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	Making Molecules Vibrate: Interactive Web Environment for the Teaching of Infrared Spectroscopy. Journal of Chemical Education, 2022, 99, 561-569.	2.3	13
2	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
3	Making the collective knowledge of chemistry open and machine actionable. Nature Chemistry, 2022, 14, 365-376.	13.6	34
4	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
5	Natureâ€Inspired Circularâ€Economy Recycling for Proteins: Proof of Concept. Advanced Materials, 2021, 33, e2104581.	21.0	14
6	A data-driven perspective on the colours of metalâ€“organic frameworks. Chemical Science, 2021, 12, 3587-3598.	7.4	16
7	Natureâ€Inspired Circularâ€Economy Recycling for Proteins: Proof of Concept (Adv. Mater. 44/2021). Advanced Materials, 2021, 33, 2170345.	21.0	0
8	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
9	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
10	Seized Ecstasy Pills: Infrared Spectra and Image Datasets. Data, 2020, 5, 116.	2.3	3
11	A biosensor for measuring NAD+ levels at the point of care. Nature Metabolism, 2019, 1, 1219-1225.	11.9	37
12	Teaching NMR spectra analysis with nmr.cheminfo.org. Magnetic Resonance in Chemistry, 2018, 56, 529-534.	1.9	5
13	Augmenting Research, Education, and Outreach with Client-Side Web Programming. Trends in Biotechnology, 2018, 36, 473-476.	9.3	13
14	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
15	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
16	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
17	Open Source Drug Discovery: Highly Potent Antimalarial Compounds Derived from the Tres Cantos Arylpyrroles. ACS Central Science, 2016, 2, 687-701.	11.3	68
18	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

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19	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
20	PDB-Explorer: a web-based interactive map of the protein data bank in shape space. BMC Bioinformatics, 2015, 16, 339.	2.6	31
21	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
22	Wikipedia Chemical Structure Explorer: substructure and similarity searching of molecules from Wikipedia. Journal of Cheminformatics, 2015, 7, 10.	6.1	29
23	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
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	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
26	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
27	Bioluminescent sensor proteins for point-of-care therapeutic drug monitoring. Nature Chemical Biology, 2014, 10, 598-603.	8.0	161
28	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
29	ChemCalc: A Building Block for Tomorrowâ€™s Chemical Infrastructure. Journal of Chemical Information and Modeling, 2013, 53, 1223-1228.	5.4	316
30	Monitoring of illicit pill distribution networks using an image collection exploration framework. Forensic Science International, 2012, 223, 298-305.	2.2	11
31	Structural Analysis from Classroom to Laboratory. Journal of Chemical Education, 2012, 89, 1083-1083.	2.3	4
32	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
33	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
34	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
35	Site Selective Functionalization of Fluorinated Nitrogen Heterocycles. ACS Symposium Series, 2009, , 23-35.	0.5	3
36	www.nmrdb.org: Resurrecting and Processing NMR Spectra On-line. Chimia, 2008, 62, 280.	0.6	126

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37	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
38	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
39	Switch Peptides In Statu Nascendi: Induction of Conformational Transitions Relevant to Degenerative Diseases. Angewandte Chemie - International Edition, 2004, 43, 4172-4178.	13.8	163
40	Pseudo-Prolines: Reversible Conformational Trap of Cyclosporin C as Novel Concept for Prodrug Design. Chimia, 2004, 58, 237-240.	0.6	2
41	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
42	Synthesis and characterization of constrained cyclosporin A derivatives containing a pseudo-proline group. Tetrahedron, 2003, 59, 5241-5249.	1.9	8
43	Preclinical Development of a Vaccine â€˜Against Smokingâ€™. Oncology Research and Treatment, 2002, 25, 406-411.	1.2	52
44	Pseudo-prolines (Î¨Pro): direct insertion of Î¨Pro systems into cysteine containing peptides. Tetrahedron Letters, 2002, 43, 4389-4390.	1.4	25
45	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
46	Pseudoproline Libraries for Tuning Inhibitors of SH3 Domain Mediated Protein-Protein Interactions. , 2001, , 185-186.		0
47	Pseudoprolines for Studying Bioactive cis-Prolyl Conformations. , 2001, , 697-698.		0
48	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
49	Pseudoprolines (Pro) in Drug Design: Direct Insertion of Pro Systems into Cyclosporinâ€…C. Chemistry - A European Journal, 2000, 6, 4358-4363.	3.3	22
50	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
51	Synthetic routes to NEtXaa4-cyclosporin A derivatives as potential anti-HIV I drugs. Tetrahedron Letters, 2000, 41, 7193-7196.	1.4	35
52	Design and Synthesis of Substrate Analogue Inhibitors of Peptide Deformylaseâ€. Biochemistry, 1999, 38, 4287-4295.	2.5	76
53	A general and practical method of synthesis of 2-disubstituted-1-chloro- and 1-bromoenamines. Tetrahedron, 1998, 54, 9207-9222.	1.9	37
54	NMRium browser-based nuclear magnetic resonance data processing. Spectroscopy Europe, 0, , 21.	0.0	2