Supporting Information

Diversity Oriented Synthesis of Densely Substituted Pyrrolo[1,2-*a*]indoles

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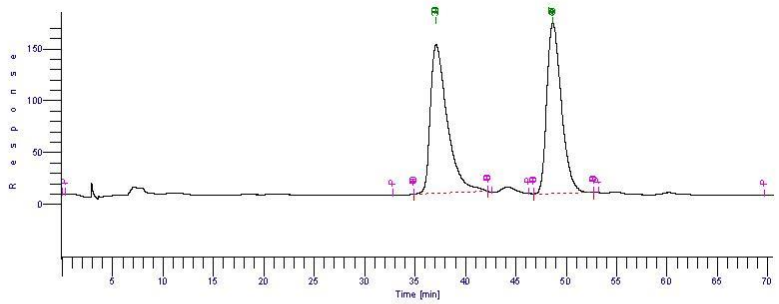
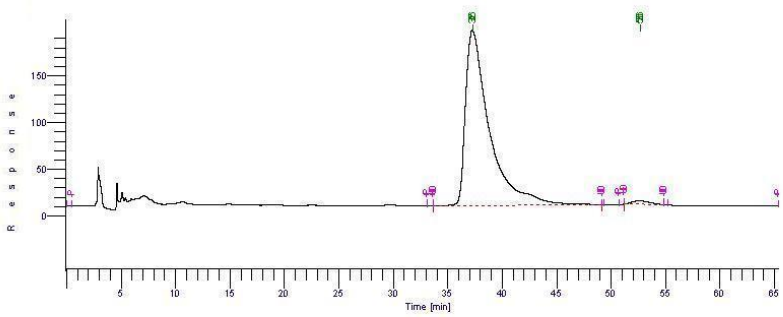


cellulose-2

Peak #	Component Name	Time [min]	Area [uV*sec]	Height [uV]	Area [%]	Norm. Area [%]
1		37.093	16733976.98	143785.84	50.39	50.39
2		48.672	16474158.60	164645.38	49.61	49.61
			33208135.58	308431.22	100.00	100.00

HPLC graph of compound (±)-19

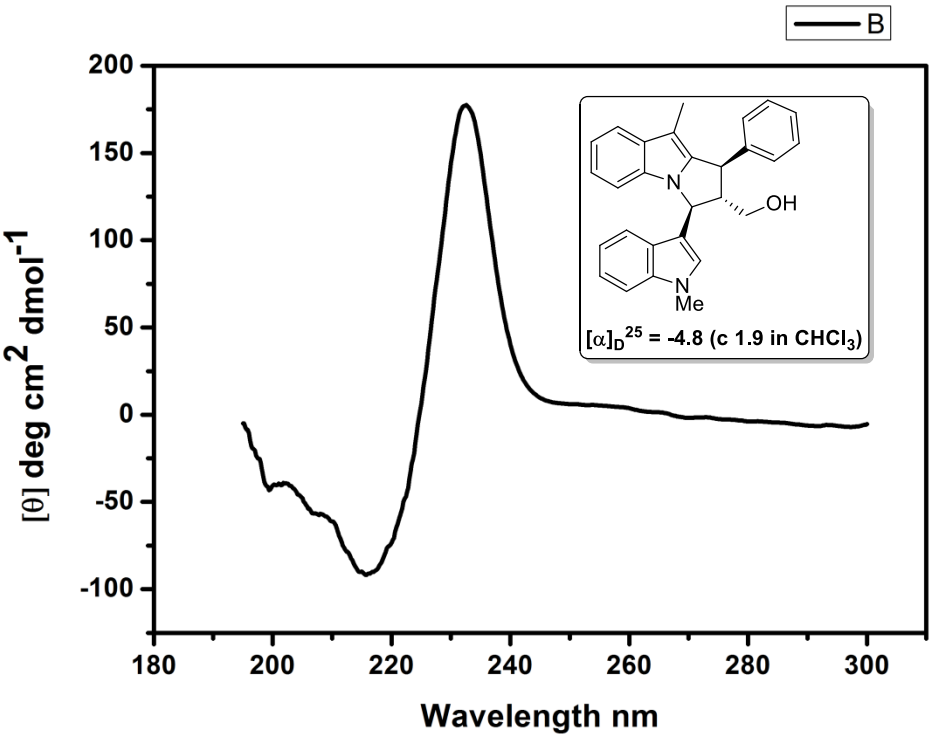


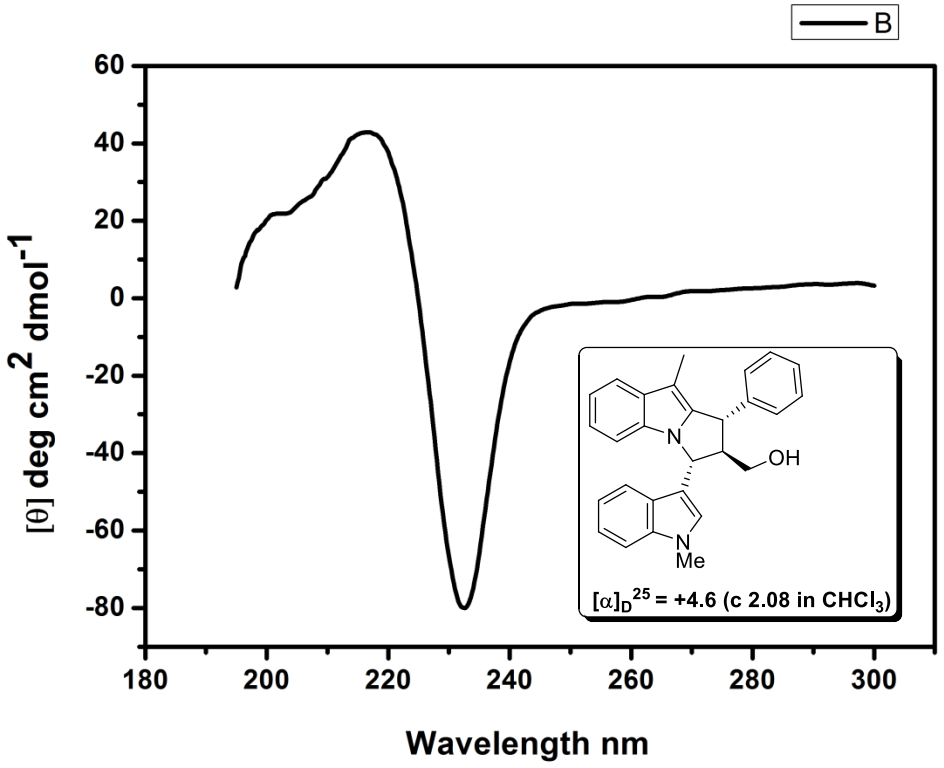
cellulose-2 ,chiral

Peak #	Component Name	Time [min]	Area [uV*sec]	Height [uV]	Area [%]	Norm. Area [%]
1		37.258	28589734.77	187597.01	98.54	98.54
2		52.657	424982.19	3771.33	1.46	1.46
			29014716.96	191368.34	100.00	100.00

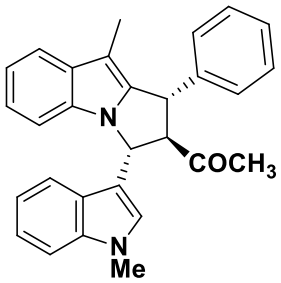
HPLC graph of compound (-)-19 (enantio enriched)

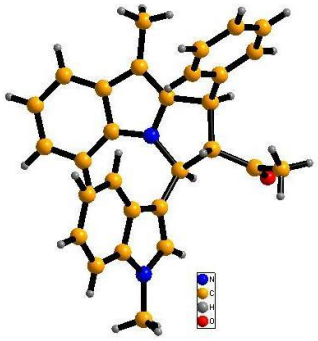
CD spectras of Compound (+)-19 and (-)-19





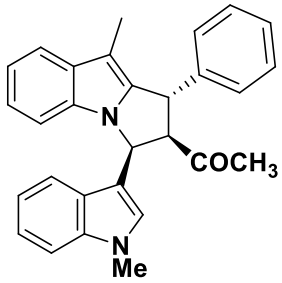
Crystal data and structure refinement for compound 8e

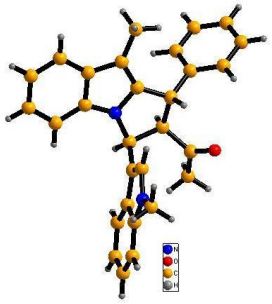




Chemical formula	$C_{29}H_{26}N_2O$
M_r	418.52
Crystal system, space group	Triclinic, P-1
Temperature (K)	100
a, *b*, *c* (Å)	9.500 (5), 11.269 (5), 12.113 (6)
α, β, γ (°)	111.974 (7), 97.280 (8), 101.443 (7)
V (Å^3)	1149.5 (10)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	0.07
Crystal size (mm)	0.16 × 0.14 × 0.11
Data collection	
Diffractometer	Bruker *SMART APEX* diffractometer
Absorption correction	Empirical (using intensity measurements) *SADABS*
T_{min}, T_{max}	0.928, 0.992
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6059, 4117, 2535
R_{int}	0.018
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.600
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.055, 0.204, 0.89
No. of reflections	4117
No. of parameters	292
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.21, −0.19

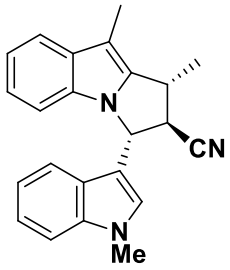
Compound 8e'

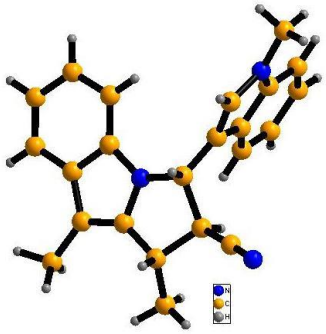




Chemical formula	$C_{29}H_{26}N_2O$
M_r	418.52
Crystal system, space group	Triclinic, P -1
Temperature (K)	100
a, *b*, *c* (Å)	9.752 (14), 11.395 (16), 12.462 (17)
α, β, γ (°)	105.79 (3), 107.47 (2), 99.95 (2)
V (Å^3)	1221 (3)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.07
Crystal size (mm)	0.12 × 0.11 × 0.10
Data collection	
Diffractometer	Bruker *SMART APEX* diffractometer
Absorption correction	Empirical (using intensity measurements) *SADABS*
T_{min}, T_{max}	0.992, 0.993
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6439, 4379, 1961
R_{int}	0.031
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.600
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.069, 0.230, 0.84
No. of reflections	4379
No. of parameters	292
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.25, −0.21

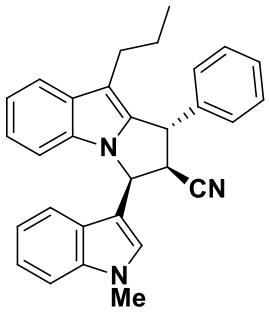
Compound 10d

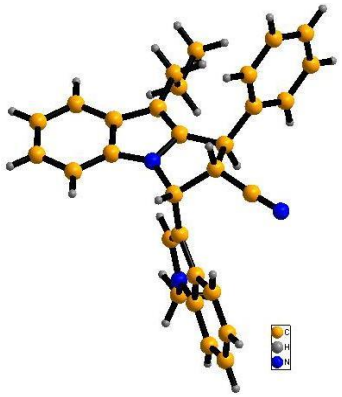




Chemical formula	$C_{23}H_{21}N_3$
M_r	339.43
Crystal system, space group	Monoclinic, C 2/c
Temperature (K)	100
a, *b*, *c* (Å)	19.869 (9), 8.329 (3), 23.300 (9)
β (°)	110.432 (12)
V (Å^3)	3613 (2)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.07
Crystal size (mm)	0.15 × 0.13 × 0.12
Data collection	
Diffractometer	Bruker *SMART APEX* diffractometer
Absorption correction	Empirical (using intensity measurements) *SADABS*
T_{min}, T_{max}	0.989, 0.991
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9601, 3345, 2361
R_{int}	0.049
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.606
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.064, 0.195, 1.04
No. of reflections	3345
No. of parameters	247
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.53, −0.52

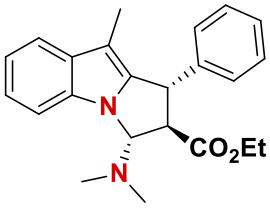
Compound 10b'

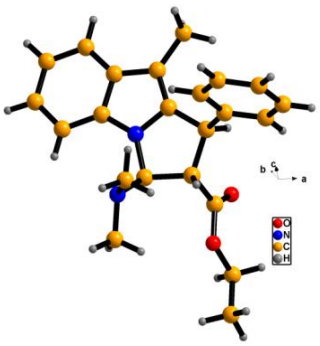




Chemical formula	$C_{30}H_{27}N_3$
M_r	429.55
Crystal system, space group	Orthorhombic, *Pbca*
Temperature (K)	100
a, *b*, *c* (Å)	9.0981 (18), 20.673 (4), 24.866 (5)
V (Å^3)	4677.0 (16)
Z	8
Radiation type	Mo *Kα*
μ (mm^{-1})	0.07
Crystal size (mm)	0.12 × 0.11 × 0.10
Data collection	
Diffractometer	Bruker *SMART APEX* diffractometer
Absorption correction	Empirical (using intensity measurements) *SADABS*
T_{min}, T_{max}	0.992, 0.993
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	25350, 4589, 2978
R_{int}	0.080
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.051, 0.150, 1.02
No. of reflections	4589
No. of parameters	300
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.24, −0.26

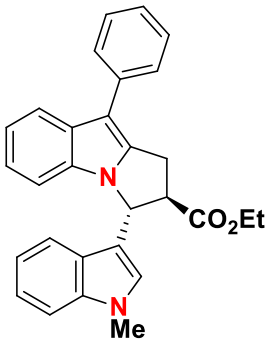
Compound 12d

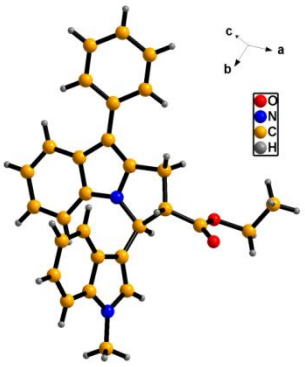




Chemical formula	$C_{23}H_{26}N_2O_2$
M_r	362.47
Crystal system, space group	Triclinic, P -1
Temperature (K)	100
a, *b*, *c* (Å)	7.845 (5), 9.525 (3), 14.475 (5)
α, β, γ (°)	102.857 (5), 103.298 (2), 104.067 (5)
V (Å^3)	975.6 (9)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	0.08
Crystal size (mm)	0.12 × 0.11 × 0.10
Data collection	
Diffractometer	Bruker *SMART APEX* diffractometer
Absorption correction	Empirical (using intensity measurements) *SADABS*
T_{min}, T_{max}	0.991, 0.992
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	12331, 3643, 2696
R_{int}	0.041
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.606
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.057, 0.168, 1.07
No. of reflections	3643
No. of parameters	244
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.60, −0.48

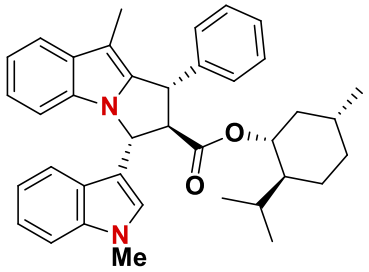
Compound 16h

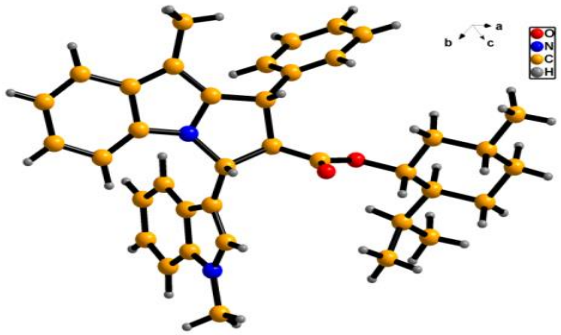




Chemical formula	$C_{29}H_{26}N_2O_2$
M_r	434.52
Crystal system, space group	Triclinic, P -1
Temperature (K)	100
a, *b*, *c* (Å)	9.929 (4), 10.675 (4), 12.143 (4)
α, β, γ (°)	90.655 (7), 113.506 (6), 109.344 (6)
V (Å^3)	1098.2 (7)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	0.08
Crystal size (mm)	0.20 × 0.20 × 0.17
Data collection	
Diffractometer	Bruker *SMART APEX* diffractometer
Absorption correction	Empirical (using intensity measurements) *SADABS*
T_{min}, T_{max}	0.984, 0.986
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5750, 3823, 3016
R_{int}	0.023
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.051, 0.150, 1.09
No. of reflections	3823
No. of parameters	300
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.23, −0.29

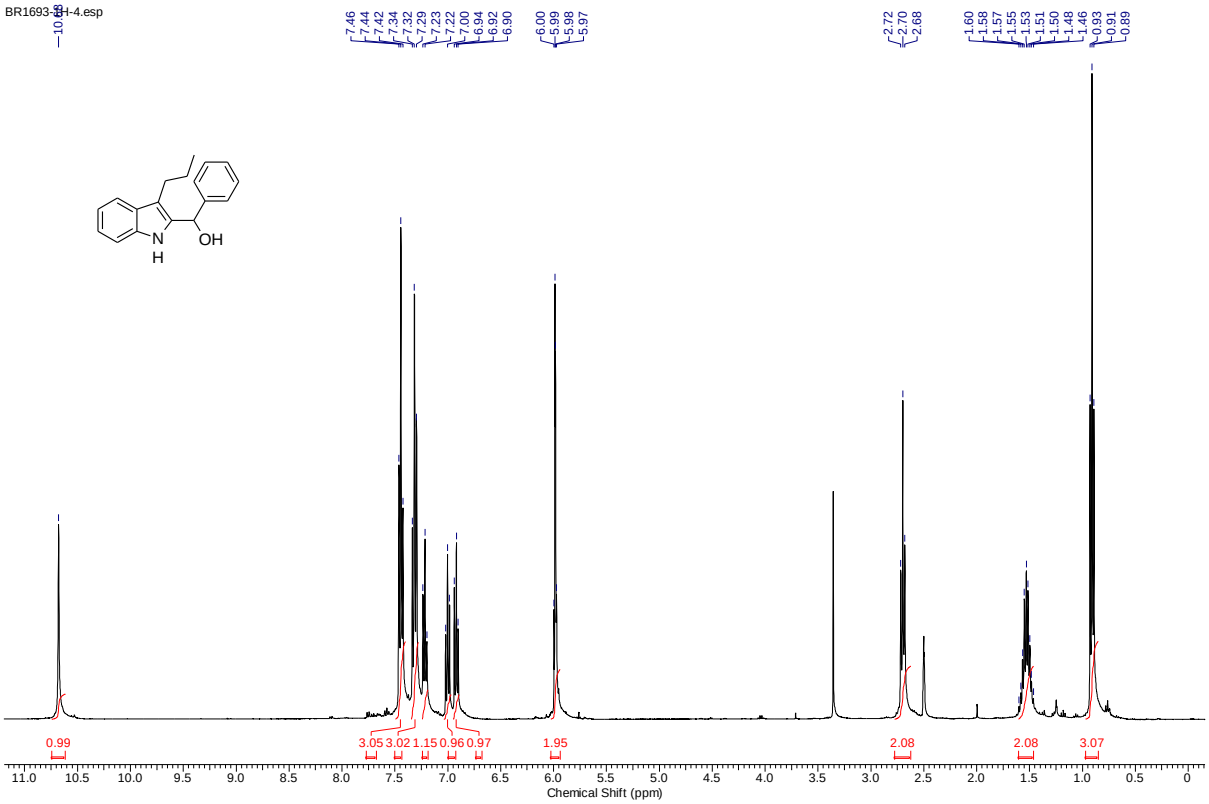
Compound 18c

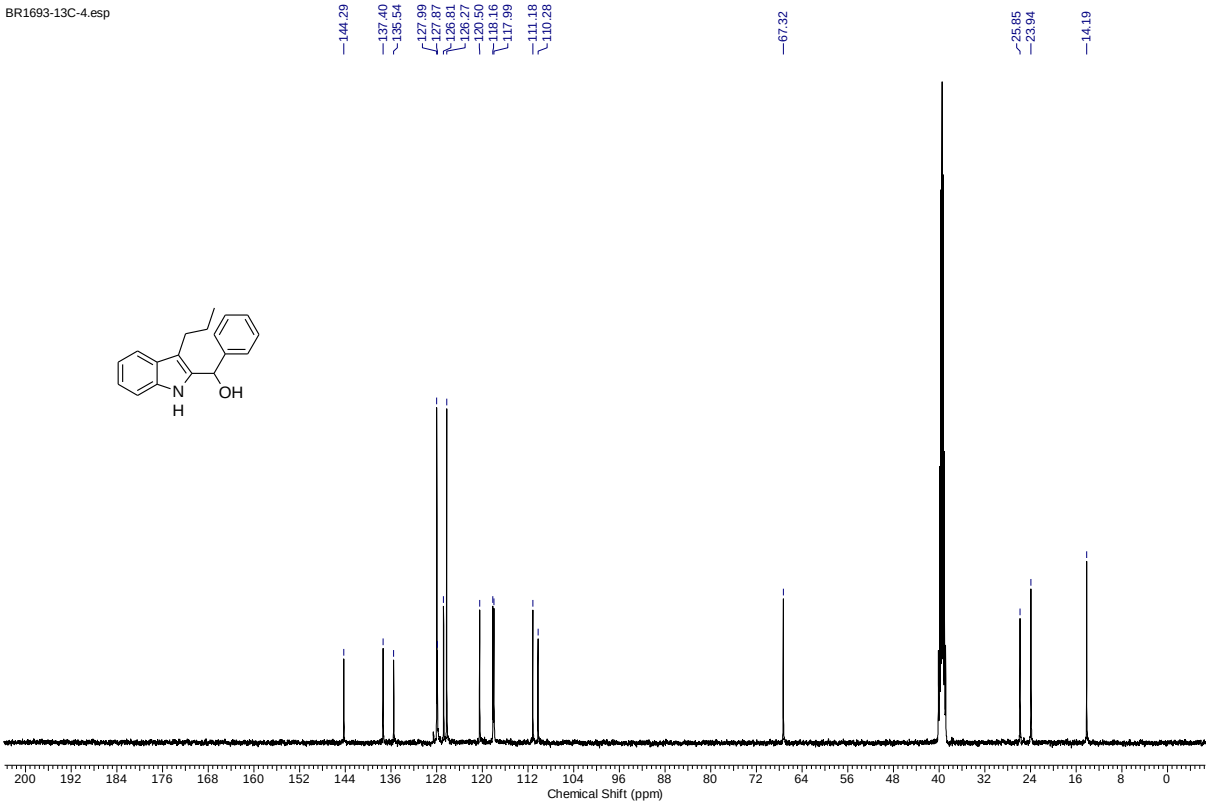




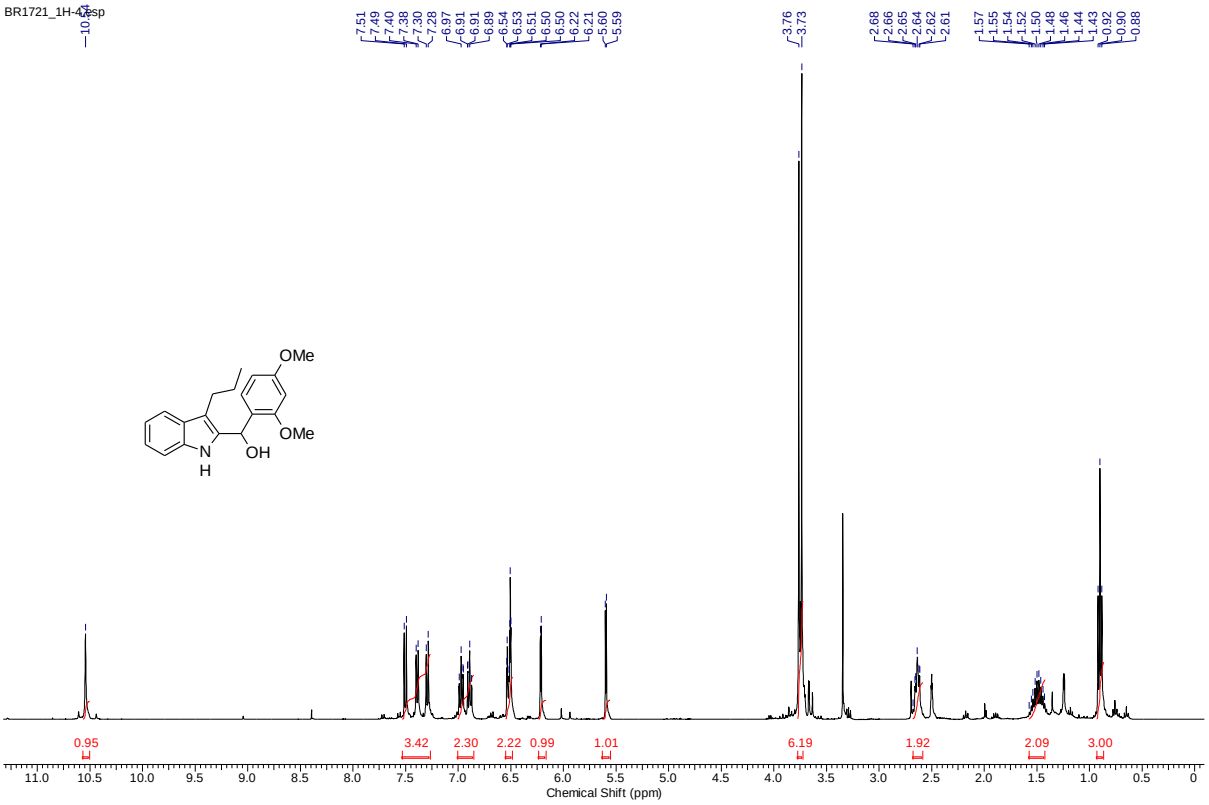
Chemical formula	$C_{38}H_{42}N_2O_2$
M_r	558.74
Crystal system, space group	Monoclinic, P 21
Temperature (K)	100
a, *b*, *c* (Å)	10.5253 (7), 19.4986 (12), 15.3673 (10)
β (°)	90.034 (2)
V (Å^3)	3153.8 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.07
Crystal size (mm)	0.25 × 0.23 × 0.21
Data collection	
Diffractometer	Bruker *SMART APEX* diffractometer
Absorption correction	Empirical (using intensity measurements) *SADABS*
T_{min}, T_{max}	0.982, 0.985
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	20849, 10249, 8489
R_{int}	0.098
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.588
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.137, 0.331, 1.08
No. of reflections	10249
No. of parameters	752
No. of restraints	1
H-atom treatment	H-atom parameters constrained
	$w = 1/[\sigma^2(F_o^2) + (0.0731P)^2 + 27.3416P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.53, −0.41
Absolute structure	Flack H D (1983), Acta Cryst. A39, 876-881
Absolute structure parameter	2 (4)

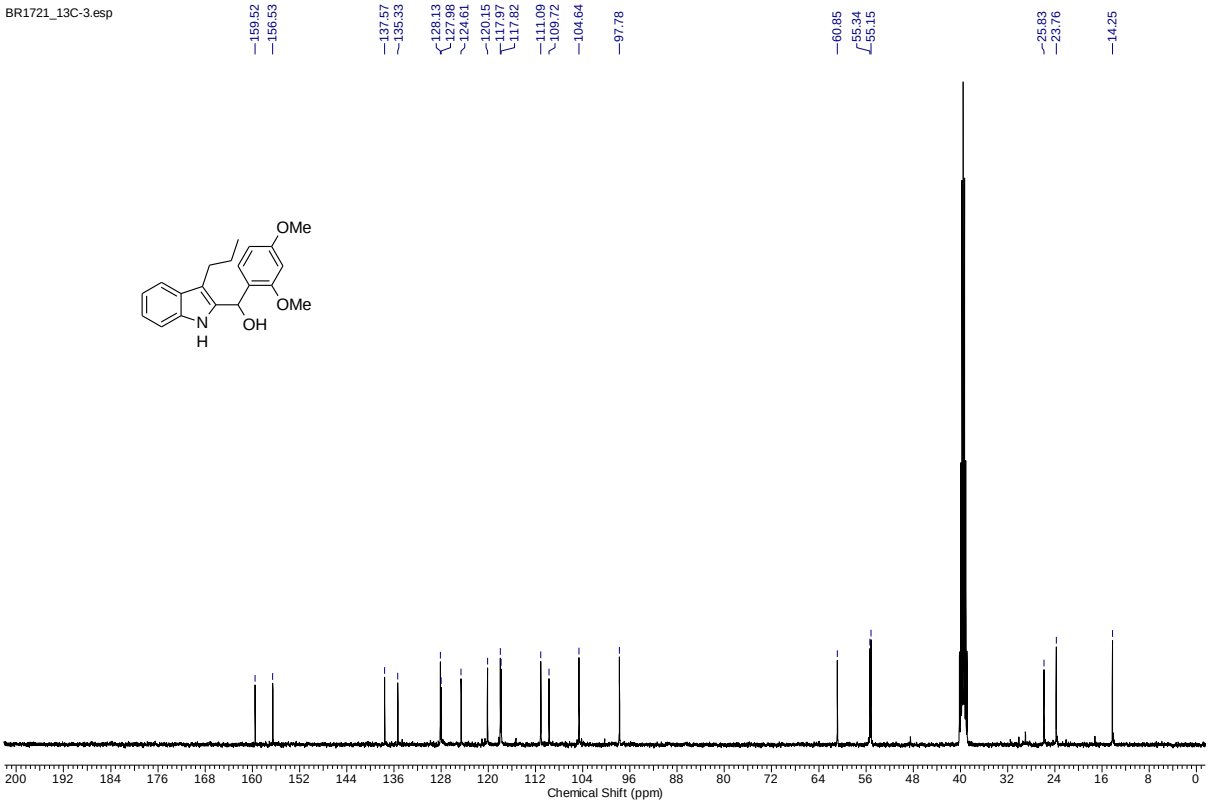
^{1}H and ^{13}C NMR of compound 4b



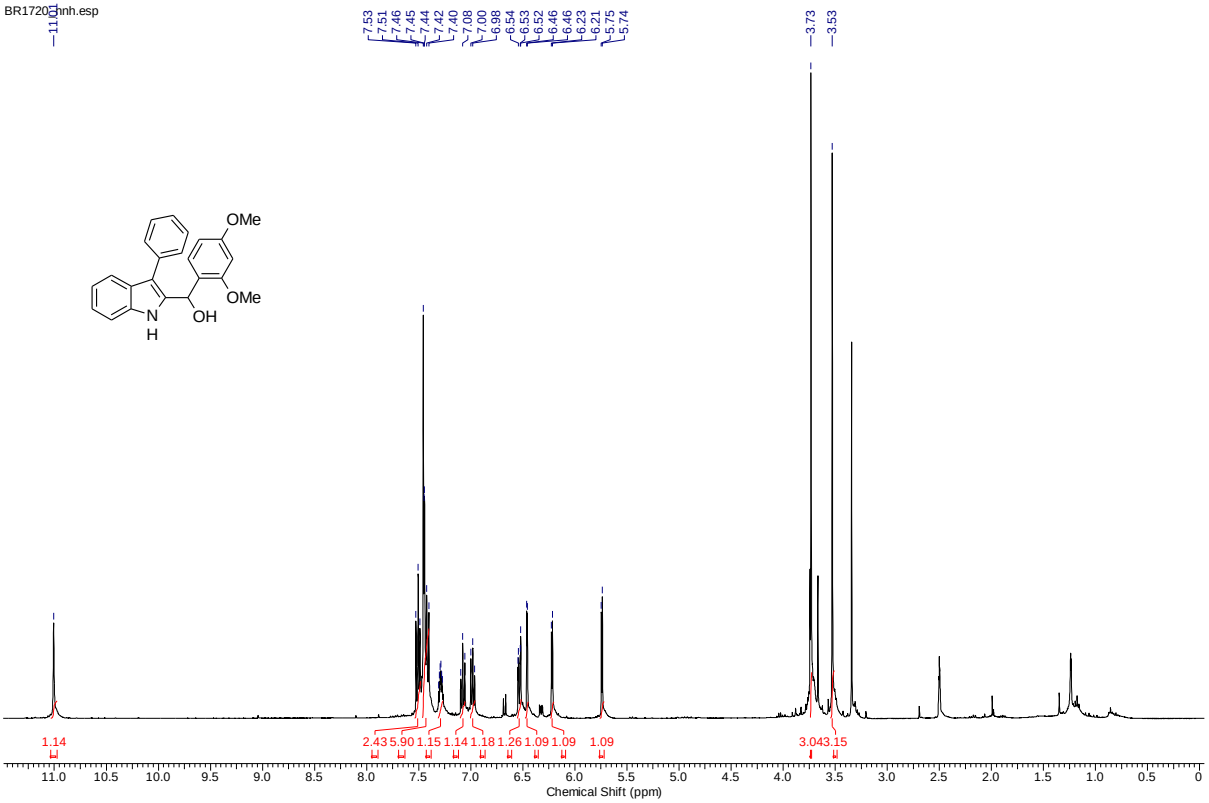


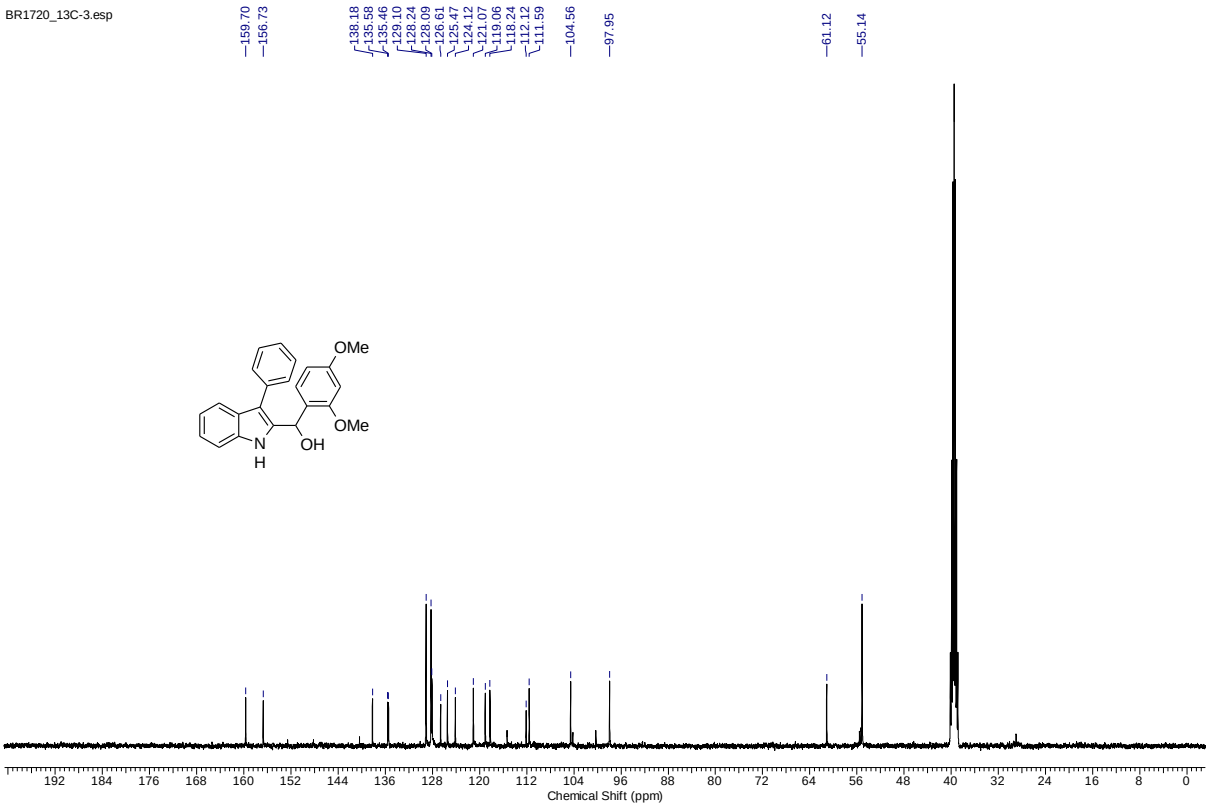
^{1}H and ^{13}C NMR of compound 4c



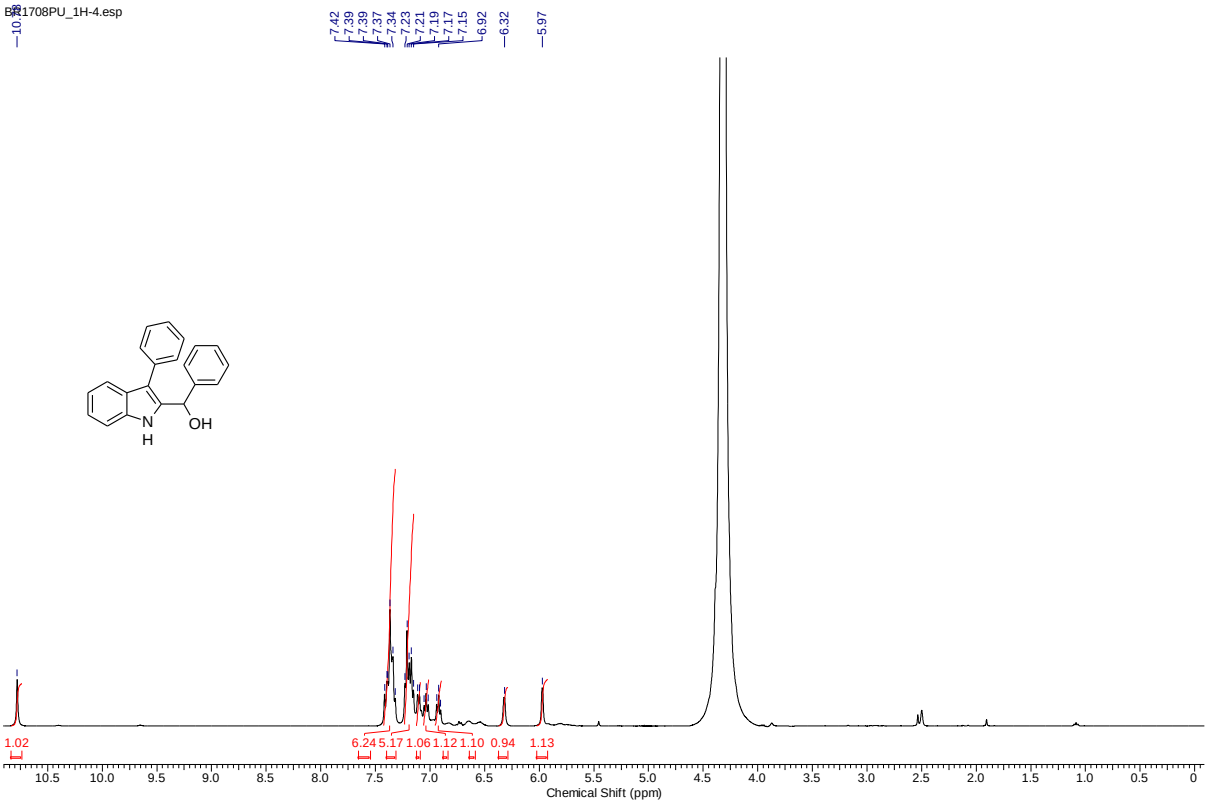


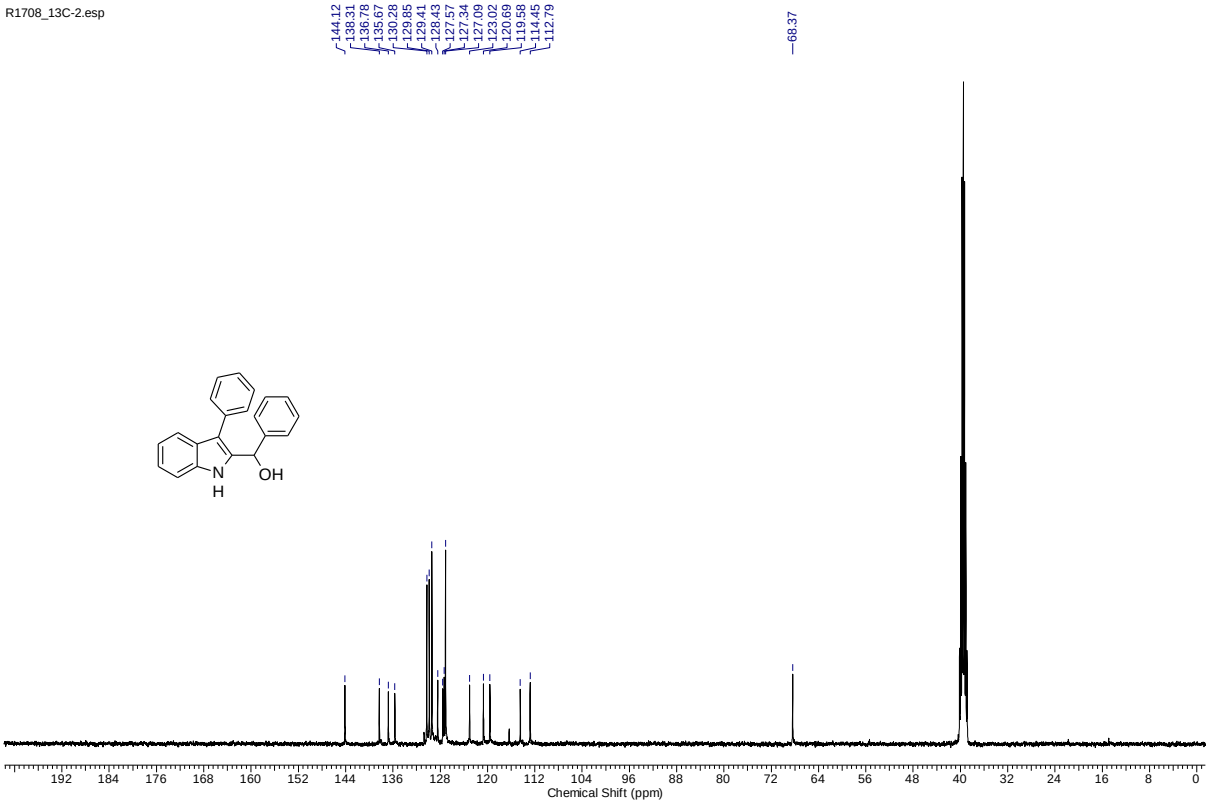
^{1}H and ^{13}C NMR of compound 4f



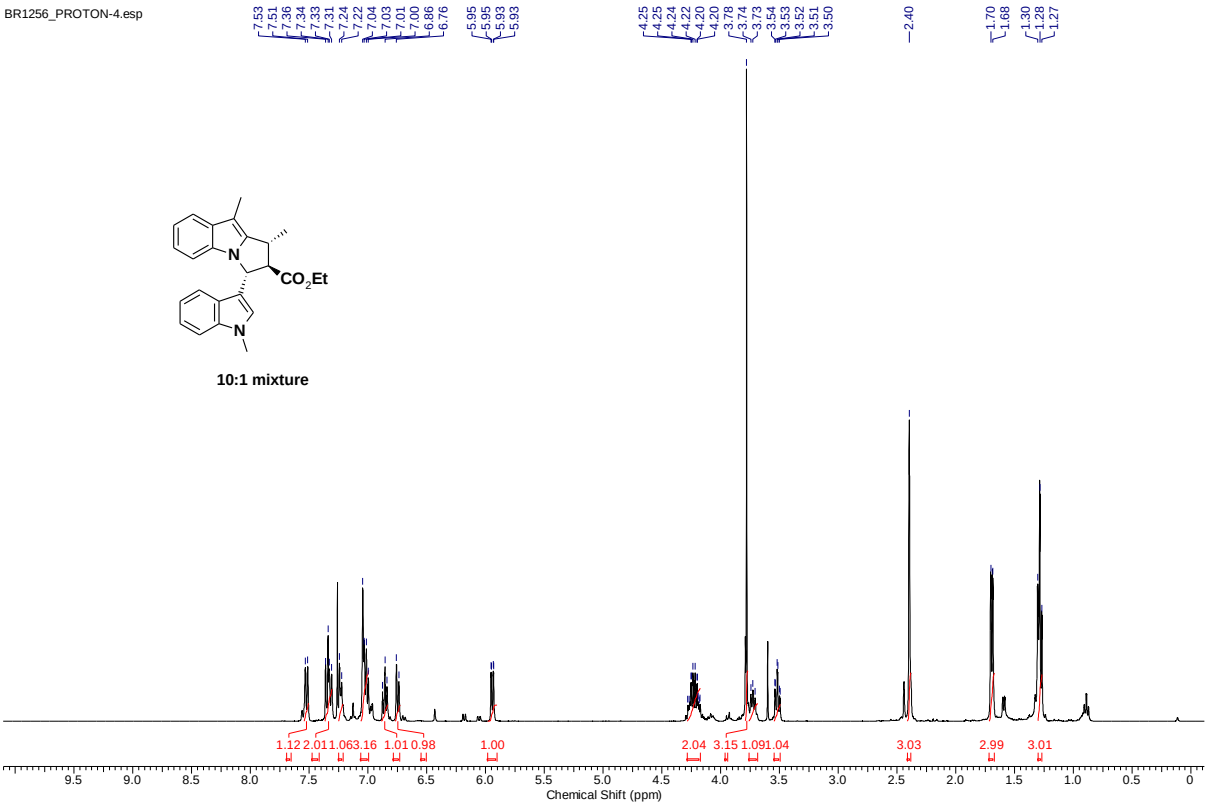


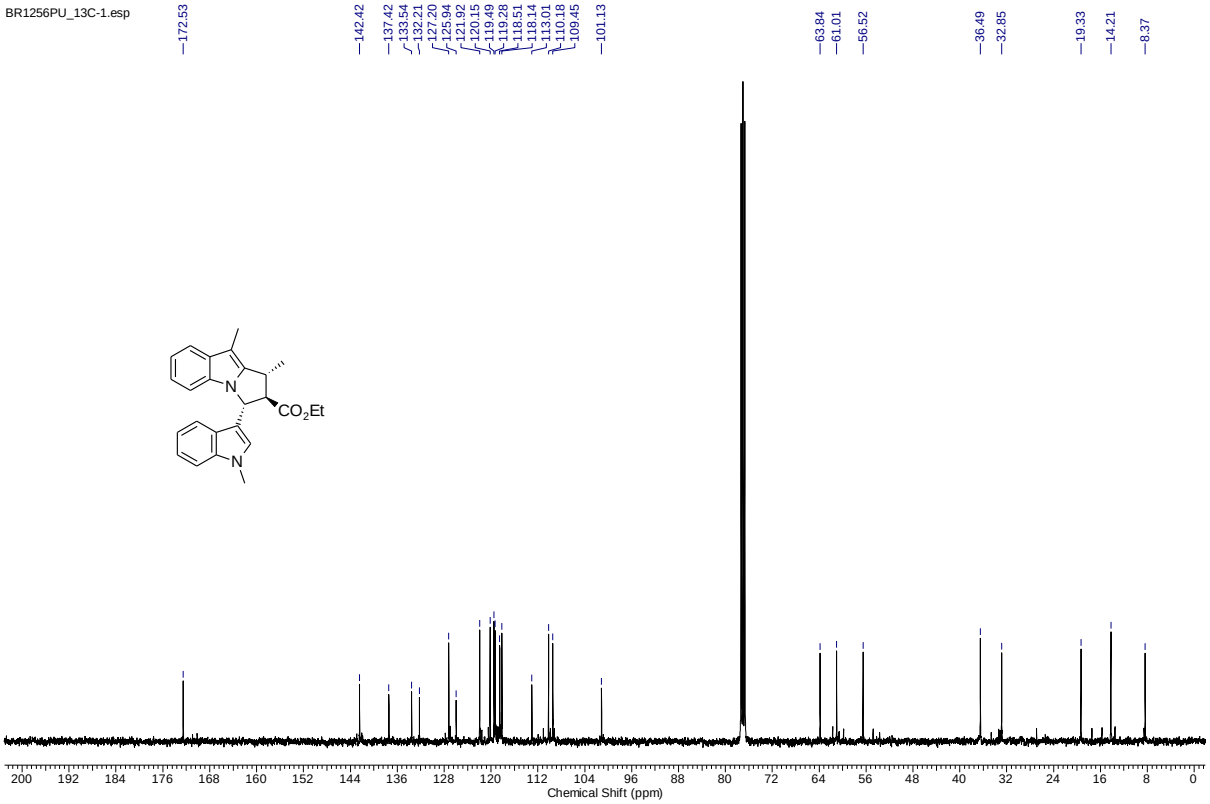
^{1}H and ^{13}C NMR of compound 4g



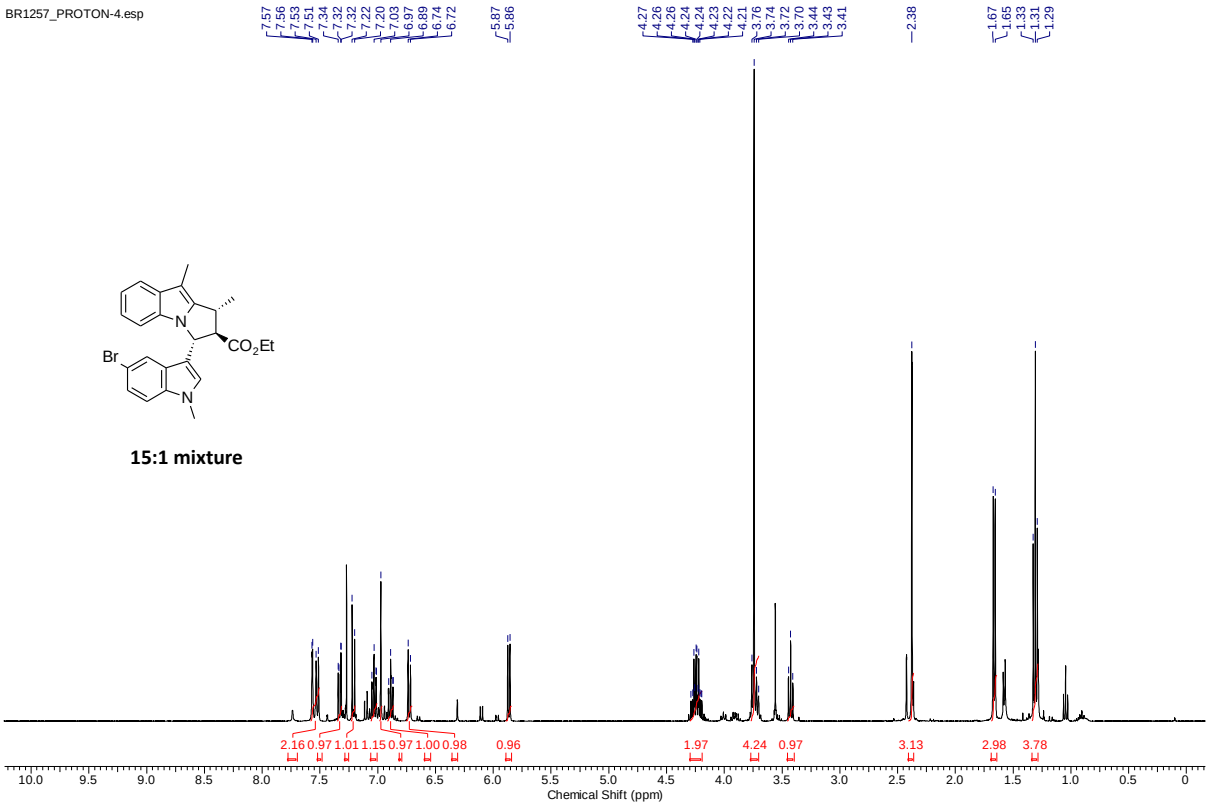


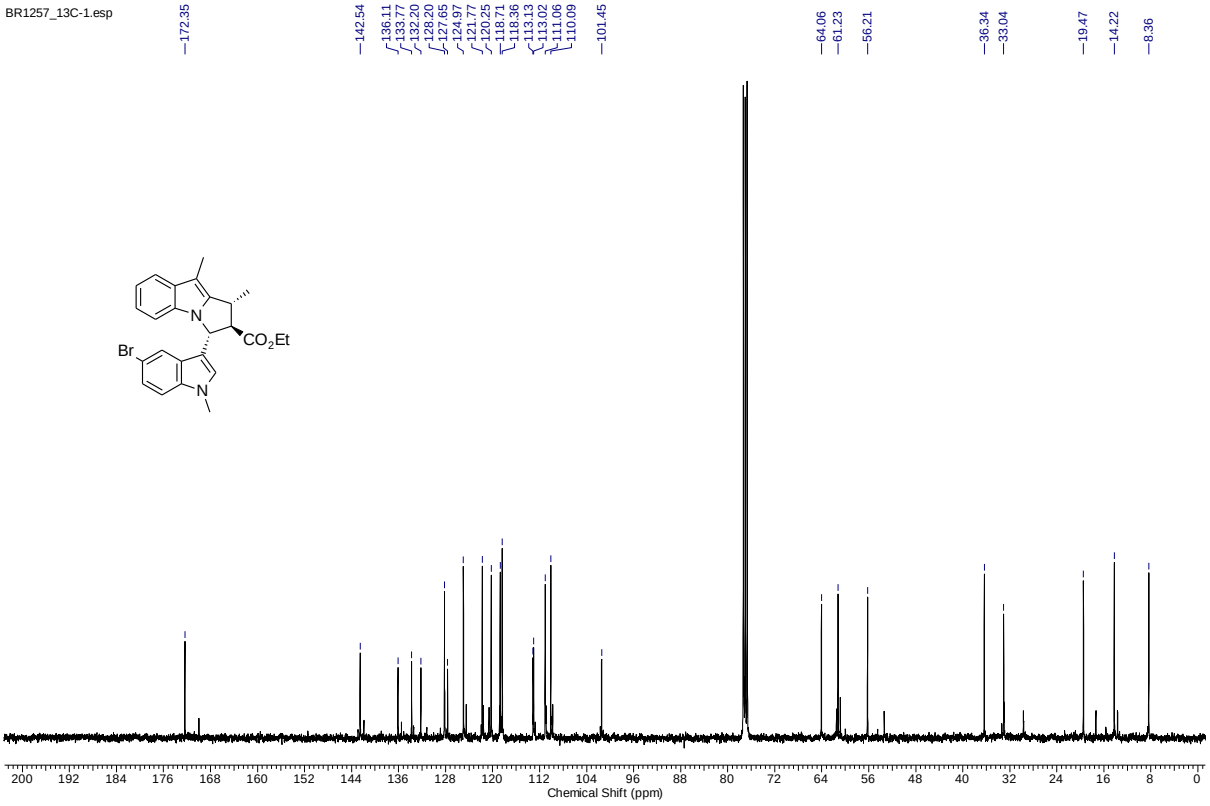
^{1}H and ^{13}C NMR of compound 6a



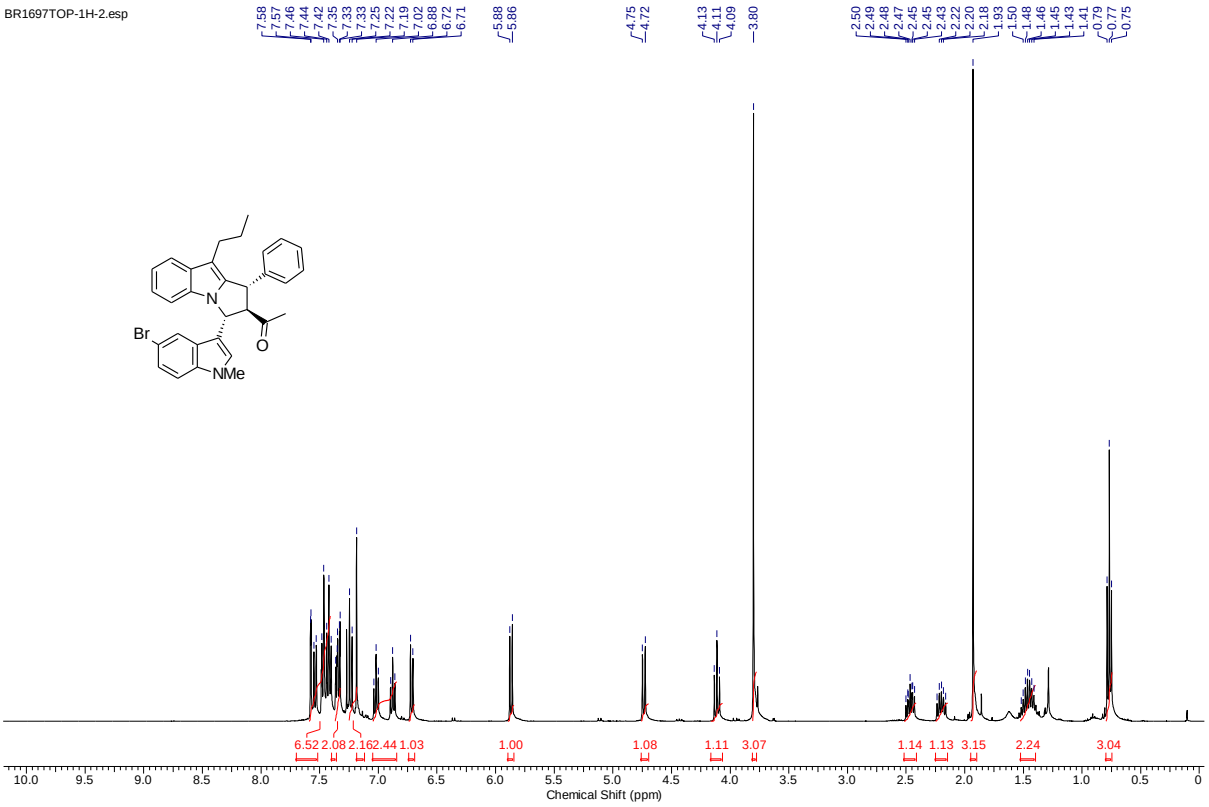


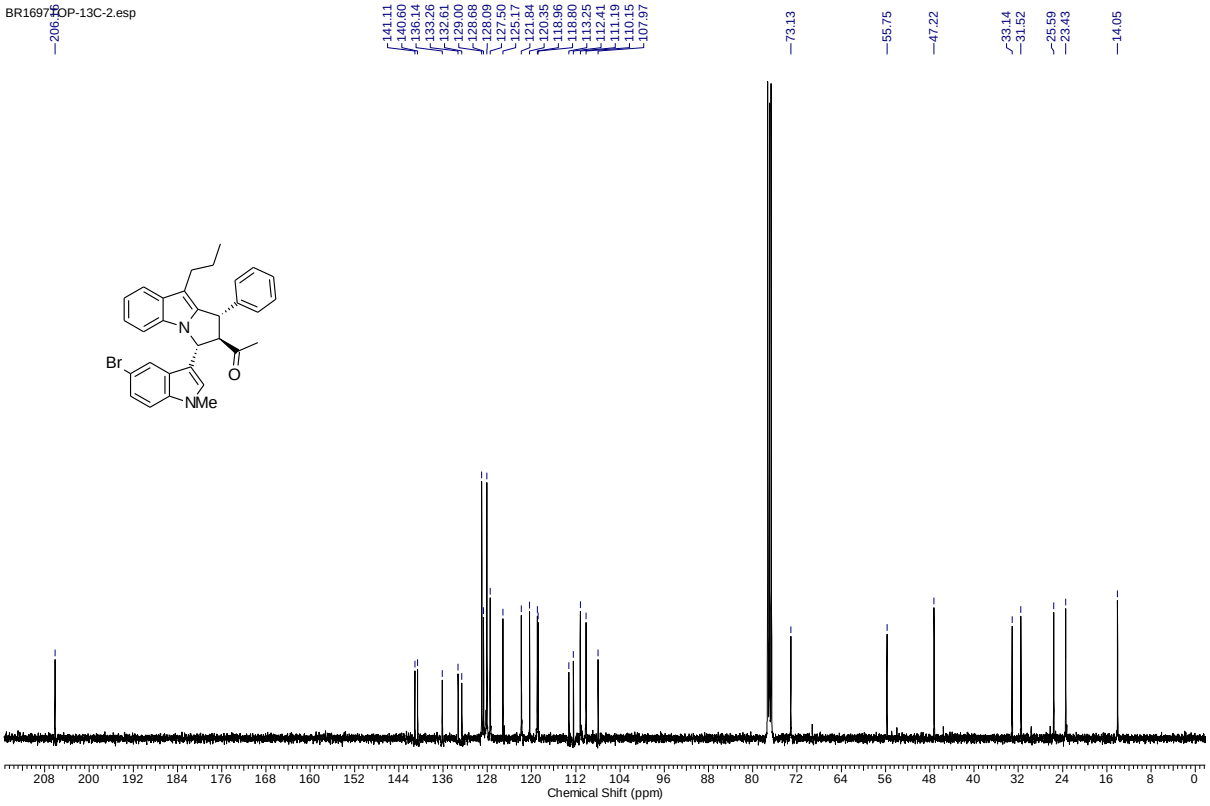
^{1}H and ^{13}C NMR of compound 6b



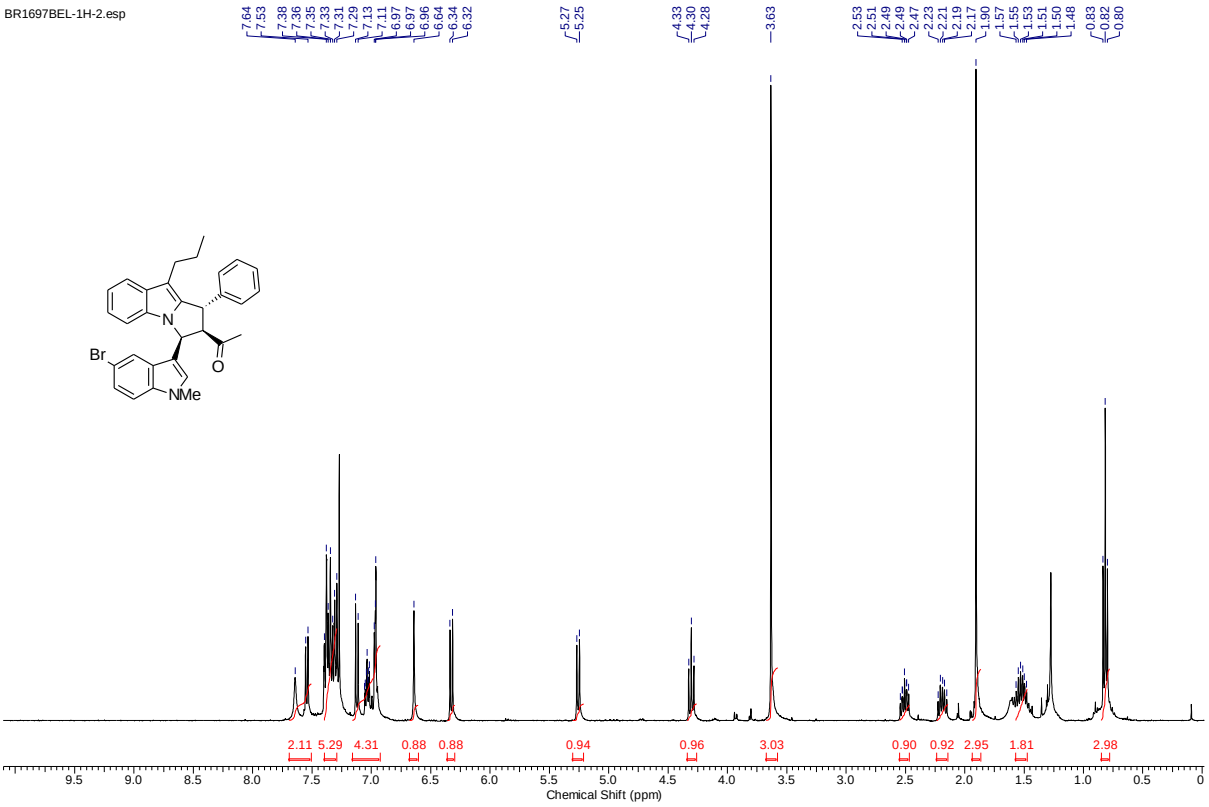


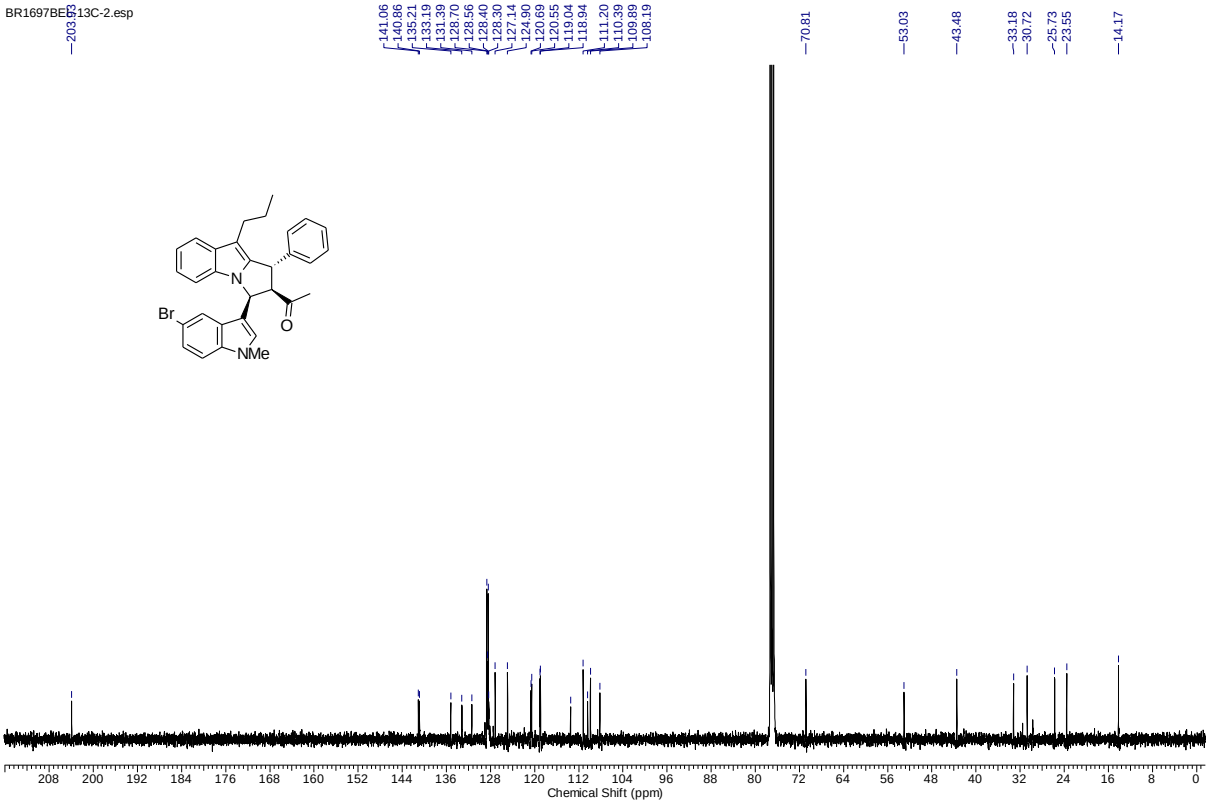
^{1}H and ^{13}C NMR of compound 8a



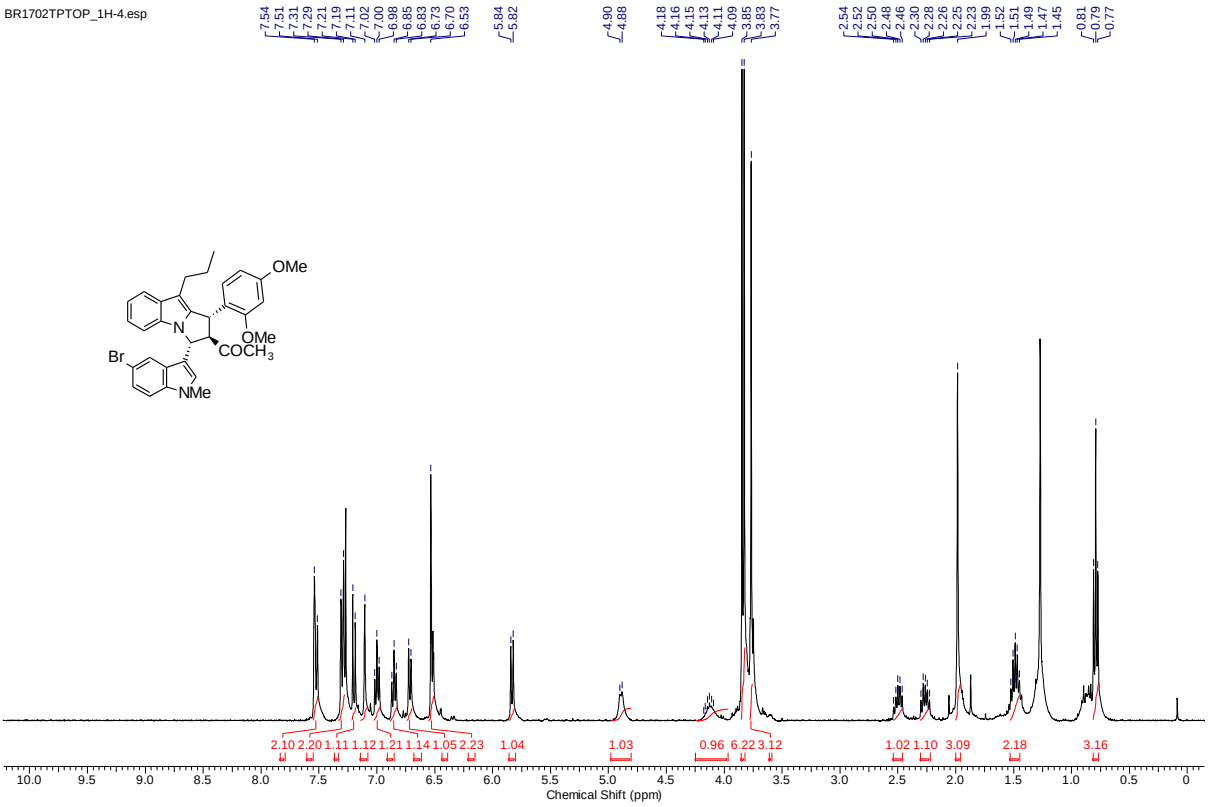


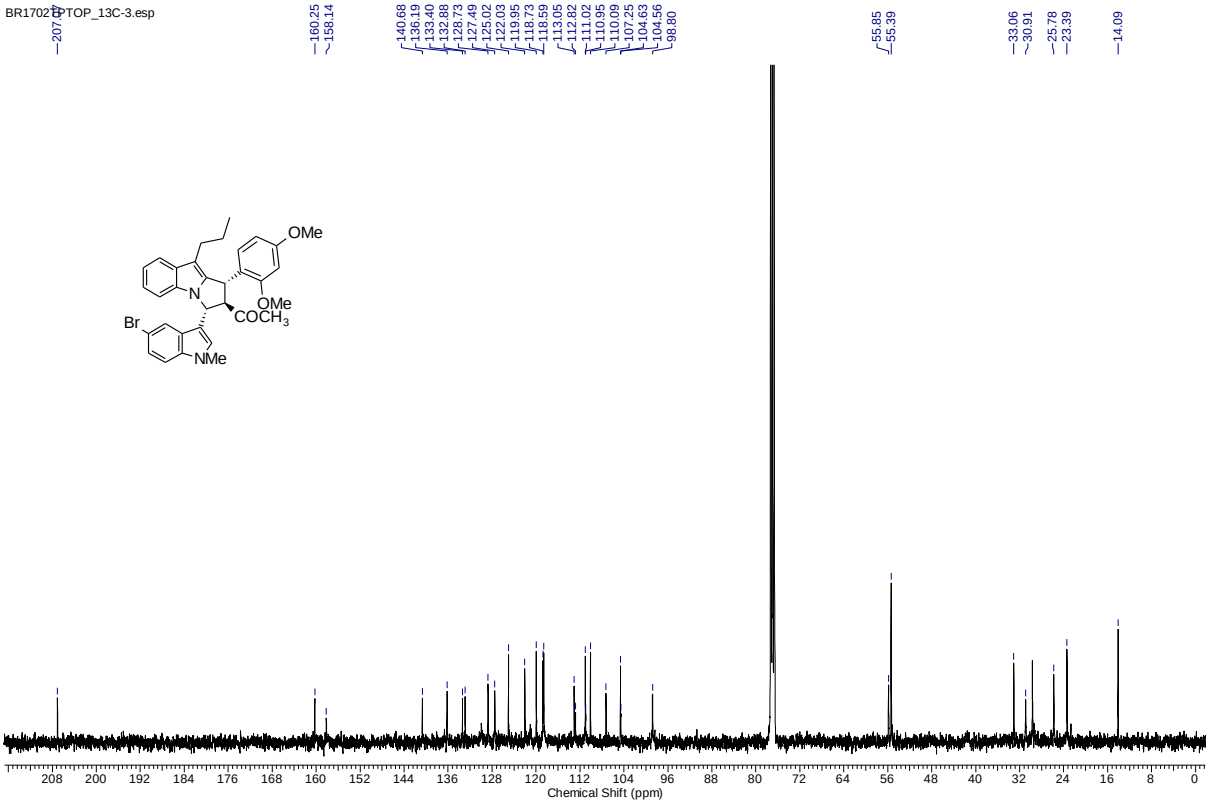
^{1}H and ^{13}C NMR of compound 8a'



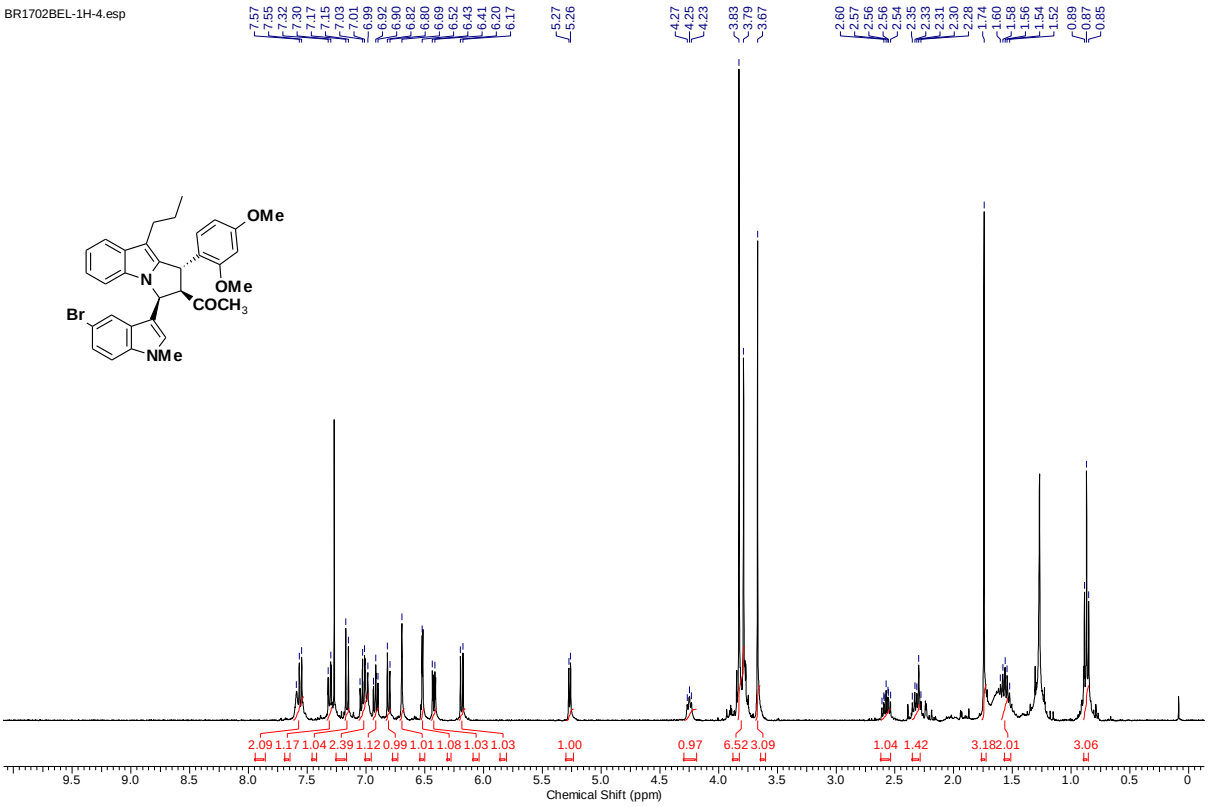


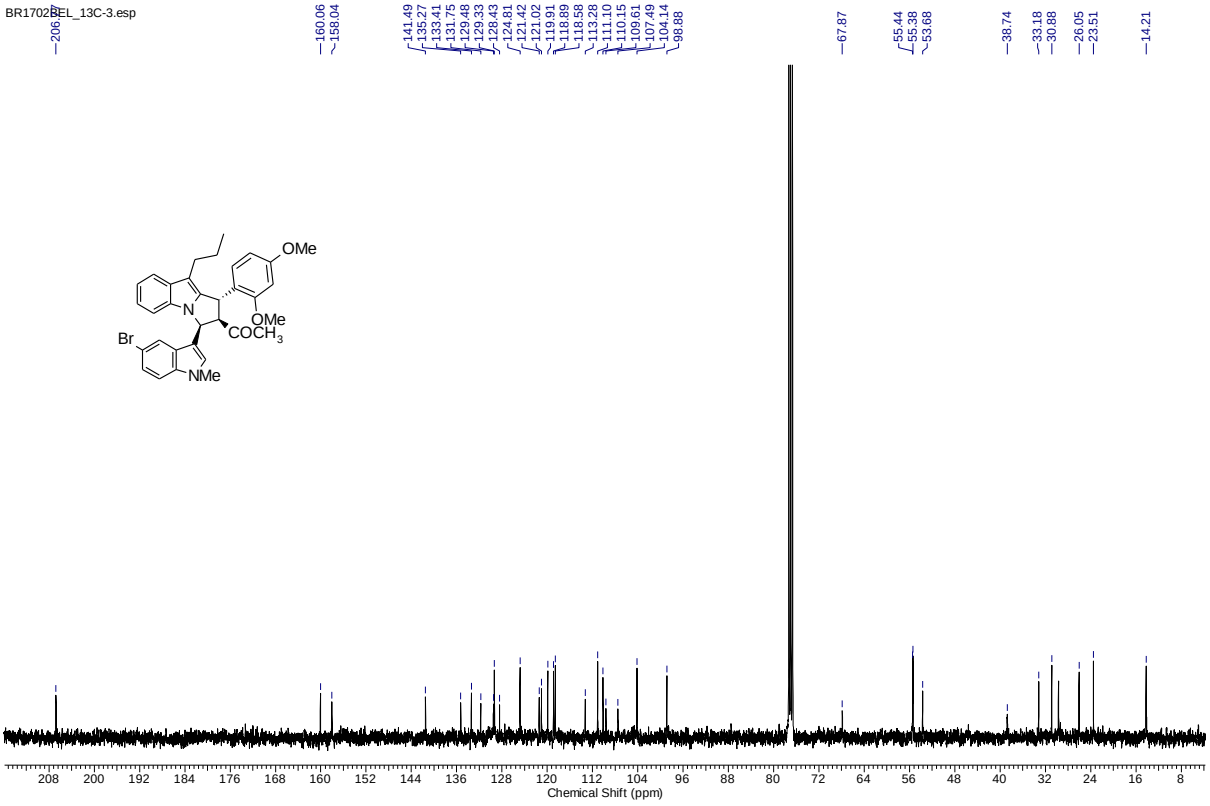
^{1}H and ^{13}C NMR of compound 8b



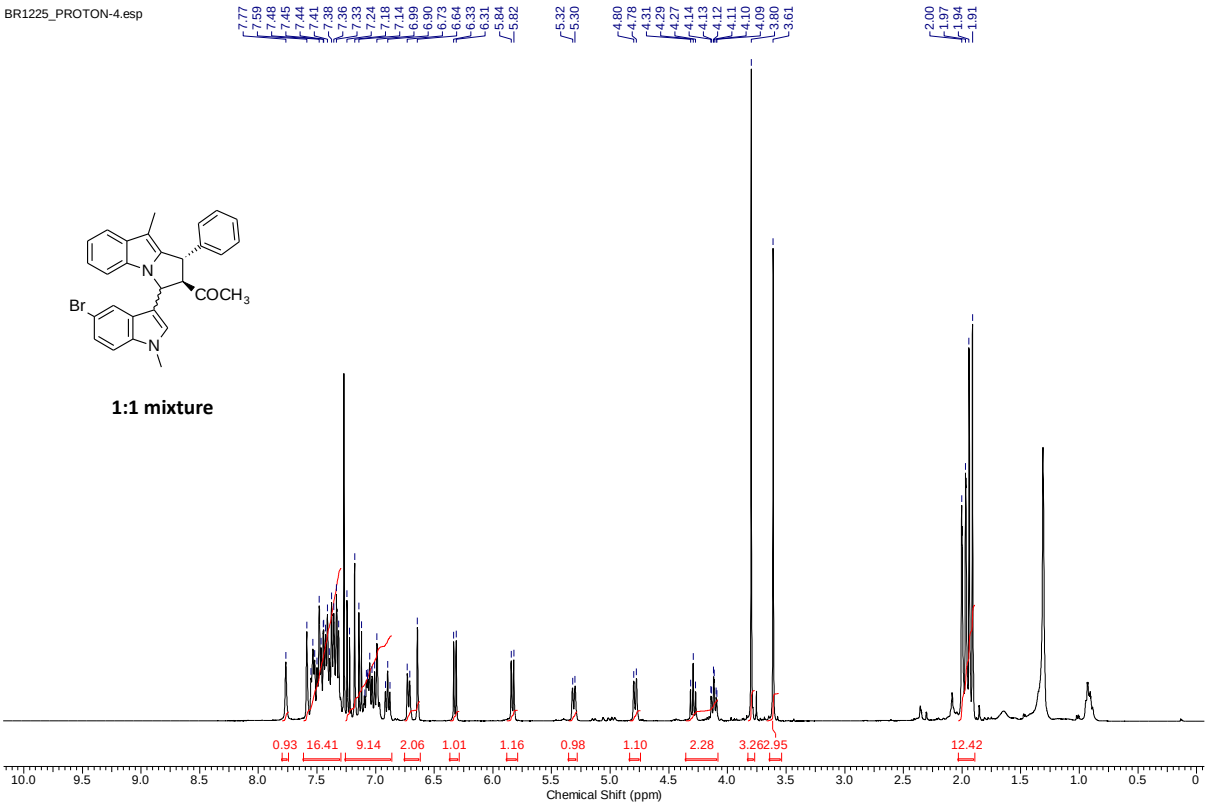


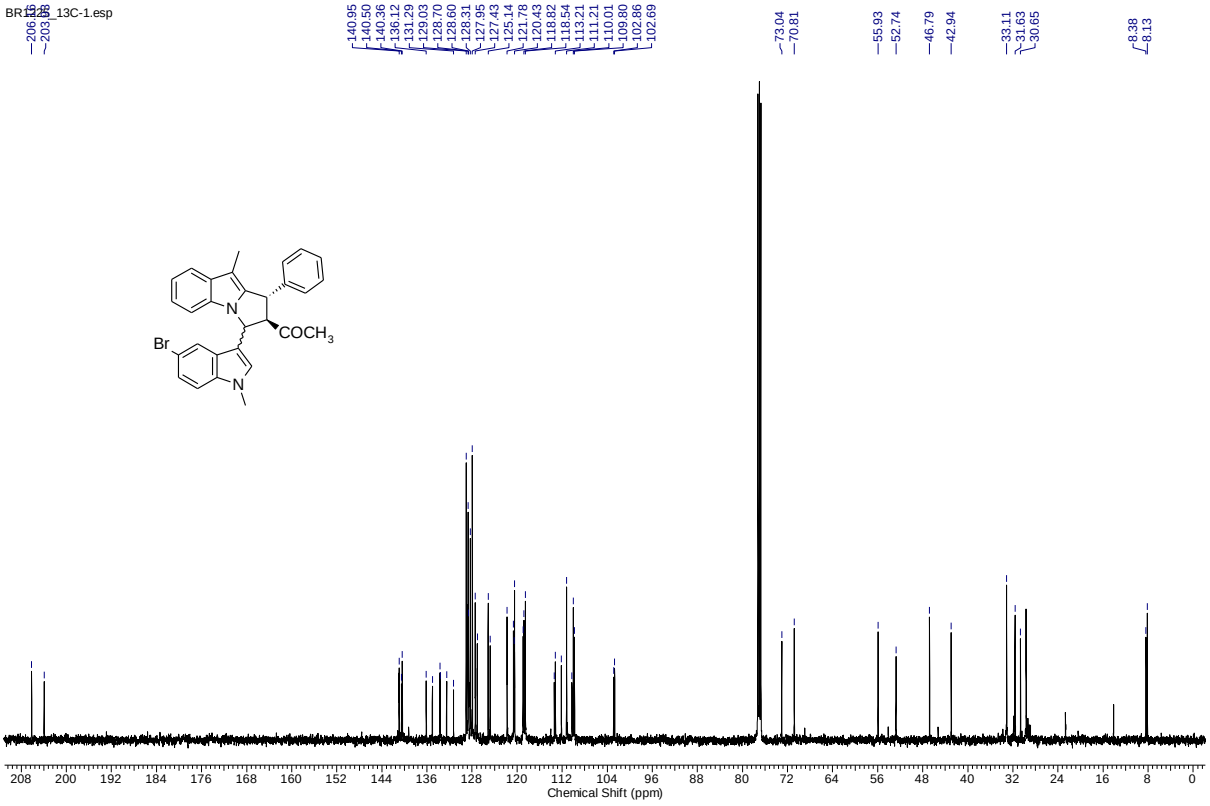
^{1}H and ^{13}C NMR of compound 8b'



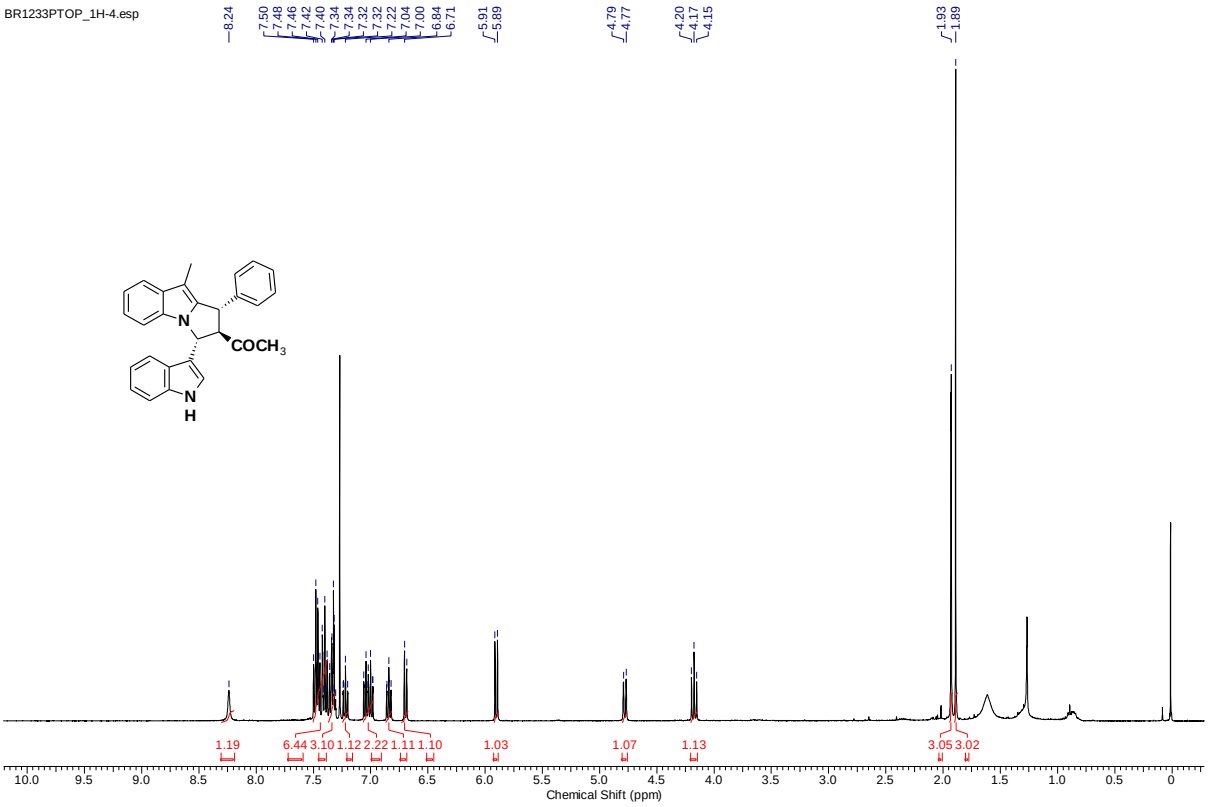


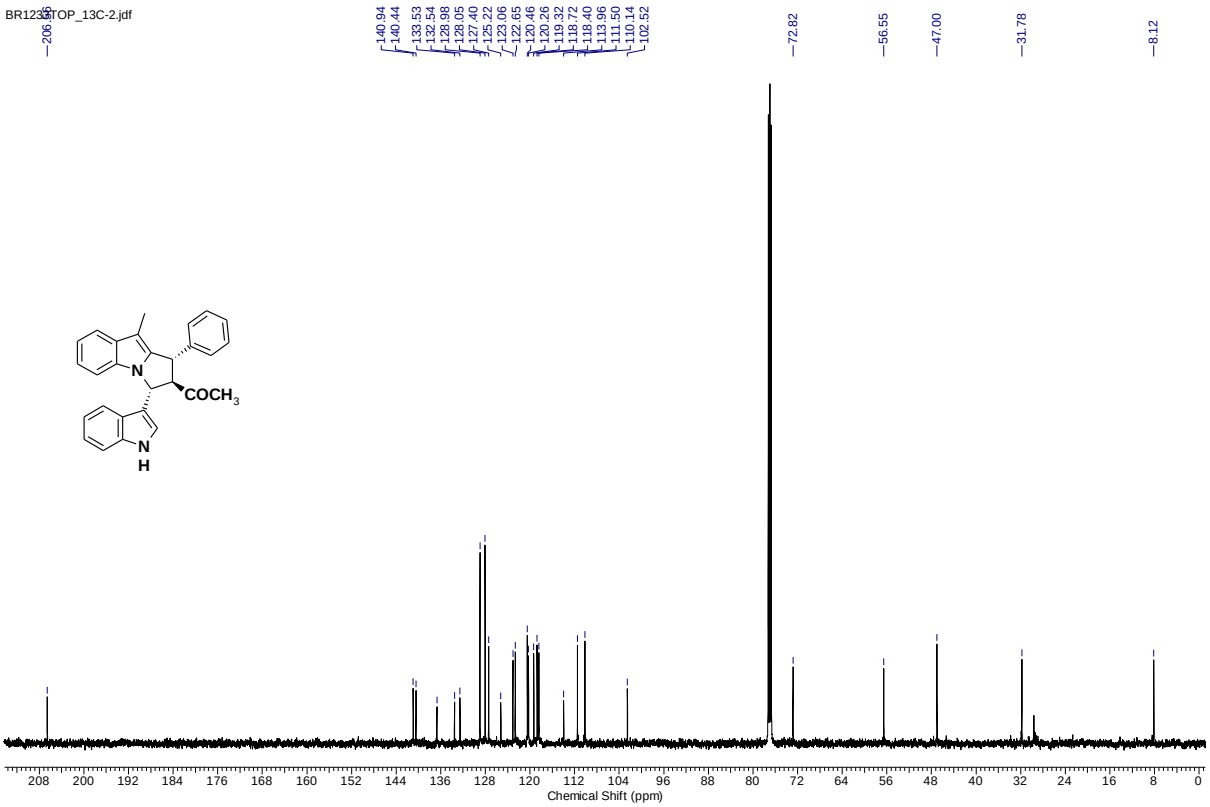
^{1}H and ^{13}C NMR of compound 8c



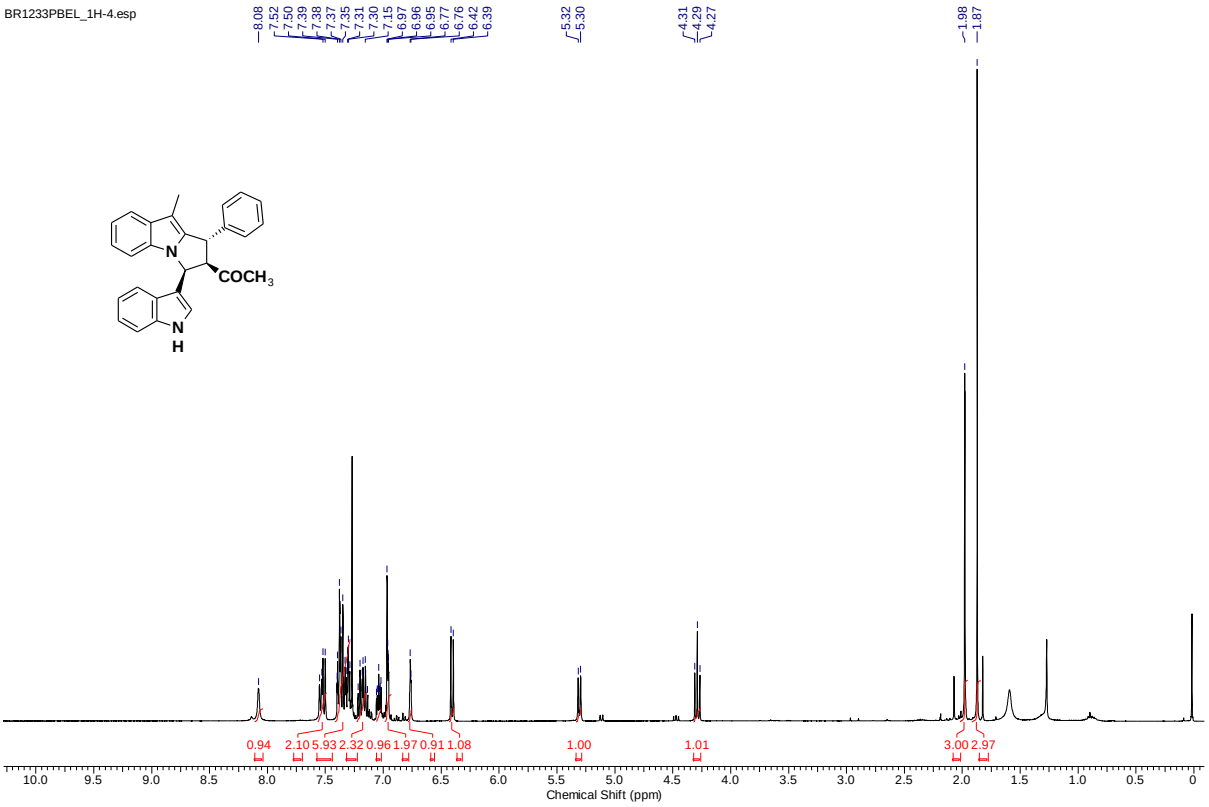


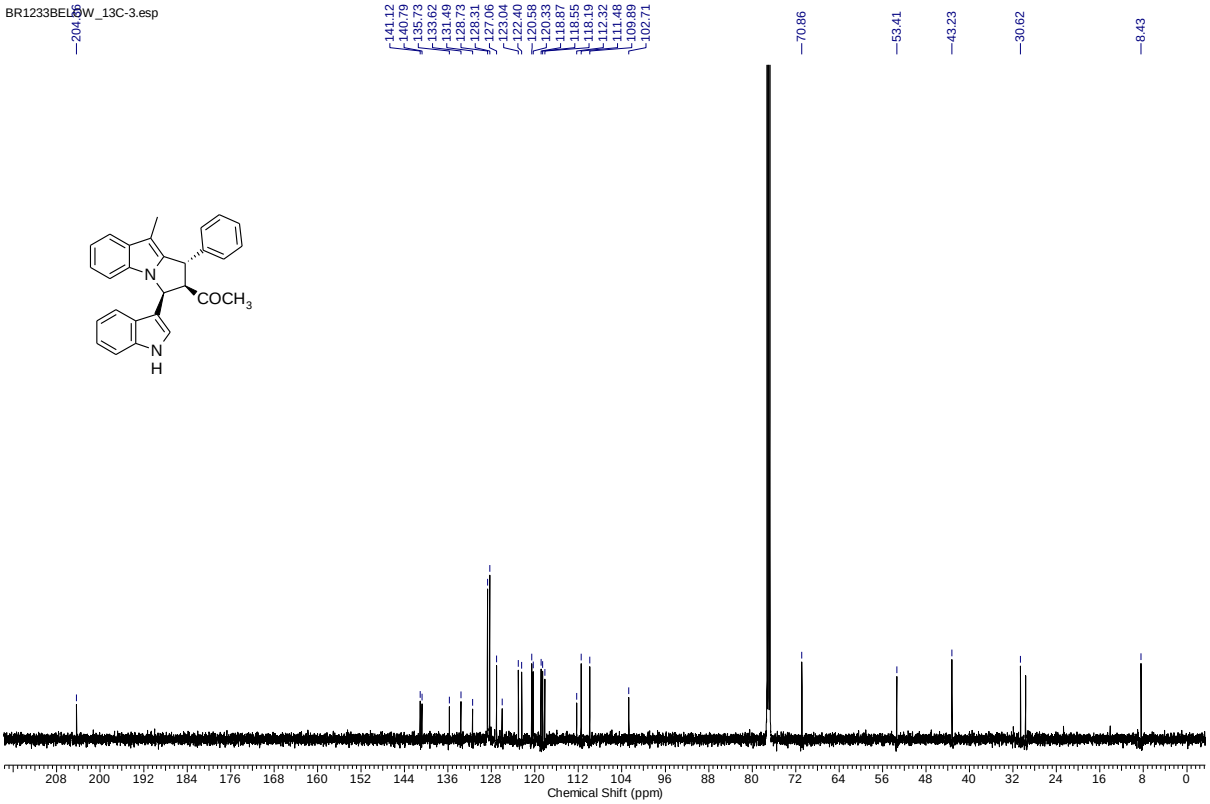
^{1}H and ^{13}C NMR of compound 8d



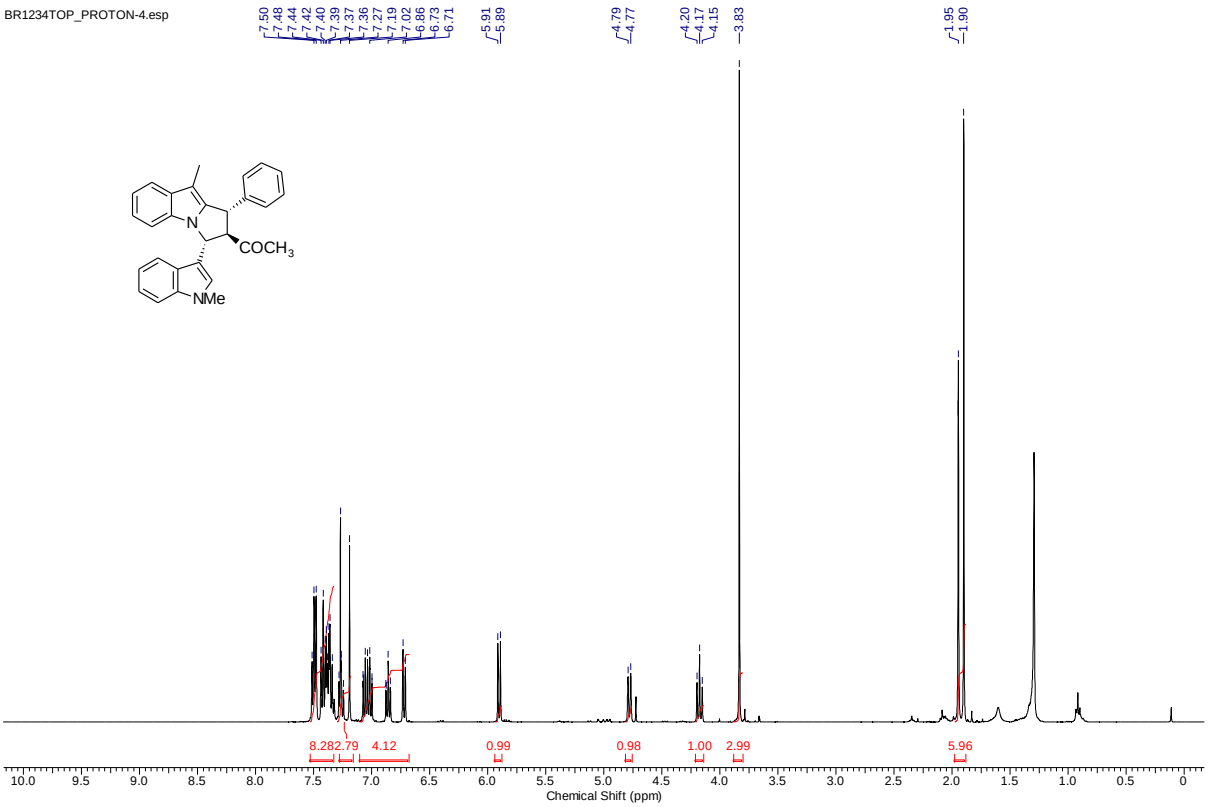


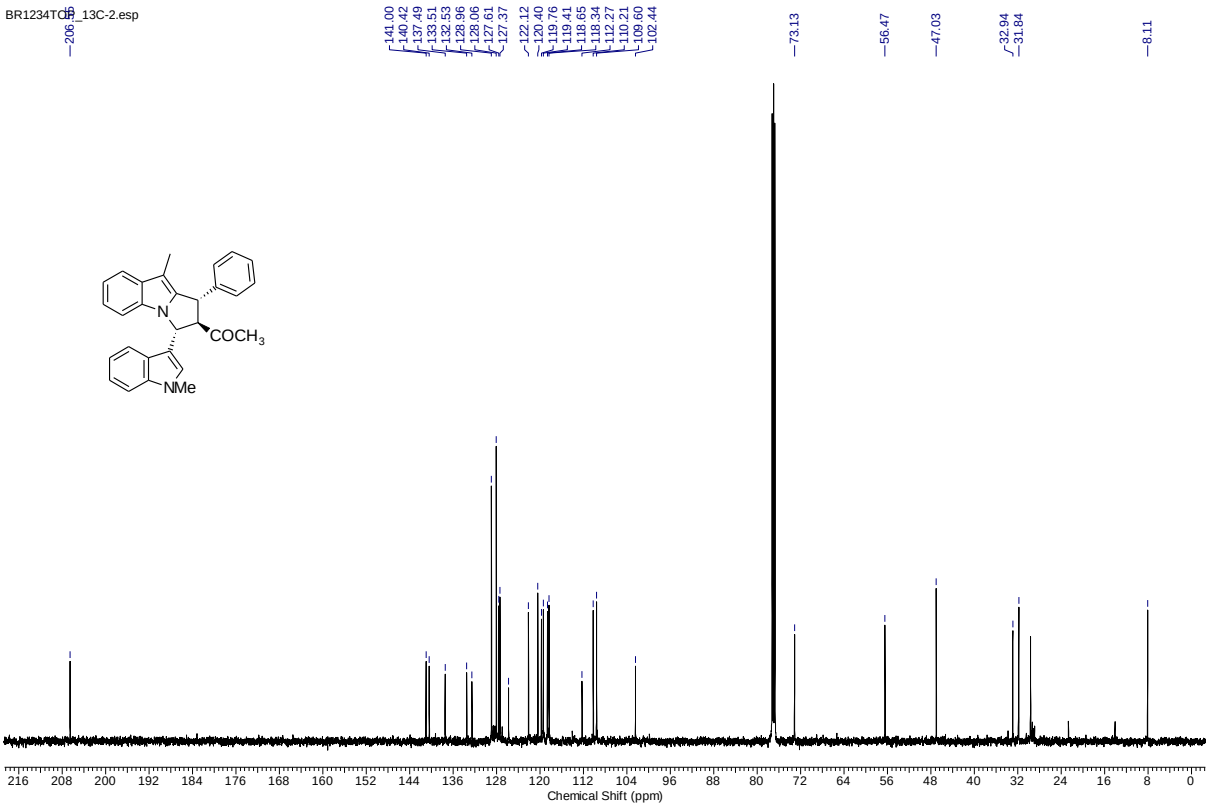
^{1}H and ^{13}C NMR of compound 8d'



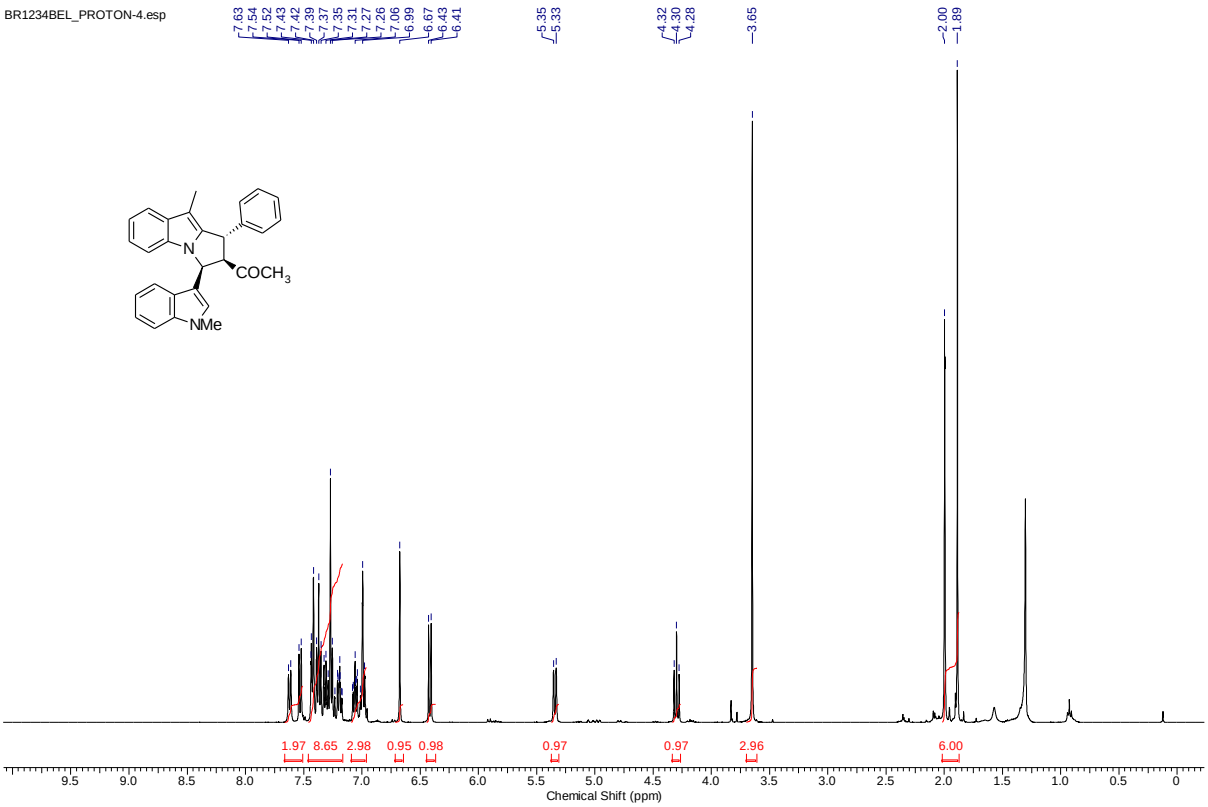


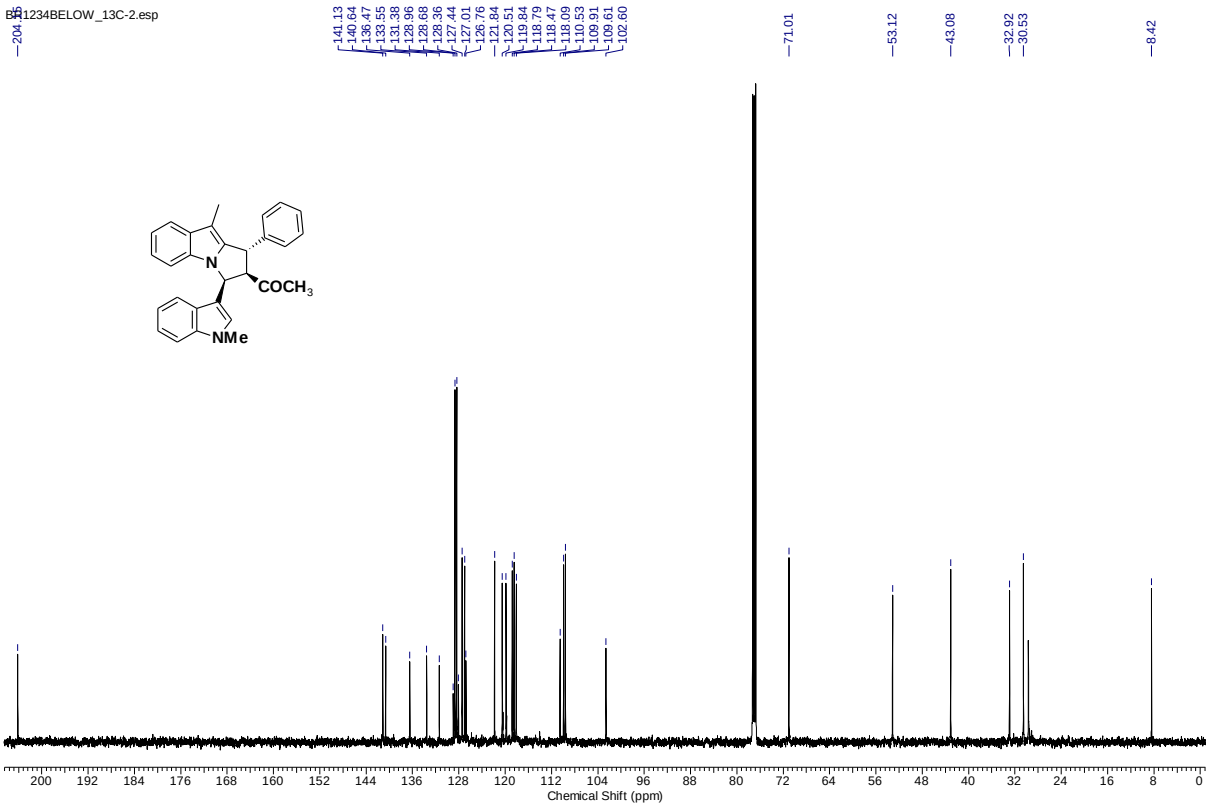
^{1}H and ^{13}C NMR of compound 8e



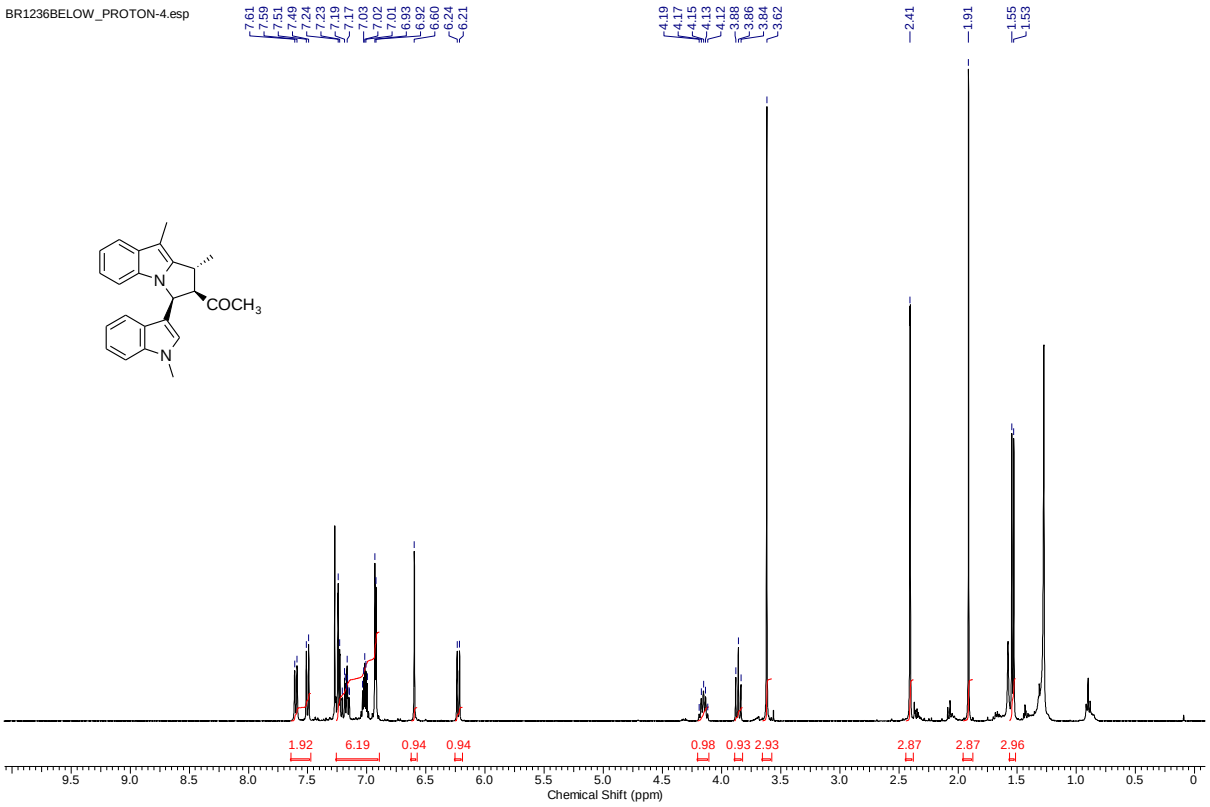


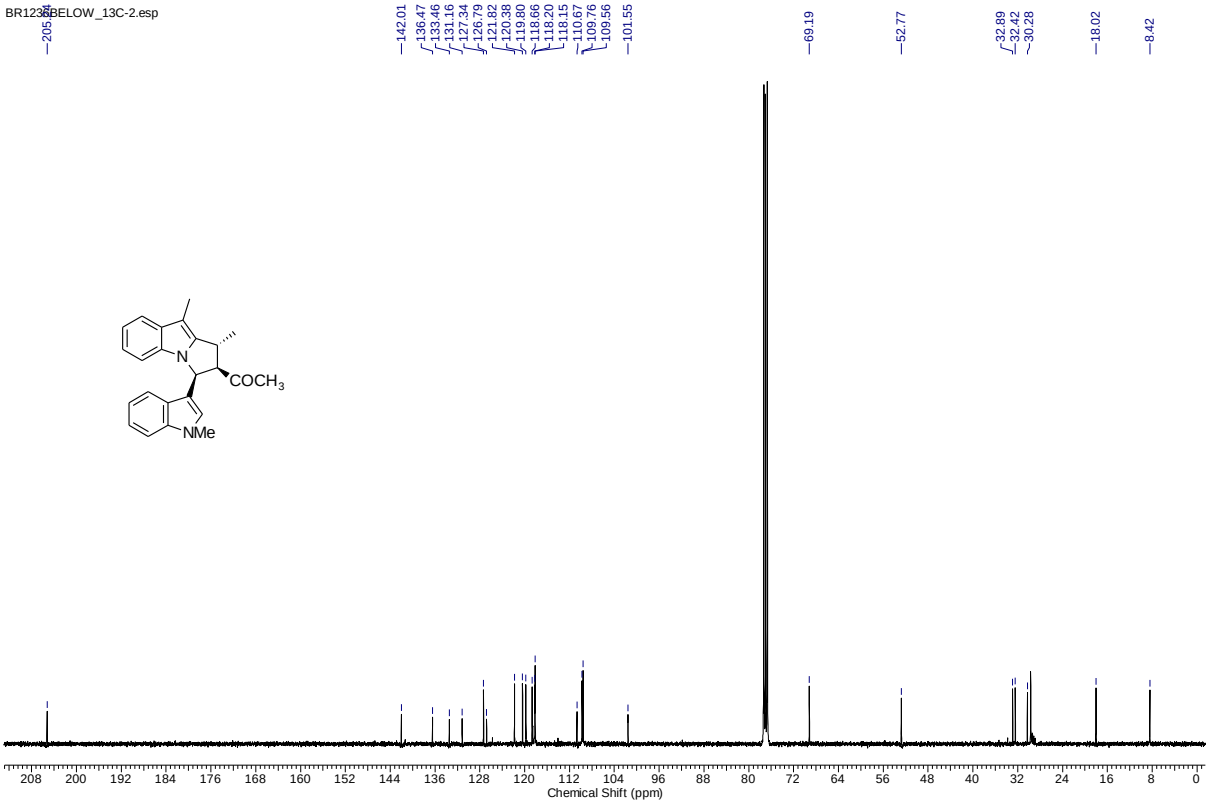
^{1}H and ^{13}C NMR of compound 8e'



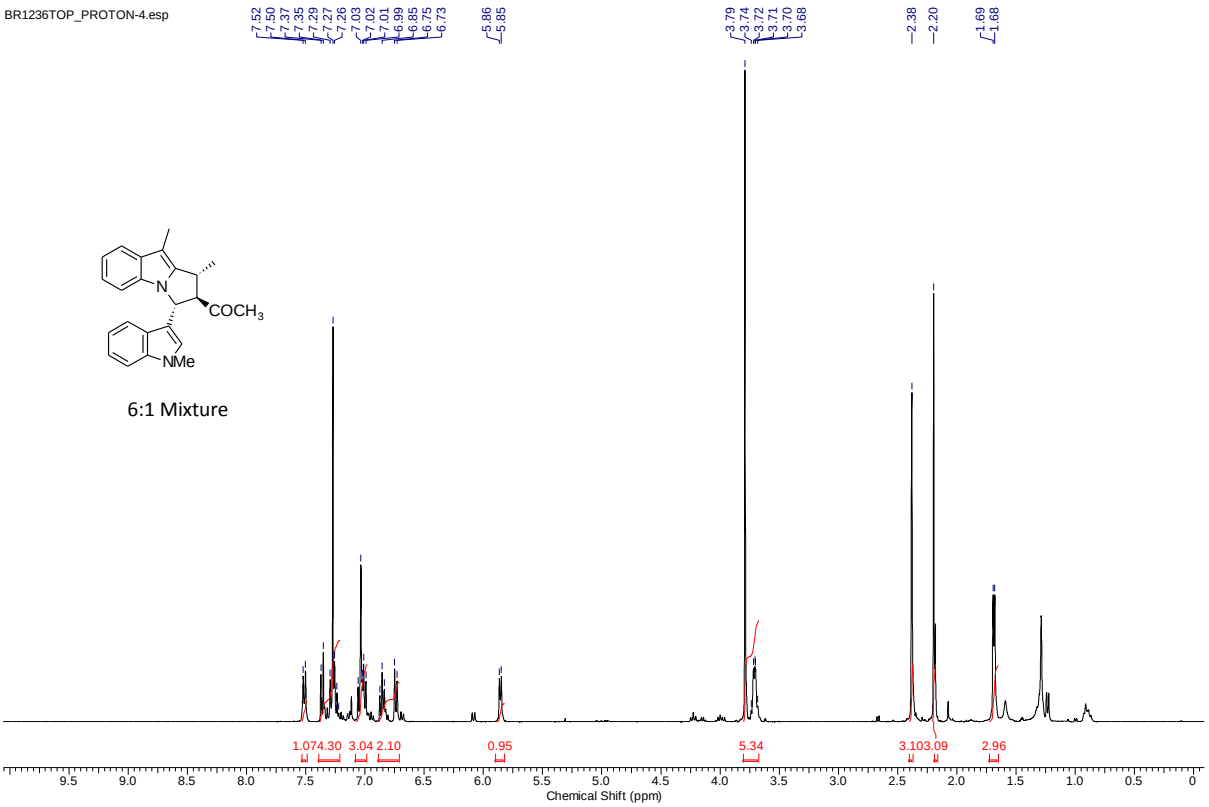


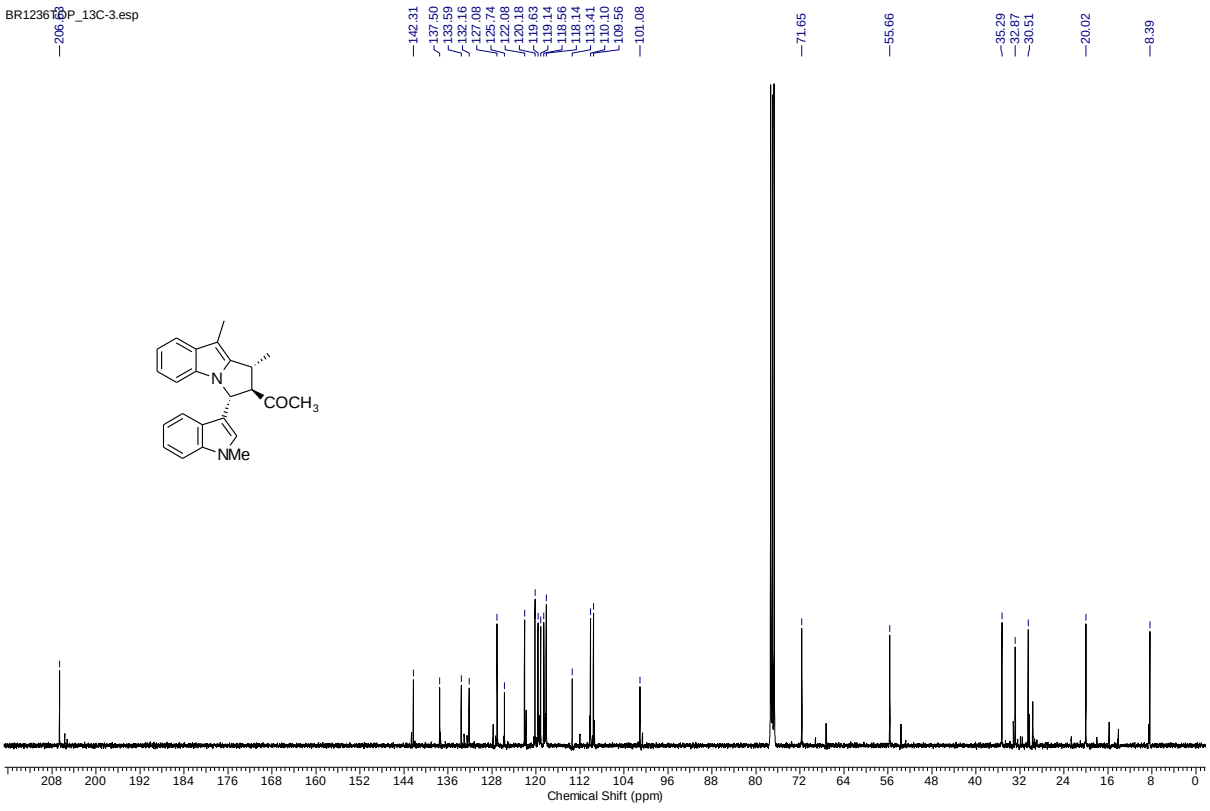
^{1}H and ^{13}C NMR of compound 8f'



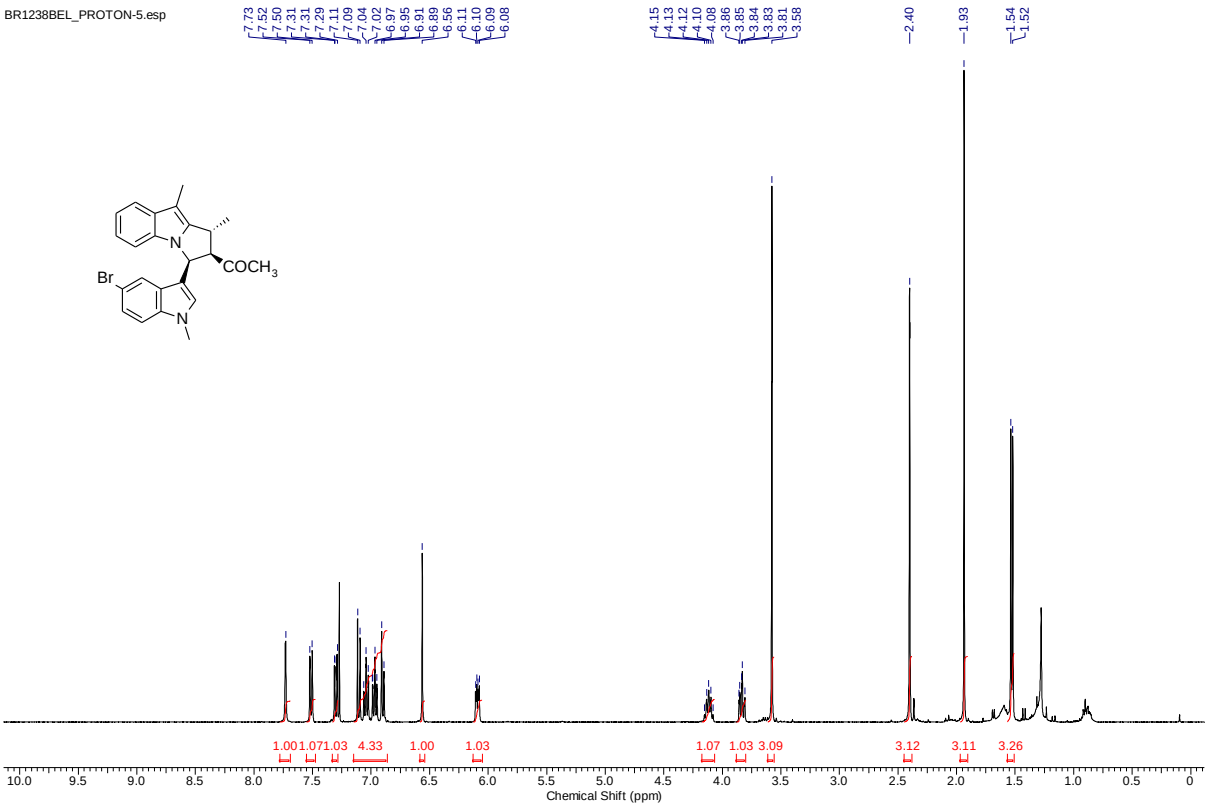


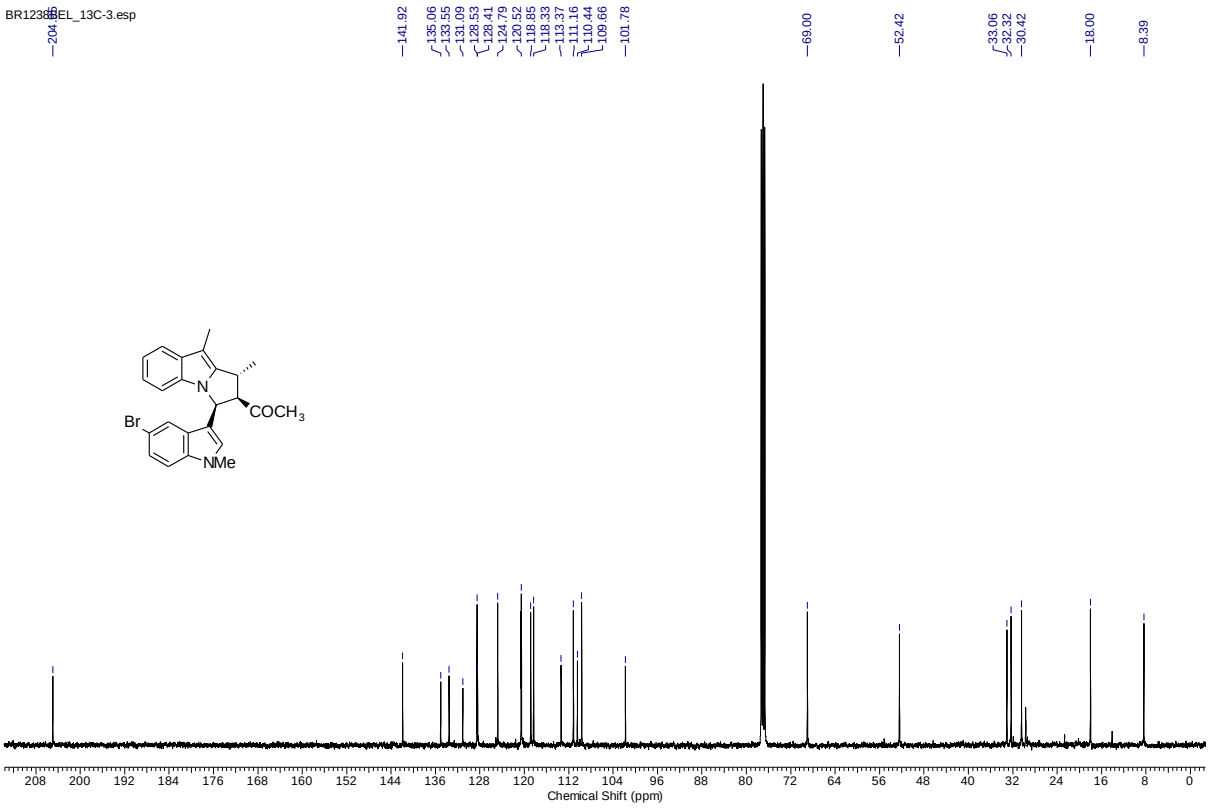
^{1}H and ^{13}C NMR of compound 8f



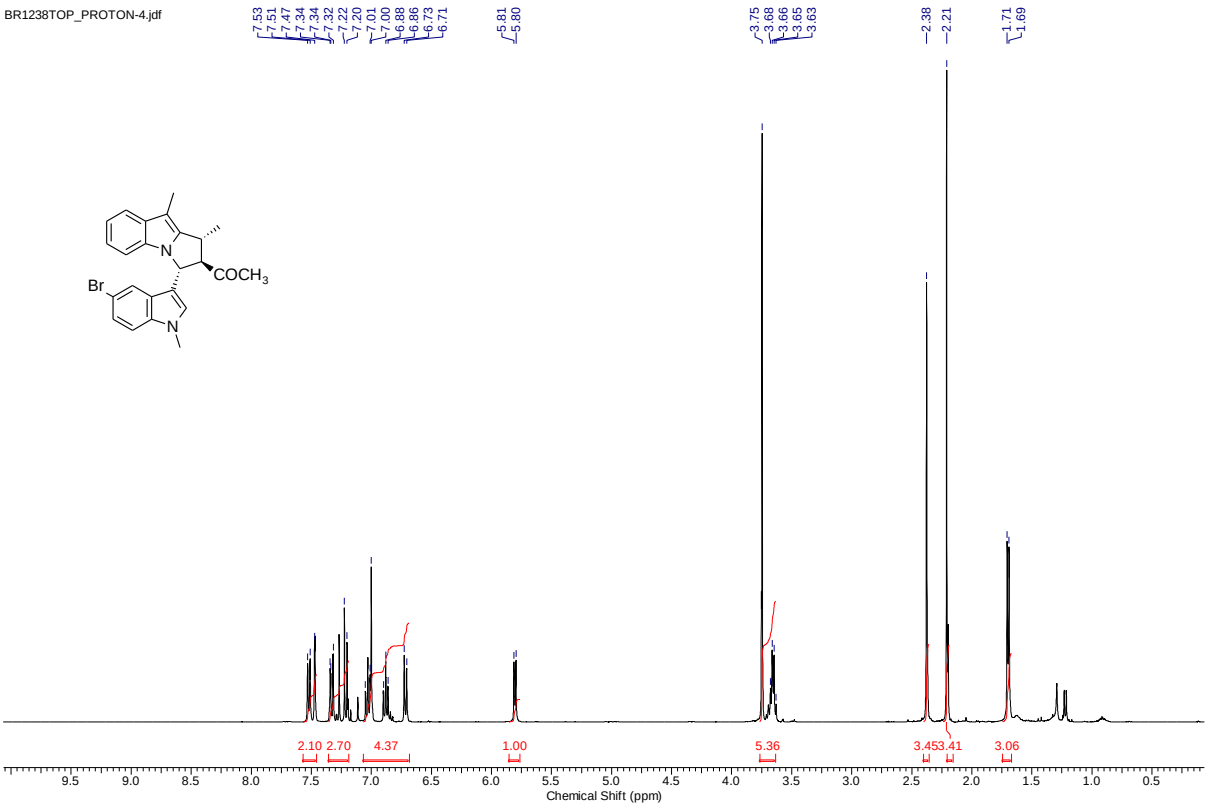


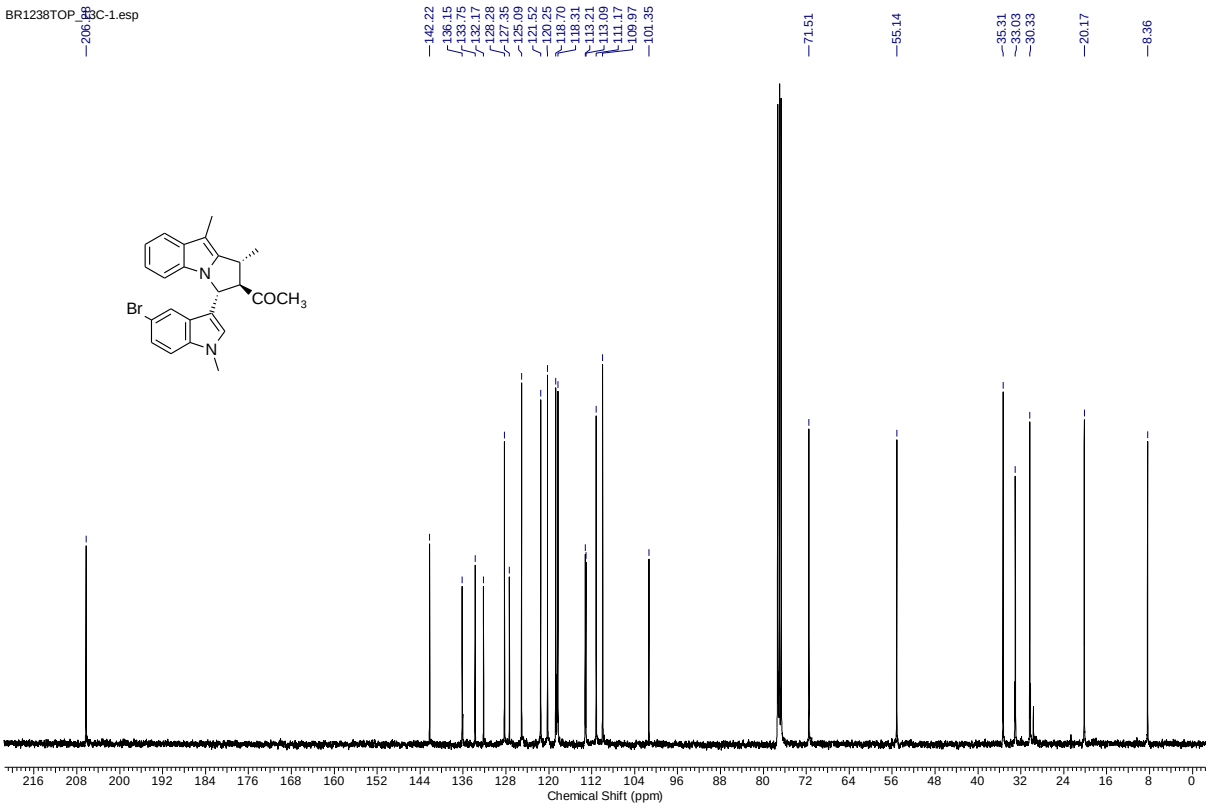
^{1}H and ^{13}C NMR of compound 8g'



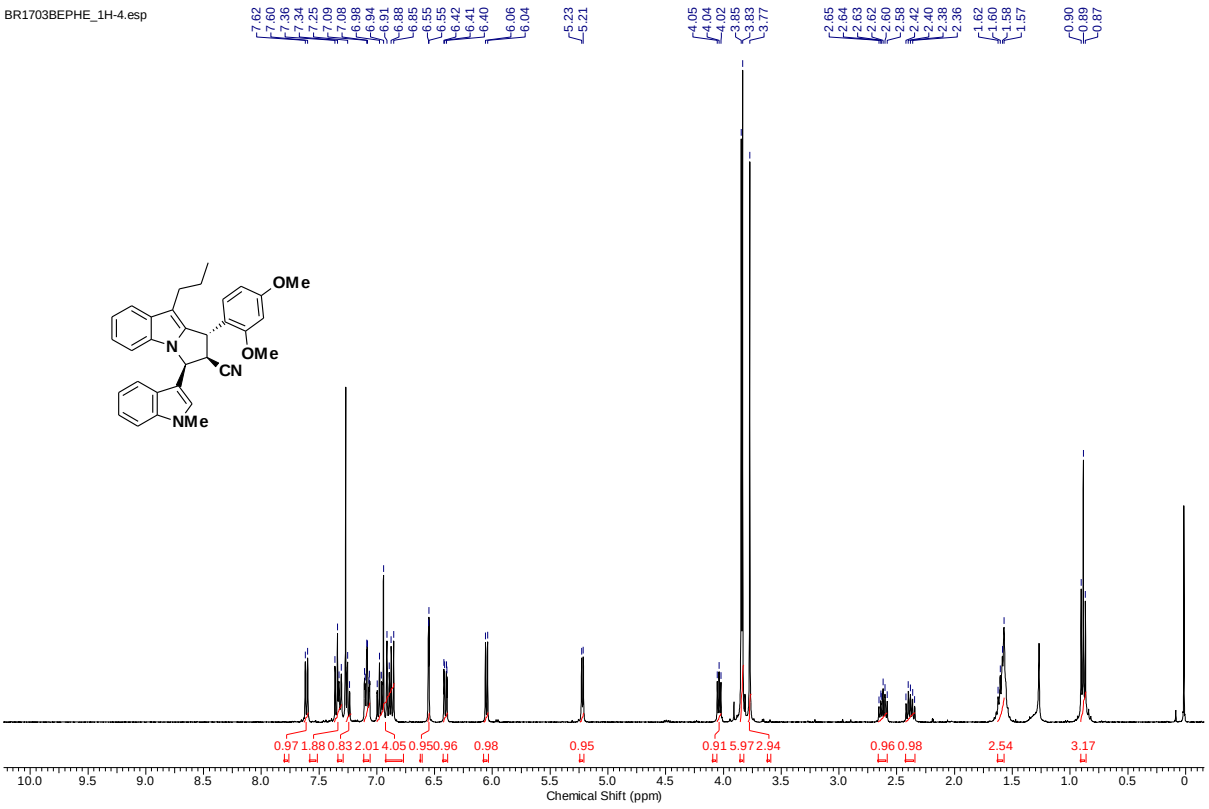


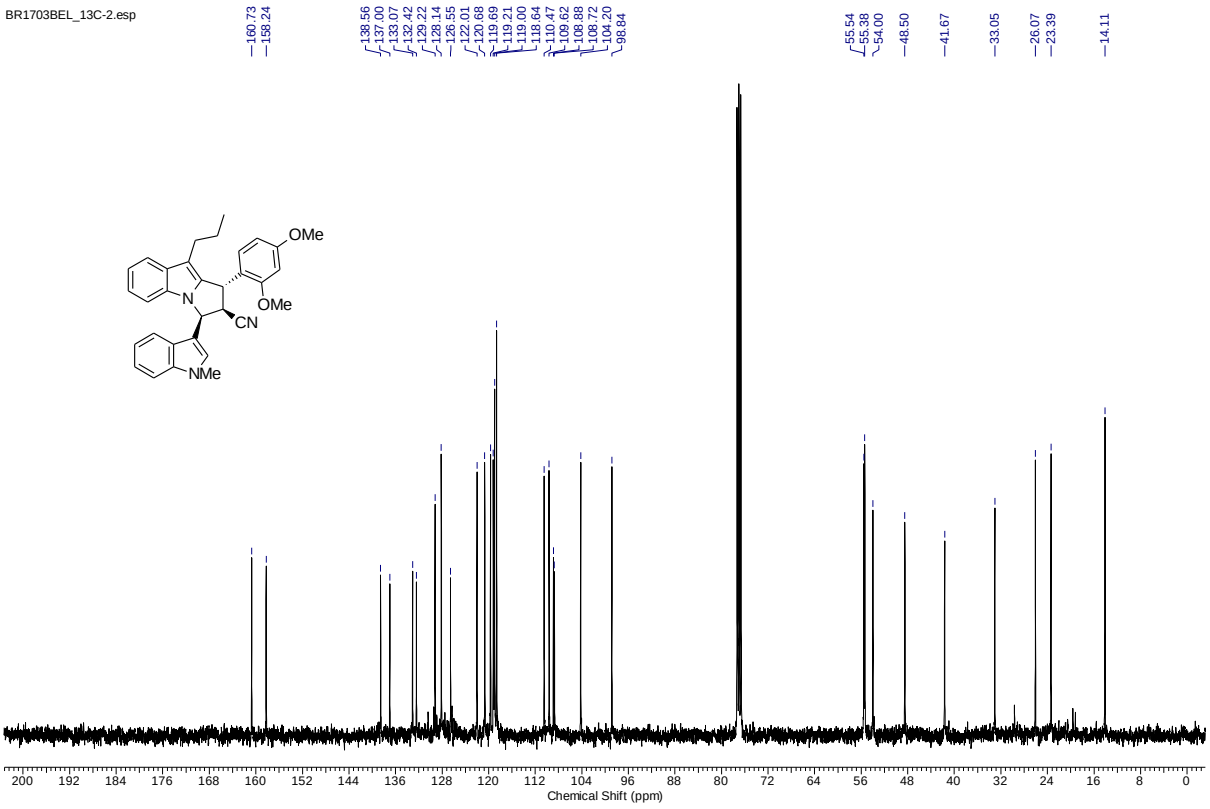
^{1}H and ^{13}C NMR of compound 8g



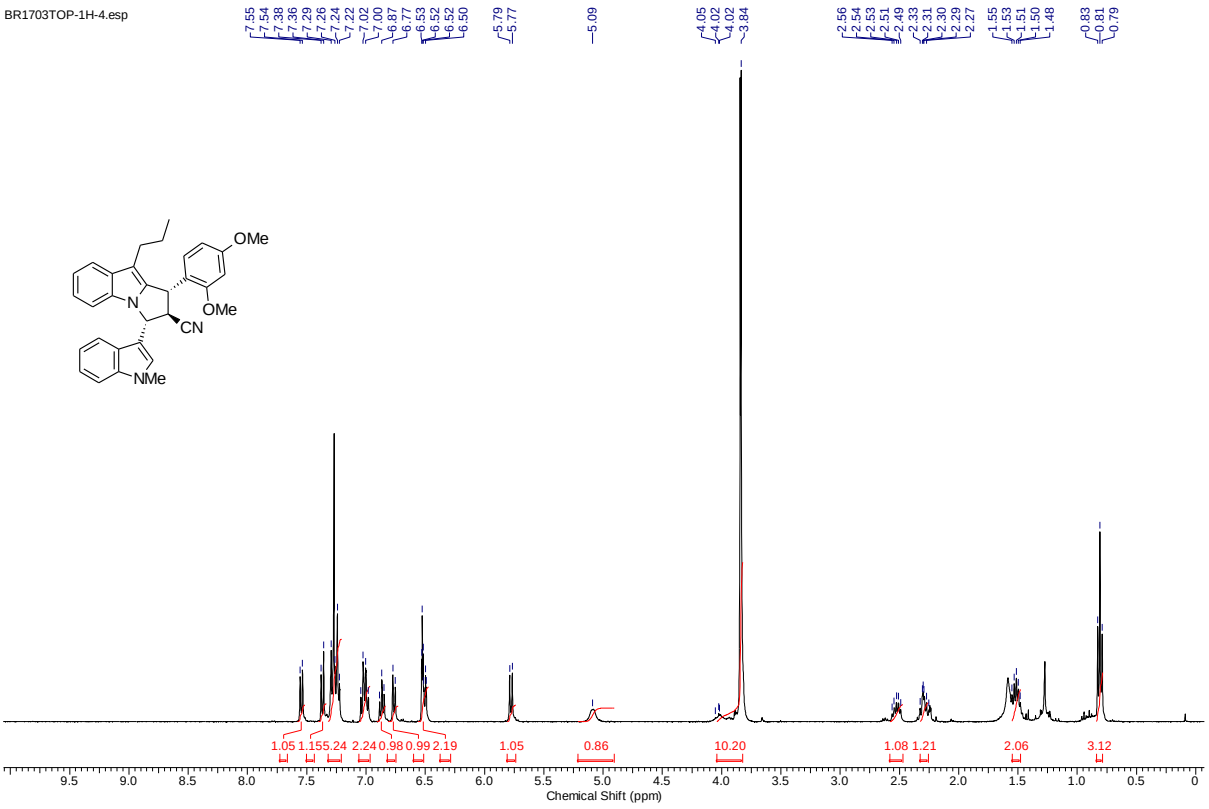


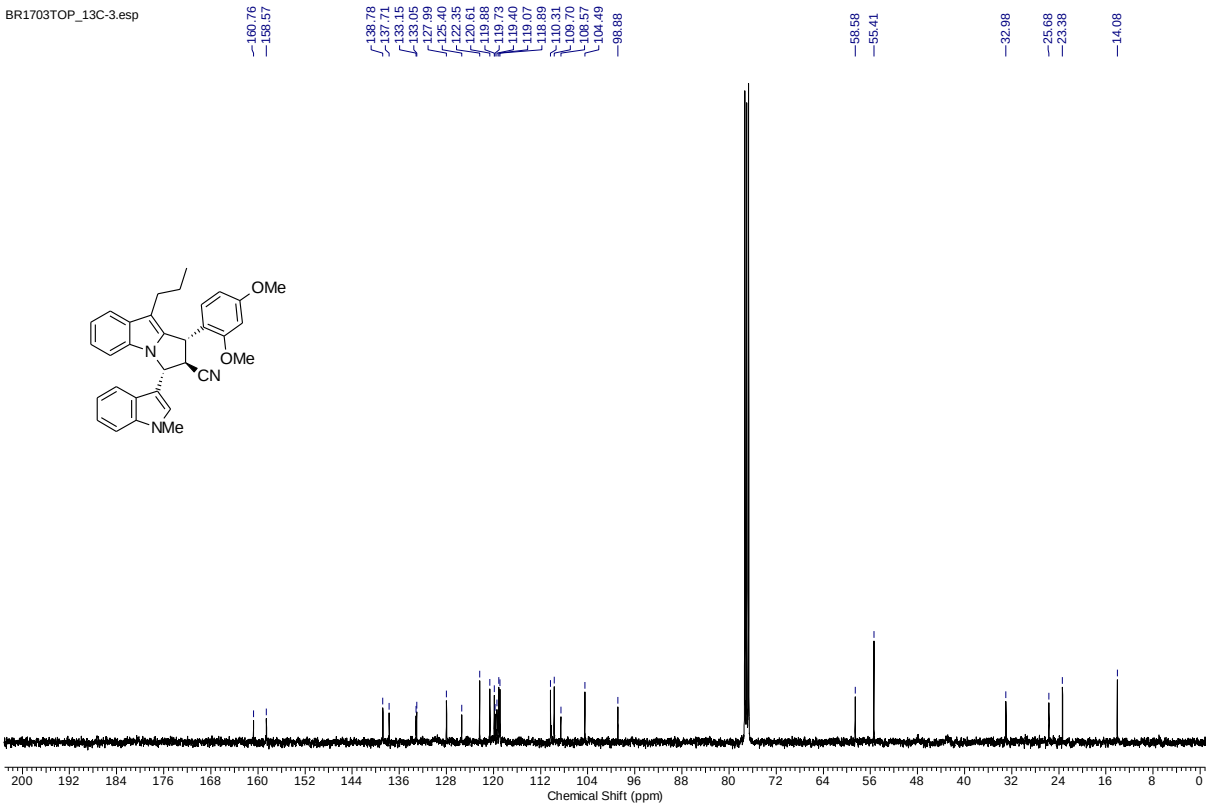
^{1}H and ^{13}C NMR of compound 10a'



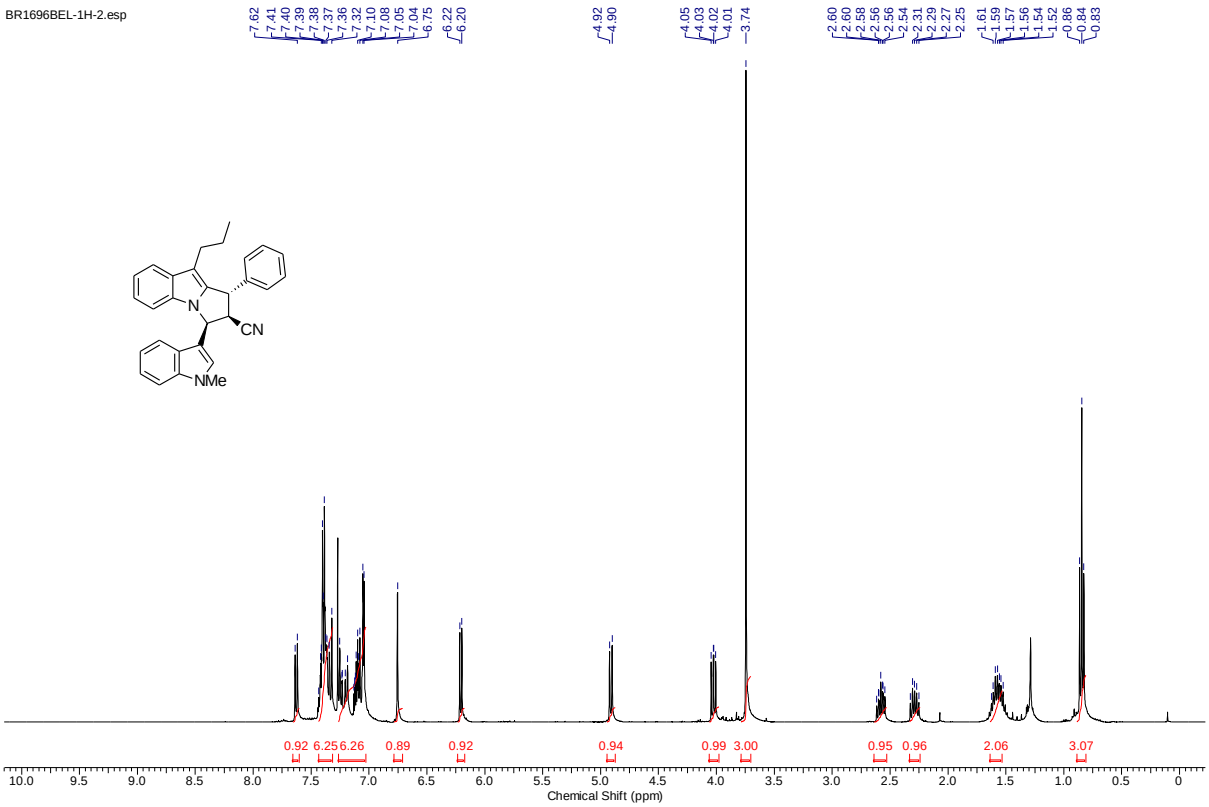


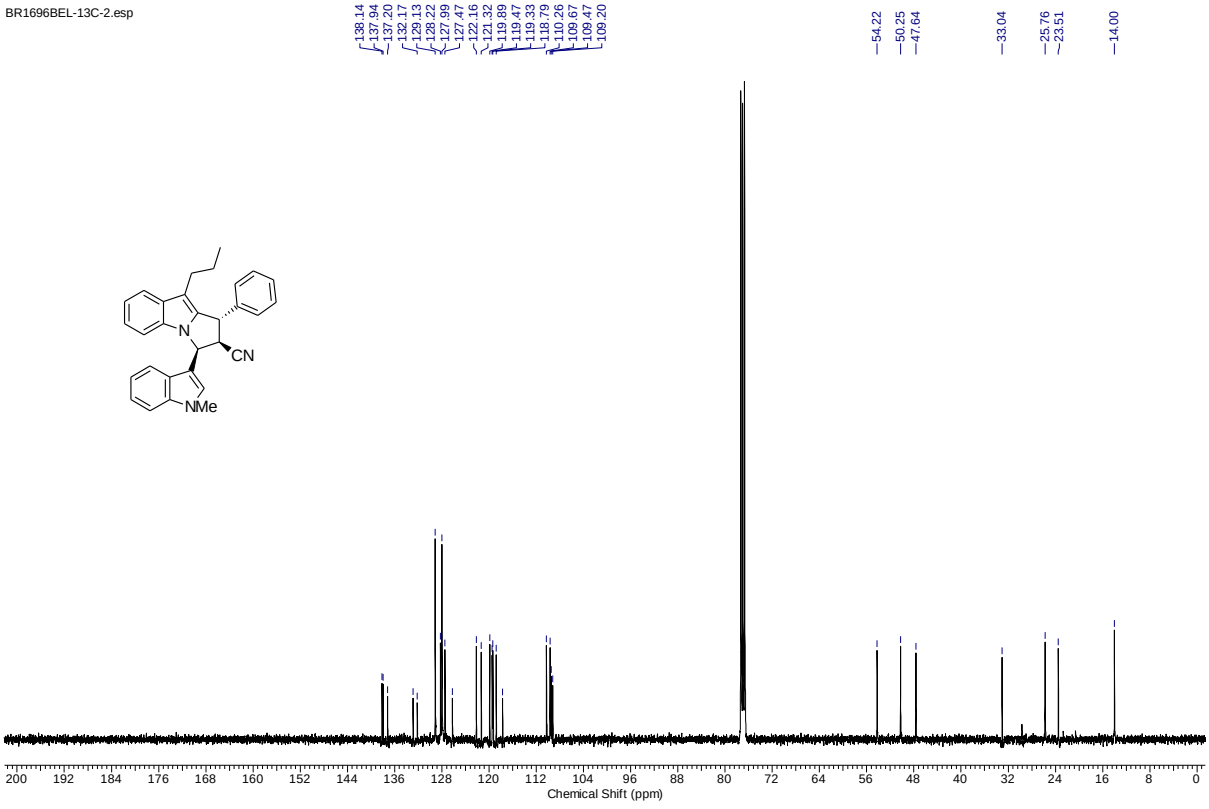
^{1}H and ^{13}C NMR of compound 10a



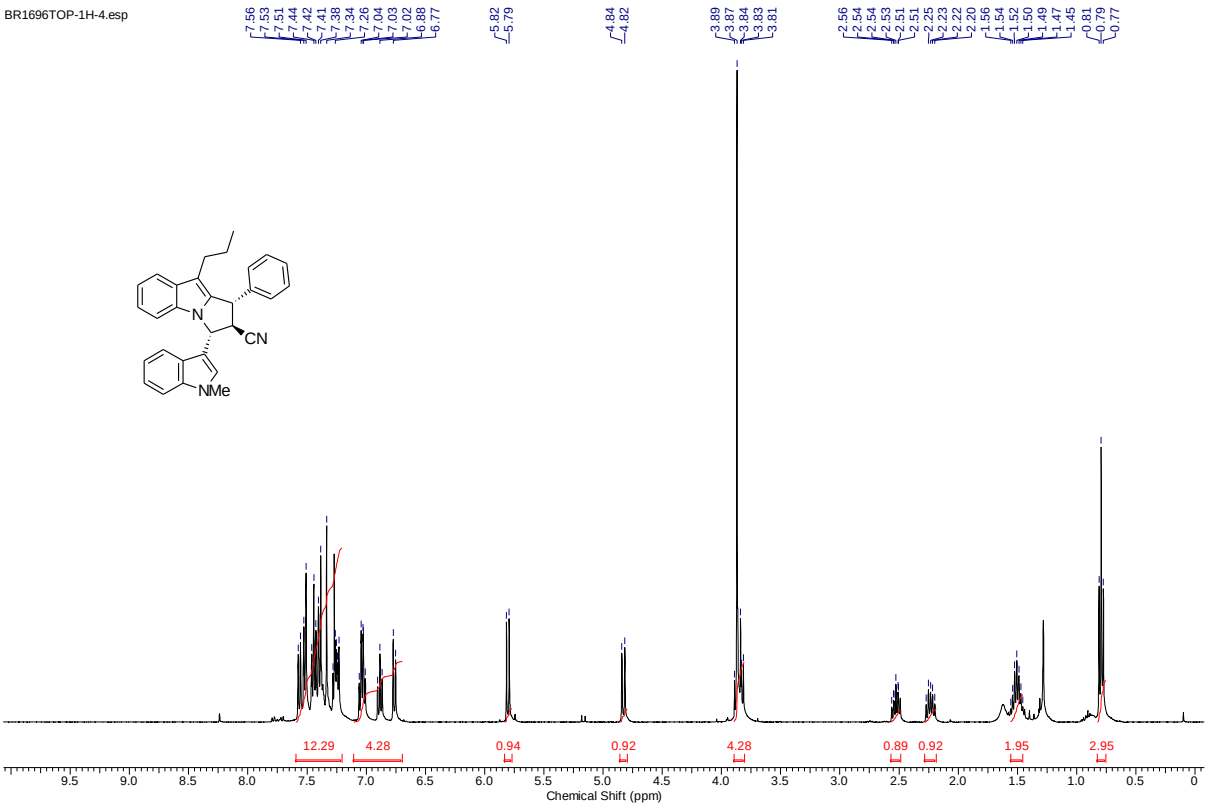


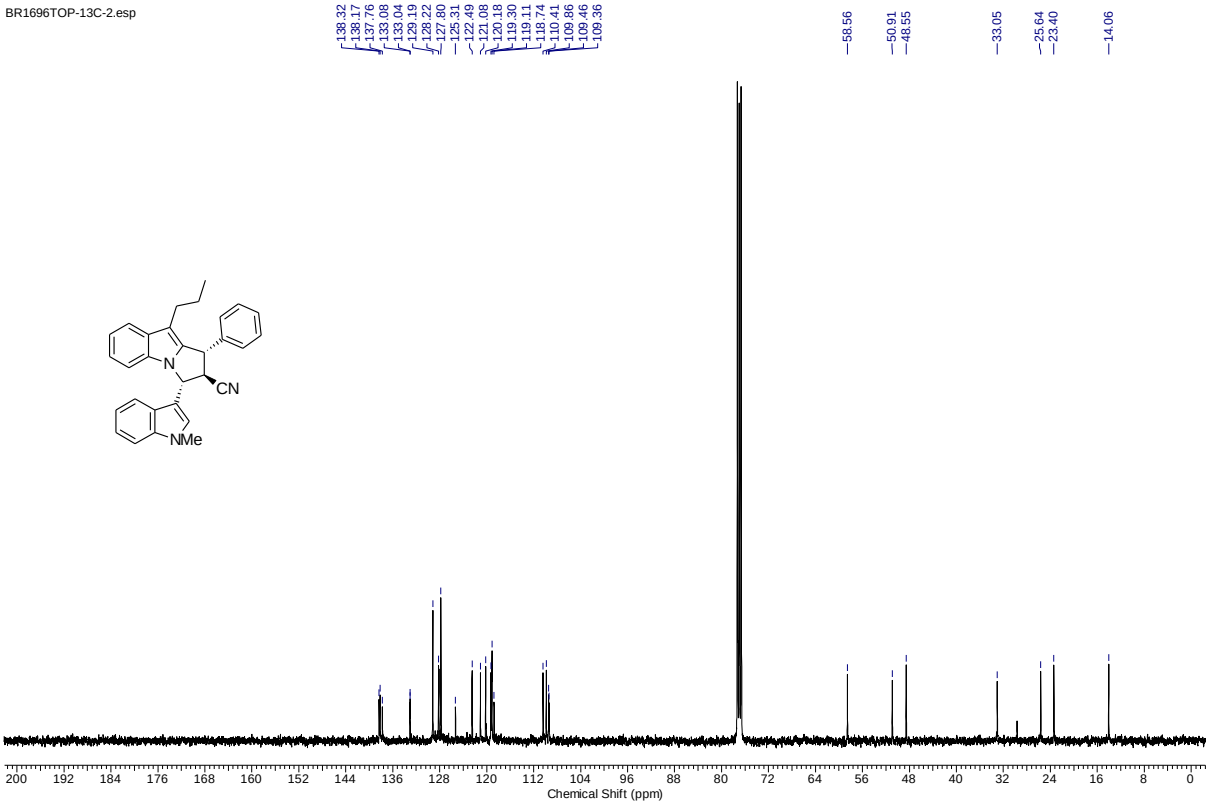
^{1}H and ^{13}C NMR of compound 10b'



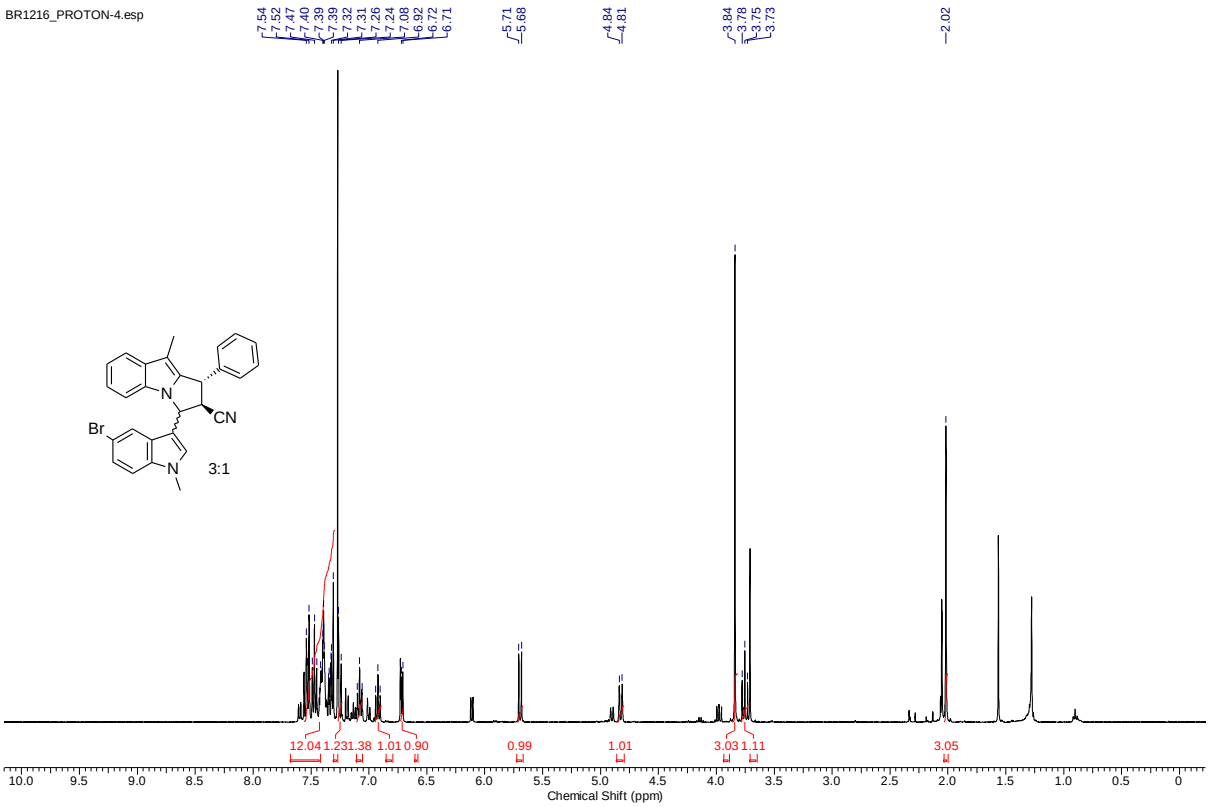


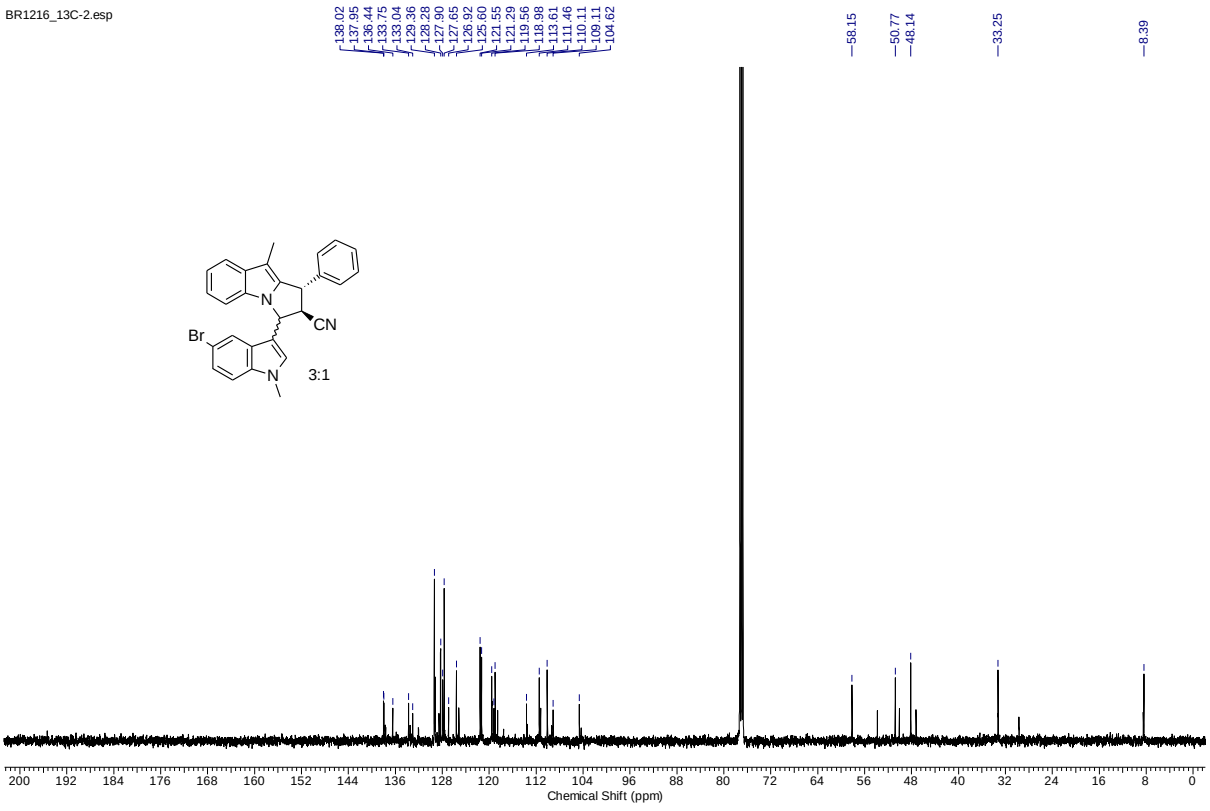
^{1}H and ^{13}C NMR of compound 10b



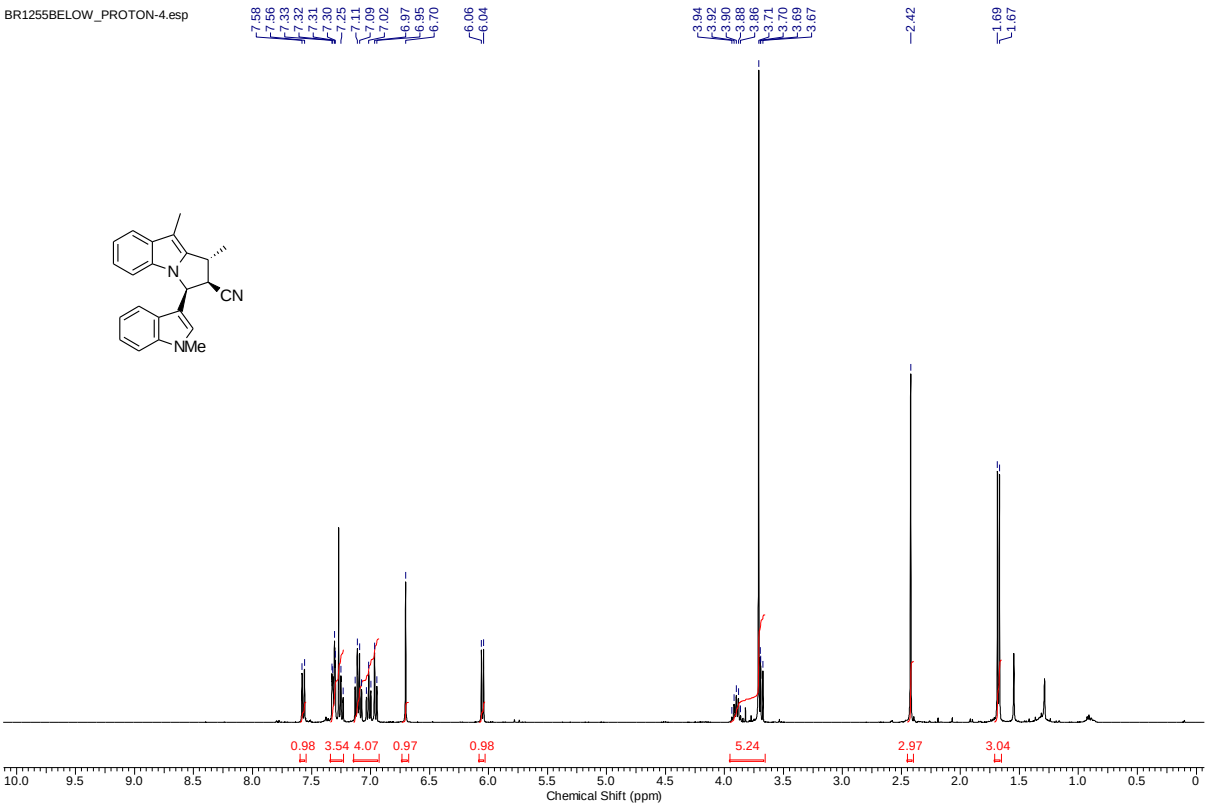


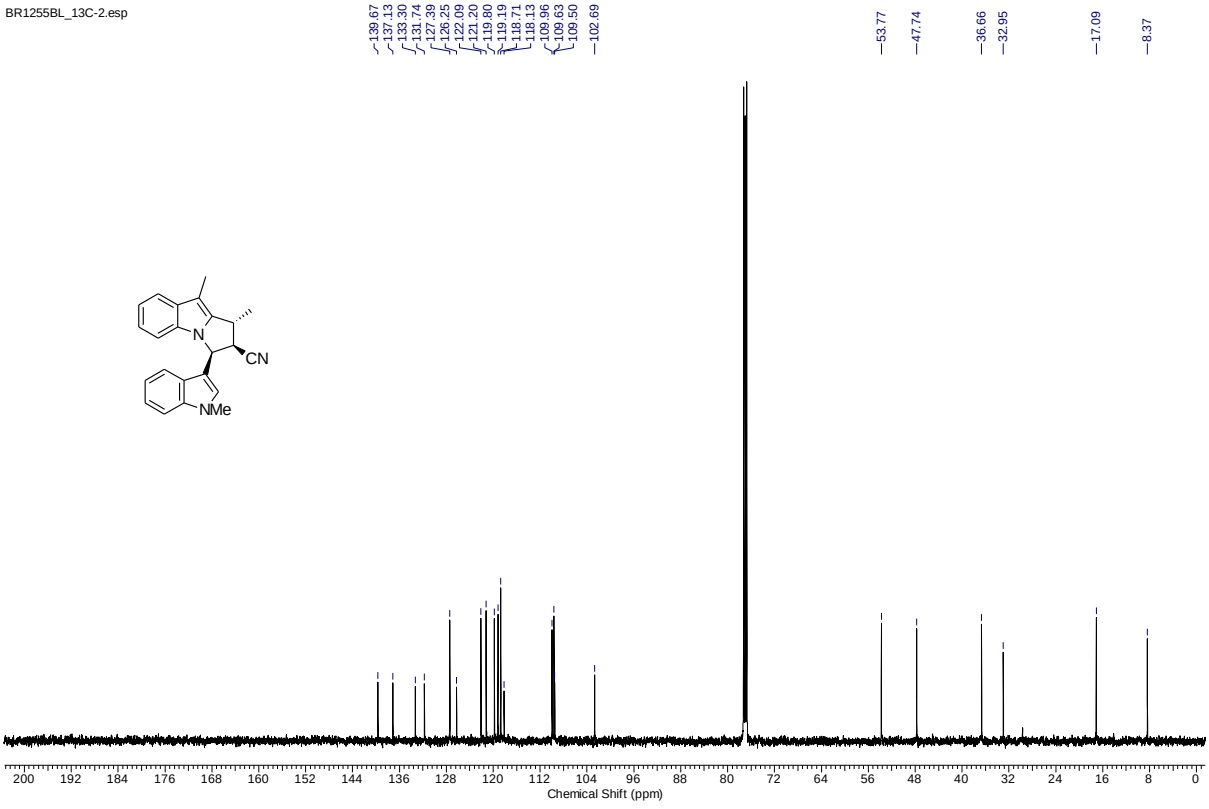
^{1}H and ^{13}C NMR of compound 10c



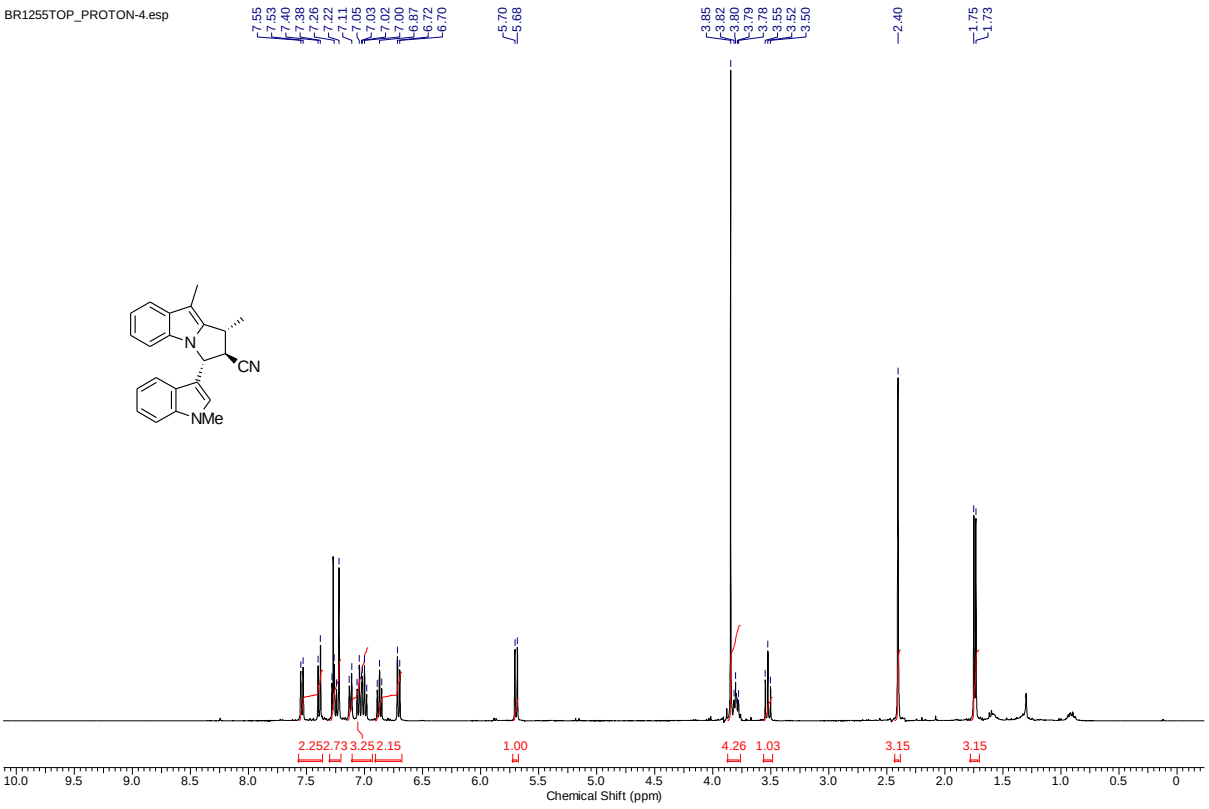


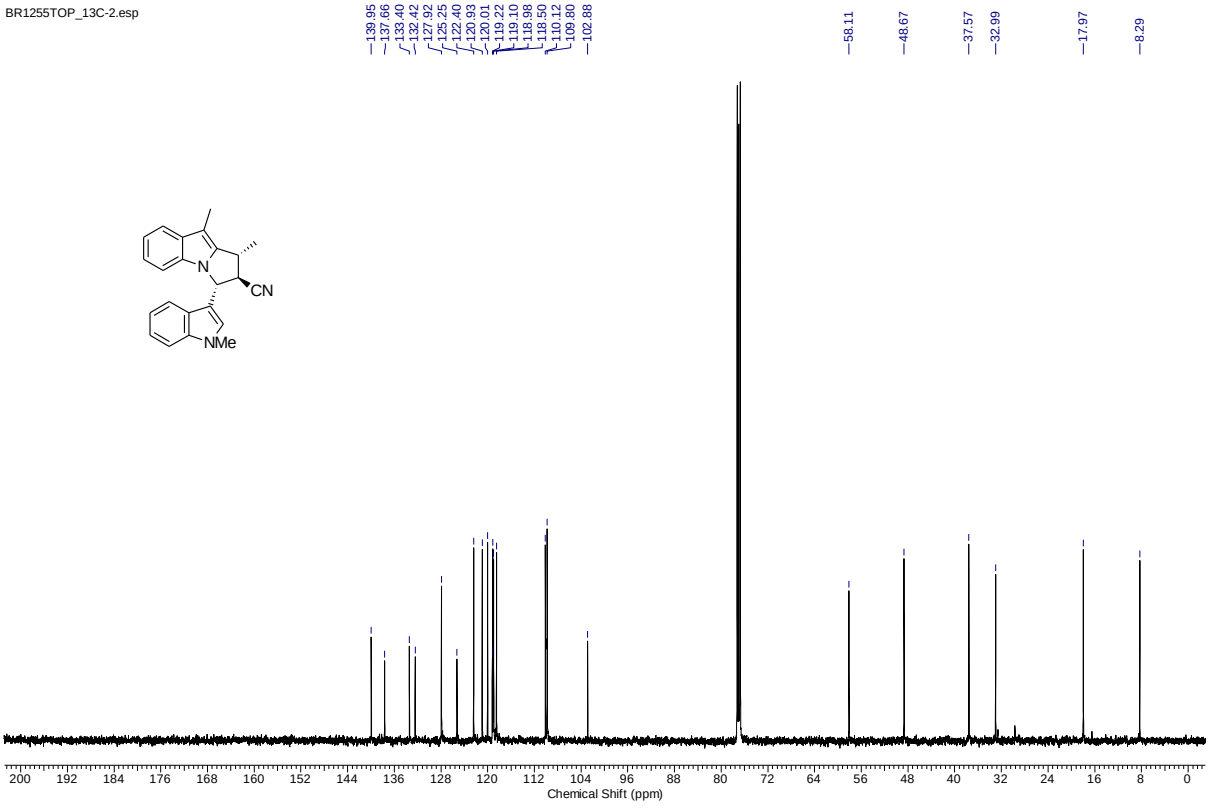
^{1}H and ^{13}C NMR of compound 10d'



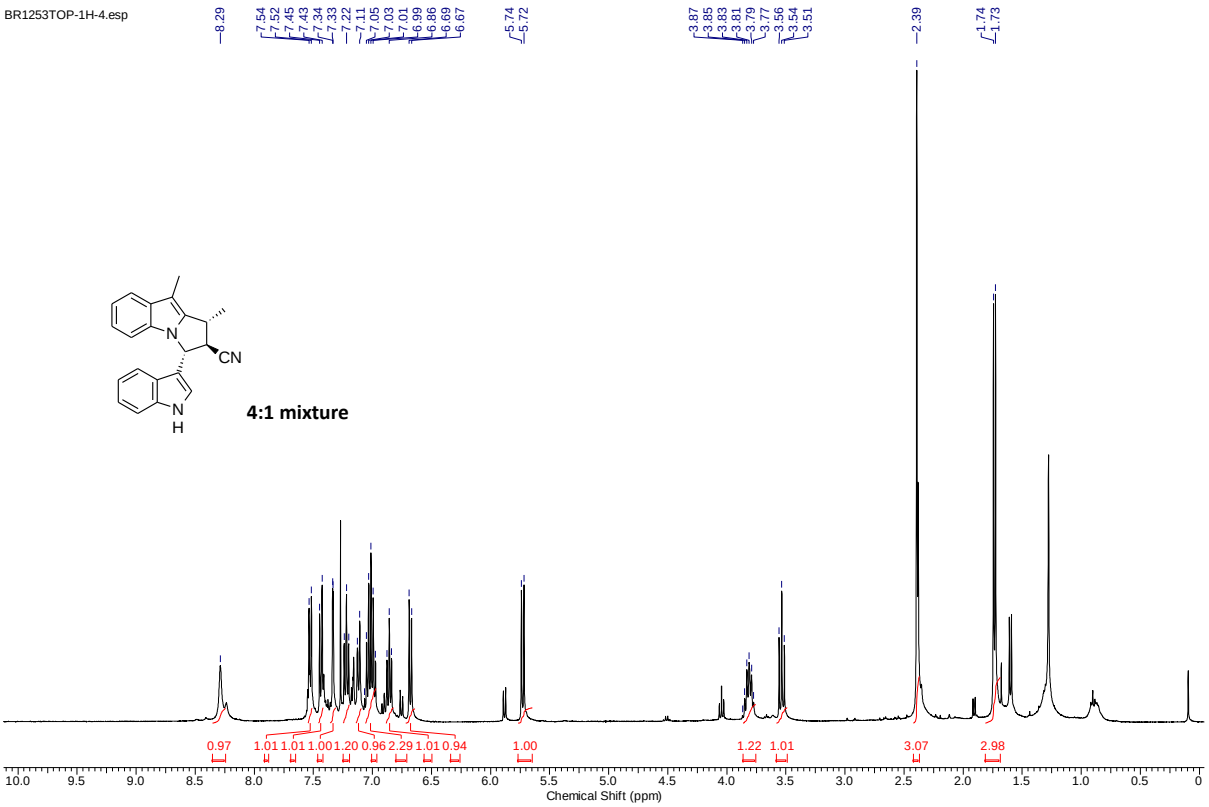


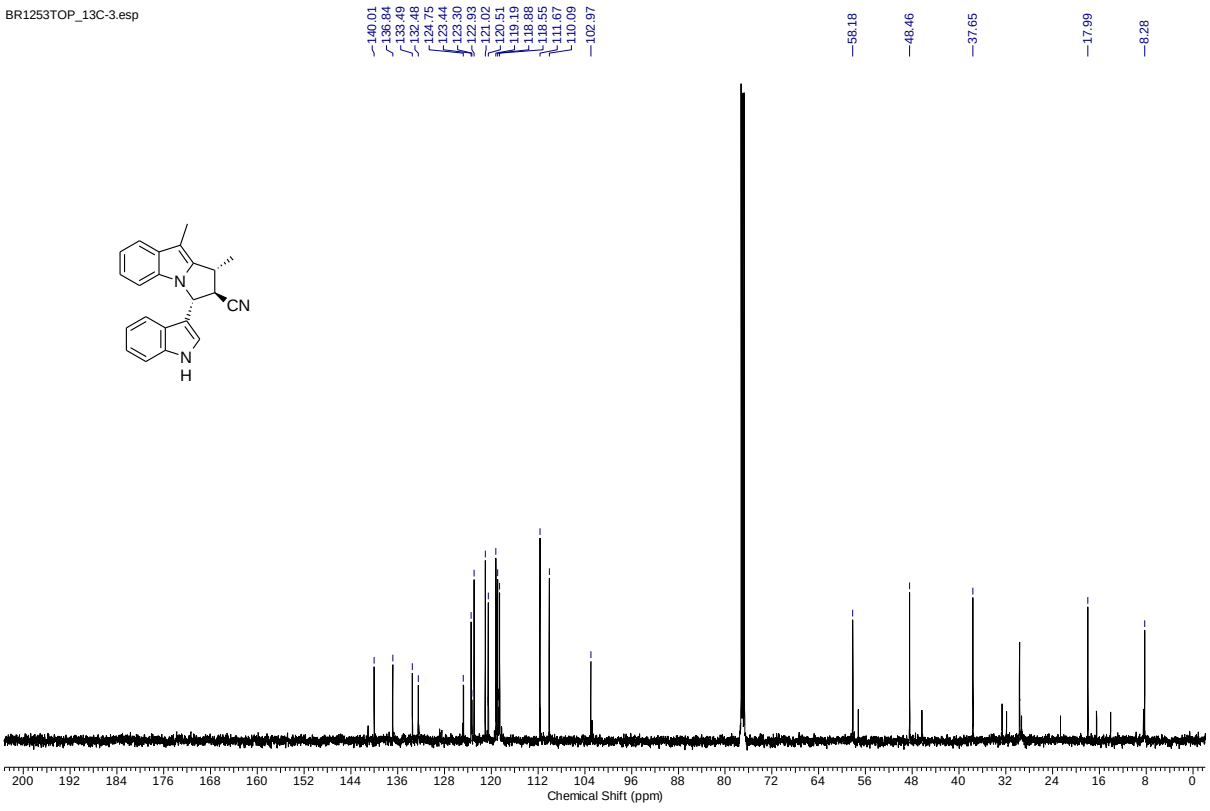
^{1}H and ^{13}C NMR of compound 10d



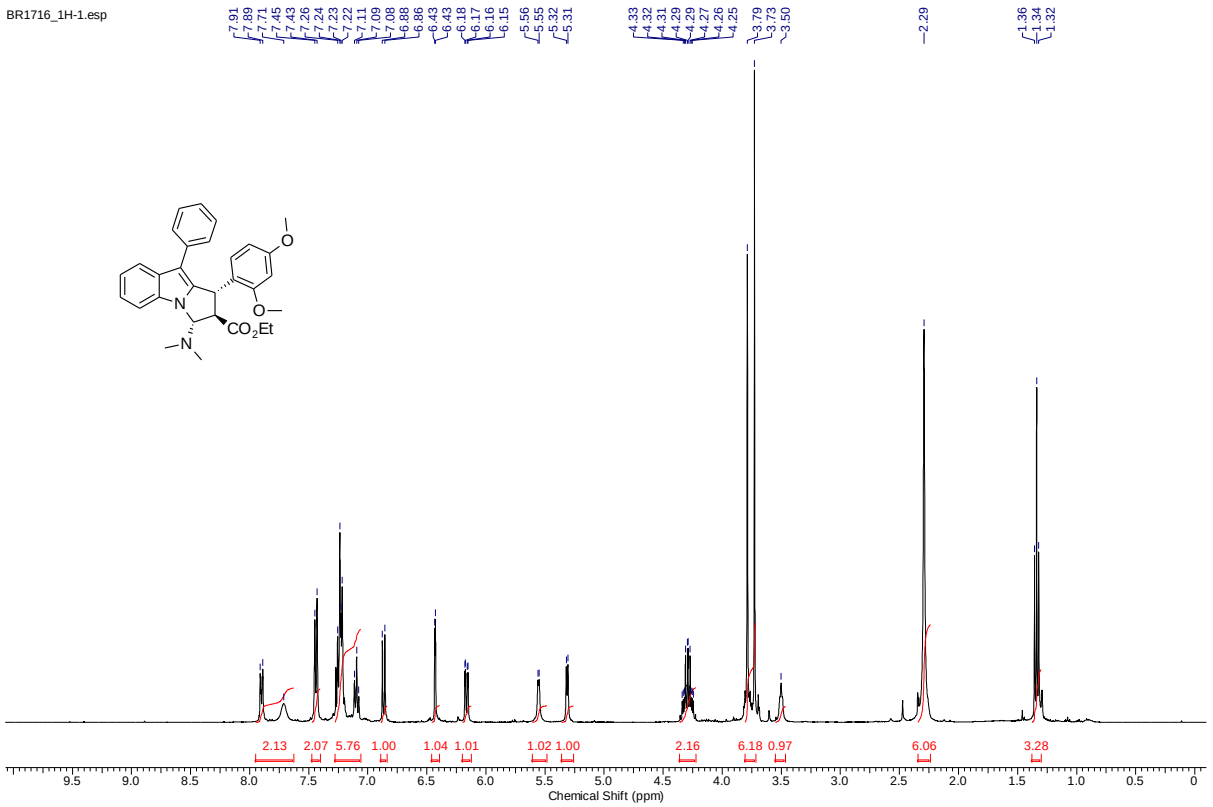


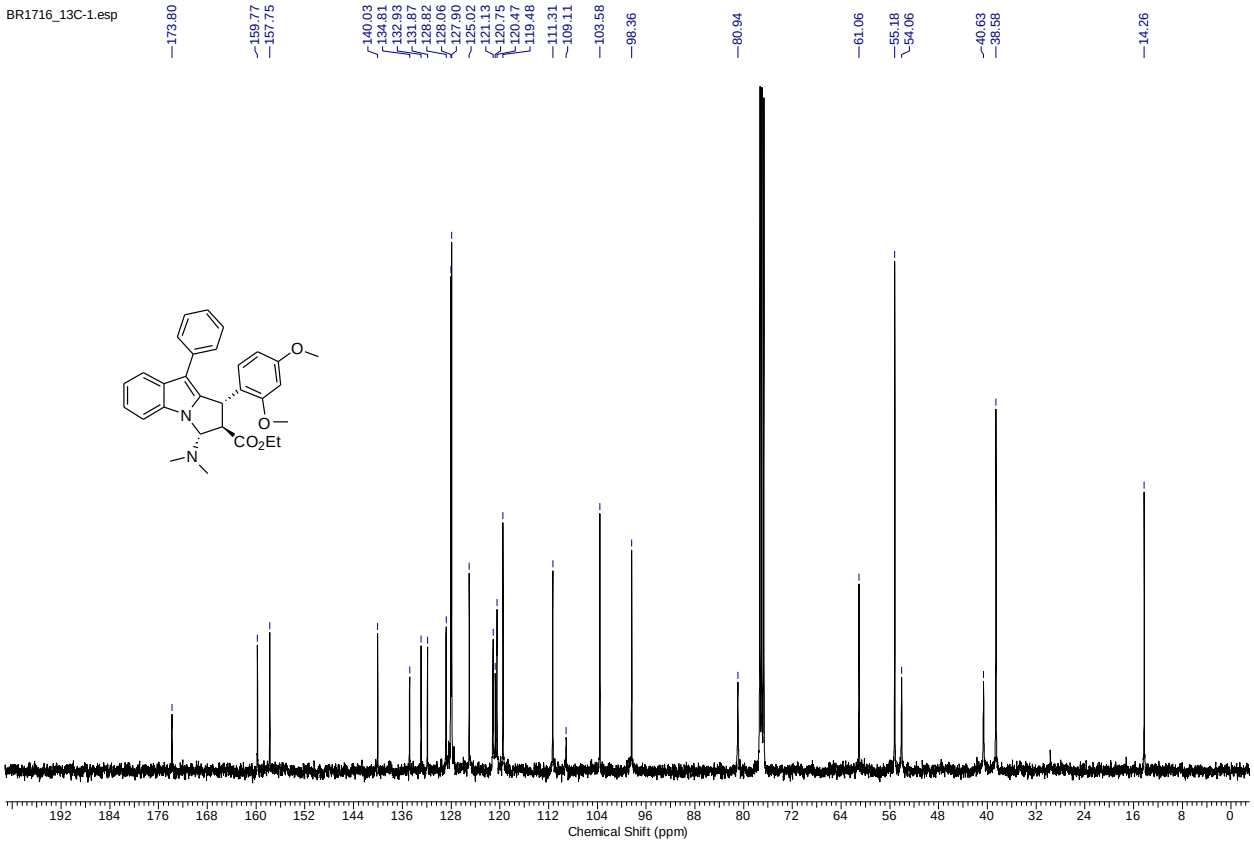
^{1}H and ^{13}C NMR of compound 10e



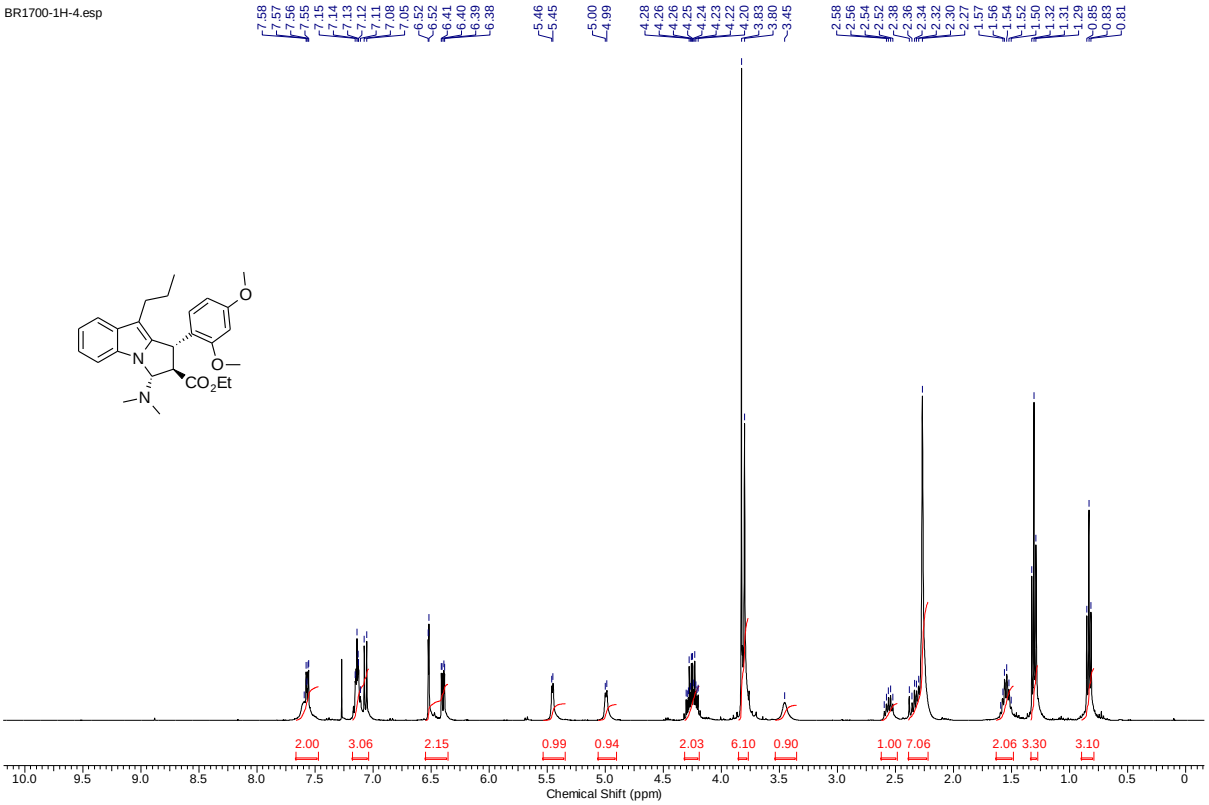


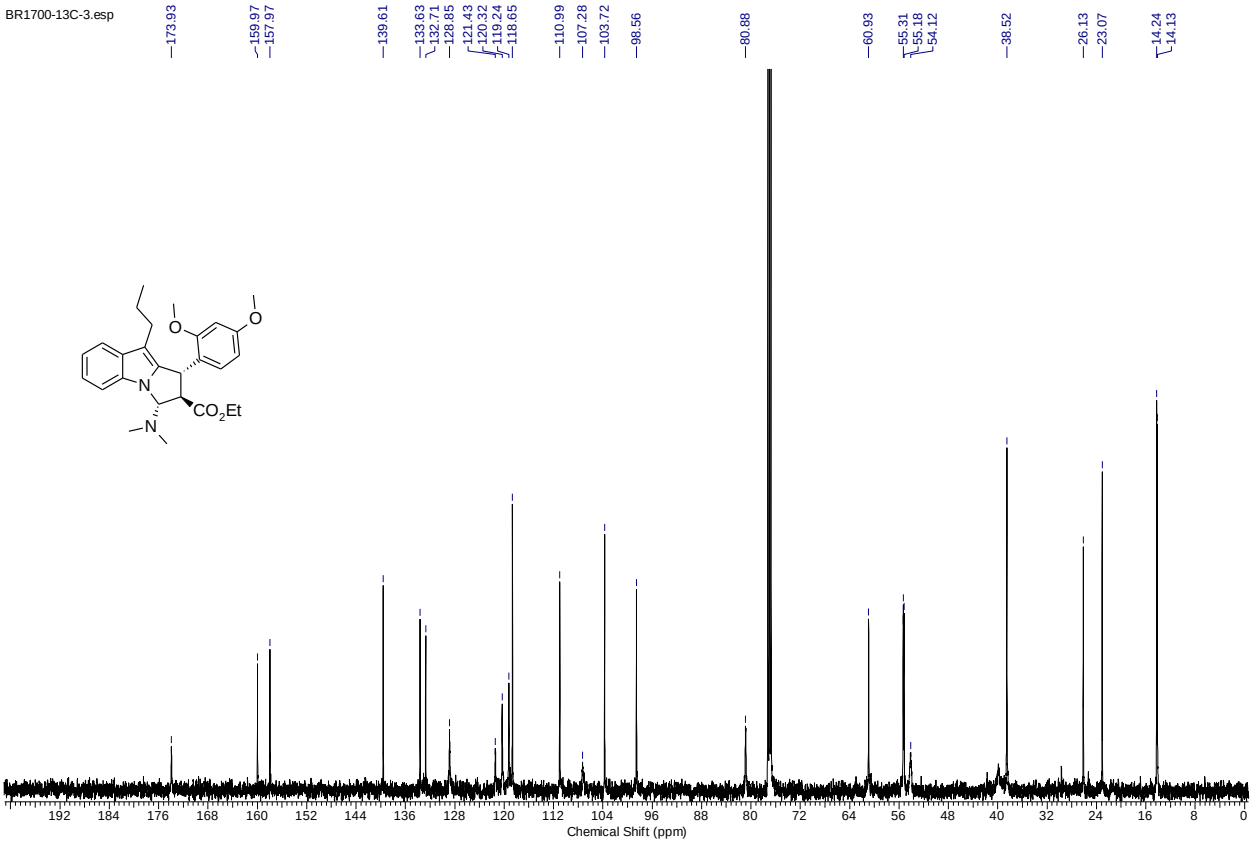
^{1}H and ^{13}C NMR of compound 12a



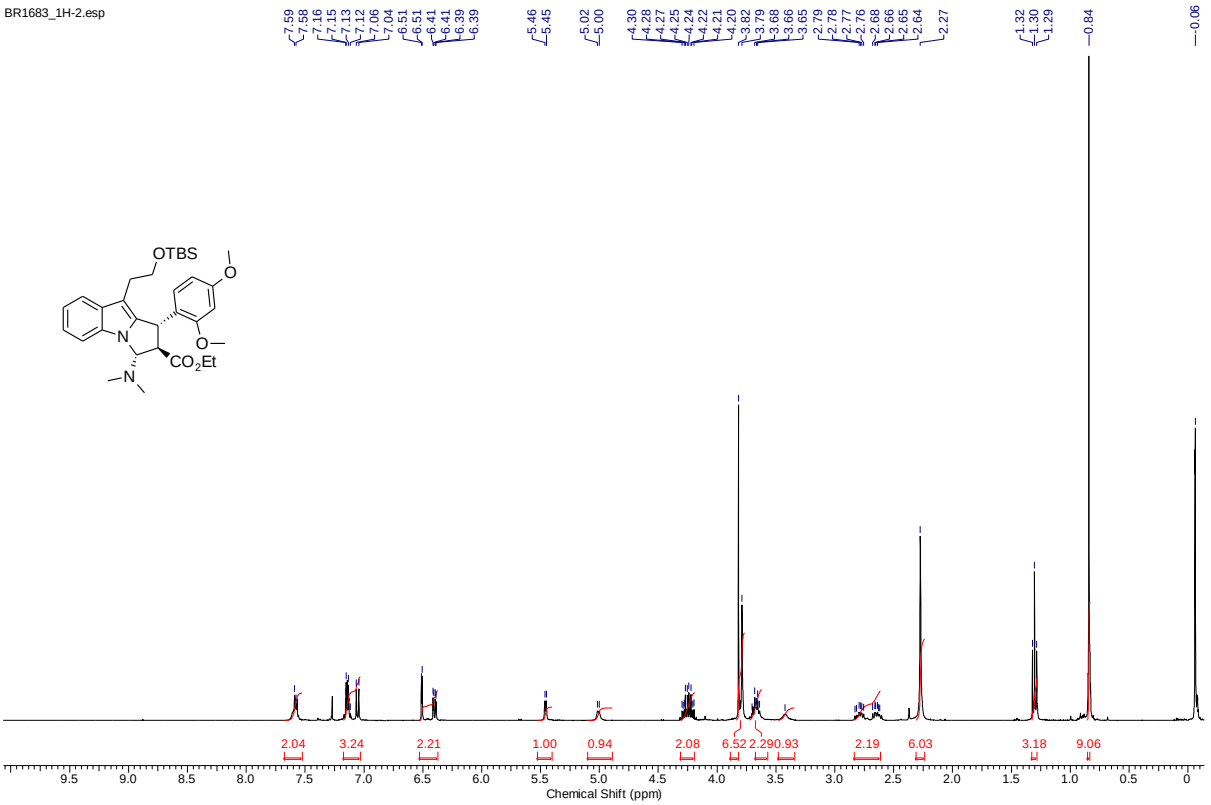


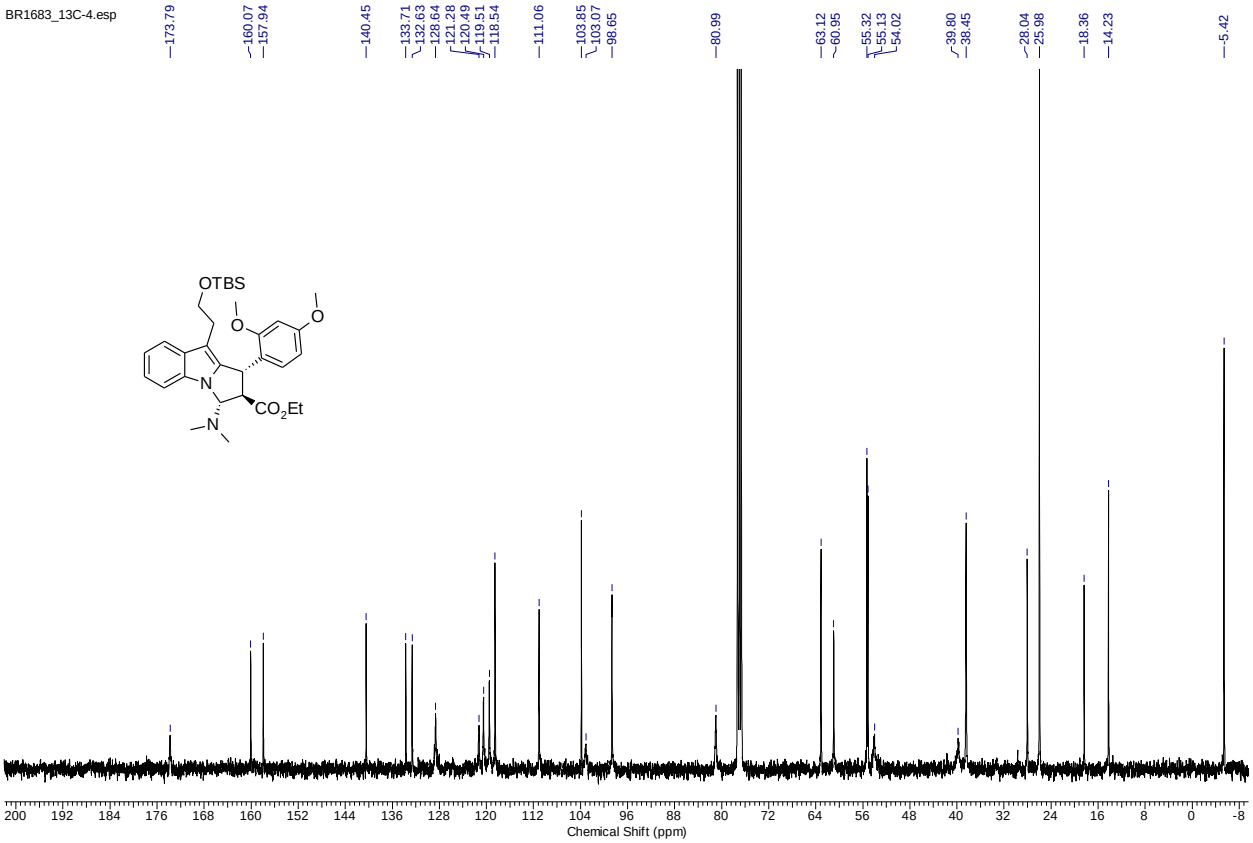
^{1}H and ^{13}C NMR of compound 12b



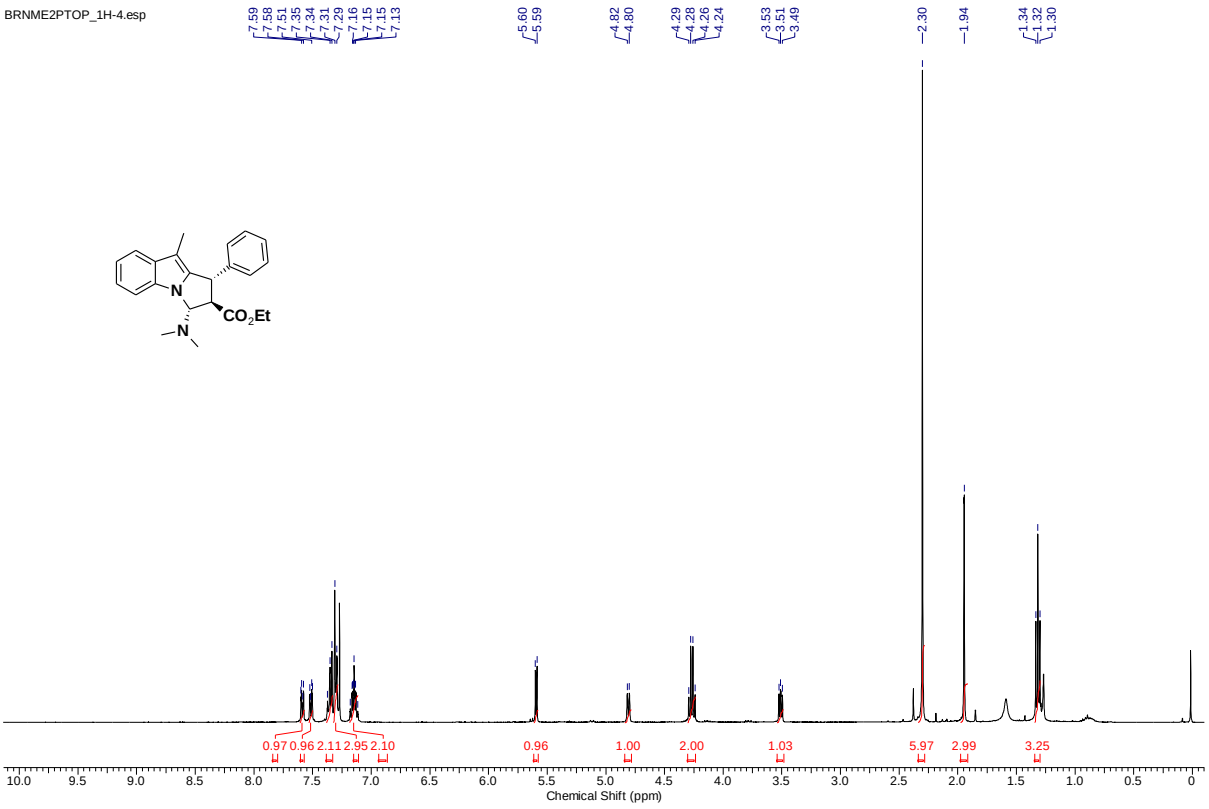


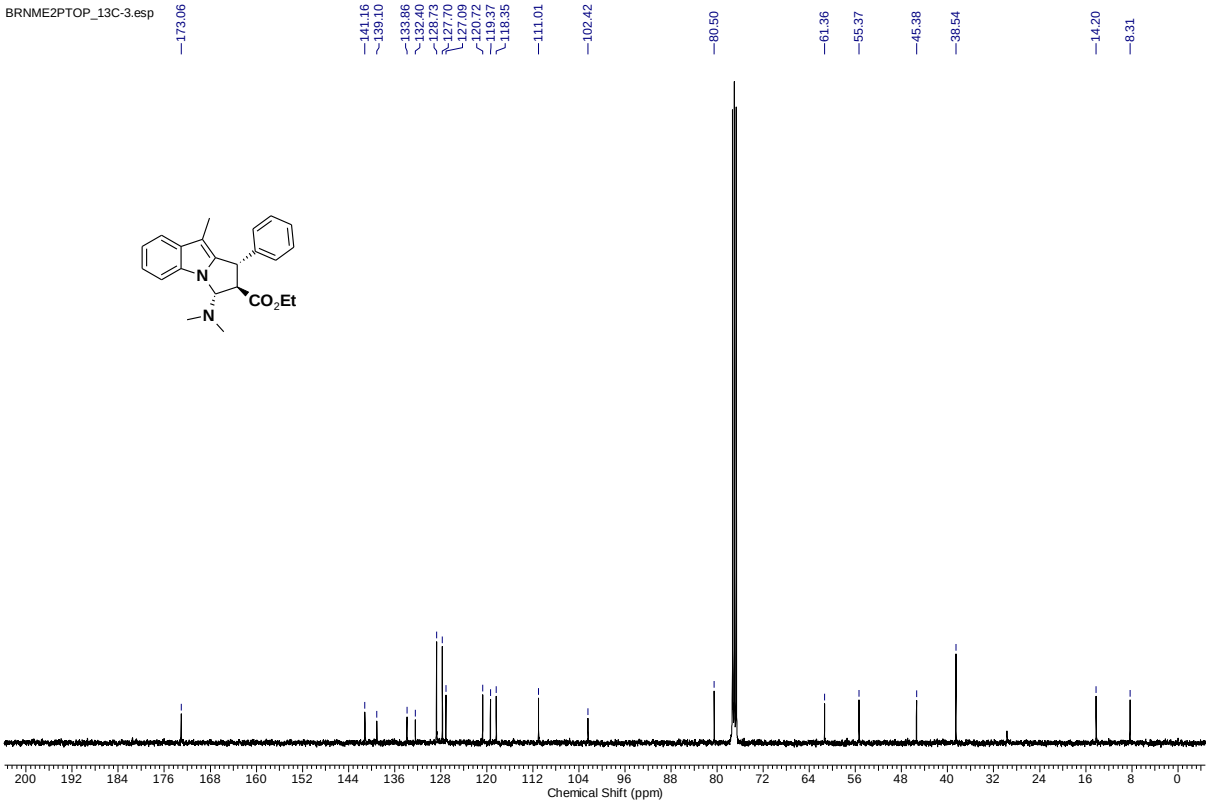
^{1}H and ^{13}C NMR of compound 12c



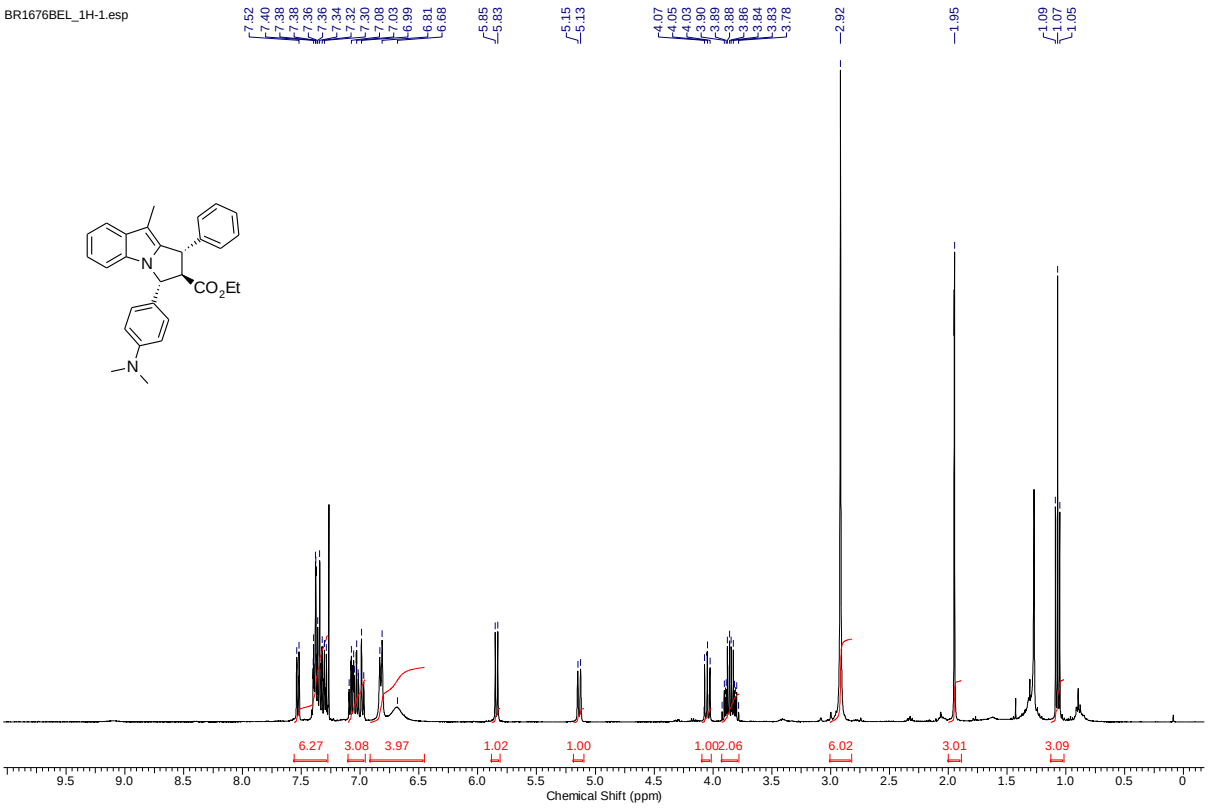


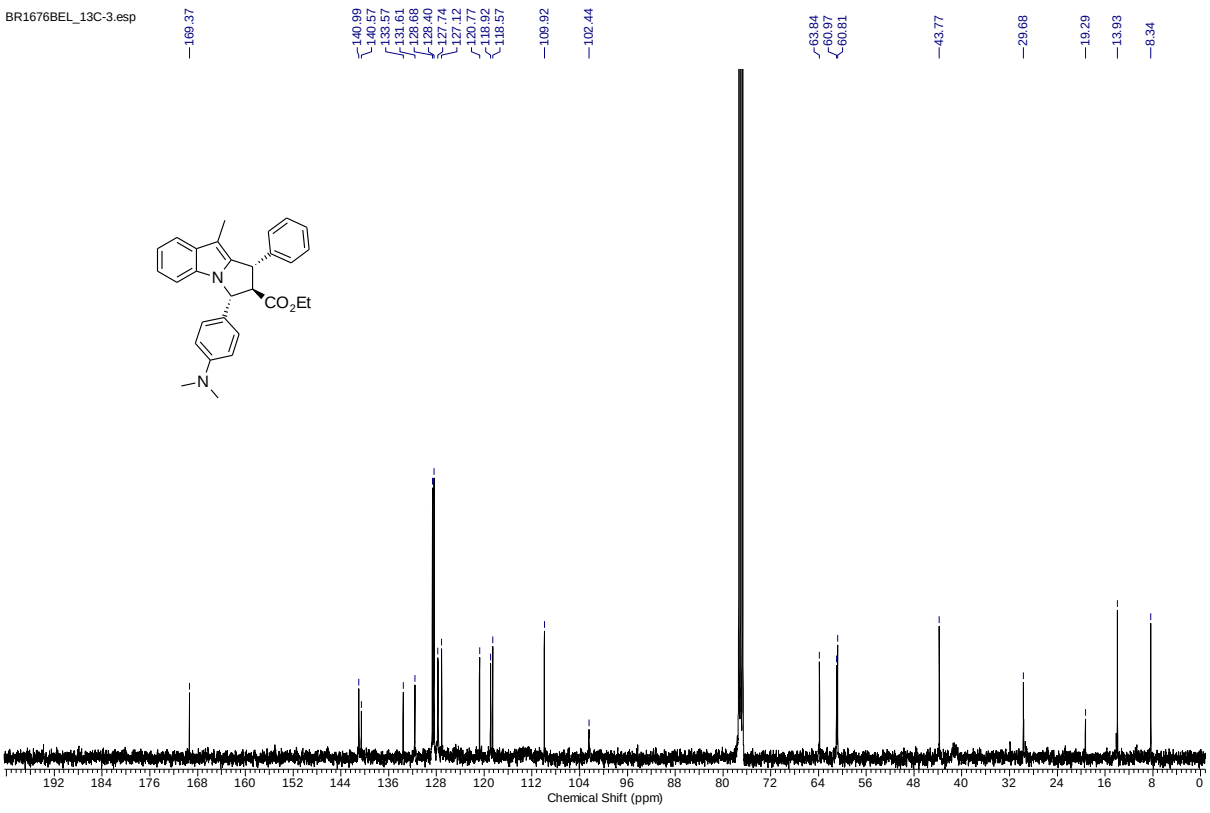
^{1}H and ^{13}C NMR of compound 12d



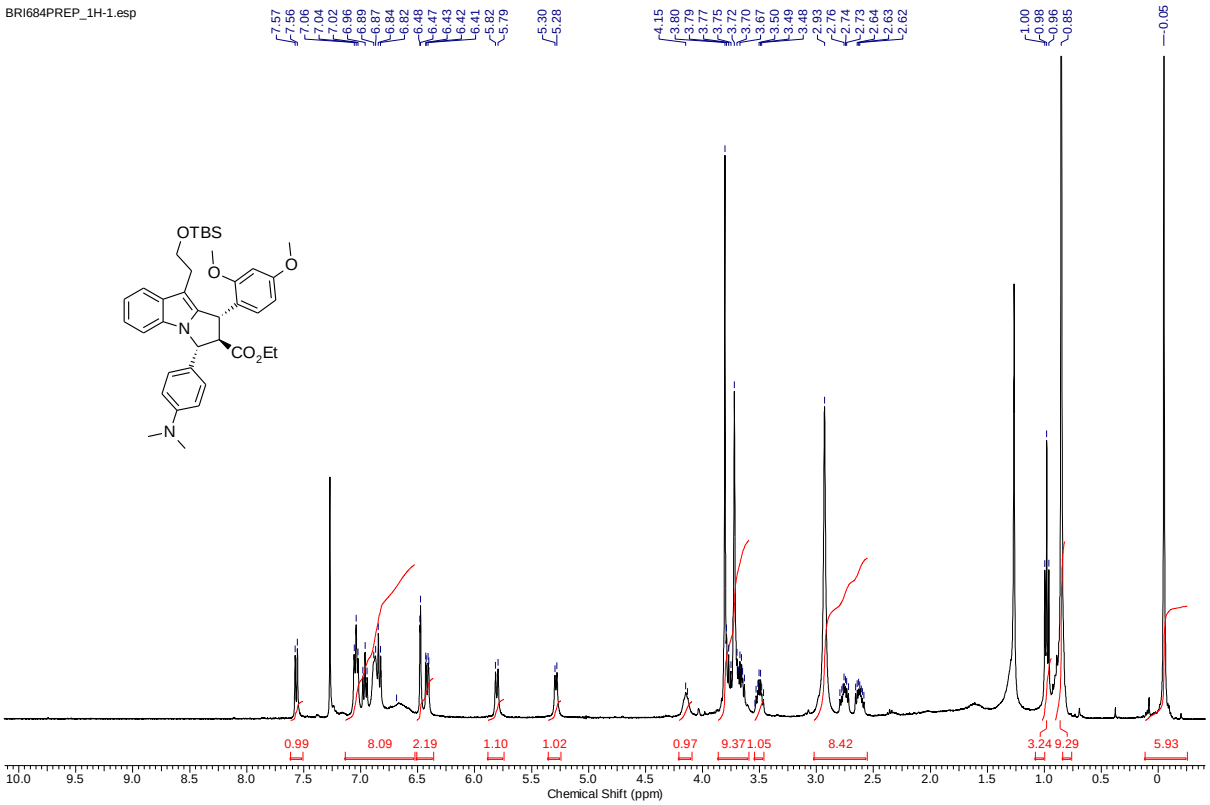


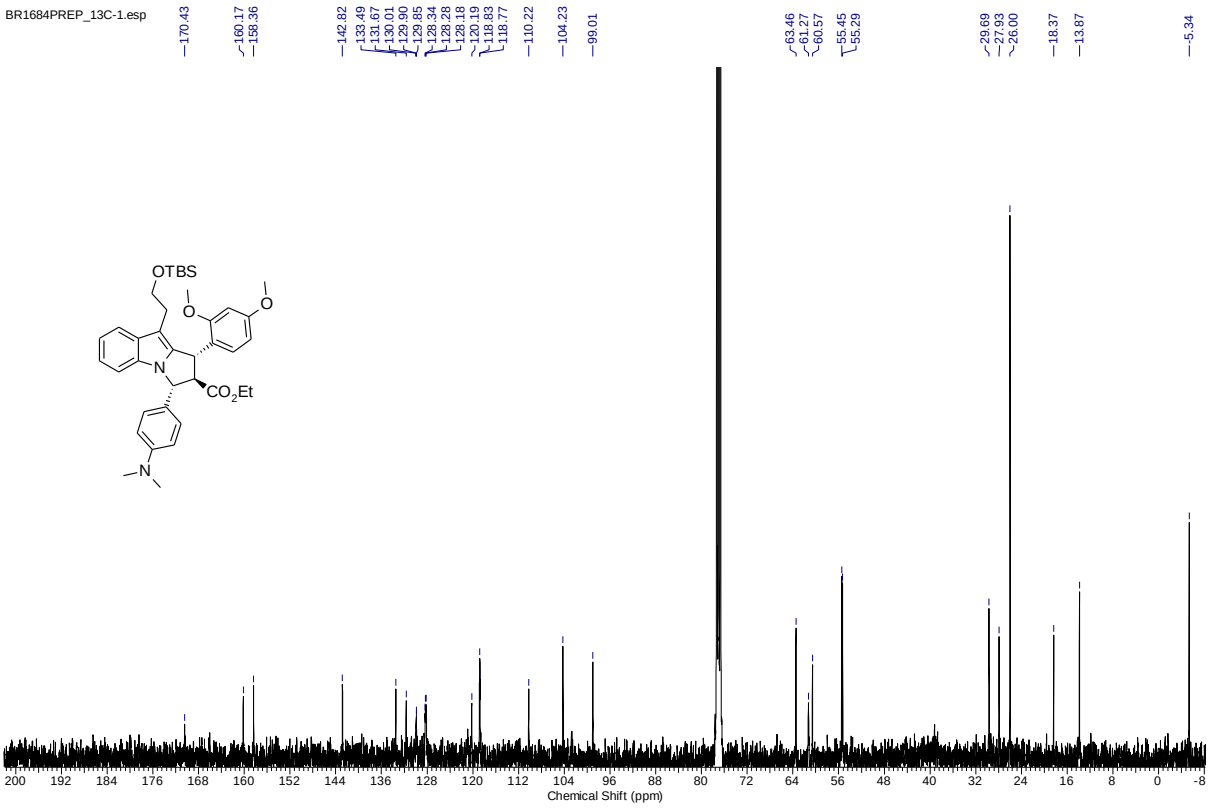
^{1}H and ^{13}C NMR of compound 14a



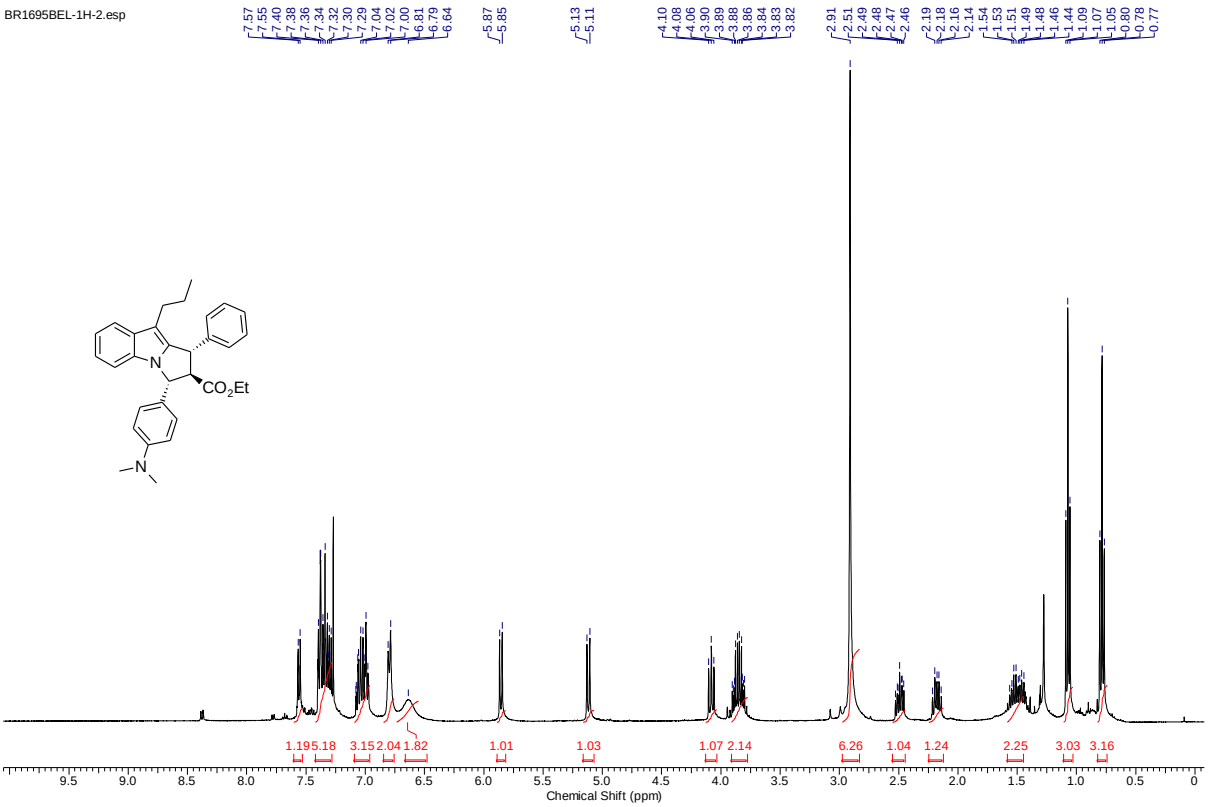


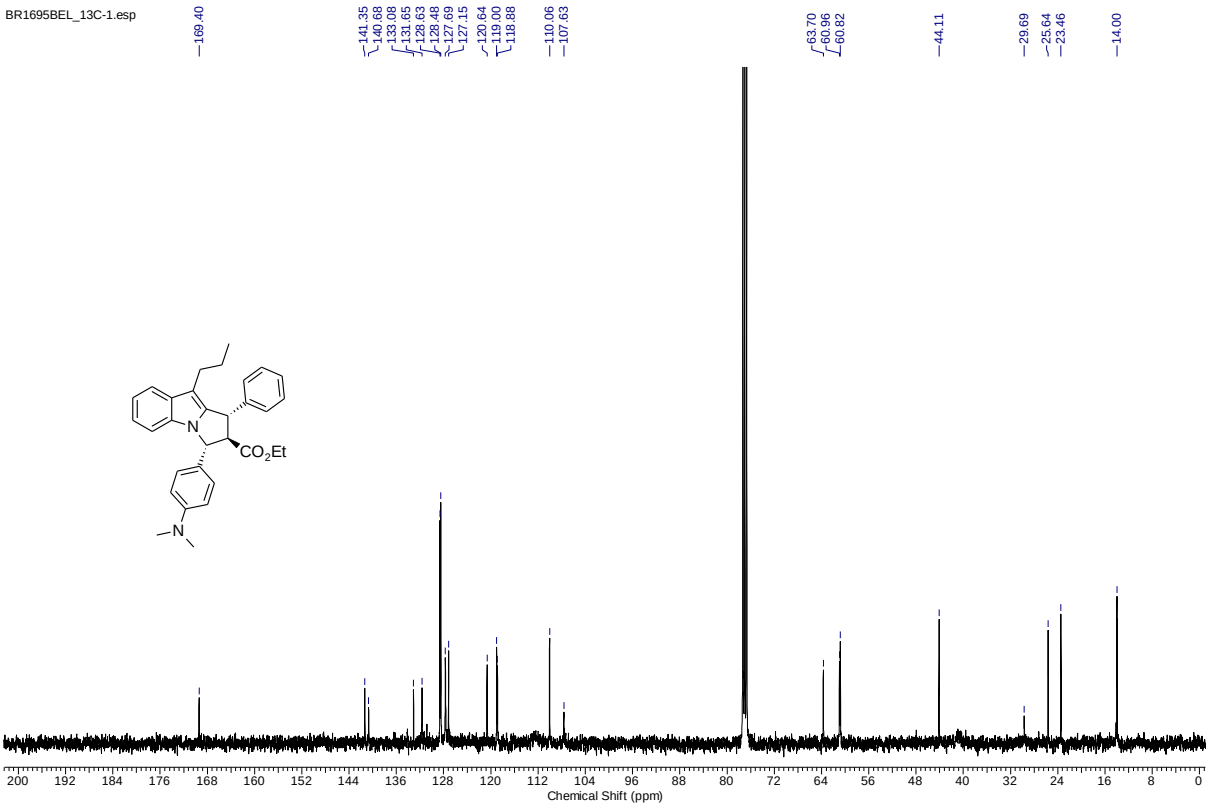
^{1}H and ^{13}C NMR of compound 14b



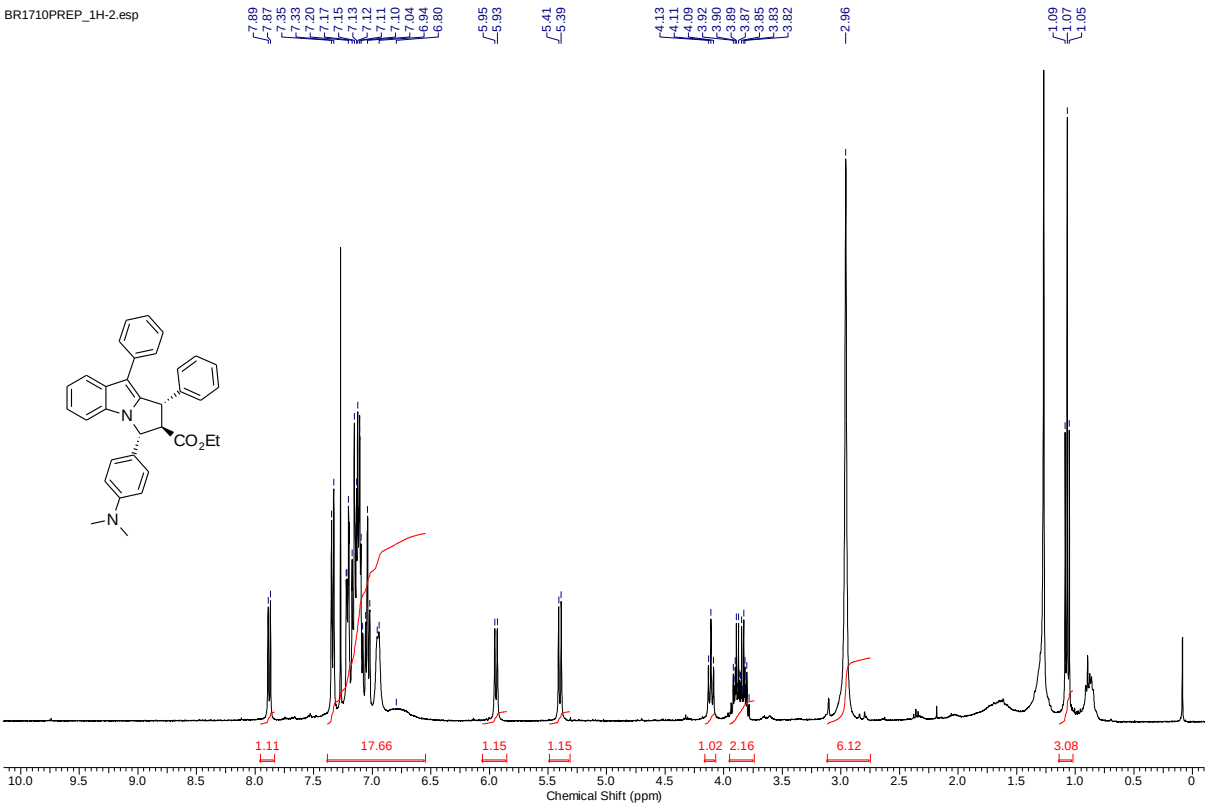


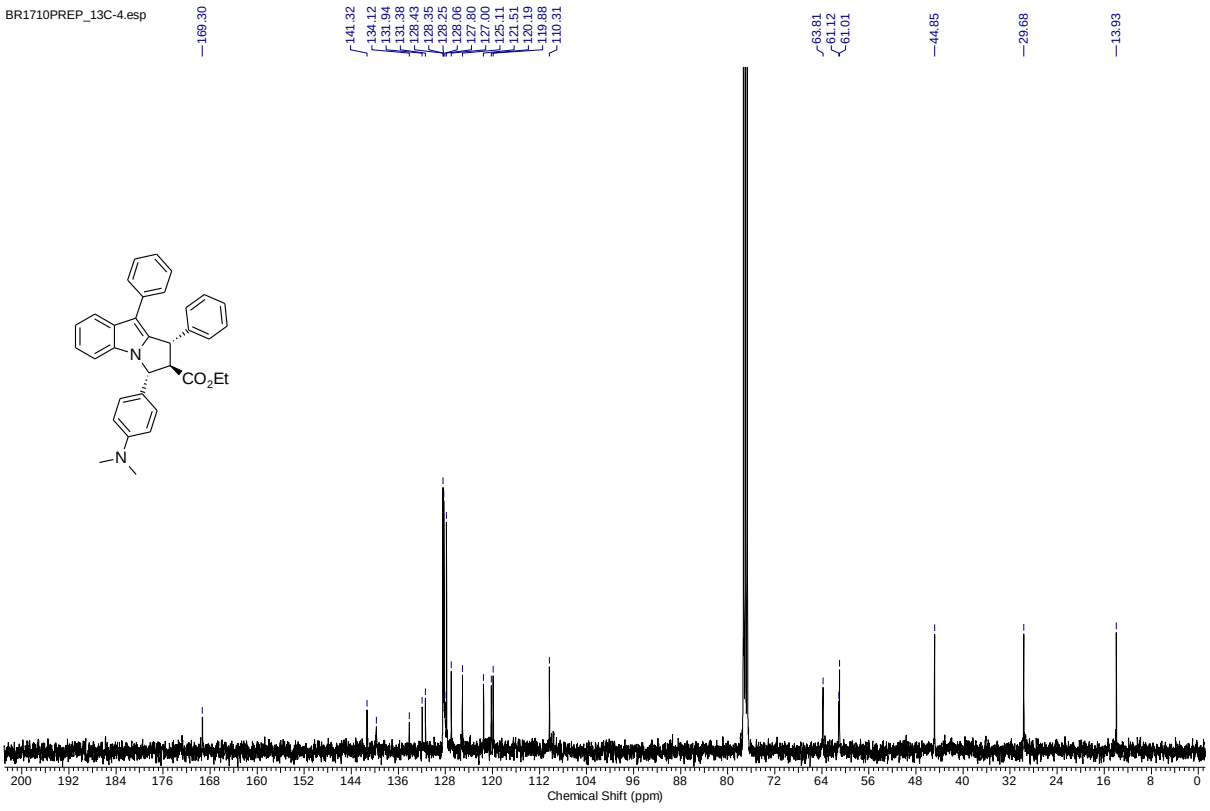
^{1}H and ^{13}C NMR of compound 14c



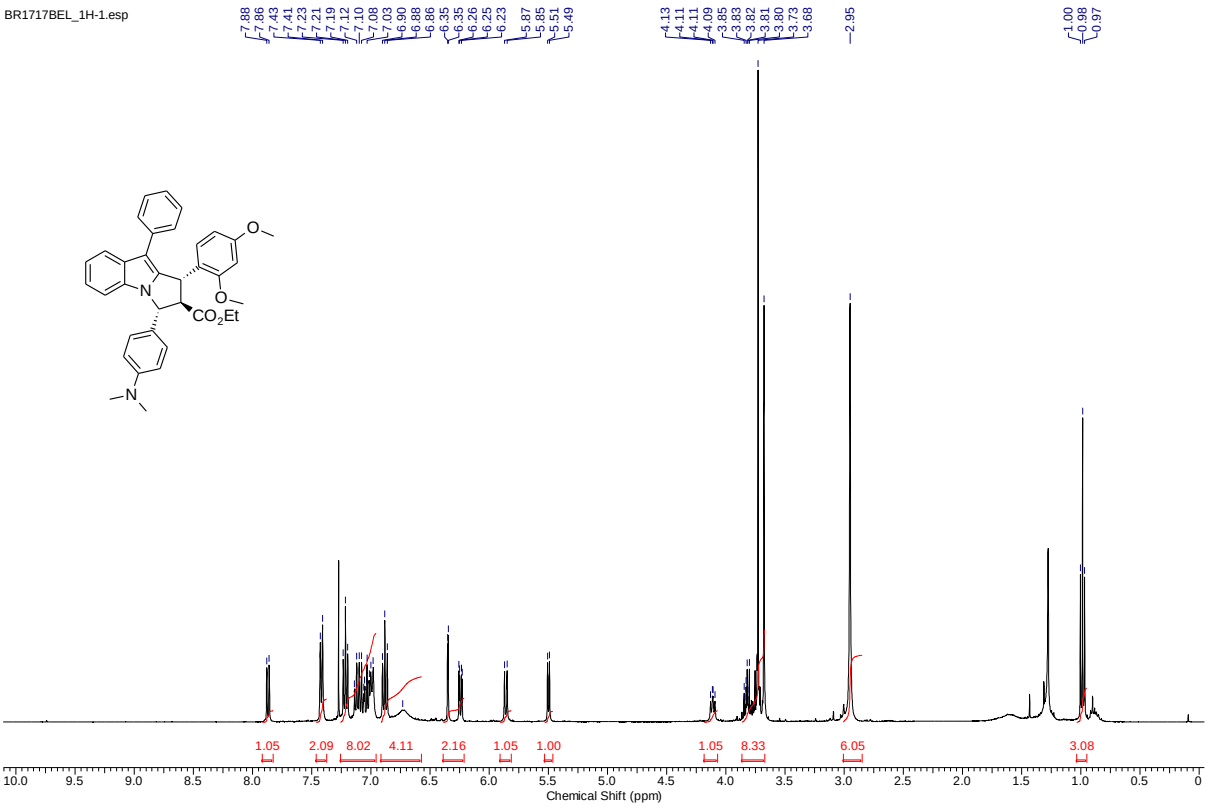


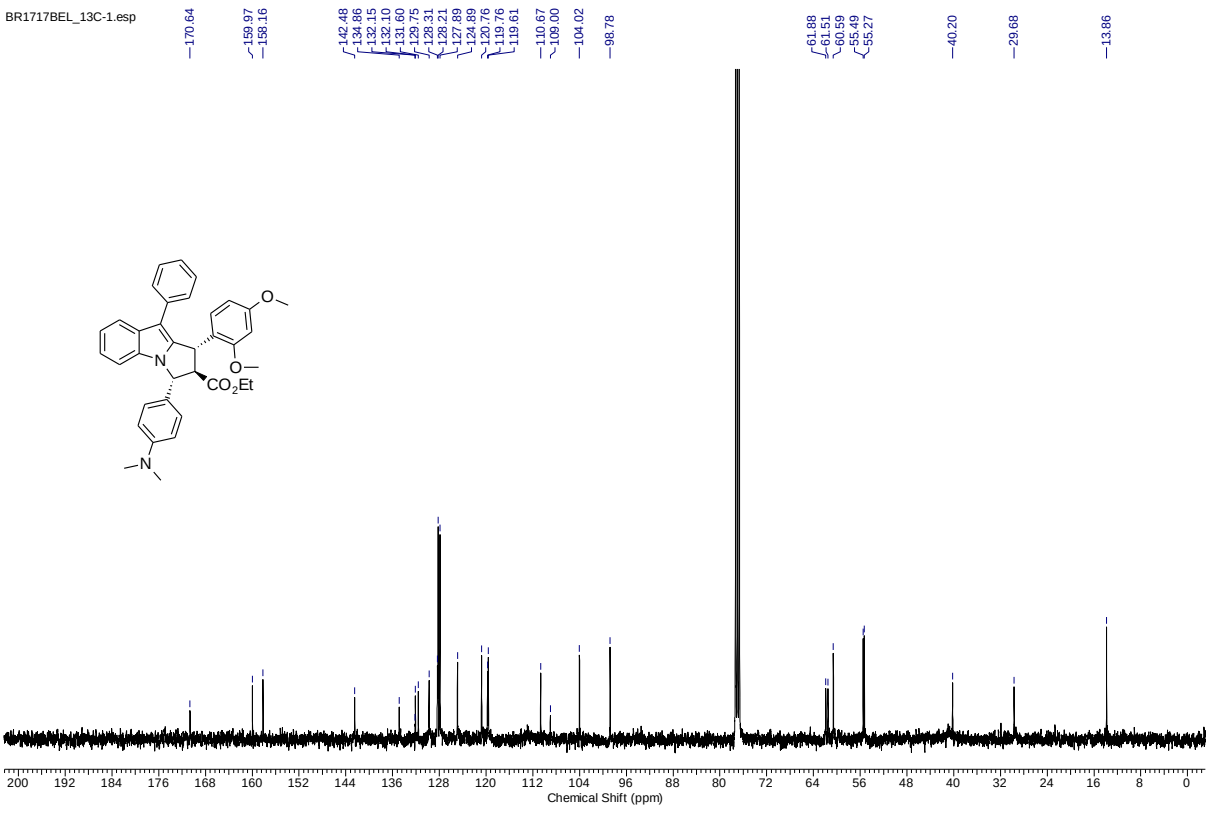
^{1}H and ^{13}C NMR of compound 14d



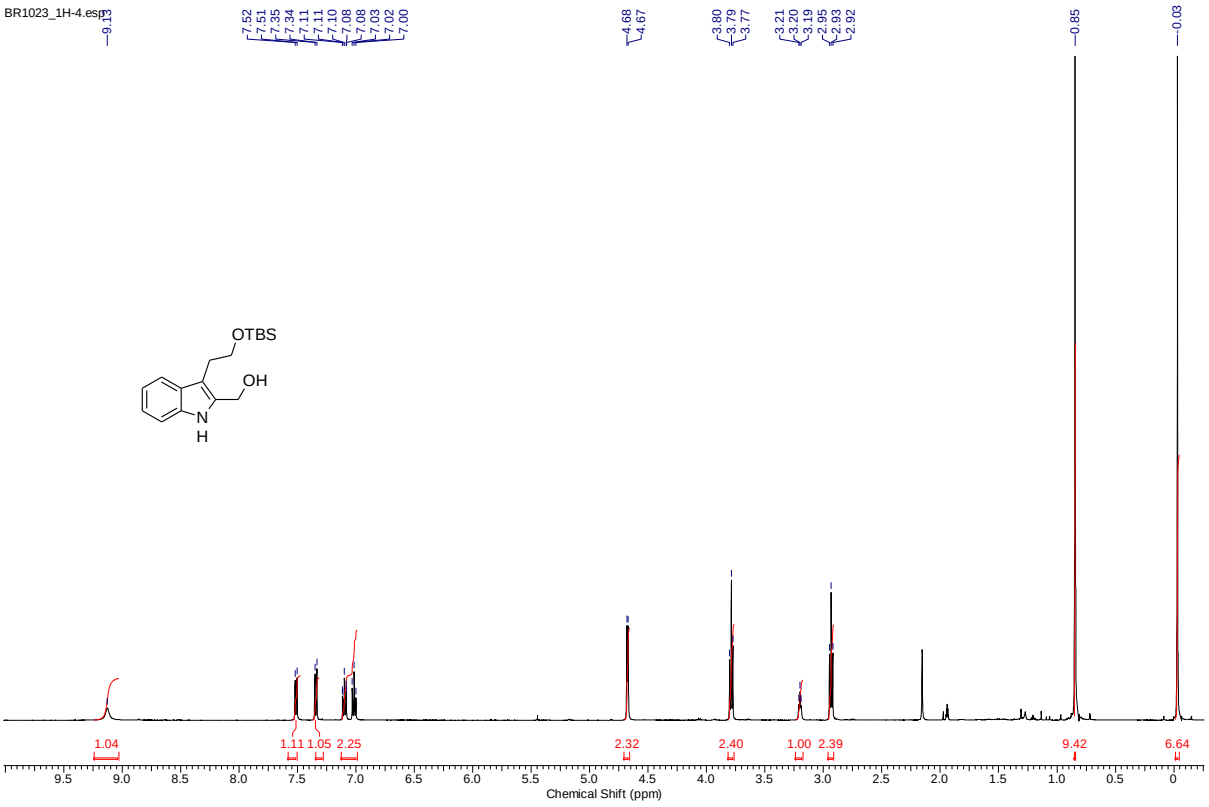


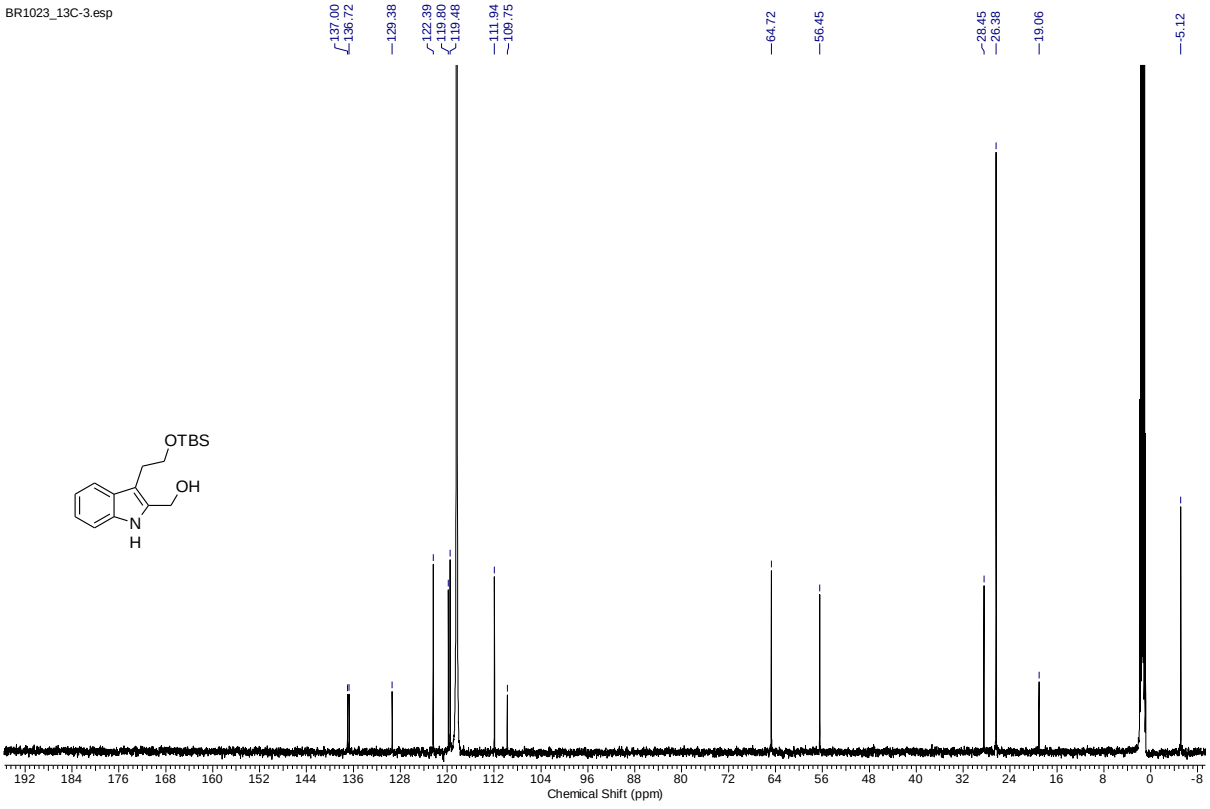
^{1}H and ^{13}C NMR of compound 14e



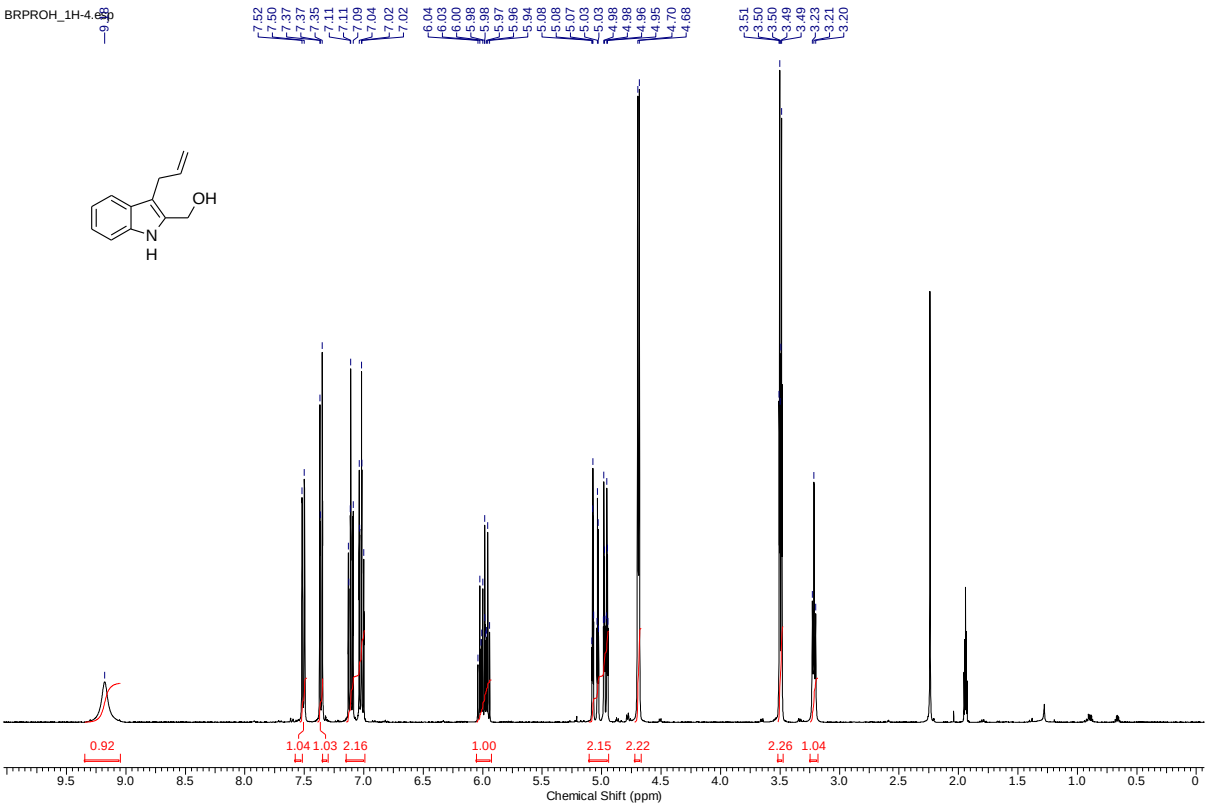


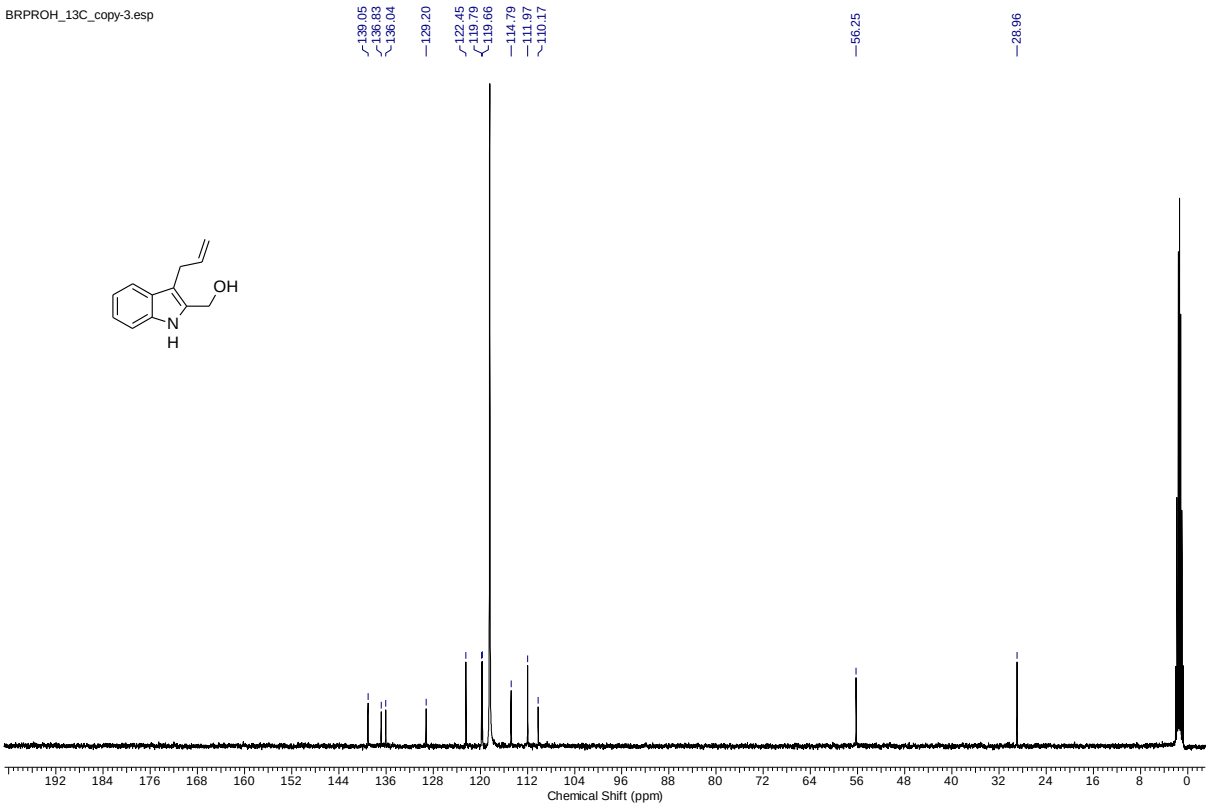
^{1}H and ^{13}C NMR of compound 15b



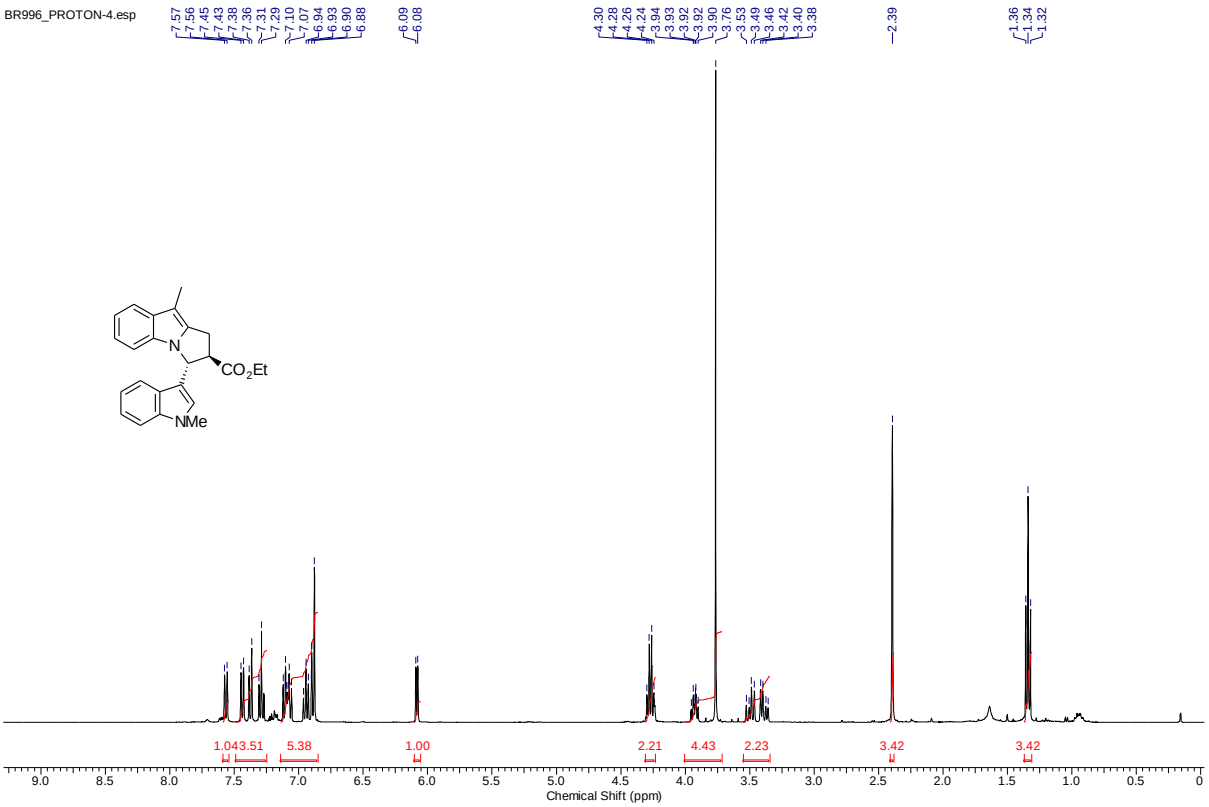


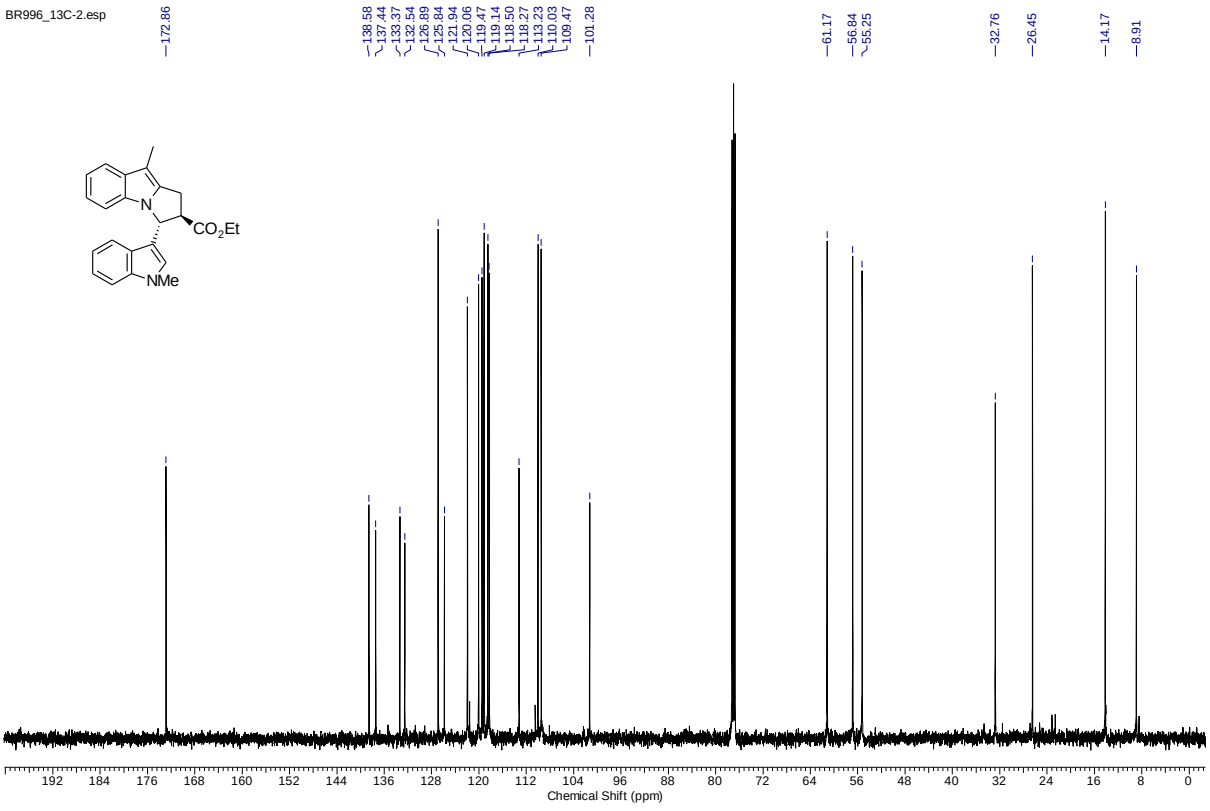
^{1}H and ^{13}C NMR of compound 15c



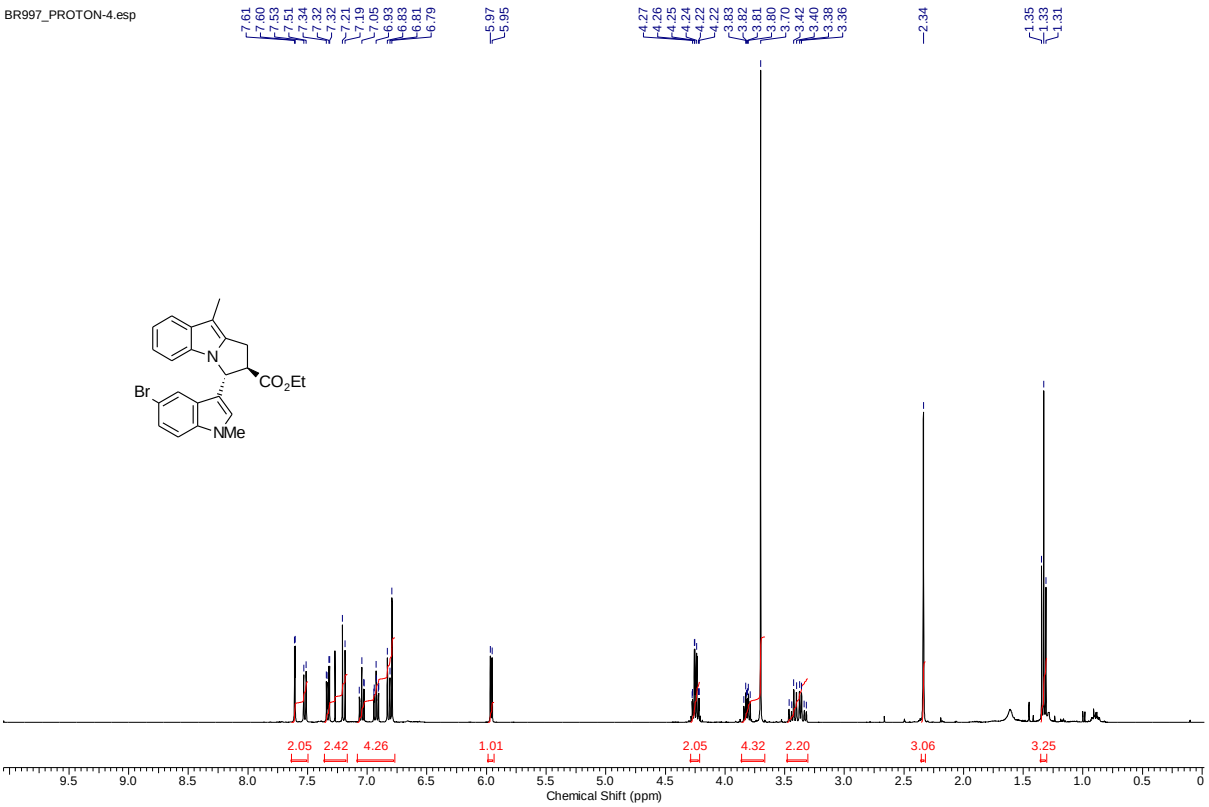


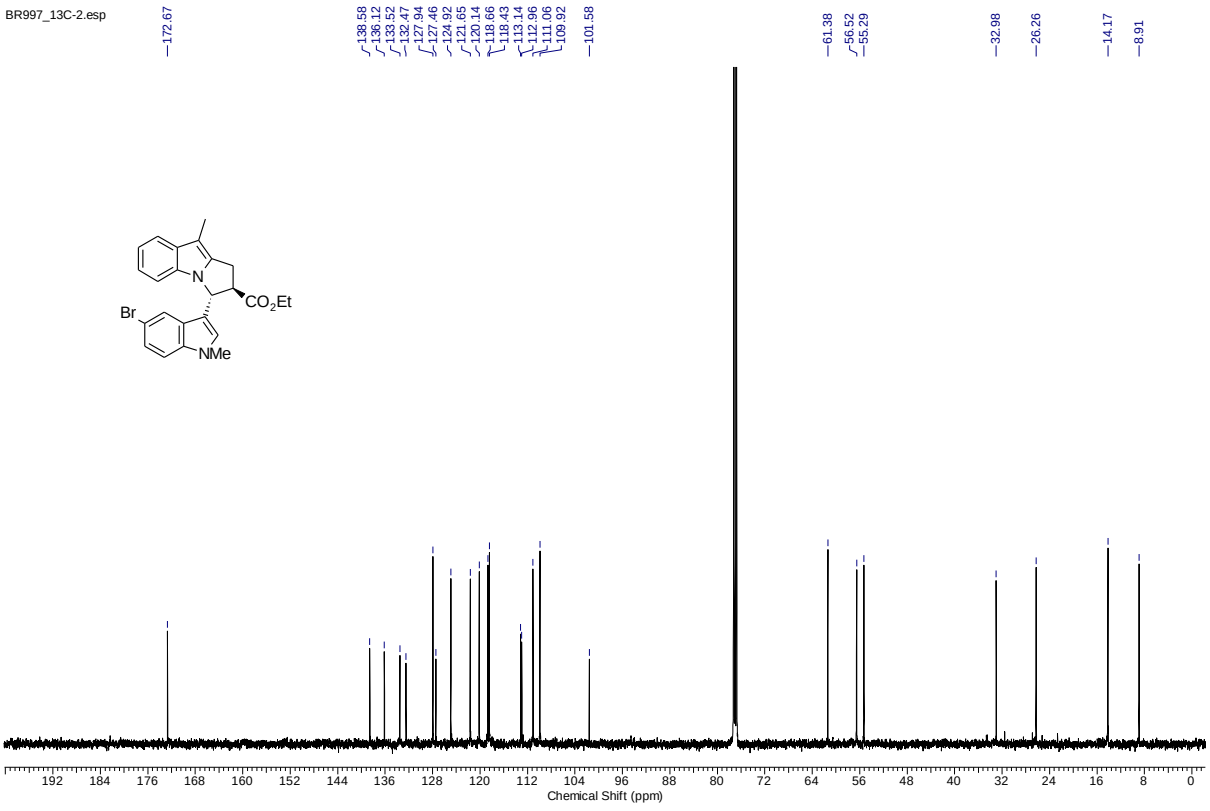
^{1}H and ^{13}C NMR of compound 16a



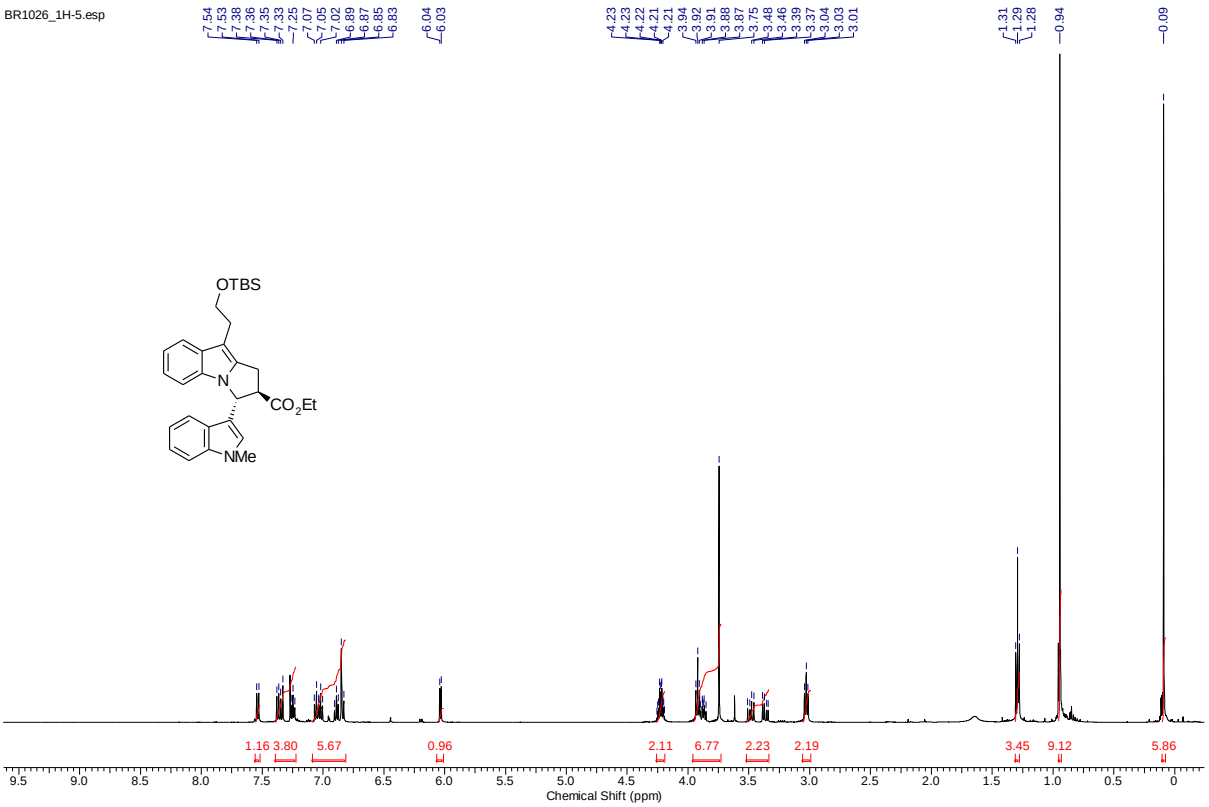


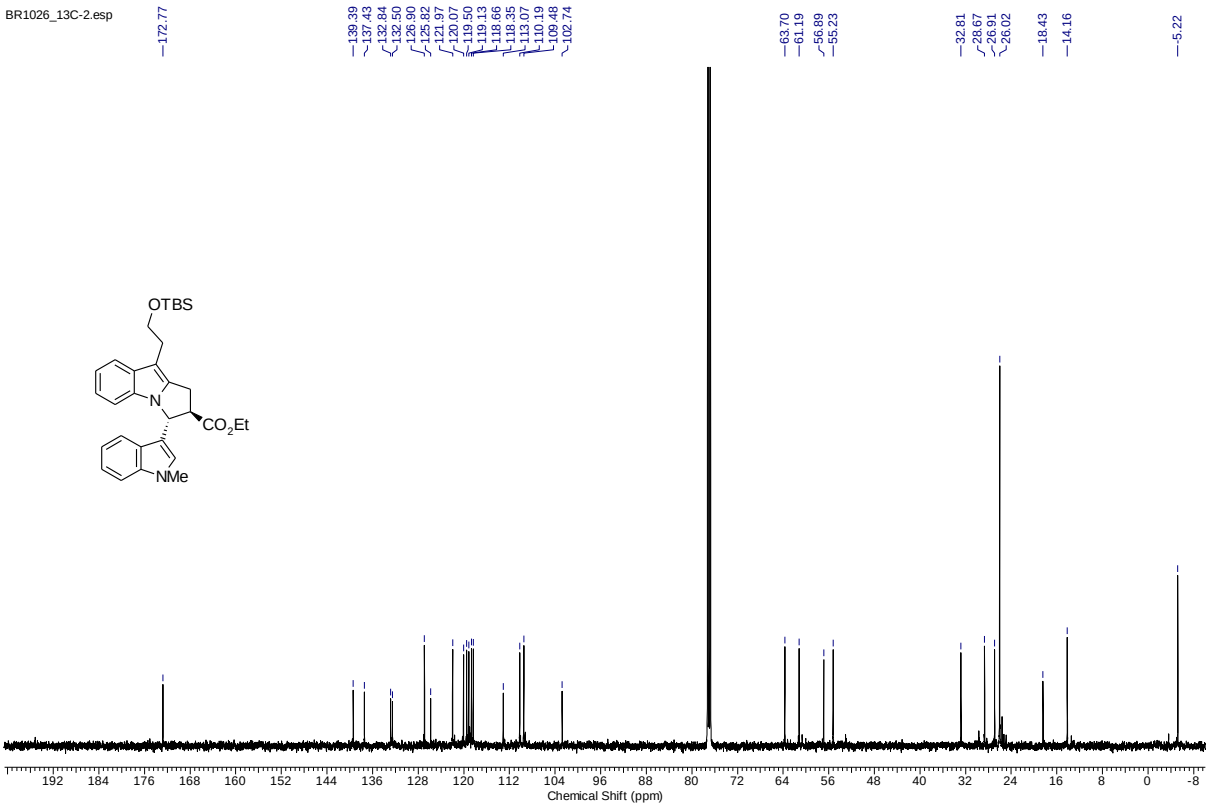
^{1}H and ^{13}C NMR of compound 16b



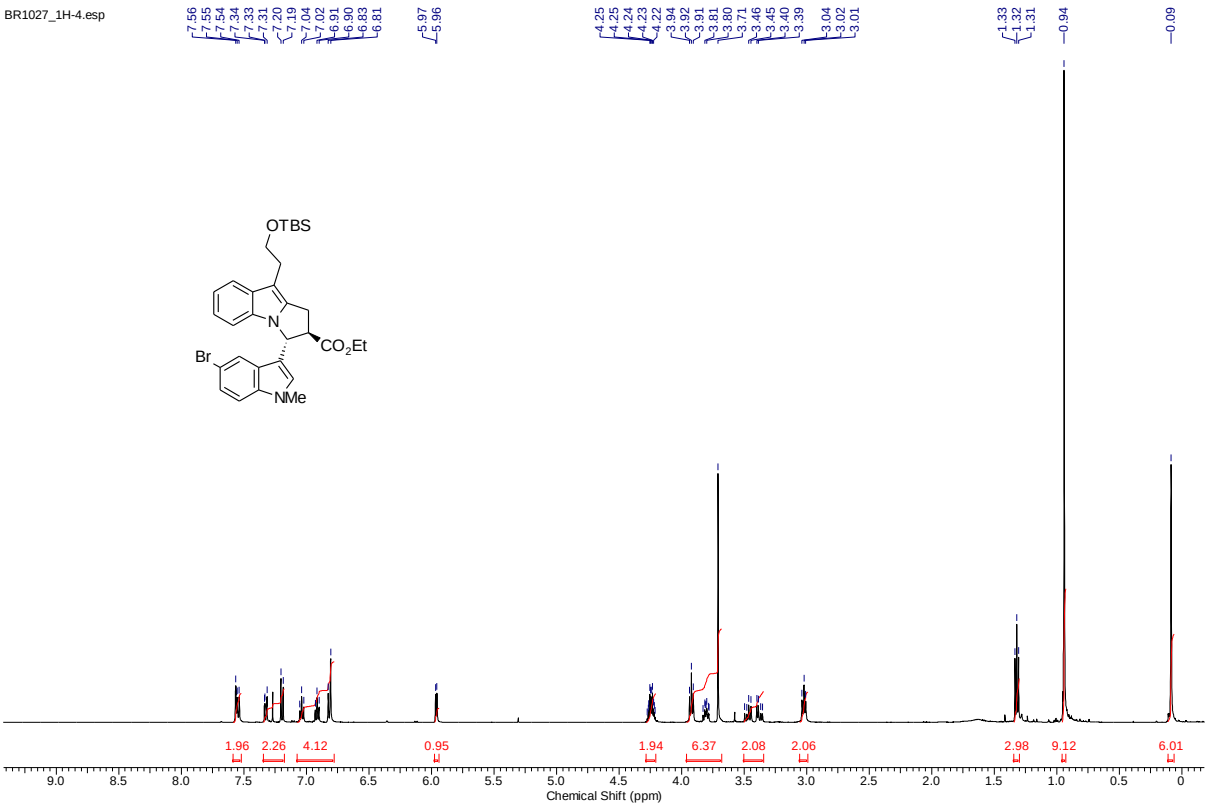


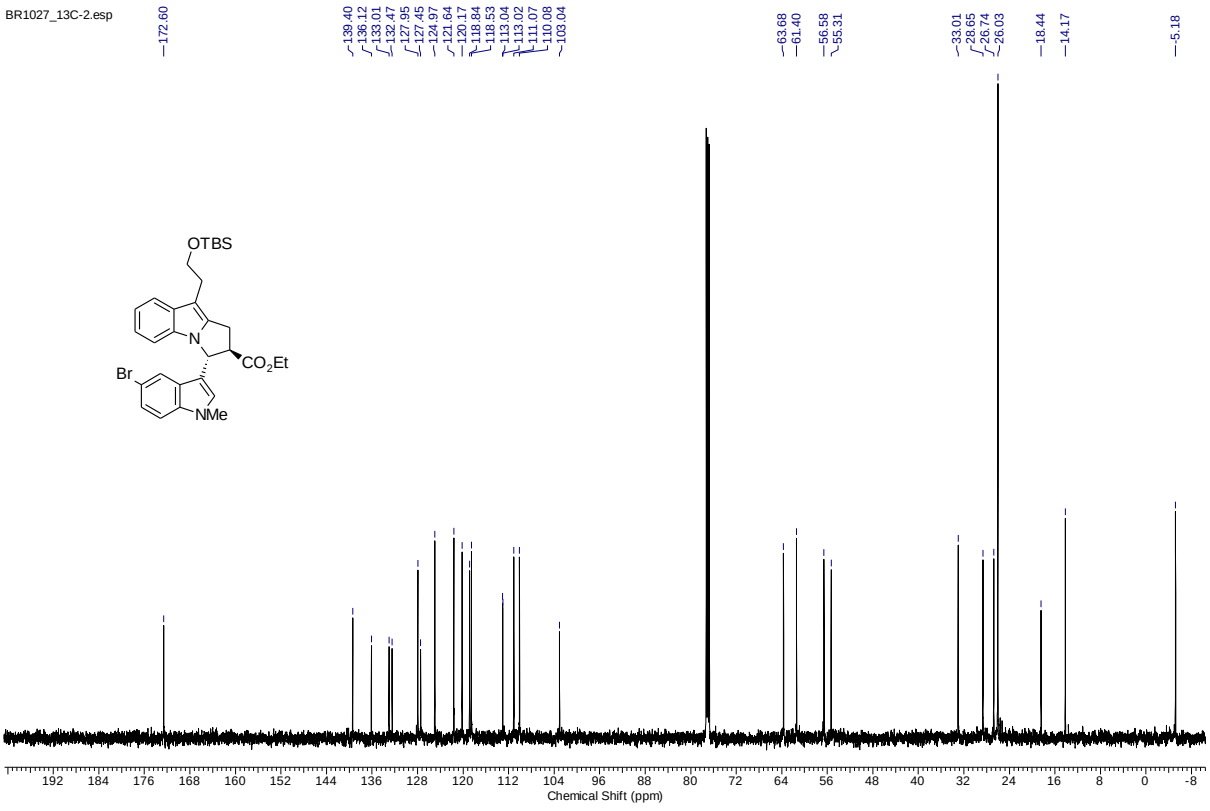
^{1}H and ^{13}C NMR of compound 16c



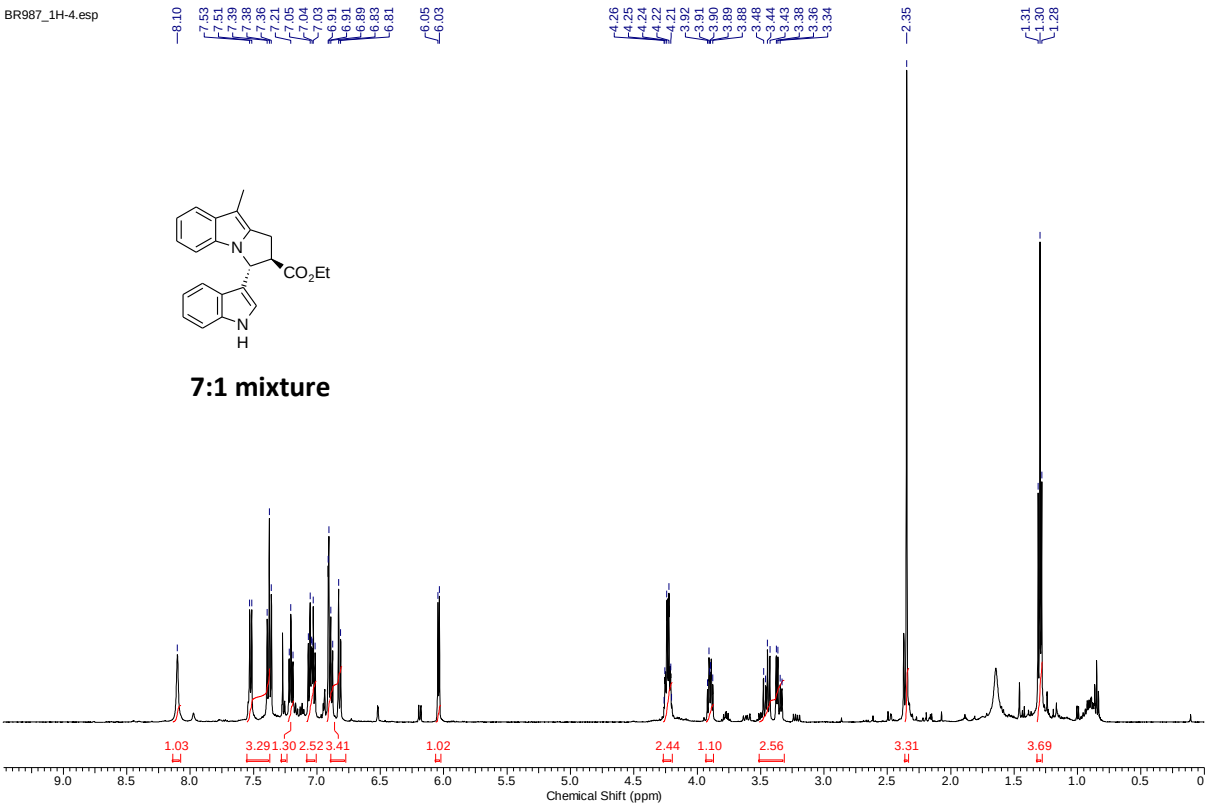


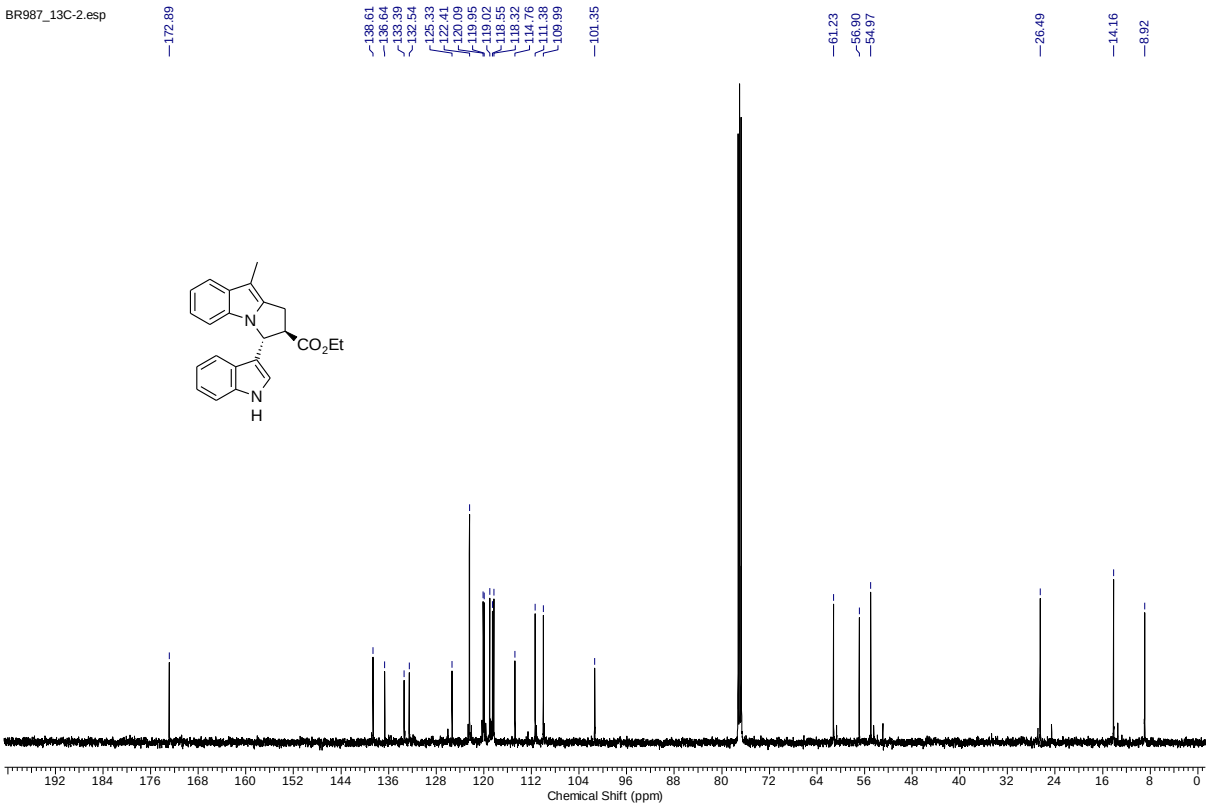
^{1}H and ^{13}C NMR of compound 16d



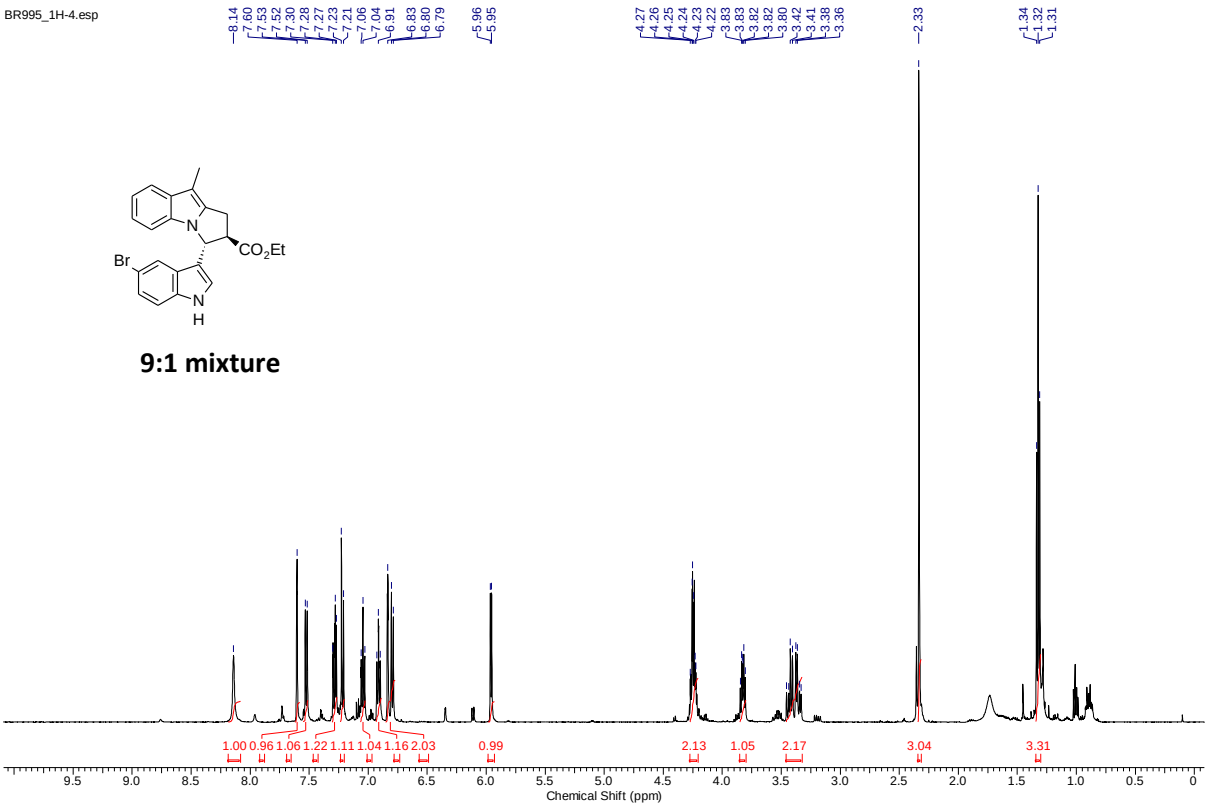


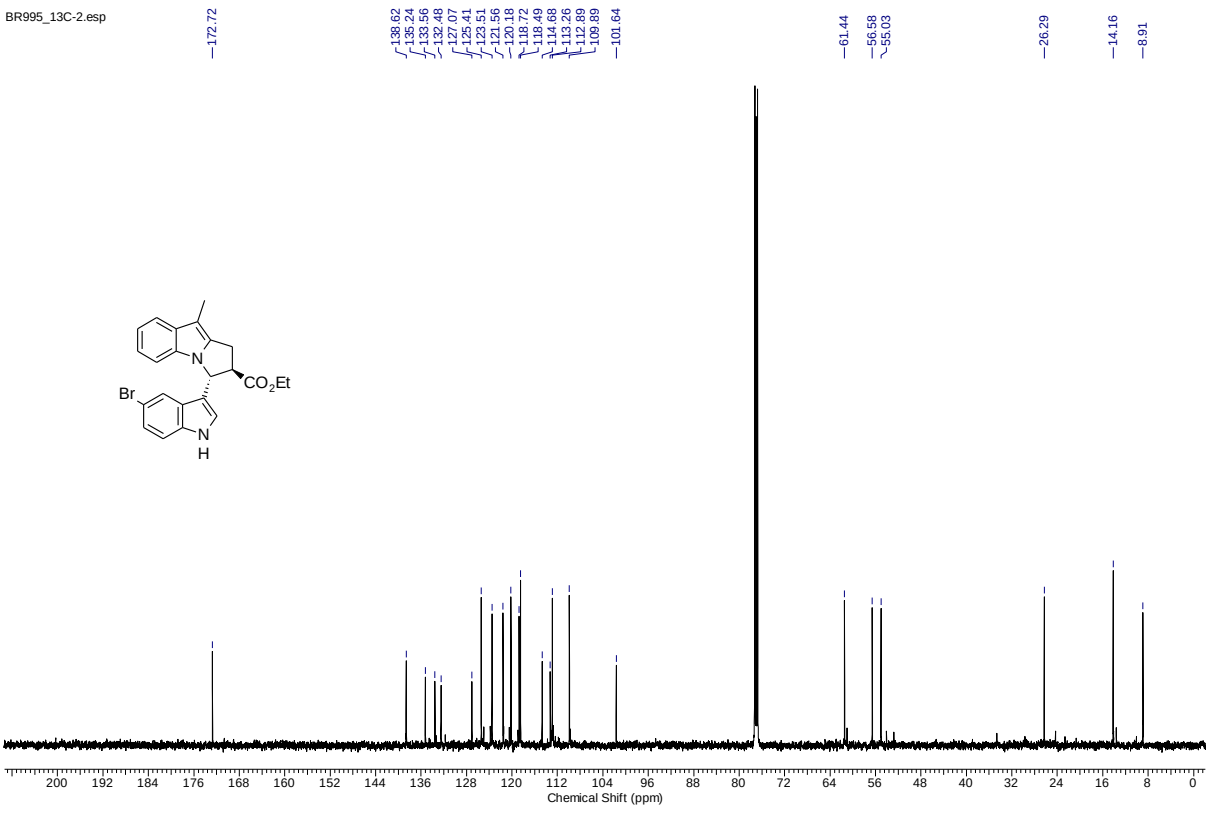
^{1}H and ^{13}C NMR of compound 16e



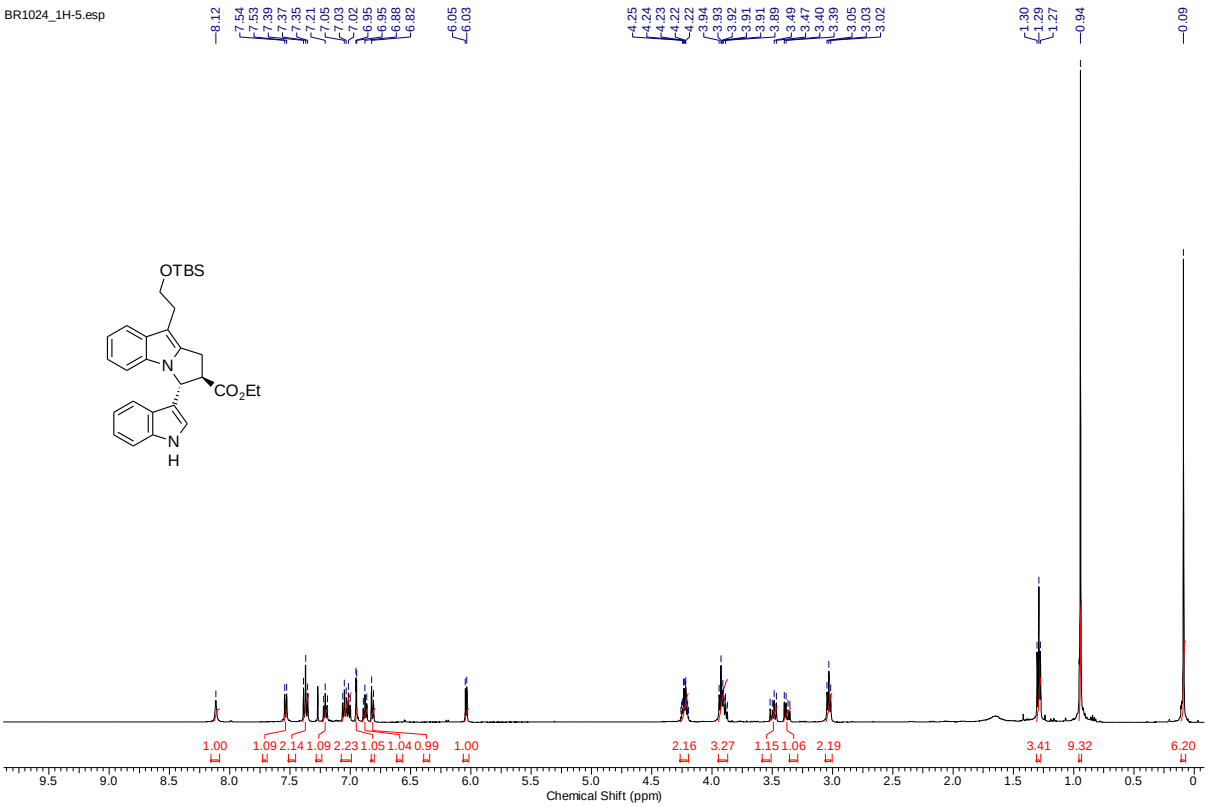


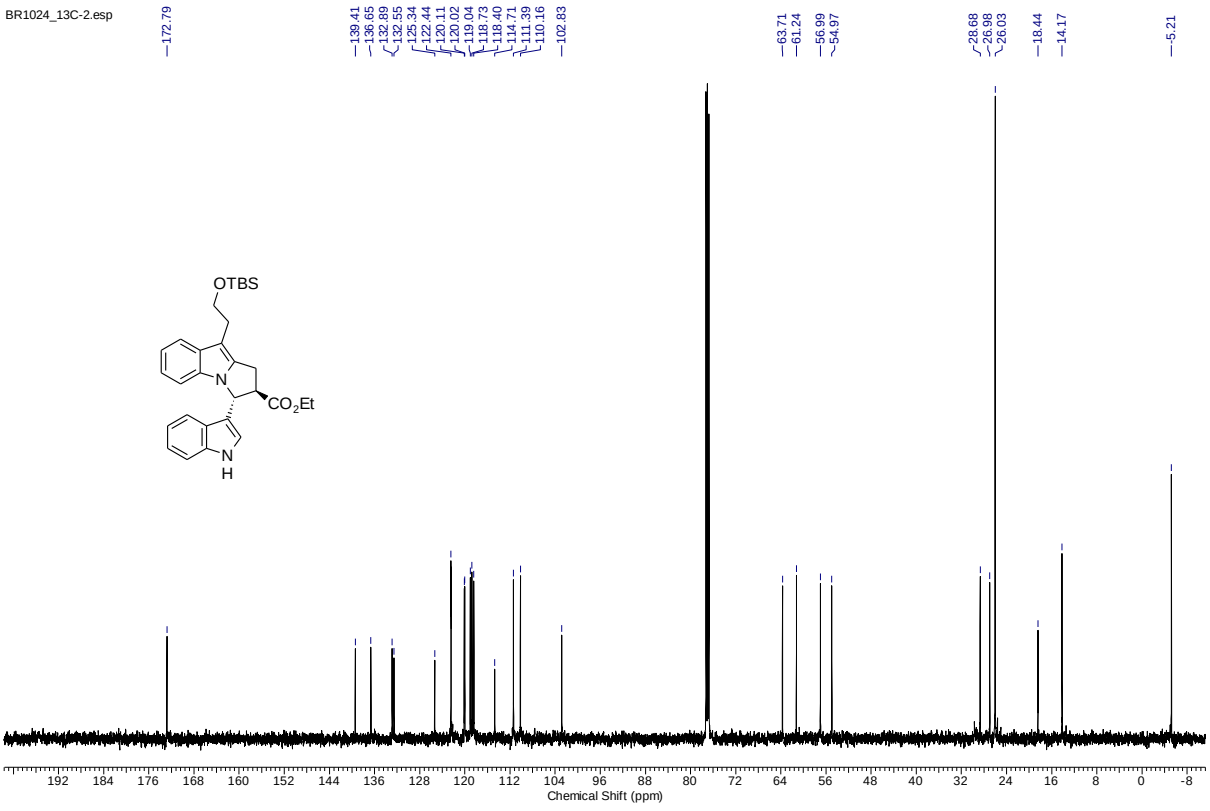
^{1}H and ^{13}C NMR of compound 16f



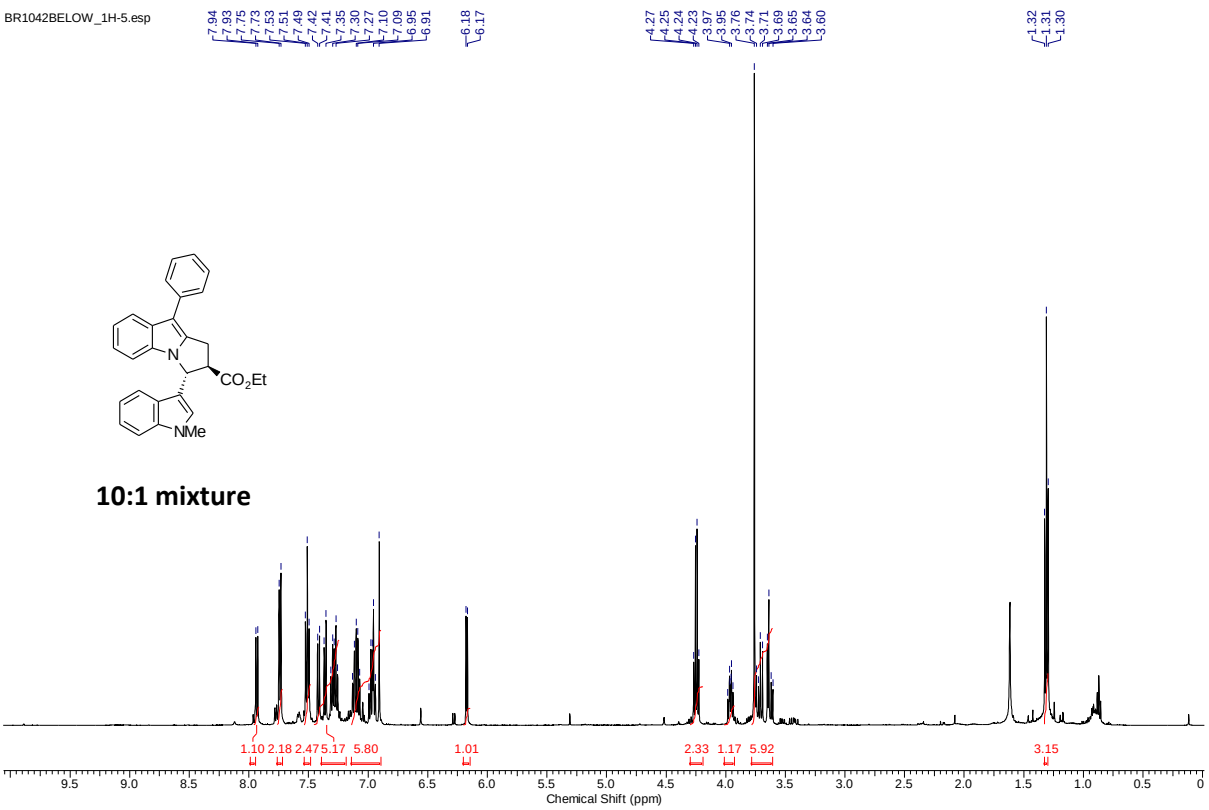


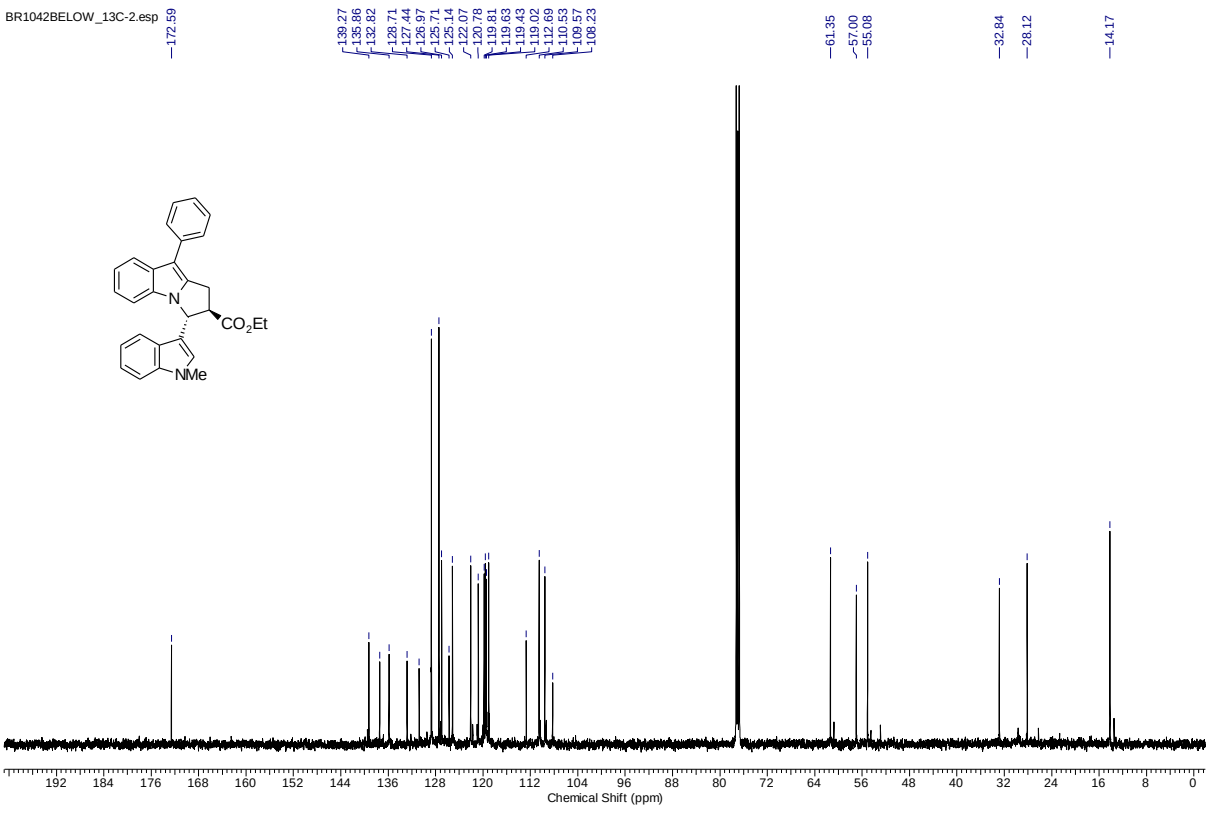
^{1}H and ^{13}C NMR of compound 16g



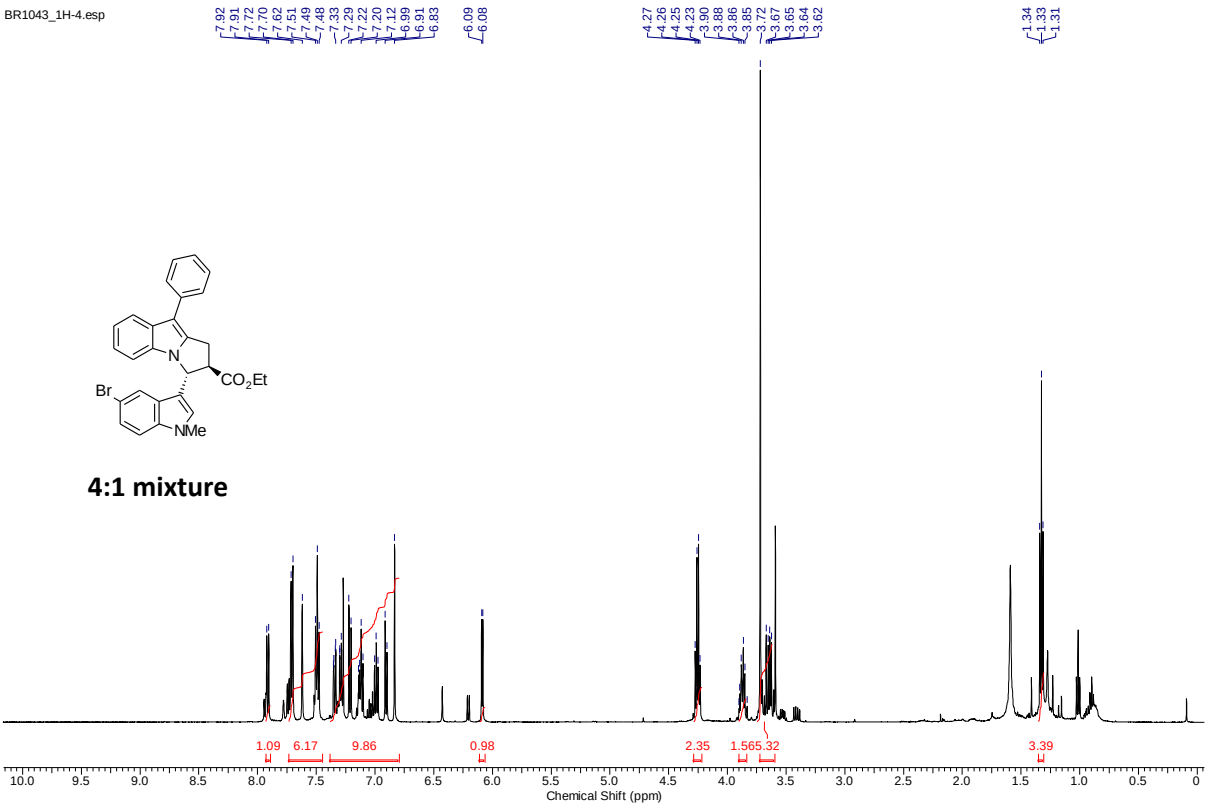


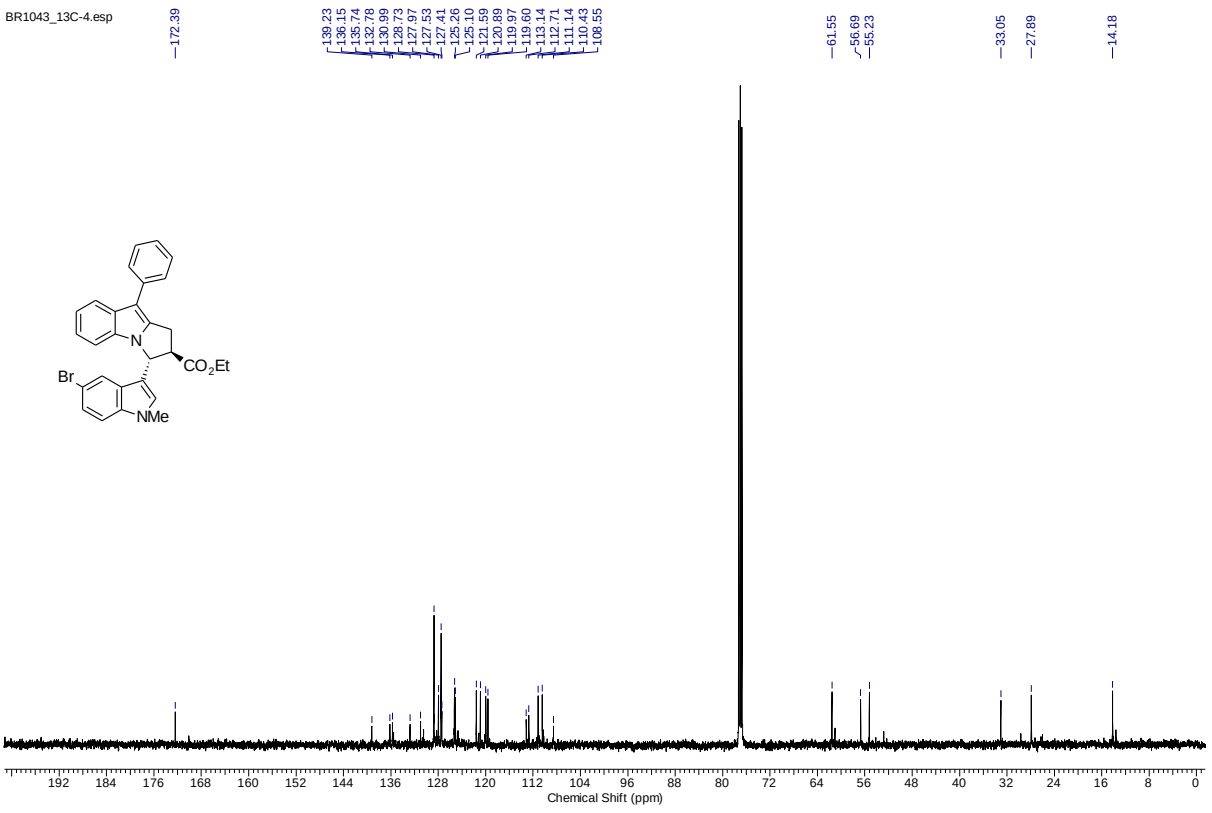
^{1}H and ^{13}C NMR of compound 16h



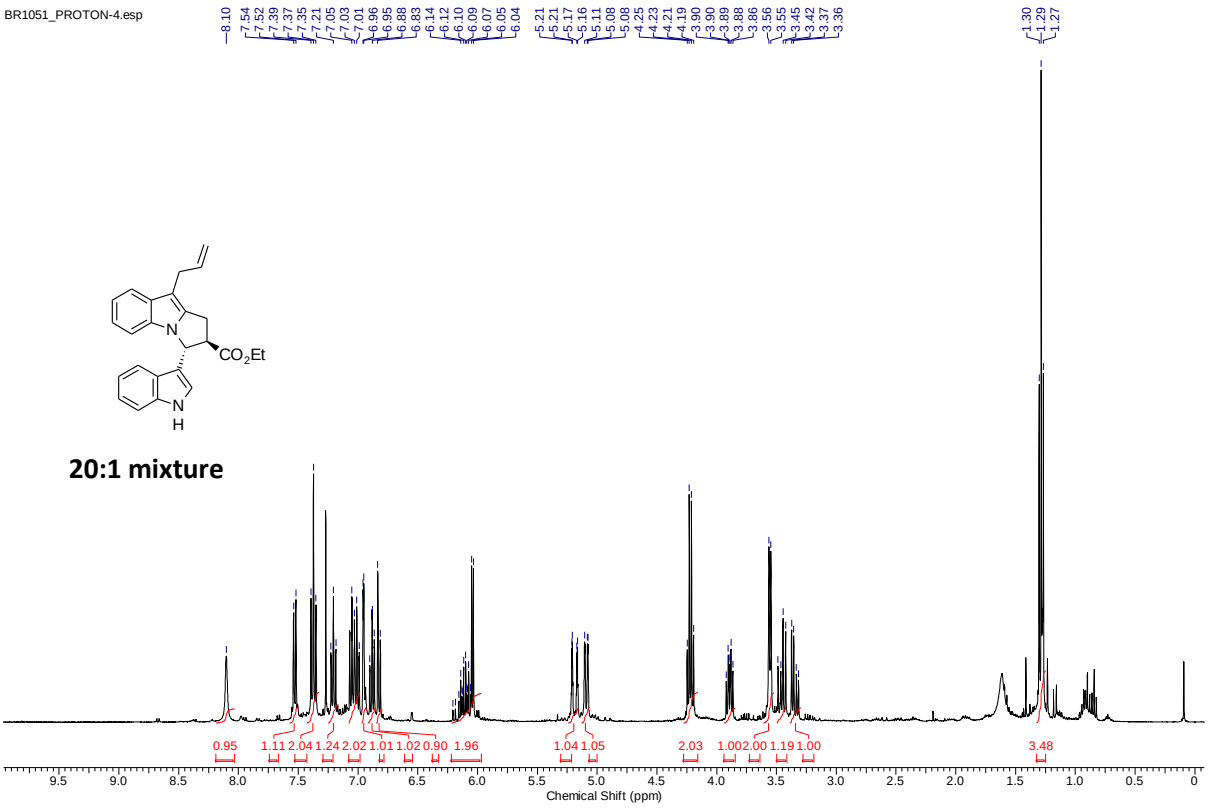


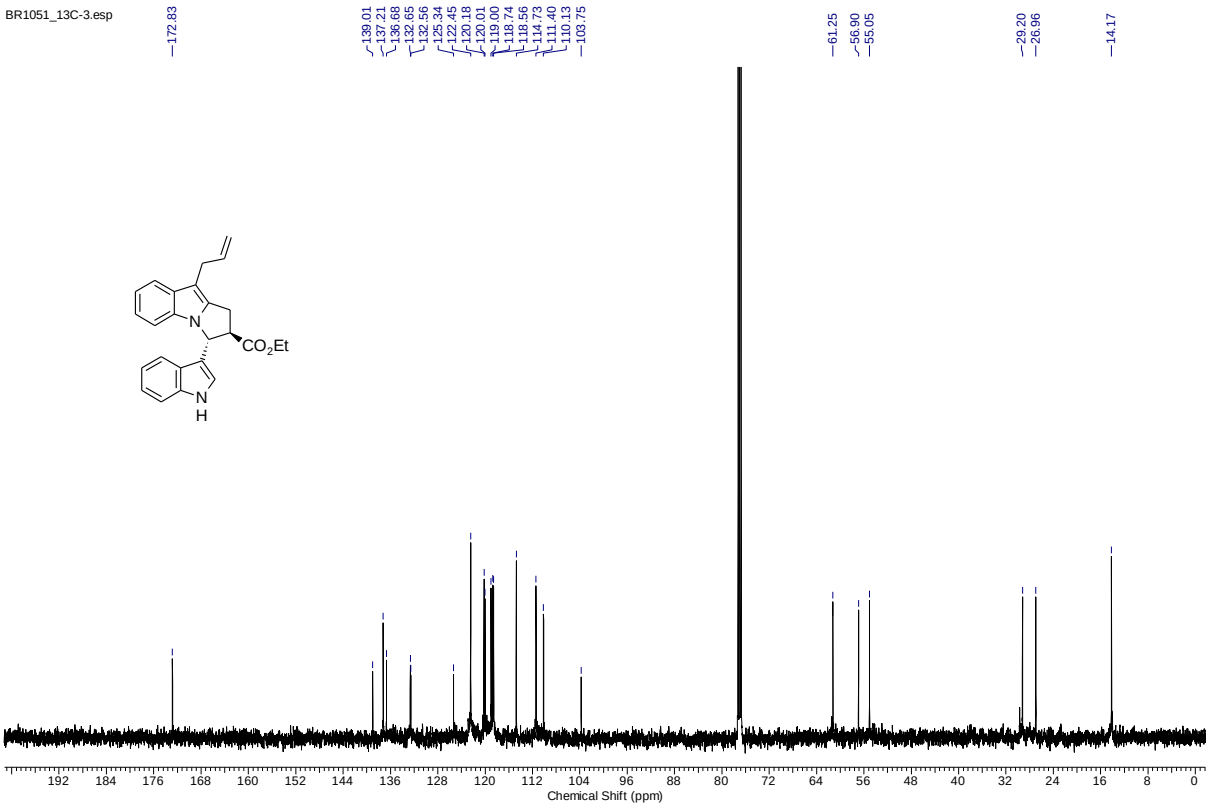
^{1}H and ^{13}C NMR of compound 16i



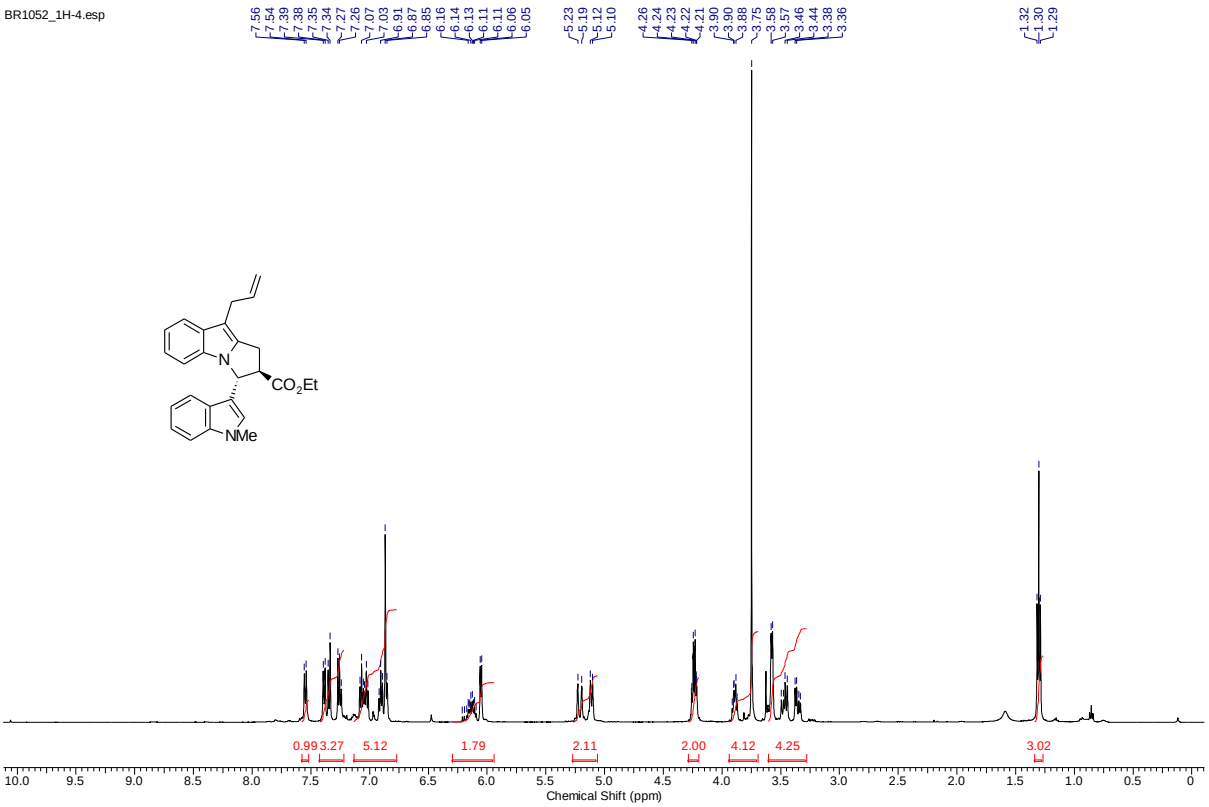


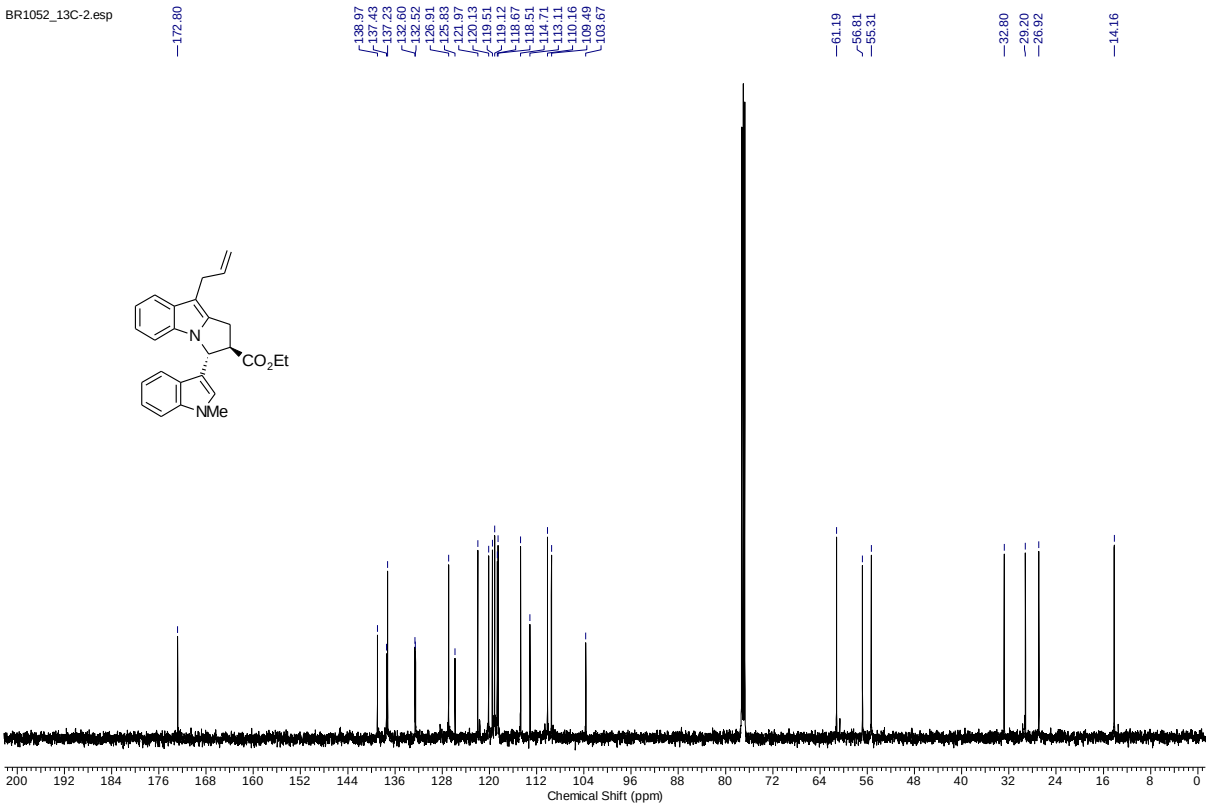
^{1}H and ^{13}C NMR of compound 16j



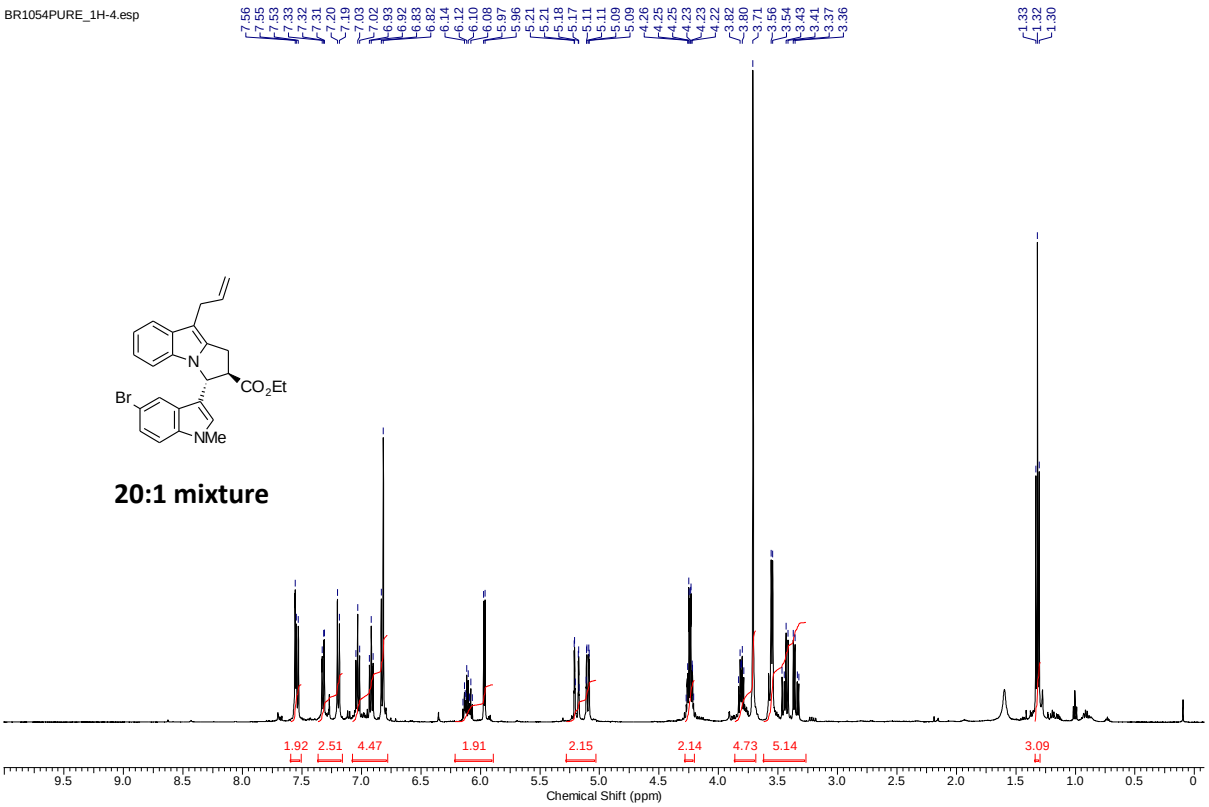


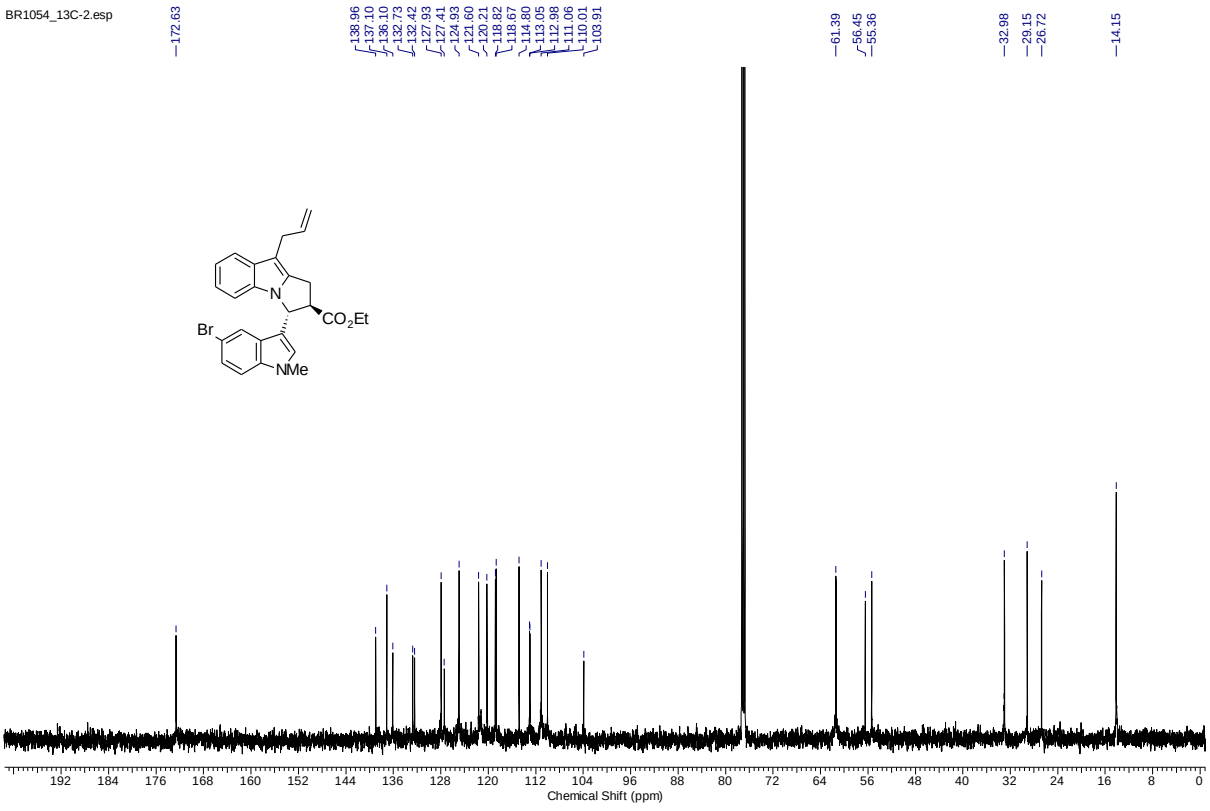
^{1}H and ^{13}C NMR of compound 16k



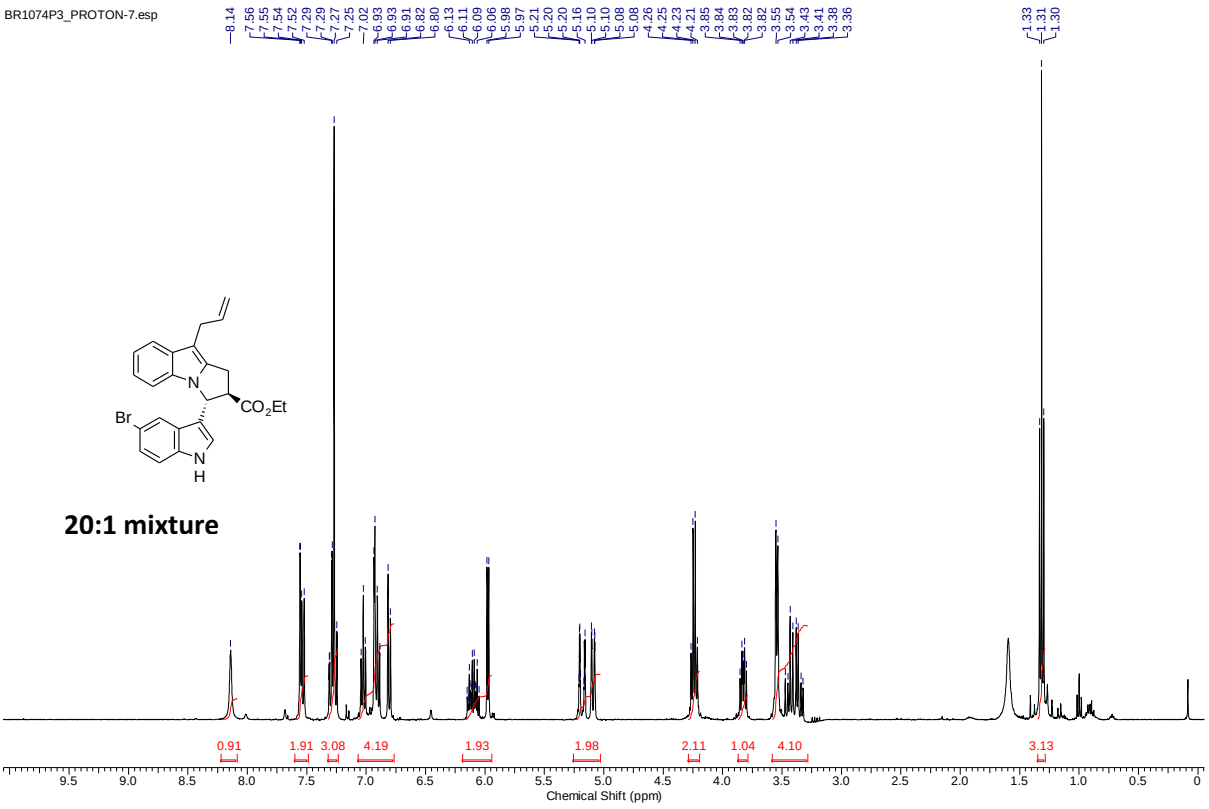


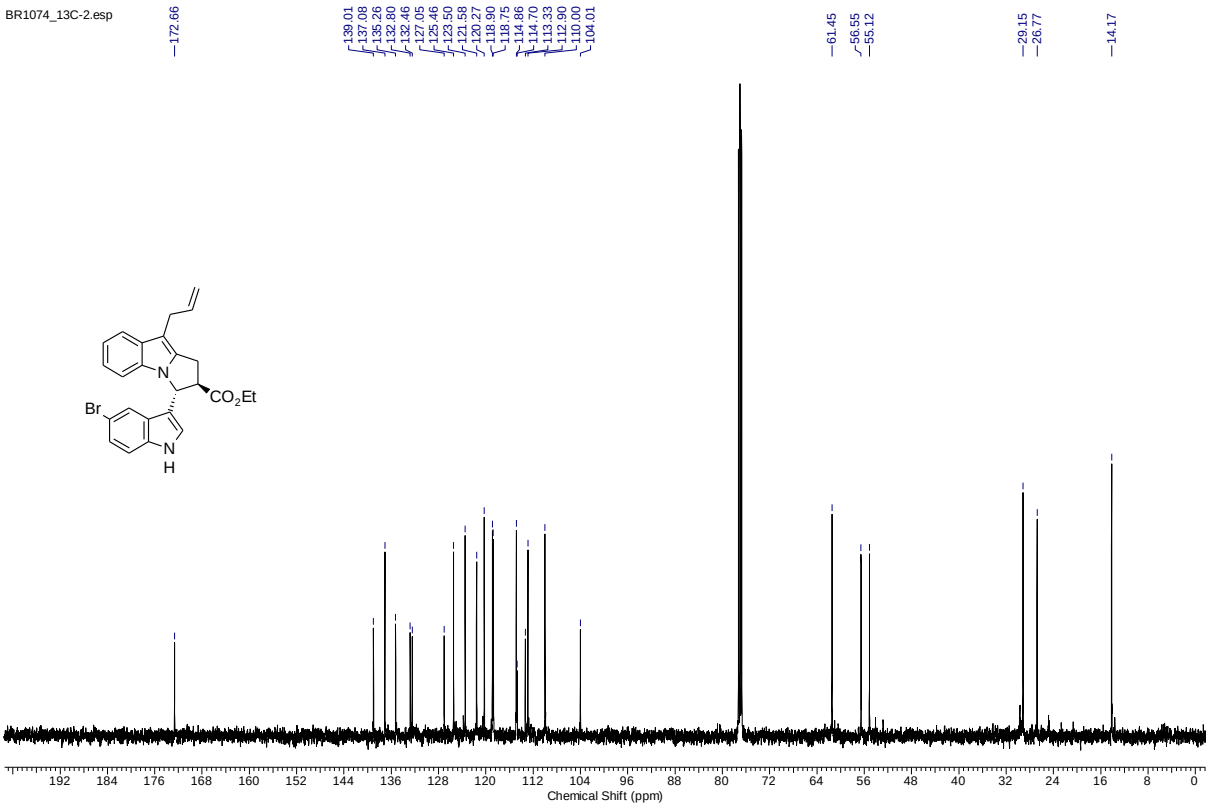
^{1}H and ^{13}C NMR of compound 16l



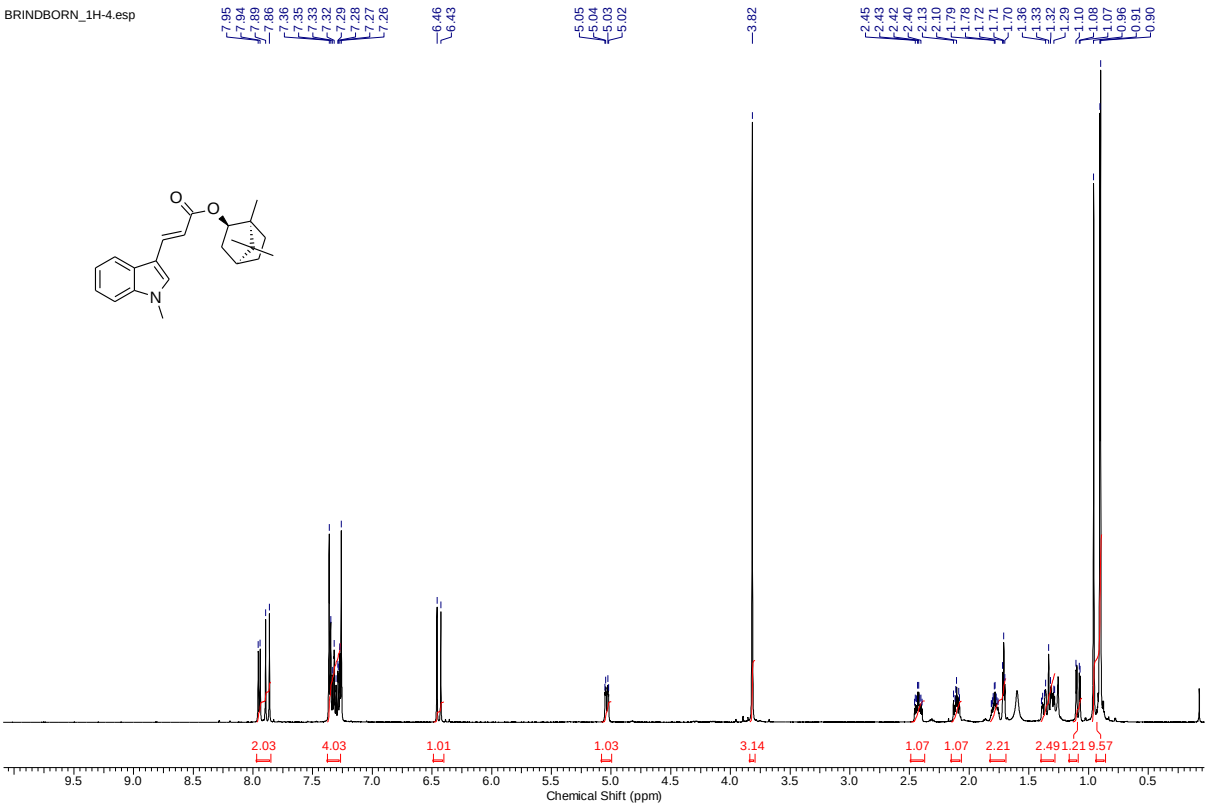


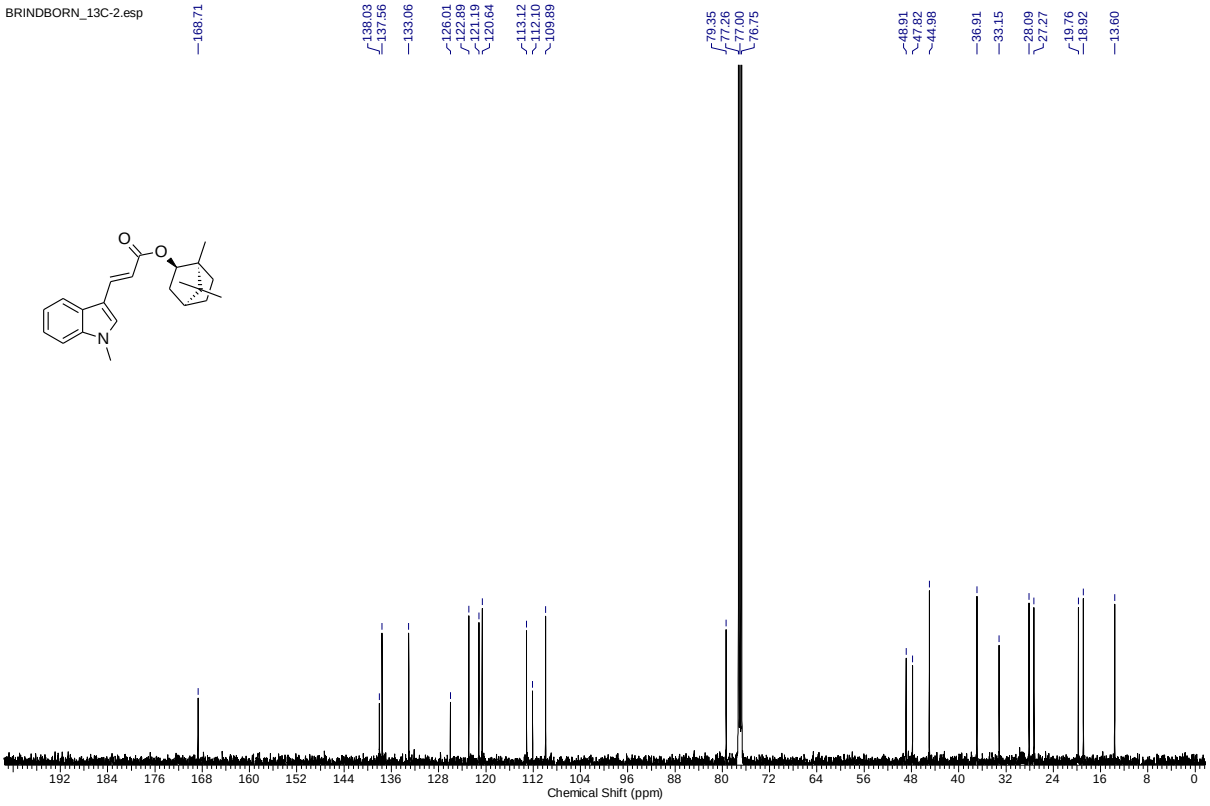
^{1}H and ^{13}C NMR of compound 16m



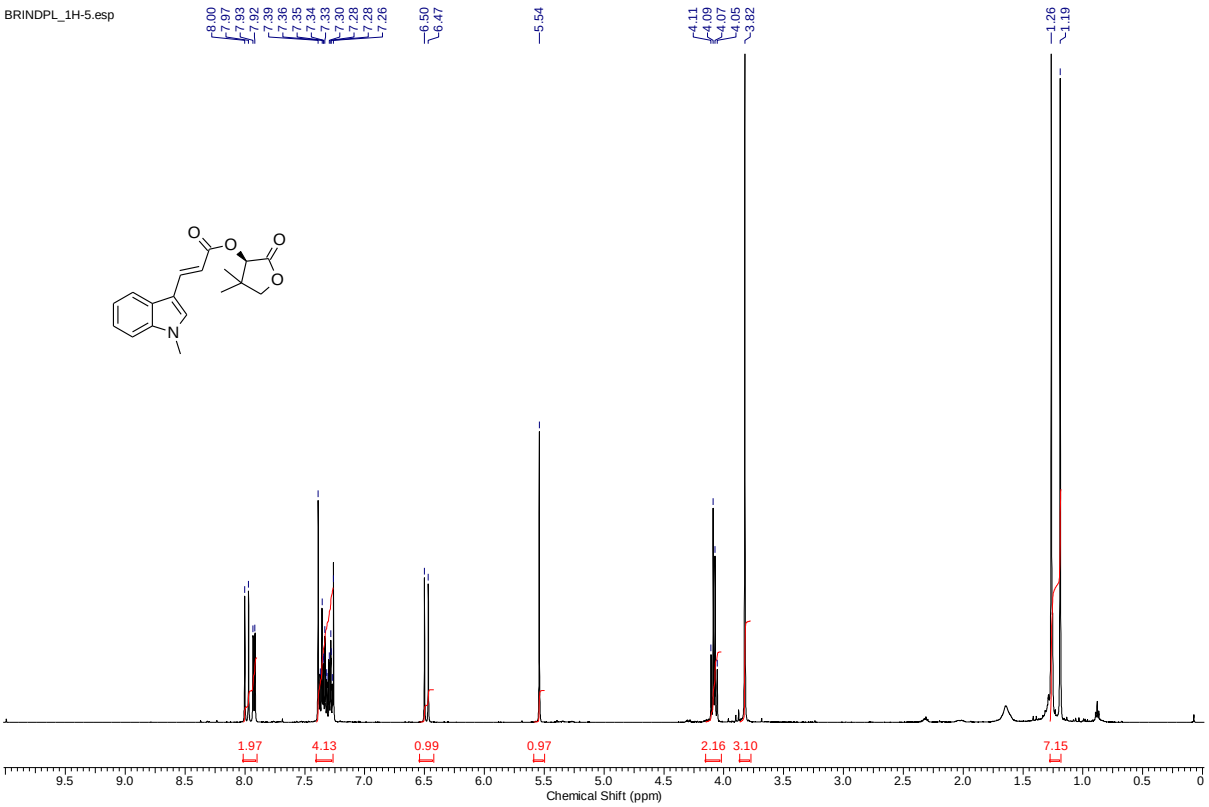


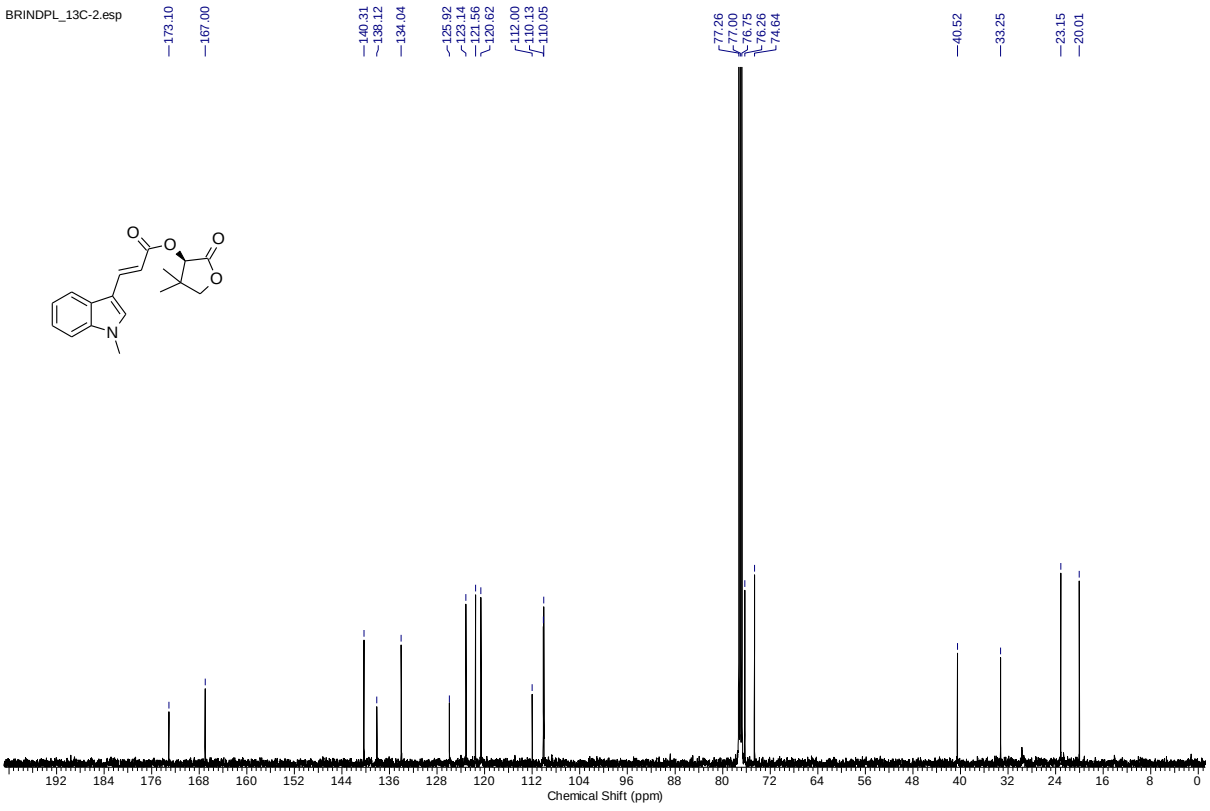
^{1}H and ^{13}C NMR of compound 17a



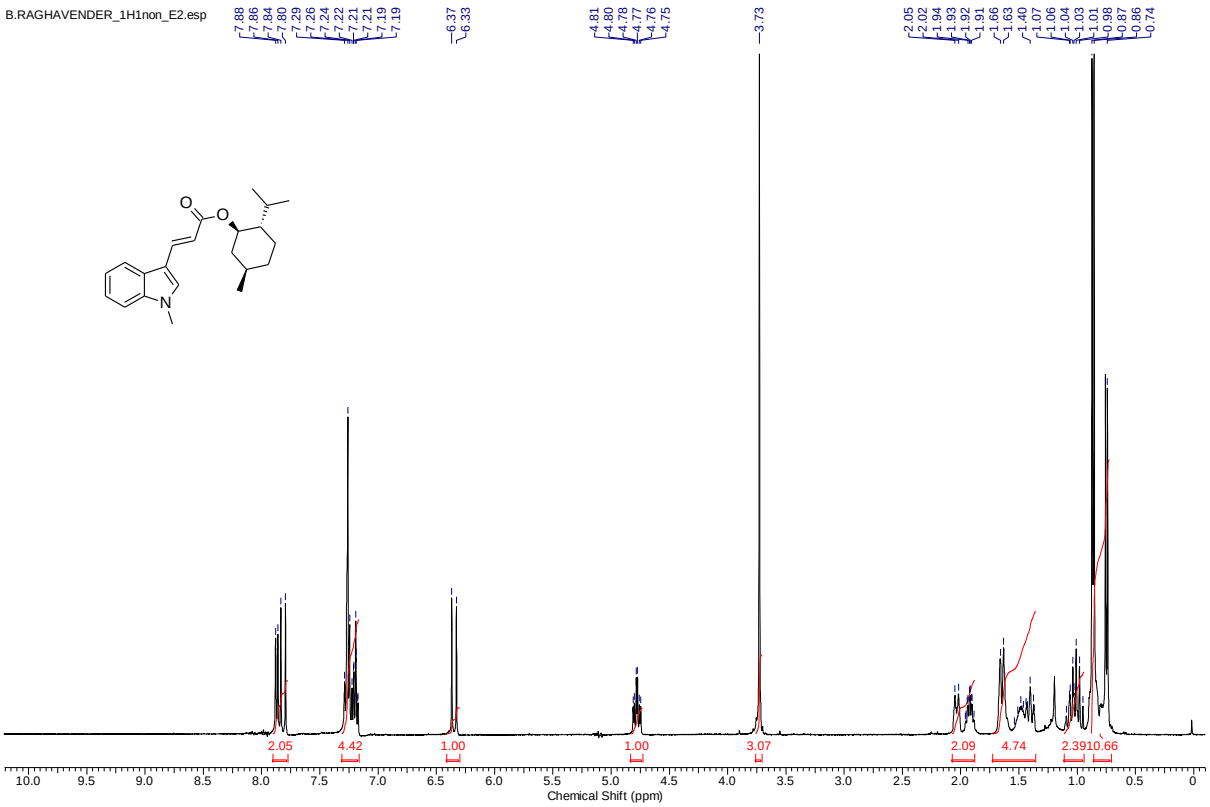


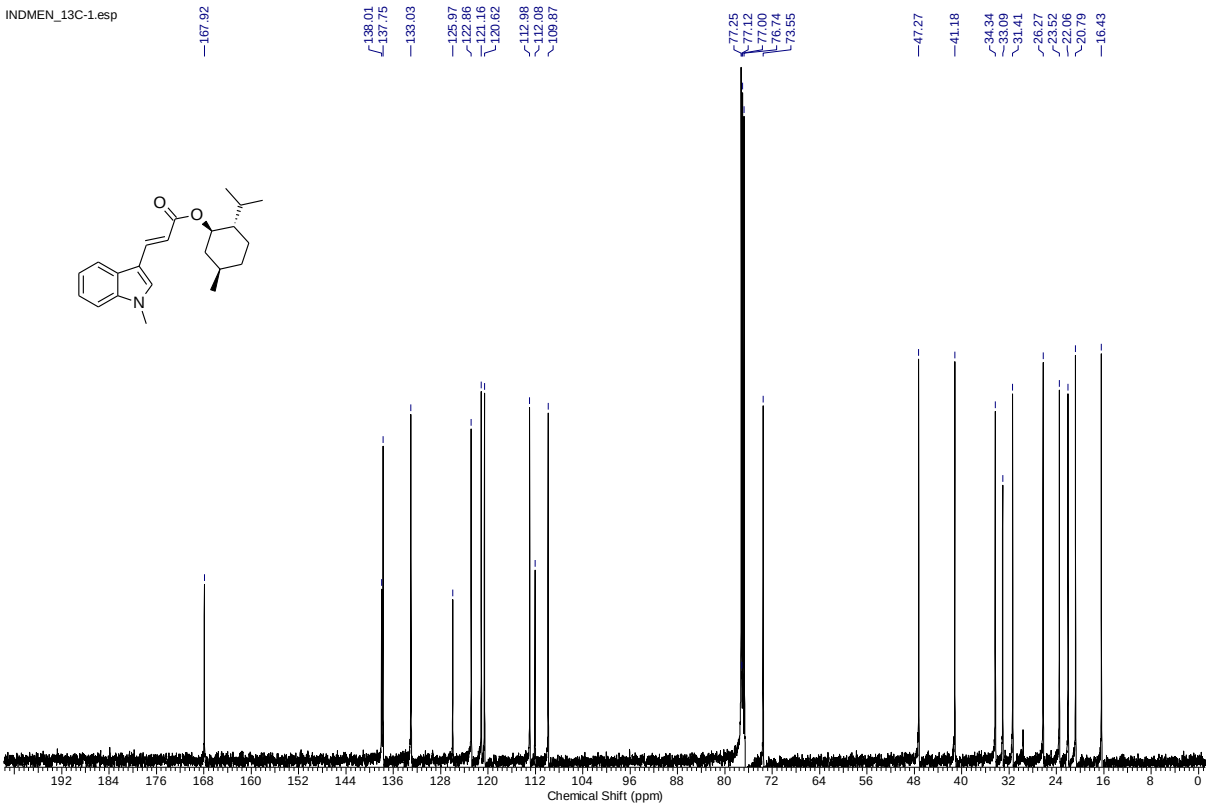
^{1}H and ^{13}C NMR of compound 17b



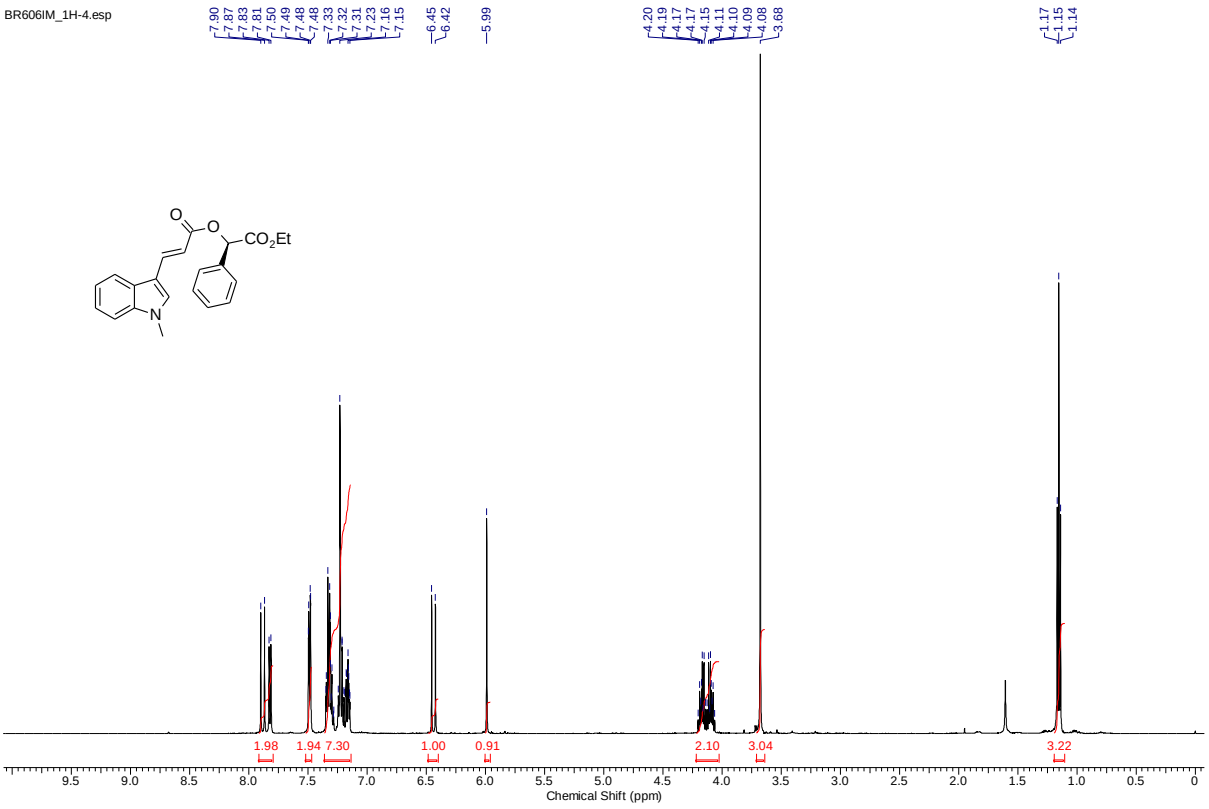


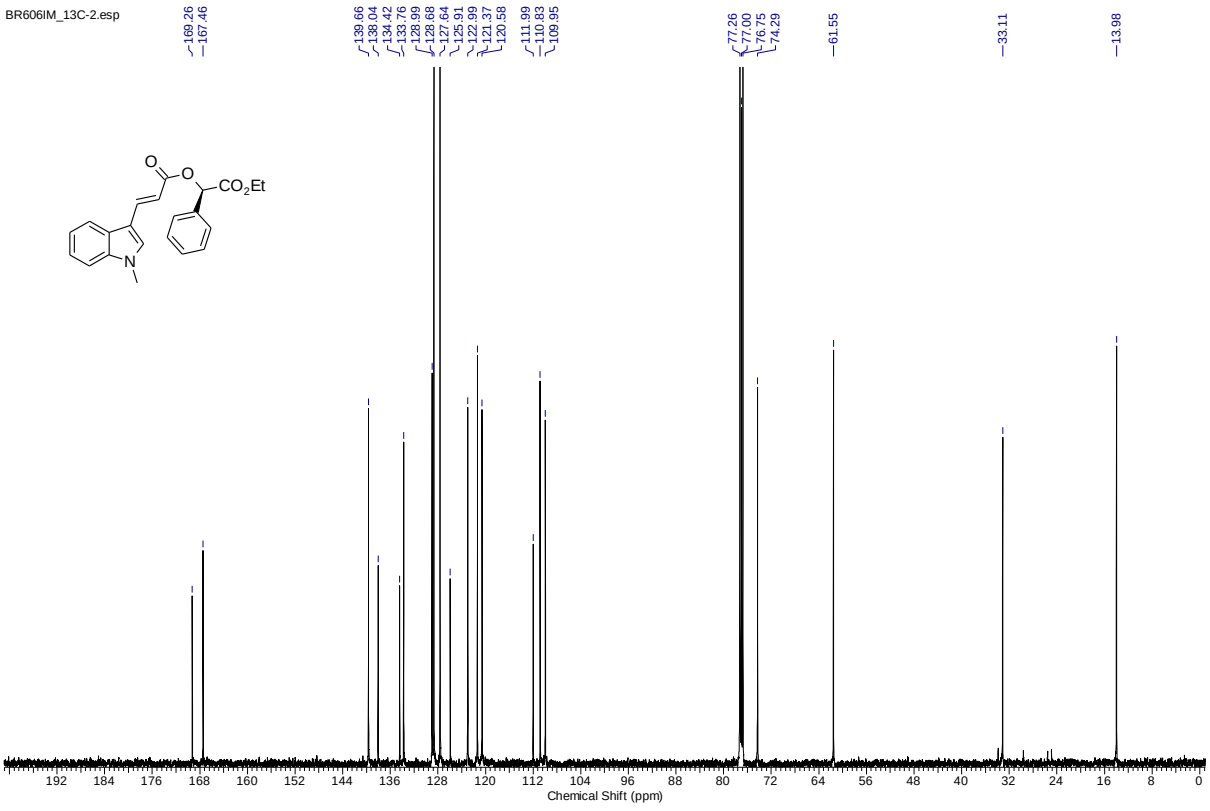
^{1}H and ^{13}C NMR of compound 17c



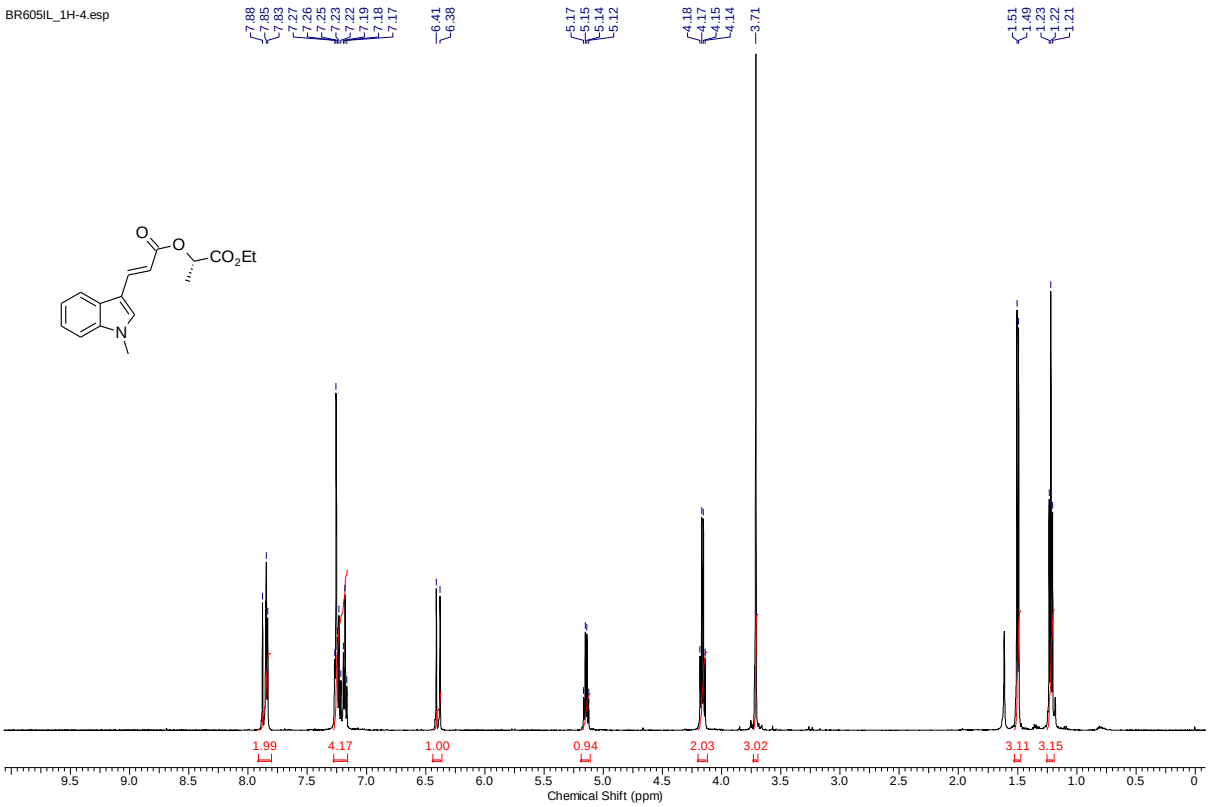


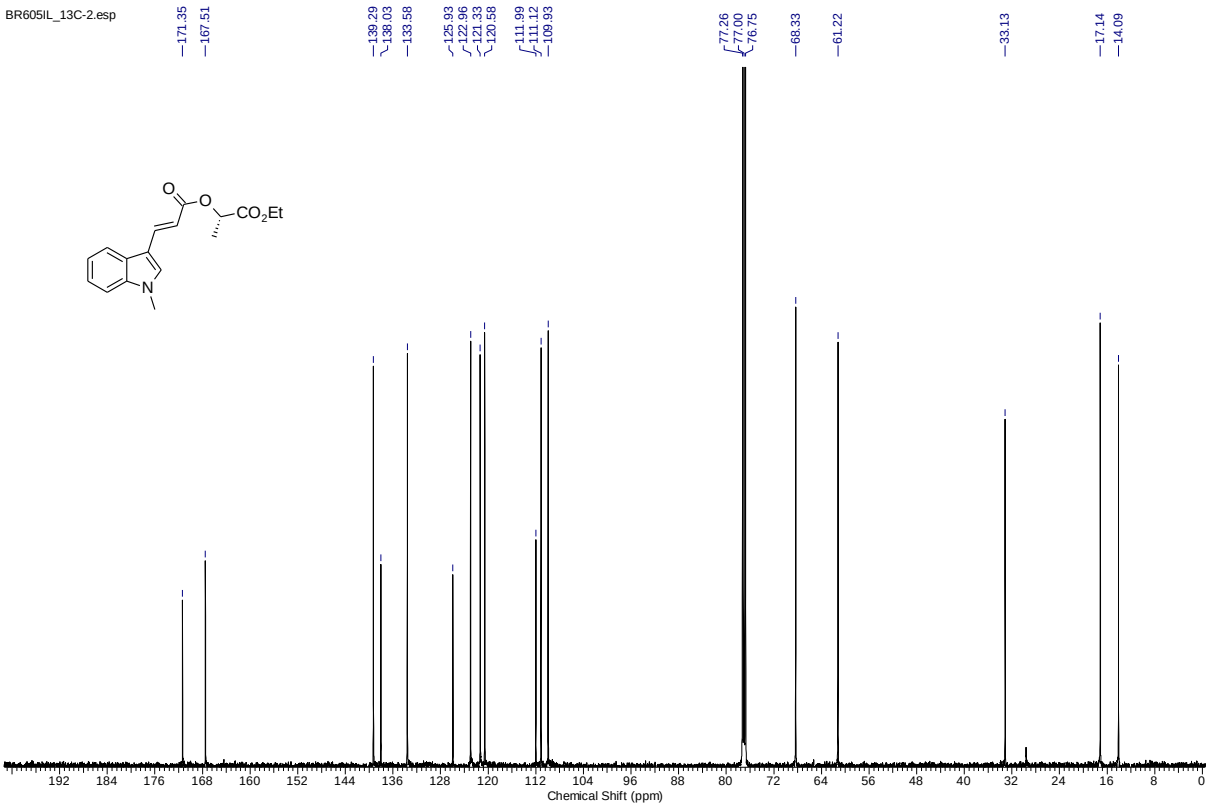
^{1}H and ^{13}C NMR of compound 17d



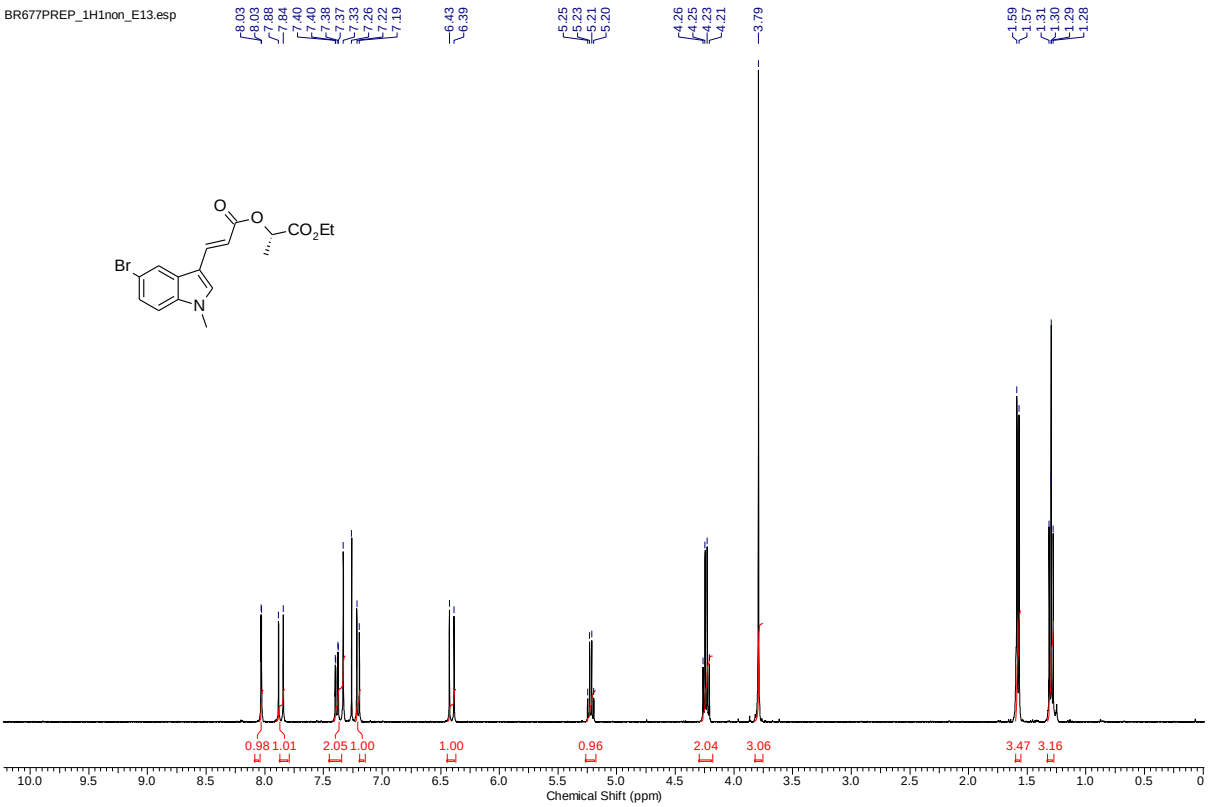


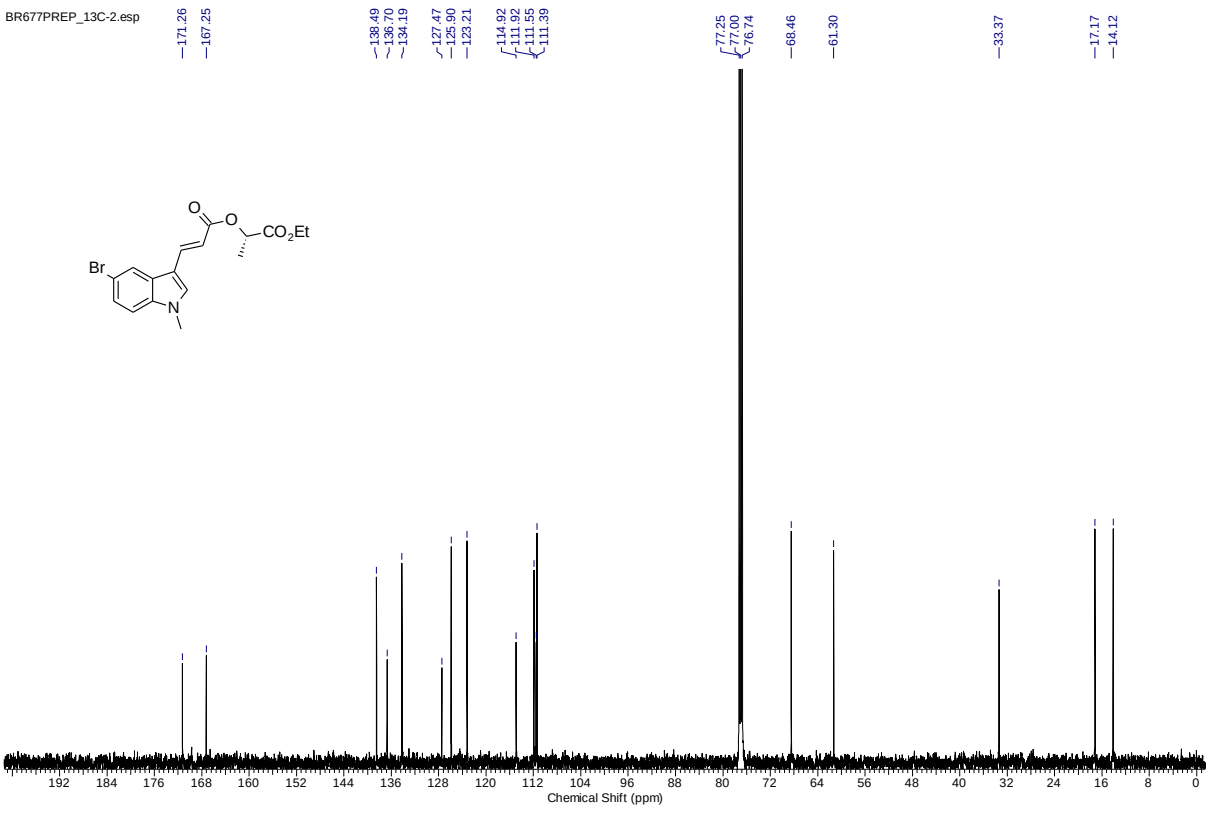
^{1}H and ^{13}C NMR of compound 17e



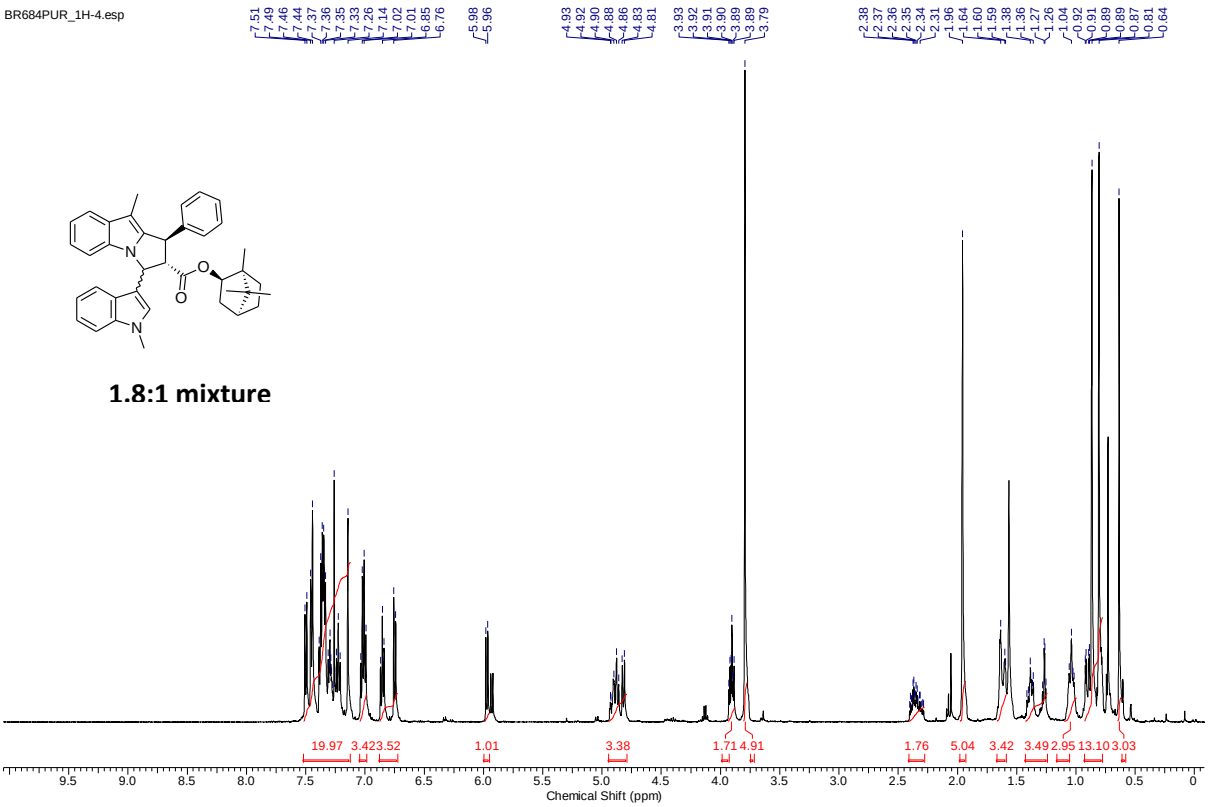


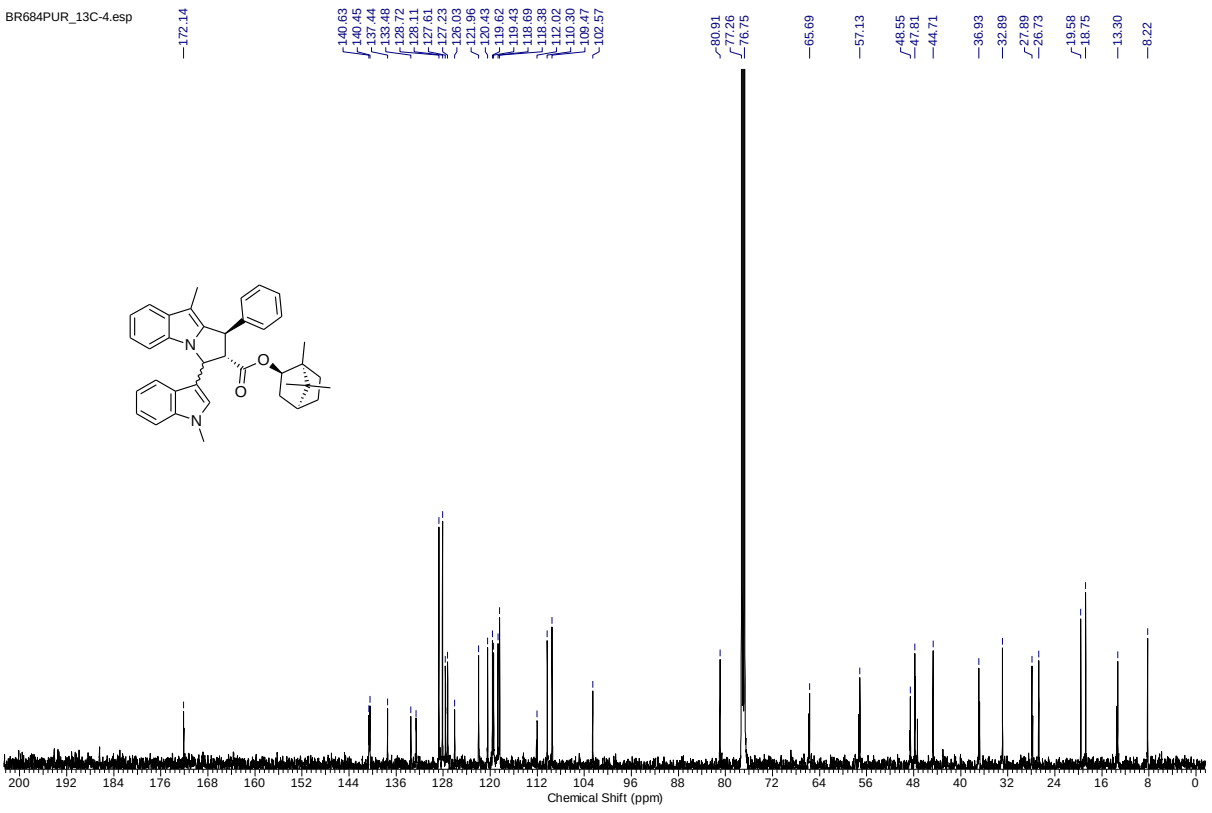
^{1}H and ^{13}C NMR of compound 17f



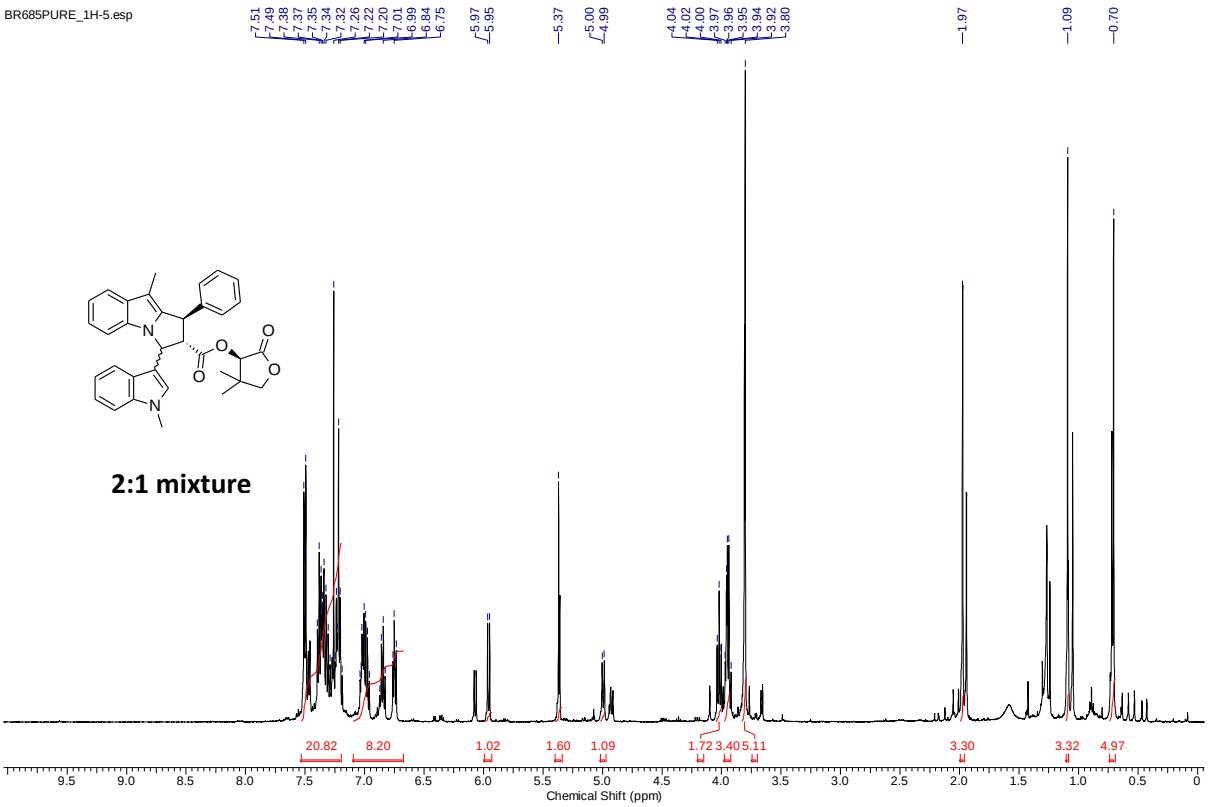


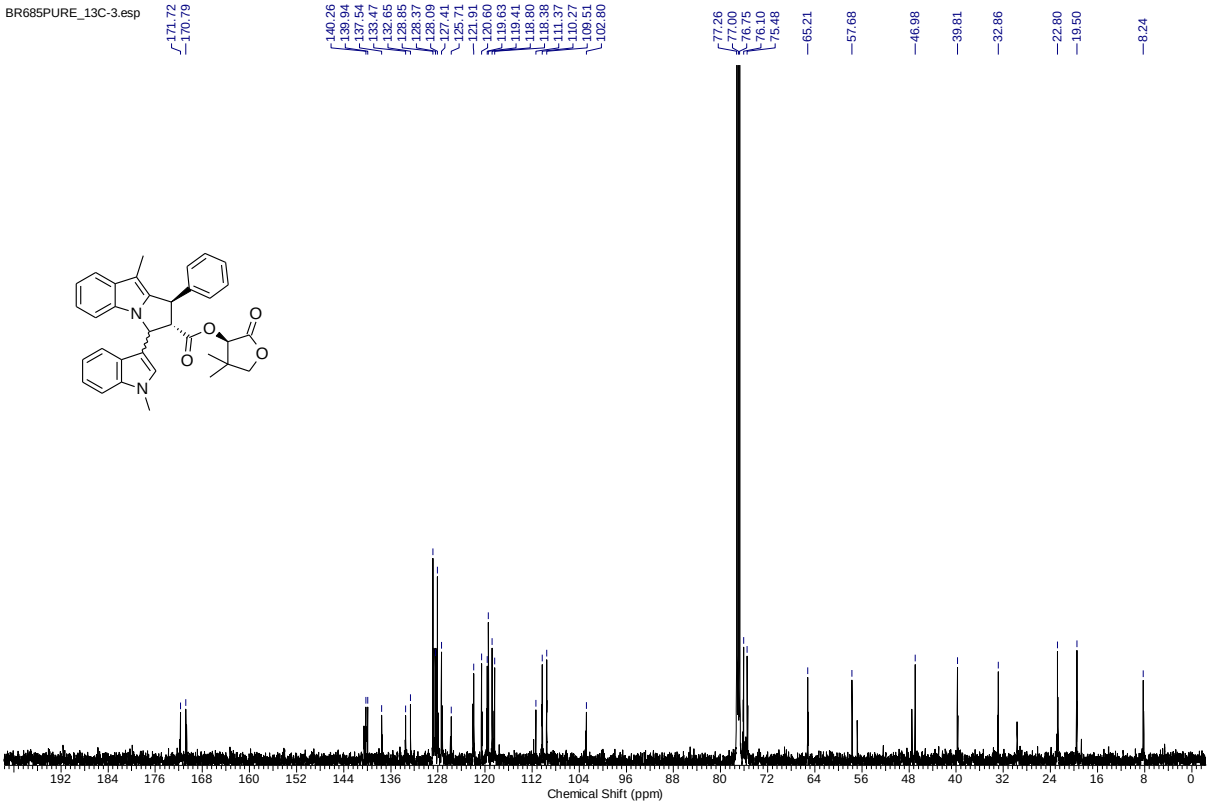
^{1}H and ^{13}C NMR of compound 18a



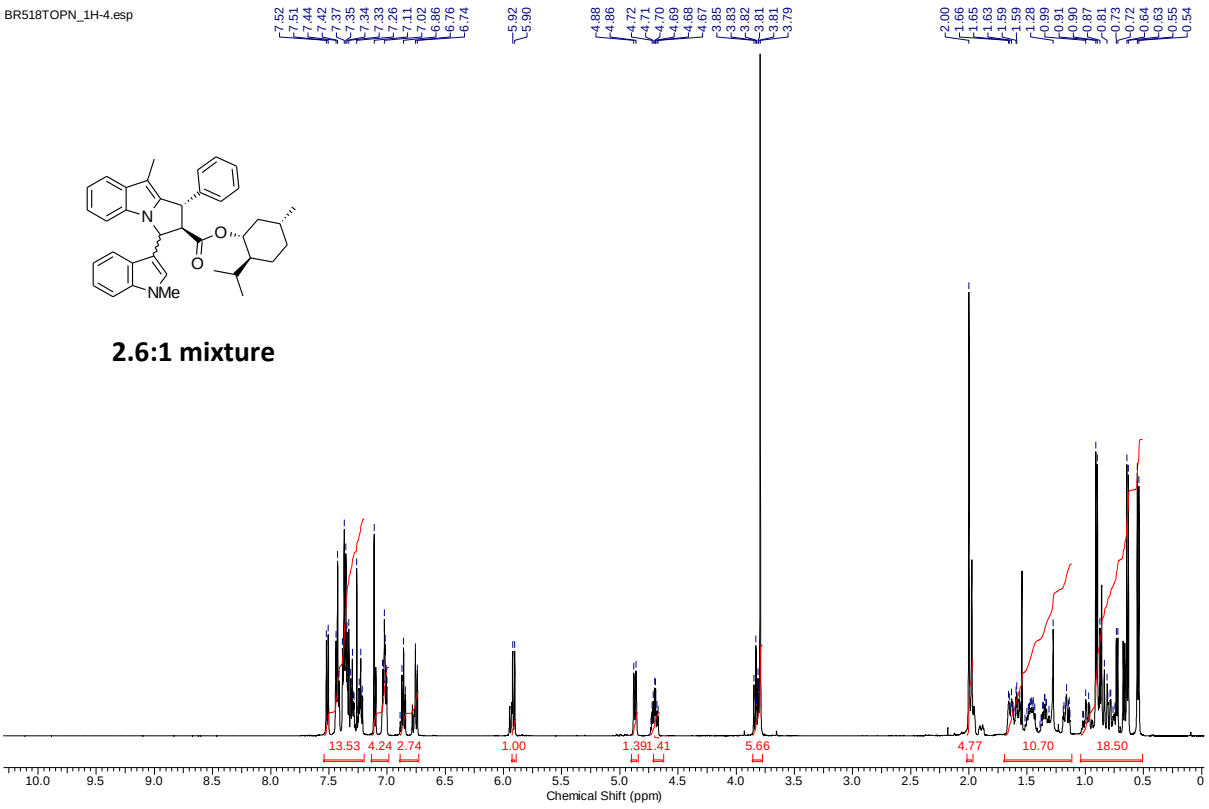


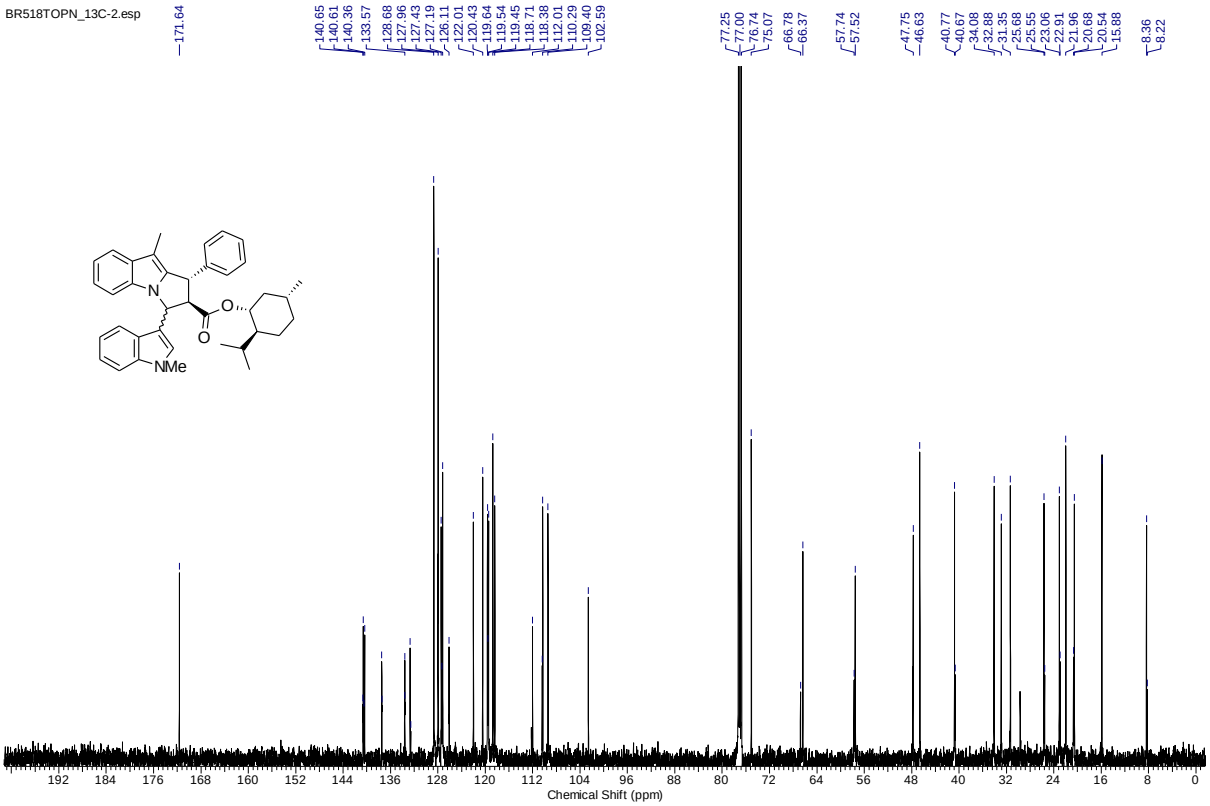
^{1}H and ^{13}C NMR of compound 18b



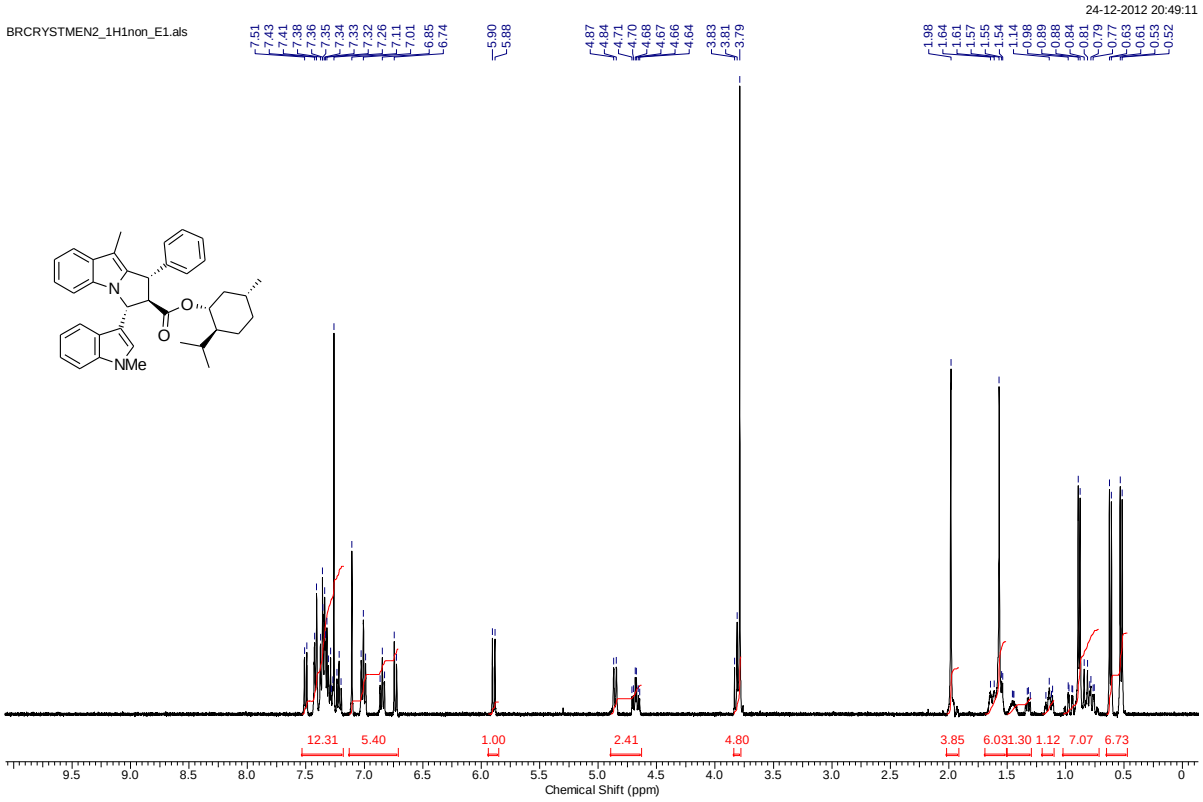


^{1}H and ^{13}C NMR of compound 18c

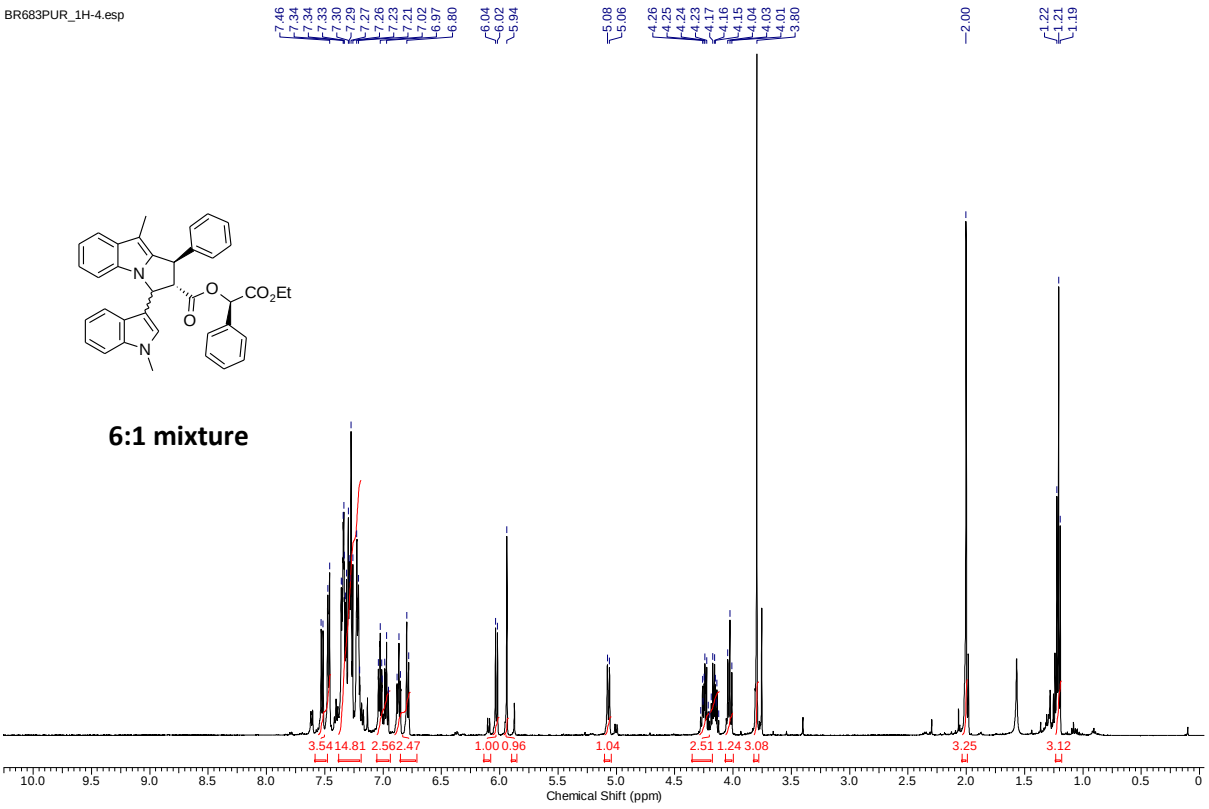


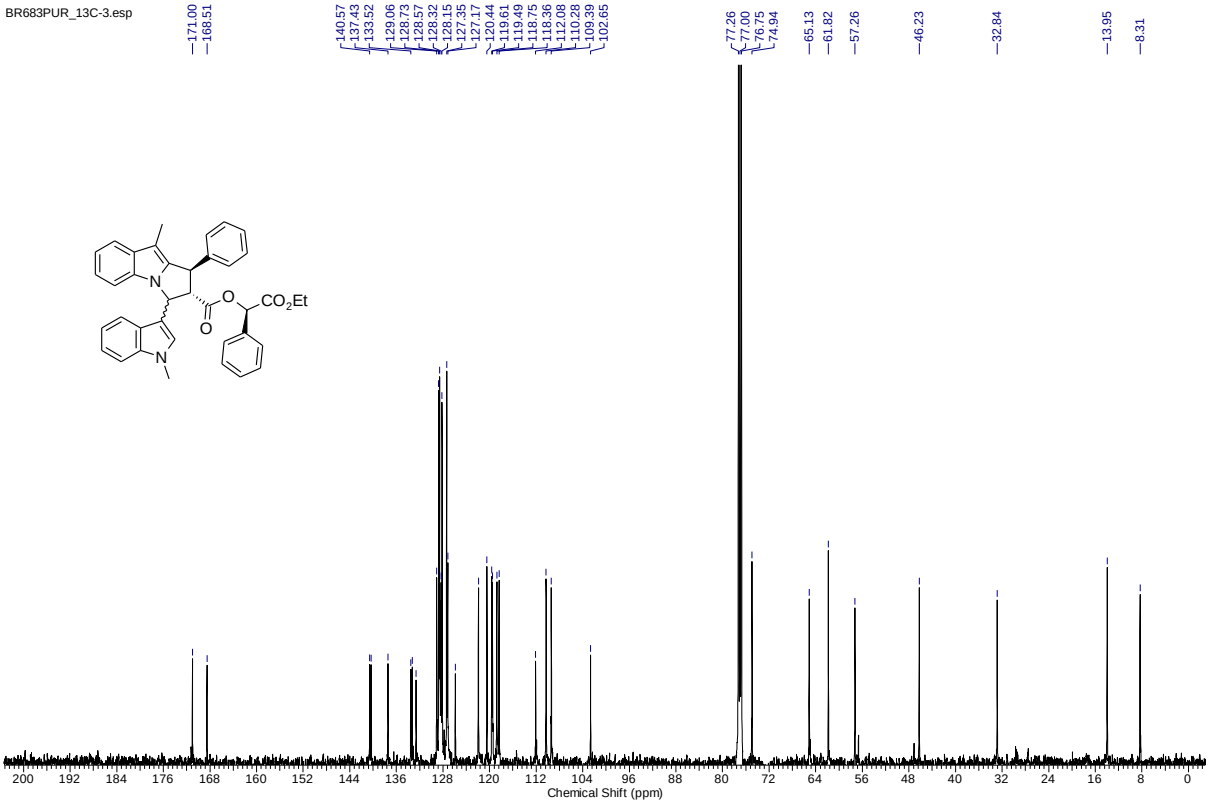


^{1}H NMR of compound 18c (Major isomer)

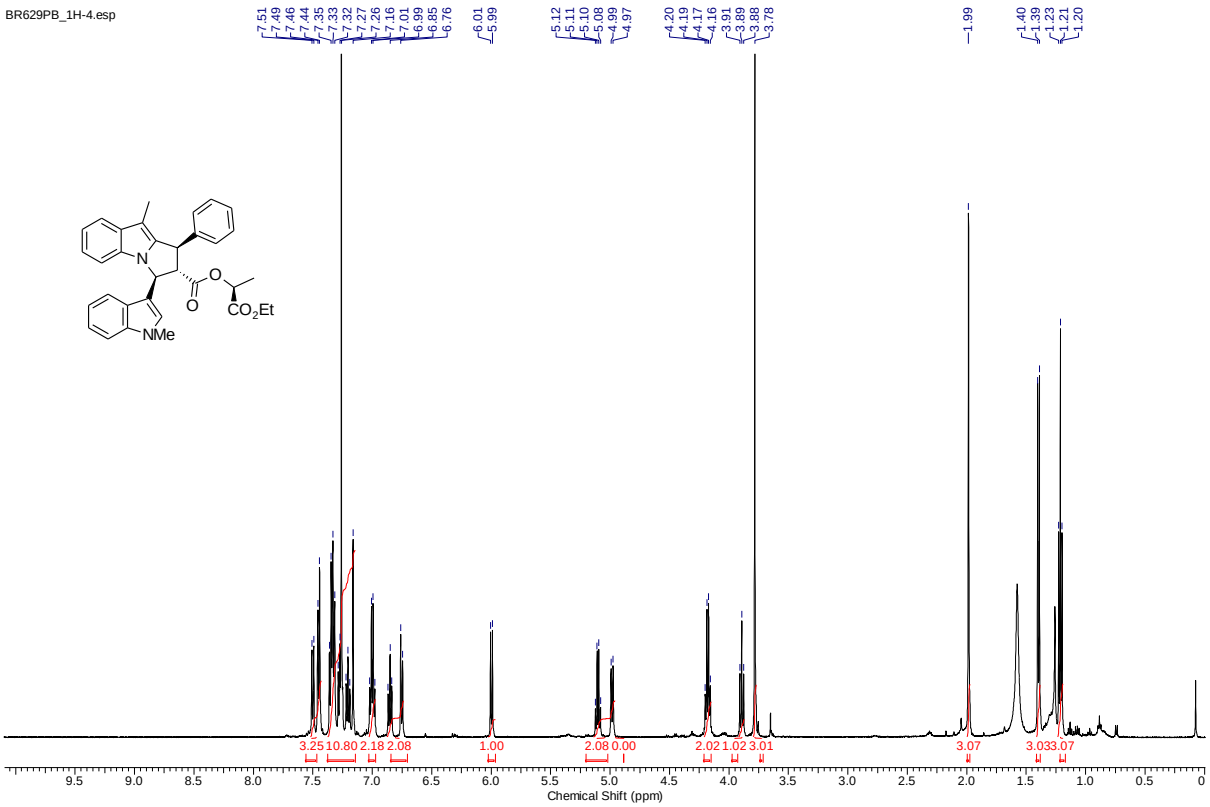


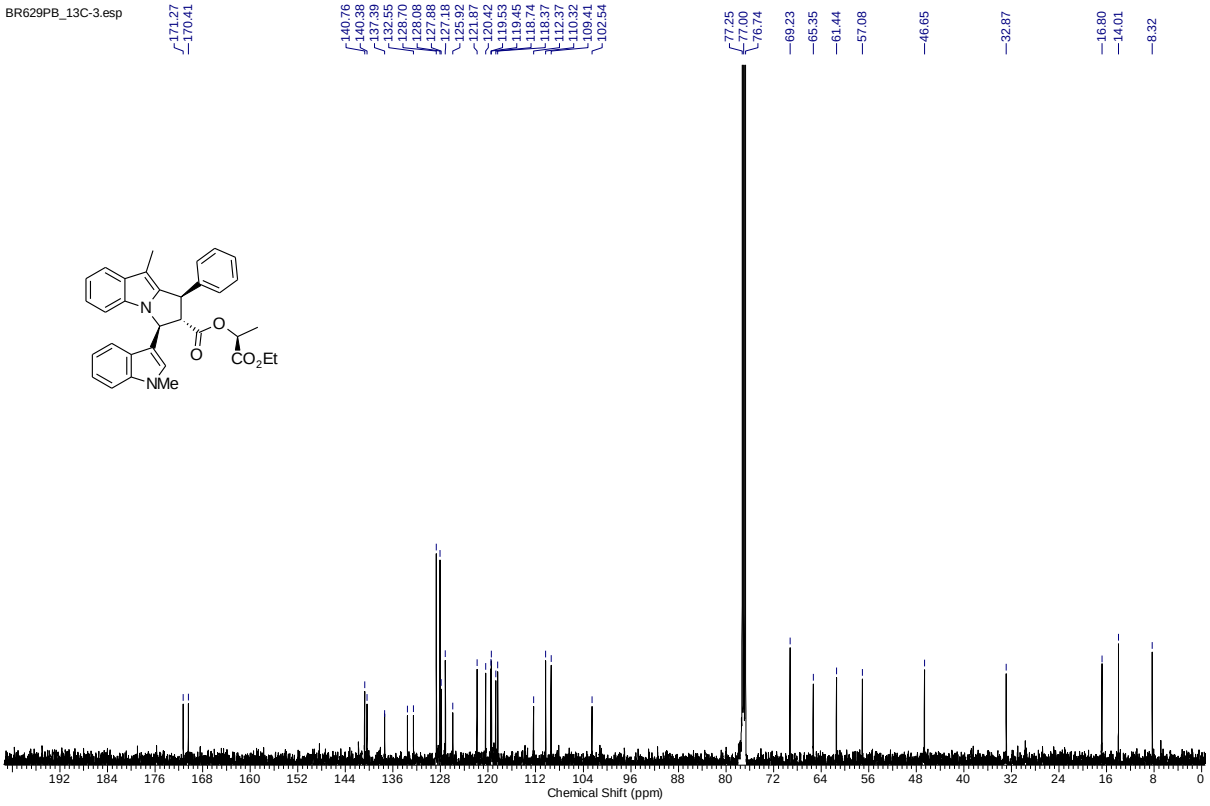
^{1}H and ^{13}C NMR of compound 18d



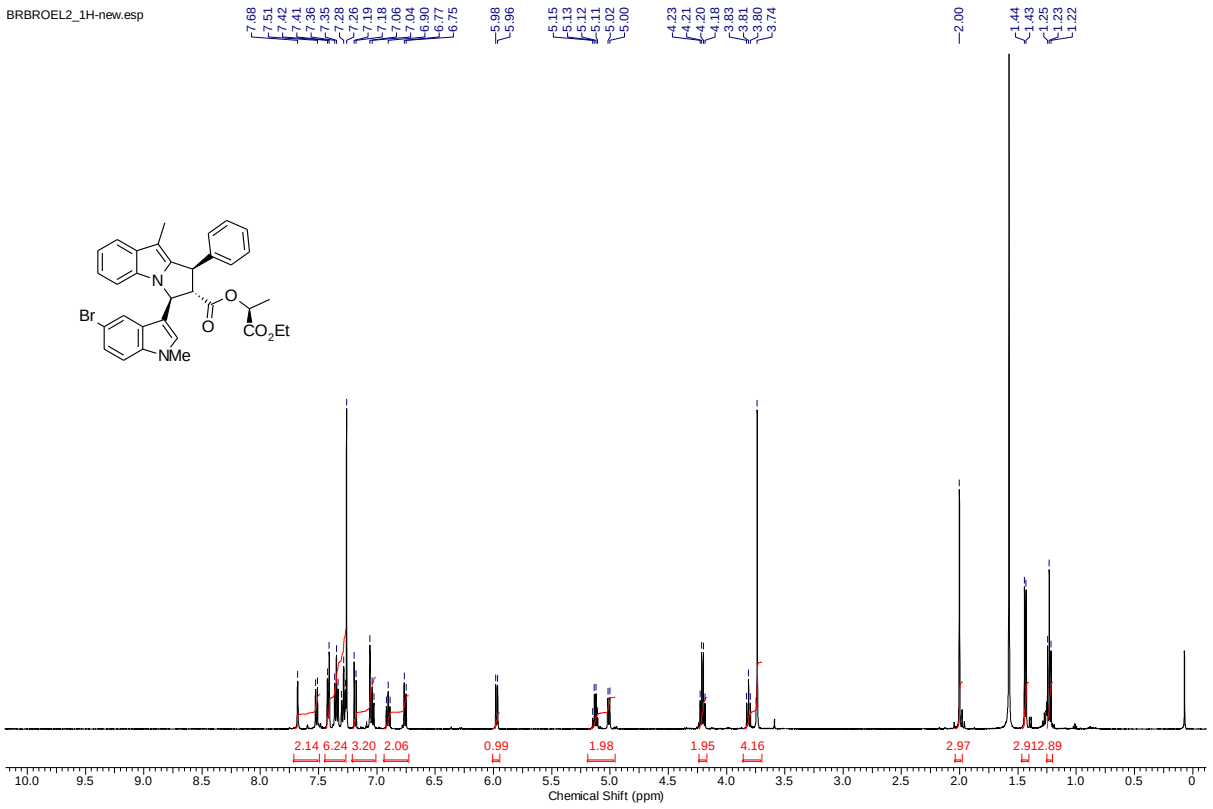


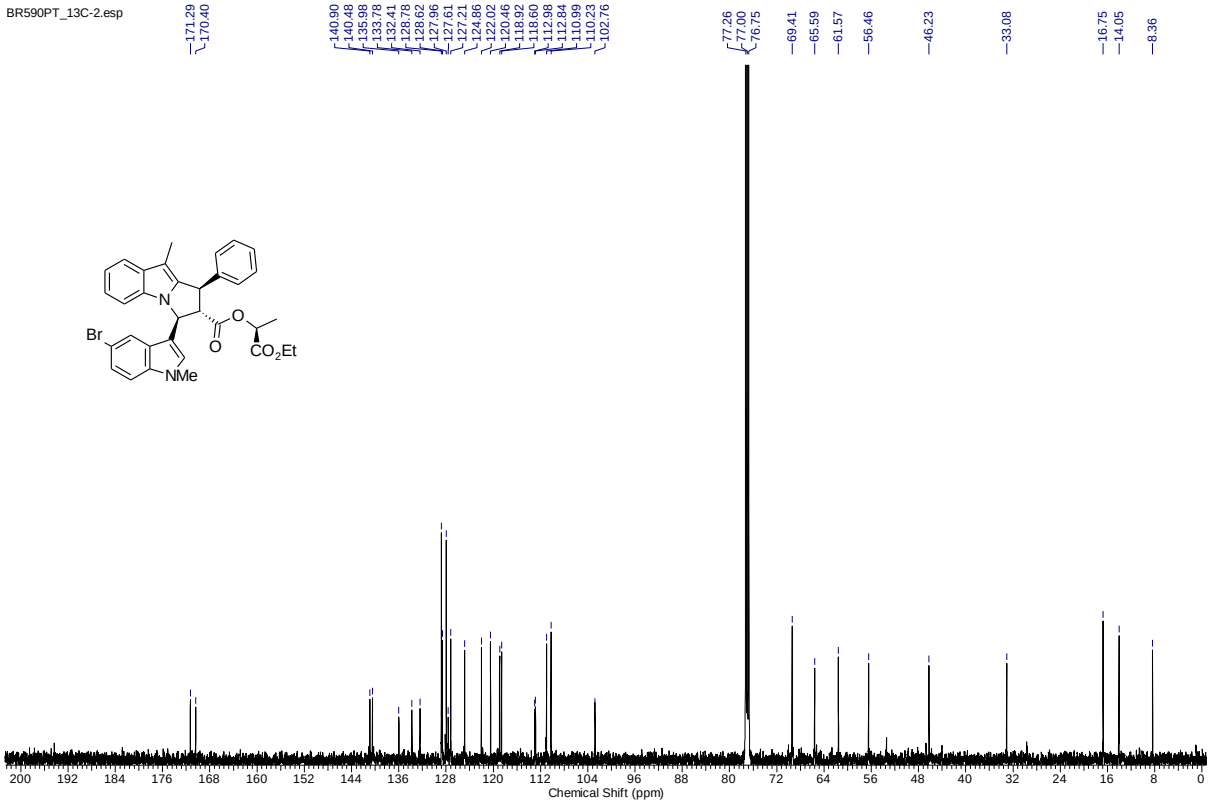
^{1}H and ^{13}C NMR of compound 18e



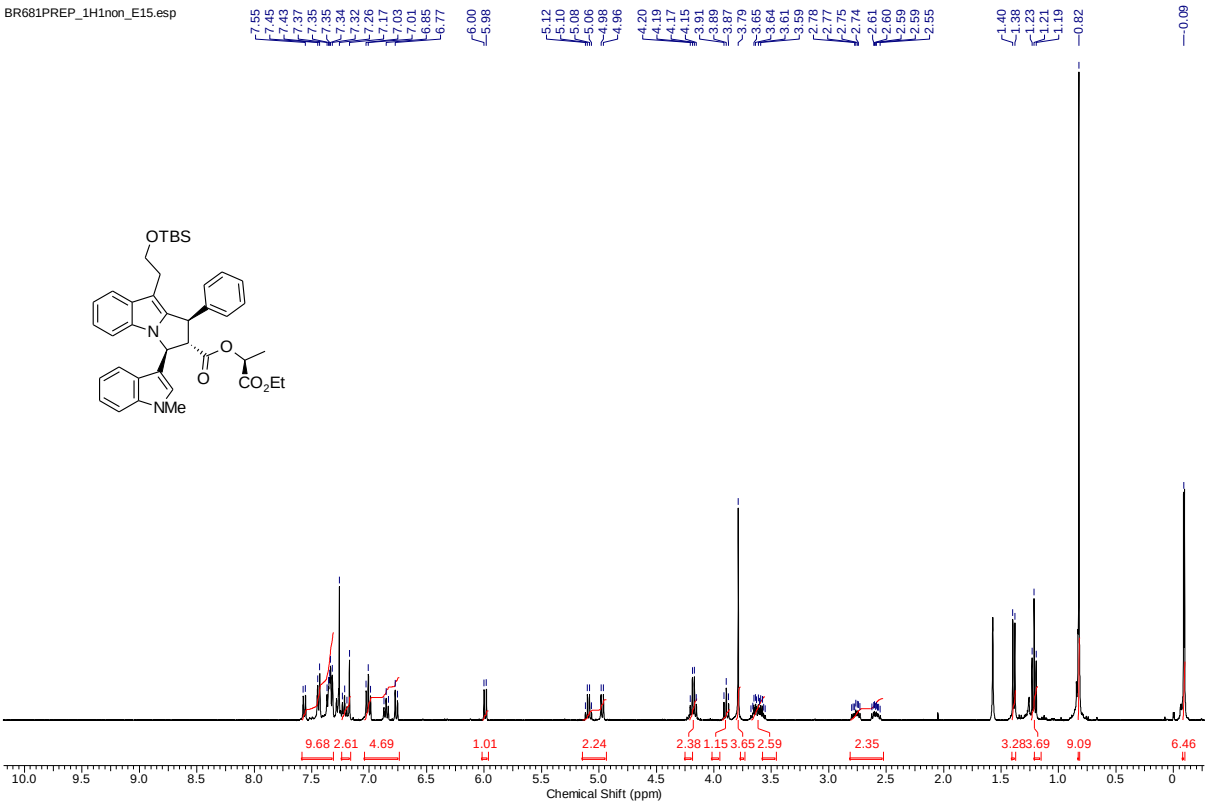


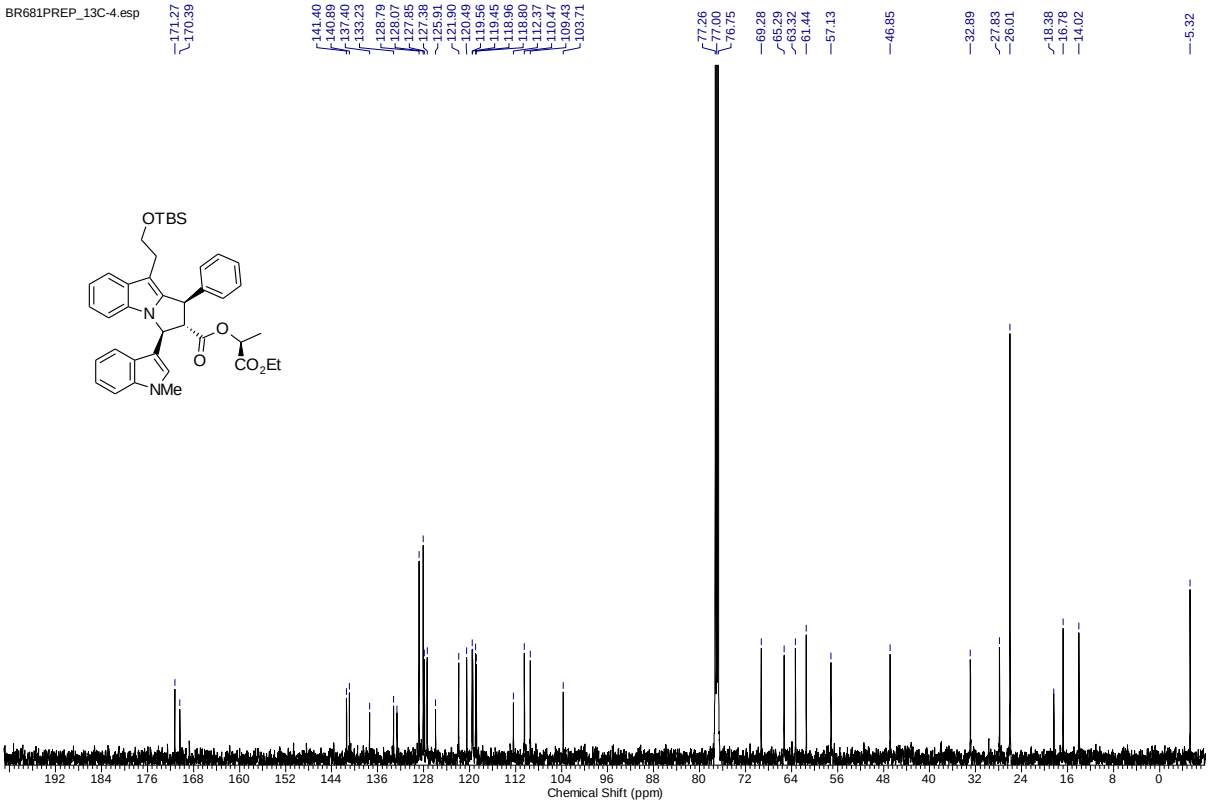
^{1}H and ^{13}C NMR of compound 18f



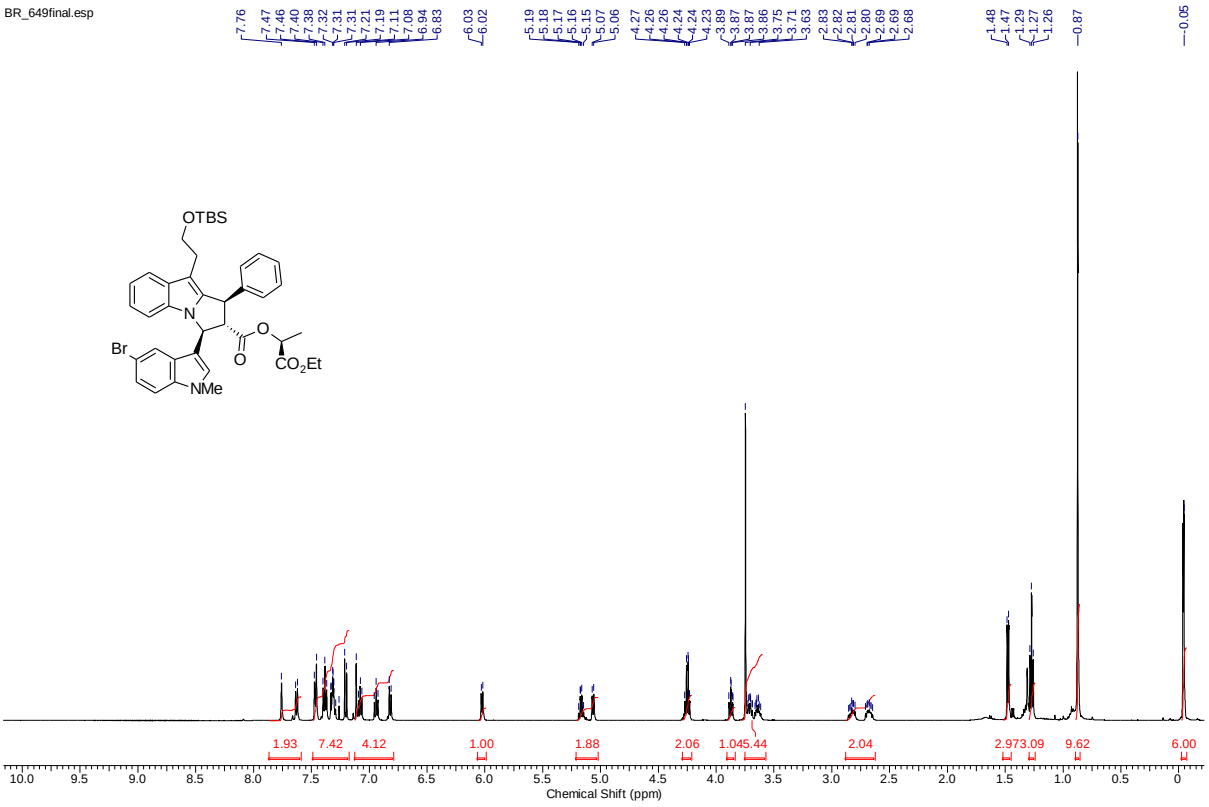


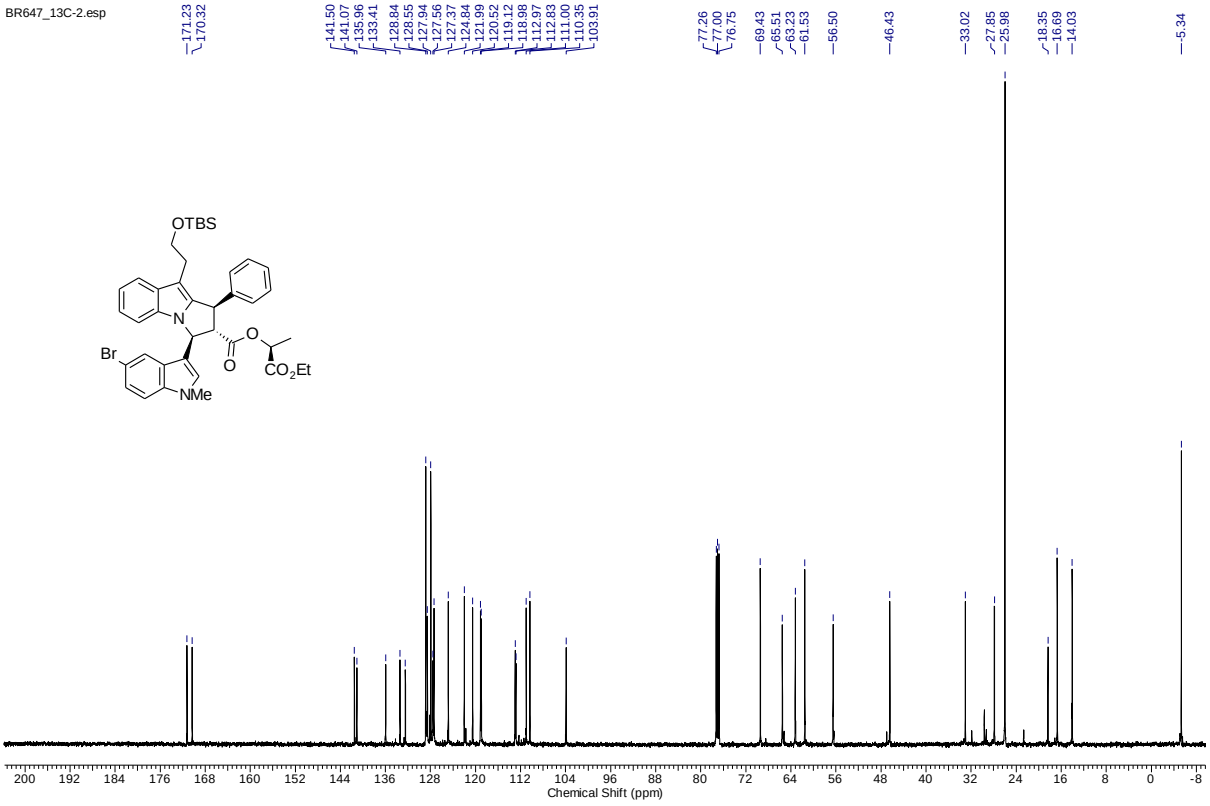
^{1}H and ^{13}C NMR of compound 18h



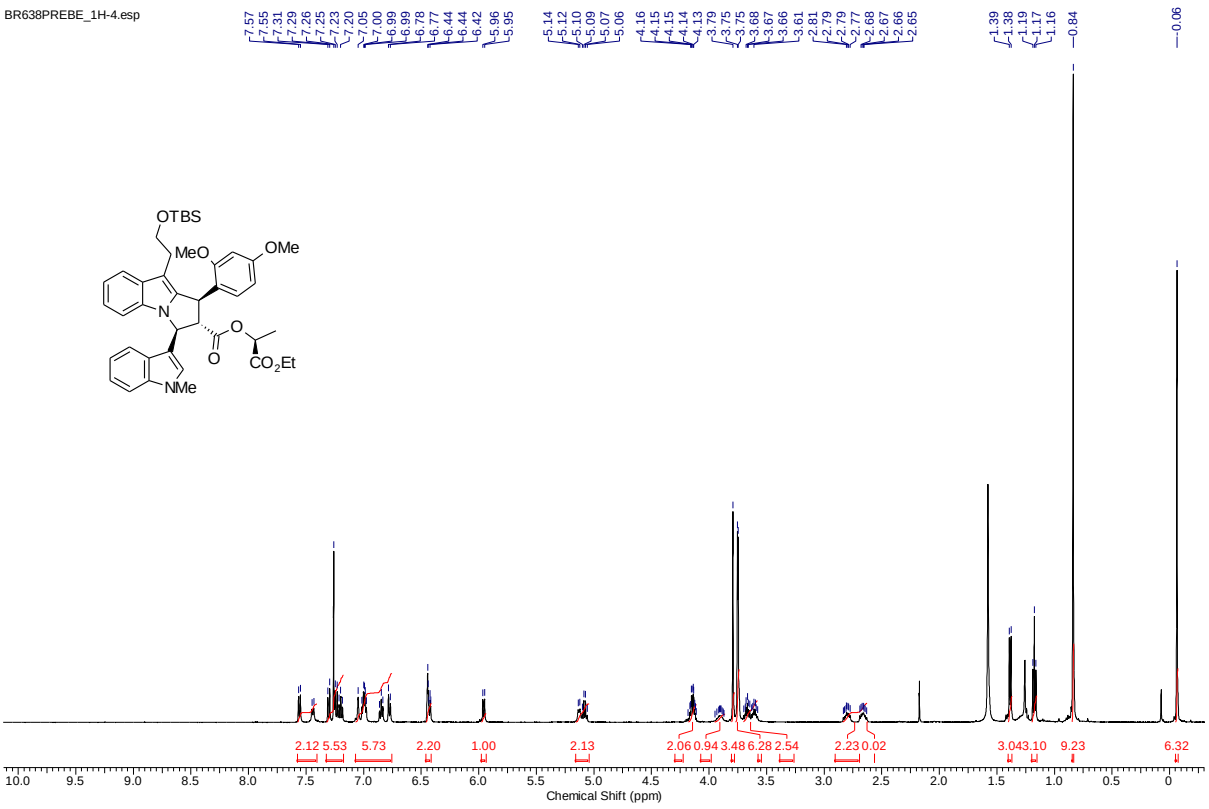


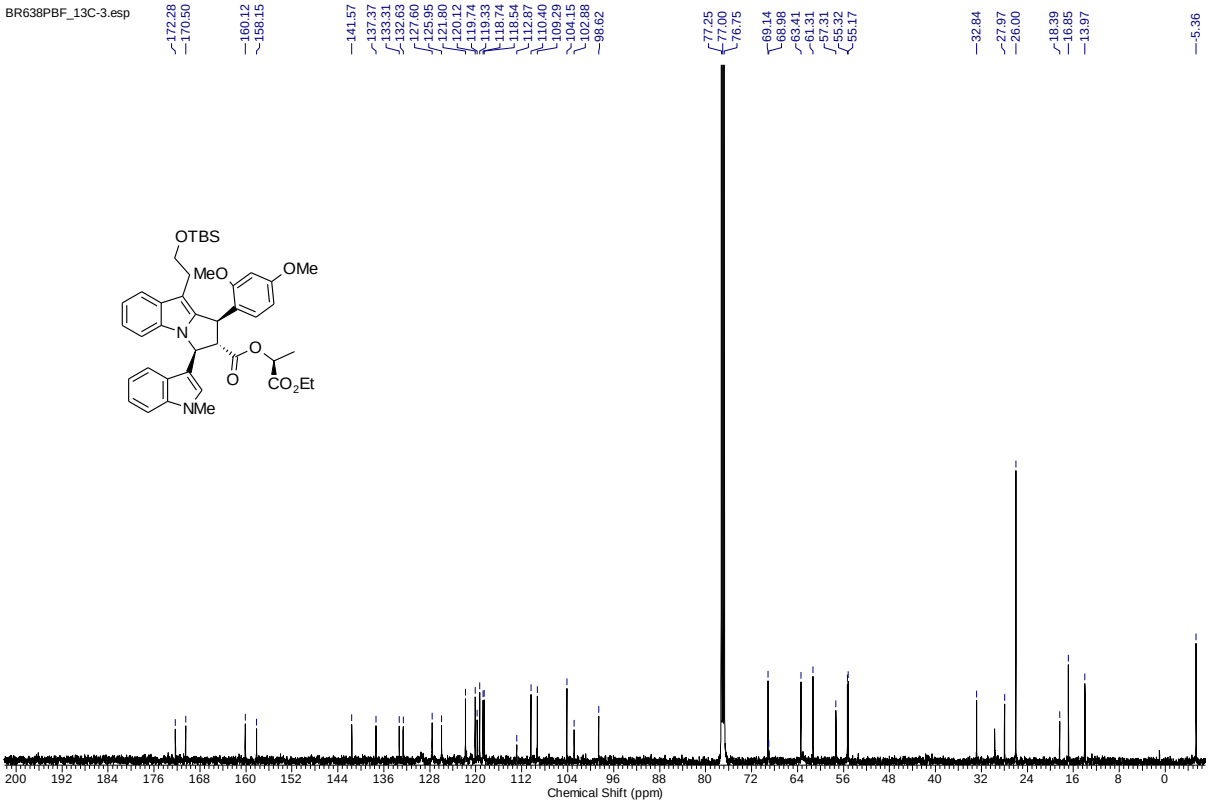
^{1}H and ^{13}C NMR of compound 18i





^{1}H and ^{13}C NMR of compound 18g





^{1}H and ^{13}C NMR of compound 19a