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List of Publications by Year
in descending order



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|---|---|---|---|
| 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<sub>BHX</sub> Hydrogen-Bond Basicity Scale: From Molecules to Anions. Journal of Organic Chemistry, 2022, 87, 7264-7273. | 1.7 | 3 |
| 2 | Hydrogen-bond acidity of silanols: A combined experimental and theoretical study. Journal of Molecular Structure, 2022, 1266, 133505. | 1.8 | 1 |
| 3 | An expanded halogen bonding scale using astatine. Chemical Science, 2021, 12, 10855-10861. | 3.7 | 7 |
| 4 | Astatine Facing Janus: Halogen Bonding vs. Charge-Shift Bonding. Molecules, 2021, 26, 4568. | 1.7 | 3 |
| 5 | 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 |
| 6 | Systematic Investigation of Lipophilicity Modulation by Aliphatic Fluorination Motifs. Journal of Medicinal Chemistry, 2020, 63, 1002-1031. | 2.9 | 83 |
| 7 | Questioning the Affinity of Electrophilic Astatine for Sulfur-containing Compounds: Unexpected Bindings Revealed. Inorganic Chemistry, 2020, 59, 13923-13932. | 1.9 | 15 |
| 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 | Cloning and Expression of Cockroach Î±7 Nicotinic Acetylcholine Receptor Subunit. Frontiers in Physiology, 2020, 11, 418. | 1.3 | 6 |
| 10 | Characterization of Steroids through Collision Cross Sections: Contribution of Quantum Chemistry Calculations. Analytical Chemistry, 2020, 92, 6034-6042. | 3.2 | 12 |
| 11 | 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 |
| 12 | 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 |
| 13 | Mechanistic and Structural Insights on the IL-15 System through Molecular Dynamics Simulations. Molecules, 2019, 24, 3261. | 1.7 | 2 |
| 14 | Di- and heptavalent nicotinic analogues to interfere with Î±7 nicotinic acetylcholine receptors. Bioorganic and Medicinal Chemistry, 2019, 27, 700-707. | 1.4 | 4 |
| 15 | 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 |
| 16 | 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 |
| 17 | Synthesis of 2,3,4-Trideoxy-2,3,4-trifluoroglucose. Journal of Organic Chemistry, 2019, 84, 5899-5906. | 1.7 | 16 |
| 18 | Influence of fluorination on alcohol hydrogen-bond donating properties. , 2019, , 301-324. | | 2 |

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| 19 | Quantum calculations of At-mediated halogen bonds: on the influence of relativistic effects. New Journal of Chemistry, 2018, 42, 10510-10517. | 1.4 | 25 |
| 20 | Spinâ€“orbit coupling as a probe to decipher halogen bonding. Physical Chemistry Chemical Physics, 2018, 20, 29616-29624. | 1.3 | 21 |
| 21 | Reducing the Lipophilicity of Perfluoroalkyl Groups by CF<sub>2</sub>â€“F/CF<sub>2</sub>â€“Me or CF<sub>3</sub>/CH<sub>3</sub> Exchange. Journal of Medicinal Chemistry, 2018, 61, 10602-10618. | 2.9 | 66 |
| 22 | 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 |
| 23 | Permethrin enhances the agonist activity of dinotefuran on insect cholinergic synaptic transmission and isolated neurons. NeuroToxicology, 2018, 67, 206-214. | 1.4 | 4 |
| 24 | Influence of Alcohol Î²â€Fluorination on Hydrogenâ€Bond Acidity of Conformationally Flexible Substrates. Chemistry - A European Journal, 2017, 23, 2811-2819. | 1.7 | 31 |
| 25 | A Study of Intramolecular Hydrogen Bonding in Levoglucosan Derivatives. Molecules, 2017, 22, 518. | 1.7 | 14 |
| 26 | 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 |
| 27 | Predictive Models for Halogenâ€bond Basicity of Binding Sites of Polyfunctional Molecules. Molecular Informatics, 2016, 35, 70-80. | 1.4 | 12 |
| 28 | 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 |
| 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 | 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 |
| 31 | 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 |
| 32 | 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 |
| 33 | 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 |
| 34 | Dissymmetric Molecular Tweezers in Hostâ€“Guest Complexes: Internal or External Complexation?. Journal of Physical Chemistry C, 2015, 119, 3771-3779. | 1.5 | 6 |
| 35 | 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 |
| 36 | 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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| 37 | Individual Hydrogenâ€Bond Strength QSPR Modelling with ISIDA Local Descriptors: a Step Towards Polyfunctional Molecules. Molecular Informatics, 2014, 33, 477-487. | 1.4 | 19 |
| 38 | Fluorescent carboxylic and phosphonic acids: comparative photophysics from solution to organic nanoparticles. Physical Chemistry Chemical Physics, 2013, 15, 12748. | 1.3 | 15 |
| 39 | Hydrogen-Bond Acidity of OH Groups in Various Molecular Environments (Phenols, Alcohols, Steroid) Tj ETQq1 1 0.784314 rgBT /Ove<br>Calculations. Journal of Physical Chemistry A, 2013, 117, 13184-13193. | 1.1 | 43 |
| 40 | 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 |
| 41 | Halogen-bond interactions: a crystallographic basicity scale towards iodoorganic compounds. CrystEngComm, 2013, 15, 3212. | 1.3 | 58 |
| 42 | Interpretation of experimental hydrogen-bond enthalpies and entropies from COSMO polarisation charge densities. Physical Chemistry Chemical Physics, 2013, 15, 7147. | 1.3 | 36 |
| 43 | 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 |
| 44 | 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 |
| 45 | 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 |
| 46 | 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 |
| 47 | 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 |
| 48 | 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 |
| 49 | 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 |
| 50 | 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 |
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| 53 | 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 |
| 54 | 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 |

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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 | 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 |
| 58 | 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 |
| 59 | The pK<sub>BHX</sub> Database: Toward a Better Understanding of Hydrogen-Bond Basicity for Medicinal Chemists. Journal of Medicinal Chemistry, 2009, 52, 4073-4086. | 2.9 | 276 |
| 60 | 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 |
| 61 | The Exceptional Hydrogen-Bond Properties of Neutral and Protonated Lobeline. Journal of Physical Chemistry A, 2007, 111, 6397-6405. | 1.1 | 22 |
| 62 | 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 |
| 63 | Structural features of neutral and protonated galanthamine: A crystallographic database and computational investigation. Chemical Physics, 2006, 328, 307-317. | 0.9 | 8 |
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| 65 | 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 |
| 66 | 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 |
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| 68 | 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 |
| 69 | 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 |
| 70 | 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 |
| 71 | Amino nitrogen and carbonyl oxygen in competitive situations: which is the best hydrogen-bond acceptor site?. CrystEngComm, 2002, 4, 326-335. | 1.3 | 22 |
| 72 | 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 |

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| 73 | 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 |
| 74 | Semiempirical and spectroscopic study of a novel porphyrin dyad. International Journal of Quantum Chemistry, 2001, 84, 259-263. | 1.0 | 7 |
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| 81 | Basicity of azoles: complexes of diiodine with imidazoles, pyrazoles and triazoles. Journal of Physical Organic Chemistry, 1997, 10, 669-674. | 0.9 | 27 |
| 82 | 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 |
| 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 |
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| 92 | 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 |
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