Patrik Rydberg

List of Publications by Citations

43 papers	1,716 citations	24 h-index	41 g-index
44 ext. papers	1,822 ext. citations	4.8 avg, IF	4.63 L-index

#	Paper	IF	Citations
43	SMARTCyp: A 2D Method for Prediction of Cytochrome P450-Mediated Drug Metabolism. *ACS Medicinal Chemistry Letters*, **2010**, 1, 96-100	4.3	186
42	On the role of the axial ligand in heme proteins: a theoretical study. *Journal of Biological Inorganic Chemistry*, **2004**, 9, 203-23	3.7	161
41	Structures of the high-valent metal-ion haem-oxygen intermediates in peroxidases, oxygenases and catalases. *Journal of Inorganic Biochemistry*, **2006**, 100, 460-76	4.2	143
40	Prediction of activation energies for hydrogen abstraction by cytochrome p450. *Journal of Medicinal Chemistry*, **2006**, 49, 6489-99	8.3	107
39	The SMARTCyp cytochrome P450 metabolism prediction server. *Bioinformatics*, **2010**, 26, 2988-9	7.2	105
38	Sulfoxide, Sulfur, and Nitrogen Oxidation and Dealkylation by Cytochrome P450. *Journal of Chemical Theory and Computation*, **2008**, 4, 1369-77	6.4	73
37	RS-predictor: a new tool for predicting sites of cytochrome P450-mediated metabolism applied to CYP 3A4. *Journal of Chemical Information and Modeling*, **2011**, 51, 1667-89	6.1	69
36	RS-Predictor models augmented with SMARTCyp reactivities: robust metabolic regioselectivity predictions for nine CYP isozymes. *Journal of Chemical Information and Modeling*, **2012**, 52, 1637-59	6.1	63
35	General Transition-State Force Field for Cytochrome P450 Hydroxylation. *Journal of Chemical Theory and Computation*, **2007**, 3, 1765-73	6.4	49
34	Prediction of activation energies for aromatic oxidation by cytochrome P450. *Journal of Physical Chemistry A*, **2008**, 112, 13058-65	2.8	48
33	RS-WebPredictor: a server for predicting CYP-mediated sites of metabolism on drug-like molecules. *Bioinformatics*, **2013**, 29, 497-8	7.2	45
32	Fast prediction of cytochrome P450 mediated drug metabolism. *ChemMedChem*, **2009**, 4, 2070-9	3.7	45
31	WhichCyp: prediction of cytochromes P450 inhibition. *Bioinformatics*, **2013**, 29, 2051-2	7.2	44
30	Predicting drug metabolism by cytochrome P450 2C9: comparison with the 2D6 and 3A4 isoforms. *ChemMedChem*, **2012**, 7, 1202-9	3.7	43
29	The accuracy of geometries for iron porphyrin complexes from density functional theory. *Journal of Physical Chemistry A*, **2009**, 113, 11949-53	2.8	43
28	FAst MEtabolizer (FAME): A rapid and accurate predictor of sites of metabolism in multiple species by endogenous enzymes. *Journal of Chemical Information and Modeling*, **2013**, 53, 2896-907	6.1	41
27	Ligand-Based Site of Metabolism Prediction for Cytochrome P450 2D6. *ACS Medicinal Chemistry Letters*, **2012**, 3, 69-73	4.3	40

26	Binding affinities in the SAMPL3 trypsin and host-guest blind tests estimated with the MM/PBSA and LIE methods. *Journal of Computer-Aided Molecular Design*, **2012**, 26, 527-41	4.2	40
25	Dynamics of water molecules in the active-site cavity of human cytochromes P450. *Journal of Physical Chemistry B*, **2007**, 111, 5445-57	3.4	39
24	The contribution of atom accessibility to site of metabolism models for cytochromes P450. *Molecular Pharmaceutics*, **2013**, 10, 1216-23	5.6	31
23	Protonation of the proximal histidine ligand in heme peroxidases. *Journal of Physical Chemistry B*, **2008**, 112, 2501-10	3.4	27
22	Do Two Different Reaction Mechanisms Contribute to the Hydroxylation of Primary Amines by Cytochrome P450?. *Journal of Chemical Theory and Computation*, **2011**, 7, 3399-404	6.4	25
21	Quantum Mechanics/Molecular Mechanics Modeling of Drug Metabolism: Mexiletine N-Hydroxylation by Cytochrome P450 1A2. *Chemical Research in Toxicology*, **2016**, 29, 963-71	4	25
20	Transition-State Docking of Flunitrazepam and Progesterone in Cytochrome P450. *Journal of Chemical Theory and Computation*, **2008**, 4, 673-81	6.4	24
19	Trends in predicted chemoselectivity of cytochrome P450 oxidation: B3LYP barrier heights for epoxidation and hydroxylation reactions. *Journal of Molecular Graphics and Modelling*, **2014**, 52, 30-5	2.8	22
18	Structural model and trans-interaction of the entire ectodomain of the olfactory cell adhesion molecule. *Structure*, **2011**, 19, 203-11	5.2	22
17	Nitrogen inversion barriers affect the N-oxidation of tertiary alkylamines by cytochromes P450. *Angewandte Chemie - International Edition*, **2013**, 52, 993-7	16.4	21
16	Mechanism of the N-hydroxylation of primary and secondary amines by cytochrome P450. *Chemical Research in Toxicology*, **2015**, 28, 597-603	4	21
15	Use of density functional theory in drug metabolism studies. *Expert Opinion on Drug Metabolism and Toxicology*, **2014**, 10, 215-27	5.5	19
14	Application of Q2MM to Stereoselective Reactions. *Current Organic Chemistry*, **2010**, 14, 1629-1645	1.7	17
13	Implicit versus explicit solvent in free energy calculations of enzyme catalysis: Methyl transfer catalyzed by catechol O-methyltransferase. *Journal of Chemical Physics*, **2006**, 124, 174503	3.9	17
12	A comparative reactivity study of microperoxidases based on hemin, mesohemin and deuterohemin. *Journal of Inorganic Biochemistry*, **2005**, 99, 852-63	4.2	15
11	Theoretical Study of the Cytochrome P450 Mediated Metabolism of Phosphorodithioate Pesticides. *Journal of Chemical Theory and Computation*, **2012**, 8, 2706-12	6.4	10
10	Branched nanotrees with immobilized acetylcholine esterase for nanobiosensor applications. *Nanotechnology*, **2010**, 21, 055102	3.4	9
9	Density functional theory study on the formation of reactive benzoquinone imines by hydrogen abstraction. *Journal of Chemical Information and Modeling*, **2015**, 55, 660-6	6.1	8

8	XMetDB: an open access database for xenobiotic metabolism. *Journal of Cheminformatics*, **2016**, 8, 47	8.6	5
7	Prediction of cytochrome p450 mediated metabolism of designer drugs. *Current Topics in Medicinal Chemistry*, **2014**, 14, 1365-73	3	5
6	Nitrogen Inversion Barriers Affect the N-Oxidation of Tertiary Alkylamines by Cytochromes P450. *Angewandte Chemie*, **2013**, 125, 1027-1031	3.6	3
5	Enrichment of True Positives from Structural Alerts Through the Use of Novel Atomic Fragment Based Descriptors. *Molecular Informatics*, **2013**, 32, 81-6	3.8	3
4	Reactivity-Based Approaches and Machine Learning Methods for Predicting the Sites of Cytochrome P450-Mediated Metabolism. *Methods and Principles in Medicinal Chemistry*, **2014**, 265-292	0.4	2
3	Comment on "binding free energies of inhibitors to iron porphyrin complex as a model for cytochrome P450". *Biopolymers*, **2012**, 97, 250-1	2.2	1
2	Fast Prediction of Cytochrome P450 Mediated Drug Metabolism. *ChemMedChem*, **2009**, 4, 1965-1965	3.7	
1	A Comparison of Tetrapyrrole Cofactors in Nature and their Tuning by Axial Ligands27-56		