

¹H NMR Analysis Report

Sample name: GVT-15

20-8-2024

Spectrometer: Bruker 600 MHz

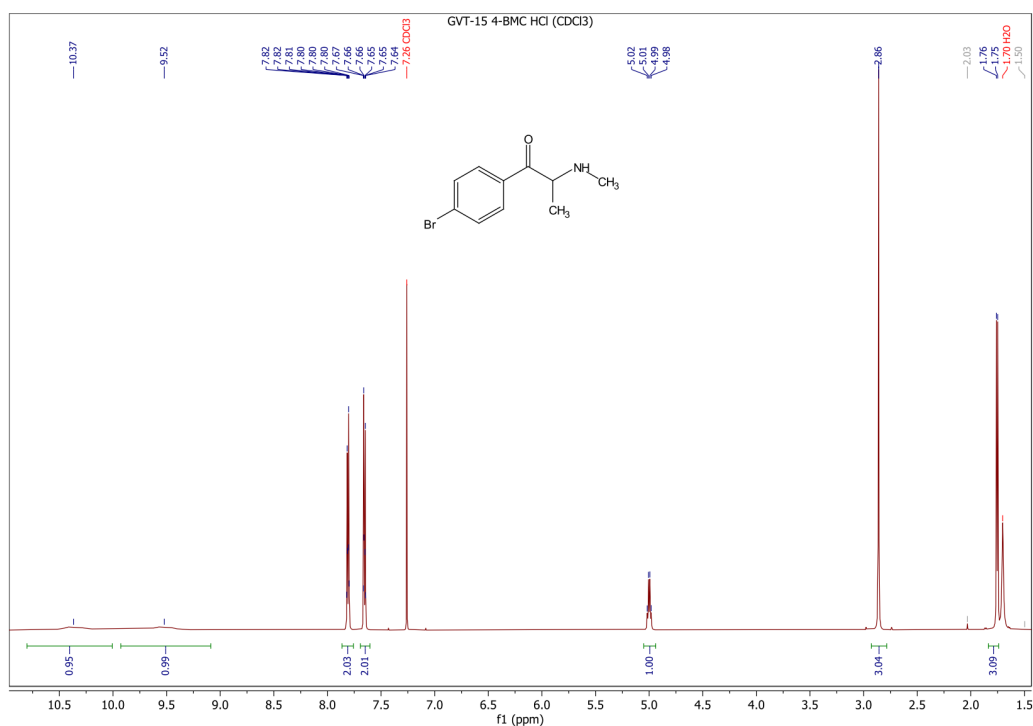
Solvent: CDCl₃ & D₂O

Expected compound: 4-BMC HCl

Identified compound: 4-BMC HCl (very likely)

2-(2-bromophenyl)-2-(methylamino)cyclohexan-1-one

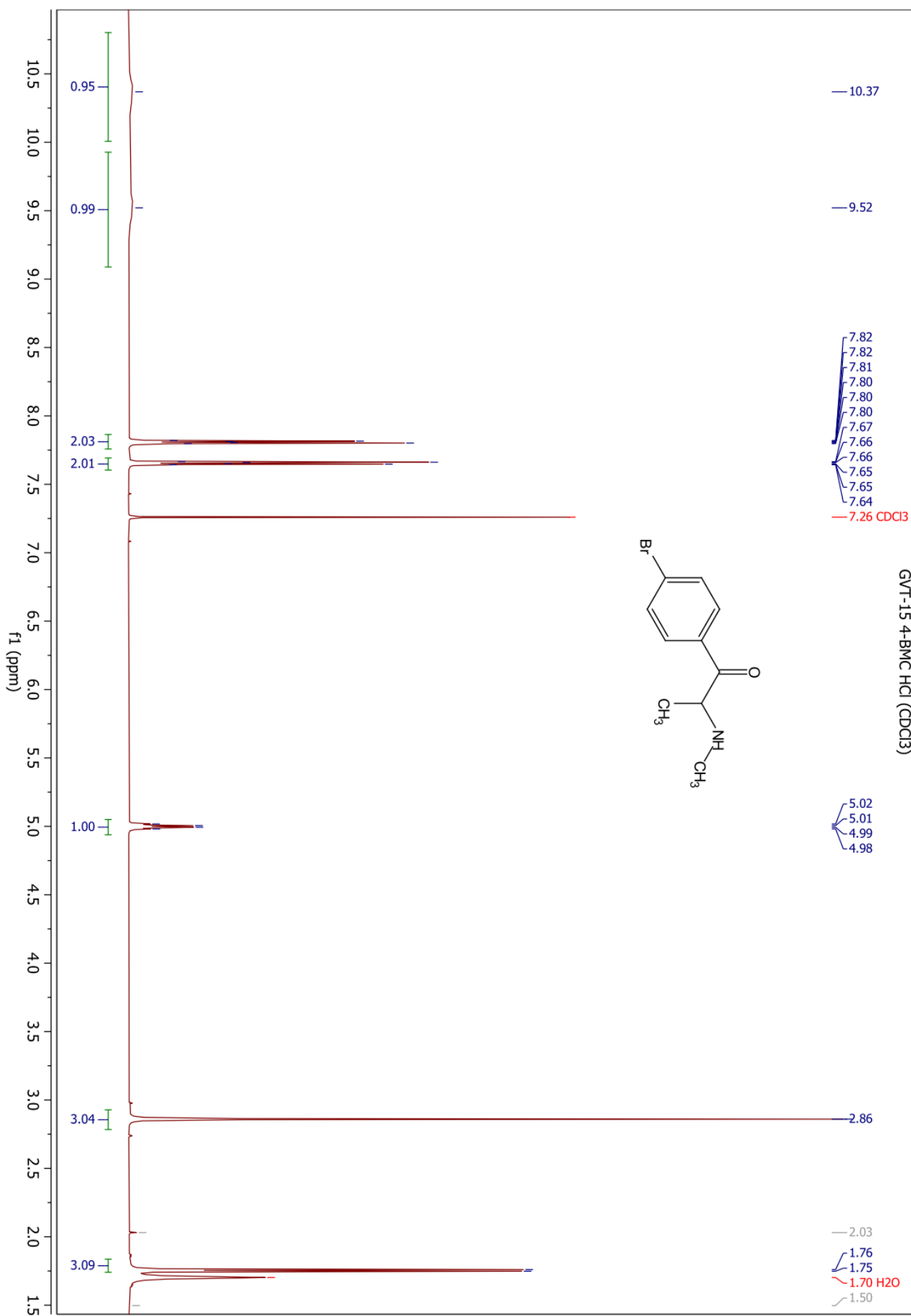
Estimated purity: ≥99%



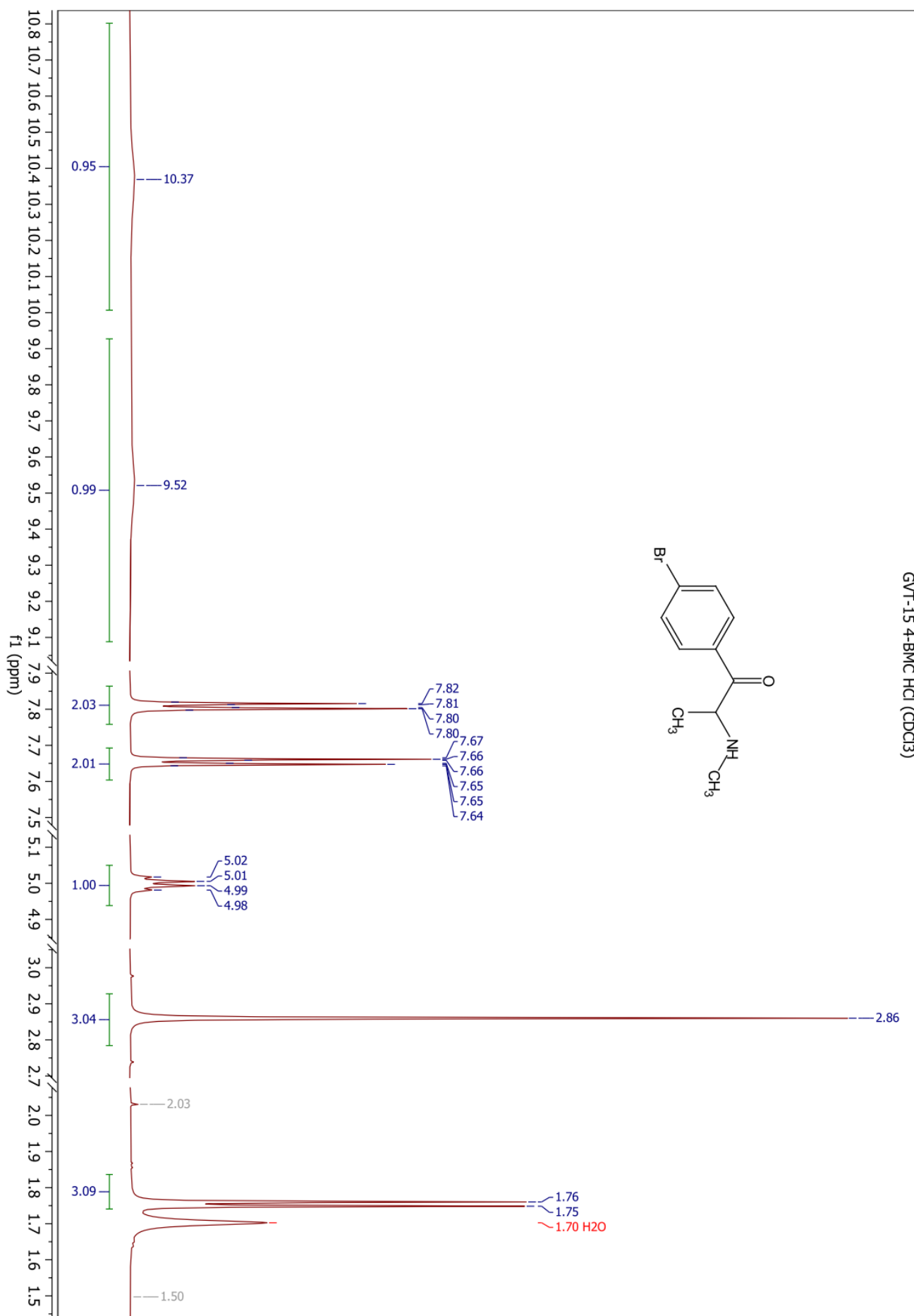
Lab Notes:

The sample was first measured in CDCl₃, which yielded a spectrum that was consistent with the expectations for the 4-BMC HCl salt. However, the difference between the spectra for 4-BMC and 4-CMC was not very pronounced, especially considering the fact that the 4-CMC spectra used as a reference were measured on a spectrometer with a lower working frequency and therefore resolution. To resolve this remaining uncertainty, a second measurement in D₂O has been performed. In D₂O, the difference between the brominated and chlorinated products was more pronounced, increasing the confidence in the results, albeit not to full certainty. For a conclusive result, additional analyses like elemental analysis or mass spectrometry are recommended. Alternatively, a mixture of the product with a known 4-CMC sample could be measured to see if one or two different products will be visible in the resulting spectrum.

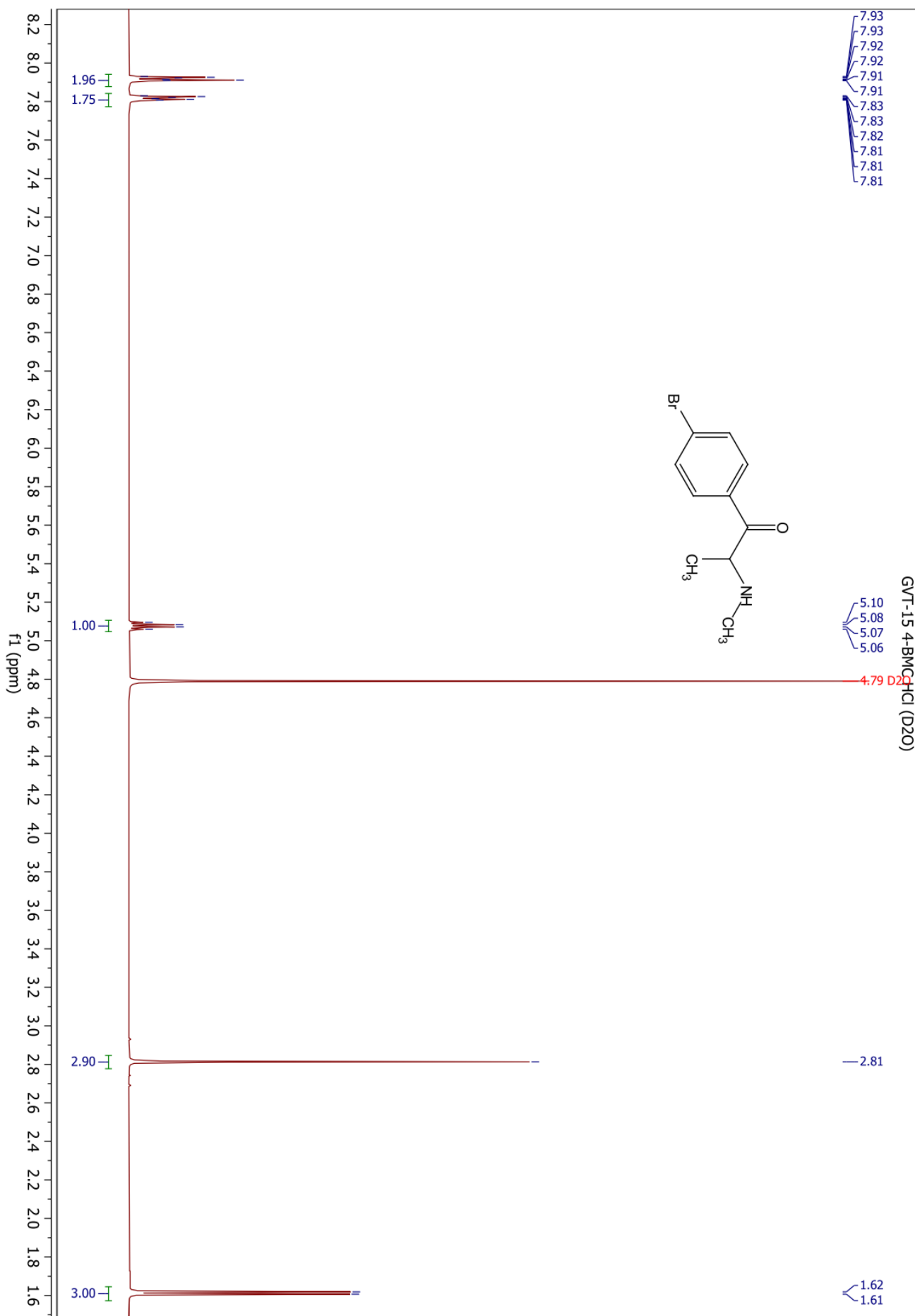
¹H NMR: full non-empty spectrum



¹H NMR: cut and zoomed spectrum



¹H NMR: full non-empty spectrum



¹H NMR: cut and zoomed spectrum

