Robert C Glen

List of Publications by Year
in descending order

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69 papers	12,769 citations	94433 37 h-index	110387 64 g-index
70 all docs	70 docs citations	70 times ranked	13844 citing authors

#	Article	IF	Citations
1	G392E neuroserpin causing the dementia FENIB is secreted from cells but is not synaptotoxic. Scientific Reports, 2021, 11, 8766.	3.3	7
2	Apelin peptides linked to antiâ€serum albumin domain antibodies retain affinity in vitro and are efficacious receptor agonists in vivo. Basic and Clinical Pharmacology and Toxicology, 2020, 126, 96-103.	2.5	14
3	The G Protein Biased Small Molecule Apelin Agonist CMF-019 is Disease Modifying in Endothelial Cell Apoptosis In Vitro and Induces Vasodilatation Without Desensitisation In Vivo. Frontiers in Pharmacology, 2020, 11, 588669.	3.5	7
4	A novel cyclic biased agonist of the apelin receptor, MM07, is disease modifying in the rat monocrotaline model of pulmonary arterial hypertension. British Journal of Pharmacology, 2019, 176, 1206-1221.	5.4	32
5	International Union of Basic and Clinical Pharmacology. CVII. Structure and Pharmacology of the Apelin Receptor with a Recommendation that Elabela/Toddler Is a Second Endogenous Peptide Ligand. Pharmacological Reviews, 2019, 71, 467-502.	16.0	64
6	Elabela/Toddler Is an Endogenous Agonist of the Apelin APJ Receptor in the Adult Cardiovascular System, and Exogenous Administration of the Peptide Compensates for the Downregulation of Its Expression in Pulmonary Arterial Hypertension. Circulation, 2017, 135, 1160-1173.	1.6	183
7	Cardiac action of the first G protein biased small molecule apelin agonist. Biochemical Pharmacology, 2016, 116, 63-72.	4.4	56
8	Improving the prediction of organism-level toxicity through integration of chemical, protein target and cytotoxicity qHTS data. Toxicology Research, 2016, 5, 883-894.	2.1	10
9	A multi-label approach to target prediction taking ligand promiscuity into account. Journal of Cheminformatics, 2015, 7, 24.	6.1	31
10	Verifying the fully â€œLaplacianisedâ€•posterior NaÃ¯ve Bayesian approach and more. Journal of Cheminformatics, 2015, 7, 27.	6.1	5
11	Design, Characterization, and First-In-Human Study of the Vascular Actions of a Novel Biased Apelin Receptor Agonist. Hypertension, 2015, 65, 834-840.	2.7	131
12	Predicting drug metabolism: experiment and/or computation?. Nature Reviews Drug Discovery, 2015, 14, 387-404.	46.4	355
13	Cheminformatics Research at the Unilever Centre for Molecular Science Informatics Cambridge. Molecular Informatics, 2015, 34, 626-633.	2.5	0
14	Extending in silico mechanism-of-action analysis by annotating targets with pathways: application to cellular cytotoxicity readouts. Future Medicinal Chemistry, 2014, 6, 2029-2056.	2.3	19
15	Investigating and Predicting how Biology Changes Molecules and Their Properties. Molecular Informatics, 2014, 33, 443-445.	2.5	4
16	How Diverse Are Diversity Assessment Methods? A Comparative Analysis and Benchmarking of Molecular Descriptor Space. Journal of Chemical Information and Modeling, 2014, 54, 230-242.	5.4	62
17	Cytochrome P450 site of metabolism prediction from 2D topological fingerprints using GPU accelerated probabilistic classifiers. Journal of Cheminformatics, 2014, 6, 29.	6.1	26
18	Quantifying the shifts in physicochemical property space introduced by the metabolism of small organic molecules. Journal of Cheminformatics, 2013, 5, .	6.1	0

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19	How Do Metabolites Differ from Their Parent Molecules and How Are They Excreted?. Journal of Chemical Information and Modeling, 2013, 53, 354-367.	5.4	33
20	In Silico Target Predictions: Defining a Benchmarking Data Set and Comparison of Performance of the Multiclass NaÃ¯ve Bayes and Parzen-Rosenblatt Window. Journal of Chemical Information and Modeling, 2013, 53, 1957-1966.	5.4	131
21	Experimental validation of in silico target predictions on synergistic protein targets. MedChemComm, 2013, 4, 278-288.	3.4	7
22	Prediction of Cytochrome P450 Xenobiotic Metabolism: Tethered Docking and Reactivity Derived from Ligand Molecular Orbital Analysis. Journal of Chemical Information and Modeling, 2013, 53, 1294-1305.	5.4	38
23	Diversity Selection of Compounds Based on â€˜Protein Affinity Fingerprintsâ€™ Improves Sampling of Bioactive Chemical Space. Chemical Biology and Drug Design, 2013, 82, 252-266.	3.2	19
24	FAst MEtabolizer (FAME): A Rapid and Accurate Predictor of Sites of Metabolism in Multiple Species by Endogenous Enzymes. Journal of Chemical Information and Modeling, 2013, 53, 2896-2907.	5.4	47
25	Anti-cancer Drug Development: Computational Strategies to Identify and Target Proteins Involved in Cancer Metabolism. Current Pharmaceutical Design, 2013, 19, 532-577.	1.9	30
26	The Challenges Involved in Modeling Toxicity Data In Silico: A Review. Current Drug Metabolism, 2012, 18, 1266-1291.	1.2	4
27	The Challenges Involved in Modeling Toxicity Data In Silico: A Review. Current Pharmaceutical Design, 2012, 18, 1266-1291.	1.9	80
28	Computational Prediction of Metabolism: Sites, Products, SAR, P450 Enzyme Dynamics, and Mechanisms. Journal of Chemical Information and Modeling, 2012, 52, 617-648.	5.4	246
29	Predicting the mechanism of phospholipidosis. Journal of Cheminformatics, 2012, 4, 2.	6.1	49
30	Classifying Large Chemical Data Sets: Using A Regularized Potential Function Method. Journal of Chemical Information and Modeling, 2011, 51, 4-14.	5.4	11
31	Classifying Molecules Using a Sparse Probabilistic Kernel Binary Classifier. Journal of Chemical Information and Modeling, 2011, 51, 1539-1544.	5.4	24
32	From in silico target prediction to multi-target drug design: Current databases, methods and applications. Journal of Proteomics, 2011, 74, 2554-2574.	2.4	243
33	Connecting the virtual world of computers to the real world of medicinal chemistry. Future Medicinal Chemistry, 2011, 3, 399-403.	2.3	0
34	Use of historic metabolic biotransformation data as a means of anticipating metabolic sites using MetaPrint2D and Bioclipse. BMC Bioinformatics, 2010, 11, 362.	2.6	66
35	Exploring the â€˜RPRLâ€™ Motif of Apelinâ€13 through Molecular Simulation and Biological Evaluation of Cyclic Peptide Analogues. ChemMedChem, 2010, 5, 1247-1253.	3.2	35
36	Predicting Phospholipidosis Using Machine Learning. Molecular Pharmaceutics, 2010, 7, 1708-1714.	4.6	49

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37	Predicting Intrinsic Aqueous Solubility by a Thermodynamic Cycle. Molecular Pharmaceutics, 2008, 5, 266-279.	4.6	104
38	Solubility Challenge: Can You Predict Solubilities of 32 Molecules Using a Database of 100 Reliable Measurements?. Journal of Chemical Information and Modeling, 2008, 48, 1289-1303.	5.4	166
39	Ab Initio potential grid based docking: From High Performance Computing to In Silico Screening. AIP Conference Proceedings, 2007, , .	0.4	3
40	Diclofenac Solubility:Â Independent Determination of the Intrinsic Solubility of Three Crystal Forms. Journal of Medicinal Chemistry, 2007, 50, 979-983.	6.4	109
41	Random Forest Models To Predict Aqueous Solubility. Journal of Chemical Information and Modeling, 2007, 47, 150-158.	5.4	277
42	A new method for the reproducible generation of polymorphs: two forms of sulindac with very different solubilities. Journal of Applied Crystallography, 2007, 40, 379-381.	4.5	44
43	Reaction Site Mapping of Xenobiotic Biotransformations. Journal of Chemical Information and Modeling, 2007, 47, 583-590.	5.4	100
44	Support vector inductive logic programming outperforms the naive Bayes classifier and inductive logic programming for the classification of bioactive chemical compounds. Journal of Computer-Aided Molecular Design, 2007, 21, 269-280.	2.9	40
45	Chapter 9 Molecular Similarity: Advances in Methods, Applications and Validations in Virtual Screening and QSAR. Annual Reports in Computational Chemistry, 2006, 2, 141-168.	1.7	10
46	Characterizing Bitterness:Â Identification of Key Structural Features and Development of a Classification Model. Journal of Chemical Information and Modeling, 2006, 46, 569-576.	5.4	54
47	Analysis of Activity Space by Fragment Fingerprints, 2D Descriptors, and Multitarget Dependent Transformation of 2D Descriptors. Journal of Chemical Information and Modeling, 2006, 46, 1078-1083.	5.4	15
48	A Discussion of Measures of Enrichment in Virtual Screening:â€‰ Comparing the Information Content of Descriptors with Increasing Levels of Sophistication. Journal of Chemical Information and Modeling, 2005, 45, 1369-1375.	5.4	167
49	Molecular Similarity: A Key Technique in Molecular Informatics.. ChemInform, 2005, 36, no.	0.0	0
50	Screening for Dihydrofolate Reductase Inhibitors Using MOLPRINT 2D, a Fast Fragment-Based Method Employing the NaÃ¯ve Bayesian Classifier: Limitations of the Descriptor and the Importance of Balanced Chemistry in Training and Test Sets. Journal of Biomolecular Screening, 2005, 10, 658-666.	2.6	30
51	General Melting Point Prediction Based on a Diverse Compound Data Set and Artificial Neural Networks. Journal of Chemical Information and Modeling, 2005, 45, 581-590.	5.4	114
52	Molecular Similarity Searching Using COSMO Screening Charges (COSMO/3PP). Lecture Notes in Computer Science, 2005, , 175-185.	1.3	1
53	Similarity Searching of Chemical Databases Using Atom Environment Descriptors (MOLPRINT 2D):â€‰ Evaluation of Performance. Journal of Chemical Information and Computer Sciences, 2004, 44, 1708-1718.	2.8	307
54	Molecular Similarity Searching Using Atom Environments, Information-Based Feature Selection, and a NaÃ¯ve Bayesian Classifier. Journal of Chemical Information and Computer Sciences, 2004, 44, 170-178.	2.8	249

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55	Molecular similarity: a key technique in molecular informatics. Organic and Biomolecular Chemistry, 2004, 2, 3204.	2.8	527
56	Molecular Surface Point Environments for Virtual Screening and the Elucidation of Binding Patterns (MOLPRINT 3D). Journal of Medicinal Chemistry, 2004, 47, 6569-6583.	6.4	49
57	Predicting proteinâ€“ligand binding affinities: a low scoring game?. Organic and Biomolecular Chemistry, 2004, 2, 3267-3273.	2.8	49
58	Predicting pKaby Molecular Tree Structured Fingerprints and PLS. Journal of Chemical Information and Computer Sciences, 2003, 43, 870-879.	2.8	64
59	Novel Methods for the Prediction of logP, pKa, and logD. Journal of Chemical Information and Computer Sciences, 2002, 42, 796-805.	2.8	151
60	Novel Methods for the Prediction of logP, pK_a, and logD.. ChemInform, 2002, 33, 231-231.	0.0	0
61	Synthesis and Biological Evaluation of Novel Pyrazoles and Indazoles as Activators of the Nitric Oxide Receptor, Soluble Guanylate Cyclase. Journal of Medicinal Chemistry, 2001, 44, 78-93.	6.4	92
62	Solution-phase parallel synthesis of 5-carboxamido 1-benzyl-3-(3-dimethylaminopropyloxy)-1H-pyrazoles as activators of soluble guanylate cyclase with improved oral bioavailability. Bioorganic and Medicinal Chemistry Letters, 2001, 11, 1089-1092.	2.2	20
63	Development and validation of a genetic algorithm for flexible docking 1 1Edited by F. E. Cohen. Journal of Molecular Biology, 1997, 267, 727-748.	4.2	5,937
64	A genetic algorithm for flexible molecular overlay and pharmacophore elucidation. Journal of Computer-Aided Molecular Design, 1995, 9, 532-549.	2.9	350
65	Molecular recognition of receptor sites using a genetic algorithm with a description of desolvation. Journal of Molecular Biology, 1995, 245, 43-53.	4.2	1,462
66	A fast empirical method for the calculation of molecular polarizability. Journal of Computer-Aided Molecular Design, 1994, 8, 457-466.	2.9	23
67	Pharmacophoric pattern matching in files of three-dimensional chemical structures: Comparison of conformational-searching algorithms for flexible searching. Journal of Chemical Information and Modeling, 1994, 34, 197-206.	5.4	82
68	Matching two-dimensional chemical graphs using genetic algorithms. Journal of Chemical Information and Modeling, 1994, 34, 63-70.	5.4	38
69	Applications of rule-induction in the derivation of quantitative structure-activity relationships. Journal of Computer-Aided Molecular Design, 1992, 6, 349-383.	2.9	17