$^{1}H–^{15}N$ HMBC NMR AS A TOOL FOR RAPID IDENTIFICATION OF AZAINDOLE CANNABINOID DRUGS

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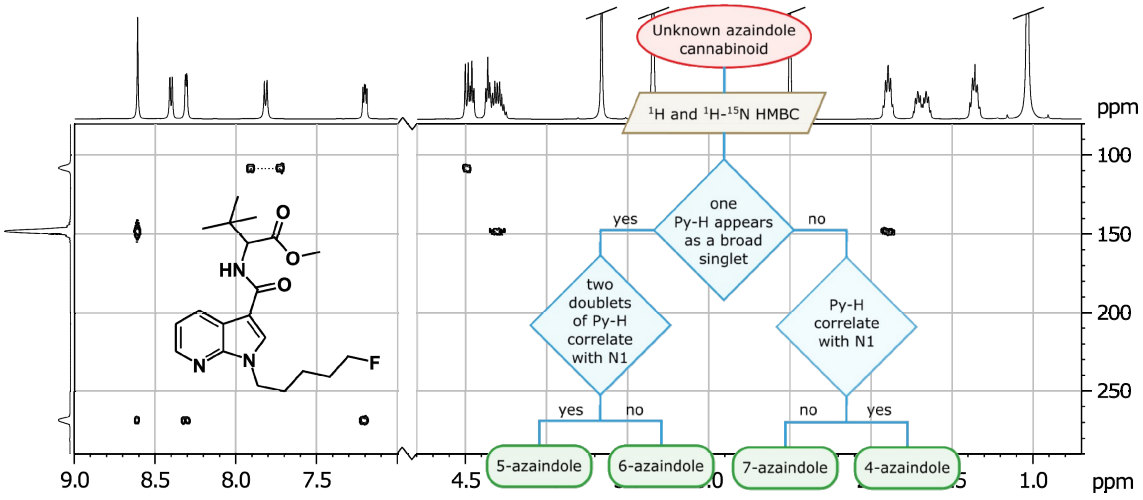
A rapid growth in the number of new synthetic cannabinoid receptor agonists (SCARs) renders this group of new psychoactive substances particularly demanding in terms of detection, identification, and responding. With almost no reference data available, differentiation and structural elucidation of constitutional isomers represents one of the major obstacles [1]. Amongst different 2D NMR techniques, HMBC experiment, introduced by Summers and Bax in 1986 [2], become a corner stone in the molecular structure determination process [3]. Since nitrogen is a common element in biological organic compounds, $^{1}H–^{15}N$ HMBC plays an important role in structural identification. Herein, we present a simple and efficient flow chart diagram, based on ^{1}H and $^{1}H–^{15}N$ HMBC NMR spectra, for distinguishing between isomeric azaindoles, which is a common heterocyclic framework in new synthetic cannabinoids. The concept was also tested on 5F-MDMB-P7AICA, newly launched on illegal drug market.



[1] Martek, B. A.; Mihelač, M.; Gazvoda, M.; Virant, M.; Urankar, D.; Krivec, M.; Gostič, M.; Nemec, B.; Koštrun, B.; Janežič, M.; Klemenc, S.; Košmrlj, J. *Drug Test. Anal*. **2019**, 1–9.

[2] Bax, A.; Summers, M. F. *J. Am. Chem. Soc.* **1986**, *108*, 2093–2094.

[3] Furrer, J. *Chem. Commun.* **2010**, *46*, 3396–3398.