Gabriela L Borosky

List of Publications by Year
in descending order

44 papers	527 citations	687363 13 h-index	713466 21 g-index
50 all docs	50 docs citations	50 times ranked	555 citing authors

#	Article	IF	Citations
1	Novel fluorinated curcuminoids and their pyrazole and isoxazole derivatives: Synthesis, structural studies, Computational/Docking and in-vitro bioassay. Journal of Fluorine Chemistry, 2018, 206, 82-98.	1.7	51
2	Ultimate Carcinogenic Metabolites from Aromatic and Heterocyclic Aromatic Amines:â€‰ A Computational Study in Relation to Their Mutagenic Potency. Chemical Research in Toxicology, 2007, 20, 171-180.	3.3	50
3	Theoretical Study Related to the Carcinogenic Activity of Polycyclic Aromatic Hydrocarbon Derivatives. Journal of Organic Chemistry, 1999, 64, 7738-7744.	3.2	40
4	Synthesis, trypanocidal activity and molecular modeling studies of 2-alkylaminomethylquinoline derivatives. European Journal of Medicinal Chemistry, 2011, 46, 3696-3703.	5.5	31
5	Carcinogenic carbocyclic and heterocyclic aromatic amines: A DFT study concerning their mutagenic potency. Journal of Molecular Graphics and Modelling, 2008, 27, 459-465.	2.4	30
6	Oxidized metabolites from benzo[a]pyrene, benzo[e]pyrene, and aza-benzo[a]pyrenes. A computational study of their carbocations formed by epoxide ring opening reactions. Organic and Biomolecular Chemistry, 2007, 5, 2234.	2.8	28
7	Electrophilic Chemistry of Thia-PAHs:â€‰ Stable Carbocations (NMR and DFT), S-Alkylated Onium Salts, Model Electrophilic Substitutions (Nitration and Bromination), and Mutagenicity Assay. Journal of Organic Chemistry, 2007, 72, 8383-8393.	3.2	26
8	Theoretical study of aza-polycyclic aromatic hydrocarbons (aza-PAHs), modelling carbocations from oxidized metabolites and their covalent adducts with representative nucleophiles. Organic and Biomolecular Chemistry, 2005, 3, 1180.	2.8	23
9	Fluoro-curcuminoids and curcuminoid-BF2 adducts: Synthesis, X-ray structures, bioassay, and computational/docking study. Journal of Fluorine Chemistry, 2016, 191, 29-41.	1.7	21
10	Catalytic, regioselective, and green methods for rearrangement of 1,2-diaryl epoxides to carbonyl compounds employing metallic triflates, BrÃ¸nsted-acidic ionic liquids (ILs), and IL/microwave; experimental and computational substituent effect study on aryl versus hydrogen migration. Applied Catalysis A: General, 2014, 486, 1-11.	4.3	18
11	A Computational Study of Carbocations from Oxidized Metabolites of Dibenzo[a,h]acridine and Their Fluorinated and Methylated Derivatives. Chemical Research in Toxicology, 2005, 18, 1876-1886.	3.3	14
12	Carbocations from Oxidized Metabolites of Benzo[a]anthracene:Â A Computational Study of Their Methylated and Fluorinated Derivatives and Guanine Adducts. Chemical Research in Toxicology, 2006, 19, 899-907.	3.3	13
13	Experimental and GIAO ¹⁵N NMR Study of Substituent Effects in 1H-Tetrazoles. Journal of Organic Chemistry, 2012, 77, 4152-4155.	3.2	13
14	Oxidized metabolites from cyclopentaâ€fused polycyclic aromatic hydrocarbons (CPâ€PAHs). A DFT model study of their carbocations formed by epoxide ring opening. Journal of Physical Organic Chemistry, 2010, 23, 810-818.	1.9	12
15	Computational Modeling of the Catalytic Mechanism of Human Placental Alkaline Phosphatase (PLAP). Journal of Chemical Information and Modeling, 2011, 51, 2538-2548.	5.4	12
16	Theoretical study concerning the reactivity of imine derivatives of polycyclic aromatic hydrocarbons. Journal of Computational Chemistry, 2003, 24, 601-608.	3.3	11
17	Synthesis and Structure of the First Bridgehead Silylium Ion. Organometallics, 2014, 33, 2146-2149.	2.3	11
18	Synthesis, Computational Docking Study, and Biological Evaluation of a Library of Heterocyclic Curcuminoids with Remarkable Antitumor Activity. ChemMedChem, 2018, 13, 1895-1908.	3.2	10

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19	Catalytic Activity of Human Placental Alkaline Phosphatase (PLAP): Insights from a Computational Study. Journal of Physical Chemistry B, 2014, 118, 14302-14313.	2.6	9
20	Catalyst-free assembly of giant tris(heteroaryl)methanes: synthesis of novel pharmacophoric triads and model sterically crowded tris(heteroaryl/aryl)methyl cation salts. Beilstein Journal of Organic Chemistry, 2019, 15, 642-654.	2.2	9
21	Deuterated Curcuminoids: Synthesis, Structures, Computational/Docking and Comparative Cell Viability Assays against Colorectal Cancer. ChemMedChem, 2019, 14, 1173-1184.	3.2	8
22	Curcumin Conjugates of Nonâ€steroidal Antiâ€inflammatory Drugs: Synthesis, Structures, Antiâ€proliferative Assays, Computational Docking, and Inflammatory Response. ChemistryOpen, 2020, 9, 822-834.	1.9	8
23	Design, synthesis, and molecular docking study of novel quinolineâ€based bisâ€chalcones as potential antitumor agents. Archiv Der Pharmazie, 2021, 354, e2100094.	4.1	8
24	A DFT Model Study of the Carbocations Formed via the Fjordâ€and Bayâ€Region Diol Epoxide Metabolites of Isomeric Dibenzopyrenes and Naphthopyrene. European Journal of Organic Chemistry, 2009, 2009, 3331-3339.	2.4	7
25	Electrophilic Addition of Propargylic Cations to Allenes: Formation of Crowded Chloroâ€and Azidoâ€Enynes by Trapping of the Resulting Allylic Cations with TMSX (X = Cl, N₃): A Synthetic and Computational Study. European Journal of Organic Chemistry, 2013, 2013, 5455-5463.	2.4	7
26	Quantum-Mechanical Study on the Catalytic Mechanism of Alkaline Phosphatases. Journal of Chemical Information and Modeling, 2017, 57, 540-549.	5.4	7
27	A Computational (DFT, MP2) and GIAO NMR Study of Substituent Effects in Benzenediazonium Mono- and Dications. European Journal of Organic Chemistry, 2011, 2011, 1771-1775.	2.4	6
28	Ionic liquid catalyzed Ritter reaction/Pd-catalyzed directed Ortho-arylation; facile access to diverse libraries of biaryl-amides from Aryl-nitriles. Tetrahedron Letters, 2020, 61, 152553.	1.4	6
29	Stable carbocations and onium ions from polycondensed aromatic and heteroaromatic compounds as models for biological electrophiles and DNA-transalkylating agents. Advances in Physical Organic Chemistry, 2009, 43, 135-176.	0.5	4
30	Î±-Sulfur or Î±-fluorineâ€"Which is more stabilizing for a carbocation? A computational study of electrophilic addition to HFCCH(SMe) and FC(R1)CR2(SMe) and related model systems. Journal of Fluorine Chemistry, 2013, 151, 26-31.	1.7	4
31	Quantum-chemical studies on mutagenicity of aromatic and heteroaromatic amines. Frontiers in Bioscience - Scholar, 2013, S5, 600-610.	2.1	4
32	Iodine Activation of Alcohols: A Computational Study. Topics in Catalysis, 2018, 61, 636-642.	2.8	4
33	Recent Advances in the Development of â€œCurcumin Inspiredâ€Compounds as New Therapeutic Agents. Mini-Reviews in Medicinal Chemistry, 2020, 20, 1543-1558.	2.4	4
34	Phospha- and arsa-bridged cyclononatetraenides: novel zwitterionic 10Ï€ aromatic hemispheres. New Journal of Chemistry, 2019, 43, 6267-6273.	2.8	3
35	TQuantum Chemical Studies of Carbocations from Oxidized Metabolites of Aza-Polycyclic Aromatic Hydrocarbons. ACS Symposium Series, 2007, , 329-363.	0.5	2
36	Quantum Chemical Studies on Ultimate Carcinogenic Metabolites from Polycyclic Aromatic Hydrocarbons. Current Medicinal Chemistry, 2008, 15, 2901-2920.	2.4	2

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37	A computational study (DFT, MP2, and GIAOâ€DFT) of substituent effects on protonation regioselectivity in Î²,Î²â€disubstituted vinyldiazonium cations: formation of highly delocalized carbenium/diazonium dications. Journal of Physical Organic Chemistry, 2010, 23, 115-125.	1.9	2
38	In Silico study of carcinogenic oâ€Quinone metabolites derived from polycyclic aromatic hydrocarbons (PAHs). Journal of Physical Organic Chemistry, 2012, 25, 720-728.	1.9	2
39	Piperidineâ€appended imidazolium ionic liquids as taskâ€specific catalysts: computational study, synthesis, and multinuclear NMR. Journal of Physical Organic Chemistry, 2016, 29, 346-351.	1.9	2
40	A computational study of SF5-substituted carbocations. Journal of Fluorine Chemistry, 2017, 197, 118-133.	1.7	2
41	Mutagenicity of heteroaromatic amines: Computational study on the influence of methyl substituents. Journal of Molecular Graphics and Modelling, 2016, 69, 92-102.	2.4	1
42	Computational study on the role of residue Arg166 in alkaline phosphatases. Arkivoc, 2018, 2018, 114-121.	0.5	1
43	Alkaline Phosphatases: in Silico Study on the Catalytic Effect of Conserved Active Site Residues Using Human Placental Alkaline Phosphatase (PLAP) As a Model Protein. Journal of Chemical Information and Modeling, 2020, 60, 6228-6241.	5.4	1
44	In Silico Study on Chemical Properties and Reactivity of Enal Derivatives. European Journal of Organic Chemistry, 2015, 2015, 6615-6623.	2.4	0