

Luc M Leblanc

List of Publications by Year in descending order

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Version: 2024-02-01

21
papers

443
citations

759233

12
h-index

713466

21
g-index

21
all docs

21
docs citations

21
times ranked

661
citing authors

#	ARTICLE	IF	CITATIONS
1	Ketone Analog of Caffeic Acid Phenethyl Ester Exhibits Antioxidant Activity via Activation of ERK-Dependent Nrf2 Pathway. <i>Applied Sciences (Switzerland)</i> , 2022, 12, 3062.	2.5	2
2	A Universal Force Field for Materials, Periodic GFN-FF: Implementation and Examination. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 7827-7849.	5.3	10
3	Asymptotic Pairwise Dispersion Corrections Can Describe Layered Materials Accurately. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 2298-2302.	4.6	17
4	What is "many-body" dispersion and should I worry about it?. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 8266-8276.	2.8	30
5	Dispersion XDM with Hybrid Functionals: Delocalization Error and Halogen Bonding in Molecular Crystals. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4933-4944.	5.3	22
6	Clusters in Liquid Fatty Acids: Structure and Role in Nucleation. <i>Journal of Physical Chemistry B</i> , 2019, 123, 7043-7054.	2.6	8
7	Crystal-energy landscapes of active pharmaceutical ingredients using composite approaches. <i>CrystEngComm</i> , 2019, 21, 5995-6009.	2.6	14
8	Composite and Low-Cost Approaches for Molecular Crystal Structure Prediction. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2265-2276.	5.3	18
9	A computational exploration of the crystal energy and charge-carrier mobility landscapes of the chiral [6]helicene molecule. <i>Nanoscale</i> , 2018, 10, 1865-1876.	5.6	48
10	Pervasive Delocalisation Error Causes Spurious Proton Transfer in Organic Acid-Base Co-Crystals. <i>Angewandte Chemie</i> , 2018, 130, 15122-15126.	2.0	10
11	Pervasive Delocalisation Error Causes Spurious Proton Transfer in Organic Acid-Base Co-Crystals. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 14906-14910.	13.8	45
12	Non-Covalent Interactions in Molecular Crystals: Exploring the Accuracy of the Exchange-Hole Dipole Moment Model with Local Orbitals. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5715-5724.	5.3	9
13	Structure-activity relationship of caffeic acid phenethyl ester analogs as new 5-lipoxygenase inhibitors. <i>Chemical Biology and Drug Design</i> , 2017, 89, 514-528.	3.2	24
14	Competing fragmentation processes of β -substituted propanoate ions upon collision-induced dissociation. <i>Rapid Communications in Mass Spectrometry</i> , 2016, 30, 2133-2144.	1.5	4
15	Evaluation of Shear-Slip Transitions in Crystalline Aspirin by Density-Functional Theory. <i>Crystal Growth and Design</i> , 2016, 16, 6867-6873.	3.0	17
16	Phenyl group participation in rearrangements during collision-induced dissociation of deprotonated phenoxyacetic acid. <i>Rapid Communications in Mass Spectrometry</i> , 2015, 29, 2293-2301.	1.5	3
17	Torquoselectivity in the Nazarov Reactions of Allenyl Vinyl Ketones. <i>Journal of Organic Chemistry</i> , 2015, 80, 1042-1051.	3.2	29
18	Density Functional Theory Study of BF_3 -Mediated Additions of Enols and [(Trimethylsilyl)oxy]alkenes to an Oxyallyl Cation: Homologous Mukaiyama Reactions. <i>Journal of Physical Chemistry A</i> , 2015, 119, 6714-6722.	2.5	6

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19	NMR Metabolomics Analysis of the Effects of 5-Lipoxygenase Inhibitors on Metabolism in Glioblastomas. <i>Journal of Proteome Research</i> , 2013, 12, 2165-2176.	3.7	19
20	Synthesis and Antiradical/Antioxidant Activities of Caffeic Acid Phenethyl Ester and Its Related Propionic, Acetic, and Benzoic Acid Analogues. <i>Molecules</i> , 2012, 17, 14637-14650.	3.8	50
21	Caffeic Acid Phenethyl Ester and Its Amide Analogue Are Potent Inhibitors of Leukotriene Biosynthesis in Human Polymorphonuclear Leukocytes. <i>PLoS ONE</i> , 2012, 7, e31833.	2.5	58