Luis R Domingo

List of Publications by Citations

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	Understanding the reactivity of captodative ethylenes in polar cycloaddition reactions. A theoretical study. *Journal of Organic Chemistry*, **2008**, 73, 4615-24	4.2	671
353	Quantitative characterization of the global electrophilicity power of common diene/dienophile pairs in Diels□Alder reactions. *Tetrahedron*, **2002**, 58, 4417-4423	2.4	652
352	Applications of the Conceptual Density Functional Theory Indices to Organic Chemistry Reactivity. *Molecules*, **2016**, 21,	4.8	475
351	Understanding the local reactivity in polar organic reactions through electrophilic and nucleophilic Parr functions. *RSC Advances*, **2013**, 3, 1486-1494	3.7	471
350	A new C□□ bond formation model based on the quantum chemical topology of electron density. *RSC Advances*, **2014**, 4, 32415-32428	3.7	347
349	Understanding the mechanism of polar Diels-Alder reactions. *Organic and Biomolecular Chemistry*, **2009**, 7, 3576-83	3.9	346
348	The nucleophilicity N index in organic chemistry. *Organic and Biomolecular Chemistry*, **2011**, 9, 7168-75	3.9	318
347	Quantitative Characterization of the Local Electrophilicity of Organic Molecules. Understanding the Regioselectivity on Diels□Alder Reactions. *Journal of Physical Chemistry A*, **2002**, 106, 6871-6875	2.8	313
346	A further exploration of a nucleophilicity index based on the gas-phase ionization potentials. *Computational and Theoretical Chemistry*, **2008**, 865, 68-72		293
345	Quantitative characterization of the global electrophilicity pattern of some reagents involved in 1,3-dipolar cycloaddition reactions. *Tetrahedron*, **2003**, 59, 3117-3125	2.4	257
344	Molecular Electron Density Theory: A Modern View of Reactivity in Organic Chemistry. *Molecules*, **2016**, 21,	4.8	218
343	Understanding the participation of quadricyclane as nucleophile in polar [2sigma + 2sigma + 2pi] cycloadditions toward electrophilic pi molecules. *Journal of Organic Chemistry*, **2008**, 73, 8791-9	4.2	183
342	New highly asymmetric Henry reaction catalyzed by Cu(II) and a C(1)-symmetric aminopyridine ligand, and its application to the synthesis of miconazole. *Chemistry - A European Journal*, **2008**, 14, 4725-30	5.8	166
341	A condensed-to-atom nucleophilicity index. An application to the director effects on the electrophilic aromatic substitutions. *Computational and Theoretical Chemistry*, **2009**, 895, 86-91		164
340	Understanding reaction mechanisms in organic chemistry from catastrophe theory applied to the electron localization function topology. *Journal of Physical Chemistry A*, **2008**, 112, 7128-36	2.8	147
339	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. *Journal of Physical Chemistry A*, **2003**, 107, 6014-6024	2.8	134
338	A theoretical study on the regioselectivity of 1,3-dipolar cycloadditions using DFT-based reactivity indexes. *Tetrahedron*, **2004**, 60, 11503-11509	2.4	128

337	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. *Journal of Organic Chemistry*, **1999**, 64, 5867-5875	4.2	122
336	New findings on the Diels-Alder reactions. An analysis based on the bonding evolution theory. *Journal of Physical Chemistry A*, **2006**, 110, 13939-47	2.8	114
335	Origin of the synchronicity on the transition structures of polar Diels-Alder reactions. Are these reactions [4 + 2] processes?. *Journal of Organic Chemistry*, **2003**, 68, 3884-90	4.2	109
334	Unravelling the Mysteries of the [3+2] Cycloaddition Reactions. *European Journal of Organic Chemistry*, **2019**, 2019, 267-282	3.2	102
333	Understanding the High Reactivity of the Azomethine Ylides in [3 + 2] Cycloaddition Reactions. *Letters in Organic Chemistry*, **2010**, 7, 432-439	0.6	99
332	Global and local reactivity indices for electrophilic/nucleophilic free radicals. *Organic and Biomolecular Chemistry*, **2013**, 11, 4350-8	3.9	97
331	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. *Journal of Physical Chemistry A*, **2008**, 112, 4046-53	2.8	92
330	Understanding the mechanisms of [3+2] cycloaddition reactions. The pseudoradical versus the zwitterionic mechanism. *Tetrahedron*, **2014**, 70, 1267-1273	2.4	83
329	On the nature of Parr functions to predict the most reactive sites along organic polar reactions. *Chemical Physics Letters*, **2013**, 582, 141-143	2.5	82
328	Density functional theory study of the mechanism of the proline-catalyzed intermolecular aldol reaction. *Theoretical Chemistry Accounts*, **2002**, 108, 232-239	1.9	82
327	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. *Journal of Organic Chemistry*, **2003**, 68, 8662-8	4.2	81
326	Toward an understanding of the unexpected regioselective hetero-Diels-Alder reactions of asymmetric tetrazines with electron-rich ethylenes: a DFT study. *Journal of Organic Chemistry*, **2009**, 74, 2726-35	4.2	80
325	Theoretical studies on cycloaddition reactions. *Journal of Cheminformatics*, **2014**, 6,	8.6	78
324	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. *Tetrahedron*, **2002**, 58, 3765-3774	2.4	78
323	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?. *Journal of Organic Chemistry*, **2002**, 67, 959-65	4.2	77
322	Understanding the mechanism of non-polar Diels-Alder reactions. A comparative ELF analysis of concerted and stepwise diradical mechanisms. *Organic and Biomolecular Chemistry*, **2010**, 8, 5495-504	3.9	73
321	A Molecular Electron Density Theory Study of the Reactivity and Selectivities in [3 + 2] Cycloaddition Reactions of C,N-Dialkyl Nitrones with Ethylene Derivatives. *Journal of Organic Chemistry*, **2018**, 83, 2182-2197	4.2	72
320	Reactivity of the carbon–carbon double bond towards nucleophilic additions. A DFT analysis. *Tetrahedron*, **2004**, 60, 6585-6591	2.4	72

319	Density Functional Theory Study for the Cycloaddition of 1,3-Butadienes with Dimethyl Acetylenedicarboxylate. Polar Stepwise vs Concerted Mechanisms. *Journal of Physical Chemistry A*, **2002**, 106, 952-961	2.8	72
318	Describing the Molecular Mechanism of Organic Reactions by Using Topological Analysis of Electronic Localization Function. *Current Organic Chemistry*, **2011**, 15, 3566-3575	1.7	71
317	Chapter 9 The electrophilicity index in organic chemistry. *Theoretical and Computational Chemistry*, **2007**, 139-201		71
316	Electronic contributions to the sigma(p) parameter of the Hammett equation. *Journal of Organic Chemistry*, **2003**, 68, 6060-2	4.2	70
315	Understanding the kinetic solvent effects on the 1,3-dipolar cycloaddition of benzonitrile N-oxide: a DFT study. *Journal of Physical Organic Chemistry*, **2011**, 24, 611-618	2.1	69
314	An Analysis of the Regioselectivity of 1,3-Dipolar Cycloaddition Reactions of Benzonitrile N-Oxides Based on Global and Local Electrophilicity and Nucleophilicity Indices. *European Journal of Organic Chemistry*, **2009**, 2009, 3036-3044	3.2	67
313	Understanding the electronic reorganization along the nonpolar [3 + 2] cycloaddition reactions of carbonyl ylides. *Journal of Organic Chemistry*, **2011**, 76, 373-9	4.2	65
312	Theoretical Study of the 1,3-Dipolar Cycloaddition Reactions of Azomethine Ylides. A DFT Study of Reaction between Trifluoromethyl Thiomethyl Azomethine Ylide and Acronitrile. *Journal of Organic Chemistry*, **1999**, 64, 3922-3929	4.2	65
311	A DFT analysis of the participation of zwitterionic TACs in polar [3+2] cycloaddition reactions. *Tetrahedron*, **2014**, 70, 4519-4525	2.4	64
310	Stereoselective 1,3-dipolar cycloadditions of a chiral nitrone derived from erythrulose. An experimental and DFT theoretical study. *Journal of Organic Chemistry*, **2000**, 65, 7000-9	4.2	61
309	Toward an Understanding of Molecular Mechanism of Domino Cycloadditions. Density Functional Theory Study of the Reaction between Hexafluorobut-2-yne and N,N□Dipyrrolylmethane. *Journal of the American Chemical Society*, **1998**, 120, 1617-1618	16.4	59
308	A molecular electron density theory study of the participation of tetrazines in aza-Diels-Alder reactions.. *RSC Advances*, **2020**, 10, 15394-15405	3.7	57
307	Understanding the mechanism of stereoselective synthesis of cyclopentenes via N-heterocyclic carbene catalyzed reactions of enals with enones. *Organic and Biomolecular Chemistry*, **2010**, 8, 4884-91	3.9	56
306	A DFT study of the Huisgen 1,3-dipolar cycloaddition between hindered thiocarbonyl ylides and tetracyanoethylene. *Tetrahedron*, **2004**, 60, 5053-5058	2.4	56
305	Understanding the mechanism of the N-heterocyclic carbene-catalyzed ring-expansion of 4-formyl-□lactams to succinimide derivatives. *Tetrahedron*, **2009**, 65, 3432-3440	2.4	55
304	A DFT study of the polar Diels□Alder reaction between 4-aza-6-nitrobenzofuroxan and cyclopentadiene. *Tetrahedron*, **2005**, 61, 7359-7365	2.4	54
303	How does the global electron density transfer diminish activation energies in polar cycloaddition reactions? A Molecular Electron Density Theory study. *Tetrahedron*, **2017**, 73, 1718-1724	2.4	52
302	A new model for C□□ 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. *Tetrahedron*, **2016**, 72, 1524-1532	2.4	52

301	1,3-Dipolar cycloadditions of electrophilically activated benzonitrile N-oxides. Polar cycloaddition versus oxime formation. *Journal of Organic Chemistry*, **2006**, 71, 9319-30	4.2	51
300	Theoretical Study of the Gas Phase Decomposition of Glycolic, Lactic, and 2-Hydroxyisobutyric Acids. *Journal of the American Chemical Society*, **1997**, 119, 6415-6422	16.4	49
299	A Molecular Electron Density Theory Study of the Reactivity of Azomethine Imine in [3+2] Cycloaddition Reactions. *Molecules*, **2017**, 22,	4.8	48
298	Complementarity of reaction force and electron localization function analyses of asynchronicity in bond formation in Diels-Alder reactions. *Physical Chemistry Chemical Physics*, **2014**, 16, 6726-34	3.6	48
297	Origin of the synchronicity in bond formation in polar Diels-Alder reactions: an ELF analysis of the reaction between cyclopentadiene and tetracyanoethylene. *Organic and Biomolecular Chemistry*, **2012**, 10, 3841-51	3.9	48
296	The Mysticism of Pericyclic Reactions: A Contemporary Rationalisation of Organic Reactivity Based on Electron Density Analysis. *European Journal of Organic Chemistry*, **2018**, 2018, 1107-1120	3.2	47
295	A combined experimental and theoretical study of the polar [3 + 2] cycloaddition of electrophilically activated carbonyl ylides with aldehydes and imines. *Journal of Organic Chemistry*, **2009**, 74, 2120-33	4.2	47
294	Why do Electron-Deficient Dienes React Rapidly in Diels–Alder Reactions with Electron-Deficient Ethylenes? A Density Functional Theory Analysis. *European Journal of Organic Chemistry*, **2004**, 2004, 4788-4793	3.2	47
293	A theoretical study of the molecular mechanism of the reaction between N,N-dimethylmethyleneammonium cation and cyclopentadiene. *Journal of Organic Chemistry*, **2001**, 66, 3211-4	4.2	47
292	Toward an Understanding of the Molecular Mechanism of the Reaction between 1-Methylpyrrole and Dimethyl Acetylenedicarboxylate. An ab Initio Study. *Journal of Organic Chemistry*, **1998**, 63, 9183-9189	4.2	47
291	Synthesis of (+)-podocarp-8(14)-en-13-one and methyl-(+)-13-oxo-podocarp-8(14)-en-18-oate from abietic acid. *Tetrahedron*, **1985**, 41, 4937-4940	2.4	47
290	Understanding local electrophilicity/nucleophilicity activation through a single reactivity difference index. *Organic and Biomolecular Chemistry*, **2012**, 10, 2855-61	3.9	46
289	Density functional theory study of the Lewis acid-catalyzed Diels–Alder reaction of nitroalkenes with vinyl ethers using aluminum derivatives. *Journal of Physical Organic Chemistry*, **2002**, 15, 660-666	2.1	46
288	Photoreaction between 2-benzoylthiophene and phenol or indole. *Journal of Organic Chemistry*, **2003**, 68, 5104-13	4.2	45
287	Understanding the mechanism and regioselectivity of the copper(i) catalyzed [3 + 2] cycloaddition reaction between azide and alkyne: a systematic DFT study.. *RSC Advances*, **2018**, 8, 7670-7678	3.7	44
286	Theoretical Study of the Elimination Kinetics of Carboxylic Acid Derivatives in the Gas Phase. Decomposition of 2-Chloropropionic Acid. *Journal of Physical Chemistry A*, **1997**, 101, 1859-1865	2.8	44
285	A bonding evolution theory study of the mechanism of [3+2] cycloaddition reactions of nitrones with electron-deficient ethylenes. *RSC Advances*, **2015**, 5, 58464-58477	3.7	43
284	Understanding the origin of the asynchronicity in bond-formation in polar cycloaddition reactions. A DFT study of the 1,3-dipolar cycloaddition reaction of carbonyl ylides with 1,2-benzoquinones. *RSC Advances*, **2012**, 2, 1334-1342	3.7	43

283	Understanding the regioselectivity in hetero Diels–Alder reactions. An ELF analysis of the reaction between nitrosoethylene and 1-vinylpyrrolidine. *Tetrahedron*, **2013**, 69, 107-114	2.4	43
282	Nonlocal (Pair Site) Reactivity from Second-Order Static Density Response Function: Gas- and Solution-Phase Reactivity of the Acetaldehyde Enolate as a Test Case. *Journal of Physical Chemistry A*, **1999**, 103, 1367-1375	2.8	43
281	Understanding the mechanism of the Povarov reaction. A DFT study. *RSC Advances*, **2014**, 4, 25268	3.7	41
280	Understanding the cooperative NHC/LA catalysis for stereoselective annulation reactions with homoenolates. A DFT study. *Organic and Biomolecular Chemistry*, **2011**, 9, 6616-22	3.9	41
279	Biosynthesis of the Brevianamides. An ab Initio Study of the Biosynthetic Intramolecular Diels–Alder Cycloaddition. *Journal of Organic Chemistry*, **1997**, 62, 1662-1667	4.2	41
278	A comparative analysis of the electrophilicity of organic molecules between the computed IPs and EAs and the HOMO and LUMO energies. *Chemical Physics Letters*, **2007**, 438, 341-345	2.5	41
277	Toward an understanding of the catalytic role of hydrogen-bond donor solvents in the hetero-Diels-Alder reaction between acetone and butadiene derivative. *Journal of Physical Chemistry A*, **2005**, 109, 10438-44	2.8	40
276	Towards an intrinsic nucleofugality scale: The leaving group (LG) ability in CH3LG model system. *Chemical Physics Letters*, **2006**, 420, 95-99	2.5	40
275	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. *Journal of Computational Chemistry*, **2012**, 33, 748-56	3.5	39
274	Why do five-membered heterocyclic compounds sometimes not participate in polar Diels-Alder reactions?. *Journal of Organic Chemistry*, **2013**, 78, 2462-71	4.2	38
273	Towards an Understanding of the Polar Diels–Alder Reactions of Nitrosoalkenes with Enamines: A Theoretical Study. *European Journal of Organic Chemistry*, **2006**, 2006, 2570-2580	3.2	38
272	Ring Expansion versus Cyclization in 4-Oxoazetidine-2- carbaldehydes Catalyzed by Molecular Iodine: Experimental and Theoretical Study in Concert. *Advanced Synthesis and Catalysis*, **2010**, 352, 1688-1700	5.6	37
271	Studies on the biosynthesis of paraherquamide A and VM99955. A theoretical study of intramolecular Diels-Alder cycloaddition. *Journal of Organic Chemistry*, **2003**, 68, 2895-902	4.2	37
270	A theoretical study of the reaction between cyclopentadiene and protonated imine derivatives: a shift from a concerted to a stepwise molecular mechanism. *Journal of Organic Chemistry*, **2001**, 66, 6151-7	4.2	37
269	Triplet reactivity and regio-/stereoselectivity in the macrocyclization of diastereomeric ketoprofen-quencher conjugates via remote hydrogen abstractions. *Journal of the American Chemical Society*, **2007**, 129, 7407-20	16.4	36
268	Understanding the role of the Lewis acid catalyst on the 1,3-dipolar cycloaddition of N-benzylideneaniline N-oxide with acrolein: a DFT study. *Tetrahedron*, **2007**, 63, 4464-4471	2.4	36
267	Lewis acid-catalyzed [4 + 3] cycloaddition of 2-(trimethyl silyloxy)acrolein with furan. Insight on the nature of the mechanism from a DFT analysis. *Organic Letters*, **2003**, 5, 4117-20	6.2	36
266	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. *Tetrahedron*, **2006**, 62, 5502-5509	2.4	35

265	The domino reaction between 4,6-dinitrobenzofuroxan and cyclopentadiene. Insights on the nature of the molecular mechanism. *Computational and Theoretical Chemistry*, **2004**, 709, 45-52		35
264	Density functional theory study of the 5-pyrrolidin-2-yltetrazole-catalyzed aldol reaction. *Tetrahedron: Asymmetry*, **2005**, 16, 2764-2770		35
263	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		33
262	Theoretical Study of the Mechanisms for the Alkoxyacetic Acids Decomposition. *Journal of Physical Chemistry A*, **1999**, 103, 3935-3943	2.8	33
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260	Understanding the polar mechanism of the ene reaction. A DFT study. *Organic and Biomolecular Chemistry*, **2014**, 12, 7581-90	3.9	31
259	Understanding the regio- and chemoselective polar [3+2] cycloaddition of the Padwa carbonyl ylides with □methylene ketones. A DFT study. *Tetrahedron*, **2009**, 65, 4644-4651	2.4	31
258	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	2.8	31
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256	Understanding the mechanism of the intramolecular stetter reaction. A DFT study. *Molecules*, **2012**, 17, 1335-53	4.8	30
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254	A DFT study of the asymmetric (S)-5-(pyrrolidin-2-yl)-1H-tetrazole catalyzed Michael addition of carbonyl compounds to nitroalkenes. *Tetrahedron: Asymmetry*, **2007**, 18, 157-164		30
253	On Transition Structures for Hydride Transfer Step: A Theoretical Study of the Reaction Catalyzed by Dihydrofolate Reductase Enzyme. *Bioorganic Chemistry*, **1996**, 24, 10-18	5.1	30
252	Theoretical study of the solvent effects on the mechanisms of addition of dimethyl acetylenedicarboxylate to 1-methyl-2-vinylpyrrole. *Tetrahedron*, **1996**, 52, 10693-10704	2.4	30
251	Non-classical CH?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. *RSC Advances*, **2015**, 5, 99299-99311	3.7	29
250	Controlled rearrangement of lactam-tethered allenols with brominating reagents: a combined experimental and theoretical study on □versus □keto lactam formation. *Chemistry - A European Journal*, **2011**, 17, 11559-66	4.8	29
249	Toward an understanding of the acceleration of Diels-Alder reactions by a pseudo-intramolecular process achieved by molecular recognition. A DFT study. *Journal of Organic Chemistry*, **2007**, 72, 4220-7	4.2	29
248	Experimental and theoretical study on the substitution reactions of aryl 2,4-dinitrophenyl carbonates with quinuclidines. *Tetrahedron*, **2006**, 62, 2555-2562	2.4	29

247	A DFT study for the regioselective 1,3-dipolar cycloadditions of nitrile N-oxides toward alkynylboronates. *Tetrahedron*, **2003**, 59, 9167-9171	2.4	29
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243	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. *Organic and Biomolecular Chemistry*, **2014**, 12, 895-904	3.9	28
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241	Comparative theoretical study of transition structures, barrier heights, and reaction energies for the intramolecular tautomerization in acetaldehyde/vinyl alcohol and acetaldimine/vinylamine systems. *International Journal of Quantum Chemistry*, **1998**, 66, 9-24	2.1	28
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238	Experimental and theoretical studies on the radical-cation-mediated imino-Diels-Alder reaction. *Organic Letters*, **2011**, 13, 5116-9	6.2	26
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228	A DFT Study of Inter- and Intramolecular Aryne Ene Reactions. *European Journal of Organic Chemistry*, **2015**, 2015, 2826-2834	3.2	23
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226	DFT study of the molecular mechanism of Lewis acid induced [4 + 3] cycloadditions of 2-alkylacroleins with cyclopentadiene. *Journal of Organic Chemistry*, **2009**, 74, 5934-40	4.2	23
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222	A DFT study of the domino inter. *Journal of Organic Chemistry*, **2000**, 65, 1076-83	4.2	23
221	Unravelling the mechanism of the ketene-imine Staudinger reaction. An ELF quantum topological analysis. *RSC Advances*, **2015**, 5, 37119-37129	3.7	22
220	The mechanism of ionic Diels–Alder reactions. A DFT study of the oxa-Povarov reaction. *RSC Advances*, **2014**, 4, 16567-16577	3.7	22
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