

Emilia Sicilia

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122
papers

2,471
citations

29
h-index

42
g-index

129
ext. papers

2,819
ext. citations

4.7
avg, IF

5.2
L-index

#	Paper	IF	Citations
122	Theoretical Study of Two-State Reactivity of Transition Metal Cations: The Difficult Case of Iron Ion Interacting with Water, Ammonia, and Methane. <i>Journal of Physical Chemistry A</i> , 2004 , 108, 1069-1081	2.8	106
121	Structures and electronic absorption spectra of a recently synthesised class of photodynamic therapy agents. <i>Chemistry - A European Journal</i> , 2006 , 12, 6797-803	4.8	94
120	Reaction of SC+(1D,3D) with H ₂ O, NH ₃ , and CH ₄ : a density functional study. <i>Journal of the American Chemical Society</i> , 2001 , 123, 2588-96	16.4	90
119	Theoretical study of ammonia and methane activation by first-row transition metal cations M(+) (M = Ti, V, Cr). <i>Journal of the American Chemical Society</i> , 2002 , 124, 1471-80	16.4	89
118	About the Mulliken electronegativity in DFT. <i>Theoretical Chemistry Accounts</i> , 2005 , 114, 38-45	1.9	81
117	Geometries, singlet-triplet separations, dipole moments, ionization potentials, and vibrational frequencies in methylene (CH ₂) and halocarbenes (CHF, CF ₂ , CCl ₂ , CBr ₂ , and Cl ₂). <i>Journal of Chemical Physics</i> , 1992 , 97, 5031-5036	3.9	80
116	Gas-phase chemistry of actinides ions: new insights into the reaction of UO ⁺ and UO ₂ ⁺ with water. <i>Journal of the American Chemical Society</i> , 2007 , 129, 4229-39	16.4	67
115	Topological Analysis of the Reaction of Mn ⁺ (7S,5S) with H ₂ O, NH ₃ , and CH ₄ Molecules. <i>Journal of Physical Chemistry A</i> , 2003 , 107, 4862-4868	2.8	62
114	On the applicability of the HSAB principle through the use of improved computational schemes for chemical hardness evaluation. <i>Journal of Computational Chemistry</i> , 2004 , 25, 994-1003	3.5	53
113	Atomic Radii Scale and Related Size Properties from Density Functional Electronegativity Formulation. <i>Journal of Physical Chemistry A</i> , 2003 , 107, 5461-5465	2.8	53
112	First-principle time-dependent study of magnesium-containing porphyrin-like compounds potentially useful for their application in photodynamic therapy. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 4123-30	3.4	47
111	Insertion Reaction of Mn ⁺ Bare Metal Cation into the N-H and C-H Bonds of Ammonia and Methane. <i>Journal of Physical Chemistry A</i> , 2002 , 106, 8937-8944	2.8	43
110	The heavy atom effect on Zn(II) phthalocyanine derivatives: a theoretical exploration of the photophysical properties. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 23595-601	3.6	41
109	On the Potential Use of Squaraine Derivatives as Photosensitizers in Photodynamic Therapy: A TDDFT and RIC2 Survey. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 1849-57	6.4	40
108	Homogeneous Gold Catalysis: Hydration of 1,2-Diphenylacetylene with Methanol in Aqueous Media. A Theoretical Viewpoint. <i>Organometallics</i> , 2012 , 31, 3074-3080	3.8	39
107	Hydration of ionic species studied by the reference interaction site model with a repulsive bridge correction. <i>Journal of Computational Chemistry</i> , 2008 , 29, 2406-15	3.5	38
106	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

105	Interaction of CO with PdAu(111) and PdAu(100) Bimetallic Surfaces: A Theoretical Cluster Model Study. <i>Journal of Physical Chemistry C</i> , 2008 , 112, 6073-6081	3.8	35
104	Metal Atom Effect on the Photophysical Properties of Mg(II), Zn(II), Cd(II), and Pd(II) Tetrphenylporphyrin Complexes Proposed as Possible Drugs in Photodynamic Therapy. <i>Molecules</i> , 2017 , 22,	4.8	34
103	Absorption Spectra of the Potential Photodynamic Therapy Photosensitizers Texaphyrins Complexes: A Theoretical Analysis. <i>Journal of Chemical Theory and Computation</i> , 2007 , 3, 860-9	6.4	34
102	Density functional study of ammonia activation by late first-row transition metal cations. <i>Inorganic Chemistry</i> , 2004 , 43, 4944-52	5.1	34
101	B,N-Codoped graphene as catalyst for the oxygen reduction reaction: Insights from periodic and cluster DFT calculations. <i>Journal of Computational Chemistry</i> , 2018 , 39, 637-647	3.5	32
100	Mechanistic investigation of the hydrogenation of O(2) by a transfer hydrogenation catalyst. <i>Journal of the American Chemical Society</i> , 2010 , 132, 4178-90	16.4	32
99	On the interaction between manganese cation (Mn ²⁺) and the nucleic acid bases (T, U, C, A, G) in the gas phase. <i>International Journal of Quantum Chemistry</i> , 2002 , 90, 903-909	2.1	32
98	Oxidation of Ethylbenzene to Acetophenone with N-Doped Graphene: Insight from Theory. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 12275-12284	3.8	31
97	Investigation of the host-guest complexation between 4-sulfocalix[4]arene and nedaplatin for potential use in drug delivery. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018 , 193, 528-536	4.4	30
96	Electronic spectra and intersystem spin-orbit coupling in 1,2- and 1,3-squaraines. <i>Journal of Computational Chemistry</i> , 2014 , 35, 2107-13	3.5	30
95	Mechanistic aspects of the reaction of Th ⁺ and Th ²⁺ with water in the gas phase. <i>Inorganic Chemistry</i> , 2008 , 47, 2083-8	5.1	30
94	Methane activation by chromium oxide cations in the gas phase: a theoretical study. <i>Journal of Computational Chemistry</i> , 2006 , 27, 174-87	3.5	30
93	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
92	beta-Hydrogen Kinetic Effect. <i>Journal of the American Chemical Society</i> , 2007 , 129, 5744-55	16.4	27
91	Reaction of bare VO ⁺ and FeO ⁺ with ammonia: a theoretical point of view. <i>Inorganic Chemistry</i> , 2003 , 42, 8773-82	5.1	26
90	Acetylene cyclotrimerization by early second-row transition metals in the gas phase. A theoretical study. <i>Inorganic Chemistry</i> , 2005 , 44, 9807-16	5.1	26
89	EH ₃ (E = N, P, As) and H ₂ activation with N-heterocyclic silylene and germylene homologues. <i>Chemistry - A European Journal</i> , 2013 , 19, 7835-46	4.8	25
88	Experimental and Theoretical Investigation on the Catalytic Generation of Environmentally Persistent Free Radicals from Benzene. <i>Journal of Physical Chemistry C</i> , 2017 , 121, 9381-9393	3.8	24

87	Investigation of the Inertness to Hydrolysis of Platinum(IV) Prodrugs. <i>Inorganic Chemistry</i> , 2016 , 55, 1580-6	2.5	24
86	On the insertion mechanism of molecular oxygen into a Pd(II)H bond. Something to add. <i>Chemical Physics Letters</i> , 2007 , 443, 183-189	2.5	24
85	Molecular quadrupole moments, second moments, and diamagnetic susceptibilities evaluated using the generalized gradient approximation in the framework of Gaussian density functional method. <i>Journal of Chemical Physics</i> , 1996 , 105, 3206-3210	3.9	24
84	DFT Investigation of the Mechanism of Action of Organoiridium(III) Complexes As Anticancer Agents. <i>Inorganic Chemistry</i> , 2015 , 54, 10801-10	5.1	23
83	Adsorption of Ethylene, Vinyl, Acetic Acid, and Acetate Species on PdAu(111) and PdAu(100) Surface Alloys: A Cluster Model Study. <i>Journal of Chemical Theory and Computation</i> , 2009 , 5, 1350-60	6.4	23
82	Activation of methane by the iron dimer cation. A theoretical study. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 12501-11	2.8	23
81	Dimethylplatinum(II) complexes: computational insights into Pt-C bond protonolysis. <i>Inorganic Chemistry</i> , 2011 , 50, 10091-101	5.1	21
80	Theoretical Investigation of the Mechanism of Acid-Catalyzed Oxygenation of a Pd(II)-Hydride To Produce a Pd(II)-Hydroperoxide. <i>Journal of Chemical Theory and Computation</i> , 2008 , 4, 1283-92	6.4	21
79	Hydrogen release from dialkylamine-boranes promoted by Mg and Ca complexes: a DFT analysis of the reaction mechanism. <i>Chemistry - A European Journal</i> , 2014 , 20, 5967-76	4.8	20
78	Theoretical investigation of the absorption spectra and singlet-triplet energy gap of positively charged tetraphenylporphyrins as potential photodynamic therapy photosensitizers. <i>Canadian Journal of Chemistry</i> , 2013 , 91, 902-906	0.9	20
77	Can phthalocyanines and their substituted alpha-para-(methoxy)phenyl derivatives act as photosensitizers in photodynamic therapy? A TD-DFT study. <i>Physical Chemistry Chemical Physics</i> , 2009 , 11, 4586-92	3.6	20
76	The Role of Chelating Phosphine Rhodium Complexes in Dehydrocoupling Reactions of Amine-Boranes: A Theoretical Investigation Attempting To Rationalize the Observed Behaviors. <i>ACS Catalysis</i> , 2014 , 4, 1104-1113	13.1	18
75	The electronic states of Fe ²⁺ . <i>Chemical Physics Letters</i> , 2003 , 376, 310-317	2.5	18
74	The Onset of Dehydrogenation in Solid Ammonia Borane: An Ab Initio Metadynamics Study. <i>Angewandte Chemie - International Edition</i> , 2019 , 58, 3976-3980	16.4	17
73	Computational Insight on CO ₂ Fixation to Produce Styrene Carbonate Assisted by a Single-Center Aluminum(III) Catalyst and Quaternary Ammonium Salts. <i>ChemCatChem</i> , 2016 , 8, 1167-1175	5.2	17
72	Computational study of alkynes insertion into metal-hydride bonds catalyzed by bimetallic complexes. <i>Inorganic Chemistry</i> , 2010 , 49, 9875-83	5.1	17
71	Density functional potential-energy hypersurface and reactivity indices in the isomerization of X ₃ H ⁺ (X = O, S, Se, Te). <i>Journal of the Chemical Society, Faraday Transactions</i> , 1997 , 93, 3309-3312		17
70	Catalytic role of dinuclear μ -acetylide gold(I) complexes in the hydroamination of terminal alkynes: theoretical insights. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 581-90	6.4	16

69	A time-dependent density functional study of a non-aromatic [1.1.1.1]-pentaphyrin and its lutetium complex. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 10816-23	3.4	16
68	Gold(I)-Catalyzed Hydration of 1,2-Diphenylacetylene: Computational Insights. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 2782-9	6.4	16
67	Solvation properties of N-substituted cis and trans amides are not identical: significant enthalpy and entropy changes are revealed by the use of variable temperature ¹ H NMR in aqueous and chloroform solutions and ab initio calculations. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 11878-84	2.8	16
66	Excitation energies, singlet-triplet energy gaps, spin-orbit matrix elements and heavy atom effects in BOIMPYs as possible photosensitizers for photodynamic therapy: a computational investigation. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 2656-2661	3.6	15
65	The recognition of a new pathway for the reaction of molecular oxygen with a Pd(II)-hydride to produce a Pd(II)-hydroperoxide. <i>Chemical Physics Letters</i> , 2008 , 456, 41-46	2.5	15
64	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
63	Ligand-centred redox activation of inert organoiridium anticancer catalysts. <i>Chemical Science</i> , 2020 , 11, 5466-5480	9.4	14
62	Do rhodium bis(amine-borane) complexes play a role as intermediates in dehydrocoupling reactions of amine-boranes?. <i>Chemistry - A European Journal</i> , 2011 , 17, 14586-92	4.8	14
61	Mechanistic insight into protonolysis and cis-trans isomerization of benzylplatinum(II) complexes assisted by weak ligand-to-metal interactions. A combined kinetic and DFT study. <i>Inorganic Chemistry</i> , 2011 , 50, 2224-39	5.1	14
60	A theoretical study of ethylene dehydrogenation by bare Niobium atom and cation. <i>Computational and Theoretical Chemistry</i> , 2006 , 762, 25-31		14
59	Glutathione activation of an organometallic half-sandwich anticancer drug candidate by ligand attack. <i>Chemical Communications</i> , 2019 , 55, 14602-14605	5.8	14
58	Antitumor Platinum(IV) Prodrugs: A Systematic Computational Exploration of Their Reduction Mechanism by l-Ascorbic Acid. <i>Inorganic Chemistry</i> , 2019 , 58, 3851-3860	5.1	13
57	Blind Search for Complex Chemical Pathways Using Harmonic Linear Discriminant Analysis. <i>Journal of Chemical Theory and Computation</i> , 2019 , 15, 4507-4515	6.4	13
56	Complexation of Al and Ni by l-Ascorbic Acid: An Experimental and Theoretical Investigation. <i>Journal of Physical Chemistry A</i> , 2017 , 121, 9773-9781	2.8	13
55	On the Nature of the CP Bond in Phosphaalkynes. <i>Journal of Chemical Theory and Computation</i> , 2008 , 4, 397-403	6.4	13
54	Structures, binding energies, temperature effects, infrared spectroscopy of [Mg(NH ₃) ₂] clusters from DFT and MP2 investigations. <i>Journal of Computational Chemistry</i> , 2019 , 40, 1707-1717	3.5	11
53	Totally green cellulose conversion into bio-oil and cellulose citrate using molten citric acid in an open system: synthesis, characterization and computational investigation of reaction mechanisms.. <i>RSC Advances</i> , 2020 , 10, 34738-34751	3.7	11
52	Computational Investigation of the Influence of Halogen Atoms on the Photophysical Properties of Tetraphenylporphyrin and Its Zinc(II) Complexes. <i>Journal of Physical Chemistry A</i> , 2018 , 122, 2809-2815	2.8	11

51	Ab initio calculations on the (1)O ₂ quenching mechanism by trans-resveratrol. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 12773-81	3.6	11
50	Insights from Computations on the Mechanism of Reduction by Ascorbic Acid of Pt Prodrugs with Asplatin and Its Chlorido and Bromido Analogues as Model Systems. <i>Chemistry - A European Journal</i> , 2018 , 24, 9572-9580	4.8	10
49	Photophysical Exploration of Dual-Approach Pt-BODIPY Conjugates: Theoretical Insights. <i>Inorganic Chemistry</i> , 2019 , 58, 9882-9889	5.1	10
48	Experimental and Computational Investigations of Carboplatin Supramolecular Complexes. <i>ACS Omega</i> , 2020 , 5, 31456-31466	3.9	10
47	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
46	A multi-methodological inquiry of the behavior of cisplatin-based Pt(IV) derivatives in the presence of bioreductants with a focus on the isolated encounter complexes. <i>Journal of Biological Inorganic Chemistry</i> , 2020 , 25, 655-670	3.7	10
45	Quantum mechanical DFT elucidation of CO ₂ catalytic conversion mechanisms: Three examples. <i>International Journal of Quantum Chemistry</i> , 2018 , 118, e25572	2.1	9
44	Host-Guest Complexation of Oxaliplatin and Sulfonatocalix[n]Arenes for Potential Use in Cancer Therapy. <i>Molecules</i> , 2020 , 25,	4.8	9
43	Hydrolysis in Acidic Environment and Degradation of Satraplatin: A Joint Experimental and Theoretical Investigation. <i>Inorganic Chemistry</i> , 2017 , 56, 6013-6026	5.1	8
42	BODIPY for photodynamic therapy applications: computational study of the effect of bromine substitution on O photosensitization. <i>Journal of Molecular Modeling</i> , 2018 , 24, 183	2	8
41	Hydrophilic annulated dinuclear zinc(II) phthalocyanine as Type II photosensitizers for PDT: a combined experimental and (TD)-DFT investigation. <i>Journal of Porphyrins and Phthalocyanines</i> , 2013 , 17, 980-988	1.8	8
40	Can subpyrriporphyrin and its boron complex be proposed as photosensitizers in photodynamic therapy? A first principle time dependent study. <i>Photochemical and Photobiological Sciences</i> , 2009 , 8, 386-90	4.2	8
39	Rationalization of the Superior Anticancer Activity of Phenanthriplatin: An In-Depth Computational Exploration. <i>Chemistry - A European Journal</i> , 2020 , 26, 259-268	4.8	8
38	Novel choline selective electrochemical membrane sensor with application in milk powders and infant formulas. <i>Talanta</i> , 2021 , 221, 121409	6.2	8
37	Can BODIPY Dimers Act as Photosensitizers in Photodynamic Therapy? A Theoretical Prediction. <i>Frontiers in Physics</i> , 2018 , 6,	3.9	8
36	Spectrophotometric determination of choline in pharmaceutical formulations via host-guest complexation with a biomimetic calixarene receptor. <i>Microchemical Journal</i> , 2019 , 146, 735-741	4.8	7
35	Anionic cyclometalated Pt(II) and Pt(IV) complexes respectively bearing one or two 1,2-benzenedithiolate ligands. <i>Dalton Transactions</i> , 2018 , 47, 11645-11657	4.3	7
34	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

33	The Onset of Dehydrogenation in Solid Ammonia Borane: An Ab Initio Metadynamics Study. <i>Angewandte Chemie</i> , 2019 , 131, 4016-4020	3.6	7
32	Elusive Intermediates in the Breakdown Reactivity Patterns of Prodrug Platinum(IV) Complexes. <i>Journal of the American Society for Mass Spectrometry</i> , 2019 , 30, 1881-1894	3.5	6
31	A study on the physicochemical properties and cytotoxic activity of p-sulfocalix[4]arene-nedaplatin complex. <i>Journal of Physics: Conference Series</i> , 2019 , 1310, 012011	0.3	6
30	Structures, harmonic vibrational frequencies and interconversion potential energy profile of Ni+(C2H2)2 complexes. <i>Computational and Theoretical Chemistry</i> , 2004 , 709, 167-170		6
29	A Boron-Containing Compound Acting on Multiple Targets Against Alzheimer's Disease. Insights from Ab Initio and Molecular Dynamics Simulations. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 3397-3410	6.1	6
28	Direct and cluster-assisted dehydrogenation of methane by Nb and Ta: a theoretical investigation. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 16178-16188	3.6	5
27	Rational Design of Modified Oxobacteriochlorins as Potential Photodynamic Therapy Photosensitizers. <i>International Journal of Molecular Sciences</i> , 2019 , 20,	6.3	5
26	Collision-induced dissociation products of the protonated dipeptide carnosine: structural elucidation, fragmentation pathways and potential energy surface analysis. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 12673-82	3.6	5
25	The influence of surface oxygen and hydroxyl groups on the dehydrogenation of ethylene on PdAu surface alloys. A theoretical cluster model study. <i>Chemical Physics Letters</i> , 2010 , 493, 87-93	2.5	5
24	Anticancer Activity, DNA Binding, and Photodynamic Properties of a N?C?N-Coordinated Pt(II) Complex. <i>Inorganic Chemistry</i> , 2021 , 60, 10350-10360	5.1	5
23	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
22	Conformation and structure of ethane-1,2-dithiol from ab initio HF and MP3 study. <i>Computational and Theoretical Chemistry</i> , 1992 , 257, 485-490		4
21	Is the cytotoxic activity of phenanthriplatin dependent on the specific size of the phenanthridine ligand system?. <i>Journal of Inorganic Biochemistry</i> , 2021 , 219, 111447	4.2	4
20	Betaine host-guest complexation with a calixarene receptor: enhanced anticancer effect.. <i>RSC Advances</i> , 2021 , 11, 24673-24680	3.7	4
19	A novel catalytic two-step process for the preparation of rigid polyurethane foams: synthesis, mechanism and computational studies. <i>Reaction Chemistry and Engineering</i> ,	4.9	4
18	Mass Spectrometric and Computational Investigation of the Protonated Carnosine-Carboplatin Complex Fragmentation. <i>Inorganic Chemistry</i> , 2015 , 54, 7885-97	5.1	3
17	Mechanism of action of the curcumin cis-diammineplatinum(II) complex as a photocytotoxic agent. <i>Inorganic Chemistry Frontiers</i> , 2020 , 7, 2759-2769	6.8	3
16	Exploring the Structure-Performance Relationship of Sulfonated Polysulfone Proton Exchange Membrane by a Combined Computational and Experimental Approach. <i>Polymers</i> , 2021 , 13,	4.5	3

15	A DFT investigation of a bulky biomimetic model catalyzing the 5'-outer ring deiodination of thyroxine. <i>Journal of Molecular Modeling</i> , 2016 , 22, 287	2	2
14	Theoretical determination of the aquation reaction mechanism of cyclometalated benzimidazole Ru(II) and Ir(III) anticancer complexes. <i>Inorganica Chimica Acta</i> , 2018 , 470, 325-330	2.7	2
13	Sequestering Ability of a Synthetic Chelating Agent towards Copper(II) and Iron(III): A Detailed Theoretical and Experimental Analysis. <i>Chemistry - an Asian Journal</i> , 2020 , 15, 3266-3274	4.5	2
12	Theoretical exploration of the photophysical properties of two-component Ru-porphyrin dyes as promising assemblies for a combined antitumor effect. <i>Dalton Transactions</i> , 2020 , 49, 12653-12661	4.3	2
11	A comparative computational mechanistic study on derivatives of pyriplatin, modified with the $\text{CH}_2\text{Ph}_3\text{P}^+$ group, as anticancer complexes targeting mitochondria. <i>Inorganica Chimica Acta</i> , 2020 , 512, 119863	2.7	1
10	Computation modeling as a tool for the exploration of complex multistep reaction cycles in homogeneous catalysis. Some selected examples in the framework of the use of hydrogen as a fuel of the future. <i>International Journal of Quantum Chemistry</i> , 2016 , 116, 1507-1512	2.1	1
9	Computational Analysis of Photophysical Properties and Reactivity of a New Phototherapeutic Cyclometalated Au(III)-Hydride Complex. <i>Chemistry - A European Journal</i> , 2021 , 27, 15528-15535	4.8	1
8	Cyclopentadienone-NHC iron(0) complexes as low valent electrocatalysts for water oxidation. <i>Catalysis Science and Technology</i> , 2021 , 11, 1407-1418	5.5	1
7	Iodido equatorial ligands influence on the mechanism of action of Pt(IV) and Pt(II) anti-cancer complexes: A DFT computational study. <i>Journal of Computational Chemistry</i> , 2021 , 42, 608-619	3.5	1
6	Theoretical exploration of the reduction reaction of monofunctional phenanthriplatin Pt(IV) prodrugs. <i>Inorganica Chimica Acta</i> , 2019 , 495, 118951	2.7	0
5	A metadynamics perspective on the reduction mechanism of the Pt(IV) asplatin prodrug. <i>Journal of Computational Chemistry</i> , 2020 , 41, 290-294	3.5	0
4	Experimental and theoretical study of the complexation of Fe^{3+} and Cu^{2+} by l-ascorbic acid in aqueous solution. <i>Journal of Molecular Liquids</i> , 2022 , 355, 118973	6	0
3	Two State Reactivity Paradigm in Catalysis. The Example of X^*H ($\text{X} = \text{O}, \text{N}, \text{C}$) and C^*C Bonds Activation Mediated by Transition Metal Compounds 337-366		
2	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	
1	Computational Studies of the Photogeneration from Dihydrosanguinarine and the Probable Cytotoxicity Mechanism of Sanguinarine. <i>Applied Sciences (Switzerland)</i> , 2022 , 12, 1095	2.6	