Paul Selzer

List of Publications by Year
in descending order

21 papers	3,977 citations	430874 18 h-index	713466 21 g-index
27 all docs	27 docs citations	27 times ranked	5490 citing authors

#	Article	IF	Citations
1	Fast Calculation of Molecular Polar Surface Area as a Sum of Fragment-Based Contributions and Its Application to the Prediction of Drug Transport Properties. Journal of Medicinal Chemistry, 2000, 43, 3714-3717.	6.4	2,413
2	The Coding of the Three-Dimensional Structure of Molecules by Molecular Transforms and Its Application to Structure-Spectra Correlations and Studies of Biological Activity. Journal of Chemical Information and Computer Sciences, 1996, 36, 334-344.	2.8	314
3	Quest for the Rings. In Silico Exploration of Ring Universe To Identify Novel Bioactive Heteroaromatic Scaffolds. Journal of Medicinal Chemistry, 2006, 49, 4568-4573.	6.4	221
4	Library Design for Fragment Based Screening. Current Topics in Medicinal Chemistry, 2005, 5, 751-762.	2.1	195
5	Chemical Information in 3D Space. Journal of Chemical Information and Computer Sciences, 1996, 36, 1030-1037.	2.8	176
6	Relationships between Molecular Complexity, Biological Activity, and Structural Diversity. Journal of Chemical Information and Modeling, 2006, 46, 525-535.	5.4	88
7	Estimation of pKa for Druglike Compounds Using Semiempirical and Information-Based Descriptors. Journal of Chemical Information and Modeling, 2007, 47, 450-459.	5.4	70
8	Complex molecules: do they add value?. Current Opinion in Chemical Biology, 2005, 9, 310-316.	6.1	69
9	Linking Phenotypes and Modes of Action Through High-Content Screen Fingerprints. Assay and Drug Development Technologies, 2015, 13, 415-427.	1.2	67
10	How Phenotypic Screening Influenced Drug Discovery: Lessons from Five Years of Practice. Assay and Drug Development Technologies, 2017, 15, 239-246.	1.2	58
11	Biodiversity of small molecules â€“ a new perspective in screening set selection. Drug Discovery Today, 2013, 18, 674-680.	6.4	51
12	Clustering and Rule-Based Classifications of Chemical Structures Evaluated in the Biological Activity Space. Journal of Chemical Information and Modeling, 2007, 47, 325-336.	5.4	50
13	Applications of Self-Organizing Neural Networks in Virtual Screening and Diversity Selection. Journal of Chemical Information and Modeling, 2006, 46, 2319-2323.	5.4	35
14	Rapid Access to Infrared Reference Spectra of Arbitrary Organic Compounds: Scope and Limitations of an Approach to the Simulation of Infrared Spectra by Neural Networks. Chemistry - A European Journal, 2000, 6, 920-927.	3.3	32
15	Benchmarking of Multivariate Similarity Measures for High-Content Screening Fingerprints in Phenotypic Drug Discovery. Journal of Biomolecular Screening, 2013, 18, 1284-1297.	2.6	32
16	Comparison of Multivariate Data Analysis Strategies for High-Content Screening. Journal of Biomolecular Screening, 2011, 16, 338-347.	2.6	31
17	Web-based cheminformatics tools deployed via corporate Intranets. Drug Discovery Today Biosilico, 2004, 2, 201-207.	0.7	24
18	Identification and Classification of GPCR Ligands Using Self-Organizing Neural Networks. QSAR and Combinatorial Science, 2005, 24, 270-276.	1.4	20

#	Article	IF	Citations
19	Differentiation and Visualization of Diverse Cellular Phenotypic Responses in Primary High-Content Screening. Journal of Biomolecular Screening, 2012, 17, 843-849.	2.6	18
20	A Combined Application of Reaction Prediction and Infrared Spectra Simulation for the Identification of Degradation Products ofs-Triazine Herbicides. Chemistry - A European Journal, 2001, 7, 2254-2260.	3.3	8
21	ToxizitÃtsvorhersage im Intranet. Nachrichten Aus Der Chemie, 2004, 52, 162-164.	0.0	2