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Endogenous water-triggered and ultrasound accelerated synthesis of 1, 5-disubstituted tetrazoles via a solvent and catalyst-free Ugi-azide reaction

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1,5-disubstituted tetrazoles (1,5-DS Ts) are the bioisosteres of the cis amide bond in peptides due to their similar physicochemical properties in living systems. They are an important class of heterocycles with wide range of applications in the medicinal chemistry, for example, antifungal agents. Additionally, 1,5-DS-Ts are used as bidentate ligands, as a metal-organic frameworks precursor, an bioimaging agents, as a photoimaging agents and in high energy materials. The main routes for the synthesis of 1,5-DS-T's are [3+2] intermolecular cycloadditions and Ugi-azide reaction UA). Anilines have received limited attention in isocyanide based multicomponent reactions (I-MCRs) like the UA reactions due to the low concentration of iminium ions in the reaction medium because of the low basicity of Schiff bases. There is one report by our group of catalyst assisted UA reaction using anilines, in which InCl3 played a key role to activate the weak basic Schiff base towards iminium ion formation and hence to continue the UA reaction in the forward direction. To the best of our knowledge, only the reports by Shahrisa and Safa describe the development of a solvent-free UA-reaction using Lewis acid catalysts towards 1,5-DS-T's. However, both reports gave an undetailed reaction mechanism and little explanation for hydrazoic acid formation. The synthesis of 1,5-DS-T's has not been reported under solvent and catalyst-free conditions neither via one-pot nor stepwise methods. As a part of our ongoing research programme towards sustainable strategies based on I-MCRs, we have recently reported the first synthesis of 1,5-DS-T's via a USI assisted UA reaction with a short reaction time and a water triggered USI-assisted protocol towards 1,5-DS-T's via the UA reaction under solvent-free and catalyst-free conditions with a wide substrate scope in moderate to excellent yields. This protocol is the first report of endogenous water-triggered formation of hydrazoic acid via single proton exchange with TMSN3 and the first solvent and catalyst free approach for the UA-reaction. The main features such as green conditions and environmental friendliness make this method a sustainable alternative towards the synthesis of 1,5-DS-T's.

Biography

Gámez-Montaño Rocío has got her PhD under guidance of Professor Raymundo Cruz-Almanza in UNAM, CDMX, México. After a Post-doctoral fellow under guidance of Professor Jieping Zhu at Gif-Sur-Yvette, France, she was incorporated to University of Guanajuato, México, where she is actually full-time Research-Professor (Class B). Her scientific interest includes design and development of efficient synthesis of heterocycles and poly-heterocycles via MCR, in vitro and in silico studies of biological properties, applications in optics, as well as study of reaction mechanisms

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