacetylation Inhibitors. ACS Medicinal Chemistry Letters, 2012, 3, 969-974.	1.3	34
61	Robust Hydrolysis of Prostaglandin Glycerol Esters by Human Monoacylglycerol Lipase (MAGL). Molecular Pharmacology, 2014, 86, 522-535.	1.0	34
62	Binding of some dioxins and dibenzofurans to the Ah receptor. A QSAR model based on comparative molecular field analysis (CoMFA). Computational and Theoretical Chemistry, 1993, 282, 259-264.	1.5	33
63	Identification of structural features in chemicals associated with cancer drug response: a systematic data-driven analysis. Bioinformatics, 2014, 30, i497-i504.	1.8	33
64	Discovery of substituted sulfonamides and thiazolidin-4-one derivatives as agonists of human constitutive androstane receptor. Biochemical Pharmacology, 2008, 76, 1288-1297.	2.0	32
65	A structure-activity relationship study of catechol-O-methyltransferase inhibitors combining molecular docking and 3D QSAR methods. Journal of Computer-Aided Molecular Design, 2003, 17, 797-810.	1.3	31
66	Molecular Determinants of Steroid Inhibition for the Mouse Constitutive Androstane Receptor. Journal of Medicinal Chemistry, 2003, 46, 4687-4695.	2.9	31
67	NÎµ-Modified lysine containing inhibitors for SIRT1 and SIRT2. Bioorganic and Medicinal Chemistry, 2010, 18, 5616-5625.	1.4	31
68	Identification of novel SIRT3 inhibitor scaffolds by virtual screening. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 2990-2995.	1.0	31
69	Deep Transferable Compound Representation across Domains and Tasks for Low Data Drug Discovery. Journal of Chemical Information and Modeling, 2019, 59, 4528-4539.	2.5	31
70	The Effects of Sequence Variation on Genome-wide NRF2 Bindingâ€”New Target Genes and Regulatory SNPs. Nucleic Acids Research, 2016, 44, 1760-1775.	6.5	30
71	The application of machine learning techniques to innovative antibacterial discovery and development. Expert Opinion on Drug Discovery, 2020, 15, 1165-1180.	2.5	30
72	The effect of powder blend and tablet structure on drug release mechanisms of hydrophobic starch acetate matrix tablets. European Journal of Pharmaceutics and Biopharmaceutics, 2005, 61, 149-157.	2.0	29

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73	Comparative molecular field analysis and molecular dynamics studies of Î±/Î² hydrolase domain containing 6 (ABHD6) inhibitors. Journal of Molecular Modeling, 2015, 21, 250.	0.8	29
74	The use of molecular descriptors in the development of co-amorphous formulations. European Journal of Pharmaceutical Sciences, 2018, 119, 31-38.	1.9	28
75	Structure-Based Design of Selective Salt-Inducible Kinase Inhibitors. Journal of Medicinal Chemistry, 2021, 64, 8142-8160.	2.9	28
76	Competitive inhibition of coumarin 7â€hydroxylation by pilocarpine and its interaction with mouse CYP 2A5 and human CYP₂A6. British Journal of Pharmacology, 1995, 116, 2625-2630.	2.7	27
77	LXRÎ± activation and Raf inhibition trigger lethal lipotoxicity in liver cancer. Nature Cancer, 2021, 2, 201-217.	5.7	27
78	More potent inhibition of human CYP2A6 than mouse CYP2A5 enzyme activities by derivatives of phenylethylamine and benzaldehyde. Xenobiotica, 2003, 33, 529-539.	0.5	26
79	Development of Pharmacophore Model for Indeno[1,2-b]indoles as Human Protein Kinase CK2 Inhibitors and Database Mining. Pharmaceuticals, 2017, 10, 8.	1.7	26
80	Pyridinylimidazoles as dual glycogen synthase kinase 3Î²/p38Î± mitogen-activated protein kinase inhibitors. European Journal of Medicinal Chemistry, 2019, 175, 309-329.	2.6	26
81	Predicting the drug concentration in starch acetate matrix tablets from ATR-FTIR spectra using multi-way methods. Analytica Chimica Acta, 2007, 595, 190-197.	2.6	25
82	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.	1.0	25
83	Modelling of molecular mutagenicity with comparative molecular field analysis (CoMFA). Structural and electronic properties of MX compounds related to TA 100 mutagenicity. Computational and Theoretical Chemistry, 1994, 304, 255-260.	1.5	24
84	Molecular dynamics simulations of the human CAR ligand-binding domain: deciphering the molecular basis for constitutive activity. Journal of Molecular Modeling, 2005, 11, 69-79.	0.8	24
85	3D-QSAR Studies on Cannabinoid CB1 Receptor Agonists:Â G-Protein Activation as Biological Data. Journal of Medicinal Chemistry, 2006, 49, 554-566.	2.9	24
86	Characterization of the binding properties of SIRT2 inhibitors with a N-(3-phenylpropenoyl)-glycine tryptamide backbone. Bioorganic and Medicinal Chemistry, 2008, 16, 8054-8062.	1.4	24
87	Whole grain intake associated molecule 5-aminovaleric acid betaine decreases Î²-oxidation of fatty acids in mouse cardiomyocytes. Scientific Reports, 2018, 8, 13036.	1.6	24
88	Pronounced differences in inhibition potency of lactone and non-lactone compounds for mouse and human coumarin 7-hydroxylases (CYP2A5 and CYP2A6). Xenobiotica, 2000, 30, 81-92.	0.5	23
89	The functional role of cysteines adjacent to the NRY motif of the human MT1 melatonin receptor. Journal of Pineal Research, 2005, 39, 1-11.	3.4	23
90	Identification of inhibitors of the nicotine metabolising CYP2A6 enzymeâ€"an in silico approach. Pharmacogenomics Journal, 2008, 8, 328-338.	0.9	23

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91	Chiral 3-(4,5-dihydrooxazol-2-yl)phenyl alkylcarbamates as novel FAAH inhibitors: Insight into FAAH enantioselectivity by molecular docking and interaction fields. European Journal of Medicinal Chemistry, 2009, 44, 4179-4191.	2.6	23
92	Investigation of novel ropinirole analogues: synthesis, pharmacological evaluation and computational analysis of dopamine D2 receptor functionalized congeners and homobivalent ligands. MedChemComm, 2014, 5, 891-898.	3.5	23
93	BRUTUS: Optimization of a grid-based similarity function for rigid-body molecular superposition. II. Description and characterization. Journal of Computer-Aided Molecular Design, 2006, 20, 227-236.	1.3	21
94	Ultrasound Transmission Technique as a Potential Tool for Physical Evaluation of Monolithic Matrix Tablets. AAPS PharmSciTech, 2008, 9, 267-273.	1.5	21
95	Pharmacological and molecular studies on the interaction of varenicline with different nicotinic acetylcholine receptor subtypes. Potential mechanism underlying partial agonism at human Î±4Î²2 and Î±3Î²4 subtypes. Biochimica Et Biophysica Acta - Biomembranes, 2015, 1848, 731-741.	1.4	21
96	DPD-Inspired Discovery of Novel LsrK Kinase Inhibitors: An Opportunity To Fight Antimicrobial Resistance. Journal of Medicinal Chemistry, 2019, 62, 2720-2737.	2.9	21
97	Acylated 1H-1,2,4-Triazol-5-amines Targeting Human Coagulation Factor XIIa and Thrombin: Conventional and Microscale Synthesis, Anticoagulant Properties, and Mechanism of Action. Journal of Medicinal Chemistry, 2020, 63, 13159-13186.	2.9	21
98	Comparison of homology models and X-ray structures of the nuclear receptor CAR: Assessing the structural basis of constitutive activity. Journal of Molecular Graphics and Modelling, 2007, 25, 644-657.	1.3	20
99	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.	1.6	20
100	The inner rod of virulenceâ€associated type III secretion systems constitutes a needle adapter of one helical turn that is deeply integrated into the system's export apparatus. Molecular Microbiology, 2019, 112, 918-931.	1.2	20
101	Potent and selective N-(4-sulfamoylphenyl)thiourea-based GPR55 agonists. European Journal of Medicinal Chemistry, 2016, 107, 119-132.	2.6	18
102	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.	1.6	18
103	Changes in solid-state structure of cyclophosphamide monohydrate induced by mechanical treatment and storage. Pharmaceutical Research, 1995, 12, 299-304.	1.7	17
104	Comparative Molecular Field Analysis (CoMFA) of MX Compounds using different Semi-empirical Methods: LUMO Field and its Correlation with Mutagenic Activity. QSAR and Combinatorial Science, 1996, 15, 189-193.	1.4	17
105	Monitoring the wetting phase of fluidized bed granulation process using multi-way methods: The separation of successful from unsuccessful batches. Chemometrics and Intelligent Laboratory Systems, 2009, 96, 88-93.	1.8	17
106	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.	1.0	17
107	New, Nonâ€quinone Fluorogeldanamycin Derivatives Strongly Inhibit Hsp90. ChemBioChem, 2015, 16, 302-311.	1.3	17
108	In Vitro and in Silico Evaluation of Bikaverin as a Potent Inhibitor of Human Protein Kinase CK2. Molecules, 2019, 24, 1380.	1.7	17

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109	Comprehensive data-driven analysis of the impact of chemoinformatic structure on the genome-wide biological response profiles of cancer cells to 1159 drugs. BMC Bioinformatics, 2012, 13, 112.	1.2	16
110	Molecular Dynamics Simulations for Human CAR Inverse Agonists. Journal of Chemical Information and Modeling, 2012, 52, 457-464.	2.5	16
111	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.	1.0	16
112	Virtual screening approach of sirtuin inhibitors results in two new scaffolds. European Journal of Pharmaceutical Sciences, 2015, 76, 27-32.	1.9	16
113	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.	1.0	16
114	The Future of Medicinal Chemistry, PROTAC, and Undruggable Drug Targets. Journal of Medicinal Chemistry, 2021, 64, 10680-10681.	2.9	16
115	3â€Heterocycleâ€Phenyl Nâ€Alkylcarbamates as FAAH Inhibitors: Design, Synthesis and 3Dâ€QSAR Studies. ChemMedChem, 2010, 5, 213-231.	1.6	15
116	Estimation of granule size distribution for batch fluidized bed granulation process using acoustic emission and Nâ€way PLS. Journal of Chemometrics, 2010, 24, 464-471.	0.7	15
117	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.	1.9	15
118	1,3,4-Oxadiazol-2-ones as fatty-acid amide hydrolase and monoacylglycerol lipase inhibitors: Synthesis, in vitro evaluation and insight into potency and selectivity determinants by molecular modelling. European Journal of Pharmaceutical Sciences, 2013, 49, 423-433.	1.9	15
119	Multiâ€Component Protein â€“ Protein Docking Based Protocol with External Scoring for Modeling Dimers of G Proteinâ€Coupled Receptors. Molecular Informatics, 2015, 34, 246-255.	1.4	15
120	SARS-COV-2 M^{pro} conformational changes induced by covalently bound ligands. Journal of Biomolecular Structure and Dynamics, 2022, 40, 12347-12357.	2.0	15
121	A Proton Relay Process as the Mechanism of Activation of the Histamine H3-Receptor Determined by 1H NMR and ab Initio Quantum Mechanical Calculations. Journal of the American Chemical Society, 2000, 122, 6989-6996.	6.6	14
122	Dicarboxylic Acid Azacyclel-Prolyl-pyrrolidine Amides as Prolyl Oligopeptidase Inhibitors and Three-Dimensional Quantitative Structureâ^'Activity Relationship of the Enzymeâ^'Inhibitor Interactions. Journal of Medicinal Chemistry, 2005, 48, 4772-4782.	2.9	14
123	Identification of novel CYP2A6 inhibitors by virtual screening. Bioorganic and Medicinal Chemistry, 2011, 19, 7186-7193.	1.4	14
124	Structural studies, homology modeling and molecular docking of novel non-competitive antagonists of GluK1/GluK2 receptors. Bioorganic and Medicinal Chemistry, 2014, 22, 787-795.	1.4	14
125	Comparative Molecular Field Analysis of Compounds with CYP2A5 Binding Affinity. QSAR and Combinatorial Science, 1995, 14, 507-511.	1.4	13
126	Calculated molecular properties for different alkanoic acidâ€“alkylamine complexes: A comparison with measured FTIR and Raman spectra. Chemical Physics, 2001, 263, 127-138.	0.9	13

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127	Partial least square projections to latent structures analysis (PLS) in evaluating and predicting drug release from starch acetate matrix tablets. Journal of Pharmaceutical Sciences, 2005, 94, 2716-2730.	1.6	12
128	Structureâ€Based Virtual Screening of LsrK Kinase Inhibitors to Target Quorum Sensing. ChemMedChem, 2018, 13, 2400-2407.	1.6	12
129	Ligand Accessibility Insights to the Dengue Virus NS3â€NS2B Protease Assessed by Longâ€Timescale Molecular Dynamics Simulations. ChemMedChem, 2021, 16, 2524-2534.	1.6	12
130	Structural and Functional Characterization of Malate Synthase G from Opportunistic Pathogen Pseudomonas aeruginosa. Biochemistry, 2017, 56, 5539-5549.	1.2	12
131	Synthesis and CB1 receptor activities of dimethylheptyl derivatives of 2-arachidonoyl glycerol (2-AG) and 2-arachidonyl glyceryl ether (2-AGE). Bioorganic and Medicinal Chemistry, 2006, 14, 2850-2858.	1.4	11
132	Experimental and computational studies on the tautomerism of N-substituted 3-amino-5-oxo-4-phenyl-1H-pyrazolo-1-carboxamides with antibacterial activity. Journal of Molecular Structure, 2013, 1051, 188-196.	1.8	11
133	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.	1.9	11
134	Exploring the chemical space for freeze-drying excipients. International Journal of Pharmaceutics, 2019, 566, 254-263.	2.6	11
135	Potent Inhibitor of Human Trypsins from the Aeruginosin Family of Natural Products. ACS Chemical Biology, 2021, 16, 2537-2546.	1.6	11
136	Prediction of Contact Angle for Pharmaceutical Solids from Their Molecular Structure. Journal of Pharmaceutical Sciences, 2005, 94, 745-758.	1.6	10
137	Synthesis and Characterization of the Novel Fluorescent Prolyl Oligopeptidase Inhibitor 4-Fluoresceinthiocarbamoyl- 6-aminocaproyl-l-prolyl-2(S)-(Hydroxy- acetyl)pyrrolidine. Journal of Medicinal Chemistry, 2005, 48, 7093-7095.	2.9	10
138	Uncertainty in dissolution test of drug release. Chemometrics and Intelligent Laboratory Systems, 2009, 97, 82-90.	1.8	10
139	Structure-Based Molecular Modeling Approaches to GPCR Oligomerization. Methods in Cell Biology, 2013, 117, 91-104.	0.5	10
140	Quantitative insights for the design of substrate-based SIRT1 inhibitors. European Journal of Pharmaceutical Sciences, 2014, 59, 12-19.	1.9	10
141	Targeting extracellular and juxtamembrane FGFR2 mutations in chemotherapy-refractory cholangiocarcinoma. Npj Precision Oncology, 2021, 5, 80.	2.3	10
142	Comparison of structure fingerprint and molecular interaction field based methods in explaining biological similarity of small molecules in cell-based screens. Journal of Computer-Aided Molecular Design, 2009, 23, 227-239.	1.3	9
143	Constitutive activity and ligandâ€dependent activation of the nuclear receptor CARâ€”insights from molecular dynamics simulations. Journal of Molecular Recognition, 2011, 24, 875-882.	1.1	9
144	Correlation between calculated molecular descriptors of excipient amino acids and experimentally observed thermal stability of lysozyme. International Journal of Pharmaceutics, 2017, 523, 238-245.	2.6	9

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145	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.	1.6	9
146	The autoinhibited state of MKK4: Phosphorylation, putative dimerization and R134W mutant studied by molecular dynamics simulations. Computational and Structural Biotechnology Journal, 2020, 18, 2687-2698.	1.9	9
147	Targeting the Water Network in Cyclin Gâ€Associated Kinase (GAK) with 4â€Anilinoâ€quin(az)oline Inhibitors. ChemMedChem, 2020, 15, 1200-1215.	1.6	9
148	Docking-Based 3D-QSAR Studies for 1,3,4-oxadiazol-2-one Derivatives as FAAH Inhibitors. International Journal of Molecular Sciences, 2021, 22, 6108.	1.8	9
149	Virus structure and structure-based antivirals. Current Opinion in Virology, 2021, 51, 16-24.	2.6	9
150	Chemical space of orally active compounds. Chemometrics and Intelligent Laboratory Systems, 2006, 84, 134-141.	1.8	8
151	Estimation of drug release profiles of a heterogeneous set of drugs from a hydrophobic matrix tablet using molecular descriptors. Journal of Chemometrics, 2008, 22, 653-660.	0.7	8
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