Supporting Information for

One-pot four-component assembling for selenoureas

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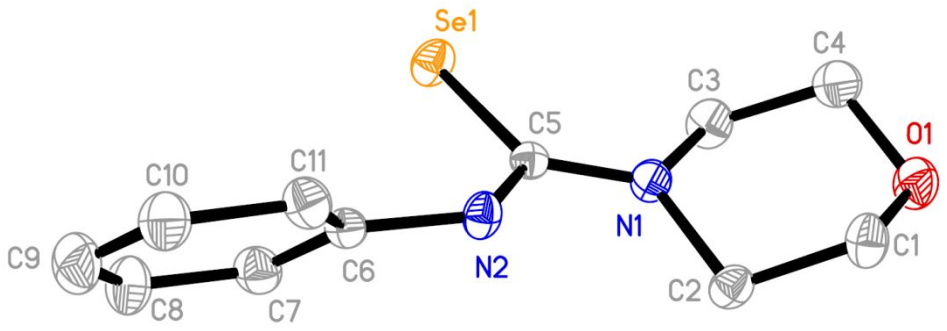
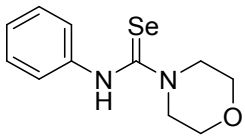


Fig. SI The molecular structure of product **3a** showing 30% probability ellipsoids; all hydrogen atoms are omitted for clarity.

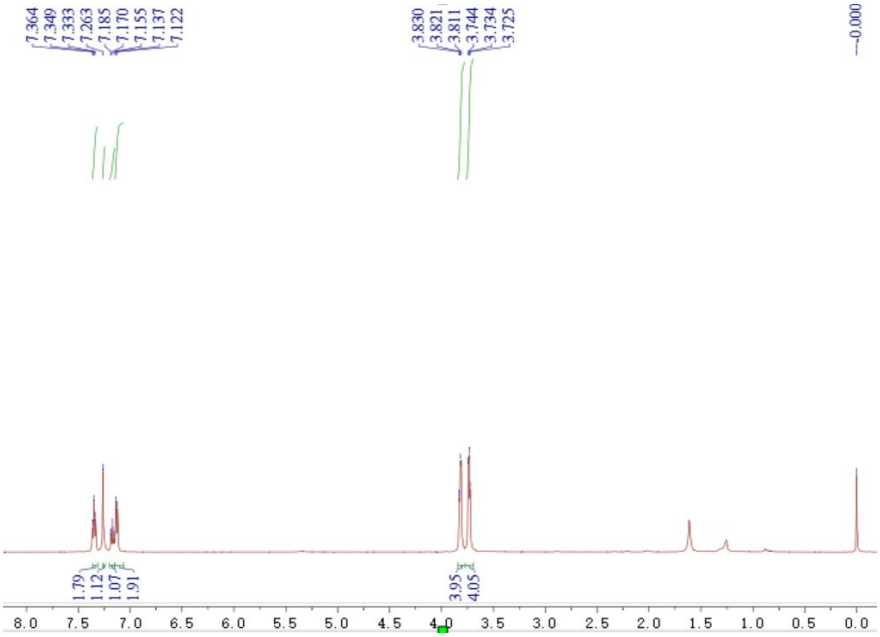
Table S1: Crystal data and refinement details for the X-ray structure determinations of compound **3a**.

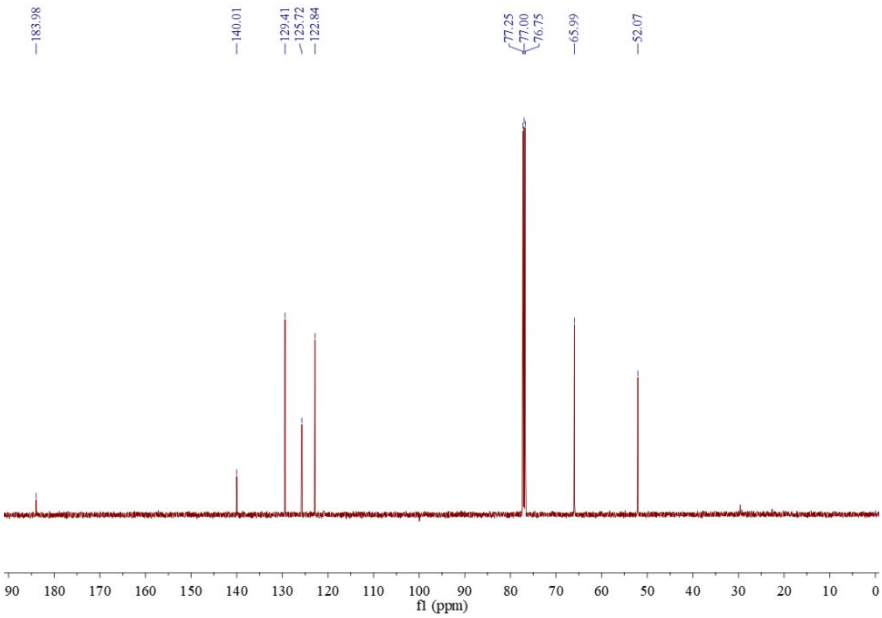
Identification code	Shelx	
Empirical formula	$C_{11}H_{14}N_2OSe$	
Formula weight	269.20	
Temperature	296(2) K	
Wavelength	71.073 pm	
Crystal system	Orthorhombic	
Space group	P c a 21	
Unit cell dimensions	a = 2782.8(8) pm	α = 90°
	b = 827.7(2) pm	β = 90°
	c = 987.7(3) pm	γ = 90°
Volume	2.2751(11) nm^3	
Z	8	
Density (calculated)	1.572 Mg/m^3	
Absorption coefficient	3.276 mm^{-1}	
F(000)	1088	
Crystal size	0.330x0.250x0.220 mm^3	
Theta range for data collection	2.461 to 25.998°	

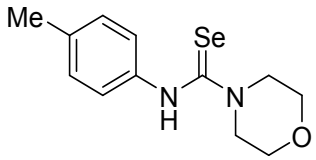
Index ranges	-34<=h<=34, -6<=k<=10, -8<=l<=12
Reflections collected	6626
Independent reflections	3299 [R(int) = 0.0244]
Completeness to theta = 25.242°	98.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.489 and 0.379
Refinement method	Full-matrix least-squares on F^2
Data/restraints/parameters	3299/1/272
Goodness-of-fit on F^2	1.056
Final R indices [I>2sigma(I)]	R^1 = 0.0287, wR2 = 0.0807
R indices (all data)	R^1 = 0.0348, wR2 = 0.0829
Absolute structure parameter	0.018(11)
Extinction coefficient	0.0124(9)
Largest diff. peak and hole	0.329 and -0.262 e·Å^{-3}



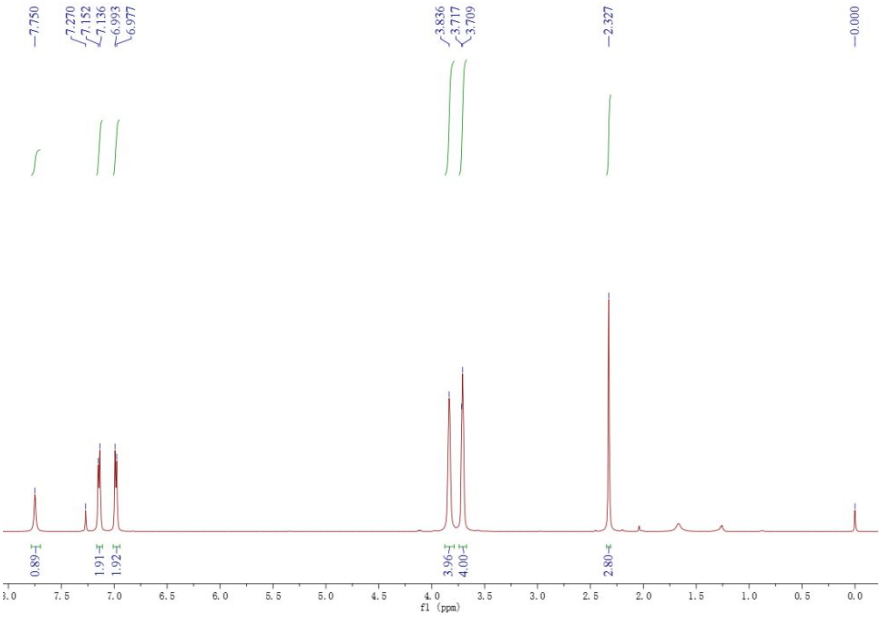
3a ($CDCl_3$, 500 MHz for ^1H NMR and 125 MHz for ^{13}C NMR)

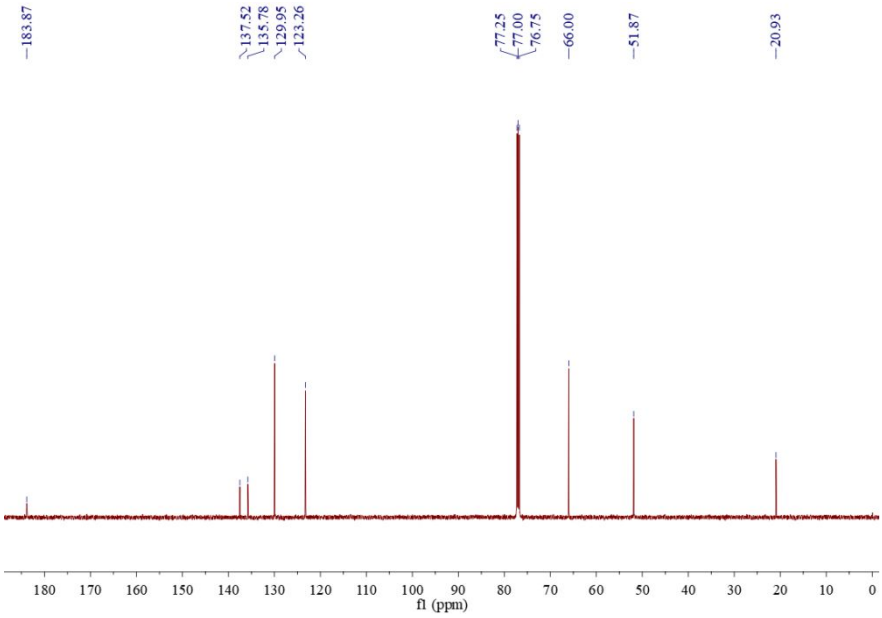


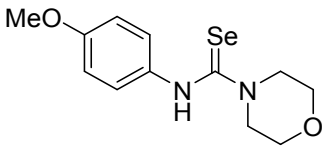




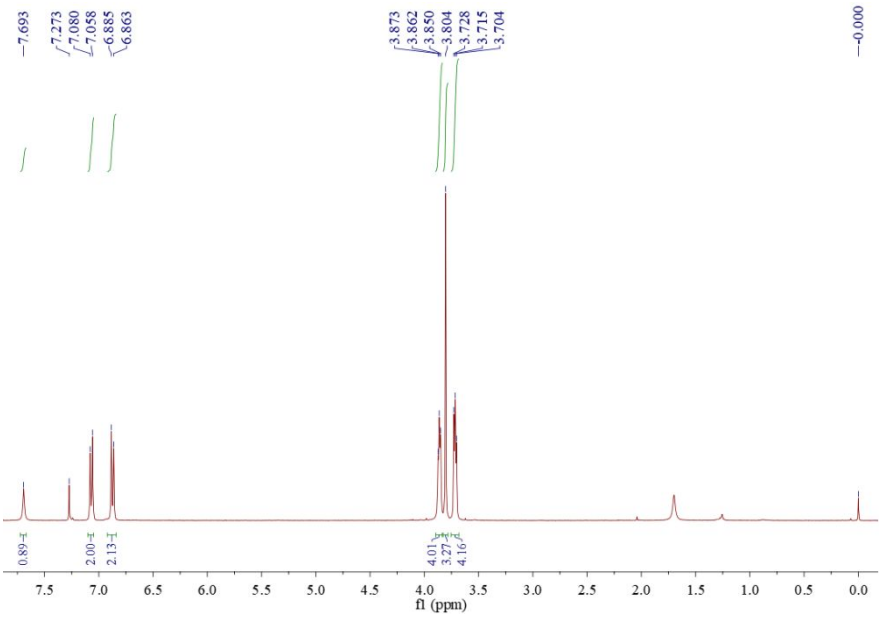
3b ($CDCl_3$, 500 MHz for ^1H NMR and 125 MHz for ^{13}C NMR)

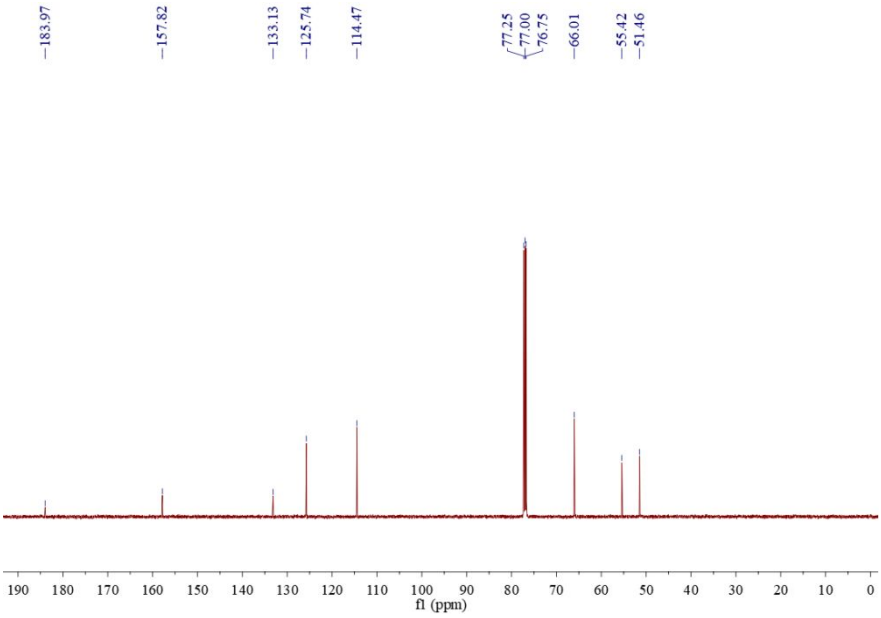


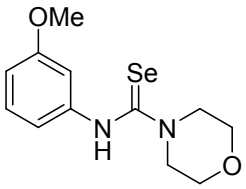




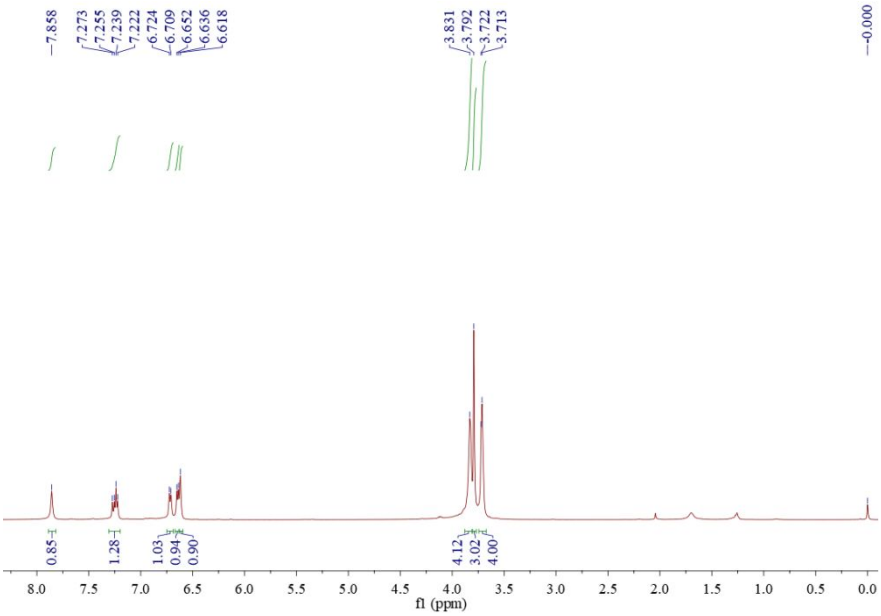
3c ($CDCl_3$, 400 MHz for ^1H NMR and 125 MHz for ^{13}C NMR)

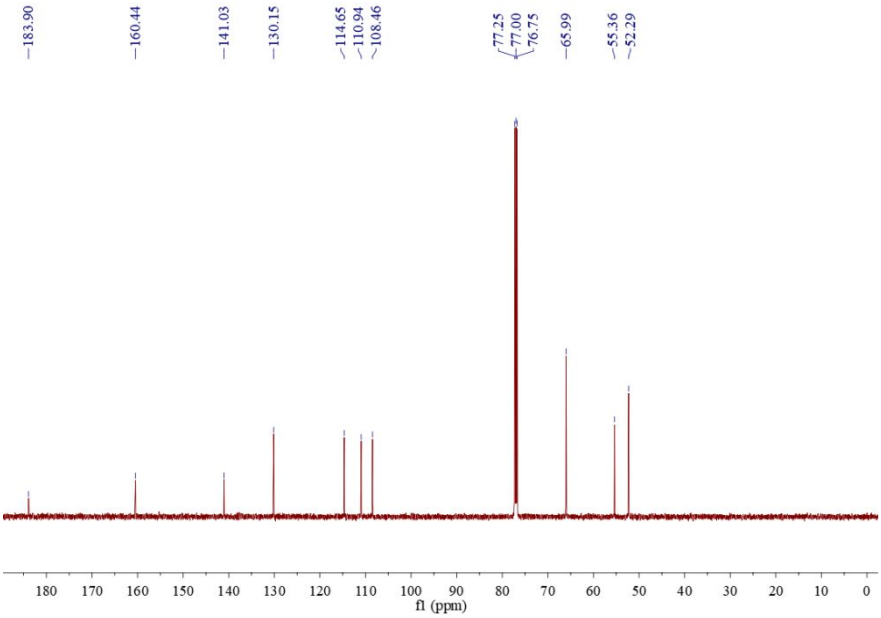


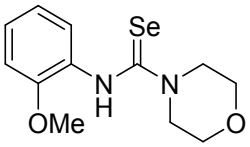




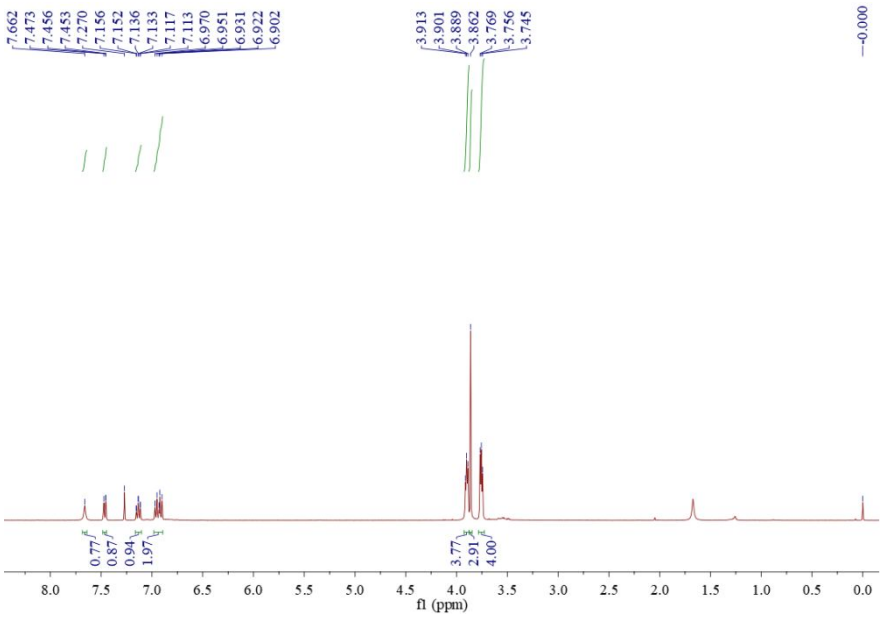
3d ($CDCl_3$, 500 MHz for ^1H NMR and 125 MHz for ^{13}C NMR)

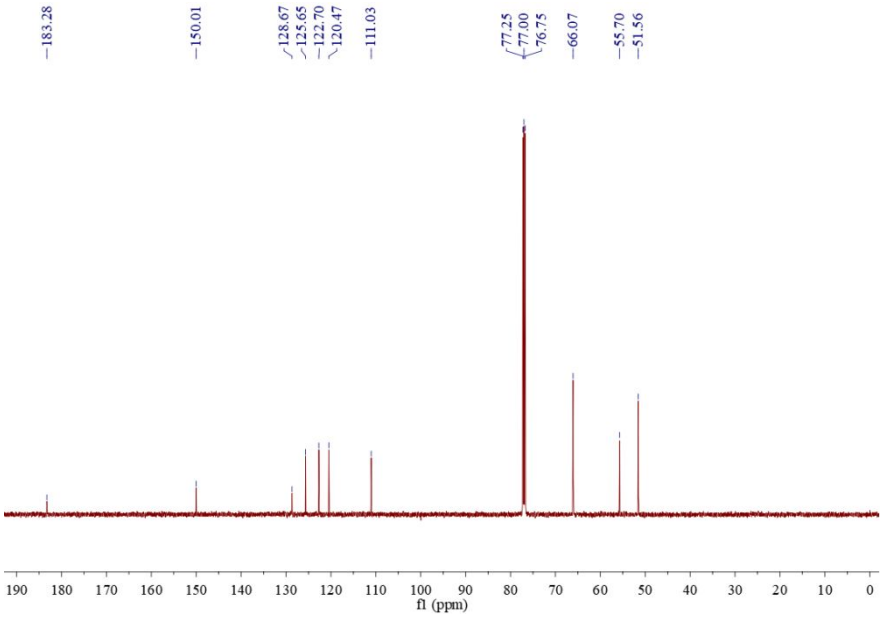


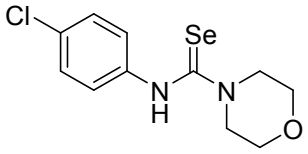




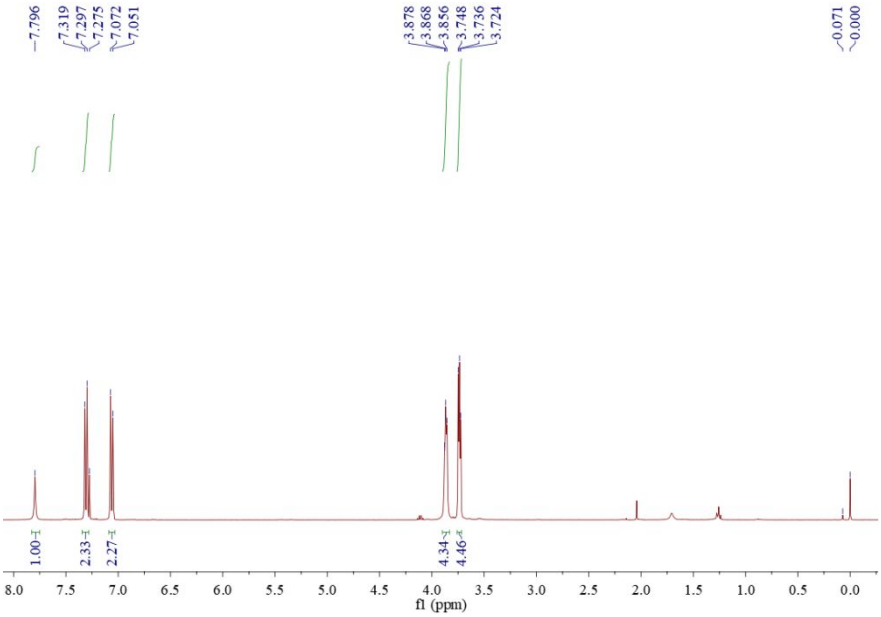
3e ($CDCl_3$, 500 MHz for ^1H NMR and 125 MHz for ^{13}C NMR)

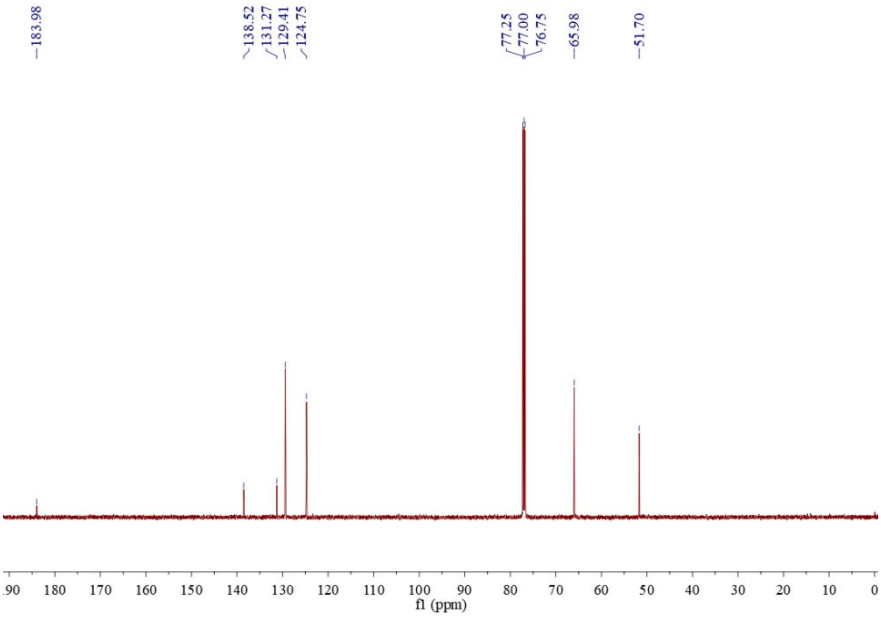


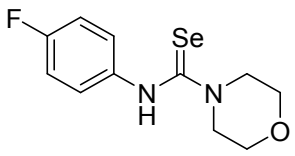




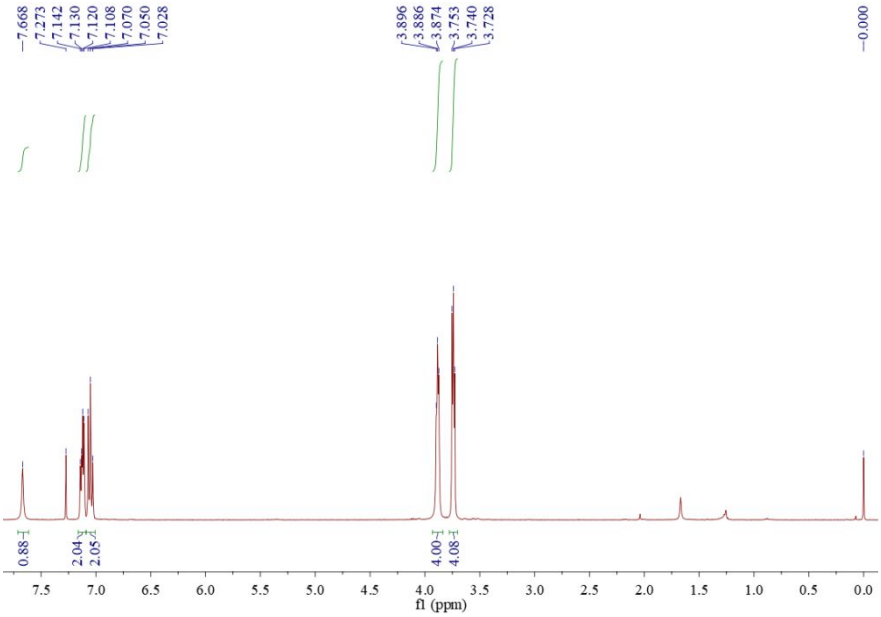
3f ($CDCl_3$, 400 MHz for ^1H NMR and 125 MHz for ^{13}C NMR)

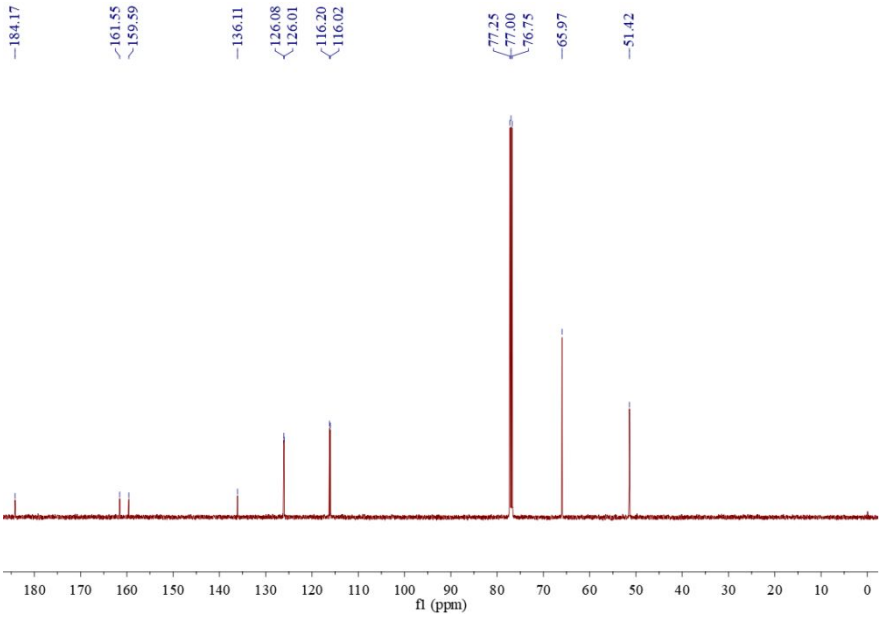


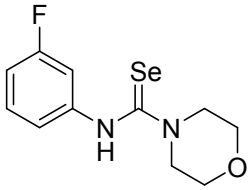




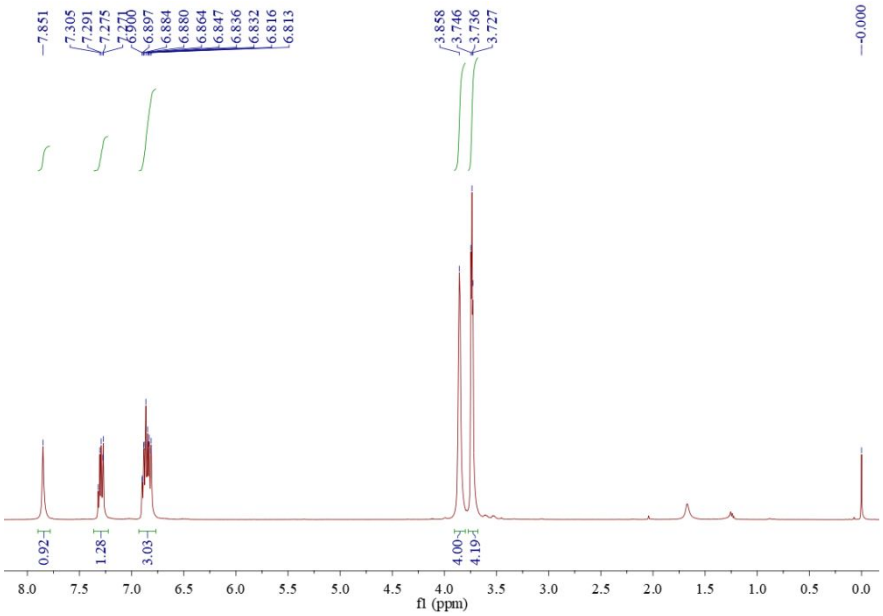
3g ($CDCl_3$, 400 MHz for ^1H NMR and 125 MHz for ^{13}C NMR)

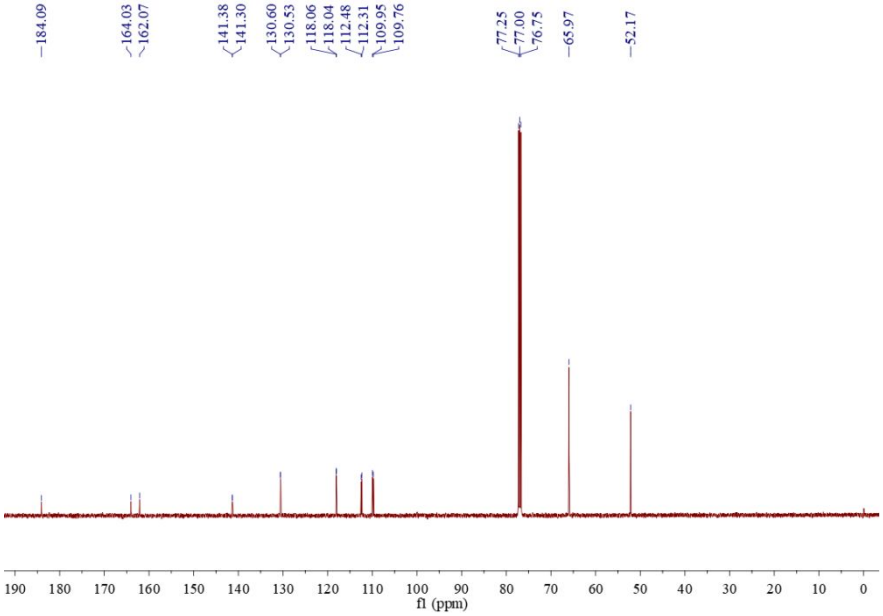


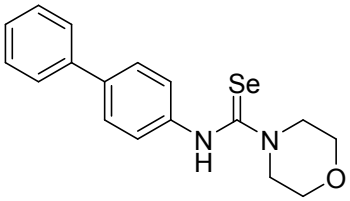




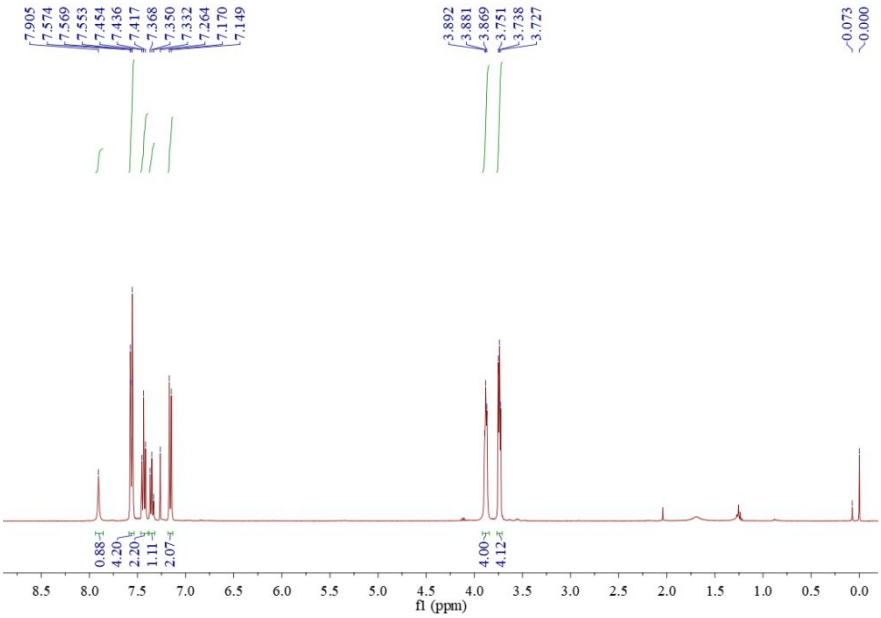
3h ($CDCl_3$, 500 MHz for ^1H NMR and 125 MHz for ^{13}C NMR)

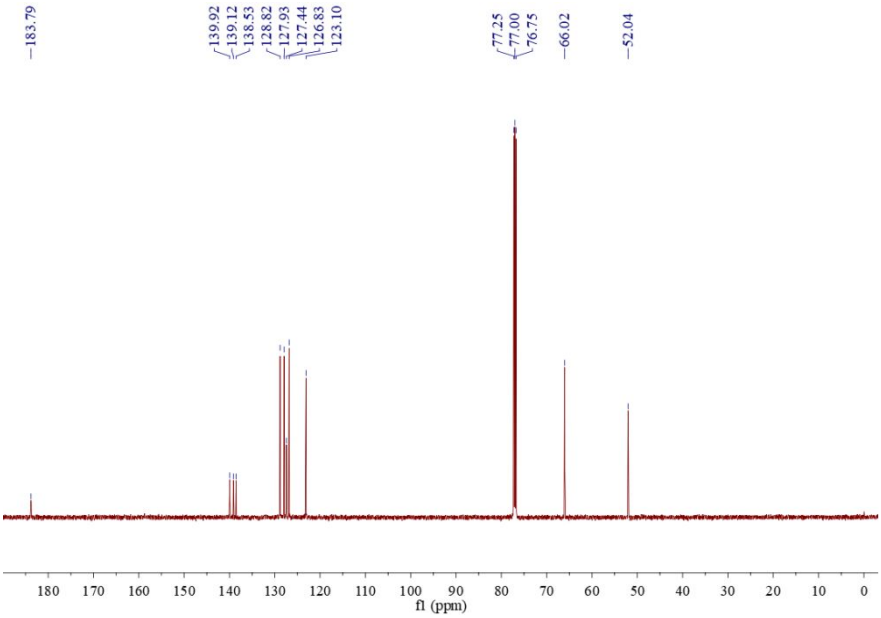


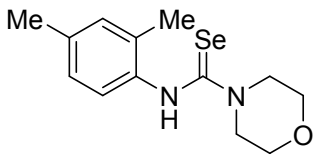




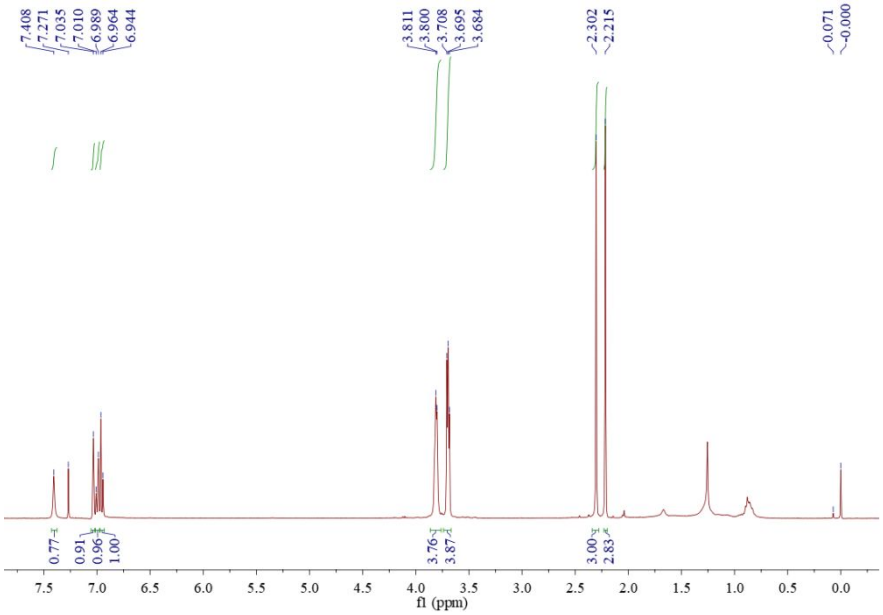
3i ($CDCl_3$, 400 MHz for ^1H NMR and 125 MHz for ^{13}C NMR)

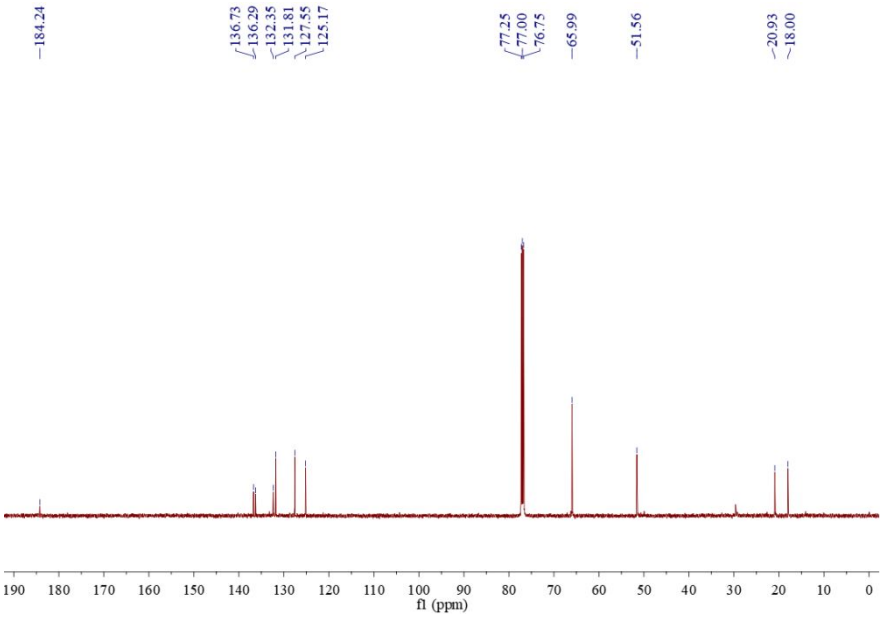


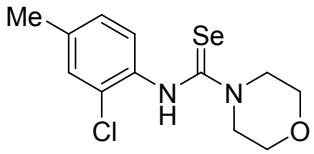




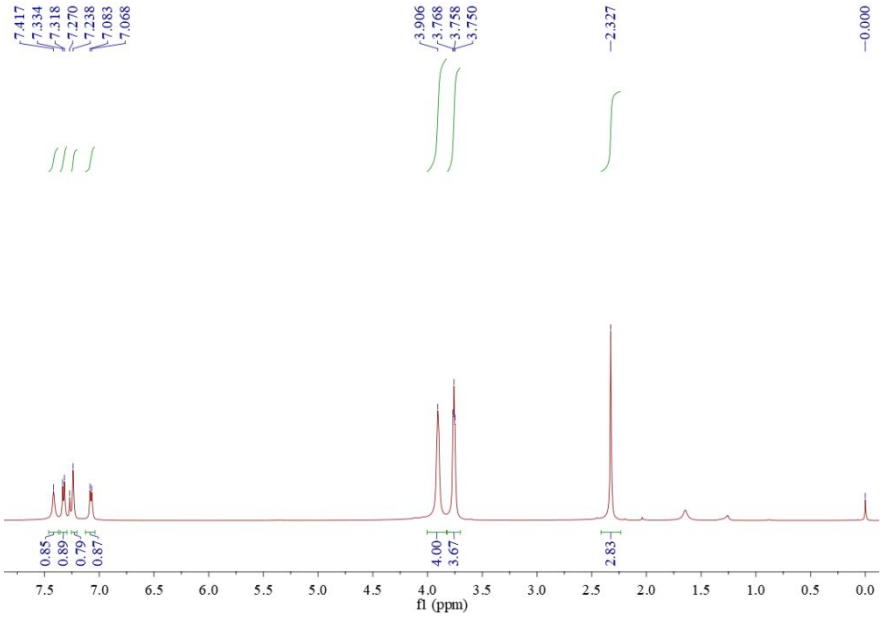
3j ($CDCl_3$, 400 MHz for ^1H NMR and 125 MHz for ^{13}C NMR)

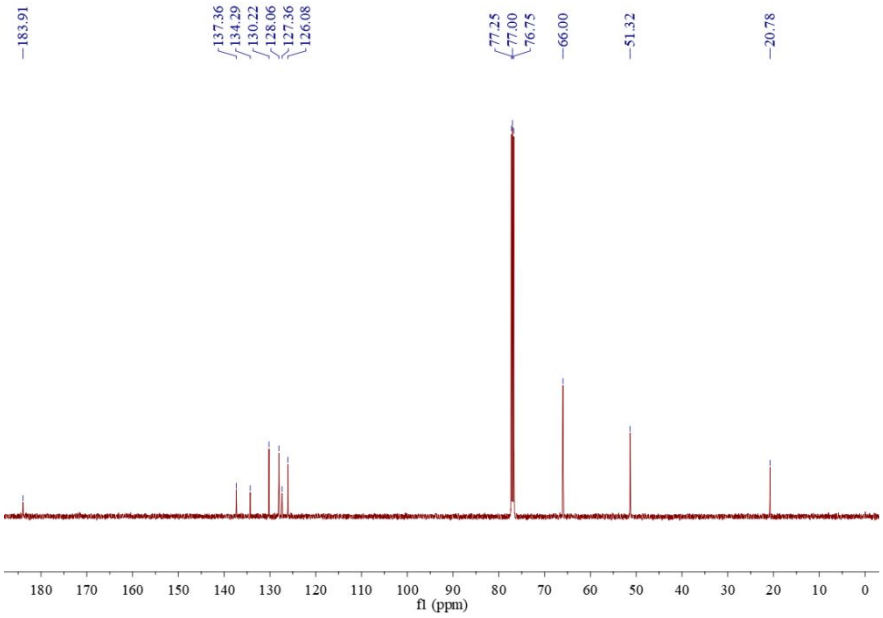


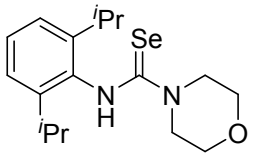




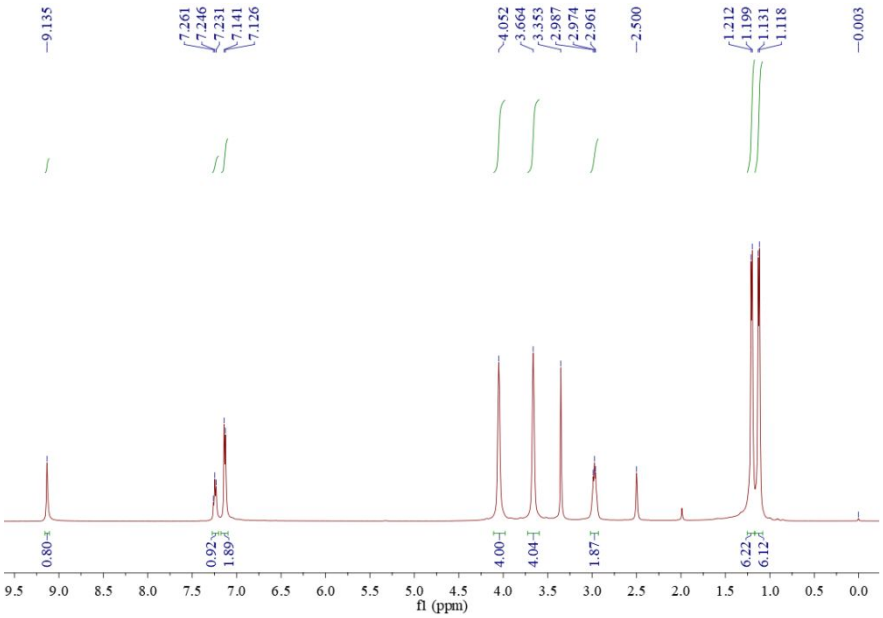
3k ($CDCl_3$, 500 MHz for ^{1}H NMR and 125 MHz for ^{13}C NMR)

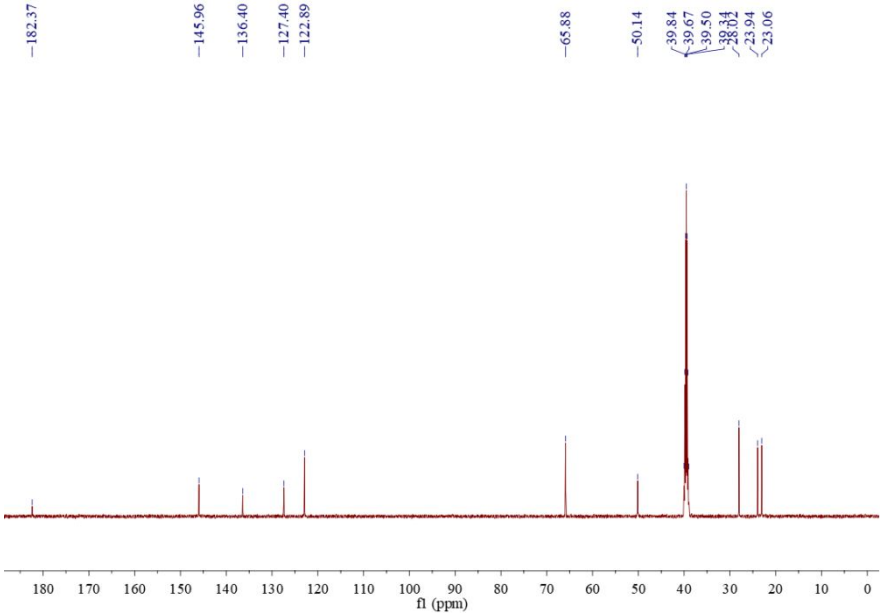


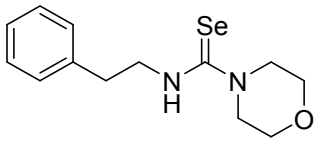




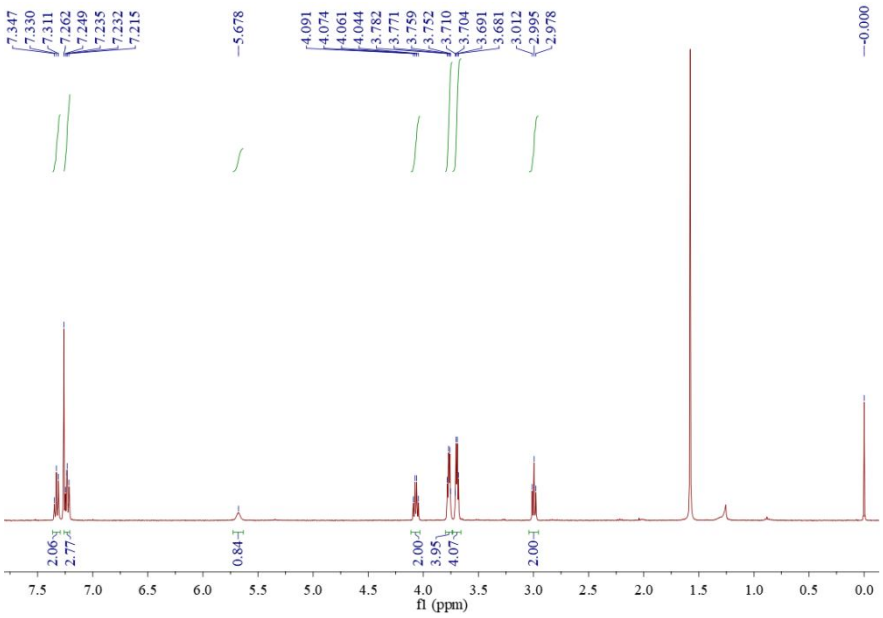
3l (DMSO-d_6, 500 MHz for ^{1}H NMR and 125 MHz for ^{13}C NMR)

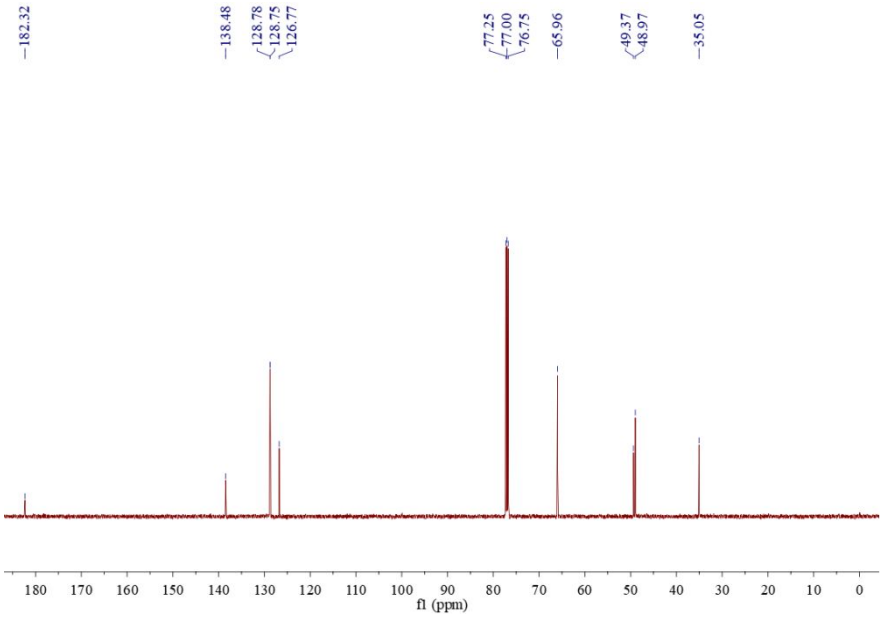


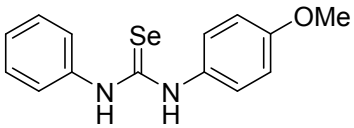




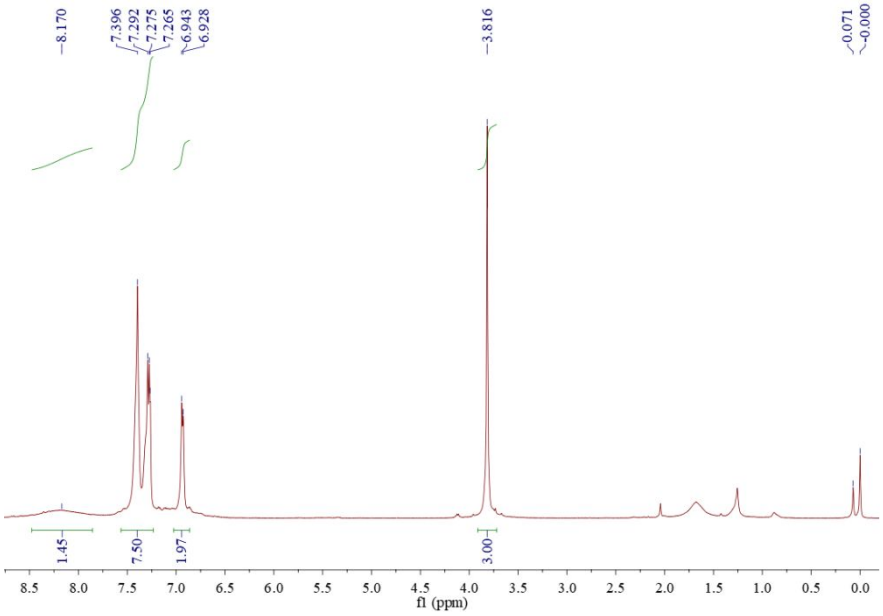
3m ($CDCl_3$, 400 MHz for ^1H NMR and 125 MHz for ^{13}C NMR)

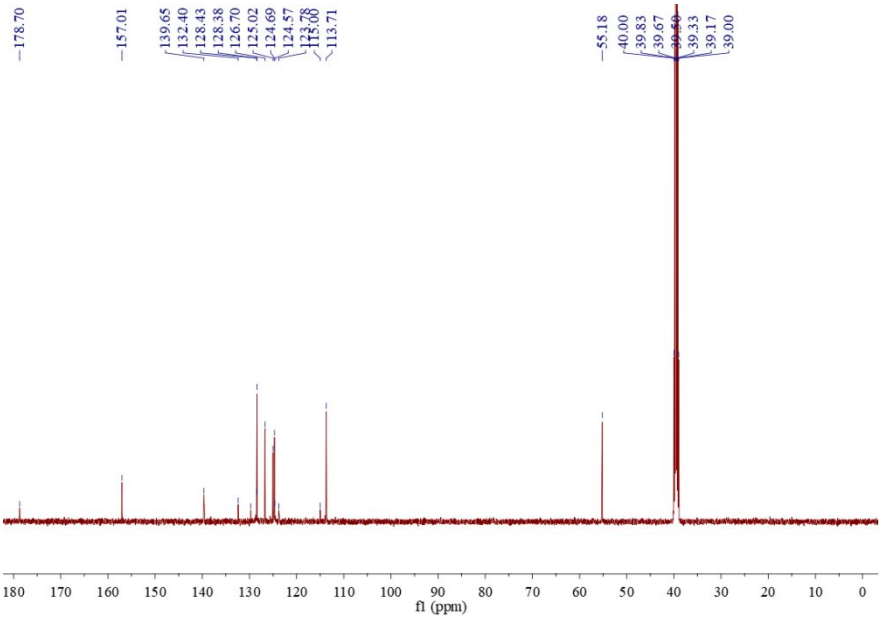


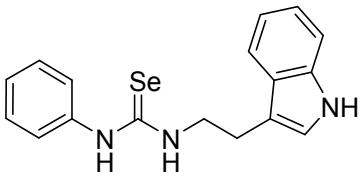




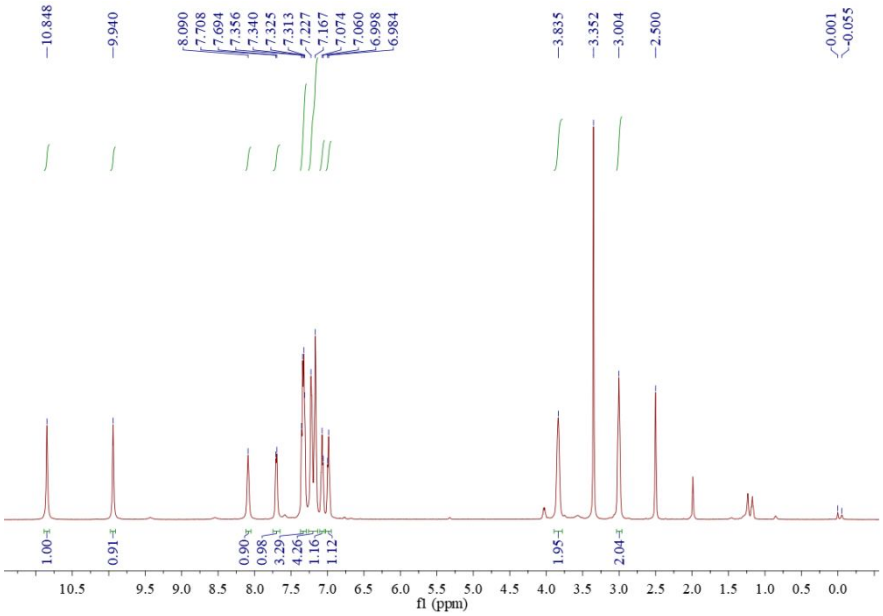
3n ($CDCl_3$, 500 MHz for ^{1}H NMR and DMSO-d_6, 125 MHz for ^{13}C NMR)

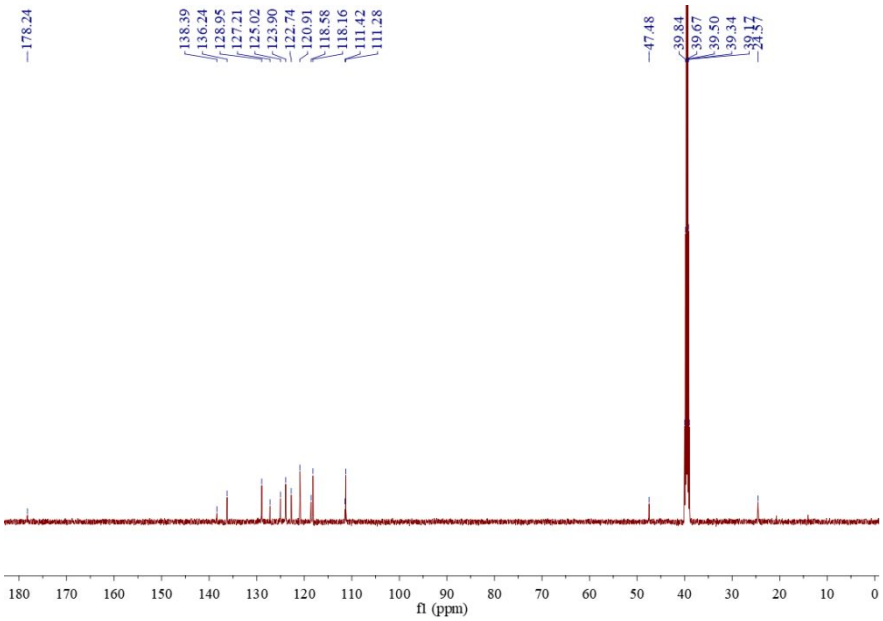


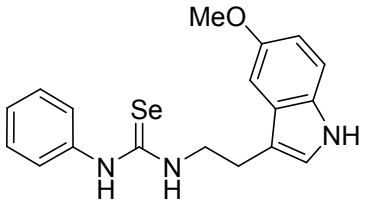




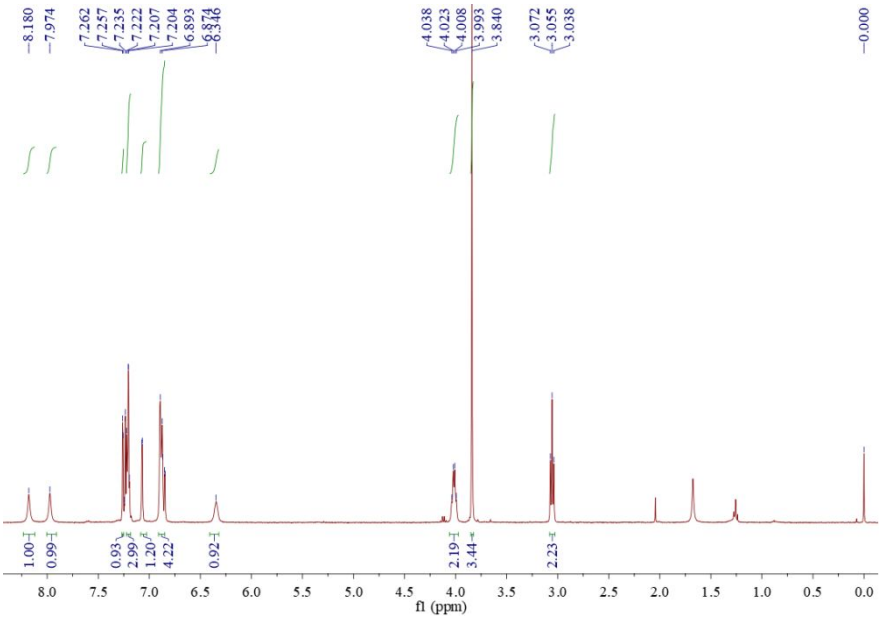
3o (DMSO-d_6, 500 MHz for ^{1}H NMR and 125 MHz for ^{13}C NMR)

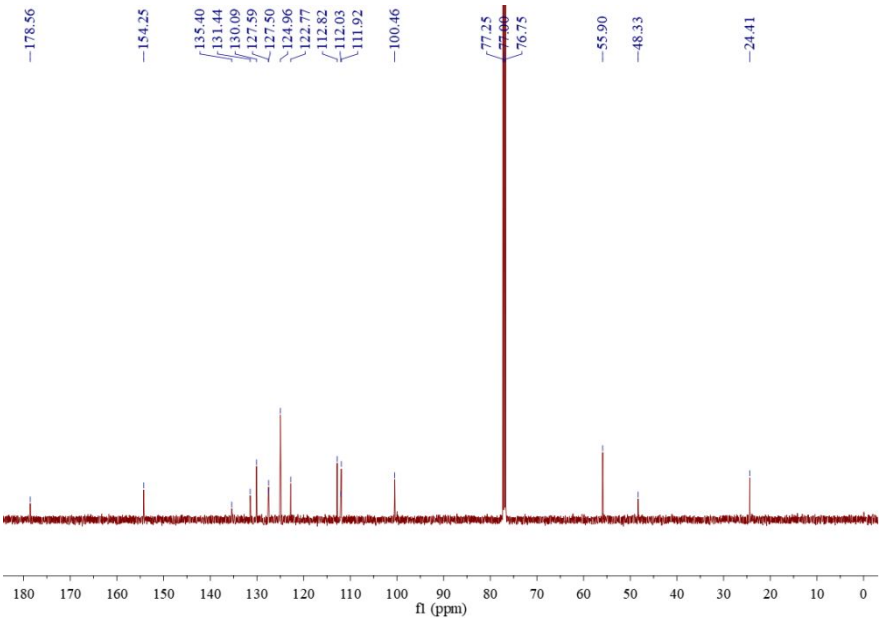


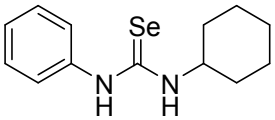




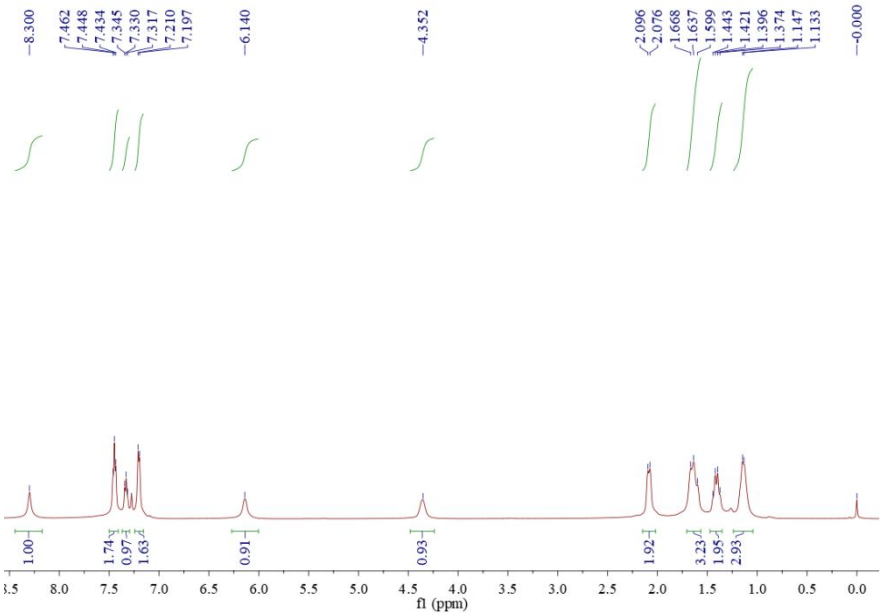
3p ($CDCl_3$, 400 MHz for ^{1}H NMR and 125 MHz for ^{13}C NMR)

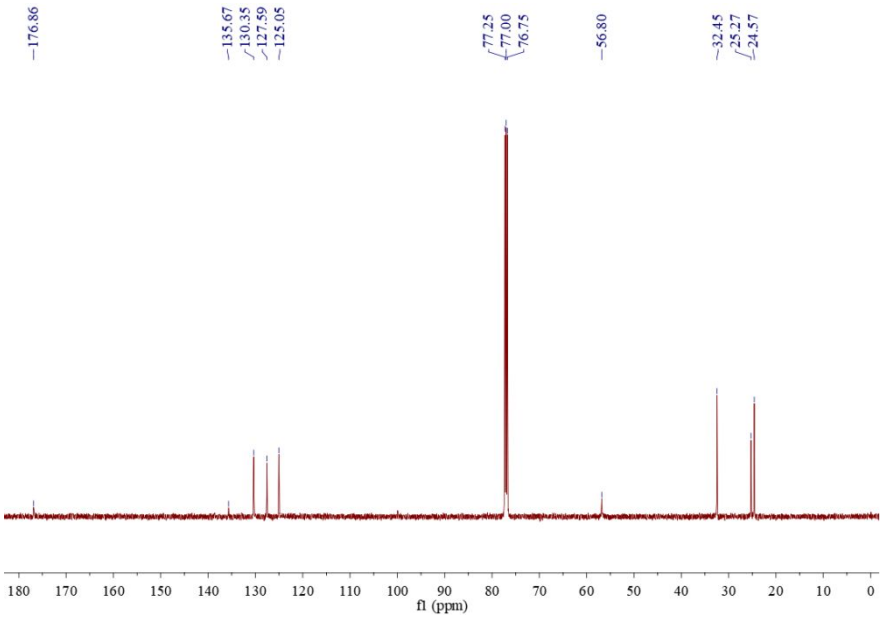


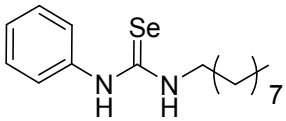




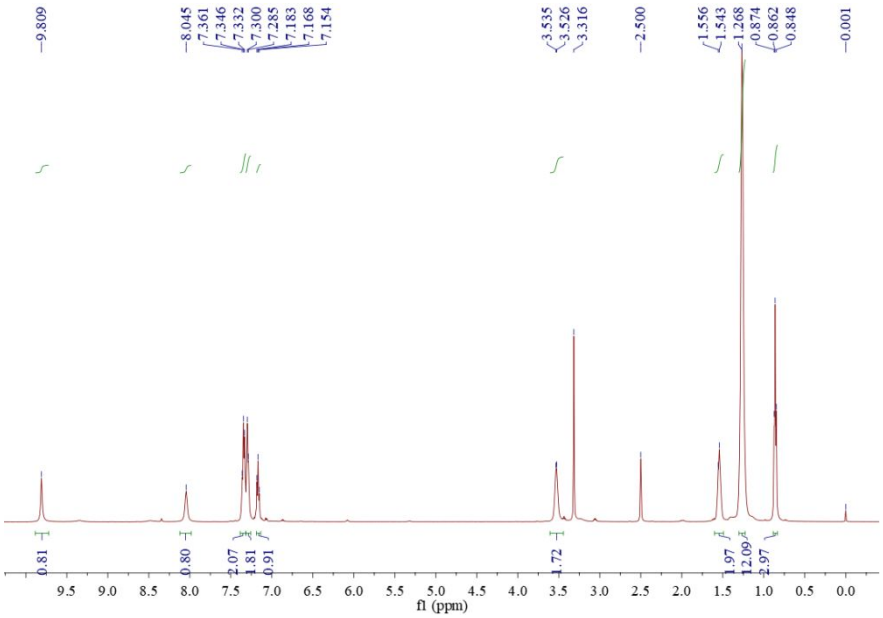
3q ($CDCl_3$, 500 MHz for ^1H NMR and 125 MHz for ^{13}C NMR)

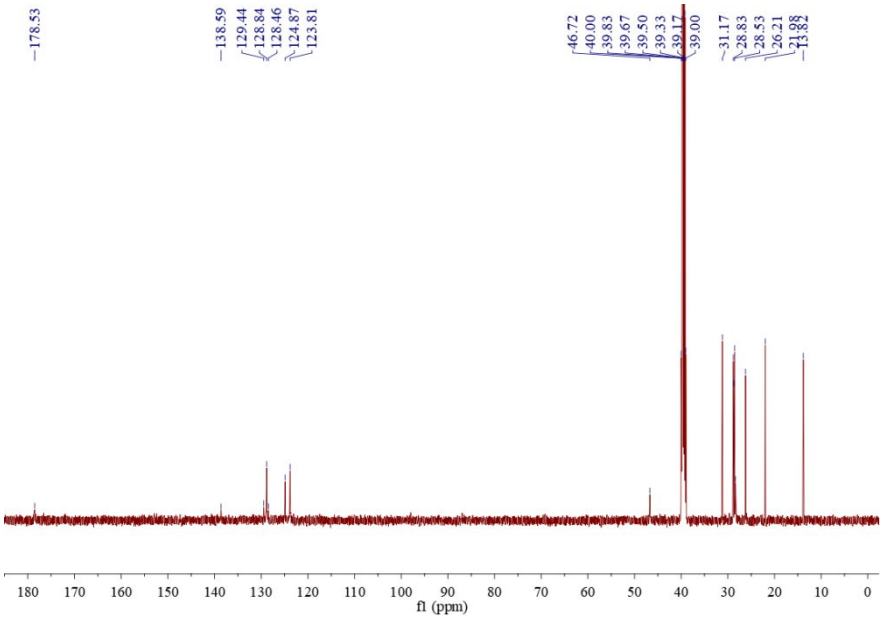


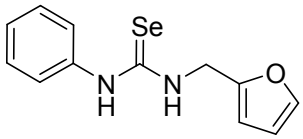




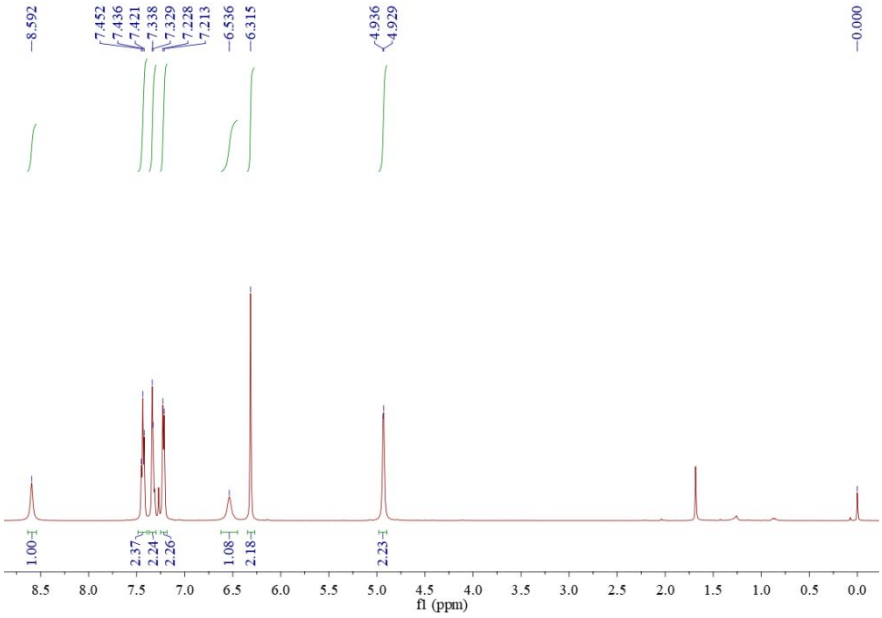
3r (DMSO-d_6, 500 MHz for ^{1}H NMR and 125 MHz for ^{13}C NMR)

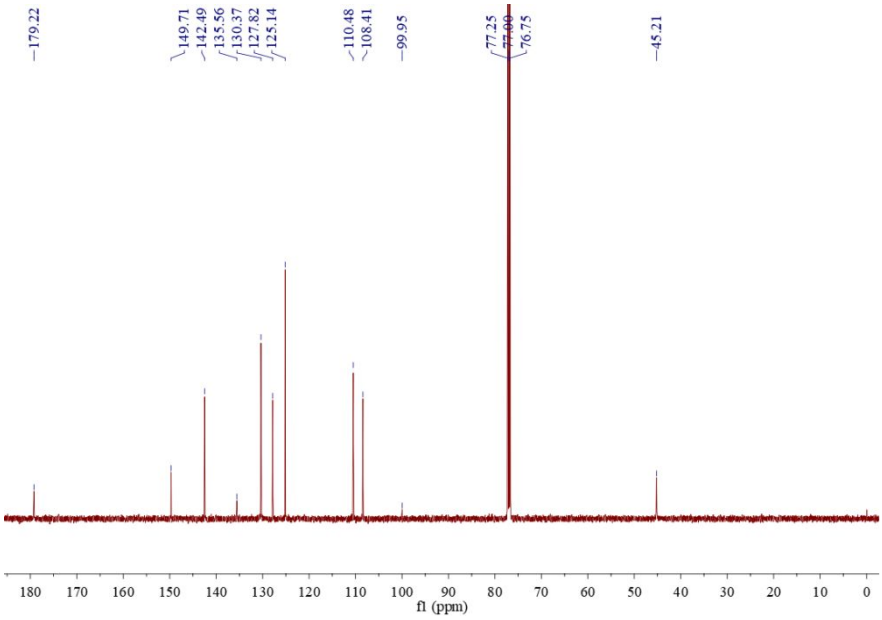


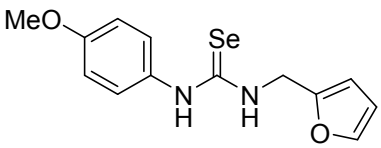




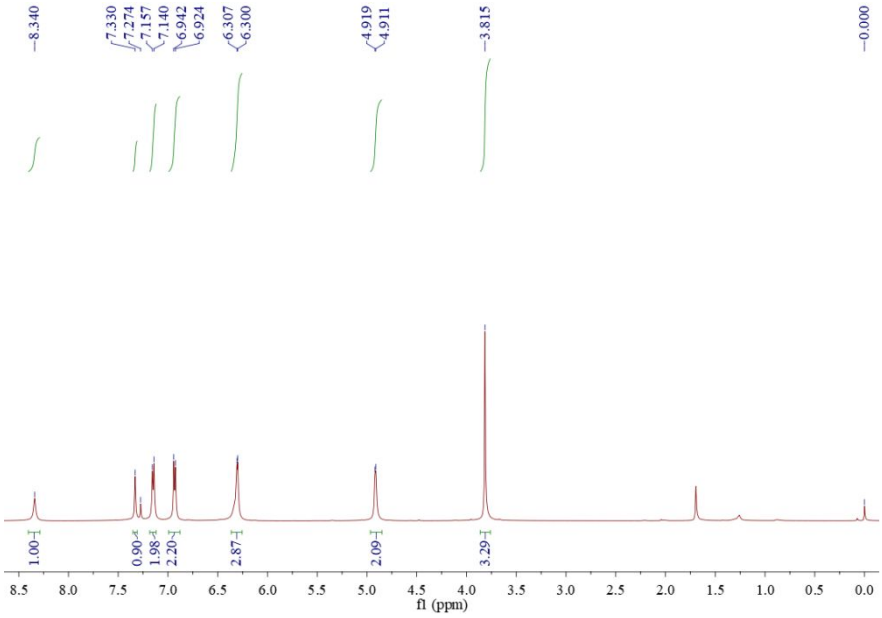
3s ($CDCl_3$, 500 MHz for ^1H NMR and 125 MHz for ^{13}C NMR)

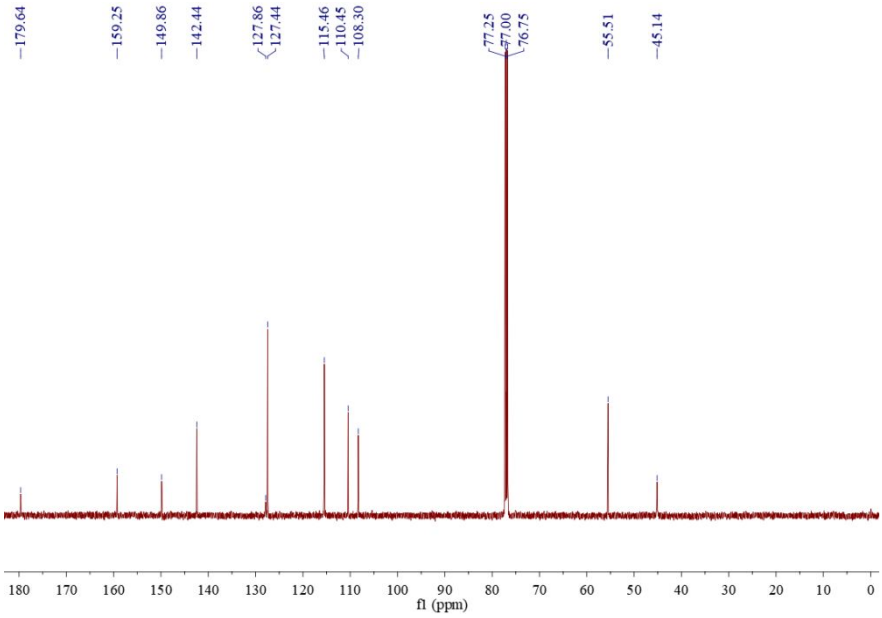


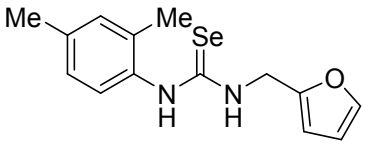




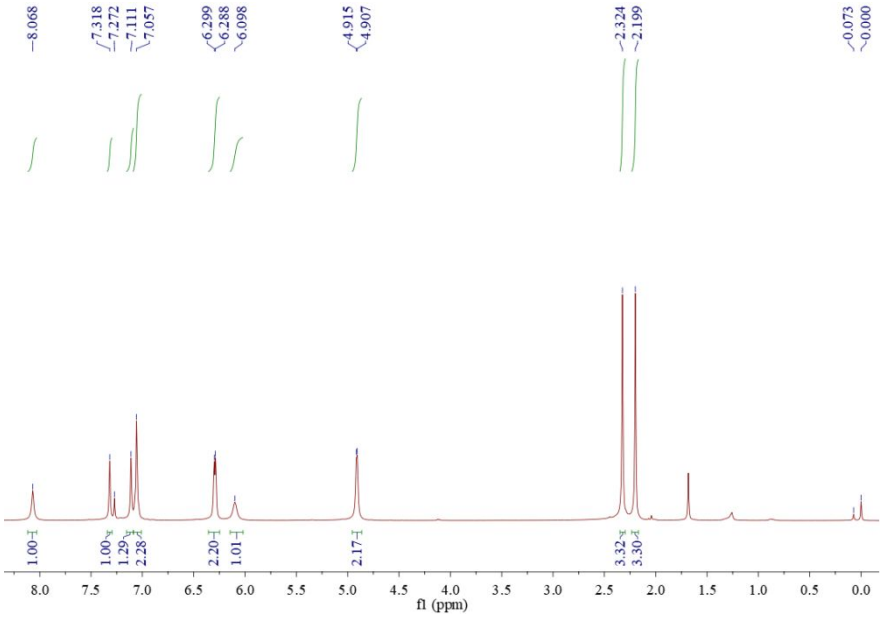
3t ($CDCl_3$, 500 MHz for ^1H NMR and 125 MHz for ^{13}C NMR)

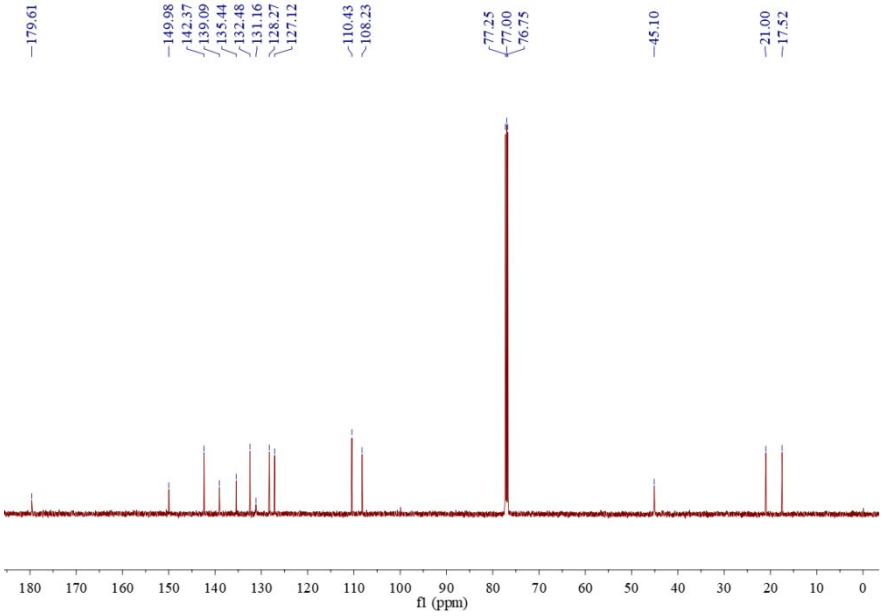


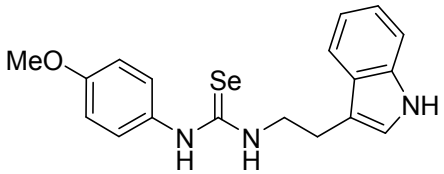




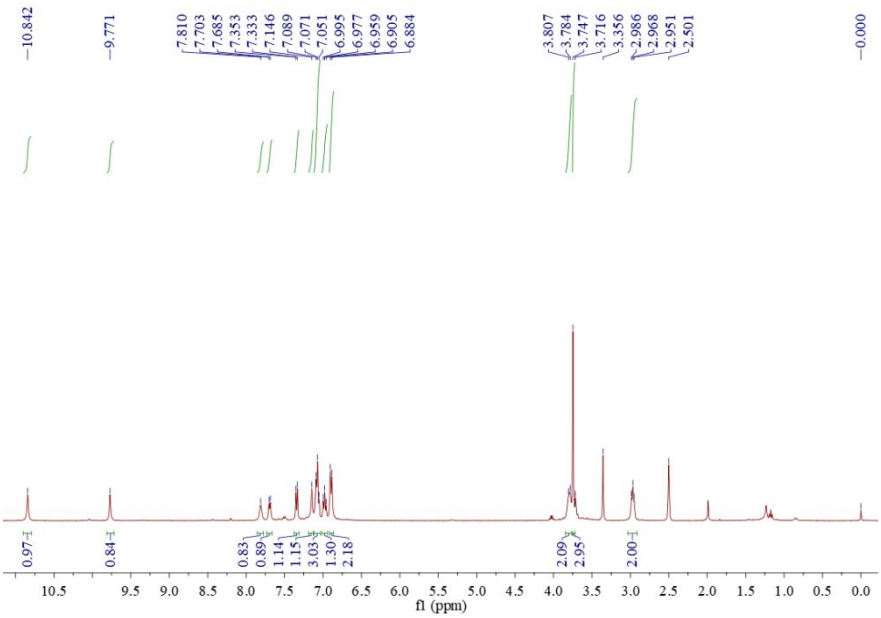
3u ($CDCl_3$, 500 MHz for ^1H NMR and 125 MHz for ^{13}C NMR)

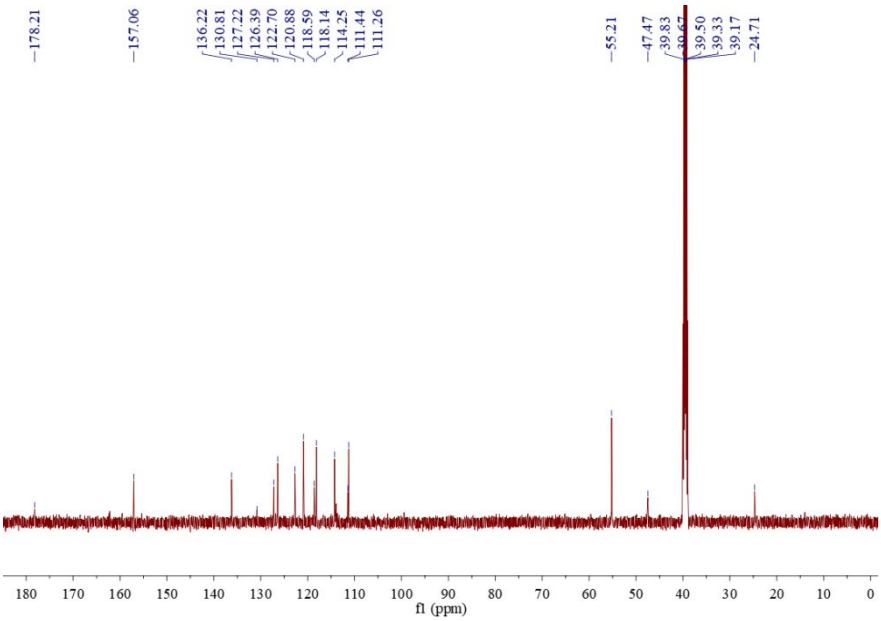


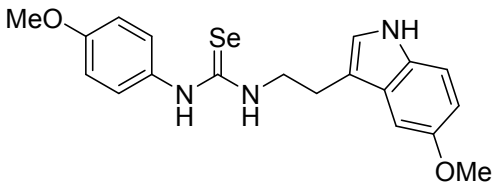




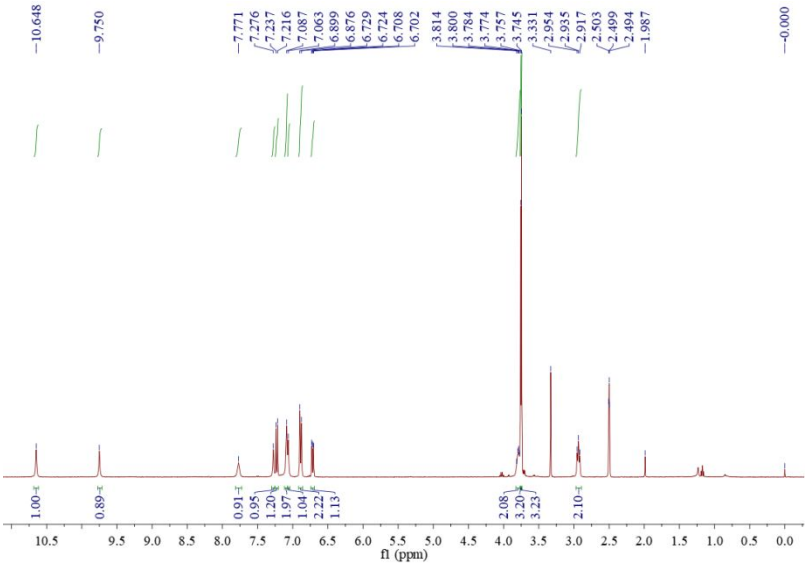
3v (DMSO-d_6, 400 MHz for ^{1}H NMR and 125 MHz for ^{13}C NMR)

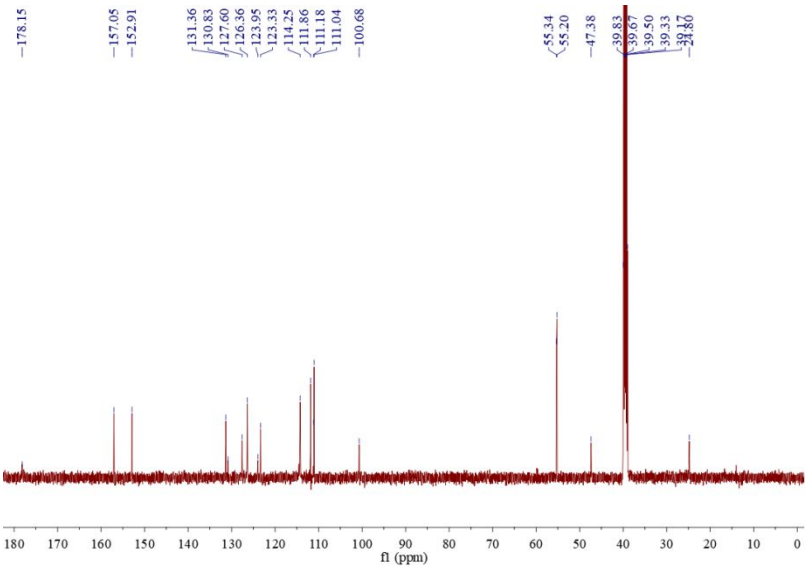


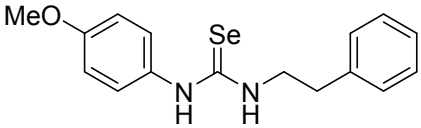




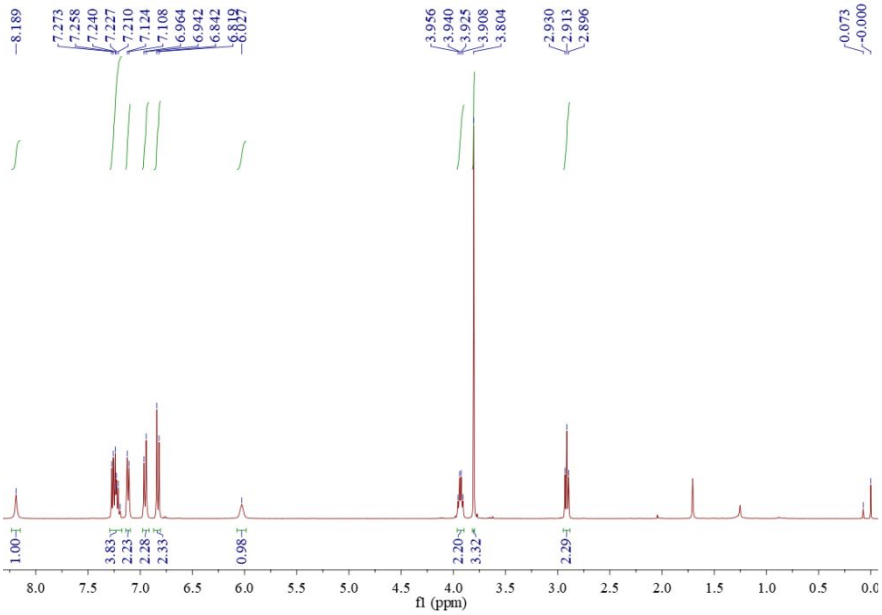
3w (DMSO-d_6, 400 MHz for ^{1}H NMR and 125 MHz for ^{13}C NMR)

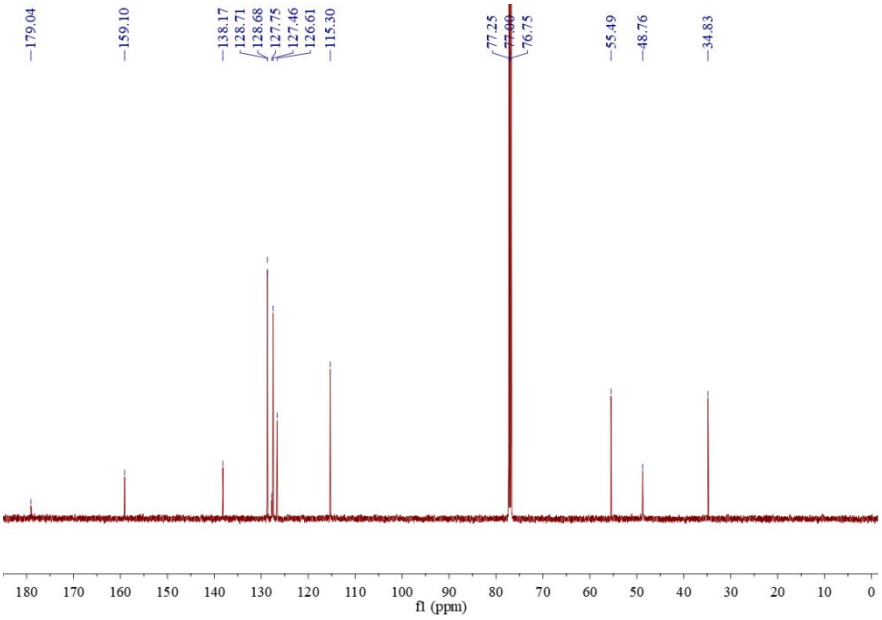


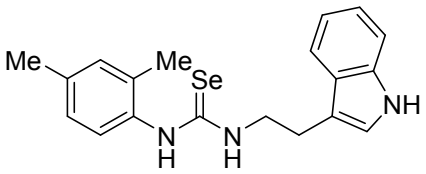




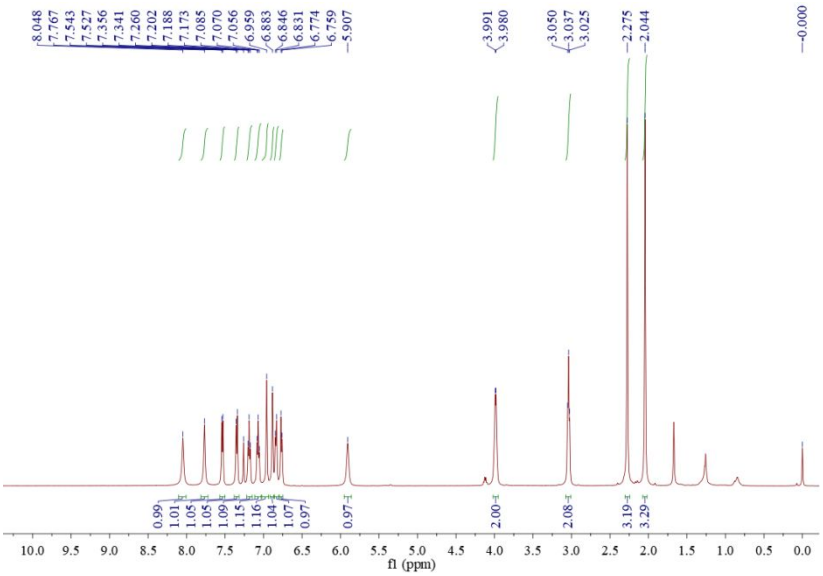
3x ($CDCl_3$, 400 MHz for ^1H NMR and 125 MHz for ^{13}C NMR)

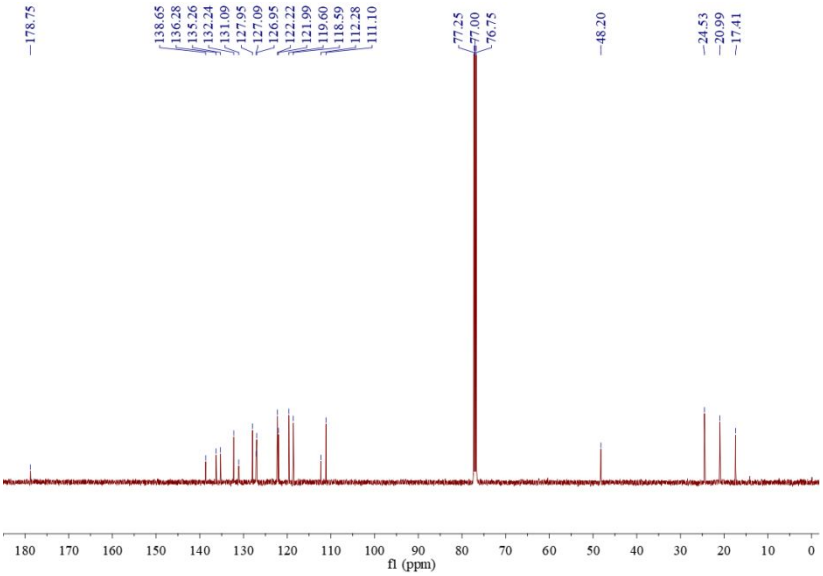


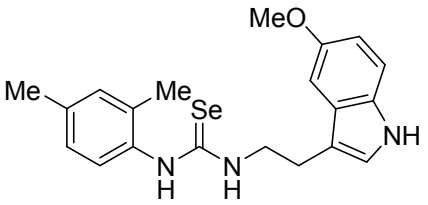




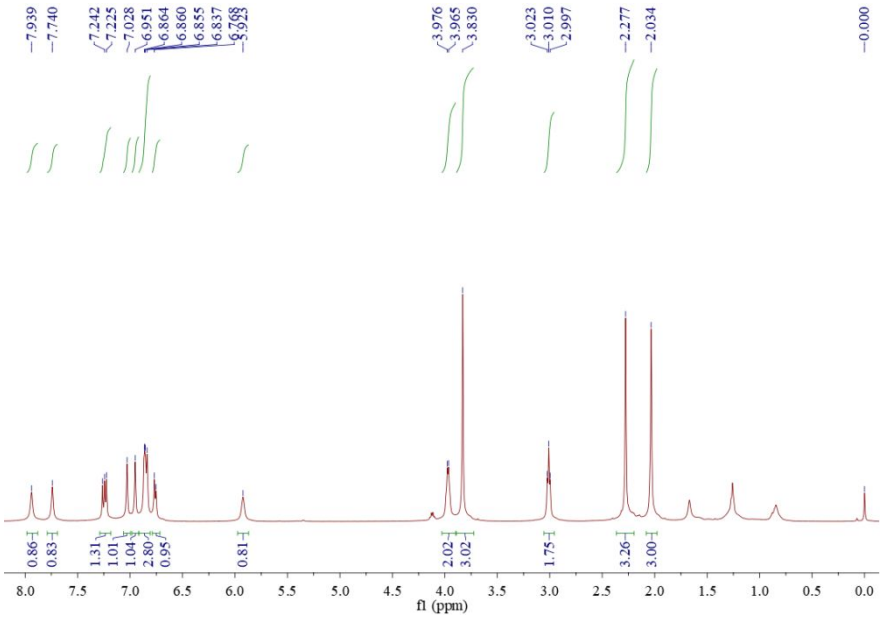
3y ($CDCl_3$, 500 MHz for ^{1}H NMR and 125 MHz for ^{13}C NMR)

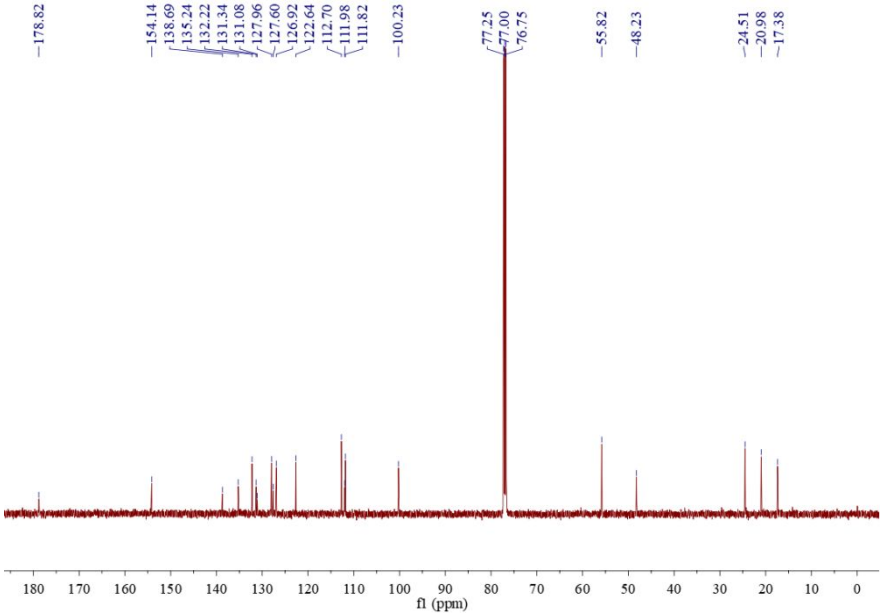


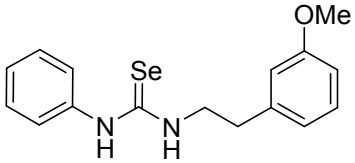




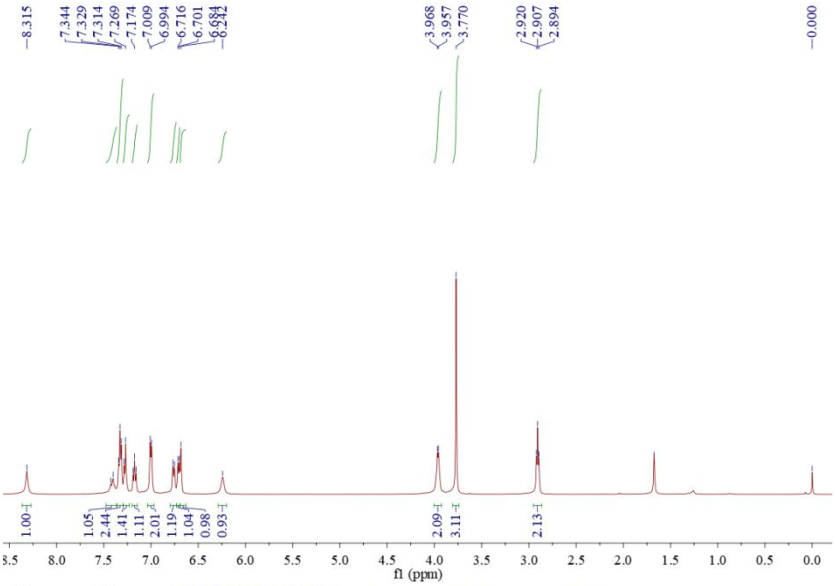
3z ($CDCl_3$, 500 MHz for ^1H NMR and 125 MHz for ^{13}C NMR)

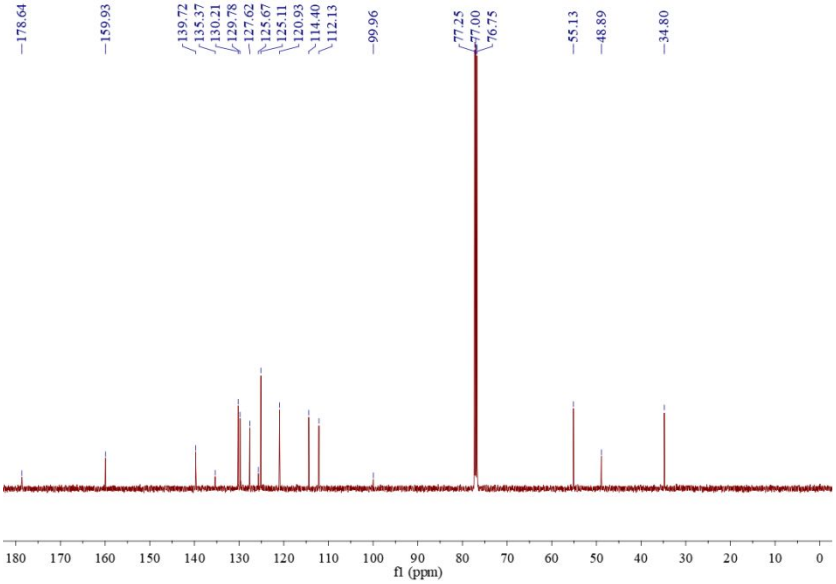


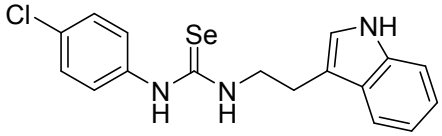




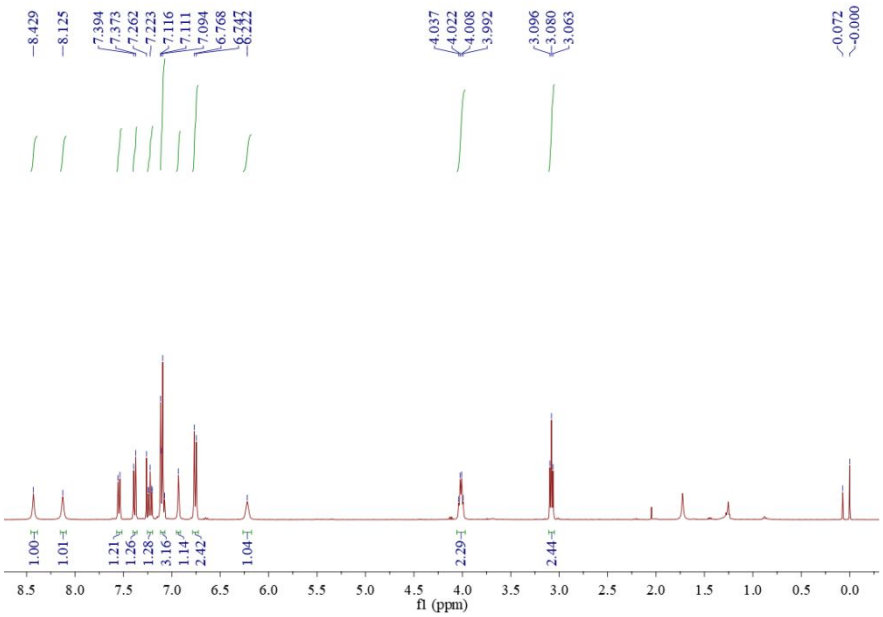
3aa ($CDCl_3$, 500 MHz for ^1H NMR and 125 MHz for ^{13}C NMR)

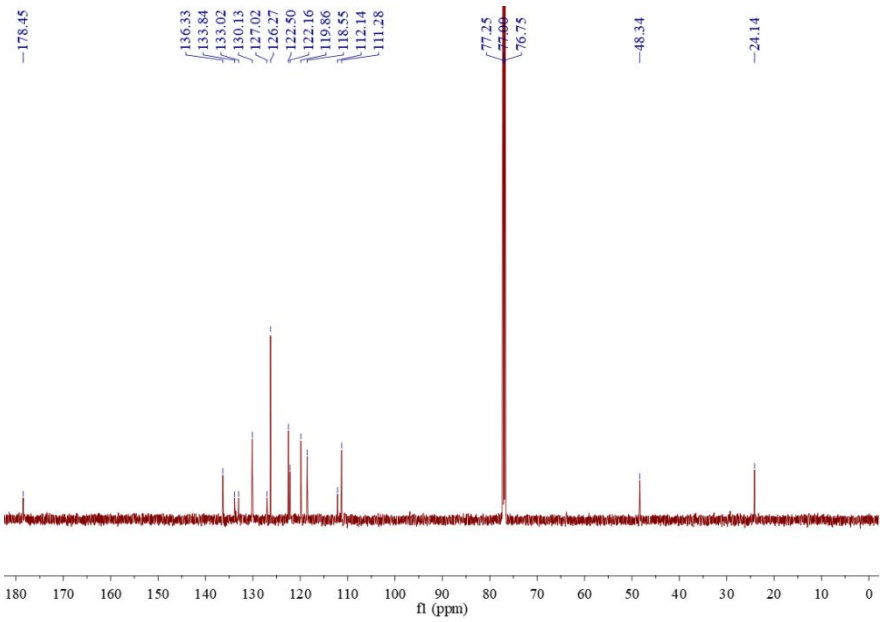


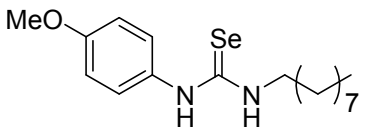




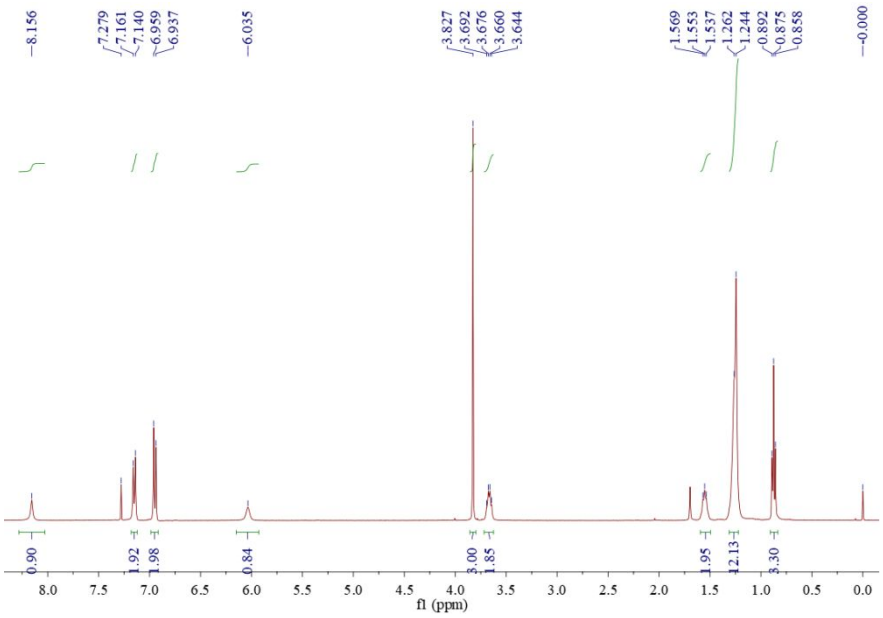
3ab ($CDCl_3$, 400 MHz for ^1H NMR and 125 MHz for ^{13}C NMR)

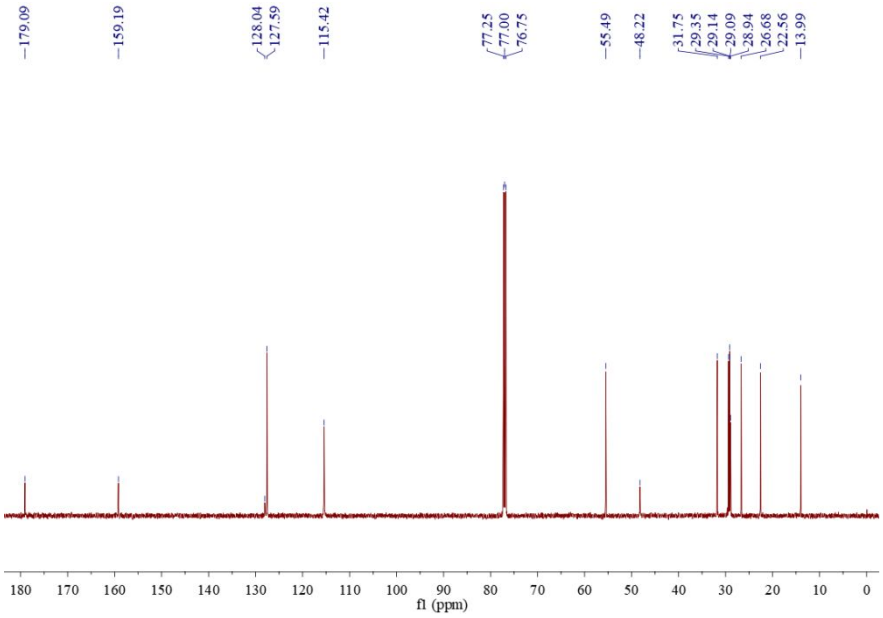


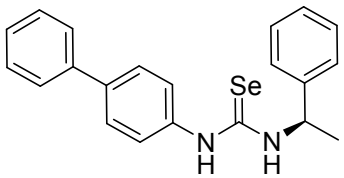




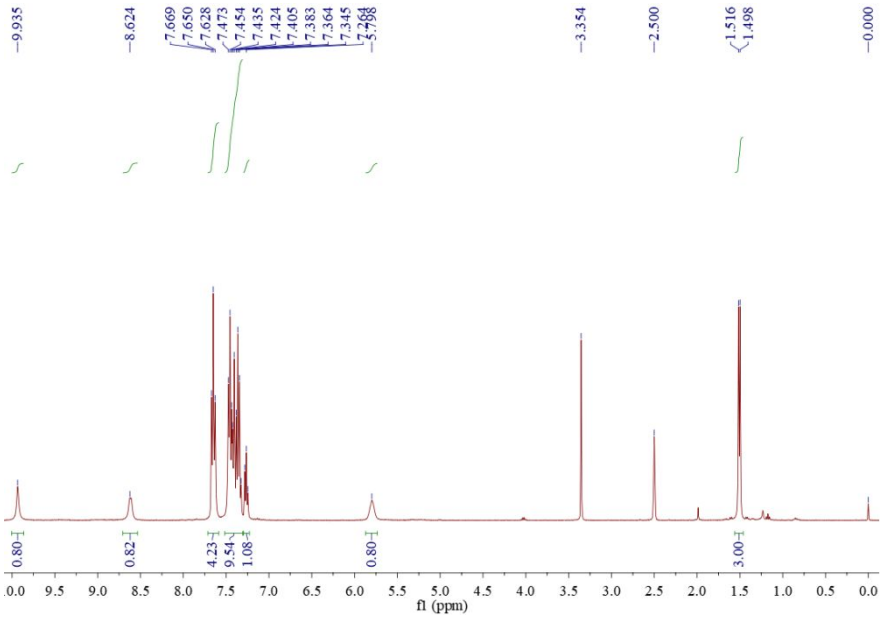
3ac ($CDCl_3$, 400 MHz for ^1H NMR and 125 MHz for ^{13}C NMR)

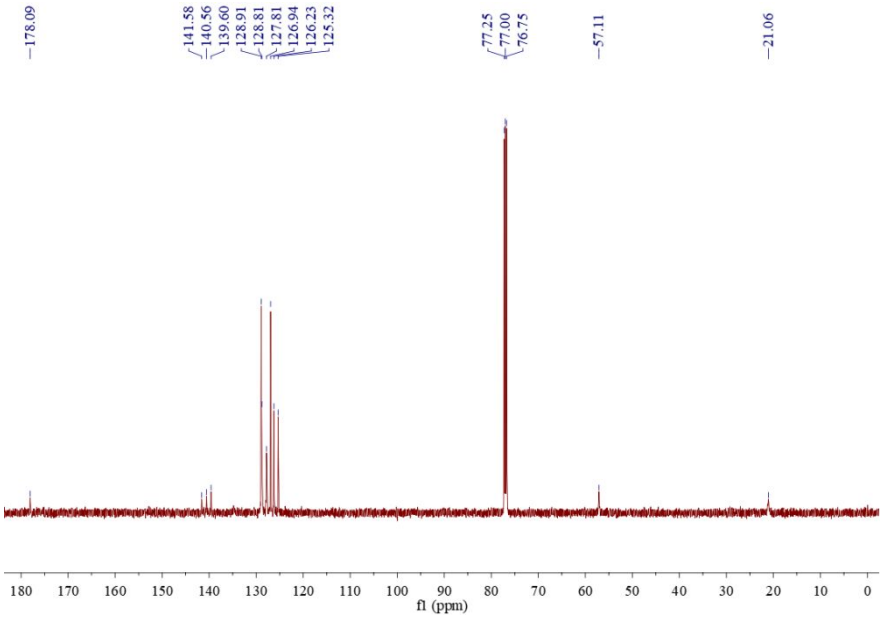


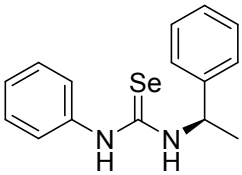




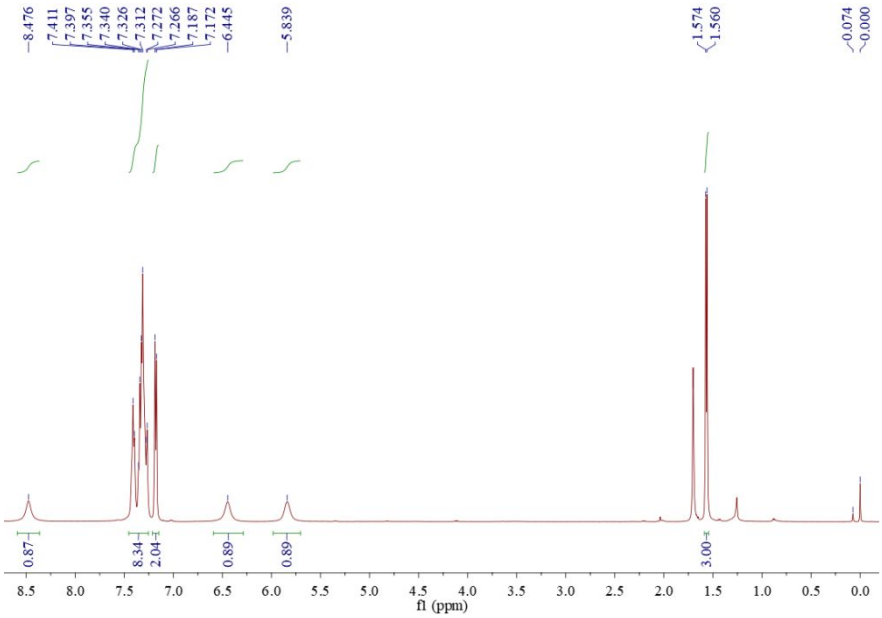
3ad (DMSO-d_6, 400 MHz for ^{1}H NMR and $CDCl_3$, 125 MHz for ^{13}C NMR)

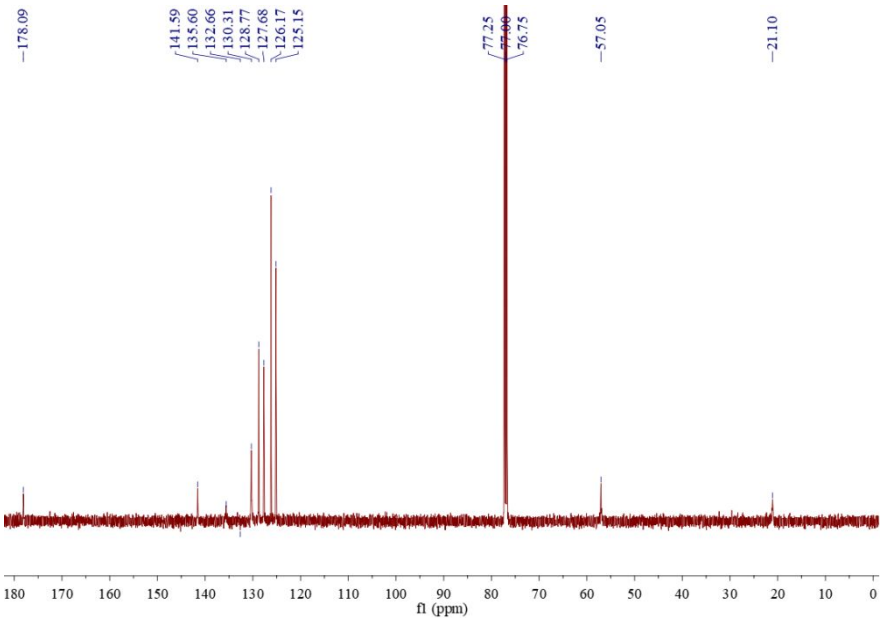


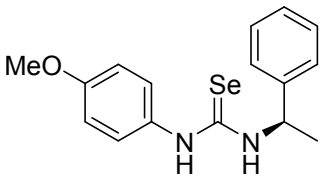




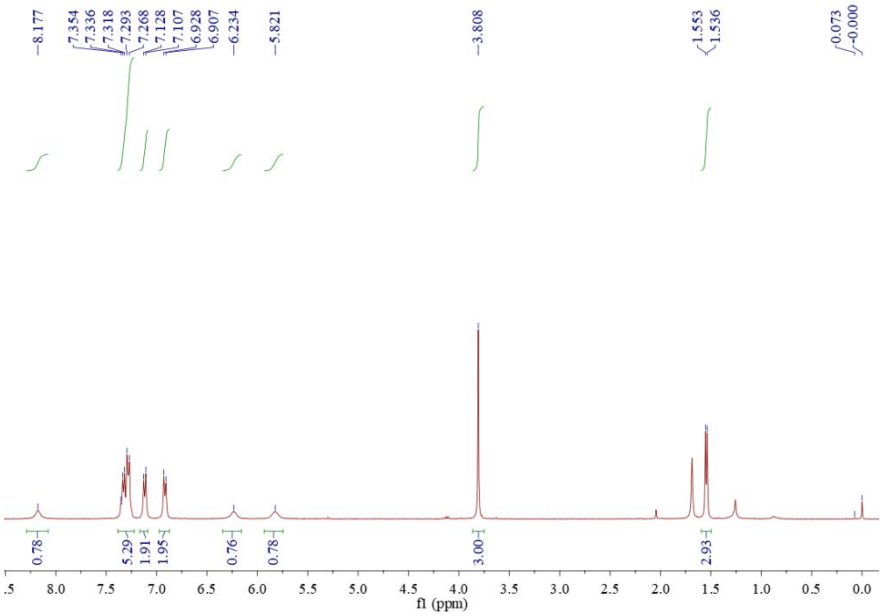
3ae ($CDCl_3$, 500 MHz for ^1H NMR and 125 MHz for ^{13}C NMR)

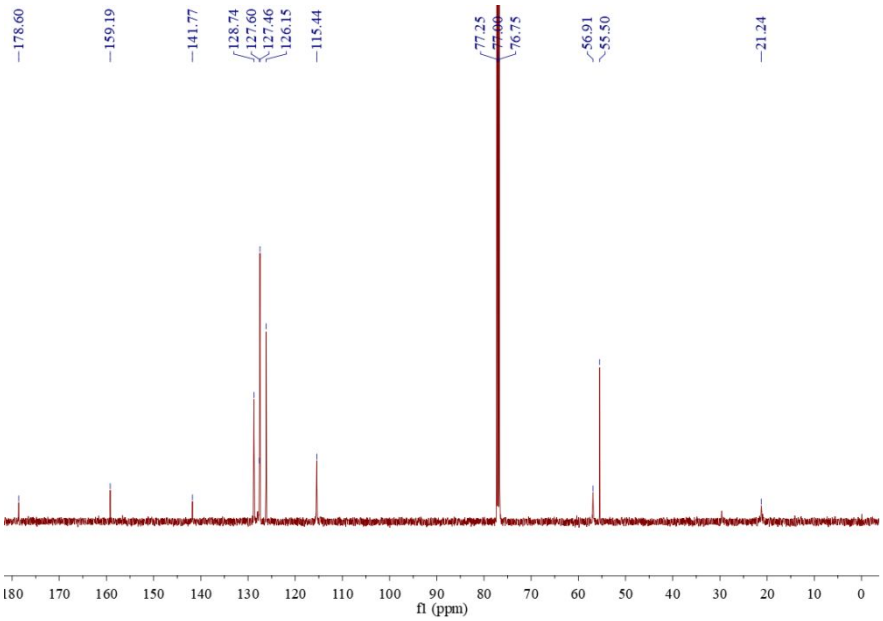


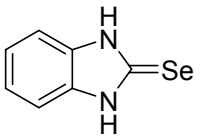




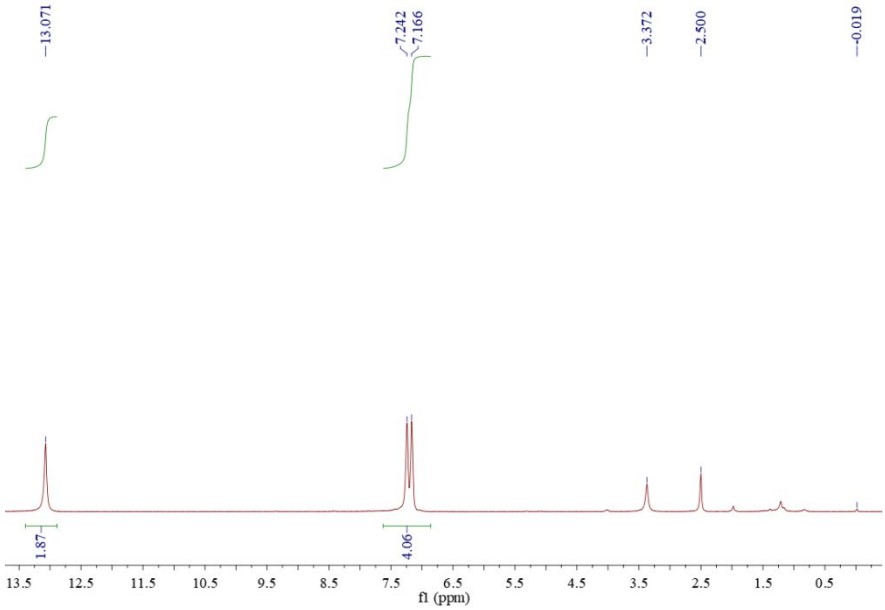
3af ($CDCl_3$, 400 MHz for ^1H NMR and 125 MHz for ^{13}C NMR)

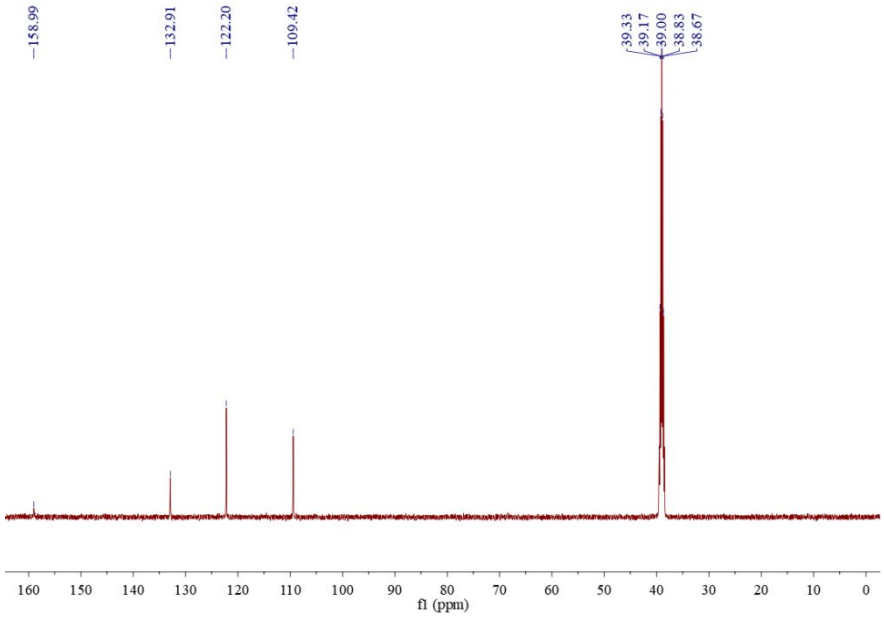


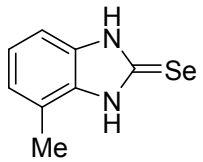




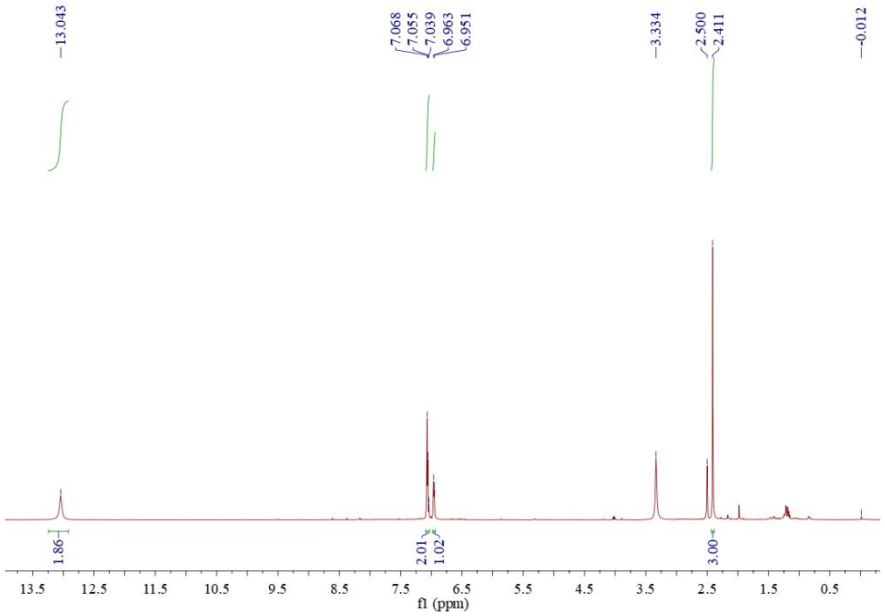
3ag (DMSO-d_6, 400 MHz for ^{1}H NMR and 125 MHz for ^{13}C NMR)

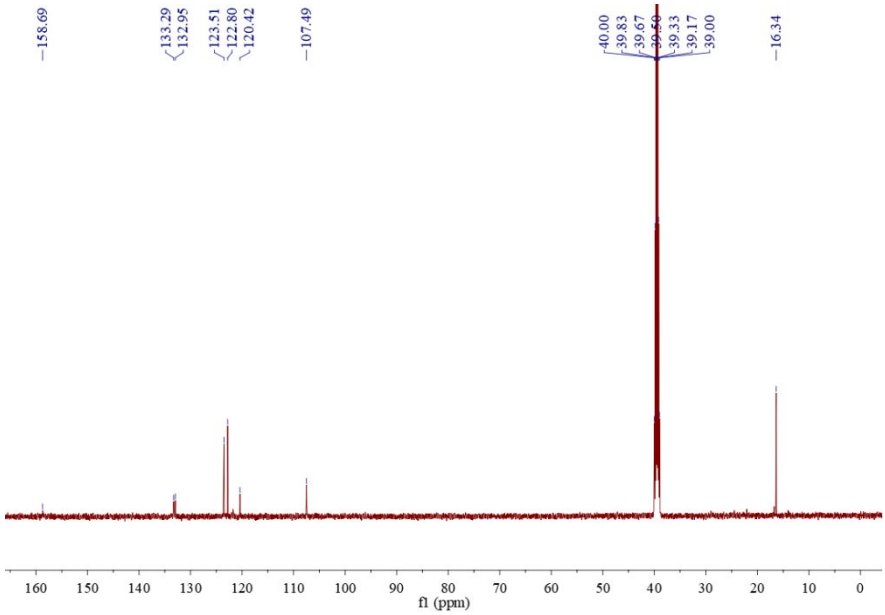


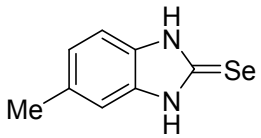




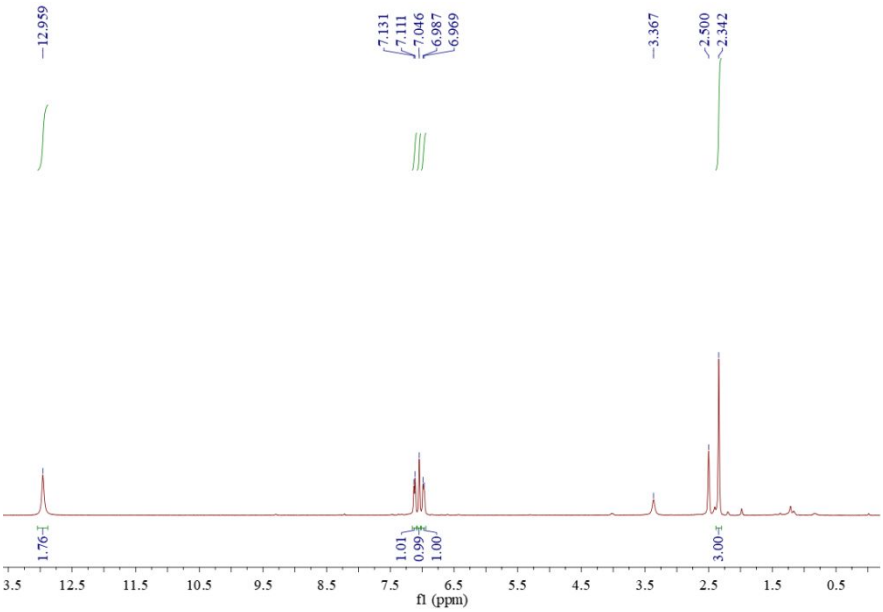
3ah (DMSO-d_6, 500 MHz for ^{1}H NMR and 125 MHz for ^{13}C NMR)

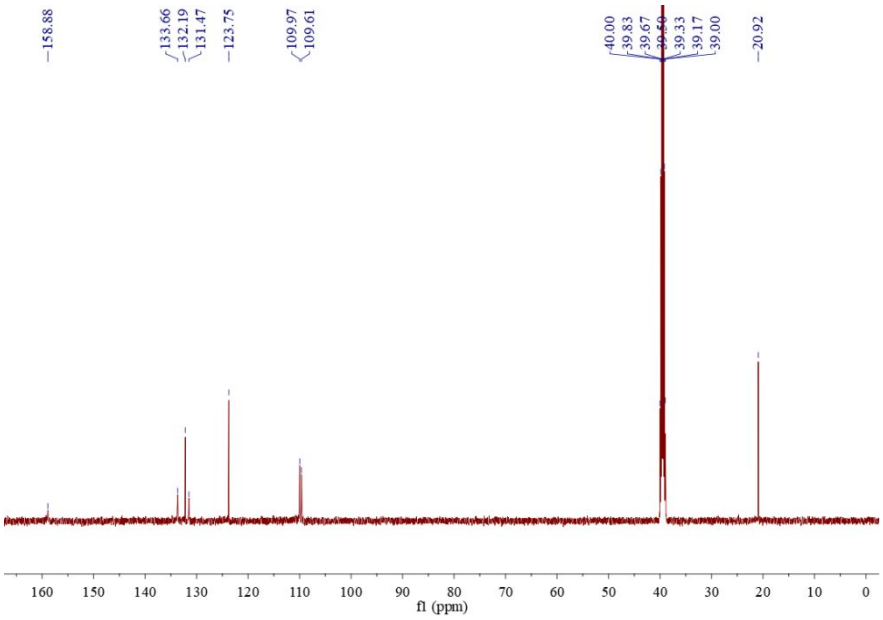


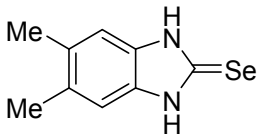




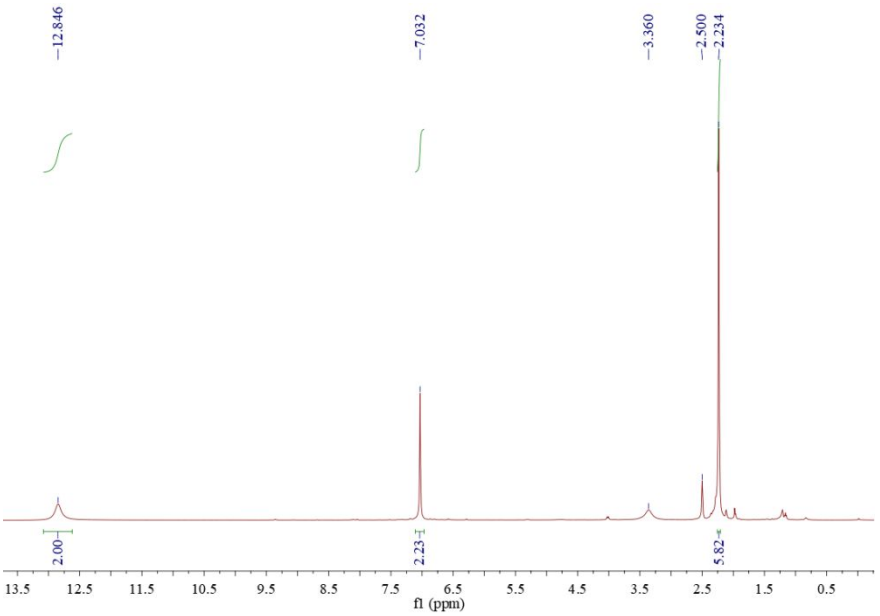
3ai (DMSO-d_6, 400 MHz for ^{1}H NMR and 125 MHz for ^{13}C NMR)

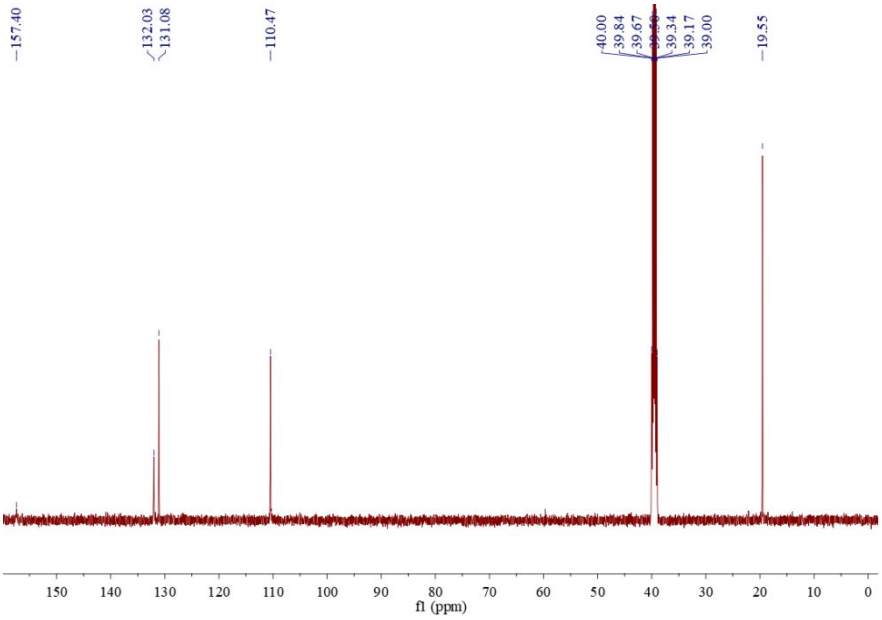


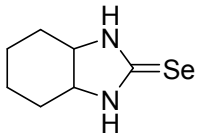




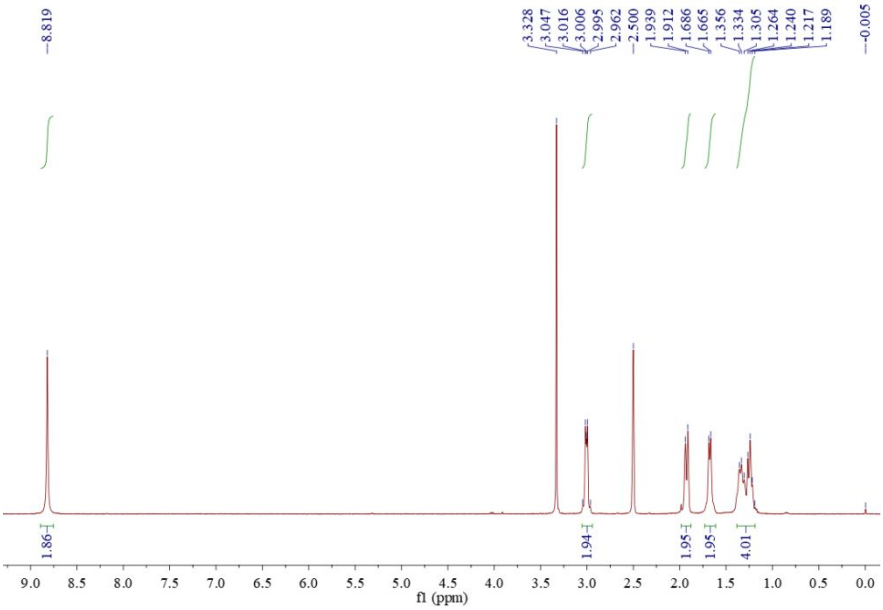
3aj (DMSO-d_6, 500 MHz for ^{1}H NMR and 125 MHz for ^{13}C NMR)

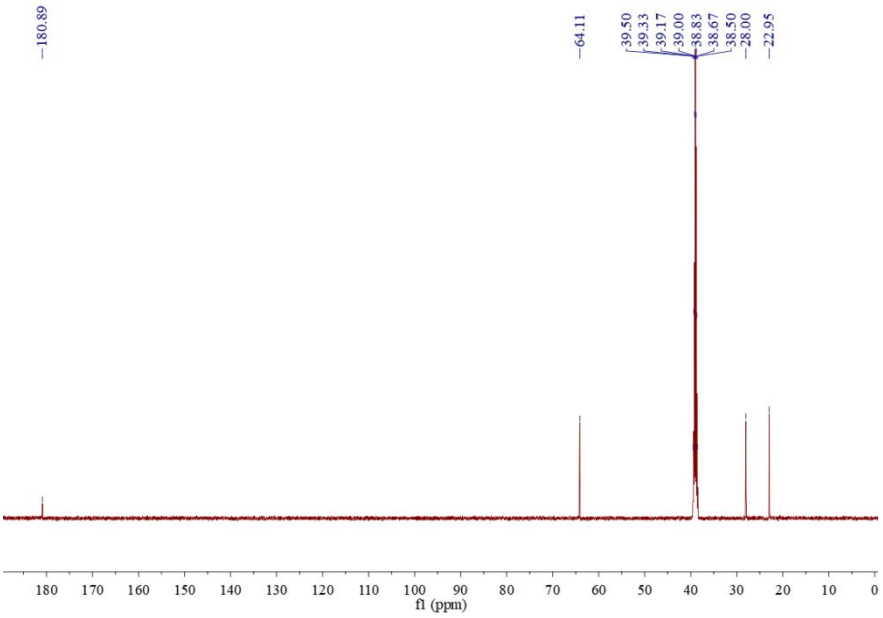


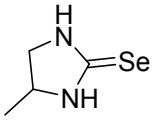




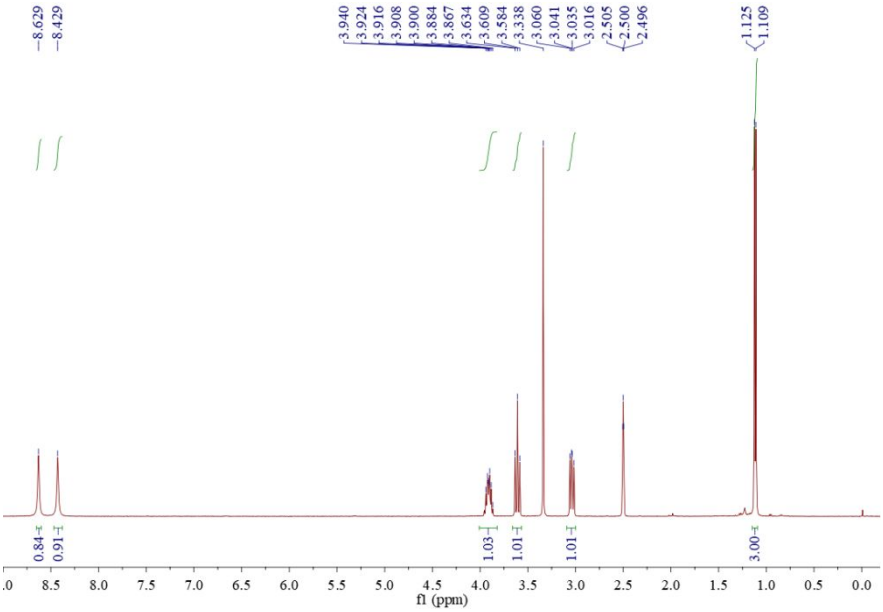
3ak (DMSO-d_6, 400 MHz for ^{1}H NMR and 125 MHz for ^{13}C NMR)

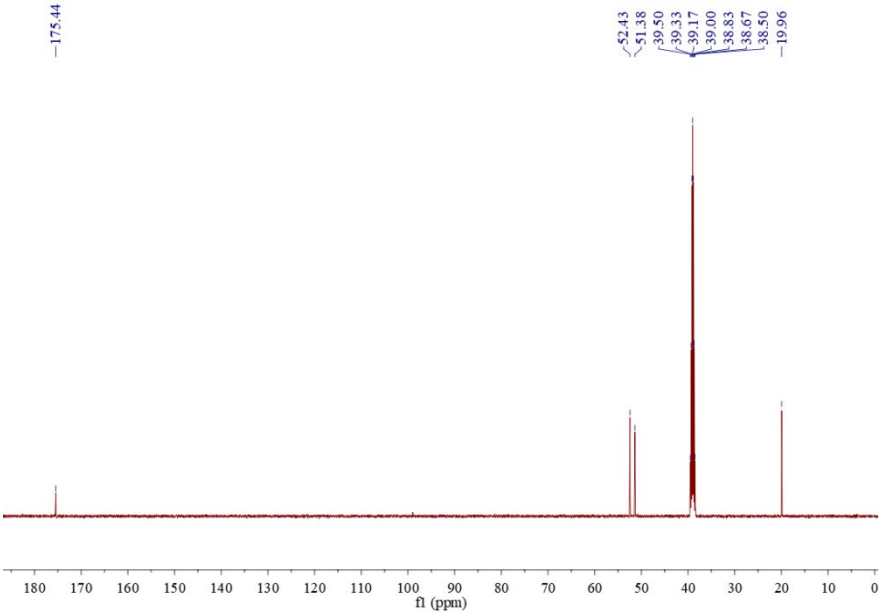


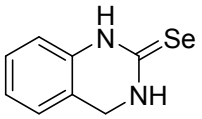




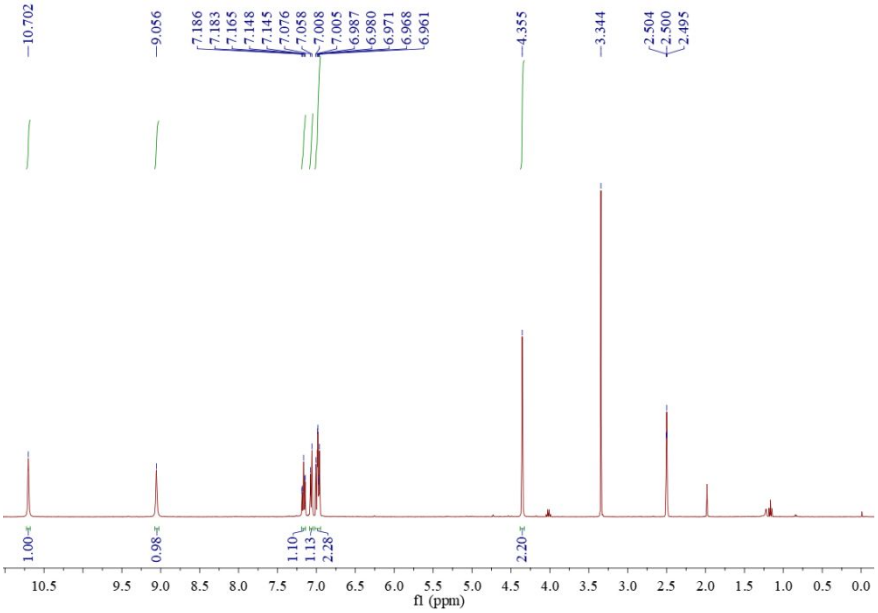
3al (DMSO-d_6, 400 MHz for ^{1}H NMR and 125 MHz for ^{13}C NMR)

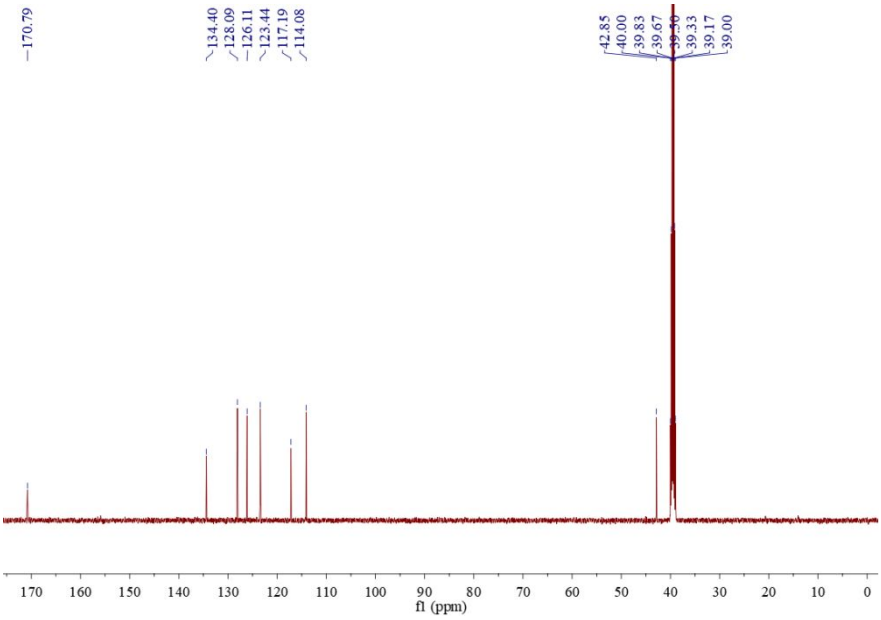


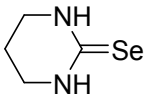




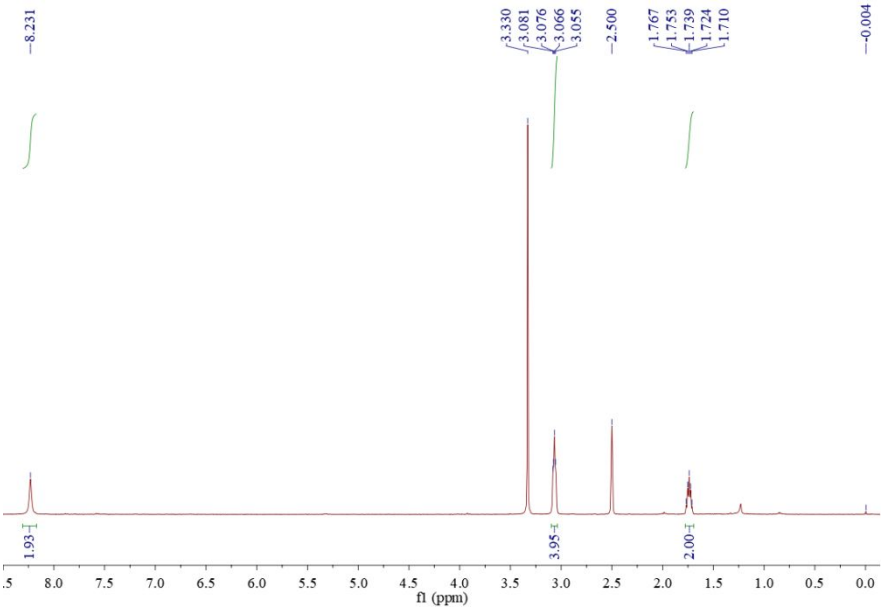
3am (DMSO-d_6, 400 MHz for ^{1}H NMR and 125 MHz for ^{13}C NMR)

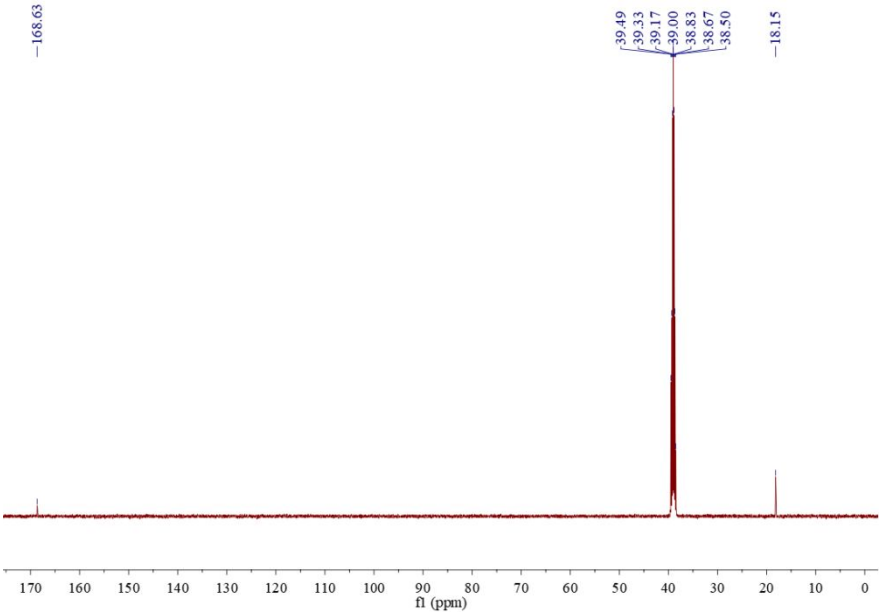


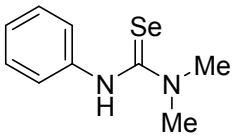




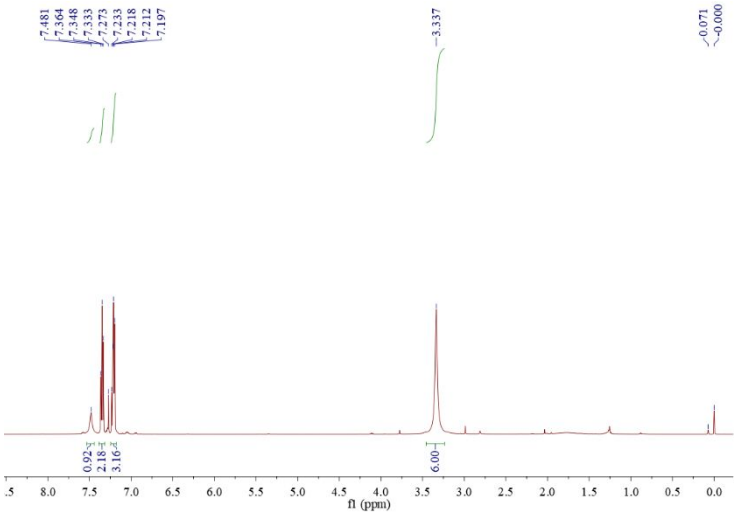
3an (DMSO-d_6, 400 MHz for ^{1}H NMR and 125 MHz for ^{13}C NMR)

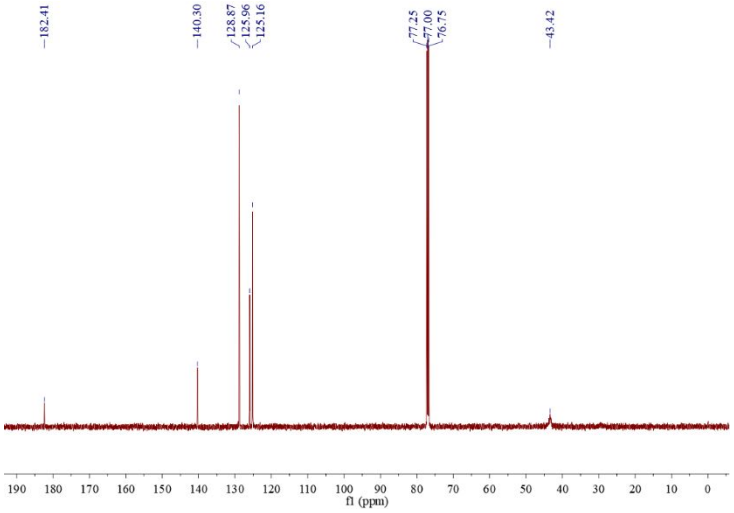


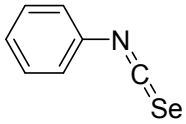




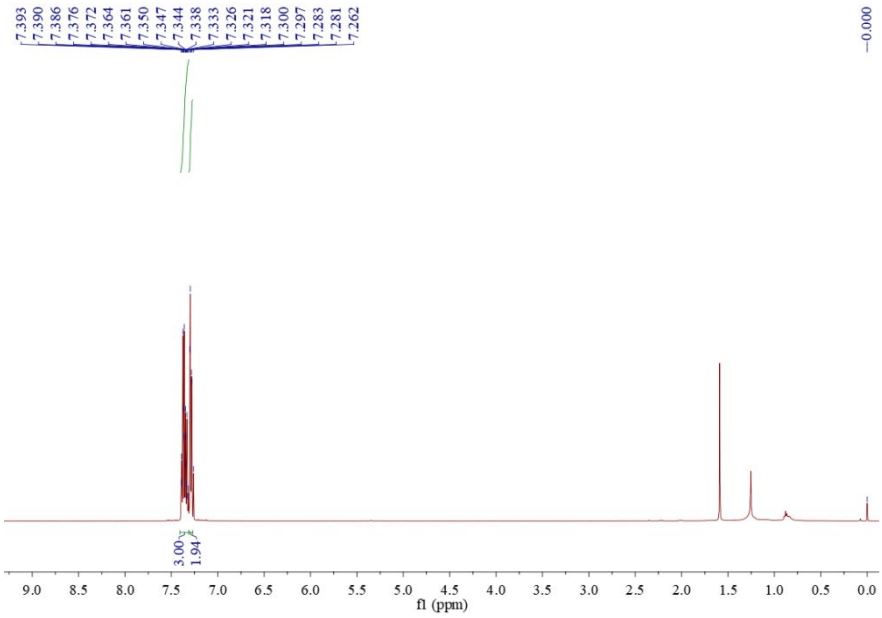
II ($CDCl_3$, 500 MHz for ^1H NMR and 125 MHz for ^{13}C NMR)

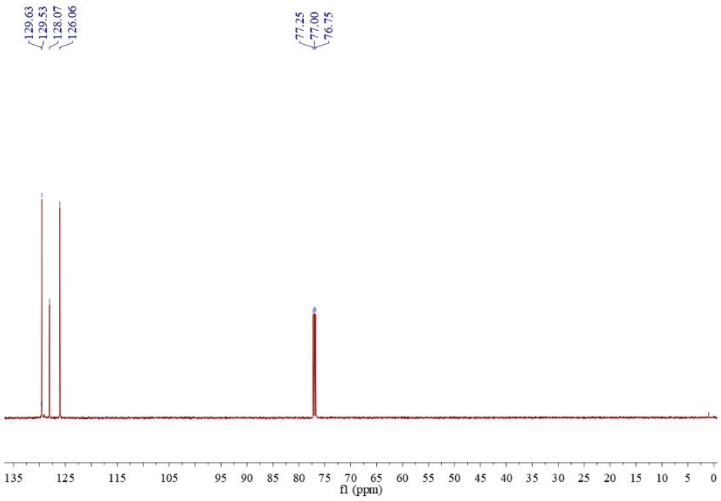


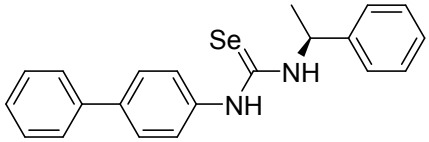




4 ($CDCl_3$, 500 MHz for ^1H NMR and 125 MHz for ^{13}C NMR)







3ad

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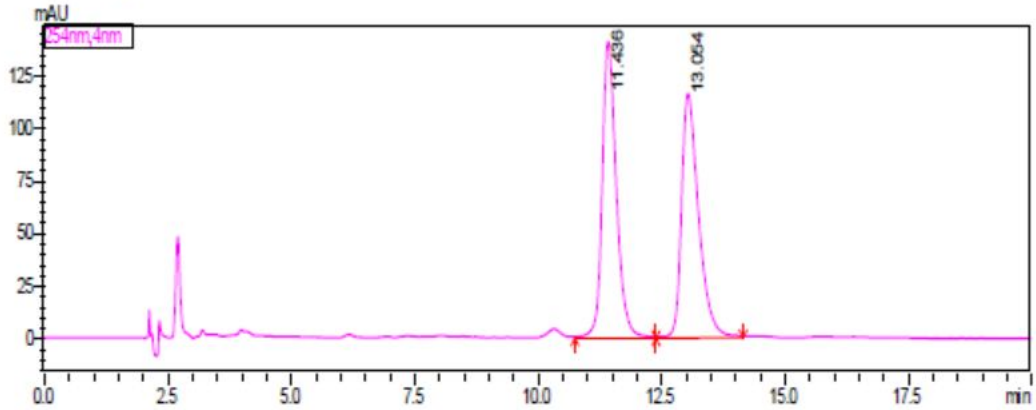

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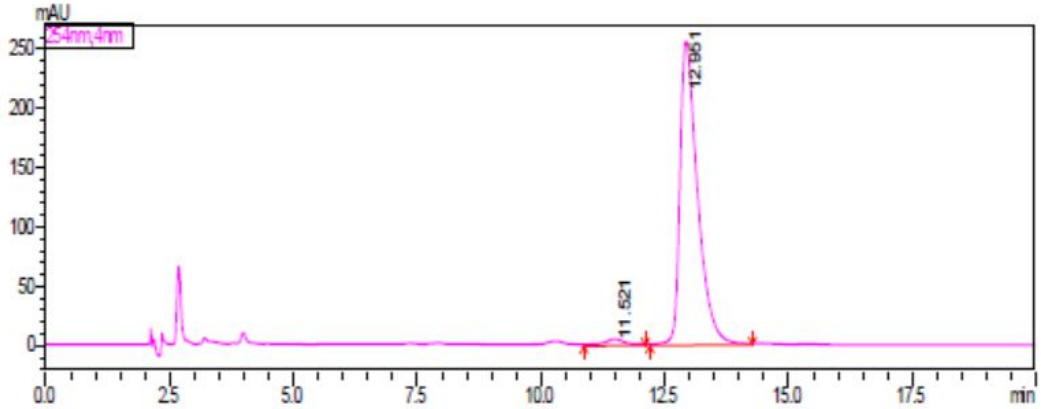

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