Luc Patiny

List of Publications by Year
in descending order

54 papers	2,795 citations	257450 24 h-index	182427 51 g-index
62 all docs	62 docs citations	62 times ranked	4283 citing authors

#	Article	IF	Citations
1	Online chemical modeling environment (OCHEM): web platform for data storage, model development and publishing of chemical information. Journal of Computer-Aided Molecular Design, 2011, 25, 533-554.	2.9	453
2	EcoScale, a semi-quantitative tool to select an organic preparation based on economical and ecological parameters. Beilstein Journal of Organic Chemistry, 2006, 2, 3.	2.2	401
3	ChemCalc: A Building Block for Tomorrowâ€™s Chemical Infrastructure. Journal of Chemical Information and Modeling, 2013, 53, 1223-1228.	5.4	316
4	Switch Peptides In Statu Nascendi: Induction of Conformational Transitions Relevant to Degenerative Diseases. Angewandte Chemie - International Edition, 2004, 43, 4172-4178.	13.8	163
5	Bioluminescent sensor proteins for point-of-care therapeutic drug monitoring. Nature Chemical Biology, 2014, 10, 598-603.	8.0	161
6	www.nmrdb.org: Resurrecting and Processing NMR Spectra On-line. Chimia, 2008, 62, 280.	0.6	126
7	Fast and accurate algorithm for the simulation of NMR spectra of large spin systems. Journal of Magnetic Resonance, 2011, 209, 123-130.	2.1	119
8	Pseudoproline-Containing Analogues of Morphiceptin and Endomorphin-2: Evidence for aCisTyrâ^'Pro Amide Bond in the Bioactive Conformation. Journal of Medicinal Chemistry, 2001, 44, 3896-3903.	6.4	96
9	Design and Synthesis of Substrate Analogue Inhibitors of Peptide Deformylaseâ€. Biochemistry, 1999, 38, 4287-4295.	2.5	76
10	How Accurately Can We Predict the Melting Points of Drug-like Compounds?. Journal of Chemical Information and Modeling, 2014, 54, 3320-3329.	5.4	70
11	Open Source Drug Discovery: Highly Potent Antimalarial Compounds Derived from the Tres Cantos Arylpyrroles. ACS Central Science, 2016, 2, 687-701.	11.3	68
12	Pseudoprolines: Targeting acis Conformation in a Mimetic of the gp120 V3 Loop of HIV-1. Angewandte Chemie - International Edition, 2000, 39, 1111-1115.	13.8	58
13	Preclinical Development of a Vaccine â€˜Against Smokingâ€™. Oncology Research and Treatment, 2002, 25, 406-411.	1.2	52
14	A general and practical method of synthesis of 2-disubstituted-1-chloro- and 1-bromoenamines. Tetrahedron, 1998, 54, 9207-9222.	1.9	37
15	A biosensor for measuring NAD+ levels at the point of care. Nature Metabolism, 2019, 1, 1219-1225.	11.9	37
16	Synthetic routes to NEtXaa4-cyclosporin A derivatives as potential anti-HIV I drugs. Tetrahedron Letters, 2000, 41, 7193-7196.	1.4	35
17	Antimalarial and antitubercular nostocarboline and eudistomin derivatives: Synthesis, in vitro and in vivo biological evaluation. Bioorganic and Medicinal Chemistry, 2010, 18, 1464-1476.	3.0	35
18	Making the collective knowledge of chemistry open and machine actionable. Nature Chemistry, 2022, 14, 365-376.	13.6	34

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19	PDB-Explorer: a web-based interactive map of the protein data bank in shape space. BMC Bioinformatics, 2015, 16, 339.	2.6	31
20	Introduction of acis-Prolyl Mimic in Position 7 of the Peptide Hormone Oxytocin Does Not Result in Antagonistic Activity. Journal of Medicinal Chemistry, 2005, 48, 6553-6562.	6.4	30
21	Versatile Tool for the Analysis of Metalâ€“Protein Interactions Reveals the Promiscuity of Metallodrugâ€“Protein Interactions. Analytical Chemistry, 2017, 89, 11985-11989.	6.5	30
22	Wikipedia Chemical Structure Explorer: substructure and similarity searching of molecules from Wikipedia. Journal of Cheminformatics, 2015, 7, 10.	6.1	29
23	Pseudo-prolines (Î¨Pro): direct insertion of Î¨Pro systems into cysteine containing peptides. Tetrahedron Letters, 2002, 43, 4389-4390.	1.4	25
24	A virtual screening approach to identifying the greenest compound for a task: application to switchable-hydrophilicity solvents. Green Chemistry, 2015, 17, 5182-5188.	9.0	23
25	Pseudoprolines (Pro) in Drug Design: Direct Insertion of Pro Systems into Cyclosporinâ€...C. Chemistry - A European Journal, 2000, 6, 4358-4363.	3.3	22
26	Dielsâ€“Alder reactions of activated furans to cyclopentenone derivatives: a regiodivergent Dielsâ€“Alder approach towards polyfunctionalised cis-hydrindanones. Tetrahedron Letters, 2000, 41, 6377-6381.	1.4	19
27	The C6H6 NMR repository: An integral solution to control the flow of your data from the magnet to the public. Magnetic Resonance in Chemistry, 2018, 56, 520-528.	1.9	19
28	A data-driven perspective on the colours of metalâ€“organic frameworks. Chemical Science, 2021, 12, 3587-3598.	7.4	16
29	Development of a systematic computer vision-based method to analyse and compare images of false identity documents for forensic intelligence purposesâ€“Part I: Acquisition, calibration and validation issues. Forensic Science International, 2016, 260, 74-84.	2.2	14
30	Aom²S: A new webâ€based application for DNA/RNA tandem mass spectrometry data interpretation. Rapid Communications in Mass Spectrometry, 2020, 34, e8927.	1.5	14
31	Natureâ€Inspired Circularâ€Economy Recycling for Proteins: Proof of Concept. Advanced Materials, 2021, 33, e2104581.	21.0	14
32	Augmenting Research, Education, and Outreach with Client-Side Web Programming. Trends in Biotechnology, 2018, 36, 473-476.	9.3	13
33	Making Molecules Vibrate: Interactive Web Environment for the Teaching of Infrared Spectroscopy. Journal of Chemical Education, 2022, 99, 561-569.	2.3	13
34	Monitoring of illicit pill distribution networks using an image collection exploration framework. Forensic Science International, 2012, 223, 298-305.	2.2	11
35	MSPolyCalc: A webâ€based App for polymer mass spectrometry data interpretation. The case study of a pharmaceutical excipient. Rapid Communications in Mass Spectrometry, 2020, 34, e8652.	1.5	11
36	Synthesis and characterization of constrained cyclosporin A derivatives containing a pseudo-proline group. Tetrahedron, 2003, 59, 5241-5249.	1.9	8

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37	â€œAsk ErnÃ¶â€: a self-learning tool for assignment and prediction of nuclear magnetic resonance spectra. Journal of Cheminformatics, 2016, 8, 26.	6.1	8
38	Fully automatic assignment of small molecules' NMR spectra without relying on chemical shift predictions. Magnetic Resonance in Chemistry, 2015, 53, 603-611.	1.9	7
39	Biochemical and biophysical characterization of ruthenation of BRCA1 RING protein by RAPTA complexes and its E3 ubiquitin ligase activity. Biochemical and Biophysical Research Communications, 2017, 488, 355-361.	2.1	7
40	Versatile Synthesis of Boc Protected Hydrazinoacetic Acid and its Application to the Chemoselective Ligation of Tasp Molecules. Protein and Peptide Letters, 2004, 11, 539-542.	0.9	7
41	Fast and shift-insensitive similarity comparisons of NMR using a tree-representation of spectra. Chemometrics and Intelligent Laboratory Systems, 2013, 127, 1-6.	3.5	6
42	Teaching NMR spectra analysis with nmr.cheminfo.org. Magnetic Resonance in Chemistry, 2018, 56, 529-534.	1.9	5
43	Structural Analysis from Classroom to Laboratory. Journal of Chemical Education, 2012, 89, 1083-1083.	2.3	4
44	A new method for the comparison of 1H NMR predictors based on tree-similarity of spectra. Journal of Cheminformatics, 2014, 6, 9.	6.1	4
45	Site Selective Functionalization of Fluorinated Nitrogen Heterocycles. ACS Symposium Series, 2009, , 23-35.	0.5	3
46	Seized Ecstasy Pills: Infrared Spectra and Image Datasets. Data, 2020, 5, 116.	2.3	3
47	Pseudo-Prolines: Reversible Conformational Trap of Cyclosporin C as Novel Concept for Prodrug Design. Chimia, 2004, 58, 237-240.	0.6	2
48	Improving the efficiency of branch-and-bound complete-search NMR assignment using the symmetry of molecules and spectra. Journal of Chemical Physics, 2015, 142, 074103.	3.0	2
49	A mild method for the replacement of a hydroxyl group by halogen: 3. the dichotomous behavior of Î±-haloenamines towards allylic and propargylic alcohols. Tetrahedron, 2021, 89, 132148.	1.9	2
50	NMRium browser-based nuclear magnetic resonance data processing. Spectroscopy Europe, 0, , 21.	0.0	2
51	Simultaneous mass spectrometry analysis of cisplatin with oligonucleotide-peptide mixtures: implications for the mechanism of action. Journal of Biological Inorganic Chemistry, 2022, 27, 239.	2.6	1
52	Pseudoproline Libraries for Tuning Inhibitors of SH3 Domain Mediated Protein-Protein Interactions. , 2001, , 185-186.		0
53	Pseudoprolines for Studying Bioactive cis-Prolyl Conformations. , 2001, , 697-698.		0
54	Natureâ€Inspired Circularâ€Economy Recycling for Proteins: Proof of Concept (Adv. Mater. 44/2021). Advanced Materials, 2021, 33, 2170345.	21.0	0