Gerhard F Ecker

List of Publications by Year in Descending Order

218 papers	5,958 citations	42 h-index	68 g-index
245 ext. papers	6,836 ext. citations	5.5 avg, IF	5.81 L-index

#	Paper	IF	Citations
218	CACHE (Critical Assessment of Computational Hit-finding Experiments): A public–private partnership benchmarking initiative to enable the development of computational methods for hit-finding. *Nature Reviews Chemistry*, **2022**, 6, 287-295	34.6	1
217	Off-targetP ML: an open source machine learning framework for off-target panel safety assessment of small molecules.. *Journal of Cheminformatics*, **2022**, 14, 27	8.6	
216	Acute effects of the imidacloprid metabolite desnitro-imidacloprid on human nACh receptors relevant for neuronal signaling. *Archives of Toxicology*, **2021**, 95, 3695-3716	5.8	3
215	Effects of Hydroxylated Mephedrone Metabolites on Monoamine Transporter Activity. *Frontiers in Pharmacology*, **2021**, 12, 654061	5.6	1
214	New approach methods (NAMs) supporting read-across: Two neurotoxicity AOP-based IATA case studies. *ALTEX: Alternatives To Animal Experimentation*, **2021**, 38, 615-635	4.3	2
213	Molecular Determinants and Pharmacological Analysis for a Class of Competitive Non-transported Bicyclic Inhibitors of the Betaine/GABA Transporter BGT1. *Frontiers in Chemistry*, **2021**, 9, 736457	5	0
212	A widespread role for SLC transmembrane transporters in resistance to cytotoxic drugs. *Nature Chemical Biology*, **2020**, 16, 469-478	11.7	42
211	COVER: conformational oversampling as data augmentation for molecules. *Journal of Cheminformatics*, **2020**, 12, 18	8.6	10
210	In silico toxicology: From structure–activity relationships towards deep learning and adverse outcome pathways. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2020**, 10, e1475	7.9	21
209	Using Machine Learning Methods and Structural Alerts for Prediction of Mitochondrial Toxicity. *Molecular Informatics*, **2020**, 39, e2000005	3.8	16
208	Image Based Liver Toxicity Prediction. *Journal of Chemical Information and Modeling*, **2020**, 60, 1111-1121	6.1	9
207	Pharmacological Characterization of a Betaine/GABA Transporter 1 (BGT1) Inhibitor Displaying an Unusual Biphasic Inhibition Profile and Anti-seizure Effects. *Neurochemical Research*, **2020**, 45, 1551-1565	4.6	2
206	Identification of mitochondrial toxicants by combined in silico and in vitro studies – A structure-based view on the adverse outcome pathway. *Computational Toxicology*, **2020**, 14, 100123	3.1	7
205	The RESOLUTE consortium: unlocking SLC transporters for drug discovery. *Nature Reviews Drug Discovery*, **2020**, 19, 429-430	64.1	28
204	Propafenone analogue with additional H-bond acceptor group shows increased inhibitory activity on P-glycoprotein. *Archiv Der Pharmazie*, **2020**, 353, e1900269	4.3	0
203	Exploring the molecular determinants for subtype-selectivity of 2-amino-1,4,5,6-tetrahydropyrimidine-5-carboxylic acid analogs as betaine/GABA transporter 1 (BGT1) substrate-inhibitors. *Scientific Reports*, **2020**, 10, 12992	4.9	2
202	ATP modulates SLC7A5 (LAT1) synergistically with cholesterol. *Scientific Reports*, **2020**, 10, 16738	4.9	11

201	A structure-kinetic relationship study using matched molecular pair analysis. *RSC Medicinal Chemistry*, **2020**, 11, 1285-1294	3.5	2
200	Studies of structural determinants of substrate binding in the Creatine Transporter (CreaT, SLC6A8) using molecular models. *Scientific Reports*, **2020**, 10, 6241	4.9	8
199	Structural and molecular aspects of betaine-GABA transporter 1 (BGT1) and its relation to brain function. *Neuropharmacology*, **2019**, 161, 107644	5.5	16
198	In Silico Approaches to Predict Drug-Transporter Interaction Profiles: Data Mining, Model Generation, and Link to Cholestasis. *Methods in Molecular Biology*, **2019**, 1981, 383-396	1.4	2
197	para-Trifluoromethyl-methcathinone is an allosteric modulator of the serotonin transporter. *Neuropharmacology*, **2019**, 161, 107615	5.5	11
196	Vienna LiverTox Workspace-A Set of Machine Learning Models for Prediction of Interactions Profiles of Small Molecules With Transporters Relevant for Regulatory Agencies. *Frontiers in Chemistry*, **2019**, 7, 899	5	8
195	A structural model of the human serotonin transporter in an outward-occluded state. *PLoS ONE*, **2019**, 14, e0217377	3.7	10
194	Rigorous sampling of docking poses unveils binding hypothesis for the halogenated ligands of L-type Amino acid Transporter 1 (LAT1). *Scientific Reports*, **2019**, 9, 15061	4.9	13
193	Structural Insight into the In Vitro Anti-Intravasative Properties of Flavonoids. *Scientia Pharmaceutica*, **2019**, 87, 23	4.3	7
192	Conformational Oversampling as Data Augmentation for Molecules. *Lecture Notes in Computer Science*, **2019**, 788-792	0.9	3
191	Predicting Residence Time and Drug Unbinding Pathway through Scaled Molecular Dynamics. *Journal of Chemical Information and Modeling*, **2019**, 59, 535-549	6.1	37
190	Comparing the performance of meta-classifiers-a case study on selected imbalanced data sets relevant for prediction of liver toxicity. *Journal of Computer-Aided Molecular Design*, **2018**, 32, 583-590	4.2	29
189	Translation Termination Factor GSPT1 Is a Phenotypically Relevant Off-Target of Heterobifunctional Phthalimide Degraders. *ACS Chemical Biology*, **2018**, 13, 553-560	4.9	78
188	Transporters in Hepatotoxicity **2018**, 145-174		
187	Predicting drug resistance related to ABC transporters using unsupervised Consensus Self-Organizing Maps. *Scientific Reports*, **2018**, 8, 6803	4.9	4
186	Ligand Desolvation Steers On-Rate and Impacts Drug Residence Time of Heat Shock Protein 90 (Hsp90) Inhibitors. *Journal of Medicinal Chemistry*, **2018**, 61, 4397-4411	8.3	23
185	GRAIL: GRids of phArmacophore Interaction fieLds. *Journal of Chemical Theory and Computation*, **2018**, 14, 4958-4970	6.4	12
184	Insights into the Structure, Function, and Ligand Discovery of the Large Neutral Amino Acid Transporter 1, LAT1. *International Journal of Molecular Sciences*, **2018**, 19,	6.3	60

183	SAR-Guided Scoring Function and Mutational Validation Reveal the Binding Mode of CGS-8216 at the 1+/2- Benzodiazepine Site. *Journal of Chemical Information and Modeling*, **2018**, 58, 1682-1696	6.1	3
182	Discovery of Potent Inhibitors for the Large Neutral Amino Acid Transporter 1 (LAT1) by Structure-Based Methods. *International Journal of Molecular Sciences*, **2018**, 20,	6.3	21
181	Linked Open Data: Ligand-Transporter Interaction Profiling and Beyond. *Methods in Pharmacology and Toxicology*, **2018**, 405-417	1.1	
180	Interspecies comparison of putative ligand binding sites of human, rat and mouse P-glycoprotein. *European Journal of Pharmaceutical Sciences*, **2018**, 122, 134-143	5.1	12
179	Linking organic anion transporting polypeptide 1B1 and 1B3 (OATP1B1 and OATP1B3) interaction profiles to hepatotoxicity - The hyperbilirubinemia use case. *European Journal of Pharmaceutical Sciences*, **2017**, 100, 9-16	5.1	10
178	Organic Anion Transporting Polypeptides as Drug Targets. *Methods and Principles in Medicinal Chemistry*, **2017**, 271-324	0.4	5
177	Recent Advances in Structural Modeling of ABC Transporters. *Methods and Principles in Medicinal Chemistry*, **2017**, 167-178	0.4	
176	ABC Transporters: From Targets to Antitargets and Back. *Methods and Principles in Medicinal Chemistry*, **2017**, 107-118	0.4	1
175	Curated human hyperbilirubinemia data and the respective OATP1B1 and 1B3 inhibition predictions. *Data in Brief*, **2017**, 11, 204-207	1.2	2
174	Predicting Drug-Induced Cholestasis with the Help of Hepatic Transporters-An in Silico Modeling Approach. *Journal of Chemical Information and Modeling*, **2017**, 57, 608-615	6.1	26
173	Kinetics for Drug Discovery: an industry-driven effort to target drug residence time. *Drug Discovery Today*, **2017**, 22, 896-911	8.8	113
172	Structure based classification for bile salt export pump (BSEP) inhibitors using comparative structural modeling of human BSEP. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 507-521	4.2	13
171	Folding correction of ABC-transporter ABCB1 by pharmacological chaperones: a mechanistic concept. *Pharmacology Research and Perspectives*, **2017**, 5, e00325	3.1	5
170	Aminobutyric Acid and Glycine Neurotransmitter Transporters. *Methods and Principles in Medicinal Chemistry*, **2017**, 69-106	0.4	4
169	Structure-Activity Relationship, Pharmacological Characterization, and Molecular Modeling of Noncompetitive Inhibitors of the Betaine/Aminobutyric Acid Transporter 1 (BGT1). *Journal of Medicinal Chemistry*, **2017**, 60, 8834-8846	8.3	15
168	Legacy data sharing to improve drug safety assessment: the eTOX project. *Nature Reviews Drug Discovery*, **2017**, 16, 811-812	64.1	37
167	Adverse outcome pathways: opportunities, limitations and open questions. *Archives of Toxicology*, **2017**, 91, 3477-3505	5.8	174
166	Virtual Screening of DrugBank Reveals Two Drugs as New BCRP Inhibitors. *SLAS Discovery*, **2017**, 22, 86-93	3.4	16

165	Development of Non-GAT1-Selective Inhibitors: Challenges and Achievements. *Advances in Neurobiology*, **2017**, 16, 315-332	2.1	9
164	Predicting drug-induced liver injury: The importance of data curation. *Toxicology*, **2017**, 389, 139-145	4.4	38
163	Empowering pharmacoinformatics by linked life science data. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 319-328	4.2	1
162	Combined Simulation and Mutation Studies to Elucidate Selectivity of Unsubstituted Amphetamine-like Cathinones at the Dopamine Transporter. *Molecular Informatics*, **2017**, 36, 1600094	3.8	8
161	Subtle Structural Differences Trigger Inhibitory Activity of Propafenone Analogues at the Two Polyspecific ABC Transporters: P-Glycoprotein (P-gp) and Breast Cancer Resistance Protein (BCRP). *ChemMedChem*, **2016**, 11, 1380-94	3.7	13
160	11th German Conference on Chemoinformatics (GCC 2015) : Fulda, Germany. 8-10 November 2015. *Journal of Cheminformatics*, **2016**, 8, 18	8.6	
159	Selectivity profiling of BCRP versus P-gp inhibition: from automated collection of polypharmacology data to multi-label learning. *Journal of Cheminformatics*, **2016**, 8, 7	8.6	19
158	Flagging Drugs That Inhibit the Bile Salt Export Pump. *Molecular Pharmaceutics*, **2016**, 13, 163-71	5.6	20
157	Interaction of ABC Transporters with Drugs **2016**, 135-151		
156	Binding Mode Selection Determines the Action of Ecstasy Homologs at Monoamine Transporters. *Molecular Pharmacology*, **2016**, 89, 165-75	4.3	36
155	A heterocyclic compound CE-103 inhibits dopamine reuptake and modulates dopamine transporter and dopamine D1-D3 containing receptor complexes. *Neuropharmacology*, **2016**, 102, 186-96	5.5	12
154	Structural Studies of GABAA Receptor Binding Sites: Which Experimental Structure Tells us What?. *Frontiers in Molecular Neuroscience*, **2016**, 9, 44	6.1	57
153	From linked open data to molecular interaction: studying selectivity trends for ligands of the human serotonin and dopamine transporter. *MedChemComm*, **2016**, 7, 1819-1831	5	8
152	Experimental Data Guided Docking of Small Molecules into Homology Models of Neurotransmitter Transporters. *Neuromethods*, **2016**, 83-89	0.4	
151	Identification of the First Highly Subtype-Selective Inhibitor of Human GABA Transporter GAT3. *ACS Chemical Neuroscience*, **2015**, 6, 1591-9	5.7	31
150	A eudesmane-type sesquiterpene isolated from Pluchea odorata (L.) Cass. combats three hallmarks of cancer cells: Unrestricted proliferation, escape from apoptosis and early metastatic outgrowth in vitro. *Mutation Research - Fundamental and Molecular Mechanisms of Mutagenesis*, **2015**, 777, 79-90	3.3	5
149	Medicinal chemistry in the era of big data. *Drug Discovery Today: Technologies*, **2015**, 14, 37-41	7.1	19
148	The ABC of Phytohormone Translocation. *Planta Medica*, **2015**, 81, 474-87	3.1	14

147	Novel scaffolds for modulation of TRPV1 identified with pharmacophore modeling and virtual screening. *Future Medicinal Chemistry*, **2015**, 7, 243-56	4.1	14
146	Prediction of drug-ABC-transporter interaction--Recent advances and future challenges. *Advanced Drug Delivery Reviews*, **2015**, 86, 17-26	18.5	119
145	Structure activity relationship of selective GABA uptake inhibitors. *Bioorganic and Medicinal Chemistry*, **2015**, 23, 2480-8	3.4	23
144	Identification of Novel Inhibitors of Organic Anion Transporting Polypeptides 1B1 and 1B3 (OATP1B1 and OATP1B3) Using a Consensus Vote of Six Classification Models. *Molecular Pharmaceutics*, **2015**, 12, 4395-404	5.6	30
143	Second-generation mephedrone analogs, 4-MEC and 4-MePPP, differentially affect monoamine transporter function. *Neuropsychopharmacology*, **2015**, 40, 1321-31	8.7	74
142	Integrative Modeling Strategies for Predicting Drug Toxicities at the eTOX Project. *Molecular Informatics*, **2015**, 34, 477-84	3.8	17
141	Synthesis and in silico evaluation of novel compounds for PET-based investigations of the norepinephrine transporter. *Molecules*, **2015**, 20, 1712-30	4.8	6
140	Refinement of the Central Steps of Substrate Transport by the Aspartate Transporter GltPh: Elucidating the Role of the Na2 Sodium Binding Site. *PLoS Computational Biology*, **2015**, 11, e1004551	5	17
139	A binding mode hypothesis of tiagabine confirms liothyronine effect on γ-aminobutyric acid transporter 1 (GAT1). *Journal of Medicinal Chemistry*, **2015**, 58, 2149-58	8.3	23
138	Computational models for predicting the interaction with ABC transporters. *Drug Discovery Today: Technologies*, **2014**, 12, e69-77	7.1	12
137	Applicability Domain ANalysis (ADAN): a robust method for assessing the reliability of drug property predictions. *Journal of Chemical Information and Modeling*, **2014**, 54, 1500-11	6.1	46
136	Exploiting open data: a new era in pharmacoinformatics. *Future Medicinal Chemistry*, **2014**, 6, 503-14	4.1	16
135	Big data in pharmaceutical science: challenges and opportunities. *Future Medicinal Chemistry*, **2014**, 6, 857-64	4.1	6
134	Efficient modulation of γ-aminobutyric acid type A receptors by piperine derivatives. *Journal of Medicinal Chemistry*, **2014**, 57, 5602-19	8.3	47
133	A multivariate approach linking reported side effects of clinical antidepressant and antipsychotic trials to in vitro binding affinities. *European Neuropsychopharmacology*, **2014**, 24, 1463-74	1.2	13
132	Passive lipoidal diffusion and carrier-mediated cell uptake are both important mechanisms of membrane permeation in drug disposition. *Molecular Pharmaceutics*, **2014**, 11, 1727-38	5.6	87
131	Development of potential selective and reversible pyrazoline based MAO-B inhibitors as MAO-B PET tracer precursors and reference substances for the early detection of Alzheimer's disease. *Bioorganic and Medicinal Chemistry Letters*, **2014**, 24, 4490-4495	2.9	8
130	Aminorex, a metabolite of the cocaine adulterant levamisole, exerts amphetamine like actions at monoamine transporters. *Neurochemistry International*, **2014**, 73, 32-41	4.4	71

129	Synthesis, biological evaluation and 3D-QSAR studies of new chalcone derivatives as inhibitors of human P-glycoprotein. *Bioorganic and Medicinal Chemistry*, **2014**, 22, 2311-9	3.4	33
128	BCRP Inhibition: from Data Collection to Ligand-Based Modeling. *Molecular Informatics*, **2014**, 33, 322-31	3.8	19
127	Transporter taxonomy - a comparison of different transport protein classification schemes. *Drug Discovery Today: Technologies*, **2014**, 12, e37-46	7.1	6
126	The application of the open pharmacological concepts triple store (open PHACTS) to support drug discovery research. *PLoS ONE*, **2014**, 9, e115460	3.7	30
125	Pore-exposed tyrosine residues of P-glycoprotein are important hydrogen-bonding partners for drugs. *Molecular Pharmacology*, **2014**, 85, 420-8	4.3	24
124	Ligand and structure-based classification models for prediction of P-glycoprotein inhibitors. *Journal of Chemical Information and Modeling*, **2014**, 54, 218-29	6.1	81
123	Development of Refined Homology Models: Adding the Missing Information to the Medically Relevant Neurotransmitter Transporters. *Springer Series in Biophysics*, **2014**, 99-120		2
122	Lanthanide resonance energy transfer-based distance measurements in the mammalian glutamate transporter excitatory amino acid transporter 3 (1064.12). *FASEB Journal*, **2014**, 28, 1064.12	0.9	
121	2D- and 3D-QSAR studies of a series of benzopyranes and benzopyrano[3,4b][1,4]-oxazines as inhibitors of the multidrug transporter P-glycoprotein. *Journal of Computer-Aided Molecular Design*, **2013**, 27, 161-71	4.2	13
120	Classification of High-Activity Tiagabine Analogs by Binary QSAR Modeling. *Molecular Informatics*, **2013**, 32, 415-419	3.8	8
119	Experimental characterization of the human non-sequence-specific nucleic acid interactome. *Genome Biology*, **2013**, 14, R81	18.3	3
118	Identification of novel positive allosteric modulators and null modulators at the GABAA receptor ββinterface. *British Journal of Pharmacology*, **2013**, 169, 371-83	8.6	39
117	How Far Could We Go with Open Data - A Case Study for TRPV1 Antagonists. *Molecular Informatics*, **2013**, 32, 555-562	3.8	6
116	Scientific competency questions as the basis for semantically enriched open pharmacological space development. *Drug Discovery Today*, **2013**, 18, 843-52	8.8	40
115	Mutational analysis of the high-affinity zinc binding site validates a refined human dopamine transporter homology model. *PLoS Computational Biology*, **2013**, 9, e1002909	5	53
114	Amphetamine actions at the serotonin transporter rely on the availability of phosphatidylinositol-4,5-bisphosphate. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, 11642-7	11.5	48
113	How to solve the problems of docking into a symmetric binding site: the example of the HERG channel. *Scientia Pharmaceutica*, **2013**, 81, 677-82	4.3	1
112	Probing the Selectivity of Monoamine Transporter Substrates by Means of Molecular Modeling. *Molecular Informatics*, **2013**, 32, 409-413	3.8	12

111	Molecular analysis of the site for 2-arachidonylglycerol (2-AG) on the β subunit of GABA(A) receptors. *Journal of Neurochemistry*, **2013**, 126, 29-36	6	19
110	Evidence-based approach to assess passive diffusion and carrier-mediated drug transport. *Drug Discovery Today*, **2012**, 17, 905-12	8.8	91
109	Taking Open Innovation to the Molecular Level - Strengths and Limitations. *Molecular Informatics*, **2012**, 31, 528-535	3.8	8
108	An In Silico Classification Model for Putative ABCC2 Substrates. *Molecular Informatics*, **2012**, 31, 547-553	3.8	15
107	Annotating Human P-Glycoprotein Bioassay Data. *Molecular Informatics*, **2012**, 31, 599-609	3.8	27
106	Fingerprint-based in silico models for the prediction of P-glycoprotein substrates and inhibitors. *Bioorganic and Medicinal Chemistry*, **2012**, 20, 5388-95	3.4	55
105	Open PHACTS: semantic interoperability for drug discovery. *Drug Discovery Today*, **2012**, 17, 1188-98	8.8	229
104	Structure-activity relationships, ligand efficiency, and lipophilic efficiency profiles of benzophenone-type inhibitors of the multidrug transporter P-glycoprotein. *Journal of Medicinal Chemistry*, **2012**, 55, 3261-73	8.3	76
103	Diazepam-bound GABAA receptor models identify new benzodiazepine binding-site ligands. *Nature Chemical Biology*, **2012**, 8, 455-64	11.7	150
102	Modulation of GABAA-receptors by honokiol and derivatives: subtype selectivity and structure-activity relationship. *Journal of Medicinal Chemistry*, **2011**, 54, 5349-61	8.3	48
101	Probing the stereoselectivity of P-glycoprotein-synthesis, biological activity and ligand docking studies of a set of enantiopure benzopyrano[3,4-b][1,4]oxazines. *Chemical Communications*, **2011**, 47, 2586-8	5.8	16
100	Prediction of hERG Channel Inhibition Using In Silico Techniques **2011**, 191-239		1
99	Trapping and dissociation of propafenone derivatives in HERG channels. *British Journal of Pharmacology*, **2011**, 162, 1542-52	8.6	22
98	Insights into structure-activity relationship of GABAA receptor modulating coumarins and furanocoumarins. *European Journal of Pharmacology*, **2011**, 668, 57-64	5.3	32
97	Synthesis, spasmolytic activity and structure-activity relationship study of a series of polypharmacological thiobenzanilides. *European Journal of Pharmaceutical Sciences*, **2011**, 42, 37-44	5.1	12
96	Amphetamine actions rely on the availability of phosphatidylinositol-4,5-bisphosphate. *BMC Pharmacology*, **2011**, 11, A19		78
95	Self-Organizing Maps for In Silico Screening and Data Visualization. *Molecular Informatics*, **2011**, 30, 838-48	3.8	21
94	Use of shape similarities for the classification of P-glycoprotein substrates and nonsubstrates. *Future Medicinal Chemistry*, **2011**, 3, 1117-28	4.1	6

93	Molecular dissection of dual pseudosymmetric solute translocation pathways in human P-glycoprotein. *Molecular Pharmacology*, **2011**, 79, 443-52	4.3	42
92	Random mutagenesis of the prokaryotic peptide transporter YdgR identifies potential periplasmic gating residues. *Journal of Biological Chemistry*, **2011**, 286, 23121-31	5.4	10
91	Exhaustive sampling of docking poses reveals binding hypotheses for propafenone type inhibitors of P-glycoprotein. *PLoS Computational Biology*, **2011**, 7, e1002036	5	65
90	Coexistence of passive and carrier-mediated processes in drug transport. *Nature Reviews Drug Discovery*, **2010**, 9, 597-614	64.1	428
89	The high-affinity binding site for tricyclic antidepressants resides in the outer vestibule of the serotonin transporter. *Molecular Pharmacology*, **2010**, 78, 1026-35	4.3	64
88	Using structural and mechanistic information to design novel inhibitors/substrates of P-glycoprotein. *Current Topics in Medicinal Chemistry*, **2010**, 10, 1769-74	3	7
87	Cancer Drug Resistance: Targets and Therapies **2010**, 361-382		1
86	The N terminus of monoamine transporters is a lever required for the action of amphetamines. *Journal of Biological Chemistry*, **2010**, 285, 10924-38	5.4	106
85	The hERG potassium channel and drug trapping: insight from docking studies with propafenone derivatives. *ChemMedChem*, **2010**, 5, 436-42	3.7	18
84	Ensemble Rule-Based Classification of Substrates of the Human ABC-Transporter ABCB1 Using Simple Physicochemical Descriptors. *Molecular Informatics*, **2010**, 29, 233-42	3.8	15
83	Impact of the Recent Mouse P-Glycoprotein Structure for Structure-Based Ligand Design. *Molecular Informatics*, **2010**, 29, 276-86	3.8	19
82	Predicting ligand interactions with ABC transporters in ADME. *Chemistry and Biodiversity*, **2009**, 6, 1960-9	2.5	36
81	Similarity-based SIBAR descriptors for classification of chemically diverse hERG blockers. *Molecular Diversity*, **2009**, 13, 321-36	3.1	36
80	Comparison of Contemporary Feature Selection Algorithms: Application to the Classification of ABC-Transporter Substrates. *QSAR and Combinatorial Science*, **2009**, 28, 1087-1091		5
79	Similarity Based Descriptors Useful for Classification of Substrates of the Human Multidrug Transporter P-Glycoprotein?. *QSAR and Combinatorial Science*, **2009**, 28, 834-839		6
78	Data-driven homology modelling of P-glycoprotein in the ATP-bound state indicates flexibility of the transmembrane domains. *FEBS Journal*, **2009**, 276, 964-72	5.7	32
77	Synthesis and antitumor-evaluation of cyclopropyl-containing combretastatin analogs. *Bioorganic and Medicinal Chemistry Letters*, **2009**, 19, 6948-51	2.9	37
76	Inhibitory activity of prostaglandin E2 production by the synthetic 2Shydroxychalcone analogues: Synthesis and SAR study. *Bioorganic and Medicinal Chemistry Letters*, **2009**, 19, 1650-3	2.9	36

75	Transport at the Blood–Brain Barrier. *Methods and Principles in Medicinal Chemistry*, **2009**, 263-298	0.4	6
74	Syntheses and antigestagenic activity of mifepristone derivatives. *Journal of Medicinal Chemistry*, **2009**, 52, 1268-74	8.3	8
73	Drug Transporters in Health and Disease. *Methods and Principles in Medicinal Chemistry*, **2009**, 387-415	0.4	
72	Biological Membranes and Drug Transport. *Methods and Principles in Medicinal Chemistry*, **2009**, 229-262	0.4	
71	Membrane Transporters in Pleiotropic Drug Resistance and Stress Response in Yeast and Fungal Pathogens. *Methods and Principles in Medicinal Chemistry*, **2009**, 159-193	0.4	
70	Organic Anion Transporting Polypeptides (Oatps/OATPs). *Methods and Principles in Medicinal Chemistry*, **2009**, 81-112	0.4	
69	QSAR Studies on ABC Transporter – How to Deal with Polyspecificity. *Methods and Principles in Medicinal Chemistry*, **2009**, 195-214	0.4	
68	CNS - Transporters as Drug Targets. *Methods and Principles in Medicinal Chemistry*, **2009**, 113-117	0.4	
67	Interplay of Drug Metabolizing Enzymes and ABC Transporter. *Methods and Principles in Medicinal Chemistry*, **2009**, 325-347	0.4	
66	Bile Canalicular Transporters. *Methods and Principles in Medicinal Chemistry*, **2009**, 299-324	0.4	
65	A Systems Biology View of Drug Transporters. *Methods and Principles in Medicinal Chemistry*, **2009**, 363-385	0.4	
64	The ABC Transporters: Structural Insights into Drug Transport. *Methods and Principles in Medicinal Chemistry*, **2009**, 1-48	0.4	2
63	ABC Transporters – From Targets to Antitargets?. *Methods and Principles in Medicinal Chemistry*, **2009**, 349-362	0.4	2
62	Biochemistry, Physiology, and Pharmacology of Nucleoside and Nucleobase Transporters. *Methods and Principles in Medicinal Chemistry*, **2009**, 49-80	0.4	1
61	Bacterial Multidrug Transporters: Molecular and Clinical Aspects. *Methods and Principles in Medicinal Chemistry*, **2009**, 119-157	0.4	4
60	Drug Transporter Pharmacophores. *Methods and Principles in Medicinal Chemistry*, **2009**, 215-227	0.4	5
59	Computational models for prediction of interactions with ABC-transporters. *Drug Discovery Today*, **2008**, 13, 311-7	8.8	65
58	In silico prediction of substrate properties for ABC-multidrug transporters. *Expert Opinion on Drug Metabolism and Toxicology*, **2008**, 4, 1167-80	5.5	42

57	Predictive QSAR Models for Polyspecific Drug Targets: The Importance of Feature Selection. *Current Computer-Aided Drug Design*, **2008**, 4, 91-110	1.4	18
56	The Similarity Principle □New Trends and Applications in Ligand-Based Drug Discovery and ADMET Profiling. *Scientia Pharmaceutica*, **2008**, 76, 5-18	4.3	3
55	Hydrophobic moments as physicochemical descriptors in structure-activity relationship studies of P-glycoprotein inhibitors. *Monatshefte F□ Chemie*, **2008**, 139, 401-405	1.4	7
54	A binary QSAR model for classification of hERG potassium channel blockers. *Bioorganic and Medicinal Chemistry*, **2008**, 16, 4107-19	3.4	75
53	Classification models for HERG inhibitors by counter-propagation neural networks. *Chemical Biology and Drug Design*, **2008**, 72, 279-89	2.9	25
52	Multispecificity of drug transporters: probing inhibitor selectivity for the human drug efflux transporters ABCB1 and ABCG2. *ChemMedChem*, **2007**, 2, 1783-8	3.7	39
51	Similarity-Based Descriptors (SIBAR) as Tool for QSAR Studies on P-Glycoprotein Inhibitors: Influence of the Reference Set. *QSAR and Combinatorial Science*, **2007**, 26, 669-678		9
50	Characterization of a novel class of antimalarials and its applicability to plasmodial target identification. *Wiener Klinische Wochenschrift*, **2007**, 119, 83-7	2.3	1
49	Predictive models for HERG channel blockers: ligand-based and structure-based approaches. *Current Medicinal Chemistry*, **2007**, 14, 3003-26	4.3	40
48	Self-organizing maps for identification of new inhibitors of P-glycoprotein. *Journal of Medicinal Chemistry*, **2007**, 50, 1698-702	8.3	47
47	Role of transmembrane domain/transmembrane domain interfaces of P-glycoprotein (ABCB1) in solute transport. Convergent information from photoaffinity labeling, site directed mutagenesis and in silico importance prediction. *Current Medicinal Chemistry*, **2006**, 13, 793-805	4.3	13
46	A novel flow based hollow-fiber blood-brain barrier in vitro model with immortalised cell line PBMEC/C1-2. *Journal of Biotechnology*, **2006**, 125, 127-41	3.7	68
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