Carolina Estarellas

List of Publications by Year
in descending order

57 papers	2,318 citations	257450 24 h-index	206112 48 g-index
62 all docs	62 docs citations	62 times ranked	2233 citing authors

#	Article	IF	Citations
1	Supramolecular Self-Assembly of M-IDA Complexes Involving Lone-PairÂ·Â·Â·Ï€ Interactions: Crystal Structures, Hirshfeld Surface Analysis, and DFT Calculations [H₂IDA = iminodiacetic acid, M = Cu(II), Ni(II)]. Crystal Growth and Design, 2011, 11, 3250-3265.	3.0	304
2	Cooperativity in multiple unusual weak bonds. Theoretical Chemistry Accounts, 2010, 126, 1-14.	1.4	254
3	Relevant Anionâ€“Ï€ Interactions in Biological Systems: The Case of Urate Oxidase. Angewandte Chemie - International Edition, 2011, 50, 415-418.	13.8	164
4	Quantification of Nitrateâˆ’Ï€ Interactions and Selective Transport of Nitrate Using Calix[4]pyrroles with Two Aromatic Walls. Journal of the American Chemical Society, 2013, 135, 8324-8330.	13.7	147
5	Supramolecular assemblies involving anionâ€“Ï€ and lone pairâ€“Ï€ interactions: experimental observation and theoretical analysis. CrystEngComm, 2011, 13, 4519.	2.6	86
6	Very Longâ€Range Effects: Cooperativity between Anionâ€“Ï€ and Hydrogenâ€Bonding Interactions. ChemPhysChem, 2009, 10, 2256-2264.	2.1	80
7	Theoretical Study on Cooperativity Effects between Anionâ€“Ï€ and Halogenâ€Bonding Interactions. ChemPhysChem, 2011, 12, 2742-2750.	2.1	79
8	Supramolecular Assembly of Mg(II) Complexes Directed by Associative Lone Pairâˆ’Ï€/Ï€âˆ’Ï€/Ï€âˆ’Anionâˆ’Ï€/Ï€âˆ’Lone Pair Interactions. Journal of Physical Chemistry B, 2010, 114, 4998-5009.	2.6	78
9	On the directionality of anionâ€“Ï€ interactions. Physical Chemistry Chemical Physics, 2011, 13, 5696.	2.8	78
10	Experimental and theoretical study of uracil derivatives: the crucial role of weak fluorineâ€“fluorine noncovalent interactions. CrystEngComm, 2010, 12, 3758.	2.6	60
11	Simultaneous Interaction of Tetrafluoroethene with Anions and Hydrogen-Bond Donors: A Cooperativity Study. Journal of Chemical Theory and Computation, 2009, 5, 1186-1194.	5.3	52
12	Energetic vs Synergetic Stability: A Theoretical Study. Journal of Physical Chemistry A, 2009, 113, 3266-3273.	2.5	52
13	Anionï£¿Ï€ Interactions in Flavoproteins. Chemistry - an Asian Journal, 2011, 6, 2316-2318.	3.3	52
14	Trinuclear and tetranuclear adduct formation between sodium perchlorate and copper(II) complexes of salicylaldimine type ligands: Structural characterization and theoretical investigation. Inorganica Chimica Acta, 2011, 366, 219-226.	2.4	51
15	Concurrent mutations in RNA-dependent RNA polymerase and spike protein emerged as the epidemiologically most successful SARS-CoV-2 variant. Scientific Reports, 2021, 11, 13705.	3.3	45
16	Interplay between cationâ€“Ï€ and hydrogen bonding interactions: Are non-additivity effects additive?. Chemical Physics Letters, 2009, 479, 316-320.	2.6	42
17	2-Aminopyrimidine Derivatives Exhibiting Anion-Ï€ Interactions: A Combined Crystallographic and Theoretical Study. Crystal Growth and Design, 2009, 9, 2363-2376.	3.0	39
18	Lone pairâ€“Ï€ vs Ï€â€“Ï€ interactions in 5-fluoro-1-hexyluracil and 1-hexyluracil: a combined crystallographic and computational study. CrystEngComm, 2010, 12, 362-365.	2.6	39

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19	Anionâ^Ï€ Interactions in Four-Membered Rings. Organic Letters, 2009, 11, 1987-1990.	4.6	38
20	Design of a dual sensing highly selective cyanide chemodosimeter based on pyridinium ring chemistry. New Journal of Chemistry, 2011, 35, 57-60.	2.8	34
21	Theoretical ab initio study of the interplay between hydrogen bonding, cationâ€“Ï€ and Ï€â€“Ï€ interactions. Theoretical Chemistry Accounts, 2009, 122, 325-332.	1.4	31
22	Multiple Multicomponent Reactions: Unexplored Substrates, Selective Processes, and Versatile Chemotypes in Biomedicine. Chemistry - A European Journal, 2018, 24, 14513-14521.	3.3	31
23	Insertion of Isocyanides into Nâ^Si Bonds: Multicomponent Reactions with Azines Leading to Potent Antiparasitic Compounds. Angewandte Chemie - International Edition, 2016, 55, 8994-8998.	13.8	28
24	Combining Machine Learning and Enhanced Sampling Techniques for Efficient and Accurate Calculation of Absolute Binding Free Energies. Journal of Chemical Theory and Computation, 2020, 16, 4641-4654.	5.3	26
25	Synthesis and Crystal Structures of Î¼â€Oxidoâ€•and Î¼â€Hydroxidoâ€Bridged Dinuclear Iron(III) Complexes with an N₂O Donor Ligand â€“ A Theoretical Study on the Influence of Weak Forces on the Feâ€“Oâ€“Fe Bridging Angle. European Journal of Inorganic Chemistry, 2011, 2011, 2558-2566.	2.0	24
26	Hydrogen-bond assisted stabilization of the less favored conformation of a tridentate Schiff base ligand in dinuclear nickel(II) complex: An experimental and theoretical study. Inorganica Chimica Acta, 2010, 363, 3904-3913.	2.4	23
27	Unexpected Nonadditivity Effects in Anionâ^Ï€ Complexes. Journal of Physical Chemistry A, 2011, 115, 7849-7857.	2.5	23
28	A methodological analysis for the assessment of non-covalent Ï€ interactions. Chemical Physics Letters, 2011, 508, 144-148.	2.6	23
29	Theoretical and Crystallographic Study of the Dual Ïƒ/Ï€ Anion Binding Affinity of Quinolizinylium Cation. Journal of Chemical Theory and Computation, 2008, 4, 1981-1989.	5.3	21
30	Theoretical and crystallographic study of edge-to-face aromatic interactions between pyridine moieties and benzene. Chemical Physics Letters, 2009, 468, 280-285.	2.6	21
31	Erroneous behaviour of the widely used MP2(full)/aug-cc-pVXZ (X=D,T) level of theory for evaluating the BSSE in ionâ€“Ï€ complexes. Chemical Physics Letters, 2010, 489, 254-258.	2.6	20
32	Molecular dynamic simulations of protein/RNA complexes: CRISPR/Csy4 endoribonuclease. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 1072-1090.	2.4	20
33	A Combined Experimental and Theoretical Study of Anionâ€“Ï€ Interactions inN⁶â€• andN⁹â€Decyladenine Salts. European Journal of Organic Chemistry, 2010, 2010, 5171-5180.	2.4	19
34	Easy access to (2-imidazolin-4-yl)phosphonates by a microwave assisted multicomponent reaction. Tetrahedron, 2015, 71, 2872-2881.	1.9	19
35	RNAs' uracil quartet model with a non-essential metal ion. Chemical Communications, 2011, 47, 4646.	4.1	16
36	Can lone pair-Ï€ and cation-Ï€ interactions coexist? A theoretical study. Open Chemistry, 2011, 9, 25-34.	1.9	14

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37	Cooperativity effects between non-covalent interactions: Are they important for Z-DNA stability?. Chemical Physics Letters, 2010, 485, 221-225.	2.6	13
38	Radical cation (CË™+â€“Ï€) and radical anion (AË™â^'â€“Ï€) interactions with aromatic rings: energetic, orbitalic and spin density considerations. Physical Chemistry Chemical Physics, 2011, 13, 16698.	2.8	13
39	Effect of a methyl group on the spontaneous resolution of a square-pyramidal coordination compound: crystal packing and conglomerate formation. CrystEngComm, 2012, 14, 5854.	2.6	13
40	MP2 Study of the Dual Ïƒ/Ï€â^'Anion-Binding Affinity of Fluorinated Phthallic Acid Anhydrides. Journal of Physical Chemistry A, 2008, 112, 1622-1626.	2.5	12
41	Anionâ€“Ï€ Interactions Involving [MX_n]^{mâ^'} Anions: A Comprehensive Theoretical Study. ChemPhysChem, 2013, 14, 145-154.	2.1	11
42	New Chlorido(dimethyl sulfoxide)iridium(III) Complexes with N6-Substituted Adenines - Kinetic N(7) versus Thermodynamic N(9) Coordinated Adenine Isomers. European Journal of Inorganic Chemistry, 2010, 2010, 5617-5628.	2.0	10
43	Understanding the Mechanism of Direct Activation of AMP-Kinase: Toward a Fine Allosteric Tuning of the Kinase Activity. Journal of Chemical Information and Modeling, 2019, 59, 2859-2870.	5.4	10
44	Structural basis of the selective activation of enzyme isoforms: Allosteric response to activators of Î²1- and Î²2-containing AMPK complexes. Computational and Structural Biotechnology Journal, 2021, 19, 3394-3406.	4.1	10
45	Synthesis, X-ray characterization and computational Studies of N-imidazolyl and N-pyrazolyl pyrimidine derivatives. Tetrahedron, 2012, 68, 2374-2382.	1.9	8
46	Amphiphilic Histidine-Based Oligopeptides Exhibit pH-Reversible Fibril Formation. ACS Macro Letters, 2021, 10, 984-989.	4.8	8
47	Theoretical ab initio study of substituted benzene trimer: Interplay between hydrogen bonding and Ï€â€“Ï€ interactions. Computational and Theoretical Chemistry, 2011, 975, 106-110.	2.5	7
48	Stereocontrolled Annulations of Indolo[2,3â€a]quinolizidineâ€Derived Lactams with a Silylated Nazarov Reagent: Access to Allo and Epiallo Yohimbineâ€Type Derivatives. Chemistry - A European Journal, 2015, 21, 13382-13389.	3.3	7
49	Insertion of Isocyanides into Nâ^'Si Bonds: Multicomponent Reactions with Azines Leading to Potent Antiparasitic Compounds. Angewandte Chemie, 2016, 128, 9140-9144.	2.0	7
50	Origin of the Baseâ€Dependent Facial Selectivity in Annulation Reactions of Nazarovâ€Type Reagents with Unsaturated Indolo[2,3â€a]quinolizidine Lactams. European Journal of Organic Chemistry, 2017, 2017, 3969-3979.	2.4	5
51	Modulating Ligand Dissociation through Methyl Isomerism in Accessory Sites: Binding of Retinol to Cellular Carriers. Journal of Physical Chemistry Letters, 2019, 10, 7333-7339.	4.6	5
52	Kinetics and mechanism of the oxidation of hydroxylamine by a {Mn3O4}4+ core in aqueous acidic media. Dalton Transactions, 2011, 40, 9571.	3.3	2
53	A Highly Selective Fluorescence Turn-on Probe for Zn2+ Based on New Diaryloxadiazole Chelate. Chemistry Letters, 2011, 40, 1163-1164.	1.3	2
54	Short Access to Belt Compounds with Spatially Close Cï£¾C Bonds and Their Transannular Reactions. Chemistry - A European Journal, 2015, 21, 14036-14046.	3.3	2

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55	Novel indolic AMPK modulators induce vasodilatation through activation of the AMPKâ€“eNOSâ€“NO pathway. Scientific Reports, 2022, 12, 4225.	3.3	2
56	Generation and Reactions of an Octacyclic Hindered Pyramidalized Alkene. Journal of Organic Chemistry, 2018, 83, 5420-5430.	3.2	1
57	Elucidating the Activation Mechanism of AMPK by Direct Pan-Activator PF-739. Frontiers in Molecular Biosciences, 2021, 8, 760026.	3.5	1