

# Patrik Rydberg

## List of Publications by Year in Descending Order

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**Version:** 2024-04-28

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	XMetDB: an open access database for xenobiotic metabolism. <i>Journal of Cheminformatics</i> , <b>2016</b> , 8, 47	8.6	5
42	Quantum Mechanics/Molecular Mechanics Modeling of Drug Metabolism: Mexiletine N-Hydroxylation by Cytochrome P450 1A2. <i>Chemical Research in Toxicology</i> , <b>2016</b> , 29, 963-71	4	25
41	Mechanism of the N-hydroxylation of primary and secondary amines by cytochrome P450. <i>Chemical Research in Toxicology</i> , <b>2015</b> , 28, 597-603	4	21
40	Density functional theory study on the formation of reactive benzoquinone imines by hydrogen abstraction. <i>Journal of Chemical Information and Modeling</i> , <b>2015</b> , 55, 660-6	6.1	8
39	Trends in predicted chemoselectivity of cytochrome P450 oxidation: B3LYP barrier heights for epoxidation and hydroxylation reactions. <i>Journal of Molecular Graphics and Modelling</i> , <b>2014</b> , 52, 30-5	2.8	22
38	Use of density functional theory in drug metabolism studies. <i>Expert Opinion on Drug Metabolism and Toxicology</i> , <b>2014</b> , 10, 215-27	5.5	19
37	Reactivity-Based Approaches and Machine Learning Methods for Predicting the Sites of Cytochrome P450-Mediated Metabolism. <i>Methods and Principles in Medicinal Chemistry</i> , <b>2014</b> , 265-292	0.4	2
36	Prediction of cytochrome p450 mediated metabolism of designer drugs. <i>Current Topics in Medicinal Chemistry</i> , <b>2014</b> , 14, 1365-73	3	5
35	WhichCyp: prediction of cytochromes P450 inhibition. <i>Bioinformatics</i> , <b>2013</b> , 29, 2051-2	7.2	44
34	RS-WebPredictor: a server for predicting CYP-mediated sites of metabolism on drug-like molecules. <i>Bioinformatics</i> , <b>2013</b> , 29, 497-8	7.2	45
33	Nitrogen Inversion Barriers Affect the N-Oxidation of Tertiary Alkylamines by Cytochromes P450. <i>Angewandte Chemie</i> , <b>2013</b> , 125, 1027-1031	3.6	3
32	Nitrogen inversion barriers affect the N-oxidation of tertiary alkylamines by cytochromes P450. <i>Angewandte Chemie - International Edition</i> , <b>2013</b> , 52, 993-7	16.4	21
31	Enrichment of True Positives from Structural Alerts Through the Use of Novel Atomic Fragment Based Descriptors. <i>Molecular Informatics</i> , <b>2013</b> , 32, 81-6	3.8	3
30	The contribution of atom accessibility to site of metabolism models for cytochromes P450. <i>Molecular Pharmaceutics</i> , <b>2013</b> , 10, 1216-23	5.6	31
29	FAst MEtabolizer (FAME): A rapid and accurate predictor of sites of metabolism in multiple species by endogenous enzymes. <i>Journal of Chemical Information and Modeling</i> , <b>2013</b> , 53, 2896-907	6.1	41
28	Comment on "binding free energies of inhibitors to iron porphyrin complex as a model for cytochrome P450". <i>Biopolymers</i> , <b>2012</b> , 97, 250-1	2.2	1
27	Ligand-Based Site of Metabolism Prediction for Cytochrome P450 2D6. <i>ACS Medicinal Chemistry Letters</i> , <b>2012</b> , 3, 69-73	4.3	40

26	RS-Predictor models augmented with SMARTCyp reactivities: robust metabolic regioselectivity predictions for nine CYP isozymes. <i>Journal of Chemical Information and Modeling</i> , <b>2012</b> , 52, 1637-59	6.1	63
25	Theoretical Study of the Cytochrome P450 Mediated Metabolism of Phosphorodithioate Pesticides. <i>Journal of Chemical Theory and Computation</i> , <b>2012</b> , 8, 2706-12	6.4	10
24	Predicting drug metabolism by cytochrome P450 2C9: comparison with the 2D6 and 3A4 isoforms. <i>ChemMedChem</i> , <b>2012</b> , 7, 1202-9	3.7	43
23	Binding affinities in the SAMPL3 trypsin and host-guest blind tests estimated with the MM/PBSA and LIE methods. <i>Journal of Computer-Aided Molecular Design</i> , <b>2012</b> , 26, 527-41	4.2	40
22	RS-predictor: a new tool for predicting sites of cytochrome P450-mediated metabolism applied to CYP 3A4. <i>Journal of Chemical Information and Modeling</i> , <b>2011</b> , 51, 1667-89	6.1	69
21	Structural model and trans-interaction of the entire ectodomain of the olfactory cell adhesion molecule. <i>Structure</i> , <b>2011</b> , 19, 203-11	5.2	22
20	Do Two Different Reaction Mechanisms Contribute to the Hydroxylation of Primary Amines by Cytochrome P450?. <i>Journal of Chemical Theory and Computation</i> , <b>2011</b> , 7, 3399-404	6.4	25
19	Branched nanotrees with immobilized acetylcholine esterase for nanobiosensor applications. <i>Nanotechnology</i> , <b>2010</b> , 21, 055102	3.4	9
18	The SMARTCyp cytochrome P450 metabolism prediction server. <i>Bioinformatics</i> , <b>2010</b> , 26, 2988-9	7.2	105
17	SMARTCyp: A 2D Method for Prediction of Cytochrome P450-Mediated Drug Metabolism. <i>ACS Medicinal Chemistry Letters</i> , <b>2010</b> , 1, 96-100	4.3	186
16	Application of Q2MM to Stereoselective Reactions. <i>Current Organic Chemistry</i> , <b>2010</b> , 14, 1629-1645	1.7	17
15	Fast prediction of cytochrome P450 mediated drug metabolism. <i>ChemMedChem</i> , <b>2009</b> , 4, 2070-9	3.7	45
14	Fast Prediction of Cytochrome P450 Mediated Drug Metabolism. <i>ChemMedChem</i> , <b>2009</b> , 4, 1965-1965	3.7	
13	The accuracy of geometries for iron porphyrin complexes from density functional theory. <i>Journal of Physical Chemistry A</i> , <b>2009</b> , 113, 11949-53	2.8	43
12	Sulfoxide, Sulfur, and Nitrogen Oxidation and Dealkylation by Cytochrome P450. <i>Journal of Chemical Theory and Computation</i> , <b>2008</b> , 4, 1369-77	6.4	73
11	Prediction of activation energies for aromatic oxidation by cytochrome P450. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 13058-65	2.8	48
10	Transition-State Docking of Flunitrazepam and Progesterone in Cytochrome P450. <i>Journal of Chemical Theory and Computation</i> , <b>2008</b> , 4, 673-81	6.4	24
9	Protonation of the proximal histidine ligand in heme peroxidases. <i>Journal of Physical Chemistry B</i> , <b>2008</b> , 112, 2501-10	3.4	27

8	Dynamics of water molecules in the active-site cavity of human cytochromes P450. <i>Journal of Physical Chemistry B</i> , <b>2007</b> , 111, 5445-57	3.4	39
7	General Transition-State Force Field for Cytochrome P450 Hydroxylation. <i>Journal of Chemical Theory and Computation</i> , <b>2007</b> , 3, 1765-73	6.4	49
6	Structures of the high-valent metal-ion haem-oxygen intermediates in peroxidases, oxygenases and catalases. <i>Journal of Inorganic Biochemistry</i> , <b>2006</b> , 100, 460-76	4.2	143
5	Implicit versus explicit solvent in free energy calculations of enzyme catalysis: Methyl transfer catalyzed by catechol O-methyltransferase. <i>Journal of Chemical Physics</i> , <b>2006</b> , 124, 174503	3.9	17
4	Prediction of activation energies for hydrogen abstraction by cytochrome p450. <i>Journal of Medicinal Chemistry</i> , <b>2006</b> , 49, 6489-99	8.3	107
3	A comparative reactivity study of microperoxidases based on hemin, mesohemin and deuterohemin. <i>Journal of Inorganic Biochemistry</i> , <b>2005</b> , 99, 852-63	4.2	15
2	On the role of the axial ligand in heme proteins: a theoretical study. <i>Journal of Biological Inorganic Chemistry</i> , <b>2004</b> , 9, 203-23	3.7	161
1	A Comparison of Tetrapyrrole Cofactors in Nature and their Tuning by Axial Ligands 27-56		