

Marc Garcia-Borràs

List of Publications by Year in descending order

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79
papers

2,752
citations

126901

33
h-index

206102

48
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99
all docs

99
docs citations

99
times ranked

2952
citing authors

#	ARTICLE	IF	CITATIONS
1	Sponge-like molecular cage for purification of fullerenes. <i>Nature Communications</i> , 2014, 5, 5557.	12.8	162
2	A promiscuous cytochrome P450 aromatic O-demethylase for lignin bioconversion. <i>Nature Communications</i> , 2018, 9, 2487.	12.8	135
3	Role of Conformational Dynamics in the Evolution of Retro-Aldolase Activity. <i>ACS Catalysis</i> , 2017, 7, 8524-8532.	11.2	103
4	The role of aromaticity in determining the molecular structure and reactivity of (endohedral) Tj ETQq0 0 0 rgBT /OvgrJlock 10 Tf 50 622 T	38.1	97
5	Catalytic iron-carbene intermediate revealed in a cytochrome <i>c</i> carbene transferase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 7308-7313.	7.1	95
6	Computational tools for the evaluation of laboratory-engineered biocatalysts. <i>Chemical Communications</i> , 2017, 53, 284-297.	4.1	84
7	Regio- and Stereoselective Steroid Hydroxylation at C7 by Cytochrome...P450 Monooxygenase Mutants. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 12499-12505.	13.8	83
8	Electronic and Vibrational Nonlinear Optical Properties of Five Representative Electrides. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 2688-2697.	5.3	78
9	A Biocatalytic Platform for Synthesis of Chiral α -Trifluoromethylated Organoborons. <i>ACS Central Science</i> , 2019, 5, 270-276.	11.3	77
10	Pervasive cooperative mutational effects on multiple catalytic enzyme traits emerge via long-range conformational dynamics. <i>Nature Communications</i> , 2021, 12, 1621.	12.8	72
11	On the existence and characterization of molecular electrides. <i>Chemical Communications</i> , 2015, 51, 4865-4868.	4.1	68
12	Supramolecular Fullerene Sponges as Catalytic Masks for Regioselective Functionalization of C60. <i>Chem</i> , 2020, 6, 169-186.	11.7	65
13	Function and Structure of MalA/MalA ² , Iterative Halogenases for Late-Stage C-H Functionalization of Indole Alkaloids. <i>Journal of the American Chemical Society</i> , 2017, 139, 12060-12068.	13.7	56
14	Maximum Aromaticity as a Guiding Principle for the Most Suitable Hosting Cages in Endohedral Metallofullerenes. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 9275-9278.	13.8	55
15	The Exohedral Diels-Alder Reactivity of the Titanium Carbide Endohedral Metallofullerene Ti ₂ C ₂ @D _{3h} -C ₇₈ : Comparison with D _{3h} -C ₇₈ and M ₃ N@D _{3h} -C ₇₈ (M=Sc and Y) Reactivity. <i>Chemistry - A European Journal</i> , 2012, 18, 7141-7154.	3.3	54
16	Ambimodal Trispericyclic Transition State and Dynamic Control of Periselectivity. <i>Journal of the American Chemical Society</i> , 2019, 141, 1217-1221.	13.7	51
17	<i>In Vivo</i> Selection for Formate Dehydrogenases with High Efficiency and Specificity toward NADP ⁺ . <i>ACS Catalysis</i> , 2020, 10, 7512-7525.	11.2	51
18	Selective Enzymatic Oxidation of Silanes to Silanols. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 15507-15511.	13.8	48

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19	Dual-function enzyme catalysis for enantioselective carbon–nitrogen bond formation. <i>Nature Chemistry</i> , 2021, 13, 1166-1172.	13.6	48
20	Electrochemical control of the regioselectivity in the exohedral functionalization of C ₆₀ : the role of aromaticity. <i>Chemical Communications</i> , 2013, 49, 1220.	4.1	44
21	Enzyme-catalyzed cationic epoxide rearrangements in quinolone alkaloid biosynthesis. <i>Nature Chemical Biology</i> , 2017, 13, 325-332.	8.0	44
22	Mechanisms and Dynamics of Reactions Involving Entropic Intermediates. <i>Trends in Chemistry</i> , 2019, 1, 22-34.	8.5	44
23	Overriding Traditional Electronic Effects in Biocatalytic Baeyer–Villiger Reactions by Directed Evolution. <i>Journal of the American Chemical Society</i> , 2018, 140, 10464-10472.	13.7	43
24	Biosynthesis of Heptacyclic Duclauxins Requires Extensive Redox Modifications of the Phenalenone Aromatic Polyketide. <i>Journal of the American Chemical Society</i> , 2018, 140, 6991-6997.	13.7	42
25	Structural basis for stereoselective dehydration and hydrogen-bonding catalysis by the SAM-dependent pericyclase LepI. <i>Nature Chemistry</i> , 2019, 11, 812-820.	13.6	42
26	Enabling microbial syringol conversion through structure-guided protein engineering. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 13970-13976.	7.1	41
27	An Enzymatic Platform for Primary Amination of 1-Aryl-2-alkyl Alkynes. <i>Journal of the American Chemical Society</i> , 2022, 144, 80-85.	13.7	41
28	Enantiospecific <i>cis</i> – <i>trans</i> Isomerization in Chiral Fulleropyrrolidines: Hydrogen-Bonding Assistance in the Carbanion Stabilization in H ₂ O@C ₆₀ . <i>Journal of the American Chemical Society</i> , 2015, 137, 1190-1197.	13.7	40
29	Self-Assembled Tetragonal Prismatic Molecular Cage Highly Selective for Anionic I ⁻ Guests. <i>Chemistry - A European Journal</i> , 2013, 19, 1445-1456.	3.3	38
30	A Complete Guide on the Influence of Metal Clusters in the Diels–Alder Regioselectivity of <i>h</i> -C ₈₀ Endohedral Metallofullerenes. <i>Chemistry - A European Journal</i> , 2013, 19, 14931-14940.	3.3	37
31	The Regioselectivity of Bingel–Hirsch Cycloadditions on Isolated Pentagon Rule Endohedral Metallofullerenes. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 2374-2377.	13.8	37
32	Directed evolution of nonheme iron enzymes to access abiological radical-relay C(sp ³)–H azidation. <i>Science</i> , 2022, 376, 869-874.	12.6	36
33	Bis-1,3-dipolar Cycloadditions on Endohedral Fullerenes M ₃ N@Ih-C ₈₀ (M = Sc, Lu): Remarkable Endohedral-Cluster Regiochemical Control. <i>Journal of the American Chemical Society</i> , 2015, 137, 11775-11782.	13.7	34
34	Structural basis of the Cope rearrangement and cyclization in hapalindole biogenesis. <i>Nature Chemical Biology</i> , 2018, 14, 345-351.	8.0	34
35	Endohedral Metal-Induced Regioselective Formation of Bis-Prato Adduct of Y ₃ N@Ih-C ₈₀ and Gd ₃ N@Ih-C ₈₀ . <i>Journal of the American Chemical Society</i> , 2015, 137, 58-61.	13.7	33
36	Accessing Chemo- and Regioselective Benzylic and Aromatic Oxidations by Protein Engineering of an Unspecific Peroxygenase. <i>ACS Catalysis</i> , 2021, 11, 7327-7338.	11.2	31

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37	Metal Cluster Electrides: A New Type of Molecular Electride with Delocalised Polyattractor Character. <i>Chemistry - A European Journal</i> , 2018, 24, 9853-9859.	3.3	28
38	Diels-Alder and Retro-Diels-Alder Cycloadditions of (1,2,3,4,5-Pentamethyl)cyclopentadiene to $\text{La} @ \text{C}_{20}$: Regioselectivity and Product Stability. <i>Chemistry - A European Journal</i> , 2013, 19, 4468-4479.	3.3	27
39	Size-selective encapsulation of C_{60} and C_{60} -derivatives within an adaptable naphthalene-based tetragonal prismatic supramolecular nanocapsule. <i>Chemical Communications</i> , 2019, 55, 798-801.	4.1	27
40	Origin and Control of Chemoselectivity in Cytochrome <i>c</i> Catalyzed Carbene Transfer into Si-H and N-H bonds. <i>Journal of the American Chemical Society</i> , 2021, 143, 7114-7123.	13.7	27
41	Effect of incarcerated HF on the exohedral chemical reactivity of $\text{HF} @ \text{C}_{60}$. <i>Chemical Communications</i> , 2017, 53, 10993-10996.	4.1	26
42	Essential Factors for Control of the Equilibrium in the Reversible Rearrangement of $\text{M}_3\text{N} @ \text{Ih} @ \text{C}_{80}$ Fulleropyrrolidines: Exohedral Functional Groups versus Endohedral Metal Clusters. <i>Chemistry - A European Journal</i> , 2014, 20, 14032-14039.	3.3	25
43	Reaction Mechanism and Regioselectivity of the Bingel-Hirsch Addition of Dimethyl Bromomalonate to $\text{La} @ \text{C}_{20}$. <i>Chemistry - A European Journal</i> , 2016, 22, 5953-5962.	3.3	23
44	Machine Learning Enables Selection of Epistatic Enzyme Mutants for Stability Against Unfolding and Detrimental Aggregation. <i>ChemBioChem</i> , 2021, 22, 904-914.	2.6	22
45	Simultaneous screening of multiple substrates with an unspecific peroxygenase enabled modified alkane and alkene oxyfunctionalisations. <i>Catalysis Science and Technology</i> , 2021, 11, 6058-6064.	4.1	22
46	Aromaticity as the driving force for the stability of non-IPR endohedral metallofullerene Bingel-Hirsch adducts. <i>Chemical Communications</i> , 2013, 49, 8767.	4.1	21
47	Reactivity of Single-Walled Carbon Nanotubes in the Diels-Alder Cycloaddition Reaction: Distortion-Interaction Analysis along the Reaction Pathway. <i>Chemistry - A European Journal</i> , 2016, 22, 12819-12824.	3.3	21
48	Enzyme-Catalyzed Intramolecular Enantioselective Hydroalkoxylation. <i>Journal of the American Chemical Society</i> , 2017, 139, 3639-3642.	13.7	20
49	Molecular Basis of Iterative C-H Oxidation by TamI, a Multifunctional P450 Monooxygenase from the Tirandamycin Biosynthetic Pathway. <i>ACS Catalysis</i> , 2020, 10, 13445-13454.	11.2	20
50	Regio- and Stereoselective Steroid Hydroxylation at C7 by Cytochrome...P450 Monooxygenase Mutants. <i>Angewandte Chemie</i> , 2020, 132, 12599-12605.	2.0	19
51	The Unexplored Importance of Fleeting Chiral Intermediates in Enzyme-Catalyzed Reactions. <i>Journal of the American Chemical Society</i> , 2021, 143, 14939-14950.	13.7	19
52	The Frozen Cage Model: A Computationally Low-Cost Tool for Predicting the Exohedral Regioselectivity of Cycloaddition Reactions Involving Endohedral Metallofullerenes. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1671-1683.	5.3	18
53	Engineering P450 TamI as an Iterative Biocatalyst for Selective Late-Stage C-H Functionalization and Epoxidation of Tirandamycin Antibiotics. <i>ACS Catalysis</i> , 2021, 11, 8304-8316.	11.2	18
54	On the physical origins of interaction-induced vibrational (hyper)polarizabilities. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 22467-22477.	2.8	16

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55	Structures of Gd ₃ N@C ₈₀ Prato Bis-Adducts: Crystal Structure, Thermal Isomerization, and Computational Study. <i>Journal of the American Chemical Society</i> , 2019, 141, 10988-10993.	13.7	16
56	Exploring the origins of selectivity in soluble epoxide hydrolase from <i>Bacillus megaterium</i> . <i>Organic and Biomolecular Chemistry</i> , 2017, 15, 8827-8835.	2.8	14
57	Regioselective Synthesis and Characterization of Tris- and Tetra-Prato Adducts of M ₃ N@C ₈₀ (M = Y, Tj ETQq1 1 0.784314 rgBT /Over	13.7	14
58	Site-Selectivity of Prato Additions to C ₇₀ : Experimental and Theoretical Studies of a New Thermodynamic Product at the <i>dd</i> -[5,6]-Junction. <i>Organic Letters</i> , 2019, 21, 5162-5166.	4.6	13
59	Computational Protocol to Understand P450 Mechanisms and Design of Efficient and Selective Biocatalysts. <i>Frontiers in Chemistry</i> , 2018, 6, 663.	3.6	12
60	Thermodynamic consequences of Tyr to Trp mutations in the cation ⁺ -mediated binding of trimethyllysine by the HP1 chromodomain. <i>Chemical Science</i> , 2020, 11, 3495-3500.	7.4	12
61	Engineered P450 Atom-Transfer Radical Cyclases are Bifunctional Biocatalysts: Reaction Mechanism and Origin of Enantioselectivity. <i>Journal of the American Chemical Society</i> , 2022, 144, 13344-13355.	13.7	12
62	On the regioselectivity of the Diels ⁺ -Alder cycloaddition to C ₆₀ in high spin states. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 11577-11585.	2.8	10
63	A Full Dimensionality Approach to Evaluate the Nonlinear Optical Properties of Molecules with Large Amplitude Anharmonic Tunneling Motions. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 520-532.	5.3	9
64	The Regioselectivity of Bingel ⁺ -Hirsch Cycloadditions on Isolated Pentagon Rule Endohedral Metallofullerenes. <i>Angewandte Chemie</i> , 2016, 128, 2420-2423.	2.0	9
65	Selective Enzymatic Oxidation of Silanes to Silanols. <i>Angewandte Chemie</i> , 2020, 132, 15637-15641.	2.0	9
66	The key role of aromaticity in the structure and reactivity of C ₆₀ and endohedral metallofullerenes. <i>Inorganica Chimica Acta</i> , 2017, 468, 38-48.	2.4	8
67	Epoxide Hydrolase Conformational Heterogeneity for the Resolution of Bulky Pharmacologically Relevant Epoxide Substrates. <i>Chemistry - A European Journal</i> , 2018, 24, 12254-12258.	3.3	8
68	Exploring the molecular basis for substrate specificity in homologous macrolide biosynthetic cytochromes P450. <i>Journal of Biological Chemistry</i> , 2019, 294, 15947-15961.	3.4	8
69	Tautomerization and Dimerization of 6,13 ⁺ -Disubstituted Derivatives of Pentacene. <i>Chemistry - A European Journal</i> , 2017, 23, 6111-6117.	3.3	7
70	A shared mechanistic pathway for pyridoxal phosphate ⁺ -dependent arginine oxidases. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	7.1	7
71	Chapter 4. Computational Design of Protein Function. <i>Chemical Biology</i> , 0, , 87-107.	0.2	6
72	Computation of Nonlinear Optical Properties of Molecules with Large Amplitude Anharmonic Motions. III. Arbitrary Double-Well Potentials. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 236-242.	5.3	5

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73	Rationalizing the relative abundances of trimetallic nitride template-based endohedral metallofullerenes from aromaticity measures. <i>Chemical Communications</i> , 2017, 53, 4140-4143.	4.1	5
74	Understanding the Exohedral Functionalization of Endohedral Metallofullerenes Metallofullerenes. <i>Carbon Materials</i> , 2015, , 67-99.	1.2	0
75	(Invited) 1,3-Dipolar Cycloadditions on Endohedral Fullerenes M ₃ N@I _h -C ₈₀ (M = Sc-Gd): Remarkable Endohedral-Cluster Regiochemical Control. <i>ECS Meeting Abstracts</i> , 2016, , .	0.0	0
76	(Invited) The Regioselectivity of the Diels-Alder and Bingel-Hirsch Additions to La@C _{2v} -C ₈₂ . <i>ECS Meeting Abstracts</i> , 2016, , .	0.0	0
77	(Invited) Aromaticity, Cage Structure, and Relative Abundancy of Endohedral Metallofullerenes. <i>ECS Meeting Abstracts</i> , 2016, , .	0.0	0
78	(Invited) The Regioselectivity of Bingel-Hirsch Cycloadditions on IPR Endohedral Metallofullerenes. <i>ECS Meeting Abstracts</i> , 2016, , .	0.0	0
79	(Invited) Molecular Recognition and Assembly of Fullerene and Carbon-Based Materials with Biomolecules. <i>ECS Meeting Abstracts</i> , 2017, , .	0.0	0