

Jose Manuel Otero Casas

List of Publications by Year in descending order

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#	ARTICLE	IF	CITATIONS
1	Structure of the bacteriophage T4 long tail fiber receptor-binding tip. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 20287-20292.	7.1	159
2	Adsorption of Pharmaceutical Pollutants from Water Using Covalent Organic Frameworks. Chemistry - A European Journal, 2018, 24, 10601-10605.	3.3	106
3	Effect of the Protonation State of the Titratable Residues on the Inhibitor Affinity to BACE-1. Biochemistry, 2010, 49, 7255-7263.	2.5	51
4	Mycobacterium tuberculosis Shikimate Kinase Inhibitors: Design and Simulation Studies of the Catalytic Turnover. Journal of the American Chemical Society, 2013, 135, 12366-12376.	13.7	51
5	Synthetic Chemical Inducers and Genetic Decoupling Enable Orthogonal Control of the <i>rhaBAD</i> Promoter. ACS Synthetic Biology, 2016, 5, 1136-1145.	3.8	47
6	Structure of the Receptor-Binding Carboxy-Terminal Domain of the Bacteriophage T5 L-Shaped Tail Fibre with and without Its Intra-Molecular Chaperone. Viruses, 2015, 7, 6424-6440.	3.3	46
7	Inhibiting and Reversing Amyloid β Peptide (1-40) Fibril Formation with Gramicidin S and Engineered Analogues. Chemistry - A European Journal, 2013, 19, 17338-17348.	3.3	39
8	An Adamantyl Amino Acid Containing Gramicidin S Analogue with Broad Spectrum Antibacterial Activity and Reduced Hemolytic Activity. Chemistry - A European Journal, 2010, 16, 12174-12181.	3.3	33
9	Exploring the Conformational and Biological Versatility of Turn-Modified Gramicidin S by Using Sugar Amino Acid Homologues that Vary in Ring Size. Chemistry - A European Journal, 2011, 17, 3995-4004.	3.3	33
10	A Prodrug Approach for Improving Antituberculosis Activity of Potent Mycobacterium tuberculosis Type II Dehydroquinase Inhibitors. Journal of Medicinal Chemistry, 2011, 54, 6063-6084.	6.4	32
11	Preliminary Studies on the Transformation of Nitrosugars into Branched Chain Iminosugars: Synthesis of 1,4-Dideoxy-4-C-hydroxymethyl-1,4-imino-pentanol. Organic Letters, 2007, 9, 623-626.	4.6	25
12	Studies on the transformation of nitrosugars into branched chain iminosugars. Part II: Synthesis of (3R,4R,5R,6S)-2,2-bis(hydroxymethyl)azepane-3,4,5,6-tetraol. Tetrahedron: Asymmetry, 2008, 19, 2443-2446.	1.8	22
13	Understanding the Key Factors that Control the Inhibition of Type II Dehydroquinase by (2 <i>R</i> ,3 <i>R</i> ,4 <i>R</i> ,5 <i>R</i> ,6 <i>S</i>)-2-bis(hydroxymethyl)azepane-3,4,5,6-tetraol. ChemMedChem, 2010, 5, 1726-1733.	3.2	22
14	Synthesis and Biological Evaluation of New Nanomolar Competitive Inhibitors of Helicobacter pylori Type II Dehydroquinase. Structural Details of the Role of the Aromatic Moieties with Essential Residues. Journal of Medicinal Chemistry, 2010, 53, 191-200.	6.4	21
15	Target highlights in CASP9: Experimental target structures for the critical assessment of techniques for protein structure prediction. Proteins: Structure, Function and Bioinformatics, 2011, 79, 6-20.	2.6	19
16	Bisphosphine-Functionalized Cyclic Decapeptides Based on the Natural Product Gramicidin S : A Potential Scaffold for Transition-Metal Coordination. Chemistry - A European Journal, 2009, 15, 8134-8145.	3.3	17
17	Studies on the transformation of nitrosugars into iminosugars III: synthesis of (2 <i>R</i> ,3 <i>R</i> ,4 <i>R</i> ,5 <i>R</i> ,6 <i>R</i>)-2-(hydroxymethyl)azepane-3,4,5,6-tetraol and (2 <i>R</i> ,3 <i>R</i> ,4 <i>R</i> ,5 <i>R</i> ,6 <i>S</i>)-2-(hydroxymethyl)azepane-3,4,5,6-tetraol. Tetrahedron: Asymmetry, 2010, 21, 21-26.	1.8	17
18	Evaluation of Readily Accessible Azoles as Mimics of the Aromatic Ring of <i>D</i> -Phenylalanine in the Turn Region of Gramicidin S . ChemMedChem, 2011, 6, 840-847.	3.2	17

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19	Gramicidin S Derivatives Containing <i>cis</i> - and <i>trans</i> -Morpholine Amino Acids (MAAs) as Turn Mimetics. <i>Chemistry - A European Journal</i> , 2010, 16, 4259-4265.	3.3	15
20	Tetrahydrobenzothiophene Derivatives: Conformationally Restricted Inhibitors of Type II Dehydroquinase. <i>ChemMedChem</i> , 2011, 6, 266-272.	3.2	15
21	Studies on the Michael addition of naphthoquinones to sugar nitro olefins: first synthesis of polyhydroxylated hexahydro-11H-benzo[a]carbazole-5,6-diones and hexahydro-11bH-benzo[b]carbazole-6,11-diones. <i>Tetrahedron</i> , 2012, 68, 1612-1621.	1.9	15
22	Synthesis and biological evaluation of asymmetric gramicidin S analogues containing modified d-phenylalanine residues. <i>Bioorganic and Medicinal Chemistry</i> , 2009, 17, 6318-6328.	3.0	14
23	On a Possible Neutral Charge State for the Catalytic Dyad in β -Secretase When Bound to Hydroxyethylene Transition State Analogue Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2011, 54, 3081-3085.	6.4	13
24	An overview of key routes for the transformation of sugars into carbasugars and related compounds. <i>Carbohydrate Chemistry</i> , 2012, , 263-302.	0.3	13
25	Design, synthesis and structural analysis of mixed β/α -peptides that adopt stable cyclic hairpin-like conformations. <i>Tetrahedron</i> , 2012, 68, 2391-2400.	1.9	12
26	Chemical Modification of a Dehydratase Enzyme Involved in Bacterial Virulence by an Ammonium Derivative: Evidence of its Active Site Covalent Adduct. <i>Journal of the American Chemical Society</i> , 2015, 137, 9333-9343.	13.7	12
27	Preliminary studies on the incorporation of sugars into naphthoquinones: synthesis of (1R,2S,3S,4R,4aS,11bS)-2-(benzyloxy)-1,2,3,4,4a,5-hexahydro-1,3,4-trihydroxy-11bH-benzo[b]carbazole-6,11-dione. <i>Tetrahedron: Asymmetry</i> , 2005, 16, 11-14.	1.8	11
28	Preliminary studies on the synthesis of rancinamycins from nitrosugars: first total synthesis of (3S,4S,5S,6R)-5-benzyloxy-6-hydroxy-3,4-(isopropylidendioxy)-cyclohex-1-enecarbaldehyde. <i>Tetrahedron: Asymmetry</i> , 2005, 16, 4045-4049.	1.8	11
29	Mechanistic Basis of the Inhibition of Type II Dehydroquinase by (2 <i>S</i>)- and (2 <i>R</i>)-2-Benzyl-3-dehydroquinic Acids. <i>ACS Chemical Biology</i> , 2013, 8, 568-577.	3.4	11
30	Preliminary studies on a novel synthesis of β -amino acids: stereocontrolled transformation of d- and l-glyceraldehyde into 3-amino-2-(2-dimethyl-1,3-dioxolan-4-yl)propanoic acids. <i>Tetrahedron: Asymmetry</i> , 2006, 17, 3063-3066.	1.8	9
31	Synthesis and evaluation of strand and turn modified ring-extended gramicidin S derivatives. <i>Bioorganic and Medicinal Chemistry</i> , 2011, 19, 3402-3409.	3.0	9
32	Inverted analogs of the antibiotic gramicidin S with an improved biological profile. <i>Bioorganic and Medicinal Chemistry</i> , 2012, 20, 6059-6062.	3.0	8
33	Exploring the Water-Binding Pocket of the Type II Dehydroquinase Enzyme in the Structure-Based Design of Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 3494-3510.	6.4	8
34	Insights into substrate binding and catalysis in bacterial type II dehydroquinase. <i>Biochemical Journal</i> , 2014, 462, 415-424.	3.7	8
35	Irreversible covalent modification of type I dehydroquinase with a stable Schiff base. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 706-716.	2.8	8
36	Deoxyhexoses from Rhamnose in the Search for Inducers of the Rhamnose Operon: Synergy of Chemistry and Biotechnology. <i>Chemistry - A European Journal</i> , 2016, 22, 12557-12565.	3.3	8

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37	High-resolution structures of <i>Thermus thermophilus</i> enoyl-acyl carrier protein reductase in the apo form, in complex with NAD ⁺ and in complex with NAD ⁺ and triclosan. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2012, 68, 1139-1148.	0.7	7
38	Design, Synthesis, and Structural Analysis of Turn Modified α -Cyclodextrin- β -Cyclodextrin Peptide Derivatives toward Crystalline Hexagon-Shaped Cationic Nanochannel Assemblies. <i>Crystal Growth and Design</i> , 2013, 13, 4355-4367.	3.0	6
39	Hydroxylammonium derivatives for selective active-site lysine modification in the anti-virulence bacterial target DHQ1 enzyme. <i>Organic Chemistry Frontiers</i> , 2019, 6, 3127-3135.	4.5	4
40	A Nitro Sugar-Mediated Stereocontrolled Synthesis of α -Amino Acids: Synthesis of a Polyhydroxylated <i>trans</i> - α -2-Amino- β -Cyclohexanecarboxylic Acid. <i>European Journal of Organic Chemistry</i> , 2012, 2012, 2969-2979.	2.4	3
41	Preliminary Studies on the Michael Addition of Quinones to Nitroolefins: (6bR,10aS)-7,8,9,10,10a,11-Hexahydro-6bH-benzo[a]carbazole-5,6-diones, (4aR,11bS)-1,2,3,4,4a,5-Hexahydro-11bH-benzo[b]carbazole-6,11-diones, and 1,2,3,4-Tetrahydro-5H-benzo[b]carbazole-6,11-diones. <i>Synlett</i> , 2007, 2007, 1399-1402.	1.8	1
42	Highly functionalized cyclic and bicyclic α -amino acids from sugar α -nitroesters. <i>Tetrahedron</i> , 2020, 76, 130837.	1.9	0
43	Total synthesis of (5S,6S)-6-amino-2,8-dimethylnonan-5-ol and (5S,6S)-6-amino-7-cyclohexyl-2-methylheptan-5-ol. <i>Arkivoc</i> , 2007, 2007, 380-388.	0.5	0