

Giuseppe Sciortino

List of Publications by Year in descending order

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66
papers

1,366
citations

279701

23
h-index

414303

32
g-index

74
all docs

74
docs citations

74
times ranked

1079
citing authors

#	ARTICLE	IF	CITATIONS
1	Polyoxovanadates with emerging biomedical activities. <i>Coordination Chemistry Reviews</i> , 2021, 447, 214143.	9.5	115
2	Polyoxidovanadates' interactions with proteins: An overview. <i>Coordination Chemistry Reviews</i> , 2022, 454, 214344.	9.5	78
3	Prediction of the interaction of metallic moieties with proteins: An update for protein–ligand docking techniques. <i>Journal of Computational Chemistry</i> , 2018, 39, 42-51.	1.5	54
4	Direct Asymmetric Hydrogenation of <i>N</i> -Methyl and <i>N</i> -Alkyl Imines with an Ir(III)H Catalyst. <i>Journal of the American Chemical Society</i> , 2018, 140, 16967-16970.	6.6	47
5	New V^{IV} , $V^{IV}O$, V^{VO} , and V^{VO}_2 Systems: Exploring their Interconversion in Solution, Protein Interactions, and Cytotoxicity. <i>Inorganic Chemistry</i> , 2020, 59, 14042-14057.	1.9	46
6	Elucidation of Binding Site and Chiral Specificity of Oxidovanadium Drugs with Lysozyme through Theoretical Calculations. <i>Inorganic Chemistry</i> , 2017, 56, 12938-12951.	1.9	40
7	Binding of vanadium ions and complexes to proteins and enzymes in aqueous solution. <i>Coordination Chemistry Reviews</i> , 2021, 449, 214192.	9.5	40
8	GaudiMM: A modular multi-objective platform for molecular modeling. <i>Journal of Computational Chemistry</i> , 2017, 38, 2118-2126.	1.5	37
9	$V^{IV}O$ complexes with antibacterial quinolone ligands and their interaction with serum proteins. <i>Dalton Transactions</i> , 2018, 47, 2164-2182.	1.6	36
10	Nonoxido V^{IV} Complexes: Prediction of the EPR Spectrum and Electronic Structure of Simple Coordination Compounds and Amavadin. <i>Inorganic Chemistry</i> , 2016, 55, 7373-7387.	1.9	35
11	Validation and Applications of Protein–Ligand Docking Approaches Improved for Metalloligands with Multiple Vacant Sites. <i>Inorganic Chemistry</i> , 2019, 58, 294-306.	1.9	35
12	DFT Protocol for EPR Prediction of Paramagnetic Cu(II) Complexes and Application to Protein Binding Sites. <i>Magnetochemistry</i> , 2018, 4, 55.	1.0	30
13	Copper(II) <i>N,N,O</i> -Chelating Complexes as Potential Anticancer Agents. <i>Inorganic Chemistry</i> , 2021, 60, 2939-2952.	1.9	30
14	Rationalizing the Decavanadate(V) and Oxidovanadium(IV) Binding to G-Actin and the Competition with Decaniobate(V) and ATP. <i>Inorganic Chemistry</i> , 2021, 60, 334-344.	1.9	29
15	Dynamic Stereoselection of Peptide Helicates and Their Selective Labeling of DNA Replication Foci in Cells**. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 8859-8866.	7.2	29
16	Decoding Surface Interaction of $V^{IV}O$ Metallodrug Candidates with Lysozyme. <i>Inorganic Chemistry</i> , 2018, 57, 4456-4469.	1.9	28
17	Interaction of Vanadium(IV) Species with Ubiquitin: A Combined Instrumental and Computational Approach. <i>Inorganic Chemistry</i> , 2019, 58, 8064-8078.	1.9	28
18	ESI-MS Study of the Interaction of Potential Oxidovanadium(IV) Drugs and Amavadin with Model Proteins. <i>Inorganic Chemistry</i> , 2020, 59, 9739-9755.	1.9	28

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19	Chemistry of mixed-ligand oxidovanadium(IV) complexes of aroylhydrazones incorporating quinoline derivatives: Study of solution behavior, theoretical evaluation and protein/DNA interaction. <i>Journal of Inorganic Biochemistry</i> , 2019, 199, 110786.	1.5	27
20	Quantitative prediction of electronic absorption spectra of copper(II)â€“bioligand systems: Validation and applications. <i>Journal of Inorganic Biochemistry</i> , 2020, 204, 110953.	1.5	27
21	Iridium-Catalyzed Isomerization of <i>N</i> -Sulfonyl Aziridines to Allyl Amines. <i>Organic Letters</i> , 2018, 20, 5747-5751.	2.4	25
22	BioMetAll: Identifying Metal-Binding Sites in Proteins from Backbone Preorganization. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 311-323.	2.5	25
23	Integrated ESI-MS/EPR/computational characterization of the binding of metal species to proteins: vanadium drugâ€“myoglobin application. <i>Inorganic Chemistry Frontiers</i> , 2019, 6, 1561-1578.	3.0	24
24	Integrated experimental/computational approaches to characterize the systems formed by vanadium with proteins and enzymes. <i>Inorganic Chemistry Frontiers</i> , 2021, 8, 1951-1974.	3.0	24
25	Unveiling V ^{IV} O ²⁺ Binding Modes to Human Serum Albumins by an Integrated Spectroscopicâ€“Computational Approach. <i>Chemistry - A European Journal</i> , 2020, 26, 11316-11326.	1.7	23
26	Effect of secondary interactions, steric hindrance and electric charge on the interaction of V ^{IV} O species with proteins. <i>New Journal of Chemistry</i> , 2019, 43, 17647-17660.	1.4	22
27	Functionalized Artificial Bidomain Proteins Based on an Î±-Solenoid Protein Repeat Scaffold: A New Class of Artificial Dielsâ€“Alderses. <i>ACS Omega</i> , 2019, 4, 4437-4447.	1.6	21
28	Simple Coordination Geometry Descriptors Allow to Accurately Predict Metal-Binding Sites in Proteins. <i>ACS Omega</i> , 2019, 4, 3726-3731.	1.6	20
29	Throughâ€“Space Spin Coupling in a Silver(II) Porphyrin Dimer upon Stepwise Oxidations: Ag II â€“â€“â€“â€“Ag II, Ag II ₇ â€“â€“â€“â€“Ag III, and Ag III â€“â€“â€“â€“Ag III Metallophilic Interactions. <i>Chemistry - A European Journal</i> , 2019, 25, 10098-10110.	1.7	19
30	The binding modes of V ^{IV} O ²⁺ ions in blood proteins and enzymes. <i>Chemical Communications</i> , 2020, 56, 12218-12221.	2.2	17
31	Covalent and non-covalent binding in vanadiumâ€“protein adducts. <i>Inorganic Chemistry Frontiers</i> , 2021, 8, 1189-1196.	3.0	17
32	Accurate prediction of vertical electronic transitions of Ni(II) coordination compounds via time dependent density functional theory. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25655.	1.0	16
33	Catalytic Regioselective Isomerization of 2,2â€“Disubstituted Oxetanes to Homoallylic Alcohols. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 7521-7527.	7.2	16
34	Stepwise Oxidations in a Cofacial Copper(II) Porphyrin Dimer: Throughâ€“Space Spinâ€“Coupling and Interplay between Metal and Radical Spins. <i>Chemistry - A European Journal</i> , 2020, 26, 7869-7880.	1.7	15
35	GPathFinder: Identification of Ligand-Binding Pathways by a Multi-Objective Genetic Algorithm. <i>International Journal of Molecular Sciences</i> , 2019, 20, 3155.	1.8	14
36	Bonding rearrangements in organometallic reactions: from orbitals to curly arrows. <i>Dalton Transactions</i> , 2019, 48, 15740-15752.	1.6	14

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37	Comparative Mechanistic Study on the [Au(NHC)] ⁺ -Catalyzed Hydration of Alkynes, Alkenes, and Allenes. <i>Organometallics</i> , 2020, 39, 3469-3479.	1.1	14
38	Mild Iridium-Catalysed Isomerization of Epoxides. Computational Insights and Application to the Synthesis of β -Alkyl Amines. <i>Advanced Synthesis and Catalysis</i> , 2019, 361, 3624-3631.	2.1	12
39	Spectroscopic/Computational Characterization and the X-ray Structure of the Adduct of the V ^{IV} -O=Picolinato Complex with RNase A. <i>Inorganic Chemistry</i> , 2021, 60, 19098-19109.	1.9	12
40	Mo(VI) Potential Metallodrugs: Explaining the Transport and Cytotoxicity by Chemical Transformations. <i>Inorganic Chemistry</i> , 2022, 61, 4513-4532.	1.9	12
41	Solution chemical properties and anticancer potential of 8-hydroxyquinoline hydrazones and their oxidovanadium(IV) complexes. <i>Journal of Inorganic Biochemistry</i> , 2022, 235, 111932.	1.5	12
42	Directed Self-Assembly of Trimeric DNA-Binding chiral Mini-protein Helicates. <i>Frontiers in Chemistry</i> , 2018, 6, 520.	1.8	11
43	Studying the reactivity of λ^5 -Cu(II) complexes for α -antitumor purposes. <i>Journal of Inorganic Biochemistry</i> , 2019, 195, 51-60.	1.5	11
44	Biospeciation of Potential Vanadium Drugs of Acetylacetonate in the Presence of Proteins. <i>Frontiers in Chemistry</i> , 2020, 8, 345.	1.8	11
45	Computational Study of Homogeneous Multimetallic Cooperative Catalysis. <i>Topics in Catalysis</i> , 0, , 1.	1.3	11
46	Ambiphilic boryl groups in a neutral Ni(ⁱⁱ) complex: a new activation mode of H ₂ . <i>Chemical Science</i> , 2021, 12, 2540-2548.	3.7	11
47	Mechanistic Insights on the Hydration of Terminal and Internal Allenes Catalyzed by [(NHC)Au] ⁺ . <i>Organometallics</i> , 2018, 37, 3543-3551.	1.1	10
48	Computational insight into the interaction of oxaliplatin with insulin. <i>Metallomics</i> , 2019, 11, 765-773.	1.0	10
49	Integrated Computational Study of the Cu-Catalyzed Hydration of Alkenes in Water Solvent and into the Context of an Artificial Metallohydratase. <i>ACS Catalysis</i> , 2019, 9, 4616-4626.	5.5	10
50	Binding of V ^{IV} O ₂ , V ^{IV} OL, V ^{IV} OL ₂ and V ^{IV} O ₂ L Moieties to Proteins: X-ray/Theoretical Characterization and Biological Implications. <i>Chemistry - A European Journal</i> , 2022, 28, .	1.7	10
51	New mixed ligand oxidovanadium(IV) complexes: Solution behavior, protein interaction and cytotoxicity. <i>Journal of Inorganic Biochemistry</i> , 2022, 233, 111853.	1.5	10
52	V ^{IV} O and V ^{IV} Species Formed in Aqueous Solution by the Tridentate Glutaroimide α -Dioxime Ligand α . An Instrumental and Computational Characterization. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 1805-1816.	1.0	9
53	An Artificial Hemoprotein with Inducible Peroxidase- and Monooxygenase-Like Activities. <i>Chemistry - A European Journal</i> , 2020, 26, 14929-14937.	1.7	9
54	Dynamic Stereoselection of Peptide Helicates and Their Selective Labeling of DNA Replication Foci in Cells**. <i>Angewandte Chemie</i> , 2021, 133, 8941-8948.	1.6	7

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55	Impact of Cu(II) and Al(III) on the conformational landscape of amyloid β ₁₋₄₂ . <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 13023-13032.	1.3	7
56	Tridentate (O,N,O) ligands as potential chelator compounds for iron overload. <i>Polyhedron</i> , 2017, 123, 192-205.	1.0	6
57	GARLEEK: Adding an extra flavor to ONIOM. <i>Journal of Computational Chemistry</i> , 2019, 40, 381-386.	1.5	6
58	Chiral Cyclobutane-Containing Cell-Penetrating Peptides as Selective Vectors for Anti-Leishmania Drug Delivery Systems. <i>International Journal of Molecular Sciences</i> , 2020, 21, 7502.	1.8	4
59	Synthesis and characterization of new Pd(II) and Pt(II) complexes with 3-substituted 1-(2-pyridyl)imidazo[1,5-a]pyridine ligands. <i>Dalton Transactions</i> , 2021, 50, 4859-4873.	1.6	4
60	Stereoselective Self-Assembly of DNA Binding Helicates Directed by the Viral β -Annulus Trimeric Peptide Motif. <i>Bioconjugate Chemistry</i> , 2021, 32, 1564-1569.	1.8	3
61	Ferromagnetic Coupling in Oxidovanadium(IV)–Porphyrin Radical Dimers. <i>Inorganic Chemistry</i> , 2021, 60, 16492-16506.	1.9	3
62	Introducing the penicillamine moiety into a metalloprotein mimicking the NiSOD enzyme: electronic and kinetic effects. <i>Inorganic Chemistry Frontiers</i> , 2022, 9, 310-322.	3.0	3
63	Catalytic Regioselective Isomerization of 2,2-Disubstituted Oxetanes to Homoallylic Alcohols. <i>Angewandte Chemie</i> , 2020, 132, 7591-7597.	1.6	1
64	Successes and Challenges in Multiscale Modelling of Artificial Metalloenzymes: the Case Study of POP-Rh2 Cyclopropanase. <i>Faraday Discussions</i> , 2022, , .	1.6	1
65	Controlling oncogenic KRAS signaling pathways with a Palladium-responsive peptide. <i>Communications Chemistry</i> , 2022, 5, .	2.0	1
66	Through-space Spin Coupling in a Silver(II) Porphyrin Dimer upon Stepwise Oxidations: Ag II \cdots Ag II, Ag II \cdots Ag III, and Ag III \cdots Ag III Metallophilic Interactions. <i>Chemistry - A European Journal</i> , 2019, 25, 10025-10025.	1.0	0