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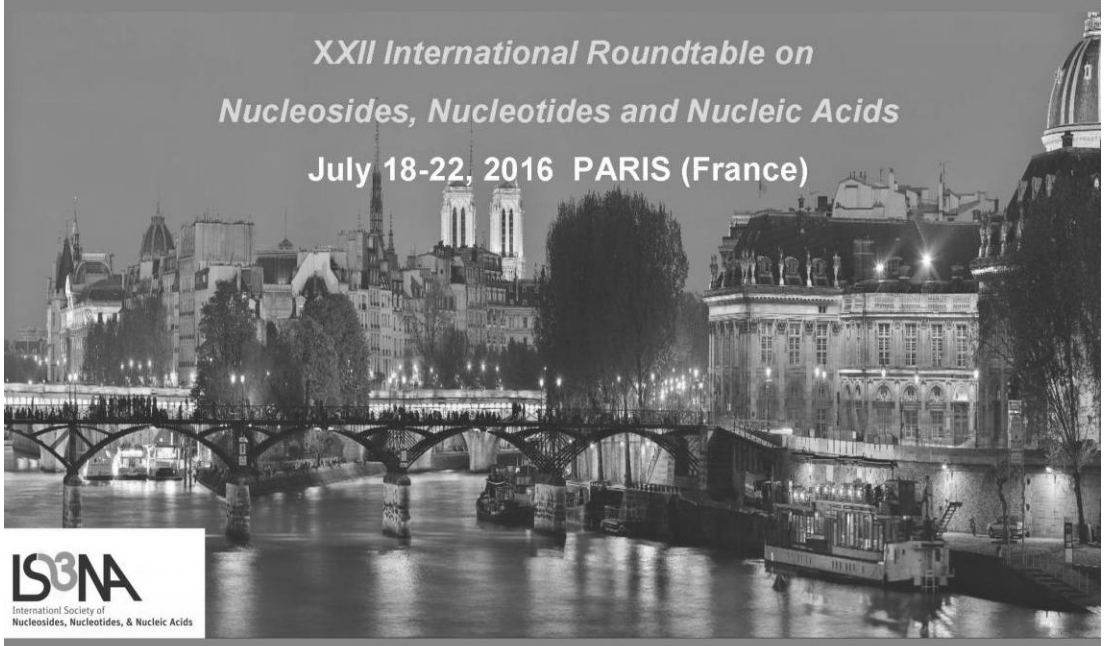

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ABSTRACT BOOK

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Novel fluorescent 2-(1,2,3-triazolyl)adenine analogs

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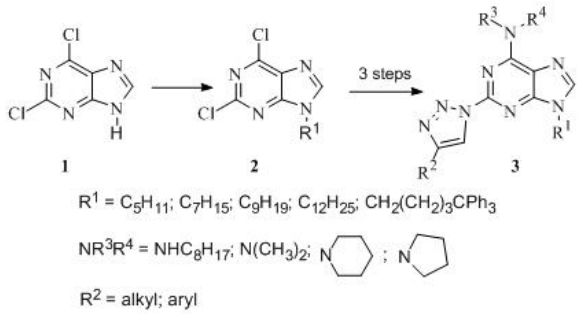
Introduction: Push-pull purine derivatives are attractive as sensors and reporters for biological applications. Recently the fluorescent purines as materials for electronic devices have also been developed.[1] Different combinations of electron donor and acceptor substituents allow fluorescence emission tuning in the range of 350-450 nm, making the purines good candidates for the construction of OLED devices.[1] Earlier we have reported that N^6-substituted 2-triazolyl-adenine nucleosides exhibit strong fluorescence with emission maxima around 400 nm and quantum yields up to 53%.[2]

The aim of this research was to synthesize 9-alkyl purines with electron donor at C(6) and 4-substituted 1,2,3-triazol-1-yl group as acceptor at C(2) and investigate their fluorescence properties.

Results and discussion: Target products **3** were obtained in four-step synthesis. Alkylation of **1** with a long chain alkyl halogenide or alcohol (Mitsunobu reaction) provided **2.** A nucleophilic substitution with NaN_3 gave 2,6-diazido-9-alkylpurines. Further, two synthetic routs toward **3** were developed: 1) nucleophilic substitution of azido group with amine at C(6) followed by a CuAAC reaction with terminal alkynes and 2) reaction of diazide to afford bis-triazolylpurines, followed by S_NAr reaction on C(6)-triazolyl group with amine. CuAAC reactions with terminal alkynes proceeded in DMF at 60-90 °C or in THF, in the presence of 10% acetic acid, using $CuSO_4 \cdot 5H_2O$ and sodium ascorbate as catalyst generating system.



Scheme 1. The synthesis of fluorescent purine derivatives

Purine derivatives **3** showed bright blue fluorescence with emission maxima at 420-450 nm. Fluorescence properties of **3** will be further investigated and discussed.

Alkylation of 2,6-dichloropurine **1** with diethyl(2-(2-hydroxyethoxy)ethyl) or diisopropyl(2-(2-hydroxyethoxy) methyl) phosphonates under Mitsunobu conditions gave acyclic nucleoside phosphonates (ANPs) **4** and **5.** Synthetic route used for synthesis of **3** was also applied to obtain ANPs **6.** Ester hydrolysis of **6** gave, as example, compound **7.** Thus, new ANPs with free phosphonic acid moiety were obtained.

Acyclic nucleoside phosphonates (ANPs) represent an important class of antiviral nucleoside derivatives, many of them have become important therapies for virus infections.[3]

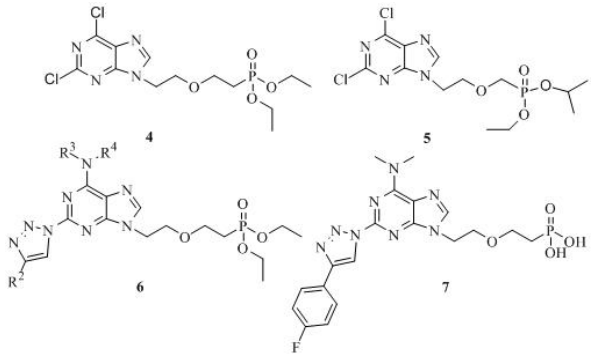


Figure 1. The structures of obtained ANPs.

Conclusion: We have developed an efficient route for synthesis of fluorescent 2-(1,2,3-triazol-1-yl)adenine derivatives suitable for obtaining push-pull purines possessing various combinations of electron donor and acceptor substituents.

References

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