NMR Measurement Report

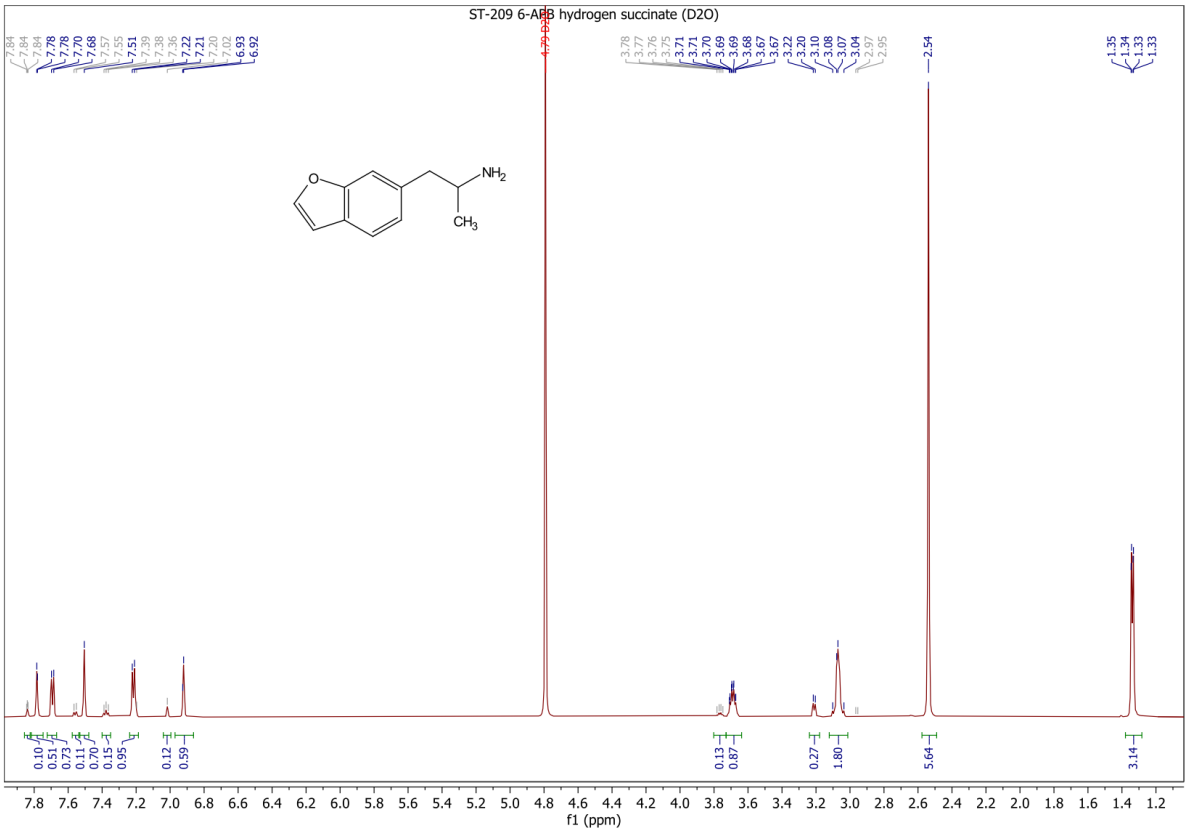
Sample name: ST-209 20-7-2022

Spectrometer: Bruker 600 MHz **Solvent**: D_2O

Expected compound: 6-APB

Identified compound: 6-APB hydrogen succinate (6-APB HS)

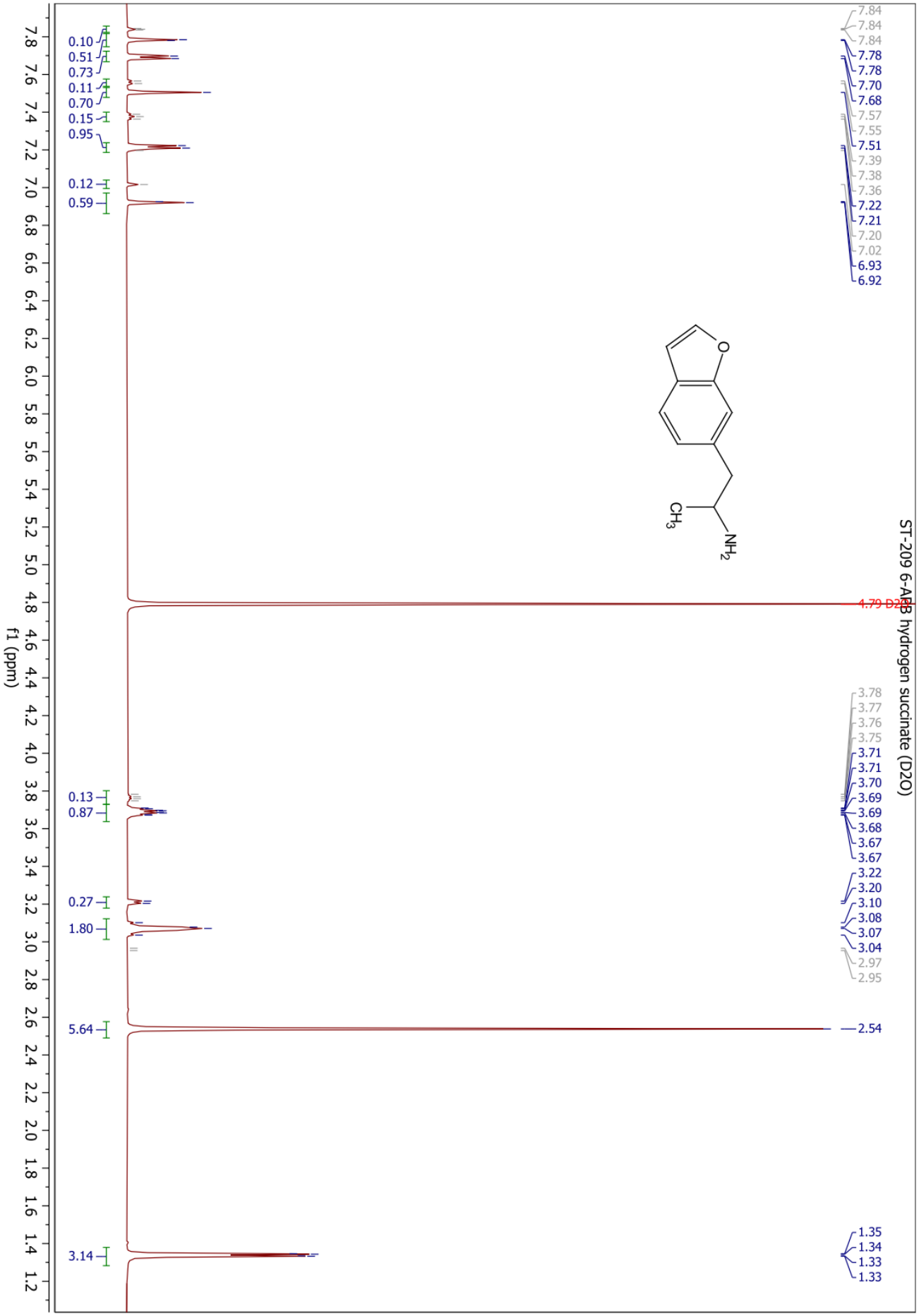
Estimated purity: ≤74%



Lab Notes: The sample contained around 13% of the isomer 4-APB (about market standard), as well as excess succinic acid (SA). The mass percentage of the two APB isomer HS relative to the SA excess was calculated as follows: The molecular mass of 4/6-APB HS is 293.32 g/mol, that of SA is 118.09 g/mol. The large singlet at 2.60 ppm belongs to succinate's CH_2-CH_2 protons and should therefore have an integral of 4. Thus, $Q_{APB\ HS}$, representing the mass percentage of 4/6-APB HS in the mixture, can be calculated: $Q_{APB\ HS} = \frac{293.32\,\frac{g}{mol}}{293.32\frac{g}{mol}+118.09\frac{g}{mol}\times\frac{5.64-4}{4}} \approx 0.858 = 85.8\%$. The maximal possible purity was calculated by multiplying $Q_{APB\ HS}$ with the percentage of 6-APB relative to 4-APB: 0.87 × 0.858 ≈ 0.747 = 74.7%. After sample preparation, small flakes of a solid precipitated (likely succinic acid). This indicates a lower than calculated total purity.

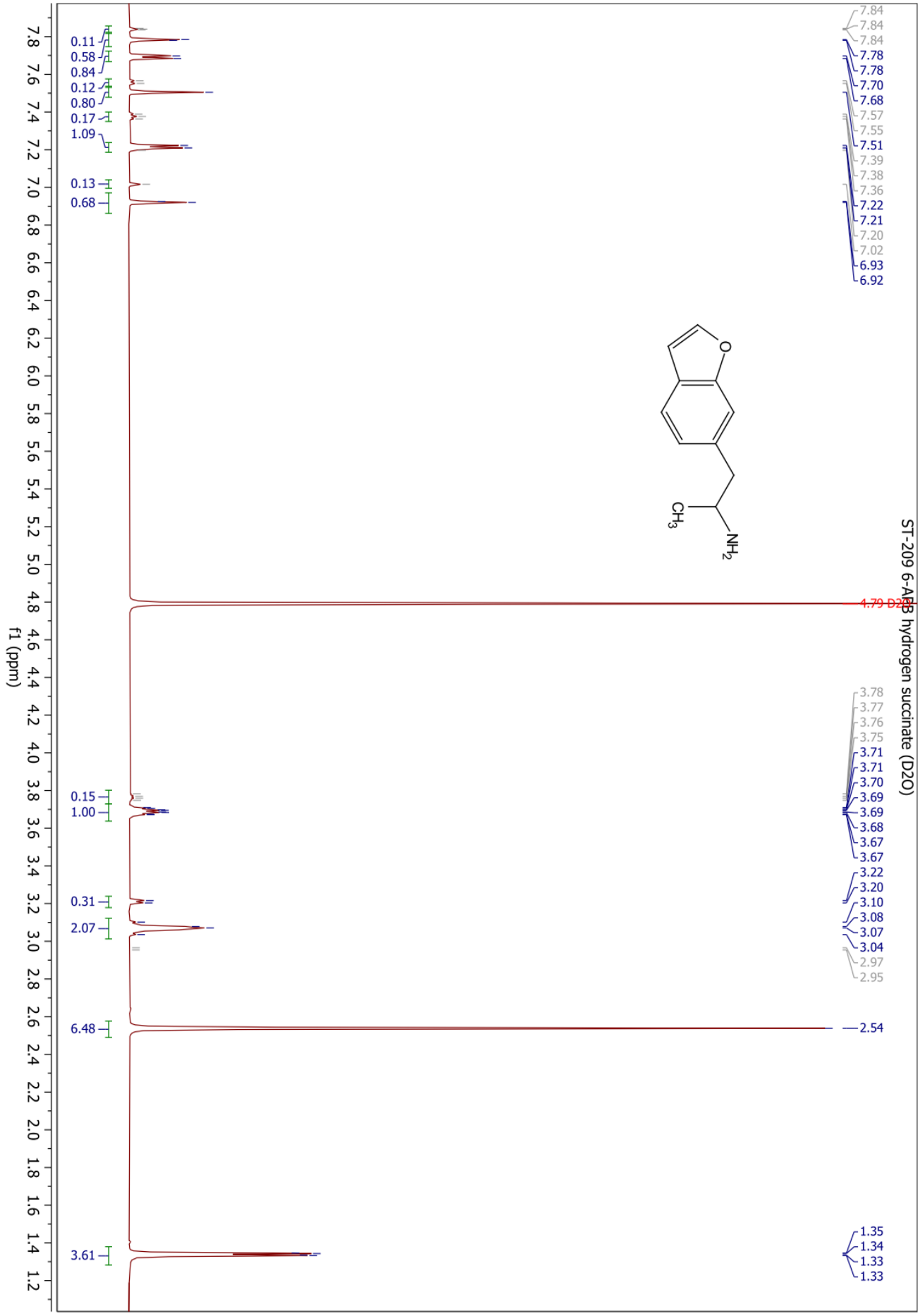
Analysis performed by Dr. Leonid Pevzner

^{1}H NMR: full non-empty spectrum, normalized to sum of isomers



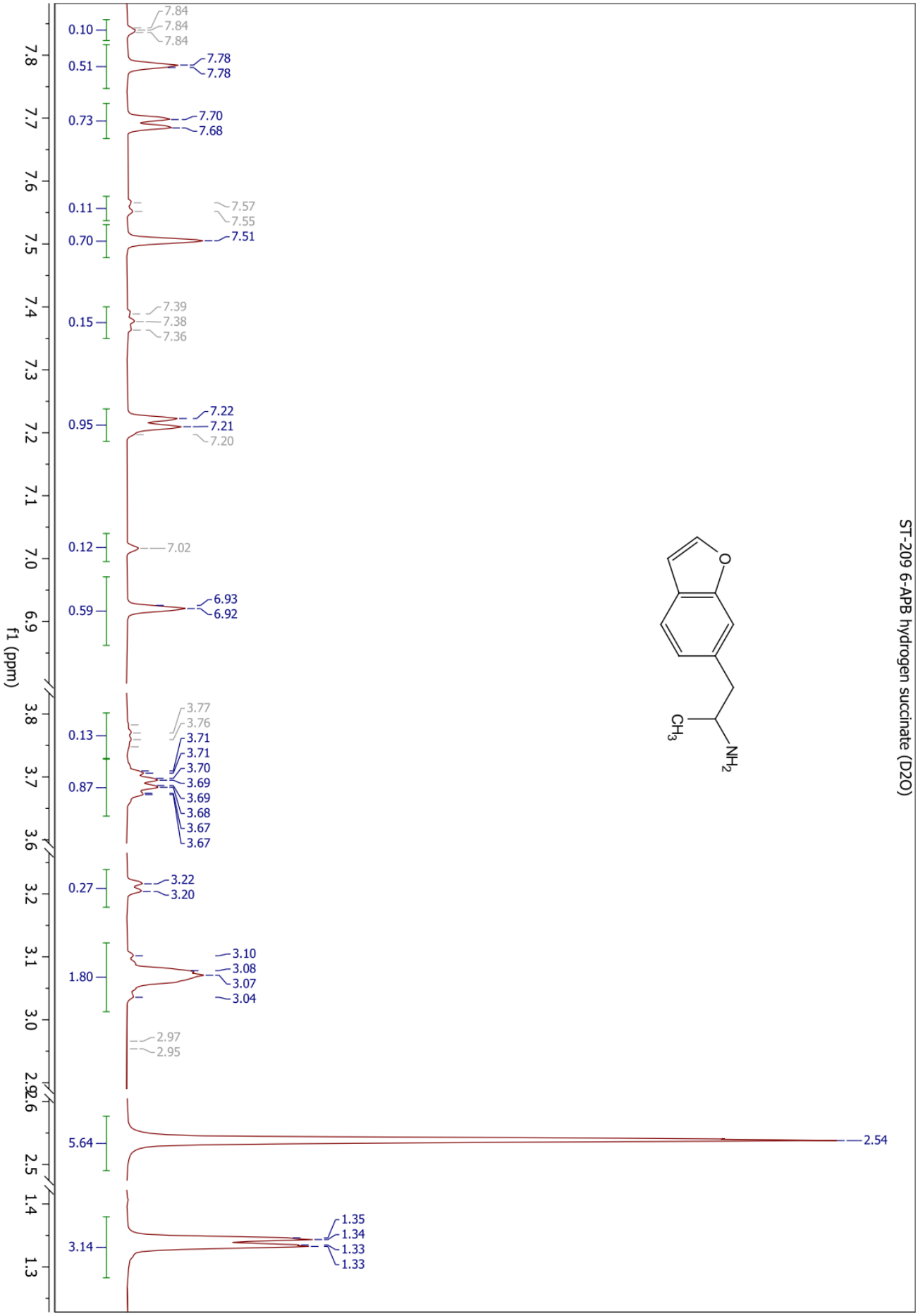
Analysis performed by Dr. Leonid Pevzner

^{1}H NMR: full non-empty spectrum, normalized to 6-APB



Analysis performed by Dr. Leonid Pevzner

[1]H NMR: Cut & enlarged, normalized to sum of isomers



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