

Giampaolo Barone

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.

148
papers

3,581
citations

34
h-index

53
g-index

174
ext. papers

4,068
ext. citations

4.6
avg, IF

5.25
L-index

#	Paper	IF	Citations
148	B-DNA Structure and Stability: The Role of Nucleotide Composition and Order.. <i>ChemistryOpen</i> , 2022 , e202100231	2.3	
147	Structure of the 5' untranslated region in SARS-CoV-2 genome and its specific recognition by innate immune system the human oligoadenylate synthase 1.. <i>Chemical Communications</i> , 2022 ,	5.8	3
146	B-DNA Structure and Stability: The Role of Nucleotide Composition and Order.. <i>ChemistryOpen</i> , 2022 , 11, e202200013	2.3	
145	Chitosan Film Functionalized with Grape Seed OilPreliminary Evaluation of Antimicrobial Activity. <i>Sustainability</i> , 2022 , 14, 5410	3.6	2
144	Never Cared for What They Do: High Structural Stability of Guanine-Quadruplexes in the Presence of Strand-Break Damage. <i>Molecules</i> , 2022 , 27, 3256	4.8	0
143	Microscopic interactions between ivermectin and key human and viral proteins involved in SARS-CoV-2 infection. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 22957-22971	3.6	4
142	Structure and Dynamics of RNA Guanine Quadruplexes in SARS-CoV-2 Genome. Original Strategies against Emerging Viruses. <i>Journal of Physical Chemistry Letters</i> , 2021 , 12, 10277-10283	6.4	4
141	Pyrazole[3,4-d]pyrimidine derivatives loaded into halloysite as potential CDK inhibitors. <i>International Journal of Pharmaceutics</i> , 2021 , 599, 120281	6.5	5
140	Forever Young: Structural Stability of Telomeric Guanine Quadruplexes in the Presence of Oxidative DNA Lesions*. <i>Chemistry - A European Journal</i> , 2021 , 27, 8865-8874	4.8	2
139	Synthesis, characterization, and cellular investigations of porphyrin- and chlorin-indomethacin conjugates for photodynamic therapy of cancer. <i>Organic and Biomolecular Chemistry</i> , 2021 , 19, 6501-6512	3.9	3
138	Organoplatinum(II) Complexes Self-Assemble and Recognize AT-Rich Duplex DNA Sequences. <i>Inorganic Chemistry</i> , 2021 , 60, 2178-2187	5.1	6
137	On the G-Quadruplex Binding of a New Class of Nickel(II), Copper(II), and Zinc(II) Salphen-Like Complexes. <i>European Journal of Inorganic Chemistry</i> , 2021 , 2021, 1332-1336	2.3	2
136	A Simple Entropic-Driving Separation Procedure of Low-Size Silver Clusters, Through Interaction with DNA. <i>ChemistryOpen</i> , 2021 , 10, 760-763	2.3	
135	C-C Cross-Couplings from a Cyclometalated Au(III) C N Complex: Mechanistic Insights and Synthetic Developments. <i>Chemistry - A European Journal</i> , 2021 , 27, 14322-14334	4.8	3
134	Combined spectroscopic and theoretical analysis of the binding of a water-soluble perylene diimide to DNA/RNA polynucleotides and G-quadruplexes. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021 , 260, 119914	4.4	0
133	Identification of New Antimicrobial Peptides from Mediterranean Medical Plant (Steinh.) Speta. <i>Antibiotics</i> , 2020 , 9,	4.9	5
132	Role of RNA Guanine Quadruplexes in Favoring the Dimerization of SARS Unique Domain in Coronaviruses. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 5661-5667	6.4	17

131	DNA-binding of zinc(II) and nickel(II) salphen-like complexes extrapolated at 1M salt concentration: Removing the ionic strength bias in physiological conditions. <i>Journal of Inorganic Biochemistry</i> , 2020 , 207, 111064	4.2	3
130	Exploring the Chemoselectivity towards Cysteine Arylation by Cyclometallated Au Compounds: New Mechanistic Insights. <i>ChemBioChem</i> , 2020 , 21, 3071-3076	3.8	12
129	Carbon-Phosphorus Coupling from C ^N Cyclometalated Au Complexes. <i>Chemistry - A European Journal</i> , 2020 , 26, 4226-4231	4.8	15
128	Modification of DNA structure by reactive nitrogen species as a result of 2-methoxyestradiol-induced neuronal nitric oxide synthase uncoupling in metastatic osteosarcoma cells. <i>Redox Biology</i> , 2020 , 32, 101522	11.3	5
127	Thermodynamics of the Interaction between the Spike Protein of Severe Acute Respiratory Syndrome Coronavirus-2 and the Receptor of Human Angiotensin-Converting Enzyme 2. Effects of Possible Ligands. <i>Journal of Physical Chemistry Letters</i> , 2020 , 11, 9272-9281	6.4	18
126	Green Tea Catechins Induce Inhibition of PTP1B Phosphatase in Breast Cancer Cells with Potent Anti-Cancer Properties: In Vitro Assay, Molecular Docking, and Dynamics Studies. <i>Antioxidants</i> , 2020 , 9,	7.1	5
125	Molecular Basis of SARS-CoV-2 Infection and Rational Design of Potential Antiviral Agents: Modeling and Simulation Approaches. <i>Journal of Proteome Research</i> , 2020 , 19, 4291-4315	5.6	36
124	Experimental and theoretical characterization of the strong effects on DNA stability caused by half-sandwich Ru(II) and Ir(III) bearing thiabendazole complexes. <i>Journal of Biological Inorganic Chemistry</i> , 2020 , 25, 1067-1083	3.7	2
123	Human DNA Telomeres in Presence of Oxidative Lesions: The Crucial Role of Electrostatic Interactions on the Stability of Guanine Quadruplexes. <i>Antioxidants</i> , 2019 , 8,	7.1	5
122	PTP1B phosphatase as a novel target of oleuropein activity in MCF-7 breast cancer model. <i>Toxicology in Vitro</i> , 2019 , 61, 104624	3.6	11
121	Halloysite nanotubes-carbon dots hybrids multifunctional nanocarrier with positive cell target ability as a potential non-viral vector for oral gene therapy. <i>Journal of Colloid and Interface Science</i> , 2019 , 552, 236-246	9.3	36
120	Cyclometalated Au Complexes for Cysteine Arylation in Zinc Finger Protein Domains: towards Controlled Reductive Elimination. <i>Chemistry - A European Journal</i> , 2019 , 25, 7628-7634	4.8	34
119	A Synthetic Derivative of Antimicrobial Peptide Holothuroidin 2 from Mediterranean Sea Cucumber () in the Control of. <i>Marine Drugs</i> , 2019 , 17,	6	16
118	DHFR Inhibitors: Reading the Past for Discovering Novel Anticancer Agents. <i>Molecules</i> , 2019 , 24,	4.8	73
117	Novel Sortase A Inhibitors to Counteract Gram-Positive Bacterial Biofilms. <i>Proceedings (mdpi)</i> , 2019 , 22, 23	0.3	2
116	Targeting G-quadruplexes with Organic Dyes: Chelerythrine-DNA Binding Elucidated by Combining Molecular Modeling and Optical Spectroscopy. <i>Antioxidants</i> , 2019 , 8,	7.1	8
115	Pyrrrolomycins as antimicrobial agents. Microwave-assisted organic synthesis and insights into their antimicrobial mechanism of action. <i>Bioorganic and Medicinal Chemistry</i> , 2019 , 27, 721-728	3.4	15
114	Selective targeting of PARP-1 zinc finger recognition domains with Au(III) organometallics. <i>Chemical Communications</i> , 2018 , 54, 611-614	5.8	33

113	Role of Seroalbumin in the Cytotoxicity of cis-Dichloro Pt(II) Complexes with (N^N)-Donor Ligands Bearing Functionalized Tails. <i>Inorganic Chemistry</i> , 2018 , 57, 6124-6134	5.1	18
112	Kinetic evidence for interaction of TMPyP4 with two different G-quadruplex conformations of human telomeric DNA. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2018 , 1862, 522-531	4	15
111	Perturbation of Developmental Regulatory Gene Expression by a G-Quadruplex DNA Inducer in the Sea Urchin Embryo. <i>Biochemistry</i> , 2018 , 57, 4391-4394	3.2	4
110	2-Methoxyestradiol Affects Mitochondrial Biogenesis Pathway and Succinate Dehydrogenase Complex Flavoprotein Subunit A in Osteosarcoma Cancer Cells. <i>Cancer Genomics and Proteomics</i> , 2018 , 15, 73-89	3.3	11
109	The interaction of Schiff Base complexes of nickel(II) and zinc(II) with duplex and G-quadruplex DNA. <i>Journal of Inorganic Biochemistry</i> , 2018 , 178, 106-114	4.2	20
108	Antimicrobial and Antibiofilm Activity of a Recombinant Fragment of Φ Thymosin of Sea Urchin. <i>Marine Drugs</i> , 2018 , 16,	6	11
107	Fishing for G-Quadruplexes in Solution with a Perylene Diimide Derivative Labeled with Biotins. <i>Chemistry - A European Journal</i> , 2018 , 24, 11292-11296	4.8	8
106	Silver Atomic Quantum Clusters of Three Atoms for Cancer Therapy: Targeting Chromatin Compaction to Increase the Therapeutic Index of Chemotherapy. <i>Advanced Materials</i> , 2018 , 30, e18013174		14
105	1,3-Dipolar cycloadditions with meso-tetraarylchlorins Φ ite selectivity and mixed bisadducts. <i>Organic Chemistry Frontiers</i> , 2017 , 4, 534-544	5.2	10
104	2-methoxyestradiol impacts on amino acids-mediated metabolic reprogramming in osteosarcoma cells by its interaction with NMDA receptor. <i>Journal of Cellular Physiology</i> , 2017 , 232, 3030-3049	7	10
103	The mechanism of aquaporin inhibition by gold compounds elucidated by biophysical and computational methods. <i>Chemical Communications</i> , 2017 , 53, 3830-3833	5.8	35
102	The dissociation of the Hsp60/pro-Caspase-3 complex by bis(pyridyl)oxadiazole copper complex (CubipyOXA) leads to cell death in NCI-H292 cancer cells. <i>Journal of Inorganic Biochemistry</i> , 2017 , 170, 8-16	4.2	35
101	Targeting G-quadruplex DNA as Potential Anti-cancer Therapy 2017 , 129-162		
100	A novel compound of triphenyltin(IV) with N-tert-butoxycarbonyl-L-ornithine causes cancer cell death by inducing a p53-dependent activation of the mitochondrial pathway of apoptosis. <i>Inorganica Chimica Acta</i> , 2017 , 456, 1-8	2.7	13
99	A peptide from human Φ thymosin as a platform for the development of new anti-biofilm agents for Staphylococcus spp. and Pseudomonas aeruginosa. <i>World Journal of Microbiology and Biotechnology</i> , 2016 , 32, 124	4.4	11
98	Circular Dichroism of DNA G-Quadruplexes: Combining Modeling and Spectroscopy To Unravel Complex Structures. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 3113-21	3.4	30
97	The inhibition of glycerol permeation through aquaglyceroporin-3 induced by mercury(II): A molecular dynamics study. <i>Journal of Inorganic Biochemistry</i> , 2016 , 160, 78-84	4.2	22
96	Molecular recognition of naphthalene diimide ligands by telomeric quadruplex-DNA: the importance of the protonation state and mediated hydrogen bonds. <i>Physical Chemistry Chemical Physics</i> , 2016 , 18, 2871-7	3.6	24

95	Interaction of Cd(II) and Ni(II) terpyridine complexes with model polynucleotides: a multidisciplinary approach. <i>RSC Advances</i> , 2016 , 6, 4936-4945	3.7	9
94	Teaching Inorganic Photophysics and Photochemistry with Three Ruthenium(II) Polypyridyl Complexes: A Computer-Based Exercise. <i>Journal of Chemical Education</i> , 2016 , 93, 292-298	2.4	12
93	Metal Ions and Metal Complexes in Alzheimer's Disease. <i>Current Pharmaceutical Design</i> , 2016 , 22, 3996-4010	4.1	27
92	DNA-Binding and Anticancer Activity of Pyrene-Imidazolium Derivatives. <i>ChemistrySelect</i> , 2016 , 1, 6755-6761	6.7	5
91	Another step toward DNA selective targeting: Ni(II) and Cu(II) complexes of a Schiff base ligand able to bind gene promoter G-quadruplexes. <i>Dalton Transactions</i> , 2016 , 45, 7758-67	4.3	35
90	G-quadruplex vs. duplex-DNA binding of nickel(II) and zinc(II) Schiff base complexes. <i>Journal of Inorganic Biochemistry</i> , 2016 , 161, 115-21	4.2	34
89	The Binding Mechanism of Epolactaene to Hsp60 Unveiled by in Silico Modelling. <i>ChemistrySelect</i> , 2016 , 1, 759-765	1.8	4
88	Enhancement of premature stop codon readthrough in the CFTR gene by Ataluren (PTC124) derivatives. <i>European Journal of Medicinal Chemistry</i> , 2015 , 101, 236-44	6.8	34
87	Zinc complexes as fluorescent chemosensors for nucleic acids: new perspectives for a "boring" element. <i>Dalton Transactions</i> , 2015 , 44, 3527-35	4.3	23
86	Ag ₂ and Ag ₃ clusters: synthesis, characterization, and interaction with DNA. <i>Angewandte Chemie - International Edition</i> , 2015 , 54, 7612-6	16.4	47
85	The Influence of the Amide Linkage in the Fe(III) -Binding Properties of Catechol-Modified Rosamine Derivatives. <i>Chemistry - A European Journal</i> , 2015 , 21, 15692-704	4.8	6
84	Quaternary structures of GroEL and naïve-Hsp60 chaperonins in solution: a combined SAXS-MD study. <i>RSC Advances</i> , 2015 , 5, 49871-49879	3.7	11
83	1,2,3-Triazole in Heterocyclic Compounds, Endowed with Biological Activity, through 1,3-Dipolar Cycloadditions. <i>European Journal of Organic Chemistry</i> , 2014 , 2014, 3289-3306	3.2	215
82	Interaction of doxorubicin with polynucleotides. A spectroscopic study. <i>Biochemistry</i> , 2014 , 53, 2197-2073	3.2	55
81	Multivariate analysis in the identification of biological targets for designed molecular structures: the BIOTA protocol. <i>European Journal of Medicinal Chemistry</i> , 2014 , 75, 106-10	6.8	18
80	Selective G-quadruplex stabilizers: Schiff-base metal complexes with anticancer activity. <i>RSC Advances</i> , 2014 , 4, 33245-33256	3.7	62
79	Paracentrin 1, a synthetic antimicrobial peptide from the sea-urchin <i>Paracentrotus lividus</i> , interferes with staphylococcal and <i>Pseudomonas aeruginosa</i> biofilm formation. <i>AMB Express</i> , 2014 , 4, 78	4.1	16
78	The Right Answer for the Right Electrostatics: Force Field Methods Are Able to Describe Relative Energies of DNA Guanine Quadruplexes. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 2901-5	6.4	11

77	A theoretical and experimental investigation of the spectroscopic properties of a DNA-intercalator salphen-type Zn(II) complex. <i>Chemistry - A European Journal</i> , 2014 , 20, 7439-47	4.8	21
76	Structure-directing and high-efficiency photocatalytic hydrogen production by Ag clusters. <i>Journal of the American Chemical Society</i> , 2014 , 136, 1182-5	16.4	62
75	Toward a rationale for the PTC124 (Ataluren) promoted readthrough of premature stop codons: a computational approach and GFP-reporter cell-based assay. <i>Molecular Pharmaceutics</i> , 2014 , 11, 653-64	5.6	63
74	New benzothieno[3,2-d]-1,2,3-triazines with antiproliferative activity: synthesis, spectroscopic studies, and biological activity. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2014 , 24, 3291-7	2.9	19
73	Nickel(II), copper(II) and zinc(II) metallo-intercalators: structural details of the DNA-binding by a combined experimental and computational investigation. <i>Dalton Transactions</i> , 2014 , 43, 6108-19	4.3	72
72	Does ligand symmetry play a role in the stabilization of DNA G-quadruplex host-guest complexes?. <i>Current Medicinal Chemistry</i> , 2014 , 21, 2665-90	4.3	9
71	DNA interaction of CuII, NiII and ZnII functionalized salphen complexes: studies by linear dichroism, gel electrophoresis and PCR. <i>Dalton Transactions</i> , 2013 , 42, 11220-6	4.3	26
70	The influence of substitution in the quinoxaline nucleus on 1,3-dipolar cycloaddition reactions: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2013 , 1013, 116-122	2	6
69	Photochemical functionalization of allyl benzoates by C _H insertion. <i>Tetrahedron</i> , 2013 , 69, 6065-6069	2.4	2
68	Are compliance constants ill-defined descriptors for weak interactions?. <i>RSC Advances</i> , 2013 , 3, 4757	3.7	29
67	Metal complex-DNA binding: Insights from molecular dynamics and DFT/MM calculations. <i>Journal of Inorganic Biochemistry</i> , 2013 , 124, 63-9	4.2	28
66	DNA-binding of nickel(II), copper(II) and zinc(II) complexes: Structure–affinity relationships. <i>Coordination Chemistry Reviews</i> , 2013 , 257, 2848-2862	23.2	197
65	B-DNA Structure and Stability as Function of Nucleic Acid Composition: Dispersion-Corrected DFT Study of Dinucleoside Monophosphate Single and Double Strands. <i>ChemistryOpen</i> , 2013 , 2, 186-93	2.3	26
64	In Silico, Spectroscopic, and Biological Insights on Annelated Pyrrolo[3,2- e]Pyrimidines with Antiproliferative Activity. <i>Letters in Drug Design and Discovery</i> , 2013 , 11, 15-26	0.8	9
63	Hsp60, a novel target for antitumor therapy: structure-function features and prospective drugs design. <i>Current Pharmaceutical Design</i> , 2013 , 19, 2757-64	3.3	55
62	DNA binding and antiproliferative activity toward human carcinoma cells of copper(II) and zinc(II) complexes of a 2,5-diphenyl[1,3,4]oxadiazole derivative. <i>Dalton Transactions</i> , 2012 , 41, 4389-95	4.3	46
61	(Dipyrido[3,2-a:2',3'-c]phenazine)(glycinato)copper(II) perchlorate: a novel DNA-intercalator with anti-proliferative activity against thyroid cancer cell lines. <i>Journal of Inorganic Biochemistry</i> , 2012 , 117, 103-10	4.2	25
60	DNA binding studies and cytotoxicity of a dinuclear PtII diazapyrenium-based metallo-supramolecular rectangular box. <i>Chemistry - A European Journal</i> , 2012 , 18, 10983-90	4.8	32

59	Relativistic coupled cluster calculations of the electronic structure of KrH ⁺ , XeH ⁺ and RnH ⁺ . <i>Theoretical Chemistry Accounts</i> , 2012 , 131, 1	1.9	4
58	Synthesis and chemical characterization of CuII, NiII and ZnII complexes of 3,5-bis(2?-pyridyl)-1,2,4-oxadiazole and 3-(2?-pyridyl)5-(phenyl)-1,2,4-oxadiazole ligands. <i>Inorganica Chimica Acta</i> , 2011 , 373, 62-67	2.7	22
57	Synthesis, characterization, cellular uptake and interaction with native DNA of a bis(pyridyl)-1,2,4-oxadiazole copper(II) complex. <i>Dalton Transactions</i> , 2010 , 39, 9140-5	4.3	42
56	Fluorescence emission and enhanced photochemical stability of Zn(II)-5-triethyl ammonium methyl salicylidene ortho-phenylendiiminate interacting with native DNA. <i>Journal of Inorganic Biochemistry</i> , 2010 , 104, 765-73	4.2	12
55	Hydrogenolysis of hydroxymatairesinol on Y derived catalysts: A computational study. <i>Journal of Molecular Catalysis A</i> , 2010 , 333, 136-144		7
54	Systematic conformational search analysis of the SRR and RRR epimers of 7-hydroxymatairesinol. <i>Journal of Physical Organic Chemistry</i> , 2010 , 23, 141-147	2.1	5
53	CASSCF/CASPT2 analysis of the fragmentation of H ₂ on a Pd ₄ cluster. <i>International Journal of Quantum Chemistry</i> , 2010 , 110, 558-562	2.1	17
52	Structural and Kinetic DFT Characterization of Materials to Rationalize Catalytic Performance. <i>Topics in Catalysis</i> , 2009 , 52, 444-455	2.3	10
51	Molecular-Level Characterization of Heterogeneous Catalytic Systems by Algorithmic Time Dependent Monte Carlo. <i>Topics in Catalysis</i> , 2009 , 52, 431-443	2.3	3
50	On the structure of 3-acetylamino-5-methyl-1,2,4-oxadiazole and on the fully degenerate rearrangements (FDR) of its anion: a stimulating comparison between the results of η -silicon chemistry and laboratory chemistry. <i>Journal of Physical Organic Chemistry</i> , 2009 , 22, 1086-1093	2.1	9
49	Computational study of the interaction of proflavine with d(ATATATATAT)2 and d(GCGCGCGCGC)2. <i>Computational and Theoretical Chemistry</i> , 2009 , 915, 86-92		22
48	The interaction of native calf thymus DNA with Fe(III)-dipyrido[3,2-a:2',3'-c]phenazine. <i>Journal of Inorganic Biochemistry</i> , 2009 , 103, 1-9	4.2	45
47	Spectroscopic study of the interaction of Ni(II)-5-triethyl ammonium methyl salicylidene ortho-phenylendiiminate with native DNA. <i>Journal of Inorganic Biochemistry</i> , 2009 , 103, 731-7	4.2	67
46	Confined But-2-ene Catalytic Isomerization Inside H-ZSM-5 Models: A DFT Study. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 1274-83	6.4	12
45	Adsorbed CO on group 10 metal fragments: a DFT study. <i>Journal of Chemical Information and Modeling</i> , 2009 , 49, 1223-33	6.1	5
44	Experimental and DFT studies on competitive heterocyclic rearrangements. 3. A cascade isoxazole-1,2,4-oxadiazole-oxazole rearrangement. <i>Journal of Organic Chemistry</i> , 2009 , 74, 351-8	4.2	31
43	Nuclear quadrupole moment of ¹¹⁹ Sn. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 1666-72	2.8	36
42	Confinement effects on the interaction of native DNA with Cu(II)-5-(triethylammoniummethyl)salicylidene ortho-phenylendiiminate in C(12)E(4) liquid crystals. <i>Dalton Transactions</i> , 2008 , 4172-8	4.3	14

41	Intercalation of daunomycin into stacked DNA base pairs. DFT study of an anticancer drug. <i>Journal of Biomolecular Structure and Dynamics</i> , 2008 , 26, 115-30	3.6	41
40	Pyrazolo[3,4-d][1,2,3]triazolo[1,5-a]pyrimidine: a new ring system through Dimroth rearrangement. <i>Tetrahedron Letters</i> , 2008 , 49, 5125-5128	2	18
39	H β SM-5 Modified Zeolite: Quantum Chemical Models of Acidic Sites. <i>Journal of Physical Chemistry C</i> , 2007 , 111, 13033-13043	3.8	35
38	Experimental and DFT studies on competitive heterocyclic rearrangements. Part 2: a one-atom side-chain versus the classic three-atom side-chain (Boulton-Katritzky) ring rearrangement of 3-acylamino-1,2,4-oxadiazoles. <i>Journal of Organic Chemistry</i> , 2007 , 72, 7656-66	4.2	29
37	IDEA: interface dynamics and energetics algorithm. <i>Journal of Computational Chemistry</i> , 2007 , 28, 2483-995	9	9
36	Dynamics of metal centers monitored by nuclear inelastic scattering. <i>Hyperfine Interactions</i> , 2007 , 165, 17-24	0.8	2
35	Tin-DNA complexes investigated by nuclear inelastic scattering of synchrotron radiation. <i>Hyperfine Interactions</i> , 2007 , 165, 299-302	0.8	1
34	The interaction of native DNA with Zn(II) and Cu(II) complexes of 5-triethyl ammonium methyl salicylidene orto-phenylendiimine. <i>Journal of Inorganic Biochemistry</i> , 2007 , 101, 841-8	4.2	100
33	Analytic high-order Douglas-Kroll-Hess electric field gradients. <i>Journal of Chemical Physics</i> , 2007 , 127, 074105	3.9	60
32	Synthesis, spectroscopic characterization and in vitro antimicrobial activity of diorganotin(IV) dichloride adducts with [1,2,4]triazolo-[1,5-a]pyrimidine and 5,7-dimethyl-[1,2,4]triazolo-[1,5-a]pyrimidine. <i>Journal of Organometallic Chemistry</i> , 2006 , 691, 693-701	2.3	30
31	The prediction of the nuclear quadrupole splitting of ¹¹⁹ Sn Mössbauer spectroscopy data by scalar relativistic DFT calculations. <i>Chemistry - A European Journal</i> , 2006 , 12, 5116-21	4.8	10
30	Photochemistry of 1,2,4-oxadiazoles. A DFT study on photoinduced competitive rearrangements of 3-amino- and 3-n-methylamino-5-perfluoroalkyl-1,2,4-oxadiazoles. <i>Journal of Organic Chemistry</i> , 2006 , 71, 2740-9	4.2	14
29	Structural investigations on diorgano- and triorganotin(IV) derivatives of [meso-tetra(4-sulfonatophenyl)porphine] metal chlorides. <i>Journal of Organometallic Chemistry</i> , 2006 , 691, 1573-1583	2.3	5
28	Ground state and electronic spectrum of Cu(II) and Cu(III) complexes of N,N'-1,2-phenylenebis-2-mercaptoacetamide. <i>Physical Chemistry Chemical Physics</i> , 2005 , 7, 2126-30	3.6	6
27	Synthesis, characterization, and in vitro antimicrobial activity of organotin(IV) complexes with triazolo-pyrimidine ligands containing exocyclic oxygen atoms. <i>Journal of Organometallic Chemistry</i> , 2005 , 690, 4773-4783	2.3	38
26	DFT computational study on Fe(III)-N,N'-ethylene-bis(salicylideneiminato) derivatives. <i>Computational and Theoretical Chemistry</i> , 2005 , 715, 79-83		7
25	X-ray Absorption Spectra of Cu(II) and Cu(III) Complexes of N,N'-1,2-Phenylenebis(2-mercapto-2-methylpropionamide). <i>European Journal of Inorganic Chemistry</i> , 2005 , 2005, 410-415	2.3	1
24	DFT calculations of the electric field gradient at the tin nucleus as a support of structural interpretation by ¹¹⁹ Sn Mössbauer spectroscopy. <i>Chemistry - A European Journal</i> , 2005 , 11, 6185-91	4.8	18

23	Conformational analysis and DFT calculations of 8-hydroxy-germacradiene-6,12-olide derivatives. <i>Journal of Physical Organic Chemistry</i> , 2005 , 18, 1116-1122	2.1	7
22	The interaction of native DNA with iron(III)-N,N'-ethylene-bis(salicylideneiminato)-chloride. <i>Journal of Inorganic Biochemistry</i> , 2004 , 98, 589-94	4.2	126
21	SCSA code: applications on the cyclopeptide renieramide. <i>Journal of Chemical Information and Computer Sciences</i> , 2004 , 44, 1024-30		9
20	New time-dependent Monte Carlo algorithm designed to model three-phase batch reactor processes: applications on 2,4-dinitro-toluene hydrogenation on Pd/C catalysts. <i>Chemical Engineering Journal</i> , 2003 , 91, 133-142	14.7	3
19	Structure validation of natural products by quantum-mechanical GIAO calculations of ¹³ C NMR chemical shifts. <i>Chemistry - A European Journal</i> , 2002 , 8, 3233-9	4.8	197
18	Determination of the relative stereochemistry of flexible organic compounds by Ab initio methods: conformational analysis and Boltzmann-averaged GIAO ¹³ C NMR chemical shifts. <i>Chemistry - A European Journal</i> , 2002 , 8, 3240-5	4.8	153
17	Ab initio study of structure and energetics of species involved in the 2,4-dinitro-toluene hydrogenation on Pd catalysts. <i>Computational and Theoretical Chemistry</i> , 2002 , 584, 211-220		6
16	Hydrogenation of 2,4-Dinitro-toluene on Pd/C Catalysts: Computational Study on the Influence of the Molecular Adsorption Modes and of Steric Hindrance and Metal Dispersion on the Reaction Mechanism. <i>Journal of Catalysis</i> , 2002 , 211, 296-307	7.3	2
15	Synthesis and thermal decomposition studies of homo- and heteroleptic tin(IV) thiolates and dithiocarbamates: molecular precursors for tin sulfides. <i>Dalton Transactions RSC</i> , 2002 , 1085-1092		67
14	Hydrogenation of 2,4-Dinitro-toluene on Pd/C Catalysts: Computational Study on the Influence of the Molecular Adsorption Modes and of Steric Hindrance and Metal Dispersion on the Reaction Mechanism. <i>Journal of Catalysis</i> , 2002 , 211, 296-307	7.3	11
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8	Deposition of tin sulfide thin films from tin(IV) thiolate precursors. <i>Journal of Materials Chemistry</i> , 2001 , 11, 464-468		57
7	Structural distortions in homoleptic (RE) ₄ A (E = O, S, Se; A = C, Si, Ge, Sn): implications for the CVD of tin sulfides. <i>Dalton Transactions RSC</i> , 2001 , 3435-3445		11
6	The interaction of deoxyribonucleic acid with methyltin(IV) moieties in solution studied by small-angle X-ray scattering, circular dichroism and UV spectroscopy. <i>Applied Organometallic Chemistry</i> , 2000 , 14, 189-196	3.1	12

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4	Semiempirical calculations on the interaction between dimethyltin(IV) and DNA model system. <i>Computational and Theoretical Chemistry</i> , 1999 , 469, 143-149		20
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2	Outstanding Nobility Observed in Cu ₅ Clusters Reveals the Key Role of Collective Quantum Effects		2
1	Silver Clusters of Five Atoms as Highly Selective Antitumoral Agents Through Irreversible Oxidation of Thiols. <i>Advanced Functional Materials</i> , 2113028	15.6	0