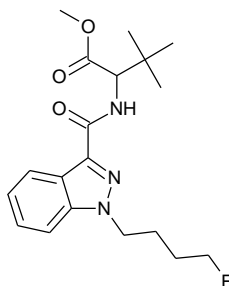


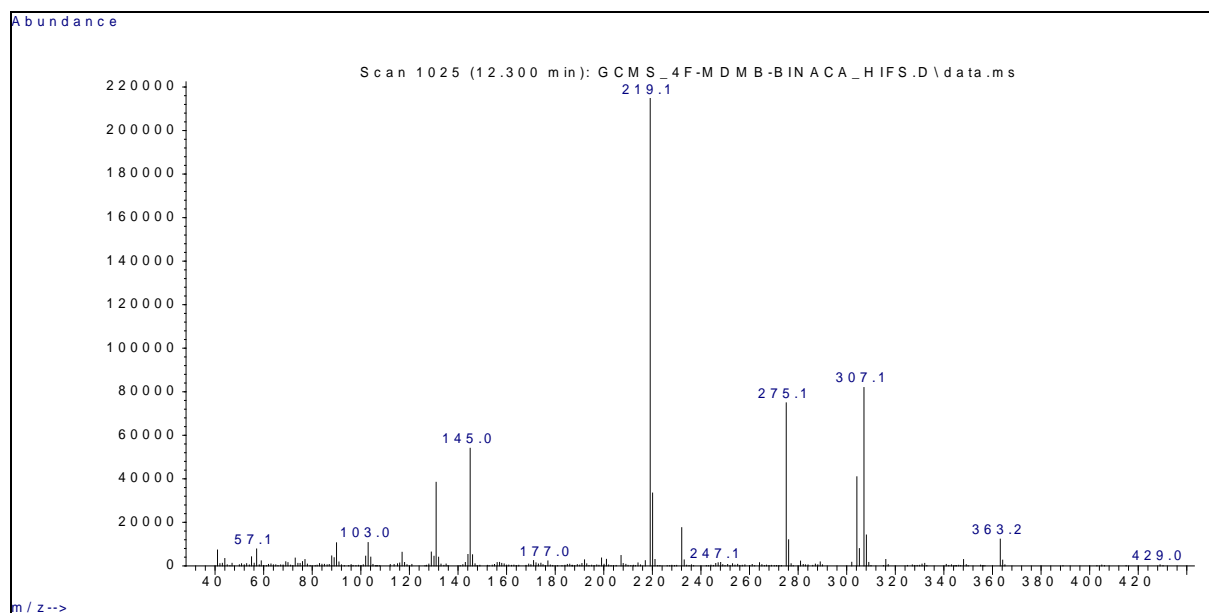
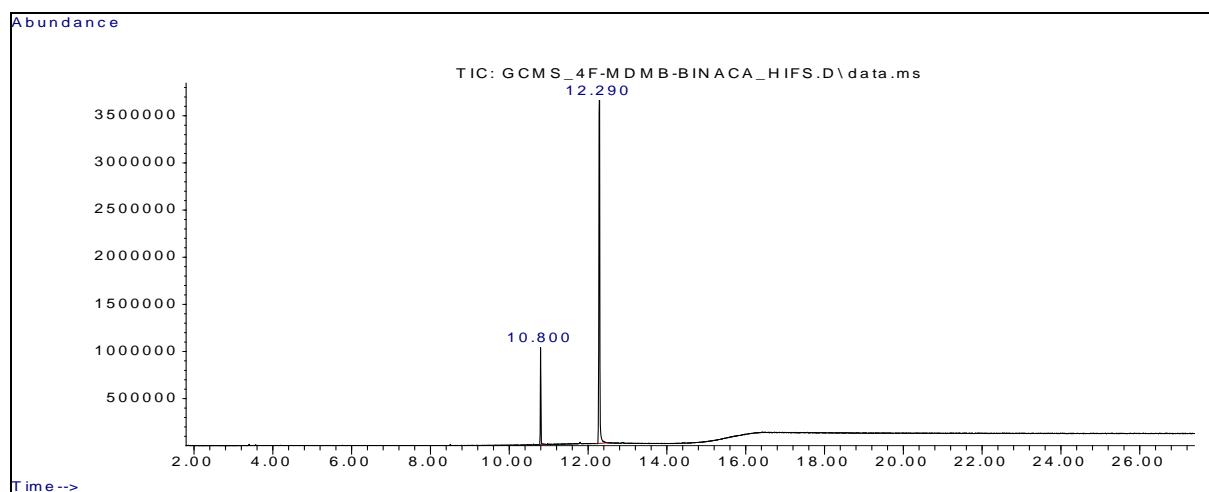
4F-MDMB-BINACA

methyl 2-(1-(4-fluorobutyl)-1H-indazole-3-carboxamido)-3,3-dimethylbutanoate

StdInChIKey: GZGKSDAMWRWYOZ-UHFFFAOYSA-N

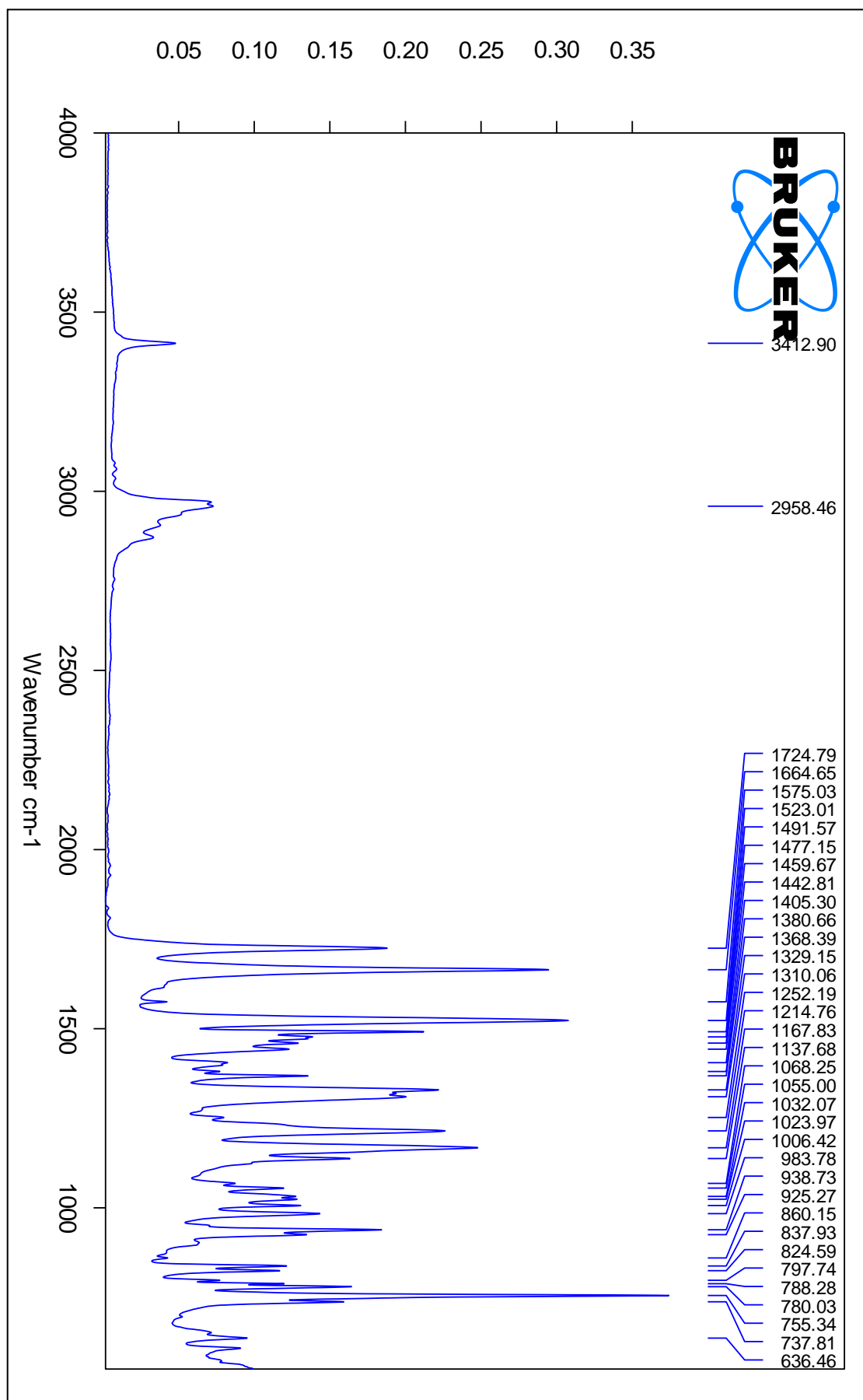
GC-MS

Rt.: 12.29 min



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.

ATR-FTIR



U:\Standard\EW\S\Bejelentendő\4F-MDMB-BINACA\ATR-FTIR_4F-MDMB-BINACA_HIFS.SPA

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2018.11.28.

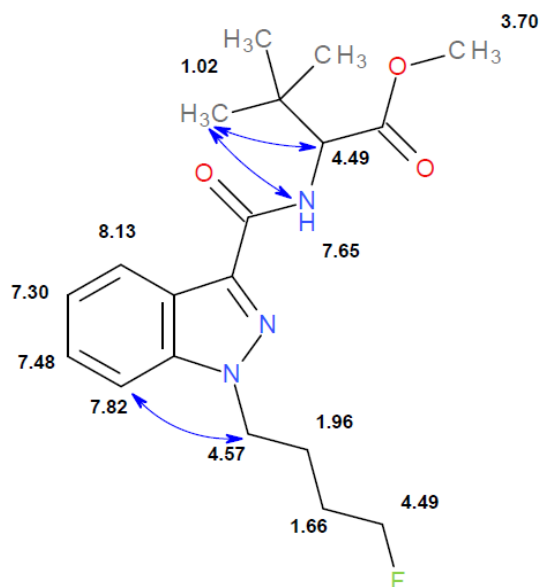
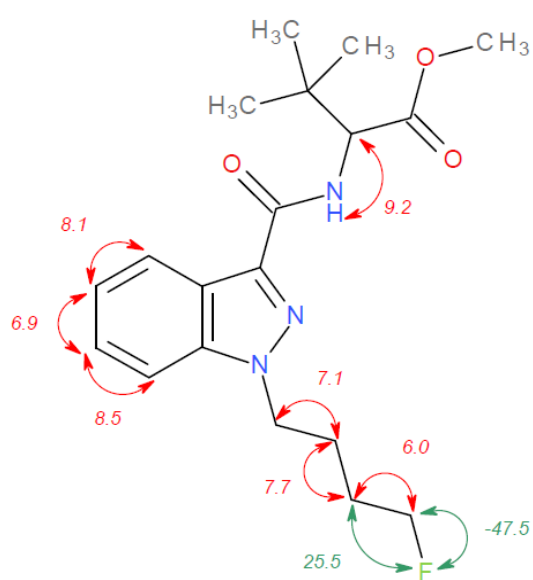
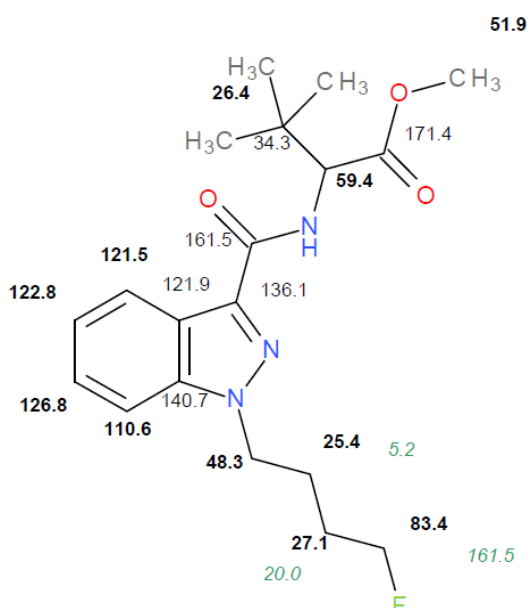
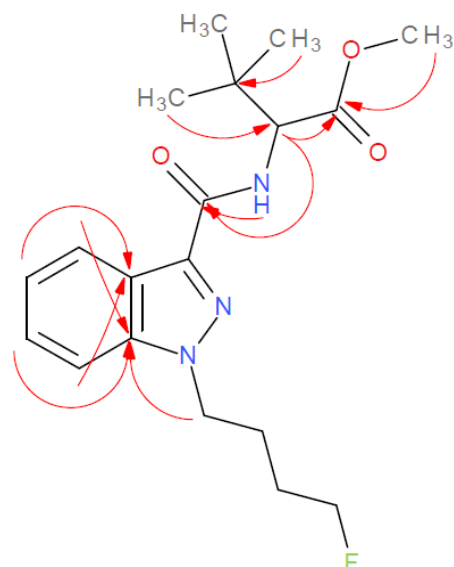
NMR

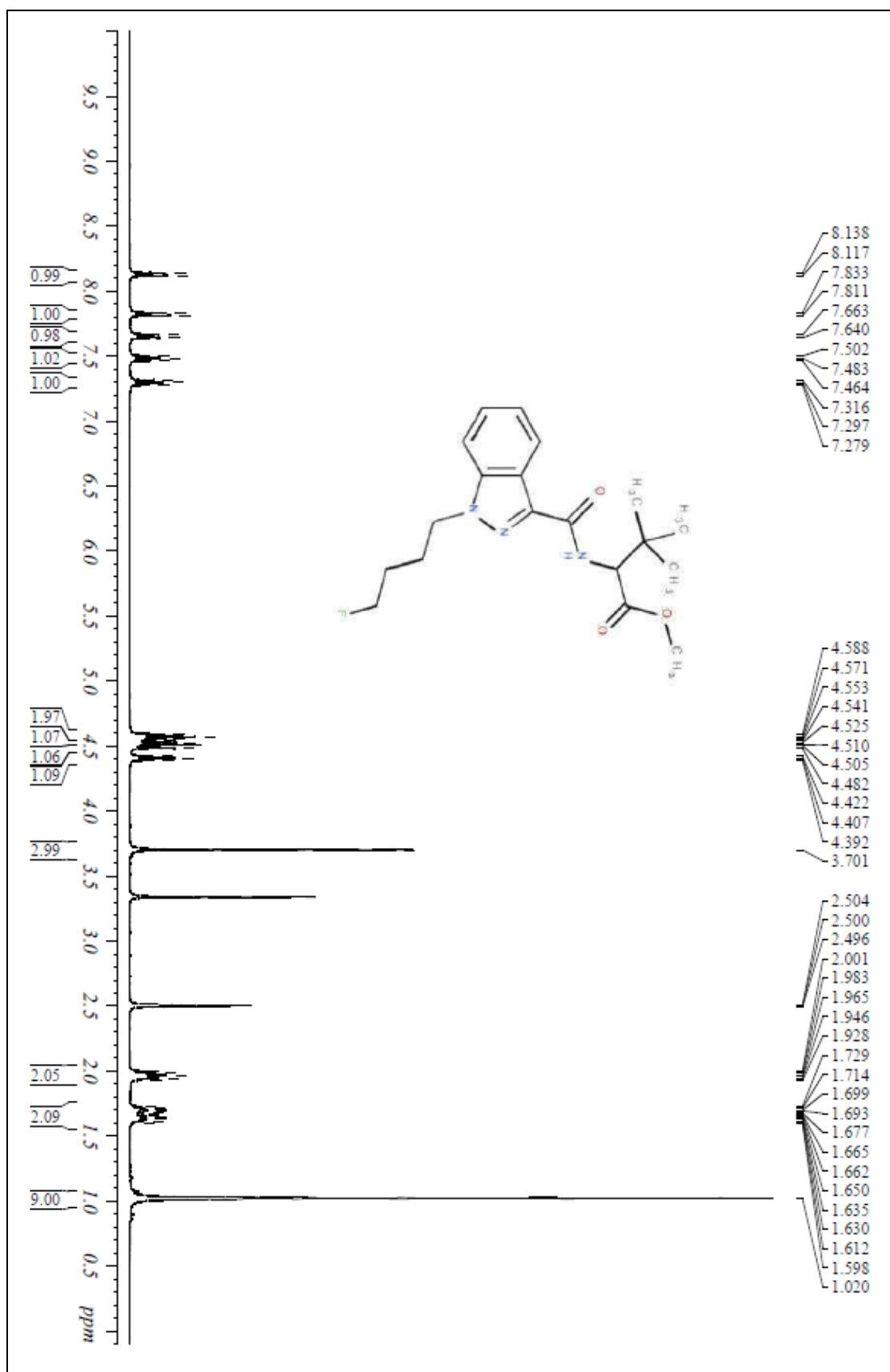
4F-MDMB-BINACA

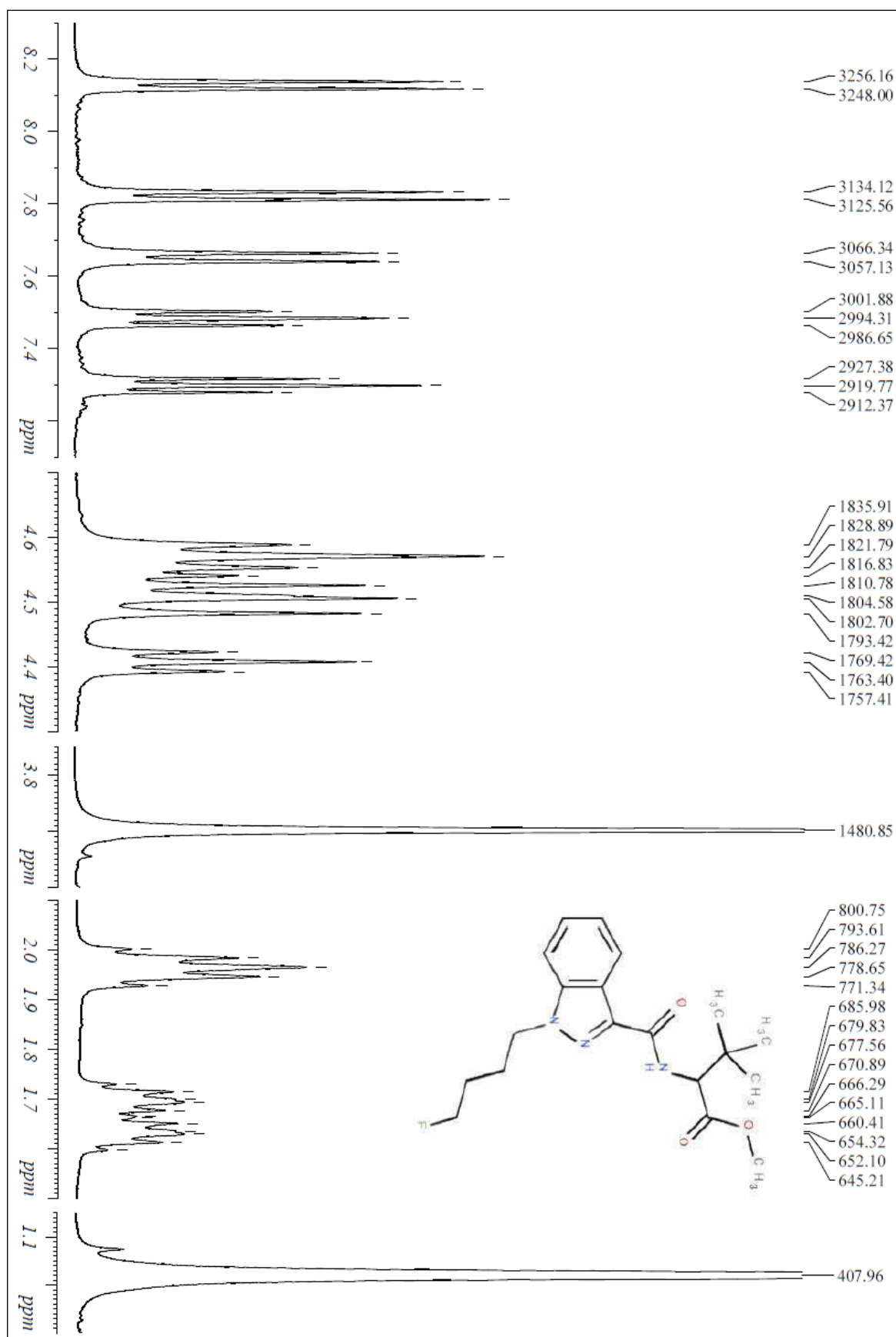
in DMSO- d_6 solution

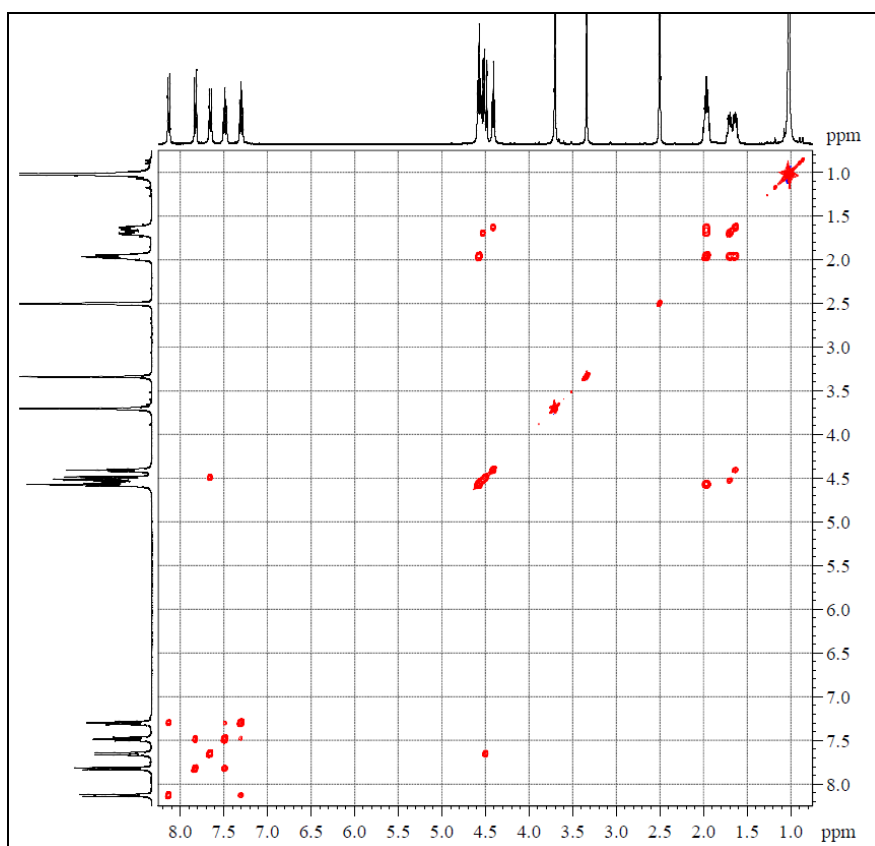
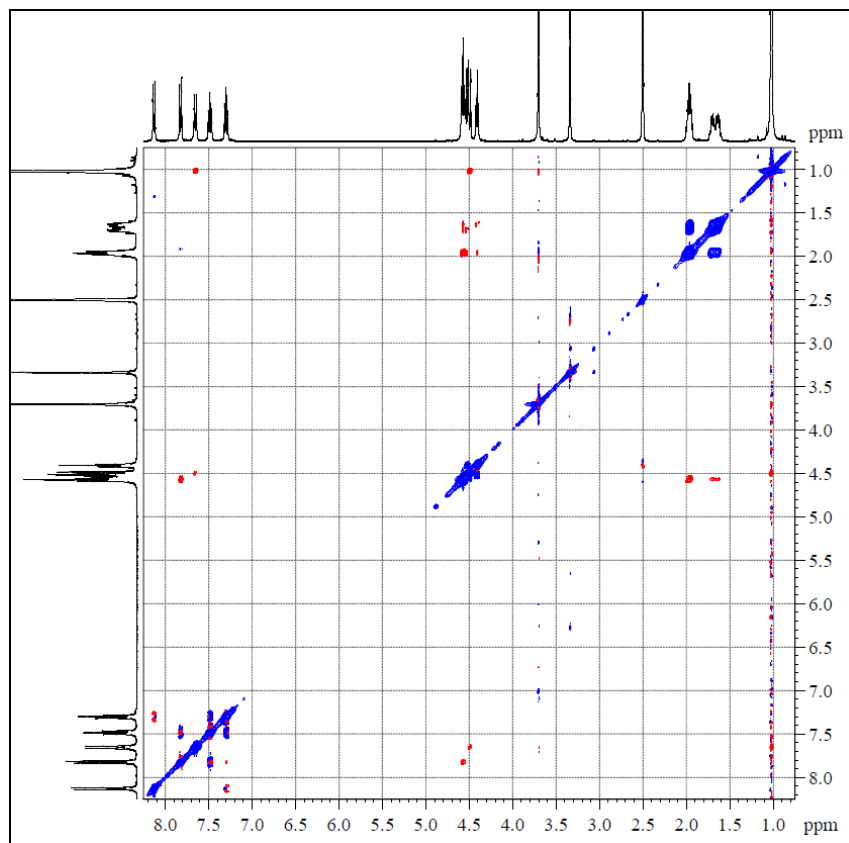
Formula Weight: 363,42644

Exact Mass: 363,195819922

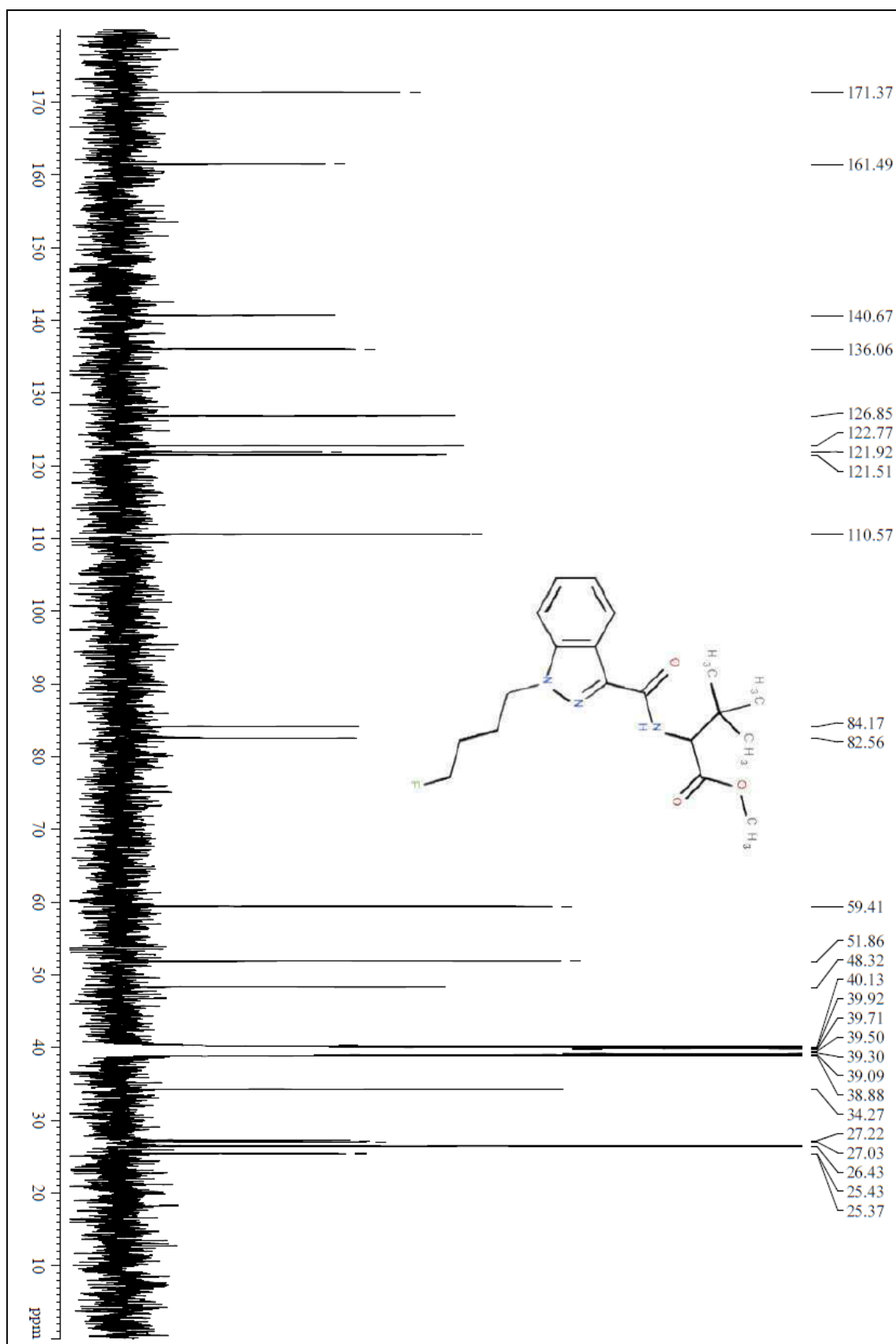
Molecular Formula: $C_{19}H_{26}FN_3O_3$ 1H -NMR chemical shifts δ [ppm]Characteristic 1H - 1H steric proximities
detected by ROESY $J(H,H)$ coupling constants [Hz] $J(H,F)$ coupling constants [Hz] ^{13}C -NMR chemical shifts δ [ppm] $J(C,F)$ coupling constants [Hz]Characteristic heteronuclear long-range
couplings detected by HMBC experiment
H \rightarrow CBruker AVANCE NEO, 400MHz, CryoProbe Prodigy; solvent: DMSO- d_6

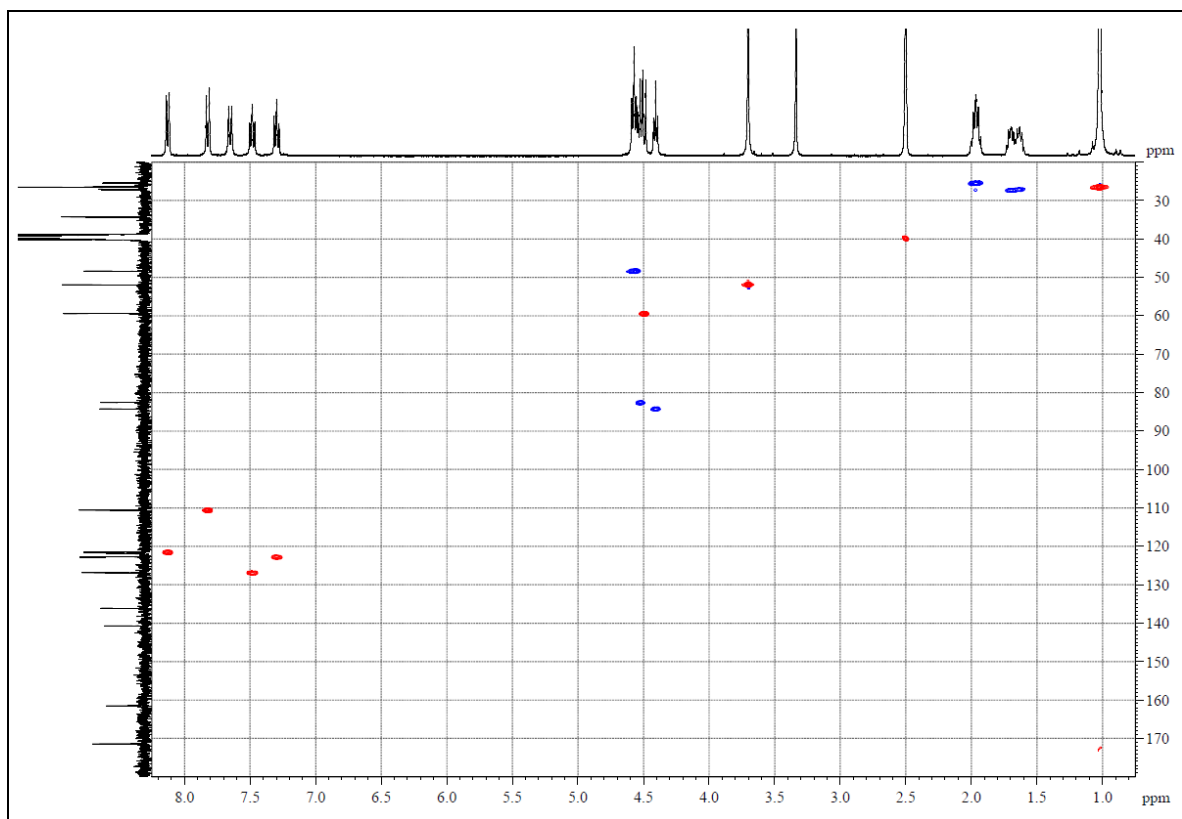
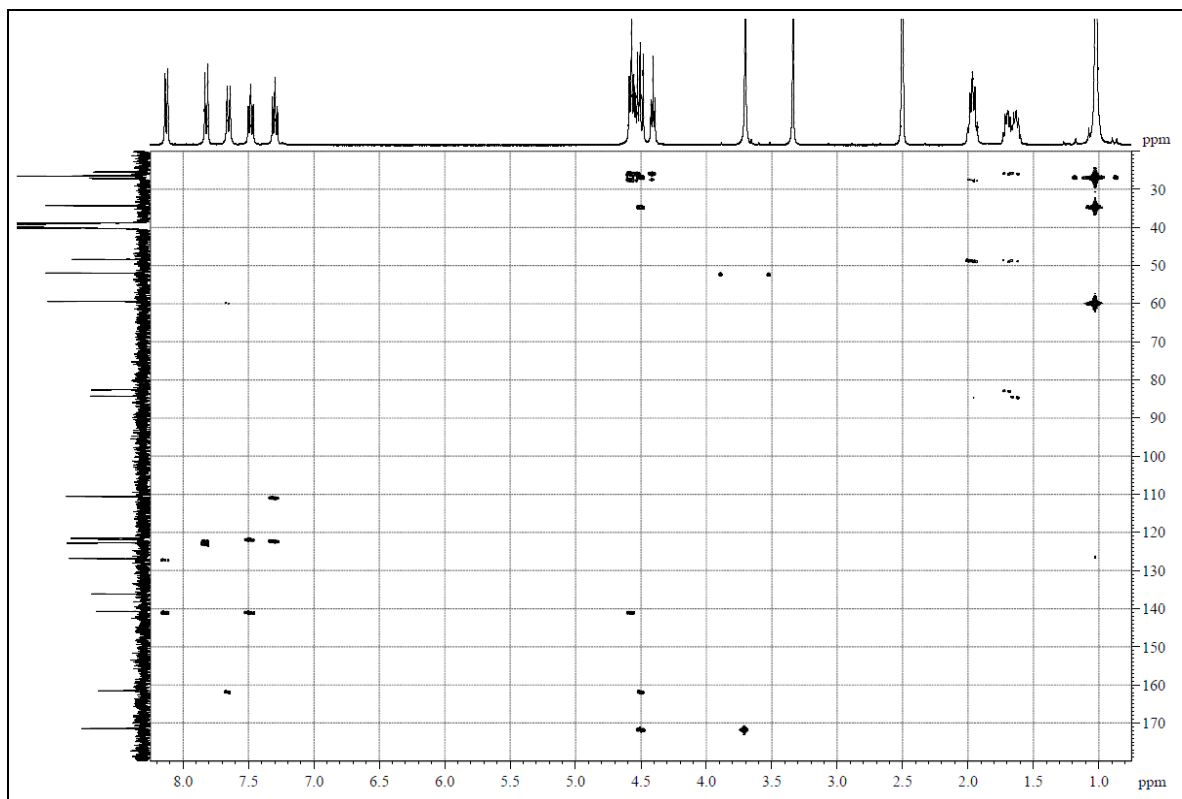
^1H NMRBruker AVANCE NEO, 400MHz, CryoProbe Prodigy; solvent: DMSO-d₆

¹H NMRBruker AVANCE NEO, 400MHz, CryoProbe Prodigy; solvent: DMSO-d₆

clip-zqs-COSY**zqs-easy-ROESY**

Bruker AVANCE NEO, 400MHz, CryoProbe Prodigy; solvent: DMSO-d6

^{13}C NMRBruker AVANCE NEO, 400MHz, CryoProbe Prodigy; solvent: DMSO- d_6

ed-HSQC**HMBC**Bruker AVANCE NEO, 400MHz, CryoProbe Prodigy; solvent: DMSO-*d*₆