

Tiziana Marino

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	On the Scavenging Ability of Scutellarein against the OOH Radical in Water and Lipid-like Environments: A Theoretical Study.. <i>Antioxidants</i> , 2022 , 11,	7.1	2
121	Aluminum(III), iron(III) and copper(II) complexes of luteolin: Stability, antioxidant, and anti-inflammatory properties. <i>Journal of Molecular Liquids</i> , 2022 , 345, 117895	6	2
120	Computational Study Reveals the Role of Water Molecules in the Inhibition Mechanism of LAT1 by 1,2,3-Dithiazoles. <i>Journal of Chemical Information and Modeling</i> , 2021 ,	6.1	5
119	Experimental and theoretical study on the coordination properties of quercetin towards aluminum(III), iron(III) and copper(II) in aqueous solution. <i>Journal of Molecular Liquids</i> , 2021 , 325, 115171 ⁶	6	5
118	A Review on Coordination Properties of Al(III) and Fe(III) toward Natural Antioxidant Molecules: Experimental and Theoretical Insights. <i>Molecules</i> , 2021 , 26,	4.8	9
117	Quantum Mechanical Predictions of the Antioxidant Capability of Moracin C Isomers. <i>Frontiers in Chemistry</i> , 2021 , 9, 666647	5	3
116	Dehydrogenation of Formic Acid to CO ₂ and H ₂ by Manganese(I) Complex: Theoretical Insights for Green and Sustainable Route. <i>Catalysts</i> , 2021 , 11, 141	4	1
115	Computationally designed p-coumaric acid analogs: searching for neuroprotective antioxidants. <i>New Journal of Chemistry</i> , 2021 , 45, 14369-14380	3.6	5
114	The platination mechanism of RNase A by arsenoplatin: insight from the theoretical study. <i>Inorganic Chemistry Frontiers</i> , 2021 , 8, 1795-1803	6.8	2
113	Theoretical investigation on bisarylselanylbenzo-2,1,3-selenadiazoles as potential photosensitizers in photodynamic therapy. <i>Journal of Chemical Physics</i> , 2021 , 154, 084113	3.9	0
112	Insights into the Catalytic Mechanism of Domains CD1 and CD2 in Histone Deacetylase 6 from Quantum Calculations. <i>ACS Catalysis</i> , 2021 , 11, 3084-3093	13.1	3
111	Photophysical properties of methyl ketone based multi-responsive electrochromic materials: A theoretical investigation. <i>Journal of Molecular Liquids</i> , 2021 , 338, 116576	6	1
110	The Se-S Bond Formation in the Covalent Inhibition Mechanism of SARS-CoV-2 Main Protease by Ebselen-like Inhibitors: A Computational Study. <i>International Journal of Molecular Sciences</i> , 2021 , 22,	6.3	3
109	Capsaicin, a Powerful OH-Inactivating Ligand. <i>Antioxidants</i> , 2020 , 9,	7.1	5
108	How Lanthanide Ions Affect the Addition-Elimination Step of Methanol Dehydrogenases. <i>Chemistry - A European Journal</i> , 2020 , 26, 11334-11339	4.8	9
107	Chalcogen effects on the primary antioxidant activity of chrysin and quercetin. <i>New Journal of Chemistry</i> , 2020 , 44, 9073-9082	3.6	11
106	Effect of Copper on the Mitochondrial Carnitine/Acylcarnitine Carrier Via Interaction with Cys136 and Cys155. Possible Implications in Pathophysiology. <i>Molecules</i> , 2020 , 25,	4.8	6

105	The Generation of the Oxidant Agent of a Mononuclear Nonheme Fe(II) Biomimetic Complex by Oxidative Decarboxylation. A DFT Investigation. <i>Molecules</i> , 2020 , 25,	4.8	1
104	How the Destabilization of a Reaction Intermediate Affects Enzymatic Efficiency: The Case of Human Transketolase. <i>ACS Catalysis</i> , 2020 , 10, 2872-2881	13.1	9
103	Iodine substituted phosphorus corrole complexes as possible photosensitizers in photodynamic therapy: Insights from theory. <i>Journal of Computational Chemistry</i> , 2020 , 41, 1395-1401	3.5	8
102	The Antioxidant Capability of Higenamine: Insights from Theory. <i>Antioxidants</i> , 2020 , 9,	7.1	11
101	The Effects of the Metal Ion Substitution into the Active Site of Metalloenzymes: A Theoretical Insight on Some Selected Cases. <i>Catalysts</i> , 2020 , 10, 1038	4	10
100	On the Catalytic Activity of the Engineered Coiled-Coil Heptamer Mimicking the Hydrolase Enzymes: Insights from a Computational Study. <i>International Journal of Molecular Sciences</i> , 2020 , 21,	6.3	4
99	Hydration of Aromatic Nitriles Catalyzed by Mn-OH Complexes: A Rationalization from Quantum Chemical Investigations. <i>Organometallics</i> , 2020 , 39, 3352-3361	3.8	3
98	Computational Mechanistic Insights on the NO Oxidation Reaction Catalyzed by Non-Heme Biomimetic Cr-N-Tetramethylated Cyclam Complexes. <i>International Journal of Molecular Sciences</i> , 2019 , 20,	6.3	2
97	How Metal Coordination in the Ca-, Ce-, and Eu-Containing Methanol Dehydrogenase Enzymes Can Influence the Catalysis: A Theoretical Point of View. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2019 , 487-501	0.7	3
96	Insight on the chelation of aluminum(III) and iron(III) by curcumin in aqueous solution. <i>Journal of Molecular Liquids</i> , 2019 , 296, 111805	6	19
95	The Catalytic Mechanism of Human Transketolase. <i>ChemPhysChem</i> , 2019 , 20, 2881-2886	3.2	10
94	The role of the halogen bond in iodothyronine deiodinase: Dependence on chalcogen substitution in naphthyl-based mimetics. <i>Journal of Computational Chemistry</i> , 2019 , 40, 944-951	3.5	10
93	Why hydroxy-proline improves the catalytic power of the peptidoglycan N-deacetylase enzyme: insight from theory. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 23338-23345	3.6	9
92	Theoretical insight into joint photodynamic action of a gold(i) complex and a BODIPY chromophore for singlet oxygen generation. <i>Physical Chemistry Chemical Physics</i> , 2019 , 21, 3446-3452	3.6	5
91	Chemical Insights into the Antioxidant Mechanisms of Alkylseleno and Alkyltelluro Phenols: Periodic Relatives Behaving Differently. <i>Chemistry - A European Journal</i> , 2018 , 24, 8686-8691	4.8	9
90	Quantum mechanical DFT elucidation of CO2 catalytic conversion mechanisms: Three examples. <i>International Journal of Quantum Chemistry</i> , 2018 , 118, e25572	2.1	9
89	QM Cluster or QM/MM in Computational Enzymology: The Test Case of LigW-Decarboxylase. <i>Frontiers in Chemistry</i> , 2018 , 6, 249	5	10
88	On the Inhibition Mechanism of Glutathione Transferase P1 by Piperlongumine. Insight From Theory. <i>Frontiers in Chemistry</i> , 2018 , 6, 606	5	13

87	Antioxidant Properties of the Vam3 Derivative of Resveratrol. <i>Molecules</i> , 2018 , 23,	4.8	4
86	On the Electrochromic Properties of Borepins: A Computational Prediction. <i>ACS Omega</i> , 2018 , 3, 9556-9563	3.6	1
85	Structural characterization of aluminium(III) and iron(III) complexes of coumarinic acid in aqueous solutions from combined experimental and theoretical investigations. <i>New Journal of Chemistry</i> , 2018 , 42, 11006-11012	3.6	10
84	Complexation behaviour of caffeic, ferulic and p-coumaric acids towards aluminium cations: a combined experimental and theoretical approach. <i>New Journal of Chemistry</i> , 2017 , 41, 5182-5190	3.6	29
83	How Can Methanol Dehydrogenase from <i>Methylobacterium</i> Work with the Alien Ce Ion in the Active Center? A Theoretical Study. <i>Chemistry - A European Journal</i> , 2017 , 23, 8652-8657	4.8	29
82	The ability of a zinc pyrrolidine complex to catalyze the synthesis of cyclic carbonates from carbon dioxide and epoxides: a mechanistic theoretical investigation. <i>Dalton Transactions</i> , 2017 , 46, 9030-9035	4.3	14
81	The role of metal substitution in the promiscuity of natural and artificial carbonic anhydrases. <i>Coordination Chemistry Reviews</i> , 2017 , 345, 73-85	23.2	8
80	Explicit Water Molecules Play a Key Role in the Mechanism of Rhodium-Substituted Human Carbonic Anhydrase. <i>ChemCatChem</i> , 2017 , 9, 1047-1053	5.2	10
79	The role of arsenic in the hydrolysis and DNA metalation processes in an arsenous acid-platinum(ii) anticancer complex. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 1328-1334	3.6	8
78	Reaction Mechanism of Low-Spin Iron(III)- and Cobalt(III)-Containing Nitrile Hydratases: A Quantum Mechanics Investigation. <i>Inorganic Chemistry</i> , 2017 , 56, 13390-13400	5.1	16
77	Time-Dependent Density Functional Computations of the Spectrochemical Properties of Dithiolodithiole and Thiophene Electrochromic Systems. <i>Materials</i> , 2017 , 10,	3.5	2
76	Mechanistic Explanation of the Weak Carbonic Anhydrase Esterase Activity. <i>Molecules</i> , 2017 , 22,	4.8	3
75	A DFT investigation of a bulky biomimetic model catalyzing the 5Souter ring deiodination of thyroxine. <i>Journal of Molecular Modeling</i> , 2016 , 22, 287	2	2
74	Food Antioxidants: Chemical Insights at the Molecular Level. <i>Annual Review of Food Science and Technology</i> , 2016 , 7, 335-52	14.7	222
73	A deeper insight on the radical scavenger activity of two simple coumarins toward OOH radical. <i>Computational and Theoretical Chemistry</i> , 2016 , 1077, 133-138	2	8
72	Can Expanded Bacteriochlorins Act as Photosensitizers in Photodynamic Therapy? Good News from Density Functional Theory Computations. <i>Molecules</i> , 2016 , 21, 288	4.8	29
71	Mechanistic investigation of trimethylamine-N-oxide reduction catalysed by biomimetic molybdenum enzyme models. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 8428-36	3.6	3
70	TDDFT investigation on methylviologen, 3,7-diazabenzophosphole, and helical helquat electrochromic systems. <i>Theoretical Chemistry Accounts</i> , 2016 , 135, 1	1.9	7

69	Structure and properties of a copper-mediated nucleobase pair from density functional theory investigation. <i>Inorganica Chimica Acta</i> , 2016 , 452, 194-198	2.7	1
68	Can fused thiophene-pyrrole-containing rings act as possible new electrochromic dyes? A computational prediction. <i>Theoretical Chemistry Accounts</i> , 2016 , 135, 1	1.9	7
67	Photophysical properties of free and metallated meso-substituted tetrabenzotriazaporphyrin from density functional theory investigation. <i>Dyes and Pigments</i> , 2015 , 120, 335-339	4.6	36
66	Theoretical investigation on the restoring step of the carbonic anhydrase catalytic cycle for natural and promiscuous substrates. <i>Archives of Biochemistry and Biophysics</i> , 2015 , 582, 101-6	4.1	6
65	Direct Hydrogenation of Carbon Dioxide by an Artificial Reductase Obtained by Substituting Rhodium for Zinc in the Carbonic Anhydrase Catalytic Center. A Mechanistic Study. <i>ACS Catalysis</i> , 2015 , 5, 5397-5409	13.1	19
64	Mechanism of thyroxine deiodination by naphthyl-based iodothyronine deiodinase mimics and the halogen bonding role: a DFT investigation. <i>Chemistry - A European Journal</i> , 2015 , 21, 8554-60	4.8	7
63	The working mechanism of the β -carbonic anhydrase degrading carbonyl sulphide (COSase): a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 14843-8	3.6	13
62	Theoretical study of silver-ion-mediated base pairs: the case of C-Ag-C and C-Ag-A systems. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 5153-7	2.8	34
61	Insights into the coordination mode of quercetin with the Al(III) ion from a combined experimental and theoretical study. <i>Dalton Transactions</i> , 2014 , 43, 7269-74	4.3	33
60	Insight into the promiscuous activity of human carbonic anhydrase against the cyanic acid substrate from a combined QM and QM/MM investigation. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 16671-6	3.6	17
59	Promiscuous ability of human carbonic anhydrase: QM and QM/MM investigation of carbon dioxide and carbodiimide hydration. <i>Inorganic Chemistry</i> , 2014 , 53, 3488-93	5.1	24
58	Radical scavenging ability of gallic acid toward OH and OOH radicals. Reaction mechanism and rate constants from the density functional theory. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 10380-9	3.4	101
57	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 . <i>Journal of Molecular Modeling</i> , 2014 , 20, 2303	2	10
56	Photophysical origin of the reduced photodynamic therapy activity of temocene compared to Foscan : insights from theory. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 16167-71	3.6	34
55	What occurs by replacing Mn ²⁺ with Co ²⁺ in human arginase I: first-principles computational analysis. <i>Inorganic Chemistry</i> , 2013 , 52, 655-9	5.1	18
54	A micro-environmental study of the Zn(+2)-A β -16 structural properties. <i>Biophysical Chemistry</i> , 2013 , 182, 86-93	3.5	4
53	Catalytic mechanism of the arylsulfatase promiscuous enzyme from <i>Pseudomonas aeruginosa</i> . <i>Chemistry - A European Journal</i> , 2013 , 19, 2185-92	4.8	46
52	Oxidation mechanism of methionine by HO \cdot radical: a theoretical study. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 5349-54	3.4	9

51	The performance of density functional based methods in the description of selected biological systems and processes. <i>Physical Chemistry Chemical Physics</i> , 2012 , 14, 14943-53	3.6	27
50	Structural and binding properties of metal ion chelators relevant to Alzheimer's disease. A theoretical investigation. <i>International Journal of Quantum Chemistry</i> , 2012 , 112, 2109-2114	2.1	3
49	Theoretical investigation on DNA/RNA base pairs mediated by copper, silver, and gold cations. <i>Dalton Transactions</i> , 2012 , 41, 1816-23	4.3	19
48	The nature of the CAs bonds in arsaalkynes: an atoms in molecules and electron localization function study. <i>Theoretical Chemistry Accounts</i> , 2012 , 131, 1	1.9	8
47	Catalytic activity of a class zinc and cadmium containing carbonic anhydrase. Compared work mechanisms. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 3468-77	3.6	45
46	Interaction of the Mn ²⁺ , Co ²⁺ , Ni ²⁺ , and Zn ²⁺ with prion protein HGGGW pentapeptide model. <i>International Journal of Quantum Chemistry</i> , 2011 , 111, 1152-1162	2.1	8
45	A proposal for mitochondrial processing peptidase catalytic mechanism. <i>Journal of the American Chemical Society</i> , 2011 , 133, 17824-31	16.4	33
44	Ab initio study of microsolvated Al ³⁺ -aromatic amino acid complexes. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 9017-22	3.4	13
43	Atomistic details of the Catalytic Mechanism of Fe(III)-Zn(II) Purple Acid Phosphatase. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 2424-33	6.4	32
42	Site-selective methylation of N(beta)-nosyl hydrazides of N-nosyl protected alpha-amino acids. <i>Journal of Organic Chemistry</i> , 2010 , 75, 3381-6	4.2	5
41	On the metal ion (Zn(2+), Cu(2+)) coordination with beta-amyloid peptide: DFT computational study. <i>Interdisciplinary Sciences, Computational Life Sciences</i> , 2010 , 2, 57-69	3.5	26
40	On the interaction of rubidium and cesium mono-, strontium and barium bi-cations with DNA and RNA bases. A theoretical study. <i>International Journal of Quantum Chemistry</i> , 2010 , 110, 138-147	2.1	13
39	The role of glutathione in cadmium ion detoxification: coordination modes and binding properties—a density functional study. <i>Journal of Inorganic Biochemistry</i> , 2009 , 103, 50-7	4.2	40
38	Human insulin-degrading enzyme working mechanism. <i>Journal of the American Chemical Society</i> , 2009 , 131, 14804-11	16.4	52
37	Potential Energy Surfaces for Reaction Catalyzed by Metalloenzymes from Quantum Chemical Computations. <i>NATO Science for Peace and Security Series A: Chemistry and Biology</i> , 2009 , 275-313	0.1	1
36	Peptide hydrolysis by the binuclear zinc enzyme aminopeptidase from <i>Aeromonas proteolytica</i> : a density functional theory study. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 2494-500	3.4	58
35	Theoretical investigation of the catalytic mechanism of the protein arginine deiminase 4 enzyme. <i>Theoretical Chemistry Accounts</i> , 2008 , 120, 459-466	1.9	13
34	On the binding mode of urease active site inhibitors: A density functional study. <i>International Journal of Quantum Chemistry</i> , 2008 , 108, 2023-2029	2.1	8

33	On the copper(II) ion coordination by prion protein HGGGW pentapeptide model. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 635-40	3.4	29
32	CO ₂ Activation by Nb(+) and NbO(+) in the Gas Phase. A Case of Two-State Reactivity Process. <i>Journal of Chemical Theory and Computation</i> , 2007 , 3, 811-5	6.4	18
31	Complexation of Al(III) by aromatic amino acids in the gas phase. <i>Inorganic Chemistry</i> , 2007 , 46, 6413-9	5.1	11
30	Assessment of Approximate Density Functional Methods for the Study of the Interactions of Al(III) with Aromatic Amino Acids. <i>Journal of Chemical Theory and Computation</i> , 2007 , 3, 1830-6	6.4	8
29	A theoretical study on tautomerization processes of dehydrated and monohydrated cytosine. <i>Computational and Theoretical Chemistry</i> , 2007 , 811, 161-167		25
28	Gas phase interaction of zinc ion with purine and pyrimidine DNA and RNA bases. <i>International Journal of Quantum Chemistry</i> , 2007 , 107, 311-317	2.1	20
27	Conformational behavior of antineoplastic peptides Dolastatin 10 and Dolastatin 15 from Monte Carlo and molecular dynamics simulations. <i>International Journal of Quantum Chemistry</i> , 2007 , 107, 318-325	2.1	1
26	The role of quantum chemistry in the elucidation of the elementary mechanisms of catalytic processes: from atoms, to surfaces, to enzymes. <i>Theoretical Chemistry Accounts</i> , 2007 , 117, 765-779	1.9	36
25	Structural and Electronic Characterization of Antioxidants from Marine Organisms. <i>Theoretical Chemistry Accounts</i> , 2006 , 115, 361-369	1.9	59
24	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. <i>Journal of Physical Chemistry B</i> , 2006 , 110, 24666-73	3.4	97
23	A comparative study of the catalytic mechanisms of the zinc and cadmium containing carbonic anhydrase. <i>Journal of the American Chemical Society</i> , 2005 , 127, 4242-53	16.4	69
22	Interaction of cysteine with Cu ²⁺ and group IIb (Zn ²⁺ , Cd ²⁺ , Hg ²⁺) metal cations: a theoretical study. <i>Journal of Mass Spectrometry</i> , 2005 , 40, 300-6	2.2	111
21	Antioxidant Properties of Phenolic Compounds: H-Atom versus Electron Transfer Mechanism. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 4916-4922	2.8	481
20	Density functional computations of the energetic and spectroscopic parameters of quercetin and its radicals in the gas phase and in solvent. <i>Theoretical Chemistry Accounts</i> , 2004 , 111, 210-216	1.9	135
19	Gas-phase interaction between DNA and RNA bases and copper (II) ion: A density functional study. <i>International Journal of Quantum Chemistry</i> , 2004 , 98, 347-354	2.1	38
18	Combined molecular mechanics, molecular dynamics and quantum mechanical study of (+)-multifidene structure and conformation. <i>Chemistry and Ecology</i> , 2004 , 20, 157-165	2.3	
17	Structure and Coordination Modes in the Interaction between Cd ²⁺ and 3-Mercaptopropionic Acid. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 8407-8410	2.8	15
16	Theoretical comparison between structural and dynamical features of Dolastatins 11 and 12 antineoplastic depsipeptides. <i>SAR and QSAR in Environmental Research</i> , 2003 , 14, 475-84	3.5	2

15	Interaction of Li ⁺ , Na ⁺ , and K ⁺ with the Proline Amino Acid. Complexation Modes, Potential Energy Profiles, and Metal Ion Affinities. <i>Journal of Physical Chemistry B</i> , 2003 , 107, 2588-2594	3.4	98
14	Density Functional Theory Performance in Metal Containing Systems 2003 , 1117-1139		
13	On the Use of Density Functional Theory in the Study of Metal-Ligand Interactions. Some Studied Cases 2003 , 1-19		
12	Interaction of Cu(+) and Cu(2+) ions with alpha-alanine. A density functional study. <i>Journal of Mass Spectrometry</i> , 2002 , 37, 786-91	2.2	36
11	Molecular dynamics, density functional and second-order Møller-Plesset theory study of the structure and conformation of acetylcholine in vacuo and in solution. <i>Theoretical Chemistry Accounts</i> , 2001 , 107, 8-14	1.9	22
10	On the fragmentation pathway of the ionized enol of glycine in the gas phase. <i>Rapid Communications in Mass Spectrometry</i> , 2001 , 15, 541-5	2.2	2
9	Gas-phase acidity of proline from density functional computations. <i>International Journal of Quantum Chemistry</i> , 2001 , 84, 264-268	2.1	18
8	Density functional computations of proton affinity and gas-phase basicity of proline. <i>Journal of Mass Spectrometry</i> , 2001 , 36, 301-5	2.2	26
7	Potential energy surfaces for the gas-phase interaction between alpha-alanine and alkali metal ions (Li ⁺ , Na ⁺ , K ⁺). A density functional study. <i>Inorganic Chemistry</i> , 2001 , 40, 6439-43	5.1	62
6	Gas-phase metal ion (Li ⁺ , Na ⁺ , Cu ⁺) affinities of glycine and alanine. <i>Journal of Inorganic Biochemistry</i> , 2000 , 79, 179-85	4.2	107
5	Conformational behaviour of 1,4-dihydronicotinamide and protonated nicotinamide in vacuo and in solvent: a density functional study. <i>Computational and Theoretical Chemistry</i> , 2000 , 501-502, 215-220		6
4	Density functional computations and mass spectrometric measurements. Can this coupling enlarge the knowledge of gas-phase chemistry?. <i>Advances in Quantum Chemistry</i> , 2000 , 36, 93-120	1.4	15
3	Density Functional Theory as a Tool for the Prediction of the Properties in Molecules with Biological and Pharmacological Significance. <i>Theoretical and Computational Chemistry</i> , 1996 , 743-772		10
2	Conformational behaviour of the antineoplastic peptide dolastatin-10 and of two mutated derivatives. <i>Journal of Computer-Aided Molecular Design</i> , 1995 , 9, 425-38	4.2	7
1	Molecular orbital study of the protonation of dA, dG, dC and dT 2'Sdeoxyribonucleosides. <i>Computational and Theoretical Chemistry</i> , 1994 , 306, 185-195		7