NMR Characterization of New 2,6- and 6,8-Diaminopurines

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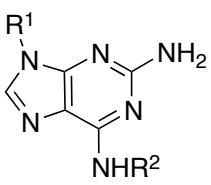
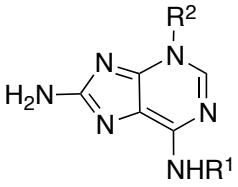
Purine-based compounds display a wide range of biological activities.[1] Their potency and selectivity depends on the position and nature of the substituents on the ring.

Adenine is one of the most important naturally occurring nitrogen heterocycles. This purine nucleobase plays a fundamental role in the nucleic acid chemistry and cellular biochemistry. In fact, the function of a remarkable number of proteins is governed by adenine nucleotides (ATP, cAMP, NAD, FAD, PAPS. . .) as co-factors or co-substrates. Moreover, the increasing number of reports describing new biological activities of synthetic adenine derivatives reveals the great potential of these compounds as new chemical-biology tools and therapeutic target as enzyme inhibitors or receptor agonists/antagonists. [1]

As part of a new research program aiming to develop new purine derivatives, we planned a synthetic strategy that enables the synthesis of adenine derivatives **1**. A series of compounds **1** were obtained in very good yield and the new products could be assigned to structures **1** on the basis of the IR and NMR techniques.



1



2

Attempts to prepare compounds **1** led us to isolate a different class of compounds. From the ^{1}H and ^{13}C NMR data we confirmed that both products should have in common a purine structure. Finally, 2D NMR spectra evidenced a completely different pattern of correlations, which were determinant to propose structure **2** to these new products. The ^{1}H, ^{13}C and 2D NMR data will be presented and discussed.

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References:

[1] Legraverend, M; Grierson, D. S; *Bioorg. Med. Chem*., (2006) *14*, 3987.