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	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
2	The Diiodine Basicity Scale: Toward a General Halogenâ€Bond Basicity Scale. Chemistry - A European Journal, 2011, 17, 10431-10444.	1.7	119
3	Systematic Investigation of Lipophilicity Modulation by Aliphatic Fluorination Motifs. Journal of Medicinal Chemistry, 2020, 63, 1002-1031.	2.9	83
4	An Unexpected and Significantly Lower Hydrogenâ€Bondâ€Donating Capacity of Fluorohydrins Compared to Nonfluorinated Alcohols. Angewandte Chemie - International Edition, 2012, 51, 6176-6180.	7.2	80
5	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
6	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
7	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
8	Hydrogen-bond basicity pKHB scale of secondary amines. Perkin Transactions II RSC, 2001, , 2130.	1.1	70
9	An Overview of Lewis Basicity and Affinity Scales. Journal of Chemical Education, 2011, 88, 1651-1657.	1.1	67
10	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
11	Experimental and computational evidence of halogen bonds involving astatine. Nature Chemistry, 2018, 10, 428-434.	6.6	63
12	Halogen-bond interactions: a crystallographic basicity scale towards iodoorganic compounds. CrystEngComm, 2013, 15, 3212.	1.3	58
13	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
14	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
15	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
16	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
17	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
18	Hydrogen-bond basicity pKHB scale of aliphatic primary amines. Journal of the Chemical Society Perkin Transactions II, 1999, , 997.	0.9	36

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19	Interpretation of experimental hydrogen-bond enthalpies and entropies from COSMO polarisation charge densities. Physical Chemistry Chemical Physics, 2013, 15, 7147.	1.3	36
20	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
21	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
22	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
23	Influence of Alcohol Î²â€Fluorination on Hydrogenâ€Bond Acidity of Conformationally Flexible Substrates. Chemistry - A European Journal, 2017, 23, 2811-2819.	1.7	31
24	Functionalized 2,5â€Dipyridinylpyrroles by Electrochemical Reduction of 3,6â€Dipyridinylpyridazine Precursors. European Journal of Organic Chemistry, 2008, 2008, 2156-2166.	1.2	30
25	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
26	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
27	Influence of Fluorination on the Conformational Properties and Hydrogenâ€Bond Acidity of Benzyl Alcohol Derivatives. Chemistry - A European Journal, 2015, 21, 11462-11474.	1.7	25
28	Quantum calculations of At-mediated halogen bonds: on the influence of relativistic effects. New Journal of Chemistry, 2018, 42, 10510-10517.	1.4	25
29	Interference between the Hydrogen Bonds to the Two Rings of Nicotine. Journal of the American Chemical Society, 2003, 125, 5988-5997.	6.6	23
30	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
31	The Exceptional Hydrogen-Bond Properties of Neutral and Protonated Lobeline. Journal of Physical Chemistry A, 2007, 111, 6397-6405.	1.1	22
32	Spinâ€“orbit coupling as a probe to decipher halogen bonding. Physical Chemistry Chemical Physics, 2018, 20, 29616-29624.	1.3	21
33	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
34	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
35	Individual Hydrogenâ€Bond Strength QSPR Modelling with ISIDA Local Descriptors: a Step Towards Polyfunctional Molecules. Molecular Informatics, 2014, 33, 477-487.	1.4	19
36	On the Interplay between Chargeâ€Shift Bonding and Halogen Bonding. ChemPhysChem, 2020, 21, 240-250.	1.0	18

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37	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
38	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
39	Synthesis of 2,3,4-Trideoxy-2,3,4-trifluoroglucose. Journal of Organic Chemistry, 2019, 84, 5899-5906.	1.7	16
40	Liaison hydrogÃ¨ne des arylamines : compÃ©tition des sites Ï€ et N. Canadian Journal of Chemistry, 2004, 82, 1413-1422.	0.6	15
41	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
42	A Study of Intramolecular Hydrogen Bonding in Levoglucosan Derivatives. Molecules, 2017, 22, 518.	1.7	14
43	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
44	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
45	Lipophilicity trends upon fluorination of isopropyl, cyclopropyl and 3-oxetanyl groups. Beilstein Journal of Organic Chemistry, 2020, 16, 2141-2150.	1.3	13
46	Î±â€Fluoroâ€oâ€cresols: The Key Role of Intramolecular Hydrogen Bonding in Conformational Preference and Hydrogenâ€Bond Acidity. ChemPhysChem, 2016, 17, 2702-2709.	1.0	12
47	Predictive Models for Halogenâ€bond Basicity of Binding Sites of Polyfunctional Molecules. Molecular Informatics, 2016, 35, 70-80.	1.4	12
48	Characterization of Steroids through Collision Cross Sections: Contribution of Quantum Chemistry Calculations. Analytical Chemistry, 2020, 92, 6034-6042.	3.2	12
49	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
50	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
51	Delocalized relativistic effects, from the viewpoint of halogen bonding. Physical Chemistry Chemical Physics, 2021, 23, 4064-4074.	1.3	10
52	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
53	Structural features of neutral and protonated galanthamine: A crystallographic database and computational investigation. Chemical Physics, 2006, 328, 307-317.	0.9	8
54	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

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55	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
56	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
57	An expanded halogen bonding scale using astatine. Chemical Science, 2021, 12, 10855-10861.	3.7	7
58	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
59	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
60	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
61	Radical Cyclisation of Î±â€Halo Aluminium Acetals: A Mechanistic Study. Chemistry - A European Journal, 2016, 22, 4809-4824.	1.7	1
62	Hydrogen-bond acidity of silanols: A combined experimental and theoretical study. Journal of Molecular Structure, 2022, 1266, 133505.	1.8	1