Gerhard F Ecker

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/9196830/publications.pdf

Version: 2024-02-01

213 papers	7,536 citations	53660 45 h-index	71532 76 g-index
245 all docs	245 docs citations	245 times ranked	9158 citing authors

#	Article	IF	Citations
1	Coexistence of passive and carrier-mediated processes in drug transport. Nature Reviews Drug Discovery, 2010, 9, 597-614.	21.5	526
2	Adverse outcome pathways: opportunities, limitations and open questions. Archives of Toxicology, 2017, 91, 3477-3505.	1.9	282
3	Open PHACTS: semantic interoperability for drug discovery. Drug Discovery Today, 2012, 17, 1188-1198.	3.2	274
4	Resveratrol analogues as selective cyclooxygenase-2 inhibitors: synthesis and structureâ€“activity relationship. Bioorganic and Medicinal Chemistry, 2004, 12, 5571-5578.	1.4	262
5	Diazepam-bound GABAA receptor models identify new benzodiazepine binding-site ligands. Nature Chemical Biology, 2012, 8, 455-464.	3.9	175
6	Prediction of drugâ€“ABC-transporter interaction â€” Recent advances and future challenges. Advanced Drug Delivery Reviews, 2015, 86, 17-26.	6.6	169
7	Kinetics for Drug Discovery: an industry-driven effort to target drug residence time. Drug Discovery Today, 2017, 22, 896-911.	3.2	165
8	Translation Termination Factor GSPT1 Is a Phenotypically Relevant Off-Target of Heterobifunctional Phthalimide Degraders. ACS Chemical Biology, 2018, 13, 553-560.	1.6	128
9	Evidence-based approach to assess passive diffusion and carrier-mediated drug transport. Drug Discovery Today, 2012, 17, 905-912.	3.2	125
10	The N Terminus of Monoamine Transporters Is a Lever Required for the Action of Amphetamines. Journal of Biological Chemistry, 2010, 285, 10924-10938.	1.6	123
11	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, 365-374.	1.0	122
12	Passive Lipoidal Diffusion and Carrier-Mediated Cell Uptake Are Both Important Mechanisms of Membrane Permeation in Drug Disposition. Molecular Pharmaceutics, 2014, 11, 1727-1738.	2.3	106
13	Insights into the Structure, Function, and Ligand Discovery of the Large Neutral Amino Acid Transporter 1, LAT1. International Journal of Molecular Sciences, 2018, 19, 1278.	1.8	102
14	Structureâ€“Activity Relationships, Ligand Efficiency, and Lipophilic Efficiency Profiles of Benzophenone-Type Inhibitors of the Multidrug Transporter P-Glycoprotein. Journal of Medicinal Chemistry, 2012, 55, 3261-3273.	2.9	99
15	Ligand and Structure-Based Classification Models for Prediction of P-Glycoprotein Inhibitors. Journal of Chemical Information and Modeling, 2014, 54, 218-229.	2.5	95
16	Aminorex, a metabolite of the cocaine adulterant levamisole, exerts amphetamine like actions at monoamine transporters. Neurochemistry International, 2014, 73, 32-41.	1.9	95
17	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.	1.1	89
18	A binary QSAR model for classification of hERG potassium channel blockers. Bioorganic and Medicinal Chemistry, 2008, 16, 4107-4119.	1.4	87

#	Article	IF	Citations
19	â€˜Second-Generationâ€™ Mephedrone Analogs, 4-MEC and 4-MePPP, Differentially Affect Monoamine Transporter Function. Neuropsychopharmacology, 2015, 40, 1321-1331.	2.8	86
20	A widespread role for SLC transmembrane transporters in resistance to cytotoxic drugs. Nature Chemical Biology, 2020, 16, 469-478.	3.9	84
21	Substituted 4-Acylpyrazoles and 4-Acylpyrazolones:â€‰ Synthesis and Multidrug Resistance-Modulating Activity. Journal of Medicinal Chemistry, 1998, 41, 4001-4011.	2.9	83
22	Structureâ€“activity relationship studies of propafenone analogs based on P-glycoprotein ATPase activity measurements. Biochemical Pharmacology, 1999, 58, 1447-1456.	2.0	81
23	In Silico Prediction Models for Blood-Brain Barrier Permeation. Current Medicinal Chemistry, 2004, 11, 1617-1528.	1.2	81
24	In silico toxicology: From structureâ€“activity relationships towards deep learning and adverse outcome pathways. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1475.	6.2	80
25	Predicting drug-induced liver injury: The importance of data curation. Toxicology, 2017, 389, 139-145.	2.0	78
26	A novel flow based hollow-fiber bloodâ€“brain barrier in vitro model with immortalised cell line PBMEC/C1â€“2. Journal of Biotechnology, 2006, 125, 127-141.	1.9	77
27	Structural Studies of GABAA Receptor Binding Sites: Which Experimental Structure Tells us What?. Frontiers in Molecular Neuroscience, 2016, 9, 44.	1.4	76
28	Synthesis and in Vitro Multidrug Resistance Modulating Activity of a Series of Dihydrobenzopyrans and Tetrahydroquinolinesâ€. Journal of Medicinal Chemistry, 1999, 42, 1921-1926.	2.9	73
29	Computational models for prediction of interactions with ABC-transporters. Drug Discovery Today, 2008, 13, 311-317.	3.2	73
30	The High-Affinity Binding Site for Tricyclic Antidepressants Resides in the Outer Vestibule of the Serotonin Transporter. Molecular Pharmacology, 2010, 78, 1026-1035.	1.0	71
31	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, 11642-11647.	3.3	71
32	Fingerprint-based in silico models for the prediction of P-glycoprotein substrates and inhibitors. Bioorganic and Medicinal Chemistry, 2012, 20, 5388-5395.	1.4	70
33	Structureâ^'Activity Relationship Studies on Benzofuran Analogs of Propafenone-Type Modulators of Tumor Cell Multidrug Resistance. Journal of Medicinal Chemistry, 1996, 39, 4767-4774.	2.9	67
34	Exhaustive Sampling of Docking Poses Reveals Binding Hypotheses for Propafenone Type Inhibitors of P-Glycoprotein. PLoS Computational Biology, 2011, 7, e1002036.	1.5	67
35	Predicting Residence Time and Drug Unbinding Pathway through Scaled Molecular Dynamics. Journal of Chemical Information and Modeling, 2019, 59, 535-549.	2.5	64
36	Lead Identification for Modulators of Multidrug Resistance based onin silico Screening with a Pharmacophoric Feature Model. Archiv Der Pharmazie, 2004, 337, 317-327.	2.1	61

#	Article	IF	Citations
37	Modulation of GABA_A-Receptors by Honokiol and Derivatives: Subtype Selectivity and Structureâ€“Activity Relationship. Journal of Medicinal Chemistry, 2011, 54, 5349-5361.	2.9	61
38	Synthesis, Pharmacologic Activity, and Structure-Activity Relationships of a Series of Propafenone-Related Modulators of Multidrug Resistance. Journal of Medicinal Chemistry, 1995, 38, 2789-2793.	2.9	60
39	Mutational Analysis of the High-Affinity Zinc Binding Site Validates a Refined Human Dopamine Transporter Homology Model. PLoS Computational Biology, 2013, 9, e1002909.	1.5	60
40	Legacy data sharing to improve drug safety assessment: the eTOX project. Nature Reviews Drug Discovery, 2017, 16, 811-812.	21.5	56
41	Self-Organizing Maps for Identification of New Inhibitors of P-Glycoprotein. Journal of Medicinal Chemistry, 2007, 50, 1698-1702.	2.9	55
42	Efficient Modulation of Î³-Aminobutyric Acid Type A Receptors by Piperine Derivatives. Journal of Medicinal Chemistry, 2014, 57, 5602-5619.	2.9	54
43	Identification of Ligand-Binding Regions of P-Glycoprotein by Activated-Pharmacophore Photoaffinity Labeling and Matrix-Assisted Laser Desorption/Ionizationâ€“Time-of-Flight Mass Spectrometry. Molecular Pharmacology, 2002, 61, 637-648.	1.0	53
44	Binding Mode Selection Determines the Action of Ecstasy Homologs at Monoamine Transporters. Molecular Pharmacology, 2016, 89, 165-175.	1.0	53
45	The RESOLUTE consortium: unlocking SLC transporters for drug discovery. Nature Reviews Drug Discovery, 2020, 19, 429-430.	21.5	53
46	Applicability Domain Analysis (ADAN): A Robust Method for Assessing the Reliability of Drug Property Predictions. Journal of Chemical Information and Modeling, 2014, 54, 1500-1511.	2.5	51
47	Molecular Dissection of Dual Pseudosymmetric Solute Translocation Pathways in Human P-Glycoprotein. Molecular Pharmacology, 2011, 79, 443-452.	1.0	48
48	Identification of novel positive allosteric modulators and null modulators at the <scp>GABA_A</scp> receptor Î±+Î²â˜ interface. British Journal of Pharmacology, 2013, 169, 371-383.	2.7	47
49	In silicoprediction of substrate properties for ABC-multidrug transporters. Expert Opinion on Drug Metabolism and Toxicology, 2008, 4, 1167-1180.	1.5	44
50	Scientific competency questions as the basis for semantically enriched open pharmacological space development. Drug Discovery Today, 2013, 18, 843-852.	3.2	44
51	A Binding Mode Hypothesis of Tiagabine Confirms Liothyronine Effect on Î³-Aminobutyric Acid Transporter 1 (GAT1). Journal of Medicinal Chemistry, 2015, 58, 2149-2158.	2.9	44
52	Predicting Ligand Interactions with ABC Transporters in ADME. Chemistry and Biodiversity, 2009, 6, 1960-1969.	1.0	43
53	Insights into structureâ€“activity relationship of GABAA receptor modulating coumarins and furanocoumarins. European Journal of Pharmacology, 2011, 668, 57-64.	1.7	43
54	Predictive Models for hERG Channel Blockers: Ligand-Based and Structure-Based Approaches. Current Medicinal Chemistry, 2007, 14, 3003-3026.	1.2	42

#	Article	IF	Citations
55	A Combined Hansch/Free-Wilson Approach as Predictive Tool in QSAR Studies on Propafenone-Type Modulators of Multidrug Resistance. Archiv Der Pharmazie, 1998, 331, 233-240.	2.1	41
56	Multispecificity of Drug Transporters: Probing Inhibitor Selectivity for the Human Drug Efflux Transporters ABCB1 and ABCG2. ChemMedChem, 2007, 2, 1783-1788.	1.6	41
57	Inhibitory activity of prostaglandin E2 production by the synthetic 2â€²-hydroxychalcone analogues: Synthesis and SAR study. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 1650-1653.	1.0	40
58	Predicting Drug-Induced Cholestasis with the Help of Hepatic Transportersâ€"An in Silico Modeling Approach. Journal of Chemical Information and Modeling, 2017, 57, 608-615.	2.5	40
59	Inhibitors of P-Glycoprotein - Lead Identification and Optimisation. Mini-Reviews in Medicinal Chemistry, 2005, 5, 153-163.	1.1	39
60	Similarity-based SIBAR descriptors for classification of chemically diverse hERG blockers. Molecular Diversity, 2009, 13, 321-336.	2.1	39
61	Synthesis and antitumor-evaluation of cyclopropyl-containing combretastatin analogs. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 6948-6951.	1.0	38
62	Synthesis, biological evaluation and 3D-QSAR studies of new chalcone derivatives as inhibitors of human P-glycoprotein. Bioorganic and Medicinal Chemistry, 2014, 22, 2311-2319.	1.4	38
63	Comparing the performance of meta-classifiersâ€"a case study on selected imbalanced data sets relevant for prediction of liver toxicity. Journal of Computer-Aided Molecular Design, 2018, 32, 583-590.	1.3	38
64	Discovery of Potent Inhibitors for the Large Neutral Amino Acid Transporter 1 (LAT1) by Structure-Based Methods. International Journal of Molecular Sciences, 2019, 20, 27.	1.8	38
65	Dataâ€driven homology modelling of Pâ€glycoprotein in the ATPâ€bound state indicates flexibility of the transmembrane domains. FEBS Journal, 2009, 276, 964-972.	2.2	37
66	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.	2.9	37
67	Topological Distance Based 3D Descriptors for Use in QSAR and Diversity Analysis. Journal of Chemical Information and Computer Sciences, 2004, 44, 200-209.	2.8	36
68	Identification of Novel Inhibitors of Organic Anion Transporting Polypeptides 1B1 and 1B3 (OATP1B1 and) Tj ETQq0 0 0 rgBT /Overlock 4395-4404.	2.3	36
69	Using Machine Learning Methods and Structural Alerts for Prediction of Mitochondrial Toxicity. Molecular Informatics, 2020, 39, e2000005.	1.4	36
70	Identification of the First Highly Subtype-Selective Inhibitor of Human GABA Transporter GAT3. ACS Chemical Neuroscience, 2015, 6, 1591-1599.	1.7	33
71	Prediction of the Aroma Quality and the Threshold Values of Some Pyrazines Using Artificial Neural Networks. Journal of Medicinal Chemistry, 2001, 44, 2805-2813.	2.9	31
72	Similarity based SAR (SIBAR) as tool for early ADME profiling. Journal of Computer-Aided Molecular Design, 2002, 16, 785-793.	1.3	31

#	Article	IF	Citations
73	Classification Models for hERG Inhibitors by Counterâ€Propagation Neural Networks. Chemical Biology and Drug Design, 2008, 72, 279-289.	1.5	31
74	The Application of the Open Pharmacological Concepts Triple Store (Open PHACTS) to Support Drug Discovery Research. PLoS ONE, 2014, 9, e115460.	1.1	31
75	Annotating Human Pâ€Glycoprotein Bioassay Data. Molecular Informatics, 2012, 31, 599-609.	1.4	30
76	Pore-Exposed Tyrosine Residues of P-Glycoprotein Are Important Hydrogen-Bonding Partners for Drugs. Molecular Pharmacology, 2014, 85, 420-428.	1.0	30
77	Trapping and dissociation of propafenone derivatives in HERG channels. British Journal of Pharmacology, 2011, 162, 1542-1552.	2.7	29
78	Acute effects of the imidacloprid metabolite desnitro-imidacloprid on human nACh receptors relevant for neuronal signaling. Archives of Toxicology, 2021, 95, 3695-3716.	1.9	28
79	BCRP Inhibition: from Data Collection to Ligandâ€Based Modeling. Molecular Informatics, 2014, 33, 322-331.	1.4	27
80	Structure activity relationship of selective GABA uptake inhibitors. Bioorganic and Medicinal Chemistry, 2015, 23, 2480-2488.	1.4	27
81	Molecular analysis of the site for 2â€arachidonylglycerol (2â€<scp>AG</scp>) on the Î²₂ subunit of <scp>GABA_A</scp> receptors. Journal of Neurochemistry, 2013, 126, 29-36.	2.1	26
82	Selectivity profiling of BCRP versus P-gp inhibition: from automated collection of polypharmacology data to multi-label learning. Journal of Cheminformatics, 2016, 8, 7.	2.8	26
83	para-Trifluoromethyl-methcathinone is an allosteric modulator of the serotonin transporter. Neuropharmacology, 2019, 161, 107615.	2.0	26
84	Structural and molecular aspects of betaine-GABA transporter 1 (BGT1) and its relation to brain function. Neuropharmacology, 2019, 161, 107644.	2.0	25
85	A Three-Dimensional Model for the Substrate Binding Domain of the Multidrug ATP Binding Cassette Transporter LmrA. Molecular Pharmacology, 2004, 66, 1169-1179.	1.0	24
86	Medicinal chemistry in the era of big data. Drug Discovery Today: Technologies, 2015, 14, 37-41.	4.0	24
87	Flagging Drugs That Inhibit the Bile Salt Export Pump. Molecular Pharmaceutics, 2016, 13, 163-171.	2.3	24
88	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.	1.6	23
89	Development of an in vitro bloodâ€“brain barrier model based on immortalized porcine brain microvascular endothelial cells. Il Farmaco, 2004, 59, 133-137.	0.9	22
90	The hERG Potassium Channel and Drug Trapping: Insight from Docking Studies with Propafenone Derivatives. ChemMedChem, 2010, 5, 436-442.	1.6	22

#	Article	IF	Citations
91	Selfâ€Organizing Maps for In Silico Screening and Data Visualization. Molecular Informatics, 2011, 30, 838-846.	1.4	22
92	Virtual Screening of DrugBank Reveals Two Drugs as New BCRP Inhibitors. SLAS Discovery, 2017, 22, 86-93.	1.4	22
93	CACHE (Critical Assessment of Computational Hit-finding Experiments): A publicâ€“private partnership benchmarking initiative to enable the development of computational methods for hit-finding. Nature Reviews Chemistry, 2022, 6, 287-295.	13.8	22
94	Predictive QSAR Models for Polyspecific Drug Targets: The Importance of Feature Selection. Current Computer-Aided Drug Design, 2008, 4, 91-110.	0.8	21
95	Impact of the Recent Mouse Pâ€Glycoprotein Structure for Structureâ€Based Ligand Design. Molecular Informatics, 2010, 29, 276-286.	1.4	21
96	ATP modulates SLC7A5 (LAT1) synergistically with cholesterol. Scientific Reports, 2020, 10, 16738.	1.6	21
97	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.	1.3	20
98	COVER: conformational oversampling as data augmentation for molecules. Journal of Cheminformatics, 2020, 12, 18.	2.8	20
99	Probing the stereoselectivity of P-glycoproteinâ€”synthesis, biological activity and ligand docking studies of a set of enantiopure benzopyrano[3,4-b][1,4]oxazines. Chemical Communications, 2011, 47, 2586-2588.	2.2	18
100	An In Silico Classification Model for Putative ABCC2 Substrates. Molecular Informatics, 2012, 31, 547-553.	1.4	18
101	Exploiting open data: a new era in pharmacoinformatics. Future Medicinal Chemistry, 2014, 6, 503-514.	1.1	18
102	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.	1.5	18
103	The ABC of Phytohormone Translocation. Planta Medica, 2015, 81, 474-487.	0.7	18
104	MCASE study of the multidrug resistance reversal activity of propafenone analogs. Journal of Computer-Aided Molecular Design, 2003, 17, 291-297.	1.3	17
105	Ensemble Ruleâ€Based Classification of Substrates of the Human ABCâ€Transporter ABCB1 Using Simple Physicochemical Descriptors. Molecular Informatics, 2010, 29, 233-242.	1.4	17
106	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, 161-171.	1.3	17
107	Integrative Modeling Strategies for Predicting Drug Toxicities at the eTOX Project. Molecular Informatics, 2015, 34, 477-484.	1.4	17
108	A structural model of the human serotonin transporter in an outward-occluded state. PLoS ONE, 2019, 14, e0217377.	1.1	17

#	Article	IF	Citations
109	Evaluation of the Success of High-Throughput Physiologically Based Pharmacokinetic (HT-PBPK) Modeling Predictions to Inform Early Drug Discovery. Molecular Pharmaceutics, 2022, 19, 2203-2216.	2.3	17
110	Studies on Propafenone-type Modulators of Multidrug Resistance III: Variations on the Nitrogen. QSAR and Combinatorial Science, 1997, 16, 361-366.	1.4	16
111	Studies on Propafenone-type Modulators of Multidrug-Resistance IV: Synthesis and Pharmacological Activity of 5-Hydroxy and 5-Benzyloxy Derivatives. Archiv Der Pharmazie, 1997, 330, 343-347.	2.1	16
112	Homology model of the multidrug transporter LmrA from Lactococcus lactis. Bioorganic and Medicinal Chemistry Letters, 2004, 14, 5823-5826.	1.0	16
113	Synthesis, spasmolytic activity and structureâ€“activity relationship study of a series of polypharmacological thiobenzanilides. European Journal of Pharmaceutical Sciences, 2011, 42, 37-44.	1.9	16
114	A multivariate approach linking reported side effects of clinical antidepressant and antipsychotic trials to in vitro binding affinities. European Neuropsychopharmacology, 2014, 24, 1463-1474.	0.3	16
115	Novel scaffolds for modulation of TRPV1 identified with pharmacophore modeling and virtual screening. Future Medicinal Chemistry, 2015, 7, 243-256.	1.1	16
116	Structureâ€“Activity Relationship, Pharmacological Characterization, and Molecular Modeling of Noncompetitive Inhibitors of the Betaine/Î³-Aminobutyric Acid Transporter 1 (BGT1). Journal of Medicinal Chemistry, 2017, 60, 8834-8846.	2.9	16
117	Interspecies comparison of putative ligand binding sites of human, rat and mouse P-glycoprotein. European Journal of Pharmaceutical Sciences, 2018, 122, 134-143.	1.9	16
118	Vienna LiverTox Workspaceâ€”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.	1.8	16
119	Studies of structural determinants of substrate binding in the Creatine Transporter (CreaT, SLC6A8) using molecular models. Scientific Reports, 2020, 10, 6241.	1.6	16
120	GRAIL: GRids of phArmacophore Interaction fieLds. Journal of Chemical Theory and Computation, 2018, 14, 4958-4970.	2.3	15
121	Recent developments in overcoming tumour cell multi-drug resistance. Expert Opinion on Therapeutic Patents, 1997, 7, 589-599.	2.4	14
122	In silico screening with benzofurane- and benzopyrane-type MDR-modulators. Il Farmaco, 2003, 58, 185-191.	0.9	14
123	Insights into Phenylalanine Derivatives Recognition of VLA-4 Integrin:â€‰ From a Pharmacophoric Study to 3D-QSAR and Molecular Docking Analyses. Journal of Chemical Information and Computer Sciences, 2004, 44, 1829-1839.	2.8	14
124	Role of Transmembrane Domain/Transmembrane Domain Interfaces of PGlycoprotein (ABCB1) in Solute Transport. Convergent Information from Photoaffinity Labeling, Site Directed Mutagenesis and in Silico Importance Prediction. Current Medicinal Chemistry, 2006, 13, 793-805.	1.2	14
125	Computational models for predicting the interaction with ABC transporters. Drug Discovery Today: Technologies, 2014, 12, e69-e77.	4.0	14
126	Subtle Structural Differences Trigger Inhibitory Activity of Propafenone Analogues at the Two Polyspecific ABC Transporters: Pâ€Glycoprotein (Pâ€gp) and Breast Cancer Resistance Protein (BCRP). ChemMedChem, 2016, 11, 1380-1394.	1.6	14

#	Article	IF	Citations
127	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.	1.9	14
128	Image Based Liver Toxicity Prediction. Journal of Chemical Information and Modeling, 2020, 60, 1111-1121.	2.5	14
129	Improved synthesis and pharmacologic activity of the enantiomers of a new benzofurane type antiarrhythmic compound. Chirality, 1994, 6, 329-336.	1.3	13
130	Probing the Selectivity of Monoamine Transporter Substrates by Means of Molecular Modeling. Molecular Informatics, 2013, 32, 409-413.	1.4	13
131	A heterocyclic compound CE-103 inhibits dopamine reuptake and modulates dopamine transporter and dopamine D1-D3 containing receptor complexes. Neuropharmacology, 2016, 102, 186-196.	2.0	13
132	Identification of mitochondrial toxicants by combined in silico and in vitro studies â€“ A structure-based view on the adverse outcome pathway. Computational Toxicology, 2020, 14, 100123.	1.8	13
133	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.	0.9	12
134	Synthesis and pharmacological activity of the stereoisomers of GP-88, a propafenone-type modulator of multidrug resistance. Bioorganic and Medicinal Chemistry Letters, 1998, 8, 829-832.	1.0	12
135	Inhibitors of ABC-type drug efflux pumps: an overview of the current patent situation. Expert Opinion on Therapeutic Patents, 2004, 14, 499-508.	2.4	12
136	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.	1.5	12
137	Random Mutagenesis of the Prokaryotic Peptide Transporter YdgR Identifies Potential Periplasmic Gating Residues. Journal of Biological Chemistry, 2011, 286, 23121-23131.	1.6	11
138	Classification of Highâ€Activity Tiagabine Analogs by Binary QSAR Modeling. Molecular Informatics, 2013, 32, 415-419.	1.4	11
139	Development of Non-GAT1-Selective Inhibitors: Challenges and Achievements. Advances in Neurobiology, 2017, 16, 315-332.	1.3	11
140	Ein Verfahren zur Synthese der Enantiomere von Propafenon. Archiv Der Pharmazie, 1994, 327, 691-695.	2.1	10
141	Intramolecular Distribution of Hydrophobicity Influences Pharmacological Activity of Propafenone-type MDR Modulators. Archiv Der Pharmazie, 2004, 337, 328-334.	2.1	10
142	Structural Insight into the In Vitro Anti-Intravasative Properties of Flavonoids. Scientia Pharmaceutica, 2019, 87, 23.	0.7	10
143	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, 2011, 49, 305-309.	1.2	9
144	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 Alzheimerâ€™s disease. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 4490-4495.	1.0	9

#	Article	IF	Citations
145	From linked open data to molecular interaction: studying selectivity trends for ligands of the human serotonin and dopamine transporter. MedChemComm, 2016, 7, 1819-1831.	3.5	9
146	Combined Simulation and Mutation Studies to Elucidate Selectivity of Unsubstituted Amphetamineâ€like Cathinones at the Dopamine Transporter. Molecular Informatics, 2017, 36, 1600094.	1.4	9
147	A structureâ€“kinetic relationship study using matched molecular pair analysis. RSC Medicinal Chemistry, 2020, 11, 1285-1294.	1.7	9
148	New approach methods supporting read-across: Two neurotoxicity AOP-based IATA case studies. ALTEX: Alternatives To Animal Experimentation, 2021, 38, 615-635.	0.9	9
149	Effects of Hydroxylated Mephedrone Metabolites on Monoamine Transporter Activity in vitro. Frontiers in Pharmacology, 2021, 12, 654061.	1.6	9
150	Similarity-based descriptors (SIBAR) â€“ A tool for safe exchange of chemical information?. Journal of Computer-Aided Molecular Design, 2005, 19, 687-692.	1.3	8
151	Syntheses and Antigestagenic Activity of Mifepristone Derivatives. Journal of Medicinal Chemistry, 2009, 52, 1268-1274.	2.9	8
152	Using Structural and Mechanistic Information to Design Novel Inhibitors/Substrates of P-Glycoprotein. Current Topics in Medicinal Chemistry, 2010, 10, 1769-1774.	1.0	8
153	Taking Open Innovation to the Molecular Level â€•Strengths and Limitations. Molecular Informatics, 2012, 31, 528-535.	1.4	8
154	â€˜Big dataâ€™ in pharmaceutical science: challenges and opportunities. Future Medicinal Chemistry, 2014, 6, 857-864.	1.1	8
155	Hydrophobic moments as physicochemical descriptors in structure-activity relationship studies of P-glycoprotein inhibitors. Monatshefte FÃ¼r Chemie, 2008, 139, 401-405.	0.9	7
156	Experimental characterization of the human non-sequence-specific nucleic acid interactome. Genome Biology, 2013, 14, R81.	13.9	7
157	Transporter taxonomy â€“ a comparison of different transport protein classification schemes. Drug Discovery Today: Technologies, 2014, 12, e37-e46.	4.0	7
158	Predicting drug resistance related to ABC transporters using unsupervised Consensus Self-Organizing Maps. Scientific Reports, 2018, 8, 6803.	1.6	7
159	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.	0.4	7
160	Similarity Based Descriptors â€“ Useful for Classification of Substrates of the Human Multidrug Transporter Pâ€Glycoprotein?. QSAR and Combinatorial Science, 2009, 28, 834-839.	1.5	6
161	Use of shape similarities for the classification of P-glycoprotein substrates and nonsubstrates. Future Medicinal Chemistry, 2011, 3, 1117-1128.	1.1	6
162	How Far Could We Go with Open Data â€“ A Case Study for TRPV1 Antagonists. Molecular Informatics, 2013, 32, 555-562.	1.4	6

#	Article	IF	Citations
163	Synthesis and in Silico Evaluation of Novel Compounds for PET-Based Investigations of the Norepinephrine Transporter. Molecules, 2015, 20, 1712-1730.	1.7	6
164	Folding correction of ABCâ€transporter ABCB1 by pharmacological chaperones: a mechanistic concept. Pharmacology Research and Perspectives, 2017, 5, e00325.	1.1	6
165	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, 589-596.	1.3	5
166	The Similarity Principle â€“ New Trends and Applications in Ligand-Based Drug Discovery and ADMET Profiling. Scientia Pharmaceutica, 2008, 76, 5-18.	0.7	5
167	Comparison of Contemporary Feature Selection Algorithms: Application to the Classification of ABCâ€Transporter Substrates. QSAR and Combinatorial Science, 2009, 28, 1087-1091.	1.5	5
168	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.	0.4	5
169	SAR-Guided Scoring Function and Mutational Validation Reveal the Binding Mode of CGS-8216 at the Î±1+Í²2â€“ Benzodiazepine Site. Journal of Chemical Information and Modeling, 2018, 58, 1682-1696.	2.5	5
170	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.	1.6	5
171	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.	1.8	5
172	Off-targetP ML: an open source machine learning framework for off-target panel safety assessment of small molecules. Journal of Cheminformatics, 2022, 14, 27.	2.8	5
173	Patent focus on agents for tumour therapy: May - October 1999. Expert Opinion on Therapeutic Patents, 1999, 9, 1627-1639.	2.4	4
174	Synthesis and Multidrug-Resistance Modulating Activity of a Series of Thienothiazines. Archiv Der Pharmazie, 2002, 335, 223.	2.1	4
175	QSAR Studies on Drug Transporters Involved in Toxicology. , 0, , 295-314.		4
176	Curated human hyperbilirubinemia data and the respective OATP1B1 and 1B3 inhibition predictions. Data in Brief, 2017, 11, 204-207.	0.5	4
177	Determination of the New MDR-Modifier PFP 6 and its Metabolites in Human Liver Microsomes by High-Performance Liquid Chromatography. , 1996, 10, 127-130.		3
178	A Method for the Synthesis of 2,3-Disubstituted 2,3-Dihydrobenzofurans. Monatshefte FÃ¼r Chemie, 2000, 131, 0375-0382.	0.9	3
179	Open Innovation in Drug Discovery. Molecular Informatics, 2012, 31, 519-520.	1.4	3
180	Propafenone analogue with additional Hâ€bond acceptor group shows increased inhibitory activity on Pâ€glycoprotein. Archiv Der Pharmazie, 2020, 353, e1900269.	2.1	3

#	Article	IF	Citations
181	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.	1.6	3
182	Levcromakalim Revisited: NMR Spectroscopic and Theoretical Investigations. Monatshefte FÃ¼r Chemie, 2001, 132, 373-386.	0.9	2
183	Transmembrane drug transporter â€“ taxonomy, assays, and their role in drug discovery. Drug Discovery Today: Technologies, 2014, 12, e35-e36.	4.0	2
184	Systems Approaches and Big Data in Molecular Informatics. Molecular Informatics, 2015, 34, 2-2.	1.4	2
185	Empowering pharmacoinformatics by linked life science data. Journal of Computer-Aided Molecular Design, 2017, 31, 319-328.	1.3	2
186	Development of Refined Homology Models: Adding the Missing Information to the Medically Relevant Neurotransmitter Transporters. Springer Series in Biophysics, 2014, , 99-120.	0.4	2
187	Structure-based peptide ligand design for improved epidermal growth factor receptor targeted gene delivery. European Journal of Pharmaceutics and Biopharmaceutics, 2022, 176, 211-221.	2.0	2
188	State-dependent dissociation of HERG channel inhibitors. BMC Pharmacology, 2007, 7, A13.	0.4	1
189	Characterization of a novel class of antimalarials and its applicability to plasmodial target identification. Wiener Klinische Wochenschrift, 2007, 119, 83-87.	1.0	1
190	Prediction of hERG Channel Inhibition Using In Silico Techniques. , 2011, , 191-239.		1
191	How to Solve the Problems of Docking into a Symmetric Binding Site: The Example of the hERG Channel. Scientia Pharmaceutica, 2013, 81, 677-682.	0.7	1
192	Molecular Informatics Going â€œFully Onlineâ€• Molecular Informatics, 2014, 33, 2-2.	1.4	1
193	11th German Conference on Chemoinformatics (GCC 2015). Journal of Cheminformatics, 2016, 8, 18.	2.8	1
194	Quantenchemische Untersuchungen an Levcromakalim. Monatshefte FÃ¼r Chemie, 1998, 129, 633.	0.9	1
195	KNIME workflow for retrieving causal drug and protein interactions, building networks, and performing topological enrichment analysis demonstrated by a DILI case study. Journal of Cheminformatics, 2022, 14, .	2.8	1
196	Troxacitabine Shire Pharmaceuticals. ChemInform, 2003, 34, no.	0.1	0
197	In silico Screening with Benzofuran- and Benzopyran-Type MDR-Modulators.. ChemInform, 2003, 34, no.	0.1	0
198	Topological Distance Based 3D Descriptors for Use in QSAR and Diversity Analysis.. ChemInform, 2004, 35, no.	0.1	0

#	Article	IF	Citations
199	Insights into Phenylalanine Derivatives Recognition of VLA-4 Integrin: From a Pharmacophoric Study to 3D-QSAR and Molecular Docking Analyses.. ChemInform, 2004, 35, no.	0.1	0
200	Editorial [Hot Topic: Drug Efflux Pumps - A Continuing Challenge (Executive Editors: Gerhard F. Ecker /) Tj ETQq0 0 0 rgBT /Overlock 10 T	1.1	0
201	Synthesis and Multidrugâ€Resistance Modulating Activity of a Series of Thienothiazines.. ChemInform, 2002, 33, 200-200.	0.1	0
202	Molecular Informatics- From Models to Molecules and Systems. Molecular Informatics, 2010, 29, 9-9.	1.4	0
203	Amphetamine actions rely on the availability of phosphatidylinositol-4,5-bisphosphate. BMC Pharmacology, 2011, 11, .	0.4	0
204	Molecular Informatics â€“ The First Year. Molecular Informatics, 2011, 30, 3-3.	1.4	0
205	Editorial:Molecular InformaticsGaining Impact. Molecular Informatics, 2012, 31, 615-615.	1.4	0
206	Editorial: Sustained Success of Molecular Informatics. Molecular Informatics, 2013, 32, 3-3.	1.4	0
207	Experimental Data Guided Docking of Small Molecules into Homology Models of Neurotransmitter Transporters. Neuromethods, 2016, , 83-89.	0.2	0
208	Molecular Informatics: From Models to Systems and Beyond. Molecular Informatics, 2016, 35, 2-2.	1.4	0
209	Interaction of ABC Transporters with Drugs. , 2016, , 135-151.		0
210	Linked Open Data: Ligand-Transporter Interaction Profiling and Beyond. Methods in Pharmacology and Toxicology, 2018, , 405-417.	0.1	0
211	Lanthanide resonance energy transferâ€based distance measurements in the mammalian glutamate transporter excitatory amino acid transporter 3 (1064.12). FASEB Journal, 2014, 28, 1064.12.	0.2	0
212	Troxacitabine (Shire Pharmaceuticals). Current Opinion in Investigational Drugs, 2002, 3, 1533-8.	2.3	0
213	EUFEPS 2002 - new safe medicines faster. IDrugs: the Investigational Drugs Journal, 2002, 5, 1134-7.	0.7	0