

Abstract

Chiral Recognition by Dissolution Dynamic Nuclear Polarization NMR Spectroscopy [†]

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The recognition of enantiomeric molecules by chemical analytical techniques is still a challenge. A method based on d-DNP (dissolution dynamic nuclear polarization) NMR spectroscopy to study chiral recognition was described for the first time [1]. DNP allows NMR sensitivity to be boosted by several orders of magnitude, overcoming one of the main limitations of NMR spectroscopy [2]. A method integrating d-DNP and ¹³C-NMR-aided enantiodifferentiation using chiral solvating agents (CSA) was developed, in which only the chiral analyte was hyperpolarized and selectively observed by NMR. The described method enhances the sensitivity of the conventional NMR-based procedure [3] and lightens the common problem of signal overlapping between analyte and CSA. As proof of concept, racemic metabolite ¹³C-labeled DL-methionine was enantiodifferentiated by a single-scan ¹³C-NMR experiment. This method entails a step forward in the chiral recognition of small molecules by NMR spectroscopy; it opens new possibilities in situations where the sensitivity is limited, for example, when low analyte concentration is available or when measurement of an insensitive nucleus is required. The advantages and current limitations of the method, as well as future perspectives, are discussed.

References

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