Access to Fused Pyrroles from Cyclic 1,3-Dienyl Boronic Esters and Arylnitroso Compounds

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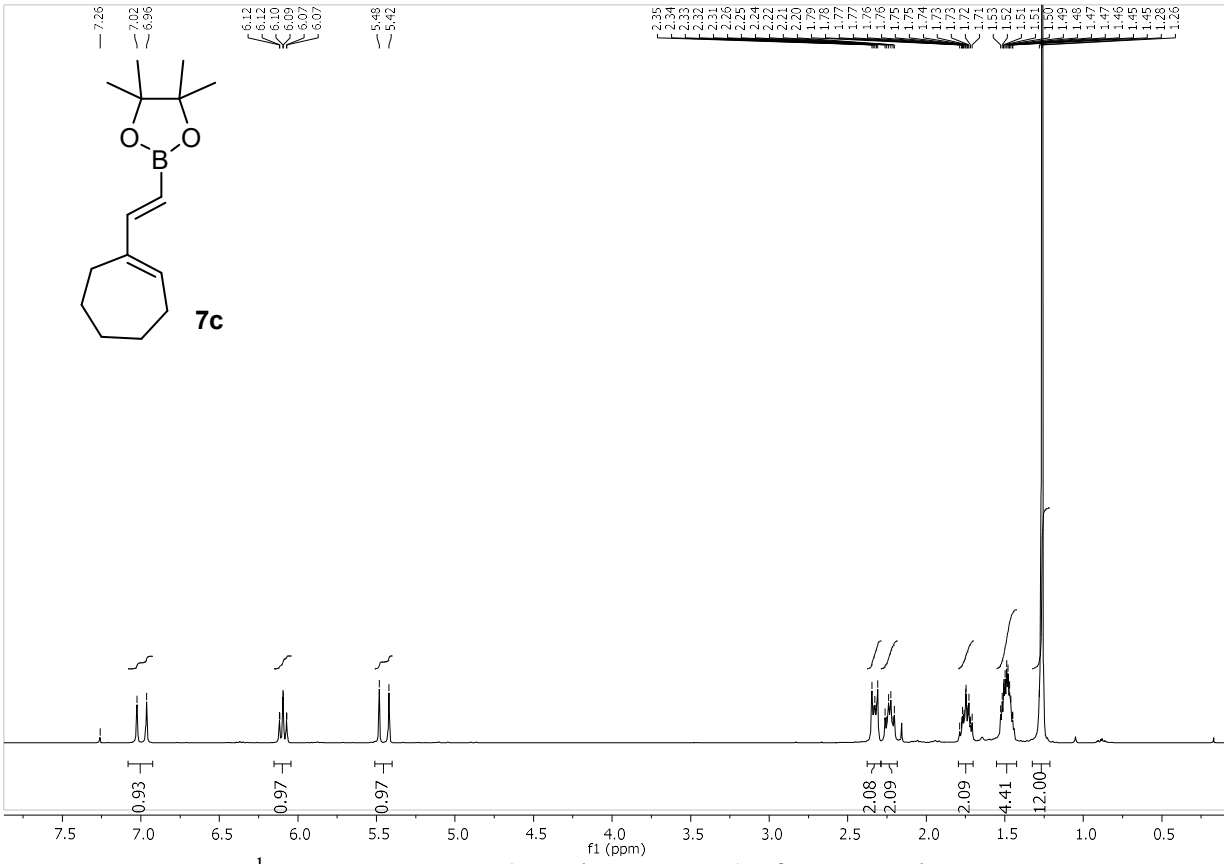
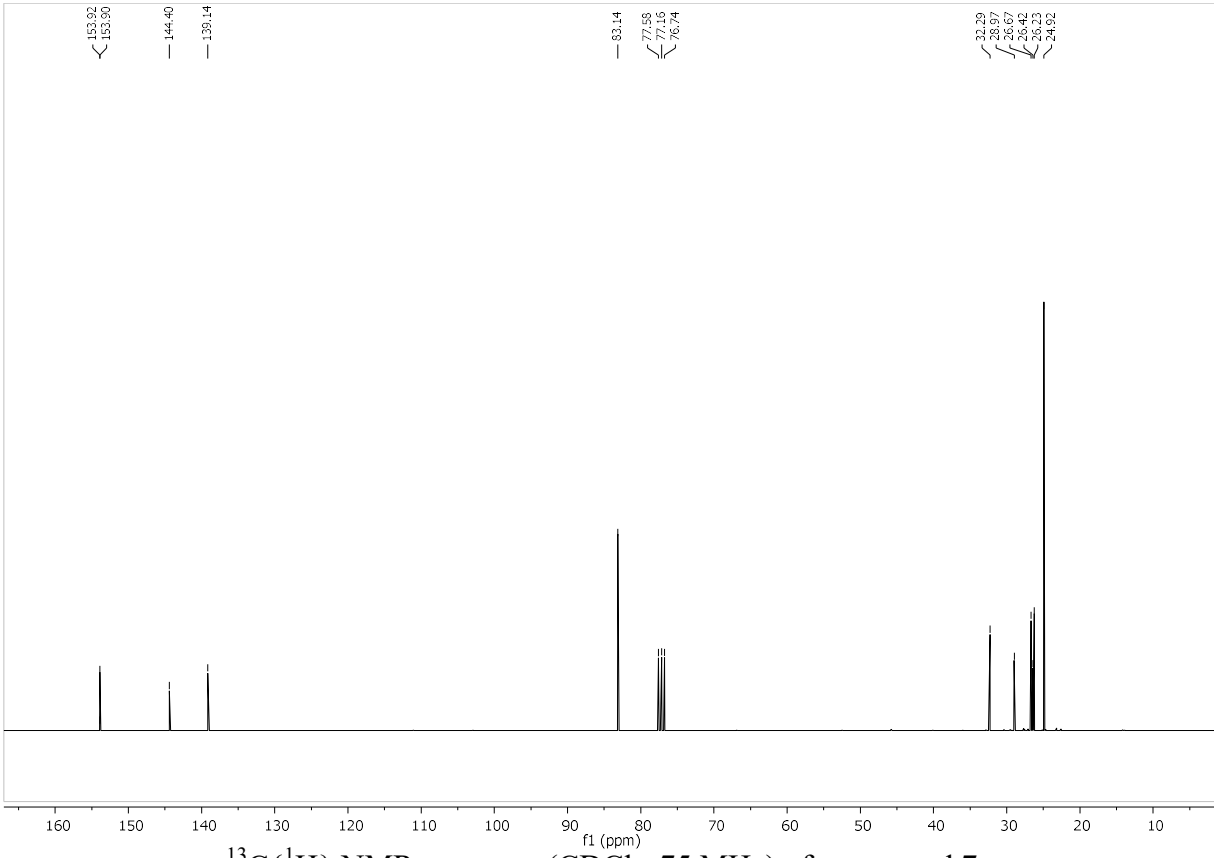
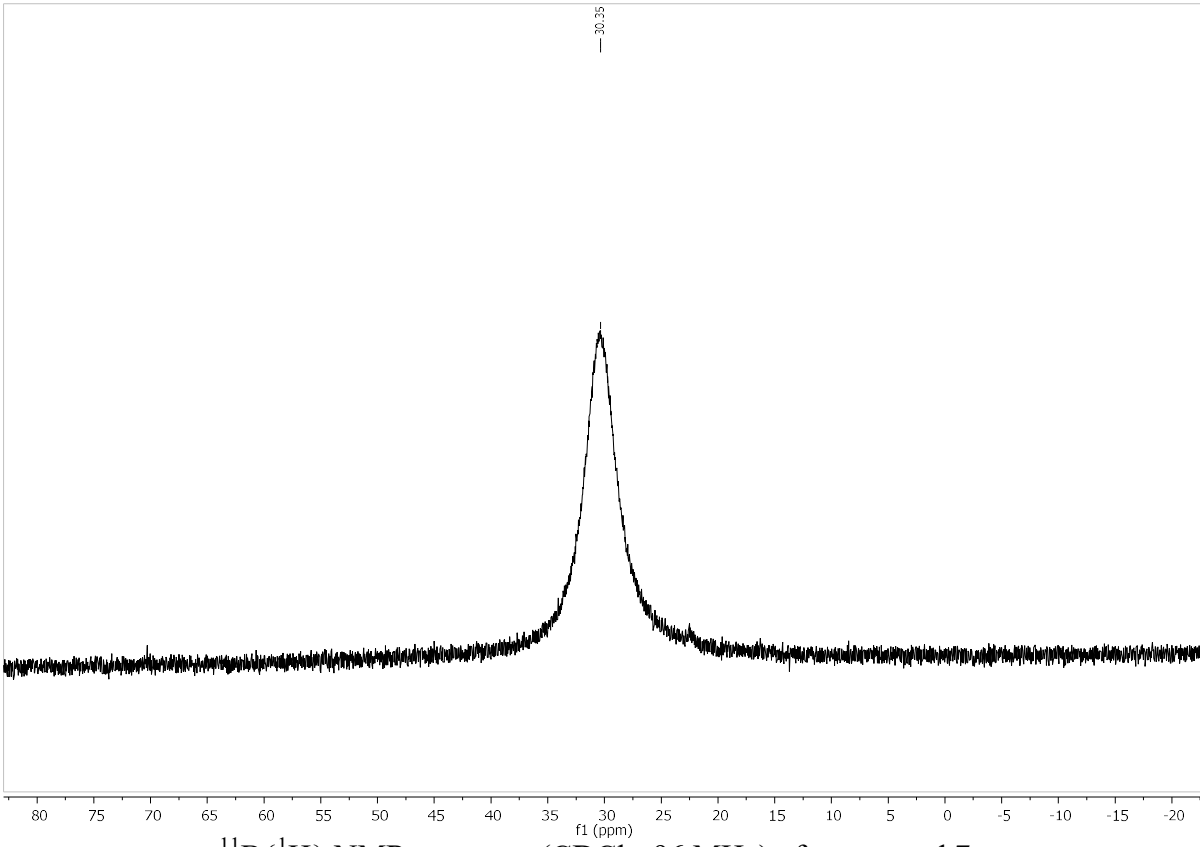


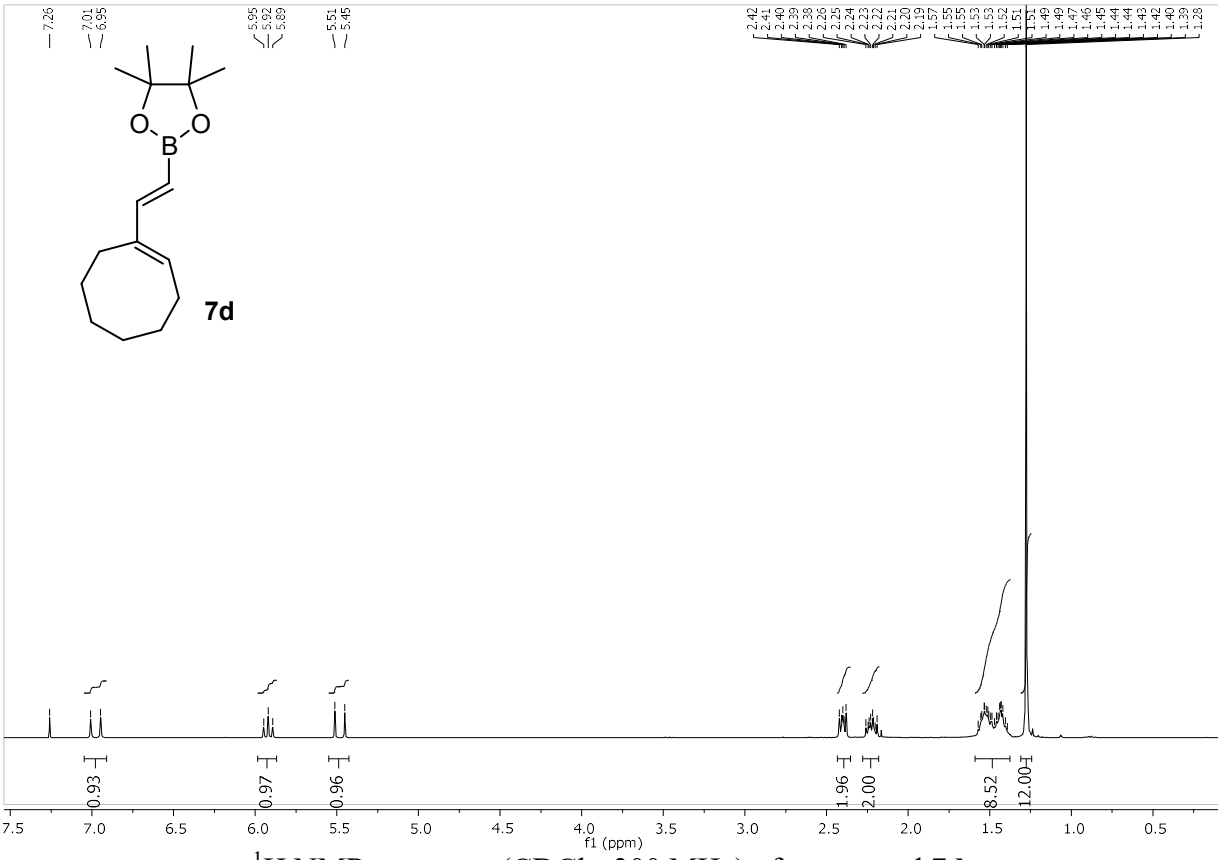
^{1}H NMR spectrum ($CDCl_3$, 300 MHz) of compound **7c**



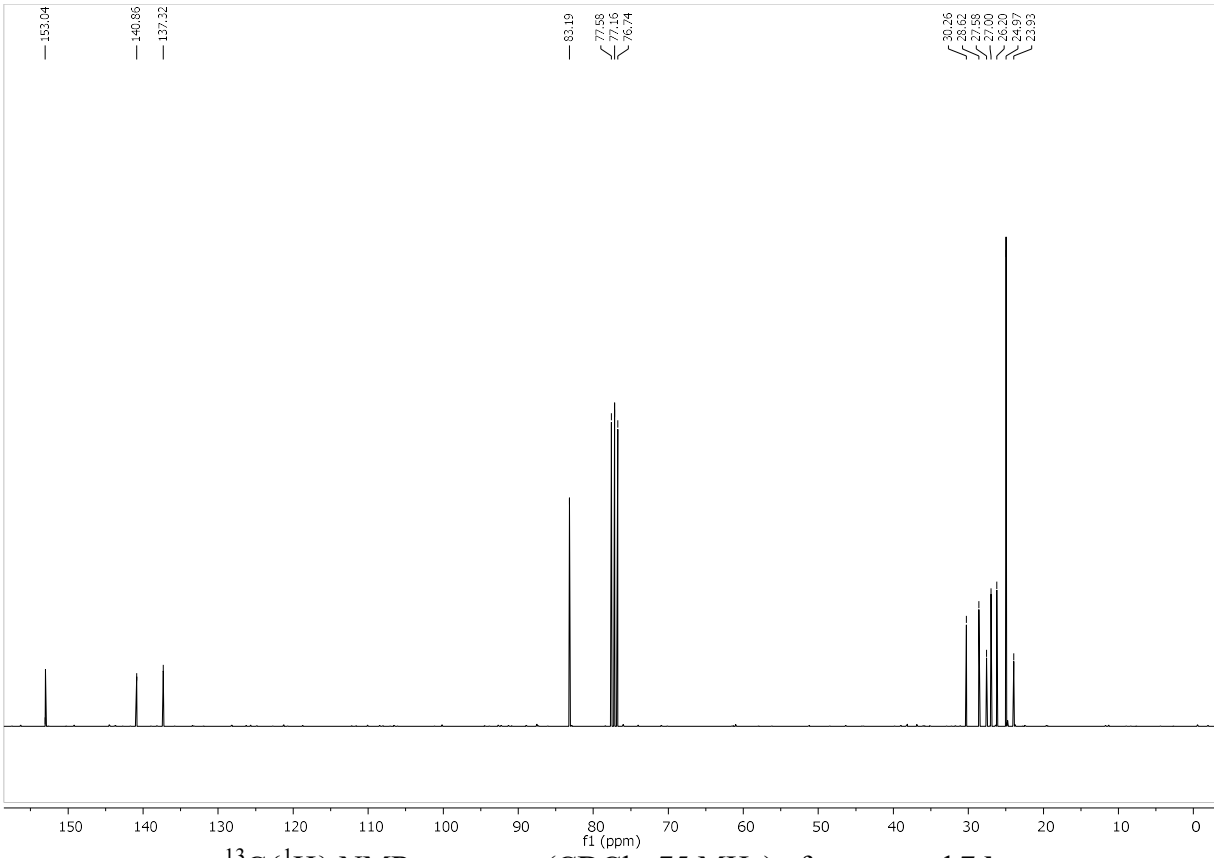
^{13}C{^{1}H} NMR spectrum ($CDCl_3$, 75 MHz) of compound **7c**



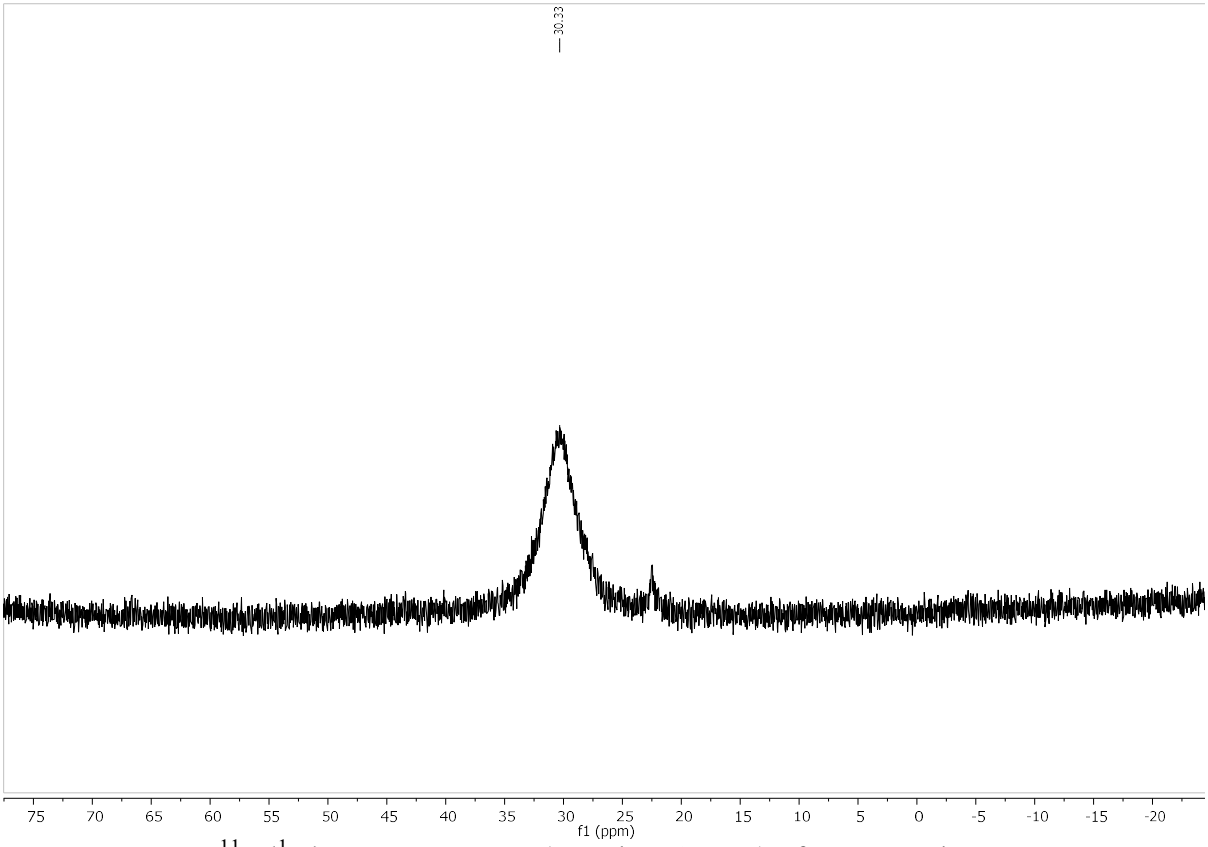
$^{11}B\{^{1}H\}$ NMR spectrum ($CDCl_3$, 96 MHz) of compound **7c**



^{1}H NMR spectrum ($CDCl_3$, 300 MHz) of compound **7d**



^{13}C{^{1}H} NMR spectrum ($CDCl_3$, 75 MHz) of compound **7d**



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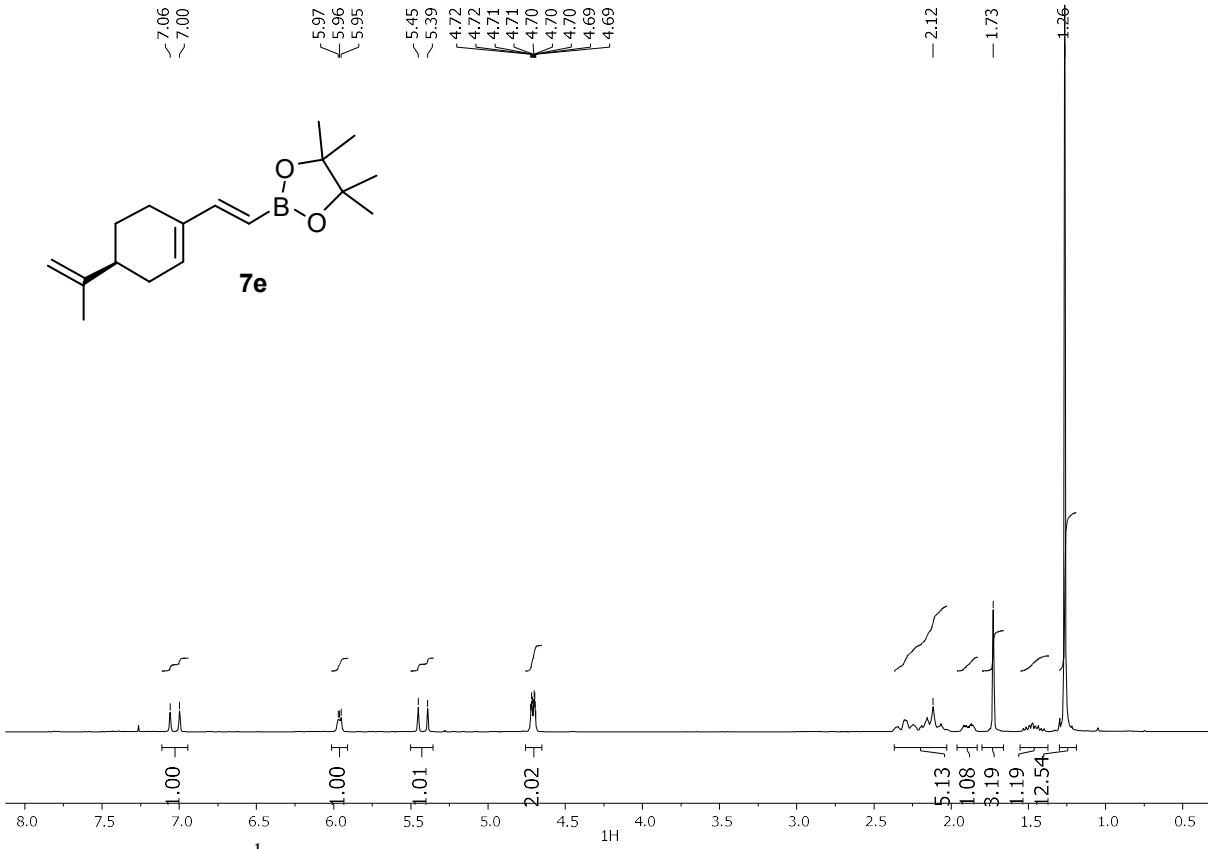

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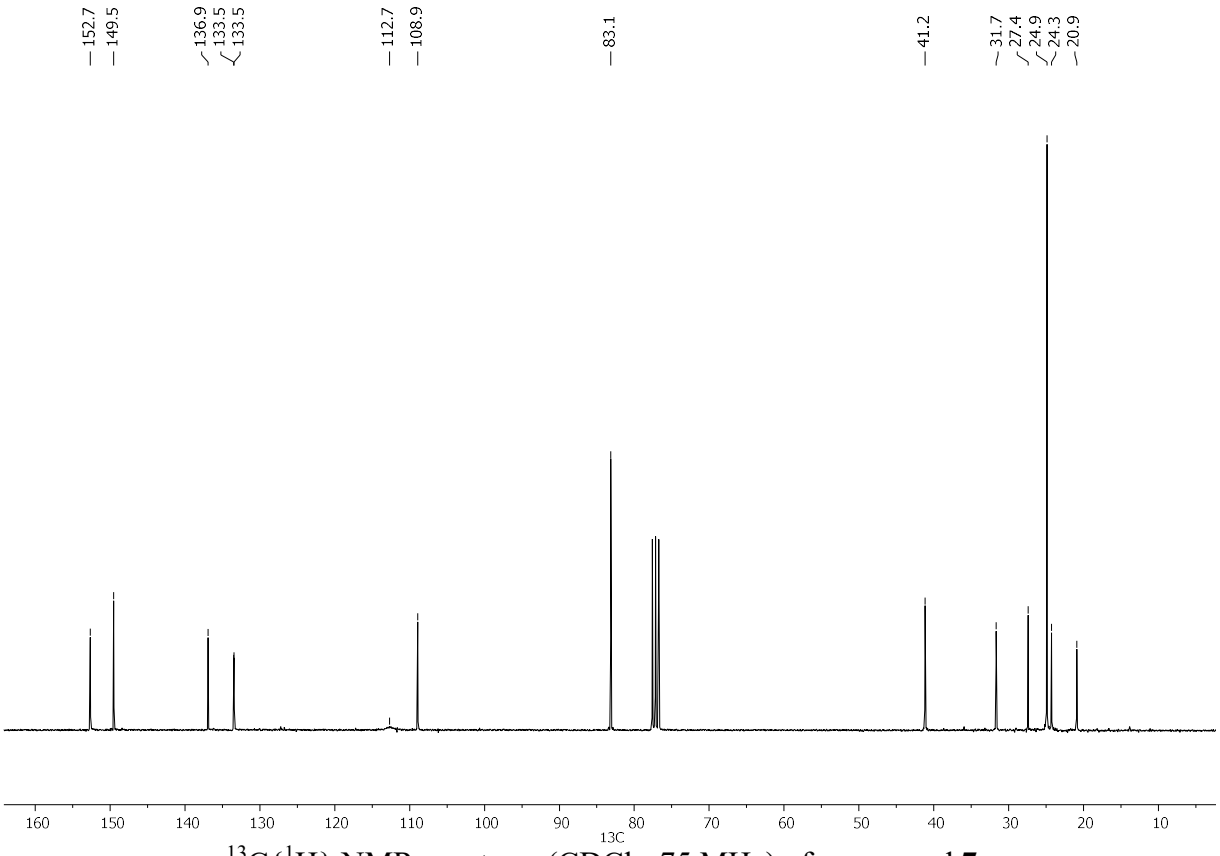
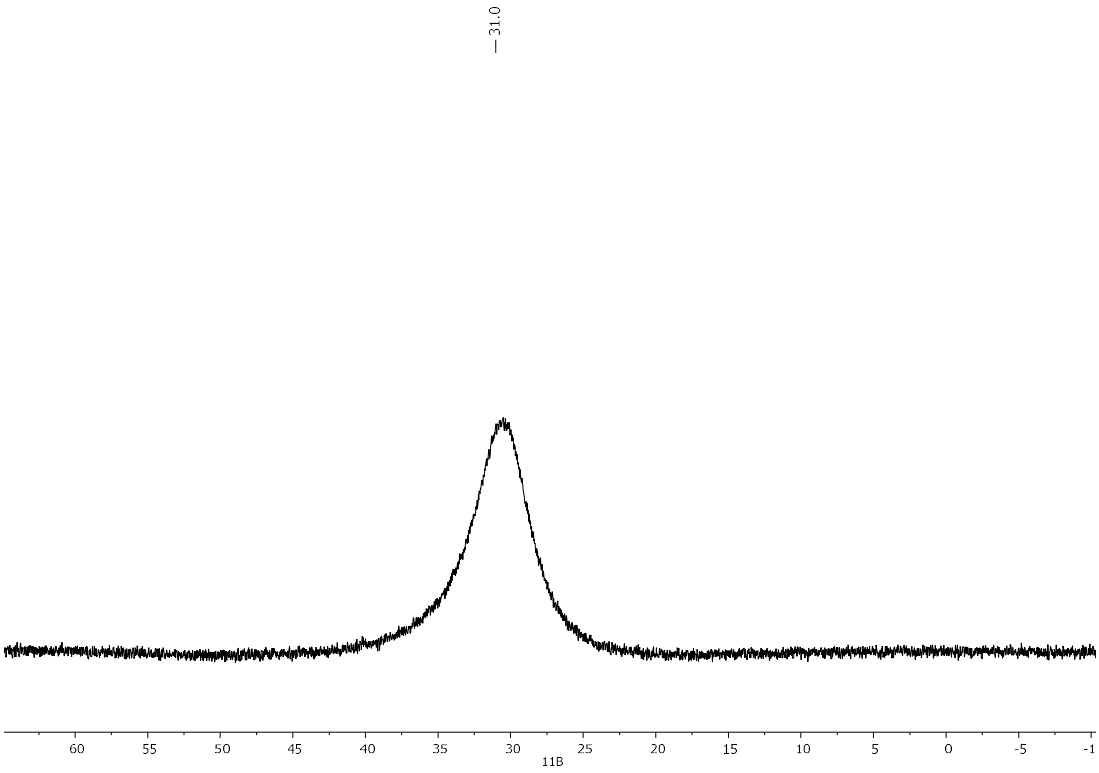


^{13}C{^{1}H} NMR spectrum ($CDCl_3$, 75 MHz) of compound **7e**



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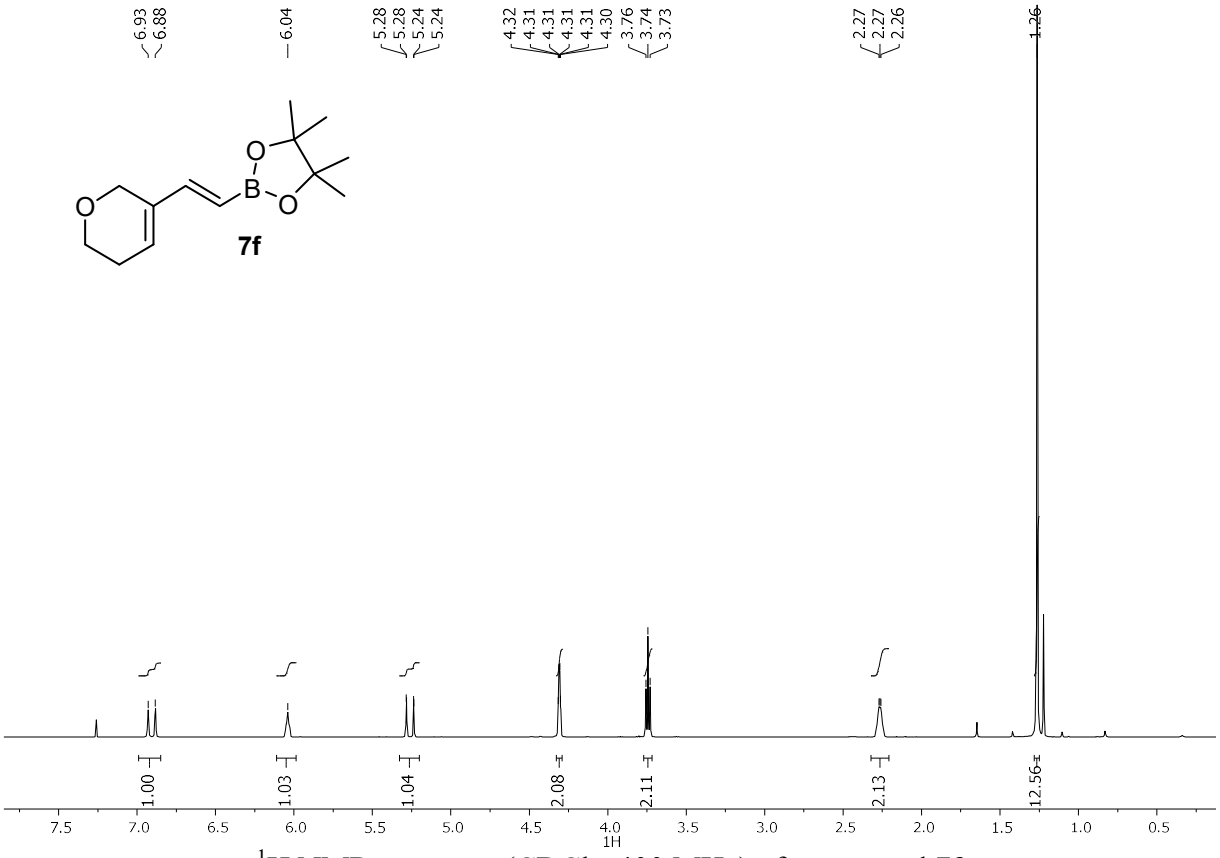

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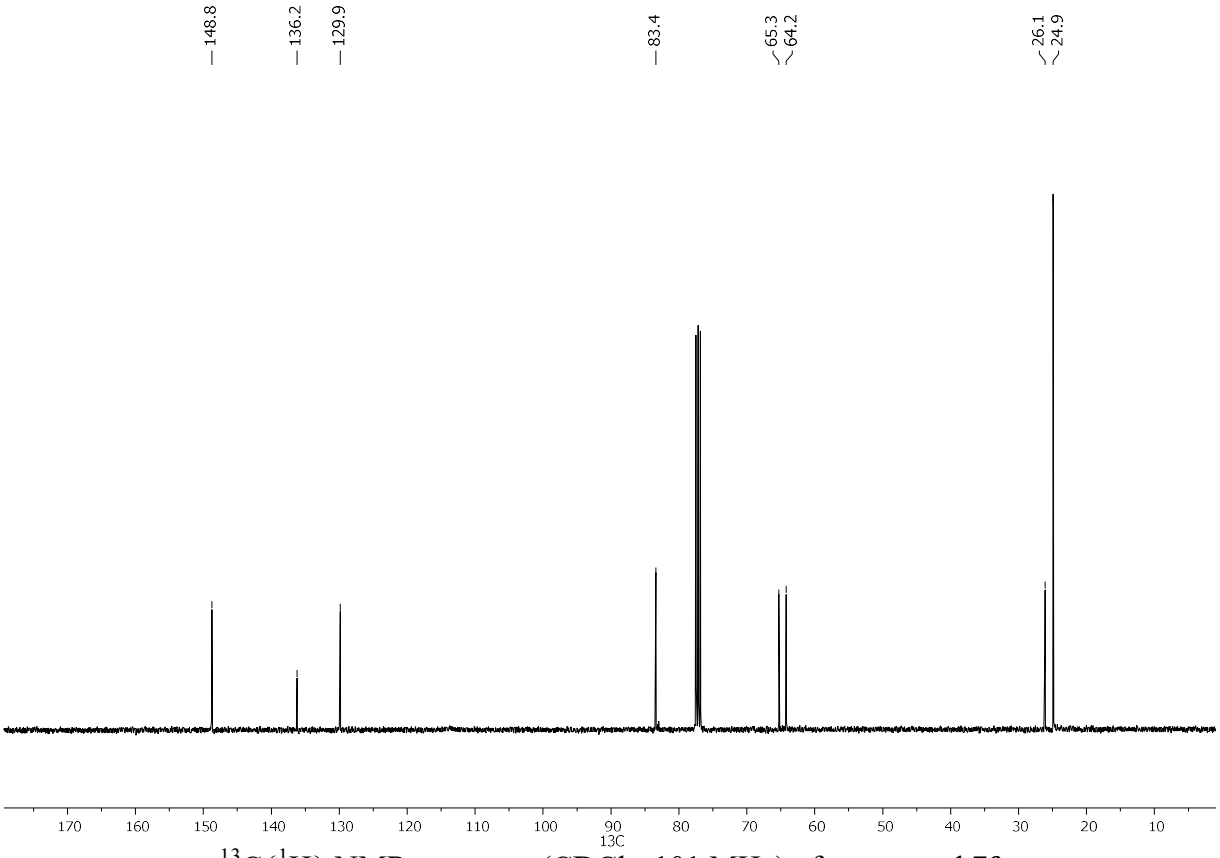

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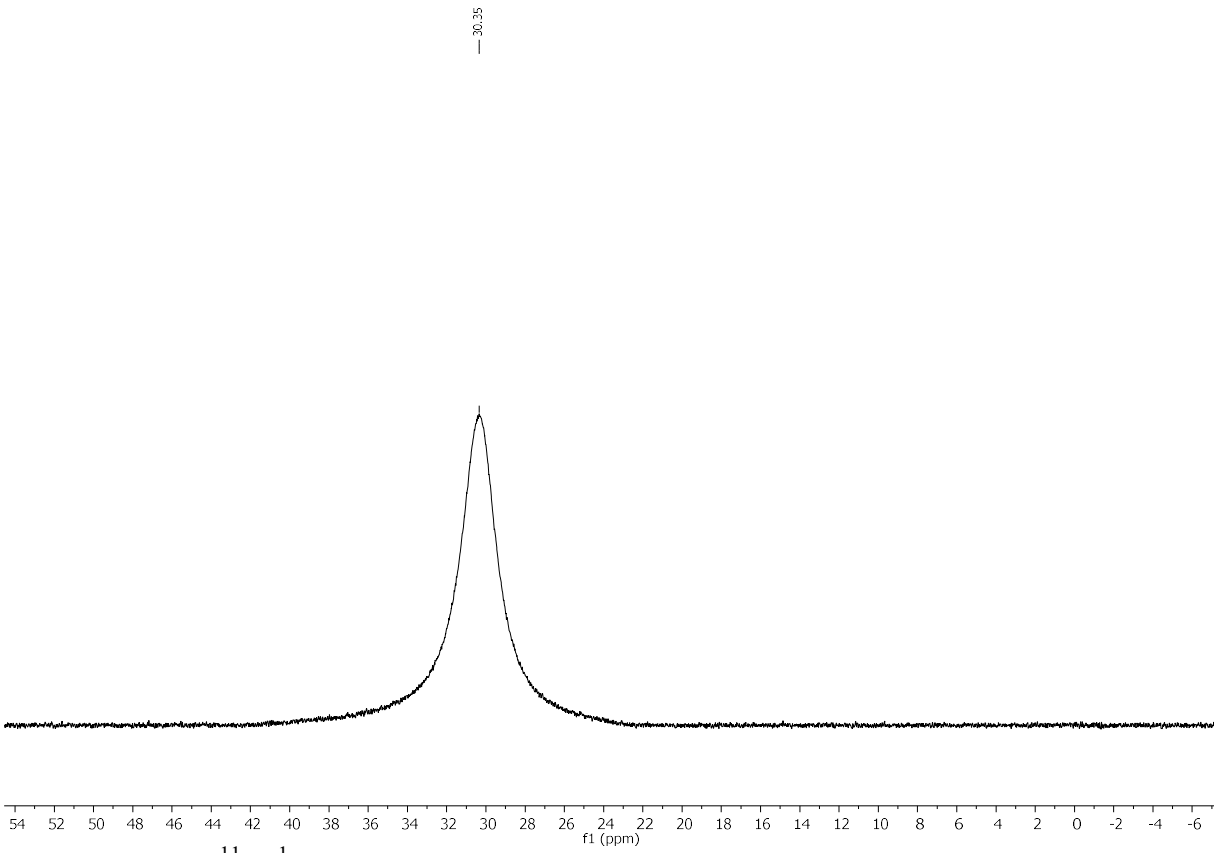
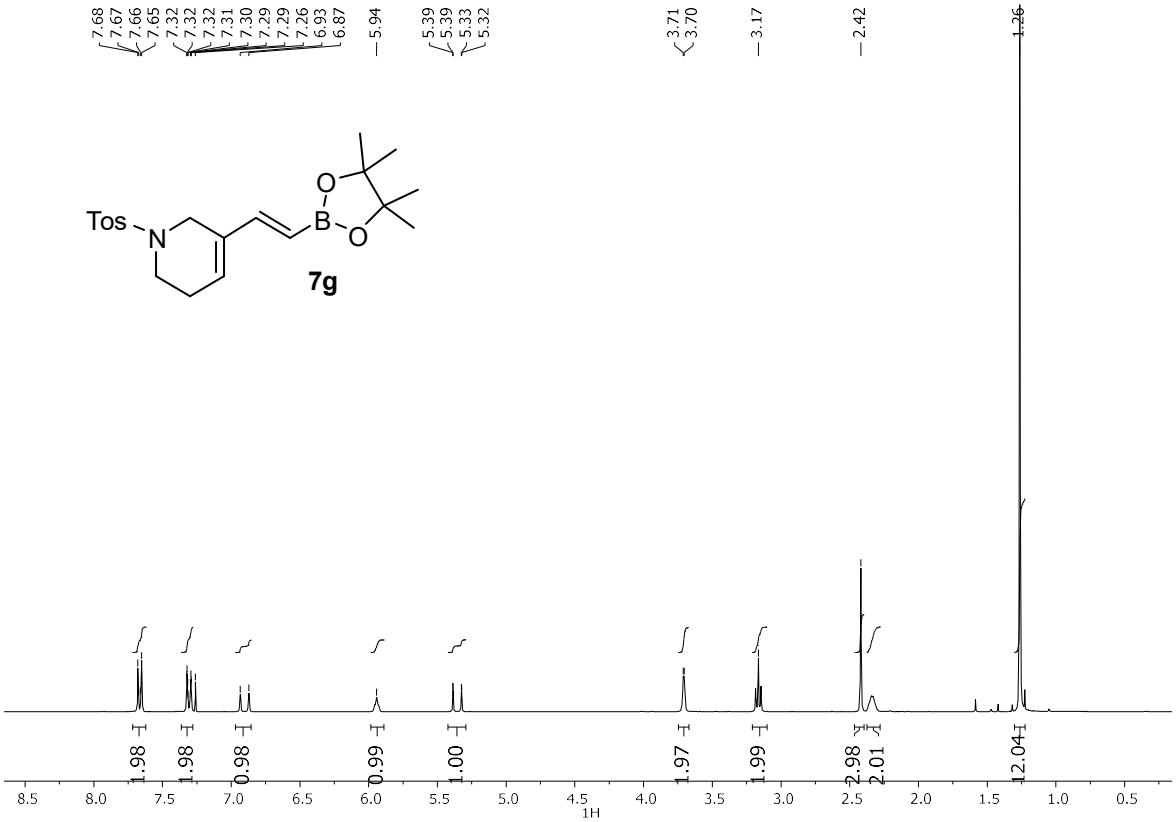
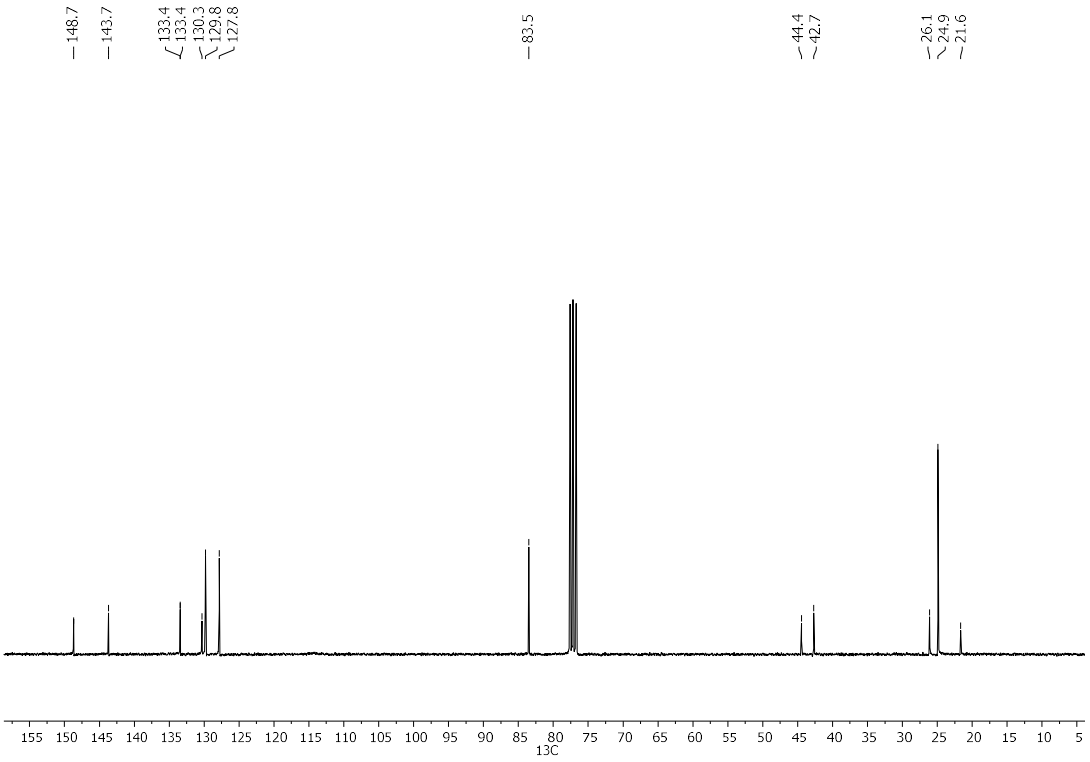


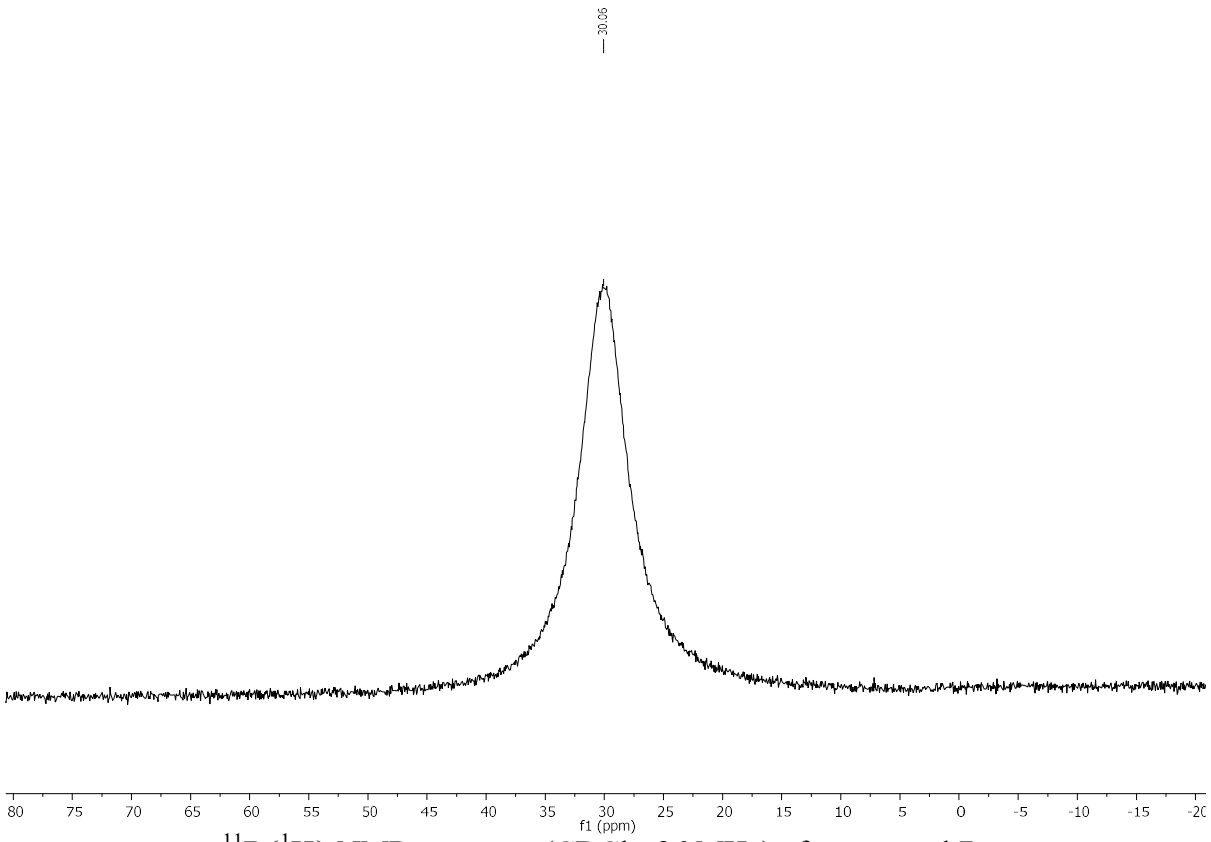
$^{11}B\{^{1}H\}$ NMR spectrum ($CDCl_3$, 128 MHz) of compound **7f**



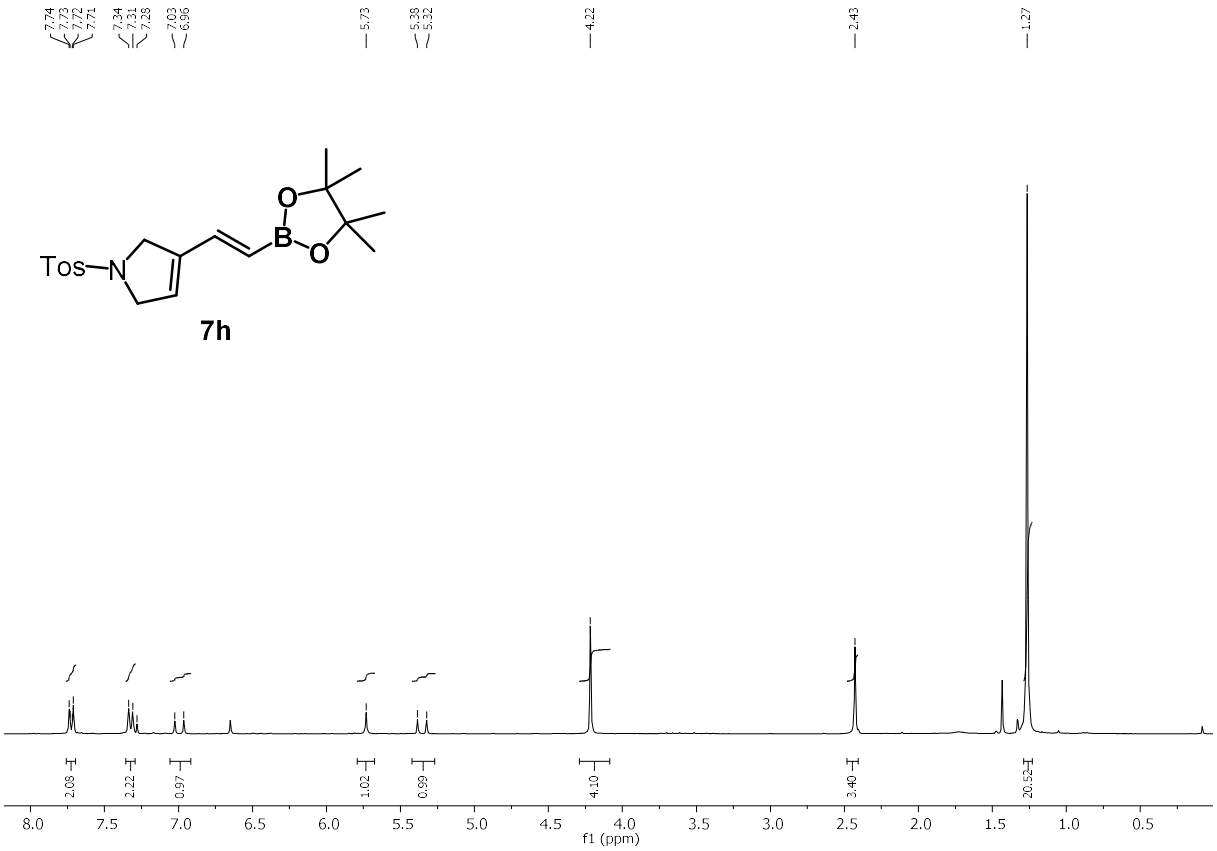
^{1}H NMR spectrum ($CDCl_3$, 300 MHz) of compound **7g**



^{13}C{^{1}H} NMR spectrum ($CDCl_3$, 75 MHz) of compound **7g**



$^{11}B\{^{1}H\}$ NMR spectrum ($CDCl_3$, 96 MHz) of compound **7g**



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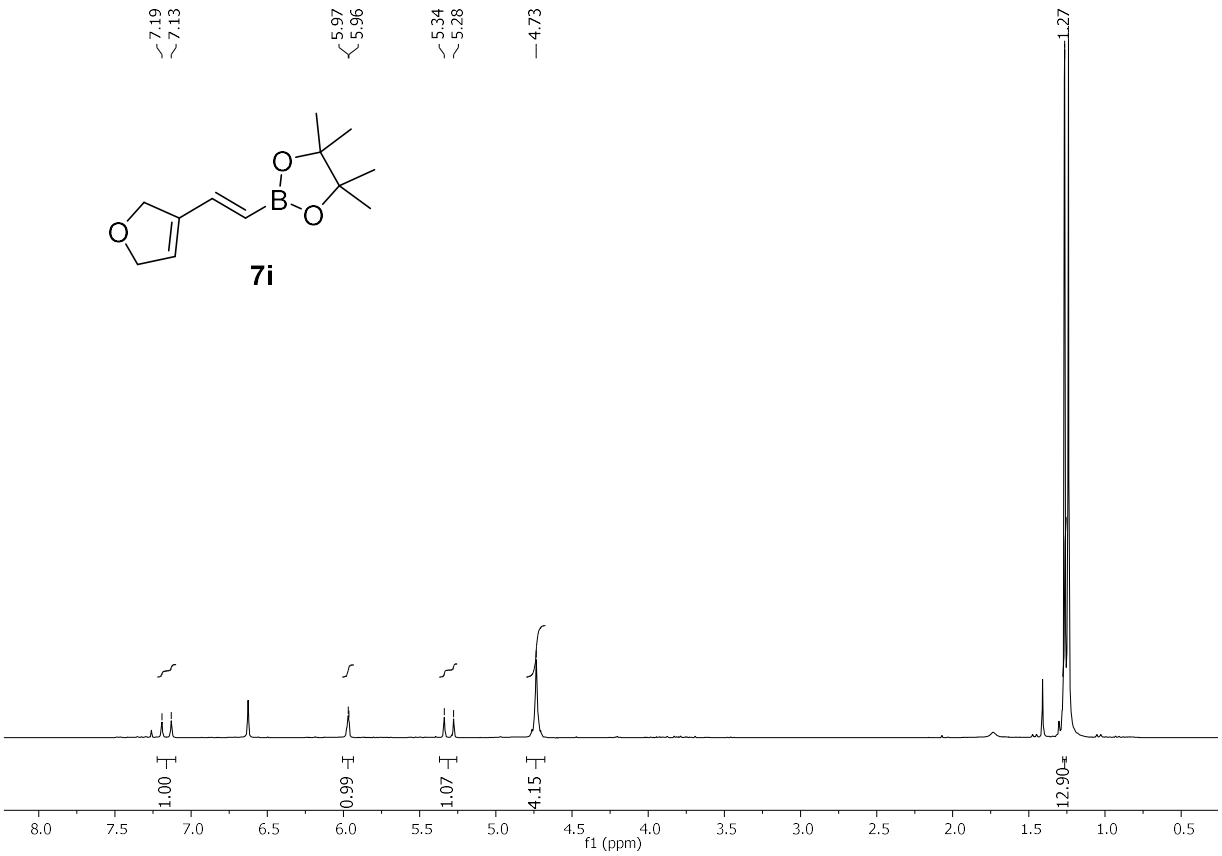

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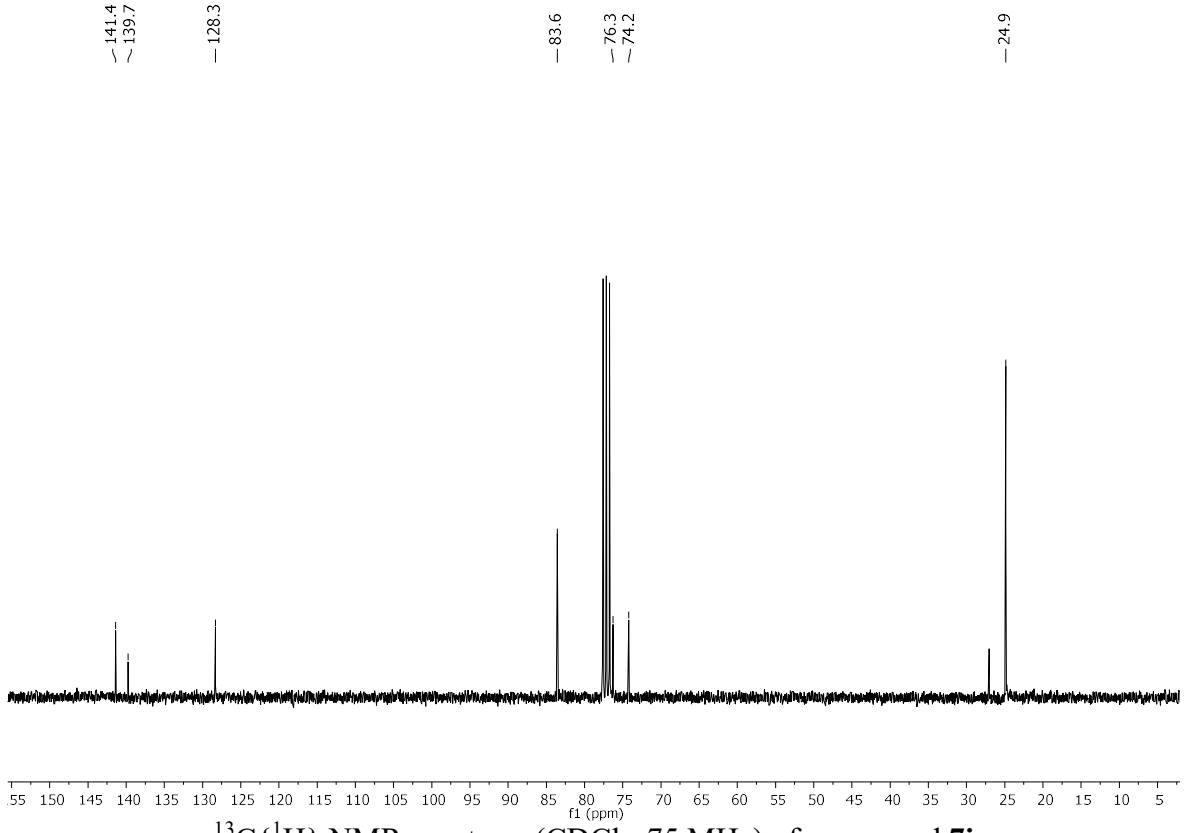
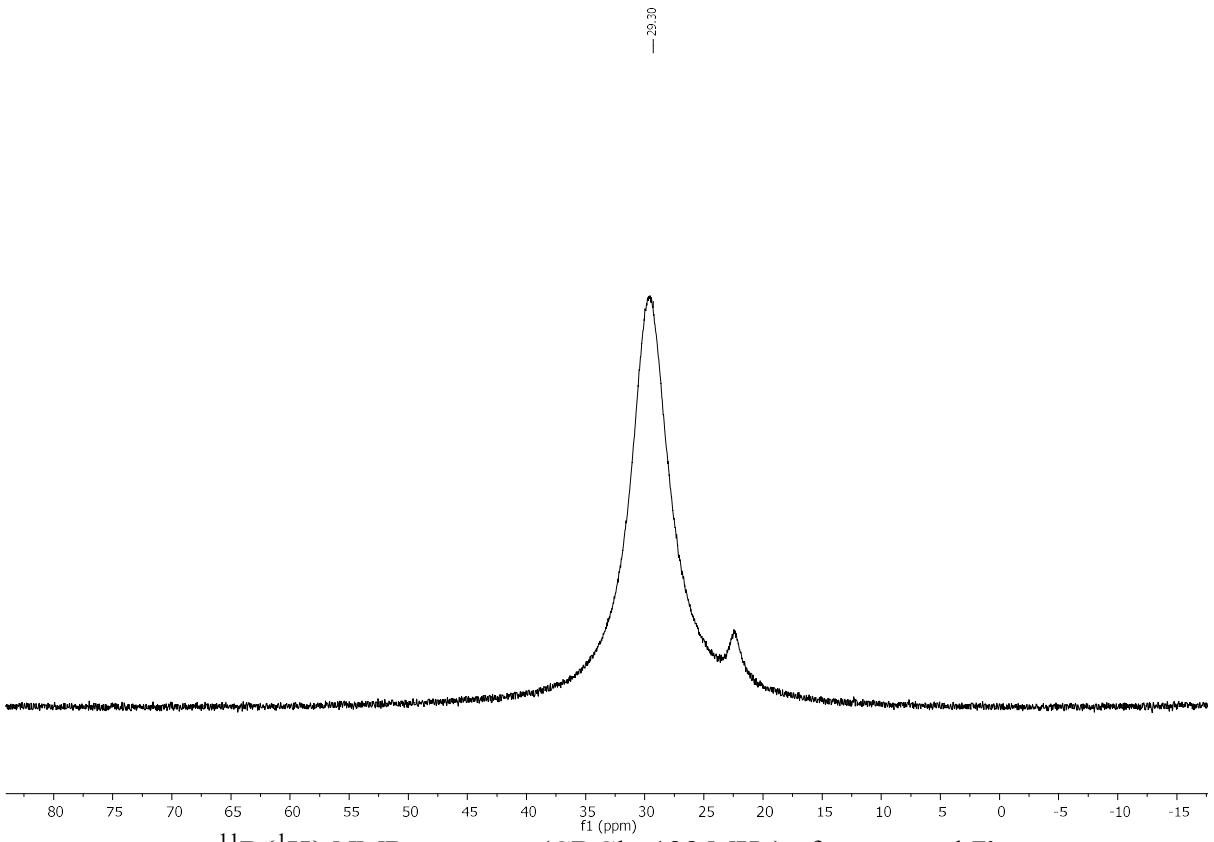
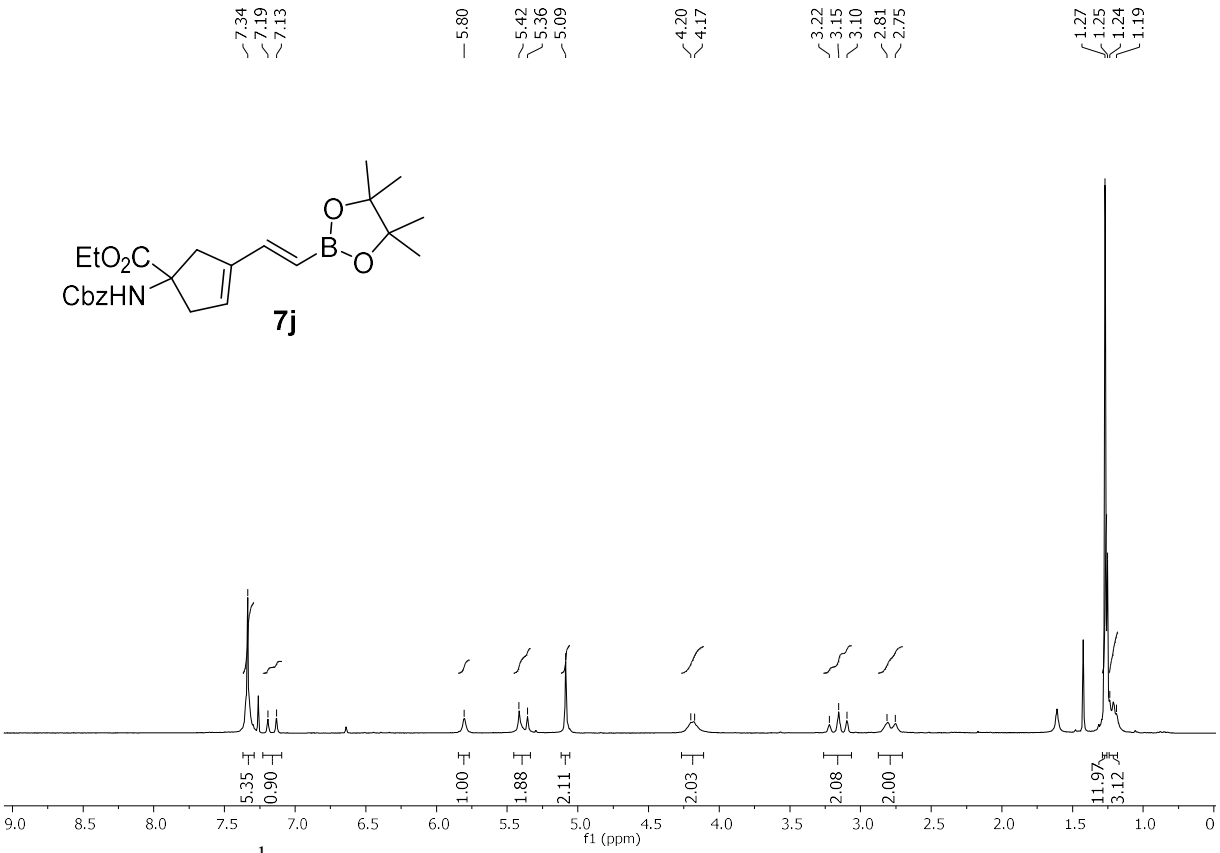


^{13}C{^{1}H} NMR spectrum ($CDCl_3$, 75 MHz) of compound **7i**



$^{11}B\{^{1}H\}$ NMR spectrum ($CDCl_3$, 128 MHz) of compound **7i**



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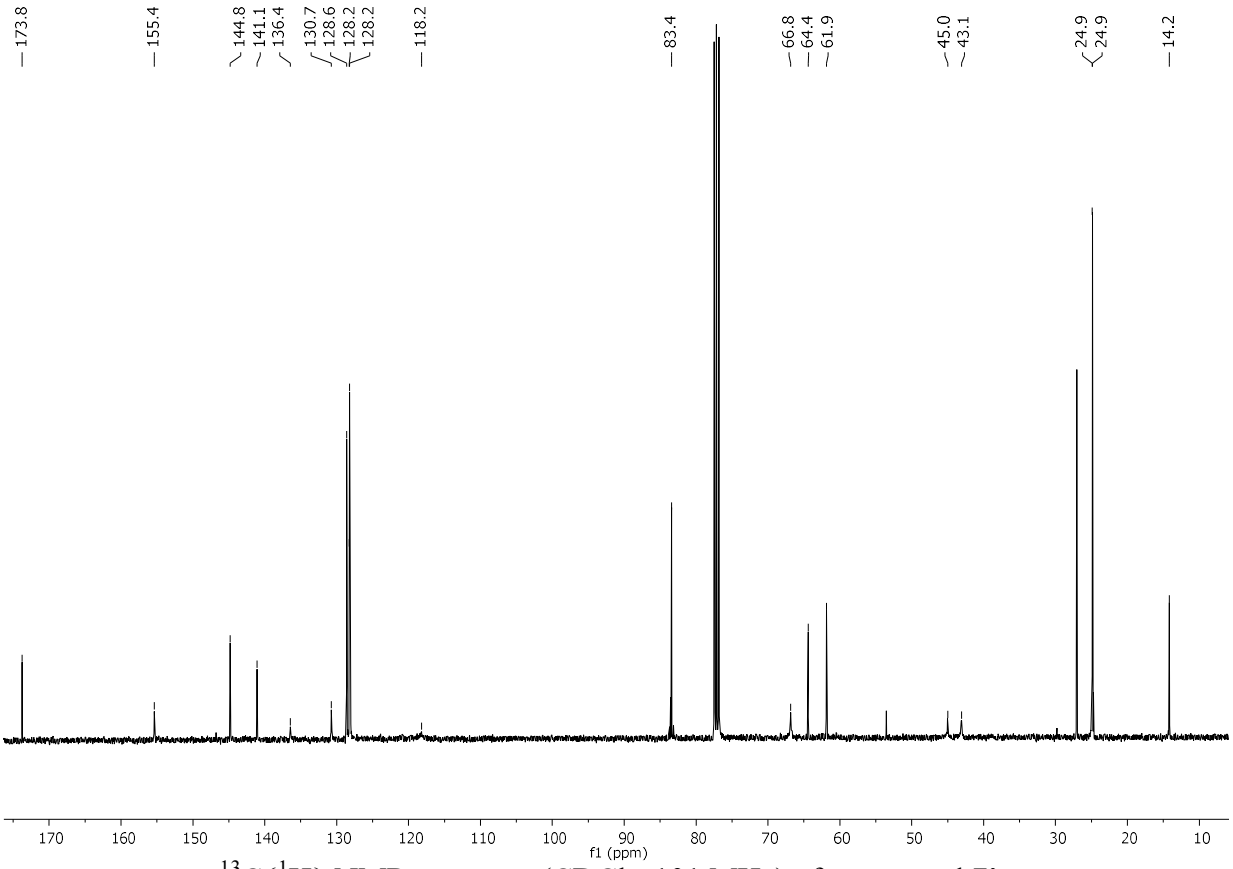
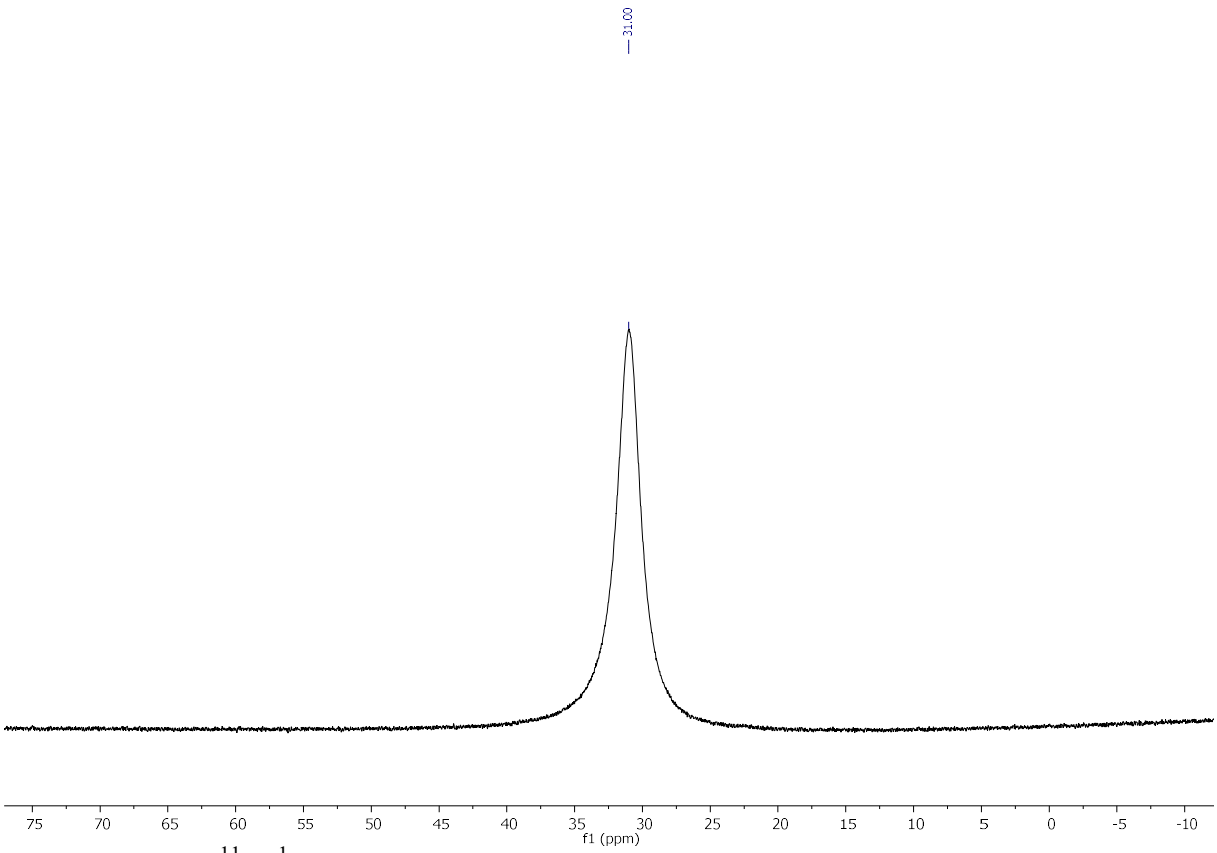
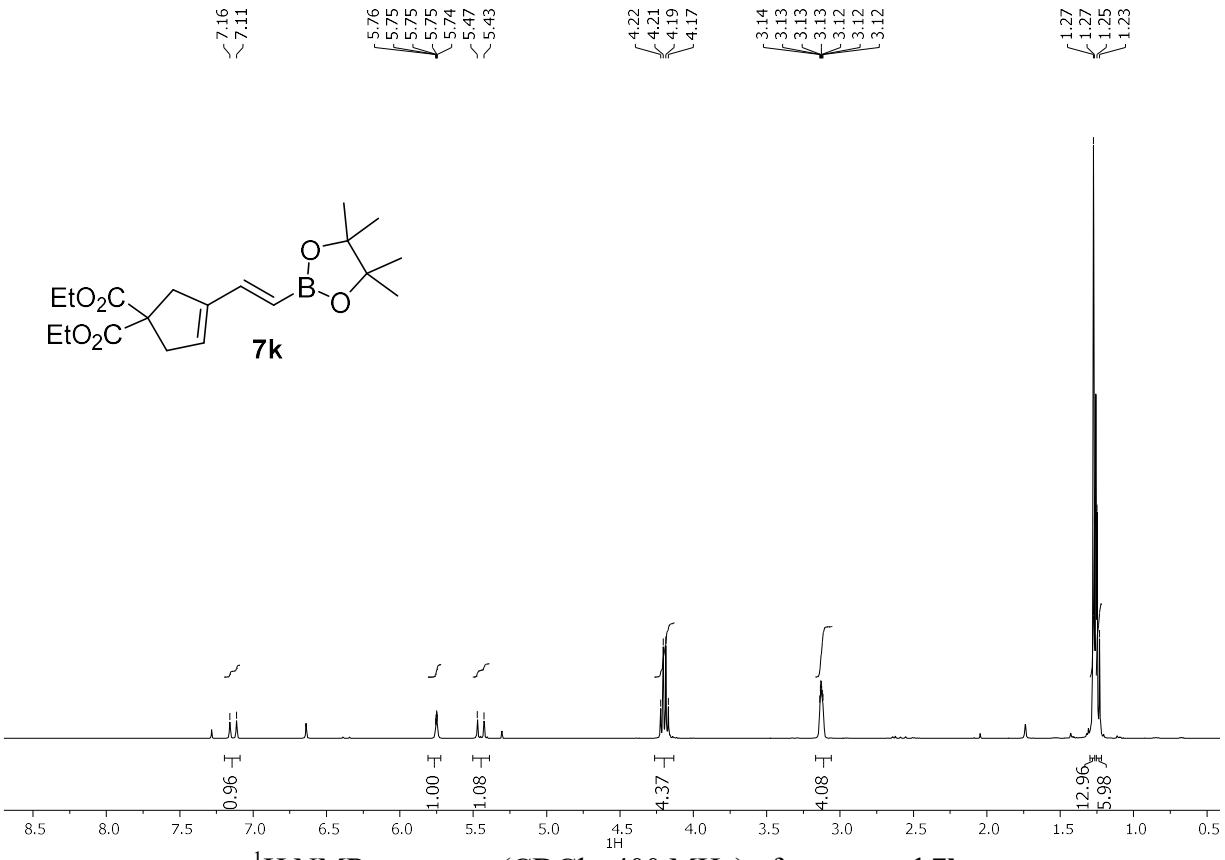


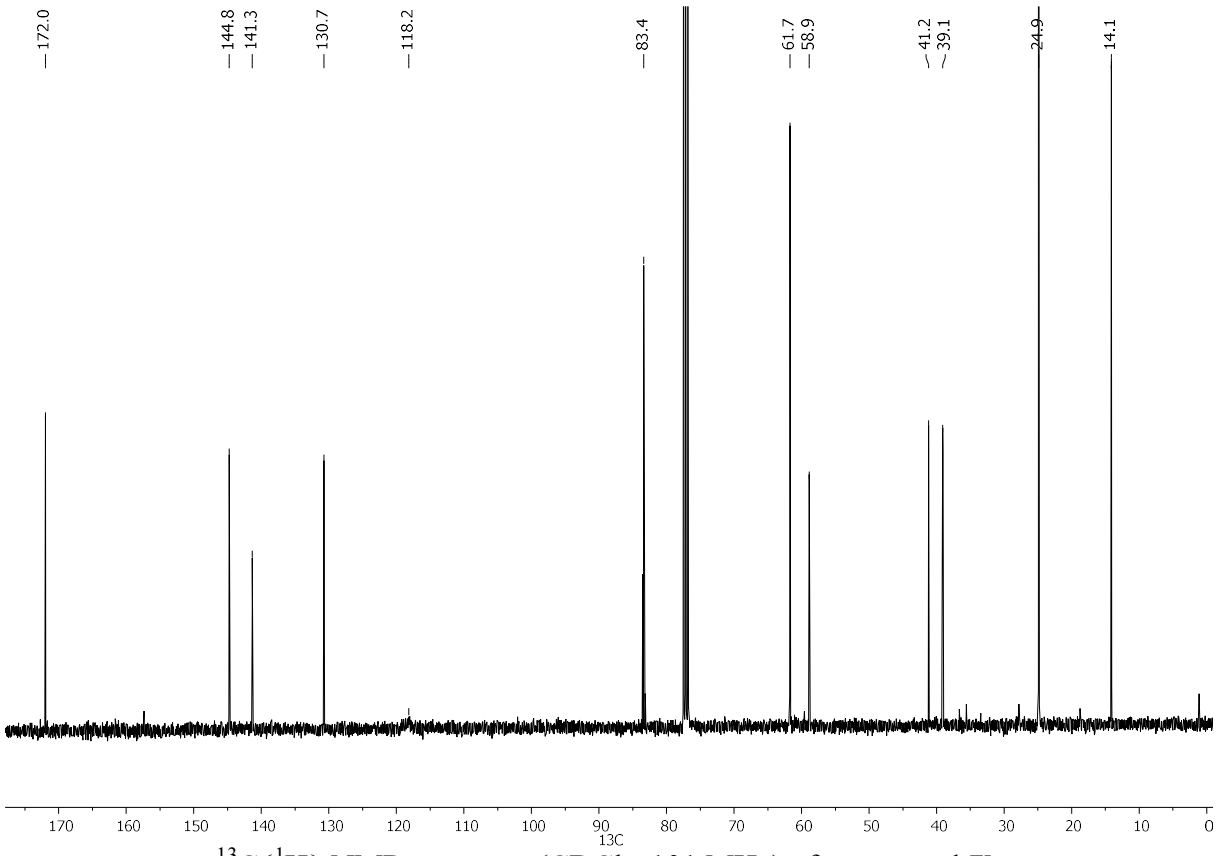
^{13}C{^{1}H} NMR spectrum ($CDCl_3$, 101 MHz) of compound **7j**



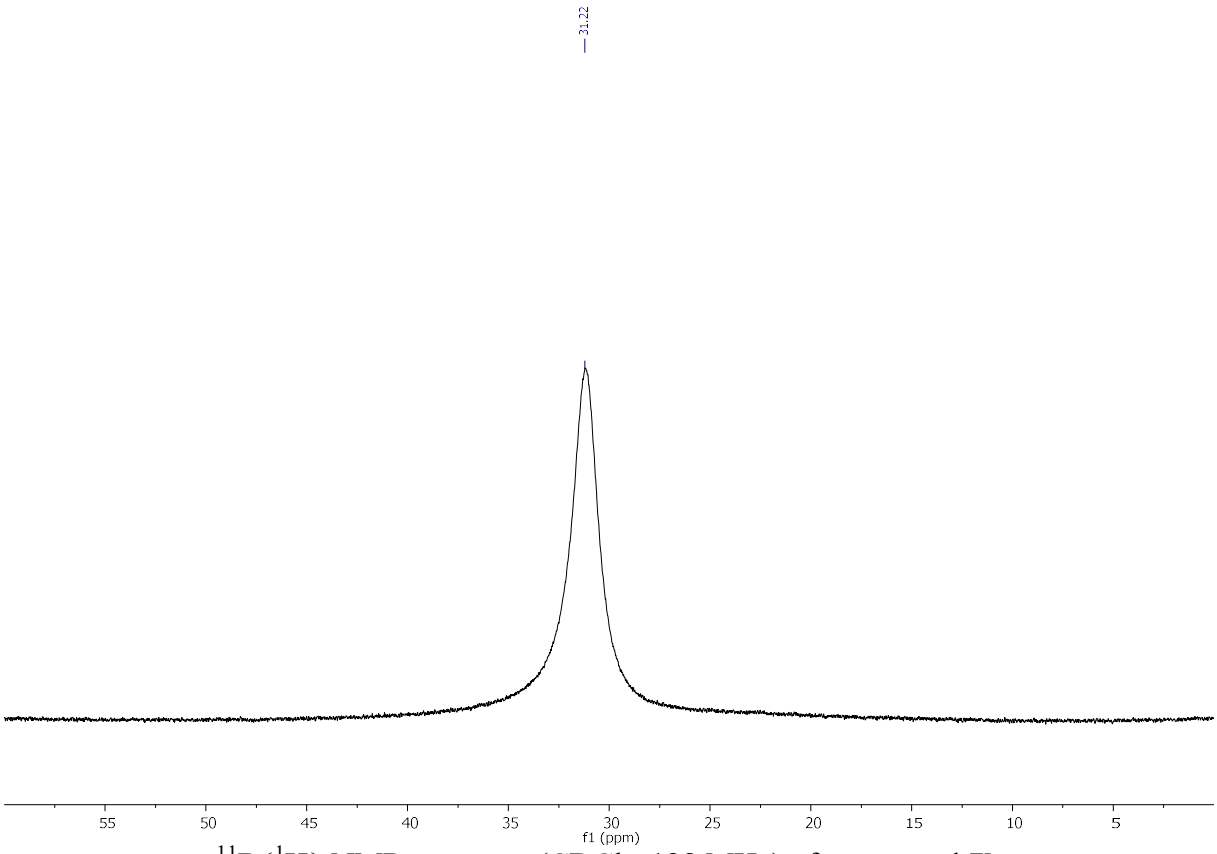
$^{11}B\{^{1}H\}$ NMR spectrum ($CDCl_3$, 128 MHz) of compound **7j**



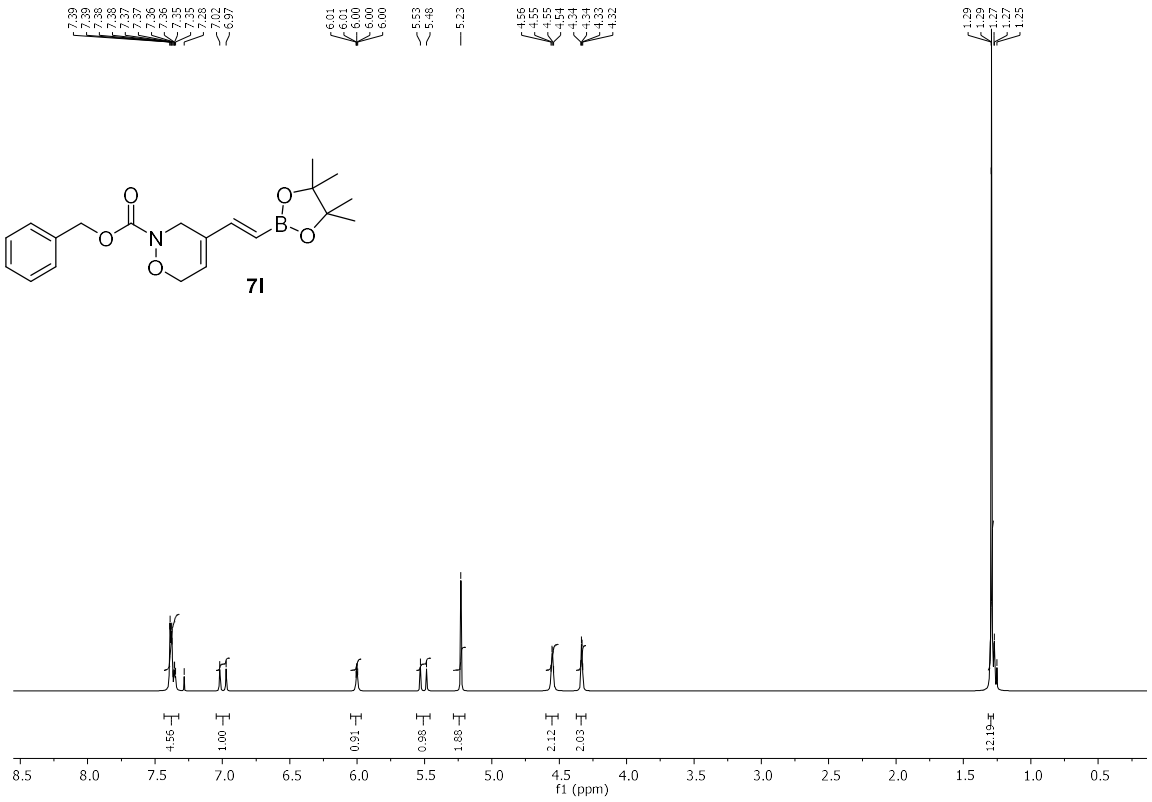
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound **7k**



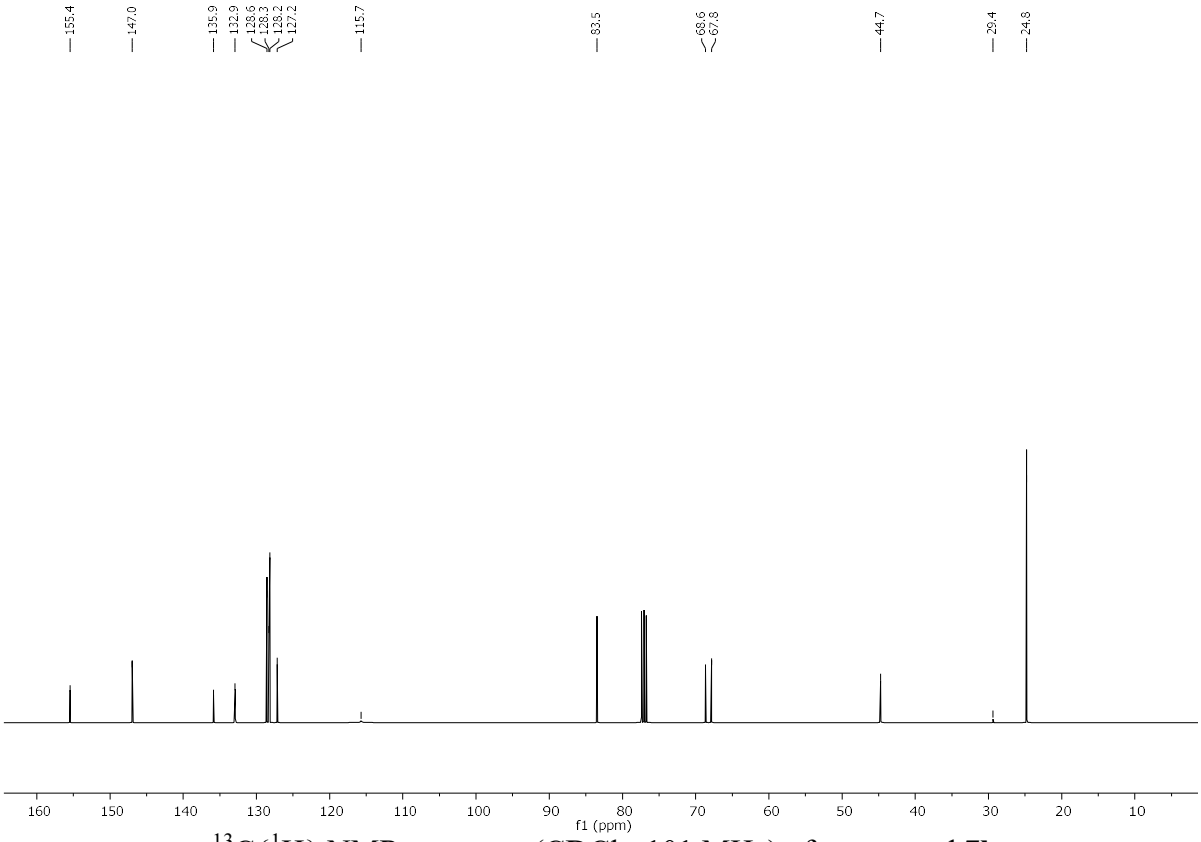
^{13}C{^{1}H} NMR spectrum ($CDCl_3$, 101 MHz) of compound **7k**



$^{11}B\{^{1}H\}$ NMR spectrum ($CDCl_3$, 128 MHz) of compound **7k**



^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound **7l**



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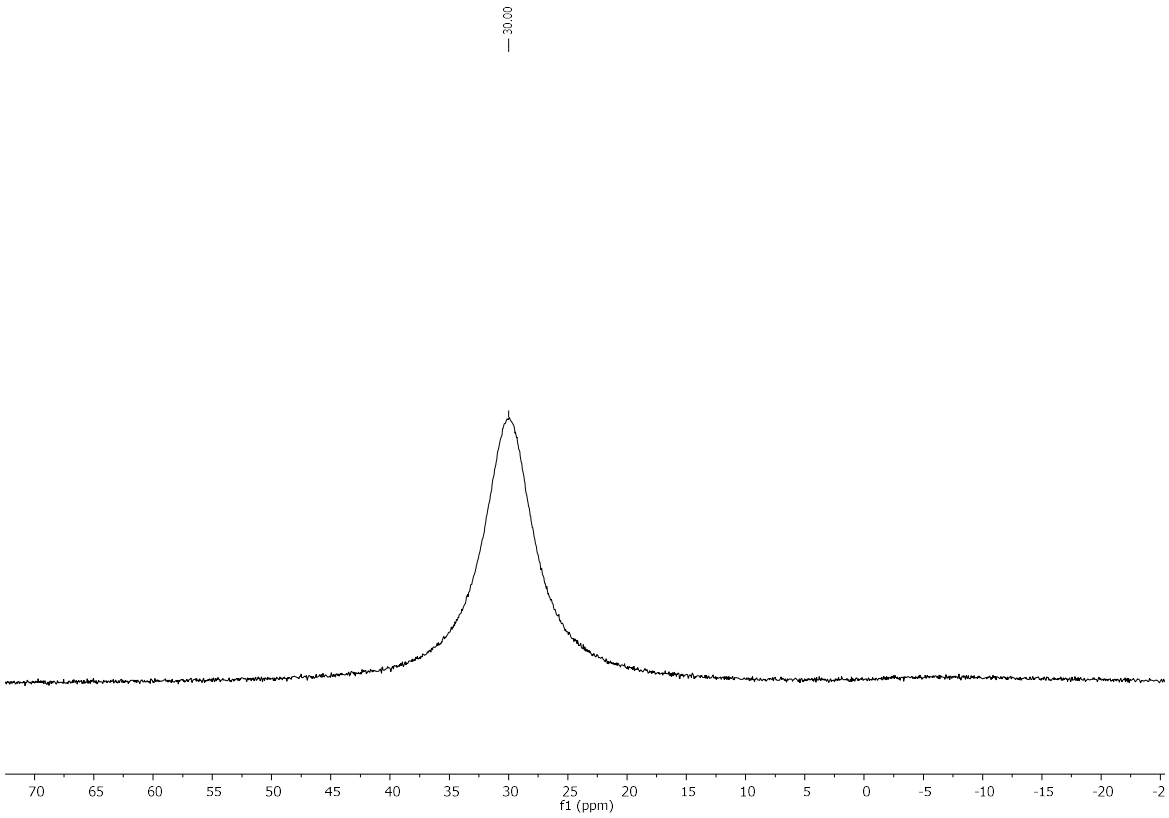
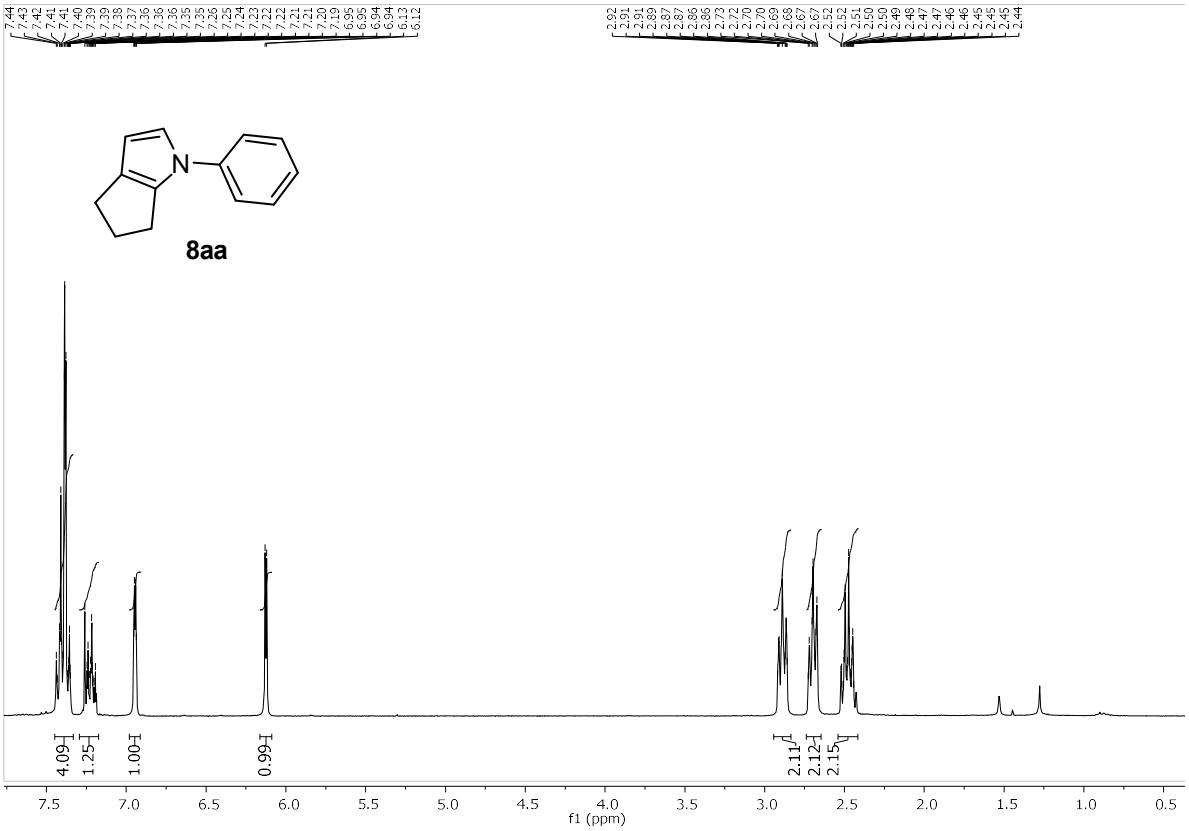
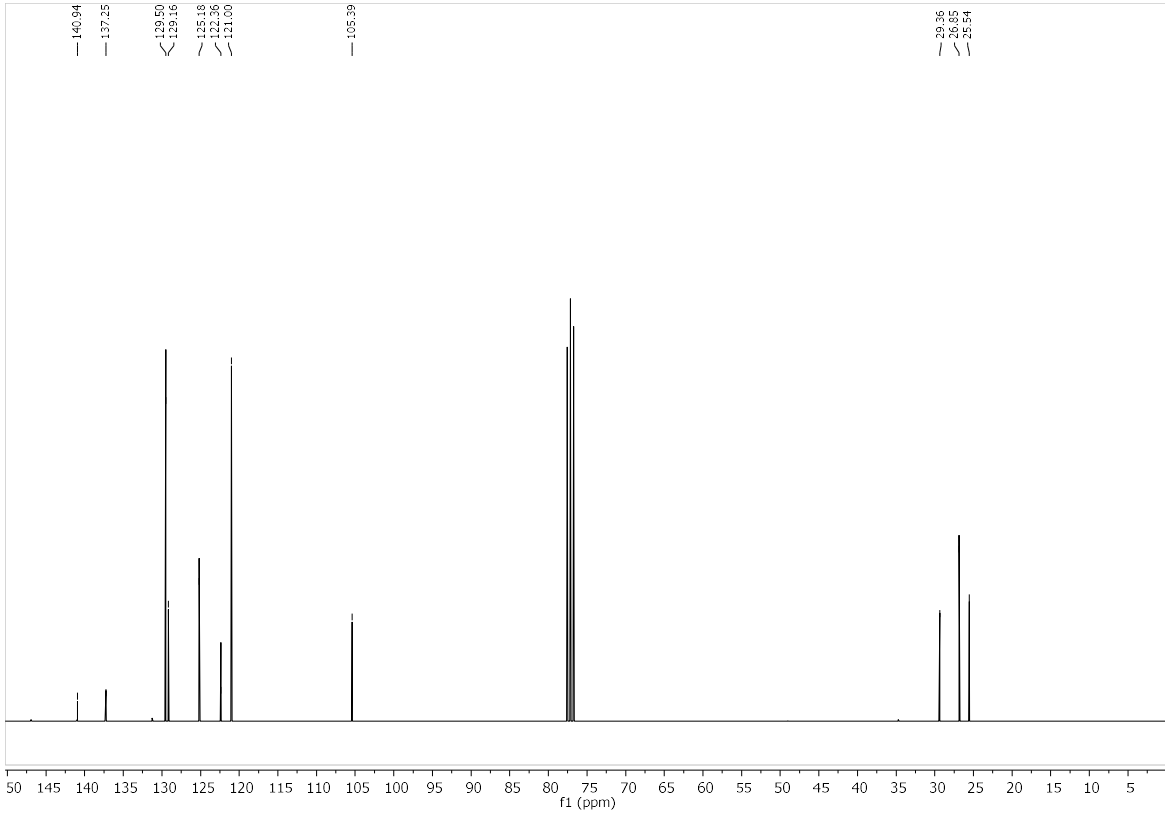


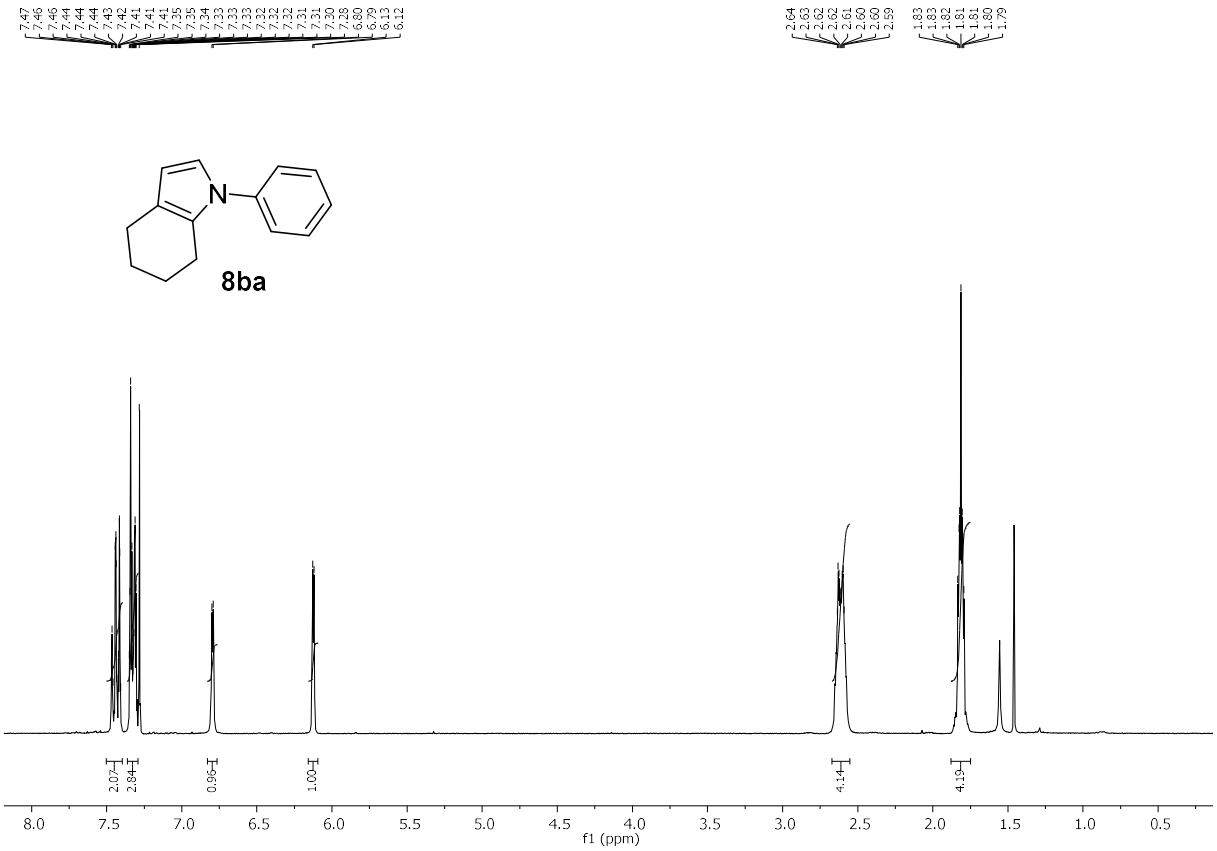
$^{11}B\{^{1}H\}$ NMR spectrum ($CDCl_3$, 96 MHz) of compound **7l**



^{1}H NMR spectrum ($CDCl_3$, 300 MHz) of compound **8aa**



^{13}C{^{1}H} NMR spectrum ($CDCl_3$, 75 MHz) of compound **8aa**



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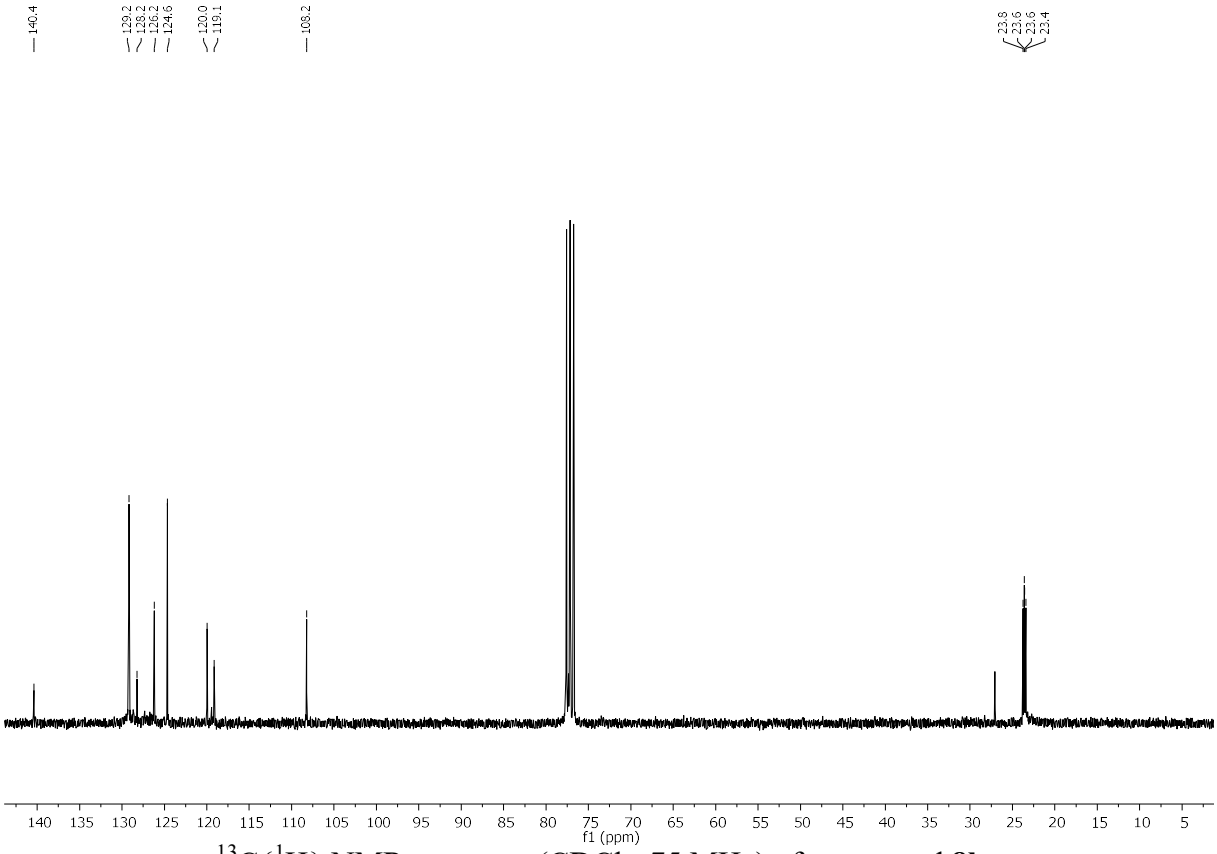

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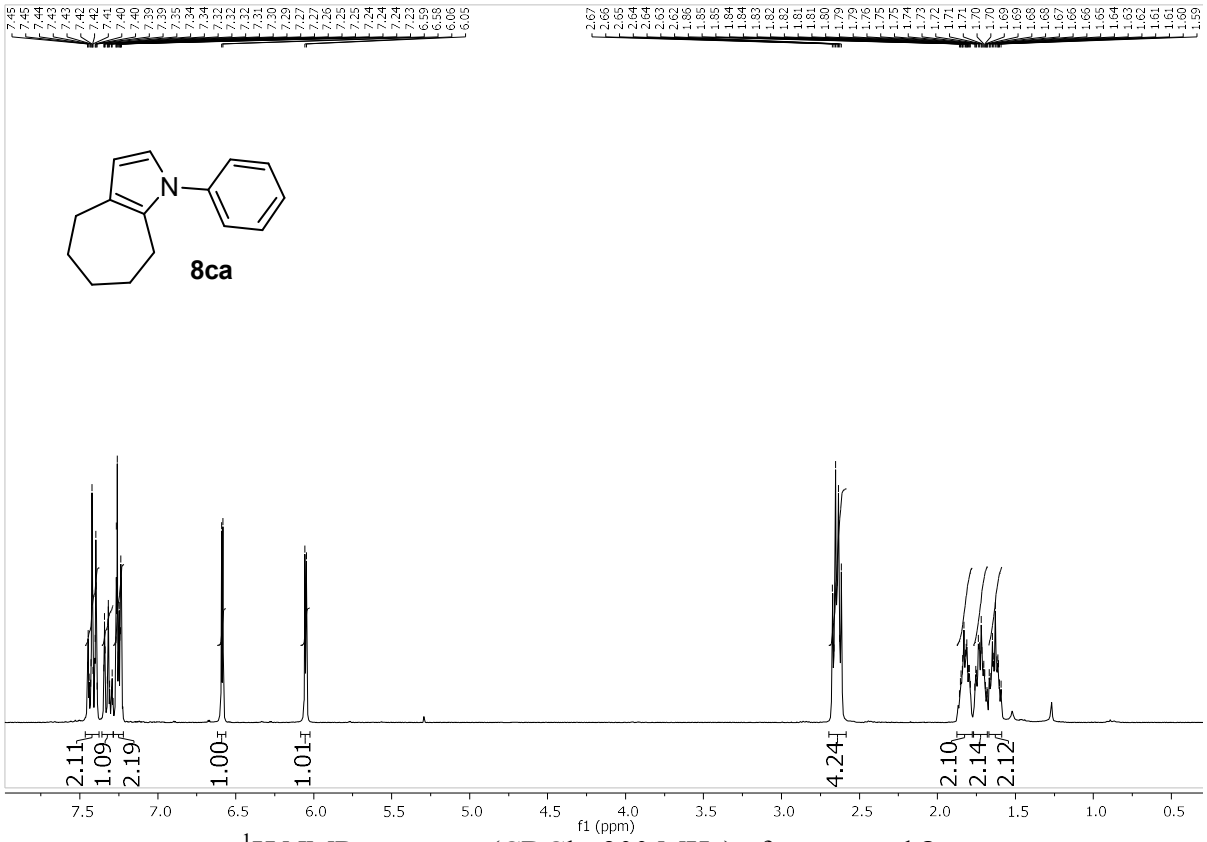

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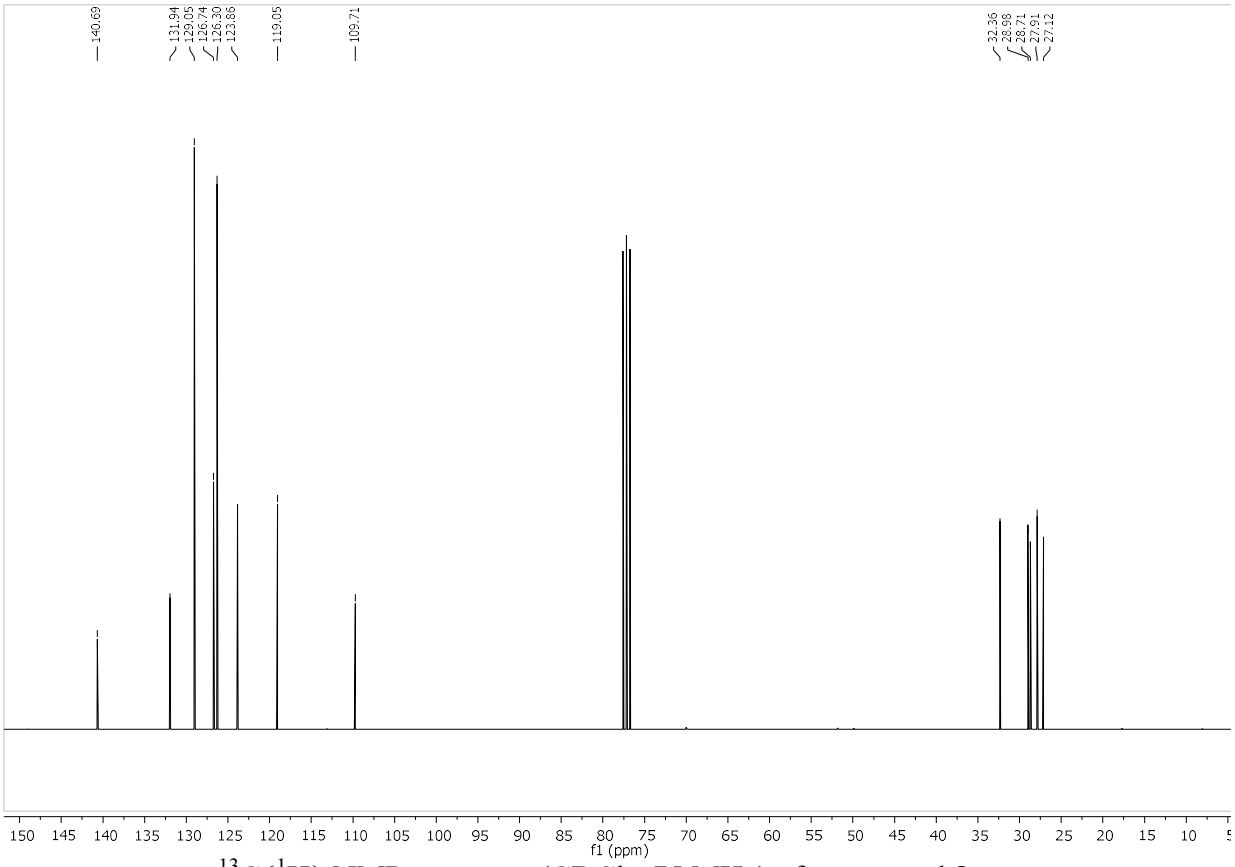

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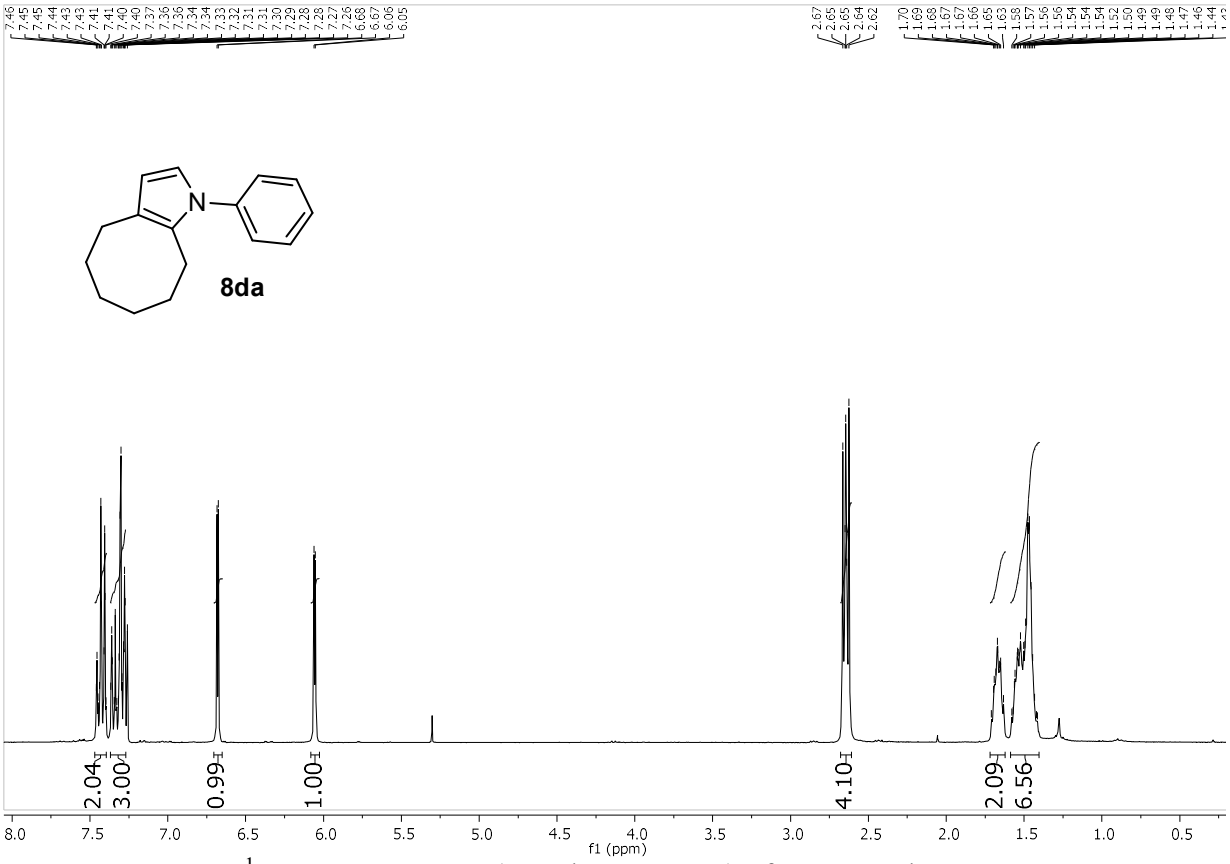

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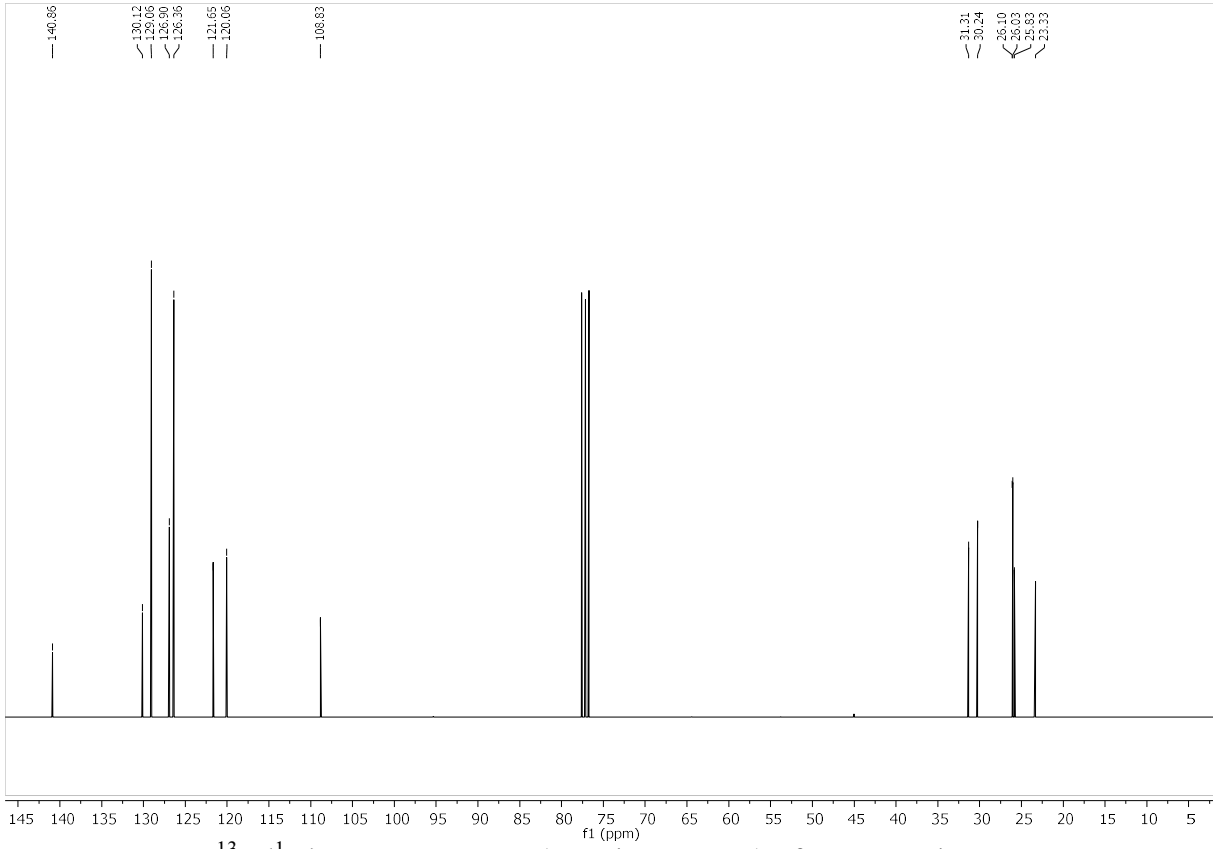

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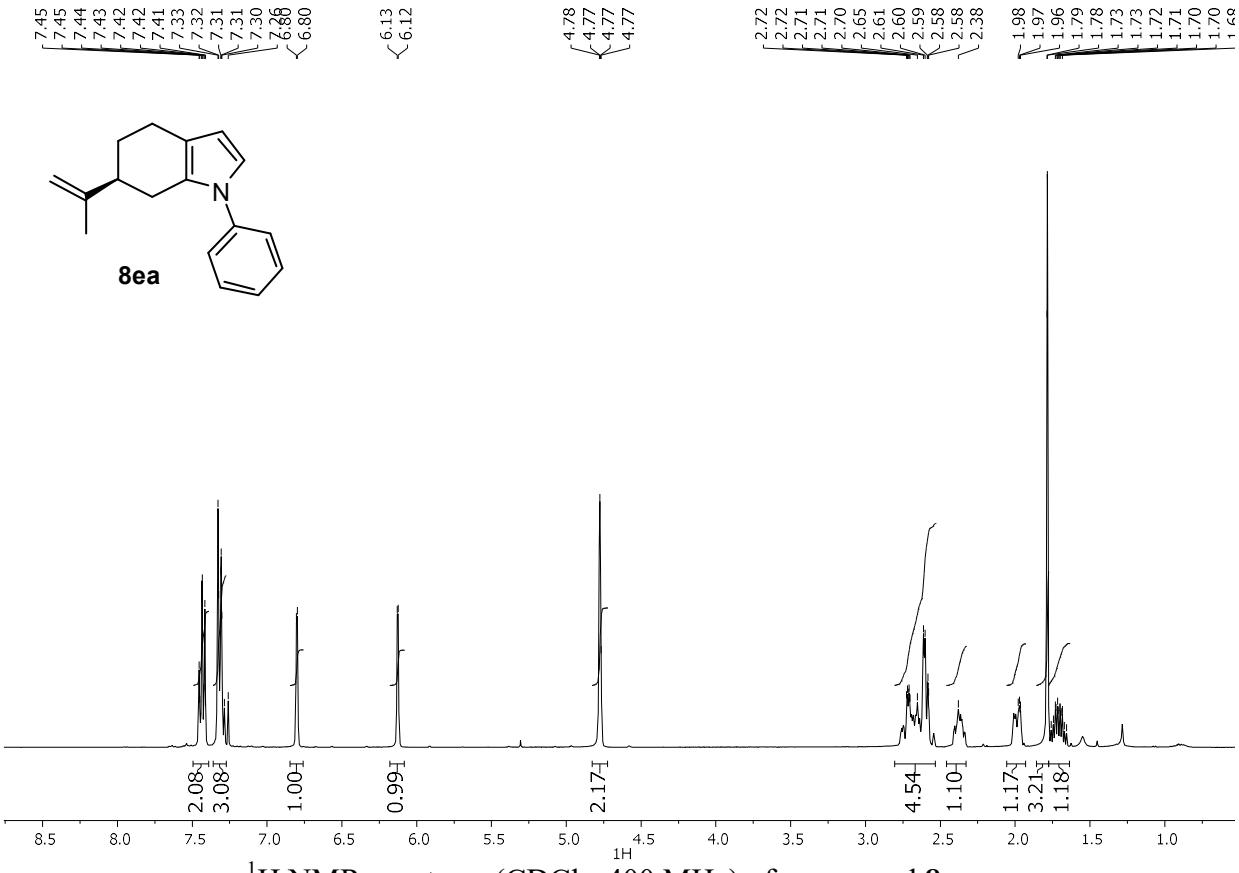

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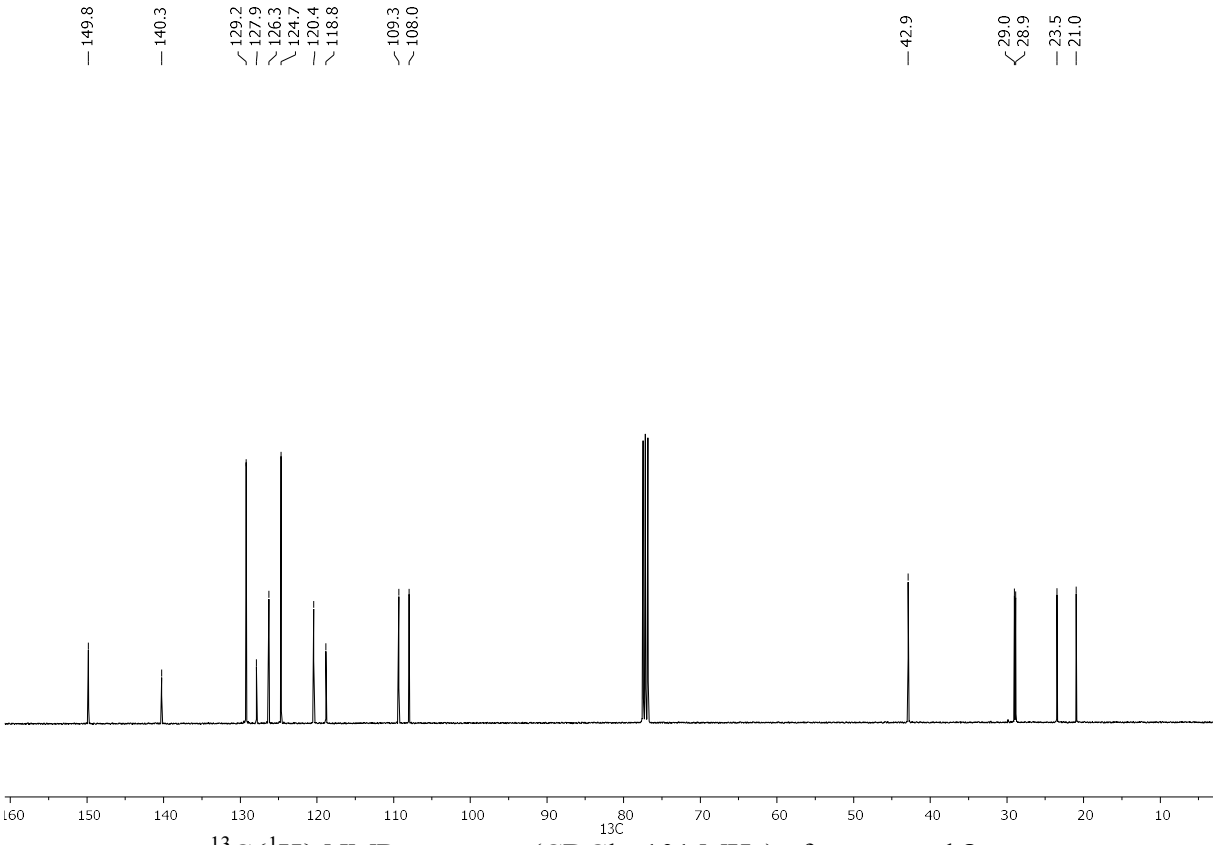
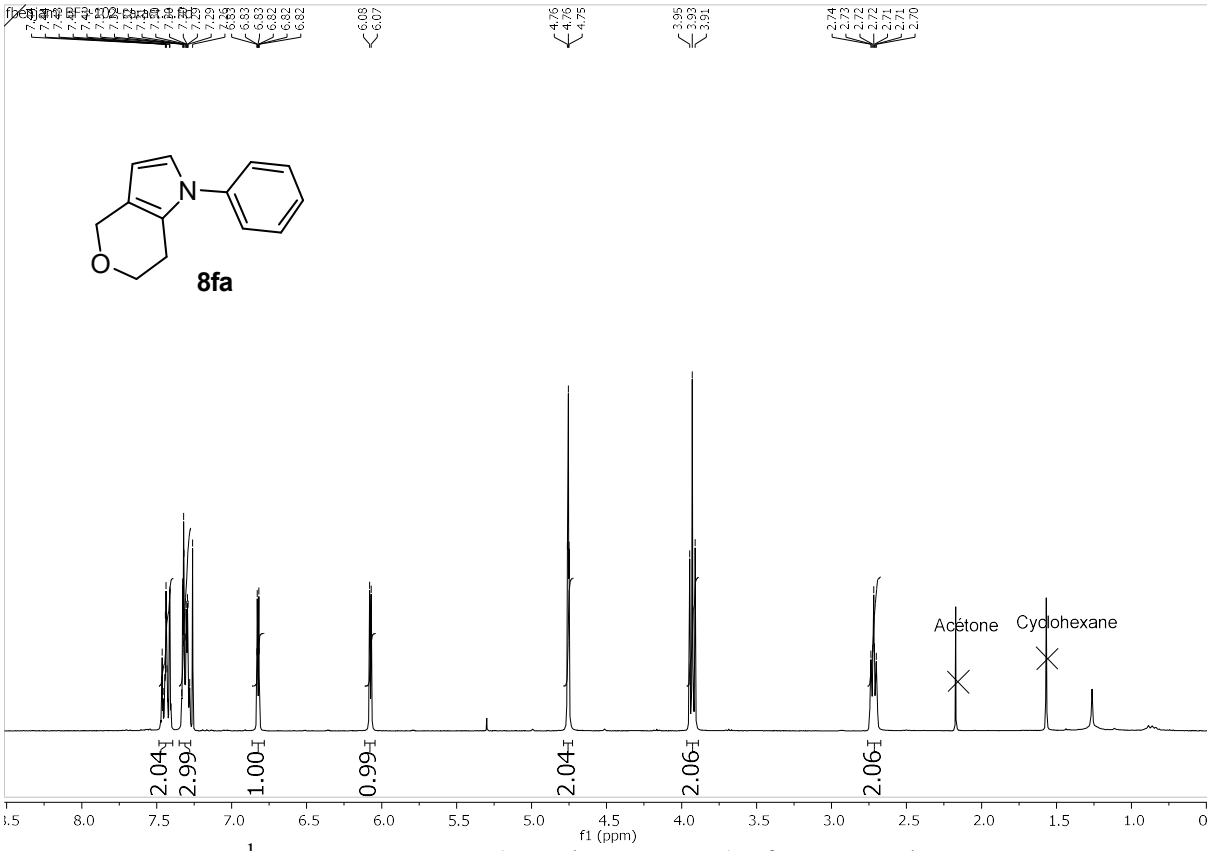


^{13}C{^{1}H} NMR spectrum ($CDCl_3$, 101 MHz) of compound **8ea**



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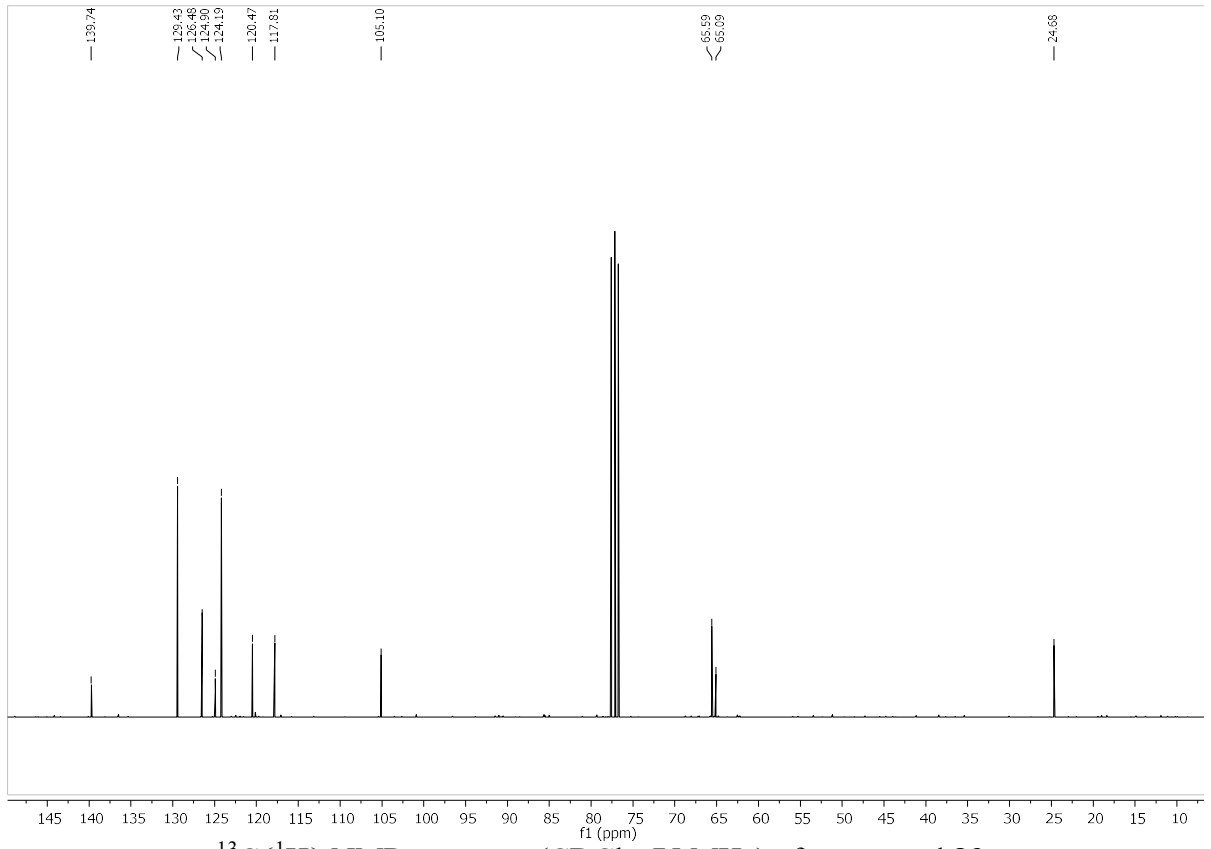
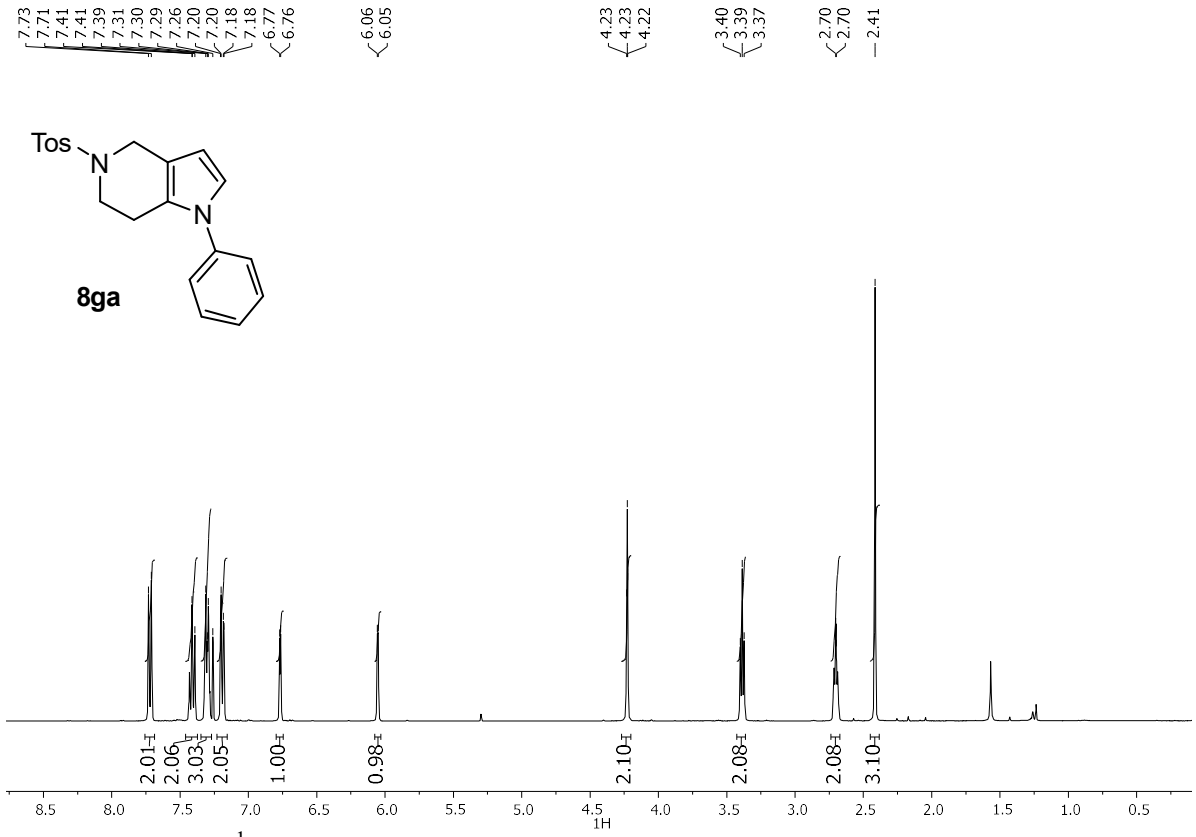
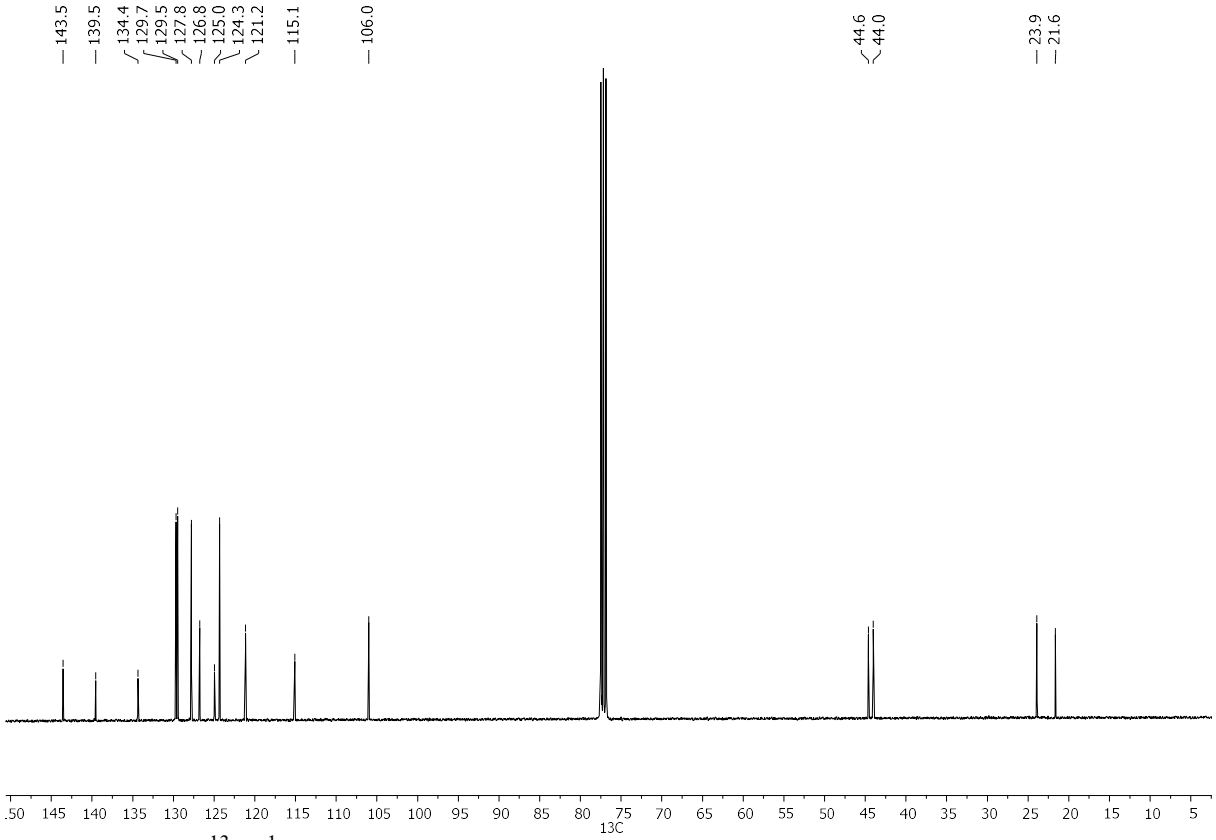


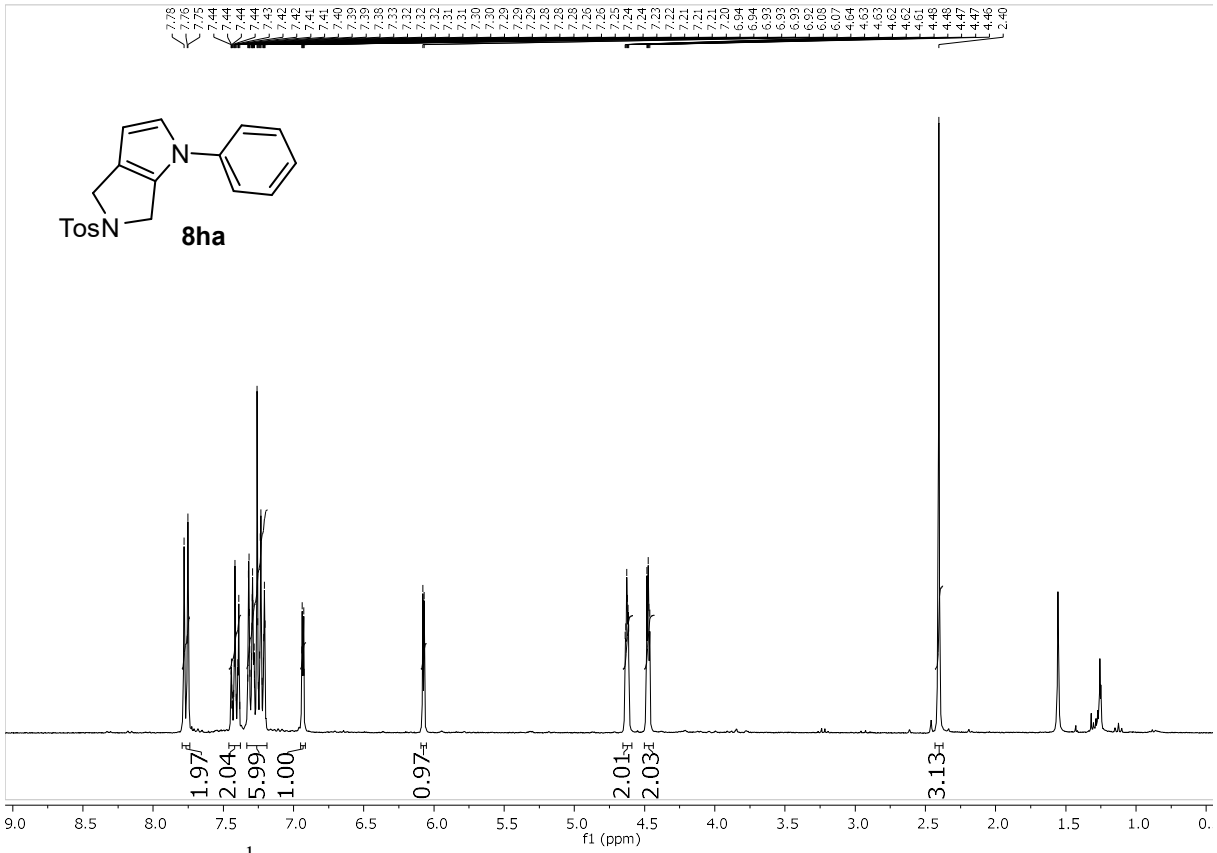
^{13}C{^{1}H} NMR spectrum ($CDCl_3$, 75 MHz) of compound **8fa**



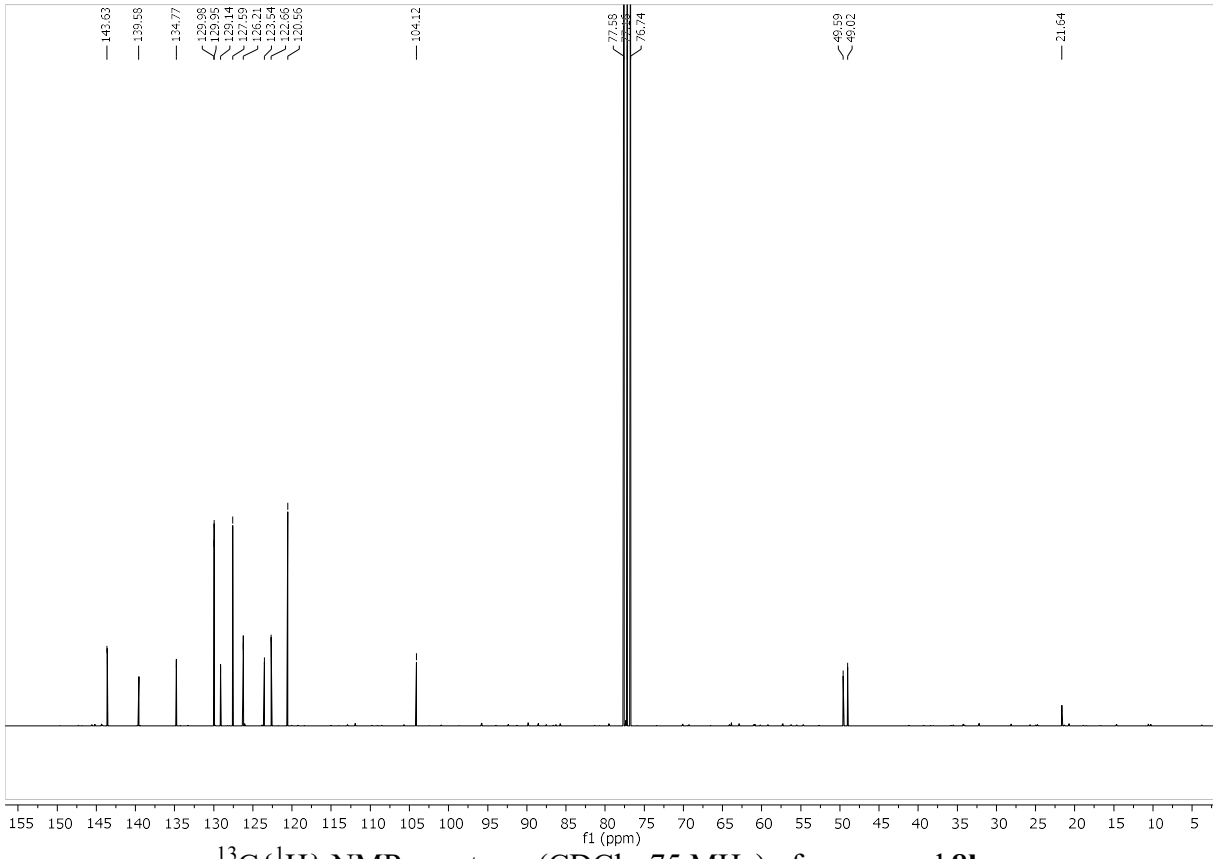
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound **8ga**



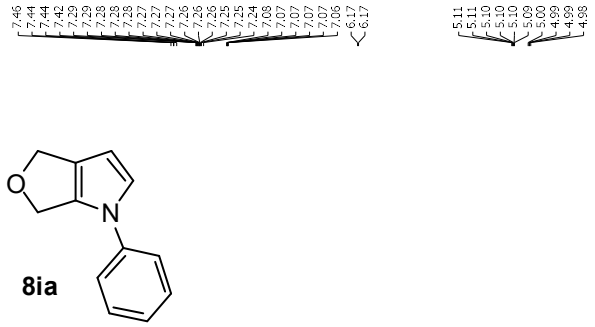
^{13}C{^{1}H} NMR spectrum ($CDCl_3$, 101 MHz) of compound **8ga**



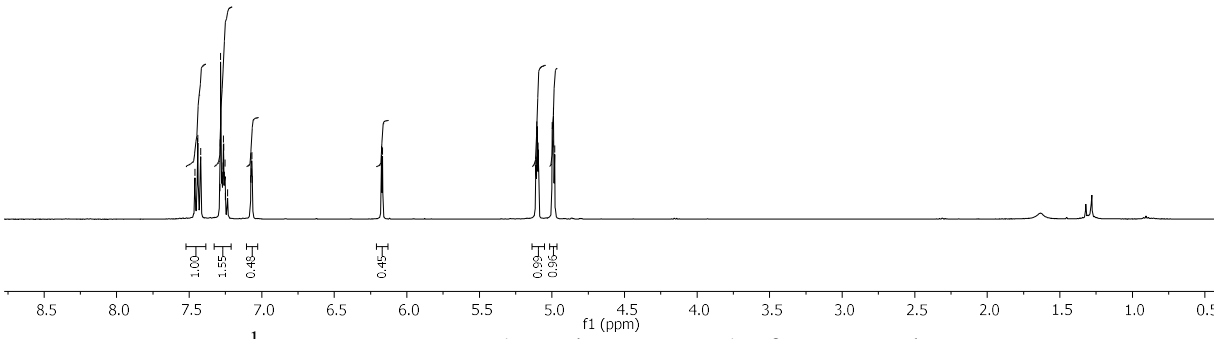
^{1}H NMR spectrum ($CDCl_3$, 300 MHz) of compound **8ha**



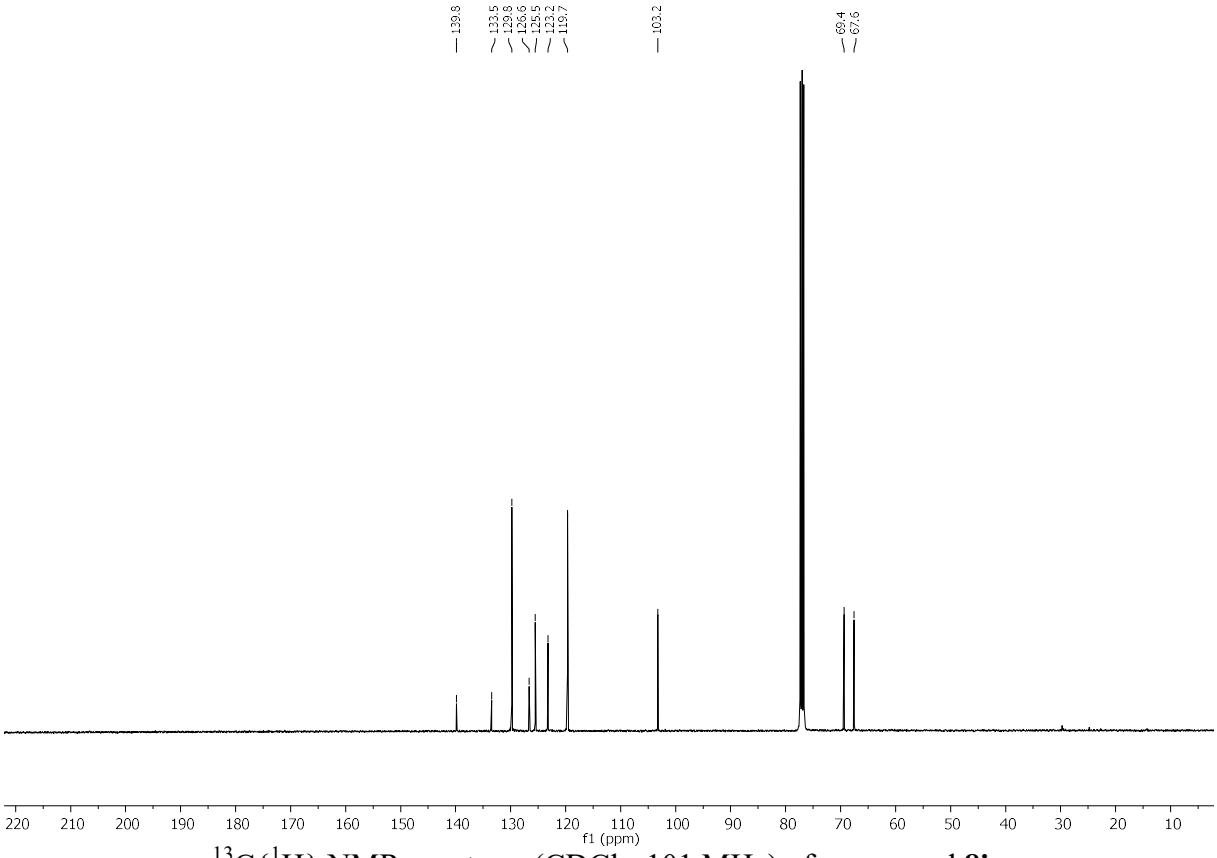
^{13}C{^{1}H} NMR spectrum ($CDCl_3$, 75 MHz) of compound **8ha**



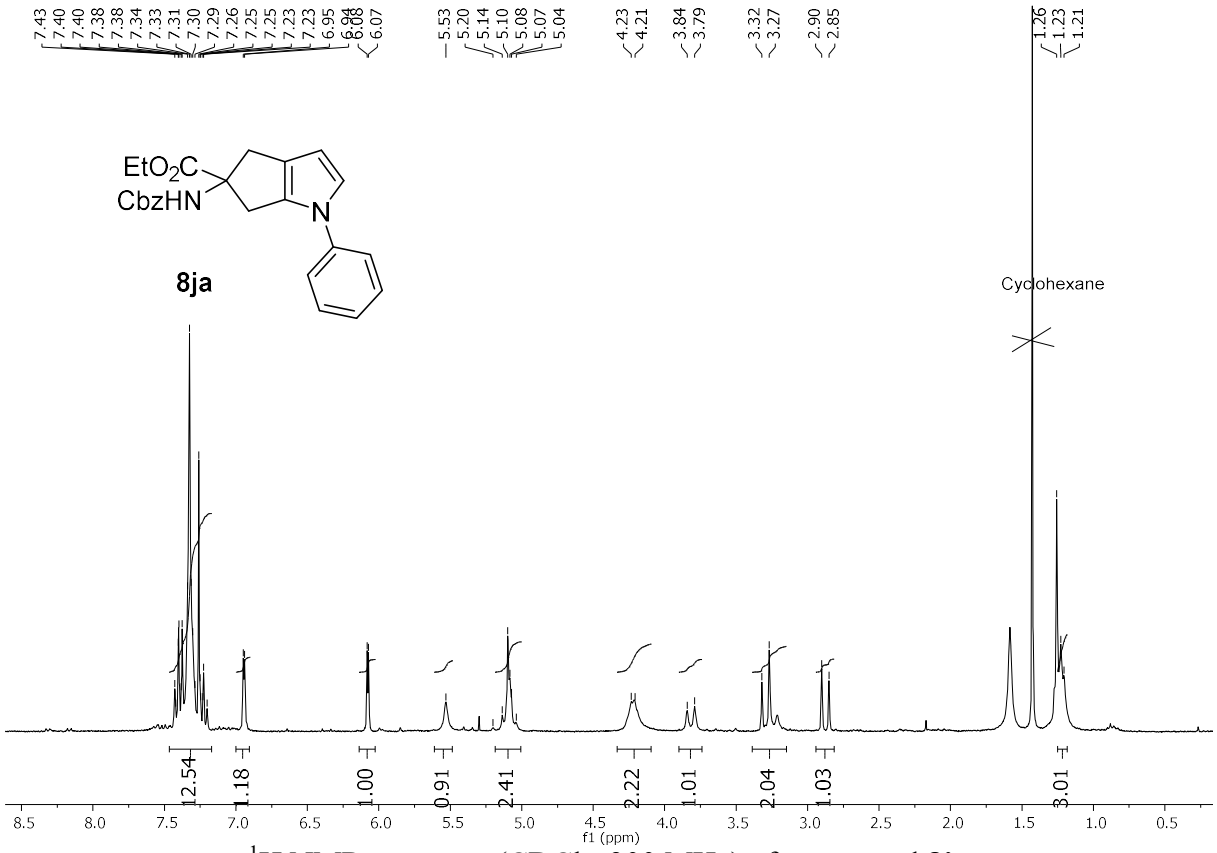
8ia



^{1}H NMR spectrum ($CDCl_3$, 300 MHz) of compound **8ia**



$^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$, 101 MHz) of compound **8ia**



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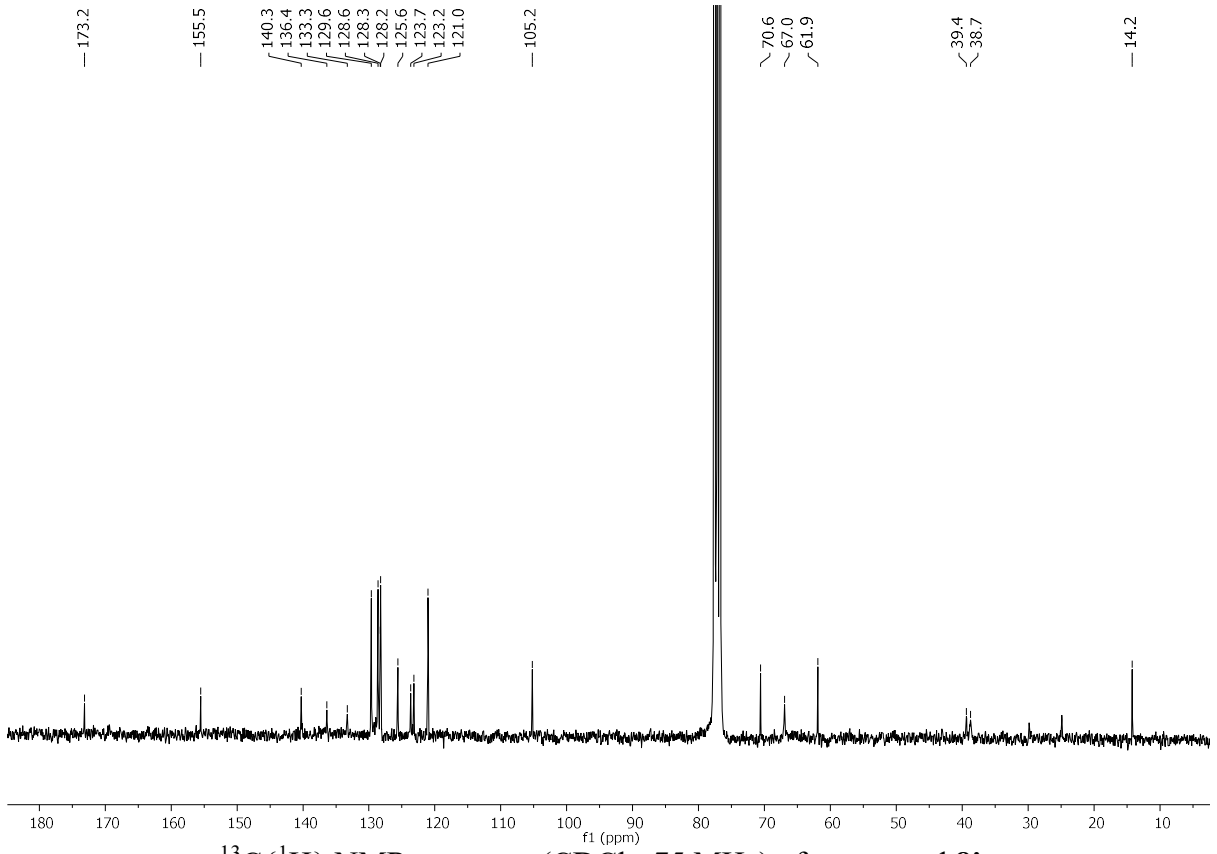
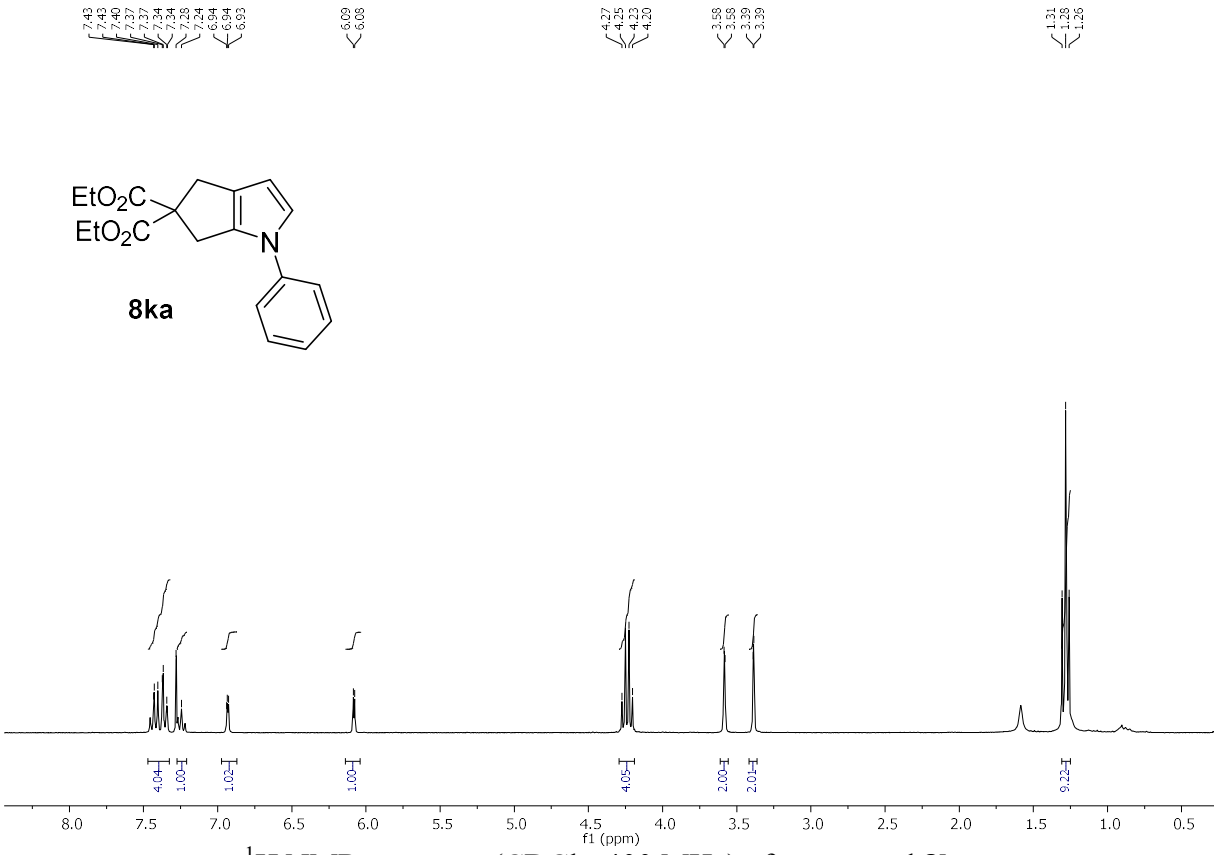
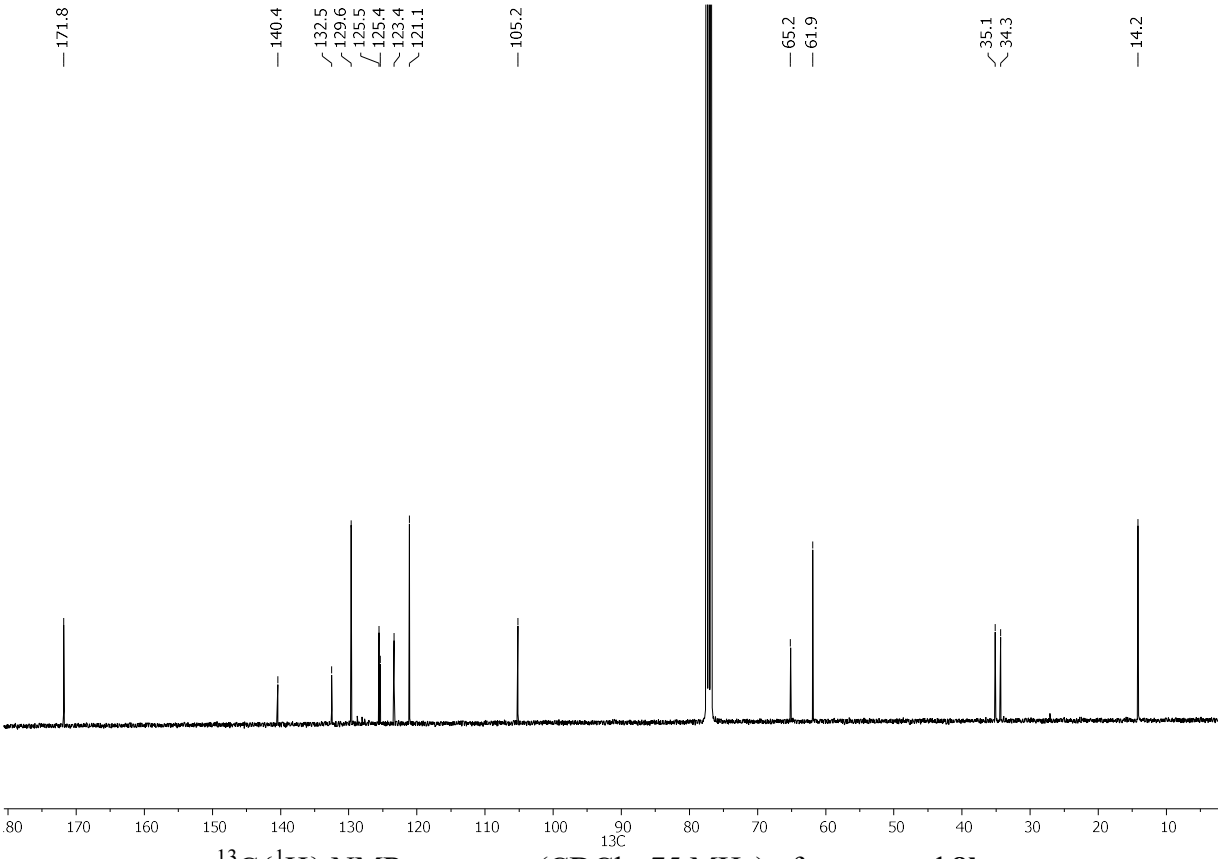


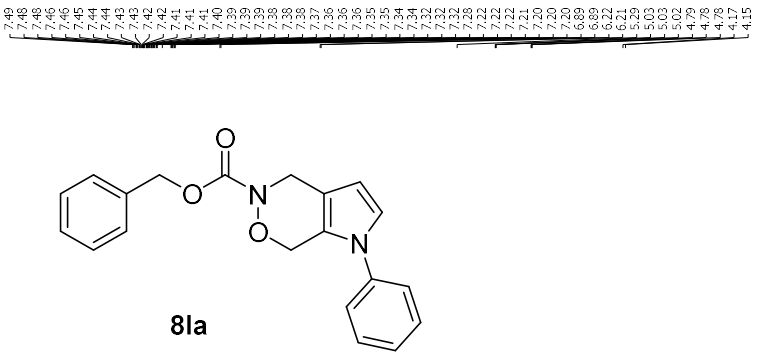
^{13}C{^{1}H} NMR spectrum ($CDCl_3$, 75 MHz) of compound **8ja**



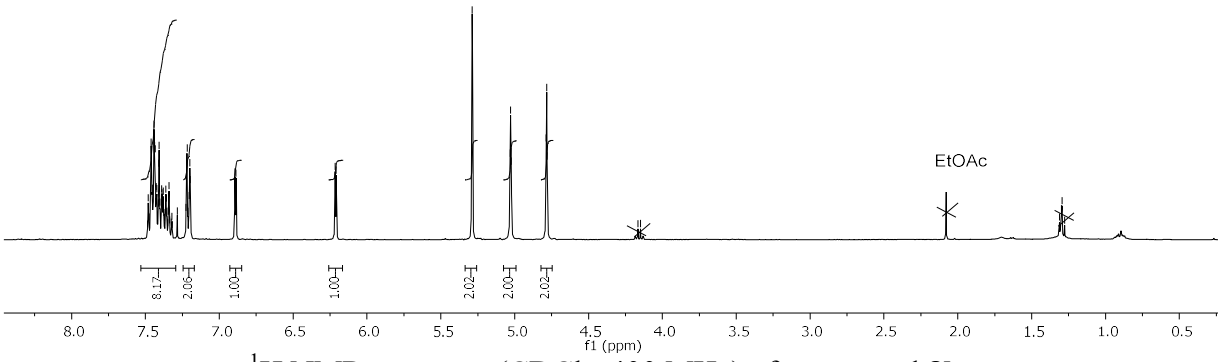
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound **8ka**



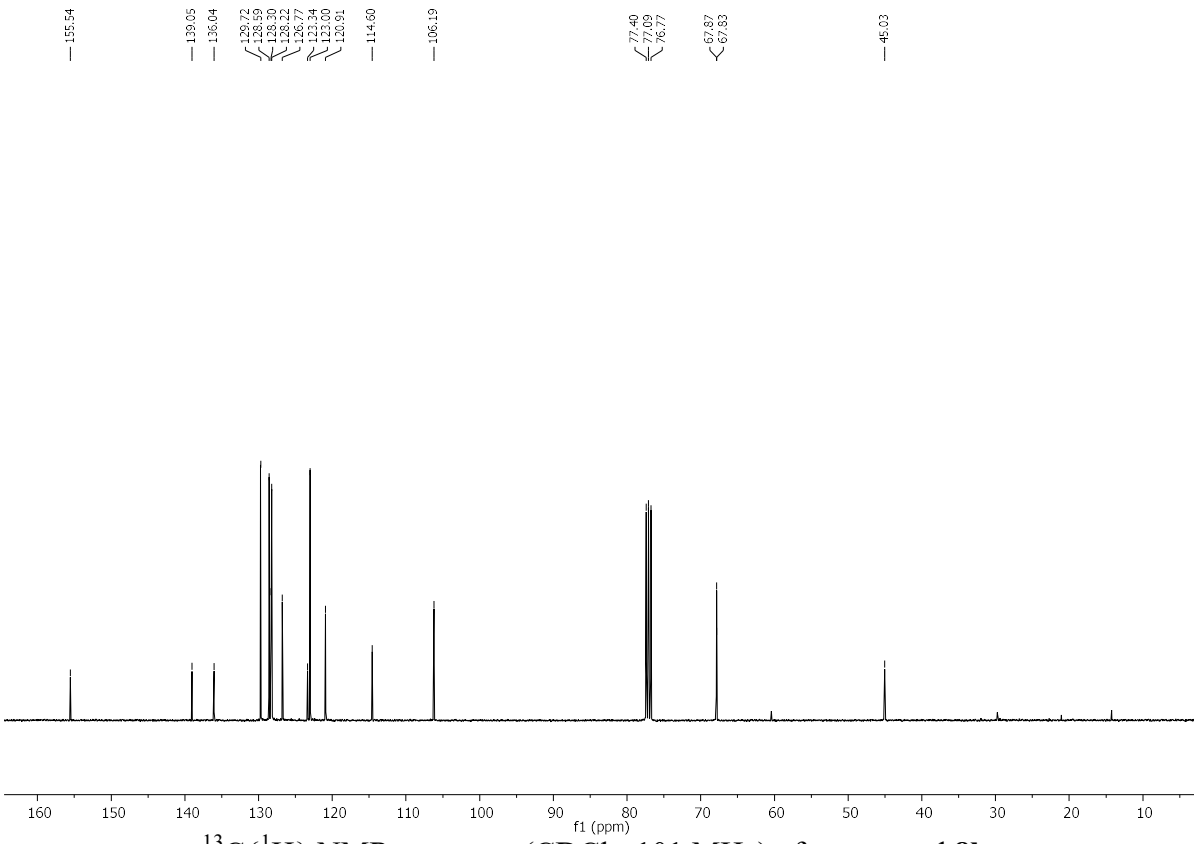
^{13}C{^{1}H} NMR spectrum ($CDCl_3$, 75 MHz) of compound **8ka**



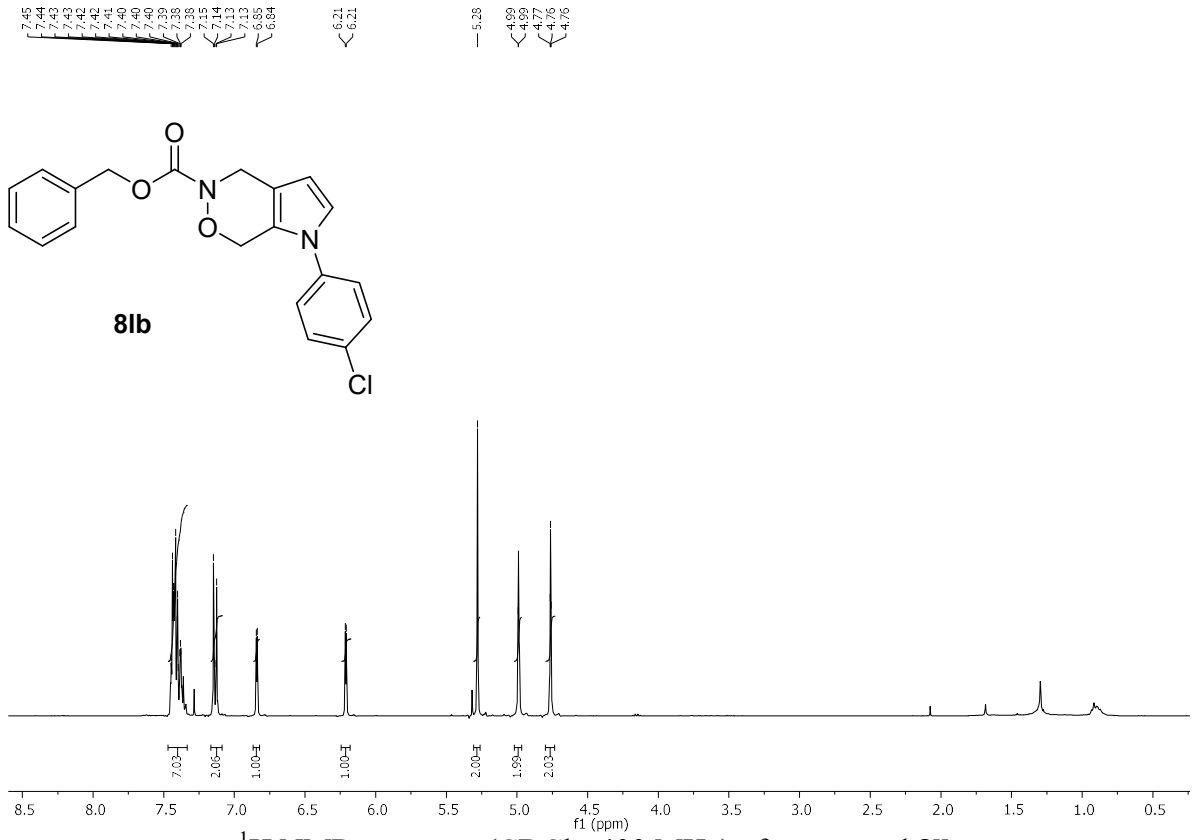
8la



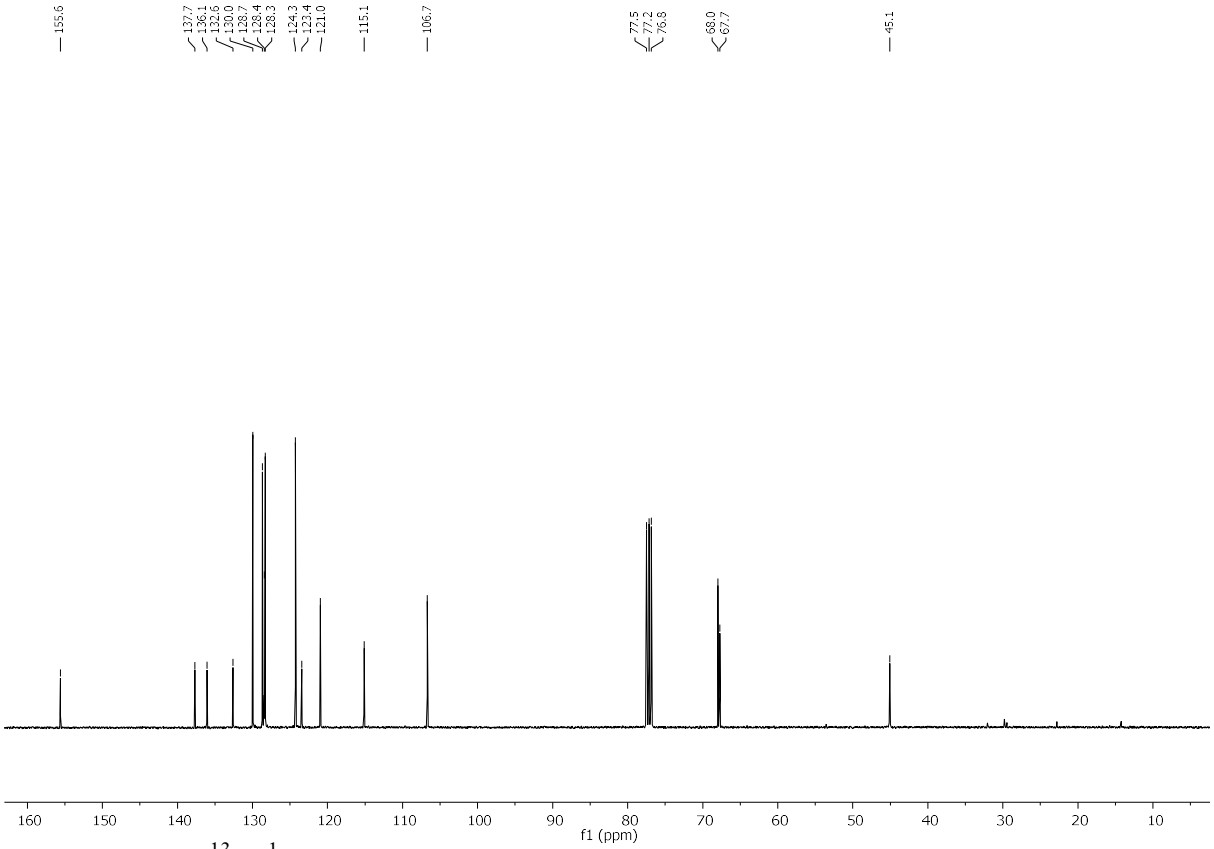
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound **8la**



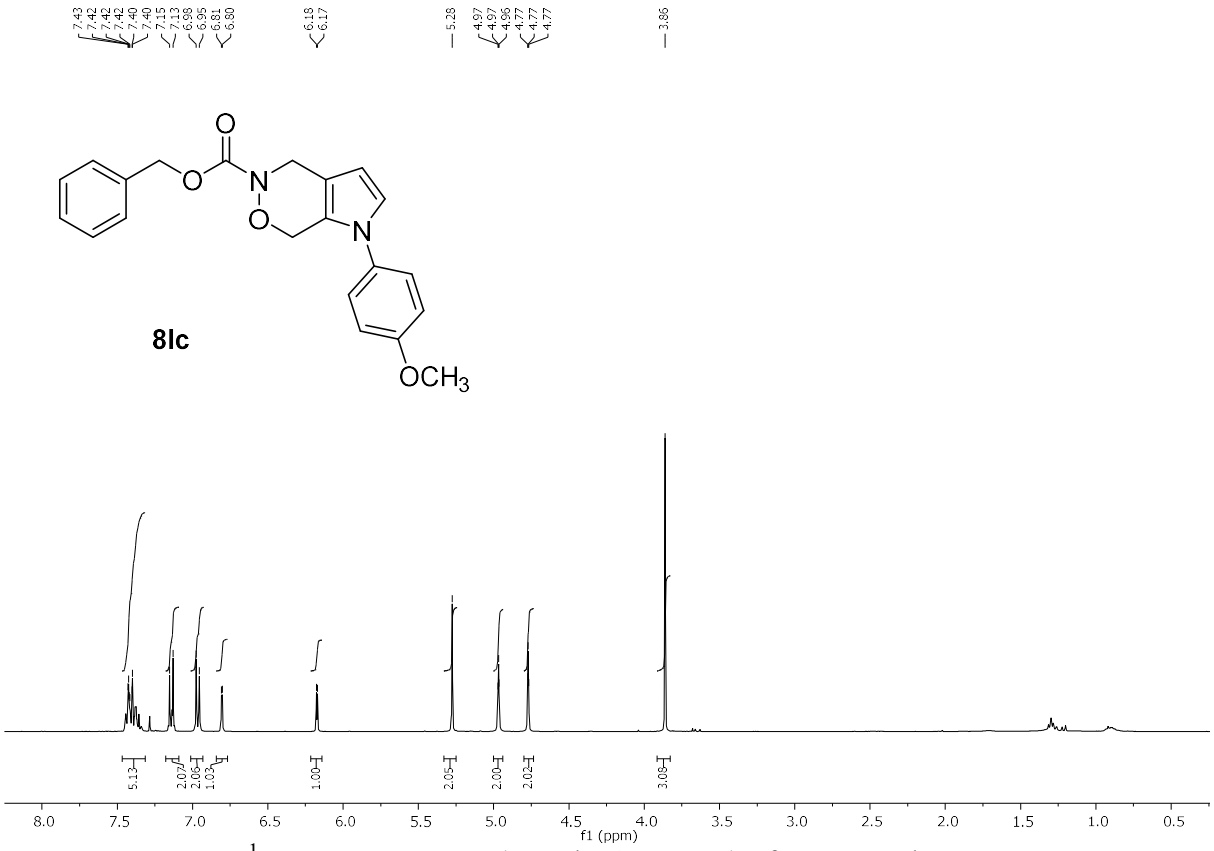
$^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$, 101 MHz) of compound **8la**



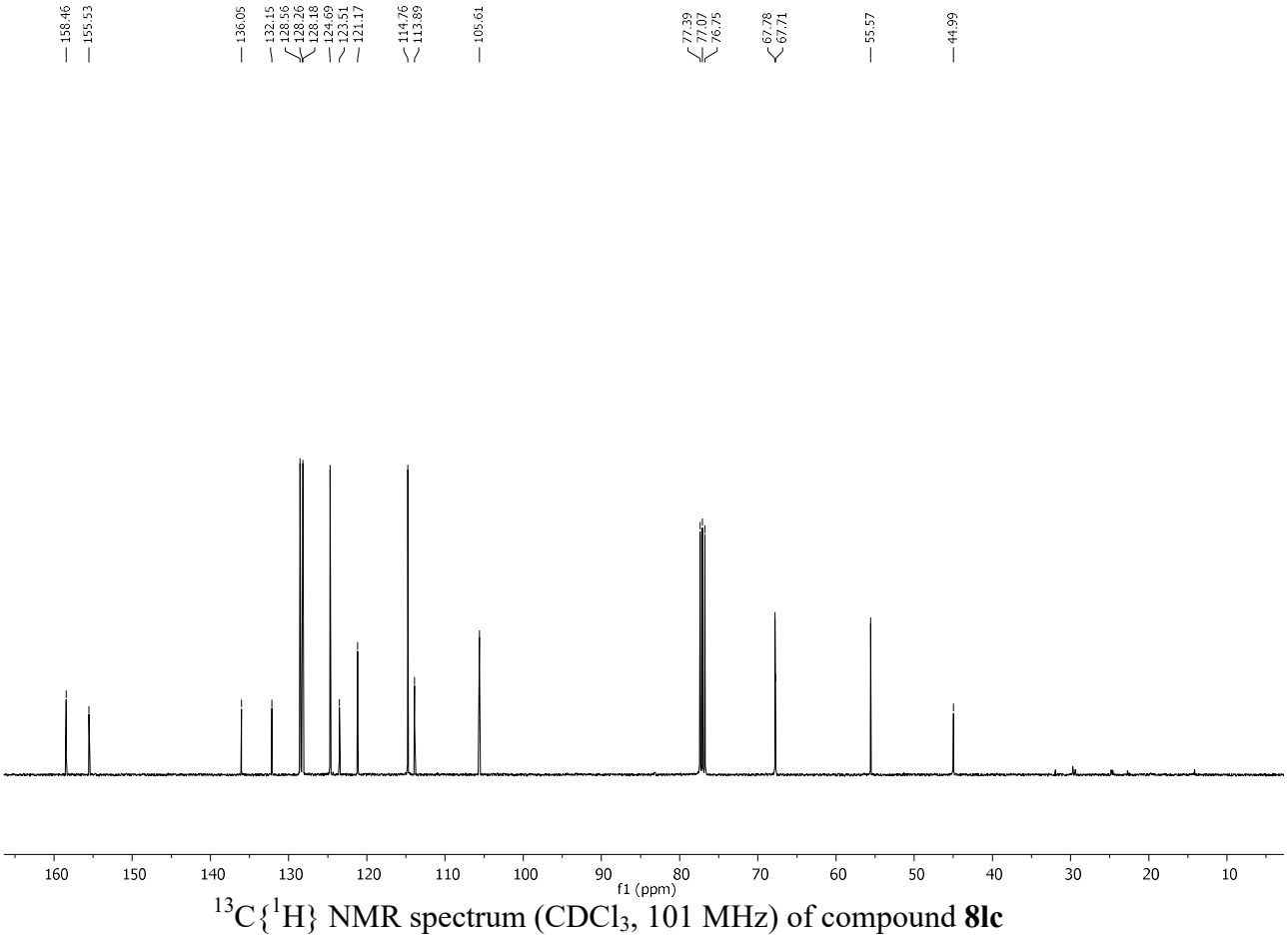
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound **8lb**



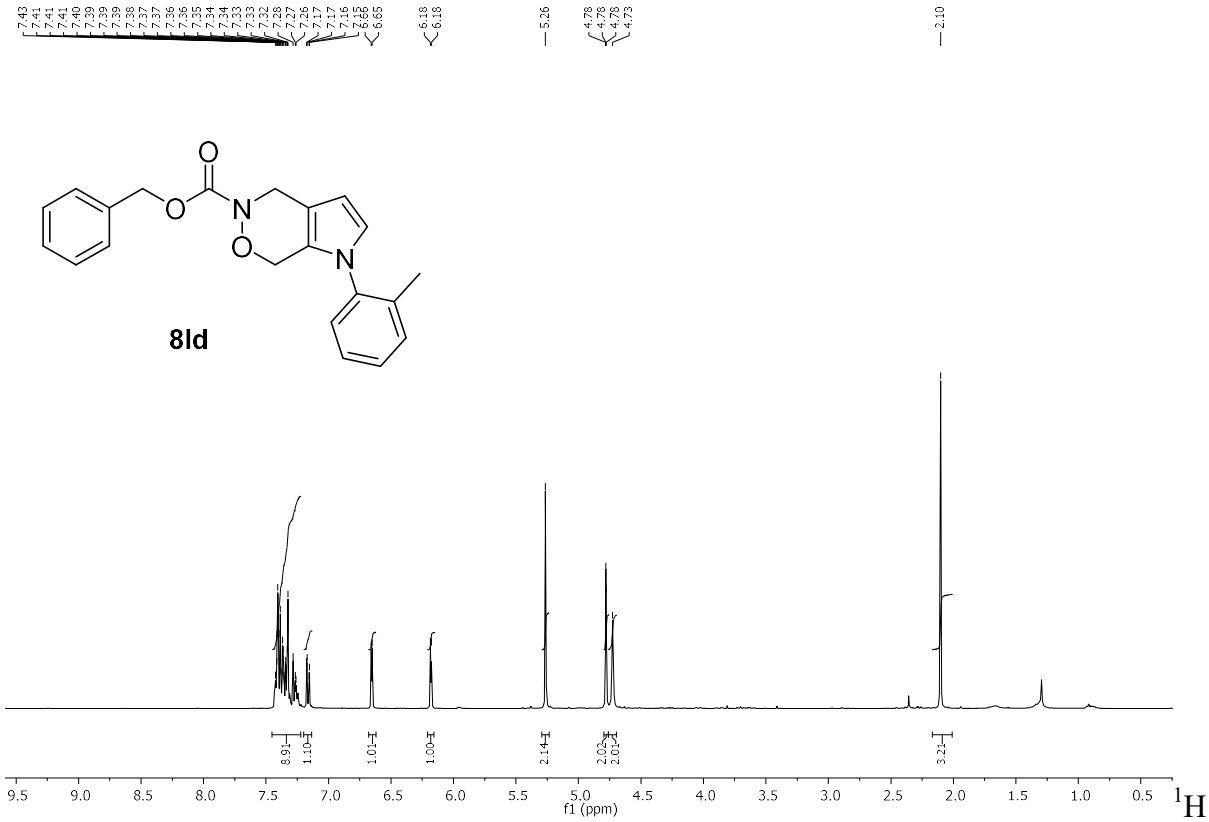
^{13}C{^{1}H} NMR spectrum ($CDCl_3$, 101 MHz) of compound **8lb**



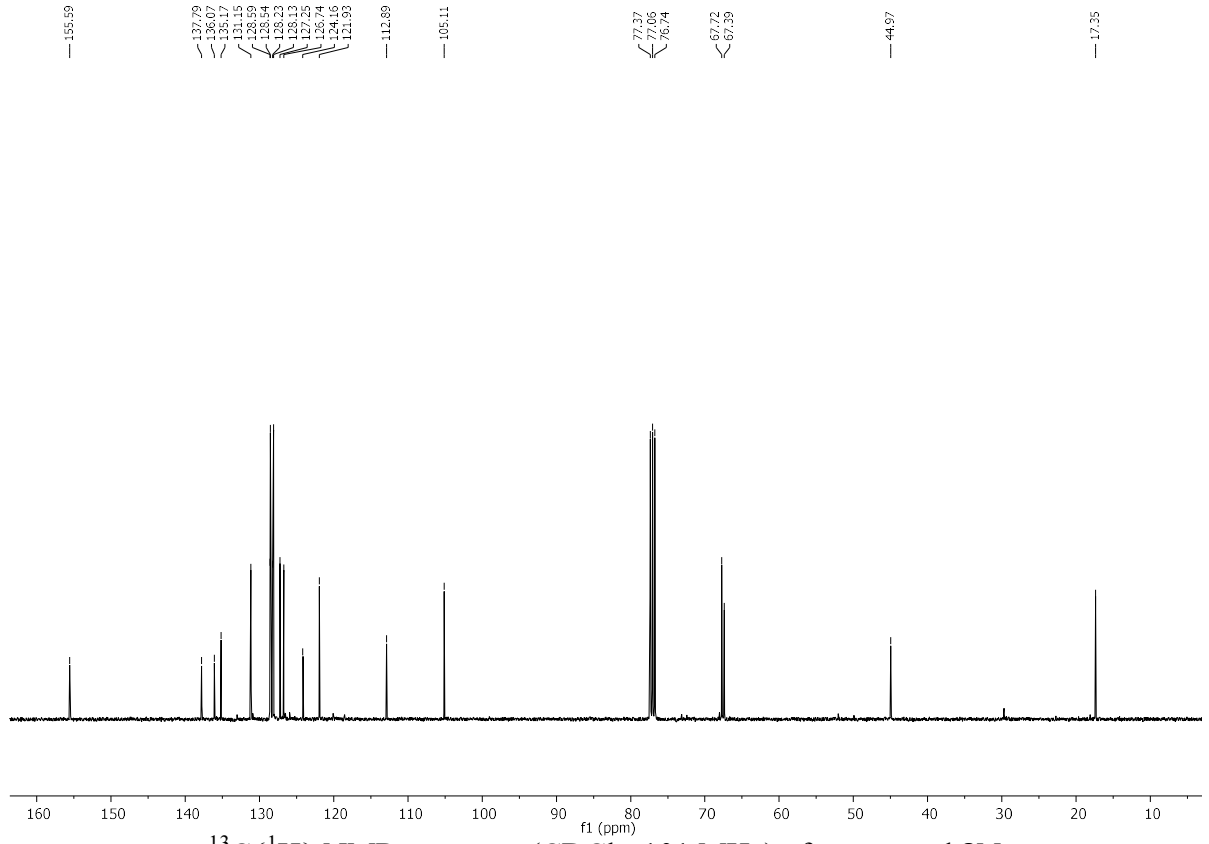
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound **8lc**



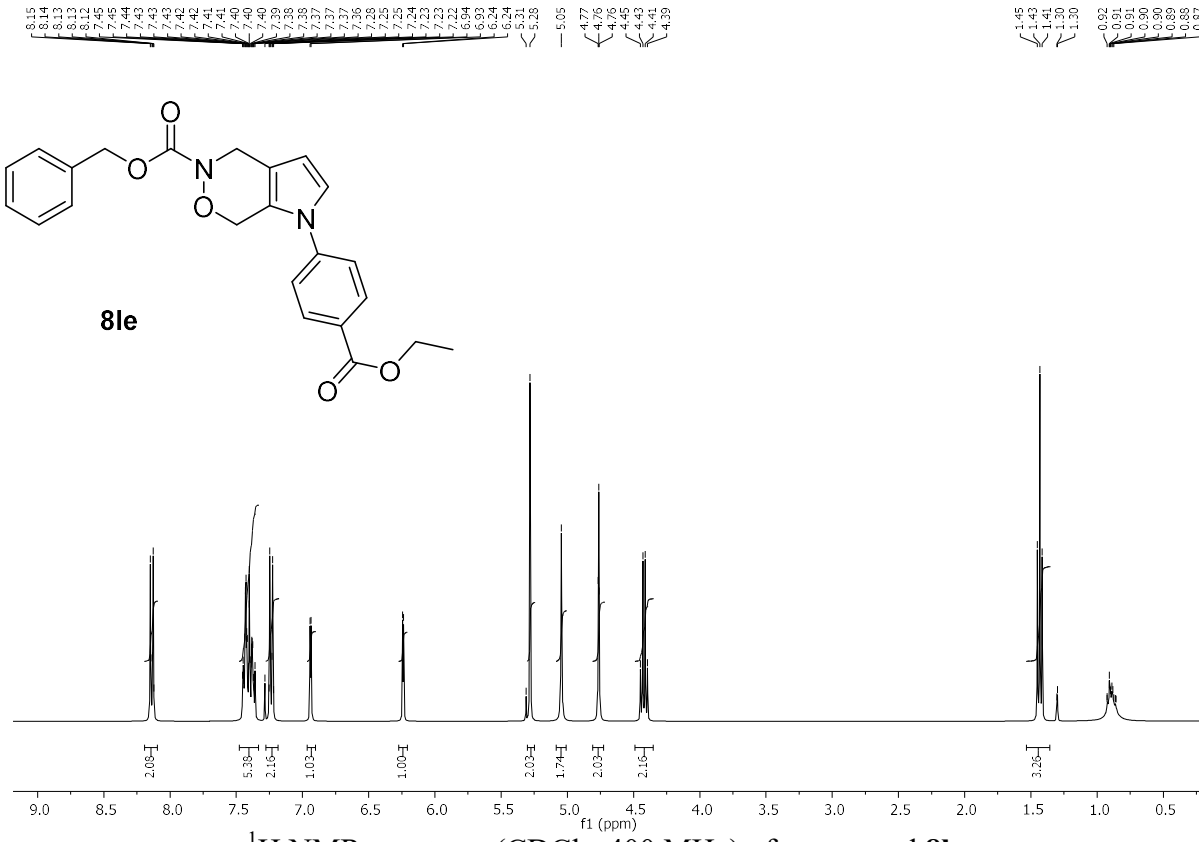
^{13}C{^{1}H} NMR spectrum ($CDCl_3$, 101 MHz) of compound **8lc**



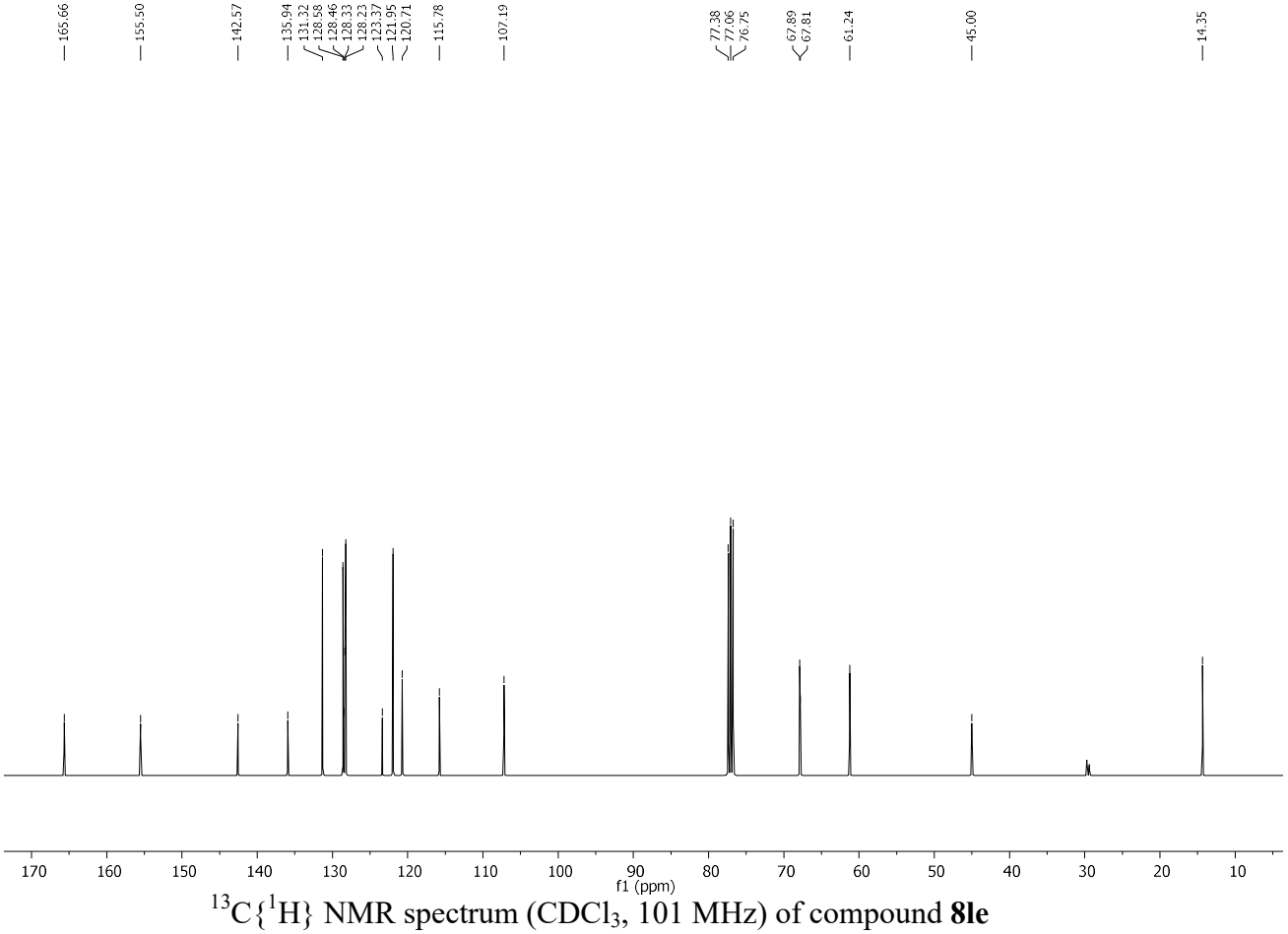
NMR spectrum ($CDCl_3$, 400 MHz) of compound **8ld**



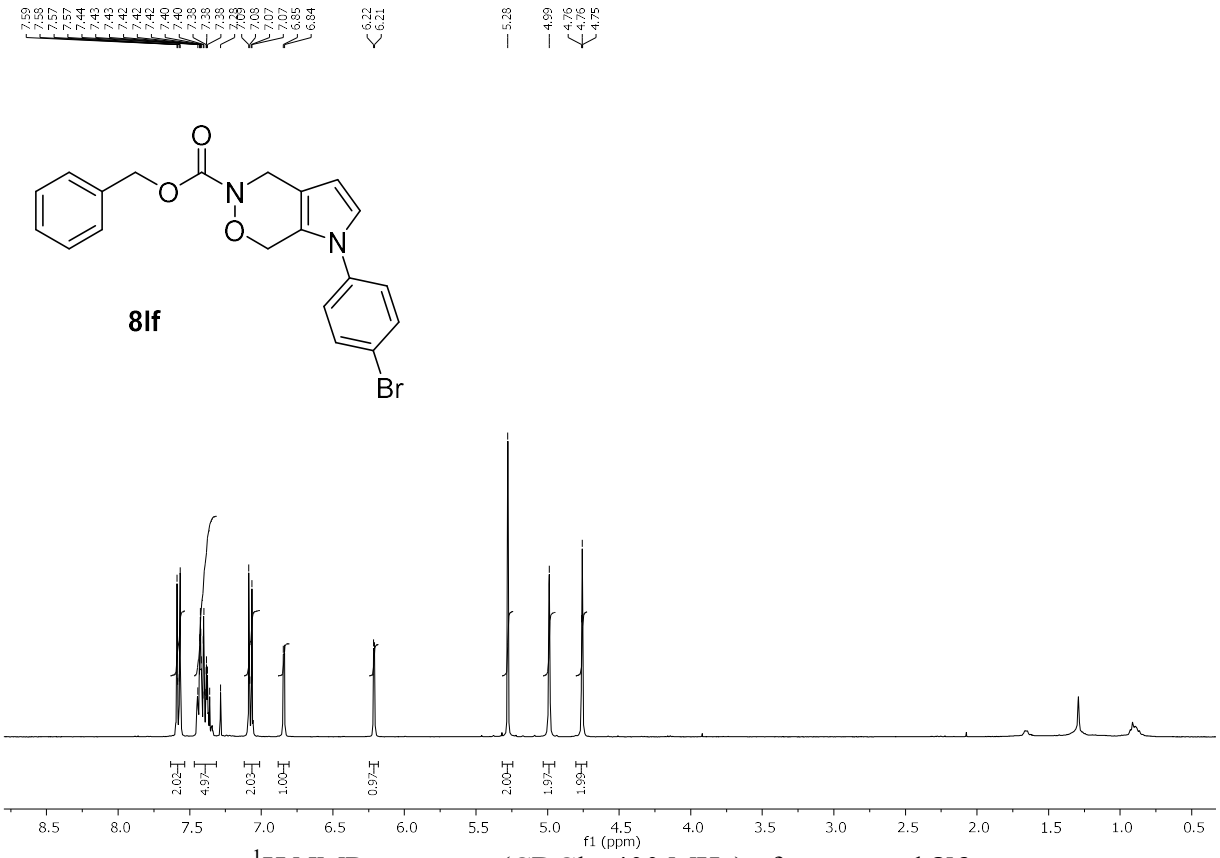
$^{13}C\{^1H\}$ NMR spectrum ($CDCl_3$, 101 MHz) of compound **8ld**



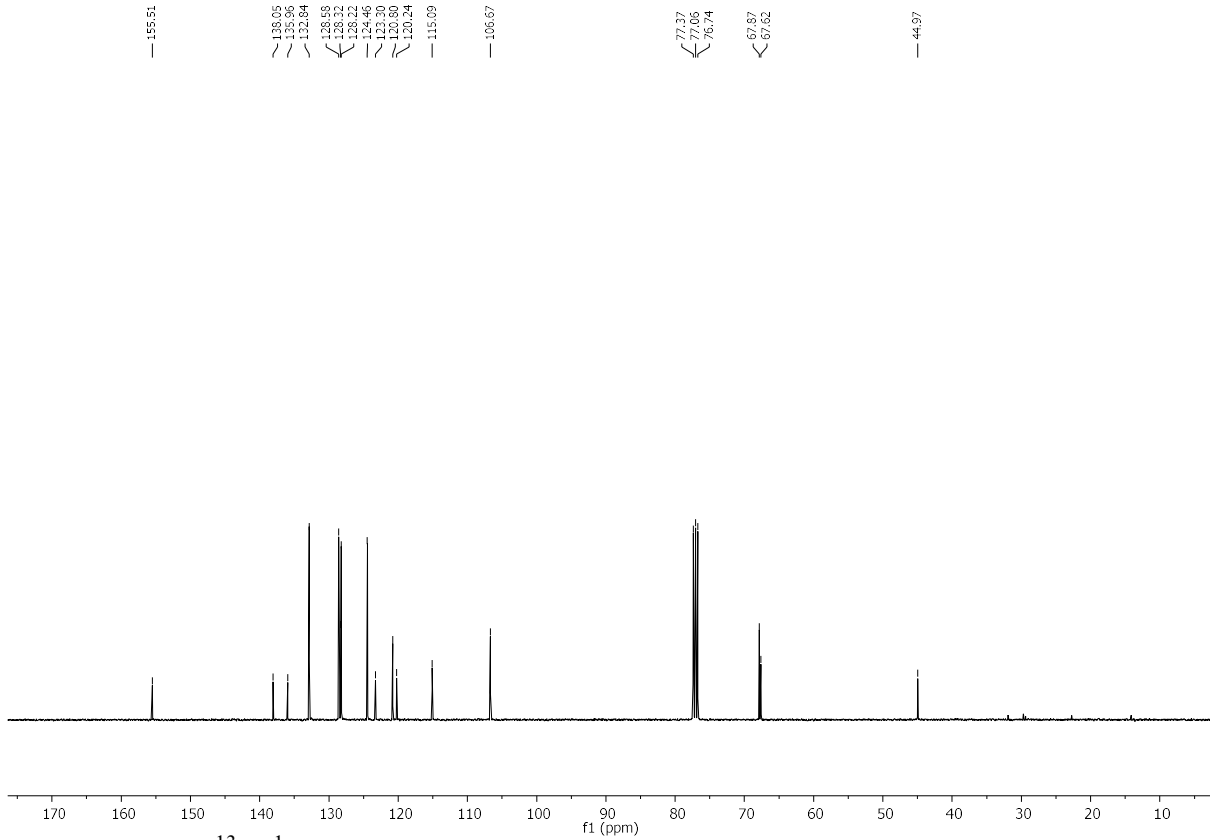
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound **8le**



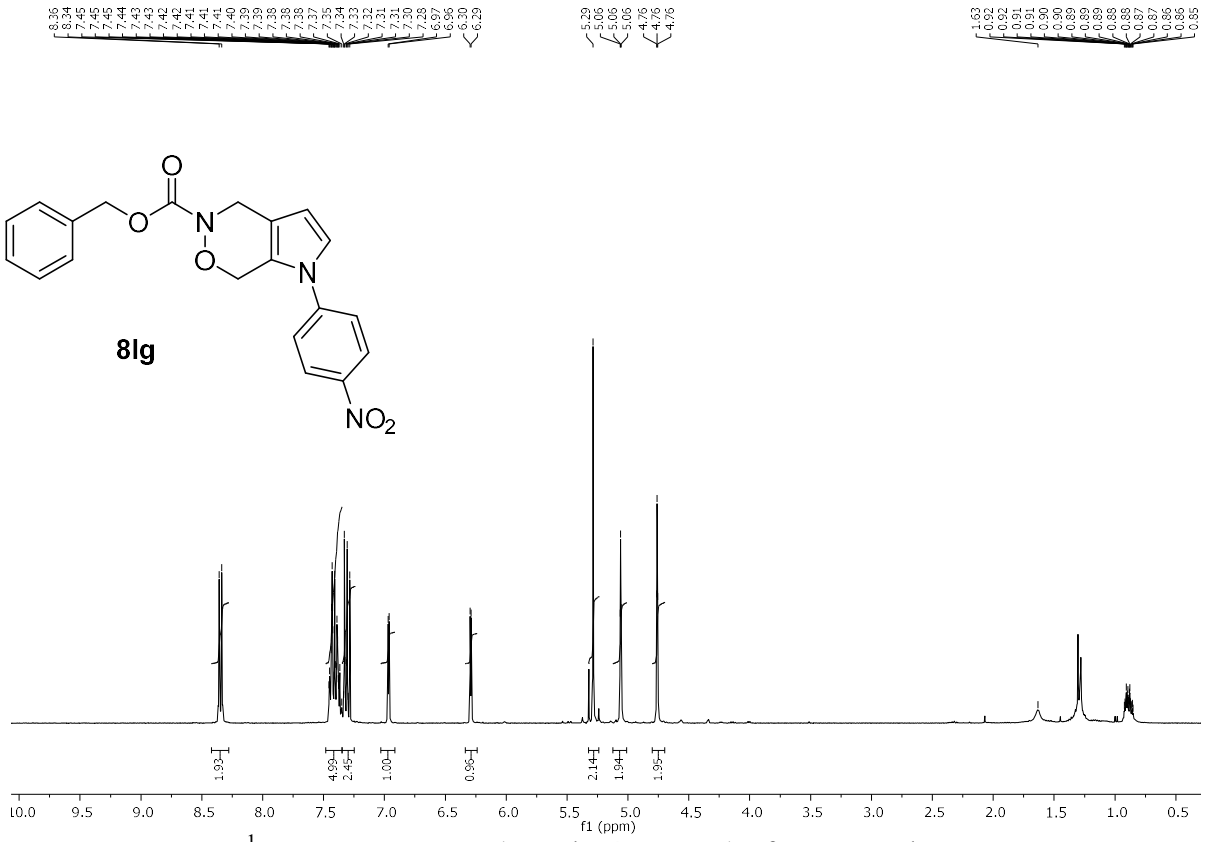
^{13}C{^{1}H} NMR spectrum ($CDCl_3$, 101 MHz) of compound **8le**



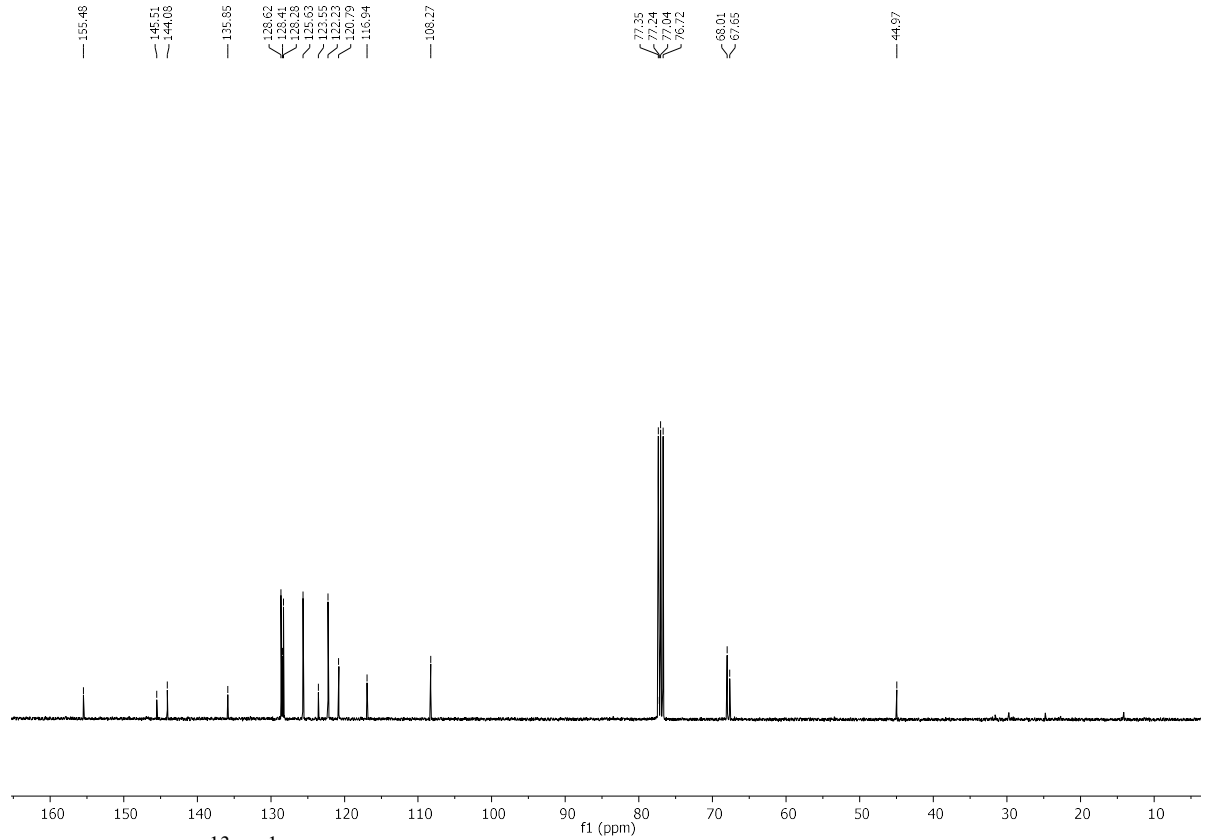
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound **8lf**



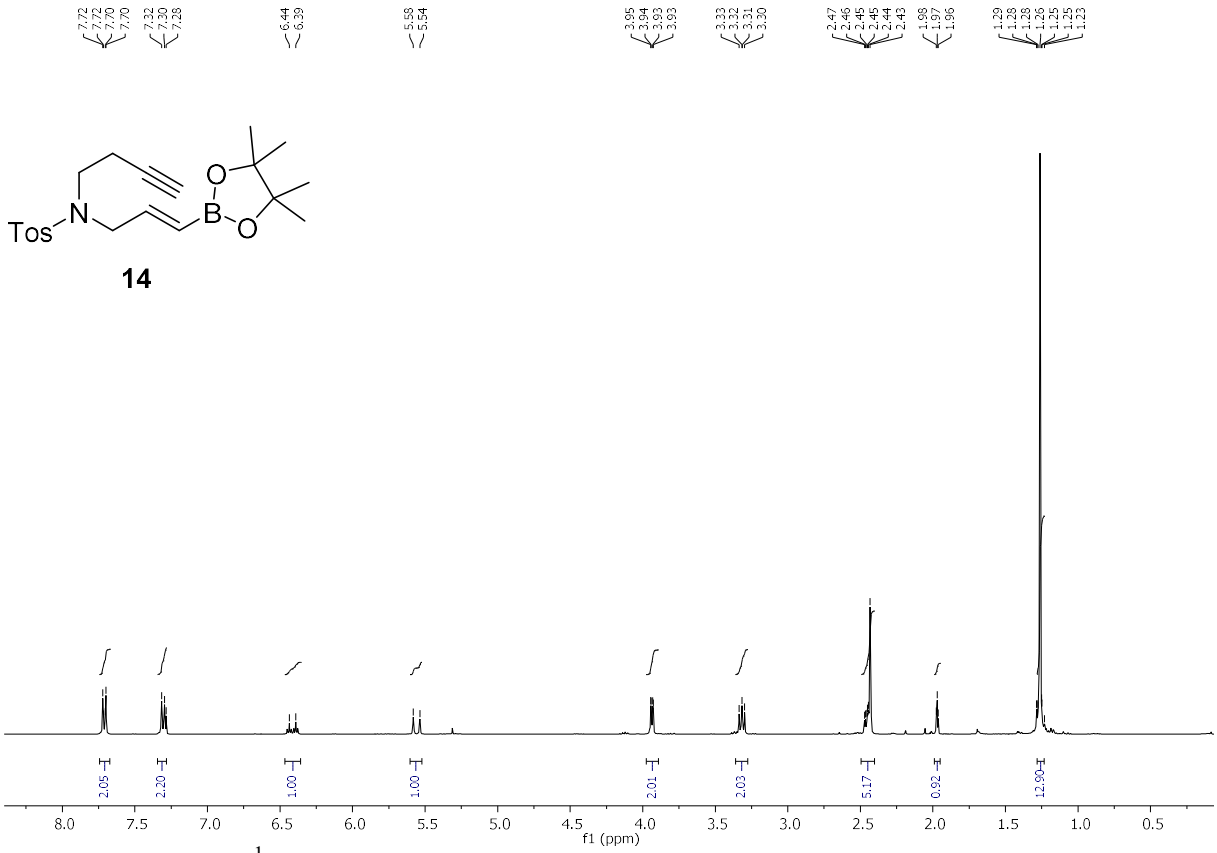
$^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$, 101 MHz) of compound **8lf**



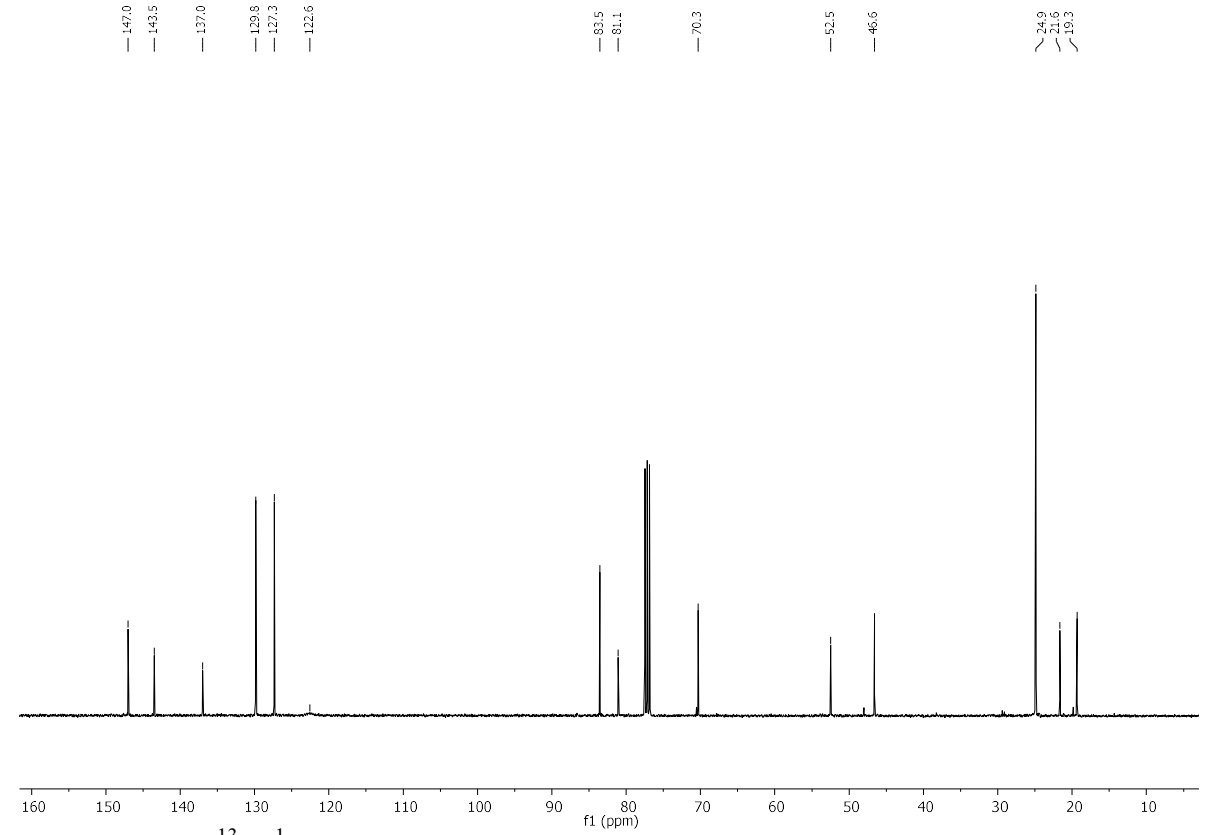
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound **8lg**



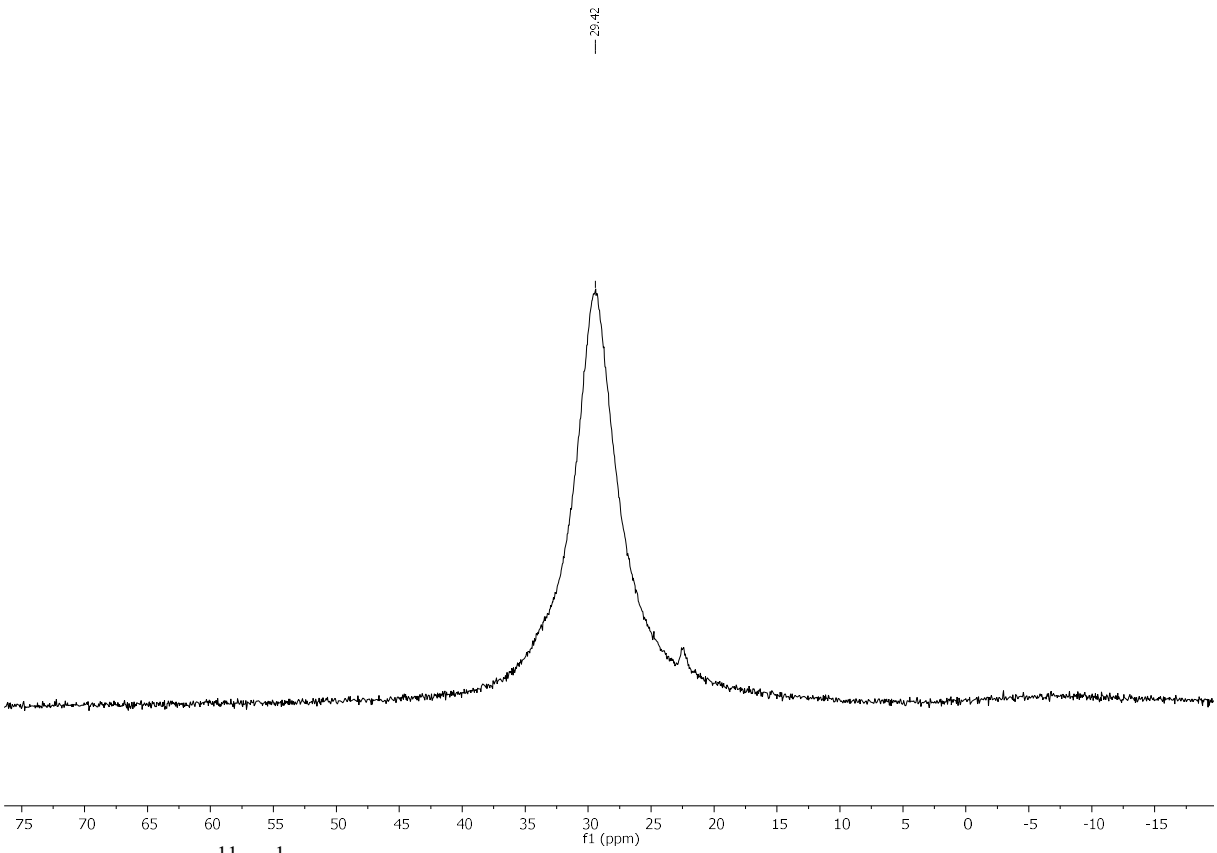
$^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$, 101 MHz) of compound **8lg**



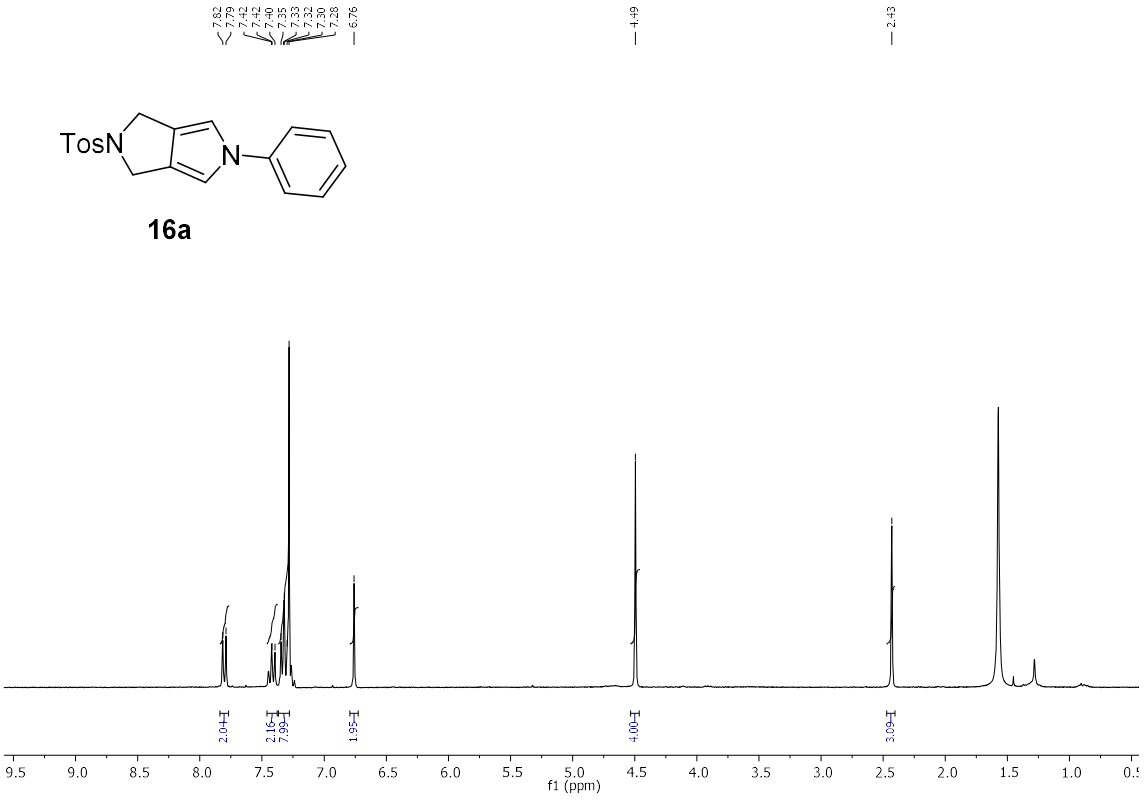
^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound **14**



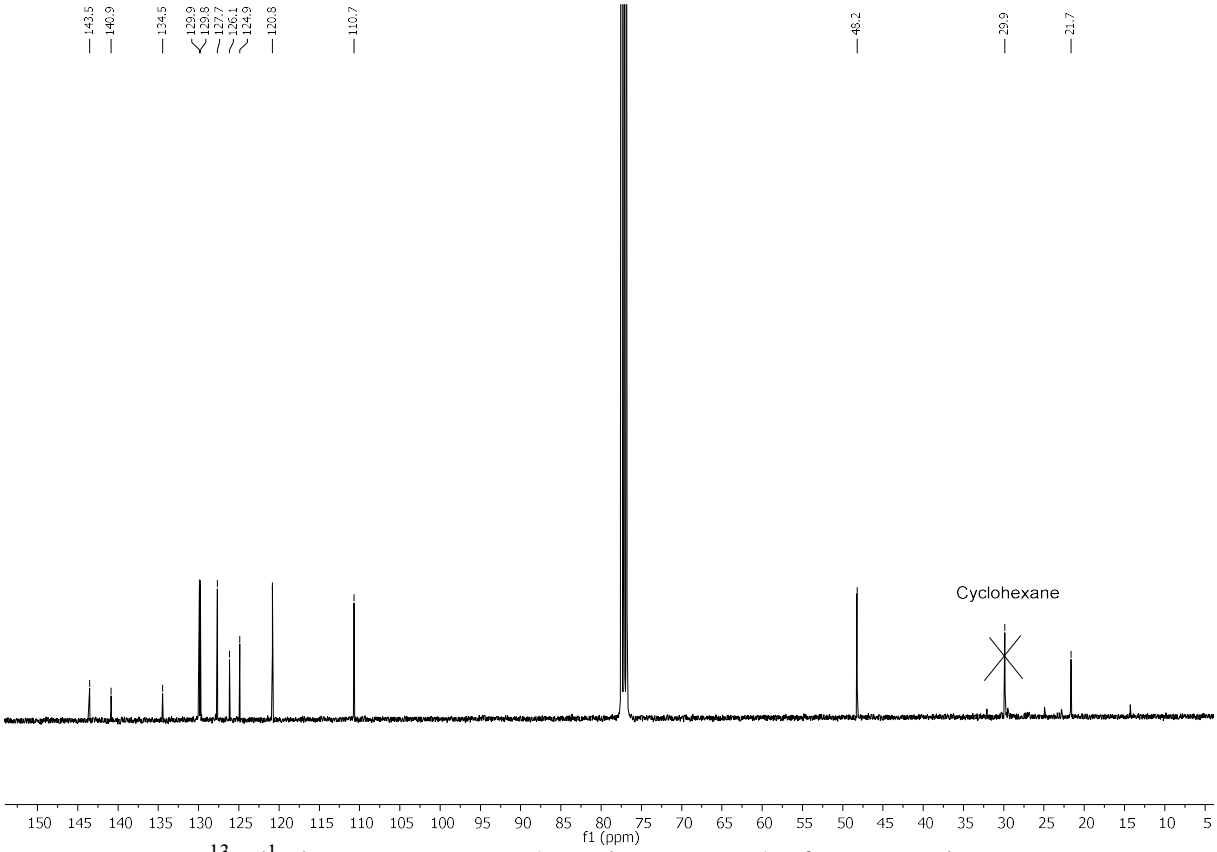
^{13}C{^{1}H} NMR spectrum ($CDCl_3$, 101 MHz) of compound **14**



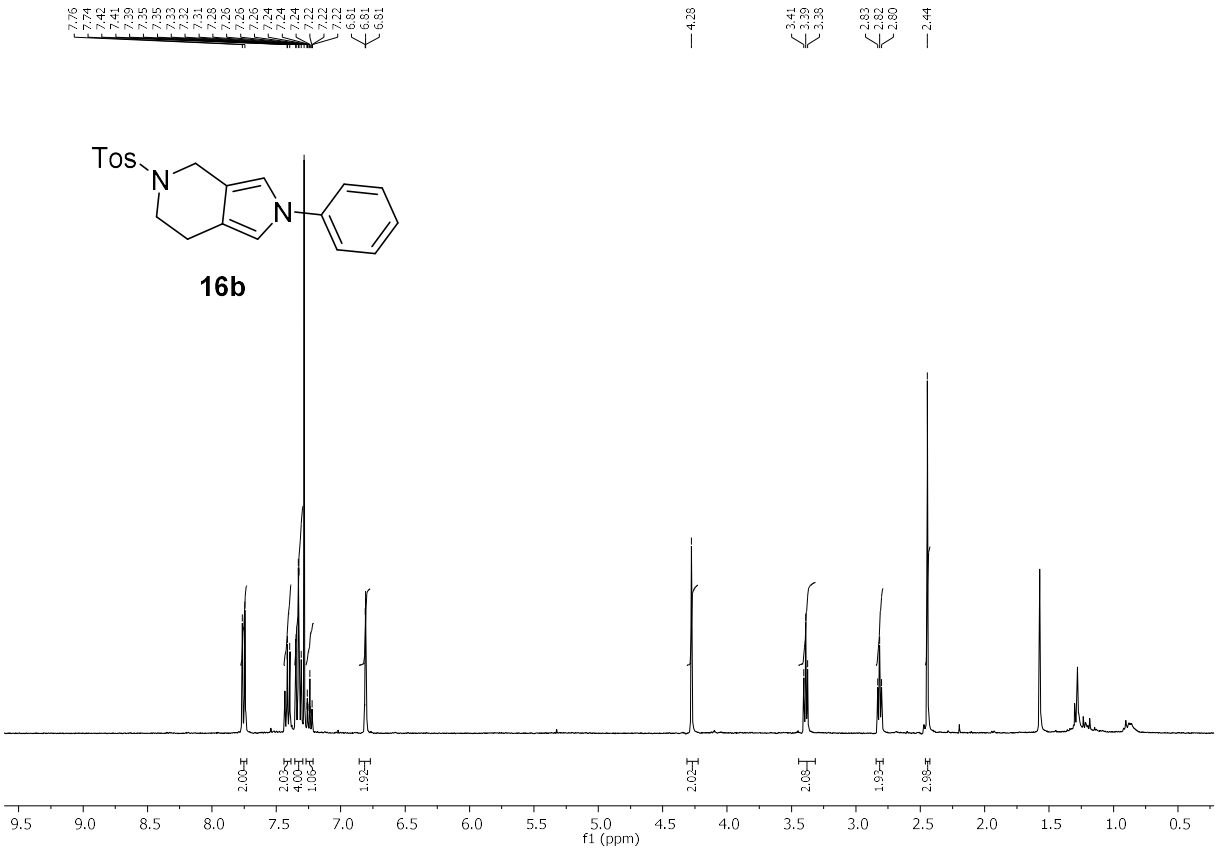
$^{11}B\{^{1}H\}$ NMR spectrum ($CDCl_3$, 128 MHz) of compound **14**



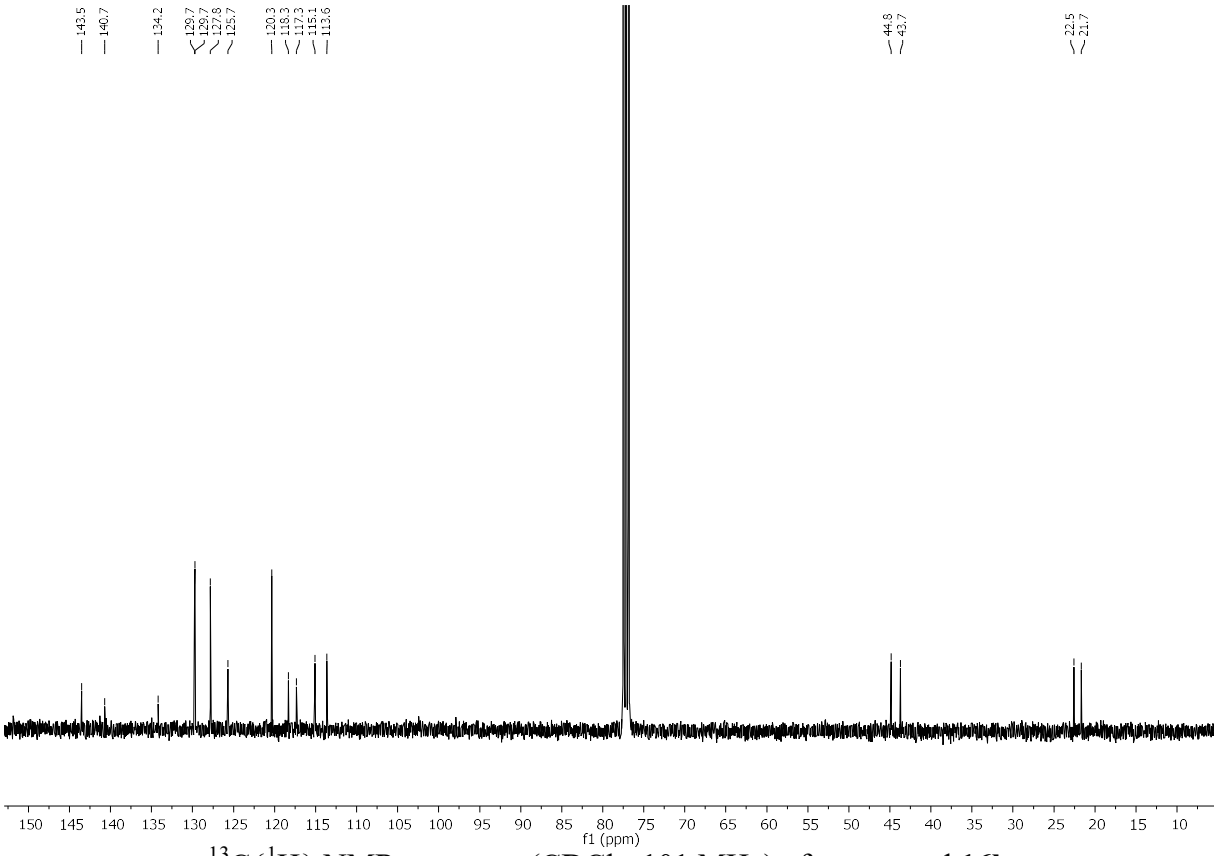
^{1}H NMR spectrum ($CDCl_3$, 300 MHz) of compound **16a**



^{13}C{^{1}H} NMR spectrum ($CDCl_3$, 101 MHz) of compound **16a**

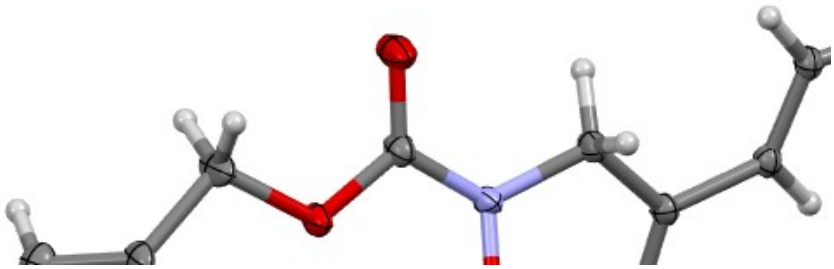


^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of compound **16b**



$^{13}C\{^{1}H\}$ NMR spectrum ($CDCl_3$, 101 MHz) of compound **16b**

Single crystal X-ray crystal structure of 7l



Thermal ellipsoids are shown at the 50% probability level

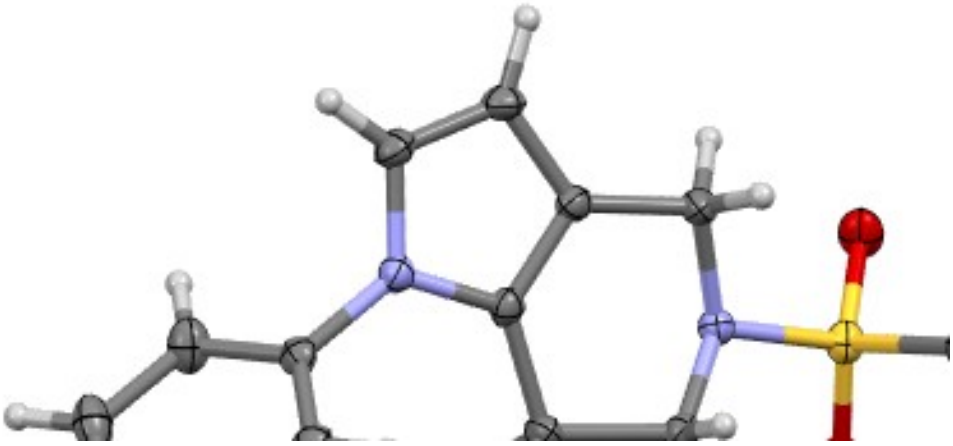
A suitable crystal obtained by slow evaporation of a methylene chloride solution of **7l** was selected and measured on a D8V_Mo diffractometer. The crystal was kept at 120 K during data collection. Using Olex2,[1] the structure was solved with the ShelXS structure solution program, using Direct Methods and refined with the ShelXL refinement package using Least Squares minimisation.[2]

Table. Crystal data and structure refinement.

Empirical formula	$C_{20}H_{26}BNO_5$
Formula weight	371.23
Temperature/K	120
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	12.8072(10)
b/Å	10.7432(9)
c/Å	14.2090(11)
α/°	90
β/°	98.573(3)
γ/°	90
Volume/Å^3	1933.2(3)
Z	4
ρ_{calc}g/cm^3	1.275
μ/mm^{-1}	0.090

F(000)	792.0
Crystal size/mm^3	0.316 × 0.311 × 0.257
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.64 to 61.886
Index ranges	-18 ≤ h ≤ 18, -15 ≤ k ≤ 15, -20 ≤ l ≤ 20
Reflections collected	44140
Independent reflections	6129 [R_{int} = 0.0325, R_{sigma} = 0.0206]
Data/restraints/parameters	6129/2/256
Goodness-of-fit on F^2	1.038
Final R indexes [I>=2σ (I)]	R_1 = 0.0455, wR_2 = 0.1184
Final R indexes [all data]	R_1 = 0.0543, wR_2 = 0.1247
Largest diff. peak/hole / e Å^{-3}	0.56/-0.34

Single crystal X-ray crystal structure of 8ga



Thermal ellipsoids are shown at the 50% probability level

A suitable crystal obtained by slow evaporation of a methylene chloride solution of **8ga** was selected and measured on a D8V_Mo diffractometer. The structure was solved by dual-space algorithm using the *SHELXT* program,[1] and then refined with full-matrix least-squares methods based on F^2 (*SHELXL*).[2]

Table. Crystal data and structure refinement.

Empirical formula	$C_{20}H_{20}N_2O_2S$
Formula weight	352.44 g/mol
Temperature/K	150 *K*
Crystal system	monoclinic
Space group	*P* $2_1/n$
a/Å	10.986(4)
b/Å	9.394(3)
c/Å	17.213(7)
α/°	90
β/°	103.123(13)
γ/°	90
Volume/$Å^3$	1730.0(11)
Z	4
$\rho_{calc}g/cm^3$	1.353
μ/mm^{-1}	0.203
F(000)	744
Crystal size/mm^3	0.380 x 0.280 x 0.260
Radiation	MoKα (λ = 0.71073)
Θ range for data collection/°	2.430 to 27.596
Index ranges	-14 ≤ h ≤ 14, -12 ≤ k ≤ 9, -22 ≤ l ≤ 22
Reflections collected / unique	24935 / 3974 [R(int)[a] = 0.1128]
Reflections [I>2σ]	2808
Data/restraints/parameters	3974 / 0 / 226
Goodness-of-fit on F^2	1.003
Final R indexes [I>=2σ]	$R1^c$ = 0.0486, $wR2^d$ = 0.1071
Final R indexes [all data]	$R1^c$ = 0.0852, $wR2^d$ = 0.1244
Largest diff. peak/hole / e^-. $Å^{-3}$	0.311 and -0.446

[1] Dolomanov, O. V.; Bourhis, L. J.; Gildea, R. J.; Howard, J. A. K.; Puschmann, H. *J. Appl. Cryst.* **2009**, *42*, 339.
[2] Sheldrick G. M. *Acta Cryst. A64*, **2008**, *64*, 112.