Sonia Ilieva

List of Publications by Year
in descending order

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45 papers	1,039 citations	361413 20 h-index	414414 32 g-index
46 all docs	46 docs citations	46 times ranked	1072 citing authors

#	Article	IF	Citations
1	An Efficient Computational Approach for the Evaluation of Substituent Constants. Journal of Organic Chemistry, 2006, 71, 6382-6387.	3.2	105
2	Computational Study of the Aminolysis of Esters. The Reaction of Methylformate with Ammonia. Journal of Organic Chemistry, 2003, 68, 1496-1502.	3.2	87
3	Electrostatic Potential at Atomic Sites as a Reactivity Descriptor for Hydrogen Bonding. Complexes of Monosubstituted Acetylenes and Ammonia. Journal of Physical Chemistry A, 2002, 106, 11801-11805.	2.5	75
4	Predicting Reactivities of Organic Molecules. Theoretical and Experimental Studies on the Aminolysis of Phenyl Acetates. Journal of Physical Chemistry A, 2008, 112, 6700-6707.	2.5	66
5	QSAR analysis of 1,4-dihydro-4-oxo-1-(2-thiazolyl)-1,8-naphthyridines with anticancer activity. European Journal of Medicinal Chemistry, 2007, 42, 1184-1192.	5.5	65
6	Computational Study of the Reactivity ofN-Phenylacetamides in the Alkaline Hydrolysis Reaction. Journal of Physical Chemistry A, 2004, 108, 11457-11462.	2.5	61
7	Mechanism of the Aminolysis of Methyl Benzoate:Â A Computational Studyâ€. Journal of Physical Chemistry A, 2005, 109, 11470-11474.	2.5	41
8	Experimental and theoretical study on the absorption and fluorescence properties of substituted aryl hydrazones of 1,8-naphthalimide. Physical Chemistry Chemical Physics, 2011, 13, 18530.	2.8	35
9	Does the Molecular Electrostatic Potential Reflect the Effects of Substituents in Aromatic Systems?. Chemistry - A European Journal, 2013, 19, 5149-5155.	3.3	35
10	Atomic Charges in Describing Properties of Aromatic Molecules. Journal of Organic Chemistry, 2019, 84, 1908-1915.	3.2	35
11	The mechanism of alkaline hydrolysis of amides: a comparative computational and experimental study of the hydrolysis of Nâ€methylacetamide, Nâ€methylbenzamide, and acetanilide. Journal of Physical Organic Chemistry, 2009, 22, 619-631.	1.9	31
12	Structureâ€“reactivity relationships for aromatic molecules: electrostatic potentials at nuclei and electrophile affinity indices. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 37-55.	14.6	31
13	Theory Supplemented by Experiment. Electronic Effects on the Rotational Stability of the Amide Group inp-Substituted Acetanilides. Journal of Organic Chemistry, 2002, 67, 6210-6215.	3.2	27
14	Computational Study of the Aminolysis of 2-Benzoxazolinone. Journal of Organic Chemistry, 2003, 68, 3406-3412.	3.2	27
15	On the Origin of Higher Rotational Barriers in Thioamides than in Amides. Remote Substituent Effects on the Conformational Stability of the Thioamide Group in Thioacetanilides. Journal of Physical Chemistry A, 2003, 107, 5854-5861.	2.5	26
16	Communication: Energetics of reaction pathways for reactions of ethenol with the hydroxyl radical: The importance of internal hydrogen bonding at the transition state. Journal of Chemical Physics, 2010, 133, 021102.	3.0	24
17	Initiation of ring-opening polymerization of lactide: The effect of metal alkoxide catalyst. Computational and Theoretical Chemistry, 2012, 995, 8-16.	2.5	24
18	Aminolysis of Phenyl N-Phenylcarbamate via an Isocyanate Intermediate: Theory and Experiment. Journal of Organic Chemistry, 2013, 78, 6440-6449.	3.2	23

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19	Experimental Measurement and Theory of Substituent Effects in Ï€-Hydrogen Bonding: Complexes of Substituted Phenols with Benzene. Journal of Organic Chemistry, 2014, 79, 6823-6831.	3.2	23
20	Electrostatic potential at nuclei as a reactivity index in hydrogen bond formation. Complexes of ammonia with Câ€“H, Nâ€“H and Oâ€“H proton donor molecules. Computational and Theoretical Chemistry, 2003, 637, 73-80.	1.5	20
21	Do Ï€-Conjugative Effects Facilitate SN2 Reactions?. Journal of the American Chemical Society, 2014, 136, 3118-3126.	13.7	20
22	How an electric field can modulate the metal ion selectivity of protein binding sites: insights from DFT/PCM calculations. Physical Chemistry Chemical Physics, 2018, 20, 24633-24640.	2.8	19
23	Ca2+/Sr2+ Selectivity in Calcium-Sensing Receptor (CaSR): Implications for Strontiumâ€™s Anti-Osteoporosis Effect. Biomolecules, 2021, 11, 1576.	4.0	19
24	Reactivity of acetanilides in the alkaline hydrolysis reaction: theory vs. experiment. Molecular Physics, 2009, 107, 1187-1192.	1.7	15
25	Computational study of the alkaline hydrolysis of acetanilide. Computational and Theoretical Chemistry, 2004, 681, 105-112.	1.5	13
26	Computational evaluation of ÏƒI and ÏƒR substituent constants. Journal of Molecular Structure, 2010, 976, 427-430.	3.6	13
27	Computational study of the general base catalysed aminolysis of 2-benzoxazolinone. Computational and Theoretical Chemistry, 2003, 633, 49-55.	1.5	9
28	Ab initio molecular orbital study of the conformation of amide group: o-methylformanilide. Journal of Molecular Structure, 1999, 476, 151-156.	3.6	8
29	Electric field influence on the helical structure of peptides: insights from DFT/PCM computations. Physical Chemistry Chemical Physics, 2019, 21, 16198-16206.	2.8	8
30	The origin of diastereoselectivity in the Michael addition reaction: a computational study of the interaction between CH-acidic Schiff base and Î±,Î²-unsaturated ketones. Tetrahedron, 2010, 66, 5168-5172.	1.9	6
31	Reactivity of phenyl Nâ€phenylcarbamates in the alkaline hydrolysis reaction. Journal of Physical Organic Chemistry, 2011, 24, 1166-1171.	1.9	6
32	Synthesis, structural analysis and application of a series of solid-state fluorochromesâ€”aryl hydrazones of 4-hydrazino-N-hexyl-1,8-naphthalimide. Tetrahedron, 2013, 69, 712-721.	1.9	6
33	Quantitative Structure-Activity Relationship Analysis of the Substituent Effects on the Binding Affinity of Derivatives of Trimetazidine. Arzneimittelforschung, 2004, 54, 9-14.	0.4	5
34	Theoretical Modeling of Absorption and Fluorescent Characteristics of Cyanine Dyes. Photochem, 2022, 2, 202-216.	2.2	5
35	Creation of intensity theory in vibrational spectroscopy: Key role of ab initio quantum mechanical calculations. International Journal of Quantum Chemistry, 1998, 70, 331-339.	2.0	4
36	Reactivity descriptors for the hydrogen bonding ability of aliphatic alcohols. Journal of Molecular Structure, 2003, 657, 317-324.	3.6	4

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37	Assembly of New Merocyanine Chromophores with a 1,8-Naphthalimide Core by a New Method for the Synthesis of the Methine Function. Australian Journal of Chemistry, 2015, 68, 1399.	0.9	4
38	Conformation of some biologically active aromatic ureas. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2005, 61, 1321-1326.	3.9	3
39	Hydrogen bonding probes electron density variations at the basic center in substituted alkyl benzoates: Theory and experiment. Journal of Physical Organic Chemistry, 2021, 34, e4258.	1.9	3
40	Hydrogen bonding as a probe of electron density Variations: Substituted pyridines. Chemical Physics Letters, 2022, 791, 139378.	2.6	3
41	The nature of intramolecular interactions determining the Ïƒâ^' constants for aromatic systems. Journal of Molecular Structure, 2012, 1023, 31-36.	3.6	2
42	Mini-Review on Structureâ€"Reactivity Relationship for Aromatic Molecules: Recent Advances. ACS Omega, 2022, 7, 8199-8208.	3.5	2
43	Rationalizing IR intensities in terms of electronic parameters. Journal of Molecular Structure, 2012, 1009, 69-73.	3.6	1
44	Electrostatic Potential at Nuclei. , 0, , 87-122.		0
45	Electrostatic Potential at Nuclei. , 0, , 280-317.		0