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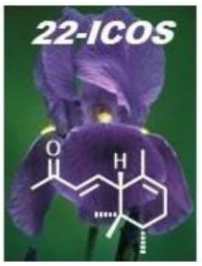

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Azidopurines and 1,2,3-Triazolylpurines as Novel Synthetic Tools for Bioorganic and Materials Chemistry

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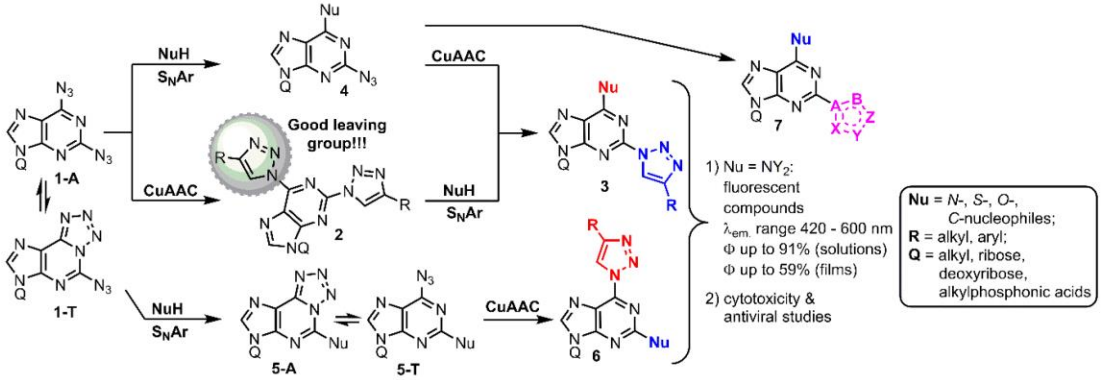
Azolylpurines and azolylpurine nucleosides have important medicinal and biological applications [1]. We have developed a novel approach for the synthesis of C(2) and C(6) modified purines and purine nucleoside analogues of type **3** containing 1,2,3-triazolyl substituents [2,3]. The method uses 2,6-diazidopurine derivatives **1** as the key starting materials. The latter can be transformed into novel structural entities – 2,6-bis(1,2,3-triazol-1-yl)purine derivatives **2** – including ribo-, deoxyribo-, and arabino-nucleoside analogs. It was found that 1,2,3-triazolyl substituent acts as excellent leaving group and permits nucleophilic aromatic substitution (**2→3**). Thus, regioselective S_NAr reactions with various nucleophiles like amines [2,4], thiols [3], amino acids and peptides [5], hydrazines, anilines, alcohols and deprotonated C-H acids are possible for compounds **2** at C(6).
Further investigations lead to the use of diazide **1** as a substrate for S_NAr reactions. Depending on the nature of N(9) substituent (Q), the incoming nucleophile and the experimental conditions, selectivity towards differently substituted compounds **4** and **5** can be achieved. This is mainly determined by azide-tetrazole tautomerism **1-A** ↔ **1-T**. To get a deeper insight, 2,6-disubstituted purine reactivity trends are explored by DFT methods and the utility of these reactions is demonstrated by the synthesis of 2/6-azido-6/2-alkylthio-purine derivatives [6]. In this context tautomerism **5-A** ↔ **5-T** is studied in detail. We have also found that 2-(1,2,3-triazolyl)adenine/adenosine analogs **3** (Nu = NY_2) and their regioisomers **6** possess excellent fluorescent properties. Compounds **3** and **6** can be applied both for fluorescent oligonucleotide synthesis [4] and for OLED technologies. Moreover, the developed chemistry permits synthesis of novel purine conjugates containing 5-membered heterocycles at C(2). Biological activity profile of the disclosed compounds will be also discussed.



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