MarÃ-a J Aurell

List of Publications by Year
in descending order

70 papers	2,928 citations	304368 22 h-index	168136 53 g-index
72 all docs	72 docs citations	72 times ranked	1903 citing authors

#	Article	IF	Citations
1	Acceptorless dehydrogenative condensation: synthesis of indoles and quinolines from diols and anilines. Organic and Biomolecular Chemistry, 2021, 19, 677-683.	1.5	13
2	Unveiling the Ionic Dielsâ€“Alder Reactions within the Molecular Electron Density Theory. Molecules, 2021, 26, 3638.	1.7	3
3	Unveiling the Intramolecular Ionic Dielsâ€“Alder Reactions within Molecular Electron Density Theory. Chemistry, 2021, 3, 834-853.	0.9	0
4	Unveiling the regioselectivity in electrophilic aromatic substitution reactions of deactivated benzenes through molecular electron density theory. New Journal of Chemistry, 2021, 45, 13626-13638.	1.4	10
5	Empirical modeling of material composition and size in MOFs prepared with ligand mixtures. Dalton Transactions, 2019, 48, 2881-2885.	1.6	2
6	A new mechanism for internal nucleophilic substitution reactions. Organic and Biomolecular Chemistry, 2018, 16, 1101-1112.	1.5	1
7	A theoretical study on NHC-catalysed enantioselective cycloaddition of ketenes and 3-aroylcoumarins: mechanism and enantioselectivity. Organic and Biomolecular Chemistry, 2018, 16, 5474-5482.	1.5	6
8	Synthesis, Optical Properties, and DNA Interaction of New Diquats Based on Triazolopyridines and Triazoloquinolines. Chemistry - A European Journal, 2017, 23, 12825-12832.	1.7	8
9	A DFT study of the mechanism of NHC catalysed annulation reactions involving Î±,Î²-unsaturated acyl azoliums and Î²-naphthol. Organic and Biomolecular Chemistry, 2016, 14, 8338-8345.	1.5	11
10	Theoretical study of the regio- and stereoselectivity of the intramolecular Povarov reactions yielding 5H-chromeno[2,3-c] acridine derivatives. RSC Advances, 2016, 6, 15759-15769.	1.7	10
11	A mechanistic study of the participation of azomethine ylides and carbonyl ylides in [3+2] cycloaddition reactions. Tetrahedron, 2015, 71, 1050-1057.	1.0	24
12	A DFT study of the domino reactions between imidazole NHC, ketenimines and DMAD or MP acetylene derivatives yielding spiro-pyrroles. Computational and Theoretical Chemistry, 2014, 1030, 25-32.	1.1	4
13	The mechanism of ionic Dielsâ€“Alder reactions. A DFT study of the oxa-Povarov reaction. RSC Advances, 2014, 4, 16567-16577.	1.7	26
14	Understanding the mechanism of the Povarov reaction. A DFT study. RSC Advances, 2014, 4, 25268.	1.7	54
15	Understanding the polar mechanism of the ene reaction. A DFT study. Organic and Biomolecular Chemistry, 2014, 12, 7581-7590.	1.5	36
16	A DFT analysis of the participation of zwitterionic TACs in polar [3+2] cycloaddition reactions. Tetrahedron, 2014, 70, 4519-4525.	1.0	68
17	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.	0.9	19
18	A DFT study of the role of Lewis acid catalysts in the mechanism of the 1,3-dipolar cycloaddition of nitrile imines towards electron-deficient acryloyl derivatives. Computational and Theoretical Chemistry, 2012, 986, 6-13.	1.1	9

#	Article	IF	Citations
19	The role of the trifluoromethyl group in reactivity and selectivity in polar cycloaddition reactions. A DFT study. Tetrahedron, 2012, 68, 8457-8462.	1.0	20
20	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.	1.7	53
21	Understanding the kinetic solvent effects on the 1,3â€dipolar cycloaddition of benzonitrile Nâ€oxide: a DFT study. Journal of Physical Organic Chemistry, 2011, 24, 611-618.	0.9	79
22	A DFT Explanation of the Reactivity and Regioselectivity of the Diels- Alder Reactions Between 2,3,4,4a-Tetrahydroquinoline and some Electron-Deficient Dienophiles. Letters in Organic Chemistry, 2011, 8, 119-124.	0.2	0
23	A DFT study of the role of the Mg complex formation on the mechanism of the 1,3-dipolar cycloadditions of benzonitrile oxides with acryloylpyrazolidinone. Computational and Theoretical Chemistry, 2010, 942, 26-31.	1.5	11
24	Understanding the mechanism of the N-heterocyclic carbene-catalyzed ring-expansion of 4-formyl-Î²-lactams to succinimide derivatives. Tetrahedron, 2009, 65, 3432-3440.	1.0	59
25	Understanding the regio- and chemoselective polar [3+2] cycloaddition of the Padwa carbonyl ylides with Î±-methylene ketones. A DFT study. Tetrahedron, 2009, 65, 4644-4651.	1.0	31
26	A combined experimental and theoretical study of the alkylation of 3,5â€dithioxoâ€[1,2,4]triazepines. Journal of Physical Organic Chemistry, 2008, 21, 457-463.	0.9	3
27	Mechanistic details of the domino reaction of nitronaphthalenes with the electron-rich dienes. A DFT study. Computational and Theoretical Chemistry, 2008, 853, 68-76.	1.5	27
28	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.	1.7	32
29	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
30	Experimental and theoretical push-pull Chemo- and regioselectivity in 1,3-Dipolar cycloaddition reactions: the case of benzotriazepin-5-one with mesitylnitrile oxide. Journal of Physical Organic Chemistry, 2007, 20, 245-254.	0.9	7
31	4,4â€²-Substituted biphenyl coronands. Preparation of a new selective fluorescent sensor for mercury salts. Tetrahedron, 2006, 62, 11972-11978.	1.0	11
32	Biphenyl Macrolactams as Colorimetric Sensors for Anions through Displacement Reactions. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2006, 54, 61-66.	1.6	5
33	Magnetoelectrochemistry of 4,4â€²-bis(dimethylamino)biphenyl and 4,4â€²-dinitrobiphenyl azacrown macrocyclic lactams. Electrochimica Acta, 2005, 50, 4063-4075.	2.6	2
34	Cation and anion fluorescent and electrochemical sensors derived from 4,4â€²-substituted biphenyl. Tetrahedron, 2005, 61, 10309-10320.	1.0	15
35	The role of the transfer group in the intramolecular [5+2] cycloadditions of substituted Î²-hydroxy-Î³-pyrones: a DFT analysis. Journal of Physical Organic Chemistry, 2005, 18, 610-615.	0.9	8
36	Biphenyl macrolactams in anion complexation. Selective naked-eye fluoride recognition. Tetrahedron, 2004, 60, 9471-9478.	1.0	61

#	Article	IF	Citations
37	Magnetoelectrochemical modulation of pre-organization processes in a 4,4?-dinitrobiphenyl azacrown macrocyclic lactam. Electrochemistry Communications, 2004, 6, 908-912.	2.3	3
38	A theoretical study on the regioselectivity of 1,3-dipolar cycloadditions using DFT-based reactivity indexes. Tetrahedron, 2004, 60, 11503-11509.	1.0	150
39	Origin of the Synchronicity on the Transition Structures of Polar Dielsâ^'Alder Reactions. Are These Reactions [4 + 2] Processes?. Journal of Organic Chemistry, 2003, 68, 3884-3890.	1.7	119
40	Title is missing!. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2003, 45, 241-249.	1.6	8
41	Origin of the Synchronicity on the Transition Structures of Polar Dielsâ€"Alder Reactions. Are these Reactions [4 + 2] Processes?. ChemInform, 2003, 34, no.	0.1	0
42	Quantitative characterization of the global electrophilicity pattern of some reagents involved in 1,3-dipolar cycloaddition reactions. Tetrahedron, 2003, 59, 3117-3125.	1.0	301
43	Quantitative Characterization of the Local Electrophilicity of Organic Molecules. Understanding the Regioselectivity on Dielsâ^'Alder Reactions. Journal of Physical Chemistry A, 2002, 106, 6871-6875.	1.1	357
44	Density Functional Theory Study of the Cycloaddition Reaction of Furan Derivatives with Maskedo-Benzoquinones. Does the Furan Act as a Dienophile in the Cycloaddition Reaction?. Journal of Organic Chemistry, 2002, 67, 959-965.	1.7	84
45	Quantitative characterization of the global electrophilicity power of common diene/dienophile pairs in Dielsâ€"Alder reactions. Tetrahedron, 2002, 58, 4417-4423.	1.0	832
46	Crown ethers derived from cyclohexane. Influence of their stereochemistry in complexation and transport. Tetrahedron, 2002, 58, 6729-6734.	1.0	16
47	Synthesis, configurational analysis and single-crystal structure of one azacrownlactame derived from biphenyl. Acta Crystallographica Section A: Foundations and Advances, 2002, 58, c311-c311.	0.3	0
48	Theoretical study on the mechanism of the domino reactions of tertiary Î±-cyano-enamines and dimethyl acetylenedicarboxylate. Tetrahedron, 2001, 57, 169-177.	1.0	4
49	On the mechanism of the addition of organolithium reagents to cinnamic acids. Tetrahedron, 2001, 57, 1067-1074.	1.0	13
50	Conjugate addition of organolithium reagents to Î±,Î²-unsaturated carboxylic acids. Tetrahedron, 1999, 55, 815-830.	1.0	20
51	Addition of organolithium reagents to cinnamic acids. Tetrahedron, 1999, 55, 831-846.	1.0	14
52	A DFT Characterization of the Mechanism for the Cycloaddition Reaction between 2-Methylfuran and Acetylenedicarboxylic Acid. Journal of Physical Chemistry A, 1999, 103, 11425-11430.	1.1	33
53	Conjugate addition of organolithium reagents to Î±,Î²-unsaturated carboxylic acids. Tetrahedron Letters, 1998, 39, 6351-6354.	0.7	14
54	Alkylation of lithium dienediolates of butenoic acids. Regioselectivity effects of structure and leaving group of the alkylating agent. Tetrahedron, 1998, 54, 4357-4366.	1.0	36

#	Article	IF	Citations
55	The Diels-Alder cycloaddition, an intriguing problem in organic sonochemistry. Ultrasonics Sonochemistry, 1996, 3, 7-13.	3.8	25
56	Trienediolates of hexadienoic acids in synthesis. Addition to unsaturated ketones. A convergent approach to the synthesis of retinoic acids. Tetrahedron, 1995, 51, 3915-3928.	1.0	15
57	A Direct Access to Ketones from Lithium Carboxylates via the Sonochemical Barbier Reaction. Synlett, 1995, 1995, 459-460.	1.0	11
58	The Sonochemical Barbier Reaction Extended to Carboxylate Salts. An Easy Access to 2-Furanyl Ketones. Journal of Organic Chemistry, 1995, 60, 8-9.	1.7	21
59	13C NMR studies of dianions of unsaturated carboxylic acids. Tetrahedron, 1994, 50, 5109-5118.	1.0	15
60	Dienediolates of unsaturated carboxylic acids in synthesis. Synthesis of cyclohexenones and polycyclic ketones by tandem Michael-Dieckmann decarboxylative annulation of unsaturated carboxylic acids.. Tetrahedron, 1994, 50, 2571-2582.	1.0	13
61	The sonochemical barbier reaction applied to carboxylates. Study of a model case. Journal of the Chemical Society Chemical Communications, 1994, , 1815.	2.0	1
62	Trienediolates of hexadienoic acids in synthesis. synthesis of retinoic and nor-retinoic acids.. Tetrahedron, 1993, 49, 6089-6100.	1.0	10
63	Synthesis of Dienedioic and Tetraenedioic Acids by Oxidative Coupling of Unsaturated Carboxylic Acid Dienediolates by 1,2-Diiodoethane. Synthetic Communications, 1993, 23, 2827-2831.	1.1	2
64	SYNTHESE DE THIENO [2,3-a] QUINOLIZIDINES. Phosphorus, Sulfur and Silicon and the Related Elements, 1993, 85, 17-21.	0.8	5
65	Iodine oxidative coupling of diene and triene-diolates of unsaturated carboxylic acids.. Tetrahedron, 1991, 47, 1997-2004.	1.0	4
66	Polyenolates of Unsaturated Carboxylic Acids in Synthesis. Synthesis of Unsaturated Î±-Amino Acids and Î²-Hydrazing Acids. Synthetic Communications, 1991, 21, 1833-1839.	1.1	8
67	Dienediolates of Unsaturated Carboxylic Acids in Synthesis. Tandem Michael Diechmann Synthesis of Substituted 2-Cyclohexenones. Synthetic Communications, 1991, 21, 1825-1831.	1.1	8
68	Polyenolates of unsaturated carboxylic acids in synthesis. A straightforward synthesis of retinoic acids.. Tetrahedron Letters, 1990, 31, 5791-5794.	0.7	8
69	The Synthesis of 1,8-Dihydroxy-2,3,4,6-tetramethoxyxanthone and 1,6-Dihydroxy-3,5,7,8-tetramethoxy-xanthone, a Confirmation of Structure. Journal of Natural Products, 1989, 52, 852-857.	1.5	1
70	Silver ion oxidative coupling of diene and triene-diolates of unsaturated carboxylic acids. A facile synthesis of octa- and dodeca-dienedioic acids. Tetrahedron Letters, 1988, 29, 6181-6182.	0.7	11