Dilyana Dimova

List of Publications by Year
in descending order

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		758635	752256
28	427	12	20
papers	citations	h-index	g-index

28	28	28	459
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Computational Method for the Systematic Identification of Analog Series and Key Compounds Representing Series and Their Biological Activity Profiles. Journal of Medicinal Chemistry, 2016, 59, 7667-7676.	2.9	50
2	Matched Molecular Pair Analysis of Small Molecule Microarray Data Identifies Promiscuity Cliffs and Reveals Molecular Origins of Extreme Compound Promiscuity. Journal of Medicinal Chemistry, 2012, 55, 10220-10228.	2.9	41
3	Highly Promiscuous Small Molecules from Biological Screening Assays Include Many Pan-Assay Interference Compounds but Also Candidates for Polypharmacology. Journal of Medicinal Chemistry, 2016, 59, 10285-10290.	2.9	38
4	Analog series-based scaffolds: computational design and exploration of a new type of molecular scaffolds for medicinal chemistry. Future Science OA, 2016, 2, FSO149.	0.9	28
5	Monitoring the Progression of Structureâ€“Activity Relationship Information during Lead Optimization. Journal of Medicinal Chemistry, 2016, 59, 4235-4244.	2.9	27
6	Assessing the Target Differentiation Potential of Imidazole-Based Protein Kinase Inhibitors. Journal of Medicinal Chemistry, 2012, 55, 11067-11071.	2.9	24
7	Do Medicinal Chemists Learn from Activity Cliffs? A Systematic Evaluation of Cliff Progression in Evolving Compound Data Sets. Journal of Medicinal Chemistry, 2013, 56, 3339-3345.	2.9	23
8	Advancing the activity cliff concept, part II. F1000Research, 2014, 3, 75.	0.8	23
9	Advances in Computational Medicinal Chemistry: Matched Molecular Pair Analysis. Drug Development Research, 2012, 73, 518-527.	1.4	21
10	Method for the Evaluation of Structureâ€“Activity Relationship Information Associated with Coordinated Activity Cliffs. Journal of Medicinal Chemistry, 2014, 57, 6553-6563.	2.9	17
11	Identification and analysis of promiscuity cliffs formed by bioactive compounds and experimental implications. RSC Advances, 2017, 7, 58-66.	1.7	15
12	Application of a New Scaffold Concept for Computational Target Deconvolution of Chemical Cancer Cell Line Screens. ACS Omega, 2017, 2, 1463-1468.	1.6	14
13	Quantifying the Fingerprint Descriptor Dependence of Structureâ€“Activity Relationship Information on a Large Scale. Journal of Chemical Information and Modeling, 2013, 53, 2275-2281.	2.5	12
14	Extraction of SAR information from activity cliff clusters via matching molecular series. European Journal of Medicinal Chemistry, 2014, 87, 454-460.	2.6	12
15	Activity cliff clusters as a source of structureâ€“activity relationship information. Expert Opinion on Drug Discovery, 2015, 10, 441-447.	2.5	12
16	Assessing Scaffold Diversity of Kinase Inhibitors Using Alternative Scaffold Concepts and Estimating the Scaffold Hopping Potential for Different Kinases. Molecules, 2017, 22, 730.	1.7	12
17	Systematic assessment of coordinated activity cliffs formed by kinase inhibitors and detailed characterization of activity cliff clusters and associated SAR information. European Journal of Medicinal Chemistry, 2015, 90, 414-427.	2.6	9
18	Classification of matching molecular series on the basis of SAR phenotypes and structural relationships. MedChemComm, 2016, 7, 237-246.	3.5	8

#	Article	IF	Citations
19	Redundancy in two major compound databases. Drug Discovery Today, 2018, 23, 1183-1186.	3.2	8
20	Collection of analog series-based scaffolds from public compound sources. Future Science OA, 2018, 4, FSO287.	0.9	8
21	Computational design of new molecular scaffolds for medicinal chemistry, part II: generalization of analog series-based scaffolds. Future Science OA, 2018, 4, FSO267.	0.9	8
22	Systematic assessment of scaffold hopping versus activity cliff formation across bioactive compound classes following a molecular hierarchy. Bioorganic and Medicinal Chemistry, 2015, 23, 3183-3191.	1.4	4
23	Computational Chemical Biology: Identification of Small Molecular Probes that Discriminate between Members of Target Protein Families. Chemical Biology and Drug Design, 2012, 79, 369-375.	1.5	3
24	Systematic analysis of structural and activity relationships between conventional hierarchical and analog series-based scaffolds. RSC Advances, 2017, 7, 18718-18723.	1.7	3
25	Identification of Orthologous Target Pairs with SharedÂActive Compounds and Comparison of Organismâ€specific Activity Patterns. Chemical Biology and Drug Design, 2015, 86, 1105-1114.	1.5	2
26	Is scaffold hopping a reliable indicator for the ability of computational methods to identify structurally diverse active compounds?. Journal of Computer-Aided Molecular Design, 2017, 31, 603-608.	1.3	2
27	Exploring Structural Relationships between Bioactive and Commercial Chemical Space and Developing Target Hypotheses for Compound Acquisition. ACS Omega, 2017, 2, 7760-7766.	1.6	2
28	Mapping Biological Activities to Different Types of Molecular Scaffolds: Exemplary Application to Protein Kinase Inhibitors. Methods in Molecular Biology, 2018, 1825, 327-337.	0.4	1