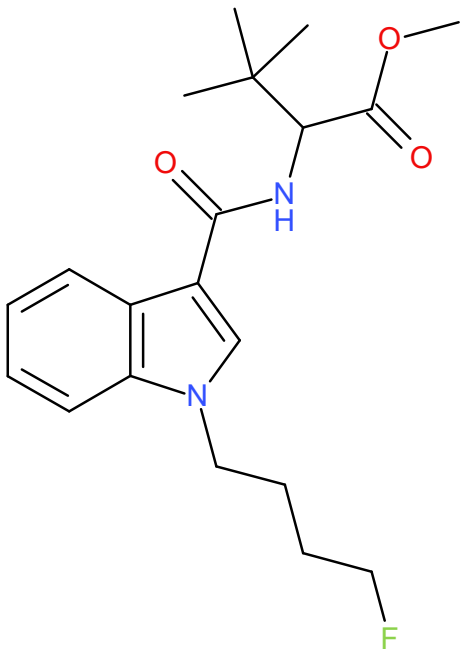
4F-MDMB-BICA



methyl 2-({[1-(4-fluorobutyl)-1*H*-indol-3-yl]carbonyl}amino)-3,3-dimethylbutanoate

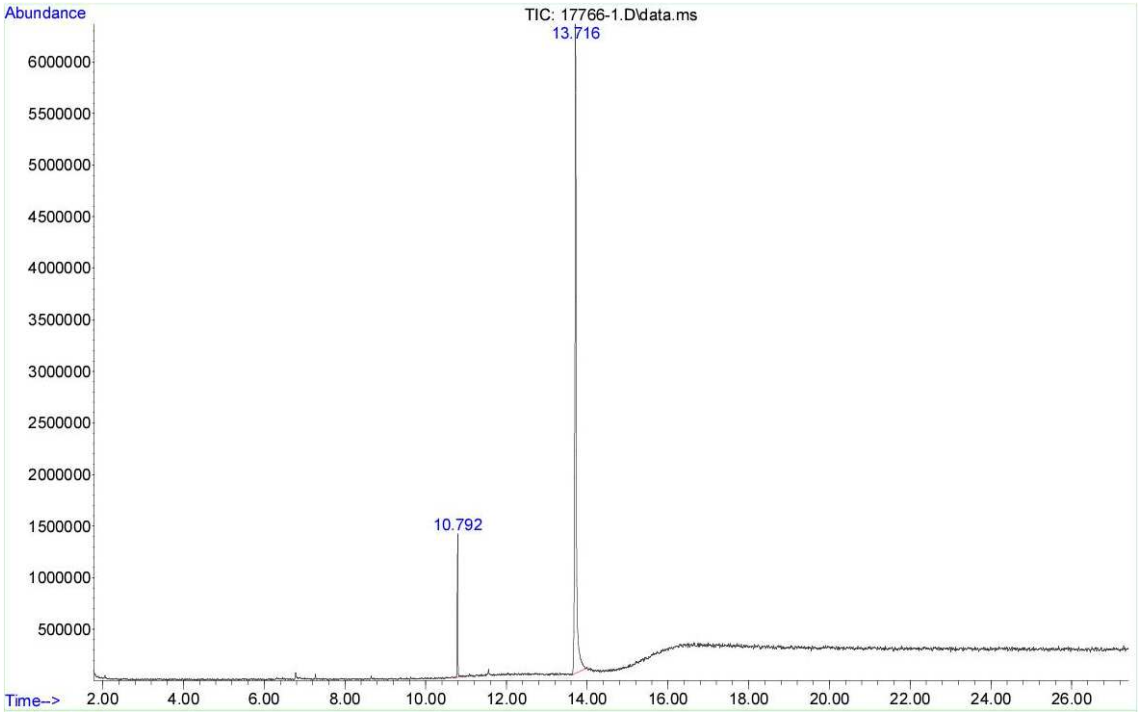
Formula: $C_{20}H_{27}FN_2O_3$
Molecular weight: 362.44
Chemical Abstracts No.: *n. a.*
Smiles code: OC(=O)C(NC(=O)c1cn(CCCCF)c2ccccc12)C(C)(C)C
InChi key: QIKHYQCWGUGFBB-UHFFFAOYSA-N
Other names: MDMB-4F-BICA, 4F-MDMB-BUTICA, MDMB-4F-BUTICA

The seized material was 53.09 grams orange colored amorphous solid material.

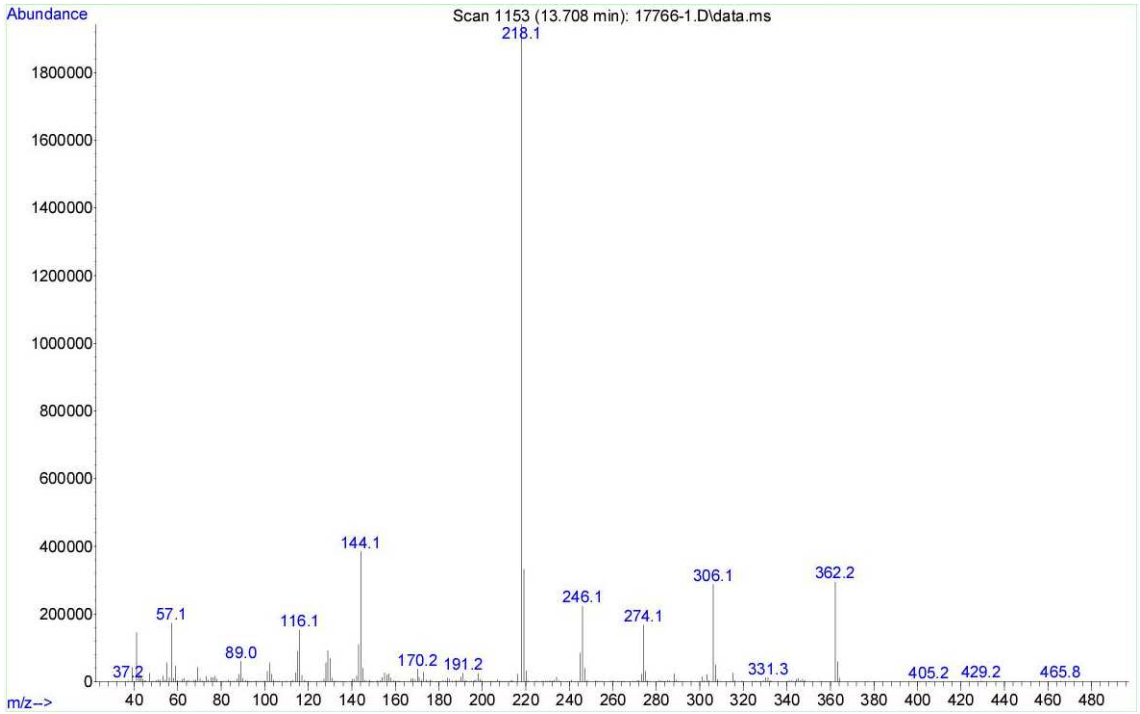
GC-MS

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 ℃ (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 13.71 min. retention time

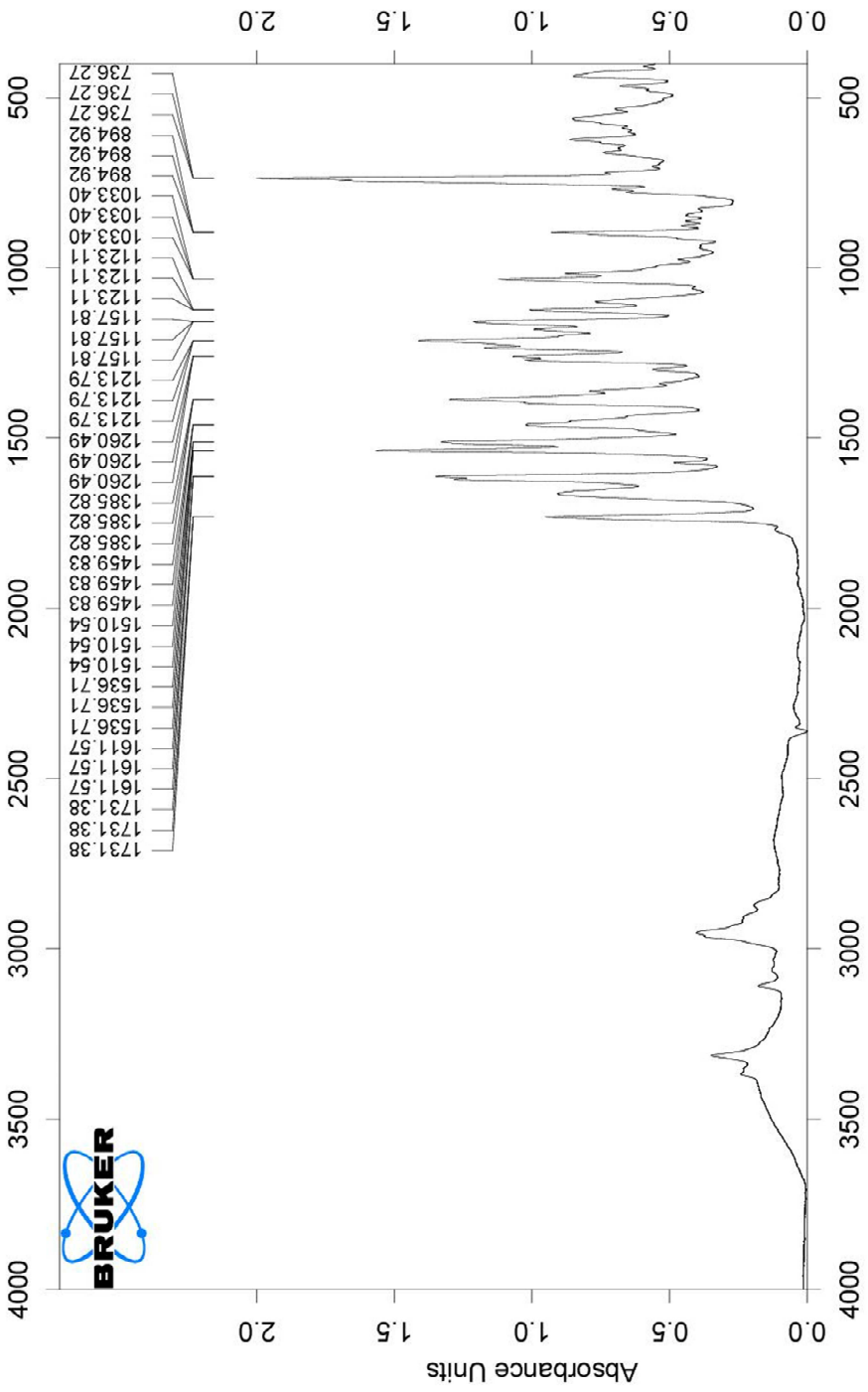


Agilent 6890N Network GC system set up with Agilent HP-5MS

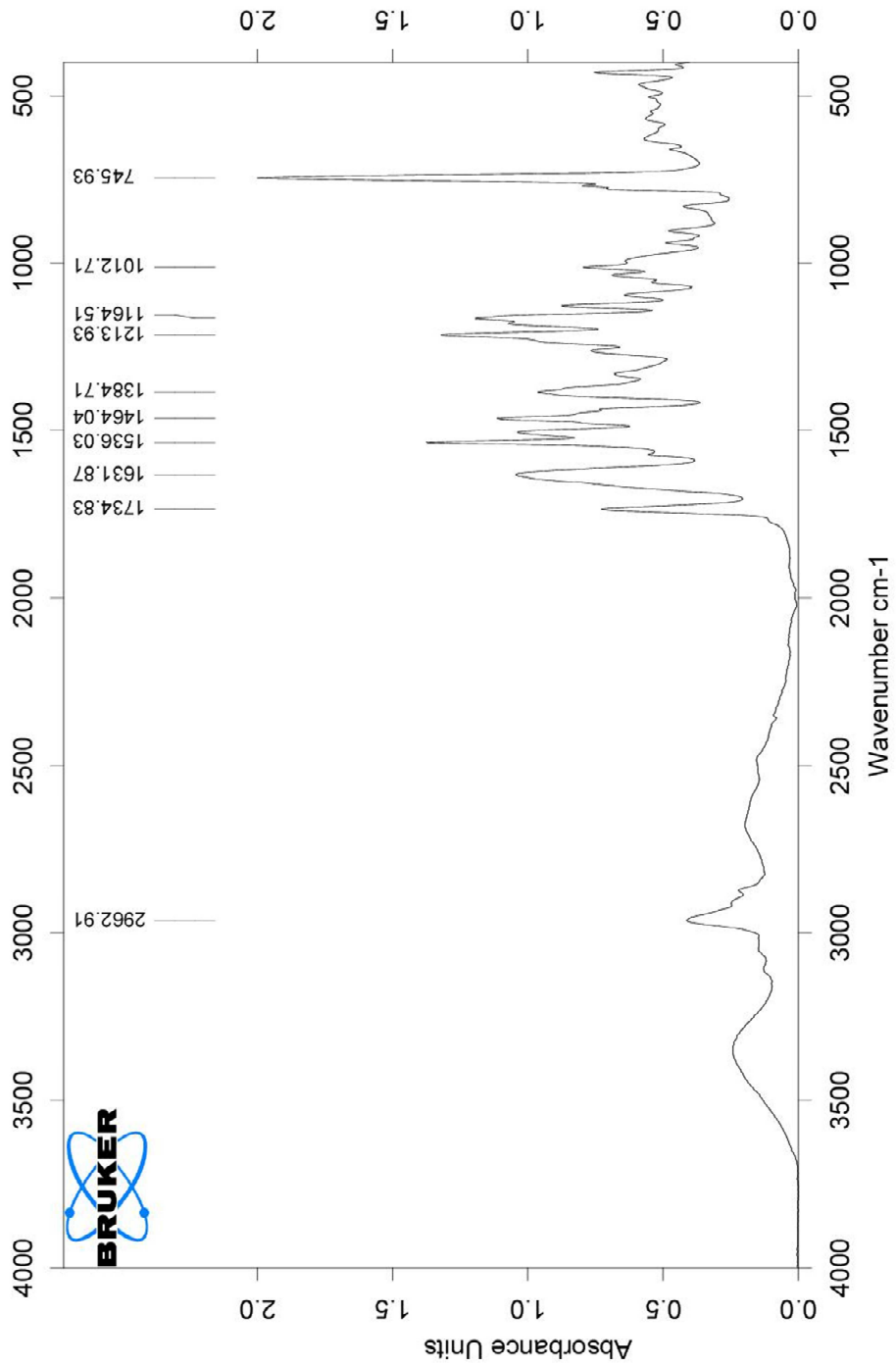
IR

The IR spectrum was recorded on a Bruker Tensor 27 IR spectrometer equipped with a Platinum ATR accessory, in absorbance mode. Az first the sized powder was measured directly, than the evaporated acetone extract was also measured. The digital resolution is 4 cm^{-1}. The spectrometer was controlled, and the data were processed using Opus 6.5 software package.

IR spectrum of the seized material



IR spectrum of the sized material evaporated acetone extract on the ATR plate

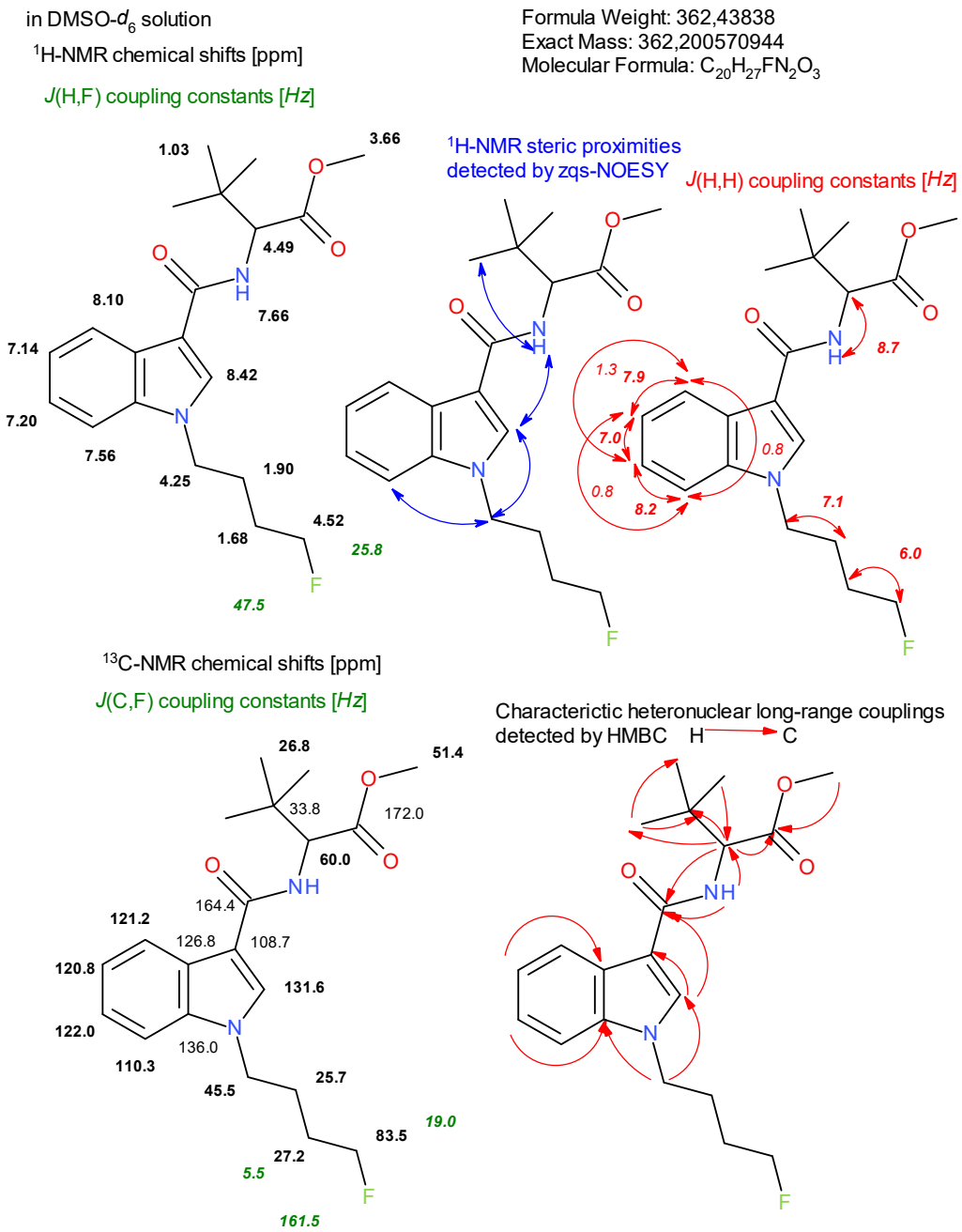


Bruker tensor 27 FT-IR spectrometer

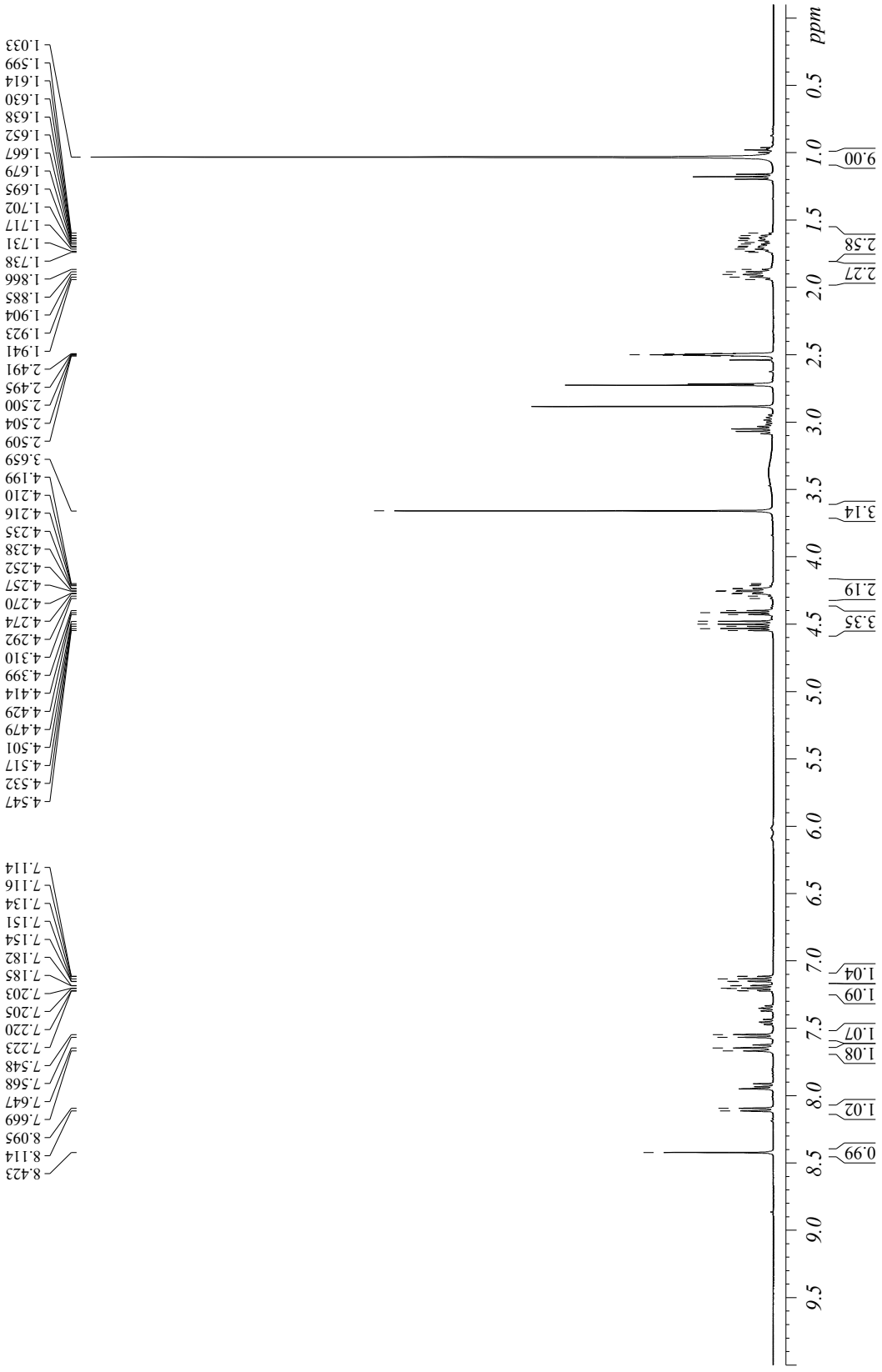
NMR

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 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, DOSY difference as well as ^{13}C, multiplicity edited HSQC, HMBC and double-edited HSQC-zqs-clip-COSY spectra.

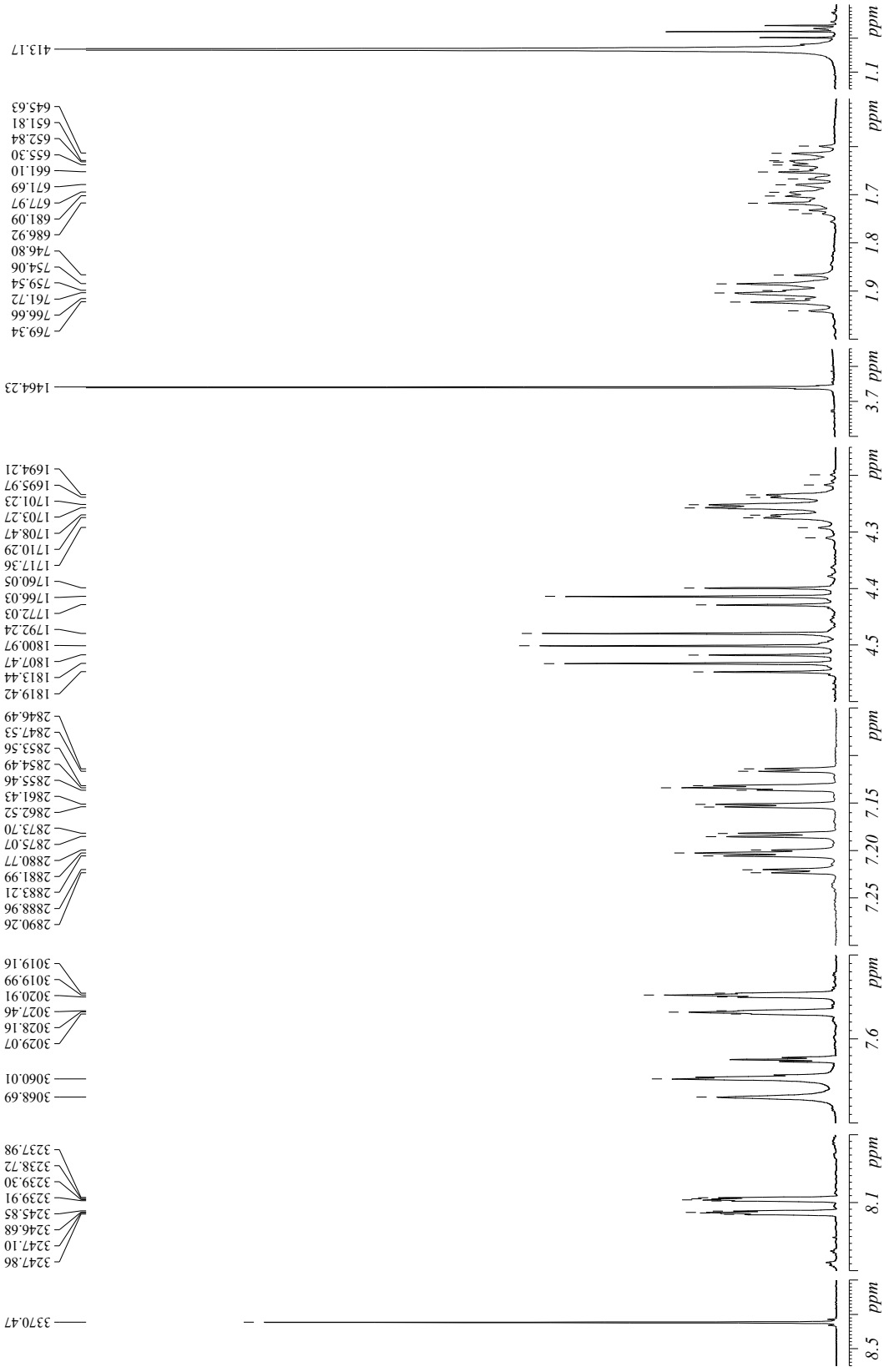
Interpretation of the NMR spectra



^{1}H-NMR spectrum (overview)

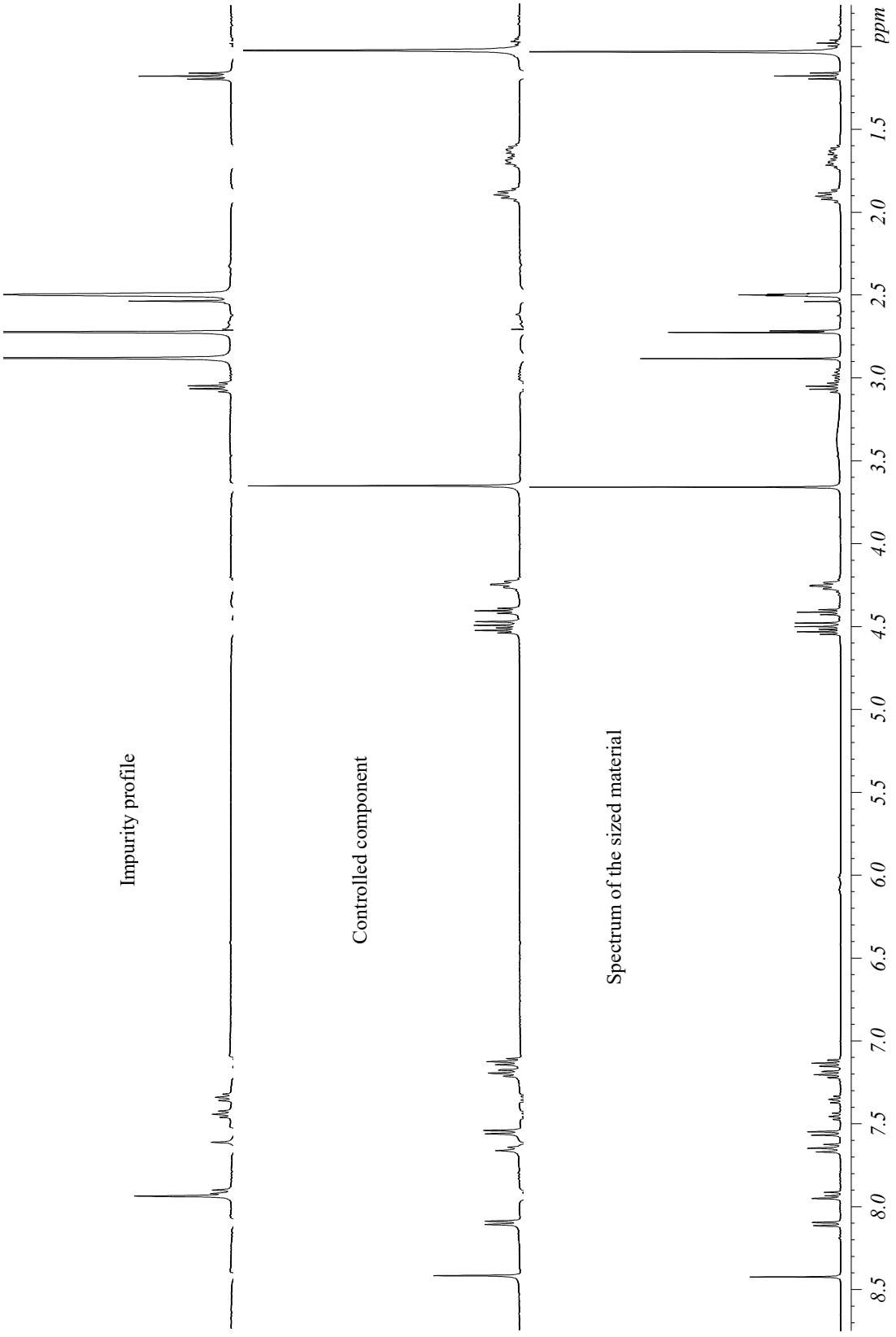


^{1}H-NMR spectrum (characteristic sections)



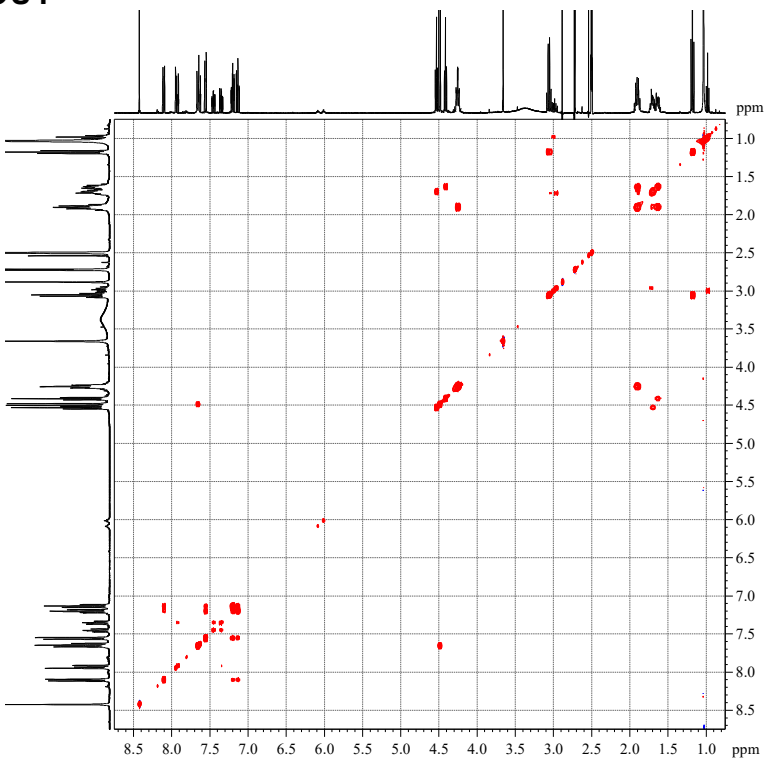
Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6

Diffusion ordered spectroscopy (DOSY) difference spectra

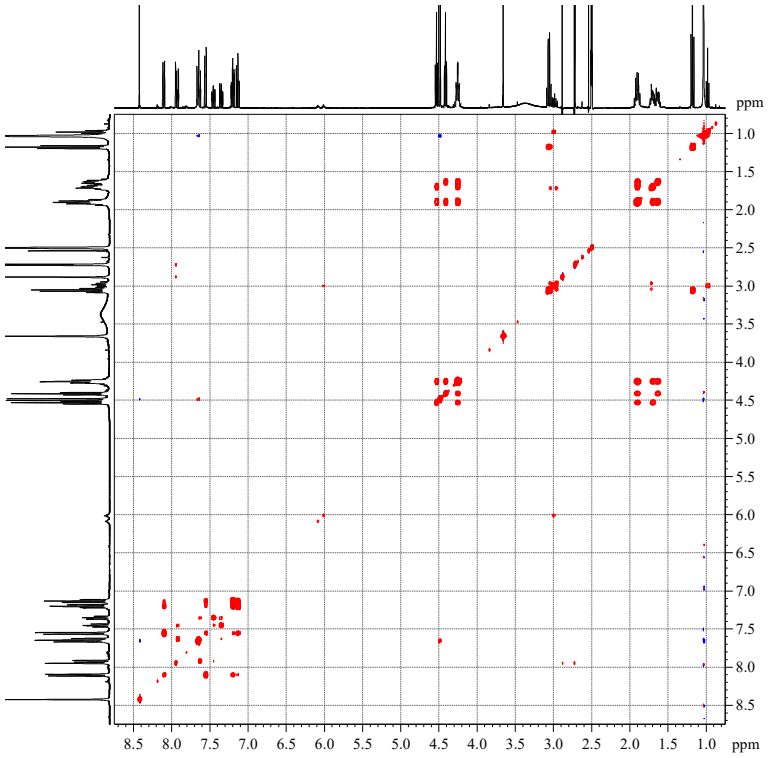


Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6

zqs-clip-COSY

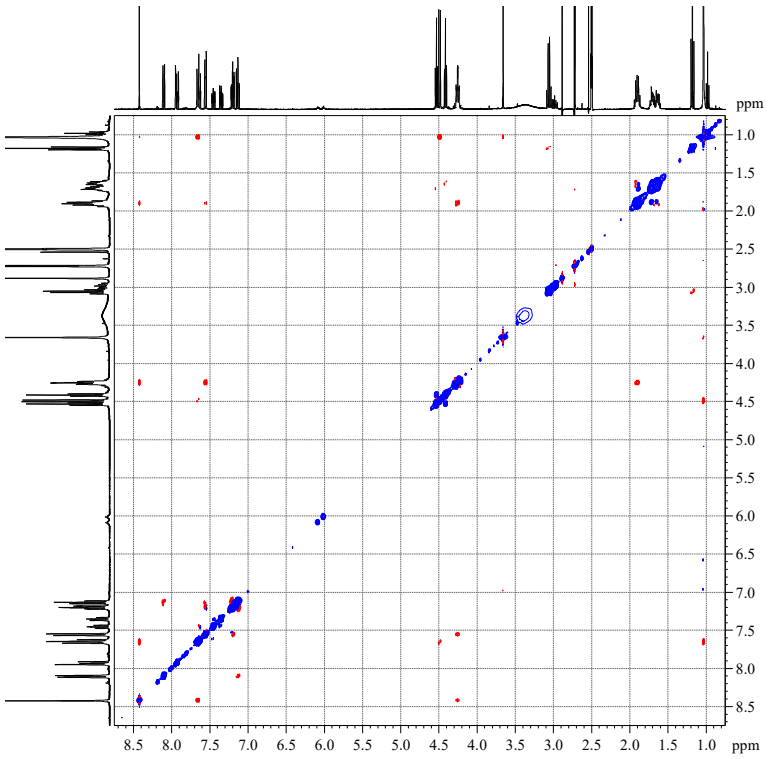


zqs-TOCSY

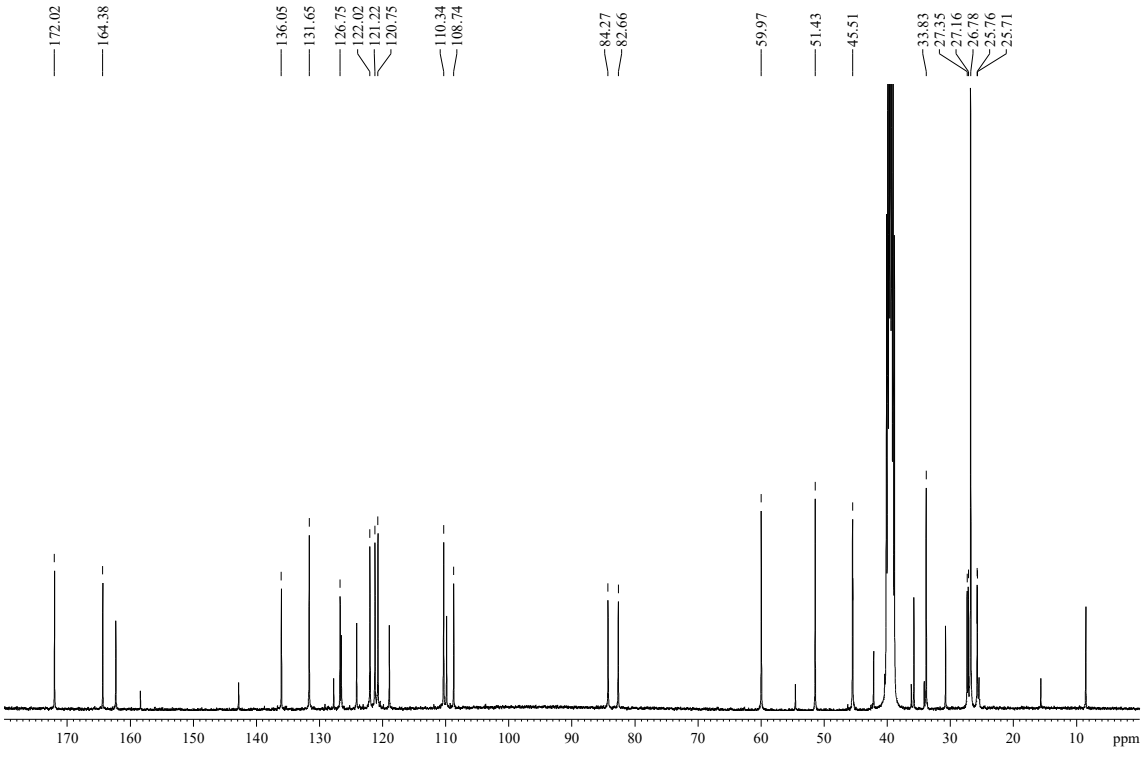


Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6

zqs-NOESY

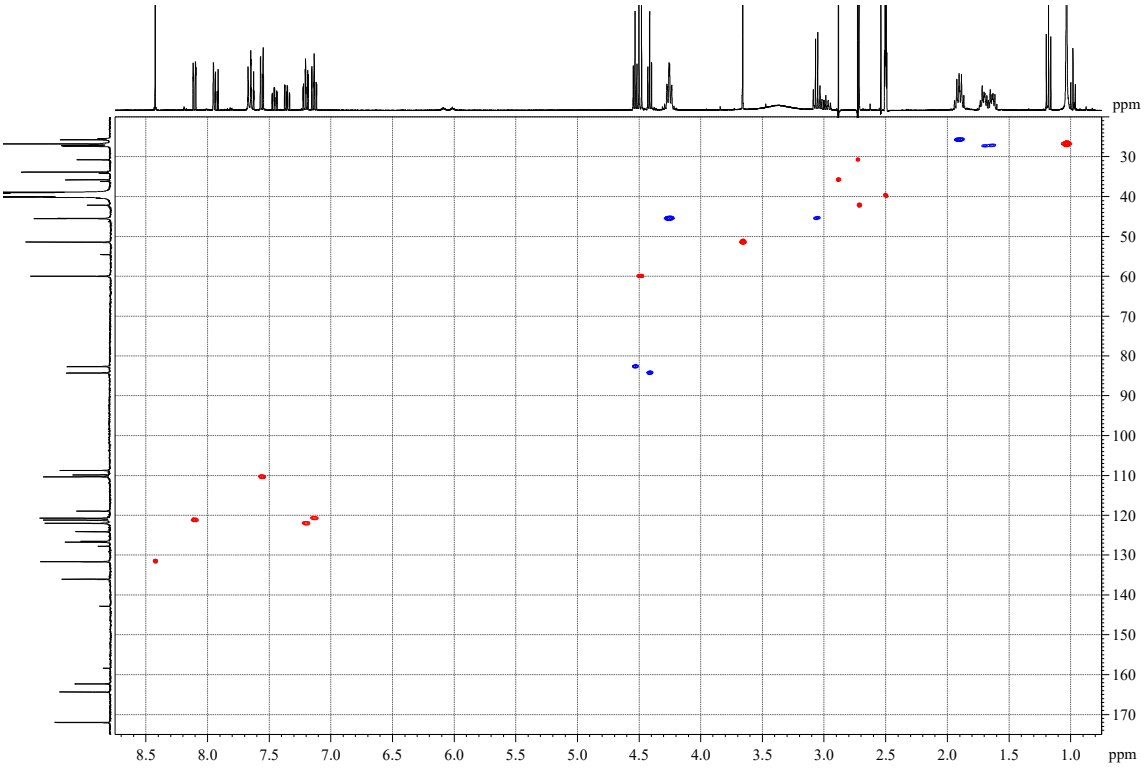


^{13}C-NMR

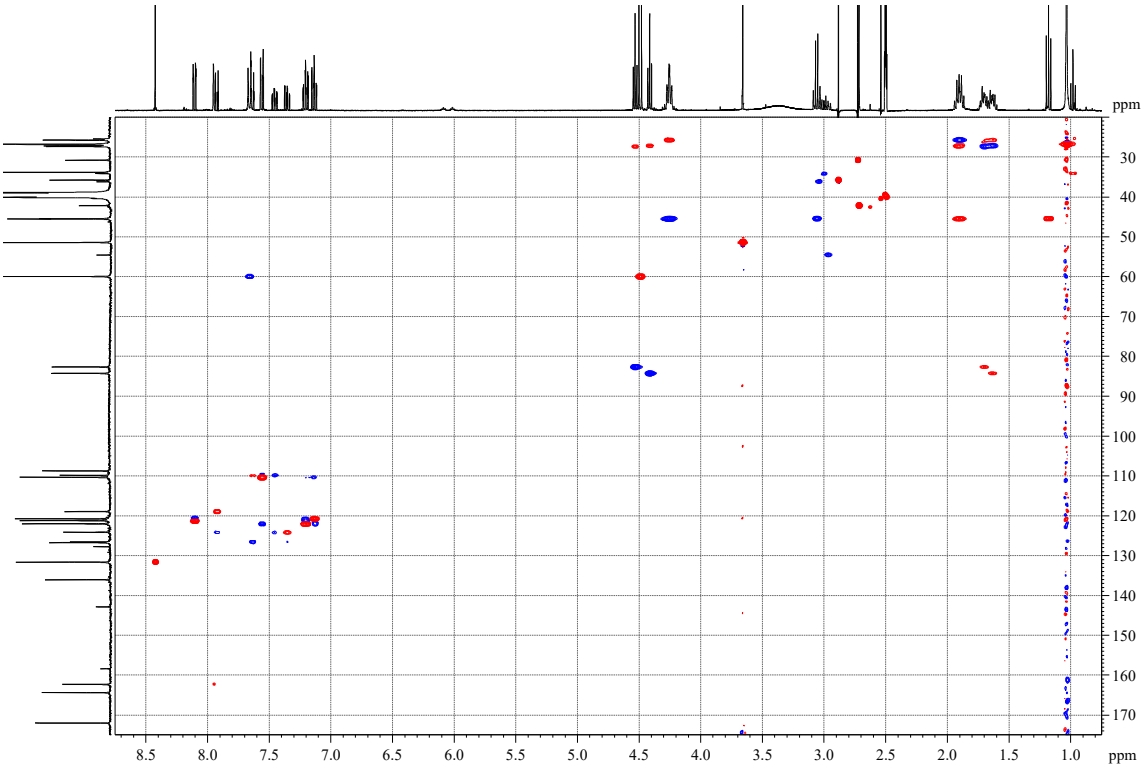


Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6

ed-HSQC

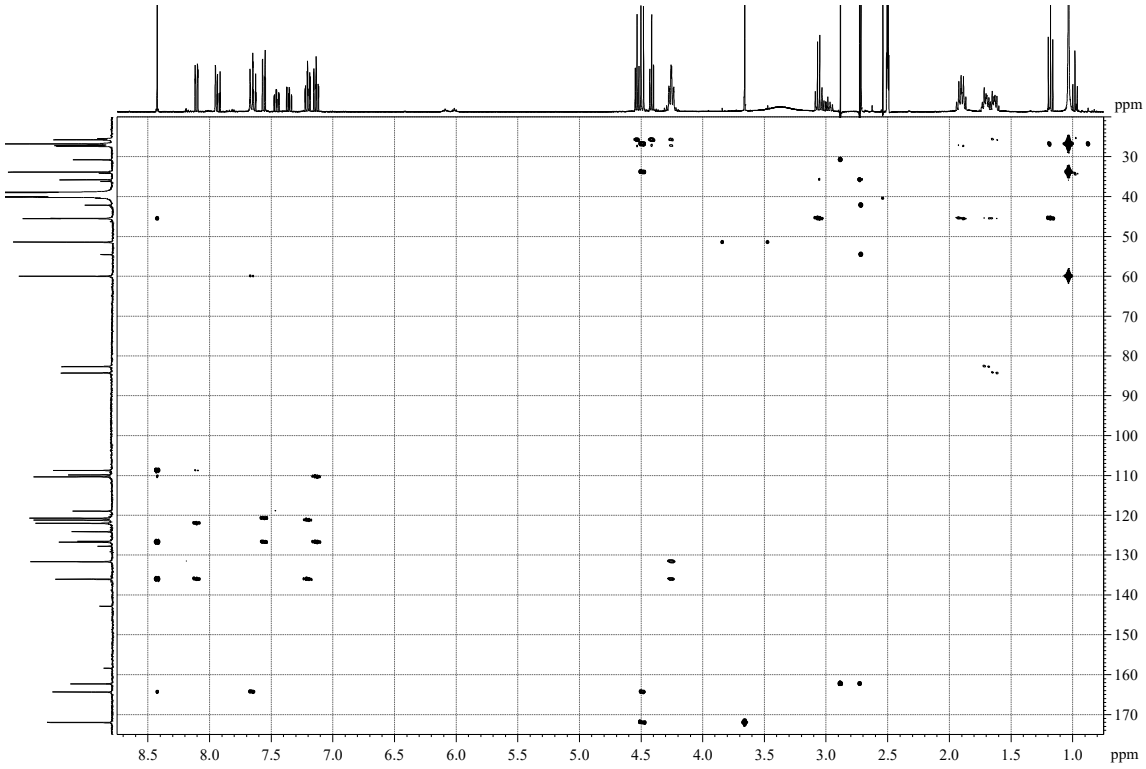


double edited-HSQC-zqs-clip-COSY



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

HMBC



Triethylamine salt and dimethylformamide impurity components were identified, two other impurity components were detected but not identified.
Only the peaks of the controlled component (and the solvent DMSO-d_6 used as secondary internal reference) are picked on the ^{1}H- and ^{13}C-NMR spectra.

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