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	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
2	Directed evolution of nonheme iron enzymes to access abiological radical-relay C(sp ³)âˆ’H azidation. Science, 2022, 376, 869-874.	12.6	36
3	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
4	Machine Learning Enables Selection of Epistatic Enzyme Mutants for Stability Against Unfolding and Detrimental Aggregation. ChemBioChem, 2021, 22, 904-914.	2.6	22
5	Pervasive cooperative mutational effects on multiple catalytic enzyme traits emerge via long-range conformational dynamics. Nature Communications, 2021, 12, 1621.	12.8	72
6	Origin and Control of Chemoselectivity in Cytochrome <i>c</i> Catalyzed Carbene Transfer into Siâ€“H and Nâ€“H bonds. Journal of the American Chemical Society, 2021, 143, 7114-7123.	13.7	27
7	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
8	Accessing Chemo- and Regioselective Benzylic and Aromatic Oxidations by Protein Engineering of an Unspecific Peroxygenase. ACS Catalysis, 2021, 11, 7327-7338.	11.2	31
9	The Unexplored Importance of Fleeting Chiral Intermediates in Enzyme-Catalyzed Reactions. Journal of the American Chemical Society, 2021, 143, 14939-14950.	13.7	19
10	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
11	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
12	Dual-function enzyme catalysis for enantioselective carbonâ€“nitrogen bond formation. Nature Chemistry, 2021, 13, 1166-1172.	13.6	48
13	Supramolecular Fullerene Sponges as Catalytic Masks for Regioselective Functionalization of C60. CheM, 2020, 6, 169-186.	11.7	65
14	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
15	<i>In Vivo</i> Selection for Formate Dehydrogenases with High Efficiency and Specificity toward NADP⁺. ACS Catalysis, 2020, 10, 7512-7525.	11.2	51
16	Selective Enzymatic Oxidation of Silanes to Silanols. Angewandte Chemie - International Edition, 2020, 59, 15507-15511.	13.8	48
17	Regioâ€•and Stereoselective Steroid Hydroxylation at C7 by Cytochromeâ€…P450 Monooxygenase Mutants. Angewandte Chemie - International Edition, 2020, 59, 12499-12505.	13.8	83
18	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

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19	Regioselective Synthesis and Characterization of Tris- and Tetra-Prato Adducts of M3N@C80 (M = Y,) Tj ETQq1 1 0.784314 rgBT /Overlo	13.7	14
20	Selective Enzymatic Oxidation of Silanes to Silanols. Angewandte Chemie, 2020, 132, 15637-15641.	2.0	9
21	Regioâ€•and Stereoselective Steroid Hydroxylation at C7 by Cytochromeâ€…P450 Monooxygenase Mutants. Angewandte Chemie, 2020, 132, 12599-12605.	2.0	19
22	Structural basis for stereoselective dehydration and hydrogen-bonding catalysis by the SAM-dependent pericyclase LepI. Nature Chemistry, 2019, 11, 812-820.	13.6	42
23	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
24	Exploring the molecular basis for substrate specificity in homologous macrolide biosynthetic cytochromes P450. Journal of Biological Chemistry, 2019, 294, 15947-15961.	3.4	8
25	A Biocatalytic Platform for Synthesis of Chiral <i>Î±-</i>Trifluoromethylated Organoborons. ACS Central Science, 2019, 5, 270-276.	11.3	77
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	Site-Selectivity of Prato Additions to C₇₀: Experimental and Theoretical Studies of a New Thermodynamic Product at the <i>dd</i>-[5,6]-Junction. Organic Letters, 2019, 21, 5162-5166.	4.6	13
28	Mechanisms and Dynamics of Reactions Involving Entropic Intermediates. Trends in Chemistry, 2019, 1, 22-34.	8.5	44
29	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
30	Ambimodal Trispericyclic Transition State and Dynamic Control of Periselectivity. Journal of the American Chemical Society, 2019, 141, 1217-1221.	13.7	51
31	Metal Cluster Electrides: A New Type of Molecular Electride with Delocalised Polyattractor Character. Chemistry - A European Journal, 2018, 24, 9853-9859.	3.3	28
32	Epoxide Hydrolase Conformational Heterogeneity for the Resolution of Bulky Pharmacologically Relevant Epoxide Substrates. Chemistry - A European Journal, 2018, 24, 12254-12258.	3.3	8
33	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
34	Structural basis of the Cope rearrangement and cyclization in hapalindole biogenesis. Nature Chemical Biology, 2018, 14, 345-351.	8.0	34
35	Catalytic iron-carbene intermediate revealed in a cytochrome <i>c</i> carbene transferase. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 7308-7313.	7.1	95
36	A promiscuous cytochrome P450 aromatic O-demethylase for lignin bioconversion. Nature Communications, 2018, 9, 2487.	12.8	135

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37	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
38	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
39	Computational Protocol to Understand P450 Mechanisms and Design of Efficient and Selective Biocatalysts. Frontiers in Chemistry, 2018, 6, 663.	3.6	12
40	Enzyme-catalyzed cationic epoxide rearrangements in quinolone alkaloid biosynthesis. Nature Chemical Biology, 2017, 13, 325-332.	8.0	44
41	Enzyme-Catalyzed Intramolecular Enantioselective Hydroalkoxylation. Journal of the American Chemical Society, 2017, 139, 3639-3642.	13.7	20
42	Rationalizing the relative abundances of trimetallic nitride template-based endohedral metallofullerenes from aromaticity measures. Chemical Communications, 2017, 53, 4140-4143.	4.1	5
43	Exploring the origins of selectivity in soluble epoxide hydrolase from Bacillus megaterium. Organic and Biomolecular Chemistry, 2017, 15, 8827-8835.	2.8	14
44	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
45	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
46	Effect of incarcerated HF on the exohedral chemical reactivity of HF@C₆₀. Chemical Communications, 2017, 53, 10993-10996.	4.1	26
47	Role of Conformational Dynamics in the Evolution of Retro-Aldolase Activity. ACS Catalysis, 2017, 7, 8524-8532.	11.2	103
48	Tautomerization and Dimerization of 6,13â€Disubstituted Derivatives of Pentacene. Chemistry - A European Journal, 2017, 23, 6111-6117.	3.3	7
49	Computational tools for the evaluation of laboratory-engineered biocatalysts. Chemical Communications, 2017, 53, 284-297.	4.1	84
50	(Invited) Molecular Recognition and Assembly of Fullerene and Carbon-Based Materials with Biomolecules. ECS Meeting Abstracts, 2017, , .	0.0	0
51	Reaction Mechanism and Regioselectivity of the Bingelâ€“Hirsch Addition of Dimethyl Bromomalonate to La@<i>C</i>_{2<i>v</i>}â€C₈₂. Chemistry - A European Journal, 2016, 22, 5953-5962.	3.3	23
52	The Regioselectivity of Bingelâ€“Hirsch Cycloadditions on Isolated Pentagon Rule Endohedral Metallofullerenes. Angewandte Chemie, 2016, 128, 2420-2423.	2.0	9
53	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
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	The Regioselectivity of Bingelâ€“Hirsch Cycloadditions on Isolated Pentagon Rule Endohedral Metallofullerenes. Angewandte Chemie - International Edition, 2016, 55, 2374-2377.	13.8	37
56	(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
57	(Invited) The Regioselectivity of the Diels-Alder and Bingel-Hirsch Additions to La@C2v -C82. ECS Meeting Abstracts, 2016, , .	0.0	0
58	(Invited) Aromaticity, Cage Structure, and Relative Abundancy of Endohedral Metallofullerenes. ECS Meeting Abstracts, 2016, , .	0.0	0
59	(Invited) The Regioselectivity of Bingel-Hirsch Cycloadditions on IPR Endohedral Metallofullerenes. ECS Meeting Abstracts, 2016, , .	0.0	0
60	Enantiospecific <i>cis</i>â€“<i>trans</i> 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
61	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
62	On the existence and characterization of molecular electrides. Chemical Communications, 2015, 51, 4865-4868.	4.1	68
63	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
64	Understanding the Exohedral Functionalization of Endohedral Metallofullerenes Metallofullerenes. Carbon Materials, 2015, , 67-99.	1.2	0
65	Sponge-like molecular cage for purification of fullerenes. Nature Communications, 2014, 5, 5557.	12.8	162
66	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
67	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
68	The role of aromaticity in determining the molecular structure and reactivity of (endohedral) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 222 T	38.1	97
69	Aromaticity as the driving force for the stability of non-IPR endohedral metallofullerene Bingelâ€“Hirsch adducts. Chemical Communications, 2013, 49, 8767.	4.1	21
70	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
71	A Complete Guide on the Influence of Metal Clusters in the Dielsâ€“Alder Regioselectivity of <i>I_h</i>â€C₈₀ Endohedral Metallofullerenes. Chemistry - A European Journal, 2013, 19, 14931-14940.	3.3	37
72	Electrochemical control of the regioselectivity in the exohedral functionalization of C60: the role of aromaticity. Chemical Communications, 2013, 49, 1220.	4.1	44

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73	Selfâ€Assembled Tetragonal Prismatic Molecular Cage Highly Selective for Anionic Ï€ Guests. Chemistry - A European Journal, 2013, 19, 1445-1456.	3.3	38
74	Dielsâ€“Alder and Retroâ€Dielsâ€“Alder Cycloadditions of (1,2,3,4,5â€Pentamethyl)cyclopentadiene to La@<i>C</i>_{2<i>v</i>}â€C₈₂: Regioselectivity and Product Stability. Chemistry - A European Journal, 2013, 19, 4468-4479.	3.3	27
75	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
76	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
77	Electronic and Vibrational Nonlinear Optical Properties of Five Representative Electrides. Journal of Chemical Theory and Computation, 2012, 8, 2688-2697.	5.3	78
78	The Exohedral Dielsâ€“Alder Reactivity of the Titanium Carbide Endohedral Metallofullerene Ti₂C₂@<i>D</i>_{3<i>h</i>}â€C₇₈: Comparison with <i>D</i>_{3<i>h</i>}â€C₇₈ and M₃N@<i>D</i>_{3<i>h</i>}â€C₇₈ (M=Sc and Y) Reactivity. Chemistry - A European Journal, 2012, 18, 7141-7154.	3.3	54
79	Chapter 4. Computational Design of Protein Function. Chemical Biology, 0, , 87-107.	0.2	6