Giampaolo Barone

List of Publications by Year
in descending order

154 papers	4,549 citations	101543 36 h-index	133252 59 g-index
174 all docs	174 docs citations	174 times ranked	5861 citing authors

#	Article	IF	Citations
1	1,2,3â€Triazole in Heterocyclic Compounds, Endowed with Biological Activity, through 1,3â€Dipolar Cycloadditions. European Journal of Organic Chemistry, 2014, 2014, 3289-3306.	2.4	271
2	DNA-binding of nickel(II), copper(II) and zinc(II) complexes: Structureâ€“affinity relationships. Coordination Chemistry Reviews, 2013, 257, 2848-2862.	18.8	240
3	Structure Validation of Natural Products by Quantum-Mechanical GIAO Calculations of 13C NMR Chemical Shifts GIAO=gauge including atomic orbitals.. Chemistry - A European Journal, 2002, 8, 3233.	3.3	221
4	Determination of the Relative Stereochemistry of Flexible Organic Compounds by Ab Initio Methods: Conformational Analysis and Boltzmann-Averaged GIAO 13C NMR Chemical Shifts GIAO=gauge including atomic orbitals.. Chemistry - A European Journal, 2002, 8, 3240.	3.3	167
5	DHFR Inhibitors: Reading the Past for Discovering Novel Anticancer Agents. Molecules, 2019, 24, 1140.	3.8	149
6	The interaction of native DNA with iron(III)-N,Nâ€²-ethylene-bis(salicylideneiminato)-chloride. Journal of Inorganic Biochemistry, 2004, 98, 589-594.	3.5	133
7	The interaction of native DNA with Zn(II) and Cu(II) complexes of 5-triethyl ammonium methyl salicylidene orto-phenylendiimine. Journal of Inorganic Biochemistry, 2007, 101, 841-848.	3.5	108
8	Nickel(ii), copper(ii) and zinc(ii) metallo-intercalators: structural details of the DNA-binding by a combined experimental and computational investigation. Dalton Transactions, 2014, 43, 6108.	3.3	79
9	Selective G-quadruplex stabilizers: Schiff-base metal complexes with anticancer activity. RSC Advances, 2014, 4, 33245-33256.	3.6	78
10	Spectroscopic study of the interaction of NiII-5-triethyl ammonium methyl salicylidene ortho-phenylendiiminate with native DNA. Journal of Inorganic Biochemistry, 2009, 103, 731-737.	3.5	77
11	Toward a Rationale for the PTC124 (Ataluren) Promoted Readthrough of Premature Stop Codons: A Computational Approach and GFP-Reporter Cell-Based Assay. Molecular Pharmaceutics, 2014, 11, 653-664.	4.6	73
12	Synthesis and thermal decomposition studies of homo- and heteroleptic tin(iv) thiolates and dithiocarbamates: molecular precursors for tin sulfides. Dalton Transactions RSC, 2002, , 1085-1092.	2.3	71
13	Molecular Basis of SARS-CoV-2 Infection and Rational Design of Potential Antiviral Agents: Modeling and Simulation Approaches. Journal of Proteome Research, 2020, 19, 4291-4315.	3.7	68
14	Deposition of tin sulfide thin films from tin(iv) thiolate precursors. Journal of Materials Chemistry, 2001, 11, 464-468.	6.7	65
15	Hsp60, a Novel Target for Antitumor Therapy: Structure-Function Features and Prospective Drugs Design. Current Pharmaceutical Design, 2013, 19, 2757-2764.	1.9	65
16	Analytic high-order Douglas-Kroll-Hess electric field gradients. Journal of Chemical Physics, 2007, 127, 074105.	3.0	64
17	Structure-Directing and High-Efficiency Photocatalytic Hydrogen Production by Ag Clusters. Journal of the American Chemical Society, 2014, 136, 1182-1185.	13.7	64
18	Ag₂ and Ag₃ Clusters: Synthesis, Characterization, and Interaction with DNA. Angewandte Chemie - International Edition, 2015, 54, 7612-7616.	13.8	63

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19	Interaction of Doxorubicin with Polynucleotides. A Spectroscopic Study. Biochemistry, 2014, 53, 2197-2207.	2.5	61
20	Cyclometalated Au^{III} Complexes for Cysteine Arylation in Zinc Finger Protein Domains: towards Controlled Reductive Elimination. Chemistry - A European Journal, 2019, 25, 7628-7634.	3.3	53
21	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. Dalton Transactions, 2012, 41, 4389.	3.3	51
22	The mechanism of aquaporin inhibition by gold compounds elucidated by biophysical and computational methods. Chemical Communications, 2017, 53, 3830-3833.	4.1	50
23	The interaction of native calf thymus DNA with FeIII-dipyrido[3,2-a:2â€²,3â€²-c]phenazine. Journal of Inorganic Biochemistry, 2009, 103, 1-9.	3.5	49
24	Another step toward DNA selective targeting: Ni^{II} and Cu^{II} complexes of a Schiff base ligand able to bind gene promoter G-quadruplexes. Dalton Transactions, 2016, 45, 7758-7767.	3.3	49
25	Intercalation of Daunomycin into Stacked DNA Base Pairs. DFT Study of an Anticancer Drug. Journal of Biomolecular Structure and Dynamics, 2008, 26, 115-129.	3.5	47
26	Selective targeting of PARP-1 zinc finger recognition domains with Au(<scp>iii</scp>) organometallics. Chemical Communications, 2018, 54, 611-614.	4.1	47
27	Halloysite nanotubes-carbon dots hybrids multifunctional nanocarrier with positive cell target ability as a potential non-viral vector for oral gene therapy. Journal of Colloid and Interface Science, 2019, 552, 236-246.	9.4	47
28	Synthesis, characterization, cellular uptake and interaction with native DNA of a bis(pyridyl)-1,2,4-oxadiazole copper(ii) complex. Dalton Transactions, 2010, 39, 9140.	3.3	46
29	Title is missing!. Catalysis Letters, 2001, 72, 17-23.	2.6	45
30	Enhancement of premature stop codon readthrough in the CFTR gene by Ataluren (PTC124) derivatives. European Journal of Medicinal Chemistry, 2015, 101, 236-244.	5.5	42
31	Circular Dichroism of DNA G-Quadruplexes: Combining Modeling and Spectroscopy To Unravel Complex Structures. Journal of Physical Chemistry B, 2016, 120, 3113-3121.	2.6	42
32	G-quadruplex vs. duplex-DNA binding of nickel(II) and zinc(II) Schiff base complexes. Journal of Inorganic Biochemistry, 2016, 161, 115-121.	3.5	41
33	The dissociation of the Hsp60/pro-Caspase-3 complex by bis(pyridyl)oxadiazole copper complex () Tj ETQq1 1 0.784314 rgBT /Overlo 8-16.	3.5	40
34	Synthesis, characterization, and in vitro antimicrobial activity of organotin(IV) complexes with triazolo-pyrimidine ligands containing exocyclic oxygen atoms. Journal of Organometallic Chemistry, 2005, 690, 4773-4783.	1.8	39
35	Nuclear Quadrupole Moment of ¹¹⁹Sn. Journal of Physical Chemistry A, 2008, 112, 1666-1672.	2.5	39
36	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. Journal of Physical Chemistry Letters, 2020, 11, 9272-9281.	4.6	39

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37	DNA Binding Studies and Cytotoxicity of a Dinuclear Pt^{II} Diazapyreniumâ€Based Metalloâ€supramolecular Rectangular Box. Chemistry - A European Journal, 2012, 18, 10983-10990.	3.3	37
38	Hâ^'ZSM-5 Modified Zeolite:â€‰ Quantum Chemical Models of Acidic Sites. Journal of Physical Chemistry C, 2007, 111, 13033-13043.	3.1	36
39	Experimental and DFT Studies on Competitive Heterocyclic Rearrangements. 3. A Cascade Isoxazoleâ^'1,2,4-Oxadiazoleâ^'Oxazole Rearrangement. Journal of Organic Chemistry, 2009, 74, 351-358.	3.2	36
40	Pyrrolomycins as antimicrobial agents. Microwave-assisted organic synthesis and insights into their antimicrobial mechanism of action. Bioorganic and Medicinal Chemistry, 2019, 27, 721-728.	3.0	34
41	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. Journal of Organometallic Chemistry, 2006, 691, 693-701.	1.8	33
42	Are compliance constants ill-defined descriptors for weak interactions?. RSC Advances, 2013, 3, 4757.	3.6	33
43	Role of RNA Guanine Quadruplexes in Favoring the Dimerization of SARS Unique Domain in Coronaviruses. Journal of Physical Chemistry Letters, 2020, 11, 5661-5667.	4.6	33
44	Experimental and DFT Studies on Competitive Heterocyclic Rearrangements. Part 2:¹ A One-Atom Side-Chain versus the Classic Three-Atom Side-Chain (Boultonâ^'Katritzky) Ring Rearrangement of 3-Acylamino-1,2,4-oxadiazoles. Journal of Organic Chemistry, 2007, 72, 7656-7666.	3.2	32
45	Bâ€DNA Structure and Stability as Function of Nucleic Acid Composition: Dispersionâ€Corrected DFT Study of Dinucleoside Monophosphate Single and Double Strands. ChemistryOpen, 2013, 2, 186-193.	1.9	32
46	Zinc complexes as fluorescent chemosensors for nucleic acids: new perspectives for a â€œboringâ€• element. Dalton Transactions, 2015, 44, 3527-3535.	3.3	32
47	DNA interaction of CuII, NiII and ZnII functionalized salphen complexes: studies by linear dichroism, gel electrophoresis and PCR. Dalton Transactions, 2013, 42, 11220.	3.3	30
48	Metal complexâ€“DNA binding: Insights from molecular dynamics and DFT/MM calculations. Journal of Inorganic Biochemistry, 2013, 124, 63-69.	3.5	29
49	Molecular recognition of naphthalene diimide ligands by telomeric quadruplex-DNA: the importance of the protonation state and mediated hydrogen bonds. Physical Chemistry Chemical Physics, 2016, 18, 2871-2877.	2.8	29
50	The interaction of Schiff Base complexes of nickel(II) and zinc(II) with duplex and G-quadruplex DNA. Journal of Inorganic Biochemistry, 2018, 178, 106-114.	3.5	29
51	Metal Ions and Metal Complexes in Alzheimer's Disease. Current Pharmaceutical Design, 2016, 22, 3996-4010.	1.9	28
52	(Dipyrido[3,2-a:2â€²,3â€²-c]phenazine)(glycinato)copper(II) perchlorate: A novel DNA-intercalator with anti-proliferative activity against thyroid cancer cell lines. Journal of Inorganic Biochemistry, 2012, 117, 103-110.	3.5	27
53	The inhibition of glycerol permeation through aquaglyceroporin-3 induced by mercury(II): A molecular dynamics study. Journal of Inorganic Biochemistry, 2016, 160, 78-84.	3.5	27
54	Role of Seroalbumin in the Cytotoxicity of cis-Dichloro Pt(II) Complexes with (N^N)-Donor Ligands Bearing Functionalized Tails. Inorganic Chemistry, 2018, 57, 6124-6134.	4.0	27

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55	New benzothieno[3,2-d]-1,2,3-triazines with antiproliferative activity: Synthesis, spectroscopic studies, and biological activity. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 3291-3297.	2.2	25
56	A Synthetic Derivative of Antimicrobial Peptide Holothuroidin 2 from Mediterranean Sea Cucumber (Holothuria tubulosa) in the Control of Listeria monocytogenes. Marine Drugs, 2019, 17, 159.	4.6	25
57	Exploring the Chemoselectivity towards Cysteine Arylation by Cyclometallated Au^{III} Compounds: New Mechanistic Insights. ChemBioChem, 2020, 21, 3071-3076.	2.6	25
58	Computational study of the interaction of proflavine with d(ATATATATAT)2 and d(GCGCGCGCGC)2. Computational and Theoretical Chemistry, 2009, 915, 86-92.	1.5	24
59	Multivariate analysis in the identification of biological targets for designed molecular structures: The BIOTA protocol. European Journal of Medicinal Chemistry, 2014, 75, 106-110.	5.5	24
60	Synthesis and chemical characterization of CuII, NiII and ZnII complexes of 3,5-bis(2â€²-pyridyl)-1,2,4-oxadiazole and 3-(2â€²-pyridyl)5-(phenyl)-1,2,4-oxadiazole ligands. Inorganica Chimica Acta, 2011, 373, 62-67.	2.4	23
61	A Theoretical and Experimental Investigation of the Spectroscopic Properties of a DNAâ€Intercalator Salphenâ€Type Zn^{II} Complex. Chemistry - A European Journal, 2014, 20, 7439-7447.	3.3	23
62	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. Antioxidants, 2020, 9, 1208.	5.1	23
63	Semiempirical calculations on the interaction between dimethyltin(IV) and DNA model system. Computational and Theoretical Chemistry, 1999, 469, 143-149.	1.5	22
64	Pyrazolo[3,4-d][1,2,3]triazolo[1,5-a]pyrimidine: a new ring system through Dimroth rearrangement. Tetrahedron Letters, 2008, 49, 5125-5128.	1.4	22
65	Kinetic evidence for interaction of TMPyP4 with two different G-quadruplex conformations of human telomeric DNA. Biochimica Et Biophysica Acta - General Subjects, 2018, 1862, 522-531.	2.4	22
66	Paracentrin 1, a synthetic antimicrobial peptide from the sea-urchin Paracentrotus lividus, interferes with staphylococcal and Pseudomonas aeruginosa biofilm formation. AMB Express, 2014, 4, 78.	3.0	21
67	Carbonâ€“Phosphorus Coupling from C^N Cyclometalated Au^{III} Complexes. Chemistry - A European Journal, 2020, 26, 4226-4231.	3.3	21
68	Structure and Dynamics of RNA Guanine Quadruplexes in SARS-CoV-2 Genome. Original Strategies against Emerging Viruses. Journal of Physical Chemistry Letters, 2021, 12, 10277-10283.	4.6	21
69	Silver Atomic Quantum Clusters of Three Atoms for Cancer Therapy: Targeting Chromatin Compaction to Increase the Therapeutic Index of Chemotherapy. Advanced Materials, 2018, 30, e1801317.	21.0	20
70	DFT Calculations of the Electric Field Gradient at the Tin Nucleus as a Support of Structural Interpretation by119Sn MÃ¶ssbauer Spectroscopy. Chemistry - A European Journal, 2005, 11, 6185-6191.	3.3	19
71	CASSCF/CASPT2 analysis of the fragmentation of H₂ on a Pd₄ cluster. International Journal of Quantum Chemistry, 2010, 110, 558-562.	2.0	19
72	2-Methoxyestradiol Affects Mitochondrial Biogenesis Pathway and Succinate Dehydrogenase Complex Flavoprotein Subunit A in Osteosarcoma Cancer Cells. Cancer Genomics and Proteomics, 2018, 15, 73-89.	2.0	18

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73	The interaction of S,N-coordinated dimethyltin(IV) derivatives with deoxyribonucleic acid: structure and dynamics by119Sn MÃ¶ssbauer spectroscopy. Applied Organometallic Chemistry, 1999, 13, 595-603.	3.5	16
74	Structural distortions in homoleptic (RE)4A (E = O, S, Se; A = C, Si, Ge, Sn): implications for the CVD of tin sulfides. Dalton Transactions RSC, 2001, , 3435-3445.	2.3	16
75	Hydrogenation of light hydrocarbons on palladium: theoretical study of the local surface arrangements. Computational and Theoretical Chemistry, 2001, 542, 207-214.	1.5	16
76	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. Inorganica Chimica Acta, 2017, 456, 1-8.	2.4	16
77	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. Journal of Organic Chemistry, 2006, 71, 2740-2749.	3.2	15
78	Confined But-2-ene Catalytic Isomerization Inside H-ZSM-5 Models: A DFT Study. Journal of Chemical Theory and Computation, 2009, 5, 1274-1283.	5.3	15
79	2â€methoxyestradiol impacts on amino acidsâ€mediated metabolic reprogramming in osteosarcoma cells by its interaction with NMDA receptor. Journal of Cellular Physiology, 2017, 232, 3030-3049.	4.1	15
80	Targeting G-quadruplexes with Organic Dyes: Chelerythrineâ€“DNA Binding Elucidated by Combining Molecular Modeling and Optical Spectroscopy. Antioxidants, 2019, 8, 472.	5.1	15
81	PTP1B phosphatase as a novel target of oleuropein activity in MCF-7 breast cancer model. Toxicology in Vitro, 2019, 61, 104624.	2.4	15
82	The interaction of deoxyribonucleic acid with methyltin(IV) moieties in solution studied by small-angle X-ray scattering, circular dichroism and UV spectroscopy. Applied Organometallic Chemistry, 2000, 14, 189-196.	3.5	14
83	Confinement effects on the interaction of native DNA with Cu(ii)â€“5-(triethylammoniummethyl)salicylidene ortho-phenylendiiminate in C12E4 liquid crystals. Dalton Transactions, 2008, , 4172.	3.3	14
84	A peptide from human Î² thymosin as a platform for the development of new anti-biofilm agents for Staphylococcus spp. and Pseudomonas aeruginosa. World Journal of Microbiology and Biotechnology, 2016, 32, 124.	3.6	14
85	Antimicrobial and Antibiofilm Activity of a Recombinant Fragment of Î²-Thymosin of Sea Urchin Paracentrotus lividus. Marine Drugs, 2018, 16, 366.	4.6	14
86	Organoplatinum(II) Complexes Self-Assemble and Recognize AT-Rich Duplex DNA Sequences. Inorganic Chemistry, 2021, 60, 2178-2187.	4.0	14
87	Pyrazole[3,4-d]pyrimidine derivatives loaded into halloysite as potential CDK inhibitors. International Journal of Pharmaceutics, 2021, 599, 120281.	5.2	14
88	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. Journal of Catalysis, 2002, 211, 296-307.	6.2	13
89	Teaching Inorganic Photophysics and Photochemistry with Three Ruthenium(II) Polypyridyl Complexes: A Computer-Based Exercise. Journal of Chemical Education, 2016, 93, 292-298.	2.3	13
90	1,3-Dipolar cycloadditions with meso-tetraarylchlorins â€“ site selectivity and mixed bisadducts. Organic Chemistry Frontiers, 2017, 4, 534-544.	4.5	13

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91	Fishing for Gâ€Quadruplexes in Solution with a Perylene Diimide Derivative Labeled with Biotins. Chemistry - A European Journal, 2018, 24, 11292-11296.	3.3	13
92	Does Ligand Symmetry Play a Role in the Stabilization of DNA G-Quadruplex Host-Guest Complexes?. Current Medicinal Chemistry, 2014, 21, 2665-2690.	2.4	13
93	Structure of the 5â€² untranslated region in SARS-CoV-2 genome and its specific recognition by innate immune systemviathe human oligoadenylate synthase 1. Chemical Communications, 2022, 58, 2176-2179.	4.1	13
94	Fluorescence emission and enhanced photochemical stability of ZnII-5-triethyl ammonium methyl salicylidene ortho-phenylendiiminate interacting with native DNA. Journal of Inorganic Biochemistry, 2010, 104, 765-773.	3.5	12
95	Quaternary structures of GroEL and naÃ¯ve-Hsp60 chaperonins in solution: a combined SAXS-MD study. RSC Advances, 2015, 5, 49871-49879.	3.6	12
96	Interaction of Cd(<scp>ii</scp>) and Ni(<scp>ii</scp>) terpyridine complexes with model polynucleotides: a multidisciplinary approach. RSC Advances, 2016, 6, 4936-4945.	3.6	12
97	Chitosan Film Functionalized with Grape Seed Oilâ€"Preliminary Evaluation of Antimicrobial Activity. Sustainability, 2022, 14, 5410.	3.2	12
98	Structural and Kinetic DFT Characterization of Materials to Rationalize Catalytic Performance. Topics in Catalysis, 2009, 52, 444-455.	2.8	11
99	The Right Answer for the Right Electrostatics: Force Field Methods Are Able to Describe Relative Energies of DNA Guanine Quadruplexes. Journal of Chemical Theory and Computation, 2014, 10, 2901-2905.	5.3	11
100	Human DNA Telomeres in Presence of Oxidative Lesions: The Crucial Role of Electrostatic Interactions on the Stability of Guanine Quadruplexes. Antioxidants, 2019, 8, 337.	5.1	11
101	Synthesis, characterization, and cellular investigations of porphyrinâ€" and chlorinâ€"indomethacin conjugates for photodynamic therapy of cancer. Organic and Biomolecular Chemistry, 2021, 19, 6501-6512.	2.8	11
102	Forever Young: Structural Stability of Telomeric Guanine Quadruplexes in the Presence of Oxidative DNA Lesions**. Chemistry - A European Journal, 2021, 27, 8865-8874.	3.3	11
103	Microscopic interactions between ivermectin and key human and viral proteins involved in SARS-CoV-2 infection. Physical Chemistry Chemical Physics, 2021, 23, 22957-22971.	2.8	11
104	SCSACode:â€‰ Applications on the Cyclopeptide Renieramide. Journal of Chemical Information and Computer Sciences, 2004, 44, 1024-1030.	2.8	10
105	The Prediction of the Nuclear Quadrupole Splitting of119Sn MÃ¶ssbauer Spectroscopy Data by Scalar Relativistic DFT Calculations. Chemistry - A European Journal, 2006, 12, 5116-5121.	3.3	10
106	IDEA: Interface dynamics and energetics algorithm. Journal of Computational Chemistry, 2007, 28, 2483-2499.	3.3	10
107	On the structure of 3â€acetylaminoâ€5â€methylâ€1,2,4â€oxadiazole and on the fully degenerate rearrangements (FDR) of its anion: a stimulating comparison between the results of â€˜inâ€silicon chemistryâ€™ and â€˜laboratory chemistryâ€™. Journal of Physical Organic Chemistry, 2009, 22, 1086-1093.	1.9	10
108	In Silico, Spectroscopic, and Biological Insights on Annelated Pyrrolo[3,2- e]Pyrimidines with Antiproliferative Activity. Letters in Drug Design and Discovery, 2013, 11, 15-26.	0.7	10

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109	DNAâ€Binding and Anticancer Activity of Pyreneâ€Imidazolium Derivatives. ChemistrySelect, 2016, 1, 6755-6761.	1.5	10
110	Identification of New Antimicrobial Peptides from Mediterranean Medical Plant Charybdis pancration (Steinh.) Speta. Antibiotics, 2020, 9, 747.	3.7	10
111	Modification of DNA structure by reactive nitrogen species as a result of 2-methoxyestradiolâ€“induced neuronal nitric oxide synthase uncoupling in metastatic osteosarcoma cells. Redox Biology, 2020, 32, 101522.	9.0	10
112	DFT computational study on FeIII-N,Nâ€²-ethylene-bis(salicylideneiminato) derivatives. Computational and Theoretical Chemistry, 2005, 715, 79-83.	1.5	9
113	On the Gâ€Quadruplex Binding of a New Class of Nickel(II), Copper(II), and Zinc(II) Salphenâ€Like Complexes. European Journal of Inorganic Chemistry, 2021, 2021, 1332-1336.	2.0	9
114	Bâ€DNA Structure and Stability: The Role of Nucleotide Composition and Order. ChemistryOpen, 2022, 11, e202100231.	1.9	9
115	Conformational analysis and DFT calculations of 8Î±-hydroxy-germacradiene-6,12-olide derivatives. Journal of Physical Organic Chemistry, 2005, 18, 1116-1122.	1.9	8
116	Hydrogenolysis of hydroxymatairesinol on Y derived catalysts: A computational study. Journal of Molecular Catalysis A, 2010, 333, 136-144.	4.8	8
117	The influence of substitution in the quinoxaline nucleus on 1,3-dipolar cycloaddition reactions: A DFT study. Computational and Theoretical Chemistry, 2013, 1013, 116-122.	2.5	8
118	The Influence of the Amide Linkage in the Fe^{III}â€Binding Properties of Catecholâ€Modified Rosamine Derivatives. Chemistry - A European Journal, 2015, 21, 15692-15704.	3.3	8
119	Câ^'C Crossâ€Couplings from a Cyclometalated Au(III) CN Complex: Mechanistic Insights and Synthetic Developments. Chemistry - A European Journal, 2021, 27, 14322-14334.	3.3	8
120	Computational study of dimethyl- and trimethyl-tin(IV) complexes of porphyrin derivatives. Applied Organometallic Chemistry, 2001, 15, 581-592.	3.5	7
121	Theoretical evaluation of structures and energetics involved in the hydrogenation of hydrocarbons on palladium surfaces. Computational and Theoretical Chemistry, 2001, 548, 173-183.	1.5	7
122	Ab initio study of structure and energetics of species involved in the 2,4-dinitro-toluene hydrogenation on Pd catalysts. Computational and Theoretical Chemistry, 2002, 584, 211-220.	1.5	7
123	Ground state and electronic spectrum of Cu(ii) and Cu(iii) complexes of N,Nâ€²-1,2-phenylenebis-2-mercaptoacetamide. Physical Chemistry Chemical Physics, 2005, 7, 2126.	2.8	7
124	Silver Clusters of Five Atoms as Highly Selective Antitumoral Agents Through Irreversible Oxidation of Thiols. Advanced Functional Materials, 2022, 32, .	14.9	7
125	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. Journal of Catalysis, 2002, 211, 296-307.	6.2	6
126	Structural investigations on diorgano- and triorganotin(IV) derivatives of [meso-tetra(4-sulfonatophenyl)porphine] metal chlorides. Journal of Organometallic Chemistry, 2006, 691, 1573-1583.	1.8	6

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127	Adsorbed CO on Group 10 Metal Fragments: A DFT Study. Journal of Chemical Information and Modeling, 2009, 49, 1223-1233.	5.4	6
128	Systematic conformational search analysis of the SRR and RRR epimers of 7â€hydroxymatairesinol. Journal of Physical Organic Chemistry, 2010, 23, 141-147.	1.9	6
129	Perturbation of Developmental Regulatory Gene Expression by a G-Quadruplex DNA Inducer in the Sea Urchin Embryo. Biochemistry, 2018, 57, 4391-4394.	2.5	6
130	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. Chemical Engineering Journal, 2003, 91, 133-142.	12.7	5
131	Relativistic coupled cluster calculations of the electronic structure of KrH+,ÂXeH+ and RnH+. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	5
132	DNA-binding of zinc(II) and nickel(II) salphen-like complexes extrapolated at 1ÂM salt concentration: Removing the ionic strength bias in physiological conditions. Journal of Inorganic Biochemistry, 2020, 207, 111064.	3.5	5
133	Induction of 2-hydroxycatecholestrogens O-methylation: A missing puzzle piece in diagnostics and treatment of lung cancer. Redox Biology, 2022, 55, 102395.	9.0	5
134	The Binding Mechanism of Epolactaene to Hsp60 Unveiled by in Silico Modelling. ChemistrySelect, 2016, 1, 759-765.	1.5	4
135	Experimental and theoretical characterization of the strong effects on DNA stability caused by half-sandwich Ru(II) and Ir(III) bearing thiabendazole complexes. Journal of Biological Inorganic Chemistry, 2020, 25, 1067-1083.	2.6	4
136	Combined spectroscopic and theoretical analysis of the binding of a water-soluble perylene diimide to DNA/RNA polynucleotides and G-quadruplexes. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 260, 119914.	3.9	4
137	How Fragile We Are: Influence of Stimulator of Interferon Genes (STING) Variants on Pathogen Recognition and Immune Response Efficiency. Journal of Chemical Information and Modeling, 2022, 62, 3096-3106.	5.4	4
138	A synchrotron radiation X-ray scattering study of aqueous solutions of native DNA. Journal of Synchrotron Radiation, 1999, 6, 1031-1034.	2.4	3
139	N -Diphenylmethyl-2-propenamide: theoretical study of the structure and interaction with a DNA model system. Computational and Theoretical Chemistry, 2001, 572, 113-119.	1.5	3
140	X-ray Absorption Spectra of CuII and CuIII Complexes ofN,N?-1,2-Phenylenebis(2-mercapto-2-methylpropionamide). European Journal of Inorganic Chemistry, 2005, 2005, 410-415.	2.0	3
141	Dynamics of metal centers monitored by nuclear inelastic scattering. Hyperfine Interactions, 2007, 165, 17-24.	0.5	3
142	Molecular-Level Characterization of Heterogeneous Catalytic Systems by Algorithmic Time Dependent Monte Carlo. Topics in Catalysis, 2009, 52, 431-443.	2.8	3
143	Photochemical functionalization of allyl benzoates by Câ€“H insertion. Tetrahedron, 2013, 69, 6065-6069.	1.9	3
144	Quantitative Analysis of the Interactions of Metal Complexes and Amphiphilic Systems: Calorimetric, Spectroscopic and Theoretical Aspects. Biomolecules, 2022, 12, 408.	4.0	3

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