Gerhard F Ecker

List of Publications by Year
in descending order

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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	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
2	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
3	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
4	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
5	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
6	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
7	Effects of Hydroxylated Mephedrone Metabolites on Monoamine Transporter Activity in vitro. Frontiers in Pharmacology, 2021, 12, 654061.	1.6	9
8	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
9	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
10	Propafenone analogue with additional Hâ€bond acceptor group shows increased inhibitory activity on Pâ€glycoprotein. Archiv Der Pharmazie, 2020, 353, e1900269.	2.1	3
11	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
12	ATP modulates SLC7A5 (LAT1) synergistically with cholesterol. Scientific Reports, 2020, 10, 16738.	1.6	21
13	A structureâ€“kinetic relationship study using matched molecular pair analysis. RSC Medicinal Chemistry, 2020, 11, 1285-1294.	1.7	9
14	A widespread role for SLC transmembrane transporters in resistance to cytotoxic drugs. Nature Chemical Biology, 2020, 16, 469-478.	3.9	84
15	COVER: conformational oversampling as data augmentation for molecules. Journal of Cheminformatics, 2020, 12, 18.	2.8	20
16	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
17	Using Machine Learning Methods and Structural Alerts for Prediction of Mitochondrial Toxicity. Molecular Informatics, 2020, 39, e2000005.	1.4	36
18	Image Based Liver Toxicity Prediction. Journal of Chemical Information and Modeling, 2020, 60, 1111-1121.	2.5	14

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19	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
20	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
21	Studies of structural determinants of substrate binding in the Creatine Transporter (CreaT, SLC6A8) using molecular models. Scientific Reports, 2020, 10, 6241.	1.6	16
22	The RESOLUTE consortium: unlocking SLC transporters for drug discovery. Nature Reviews Drug Discovery, 2020, 19, 429-430.	21.5	53
23	A structural model of the human serotonin transporter in an outward-occluded state. PLoS ONE, 2019, 14, e0217377.	1.1	17
24	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
25	Structural Insight into the In Vitro Anti-Intravasative Properties of Flavonoids. Scientia Pharmaceutica, 2019, 87, 23.	0.7	10
26	Structural and molecular aspects of betaine-GABA transporter 1 (BGT1) and its relation to brain function. Neuropharmacology, 2019, 161, 107644.	2.0	25
27	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
28	para-Trifluoromethyl-methcathinone is an allosteric modulator of the serotonin transporter. Neuropharmacology, 2019, 161, 107615.	2.0	26
29	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
30	Predicting Residence Time and Drug Unbinding Pathway through Scaled Molecular Dynamics. Journal of Chemical Information and Modeling, 2019, 59, 535-549.	2.5	64
31	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
32	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
33	Translation Termination Factor GSPT1 Is a Phenotypically Relevant Off-Target of Heterobifunctional Phthalimide Degraders. ACS Chemical Biology, 2018, 13, 553-560.	1.6	128
34	Predicting drug resistance related to ABC transporters using unsupervised Consensus Self-Organizing Maps. Scientific Reports, 2018, 8, 6803.	1.6	7
35	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
36	Linked Open Data: Ligand-Transporter Interaction Profiling and Beyond. Methods in Pharmacology and Toxicology, 2018, , 405-417.	0.1	0

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37	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
38	GRAIL: GRids of phArmacophore Interaction fieLds. Journal of Chemical Theory and Computation, 2018, 14, 4958-4970.	2.3	15
39	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
40	SAR-Guided Scoring Function and Mutational Validation Reveal the Binding Mode of CGS-8216 at the Î±1+/Î²2â€“ Benzodiazepine Site. Journal of Chemical Information and Modeling, 2018, 58, 1682-1696.	2.5	5
41	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
42	Curated human hyperbilirubinemia data and the respective OATP1B1 and 1B3 inhibition predictions. Data in Brief, 2017, 11, 204-207.	0.5	4
43	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
44	Kinetics for Drug Discovery: an industry-driven effort to target drug residence time. Drug Discovery Today, 2017, 22, 896-911.	3.2	165
45	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
46	Folding correction of ABCâ€transporter ABCB1 by pharmacological chaperones: a mechanistic concept. Pharmacology Research and Perspectives, 2017, 5, e00325.	1.1	6
47	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
48	Legacy data sharing to improve drug safety assessment: the eTOX project. Nature Reviews Drug Discovery, 2017, 16, 811-812.	21.5	56
49	Adverse outcome pathways: opportunities, limitations and open questions. Archives of Toxicology, 2017, 91, 3477-3505.	1.9	282
50	Development of Non-GAT1-Selective Inhibitors: Challenges and Achievements. Advances in Neurobiology, 2017, 16, 315-332.	1.3	11
51	Predicting drug-induced liver injury: The importance of data curation. Toxicology, 2017, 389, 139-145.	2.0	78
52	Empowering pharmacoinformatics by linked life science data. Journal of Computer-Aided Molecular Design, 2017, 31, 319-328.	1.3	2
53	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
54	Virtual Screening of DrugBank Reveals Two Drugs as New BCRP Inhibitors. SLAS Discovery, 2017, 22, 86-93.	1.4	22

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55	Structural Studies of GABAA Receptor Binding Sites: Which Experimental Structure Tells us What?. Frontiers in Molecular Neuroscience, 2016, 9, 44.	1.4	76
56	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
57	Experimental Data Guided Docking of Small Molecules into Homology Models of Neurotransmitter Transporters. Neuromethods, 2016, , 83-89.	0.2	0
58	Molecular Informatics: From Models to Systems and Beyond. Molecular Informatics, 2016, 35, 2-2.	1.4	0
59	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
60	11th German Conference on Chemoinformatics (GCC 2015). Journal of Cheminformatics, 2016, 8, 18.	2.8	1
61	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
62	Flagging Drugs That Inhibit the Bile Salt Export Pump. Molecular Pharmaceutics, 2016, 13, 163-171.	2.3	24
63	Interaction of ABC Transporters with Drugs. , 2016, , 135-151.		0
64	Binding Mode Selection Determines the Action of Ecstasy Homologs at Monoamine Transporters. Molecular Pharmacology, 2016, 89, 165-175.	1.0	53
65	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
66	Integrative Modeling Strategies for Predicting Drug Toxicities at the eTOX Project. Molecular Informatics, 2015, 34, 477-484.	1.4	17
67	Synthesis and in Silico Evaluation of Novel Compounds for PET-Based Investigations of the Norepinephrine Transporter. Molecules, 2015, 20, 1712-1730.	1.7	6
68	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
69	Systems Approaches and Big Data in Molecular Informatics. Molecular Informatics, 2015, 34, 2-2.	1.4	2
70	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
71	Identification of the First Highly Subtype-Selective Inhibitor of Human GABA Transporter GAT3. ACS Chemical Neuroscience, 2015, 6, 1591-1599.	1.7	33
72	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

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73	Medicinal chemistry in the era of big data. Drug Discovery Today: Technologies, 2015, 14, 37-41.	4.0	24
74	The ABC of Phytohormone Translocation. Planta Medica, 2015, 81, 474-487.	0.7	18
75	Novel scaffolds for modulation of TRPV1 identified with pharmacophore modeling and virtual screening. Future Medicinal Chemistry, 2015, 7, 243-256.	1.1	16
76	Prediction of drugâ€“ABC-transporter interaction â€" Recent advances and future challenges. Advanced Drug Delivery Reviews, 2015, 86, 17-26.	6.6	169
77	Structure activity relationship of selective GABA uptake inhibitors. Bioorganic and Medicinal Chemistry, 2015, 23, 2480-2488.	1.4	27
78	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
79	â€˜Second-Generationâ€™ Mephedrone Analogs, 4-MEC and 4-MePPP, Differentially Affect Monoamine Transporter Function. Neuropsychopharmacology, 2015, 40, 1321-1331.	2.8	86
80	The Application of the Open Pharmacological Concepts Triple Store (Open PHACTS) to Support Drug Discovery Research. PLoS ONE, 2014, 9, e115460.	1.1	31
81	Pore-Exposed Tyrosine Residues of P-Glycoprotein Are Important Hydrogen-Bonding Partners for Drugs. Molecular Pharmacology, 2014, 85, 420-428.	1.0	30
82	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
83	Computational models for predicting the interaction with ABC transporters. Drug Discovery Today: Technologies, 2014, 12, e69-e77.	4.0	14
84	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
85	Exploiting open data: a new era in pharmacoinformatics. Future Medicinal Chemistry, 2014, 6, 503-514.	1.1	18
86	Molecular Informatics Going â€œFully Onlineâ€• Molecular Informatics, 2014, 33, 2-2.	1.4	1
87	â€˜Big dataâ€™ in pharmaceutical science: challenges and opportunities. Future Medicinal Chemistry, 2014, 6, 857-864.	1.1	8
88	Efficient Modulation of Î³-Aminobutyric Acid Type A Receptors by Piperine Derivatives. Journal of Medicinal Chemistry, 2014, 57, 5602-5619.	2.9	54
89	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
90	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

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91	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
92	Aminorex, a metabolite of the cocaine adulterant levamisole, exerts amphetamine like actions at monoamine transporters. Neurochemistry International, 2014, 73, 32-41.	1.9	95
93	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
94	BCRP Inhibition: from Data Collection to Ligandâ€Based Modeling. Molecular Informatics, 2014, 33, 322-331.	1.4	27
95	Transporter taxonomy â€“ a comparison of different transport protein classification schemes. Drug Discovery Today: Technologies, 2014, 12, e37-e46.	4.0	7
96	Transmembrane drug transporter â€“ taxonomy, assays, and their role in drug discovery. Drug Discovery Today: Technologies, 2014, 12, e35-e36.	4.0	2
97	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
98	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
99	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
100	Classification of Highâ€Activity Tiagabine Analogs by Binary QSAR Modeling. Molecular Informatics, 2013, 32, 415-419.	1.4	11
101	Experimental characterization of the human non-sequence-specific nucleic acid interactome. Genome Biology, 2013, 14, R81.	13.9	7
102	Editorial: Sustained Success of Molecular Informatics. Molecular Informatics, 2013, 32, 3-3.	1.4	0
103	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
104	How Far Could We Go with Open Data â€“ A Case Study for TRPV1 Antagonists. Molecular Informatics, 2013, 32, 555-562.	1.4	6
105	Scientific competency questions as the basis for semantically enriched open pharmacological space development. Drug Discovery Today, 2013, 18, 843-852.	3.2	44
106	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
107	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
108	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

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109	Probing the Selectivity of Monoamine Transporter Substrates by Means of Molecular Modeling. Molecular Informatics, 2013, 32, 409-413.	1.4	13
110	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
111	Evidence-based approach to assess passive diffusion and carrier-mediated drug transport. Drug Discovery Today, 2012, 17, 905-912.	3.2	125
112	Taking Open Innovation to the Molecular Level â€•Strengths and Limitations. Molecular Informatics, 2012, 31, 528-535.	1.4	8
113	An In Silico Classification Model for Putative ABCC2 Substrates. Molecular Informatics, 2012, 31, 547-553.	1.4	18
114	Annotating Human Pâ€Glycoprotein Bioassay Data. Molecular Informatics, 2012, 31, 599-609.	1.4	30
115	Open Innovation in Drug Discovery. Molecular Informatics, 2012, 31, 519-520.	1.4	3
116	Editorial:Molecular InformaticsGaining Impact. Molecular Informatics, 2012, 31, 615-615.	1.4	0
117	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
118	Open PHACTS: semantic interoperability for drug discovery. Drug Discovery Today, 2012, 17, 1188-1198.	3.2	274
119	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
120	Diazepam-bound GABAA receptor models identify new benzodiazepine binding-site ligands. Nature Chemical Biology, 2012, 8, 455-464.	3.9	175
121	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
122	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
123	Prediction of hERG Channel Inhibition Using In Silico Techniques. , 2011, , 191-239.		1
124	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
125	Trapping and dissociation of propafenone derivatives in HERG channels. British Journal of Pharmacology, 2011, 162, 1542-1552.	2.7	29
126	Insights into structureâ€“activity relationship of GABAA receptor modulating coumarins and furanocoumarins. European Journal of Pharmacology, 2011, 668, 57-64.	1.7	43

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127	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
128	Amphetamine actions rely on the availability of phosphatidylinositol-4,5-bisphosphate. BMC Pharmacology, 2011, 11, .	0.4	0
129	Selfâ€Organizing Maps for In Silico Screening and Data Visualization. Molecular Informatics, 2011, 30, 838-846.	1.4	22
130	Molecular Informatics â€“ The First Year. Molecular Informatics, 2011, 30, 3-3.	1.4	0
131	Use of shape similarities for the classification of P-glycoprotein substrates and nonsubstrates. Future Medicinal Chemistry, 2011, 3, 1117-1128.	1.1	6
132	Molecular Dissection of Dual Pseudosymmetric Solute Translocation Pathways in Human P-Glycoprotein. Molecular Pharmacology, 2011, 79, 443-452.	1.0	48
133	Random Mutagenesis of the Prokaryotic Peptide Transporter YdgR Identifies Potential Periplasmic Gating Residues. Journal of Biological Chemistry, 2011, 286, 23121-23131.	1.6	11
134	Exhaustive Sampling of Docking Poses Reveals Binding Hypotheses for Propafenone Type Inhibitors of P-Glycoprotein. PLoS Computational Biology, 2011, 7, e1002036.	1.5	67
135	The hERG Potassium Channel and Drug Trapping: Insight from Docking Studies with Propafenone Derivatives. ChemMedChem, 2010, 5, 436-442.	1.6	22
136	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
137	Impact of the Recent Mouse Pâ€Glycoprotein Structure for Structureâ€Based Ligand Design. Molecular Informatics, 2010, 29, 276-286.	1.4	21
138	Molecular Informatics- From Models to Molecules and Systems. Molecular Informatics, 2010, 29, 9-9.	1.4	0
139	Coexistence of passive and carrier-mediated processes in drug transport. Nature Reviews Drug Discovery, 2010, 9, 597-614.	21.5	526
140	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
141	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
142	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
143	Predicting Ligand Interactions with ABC Transporters in ADME. Chemistry and Biodiversity, 2009, 6, 1960-1969.	1.0	43
144	Similarity-based SIBAR descriptors for classification of chemically diverse hERG blockers. Molecular Diversity, 2009, 13, 321-336.	2.1	39

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145	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
146	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
147	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
148	Synthesis and antitumor-evaluation of cyclopropyl-containing combretastatin analogs. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 6948-6951.	1.0	38
149	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
150	Syntheses and Antigestagenic Activity of Mifepristone Derivatives. Journal of Medicinal Chemistry, 2009, 52, 1268-1274.	2.9	8
151	Hydrophobic moments as physicochemical descriptors in structure-activity relationship studies of P-glycoprotein inhibitors. Monatshefte FÃ¼r Chemie, 2008, 139, 401-405.	0.9	7
152	A binary QSAR model for classification of hERG potassium channel blockers. Bioorganic and Medicinal Chemistry, 2008, 16, 4107-4119.	1.4	87
153	Classification Models for hERG Inhibitors by Counterâ€Propagation Neural Networks. Chemical Biology and Drug Design, 2008, 72, 279-289.	1.5	31
154	Computational models for prediction of interactions with ABC-transporters. Drug Discovery Today, 2008, 13, 311-317.	3.2	73
155	In silicoprediction of substrate properties for ABC-multidrug transporters. Expert Opinion on Drug Metabolism and Toxicology, 2008, 4, 1167-1180.	1.5	44
156	Predictive QSAR Models for Polyspecific Drug Targets: The Importance of Feature Selection. Current Computer-Aided Drug Design, 2008, 4, 91-110.	0.8	21
157	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
158	Predictive Models for hERG Channel Blockers: Ligand-Based and Structure-Based Approaches. Current Medicinal Chemistry, 2007, 14, 3003-3026.	1.2	42
159	Self-Organizing Maps for Identification of New Inhibitors of P-Glycoprotein. Journal of Medicinal Chemistry, 2007, 50, 1698-1702.	2.9	55
160	Multispecificity of Drug Transporters: Probing Inhibitor Selectivity for the Human Drug Efflux Transporters ABCB1 and ABCG2. ChemMedChem, 2007, 2, 1783-1788.	1.6	41
161	State-dependent dissociation of HERG channel inhibitors. BMC Pharmacology, 2007, 7, A13.	0.4	1
162	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

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163	Characterization of a novel class of antimalarials and its applicability to plasmodial target identification. Wiener Klinische Wochenschrift, 2007, 119, 83-87.	1.0	1
164	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
165	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
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