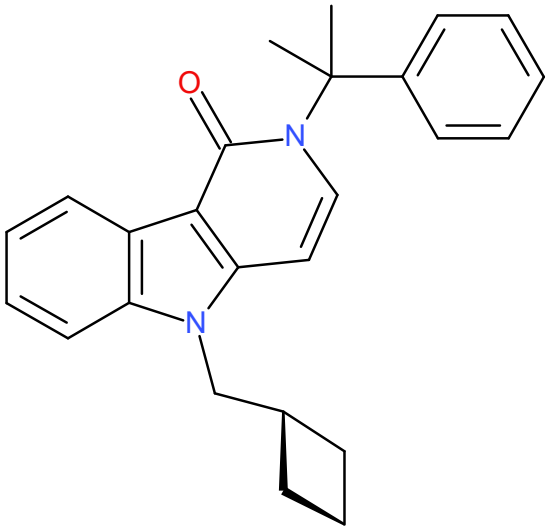
Cumyl-Cb-MeGaClone



5-(cyclobutylmethyl)-2-(1-methyl-1-phenyl-ethyl)pyrido[4,3-b]indol-1-one

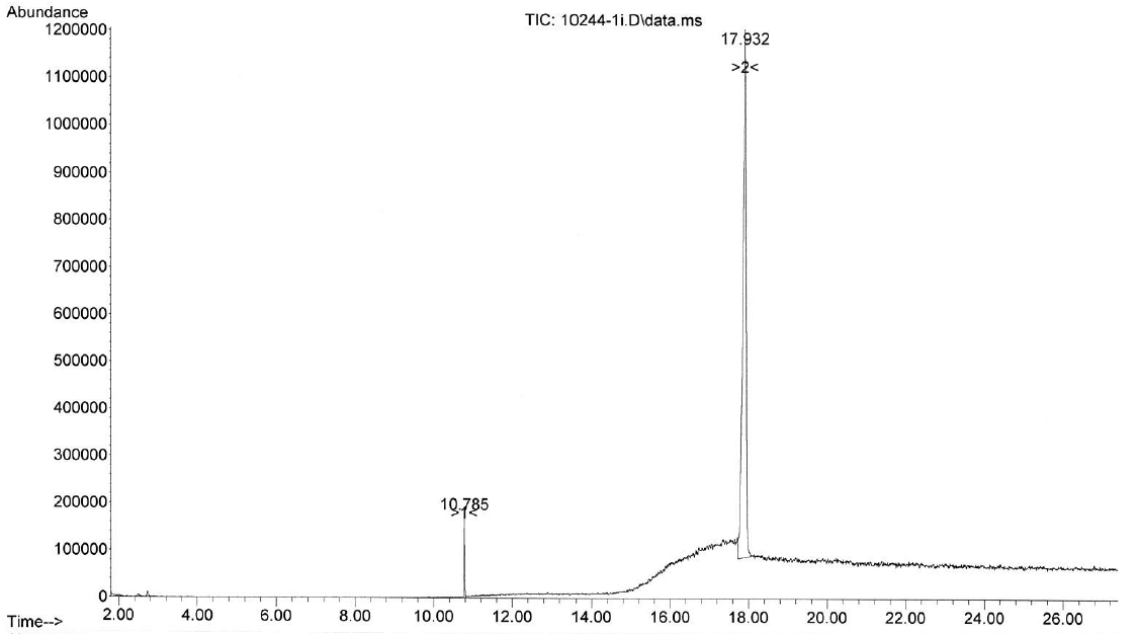
Formula: $C_{25}H_{26}N_2O$
Molecular weight: 370.49
Chemical Abstracts No.: *n. a.*
Smiles code: CC(C)(N1C=Cc2c(C1=O)c3ccccc3n2CC4CCC4)c5ccccc5
InChi key: VOCGZWPYRQJUMY-UHFFFAOYSA-N
Other names: cumyl-cyclobutylmethyl-gamma-carbolinone,
Cumyl-Cb-MeGaClone

The compound was adsorbed on herbal.

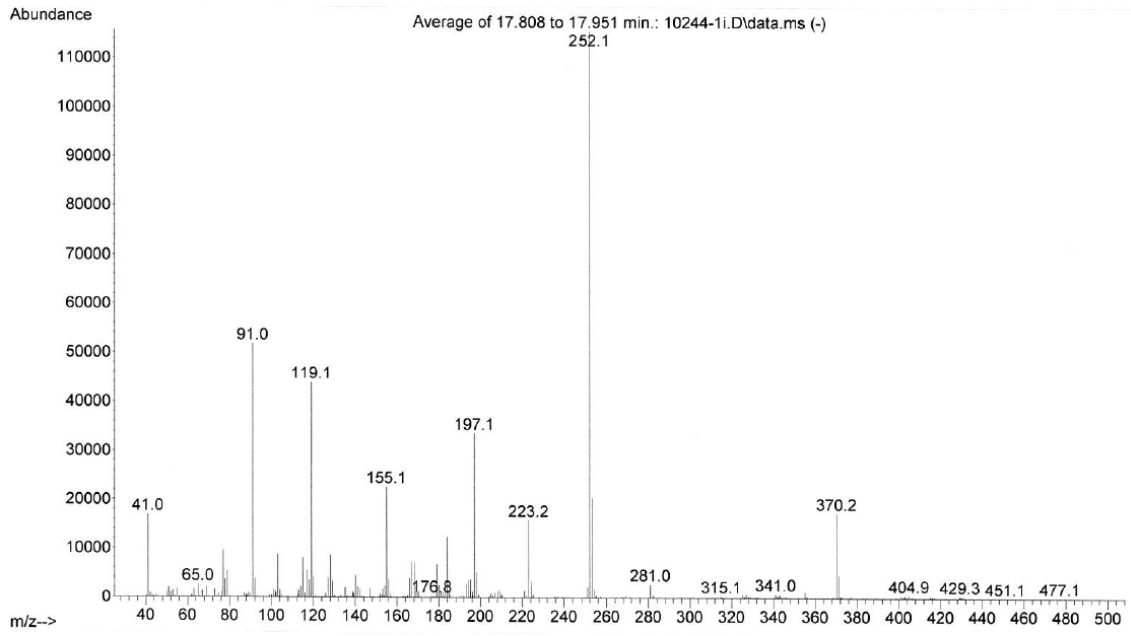
GC-MS

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. 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 chromatogram



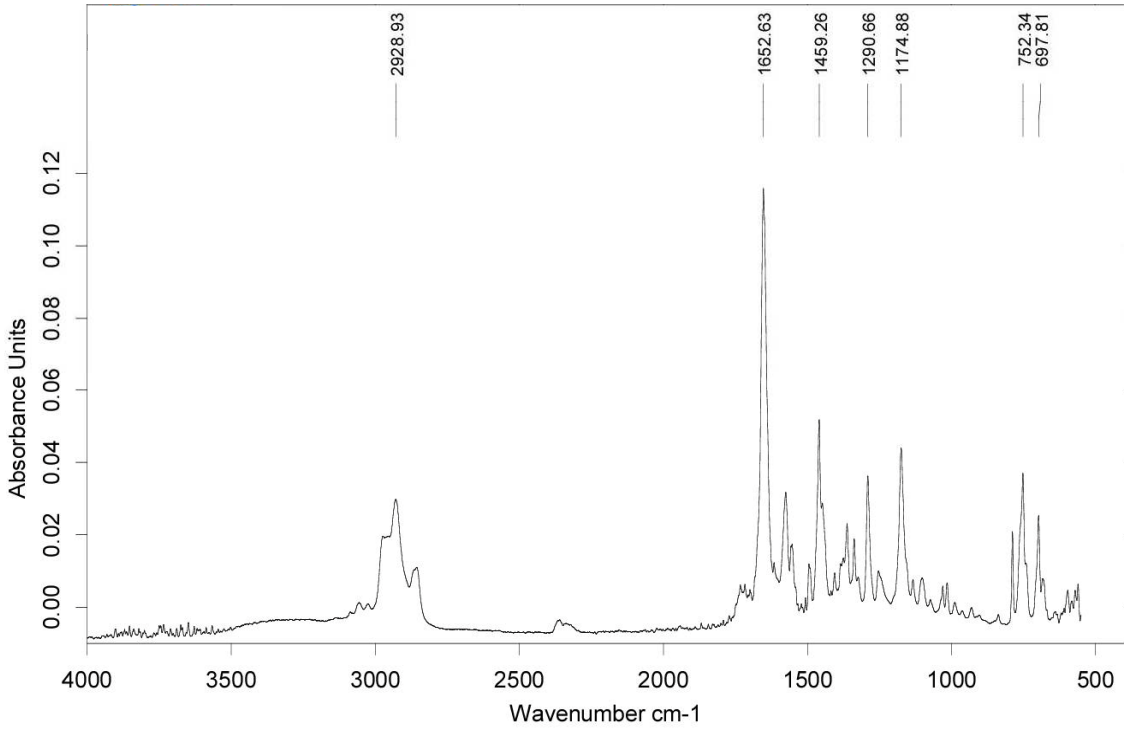
Mass spectrum at 17.95 min. retention time



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 material was extracted by acetone, the solvent was evaporated on the surface of the ATR accessory. 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.



Thermo SCIENTIFIC Nicolet iS5 FT-IR spectrometer

NMR

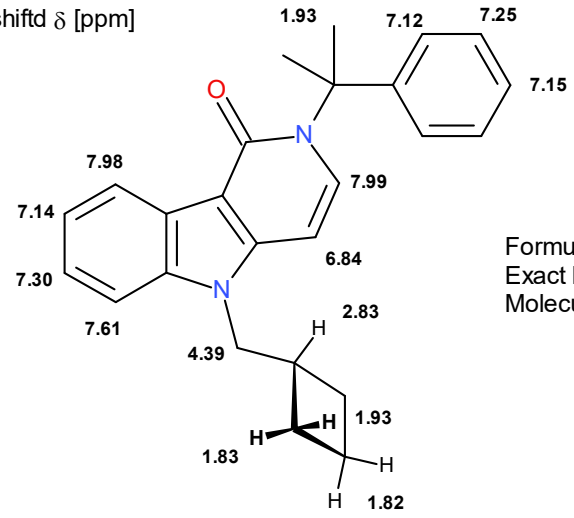
The sized material was extracted by DMSO-d_6 solvent, the filtered extract was transferred into NMR tube. The NMR spectra were recorded on a Bruker Avance Neo 400 NMR operating at 9.4 Tesla magnetic field, equipped with Prodigy BBO-H&F-D-05 Z-gradient probe. The spectra were recorded at 25°C. The spectrometer 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-easy-ROESY, as well as ^{13}C, multiplicity edited HSQC, HMBC as well as double-edited HSQC-zqs-clip-COSY spectra.

Interpretation of the NMR spectra

Cumyl-Cb-MeGaClone
5-(cyclobutylmethyl)-2-(1-methyl-1-phenyl-ethyl)pyrido[4,3-b]indol-1-one
CC(C)(N1C=Cc2c(C1=O)c3ccccc3n2CC4CCC4)c5ccccc5
VOCGZWPYRQJUMY-UHFFFAOYSA-N

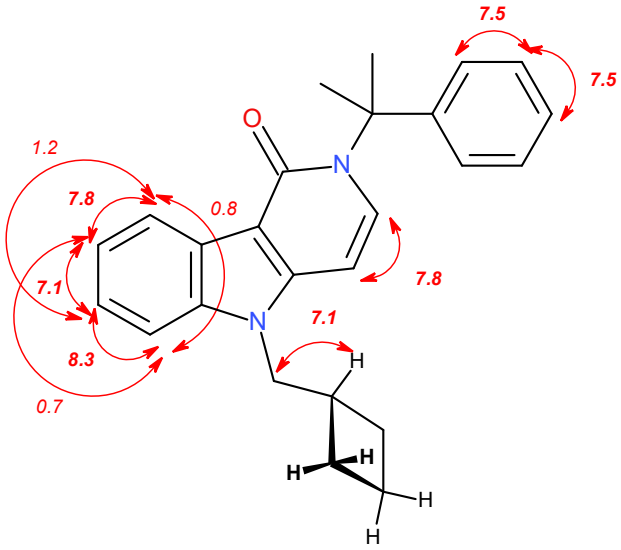
In DMSO-d_6 solution

^{1}H-NMR chemical shiftd δ [ppm]

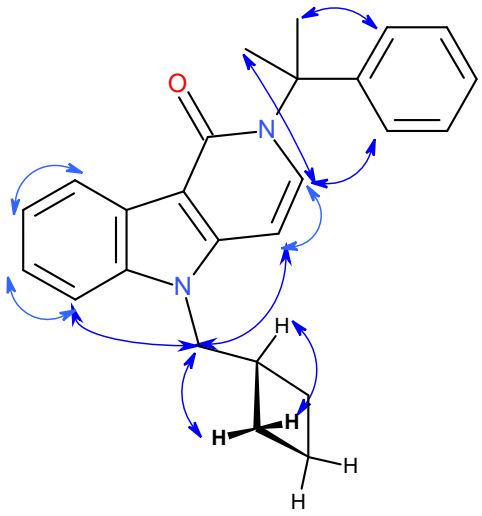


Formula Weight: 370,48674
Exact Mass: 370,204513472
Molecular Formula: $C_{25}H_{26}N_2O$

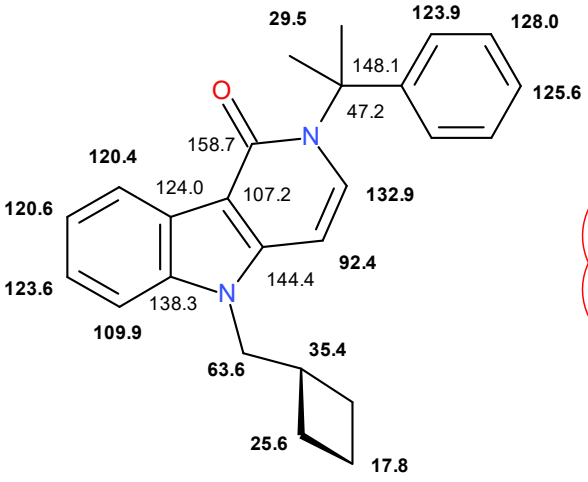
J(H,H) coupling constants [Hz]



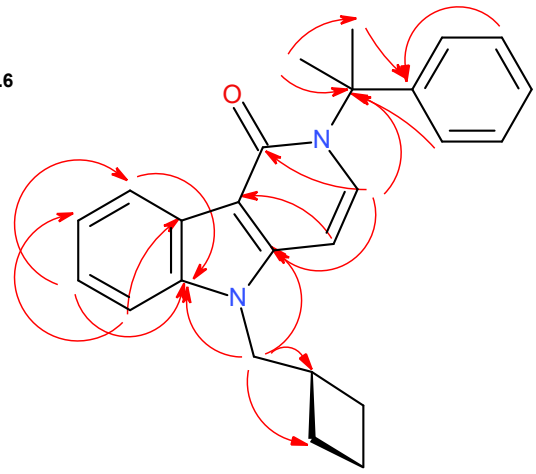
Steric proximities detected by zqs-easy-ROESY method



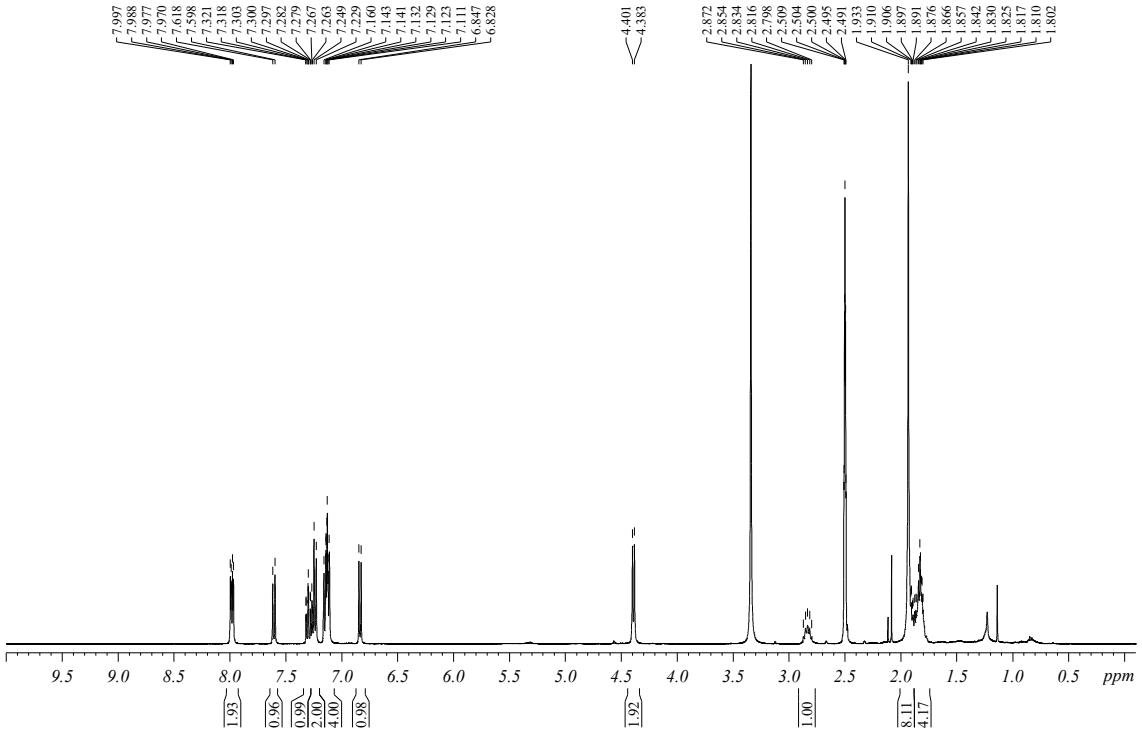
^{13}C-NMR chemical shifts δ [ppm]



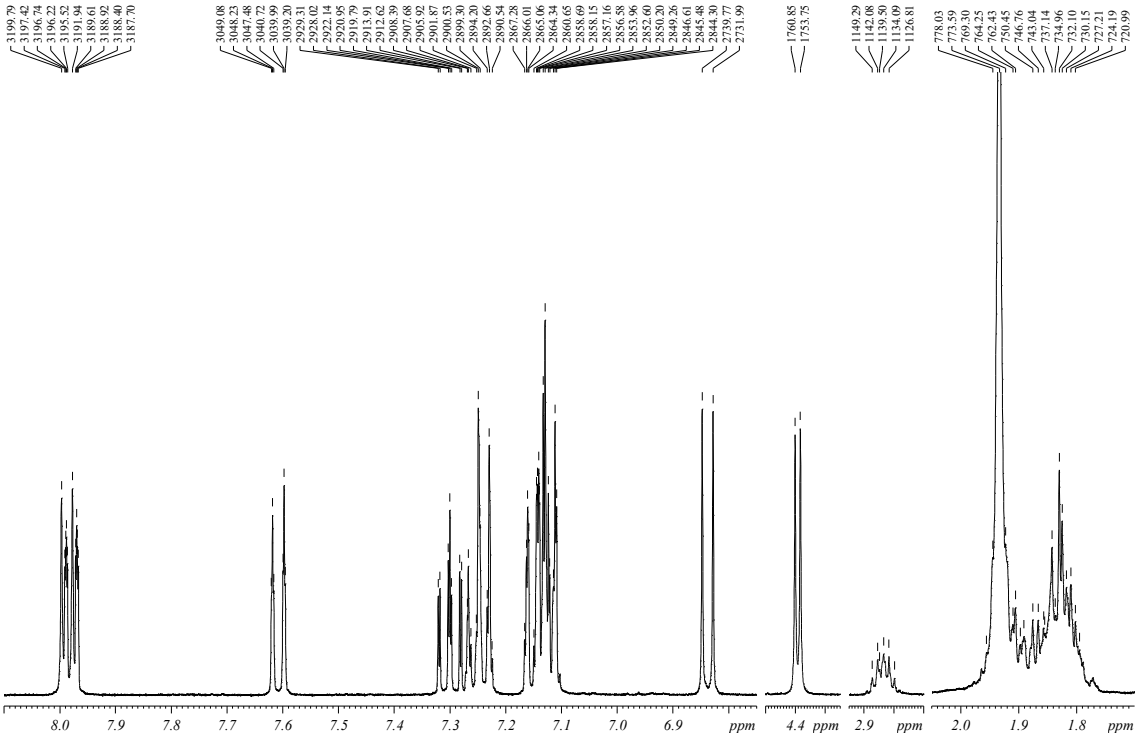
Heteronuclear long-range coupling detected by HMBC method H ⟶ C



^{1}H NMR spectrum (overview)

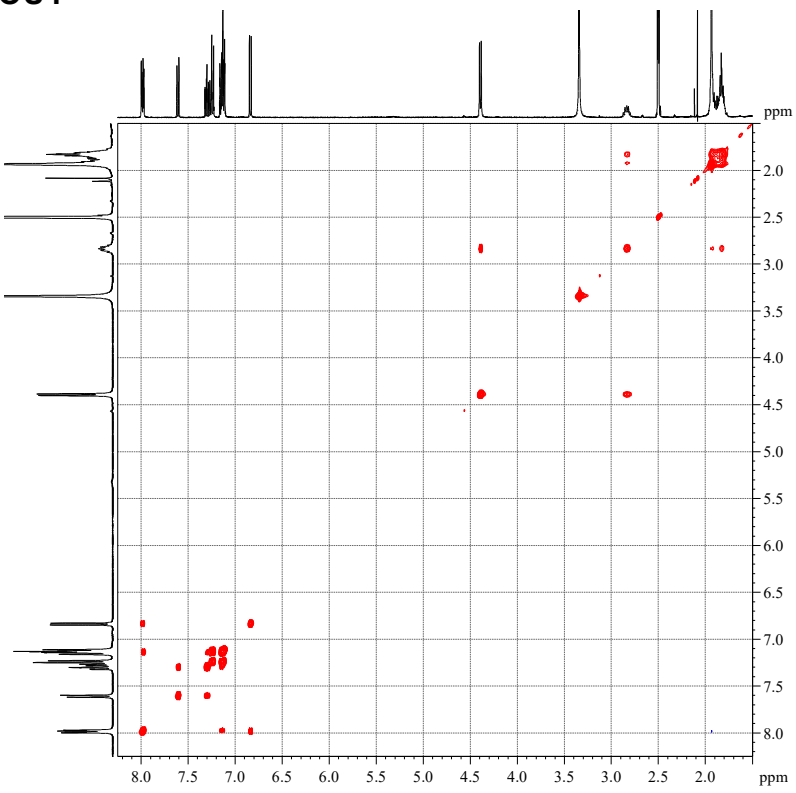


^{1}H NMR spectrum (characteristic sections)

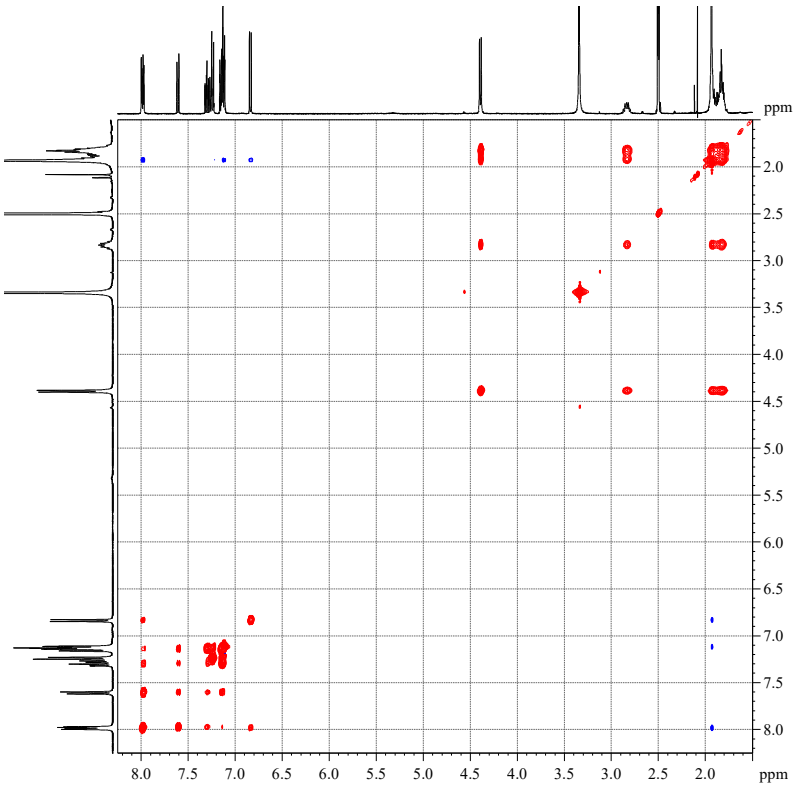


Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6

zqs-clip-COSY

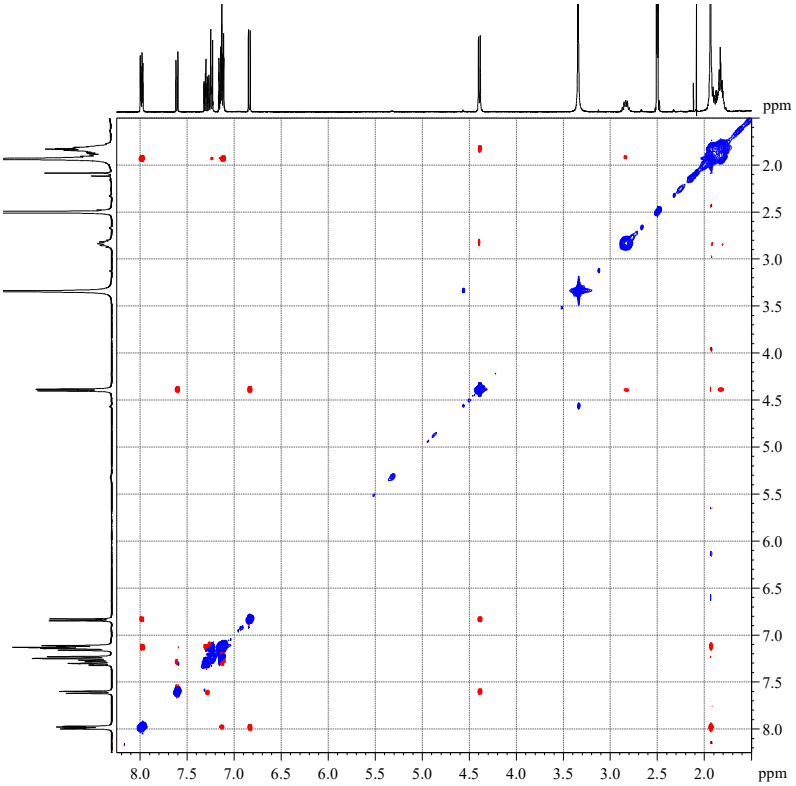


zqs-TOCSY

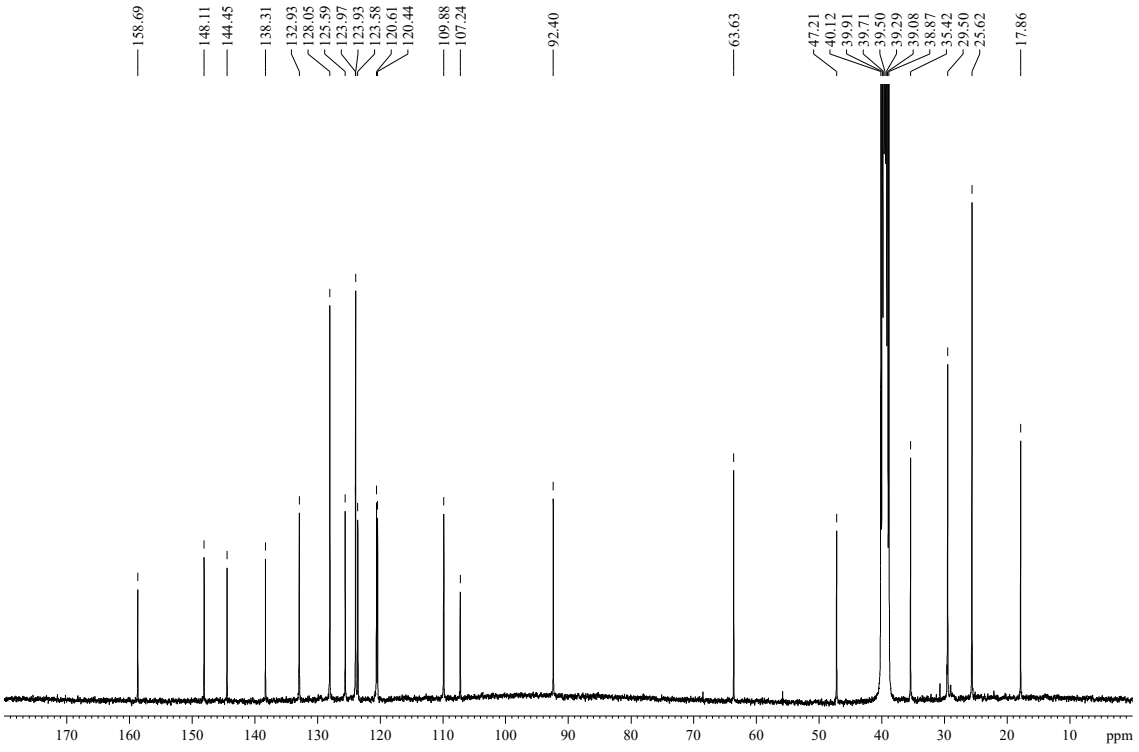


Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6

zqs-easy-ROESY

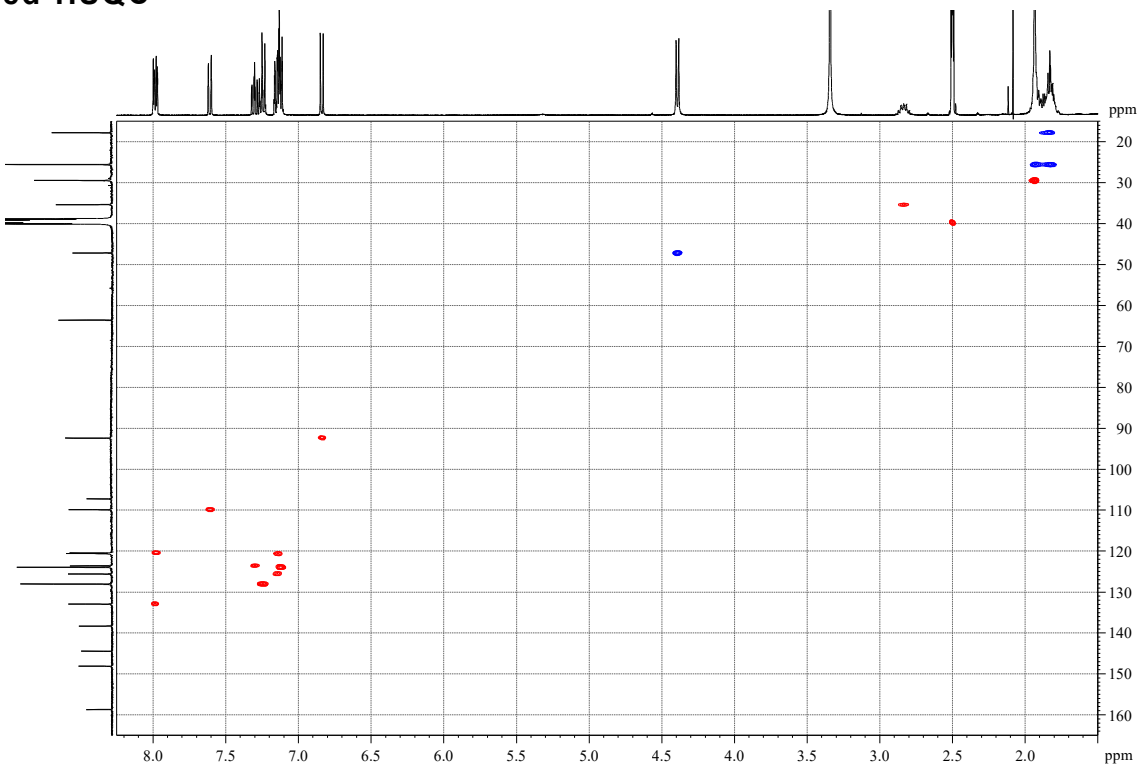


^{13}C NMR

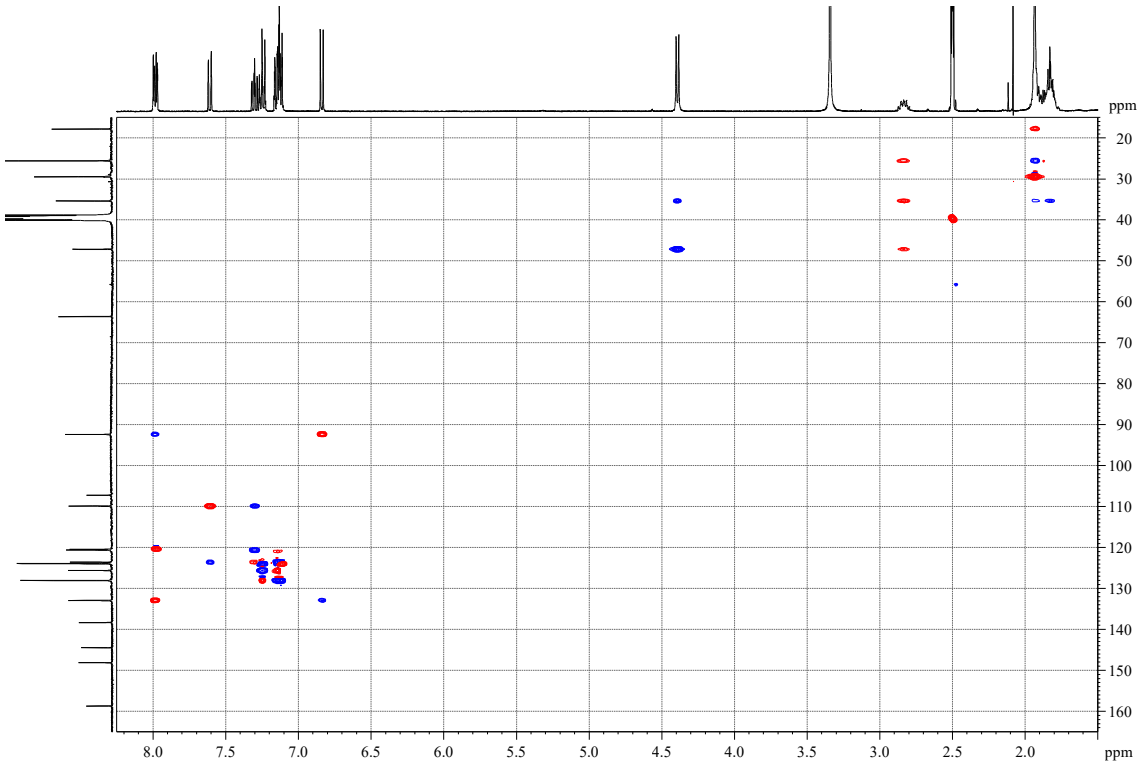


Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6

ed-HSQC

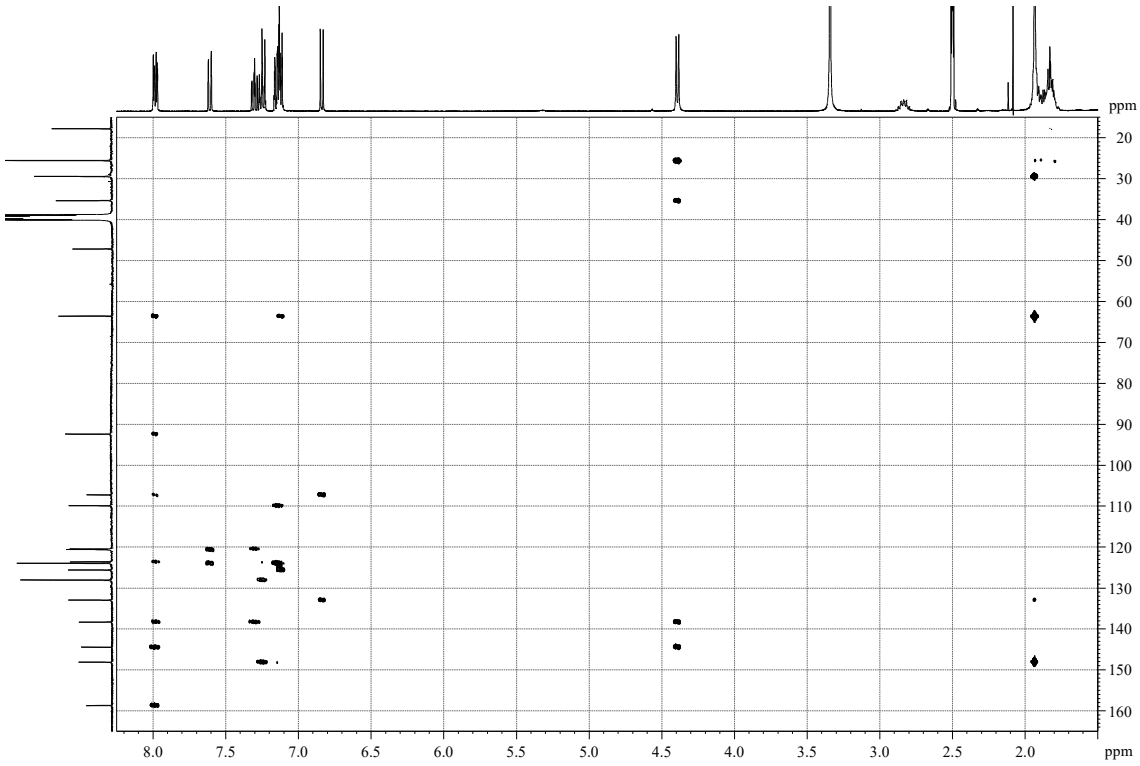


double edited-HSQC-zqs-clip-COSY



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

HMBC



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