Silvia Angelova

List of Publications by Year in descending order

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60 papers	616 citations	623734 14 h-index	713466 21 g-index
62 all docs	62 docs citations	62 times ranked	782 citing authors

#	Article	IF	Citations
1	Complexation of trivalent metal cations (Al³⁺, Ga³⁺, In³⁺,) Tj ETQq1 1 0.784314 rgBT /Overlo governing the hostâ€“guest recognition. Physical Chemistry Chemical Physics, 2022, 24, 6274-6281.	2.8	4
2	Highly efficient unbridged D-A+(D) chromophores based on the quinolizinium cation for nonlinear optical (NLO) applications. Dyes and Pigments, 2022, 205, 110323.	3.7	2
3	Theoretical Insight into the Phosphate-Targeted Silverâ€™s Antibacterial Action: Differentiation between Gram (+) and Gram (â^') Bacteria. Inorganic Chemistry, 2022, 61, 10089-10100.	4.0	6
4	Antioxidant properties of novel curcumin analogues: A combined experimental and computational study. Journal of Food Biochemistry, 2021, 45, e13584.	2.9	7
5	Hostâ€“Guest Complexation of Cucurbit[7]Uril and Cucurbit[8]Uril with the Antineoplastic and Multiple Sclerosis Agent Mitoxantrone (Novantrone). Journal of Physical Chemistry A, 2021, 125, 536-542.	2.5	6
6	Natural Chain-Breaking Antioxidants and Their Synthetic Analogs as Modulators of Oxidative Stress. Antioxidants, 2021, 10, 624.	5.1	12
7	Inclusion complexes of (S)-naproxen and native cyclodextrins: Supramolecular structure and stability. Journal of Molecular Structure, 2021, 1235, 130218.	3.6	6
8	Halide anion solvation and recognition by bambusurils: A DFT study. Journal of Molecular Liquids, 2021, 335, 116160.	4.9	0
9	Unusual Para-Substituent Effects on the Intramolecular Hydrogen Bond in Hydrazone-Based Switches: Insights from Chemical Landscape Analysis and DFT Calculations. Physchem, 2021, 1, 189-201.	1.1	1
10	Molecular insights into the interaction of angiotensin I-converting enzyme (ACE) inhibitors and HEXXH motif. Biophysical Chemistry, 2021, 276, 106626.	2.8	6
11	Inclusion complexes of ibuprofen and Î²-cyclodextrin: Supramolecular structure and stability. Journal of Molecular Structure, 2020, 1205, 127575.	3.6	21
12	Synthesis, photophysical characterisation and antimicrobial activity of a new anionic PAMAM dendrimer. Journal of Photochemistry and Photobiology A: Chemistry, 2020, 403, 112878.	3.9	4
13	Zinc and Its Critical Role in Retinitis pigmentosa: Insights from DFT/SMD Calculations. Inorganic Chemistry, 2020, 59, 17347-17355.	4.0	10
14	Complexation of biologically essential (mono- and divalent) metal cations to cucurbiturils: a DFT/SMD evaluation of the key factors governing the hostâ€“guest recognition. RSC Advances, 2020, 10, 28139-28147.	3.6	10
15	Spectral Characteristics and Sensor Ability of a New 1,8-Naphthalimide and Its Copolymer with Styrene. Sensors, 2020, 20, 3501.	3.8	3
16	Bacterial Natural Disaccharide (Trehalose Tetraester): Molecular Modeling and in Vitro Study of Anticancer Activity on Breast Cancer Cells. Polymers, 2020, 12, 499.	4.5	9
17	Water inside Î²-cyclodextrin cavity: amount, stability and mechanism of binding. Beilstein Journal of Organic Chemistry, 2019, 15, 1592-1600.	2.2	43
18	Hostâ€“guest interactions between p-sulfonatocalix[4]arene and p-sulfonatothiacalix[4]arene and group IA, IIA and f-block metal cations: a DFT/SMD study. Beilstein Journal of Organic Chemistry, 2019, 15, 1321-1330.	2.2	8

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19	Precious metal-free molecular machines for solar thermal energy storage. Beilstein Journal of Organic Chemistry, 2019, 15, 1096-1106.	2.2	5
20	Complexation of IA and IIA group metal ions by N-phenylaza-15-crown-5 containing Schiff bases: A DFT study. Inorganica Chimica Acta, 2019, 487, 316-321.	2.4	4
21	DFT study of hydrazone-based molecular switches: the effect of different stators on the on/off state distribution. Molecular Physics, 2019, 117, 1604-1612.	1.7	8
22	Protective effects of new antioxidant compositions of 4â€•methylcoumarins and related compounds with <scp>dl</scp>â€‹Î±â€‹tocopherol and <scp>l</scp>â€‹ascorbic acid. Journal of the Science of Food and Agriculture, 2018, 98, 3784-3794.	3.5	8
23	Cover Image, Volume 98, Issue 10. Journal of the Science of Food and Agriculture, 2018, 98, i-i.	3.5	0
24	Factors Governing the Hostâ€“Guest Interactions between IIA/IIB Group Metal Cations and Î±-Cyclodextrin: A DFT/CDM Study. Inorganic Chemistry, 2017, 56, 1981-1987.	4.0	20
25	Determinants of the hostâ€“guest interactions between Î±-, Î²- and Î³-cyclodextrins and group IA, IIA and IIIA metal cations: a DFT/PCM study. Physical Chemistry Chemical Physics, 2017, 19, 15129-15136.	2.8	15
26	4-Carboxyl-2,6-dinitrophenylazohydroxynaphthalenes tautomerism NMR re-explained and other methods verified. Dyes and Pigments, 2017, 142, 226-229.	3.7	4
27	Molecular Insight into Inclusion Complex Formation of Curcumin and Calix[4]arene. ChemistrySelect, 2017, 2, 9658-9662.	1.5	5
28	Î±-Cyclodextrin: How Effectively Can Its Hydrophobic Cavity Be Hydrated?. Journal of Physical Chemistry B, 2017, 121, 9260-9267.	2.6	20
29	Protective effects of 4-methylcoumarins and related compounds as radical scavengers and chain-breaking antioxidants. Biochimie, 2017, 140, 133-145.	2.6	9
30	Halogen-containing thiazole orange analogues â€“ new fluorogenic DNA stains. Beilstein Journal of Organic Chemistry, 2017, 13, 2902-2914.	2.2	18
31	Gallium as a Therapeutic Agent: A Thermodynamic Evaluation of the Competition between Ga³⁺ and Fe³⁺ Ions in Metalloproteins. Journal of Physical Chemistry B, 2016, 120, 2241-2248.	2.6	44
32	Bright fluorescent ds<scp>DNA</scp> probes: novel polycationic asymmetric monomethine cyanine dyes based on thiazolopyridineâ€quinolinium chromophore. Coloration Technology, 2015, 131, 94-103.	1.5	4
33	Antioxidant potential of curcumin-related compounds studied by chemiluminescence kinetics, chain-breaking efficiencies, scavenging activity (ORAC) and DFT calculations. Beilstein Journal of Organic Chemistry, 2015, 11, 1398-1411.	2.2	45
34	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
35	Optical properties of thin merocyanine dye layers for photovoltaic applications. Journal of Physics: Conference Series, 2014, 514, 012019.	0.4	0
36	Optical modeling of bulk-heterojunction organic solar cells based on squarine dye as electron donor. Journal of Physics: Conference Series, 2014, 558, 012052.	0.4	2

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37	Solid-state structures of 2-(4-hydroxyphenyl)-substituted phenalene-1,3-dione and indan-1,3-dione. Journal of Structural Chemistry, 2014, 55, 446-455.	1.0	1
38	A model system with intramolecular hydrogen bonding: Effect of external electric field on the tautomeric conversion and electronic structures. Computational and Theoretical Chemistry, 2013, 1006, 113-122.	2.5	12
39	Excited state proton transfer in 3,6-bis(4,5-dihydroxyoxazo-2-yl)benzene-1,2-diol. Chemical Physics Letters, 2013, 563, 43-49.	2.6	12
40	Antiradical and Antioxidant Activities of New Natural-like Hydroxylated Biphenyls of Dehydrozingerone, Zingerone and Ferulic Acid. Comptes Rendus De L'Academie Bulgare Des Sciences, 2013, 66, .	0.2	3
41	Enhanced Intramolecular Charge Transfer in New Type Donorâ€“Acceptor Substituted Perylenes. Journal of Physical Chemistry C, 2012, 116, 22711-22719.	3.1	18
42	Antiradical and antioxidant activities of new bio-antioxidants. Biochimie, 2012, 94, 403-415.	2.6	26
43	Tautomerism in 1-phenylazo-4-naphthols: Experimental results vs quantum-chemical predictions. Dyes and Pigments, 2012, 92, 714-723.	3.7	33
44	Solid-State Tautomerism in 2-Carboxyindan-1,3-dione. Journal of Physical Chemistry A, 2011, 115, 2026-2034.	2.5	4
45	Aggregation of 2â€Aminobenzimidazoleâ€”A Combined Experimental and Theoretical Investigation. ChemPhysChem, 2011, 12, 1747-1755.	2.1	5
46	Ab initio study of the tautomerism of 2,5-substituted diazoles. Structural Chemistry, 2010, 21, 1053-1060.	2.0	7
47	Influence of pH on the cisâ€“trans isomerization of Valine-Proline dipeptide: An integrated NMR and theoretical investigation. Journal of Molecular Structure, 2010, 975, 330-334.	3.6	9
48	Synthesis of 1,2,3,4-substituted spiroheterocyclic tetrahydroisoquinoline-1-ones and their structural similarity in water solution and in crystallohydrate solid state. Arkivoc, 2010, 2010, 303-314.	0.5	5
49	Does tautomeric equilibrium exist in 4-nitroso-5-pyrazolones?. Computational and Theoretical Chemistry, 2009, 897, 55-60.	1.5	14
50	Mechanism and Stereoselectivity of the Phosphinylation of 3-Acyl Coumarins-Stereocontrol Via Concurrent Aromatic Interaction/Oxaphosphole Formation. Letters in Organic Chemistry, 2009, 6, 180-185.	0.5	0
51	Synthesis and characterization of cerium citric and tartaric complexes. Journal of Alloys and Compounds, 2008, 454, 491-500.	5.5	19
52	Theoretical and Spectroscopic Study of 2-Substituted Indan-1,3-diones:â€‰ A Coherent Picture of the Tautomeric Equilibrium. Journal of Physical Chemistry A, 2007, 111, 9901-9913.	2.5	9
53	Synthesis of trans/cis 4-substituted 3-furyl-2-phenethyltetrahydroisoquinolin-1-ones: conformation of the trans-4-(pyrrolidinylcarbonyl) derivative. Tetrahedron Letters, 2006, 47, 2119-2123.	1.4	4
54	Fast intramolecular proton transfer in 2-(hydroxyaminomethylidene)-indan-1,3-dione. Computational and Theoretical Chemistry, 2005, 719, 169-175.	1.5	15

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55	(3RS,4RS)-3-(2-Furyl)-2-phenethyl-4-(pyrrolidin-1-ylcarbonyl)-3,4-dihydroisoquinolin-1(2H)-one. Acta Crystallographica Section E: Structure Reports Online, 2005, 61, o2248-o2250.	0.2	1
56	Ab Initio Study of 2,4-Substituted Azolidines. II. Aminoâ^'Imino Tautomerism of 2-Aminothiazolidine-4-one and 4-Aminothiazolidine-2-one in Water Solution. Journal of Physical Chemistry A, 2005, 109, 8904-8913.	2.5	14
57	Ab initio study of 2,4-substituted azolidines. I. Tautomerism. Computational and Theoretical Chemistry, 2004, 711, 201-207.	1.5	25
58	Diastereoselectivity of tandem Michael additionâ€“alkylation reactions: a convenient method for one-pot synthesis of Î±-branched 2,3-diphenylglutaric acid derivatives. Tetrahedron, 2002, 58, 3371-3378.	1.9	4
59	Synthesis and Stereochemistry of 1,2,4,5-tetraarylimidazolidines. Journal of Chemical Research, 2001, 2001, 457-459.	1.3	1
60	Phase-transfer Catalysed Reactions of Mono- and disubstituted N-(benzylidene)-benzylamines with cinnamic acid derivatives. Journal of Chemical Research, 2000, 2000, 103-105.	1.3	2