

SÃ-ivia Osuna Oliveras

List of Publications by Year in descending order

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97
papers

4,370
citations

81900

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118850

62
g-index

107
all docs

107
docs citations

107
times ranked

4669
citing authors

#	ARTICLE	IF	CITATIONS
1	Biocatalysis. Nature Reviews Methods Primers, 2021, 1, .	21.2	255
2	The role of distant mutations and allosteric regulation on LovD active site dynamics. Nature Chemical Biology, 2014, 10, 431-436.	8.0	166
3	Sponge-like molecular cage for purification of fullerenes. Nature Communications, 2014, 5, 5557.	12.8	162
4	The reactivity of endohedral fullerenes. What can be learnt from computational studies?. Physical Chemistry Chemical Physics, 2011, 13, 3585-3603.	2.8	128
5	Intrinsic enzymatic properties modulate the self-propulsion of micromotors. Nature Communications, 2019, 10, 2826.	12.8	126
6	Role of conformational dynamics in the evolution of novel enzyme function. Chemical Communications, 2018, 54, 6622-6634.	4.1	123
7	Covalently Patterned Graphene Surfaces by a Force-Accelerated Diels-Alder Reaction. Journal of the American Chemical Society, 2013, 135, 9240-9243.	13.7	121
8	Dispersion Corrections Essential for the Study of Chemical Reactivity in Fullerenes. Journal of Physical Chemistry A, 2011, 115, 3491-3496.	2.5	117
9	Origins of stereoselectivity in evolved ketoreductases. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E7065-72.	7.1	104
10	Role of Conformational Dynamics in the Evolution of Retro-Aldolase Activity. ACS Catalysis, 2017, 7, 8524-8532.	11.2	103
11	The role of aromaticity in determining the molecular structure and reactivity of (endohedral) Tj ETQq1 1 0.784314 rBT /Overlock 10 Tf	38.1	97
12	Cycloaddition Reactions of Butadiene and 1,3-dipoles to Curved Arenes, Fullerenes, and Nanotubes: Theoretical Evaluation of the Role of Distortion Energies on Activation Barriers. Chemistry - A European Journal, 2009, 15, 13219-13231.	3.3	92
13	Scalable and Selective Dispersion of Semiconducting Arc-Discharged Carbon Nanotubes by Dithiafulvalene/Thiophene Copolymers for Thin Film Transistors. ACS Nano, 2013, 7, 2659-2668.	14.6	88
14	Molecular Dynamics Explorations of Active Site Structure in Designed and Evolved Enzymes. Accounts of Chemical Research, 2015, 48, 1080-1089.	15.6	86
15	Computational tools for the evaluation of laboratory-engineered biocatalysts. Chemical Communications, 2017, 53, 284-297.	4.1	84
16	Regio- and Stereoselective Steroid Hydroxylation at C7 by Cytochrome P450 Monooxygenase Mutants. Angewandte Chemie - International Edition, 2020, 59, 12499-12505.	13.8	83
17	Diels-Alder Reactions of Graphene: Computational Predictions of Products and Sites of Reaction. Journal of the American Chemical Society, 2013, 135, 17643-17649.	13.7	82
18	The Diels-Alder Reaction on Endohedral Y ₃ N@C ₇₈ : The Importance of the Fullerene Strain Energy. Journal of the American Chemical Society, 2009, 131, 129-139.	13.7	76

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19	Chemical Reactivity of D3h C78 (Metallo)Fullerene: Regioselectivity Changes Induced by Sc3N Encapsulation. <i>Journal of the American Chemical Society</i> , 2008, 130, 6206-6214.	13.7	75
20	p38 ^{Î³} is essential for cell cycle progression and liver tumorigenesis. <i>Nature</i> , 2019, 568, 557-560.	27.8	72
21	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
22	Density Functional Study of the [2+2+2] Cyclootrimerization of Acetylene Catalyzed by Wilkinson's Catalyst, RhCl(PPh ₃) ₃ . <i>Organometallics</i> , 2010, 29, 562-569.	2.3	68
23	Efficient reductive desymmetrization of bulky 1,3-cyclodiketones enabled by structure-guided directed evolution of a carbonyl reductase. <i>Nature Catalysis</i> , 2019, 2, 931-941.	34.4	68
24	Diels-Alder Reaction between Cyclopentadiene and C ₆₀ : An Analysis of the Performance of the ONIOM Method for the Study of Chemical Reactivity in Fullerenes and Nanotubes. <i>Journal of Physical Chemistry A</i> , 2009, 113, 9721-9726.	2.5	63
25	The challenge of predicting distal active site mutations in computational enzyme design. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021, 11, e1502.	14.6	61
26	Enzyme Conformation Influences the Performance of Lipase-powered Nanomotors. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 21080-21087.	13.8	58
27	On the Mechanism of the Thermal Retrocycloaddition of Pyrrolidinofullerenes (Retro-Prato) Tj ETQq1 1 0.784314.rgBT / Overlock 10	3.5	56
28	Reaction Mechanisms for Graphene and Carbon Nanotube Fluorination. <i>Journal of Physical Chemistry C</i> , 2010, 114, 3340-3345.	3.1	56
29	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
30	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
31	Why Bistetracenes Are Much Less Reactive Than Pentacenes in Diels-Alder Reactions with Fullerenes. <i>Journal of the American Chemical Society</i> , 2014, 136, 10743-10751.	13.7	52
32	In Vivo Selection for Formate Dehydrogenases with High Efficiency and Specificity toward NADP ⁺ . <i>ACS Catalysis</i> , 2020, 10, 7512-7525.	11.2	51
33	Rhodium(I)-Catalysed Intramolecular [2+2+2] Cyclootrimerisations of 15-, 20- and 25-Membered Azamacrocycles: Experimental and Theoretical Mechanistic Studies. <i>Chemistry - A European Journal</i> , 2009, 15, 5289-5300.	3.3	49
34	On the Mechanism of Action of Fullerene Derivatives in Superoxide Dismutation. <i>Chemistry - A European Journal</i> , 2010, 16, 3207-3214.	3.3	49
35	Full Exploration of the Diels-Alder Cycloaddition on Metallofullerenes M ₃ N@C ₈₀ (M=Sc, Lu, Gd): The D _{5h} versus I _h Isomer and the Influence of the Metal Cluster. <i>Chemistry - A European Journal</i> , 2012, 18, 8944-8956.	3.3	49
36	Deciphering the Allosterically Driven Conformational Ensemble in Tryptophan Synthase Evolution. <i>Journal of the American Chemical Society</i> , 2019, 141, 13049-13056.	13.7	49

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37	Reactivity and Regioselectivity of Noble Gas Endohedral Fullerenes Ng@C ₆₀ and Ng ₂ @C ₆₀ (Ng=He, Xe). Chemistry - A European Journal, 2009, 15, 13111-13123.	3.3	45
38	Electrochemical control of the regioselectivity in the exohedral functionalization of C ₆₀ : the role of aromaticity. Chemical Communications, 2013, 49, 1220.	4.1	44
39	Inducing high activity of a thermophilic enzyme at ambient temperatures by directed evolution. Chemical Communications, 2017, 53, 9454-9457.	4.1	41
40	Enantiospecific <i>cis</i> → <i>trans</i> Isomerization in Chiral Fulleropyrrolidines: Hydrogen-Bonding Assistance in the Carbanion Stabilization in H ₂ O@C ₆₀ . Journal of the American Chemical Society, 2015, 137, 1190-1197.	13.7	40
41	Self-Assembled Tetragonal Prismatic Molecular Cage Highly Selective for Anionic I ⁻ Guests. Chemistry - A European Journal, 2013, 19, 1445-1456.	3.3	38
42	H-Bond-Assisted Regioselective (<i>cis</i> -1) Intramolecular Nucleophilic Addition of the Hydroxyl Group to [60]Fullerene. Journal of Organic Chemistry, 2009, 74, 1480-1487.	3.2	37
43	A Complete Guide on the Influence of Metal Clusters in the Diels-Alder Regioselectivity of <i>h</i> -C ₈₀ Endohedral Metallofullerenes. Chemistry - A European Journal, 2013, 19, 14931-14940.	3.3	37
44	The Regioselectivity of Bingel-Hirsch Cycloadditions on Isolated Pentagon Rule Endohedral Metallofullerenes. Angewandte Chemie - International Edition, 2016, 55, 2374-2377.	13.8	37
45	Exploring the reversal of enantioselectivity on a zinc-dependent alcohol dehydrogenase. Organic and Biomolecular Chemistry, 2017, 15, 4122-4129.	2.8	36
46	Bis-1,3-dipolar Cycloadditions on Endohedral Fullerenes M ₃ N@Ih-C ₈₀ (M = Sc, Lu): Remarkable Endohedral-Cluster Regiochemical Control. Journal of the American Chemical Society, 2015, 137, 11775-11782.	13.7	34
47	(4 + 2) and (2 + 2) Cycloadditions of Benzyne to C ₆₀ and Zig-Zag Single-Walled Carbon Nanotubes: The Effect of the Curvature. Journal of Physical Chemistry C, 2016, 120, 1716-1726.	3.1	34
48	Are nucleus-independent (NICS) and ¹ H NMR chemical shifts good indicators of aromaticity in I ⁻ -stacked polyfluorenes?. Chemical Physics Letters, 2006, 428, 191-195.	2.6	33
49	Regioselective Intramolecular Nucleophilic Addition of Alcohols to C ₆₀ : One-Step Formation of a <i>cis</i> -1 Bicyclic-Fused Fullerene. Journal of Organic Chemistry, 2009, 74, 6253-6259.	3.2	33
50	The Roles of Counterion and Water in a Stereoselective Cysteine-Catalyzed Rauht-Currier Reaction: A Challenge for Computational Chemistry. Chemistry - A European Journal, 2013, 19, 14245-14253.	3.3	33
51	Endohedral Metal-Induced Regioselective Formation of Bis-Prato Adduct of Y ₃ N@Ih-C ₈₀ and Gd ₃ N@Ih-C ₈₀ . Journal of the American Chemical Society, 2015, 137, 58-61.	13.7	33
52	<i>In Silico</i> Identification and Experimental Validation of Distal Activity-Enhancing Mutations in Tryptophan Synthase. ACS Catalysis, 2021, 11, 13733-13743.	11.2	30
53	Improved Electro- and Photocatalytic Water Reduction by Confined Cobalt Catalysts in Streptavidin. ACS Catalysis, 2019, 9, 5837-5846.	11.2	28
54	Acceleration of an Aromatic Claisen Rearrangement via a Designed Spirolygozyme Catalyst that Mimics the Ketosteroid Isomerase Catalytic Dyad. Journal of the American Chemical Society, 2014, 136, 3817-3827.	13.7	27

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55	Product formation in the Prato reaction on Sc ₃ N@D ₅ h-C ₈₀ : preference for [5,6]-bonds, and not pyracylenic bonds. <i>Chemical Communications</i> , 2012, 48, 2486.	4.1	26
56	Effect of incarcerated HF on the exohedral chemical reactivity of HF@C ₆₀ . <i>Chemical Communications</i> , 2017, 53, 10993-10996.	4.1	26
57	Competitive Retro-Cycloaddition Reaction in Fullerene Dimers Connected through Pyrrolidinopyrazolino Rings. <i>Journal of Organic Chemistry</i> , 2009, 74, 8174-8180.	3.2	25
58	Essential Factors for Control of the Equilibrium in the Reversible Rearrangement of M ₃ N@I _h -C ₈₀ Fullerenopyrrolidines: Exohedral Functional Groups versus Endohedral Metal Clusters. <i>Chemistry - A European Journal</i> , 2014, 20, 14032-14039.	3.3	25
59	Toward Bioelectronic Nanomaterials: Photoconductivity in Protein-Porphyrin Hybrids Wrapped around SWCNT. <i>Advanced Functional Materials</i> , 2018, 28, 1704031.	14.9	25
60	Time Evolution of the Millisecond Allosteric Activation of Imidazole Glycerol Phosphate Synthase. <i>Journal of the American Chemical Society</i> , 2022, 144, 7146-7159.	13.7	24
61	Interplay between R513 methylation and S516 phosphorylation of the cardiac voltage-gated sodium channel. <i>Amino Acids</i> , 2015, 47, 429-434.	2.7	23
62	Reaction Mechanism and Regioselectivity of the Bingel-Hirsch Addition of Dimethyl Bromomalonate to La@C _{2v} -C ₈₂ . <i>Chemistry - A European Journal</i> , 2016, 22, 5953-5962.	3.3	23
63	Discovery and In Vivo Proof of Concept of a Highly Potent Dual Inhibitor of Soluble Epoxide Hydrolase and Acetylcholinesterase for the Treatment of Alzheimer's Disease. <i>Journal of Medicinal Chemistry</i> , 2022, 65, 4909-4925.	6.4	22
64	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
65	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
66	Regio- and Stereoselective Steroid Hydroxylation at C7 by Cytochrome P450 Monooxygenase Mutants. <i>Angewandte Chemie</i> , 2020, 132, 12599-12605.	2.0	19
67	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
68	Aromatic Claisen Rearrangements of Prenylated Tyrosine and Model Prenyl Aryl Ethers: Computational Study of the Role of Water on Acceleration of Claisen Rearrangements. <i>European Journal of Organic Chemistry</i> , 2013, 2013, 2823-2831.	2.4	18
69	Hidden Conformations in <i>Aspergillus niger</i> Monoamine Oxidase are Key for Catalytic Efficiency. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 3097-3101.	13.8	18
70	On the Regioselective Intramolecular Nucleophilic Addition of Thiols to C ₆₀ . <i>European Journal of Organic Chemistry</i> , 2009, 2009, 6231-6238.	2.4	16
71	Confined organization of fullerene units along high polymer chains. <i>Journal of Materials Chemistry C</i> , 2013, 1, 5747.	5.5	16
72	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

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73	Homolytic versus Heterolytic Dissociation of Alkalimetal Halides: The Effect of Microsolvation. <i>ChemPhysChem</i> , 2009, 10, 2955-2965.	2.1	14
74	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
75	2-Oxaadamant-1-yl Ureas as Soluble Epoxide Hydrolase Inhibitors: <i>In Vivo</i> Evaluation in a Murine Model of Acute Pancreatitis. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 9237-9257.	6.4	14
76	Regioselective Synthesis and Characterization of Tris- and Tetra-Prato Adducts of M ₃ N@C ₈₀ (M = Y, Tj ETQq0 0 0 18.7 / Overlock 10 TF	18.7	14
77	Extent of charge separation and exciton delocalization for electronically excited states in a triphenylamine-C ₆₀ donor-acceptor conjugate: a combined molecular dynamics and TD-DFT study. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	1.4	13
78	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
79	From the Design to the <i>In Vivo</i> Evaluation of Benzohomoadamantane-Derived Soluble Epoxide Hydrolase Inhibitors for the Treatment of Acute Pancreatitis. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 5429-5446.	6.4	12
80	Protein-directed crystalline 2D fullerene assemblies. <i>Nanoscale</i> , 2020, 12, 3614-3622.	5.6	11
81	The Regioselectivity of Bingel-Hirsch Cycloadditions on Isolated Pentagon Rule Endohedral Metallofullerenes. <i>Angewandte Chemie</i> , 2016, 128, 2420-2423.	2.0	9
82	Conformational Landscapes of Halohydrin Dehalogenases and Their Accessible Active Site Tunnels. <i>Catalysts</i> , 2020, 10, 1403.	3.5	9
83	Local Aromaticity of Pristine and Fluorinated Carbon Nanotubes. <i>Journal of Nanoscience and Nanotechnology</i> , 2009, 9, 6078-6083.	0.9	8
84	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
85	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
86	Reactivity and Regioselectivity of Noble Gas Endohedral Fullerenes Ng@C ₆₀ and Ng ₂ @C ₆₀ (Ng=He-Xe). <i>Chemistry - A European Journal</i> , 2010, 16, 3878-3878.	3.3	6
87	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
88	Insights into the molecular determinants of thermal stability in halohydrin dehalogenase HheD2. <i>FEBS Journal</i> , 2021, 288, 4683-4701.	4.7	5
89	Exploring the Conversion of a <i>d</i> -Sialic Acid Aldolase into a <i>l</i> -KDO Aldolase. <i>European Journal of Organic Chemistry</i> , 2018, 2018, 2603-2608.	2.4	4
90	Computational NMR Spectra of <i>o</i> -Benzynes and Stable Guests and Their Hemiarceplexes. <i>Chemistry - A European Journal</i> , 2020, 26, 2626-2634.	3.3	4

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91	Mutational Analysis of Linalool Dehydratase Isomerase Suggests That Alcohol and Alkene Transformations Are Catalyzed Using Noncovalent Mechanisms. <i>ACS Catalysis</i> , 2020, 10, 11136-11146.	11.2	4
92	Molecular Dynamics Simulations on <i>Aspergillus niger</i> Monoamine Oxidase: Conformational Dynamics and Intermonomer Communication Essential for Its Efficient Catalysis. <i>Advanced Synthesis and Catalysis</i> , 2019, 361, 2718.	4.3	3
93	SBMOpenMM: A Builder of Structure-Based Models for OpenMM. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 3166-3171.	5.4	3
94	The Chemical Reactivity of Fullerenes and Endohedral Fullerenes: A Theoretical Perspective. <i>Carbon Materials</i> , 2011, , 57-78.	1.2	2
95	Editorial (Hot Topic: Nanoreactors and Molecular Prisons). <i>Current Organic Chemistry</i> , 2013, 17, 1469-1469.	1.6	0
96	Hidden Conformations in <i>Aspergillus niger</i> Monoamine Oxidase are Key for Catalytic Efficiency. <i>Angewandte Chemie</i> , 2019, 131, 3129-3133.	2.0	0
97	Understanding the Exohedral Functionalization of Endohedral Metallofullerenes Metallofullerenes. <i>Carbon Materials</i> , 2015, , 67-99.	1.2	0