

NMR Measurement Report

Sample name: AC-15

10-9-2023

Spectrometer: Bruker 600 MHz

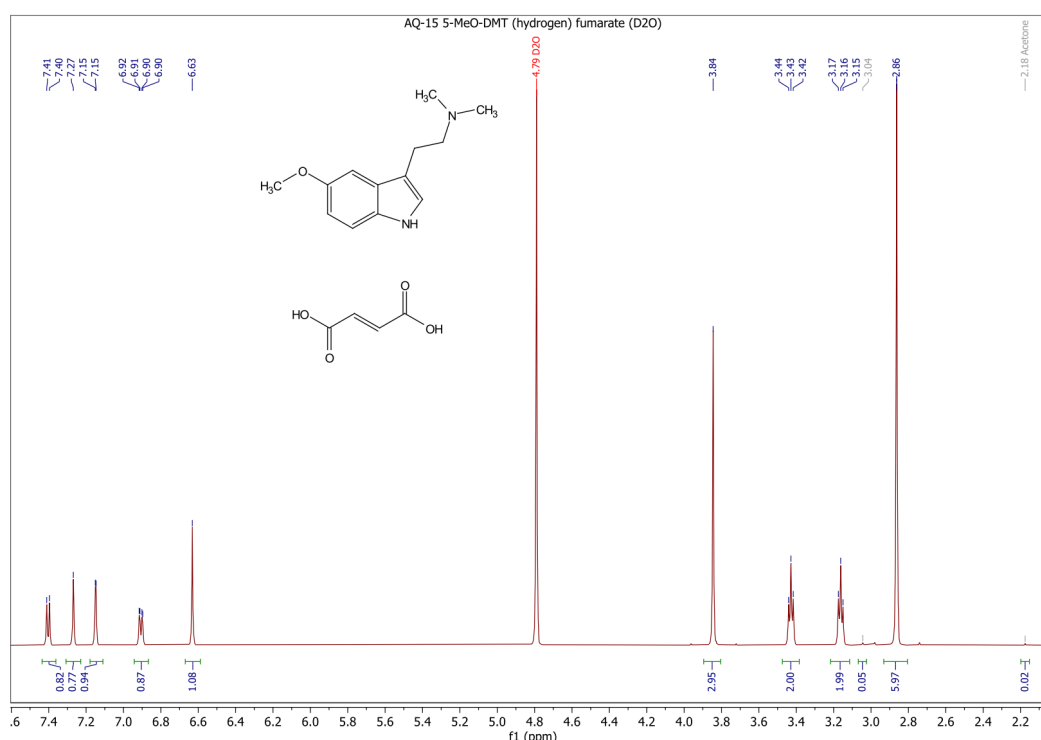
Solvent: DMSO-*d*₆ & D₂O

Expected compound: 5-MeO-DMT (hydrogen) fumarate

Identified compound: 5-MeO-DMT (hydrogen) fumarate

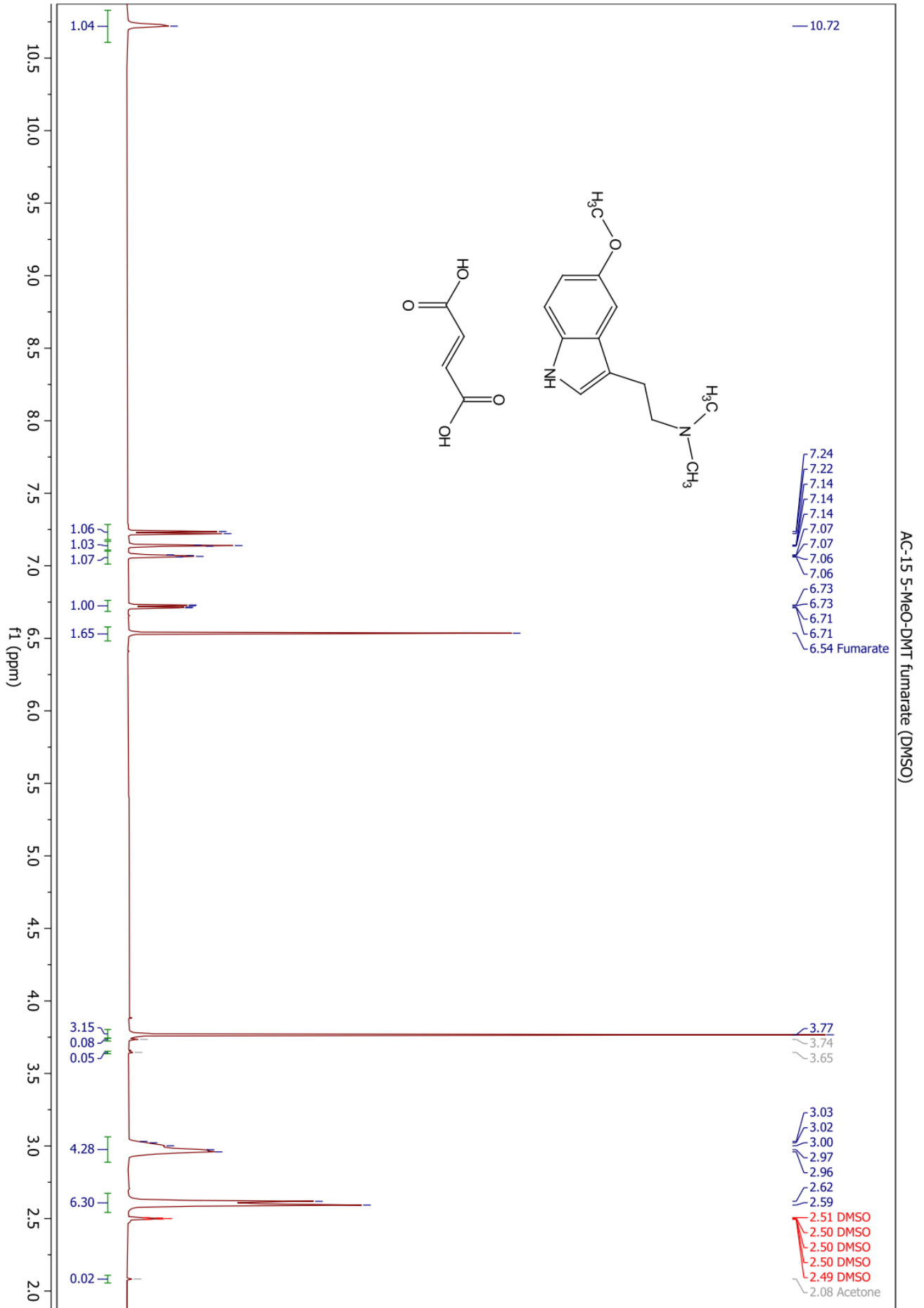
2-(5-methoxy-1*H*-indol-3-yl)-*N,N*-dimethylethan-1-amine

Estimated purity: >98%

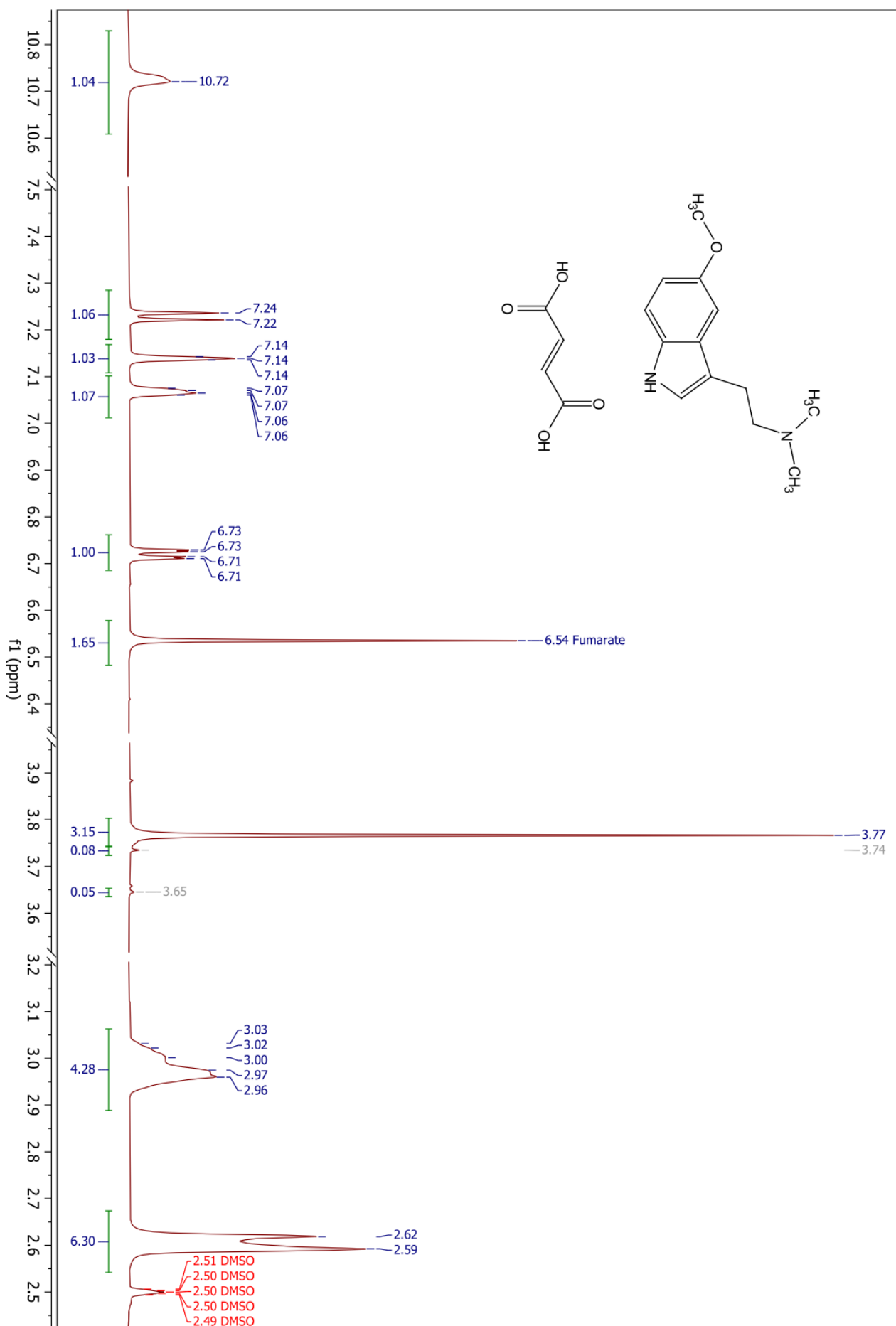


Lab Notes: The sample contained the expected product 5-MeO-DMT as a mixture of the fumarate (FM) and hydrogen fumarate (HFM) salts (1 to 0.65 ratio). The sample also contained a minor unidentified impurity and minimal traces of acetone. The difference in appearance and chemical shifts of the aliphatic proton peaks (CH₂ and N-CH₃) was due to formation of fumarate adducts in solution, leading in turn to an increase of the rotational energy barrier around the CH₂-N bond. As expected, this effect was not observed D₂O where the ions dissociate in solution. This confirmed the initial conclusions and identity of the product. For the measurement in D₂O, the sample was homogenized by grinding, whereafter a considerably higher FM to HFM ratio (1 to 0.05) was found.

¹H NMR: full non-empty spectrum

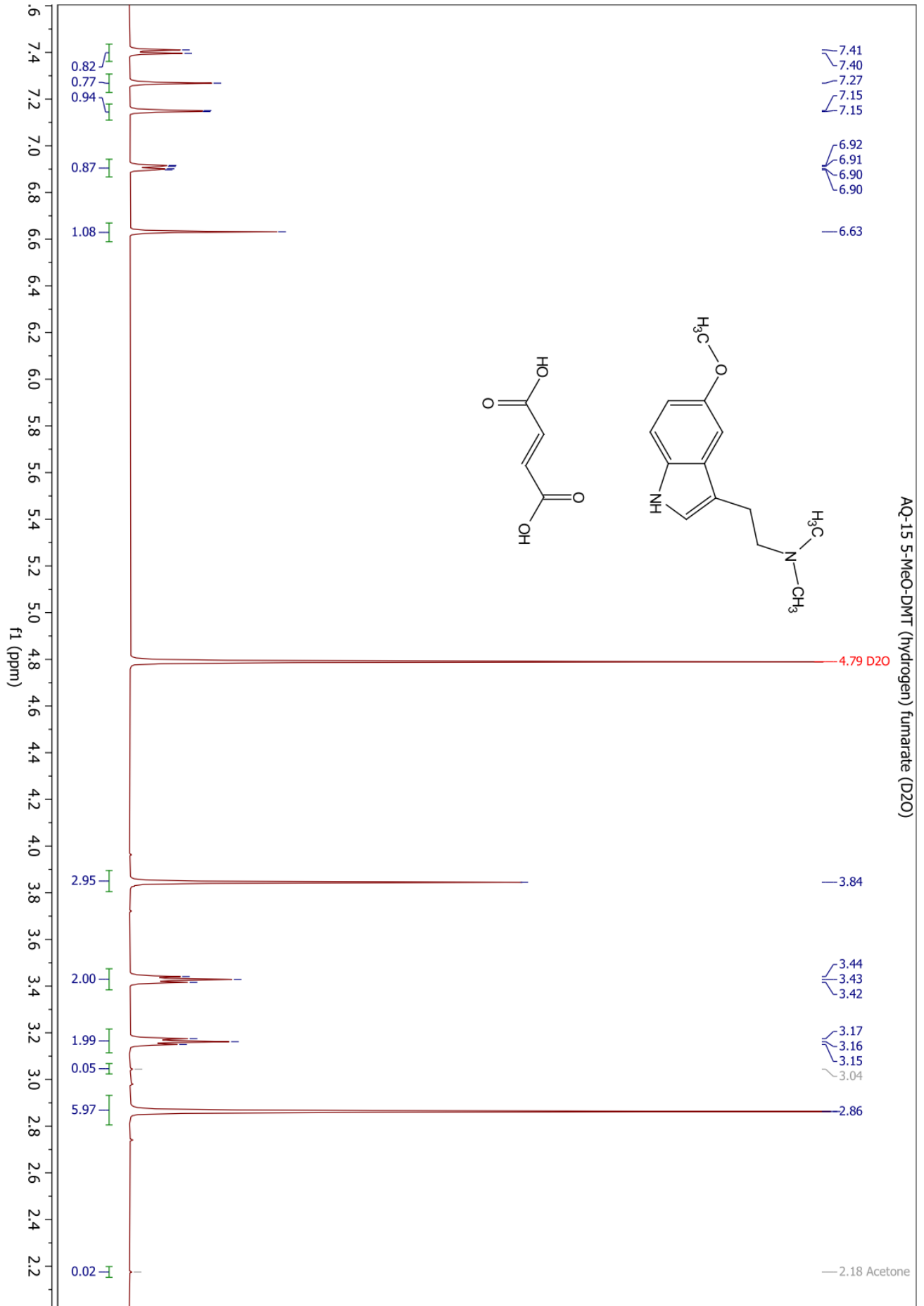


¹H NMR: cut and zoomed spectrum

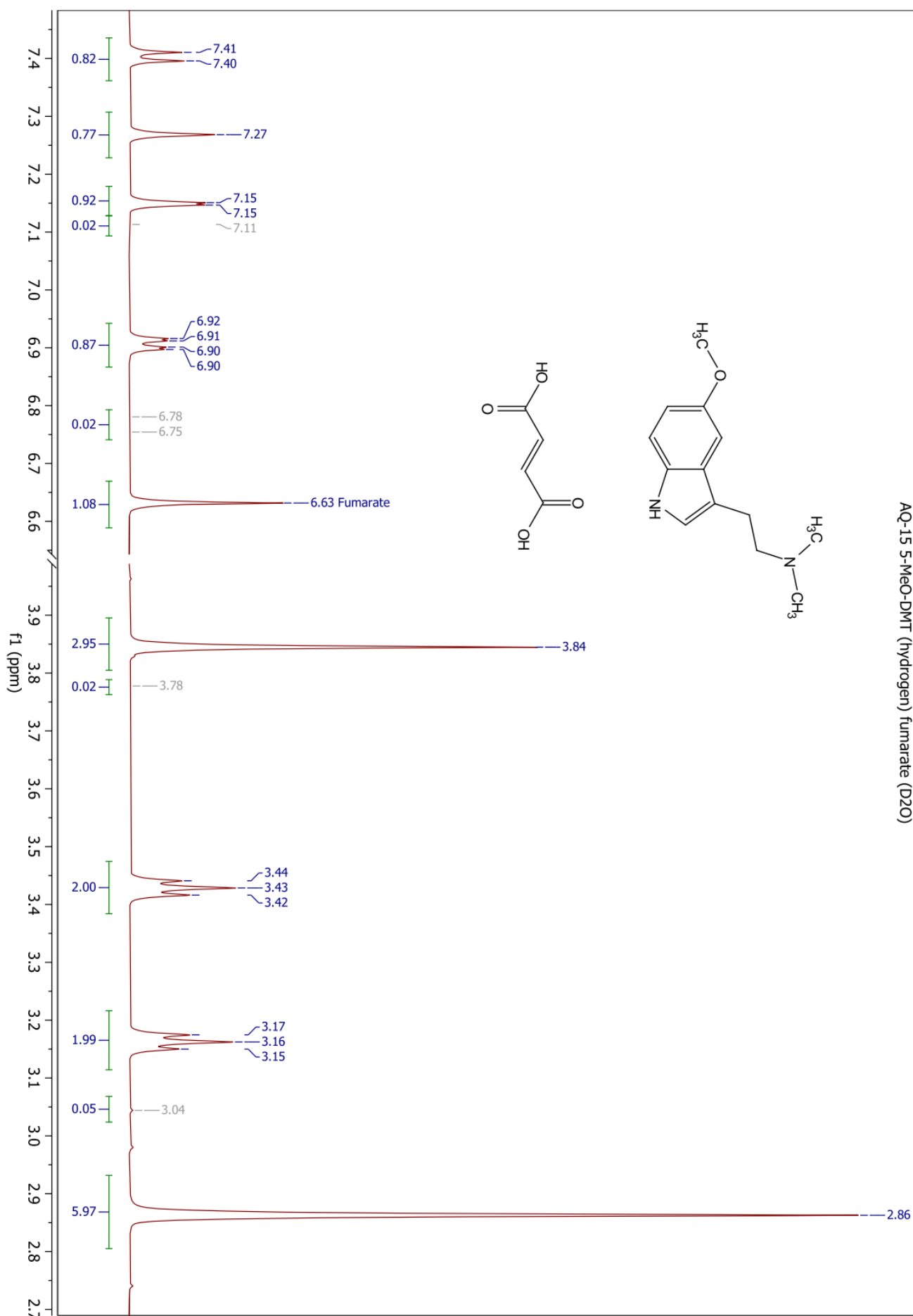


AC-15 5-MeO-DMT fumarate (DMSO)

¹H NMR: full non-empty spectrum



¹H NMR: cut and zoomed spectrum



AQ-15 5-MeO-DMT (hydrogen) fumarate (D₂O)