Luigi Di Costanzo

List of Publications by Year
in descending order

84 papers	7,136 citations	109321 35 h-index	60623 81 g-index
86 all docs	86 docs citations	86 times ranked	9484 citing authors

#	Article	IF	Citations
1	RCSB Protein Data Bank: biological macromolecular structures enabling research and education in fundamental biology, biomedicine, biotechnology and energy. Nucleic Acids Research, 2019, 47, D464-D474.	14.5	918
2	RCSB Protein Data Bank: powerful new tools for exploring 3D structures of biological macromolecules for basic and applied research and education in fundamental biology, biomedicine, biotechnology, bioengineering and energy sciences. Nucleic Acids Research, 2021, 49, D437-D451.	14.5	918
3	Protein Data Bank: the single global archive for 3D macromolecular structure data. Nucleic Acids Research, 2019, 47, D520-D528.	14.5	671
4	OUP accepted manuscript. Nucleic Acids Research, 2017, 45, D271-D281.	14.5	619
5	Structural basis for the function and inhibition of an influenza virus proton channel. Nature, 2008, 451, 596-599.	27.8	549
6	RCSB Protein Data Bank: Enabling biomedical research and drug discovery. Protein Science, 2020, 29, 52-65.	7.6	223
7	Inducible NO Synthaseâ€“Dependent S -Nitrosylation and Activation of Arginase1 Contribute to Age-Related Endothelial Dysfunction. Circulation Research, 2007, 101, 692-702.	4.5	177
8	Crystal structure of human arginase I at 1.29-A resolution and exploration of inhibition in the immune response. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 13058-13063.	7.1	164
9	X-ray Crystal Structure of Aristolochene Synthase from Aspergillus terreus and Evolution of Templates for the Cyclization of Farnesyl Diphosphate,. Biochemistry, 2007, 46, 1941-1951.	2.5	161
10	Guest Encapsulation in a Water-Soluble Molecular Capsule Based on Ionic Interactions. Journal of the American Chemical Society, 2003, 125, 9946-9947.	13.7	145
11	OneDep: Unified wwPDB System for Deposition, Biocuration, and Validation of Macromolecular Structures in the PDB Archive. Structure, 2017, 25, 536-545.	3.3	130
12	Crystal Structure of (+)-Î´-Cadinene Synthase from Gossypium arboreum and Evolutionary Divergence of Metal Binding Motifs for Catalysis. Biochemistry, 2009, 48, 6175-6183.	2.5	122
13	Toward the de Novo Design of a Catalytically Active Helix Bundle:Â A Substrate-Accessible Carboxylate-Bridged Dinuclear Metal Center. Journal of the American Chemical Society, 2001, 123, 12749-12757.	13.7	100
14	Directing Noble Metal Ion Chemistry within a Designed Ferritin Protein[,]. Biochemistry, 2008, 47, 12729-12739.	2.5	84
15	Calixareneâ€“Porphyrin Supramolecular Complexes: pHâ€Tuning of the Complex Stoichiometry. Angewandte Chemie - International Edition, 2001, 40, 4245-4247.	13.8	78
16	Trendspotting in the Protein Data Bank. FEBS Letters, 2013, 587, 1036-1045.	2.8	74
17	Crystal Structure of Human Liver Î”4-3-Ketosteroid 5Î²-Reductase (AKR1D1) and Implications for Substrate Binding and Catalysis. Journal of Biological Chemistry, 2008, 283, 16830-16839.	3.4	67
18	Miniaturized metalloproteins: Application to iron-sulfur proteins. Proceedings of the National Academy of Sciences of the United States of America, 2000, 97, 11922-11927.	7.1	66

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19	Expression, purification, assay, and crystal structure of perdeuterated human arginase I. Archives of Biochemistry and Biophysics, 2007, 465, 82-89.	3.0	65
20	Evolution of the arginase fold and functional diversity. Cellular and Molecular Life Sciences, 2008, 65, 2039-2055.	5.4	64
21	Binding of Î±,Î±-Disubstituted Amino Acids to Arginase Suggests New Avenues for Inhibitor Design. Journal of Medicinal Chemistry, 2011, 54, 5432-5443.	6.4	62
22	Inhibition of human arginase I by substrate and product analogues. Archives of Biochemistry and Biophysics, 2010, 496, 101-108.	3.0	59
23	Structure of a 129Xe-Cryptophane Biosensor Complexed with Human Carbonic Anhydrase II. Journal of the American Chemical Society, 2008, 130, 6942-6943.	13.7	58
24	Crystal Structure of Human Arginase I Complexed with Thiosemicarbazide Reveals an Unusual Thiocarbonyl Î¼-Sulfide Ligand in the Binuclear Manganese Cluster. Journal of the American Chemical Society, 2007, 129, 6388-6389.	13.7	57
25	Noncovalent Synthesis in Aqueous Solution and Spectroscopic Characterization of Multi-Porphyrin Complexes. Chemistry - A European Journal, 2006, 12, 2722-2729.	3.3	53
26	Sliding Helix and Change of Coordination Geometry in a Model Di-MnII Protein. Angewandte Chemie - International Edition, 2003, 42, 417-420.	13.8	52
27	Inhibition of Human Steroid 5Î²-Reductase (AKR1D1) by Finasteride and Structure of the Enzyme-Inhibitor Complex. Journal of Biological Chemistry, 2009, 284, 19786-19790.	3.4	50
28	Response of a Designed Metalloprotein to Changes in Metal Ion Coordination, Exogenous Ligands, and Active Site Volume Determined by X-ray Crystallography. Journal of the American Chemical Society, 2005, 127, 17266-17276.	13.7	49
29	Crystal Structure of Lactaldehyde Dehydrogenase from Escherichia coli and Inferences Regarding Substrate and Cofactor Specificity. Journal of Molecular Biology, 2007, 366, 481-493.	4.2	49
30	Worldwide Protein Data Bank biocuration supporting open access to high-quality 3D structural biology data. Database: the Journal of Biological Databases and Curation, 2018, 2018, .	3.0	45
31	Structure of anticancer ruthenium half-sandwich complex bound to glycogen synthase kinase 3Î². Journal of Biological Inorganic Chemistry, 2011, 16, 45-50.	2.6	44
32	2-Aminoimidazole Amino Acids as Inhibitors of the Binuclear Manganese Metalloenzyme Human Arginase I. Journal of Medicinal Chemistry, 2010, 53, 4266-4276.	6.4	42
33	A real-time tripodal colorimetric/fluorescence sensor for multiple target metal ions. Dyes and Pigments, 2018, 155, 249-257.	3.7	40
34	Miniaturized heme proteins: crystal structure of Co(III)-mimochrome IV. Journal of Biological Inorganic Chemistry, 2004, 9, 1017-1027.	2.6	37
35	AIE/ACQ Effects in Two DR/NIR Emitters: A Structural and DFT Comparative Analysis. Molecules, 2018, 23, 1947.	3.8	37
36	Probing the Specificity Determinants of Amino Acid Recognition by Arginase. Biochemistry, 2009, 48, 121-131.	2.5	35

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37	Stereochemistry of guanidine-metal interactions: Implications for L-arginine-metal interactions in protein structure and function. Proteins: Structure, Function and Bioinformatics, 2006, 65, 637-642.	2.6	34
38	Fluorescence pH-dependent sensing of Zn(II) by a tripodal ligand. A comparative X-ray and DFT study. Journal of Luminescence, 2019, 212, 200-206.	3.1	34
39	Visual pH Sensors: From a Chemical Perspective to New Bioengineered Materials. Molecules, 2021, 26, 2952.	3.8	34
40	Photophysical Properties of Luminescent Zinc(II)â€'Pyridinyloxadiazole Complexes and their Glassy Selfâ€Assembly Networks. European Journal of Inorganic Chemistry, 2018, 2018, 2709-2716.	2.0	33
41	Structure and catalytic mechanism of human steroid 5Î²-reductase (AKR1D1). Molecular and Cellular Endocrinology, 2009, 301, 191-198.	3.2	31
42	Two aminobenzothiazole derivatives for Pd(II) and Zn(II) coordination. Inorganic Chemistry Communication, 2011, 14, 46-48.	3.9	31
43	Fluorescent metallopolymers with Zn(II) in a Schiff base/phenoxide coordination environment. Inorganic Chemistry Communication, 2013, 29, 138-140.	3.9	31
44	Series of O,N,Oâ€Tridentate Ligands Zinc(II) Complexes with High Solidâ€State Photoluminescence Quantum Yield. European Journal of Inorganic Chemistry, 2014, 2014, 2695-2703.	2.0	31
45	High Solid State Photoluminescence Quantum Yields and Effective Color Tuning in Polyvinylpyridine Based Zinc(II) Metallopolymers. Macromolecular Chemistry and Physics, 2015, 216, 1516-1522.	2.2	31
46	Vision, challenges and opportunities for a Plant Cell Atlas. ELife, 2021, 10, .	6.0	31
47	Synthesis, structure and reactivity of amino-benzodifurane derivatives. Comptes Rendus Chimie, 2009, 12, 622-634.	0.5	30
48	Facile synthesis of new Pd(II) and Cu(II) based metallomesogens from ligands containing thiophene rings. Inorganic Chemistry Communication, 2009, 12, 1135-1138.	3.9	30
49	Color Tuning and Noteworthy Photoluminescence Quantum Yields in Crystalline Monoâ€/Dinuclear Zn^{II} Complexes. European Journal of Inorganic Chemistry, 2014, 2014, 5916-5924.	2.0	30
50	Synthesis, spectroscopic properties and DFT calculations of a novel multipolar azo dye and its zinc(II) complex. Inorganic Chemistry Communication, 2017, 84, 103-108.	3.9	30
51	Highly efficient dicyano-phenylenevinylene fluorophore as polymer dopant or zinc-driven self-assembling building block. Inorganic Chemistry Communication, 2019, 104, 145-149.	3.9	30
52	Second order nonlinear optical networks with excellent poling stability from a new trifunctional thiophene based chromophore. Organic Electronics, 2009, 10, 53-60.	2.6	29
53	From cadmium(II)-aroylhydrazone complexes to metallopolymers with enhanced photoluminescence. A structural and DFT study. Inorganica Chimica Acta, 2017, 458, 129-137.	2.4	29
54	Solid-State Highly Efficient DR Mono and Poly-dicyano-phenylenevinylene Fluorophores. Molecules, 2018, 23, 1505.	3.8	28

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55	Small molecule annotation for the Protein Data Bank. Database: the Journal of Biological Databases and Curation, 2014, 2014, bau116-bau116.	3.0	26
56	Two tridentate pyridinyl-hydrazone zinc(II) complexes as fluorophores for blue emitting layers. Journal of Molecular Structure, 2019, 1197, 672-680.	3.6	26
57	An Amphiphilic Pyridinoyl-hydrazone Probe for Colorimetric and Fluorescence pH Sensing. Molecules, 2019, 24, 3833.	3.8	26
58	The Effect of Bulky Substituents on Two Ï€-Conjugated Mesogenic Fluorophores. Their Organic Polymers and Zinc-Bridged Luminescent Networks. Polymers, 2019, 11, 1379.	4.5	26
59	A symmetrical azo-based fluorophore and the derived salen multipurpose framework for emissive layers. Inorganic Chemistry Communication, 2019, 104, 186-189.	3.9	26
60	Analysis of impact metrics for the Protein Data Bank. Scientific Data, 2018, 5, 180212.	5.3	24
61	A Novel DR/NIR T-Shaped AIEgen: Synthesis and X-Ray Crystal Structure Study. Crystals, 2020, 10, 269.	2.2	20
62	Assembly of Positively Charged Porphyrins Driven by Metal Ions:Â A Novel Polymeric Arrangement of Cationic Metalloporphyrin. Inorganic Chemistry, 2004, 43, 7579-7581.	4.0	17
63	(S)-2-Amino-6-nitrohexanoic Acid Binds to Human Arginase I through Multiple Nitroâ^'Metal Coordination Interactions in the Binuclear Manganese Cluster. Journal of the American Chemical Society, 2008, 130, 17254-17255.	13.7	17
64	Aldo-keto reductases in which the conserved catalytic histidine is substituted. Chemico-Biological Interactions, 2009, 178, 127-133.	4.0	17
65	A Highly Efficient White Luminescent Zinc (II) Based Metallopolymer by RGB Approach. Polymers, 2019, 11, 1712.	4.5	17
66	Impact of the Protein Data Bank Across Scientific Disciplines. Data Science Journal, 2020, 19, 25.	1.3	17
67	Colorimetric recognition of multiple first-row transition metals: A single water-soluble chemosensor in acidic and basic conditions. Dyes and Pigments, 2021, 184, 108832.	3.7	15
68	The crystal structure of Afc-containing peptides. Biopolymers, 2000, 53, 150-160.	2.4	14
69	Atomic Details of Carbon-Based Nanomolecules Interacting with Proteins. Molecules, 2020, 25, 3555.	3.8	13
70	The crystal structure of aDcp-containing peptide. Biopolymers, 2000, 53, 182-188.	2.4	12
71	Conformational and coordination properties of a peptide containing the novel Î±,Î±-bis(2-pyridyl)glycine amino acidElectronic supplementary information (ESI) available: Figs. 1S, 2S. See http://www.rsc.org/suppdata/dt/b2/b209199b/. Dalton Transactions, 2003, , 787-792.	3.3	11
72	Data on a real-time tripodal colorimetric/fluorescence sensor for multiple target metal ions. Data in Brief, 2018, 19, 2119-2125.	1.0	11

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73	A Highly Water-Soluble Fluorescent and Colorimetric pH Probe. Crystals, 2020, 10, 83.	2.2	11
74	Stimuli-Responsive Zinc (II) Coordination Polymers: A Novel Platform for Supramolecular Chromic Smart Tools. Polymers, 2021, 13, 3712.	4.5	9
75	Using the Tools and Resources of the RCSB Protein Data Bank. Current Protocols in Bioinformatics, 2016, 55, 1.9.1-1.9.35.	25.8	8
76	Phasing protein structures using the groupâ€“subgroup relation. Acta Crystallographica Section D: Biological Crystallography, 2003, 59, 1435-1439.	2.5	7
77	Design, Synthesis, and Structural Analysis of <scp>d</scp>,<scp>l</scp>-Mixed Polypyrrolinones. 2. Macrocyclic Hexapyrrolinones. Organic Letters, 2010, 12, 2994-2997.	4.6	6
78	Amino acid modifications for conformationally constraining naturally occurring and engineered peptide backbones: Insights from the Protein Data Bank. Biopolymers, 2018, 109, e23230.	2.4	6
79	A Novel L-Shaped Fluorescent Probe for AIE Sensing of Zinc (II) Ion by a DR/NIR Response. Molecules, 2021, 26, 7347.	3.8	6
80	Synthesis of (2S)-2-amino-7,8-epoxyoctanoic acid and structure of its metal-bridging complex with human arginase I. Organic and Biomolecular Chemistry, 2008, 6, 3240.	2.8	5
81	A Water Soluble 2-Phenyl-5-(pyridin-3-yl)-1,3,4-oxadiazole Based Probe: Antimicrobial Activity and Colorimetric/Fluorescence pH Response. Molecules, 2022, 27, 1824.	3.8	5
82	Novel Solid-State Emissive Polymers and Polymeric Blends from a T-Shaped Benzodifuran Scaffold: A Comparative Study. Polymers, 2020, 12, 718.	4.5	3
83	Benzodifuran-based fluorescent brighteners: A novel platform for plant cell wall imaging. Dyes and Pigments, 2022, 199, 110071.	3.7	3
84	Thermo-Induced Fluorochromism in Two AIE Zinc Complexes: A Deep Insight into the Structure-Property Relationship. Molecules, 2022, 27, 2551.	3.8	3