JÃ©rÃ´me Graton

List of Publications by Year
in descending order

62 papers	2,097 citations	218381 26 h-index	243296 44 g-index
65 all docs	65 docs citations	65 times ranked	2527 citing authors

#	Article	IF	Citations
1	Hydrogen-bond acidity of silanols: A combined experimental and theoretical study. Journal of Molecular Structure, 2022, 1266, 133505.	1.8	1
2	An expanded halogen bonding scale using astatine. Chemical Science, 2021, 12, 10855-10861.	3.7	7
3	Delocalized relativistic effects, from the viewpoint of halogen bonding. Physical Chemistry Chemical Physics, 2021, 23, 4064-4074.	1.3	10
4	A regioselective C7 bromination and C7 palladium-catalyzed Suzukiâ€“Miyaura cross-coupling arylation of 4-substituted NH-free indazoles. RSC Advances, 2021, 11, 7107-7114.	1.7	7
5	Systematic Investigation of Lipophilicity Modulation by Aliphatic Fluorination Motifs. Journal of Medicinal Chemistry, 2020, 63, 1002-1031.	2.9	83
6	Towards a Stronger Halogen Bond Involving Astatine: Unexpected Adduct with Bu₃PO Stabilized by Hydrogen Bonding. Chemistry - A European Journal, 2020, 26, 3713-3717.	1.7	13
7	On the Interplay between Chargeâ€Shift Bonding and Halogen Bonding. ChemPhysChem, 2020, 21, 240-250.	1.0	18
8	Lipophilicity trends upon fluorination of isopropyl, cyclopropyl and 3-oxetanyl groups. Beilstein Journal of Organic Chemistry, 2020, 16, 2141-2150.	1.3	13
9	Characterization of Steroids through Collision Cross Sections: Contribution of Quantum Chemistry Calculations. Analytical Chemistry, 2020, 92, 6034-6042.	3.2	12
10	Binding of Sulfoxaflor to Aplysia californica-AChBP: Computational Insights from Multiscale Approaches. Journal of Chemical Information and Modeling, 2019, 59, 3755-3769.	2.5	8
11	3,4-Dideoxy-3,3,4,4-tetrafluoro- and 4-OH epimeric 3-deoxy-3,3-difluoro-Î±-GalCer analogues: Synthesis and biological evaluation on human iNKT cells stimulation. European Journal of Medicinal Chemistry, 2019, 178, 195-213.	2.6	11
12	Synthesis of 2,3,4-Trideoxy-2,3,4-trifluoroglucose. Journal of Organic Chemistry, 2019, 84, 5899-5906.	1.7	16
13	Quantum calculations of At-mediated halogen bonds: on the influence of relativistic effects. New Journal of Chemistry, 2018, 42, 10510-10517.	1.4	25
14	Experimental and computational evidence of halogen bonds involving astatine. Nature Chemistry, 2018, 10, 428-434.	6.6	63
15	Spinâ€“orbit coupling as a probe to decipher halogen bonding. Physical Chemistry Chemical Physics, 2018, 20, 29616-29624.	1.3	21
16	Reducing the Lipophilicity of Perfluoroalkyl Groups by CF₂â€“F/CF₂â€“Me or CF₃/CH₃ Exchange. Journal of Medicinal Chemistry, 2018, 61, 10602-10618.	2.9	66
17	Conformations and Binding Properties of Thiametoxam and Clothianidin Neonicotinoid Insecticides to Nicotinic Acetylcholine Receptors: The Contribution of Ïƒâ€Hole Interactions. ChemPhysChem, 2018, 19, 3069-3083.	1.0	7
18	Influence of Alcohol Î²â€Fluorination on Hydrogenâ€Bond Acidity of Conformationally Flexible Substrates. Chemistry - A European Journal, 2017, 23, 2811-2819.	1.7	31

#	ARTICLE	IF	CITATIONS
19	A Study of Intramolecular Hydrogen Bonding in Levoglucosan Derivatives. Molecules, 2017, 22, 518.	1.7	14
20	Radical Cyclisation of Î±â€Halo Aluminium Acetals: A Mechanistic Study. Chemistry - A European Journal, 2016, 22, 4809-4824.	1.7	1
21	Î±â€Fluoroâ€‹i>o</i>â€cresols: The Key Role of Intramolecular Hydrogen Bonding in Conformational Preference and HydrogenâEBond Acidity. ChemPhysChem, 2016, 17, 2702-2709.	1.0	12
22	Predictive Models for Halogenâ€bond Basicity of Binding Sites of Polyfunctional Molecules. Molecular Informatics, 2016, 35, 70-80.	1.4	12
23	Hydrogen-Bond Accepting Properties of New Heteroaromatic Ring Chemical Motifs: A Theoretical Study. Journal of Chemical Information and Modeling, 2016, 56, 322-334.	2.5	31
24	Influence of Fluorination on the Conformational Properties and HydrogenâEBond Acidity of Benzyl Alcohol Derivatives. Chemistry - A European Journal, 2015, 21, 11462-11474.	1.7	25
25	Intramolecular OHâ‹…â‹…â‹…Fluorine Hydrogen Bonding in Saturated, Acyclic Fluorohydrins: The Î³â€Fluoropropanol Motif. Chemistry - A European Journal, 2015, 21, 17808-17816.	1.7	41
26	Molecular recognition of thiaclopride by Aplysia californica AChBP: new insights from a computational investigation. Journal of Computer-Aided Molecular Design, 2015, 29, 1151-1167.	1.3	8
27	Molecular features and toxicological properties of four common pesticides, acetamiprid, deltamethrin, chlorpyriphos and fipronil. Bioorganic and Medicinal Chemistry, 2015, 23, 1540-1550.	1.4	23
28	Imidacloprid and thiacloprid neonicotinoids bind more favourably to cockroach than to honeybee Î±6 nicotinic acetylcholine receptor: Insights from computational studies. Journal of Molecular Graphics and Modelling, 2015, 55, 1-12.	1.3	13
29	Insights into a highly conserved network of hydrogen bonds in the agonist binding site of nicotinic acetylcholine receptors: A structural and theoretical study. Proteins: Structure, Function and Bioinformatics, 2014, 82, 2303-2317.	1.5	1
30	Individual HydrogenâEBond Strength QSPR Modelling with ISIDA Local Descriptors: a Step Towards Polyfunctional Molecules. Molecular Informatics, 2014, 33, 477-487.	1.4	19
31	Hydrogen-Bond Acidity of OH Groups in Various Molecular Environments (Phenols, Alcohols, Steroid) Tj ETQq1 1 0.784314 rgBT /Ove Calculations. Journal of Physical Chemistry A, 2013, 117, 13184-13193.	1.1	43
32	Halogen-bond interactions: a crystallographic basicity scale towards iodoorganic compounds. CrystEngComm, 2013, 15, 3212.	1.3	58
33	Interpretation of experimental hydrogen-bond enthalpies and entropies from COSMO polarisation charge densities. Physical Chemistry Chemical Physics, 2013, 15, 7147.	1.3	36
34	New Insights on the Molecular Recognition of Imidacloprid with Aplysia californica AChBP: A Computational Study. Journal of Physical Chemistry B, 2013, 117, 3944-3953.	1.2	20
35	An Unexpected and Significantly Lower HydrogenâEBondâEDonating Capacity of Fluorohydrins Compared to Nonfluorinated Alcohols. Angewandte Chemie - International Edition, 2012, 51, 6176-6180.	7.2	80
36	Structural features and protonation site of epibatidine in the gas phase: an investigation through infrared multiphoton dissociation spectroscopy and computational chemistry. Physical Chemistry Chemical Physics, 2011, 13, 2272-2277.	1.3	1

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37	Can Quantum-Mechanical Calculations Yield Reasonable Estimates of Hydrogen-Bonding Acceptor Strength? The Case of Hydrogen-Bonded Complexes of Methanol. Journal of Physical Chemistry A, 2011, 115, 13975-13985.	1.1	31
38	New insights on the molecular features and electrophysiological properties of dinotefuran, imidacloprid and acetamiprid neonicotinoid insecticides. Bioorganic and Medicinal Chemistry, 2011, 19, 7623-7634.	1.4	39
39	An Overview of Lewis Basicity and Affinity Scales. Journal of Chemical Education, 2011, 88, 1651-1657.	1.1	67
40	Structural Features and Hydrogenâ€Bond Properties of Galanthamine and Codeine: An Experimental and Theoretical Study. Chemistry - A European Journal, 2011, 17, 11637-11649.	1.7	15
41	The Diiodine Basicity Scale: Toward a General Halogenâ€Bond Basicity Scale. Chemistry - A European Journal, 2011, 17, 10431-10444.	1.7	119
42	An Enthalpic Scale of Hydrogen-Bond Basicity. 4. Carbon Ï€ Bases, Oxygen Bases, and Miscellaneous Second-Row, Third-Row, and Fourth-Row Bases and a Survey of the 4-Fluorophenol Affinity Scale. Journal of Organic Chemistry, 2010, 75, 4105-4123.	1.7	79
43	Hydrogenâ€Bond Accepting Strength of Fiveâ€Membered Nâ€Heterocycles:The Case of Substituted Phenylpyrrolines and Myosmines. European Journal of Organic Chemistry, 2009, 2009, 4939-4948.	1.2	9
44	The pK_{BHX} Database: Toward a Better Understanding of Hydrogen-Bond Basicity for Medicinal Chemists. Journal of Medicinal Chemistry, 2009, 52, 4073-4086.	2.9	276
45	A Theoretical Evaluation of the pK_{HB} and Î”$H{{{,ominus}hfill atop {m HB}hfill}}}$ Hydrogenâ€Bond Scales of Nitrogen Bases. Chemistry - A European Journal, 2008, 14, 10656-10669.	1.7	25
46	Functionalized 2,5â€Dipyridinylpyrroles by Electrochemical Reduction of 3,6â€Dipyridinylpyridazine Precursors. European Journal of Organic Chemistry, 2008, 2008, 2156-2166.	1.2	30
47	The Exceptional Hydrogen-Bond Properties of Neutral and Protonated Lobeline. Journal of Physical Chemistry A, 2007, 111, 6397-6405.	1.1	22
48	Hydrogen-Bond Interactions of Nicotine and Acetylcholine Salts: A Combined Crystallographic, Spectroscopic, Thermodynamic and Theoretical Study. Chemistry - A European Journal, 2007, 13, 1499-1510.	1.7	17
49	Structural features of neutral and protonated galanthamine: A crystallographic database and computational investigation. Chemical Physics, 2006, 328, 307-317.	0.9	8
50	An Enthalpic Scale of Hydrogen-Bond Basicity. 3. Ammonia, Primary, Secondary, and Tertiary Amines. Journal of Organic Chemistry, 2005, 70, 7892-7901.	1.7	37
51	Three-centre hydrogen bonding in the complexes ofsyn-2,4-difluoroadamantane with 4-fluorophenol and hydrogen fluoride. Journal of Physical Organic Chemistry, 2005, 18, 227-234.	0.9	19
52	B3LYP and MP2 Calculations of the Enthalpies of Hydrogen-Bonded Complexes of Methanol with Neutral Bases and Anions:â€‰Comparison with Experimental Data. Journal of Physical Chemistry A, 2005, 109, 11907-11913.	1.1	75
53	Determination of the hydrogen-bond basicity of weak and multifunctional bases: the case of lindane(Î³-hexachlorocyclohexane). Journal of Physical Organic Chemistry, 2004, 17, 56-64.	0.9	17
54	Liaison hydrogÃ¨ne des arylamines : compÃ©tition des sites Ï€ et N. Canadian Journal of Chemistry, 2004, 82, 1413-1422.	0.6	15

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55	Interference between the Hydrogen Bonds to the Two Rings of Nicotine. Journal of the American Chemical Society, 2003, 125, 5988-5997.	6.6	23
56	The Nicotinic Pharmacophore:Â Thermodynamics of the Hydrogen-Bonding Complexation of Nicotine, Nornicotine, and Models. Journal of Organic Chemistry, 2003, 68, 8208-8221.	1.7	42
57	Site of Protonation of Nicotine and Nornicotine in the Gas Phase: Pyridine or Pyrrolidine Nitrogen?. Journal of the American Chemical Society, 2002, 124, 10552-10562.	6.6	77
58	L'Ã©chelle pKHB de basicitÃ© de liaison hydrogÃ¨ne des amines tertiaires aliphatiques. Canadian Journal of Chemistry, 2002, 80, 1375-1385.	0.6	28
59	Hydrogen-bond basicity of solutes in hydroxylic solvents from octanol-water partition coefficients. Journal of Physical Organic Chemistry, 2002, 15, 218-228.	0.9	10
60	Hydrogen-bond basicity pKHB scale of secondary amines. Perkin Transactions II RSC, 2001, , 2130.	1.1	70
61	Amino and cyano N atoms in competitive situations: which is the best hydrogen-bond acceptor? A crystallographic database investigation. Acta Crystallographica Section B: Structural Science, 2001, 57, 850-858.	1.8	34
62	Hydrogen-bond basicity pKHB scale of aliphatic primary amines. Journal of the Chemical Society Perkin Transactions II, 1999, , 997.	0.9	36