

Marcel J De Groot

List of Publications by Year in descending order

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31
papers

2,179
citations

331670

21
h-index

454955

30
g-index

31
all docs

31
docs citations

31
times ranked

1911
citing authors

#	ARTICLE	IF	CITATIONS
1	Discovery of a novel binding pocket for CYP 2C9 inhibitors: crystallography, pharmacophore modelling and inhibitor SAR. <i>MedChemComm</i> , 2016, 7, 813-819.	3.4	6
2	Quantum Mechanics/Molecular Mechanics Modeling of Regioselectivity of Drug Metabolism in Cytochrome P450 2C9. <i>Journal of the American Chemical Society</i> , 2013, 135, 8001-8015.	13.7	110
3	In Silico Methods for Predicting Ligand Binding Determinants of Cytochromes P450. , 2012, , 615-652.		1
4	Understanding ion channels using computational approaches. <i>Future Medicinal Chemistry</i> , 2010, 2, 697-701.	2.3	1
5	Understanding CYP2D6 interactions. <i>Drug Discovery Today</i> , 2009, 14, 964-972.	6.4	31
6	Fluorescently Labeled Analogues of Dofetilide as High-Affinity Fluorescence Polarization Ligands for the Human Ether-a-go-go-Related Gene (hERG) Channel. <i>Journal of Medicinal Chemistry</i> , 2007, 50, 2931-2941.	6.4	41
7	Pharmacophoric Fingerprint Method (TOPP) for 3D-QSAR Modeling: Application to CYP2D6 Metabolic Stability. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 76-84.	5.4	31
8	The Discovery of Tropane-derived CCR5 Receptor Antagonists. <i>Chemical Biology and Drug Design</i> , 2006, 67, 305-308.	3.2	19
9	Designing better drugs: predicting cytochrome P450 metabolism. <i>Drug Discovery Today</i> , 2006, 11, 601-606.	6.4	112
10	The Discovery of CCR5 Receptor Antagonists for the Treatment of HIV Infection: Hit-to-Lead Studies. <i>ChemMedChem</i> , 2006, 1, 706-709.	3.2	33
11	Drug Binding Interactions in the Inner Cavity of hERG Channels: Molecular Insights from Structure-Activity Relationships of Clofilium and Ibutilide Analogs. <i>Molecular Pharmacology</i> , 2006, 69, 509-519.	2.3	84
12	Surface-Integral QSPR Models: Local Energy Properties. <i>Journal of Chemical Information and Modeling</i> , 2005, 45, 1053-1060.	5.4	14
13	Greater Than the Sum of Its Parts: Combining Models for Useful ADMET Prediction. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 1287-1291.	6.4	127
14	In Silico Methods for Predicting Ligand Binding Determinants of Cytochromes P450. <i>Current Topics in Medicinal Chemistry</i> , 2004, 4, 1803-1824.	2.1	67
15	Structural Determinants of HERG Channel Block by Clofilium and Ibutilide. <i>Molecular Pharmacology</i> , 2004, 66, 240-249.	2.3	161
16	New Molecular Descriptors Based on Local Properties at the Molecular Surface and a Boiling-Point Model Derived from Them. <i>Journal of Chemical Information and Computer Sciences</i> , 2004, 44, 658-668.	2.8	43
17	Development of a Combined Protein and Pharmacophore Model for Cytochrome P450 2C9. <i>Journal of Medicinal Chemistry</i> , 2002, 45, 1983-1993.	6.4	110
18	Pharmacophore modeling of cytochromes P450. <i>Advanced Drug Delivery Reviews</i> , 2002, 54, 367-383.	13.7	123

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19	Novel Approach To Predicting P450-Mediated Drug Metabolism:Â Development of a Combined Protein and Pharmacophore Model for CYP2D6. <i>Journal of Medicinal Chemistry</i> , 1999, 42, 1515-1524.	6.4	199
20	A Novel Approach to Predicting P450 Mediated Drug Metabolism. CYP2D6 Catalyzed N-Dealkylation Reactions and Qualitative Metabolite Predictions Using a Combined Protein and Pharmacophore Model for CYP2D6. <i>Journal of Medicinal Chemistry</i> , 1999, 42, 4062-4070.	6.4	172
21	Ab initio calculations on iron-porphyrin model systems for intermediates in the oxidative cycle of cytochrome P450s. <i>Journal of Computer-Aided Molecular Design</i> , 1998, 12, 183-193.	2.9	23
22	Oxidative N-Dealkylation of p-Cyclopropyl-N,N-dimethylaniline. A Substituent Effect on a Radical-Clock Reaction Rationalized by Ab Initio Calculations on Radical Cation Intermediates. <i>Journal of Organic Chemistry</i> , 1997, 62, 8227-8230.	3.2	31
23	4-Substituted 1-Chloro-2-nitrobenzenes:Â Structure-Activity Relationships and Extension of the Substrate Model of Rat Glutathione S-Transferase 4-4. <i>Chemical Research in Toxicology</i> , 1997, 10, 439-449.	3.3	9
24	A Refined Substrate Model for Human Cytochrome P450 2D6. <i>Chemical Research in Toxicology</i> , 1997, 10, 41-48.	3.3	71
25	Modeling the Active Sites of Cytochrome P450s and Glutathione S-Transferases, two of the Most Important Biotransformation Enzymes. <i>Drug Metabolism Reviews</i> , 1997, 29, 747-799.	3.6	33
26	A Three-Dimensional Protein Model for Human Cytochrome P450 2D6 Based on the Crystal Structures of P450 101, P450 102, and P450 108. <i>Chemical Research in Toxicology</i> , 1996, 9, 1079-1091.	3.3	97
27	Structure-Activity Relationships for the Glutathione Conjugation of 2-Substituted 1-Chloro-4-nitrobenzenes by Rat Glutathione S-Transferase 4-4. <i>Chemical Research in Toxicology</i> , 1996, 9, 527-534.	3.3	8
28	A Homology Model for Rat Mu Class Glutathione S-Transferase 4-4. <i>Chemical Research in Toxicology</i> , 1996, 9, 28-40.	3.3	16
29	A Quantum Chemical Explanation of the Antioxidant Activity of Flavonoids. <i>Chemical Research in Toxicology</i> , 1996, 9, 1305-1312.	3.3	378
30	Metabolite Predictions for Para-Substituted Anisoles Based on ab Initio Complete Active Space Self-Consistent Field Calculations. <i>Chemical Research in Toxicology</i> , 1995, 8, 437-443.	3.3	17
31	A Predictive Substrate Model for Rat Glutathione S-Transferase 4-4. <i>Chemical Research in Toxicology</i> , 1995, 8, 649-658.	3.3	11