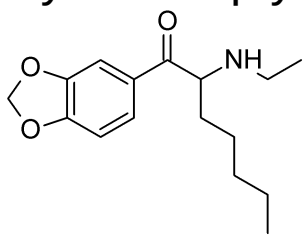
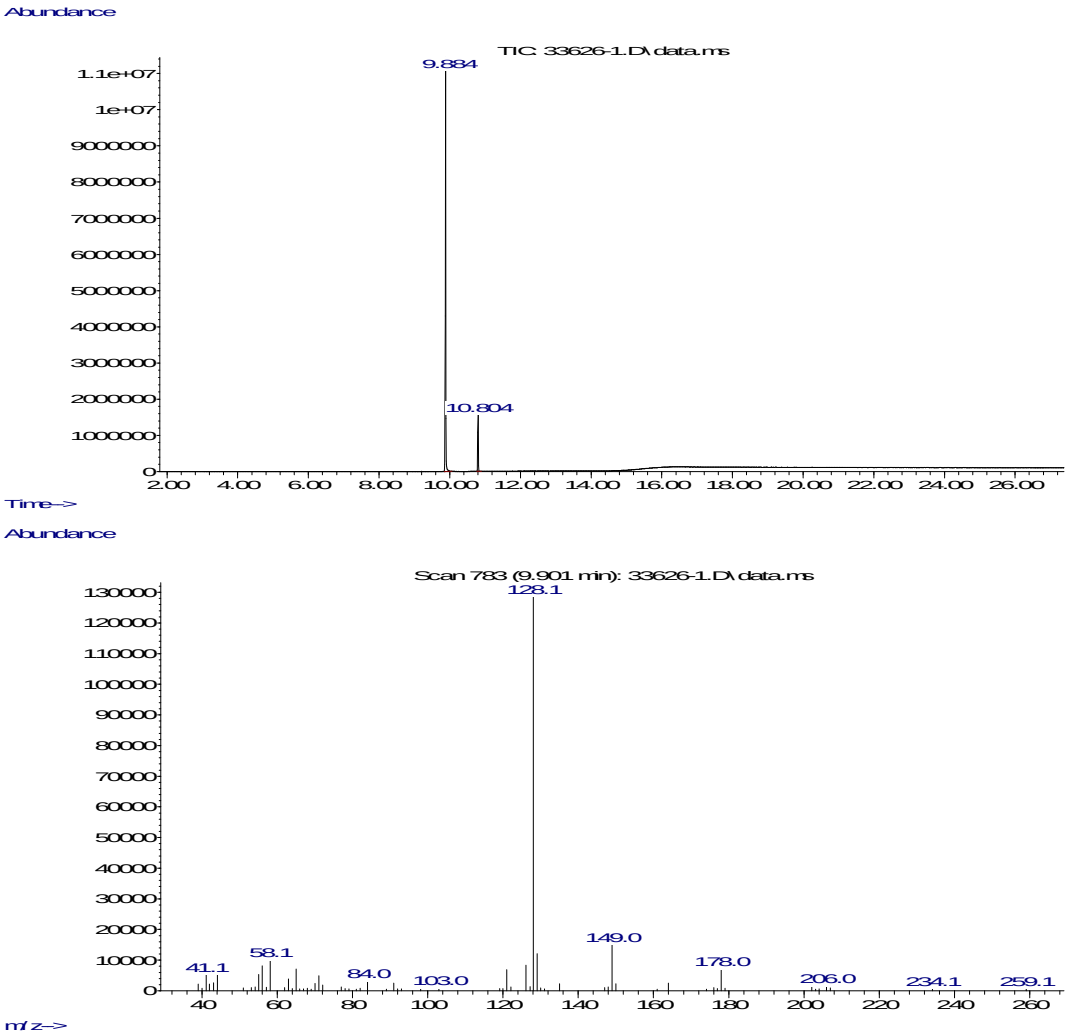
N-ethyl-*nor*-heptylone



1-(1,3-benzodioxol-5-yl)-2-(ethylamino)heptan-1-one

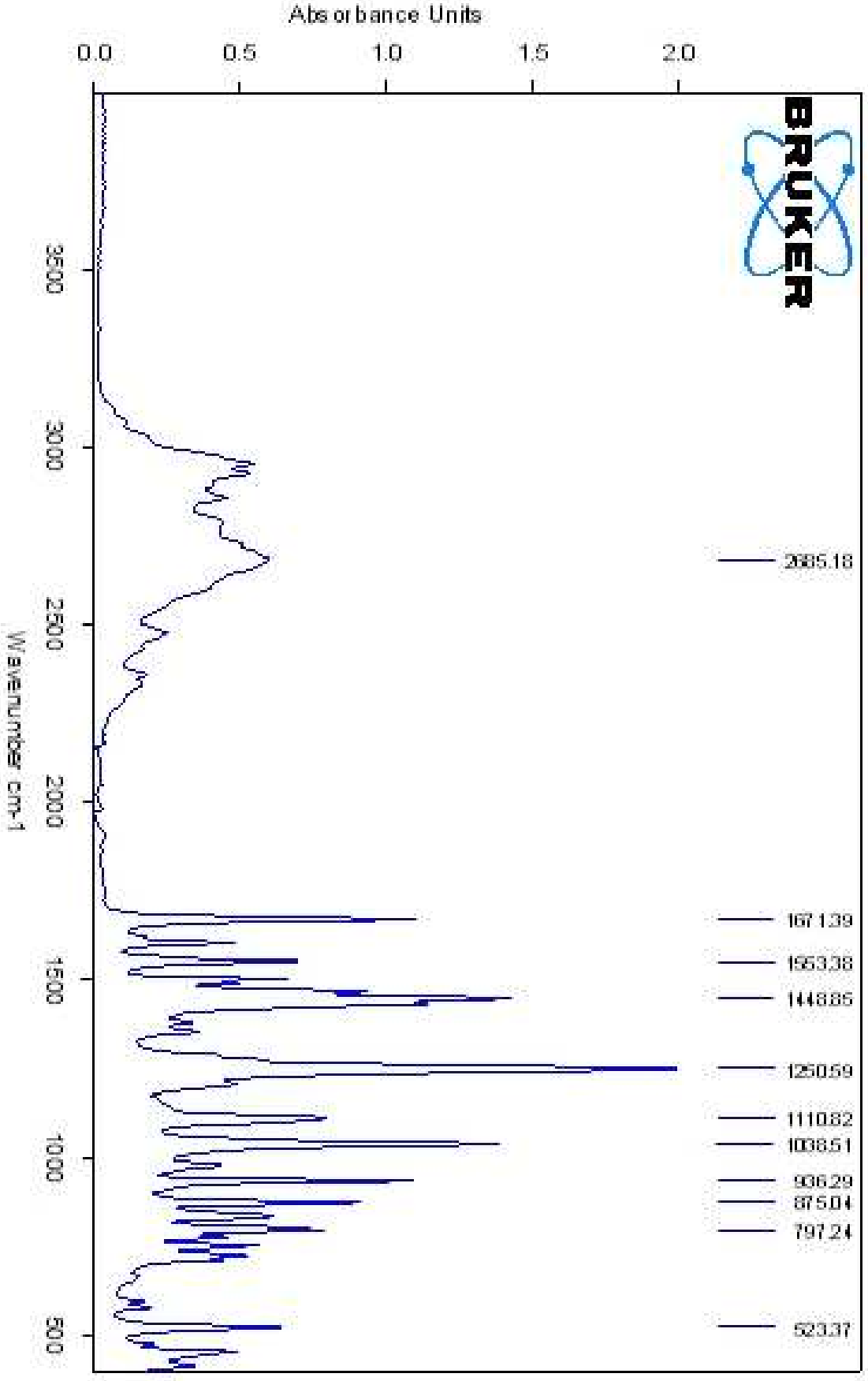
GC-MS

Rt.: 9.90 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 ℃ (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 softare.

ATR-FTIR (powder)



NMR

_N_-ethyl-_nor_-heptylone

In DMSO-d_6 solution

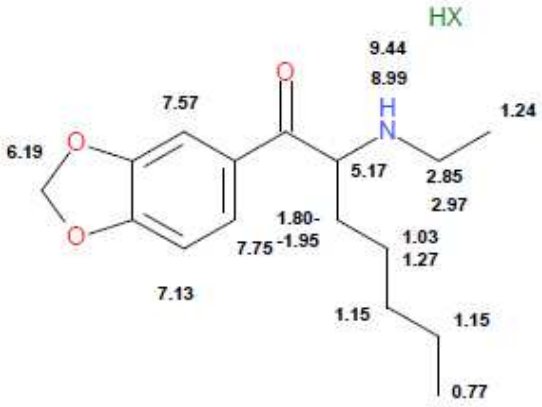
1-(1,3-benzodioxol-5-yl)-2-(ethylamino)heptan-1-one

CCCCCC(NCC)C(=O)c1ccc2OCOc2c1

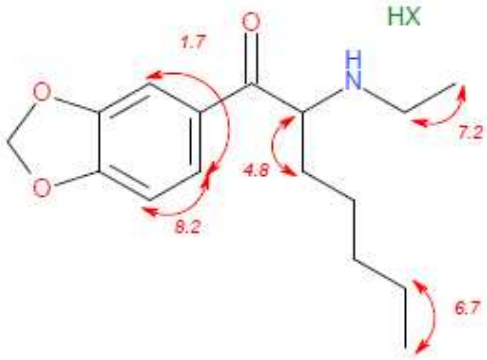
ZYFSMTZZSZKLKU-UHFFFAOYSA-N

Formula Weight: 277,35872
Exact Mass: 277,167793606
Molecular Formula: $C_{16}H_{23}NO_3$

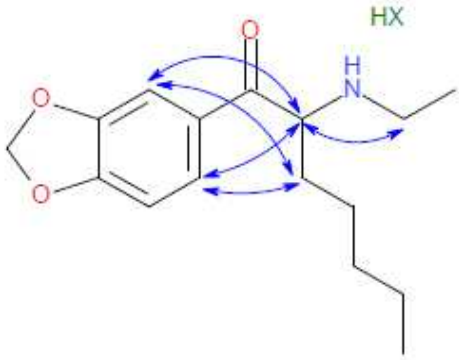
^{1}H-NMR chemical shifts δ [ppm]



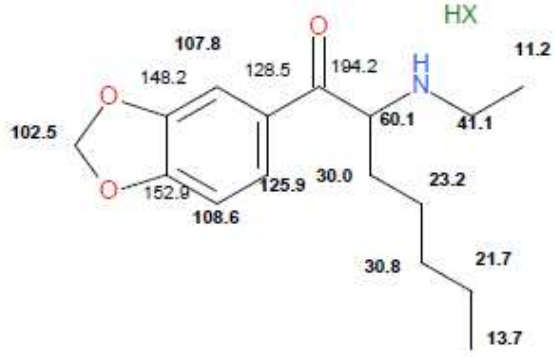
J(H,H) coupling constants [Hz]



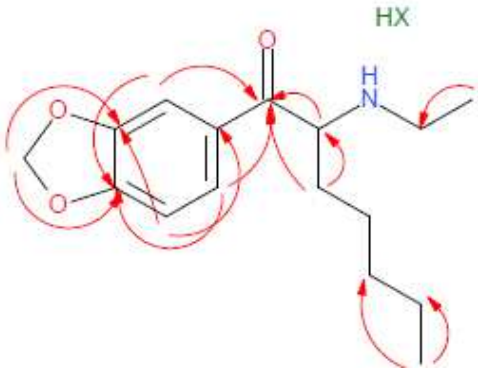
Characteristic steric proximities detected by zqs-easy-ROESY



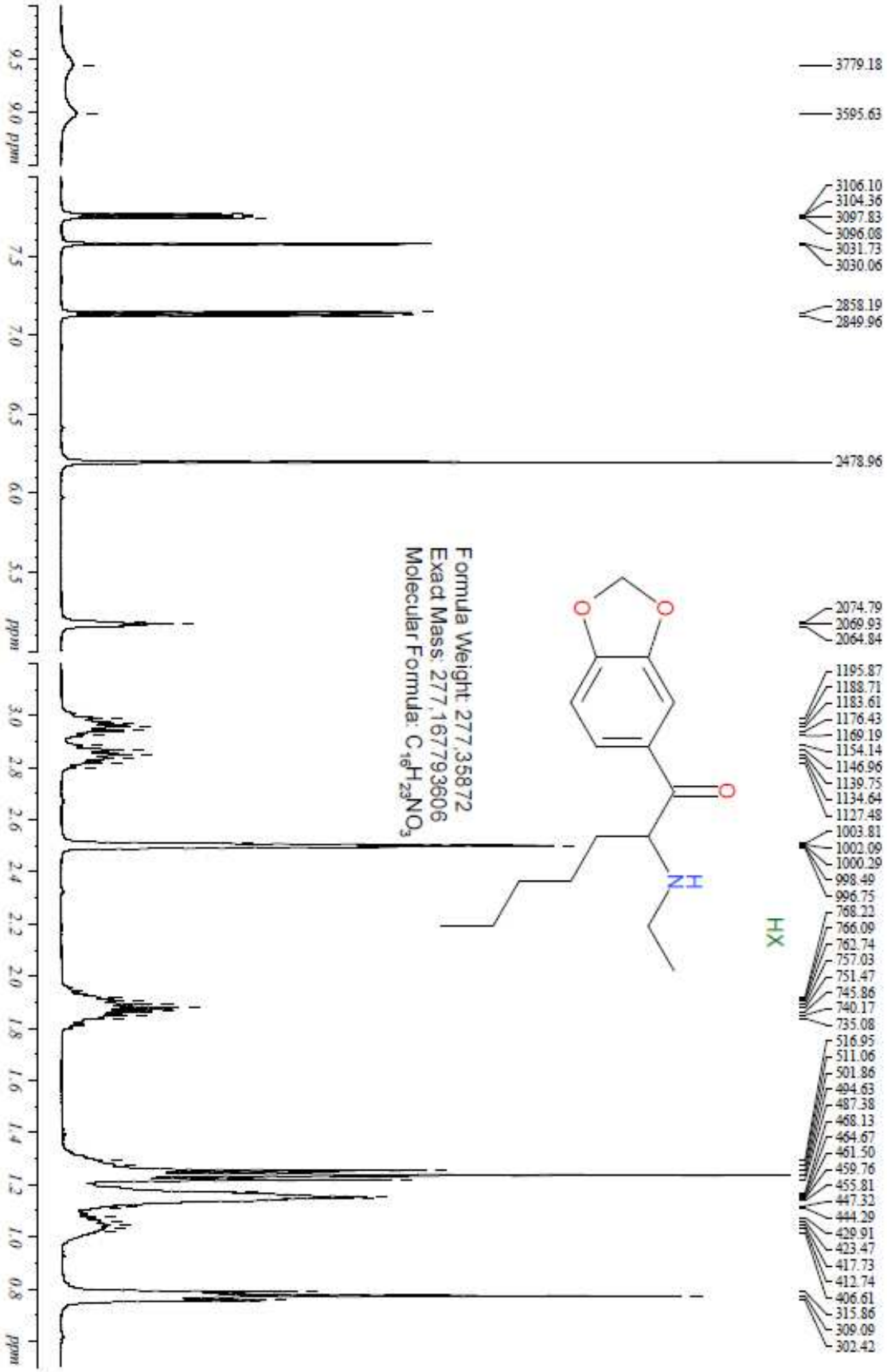
^{13}C-NMR chemical shifts δ [ppm]



Characteristic heteronucler long-range coupling detected by HMBC method H ⟶ C

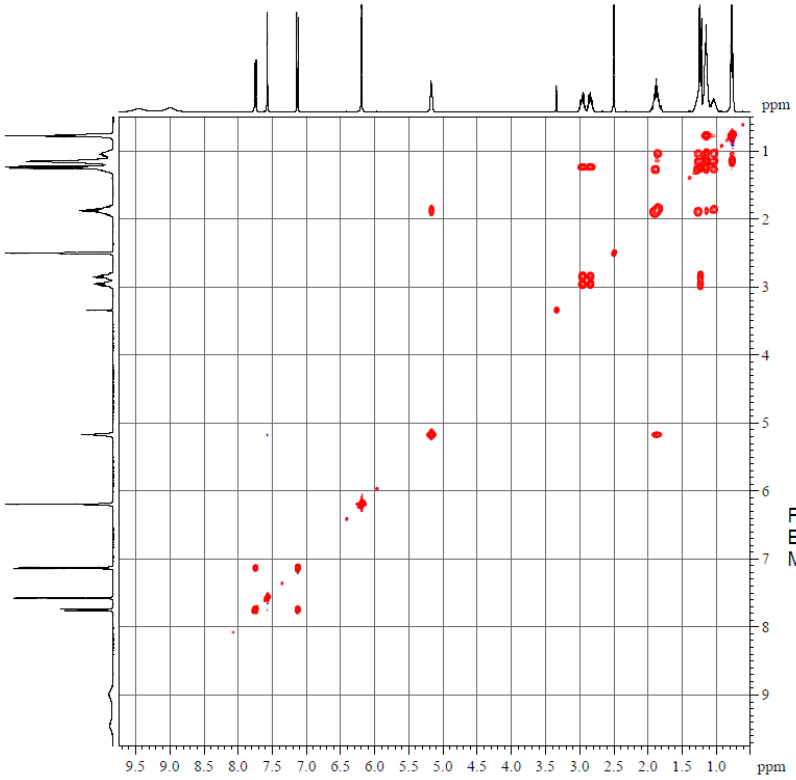


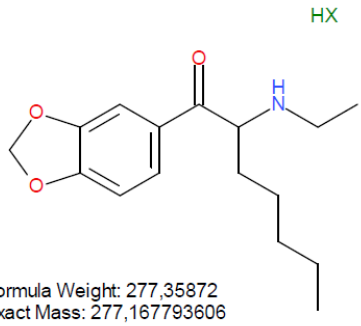
^{1}H NMR (overview and characteristic parts)



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

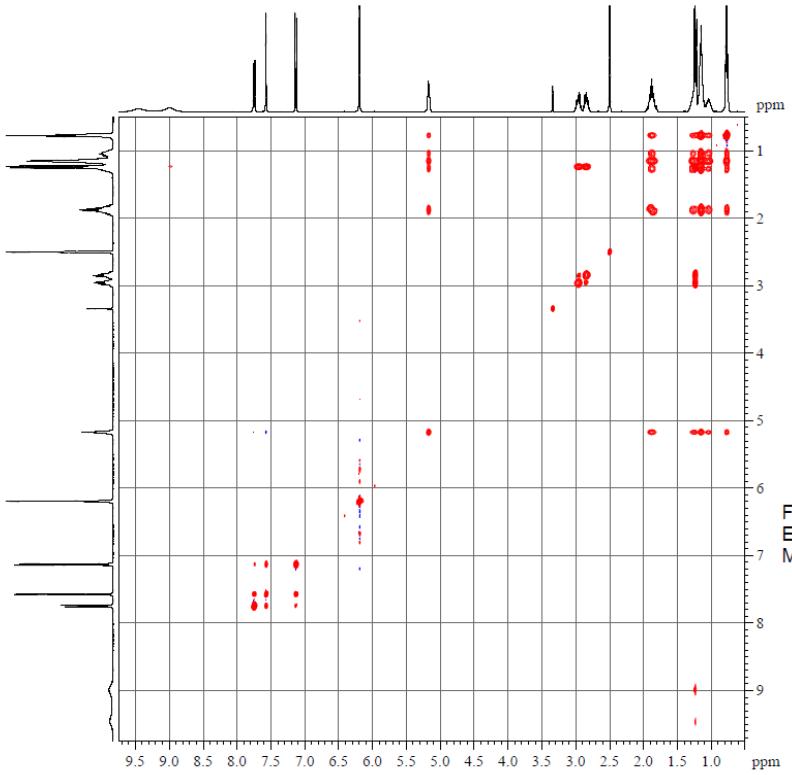
zqs-clip-COSY

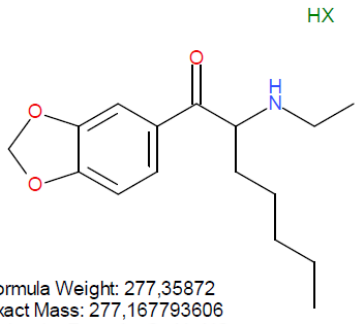




Formula Weight: 277,35872
Exact Mass: 277,167793606
Molecular Formula: $C_{16}H_{23}NO_3$

zqs-TOCSY

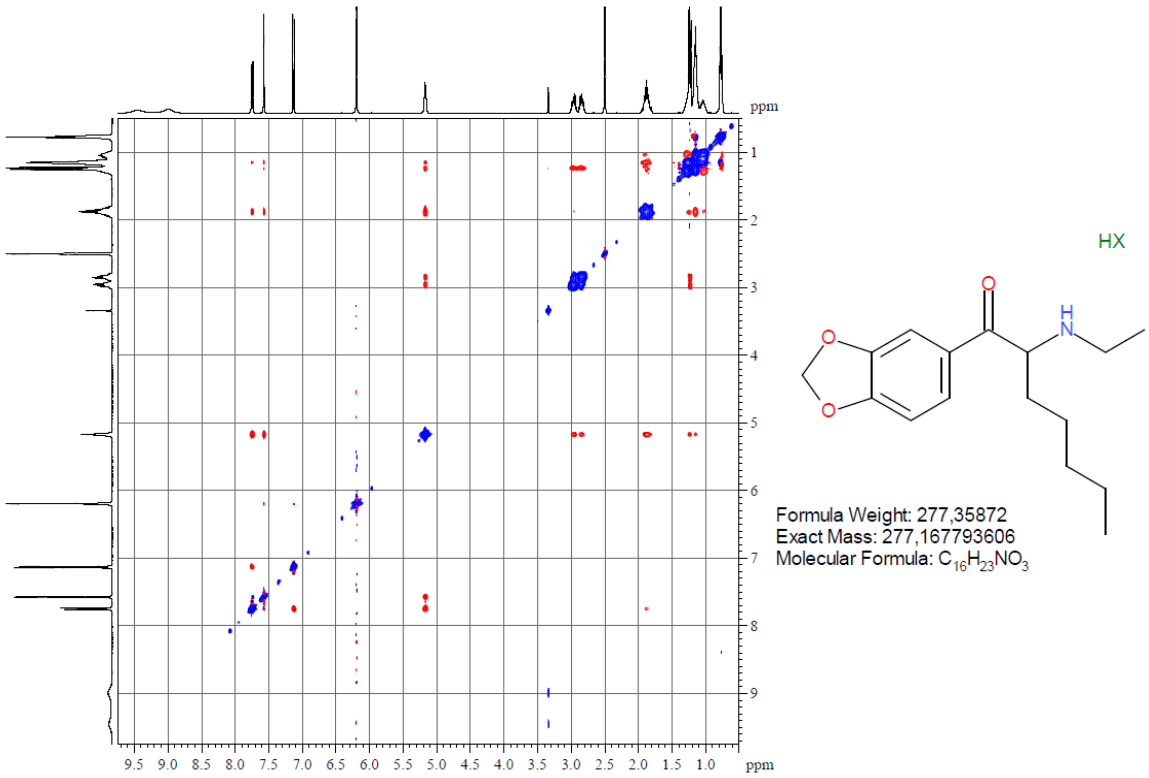




Formula Weight: 277,35872
Exact Mass: 277,167793606
Molecular Formula: $C_{16}H_{23}NO_3$

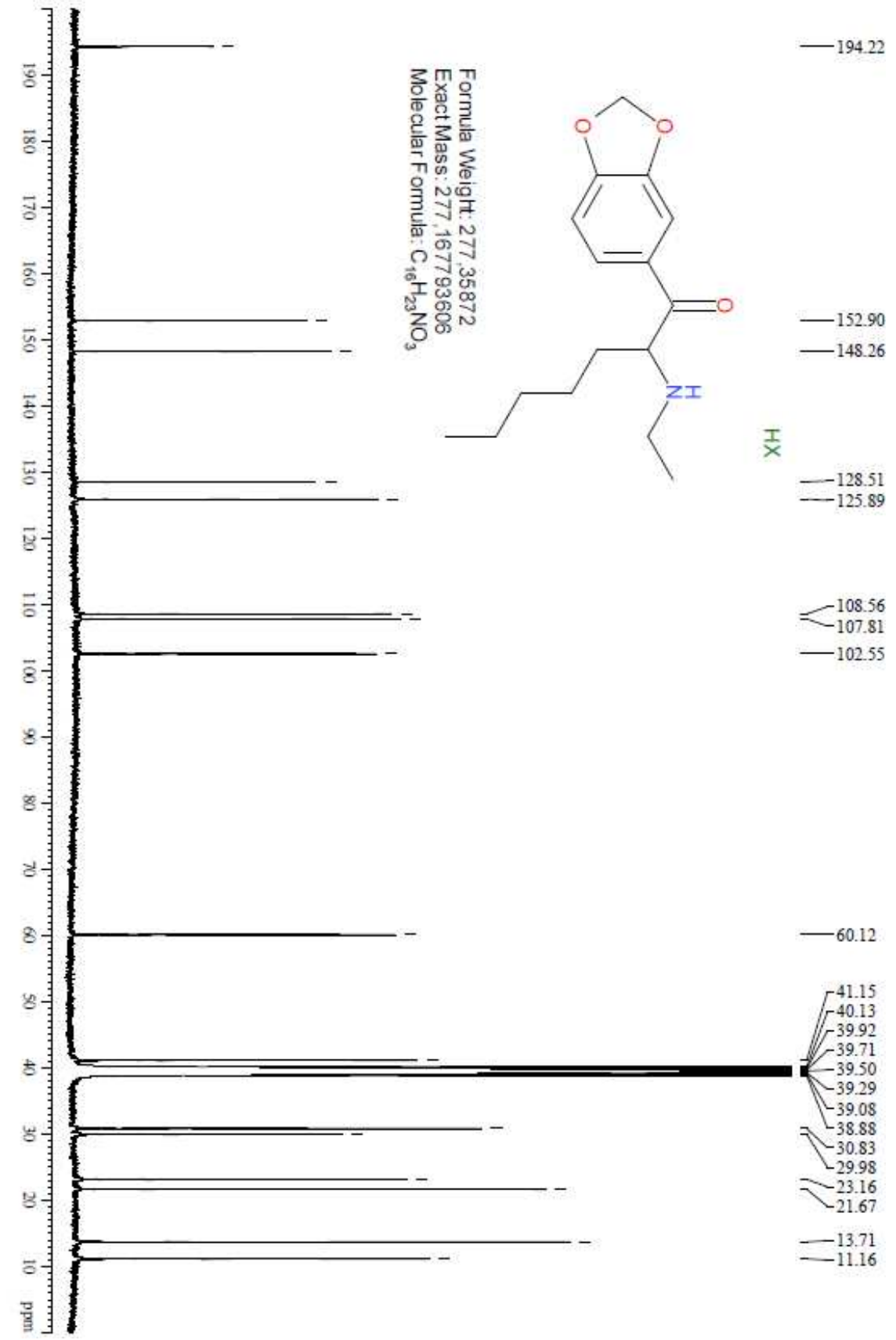
Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6

zqs-easy-ROESY



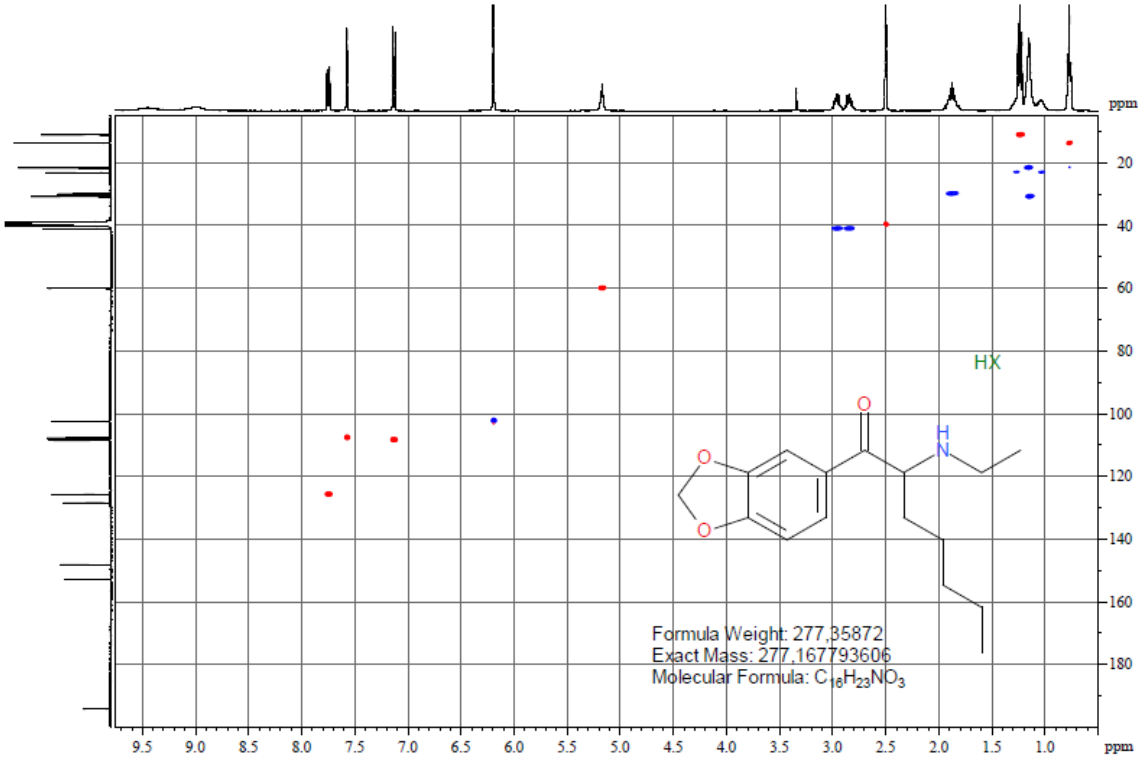
Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6

^{13}C NMR

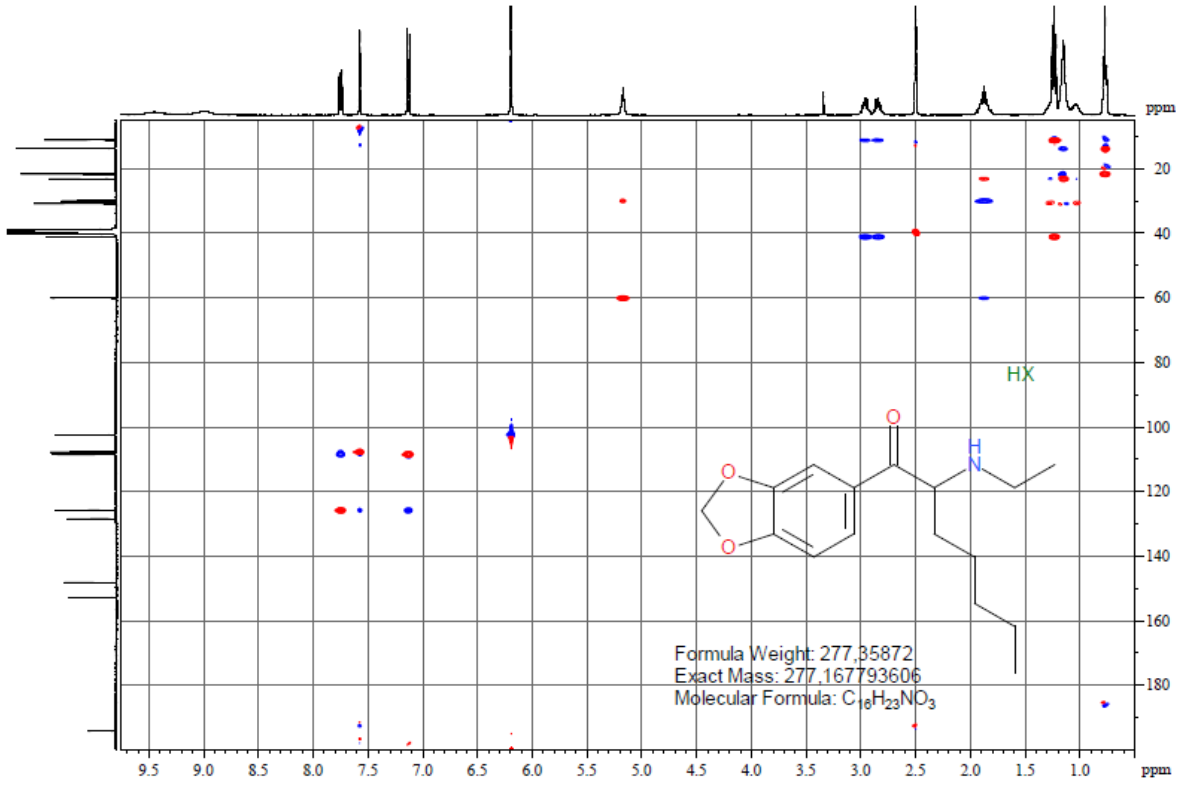


Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6

ed-HSQC

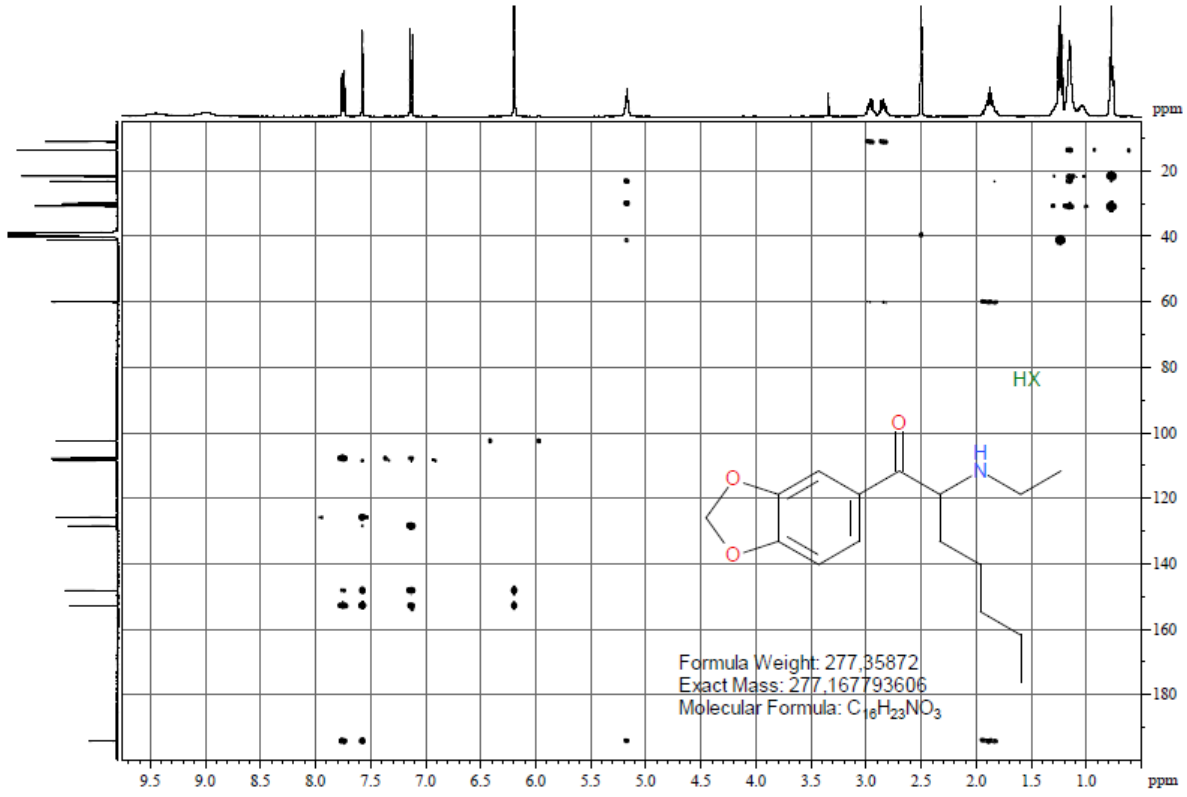


ed-HSQC-zqs-clip-COSY-ed3



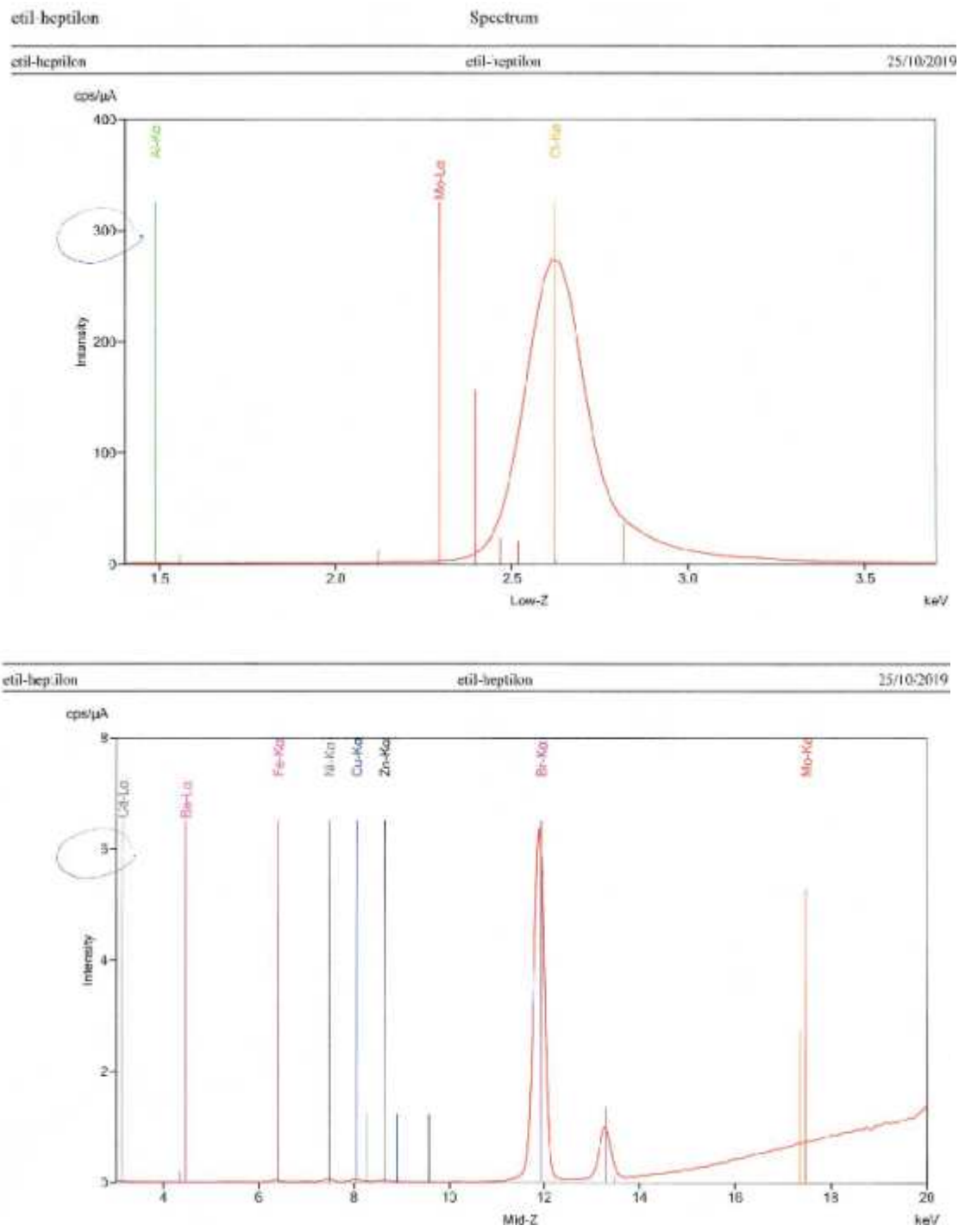
Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6

HMBC



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

XRF



Rigaku NEX QC+QuantEZ Benchtop Energy Dispersive X-rayFluorescence (EDXRF) spectrometer; measured at room temperature under He; N-ethyl-nor-heptylone is mainly in chloride salted form and slightly in bromide from.