

Supporting information

Natural compounds and their structural analogs in regio- and stereoselective synthesis of new families of water-soluble 2H,3H-[1,3]thia- and -selenazolo[3,2-a]pyridin-4-ium heterocycles by annulation reactions

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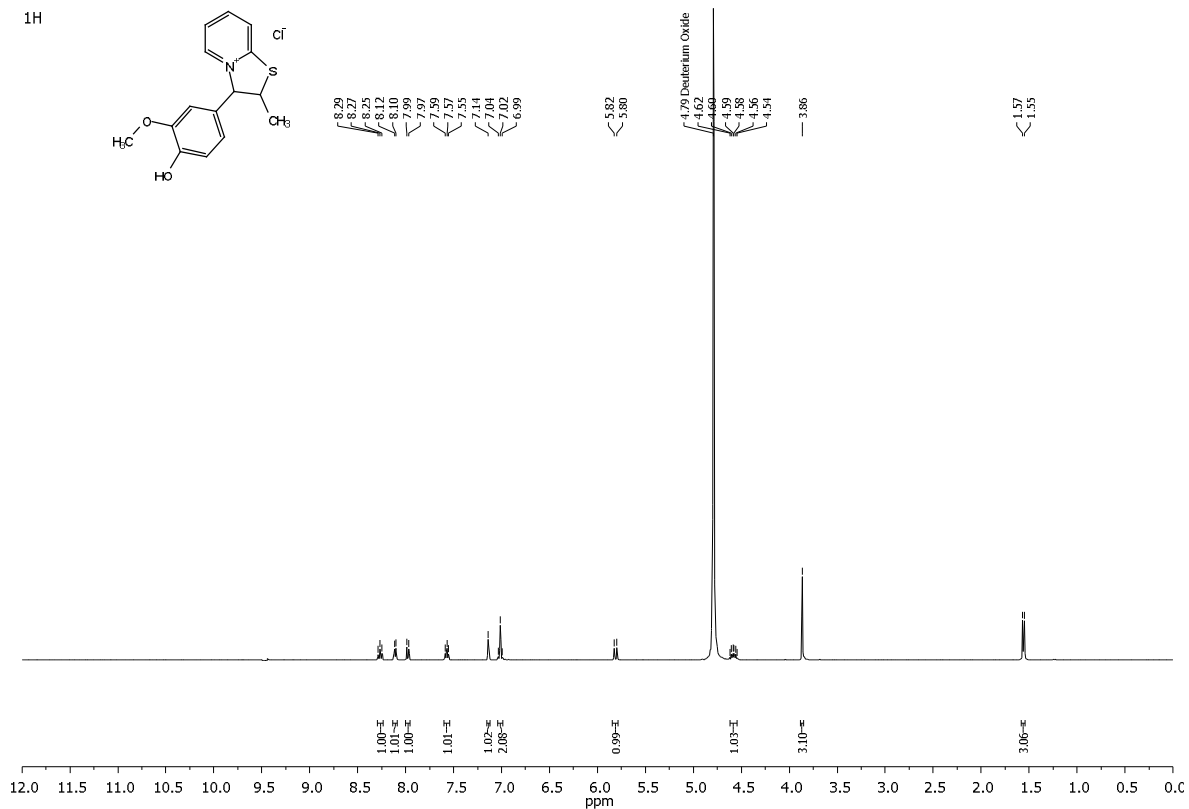
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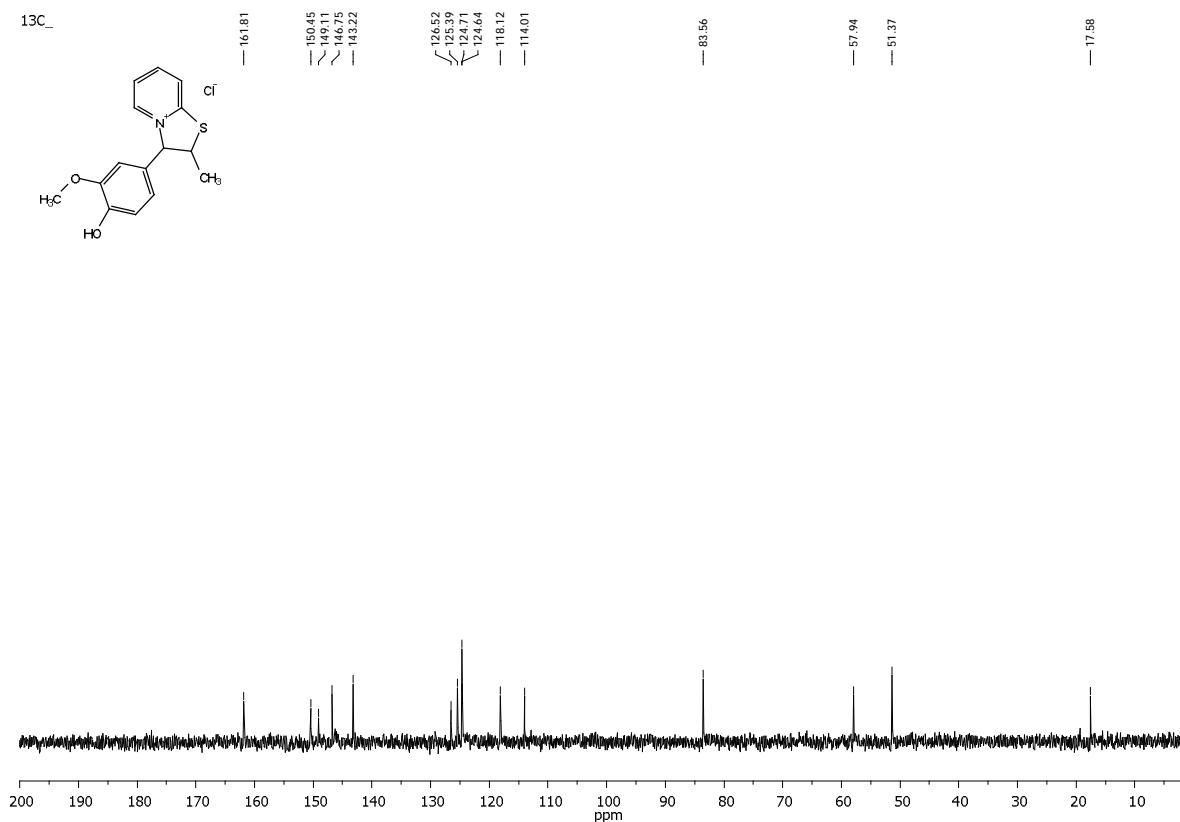
Experimental (General Information)

^1H (400.1 MHz) and ^{13}C (100.6 MHz) NMR spectra were recorded on a Bruker DPX-400 spectrometer in 5-10% solution in D_2O or $\text{DMSO-}d_6$ or CDCl_3 . ^1H and ^{13}C chemical shifts (δ) are reported in parts per million (ppm), relative to tetramethylsilane (external) or to the residual solvent peaks of $\text{DMSO-}d_6$ ($\delta = 2.50$ and 39.52 ppm in $^1\text{H-}$ and $^{13}\text{C-NMR}$, respectively) or CDCl_3 ($\delta = 7.26$ and 77.16 ppm in $^1\text{H-}$ and $^{13}\text{C-NMR}$, respectively).

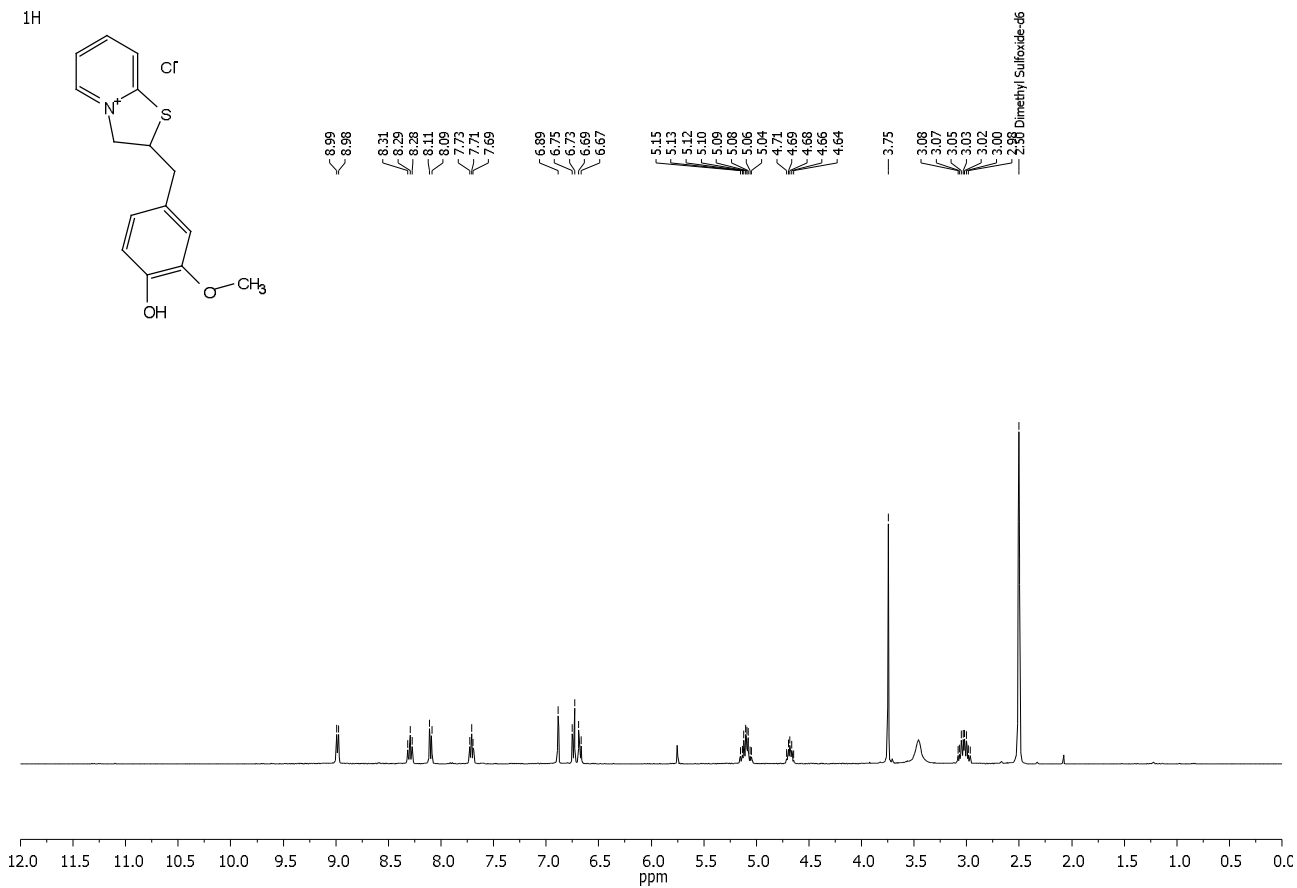
Examples of ^1H and ^{13}C -NMR spectra



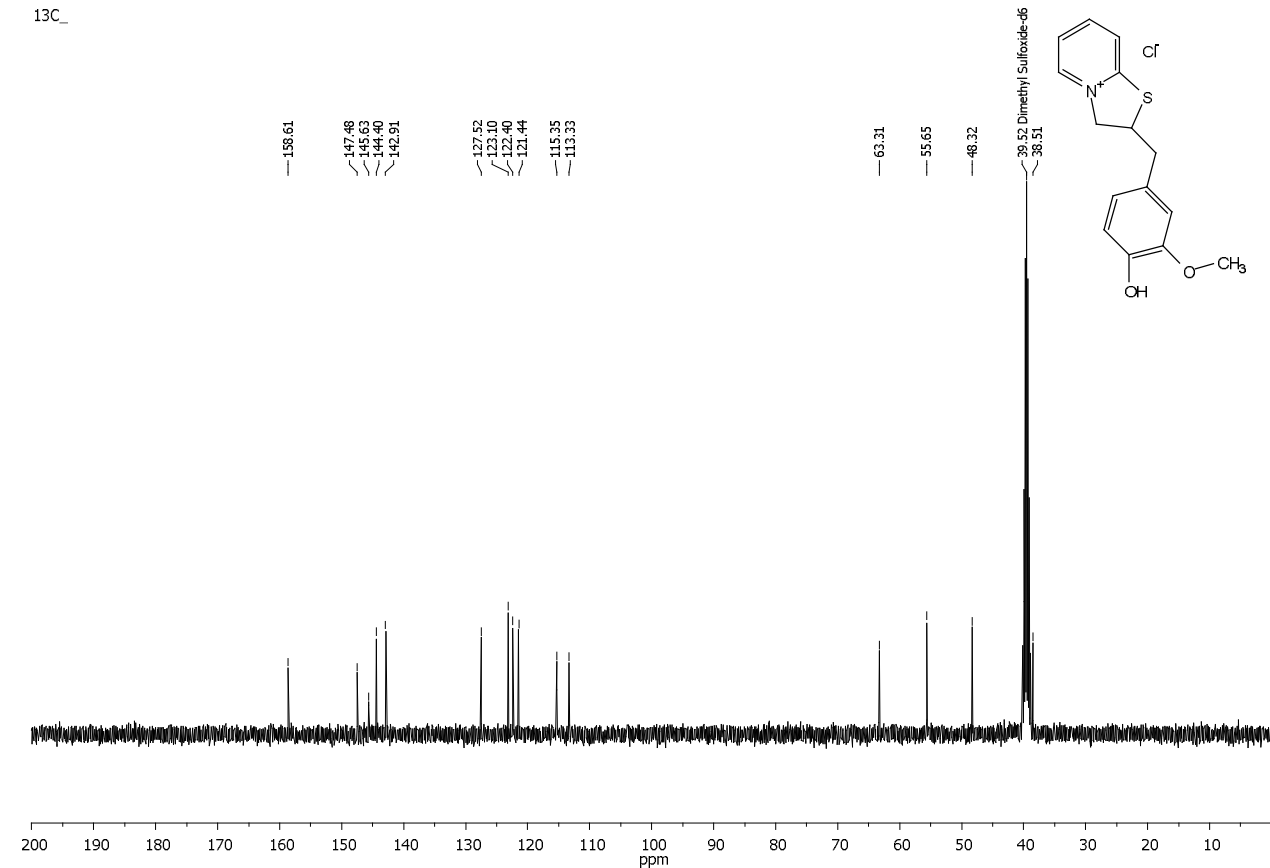
^1H -NMR (D_2O) spectrum of compound 1



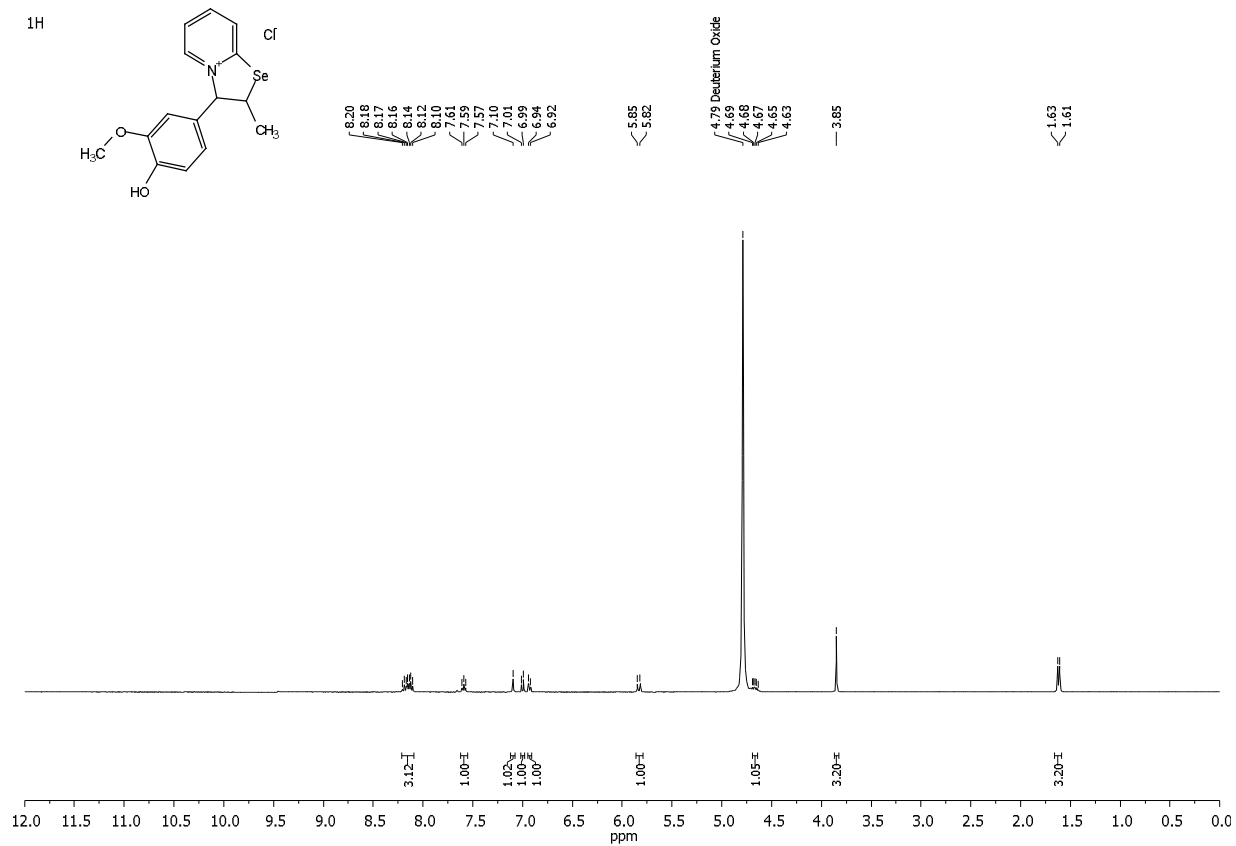
^{13}C -NMR (D_2O) spectrum of compound 1



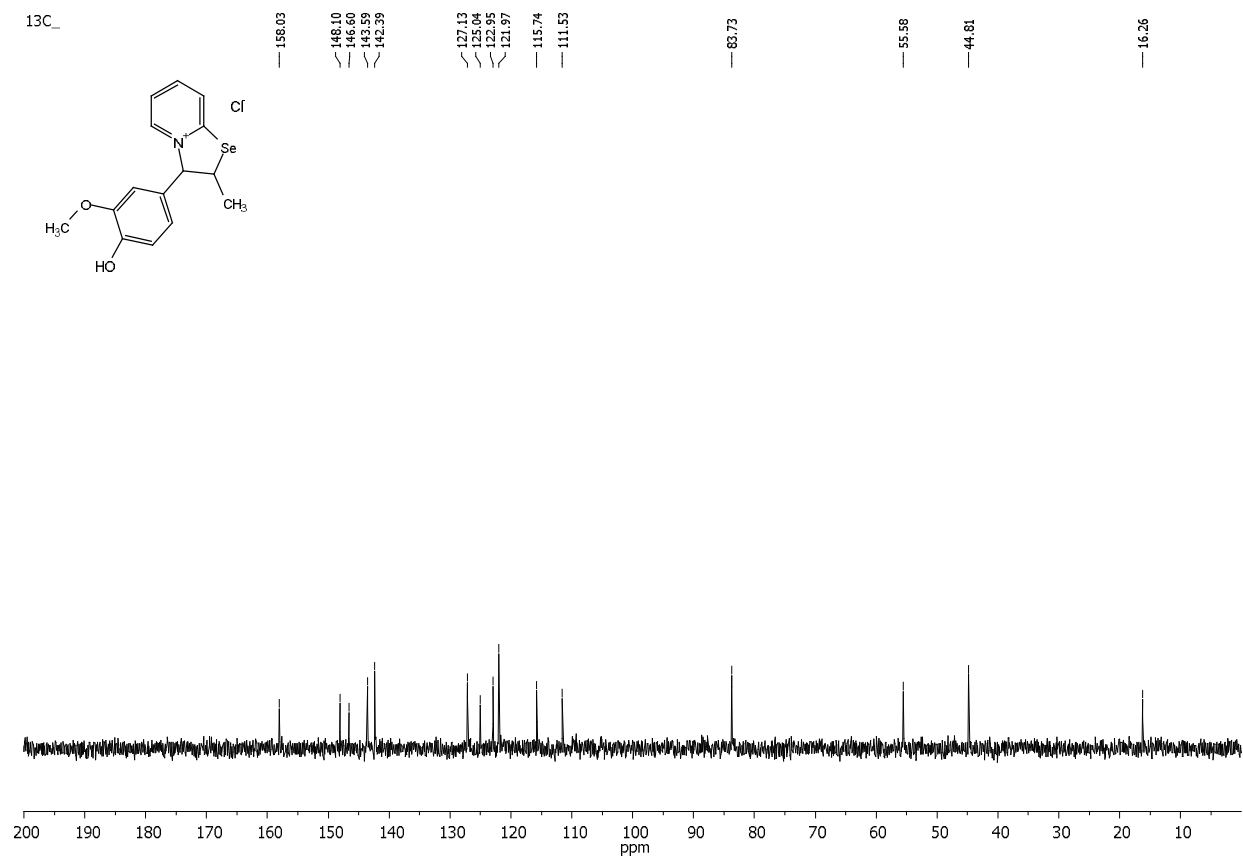
¹H-NMR (DMSO-*d*₆) spectrum of compound 2



¹³C-NMR (DMSO-*d*₆) spectrum of compound 2

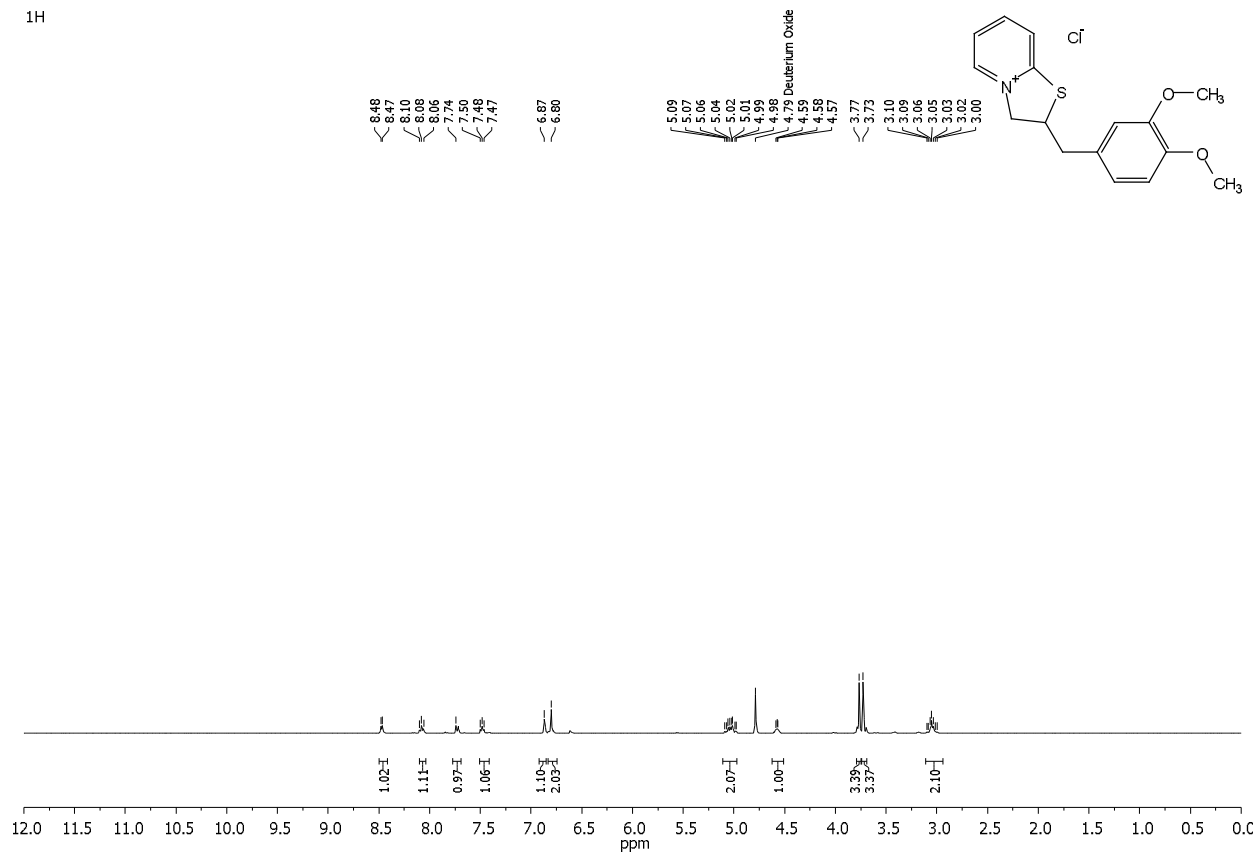


¹H-NMR (D₂O) spectrum of compound 3

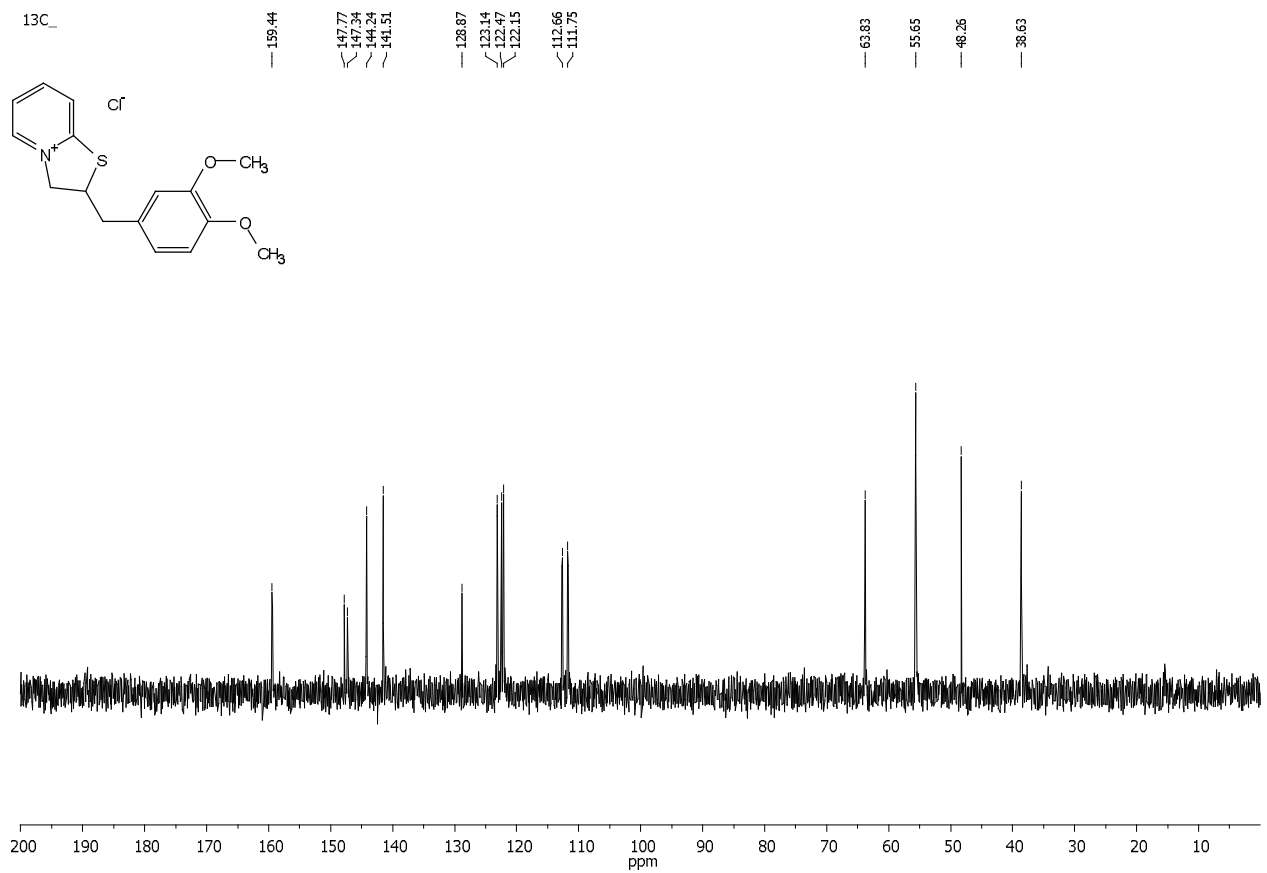


¹³C-NMR (D₂O) spectrum of compound 3

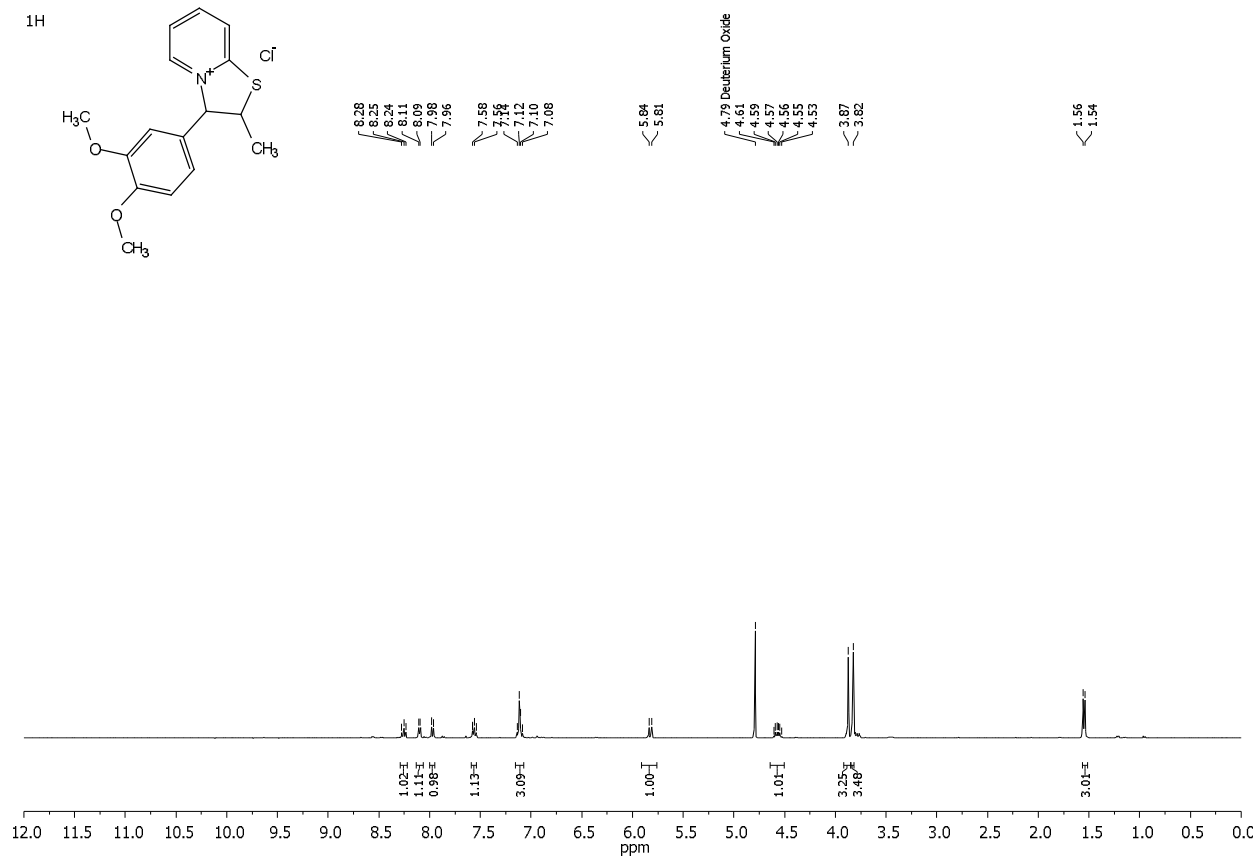
¹H



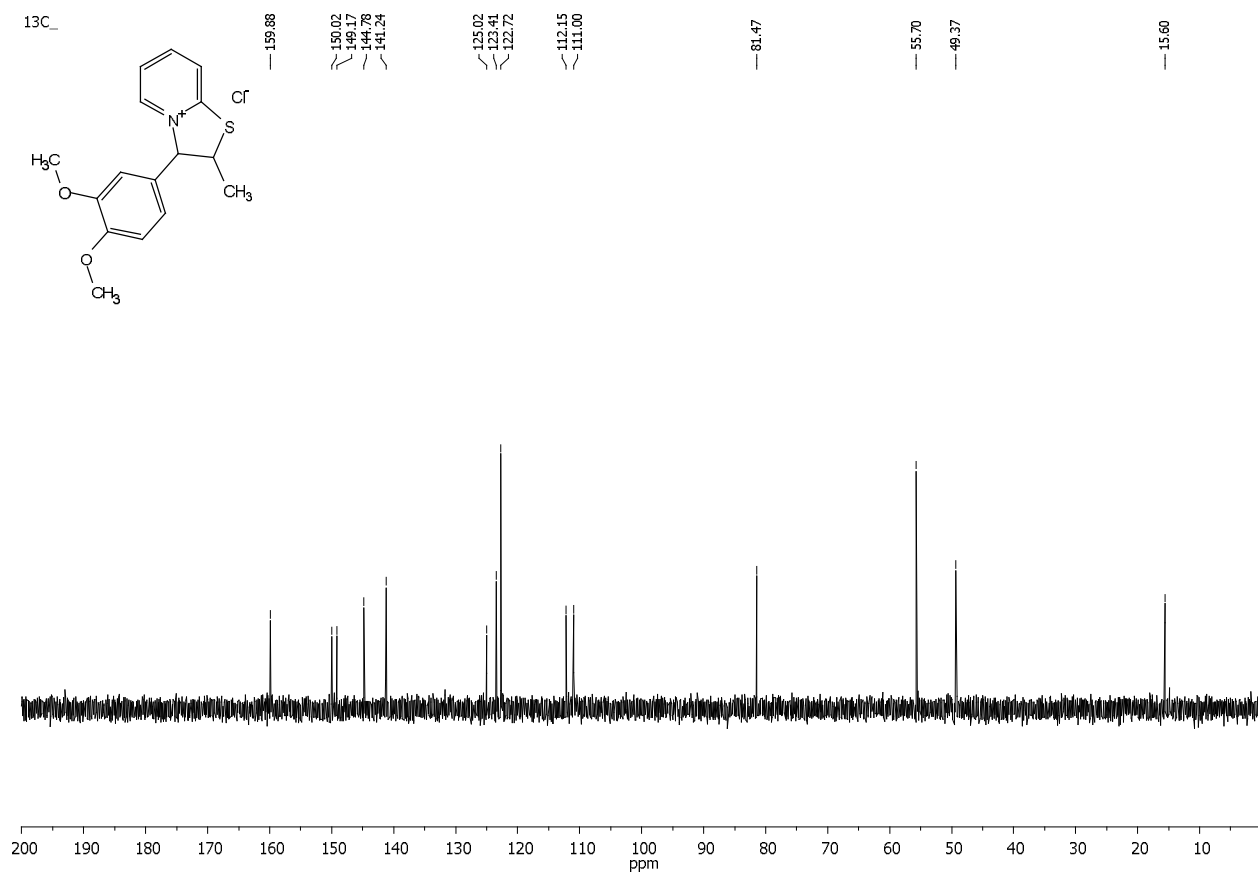
¹H-NMR (D₂O) spectrum of compound 5



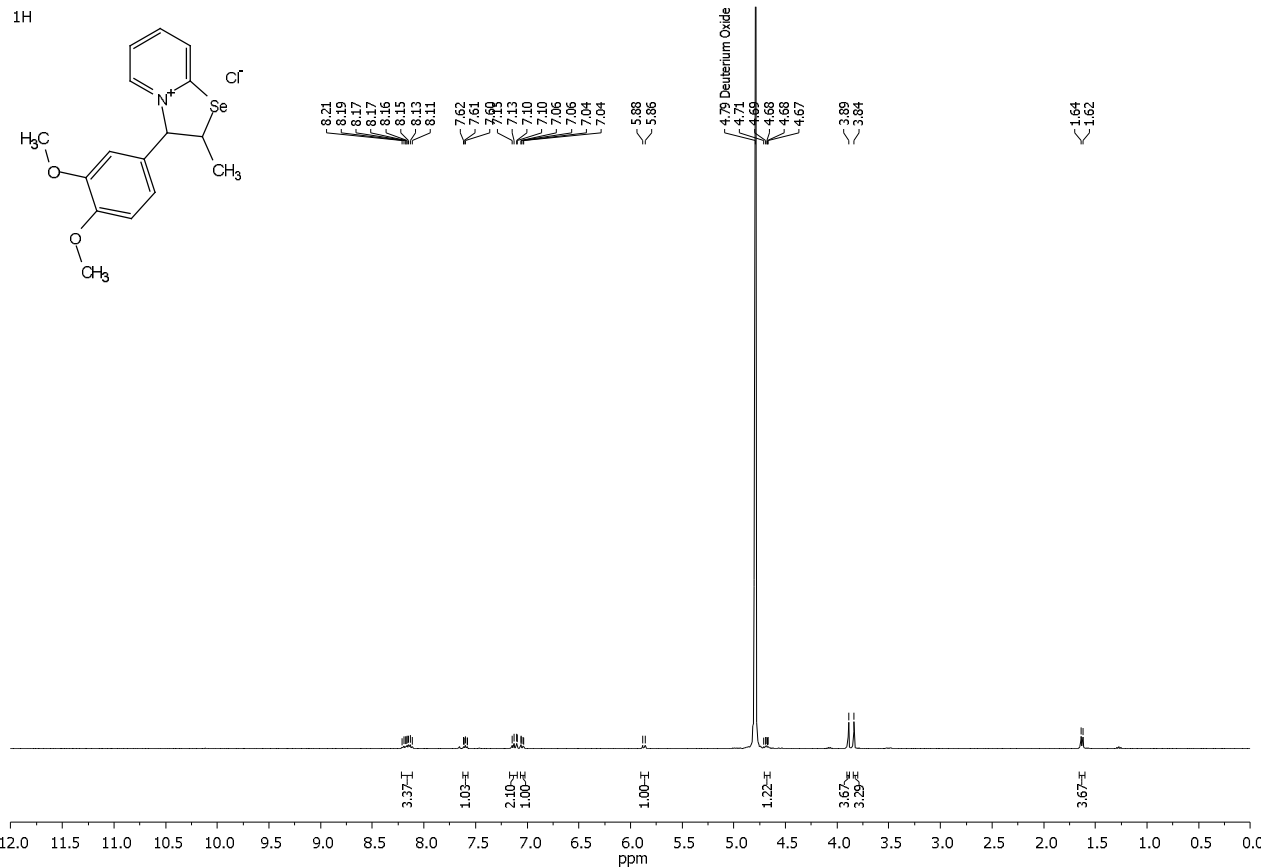
¹³C-NMR (D₂O) spectrum of compound 5



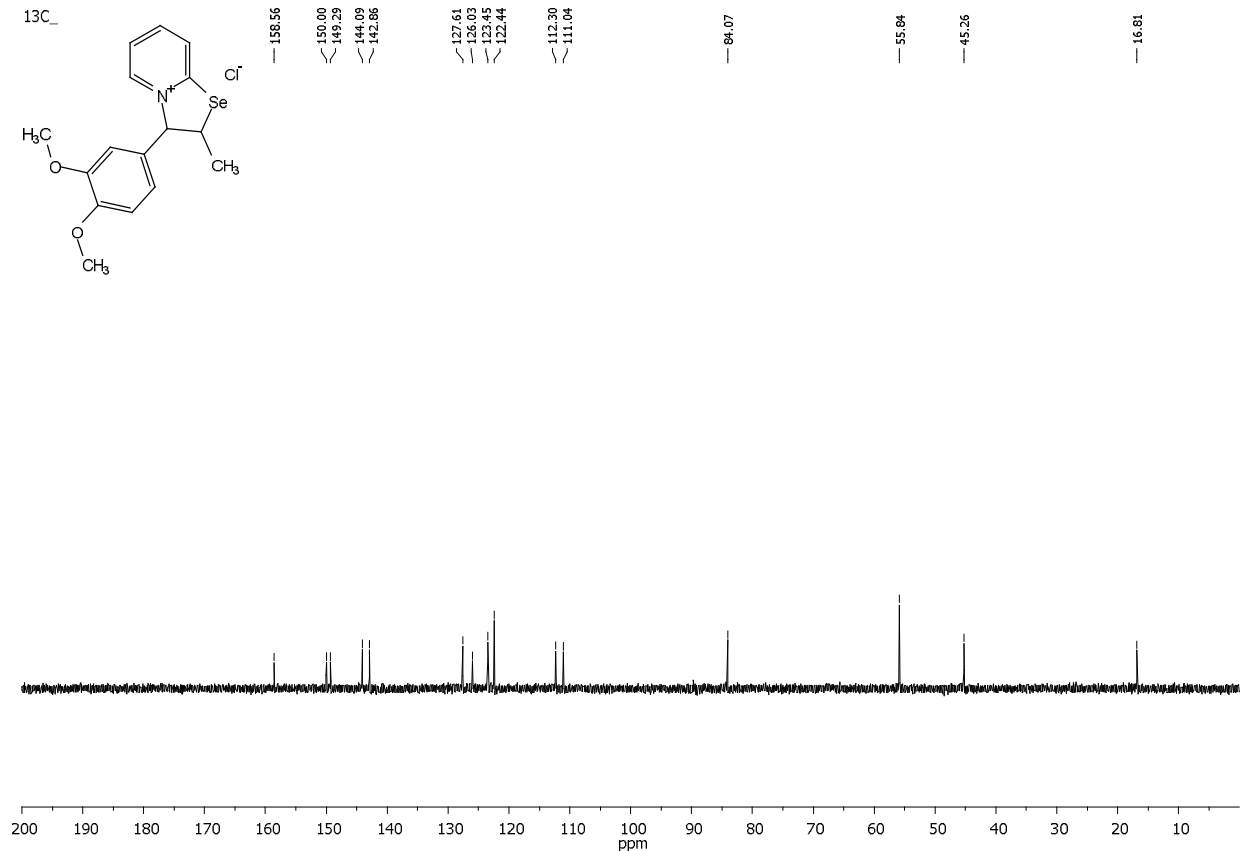
¹H-NMR (D₂O) spectrum of compound 6



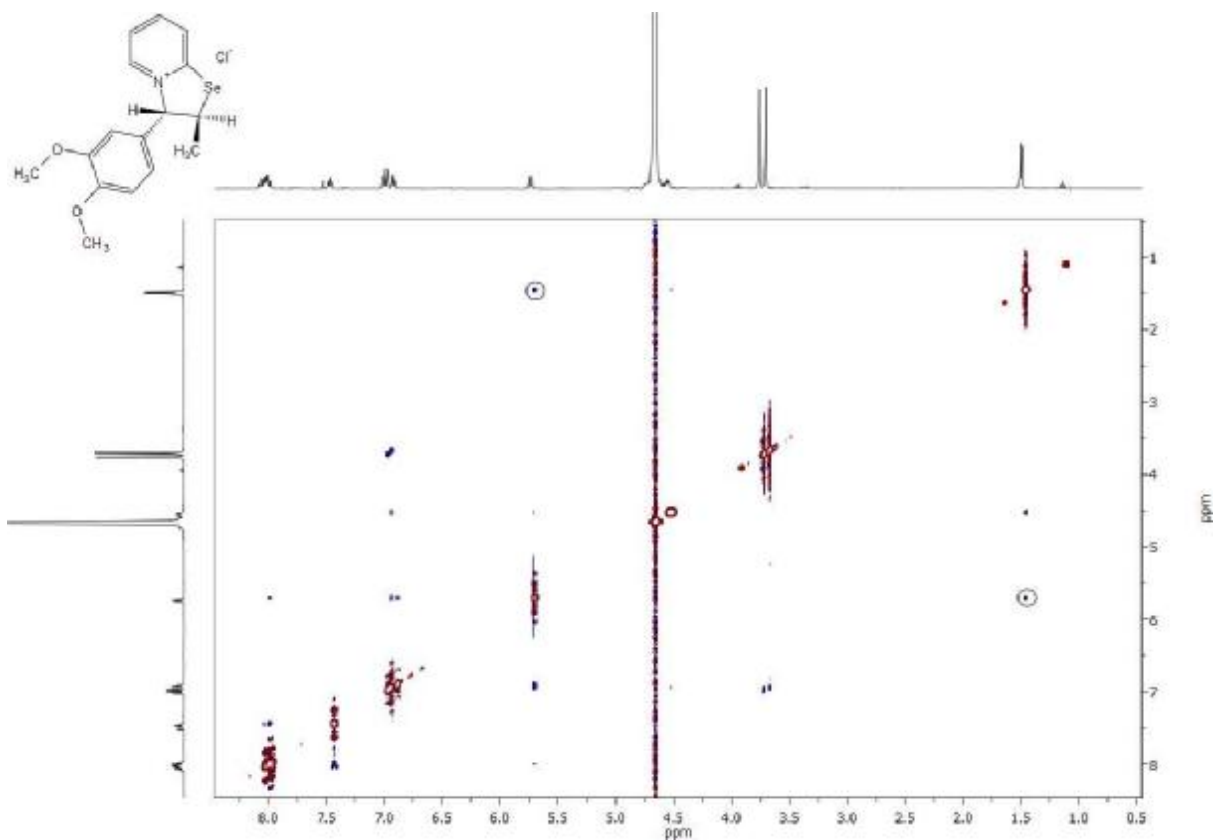
¹³C-NMR (D₂O) spectrum of compound 6



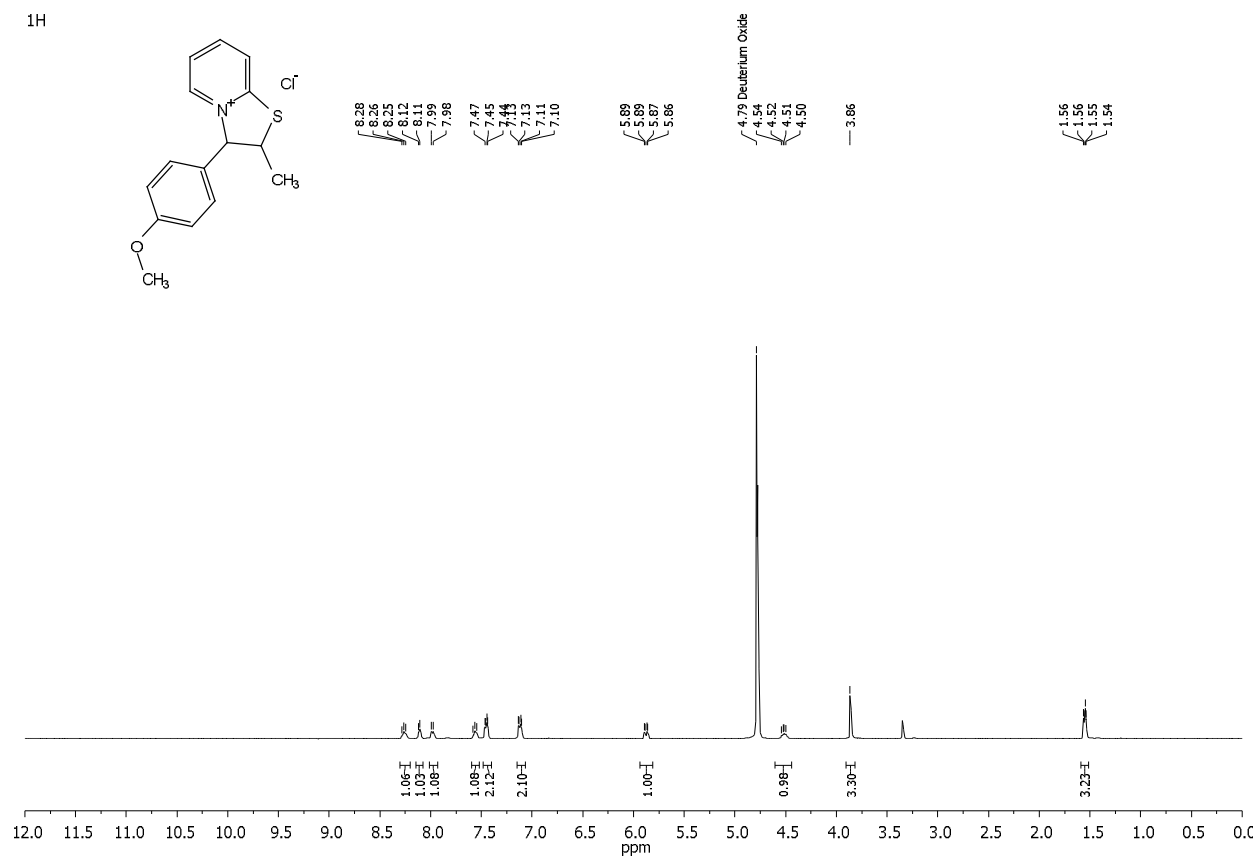
¹H-NMR (D₂O) spectrum of compound 8



¹³C-NMR (D₂O) spectrum of compound 8

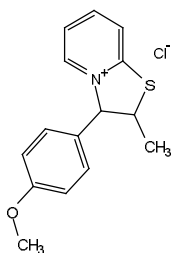


$^1\text{H-NMR NOESY (D}_2\text{O)}$ spectrum of compound 8

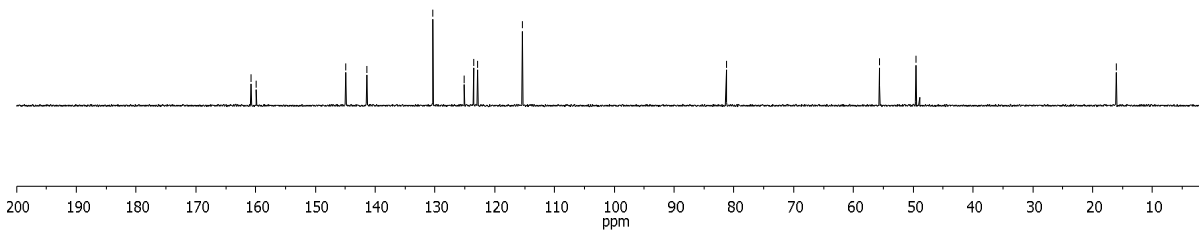


$^1\text{H-NMR (D}_2\text{O)}$ spectrum of compound 11

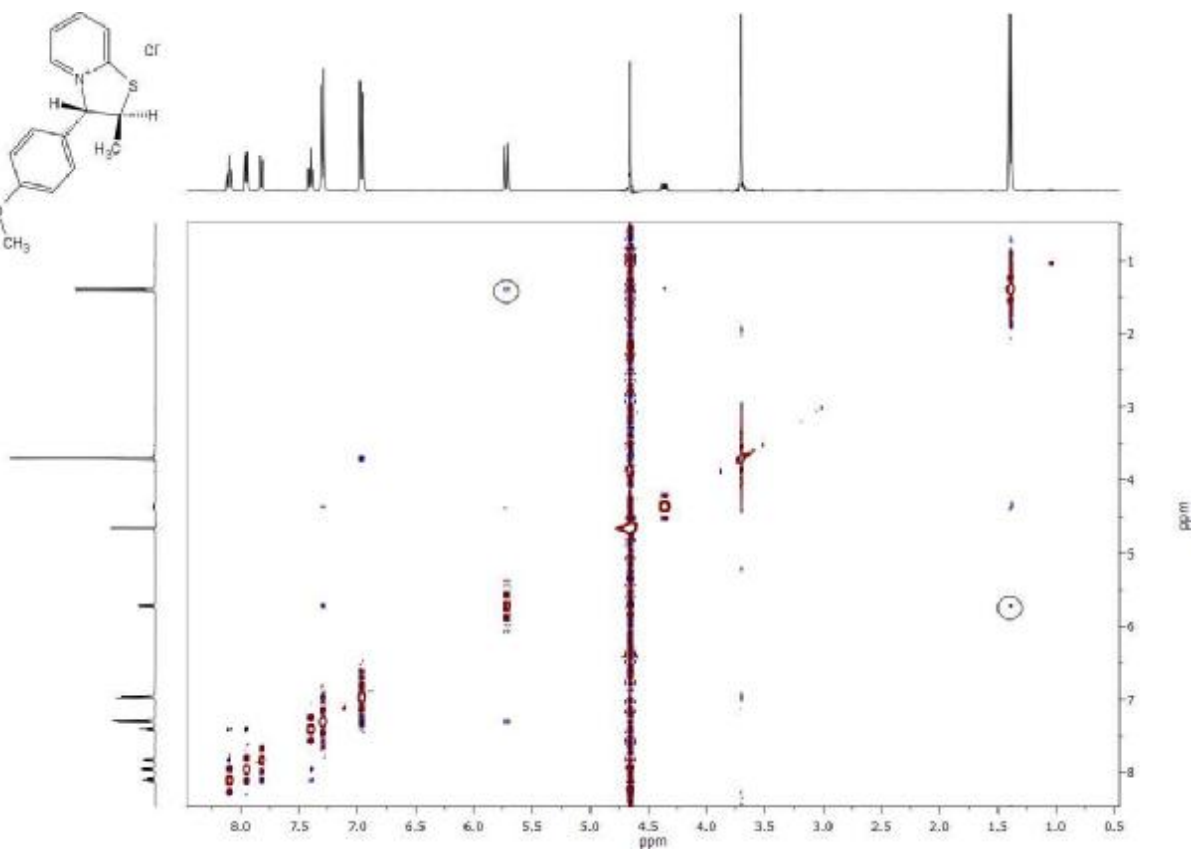
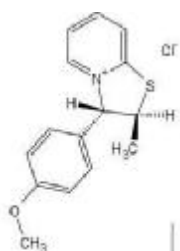
13C_



160.76
159.90
144.89
141.37
130.36
125.11
123.55
122.85
115.34
81.25
55.60
49.58
16.06

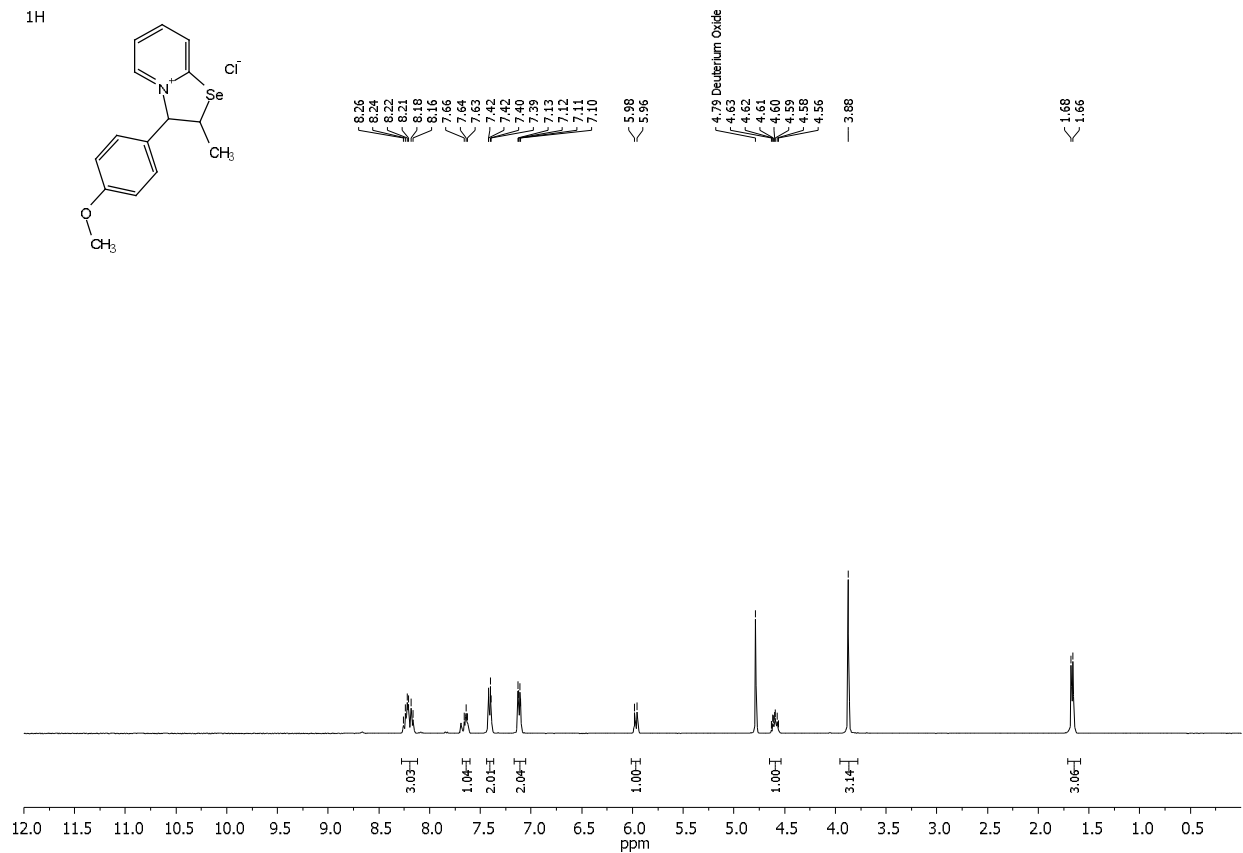
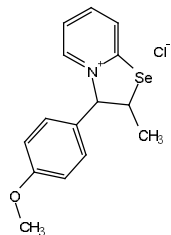


¹³C-NMR (D₂O) spectrum of compound 11



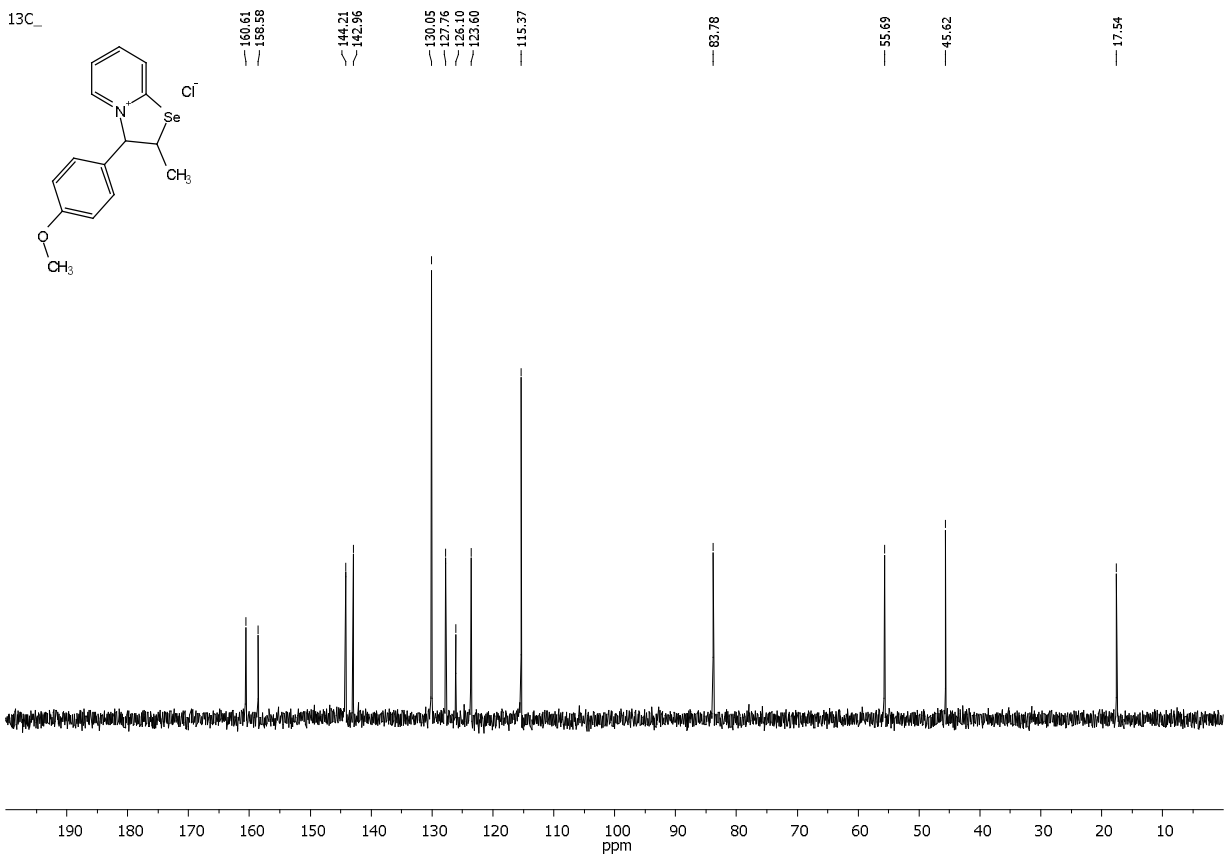
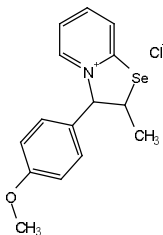
¹H-NMR NOESY (D₂O) spectrum of compound 11

¹H



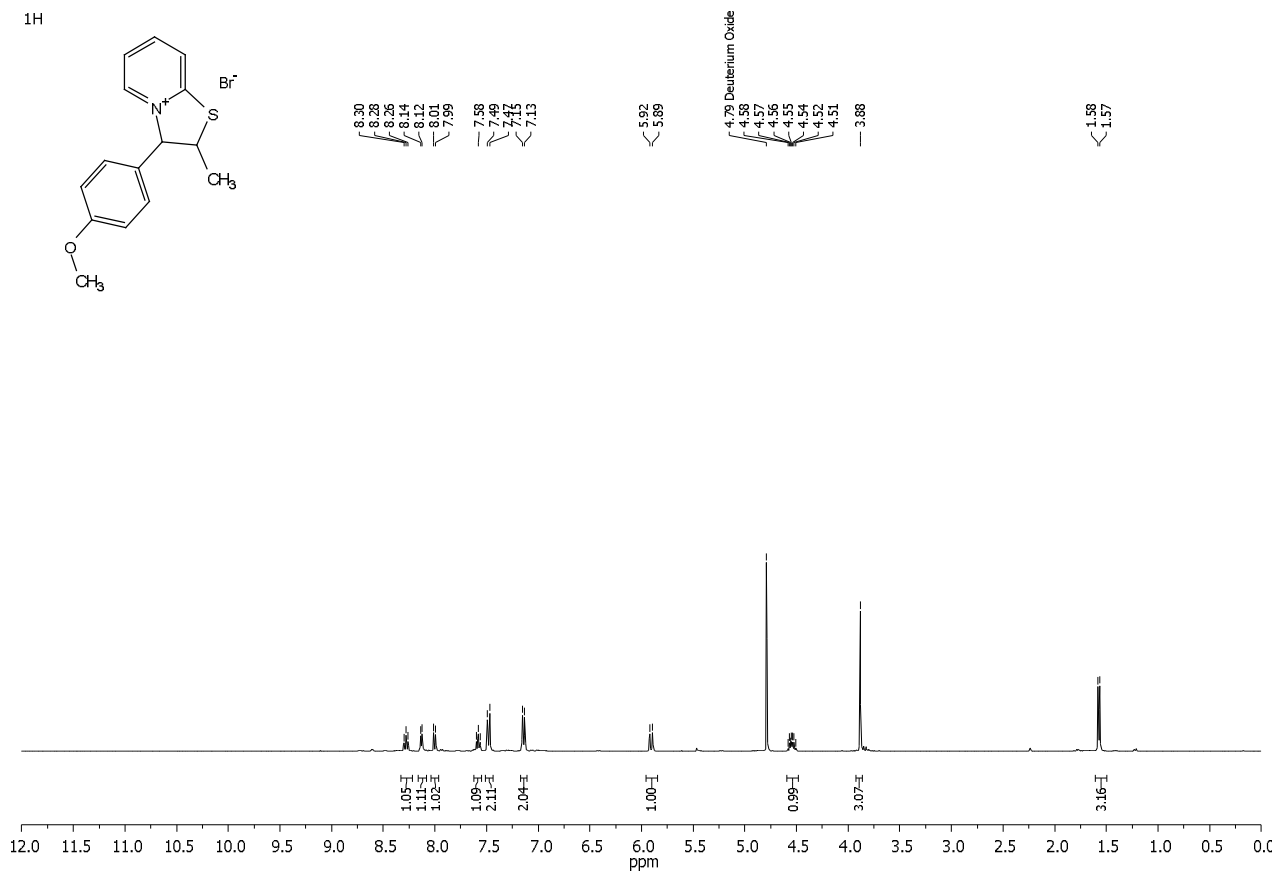
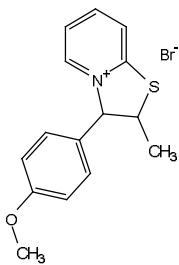
¹H-NMR (D₂O) spectrum of compound 12

¹³C



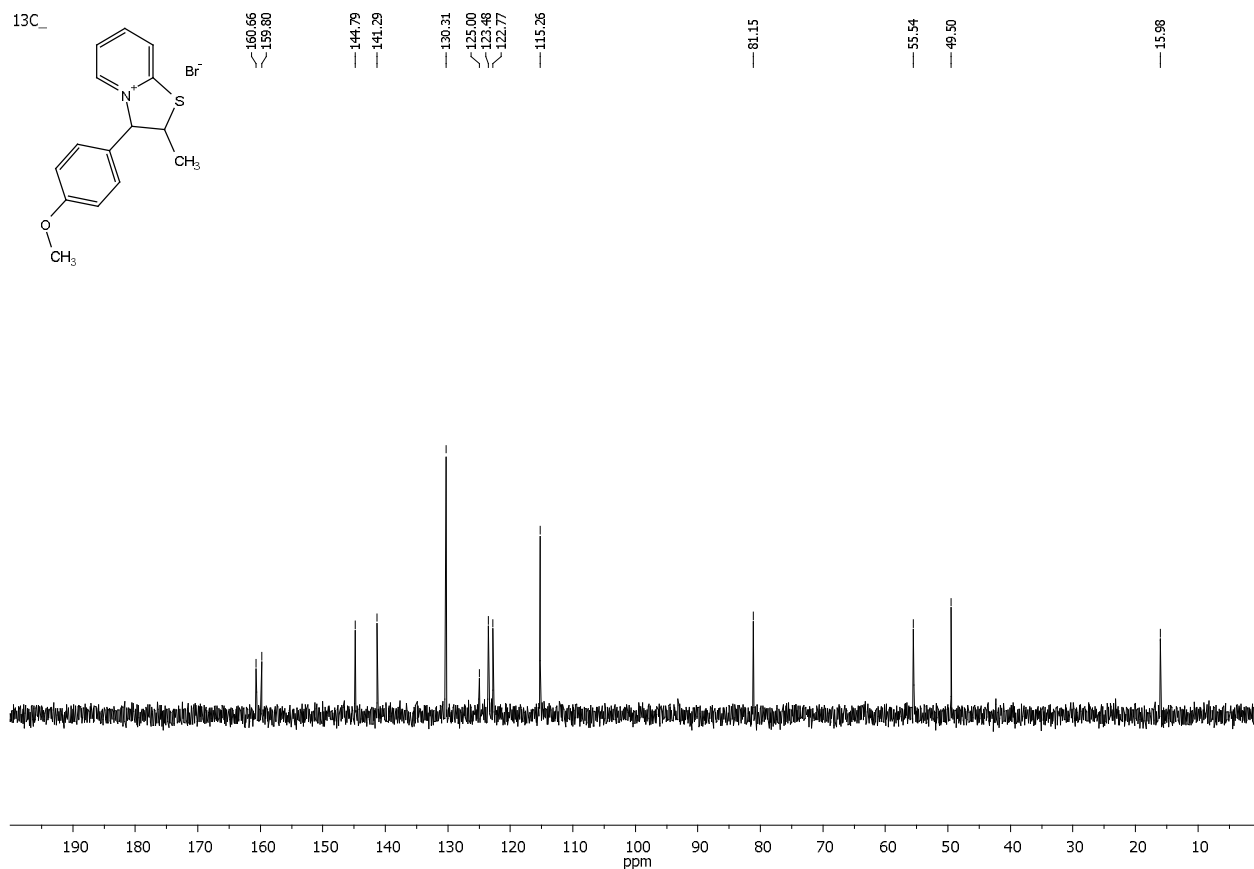
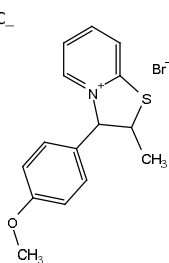
¹³C-NMR (D₂O) spectrum of compound 12

¹H

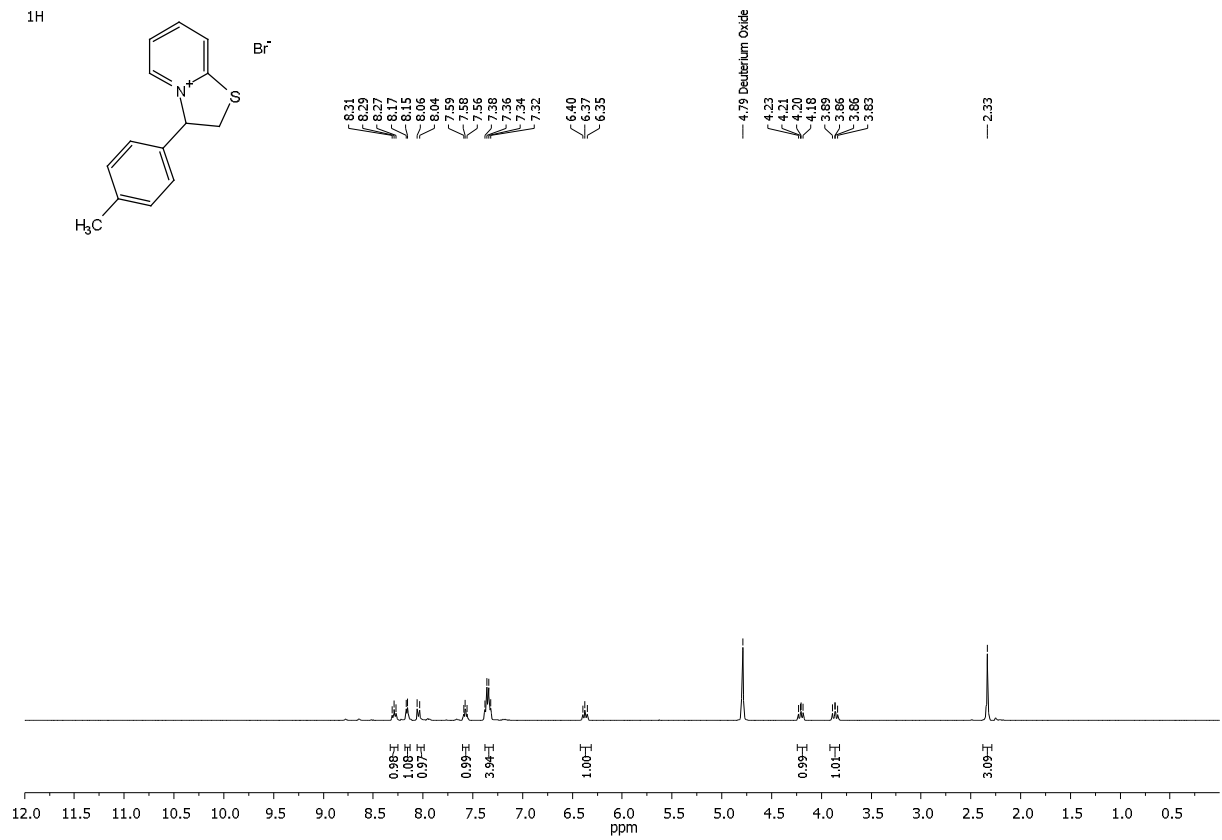


¹H-NMR (D₂O) spectrum of compound 13

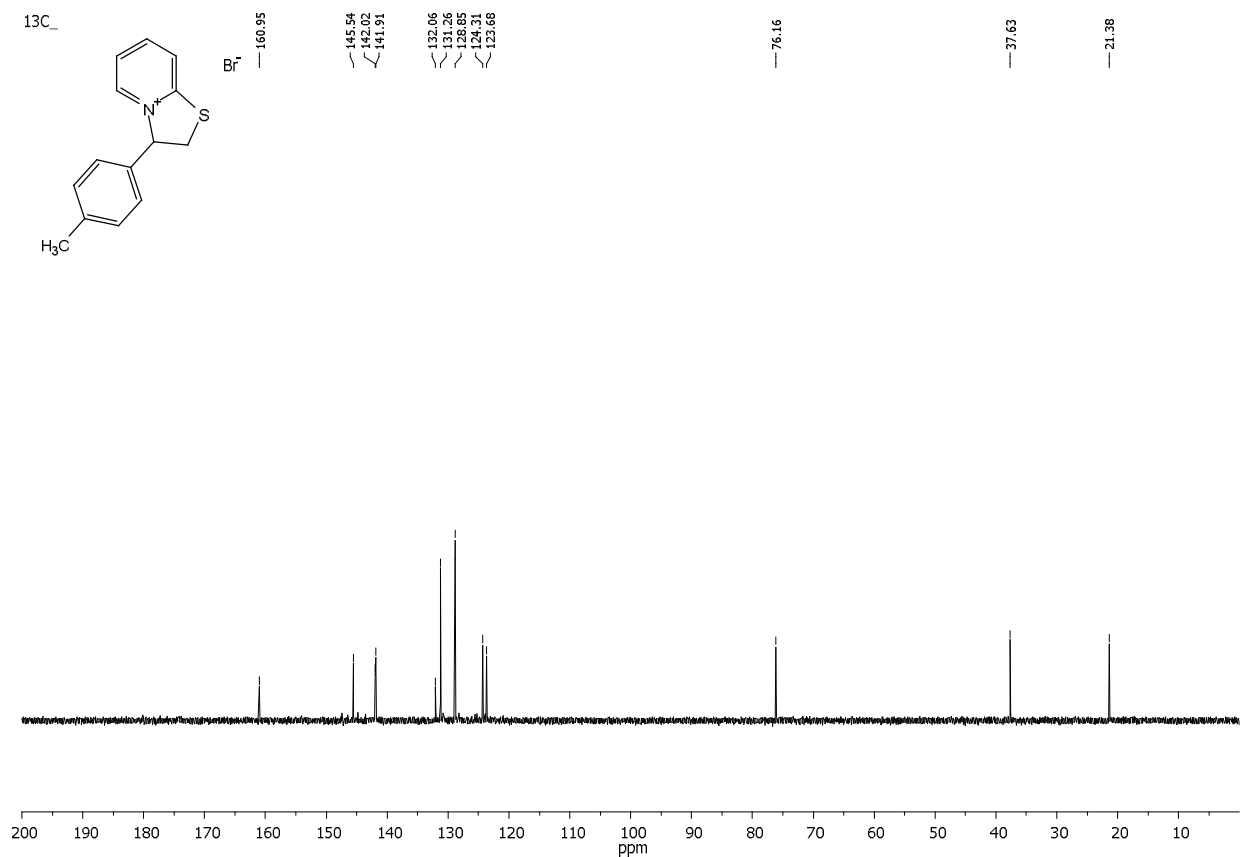
¹³C



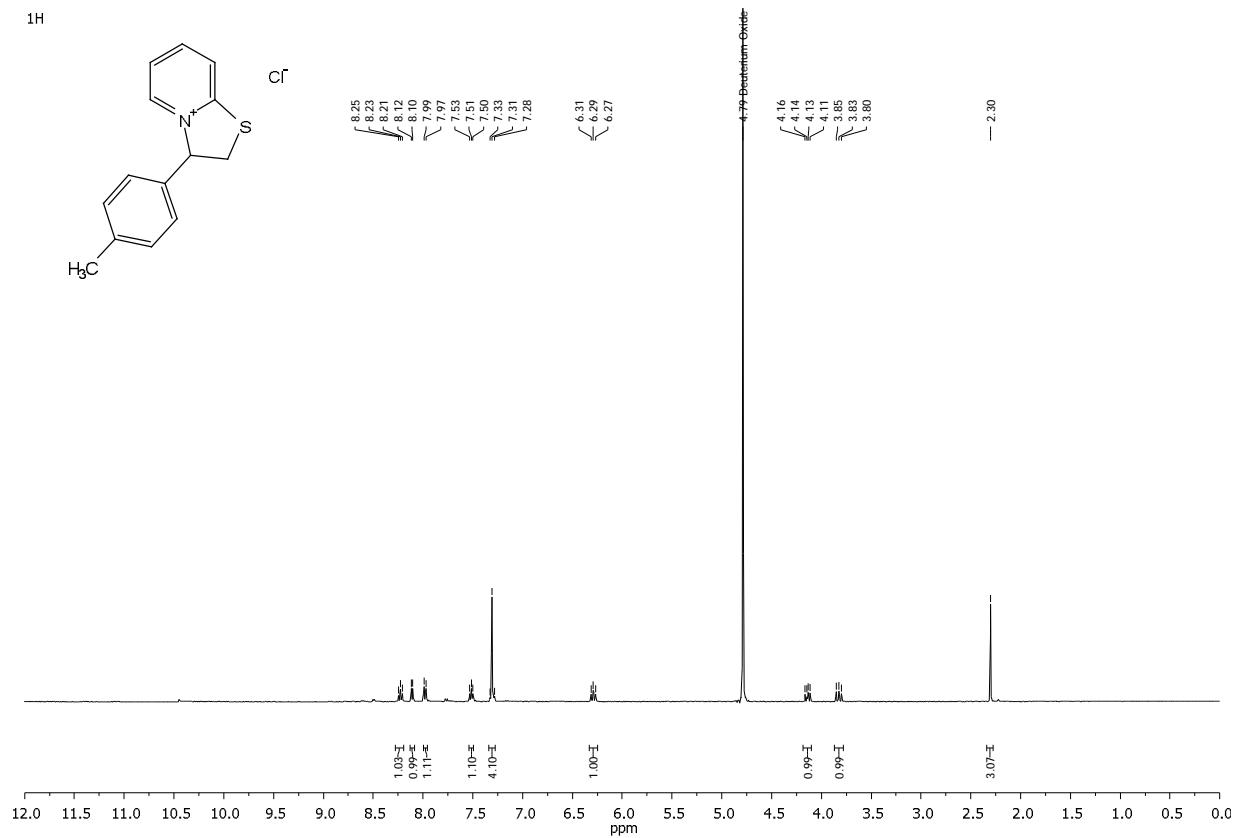
¹³C-NMR (D₂O) spectrum of compound 13



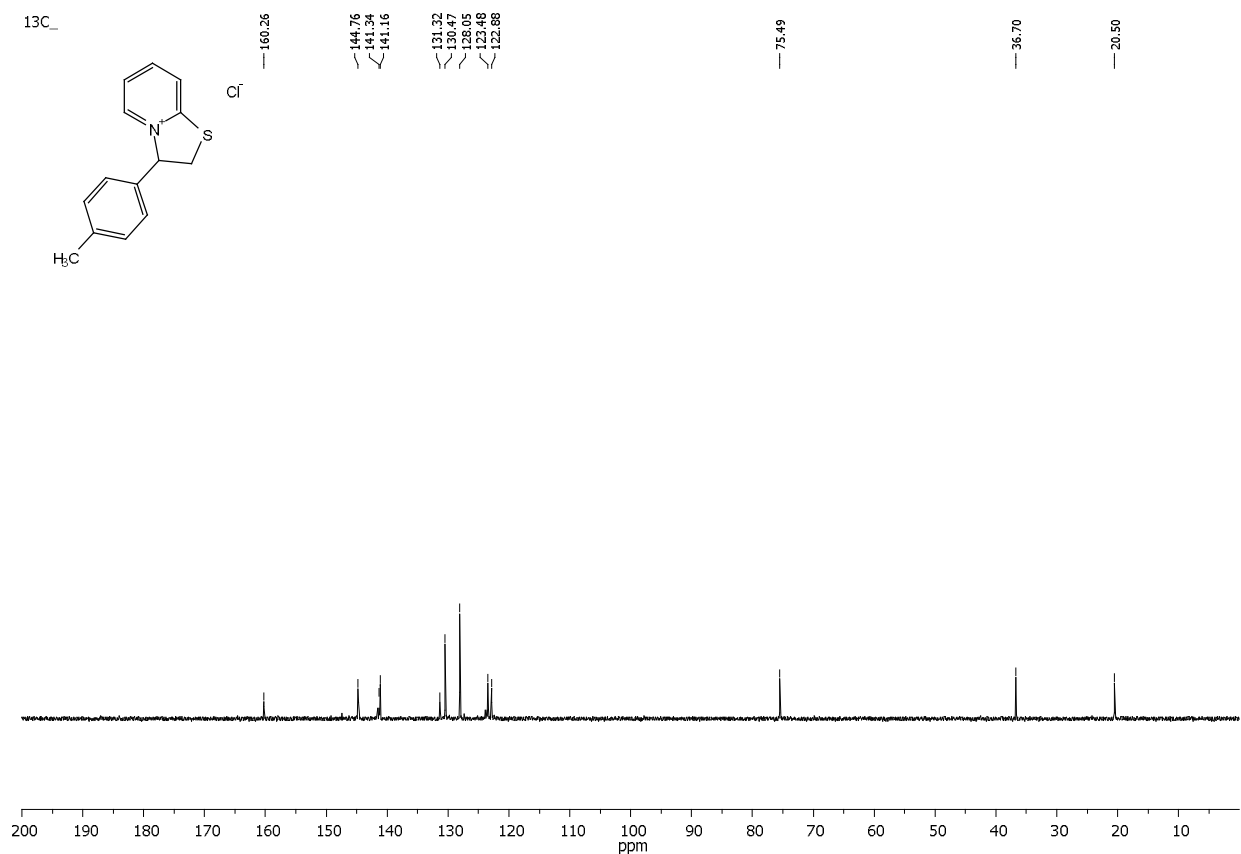
¹H-NMR (D₂O) spectrum of compound 14



¹³C-NMR (D₂O) spectrum of compound 14

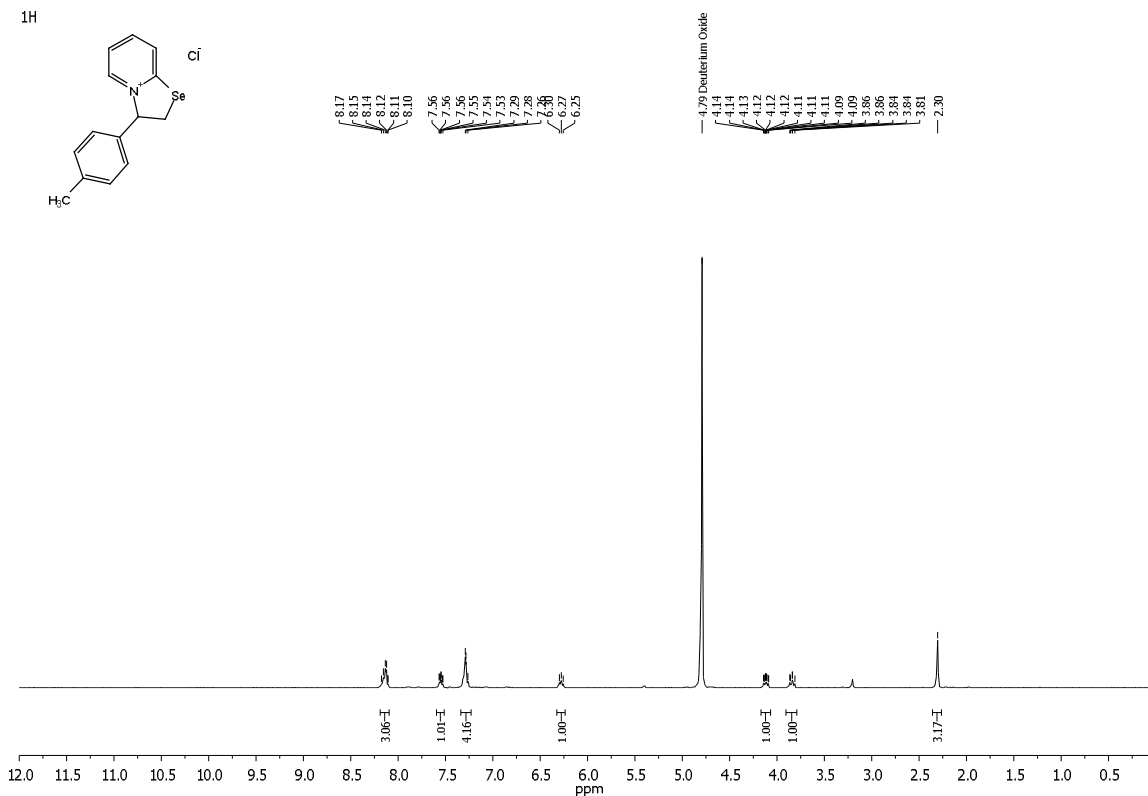
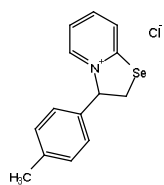


¹H-NMR (D₂O) spectrum of compound 15



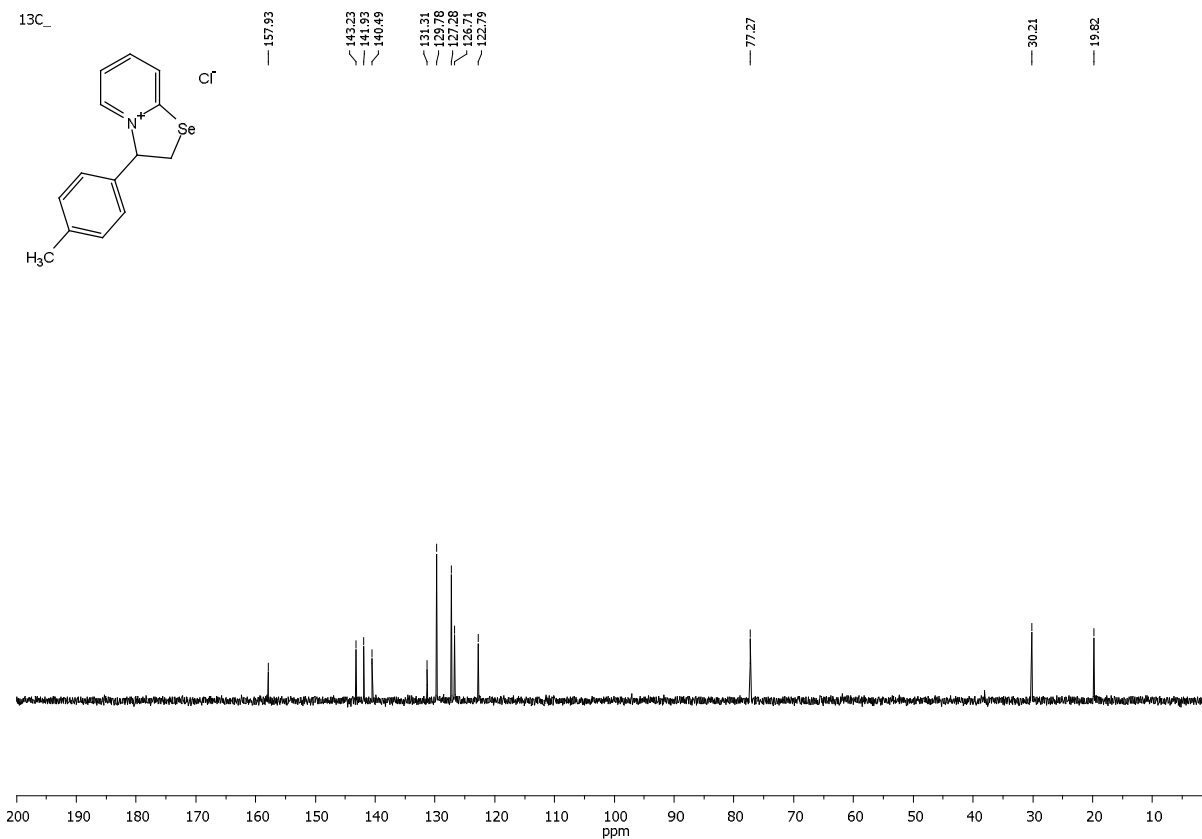
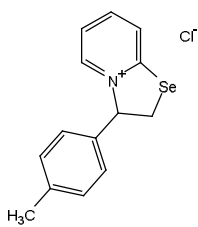
¹³C-NMR (D₂O) spectrum of compound 15

¹H



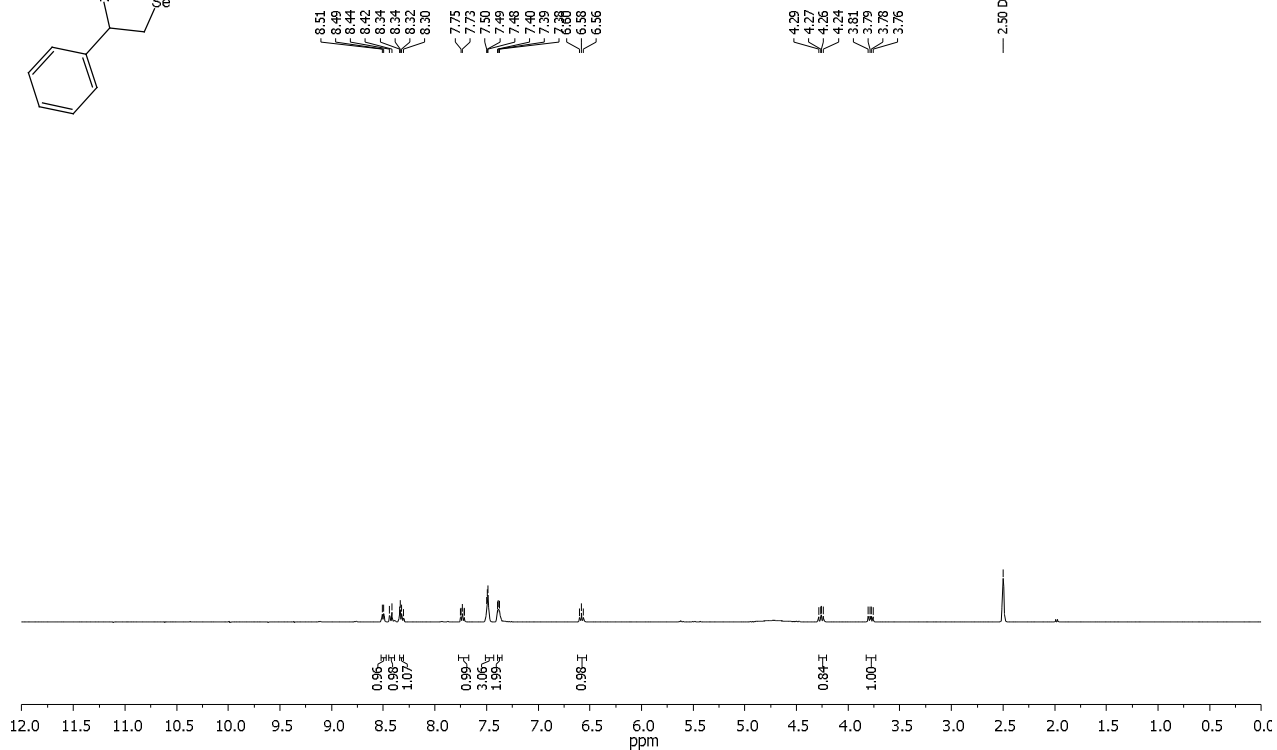
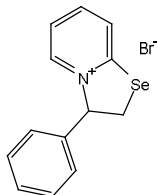
¹H-NMR (D₂O) spectrum of compound 17

¹³C



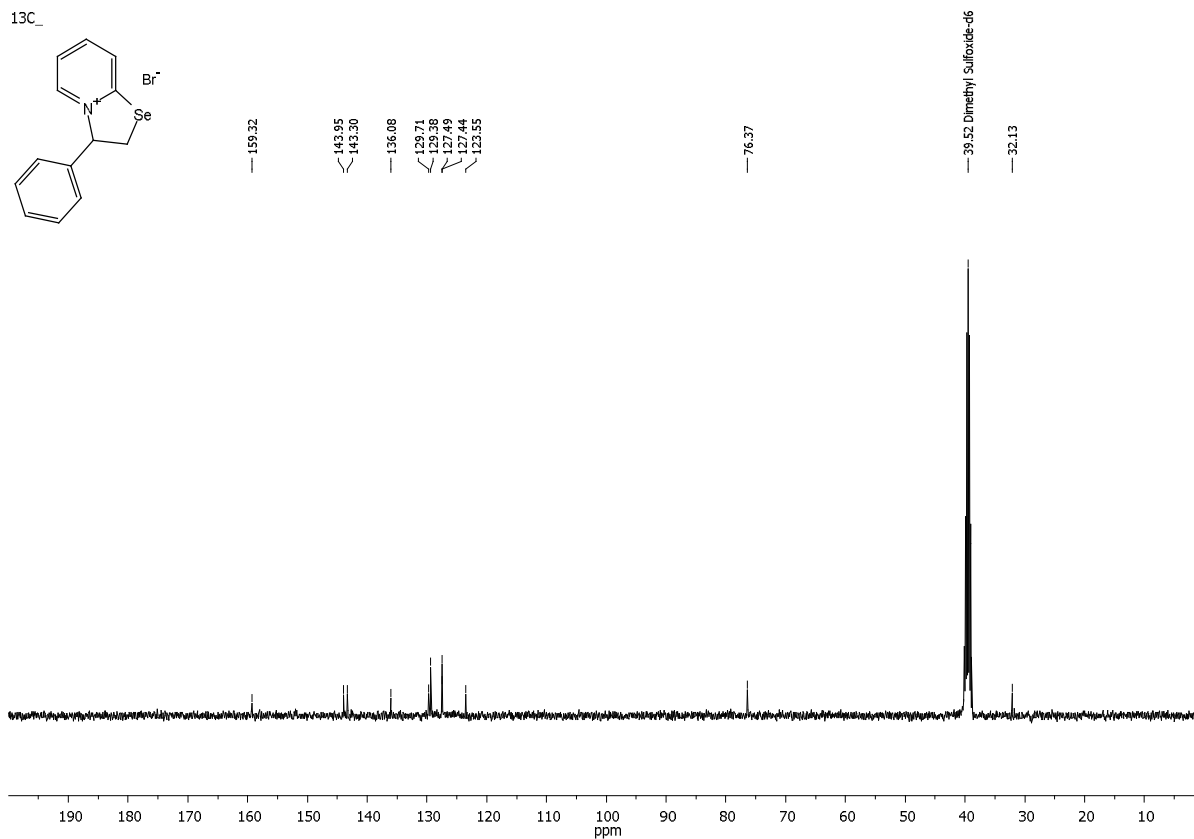
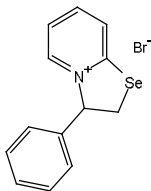
¹³C-NMR (D₂O) spectrum of compound 17

¹H



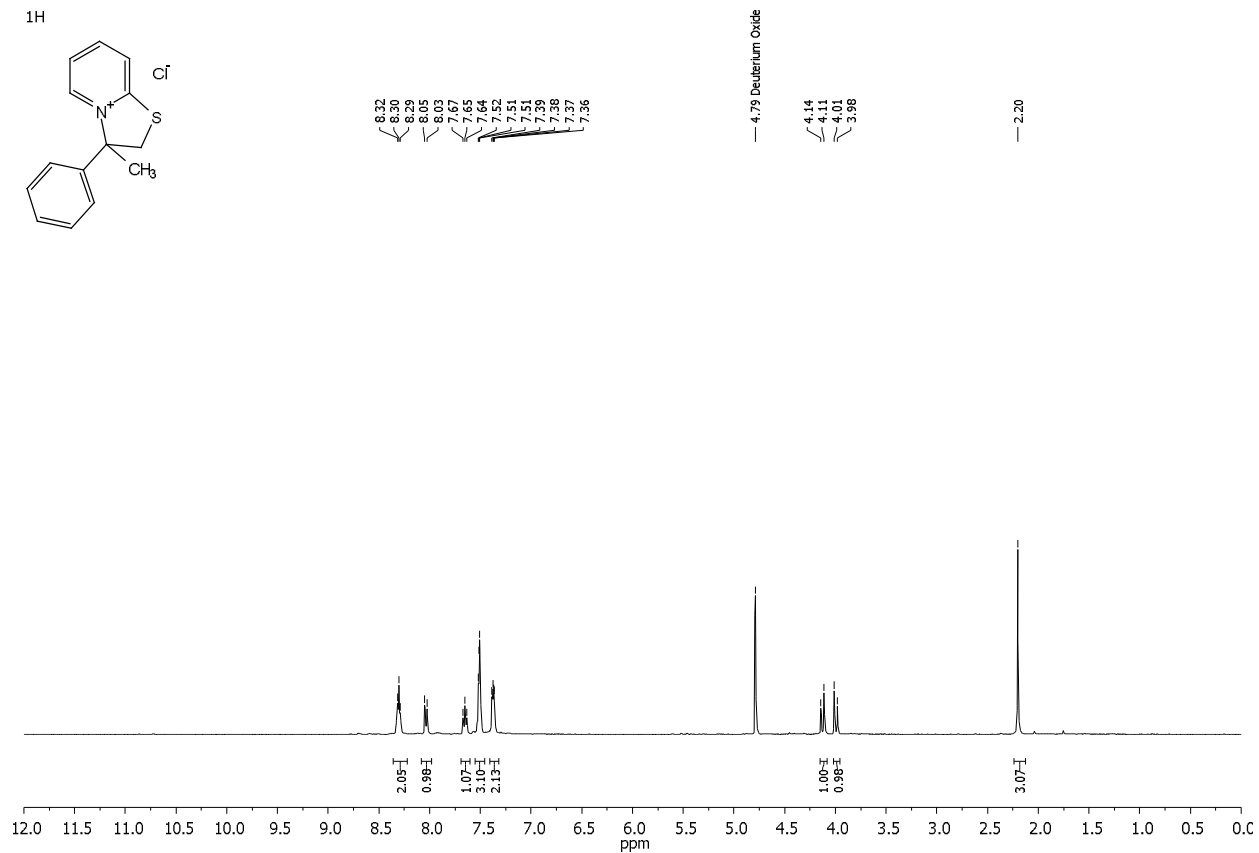
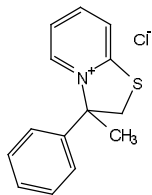
¹H-NMR (DMSO-*d*₆) spectrum of compound 18

¹³C



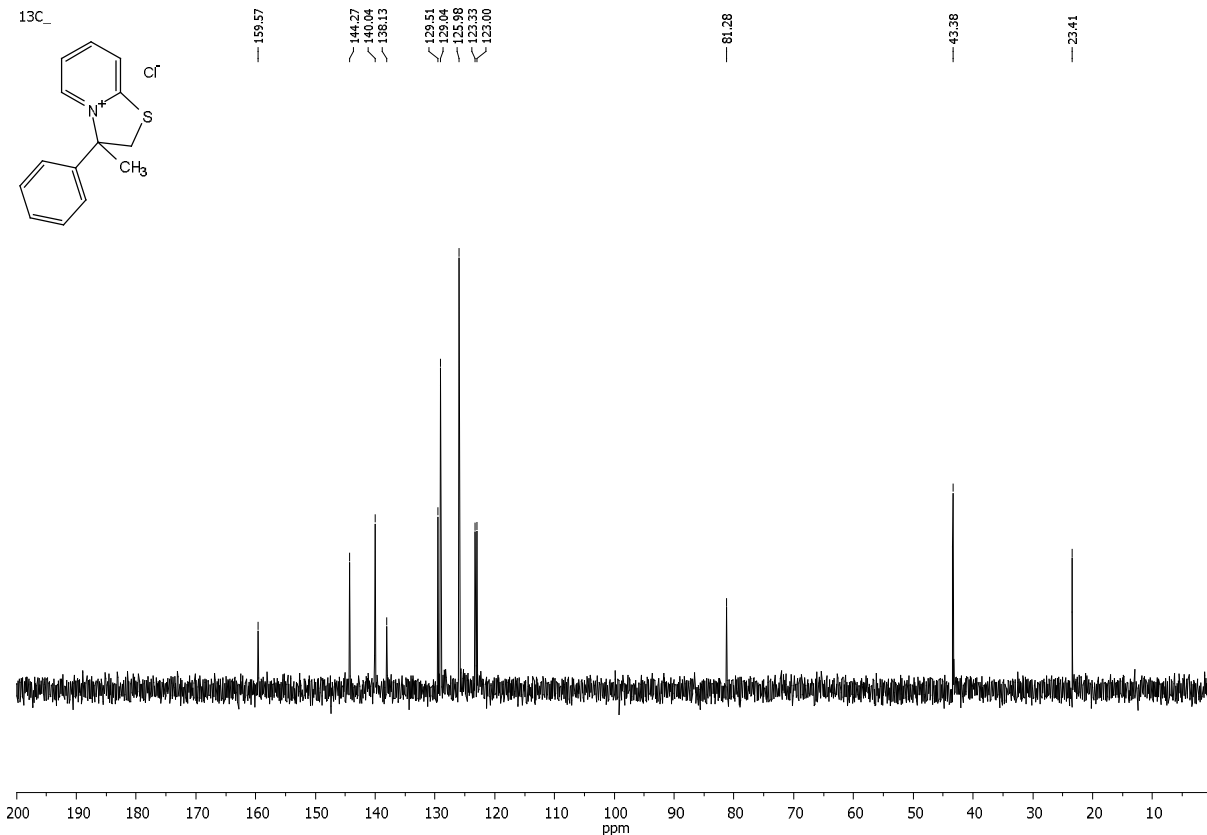
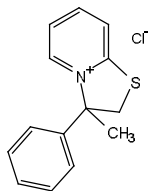
¹³C-NMR (DMSO-*d*₆) spectrum of compound 18

¹H

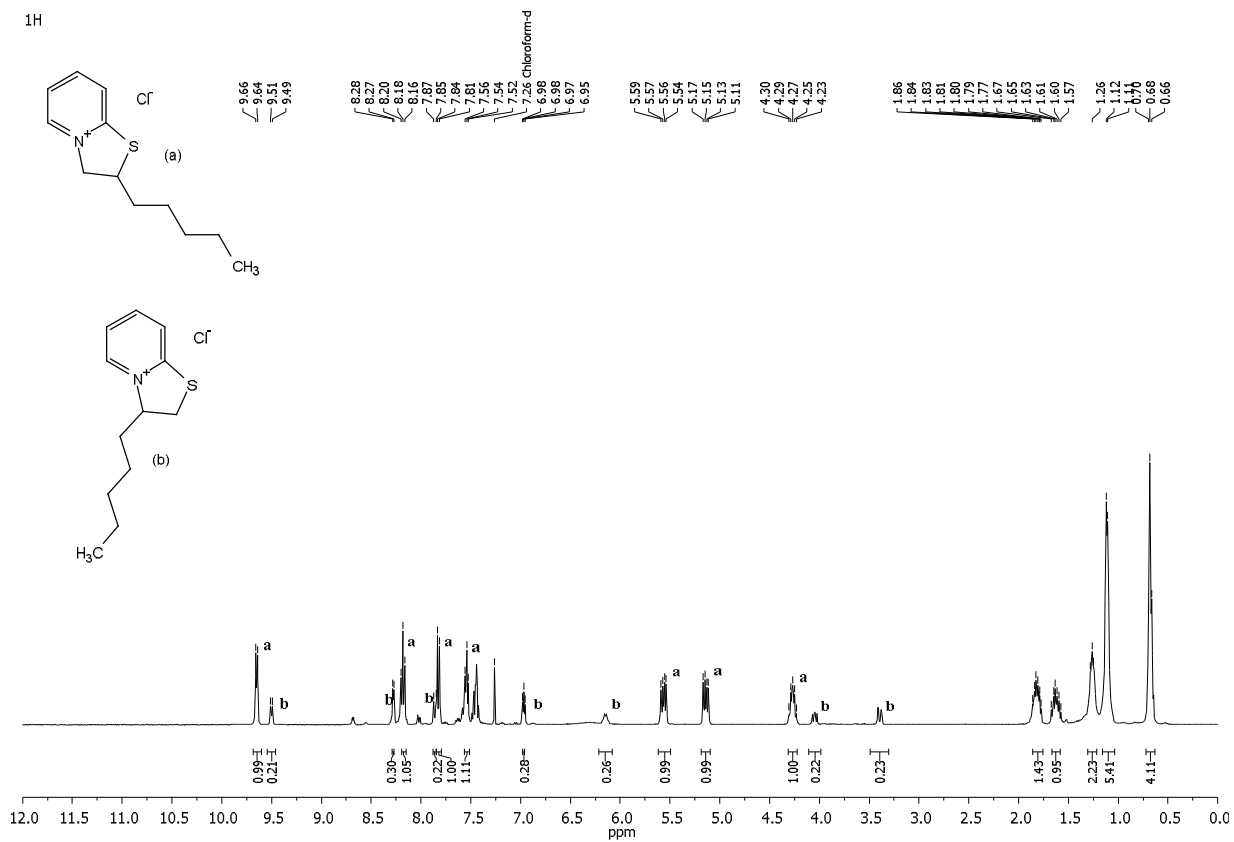


¹H-NMR (D₂O) spectrum of compound 22

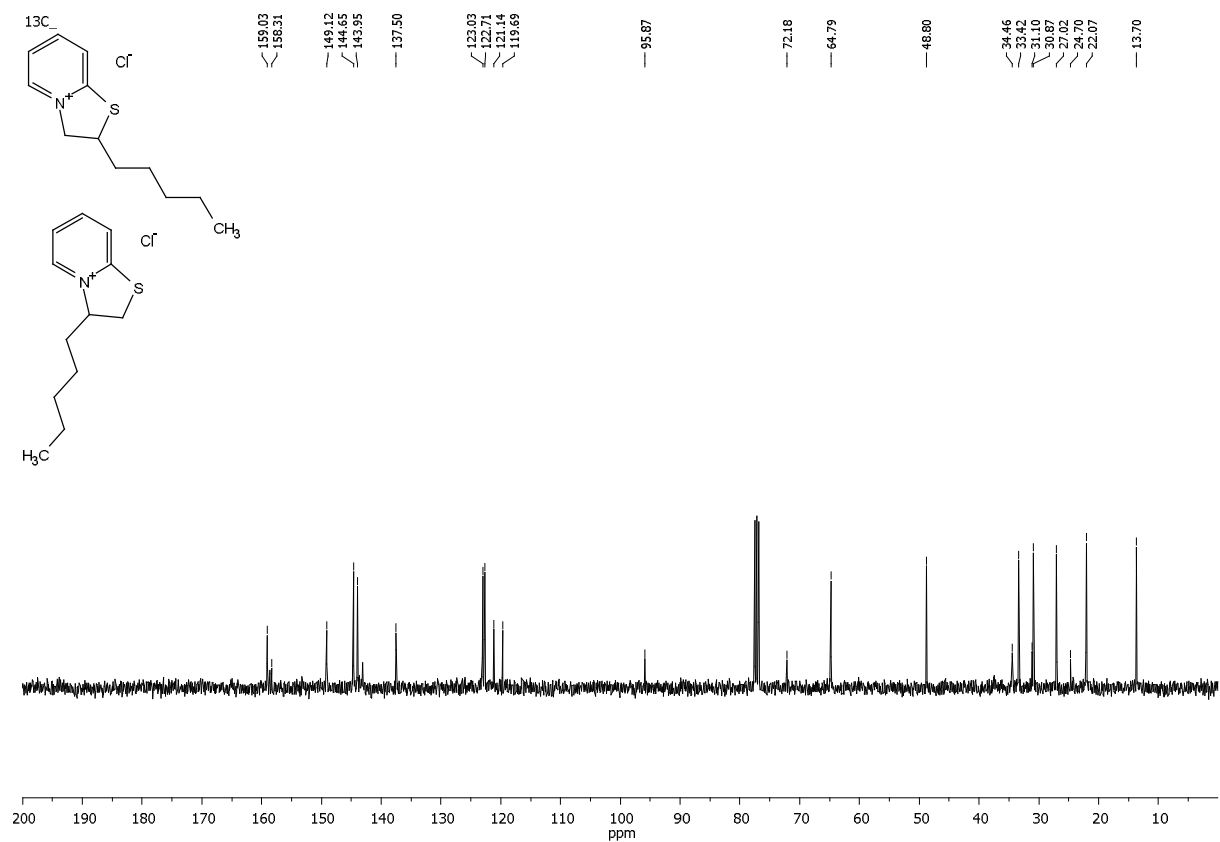
¹³C



¹³C-NMR (D₂O) spectrum of compound 22



¹H-NMR (CDCl₃) spectrum of the mixture of compounds 24 (a) and 25 (b)



¹³C-NMR (CDCl₃) spectrum of the mixture of compounds 24 and 25