Marcel J De Groot

List of Publications by Year in descending order

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Version: 2024-02-01

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	A Quantum Chemical Explanation of the Antioxidant Activity of Flavonoids. Chemical Research in Toxicology, 1996, 9, 1305-1312.	3.3	378
2	Novel Approach To Predicting P450-Mediated Drug Metabolism:Â Development of a Combined Protein and Pharmacophore Model for CYP2D6. Journal of Medicinal Chemistry, 1999, 42, 1515-1524.	6.4	199
3	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. Journal of Medicinal Chemistry, 1999, 42, 4062-4070.	6.4	172
4	Structural Determinants of HERG Channel Block by Clofilium and Ibutilide. Molecular Pharmacology, 2004, 66, 240-249.	2.3	161
5	Greater Than the Sum of Its Parts:Â Combining Models for Useful ADMET Prediction. Journal of Medicinal Chemistry, 2005, 48, 1287-1291.	6.4	127
6	Pharmacophore modeling of cytochromes P450. Advanced Drug Delivery Reviews, 2002, 54, 367-383.	13.7	123
7	Designing better drugs: predicting cytochrome P450 metabolism. Drug Discovery Today, 2006, 11, 601-606.	6.4	112
8	Development of a Combined Protein and Pharmacophore Model for Cytochrome P450 2C9. Journal of Medicinal Chemistry, 2002, 45, 1983-1993.	6.4	110
9	Quantum Mechanics/Molecular Mechanics Modeling of Regioselectivity of Drug Metabolism in Cytochrome P450 2C9. Journal of the American Chemical Society, 2013, 135, 8001-8015.	13.7	110
10	A Three-Dimensional Protein Model for Human Cytochrome P450 2D6 Based on the Crystal Structures of P450 101, P450 102, and P450 108. Chemical Research in Toxicology, 1996, 9, 1079-1091.	3.3	97
11	Drug Binding Interactions in the Inner Cavity of hERG Channels: Molecular Insights from Structure-Activity Relationships of Clofilium and Ibutilide Analogs. Molecular Pharmacology, 2006, 69, 509-519.	2.3	84
12	A Refined Substrate Model for Human Cytochrome P450 2D6. Chemical Research in Toxicology, 1997, 10, 41-48.	3.3	71
13	In Silico Methods for Predicting Ligand Binding Determinants of Cytochromes P450. Current Topics in Medicinal Chemistry, 2004, 4, 1803-1824.	2.1	67
14	New Molecular Descriptors Based on Local Properties at the Molecular Surface and a Boiling-Point Model Derived from Them. Journal of Chemical Information and Computer Sciences, 2004, 44, 658-668.	2.8	43
15	Fluorescently Labeled Analogues of Dofetilide as High-Affinity Fluorescence Polarization Ligands for the Human Ether-a-go-go-Related Gene (hERG) Channel. Journal of Medicinal Chemistry, 2007, 50, 2931-2941.	6.4	41
16	Modeling the Active Sites of Cytochrome P450s and GlutathioneS-Transferases, two of the Most Important Biotransformation Enzymes. Drug Metabolism Reviews, 1997, 29, 747-799.	3.6	33
17	The Discovery of CCR5 Receptor Antagonists for the Treatment of HIV Infection: Hit-to-Lead Studies. ChemMedChem, 2006, 1, 706-709.	3.2	33
18	Oxidative N-Dealkylation ofp-Cyclopropyl-N,N-dimethylaniline. A Substituent Effect on a Radical-Clock Reaction Rationalized by Ab Initio Calculations on Radical Cation Intermediates. Journal of Organic Chemistry, 1997, 62, 8227-8230.	3.2	31

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19	Pharmacophoric Fingerprint Method (TOPP) for 3D-QSAR Modeling:â€‰ Application to CYP2D6 Metabolic Stability. Journal of Chemical Information and Modeling, 2007, 47, 76-84.	5.4	31
20	Understanding CYP2D6 interactions. Drug Discovery Today, 2009, 14, 964-972.	6.4	31
21	Ab initio calculations on iron-porphyrin model systems for intermediates in the oxidative cycle of cytochrome P450s. Journal of Computer-Aided Molecular Design, 1998, 12, 183-193.	2.9	23
22	The Discovery of Tropane-derived CCR5 Receptor Antagonists. Chemical Biology and Drug Design, 2006, 67, 305-308.	3.2	19
23	Metabolite Predictions for Para-Substituted Anisoles Based on ab Initio Complete Active Space Self-Consistent Field Calculations. Chemical Research in Toxicology, 1995, 8, 437-443.	3.3	17
24	A Homology Model for Rat Mu Class Glutathione S-Transferase 4-4. Chemical Research in Toxicology, 1996, 9, 28-40.	3.3	16
25	Surface-Integral QSPR Models:Â Local Energy Properties. Journal of Chemical Information and Modeling, 2005, 45, 1053-1060.	5.4	14
26	A Predictive Substrate Model for Rat Glutathione S-Transferase 4-4. Chemical Research in Toxicology, 1995, 8, 649-658.	3.3	11
27	4-Substituted 1-Chloro-2-nitrobenzenes:Â Structureâ^'Activity Relationships and Extension of the Substrate Model of Rat GlutathioneS-Transferase 4-4. Chemical Research in Toxicology, 1997, 10, 439-449.	3.3	9
28	Structureâ^'Activity Relationships for the Glutathione Conjugation of 2-Substituted 1-Chloro-4-nitrobenzenes by Rat Glutathione S-Transferase 4-4. Chemical Research in Toxicology, 1996, 9, 527-534.	3.3	8
29	Discovery of a novel binding pocket for CYP 2C9 inhibitors: crystallography, pharmacophore modelling and inhibitor SAR. MedChemComm, 2016, 7, 813-819.	3.4	6
30	Understanding ion channels using computational approaches. Future Medicinal Chemistry, 2010, 2, 697-701.	2.3	1
31	In Silico Methods for Predicting Ligand Binding Determinants of Cytochromes P450. , 2012, , 615-652.		1