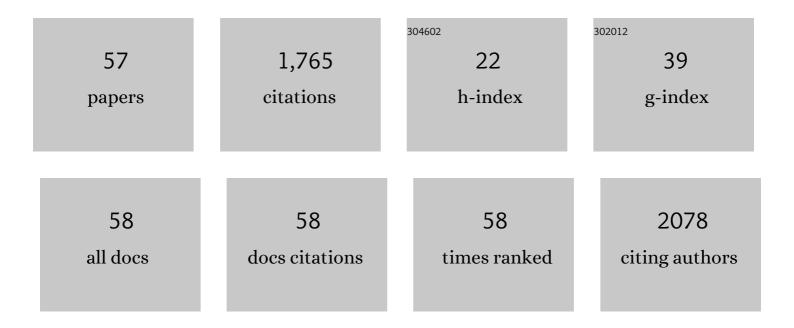
Adriana Pietropaolo

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Promoting transparency and reproducibility in enhanced molecular simulations. Nature Methods, 2019, 16, 670-673.	9.0	655
2	Copper(I) and Copper(II) Inhibit AÎ² Peptides Proteolysis by Insulinâ€Degrading Enzyme Differently: Implications for Metallostasis Alteration in Alzheimer's Disease . Chemistry - A European Journal, 2011, 17, 2752-2762.	1.7	68
3	Molecular Mechanism of Polyacrylate Helix Sense Switching across Its Free Energy Landscape. Journal of the American Chemical Society, 2013, 135, 5509-5512.	6.6	65
4	Metal ions affect insulin-degrading enzyme activity. Journal of Inorganic Biochemistry, 2012, 117, 351-358.	1.5	48
5	Predicting the Switchable Screw Sense in Fluoreneâ€Based Polymers. Angewandte Chemie - International Edition, 2015, 54, 2688-2692.	7.2	48
6	Ubiquitin binds the amyloid \hat{l}^2 peptide and interferes with its clearance pathways. Chemical Science, 2019, 10, 2732-2742.	3.7	46
7	The switching mechanism of the mitochondrial ADP/ATP carrier explored by free-energy landscapes. Biochimica Et Biophysica Acta - Bioenergetics, 2016, 1857, 772-781.	0.5	44
8	Copper(II) complexes with chicken prion repeats: influence of proline and tyrosine residues on the coordination features. Journal of Biological Inorganic Chemistry, 2005, 10, 463-475.	1.1	42
9	A chirality index for investigating protein secondary structures and their time evolution. Proteins: Structure, Function and Bioinformatics, 2008, 70, 667-677.	1.5	37
10	Formation of insulin fragments by insulinâ€degrading enzyme: the role of zinc(II) and cystine bridges. Journal of Mass Spectrometry, 2013, 48, 135-140.	0.7	36
11	Copper, BDNF and Its Nâ€ŧerminal Domain: Inorganic Features and Biological Perspectives. Chemistry - A European Journal, 2012, 18, 15618-15631.	1.7	35
12	Rationalizing the design and implementation of chiral hybrid perovskites. CheM, 2022, 8, 1231-1253.	5.8	35
13	Unusual Cyclodextrin Derivatives as a New Avenue to Modulate Self―and Metalâ€Induced Aβ Aggregation. Chemistry - A European Journal, 2015, 21, 14047-14059.	1.7	33
14	Copper(II) complexes with an avian prion N-terminal region and their potential SOD-like activity. Journal of Inorganic Biochemistry, 2009, 103, 195-204.	1.5	27
15	The inorganic perspectives of neurotrophins and Alzheimer's disease. Journal of Inorganic Biochemistry, 2012, 111, 130-137.	1.5	27
16	Zinc(II) Interactions with Brain-Derived Neurotrophic Factor N-Terminal Peptide Fragments: Inorganic Features and Biological Perspectives. Inorganic Chemistry, 2013, 52, 11075-11083.	1.9	27
17	The insulin degrading enzyme activates ubiquitin and promotes the formation of K48 and K63 diubiquitin. Chemical Communications, 2015, 51, 15724-15727.	2.2	26
18	The Inorganic Side of NGF: Copper(II) and Zinc(II) Affect the NGF Mimicking Signaling of the N-Terminus Peptides Encompassing the Recognition Domain of TrkA Receptor. Frontiers in Neuroscience, 2016, 10, 569	1.4	26

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19	Structural Role of Compensatory Amino Acid Replacements in the α-Synuclein Protein. Biochemistry, 2011, 50, 6994-7001.	1.2	25
20	A chiralityâ€based metrics for freeâ€energy calculations in biomolecular systems. Journal of Computational Chemistry, 2011, 32, 2627-2637.	1.5	25
21	The copper(II) and zinc(II) coordination mode of HExxH and HxxEH motif in small peptides: The role of carboxylate location and hydrogen bonding network. Journal of Inorganic Biochemistry, 2014, 130, 92-102.	1.5	25
22	The Copper(II)-Assisted Connection between NGF and BDNF by Means of Nerve Growth Factor-Mimicking Short Peptides. Cells, 2019, 8, 301.	1.8	25
23	Intramolecular Weak Interactions in the Thermodynamic Stereoselectivity of Copper(II) Complexes with Carnosine–Trehalose Conjugates. Chemistry - A European Journal, 2011, 17, 9448-9455.	1.7	24
24	Synergistic Approach of Ultrafast Spectroscopy and Molecular Simulations in the Characterization of Intramolecular Charge Transfer in Push-Pull Molecules. Molecules, 2020, 25, 430.	1.7	24
25	Unveiling the Role of Histidine and Tyrosine Residues on the Conformation of the Avian Prion Hexarepeat Domain. Journal of Physical Chemistry B, 2008, 112, 5182-5188.	1.2	21
26	Prion Proteins Leading to Neurodegeneration. Current Alzheimer Research, 2008, 5, 579-590.	0.7	20
27	A Small Linear Peptide Encompassing the NGF N-Terminus Partly Mimics the Biological Activities of the Entire Neurotrophin in PC12 Cells. ACS Chemical Neuroscience, 2015, 6, 1379-1392.	1.7	20
28	Different zinc(II) complex species and binding modes at AÎ ² N-terminus drive distinct long range cross-talks in the AÎ ² monomers. Journal of Inorganic Biochemistry, 2015, 153, 367-376.	1.5	18
29	Zinc Complexes of Cyclodextrinâ€bearing 8â€Hydroxyquinoline Ligands: A Comparative Study. Chemistry - an Asian Journal, 2017, 12, 110-115.	1.7	15
30	Pyrazolones Activate the Proteasome by Gating Mechanisms and Protect Neuronal Cells from βâ€Amyloid Toxicity. ChemMedChem, 2020, 15, 302-316.	1.6	15
31	Trehalose-8-hydroxyquinoline conjugates as antioxidant modulators of AÎ ² aggregation. RSC Advances, 2016, 6, 47229-47236.	1.7	14
32	Temperature-dependent UV absorption of biphenyl based on intra-molecular rotation investigated within a combined experimental and TD-DFT approach. Liquid Crystals, 2018, 45, 2048-2053.	0.9	13
33	An NMR and molecular dynamics investigation of the avian prion hexarepeat conformational features in solution. Chemical Physics Letters, 2007, 442, 110-118.	1.2	12
34	A Versatile Computational Strategy To Characterize the Free-Energy Landscape of Excited States in Oligofluorenes. Journal of Chemical Theory and Computation, 2018, 14, 5441-5445.	2.3	12
35	Copper, differently from zinc, affects the conformation, oligomerization state and activity of bradykinin. Metallomics, 2016, 8, 750-761.	1.0	11
36	Free-energy predictions and absorption spectra calculations for supramolecular nanocarriers and their photoactive cargo. Nanoscale, 2017, 9, 4989-4994.	2.8	11

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37	Metal ion coordination in peptide fragments of neurotrophins: A crucial step for understanding the role and signaling of these proteins in the brain. Coordination Chemistry Reviews, 2021, 435, 213790.	9.5	11
38	Predicting the Switchable Screw Sense in Fluoreneâ€Based Polymers. Angewandte Chemie, 2015, 127, 2726-2730.	1.6	10
39	From Peptide Fragments to Whole Protein: Copper(II) Load and Coordination Features of IAPP. Chemistry - A European Journal, 2017, 23, 17898-17902.	1.7	10
40	Blue circularly polarized luminescent amorphous molecules with single-handed propeller chirality induced by circularly polarized light irradiation. Chemical Communications, 2021, 57, 1794-1797.	2.2	10
41	Conformational Preferences of the Full Chicken Prion Protein in Solution and Its Differences with Respect to Mammals. ChemPhysChem, 2009, 10, 1500-1510.	1.0	8
42	A quantitative measure of chirality inside nucleic acid databank. Chirality, 2011, 23, 534-542.	1.3	7
43	Right-handed 2/1 helical arrangement of benzene molecules in cholic acid crystal established by experimental and theoretical circular dichroism spectroscopy. RSC Advances, 2015, 5, 101110-101114.	1.7	6
44	Zinc Interactions with a Soluble Mutated Rat Amylin to Mimic Whole Human Amylin: An Experimental and Simulation Approach to Understand Stoichiometry, Speciation and Coordination of the Metal Complexes. Chemistry - A European Journal, 2020, 26, 13072-13084.	1.7	6
45	Multi-replica biased sampling for photoswitchable π-conjugated polymers. Journal of Chemical Physics, 2021, 154, 174108.	1.2	6
46	Aggregation-induced chirality amplification of optically active fluorescent polyurethane and a cyclic dimer in the ground and excited states. Chemical Communications, 2022, 58, 1029-1032.	2.2	6
47	Effect of Different Zâ€Inducers on the Stabilization of Z Portion in BZâ€DNA Sequence: Correlation Between Experimental and Simulation Data. Chirality, 2015, 27, 773-778.	1.3	5
48	Photo racemization of 2,2â€2â€dihydroxyâ€1,1â€2â€binaphthyl derivatives. Chirality, 2022, 34, 317-324.	1.3	5
49	The curious case of opossum prion: a physicochemical study on copper(<scp>ii</scp>) binding to the bis-decarepeat fragment from the protein N-terminal domain. Dalton Transactions, 2019, 48, 17533-17543.	1.6	4
50	Learning how planarization can affect dichroic patterns in polyfluorenes. Chirality, 2020, 32, 661-666.	1.3	4
51	Exploring metal-driven stereoselectivity of glycopeptides by free-energy calculations. Pure and Applied Chemistry, 2012, 84, 1919-1930.	0.9	3
52	Binding of Zn(II) to Tropomyosin Receptor Kinase A in Complex with Its Cognate Nerve Growth Factor: Insights from Molecular Simulation and <i>in Vitro</i> Essays. ACS Chemical Neuroscience, 2018, 9, 1095-1103.	1.7	3
53	Optically Active Polymers with Cationic Units Connected through Neutral Spacers: Helical Conformation and Chirality Transfer to External Molecules. Macromolecules, 2020, 53, 9916-9928.	2.2	3

54 Molecular Simulations of Biological Nanoswitches. , 2020, , 1-5.

#	Article	IF	CITATIONS
55	Dataset of the AAC2 conformations in the c-, intermediate- and m-states obtained from free-energy simulations. Data in Brief, 2016, 7, 1355-1357.	0.5	0
56	Shape factors in the binding of soft fluorescent nanoshuttles with target receptors. Molecular Systems Design and Engineering, 2021, 6, 281-285.	1.7	0
57	Chirality analysis of helical polymers. Chemistry Teacher International, 2021, 3, 131-140.	0.9	0