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List of Publications by Year
in descending order

93 papers	2,511 citations	218381 26 h-index	223531 46 g-index
97 all docs	97 docs citations	97 times ranked	3208 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	Halogen-bond geometry: a crystallographic database investigation of dihalogen complexes. Acta Crystallographica Section B: Structural Science, 2003, 59, 512-526.	1.8	127
3	Hydrogen-bond acceptor properties of nitriles: a combined crystallographic andab initio theoretical investigation. Journal of Physical Organic Chemistry, 2000, 13, 347-358.	0.9	123
4	Synthesis of Oligothiophene-Bridged Bisporphyrins and Study of the Linkage Dependence of the Electronic Coupling. Chemistry - A European Journal, 2002, 8, 3027.	1.7	94
5	Systematic Investigation of Lipophilicity Modulation by Aliphatic Fluorination Motifs. Journal of Medicinal Chemistry, 2020, 63, 1002-1031.	2.9	83
6	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
7	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
8	Structure and molecular interactions of anti-thyroid drugs. Part 3.1 Methimazole: a diiodine sponge. Journal of the Chemical Society Perkin Transactions II, 1998, , 1545-1552.	0.9	78
9	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
10	Hydrogen-bond basicity of secondary and tertiary amides, carbamates, ureas and lactams. Journal of the Chemical Society Perkin Transactions II, 1992, , 2091.	0.9	74
11	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
12	Halogen-bond interactions: a crystallographic basicity scale towards iodoorganic compounds. CrystEngComm, 2013, 15, 3212.	1.3	58
13	Computer modelling of sulfated carbohydrates: Applications to carrageenans. International Journal of Biological Macromolecules, 1995, 17, 161-175.	3.6	54
14	Hydrogen-bond basicity of nitriles. Journal of Physical Organic Chemistry, 1993, 6, 302-306.	0.9	47
15	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
16	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
17	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
18	Hydrogen-bond basicity of thioamides and thioureas. Journal of the Chemical Society Perkin Transactions II, 1995, , 2075.	0.9	39

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19	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
20	Gas-phase basicity and site of protonation of polyfunctional molecules of biological interest: FT-ICR experiments and AM1 calculations on nicotines, nicotinic acid derivatives, and related compounds. Journal of Organic Chemistry, 1991, 56, 4490-4494.	1.7	37
21	Hydrogen-bond basicity pKHB scale of aliphatic primary amines. Journal of the Chemical Society Perkin Transactions II, 1999, , 997.	0.9	36
22	Interpretation of experimental hydrogen-bond enthalpies and entropies from COSMO polarisation charge densities. Physical Chemistry Chemical Physics, 2013, 15, 7147.	1.3	36
23	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
24	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
25	Influence of Alcohol Î²â€Fluorination on Hydrogenâ€Bond Acidity of Conformationally Flexible Substrates. Chemistry - A European Journal, 2017, 23, 2811-2819.	1.7	31
26	Hydrogen Bonding of Progesterone: a Combined Theoretical, Spectroscopic, Thermodynamic, and Crystallographic Database Study. Journal of Physical Chemistry B, 2000, 104, 11816-11823.	1.2	29
27	Super-basic nitriles. Journal of the Chemical Society Perkin Transactions II, 1993, , 625.	0.9	28
28	Basicity of azoles: complexes of diiodine with imidazoles, pyrazoles and triazoles. Journal of Physical Organic Chemistry, 1997, 10, 669-674.	0.9	27
29	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
30	Quantum calculations of At-mediated halogen bonds: on the influence of relativistic effects. New Journal of Chemistry, 2018, 42, 10510-10517.	1.4	25
31	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
32	Amino nitrogen and carbonyl oxygen in competitive situations: which is the best hydrogen-bond acceptor site?. CrystEngComm, 2002, 4, 326-335.	1.3	22
33	The Exceptional Hydrogen-Bond Properties of Neutral and Protonated Lobeline. Journal of Physical Chemistry A, 2007, 111, 6397-6405.	1.1	22
34	3-Fluoro- and 3,3-Difluoro-3,4-dideoxy-KRN7000 Analogues as New Potent Immunostimulator Agents: Total Synthesis and Biological Evaluation in Human Invariant Natural Killer T Cells and Mice. Journal of Medicinal Chemistry, 2012, 55, 1227-1241.	2.9	21
35	Spinâ€“orbit coupling as a probe to decipher halogen bonding. Physical Chemistry Chemical Physics, 2018, 20, 29616-29624.	1.3	21
36	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

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37	Common Ring Motifs in Proteins Involving Asparagine or Glutamine Amide Groups Hydrogen-bonded to Main-chain Atoms. Journal of Molecular Biology, 1993, 231, 888-896.	2.0	19
38	Individual Hydrogenâ€Bond Strength QSPR Modelling with ISIDA Local Descriptors: a Step Towards Polyfunctional Molecules. Molecular Informatics, 2014, 33, 477-487.	1.4	19
39	Similar Comparative Low and High Doses of Deltamethrin and Acetamiprid Differently Impair the Retrieval of the Proboscis Extension Reflex in the Forager Honey Bee (Apis mellifera). Insects, 2015, 6, 805-814.	1.0	18
40	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
41	A DFT-D evaluation of the complexation of a molecular tweezer with small aromatic molecules. Chemical Physics Letters, 2012, 522, 11-16.	1.2	17
42	Can semi-empirical calculations yield reasonable estimates of hydrogen-bonding basicity? The case of nitriles. Journal of the Chemical Society Perkin Transactions II, 1997, , 2711-2718.	0.9	16
43	Synthesis of 2,3,4-Trideoxy-2,3,4-trifluoroglucose. Journal of Organic Chemistry, 2019, 84, 5899-5906.	1.7	16
44	Multiple Hydrogen-Bond Accepting Capacities of Polybasic Molecules:â€‰ The Case of Cotinine. Journal of Physical Chemistry A, 2004, 108, 10740-10748.	1.1	15
45	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
46	Fluorescent carboxylic and phosphonic acids: comparative photophysics from solution to organic nanoparticles. Physical Chemistry Chemical Physics, 2013, 15, 12748.	1.3	15
47	Questioning the Affinity of Electrophilic Astatine for Sulfur-containing Compounds: Unexpected Bindings Revealed. Inorganic Chemistry, 2020, 59, 13923-13932.	1.9	15
48	Cytochrome P450-Catalyzed Degradation of Nicotine: Fundamental Parameters Determining Hydroxylation by Cytochrome P450 2A6 at the 5â€²-Carbon or the N-Methyl Carbon. Journal of Physical Chemistry B, 2012, 116, 7827-7840.	1.2	14
49	A Study of Intramolecular Hydrogen Bonding in Levoglucosan Derivatives. Molecules, 2017, 22, 518.	1.7	14
50	Hydrogen-Bond Accepting Strength of Protonated Nicotine. Journal of Physical Chemistry A, 2005, 109, 3767-3770.	1.1	13
51	Study of N1-alkylation of indoles from the reaction of 2(or 3)-aminoindole-3-(or 2)carbonitriles with DMF-dialkylacetals. Organic and Biomolecular Chemistry, 2012, 10, 4916.	1.5	13
52	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
53	Mode of action of sulfoxaflor on Î±-bungarotoxin-insensitive nAChR1 and nAChR2 subtypes: Inhibitory effect of imidacloprid. NeuroToxicology, 2019, 74, 132-138.	1.4	13
54	Lipophilicity trends upon fluorination of isopropyl, cyclopropyl and 3-oxetanyl groups. Beilstein Journal of Organic Chemistry, 2020, 16, 2141-2150.	1.3	13

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55	Electrochemical Synthesis and Characterisation of Alternating Tripyridylâ€“Dipyrrole Molecular Strands with Multiple Nitrogenâ€Based Donorâ€“Acceptor Binding Sites. Chemistry - A European Journal, 2010, 16, 11876-11889.	1.7	12
56	Theoretical Study of the Structures and Hydrogen-Bond Properties of New Alternated Heterocyclic Compounds. Journal of Physical Chemistry A, 2010, 114, 6413-6422.	1.1	12
57	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
58	Predictive Models for Halogenâ€bond Basicity of Binding Sites of Polyfunctional Molecules. Molecular Informatics, 2016, 35, 70-80.	1.4	12
59	Characterization of Steroids through Collision Cross Sections: Contribution of Quantum Chemistry Calculations. Analytical Chemistry, 2020, 92, 6034-6042.	3.2	12
60	Selenoxides Are Better Hydrogen-Bond Acceptors than Sulfoxides:Â a Crystallographic Database and Theoretical Investigation. Journal of Physical Chemistry A, 2004, 108, 7232-7240.	1.1	11
61	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
62	The crystal and molecular structures of 4-cyanophenyl 1,5-dithio-Î²-d-xylopyranoside S-5 oxide and 4-ethyl-2-oxo-2H- 1-benzopyran-7-yl 5-thio-Î²-d-xylopyranoside S-5 oxide. Carbohydrate Research, 1997, 302, 53-66.	1.1	10
63	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
64	Structural features of neutral and protonated galanthamine: A crystallographic database and computational investigation. Chemical Physics, 2006, 328, 307-317.	0.9	8
65	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
66	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
67	Semiempirical and spectroscopic study of a novel porphyrin dyad. International Journal of Quantum Chemistry, 2001, 84, 259-263.	1.0	7
68	Molecular Tweezers in Hostâ€“Guest Complexes: A Computational Study through a DFT-D Approach. Journal of Physical Chemistry C, 2012, 116, 23067-23074.	1.5	7
69	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
70	An expanded halogen bonding scale using astatine. Chemical Science, 2021, 12, 10855-10861.	3.7	7
71	Mode of Action of Neonicotinoid Insecticides Imidacloprid and Thiacloprid to the Cockroach PameÎ±7 Nicotinic Acetylcholine Receptor. International Journal of Molecular Sciences, 2021, 22, 9880.	1.8	7
72	The first crystal structure of a free neutral form of a nicotine derivative. Zeitschrift Fur Kristallographie - Crystalline Materials, 2003, 218, 753-760.	0.4	6

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73	Cytochrome P450 Monooxygenaseâ€Catalyzed Ring Opening of the Bicyclic Amine, Nortropine: An Experimental and DFT Computational Study. ChemCatChem, 2012, 4, 530-539.	1.8	6
74	Dissymmetric Molecular Tweezers in Hostâ€“Guest Complexes: Internal or External Complexation?. Journal of Physical Chemistry C, 2015, 119, 3771-3779.	1.5	6
75	Cloning and Expression of Cockroach Î±7 Nicotinic Acetylcholine Receptor Subunit. Frontiers in Physiology, 2020, 11, 418.	1.3	6
76	The crystal and molecular structure of 4-cyanophenyl and 4-nitrophenyl Î²-d-xylopyranosides. Carbohydrate Research, 1994, 265, 291-298.	1.1	4
77	Hydrogen-bonding properties of galanthamine: an investigation through crystallographic database observations and computational chemistry. Acta Crystallographica Section B: Structural Science, 2008, 64, 338-347.	1.8	4
78	Permethrin enhances the agonist activity of dinotefuran on insect cholinergic synaptic transmission and isolated neurons. NeuroToxicology, 2018, 67, 206-214.	1.4	4
79	Di- and heptavalent nicotinic analogues to interfere with Î±7 nicotinic acetylcholine receptors. Bioorganic and Medicinal Chemistry, 2019, 27, 700-707.	1.4	4
80	Astatine Facing Janus: Halogen Bonding vs. Charge-Shift Bonding. Molecules, 2021, 26, 4568.	1.7	3
81	The pK_{BHX} Hydrogen-Bond Basicity Scale: From Molecules to Anions. Journal of Organic Chemistry, 2022, 87, 7264-7273.	1.7	3
82	The crystal and molecular structure of 4-cyanophenyl 5-thio-Î²-d-xylopyranoside. Carbohydrate Research, 1995, 268, 127-133.	1.1	2
83	Molecular structure of [4-(4-cyanobenzoyl) phenyl] 1,5-dithio-Î²-d-xylopyranoside (naroparcil) in the solid state and in solution: An investigation by X-ray crystallography, molecular mechanics calculations, and NMR spectroscopy. Carbohydrate Research, 1996, 284, 35-49.	1.1	2
84	Mechanistic and Structural Insights on the IL-15 System through Molecular Dynamics Simulations. Molecules, 2019, 24, 3261.	1.7	2
85	Influence of fluorination on alcohol hydrogen-bond donating properties. , 2019, , 301-324.		2
86	Hydrogen-bond acceptor properties of nitriles: a combined crystallographic and ab initio theoretical investigation. , 2000, 13, 347.		2
87	Substituent effects in infrared spectroscopyâ€”XI. Field effects of 4-substituents on the Î½(OH) vibrator of isoborneols. Spectrochimica Acta Part A: Molecular Spectroscopy, 1991, 47, 1649-1652.	0.1	1
88	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
89	Mapping of the interaction sites of galanthamine: a quantitative analysis through pairwise potentials and quantum chemistry. Journal of Computer-Aided Molecular Design, 2012, 26, 1111-1126.	1.3	1
90	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

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91	Synergic effect of a quinuclidine benzamide complexed with borane, the LMA10233, in combination with seven pesticides. Pesticide Biochemistry and Physiology, 2020, 168, 104633.	1.6	1
92	Hydrogen-bond acidity of silanols: A combined experimental and theoretical study. Journal of Molecular Structure, 2022, 1266, 133505.	1.8	1
93	Pretreatment of the cockroach cercal afferent/giant interneuron synapses with nicotinoids and neonicotinoids differently affects acetylcholine and nicotine-induced ganglionic depolarizations. Invertebrate Neuroscience, 2013, 13, 91-97.	1.8	0