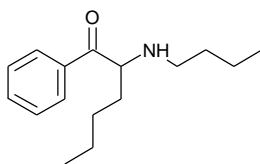


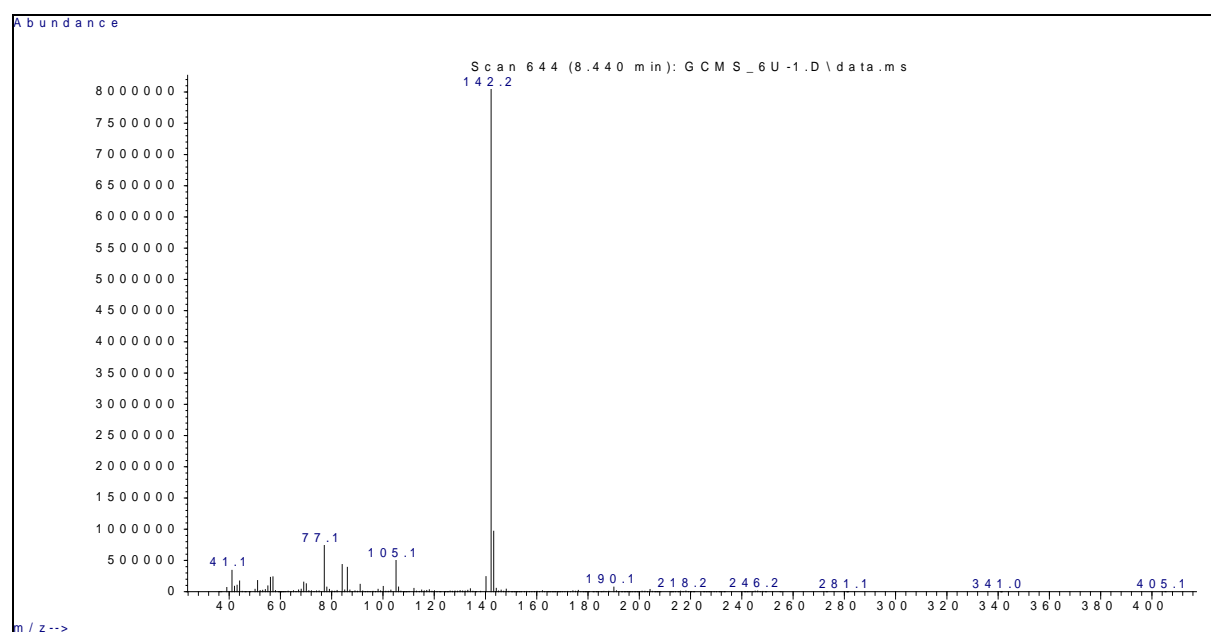
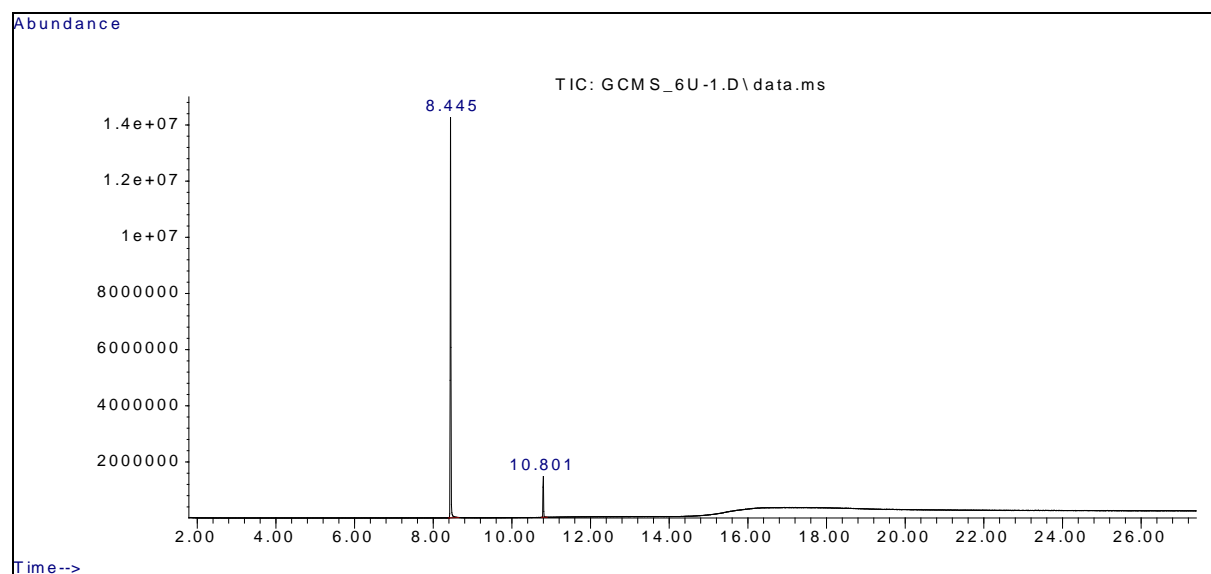
# Butyl-hexedrone



2-(butylamino)-1-phenylhexan-1-one

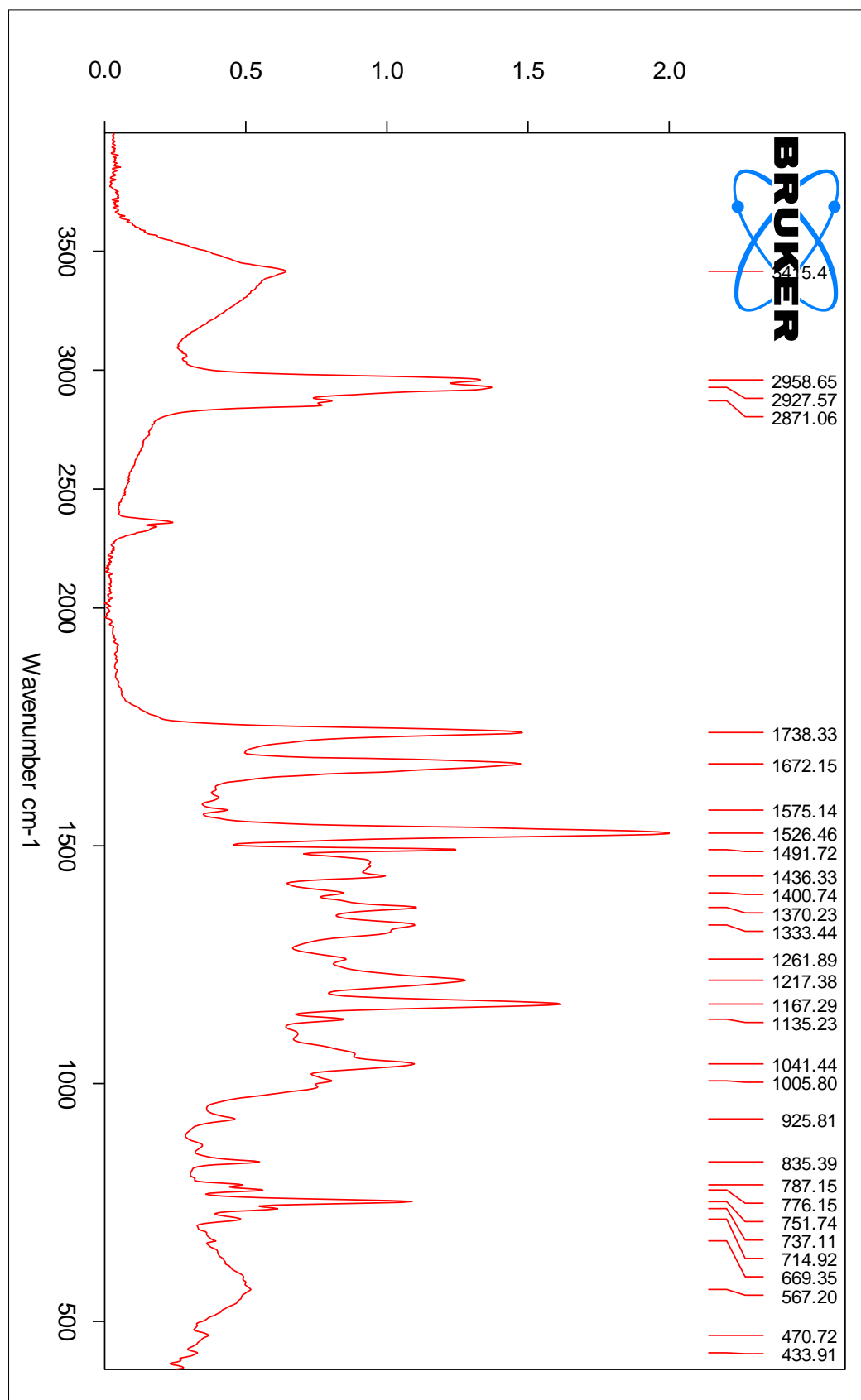
## GC-MS

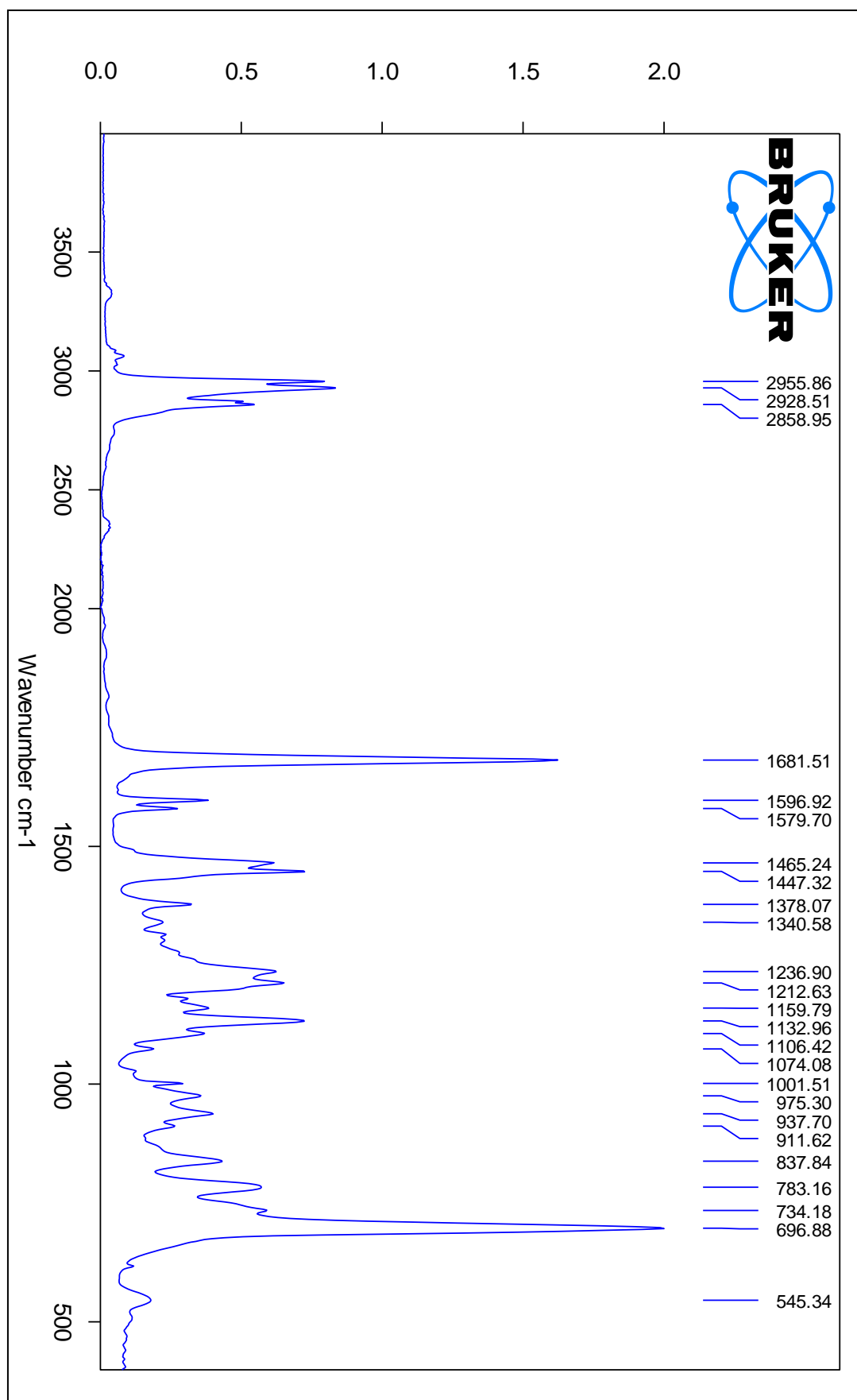
Rt.: 8.44 min



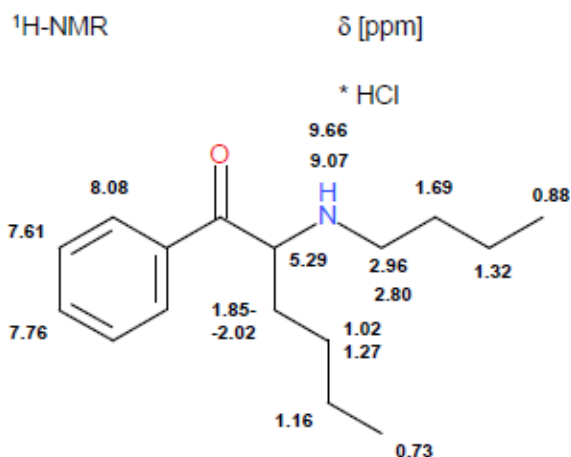
An Agilent 6890N Network GC system set up with Agilent HP-5MS (length: 30 m, diameter: 0.25 mm, film: 0.25 mm) coupled to an Agilent 5973 Network Mass Selective Detector (scan range m/z 35 – m/z 500) was used. Samples were subjected to electron ionization (EI) mode. GC-MS conditions: HP-5MS column was 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)



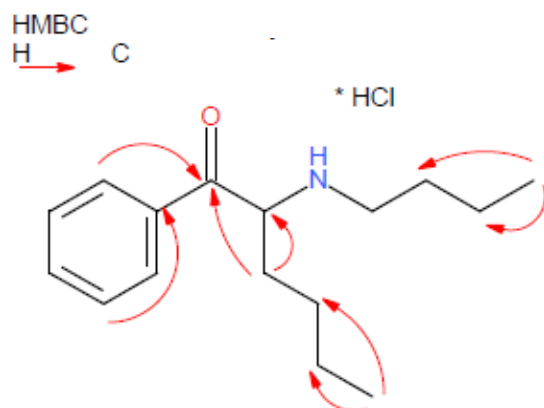
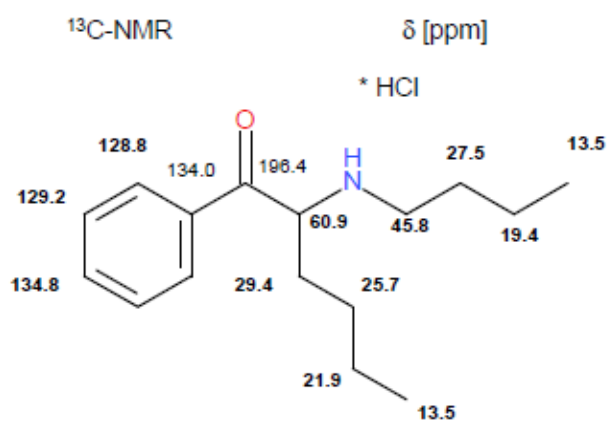
**ATR-FTIR (free-base)**

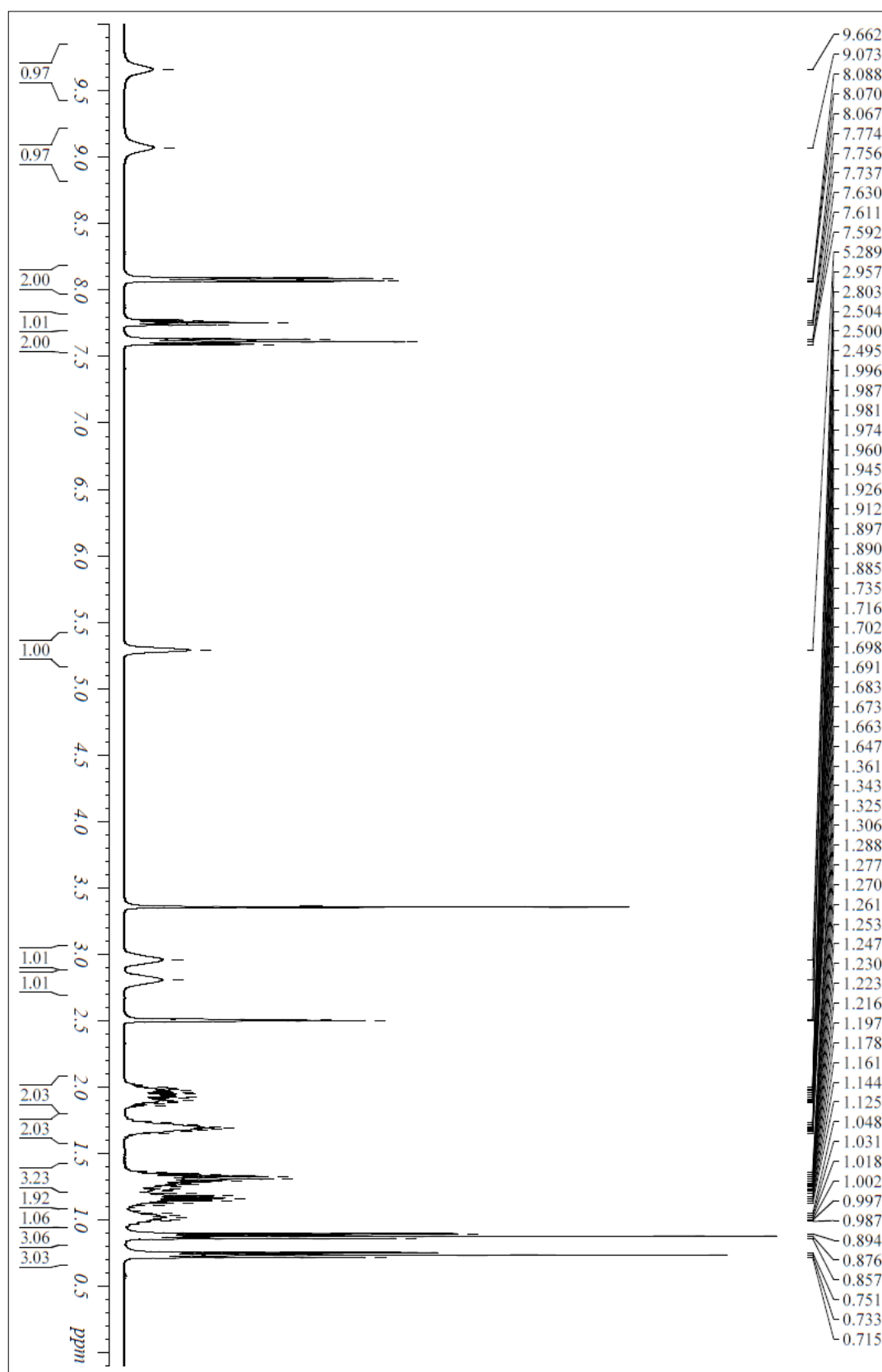
## NMR

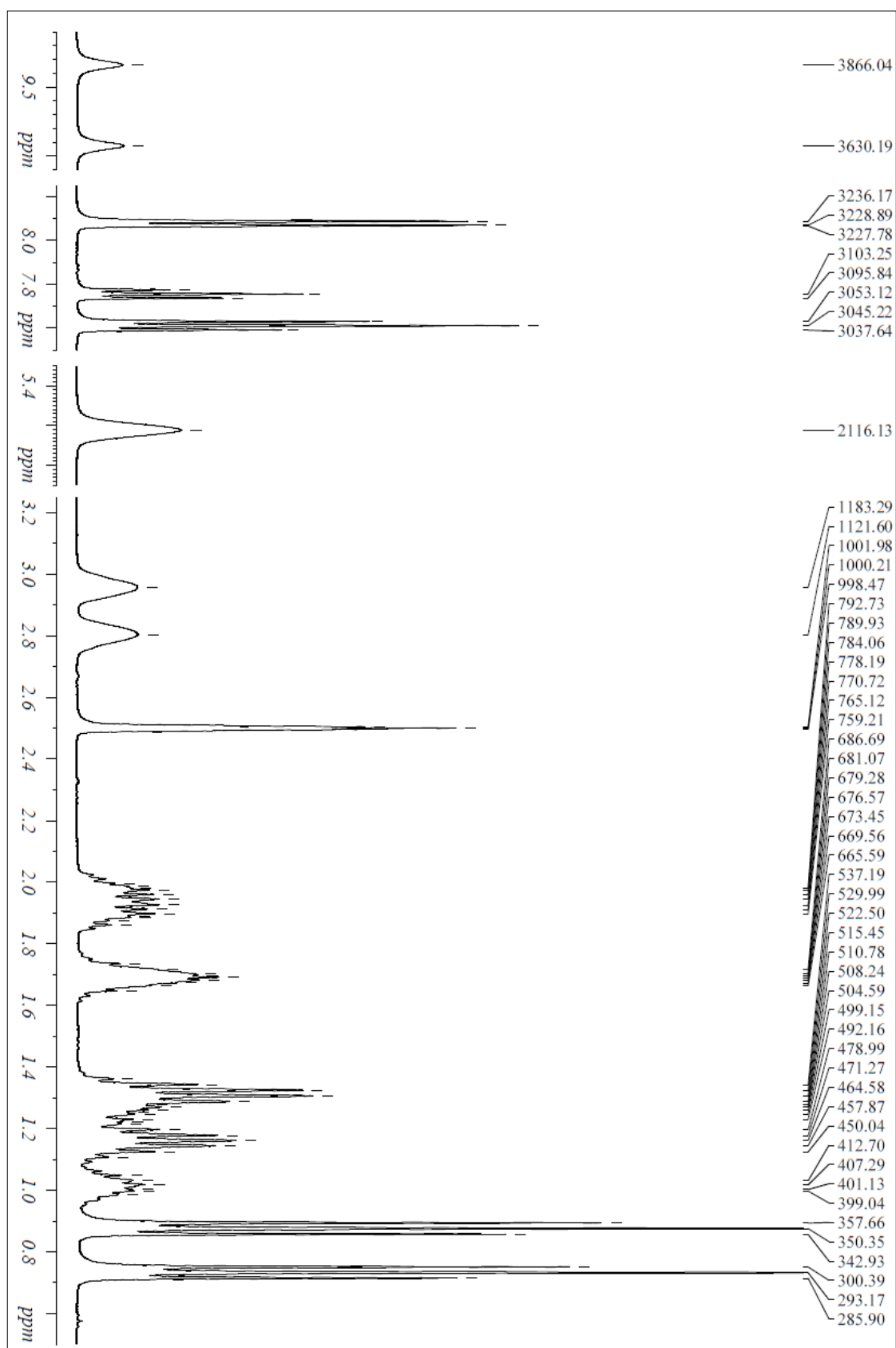


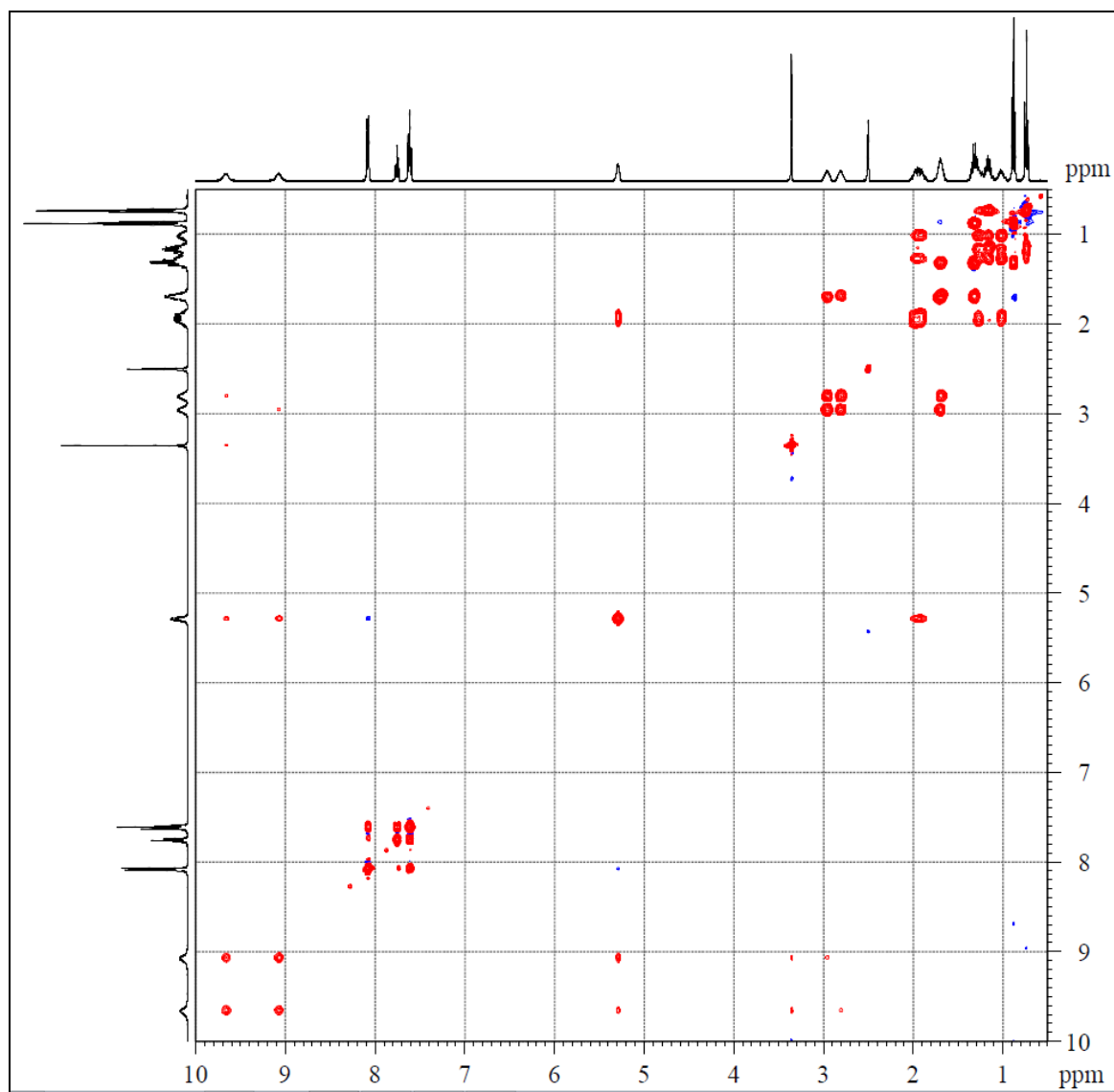
## Butyl-hexedrone

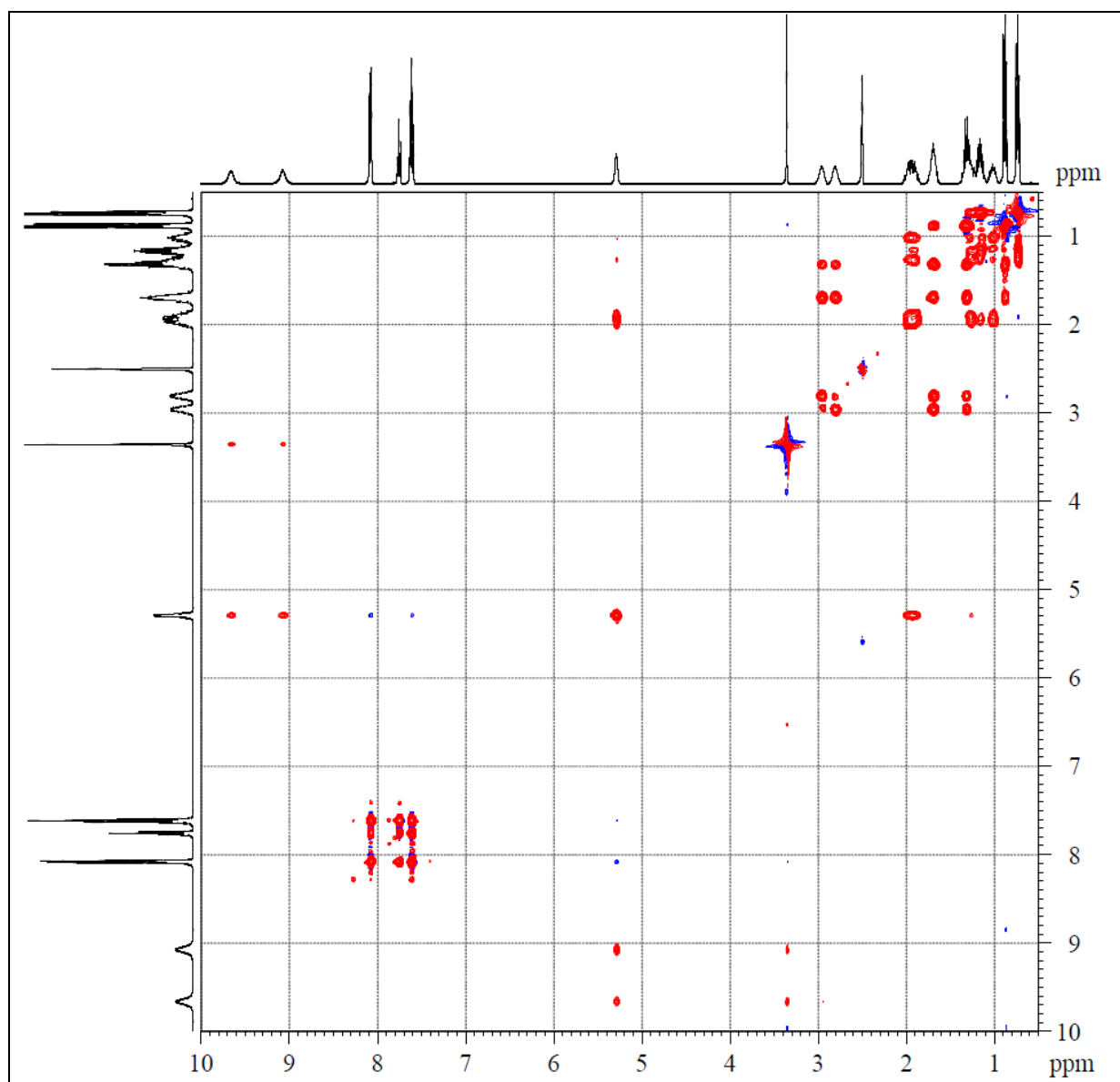
Formula Weight: 247,3758  
 Exact Mass: 247,19361443  
 Molecular Formula: C<sub>16</sub>H<sub>25</sub>NO



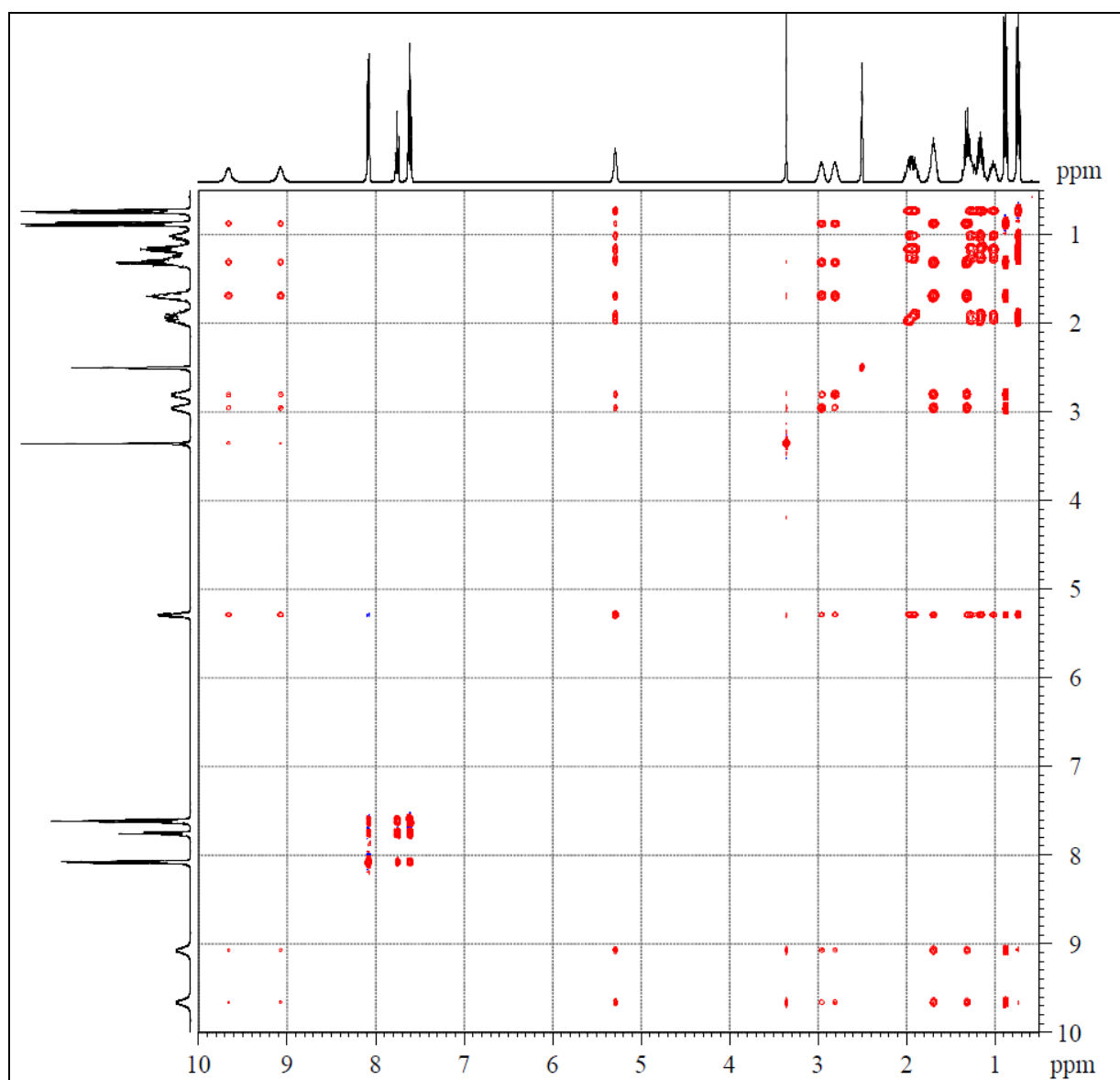
**$^1\text{H}$  NMR (overview)**Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO- $d_6$

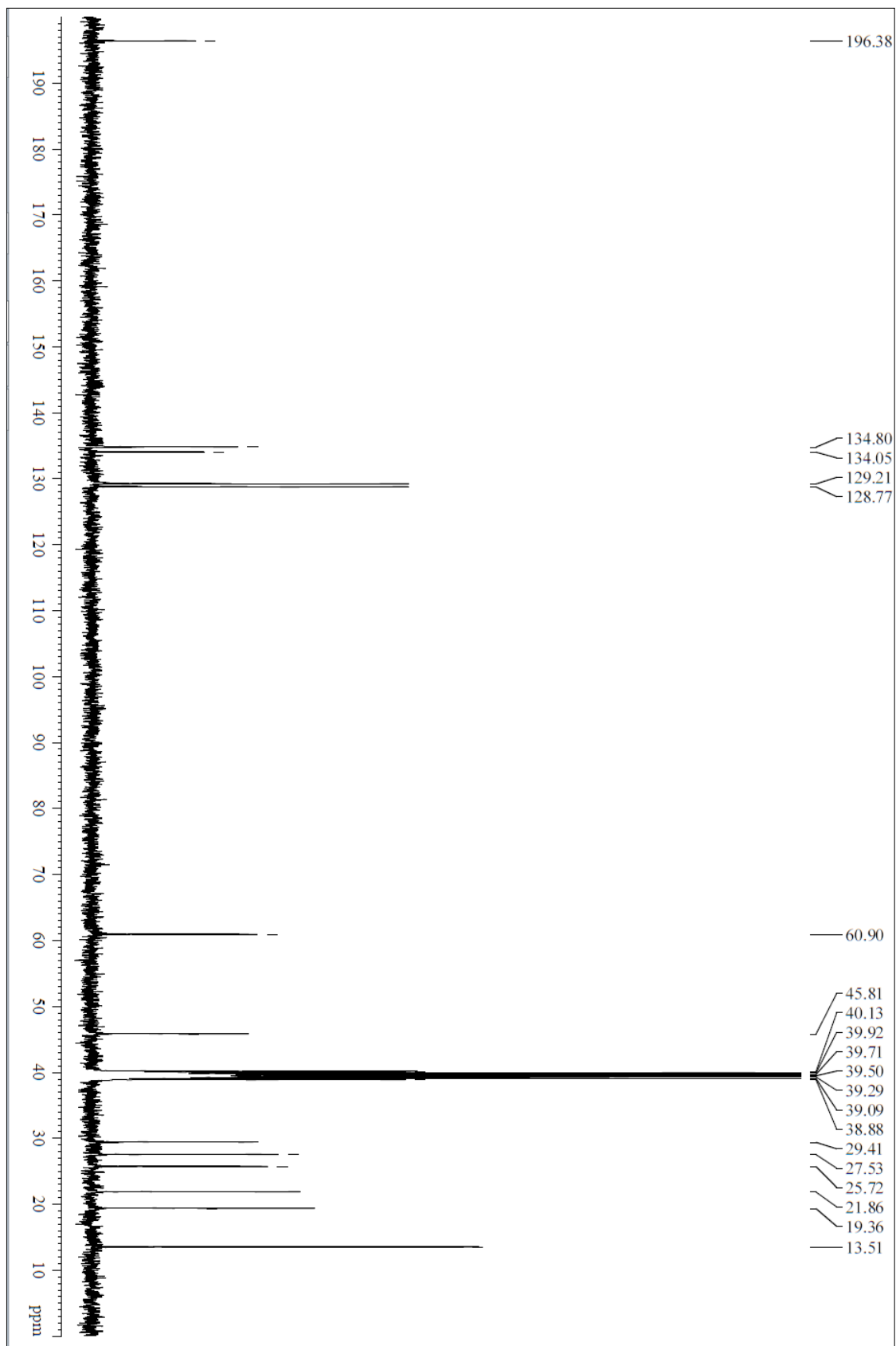
**$^1\text{H}$  NMR (characteristic parts)**Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent:  $\text{DMSO-d}_6$

***clip-zqs-COSY***Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d<sub>6</sub>

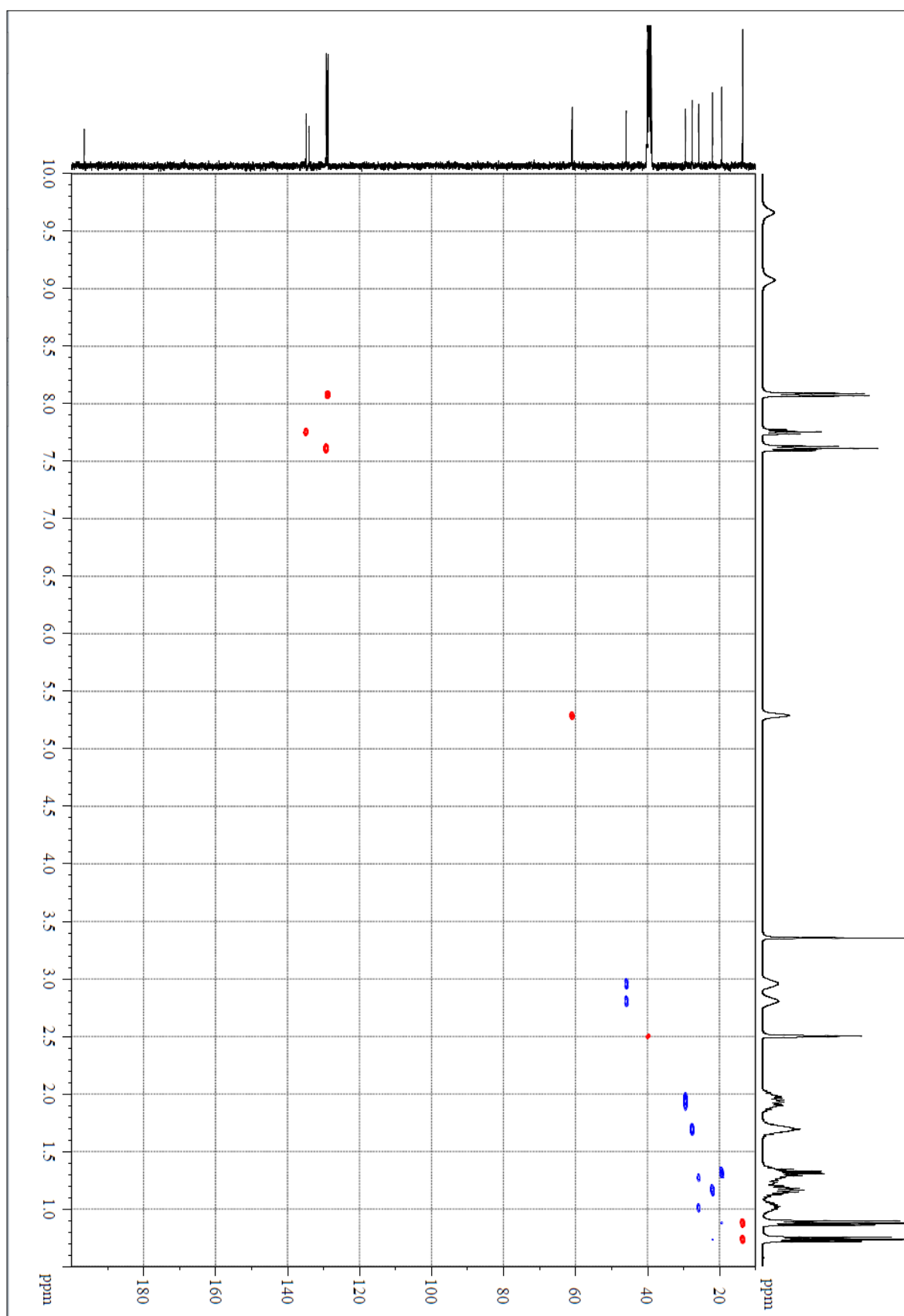
**clip-zqs-COSY-Relay**Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d<sub>6</sub>



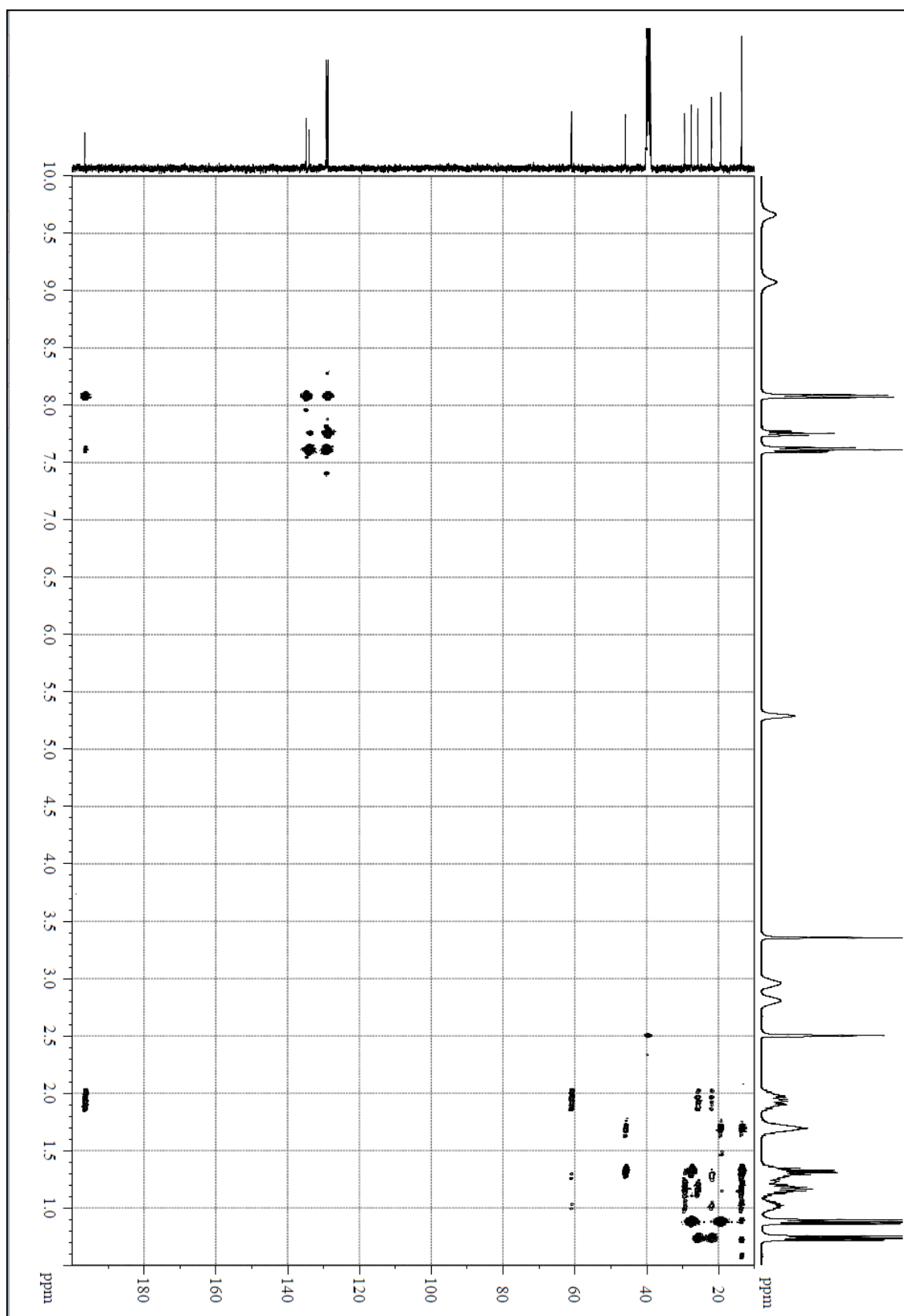
**zqs-TOCSY  $T_{mix} = 120 \text{ msec}$** Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d<sub>6</sub>

**$^{13}\text{C}$  NMR**Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO- $d_6$

## ed-HSQC

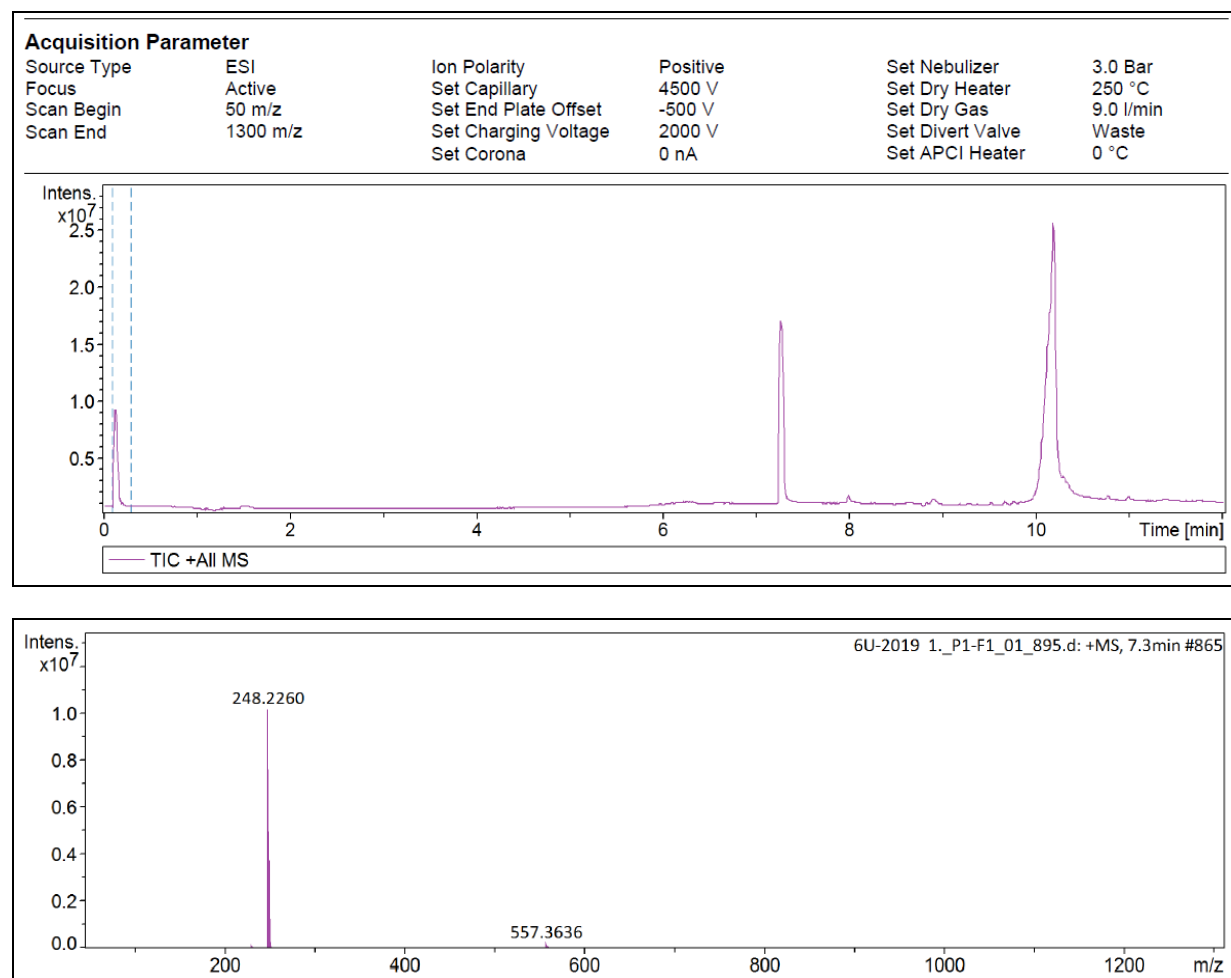
Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO- $d_6$

## HMBC



Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent:  $\text{DMSO-d}_6$

## qTOF



Bruker - QTOF compact; Agilent 1260 Infinity