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Monitoring of the ethionamide pro-drug activation in mycobacteria by ^1H high resolution magic angle spinning NMR

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Abstract

In this study, we use HRMAS NMR as a non-invasive technique to monitor the in vivo metabolism of a xenobiotic. The antituberculosis Ethionamide is a pro-drug that has to be activated in mycobacteria before inhibiting its cellular target. The use of ^1H HRMAS NMR has allowed to detect a metabolite (ETH*) of the drug directly in living bacteria, even with a spectrometer operating at the relatively low magnetic field of 300 MHz. We show that metabolism monitoring of an unlabelled drug at a therapeutically relevant concentration as low as 5 $\mu\text{g/ml}$ is within reach of the technique. ^1H HRMAS NMR in combination with diffusion filtering leads to the conclusion that the metabolite is located inside the intact cells. The comparison of the metabolite NMR signature with that of synthetic molecules proves the non-identity of ETH* with the ETH derivatives described previously in the literature.



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Keywords

HRMAS NMR; Anti-tuberculosis drug Ethionamide; Mycobacteria in vivo; Unlabelled precursor

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