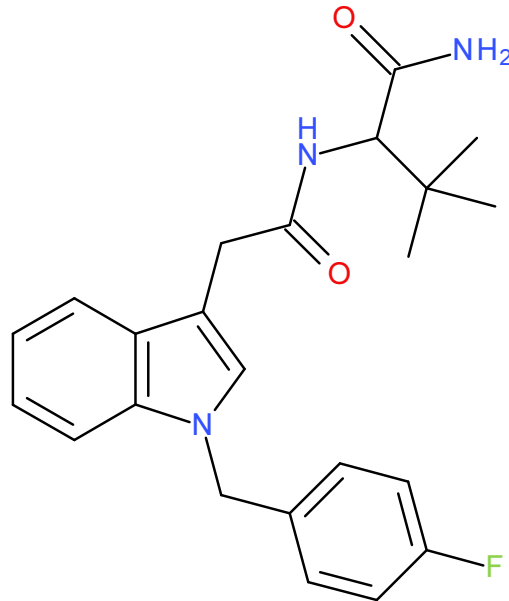


ADB-FUBIATA



2-[[2-[1-[(4-fluorophenyl)methyl]indol-3-yl]acetyl]amino]-3,3-dimethyl-butanamide

Formula: C₂₃H₂₆FN₃O₂

Formula weight: 395,47

Chemical Abstracts No.: *n. a.*

Smiles code: CC(C)(C)C(NC(=O)Cc1cn(Cc2ccc(F)cc2)c3ccccc13)C(=O)N

InChi key: KHAUCCNSUMBFOT-UHFFFAOYSA-N

Other names: ADB-FUB-Indaneacetamide, ADB-FUB-Indolylacetamide, AD-18, FUB-ACADB

Three evidences were investigated.

The first evidence was 27.55 grams impregnated, tabaco

The second evidence was 0.12 grams yellow coloured powder

The third evidence was 0.45 grams yellow coloured powder with fractured plant particles

The characterization was performed based on the second evidence and its purified fraction.

References:

Cui-Mei Liu, Zhen-Dong Hua, Wei Jia, Tao Li: Identification of AD-18, 5F-MDA-19, and pentyl MDA-19 in seized materials after the class-wide ban of synthetic cannabinoids in China.

Drug Test Anal. (2021) in press

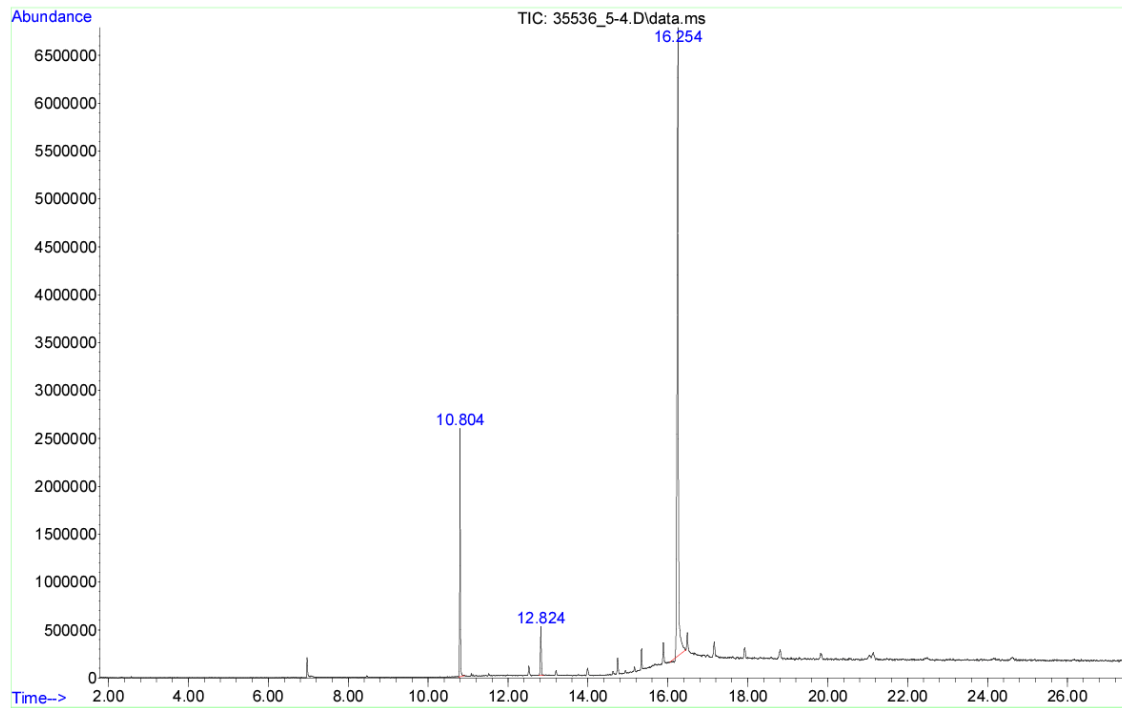
<https://doi.org/10.1002/dta.3185>

https://www.npsdiscovery.org/wp-content/uploads/2021/11/ADB-FUBIATA_111721_CFSRE-Chemistry_Report.pdf?mc_cid=50c984460f&mc_eid=604314c9a2

GC-MS

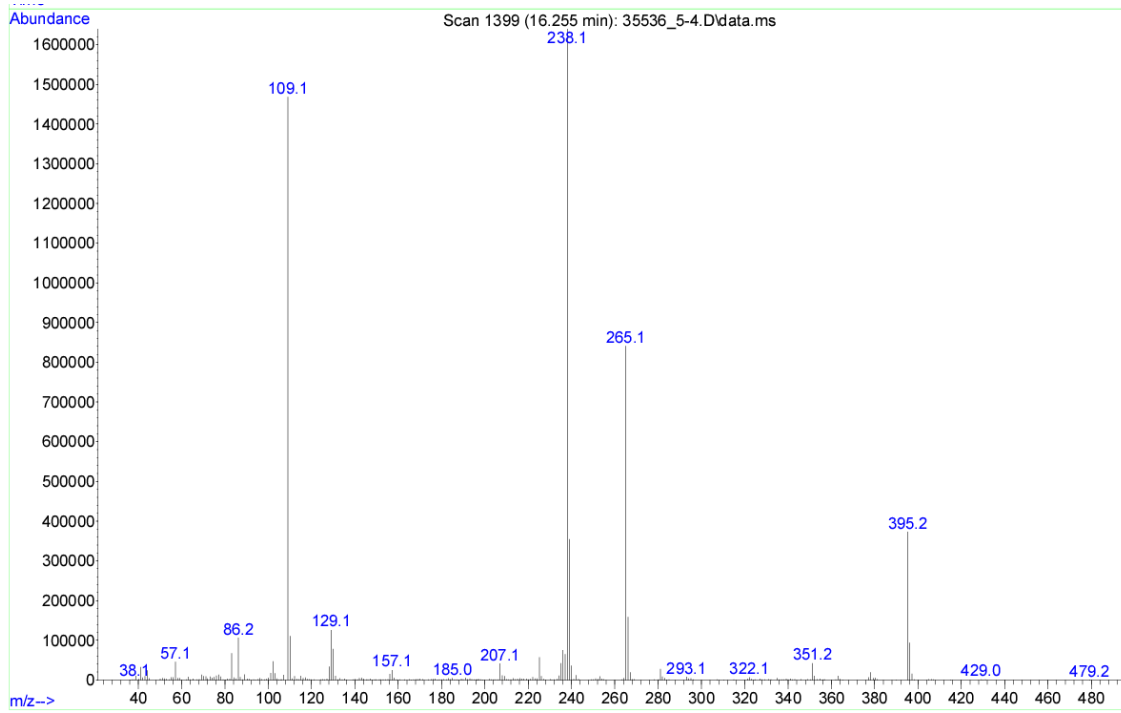
An Agilent 6890N Network GC system set up with Agilent HP-5MS (length: 30 m, diameter: 0.25 mm, film: 0.25 mm) coupled to an Agilent 5973 Network Mass Selective Detector (scan range m/z 35 – m/z 500) was used. The evidence was solved in methanol, the solution was injected. Samples were subjected to electron 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 current chromatogram of the evidence as received



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

Mass spectrum at 16.25 min retention time

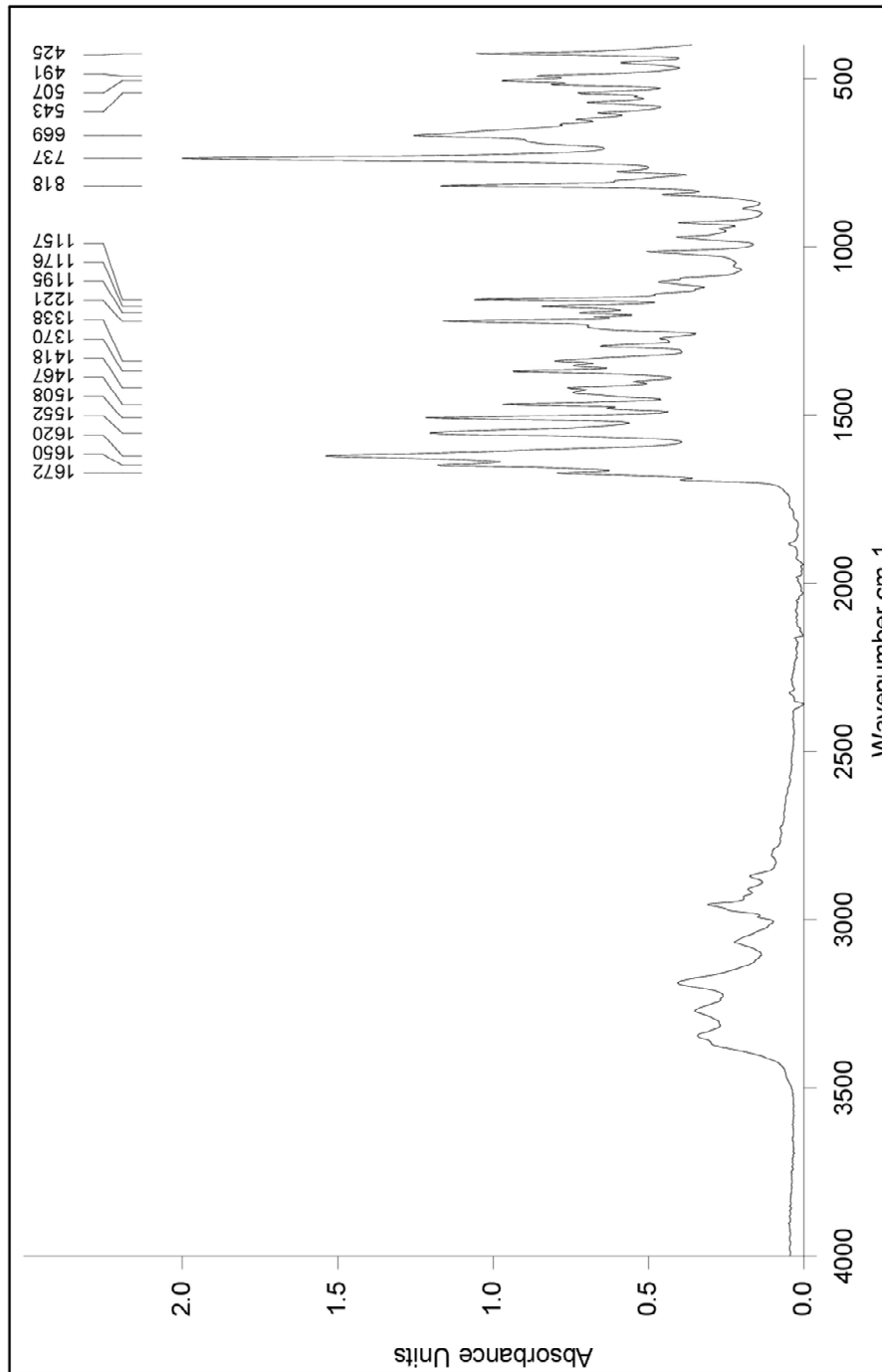


Agilent 6890N Network GC system set up with Agilent HP-5MS

IR

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

IR spectrum of the evidence as received



Bruker Tensor 27

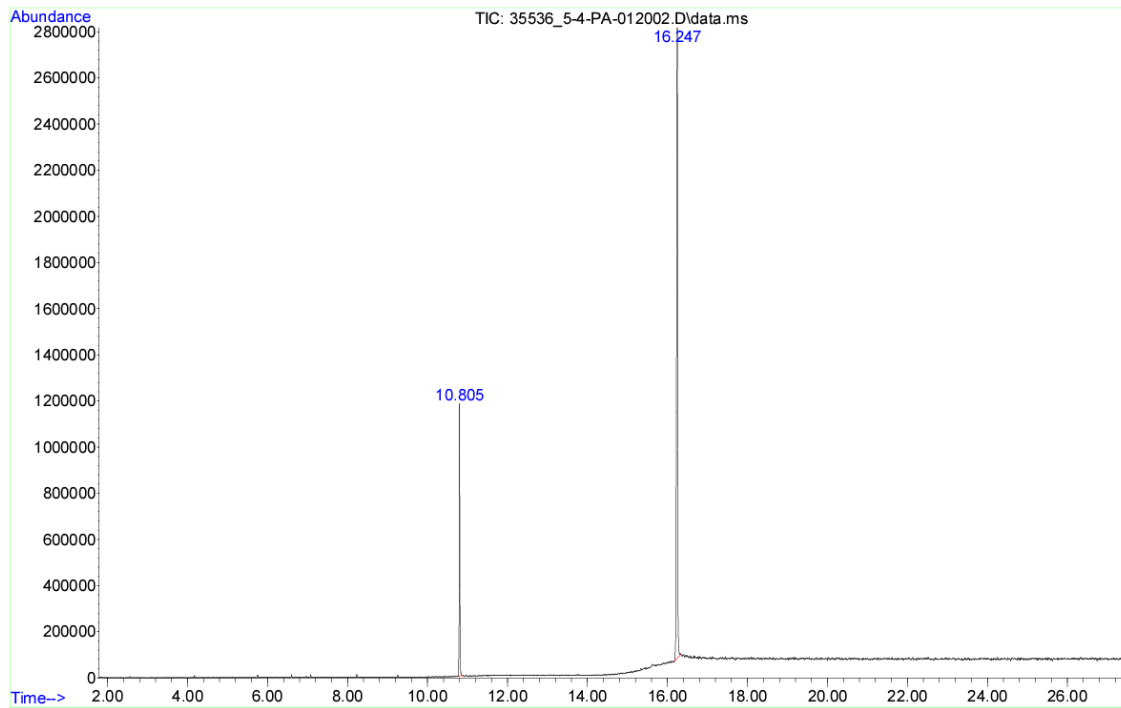
Isolation of the reported compound

50,1 mg seized sample were subjected to purification on a CombiFlash RF+ Teledyne ISCO flash chromatograph with gradient elution by up to 10 % methanol in dichloromethane through a 4 g RediSepRf SILICA column application of solid sample loading. The separated four fraction were analyzed accordingly.

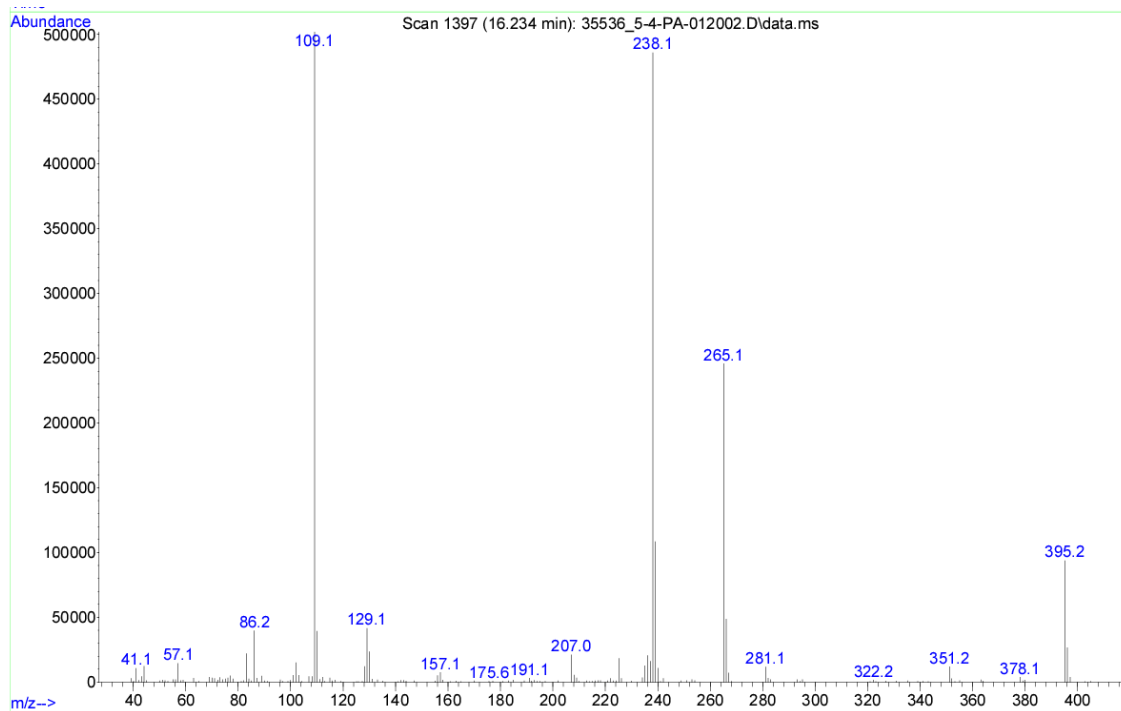
The reported compound was isolated as 2nd (major) fraction.

GC-MS of the purified fraction

GC-MS total ion current chromatogram of the 2nd fraction of the evidence



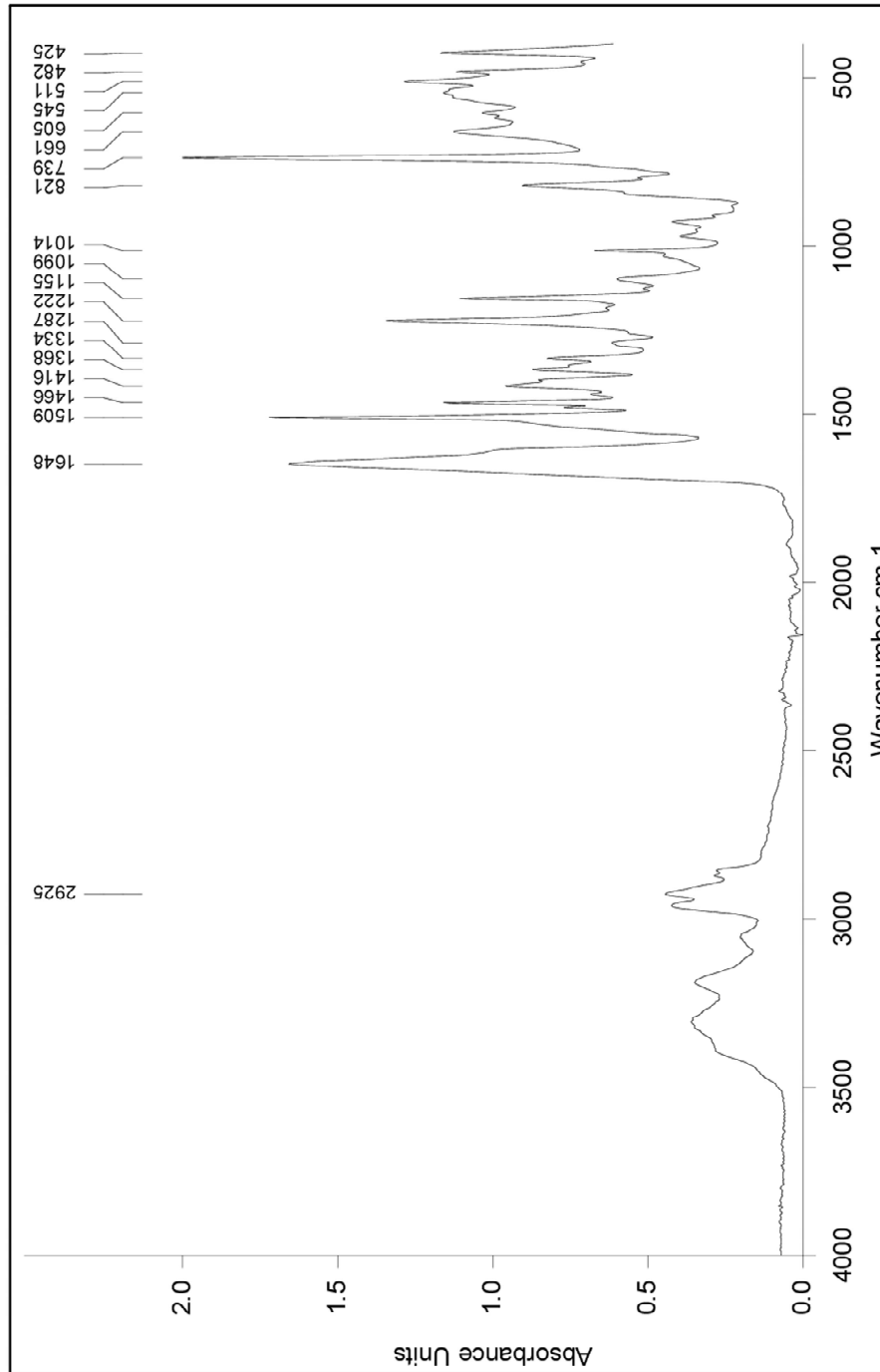
Mass spectrum at 16.25 min retention time



Agilent 6890N Network GC system set up with Agilent HP-5MS, using same conditions as the neat evidence was recorded

IR

IR spectrum of the 2nd fraction of the evidence after purification



Bruker Tensor 27, using same conditions as the neat evidence was recorded

GC-IRD

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 a Dani DiscovIR FT-IR spectrometer was used. GC conditions: Split ratio: 1:5, 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. The evidence was extracted by methanol, the filtered extractum was injected. Tribenzyl-amine was applied as an internal standard. IRD conditions: Deposition tip: 280 °C, Restrictor: 280 °C, Transfer Line: 280 °C, Disk temperature:- 40 °C, Dewar Cap temperature: 30 °C. Data handling was carried out with DiscovIR6 software.

GC-IR chromatogram of the purified 2nd fraction

GC-IR Analysis Report

DiscovIR conditions

Peaks file: C:/Data/MERESK2021/35536_5-4/reproc/35536_5-4.Peaks.spc
 Sample name: 35536_5-4
 Chemist: BD GT
 Date collected: 11/15/2021 09:44
 Date analyzed:
 Disk speed: 3 mm/min
 Vial number: 2

Run conditions	Start	End
Transfer line temperature (°C):	280	280
Oven temperature (°C):	280	280
Restrictor temperature (°C):	280	280
Disk temperature (°C):	-40	-40
Data collect (minutes):	2.50	28.01
Track pointer:	69771	133525
Chamber pressure (Torr):	2.100e-4	2.000e-4

Comment: 35536/2021 4. PA-012002 / MeOH

Chemstation conditions

Method name: KABSEQ2_5S.M

Run time: 27.40 minutes

Split mode: SPLIT

Split ratio: 5 : 1

GC column: HP-5ms Ultra Inert : 30 m x 250 µm x 0.25 µm film

Oven Temperature: 100°C for 2 min, then 20°C/min to 280°C, hold 3 min, then 25°C/min to 315°C, hold 12 min

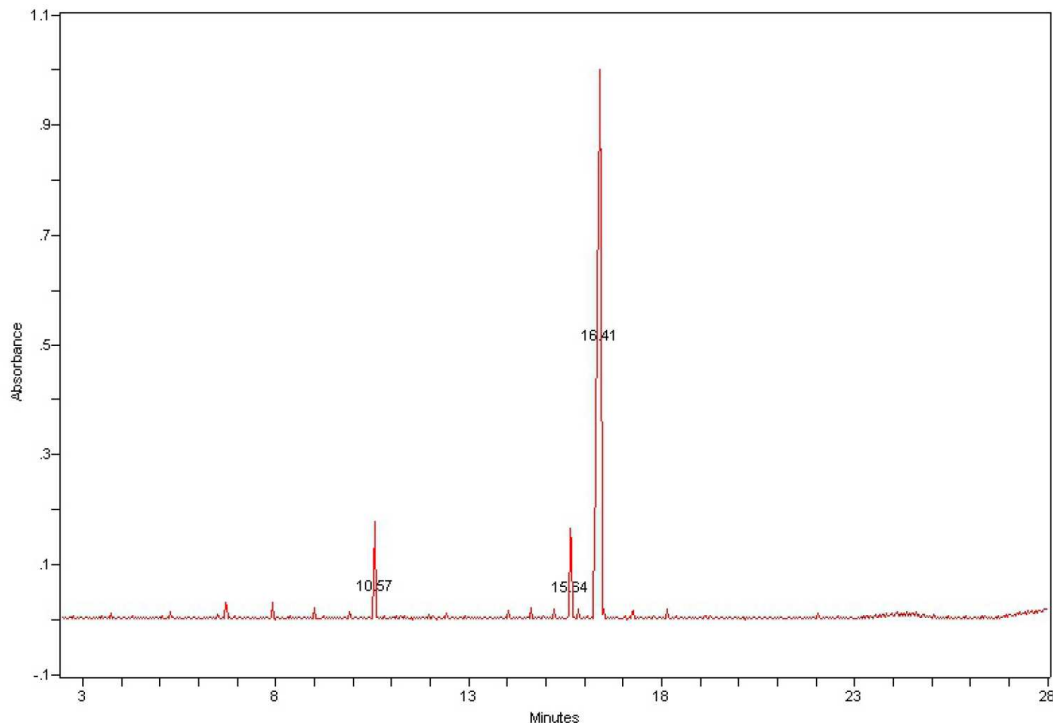
Injection port temperature (°C): 300

Injection volume (µL): 1

Gas pressure (psi): 24.10

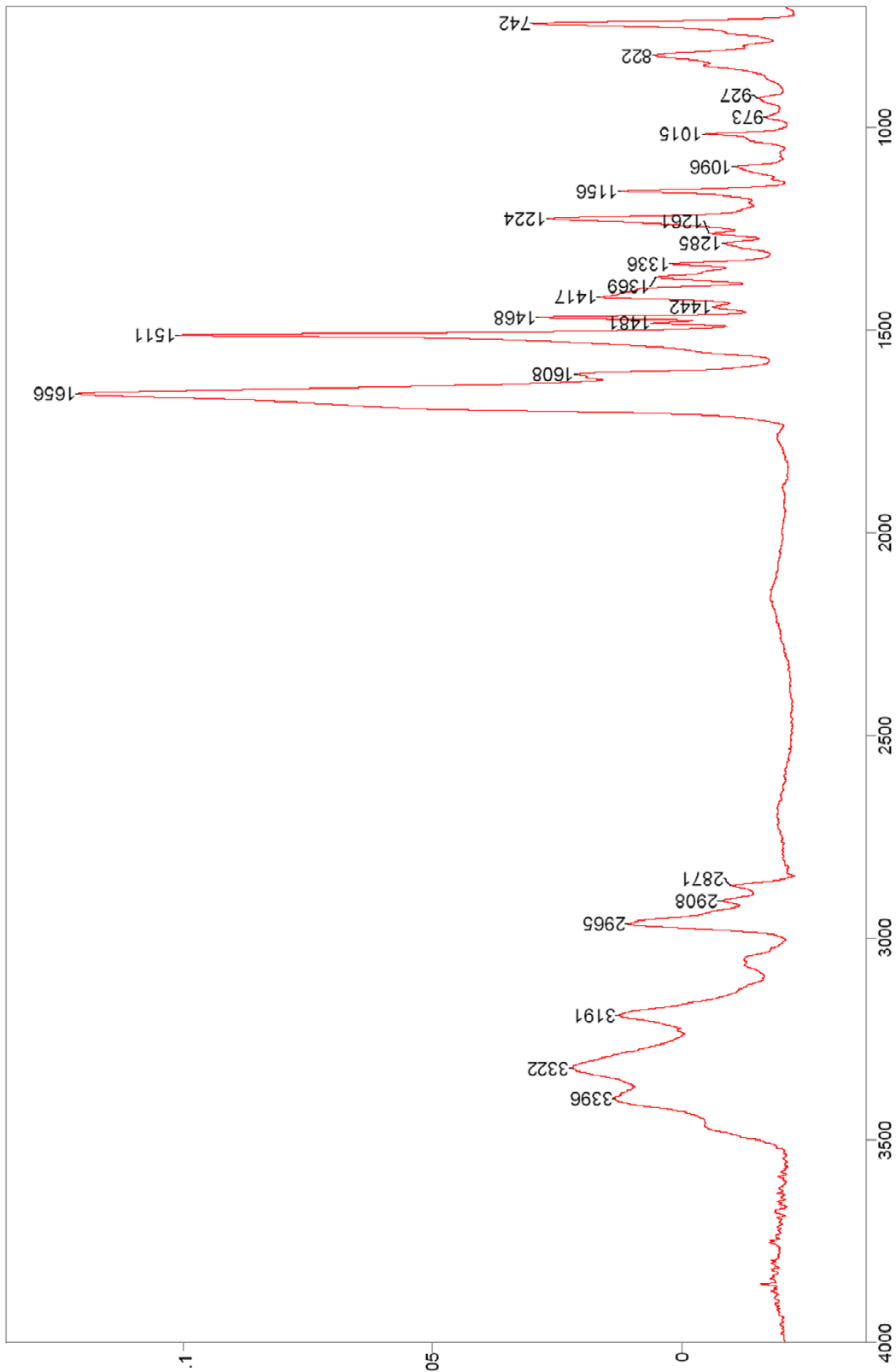
Chromatogram

Data file: C:/Data/MERESK2021/35536_5-4/reproc/35536_5-4.Multifile.cgm



Agilent 6890N Network GC system coupled to Dani DiscovIR FT-IR spectrometer

IR spectrum of the reported component at 16.41 min retention time

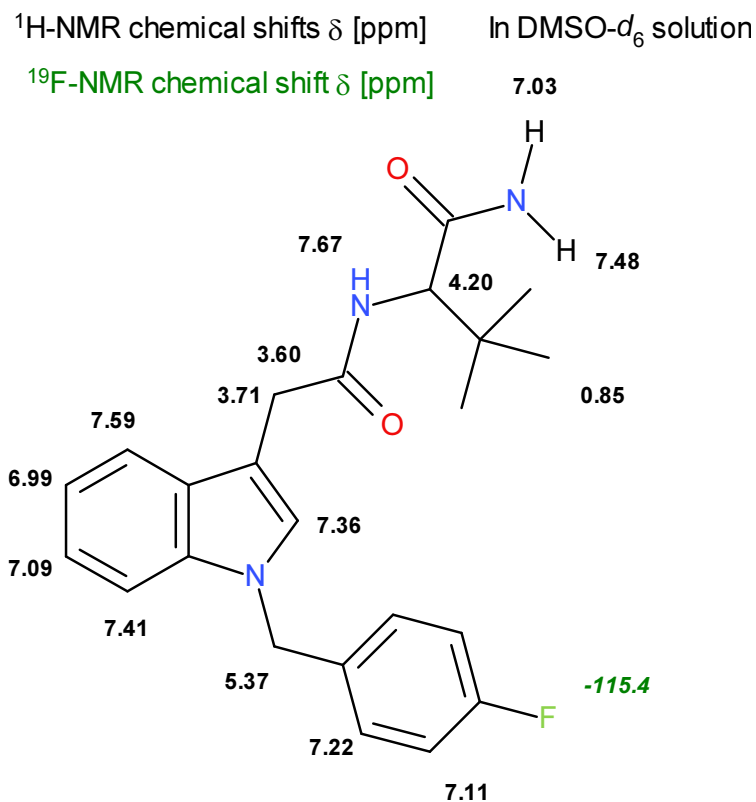


Agilent 6890N Network GC system coupled to Dani DiscovIR FT-IR spectrometer

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 fraction was measured in DMSO- d_6 solvent. 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 ($\delta_{\text{TMS}} = 0.00$ ppm). The determination of the structure was based on ^1H , zqs-clip-COSY, zqs-TOCSY, zqs-easy-ROESY, ^{19}F , as well as ^{13}C , multiplicity edited HSQC and HMBC spectra.

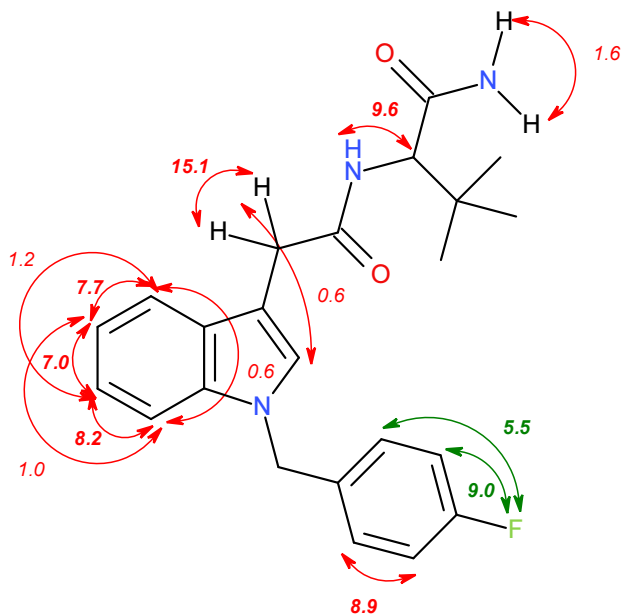
Interpretation of the NMR spectra



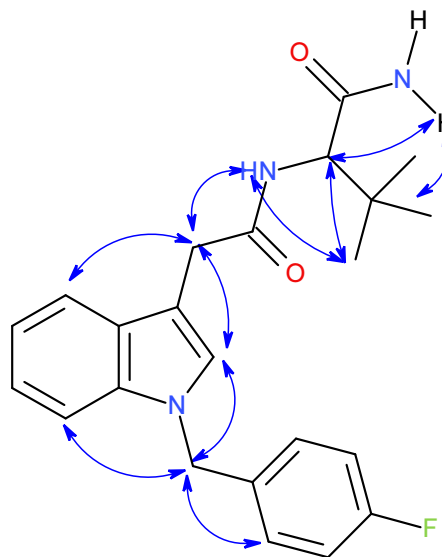
Interpretation of the NMR spectra (continued)

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

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

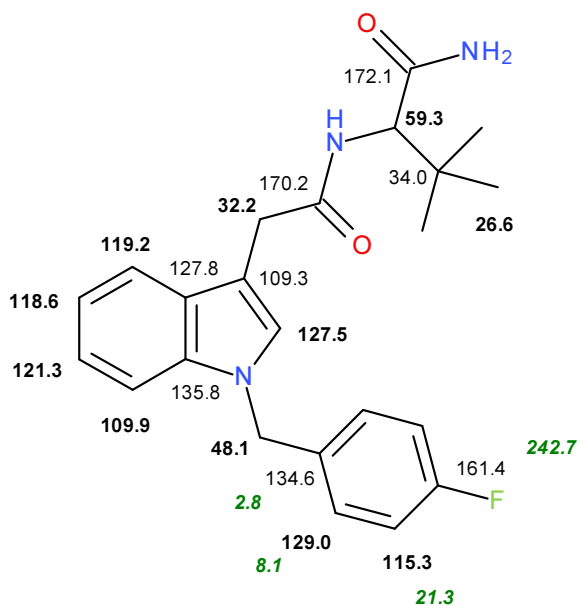


Characteristic H-H steric proximities detected by zqs-NOESY measurement

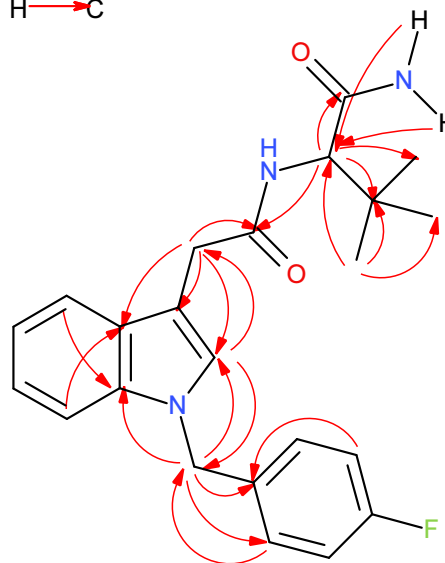


^{13}C -NMR chemical shifts δ [ppm]

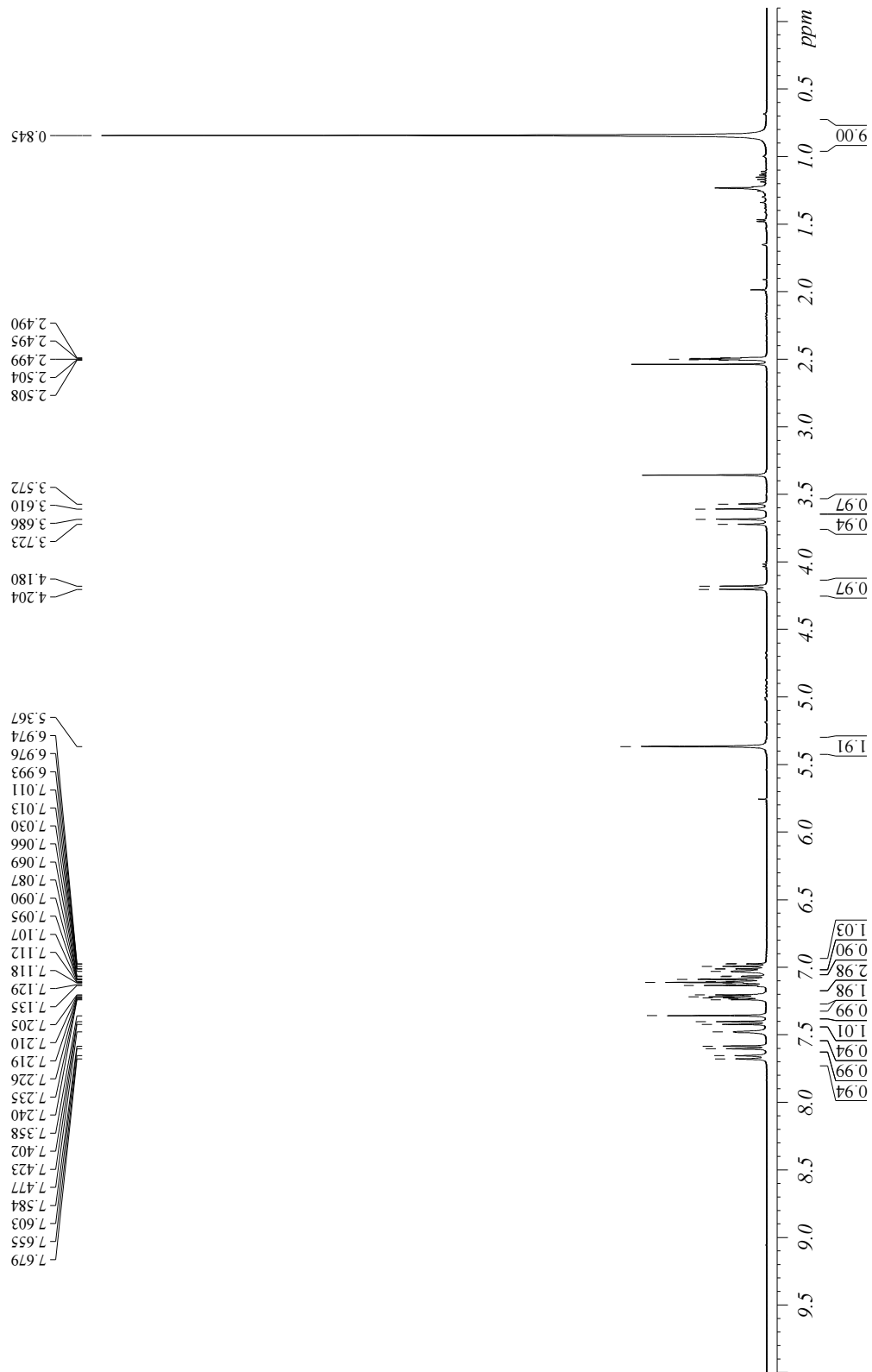
$J(C,F)$ coupling constants [Hz]



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

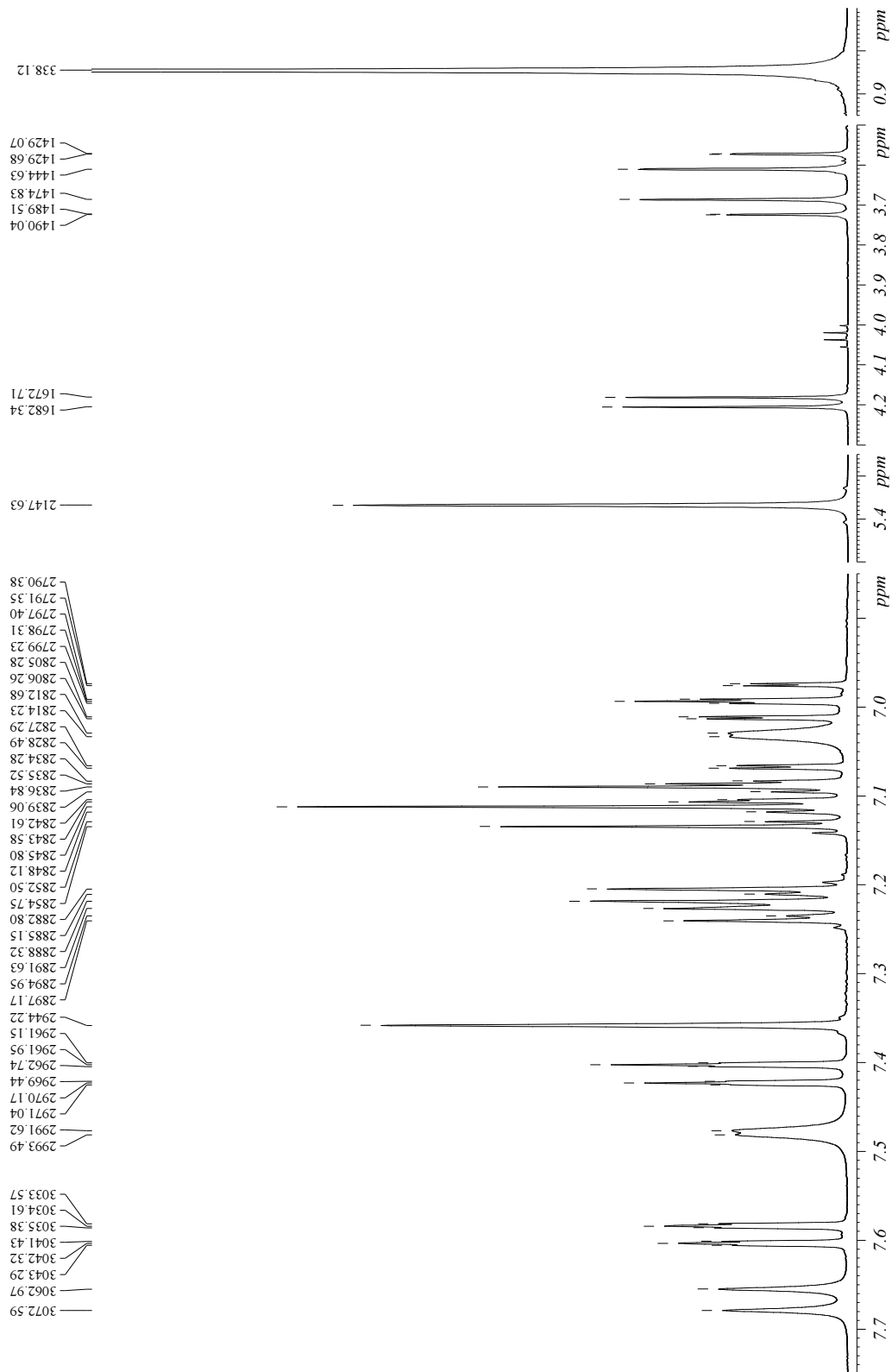


¹H-NMR spectrum (overview)



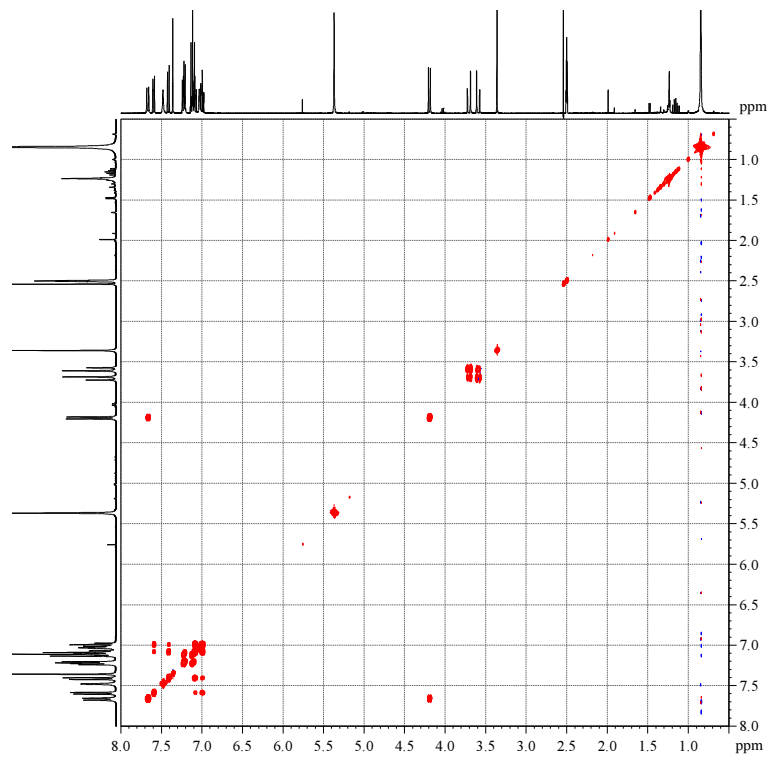
Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-*d*₆

Characteristic sections of the $^1\text{H-NMR}$ spectrum

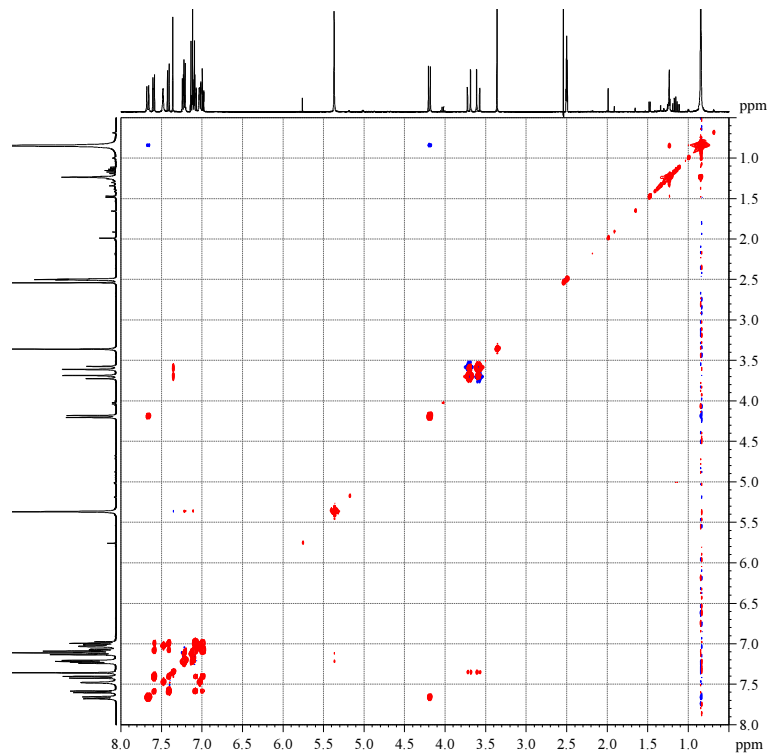


Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: $\text{DMSO-}d_6$

zqs-clip-COSY

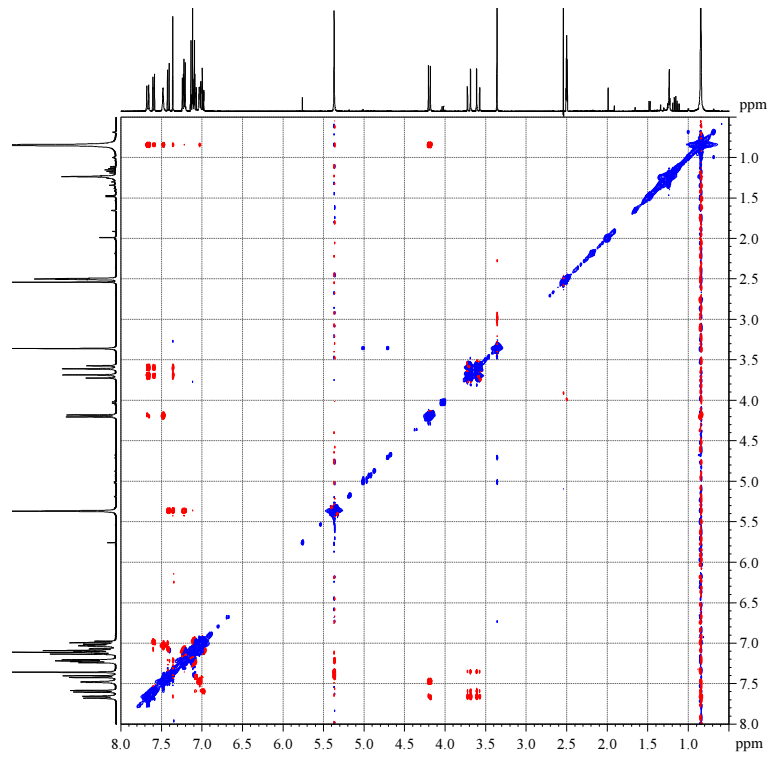


zqs-TOCSY

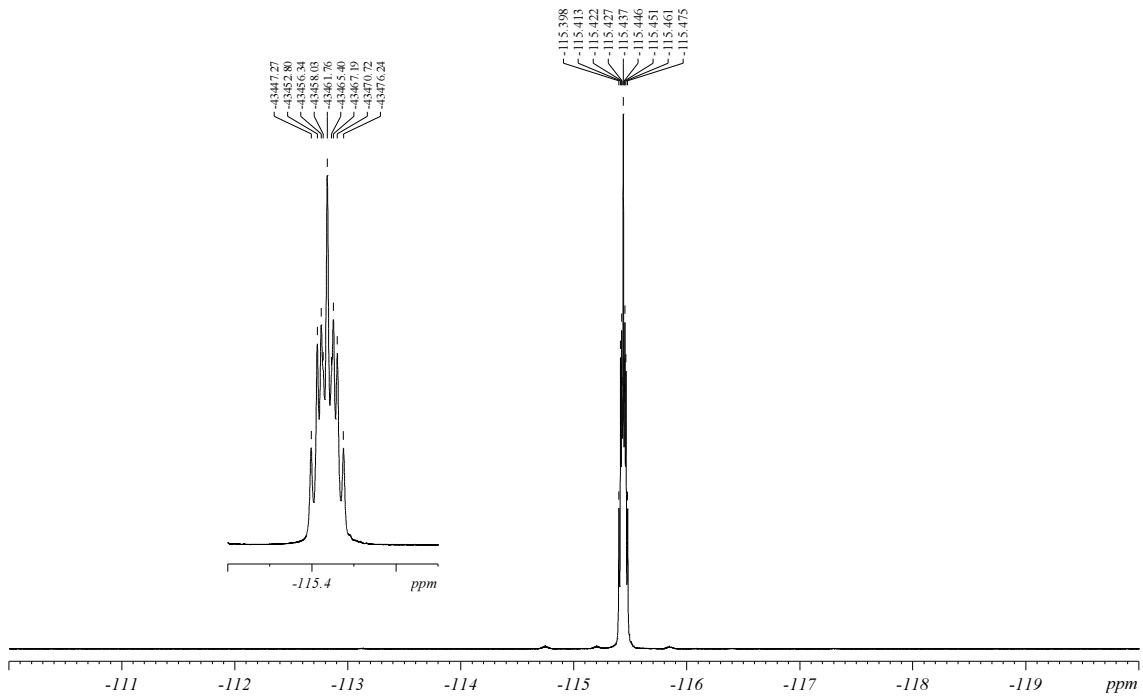


Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-*d*₆

zqs-easy-ROESY

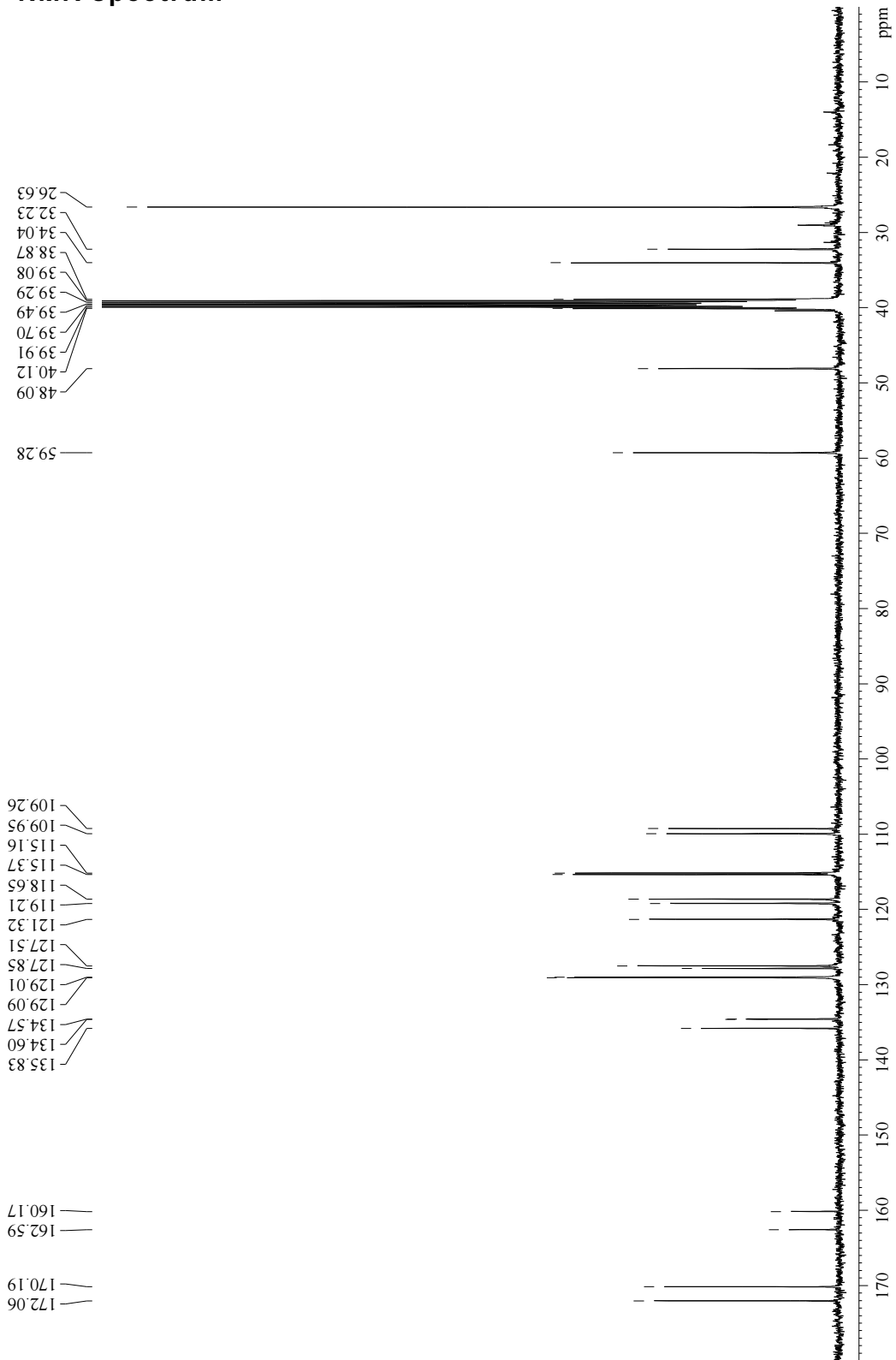


¹⁹F-NMR spectrum with expanded regions with Hz list above



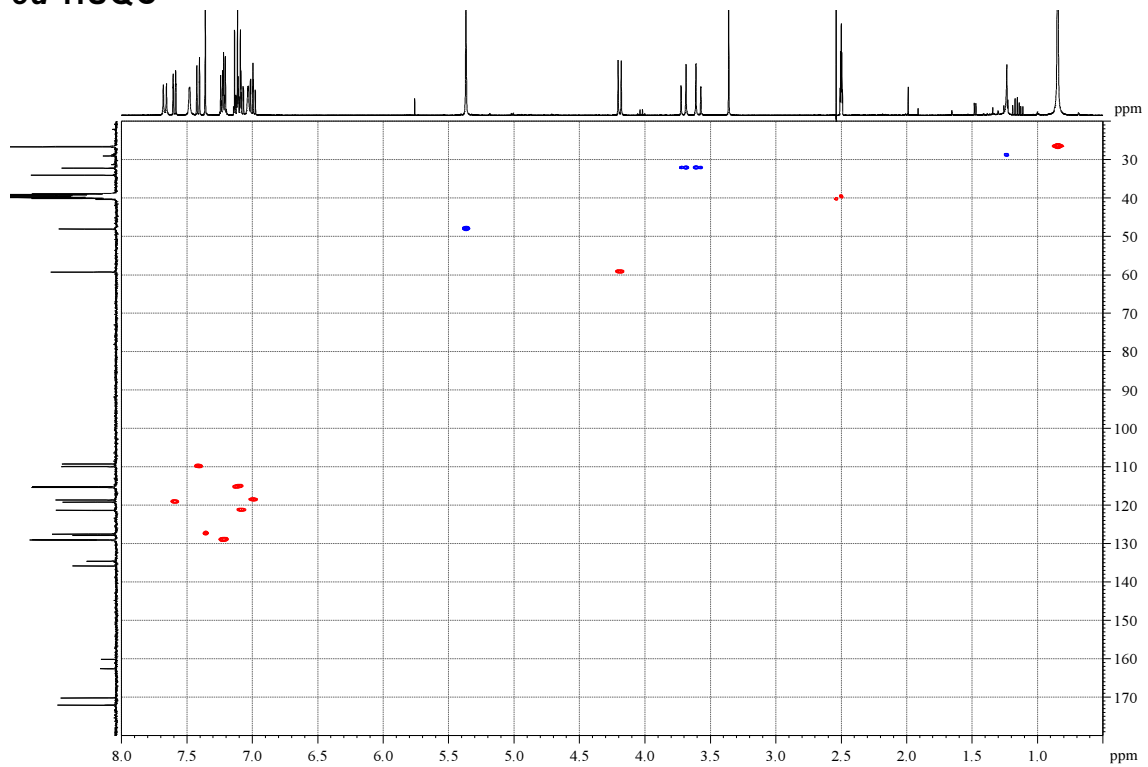
Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-*d*₆

^{13}C -NMR spectrum

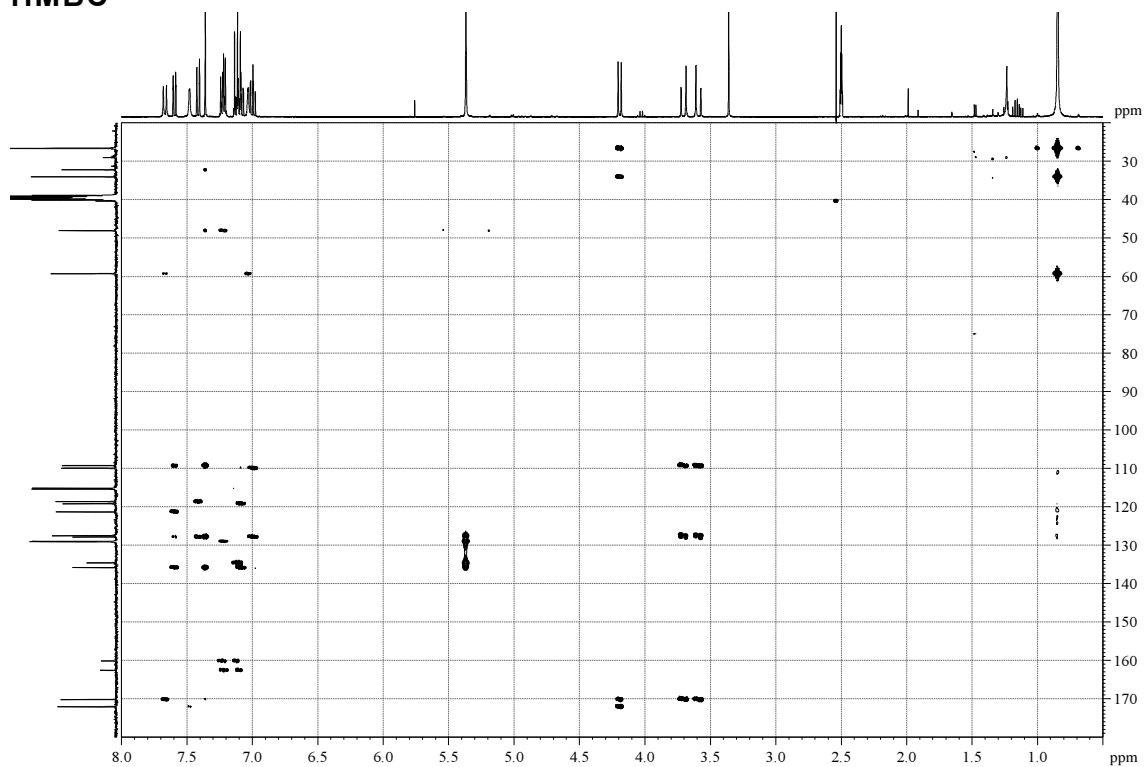


Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO- d_6

ed-HSQC



HMBC



Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-*d*₆