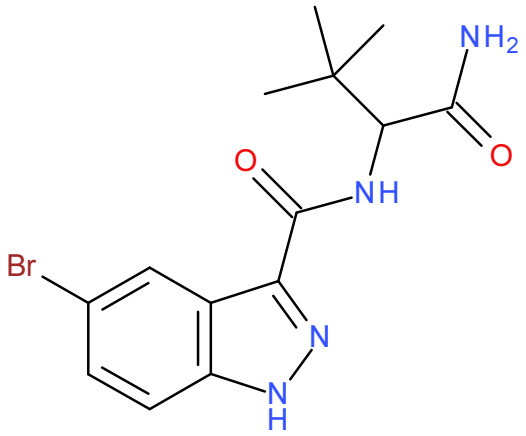
ADB-5Br-INACA



5-bromo-*N*-(1-carbamoyl-2,2-dimethyl-propyl)-1H-indazole-3-carboxamide

Formula: $C_{14}H_{17}BrN_4O_2$
Formula weight: 353.21
Chemical Abstracts No.: *n. a.*
Smiles code: CC(C)(C)C(NC(=O)c1n[nH]c2ccc(Br)cc12)C(=O)N
InChi key: AJGASUCDTSLMNP-UHFFFAOYSA-N
Other names:

Reference for the given name:

A. J. Potts, C. Cano, S. H. L. Thomas, S. L. Hill:
Synthetic cannabinoid receptor agonists: classification and nomenclature,
Clinical Toxicology, **58**(2), 89-92 (2020)
https://doi.org/10.1080/15563650.2019.1661425

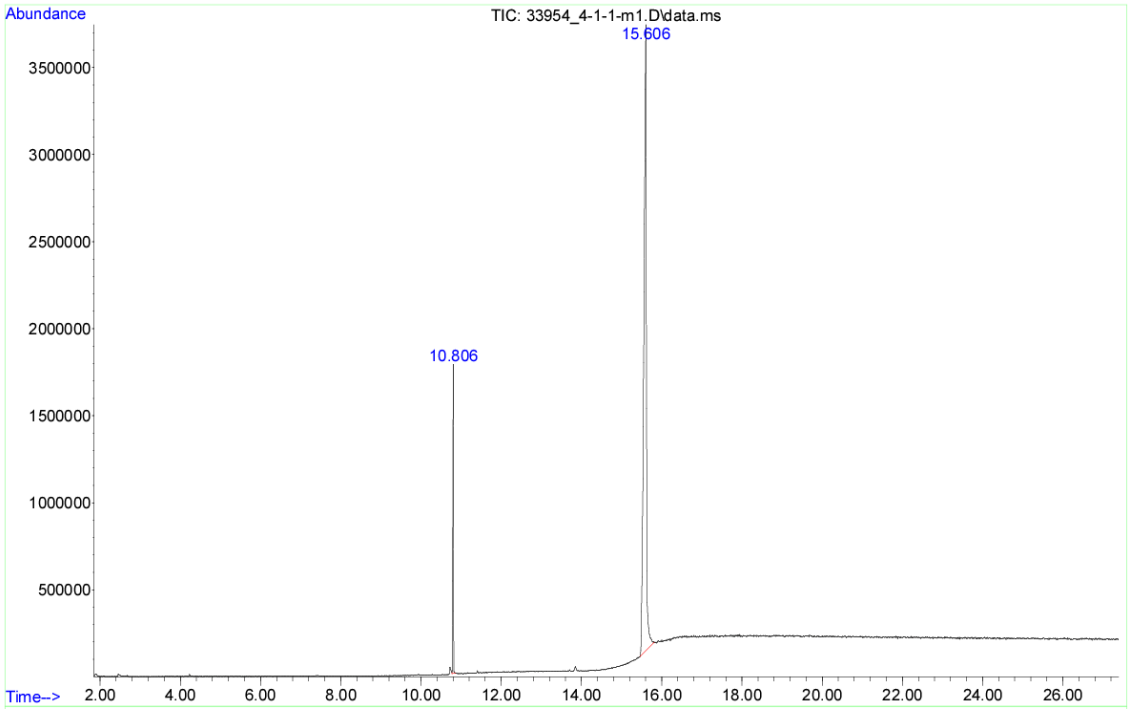
The evidence was 4.58 grams off-white powder.

< No characteristic photo available >

GC-MS

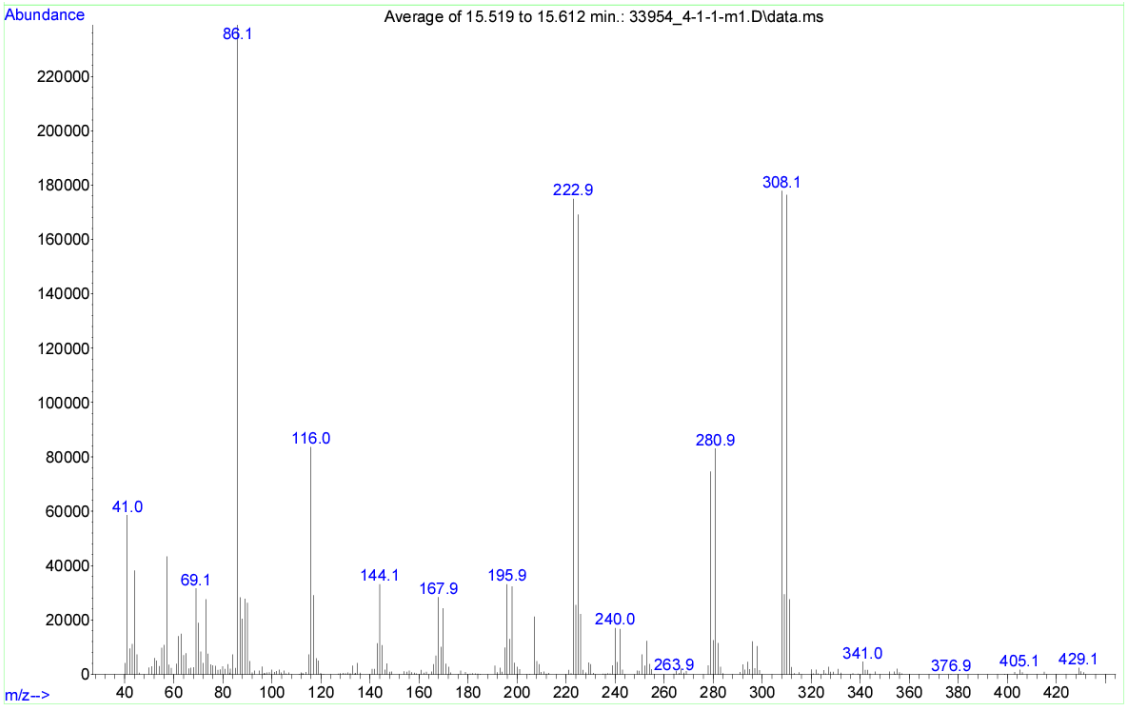
An Agilent 6890N Network GC system set up with Agilent HP-5MS (length: 30 m, diameter: 0.25 mm, film: 0.25 mm) coupled to an Agilent 5973 Network Mass Selective Detector (scan range m/z 35 – m/z 500) was used. The methanolic solution of the evidence was injected. Samples were subjected to electron ionization (EI) mode. GC-MS conditions: HP-5MS column was temperature programmed from 100 ℃ (which was held for 2 minutes) to 280 ℃ at 20 ℃/min, 280°C was held for 3 minutes, then to 315 ℃ at 25 ℃/min, the temperature was stated at 315 ℃ 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 current chromatogram



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

Mass spectrum at 15.60 min retention time



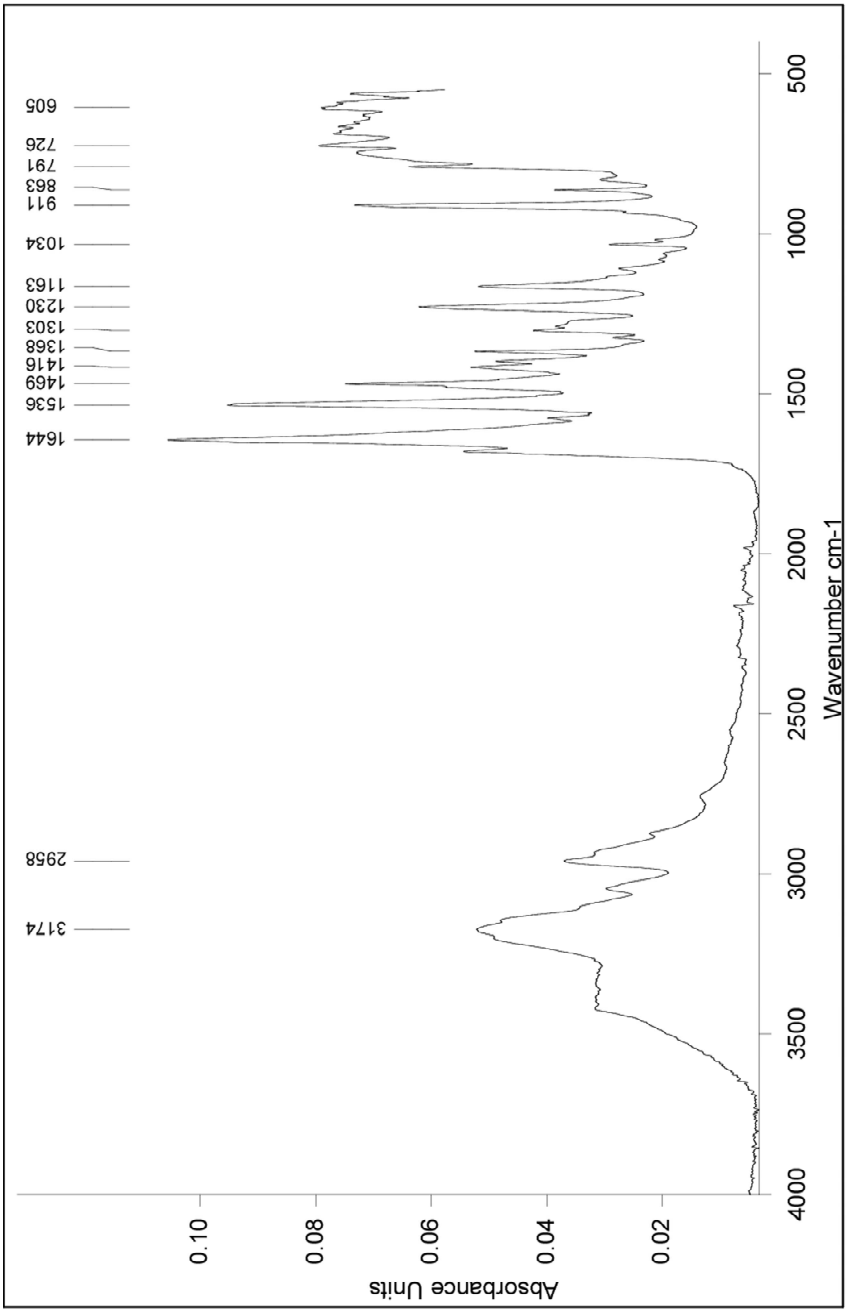
Interpretation of the mass spectrum

Some peak pairs indicate bromine content in the molecule.

IR

The IR spectrum of the evidence 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 spectrometer was controlled, and the data were processed using Omnic 9 software package. The spectrum was off-line imported into Bruker OPUS software, and the output below was performed by OPUS 7.5 software.

IR spectrum of the evidence as received



Thermo SCIENTIFIC Nicolet iS5 FT-IR spectrometer

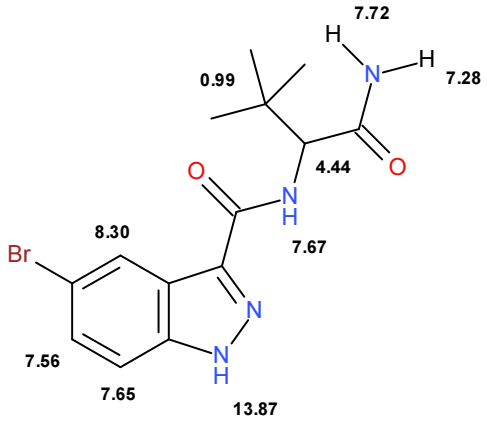
NMR

The NMR spectra were recorded on a Bruker Avance Neo 400 NMR spectrometer 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-easy-ROESY, as well as ^{13}C, multiplicity edited HSQC and HMBC spectra.

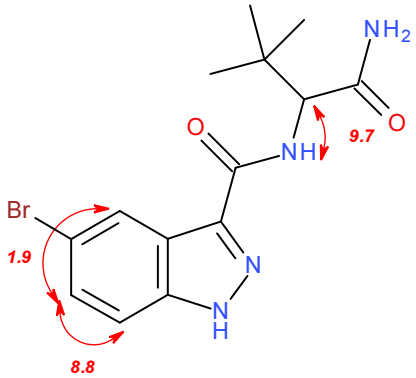
Interpretation of the NMR spectra

^{1}H-NMR chemical shifts δ [ppm]

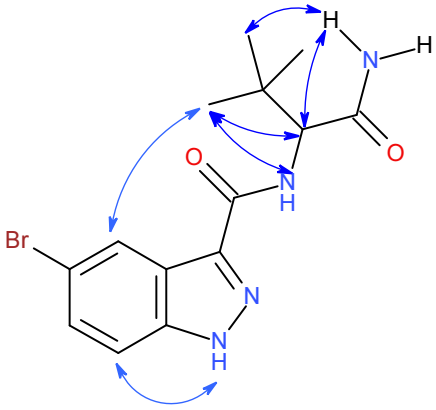
In DMSO-d_6 solution



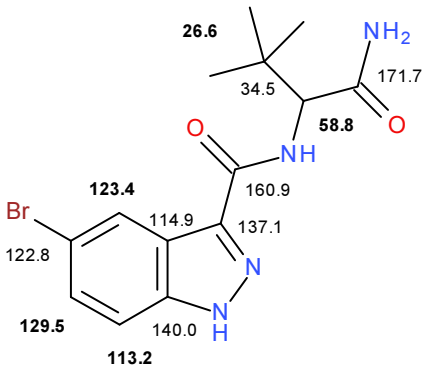
Characteristic J(H,H) coupling constants [Hz]



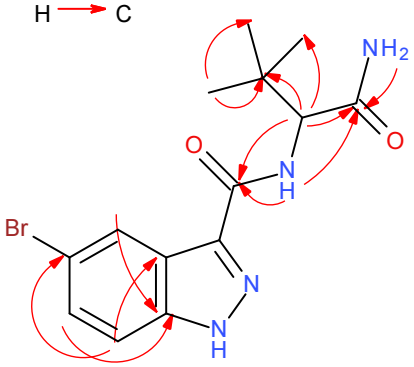
Characteristic H-H steric proximities detected by zqs-easy-ROESY measurement



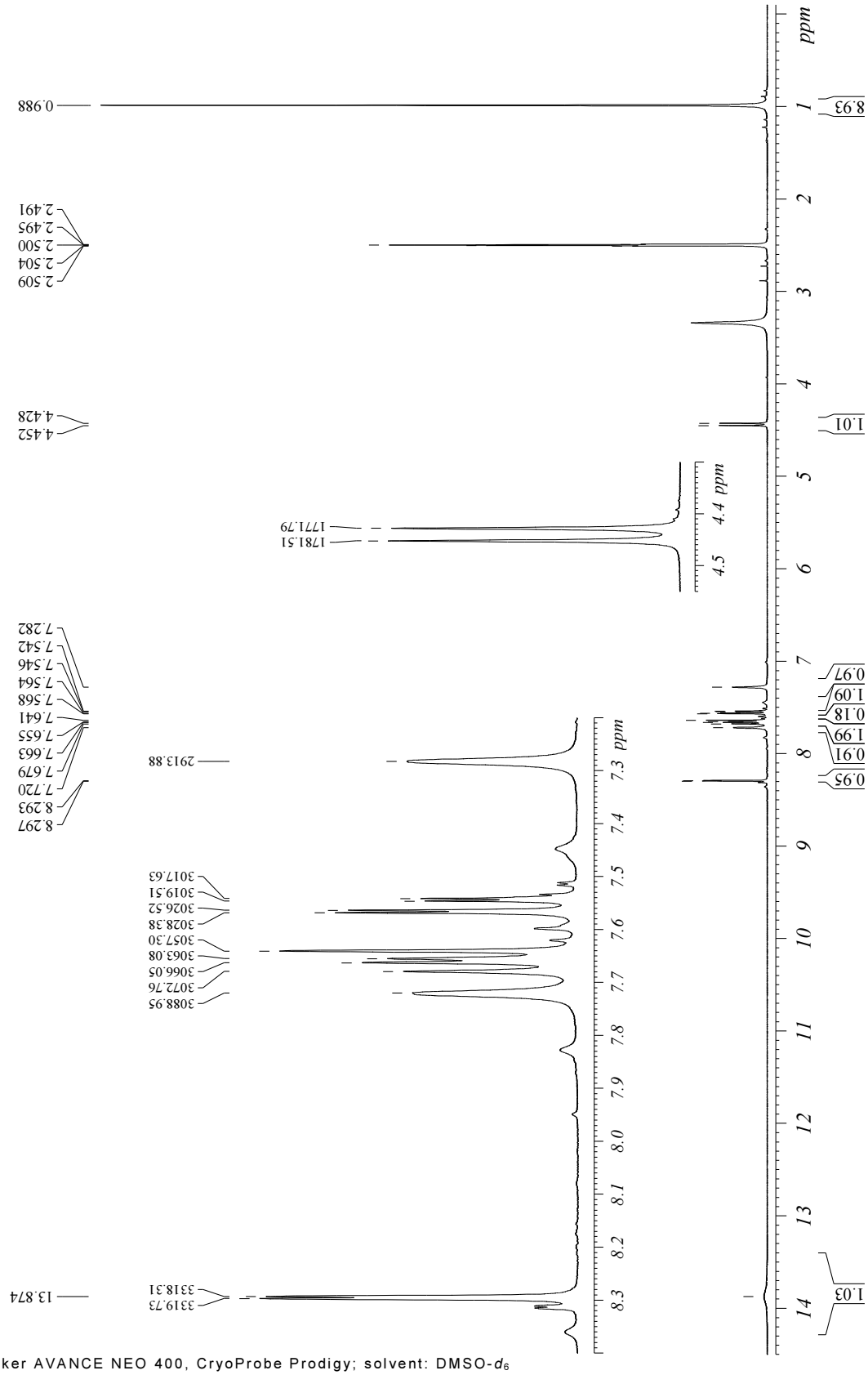
^{13}C-NMR chemical shifts δ [ppm]



Characteristic heteronuclear long-range couplings detected by HMBC measurement
H → C

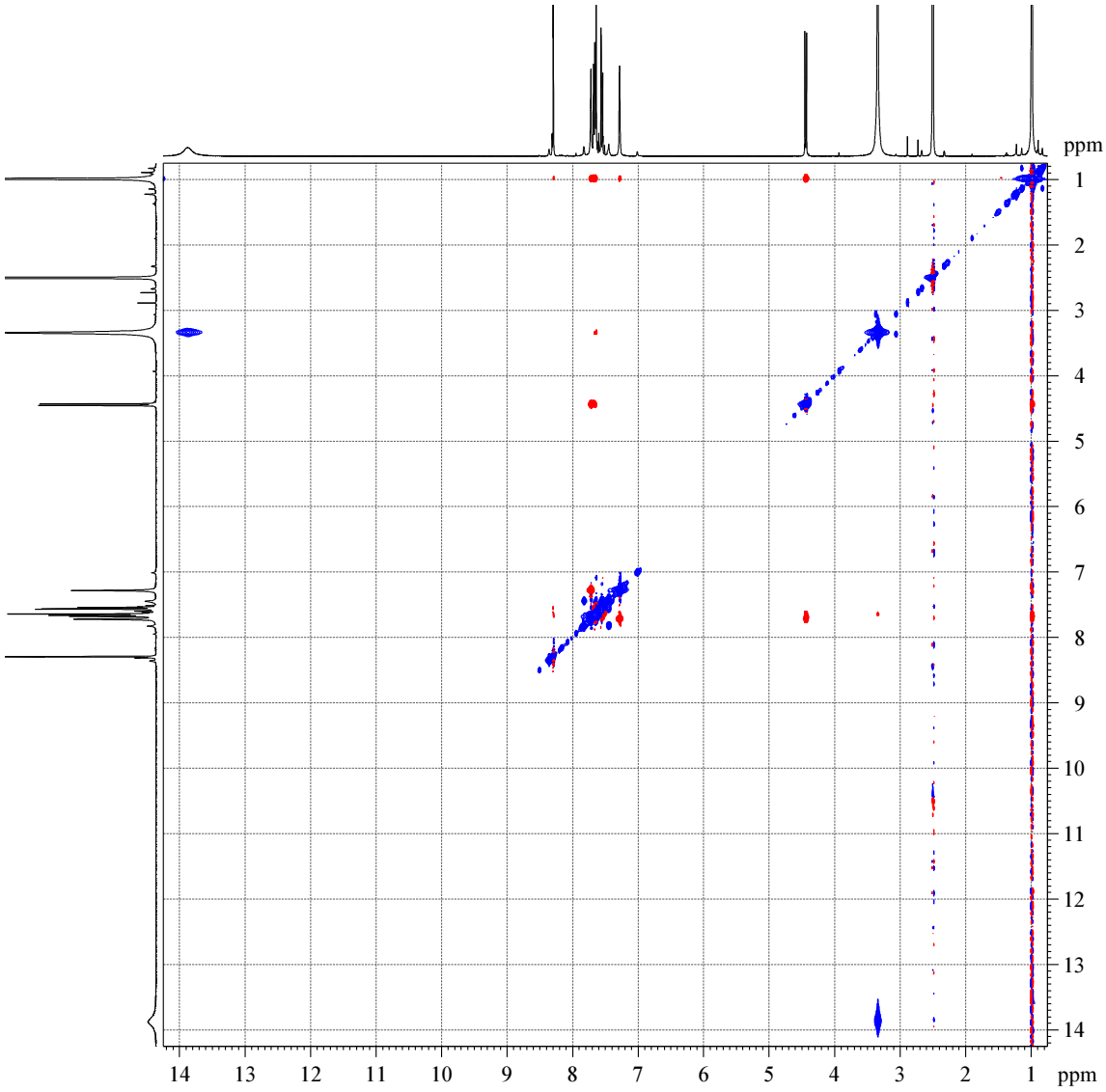


^{1}H-NMR spectrum (overview and characteristic sections)



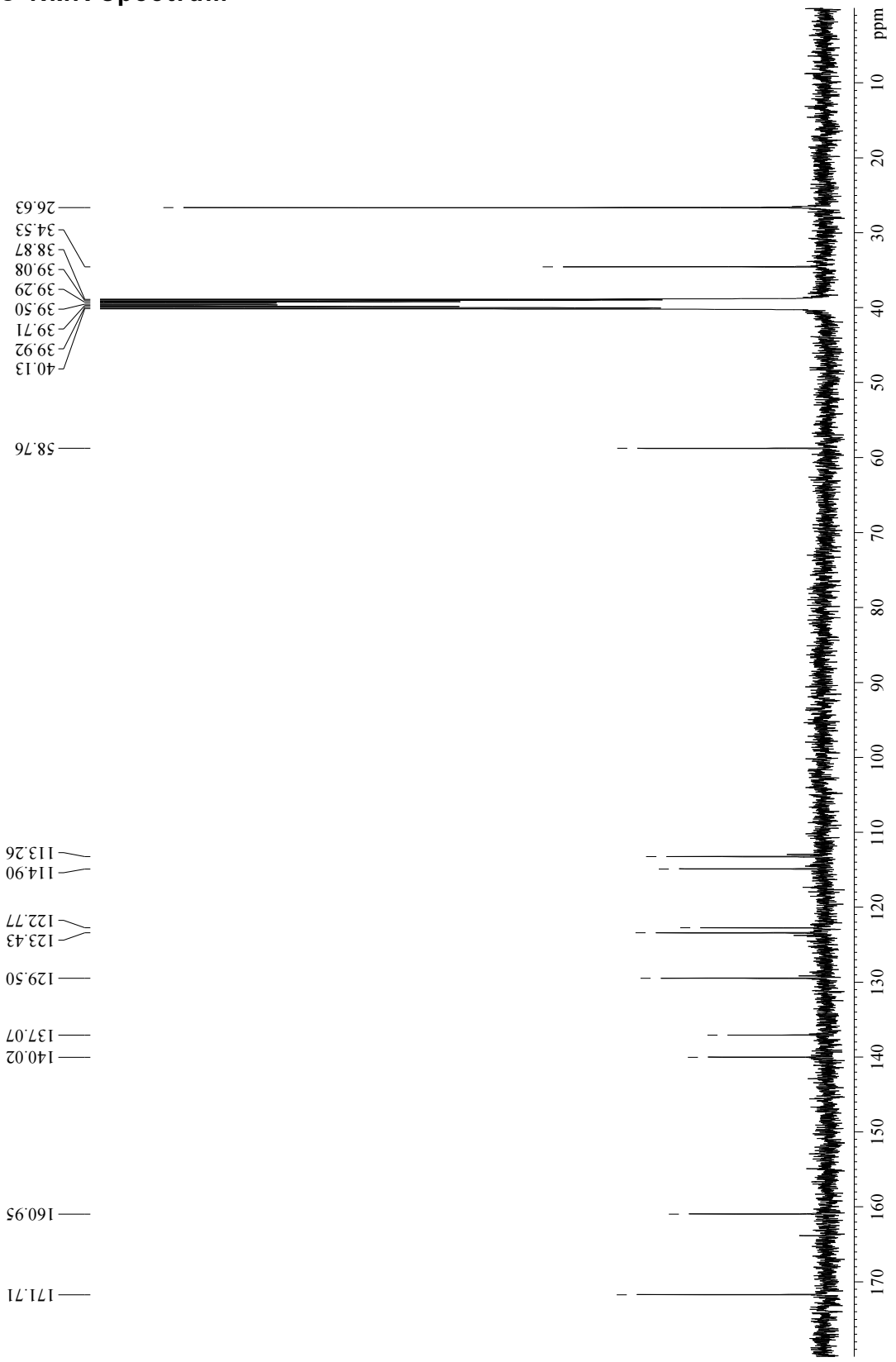
Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6

***zqs-easy*-ROESY**



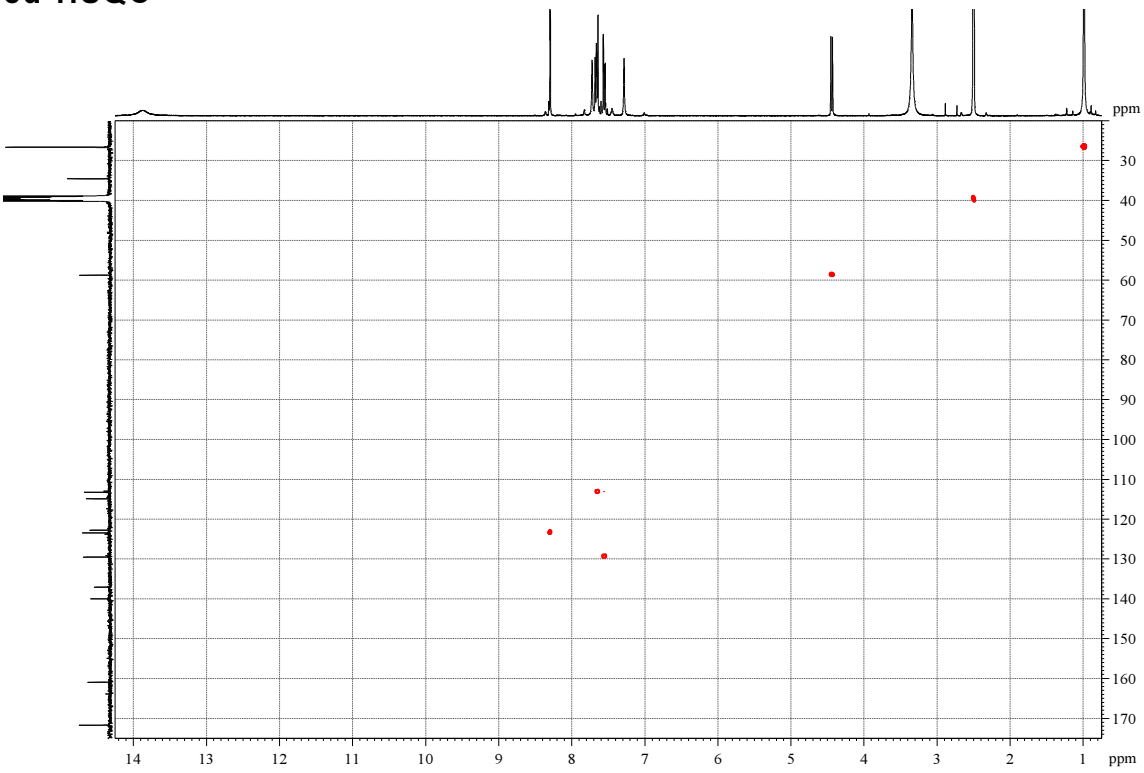
Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6

^{13}C-NMR spectrum

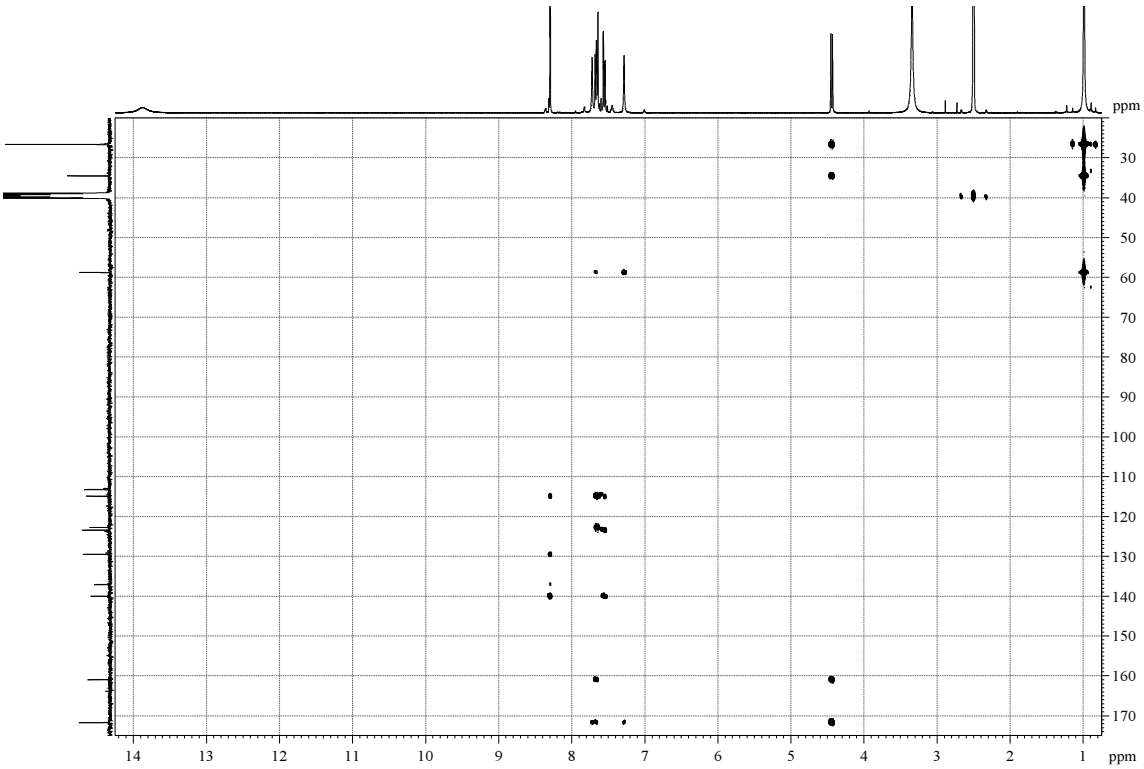


Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6

ed-HSQC



HMBC



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