

Supporting Information

Facile Assembly of Structurally Diverse 2H-Pyrans Enabled by Chloropalladation-Initiated Carboetherification of Alkenes

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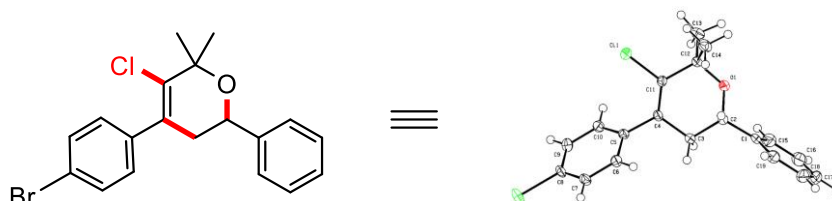
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X-ray Crystallographic analysis for product **3k**

The CCDC number of the compound **3k** is 2534149.

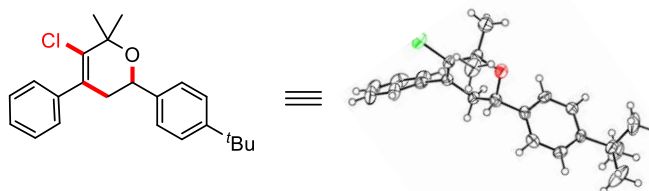


Crystal Data and Structure Refinement for Product **3k**

Empirical formula	C ₁₉ H ₁₈ BrClO
Formula weight	377.69
Temperature	170 K
Wavelength	0.71073 Å
Crystal system	triclinic
Space group	P-1
Unit cell dimensions	a = 5.8690(2) Å, α = 104.8380(10)°
	b = 10.1522(4) Å, β = 94.280(2)°
	c = 14.6162(6) Å, γ = 96.306(2)°
Density (calculated)	1.508
Absorption coefficient	0.083
F(000)	384.0
Crystal size(mm ³)	0.15 × 0.06 × 0.05
Theta range for data collection	4.188 to 52.852
Index ranges	-7 ≤ h ≤ 7, -12 ≤ k ≤ 12, -18 ≤ l ≤ 18
Reflections collected	10135
Independent reflections	3421
Completeness to theta = 29.55°	98.03%
Absorption correction	multi-scan
Refinement method	Full-matrix least-squares on F ²
Data/restraints/parameters	3421/0/201
Goodness-of-fit on F ²	1.031
Final R indices [I > 2σ(I)]	R ₁ = 0.0362, wR ₂ = 0.0857
R indices (all data)	R ₁ = 0.0452, wR ₂ = 0.0910

X-ray Crystallographic analysis for product 4d

The CCDC number of the compound **4d** is 2534152.

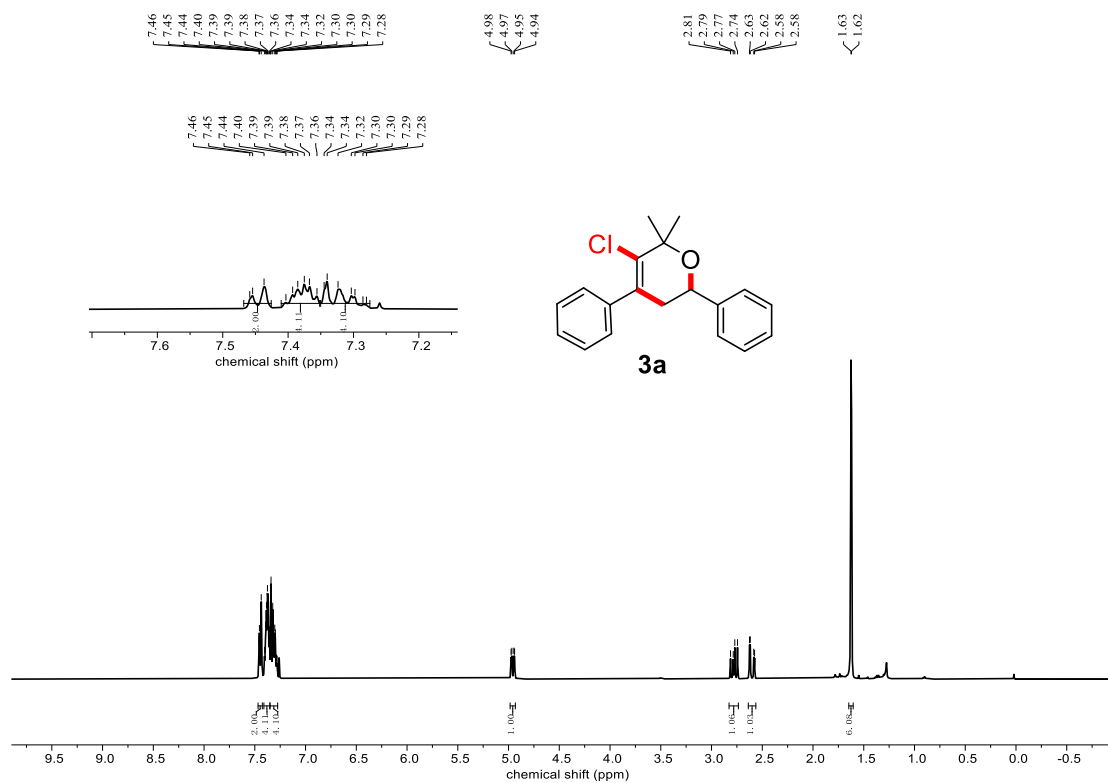


Crystal Data and Structure Refinement for Product **4d**

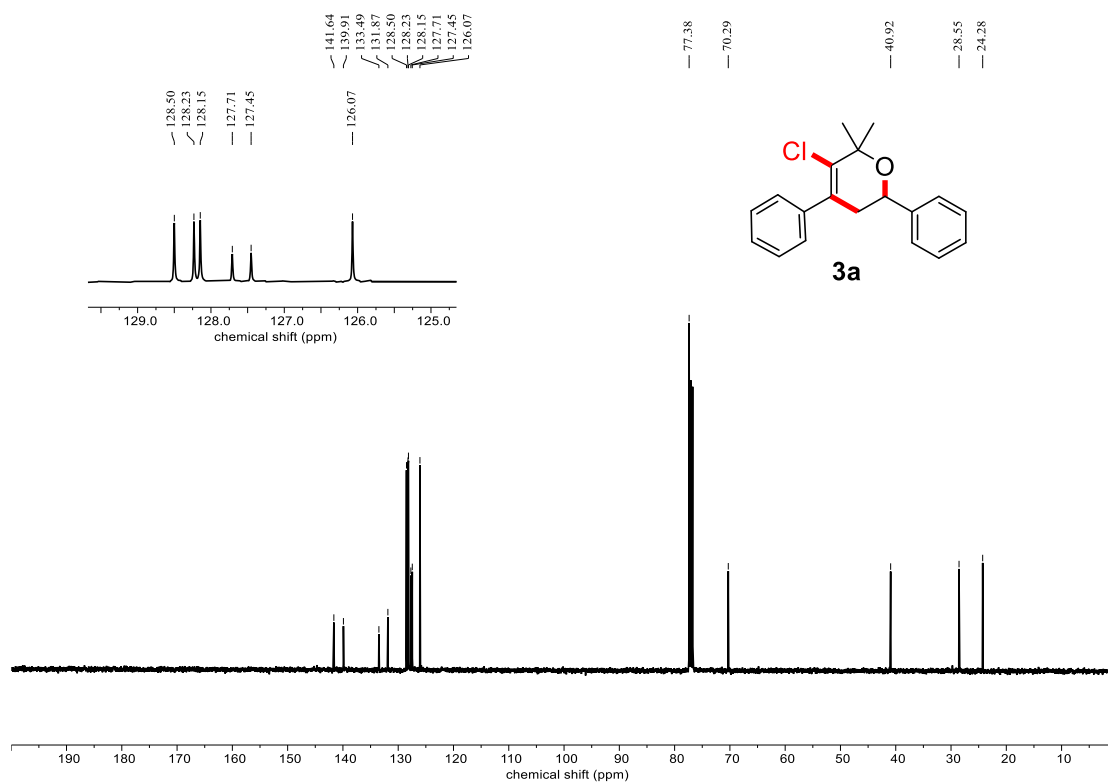
Empirical formula	C ₂₃ H ₂₇ ClO
Formula weight	354.89
Temperature	170 K
Wavelength	0.71073 Å
Crystal system	triclinic
Space group	P-1
Unit cell dimensions	a = 10.1041(18) Å, α = 71.017(6)°
	b = 13.308(2) Å, β = 76.649(6)°
	c = 16.926(3) Å, γ = 72.312(6)°
Density (calculated)	1.162
Absorption coefficient	0.083
F(000)	760.0
Crystal size	0.12 × 0.06 × 0.05
Theta range for data collection	4.658 to 52.946
Index ranges	-12 ≤ h ≤ 12, -16 ≤ k ≤ 16, -21 ≤ l ≤ 21
Reflections collected	8207
Independent reflections	8207
Completeness to theta = 29.55°	98.20%
Absorption correction	multi-scan
Refinement method	Full-matrix least-squares on F ²
Data/restraints/parameters	8207/0/461
Goodness-of-fit on F ²	1.062
Final R indices [I > 2σ(I)]	R ₁ = 0.0876, wR ₂ = 0.1948
R indices (all data)	R ₁ = 0.1565, wR ₂ = 0.2239

¹H and ¹³C NMR spectra of compounds 3

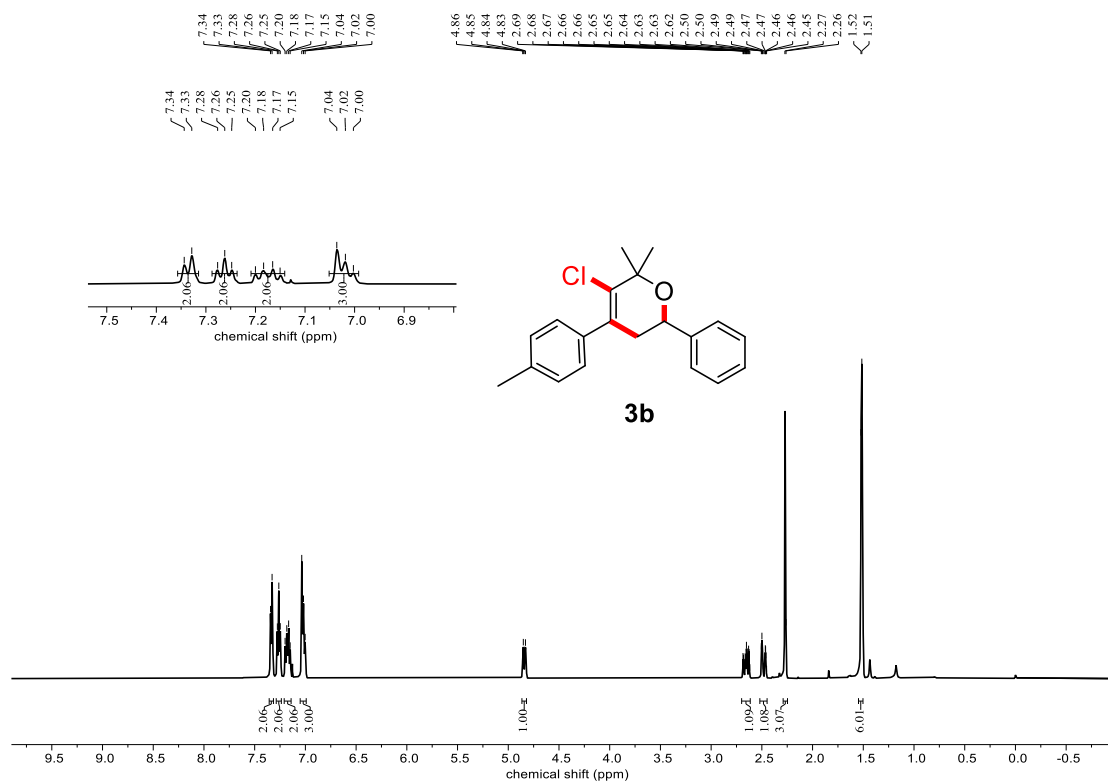
¹H NMR of 3a



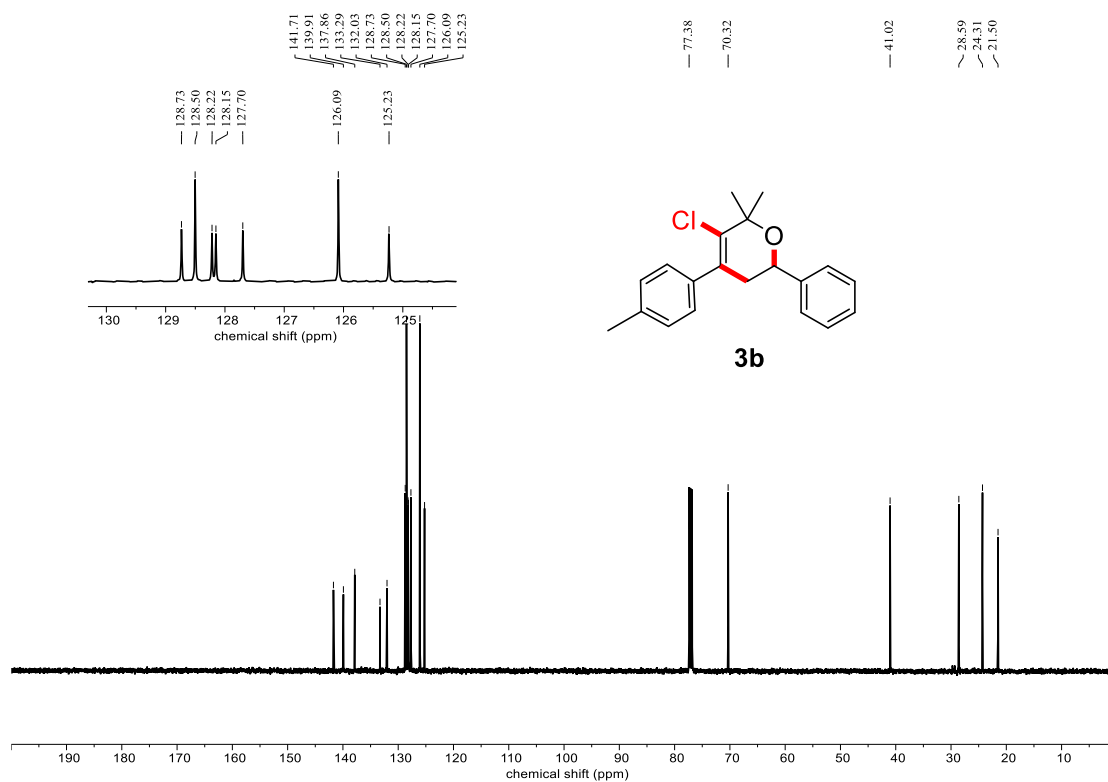
¹³C NMR of 3a



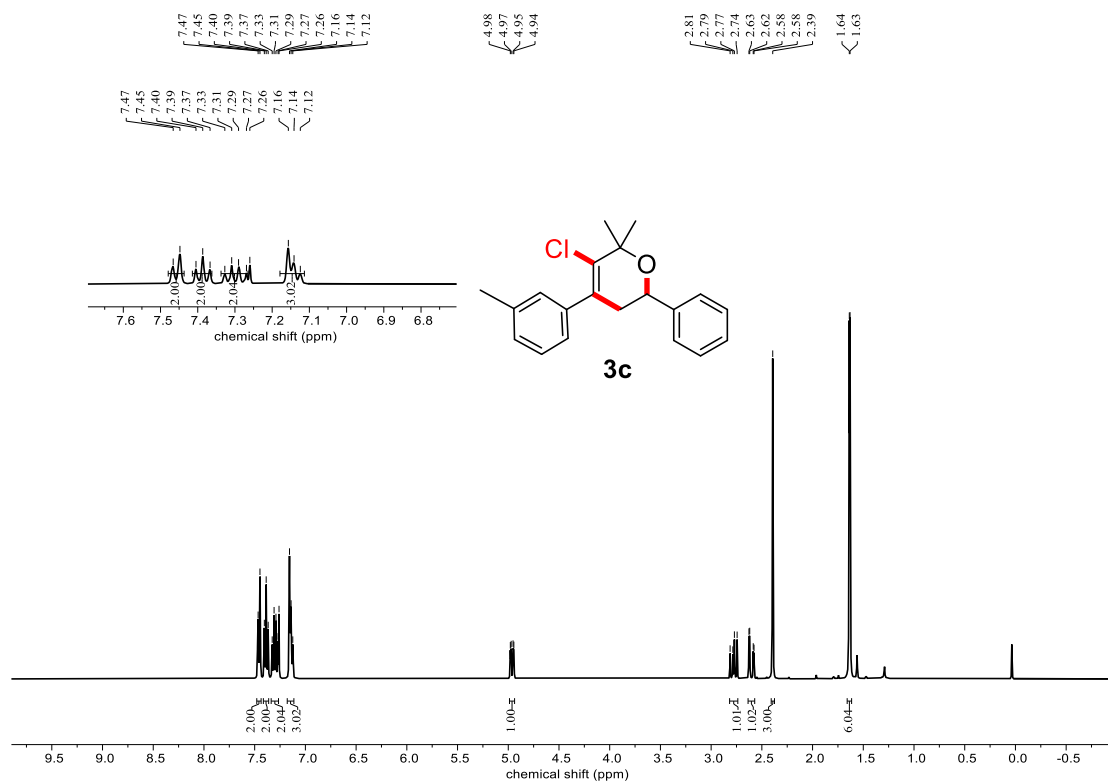
¹H NMR of 3b



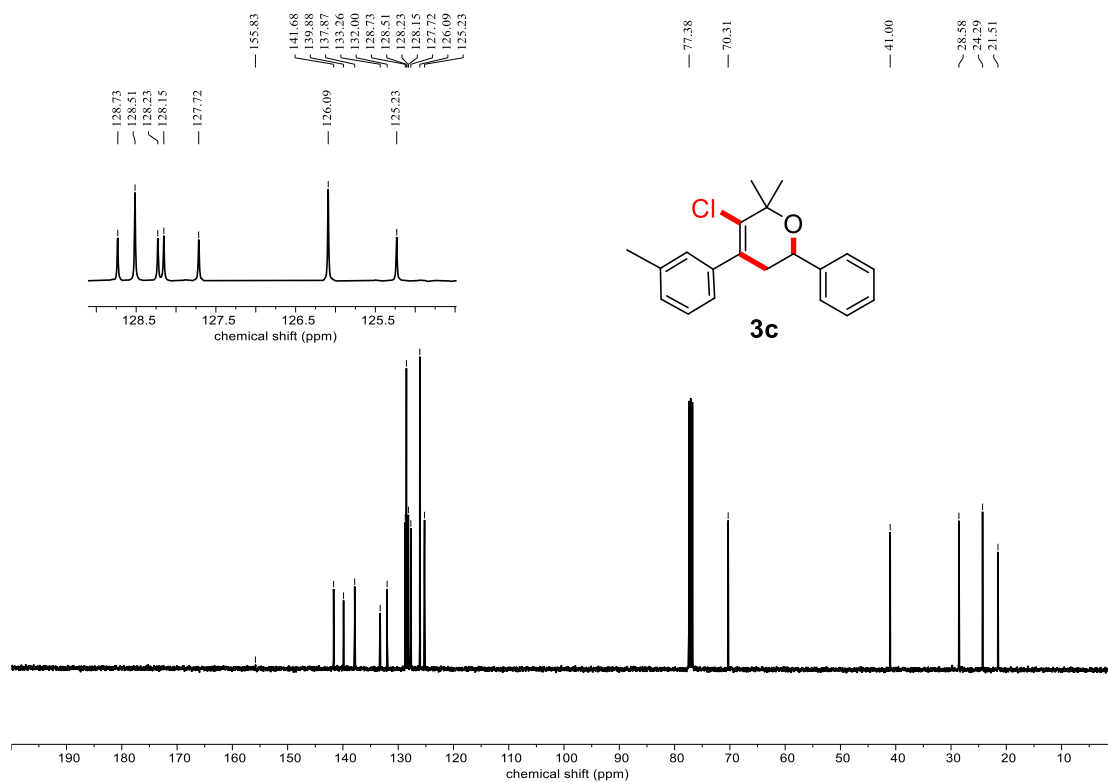
¹³C NMR of 3b



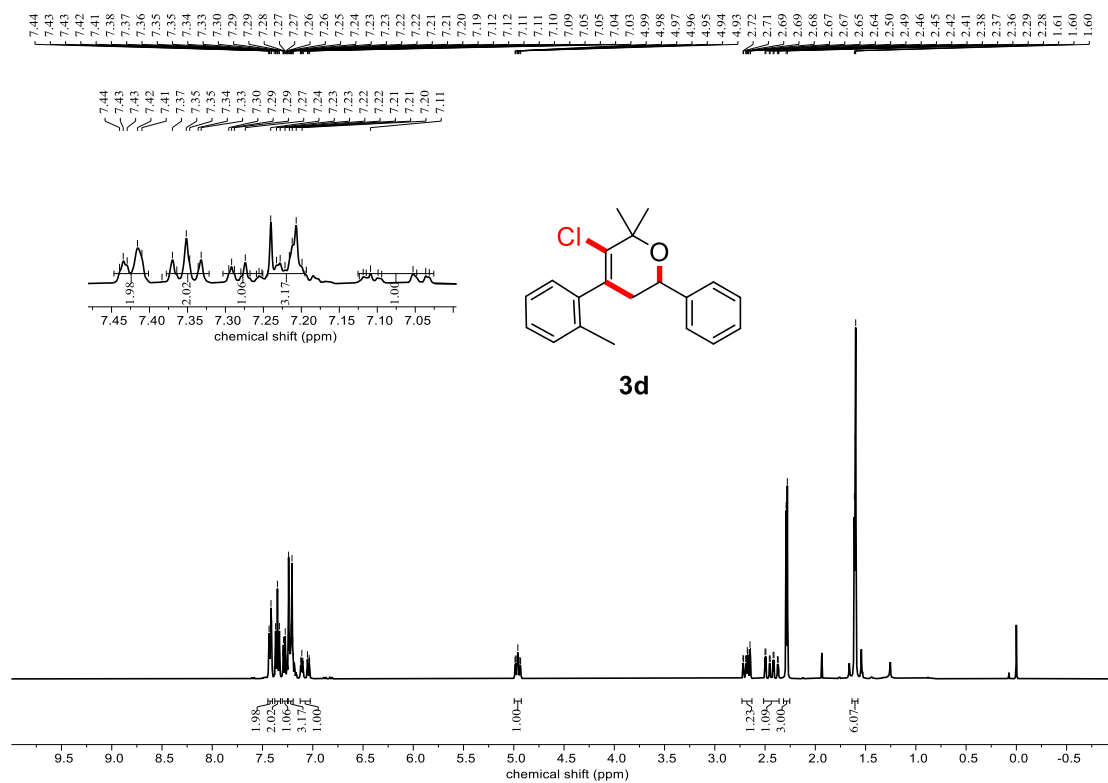
¹H NMR of 3c



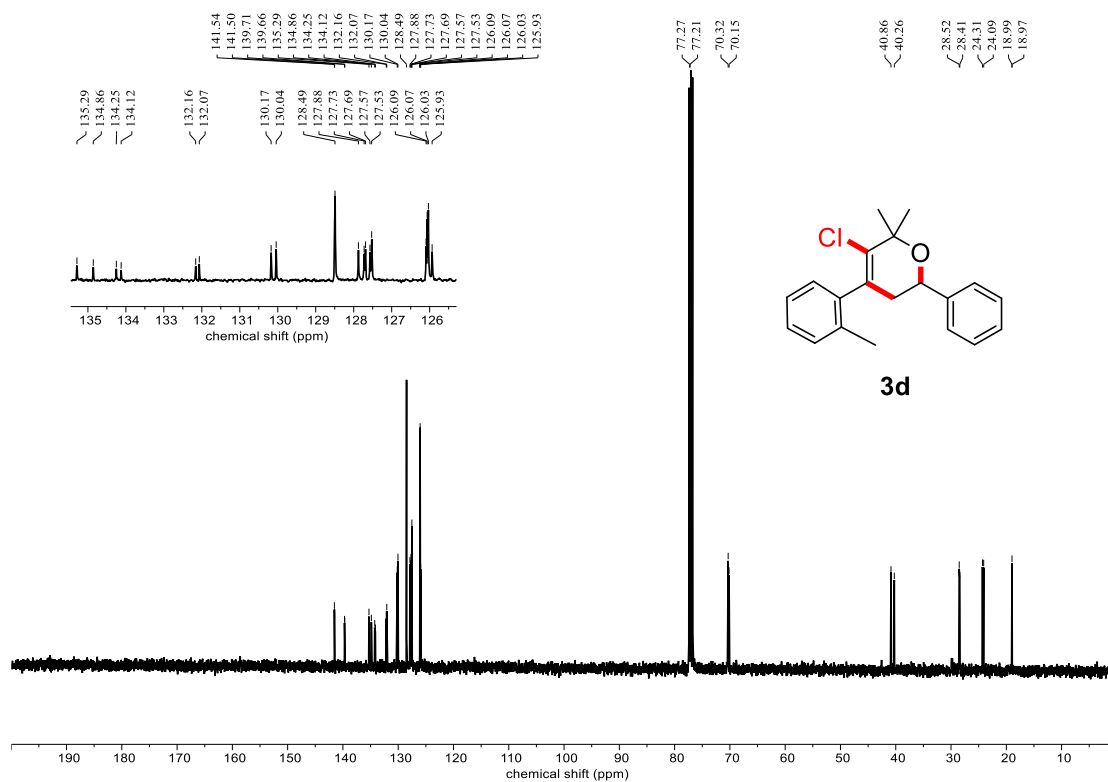
¹³C NMR of 3c



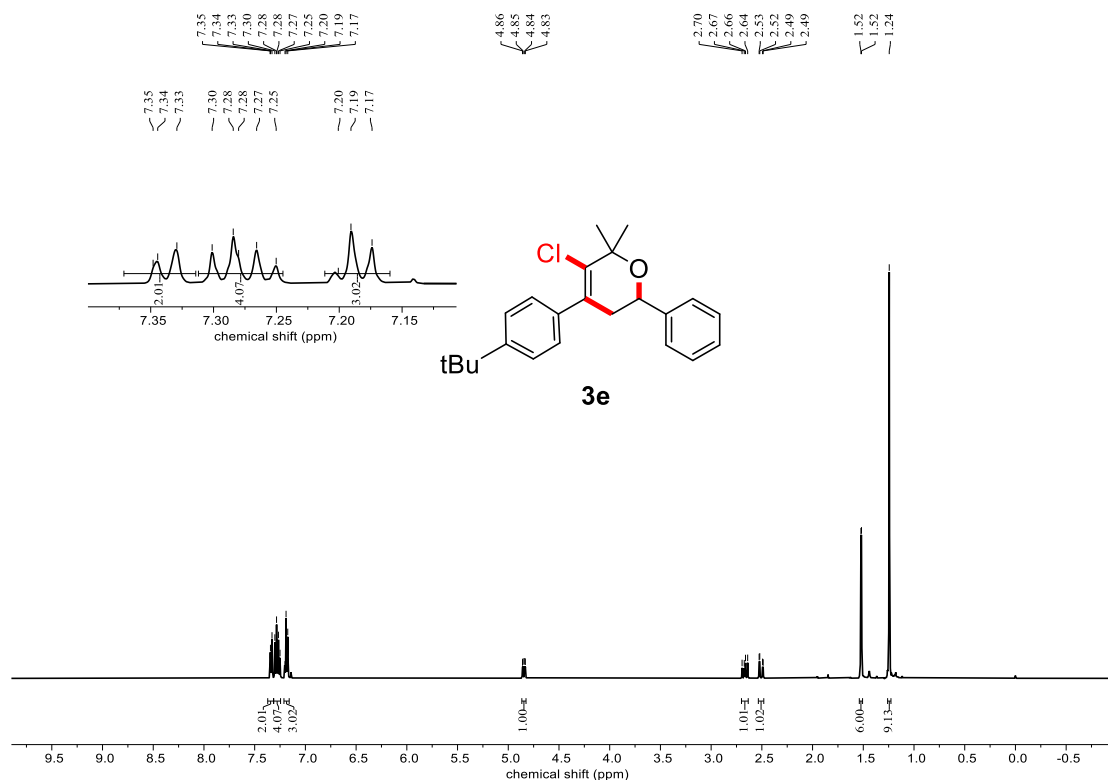
¹H NMR of 3d



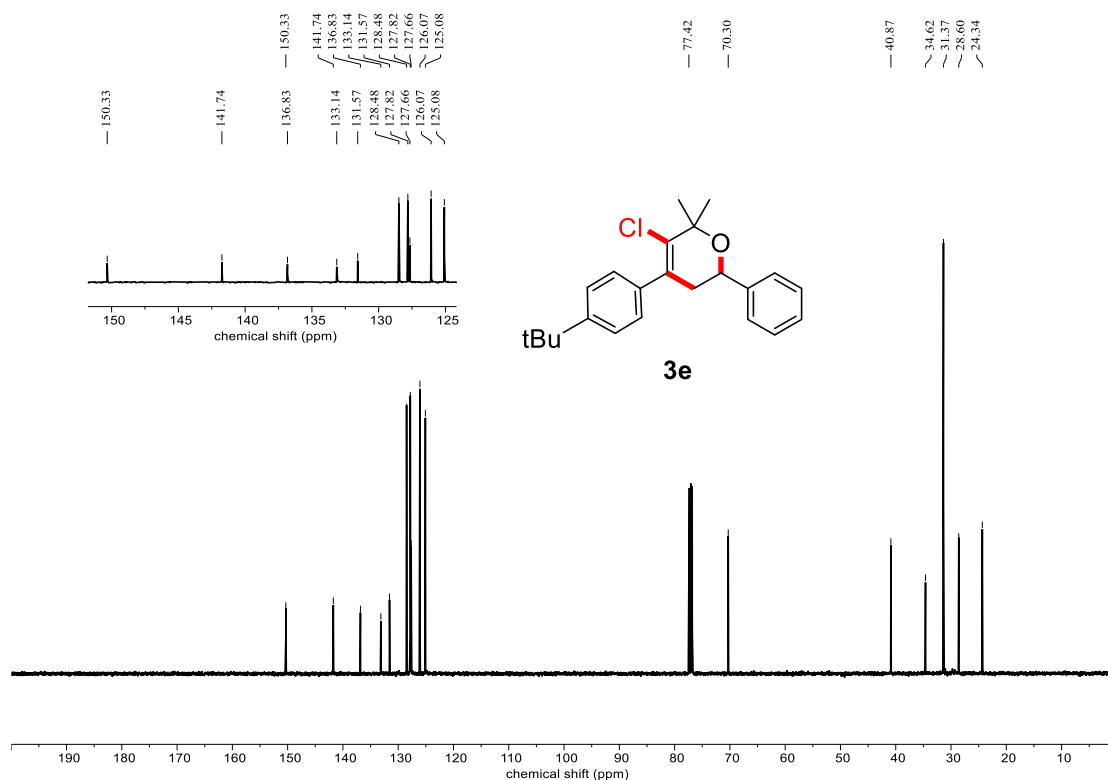
¹³C NMR of 3d



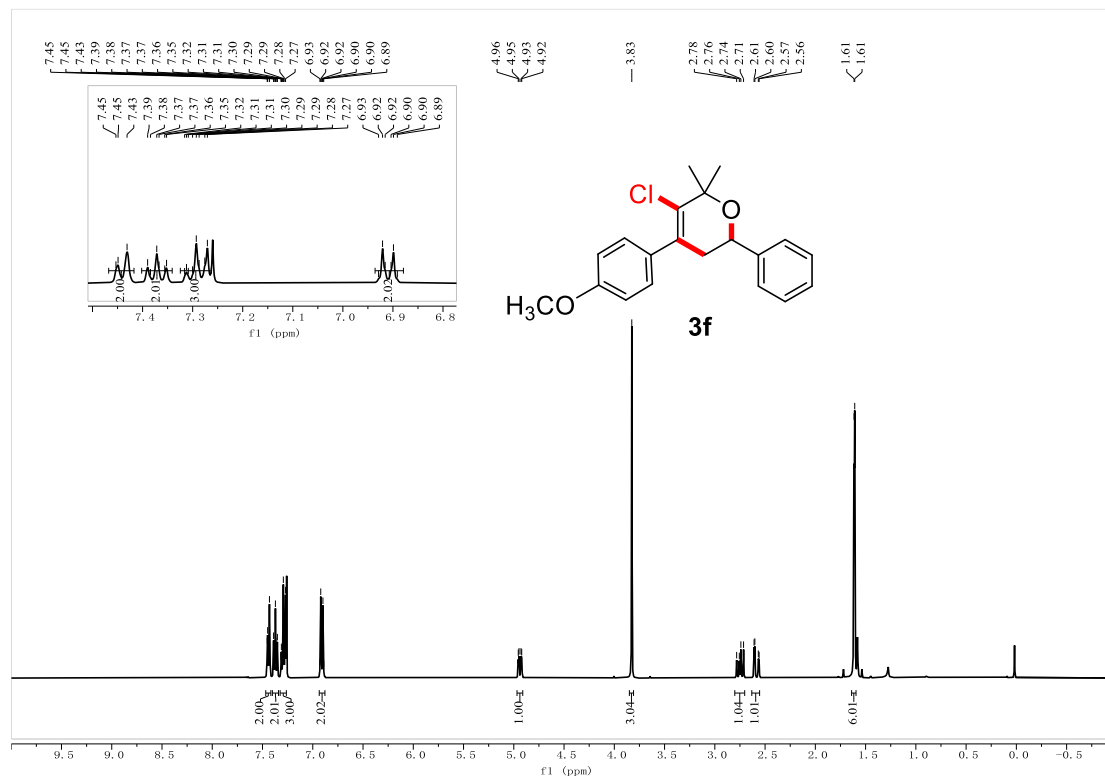
¹H NMR of 3e



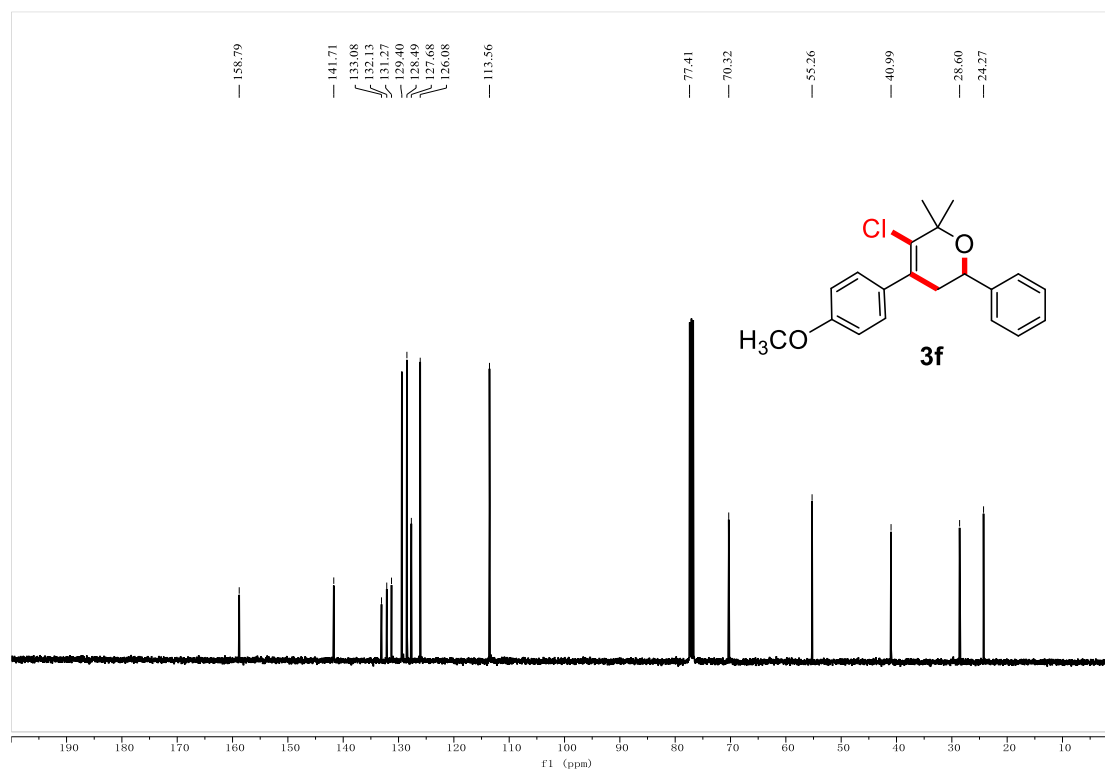
¹³C NMR of 3e



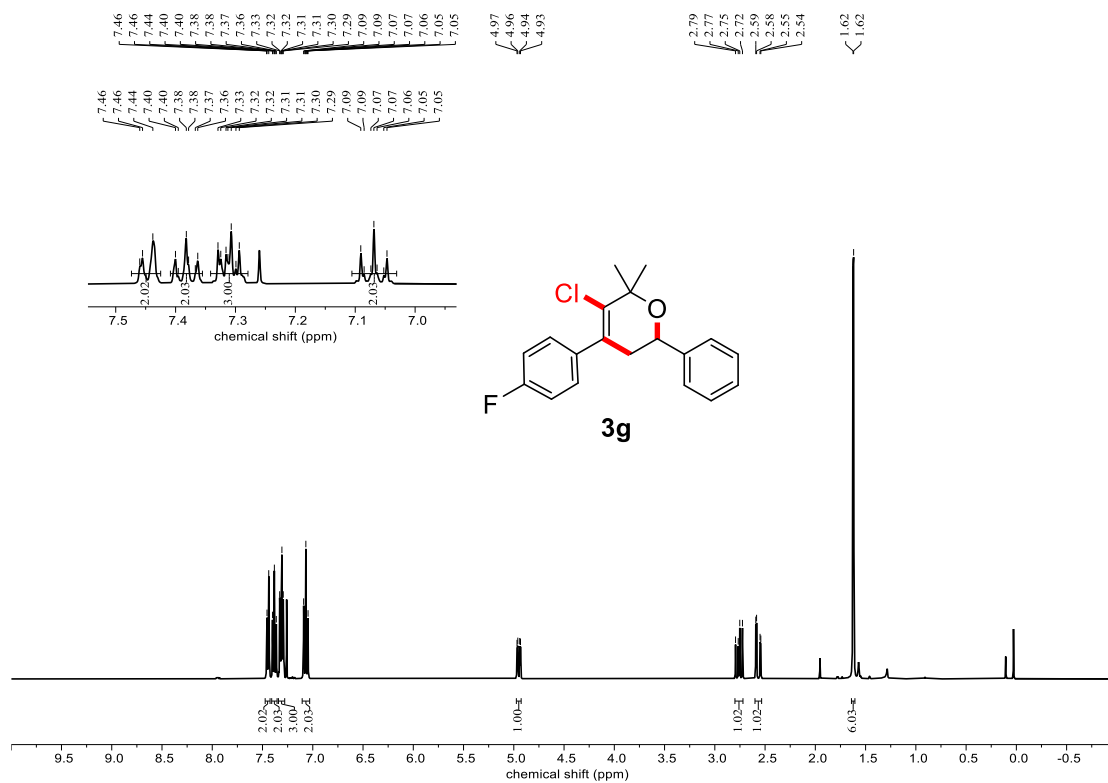
¹H NMR of 3f



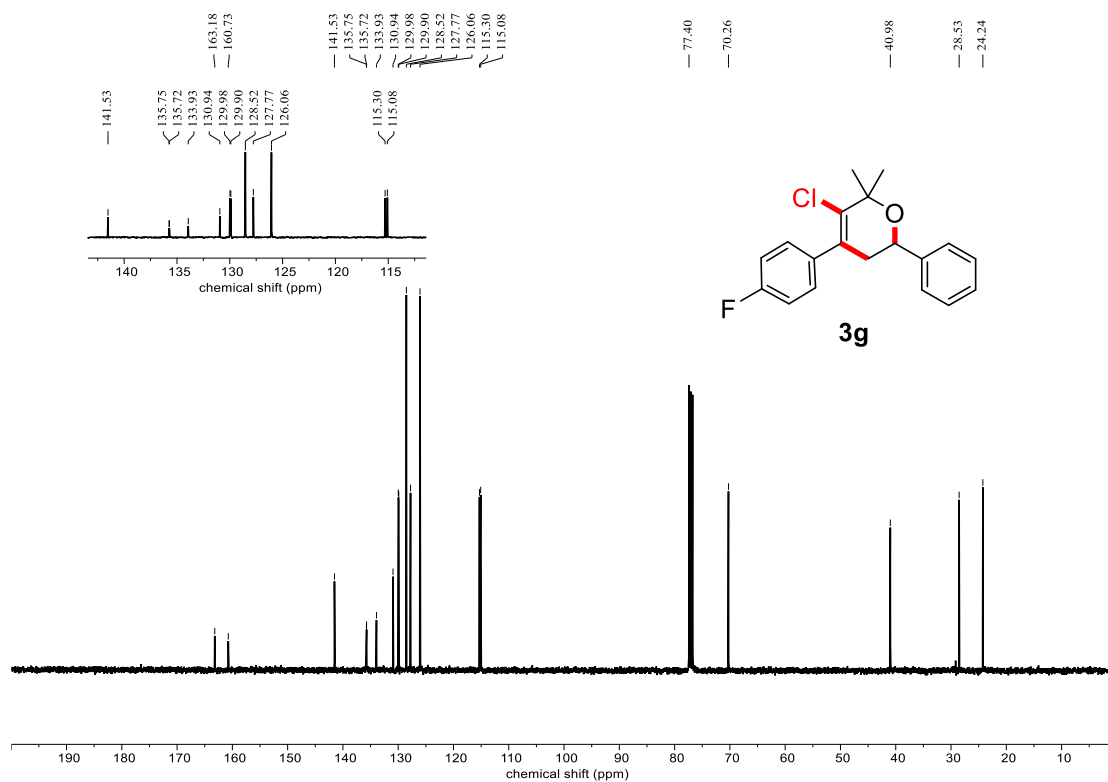
¹³C NMR of 3f



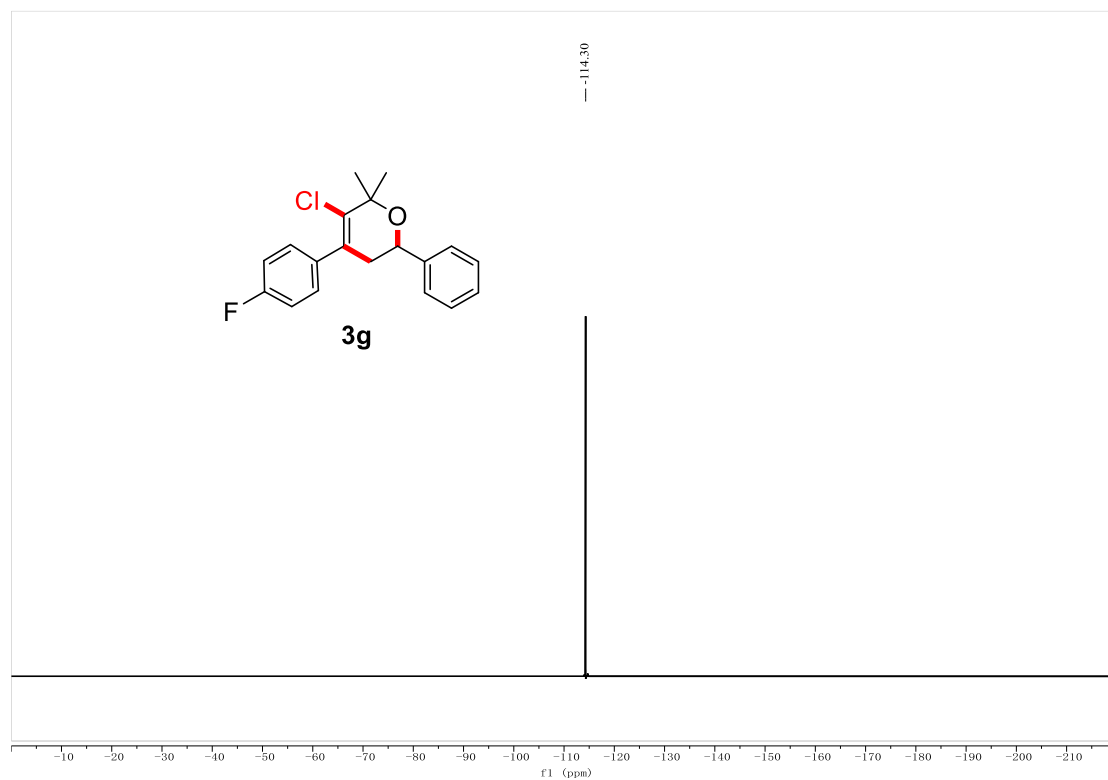
¹H NMR of 3g



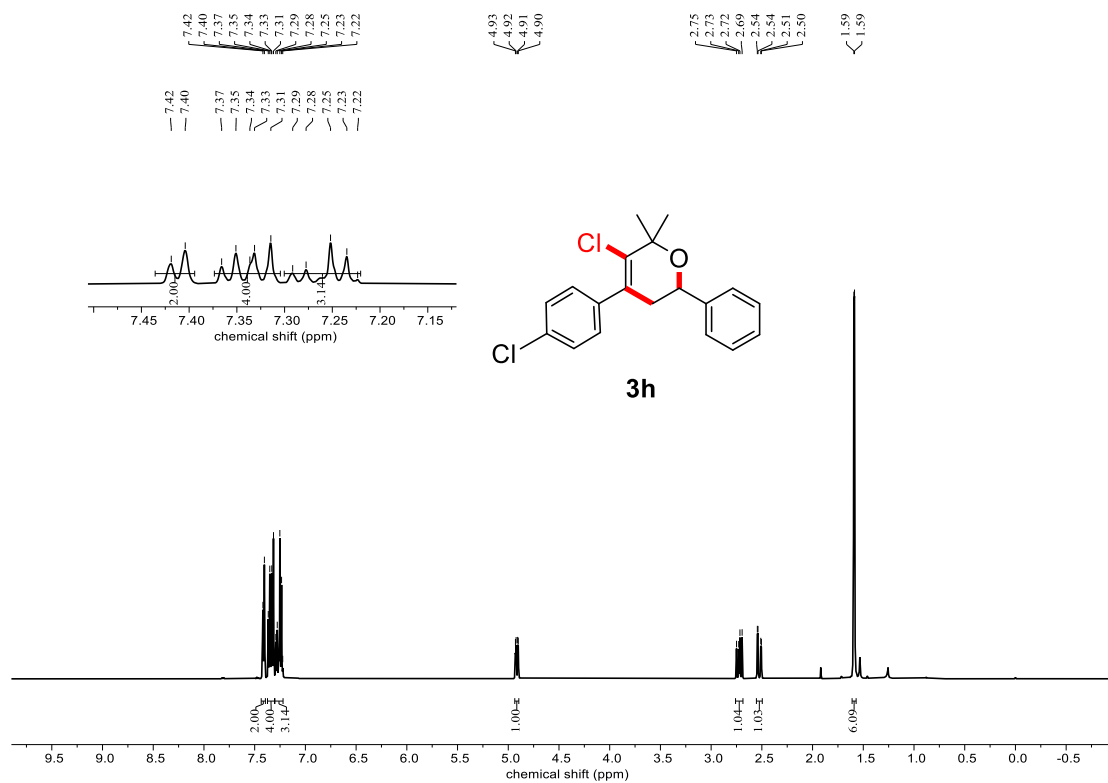
¹³C NMR of 3g



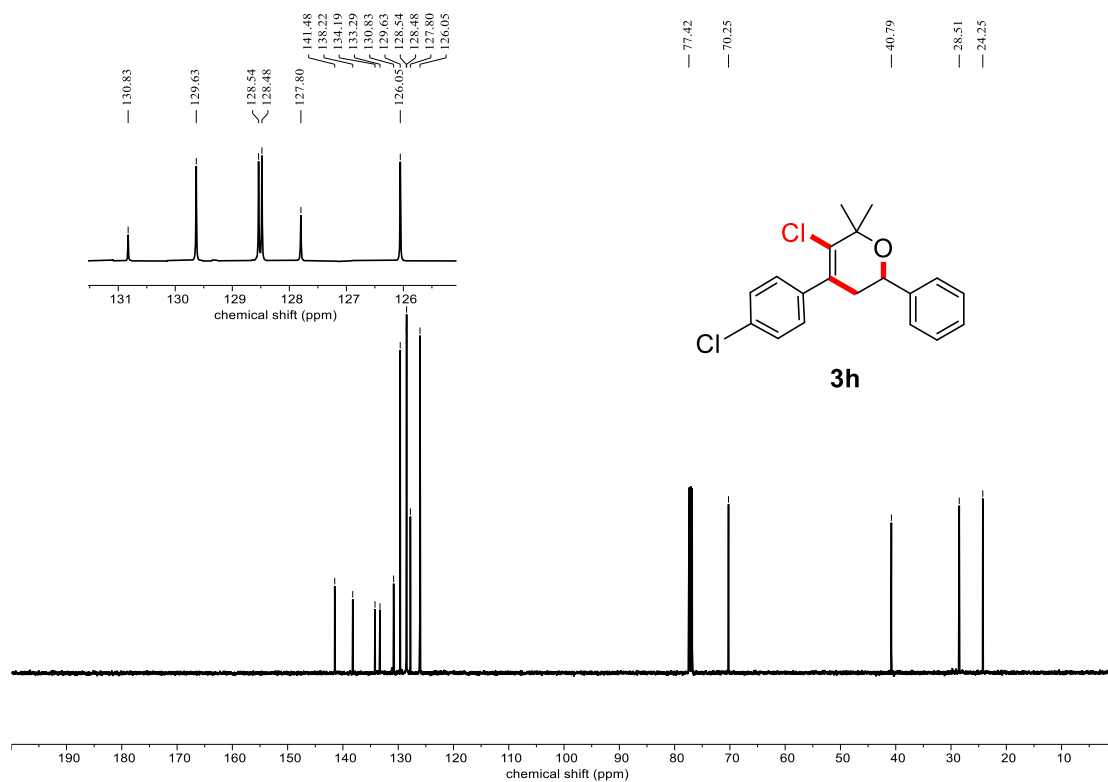
¹⁹F NMR of 3g



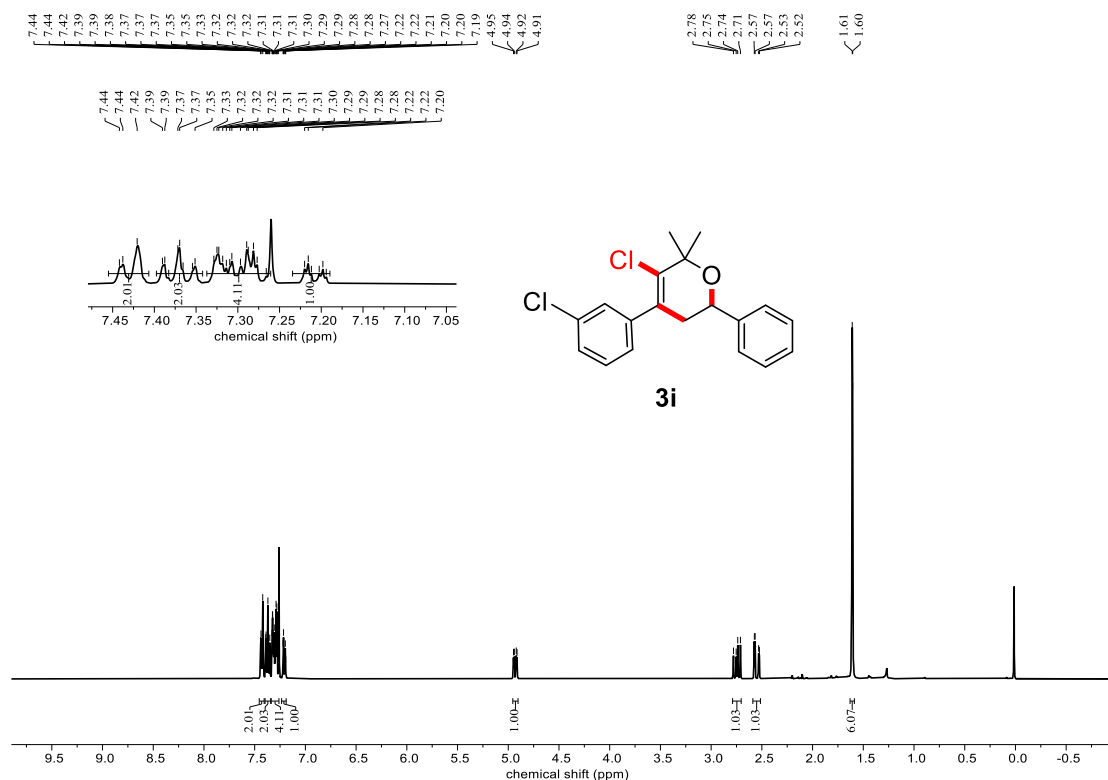
¹H NMR of 3h



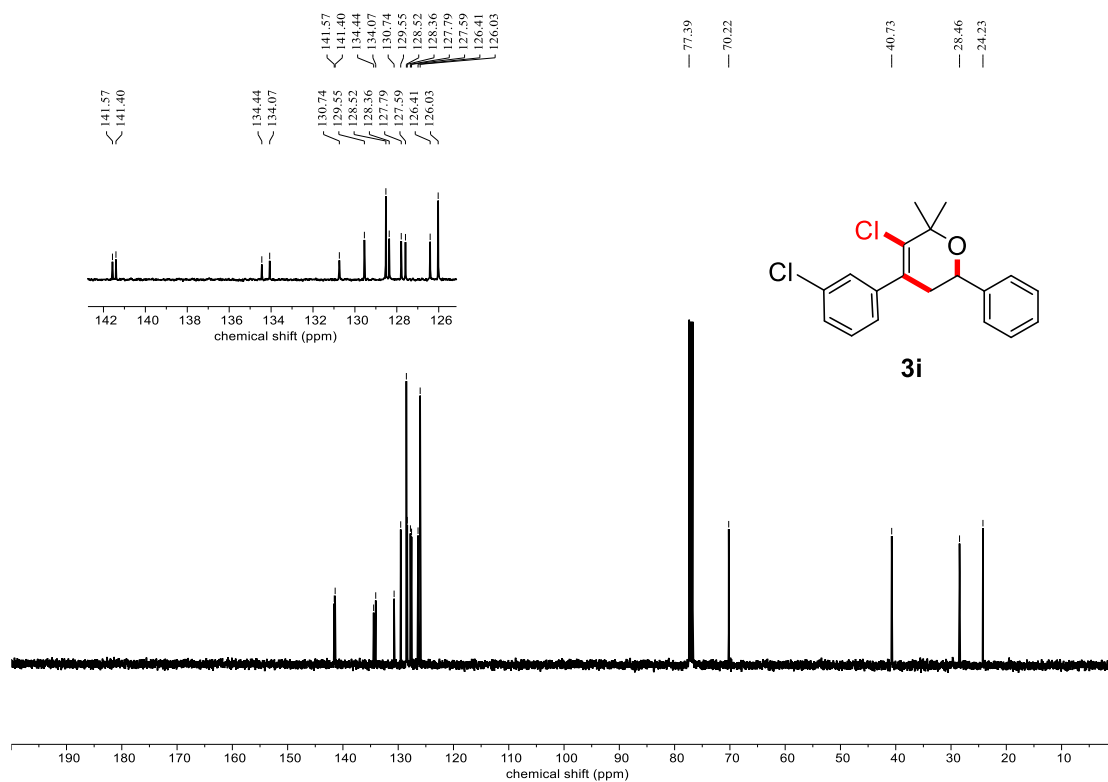
¹³C NMR of 3h



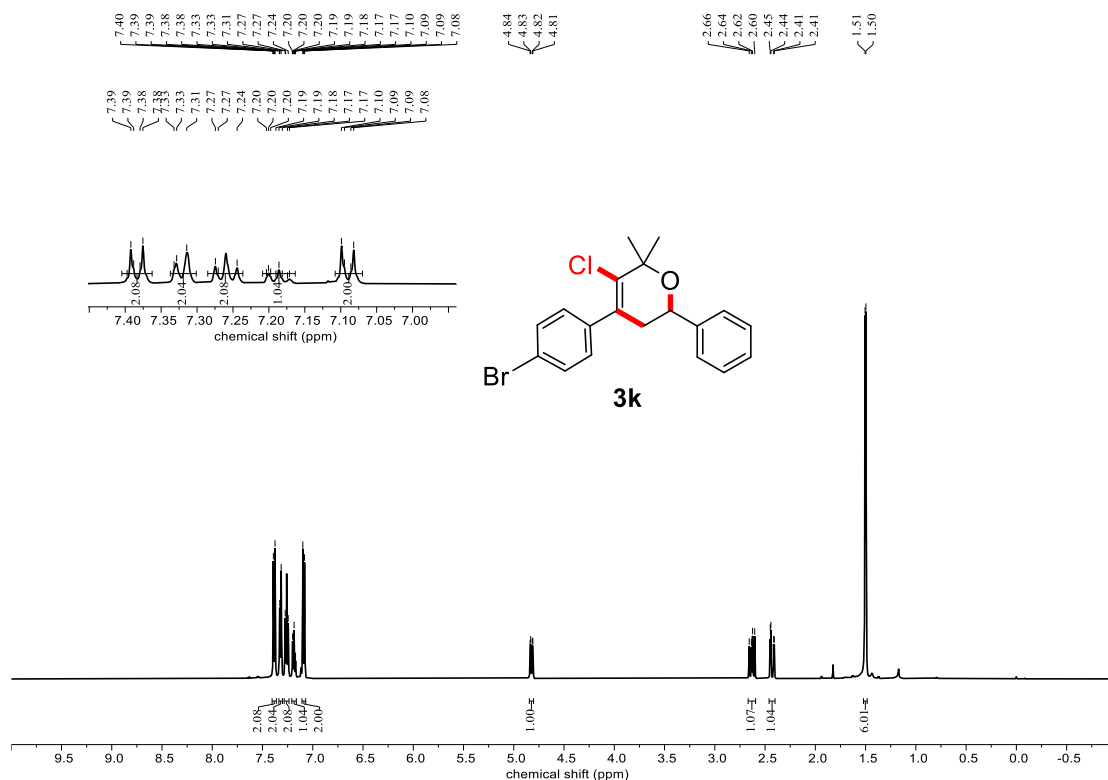
¹H NMR of 3i



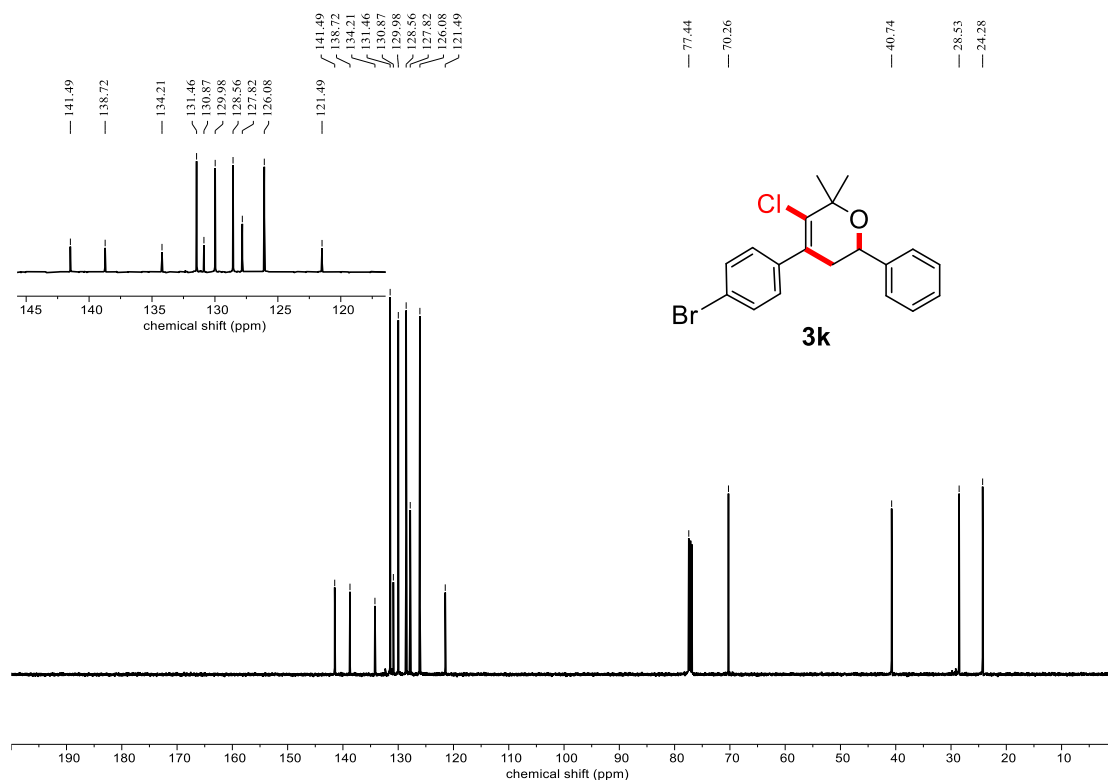
¹³C NMR of 3i



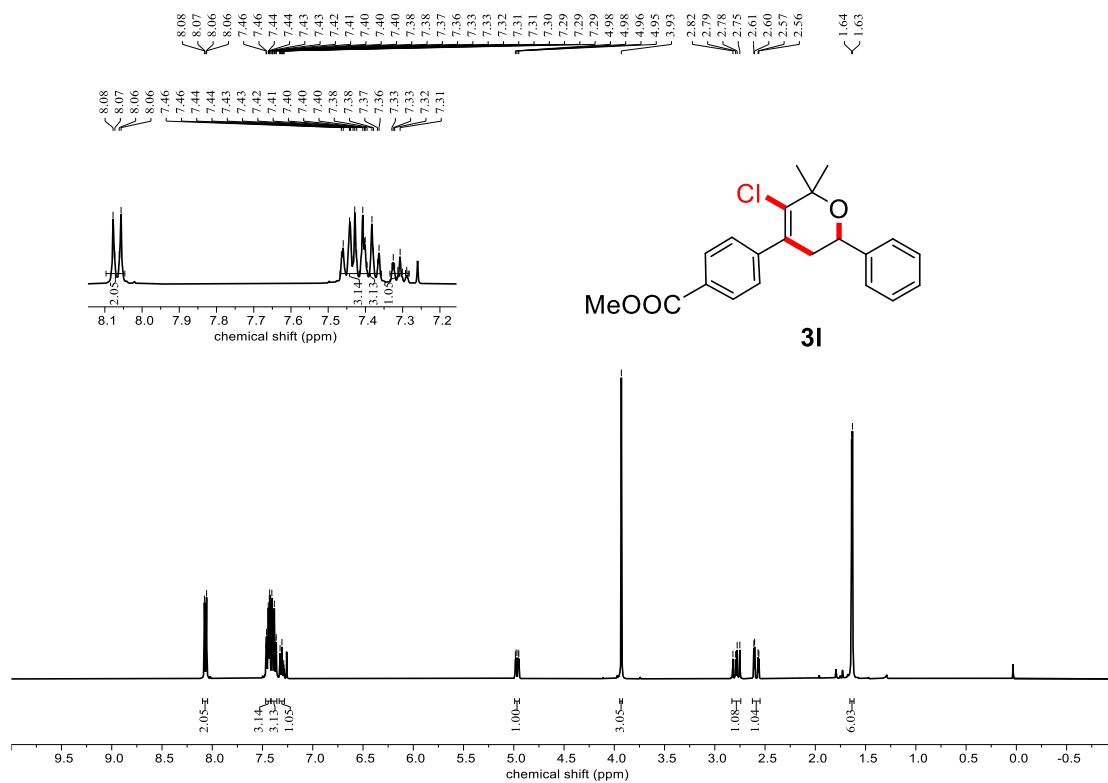
¹H NMR of 3k



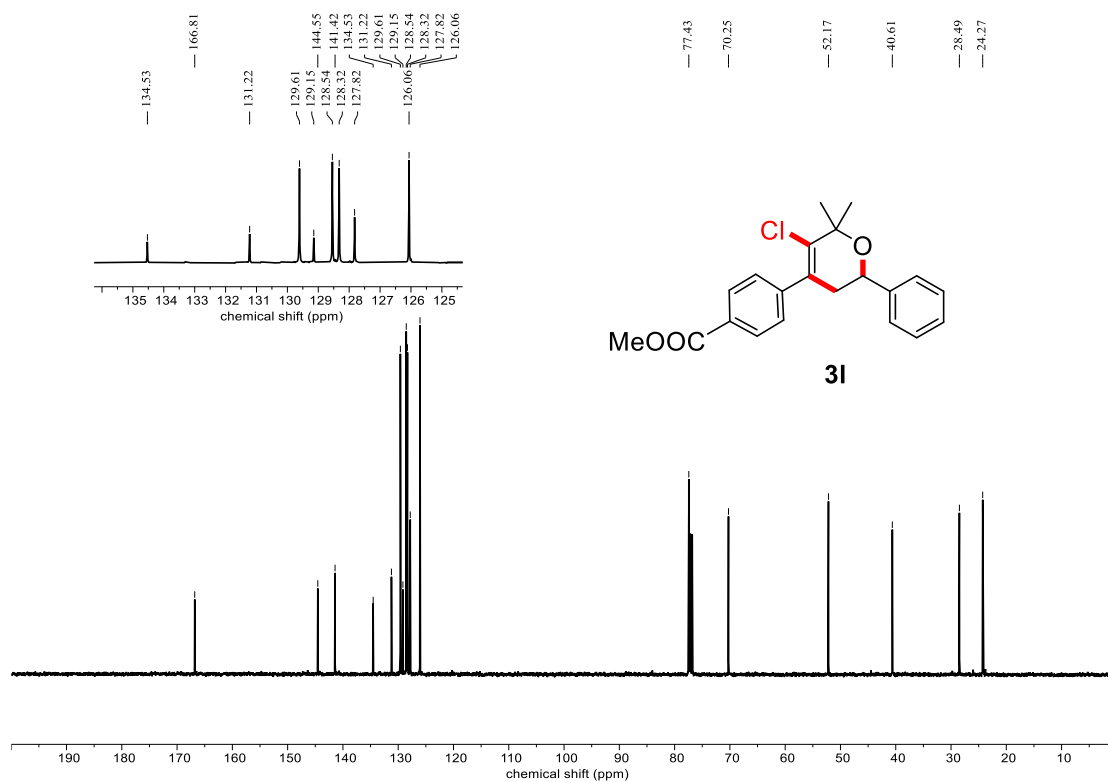
¹³C NMR of 3k



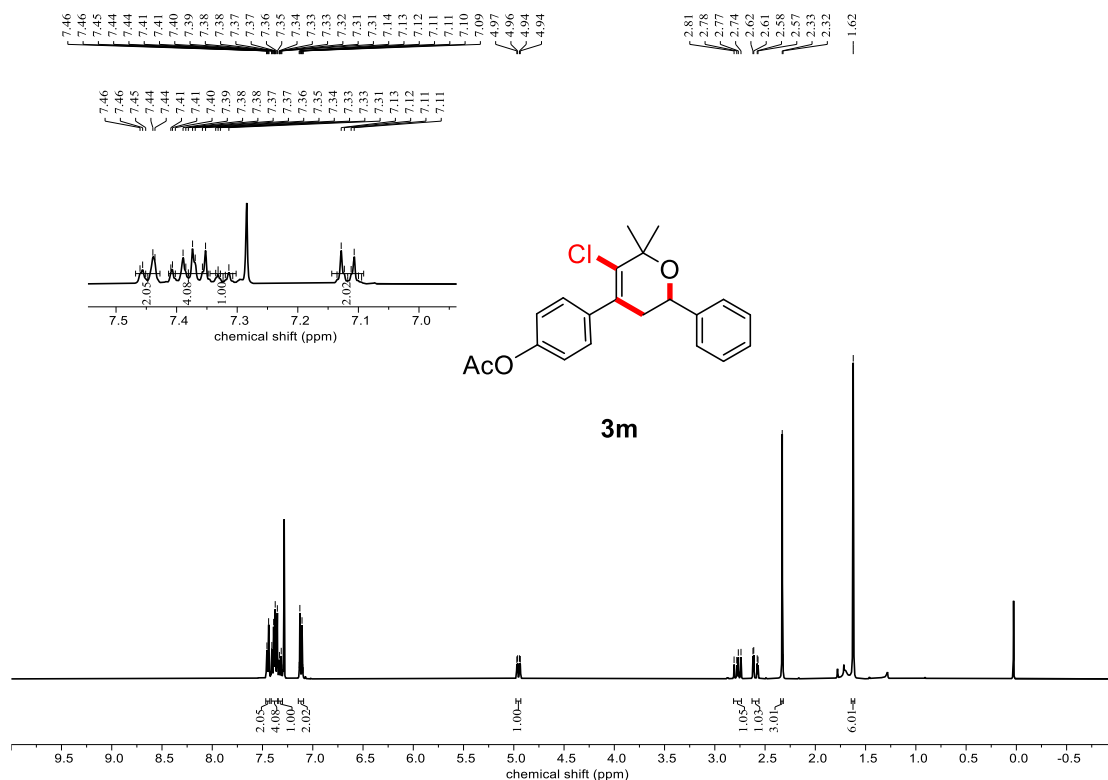
¹H NMR of 3l



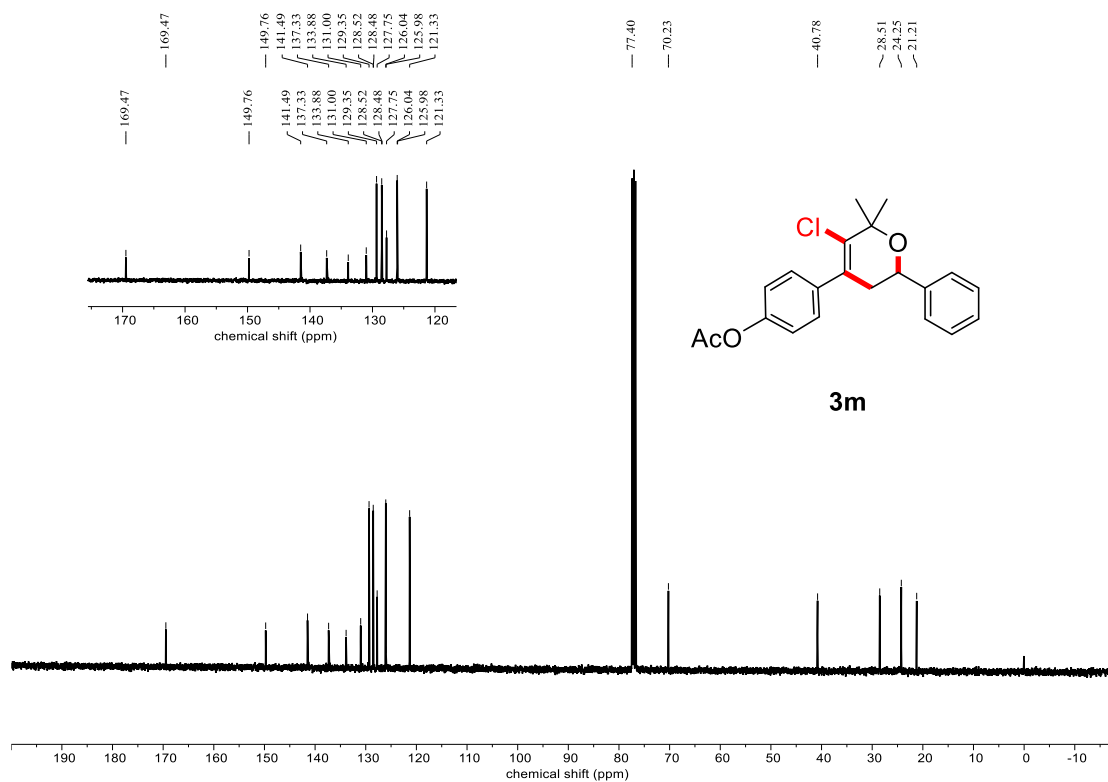
¹³C NMR of 3l



¹H NMR of 3m



¹³C NMR of 3m



Chemical structure of 3n: CC(C)OC(=O)c1ccc(C#N)cc1Cl

¹H NMR spectrum (CDCl₃):

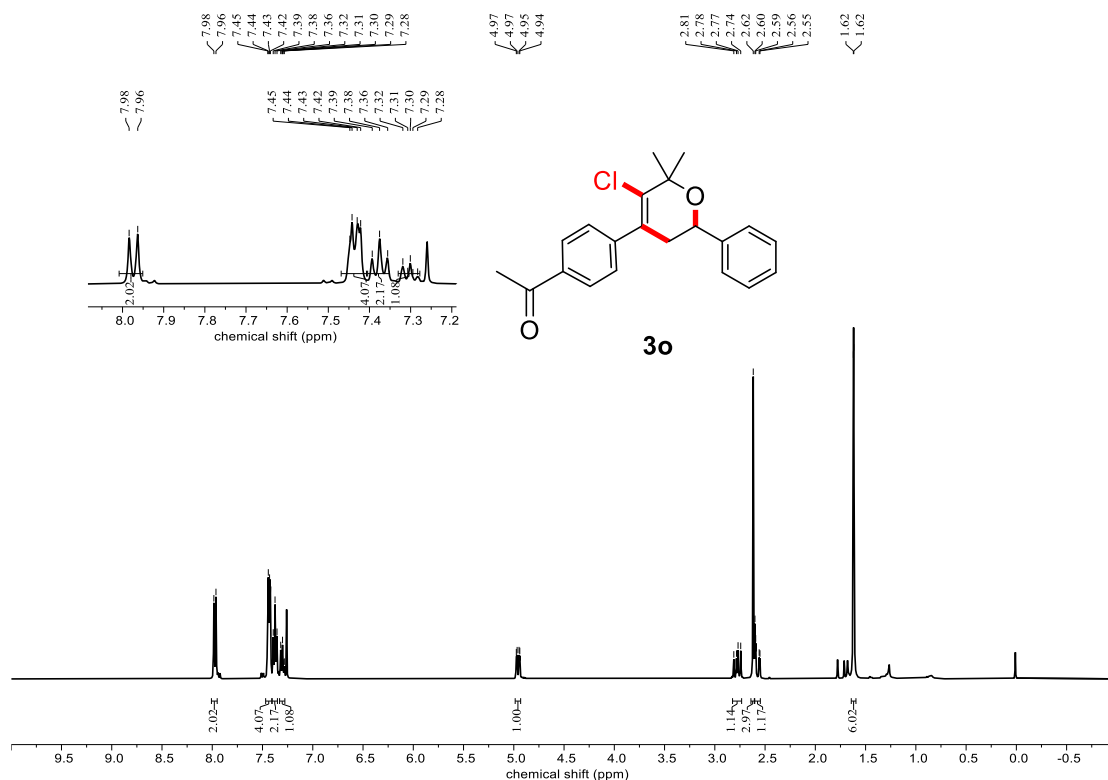
Chemical Shift (ppm)	Integration
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Chemical structure of 3n: Cc1cc(C(=O)c2ccccc2)c(Cl)c1-c3ccc(C#N)cc3

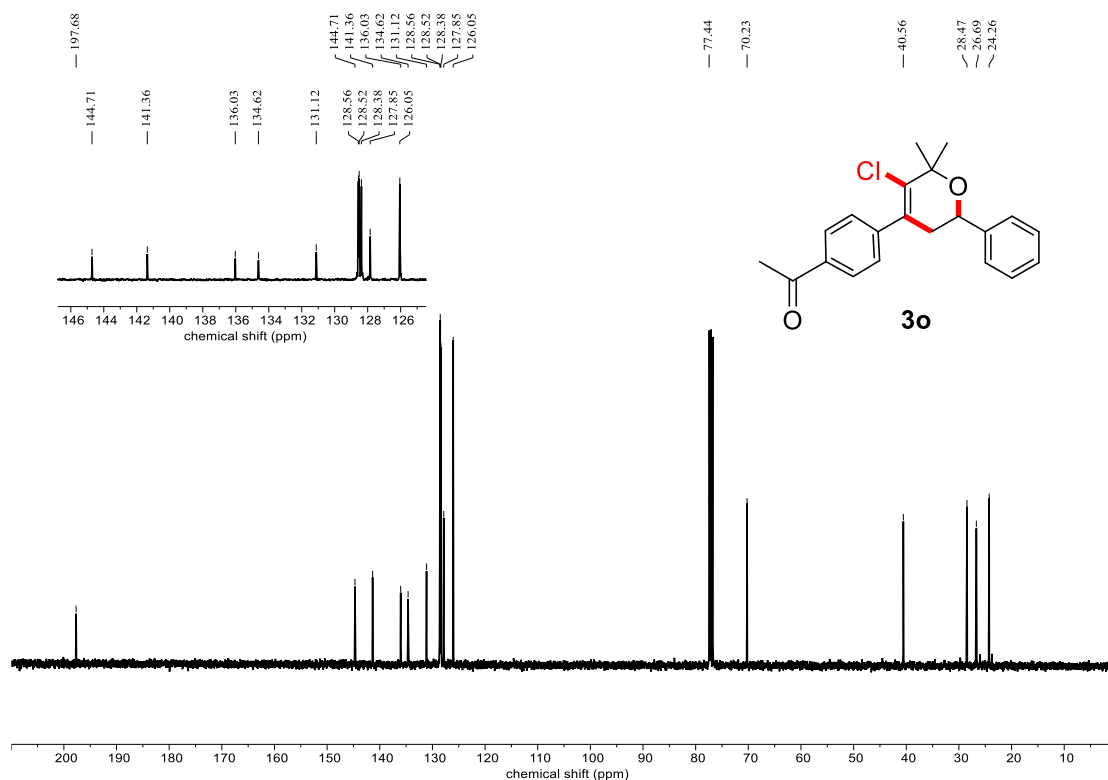
¹³C NMR peaks (ppm):

Region	Chemical Shift (ppm)
Aromatic / Nitrile	144.50, 141.17, 135.38, 132.14, 130.50, 128.57, 127.90, 125.99, 118.72, 111.26
Aliphatic / Solvent	77.44, 70.16, 40.40, 28.40, 24.21

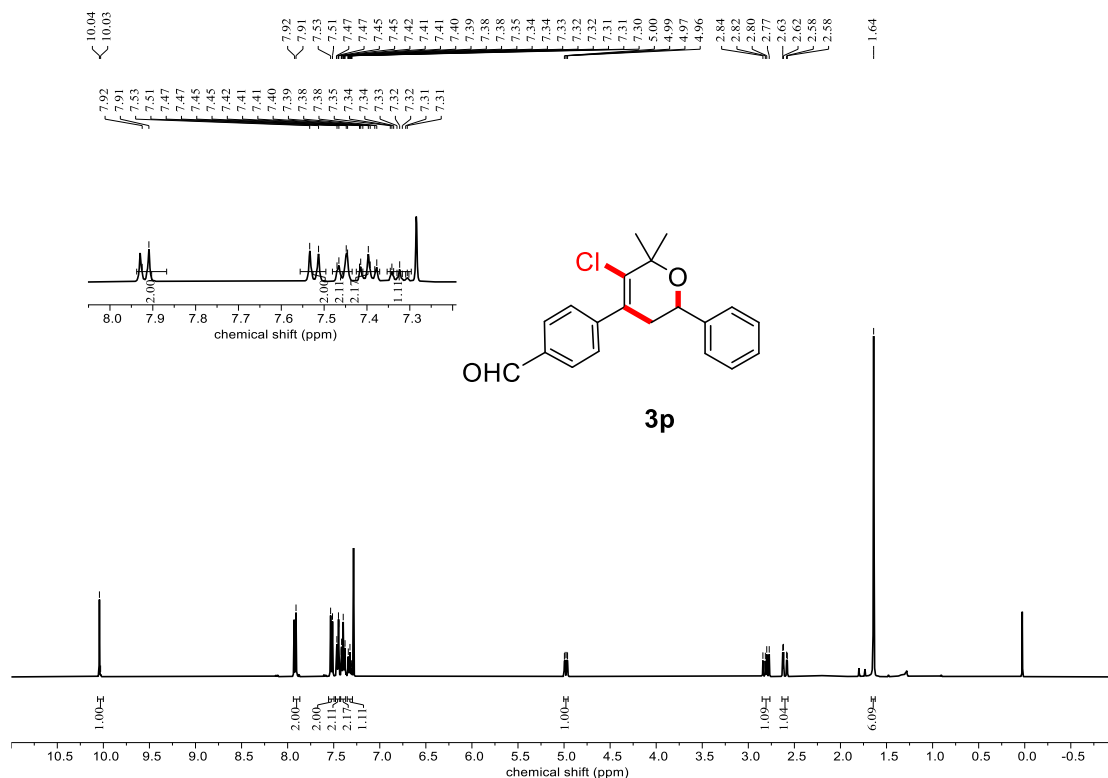
¹H NMR of 3o



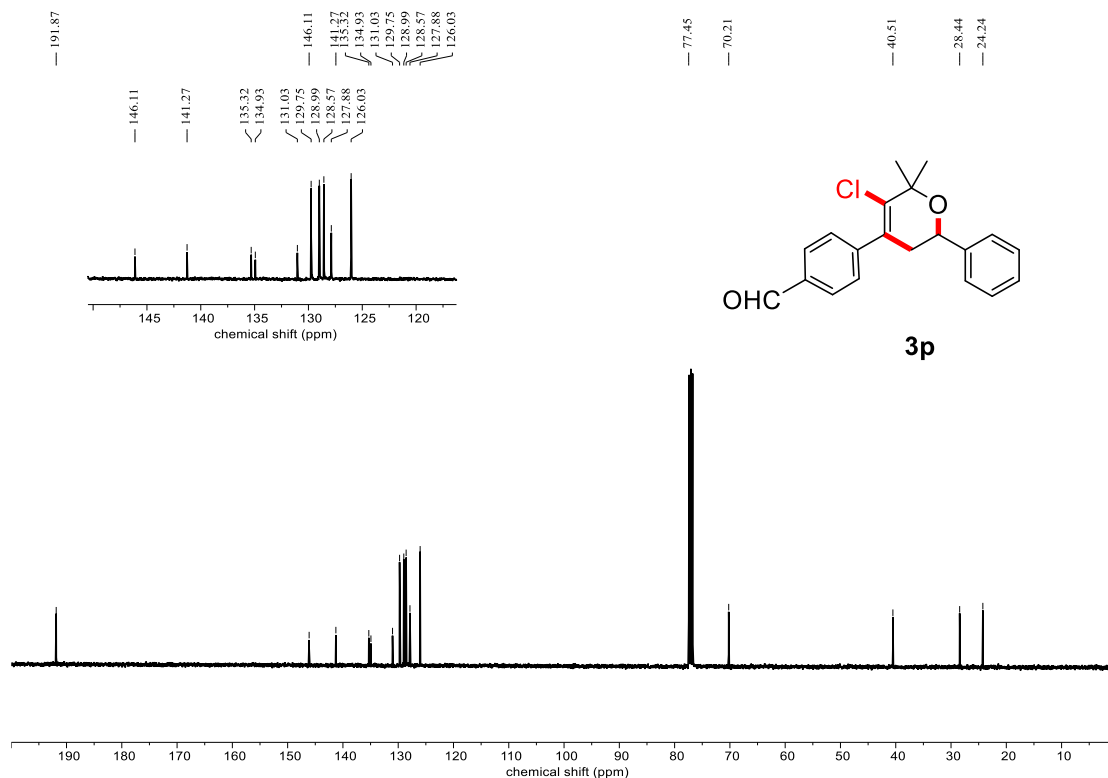
¹³C NMR of 3o



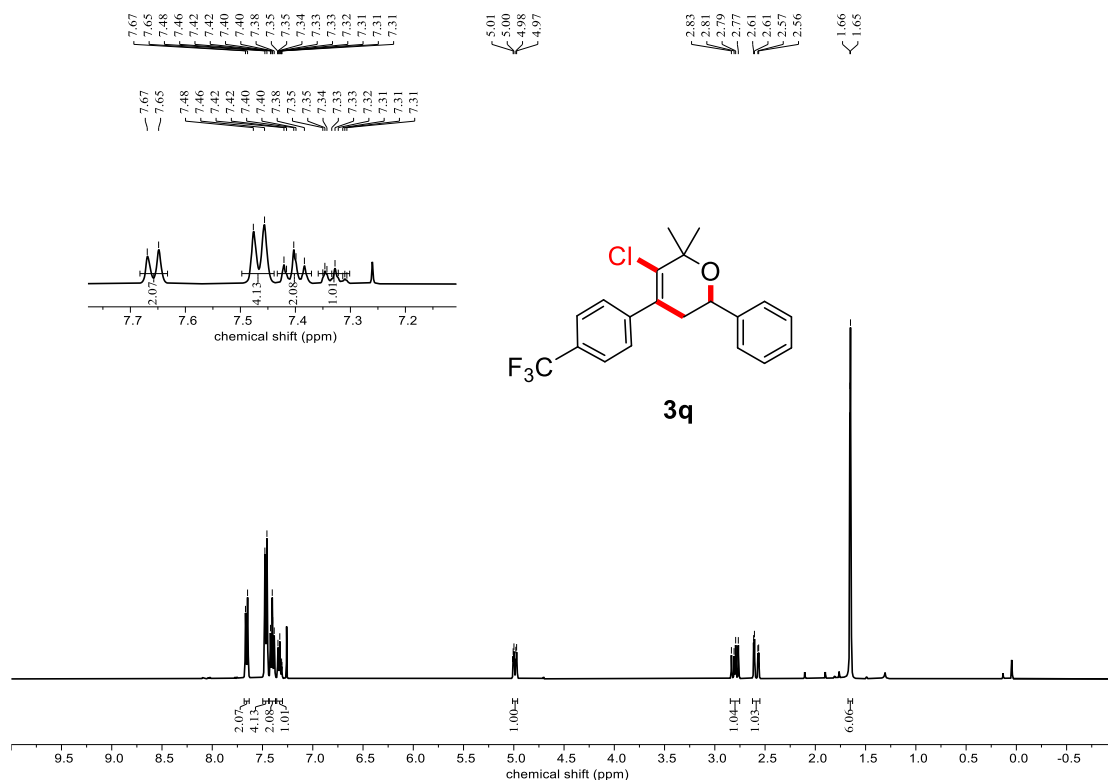
¹H NMR of 3p



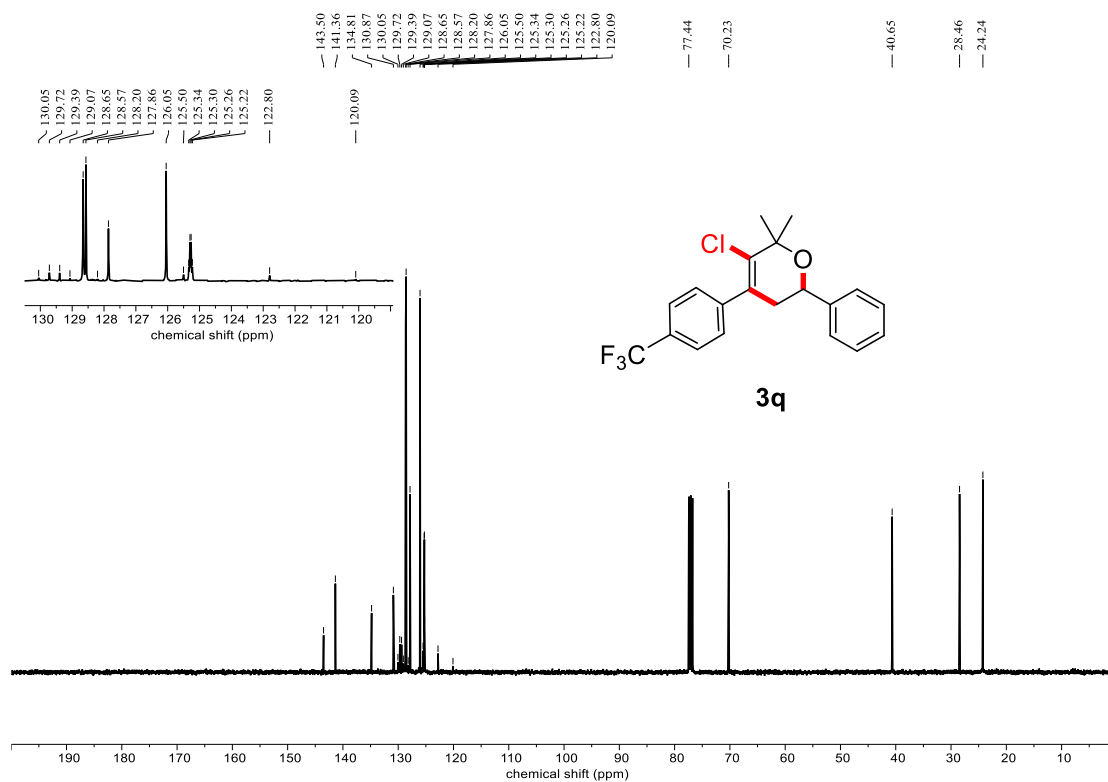
¹³C NMR of 3p



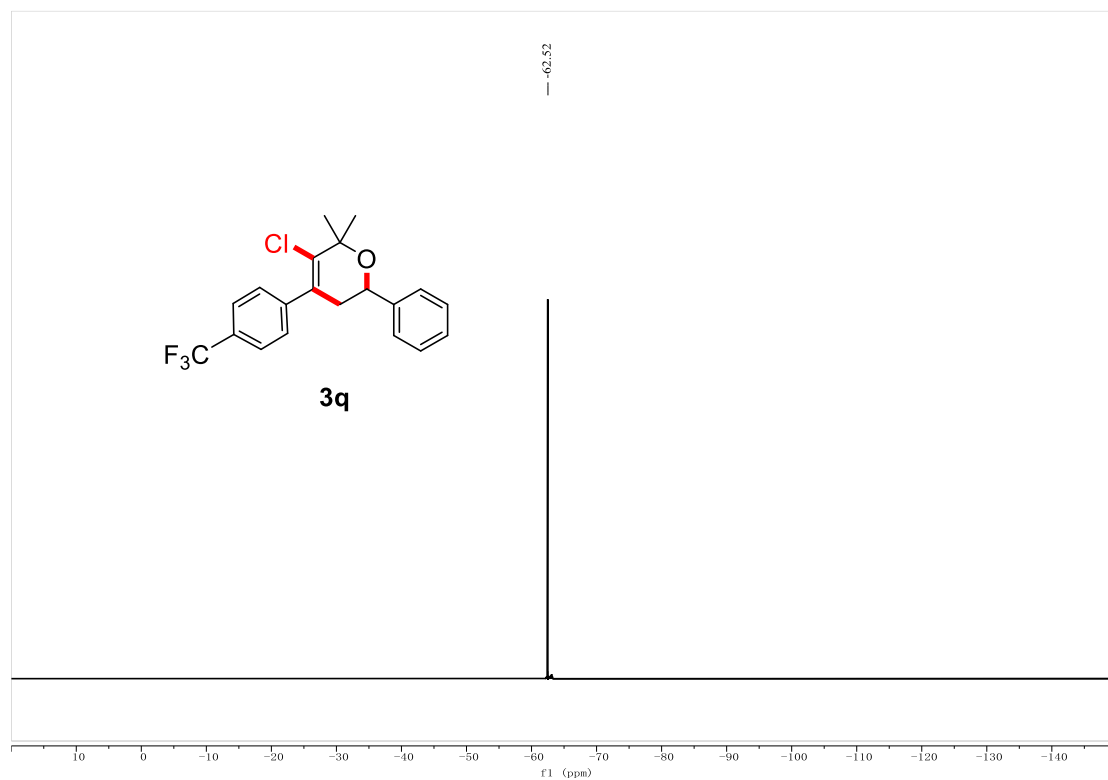
¹H NMR of 3q



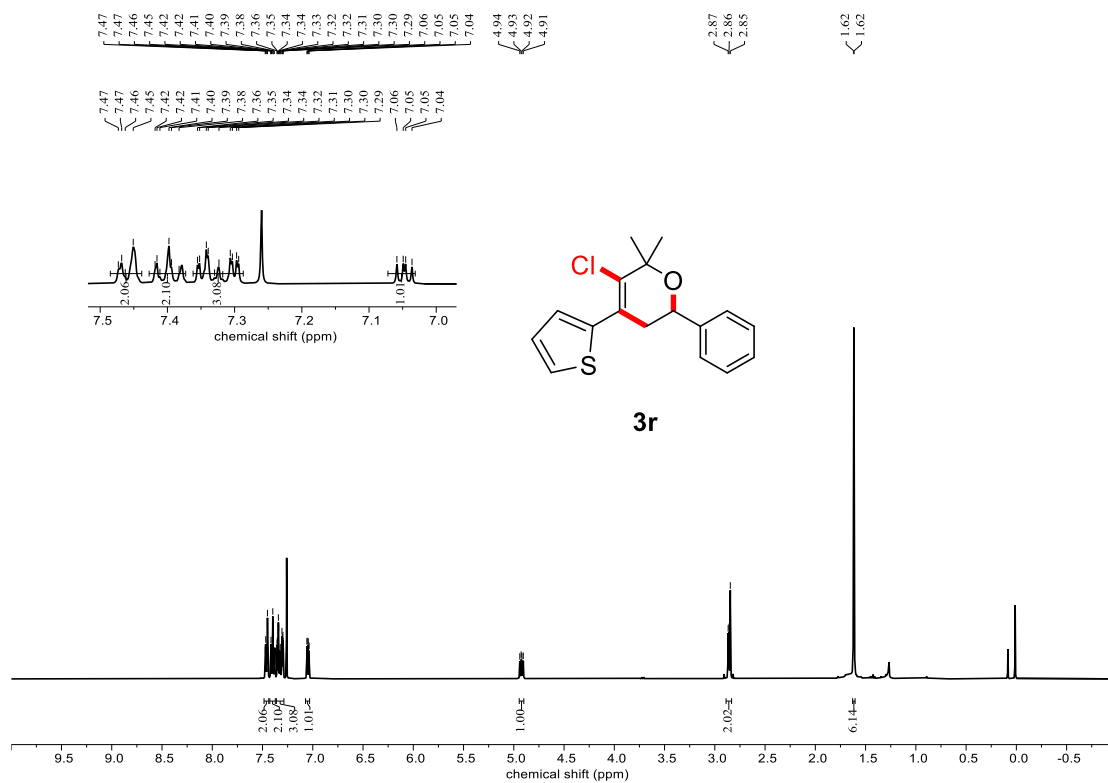
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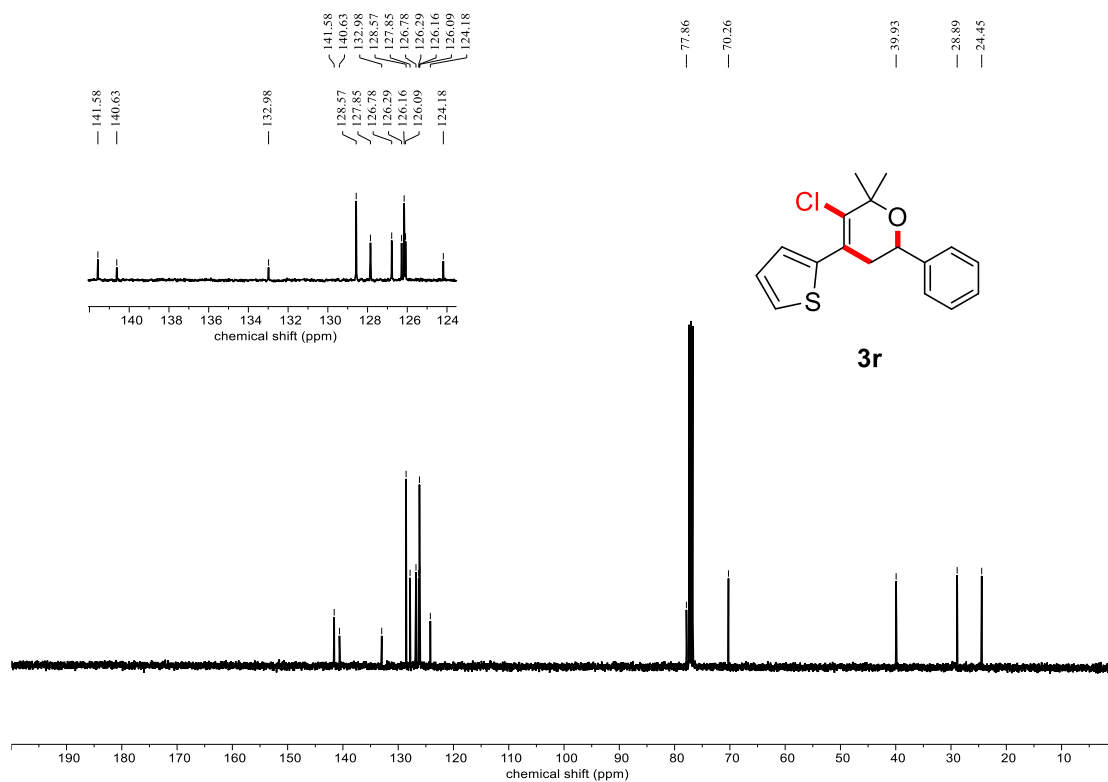
^{19}F NMR of 3q

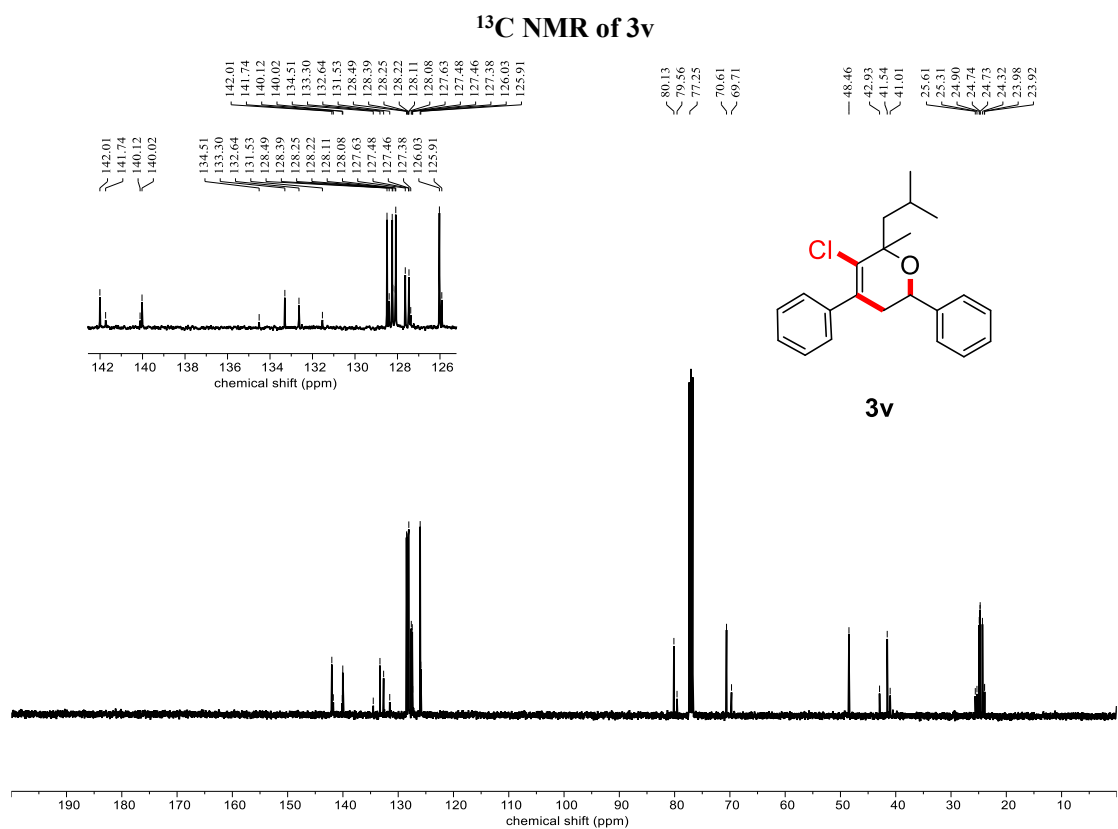
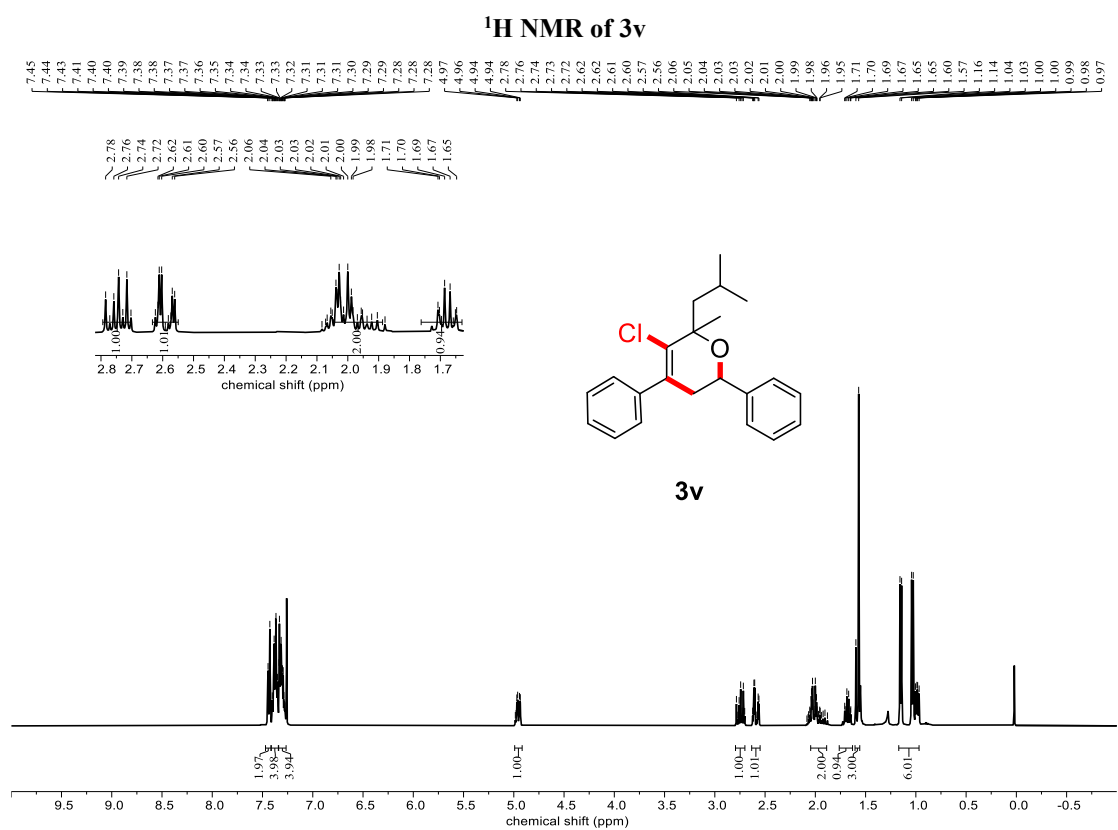


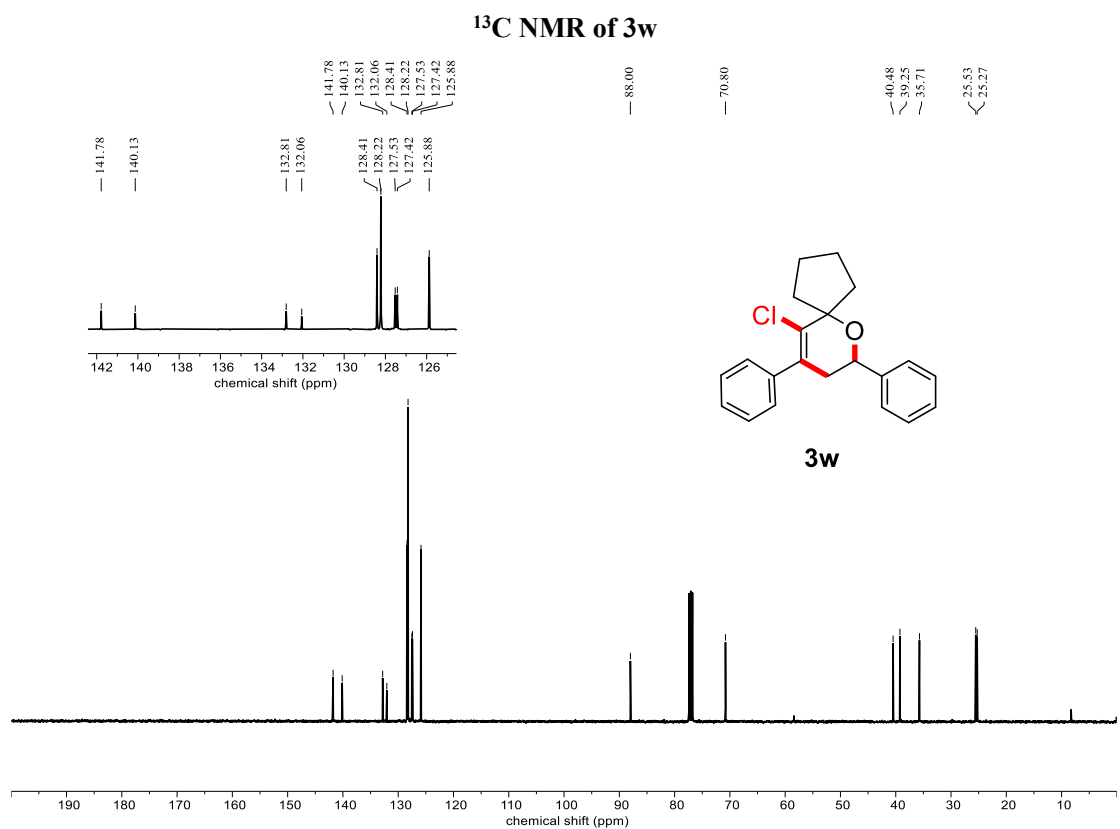
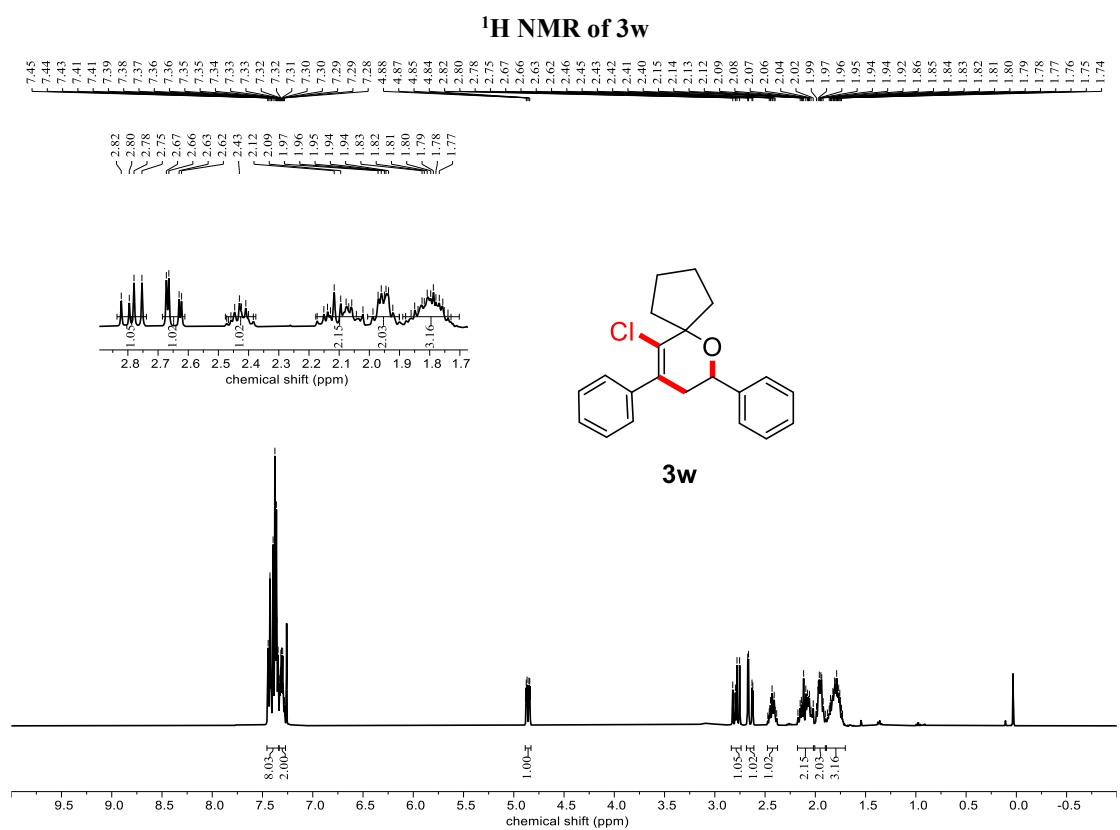
¹H NMR of 3r



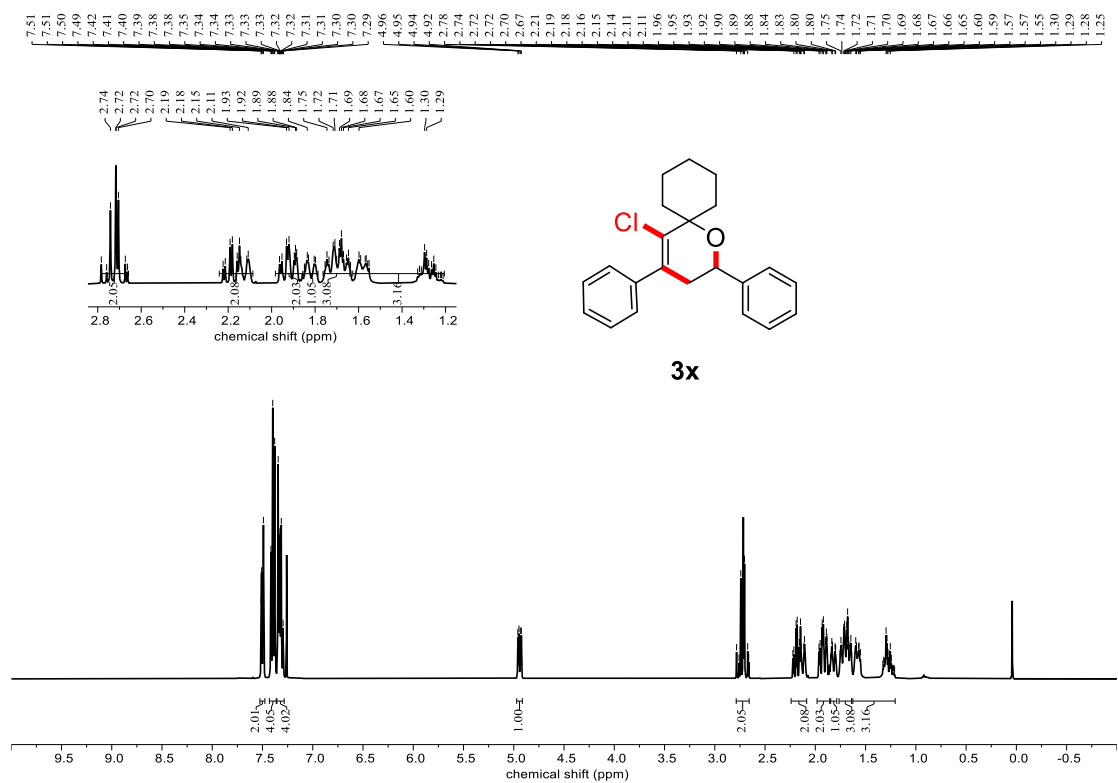
¹³C NMR of 3r



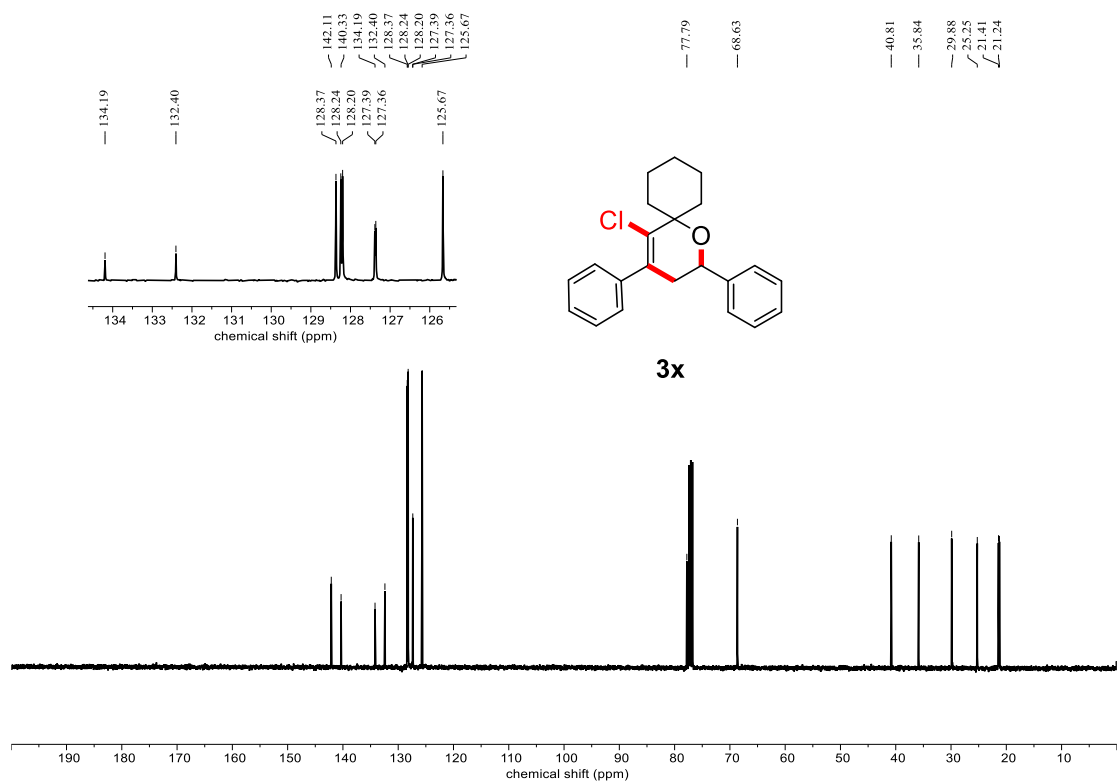




¹H NMR of 3x

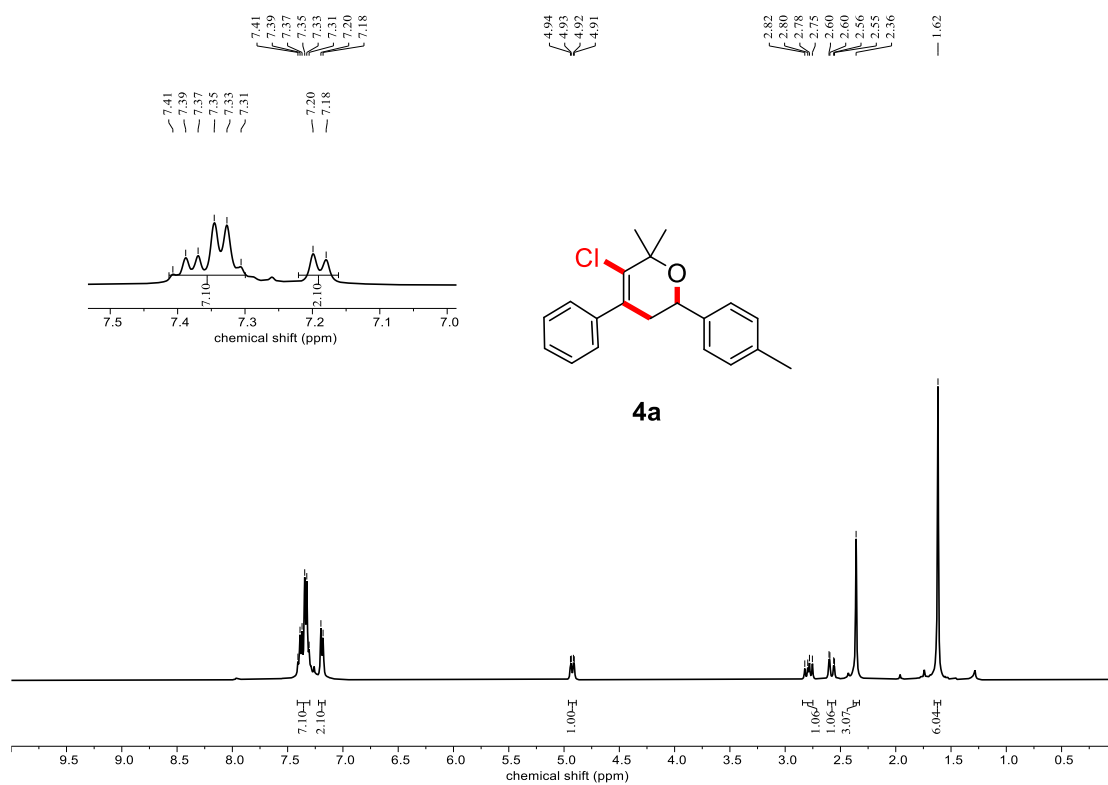


¹³C NMR of 3x

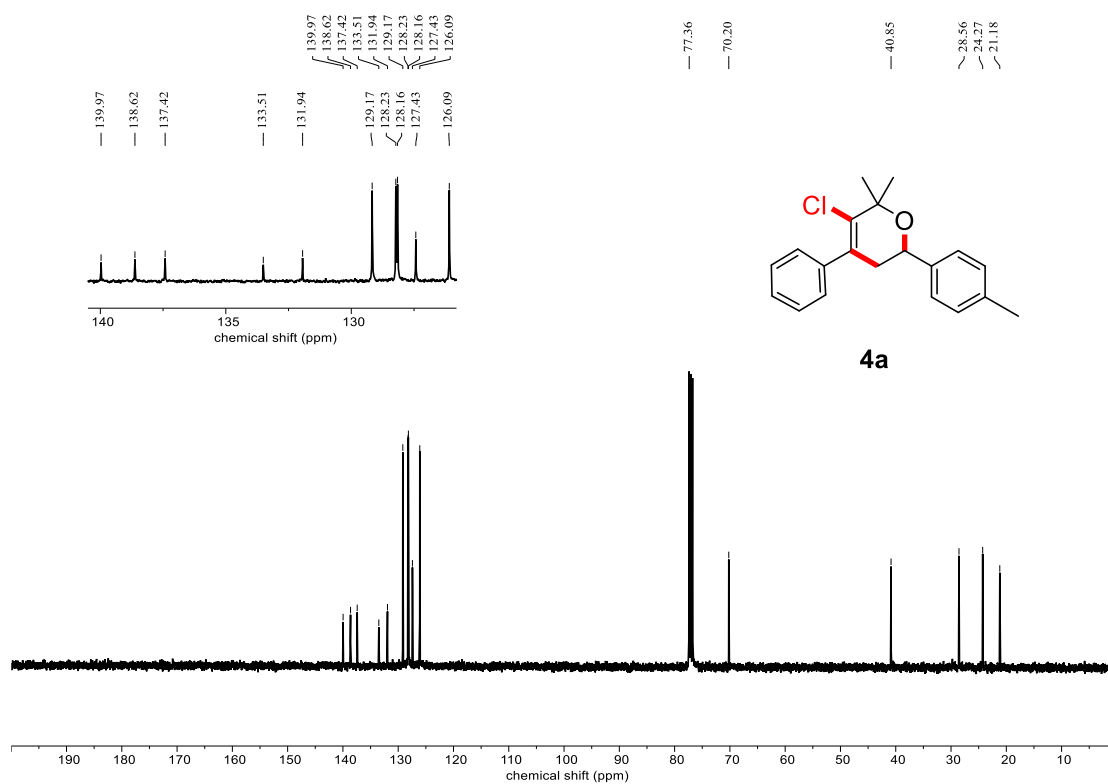


¹H and ¹³C NMR spectra of compounds 4

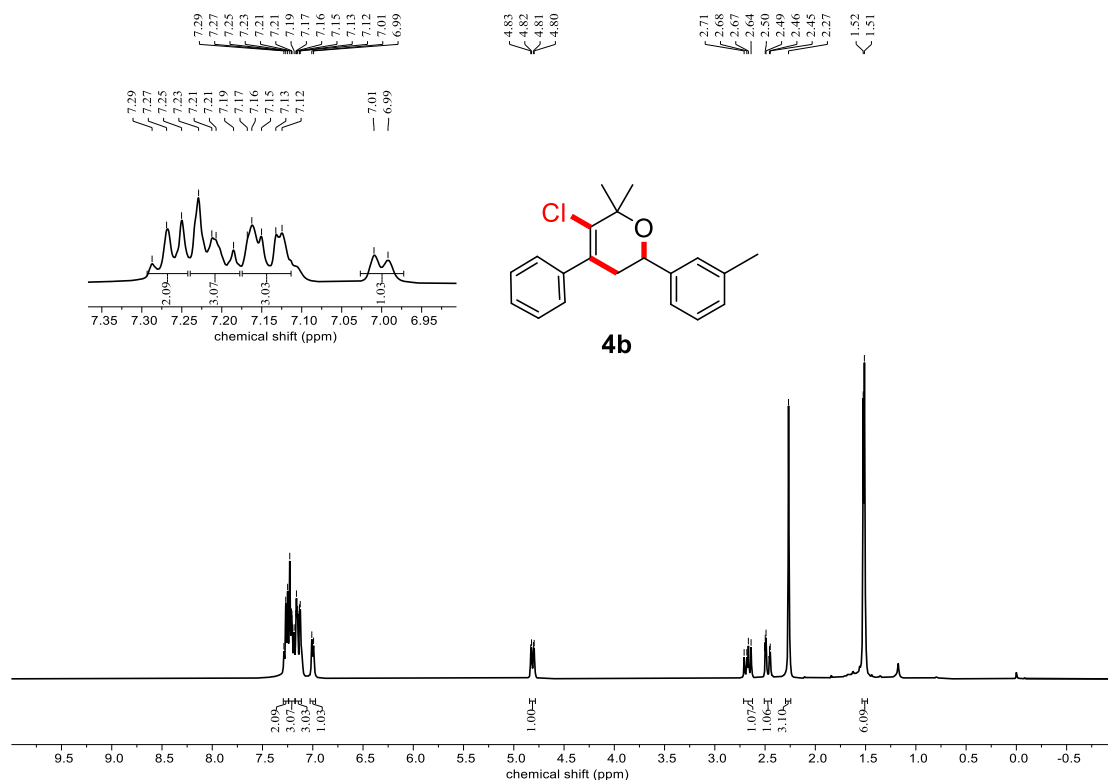
¹H NMR of 4a



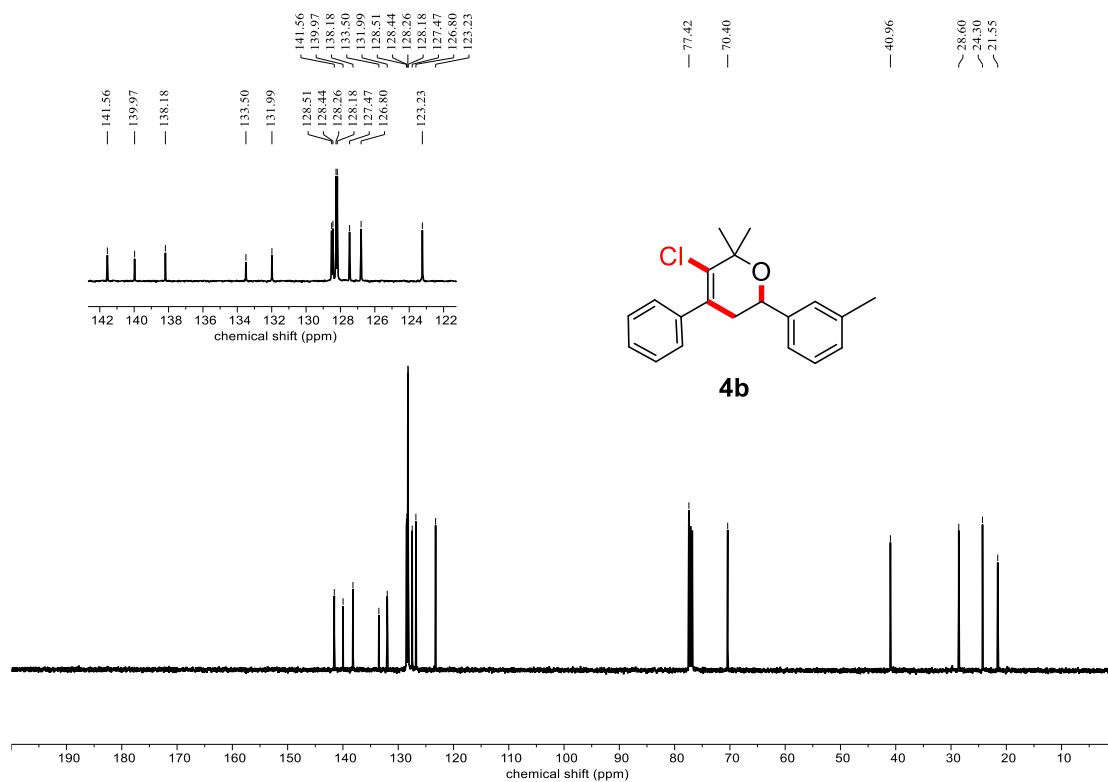
¹³C NMR of 4a



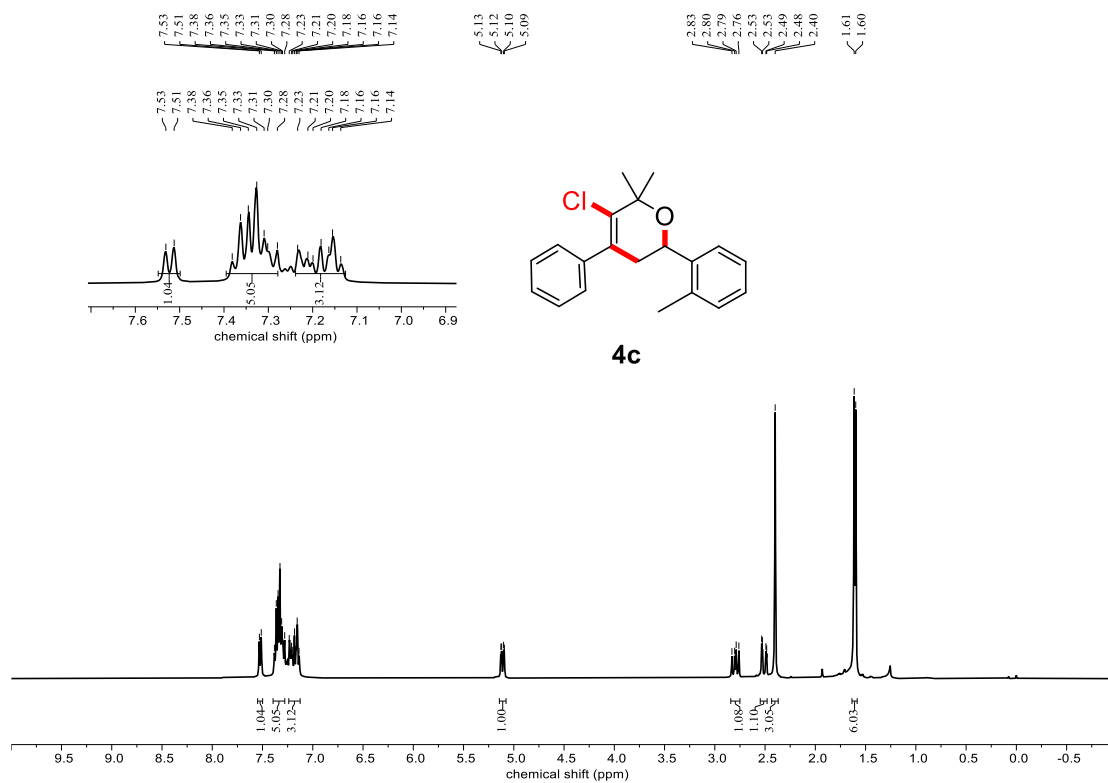
¹H NMR of 4b



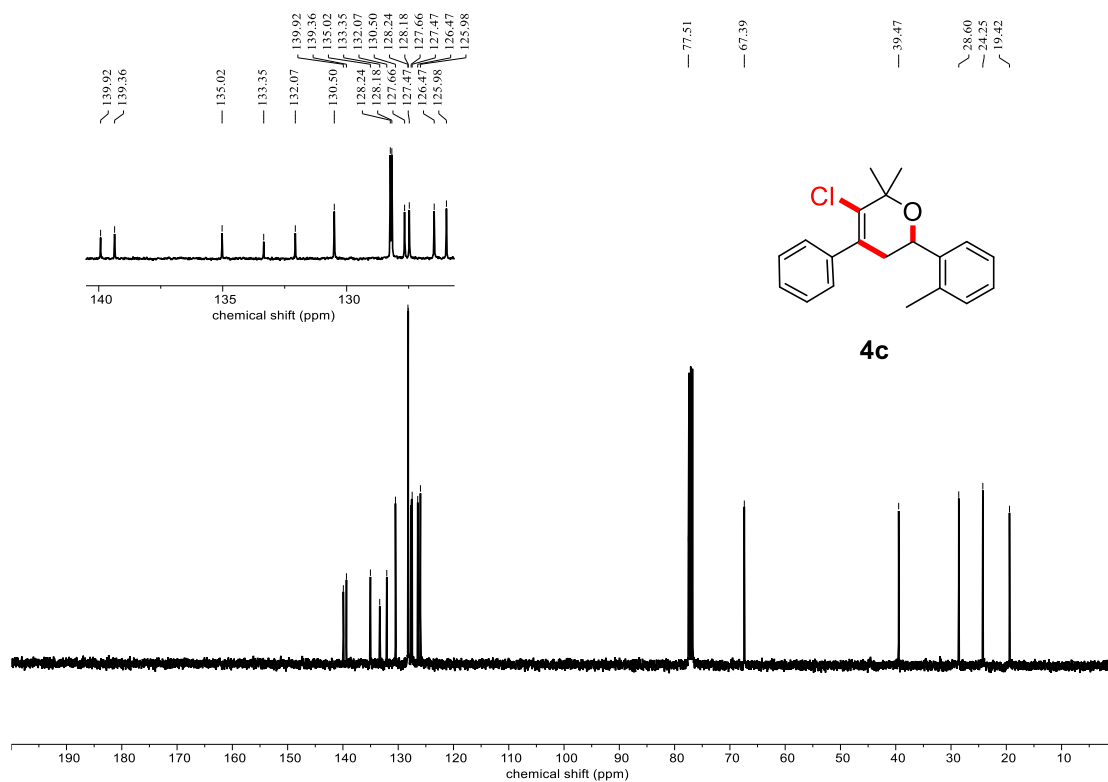
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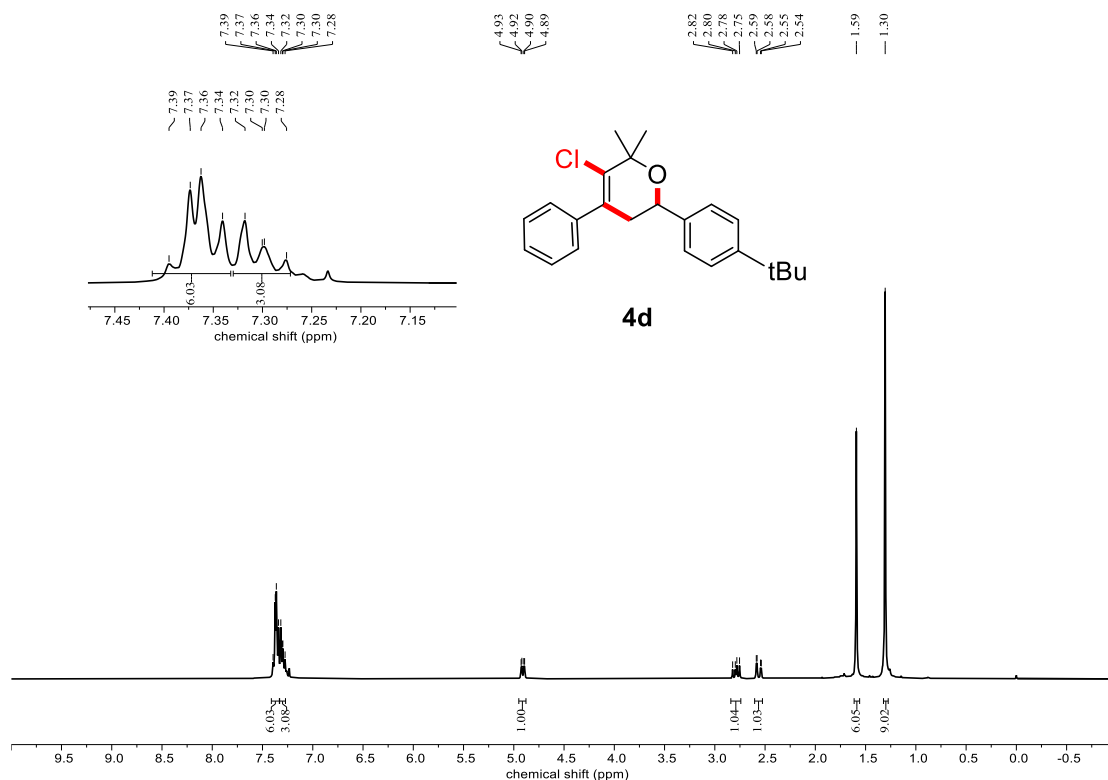
¹H NMR of 4c



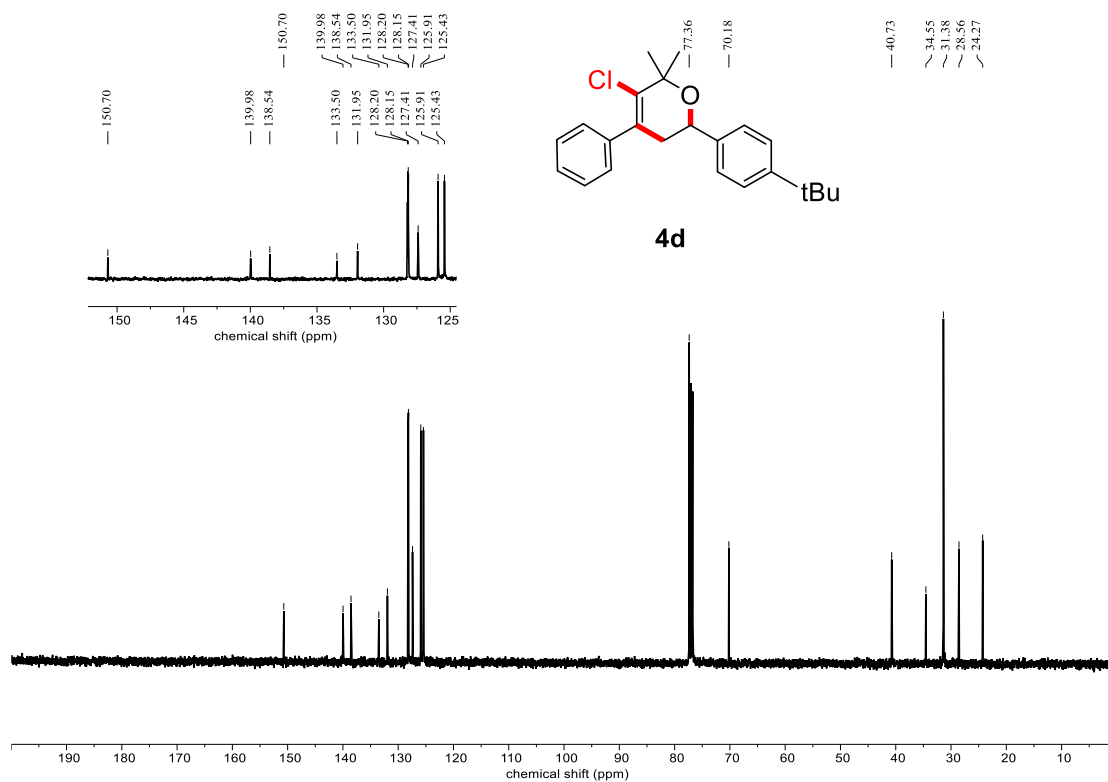
¹³C NMR of 4c



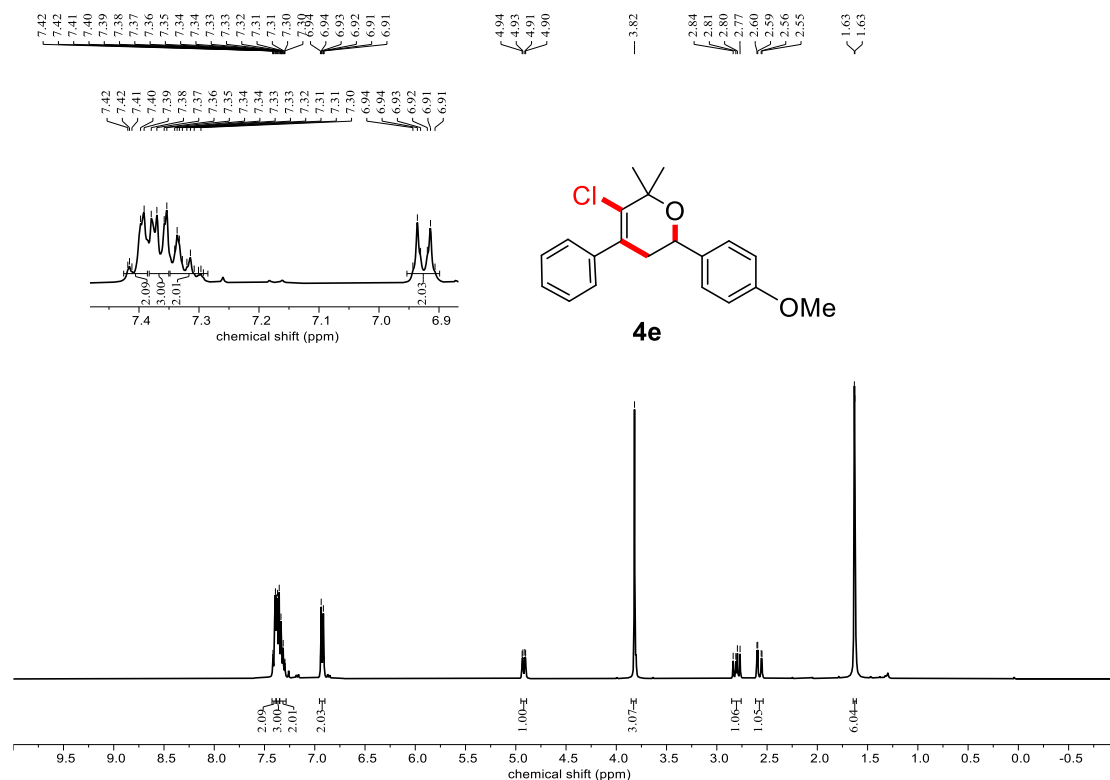
¹H NMR of 4d



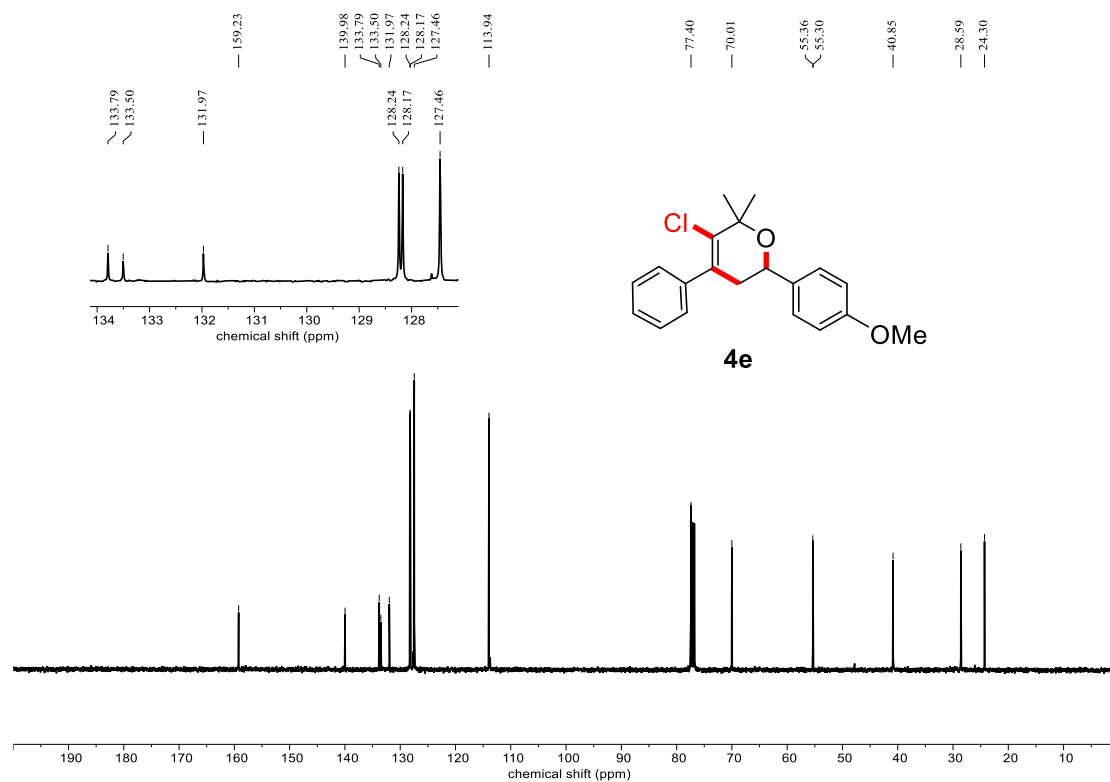
¹³C NMR of 4d



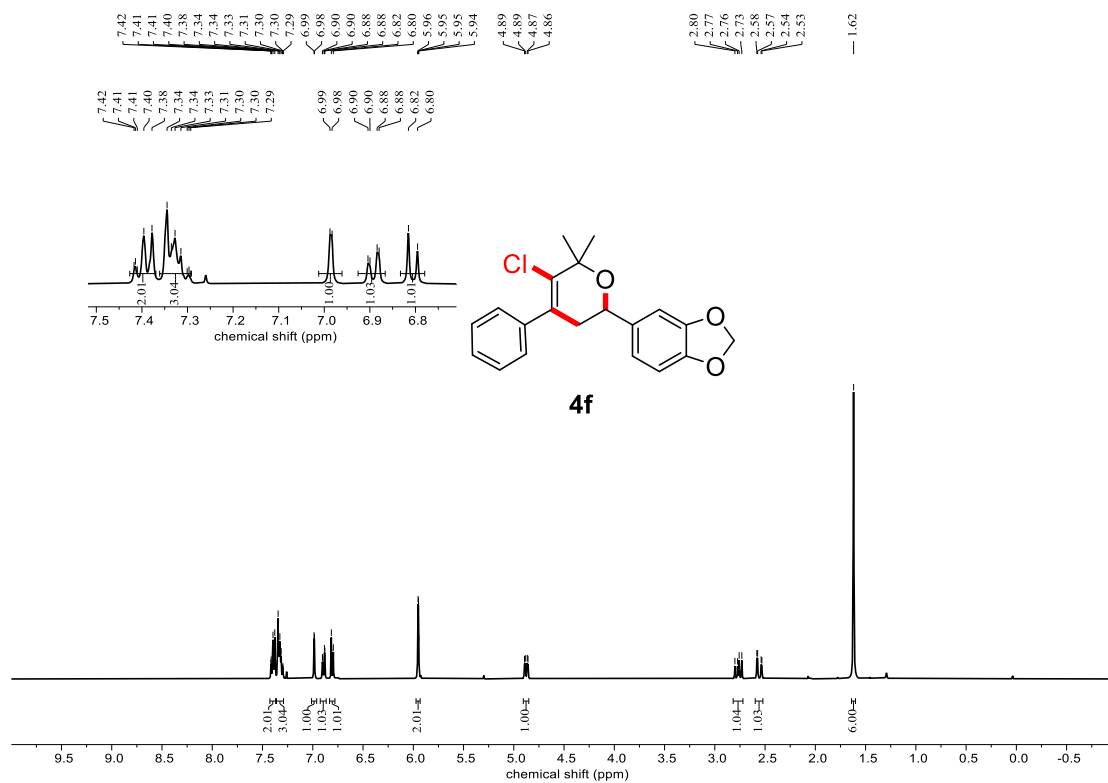
¹H NMR of 4e



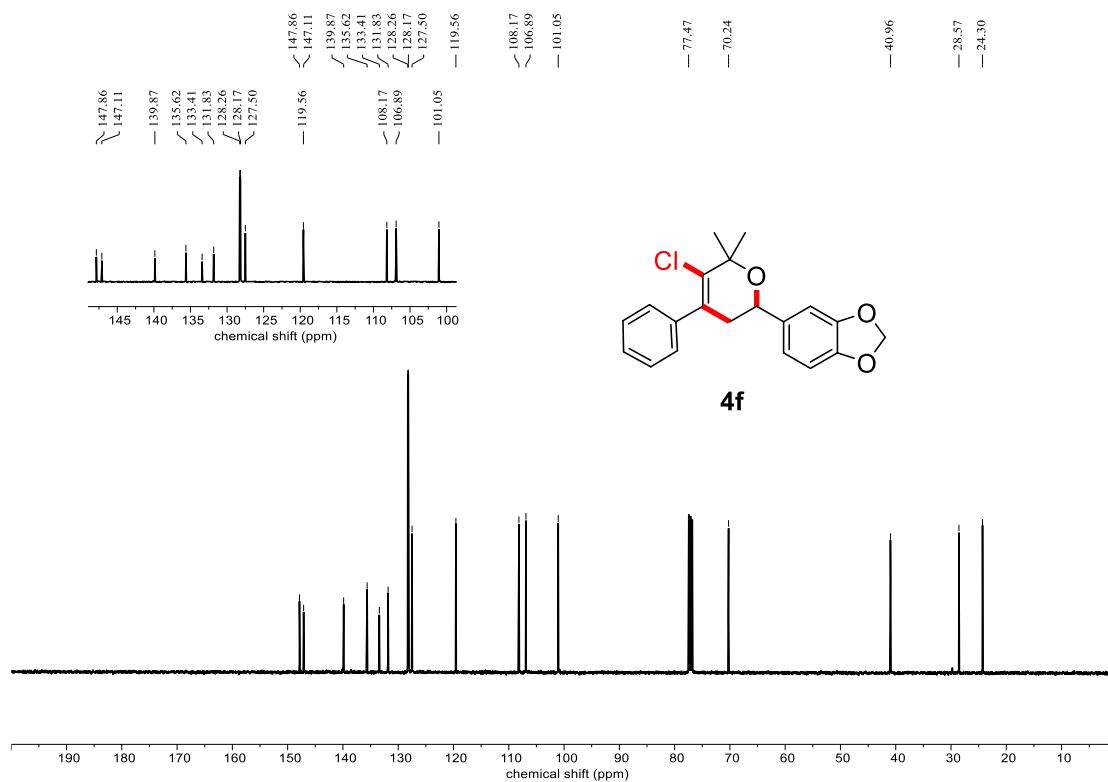
¹³C NMR of 4e

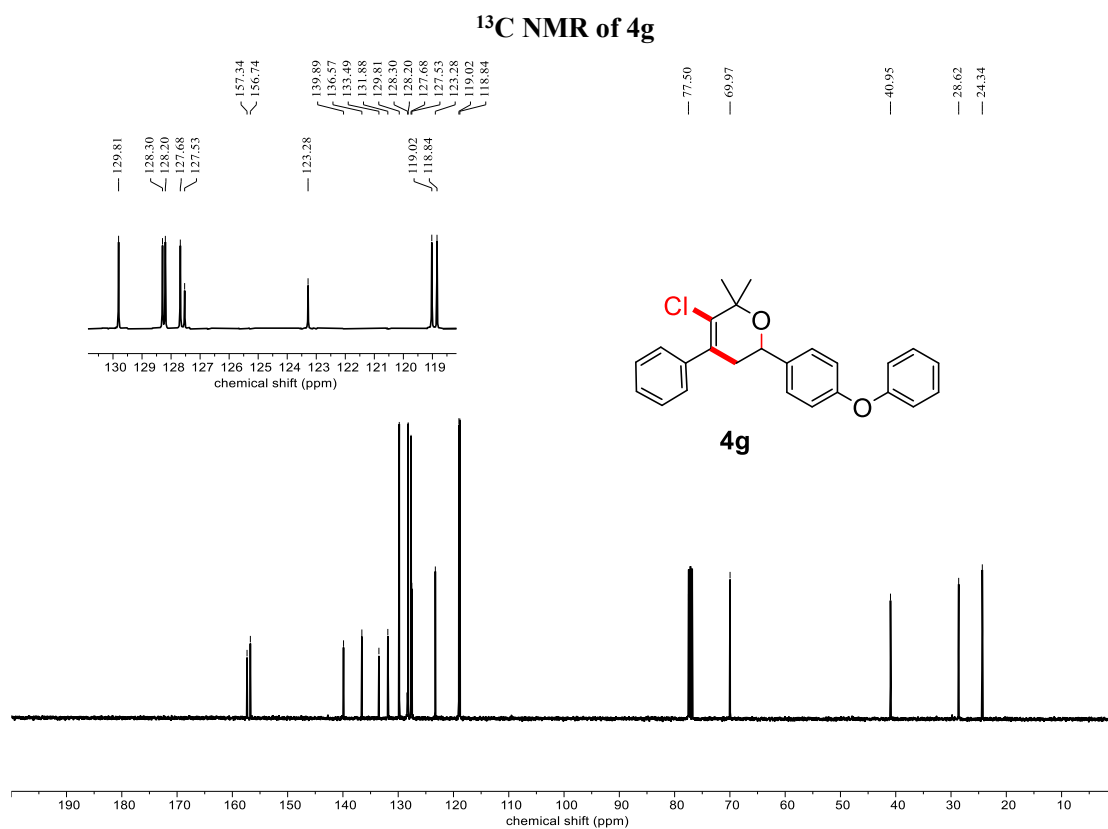
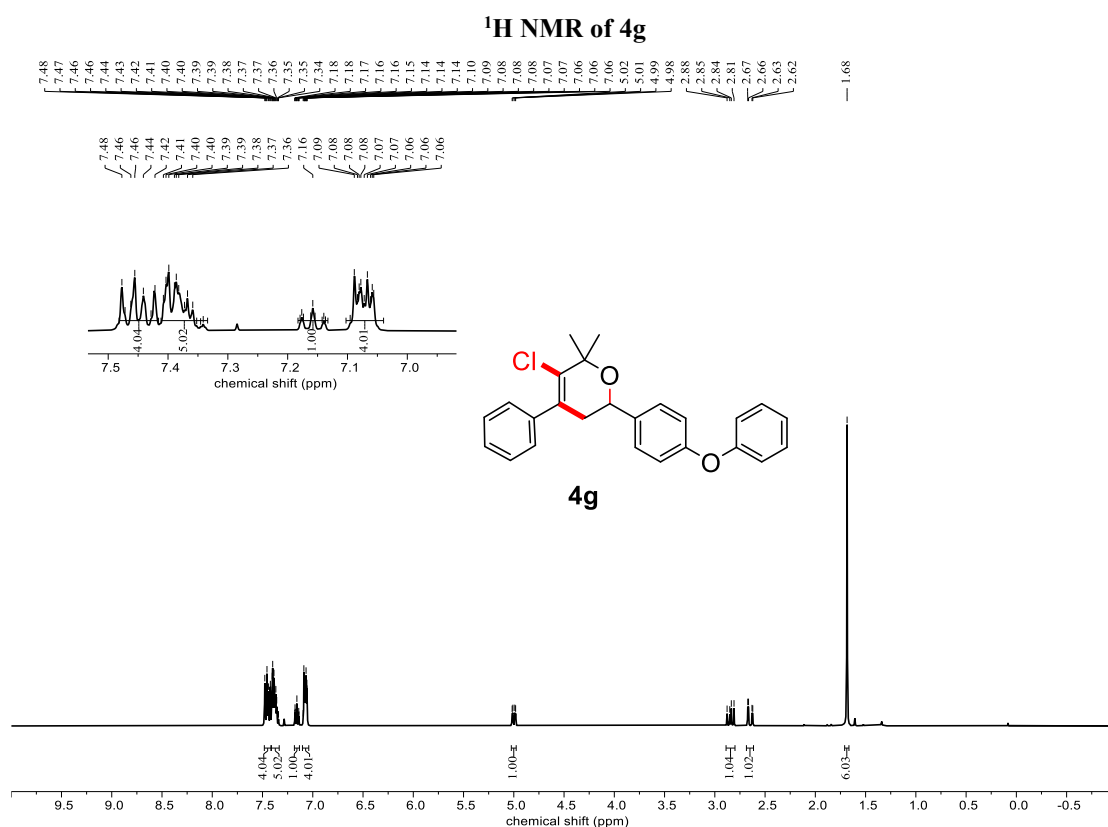


¹H NMR of 4f

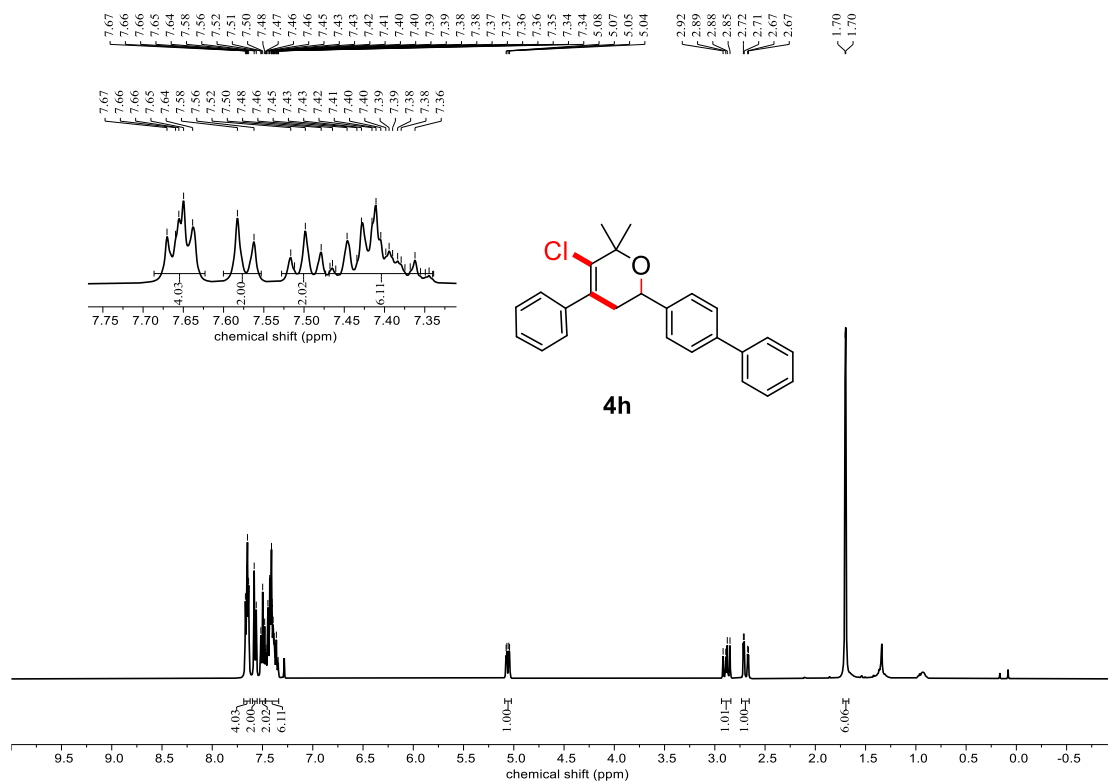


¹³C NMR of 4f

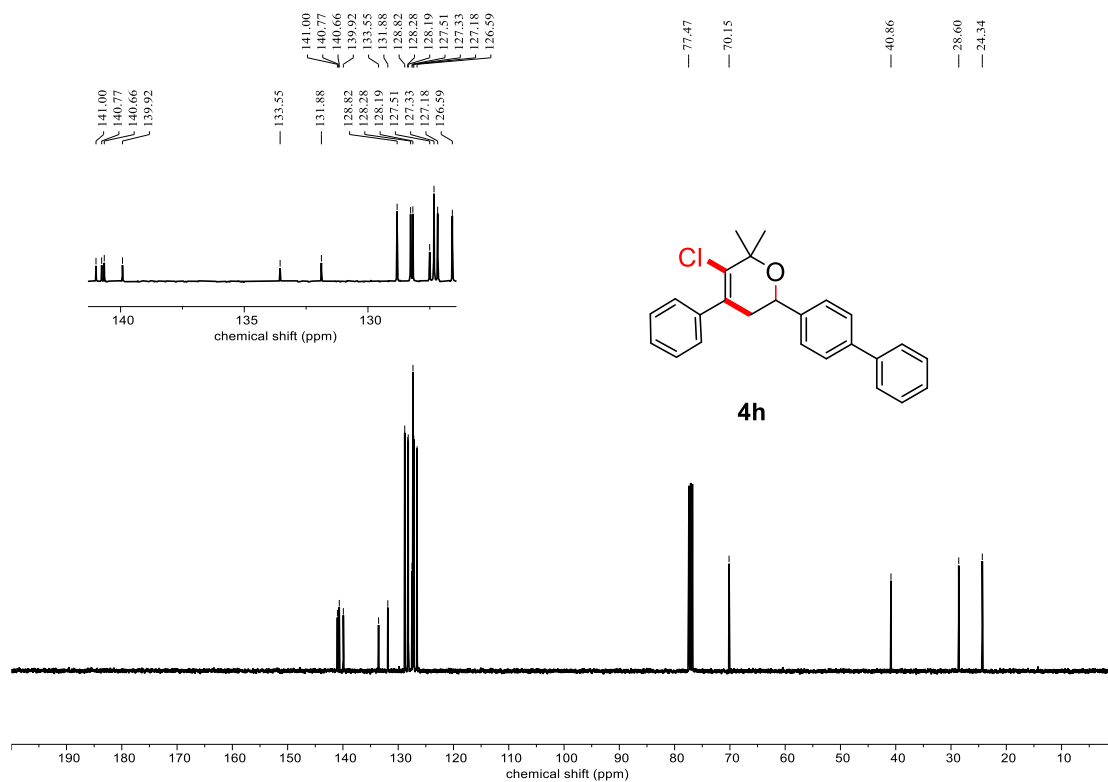




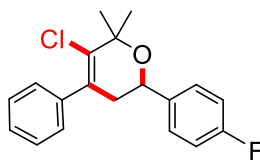
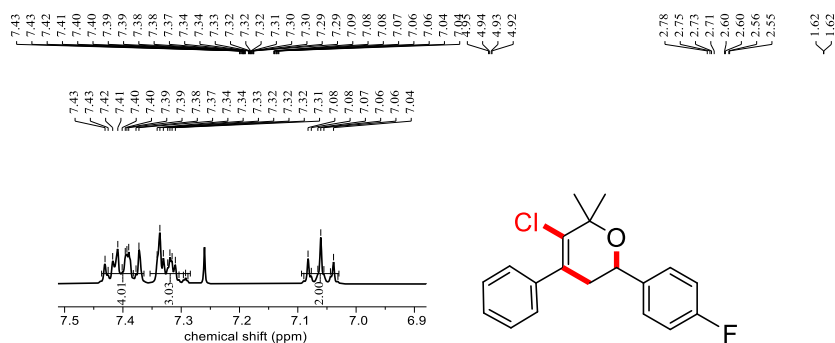
¹H NMR of 4h



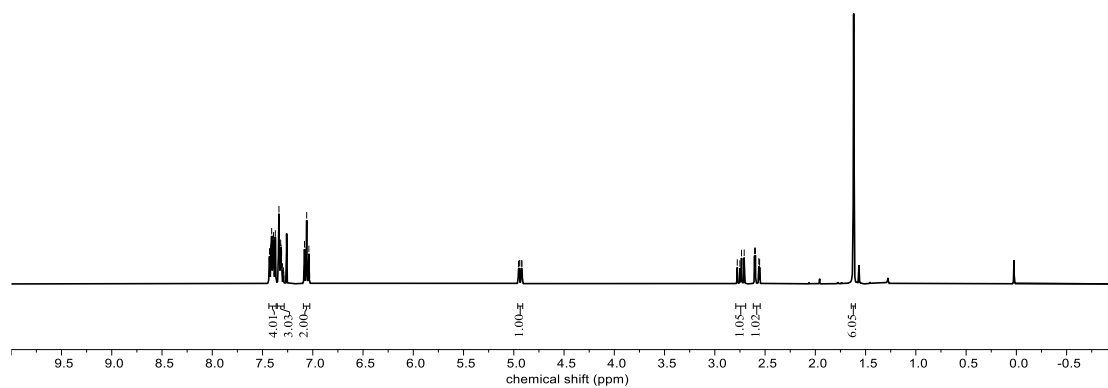
¹³C NMR of 4h



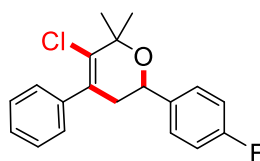
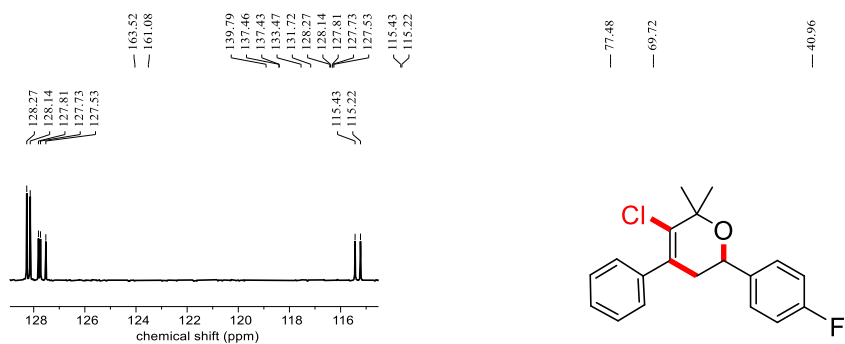
¹H NMR of 4i



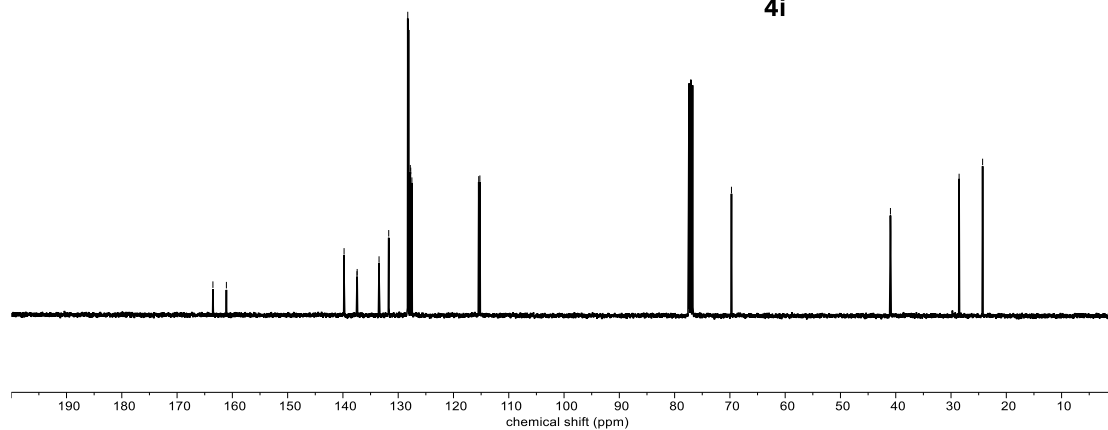
4i



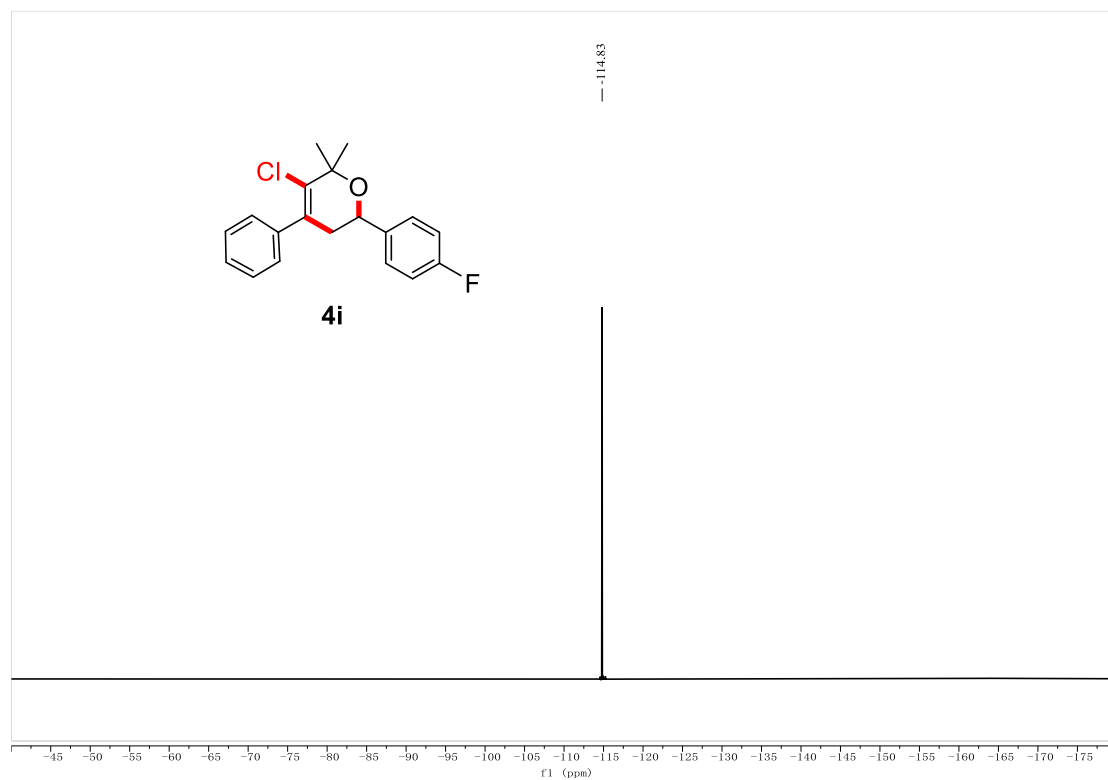
¹³C NMR of 4i



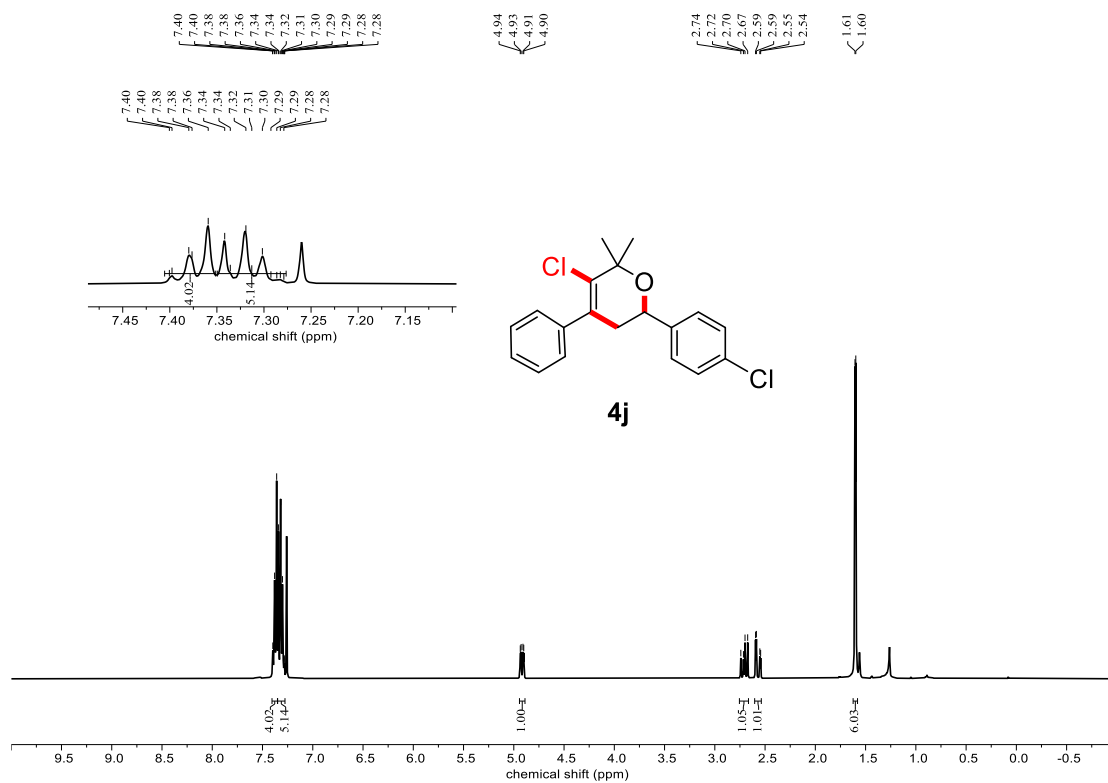
4i



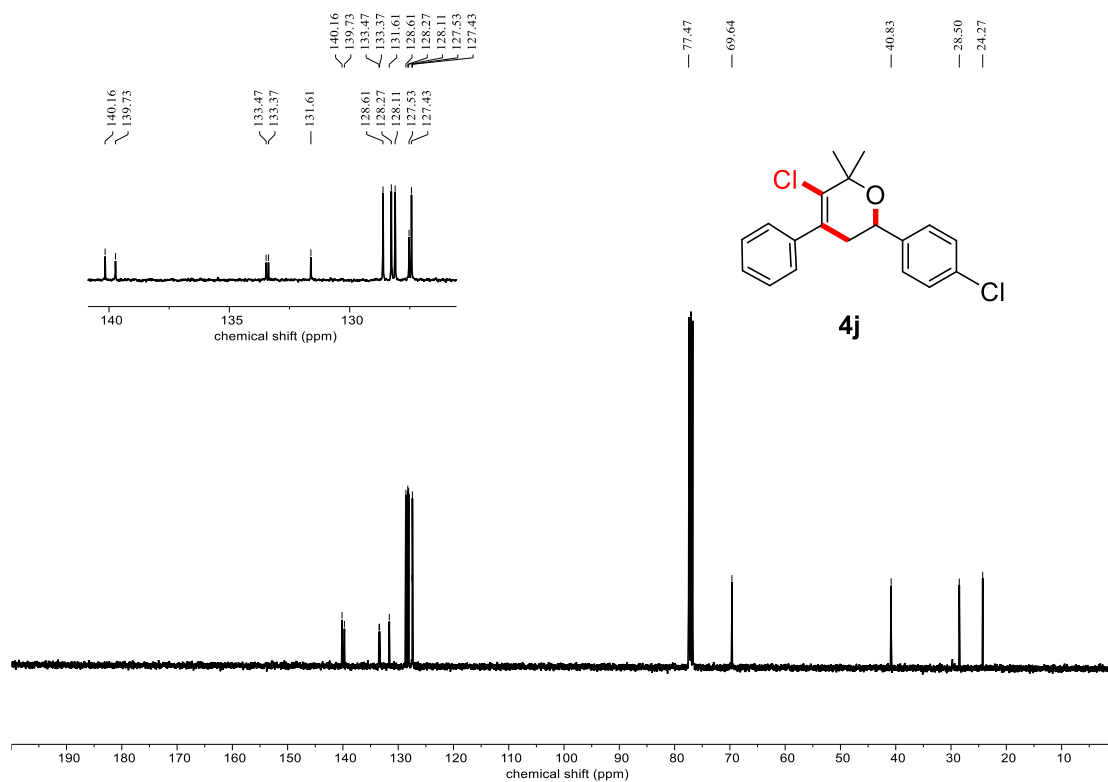
^{19}F NMR of 4i



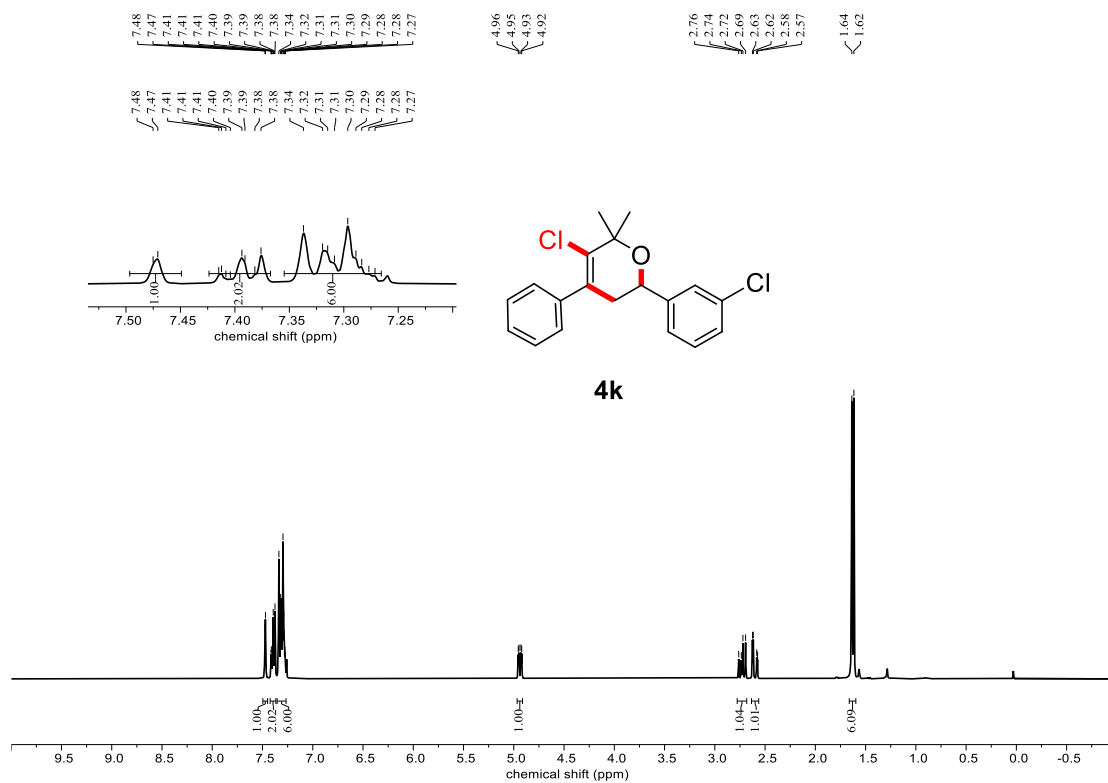
¹H NMR of 4j



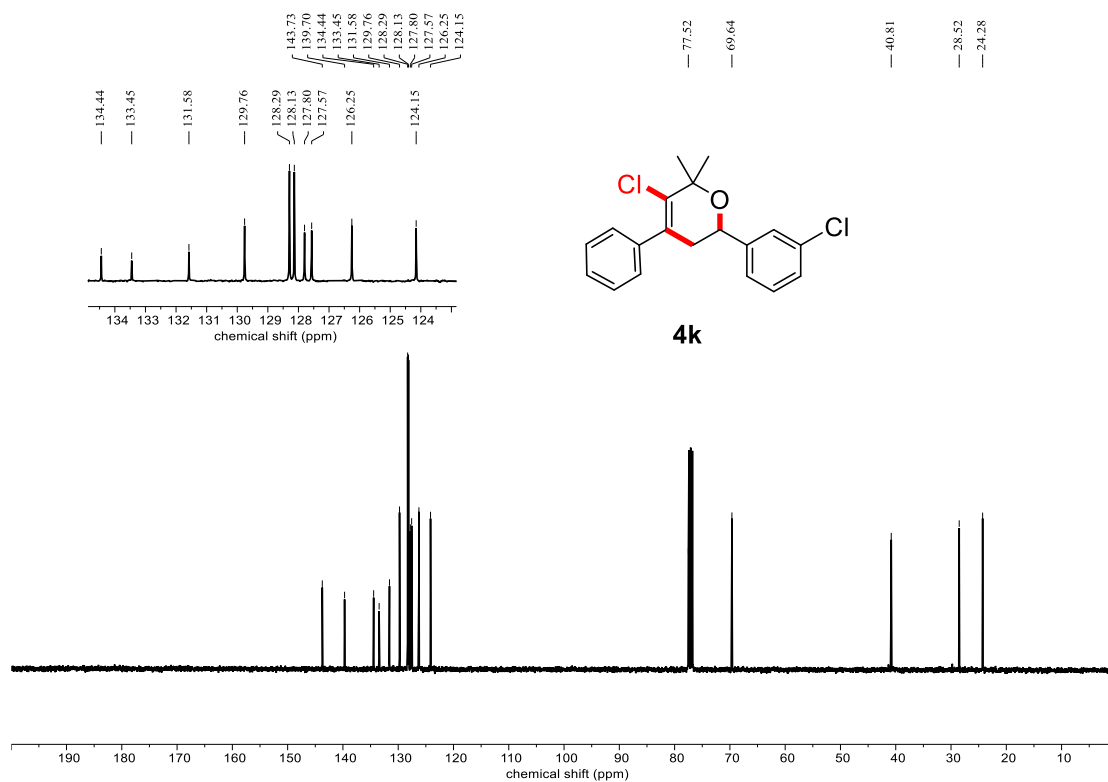
¹³C NMR of 4j



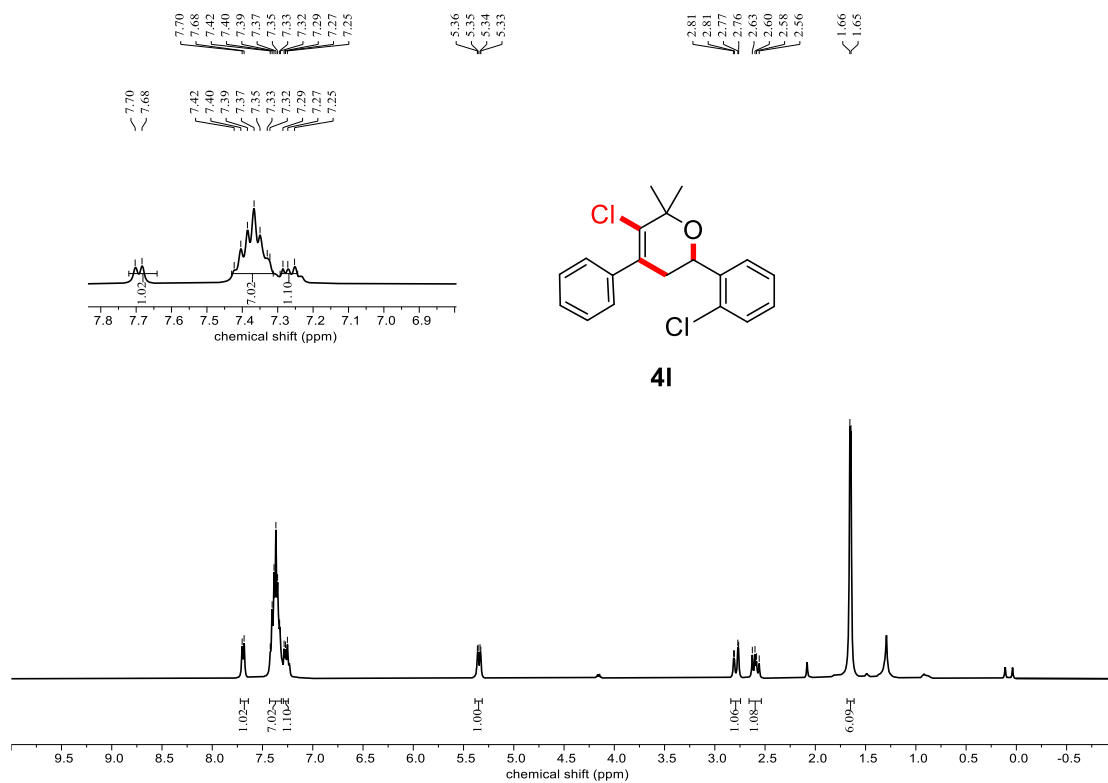
¹H NMR of 4k



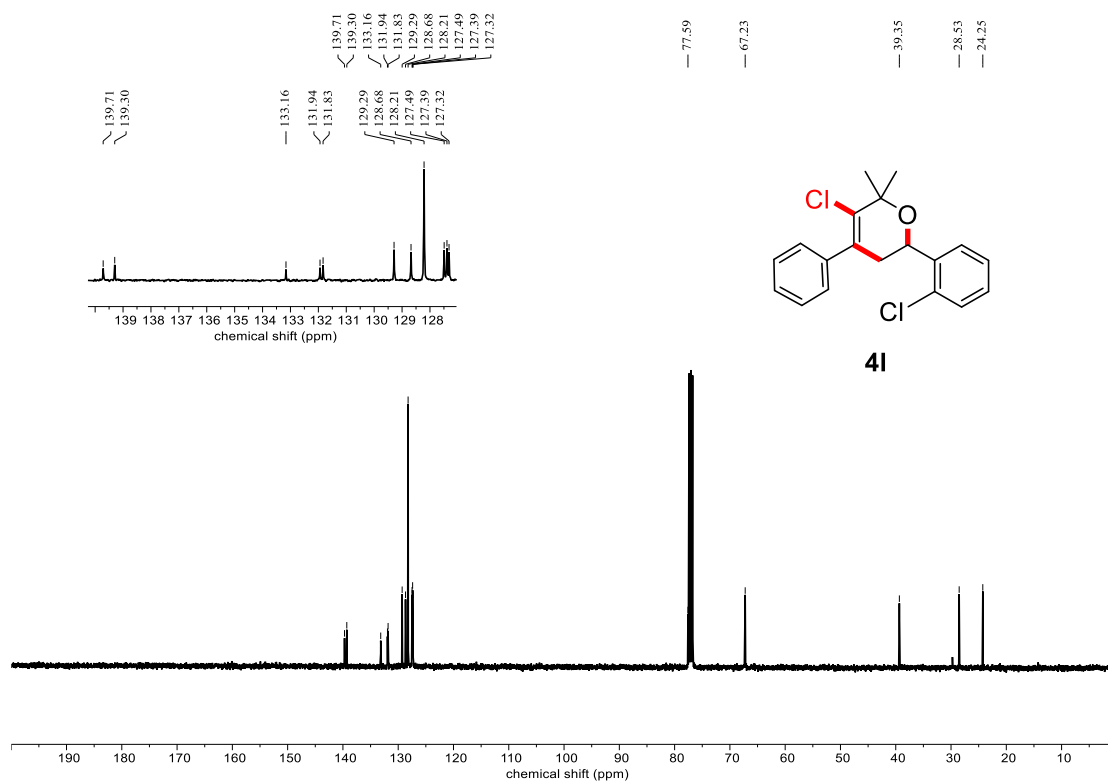
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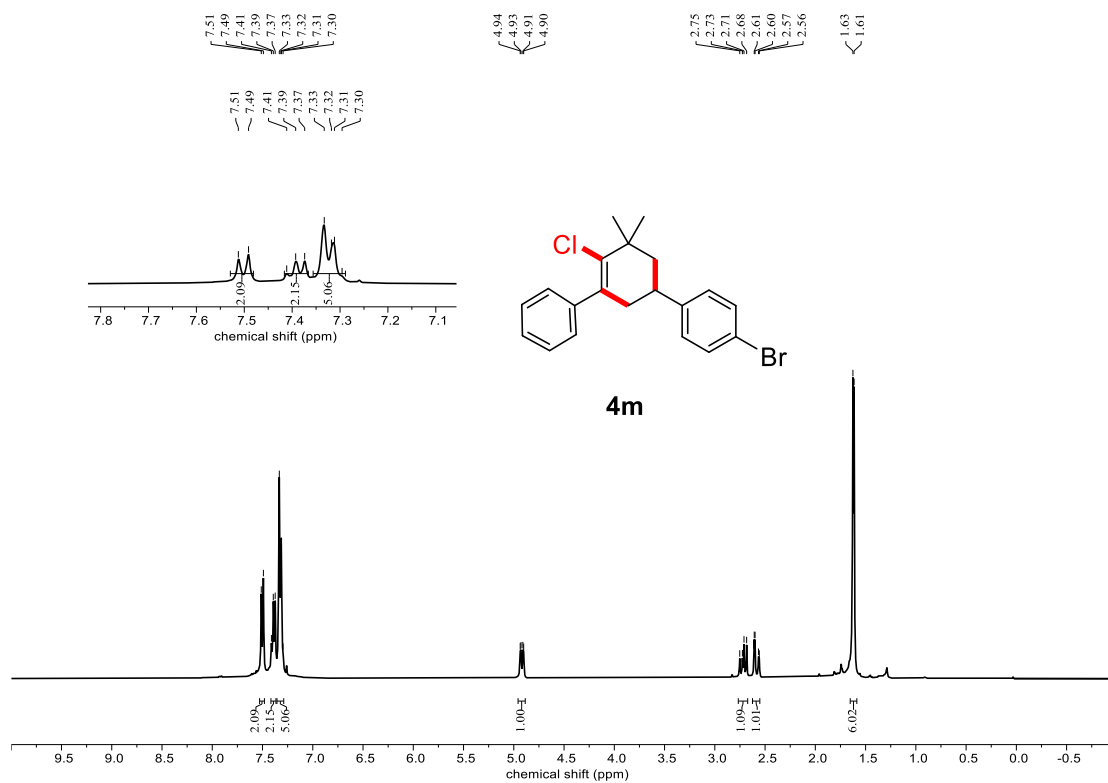
¹H NMR of 4I



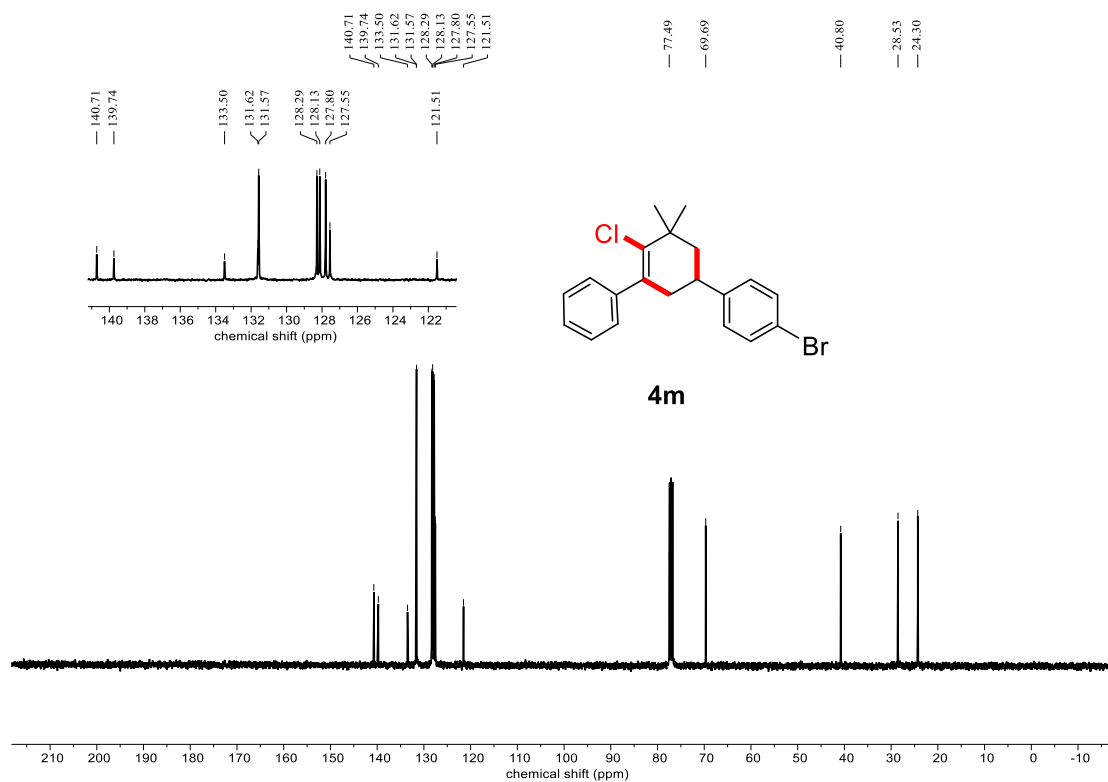
¹³C NMR of 4I



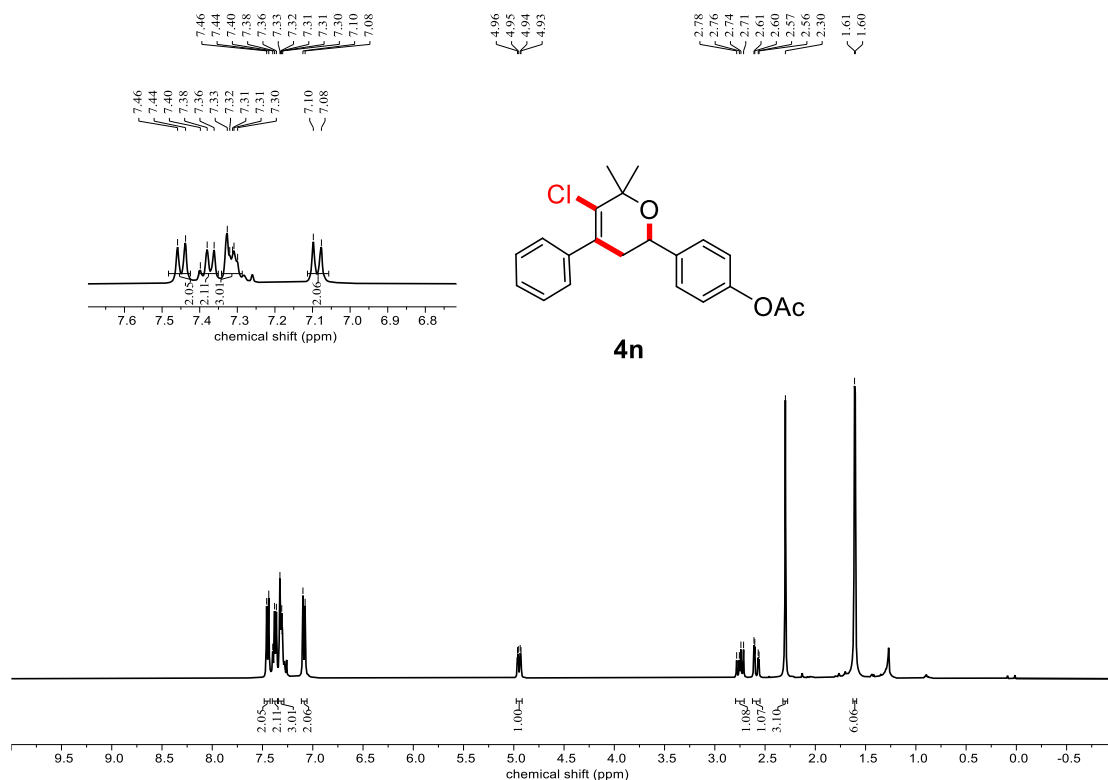
¹H NMR of 4m



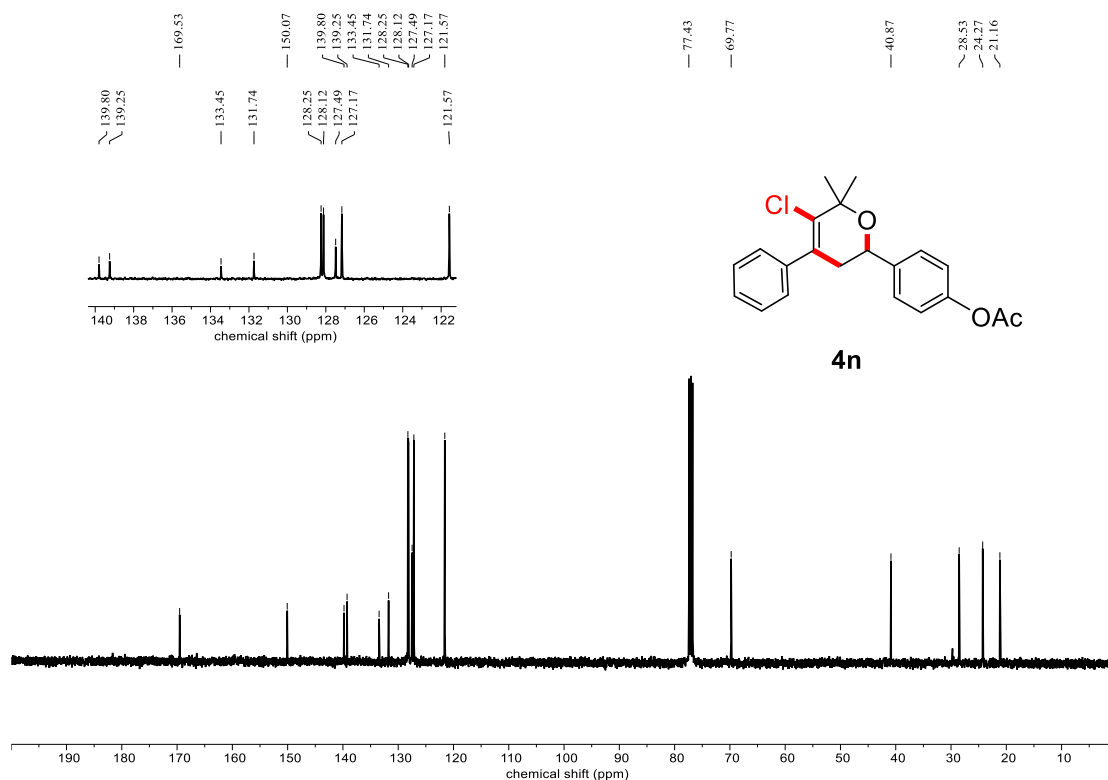
¹³C NMR of 4m



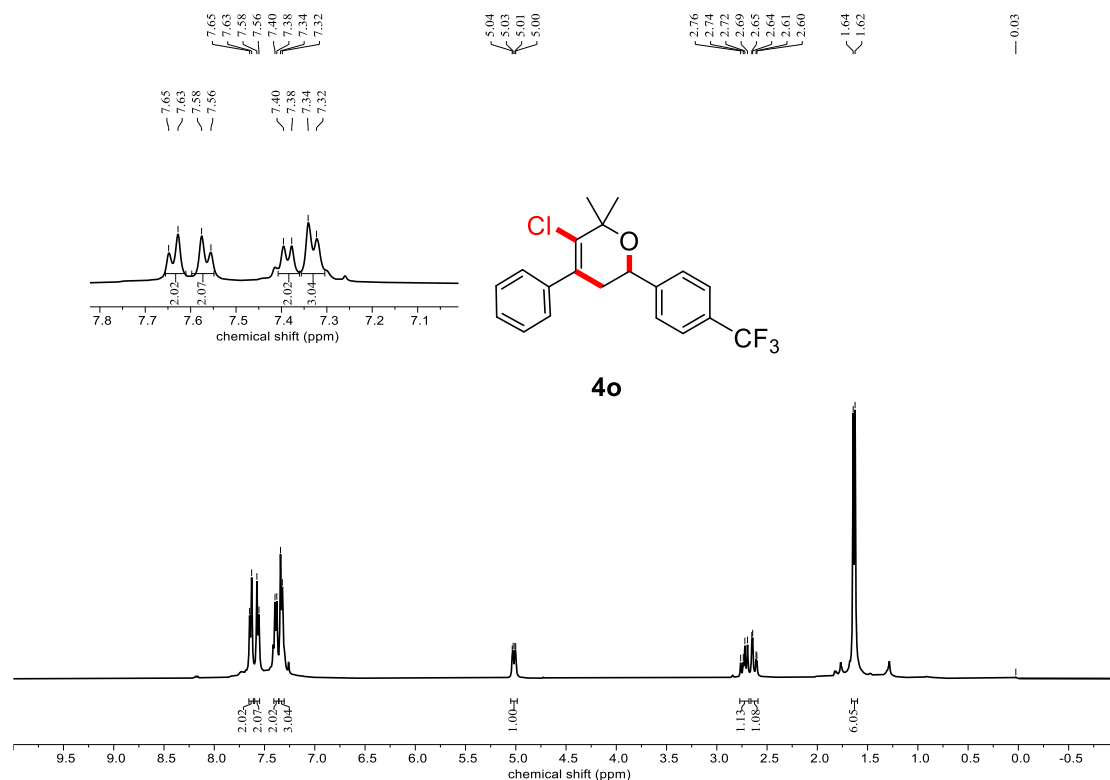
¹H NMR of 4n



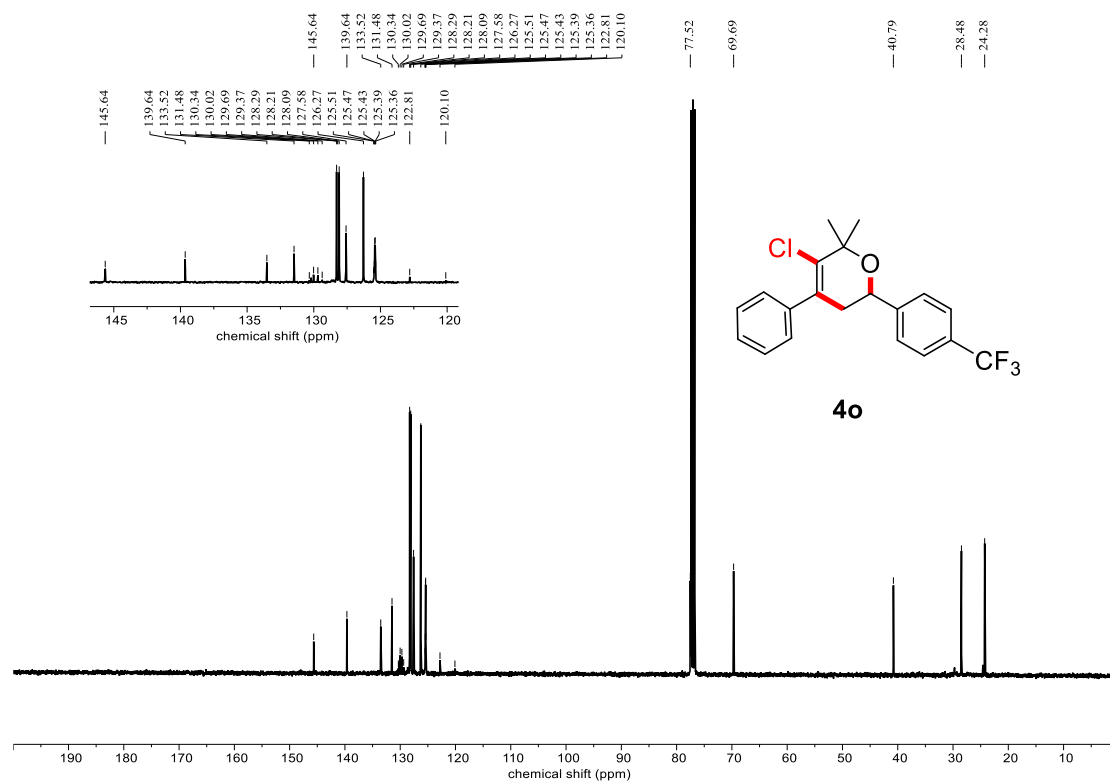
¹³C NMR of 4n



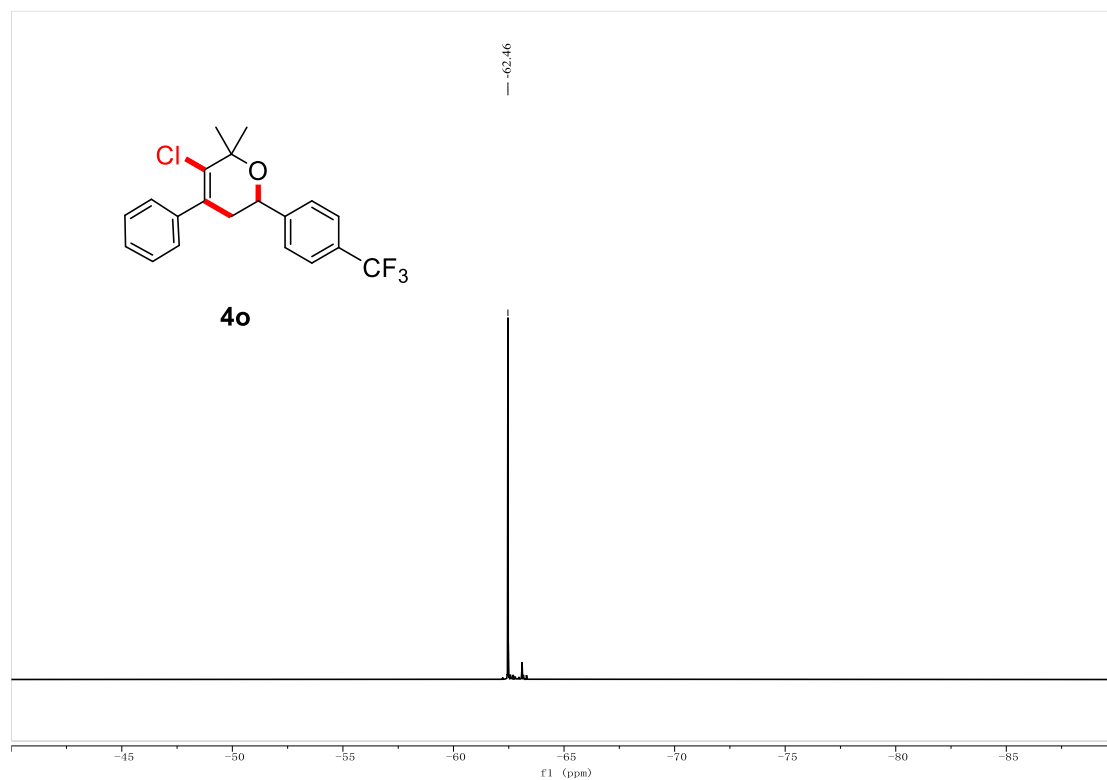
¹H NMR of 4o



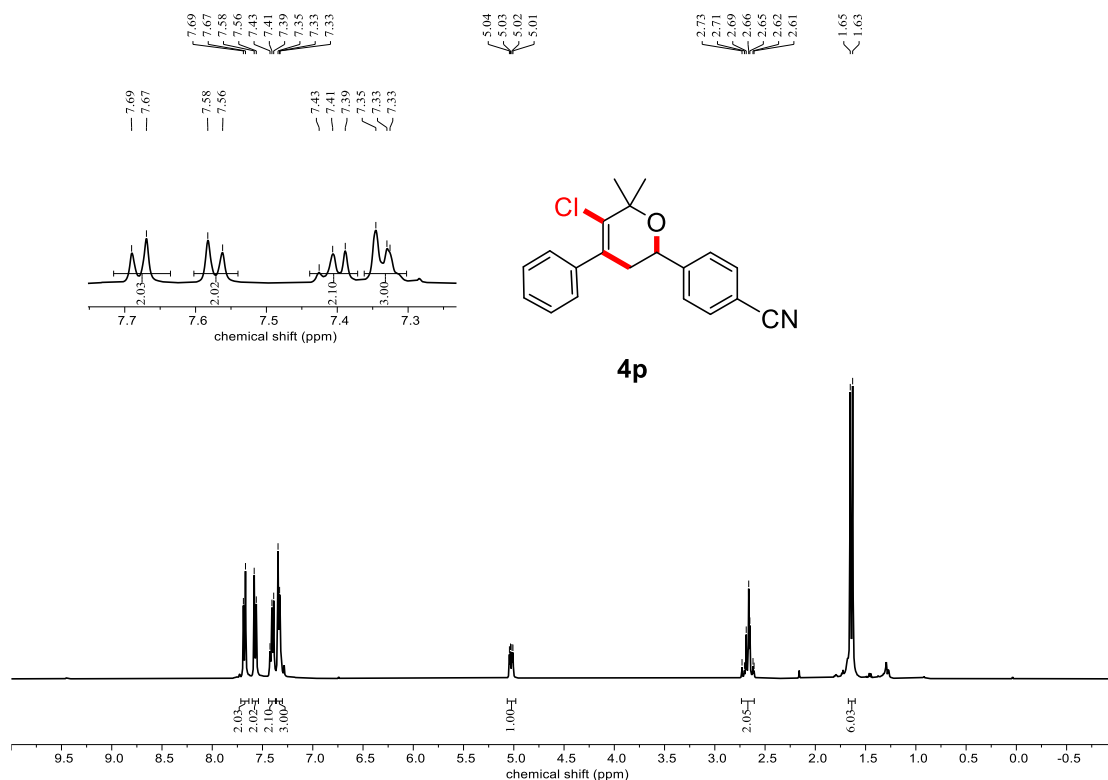
¹³C NMR of 4o



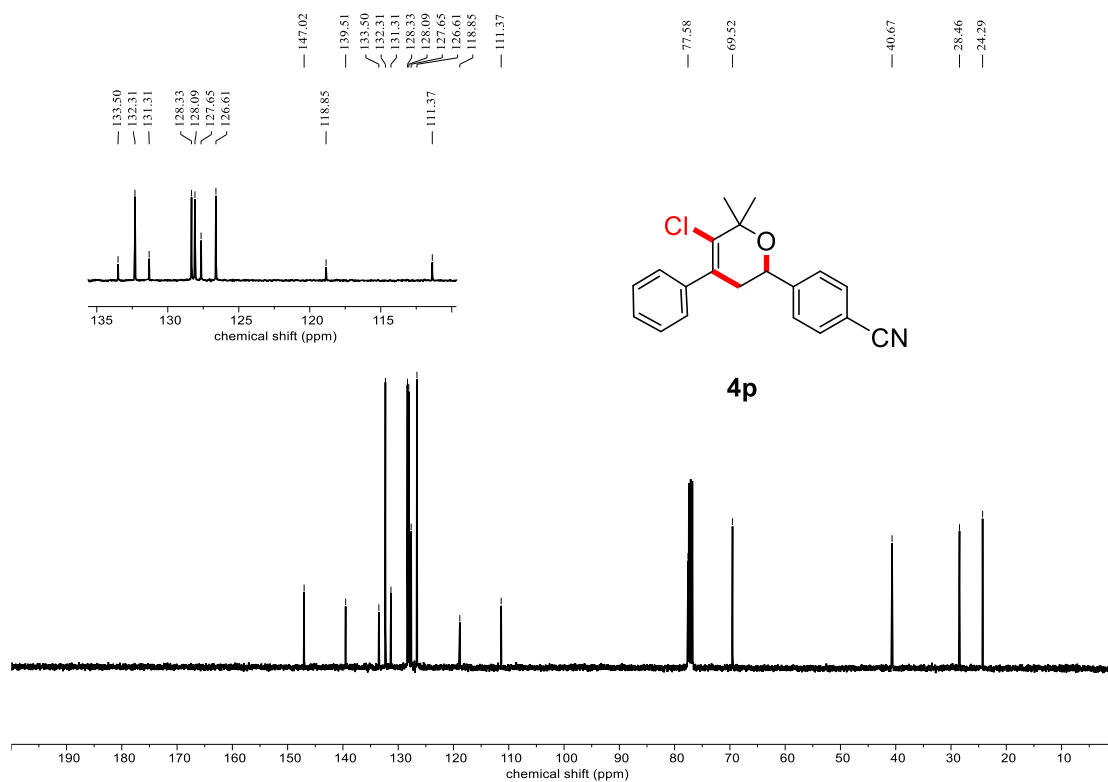
^{19}F NMR of 4o



¹H NMR of 4p



¹³C NMR of 4p



Chemical structure of **4q** is shown above the spectrum. The structure is a 2-chloro-2-methyl-5-(naphthalen-1-yl)-5-phenyl-2,5-dihydrofuran derivative.

¹H NMR spectrum (CDCl₃) of **4q** is shown below the structure. The spectrum displays peaks in the aromatic region (7.36–7.95 ppm) and a reference peak (TMS, 0 ppm). Integration values are provided below the peaks.

Chemical shift (ppm): 7.95, 7.92, 7.91, 7.88, 7.90, 7.87, 7.63, 7.63, 7.91, 7.90, 7.61, 7.61, 7.56, 7.55, 7.55, 7.54, 7.53, 7.53, 7.52, 7.51, 7.51, 7.43, 7.42, 7.41, 7.41, 7.38, 7.38, 7.41, 7.38, 7.40, 7.37, 7.36, 7.36, 5.20, 5.19, 5.17, 5.16, 2.96, 2.94, 2.92, 2.90, 2.77, 2.76, 2.73, 2.72, 1.74, 1.73.

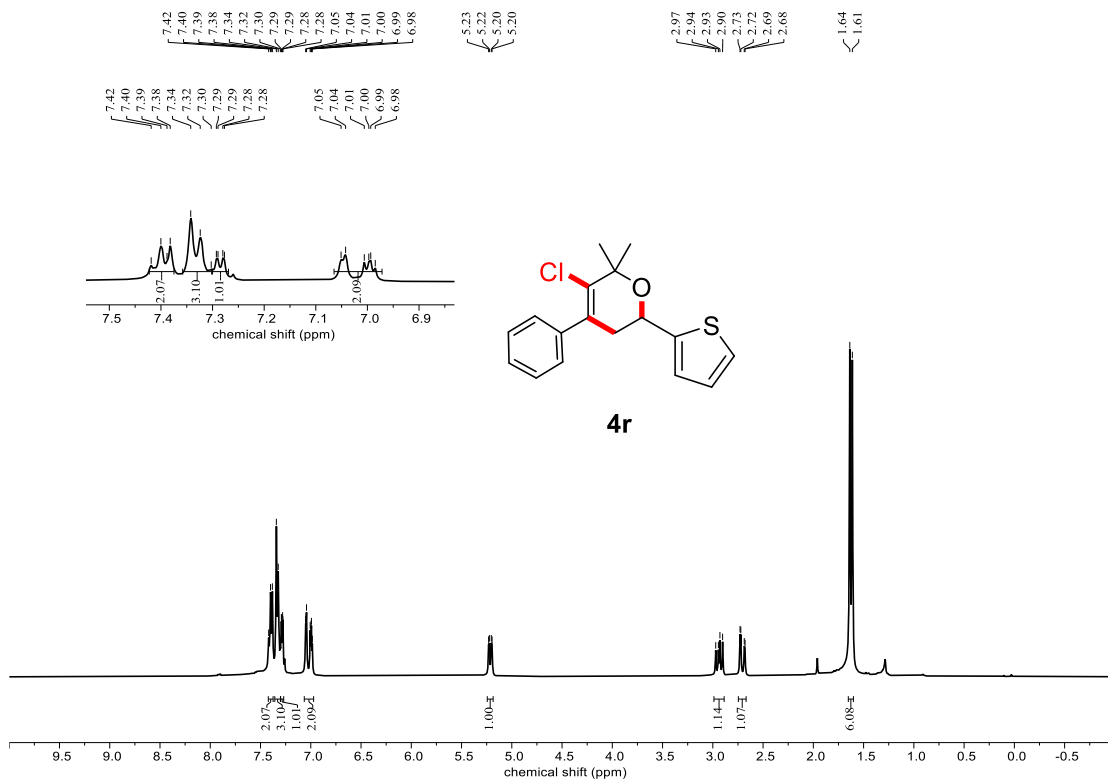
Integration values: 1.00, 3.03, 1.16, 2.06, 5.05, 1.00, 1.07, 6.06.

Chemical structure of 4q: CC1(C)C(=C(C2=CC=CC=C2)C(=O)C3=CC=CC=C3)OC1=O

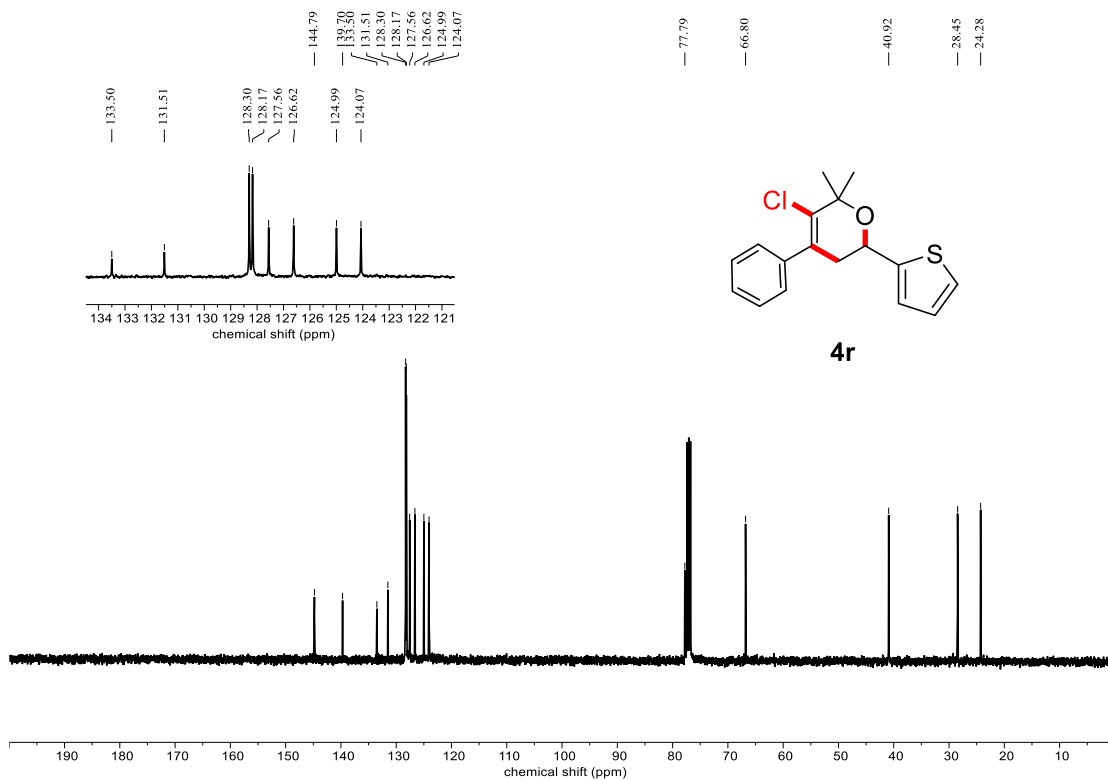
¹³C NMR spectrum (CDCl₃):

Chemical shift (ppm): 139.96, 139.04, 133.59, 133.38, 133.08, 131.94, 128.30, 128.20, 128.06, 127.72, 127.52, 128.30, 126.16, 125.92, 128.20, 127.72, 126.16, 125.92, 124.78, 124.33, 77.53, 70.43, 40.90, 28.64, 24.38.

¹H NMR of 4r

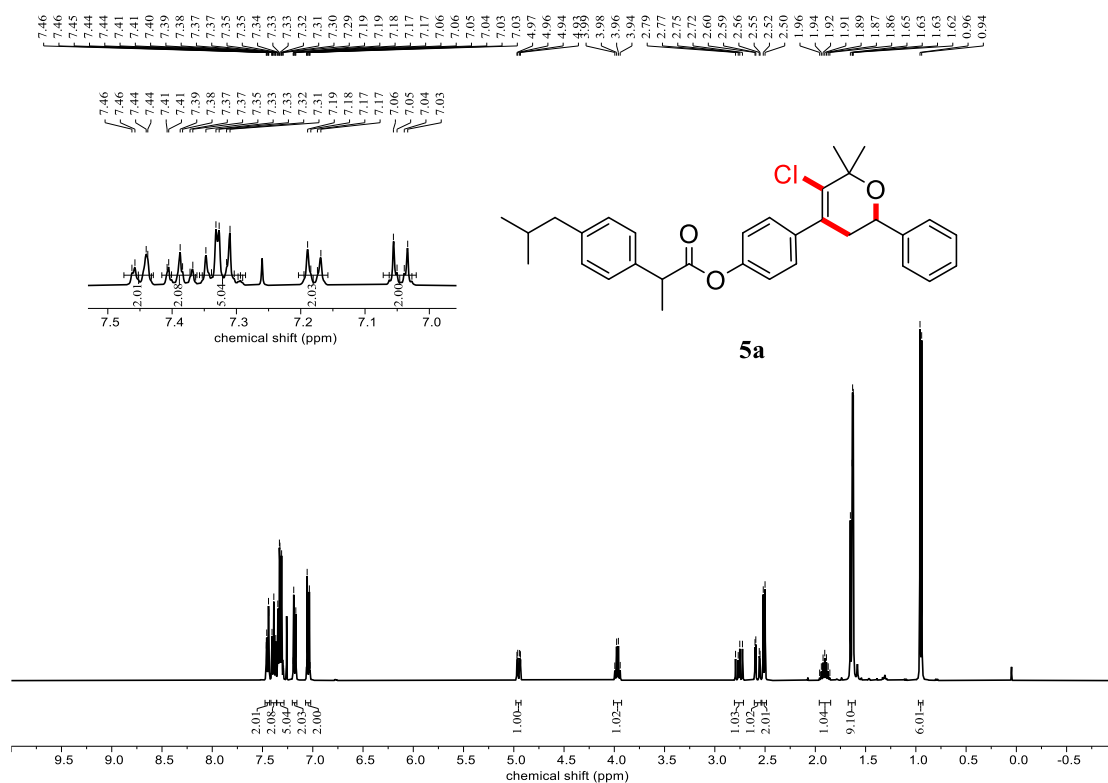


¹³C NMR of 4r

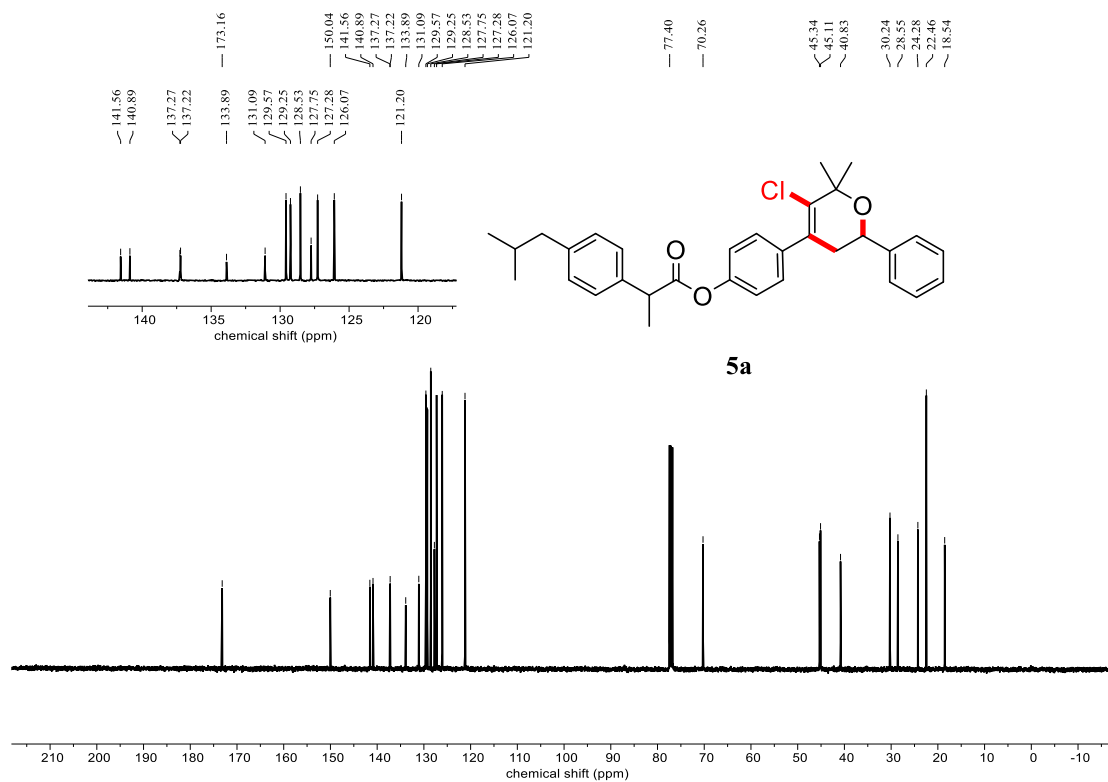


¹H and ¹³C NMR spectra of compounds 5

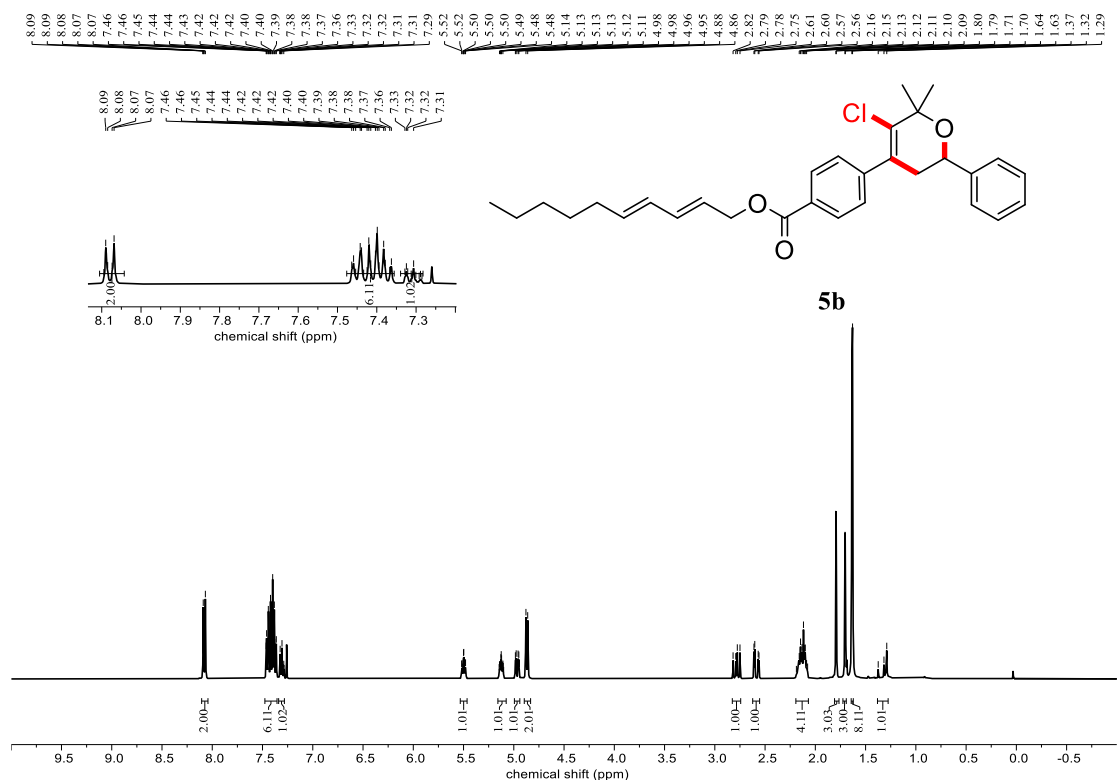
¹H NMR of 5a



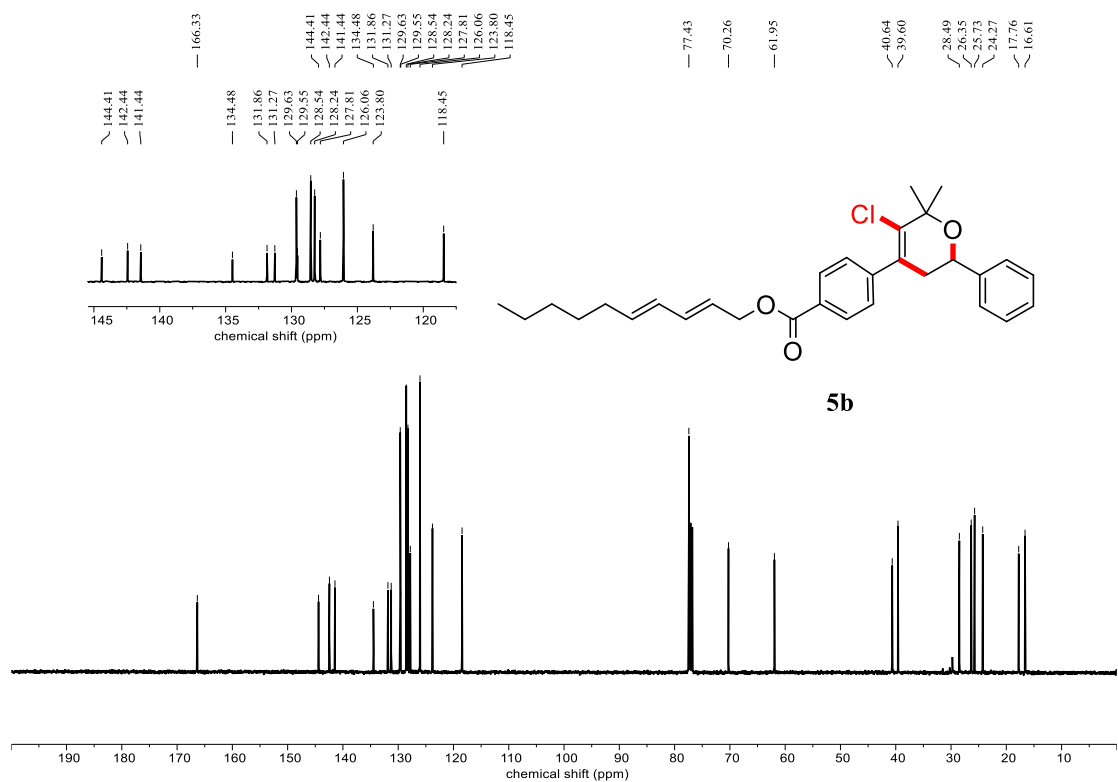
¹³C NMR of 5a



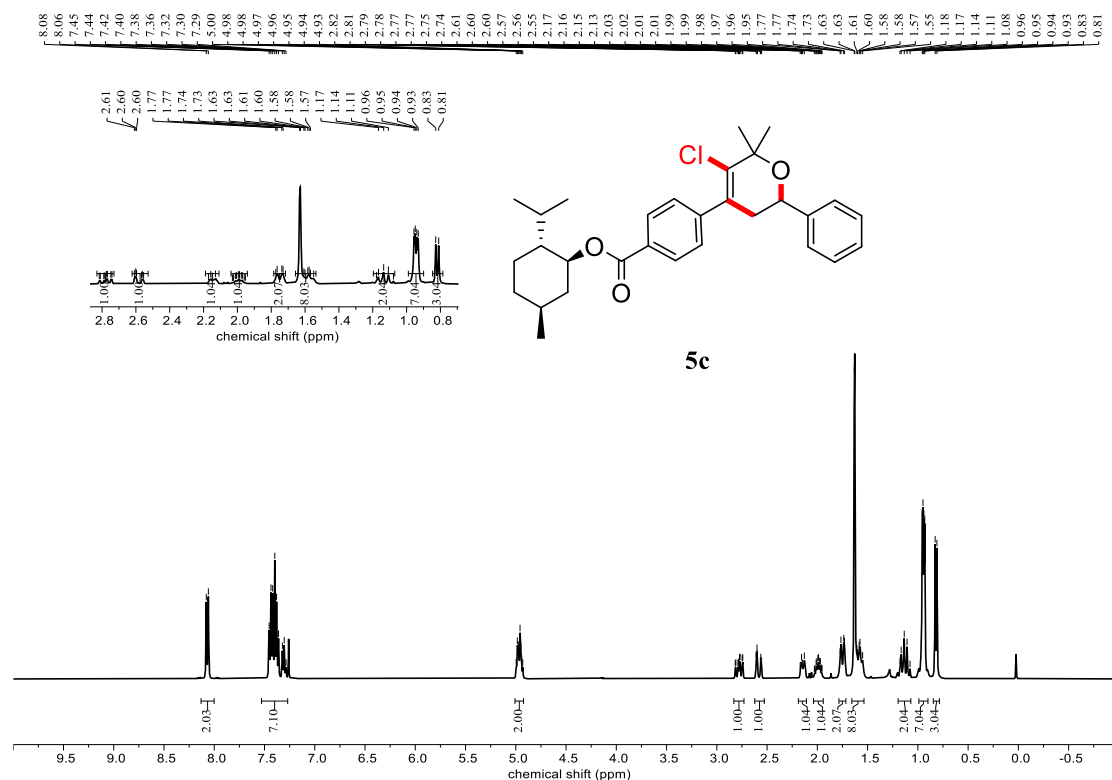
¹H NMR of 5b



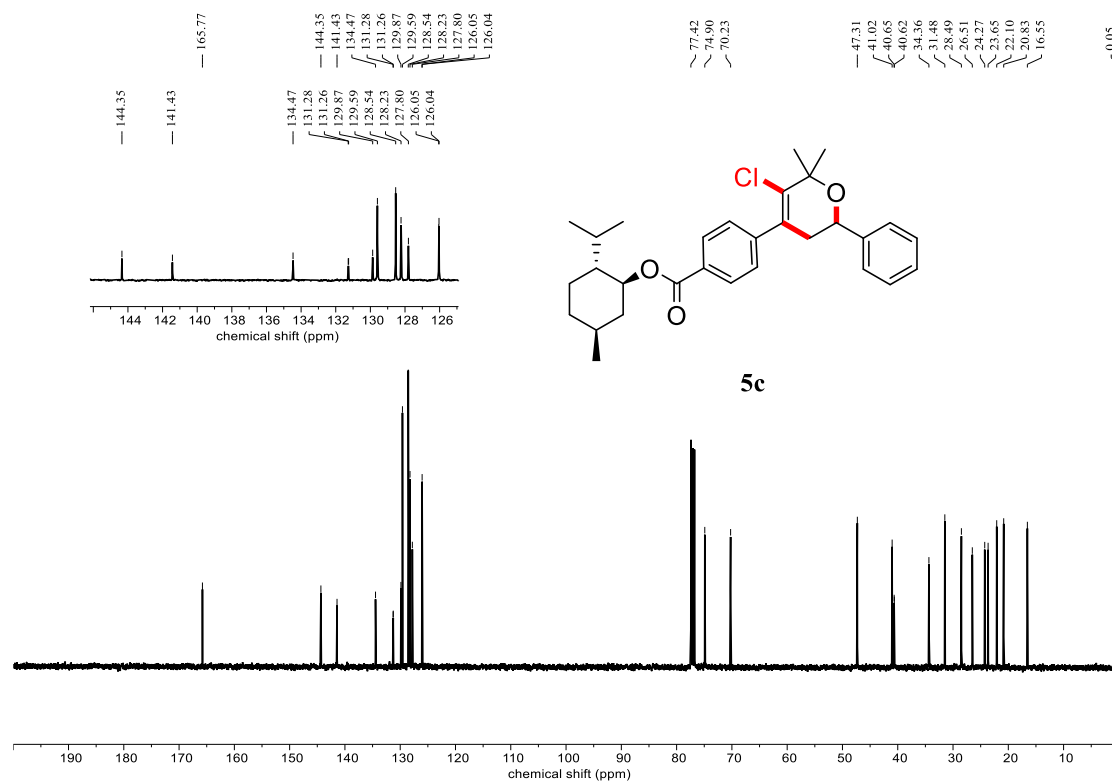
¹³C NMR of 5b

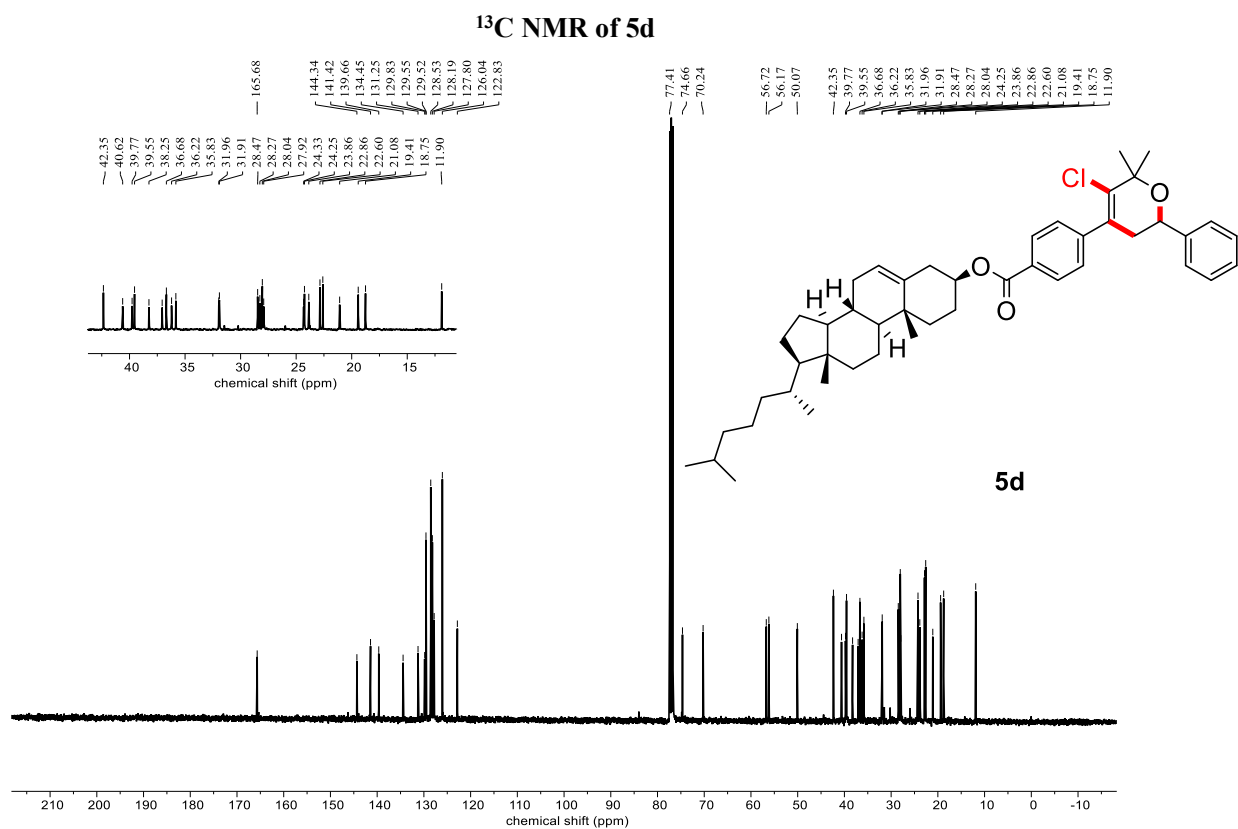
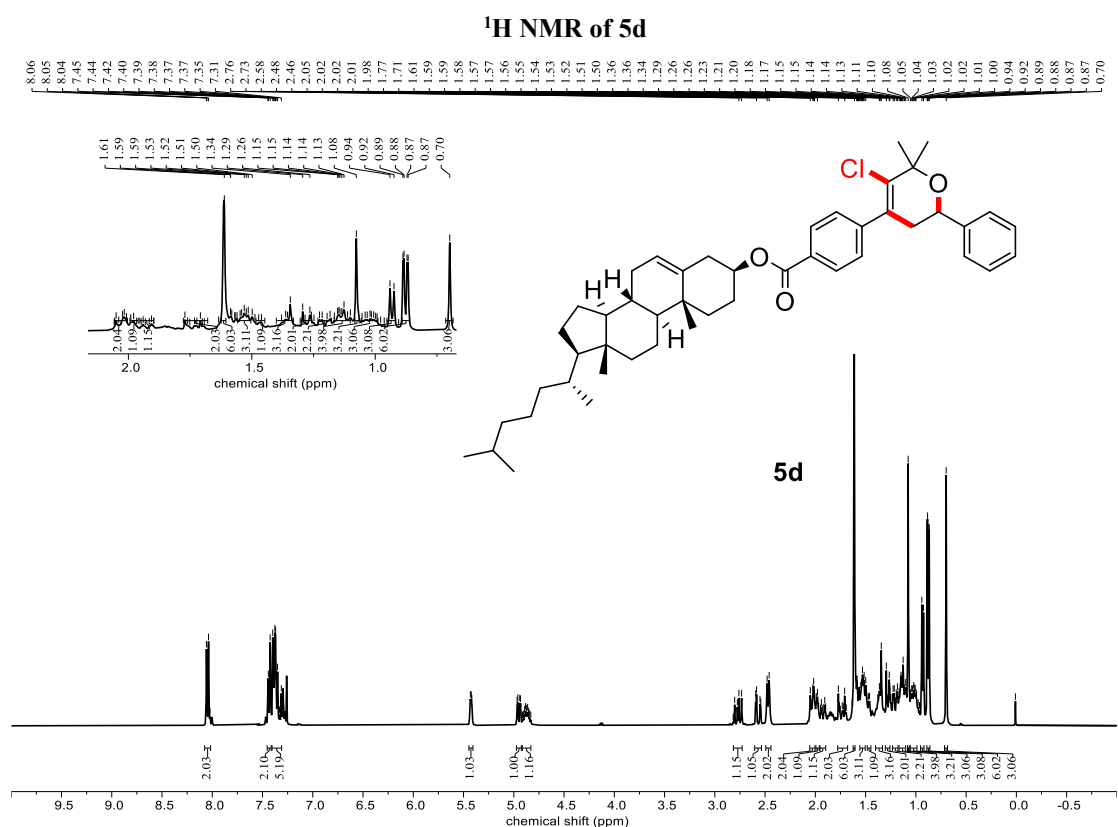


¹H NMR of 5c

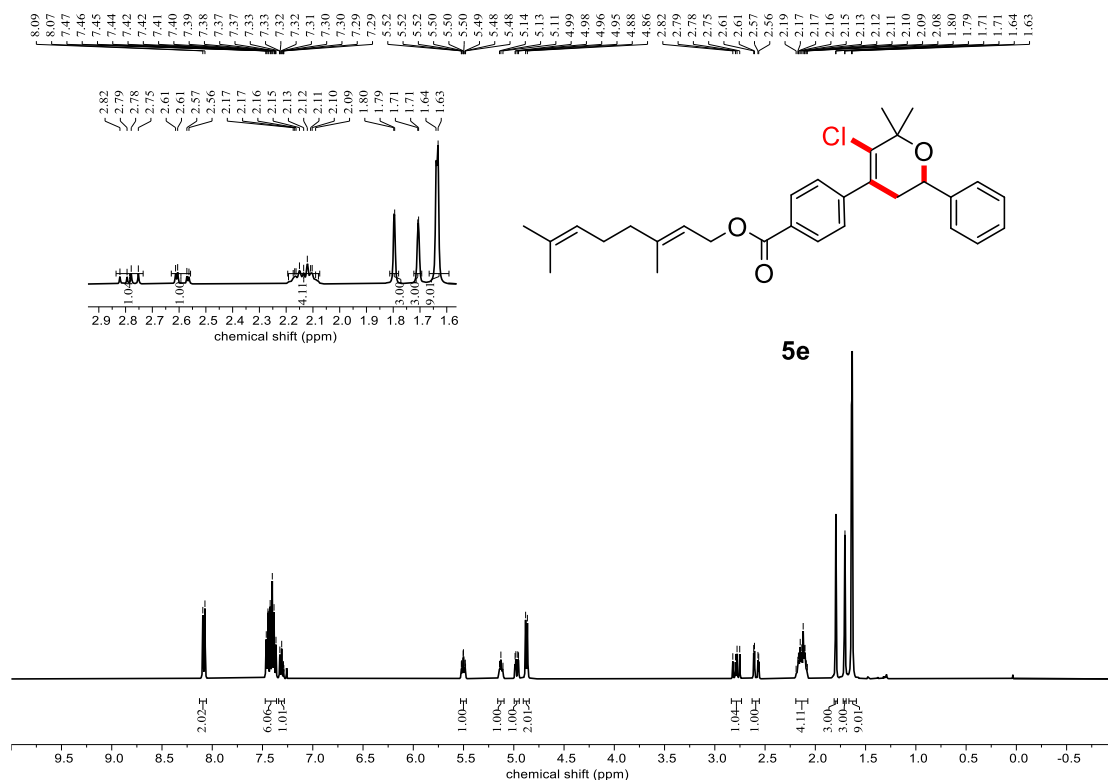


¹³C NMR of 5c

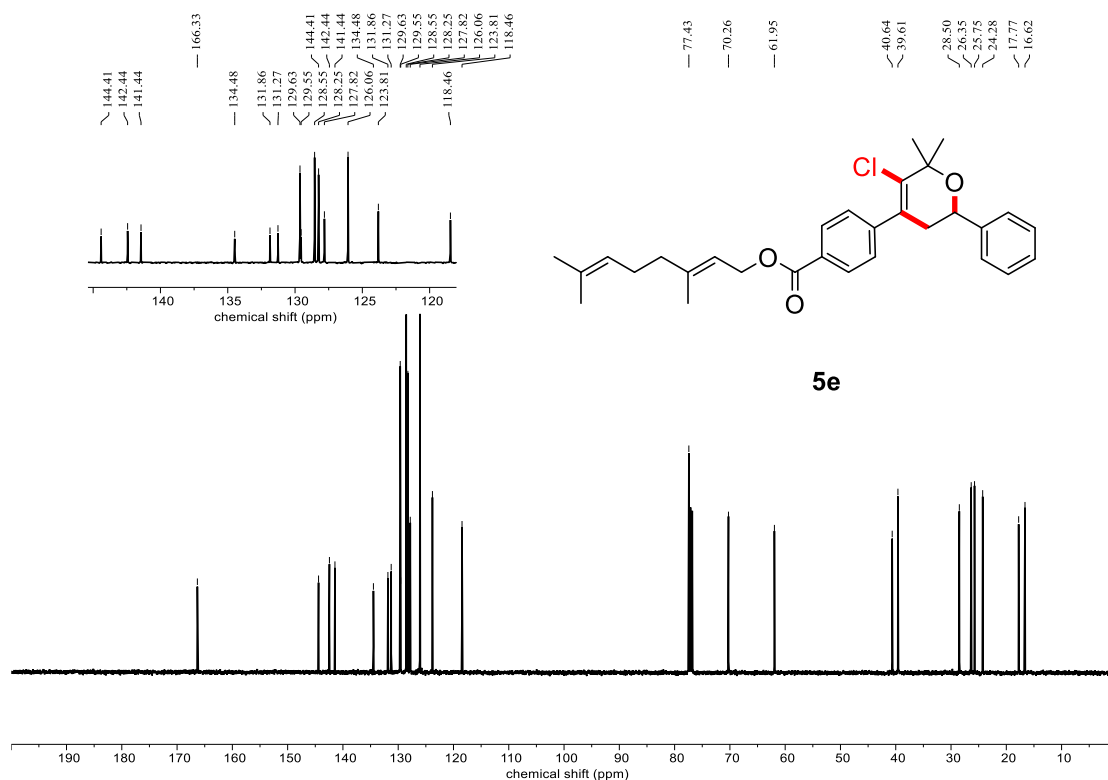




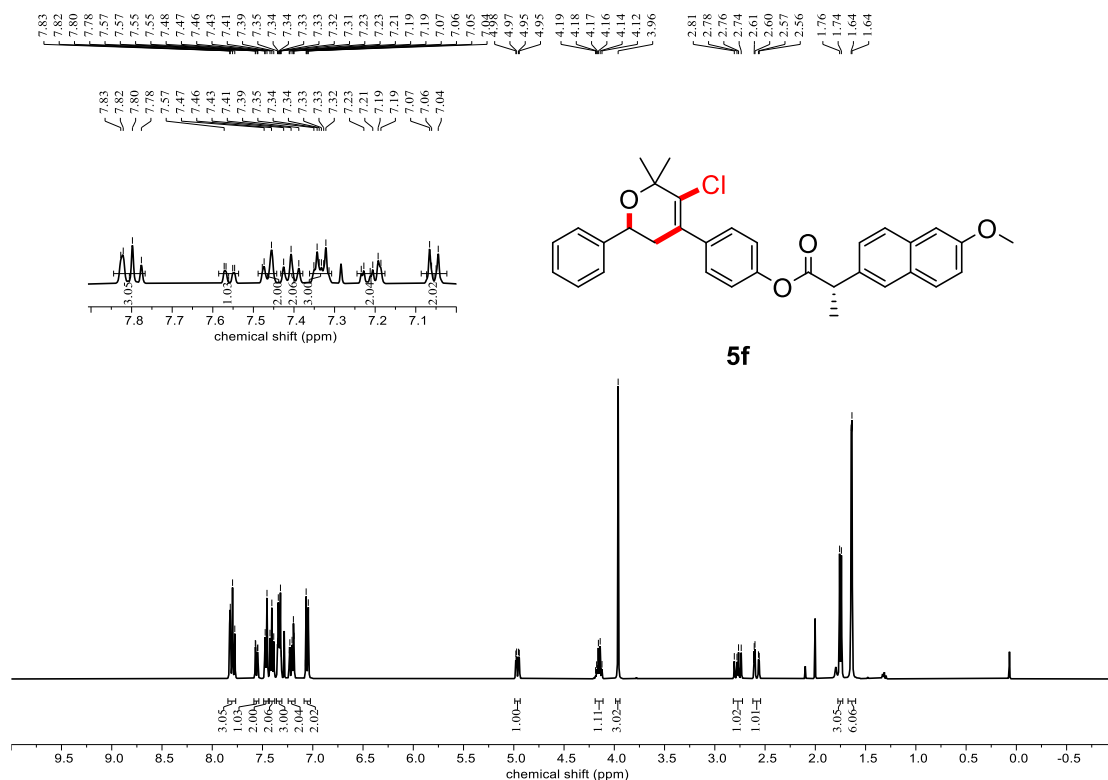
¹H NMR of 5e



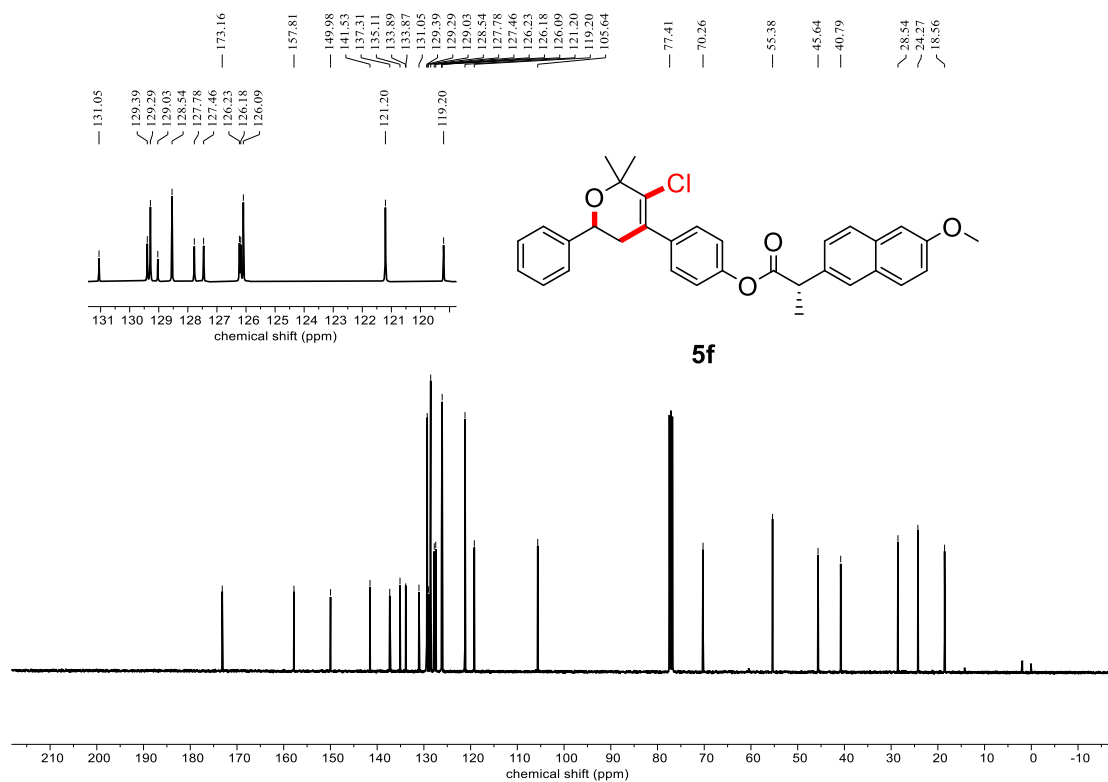
¹³C NMR of 5e



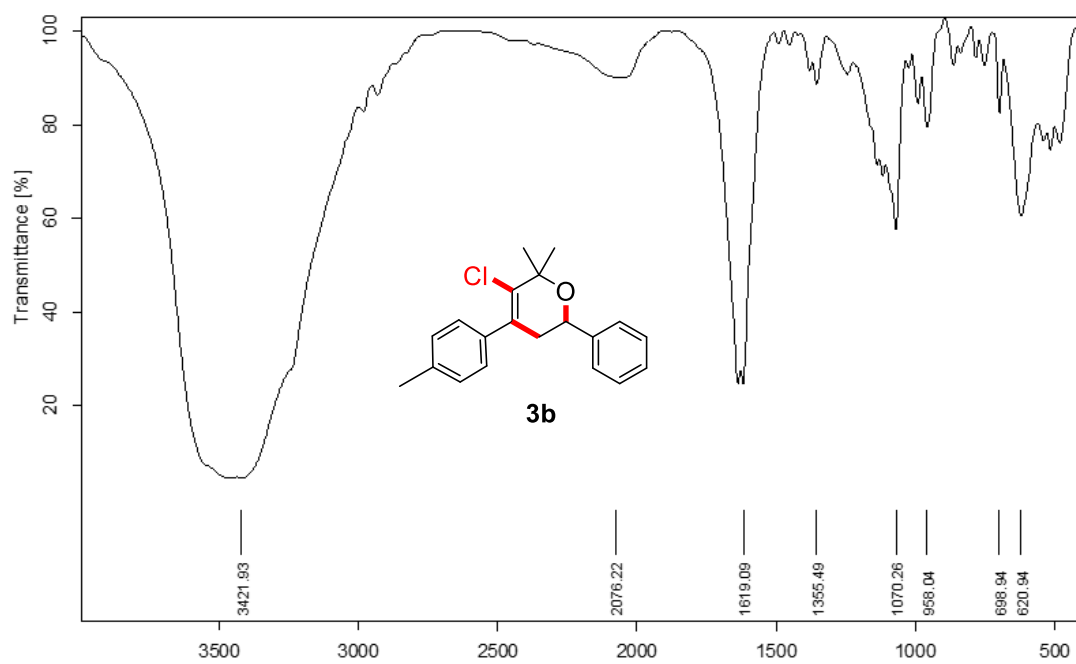
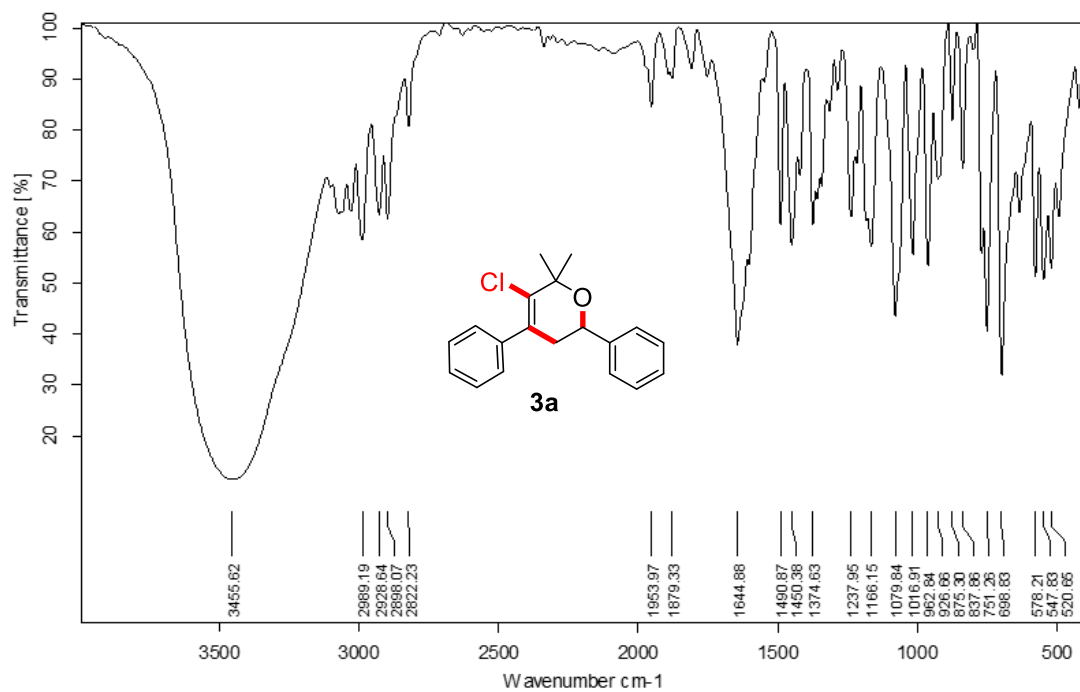
¹H NMR of 5f

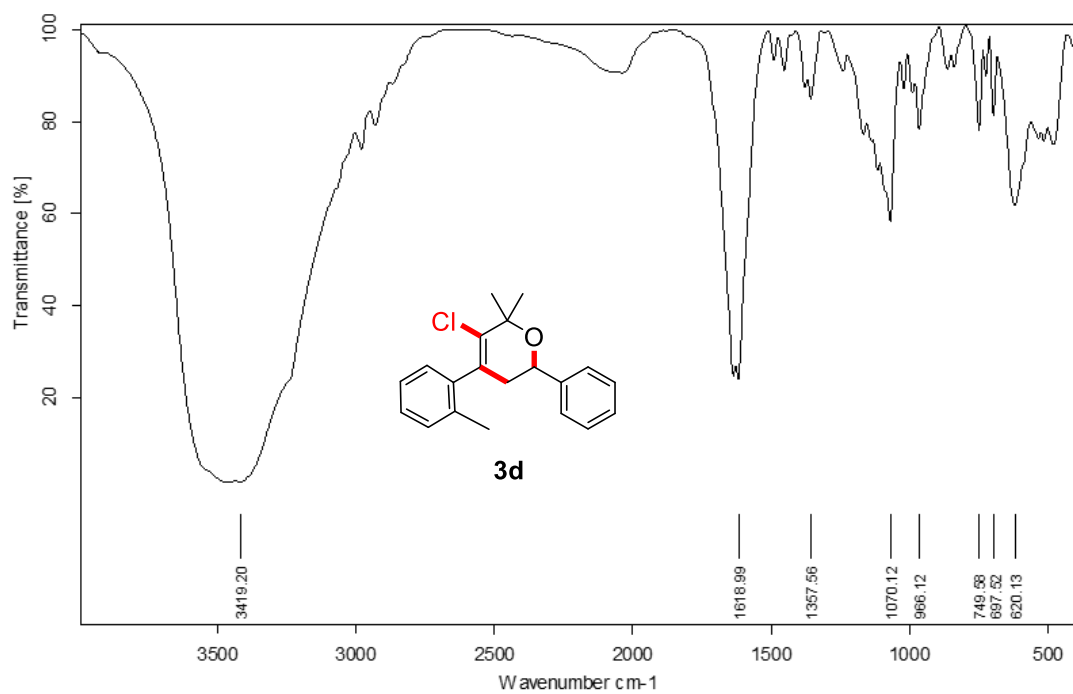
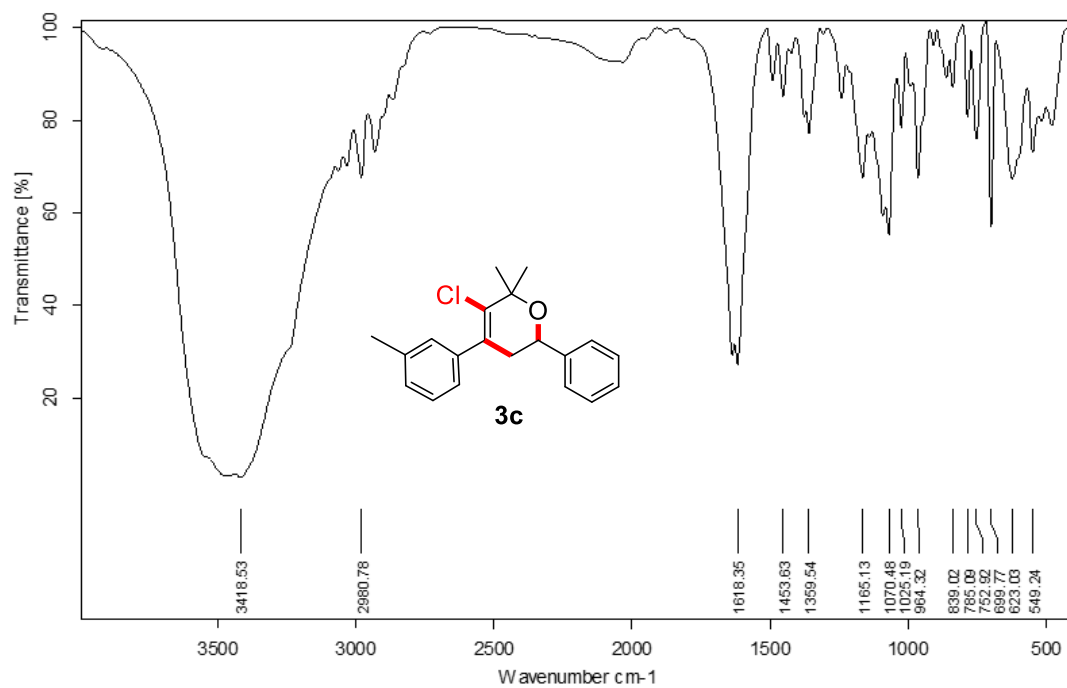


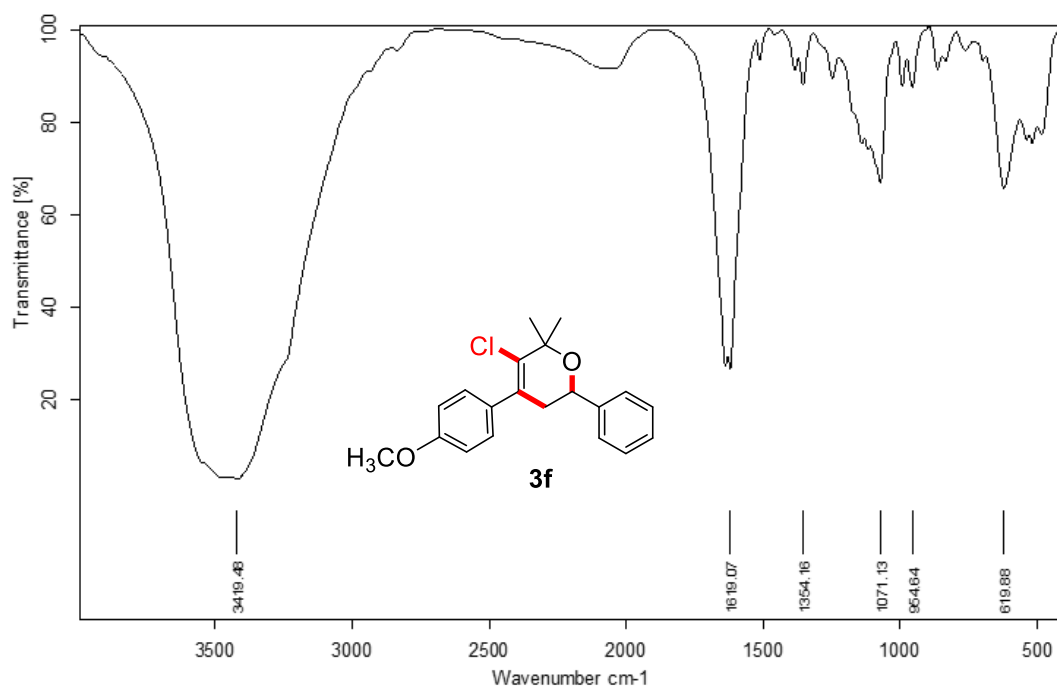
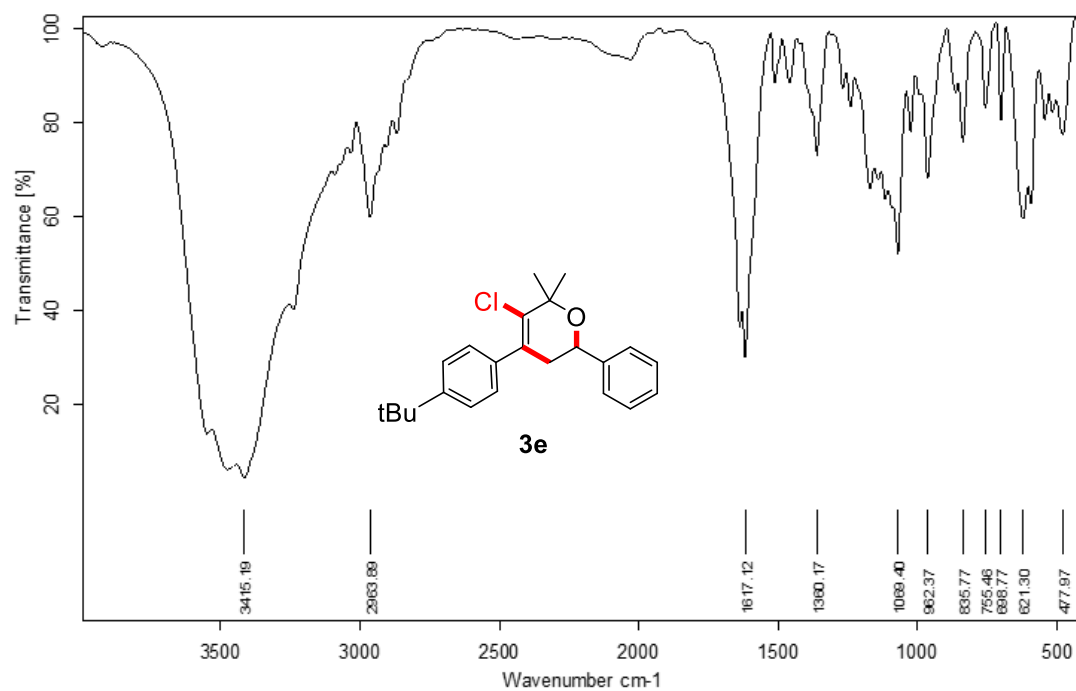
¹³C NMR of 5f

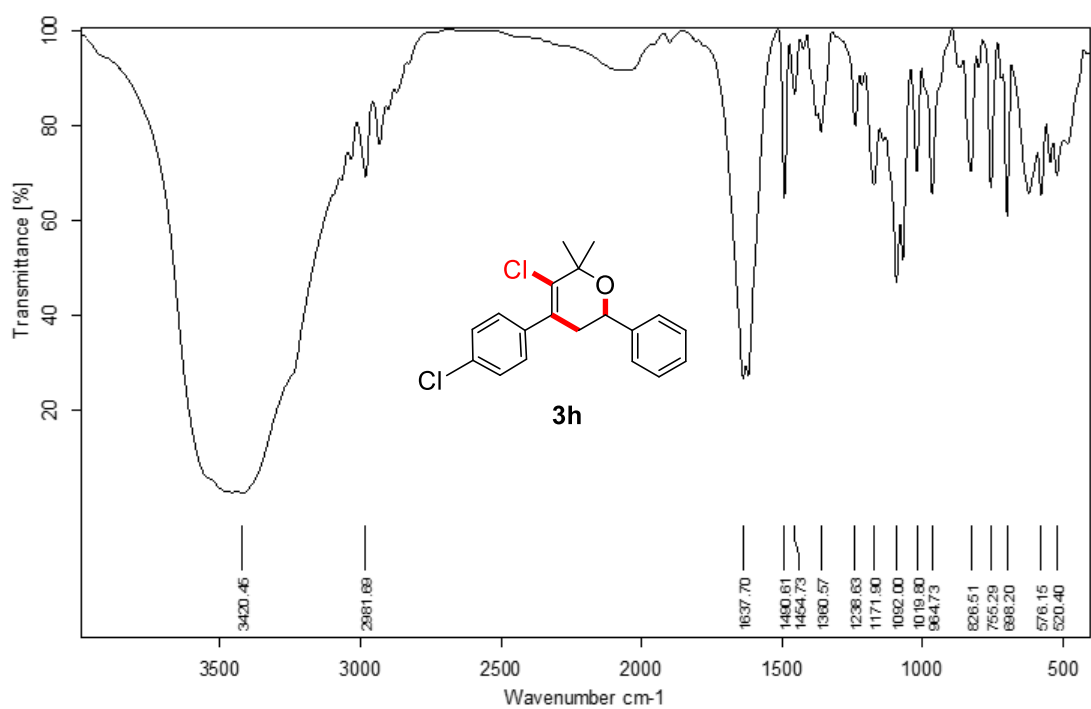
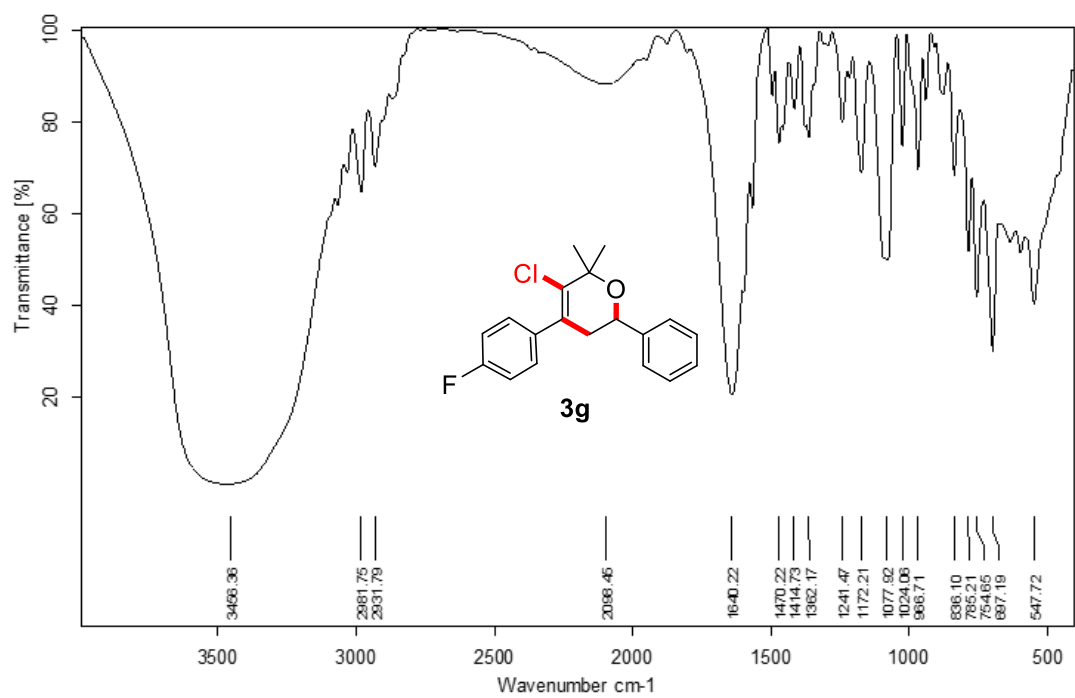


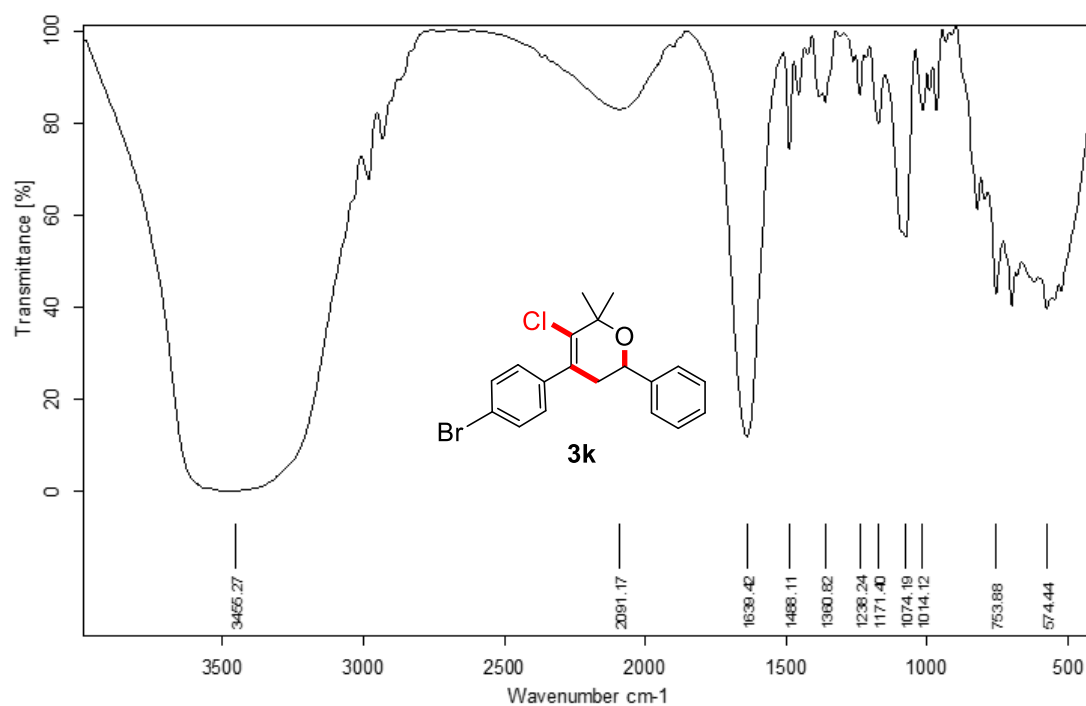
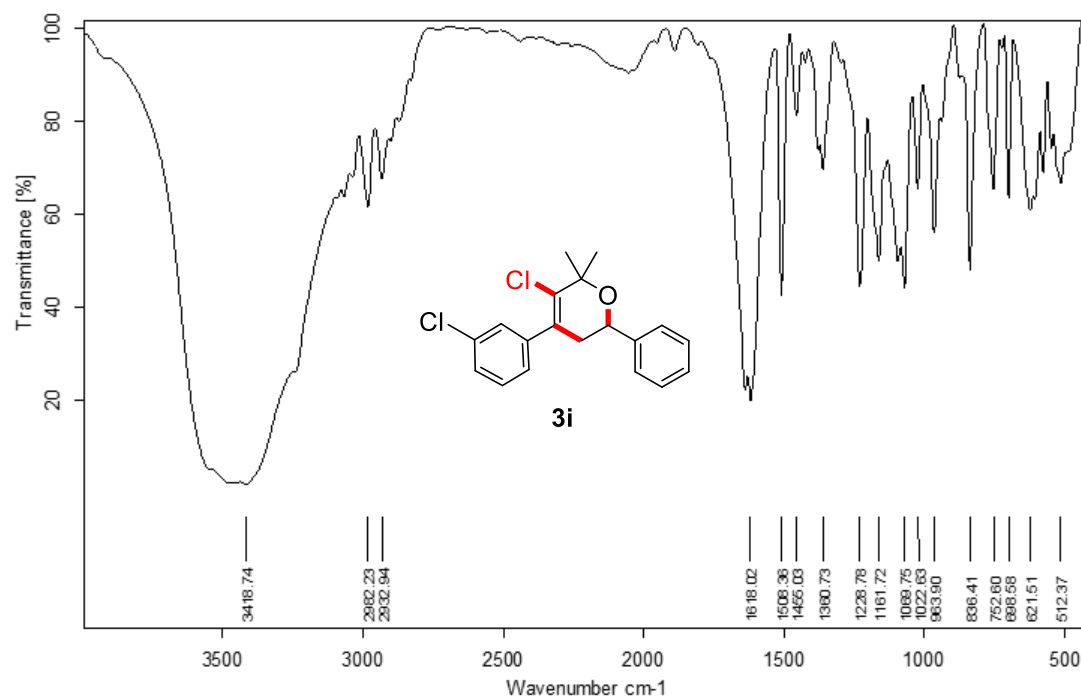
IR spectra of all compounds

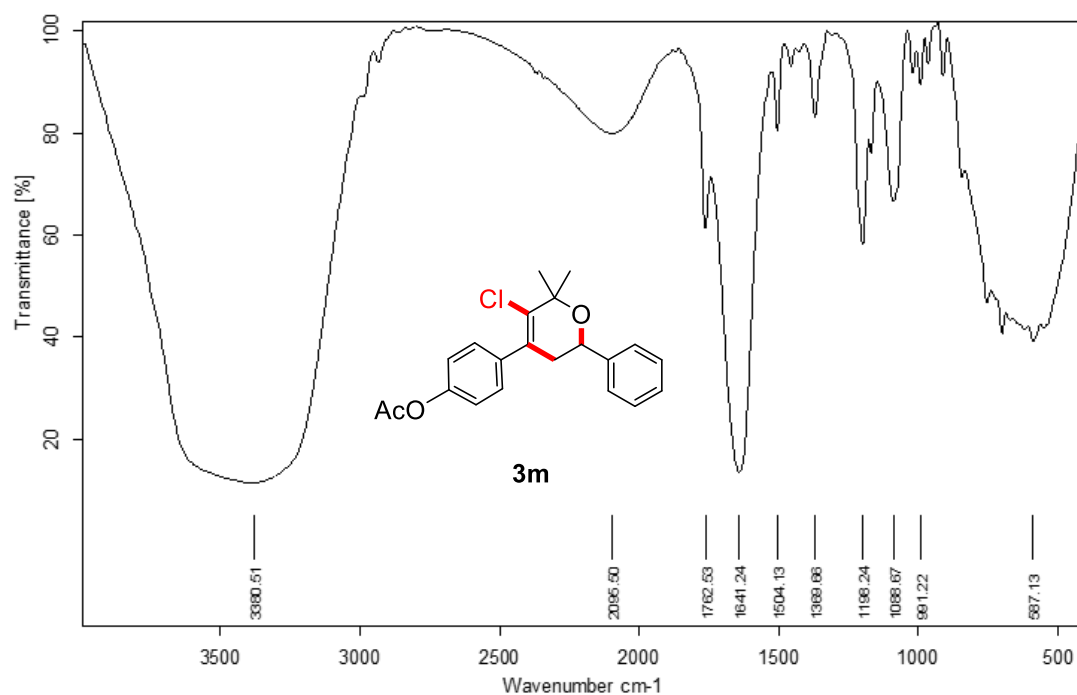
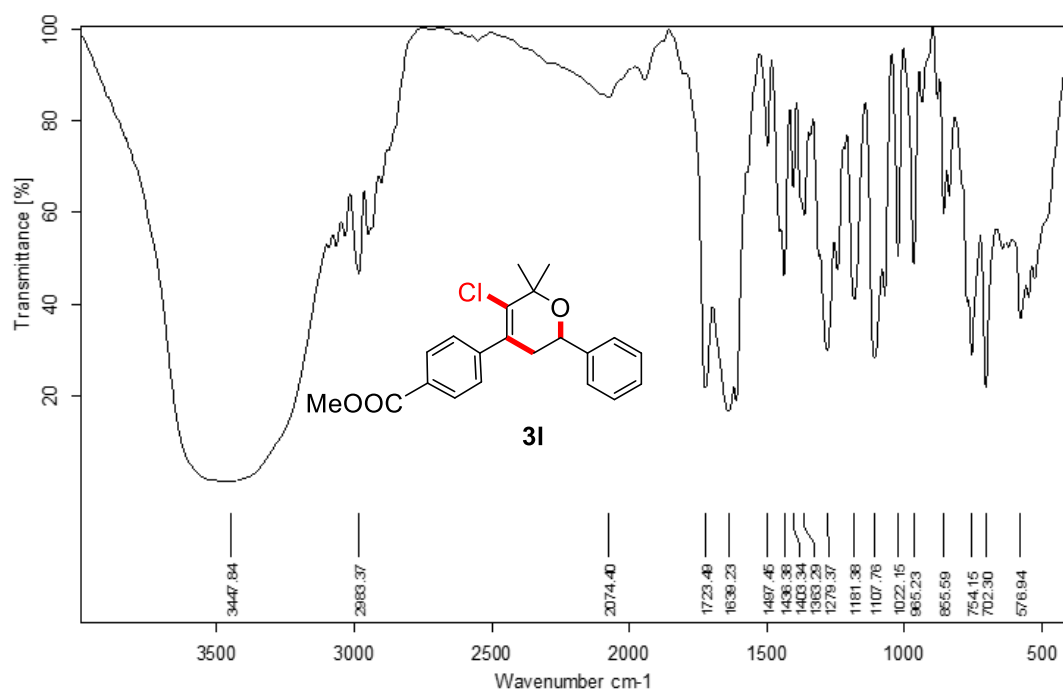


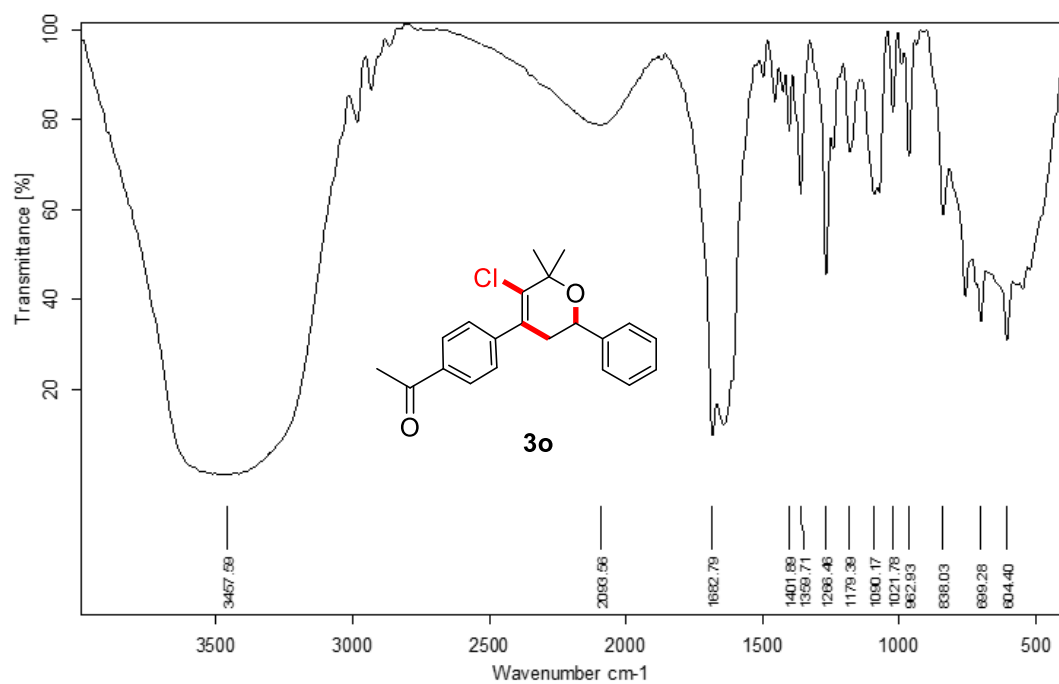
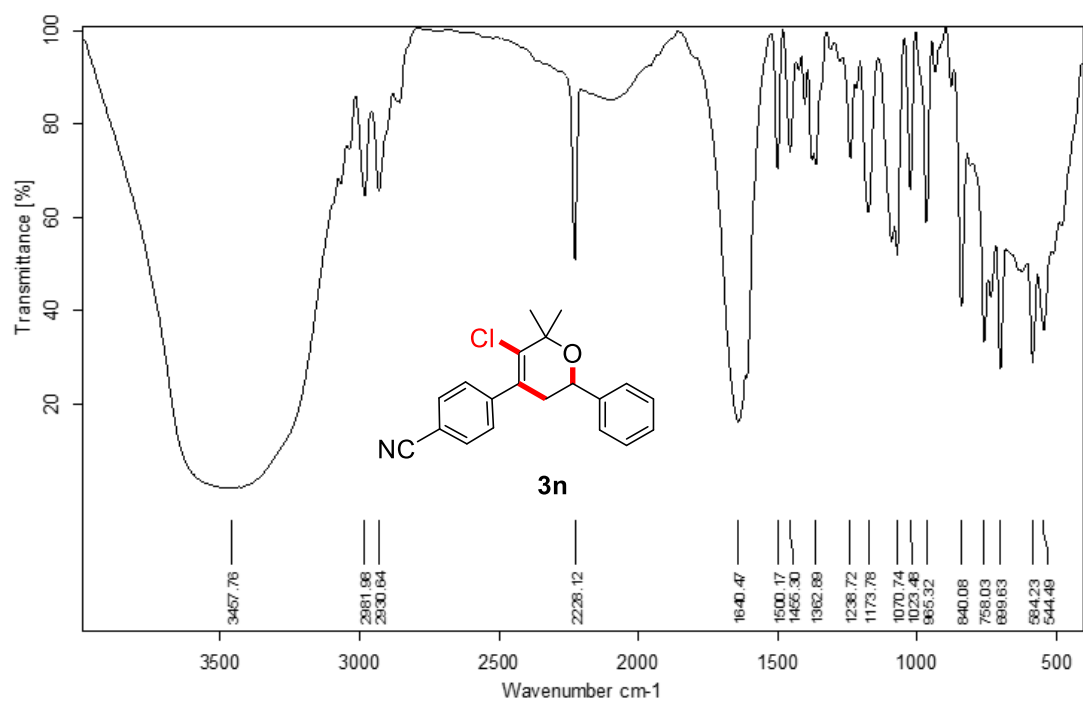


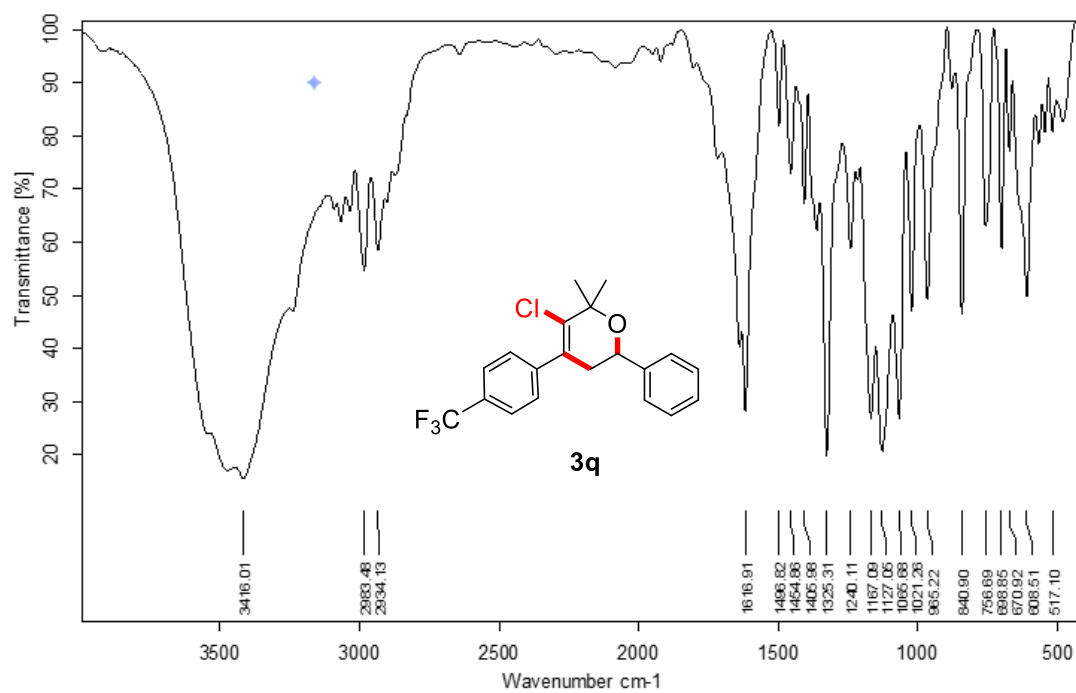
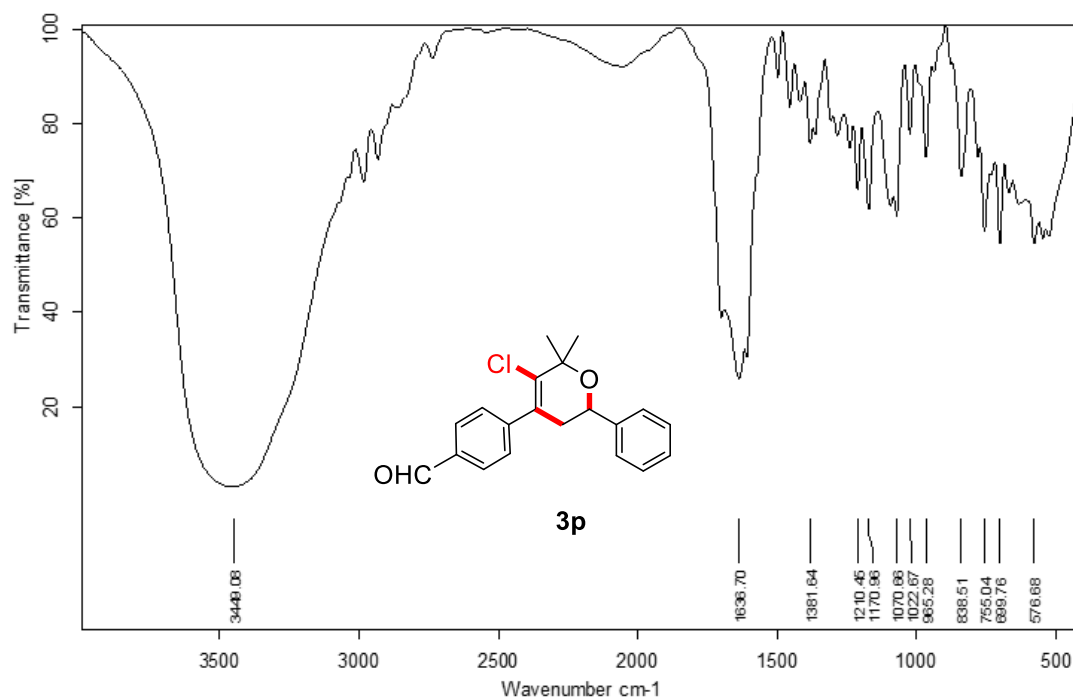


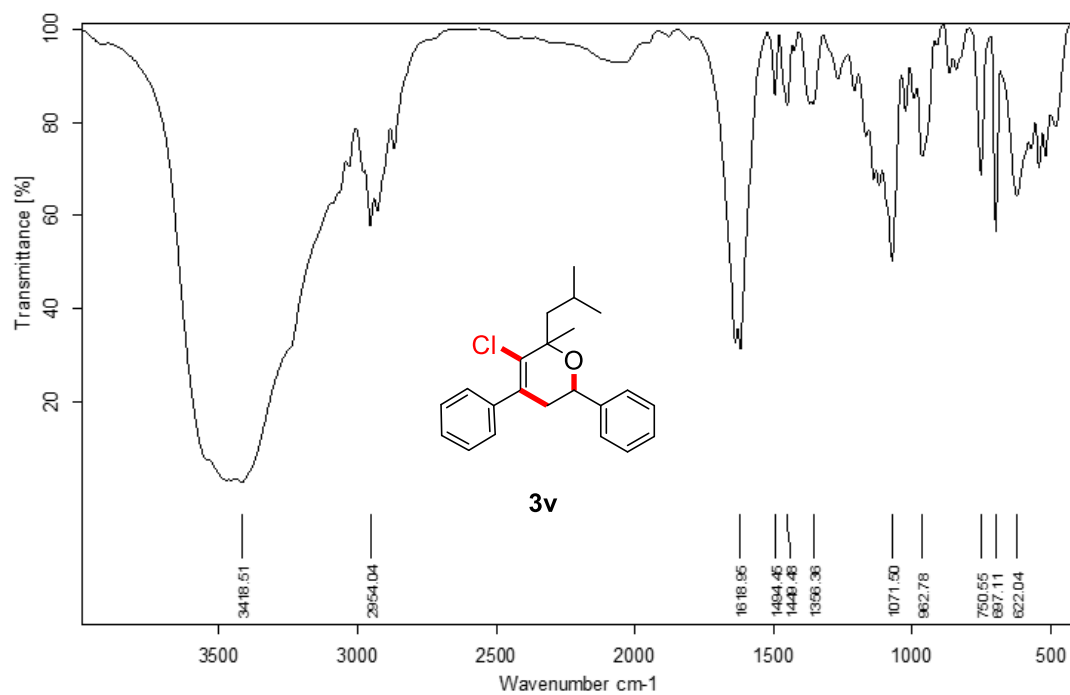
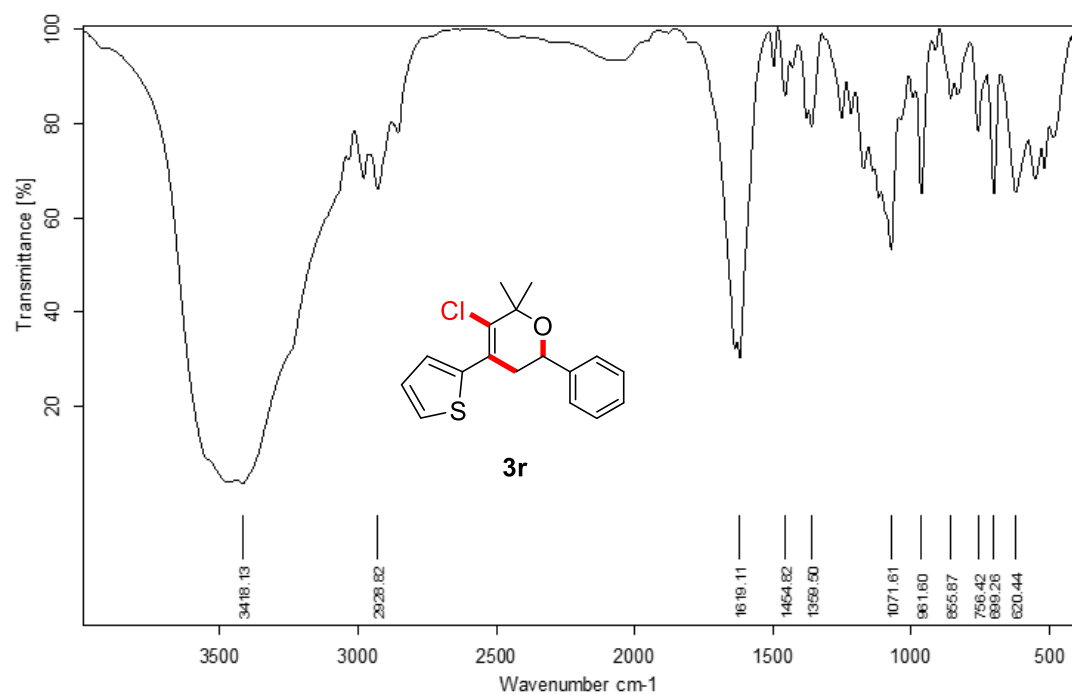


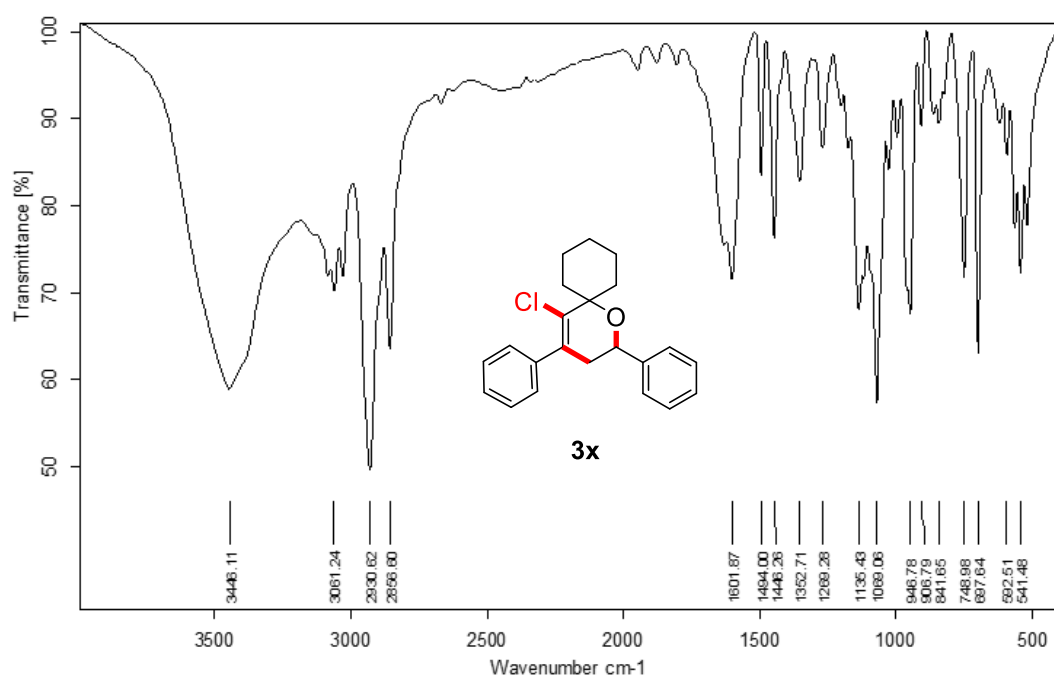
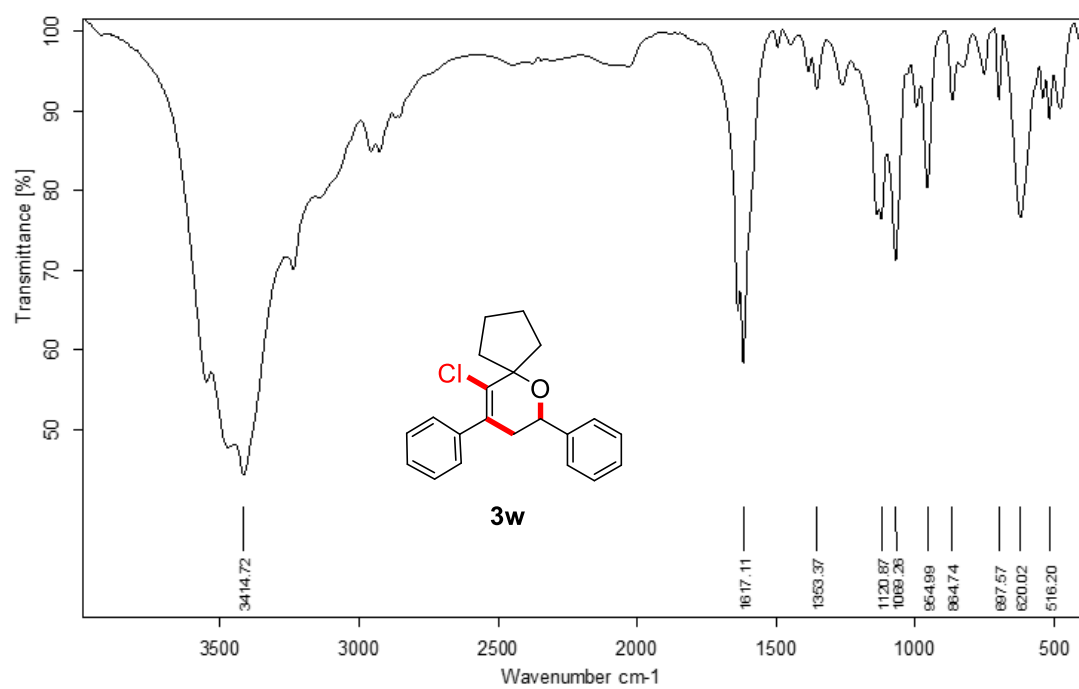


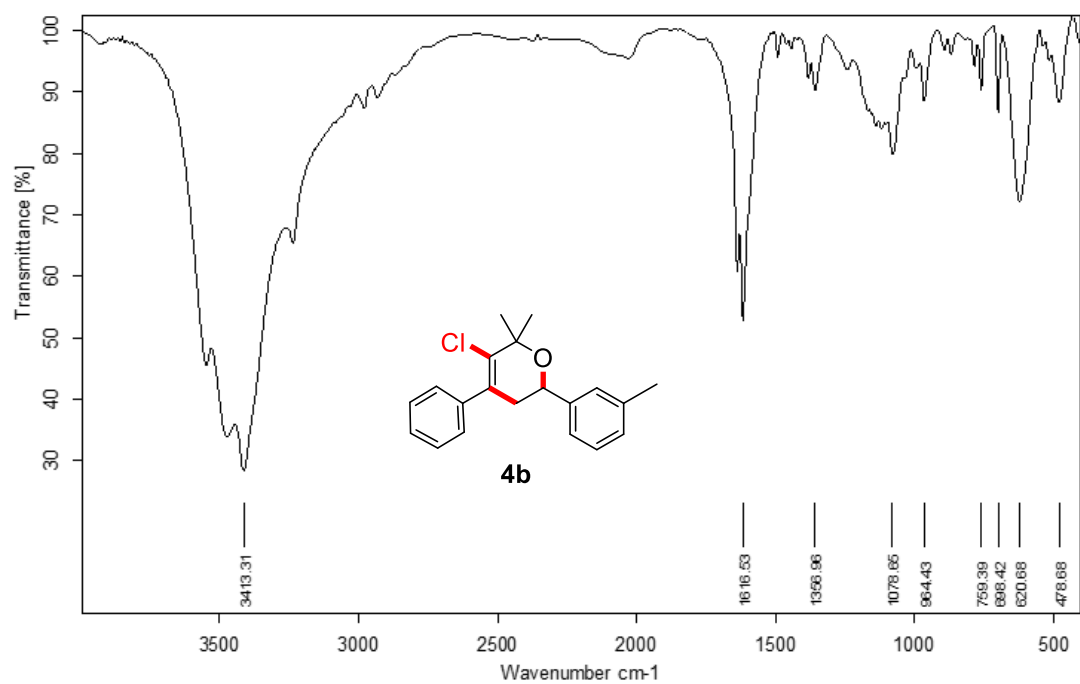
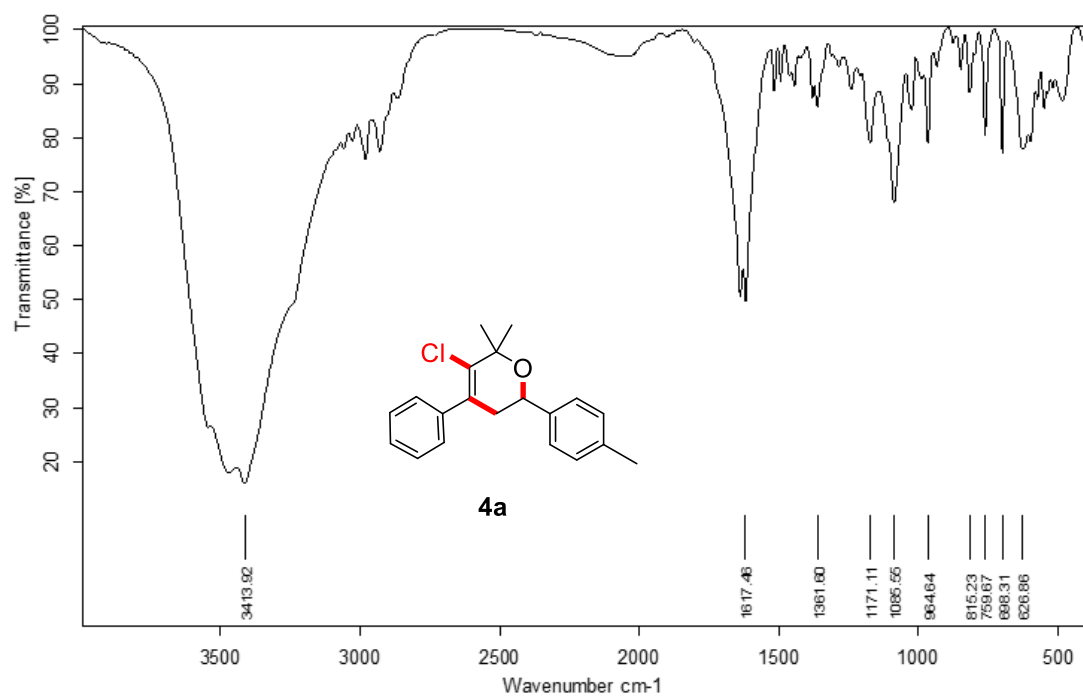


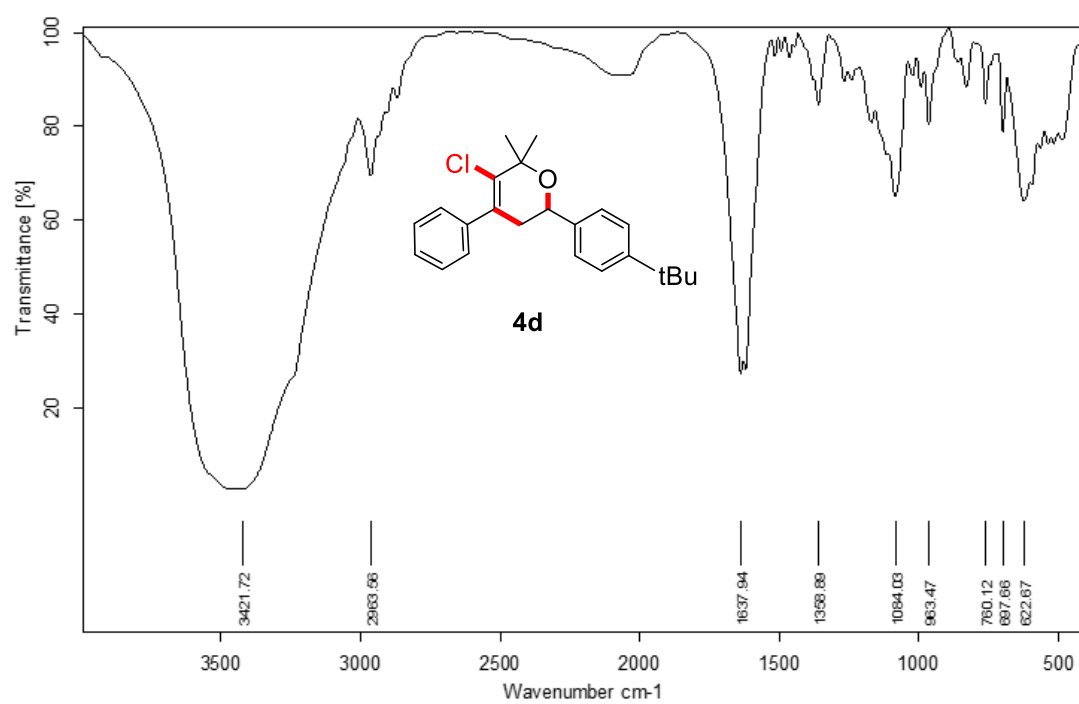
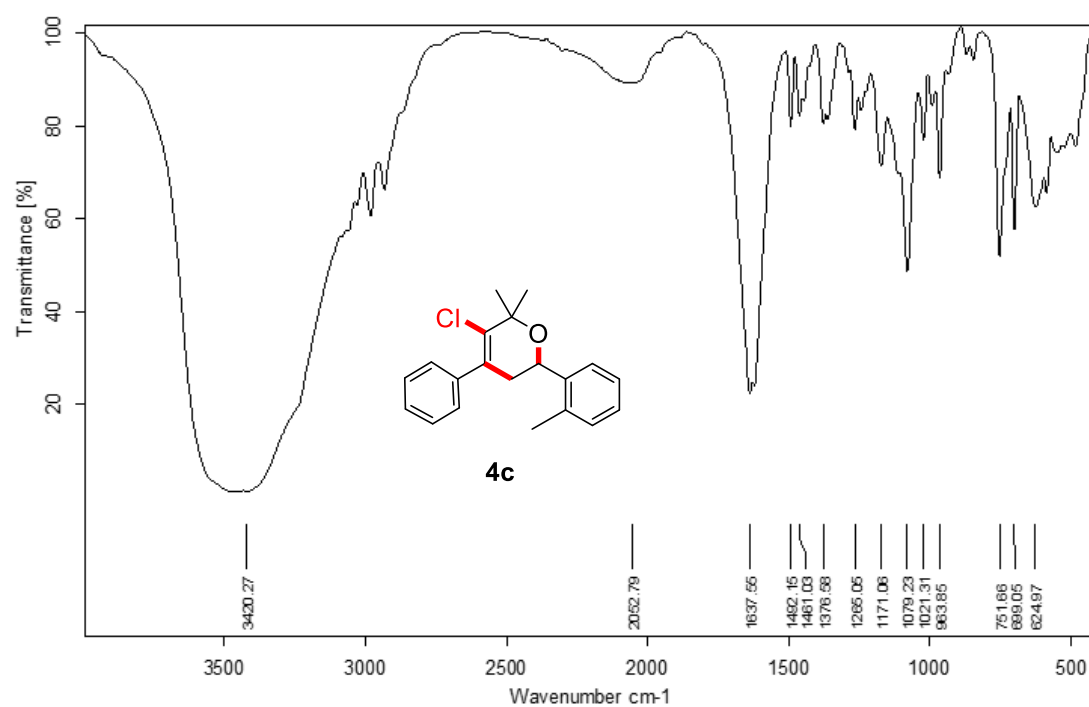


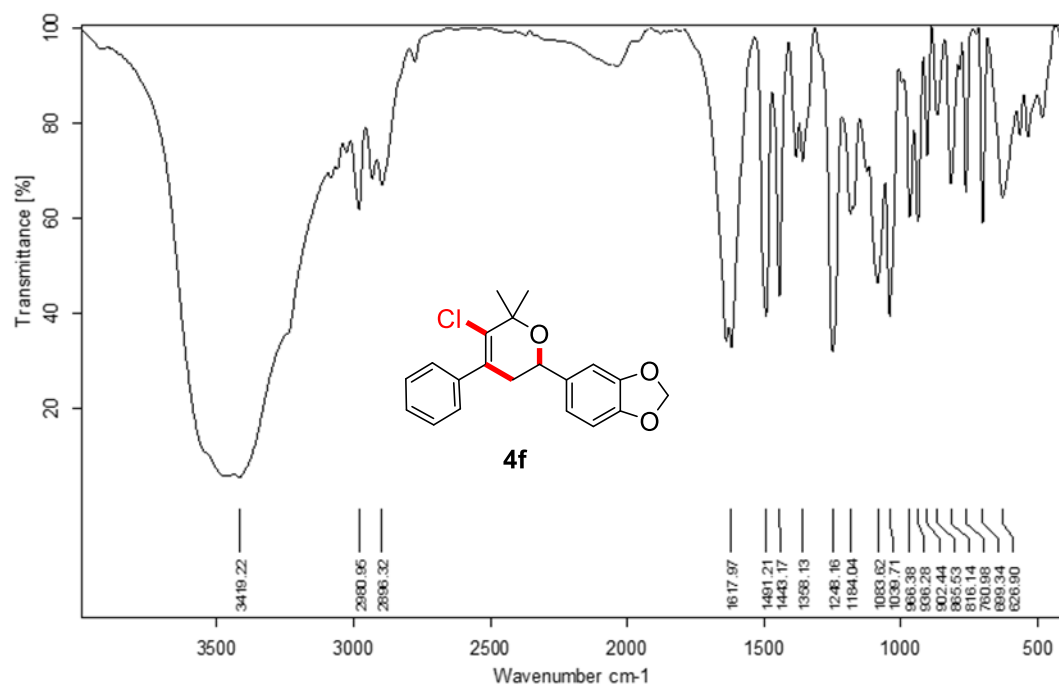
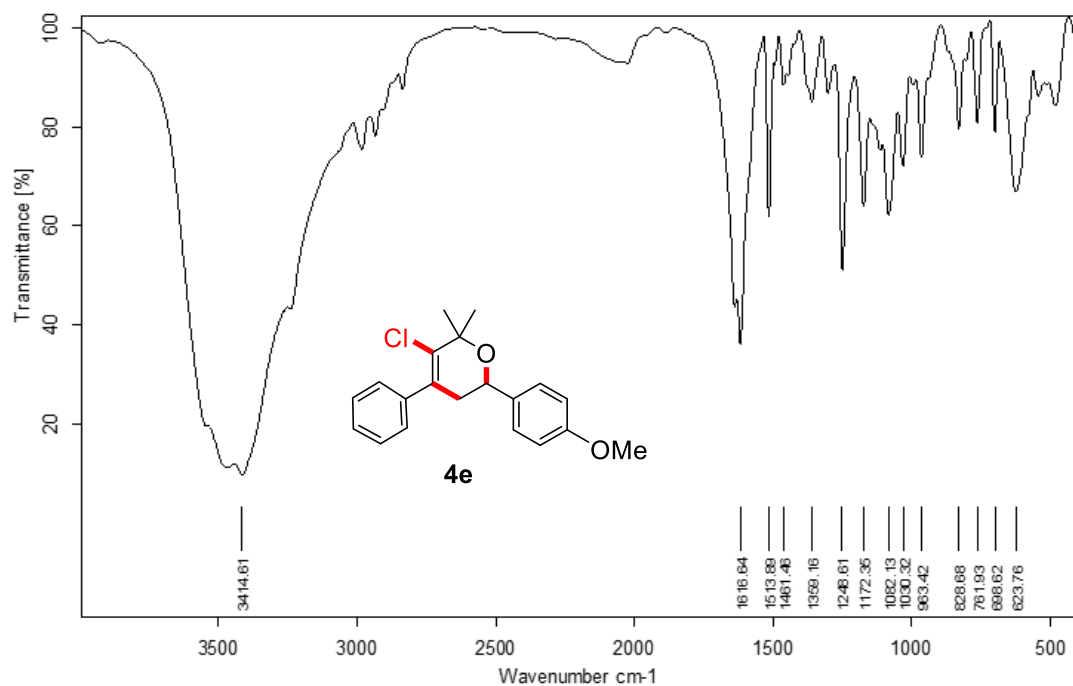


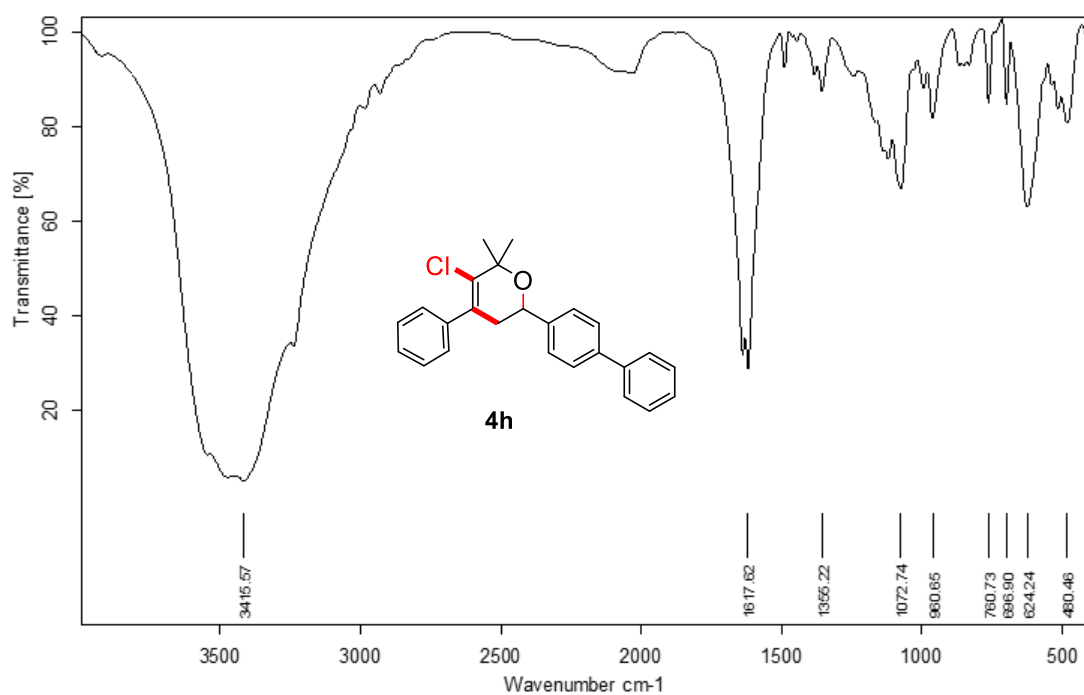
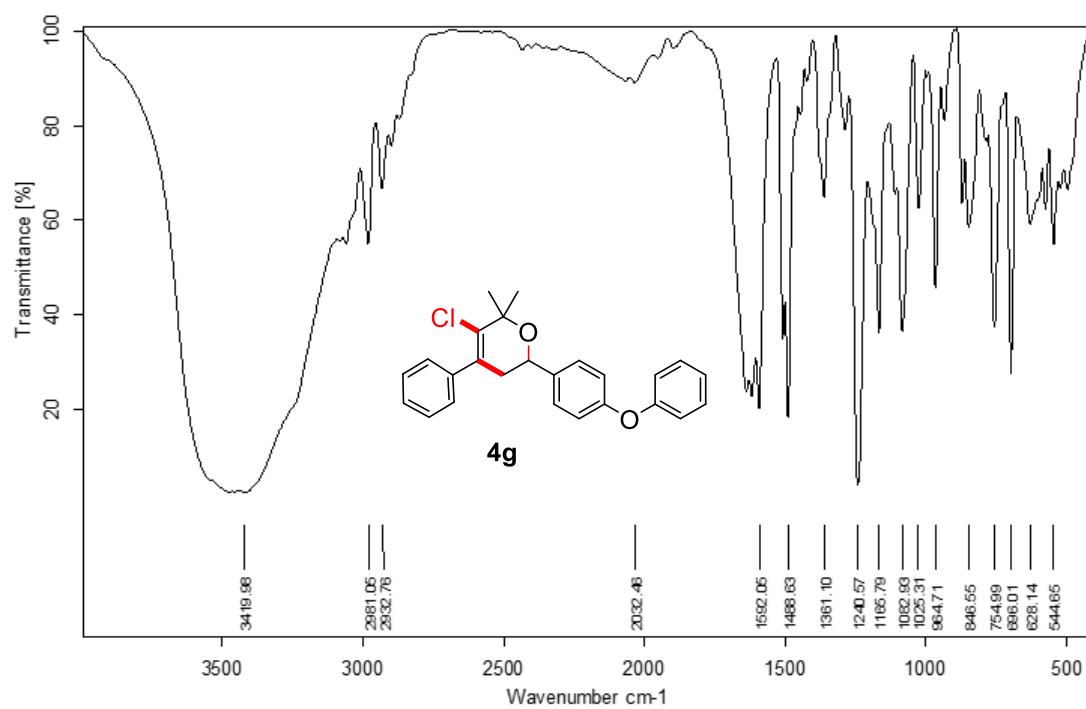


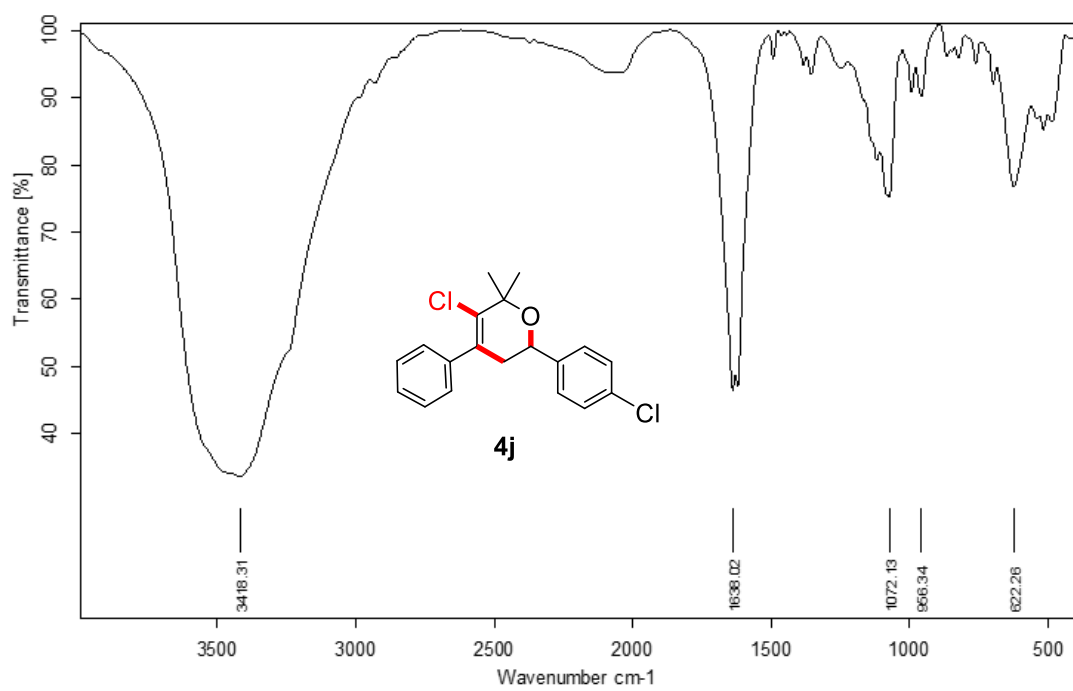
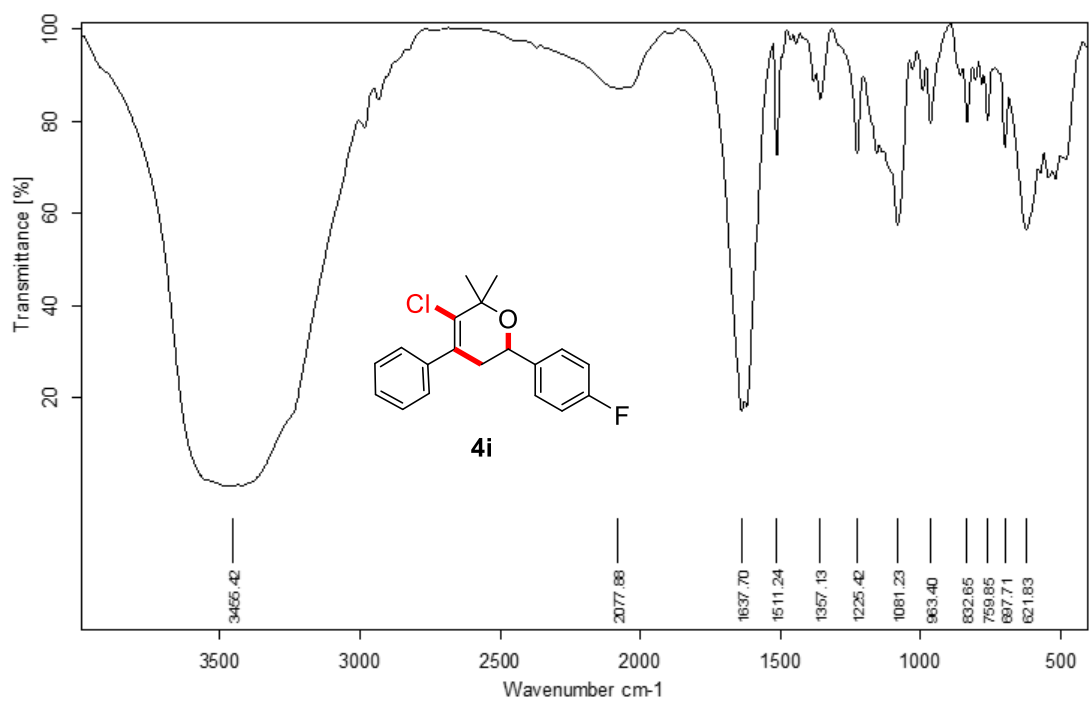


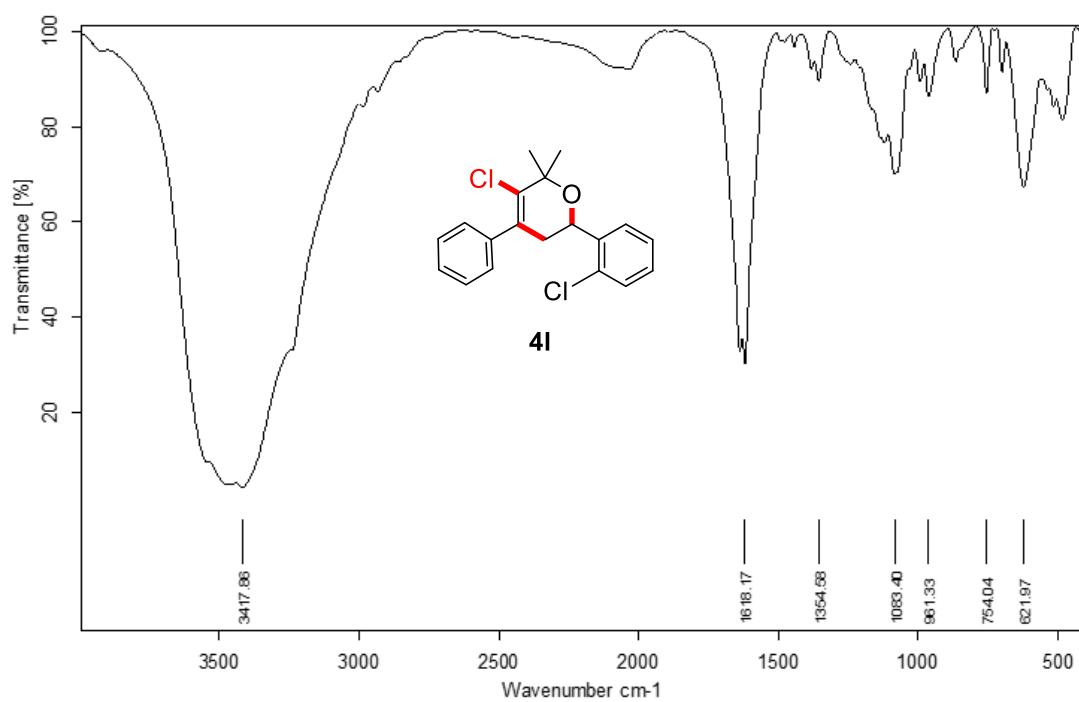
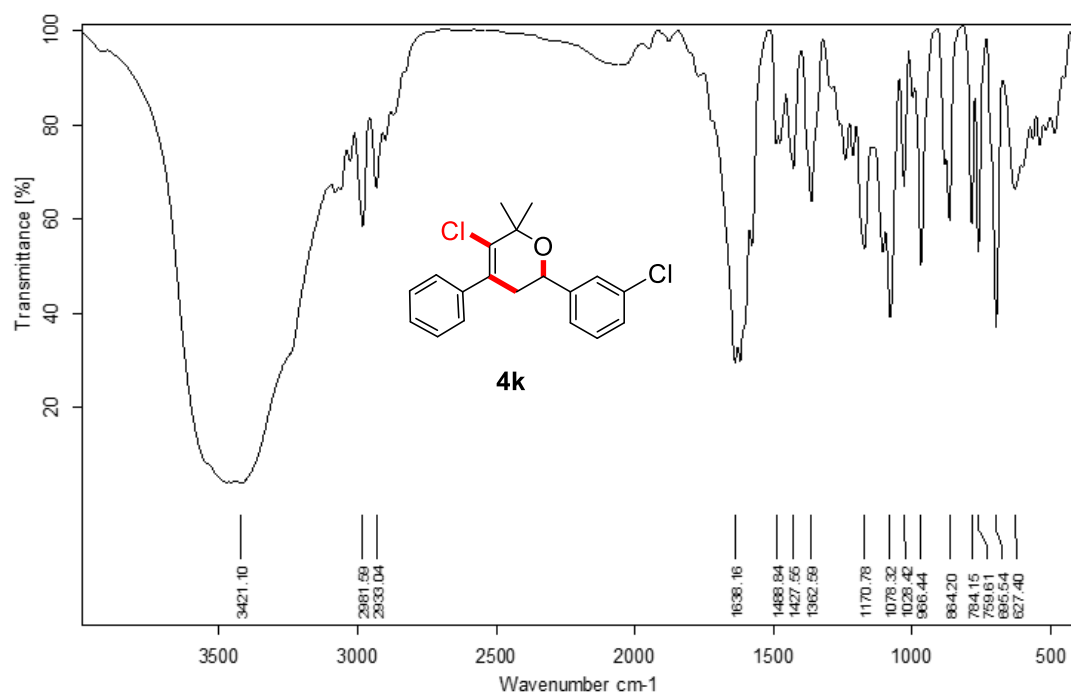


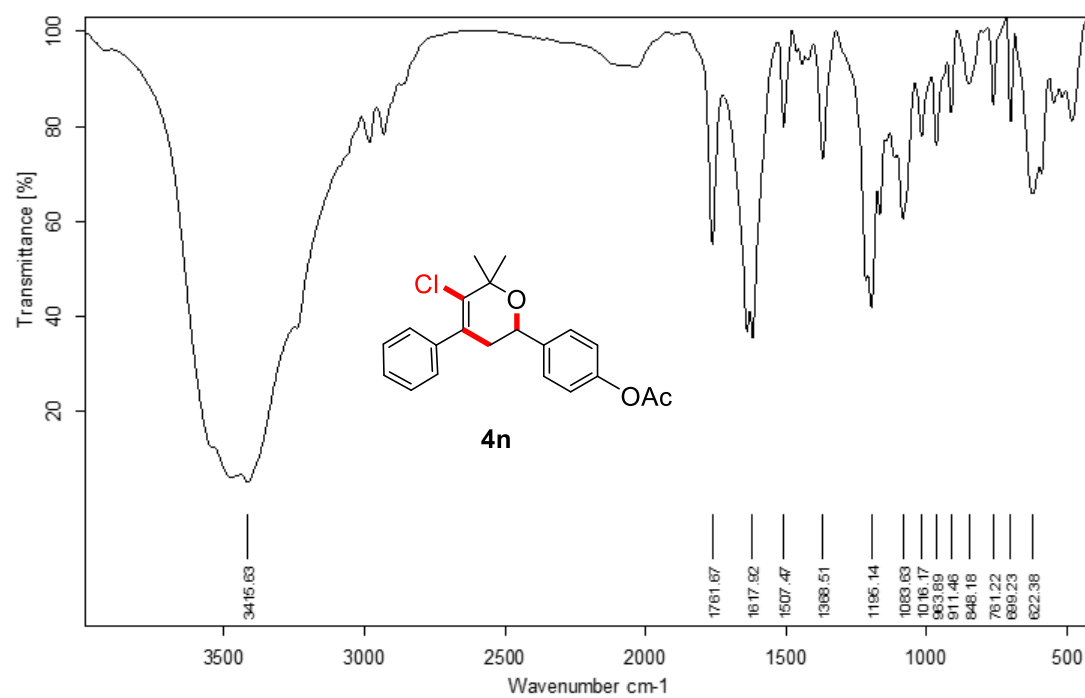
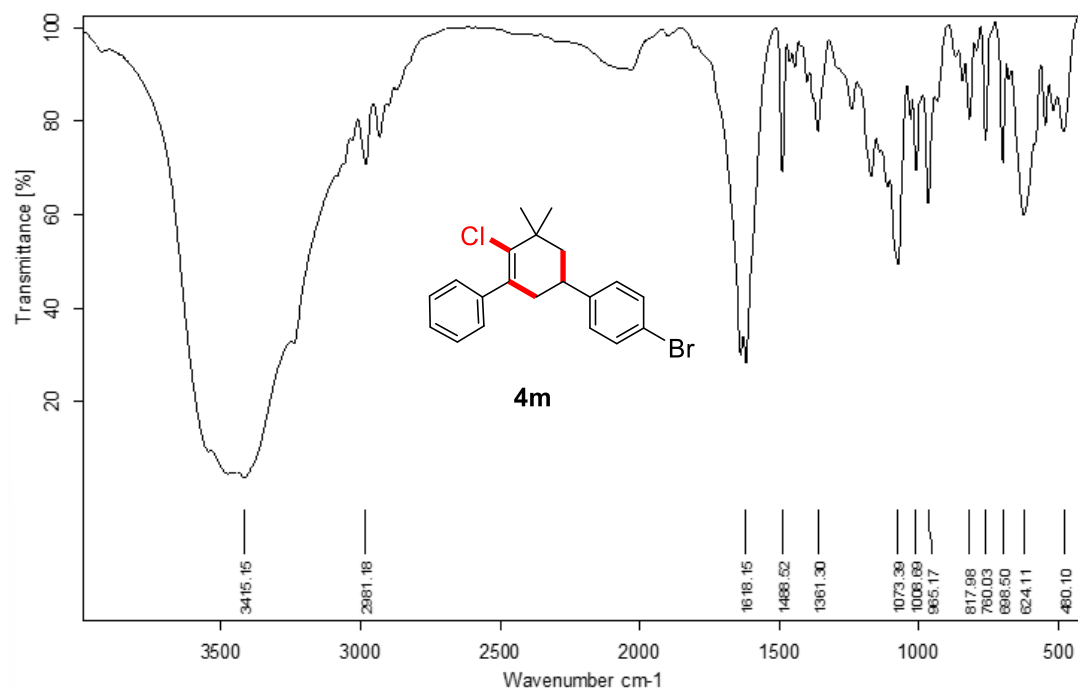


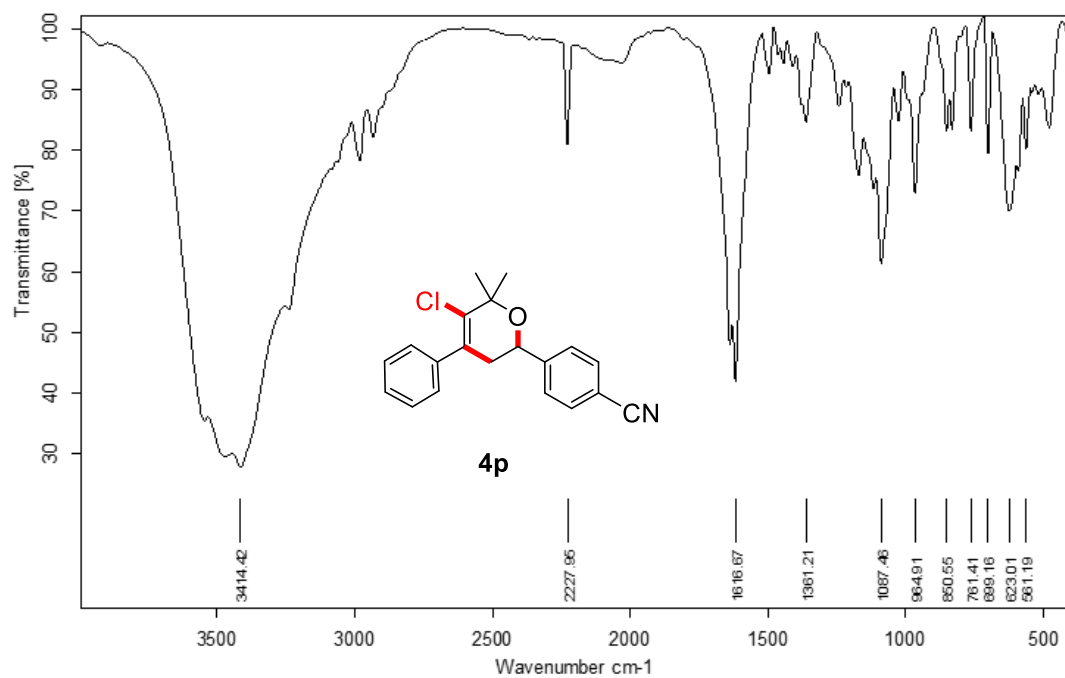
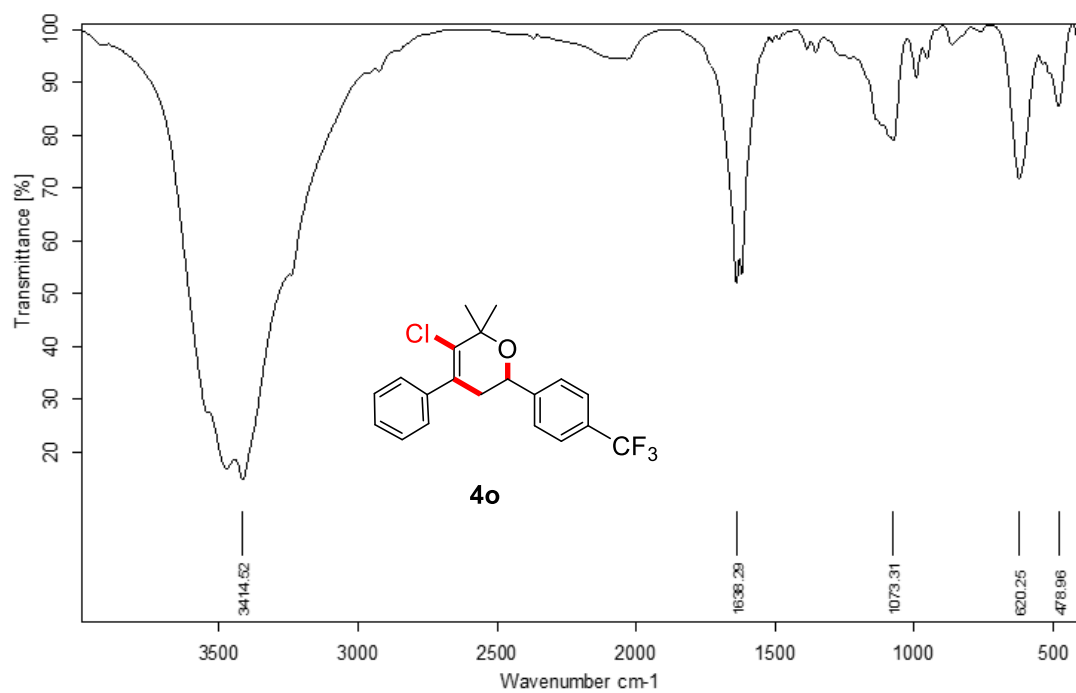


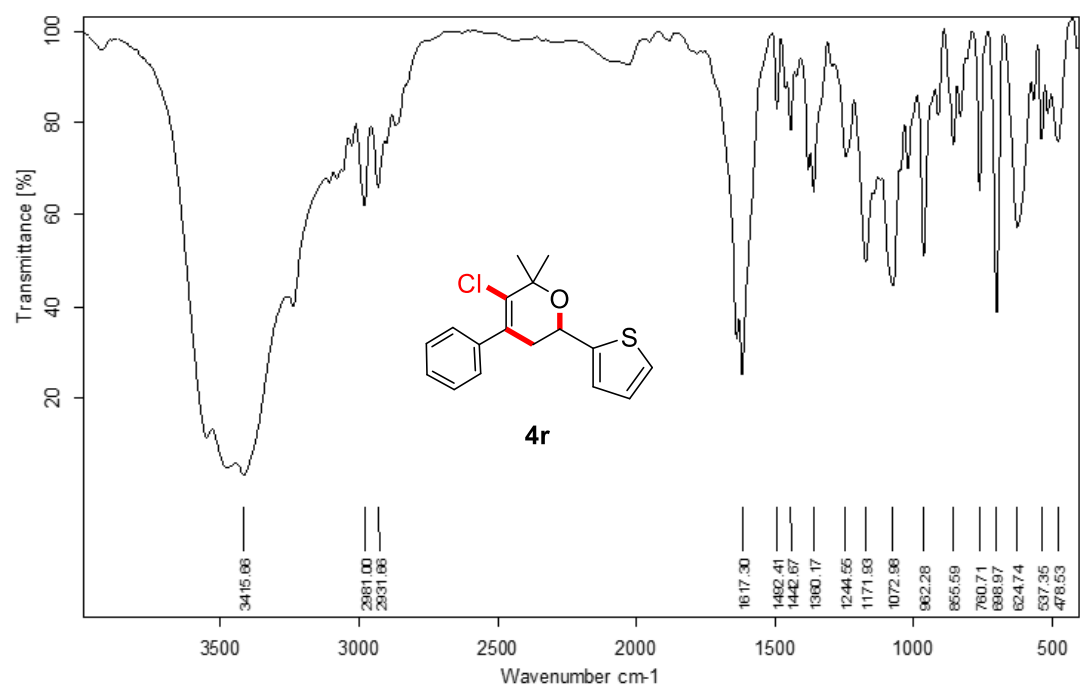
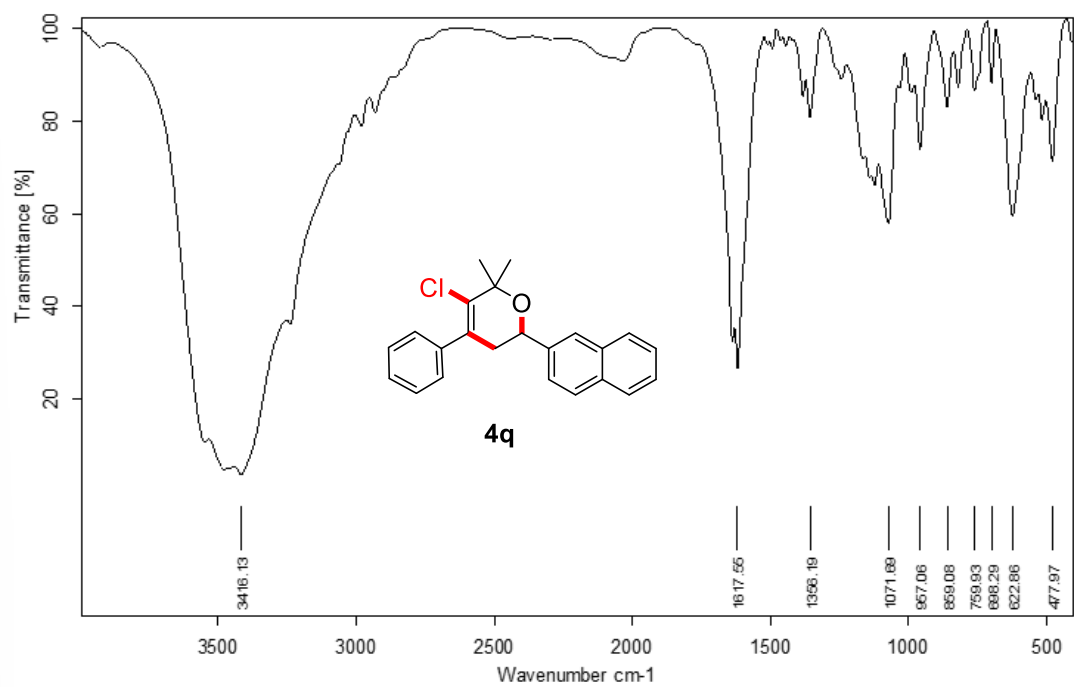


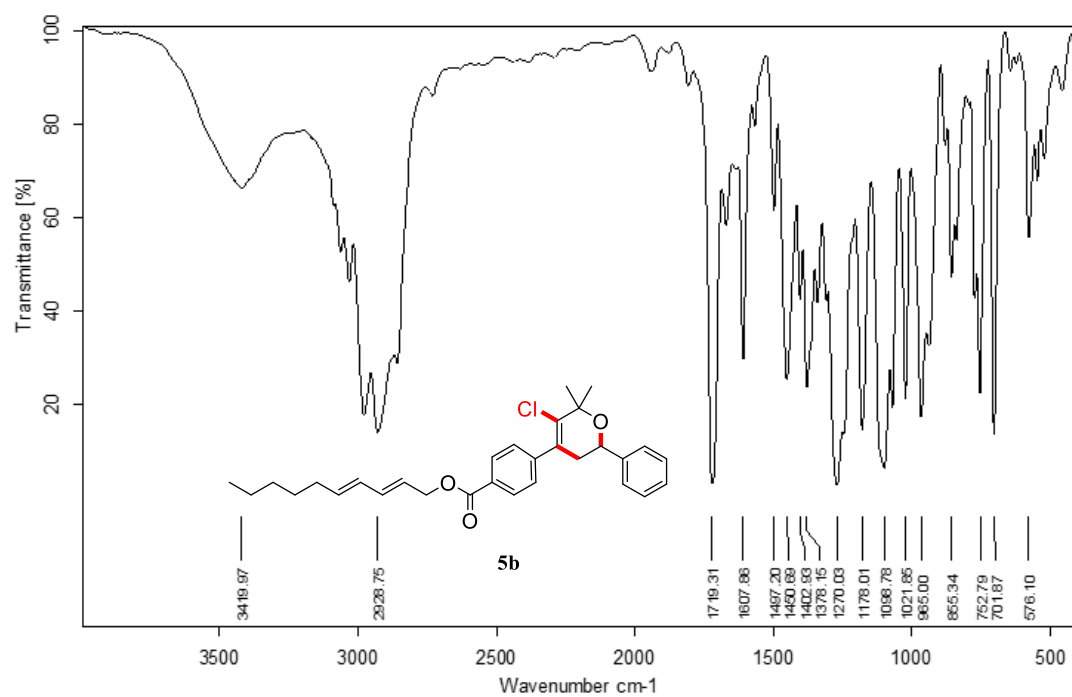
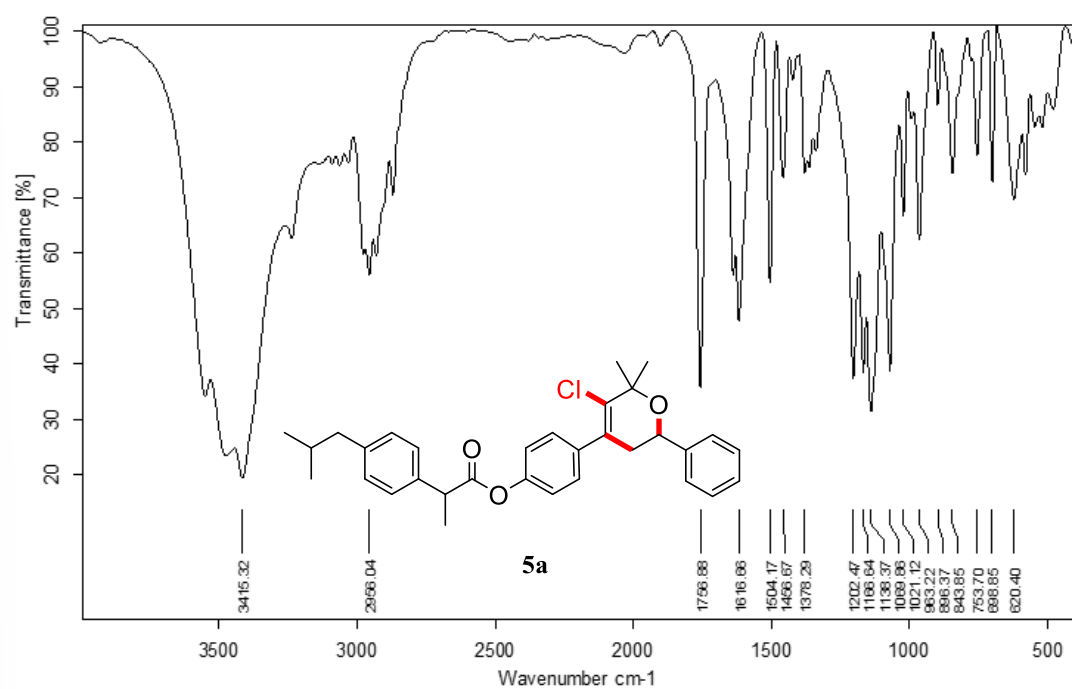


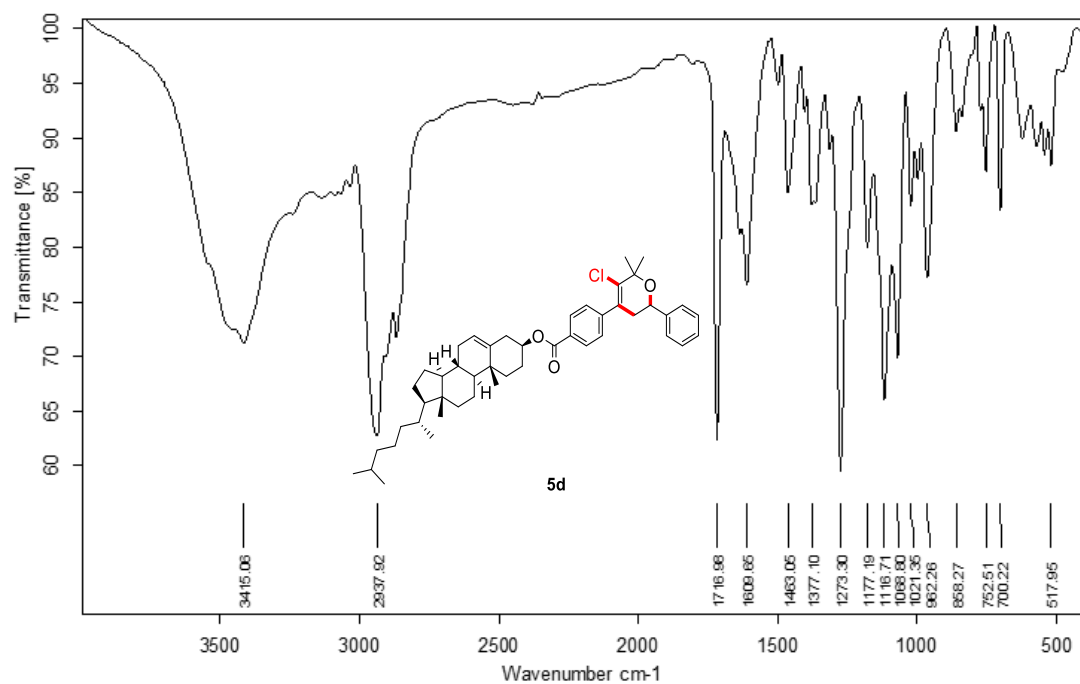
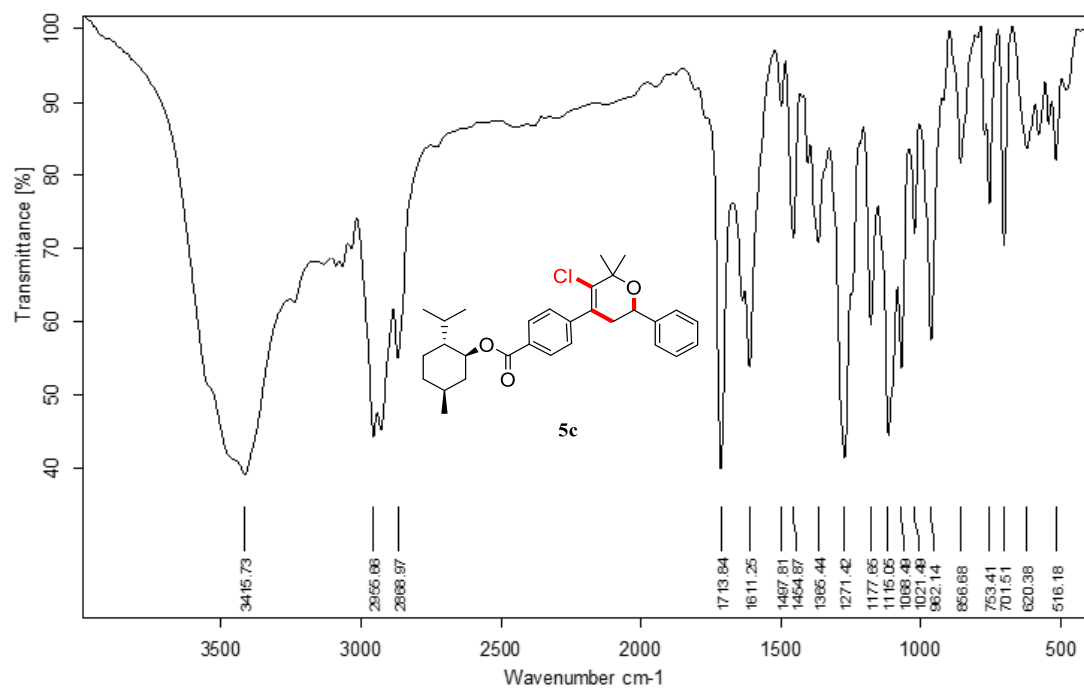


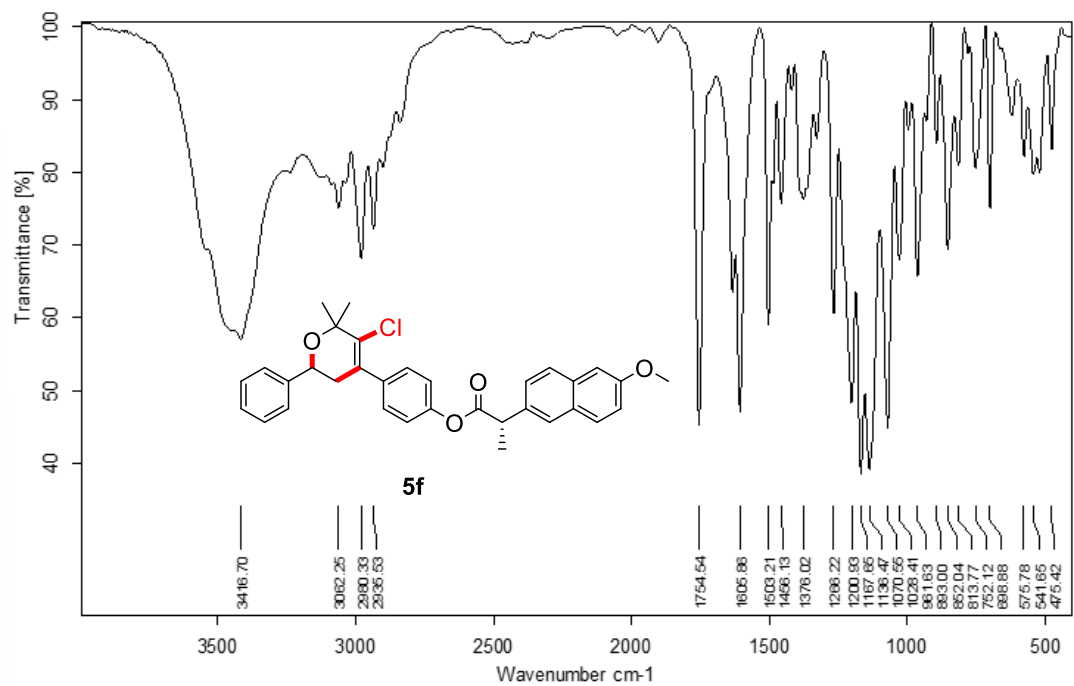
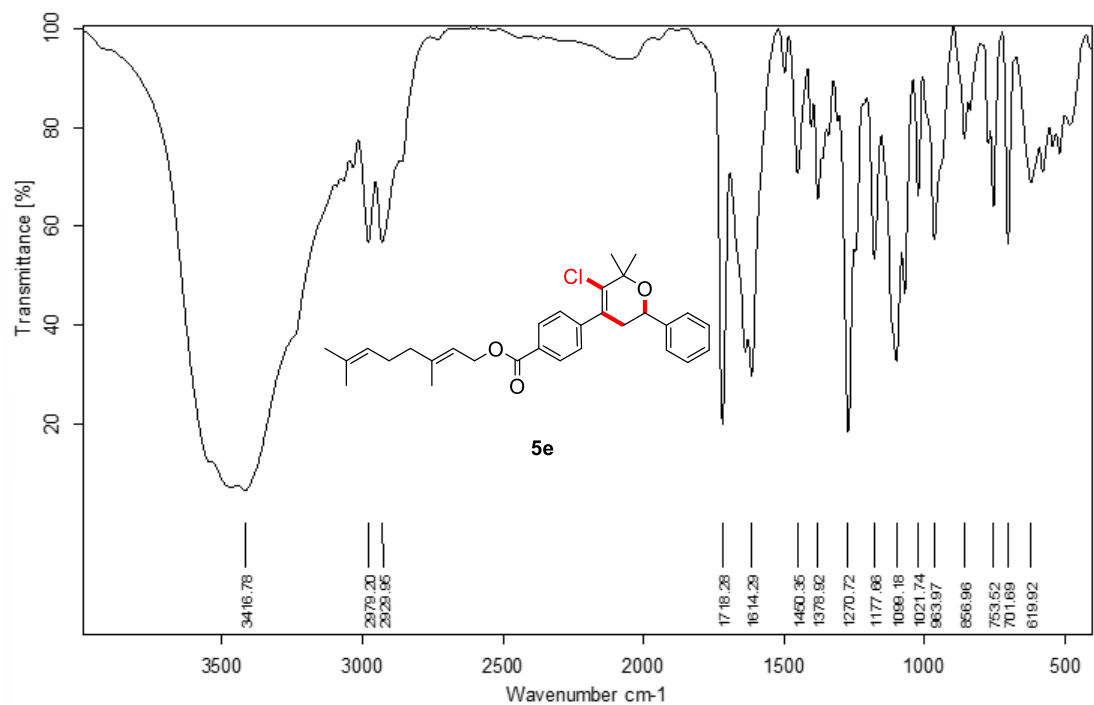




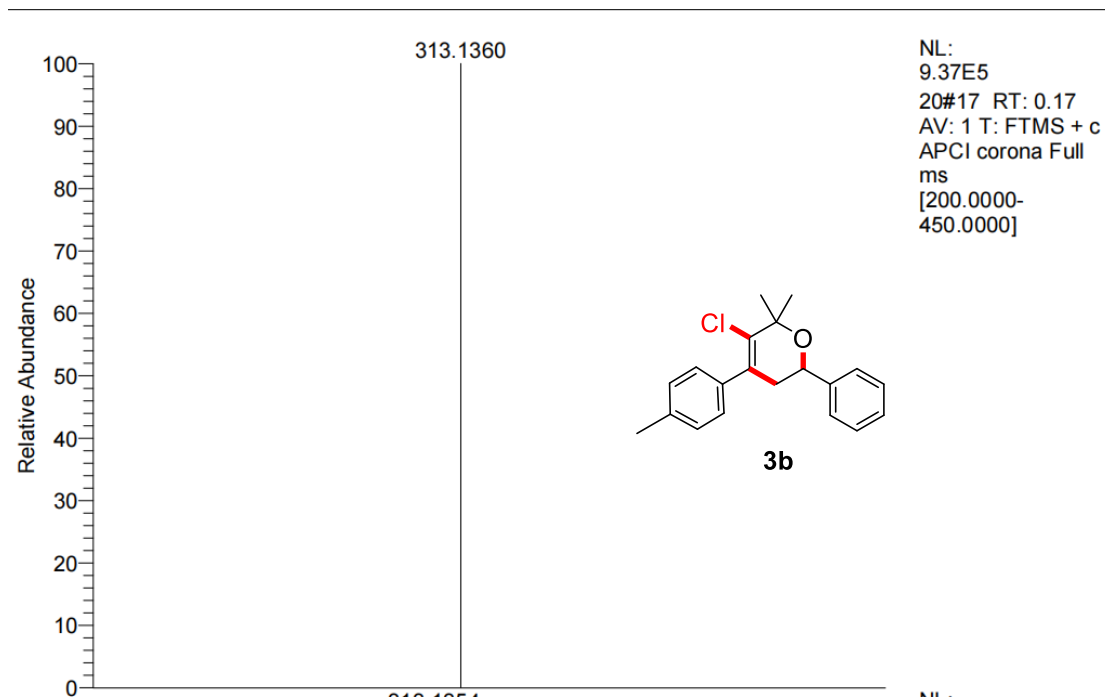
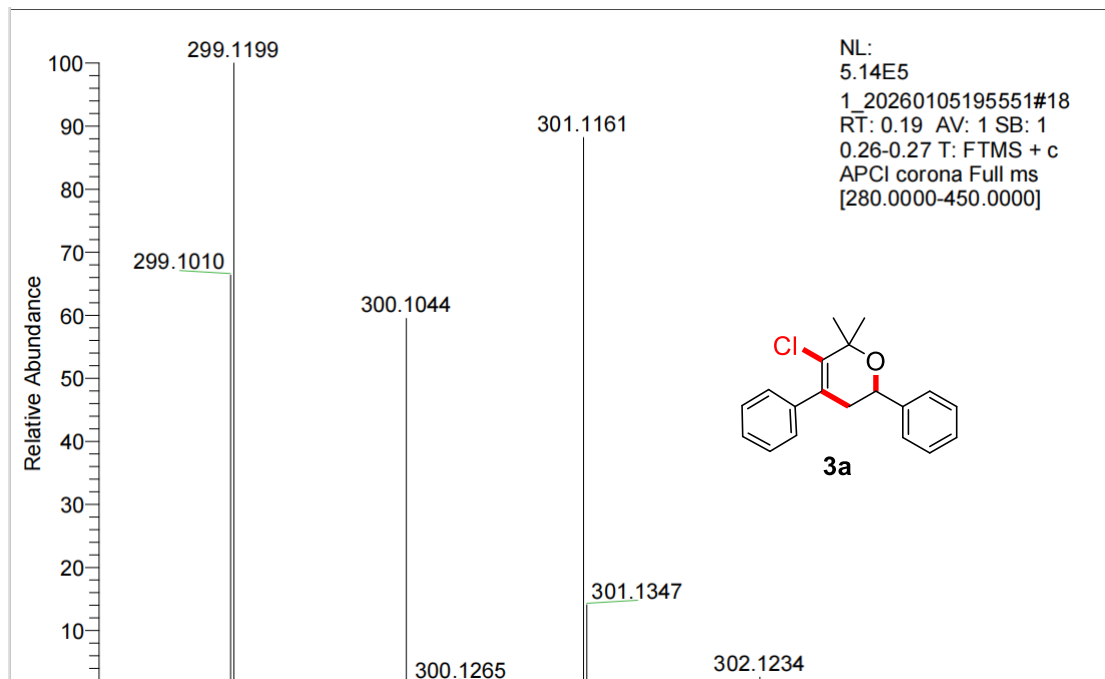


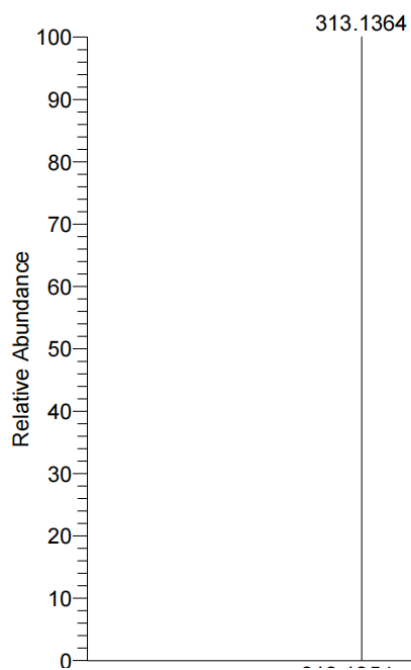




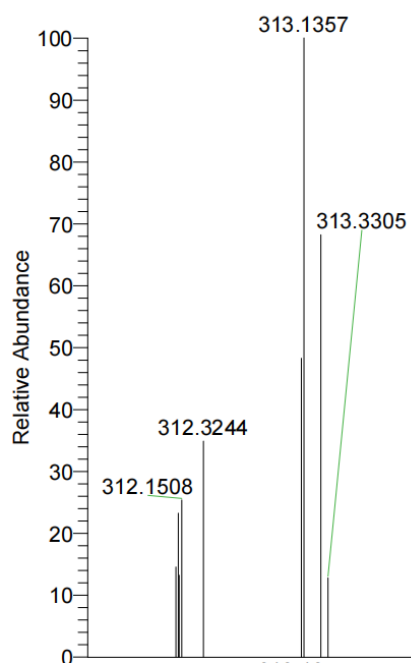
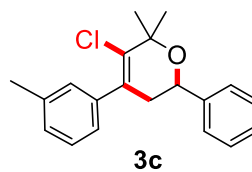


HRMS spectra of all compounds

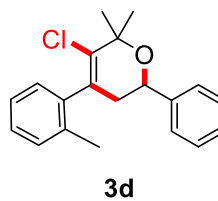


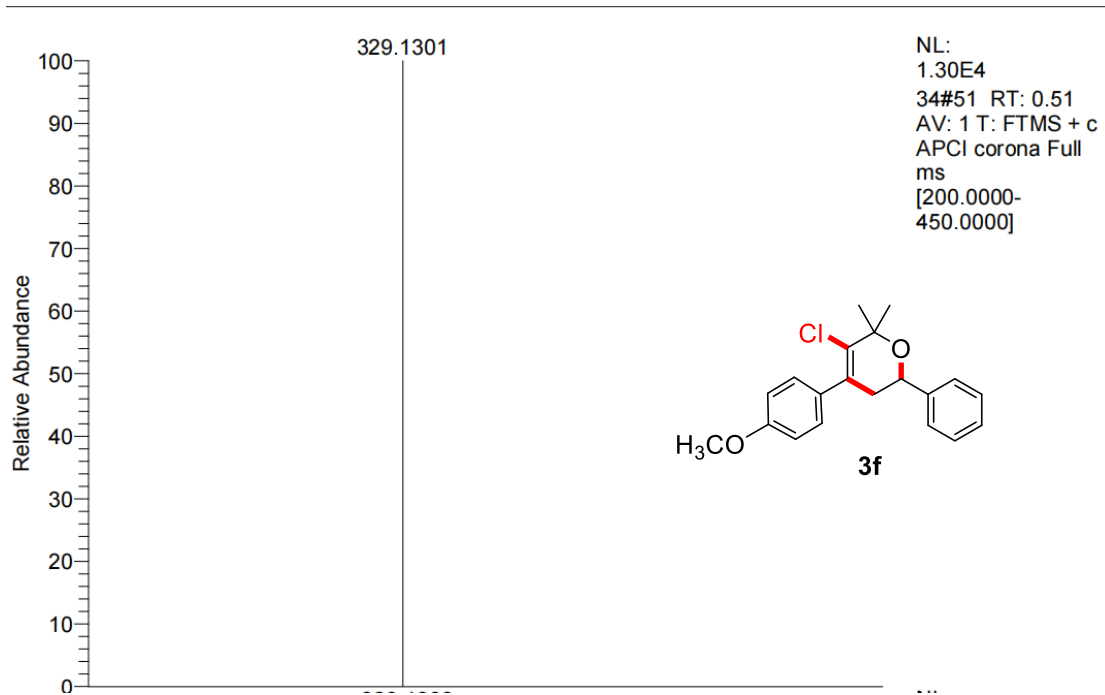
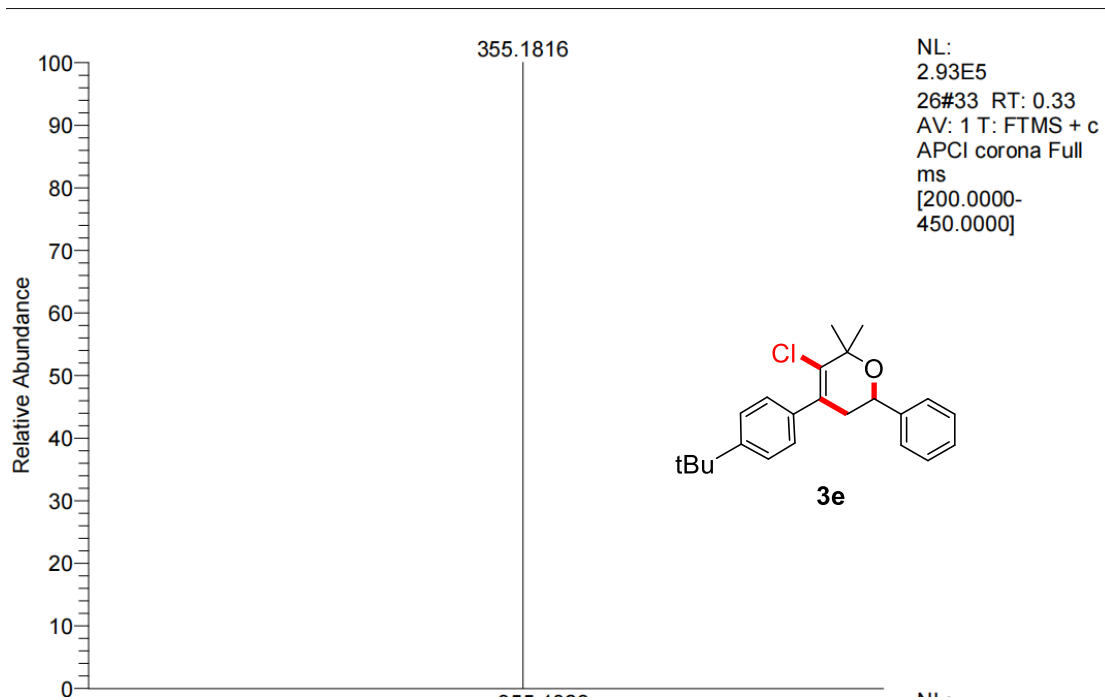


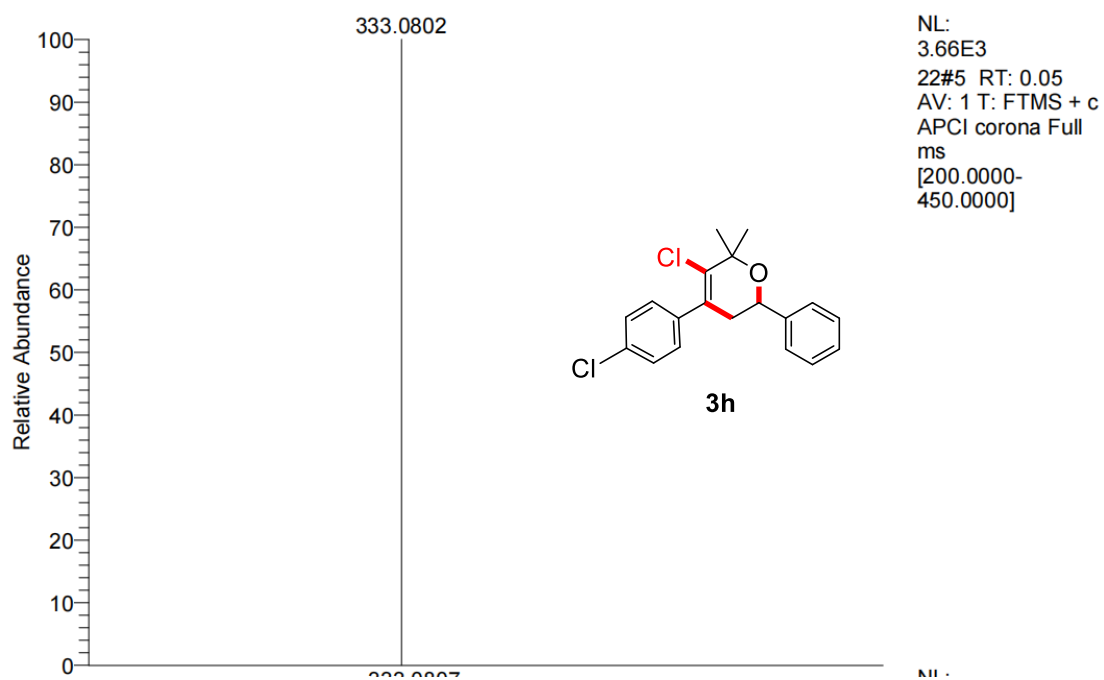
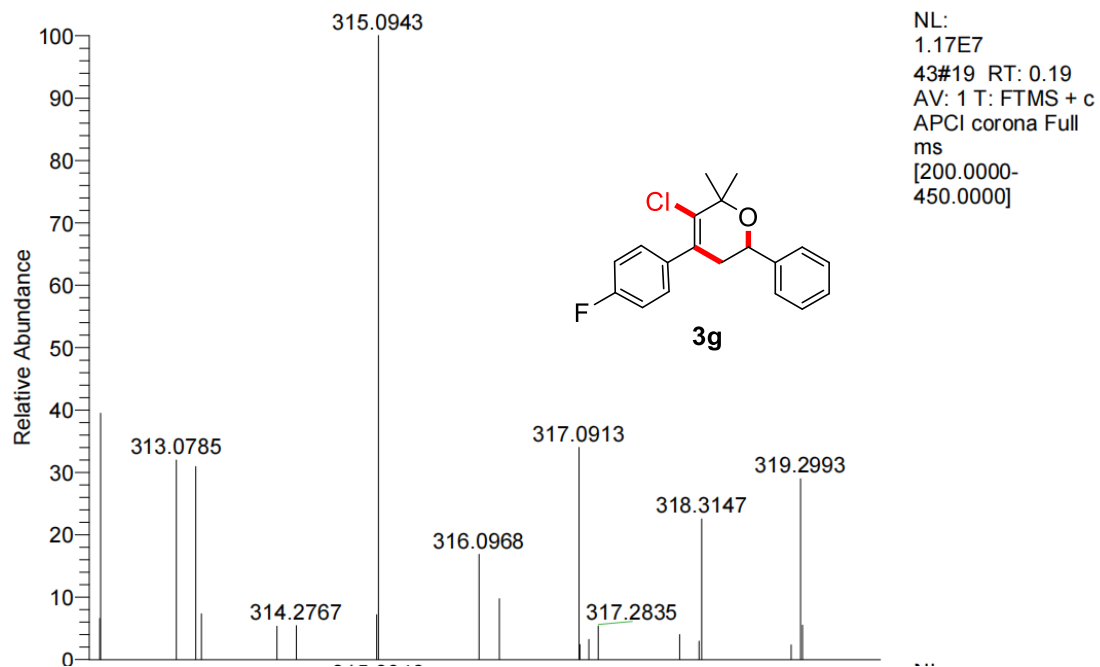
NL:
3.92E6
42#19 RT: 0.19
AV: 1 T: FTMS + c
APCI corona Full
ms
[200.0000-
450.0000]

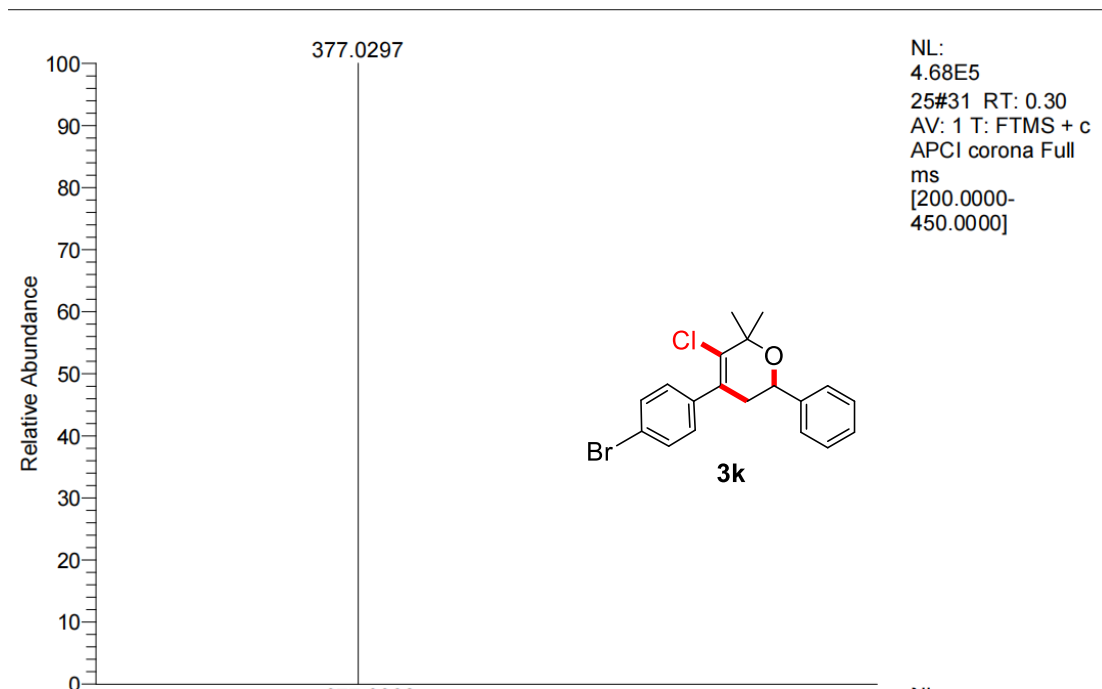
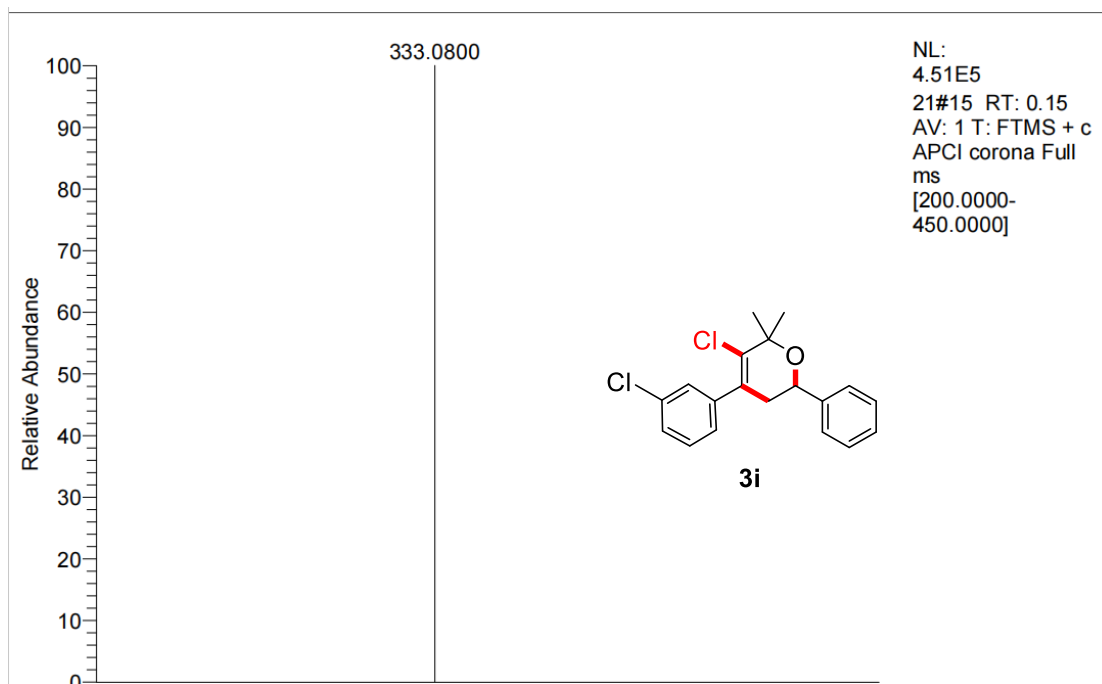


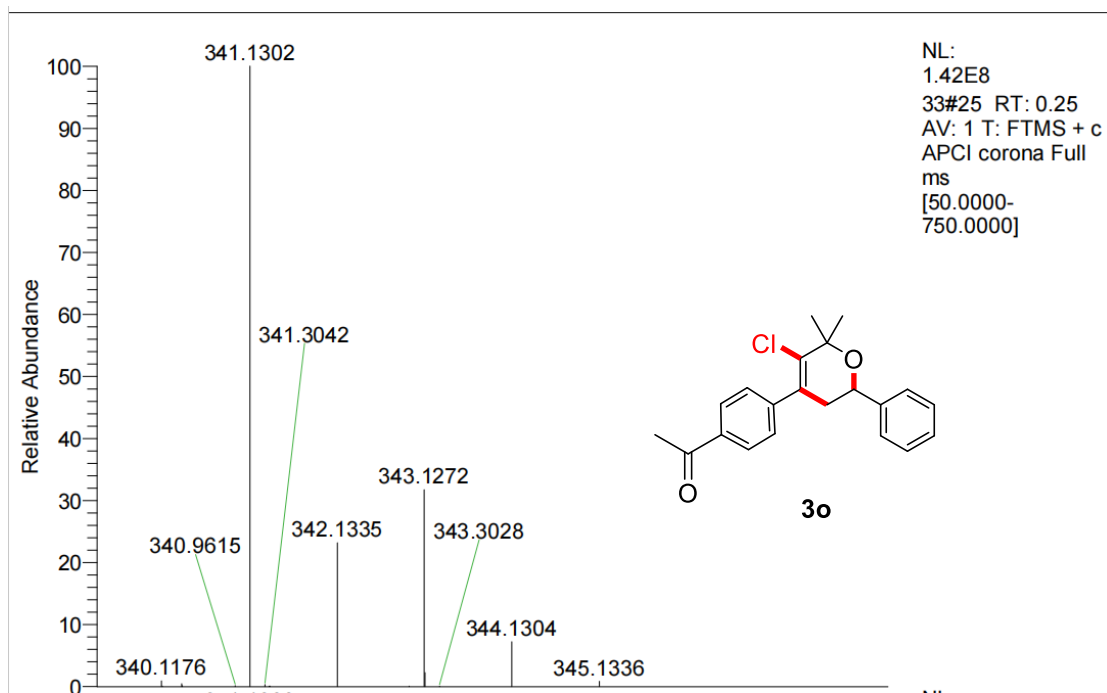
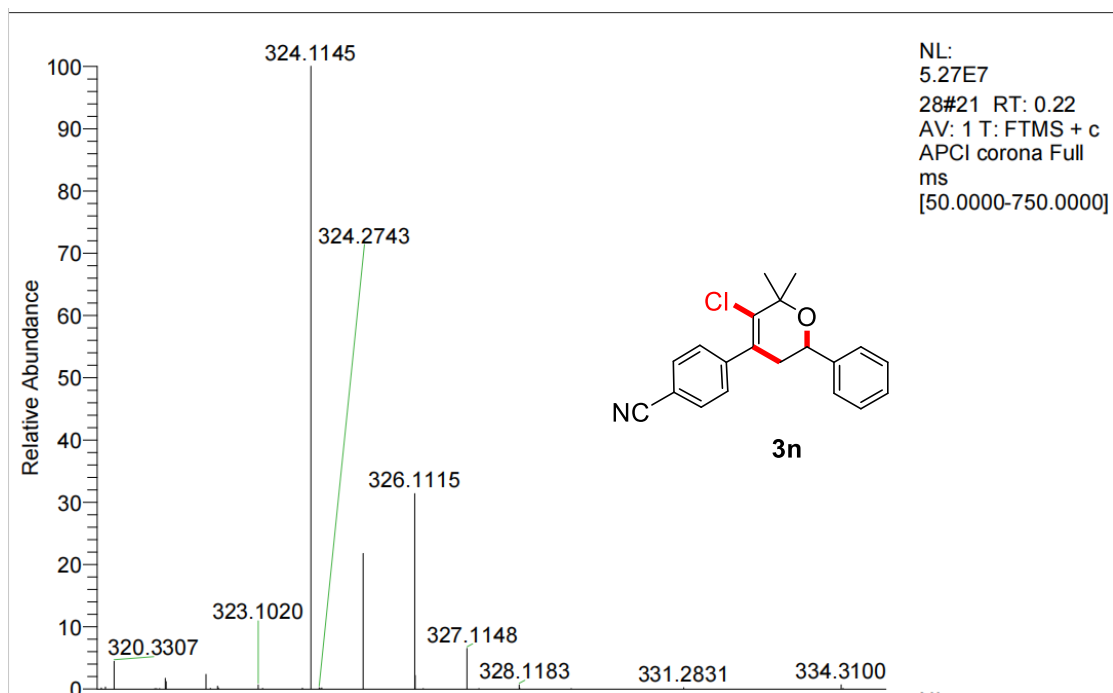
NL:
8.08E6
44#23 RT: 0.23
AV: 1 T: FTMS + c
APCI corona Full
ms
[200.0000-
450.0000]

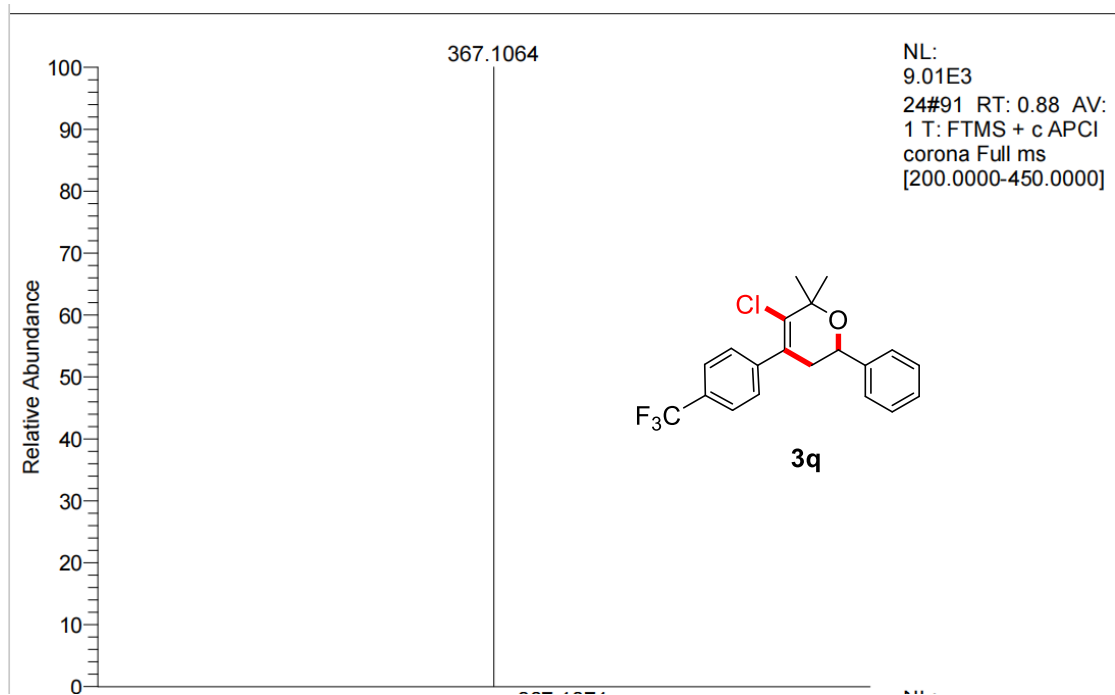
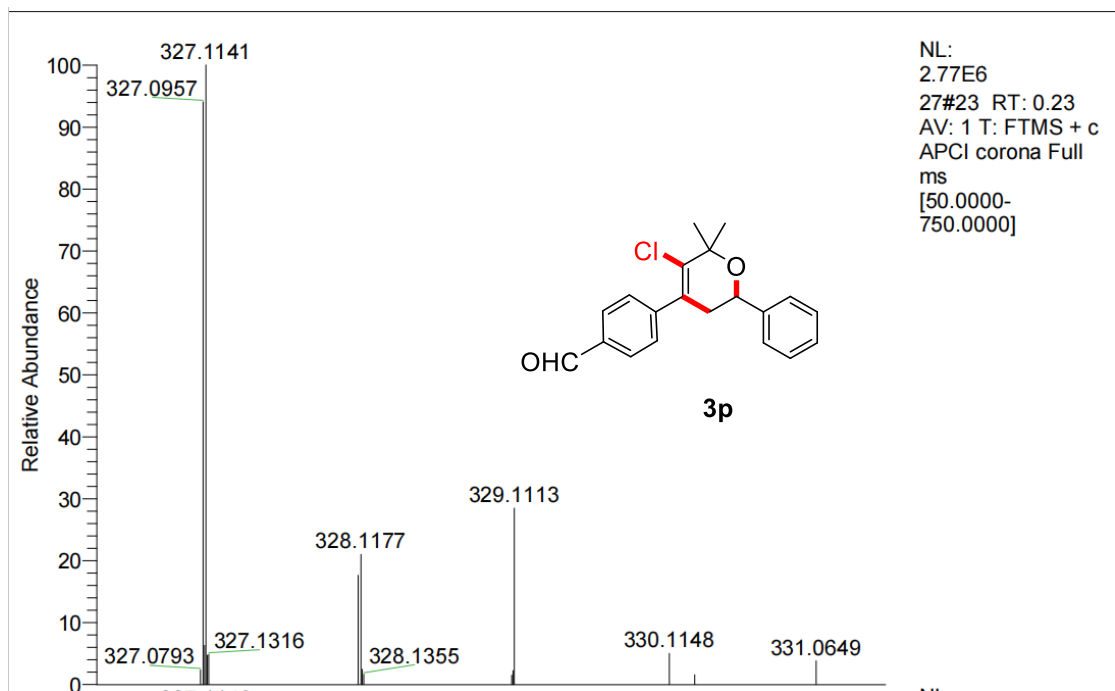


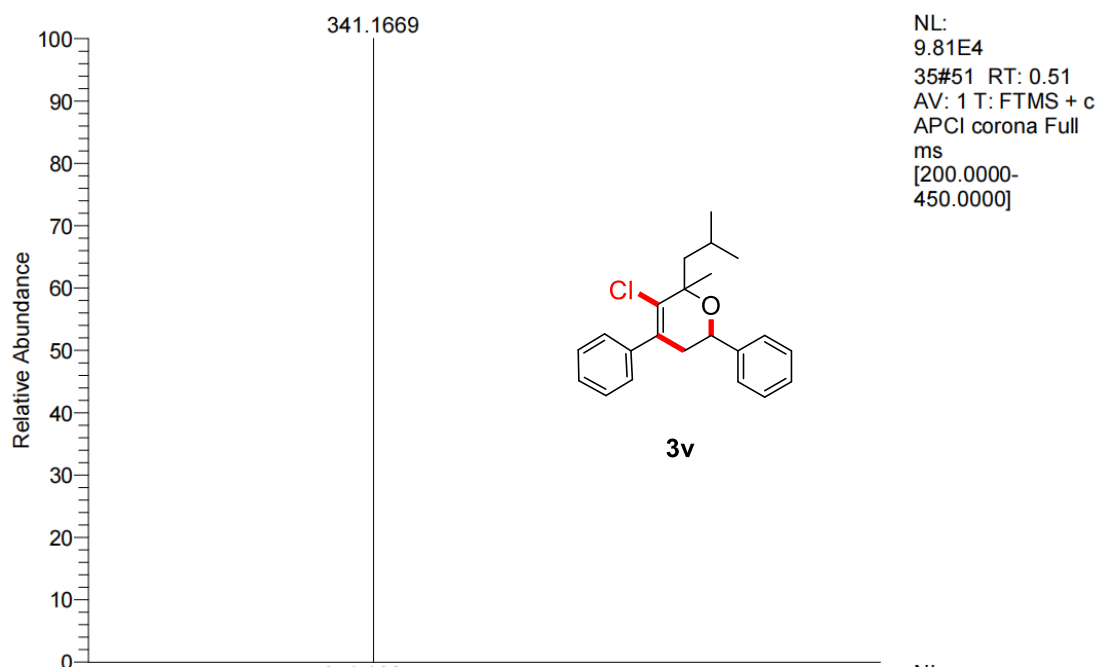
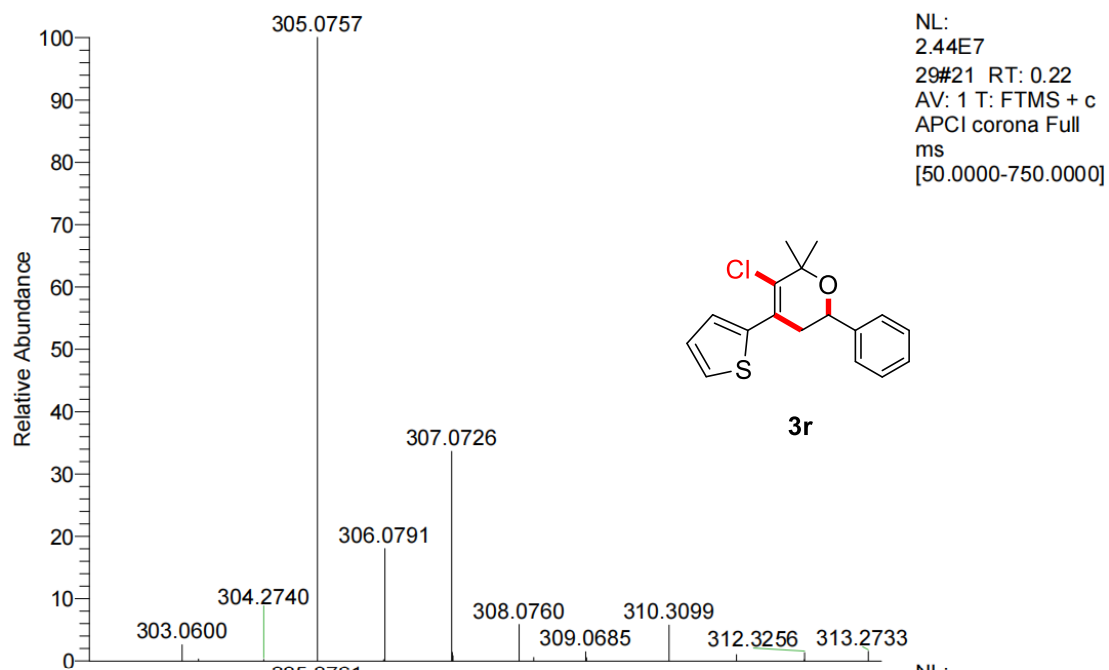


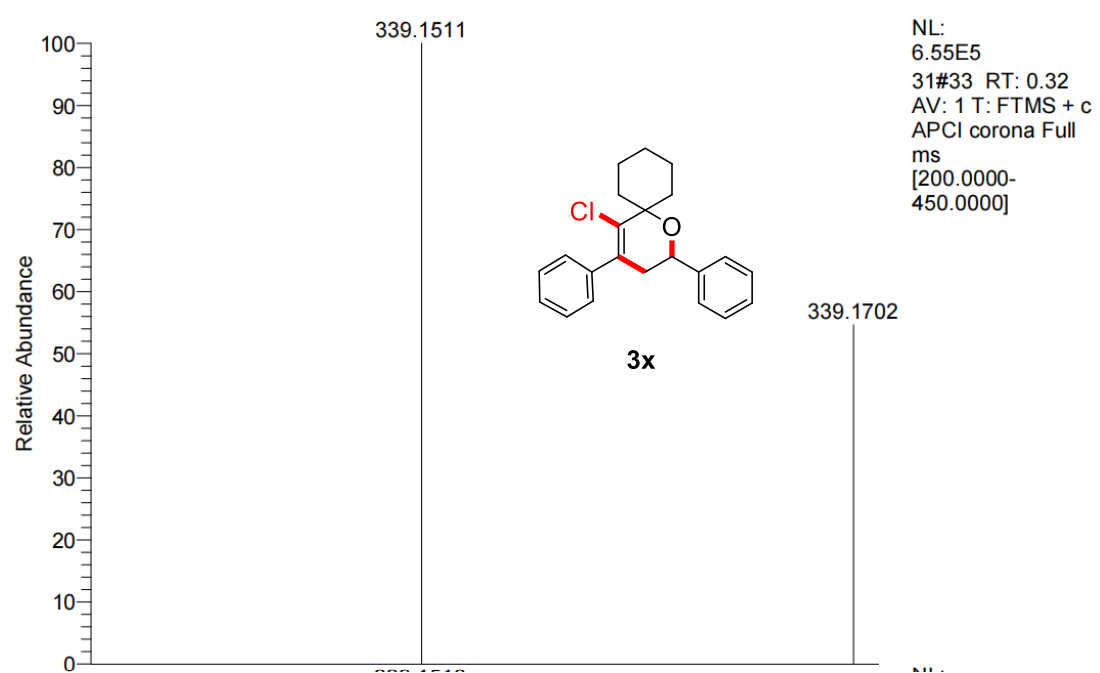
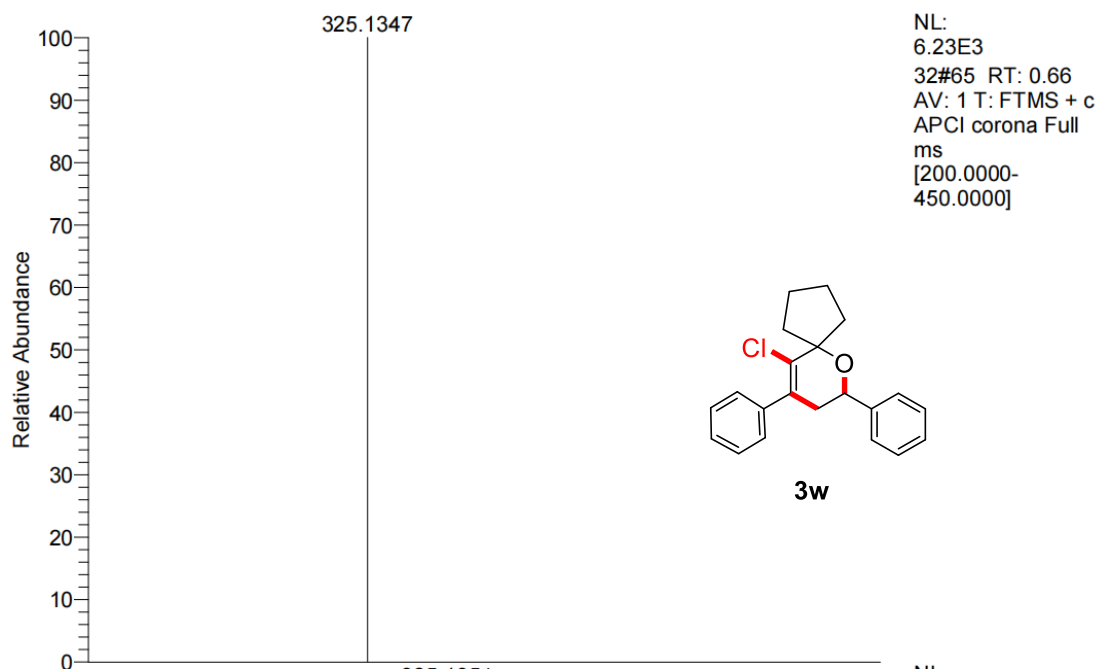


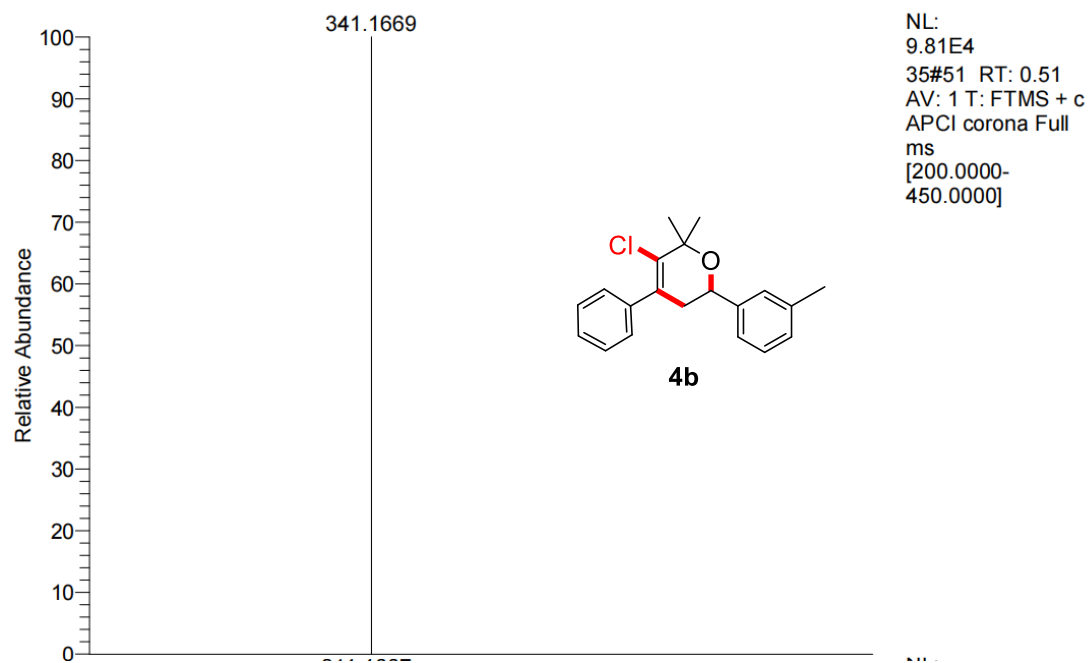
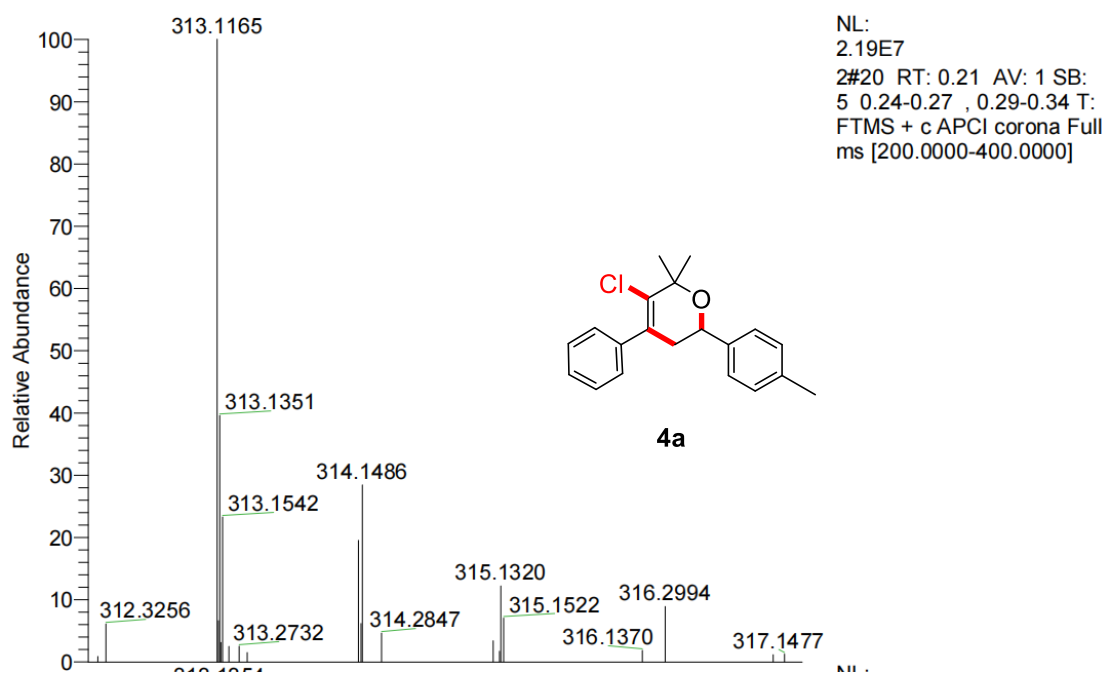


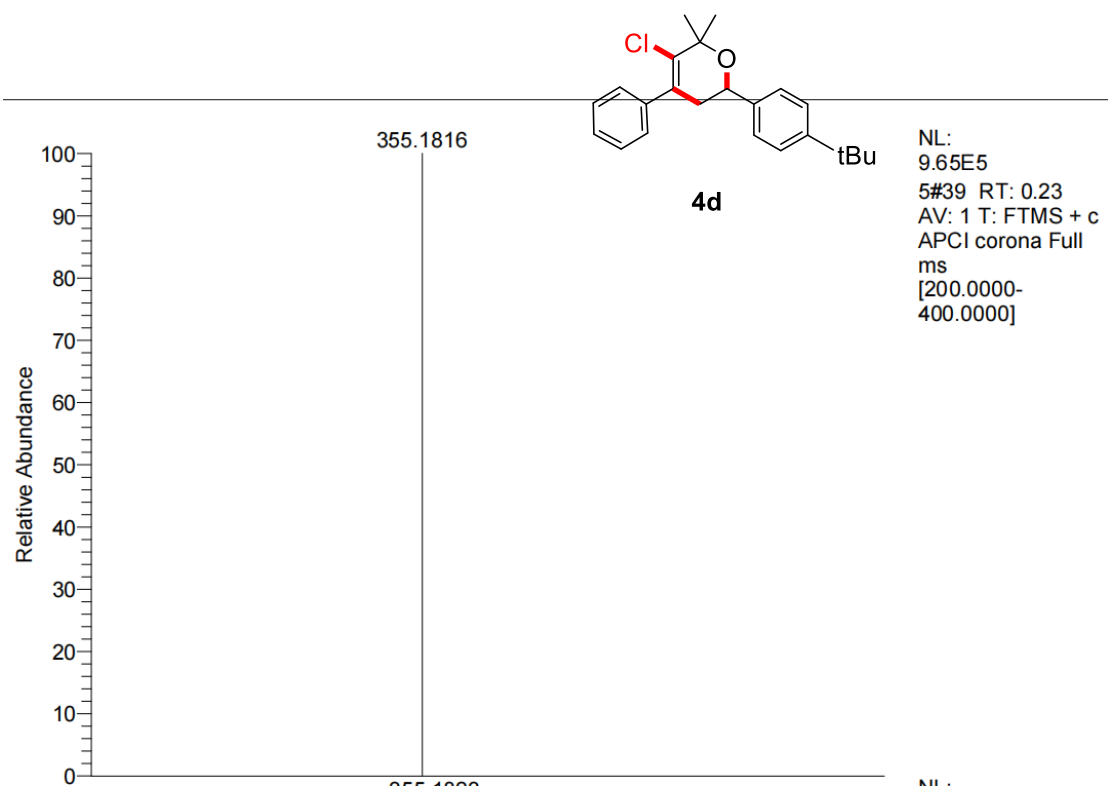
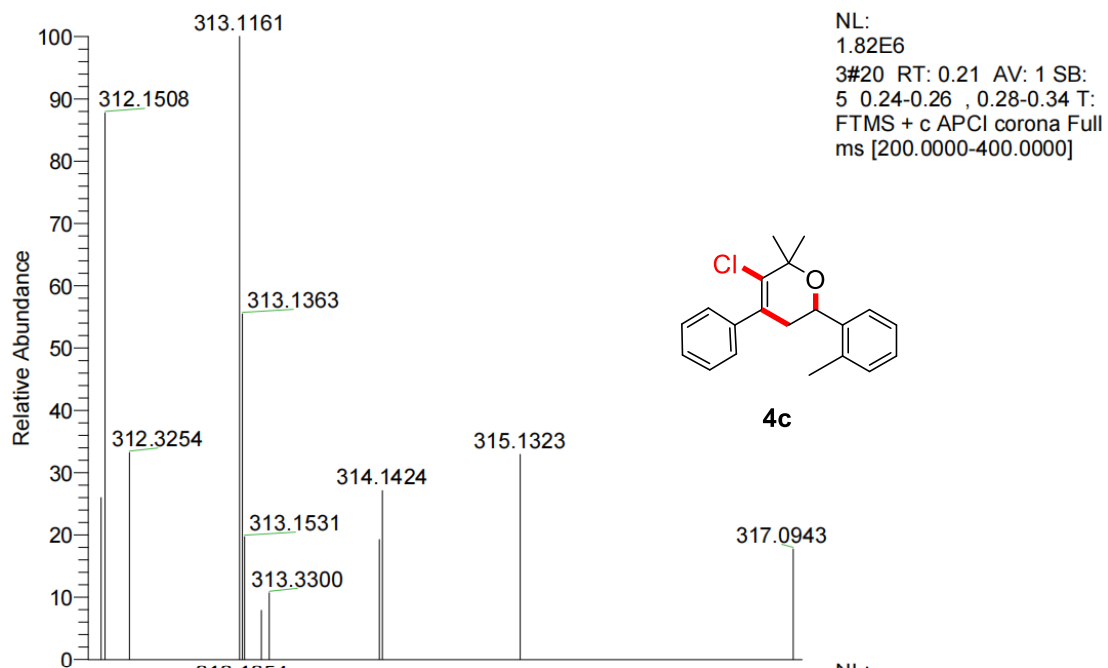


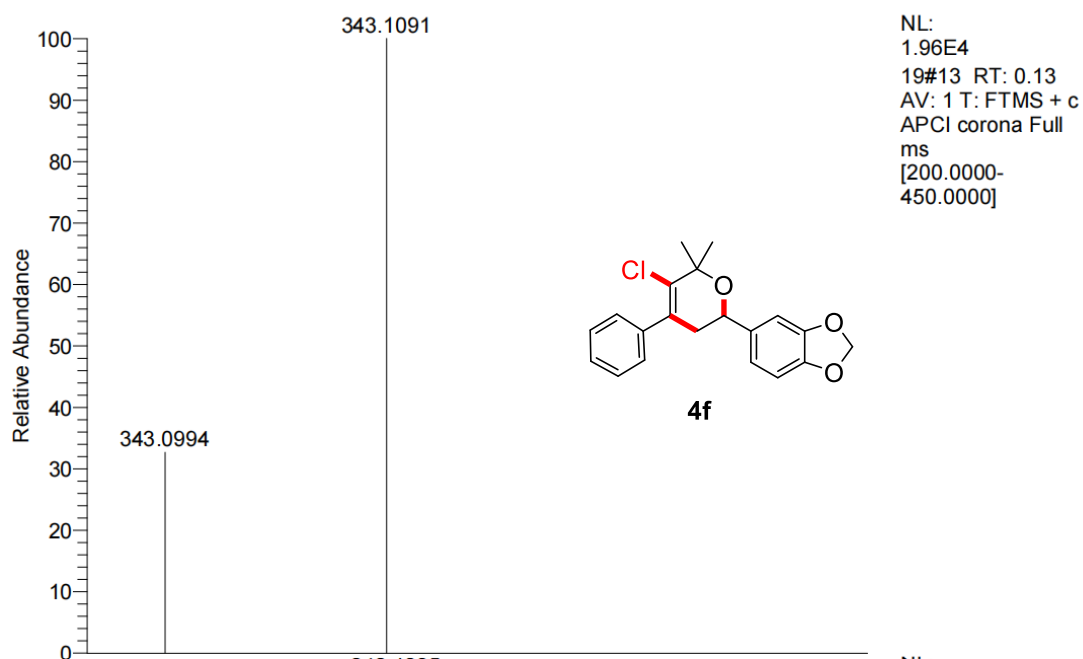
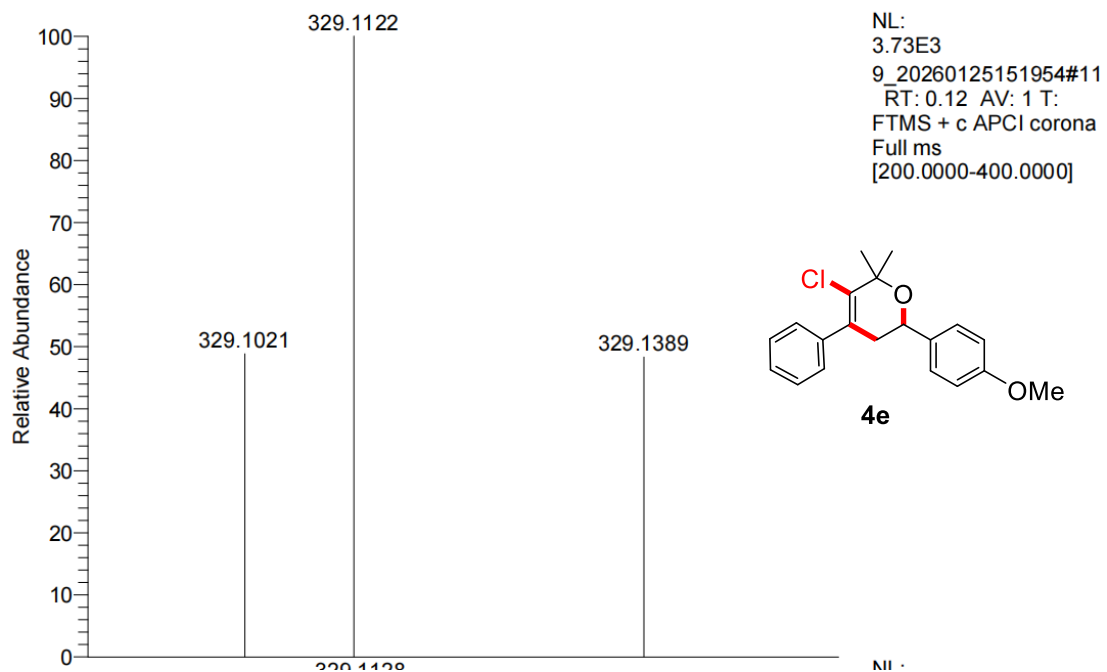


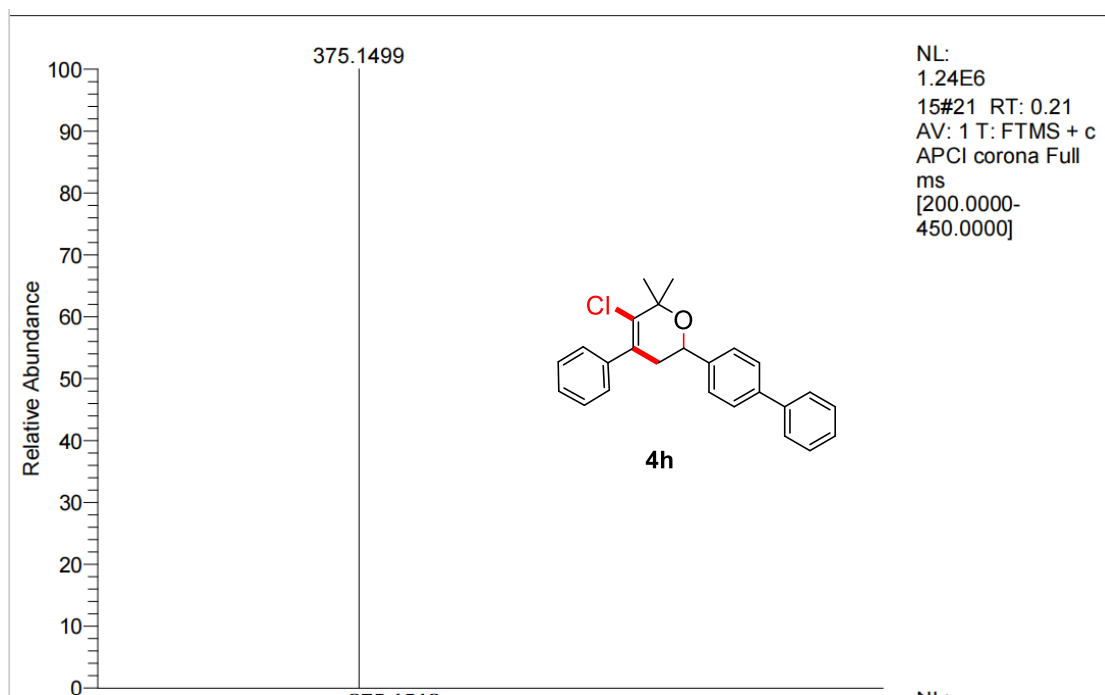
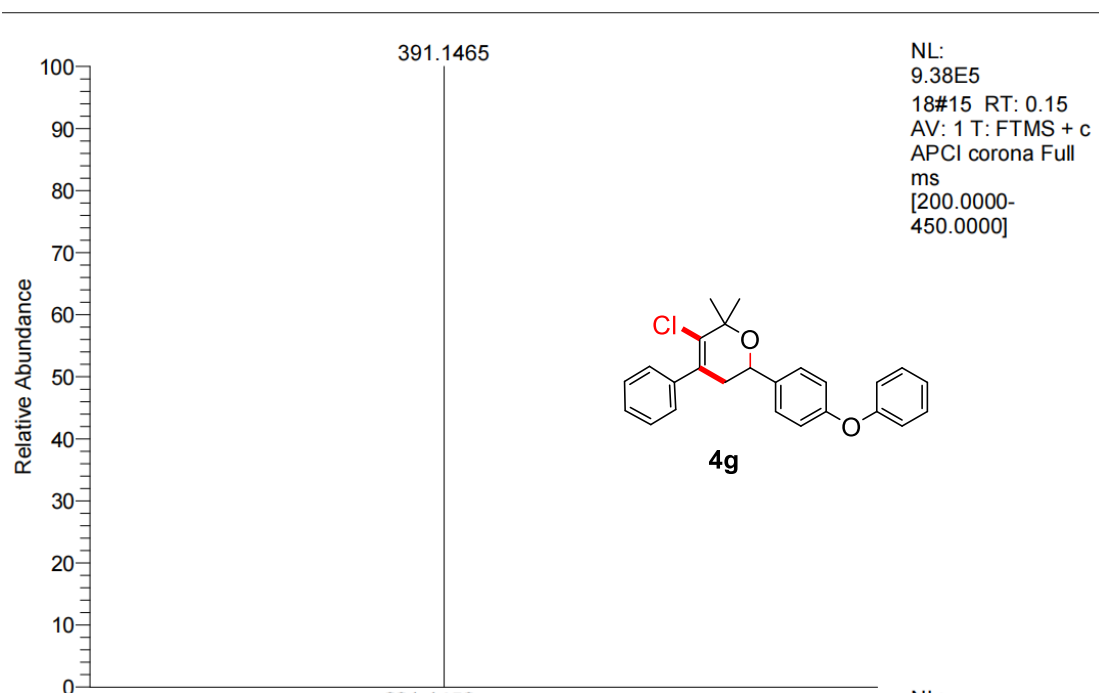


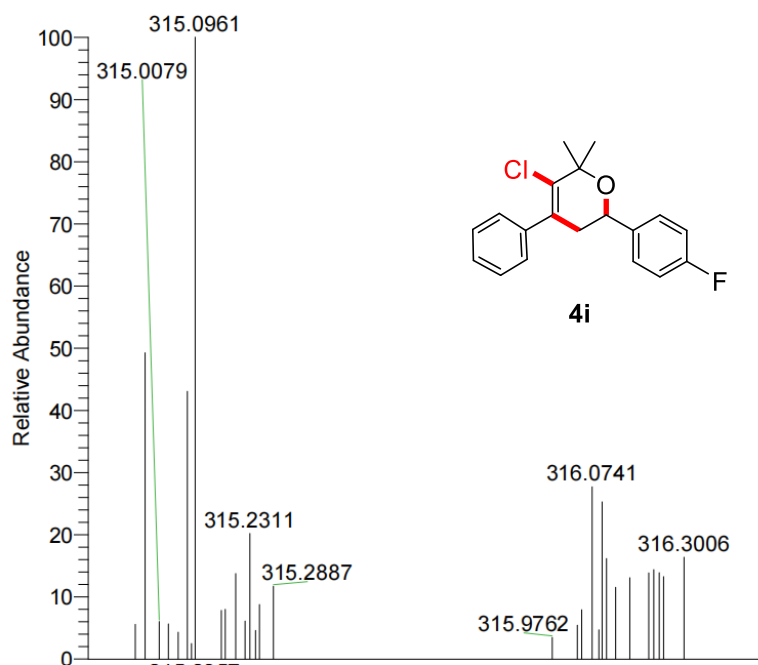




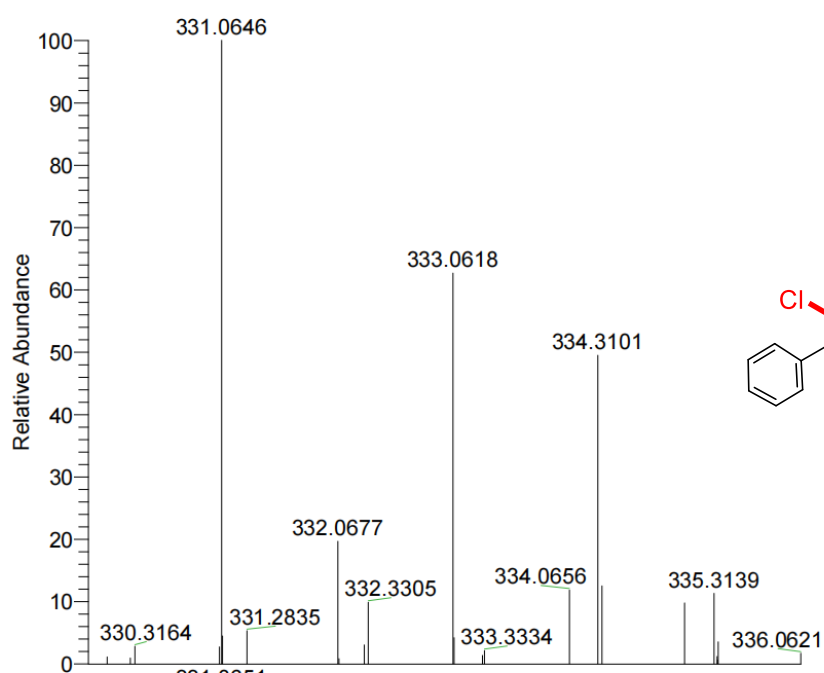








NL:
1.15E4
6_20260105192557#34 RT:
0.17 AV: 1 SB: 20 0.21-0.24 ,
0.08-0.13 T: FTMS - c APCI
corona SIM ms
[300.0000-330.0000]



NL:
4.23E7
7_20260125153134#27
RT: 0.27 AV: 1 SB: 5
0.00-0.09 T: FTMS + c
APCI corona SIM ms
[325.0000-345.0000]

