Antti T Poso

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/9190363/publications.pdf

Version: 2024-02-01

192	5,577	71102	133252
papers	citations	41 h-index	59 g-index

202	202	202	7108
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	SARS-COV-2 M^{pro} conformational changes induced by covalently bound ligands. Journal of Biomolecular Structure and Dynamics, 2022, 40, 12347-12357.	3.5	15
2	A new porphyrin as selective substrate-based inhibitor of breast cancer resistance protein (BCRP/ABCG2). Chemico-Biological Interactions, 2022, 351, 109718.	4.0	4
3	Inhibition of prolyl oligopeptidase: A promising pathway to prevent the progression of age-related macular degeneration. Biomedicine and Pharmacotherapy, 2022, 146, 112501.	5.6	3
4	WaterMapâ€Guided Structureâ€Based Virtual Screening for Acetylcholinesterase Inhibitors. ChemMedChem, 2022, 17, .	3.2	5
5	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
6	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.	6.4	35
7	Inhibitor induced conformational changes in SARS-COV-2 papain-like protease. Scientific Reports, 2022, 12, .	3.3	5
8	LXRÎ± activation and Raf inhibition trigger lethal lipotoxicity in liver cancer. Nature Cancer, 2021, 2, 201-217.	13.2	27
9	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
10	Deep Learning in Drug Target Interaction Prediction: Current and Future Perspectives. Current Medicinal Chemistry, 2021, 28, 2100-2113.	2.4	43
11	In Vitro Identification and In Vivo Confirmation of Inhibitors for Sweet Potato Chlorotic Stunt Virus RNA Silencing Suppressor, a Viral RNase III. Journal of Virology, 2021, 95, .	3.4	3
12	Ligand Accessibility Insights to the Dengue Virus NS3â€NS2B Protease Assessed by Longâ€Timescale Molecular Dynamics Simulations. ChemMedChem, 2021, 16, 2524-2534.	3.2	12
13	Tetrahydroquinoline/4,5â€Dihydroisoxazole Molecular Hybrids as Inhibitors of Breast Cancer Resistance Protein (BCRP/ABCG2). ChemMedChem, 2021, 16, 2686-2694.	3.2	6
14	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
15	Structure-Based Design of Selective Salt-Inducible Kinase Inhibitors. Journal of Medicinal Chemistry, 2021, 64, 8142-8160.	6.4	28
16	Molecular characteristics supporting l-Type amino acid transporter 1 (LAT1)-mediated translocation. Bioorganic Chemistry, 2021, 112, 104921.	4.1	7
17	The Future of Medicinal Chemistry, PROTAC, and Undruggable Drug Targets. Journal of Medicinal Chemistry, 2021, 64, 10680-10681.	6.4	16
18	Targeting extracellular and juxtamembrane FGFR2 mutations in chemotherapy-refractory cholangiocarcinoma. Npj Precision Oncology, 2021, 5, 80.	5.4	10

#	Article	IF	Citations
19	Neurosteroids: Structure-Uptake Relationships and Computational Modeling of Organic Anion Transporting Polypeptides (OATP)1A2. Molecules, 2021, 26, 5662.	3.8	6
20	Virus structure and structure-based antivirals. Current Opinion in Virology, 2021, 51, 16-24.	5.4	9
21	Potent Inhibitor of Human Trypsins from the Aeruginosin Family of Natural Products. ACS Chemical Biology, 2021, 16, 2537-2546.	3.4	11
22	SARSâ€CoVâ€2â€“host proteome interactions for antiviral drug discovery. Molecular Systems Biology, 2021, 17, e10396.	7.2	53
23	FGFR3 overexpression is a useful detection tool for FGFR3 fusions and sequence variations in glioma. Neuro-Oncology Practice, 2021, 8, 209-221.	1.6	7
24	VTT-006, an anti-mitotic compound, binds to the Ndc80 complex and suppresses cancer cell growth in vitro. Oncoscience, 2021, 8, 134-153.	2.2	1
25	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
26	Molecular Modeling of Protein Kinases: Current Status and Challenges. Topics in Medicinal Chemistry, 2020, , 25-41.	0.8	0
27	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.	6.4	21
28	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.	4.1	9
29	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
30	DeepCDA: deep cross-domain compoundâ€“protein affinity prediction through LSTM and convolutional neural networks. Bioinformatics, 2020, 36, 4633-4642.	4.1	110
31	Design, synthesis and biological activity of novel substituted 3-benzoic acid derivatives as MtDHFR inhibitors. Bioorganic and Medicinal Chemistry, 2020, 28, 115600.	3.0	7
32	The application of machine learning techniques to innovative antibacterial discovery and development. Expert Opinion on Drug Discovery, 2020, 15, 1165-1180.	5.0	30
33	Transcription and Translation Inhibitors in Cancer Treatment. Frontiers in Chemistry, 2020, 8, 276.	3.6	54
34	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
35	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
36	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

#	Article	IF	Citations
37	Ligandâ€•and Structureâ€Based Approaches of Escherichia coli FabI Inhibition by Triclosan Derivatives: From Chemical Similarity to Protein Dynamics Influence. ChemMedChem, 2019, 14, 1995-2004.	3.2	7
38	Deep Transferable Compound Representation across Domains and Tasks for Low Data Drug Discovery. Journal of Chemical Information and Modeling, 2019, 59, 4528-4539.	5.4	31
39	The Universal 3D QSAR Model for Dopamine D2 Receptor Antagonists. International Journal of Molecular Sciences, 2019, 20, 4555.	4.1	6
40	Exploring the chemical space for freeze-drying excipients. International Journal of Pharmaceutics, 2019, 566, 254-263.	5.2	11
41	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.	2.5	20
42	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
43	Pyridinylimidazoles as dual glycogen synthase kinase 3Î²/p38Î± mitogen-activated protein kinase inhibitors. European Journal of Medicinal Chemistry, 2019, 175, 309-329.	5.5	26
44	In Vitro and in Silico Evaluation of Bikaverin as a Potent Inhibitor of Human Protein Kinase CK2. Molecules, 2019, 24, 1380.	3.8	17
45	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
46	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
47	The use of molecular descriptors in the development of co-amorphous formulations. European Journal of Pharmaceutical Sciences, 2018, 119, 31-38.	4.0	28
48	Structureâ€Based Virtual Screening of LsrK Kinase Inhibitors to Target Quorum Sensing. ChemMedChem, 2018, 13, 2400-2407.	3.2	12
49	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
50	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
51	Binding Affinity via Docking: Fact and Fiction. Molecules, 2018, 23, 1899.	3.8	292
52	Discovery of Small Molecules Targeting the Synergy of Cardiac Transcription Factors GATA4 and NKX2-5. Proceedings for Annual Meeting of the Japanese Pharmacological Society, 2018, WCP2018, PO4-2-24.	0.0	0
53	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
54	Correlation between calculated molecular descriptors of excipient amino acids and experimentally observed thermal stability of lysozyme. International Journal of Pharmaceutics, 2017, 523, 238-245.	5.2	9

#	Article	IF	Citations
55	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
56	Discovery of Small Molecules Targeting the Synergy of Cardiac Transcription Factors GATA4 and NKX2-5. Journal of Medicinal Chemistry, 2017, 60, 7781-7798.	6.4	46
57	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
58	Cover Image, Volume 85, Issue 9. Proteins: Structure, Function and Bioinformatics, 2017, 85, C1-C1.	2.6	0
59	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
60	Structural and Functional Characterization of Malate Synthase G from Opportunistic Pathogen Pseudomonas aeruginosa. Biochemistry, 2017, 56, 5539-5549.	2.5	12
61	Virtual Screening of Transmembrane Serine Protease Inhibitors. Bio-protocol, 2017, 7, e2246.	0.4	0
62	Structureâ€Based Virtual Screening for Dopamine D₂ Receptor Ligands as Potential Antipsychotics. ChemMedChem, 2016, 11, 718-729.	3.2	51
63	A MYCâ€“aurora kinase A protein complex represents an actionable drug target in p53-altered liver cancer. Nature Medicine, 2016, 22, 744-753.	30.7	207
64	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
65	Virtual Screening of Small Drugâ€Like Compounds Stimulating the Enzymatic Activity of Kallikreinâ€Related Peptidaseâ€…3 (KLK3). ChemMedChem, 2016, 11, 2043-2049.	3.2	2
66	Potent and selective N-(4-sulfamoylphenyl)thiourea-based GPR55 agonists. European Journal of Medicinal Chemistry, 2016, 107, 119-132.	5.5	18
67	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
68	Deregulated hepsin protease activity confers oncogenicity by concomitantly augmenting HGF/MET signalling and disrupting epithelial cohesion. Oncogene, 2016, 35, 1832-1846.	5.9	37
69	Common and Distinct Interactions of Chemical Inhibitors with Cytochrome P450 CYP1A2, CYP2A6 and CYP2B6 Enzymes. Drug Metabolism Letters, 2016, 10, 56-64.	0.8	2
70	Prediction of human population responses to toxic compounds by a collaborative competition. Nature Biotechnology, 2015, 33, 933-940.	17.5	88
71	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.	2.6	21
72	New, Nonâ€quinone Fluorogeldanamycin Derivatives Strongly Inhibit Hsp90. ChemBioChem, 2015, 16, 302-311.	2.6	17

#	Article	IF	Citations
73	Virtual screening approach of sirtuin inhibitors results in two new scaffolds. European Journal of Pharmaceutical Sciences, 2015, 76, 27-32.	4.0	16
74	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
75	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.	2.5	15
76	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
77	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
78	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.	4.0	35
79	Robust Hydrolysis of Prostaglandin Glycerol Esters by Human Monoacylglycerol Lipase (MAGL). Molecular Pharmacology, 2014, 86, 522-535.	2.3	34
80	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.	3.2	52
81	Synthesis, in vitro and in vivo studies, and molecular modeling of N-alkylated dextromethorphan derivatives as non-competitive inhibitors of Î±3Î²4 nicotinic acetylcholine receptor. Bioorganic and Medicinal Chemistry, 2014, 22, 6846-6856.	3.0	6
82	Centmitor-1, a Novel Acridinyl-Acetohydrazide, Possesses Similar Molecular Interaction Field and Antimitotic Cellular Phenotype as Rigosertib, ON 01910.Na. Molecular Cancer Therapeutics, 2014, 13, 1054-1066.	4.1	6
83	Identification of structural features in chemicals associated with cancer drug response: a systematic data-driven analysis. Bioinformatics, 2014, 30, i497-i504.	4.1	33
84	Structural studies, homology modeling and molecular docking of novel non-competitive antagonists of GluK1/GluK2 receptors. Bioorganic and Medicinal Chemistry, 2014, 22, 787-795.	3.0	14
85	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
86	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
87	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
88	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.	3.4	23
89	Quantitative insights for the design of substrate-based SIRT1 inhibitors. European Journal of Pharmaceutical Sciences, 2014, 59, 12-19.	4.0	10
90	In Vitro Screening of Some Heterocyclic Compounds Against Human ABHD6 and ABHD12 Hydrolases. Letters in Drug Design and Discovery, 2014, 11, 944-952.	0.7	2

#	Article	IF	Citations
91	Identification of novel SIRT3 inhibitor scaffolds by virtual screening. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 2990-2995.	2.2	31
92	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.	3.6	11
93	Chiral 1,3,4-Oxadiazol-2-ones as Highly Selective FAAH Inhibitors. Journal of Medicinal Chemistry, 2013, 56, 8484-8496.	6.4	54
94	Structure-Based Molecular Modeling Approaches to GPCR Oligomerization. Methods in Cell Biology, 2013, 117, 91-104.	1.1	10
95	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
96	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.	4.0	15
97	Piperazine and Piperidine Triazole Ureas as Ultrapotent and Highly Selective Inhibitors of Monoacylglycerol Lipase. Chemistry and Biology, 2013, 20, 379-390.	6.0	80
98	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.	4.0	42
99	Synthesis and Biological Evaluation of Arylthiourea Derivatives with Antitubercular Activity. Letters in Drug Design and Discovery, 2013, 10, 640-650.	0.7	4
100	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.	2.6	16
101	Peptides and Pseudopeptides as SIRT6 Deacetylation Inhibitors. ACS Medicinal Chemistry Letters, 2012, 3, 969-974.	2.8	34
102	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.	6.4	84
103	Molecular Dynamics Simulations for Human CAR Inverse Agonists. Journal of Chemical Information and Modeling, 2012, 52, 457-464.	5.4	16
104	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
105	Structure-Based Design of Pseudopeptidic Inhibitors for SIRT1 and SIRT2. Journal of Medicinal Chemistry, 2011, 54, 6456-6468.	6.4	45
106	Identification of novel CYP2A6 inhibitors by virtual screening. Bioorganic and Medicinal Chemistry, 2011, 19, 7186-7193.	3.0	14
107	Constitutive activity and ligandâ€dependent activation of the nuclear receptor CARâ€”insights from molecular dynamics simulations. Journal of Molecular Recognition, 2011, 24, 875-882.	2.1	9
108	The Discovery of Compounds That Stimulate the Activity of Kallikreinâ€Related Peptidaseâ€…3 (KLK3). ChemMedChem, 2011, 6, 2170-2178.	3.2	8

#	Article	IF	Citations
109	Studying the catechol binding cavity in comparative models of human dopamine D2 receptor. Journal of Molecular Graphics and Modelling, 2011, 29, 685-692.	2.4	7
110	3â€Heterocycleâ€Phenyl Nâ€Alkylcarbamates as FAAH Inhibitors: Design, Synthesis and 3Dâ€QSAR Studies. ChemMedChem, 2010, 5, 213-231.	3.2	15
111	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.	1.3	15
112	Increasing the Throughput of Shapeâ€Based Virtual Screening with GPU Processing and Single Conformation Databases. Molecular Informatics, 2010, 29, 293-296.	2.5	0
113	Nε-Modified lysine containing inhibitors for SIRT1 and SIRT2. Bioorganic and Medicinal Chemistry, 2010, 18, 5616-5625.	3.0	31
114	Screening of Various Hormoneâ€Sensitive Lipase Inhibitors as Endocannabinoidâ€Hydrolyzing Enzyme Inhibitors. ChemMedChem, 2009, 4, 1253-1259.	3.2	45
115	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.	5.5	23
116	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.	2.9	9
117	The feasibility of using acoustic emissions for monitoring of fluidized bed granulation. Chemometrics and Intelligent Laboratory Systems, 2009, 97, 75-81.	3.5	46
118	Uncertainty in dissolution test of drug release. Chemometrics and Intelligent Laboratory Systems, 2009, 97, 82-90.	3.5	10
119	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.	3.5	17
120	Critical Comparison of Virtual Screening Methods against the MUV Data Set. Journal of Chemical Information and Modeling, 2009, 49, 2168-2178.	5.4	42
121	The Effect of Ligand-Based Tautomer and Protomer Prediction on Structure-Based Virtual Screening. Journal of Chemical Information and Modeling, 2009, 49, 2742-2748.	5.4	63
122	N^ε-Thioacetyl-Lysine-Containing Tri-, Tetra-, and Pentapeptides as SIRT1 and SIRT2 Inhibitors. Journal of Medicinal Chemistry, 2009, 52, 2153-2156.	6.4	56
123	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.	1.3	8
124	Characterization of the binding properties of SIRT2 inhibitors with a N-(3-phenylpropenoyl)-glycine tryptamide backbone. Bioorganic and Medicinal Chemistry, 2008, 16, 8054-8062.	3.0	24
125	Ultrasound Transmission Technique as a Potential Tool for Physical Evaluation of Monolithic Matrix Tablets. AAPS PharmSciTech, 2008, 9, 267-273.	3.3	21
126	Targeting the cannabinoid CB2 receptor: modelling and structural determinants of CB2 selective ligands. British Journal of Pharmacology, 2008, 153, 335-346.	5.4	61

#	Article	IF	Citations
127	Discovery of substituted sulfonamides and thiazolidin-4-one derivatives as agonists of human constitutive androstane receptor. Biochemical Pharmacology, 2008, 76, 1288-1297.	4.4	32
128	Discovery of Boronic Acids as Novel and Potent Inhibitors of Fatty Acid Amide Hydrolase. Journal of Medicinal Chemistry, 2008, 51, 7057-7060.	6.4	54
129	Identification of inhibitors of the nicotine metabolising CYP2A6 enzymeâ€"an in silico approach. Pharmacogenomics Journal, 2008, 8, 328-338.	2.0	23
130	FieldChopper, A New Tool for Automatic Model Generation and Virtual Screening Based on Molecular Fields. Journal of Chemical Information and Modeling, 2008, 48, 1131-1137.	5.4	3
131	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.	6.4	34
132	Oxadiazole-carbonylaminothioureas as SIRT1 and SIRT2 Inhibitors. Journal of Medicinal Chemistry, 2008, 51, 4377-4380.	6.4	72
133	N-(3-(4-Hydroxyphenyl)-propenoyl)-amino acid tryptamides as SIRT2 inhibitors. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 2448-2451.	2.2	48
134	Predicting the drug concentration in starch acetate matrix tablets from ATR-FTIR spectra using multi-way methods. Analytica Chimica Acta, 2007, 595, 190-197.	5.4	25
135	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.	2.4	20
136	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.	5.4	41
137	Synthesis and SAR Studies of 2-Oxoquinoline Derivatives as CB2 Receptor Inverse Agonists. Journal of Medicinal Chemistry, 2006, 49, 2022-2027.	6.4	57
138	Discovering Inhibitors of Human Sirtuin Type 2:â€‰ Novel Structural Scaffolds. Journal of Medicinal Chemistry, 2006, 49, 7239-7241.	6.4	52
139	Fatty Acid Amide Hydrolase Inhibitors from Virtual Screening of the Endocannabinoid System. Journal of Medicinal Chemistry, 2006, 49, 4650-4656.	6.4	58
140	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.	6.4	44
141	Chemical space of orally active compounds. Chemometrics and Intelligent Laboratory Systems, 2006, 84, 134-141.	3.5	8
142	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.	3.0	11
143	3D-QSAR Studies on Cannabinoid CB1 Receptor Agonists:Â G-Protein Activation as Biological Data. Journal of Medicinal Chemistry, 2006, 49, 554-566.	6.4	24
144	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.	2.9	21

#	Article	IF	Citations
145	Comparative and pharmacophore model for deacetylase SIRT1. Journal of Computer-Aided Molecular Design, 2006, 20, 589-599.	2.9	45
146	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.	2.4	38
147	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.	6.0	145
148	Virtual Screening of Novel CB2 Ligands Using a Comparative Model of the Human Cannabinoid CB2 Receptor. Journal of Medicinal Chemistry, 2005, 48, 7166-7171.	6.4	64
149	Identification of WIN55212-3 as a competitive neutral antagonist of the human cannabinoid CB2 receptor. British Journal of Pharmacology, 2005, 145, 636-645.	5.4	42
150	The functional role of cysteines adjacent to the NRY motif of the human MT1 melatonin receptor. Journal of Pineal Research, 2005, 39, 1-11.	7.4	23
151	Prediction of Contact Angle for Pharmaceutical Solids from Their Molecular Structure. Journal of Pharmaceutical Sciences, 2005, 94, 745-758.	3.3	10
152	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.	3.3	12
153	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.	1.8	24
154	Targeting the Cannabinoid CB2 Receptor: Mutations, Modeling and Development of CB2 Selective Ligands. Current Medicinal Chemistry, 2005, 12, 1217-1237.	2.4	59
155	Quantitative Structureâ^'Activity Relationship Analysis of Inhibitors of the Nicotine Metabolizing CYP2A6 Enzyme. Journal of Medicinal Chemistry, 2005, 48, 440-449.	6.4	47
156	Amino Acids Important for Ligand Specificity of the Human Constitutive Androstane Receptor. Journal of Biological Chemistry, 2005, 280, 5960-5971.	3.4	52
157	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.	6.4	10
158	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.	6.4	39
159	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.	4.3	29
160	Predictive Three-Dimensional Quantitative Structureâ^'Activity Relationship of Cytochrome P450 1A2 Inhibitors. Journal of Medicinal Chemistry, 2005, 48, 3808-3815.	6.4	64
161	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.	6.4	14
162	Development of a 3D Model for the Human Cannabinoid CB1 Receptor. Journal of Medicinal Chemistry, 2004, 47, 3048-3057.	6.4	83

#	Article	IF	Citations
163	Comparing the Quality and Predictiveness Between 3D QSAR Models Obtained from Manual and Automated Alignment.. ChemInform, 2004, 35, no.	0.0	0
164	Drug release from starch-acetate microparticles and films with and without incorporated Î±-amylase. Biomaterials, 2004, 25, 4355-4362.	11.4	55
165	An In Silico Approach to Discovering Novel Inhibitors of Human Sirtuin Type 2. Journal of Medicinal Chemistry, 2004, 47, 6292-6298.	6.4	105
166	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
167	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.	2.9	31
168	Molecular Determinants of Steroid Inhibition for the Mouse Constitutive Androstane Receptor. Journal of Medicinal Chemistry, 2003, 46, 4687-4695.	6.4	31
169	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.	2.4	35
170	More potent inhibition of human CYP2A6 than mouse CYP2A5 enzyme activities by derivatives of phenylethylamine and benzaldehyde. Xenobiotica, 2003, 33, 529-539.	1.1	26
171	Aggregation and Solvation of Steroid Molecules in Different Solvents. Crystal Growth and Design, 2002, 2, 121-126.	3.0	3
172	Substrate-dependent, non-hyperbolic kinetics of pig brain prolyl oligopeptidase and its tight binding inhibition by JTP-4819. Biochemical Pharmacology, 2002, 64, 463-471.	4.4	51
173	Characterization of the Phase Behavior and Complexation in the Heptanoic Acidâˆ'Heptylamineâˆ'Water System. Journal of Physical Chemistry B, 2001, 105, 7944-7949.	2.6	7
174	Predicting plasticization efficiency from three-dimensional molecular structure of a polymer plasticizer. Pharmaceutical Research, 2001, 18, 1760-1766.	3.5	48
175	A comparative molecular field analysis of cytochrome P450 2A5 and 2A6 inhibitors. Journal of Computer-Aided Molecular Design, 2001, 15, 195-202.	2.9	37
176	Calculated molecular properties for different alkanoic acidâ€“alkylamine complexes: A comparison with measured FTIR and Raman spectra. Chemical Physics, 2001, 263, 127-138.	1.9	13
177	Calculated and measured vibrational frequencies in an alkanoic acidâ€“alkylamine complex. Chemical Physics Letters, 2000, 327, 420-424.	2.6	7
178	Deformation behaviors of tolbutamide, hydroxypropyl-beta-cyclodextrin, and their dispersions. Pharmaceutical Research, 2000, 17, 942-948.	3.5	7
179	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.	1.1	23
180	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.	13.7	14

#	Article	IF	Citations
181	1H NMR study on putative intramolecular hydrogen bonding for histamine H3-receptor agonists. Tetrahedron Letters, 1999, 40, 2425-2428.	1.4	6
182	Dehydration of theophylline monohydrateâ€"a two step process. International Journal of Pharmaceutics, 1997, 158, 47-55.	5.2	52
183	A rhodopsin-based model for melatonin recognition at its G protein-coupled receptor. European Journal of Pharmacology, 1996, 304, 173-183.	3.5	61
184	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.	1.2	17
185	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.	1.0	43
186	Comparative Molecular Field Analysis of Compounds with CYP2A5 Binding Affinity. QSAR and Combinatorial Science, 1995, 14, 507-511.	1.2	13
187	Changes in solid-state structure of cyclophosphamide monohydrate induced by mechanical treatment and storage. Pharmaceutical Research, 1995, 12, 299-304.	3.5	17
188	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.	5.4	27
189	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.	4.3	39
190	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
191	The pictetâ€spengler reaction and biogenic tryptamines: Formation of tetrahydroâ€Î²â€carbolines at physiological pH. Journal of Heterocyclic Chemistry, 1994, 31, 431-435.	2.6	38
192	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