Carlos Silva-LÃ³pez

List of Publications by Year
in descending order

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102 papers	2,293 citations	201385 27 h-index	264894 42 g-index
102 all docs	102 docs citations	102 times ranked	2188 citing authors

#	Article	IF	Citations
1	Accessible triplet excited states in the photoisomerization of allenes with extended conjugation. Dalton Transactions, 2022, 51, 1357-1363.	1.6	0
2	Boosting Gold(I) Catalysis via Weak Interactions: New Fine-Tunable Impy Ligands. ACS Organic & Inorganic Au, 2022, 2, 229-235.	1.9	6
3	On the mechanism of the dyotropic expansion of hydrindanes into decalins. Organic and Biomolecular Chemistry, 2022, 20, 1073-1079.	1.5	0
4	Enantioselective CO₂ Fixation Via a Heckâ€Coupling/Carboxylation Cascade Catalyzed by Nickel. Chemistry - A European Journal, 2021, 27, 7657-7662.	1.7	32
5	The New Pharmacological Chaperones PBXs Increase Î±-Galactosidase A Activity in Fabry Disease Cellular Models. Biomolecules, 2021, 11, 1856.	1.8	1
6	Au(III) catalyzes the cross-coupling between activated methylenes and alkene derivatives. Journal of Catalysis, 2020, 392, 159-164.	3.1	4
7	The effect of solvation in torquoselectivity: ring opening of monosubstituted cyclobutenes. Organic and Biomolecular Chemistry, 2020, 18, 6287-6296.	1.5	1
8	Experimental and Computational Study of the 1,5-O â†' N Carbamoyl Snieckusâ€“Fries-Type Rearrangement. Journal of Organic Chemistry, 2020, 85, 12561-12578.	1.7	1
9	Unlocking the 5â€•exo Pathway with the Au I â€Catalyzed Alkoxycyclization of 1,3â€Dienâ€5â€ynes. Chemistry - A European Journal, 2020, 26, 8443-8451.	1.7	4
10	Photochemically Driven Tandem Process in the Construction of a Biscyclopropylcage from 2,5-Dimethoxy-p-benzoquinone and Terminal Acetylenes. Organic Letters, 2020, 22, 4527-4531.	2.4	6
11	Site-selective synthesis of 1,3-dioxin-3-ones via a gold(<scp>i</scp>) catalyzed cascade reaction. Chemical Communications, 2020, 56, 7734-7737.	2.2	4
12	The key role of protodeauration in the gold-catalyzed reaction of 1,3-diynes with pyrrole and indole to form complex heterocycles. Organic Chemistry Frontiers, 2020, 7, 997-1005.	2.3	8
13	Acetate-catalyzed hydroboration of CO₂ for the selective formation of methanol-equivalent products. Catalysis Science and Technology, 2020, 10, 2407-2414.	2.1	10
14	Double Protonation of a cis-Bipyridoallenophane Detected via Chiral-Sensing Switch: The Role of Ion Pairs. Organic Letters, 2019, 21, 5898-5902.	2.4	3
15	Scandium catalysed stereoselective thio-allylation of allenyl-imidates. Chemical Communications, 2019, 55, 9669-9672.	2.2	3
16	Pushing the limits of concertedness. A waltz of wandering carbocations. Chemical Science, 2019, 10, 2159-2170.	3.7	21
17	Gold-Catalyzed Homogeneous (Cyclo)Isomerization Reactions. Frontiers in Chemistry, 2019, 7, 296.	1.8	46
18	Phosphine-Catalyzed Stereoselective Dearomatization of 3-NO₂-Indoles with Allenoates. Journal of Organic Chemistry, 2019, 84, 6347-6355.	1.7	32

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19	Computational and experimental studies on Cu/Au-catalyzed stereoselective synthesis of 1,3-disubstituted allenes. Organic Chemistry Frontiers, 2019, 6, 1780-1786.	2.3	4
20	Lennard-Jones Intermolecular Potentials for the Description of 6-Membered Aromatic Heterocycles Interacting with the Isoelectronic CO2 and CS2. Journal of Physical Chemistry A, 2019, 123, 4475-4485.	1.1	0
21	Gold(<scp>i</scp>)-catalyzed nucleophilic cyclization of Î²-monosubstituted o-(alkynyl)styrenes: a combined experimental and computational study. Organic and Biomolecular Chemistry, 2019, 17, 9924-9932.	1.5	6
22	On the Use of Popular Basis Sets: Impact of the Intramolecular Basis Set Superposition Error. Molecules, 2019, 24, 3810.	1.7	14
23	Methanol directing the dual reactivity of 1,3-dien-5-ynes under gold(I) catalysis: A computational study. Computational and Theoretical Chemistry, 2019, 1148, 33-37.	1.1	2
24	Nitrogen doped nanohoops as promising CO₂ capturing devices. Physical Chemistry Chemical Physics, 2018, 20, 8607-8615.	1.3	7
25	Solvation. , 2018, , 97-146.		0
26	Rational Design of Efficient Environmental Sensors: Ring-Shaped Nanostructures Can Capture Quat Herbicides. ACS Omega, 2018, 3, 16976-16988.	1.6	5
27	Nickel catalyzed regio- and stereoselective arylation and methylation of allenamides via coupling reactions. An experimental and computational study. Organic Chemistry Frontiers, 2018, 5, 3231-3239.	2.3	16
28	Mechanism of the Molybdenum-Mediated Cadogan Reaction. ACS Omega, 2018, 3, 7019-7026.	1.6	14
29	Three Reaction Channels with Signature Proton Transfers in the Ni(I)-Catalyzed Decomposition of Ethyl Acetate. Organometallics, 2017, 36, 761-766.	1.1	2
30	Governing effects in the mechanism of the gold-catalyzed cycloisomerization of allenic hydroxylamine derivatives. Organic and Biomolecular Chemistry, 2017, 15, 5920-5926.	1.5	6
31	From Hydrindane to Decalin: A Mild Transformation through a Dyotropic Ring Expansion. Organic Letters, 2017, 19, 3648-3651.	2.4	8
32	Dynamic Effects Responsible for High Selectivity in a [3,3] Sigmatropic Rearrangement Featuring a Bispericyclic Transition State. Journal of Organic Chemistry, 2017, 82, 4758-4765.	1.7	22
33	Cycloreversion of the CO₂trimer: a paradigmatic pseudopericyclic [2 + 2 + 2] cycloaddition reaction. Organic and Biomolecular Chemistry, 2017, 15, 435-441.	1.5	9
34	CO₂ Complexes with Five-Membered Heterocycles: Structure, Topology, and Spectroscopic Characterization. Journal of Physical Chemistry A, 2017, 121, 9118-9130.	1.1	12
35	[MoO₂]²⁺-Mediated Oxygen Atom Transfer via an Unusual Lewis Acid Mechanism. Inorganic Chemistry, 2017, 56, 10570-10575.	1.9	7
36	Goldâ€Catalyzed Dearomatization of 2â€Naphthols with Alkynes. Chemistry - A European Journal, 2017, 23, 17473-17477.	1.7	29

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37	Lennard-Jones Potentials for the Interaction of CO₂ with Five-Membered Aromatic Heterocycles. Journal of Physical Chemistry A, 2017, 121, 9518-9530.	1.1	7
38	Exploring the Reactivity of Î±â€Lithiated Aryl Benzyl Ethers: Inhibition of the [1,2]â€Wittig Rearrangement and the Mechanistic Proposal Revisited. Chemistry - A European Journal, 2016, 22, 15058-15068.	1.7	16
39	Conformational control allows for [3,3]-sigmatropic rearrangements to proceed with torquoselectivity. RSC Advances, 2016, 6, 59181-59184.	1.7	6
40	Assessing the attractive/repulsive force balance in axial cyclohexane C-H_{ax}Â·Â·Â·Y_{ax}contacts: A combined computational analysis in monosubstituted cyclohexanes. Journal of Computational Chemistry, 2016, 37, 2647-2658.	1.5	10
41	The Outerâ€Sphere Mechanism of Nitrene Transfer onto Gold(I) Alkyne Complexes. ChemCatChem, 2016, 8, 2387-2392.	1.8	6
42	Rational Design in Catalysis: A Mechanistic Study of Î²-Hydride Eliminations in Gold(I) and Gold(III) Complexes Based on Features of the Reaction Valley. Inorganic Chemistry, 2016, 55, 8636-8645.	1.9	40
43	Copperâ€Catalyzed Skeletal Rearrangement of Oâ€Propargyl Oximes: A Mechanistic Manifold. ChemCatChem, 2016, 8, 2696-2703.	1.8	5
44	A Radical Mechanism for the Vanadium-Catalyzed Deoxydehydration of Glycols. Inorganic Chemistry, 2016, 55, 11372-11382.	1.9	16
45	Solving the Pericyclicâ€“Pseudopericyclic Puzzle in the Ring-Closure Reactions of 1,2,4,6-Heptatetraene Derivatives. Journal of Organic Chemistry, 2016, 81, 404-414.	1.7	29
46	BrÃ¸nsted Acidâ€Catalyzed Cascade Reactions Involving 1,2â€Indole Migration. Chemistry - A European Journal, 2015, 21, 12889-12893.	1.7	17
47	Diradical ring closing reactions displaying Woodwardâ€“Hoffmann behaviour and torquoselectivity. RSC Advances, 2015, 5, 30405-30408.	1.7	6
48	Accounting for Diradical Character through DFT. The Case of Vinyl Allene Oxide Rearrangement. Journal of Organic Chemistry, 2015, 80, 11206-11211.	1.7	9
49	Opening Access to New Chiral Macrocycles: From Allenes to Spiranes. Journal of Physical Chemistry A, 2015, 119, 1747-1753.	1.1	14
50	Computational Approaches to Homogeneous Gold Catalysis. Topics in Current Chemistry, 2014, 357, 213-283.	4.0	28
51	Bis(o-methylserotonin)-containing iridium(III) and ruthenium(II) complexes as new cellular imaging dyes: synthesis, applications, and photophysical and computational studies. Journal of Biological Inorganic Chemistry, 2013, 18, 679-692.	1.1	9
52	Computational insights on the mechanism of the catalytic hydrogenation with BINAPâ€“diamineâ€“Ru complexes: the role of base and origin of selectivity. Chemical Communications, 2013, 49, 4277-4279.	2.2	16
53	Computational Study of Gold-Catalyzed Homo- and Cross-Coupling Reactions. Journal of Organic Chemistry, 2013, 78, 4929-4939.	1.7	29
54	Noyori Hydrogenation: Aromaticity, Synchronicity, and Activation Strain Analysis. Journal of Organic Chemistry, 2013, 78, 5669-5676.	1.7	44

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55	Theoretical and experimental exploration of the photochemistry of resveratrol: beyond the simple double bond isomerization. Organic and Biomolecular Chemistry, 2012, 10, 9175.	1.5	37
56	Novel emissive podands based on 8-OH-quinoline: Synthesis, fluorescence materials, DFT and complexation studies. Inorganica Chimica Acta, 2012, 381, 218-228.	1.2	11
57	A stepwise retroâ€iminoâ€ene as a key step in the mechanism of allene formation via the CrabbÃ© acetylene homologation. Journal of Computational Chemistry, 2012, 33, 1236-1239.	1.5	6
58	On the Memory of Chirality in Gold(I)-Catalyzed Intramolecular Carboalkoxylation of Alkynes. Journal of Organic Chemistry, 2011, 76, 3791-3796.	1.7	41
59	Experimental and Computational Exploration of Indolizinyl Carbene Generation. A Route to Biindolizines. Journal of Organic Chemistry, 2011, 76, 3266-3273.	1.7	7
60	Performance of density functional theory on homogeneous gold catalysis. Theoretical Chemistry Accounts, 2011, 128, 647-661.	0.5	81
61	Novel versatile imineâ€"enamine chemosensor based on 6-nitro-4-oxo-4H-chromene for ion detection in solution, solid and gas-phase: synthesis, emission, computational and MALDI-TOF-MS studies. Tetrahedron, 2011, 67, 326-333.	1.0	12
62	Computational Study of the Intramolecular Pericyclic Reactions of Aldazines and Some Pseudopericyclic Variants. European Journal of Organic Chemistry, 2011, 2011, 2933-2939.	1.2	13
63	Bond Ellipticity as a Measure of Electron Delocalization in Structure and Reactivity. Current Organic Chemistry, 2011, 15, 3576-3593.	0.9	75
64	Competing Thermal Electrocyclic Ring-Closure Reactions of (2Z)-Hexa-2,4,5-trienals and Their Schiff Bases. Structural, Kinetic, and Computational Studies. Journal of Organic Chemistry, 2010, 75, 4453-4462.	1.7	16
65	Regioâ€, Periâ€, and Torquoselectivity in Hydroxy Heptatrienyl Cation Electrocyclizations: The Iso/Homoâ€Nazarov Reaction. Chemistry - A European Journal, 2009, 15, 1944-1956.	1.7	29
66	Torquoselectivity in the electrocyclic ringâ€opening of cyclopropyl anions. Journal of Physical Organic Chemistry, 2009, 22, 378-385.	0.9	10
67	Mechanism of the Gold-Catalyzed Rearrangement of (3-Acyloxyprop-1-ynyl)oxiranes: A Dual Role of the Catalyst. Journal of Organic Chemistry, 2009, 74, 2982-2991.	1.7	50
68	Allenyl Azide Cycloaddition Chemistry. 2,3-Cyclopentennelated Indole Synthesis through Indolidene Intermediates. Journal of Organic Chemistry, 2009, 74, 4958-4974.	1.7	41
69	Complex Thermal Behavior of 11-cis-Retinal, the Ligand of the Visual Pigments. Journal of Organic Chemistry, 2009, 74, 1007-1013.	1.7	10
70	Mechanistic Investigation on the Formation of Indolizines from 2-Enynylpyridines. Organic Letters, 2009, 11, 4802-4805.	2.4	16
71	Electrocyclic Ring Opening of Charged cis-Bicyclo[3.2.0]heptadiene and Heterocyclic Derivatives. The Anti-Woodwardâ"Hoffmann Quest (II). Journal of Organic Chemistry, 2009, 74, 2396-2402.	1.7	15
72	Allenyl Azide Cycloaddition Chemistry. Photochemical Initiation and CuI Mediation Leads to Improved Regioselectivity. Organic Letters, 2008, 10, 1665-1668.	2.4	41

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73	Role of Mg²⁺ in Hammerhead Ribozyme Catalysis from Molecular Simulation. Journal of the American Chemical Society, 2008, 130, 3053-3064.	6.6	102
74	Characterization of the Switch in the Mechanism of an Intramolecular Dielsâ^'Alder Reaction. Journal of Organic Chemistry, 2008, 73, 467-473.	1.7	14
75	Mechanistic Insights into the Stereocontrolled Synthesis of Hexahydropyrrolo[2,3-b]indoles by Electrophilic Activation of Tryptophan Derivatives. Organic Letters, 2008, 10, 77-80.	2.4	81
76	Allenyl Azide Cycloaddition Chemistry: Exploration of the Scope and Mechanism of Cyclopentennelated Dihydropyrrole Synthesis through Azatrimethylenemethane Intermediates. Journal of Organic Chemistry, 2008, 73, 5090-5099.	1.7	25
77	Sulfoxide-Induced Stereoselection in [1,5]-Sigmatropic Hydrogen Shifts of Vinylallenes. A Computational Study. Journal of Organic Chemistry, 2007, 72, 2617-2624.	1.7	13
78	Cyclization Cascade of Allenyl Azides:â€‰ A Dual Mechanism. Journal of the American Chemical Society, 2007, 129, 7638-7646.	6.6	35
79	Insight into the Role of Mg2+ in Hammerhead Ribozyme Catalysis from X-ray Crystallography and Molecular Dynamics Simulation. Journal of Chemical Theory and Computation, 2007, 3, 325-327.	2.3	38
80	Electrocyclic Ring Opening ofcis-Bicyclo[m.n.0]alkenes: The Anti-Woodwardâ€“Hoffmann Quest. Chemistry - A European Journal, 2007, 13, 5009-5017.	1.7	22
81	Pseudopericyclic design drives antara-antara [1,5] methylene sigmatropic shifts from a stepwise to a concerted mechanism. Journal of Computational Chemistry, 2007, 28, 1411-1416.	1.5	7
82	Computational Characterization of a Complete Palladium-Catalyzed Cross-Coupling Process:â€‰ The Associative Transmetalation in the Stille Reaction. Organic Letters, 2006, 8, 35-38.	2.4	78
83	Mechanism of the Gold(I)-Catalyzed Rautenstrauch Rearrangement:Â A Center-to-Helix-to-Center Chirality Transfer. Journal of the American Chemical Society, 2006, 128, 2434-2437.	6.6	183
84	Cycloisomerization of Activated (2E,4Z)-Heptatrienoate and Its Relevance to Crispatene (Bio)synthesis. A Case of Concerted and Stepwise Uncertainty. Journal of Organic Chemistry, 2006, 71, 4497-4501.	1.7	10
85	Computational Study and Analysis of the Kinetic Isotope Effects of the Rearrangement ofcis-Bicyclo[4.2.0]oct-7-ene tocis,cis-Cycloocta-1,3-diene. Organic Letters, 2006, 8, 2055-2058.	2.4	21
86	Multilevel and Density Functional Electronic Structure Calculations of Proton Affinities and Gas-Phase Basicities Involved in Biological Phosphoryl Transferâ€. Journal of Physical Chemistry A, 2006, 110, 791-797.	1.1	17
87	QCRNA 1.0: A database of quantum calculations for RNA catalysis. Journal of Molecular Graphics and Modelling, 2006, 25, 423-433.	1.3	26
88	Computation of vertical excitation energies of retinal and analogs: Scope and limitations. Journal of Computational Chemistry, 2006, 27, 116-123.	1.5	25
89	Synthesis of N-Heteroaryl Retinals and their Artificial Bacteriorhodopsins. ChemBioChem, 2005, 6, 2078-2087.	1.3	12
90	Pseudorotation Barriers of Biological Oxyphosphoranes: A Challenge for Simulations of Ribozyme Catalysis. Chemistry - A European Journal, 2005, 11, 2081-2093.	1.7	54

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91	Ellipticity: A Convenient Tool To Characterize Electrocyclic Reactions. Chemistry - A European Journal, 2005, 11, 1734-1738.	1.7	71
92	Mechanistic subtleties in the cyclopentannelation of allenolate allyl carbamates: the origin of the center-to-center chirality transfer. Chemical Communications, 2005, , 4285.	2.2	12
93	2-Alkylidenesulfol-3-enes by (Regio- and) Stereoselective Cheletropic Addition of SO2to (Di)vinylallenes. Organic Letters, 2005, 7, 1565-1568.	2.4	12
94	Simple Diastereoselectivity of the BF3Â·OEt2-Catalyzed Vinylogous Mukaiyama Aldol Reaction of 2-(Trimethylsiloxy)furans with Aldehydes. Journal of Organic Chemistry, 2005, 70, 3654-3659.	1.7	33
95	Pseudorotation of Natural and Chemically Modified Biological Phosphoranes: Implications for RNA Catalysis. ChemPhysChem, 2004, 5, 1045-1049.	1.0	32
96	Pseudorotation of Natural and Chemically Modified Biological Phosphoranes: Implications for RNA Catalysis. ChemPhysChem, 2004, 5, 1266-1266.	1.0	1
97	Theoretical Study of the Electrocyclic Ring Closure of Hydroxypentadienyl Cations. Chemistry - A European Journal, 2004, 10, 4324-4333.	1.7	95
98	The Woodwardâ^'Hoffmannâ^'De Puy Rule Revisitedâ€. Organic Letters, 2004, 6, 905-908.	2.4	31
99	Solvolytic Ring-Opening Reactions of Cyclopropyl Bromides. An Assessment of the Woodwardâ^'Hoffmannâ^'DePuy Rule. Journal of Organic Chemistry, 2004, 69, 9002-9010.	1.7	30
100	Conrotatory Ring-Opening Reactions of Cyclopropyl Anions in Monocyclic and Tricyclic Systems. Organic Letters, 2004, 6, 901-904.	2.4	13
101	Theoretical Study of the Vinyl Allene Oxide to Cyclopent-2-en-1-one Rearrangement:â€‰ Mechanism, Torquoselectivity and Solvent Effects. Journal of Organic Chemistry, 2004, 69, 3635-3644.	1.7	35
102	On the mechanism of the Au(I)â€mediated addition of alkynes to anthranils to furnish 7â€acylindoles. Journal of Physical Organic Chemistry, 0, , .	0.9	2