

Luis R Domingo

List of Publications by Year in Descending Order

Source: <https://exaly.com/author-pdf/3364276/luis-r-domingo-publications-by-year.pdf>

Version: 2024-04-27

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

354 papers	12,733 citations	52 h-index	99 g-index
386 ext. papers	14,263 ext. citations	3.3 avg, IF	7.13 L-index

#	Paper	IF	Citations
354	A Molecular Electron Density Theory Study of the Lewis Acid Catalyzed [3+2] Cycloaddition Reactions of Nitrones with Nucleophilic Ethylenes. <i>European Journal of Organic Chemistry</i> , 2022 , 2022,	3.2	3
353	Application of Reactivity Indices in the Study of Polar Diels-Alder Reactions 2022 , 481-502		3
352	A molecular electron density theory study of the higher-order cycloaddition reactions of tropone with electron-rich ethylenes. The role of the Lewis acid catalyst in the mechanism and pseudocyclic selectivity. <i>New Journal of Chemistry</i> , 2021 , 46, 294-308	3.6	0
351	Design, Synthesis, Chemical and Biochemical Insights Into Novel Hybrid Spirooxindole-Based p53-MDM2 Inhibitors With Potential Bcl2 Signaling Attenuation.. <i>Frontiers in Chemistry</i> , 2021 , 9, 735236 ⁵		7
350	Straightforward Regio- and Diastereoselective Synthesis, Molecular Structure, Intermolecular Interactions and Mechanistic Study of Spirooxindole-Engrafted Rhodanine Analogs. <i>Molecules</i> , 2021 , 26,	4.8	3
349	Unveiling the Substituent Effects in the Stereochemistry of [3+2] Cycloaddition Reactions of Aryl- and Alkyldiazomethylphosphonates with Norbornadiene within a MEDT Perspective. <i>ChemistrySelect</i> , 2021 , 6, 10722-10733	1.8	1
348	Theoretical Studies on the Mechanism of the Formation of Cyclopentadienes and Dihydropyridazines. <i>ChemistrySelect</i> , 2021 , 6, 9806-9813	1.8	
347	Quasi-RRHO approximation and DFT study for understanding the mechanism and kinetics of nitration reaction of benzonitrile with nitronium ion. <i>Computational and Theoretical Chemistry</i> , 2021 , 1199, 113209	2	1
346	Unveiling the Chemo- and Regioselectivity of the [3+2] Cycloaddition Reaction between 4-Chlorobenzonitrile Oxide and β -Aminocinnamitrile with a MEDT Perspective**. <i>ChemistrySelect</i> , 2021 , 6, 4521-4532	1.8	4
345	Unveiling the Ionic Diels-Alder Reactions within the Molecular Electron Density Theory. <i>Molecules</i> , 2021 , 26,	4.8	1
344	Divulging the various chemical reactivity of trifluoromethyl-4-vinyl-benzene as well as methyl-4-vinyl-benzene in [3+2] cycloaddition reactions. <i>Journal of Molecular Graphics and Modelling</i> , 2021 , 102, 107760	2.8	2
343	A molecular electron density theory study for [3 + 2] cycloaddition reactions of 1-pyrroline-1-oxide with disubstituted acetylenes leading to bicyclic 4-isoxazolines. <i>International Journal of Quantum Chemistry</i> , 2021 , 121, e26503	2.1	3
342	Unveiling the Unexpected Reactivity of Electrophilic Diazoalkanes in [3+2] Cycloaddition Reactions within Molecular Electron Density Theory. <i>Chemistry</i> , 2021 , 3, 74-93	2.1	5
341	Mpro-SARS-CoV-2 Inhibitors and Various Chemical Reactivity of 1-Bromo- and 1-Chloro-4-vinylbenzene in [3 + 2] Cycloaddition Reactions. <i>Organics</i> , 2021 , 2, 1-16	9	3
340	Unveiling the Different Reactivity of Bent and Linear Three-Atom-Components Participating in [3 + 2] Cycloaddition Reactions. <i>Organics</i> , 2021 , 2, 274-286	9	3
339	Closer Investigation of the Kinetics and Mechanism of Spirovinylcyclopropyl Oxindole Reaction with β -O by Topological Approaches and Unraveling the Role of the I Catalyst. <i>Journal of Physical Chemistry A</i> , 2021 , 125, 6913-6926	2.8	1
338	Understanding the Participation of Fluorinated Azomethine Ylides in Carbenoid-Type [3 + 2] Cycloaddition Reactions with Ynal Systems: A Molecular Electron Density Theory Study. <i>Journal of Organic Chemistry</i> , 2021 , 86, 12644-12653	4.2	5

337	Unveiling the Intramolecular Ionic Diels-Alder Reactions within Molecular Electron Density Theory. <i>Chemistry</i> , 2021 , 3, 834-853	2.1	
336	Understanding the different reactivity of (-)- and (+)-thiostyrenes in [3+2] cycloaddition reactions. An MEDT study.. <i>RSC Advances</i> , 2021 , 11, 9698-9708	3.7	1
335	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	3.6	2
334	The catalytic effects of a thiazolium salt in the oxa-Diels-Alder reaction between benzaldehyde and Danishefsky's diene: a molecular electron density theory study. <i>Organic and Biomolecular Chemistry</i> , 2021 , 19, 9306-9317	3.9	
333	Synthesis of Spirooxindole Analogs Tethered Pyrazole Scaffold as Acetylcholinesterase Inhibitors. <i>ChemistrySelect</i> , 2021 , 6, 14039-14053	1.8	2
332	Understanding the Reactivity of Trimethylsilyldiazoalkanes Participating in [3+2] Cycloaddition Reactions towards Diethylfumarate with a Molecular Electron Density Theory Perspective. <i>Organics</i> , 2020 , 1, 3-18	9	3
331	Atmospheric Oxidation Reactions of Methyl Salicylate as Green Leaf Volatiles by OH Radical: Theoretical Kinetics and Mechanism. <i>ChemistrySelect</i> , 2020 , 5, 12535-12547	1.8	2
330	A Study of the Effects of the Lewis Acid Catalysts on Oxa-Diels-Alder Reactions through Molecular Electron Density Theory. <i>ChemistrySelect</i> , 2020 , 5, 5341-5348	1.8	5
329	Unveiling the Lewis Acid Catalyzed Diels-Alder Reactions Through the Molecular Electron Density Theory. <i>Molecules</i> , 2020 , 25,	4.8	20
328	Unveiling the Different Chemical Reactivity of Diphenyl Nitrilimine and Phenyl Nitrile Oxide in [3+2] Cycloaddition Reactions with (R)-Carvone through the Molecular Electron Density Theory. <i>Molecules</i> , 2020 , 25,	4.8	19
327	A molecular electron density theory study of the [3 + 2] cycloaddition reaction of 1,4-diphosphorinium-3-olates with methyl acrylate and methyl methacrylate. <i>Theoretical Chemistry Accounts</i> , 2020 , 139, 1	1.9	0
326	A molecular electron density theory study of the Grignard reagent-mediated regioselective direct synthesis of 1,5-disubstituted-1,2,3-triazoles. <i>Journal of Physical Organic Chemistry</i> , 2020 , 33, e4062	2.1	16
325	A molecular electron density theory investigation of the molecular mechanism, regioselectivity, stereoselectivity and chemoselectivity of cycloaddition reaction between acetonitrile N-oxide and 2,5-dimethyl-2H-[1,2,3]diazarsole. <i>Theoretical Chemistry Accounts</i> , 2020 , 139, 1	1.9	6
324	Unravelling the kinetics and molecular mechanism of the degenerate Cope rearrangement of bullvalene. <i>New Journal of Chemistry</i> , 2020 , 44, 6543-6552	3.6	6
323	A molecular electron density theory study of the participation of tetrazines in aza-Diels-Alder reactions.. <i>RSC Advances</i> , 2020 , 10, 15394-15405	3.7	57
322	Molecular Electron Density Theory: A New Theoretical Outlook on Organic Chemistry 2020 , 174-227		7
321	A molecular electron density theory (MEDT) study of the role of halogens (X ₂ = F ₂ , Cl ₂ , Br ₂ and I ₂) on the aza-Michael-addition reactions. <i>New Journal of Chemistry</i> , 2020 , 44, 19002-19012	3.6	4
320	A molecular electron density theory study of the enhanced reactivity of aza aromatic compounds participating in Diels-Alder reactions. <i>Organic and Biomolecular Chemistry</i> , 2020 , 18, 292-304	3.9	19

319	Unveiling the Reactivity of Cyclic Azomethine Ylides in [3+2] Cycloaddition Reactions within the Molecular Electron Density Theory. <i>European Journal of Organic Chemistry</i> , 2020 , 2020, 5938-5948	3.2	29
318	Unveiling the high reactivity of strained dibenzocyclooctyne in [3 + 2] cycloaddition reactions with diazoalkanes through the molecular electron density theory. <i>Journal of Physical Organic Chemistry</i> , 2020 , 33, e4100	2.1	8
317	Calculation of the rate constants for hydrogen abstraction reactions by Hydroperoxyl radical from Methanol, and the investigation of stability of CH ₃ OH.HO ₂ complex. <i>Computational and Theoretical Chemistry</i> , 2020 , 1190, 113010	2	1
316	Understanding the Origin of the Regioselectivity in Non-Polar [3+2] Cycloaddition Reactions through the Molecular Electron Density Theory. <i>Organics</i> , 2020 , 1, 19-35	9	8
315	Unveiling the high reactivity of benzyne in the formal [3+2] cycloaddition reactions towards thioamides through the Molecular Electron Density Theory. <i>Tetrahedron</i> , 2020 , 76, 131458	2.4	6
314	Unravelling the strain-promoted [3+2] cycloaddition reactions of phenyl azide with cycloalkynes from the molecular electron density theory perspective. <i>New Journal of Chemistry</i> , 2020 , 44, 13633-13643	2.6	13
313	Understanding the Influence of the Trifluoromethyl Group on the Selectivities of the [3+2] Cycloadditions of Thiocarbonyl S-methanides with α,β -Unsaturated Ketones. A MEDT study. <i>ChemistrySelect</i> , 2020 , 5, 12791-12806	1.8	4
312	Lithium Cation-Catalyzed Benzene Diels-Alder Reaction: Insights on the Molecular Mechanism Within the Molecular Electron Density Theory. <i>Journal of Organic Chemistry</i> , 2020 , 85, 13121-13132	4.2	7
311	Unraveling the kinetics and molecular mechanism of gas phase pyrolysis of cubane to [8]annulene.. <i>RSC Advances</i> , 2020 , 10, 32730-32739	3.7	0
310	Deciphering the Mechanism of Silver Catalysis of Click Chemistry in Water by Combining Experimental and MEDT Studies. <i>Catalysts</i> , 2020 , 10, 956	4	5
309	A Close Look to the Oxaphosphetane Formation along the Wittig Reaction: A [2+2] Cycloaddition?. <i>Journal of Organic Chemistry</i> , 2020 , 85, 6675-6686	4.2	15
308	A molecular electron density theory study of the mechanism, chemo- and stereoselectivity of the epoxidation reaction of -carvone with peracetic acid.. <i>RSC Advances</i> , 2019 , 9, 28500-28509	3.7	5
307	Site-selectivity control in hetero-Diels-Alder reactions of methyldiene derivatives of lawsone through modification of the reactive carbonyl group: an experimental and theoretical study. <i>Organic and Biomolecular Chemistry</i> , 2019 , 17, 692-702	3.9	2
306	Unveiling the high reactivity of cyclohexynes in [3 + 2] cycloaddition reactions through the molecular electron density theory. <i>Organic and Biomolecular Chemistry</i> , 2019 , 17, 498-508	3.9	8
305	A molecular electron density theory study of the insertion of CO into frustrated Lewis pair boron-amidines: a [4 + 1] cycloaddition reaction. <i>Dalton Transactions</i> , 2019 , 48, 9214-9224	4.3	3
304	On the nature of organic electron density transfer complexes within molecular electron density theory. <i>Organic and Biomolecular Chemistry</i> , 2019 , 17, 6478-6488	3.9	6
303	An MEDT study of the mechanism and selectivities of the [3+2] cycloaddition reaction of tomentosin with benzonitrile oxide. <i>International Journal of Quantum Chemistry</i> , 2019 , 119, e25980	2.1	6
302	A molecular electron density theory study of the Lewis acid-catalyzed decomposition reaction of nitroethyl benzoate using aluminum derivatives. <i>Journal of Physical Organic Chemistry</i> , 2019 , 32, e3938	2.1	15

301	Understanding the domino reactions of alkyne-tethered N-tosylhydrazones yielding fused polycyclic pyrazoles. An MEDT study. <i>Tetrahedron</i> , 2019 , 75, 2807-2816	2.4	3
300	The carbenoid-type reactivity of simplest nitrile imine from a molecular electron density theory perspective. <i>Tetrahedron</i> , 2019 , 75, 1961-1967	2.4	18
299	A Molecular Electron Density Theory Study of the Chemoselectivity, Regioselectivity, and Diastereofacial Selectivity in the Synthesis of an Anticancer Spiroisoxazoline derived from Elantoin. <i>Molecules</i> , 2019 , 24,	4.8	21
298	An investigation of the molecular mechanism, chemoselectivity and regioselectivity of cycloaddition reaction between acetonitrile N-Oxide and 2,5-dimethyl-2H-[1,2,3]diazaphosphole: a MEDT study. <i>Journal of Chemical Sciences</i> , 2019 , 131, 1	1.8	3
297	Are one-step aromatic nucleophilic substitutions of non-activated benzenes concerted processes?. <i>Organic and Biomolecular Chemistry</i> , 2019 , 17, 8185-8193	3.9	8
296	Clicking Azides and Alkynes with Poly(pyrazolyl)borate-Copper(I) Catalysts: An Experimental and Computational Study. <i>Catalysts</i> , 2019 , 9, 687	4	4
295	A Molecular Electron Density Theory Study of the Synthesis of Spirobipyrazolines through the Domino Reaction of Nitrilimines with Allenates. <i>Molecules</i> , 2019 , 24,	4.8	5
294	Understanding the Mechanism of Nitrobenzene Nitration with Nitronium Ion: A Molecular Electron Density Theory Study. <i>ChemistrySelect</i> , 2019 , 4, 13313-13319	1.8	5
293	Unravelling the Mysteries of the [3+2] Cycloaddition Reactions. <i>European Journal of Organic Chemistry</i> , 2019 , 2019, 267-282	3.2	102
292	Aziridination of Aromatic Aldimines Through Stabilized Ammonium Ylides: A Molecular Electron Density Theory Study. <i>European Journal of Organic Chemistry</i> , 2019 , 2019, 1605-1613	3.2	4
291	Structure, Reactivity, Nonlinear Optical Properties and Vibrational Study of 5-Thioxo-1,4-thiaolidin-3-one and 5-thioxo-1,4,2-thiazasolidin-3-one (Silicon vs. Carbon). A DFT Study. <i>Silicon</i> , 2019 , 11, 2135-2147	2.4	2
290	Participation of furoxan carbonitrile oxide in [3+2] cycloaddition reaction toward C≡N triple bond: a Molecular Electron Density Theory study of regioselectivity and mechanistic aspect. <i>Structural Chemistry</i> , 2019 , 30, 317-326	1.8	5
289	A molecular electron density theory study of the [3+2] cycloaddition reaction between an azomethine imine and electron deficient ethylenes. <i>Journal of Physical Organic Chemistry</i> , 2018 , 31, e3830	2.1	18
288	Understanding the mechanism and regioselectivity of the copper(i) catalyzed [3 + 2] cycloaddition reaction between azide and alkyne: a systematic DFT study.. <i>RSC Advances</i> , 2018 , 8, 7670-7678	3.7	44
287	Experimental and Theoretical MEDT Study of the Thermal [3+2] Cycloaddition Reactions of Aryl Azides with Alkyne Derivatives. <i>ChemistrySelect</i> , 2018 , 3, 1215-1223	1.8	7
286	A Molecular Electron Density Theory Study of the Reactivity and Selectivities in [3 + 2] Cycloaddition Reactions of C,N-Dialkyl Nitrones with Ethylene Derivatives. <i>Journal of Organic Chemistry</i> , 2018 , 83, 2182-2197	4.2	72
285	A combined experimental and theoretical study of the thermal [3+2] cycloaddition of carbonyl ylides with activated alkenes. <i>Journal of Molecular Structure</i> , 2018 , 1157, 276-287	3.4	7
284	A molecular electron density theory study of the chemo- and regioselective [3 + 2] cycloaddition reactions between trifluoroacetonitrile N-oxide and thioketones. <i>Chemical Physics</i> , 2018 , 501, 128-137	2.3	9

283	The Mysticism of Pericyclic Reactions: A Contemporary Rationalisation of Organic Reactivity Based on Electron Density Analysis. <i>European Journal of Organic Chemistry</i> , 2018 , 2018, 1107-1120	3.2	47
282	Does a fluorinated Lewis acid catalyst change the molecular mechanism of the decomposition process of nitroethyl carboxylates?. <i>Research on Chemical Intermediates</i> , 2018 , 44, 325-337	2.8	10
281	[3+2] Cycloaddition Reaction of C-Phenyl-N-methyl Nitron to Acyclic-Olefin-Bearing Electron-Donating Substituent: A Molecular Electron Density Theory Study. <i>ChemistrySelect</i> , 2018 , 3, 8373-8380	1.8	12
280	DFT exploration of [3 + 2] cycloaddition reaction of 1-phosphorinium-3-olate and 1-methylphosphorinium-3-olate with methyl methacrylate.. <i>RSC Advances</i> , 2018 , 8, 27406-27416	3.7	6
279	A Molecular Electron Density Theory Study of the Role of the Copper Metalation of Azomethine Ylides in [3 + 2] Cycloaddition Reactions. <i>Journal of Organic Chemistry</i> , 2018 , 83, 10959-10973	4.2	24
278	A Molecular Electron Density Theory Study of the Competitiveness of Polar Diels-Alder and Polar Alder-ene Reactions. <i>Molecules</i> , 2018 , 23,	4.8	9
277	Molecular Electron Density Theory Study of Fused Regioselectivity in the Intramolecular [3+2] Cycloaddition Reaction of Cyclic Nitrones. <i>ChemistrySelect</i> , 2018 , 3, 5412-5420	1.8	10
276	A molecular electron density theory study of the [3 + 2] cycloaddition reaction of nitrones with ketenes. <i>Organic and Biomolecular Chemistry</i> , 2017 , 15, 1618-1627	3.9	27
275	How does the global electron density transfer diminish activation energies in polar cycloaddition reactions? A Molecular Electron Density Theory study. <i>Tetrahedron</i> , 2017 , 73, 1718-1724	2.4	52
274	Steric interactions controlling the syn diastereofacial selectivity in the [3+2] cycloaddition reaction between acetonitrile oxide and 7-oxanorborn-5-en-2-ones: A molecular electron density theory study. <i>Journal of Physical Organic Chemistry</i> , 2017 , 30, e3710	2.1	18
273	Understanding the reaction mechanism of the Lewis acid (MgBr ₂)-catalysed [3+2] cycloaddition reaction between C-methoxycarbonyl nitron and 2-propen-1-ol: a DFT study. <i>Theoretical Chemistry Accounts</i> , 2017 , 136, 1	1.9	9
272	A molecular electron density theory study of the [3 + 2] cycloaddition reaction of nitrones with strained allenes. <i>RSC Advances</i> , 2017 , 7, 26879-26887	3.7	19
271	Copper(I)-catalysed regioselective synthesis of pyrazolo[5,1-c]-1,2,4-triazoles: A DFT mechanistic study. <i>Tetrahedron</i> , 2017 , 73, 4653-4662	2.4	4
270	Understanding the domino reaction between 1-diazopropan-2-one and 1,1-dinitroethylene. A molecular electron density theory study of the [3 + 2] cycloaddition reactions of diazoalkanes with electron-deficient ethylenes. <i>RSC Advances</i> , 2017 , 7, 15586-15595	3.7	17
269	Understanding the Intramolecular Diels-Alder Reactions of N-Substituted N-Allyl-Furfurylamines: An MEDT Study. <i>ChemistrySelect</i> , 2017 , 2, 9736-9743	1.8	1
268	Understanding the mechanism of the decomposition reaction of nitroethyl benzoate through the Molecular Electron Density Theory. <i>Theoretical Chemistry Accounts</i> , 2017 , 136, 1	1.9	10
267	A Molecular Electron Density Theory Study of the Reactivity of Azomethine Imine in [3+2] Cycloaddition Reactions. <i>Molecules</i> , 2017 , 22,	4.8	48
266	A DFT Study of the Conversion of Ptaquiloside, a Bracken Fern Carcinogen, to Pterosis B in Neutral and Acidic Aqueous Medium. <i>ChemistrySelect</i> , 2017 , 2, 8178-8186	1.8	1

265	A molecular electron density theory study of [3 + 2] cycloaddition reactions of chiral azomethine ylides with β -nitrostyrene. <i>Theoretical Chemistry Accounts</i> , 2017 , 136, 1	1.9	16
264	Understanding the reactivity and regioselectivity of [3 + 2] cycloaddition reactions between substituted nitrile oxides and methyl acrylate. A molecular electron density theory study. <i>International Journal of Quantum Chemistry</i> , 2017 , 117, e25451	2.1	21
263	Nitropyrroles, Diels-Alder reactions assisted by microwave irradiation and solvent effect. An experimental and theoretical study. <i>Journal of Molecular Structure</i> , 2017 , 1147, 155-160	3.4	10
262	Electrophilic activation of CO ₂ in cycloaddition reactions towards a nucleophilic carbenoid intermediate: new defying insights from the Molecular Electron Density Theory. <i>Theoretical Chemistry Accounts</i> , 2017 , 136, 1	1.9	6
261	A DFT study of the mechanism and selectivities of the [3+2] cycloaddition reaction between 3-(benzylideneamino)oxindole and trans- β -nitrostyrene. <i>Journal of Physical Organic Chemistry</i> , 2017 , 30, e3637	2.1	17
260	Aromaticity in Pericyclic Transition State Structures? A Critical Rationalisation Based on the Topological Analysis of Electron Density. <i>ChemistrySelect</i> , 2016 , 1, 6026-6039	1.8	14
259	A DFT study of [3+2] cycloaddition reactions of an azomethine imine with N-vinyl pyrrole and N-vinyl tetrahydroindole. <i>Journal of Molecular Graphics and Modelling</i> , 2016 , 70, 296-304	2.8	16
258	Understanding the carbenoid-type reactivity of nitrile ylides in [3+2] cycloaddition reactions towards electron-deficient ethylenes: a molecular electron density theory study. <i>Theoretical Chemistry Accounts</i> , 2016 , 135, 1	1.9	20
257	Understanding the stereoselectivity in Brønsted acid catalysed Povarov reactions generating cis/trans CF ₃ -substituted tetrahydroquinolines: a DFT study. <i>RSC Advances</i> , 2016 , 6, 17064-17073	3.7	13
256	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	3.7	6
255	Understanding the [2n+2n] reaction mechanism between a carbenoid intermediate and CO ₂ . <i>Molecular Physics</i> , 2016 , 114, 1374-1391	1.7	17
254	A new model for C–N bond formation processes derived from the Molecular Electron Density Theory in the study of the mechanism of [3+2] cycloaddition reactions of carbenoid nitrile ylides with electron-deficient ethylenes. <i>Tetrahedron</i> , 2016 , 72, 1524-1532	2.4	52
253	Analysis of mebendazole binding to its target biomolecule by laser flash photolysis. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2016 , 155, 1-6	6.7	6
252	A Theoretical Study of the Relationship between the Electrophilicity Index and Hammett Constant in [3+2] Cycloaddition Reactions of Aryl Azide/Alkyne Derivatives. <i>Molecules</i> , 2016 , 21,	4.8	5
251	Applications of the Conceptual Density Functional Theory Indices to Organic Chemistry Reactivity. <i>Molecules</i> , 2016 , 21,	4.8	475
250	Molecular Electron Density Theory: A Modern View of Reactivity in Organic Chemistry. <i>Molecules</i> , 2016 , 21,	4.8	218
249	Understanding the molecular mechanism of the [3 + 2] cycloaddition reaction of benzonitrile oxide toward electron-rich N-vinylpyrrole: a DFT study. <i>Journal of Physical Organic Chemistry</i> , 2016 , 29, 368-376	2.1	11
248	[3+2] Cycloaddition reaction of 1H-phosphorinium-3-olate and 1-methylphosphorinium-3-olate with methyl acrylate: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2016 , 1087, 36-47	2	2

247	An MEDT study of the carbenoid-type [3 + 2] cycloaddition reactions of nitrile ylides with electron-deficient chiral oxazolidinones. <i>Organic and Biomolecular Chemistry</i> , 2016 , 14, 10427-10436	3.9	13
246	Intrinsic relative nucleophilicity of indoles. <i>Theoretical Chemistry Accounts</i> , 2016 , 135, 1	1.9	5
245	A DFT study of the mechanism of NHC catalysed annulation reactions involving β -unsaturated acyl azoliums and β -naphthol. <i>Organic and Biomolecular Chemistry</i> , 2016 , 14, 8338-45	3.9	7
244	A mechanistic study of the participation of azomethine ylides and carbonyl ylides in [3+2] cycloaddition reactions. <i>Tetrahedron</i> , 2015 , 71, 1050-1057	2.4	18
243	A DFT study of the ionic [2+2] cycloaddition reactions of keteniminium cations with terminal acetylenes. <i>Tetrahedron</i> , 2015 , 71, 2421-2427	2.4	20
242	A bonding evolution theory study of the mechanism of [3+2] cycloaddition reactions of nitrones with electron-deficient ethylenes. <i>RSC Advances</i> , 2015 , 5, 58464-58477	3.7	43
241	A DFT study of the role of the Lewis acid catalysts in the [3 + 2] cycloaddition reaction of the electrophilic nitrone isomer of methyl glyoxylate oxime with nucleophilic cyclopentene. <i>RSC Advances</i> , 2015 , 5, 64098-64105	3.7	18
240	A DFT Study of Inter- and Intramolecular Aryne Ene Reactions. <i>European Journal of Organic Chemistry</i> , 2015 , 2015, 2826-2834	3.2	23
239	A computational and conceptual DFT study on the mechanism of hydrogen activation by novel frustrated Lewis pairs. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 10715-25	3.6	19
238	Understanding the role of the trifluoromethyl group in reactivity and regioselectivity in [3+2] cycloaddition reactions of enol acetates with nitrones. A DFT study. <i>Journal of Molecular Modeling</i> , 2015 , 21, 104	2	3
237	A Combined Experimental and Theoretical Study of the Ammonium Bifluoride Catalyzed Regioselective Synthesis of Quinoxalines and Pyrido[2,3-b]pyrazines. <i>Synthesis</i> , 2015 , 47, 2680-2689	2.9	11
236	Unravelling the mechanism of the ketene-imine Staudinger reaction. An ELF quantum topological analysis. <i>RSC Advances</i> , 2015 , 5, 37119-37129	3.7	22
235	Understanding the participation of 3-nitropyridine in polar Diels-Alder reactions. A DFT study. <i>Computational and Theoretical Chemistry</i> , 2015 , 1072, 37-42	2	12
234	A DFT study of the mechanism of Brønsted acid catalysed Povarov reactions. <i>Tetrahedron</i> , 2015 , 71, 9339-9345	2.4	13
233	Understanding the high reactivity of carbonyl compounds towards nucleophilic carbenoid intermediates generated from carbene isocyanides. <i>RSC Advances</i> , 2015 , 5, 84797-84809	3.7	17
232	Non-classical CH \cdots O hydrogen-bond determining the regio- and stereoselectivity in the [3 + 2] cycloaddition reaction of (Z)-C-phenyl-N-methylnitrone with dimethyl 2-benzylidenecyclopropane-1,1-dicarboxylate. A topological electron-density study. <i>RSC Advances</i> , 2015 , 5, 99299-99311	3.7	29
231	Polar Diels-Alder reactions using electrophilic nitrobenzothiophenes. A combined experimental and DFT study. <i>Journal of Molecular Structure</i> , 2015 , 1079, 47-53	3.4	21
230	Diels-Alderase Catalyzing the Cyclization Step in the Biosynthesis of Spinosyn A 2015 , 169-201		

229	Synthesis, molecular structure and stability of fused bicyclic 4,1,2,4-oxadiazoline Pt(II) complexes. <i>Polyhedron</i> , 2015 , 98, 55-63	2.7	7
228	Understanding the domino reaction between 3-chloroindoles and methyl coumalate yielding carbazoles. A DFT study. <i>Organic and Biomolecular Chemistry</i> , 2015 , 13, 2034-43	3.9	14
227	Efficient Synthesis of 5-Chalcogenyl-1,3-oxazin-2-ones by Chalcogen-Mediated Yne-Carbamate Cyclisation: An Experimental and Theoretical Study. <i>European Journal of Organic Chemistry</i> , 2015 , 2015, 1020-1027	3.2	11
226	A DFT study of the domino reactions between imidazole NHC, ketenimines and DMAD or MP acetylene derivatives yielding spiro-pyrroles. <i>Computational and Theoretical Chemistry</i> , 2014 , 1030, 25-32	2	4
225	Understanding the high reactivity of triazolinones in Diels-Alder reactions. A DFT study. <i>Journal of Molecular Modeling</i> , 2014 , 20, 2207	2	6
224	The mechanism of ionic Diels-Alder reactions. A DFT study of the oxa-Povarov reaction. <i>RSC Advances</i> , 2014 , 4, 16567-16577	3.7	22
223	Understanding the mechanisms of [3+2] cycloaddition reactions. The pseudoradical versus the zwitterionic mechanism. <i>Tetrahedron</i> , 2014 , 70, 1267-1273	2.4	83
222	A DFT study on the NHC catalysed Michael addition of enols to α,β -unsaturated acyl-azoliums. A base catalysed C-C bond-formation step. <i>Organic and Biomolecular Chemistry</i> , 2014 , 12, 895-904	3.9	28
221	Understanding the selectivity in the formation of β -lactams vs. γ -lactams in the Staudinger reactions of chloro-cyan-ketene with unsaturated imines. A DFT study. <i>RSC Advances</i> , 2014 , 4, 58559-58566	3.7	13
220	Understanding the mechanism of the Povarov reaction. A DFT study. <i>RSC Advances</i> , 2014 , 4, 25268	3.7	41
219	A new C-C bond formation model based on the quantum chemical topology of electron density. <i>RSC Advances</i> , 2014 , 4, 32415-32428	3.7	347
218	A quantum chemical topological analysis of the C-C bond formation in organic reactions involving cationic species. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 14108-15	3.6	12
217	Understanding the polar mechanism of the ene reaction. A DFT study. <i>Organic and Biomolecular Chemistry</i> , 2014 , 12, 7581-90	3.9	31
216	Complementarity of reaction force and electron localization function analyses of asynchronicity in bond formation in Diels-Alder reactions. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 6726-34	3.6	48
215	Theoretical studies on cycloaddition reactions. <i>Journal of Cheminformatics</i> , 2014 , 6,	8.6	78
214	Understanding the domino retro [3+2] cycloaddition/cyclization reaction of bicyclic isoxazolidines in the synthesis of spirocyclic alkaloids. A DFT study. <i>Journal of Molecular Modeling</i> , 2014 , 20, 2347	2	4
213	A DFT analysis of the participation of zwitterionic TACs in polar [3+2] cycloaddition reactions. <i>Tetrahedron</i> , 2014 , 70, 4519-4525	2.4	64
212	WHY DIELS-ALDER REACTIONS ARE NON-CONCERTED PROCESSES. <i>Journal of the Chilean Chemical Society</i> , 2014 , 59, 2615-2618	2.5	9

211	Tautomerism in pyridazin-3(2H)-one: a theoretical study using implicit/explicit solvation models. <i>Journal of Molecular Graphics and Modelling</i> , 2014 , 49, 47-54	2.8	16
210	On the nature of Parr functions to predict the most reactive sites along organic polar reactions. <i>Chemical Physics Letters</i> , 2013 , 582, 141-143	2.5	82
209	Experimental and theoretical studies on polar Diels-Alder reactions of 1-nitronaphthalene developed in ionic liquids. <i>RSC Advances</i> , 2013 , 3, 13825	3.7	8
208	A density functional theory study of the regio- and stereoselectivity of the 1,3-dipolar cycloaddition of C-methyl substituted pyrazinium-3-olates with methyl acrylate and methyl methacrylate. <i>Computational and Theoretical Chemistry</i> , 2013 , 1025, 58-66	2	5
207	Theoretical study on the molecular mechanism of the [5 + 2] vs. [4 + 2] cyclization mediated by Lewis acid in the quinone system. <i>Organic and Biomolecular Chemistry</i> , 2013 , 11, 8357-65	3.9	2
206	Understanding C-C bond formation in polar reactions. An ELF analysis of the Friedel-Crafts reaction between indoles and nitroolefins. <i>RSC Advances</i> , 2013 , 3, 7520	3.7	21
205	Synthesis of densely functionalised 5-halogen-1,3-oxazin-2-ones by halogen-mediated regioselective cyclisation of N-Cbz-protected propargylic amines: a combined experimental and theoretical study. <i>Chemistry - A European Journal</i> , 2013 , 19, 14852-60	4.8	23
204	Xanthone-photosensitized detoxification of the veterinary anthelmintic fenbendazole. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2013 , 264, 34-40	4.7	
203	Why do five-membered heterocyclic compounds sometimes not participate in polar Diels-Alder reactions?. <i>Journal of Organic Chemistry</i> , 2013 , 78, 2462-71	4.2	38
202	A DFT study of the [3 + 2] versus [4 + 2] cycloaddition reactions of 1,5,6-trimethylpyrazinium-3-olate with methyl methacrylate. <i>Journal of Organic Chemistry</i> , 2013 , 78, 1621-9	4.2	25
201	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. <i>RSC Advances</i> , 2013 , 3, 447-457	2.7	19
200	Understanding the local reactivity in polar organic reactions through electrophilic and nucleophilic Parr functions. <i>RSC Advances</i> , 2013 , 3, 1486-1494	3.7	471
199	Global and local reactivity indices for electrophilic/nucleophilic free radicals. <i>Organic and Biomolecular Chemistry</i> , 2013 , 11, 4350-8	3.9	97
198	Understanding the regioselectivity in hetero Diels-Alder reactions. An ELF analysis of the reaction between nitrosoethylene and 1-vinylpyrrolidine. <i>Tetrahedron</i> , 2013 , 69, 107-114	2.4	43
197	The triplet excited state of the bioactive compound thiabendazole. Characterization and suitability as reporter for cyclodextrin complexation. <i>Chemical Physics Letters</i> , 2012 , 525-526, 166-170	2.5	4
196	Nature of the ring-closure process along the rearrangement of octa-1,3,5,7-tetraene to cycloocta-1,3,5-triene from the perspective of the electron localization function and catastrophe theory. <i>Journal of Computational Chemistry</i> , 2012 , 33, 748-56	3.5	39
195	Oxetane ring enlargement through nucleophilic trapping of radical cations by acetonitrile. <i>Organic Letters</i> , 2012 , 14, 5700-3	6.2	8
194	Origin of the synchronicity in bond formation in polar Diels-Alder reactions: an ELF analysis of the reaction between cyclopentadiene and tetracyanoethylene. <i>Organic and Biomolecular Chemistry</i> , 2012 , 10, 3841-51	3.9	48

193	Computational Assessment of 1,3-Dipolar Cycloaddition of Nitrile Oxides with Ethene and [60]Fullerene. <i>Heterocycles</i> , 2012 , 84, 719	0.8	7
192	An ELF analysis of the C≡ bond formation step in the N-heterocyclic carbene-catalyzed hydroacylation of unactivated C≡ double bonds. <i>RSC Advances</i> , 2012 , 2, 7127	3.7	20
191	Azo-hydrazo conversion via [1,5]-hydrogen shifts. A combined experimental and theoretical study. <i>Tetrahedron</i> , 2012 , 68, 6902-6907	2.4	7
190	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	6
189	Electronic fluxes during Diels-Alder reactions involving 1,2-benzoquinones: mechanistic insights from the analysis of electron localization function and catastrophe theory. <i>Journal of Computational Chemistry</i> , 2012 , 33, 2400-11	3.5	21
188	Understanding local electrophilicity/nucleophilicity activation through a single reactivity difference index. <i>Organic and Biomolecular Chemistry</i> , 2012 , 10, 2855-61	3.9	46
187	Ionic liquids and microwave irradiation as synergistic combination for polar Diels-Alder reactions using properly substituted heterocycles as dienophiles. A DFT study related. <i>Tetrahedron Letters</i> , 2012 , 53, 6508-6511	2	17
186	The role of the trifluoromethyl group in reactivity and selectivity in polar cycloaddition reactions. A DFT study. <i>Tetrahedron</i> , 2012 , 68, 8457-8462	2.4	12
185	Experimental and theoretical study of the [3 + 2] cycloaddition of carbonyl ylides with alkynes. <i>Organic and Biomolecular Chemistry</i> , 2012 , 10, 8434-44	3.9	10
184	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	3.7	43
183	Ring splitting of azetidin-2-ones via radical anions. <i>Organic and Biomolecular Chemistry</i> , 2012 , 10, 7928-33.9	3.9	11
182	Scandium-Catalyzed Preparation of Cytotoxic 3-Functionalized Quinolin-2-ones: Regioselective Ring Enlargement of Isatins or Imino Isatins. <i>ChemPlusChem</i> , 2012 , 77, 563-569	2.8	21
181	Polar Diels-Alder Reactions Developed in a Protic Ionic Liquid: 3-Nitroindole as Dienophile. Theoretical Studies Using DFT Methods. <i>Letters in Organic Chemistry</i> , 2012 , 9, 691-695	0.6	11
180	Regio- and Stereoselectivity of the 1,3-Dipolar Cycloaddition of Pyridinium-3-olates and Pyrazinium-3-olates with Methyl Methacrylate: A Density Functional Theory Exploration. <i>Current Organic Chemistry</i> , 2012 , 16, 1711-1722	1.7	6
179	Understanding the Bond Formation in Hetero-Diels-Alder Reactions. An ELF Analysis of the Reaction of Nitroethylene with Dimethylvinylamine. <i>Current Organic Chemistry</i> , 2012 , 16, 2343-2351	1.7	17
178	On the catalytic effect of water in the intramolecular Diels-Alder reaction of quinone systems: a theoretical study. <i>Molecules</i> , 2012 , 17, 13687-703	4.8	14
177	Understanding the mechanism of the intramolecular stetter reaction. A DFT study. <i>Molecules</i> , 2012 , 17, 1335-53	4.8	30
176	Understanding the electronic reorganization along the nonpolar [3 + 2] cycloaddition reactions of carbonyl ylides. <i>Journal of Organic Chemistry</i> , 2011 , 76, 373-9	4.2	65

175	A combined experimental and theoretical study of the thermal cycloaddition of aryl azides with activated alkenes. <i>Organic and Biomolecular Chemistry</i> , 2011 , 9, 4295-305	3.9	28
174	Understanding the cooperative NHC/LA catalysis for stereoselective annulation reactions with homoenolates. A DFT study. <i>Organic and Biomolecular Chemistry</i> , 2011 , 9, 6616-22	3.9	41
173	Experimental and theoretical studies on the radical-cation-mediated imino-Diels-Alder reaction. <i>Organic Letters</i> , 2011 , 13, 5116-9	6.2	26
172	Describing the Molecular Mechanism of Organic Reactions by Using Topological Analysis of Electronic Localization Function. <i>Current Organic Chemistry</i> , 2011 , 15, 3566-3575	1.7	71
171	1,3-Dipolar cycloaddition of 1H-pyrazinium-3-olate and N1- and C-methyl substituted pyrazinium-3-olates with methyl acrylate: a density functional theory study. <i>Tetrahedron</i> , 2011 , 67, 8383-8391	2.4	7
170	The nucleophilicity N index in organic chemistry. <i>Organic and Biomolecular Chemistry</i> , 2011 , 9, 7168-75	3.9	318
169	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	2.1	69
168	Controlled rearrangement of lactam-tethered allenols with brominating reagents: a combined experimental and theoretical study on E versus E keto lactam formation. <i>Chemistry - A European Journal</i> , 2011 , 17, 11559-66	4.8	29
167	DFT study on the cycloreversion of thietane radical cations. <i>Journal of Physical Chemistry A</i> , 2011 , 115, 5443-8	2.8	4
166	Understanding the High Reactivity of the Azomethine Ylides in [3 + 2] Cycloaddition Reactions. <i>Letters in Organic Chemistry</i> , 2010 , 7, 432-439	0.6	99
165	Experimental and theoretical (DFT) characterization of the excited states and N-centered radical species derived from 2-aminobenzimidazole, the core substructure of a family of bioactive compounds. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 6608-13	3.4	5
164	Experimental and theoretical studies on the mechanism of photochemical hydrogen transfer from 2-aminobenzimidazole to α and β aromatic ketones. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 11920-6	3.4	14
163	Understanding the mechanism of non-polar Diels-Alder reactions. A comparative ELF analysis of concerted and stepwise diradical mechanisms. <i>Organic and Biomolecular Chemistry</i> , 2010 , 8, 5495-504	3.9	73
162	Understanding the mechanism of stereoselective synthesis of cyclopentenones via N-heterocyclic carbene catalyzed reactions of enals with enones. <i>Organic and Biomolecular Chemistry</i> , 2010 , 8, 4884-91	3.9	56
161	Quantitative characterization of group electrophilicity and nucleophilicity for intramolecular Diels-Alder reactions. <i>Organic and Biomolecular Chemistry</i> , 2010 , 8, 3678-83	3.9	18
160	Alkoxy-styryl DCDHF fluorophores. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 7768-71	3.6	11
159	General and Theoretical Aspects of the Metal Enolates 2010 ,		1
158	Invariance of electrophilicity of independent fragments. Application to intramolecular Diels-Alder reactions. <i>Chemical Physics Letters</i> , 2010 , 499, 272-277	2.5	6

157	Ring Expansion versus Cyclization in 4-Oxoazetidine-2- carbaldehydes Catalyzed by Molecular Iodine: Experimental and Theoretical Study in Concert. <i>Advanced Synthesis and Catalysis</i> , 2010 , 352, 1688-1700	5.6	37
156	The 1,3-dipolar cycloaddition of 1H-pyridinium-3-olate and 1-methylpyridinium-3-olate with methyl acrylate: a density functional theory study. <i>Tetrahedron</i> , 2010 , 66, 9187-9193	2.4	14
155	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		9
154	An Analysis of the Regioselectivity of 1,3-Dipolar Cycloaddition Reactions of Benzonitrile N-Oxides Based on Global and Local Electrophilicity and Nucleophilicity Indices. <i>European Journal of Organic Chemistry</i> , 2009 , 2009, 3036-3044	3.2	67
153	Formation of pyrazol-1,3,4-thiadiazoles through 1,3-dipolar cycloadditions of 3-thioxo-[1,2,4]-triazepin-5-one with nitrilimines: an experimental and computational study. <i>Journal of Physical Organic Chemistry</i> , 2009 , 22, 31-41	2.1	7
152	Understanding the stereo- and regioselectivities of the polar Diels-Alder reactions between 2-acetyl-1,4-benzoquinone and methyl substituted 1,3-butadienes: a DFT study. <i>Journal of Physical Organic Chemistry</i> , 2009 , 22, 578-584	2.1	8
151	Understanding the mechanism of the N-heterocyclic carbene-catalyzed ring-expansion of 4-formyl-lactams to succinimide derivatives. <i>Tetrahedron</i> , 2009 , 65, 3432-3440	2.4	55
150	Understanding the regio- and chemoselective polar [3+2] cycloaddition of the Padwa carbonyl ylides with methylene ketones. A DFT study. <i>Tetrahedron</i> , 2009 , 65, 4644-4651	2.4	31
149	A condensed-to-atom nucleophilicity index. An application to the director effects on the electrophilic aromatic substitutions. <i>Computational and Theoretical Chemistry</i> , 2009 , 895, 86-91		164
148	Understanding the influence of Lewis acids in the regioselectivity of the Diels-Alder reactions of 2-methoxy-5-methyl-1,4-benzoquinone: A DFT study. <i>Computational and Theoretical Chemistry</i> , 2009 , 902, 103-108		9
147	DFT study of the molecular mechanism of Lewis acid induced [4 + 3] cycloadditions of 2-alkylacroleins with cyclopentadiene. <i>Journal of Organic Chemistry</i> , 2009 , 74, 5934-40	4.2	23
146	DFT study on the molecular mechanism of the [4 + 2] cycloaddition between thiobenzophenone and arylalkenes via radical cations. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 5718-22	2.8	12
145	Understanding the mechanism of polar Diels-Alder reactions. <i>Organic and Biomolecular Chemistry</i> , 2009 , 7, 3576-83	3.9	346
144	Toward an understanding of the unexpected regioselective hetero-Diels-Alder reactions of asymmetric tetrazines with electron-rich ethylenes: a DFT study. <i>Journal of Organic Chemistry</i> , 2009 , 74, 2726-35	4.2	80
143	A combined experimental and theoretical study of the polar [3 + 2] cycloaddition of electrophilically activated carbonyl ylides with aldehydes and imines. <i>Journal of Organic Chemistry</i> , 2009 , 74, 2120-33	4.2	47
142	Understanding reaction mechanisms in organic chemistry from catastrophe theory applied to the electron localization function topology. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 7128-36	2.8	147
141	An understanding of the electrophilic/nucleophilic behavior of electro-deficient 2,3-disubstituted 1,3-butadienes in polar diels-alder reactions. A density functional theory study. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 4046-53	2.8	92
140	Understanding the reactivity of captodative ethylenes in polar cycloaddition reactions. A theoretical study. <i>Journal of Organic Chemistry</i> , 2008 , 73, 4615-24	4.2	671

139	Polar [3 + 2] cycloaddition of ketones with electrophilically activated carbonyl ylides. Synthesis of spirocyclic dioxolane indolinones. <i>Organic and Biomolecular Chemistry</i> , 2008 , 6, 3144-57	3.9	25
138	Understanding the participation of quadricyclane as nucleophile in polar [2sigma + 2sigma + 2pi] cycloadditions toward electrophilic pi molecules. <i>Journal of Organic Chemistry</i> , 2008 , 73, 8791-9	4.2	183
137	Unusual regioselectivity in the opening of epoxides by carboxylic acid enediolates. <i>Molecules</i> , 2008 , 13, 1303-11	4.8	4
136	A further exploration of a nucleophilicity index based on the gas-phase ionization potentials. <i>Computational and Theoretical Chemistry</i> , 2008 , 865, 68-72		293
135	A combined experimental and theoretical study of the alkylation of 3,5-dithio-[1,2,4]triazepines. <i>Journal of Physical Organic Chemistry</i> , 2008 , 21, 457-463	2.1	3
134	New highly asymmetric Henry reaction catalyzed by Cu(II) and a C(1)-symmetric aminopyridine ligand, and its application to the synthesis of miconazole. <i>Chemistry - A European Journal</i> , 2008 , 14, 4725-480	4.8	166
133	Mechanistic details of the domino reaction of nitronaphthalenes with the electron-rich dienes. A DFT study. <i>Computational and Theoretical Chemistry</i> , 2008 , 853, 68-76		25
132	A bibracchial lariat aza-crown ether as an abiotic catalyst of malonic acid enolization. <i>New Journal of Chemistry</i> , 2007 , 31, 2065	3.6	
131	Triplet reactivity and regio-/stereoselectivity in the macrocyclization of diastereomeric ketoprofen-quencher conjugates via remote hydrogen abstractions. <i>Journal of the American Chemical Society</i> , 2007 , 129, 7407-20	16.4	36
130	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, 4220-7	4.2	29
129	Chapter 9 The electrophilicity index in organic chemistry. <i>Theoretical and Computational Chemistry</i> , 2007 , 139-201		71
128	Understanding the role of the Lewis acid catalyst on the 1,3-dipolar cycloaddition of N-benzylideneaniline N-oxide with acrolein: a DFT study. <i>Tetrahedron</i> , 2007 , 63, 4464-4471	2.4	36
127	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. <i>Computational and Theoretical Chemistry</i> , 2007 , 811, 125-133		33
126	A comparative analysis of the electrophilicity of organic molecules between the computed IPs and EAs and the HOMO and LUMO energies. <i>Chemical Physics Letters</i> , 2007 , 438, 341-345	2.5	41
125	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	2.1	6
124	A DFT study of the asymmetric (S)-5-(pyrrolidin-2-yl)-1H-tetrazole catalyzed Michael addition of carbonyl compounds to nitroalkenes. <i>Tetrahedron: Asymmetry</i> , 2007 , 18, 157-164		30
123	Strain-Induced Electrophilicity in Small Cycloalkynes: A DFT Analysis of the Polar Cycloaddition of Cyclopentyne towards Enol Ethers. <i>European Journal of Organic Chemistry</i> , 2006 , 2006, 498-506	3.2	25
122	Towards an Understanding of the Polar Diels-Alder Reactions of Nitrosoalkenes with Enamines: A Theoretical Study. <i>European Journal of Organic Chemistry</i> , 2006 , 2006, 2570-2580	3.2	38

121	A DFT Study of the Molecular Mechanisms of the Nucleophilic Addition of Ester-Derived Lithium Enolates and Silyl Ketene Acetals to Nitrones: Effects of the Lewis Acid Catalyst. <i>European Journal of Organic Chemistry</i> , 2006 , 2006, 3464-3472	3.2	23
120	Exploring two-state reaction pathways in the photodimerization of cyclohexadiene. <i>ChemPhysChem</i> , 2006 , 7, 614-8	3.2	6
119	New findings on the Diels-Alder reactions. An analysis based on the bonding evolution theory. <i>Journal of Physical Chemistry A</i> , 2006 , 110, 13939-47	2.8	114
118	Better understanding of the ring-cleavage process of cyanocyclopropyl anionic derivatives. A theoretical study based on the electron localization function. <i>Journal of Organic Chemistry</i> , 2006 , 71, 754-62	4.2	24
117	1,3-Dipolar cycloadditions of electrophilically activated benzonitrile N-oxides. Polar cycloaddition versus oxime formation. <i>Journal of Organic Chemistry</i> , 2006 , 71, 9319-30	4.2	51
116	Highly diastereoselective one-pot synthesis of spiro[cyclopenta[a]indene-2,2'-indene]diones from 1-indanones and aromatic aldehydes. <i>Journal of Organic Chemistry</i> , 2006 , 71, 3464-71	4.2	15
115	Photogeneration and reactivity of 1,n-diphenyl-1,n-azabiradicals. <i>Journal of Organic Chemistry</i> , 2006 , 71, 4439-44	4.2	2
114	Mechanism of triplet photosensitized Diels-Alder Reaction between indoles and cyclohexadienes: theoretical support for an adiabatic pathway. <i>Journal of Organic Chemistry</i> , 2006 , 71, 6932-41	4.2	23
113	Towards an intrinsic nucleofugality scale: The leaving group (LG) ability in CH3LG model system. <i>Chemical Physics Letters</i> , 2006 , 420, 95-99	2.5	40
112	Experimental and theoretical study on the substitution reactions of aryl 2,4-dinitrophenyl carbonates with quinuclidines. <i>Tetrahedron</i> , 2006 , 62, 2555-2562	2.4	29
111	A DFT study of the Diels-Alder reaction between methyl acrolein derivatives and cyclopentadiene. Understanding the effects of Lewis acids catalysts based on sulfur containing boron heterocycles. <i>Tetrahedron</i> , 2006 , 62, 5502-5509	2.4	35
110	A DFT study for the formation of imidazo[1,2-c]pyrimidines through an intramolecular Michael addition. <i>Tetrahedron</i> , 2006 , 62, 10408-10416	2.4	9
109	Theoretical calculations on the cycloreversion of oxetane radical cations. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 2602-7	2.8	15
108	Toward an understanding of the catalytic role of hydrogen-bond donor solvents in the hetero-Diels-Alder reaction between acetone and butadiene derivative. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 10438-44	2.8	40
107	Intramolecular NH/pi complexes of 2-allylaniline derivatives in the ground and excited states. <i>Journal of Physical Chemistry A</i> , 2005 , 109, 1758-63	2.8	1
106	Density functional theory study of the 5-pyrrolidin-2-yltetrazole-catalyzed aldol reaction. <i>Tetrahedron: Asymmetry</i> , 2005 , 16, 2764-2770		35
105	Effect of electron-withdrawing substituents on the electrophilicity of carbonyl carbons. <i>Tetrahedron</i> , 2005 , 61, 417-422	2.4	29
104	Lewis acid induced [4+3] cycloadditions of 2-silyloxyacroleins. Insights on the mechanism from a DFT analysis. <i>Tetrahedron</i> , 2005 , 61, 7538-7545	2.4	18

103	A DFT study of the polar Diels-Alder reaction between 4-aza-6-nitrobenzofuroxan and cyclopentadiene. <i>Tetrahedron</i> , 2005 , 61, 7359-7365	2.4	54
102	Lewis Acid Induced [2+2] Cycloadditions of Silyl Enol Ethers with α,β -Unsaturated Esters: A DFT Analysis. <i>European Journal of Organic Chemistry</i> , 2005 , 2005, 3973-3979	3.2	13
101	Lewis Acid Mediated Domino Reaction between 2-Cyclohexenone and Methyl Azide [A DFT Study. <i>European Journal of Organic Chemistry</i> , 2005 , 2005, 4705-4709	3.2	16
100	High chemoselectivity of C=S dipolarophile in 1,3-dipolar cycloaddition of nitrilimines and 1,2,4-triazepin-5-one derivatives: experimental, theoretical and X-ray study. <i>Journal of Physical Organic Chemistry</i> , 2005 , 18, 522-528	2.1	8
99	The role of the transfer group in the intramolecular [5+2] cycloadditions of substituted Hydroxy-Epyrones: a DFT analysis. <i>Journal of Physical Organic Chemistry</i> , 2005 , 18, 610-615	2.1	6
98	Theoretical Studies on Domino Cycloaddition Reactions. <i>Mini-Reviews in Organic Chemistry</i> , 2005 , 2, 47-57.	2.7	12
97	A DFT Analysis of the Strain-Induced Regioselective [2+2] Cycloaddition of Benzyne Possessing Fused Four-Membered Ring. <i>Letters in Organic Chemistry</i> , 2005 , 2, 68-73	0.6	14
96	The nucleophilic addition of nitrones to carbonyl compounds: insights on the nature of the mechanism of the l-proline induced asymmetric reaction from a DFT analysis. <i>Tetrahedron: Asymmetry</i> , 2004 , 15, 1541-1549		17
95	Why do Electron-Deficient Dienes React Rapidly in Diels-Alder Reactions with Electron-Deficient Ethylenes? A Density Functional Theory Analysis. <i>European Journal of Organic Chemistry</i> , 2004 , 2004, 4788-4793	3.2	47
94	Understanding the nature of the molecular mechanisms associated with the competitive Lewis acid catalyzed [4+2] and [4+3] cycloadditions between arylidenoxazolone systems and cyclopentadiene: a DFT analysis. <i>Chemistry - A European Journal</i> , 2004 , 10, 4742-9	4.8	26
93	The domino reaction between 4,6-dinitrobenzofuroxan and cyclopentadiene. Insights on the nature of the molecular mechanism. <i>Computational and Theoretical Chemistry</i> , 2004 , 709, 45-52		35
92	A DFT study of the Huisgen 1,3-dipolar cycloaddition between hindered thiocarbonyl ylides and tetracyanoethylene. <i>Tetrahedron</i> , 2004 , 60, 5053-5058	2.4	56
91	Reactivity of the carbon-carbon double bond towards nucleophilic additions. A DFT analysis. <i>Tetrahedron</i> , 2004 , 60, 6585-6591	2.4	72
90	A theoretical study on the regioselectivity of 1,3-dipolar cycloadditions using DFT-based reactivity indexes. <i>Tetrahedron</i> , 2004 , 60, 11503-11509	2.4	128
89	Novel examples of the N-methyl effect on cyclisations of N-Boc derivatives of amino alcohols. A theoretical study. <i>Tetrahedron</i> , 2004 , 60, 12067-12073	2.4	5
88	Geometrical effects on the intramolecular quenching of π,π^* aromatic ketones by phenols and indoles. <i>Journal of Organic Chemistry</i> , 2004 , 69, 8618-25	4.2	19
87	Diels-Alder reaction between indoles and cyclohexadienes photocatalyzed by π,π aromatic ketones. <i>Organic Letters</i> , 2004 , 6, 3905-8	6.2	12
86	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, 3884-90	4.2	109

85	Photogeneration of o-quinone methides from o-cycloalkenylphenols. <i>Journal of Organic Chemistry</i> , 2003 , 68, 9643-7	4.2	11
84	A DFT study for the regioselective 1,3-dipolar cycloadditions of nitrile N-oxides toward alkynylboronates. <i>Tetrahedron</i> , 2003 , 59, 9167-9171	2.4	29
83	Diastereomeric differentiation in the quenching of excited states by hydrogen donors. <i>Angewandte Chemie - International Edition</i> , 2003 , 42, 2531-4	16.4	27
82	Experimental and theoretical investigations for the regio and stereoselective transformation of trans 1,2,3-trisubstituted aziridines into trans oxazolidin-2-ones. <i>Tetrahedron</i> , 2003 , 59, 677-683	2.4	23
81	Quantitative characterization of the global electrophilicity pattern of some reagents involved in 1,3-dipolar cycloaddition reactions. <i>Tetrahedron</i> , 2003 , 59, 3117-3125	2.4	257
80	Experimental and theoretical investigations for the tandem alkylation-isomerization reactions between unsaturated carboxylic acids and allyl halides. <i>Tetrahedron</i> , 2003 , 59, 6233-6239	2.4	20
79	Studies on the biosynthesis of paraherquamide A and VM99955. A theoretical study of intramolecular Diels-Alder cycloaddition. <i>Journal of Organic Chemistry</i> , 2003 , 68, 2895-902	4.2	37
78	Lewis acid-catalyzed [4 + 3] cycloaddition of 2-(trimethyl silyloxy)acrolein with furan. Insight on the nature of the mechanism from a DFT analysis. <i>Organic Letters</i> , 2003 , 5, 4117-20	6.2	36
77	Photoreaction between 2-benzoylthiophene and phenol or indole. <i>Journal of Organic Chemistry</i> , 2003 , 68, 5104-13	4.2	45
76	Enhancing reactivity of carbonyl compounds via hydrogen-bond formation. A DFT study of the hetero-Diels-Alder reaction between butadiene derivative and acetone in chloroform. <i>Journal of Organic Chemistry</i> , 2003 , 68, 8662-8	4.2	81
75	The Joint Use of Catastrophe Theory and Electron Localization Function to Characterize Molecular Mechanisms. A Density Functional Study of the Diels-Alder Reaction between Ethylene and 1,3-Butadiene. <i>Journal of Physical Chemistry A</i> , 2003 , 107, 6014-6024	2.8	134
74	Electronic contributions to the sigma(p) parameter of the Hammett equation. <i>Journal of Organic Chemistry</i> , 2003 , 68, 6060-2	4.2	70
73	Theozyme for antibody aldolases. Characterization of the transition-state analogue. <i>Organic and Biomolecular Chemistry</i> , 2003 , 1, 637-43	3.9	13
72	A DFT Study of the Molecular Mechanisms of the Diels-Alder Reaction between Cyclopentadiene and 3-Phenyl-1-(2-pyridyl)-2-propen-1-one [Role of the Zn ²⁺ Lewis Acid Catalyst and Water Solvent. <i>European Journal of Organic Chemistry</i> , 2002 , 2002, 2557	3.2	16
71	Density functional theory study of the mechanism of the proline-catalyzed intermolecular aldol reaction. <i>Theoretical Chemistry Accounts</i> , 2002 , 108, 232-239	1.9	82
70	Density functional theory study of the Lewis acid-catalyzed Diels-Alder reaction of nitroalkenes with vinyl ethers using aluminum derivatives. <i>Journal of Physical Organic Chemistry</i> , 2002 , 15, 660-666	2.1	46
69	An AM1 theoretical study on the effect of Zn ²⁺ Lewis acid catalysis on the mechanism of the cycloaddition between 3-phenyl-1-(2-pyridyl)-2-propen-1-one and cyclopentadiene. <i>Tetrahedron</i> , 2002 , 58, 2695-2700	2.4	14
68	A density functional theory study for the Diels-Alder reaction between N-acyl-1-aza-1,3-butadienes and vinylamines. Lewis acid catalyst and solvent effects. <i>Tetrahedron</i> , 2002 , 58, 3765-3774	2.4	78

67	Quantitative characterization of the global electrophilicity power of common diene/dienophile pairs in Diels-Alder reactions. <i>Tetrahedron</i> , 2002 , 58, 4417-4423	2.4	652
66	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	2.8	313
65	Density Functional Theory Study for the Cycloaddition of 1,3-Butadienes with Dimethyl Acetylenedicarboxylate. Polar Stepwise vs Concerted Mechanisms. <i>Journal of Physical Chemistry A</i> , 2002 , 106, 952-961	2.8	72
64	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, 959-65	4.2	77
63	Theoretical study on the mechanism of the domino reactions of tertiary β -cyano-enamines and dimethyl acetylenedicarboxylate. <i>Tetrahedron</i> , 2001 , 57, 169-177	2.4	4
62	A theoretical study of the selectivity for the domino [5+2]/[4+2] cycloadditions of β -pyrones bearing tethered alkenes with substituted 1,3-butadienes. <i>Tetrahedron</i> , 2001 , 57, 5597-5606	2.4	4
61	Using theozymes for designing transition-state analogs for the intramolecular aldol reaction of β -diketones. <i>International Journal of Quantum Chemistry</i> , 2001 , 83, 338-347	2.1	5
60	A PM3 study of the molecular mechanism for the cycloaddition between cyclopentadiene and protonated pyridine-imine derivatives. <i>Computational and Theoretical Chemistry</i> , 2001 , 544, 79-90		5
59	A theoretical study of the molecular mechanism of the reaction between N,N-dimethylmethyleammonium cation and cyclopentadiene. <i>Journal of Organic Chemistry</i> , 2001 , 66, 3211-4	4.2	47
58	A Combined Experimental and Theoretical Study of the Homogeneous, Unimolecular Decomposition Kinetics of 3-Chloropivalic Acid in the Gas Phase. <i>Journal of Physical Chemistry A</i> , 2001 , 105, 1869-1875	2.8	4
57	A theoretical study of the reaction between cyclopentadiene and protonated imine derivatives: a shift from a concerted to a stepwise molecular mechanism. <i>Journal of Organic Chemistry</i> , 2001 , 66, 6151-7 ²	4.2	37
56	First synthesis of the chiral mixed O/S ligands, 1,2-sulfinyl thiols: application as chiral proton sources in enantioselective protonations of enolates. <i>Tetrahedron: Asymmetry</i> , 2000 , 11, 3481-3493		14
55	Toward an understanding of the mechanisms of the intramolecular. <i>Journal of Organic Chemistry</i> , 2000 , 65, 5480-6	4.2	18
54	A density functional theory study of the chemoselectivity and regioselectivity of the domino cycloaddition reactions of nitroalkenes with substituted alkenes. <i>Theoretical Chemistry Accounts</i> , 2000 , 104, 240-246	1.9	15
53	Toward an understanding of the selectivity in domino reactions. A DFT study of the reaction between acetylenedicarboxylic acid and 1, 3-Bis(2-furyl)propane. <i>Journal of Organic Chemistry</i> , 2000 , 65, 3473-7	4.2	18
52	A DFT study of the domino inter. <i>Journal of Organic Chemistry</i> , 2000 , 65, 1076-83	4.2	23
51	Stereoselective 1,3-dipolar cycloadditions of a chiral nitron derived from erythrulose. An experimental and DFT theoretical study. <i>Journal of Organic Chemistry</i> , 2000 , 65, 7000-9	4.2	61
50	Conjugate addition of organolithium reagents to α,β -unsaturated carboxylic acids. <i>Tetrahedron</i> , 1999 , 55, 815-830	2.4	16

49	Ring opening of cyclopropane in tricyclo[4.3.0.0 ^{2,9}]nonan-3-one with electrophile-nucleophile reagents. <i>Tetrahedron</i> , 1999 , 55, 847-860	2.4	3
48	A combined experimental and theoretical study of the unimolecular elimination kinetics of 2-alkoxypropionic acids in the gas phase. <i>Chemical Physics</i> , 1999 , 246, 1-12	2.3	24
47	Influence of Reactant Polarity on the Course of the Inverse-Electron-Demand Diels-Alder Reaction. A DFT Study of Regio- and Stereoselectivity, Presence of Lewis Acid Catalyst, and Inclusion of Solvent Effects in the Reaction between Nitroethene and Substituted Ethenes. <i>Journal of Organic Chemistry</i> , 1999 , 64, 5867-5875	4.2	122
46	PM3 study of the domino reaction of nitroalkenes with silyl enol ethers. <i>Journal of Physical Organic Chemistry</i> , 1999 , 12, 24-30	2.1	6
45	Theoretical study of the molecular mechanism of the domino pathways for squarate ester sequential reactions. <i>Journal of Physical Organic Chemistry</i> , 1999 , 12, 61-68	2.1	2
44	Domino reaction between 2-acylfurans and diethyl azodicarboxylate: a combined experimental, theoretical, X-ray and dynamic NMR study. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1999 , 73-80		6
43	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	2.8	31
42	Theoretical Study of the 1,3-Dipolar Cycloaddition Reactions of Azomethine Ylides. A DFT Study of Reaction between Trifluoromethyl Thiomethyl Azomethine Ylide and Acronitrile. <i>Journal of Organic Chemistry</i> , 1999 , 64, 3922-3929	4.2	65
41	Theoretical Study of the Mechanisms for the Alkoxyacetic Acids Decomposition. <i>Journal of Physical Chemistry A</i> , 1999 , 103, 3935-3943	2.8	33
40	Theoretical Study on the Molecular Mechanism of the Domino Cycloadditions between Dimethyl Acetylenedicarboxylate and Naphthaleno- and Anthracenofuranophane. <i>Journal of Organic Chemistry</i> , 1999 , 64, 3026-3033	4.2	8
39	Designing a Transition State Analogue for the Disfavored Intramolecular Michael Addition of 2-(2-Hydroxyethyl)acrylate Esters. <i>Journal of Organic Chemistry</i> , 1999 , 64, 9164-9169	4.2	3
38	Nonlocal (Pair Site) Reactivity from Second-Order Static Density Response Function: Gas- and Solution-Phase Reactivity of the Acetaldehyde Enolate as a Test Case. <i>Journal of Physical Chemistry A</i> , 1999 , 103, 1367-1375	2.8	43
37	A theoretical study on the decomposition mechanism of ϵ -propiolactone and ϵ -butyrolactone. <i>Chemical Physics Letters</i> , 1998 , 288, 261-269	2.5	7
36	Synthesis and characterization of molybdenum(VI)-dioxo complexes containing both coordinated thiolate and carboxylate groups. Reactions with their own free ligands. <i>Inorganica Chimica Acta</i> , 1998 , 268, 145-150	2.7	4
35	The tandem Diels-Alder reaction between acetylenedicarboxyaldehyde and N,N'-dipyrrolylmethane. An ab initio study of the molecular mechanisms. <i>Computational and Theoretical Chemistry</i> , 1998 , 426, 257-262		8
34	A theoretical study of the addition of CH ₃ MgCl to chiral β -alkoxy carbonyl compounds. <i>Computational and Theoretical Chemistry</i> , 1998 , 426, 263-275		3
33	Comparative theoretical study of transition structures, barrier heights, and reaction energies for the intramolecular tautomerization in acetaldehyde/vinyl alcohol and acetaldimine/vinylamine systems. <i>International Journal of Quantum Chemistry</i> , 1998 , 66, 9-24	2.1	28
32	Remarkable effect of lithium bromide in the enantioselective protonation with β -ulfinyl alcohols. <i>Tetrahedron Letters</i> , 1998 , 39, 3277-3280	2	25

31	Ground and excited-state intramolecular interactions in phenol-olefin bichromophoric compounds. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1998 , 2175-2180		9
30	Stereoselection Parameters and Theoretical Model in the Enantioselective Protonation of Enolates with β -Sulfinyl Alcohols. <i>Journal of Organic Chemistry</i> , 1998 , 63, 9342-9347	4.2	29
29	Toward an Understanding of the Molecular Mechanism of the Reaction between 1-Methylpyrrole and Dimethyl Acetylenedicarboxylate. An ab Initio Study. <i>Journal of Organic Chemistry</i> , 1998 , 63, 9183-9189	4.2	47
28	Toward an Understanding of Molecular Mechanism of Domino Cycloadditions. Density Functional Theory Study of the Reaction between Hexafluorobut-2-yne and N,N-Dipyrrolylmethane. <i>Journal of the American Chemical Society</i> , 1998 , 120, 1617-1618	16.4	59
27	Ab Initio Study of Stereo- and Regioselectivity in the Diels-Alder Reaction between 2-Phenylcyclopentadiene and β -(Methylthio)acrylonitrile. <i>Journal of Organic Chemistry</i> , 1997 , 62, 1775-1778	4.2	30
26	Theoretical Study of the Gas Phase Decomposition of Glycolic, Lactic, and 2-Hydroxyisobutyric Acids. <i>Journal of the American Chemical Society</i> , 1997 , 119, 6415-6422	16.4	49
25	Theoretical Study of the Elimination Kinetics of Carboxylic Acid Derivatives in the Gas Phase. Decomposition of 2-Chloropropionic Acid. <i>Journal of Physical Chemistry A</i> , 1997 , 101, 1859-1865	2.8	44
24	Biosynthesis of the Brevianamides. An ab Initio Study of the Biosynthetic Intramolecular Diels-Alder Cycloaddition. <i>Journal of Organic Chemistry</i> , 1997 , 62, 1662-1667	4.2	41
23	Diastereoselectivity of the reactions of organometallic reagents with protected d- and l-erythrose 1,3-O-ethylidene acetals. <i>Tetrahedron: Asymmetry</i> , 1997 , 8, 559-577		12
22	Potential energy surface for the decomposition of mandelic acid. <i>Chemical Physics Letters</i> , 1997 , 274, 422-428	2.5	32
21	On Transition Structures for Hydride Transfer Step in Enzyme Catalysis. A Comparative Study on Models of Glutathione Reductase Derived from Semiempirical, HF, and DFT Methods. <i>Journal of Organic Chemistry</i> , 1996 , 61, 7777-7783	4.2	20
20	Theoretical study of the reactions of 1-methyl-2-vinylpyrrole with methyl propiolate and with dimethyl acetylenedicarboxylate. <i>Computational and Theoretical Chemistry</i> , 1996 , 362, 209-213		4
19	Transition structure for hydride transfer from cyclopropene to azirinium cation. <i>Computational and Theoretical Chemistry</i> , 1996 , 363, 257-261		1
18	On Transition Structures for Hydride Transfer Step: A Theoretical Study of the Reaction Catalyzed by Dihydrofolate Reductase Enzyme. <i>Bioorganic Chemistry</i> , 1996 , 24, 10-18	5.1	30
17	Theoretical study of the solvent effects on the mechanisms of addition of dimethyl acetylenedicarboxylate to 1-methyl-2-vinylpyrrole. <i>Tetrahedron</i> , 1996 , 52, 10693-10704	2.4	30
16	Theoretical model of solvated lithium dienediolates of methyl substituted 2-butenic acids. <i>Tetrahedron</i> , 1996 , 52, 11105-11112	2.4	14
15	The tandem Diels-Alder reaction of dimethyl acetylenedicarboxylate to bicyclopentadiene. A theoretical study of the molecular mechanisms. <i>Tetrahedron Letters</i> , 1996 , 37, 7573-7576	2	8
14	Theoretical Study of the Reaction of Dimethyl Acetylenedicarboxylate with 1-Methyl-2-(1-substituted vinyl)pyrroles. <i>Tetrahedron</i> , 1995 , 51, 8739-8748	2.4	31

13	[MoO ₂ (SCPh ₂ CO ₂) ₂] ₂ and [MoO(SCPh ₂ CO ₂) ₂] ₂ anion complexes. A theoretical structure characterization. <i>Computational and Theoretical Chemistry</i> , 1995 , 339, 201-208		2
12	A theoretical study of the molecular mechanism for the oxidation of methanol by PQQ. <i>Journal of the American Chemical Society</i> , 1995 , 117, 8807-8815	16.4	22
11	Influence of conformational factors on acid-catalyzed cyclizations of germacranolides: Molecular structure of the cyclization products of gallicin and 8-hydroxygallicin (shonachalin a). <i>Liebigs Annalen</i> , 1995 , 1995, 1837-1841		13
10	Theoretical model of solvated lithium dienediolate of 2-butenic acid. <i>Tetrahedron</i> , 1995 , 51, 7207-7214	2.4	16
9	Transformation of resin abietic acid into a pregnane-type steroid. <i>Canadian Journal of Chemistry</i> , 1991 , 69, 379-382	0.9	3
8	CONVERSION OF RESIN ACIDS INTO STEROIDAL COMPOUNDS. A REVIEW. <i>Organic Preparations and Procedures International</i> , 1991 , 23, 321-356	1.1	6
7	¹³ C nuclear magnetic resonance spectra of several podocarpene and cassane diterpenoids. <i>Magnetic Resonance in Chemistry</i> , 1990 , 28, 529-532	2.1	3
6	Conversion of sandaracopimaric acid into an androstane analog steroid. <i>Journal of Organic Chemistry</i> , 1990 , 55, 2369-2373	4.2	13
5	Erythrophleum alkaloids. Synthesis of (±)-4-epi-cassamine. <i>Journal of the Chemical Society Perkin Transactions 1</i> , 1989 , 1875-1883		2
4	Conversion of dehydroabietic acid into 20-keto-C-aryl-18-norsteroids. Formation of the D ring. <i>Journal of Organic Chemistry</i> , 1988 , 53, 3761-3765	4.2	13
3	An approach to erythrophleum alkaloids. Synthesis of methyl (±)-4-epi-cassamate. <i>Tetrahedron Letters</i> , 1986 , 27, 3289-3292	2	5
2	Synthesis of (+)-podocarp-8(14)-en-13-one and methyl-(+)-13-oxo-podocarp-8(14)-en-18-oate from abietic acid. <i>Tetrahedron</i> , 1985 , 41, 4937-4940	2.4	47
1	Synthesis and anti-Cancer Activity of a New Hybrid Based Spirooxindole-Pyrrolidine -Thiochromene Scaffolds via [3 + 2] Cycloaddition Reaction: Computational Investigation. <i>Polycyclic Aromatic Compounds</i> , 1-19	1.3	0