Lars Olsen

List of Publications by Year
in descending order

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68 papers	2,593 citations	172386 29 h-index	197736 49 g-index
72 all docs	72 docs citations	72 times ranked	3174 citing authors

#	Article	IF	Citations
1	SMARTCyp: A 2D Method for Prediction of Cytochrome P450-Mediated Drug Metabolism. ACS Medicinal Chemistry Letters, 2010, 1, 96-100.	1.3	233
2	5-Carboxy-8-hydroxyquinoline is a broad spectrum 2-oxoglutarate oxygenase inhibitor which causes iron translocation. Chemical Science, 2013, 4, 3110.	3.7	142
3	Ionotropic glutamate-like receptor Î´2 binds <scp>d</scp> -serine and glycine. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 14116-14121.	3.3	138
4	The SMARTCyp cytochrome P450 metabolism prediction server. Bioinformatics, 2010, 26, 2988-2989.	1.8	129
5	Prediction of Activation Energies for Hydrogen Abstraction by Cytochrome P450. Journal of Medicinal Chemistry, 2006, 49, 6489-6499.	2.9	120
6	Classification of Cytochrome P450 1A2 Inhibitors and Noninhibitors by Machine Learning Techniques. Drug Metabolism and Disposition, 2009, 37, 658-664.	1.7	91
7	Sulfoxide, Sulfur, and Nitrogen Oxidation and Dealkylation by Cytochrome P450. Journal of Chemical Theory and Computation, 2008, 4, 1369-1377.	2.3	83
8	Virtual Screening and Prediction of Site of Metabolism for Cytochrome P450 1A2 Ligands. Journal of Chemical Information and Modeling, 2009, 49, 43-52.	2.5	78
9	Prediction of cytochrome P450 mediated metabolism. Advanced Drug Delivery Reviews, 2015, 86, 61-71.	6.6	78
10	RS-Predictor Models Augmented with SMARTCyp Reactivities: Robust Metabolic Regioselectivity Predictions for Nine CYP Isozymes. Journal of Chemical Information and Modeling, 2012, 52, 1637-1659.	2.5	69
11	Prediction of Activation Energies for Aromatic Oxidation by Cytochrome P450. Journal of Physical Chemistry A, 2008, 112, 13058-13065.	1.1	55
12	General Transition-State Force Field for Cytochrome P450 Hydroxylation. Journal of Chemical Theory and Computation, 2007, 3, 1765-1773.	2.3	54
13	The Accuracy of Geometries for Iron Porphyrin Complexes from Density Functional Theory. Journal of Physical Chemistry A, 2009, 113, 11949-11953.	1.1	53
14	SMARTCyp 3.0: enhanced cytochrome P450 site-of-metabolism prediction server. Bioinformatics, 2019, 35, 3174-3175.	1.8	53
15	The Structure of a Mixed GluR2 Ligand-binding Core Dimer in Complex with (S)-Glutamate and the Antagonist (S)-NS1209. Journal of Molecular Biology, 2006, 357, 1184-1201.	2.0	47
16	Fast Prediction of Cytochrome P450 Mediated Drug Metabolism. ChemMedChem, 2009, 4, 2070-2079.	1.6	46
17	Predicting Drug Metabolism by Cytochrome P450 2C9: Comparison with the 2D6 and 3A4 Isoforms. ChemMedChem, 2012, 7, 1202-1209.	1.6	46
18	Ligand-Based Site of Metabolism Prediction for Cytochrome P450 2D6. ACS Medicinal Chemistry Letters, 2012, 3, 69-73.	1.3	43

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19	Promising Tools in Prostate Cancer Research: Selective Non-Steroidal Cytochrome P450 17A1 Inhibitors. Scientific Reports, 2016, 6, 29468.	1.6	43
20	Prediction of pK_a Values for Druglike Molecules Using Semiempirical Quantum Chemical Methods. Journal of Physical Chemistry A, 2017, 121, 699-707.	1.1	41
21	Characterization of the hepatic cytochrome P450 enzymes involved in the metabolism of 25Iâ€NBOMe and 25Iâ€NBOH. Drug Testing and Analysis, 2017, 9, 671-679.	1.6	41
22	7-Phenoxy-Substituted 3,4-Dihydro-2H-1,2,4-benzothiadiazine 1,1-Dioxides as Positive Allosteric Modulators of Î±-Amino-3-hydroxy-5-methyl-4-isoxazolepropionic Acid (AMPA) Receptors with Nanomolar Potency. Journal of Medicinal Chemistry, 2018, 61, 251-264.	2.9	41
23	Salt Bridge Swapping in the EXXERFXYY Motif of Proton-coupled Oligopeptide Transporters. Journal of Biological Chemistry, 2015, 290, 29931-29940.	1.6	40
24	Synthesis, Pharmacological and Structural Characterization, and Thermodynamic Aspects of GluA2-Positive Allosteric Modulators with a 3,4-Dihydro-2H-1,2,4-benzothiadiazine 1,1-Dioxide Scaffold. Journal of Medicinal Chemistry, 2013, 56, 8736-8745.	2.9	38
25	The Contribution of Atom Accessibility to Site of Metabolism Models for Cytochromes P450. Molecular Pharmaceutics, 2013, 10, 1216-1223.	2.3	38
26	Thermodynamics and structural analysis of positive allosteric modulation of the ionotropic glutamate receptor GluA2. Biochemical Journal, 2012, 441, 173-178.	1.7	37
27	Computational Prediction of Binding Affinity for CYP1A2-Ligand Complexes Using Empirical Free Energy Calculations. Drug Metabolism and Disposition, 2010, 38, 1347-1354.	1.7	33
28	Aldehyde Oxidase: Reaction Mechanism and Prediction of Site of Metabolism. ACS Omega, 2017, 2, 4237-4244.	1.6	33
29	Dissecting the Cytochrome P450 1A2â€•and 3A4â€Mediated Metabolism of Aflatoxin B1 in Ligand and Protein Contributions. Chemistry - A European Journal, 2017, 23, 2884-2893.	1.7	31
30	Insights into regioselective metabolism of mefenamic acid by cytochrome <scp>P</scp>450 <scp>BM</scp>3 mutants through crystallography, docking, molecular dynamics, and free energy calculations. Proteins: Structure, Function and Bioinformatics, 2016, 84, 383-396.	1.5	29
31	Do Two Different Reaction Mechanisms Contribute to the Hydroxylation of Primary Amines by Cytochrome P450?. Journal of Chemical Theory and Computation, 2011, 7, 3399-3404.	2.3	28
32	Mechanism of the N-Hydroxylation of Primary and Secondary Amines by Cytochrome P450. Chemical Research in Toxicology, 2015, 28, 597-603.	1.7	27
33	Transition-State Docking of Flunitrazepam and Progesterone in Cytochrome P450. Journal of Chemical Theory and Computation, 2008, 4, 673-681.	2.3	26
34	Trends in predicted chemoselectivity of cytochrome P450 oxidation: B3LYP barrier heights for epoxidation and hydroxylation reactions. Journal of Molecular Graphics and Modelling, 2014, 52, 30-35.	1.3	26
35	Pharmacology and Structural Analysis of Ligand Binding to the Orthosteric Site of Glutamate-Like GluD2 Receptors. Molecular Pharmacology, 2016, 89, 253-262.	1.0	26
36	Positive Allosteric Modulators of 2-Amino-3-(3-hydroxy-5-methylisoxazol-4-yl)propionic Acid Receptors Belonging to 4-Cyclopropyl-3,4-dihydro-2H-1,2,4-pyridothiadiazine Dioxides and Diversely Chloro-Substituted 4-Cyclopropyl-3,4-dihydro-2H-1,2,4-benzothiadiazine 1,1-Dioxides. Journal of Medicinal Chemistry, 2014, 57, 9539-9553.	2.9	25

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37	Use of density functional theory in drug metabolism studies. Expert Opinion on Drug Metabolism and Toxicology, 2014, 10, 215-227.	1.5	25
38	A Quantitative Structureâ€“Activity Relationship for Translocation of Tripeptides via the Human Proton-Coupled Peptide Transporter, hPEPT1 (SLC15A1). AAPS Journal, 2010, 12, 385-396.	2.2	24
39	Mechanism of Cytochrome P450 17A1-Catalyzed Hydroxylase and Lyase Reactions. Journal of Chemical Information and Modeling, 2017, 57, 1123-1133.	2.5	24
40	Lysine demethylase inhibition protects pancreatic Î² cells from apoptosis and improves Î²-cell function. Molecular and Cellular Endocrinology, 2018, 460, 47-56.	1.6	22
41	Nitrogen Inversion Barriers Affect the Nâ€Oxidation of Tertiary Alkylamines by Cytochromesâ€...P450. Angewandte Chemie - International Edition, 2013, 52, 993-997.	7.2	21
42	Electric field gradients of water: A systematic investigation of basis set, electron correlation, and rovibrational effects. Journal of Chemical Physics, 2002, 116, 1424-1434.	1.2	20
43	Biophysical characterization of the proton-coupled oligopeptide transporter YjdL. Peptides, 2012, 38, 89-93.	1.2	20
44	Enthalpy-Entropy Compensation in the Binding of Modulators at Ionotropic Glutamate Receptor GluA2. Biophysical Journal, 2016, 110, 2397-2406.	0.2	20
45	Cytochrome P450â€mediated metabolism of the synthetic cannabinoids URâ€144 and XLRâ€11. Drug Testing and Analysis, 2016, 8, 792-800.	1.6	19
46	Thermodynamic Characterization of New Positive Allosteric Modulators Binding to the Glutamate Receptor A2 Ligand-Binding Domain: Combining Experimental and Computational Methods Unravels Differences in Driving Forces. Journal of Chemical Information and Modeling, 2014, 54, 3404-3416.	2.5	18
47	Structural Basis of Histone Demethylase KDM6B Histone 3 Lysine 27 Specificity. Biochemistry, 2018, 57, 585-592.	1.2	18
48	Enzyme kinetic studies of histone demethylases KDM4C and KDM6A: Towards understanding selectivity of inhibitors targeting oncogenic histone demethylases. FEBS Letters, 2011, 585, 1951-1956.	1.3	17
49	Quantum-Mechanical Studies of Reactions Performed by Cytochrome P450 Enzymes. Current Inorganic Chemistry, 2012, 2, 292-315.	0.2	17
50	Fast Methods for Prediction of Aldehyde Oxidase-Mediated Site-of-Metabolism. Computational and Structural Biotechnology Journal, 2019, 17, 345-351.	1.9	16
51	Enantioselective endocrine disrupting effects of omeprazole studied in the H295R cell assay and by molecular modeling. Toxicology in Vitro, 2016, 34, 71-80.	1.1	13
52	Both Reactivity and Accessibility Are Important in Cytochrome P450 Metabolism: A Combined DFT and MD Study of Fenamic Acids in BM3 Mutants. Journal of Chemical Information and Modeling, 2019, 59, 743-753.	2.5	13
53	Potent Inhibitors against Newcastle Disease Virus Hemagglutininâ€Neuraminidase. ChemMedChem, 2018, 13, 236-240.	1.6	11
54	Synthesis and chemical characterization of several perfluorinated sialic acid glycals and evaluation of their in vitro antiviral activity against Newcastle disease virus. MedChemComm, 2017, 8, 1505-1513.	3.5	10

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55	Structure-based optimisation of non-steroidal cytochrome P450 17A1 inhibitors. Chemical Communications, 2017, 53, 3118-3121.	2.2	9
56	Structureâ€Based Design of a New Scaffold for Cellâ€Penetrating Peptidic Inhibitors of the Histone Demethylase PHF8. ChemBioChem, 2017, 18, 1369-1375.	1.3	9
57	Identification of CYP1A2 ligands by structure-based and ligand-based virtual screening. MedChemComm, 2011, 2, 853.	3.5	8
58	Density Functional Theory Study on the Formation of Reactive Benzoquinone Imines by Hydrogen Abstraction. Journal of Chemical Information and Modeling, 2015, 55, 660-666.	2.5	8
59	Studies on Aryl-Substituted Phenylalanines: Synthesis, Activity, and Different Binding Modes at AMPA Receptors. Journal of Medicinal Chemistry, 2016, 59, 448-461.	2.9	8
60	The CYP79A1 catalyzed conversion of tyrosine to (E)-p-hydroxyphenylacetaldoxime unravelled using an improved method for homology modeling. Phytochemistry, 2017, 135, 8-17.	1.4	8
61	Design, synthesis and in vitro pharmacology of GluK1 and GluK3 antagonists. Studies towards the design of subtype-selective antagonists through 2-carboxyethyl-phenylalanines with substituents interacting with non-conserved residues in the GluK binding sites. Bioorganic and Medicinal Chemistry, 2014, 22, 5368-5377.	1.4	6
62	Discovery of Novel Non-Steroidal Cytochrome P450 17A1 Inhibitors as Potential Prostate Cancer Agents. International Journal of Molecular Sciences, 2020, 21, 4868.	1.8	6
63	Prediction of Cytochrome P450 Mediated Metabolism of Designer Drugs. Current Topics in Medicinal Chemistry, 2014, 14, 1365-1373.	1.0	5
64	A novel dualistic profile of an allosteric AMPA receptor modulator identified through studies on recombinant receptors, mouse hippocampal synapses and crystal structures. Neuroscience, 2015, 310, 709-722.	1.1	3
65	The anti-epileptic drug lamotrigine inhibits the CYP17A1 lyase reaction in vitroâ€. Biology of Reproduction, 2018, 99, 888-897.	1.2	3
66	Peptides Derived from Histone 3 and Modified at Position 18 Inhibit Histone Demethylase KDM6 Enzymes. ChemBioChem, 2018, 19, 1817-1822.	1.3	2
67	Pressure-Flow Studies: An Evaluation of Within-Testing Reproducibility-Validity of the Measured Parameters. Journal of Urology, 1999, 161, 1040-1041.	0.2	0
68	Fast Prediction of Cytochrome P450 Mediated Drug Metabolism. ChemMedChem, 2009, 4, 1965-1965.	1.6	0