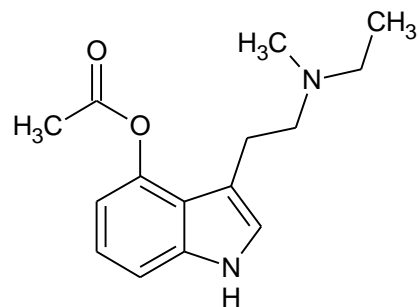


4-AcO-MET

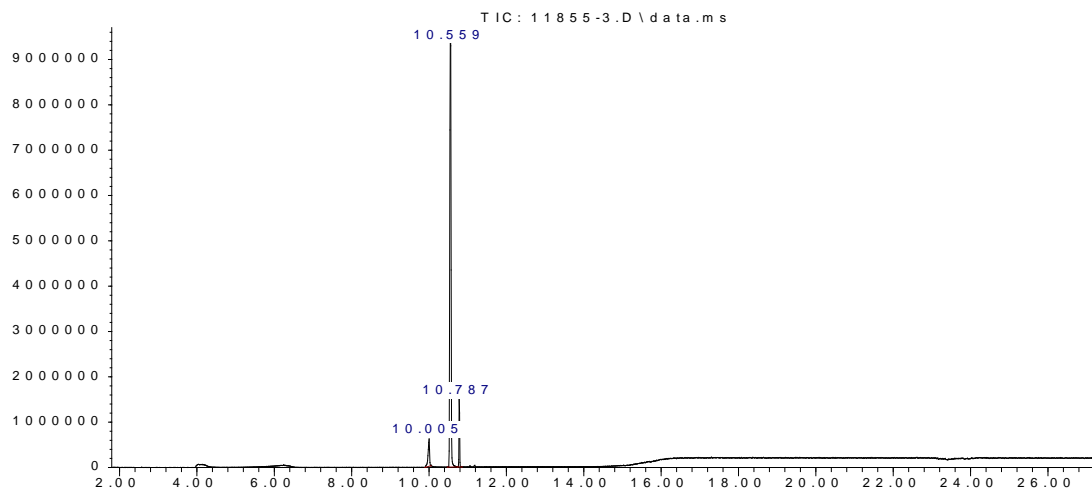


4-acetoxy-N-methyl-N-ethyltryptamine

GC-MS

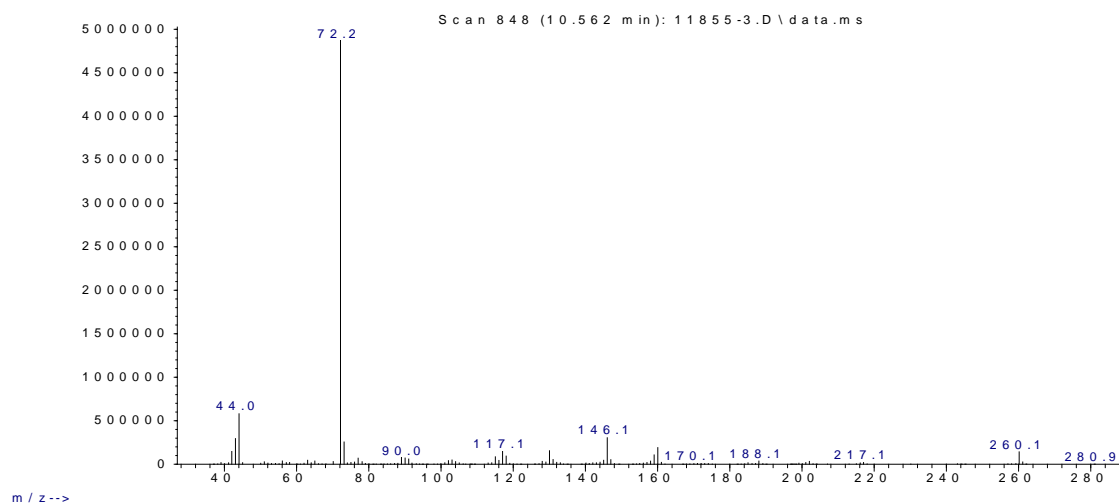
Rt.: 10.56 min

Abundance



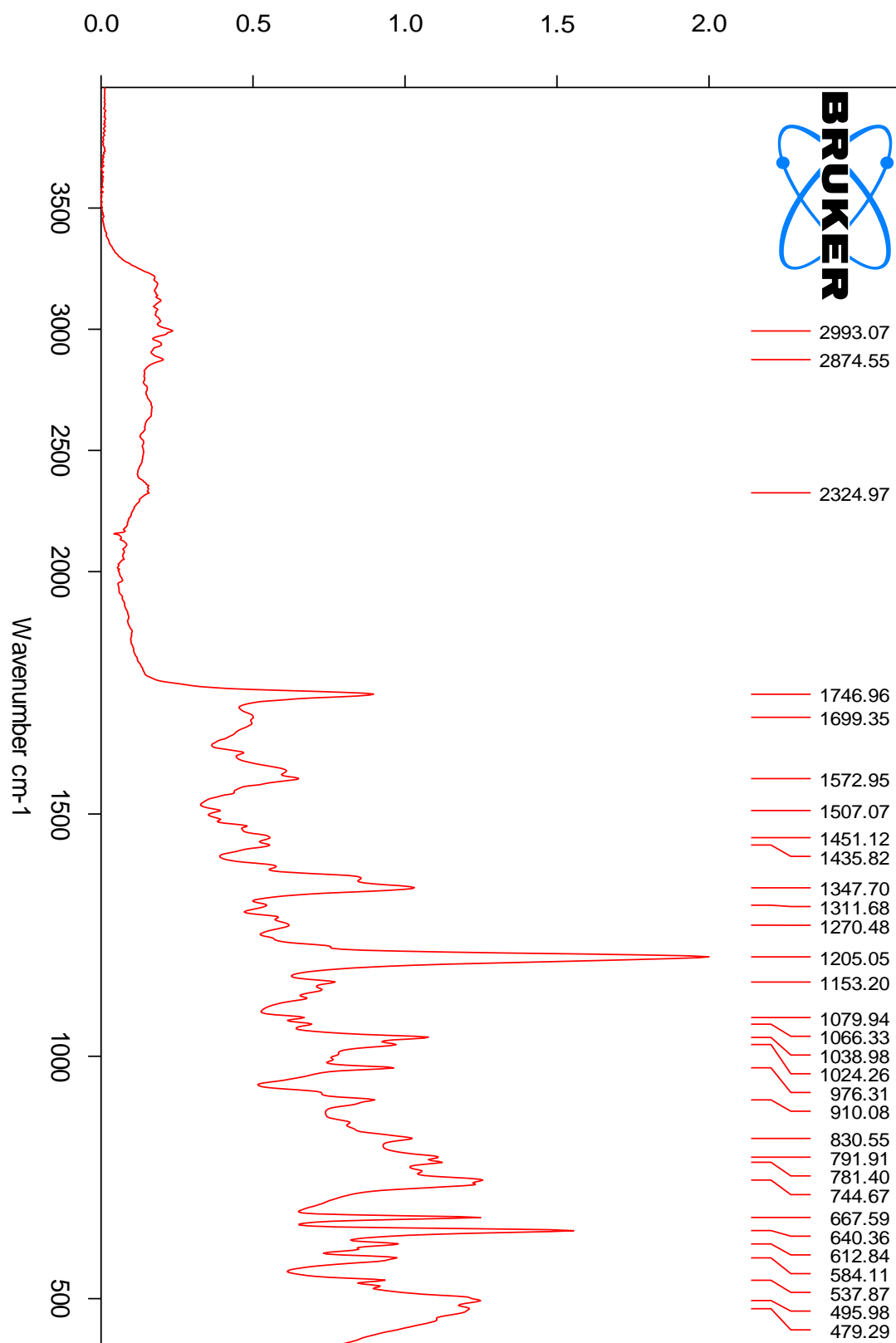
Time-->

Abundance



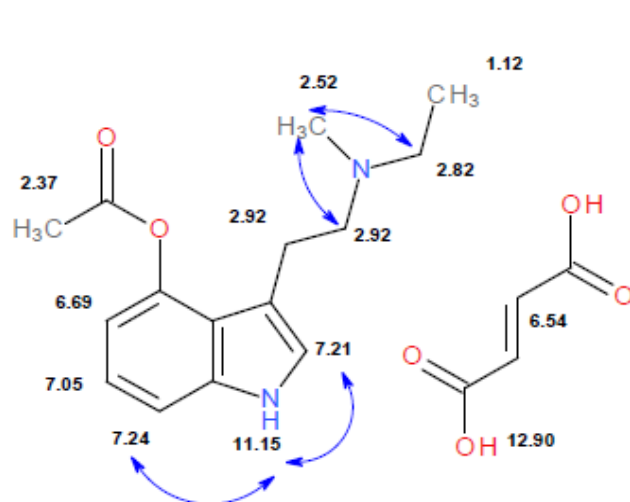
m/z-->

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.

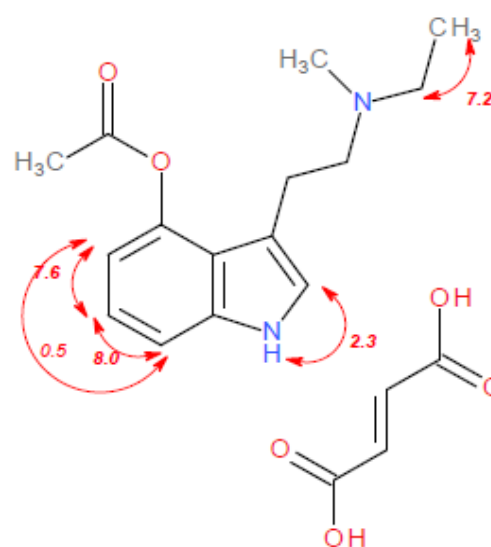
ATR-FTIR (powder, 4-AcO-MET.fumarate)

NMR

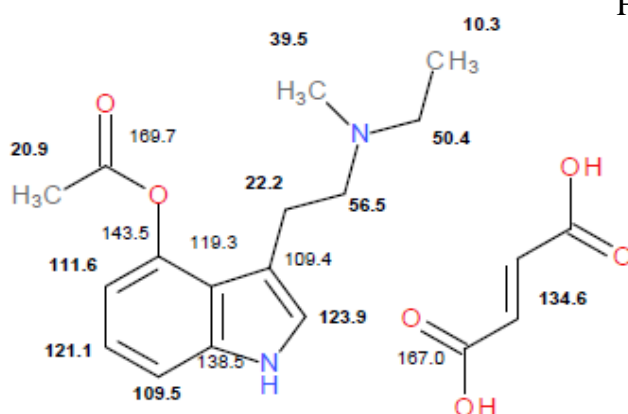
$^1\text{H-NMR}$ chemical shift δ [ppm]
Characteristic steric proximities



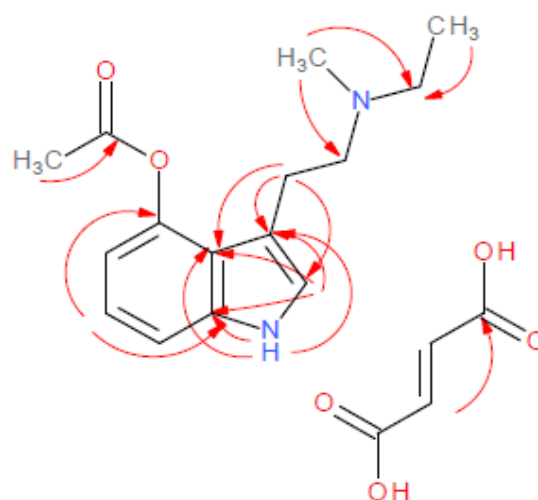
$J(\text{H,H})$ coupling constants [Hz]

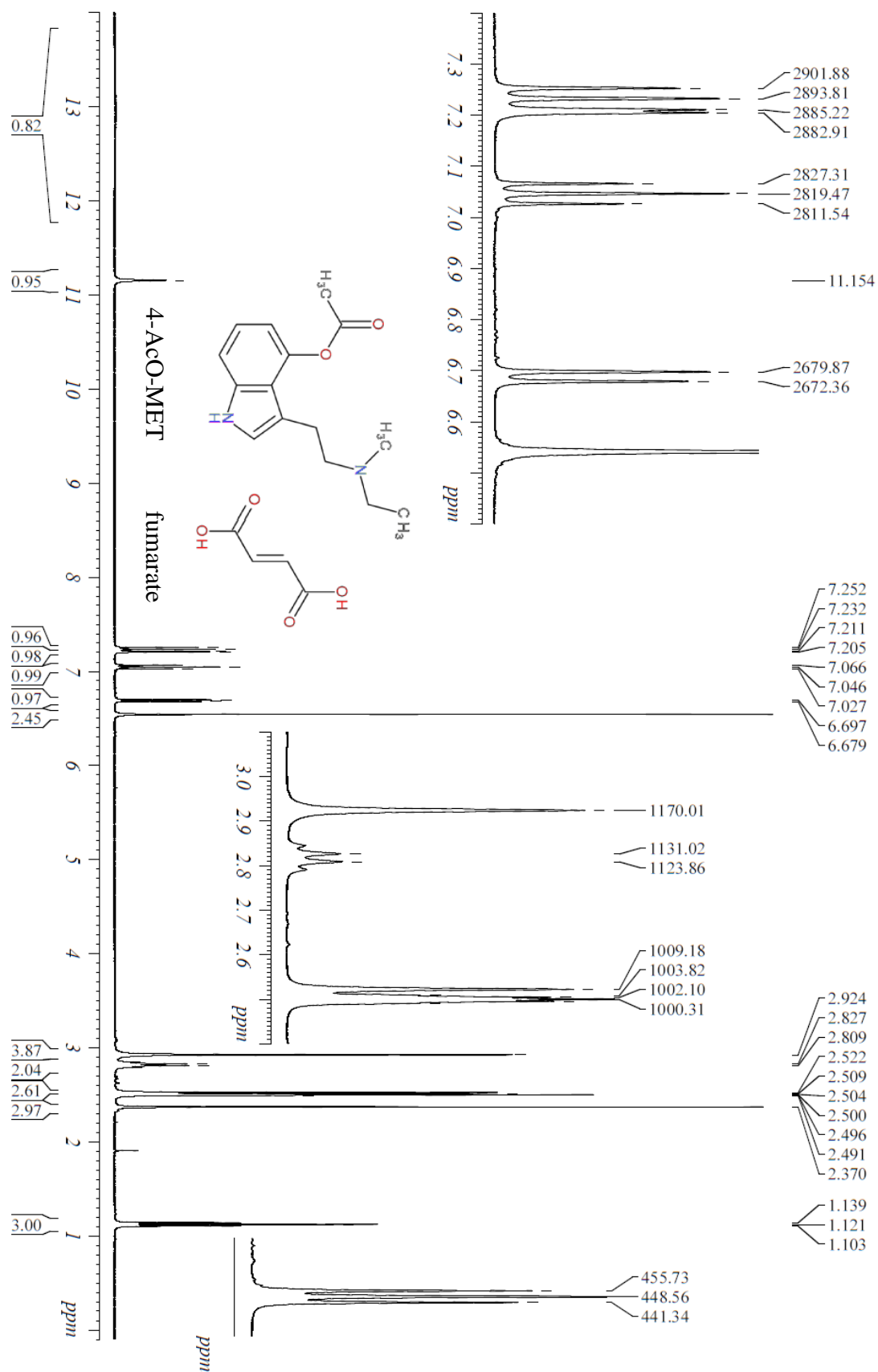


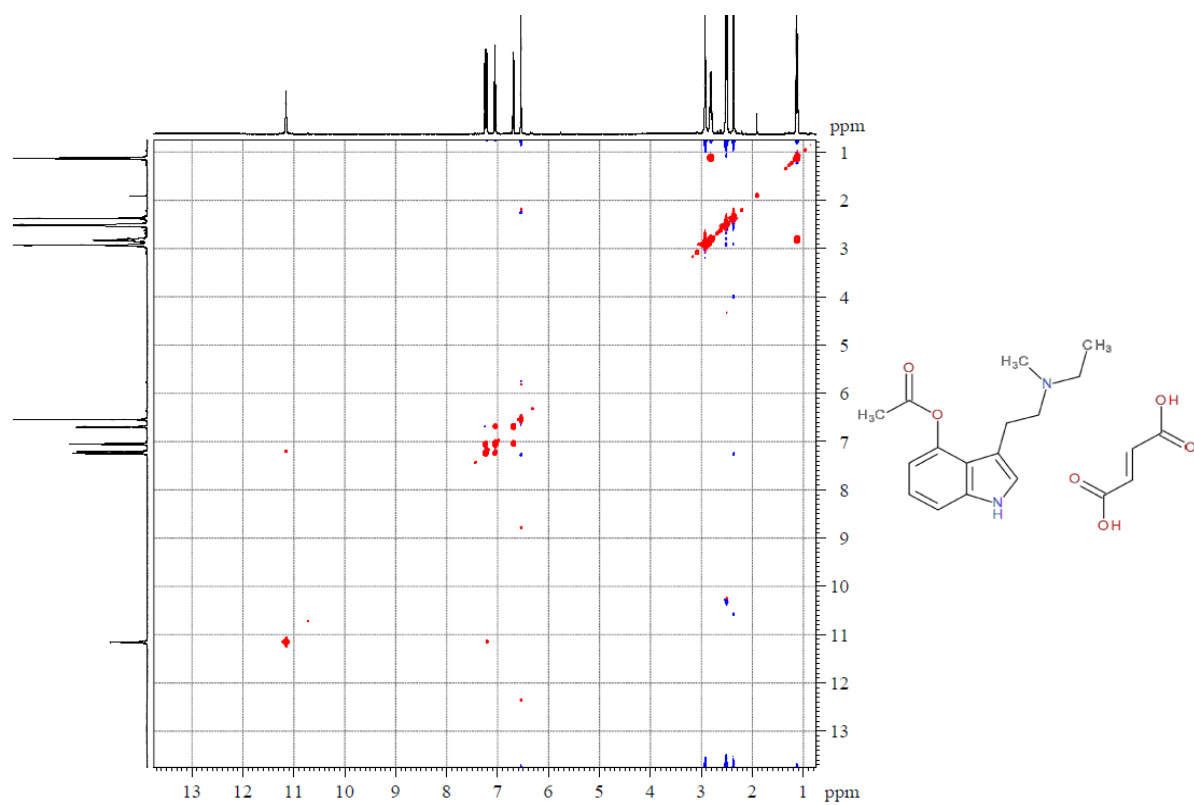
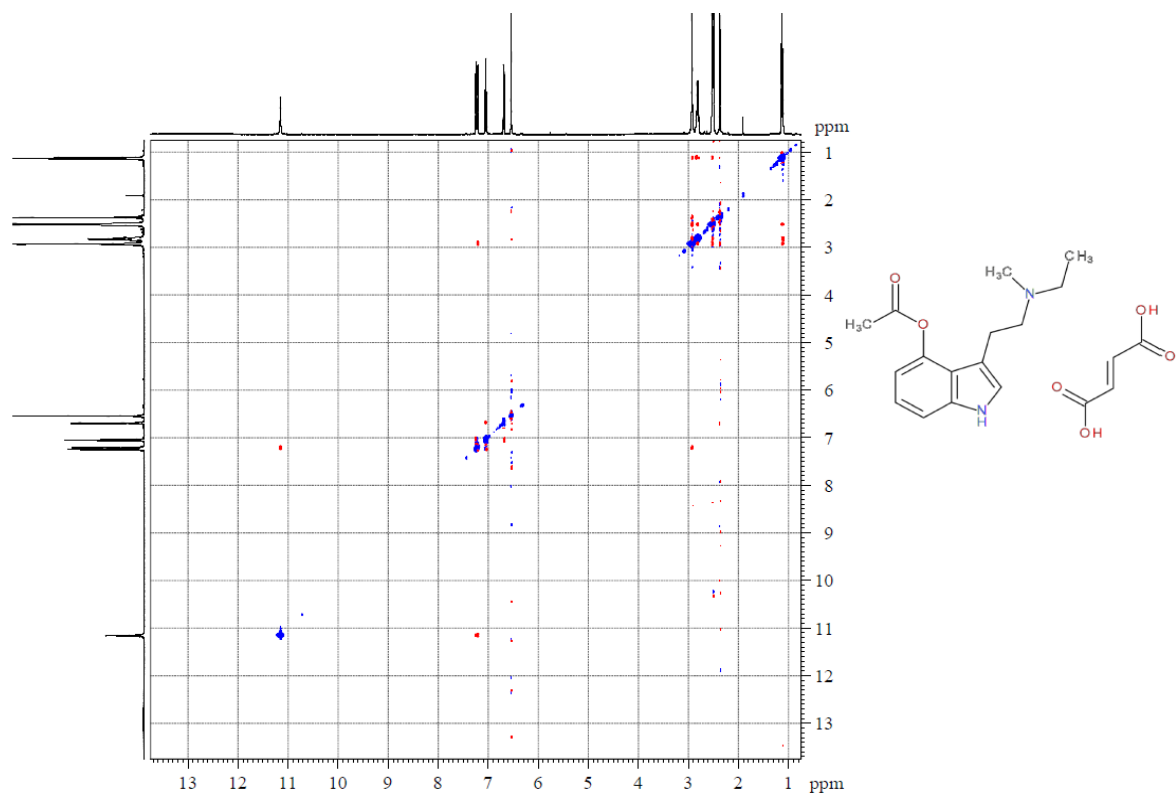
$^{13}\text{C-NMR}$ chemical shift δ [ppm]

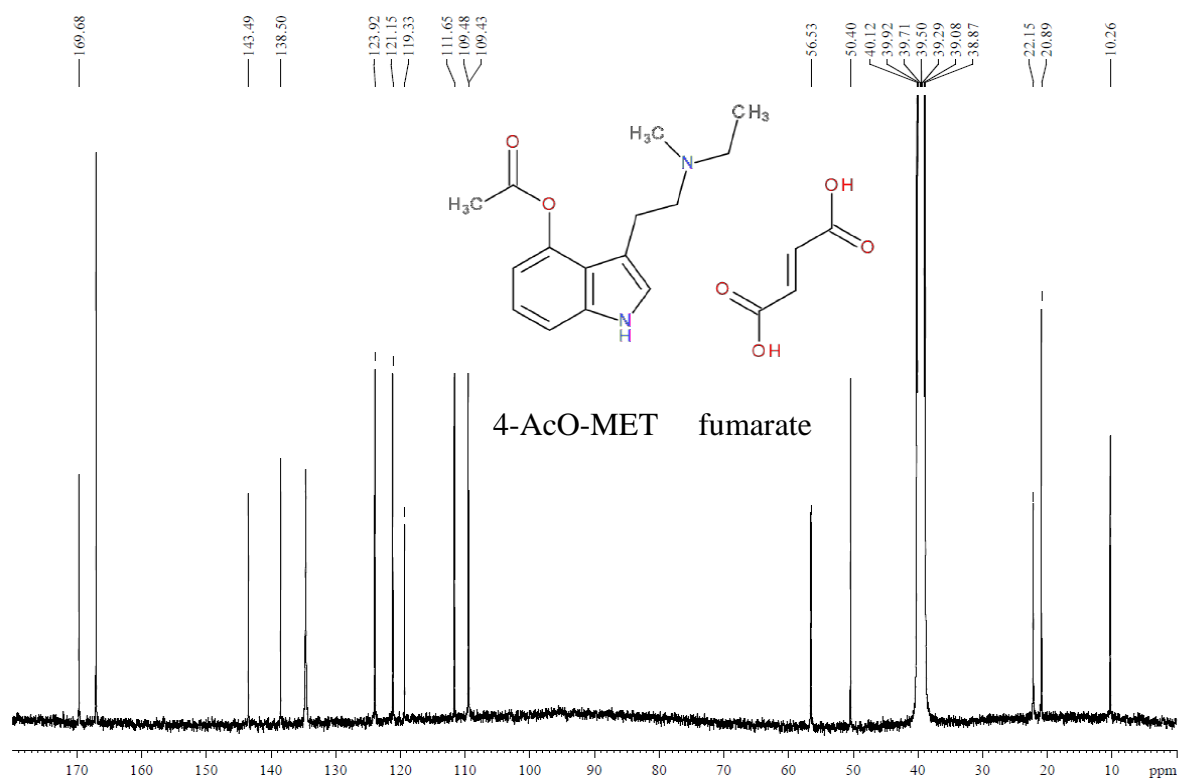
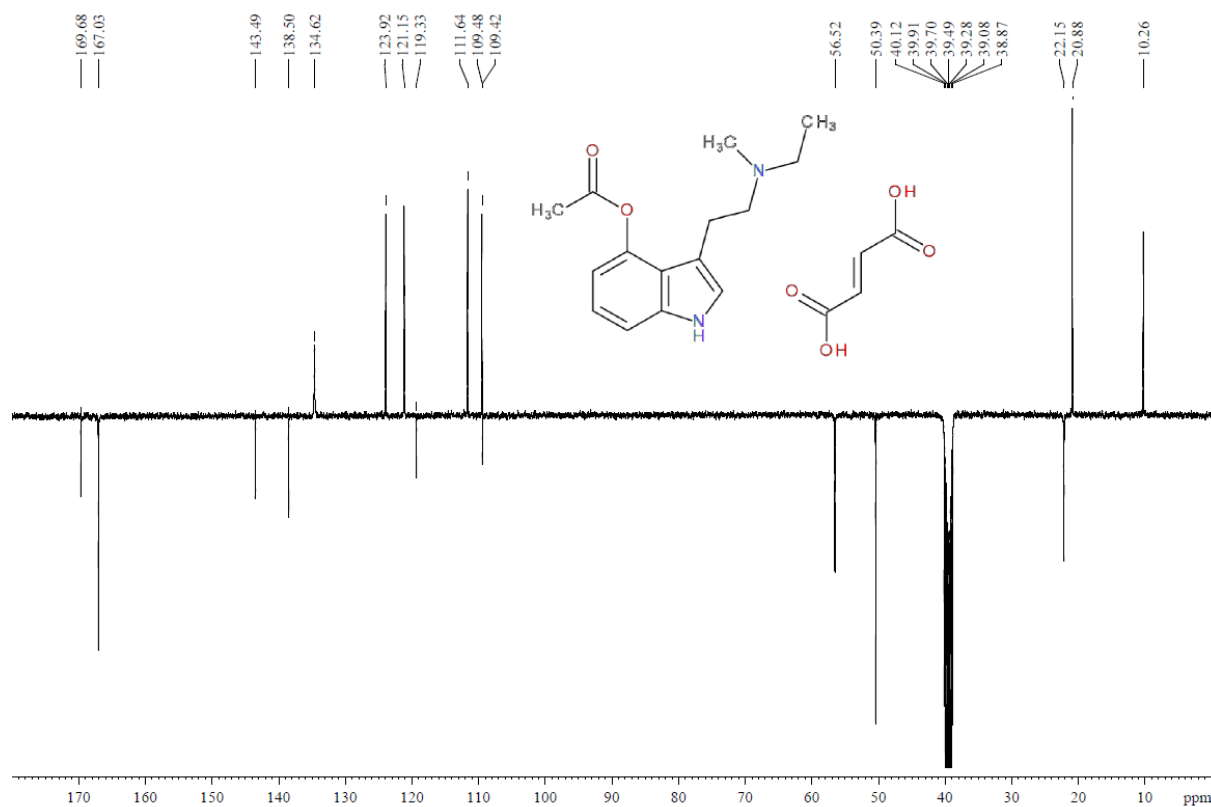


Characteristic heteronuclear long-range coupling by HMBC method
 $\text{H} \rightarrow \text{C}$

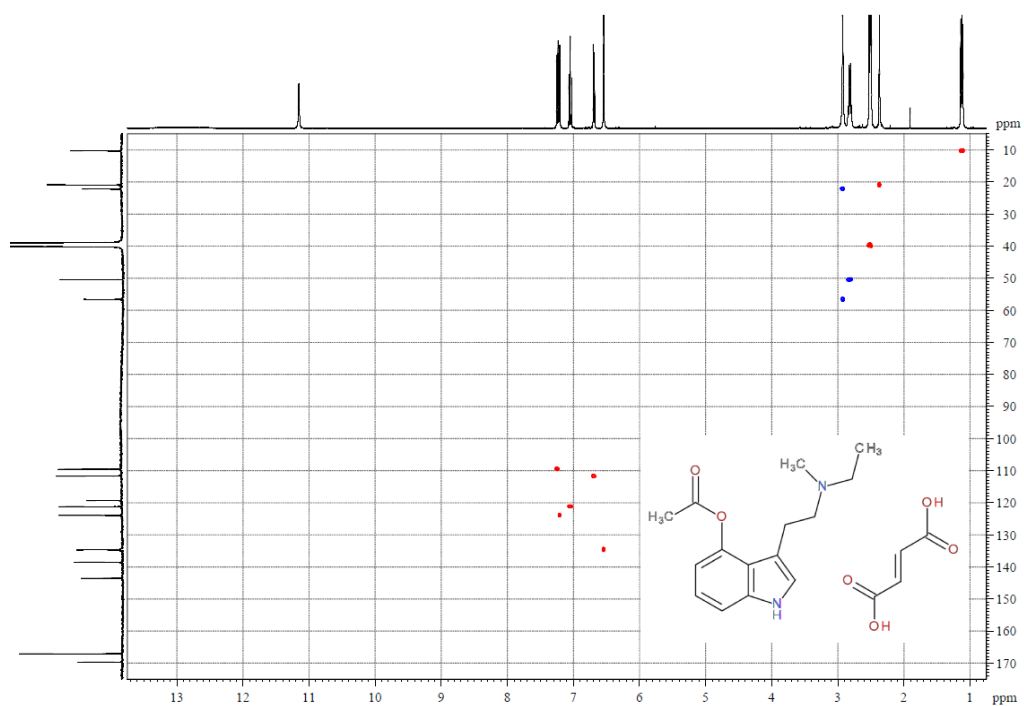


¹H NMR (overview and characteristic parts)Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d₆

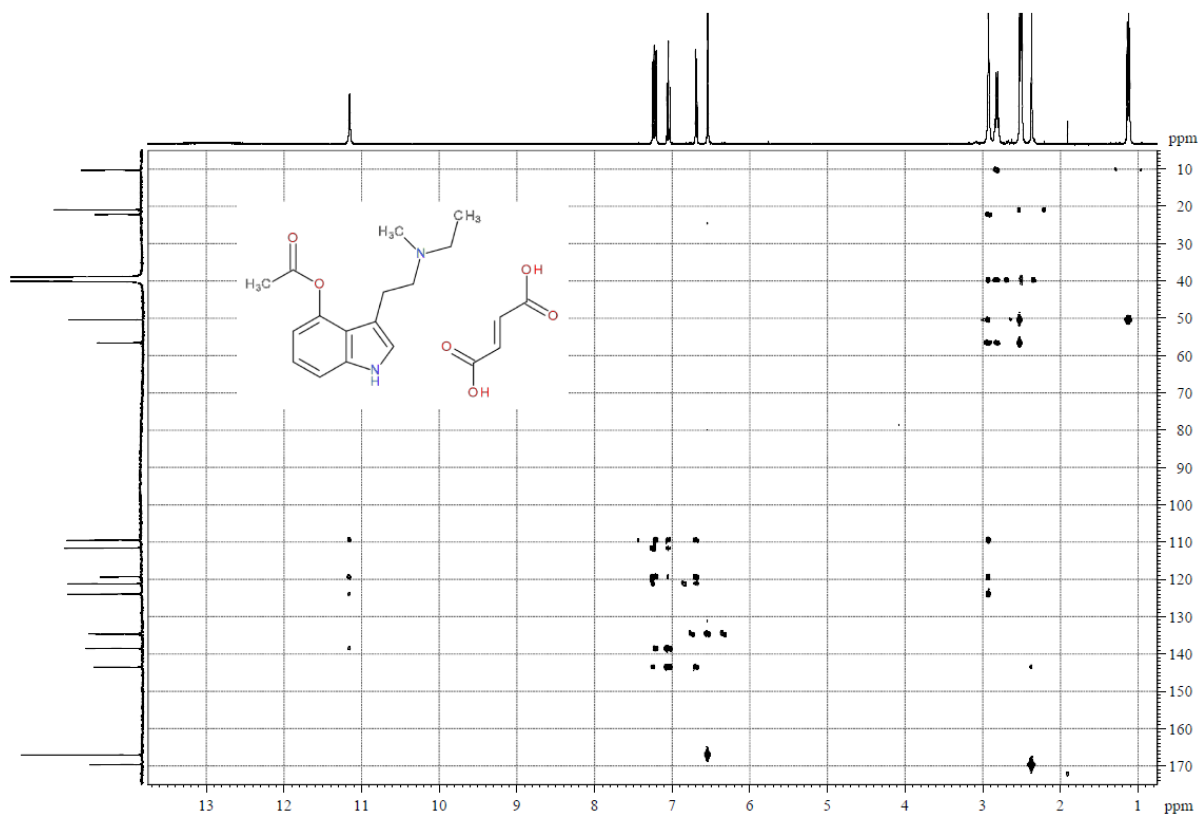
clip-zqs-COSY**zqs-easy-ROESY**Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d₆

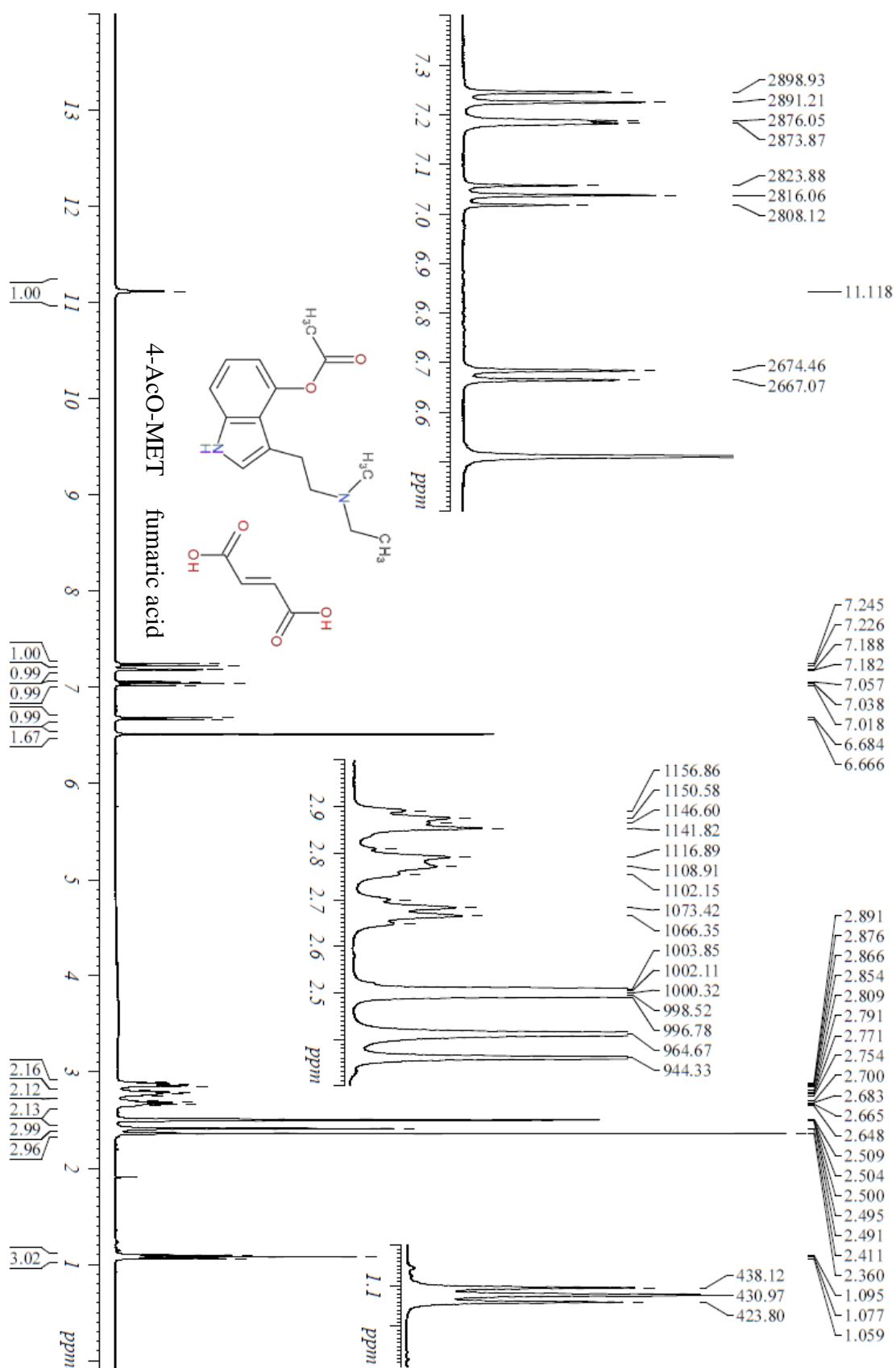
^{13}C NMR**DEPT-Q-135**Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO- d_6

ed-HSQC

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

HMBC

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

^1H NMRN neutralised with Na_2CO_3 Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6