Robert P Sheridan

List of Publications by Year
in descending order

67	9,393	93792	104191
papers	citations	39 h-index	69 g-index

75	75	75	10477
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Application of Machine Learning and Reaction Optimization for the Iterative Improvement of Enantioselectivity of Cinchona-Derived Phase Transfer Catalysts. Organic Process Research and Development, 2022, 26, 670-682.	1.3	14
2	Driving Aspirational Process Mass Intensity Using Simple Structure-Based Prediction. Organic Process Research and Development, 2022, 26, 1405-1410.	1.3	8
3	Stability of Prediction in Production ADMET Models as a Function of Version: Why and When Predictions Change. Journal of Chemical Information and Modeling, 2022, 62, 3477-3485.	2.5	5
4	Prediction Accuracy of Production ADMET Models as a Function of Version: Activity Cliffs Rule. Journal of Chemical Information and Modeling, 2022, 62, 3275-3280.	2.5	6
5	Nearest Neighbor Gaussian Process for Quantitative Structureâ€“Activity Relationships. Journal of Chemical Information and Modeling, 2020, 60, 4653-4663.	2.5	4
6	Experimental Error, Kurtosis, Activity Cliffs, and Methodology: What Limits the Predictivity of Quantitative Structureâ€“Activity Relationship Models?. Journal of Chemical Information and Modeling, 2020, 60, 1969-1982.	2.5	34
7	QSAR without borders. Chemical Society Reviews, 2020, 49, 3525-3564.	18.7	427
8	Deep Dive into Machine Learning Models for Protein Engineering. Journal of Chemical Information and Modeling, 2020, 60, 2773-2790.	2.5	134
9	Building Quantitative Structureâ€“Activity Relationship Models Using Bayesian Additive Regression Trees. Journal of Chemical Information and Modeling, 2019, 59, 2642-2655.	2.5	9
10	Interpretation of QSAR Models by Coloring Atoms According to Changes in Predicted Activity: How Robust Is It?. Journal of Chemical Information and Modeling, 2019, 59, 1324-1337.	2.5	42
11	Modeling and predicting chiral stationary phase enantioselectivity: An efficient random forest classifier using an optimally balanced training dataset and an aggregation strategy. Journal of Separation Science, 2018, 41, 1365-1375.	1.3	19
12	CHEMGENIE: integration of chemogenomics data for applications in chemical biology. Drug Discovery Today, 2018, 23, 151-160.	3.2	13
13	Response to Comment on â€œPredicting reaction performance in Câ€“N cross-coupling using machine learningâ€. Science, 2018, 362, .	6.0	49
14	Role of simple descriptors and applicability domain in predicting change in protein thermostability. PLoS ONE, 2018, 13, e0203819.	1.1	11
15	Mapping the dark space of chemical reactions with extended nanomole synthesis and MALDI-TOF MS. Science, 2018, 361, .	6.0	126
16	Informing the Selection of Screening Hit Series with in Silico Absorption, Distribution, Metabolism, Excretion, and Toxicity Profiles. Journal of Medicinal Chemistry, 2017, 60, 6771-6780.	2.9	17
17	Demystifying Multitask Deep Neural Networks for Quantitative Structureâ€“Activity Relationships. Journal of Chemical Information and Modeling, 2017, 57, 2490-2504.	2.5	178
18	Is Multitask Deep Learning Practical for Pharma?. Journal of Chemical Information and Modeling, 2017, 57, 2068-2076.	2.5	191

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19	Mining Chromatographic Enantioseparation Data Using Matched Molecular Pair Analysis. Molecules, 2016, 21, 1297.	1.7	7
20	Extreme Gradient Boosting as a Method for Quantitative Structureâ€“Activity Relationships. Journal of Chemical Information and Modeling, 2016, 56, 2353-2360.	2.5	308
21	Toward structure-based predictive tools for the selection of chiral stationary phases for the chromatographic separation of enantiomers. Journal of Chromatography A, 2016, 1467, 206-213.	1.8	29
22	Debunking the Idea that Ligand Efficiency Indices Are Superior to pIC50 as QSAR Activities. Journal of Chemical Information and Modeling, 2016, 56, 2253-2262.	2.5	11
23	Deep Neural Nets as a Method for Quantitative Structureâ€“Activity Relationships. Journal of Chemical Information and Modeling, 2015, 55, 263-274.	2.5	840
24	eCounterscreening: Using QSAR Predictions to Prioritize Testing for Off-Target Activities and Setting the Balance between Benefit and Risk. Journal of Chemical Information and Modeling, 2015, 55, 231-238.	2.5	12
25	The Relative Importance of Domain Applicability Metrics for Estimating Prediction Errors in QSAR Varies with Training Set Diversity. Journal of Chemical Information and Modeling, 2015, 55, 1098-1107.	2.5	45
26	Global Quantitative Structureâ€“Activity Relationship Models vs Selected Local Models as Predictors of Off-Target Activities for Project Compounds. Journal of Chemical Information and Modeling, 2014, 54, 1083-1092.	2.5	18
27	Modeling a Crowdsourced Definition of Molecular Complexity. Journal of Chemical Information and Modeling, 2014, 54, 1604-1616.	2.5	48
28	Using Random Forest To Model the Domain Applicability of Another Random Forest Model. Journal of Chemical Information and Modeling, 2013, 53, 2837-2850.	2.5	88
29	Time-Split Cross-Validation as a Method for Estimating the Goodness of Prospective Prediction.. Journal of Chemical Information and Modeling, 2013, 53, 783-790.	2.5	201
30	Three Useful Dimensions for Domain Applicability in QSAR Models Using Random Forest. Journal of Chemical Information and Modeling, 2012, 52, 814-823.	2.5	97
31	Comparison of Random Forest and Pipeline Pilot NaÃ¯ve Bayes in Prospective QSAR Predictions. Journal of Chemical Information and Modeling, 2012, 52, 792-803.	2.5	94
32	QSAR Prediction of Passive Permeability in the LLCâ€PK1 Cell Line: Trends in Molecular Properties and Crossâ€Prediction of Cacoâ€2 Permeabilities. Molecular Informatics, 2012, 31, 231-245.	1.4	27
33	Molecular Shape and Medicinal Chemistry: A Perspective. Journal of Medicinal Chemistry, 2010, 53, 3862-3886.	2.9	262
34	Drug-like Density: A Method of Quantifying the â€œBindabilityâ€• of a Protein Target Based on a Very Large Set of Pockets and Drug-like Ligands from the Protein Data Bank. Journal of Chemical Information and Modeling, 2010, 50, 2029-2040.	2.5	100
35	Generating hypotheses about molecular structureâ€“activity relationships (SARs) by solving an optimization problem. Statistical Analysis and Data Mining, 2009, 2, 161-174.	1.4	1
36	QSAR Models for Predicting the Similarity in Binding Profiles for Pairs of Protein Kinases and the Variation of Models between Experimental Data Sets. Journal of Chemical Information and Modeling, 2009, 49, 1974-1985.	2.5	30

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37	Multiple protein structures and multiple ligands: effects on the apparent goodness of virtual screening results. Journal of Computer-Aided Molecular Design, 2008, 22, 257-265.	1.3	52
38	Alternative Global Goodness Metrics and Sensitivity Analysis:â€‰ Heuristics to Check the Robustness of Conclusions from Studies Comparing Virtual Screening Methods. Journal of Chemical Information and Modeling, 2008, 48, 426-433.	2.5	20
39	Chemical similarity searches: when is complexity justified?. Expert Opinion on Drug Discovery, 2007, 2, 423-430.	2.5	47
40	Empirical Regioselectivity Models for Human Cytochromes P450 3A4, 2D6, and 2C9. Journal of Medicinal Chemistry, 2007, 50, 3173-3184.	2.9	105
41	Comparison of Topological, Shape, and Docking Methods in Virtual Screening. Journal of Chemical Information and Modeling, 2007, 47, 1504-1519.	2.5	384
42	Molecular Transformations as a Way of Finding and Exploiting Consistent Local QSAR. Journal of Chemical Information and Modeling, 2006, 46, 180-192.	2.5	87
43	Boosting:Â An Ensemble Learning Tool for Compound Classification and QSAR Modeling. Journal of Chemical Information and Modeling, 2005, 45, 786-799.	2.5	183
44	Calculating Similarities Between Biological Activities in the MDL Drug Data Report Database.. ChemInform, 2004, 35, no.	0.1	0
45	Calculating Similarities between Biological Activities in the MDL Drug Data Report Database. Journal of Chemical Information and Computer Sciences, 2004, 44, 727-740.	2.8	41
46	Similarity to Molecules in the Training Set Is a Good Discriminator for Prediction Accuracy in QSAR. Journal of Chemical Information and Computer Sciences, 2004, 44, 1912-1928.	2.8	251
47	Random Forest:â€‰ A Classification and Regression Tool for Compound Classification and QSAR Modeling. Journal of Chemical Information and Computer Sciences, 2003, 43, 1947-1958.	2.8	2,582
48	Finding Multiactivity Substructures by Mining Databases of Drug-Like Compounds. Journal of Chemical Information and Computer Sciences, 2003, 43, 1037-1050.	2.8	42
49	A Model for Predicting Likely Sites of CYP3A4-mediated Metabolism on Drug-like Molecules. Journal of Medicinal Chemistry, 2003, 46, 1330-1336.	2.9	141
50	The Most Common Chemical Replacements in Drug-Like Compounds. Journal of Chemical Information and Computer Sciences, 2002, 42, 103-108.	2.8	156
51	Why do we need so many chemical similarity search methods?. Drug Discovery Today, 2002, 7, 903-911.	3.2	412
52	A simple method for visualizing the differences between related receptor sites. Journal of Molecular Graphics and Modelling, 2002, 21, 71-79.	1.3	8
53	A simple method for visualizing the differences between related receptor sites. Journal of Molecular Graphics and Modelling, 2002, 21, 217-25.	1.3	2
54	Protocols for Bridging the Peptide to Nonpeptide Gap in Topological Similarity Searches. Journal of Chemical Information and Computer Sciences, 2001, 41, 1395-1406.	2.8	119

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55	Latent Semantic Structure Indexing (LaSSI) for Defining Chemical Similarity. Journal of Medicinal Chemistry, 2001, 44, 1177-1184.	2.9	37
56	Chemical Similarity Searches Using Latent Semantic Structural Indexing (LaSSI) and Comparison to TOPOSIM. Journal of Medicinal Chemistry, 2001, 44, 1185-1191.	2.9	27
57	Mining the Chemical Quarry with Joint Chemical Probes:Â An Application of Latent Semantic Structure Indexing (LaSSI) and TOPOSIM (Dice) to Chemical Database Mining. Journal of Medicinal Chemistry, 2001, 44, 1564-1575.	2.9	13
58	Designing targeted libraries with genetic algorithms11Color Plates for this article are on page 525.. Journal of Molecular Graphics and Modelling, 2000, 18, 320-334.	1.3	44
59	The Centroid Approximation for Mixtures:â€‰ Calculating Similarity and Deriving Structureâ^'Activity Relationships. Journal of Chemical Information and Computer Sciences, 2000, 40, 1456-1469.	2.8	29
60	SQ:Â A Program for Rapidly Producing Pharmacophorically Relevent Molecular Superpositions. Journal of Medicinal Chemistry, 1999, 42, 1505-1514.	2.9	122
61	A Method for Visualizing Recurrent Topological Substructures in Sets of Active Molecules. Journal of Chemical Information and Computer Sciences, 1998, 38, 915-924.	2.8	43
62	Chemical Similarity Using Physiochemical Property Descriptors. Journal of Chemical Information and Computer Sciences, 1996, 36, 118-127.	2.8	262
63	Using a Genetic Algorithm To Suggest Combinatorial Libraries. Journal of Chemical Information and Computer Sciences, 1995, 35, 310-320.	2.8	175
64	FLOG: A system to select ?quasi-flexible? ligands complementary to a receptor of known three-dimensional structure. Journal of Computer-Aided Molecular Design, 1994, 8, 153-174.	1.3	243
65	Flexibases: A way to enhance the use of molecular docking methods. Journal of Computer-Aided Molecular Design, 1994, 8, 565-582.	1.3	100
66	Extending the trend vector: The trend matrix and sample-based partial least squares. Journal of Computer-Aided Molecular Design, 1994, 8, 323-340.	1.3	57
67	PATTY: A programmable atom type and language for automatic classification of atoms in molecular databases. Journal of Chemical Information and Computer Sciences, 1993, 33, 756-762.	2.8	75