

Giampaolo Barone

List of Publications by Year in descending order

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154
papers

4,549
citations

101384

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133063

59
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174
all docs

174
docs citations

174
times ranked

5861
citing authors

#	ARTICLE	IF	CITATIONS
1	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.	1.2	271
2	DNA-binding of nickel(II), copper(II) and zinc(II) complexes: Structure-affinity relationships. <i>Coordination Chemistry Reviews</i> , 2013, 257, 2848-2862.	9.5	240
3	Structure Validation of Natural Products by Quantum-Mechanical GIAO Calculations of ¹³ C NMR Chemical Shifts GIAO=gauge including atomic orbitals.. <i>Chemistry - A European Journal</i> , 2002, 8, 3233.	1.7	221
4	Determination of the Relative Stereochemistry of Flexible Organic Compounds by Ab Initio Methods: Conformational Analysis and Boltzmann-Averaged GIAO ¹³ C NMR Chemical Shifts GIAO=gauge including atomic orbitals.. <i>Chemistry - A European Journal</i> , 2002, 8, 3240.	1.7	167
5	DHFR Inhibitors: Reading the Past for Discovering Novel Anticancer Agents. <i>Molecules</i> , 2019, 24, 1140.	1.7	149
6	The interaction of native DNA with iron(III)-N,N'-ethylene-bis(salicylideneiminato)-chloride. <i>Journal of Inorganic Biochemistry</i> , 2004, 98, 589-594.	1.5	133
7	The interaction of native DNA with Zn(II) and Cu(II) complexes of 5-triethyl ammonium methyl salicylidene ortho-phenylendiimine. <i>Journal of Inorganic Biochemistry</i> , 2007, 101, 841-848.	1.5	108
8	Nickel(ii), copper(ii) and zinc(ii) metallo-intercalators: structural details of the DNA-binding by a combined experimental and computational investigation. <i>Dalton Transactions</i> , 2014, 43, 6108.	1.6	79
9	Selective G-quadruplex stabilizers: Schiff-base metal complexes with anticancer activity. <i>RSC Advances</i> , 2014, 4, 33245-33256.	1.7	78
10	Spectroscopic study of the interaction of Ni(II)-5-triethyl ammonium methyl salicylidene ortho-phenylendiimine with native DNA. <i>Journal of Inorganic Biochemistry</i> , 2009, 103, 731-737.	1.5	77
11	Toward a Rationale for the PTC124 (Ataluren) Promoted Readthrough of Premature Stop Codons: A Computational Approach and GFP-Reporter Cell-Based Assay. <i>Molecular Pharmaceutics</i> , 2014, 11, 653-664.	2.3	73
12	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.	2.3	71
13	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.	1.8	68
14	Deposition of tin sulfide thin films from tin(IV) thiolate precursors. <i>Journal of Materials Chemistry</i> , 2001, 11, 464-468.	6.7	65
15	Hsp60, a Novel Target for Antitumor Therapy: Structure-Function Features and Prospective Drugs Design. <i>Current Pharmaceutical Design</i> , 2013, 19, 2757-2764.	0.9	65
16	Analytic high-order Douglas-Kroll-Hess electric field gradients. <i>Journal of Chemical Physics</i> , 2007, 127, 074105.	1.2	64
17	Structure-Directing and High-Efficiency Photocatalytic Hydrogen Production by Ag Clusters. <i>Journal of the American Chemical Society</i> , 2014, 136, 1182-1185.	6.6	64
18	Ag ₂ and Ag ₃ Clusters: Synthesis, Characterization, and Interaction with DNA. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 7612-7616.	7.2	63

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19	Interaction of Doxorubicin with Polynucleotides. A Spectroscopic Study. <i>Biochemistry</i> , 2014, 53, 2197-2207.	1.2	61
20	Cyclometalated Au ^{III} Complexes for Cysteine Arylation in Zinc Finger Protein Domains: towards Controlled Reductive Elimination. <i>Chemistry - A European Journal</i> , 2019, 25, 7628-7634.	1.7	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. <i>Dalton Transactions</i> , 2012, 41, 4389.	1.6	51
22	The mechanism of aquaporin inhibition by gold compounds elucidated by biophysical and computational methods. <i>Chemical Communications</i> , 2017, 53, 3830-3833.	2.2	50
23	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.	1.5	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. <i>Dalton Transactions</i> , 2016, 45, 7758-7767.	1.6	49
25	Intercalation of Daunomycin into Stacked DNA Base Pairs. DFT Study of an Anticancer Drug. <i>Journal of Biomolecular Structure and Dynamics</i> , 2008, 26, 115-129.	2.0	47
26	Selective targeting of PARP-1 zinc finger recognition domains with Au(^{III}) organometallics. <i>Chemical Communications</i> , 2018, 54, 611-614.	2.2	47
27	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.	5.0	47
28	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.	1.6	46
29	Title is missing!. <i>Catalysis Letters</i> , 2001, 72, 17-23.	1.4	45
30	Enhancement of premature stop codon readthrough in the CFTR gene by Ataluren (PTC124) derivatives. <i>European Journal of Medicinal Chemistry</i> , 2015, 101, 236-244.	2.6	42
31	Circular Dichroism of DNA G-Quadruplexes: Combining Modeling and Spectroscopy To Unravel Complex Structures. <i>Journal of Physical Chemistry B</i> , 2016, 120, 3113-3121.	1.2	42
32	G-quadruplex vs. duplex-DNA binding of nickel(II) and zinc(II) Schiff base complexes. <i>Journal of Inorganic Biochemistry</i> , 2016, 161, 115-121.	1.5	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.	1.5	40
34	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.	0.8	39
35	Nuclear Quadrupole Moment of ¹¹⁹ Sn. <i>Journal of Physical Chemistry A</i> , 2008, 112, 1666-1672.	1.1	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. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 9272-9281.	2.1	39

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37	DNA Binding Studies and Cytotoxicity of a Dinuclear Pt ^{II} Diazapyrenium-Based Metallo-supramolecular Rectangular Box. <i>Chemistry - A European Journal</i> , 2012, 18, 10983-10990.	1.7	37
38	H ⁺ ZSM-5 Modified Zeolite: Quantum Chemical Models of Acidic Sites. <i>Journal of Physical Chemistry C</i> , 2007, 111, 13033-13043.	1.5	36
39	Experimental and DFT Studies on Competitive Heterocyclic Rearrangements. 3. A Cascade Isoxazole ^{1,2,4} -Oxadiazole ^{1,2,4} -Oxazole Rearrangement. <i>Journal of Organic Chemistry</i> , 2009, 74, 351-358.	1.7	36
40	Pyrrlomycins 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.	1.4	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. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 693-701.	0.8	33
42	Are compliance constants ill-defined descriptors for weak interactions?. <i>RSC Advances</i> , 2013, 3, 4757.	1.7	33
43	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.	2.1	33
44	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, 7656-7666.	1.7	32
45	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, 186-193.	0.9	32
46	Zinc complexes as fluorescent chemosensors for nucleic acids: new perspectives for a σ -bonding element. <i>Dalton Transactions</i> , 2015, 44, 3527-3535.	1.6	32
47	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.	1.6	30
48	Metal complex-DNA binding: Insights from molecular dynamics and DFT/MM calculations. <i>Journal of Inorganic Biochemistry</i> , 2013, 124, 63-69.	1.5	29
49	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, 2871-2877.	1.3	29
50	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.	1.5	29
51	Metal Ions and Metal Complexes in Alzheimer's Disease. <i>Current Pharmaceutical Design</i> , 2016, 22, 3996-4010.	0.9	28
52	(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, 103-110.	1.5	27
53	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.	1.5	27
54	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.	1.9	27

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55	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, 3291-3297.	1.0	25
56	A Synthetic Derivative of Antimicrobial Peptide Holothuroidin 2 from Mediterranean Sea Cucumber (<i>Holothuria tubulosa</i>) in the Control of <i>Listeria monocytogenes</i> . <i>Marine Drugs</i> , 2019, 17, 159.	2.2	25
57	Exploring the Chemoselectivity towards Cysteine Arylation by Cyclometallated Au ^{III} Compounds: New Mechanistic Insights. <i>ChemBioChem</i> , 2020, 21, 3071-3076.	1.3	25
58	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.	1.5	24
59	Multivariate analysis in the identification of biological targets for designed molecular structures: The BIOTA protocol. <i>European Journal of Medicinal Chemistry</i> , 2014, 75, 106-110.	2.6	24
60	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.	1.2	23
61	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, 7439-7447.	1.7	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. <i>Antioxidants</i> , 2020, 9, 1208.	2.2	23
63	Semiempirical calculations on the interaction between dimethyltin(IV) and DNA model system. <i>Computational and Theoretical Chemistry</i> , 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. <i>Tetrahedron Letters</i> , 2008, 49, 5125-5128.	0.7	22
65	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.	1.1	22
66	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.	1.4	21
67	Carbon-Phosphorus Coupling from C ^N Cyclometallated Au ^{III} Complexes. <i>Chemistry - A European Journal</i> , 2020, 26, 4226-4231.	1.7	21
68	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.	2.1	21
69	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, e1801317.	11.1	20
70	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, 6185-6191.	1.7	19
71	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.	1.0	19
72	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.	1.0	18

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73	The interaction of S,N-coordinated dimethyltin(IV) derivatives with deoxyribonucleic acid: structure and dynamics by ^{119}Sn Mössbauer spectroscopy. <i>Applied Organometallic Chemistry</i> , 1999, 13, 595-603.	1.7	16
74	Structural distortions in homoleptic (RE)4A (E = O, S, Se; A = C, Si, Ge, Sn): implications for the CVD of tin sulfides. <i>Dalton Transactions RSC</i> , 2001, , 3435-3445.	2.3	16
75	Hydrogenation of light hydrocarbons on palladium: theoretical study of the local surface arrangements. <i>Computational and Theoretical Chemistry</i> , 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. <i>Inorganica Chimica Acta</i> , 2017, 456, 1-8.	1.2	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. <i>Journal of Organic Chemistry</i> , 2006, 71, 2740-2749.	1.7	15
78	Confined But-2-ene Catalytic Isomerization Inside H-ZSM-5 Models: A DFT Study. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1274-1283.	2.3	15
79	17 β -Ethinyl estradiol 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.	2.0	15
80	Targeting G-quadruplexes with Organic Dyes: Chelerythrine-DNA Binding Elucidated by Combining Molecular Modeling and Optical Spectroscopy. <i>Antioxidants</i> , 2019, 8, 472.	2.2	15
81	PTP1B phosphatase as a novel target of oleuropein activity in MCF-7 breast cancer model. <i>Toxicology in Vitro</i> , 2019, 61, 104624.	1.1	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. <i>Applied Organometallic Chemistry</i> , 2000, 14, 189-196.	1.7	14
83	Confinement effects on the interaction of native DNA with Cu(II)-5-(triethylammoniummethyl)salicylidene ortho-phenylendiiminate in C12E4 liquid crystals. <i>Dalton Transactions</i> , 2008, , 4172.	1.6	14
84	A peptide from human β 2 thymosin as a platform for the development of new anti-biofilm agents for <i>Staphylococcus</i> spp. and <i>Pseudomonas aeruginosa</i> . <i>World Journal of Microbiology and Biotechnology</i> , 2016, 32, 124.	1.7	14
85	Antimicrobial and Antibiofilm Activity of a Recombinant Fragment of β 2-Thymosin of Sea Urchin <i>Paracentrotus lividus</i> . <i>Marine Drugs</i> , 2018, 16, 366.	2.2	14
86	Organoplatinum(II) Complexes Self-Assemble and Recognize AT-Rich Duplex DNA Sequences. <i>Inorganic Chemistry</i> , 2021, 60, 2178-2187.	1.9	14
87	Pyrazole[3,4-d]pyrimidine derivatives loaded into halloysite as potential CDK inhibitors. <i>International Journal of Pharmaceutics</i> , 2021, 599, 120281.	2.6	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. <i>Journal of Catalysis</i> , 2002, 211, 296-307.	3.1	13
89	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.	1.1	13
90	1,3-Dipolar cycloadditions with meso-tetraarylchlorins: site selectivity and mixed bisadducts. <i>Organic Chemistry Frontiers</i> , 2017, 4, 534-544.	2.3	13

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91	Fishing for G-Quadruplexes in Solution with a Perylene Diimide Derivative Labeled with Biotins. <i>Chemistry - A European Journal</i> , 2018, 24, 11292-11296.	1.7	13
92	Does Ligand Symmetry Play a Role in the Stabilization of DNA G-Quadruplex Host-Guest Complexes?. <i>Current Medicinal Chemistry</i> , 2014, 21, 2665-2690.	1.2	13
93	Structure of the 5' untranslated region in SARS-CoV-2 genome and its specific recognition by innate immune system via the human oligoadenylate synthase 1. <i>Chemical Communications</i> , 2022, 58, 2176-2179.	2.2	13
94	Fluorescence emission and enhanced photochemical stability of ZnII-5-triethyl ammonium methyl salicylidene ortho-phenylendiiminate interacting with native DNA. <i>Journal of Inorganic Biochemistry</i> , 2010, 104, 765-773.	1.5	12
95	Quaternary structures of GroEL and Na ⁺ -Hsp60 chaperonins in solution: a combined SAXS-MD study. <i>RSC Advances</i> , 2015, 5, 49871-49879.	1.7	12
96	Interaction of Cd(II) and Ni(II) terpyridine complexes with model polynucleotides: a multidisciplinary approach. <i>RSC Advances</i> , 2016, 6, 4936-4945.	1.7	12
97	Chitosan Film Functionalized with Grape Seed Oil: Preliminary Evaluation of Antimicrobial Activity. <i>Sustainability</i> , 2022, 14, 5410.	1.6	12
98	Structural and Kinetic DFT Characterization of Materials to Rationalize Catalytic Performance. <i>Topics in Catalysis</i> , 2009, 52, 444-455.	1.3	11
99	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, 2901-2905.	2.3	11
100	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, 337.	2.2	11
101	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.	1.5	11
102	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.	1.7	11
103	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.	1.3	11
104	SCSACode: Applications on the Cyclopeptide Renieramide. <i>Journal of Chemical Information and Computer Sciences</i> , 2004, 44, 1024-1030.	2.8	10
105	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, 5116-5121.	1.7	10
106	IDEA: Interface dynamics and energetics algorithm. <i>Journal of Computational Chemistry</i> , 2007, 28, 2483-2499.	1.5	10
107	On the structure of 3-acetylaminomethyl-1,2,4-oxadiazole and on the fully degenerate rearrangements (FDR) of its anion: a stimulating comparison between the results of ²⁹ Si NMR silicon chemistry and laboratory chemistry. <i>Journal of Physical Organic Chemistry</i> , 2009, 22, 1086-1093.	0.9	10
108	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.	0.4	10

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109	DNA Binding and Anticancer Activity of Pyreneimidazolium Derivatives. <i>ChemistrySelect</i> , 2016, 1, 6755-6761.	0.7	10
110	Identification of New Antimicrobial Peptides from Mediterranean Medical Plant <i>Charybdis pancration</i> (Steinh.) Speta. <i>Antibiotics</i> , 2020, 9, 747.	1.5	10
111	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.	3.9	10
112	DFT computational study on Fe(III)-N,N'-ethylene-bis(salicylideneiminato) derivatives. <i>Computational and Theoretical Chemistry</i> , 2005, 715, 79-83.	1.5	9
113	On the 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.	1.0	9
114	B-DNA Structure and Stability: The Role of Nucleotide Composition and Order. <i>ChemistryOpen</i> , 2022, 11, e202100231.	0.9	9
115	Conformational analysis and DFT calculations of 8-hydroxy-germacradiene-6,12-olide derivatives. <i>Journal of Physical Organic Chemistry</i> , 2005, 18, 1116-1122.	0.9	8
116	Hydrogenolysis of hydroxymatairesinol on Y derived catalysts: A computational study. <i>Journal of Molecular Catalysis A</i> , 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. <i>Computational and Theoretical Chemistry</i> , 2013, 1013, 116-122.	1.1	8
118	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, 15692-15704.	1.7	8
119	C-C Cross-Couplings from a Cyclometalated Au(III) CN Complex: Mechanistic Insights and Synthetic Developments. <i>Chemistry - A European Journal</i> , 2021, 27, 14322-14334.	1.7	8
120	Computational study of dimethyl- and trimethyl-tin(IV) complexes of porphyrin derivatives. <i>Applied Organometallic Chemistry</i> , 2001, 15, 581-592.	1.7	7
121	Theoretical evaluation of structures and energetics involved in the hydrogenation of hydrocarbons on palladium surfaces. <i>Computational and Theoretical Chemistry</i> , 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. <i>Computational and Theoretical Chemistry</i> , 2002, 584, 211-220.	1.5	7
123	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.	1.3	7
124	Silver Clusters of Five Atoms as Highly Selective Antitumoral Agents Through Irreversible Oxidation of Thiols. <i>Advanced Functional Materials</i> , 2022, 32, .	7.8	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. <i>Journal of Catalysis</i> , 2002, 211, 296-307.	3.1	6
126	Structural investigations on diorgano- and triorganotin(IV) derivatives of [meso-tetra(4-sulfonatophenyl)porphyrin] metal chlorides. <i>Journal of Organometallic Chemistry</i> , 2006, 691, 1573-1583.	0.8	6

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127	Adsorbed CO on Group 10 Metal Fragments: A DFT Study. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 1223-1233.	2.5	6
128	Systematic conformational search analysis of the SRR and RRR epimers of 7- β -hydroxymatairesinol. <i>Journal of Physical Organic Chemistry</i> , 2010, 23, 141-147.	0.9	6
129	Perturbation of Developmental Regulatory Gene Expression by a G-Quadruplex DNA Inducer in the Sea Urchin Embryo. <i>Biochemistry</i> , 2018, 57, 4391-4394.	1.2	6
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