Simone Fulle

List of Publications by Year in descending order

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1040056 1281871 11 887 9 11 citations h-index g-index papers 11 11 11 1562 citing authors docs citations times ranked all docs

#	Article	IF	CITATIONS
1	Development of Cagrilintide, a Long-Acting Amylin Analogue. Journal of Medicinal Chemistry, 2021, 64, 11183-11194.	6.4	41
2	Modeling conformational flexibility of kinases in inactive states. Proteins: Structure, Function and Bioinformatics, 2019, 87, 943-951.	2.6	11
3	Mol2vec: Unsupervised Machine Learning Approach with Chemical Intuition. Journal of Chemical Information and Modeling, 2018, 58, 27-35.	5.4	398
4	Kinomeâ€Wide Profiling Prediction of Small Molecules. ChemMedChem, 2018, 13, 495-499.	3.2	27
5	From Cancer to Pain Target by Automated Selectivity Inversion of a Clinical Candidate. Journal of Medicinal Chemistry, 2018, 61, 4851-4859.	6.4	9
6	Coupling Matched Molecular Pairs with Machine Learning for Virtual Compound Optimization. Journal of Chemical Information and Modeling, 2017, 57, 3079-3085.	5.4	16
7	Profiling Prediction of Kinase Inhibitors: Toward the Virtual Assay. Journal of Medicinal Chemistry, 2017, 60, 474-485.	6.4	94
8	KinMap: a web-based tool for interactive navigation through human kinome data. BMC Bioinformatics, 2017, 18, 16.	2.6	235
9	11th German Conference on Chemoinformatics (GCC 2015). Journal of Cheminformatics, 2016, 8, 18.	6.1	1
10	Identification and Visualization of Kinase-Specific Subpockets. Journal of Chemical Information and Modeling, 2016, 56, 335-346.	5.4	18
11	Pocketome of Human Kinases: Prioritizing the ATP Binding Sites of (Yet) Untapped Protein Kinases for Drug Discovery. Journal of Chemical Information and Modeling, 2015, 55, 538-549.	5.4	37