Marc Garcia-BorrÃ s

List of Publications by Year
in descending order

79 papers	2,752 citations	126907 33 h-index	206112 48 g-index
99 all docs	99 docs citations	99 times ranked	2952 citing authors

#	Article	IF	Citations
1	Sponge-like molecular cage for purification of fullerenes. Nature Communications, 2014, 5, 5557.	12.8	162
2	A promiscuous cytochrome P450 aromatic O-demethylase for lignin bioconversion. Nature Communications, 2018, 9, 2487.	12.8	135
3	Role of Conformational Dynamics in the Evolution of Retro-Aldolase Activity. ACS Catalysis, 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 /Overlock 10 Tf 50 622 T	38.1	97
5	Catalytic iron-carbene intermediate revealed in a cytochrome c carbene transferase. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 7308-7313.	7.1	95
6	Computational tools for the evaluation of laboratory-engineered biocatalysts. Chemical Communications, 2017, 53, 284-297.	4.1	84
7	Regioâ€•and Stereoselective Steroid Hydroxylation at C7 by Cytochromeâ€…P450 Monooxygenase Mutants. Angewandte Chemie - International Edition, 2020, 59, 12499-12505.	13.8	83
8	Electronic and Vibrational Nonlinear Optical Properties of Five Representative Electrides. Journal of Chemical Theory and Computation, 2012, 8, 2688-2697.	5.3	78
9	A Biocatalytic Platform for Synthesis of Chiral Î±-Trifluoromethylated Organoborons. ACS Central Science, 2019, 5, 270-276.	11.3	77
10	Pervasive cooperative mutational effects on multiple catalytic enzyme traits emerge via long-range conformational dynamics. Nature Communications, 2021, 12, 1621.	12.8	72
11	On the existence and characterization of molecular electrides. Chemical Communications, 2015, 51, 4865-4868.	4.1	68
12	Supramolecular Fullerene Sponges as Catalytic Masks for Regioselective Functionalization of C60. CheM, 2020, 6, 169-186.	11.7	65
13	Function and Structure of MalA/MalAâ€², Iterative Halogenases for Late-Stage Câ€“H Functionalization of Indole Alkaloids. Journal of the American Chemical Society, 2017, 139, 12060-12068.	13.7	56
14	Maximum Aromaticity as a Guiding Principle for the Most Suitable Hosting Cages in Endohedral Metallofullerenes. Angewandte Chemie - International Edition, 2013, 52, 9275-9278.	13.8	55
15	The Exohedral Dielsâ€“Alder Reactivity of the Titanium Carbide Endohedral Metallofullerene Ti₂C₂@D₃h</sub>â€‘₇₈: Comparison with D₃h</sub>â€‘₇₈ and M₃N@D₃h</sub>â€‘₇₈ (M=Sc and Y) Reactivity. Chemistry - A European Journal, 2012, 18, 7141-7154.	3.3	54
16	Ambimodal Trispericyclic Transition State and Dynamic Control of Periselectivity. Journal of the American Chemical Society, 2019, 141, 1217-1221.	13.7	51
17	In Vivo Selection for Formate Dehydrogenases with High Efficiency and Specificity toward NADP⁺. ACS Catalysis, 2020, 10, 7512-7525.	11.2	51
18	Selective Enzymatic Oxidation of Silanes to Silanols. Angewandte Chemie - International Edition, 2020, 59, 15507-15511.	13.8	48

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19	Dual-function enzyme catalysis for enantioselective carbonâ€“nitrogen bond formation. Nature Chemistry, 2021, 13, 1166-1172.	13.6	48
20	Electrochemical control of the regioselectivity in the exohedral functionalization of C60: the role of aromaticity. Chemical Communications, 2013, 49, 1220.	4.1	44
21	Enzyme-catalyzed cationic epoxide rearrangements in quinolone alkaloid biosynthesis. Nature Chemical Biology, 2017, 13, 325-332.	8.0	44
22	Mechanisms and Dynamics of Reactions Involving Entropic Intermediates. Trends in Chemistry, 2019, 1, 22-34.	8.5	44
23	Overriding Traditional Electronic Effects in Biocatalytic Baeyerâ€“Villiger Reactions by Directed Evolution. Journal of the American Chemical Society, 2018, 140, 10464-10472.	13.7	43
24	Biosynthesis of Heptacyclic Duclauxins Requires Extensive Redox Modifications of the Phenalenone Aromatic Polyketide. Journal of the American Chemical Society, 2018, 140, 6991-6997.	13.7	42
25	Structural basis for stereoselective dehydration and hydrogen-bonding catalysis by the SAM-dependent pericyclase LepI. Nature Chemistry, 2019, 11, 812-820.	13.6	42
26	Enabling microbial syringol conversion through structure-guided protein engineering. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 13970-13976.	7.1	41
27	An Enzymatic Platform for Primary Amination of 1-Aryl-2-alkyl Alkynes. Journal of the American Chemical Society, 2022, 144, 80-85.	13.7	41
28	Enantiospecific cisâ€“trans Isomerization in Chiral Fulleropyrrolidines: Hydrogen-Bonding Assistance in the Carbanion Stabilization in H₂O@C₆₀. Journal of the American Chemical Society, 2015, 137, 1190-1197.	13.7	40
29	Selfâ€Assembled Tetragonal Prismatic Molecular Cage Highly Selective for Anionic Ï€ Guests. Chemistry - A European Journal, 2013, 19, 1445-1456.	3.3	38
30	A Complete Guide on the Influence of Metal Clusters in the Dielsâ€“Alder Regioselectivity of I_hâ€C₈₀ Endohedral Metallofullerenes. Chemistry - A European Journal, 2013, 19, 14931-14940.	3.3	37
31	The Regioselectivity of Bingelâ€“Hirsch Cycloadditions on Isolated Pentagon Rule Endohedral Metallofullerenes. Angewandte Chemie - International Edition, 2016, 55, 2374-2377.	13.8	37
32	Directed evolution of nonheme iron enzymes to access abiological radical-relay C(sp ³)â^'H azidation. Science, 2022, 376, 869-874.	12.6	36
33	Bis-1,3-dipolar Cycloadditions on Endohedral Fullerenes M3N@Ih-C80(M = Sc, Lu): Remarkable Endohedral-Cluster Regiochemical Control. Journal of the American Chemical Society, 2015, 137, 11775-11782.	13.7	34
34	Structural basis of the Cope rearrangement and cyclization in hapalindole biogenesis. Nature Chemical Biology, 2018, 14, 345-351.	8.0	34
35	Endohedral Metal-Induced Regioselective Formation of Bis-Prato Adduct of Y3N@Ih-C80 and Gd3N@Ih-C80. Journal of the American Chemical Society, 2015, 137, 58-61.	13.7	33
36	Accessing Chemo- and Regioselective Benzylic and Aromatic Oxidations by Protein Engineering of an Unspecific Peroxygenase. ACS Catalysis, 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. Chemistry - A European Journal, 2018, 24, 9853-9859.	3.3	28
38	Dielsâ€“Alder and Retroâ€Dielsâ€“Alder Cycloadditions of (1,2,3,4,5â€Pentamethyl)cyclopentadiene to La@C_{2v}â€C₈₂: Regioselectivity and Product Stability. Chemistry - A European Journal, 2013, 19, 4468-4479.	3.3	27
39	Size-selective encapsulation of C₆₀ and C₆₀-derivatives within an adaptable naphthalene-based tetragonal prismatic supramolecular nanocapsule. Chemical Communications, 2019, 55, 798-801.	4.1	27
40	Origin and Control of Chemoselectivity in Cytochrome c Catalyzed Carbene Transfer into Siâ€“H and Nâ€“H bonds. Journal of the American Chemical Society, 2021, 143, 7114-7123.	13.7	27
41	Effect of incarcerated HF on the exohedral chemical reactivity of HF@C₆₀. Chemical Communications, 2017, 53, 10993-10996.	4.1	26
42	Essential Factors for Control of the Equilibrium in the Reversible Rearrangement of M 3 N@ I h â€C 80 Fulleropyrrolidines: Exohedral Functional Groups versus Endohedral Metal Clusters. Chemistry - A European Journal, 2014, 20, 14032-14039.	3.3	25
43	Reaction Mechanism and Regioselectivity of the Bingelâ€“Hirsch Addition of Dimethyl Bromomalonate to La@C_{2v}â€C₈₂. Chemistry - A European Journal, 2016, 22, 5953-5962.	3.3	23
44	Machine Learning Enables Selection of Epistatic Enzyme Mutants for Stability Against Unfolding and Detrimental Aggregation. ChemBioChem, 2021, 22, 904-914.	2.6	22
45	Simultaneous screening of multiple substrates with an unspecific peroxygenase enabled modified alkane and alkene oxyfunctionalisations. Catalysis Science and Technology, 2021, 11, 6058-6064.	4.1	22
46	Aromaticity as the driving force for the stability of non-IPR endohedral metallofullerene Bingelâ€“Hirsch adducts. Chemical Communications, 2013, 49, 8767.	4.1	21
47	Reactivity of Singleâ€Walled Carbon Nanotubes in the Dielsâ€“Alder Cycloaddition Reaction: Distortionâ€“Interaction Analysis along the Reaction Pathway. Chemistry - A European Journal, 2016, 22, 12819-12824.	3.3	21
48	Enzyme-Catalyzed Intramolecular Enantioselective Hydroalkoxylation. Journal of the American Chemical Society, 2017, 139, 3639-3642.	13.7	20
49	Molecular Basis of Iterative Câ€“H Oxidation by TamI, a Multifunctional P450 Monooxygenase from the Tirandamycin Biosynthetic Pathway. ACS Catalysis, 2020, 10, 13445-13454.	11.2	20
50	Regioâ€•and Stereoselective Steroid Hydroxylation at C7 by Cytochromeâ€…P450 Monooxygenase Mutants. Angewandte Chemie, 2020, 132, 12599-12605.	2.0	19
51	The Unexplored Importance of Fleeting Chiral Intermediates in Enzyme-Catalyzed Reactions. Journal of the American Chemical Society, 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. Journal of Chemical Theory and Computation, 2012, 8, 1671-1683.	5.3	18
53	Engineering P450 TamI as an Iterative Biocatalyst for Selective Late-Stage Câ€“H Functionalization and Epoxidation of Tirandamycin Antibiotics. ACS Catalysis, 2021, 11, 8304-8316.	11.2	18
54	On the physical origins of interaction-induced vibrational (hyper)polarizabilities. Physical Chemistry Chemical Physics, 2016, 18, 22467-22477.	2.8	16

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55	Structures of Gd₃N@C₈₀ Prato Bis-Adducts: Crystal Structure, Thermal Isomerization, and Computational Study. Journal of the American Chemical Society, 2019, 141, 10988-10993.	13.7	16
56	Exploring the origins of selectivity in soluble epoxide hydrolase from Bacillus megaterium. Organic and Biomolecular Chemistry, 2017, 15, 8827-8835.	2.8	14
57	Regioselective Synthesis and Characterization of Tris- and Tetra-Prato Adducts of M3N@C80 (M = Y,) Tj ETQq1 1 0.784314 rgBT /Ove	13.7	14
58	Site-Selectivity of Prato Additions to C₇₀: Experimental and Theoretical Studies of a New Thermodynamic Product at the dd-[5,6]-Junction. Organic Letters, 2019, 21, 5162-5166.	4.6	13
59	Computational Protocol to Understand P450 Mechanisms and Design of Efficient and Selective Biocatalysts. Frontiers in Chemistry, 2018, 6, 663.	3.6	12
60	Thermodynamic consequences of Tyr to Trp mutations in the cationâ€“Ï€-mediated binding of trimethyllysine by the HP1 chromodomain. Chemical Science, 2020, 11, 3495-3500.	7.4	12
61	Engineered P450 Atom-Transfer Radical Cyclases are Bifunctional Biocatalysts: Reaction Mechanism and Origin of Enantioselectivity. Journal of the American Chemical Society, 2022, 144, 13344-13355.	13.7	12
62	On the regioselectivity of the Dielsâ€“Alder cycloaddition to C₆₀ in high spin states. Physical Chemistry Chemical Physics, 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. Journal of Chemical Theory and Computation, 2013, 9, 520-532.	5.3	9
64	The Regioselectivity of Bingelâ€“Hirsch Cycloadditions on Isolated Pentagon Rule Endohedral Metallofullerenes. Angewandte Chemie, 2016, 128, 2420-2423.	2.0	9
65	Selective Enzymatic Oxidation of Silanes to Silanols. Angewandte Chemie, 2020, 132, 15637-15641.	2.0	9
66	The key role of aromaticity in the structure and reactivity of C60 and endohedral metallofullerenes. Inorganica Chimica Acta, 2017, 468, 38-48.	2.4	8
67	Epoxide Hydrolase Conformational Heterogeneity for the Resolution of Bulky Pharmacologically Relevant Epoxide Substrates. Chemistry - A European Journal, 2018, 24, 12254-12258.	3.3	8
68	Exploring the molecular basis for substrate specificity in homologous macrolide biosynthetic cytochromes P450. Journal of Biological Chemistry, 2019, 294, 15947-15961.	3.4	8
69	Tautomerization and Dimerization of 6,13â€Disubstituted Derivatives of Pentacene. Chemistry - A European Journal, 2017, 23, 6111-6117.	3.3	7
70	A shared mechanistic pathway for pyridoxal phosphateâ€“dependent arginine oxidases. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	7
71	Chapter 4. Computational Design of Protein Function. Chemical Biology, 0, , 87-107.	0.2	6
72	Computation of Nonlinear Optical Properties of Molecules with Large Amplitude Anharmonic Motions. III. Arbitrary Double-Well Potentials. Journal of Chemical Theory and Computation, 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. Chemical Communications, 2017, 53, 4140-4143.	4.1	5
74	Understanding the Exohedral Functionalization of Endohedral Metallofullerenes Metallofullerenes. Carbon Materials, 2015, , 67-99.	1.2	0
75	(Invited) 1,3-Dipolar Cycloadditions on Endohedral Fullerenes M3N@I h -C80 (M = Sc-Gd): Remarkable Endohedral-Cluster Regiochemical Control. ECS Meeting Abstracts, 2016, , .	0.0	0
76	(Invited) The Regioselectivity of the Diels-Alder and Bingel-Hirsch Additions to La@C2v -C82. ECS Meeting Abstracts, 2016, , .	0.0	0
77	(Invited) Aromaticity, Cage Structure, and Relative Abundancy of Endohedral Metallofullerenes. ECS Meeting Abstracts, 2016, , .	0.0	0
78	(Invited) The Regioselectivity of Bingel-Hirsch Cycloadditions on IPR Endohedral Metallofullerenes. ECS Meeting Abstracts, 2016, , .	0.0	0
79	(Invited) Molecular Recognition and Assembly of Fullerene and Carbon-Based Materials with Biomolecules. ECS Meeting Abstracts, 2017, , .	0.0	0