

# Lisa M PÃ©rez

## List of Publications by Year in descending order

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80  
papers

2,838  
citations

136950

32  
h-index

182427

51  
g-index

82  
all docs

82  
docs citations

82  
times ranked

3534  
citing authors

#	ARTICLE	IF	CITATIONS
1	Cellulose Nanocrystal-Enabled Tailoring of the Interface in Carbon Nanotube- and Graphene Nanoplatelet-Carbon Fiber Polymer Composites: Implications for Structural Applications. ACS Applied Nano Materials, 2022, 5, 1284-1295.	5.0	11
2	ELIXIR-A: An Interactive Visualization Tool for Multi-Target Pharmacophore Refinement. ACS Omega, 2022, 7, 12707-12715.	3.5	6
3	Thermal Stability of Metal-Organic Frameworks (MOFs): Concept, Determination, and Model Prediction Using Computational Chemistry and Machine Learning. Industrial & Engineering Chemistry Research, 2022, 61, 5853-5862.	3.7	21
4	Regional Collaborations Supporting Cyberinfrastructure-Enabled Research During a Pandemic. , 2022, , .		4
5	Expanding the Reach of Research Computing: A Landscape Study. , 2022, , .		0
6	Minimum Ignition Energy (MIE) prediction models for ignition sensitive fuels using machine learning methods. Journal of Loss Prevention in the Process Industries, 2021, 69, 104343.	3.3	8
7	Quantum Chemical Modeling of the Effects of Hydrated Lime (Calcium Hydroxide) as a Filler in Bituminous Materials. ACS Omega, 2021, 6, 3130-3139.	3.5	5
8	Exploring Remote Learning Methods for User Training in Research Computing. Journal of Computational Science Education, 2021, 12, 11-17.	0.3	3
9	Navigating the Light-Sheet Image Analysis Software Landscape: Concepts for Driving Cohesion From Data Acquisition to Analysis. Frontiers in Cell and Developmental Biology, 2021, 9, 739079.	3.7	11
10	Metal-templated, Tight Loop Conformation of a Cys-X-Cys Biomimetic Assembles a Dimanganese Complex. Angewandte Chemie, 2020, 132, 3674-3678.	2.0	0
11	Hydrogel Synthesis and Stabilization via Tetrazine Click-Induced Secondary Interactions. Macromolecular Rapid Communications, 2020, 41, e2000287.	3.9	10
12	An amber obligate active site-directed ligand evolution technique for phage display. Nature Communications, 2020, 11, 1392.	12.8	25
13	Capture chromatography with mixed-mode resins: A case study with recombinant human thioredoxin from Escherichia coli. Journal of Chromatography A, 2020, 1625, 461327.	3.7	3
14	Quantitative Structure-Property Relationship (QSPR) models for Minimum Ignition Energy (MIE) prediction of combustible dusts using machine learning. Powder Technology, 2020, 372, 227-234.	4.2	15
15	The molecular basis of pyrazinamide activity on Mycobacterium tuberculosis PanD. Nature Communications, 2020, 11, 339.	12.8	37
16	Metal-templated, Tight Loop Conformation of a Cys-X-Cys Biomimetic Assembles a Dimanganese Complex. Angewandte Chemie - International Edition, 2020, 59, 3645-3649.	13.8	2
17	Incorporating Complexity in Computing Camps for High School Students - A Report on the Summer Computing Academy Program at Texas A&M University. Journal of Computational Science Education, 2020, 11, 12-20.	0.3	0
18	Design criteria for minimalist mimics of protein-protein interface segments. Organic and Biomolecular Chemistry, 2019, 17, 908-915.	2.8	10

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19	Correlations between secondary structure- and protein-protein interface-mimicry: the interface mimicry hypothesis. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 3267-3274.	2.8	17
20	Study of phase behavior of 2,6-lutidine, 2,6-lutidine-N-oxide and water mixture using UNIQUAC model with interaction parameters determined by molecular simulations. <i>Thermochimica Acta</i> , 2019, 671, 110-118.	2.7	1
21	Dearomatization of the PCP Pincer Ligand in a Re <sup>V</sup> Oxo Complex. <i>Chemistry - A European Journal</i> , 2018, 24, 13754-13757.	3.3	17
22	Highly Luminescent Linear Complex Arrays of up to Eight Cuprous Centers. <i>Chemistry - A European Journal</i> , 2016, 22, 2396-2405.	3.3	27
23	A Biomimetic-Computational Approach to Optimizing the Quantum Efficiency of Photovoltaics. <i>Microscopy and Microanalysis</i> , 2015, 21, 1651-1652.	0.4	0
24	Utilizing Nearest-Neighbor Interactions To Alter Charge Transport Mechanisms in Molecular Assemblies of Porphyrins on Surfaces. <i>Journal of Physical Chemistry C</i> , 2015, 119, 13569-13579.	3.1	16
25	Effects of charge states, charge sites and side chain interactions on conformational preferences of a series of model peptide ions. <i>Analyst</i> , 2015, 140, 6933-6944.	3.5	14
26	Photocrystallographic Observation of Halide-Bridged Intermediates in Halogen Photoeliminations. <i>Journal of the American Chemical Society</i> , 2014, 136, 15346-15355.	13.7	31
27	A Multifaceted Secondary Structure Mimic Based On Piperidine-piperidinones. <i>Angewandte Chemie - International Edition</i> , 2014, 53, 3594-3598.	13.8	25
28	Evaluating minimalist mimics by exploring key orientations on secondary structures (EKOS). <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 7789.	2.8	26
29	Exploring Key Orientations at Protein-Protein Interfaces with Small Molecule Probes. <i>Journal of the American Chemical Society</i> , 2013, 135, 167-173.	13.7	37
30	Expanding the Scope of Oligo-pyrrolinone-Pyrrolidines as Protein-Protein Interface Mimics. <i>Journal of Organic Chemistry</i> , 2013, 78, 4823-4833.	3.2	8
31	Measuring the internal energies of species emitted from hypervelocity nanoparticle impacts on surfaces using recalibrated benzylpyridinium probe ions. <i>Journal of Chemical Physics</i> , 2013, 138, 214301.	3.0	17
32	Mechanistic Investigations of the ZnCl <sub>2</sub> -Mediated Tandem Mukaiyama Aldol Lactonization: Evidence for Asynchronous, Concerted Transition States and Discovery of 2-Oxopyridyl Ketene Acetal Variants. <i>Journal of the American Chemical Society</i> , 2012, 134, 3084-3094.	13.7	35
33	Computational Insights into Uranium Complexes Supported by Redox-Active $\hat{\pi}$ -Diimine Ligands. <i>Inorganic Chemistry</i> , 2012, 51, 2058-2064.	4.0	25
34	Studies of Ligand Exchange in N-Heterocyclic Carbene Silver(I) Complexes. <i>Organometallics</i> , 2012, 31, 4063-4071.	2.3	88
35	Diruthenium Naphthalene and Anthracene Complexes Containing a Doubly Linked Dicyclopentadienyl Ligand. <i>Organometallics</i> , 2012, 31, 4838-4848.	2.3	14
36	Carbon-Bromine Bond Formation through a Nickel-Centered Spin-Crossing Mechanism. <i>Organometallics</i> , 2011, 30, 6365-6371.	2.3	19

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37	Synthesis and Structure of a Dinuclear Gold(II) Complex with Terminal Fluoride Ligands. <i>Inorganic Chemistry</i> , 2011, 50, 4238-4240.	4.0	31
38	Pyrrrolinoneâ€“Pyrrolidine Oligomers as Universal Peptidomimetics. <i>Journal of the American Chemical Society</i> , 2011, 133, 12350-12353.	13.7	55
39	Universal Peptidomimetics. <i>Journal of the American Chemical Society</i> , 2011, 133, 462-477.	13.7	138
40	Synthesis of Odd Generation Triazine Dendrimers Using a Divergent, Macromonomer Approach. <i>Organic Letters</i> , 2010, 12, 1148-1151.	4.6	35
41	Analysis of a Pentacoordinate Iron Dicarbonyl as Synthetic Analogue of the Hmd or Monoâ€“Iron Hydrogenase Active Site. <i>Chemistry - A European Journal</i> , 2010, 16, 3083-3089.	3.3	69
42	Cyanideâ€“Bridged [Co <sup>II</sup> ] <sub>2</sub> M <sup>II</sup> ] and [Co <sup>II</sup> ] <sub>2</sub> M <sup>II</sup> Complexes Based on the [Co <sup>II</sup> (triphos)(CN) <sub>2</sub> ] Building Block: Syntheses, Structures, Magnetic Properties, and Density Functional Theoretical Studies. <i>Chemistry - A European Journal</i> , 2010, 16, 7164-7173.	3.3	11
43	A Mercuryâ†Antimony Interaction. <i>Angewandte Chemie - International Edition</i> , 2010, 49, 6357-6360.	13.8	66
44	Divergent synthesis of triazine dendrimers using a trimethylene-dipiperidine linker that increases efficiency, simplifies analysis, and improves product solubility. <i>Tetrahedron Letters</i> , 2010, 51, 1631-1634.	1.4	12
45	Thermal Decomposition Pathways of Hydroxylamine: Theoretical Investigation on the Initial Steps. <i>Journal of Physical Chemistry A</i> , 2010, 114, 9262-9269.	2.5	52
46	Factors That Influence Helical Preferences for Singly Charged Gas-Phase Peptide Ions: The Effects of Multiple Potential Charge-Carrying Sites. <i>Journal of Physical Chemistry B</i> , 2010, 114, 809-816.	2.6	31
47	A short, unsupported Cu(i)âˆ“Cu(i) interaction, 2.65 Å..., in a dinuclear guanidine chloride complex. <i>Chemical Communications</i> , 2010, 46, 136-138.	4.1	48
48	Goldâ€“Silane and Goldâ€“Stannane Complexes: Saturated Molecules as Îƒâ€“Acceptor Ligands. <i>Angewandte Chemie - International Edition</i> , 2009, 48, 9892-9895.	13.8	119
49	A new copper containing MALDI matrix that yields high abundances of [Peptide + Cu] <sup>+</sup> ions. <i>Journal of the American Society for Mass Spectrometry</i> , 2009, 20, 1263-1271.	2.8	14
50	The contributions of molecular framework to IMS collision cross-sections of gas-phase peptide ions. <i>Journal of the American Society for Mass Spectrometry</i> , 2009, 20, 1593-1602.	2.8	22
51	Synthesis, Structures, and Properties of Mixed Dithiolene-Carbonyl and Dithiolene-Phosphine Complexes of Tungsten. <i>Inorganic Chemistry</i> , 2009, 48, 2103-2113.	4.0	41
52	Mimicking PAMAM Dendrimers with Amphoteric, Hybrid Triazine Dendrimers: A Comparison of Dispersity and Stability. <i>Macromolecules</i> , 2009, 42, 6723-6732.	4.8	19
53	Theoretical study of the biologically important dioxo diiron diamond core structures. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 467-478.	1.4	2
54	Synthesis and cellular effects of cycloterpenals: Cyclohexadienal-based activators of neurite outgrowth. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 7573-7581.	3.0	12

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55	Synthesis and Characterization of a Thiol-Tethered Tripyridyl Porphyrin on Au(111). <i>Journal of Physical Chemistry C</i> , 2008, 112, 6110-6118.	3.1	37
56	Hydrogen-Bonding and $\pi$ - $\pi$ Base-Stacking Interactions Are Coupled in DNA, As Suggested by Calculated and Experimental Trans-Hbond Deuterium Isotope Shifts. <i>Journal of the American Chemical Society</i> , 2007, 129, 11298-11299.	13.7	32
57	Dinuclear and Tetranuclear Gold $\pi$ -Nitrogen Complexes. Solvent Influences on Oxidation and Nuclearity of Gold Guanidinate Derivatives. <i>Inorganic Chemistry</i> , 2007, 46, 11165-11172.	4.0	38
58	A divergent route towards single-chemical entity triazine dendrimers with opportunities for structural diversity. <i>New Journal of Chemistry</i> , 2007, 31, 1283.	2.8	32
59	Anion $\pi$ - $\pi$ Interactions as Controlling Elements in Self-Assembly Reactions of Ag(I) Complexes with $\pi$ -Acidic Aromatic Rings. <i>Journal of the American Chemical Society</i> , 2006, 128, 5895-5912.	13.7	302
60	Genetically Engineered Synthesis and Structural Characterization of Cobalt $\pi$ -Precorrin 5A and $\pi$ 5B, Two New Intermediates on the Anaerobic Pathway to Vitamin B12: A Definition of the Roles of the CbiF and CbiG Enzymes. <i>Journal of the American Chemical Society</i> , 2006, 128, 9971-9978.	13.7	27
61	Computational and Empirical Trans-hydrogen Bond Deuterium Isotope Shifts Suggest that N1 $\pi$ -N3 A:U Hydrogen Bonds of RNA are Shorter than those of A:T Hydrogen Bonds of DNA. <i>Journal of Biomolecular NMR</i> , 2006, 34, 229-236.	2.8	13
62	Mechanistic Investigation of the Oxygen-Atom-Transfer Reactivity of Dioxo-molybdenum(VI) Complexes. <i>Chemistry - A European Journal</i> , 2006, 12, 7501-7509.	3.3	56
63	Unsupported intermolecular argentophilic interaction in the dimer of trinuclear silver(I) 3,5-diphenylpyrazolates. <i>Inorganica Chimica Acta</i> , 2005, 358, 1657-1662.	2.4	83
64	Experimental and Computational Studies of Charge-Transfer and Reduction Products of 1, 4, 5, 8, 9, 11-Hexaazatriphenylene-Hexacarbonitrile: HAT-(CN) $\pi$ . <i>Journal of Cluster Science</i> , 2004, 15, 503-530.	3.3	35
65	$^{113}\text{Cd}$ NMR Determination of the Binding Parameters of Alicyclic Epoxides to [Hydrotris(3-phenylpyrazol-1-yl)borate]Cd(II) Acetate. <i>Organometallics</i> , 2004, 23, 5286-5290.	2.3	11
66	Reaction of the 1,8-Bis(diphenylmethylium)naphthalenediyl Dication with Fluoride: $\pi$ Formation of a Cation Containing a C $\pi$ -F $\pi$ -C Bridge. <i>Journal of the American Chemical Society</i> , 2004, 126, 8189-8196.	13.7	43
67	Unprecedented Head-to-Head Conformers of d(GpG) Bound to the Antitumor Active Compound Tetrakis( $\pi$ -carboxylato)dirhodium(II,II). <i>Journal of the American Chemical Society</i> , 2003, 125, 10703-10713.	13.7	70
68	Polyunsaturated Dicarboxylate Tethers Connecting Dimolybdenum Redox and Chromophoric Centers: A Absorption Spectra and Electronic Structures. <i>Journal of the American Chemical Society</i> , 2003, 125, 5486-5492.	13.7	71
69	Evaluation of Multivalent Dendrimers Based on Melamine: A Kinetics of Thiol $\pi$ -Disulfide Exchange Depends on the Structure of the Dendrimer. <i>Journal of the American Chemical Society</i> , 2003, 125, 5086-5094.	13.7	54
70	Cyclic Polyamidato Dianions as Bridges between Mo $\pi$ 4+ Units: A Synthesis, Crystal Structures, Electrochemistry, Absorption Spectra, and Electronic Structures. <i>Journal of the American Chemical Society</i> , 2003, 125, 8900-8910.	13.7	46
71	Novel Binding Interactions of the DNA Fragment d(pGpG) Cross-Linked by the Antitumor Active Compound Tetrakis( $\pi$ -carboxylato)dirhodium(II,II). <i>Journal of the American Chemical Society</i> , 2003, 125, 10714-10724.	13.7	71
72	Triazine Dendrimers for Drug Delivery: Evaluation of Solubilization Properties, Activity in Cell Culture, and In Vivo Toxicity of a Candidate Vehicle. <i>Supramolecular Chemistry</i> , 2003, 15, 607-616.	1.2	42

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73	The role of triplet states in the long wavelength absorption region of bromine nitrate. <i>Journal of Chemical Physics</i> , 2003, 119, 7864-7870.	3.0	5
74	Homologous Series of Redox-Active, Dinuclear Cations $[M_2(O_2CCH_3)_2(pynp)_2]^{2+}$ (M = Mo, Ru, Rh) with the Bridging Ligand 2-(2-Pyridyl)-1,8-naphthyridine (pynp). <i>Inorganic Chemistry</i> , 2002, 41, 1523-1533.	4.0	82
75	Unique Reactivity of a Tetradentate $N_2S_2$ Complex of Nickel: $\hat{A}$ Intermediates in the Production of Sulfur Oxygenates. <i>Inorganic Chemistry</i> , 2002, 41, 1837-1844.	4.0	61
76	Distinguishing between Phosphorylated and Nonphosphorylated Peptides with Ion Mobility $\hat{A}$ Mass Spectrometry. <i>Journal of Proteome Research</i> , 2002, 1, 303-306.	3.7	86
77	Observation of Conserved Solution-Phase Secondary Structure in Gas-Phase Tryptic Peptides. <i>Journal of the American Chemical Society</i> , 2002, 124, 4214-4215.	13.7	60
78	A Theoretical Study of the Primary Oxo Transfer Reaction of a Dioxo Molybdenum(VI) Compound with Imine Thiolate Chelating Ligands: $\hat{A}$ A Molybdenum Oxotransferase Analogue. <i>Journal of the American Chemical Society</i> , 2001, 123, 3995-4002.	13.7	63
79	Structure and thermodynamic stability of the OsC and OsC <sub>2</sub> molecules by theoretical calculations and by Knudsen cell mass spectrometry. <i>Journal of Chemical Physics</i> , 2001, 115, 4496-4501.	3.0	32
80	Theoretical Study of the Thermal Decomposition of N,N- $\hat{E}$ -Diacyl-N,N- $\hat{E}$ -Dialkoxyhydrazines: $\hat{A}$ A Comparison of HF, MP2, and DFT. <i>Journal of Physical Chemistry A</i> , 2000, 104, 6247-6252.	2.5	15