Tiziana Marino

List of Publications by Citations

122 papers	3,019 citations	29 h-index	51 g-index
133 ext. papers	3,405 ext. citations	4.5 avg, IF	5.36 L-index

#	Paper	IF	Citations
122	Antioxidant Properties of Phenolic Compounds: H-Atom versus Electron Transfer Mechanism. *Journal of Physical Chemistry A*, **2004**, 108, 4916-4922	2.8	481
121	Food Antioxidants: Chemical Insights at the Molecular Level. *Annual Review of Food Science and Technology*, **2016**, 7, 335-52	14.7	222
120	Density functional computations of the energetic and spectroscopic parameters of quercetin and its radicals in the gas phase and in solvent. *Theoretical Chemistry Accounts*, **2004**, 111, 210-216	1.9	135
119	Interaction of cysteine with Cu2+ and group IIb (Zn2+, Cd2+, Hg2+) metal cations: a theoretical study. *Journal of Mass Spectrometry*, **2005**, 40, 300-6	2.2	111
118	Gas-phase metal ion (Li+, Na+, Cu+) affinities of glycine and alanine. *Journal of Inorganic Biochemistry*, **2000**, 79, 179-85	4.2	107
117	Radical scavenging ability of gallic acid toward OH and OOH radicals. Reaction mechanism and rate constants from the density functional theory. *Journal of Physical Chemistry B*, **2014**, 118, 10380-9	3.4	101
116	Interaction of Li+, Na+, and K+ with the Proline Amino Acid. Complexation Modes, Potential Energy Profiles, and Metal Ion Affinities. *Journal of Physical Chemistry B*, **2003**, 107, 2588-2594	3.4	98
115	Structural and electronic characterization of the complexes obtained by the interaction between bare and hydrated first-row transition-metal ions (Mn(2+), Fe(2+), Co(2+), Ni(2+), Cu(2+), Zn(2+)) and glycine. *Journal of Physical Chemistry B*, **2006**, 110, 24666-73	3.4	97
114	A comparative study of the catalytic mechanisms of the zinc and cadmium containing carbonic anhydrase. *Journal of the American Chemical Society*, **2005**, 127, 4242-53	16.4	69
113	Potential energy surfaces for the gas-phase interaction between alpha-alanine and alkali metal Ions (Li+, Na+, K+). A density functional study. *Inorganic Chemistry*, **2001**, 40, 6439-43	5.1	62
112	Structural and Electronic Characterization of Antioxidants from Marine Organisms. *Theoretical Chemistry Accounts*, **2006**, 115, 361-369	1.9	59
111	Peptide hydrolysis by the binuclear zinc enzyme aminopeptidase from Aeromonas proteolytica: a density functional theory study. *Journal of Physical Chemistry B*, **2008**, 112, 2494-500	3.4	58
110	Human insulin-degrading enzyme working mechanism. *Journal of the American Chemical Society*, **2009**, 131, 14804-11	16.4	52
109	Catalytic mechanism of the arylsulfatase promiscuous enzyme from Pseudomonas aeruginosa. *Chemistry - A European Journal*, **2013**, 19, 2185-92	4.8	46
108	Catalytic activity of a □class zinc and cadmium containing carbonic anhydrase. Compared work mechanisms. *Physical Chemistry Chemical Physics*, **2011**, 13, 3468-77	3.6	45
107	The role of glutathione in cadmium ion detoxification: coordination modes and binding properties--a density functional study. *Journal of Inorganic Biochemistry*, **2009**, 103, 50-7	4.2	40
106	Gas-phase interaction between DNA and RNA bases and copper (II) ion: A density functional study. *International Journal of Quantum Chemistry*, **2004**, 98, 347-354	2.1	38

105	Photophysical properties of free and metallated meso-substituted tetrabenzotriazaporphyrin from density functional theory investigation. *Dyes and Pigments*, **2015**, 120, 335-339	4.6	36
104	The role of quantum chemistry in the elucidation of the elementary mechanisms of catalytic processes: from atoms, to surfaces, to enzymes. *Theoretical Chemistry Accounts*, **2007**, 117, 765-779	1.9	36
103	Interaction of Cu(+) and Cu(2+) ions with alpha-alanine. A density functional study. *Journal of Mass Spectrometry*, **2002**, 37, 786-91	2.2	36
102	Photophysical origin of the reduced photodynamic therapy activity of temocene compared to Foscan : insights from theory. *Physical Chemistry Chemical Physics*, **2013**, 15, 16167-71	3.6	34
101	Theoretical study of silver-ion-mediated base pairs: the case of C-Ag-C and C-Ag-A systems. *Journal of Physical Chemistry A*, **2015**, 119, 5153-7	2.8	34
100	Insights into the coordination mode of quercetin with the Al(III) ion from a combined experimental and theoretical study. *Dalton Transactions*, **2014**, 43, 7269-74	4.3	33
99	A proposal for mitochondrial processing peptidase catalytic mechanism. *Journal of the American Chemical Society*, **2011**, 133, 17824-31	16.4	33
98	Atomistic details of the Catalytic Mechanism of Fe(III)-Zn(II) Purple Acid Phosphatase. *Journal of Chemical Theory and Computation*, **2010**, 6, 2424-33	6.4	32
97	Complexation behaviour of caffeic, ferulic and p-coumaric acids towards aluminium cations: a combined experimental and theoretical approach. *New Journal of Chemistry*, **2017**, 41, 5182-5190	3.6	29
96	How Can Methanol Dehydrogenase from Methylacidiphilum fumariolicum Work with the Alien Ce Ion in the Active Center? A Theoretical Study. *Chemistry - A European Journal*, **2017**, 23, 8652-8657	4.8	29
95	On the copper(II) ion coordination by prion protein HGGGW pentapeptide model. *Journal of Physical Chemistry B*, **2007**, 111, 635-40	3.4	29
94	Can Expanded Bacteriochlorins Act as Photosensitizers in Photodynamic Therapy? Good News from Density Functional Theory Computations. *Molecules*, **2016**, 21, 288	4.8	29
93	The performance of density functional based methods in the description of selected biological systems and processes. *Physical Chemistry Chemical Physics*, **2012**, 14, 14943-53	3.6	27
92	On the metal ion (Zn(2+), Cu(2+)) coordination with beta-amyloid peptide: DFT computational study. *Interdisciplinary Sciences, Computational Life Sciences*, **2010**, 2, 57-69	3.5	26
91	Density functional computations of proton affinity and gas-phase basicity of proline. *Journal of Mass Spectrometry*, **2001**, 36, 301-5	2.2	26
90	A theoretical study on tautomerization processes of dehydrated and monohydrated cytosine. *Computational and Theoretical Chemistry*, **2007**, 811, 161-167		25
89	Promiscuous ability of human carbonic anhydrase: QM and QM/MM investigation of carbon dioxide and carbodiimide hydration. *Inorganic Chemistry*, **2014**, 53, 3488-93	5.1	24
88	Molecular dynamics, density functional and second-order MllerPlesset theory study of the structure and conformation of acetylcholine in vacuo and in solution. *Theoretical Chemistry Accounts*, **2001**, 107, 8-14	1.9	22

87	Gas phase interaction of zinc ion with purine and pyrimidine DNA and RNA bases. *International Journal of Quantum Chemistry*, **2007**, 107, 311-317	2.1	20
86	Direct Hydrogenation of Carbon Dioxide by an Artificial Reductase Obtained by Substituting Rhodium for Zinc in the Carbonic Anhydrase Catalytic Center. A Mechanistic Study. *ACS Catalysis*, **2015**, 5, 5397-5409	13.1	19
85	Insight on the chelation of aluminum(III) and iron(III) by curcumin in aqueous solution. *Journal of Molecular Liquids*, **2019**, 296, 111805	6	19
84	Theoretical investigation on DNA/RNA base pairs mediated by copper, silver, and gold cations. *Dalton Transactions*, **2012**, 41, 1816-23	4.3	19
83	What occurs by replacing Mn2+ with Co2+ in human arginase I: first-principles computational analysis. *Inorganic Chemistry*, **2013**, 52, 655-9	5.1	18
82	CO2 Activation by Nb(+) and NbO(+) in the Gas Phase. A Case of Two-State Reactivity Process. *Journal of Chemical Theory and Computation*, **2007**, 3, 811-5	6.4	18
81	Gas-phase acidity of proline from density functional computations. *International Journal of Quantum Chemistry*, **2001**, 84, 264-268	2.1	18
80	Insight into the promiscuous activity of human carbonic anhydrase against the cyanic acid substrate from a combined QM and QM/MM investigation. *Physical Chemistry Chemical Physics*, **2014**, 16, 16671-6	3.6	17
79	Reaction Mechanism of Low-Spin Iron(III)- and Cobalt(III)-Containing Nitrile Hydratases: A Quantum Mechanics Investigation. *Inorganic Chemistry*, **2017**, 56, 13390-13400	5.1	16
78	Structure and Coordination Modes in the Interaction between Cd2+ and 3-Mercaptopropionic Acid. *Journal of Physical Chemistry A*, **2004**, 108, 8407-8410	2.8	15
77	Density functional computations and mass spectrometric measurements. Can this coupling enlarge the knowledge of gas-phase chemistry?. *Advances in Quantum Chemistry*, **2000**, 36, 93-120	1.4	15
76	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
75	The working mechanism of the Ecarbonic anhydrase degrading carbonyl sulphide (COSase): a theoretical study. *Physical Chemistry Chemical Physics*, **2015**, 17, 14843-8	3.6	13
74	Ab initio study of microsolvated Al3+-aromatic amino acid complexes. *Journal of Physical Chemistry B*, **2010**, 114, 9017-22	3.4	13
73	On the interaction of rubidium and cesium mono-, strontium and barium bi-cations with DNA and RNA bases. A theoretical study. *International Journal of Quantum Chemistry*, **2010**, 110, 138-147	2.1	13
72	Theoretical investigation of the catalytic mechanism of the protein arginine deiminase 4 enzyme. *Theoretical Chemistry Accounts*, **2008**, 120, 459-466	1.9	13
71	On the Inhibition Mechanism of Glutathione Transferase P1 by Piperlongumine. Insight From Theory. *Frontiers in Chemistry*, **2018**, 6, 606	5	13
70	Chalcogen effects on the primary antioxidant activity of chrysin and quercetin. *New Journal of Chemistry*, **2020**, 44, 9073-9082	3.6	11

69	The Antioxidant Capability of Higenamine: Insights from Theory. *Antioxidants*, **2020**, 9,	7.1	11
68	Complexation of Al(III) by aromatic amino acids in the gas phase. *Inorganic Chemistry*, **2007**, 46, 6413-9	5.1	11
67	Explicit Water Molecules Play a Key Role in the Mechanism of Rhodium-Substituted Human Carbonic Anhydrase. *ChemCatChem*, **2017**, 9, 1047-1053	5.2	10
66	QM Cluster or QM/MM in Computational Enzymology: The Test Case of LigW-Decarboxylase. *Frontiers in Chemistry*, **2018**, 6, 249	5	10
65	The Catalytic Mechanism of Human Transketolase. *ChemPhysChem*, **2019**, 20, 2881-2886	3.2	10
64	DFT investigation of the mismatched base pairs (T-Hg-T)3, (U-Hg-U)3, d(T-Hg-T)2, and d(U-Hg-U)2. *Journal of Molecular Modeling*, **2014**, 20, 2303	2	10
63	Density Functional Theory as a Tool for the Prediction of the Properties in Molecules with Biological and Pharmacological Significance. *Theoretical and Computational Chemistry*, **1996**, 743-772		10
62	The Effects of the Metal Ion Substitution into the Active Site of Metalloenzymes: A Theoretical Insight on Some Selected Cases. *Catalysts*, **2020**, 10, 1038	4	10
61	The role of the halogen bond in iodothyronine deiodinase: Dependence on chalcogen substitution in naphthyl-based mimetics. *Journal of Computational Chemistry*, **2019**, 40, 944-951	3.5	10
60	Structural characterization of aluminium(III) and iron(III) complexes of coumarinic acid in aqueous solutions from combined experimental and theoretical investigations. *New Journal of Chemistry*, **2018**, 42, 11006-11012	3.6	10
59	How Lanthanide Ions Affect the Addition-Elimination Step of Methanol Dehydrogenases. *Chemistry - A European Journal*, **2020**, 26, 11334-11339	4.8	9
58	How the Destabilization of a Reaction Intermediate Affects Enzymatic Efficiency: The Case of Human Transketolase. *ACS Catalysis*, **2020**, 10, 2872-2881	13.1	9
57	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
56	Quantum mechanical DFT elucidation of CO2 catalytic conversion mechanisms: Three examples. *International Journal of Quantum Chemistry*, **2018**, 118, e25572	2.1	9
55	Oxidation mechanism of methionine by HO□radical: a theoretical study. *Journal of Physical Chemistry B*, **2012**, 116, 5349-54	3.4	9
54	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
53	Why hydroxy-proline improves the catalytic power of the peptidoglycan N-deacetylase enzyme: insight from theory. *Physical Chemistry Chemical Physics*, **2019**, 21, 23338-23345	3.6	9
52	The role of metal substitution in the promiscuity of natural and artificial carbonic anhydrases. *Coordination Chemistry Reviews*, **2017**, 345, 73-85	23.2	8

51	The role of arsenic in the hydrolysis and DNA metalation processes in an arsenous acid-platinum(ii) anticancer complex. *Physical Chemistry Chemical Physics*, **2017**, 19, 1328-1334	3.6	8
50	Iodine substituted phosphorus corrole complexes as possible photosensitizers in photodynamic therapy: Insights from theory. *Journal of Computational Chemistry*, **2020**, 41, 1395-1401	3.5	8
49	A deeper insight on the radical scavenger activity of two simple coumarins toward OOH radical. *Computational and Theoretical Chemistry*, **2016**, 1077, 133-138	2	8
48	The nature of the C□As bonds in arsaalkynes: an atoms in molecules and electron localization function study. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	8
47	Interaction of the Mn2+, Co2+, Ni2+, and Zn2+ with prion protein HGGGW pentapeptide model. *International Journal of Quantum Chemistry*, **2011**, 111, 1152-1162	2.1	8
46	Assessment of Approximate Density Functional Methods for the Study of the Interactions of Al(III) with Aromatic Amino Acids. *Journal of Chemical Theory and Computation*, **2007**, 3, 1830-6	6.4	8
45	On the binding mode of urease active site inhibitors: A density functional study. *International Journal of Quantum Chemistry*, **2008**, 108, 2023-2029	2.1	8
44	Mechanism of thyroxine deiodination by naphthyl-based iodothyronine deiodinase mimics and the halogen bonding role: a DFT investigation. *Chemistry - A European Journal*, **2015**, 21, 8554-60	4.8	7
43	Conformational behaviour of the antineoplastic peptide dolastatin-10 and of two mutated derivatives. *Journal of Computer-Aided Molecular Design*, **1995**, 9, 425-38	4.2	7
42	Molecular orbital study of the protonation of dA, dG, dC and dT 2Sdeoxyribonucleosides. *Computational and Theoretical Chemistry*, **1994**, 306, 185-195		7
41	TDDFT investigation on methylviologen, 3,7-diazabenzophosphole, and helical helquat electrochromic systems. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	7
40	Can fused thiophene□yrrole-containing rings act as possible new electrochromic dyes? A computational prediction. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	7
39	Theoretical investigation on the restoring step of the carbonic anhydrase catalytic cycle for natural and promiscuous substrates. *Archives of Biochemistry and Biophysics*, **2015**, 582, 101-6	4.1	6
38	Effect of Copper on the Mitochondrial Carnitine/Acylcarnitine Carrier Via Interaction with Cys136 and Cys155. Possible Implications in Pathophysiology. *Molecules*, **2020**, 25,	4.8	6
37	Conformational behaviour of 1,4-dihydronicotinamide and protonated nicotinamide in vacuo and in solvent: a density functional study. *Computational and Theoretical Chemistry*, **2000**, 501-502, 215-220		6
36	Capsaicin, a Powerful OH-Inactivating Ligand. *Antioxidants*, **2020**, 9,	7.1	5
35	Site-selective methylation of N(beta)-nosyl hydrazides of N-nosyl protected alpha-amino acids. *Journal of Organic Chemistry*, **2010**, 75, 3381-6	4.2	5
34	Computational Study Reveals the Role of Water Molecules in the Inhibition Mechanism of LAT1 by 1,2,3-Dithiazoles. *Journal of Chemical Information and Modeling*, **2021**,	6.1	5

33	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
32	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
31	Computationally designed p-coumaric acid analogs: searching for neuroprotective antioxidants. *New Journal of Chemistry*, **2021**, 45, 14369-14380	3.6	5
30	A micro-environmental study of the Zn(+2)-A□-16 structural properties. *Biophysical Chemistry*, **2013**, 182, 86-93	3.5	4
29	On the Catalytic Activity of the Engineered Coiled-Coil Heptamer Mimicking the Hydrolase Enzymes: Insights from a Computational Study. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	4
28	Antioxidant Properties of the Vam3 Derivative of Resveratrol. *Molecules*, **2018**, 23,	4.8	4
27	How Metal Coordination in the Ca-, Ce-, and Eu-Containing Methanol Dehydrogenase Enzymes Can Influence the Catalysis: A Theoretical Point of View. *Challenges and Advances in Computational Chemistry and Physics*, **2019**, 487-501	0.7	3
26	Mechanistic Explanation of the Weak Carbonic Anhydrase's Esterase Activity. *Molecules*, **2017**, 22,	4.8	3
25	Structural and binding properties of metal ion chelators relevant to Alzheimer's disease. A theoretical investigation. *International Journal of Quantum Chemistry*, **2012**, 112, 2109-2114	2.1	3
24	Hydration of Aromatic Nitriles Catalyzed by Mn-OH Complexes: A Rationalization from Quantum Chemical Investigations. *Organometallics*, **2020**, 39, 3352-3361	3.8	3
23	Quantum Mechanical Predictions of the Antioxidant Capability of Moracin C Isomers. *Frontiers in Chemistry*, **2021**, 9, 666647	5	3
22	Mechanistic investigation of trimethylamine-N-oxide reduction catalysed by biomimetic molybdenum enzyme models. *Physical Chemistry Chemical Physics*, **2016**, 18, 8428-36	3.6	3
21	Insights into the Catalytic Mechanism of Domains CD1 and CD2 in Histone Deacetylase 6 from Quantum Calculations. *ACS Catalysis*, **2021**, 11, 3084-3093	13.1	3
20	The Se-S Bond Formation in the Covalent Inhibition Mechanism of SARS-CoV-2 Main Protease by Ebselen-like Inhibitors: A Computational Study. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	3
19	Computational Mechanistic Insights on the NO Oxidation Reaction Catalyzed by Non-Heme Biomimetic Cr-N-Tetramethylated Cyclam Complexes. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	2
18	A DFT investigation of a bulky biomimetic model catalyzing the 5Souter ring deiodination of thyroxine. *Journal of Molecular Modeling*, **2016**, 22, 287	2	2
17	Time-Dependent Density Functional Computations of the Spectrochemical Properties of Dithiolodithiole and Thiophene Electrochromic Systems. *Materials*, **2017**, 10,	3.5	2
16	Theoretical comparison between structural and dynamical features of Dolastatins 11 and 12 antineoplastic depsipeptides. *SAR and QSAR in Environmental Research*, **2003**, 14, 475-84	3.5	2

15	On the fragmentation pathway of the ionized enol of glycine in the gas phase. *Rapid Communications in Mass Spectrometry*, **2001**, 15, 541-5	2.2	2
14	On the Scavenging Ability of Scutellarein against the OOH Radical in Water and Lipid-like Environments: A Theoretical Study.. *Antioxidants*, **2022**, 11,	7.1	2
13	Aluminum(III), iron(III) and copper(II) complexes of luteolin: Stability, antioxidant, and anti-inflammatory properties. *Journal of Molecular Liquids*, **2022**, 345, 117895	6	2
12	The platination mechanism of RNase A by arsenoplatin: insight from the theoretical study. *Inorganic Chemistry Frontiers*, **2021**, 8, 1795-1803	6.8	2
11	The Generation of the Oxidant Agent of a Mononuclear Nonheme Fe(II) Biomimetic Complex by Oxidative Decarboxylation. A DFT Investigation. *Molecules*, **2020**, 25,	4.8	1
10	Conformational behavior of antineoplastic peptides Dolastatin 10 and Dolastatin 15 from Monte Carlo and molecular dynamics simulations. *International Journal of Quantum Chemistry*, **2007**, 107, 318-325	2.1	1
9	Potential Energy Surfaces for Reaction Catalyzed by Metalloenzymes from Quantum Chemical Computations. *NATO Science for Peace and Security Series A: Chemistry and Biology*, **2009**, 275-313	0.1	1
8	Structure and properties of a copper-mediated nucleobase pair from density functional theory investigation. *Inorganica Chimica Acta*, **2016**, 452, 194-198	2.7	1
7	Dehydrogenation of Formic Acid to CO2 and H2 by Manganese(I) Complex: Theoretical Insights for Green and Sustainable Route. *Catalysts*, **2021**, 11, 141	4	1
6	On the Electrochromic Properties of Borepins: A Computational Prediction. *ACS Omega*, **2018**, 3, 9556-9563	3.9	1
5	Photophysical properties of methyl ketone based multi-responsive electrochromic materials: A theoretical investigation. *Journal of Molecular Liquids*, **2021**, 338, 116576	6	1
4	Theoretical investigation on bisarylselanylbenzo-2,1,3-selenadiazoles as potential photosensitizers in photodynamic therapy. *Journal of Chemical Physics*, **2021**, 154, 084113	3.9	0
3	Combined molecular mechanics, molecular dynamics and quantum mechanical study of (+)-multifidene structure and conformation. *Chemistry and Ecology*, **2004**, 20, 157-165	2.3	
2	Density Functional Theory Performance in Metal Containing Systems **2003**, 1117-1139		
1	On the Use of Density Functional Theory in the Study of Metal-Ligand Interactions. Some Studied Cases **2003**, 1-19		