

## Solution to the symmetrical molecule NMR challenge

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The <sup>1</sup>H-NMR spectrum of a mixture of *trans* and *cis* isomers of an aliphatic amine hydrochloride shows three peaks at the vicinity of 10 ppm [1]. The smaller signals observed at 9.7 ppm and 10.5 ppm correspond to the *cis* isomer. This is because the *cis* configuration of the amine makes protons of the –NH<sub>2</sub><sup>+</sup>– group to become chemically non-equivalent: one of the –NH<sub>2</sub><sup>+</sup>– protons is spatially closer to the –CH<sub>2</sub>– group of cyclopropane whereas the other is closer to the protons of the CH groups. The protons of the –NH<sub>2</sub><sup>+</sup>– group of the *trans* isomer, on the other hand, are in

the same spatial environment, so they appear as one signal at 10.1 ppm. From the peak integrals given in the NMR spectrum [1], we can therefore estimate the *trans/cis* ratio to be approximately  $2.11/(0.54 + 0.42) \approx 2.2$ .

### Declarations

**Conflict of interest** The author declares no competing interests.

### Reference

1. Kozytskiy AV. Symmetrical molecule NMR challenge. *Anal Bioanal Chem.* 2023;415:3–4.

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