SÃ-lvia Osuna Oliveras

List of Publications by Year
in descending order

97 papers	4,370 citations	81900 39 h-index	118850 62 g-index
107 all docs	107 docs citations	107 times ranked	4669 citing authors

#	Article	IF	Citations
1	Discovery and In Vivo Proof of Concept of a Highly Potent Dual Inhibitor of Soluble Epoxide Hydrolase and Acetylcholinesterase for the Treatment of Alzheimerâ€™s Disease. Journal of Medicinal Chemistry, 2022, 65, 4909-4925.	6.4	22
2	Time Evolution of the Millisecond Allosteric Activation of Imidazole Glycerol Phosphate Synthase. Journal of the American Chemical Society, 2022, 144, 7146-7159.	13.7	24
3	The challenge of predicting distal active site mutations in computational enzyme design. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1502.	14.6	61
4	Insights into the molecular determinants of thermal stability in halohydrin dehalogenase HheD2. FEBS Journal, 2021, 288, 4683-4701.	4.7	5
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	From the Design to the In Vivo Evaluation of Benzohomoadamantane-Derived Soluble Epoxide Hydrolase Inhibitors for the Treatment of Acute Pancreatitis. Journal of Medicinal Chemistry, 2021, 64, 5429-5446.	6.4	12
7	Biocatalysis. Nature Reviews Methods Primers, 2021, 1, .	21.2	255
8	SBMOpenMM: A Builder of Structure-Based Models for OpenMM. Journal of Chemical Information and Modeling, 2021, 61, 3166-3171.	5.4	3
9	In Silico Identification and Experimental Validation of Distal Activity-Enhancing Mutations in Tryptophan Synthase. ACS Catalysis, 2021, 11, 13733-13743.	11.2	30
10	Protein-directed crystalline 2D fullerene assemblies. Nanoscale, 2020, 12, 3614-3622.	5.6	11
11	Computational NMR Spectra of oâ€Benzyne and Stable Guests and Their Hemicarceplexes. Chemistry - A European Journal, 2020, 26, 2626-2634.	3.3	4
12	2-Oxaadamant-1-yl Ureas as Soluble Epoxide Hydrolase Inhibitors: In Vivo Evaluation in a Murine Model of Acute Pancreatitis. Journal of Medicinal Chemistry, 2020, 63, 9237-9257.	6.4	14
13	Enzyme Conformation Influences the Performance of Lipaseâ€powered Nanomotors. Angewandte Chemie - International Edition, 2020, 59, 21080-21087.	13.8	58
14	Mutational Analysis of Linalool Dehydratase Isomerase Suggests That Alcohol and Alkene Transformations Are Catalyzed Using Noncovalent Mechanisms. ACS Catalysis, 2020, 10, 11136-11146.	11.2	4
15	Conformational Landscapes of Halohydrin Dehalogenases and Their Accessible Active Site Tunnels. Catalysts, 2020, 10, 1403.	3.5	9
16	In Vivo Selection for Formate Dehydrogenases with High Efficiency and Specificity toward NADP⁺. ACS Catalysis, 2020, 10, 7512-7525.	11.2	51
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	Regioselective Synthesis and Characterization of Tris- and Tetra-Prato Adducts of M3N@C80 (M = Y,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	13.7	14

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19	Regioâ€•and Stereoselective Steroid Hydroxylation at C7 by Cytochromeâ€…P450 Monooxygenase Mutants. Angewandte Chemie, 2020, 132, 12599-12605.	2.0	19
20	Deciphering the Allosterically Driven Conformational Ensemble in Tryptophan Synthase Evolution. Journal of the American Chemical Society, 2019, 141, 13049-13056.	13.7	49
21	Intrinsic enzymatic properties modulate the self-propulsion of micromotors. Nature Communications, 2019, 10, 2826.	12.8	126
22	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
23	Efficient reductive desymmetrization of bulky 1,3-cyclodiketones enabled by structure-guided directed evolution of a carbonyl reductase. Nature Catalysis, 2019, 2, 931-941.	34.4	68
24	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
25	Improved Electro- and Photocatalytic Water Reduction by Confined Cobalt Catalysts in Streptavidin. ACS Catalysis, 2019, 9, 5837-5846.	11.2	28
26	p38Î³ is essential for cell cycle progression and liver tumorigenesis. Nature, 2019, 568, 557-560.	27.8	72
27	Molecular Dynamics Simulations on Aspergillus niger Monoamine Oxidase: Conformational Dynamics and Interâ€•monomer Communication Essential for Its Efficient Catalysis. Advanced Synthesis and Catalysis, 2019, 361, 2718.	4.3	3
28	Hidden Conformations in Aspergillus niger Monoamine Oxidase are Key for Catalytic Efficiency. Angewandte Chemie - International Edition, 2019, 58, 3097-3101.	13.8	18
29	Hidden Conformations in Aspergillus niger Monoamine Oxidase are Key for Catalytic Efficiency. Angewandte Chemie, 2019, 131, 3129-3133.	2.0	0
30	Exploring the Conversion of a <scp>d</scp>â€Sialic Acid Aldolase into a <scp>l</scp>â€KDO Aldolase. European Journal of Organic Chemistry, 2018, 2018, 2603-2608.	2.4	4
31	Epoxide Hydrolase Conformational Heterogeneity for the Resolution of Bulky Pharmacologically Relevant Epoxide Substrates. Chemistry - A European Journal, 2018, 24, 12254-12258.	3.3	8
32	Toward Bioelectronic Nanomaterials: Photoconductivity in Proteinâ€“Porphyrin Hybrids Wrapped around SWCNT. Advanced Functional Materials, 2018, 28, 1704031.	14.9	25
33	Role of conformational dynamics in the evolution of novel enzyme function. Chemical Communications, 2018, 54, 6622-6634.	4.1	123
34	Exploring the reversal of enantioselectivity on a zinc-dependent alcohol dehydrogenase. Organic and Biomolecular Chemistry, 2017, 15, 4122-4129.	2.8	36
35	Rationalizing the relative abundances of trimetallic nitride template-based endohedral metallofullerenes from aromaticity measures. Chemical Communications, 2017, 53, 4140-4143.	4.1	5
36	Exploring the origins of selectivity in soluble epoxide hydrolase from Bacillus megaterium. Organic and Biomolecular Chemistry, 2017, 15, 8827-8835.	2.8	14

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37	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
38	Inducing high activity of a thermophilic enzyme at ambient temperatures by directed evolution. Chemical Communications, 2017, 53, 9454-9457.	4.1	41
39	Effect of incarcerated HF on the exohedral chemical reactivity of HF@C₆₀. Chemical Communications, 2017, 53, 10993-10996.	4.1	26
40	Role of Conformational Dynamics in the Evolution of Retro-Aldolase Activity. ACS Catalysis, 2017, 7, 8524-8532.	11.2	103
41	Computational tools for the evaluation of laboratory-engineered biocatalysts. Chemical Communications, 2017, 53, 284-297.	4.1	84
42	Reaction Mechanism and Regioselectivity of the Bingelâ€“Hirsch Addition of Dimethyl Bromomalonate to La@C₂v</sub>â€Œ₈₂. Chemistry - A European Journal, 2016, 22, 5953-5962.	3.3	23
43	The Regioselectivity of Bingelâ€“Hirsch Cycloadditions on Isolated Pentagon Rule Endohedral Metallofullerenes. Angewandte Chemie, 2016, 128, 2420-2423.	2.0	9
44	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
45	The Regioselectivity of Bingelâ€“Hirsch Cycloadditions on Isolated Pentagon Rule Endohedral Metallofullerenes. Angewandte Chemie - International Edition, 2016, 55, 2374-2377.	13.8	37
46	(4 + 2) and (2 + 2) Cycloadditions of Benzyne to C₆₀ and Zig-Zag Single-Walled Carbon Nanotubes: The Effect of the Curvature. Journal of Physical Chemistry C, 2016, 120, 1716-1726.	3.1	34
47	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
48	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
49	Extent of charge separation and exciton delocalization for electronically excited states in a triphenylamine-C60 donorâ€“acceptor conjugate: a combined molecular dynamics and TD-DFT study. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	13
50	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
51	Molecular Dynamics Explorations of Active Site Structure in Designed and Evolved Enzymes. Accounts of Chemical Research, 2015, 48, 1080-1089.	15.6	86
52	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
53	Interplay between R513 methylation and S516 phosphorylation of the cardiac voltage-gated sodium channel. Amino Acids, 2015, 47, 429-434.	2.7	23
54	Understanding the Exohedral Functionalization of Endohedral Metallofullerenes Metallofullerenes. Carbon Materials, 2015, , 67-99.	1.2	0

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55	Sponge-like molecular cage for purification of fullerenes. Nature Communications, 2014, 5, 5557.	12.8	162
56	The role of distant mutations and allosteric regulation on LovD active site dynamics. Nature Chemical Biology, 2014, 10, 431-436.	8.0	166
57	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
58	Why Bistetracenes Are Much Less Reactive Than Pentacenes in Dielsâ€“Alder Reactions with Fullerenes. Journal of the American Chemical Society, 2014, 136, 10743-10751.	13.7	52
59	Acceleration of an Aromatic Claisen Rearrangement via a Designed Spiroligozyme Catalyst that Mimics the Ketosteroid Isomerase Catalytic Dyad. Journal of the American Chemical Society, 2014, 136, 3817-3827.	13.7	27
60	The role of aromaticity in determining the molecular structure and reactivity of (endohedral) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 542 T	38.1	97
61	Aromaticity as the driving force for the stability of non-IPR endohedral metallofullerene Bingelâ€“Hirsch adducts. Chemical Communications, 2013, 49, 8767.	4.1	21
62	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
63	Dielsâ€“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
64	Confined organization of fullerene units along high polymer chains. Journal of Materials Chemistry C, 2013, 1, 5747.	5.5	16
65	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
66	Electrochemical control of the regioselectivity in the exohedral functionalization of C60: the role of aromaticity. Chemical Communications, 2013, 49, 1220.	4.1	44
67	Selfâ€Assembled Tetragonal Prismatic Molecular Cage Highly Selective for Anionic Ï€ Guests. Chemistry - A European Journal, 2013, 19, 1445-1456.	3.3	38
68	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
69	Covalently Patterned Graphene Surfaces by a Force-Accelerated Dielsâ€“Alder Reaction. Journal of the American Chemical Society, 2013, 135, 9240-9243.	13.7	121
70	Aromatic Claisen Rearrangements of Oâ€Prenylated Tyrosine and Model Prenyl Aryl Ethers: Computational Study of the Role of Water on Acceleration of Claisen Rearrangements. European Journal of Organic Chemistry, 2013, 2013, 2823-2831.	2.4	18
71	The Roles of Counterion and Water in a Stereoselective Cysteineâ€Catalyzed Rauhutâ€“Currier Reaction: A Challenge for Computational Chemistry. Chemistry - A European Journal, 2013, 19, 14245-14253.	3.3	33
72	Editorial (Hot Topic: Nanoreactors and Molecular Prisons). Current Organic Chemistry, 2013, 17, 1469-1469.	1.6	0

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73	Product formation in the Prato reaction on Sc3N@D5h-C80: preference for [5,6]-bonds, and not pyracylenic bonds. Chemical Communications, 2012, 48, 2486.	4.1	26
74	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
75	The Exohedral Dielsâ€“Alder Reactivity of the Titanium Carbide Endohedral Metallofullerene Ti₂C₂@D₃h</sub>â€C₇₈: Comparison with D₃h</sub>â€C₇₈ and M₃N@D₃h</sub>â€C₇₈ (M=Sc and Y) Reactivity. Chemistry - A European Journal, 2012, 18, 7141-7154.	3.3	54
76	Full Exploration of the Dielsâ€“Alder Cycloaddition on Metallofullerenes M₃N@C₈₀ (M=Sc, Lu, Gd): The D₅h</sub> versus I_h Isomer and the Influence of the Metal Cluster. Chemistry - A European Journal, 2012, 18, 8944-8956.	3.3	49
77	The reactivity of endohedral fullerenes. What can be learnt from computational studies?. Physical Chemistry Chemical Physics, 2011, 13, 3585-3603.	2.8	128
78	Dispersion Corrections Essential for the Study of Chemical Reactivity in Fullerenes. Journal of Physical Chemistry A, 2011, 115, 3491-3496.	2.5	117
79	The Chemical Reactivity of Fullerenes and Endohedral Fullerenes: A Theoretical Perspective. Carbon Materials, 2011, , 57-78.	1.2	2
80	On the Mechanism of Action of Fullerene Derivatives in Superoxide Dismutation. Chemistry - A European Journal, 2010, 16, 3207-3214.	3.3	49
81	Reactivity and Regioselectivity of Noble Gas Endohedral Fullerenes Ng@C60 and Ng2@C60 (Ng=He-Xe). Chemistry - A European Journal, 2010, 16, 3878-3878.	3.3	6
82	Density Functional Study of the [2+2+2] Cyclotrimerization of Acetylene Catalyzed by Wilkinsonâ€™s Catalyst, RhCl(PPh₃)₃. Organometallics, 2010, 29, 562-569.	2.3	68
83	Reaction Mechanisms for Graphene and Carbon Nanotube Fluorination. Journal of Physical Chemistry C, 2010, 114, 3340-3345.	3.1	56
84	Rhodium(I)â€Catalysed Intramolecular [2+2+2] Cyclotrimerisations of 15â€, 20â€•and 25â€Membered Azamacrocycles: Experimental and Theoretical Mechanistic Studies. Chemistry - A European Journal, 2009, 15, 5289-5300.	3.3	49
85	Reactivity and Regioselectivity of Noble Gas Endohedral Fullerenes Ng@C₆₀ and Ng₂@C₆₀ (Ng=Heâ€“Xe). Chemistry - A European Journal, 2009, 15, 13111-13123.	3.3	45
86	Cycloaddition Reactions of Butadiene and 1,3â€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
87	Homolytic versus Heterolytic Dissociation of Alkalimetal Halides: The Effect of Microsolvation. ChemPhysChem, 2009, 10, 2955-2965.	2.1	14
88	On the Regioselective Intramolecular Nucleophilic Addition of Thiols to C₆₀. European Journal of Organic Chemistry, 2009, 2009, 6231-6238.	2.4	16
89	Dielsâ€™Alder Reaction between Cyclopentadiene and C₆₀: An Analysis of the Performance of the ONIOM Method for the Study of Chemical Reactivity in Fullerenes and Nanotubes. Journal of Physical Chemistry A, 2009, 113, 9721-9726.	2.5	63
90	The Dielsâ€™Alder Reaction on Endohedral Y₃N@C₇₈: The Importance of the Fullerene Strain Energy. Journal of the American Chemical Society, 2009, 131, 129-139.	13.7	76

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91	H-Bond-Assisted Regioselective (cis-1) Intramolecular Nucleophilic Addition of the Hydroxyl Group to [60]Fullerene. Journal of Organic Chemistry, 2009, 74, 1480-1487.	3.2	37
92	Competitive Retro-Cycloaddition Reaction in Fullerene Dimers Connected through Pyrrolidinopyrazolino Rings. Journal of Organic Chemistry, 2009, 74, 8174-8180.	3.2	25
93	Regioselective Intramolecular Nucleophilic Addition of Alcohols to C₆₀: One-Step Formation of acis-1 Bicyclic-Fused Fullerene. Journal of Organic Chemistry, 2009, 74, 6253-6259.	3.2	33
94	Local Aromaticity of Pristine and Fluorinated Carbon Nanotubes. Journal of Nanoscience and Nanotechnology, 2009, 9, 6078-6083.	0.9	8
95	On the Mechanism of the Thermal Retrocycloaddition of Pyrrolidinofullerenes (Retroâ€Prato) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf	3.3	56
96	Chemical Reactivity of D3h C78 (Metallo)Fullerene: Regioselectivity Changes Induced by Sc3N Encapsulation. Journal of the American Chemical Society, 2008, 130, 6206-6214.	13.7	75
97	Are nucleus-independent (NICS) and 1H NMR chemical shifts good indicators of aromaticity in Ï€-stacked polyfluorenes?. Chemical Physics Letters, 2006, 428, 191-195.	2.6	33