Gerhard F Ecker

List of Publications by Citations

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	Coexistence of passive and carrier-mediated processes in drug transport. *Nature Reviews Drug Discovery*, **2010**, 9, 597-614	64.1	428
217	Resveratrol analogues as selective cyclooxygenase-2 inhibitors: synthesis and structure-activity relationship. *Bioorganic and Medicinal Chemistry*, **2004**, 12, 5571-8	3.4	239
216	Open PHACTS: semantic interoperability for drug discovery. *Drug Discovery Today*, **2012**, 17, 1188-98	8.8	229
215	Adverse outcome pathways: opportunities, limitations and open questions. *Archives of Toxicology*, **2017**, 91, 3477-3505	5.8	174
214	Diazepam-bound GABAA receptor models identify new benzodiazepine binding-site ligands. *Nature Chemical Biology*, **2012**, 8, 455-64	11.7	150
213	Prediction of drug-ABC-transporter interaction--Recent advances and future challenges. *Advanced Drug Delivery Reviews*, **2015**, 86, 17-26	18.5	119
212	P-glycoprotein substrate binding domains are located at the transmembrane domain/transmembrane domain interfaces: a combined photoaffinity labeling-protein homology modeling approach. *Molecular Pharmacology*, **2005**, 67, 365-74	4.3	114
211	Kinetics for Drug Discovery: an industry-driven effort to target drug residence time. *Drug Discovery Today*, **2017**, 22, 896-911	8.8	113
210	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
209	Evidence-based approach to assess passive diffusion and carrier-mediated drug transport. *Drug Discovery Today*, **2012**, 17, 905-12	8.8	91
208	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
207	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
206	Reversal of antifungal resistance mediated by ABC efflux pumps from Candida albicans functionally expressed in yeast. *International Journal of Antimicrobial Agents*, **2003**, 22, 291-300	14.3	80
205	Translation Termination Factor GSPT1 Is a Phenotypically Relevant Off-Target of Heterobifunctional Phthalimide Degraders. *ACS Chemical Biology*, **2018**, 13, 553-560	4.9	78
204	Amphetamine actions rely on the availability of phosphatidylinositol-4,5-bisphosphate. *BMC Pharmacology*, **2011**, 11, A19		78
203	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
202	A binary QSAR model for classification of hERG potassium channel blockers. *Bioorganic and Medicinal Chemistry*, **2008**, 16, 4107-19	3.4	75

201	Structure-activity relationship studies of propafenone analogs based on P-glycoprotein ATPase activity measurements. *Biochemical Pharmacology*, **1999**, 58, 1447-56	6	75
200	Second-generationSmephedrone analogs, 4-MEC and 4-MePPP, differentially affect monoamine transporter function. *Neuropsychopharmacology*, **2015**, 40, 1321-31	8.7	74
199	Substituted 4-acylpyrazoles and 4-acylpyrazolones: synthesis and multidrug resistance-modulating activity. *Journal of Medicinal Chemistry*, **1998**, 41, 4001-11	8.3	74
198	Aminorex, a metabolite of the cocaine adulterant levamisole, exerts amphetamine like actions at monoamine transporters. *Neurochemistry International*, **2014**, 73, 32-41	4.4	71
197	In silico prediction models for blood-brain barrier permeation. *Current Medicinal Chemistry*, **2004**, 11, 1617-28	4.3	70
196	Synthesis and in vitro multidrug resistance modulating activity of a series of dihydrobenzopyrans and tetrahydroquinolines. *Journal of Medicinal Chemistry*, **1999**, 42, 1921-6	8.3	70
195	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
194	Exhaustive sampling of docking poses reveals binding hypotheses for propafenone type inhibitors of P-glycoprotein. *PLoS Computational Biology*, **2011**, 7, e1002036	5	65
193	Computational models for prediction of interactions with ABC-transporters. *Drug Discovery Today*, **2008**, 13, 311-7	8.8	65
192	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
191	Structure-activity relationship studies on benzofuran analogs of propafenone-type modulators of tumor cell multidrug resistance. *Journal of Medicinal Chemistry*, **1996**, 39, 4767-74	8.3	63
190	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
189	Structural Studies of GABAA Receptor Binding Sites: Which Experimental Structure Tells us What?. *Frontiers in Molecular Neuroscience*, **2016**, 9, 44	6.1	57
188	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
187	Lead identification for modulators of multidrug resistance based on in silico screening with a pharmacophoric feature model. *Archiv Der Pharmazie*, **2004**, 337, 317-27	4.3	55
186	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
185	Synthesis, pharmacologic activity, and structure-activity relationships of a series of propafenone-related modulators of multidrug resistance. *Journal of Medicinal Chemistry*, **1995**, 38, 2789-93	8.3	52
184	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

183	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
182	Efficient modulation of □aminobutyric acid type A receptors by piperine derivatives. *Journal of Medicinal Chemistry*, **2014**, 57, 5602-19	8.3	47
181	Self-organizing maps for identification of new inhibitors of P-glycoprotein. *Journal of Medicinal Chemistry*, **2007**, 50, 1698-702	8.3	47
180	Identification of ligand-binding regions of P-glycoprotein by activated-pharmacophore photoaffinity labeling and matrix-assisted laser desorption/ionization-time-of-flight mass spectrometry. *Molecular Pharmacology*, **2002**, 61, 637-48	4.3	47
179	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
178	A widespread role for SLC transmembrane transporters in resistance to cytotoxic drugs. *Nature Chemical Biology*, **2020**, 16, 469-478	11.7	42
177	Molecular dissection of dual pseudosymmetric solute translocation pathways in human P-glycoprotein. *Molecular Pharmacology*, **2011**, 79, 443-52	4.3	42
176	In silico prediction of substrate properties for ABC-multidrug transporters. *Expert Opinion on Drug Metabolism and Toxicology*, **2008**, 4, 1167-80	5.5	42
175	Scientific competency questions as the basis for semantically enriched open pharmacological space development. *Drug Discovery Today*, **2013**, 18, 843-52	8.8	40
174	Predictive models for HERG channel blockers: ligand-based and structure-based approaches. *Current Medicinal Chemistry*, **2007**, 14, 3003-26	4.3	40
173	Identification of novel positive allosteric modulators and null modulators at the GABAA receptor □□interface. *British Journal of Pharmacology*, **2013**, 169, 371-83	8.6	39
172	Multispecificity of drug transporters: probing inhibitor selectivity for the human drug efflux transporters ABCB1 and ABCG2. *ChemMedChem*, **2007**, 2, 1783-8	3.7	39
171	Predicting drug-induced liver injury: The importance of data curation. *Toxicology*, **2017**, 389, 139-145	4.4	38
170	A combined Hansch/Free-Wilson approach as predictive tool in QSAR studies on propafenone-type modulators of multidrug resistance. *Archiv Der Pharmazie*, **1998**, 331, 233-40	4.3	38
169	Legacy data sharing to improve drug safety assessment: the eTOX project. *Nature Reviews Drug Discovery*, **2017**, 16, 811-812	64.1	37
168	Synthesis and antitumor-evaluation of cyclopropyl-containing combretastatin analogs. *Bioorganic and Medicinal Chemistry Letters*, **2009**, 19, 6948-51	2.9	37
167	Predicting Residence Time and Drug Unbinding Pathway through Scaled Molecular Dynamics. *Journal of Chemical Information and Modeling*, **2019**, 59, 535-549	6.1	37
166	Binding Mode Selection Determines the Action of Ecstasy Homologs at Monoamine Transporters. *Molecular Pharmacology*, **2016**, 89, 165-75	4.3	36

165	Predicting ligand interactions with ABC transporters in ADME. *Chemistry and Biodiversity*, **2009**, 6, 1960-9	2.5	36
164	Similarity-based SIBAR descriptors for classification of chemically diverse hERG blockers. *Molecular Diversity*, **2009**, 13, 321-36	3.1	36
163	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
162	Inhibitors of p-glycoprotein--lead identification and optimisation. *Mini-Reviews in Medicinal Chemistry*, **2005**, 5, 153-63	3.2	35
161	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
160	Insights into structure-activity relationship of GABAA receptor modulating coumarins and furanocoumarins. *European Journal of Pharmacology*, **2011**, 668, 57-64	5.3	32
159	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
158	Identification of the First Highly Subtype-Selective Inhibitor of Human GABA Transporter GAT3. *ACS Chemical Neuroscience*, **2015**, 6, 1591-9	5.7	31
157	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
156	The application of the open pharmacological concepts triple store (open PHACTS) to support drug discovery research. *PLoS ONE*, **2014**, 9, e115460	3.7	30
155	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
154	Prediction of the aroma quality and the threshold values of some pyrazines using artificial neural networks. *Journal of Medicinal Chemistry*, **2001**, 44, 2805-13	8.3	29
153	The RESOLUTE consortium: unlocking SLC transporters for drug discovery. *Nature Reviews Drug Discovery*, **2020**, 19, 429-430	64.1	28
152	Annotating Human P-Glycoprotein Bioassay Data. *Molecular Informatics*, **2012**, 31, 599-609	3.8	27
151	Similarity based SAR (SIBAR) as tool for early ADME profiling. *Journal of Computer-Aided Molecular Design*, **2002**, 16, 785-93	4.2	27
150	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
149	Classification models for HERG inhibitors by counter-propagation neural networks. *Chemical Biology and Drug Design*, **2008**, 72, 279-89	2.9	25
148	Pore-exposed tyrosine residues of P-glycoprotein are important hydrogen-bonding partners for drugs. *Molecular Pharmacology*, **2014**, 85, 420-8	4.3	24

147	A three-dimensional model for the substrate binding domain of the multidrug ATP binding cassette transporter LmrA. *Molecular Pharmacology*, **2004**, 66, 1169-79	4.3	24
146	Structure activity relationship of selective GABA uptake inhibitors. *Bioorganic and Medicinal Chemistry*, **2015**, 23, 2480-8	3.4	23
145	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
144	A binding mode hypothesis of tiagabine confirms liothyronine effect on □aminobutyric acid transporter 1 (GAT1). *Journal of Medicinal Chemistry*, **2015**, 58, 2149-58	8.3	23
143	Trapping and dissociation of propafenone derivatives in HERG channels. *British Journal of Pharmacology*, **2011**, 162, 1542-52	8.6	22
142	Development of an in vitro blood-brain barrier model based on immortalized porcine brain microvascular endothelial cells. *Il Farmaco*, **2004**, 59, 133-7		22
141	Topological distance based 3D descriptors for use in QSAR and diversity analysis. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 200-9		22
140	In silico toxicology: From structure□ctivity relationships towards deep learning and adverse outcome pathways. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2020**, 10, e1475	7.9	21
139	Self-Organizing Maps for In Silico Screening and Data Visualization. *Molecular Informatics*, **2011**, 30, 838-46	3.8	21
138	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
137	Flagging Drugs That Inhibit the Bile Salt Export Pump. *Molecular Pharmaceutics*, **2016**, 13, 163-71	5.6	20
136	Medicinal chemistry in the era of big data. *Drug Discovery Today: Technologies*, **2015**, 14, 37-41	7.1	19
135	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
134	BCRP Inhibition: from Data Collection to Ligand-Based Modeling. *Molecular Informatics*, **2014**, 33, 322-31	3.8	19
133	Molecular analysis of the site for 2-arachidonylglycerol (2-AG) on the □subunit of GABA(A) receptors. *Journal of Neurochemistry*, **2013**, 126, 29-36	6	19
132	Impact of the Recent Mouse P-Glycoprotein Structure for Structure-Based Ligand Design. *Molecular Informatics*, **2010**, 29, 276-86	3.8	19
131	The hERG potassium channel and drug trapping: insight from docking studies with propafenone derivatives. *ChemMedChem*, **2010**, 5, 436-42	3.7	18
130	Predictive QSAR Models for Polyspecific Drug Targets: The Importance of Feature Selection. *Current Computer-Aided Drug Design*, **2008**, 4, 91-110	1.4	18

129	Integrative Modeling Strategies for Predicting Drug Toxicities at the eTOX Project. *Molecular Informatics*, **2015**, 34, 477-84	3.8	17
128	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
127	Structural and molecular aspects of betaine-GABA transporter 1 (BGT1) and its relation to brain function. *Neuropharmacology*, **2019**, 161, 107644	5.5	16
126	Using Machine Learning Methods and Structural Alerts for Prediction of Mitochondrial Toxicity. *Molecular Informatics*, **2020**, 39, e2000005	3.8	16
125	Virtual Screening of DrugBank Reveals Two Drugs as New BCRP Inhibitors. *SLAS Discovery*, **2017**, 22, 86-93	3.4	16
124	Exploiting open data: a new era in pharmacoinformatics. *Future Medicinal Chemistry*, **2014**, 6, 503-14	4.1	16
123	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
122	MCASE study of the multidrug resistance reversal activity of propafenone analogs. *Journal of Computer-Aided Molecular Design*, **2003**, 17, 291-7	4.2	16
121	Structure-Activity Relationship, Pharmacological Characterization, and Molecular Modeling of Noncompetitive Inhibitors of the Betaine/γ-Aminobutyric Acid Transporter 1 (BGT1). *Journal of Medicinal Chemistry*, **2017**, 60, 8834-8846	8.3	15
120	An In Silico Classification Model for Putative ABCC2 Substrates. *Molecular Informatics*, **2012**, 31, 547-553	3.8	15
119	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
118	Studies on propafenone-type modulators of multidrug-resistance IV1): synthesis and pharmacological activity of 5-hydroxy and 5-benzyloxy derivatives. *Archiv Der Pharmazie*, **1997**, 330, 343-7	4.3	15
117	Homology model of the multidrug transporter LmrA from Lactococcus lactis. *Bioorganic and Medicinal Chemistry Letters*, **2004**, 14, 5823-6	2.9	15
116	The ABC of Phytohormone Translocation. *Planta Medica*, **2015**, 81, 474-87	3.1	14
115	Novel scaffolds for modulation of TRPV1 identified with pharmacophore modeling and virtual screening. *Future Medicinal Chemistry*, **2015**, 7, 243-56	4.1	14
114	Studies on Propafenone-type Modulators of Multidrug Resistance III: Variations on the Nitrogen. *QSAR and Combinatorial Science*, **1997**, 16, 361-366		14
113	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
112	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

111	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
110	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
109	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
108	Recent developments in overcoming tumour cell multi-drug resistance. *Expert Opinion on Therapeutic Patents*, **1997**, 7, 589-599	6.8	13
107	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
106	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
105	GRAIL: GRids of phArmacophore Interaction fieLds. *Journal of Chemical Theory and Computation*, **2018**, 14, 4958-4970	6.4	12
104	Computational models for predicting the interaction with ABC transporters. *Drug Discovery Today: Technologies*, **2014**, 12, e69-77	7.1	12
103	Probing the Selectivity of Monoamine Transporter Substrates by Means of Molecular Modeling. *Molecular Informatics*, **2013**, 32, 409-413	3.8	12
102	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
101	In silico screening with benzofurane- and benzopyrane-type MDR-modulators. *Il Farmaco*, **2003**, 58, 185-91		12
100	Improved synthesis and pharmacologic activity of the enantiomers of a new benzofurane type antiarrhythmic compound. *Chirality*, **1994**, 6, 329-36	2.1	12
99	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
98	para-Trifluoromethyl-methcathinone is an allosteric modulator of the serotonin transporter. *Neuropharmacology*, **2019**, 161, 107615	5.5	11
97	Insights into phenylalanine derivatives recognition of VLA-4 integrin: from a pharmacophoric study to 3D-QSAR and molecular docking analyses. *Journal of Chemical Information and Computer Sciences* , **2004**, 44, 1829-39		11
96	ATP modulates SLC7A5 (LAT1) synergistically with cholesterol. *Scientific Reports*, **2020**, 10, 16738	4.9	11
95	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
94	COVER: conformational oversampling as data augmentation for molecules. *Journal of Cheminformatics*, **2020**, 12, 18	8.6	10

93	A structural model of the human serotonin transporter in an outward-occluded state. *PLoS ONE*, **2019**, 14, e0217377	3.7	10
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	Synthesis and pharmacological activity of the stereoisomers of GP-88, a propafenone-type modulator of multidrug resistance. *Bioorganic and Medicinal Chemistry Letters*, **1998**, 8, 829-32	2.9	10
90	Intramolecular distribution of hydrophobicity influences pharmacological activity of propafenone-type MDR modulators. *Archiv Der Pharmazie*, **2004**, 337, 328-34	4.3	10
89	Inhibitors of ABC-type drug efflux pumps: an overview of the current patent situation. *Expert Opinion on Therapeutic Patents*, **2004**, 14, 499-508	6.8	10
88	Image Based Liver Toxicity Prediction. *Journal of Chemical Information and Modeling*, **2020**, 60, 1111-1121	6.1	9
87	Development of Non-GAT1-Selective Inhibitors: Challenges and Achievements. *Advances in Neurobiology*, **2017**, 16, 315-332	2.1	9
86	Estimation of the chemosensitizing activity of modulators of multi-drug resistance via combined simultaneous analysis of sigmoidal dose-response curves. *Journal of Pharmacy and Pharmacology*, **1997**, 49, 305-9	4.8	9
85	Studies on propafenone-type modulators of multidrug resistance VI. Synthesis and pharmacological activity of compounds with varied spacer length between the central aromatic ring and the nitrogen atom. *Il Farmaco*, **1998**, 53, 357-364		9
84	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
83	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
82	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
81	Classification of High-Activity Tiagabine Analogs by Binary QSAR Modeling. *Molecular Informatics*, **2013**, 32, 415-419	3.8	8
80	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
79	Taking Open Innovation to the Molecular Level - Strengths and Limitations. *Molecular Informatics*, **2012**, 31, 528-535	3.8	8
78	Syntheses and antigestagenic activity of mifepristone derivatives. *Journal of Medicinal Chemistry*, **2009**, 52, 1268-74	8.3	8
77	Similarity-based descriptors (SIBAR)--a tool for safe exchange of chemical information?. *Journal of Computer-Aided Molecular Design*, **2005**, 19, 687-92	4.2	8
76	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

75	Studies of structural determinants of substrate binding in the Creatine Transporter (CreaT, SLC6A8) using molecular models. *Scientific Reports*, **2020**, 10, 6241	4.9	8
74	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
73	Structural Insight into the In Vitro Anti-Intravasative Properties of Flavonoids. *Scientia Pharmaceutica*, **2019**, 87, 23	4.3	7
72	Using structural and mechanistic information to design novel inhibitors/substrates of P-glycoprotein. *Current Topics in Medicinal Chemistry*, **2010**, 10, 1769-74	3	7
71	Hydrophobic moments as physicochemical descriptors in structure-activity relationship studies of P-glycoprotein inhibitors. *Monatshefte F Chemie*, **2008**, 139, 401-405	1.4	7
70	Ein Verfahren zur Synthese der Enantiomere von Propafenon. *Archiv Der Pharmazie*, **1994**, 327, 691-695	4.3	7
69	Big data in pharmaceutical science: challenges and opportunities. *Future Medicinal Chemistry*, **2014**, 6, 857-64	4.1	6
68	Transporter taxonomy - a comparison of different transport protein classification schemes. *Drug Discovery Today: Technologies*, **2014**, 12, e37-46	7.1	6
67	Synthesis and in silico evaluation of novel compounds for PET-based investigations of the norepinephrine transporter. *Molecules*, **2015**, 20, 1712-30	4.8	6
66	How Far Could We Go with Open Data - A Case Study for TRPV1 Antagonists. *Molecular Informatics*, **2013**, 32, 555-562	3.8	6
65	Similarity Based Descriptors Useful for Classification of Substrates of the Human Multidrug Transporter P-Glycoprotein?. *QSAR and Combinatorial Science*, **2009**, 28, 834-839		6
64	Transport at the Blood Brain Barrier. *Methods and Principles in Medicinal Chemistry*, **2009**, 263-298	0.4	6
63	Use of shape similarities for the classification of P-glycoprotein substrates and nonsubstrates. *Future Medicinal Chemistry*, **2011**, 3, 1117-28	4.1	6
62	Organic Anion Transporting Polypeptides as Drug Targets. *Methods and Principles in Medicinal Chemistry*, **2017**, 271-324	0.4	5
61	Folding correction of ABC-transporter ABCB1 by pharmacological chaperones: a mechanistic concept. *Pharmacology Research and Perspectives*, **2017**, 5, e00325	3.1	5
60	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
59	Comparison of Contemporary Feature Selection Algorithms: Application to the Classification of ABC-Transporter Substrates. *QSAR and Combinatorial Science*, **2009**, 28, 1087-1091		5
58	A subset of highly effective propafenone-type multidrug resistance modulators lacks effects on cardiac action potential and mechanical twitch parameters of rat papillary muscles. *Journal of Pharmacology and Experimental Therapeutics*, **2003**, 307, 589-96	4.7	5

57	Drug Transporter Pharmacophores. *Methods and Principles in Medicinal Chemistry*, **2009**, 215-227	0.4	5
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55	Predicting drug resistance related to ABC transporters using unsupervised Consensus Self-Organizing Maps. *Scientific Reports*, **2018**, 8, 6803	4.9	4
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53	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
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