Jules Leguy

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/5654335/publications.pdf Version: 2024-02-01

1937685 2272923 6 120 4 4 citations h-index g-index papers 10 10 10 172 docs citations times ranked citing authors all docs

#	Article	IF	CITATIONS
1	Goal-directed generation of new molecules by AI methods. , 2022, , 39-67.		Ο
2	Scalable estimator of the diversity for de novo molecular generation resulting in a more robust QM dataset (OD9) and a more efficient molecular optimization. Journal of Cheminformatics, 2021, 13, 76.	6.1	5
3	Surrogate-Based Black-Box Optimization Method for Costly Molecular Properties. , 2021, , .		1
4	EvoMol: a flexible and interpretable evolutionary algorithm for unbiased de novo molecular generation. Journal of Cheminformatics, 2020, 12, 55.	6.1	29
5	MixONat, a Software for the Dereplication of Mixtures Based on ¹³ C NMR Spectroscopy. Analytical Chemistry, 2020, 92, 8793-8801.	6.5	27
6	Dataset's chemical diversity limits the generalizability of machine learning predictions. Journal of Cheminformatics, 2019, 11, 69.	6.1	57