Alexandre Hocquet

List of Publications by Year
in descending order

30	633	759233 12	580821 25
papers	citations	h-index	g-index

33	33	33	728
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Epistemic issues in computational reproducibility: software as the elephant in the room. European Journal for Philosophy of Science, 2021, 11, 1.	1.1	9
2	Models, Parameterization, and Software: Epistemic Opacity in Computational Chemistry. Perspectives on Science, 2020, 28, 610-629.	1.0	4
3	ParcoursÂ11. Reprenez ce texte sur la science ouverte et transformez-le. , 2019, , 527-534.		2
4	Mailing list archives as useful primary sources for historians: looking for flame wars. Internet Histories, 2018, 2, 38-54.	1.1	6
5	â€œWe were here before the Web and hypeâ€¦â€: a brief history of and tribute to the Computational Chemistry List. Journal of Cheminformatics, 2018, 10, 67.	6.1	2
6	â€œOnly the Initiates Will Have the Secrets Revealedâ€: Computational Chemists and the Openness of Scientific Software. IEEE Annals of the History of Computing, 2017, 39, 40-58.	0.2	5
7	â€œOnly the Initiates Will Have the Secrets Revealedâ€: Computational Chemists and the Openness of Scientific Software. IEEE Annals of the History of Computing, 2017, 39, 40-58.	0.2	2
8	WikipÃ©dia au prisme de lâ€™Ã©pistÃ©mologie sociale et des Ã©tudes des sciences. Cahiers Philosophiques, 2015, nÂ° 141, 68-86.	0.0	2
9	Stereodynamics of Nitrogen Chiral Centers in azaâ€Î²³â€Cyclodipeptides. Chirality, 2013, 25, 341-349.	2.6	4
10	DFT, ab initio, NMR, and NBO analyses of NÎ±-substituted hydrazino acetamides: Experimental vs theoretical values. Tetrahedron, 2010, 66, 2322-2330.	1.9	7
11	DFT and ab initio potential energy scan and hydrogen bond analysis of NÎ±-substituted hydrazino acetamides: Characterization of the â€œhydrazinoturnâ€•hydrogen bonding pattern. Computational and Theoretical Chemistry, 2009, 911, 92-97.	1.5	2
12	A conceptual DFT study of hydrazino peptides: Assessment of the nucleophilicity of the nitrogen atoms by means of the dual descriptor Î”f(r). Computational and Theoretical Chemistry, 2008, 849, 46-51.	1.5	54
13	The â€œhydrazinoturnâ€•hydrogen bonding network in hydrazinopeptides and aza-Î²3-peptides as probed by an AIM topological analysis of the electronic density. Computational and Theoretical Chemistry, 2008, 869, 41-46.	1.5	8
14	Influence of the gelator structure and solvent on the organisation and chirality of self-assembling fibrillar networks. New Journal of Chemistry, 2008, 32, 1131.	2.8	33
15	Nâ€²-(3-Amino-1H-isoindol-1-ylidene)-R-carbohydrazides and Their Amide-Type Isomerism. European Journal of Organic Chemistry, 2006, 2006, 2833-2842.	2.4	11
16	Interaction of sodium and potassium ions with sandwiched cytosine-, guanine-, thymine-, and uracil-base tetrads. Journal of Computational Chemistry, 2005, 26, 352-364.	3.3	34
17	Intramolecular interactions along the reaction path of ketoâ€“enol tautomerism: Fukui functions as local softnesses and charges as local hardnesses. Computational and Theoretical Chemistry, 2004, 686, 213-218.	1.5	32
18	Guanine tetrads interacting with metal ions. An AIM topological analysis of the electronic densityElectronic Supplementary Information (ESI) available: Geometric data, topologic data at the BCP and integrated properties of the hydrogen atom of every H1â‹¯O6 and H2â‹¯N7 hydrogen bond. See http://www.rsc.org/suppdata/qu/b2/b210911e/. PhysChemComm, 2003, 6, 1-5.	0.8	22

#	Article	IF	Citations
19	L-nucleotides and 8-methylguanine of d(C1m8G2C3G4C5LG6LC7G8C9G10)2 act cooperatively to promote a left-handed helix under physiological salt conditions. Nucleic Acids Research, 2003, 31, 6986-6995.	14.5	7
20	Intramolecular hydrogen bonding in ribonucleosides: an AIM topological study of the electronic densityElectronic supplementary information (ESI) available: Integrated properties of atomic basins, radii characterizing hydrogen bond interactions, and properties at bond critical points of hydrogen bonds (Tables 3â€“5). See http://www.rsc.org/suppdata/cp/b2/b201339h/. Physical Chemistry Chemical Physics, 2002, 4, 3843-3848.	2.8	28
21	Are guanine tetrads stabilised by bifurcated hydrogen bonds? An AIM topological analysis of the electronic density. PhysChemComm, 2002, 5, 94-98.	0.8	24
22	Intramolecular hydrogen bonding in 2â€²-deoxyribonucleosides: an AIM topological study of the electronic density. Physical Chemistry Chemical Physics, 2001, 3, 3192-3199.	2.8	69
23	The peculiar role of cytosine in nucleoside conformational behaviour: Hydrogen bond donor capacity of nucleic bases. Physical Chemistry Chemical Physics, 2000, 2, 5351-5353.	2.8	44
24	Ground-State Properties of Nucleic Acid Constituents Studied by Density Functional Calculations. 3. Role of Sugar Puckering and Base Orientation on the Energetics and Geometry of 2â€˜-Deoxyribonucleosides and Ribonucleosides. Journal of Physical Chemistry B, 2000, 104, 4560-4568.	2.6	97
25	An Evaluation of the MM+ Force Field. Journal of Molecular Modeling, 1998, 4, 94-112.	1.8	88
26	Alchemy 2000 Version 1.00 for Windows:â€‰ A Review. Journal of Chemical Information and Computer Sciences, 1997, 37, 622-623.	2.8	2
27	Magnetic properties of dinuclear copper(II) complexes with a N6 pyridazine-derived ligandâ€Š*. Journal of the Chemical Society Dalton Transactions, 1997, , 3683-3690.	1.1	19
28	Dynamic behavior of a perfunctionalized Î²-cyclodextrin as probed by NMR and molecular modeling. Carbohydrate Research, 1997, 303, 379-393.	2.3	9
29	Structures of (1) N-(2-pyridyl)-, (2) N-(3-pyridyl)- and (3) N-(4-pyridyl)-N'-(4-chlorophenyl)urea. Acta Crystallographica Section C: Crystal Structure Communications, 1994, 50, 1507-1511.	0.4	3
30	Synthesis and Spectroscopic Study of Plant Growth Regulators Phenylpyridylureas: An "Agrorganic" Undergraduate Laboratory Experiment. Journal of Chemical Education, 1994, 71, 1092.	2.3	4