Supplementary Information

Updating the list of known opioids through identification and characterization of the new opioid derivative 3,4-dichloro-N-(2-(diethylamino)cyclohexyl)-N-methylbenzamide (U-49900).

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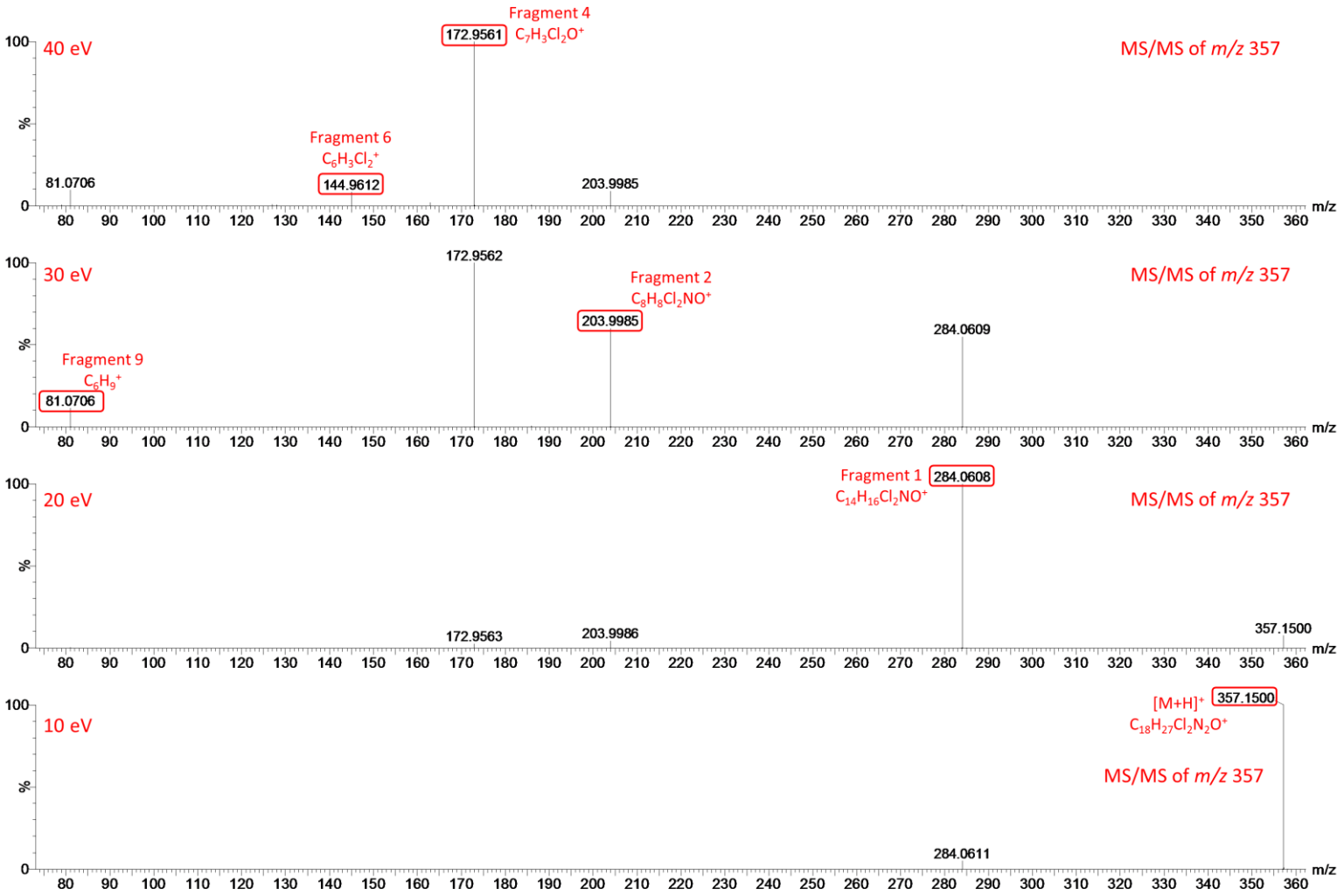
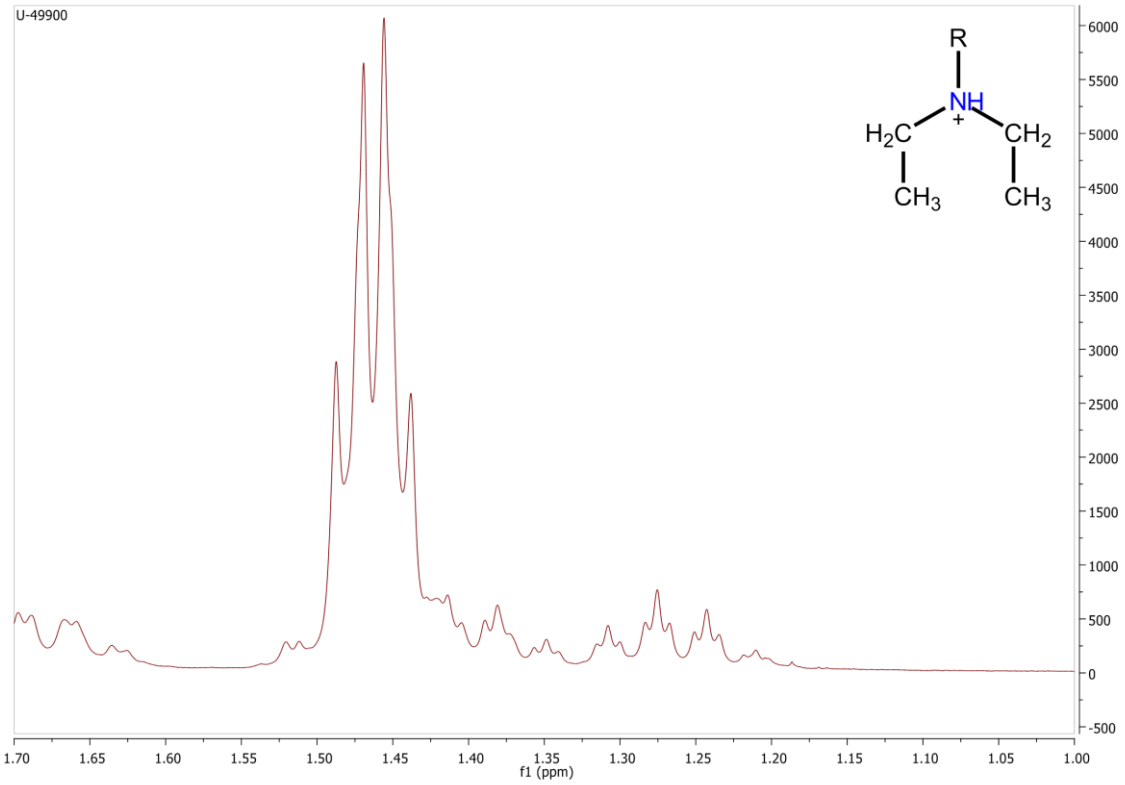
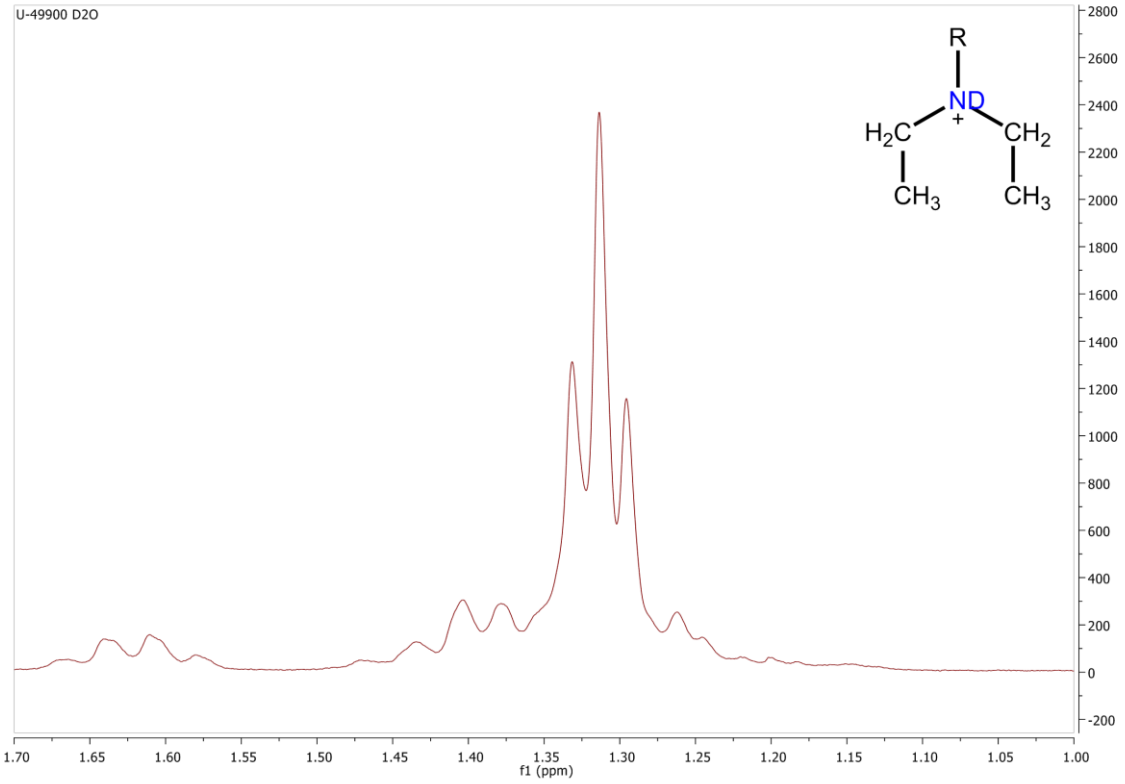
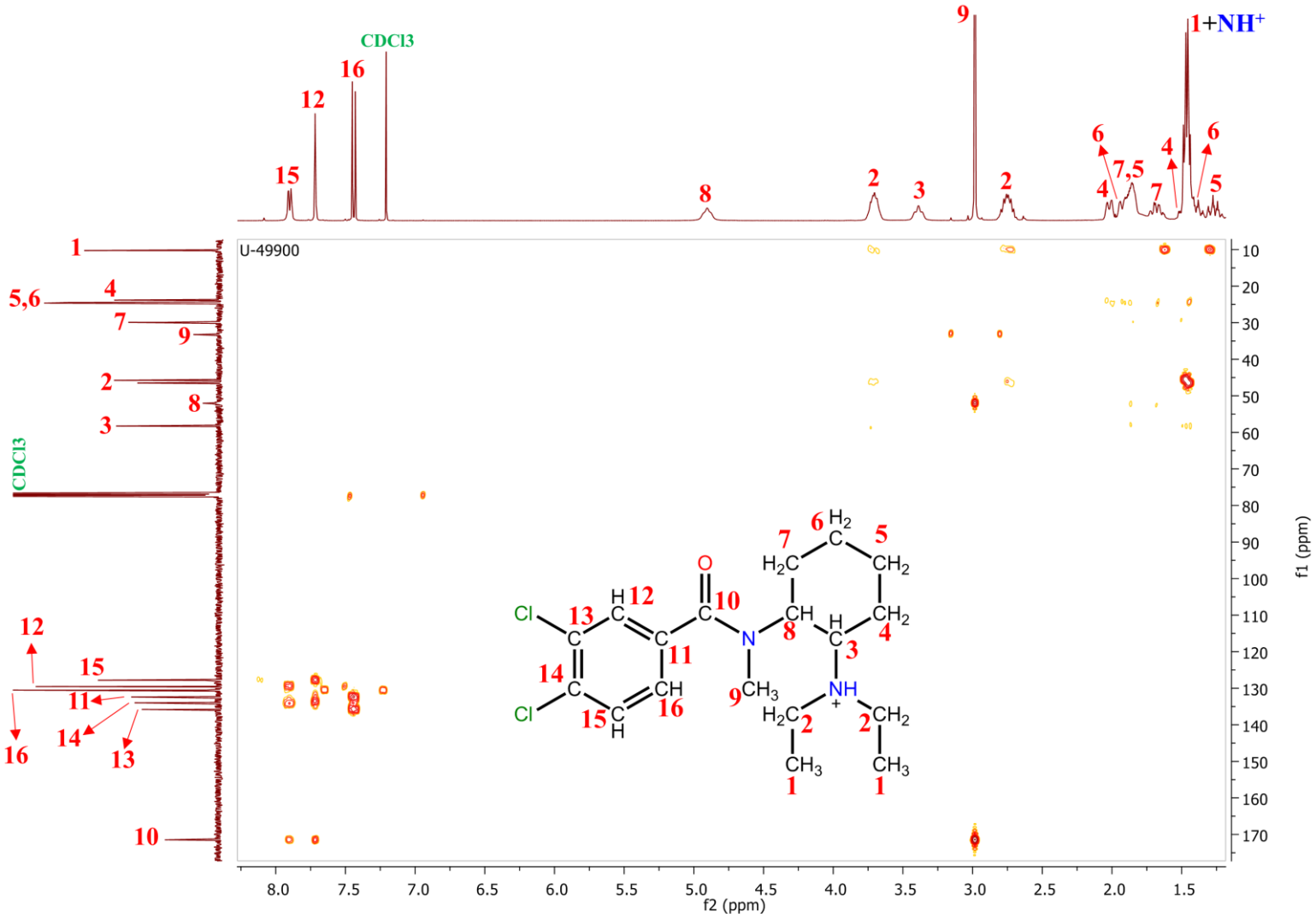


SI.1. MS/MS spectra of U-49900 at 10, 20, 30 and 40 eV collision energy.

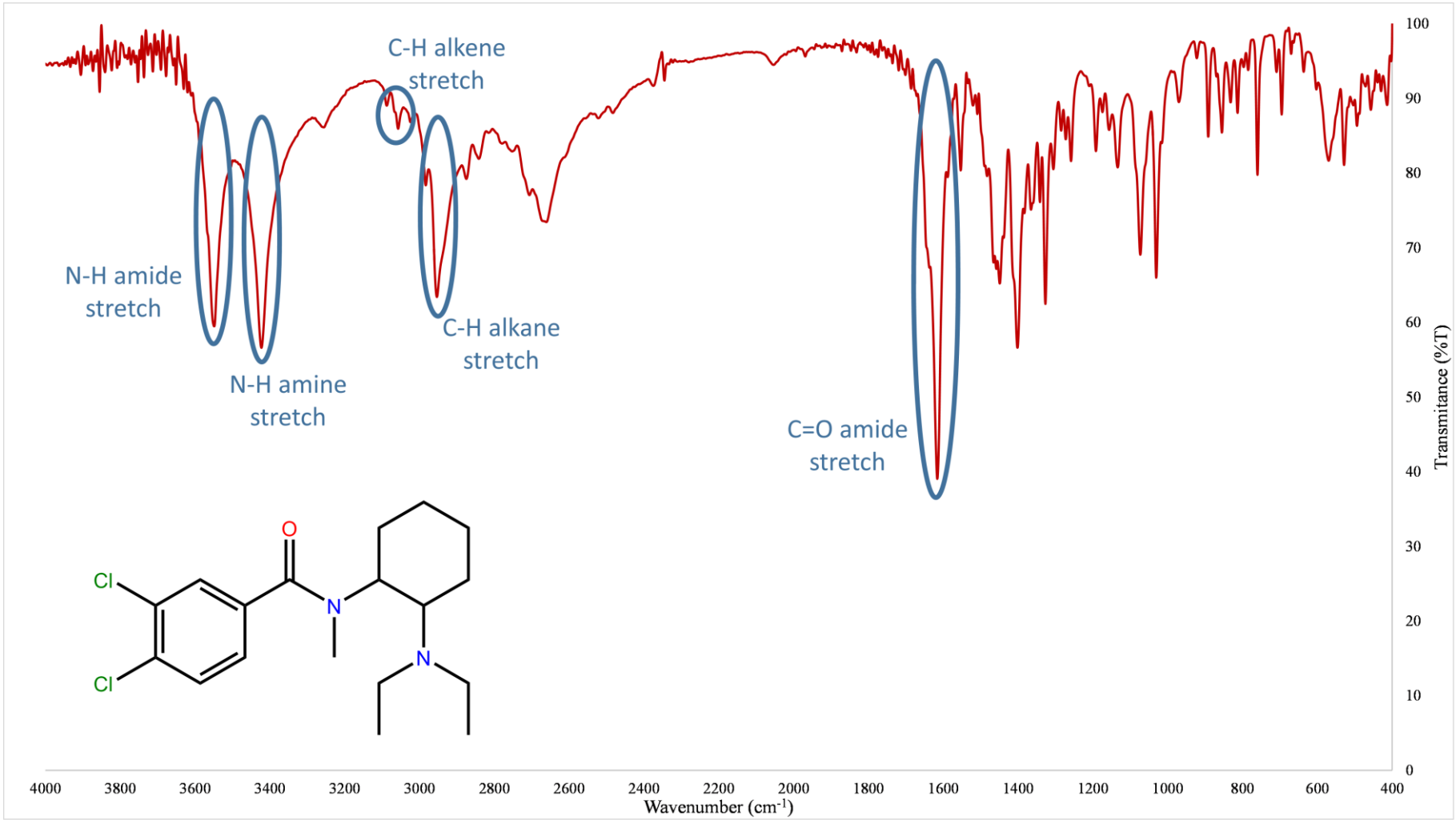




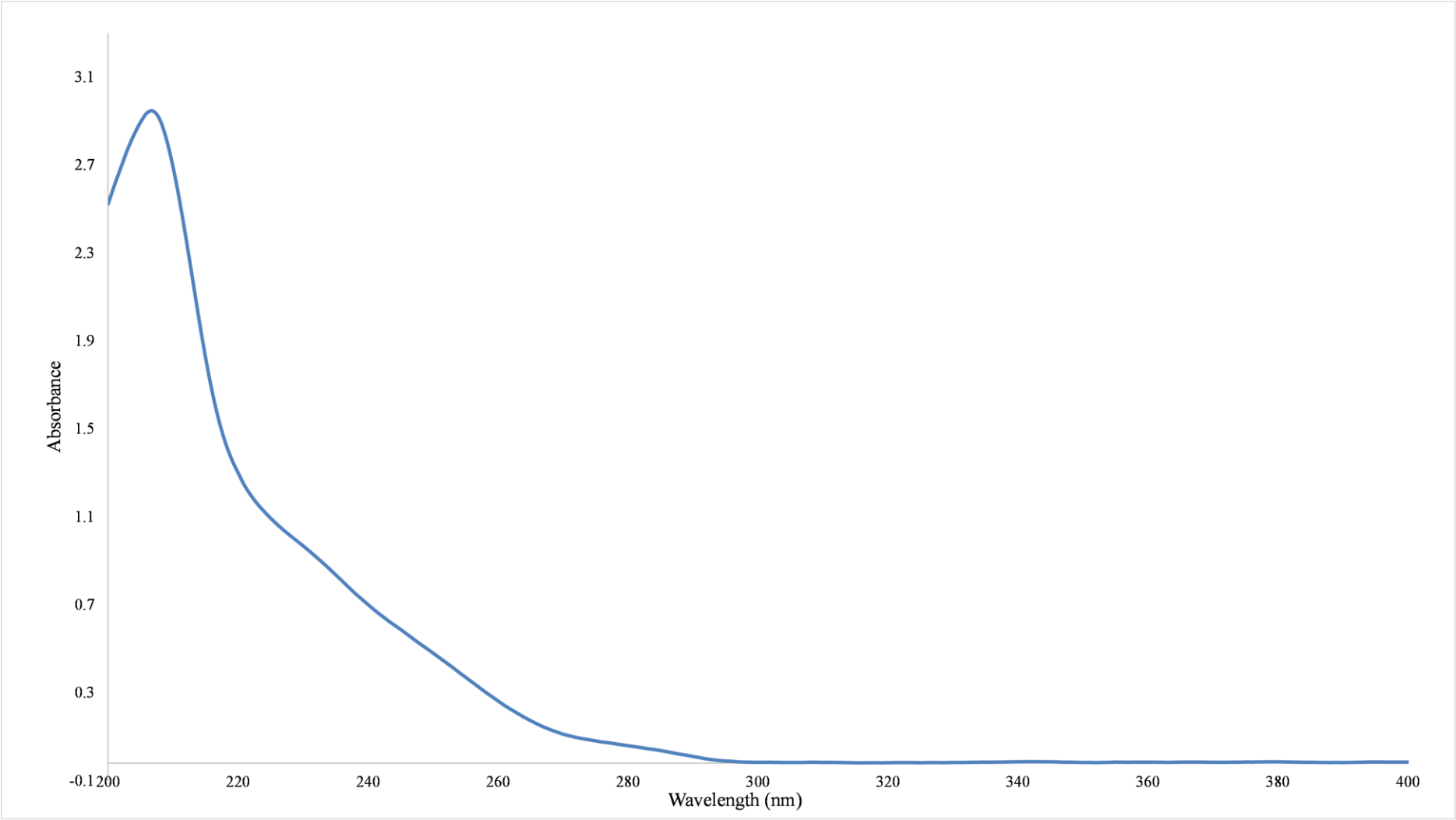
SI.2. ^{1}H-NMR signal for hydrogens of the methyl groups of diethylamine group. **Top:** Signal obtained when using $CDCl_3$ for dissolve the sample. **Bottom:** Signal obtained when using D_2O for dissolving the sample.



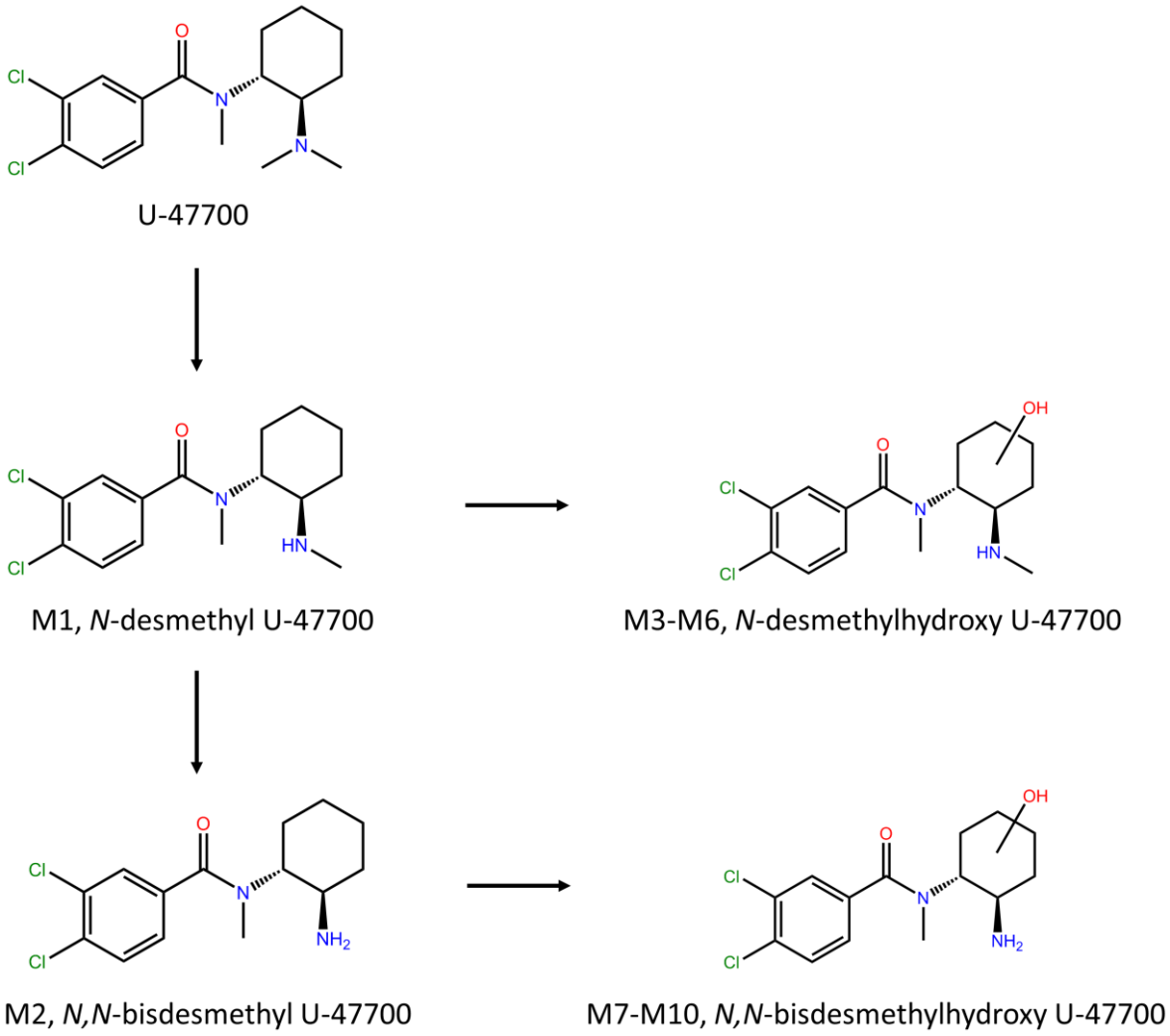
SI.3. HMBC spectra of U-49900. Correlations over 2 bonds are showed between ^{1}H and ^{13}C-NMR signals.



SI.4. FTIR spectrum of U-49900. C=O band of the amide group is observed at 1600-1650 cm^{-1}. Aliphatic C-H bands are observed down to 3000 cm^{-1}. Aromatic C-H bands are observed up to 3000 cm^{-1}. N-H band of the amine is observed around 3400 cm^{-1}. N-H band of the amide is observed around 3500 cm^{-1}.



SI.5. UV spectrum of the U-49900



SI.6. Proposed metabolic pathway of U-47700.