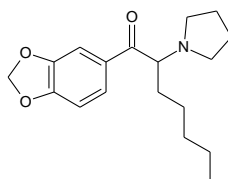


## MDPEP

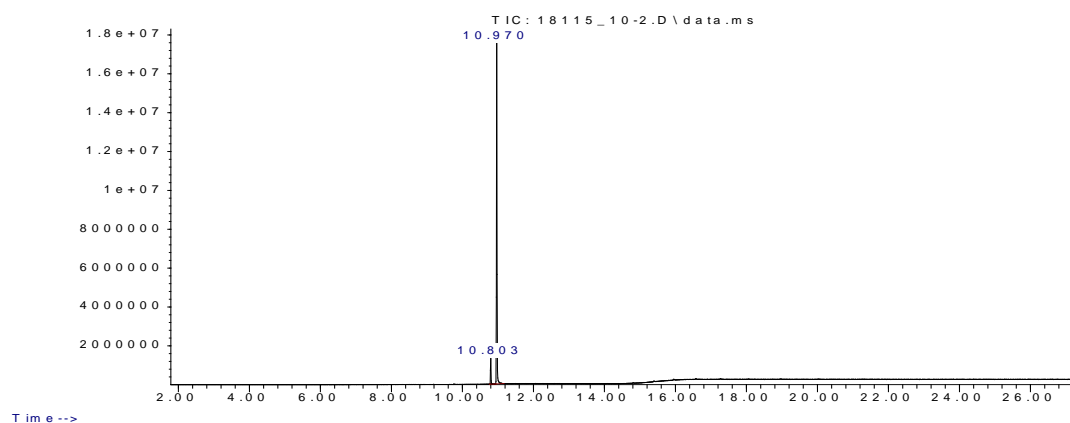


1-(1,3-benzodioxol-5-yl)-2-pyrrolidin-1-yl-heptan-1-one

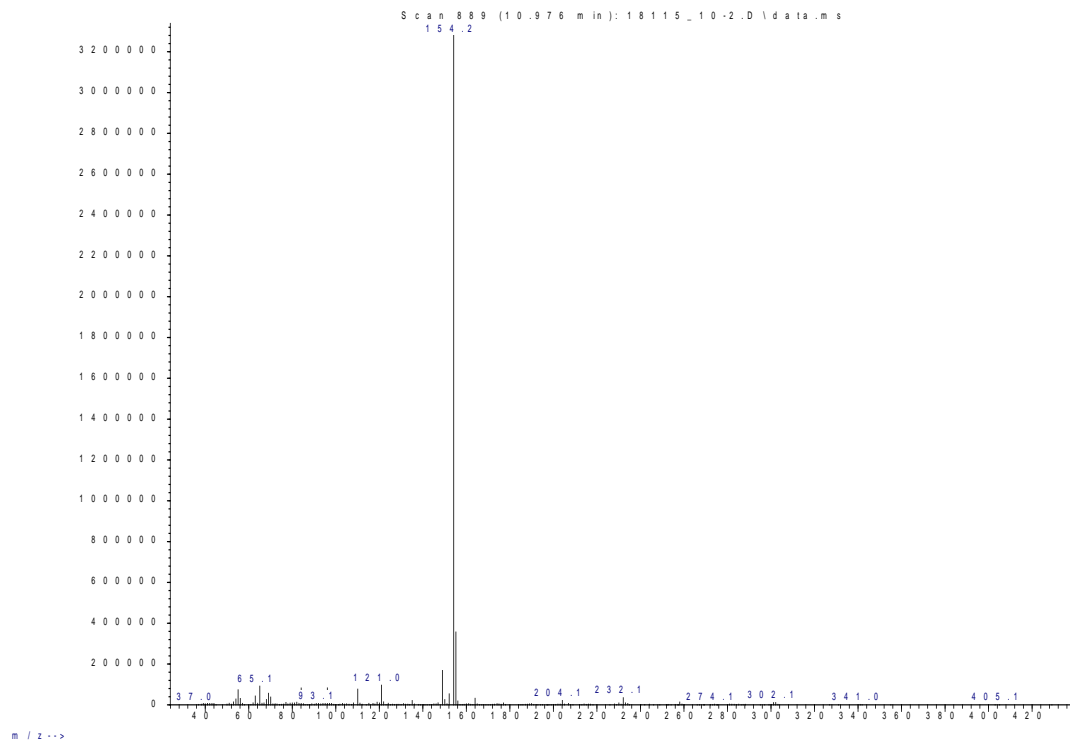
## GC-MS

Rt.: 10.97 min

Abundance

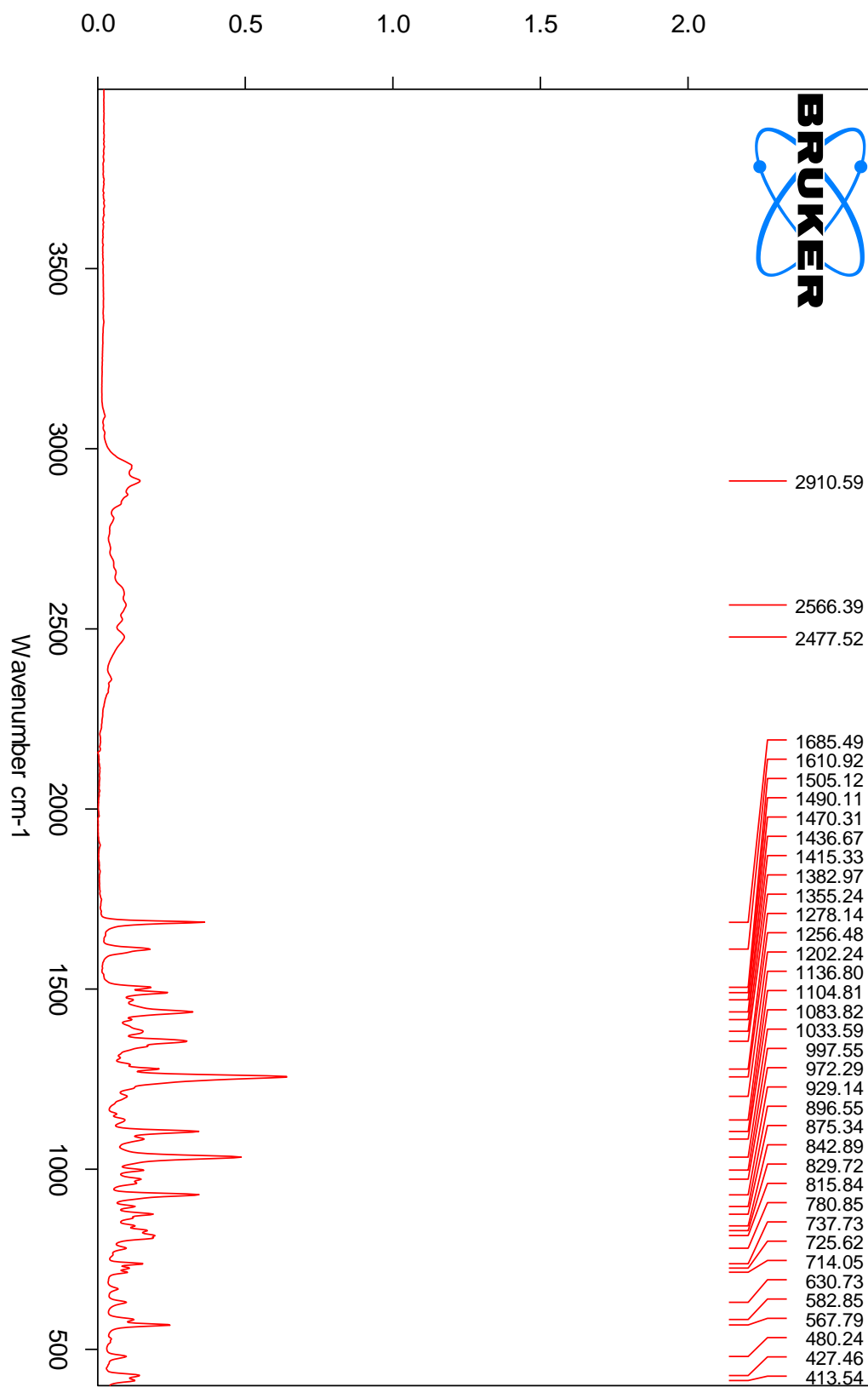


Abundance



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 (powder)

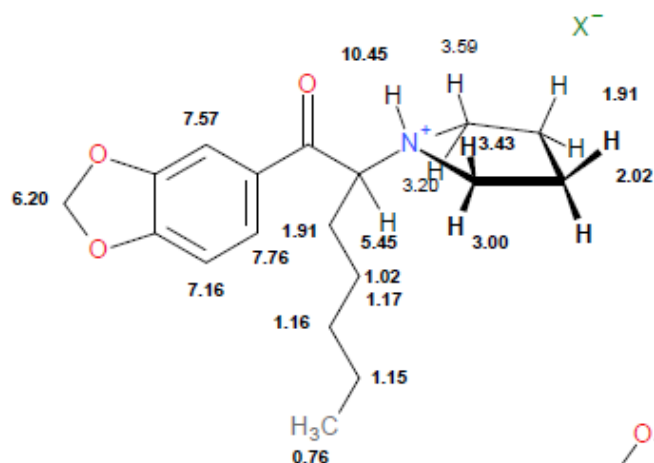


# NMR

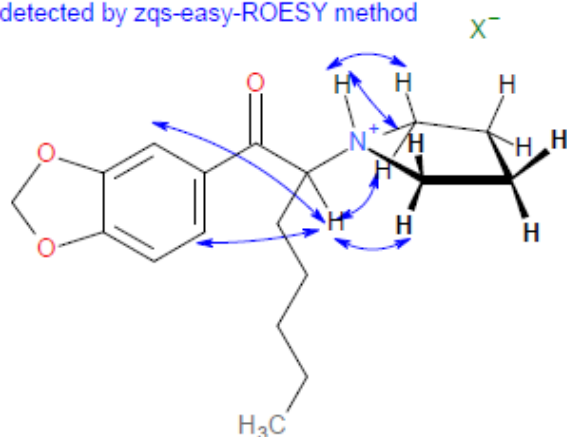
## MDPEP 3,4-methylenedioxy-PV8

in DMSO- $d_6$  solution

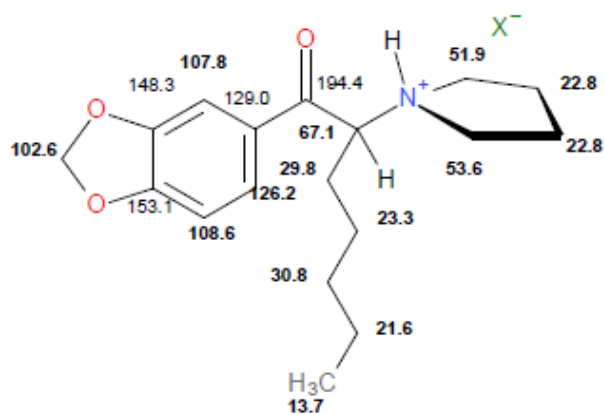
$^1\text{H}$ -NMR chemical shifts  $\delta$  [ppm]



Characteristic  $^1\text{H}/^1\text{H}$  steric proximities detected by zqs-easy-ROESY method



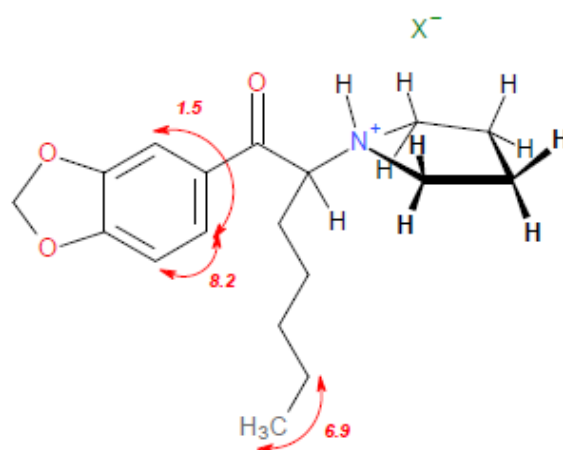
$^{13}\text{C}$ -NMR chemical shifts  $\delta$  [ppm]



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

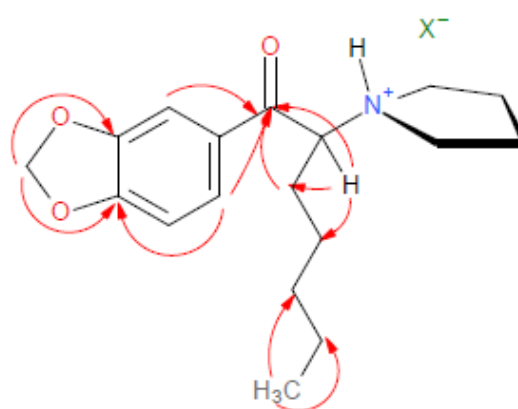
$\text{X}^-$

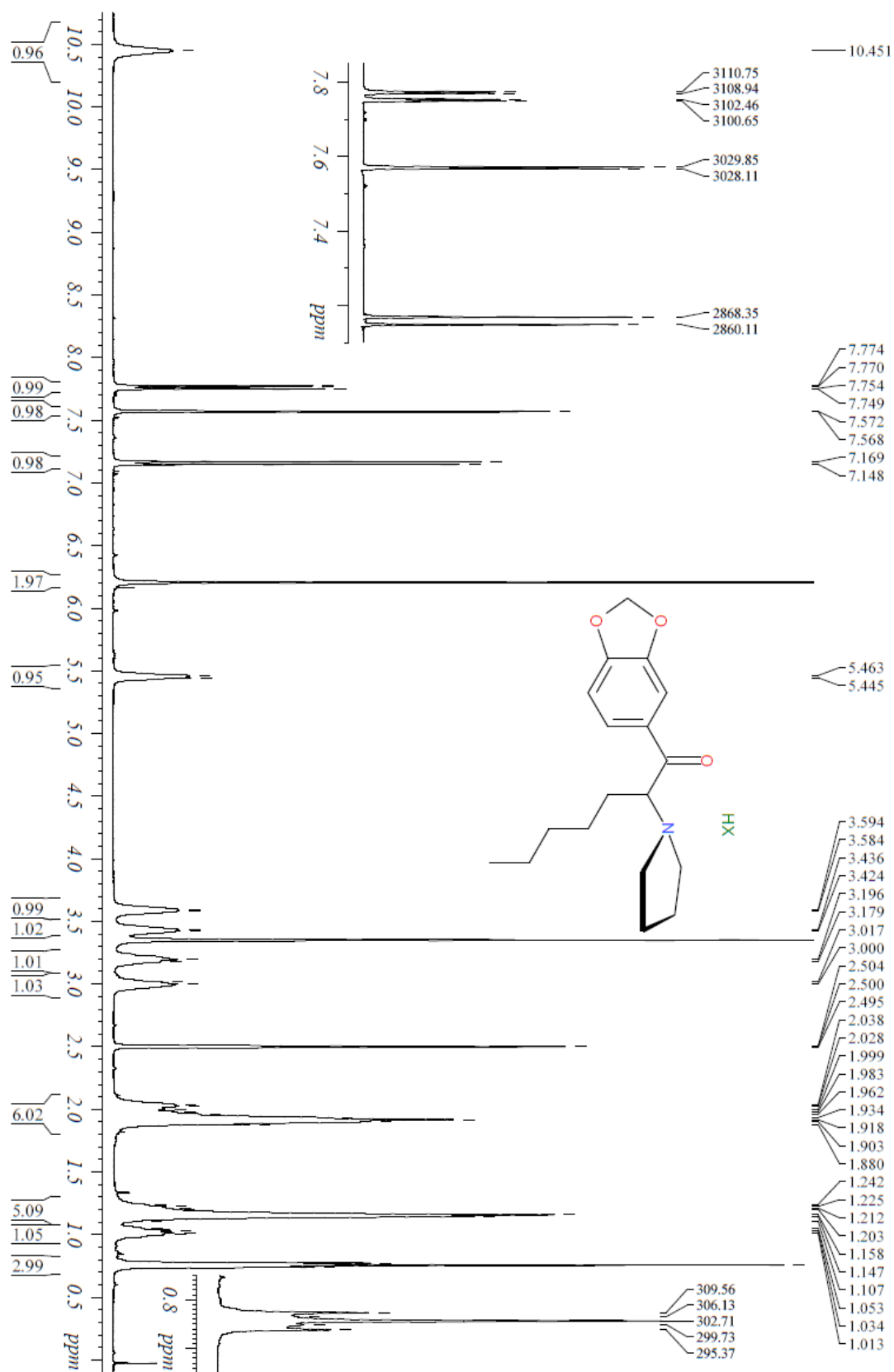
$^1\text{H}$ - $^1\text{H}$  coupling constants  $J$  [Hz]

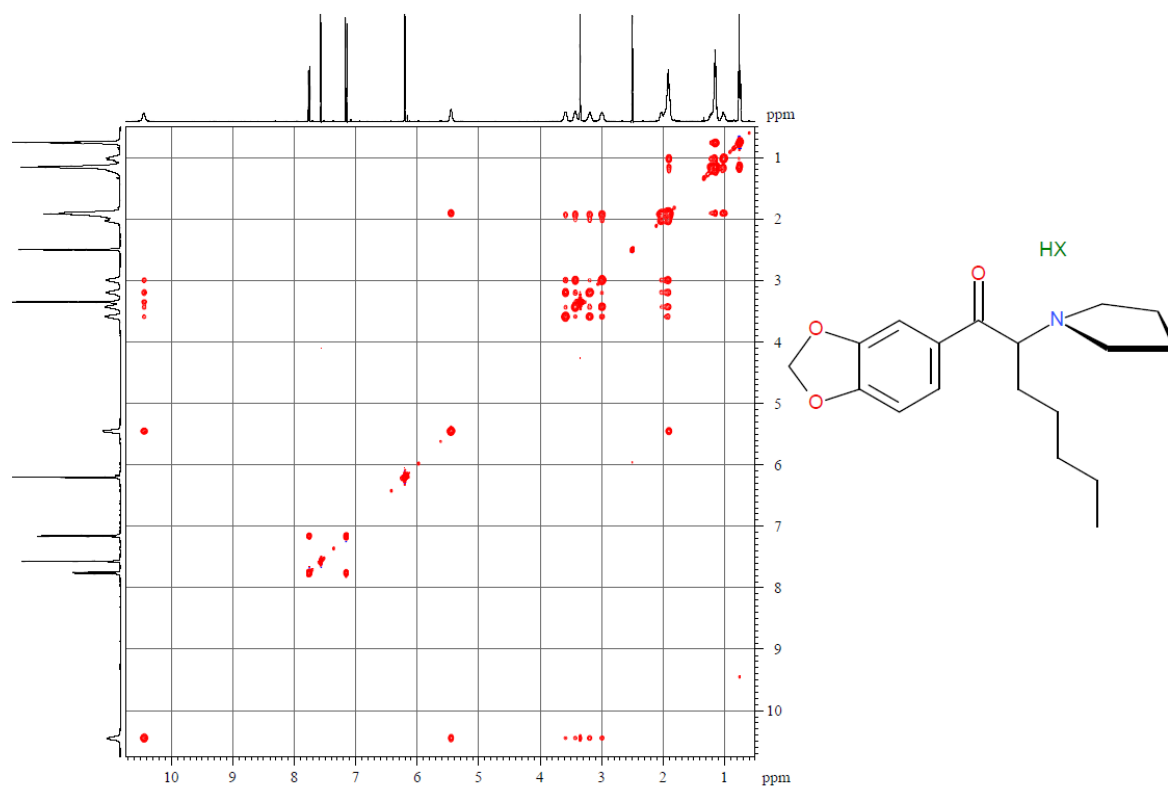
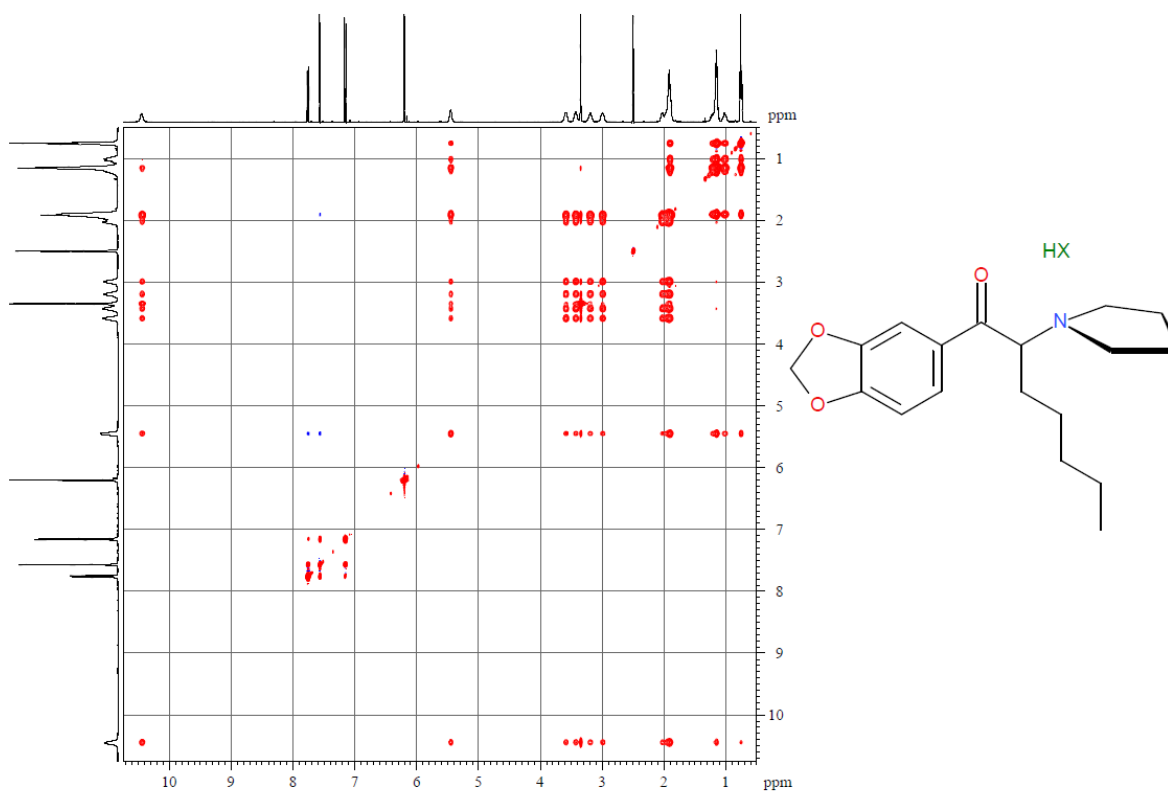


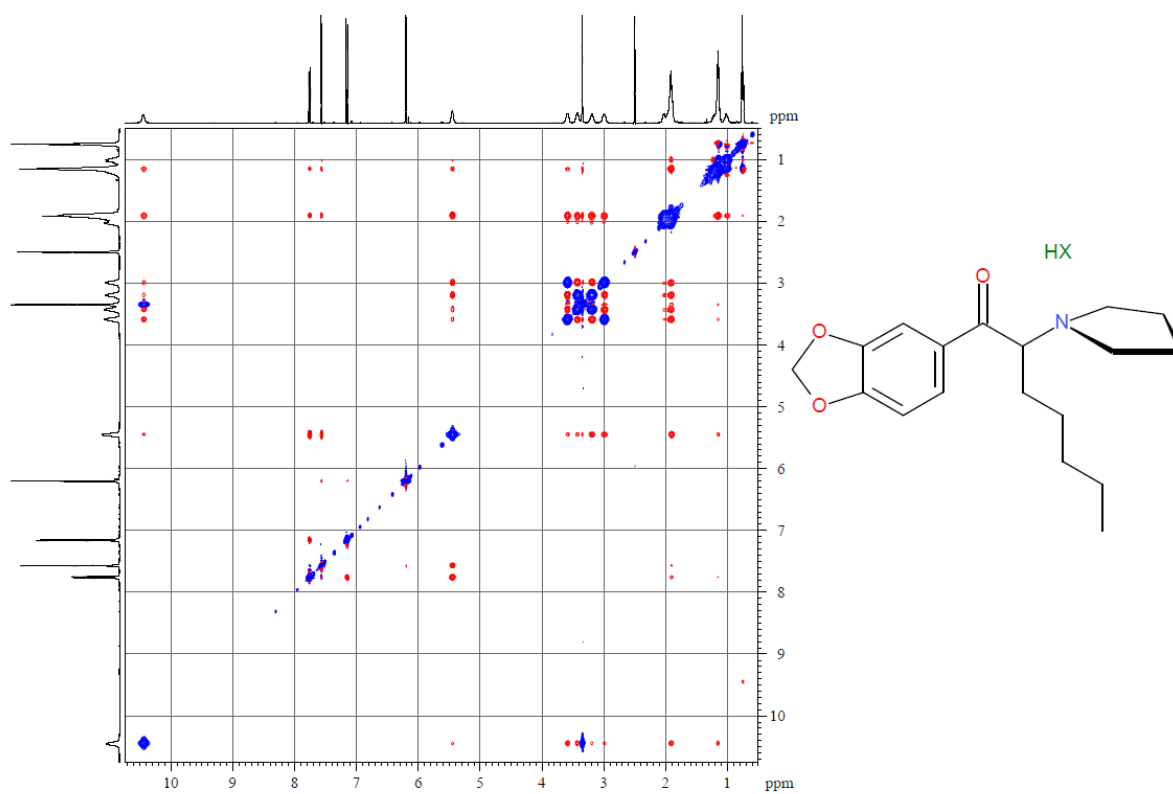
Characteristic heteronuclear long-range couplings detected by HMBC method

$\text{H} \rightarrow \text{C}$

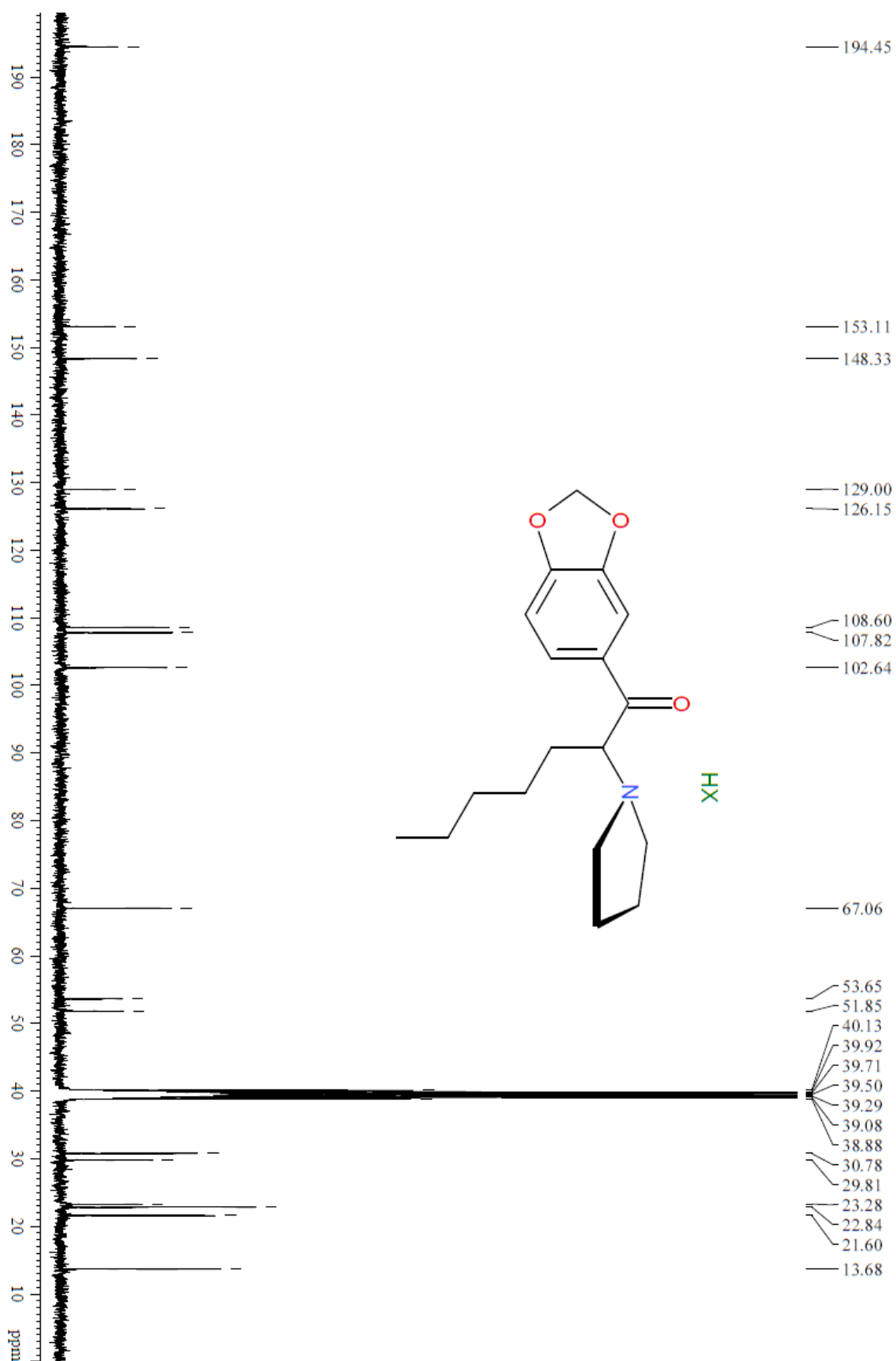


**$^1\text{H}$  NMR (overview and characteristic parts)**Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent:  $\text{DMSO-d}_6$

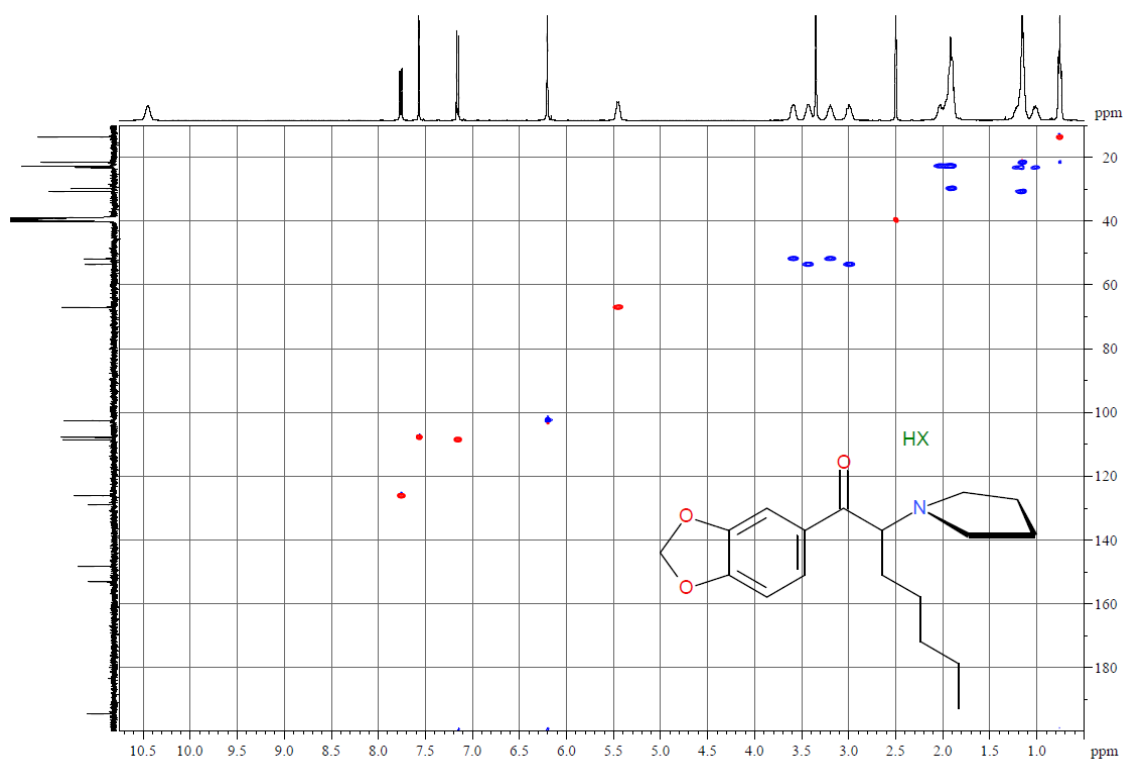
**zqs-clip-COSY****zqs-TOCSY**Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d<sub>6</sub>

**zqs-easy-ROESY**

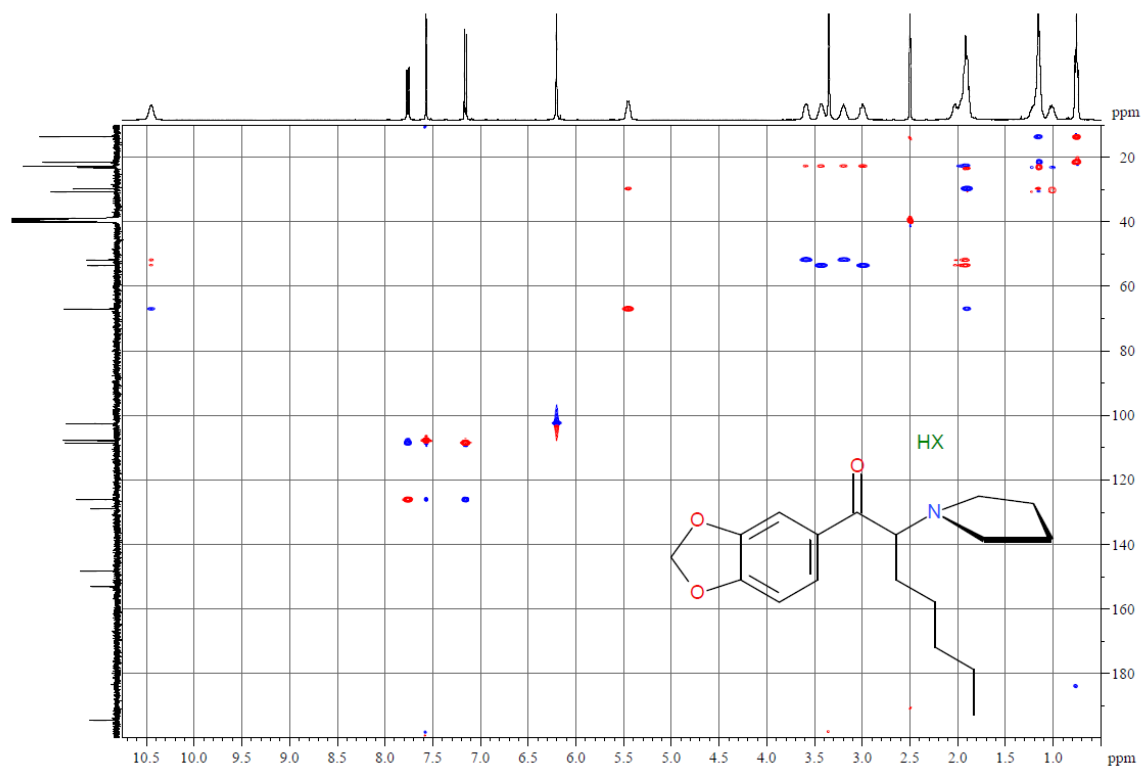
Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d<sub>6</sub>

**$^{13}\text{C}$  NMR**Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent:  $\text{DMSO-d}_6$

## ed-HSQC

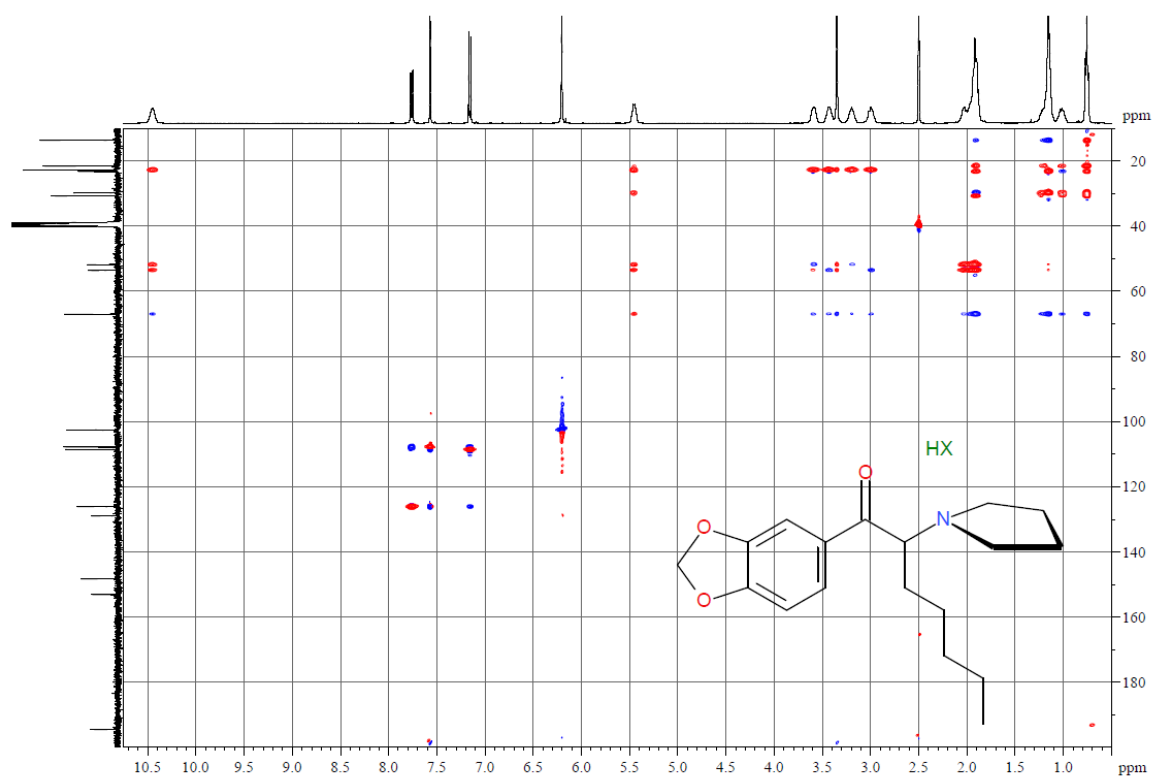


## ed-HSQC-zqs-clip-COSY-ed3

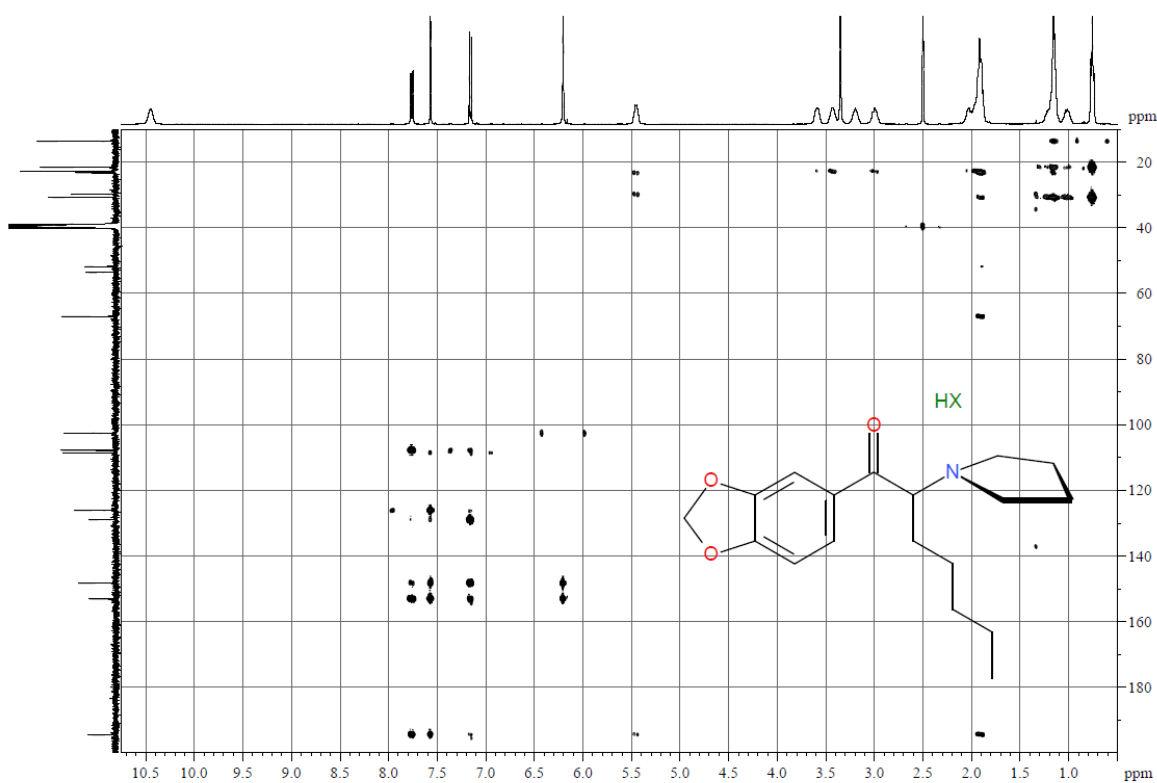
Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d<sub>6</sub>



## ed-HSQC-zqs-TOCSY-ed3



## HMBC

Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d<sub>6</sub>