JosÃ© A SÃ¡ez

List of Publications by Year
in descending order

52 papers	2,659 citations	201674 27 h-index	182427 51 g-index
55 all docs	55 docs citations	55 times ranked	1989 citing authors

#	Article	IF	Citations
1	Understanding the local reactivity in polar organic reactions through electrophilic and nucleophilic Parr functions. RSC Advances, 2013, 3, 1486-1494.	3.6	628
2	Understanding the mechanism of polar Dielsâ€“Alder reactions. Organic and Biomolecular Chemistry, 2009, 7, 3576.	2.8	427
3	Understanding the Participation of Quadricyclane as Nucleophile in Polar [2Ïƒ + 2Ïƒ + 2Ï€] Cycloadditions toward Electrophilic Ï€ Molecules. Journal of Organic Chemistry, 2008, 73, 8791-8799.	3.2	220
4	Toward an Understanding of the Unexpected Regioselective Hetero-Dielsâ^'Alder Reactions of Asymmetric Tetrazines with Electron-Rich Ethylenes: A DFT Study. Journal of Organic Chemistry, 2009, 74, 2726-2735.	3.2	92
5	Understanding the Electronic Reorganization along the Nonpolar [3 + 2] Cycloaddition Reactions of Carbonyl Ylides.. Journal of Organic Chemistry, 2011, 76, 373-379.	3.2	89
6	1,3-Dipolar Cycloadditions of Electrophilically Activated Benzonitrile N-Oxides. Polar Cycloaddition versus Oxime Formation. Journal of Organic Chemistry, 2006, 71, 9319-9330.	3.2	56
7	Understanding the mechanism of the Povarov reaction. A DFT study. RSC Advances, 2014, 4, 25268.	3.6	54
8	Understanding the origin of the asynchronicity in bond-formation in polar cycloaddition reactions. A DFT study of the 1,3-dipolar cycloaddition reaction of carbonyl ylides with 1,2-benzoquinones. RSC Advances, 2012, 2, 1334-1342.	3.6	53
9	Understanding the regioselectivity in hetero Dielsâ€“Alder reactions. AnÂELF analysis of the reaction between nitrosoethylene and 1-vinylpyrrolidine. Tetrahedron, 2013, 69, 107-114.	1.9	52
10	Origin of the synchronicity in bond formation in polar Dielsâ€“Alder reactions: an ELF analysis of the reaction between cyclopentadiene and tetracyanoethylene. Organic and Biomolecular Chemistry, 2012, 10, 3841.	2.8	51
11	A Combined Experimental and Theoretical Study of the Polar [3 + 2] Cycloaddition of Electrophilically Activated Carbonyl Ylides with Aldehydes and Imines. Journal of Organic Chemistry, 2009, 74, 2120-2133.	3.2	49
12	A comparative analysis of the electrophilicity of organic molecules between the computed IPs and EAs and the HOMO and LUMO energies. Chemical Physics Letters, 2007, 438, 341-345.	2.6	46
13	Supramolecular hydrogels for enzymatically triggered self-immolative drug delivery. Tetrahedron, 2010, 66, 2614-2618.	1.9	46
14	Selective catechol-triggered supramolecular gel disassembly. Chemical Communications, 2010, 46, 7996.	4.1	42
15	Stereoisomerization of Î²-Hydroxy-Î±-sulfenyl-Î³-butyrolactones Controlled by Two Concomitant 1,4-Type Nonbonded Sulfurâ^'Oxygen Interactions As Analyzed by X-ray Crystallography. Journal of Organic Chemistry, 2010, 75, 5888-5894.	3.2	40
16	Lewis Acid-Catalyzed [4 + 3] Cycloaddition of 2-(Trimethyl Silyloxy)acrolein with Furan. Insight on the Nature of the Mechanism from a DFT Analysis. Organic Letters, 2003, 5, 4117-4120.	4.6	39
17	Toward an understanding of the 1,3-dipolar cycloaddition between diphenylnitrone and a maleimide:bisamide complex. A DFT analysis of the reactivity of symmetrically substituted dipolarophiles. Computational and Theoretical Chemistry, 2007, 811, 125-133.	1.5	38
18	Understanding the Mechanism of the Intramolecular Stetter Reaction. A DFT Study. Molecules, 2012, 17, 1335-1353.	3.8	34

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19	A combined experimental and theoretical study of the thermal cycloaddition of aryl azides with activated alkenes. Organic and Biomolecular Chemistry, 2011, 9, 4295.	2.8	33
20	A DFT study for the regioselective 1,3-dipolar cycloadditions of nitrile N-oxides toward alkynylboronates. Tetrahedron, 2003, 59, 9167-9171.	1.9	32
21	Toward an Understanding of the Acceleration of Dielsâ^'Alder Reactions by a Pseudo-intramolecular Process Achieved by Molecular Recognition. A DFT Study. Journal of Organic Chemistry, 2007, 72, 4220-4227.	3.2	32
22	Experimental and theoretical study on the substitution reactions of aryl 2,4-dinitrophenyl carbonates with quinuclidines. Tetrahedron, 2006, 62, 2555-2562.	1.9	31
23	Polar [3 + 2] cycloaddition of ketones with electrophilically activated carbonyl ylides. Synthesis of spirocyclic dioxolane indolinones. Organic and Biomolecular Chemistry, 2008, 6, 3144.	2.8	30
24	Molecular recognition through divalent interactions with a self-assembled fibrillar network of a supramolecular organogel. Organic and Biomolecular Chemistry, 2008, 6, 4378.	2.8	30
25	A DFT study on the NHC catalysed Michael addition of enols to Î±,Î²-unsaturated acyl-azoliums. A base catalysed Câ€“C bond-formation step. Organic and Biomolecular Chemistry, 2014, 12, 895-904.	2.8	30
26	Photophysical properties of 5-substituted 2-thiopyrimidines. Photochemical and Photobiological Sciences, 2013, 12, 1460-1465.	2.9	28
27	A DFT Study of the [3 + 2] versus [4 + 2] Cycloaddition Reactions of 1,5,6-Trimethylpyrazinium-3-olate with Methyl Methacrylate. Journal of Organic Chemistry, 2013, 78, 1621-1629.	3.2	28
28	DFT Study of the Molecular Mechanism of Lewis Acid Induced [4 + 3] Cycloadditions of 2-Alkylacroleins with Cyclopentadiene. Journal of Organic Chemistry, 2009, 74, 5934-5940.	3.2	25
29	Understanding Câ€“C bond formation in polar reactions. An ELF analysis of the Friedelâ€“Crafts reaction between indoles and nitroolefins. RSC Advances, 2013, 3, 7520.	3.6	23
30	Unravelling the mechanism of the ketene-imine Staudinger reaction. An ELF quantum topological analysis. RSC Advances, 2015, 5, 37119-37129.	3.6	23
31	An ELF analysis of the Câ€“C bond formation step in the N-heterocyclic carbene-catalyzed hydroacylation of unactivated Câ€“C double bonds. RSC Advances, 2012, 2, 7127.	3.6	21
32	Experimental and theoretical investigations for the tandem alkylationâ€“isomerization reactions between unsaturated carboxylic acids and allyl halides. Tetrahedron, 2003, 59, 6233-6239.	1.9	20
33	Lewis acid induced [4+3] cycloadditions of 2-silyloxyacroleins. Insights on the mechanism from a DFT analysis. Tetrahedron, 2005, 61, 7538-7545.	1.9	20
34	Understanding the formation of [3+2] and [2+4] cycloadducts in the Lewis acid catalysed reaction between methyl glyoxylate oxime and cyclopentadiene: a theoretical study. RSC Advances, 2013, 3, 447-457.	3.6	20
35	Study of the stereoselectivity of the nucleophilic epoxidation of 3-hydroxy-2-methylene esters. Tetrahedron, 2014, 70, 97-102.	1.9	20
36	Understanding the Bond Formation in Hetero-Diels-Alder Reactions. An ELF Analysis of the Reaction of Nitroethylene with Dimethylvinylamine. Current Organic Chemistry, 2012, 16, 2343-2351.	1.6	19

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37	Solvent-free construction of self-assembled 1D nanostructures from low-molecular-weight organogelators: sublimation vs. gelation. Soft Matter, 2009, 5, 3727.	2.7	18
38	Understanding the domino reaction between 3-chloroindoles and methyl coumalate yielding carbazoles. A DFT study. Organic and Biomolecular Chemistry, 2015, 13, 2034-2043.	2.8	15
39	Understanding the selectivity in the formation of Î´-lactams vs. Î²-lactams in the Staudinger reactions of chloro-cyan-ketene with unsaturated imines. A DFT study. RSC Advances, 2014, 4, 58559-58566.	3.6	14
40	Ring splitting of azetidin-2-ones via radical anions. Organic and Biomolecular Chemistry, 2012, 10, 7928.	2.8	13
41	Experimental and theoretical study of the [3 + 2] cycloaddition of carbonyl ylides with alkynes. Organic and Biomolecular Chemistry, 2012, 10, 8434.	2.8	12
42	Protection against chemical submission: naked-eye detection of Î³-hydroxybutyric acid (GHB) in soft drinks and alcoholic beverages. Chemical Communications, 2020, 56, 12600-12603.	4.1	12
43	A DFT study for the formation of imidazo[1,2-c]pyrimidines through an intramolecular Michael addition. Tetrahedron, 2006, 62, 10408-10416.	1.9	9
44	Formation of pyrazolâ€1,3,4â€thiadiazoles through 1,3â€dipolar cycloadditions of 3â€thioxoâ€[1,2,4]â€triazepinâ€5â€one with nitrilimines: an experimental and computational study. Journal of Physical Organic Chemistry, 2009, 22, 31-41.	1.9	8
45	Oxetane Ring Enlargement through Nucleophilic Trapping of Radical Cations by Acetonitrile. Organic Letters, 2012, 14, 5700-5703.	4.6	8
46	Cycloreversion of Î²-lactams via photoinduced electron transfer. Organic and Biomolecular Chemistry, 2014, 12, 8428-8432.	2.8	8
47	Azo-hydrazo conversion via [1,5]-hydrogen shifts. A combined experimental and theoretical study. Tetrahedron, 2012, 68, 6902-6907.	1.9	7
48	Heteroditopic chemosensor to detect Î³-hydroxybutyric acid (GHB) in soft drinks and alcoholic beverages. Analyst, The, 2021, 146, 5601-5609.	3.5	5
49	Spermine and Spermidine Detection through Restricted Intramolecular Rotations in a Tetraphenylethylene Derivative. Chemosensors, 2022, 10, 8.	3.6	5
50	Theoretical study on the molecular mechanism of the [5 + 2] vs. [4 + 2] cyclization mediated by Lewis acid in the quinone system. Organic and Biomolecular Chemistry, 2013, 11, 8357.	2.8	2
51	Isomerization and Redox Tuning: Reorganizing the Maya Blue Puzzle from Synthetic, Spectral, and Electrochemical Issues. Journal of Physical Chemistry C, 2021, 125, 26188-26200.	3.1	2
52	Diels-Alderase Catalyzing the Cyclization Step in the Biosynthesis of Spinosyn A. , 2015, , 169-201.		0