ON THE UTILITY OF NONUNIFORMLY SAMPLED TWO-DIMENSIONAL NMR SPECTRA IN THE PHARMACEUTICAL INDUSTRY

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We present some intriguing examples of NMR structure elucidation – with a special pharmaceutical industrial flair. A common feature of these problems is that the use of nonuniformly sampled 2D NMR spectra substantially contributed to their successful solution. We discuss the difficulties that we encountered during the acquisition and interpretation of the 2D NMR spectra of these samples, and we suggest a novel and efficient way to overcome them.

The examples presented involve a) the determination of the constitution of a complex molecule; b) the unambiguous resonance assignment of a molecule consisting of several identical functional groups in different positions; c) the verification of the substitution pattern in aromatic rings when “routine” techniques fail due to severe signal overlap; d) proof of a four-site conformational exchange in a severely mass-limited sample; e) detection of trace impurities in a starting material used in the production of a drug substance. The theoretical background and the experimental conditions of the examples are discussed in detail in our recent publication.[1]

Áron Szigetvári’s PhD thesis (under preparation) is partly based on the presented topic.

REFERENCES

[1] Á. Szigetvári, C. Szántay Jr, *Magn. Reason. Chem.* **2021**, *59*, 264–286.