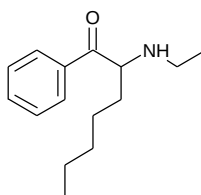


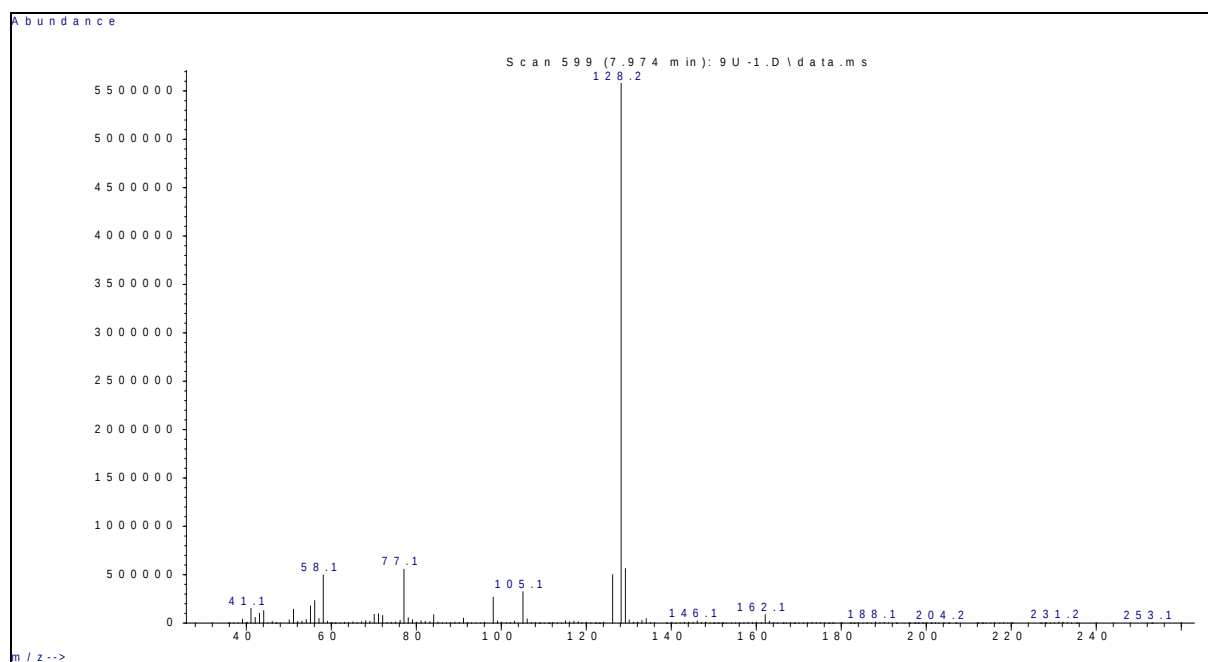
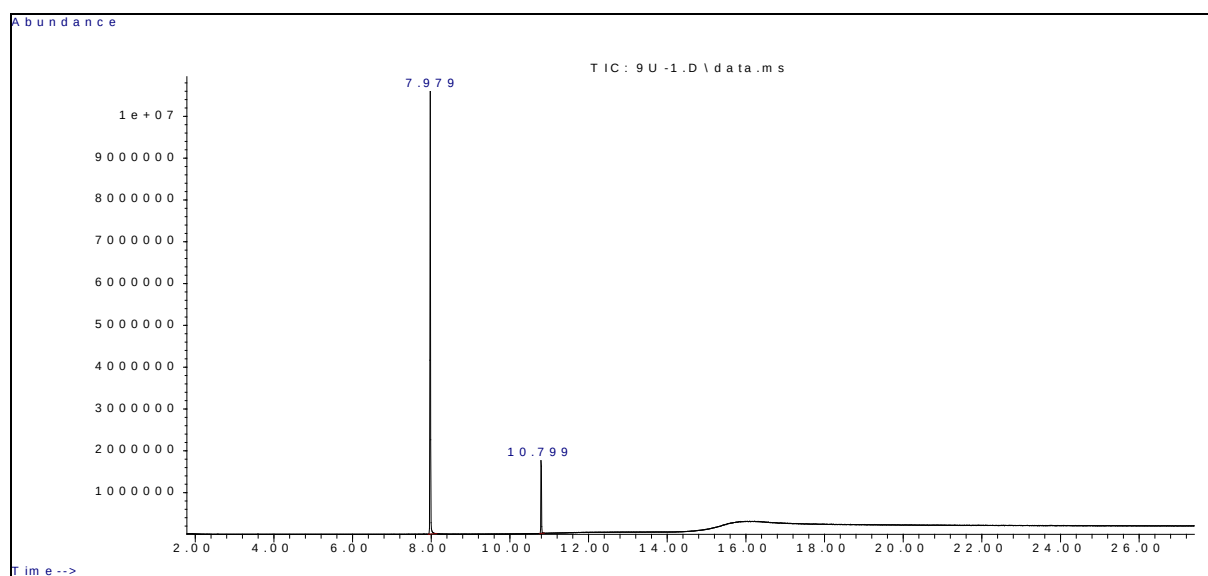
Ethyl-heptedrone



2-(ethylamino)-1-phenylheptan-1-one

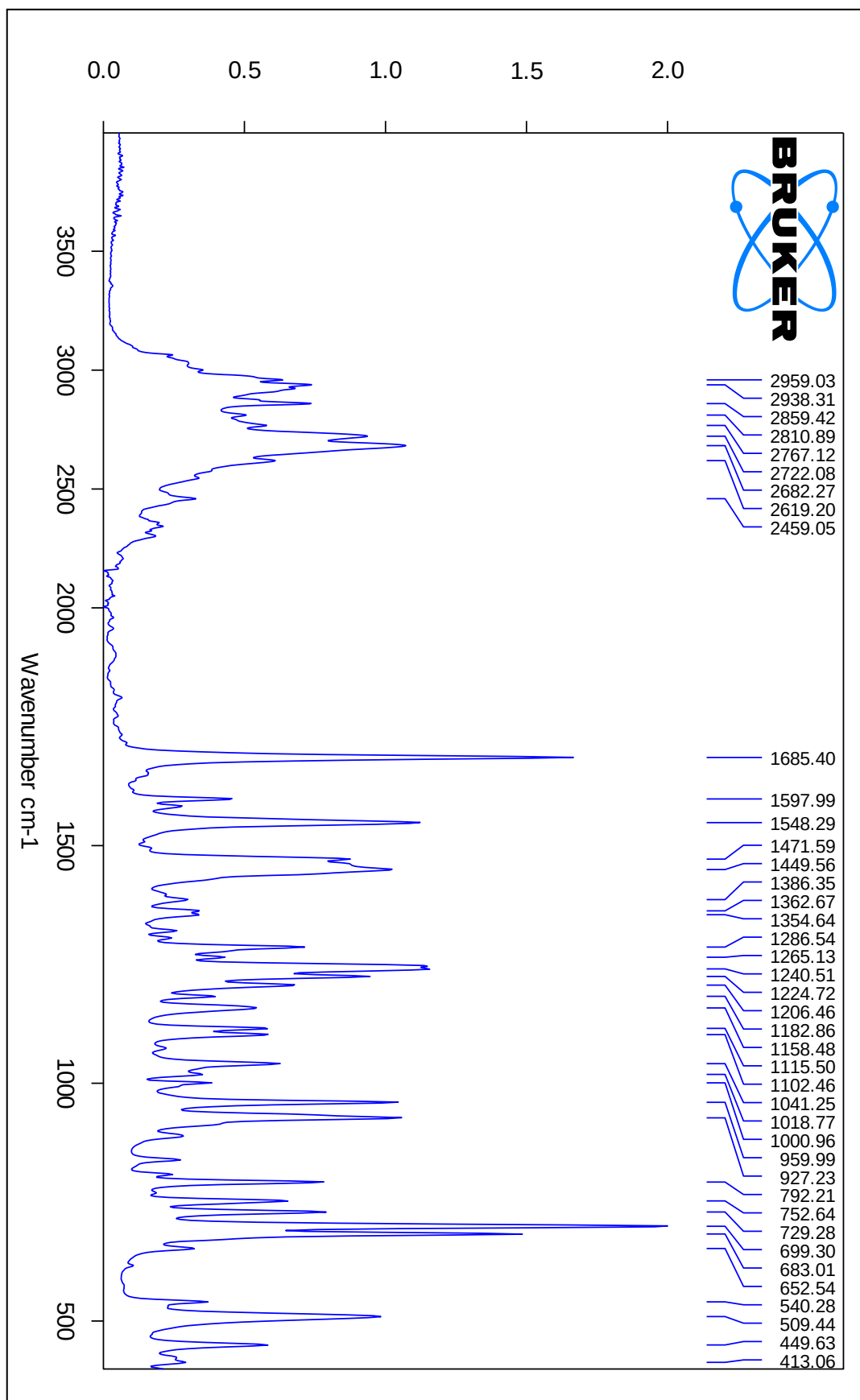
GC-MS

Rt.: 7.98 min

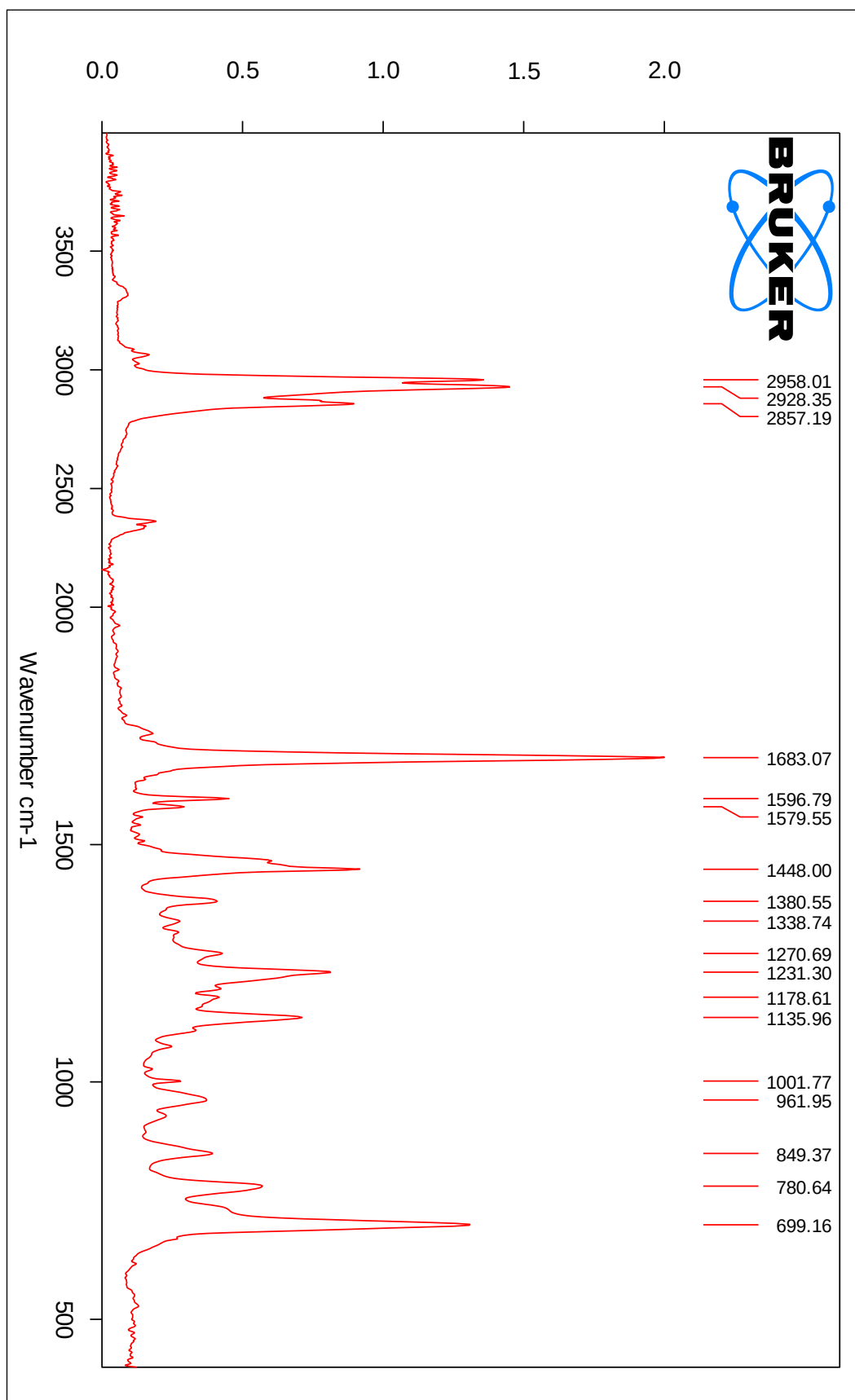


An Agilent 6890N Network GC system set up with Agilent HP-5MS (length: 30 m, diameter: 0.25 mm, film: 0.25 mm) coupled to an Agilent 5973 Network Mass Selective Detector (scan range m/z 35 – m/z 500) was used. Samples were subjected to electron ionization (EI) mode. GC-MS conditions: HP-5MS column was temperature programmed from 100 °C (which was held for 2 minutes) to 280 °C at 20 °C/min, 280 °C was held for 3 minutes, then to 315 °C at 25 °C/min, the temperature was stated at 315 °C for 12 minutes. The carrier gas was helium. Tribenzyl-amine was applied as an internal standard (locked to 10.8 minutes). Data handling was carried out with GC/MSD ChemStation software.

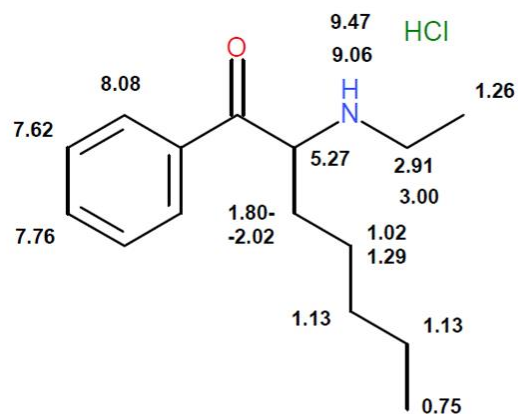
ATR-FTIR (powder)



ATR-FTIR (free-base)



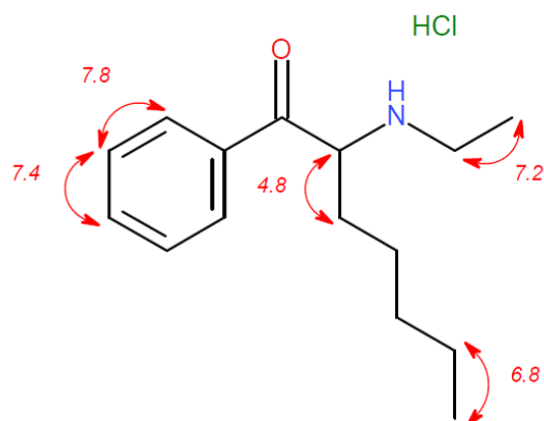
NMR

 ^1H -NMR chemical shifts δ [ppm]

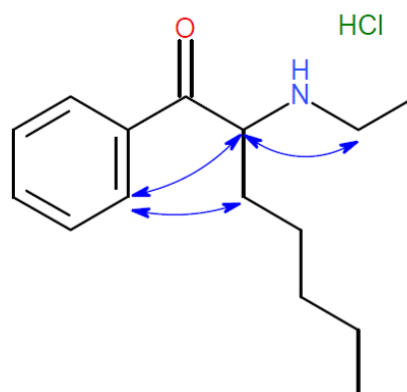
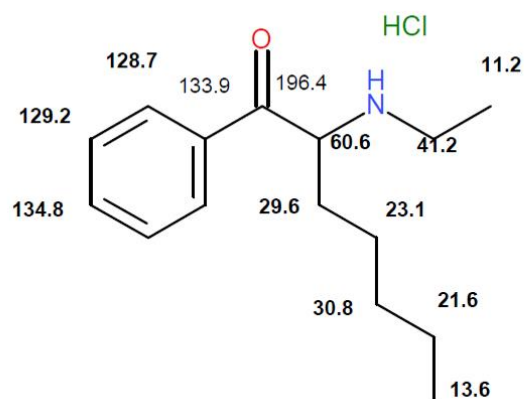
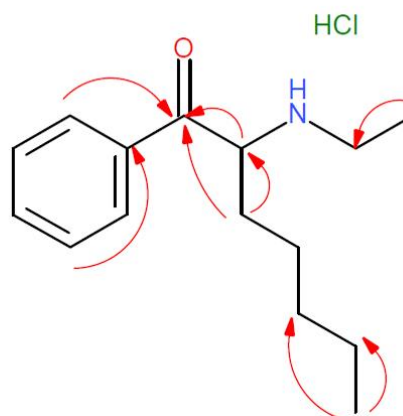
Etil-heptedron

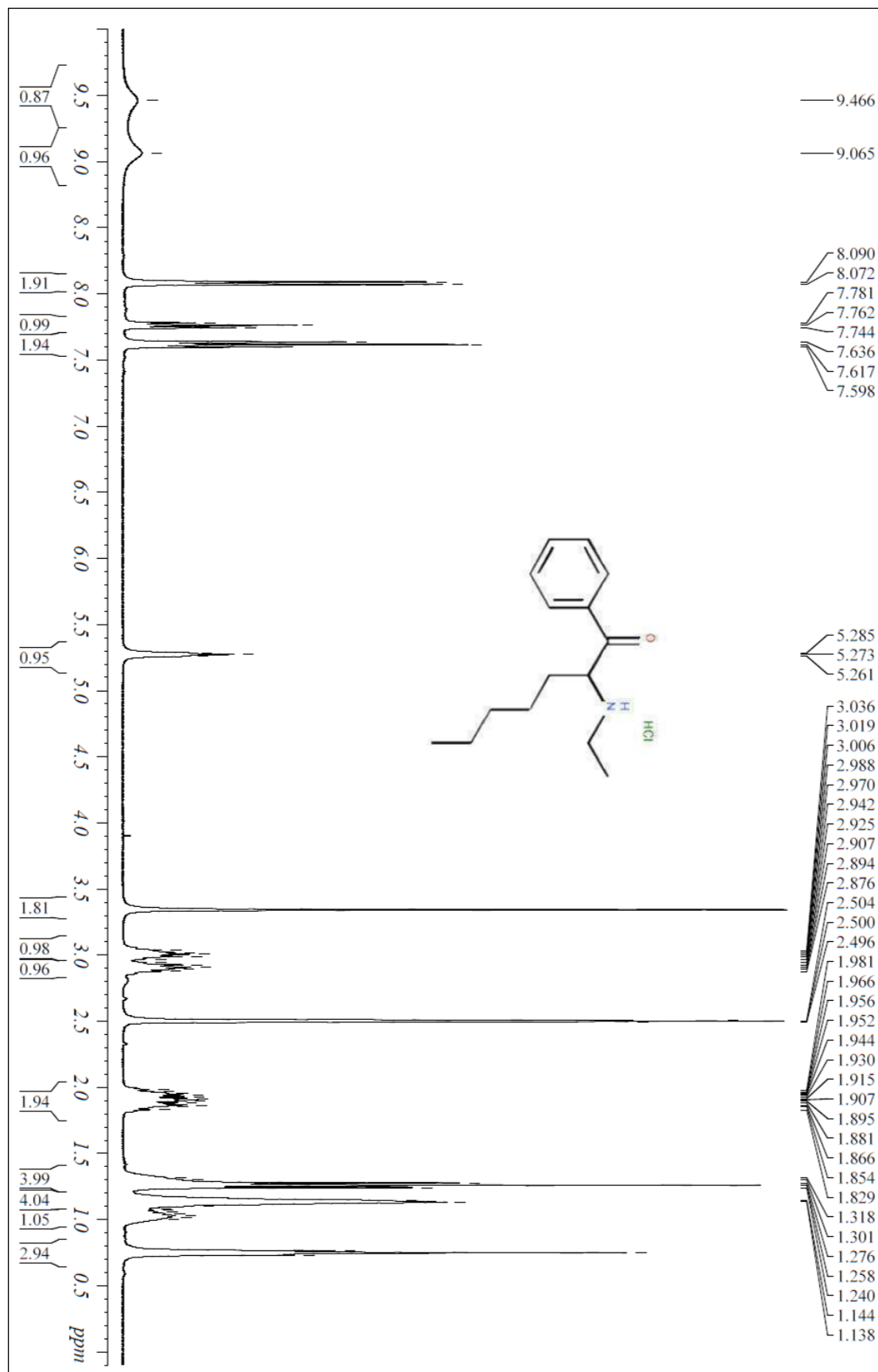
Formula Weight: 233,34922 (base)

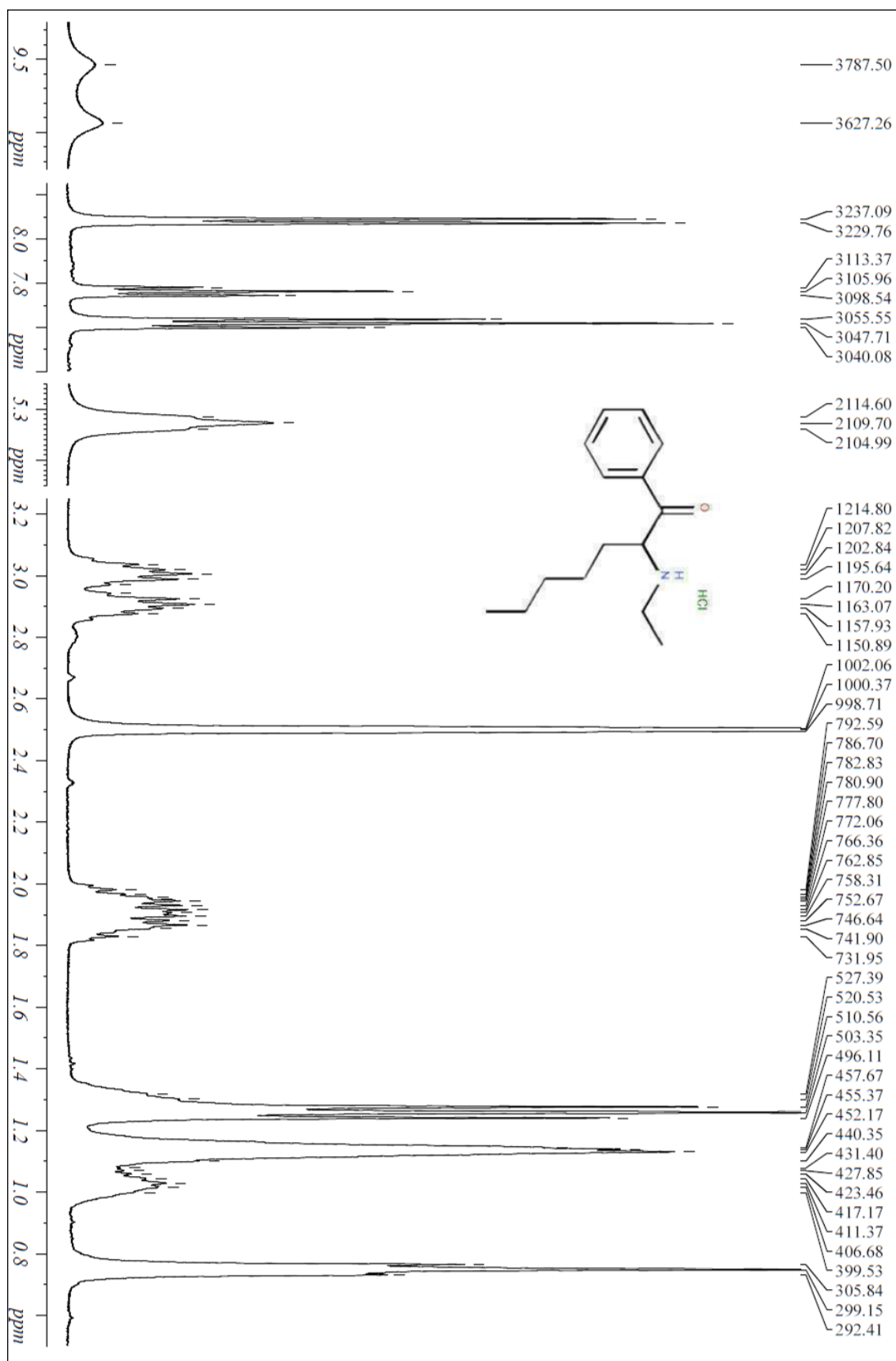
Exact Mass: 233,177964366

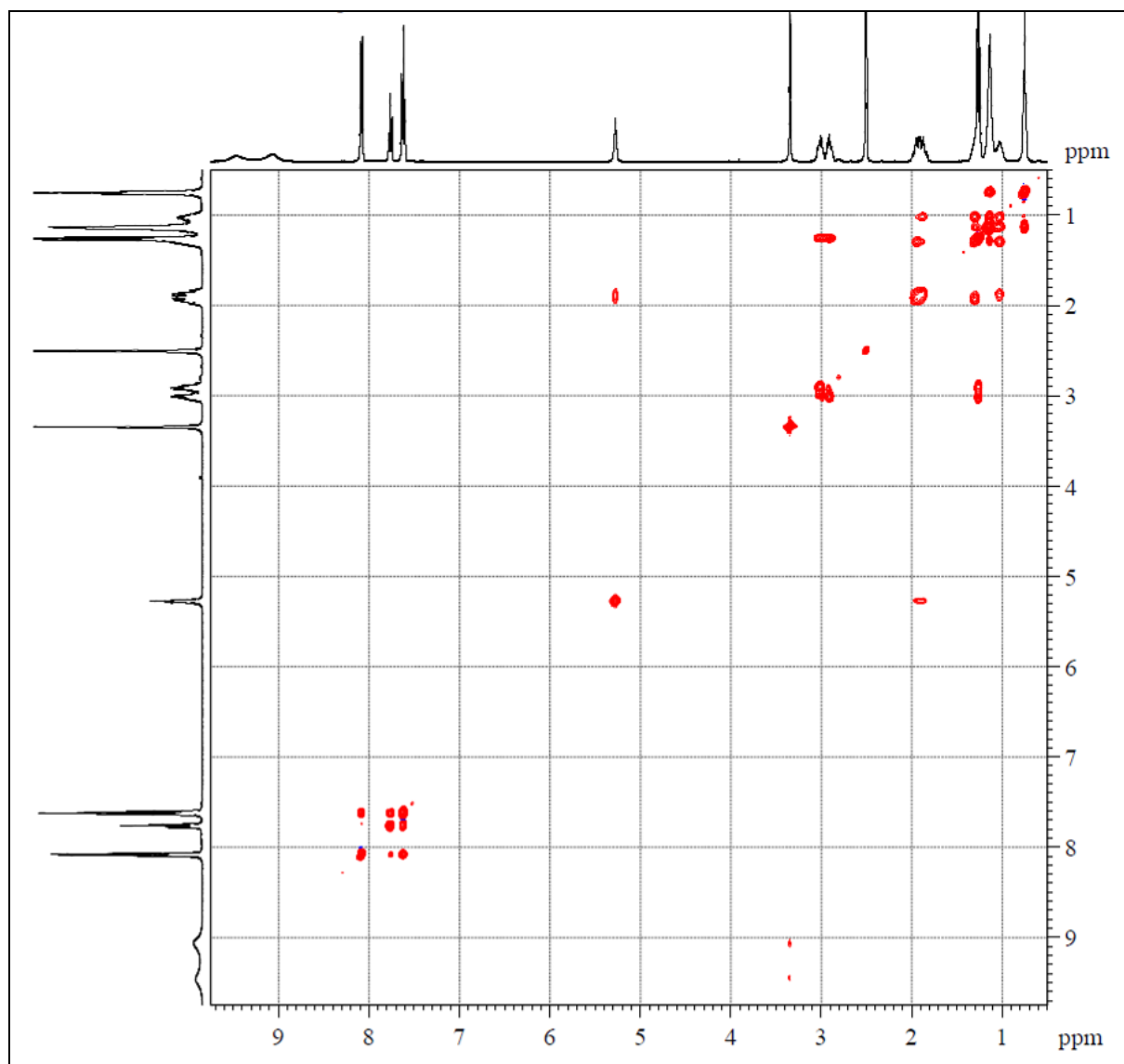
Molecular Formula: $\text{C}_{15}\text{H}_{23}\text{NO}$ $J(\text{H,H})$ couplings constants [Hz]

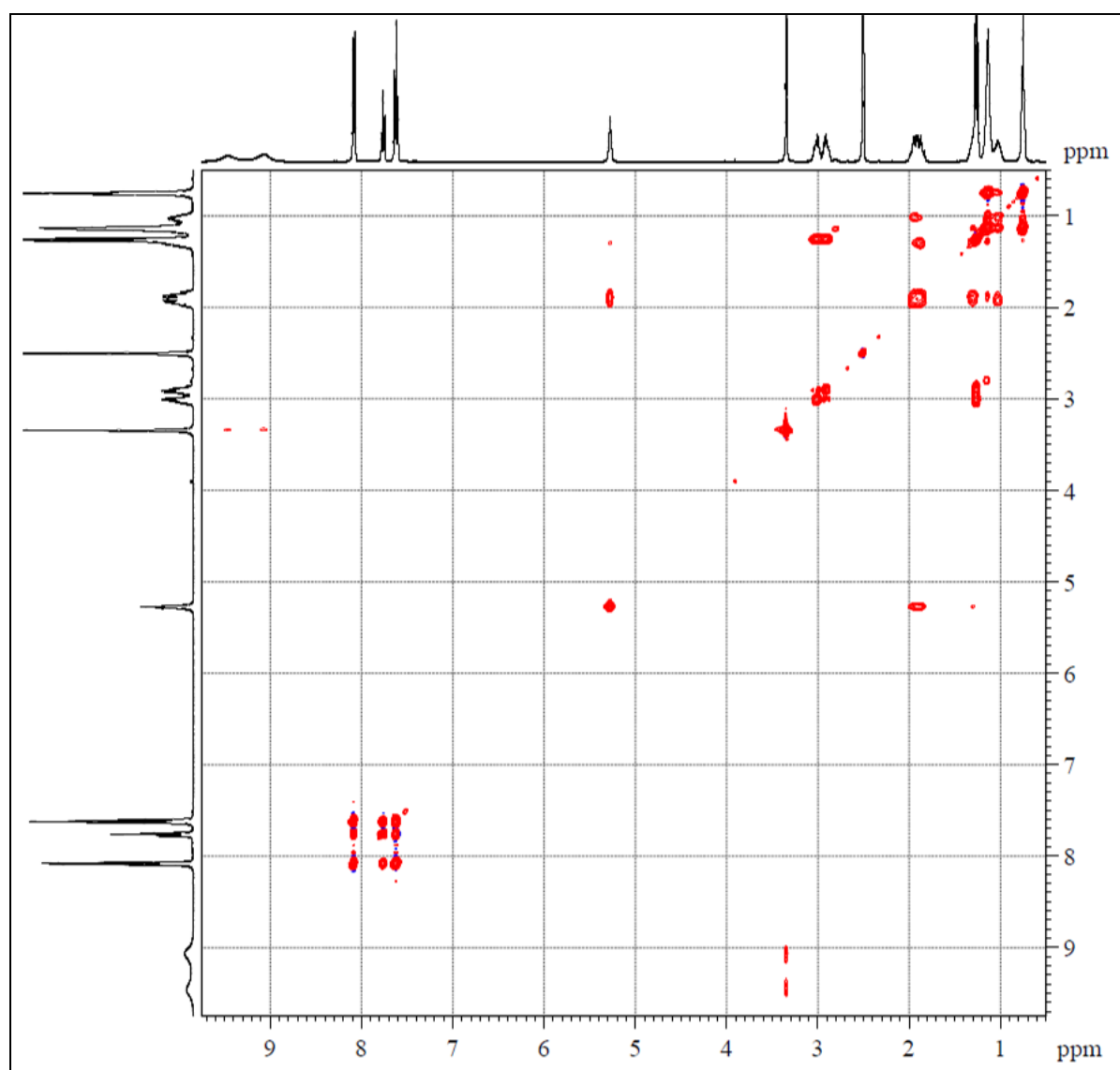
Characteristic steric proximities detected by zqs-easy-ROESY

 ^{13}C -NMR chemical shifts δ [ppm]Characteristic heteronuclear long-range coupling detected by HMBC method $\text{H} \rightarrow \text{C}$ 

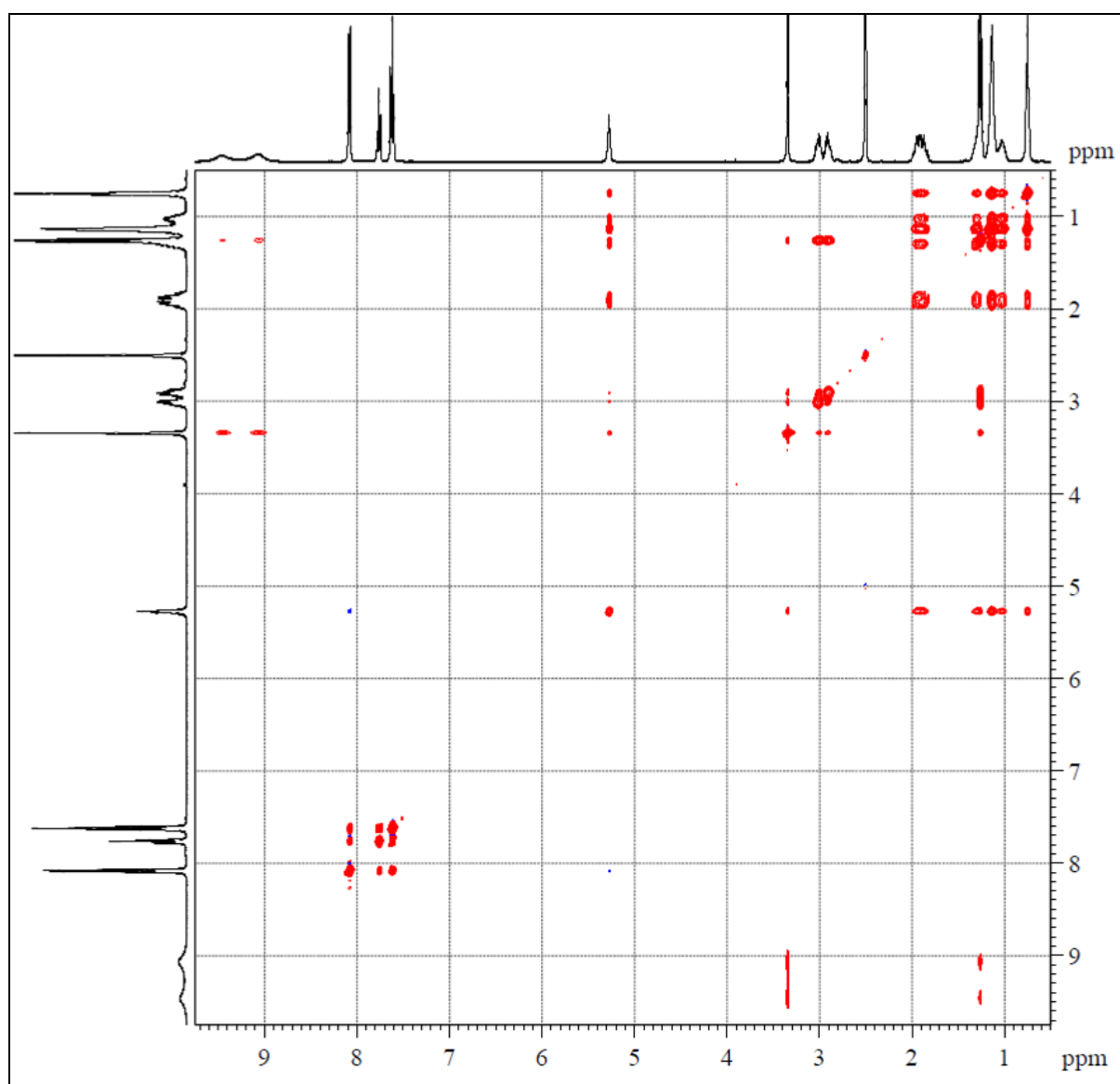
^1H NMR (overview)

Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d₆**¹H NMR (characteristic parts)**

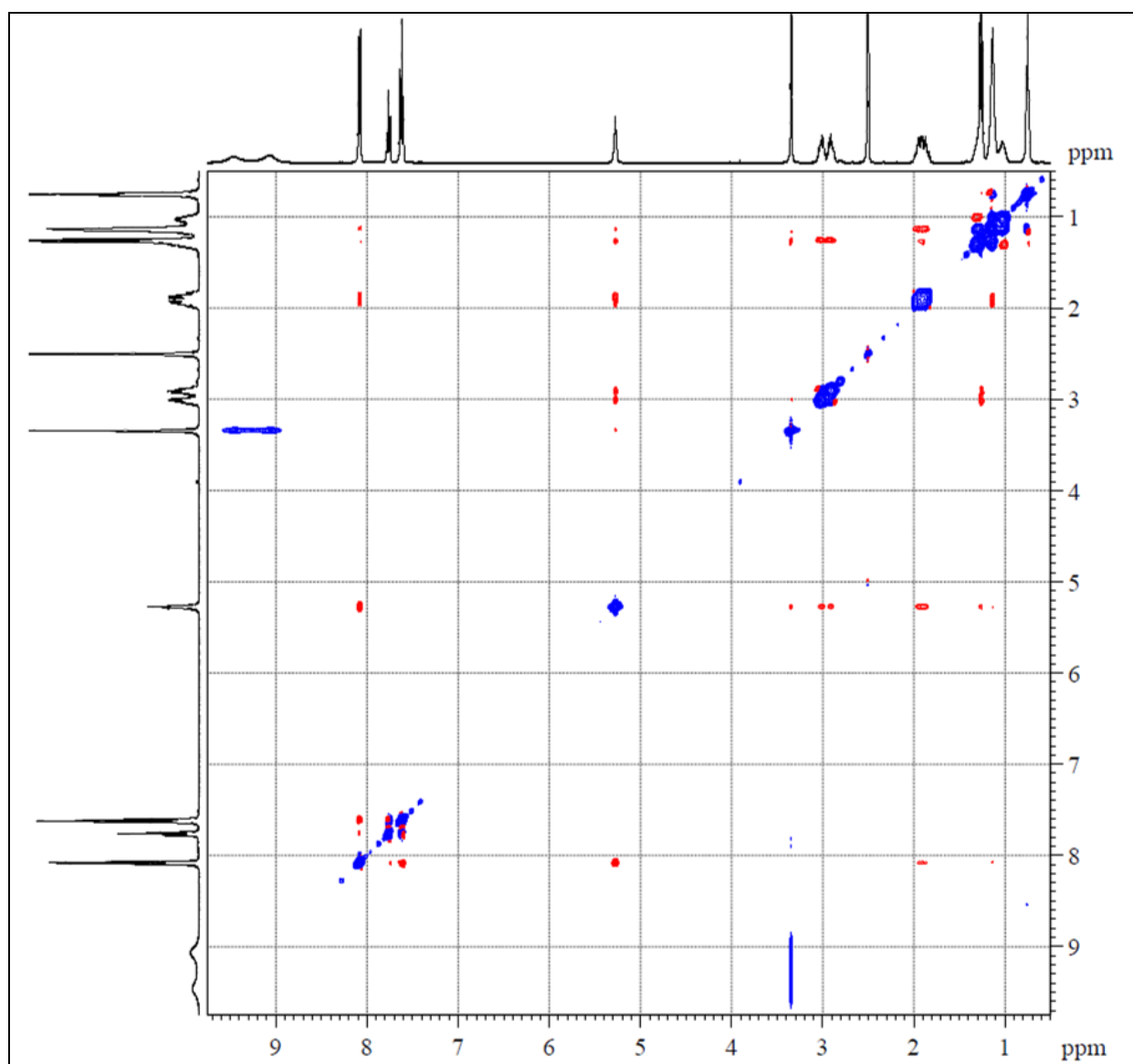
Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d₆***clip-zqs-COSY***Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d₆

clip-zqs-COSY-Relay

Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d₆

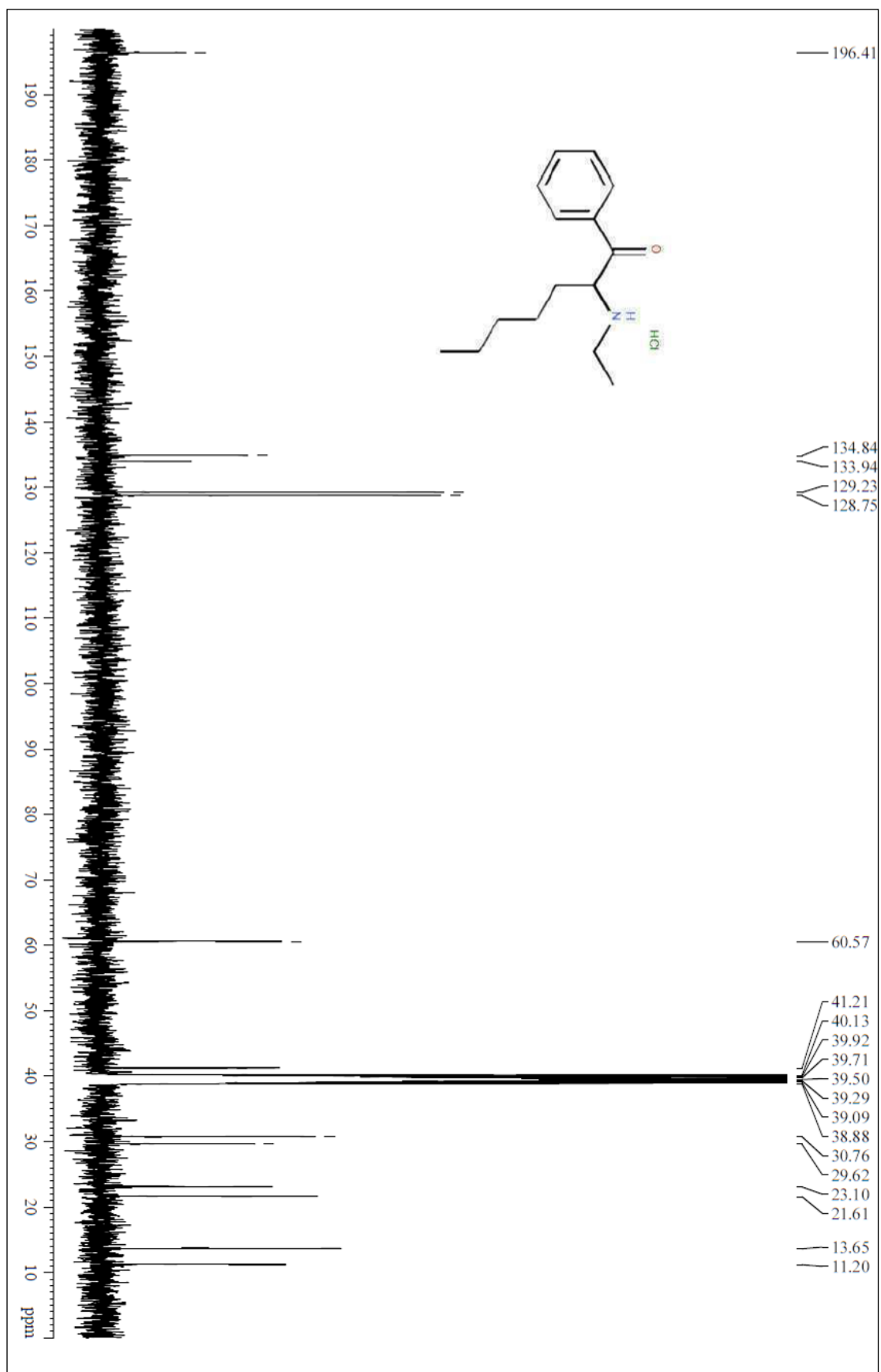
zqs-TOCSY

Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d₆

***zqs-easy*-ROESY**

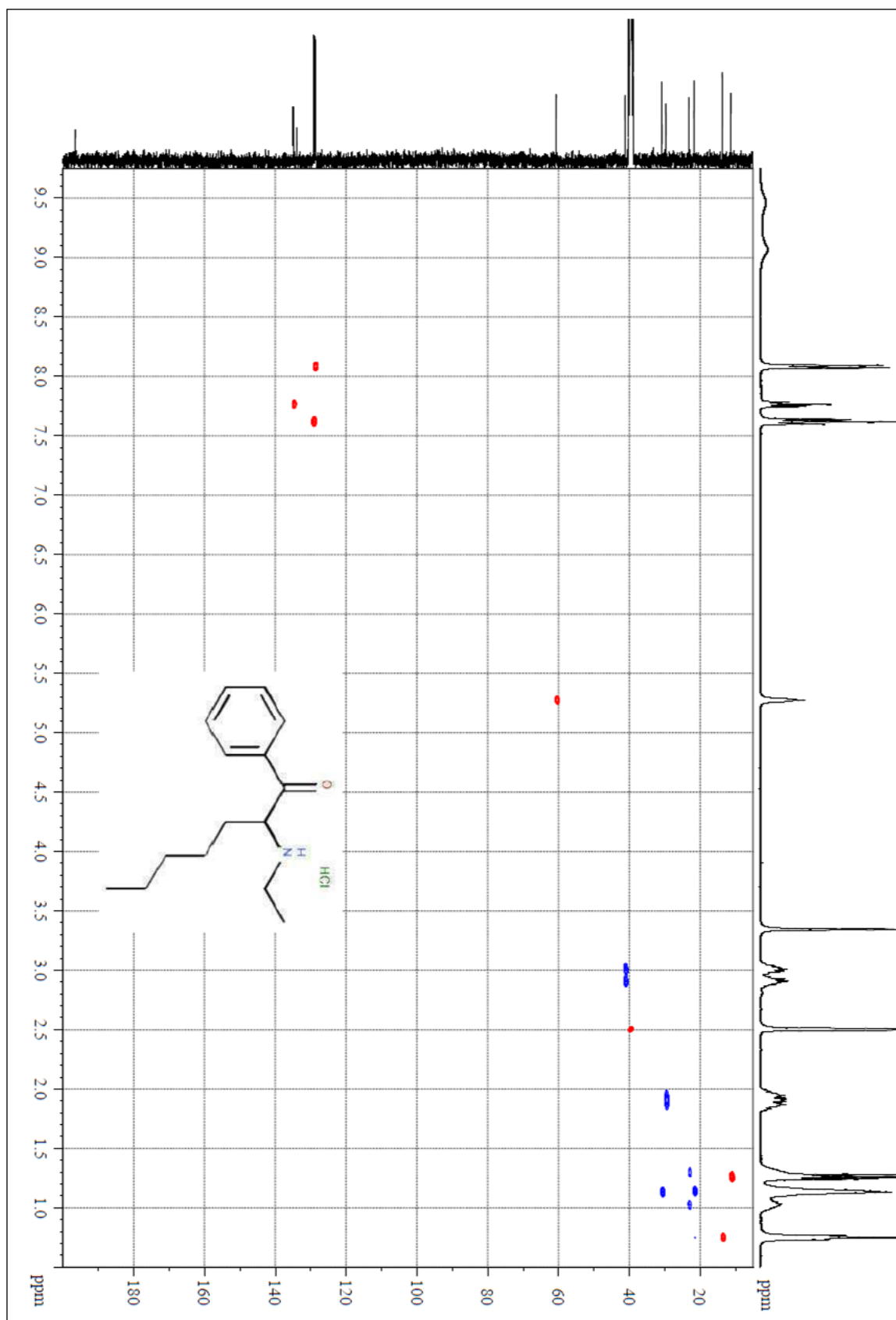
Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d₆

^{13}C NMR



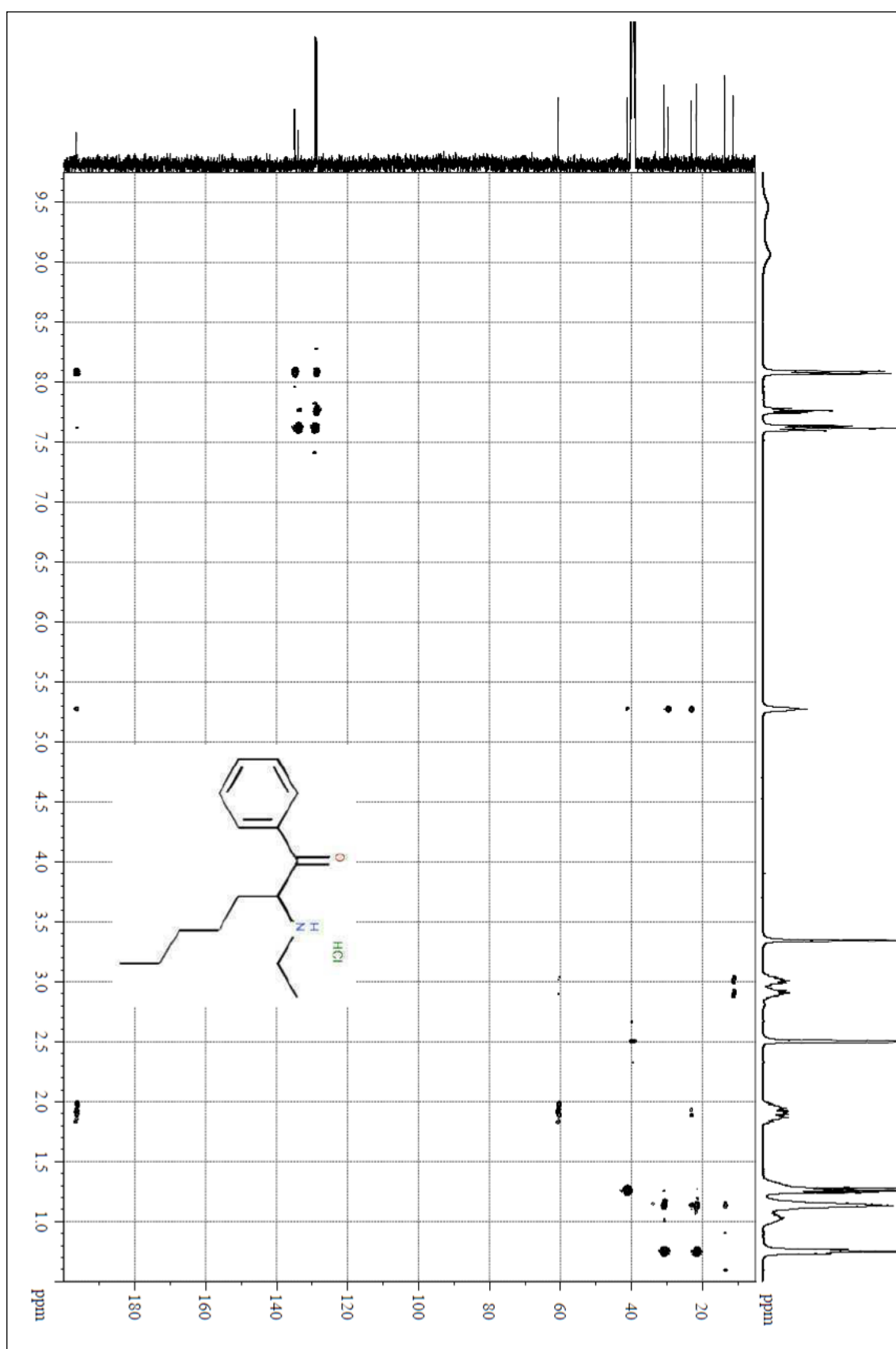
Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d₆

ed-HSQC



Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d₆

HMBC



Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6