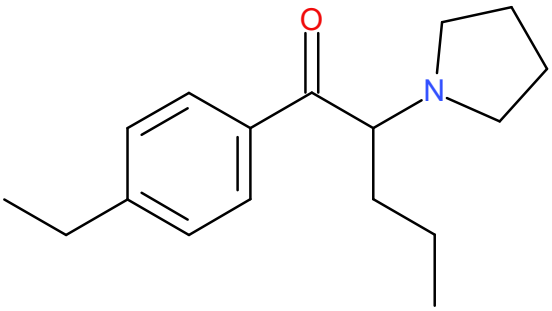
4'-Ethyl-α-PVP



1-(4-ethylphenyl)-2-(pyrrolidin-1-yl)pentan-1-one

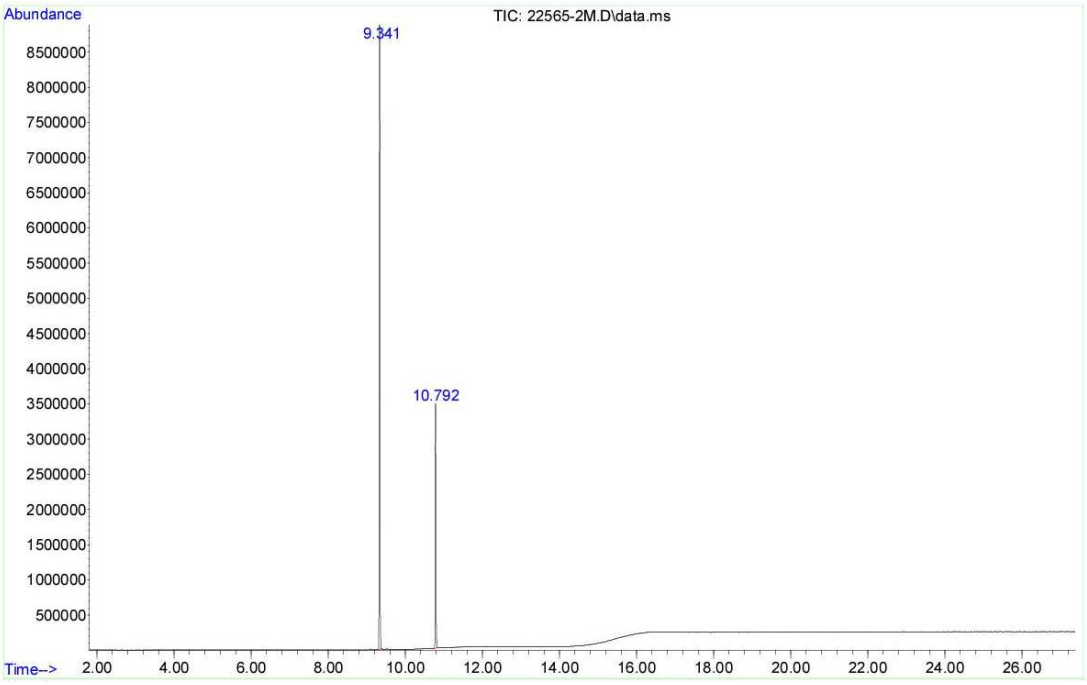
Formula: $C_{17}H_{25}NO$
Formula weight: 259.39
Chemical Abstracts No: n. a.
Smiles string: CCCC(N1CCCC1)C(=O)c2ccc(CC)cc2
InChi key: DXQSRSYIYCRPMM-UHFFFAOYSA-N
Other names:

The evidence was 9.64 grams pink powder.

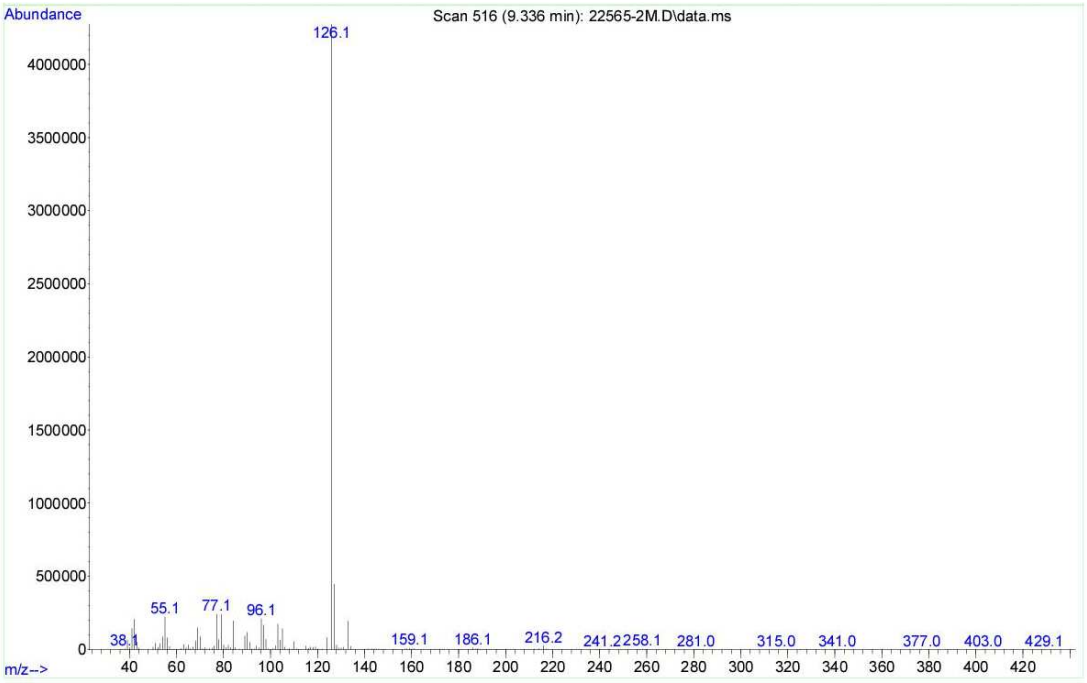
GC-MS

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. The solution of the sample in methanol was injected. 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.

GC-MS total ion chromatogram



Mass spectrum at 9.34 min retention time

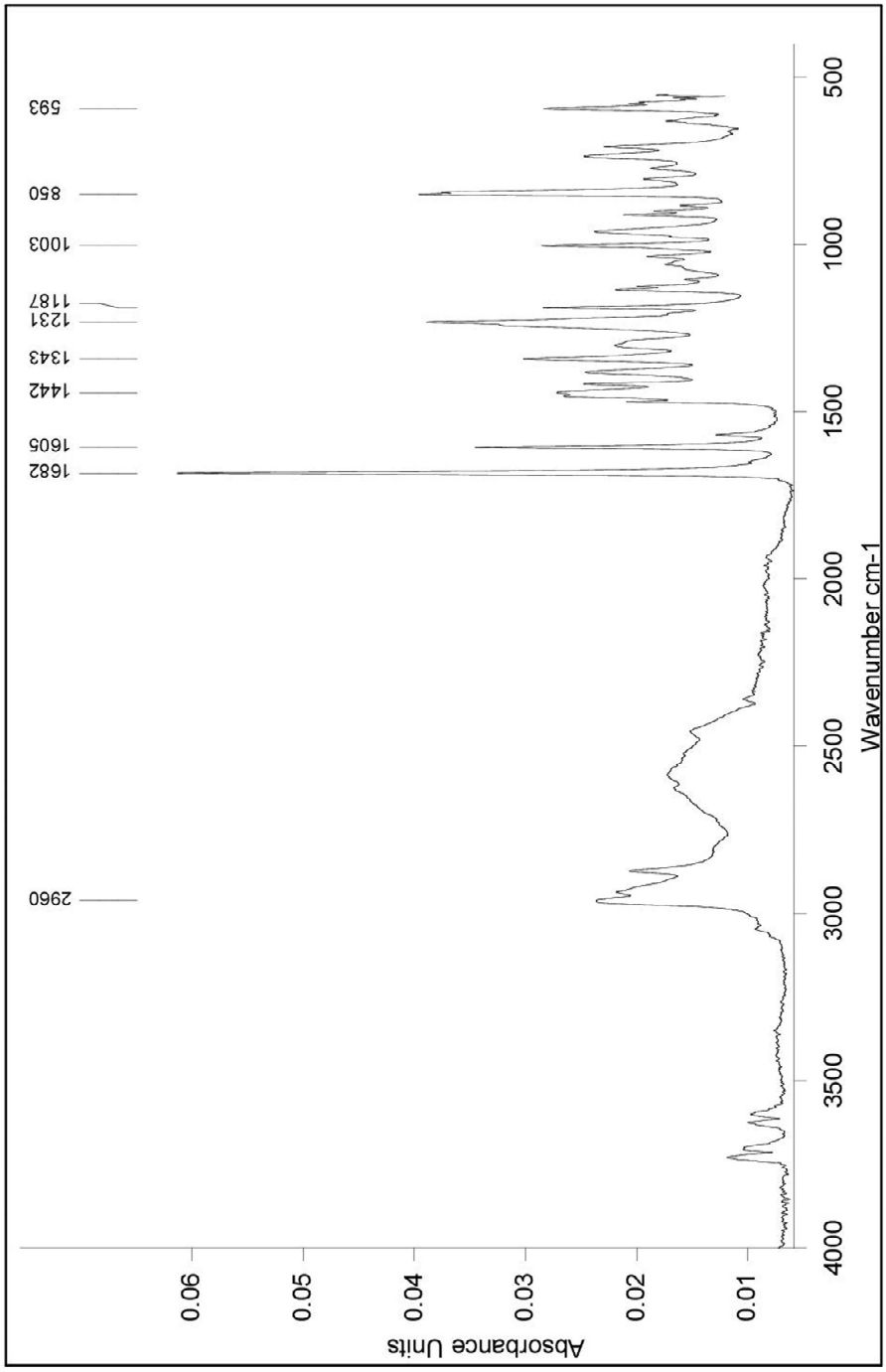


Agilent 6890N Network GC system set up with Agilent HP-5MS

IR

The IR spectrum was recorded on a Thermo SCIENTIFIC Nicolet iS5 FT-IR spectrometer equipped with an iD5 ATR accessory, in absorbance mode. The digital resolution is 4 cm^{-1}. The seized powder was measured directly. The spectrometer was controlled, and the data were processed using Omnic 9 software package. The spectrum was off-line visualized, and the output below was performed by OPUS 7.5 software.

IR spectrum



Thermo SCIENTIFIC Nicolet iS5 FT-IR spectrometer

NMR

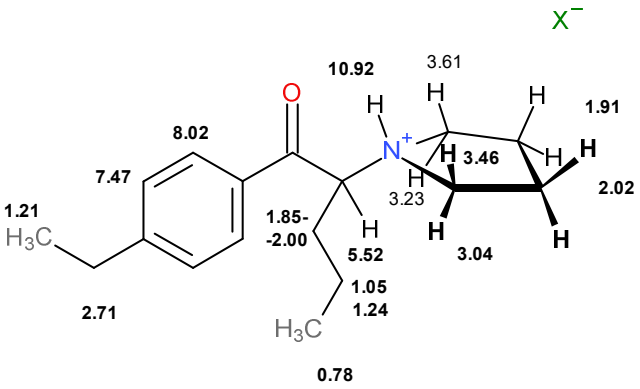
The NMR spectra were recorded on a Bruker Avance Neo 400 NMR operating at 9.4 Tesla magnetic field, equipped with Prodigy BBO-H&F-D-05 Z-gradient probe. The spectra were recorded at 25°C in DMSO-d_6 solution. The sized powder was measured directly. The spectrometer was controlled, and the data were processed using TopSpin 4.0 software package. Chemical shifts (δ) are given in parts per million unit, referenced to tetramethylsilane (δ_{TMS} = 0.00 ppm). The determination of the structure was based on ^{1}H, *zqs-clip*-COSY, *zqs*-TOCSY, *zqs*-NOESY as well as ^{13}C, multiplicity edited HSQC, double edited HSQC-*zqs-clip*-COSY and HMBC spectra.

Interpretation of the NMR spectra

In DMSO-d_6 solution

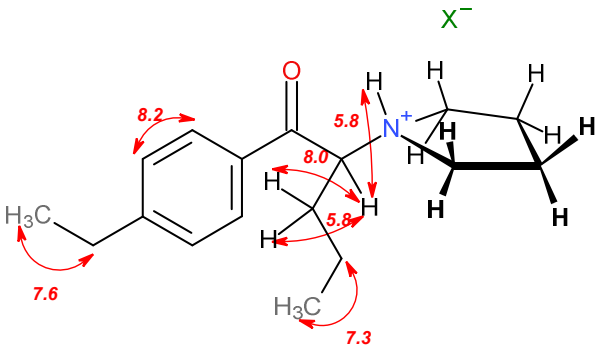
^{1}H-NMR chemical shifts δ [ppm]

4'-ethyl-α-PVP

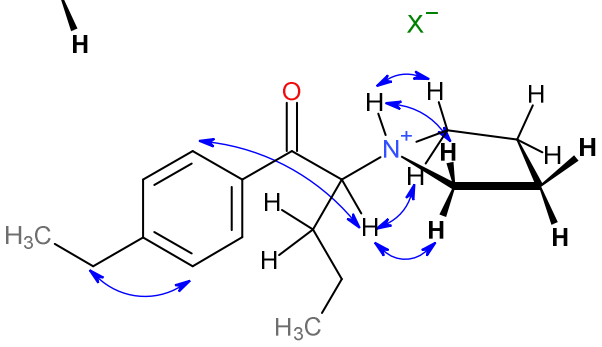


Formula Weight: 259,3865 (Base)
Exact Mass: 259,19361443
Molecular Formula: $C_{17}H_{25}NO$
Formula Weight: 295,84744 (HCl salt)

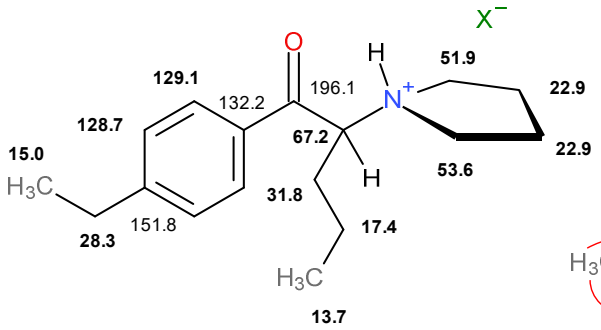
Characteristic J(H-H) coupling constants *J* [Hz]



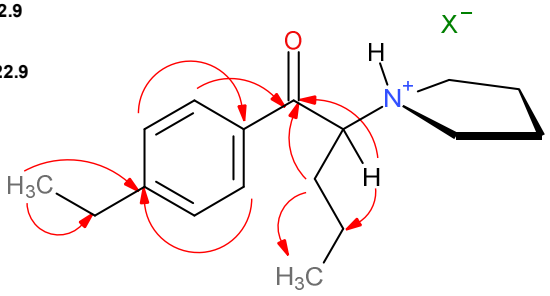
Characteristic H-H steric proximitis detected by zqs-NOESY measurement



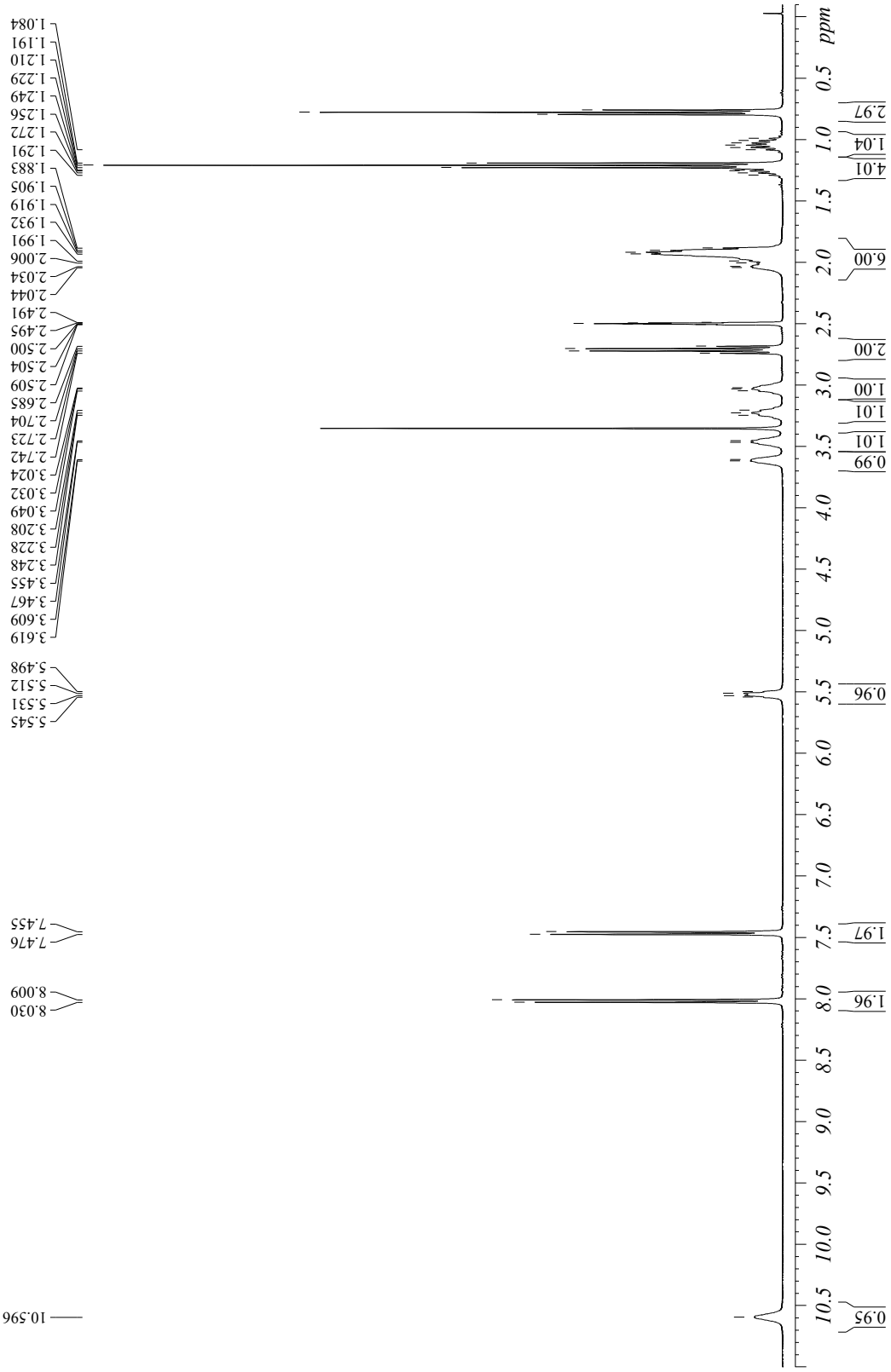
^{13}C-NMR chemical shifts δ [ppm]



Characteristic heteronuclear long-range couplings detected byHMBC measurement
H ⟶ C

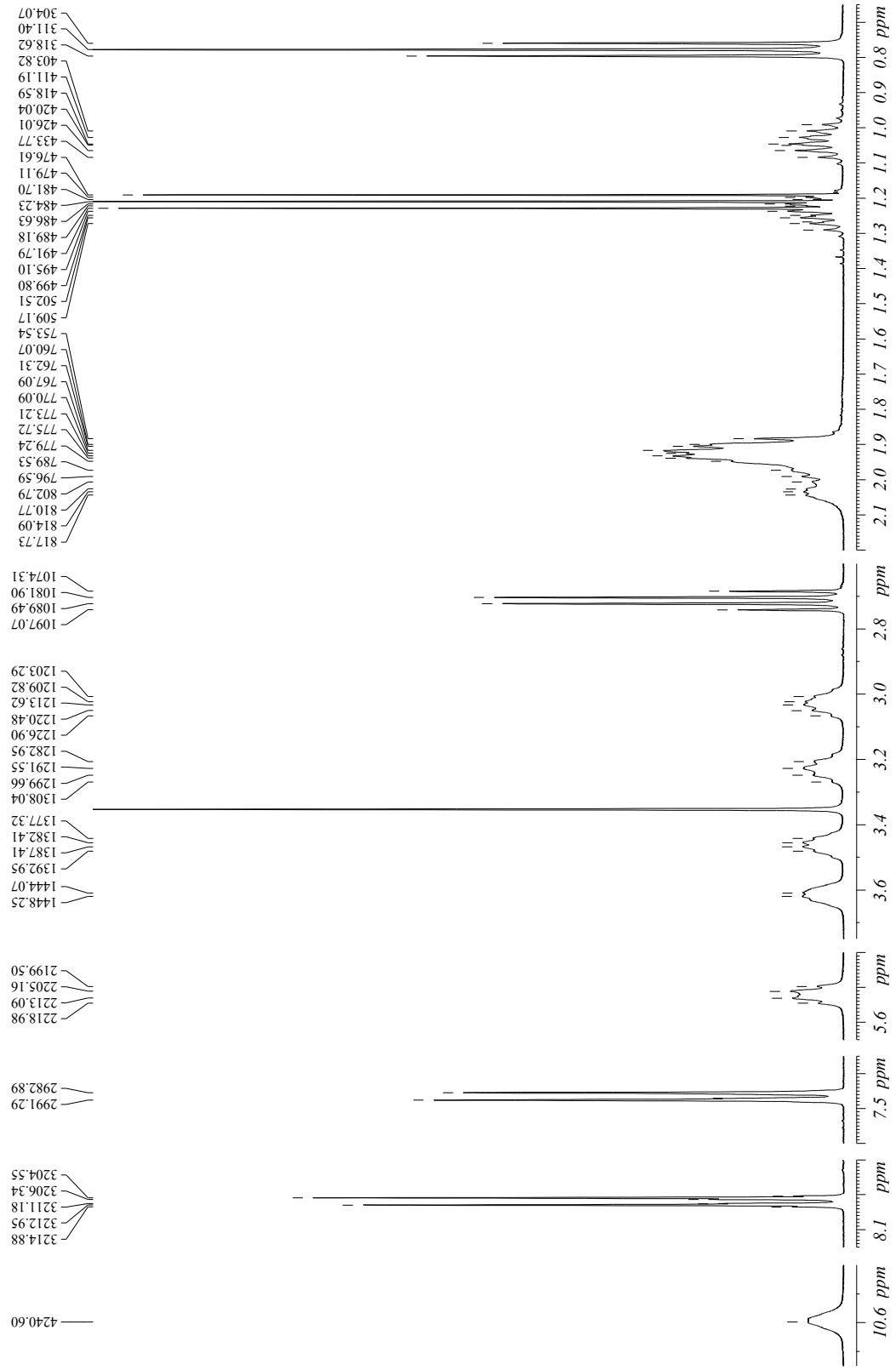


^{1}H-NMR spectrum (overview)



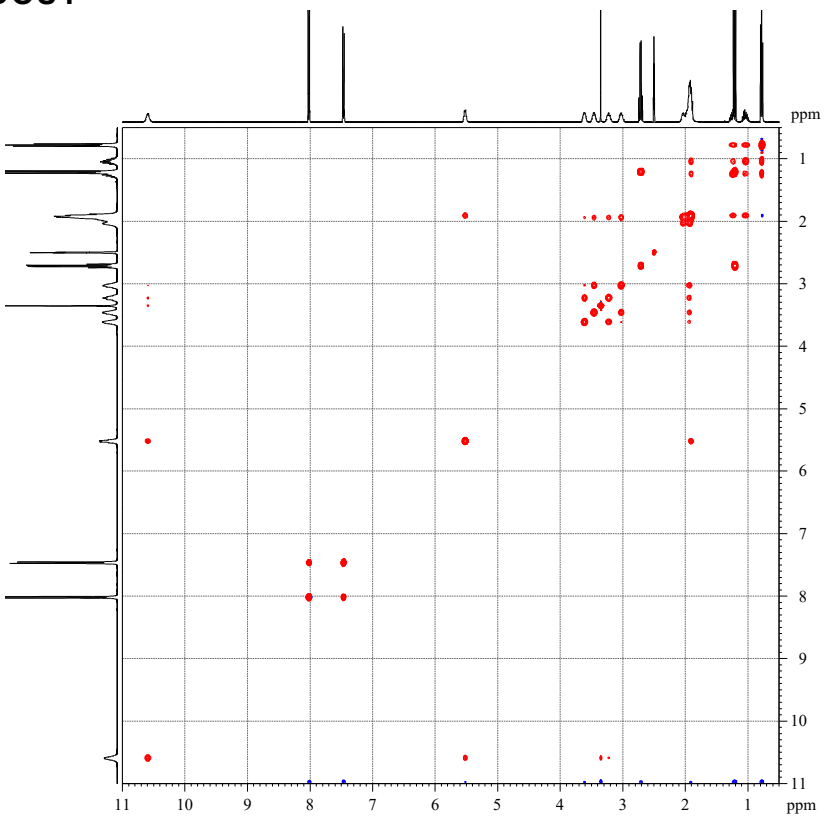
Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6

^{1}H-NMR spectrum (characteristic sections)

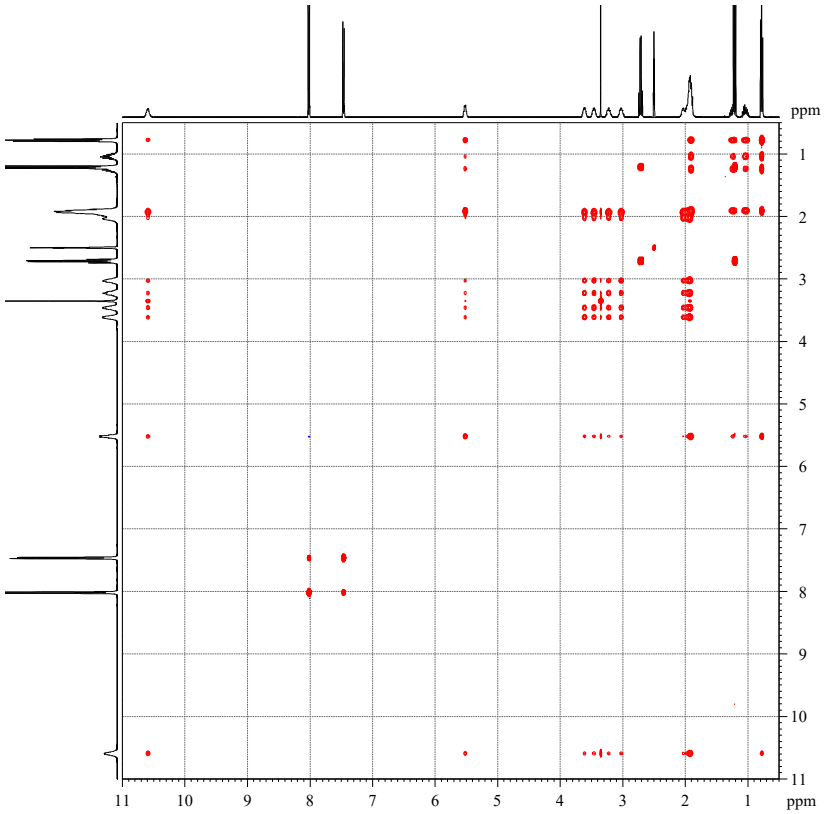


Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6

zqs-clip-COSY

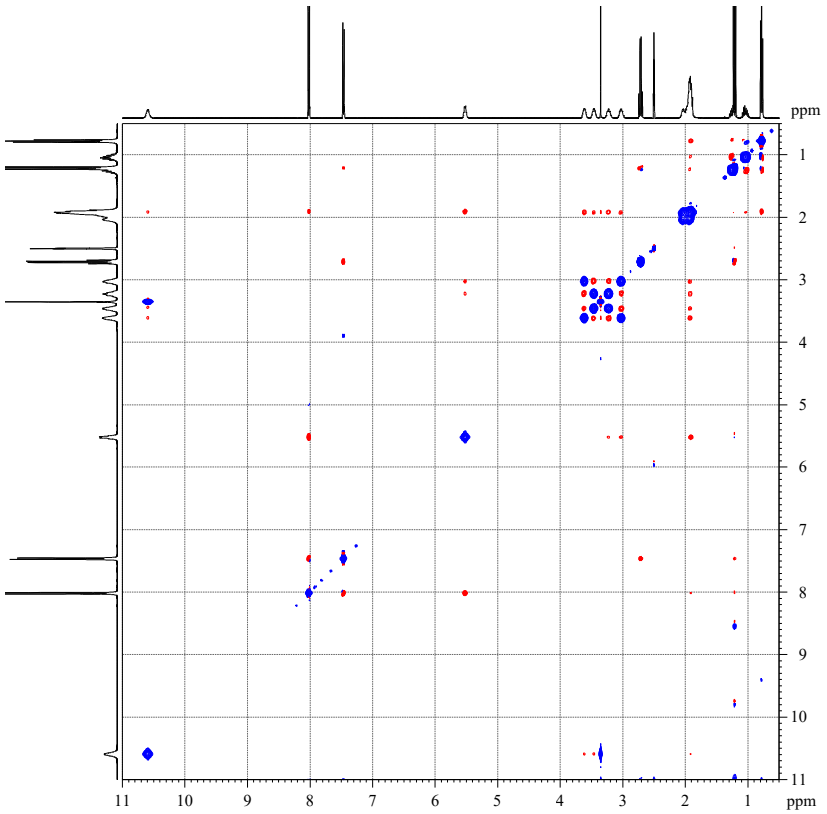


zqs-TOCSY

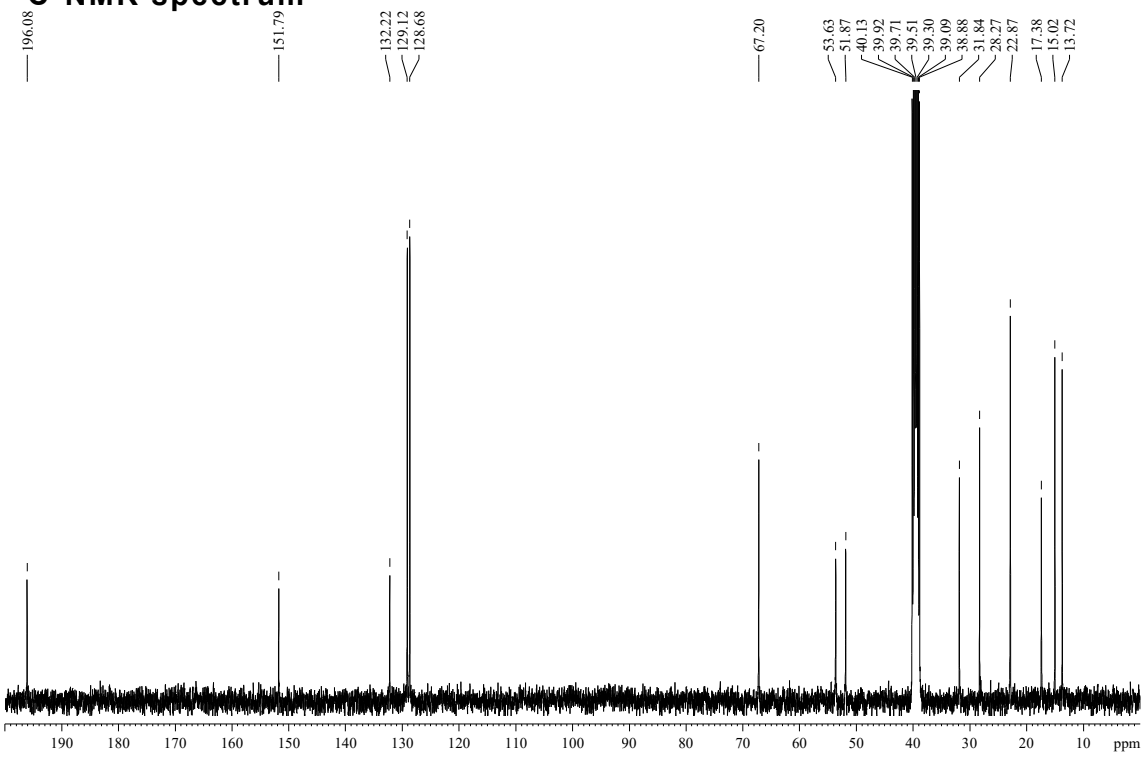


Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6

zqs-NOESY

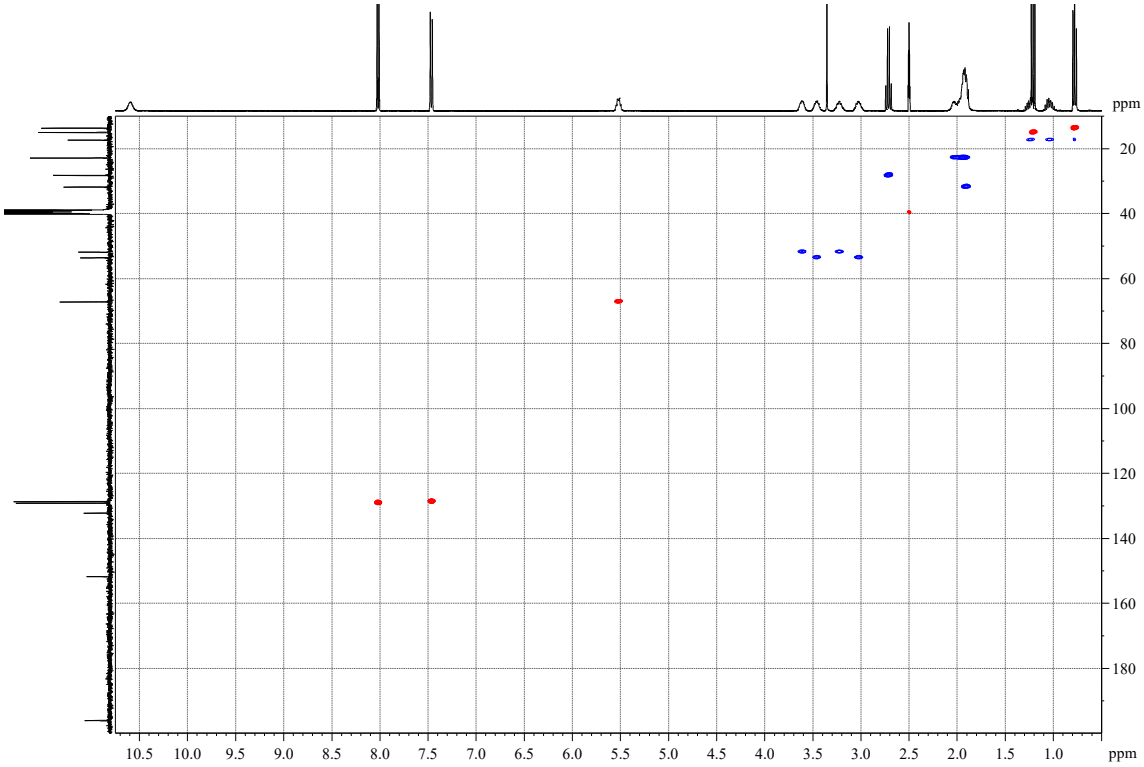


^{13}C-NMR spectrum

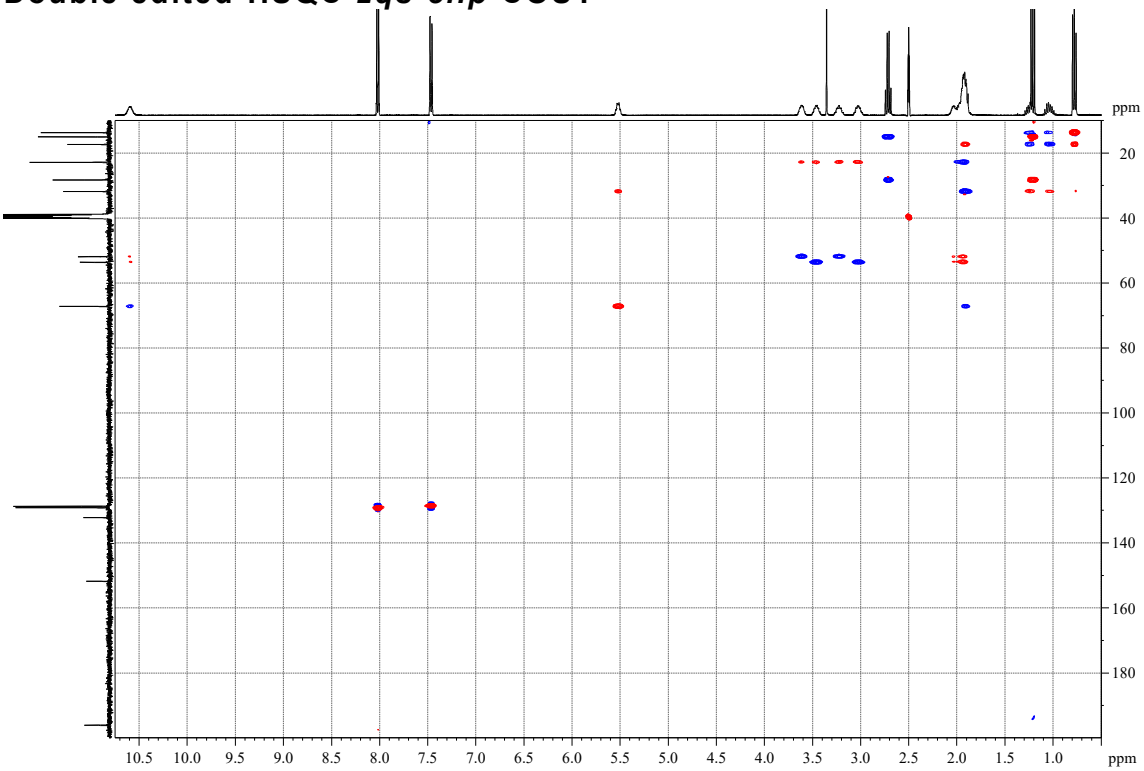


Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6

ed-HSQC

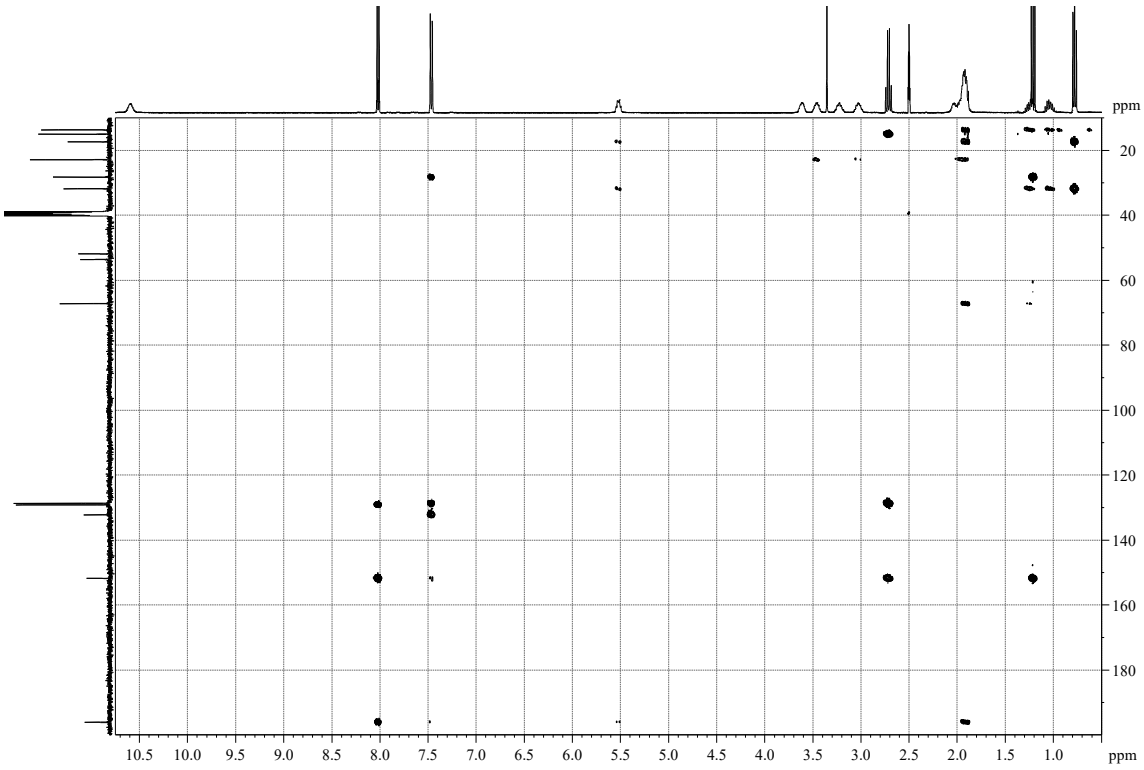


Double edited-HSQC-*zqs-clip*-COSY



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

HMBC



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