

# NMR Measurement Report

Sample name: ST-123

13-3-2021

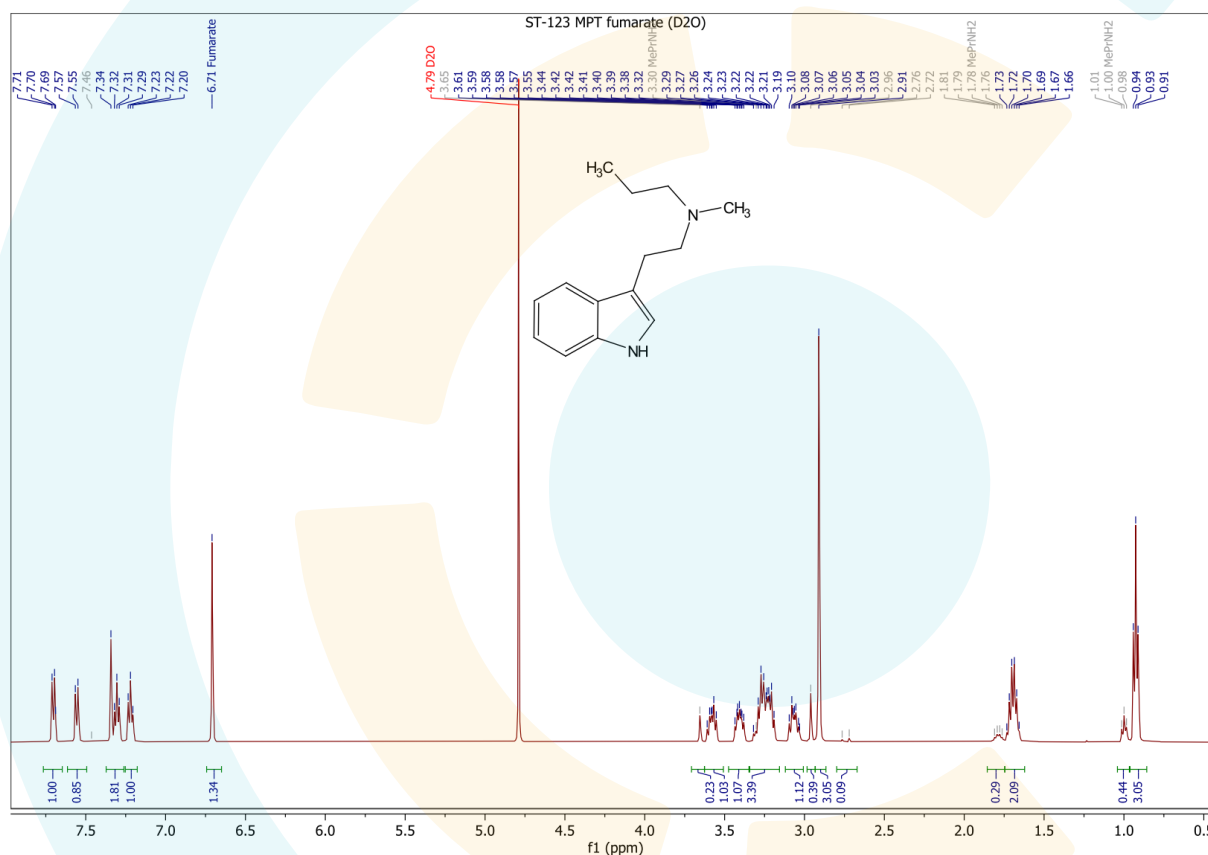
Spectrometer: Bruker 500 MHz

Solvent: D<sub>2</sub>O

Expected compound: MPT fumarate

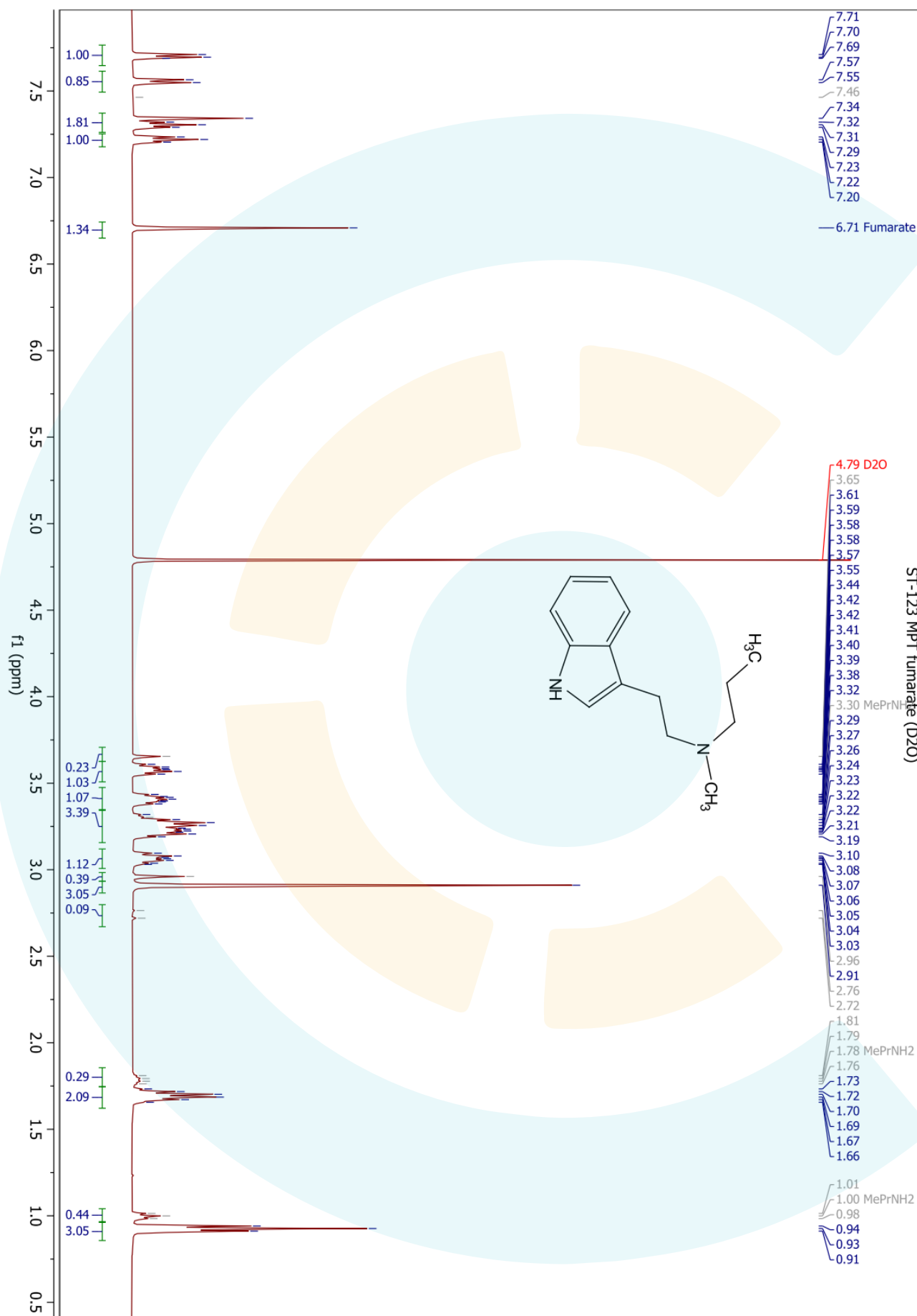
Identified compound: MPT fumarate

Estimated purity: 93%



**Lab Notes:** Right identity of the main product. The solution was opaque, indicating that something (probably an impurity) was not fully dissolved. The small peaks at 2.96, 1.78 and 1.00 ppm have similar fine structures and relative integrals to their neighboring peaks at 2.91, 1.69 and 0.93 ppm, which belong to the methyl-propyl-amino moiety. This makes it very likely that those additional peaks are caused by residual *N*-methylpropylamine that has also been co-crystallized as the fumarate salt, in which case it would amount to about 6% of the total weight. Other unidentified minor impurities/solvent residues were present as well. An additional measurement in DMSO-*d*<sub>6</sub> is recommended to obtain more information.

<sup>1</sup>H NMR: full non-empty spectrum



# <sup>1</sup>H NMR: cut and zoomed spectrum

