Luis SimÃ³n Rubio

List of Publications by Year
in descending order

63 papers	2,188 citations	304368 22 h-index	223531 46 g-index
69 all docs	69 docs citations	69 times ranked	2230 citing authors

#	Article	IF	Citations
1	Theoretical Study of the Mechanism of Hantzsch Ester Hydrogenation of Imines Catalyzed by Chiral BINOL-Phosphoric Acids. Journal of the American Chemical Society, 2008, 130, 8741-8747.	6.6	283
2	How reliable are DFT transition structures? Comparison of GGA, hybrid-meta-GGA and meta-GGA functionals. Organic and Biomolecular Chemistry, 2011, 9, 689-700.	1.5	212
3	The Mechanism of TBD-Catalyzed Ring-Opening Polymerization of Cyclic Esters. Journal of Organic Chemistry, 2007, 72, 9656-9662.	1.7	184
4	A Model for the Enantioselectivity of Imine Reactions Catalyzed by BINOLâˆ'Phosphoric Acid Catalysts. Journal of Organic Chemistry, 2011, 76, 1775-1788.	1.7	155
5	A Practical Guide for Predicting the Stereochemistry of Bifunctional Phosphoric Acid Catalyzed Reactions of Imines. Accounts of Chemical Research, 2016, 49, 1029-1041.	7.6	139
6	Enzyme Catalysis by Hydrogen Bonds: The Balance between Transition State Binding and Substrate Binding in Oxyanion Holes. Journal of Organic Chemistry, 2010, 75, 1831-1840.	1.7	110
7	DFT Study on the Factors Determining the Enantioselectivity of Friedelâˆ'Crafts Reactions of Indole with <i>N</i>-Acyl and <i>N</i>-Tosylimines Catalyzed by BINOLâˆ'Phosphoric Acid Derivatives. Journal of Organic Chemistry, 2010, 75, 589-597.	1.7	107
8	Mechanism of BINOLâˆ'Phosphoric Acid-Catalyzed Strecker Reaction of Benzyl Imines. Journal of the American Chemical Society, 2009, 131, 4070-4077.	6.6	105
9	A macrocyclic receptor for the chiral recognition of hydroxycarboxylates. Tetrahedron Letters, 2000, 41, 4563-4566.	0.7	84
10	Proline imidazolidinones and enamines in Hajosâ€"Wiechert and Wielandâ€"Miescher ketone synthesis. Tetrahedron, 2009, 65, 4841-4845.	1.0	40
11	Synthesis of Monoacylated Derivatives of 1,2- Cyclohexanediamine. Evaluation of their Catalytic Activity in the Preparation of Wielandâˆ'Miescher Ketone. Journal of Organic Chemistry, 2010, 75, 8303-8306.	1.7	39
12	Hydrogen-bond stabilization in oxyanion holes: grand jetÃ© to three dimensions. Organic and Biomolecular Chemistry, 2012, 10, 1905.	1.5	37
13	Imidazolidinone intermediates in prolinamide-catalyzed aldol reactions. Organic and Biomolecular Chemistry, 2010, 8, 2979.	1.5	33
14	Sulfonamide carbazole receptors for anion recognition. Organic and Biomolecular Chemistry, 2011, 9, 8321.	1.5	32
15	Origins of Asymmetric Phosphazene Organocatalysis: Computations Reveal a Common Mechanism for Nitro- and Phospho-Aldol Additions. Journal of Organic Chemistry, 2015, 80, 2756-2766.	1.7	30
16	Mechanism of Amination of Î²-Keto Esters by Azadicarboxylates Catalyzed by an Axially Chiral Guanidine: Acyclic Keto Esters React through an E Enolate. Journal of the American Chemical Society, 2012, 134, 16869-16876.	6.6	27
17	Acridone Heterocycles as Fluorescent Sensors for Anions. Heterocycles, 2006, 69, 73.	0.4	24
18	From Theozymes to Artificial Enzymes: Enzymeâ€Like Receptors for Michael Additions with Oxyanion Holes and Active Amino Groups. European Journal of Organic Chemistry, 2007, 2007, 4821-4830.	1.2	24

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19	Thiourea versus the oxyanion hole as a double H-bond donor. Tetrahedron Letters, 2008, 49, 5050-5052.	0.7	24
20	QM/MM study on the enantioselectivity of spiroacetalization catalysed by an imidodiphosphoric acid catalyst: how confinement works. Organic and Biomolecular Chemistry, 2016, 14, 3031-3039.	1.5	24
21	Phosphazene Catalyzed Addition to Electron-Deficient Alkynes: The Importance of Nonlinear Allenyl Intermediates upon Stereoselectivity. Journal of Organic Chemistry, 2017, 82, 3855-3863.	1.7	24
22	BIMPâ€Catalyzed 1,3â€Prototropic Shift for the Highly Enantioselective Synthesis of Conjugated Cyclohexenones. Angewandte Chemie - International Edition, 2020, 59, 17417-17422.	7.2	24
23	A xanthone-based neutral receptor for zwitterionic amino acids. Tetrahedron Letters, 2003, 44, 6983-6985.	0.7	22
24	What is the mechanism of amine conjugate additions to pyrazole crotonate catalyzed by thiourea catalysts?. Organic and Biomolecular Chemistry, 2009, 7, 483-487.	1.5	22
25	The True Catalyst Revealed: The Intervention of Chiral Ca and Mg Phosphates in BrÃ¸nsted Acid Promoted Asymmetric Mannich Reactions. Journal of the American Chemical Society, 2018, 140, 5412-5420.	6.6	21
26	Xanthone Receptors as Oxyanion-Hole Mimics in Artificial Enzymes. Helvetica Chimica Acta, 2005, 88, 1682-1701.	1.0	19
27	Ternary enantioselective complexes from Î±-amino acids, 18-crown-6 ether and a macrocyclic xanthone-based receptor. Tetrahedron Letters, 2004, 45, 4831-4833.	0.7	18
28	Synthesis of a chiral artificial receptor with catalytic activity in Michael additions and its chiral resolution by a new methodology. Organic and Biomolecular Chemistry, 2010, 8, 1763.	1.5	18
29	A Xantheneâ€“Benzimidazole Receptor with Multiple Hâ€Bond Donors for Carboxylic Acids. European Journal of Organic Chemistry, 2010, 2010, 6179-6185.	1.2	16
30	Bifunctional organocatalysts based on a carbazole scaffold for the synthesis of the Hajosâ€“Wiechert and Wielandâ€“Miescher ketones. Tetrahedron, 2015, 71, 1297-1303.	1.0	16
31	trans-Benzoxanthene receptors for enantioselective recognition of amino acid derivatives. Tetrahedron Letters, 2001, 42, 5853-5856.	0.7	15
32	Enzyme Mimics for Michael Additions with Novel Proton Transport Groups. European Journal of Organic Chemistry, 2008, 2008, 2397-2403.	1.2	15
33	Enantioselective recognition of Î±-amino acid derivatives with a cis-tetrahydrobenzoxanthene receptorElectronic supplementary information (ESI) available: binding data. See http://www.rsc.org/suppdata/p2/b2/b203054c/. Perkin Transactions II RSC, 2002, , 1050-1052.	1.1	14
34	A molecular receptor selective for zwitterionic alanine. Organic and Biomolecular Chemistry, 2017, 15, 477-485.	1.5	14
35	An Enzyme Model Which Mimics Chymotrypsin and N-Terminal Hydrolases. ACS Catalysis, 2020, 10, 11162-11170.	5.5	14
36	Assessing the Protonation State of Drug Molecules:Â The Case of Aztreonam. Journal of Medicinal Chemistry, 2006, 49, 3235-3243.	2.9	13

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37	Interaction between the N-terminal SH3 domain of NckÎ± and CD3É›-derived peptides: Non-canonical and canonical recognition motifs. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2009, 1794, 110-117.	1.1	13
38	A High Yield Procedure for the Preparation of 2â€Hydroxynitrostyrenes: Synthesis of Imines and Tetracyclic 1,3â€Benzoxazines. European Journal of Organic Chemistry, 2014, 2014, 3242-3248.	1.2	13
39	Chiral recognition with a benzofuran receptor that mimics an oxyanion hole. Organic and Biomolecular Chemistry, 2015, 13, 493-501.	1.5	13
40	Urea-tetrahydrobenzoxanthene receptors for carboxylic acids. Tetrahedron, 2004, 60, 3755-3762.	1.0	12
41	Aminopyridineâˆ’Benzoxanthene Enantioselective Receptor for Sulfonylamino Acids. Organic Letters, 2004, 6, 1155-1157.	2.4	12
42	Enantioselective Chromenone Benzoxazole Receptor for Glutamic Acid and Its Derivatives. Journal of Organic Chemistry, 2003, 68, 7513-7516.	1.7	11
43	Enantioselectivity in CPA-catalyzed Friedelâ€“Crafts reaction of indole and <i>N</i>-tosylimines: a challenge for guiding models. Organic and Biomolecular Chemistry, 2018, 16, 2225-2238.	1.5	11
44	Daxabe â€“ A Xantheneâ€Based Fluorescent Sensor for 3,5â€Dinitrobenzoic Acid and Anions. European Journal of Organic Chemistry, 2009, 2009, 1009-1015.	1.2	10
45	Highly Enantioselective Extraction of Phenylglycine by a Chiral Macrocyclic Receptor Based on Supramolecular Interactions. Organic Letters, 2020, 22, 867-872.	2.4	10
46	Chromogenic Charge Transfer Cleft-Type Tetrahydrobenzoxanthene Enantioselective Receptors for Dinitrobenzoylamino Acids. Journal of Organic Chemistry, 2004, 69, 6883-6885.	1.7	8
47	A Highly Enantioselective Receptor for Carbamoyl Lactic Acid. European Journal of Organic Chemistry, 2009, 2009, 5350-5354.	1.2	8
48	A trans-tetrahydrobenzoxanthene receptor for the resolution of racemic mixtures of sulfonylamino acids. Chemical Communications, 2004, , 426-427.	2.2	7
49	A molecular receptor for zwitterionic phenylalanine. Organic and Biomolecular Chemistry, 2016, 14, 3906-3912.	1.5	7
50	A Fluorescent Sensor for Dinitrobenzoic Acid Based on a Cyanuric Acid and Xanthene Skeleton. Sensors, 2008, 8, 1637-1644.	2.1	6
51	A Twitchell Reagent Revival: Biodiesel Generation from Low Cost Oils. Advanced Synthesis and Catalysis, 2011, 353, 2681-2690.	2.1	6
52	An Enantioselective Benzofuranâ€Based Receptor for Dinitrobenzoylâ€Substituted Amino Acids. European Journal of Organic Chemistry, 2016, 2016, 1541-1547.	1.2	6
53	Chiral Recognition of Diketopiperazines with Xanthone Receptors. Chemistry Letters, 2000, 29, 718-719.	0.7	5
54	Selective acylation of 4,5-diamino-9,9â€²-dimethylxanthene through an aggregation effect. Tetrahedron Letters, 2008, 49, 790-793.	0.7	5

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55	Preparation of cyclic boramides from salicylaldehydes, ammonium acetate and sodium borohydride. Tetrahedron, 2014, 70, 8614-8618.	1.0	5
56	A highly selective receptor for zwitterionic proline. Organic and Biomolecular Chemistry, 2016, 14, 1325-1331.	1.5	5
57	Enantioselective Lutidine-Tetrahydrobenzoxanthene Receptors for Carboxylic Acids. European Journal of Organic Chemistry, 2004, 2004, 1698-1702.	1.2	4
58	Study of a new â€˜chiral protonâ€™ organocatalyst with hydrolase activity: application in azlactone racemic dynamic resolution. Tetrahedron: Asymmetry, 2017, 28, 819-823.	1.8	4
59	A Xanthone-based Macrocyclic Receptor and Its Possible Applications. Heterocycles, 2004, 63, 2465.	0.4	4
60	A cleft type receptor which combines an oxyanion hole with electrostatic interactions. Organic and Biomolecular Chemistry, 2017, 15, 4571-4578.	1.5	3
61	A bio-inspired enantioselective small-molecule artificial receptor for Î² adrenergic agonists and antagonists and its application for enantioselective extraction. Chemical Communications, 2016, 52, 12582-12585.	2.2	2
62	A trans-Tetrahydrobenzoxanthene Receptor for the Resolution of Racemic Mixtures of Sulfonylamino Acids.. ChemInform, 2004, 35, no.	0.1	0
63	The Aggregation of 8-Formylamino-2-carboxamidochromenone Heterocycles in Solution. Heterocycles, 2003, 59, 41.	0.4	0