

# MarÃ-a J Aurell

## List of Publications by Year in descending order

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70  
papers

2,928  
citations

304743

22  
h-index

168389

53  
g-index

72  
all docs

72  
docs citations

72  
times ranked

1903  
citing authors

#	ARTICLE	IF	CITATIONS
1	Quantitative characterization of the global electrophilicity power of common diene/dienophile pairs in Diels-Alder reactions. <i>Tetrahedron</i> , 2002, 58, 4417-4423.	1.9	832
2	Quantitative Characterization of the Local Electrophilicity of Organic Molecules. Understanding the Regioselectivity on Diels-Alder Reactions. <i>Journal of Physical Chemistry A</i> , 2002, 106, 6871-6875.	2.5	357
3	Quantitative characterization of the global electrophilicity pattern of some reagents involved in 1,3-dipolar cycloaddition reactions. <i>Tetrahedron</i> , 2003, 59, 3117-3125.	1.9	301
4	A theoretical study on the regioselectivity of 1,3-dipolar cycloadditions using DFT-based reactivity indexes. <i>Tetrahedron</i> , 2004, 60, 11503-11509.	1.9	150
5	Origin of the Synchronicity on the Transition Structures of Polar Diels-Alder Reactions. Are These Reactions [4 + 2] Processes?. <i>Journal of Organic Chemistry</i> , 2003, 68, 3884-3890.	3.2	119
6	Density Functional Theory Study of the Cycloaddition Reaction of Furan Derivatives with Masked-o-Benzoquinones. Does the Furan Act as a Dienophile in the Cycloaddition Reaction?. <i>Journal of Organic Chemistry</i> , 2002, 67, 959-965.	3.2	84
7	Understanding the kinetic solvent effects on the 1,3-dipolar cycloaddition of benzonitrile N-oxide: a DFT study. <i>Journal of Physical Organic Chemistry</i> , 2011, 24, 611-618.	1.9	79
8	A DFT analysis of the participation of zwitterionic TACs in polar [3+2] cycloaddition reactions. <i>Tetrahedron</i> , 2014, 70, 4519-4525.	1.9	68
9	Biphenyl macrolactams in anion complexation. Selective naked-eye fluoride recognition. <i>Tetrahedron</i> , 2004, 60, 9471-9478.	1.9	61
10	Understanding the mechanism of the N-heterocyclic carbene-catalyzed ring-expansion of 4-formyl- $\beta$ -lactams to succinimide derivatives. <i>Tetrahedron</i> , 2009, 65, 3432-3440.	1.9	59
11	Understanding the mechanism of the Povarov reaction. A DFT study. <i>RSC Advances</i> , 2014, 4, 25268.	3.6	54
12	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. <i>RSC Advances</i> , 2012, 2, 1334-1342.	3.6	53
13	Toward an understanding of the 1,3-dipolar cycloaddition between diphenylnitron and a maleimide:bisamide complex. A DFT analysis of the reactivity of symmetrically substituted dipolarophiles. <i>Computational and Theoretical Chemistry</i> , 2007, 811, 125-133.	1.5	38
14	Alkylation of lithium dienediolates of butenoic acids. Regioselectivity effects of structure and leaving group of the alkylating agent. <i>Tetrahedron</i> , 1998, 54, 4357-4366.	1.9	36
15	Understanding the polar mechanism of the ene reaction. A DFT study. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 7581-7590.	2.8	36
16	A DFT Characterization of the Mechanism for the Cycloaddition Reaction between 2-Methylfuran and Acetylenedicarboxylic Acid. <i>Journal of Physical Chemistry A</i> , 1999, 103, 11425-11430.	2.5	33
17	Toward an Understanding of the Acceleration of Diels-Alder Reactions by a Pseudo-intramolecular Process Achieved by Molecular Recognition. A DFT Study. <i>Journal of Organic Chemistry</i> , 2007, 72, 4220-4227.	3.2	32
18	Understanding the regio- and chemoselective polar [3+2] cycloaddition of the Padwa carbonyl ylides with $\alpha$ -methylene ketones. A DFT study. <i>Tetrahedron</i> , 2009, 65, 4644-4651.	1.9	31

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19	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
20	The mechanism of ionic Diels-Alder reactions. A DFT study of the oxa-Povarov reaction. RSC Advances, 2014, 4, 16567-16577.	3.6	26
21	The Diels-Alder cycloaddition, an intriguing problem in organic sonochemistry. Ultrasonics Sonochemistry, 1996, 3, 7-13.	8.2	25
22	A mechanistic study of the participation of azomethine ylides and carbonyl ylides in [3+2] cycloaddition reactions. Tetrahedron, 2015, 71, 1050-1057.	1.9	24
23	The Sonochemical Barbier Reaction Extended to Carboxylate Salts. An Easy Access to 2-Furanyl Ketones. Journal of Organic Chemistry, 1995, 60, 8-9.	3.2	21
24	Conjugate addition of organolithium reagents to $\alpha,\beta$ -unsaturated carboxylic acids. Tetrahedron, 1999, 55, 815-830.	1.9	20
25	The role of the trifluoromethyl group in reactivity and selectivity in polar cycloaddition reactions. A DFT study. Tetrahedron, 2012, 68, 8457-8462.	1.9	20
26	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
27	Crown ethers derived from cyclohexane. Influence of their stereochemistry in complexation and transport. Tetrahedron, 2002, 58, 6729-6734.	1.9	16
28	<sup>13</sup> C NMR studies of dianions of unsaturated carboxylic acids. Tetrahedron, 1994, 50, 5109-5118.	1.9	15
29	Trienediolates of hexadienoic acids in synthesis. Addition to unsaturated ketones. A convergent approach to the synthesis of retinoic acids. Tetrahedron, 1995, 51, 3915-3928.	1.9	15
30	Cation and anion fluorescent and electrochemical sensors derived from 4,4'-substituted biphenyl. Tetrahedron, 2005, 61, 10309-10320.	1.9	15
31	Conjugate addition of organolithium reagents to $\alpha,\beta$ -unsaturated carboxylic acids. Tetrahedron Letters, 1998, 39, 6351-6354.	1.4	14
32	Addition of organolithium reagents to cinnamic acids. Tetrahedron, 1999, 55, 831-846.	1.9	14
33	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.	1.9	13
34	On the mechanism of the addition of organolithium reagents to cinnamic acids. Tetrahedron, 2001, 57, 1067-1074.	1.9	13
35	Acceptorless dehydrogenative condensation: synthesis of indoles and quinolines from diols and anilines. Organic and Biomolecular Chemistry, 2021, 19, 677-683.	2.8	13
36	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.	1.4	11

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37	A Direct Access to Ketones from Lithium Carboxylates via the Sonochemical Barbier Reaction. <i>Synlett</i> , 1995, 1995, 459-460.	1.8	11
38	4,4-Substituted biphenyl coronands. Preparation of a new selective fluorescent sensor for mercury salts. <i>Tetrahedron</i> , 2006, 62, 11972-11978.	1.9	11
39	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. <i>Computational and Theoretical Chemistry</i> , 2010, 942, 26-31.	1.5	11
40	A DFT study of the mechanism of NHC catalysed annulation reactions involving $\hat{1},\hat{2}$ -unsaturated acyl azoliums and $\hat{2}$ -naphthol. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 8338-8345.	2.8	11
41	Trienediolates of hexadienoic acids in synthesis. synthesis of retinoic and nor-retinoic acids.. <i>Tetrahedron</i> , 1993, 49, 6089-6100.	1.9	10
42	Theoretical study of the regio- and stereoselectivity of the intramolecular Povarov reactions yielding 5H-chromeno[2,3-c] acridine derivatives. <i>RSC Advances</i> , 2016, 6, 15759-15769.	3.6	10
43	Unveiling the regioselectivity in electrophilic aromatic substitution reactions of deactivated benzenes through molecular electron density theory. <i>New Journal of Chemistry</i> , 2021, 45, 13626-13638.	2.8	10
44	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. <i>Computational and Theoretical Chemistry</i> , 2012, 986, 6-13.	2.5	9
45	Polyenolates of unsaturated carboxylic acids in synthesis. A straightforward synthesis of retinoic acids.. <i>Tetrahedron Letters</i> , 1990, 31, 5791-5794.	1.4	8
46	Polyenolates of Unsaturated Carboxylic Acids in Synthesis. Synthesis of Unsaturated $\hat{1},\hat{2}$ -Amino Acids and $\hat{2}$ -Hydrazing Acids. <i>Synthetic Communications</i> , 1991, 21, 1833-1839.	2.1	8
47	Dienediolates of Unsaturated Carboxylic Acids in Synthesis. Tandem Michael Dieckmann Synthesis of Substituted 2-Cyclohexenones. <i>Synthetic Communications</i> , 1991, 21, 1825-1831.	2.1	8
48	Title is missing!. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2003, 45, 241-249.	1.6	8
49	The role of the transfer group in the intramolecular [5+2] cycloadditions of substituted $\hat{2}$ -hydroxy- $\hat{3}$ -pyrones: a DFT analysis. <i>Journal of Physical Organic Chemistry</i> , 2005, 18, 610-615.	1.9	8
50	Synthesis, Optical Properties, and DNA Interaction of New Diquats Based on Triazolopyridines and Triazoloquinolines. <i>Chemistry - A European Journal</i> , 2017, 23, 12825-12832.	3.3	8
51	Experimental and theoretical push-pull Chemo- and regioselectivity in 1,3-Dipolar cycloaddition reactions: the case of benzotriazepin-5-one with mesitylnitrile oxide. <i>Journal of Physical Organic Chemistry</i> , 2007, 20, 245-254.	1.9	7
52	A theoretical study on NHC-catalysed enantioselective cycloaddition of ketenes and 3-arylcoumarins: mechanism and enantioselectivity. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 5474-5482.	2.8	6
53	SYNTHESE DE THIENO [2,3-a] QUINOLIZIDINES. Phosphorus, Sulfur and Silicon and the Related Elements, 1993, 85, 17-21.	1.6	5
54	Biphenyl Macrolactams as Colorimetric Sensors for Anions through Displacement Reactions. <i>Journal of Inclusion Phenomena and Macrocyclic Chemistry</i> , 2006, 54, 61-66.	1.6	5

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55	Iodine oxidative coupling of diene and triene-diolates of unsaturated carboxylic acids.. Tetrahedron, 1991, 47, 1997-2004.	1.9	4
56	Theoretical study on the mechanism of the domino reactions of tertiary $\beta$ -cyano-enamines and dimethyl acetylenedicarboxylate. Tetrahedron, 2001, 57, 169-177.	1.9	4
57	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.	2.5	4
58	Magnetochemical modulation of pre-organization processes in a 4,4'-dinitrobiphenyl azacrown macrocyclic lactam. Electrochemistry Communications, 2004, 6, 908-912.	4.7	3
59	A combined experimental and theoretical study of the alkylation of 3,5-dithio- $\epsilon$ [1,2,4]triazepines. Journal of Physical Organic Chemistry, 2008, 21, 457-463.	1.9	3
60	Unveiling the Ionic Diels-Alder Reactions within the Molecular Electron Density Theory. Molecules, 2021, 26, 3638.	3.8	3
61	Synthesis of Dienedioic and Tetraenedioic Acids by Oxidative Coupling of Unsaturated Carboxylic Acid Dienediolates by 1,2-Diiodoethane. Synthetic Communications, 1993, 23, 2827-2831.	2.1	2
62	Magnetochemical chemistry of 4,4'-bis(dimethylamino)biphenyl and 4,4'-dinitrobiphenyl azacrown macrocyclic lactams. Electrochimica Acta, 2005, 50, 4063-4075.	5.2	2
63	Empirical modeling of material composition and size in MOFs prepared with ligand mixtures. Dalton Transactions, 2019, 48, 2881-2885.	3.3	2
64	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.	3.0	1
65	The sonochemical barbier reaction applied to carboxylates. Study of a model case. Journal of the Chemical Society Chemical Communications, 1994, , 1815.	2.0	1
66	A new mechanism for internal nucleophilic substitution reactions. Organic and Biomolecular Chemistry, 2018, 16, 1101-1112.	2.8	1
67	Origin of the Synchronicity on the Transition Structures of Polar Diels-Alder Reactions. Are these Reactions [4 + 2] Processes?. ChemInform, 2003, 34, no.	0.0	0
68	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.	0.5	0
69	Unveiling the Intramolecular Ionic Diels-Alder Reactions within Molecular Electron Density Theory. Chemistry, 2021, 3, 834-853.	2.2	0
70	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