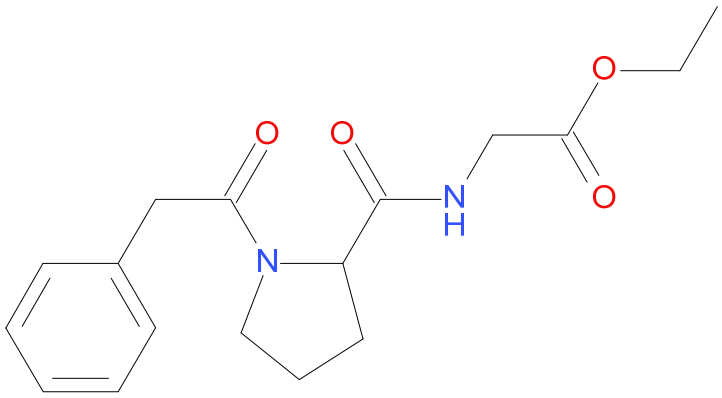
NOOPEPT



ethyl 2-[[1-(2-phenylacetyl)pyrrolidine-2-carbonyl]amino]acetate

Phenylacetyl-Pro-Gly-OEt
Formula: $C_{17}H_{22}N_2O_4$
Formula weight: 318,37
Chemical Abstracts No.: 157115-85-0
Smiles code: O=C(CC1=CC=CC=C1)N2[C@H](C(NCC(OCC)=O)=O)CCC2
InChi key: PJNSMUBMSNAEEN-AWEZNQCLSA-N
Other names: **NOOPEPT**, GVS-111, SGS 111

The seized material was 0.9364 gram white 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 ℃ (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.

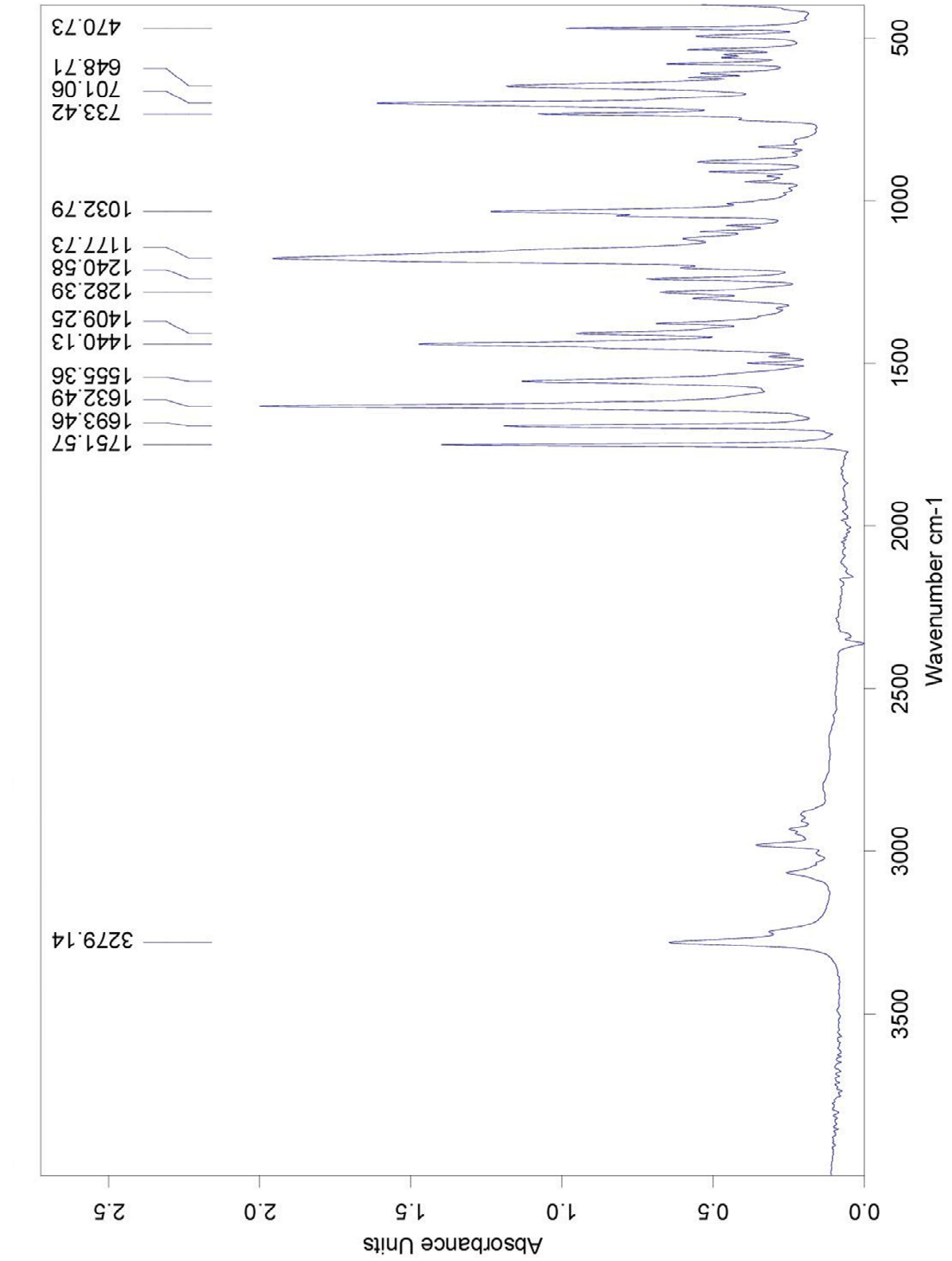
IR

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

NMR

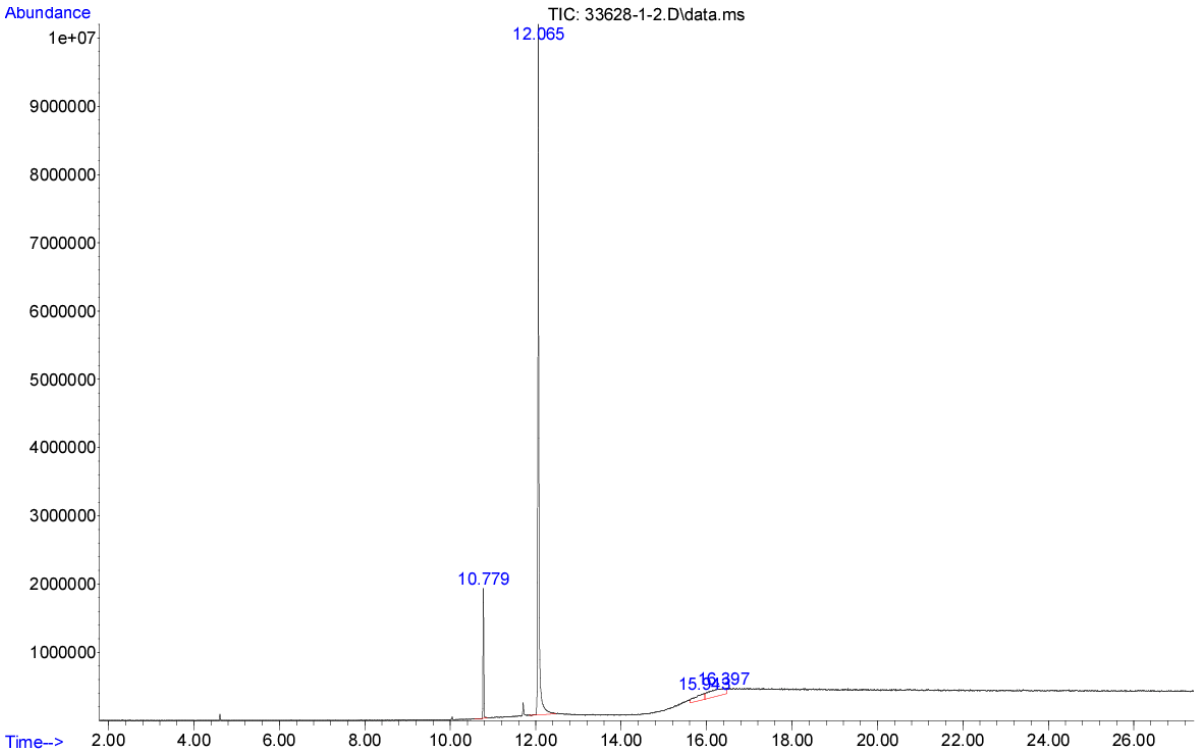
The NMR spectra were recorded on a Bruker Avance Neo 400 NMR operating at 9.4 Tesla magnetic field, equipped with Prodigy BBO-H&F-D-05 Z-gradient probe. The spectra were recorded at 25 °C in DMSO-d_6 solution. The spectrometer was controlled, and the data were processed using TopSpin 4.0 software package. 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-easy-ROESY as well as ^{13}C, multiplicity edited HSQC and HMBC spectra.

IR spectrum

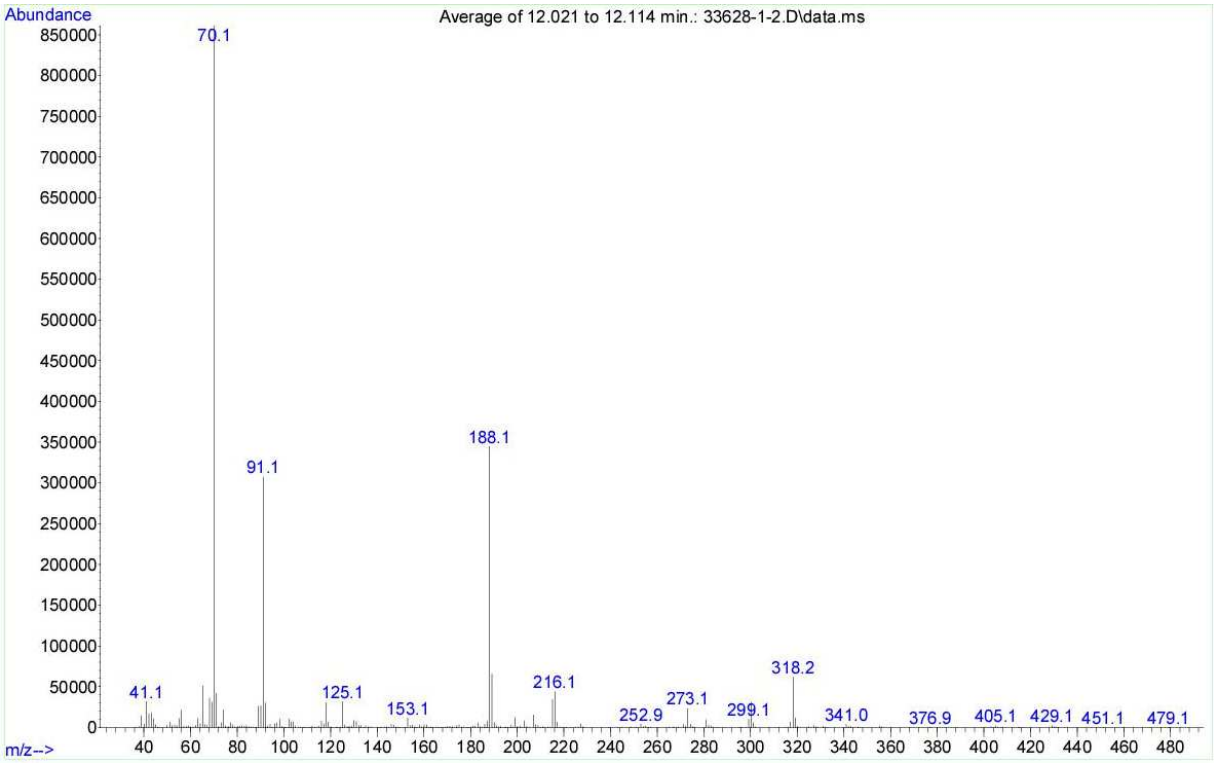


Bruker Tensor 27

GC-MS total ion chromatogram



Mass spectrum at 12,06 min retention time



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

Interpretation of the NMR spectra

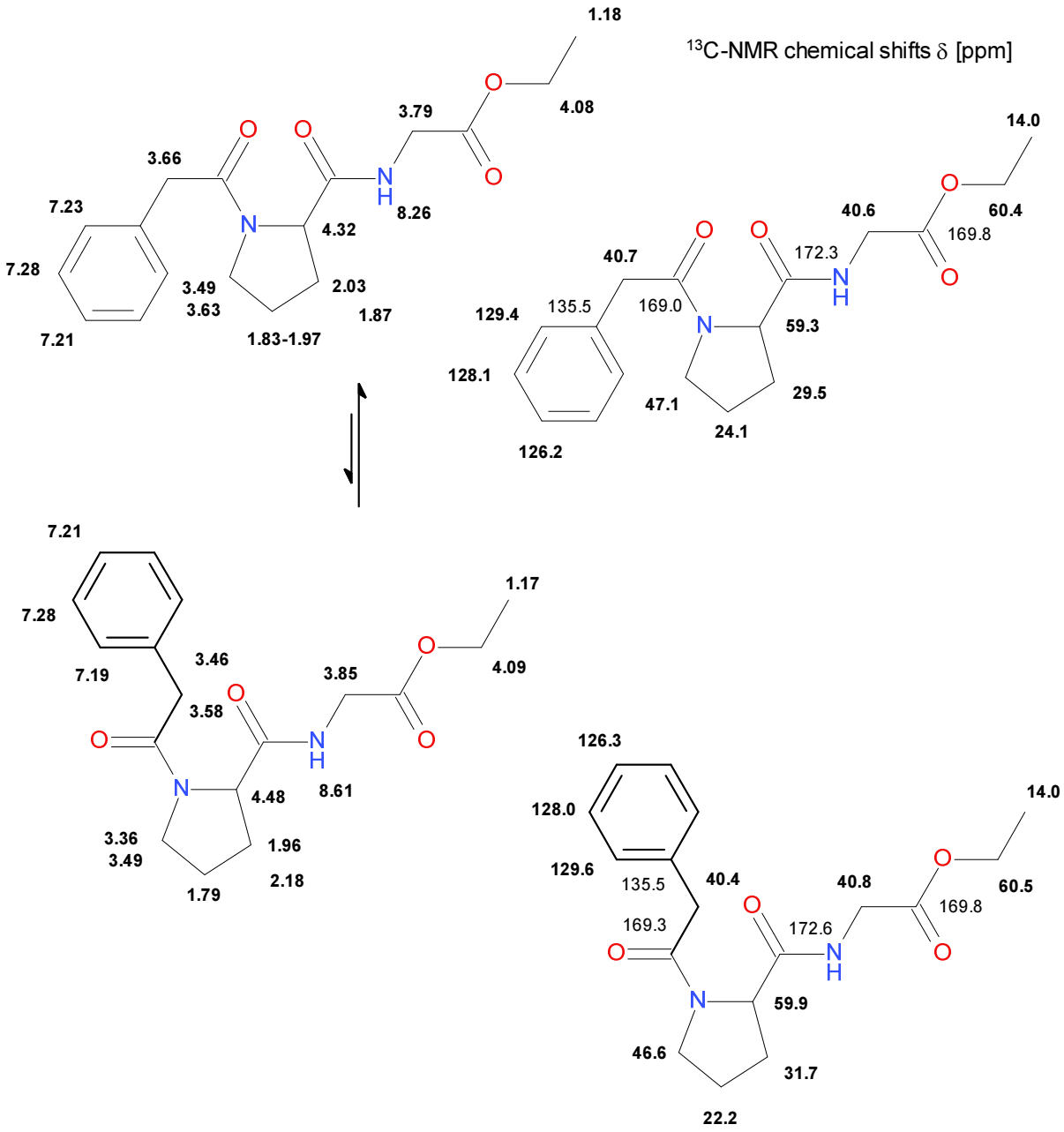
Noopept
GVS-111, SGS 111
CAS No.: 157115-85-0
ethyl 2-[[1-(2-phenylacetyl)pyrrolidine-2-carbonyl]amino]acetate
PJNSMUBMSNAEEN-AWEZNQCLSA-N
O=C(CC1=CC=CC=C1)N2[C@H](C(NCC(OCC)=O)=O)CCC2

Formula Weight: 318,36758
Exact Mass: 318,157957204
Molecular Formula: $C_{17}H_{22}N_2O_4$

In DMSO-d_6 solution

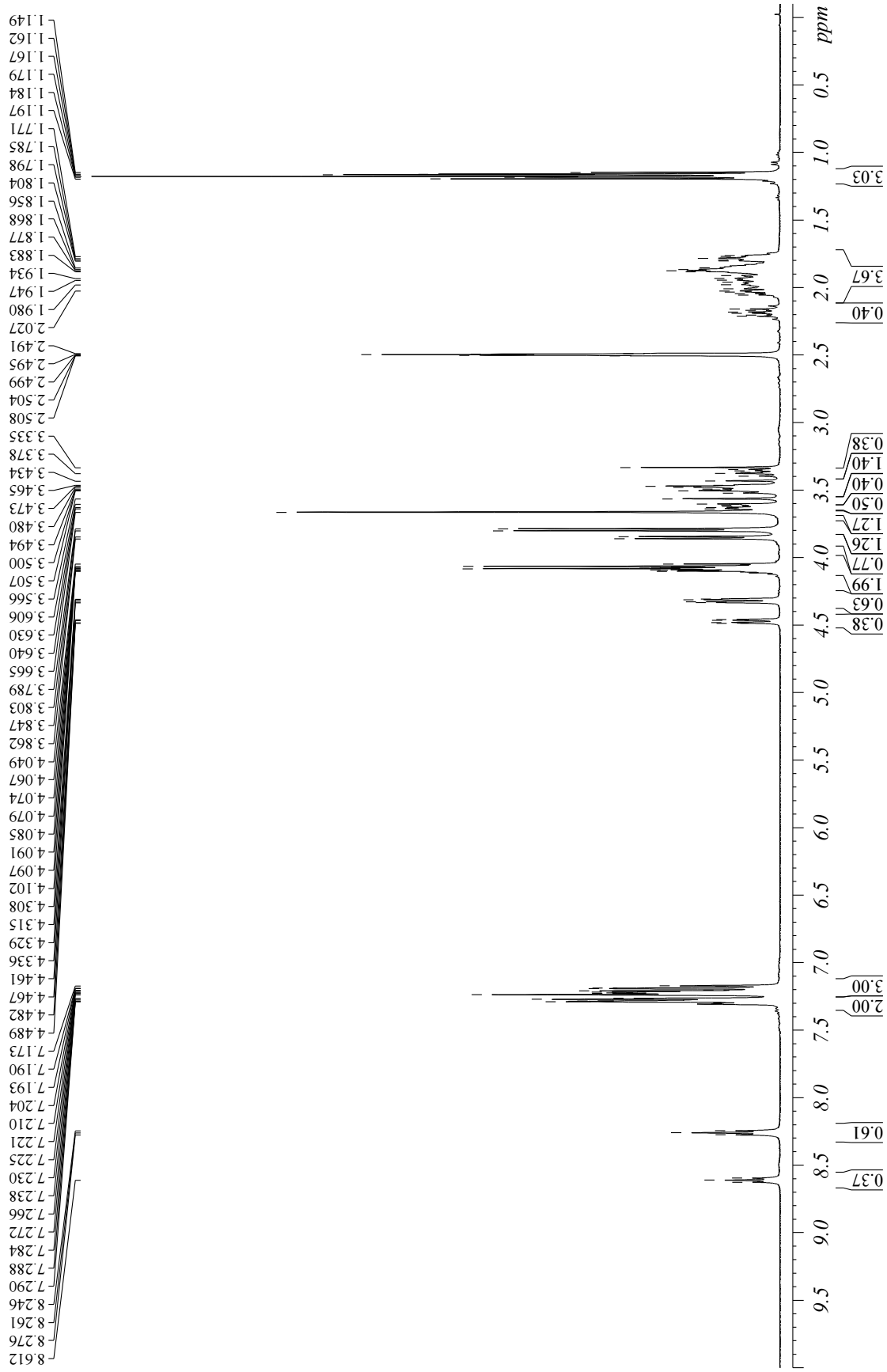
^{1}H-NMR chemical shifts δ [ppm]

^{13}C-NMR chemical shifts δ [ppm]



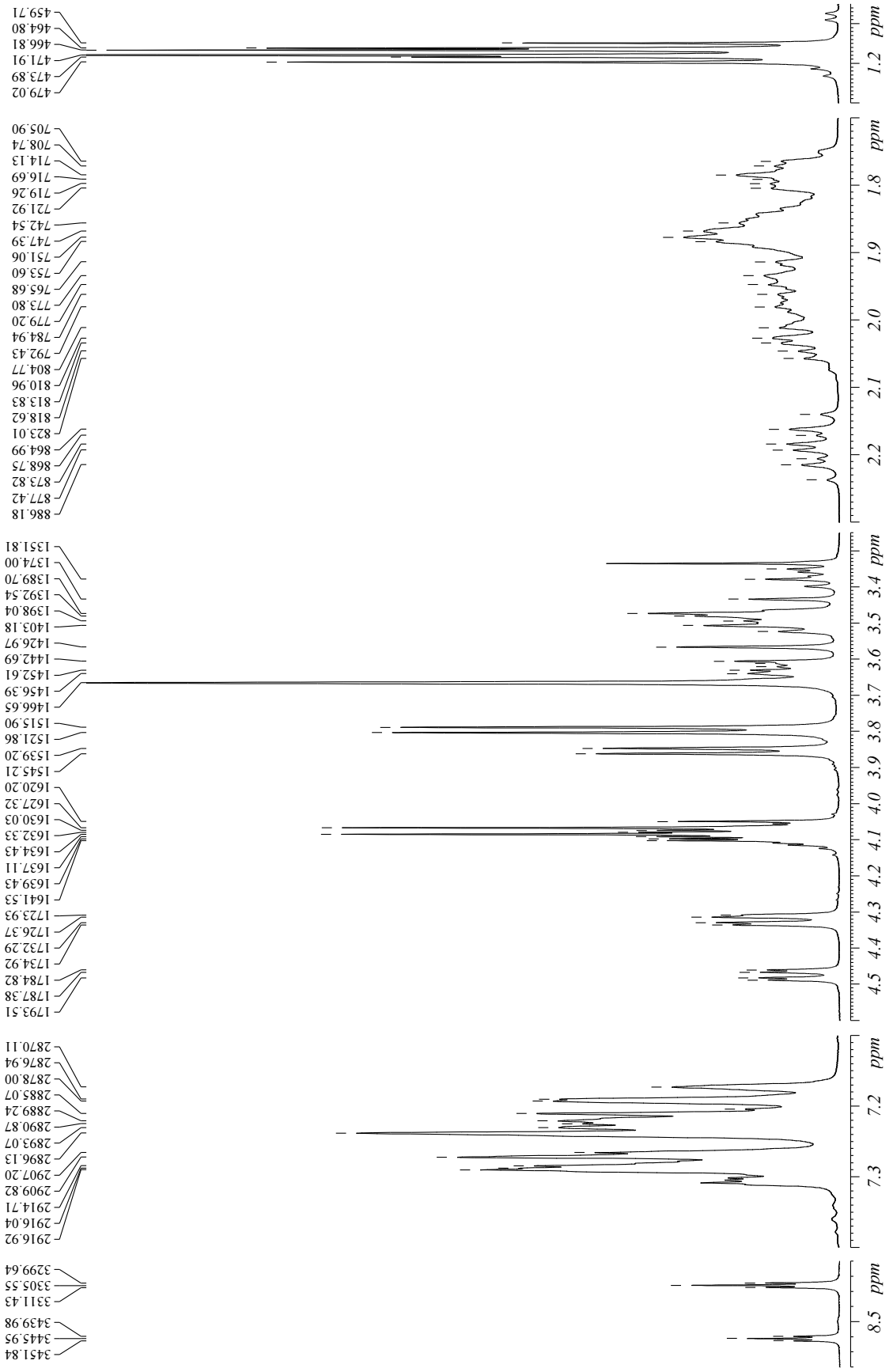
The equilibrium of the two proline amide rotamers is proven by the exchange crosspeaks in the zqs-easy-ROESY spectrum.

^{1}H-NMR spectrum (overview)



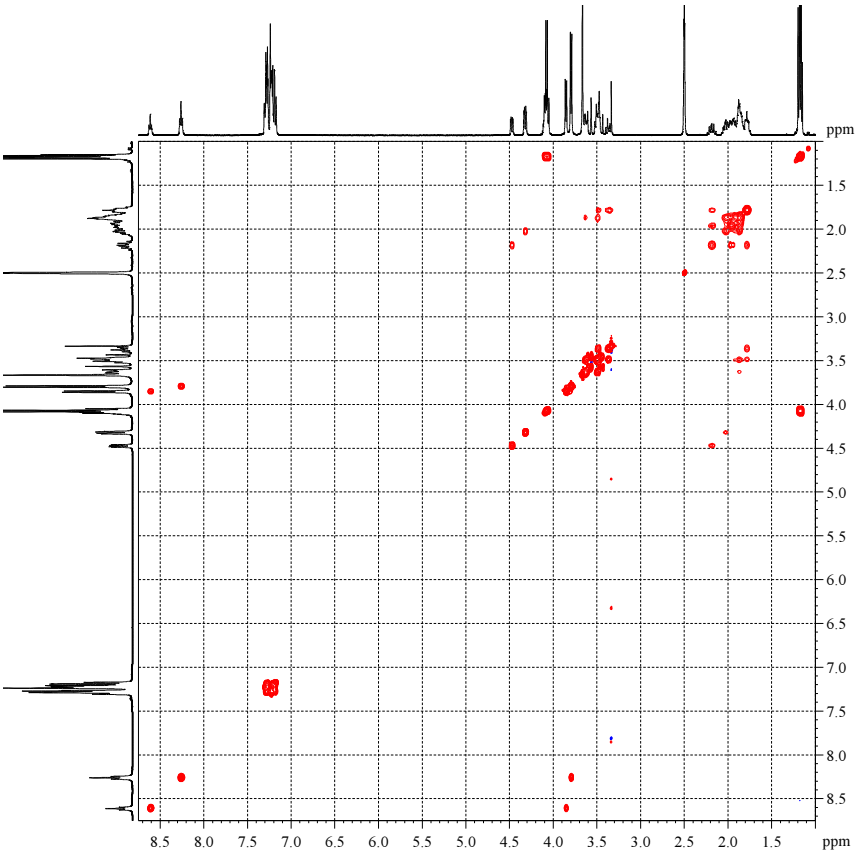
Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6

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

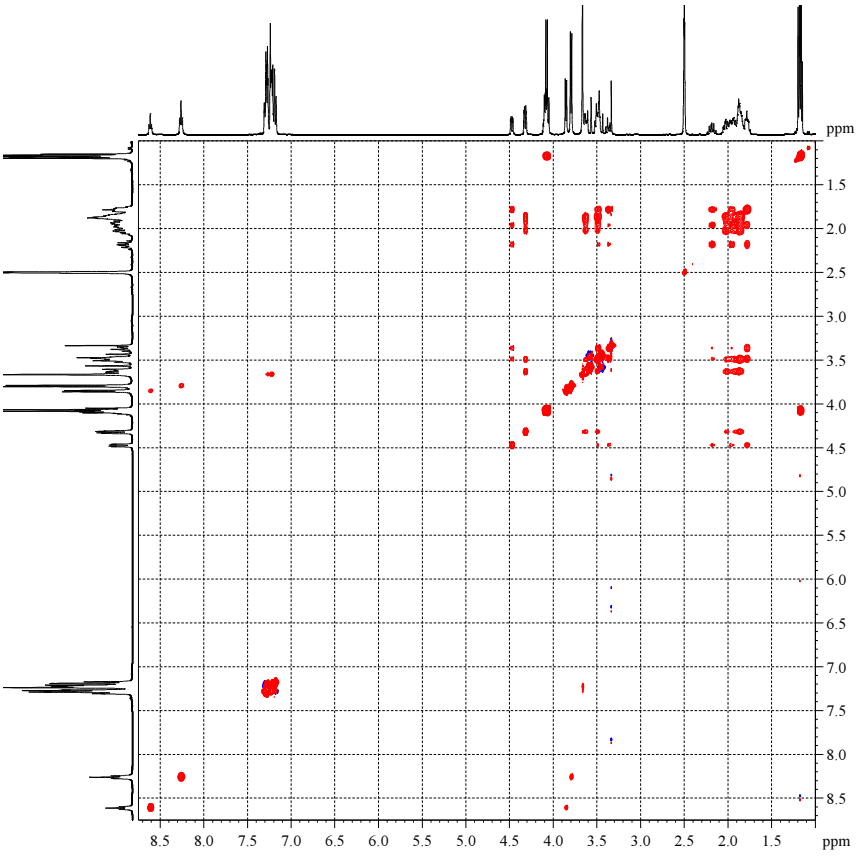


Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6

zqs-clip-COSY

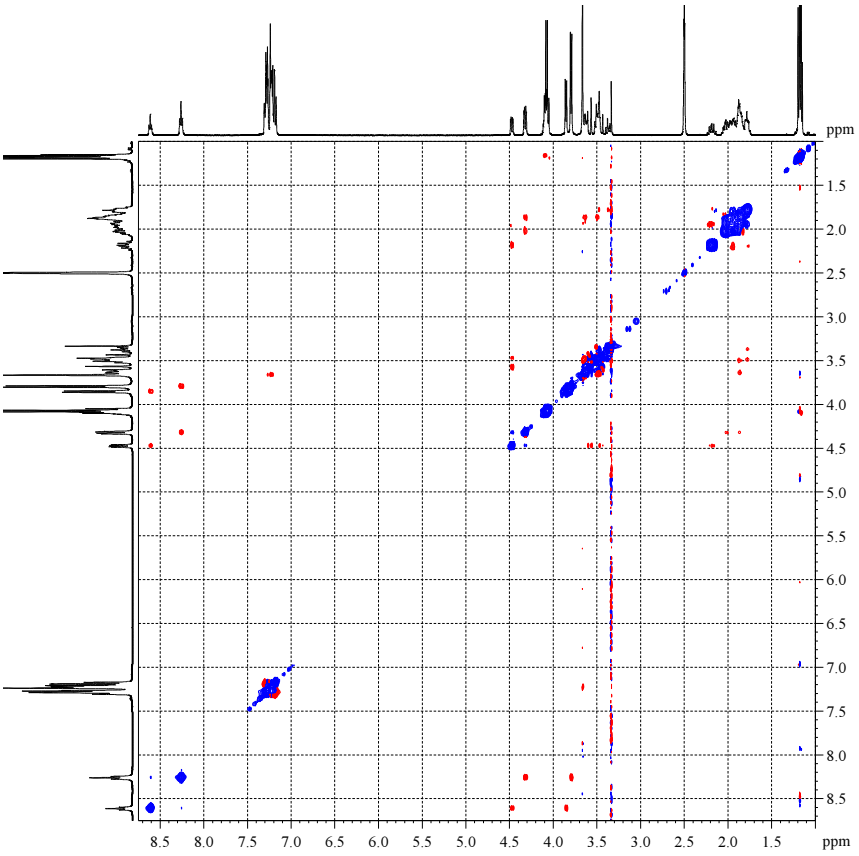


zqs-TOCSY

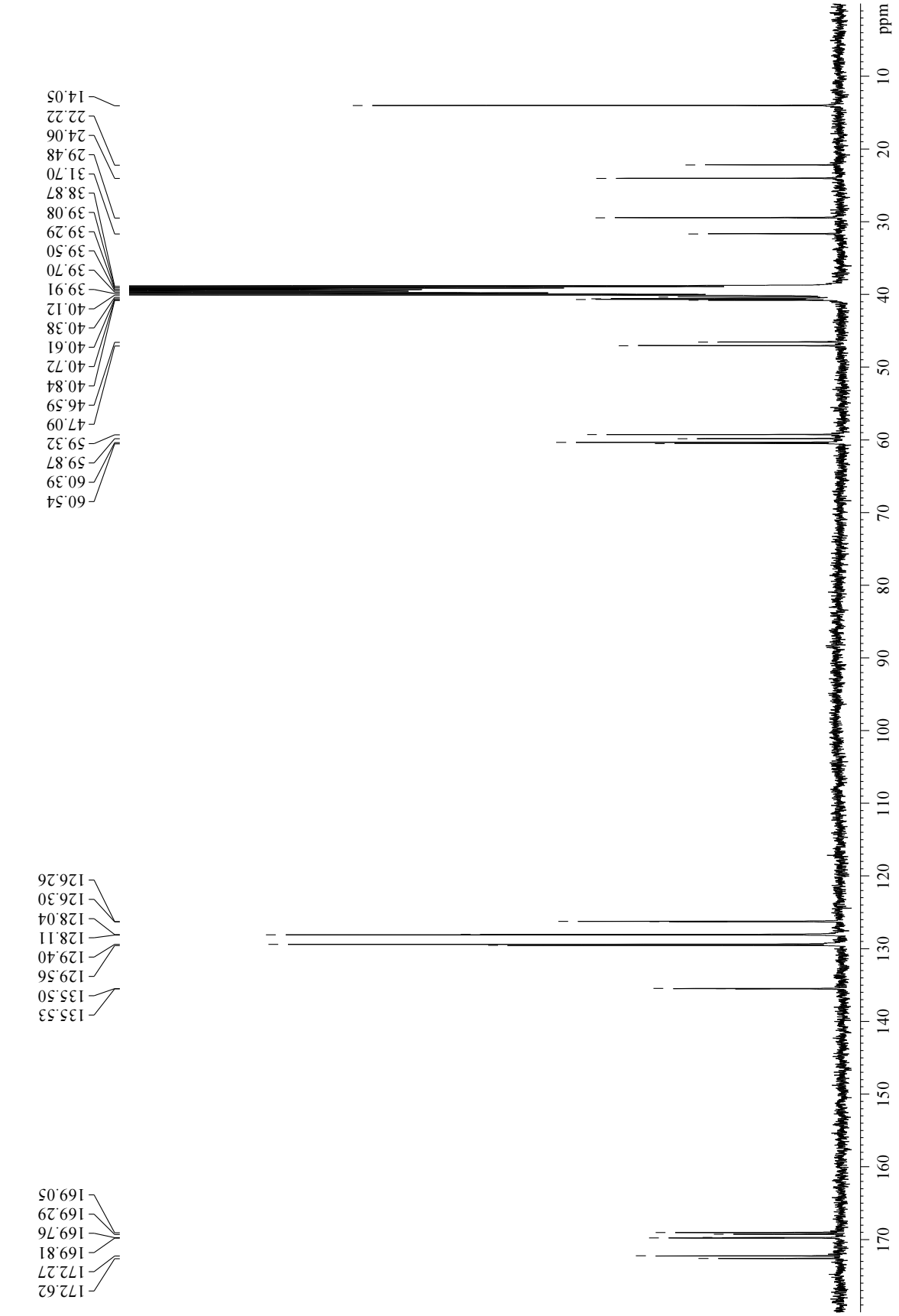


Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6

zqs-easy-ROESY

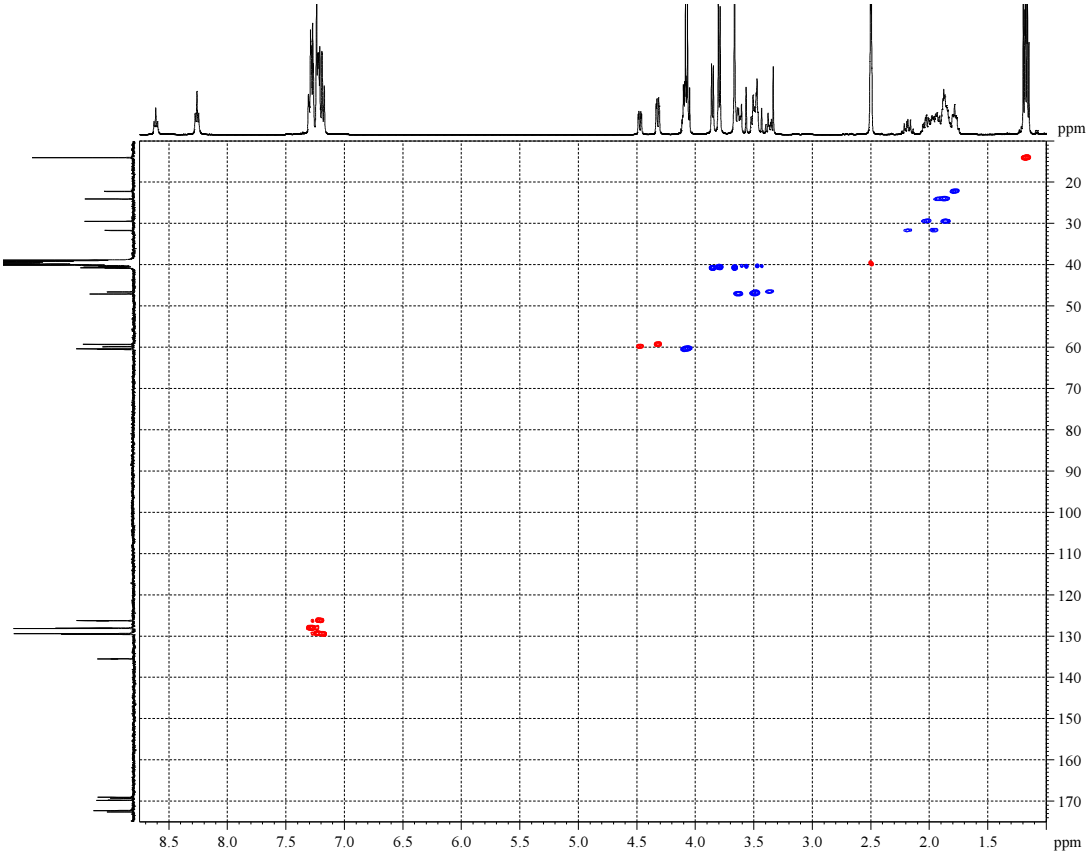


^{13}C-NMR

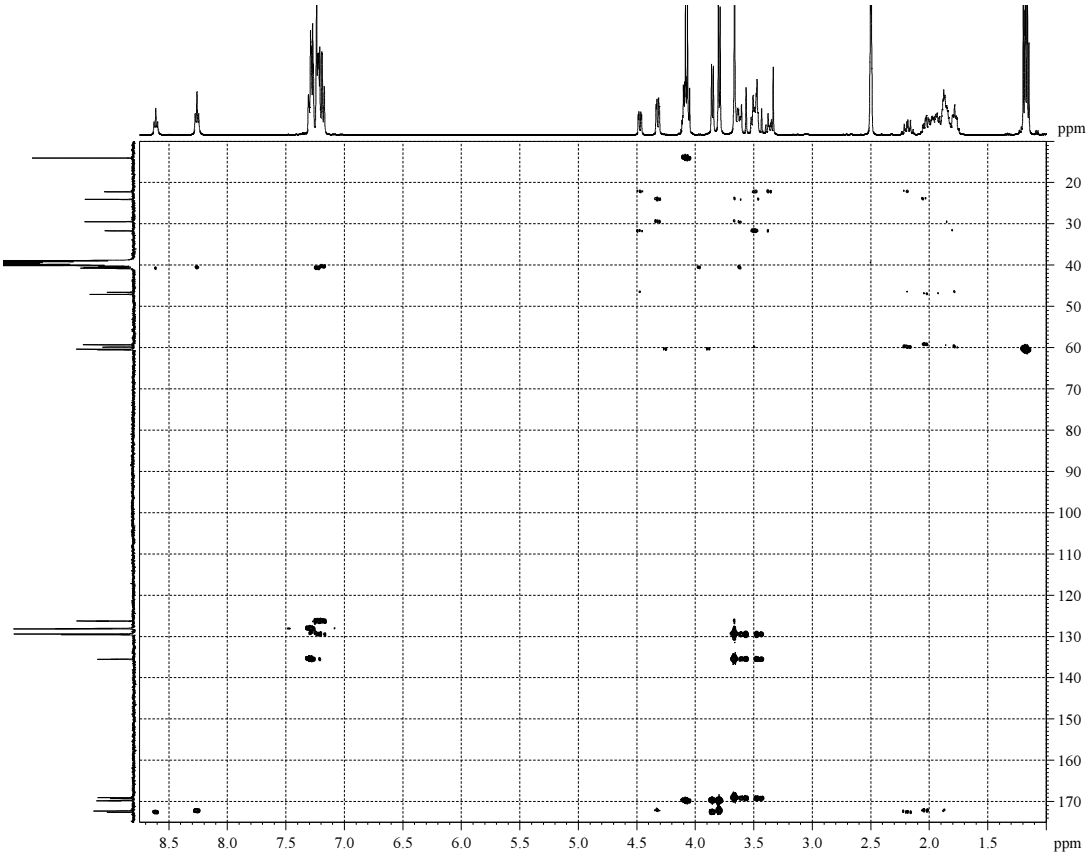


Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6

ed-HSQC



HMBC



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