NMR Measurement Report

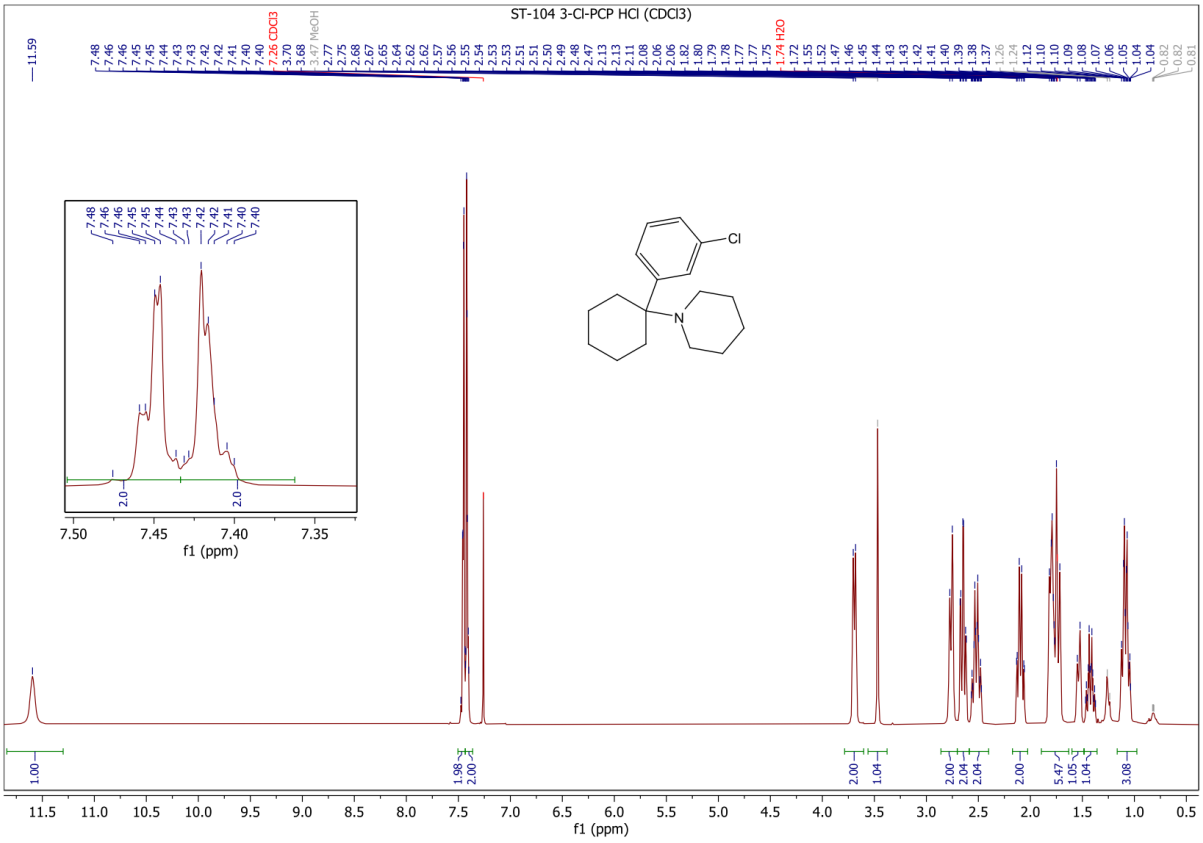
Sample name: ST-104 7-3-2021

Spectrometer: Bruker 500 MHz **Solvent**: $CDCl_3$

Expected compound: 3-Chloro-PCP (3-Cl-PCP)

Identified compound: Most like 3-Cl-PCP or isomer (s. lab notes)

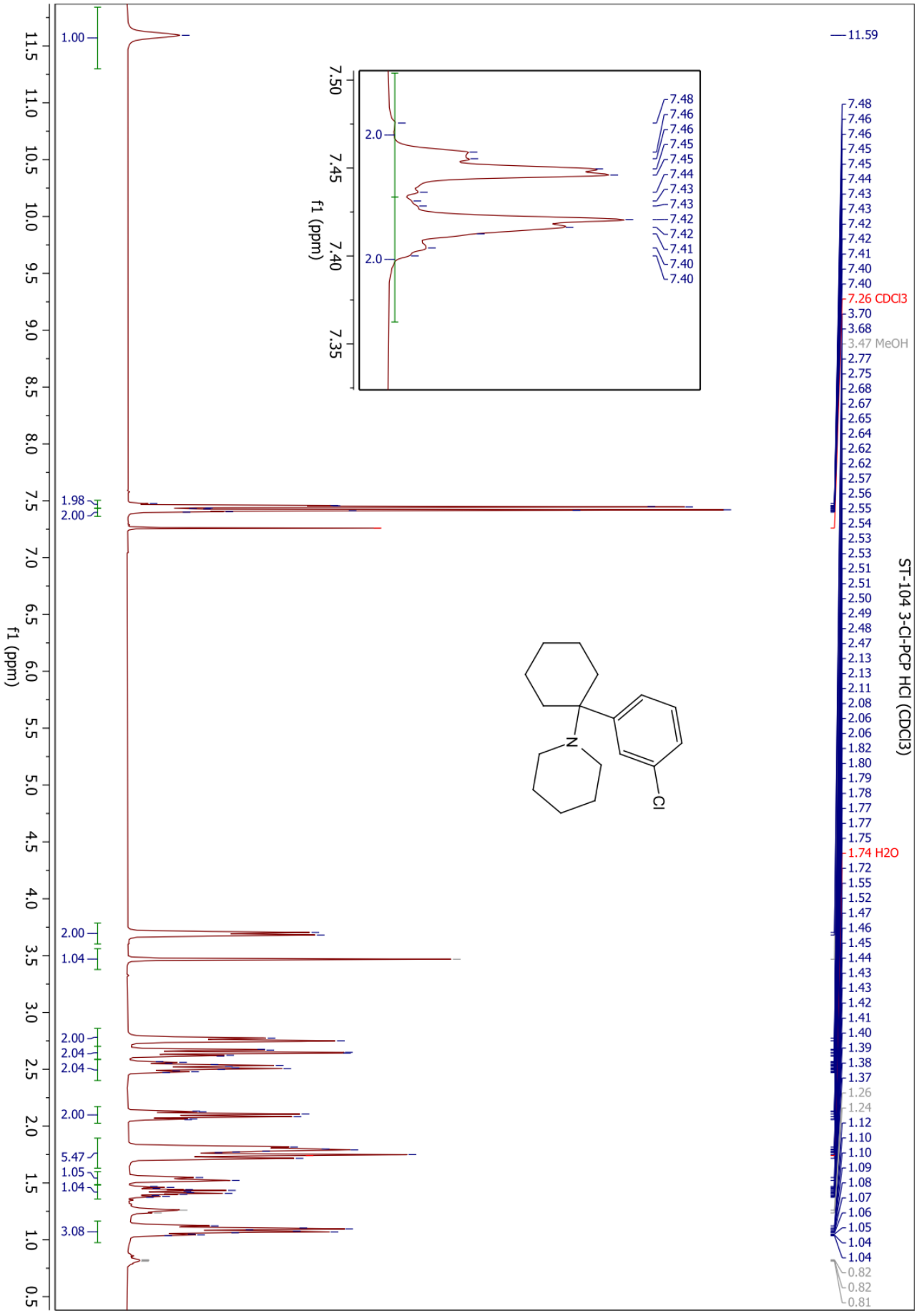
Estimated purity: 99%



Lab Notes: The acquired spectrum can be interpreted as belonging to the target compound but cannot be considered conclusive proof without additional information. In particular, the aromatic substituent (Cl) cannot be identified with ^{1}H NMR alone. A mass spectrum or elemental analysis would be helpful to verify that it is really chlorine, although it probably is. The position of the substituent presents a more serious concern. The semisymmetric structure of the aromatic proton peaks is typical for *para* or *ortho* substituted phenyl rings, but uncommon for *meta* substitution. The easiest way to verify the sample's identity would be to remeasure in DMSO-*d*6, since a forensic report containing such a ^{1}H NMR has already been published.

Analysis performed by Dr. Leonid Pevzner

^{1}H NMR: full non-empty spectrum



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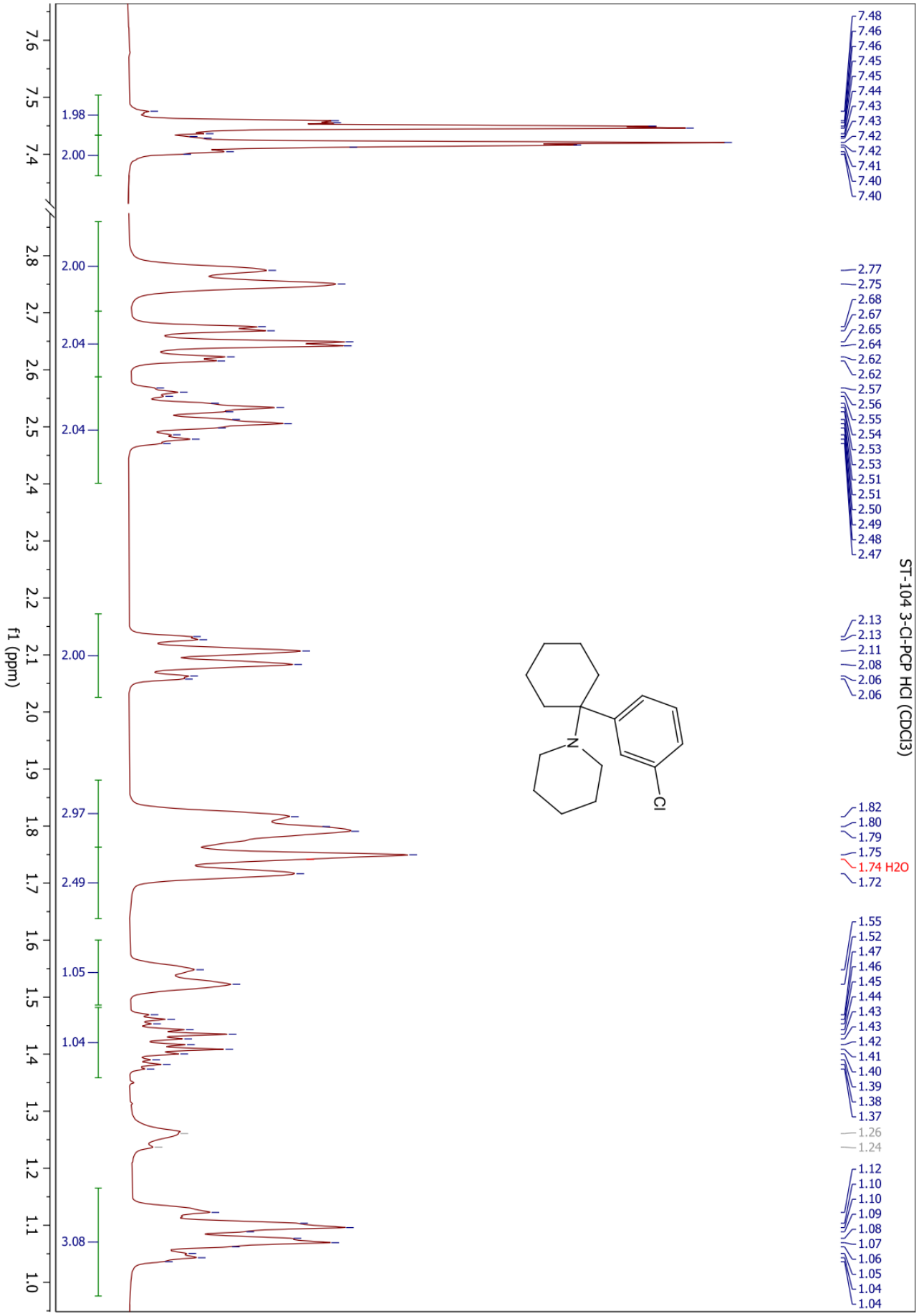
^{1}H NMR: cut and zoomed spectrum



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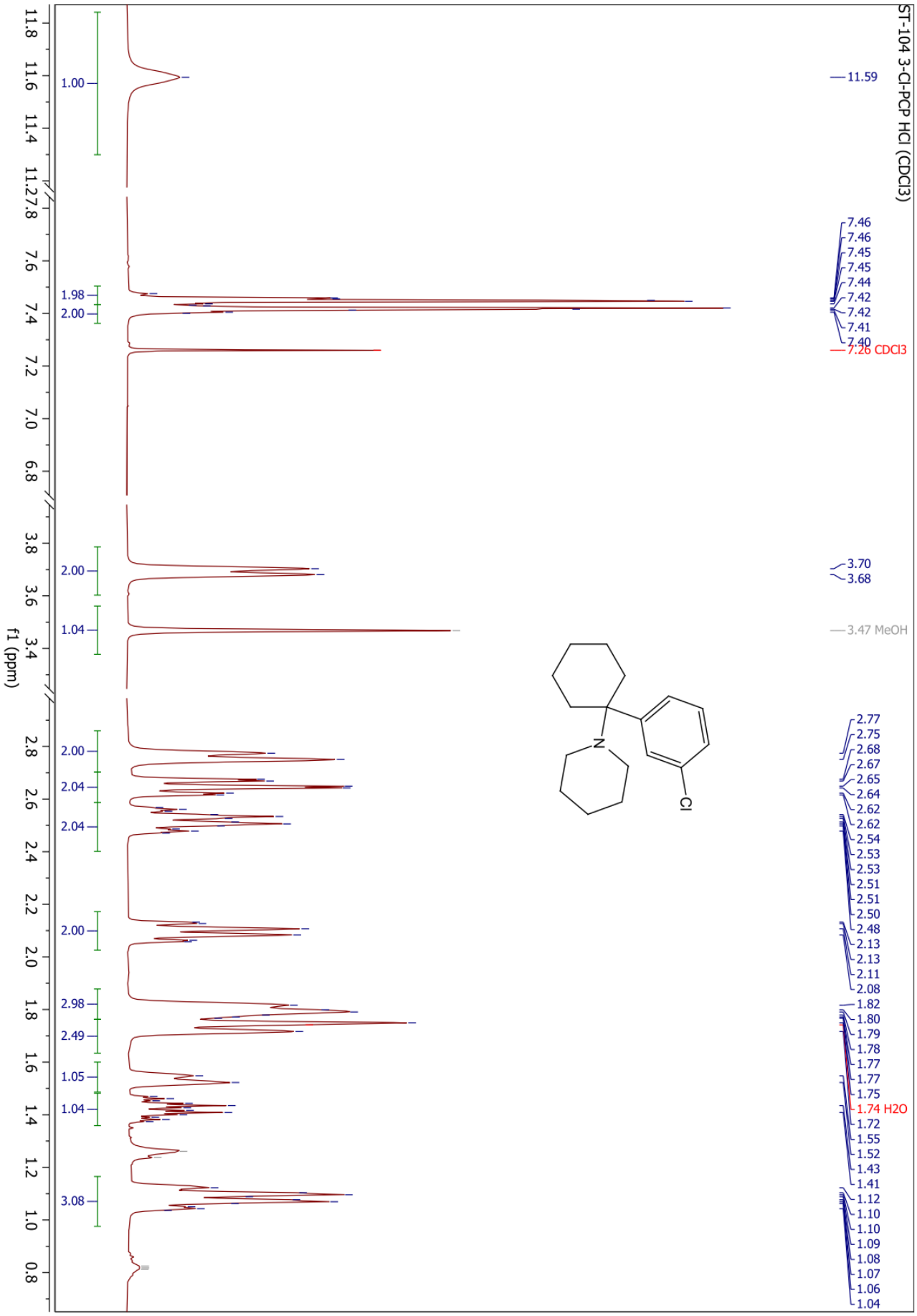
^{1}H NMR: full non-empty spectrum



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