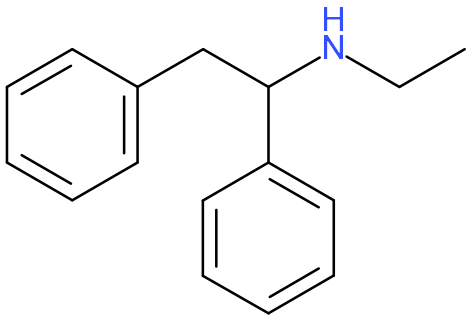
Ephenidine



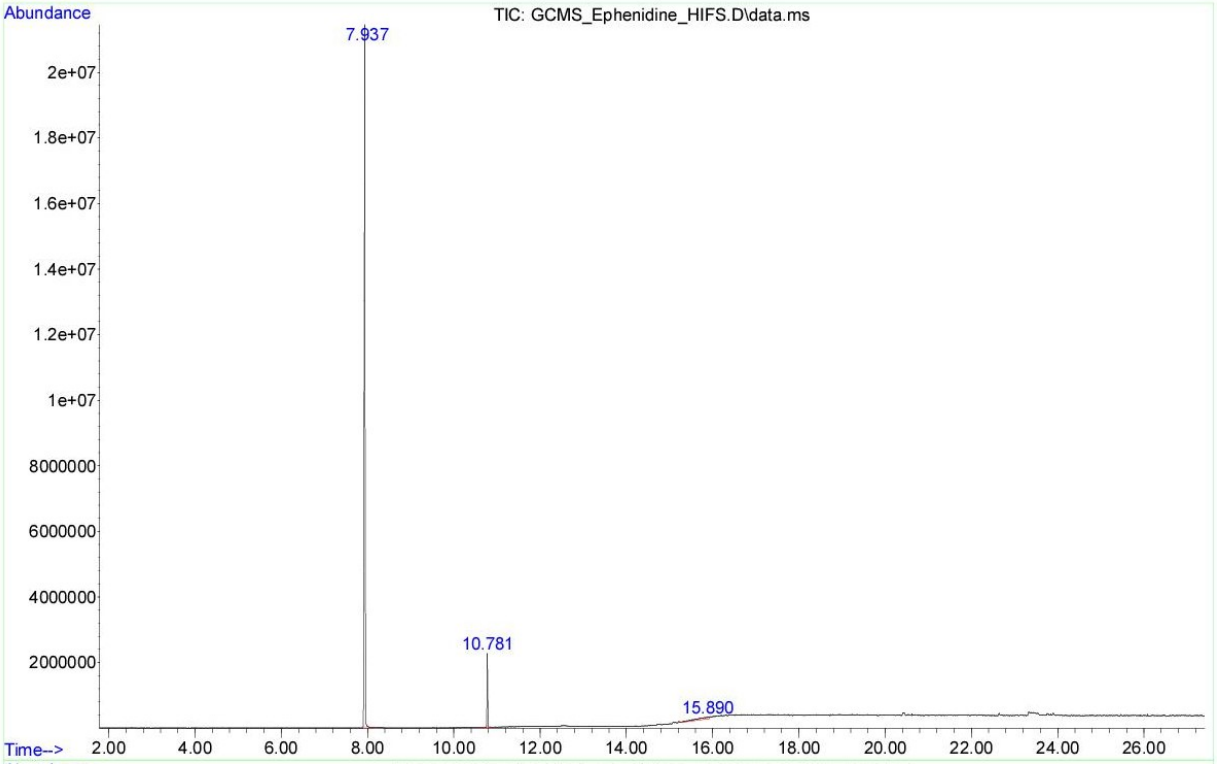
N-ethyl-1,2-diphenylethanamine
Formula: $C_{16}H_{19}N$
Formula weight: 225.33
Chemical Abstracts No.: 60951-19-1 (base), 6272-97-5 (HCl salt)
Smiles code: CCNC(Cc1ccccc1)c2ccccc2
InChi key: IGFZMQXEKIZPDR-UHFFFAOYSA-N
Other names: EPE, NEDPA, NSC 33648,
N-ethyl-α-phenyl-benzeneethanamine

The seized evidence was 0.806 grams white powder in a plastic zip-bag titled EPHENIDINE.

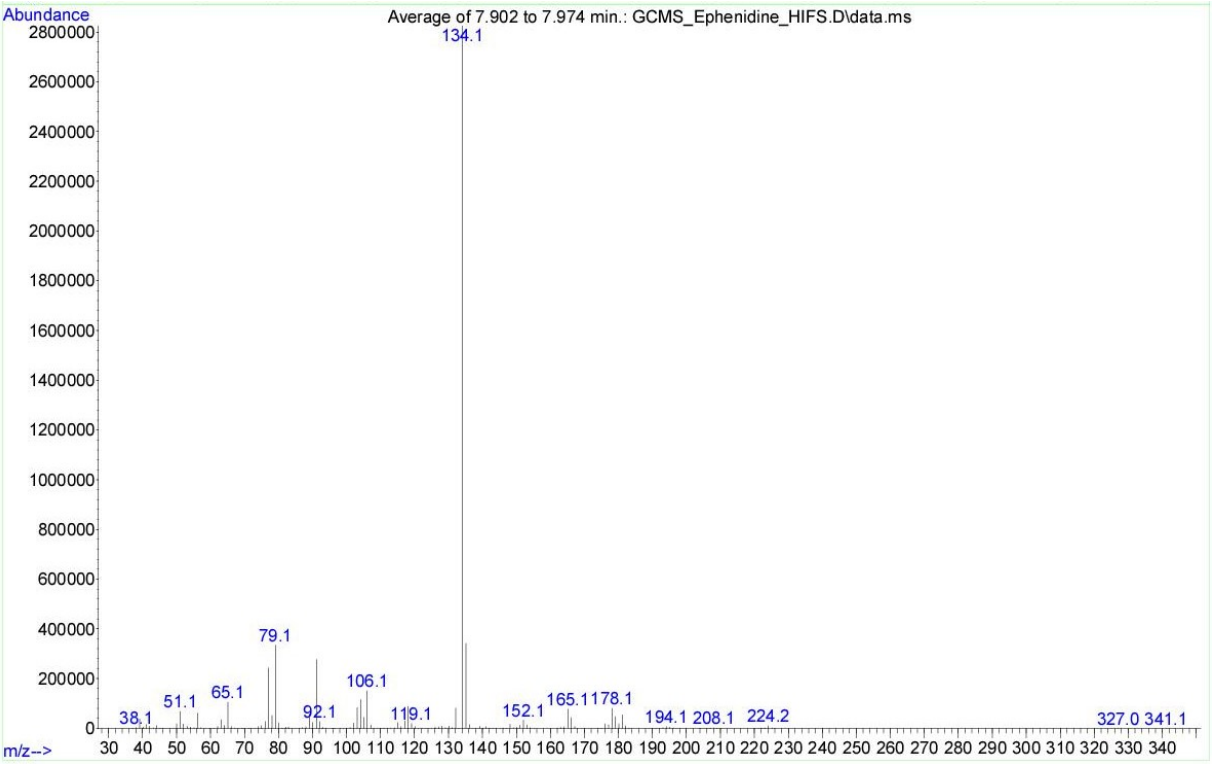
GC-MS

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. 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 softare.

GC-MS total ion chromatogram



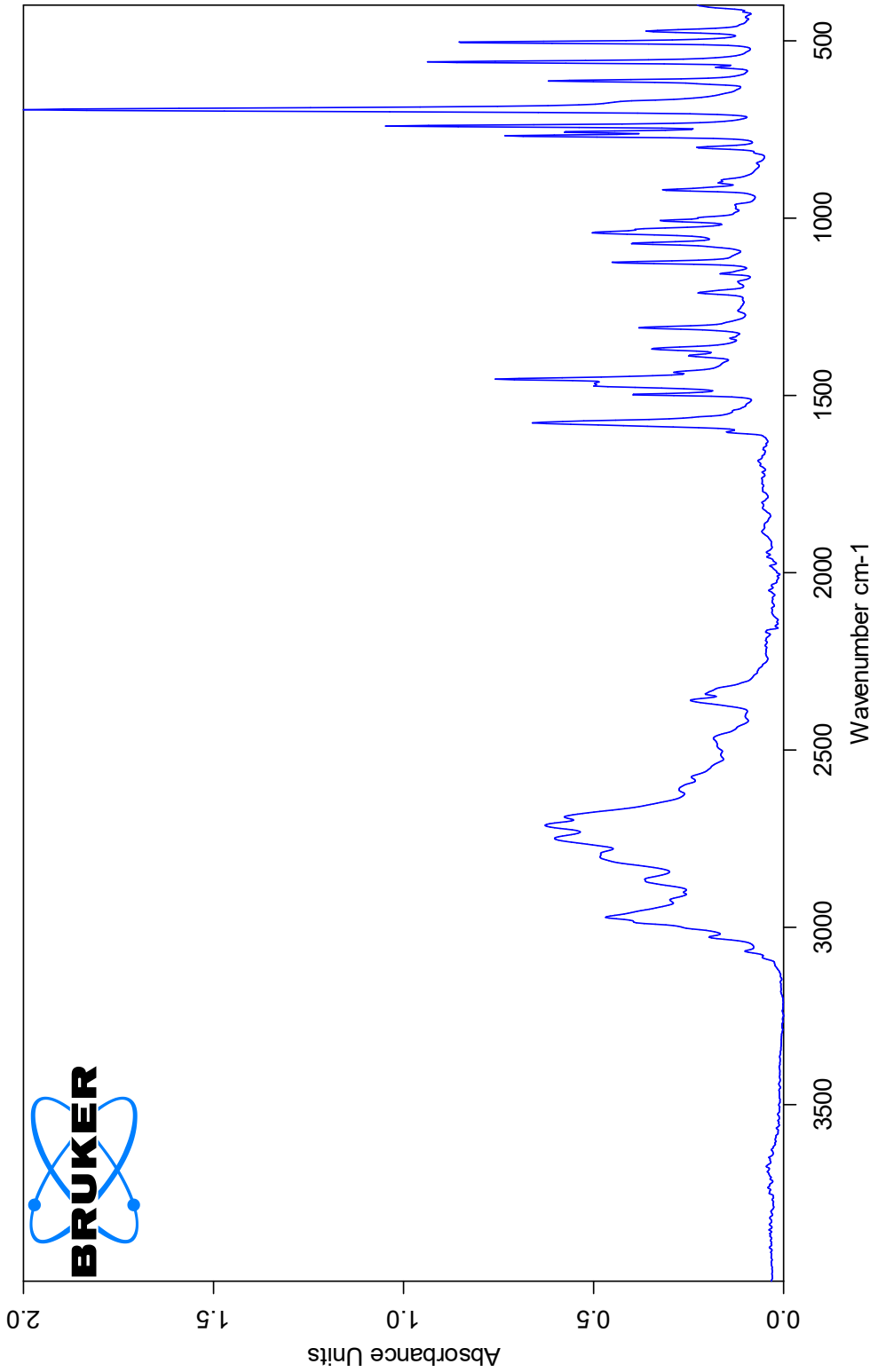
Mass spectrum at 7.93 min retention time



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

ATR-FTIR (powder)

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 spectrometer was controlled, and the data were processed using Opus 6.5 software package.



Bruker Tensor 27

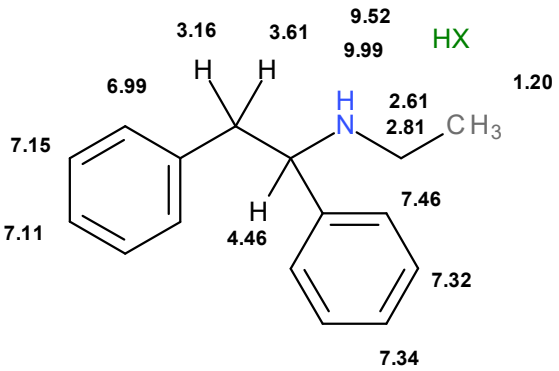
NMR

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 spectra were recorded at 25°C in DMSO-d_6 solution. 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 (δ_{TMS} = 0.00 ppm). The determination of the structure was based on ^{1}H, zqs-clip-COSY, zqs-TOCSY, zqs-easy-ROESY as well as ^{13}C, multiplicity edited HSQC, double edited HSQC-zqs-clip-COSY and magnitude mode HMBC spectra. The salt form is proven, but the counter ion was not determined.

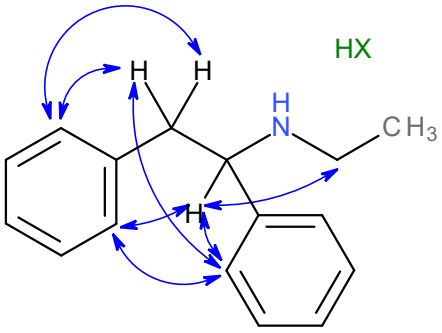
Interpretation of the NMR spectra

In DMSO-d_6 solution

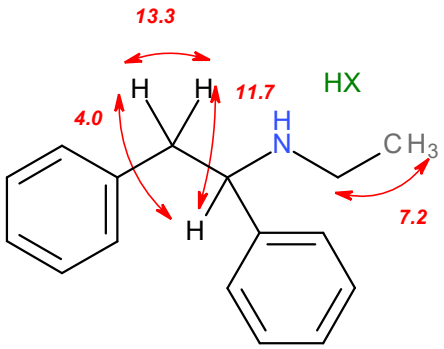
^{1}H-NMR chemical shifts δ [ppm]



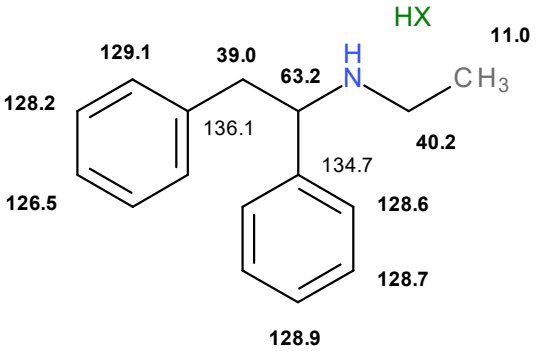
Characteristic H-H steric proximities detected by zqs-easy-ROESY measurement



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

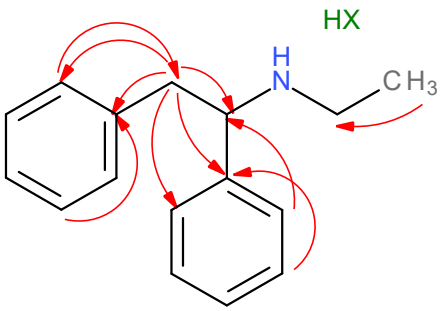


^{13}C-NMR chemical shifts δ [ppm]

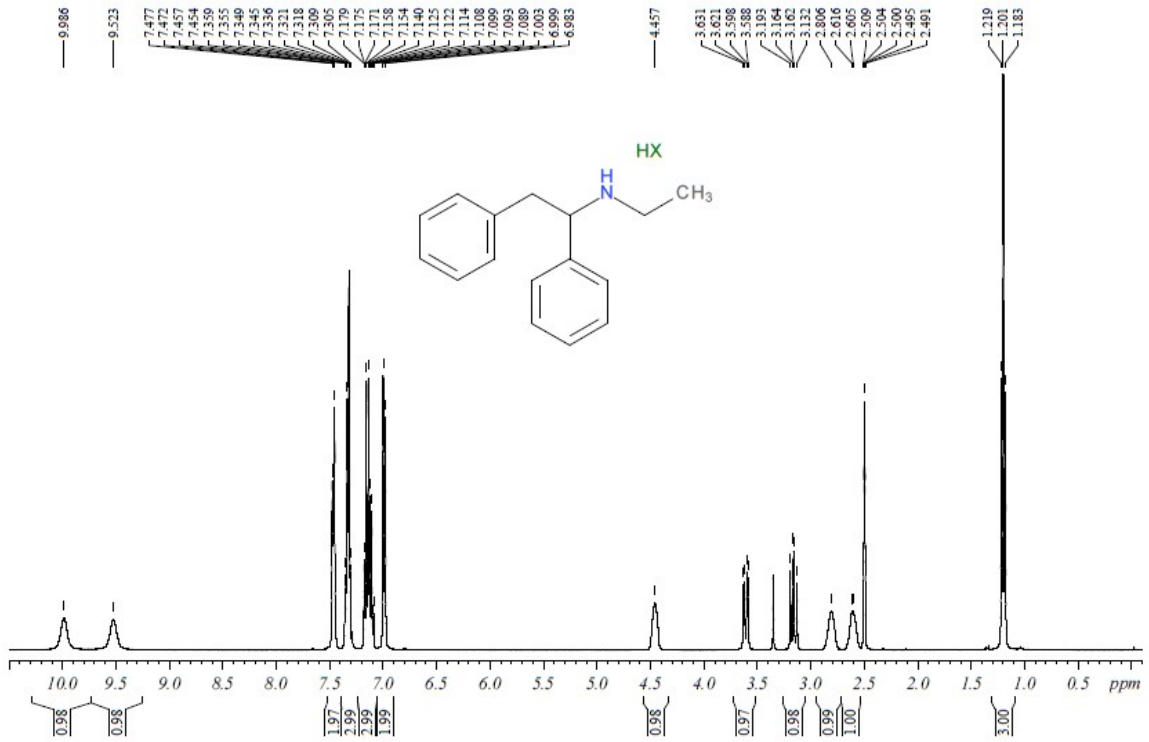


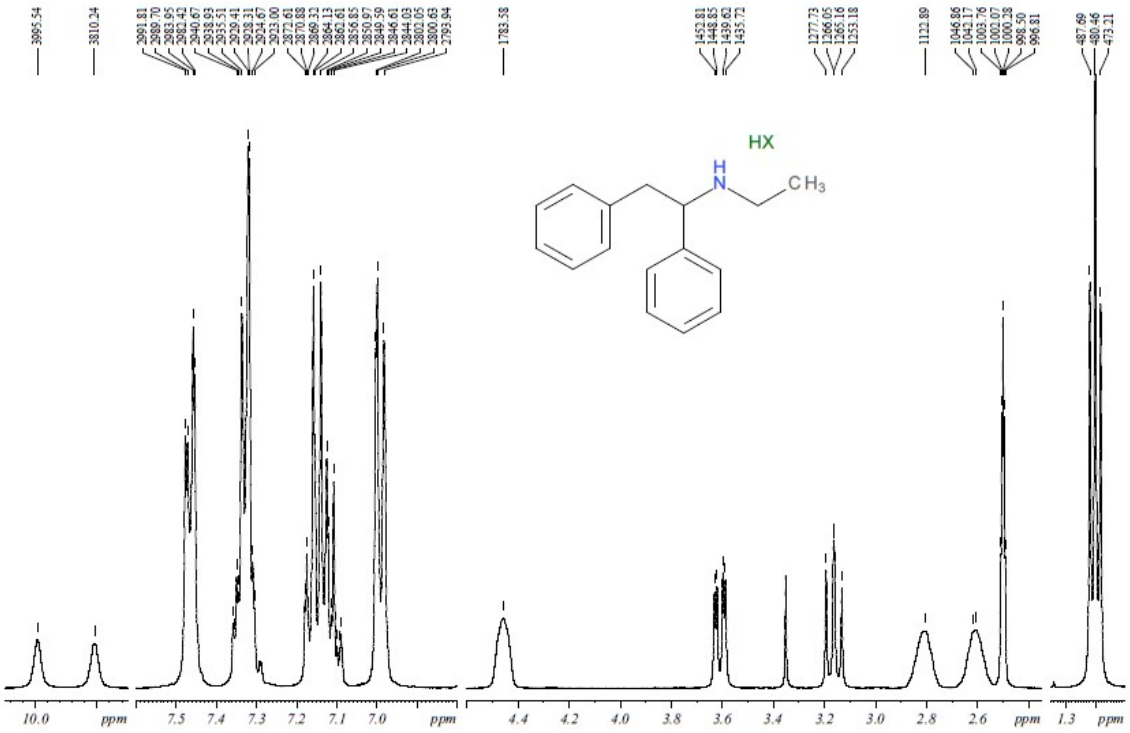
Characteristic heteronuclear long-range couplings detected by HMBC measurement

H ⟶ C



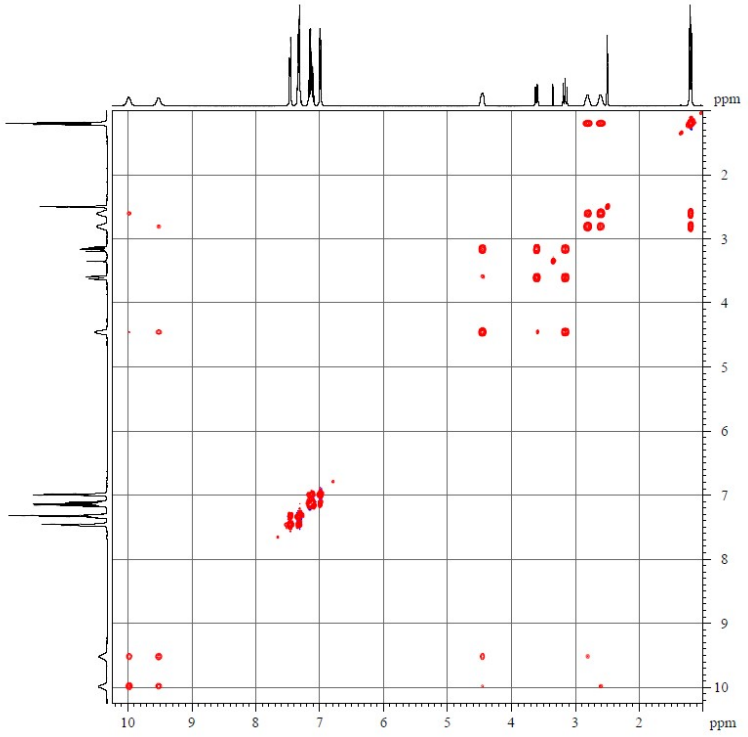
^{1}H NMR (overview and characteristic parts)

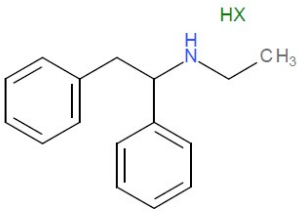




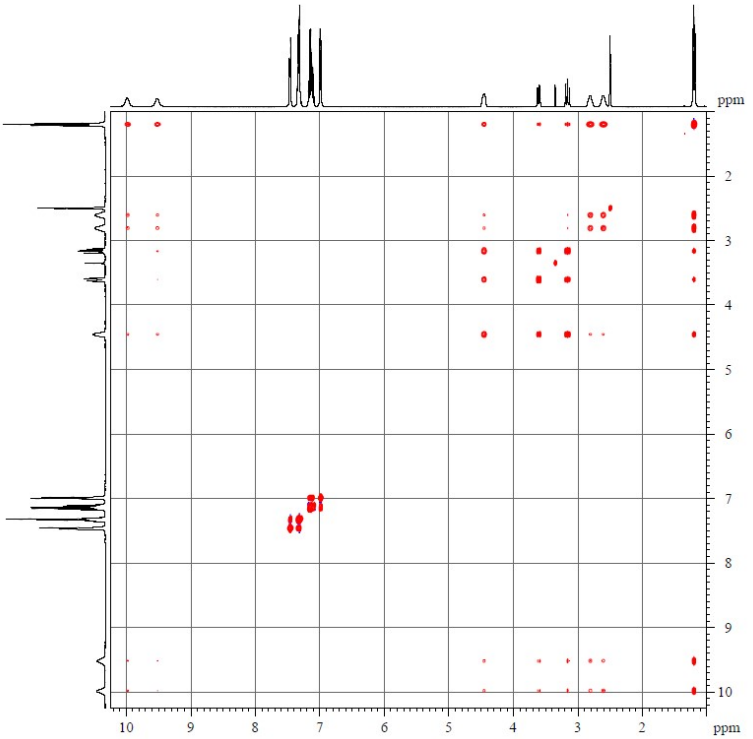
Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6

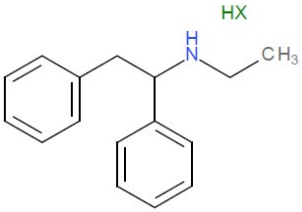
zqs-clip-COSY





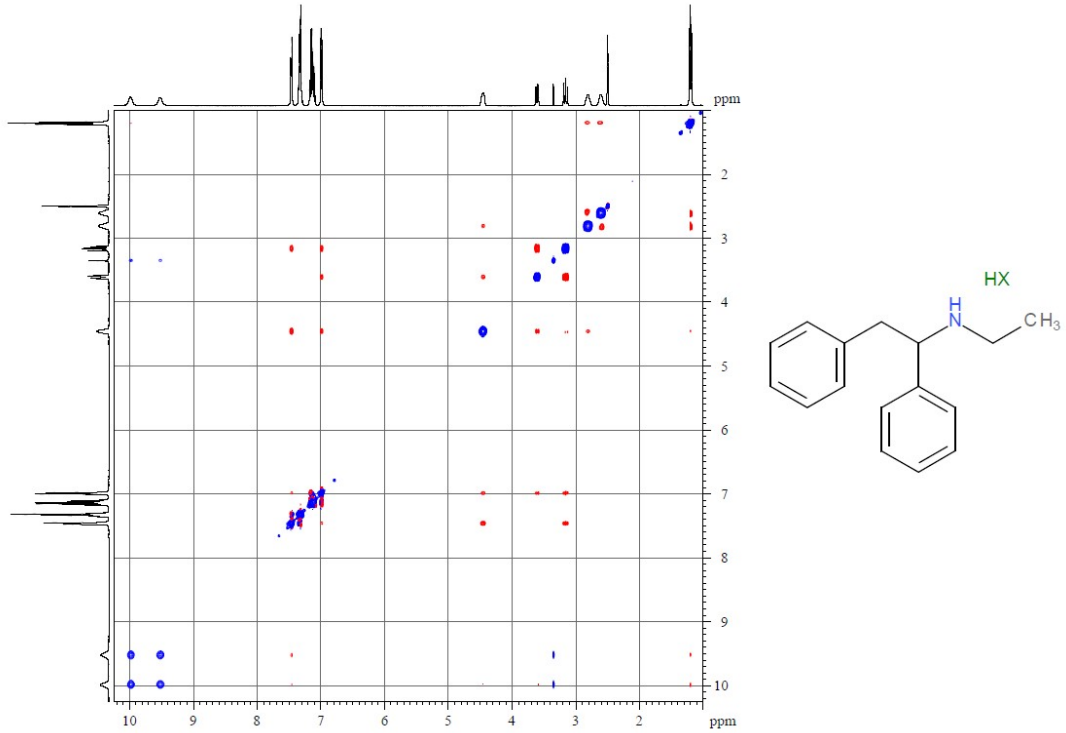
zqs-TOCSY



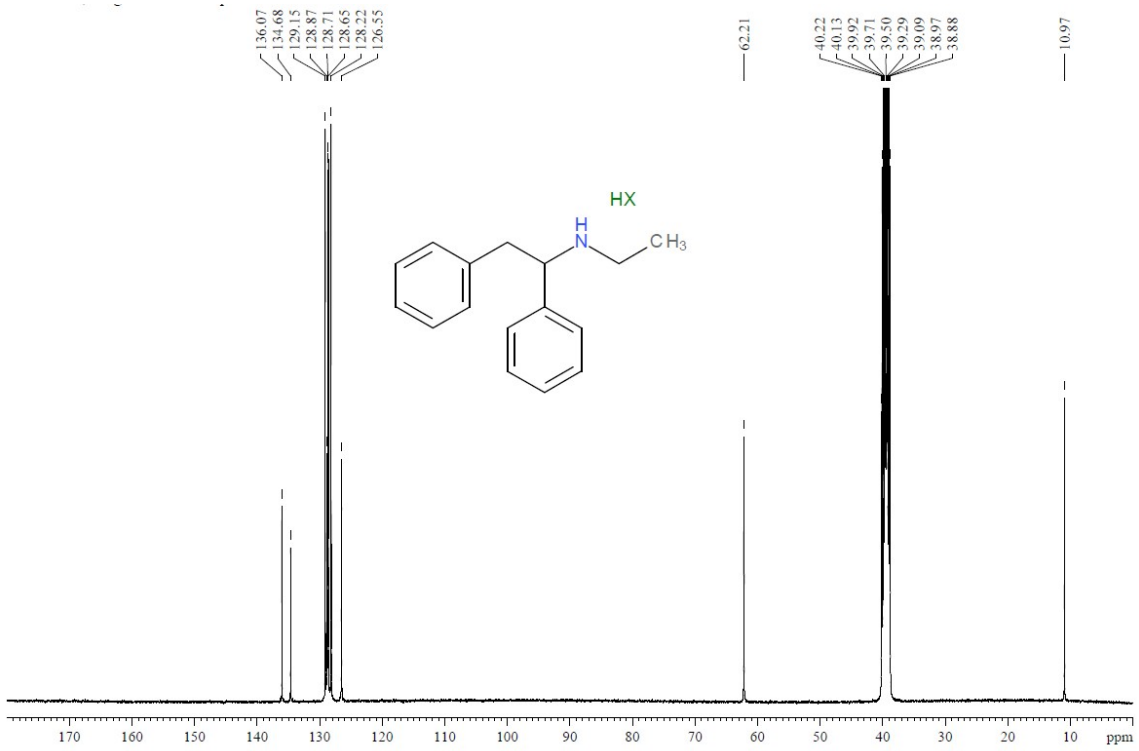


Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6

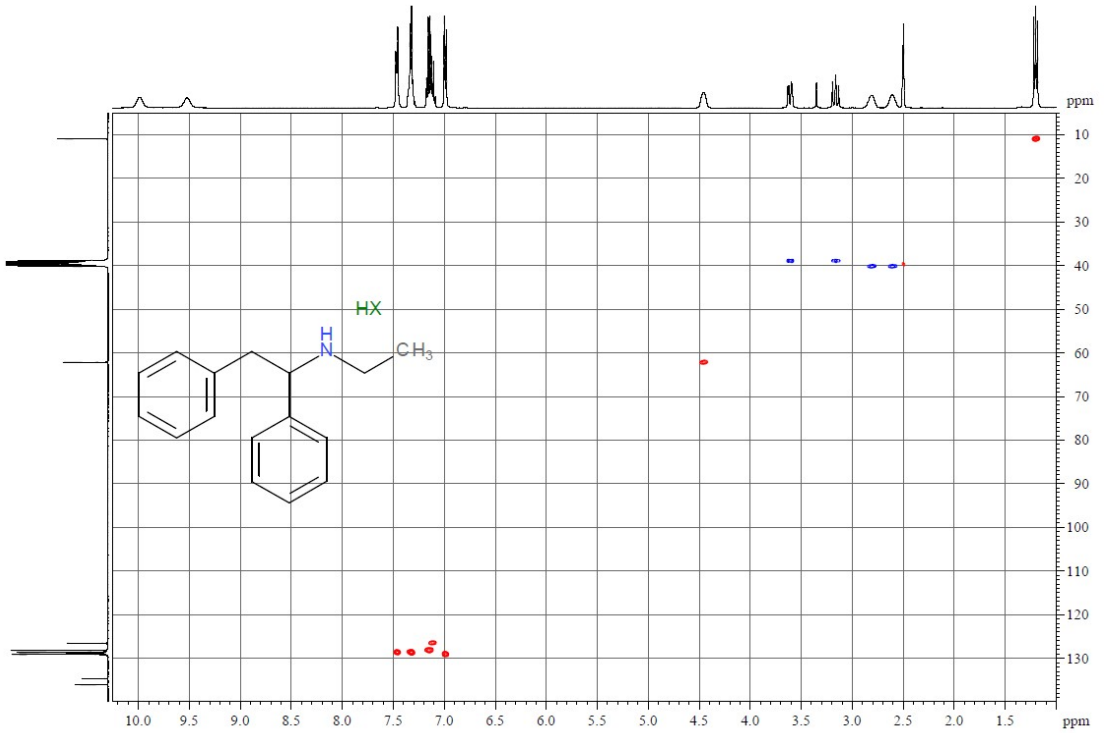
zqs-easy-ROESY



^{13}C NMR

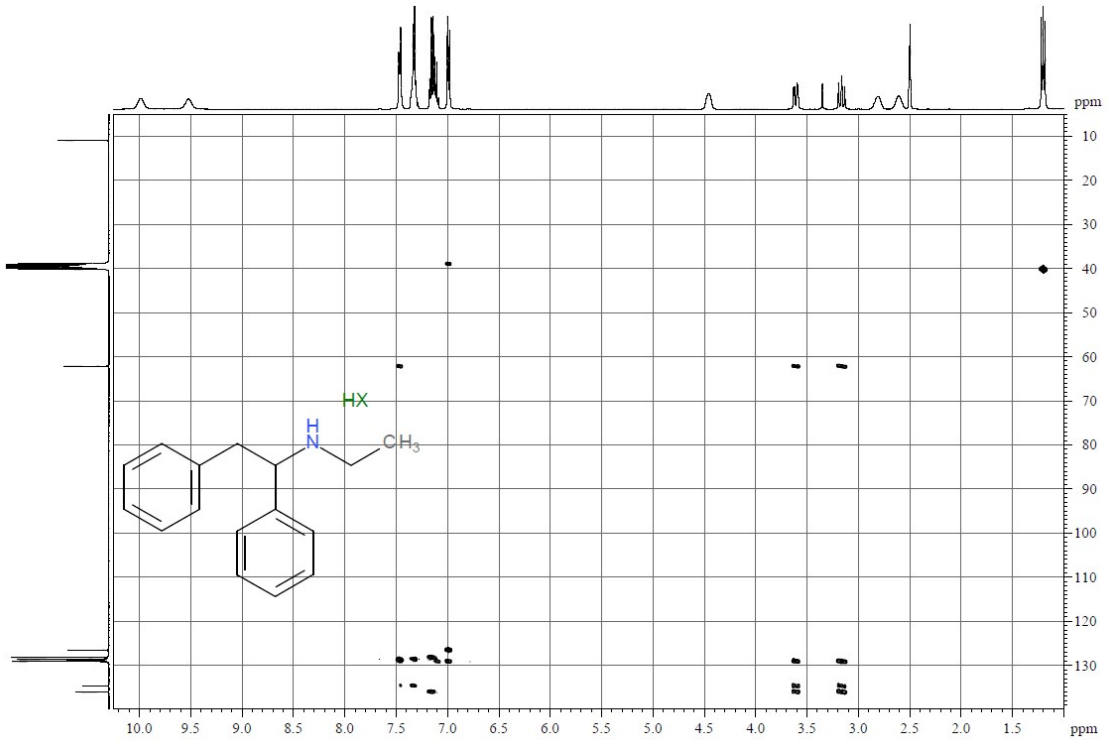


ed-HSQC



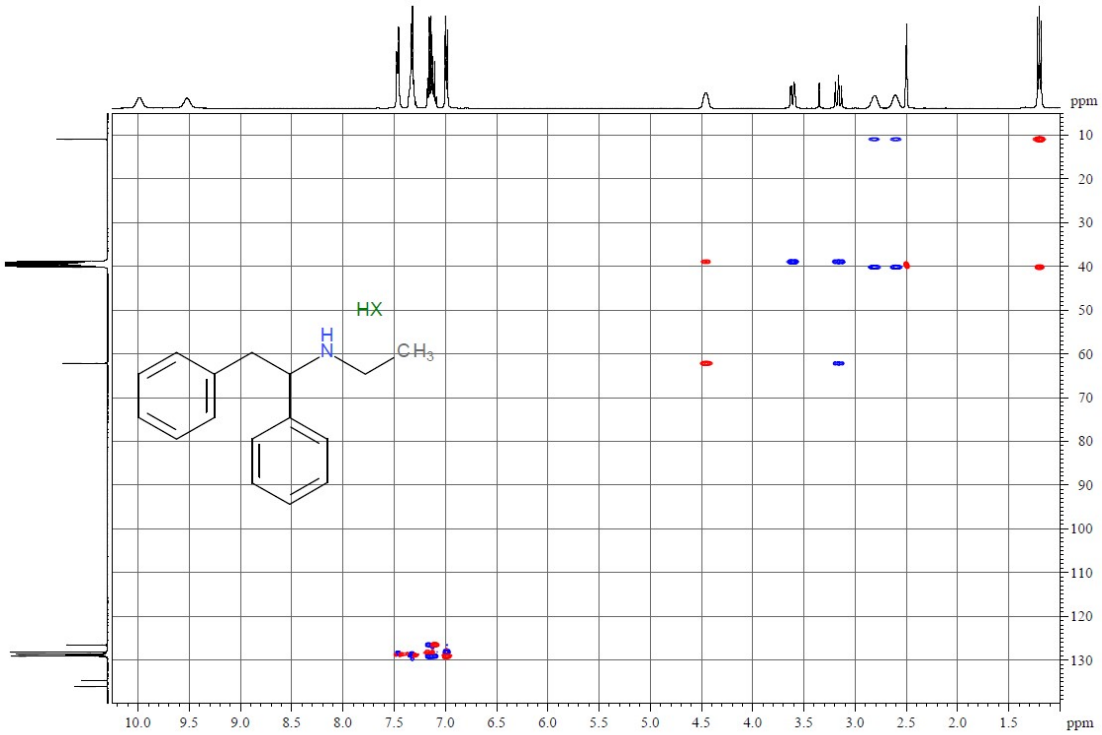
Bruker AVANCE NEO 400, CryoProbe Prodigy; solvent: DMSO-d_6

HMBC



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

ed-HSQC-zqs-clip-COSY



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

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