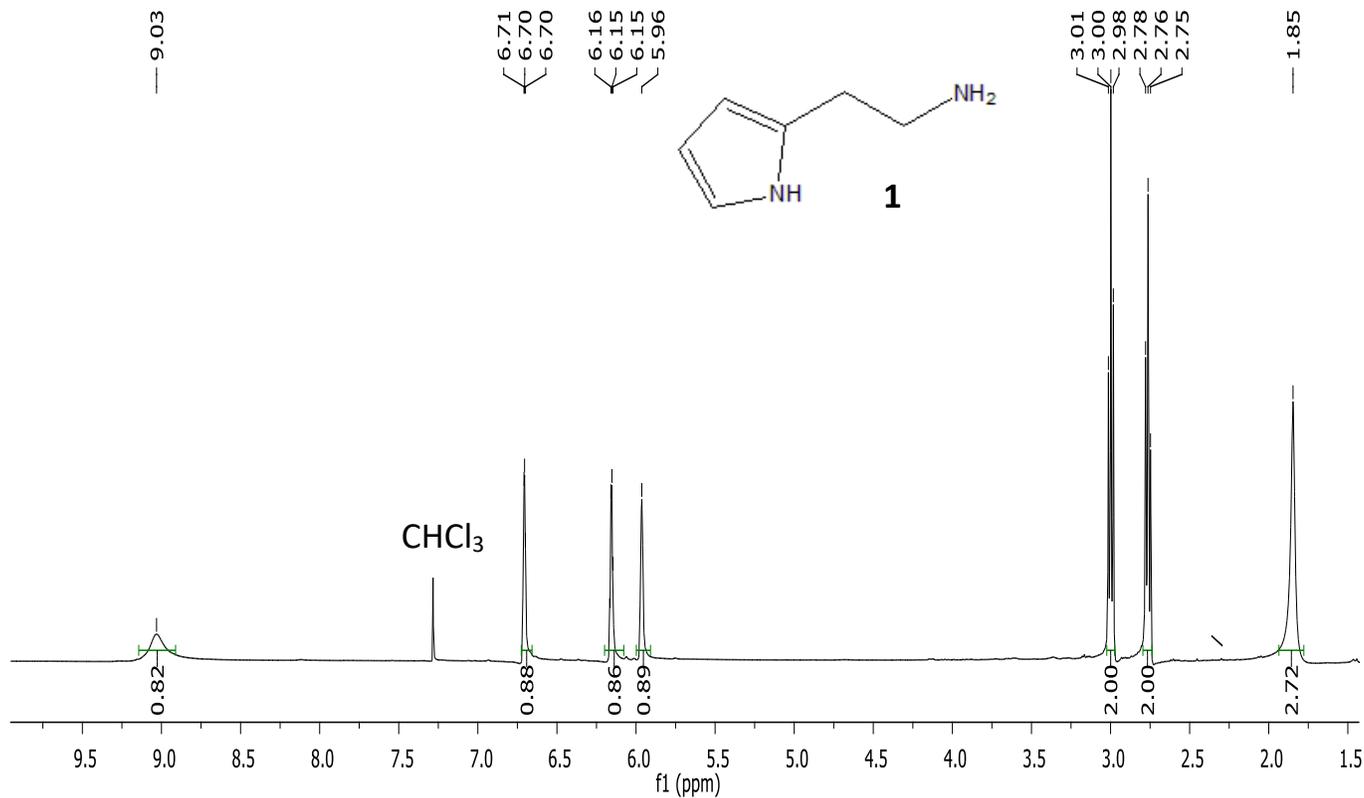


Supplementary Materials: New Histamine-Related Five-Membered N-Heterocycle Derivatives as Carbonic Anhydrase I Activators

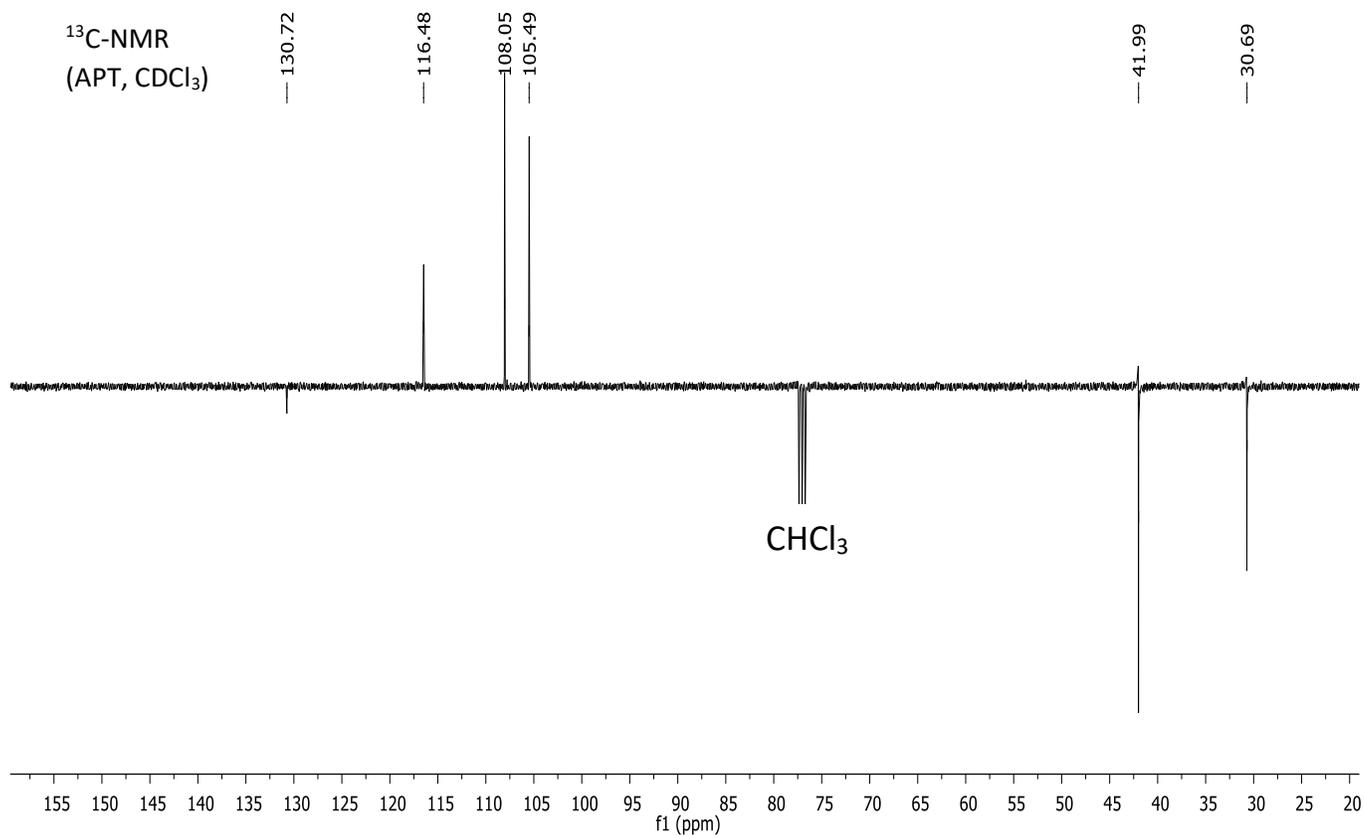
Niccolò Chiaramonte, Alessio Gabellini, Andrea Angeli, Gianluca Bartolucci, Laura Braconi, Silvia Dei, Elisabetta Teodori, Claudiu T. Supuran and Maria Novella Romanelli

¹H and ¹³C-NMR spectra of the final compounds

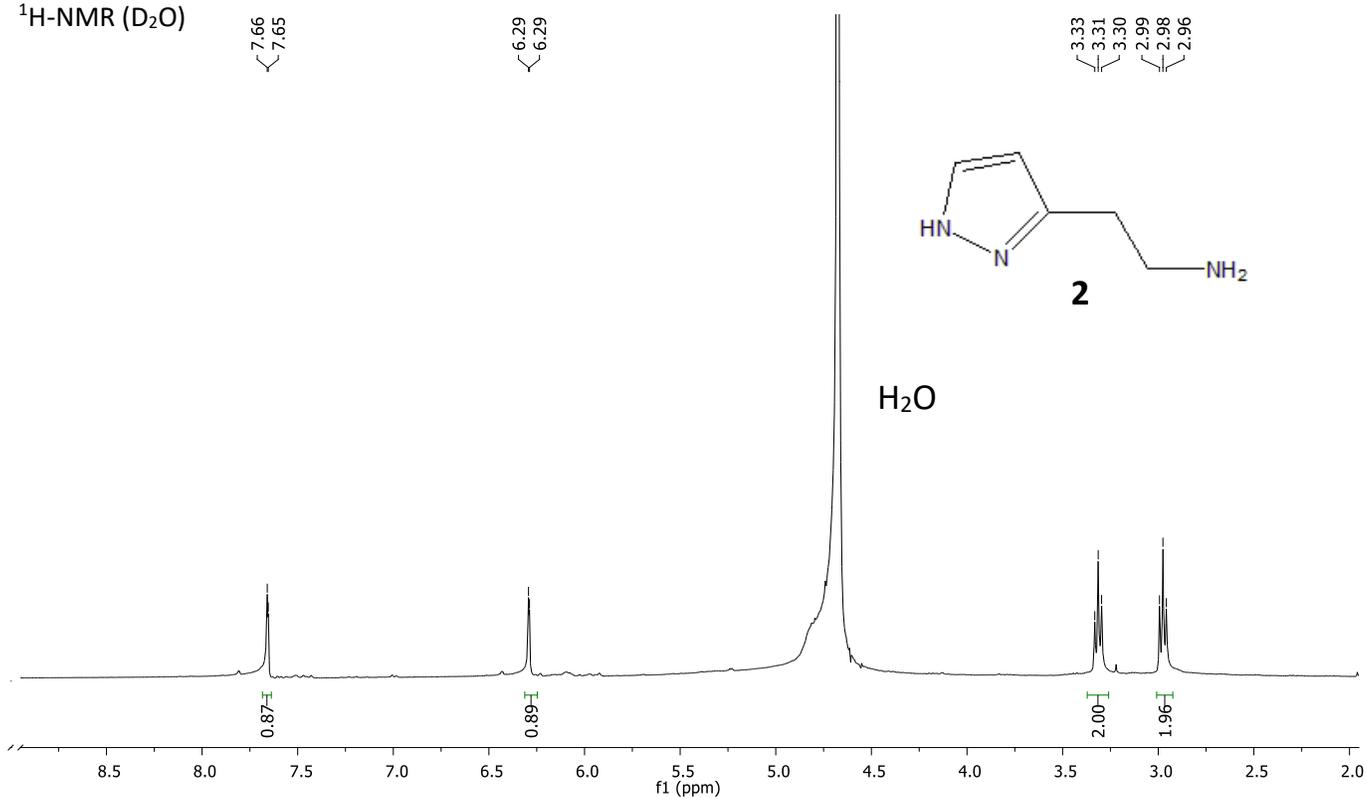
¹H-NMR (CDCl₃)



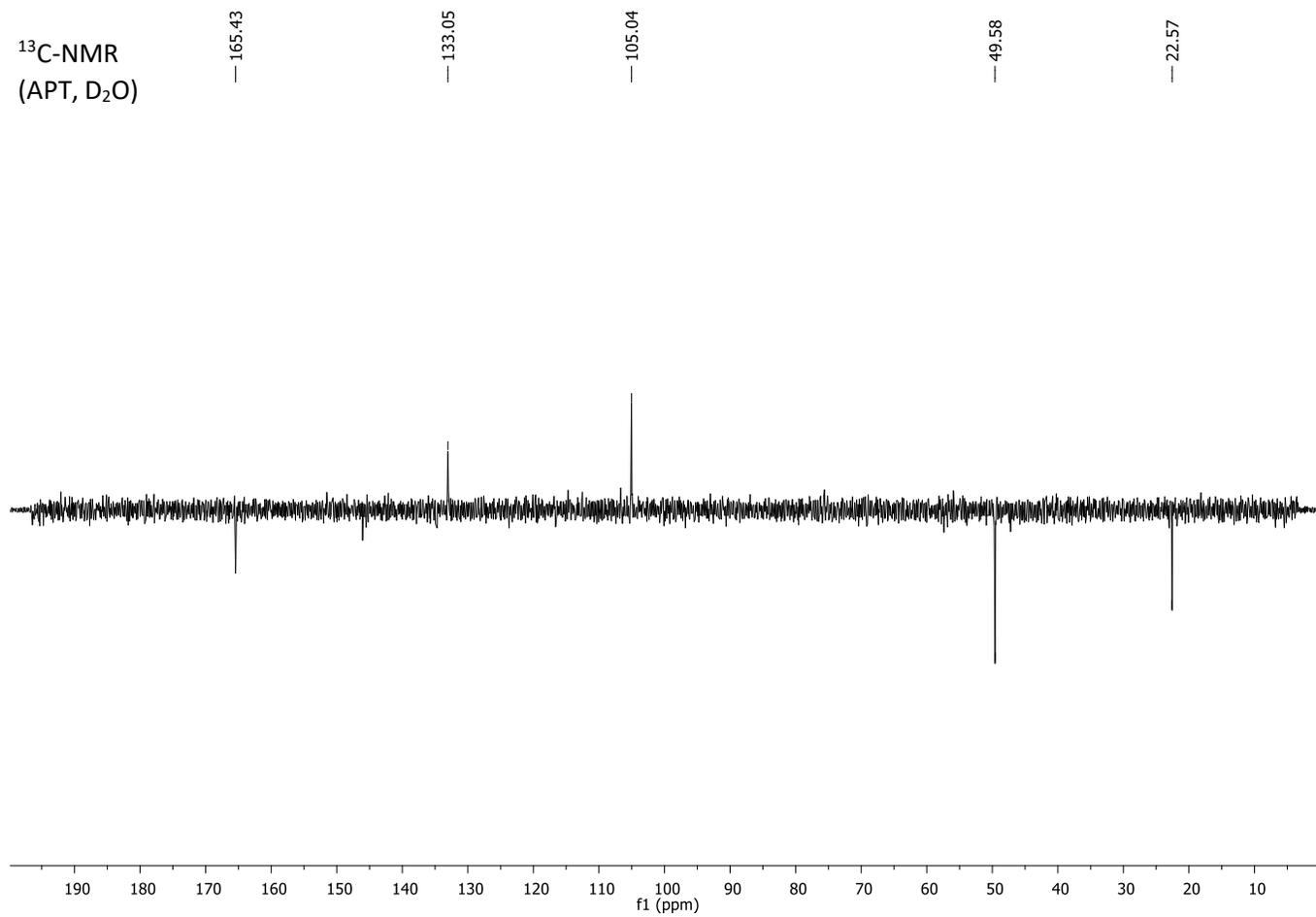
¹³C-NMR (APT, CDCl₃)



$^1\text{H-NMR}$ (D_2O)

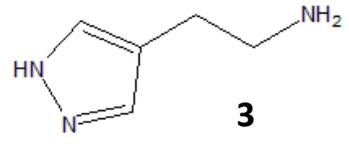


$^{13}\text{C-NMR}$
(APT, D_2O)

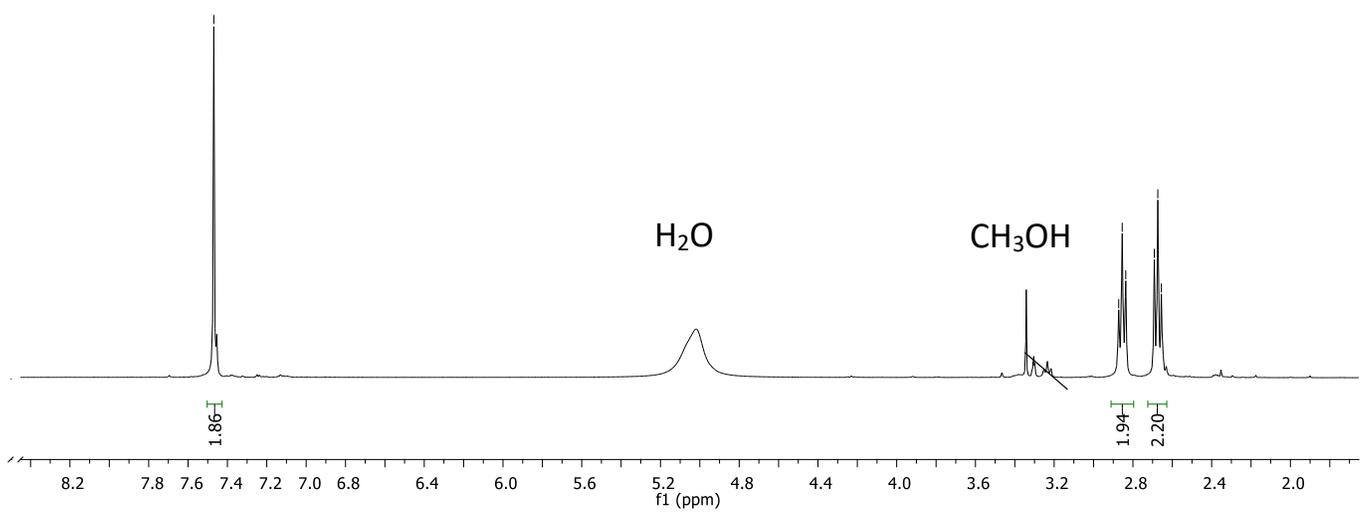


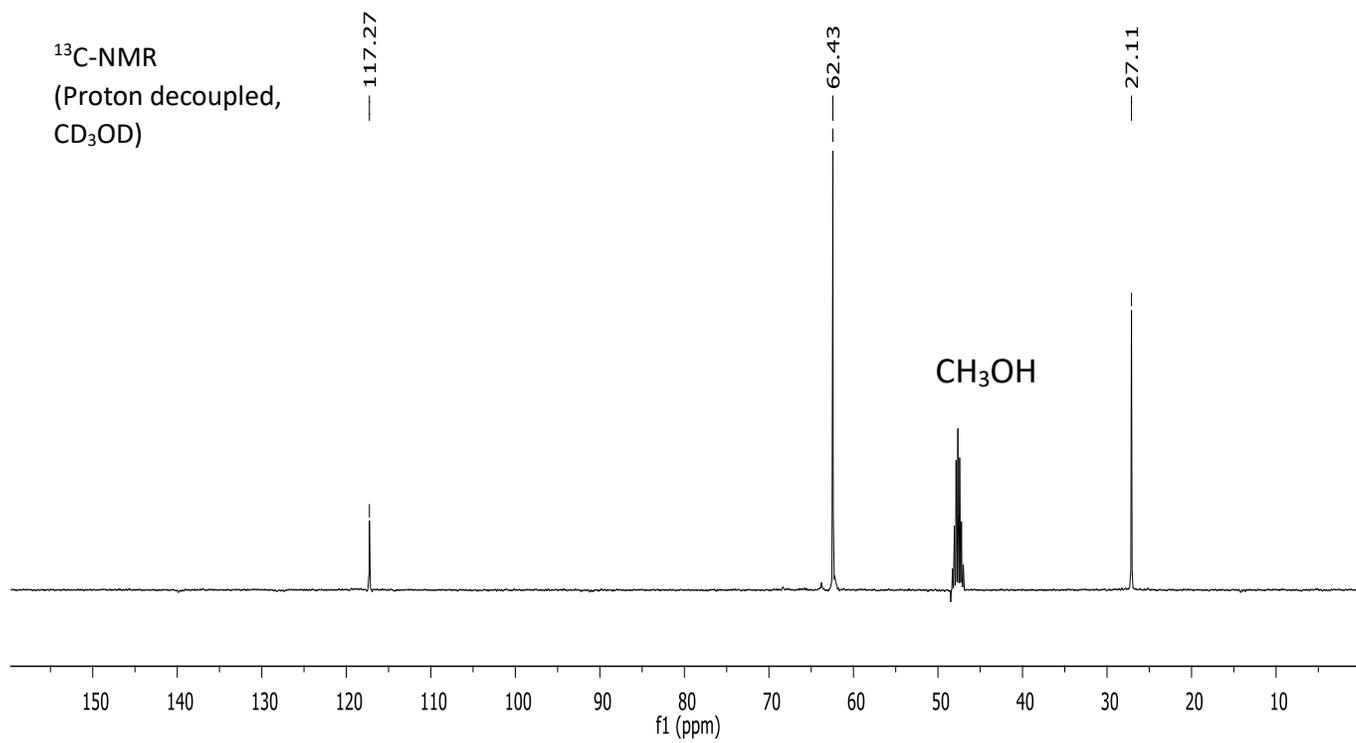
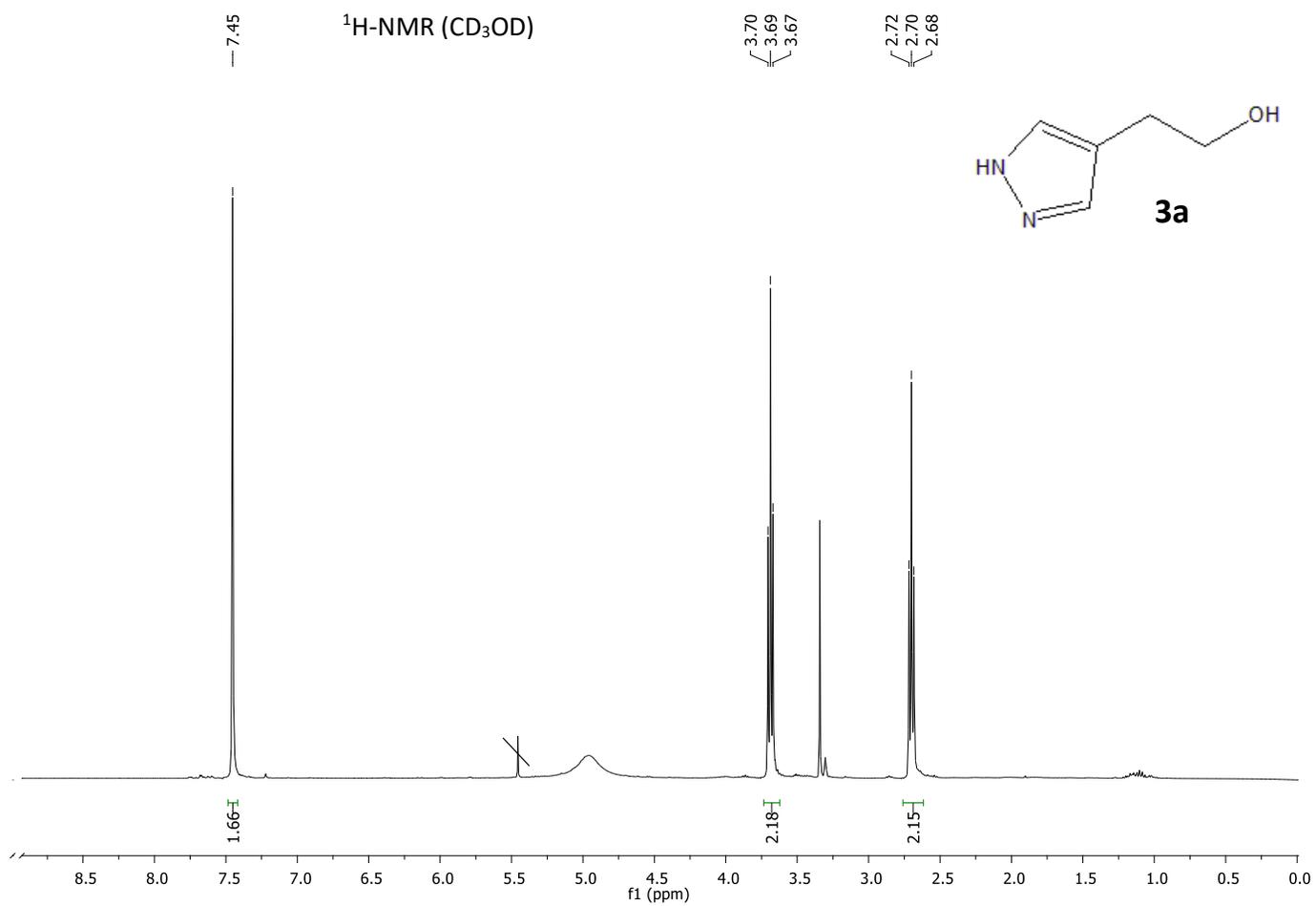
¹H-NMR (CD₃OD)

—7.47

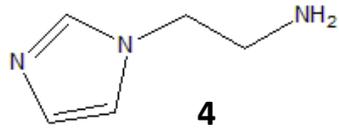


2.87
2.85
2.84
2.69
2.67
2.66





¹H-NMR (CD₃OD)



7.67

7.15

6.99

4.09

4.07

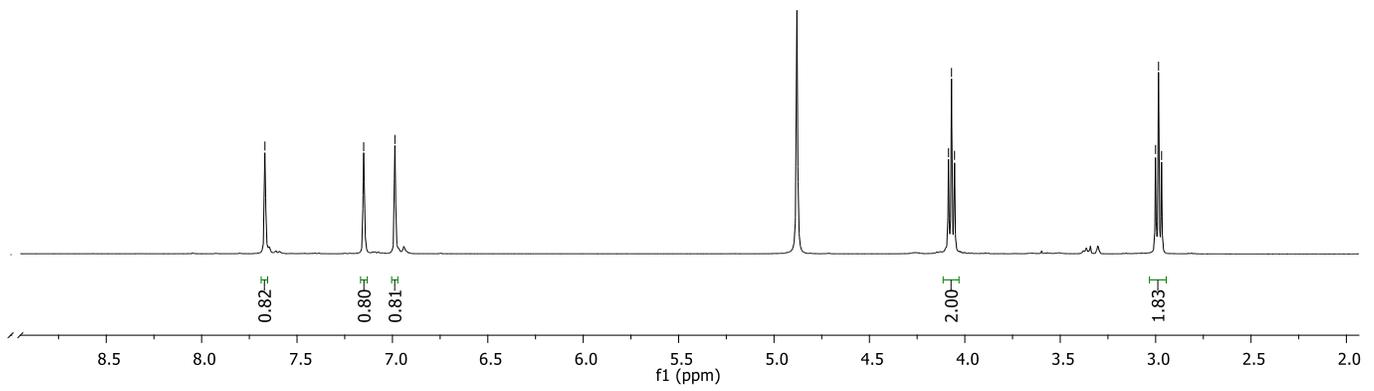
4.05

3.00

2.98

2.97

H₂O



¹³C-NMR
(APT, CD₃OD)

137.31

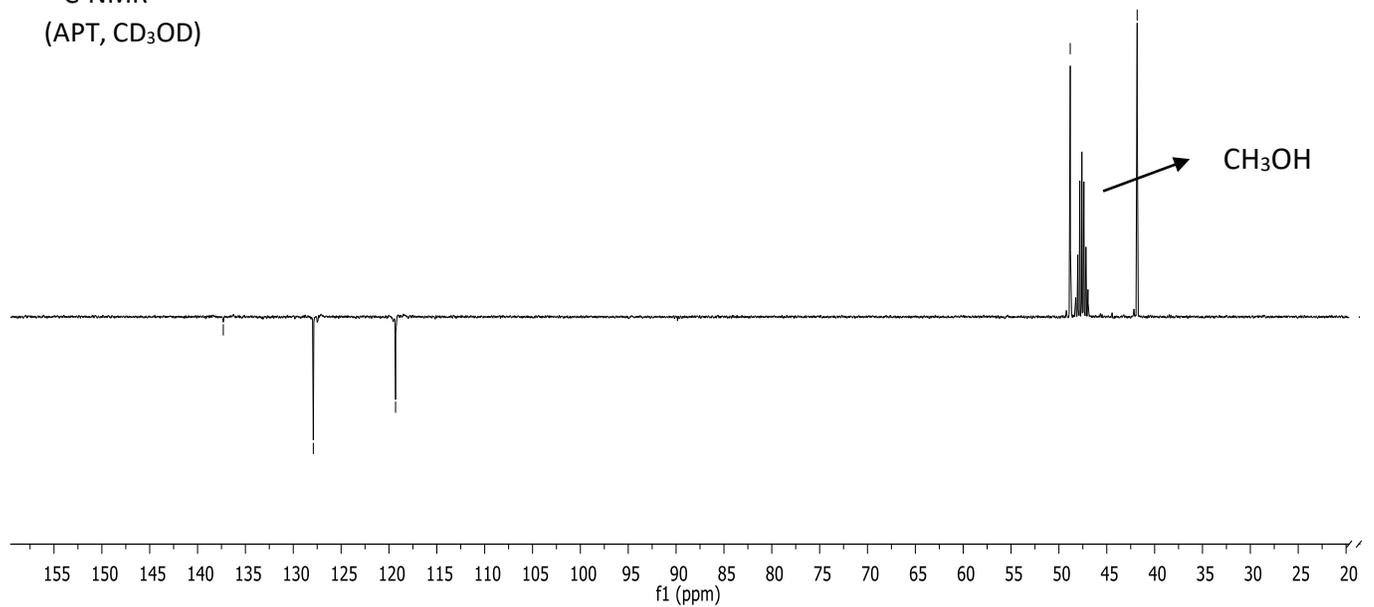
127.90

119.31

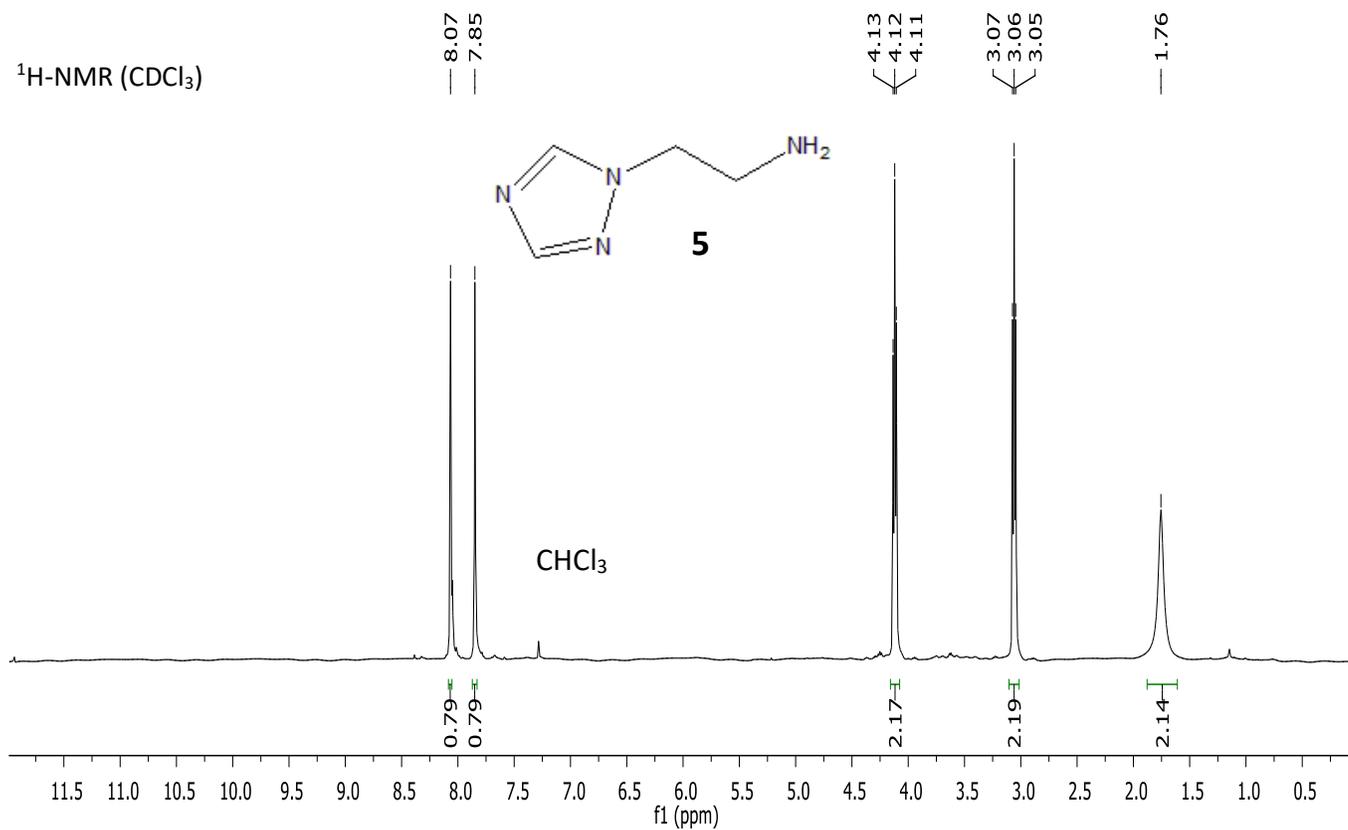
48.82

41.82

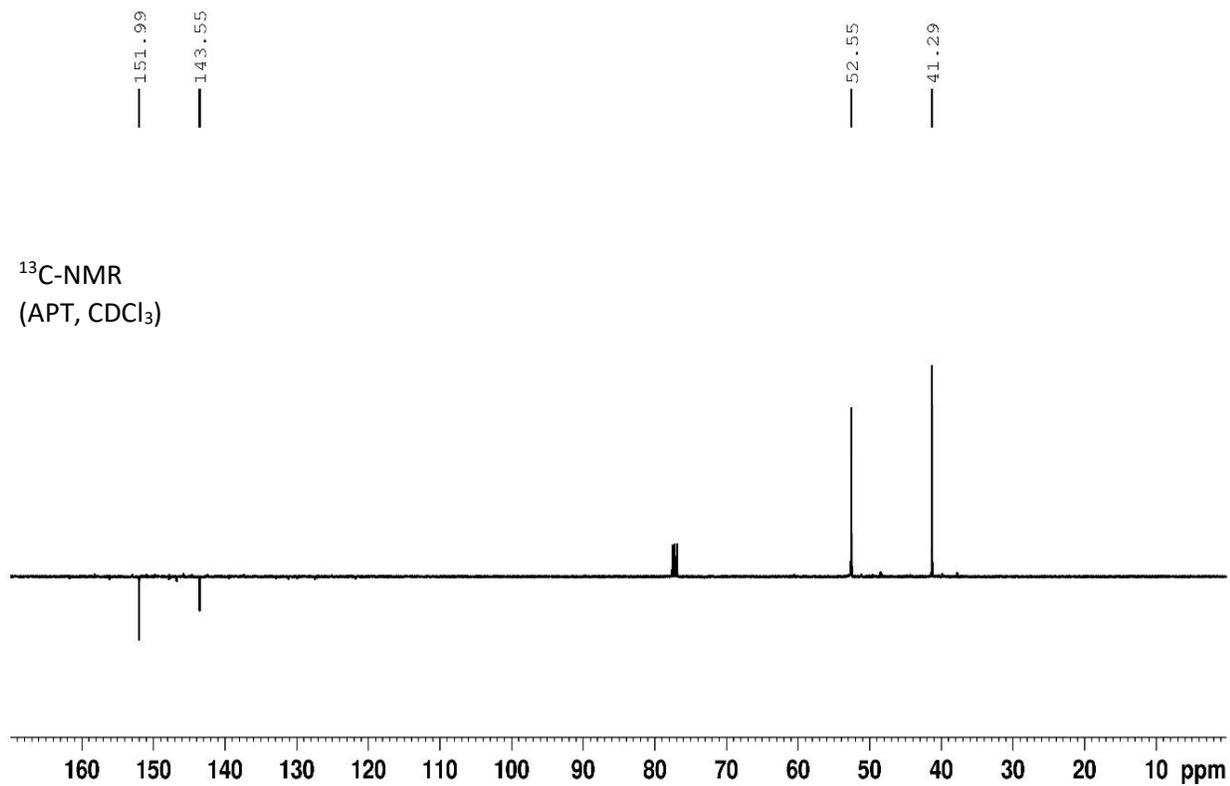
CH₃OH



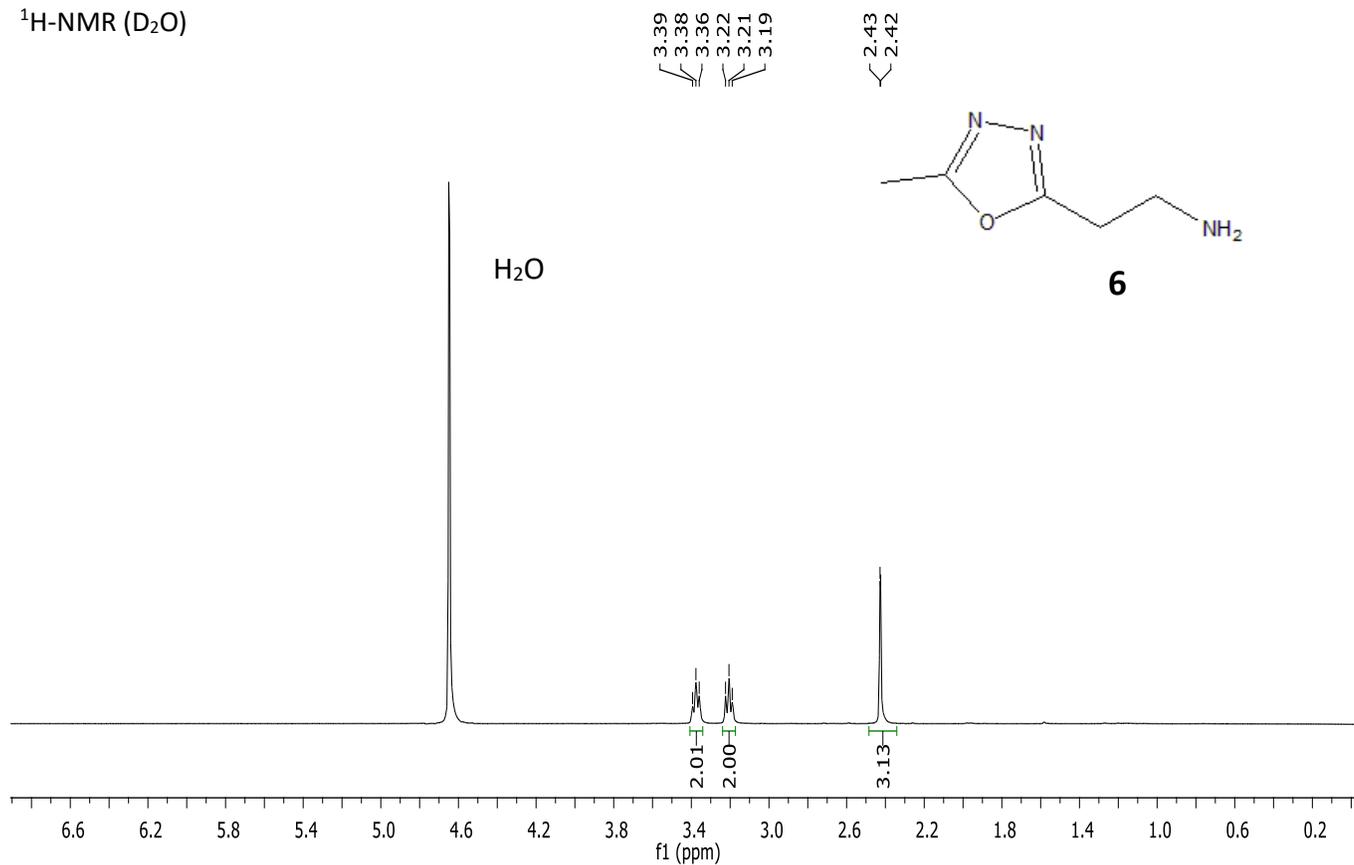
$^1\text{H-NMR}$ (CDCl_3)



$^{13}\text{C-NMR}$
(APT, CDCl_3)



$^1\text{H-NMR}$ (D_2O)



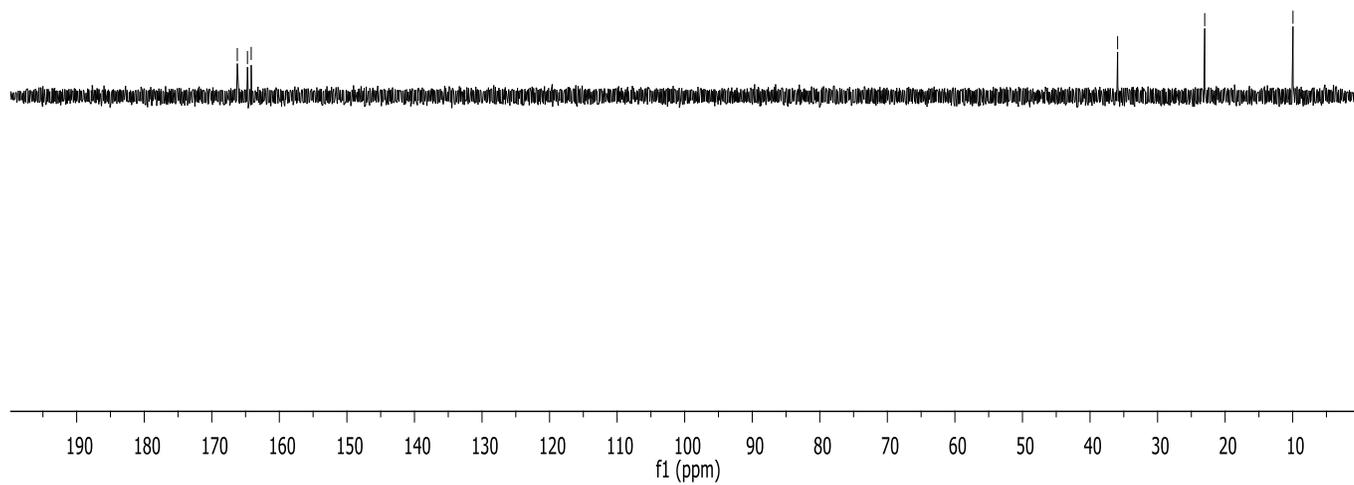
166.23
164.72
164.17

6 (oxalate salt)
 $^{13}\text{C-NMR}$
(Proton decoupled, D_2O)

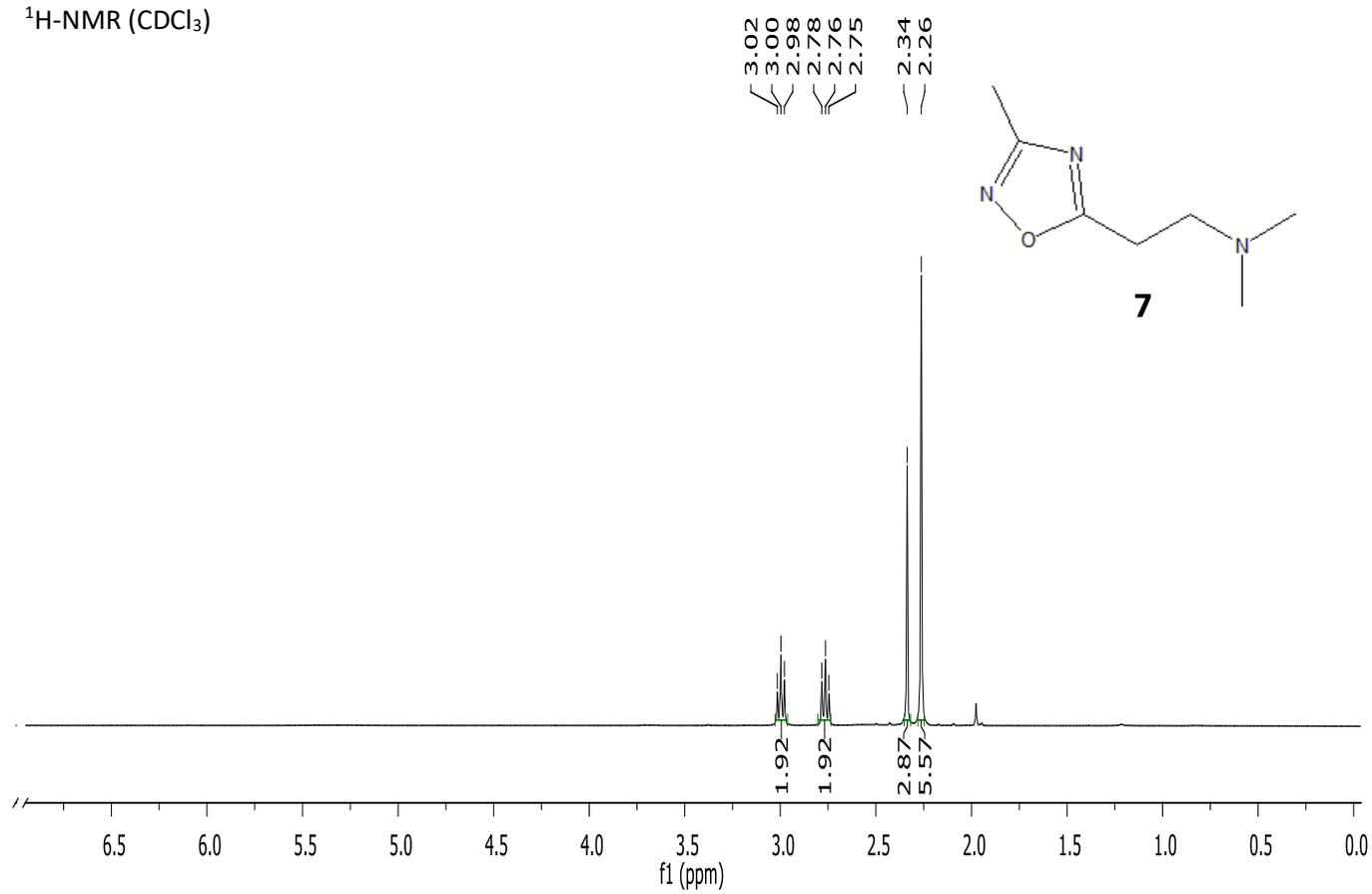
— 35.92

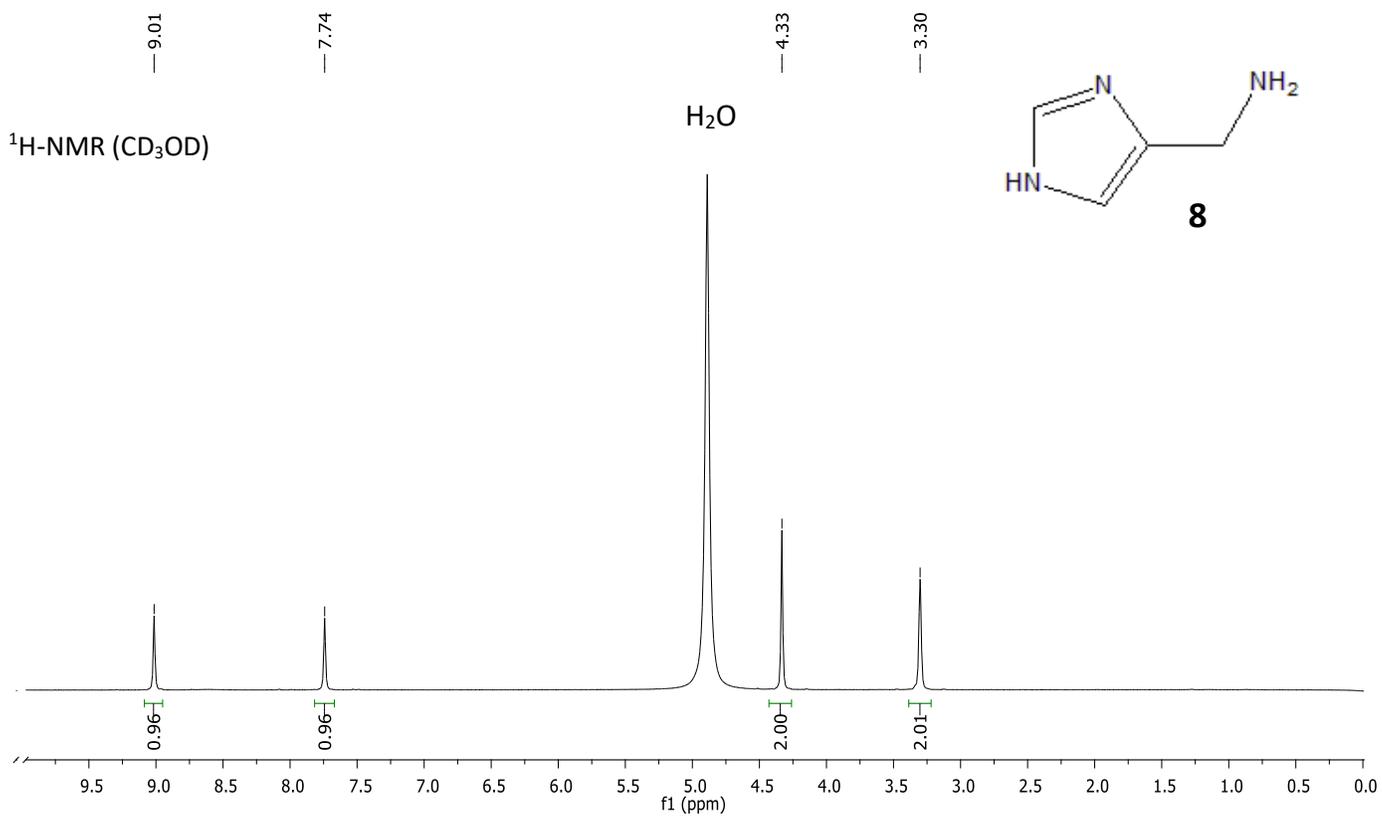
— 23.02

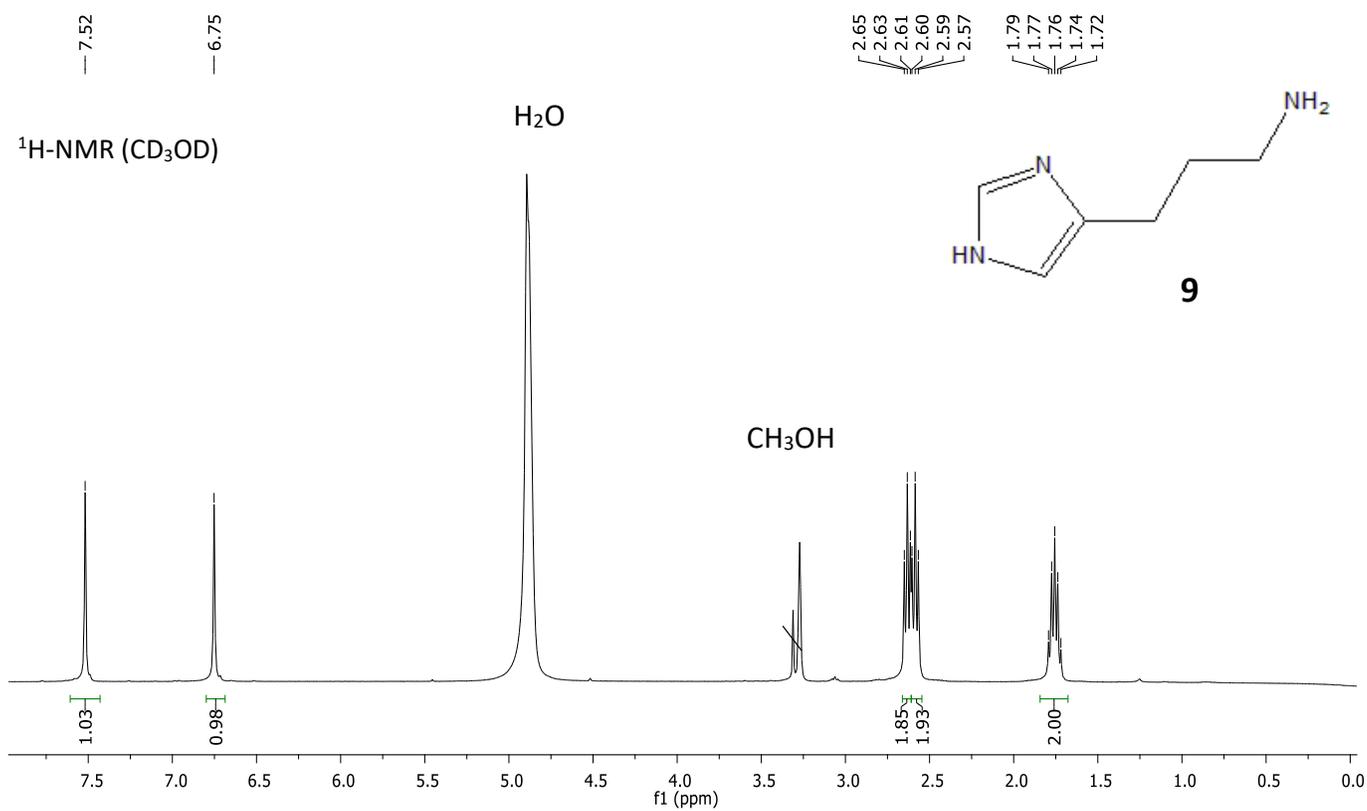
— 9.96

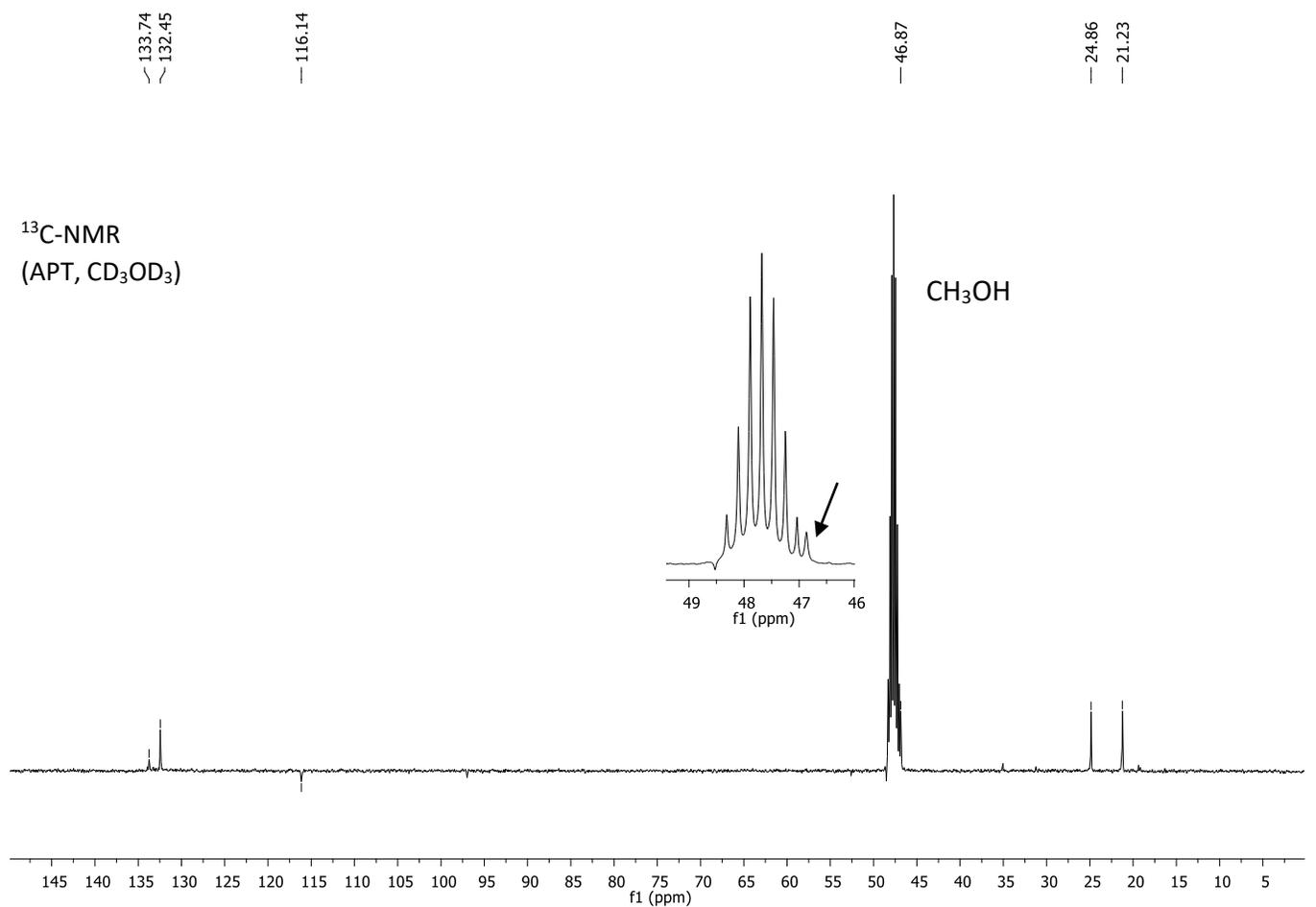
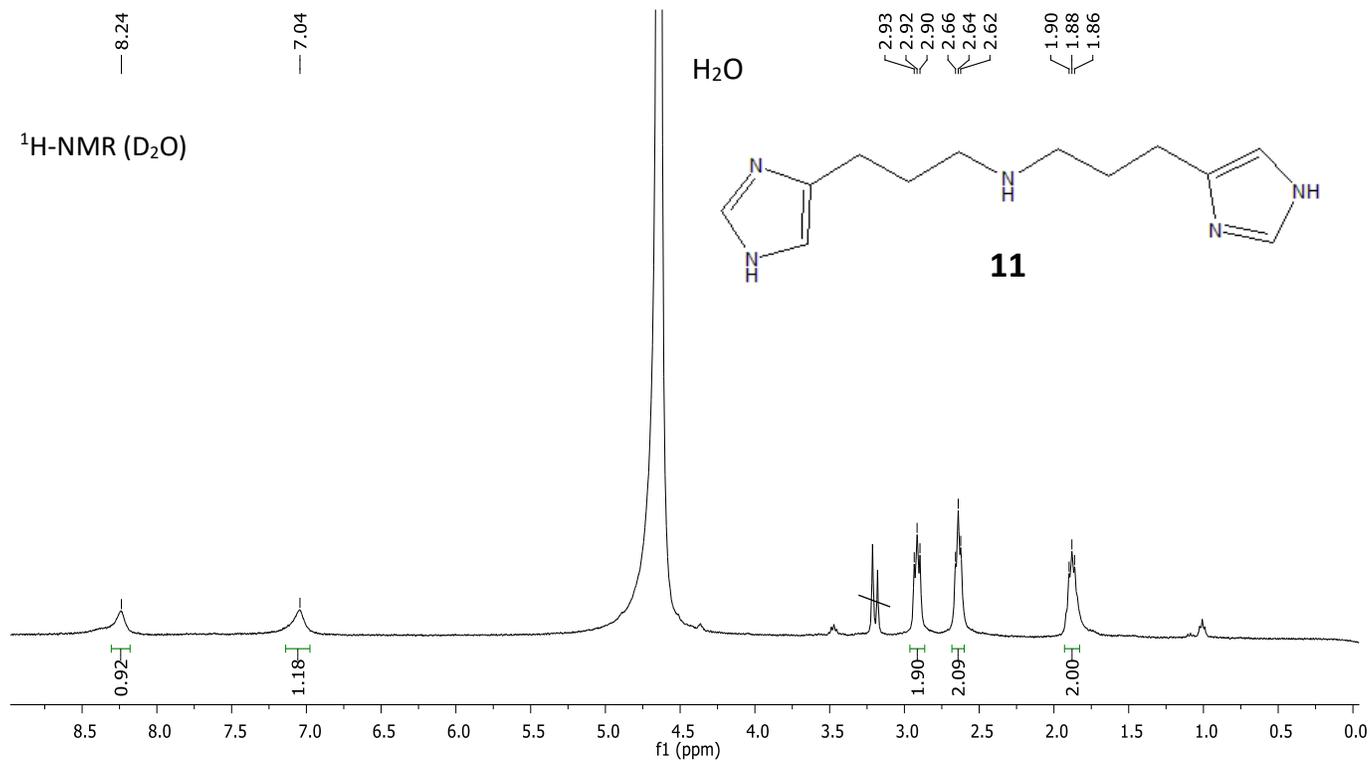


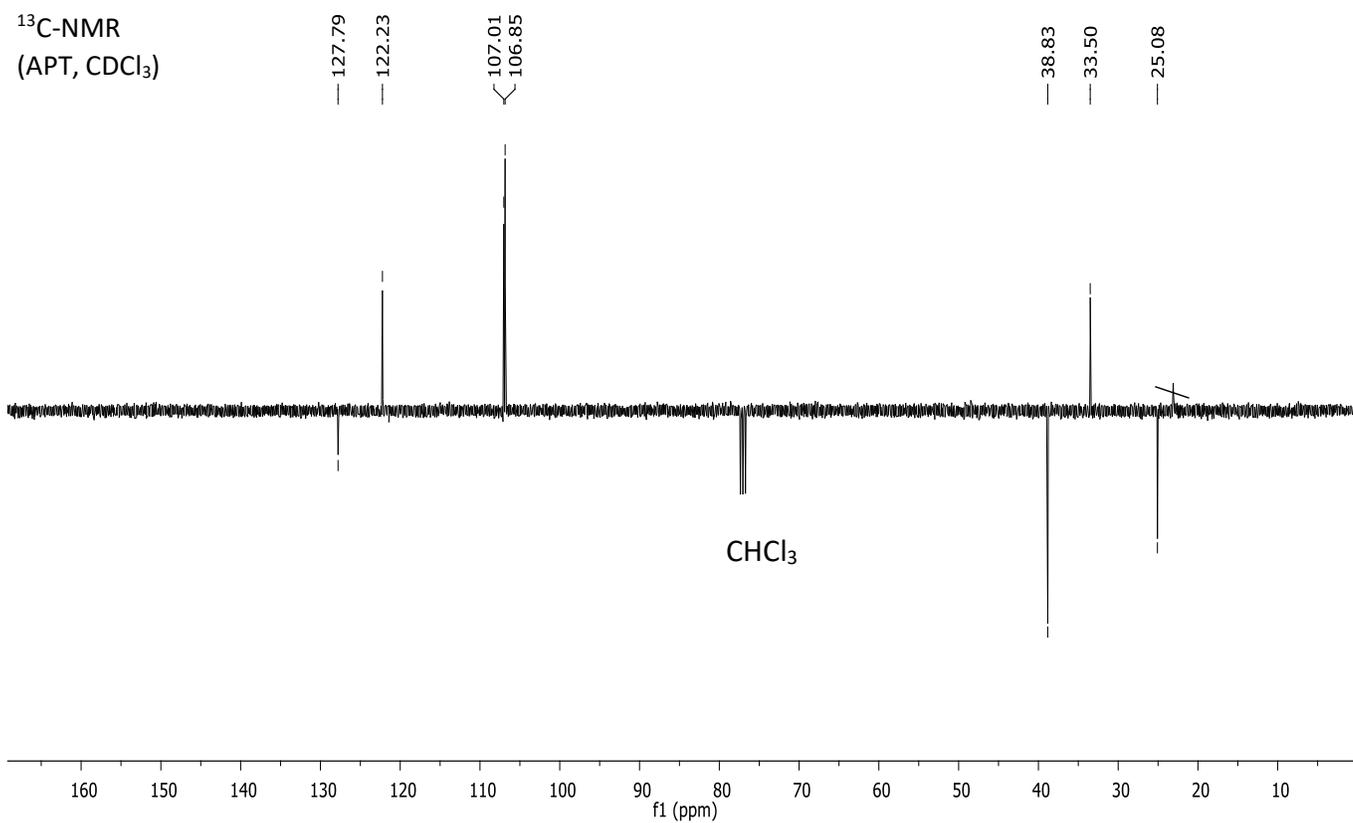
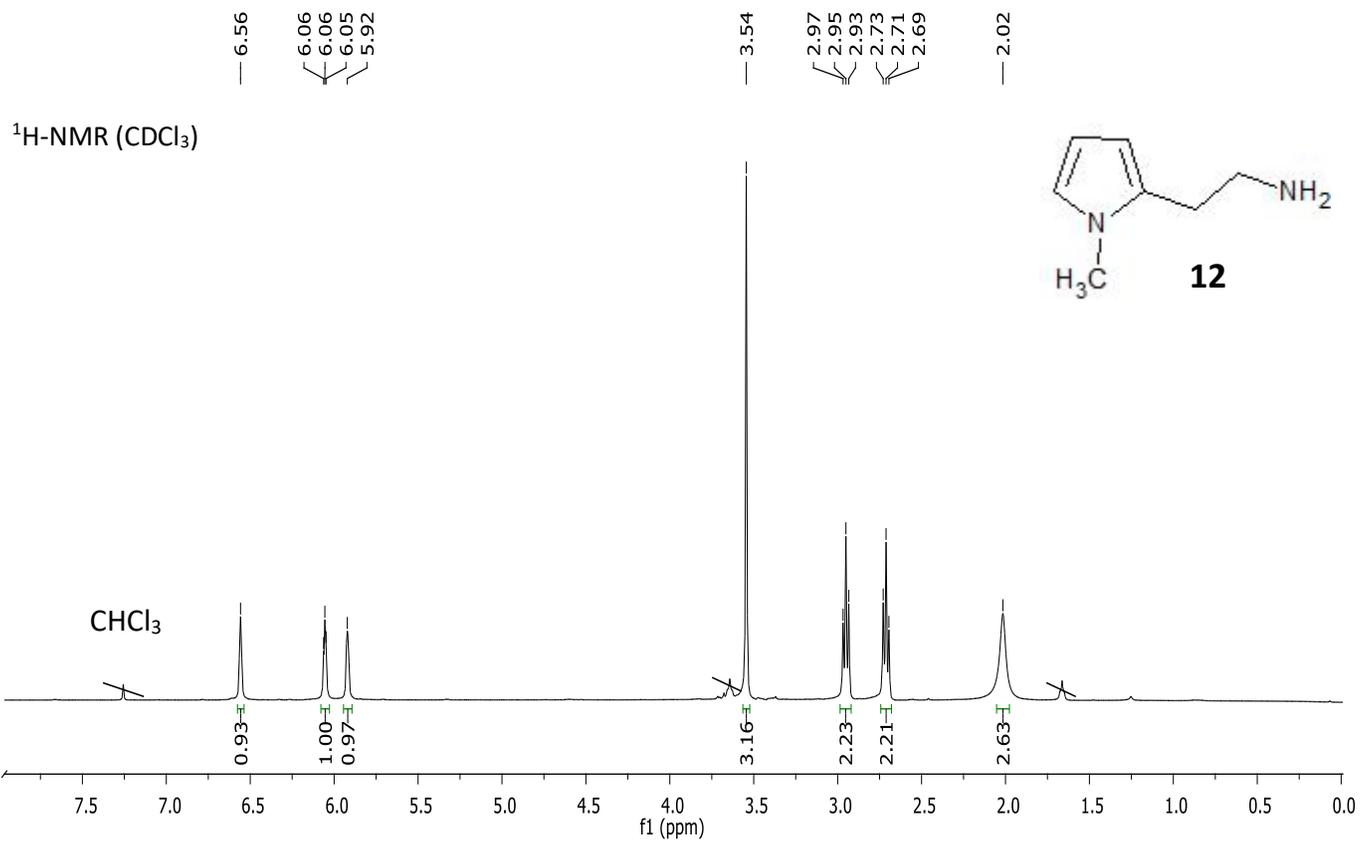
$^1\text{H-NMR}$ (CDCl_3)

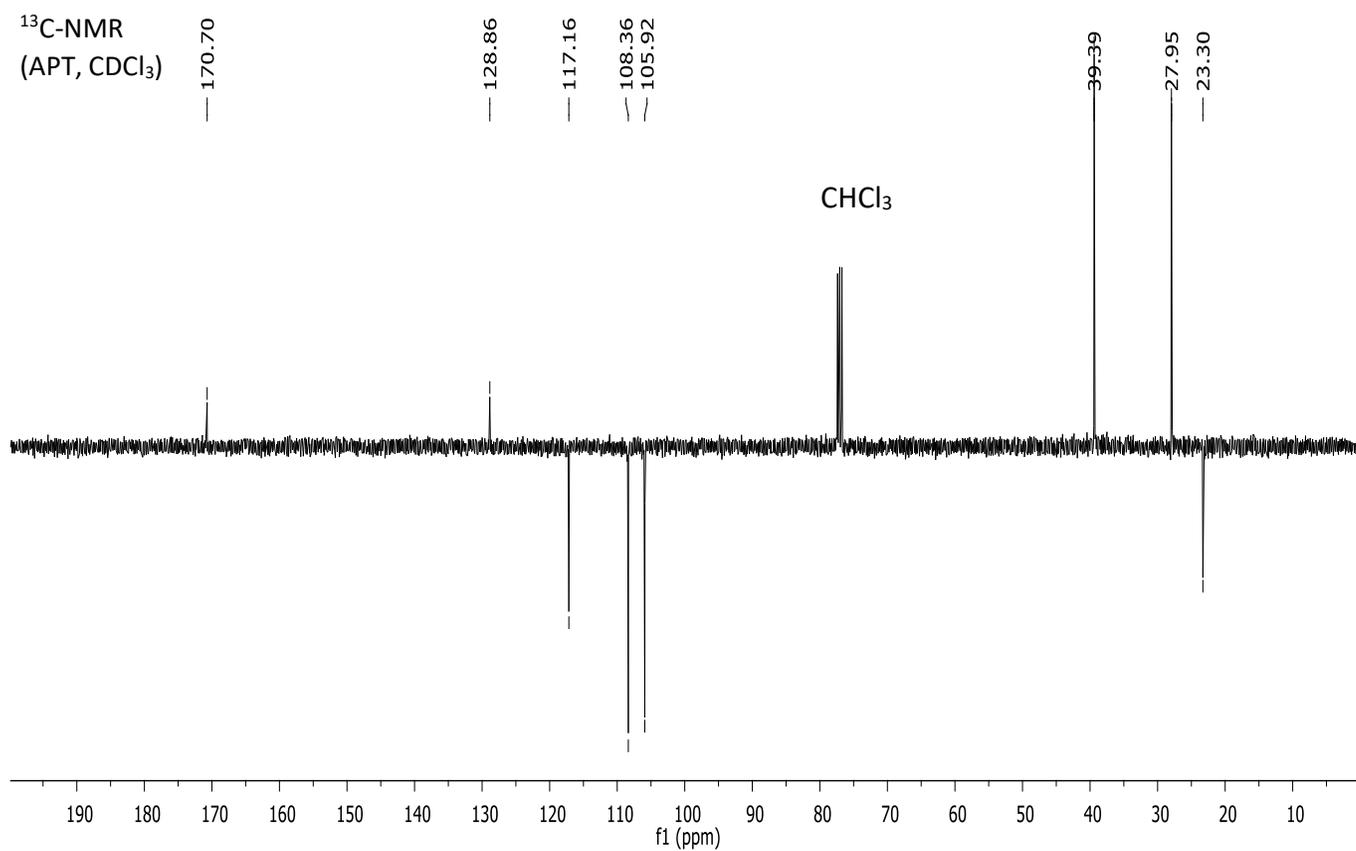
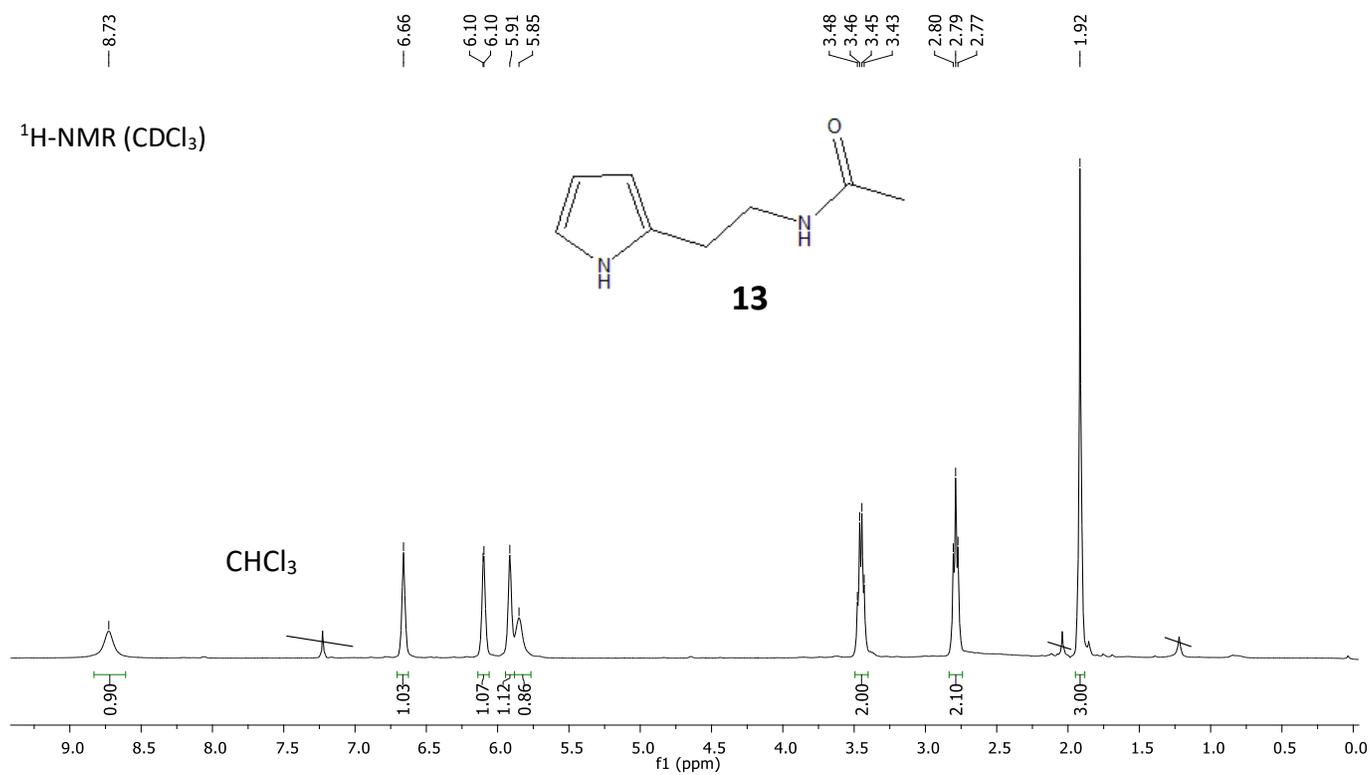


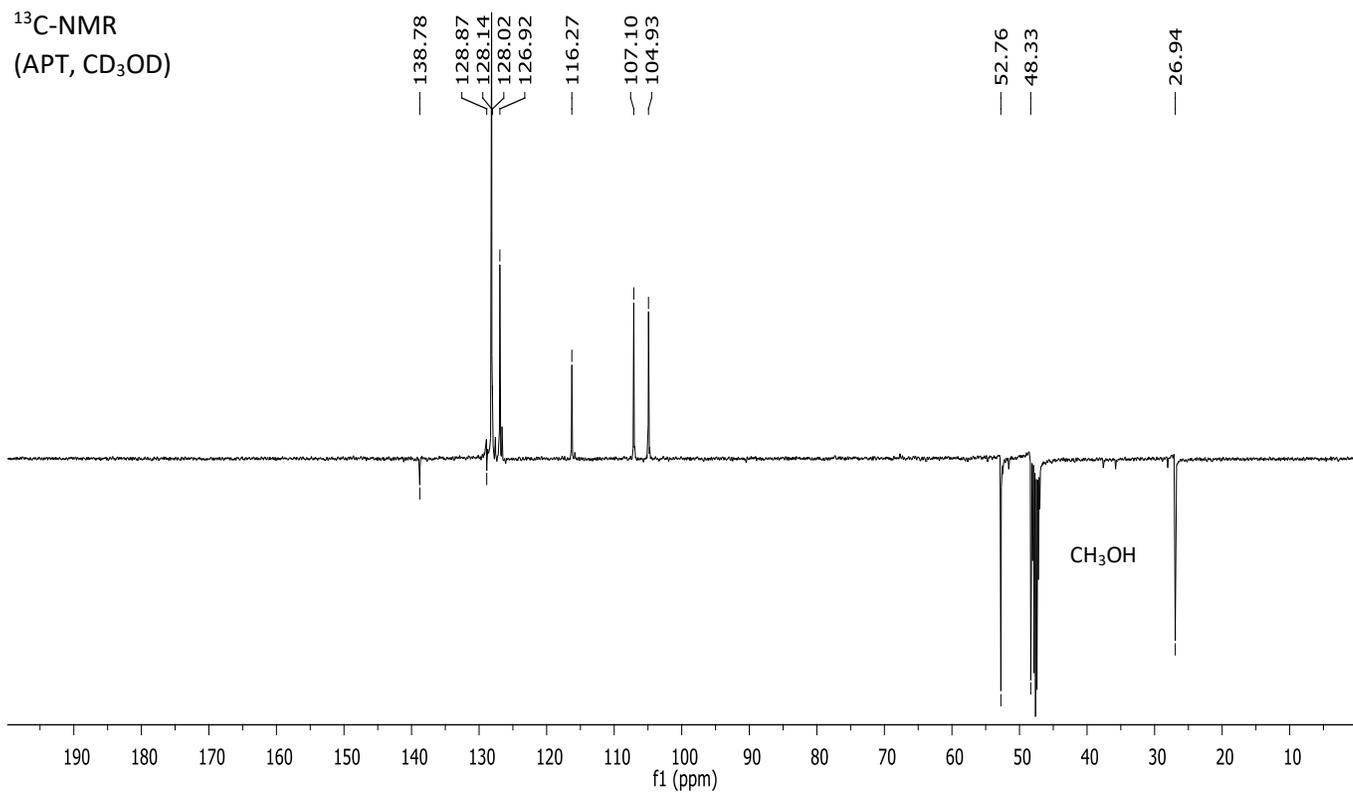
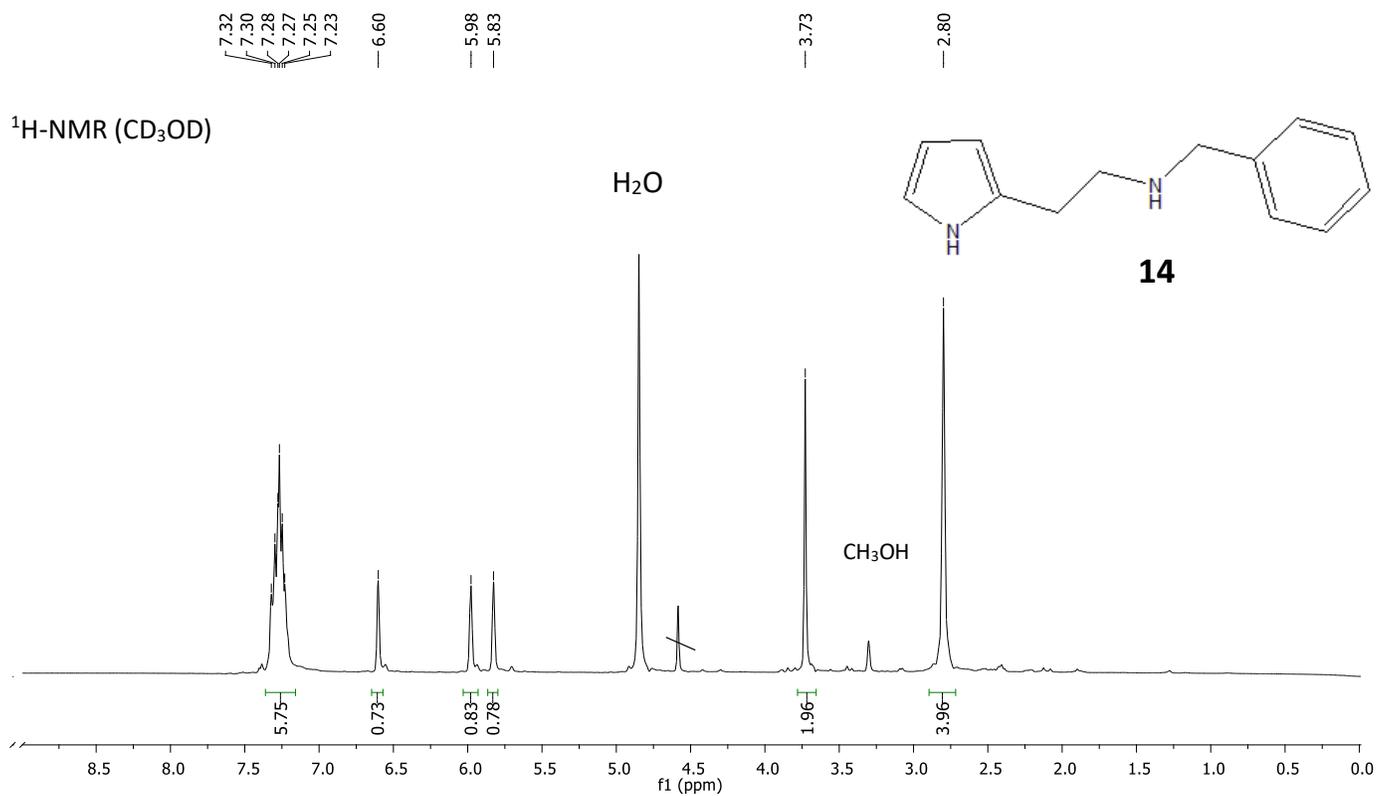


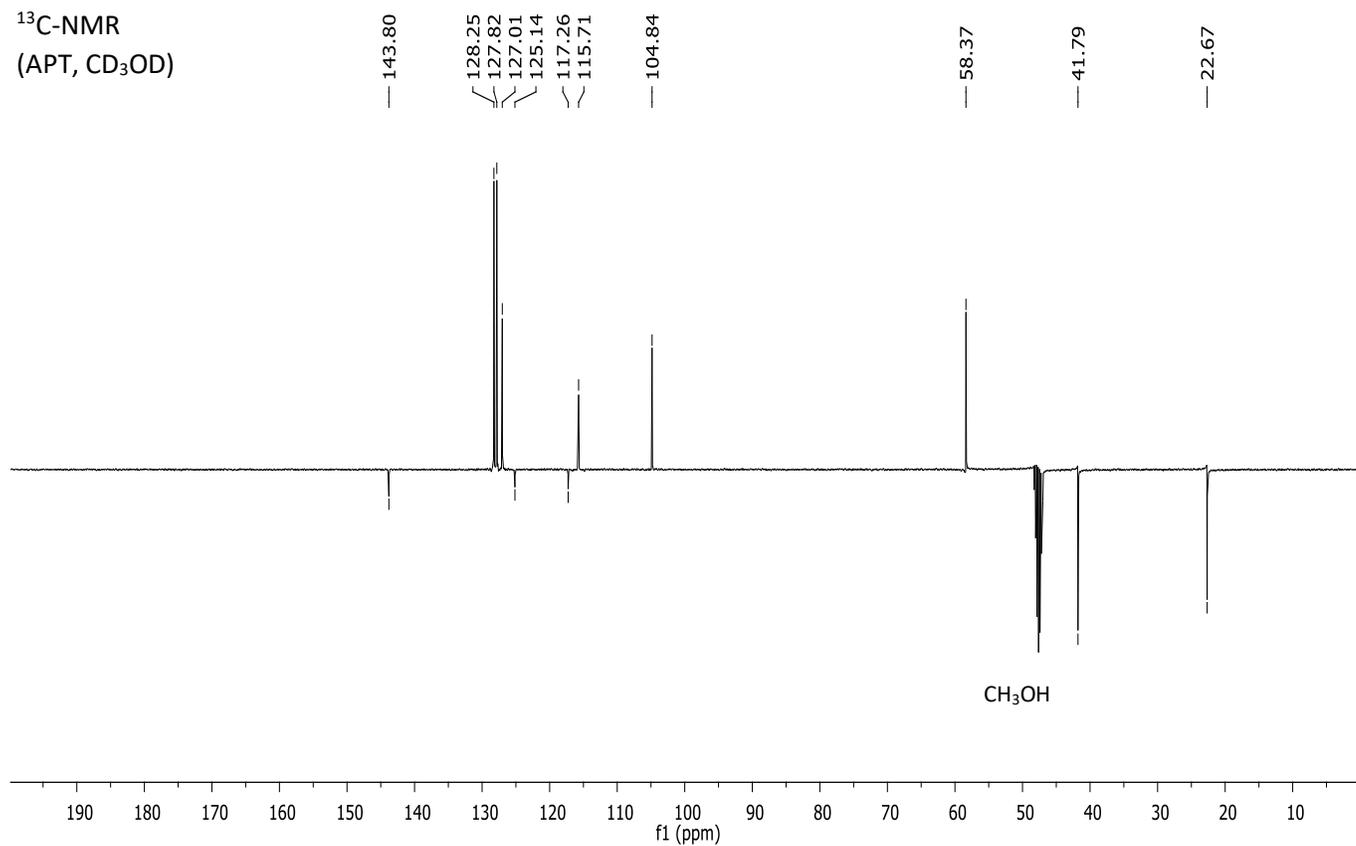
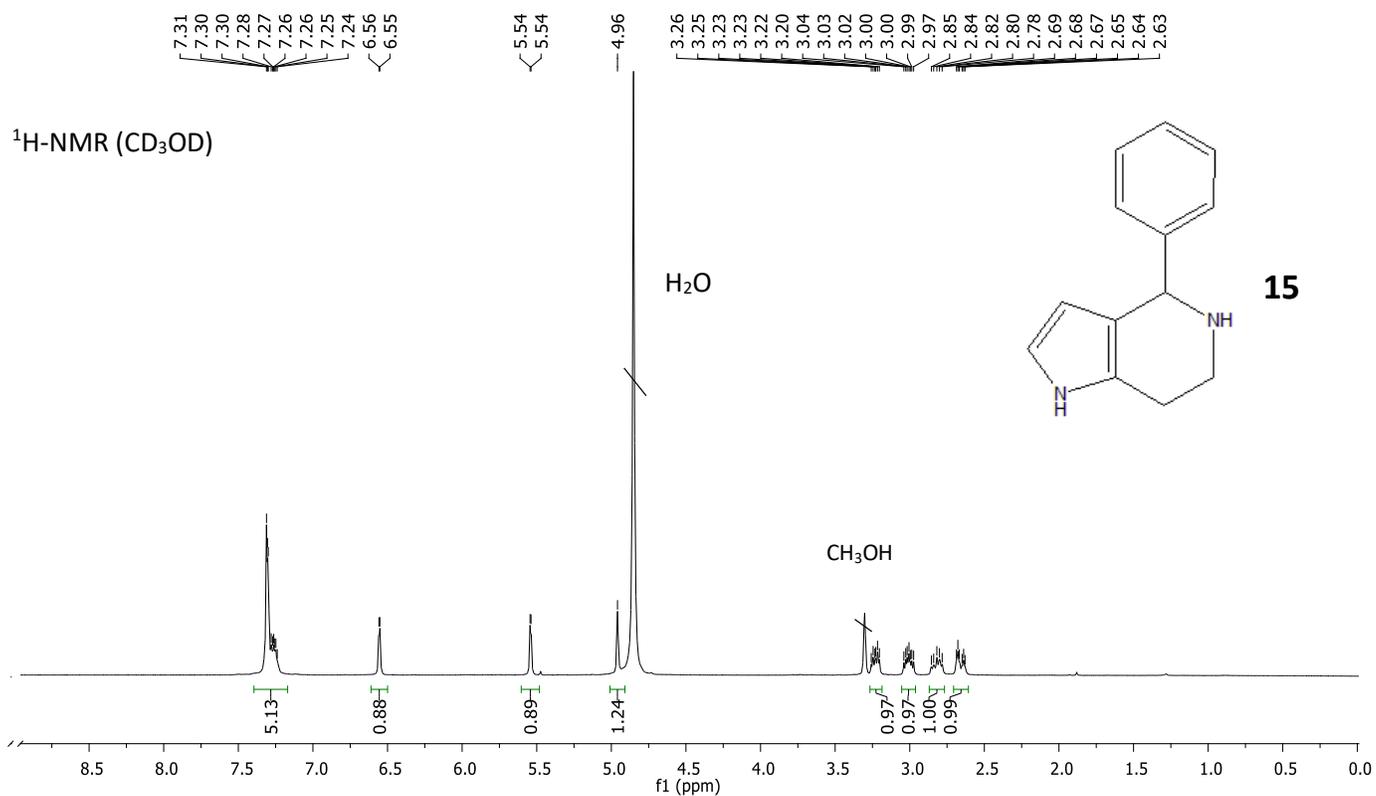


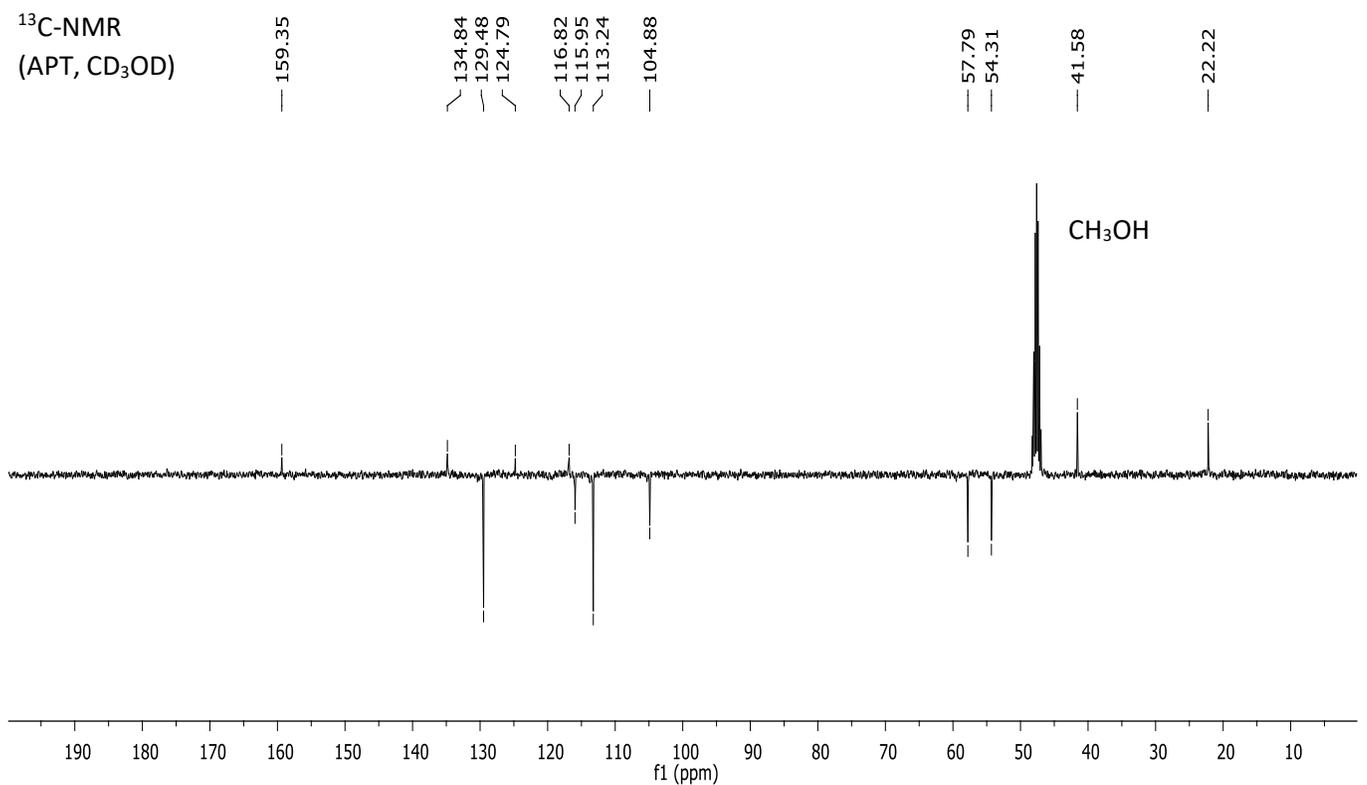
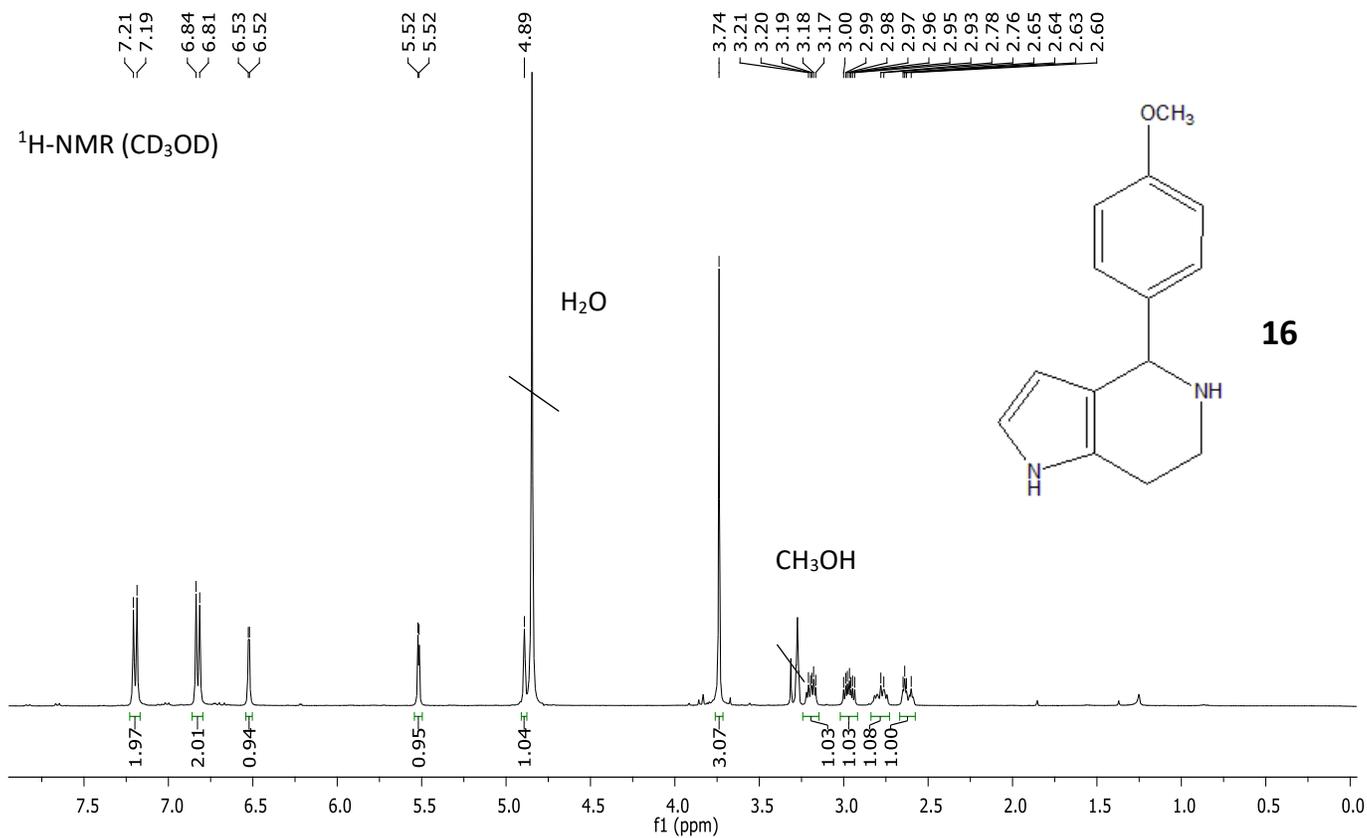


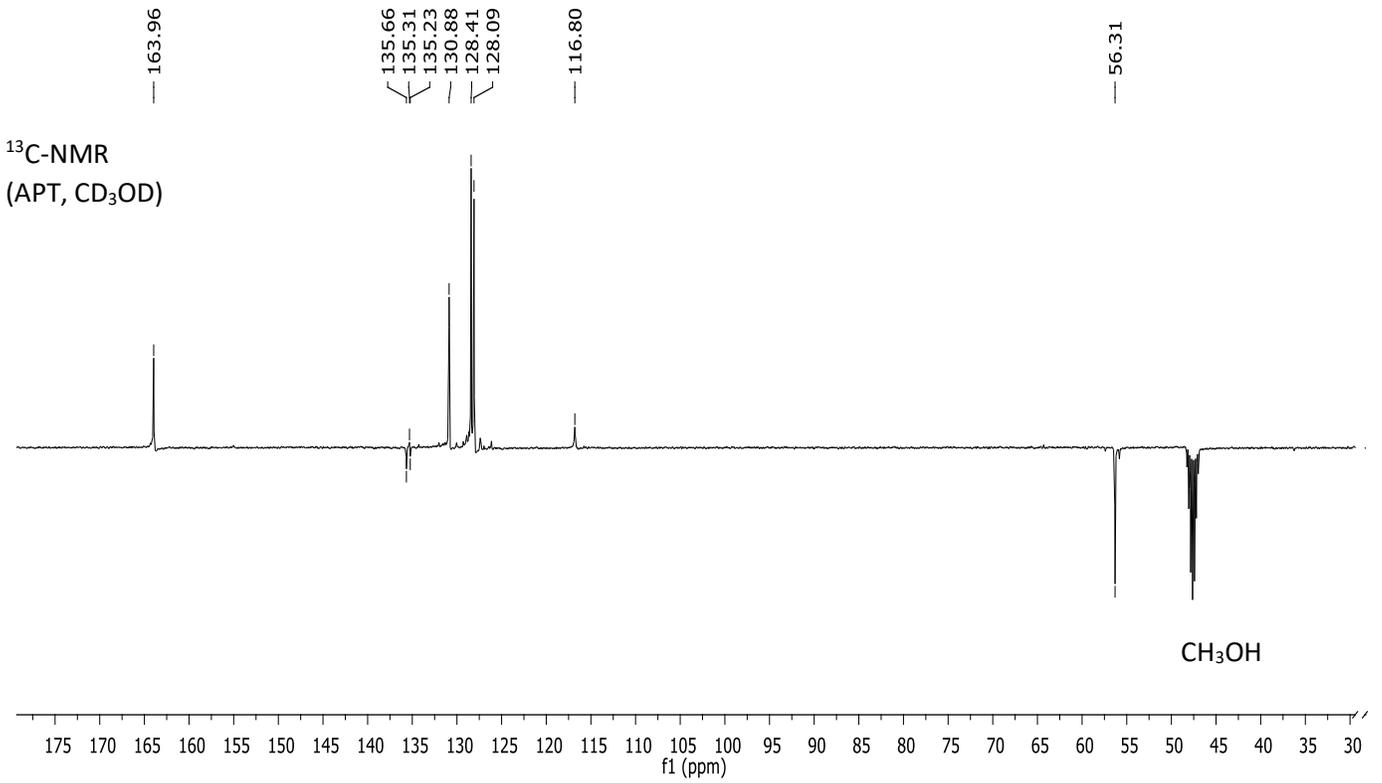
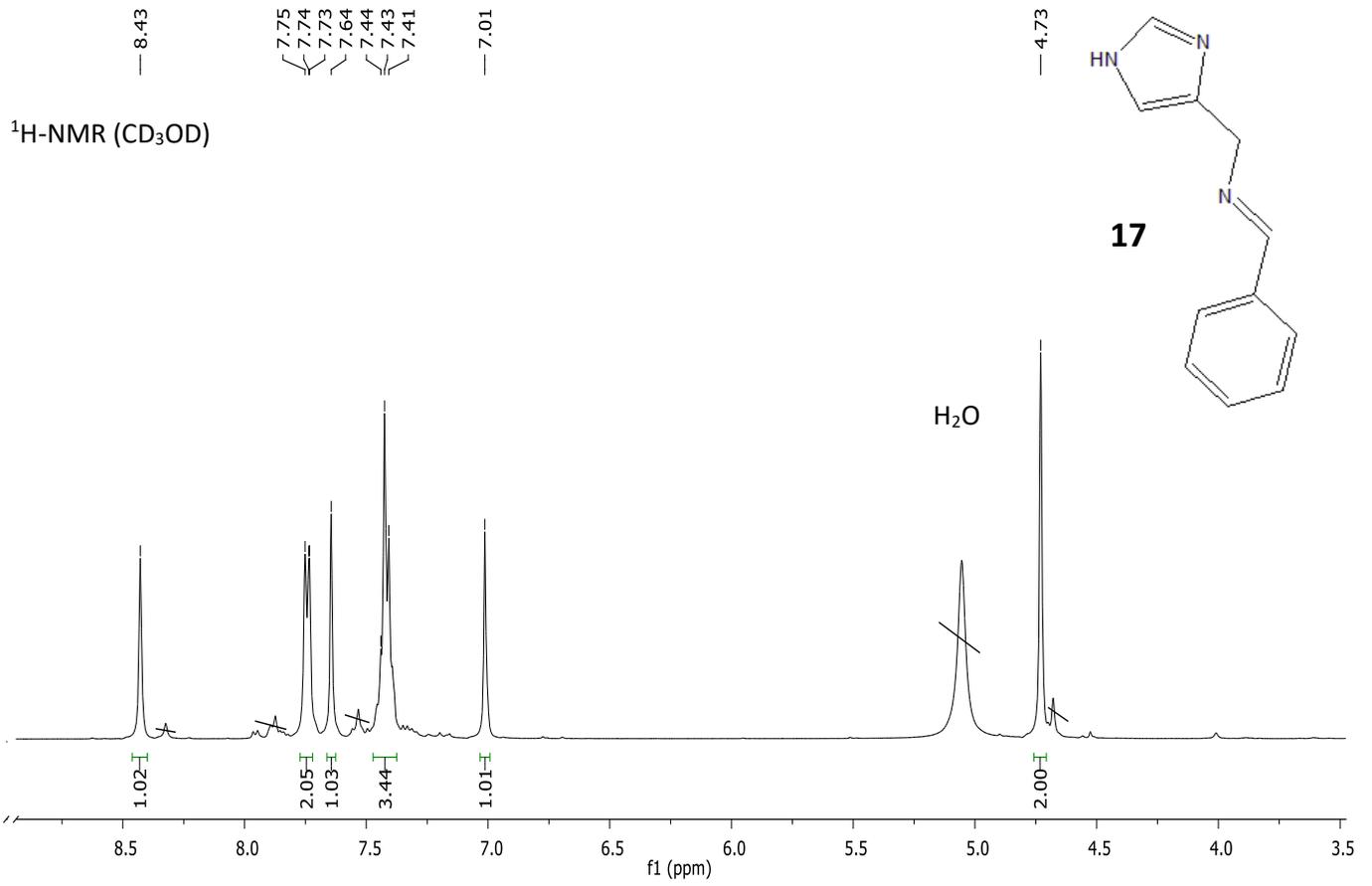


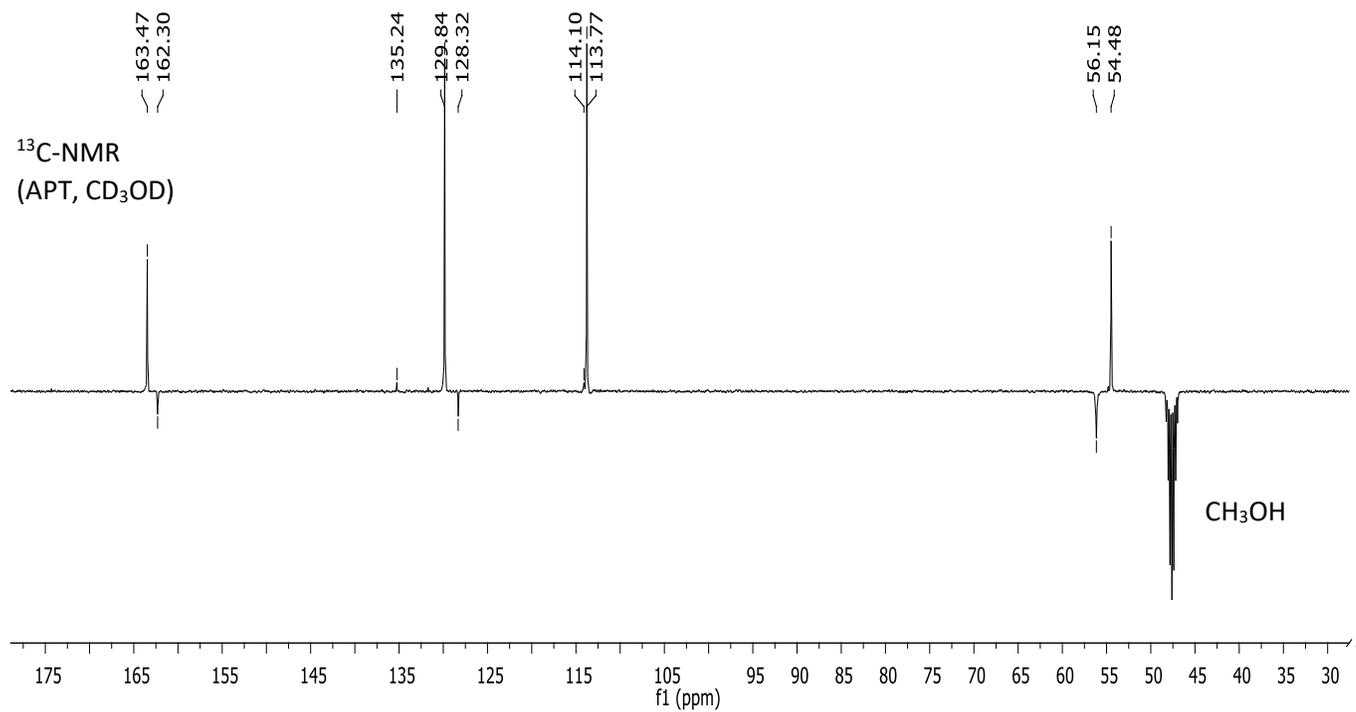
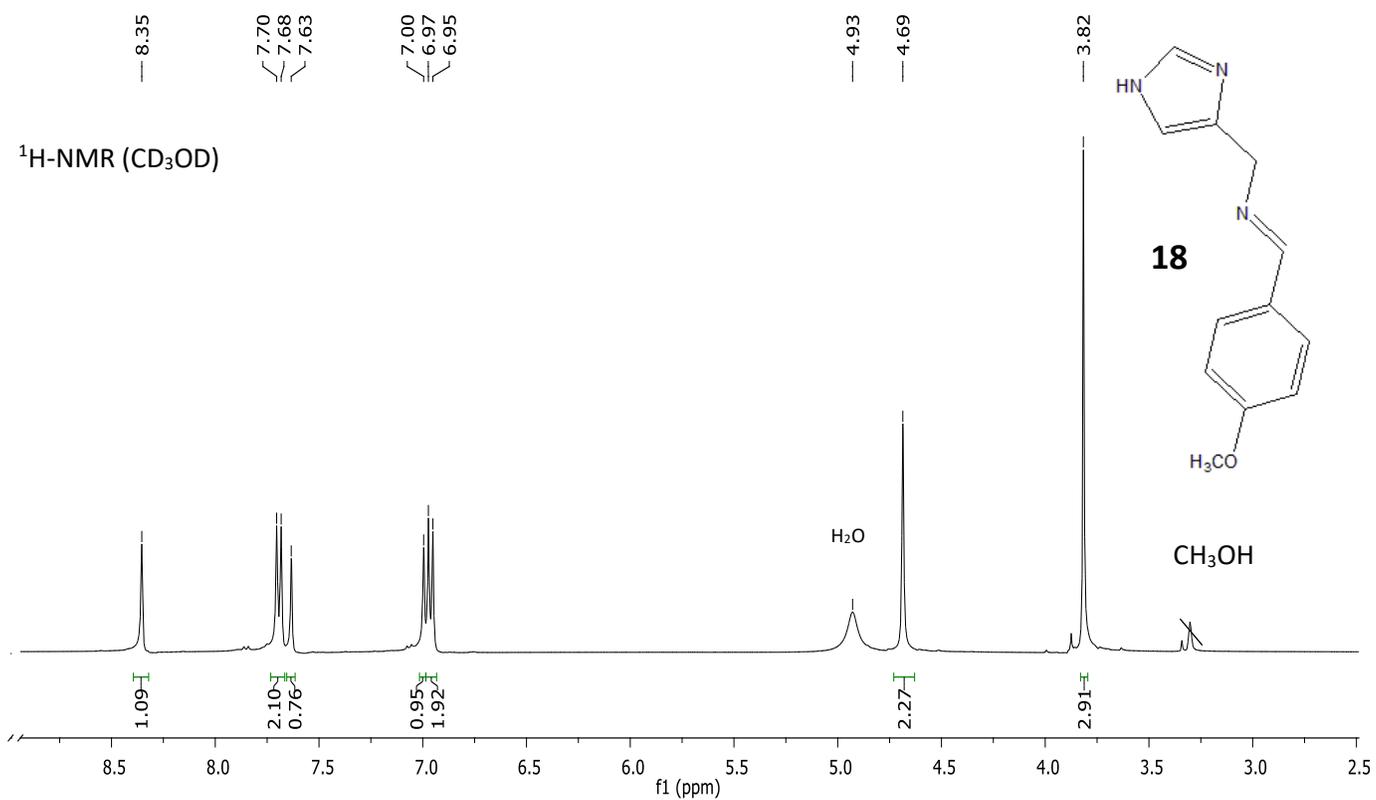


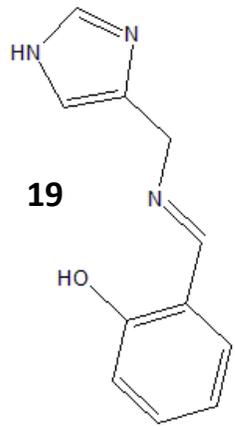




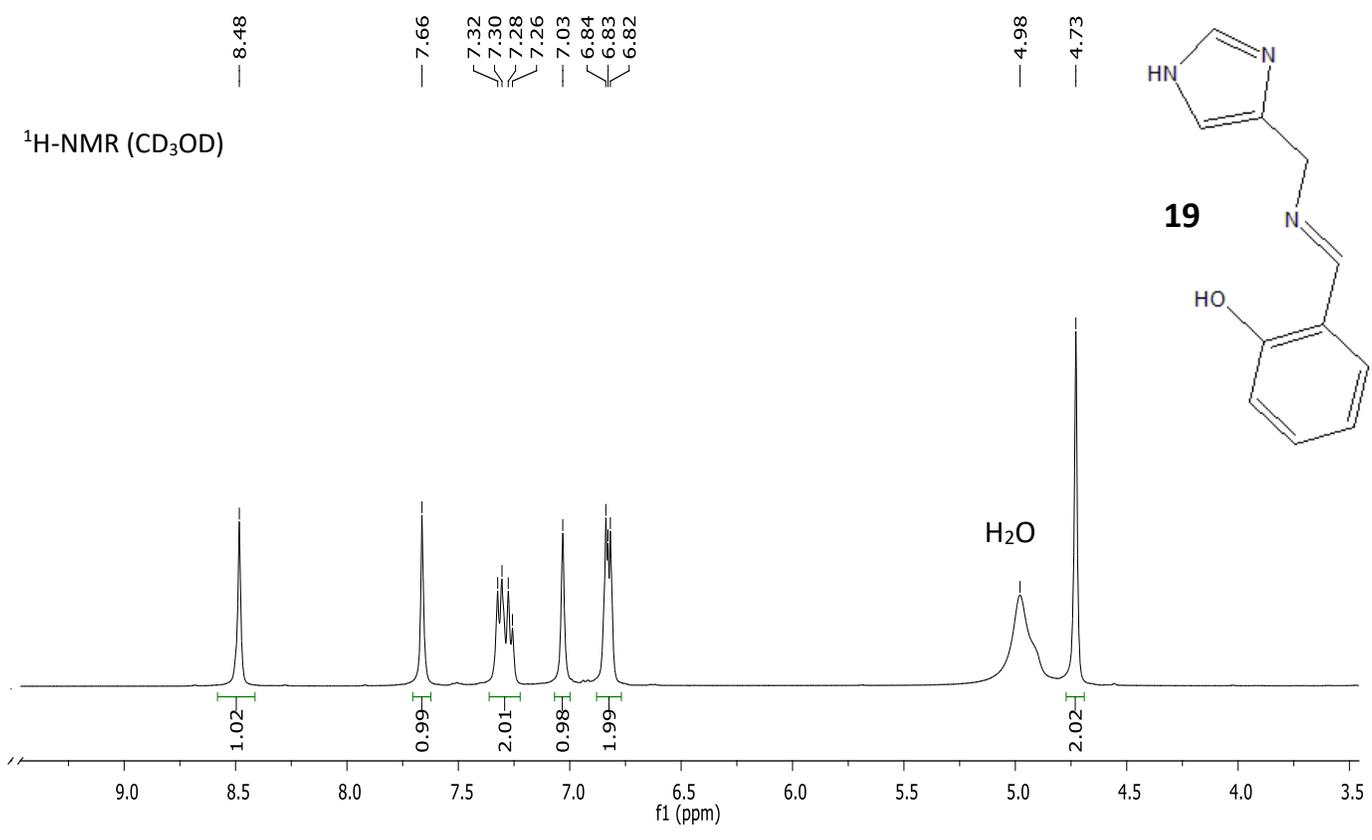




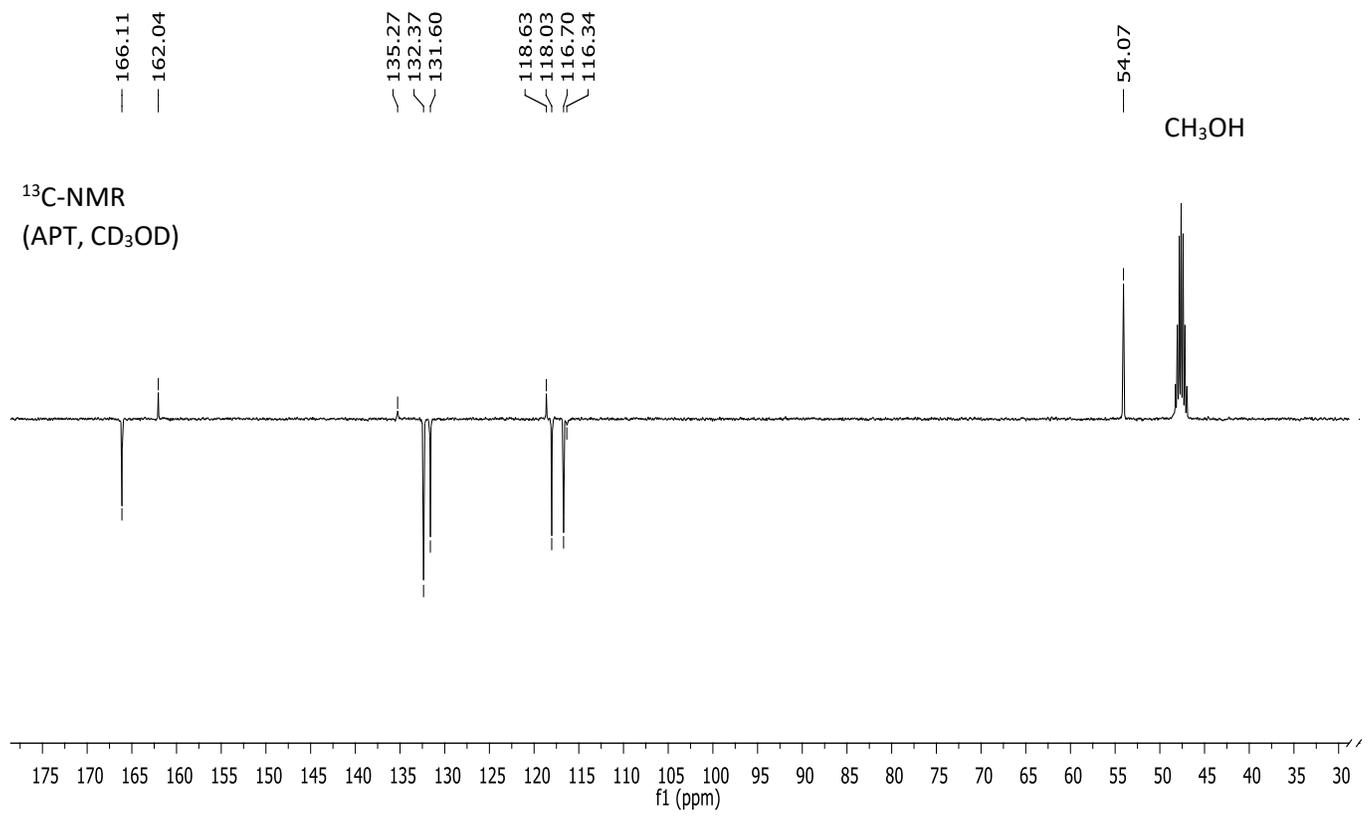


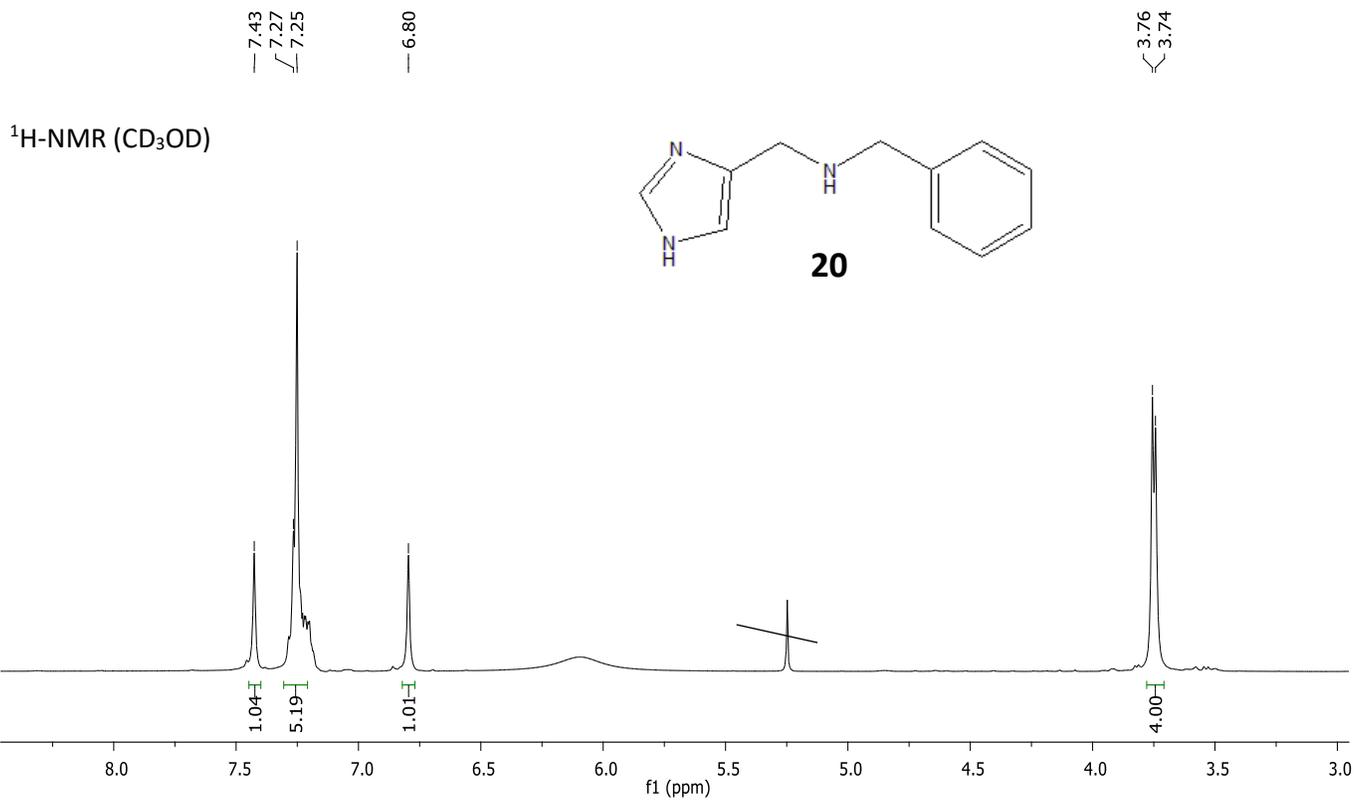


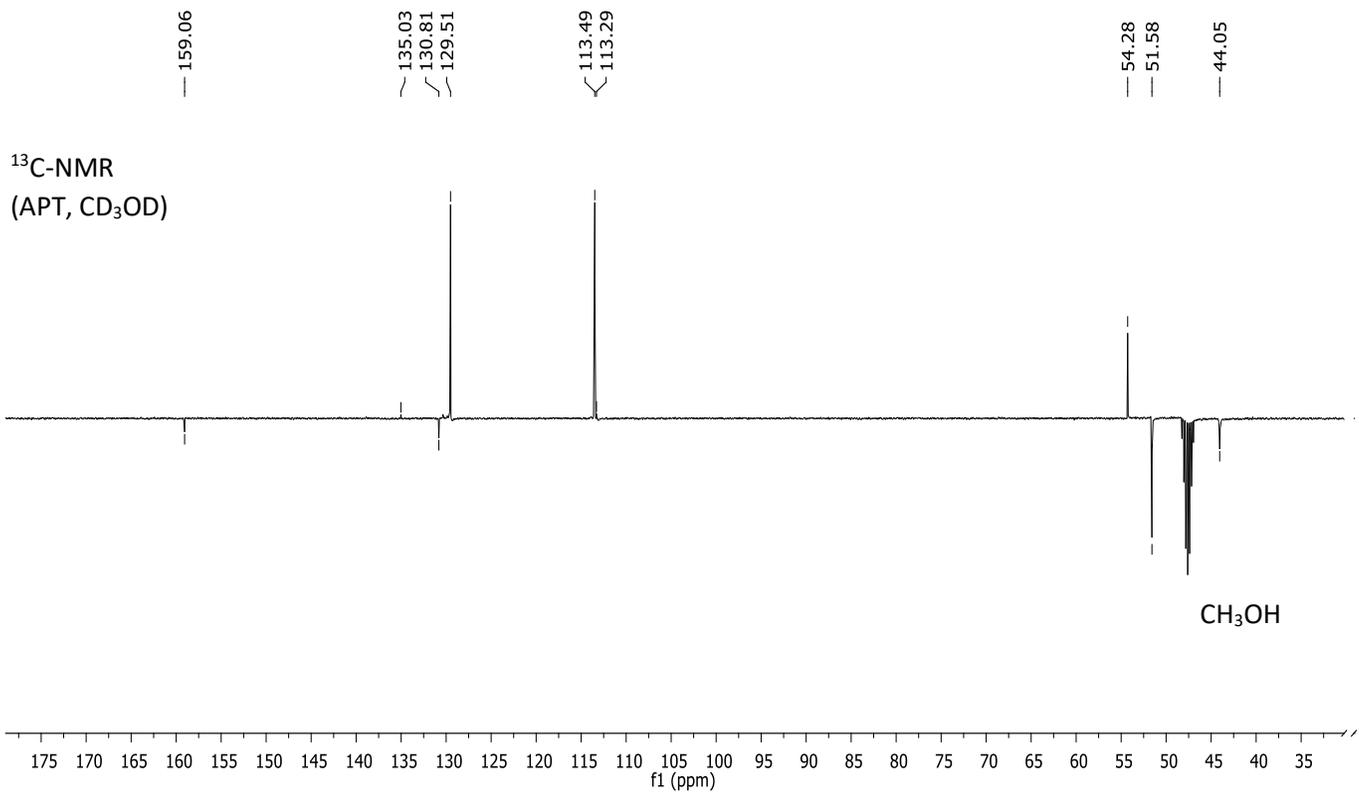
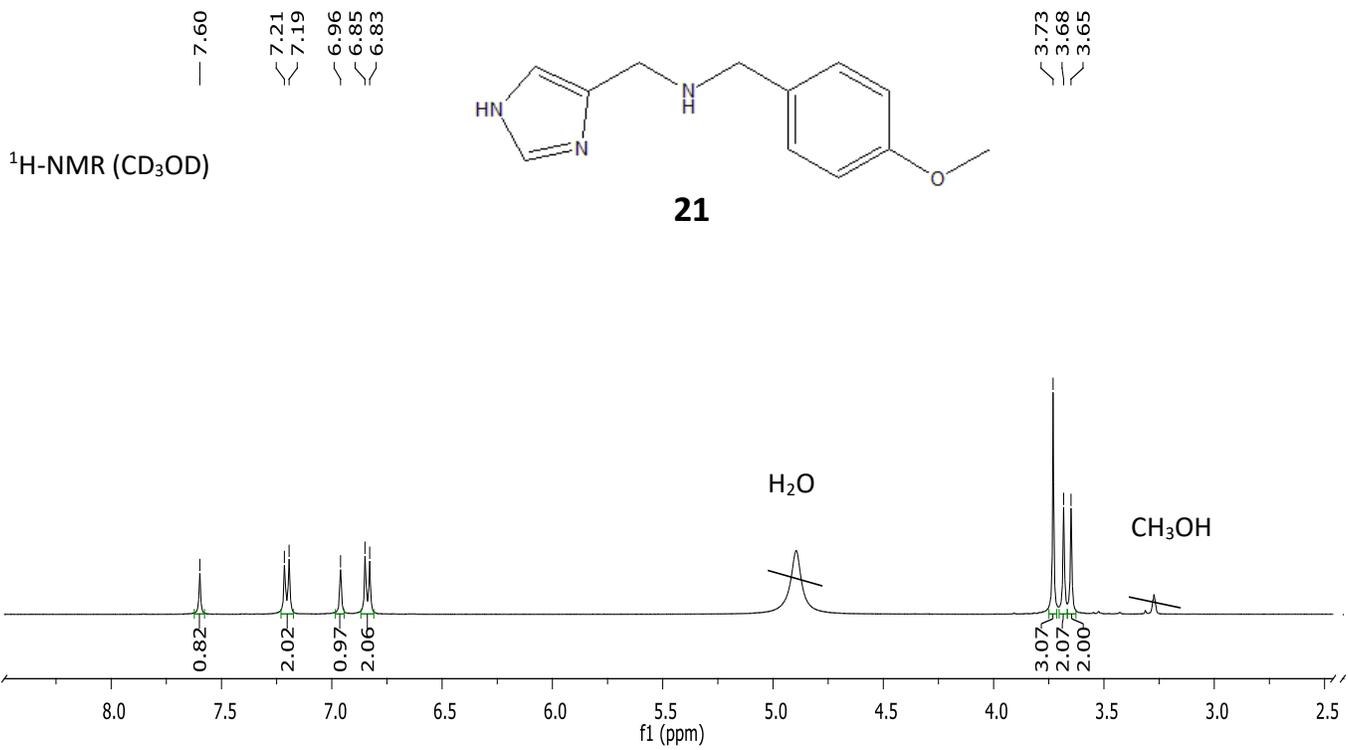
¹H-NMR (CD₃OD)



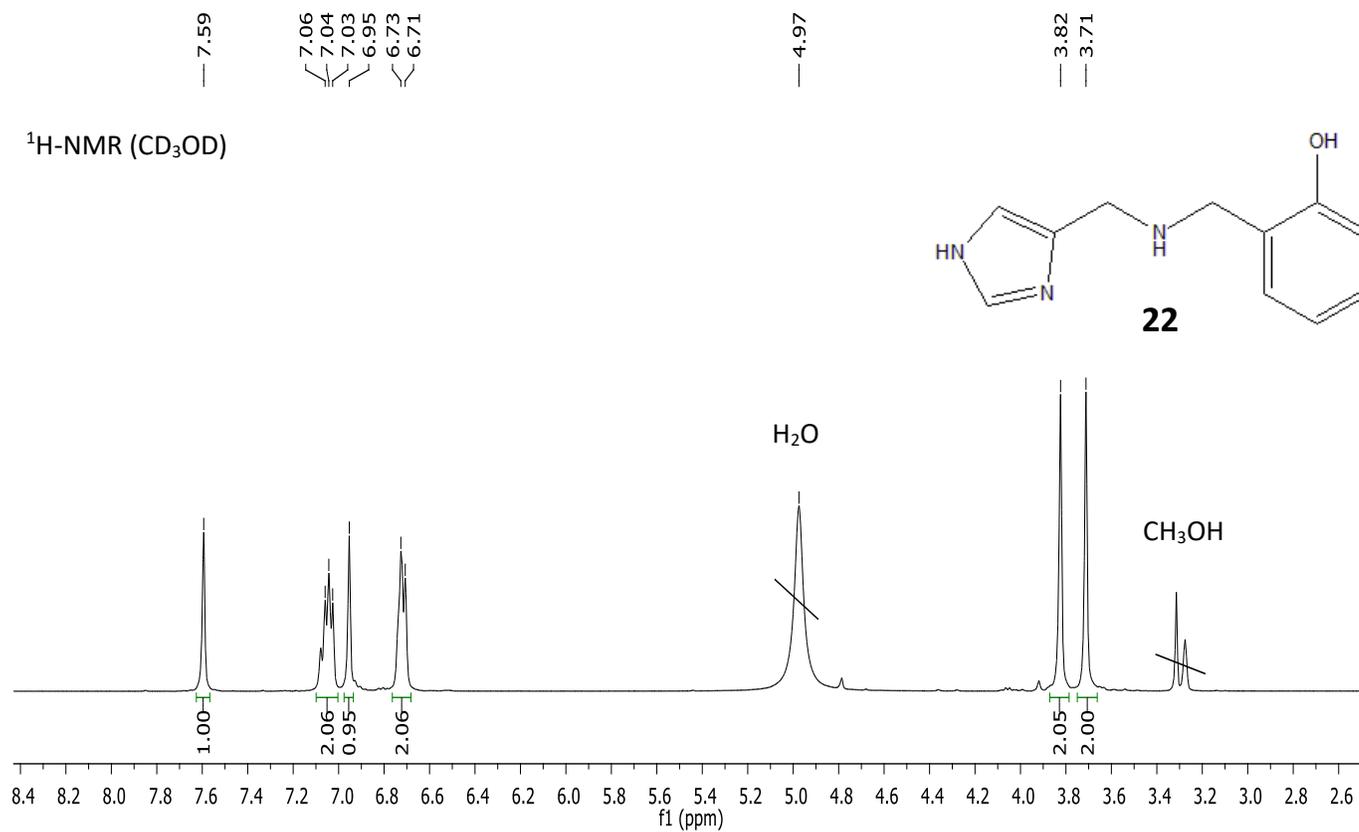
¹³C-NMR (APT, CD₃OD)



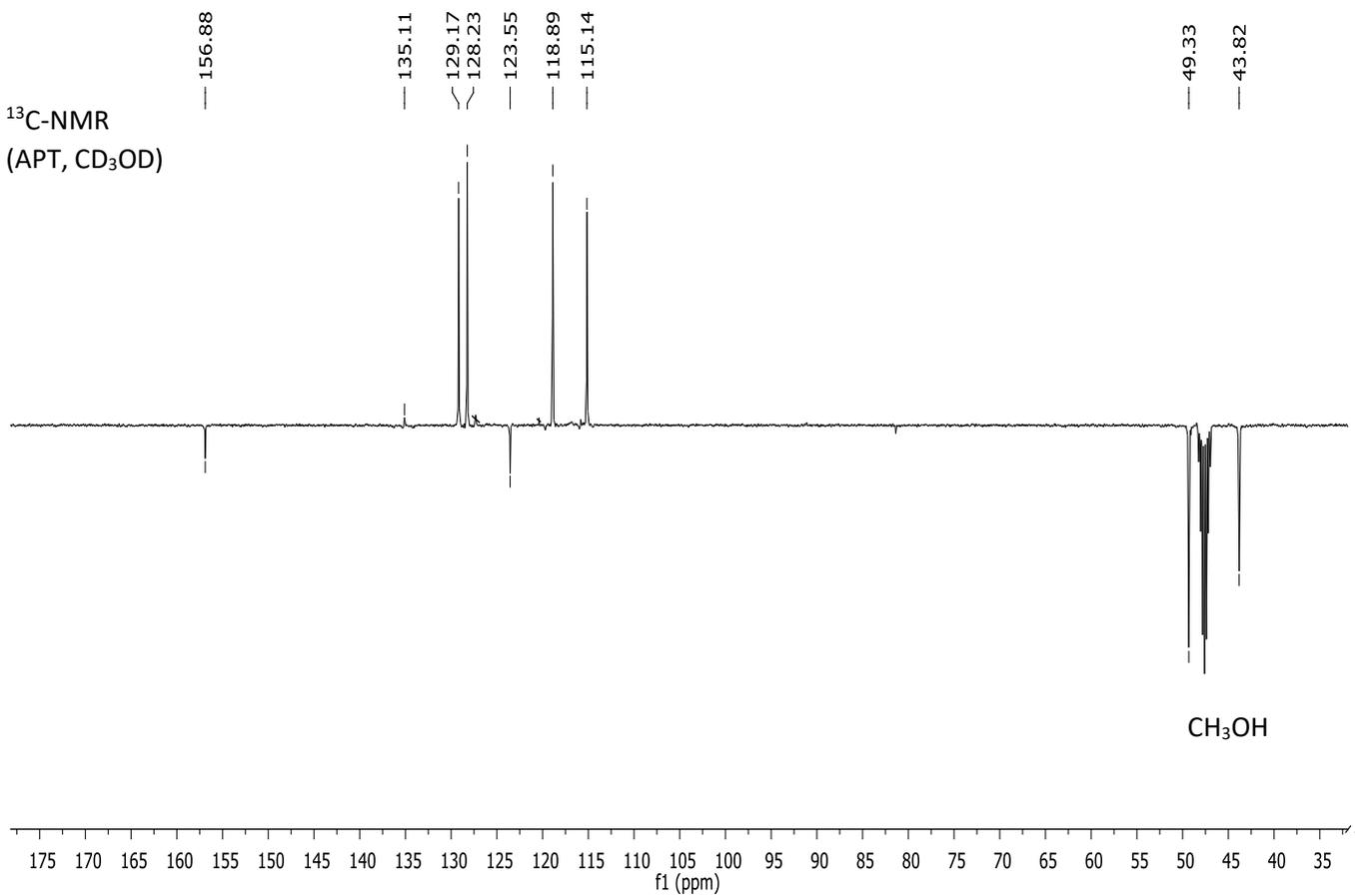


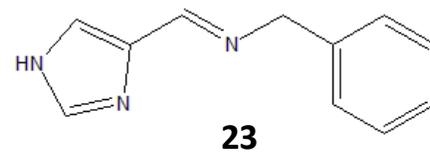


¹H-NMR (CD₃OD)

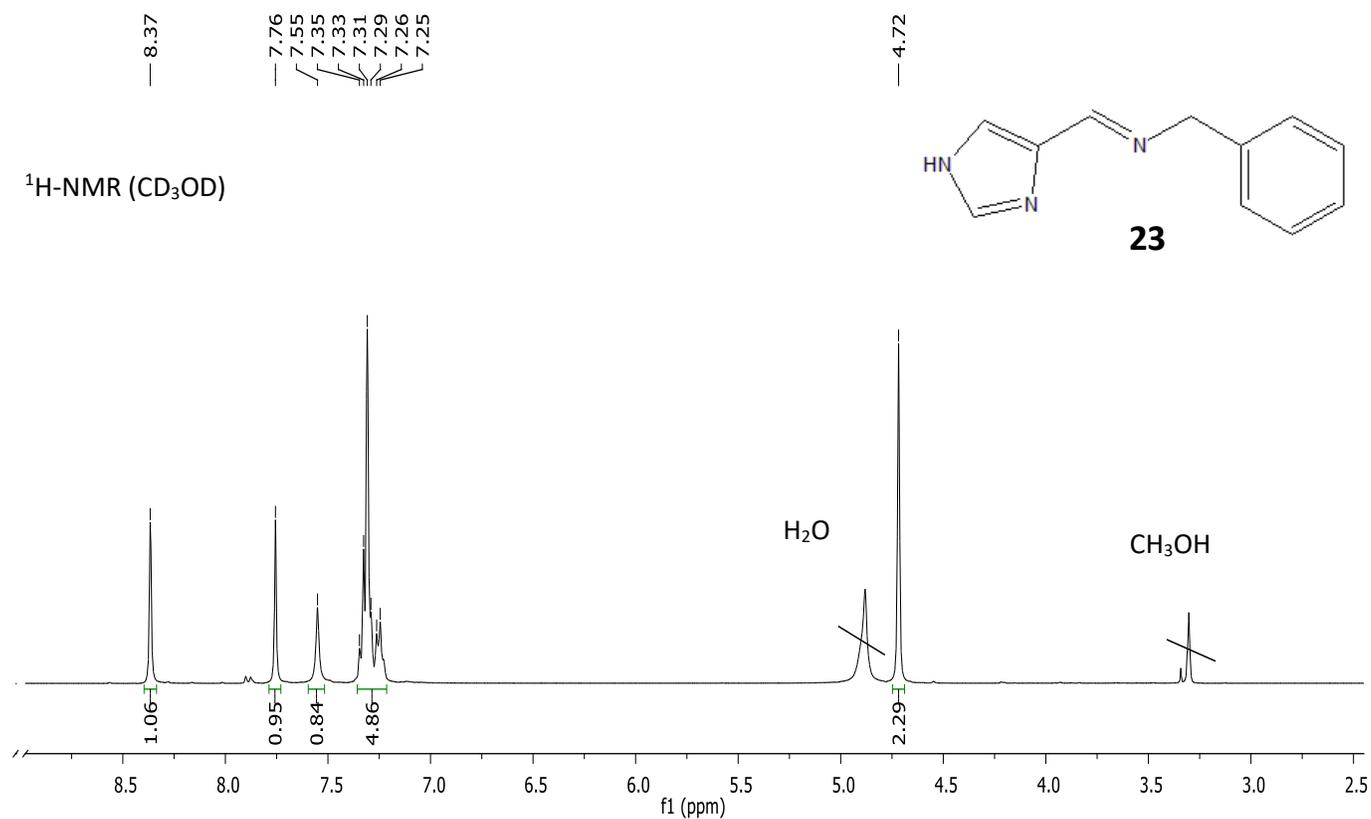


¹³C-NMR
(APT, CD₃OD)





$^1\text{H-NMR}$ (CD_3OD)



$^{13}\text{C-NMR}$
(Proton decoupled,
 CD_3OD)

