

# Paul Selzer

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/11936855/publications.pdf>

Version: 2024-02-01

21  
papers

3,977  
citations

489802

18  
h-index

799663

21  
g-index

27  
all docs

27  
docs citations

27  
times ranked

6082  
citing authors

#	ARTICLE	IF	CITATIONS
1	How Phenotypic Screening Influenced Drug Discovery: Lessons from Five Years of Practice. <i>Assay and Drug Development Technologies</i> , 2017, 15, 239-246.	0.6	58
2	Linking Phenotypes and Modes of Action Through High-Content Screen Fingerprints. <i>Assay and Drug Development Technologies</i> , 2015, 13, 415-427.	0.6	67
3	Biodiversity of small molecules – a new perspective in screening set selection. <i>Drug Discovery Today</i> , 2013, 18, 674-680.	3.2	51
4	Benchmarking of Multivariate Similarity Measures for High-Content Screening Fingerprints in Phenotypic Drug Discovery. <i>Journal of Biomolecular Screening</i> , 2013, 18, 1284-1297.	2.6	32
5	Differentiation and Visualization of Diverse Cellular Phenotypic Responses in Primary High-Content Screening. <i>Journal of Biomolecular Screening</i> , 2012, 17, 843-849.	2.6	18
6	Comparison of Multivariate Data Analysis Strategies for High-Content Screening. <i>Journal of Biomolecular Screening</i> , 2011, 16, 338-347.	2.6	31
7	Clustering and Rule-Based Classifications of Chemical Structures Evaluated in the Biological Activity Space. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 325-336.	2.5	50
8	Estimation of pKa for Druglike Compounds Using Semiempirical and Information-Based Descriptors. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 450-459.	2.5	70
9	Quest for the Rings. In Silico Exploration of Ring Universe To Identify Novel Bioactive Heteroaromatic Scaffolds. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 4568-4573.	2.9	221
10	Relationships between Molecular Complexity, Biological Activity, and Structural Diversity. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 525-535.	2.5	88
11	Applications of Self-Organizing Neural Networks in Virtual Screening and Diversity Selection. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 2319-2323.	2.5	35
12	Complex molecules: do they add value?. <i>Current Opinion in Chemical Biology</i> , 2005, 9, 310-316.	2.8	69
13	Identification and Classification of GPCR Ligands Using Self-Organizing Neural Networks. <i>QSAR and Combinatorial Science</i> , 2005, 24, 270-276.	1.5	20
14	Library Design for Fragment Based Screening. <i>Current Topics in Medicinal Chemistry</i> , 2005, 5, 751-762.	1.0	195
15	Web-based cheminformatics tools deployed via corporate Intranets. <i>Drug Discovery Today Biosilico</i> , 2004, 2, 201-207.	0.7	24
16	Toxizitätsvorhersage im Intranet. <i>Nachrichten Aus Der Chemie</i> , 2004, 52, 162-164.	0.0	2
17	A Combined Application of Reaction Prediction and Infrared Spectra Simulation for the Identification of Degradation Products of Triazine Herbicides. <i>Chemistry - A European Journal</i> , 2001, 7, 2254-2260.	1.7	8
18	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. <i>Chemistry - A European Journal</i> , 2000, 6, 920-927.	1.7	32

#	ARTICLE	IF	CITATIONS
19	Fast Calculation of Molecular Polar Surface Area as a Sum of Fragment-Based Contributions and Its Application to the Prediction of Drug Transport Properties. <i>Journal of Medicinal Chemistry</i> , 2000, 43, 3714-3717.	2.9	2,413
20	Chemical Information in 3D Space. <i>Journal of Chemical Information and Computer Sciences</i> , 1996, 36, 1030-1037.	2.8	176
21	The Coding of the Three-Dimensional Structure of Molecules by Molecular Transforms and Its Application to Structure-Spectra Correlations and Studies of Biological Activity. <i>Journal of Chemical Information and Computer Sciences</i> , 1996, 36, 334-344.	2.8	314