Synthesis and structural characterization of *N*-substituted azoles with potential pharmacological activities

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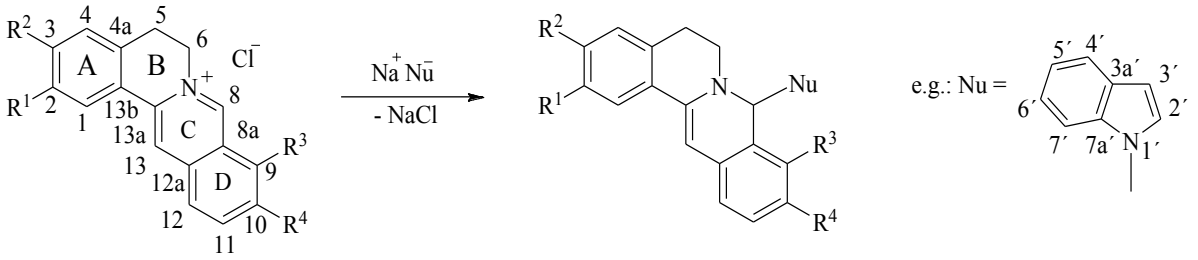
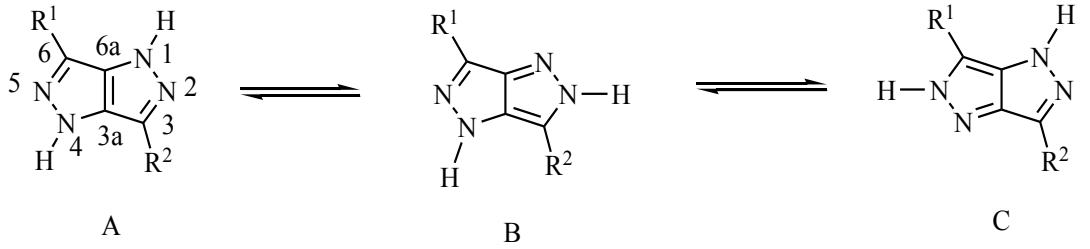
The main goal of our study is to synthesize and structurally characterize the *N*-substituted azoles. They are indispensable components of many pharmaceuticals and therapeutic drugs. This study comprises of two main projects: isoquninoline alkaloids and pyrazolopyrazoles.

The basic skeletons of quaternary protoberberine alkaloids and quaternary benzophenanthridine alkaloids contain iminium bonds ($C=N^+$), which are rather sensitivity to the nucleophilic attack resulting in the formation on covalent adducts - 8-substituted-7,8-dihydroprotoberberines and 6-substituted-5,6-dihydrobenzophenanthridines, respectively. All new compounds were characterized by using mass spectrometry, NMR spectroscopy, and some of them also by X-ray diffraction. We have found some interesting trends in the experimental NMR chemical shifts, which were rationalized by density-functional calculations.



Scheme 1. Nucleophilic addition of azoles to a quaternary protoberberine skeleton.

Substituted purines and purine analogues represent an important group of heterocyclic compounds. Generally, these compounds can exist in a number of tautomeric forms, which are relevant to any investigation of their binding modes with biological targets. We have synthesized a series of variously substituted analogs derived from pyrazolo[4,3-*c*]pyrazole and investigated their tautomeric equilibria using model systems of *N*-methylated pyrazolo[4,3-*c*]pyrazoles.



Scheme 2. Three tautomeric forms (N1H/N4H, N2H/N4H, and N1H/N5H) of pyrazolo[4,3-*c*]pyrazoles.