

# Jules Leguy

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/5654335/publications.pdf>

Version: 2024-02-01

6  
papers

120  
citations

1937685

4  
h-index

2272923

4  
g-index

10  
all docs

10  
docs citations

10  
times ranked

172  
citing authors

| # | ARTICLE                                                                                                                                                                                                 | IF  | CITATIONS |
|---|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----|-----------|
| 1 | Dataset's chemical diversity limits the generalizability of machine learning predictions. Journal of Cheminformatics, 2019, 11, 69.                                                                     | 6.1 | 57        |
| 2 | EvoMol: a flexible and interpretable evolutionary algorithm for unbiased de novo molecular generation. Journal of Cheminformatics, 2020, 12, 55.                                                        | 6.1 | 29        |
| 3 | MixONat, a Software for the Dereplication of Mixtures Based on <sup>13</sup> C NMR Spectroscopy. Analytical Chemistry, 2020, 92, 8793-8801.                                                             | 6.5 | 27        |
| 4 | 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         |
| 5 | Surrogate-Based Black-Box Optimization Method for Costly Molecular Properties. , 2021, , .                                                                                                              |     | 1         |
| 6 | Goal-directed generation of new molecules by AI methods. , 2022, , 39-67.                                                                                                                               |     | 0         |