Gloria Mazzone

List of Publications by Year in Descending Order

70 papers	1,454 citations	23 h-index	35 g-index
81 ext. papers	1,768 ext. citations	4.4 avg, IF	5.04 L-index

#	Paper	IF	Citations
70	Computational Studies of the Photogeneration from Dihydrosanguinarine and the Probable Cytotoxicity Mechanism of Sanguinarine. *Applied Sciences (Switzerland)*, **2022**, 12, 1095	2.6	
69	Experimental and theoretical study of the complexation of Fe3+ and Cu2+ by l-ascorbic acid in aqueous solution. *Journal of Molecular Liquids*, **2022**, 355, 118973	6	0
68	Experimental and theoretical study on the coordination properties of quercetin towards aluminum(III), iron(III) and copper(II) in aqueous solution. *Journal of Molecular Liquids*, **2021**, 325, 115171	6	5
67	A Review on Coordination Properties of Al(III) and Fe(III) toward Natural Antioxidant Molecules: Experimental and Theoretical Insights. *Molecules*, **2021**, 26,	4.8	9
66	A combined Monte Carlo/DFT approach to simulate UV-vis spectra of molecules and aggregates: Merocyanine dyes as a case study. *Journal of Computational Chemistry*, **2021**, 42, 1054-1063	3.5	0
65	Torsion-Induced Nonradiative Relaxation of the Singlet Excited State of -Thienyl Bodipy and Charge Separation, Charge Recombination-Induced Intersystem Crossing in Its Compact Electron Donor/Acceptor Dyads. *Journal of Physical Chemistry B*, **2021**, 125, 4779-4793	3.4	5
64	Anticancer Activity, DNA Binding, and Photodynamic Properties of a N?C?N-Coordinated Pt(II) Complex. *Inorganic Chemistry*, **2021**, 60, 10350-10360	5.1	5
63	Novel choline selective electrochemical membrane sensor with application in milk powders and infant formulas. *Talanta*, **2021**, 221, 121409	6.2	8
62	Theoretical investigation on bisarylselanylbenzo-2,1,3-selenadiazoles as potential photosensitizers in photodynamic therapy. *Journal of Chemical Physics*, **2021**, 154, 084113	3.9	0
61	A Boron-Containing Compound Acting on Multiple Targets Against Alzheimer's Disease. Insights from Ab Initio and Molecular Dynamics Simulations. *Journal of Chemical Information and Modeling*, **2021**, 61, 3397-3410	6.1	6
60	Computational Analysis of Photophysical Properties and Reactivity of a New Phototherapeutic Cyclometalated Au(III)-Hydride Complex. *Chemistry - A European Journal*, **2021**, 27, 15528-15535	4.8	1
59	Cyclopentadienone–NHC iron(0) complexes as low valent electrocatalysts for water oxidation. *Catalysis Science and Technology*, **2021**, 11, 1407-1418	5.5	1
58	Mechanism of action of the curcumin cis-diammineplatinum(II) complex as a photocytotoxic agent. *Inorganic Chemistry Frontiers*, **2020**, 7, 2759-2769	6.8	3
57	Spin-Orbit Charge-Transfer Intersystem Crossing (ISC) in Compact Electron Donor-Acceptor Dyads: ISC Mechanism and Application as Novel and Potent Photodynamic Therapy Reagents. *Chemistry - A European Journal*, **2020**, 26, 1091-1102	4.8	44
56	A comparative computational mechanistic study on derivatives of pyriplatin, modified with the [CH2Ph3P+ group, as anticancer complexes targeting mitochondria. *Inorganica Chimica Acta*, **2020**, 512, 119863	2.7	1
55	Theoretical exploration of the photophysical properties of two-component Ru-porphyrin dyes as promising assemblies for a combined antitumor effect. *Dalton Transactions*, **2020**, 49, 12653-12661	4.3	2
54	Spectrophotometric determination of choline in pharmaceutical formulations via host-guest complexation with a biomimetic calixarene receptor. *Microchemical Journal*, **2019**, 146, 735-741	4.8	7

53	Increasing the anti-Stokes shift in TTA upconversion with photosensitizers showing red-shifted spin-allowed charge transfer absorption but a non-compromised triplet state energy level. *Chemical Communications*, **2019**, 55, 1510-1513	5.8	39
52	On the Inhibition of Hydroxyl Radical Formation by Hydroxycinnamic Acids: The Case of Caffeic Acid as a Promising Chelating Ligand of a Ferrous Ion. *Journal of Physical Chemistry A*, **2019**, 123, 9560-9566	2.8	15
51	Theoretical insight into joint photodynamic action of a gold(i) complex and a BODIPY chromophore for singlet oxygen generation. *Physical Chemistry Chemical Physics*, **2019**, 21, 3446-3452	3.6	5
50	Computational Investigation of the Influence of Halogen Atoms on the Photophysical Properties of Tetraphenylporphyrin and Its Zinc(II) Complexes. *Journal of Physical Chemistry A*, **2018**, 122, 2809-2815	2.8	11
49	Chemical Insights into the Antioxidant Mechanisms of Alkylseleno and Alkyltelluro Phenols: Periodic Relatives Behaving Differently. *Chemistry - A European Journal*, **2018**, 24, 8686-8691	4.8	9
48	Quantum mechanical DFT elucidation of CO2 catalytic conversion mechanisms: Three examples. *International Journal of Quantum Chemistry*, **2018**, 118, e25572	2.1	9
47	Excitation energies, singlet-triplet energy gaps, spin-orbit matrix elements and heavy atom effects in BOIMPYs as possible photosensitizers for photodynamic therapy: a computational investigation. *Physical Chemistry Chemical Physics*, **2018**, 20, 2656-2661	3.6	15
46	Theoretical Insights into the Switching Off/On of O Photosensitization in Chemicontrolled Photodynamic Therapy. *Chemistry - A European Journal*, **2018**, 24, 3512-3519	4.8	10
45	Anion-π weak interactions in a heteroaromatic calixarene receptor. A theoretical investigation. *Inorganica Chimica Acta*, **2018**, 470, 379-384	2.7	10
44	BODIPY for photodynamic therapy applications: computational study of the effect of bromine substitution on O photosensitization. *Journal of Molecular Modeling*, **2018**, 24, 183	2	8
43	Antioxidant properties and free radical scavenging mechanisms of cyclocurcumin. *New Journal of Chemistry*, **2018**, 42, 12698-12705	3.6	8
42	Theoretical determination of the aquation reaction mechanism of cyclometalated benzimidazole Ru(II) and Ir(III) anticancer complexes. *Inorganica Chimica Acta*, **2018**, 470, 325-330	2.7	2
41	Spin–Orbit Charge Recombination Intersystem Crossing in Phenothiazine–Anthracene Compact Dyads: Effect of Molecular Conformation on Electronic Coupling, Electronic Transitions, and Electron Spin Polarizations of the Triplet States. *Journal of Physical Chemistry C*, **2018**, 122, 27850-27865	3.8	56
40	Photophysical Properties of Nitrated and Halogenated Phosphorus Tritolylcorrole Complexes: Insights from Theory. *Molecules*, **2018**, 23,	4.8	4
39	On the Electrochromic Properties of Borepins: A Computational Prediction. *ACS Omega*, **2018**, 3, 9556-9563	3.9	1
38	Direct and cluster-assisted dehydrogenation of methane by Nb and Ta: a theoretical investigation. *Physical Chemistry Chemical Physics*, **2017**, 19, 16178-16188	3.6	5
37	The ability of a zinc pyrrolidine complex to catalyze the synthesis of cyclic carbonates from carbon dioxide and epoxides: a mechanistic theoretical investigation. *Dalton Transactions*, **2017**, 46, 9030-9035	4.3	14
36	Photophysical Properties of S, Se and Te-Substituted Deoxyguanosines: Insight into Their Ability To Act as Chemotherapeutic Agents. *Journal of Chemical Information and Modeling*, **2017**, 57, 234-242	6.1	22

35	Halogen atom effect on the photophysical properties of substituted aza-BODIPY derivatives. *Physical Chemistry Chemical Physics*, **2017**, 19, 2530-2536	3.6	42
34	Bodipy-squaraine triads: Preparation and study of the intramolecular energy transfer, charge separation and intersystem crossing. *Dyes and Pigments*, **2017**, 147, 560-572	4.6	8
33	Theoretical investigation of the action mechanisms of N,N-di-alkylated diarylamine antioxidants. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	2
32	Complexation of Al and Ni by l-Ascorbic Acid: An Experimental and Theoretical Investigation. *Journal of Physical Chemistry A*, **2017**, 121, 9773-9781	2.8	13
31	Trimethylphosphate and Dimethylphosphate Hydrolysis by Binuclear Cd , Mn , and Zn -Fe Promiscuous Organophosphate-Degrading Enzyme: Reaction Mechanisms. *Chemistry - A European Journal*, **2017**, 23, 13742-13753	4.8	6
30	Time-Dependent Density Functional Computations of the Spectrochemical Properties of Dithiolodithiole and Thiophene Electrochromic Systems. *Materials*, **2017**, 10,	3.5	2
29	Metal Atom Effect on the Photophysical Properties of Mg(II), Zn(II), Cd(II), and Pd(II) Tetraphenylporphyrin Complexes Proposed as Possible Drugs in Photodynamic Therapy. *Molecules*, **2017**, 22,	4.8	34
28	Investigation of the Inertness to Hydrolysis of Platinum(IV) Prodrugs. *Inorganic Chemistry*, **2016**, 55, 1580-6	5.6	24
27	Food Antioxidants: Chemical Insights at the Molecular Level. *Annual Review of Food Science and Technology*, **2016**, 7, 335-52	14.7	222
26	Coumarin-Chalcone Hybrids as Peroxyl Radical Scavengers: Kinetics and Mechanisms. *Journal of Chemical Information and Modeling*, **2016**, 56, 662-70	6.1	32
25	Antioxidant properties comparative study of natural hydroxycinnamic acids and structurally modified derivatives: Computational insights. *Computational and Theoretical Chemistry*, **2016**, 1077, 39-47	2	34
24	Can Expanded Bacteriochlorins Act as Photosensitizers in Photodynamic Therapy? Good News from Density Functional Theory Computations. *Molecules*, **2016**, 21, 288	4.8	29
23	PDT-correlated photophysical properties of thienopyrrole BODIPY derivatives. Theoretical insights. *Dyes and Pigments*, **2016**, 130, 9-15	4.6	37
22	Catalytic role of dinuclear acetylide gold(I) complexes in the hydroamination of terminal alkynes: theoretical insights. *Journal of Chemical Theory and Computation*, **2015**, 11, 581-90	6.4	16
21	Photophysical properties of free and metallated meso-substituted tetrabenzotriazaporphyrin from density functional theory investigation. *Dyes and Pigments*, **2015**, 120, 335-339	4.6	36
20	The heavy atom effect on Zn(ii) phthalocyanine derivatives: a theoretical exploration of the photophysical properties. *Physical Chemistry Chemical Physics*, **2015**, 17, 23595-601	3.6	41
19	Understanding zinc(II) chelation with quercetin and luteolin: a combined NMR and theoretical study. *Journal of Physical Chemistry B*, **2015**, 119, 83-95	3.4	50
18	Antioxidant properties of several coumarin–chalcone hybrids from theoretical insights. *RSC Advances*, **2015**, 5, 565-575	3.7	61

17	Ab initio calculations on the (1)O2 quenching mechanism by trans-resveratrol. *Physical Chemistry Chemical Physics*, **2014**, 16, 12773-81	3.6	11
16	Electronic spectra and intersystem spin-orbit coupling in 1,2- and 1,3-squaraines. *Journal of Computational Chemistry*, **2014**, 35, 2107-13	3.5	30
15	Theoretical mechanistic study of the formic acid decomposition assisted by a Ru(II)-phosphine catalyst. *Journal of Molecular Modeling*, **2014**, 20, 2250	2	9
14	Theoretical Determination of Electronic Spectra and Intersystem Spin-Orbit Coupling: The Case of Isoindole-BODIPY Dyes. *Journal of Chemical Theory and Computation*, **2014**, 10, 4006-13	6.4	45
13	Density functional study of the antioxidant activity of some recently synthesized resveratrol analogues. *Food Chemistry*, **2013**, 141, 2017-24	8.5	46
12	Theoretical investigation of the absorption spectra and singlet-triplet energy gap of positively charged tetraphenylporphyrins as potential photodynamic therapy photosensitizers. *Canadian Journal of Chemistry*, **2013**, 91, 902-906	0.9	20
11	Density functional predictions of antioxidant activity and UV spectral features of nasutin A, isonasutin, ellagic acid, and one of its possible derivatives. *Journal of Agricultural and Food Chemistry*, **2013**, 61, 9650-7	5.7	36
10	Homogeneous Gold Catalysis: Hydration of 1,2-Diphenylacetylene with Methanol in Aqueous Media. A Theoretical Viewpoint. *Organometallics*, **2012**, 31, 3074-3080	3.8	39
9	Dimethylplatinum(II) complexes: computational insights into Pt-C bond protonolysis. *Inorganic Chemistry*, **2011**, 50, 10091-101	5.1	21
8	The mutual influence of non-covalent interactions in pi-electron deficient cavities: the case of anion recognition by tetraoxacalix[2]arene[2]triazine. *Chemical Communications*, **2010**, 46, 5894-6	5.8	37
7	Gold(I)-Catalyzed Hydration of 1,2-Diphenylacetylene: Computational Insights. *Journal of Chemical Theory and Computation*, **2010**, 6, 2782-9	6.4	16
6	The influence of surface oxygen and hydroxyl groups on the dehydrogenation of ethylene on PdAu surface alloys. A theoretical cluster model study. *Chemical Physics Letters*, **2010**, 493, 87-93	2.5	5
5	Adsorption of Ethylene, Vinyl, Acetic Acid, and Acetate Species on PdAu(111) and PdAu(100) Surface Alloys: A Cluster Model Study. *Journal of Chemical Theory and Computation*, **2009**, 5, 1350-60	6.4	23
4	The geometric effect in palladium-gold catalysis. Is the coupling the rate-determining step in the vinyl-acetate synthesis?. *Chemical Communications*, **2009**, 1852-4	5.8	14
3	Interaction of CO with PdAu(111) and PdAu(100) Bimetallic Surfaces: A Theoretical Cluster Model Study. *Journal of Physical Chemistry C*, **2008**, 112, 6073-6081	3.8	35
2	Mechanistic aspects of the reaction of Th+ and Th2+ with water in the gas phase. *Inorganic Chemistry*, **2008**, 47, 2083-8	5.1	30
1	The combined use of deuterium NMR and computer simulations for conformational investigation of flexible molecules in nematic solutions. *Computational and Theoretical Chemistry*, **2005**, 728, 209-214		5