

## Supplementary Material

### Samarium triflate-catalyzed dimerization of vinylarenes

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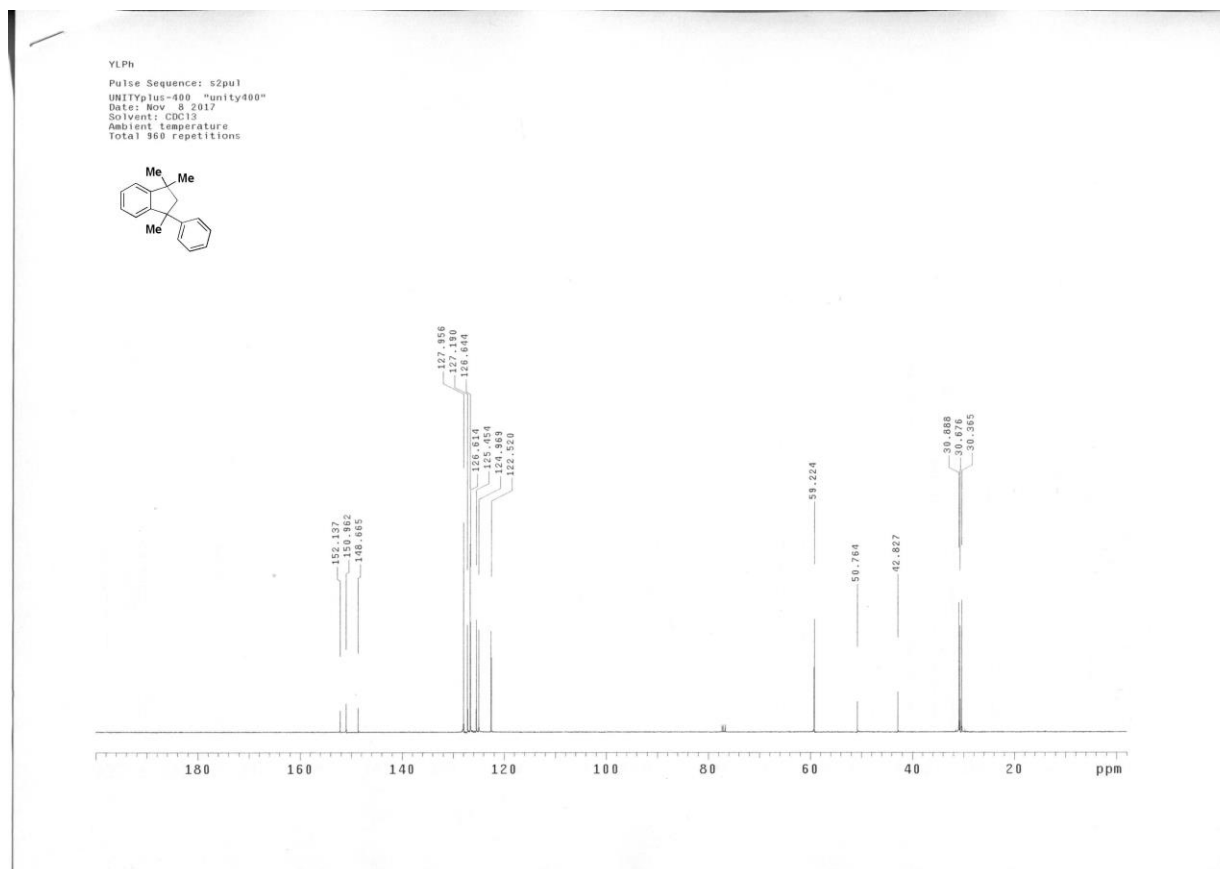
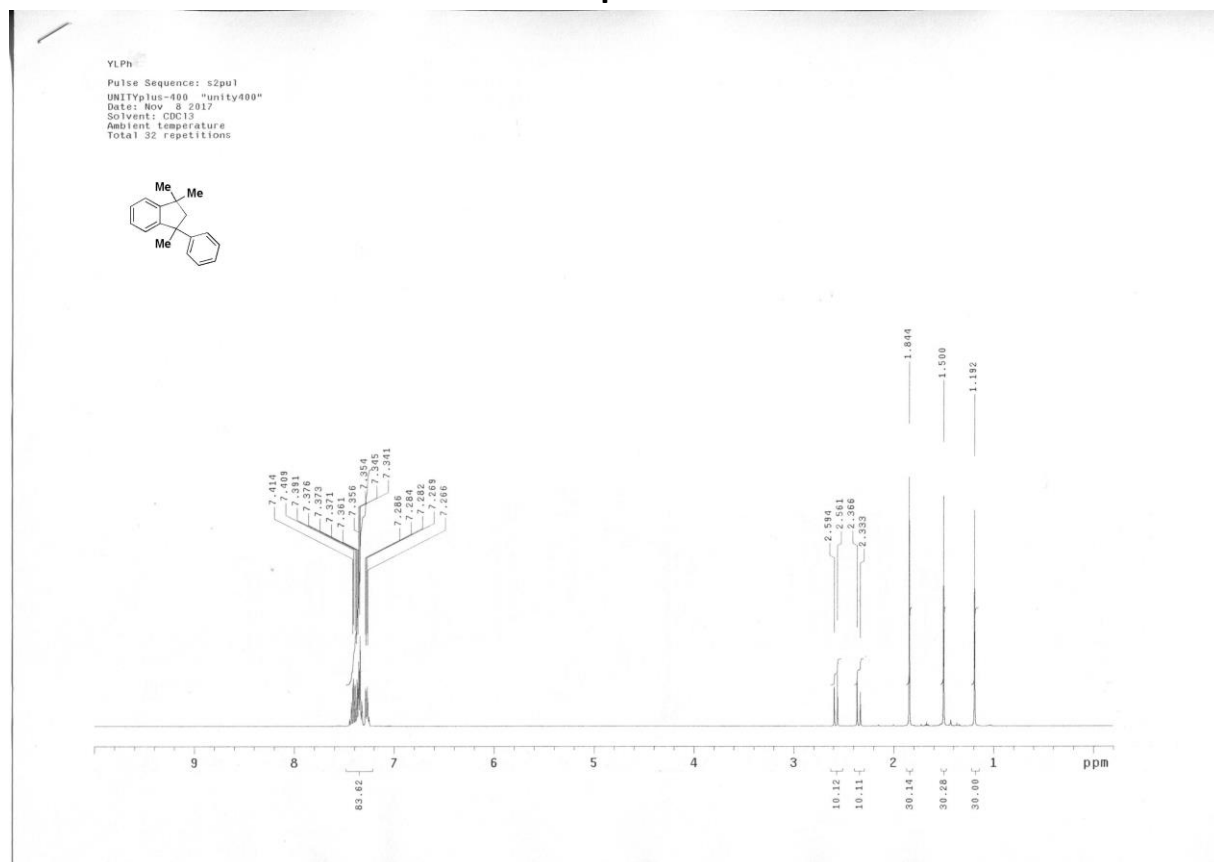
<sup>b</sup> Department of Medical Research, Kaohsiung Medical University Hospital, Kaohsiung 807, Taiwan

Email: [mychang@kmu.edu.tw](mailto:mychang@kmu.edu.tw)

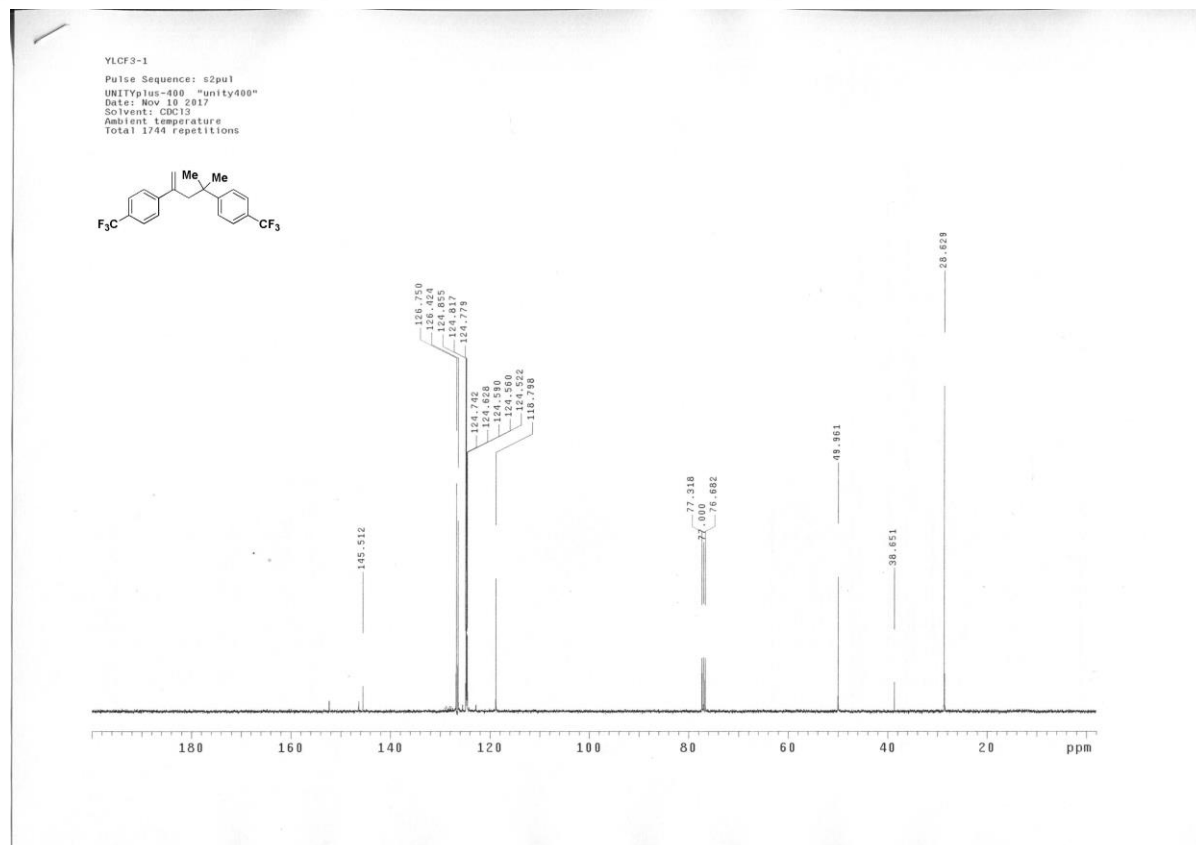
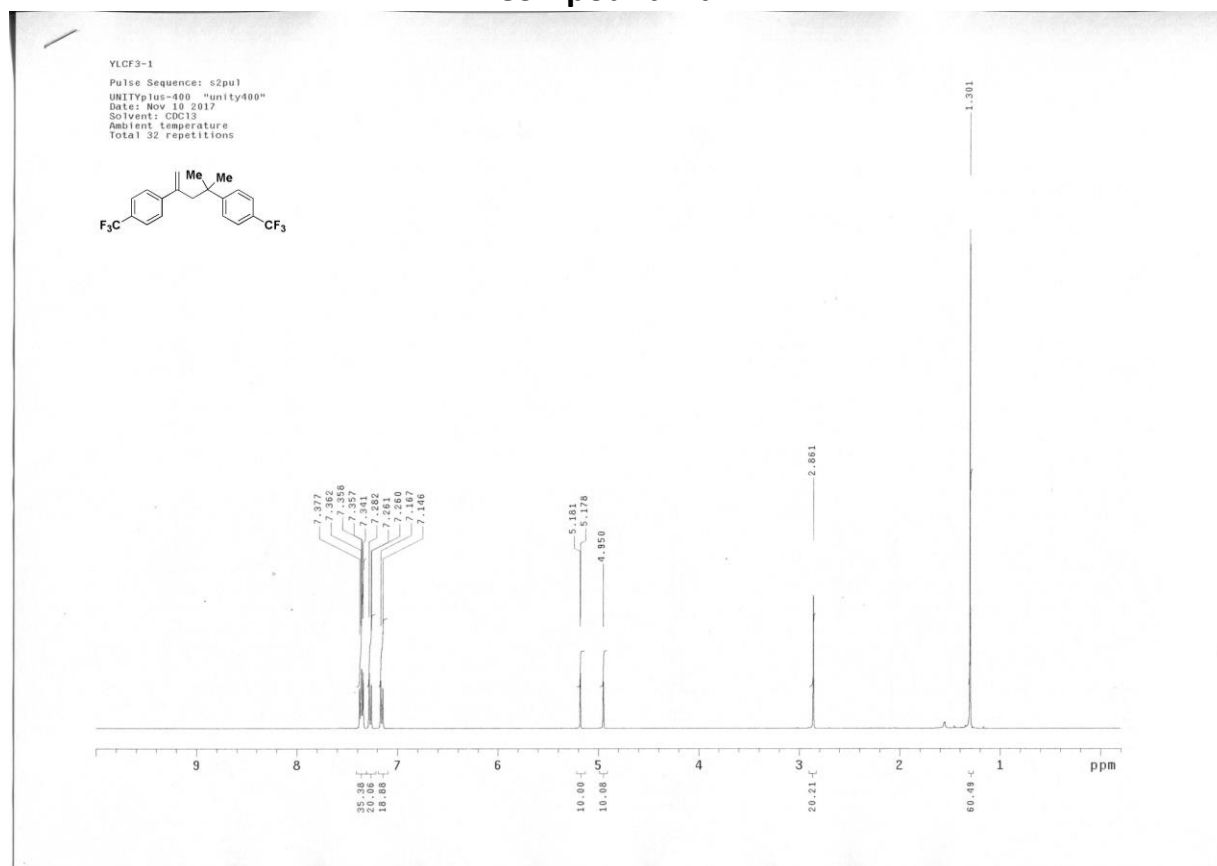
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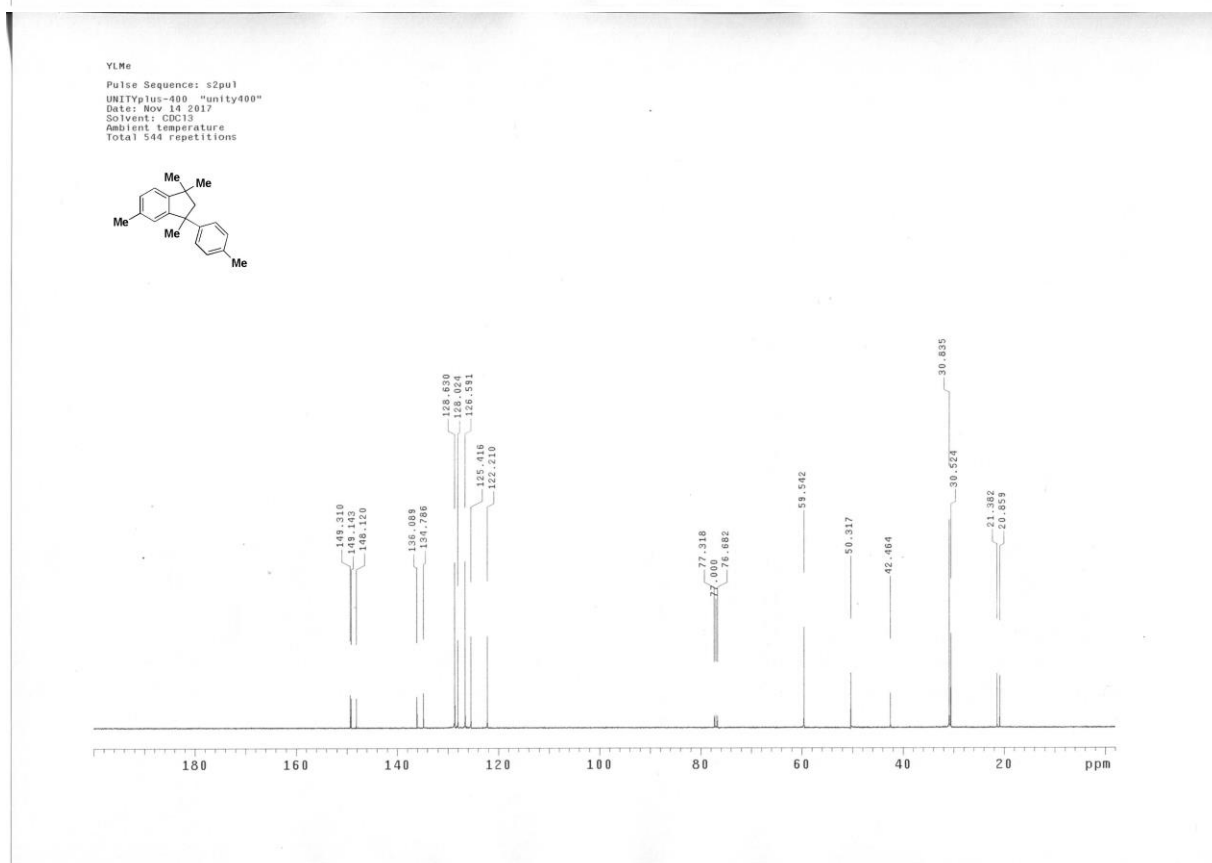
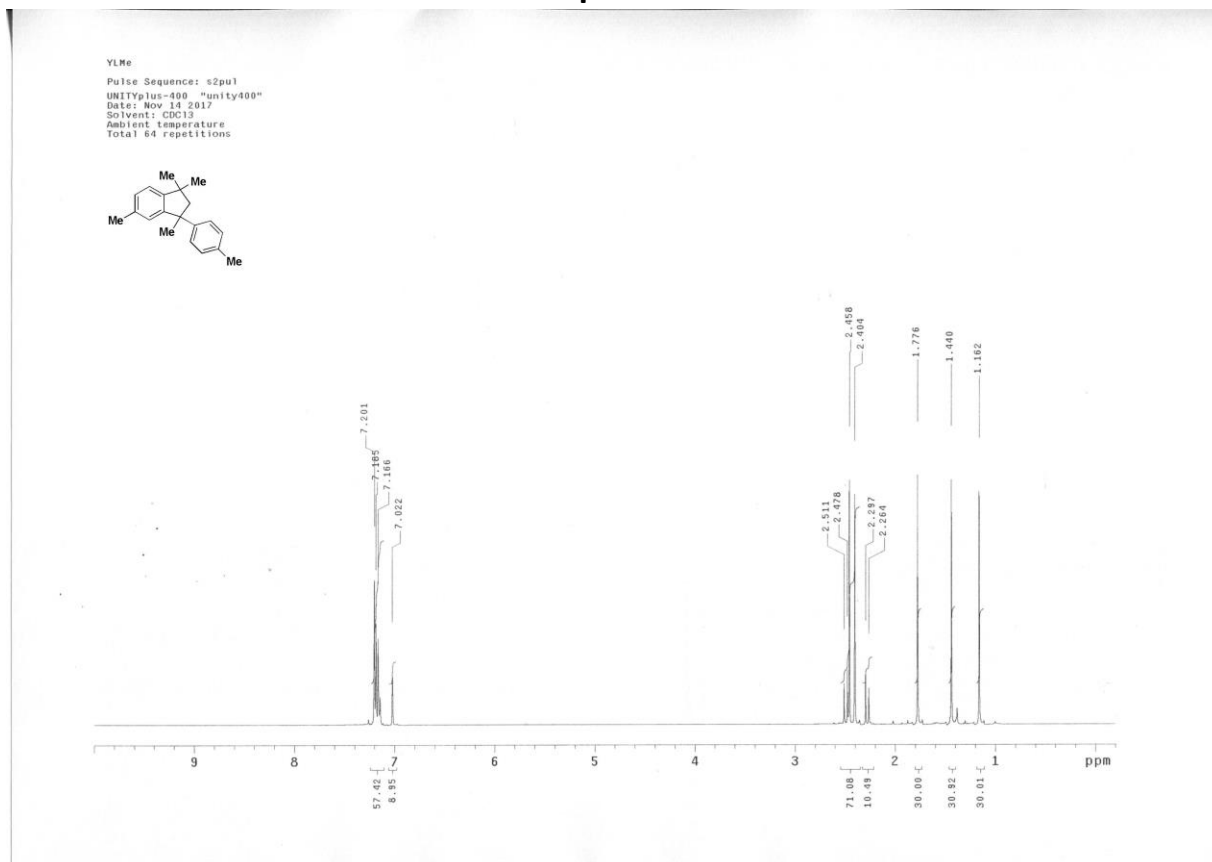
## Compound 4a



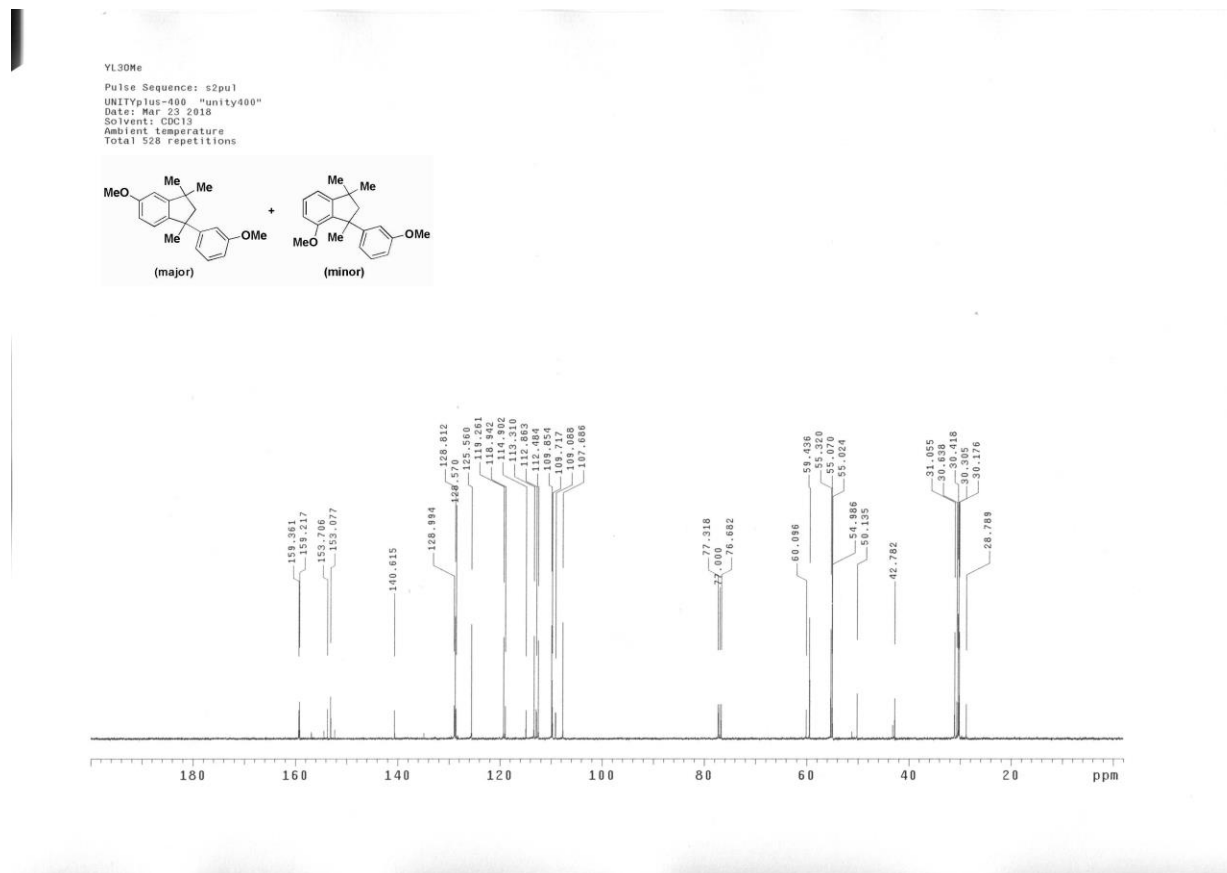
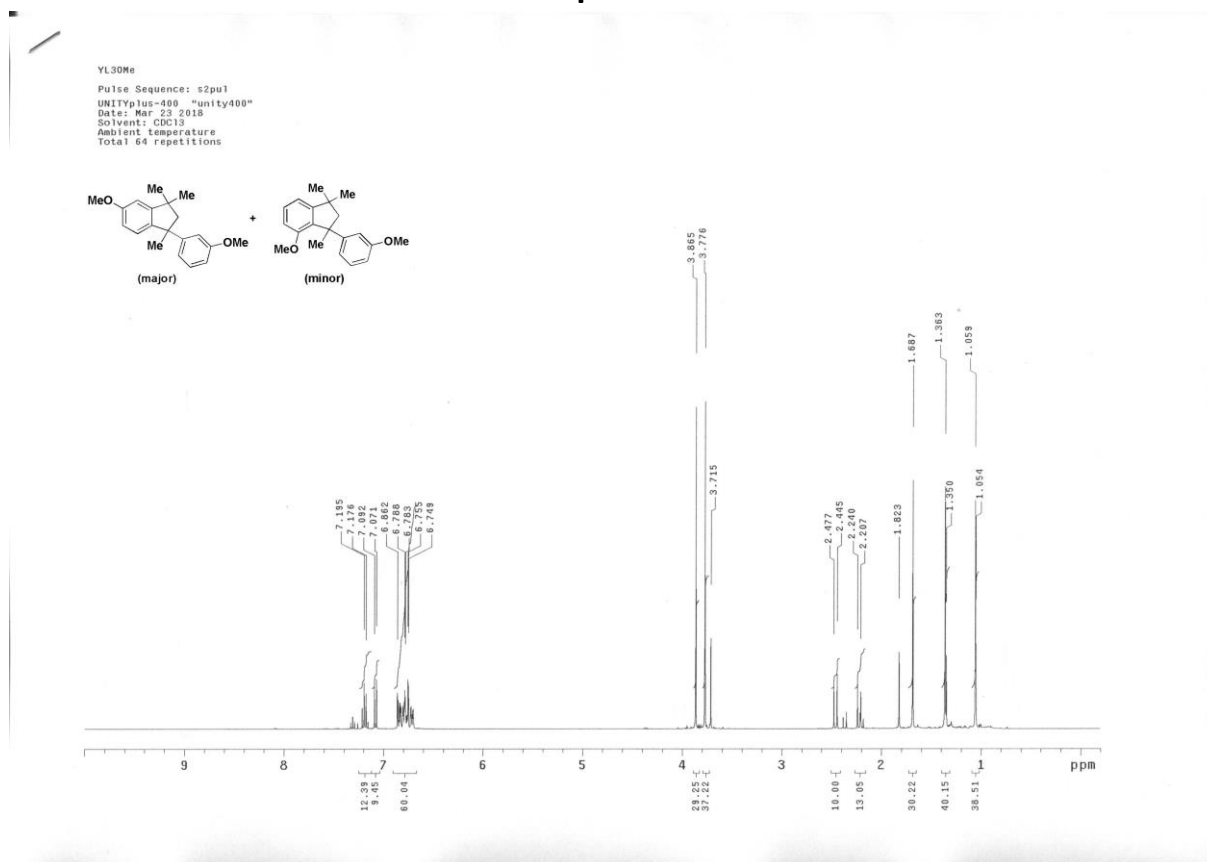
## Compound 4b-1



## Compound 4c

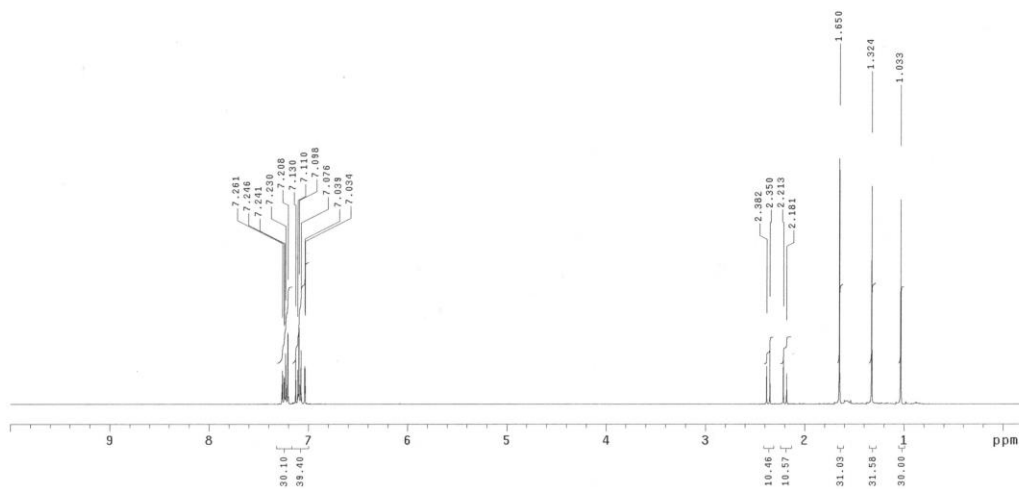
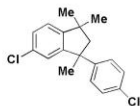


## Compound 4d

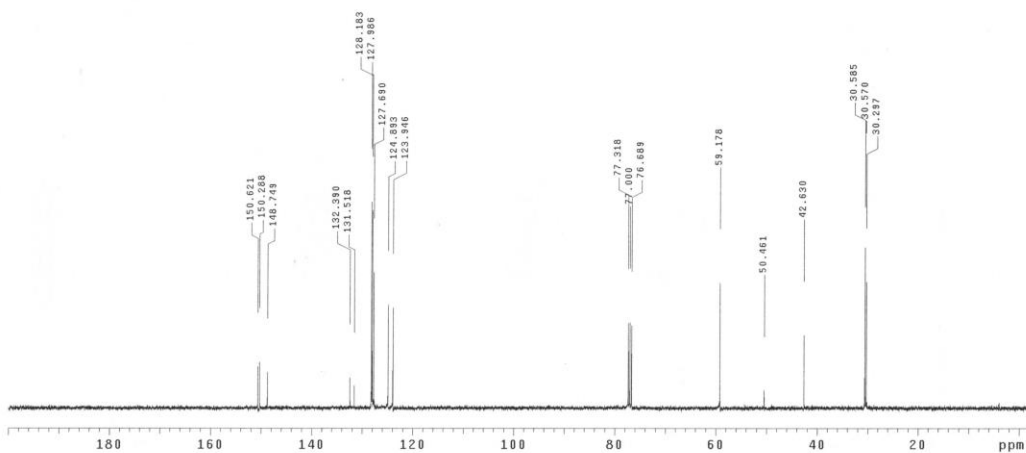
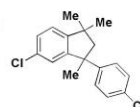


Compound 4e

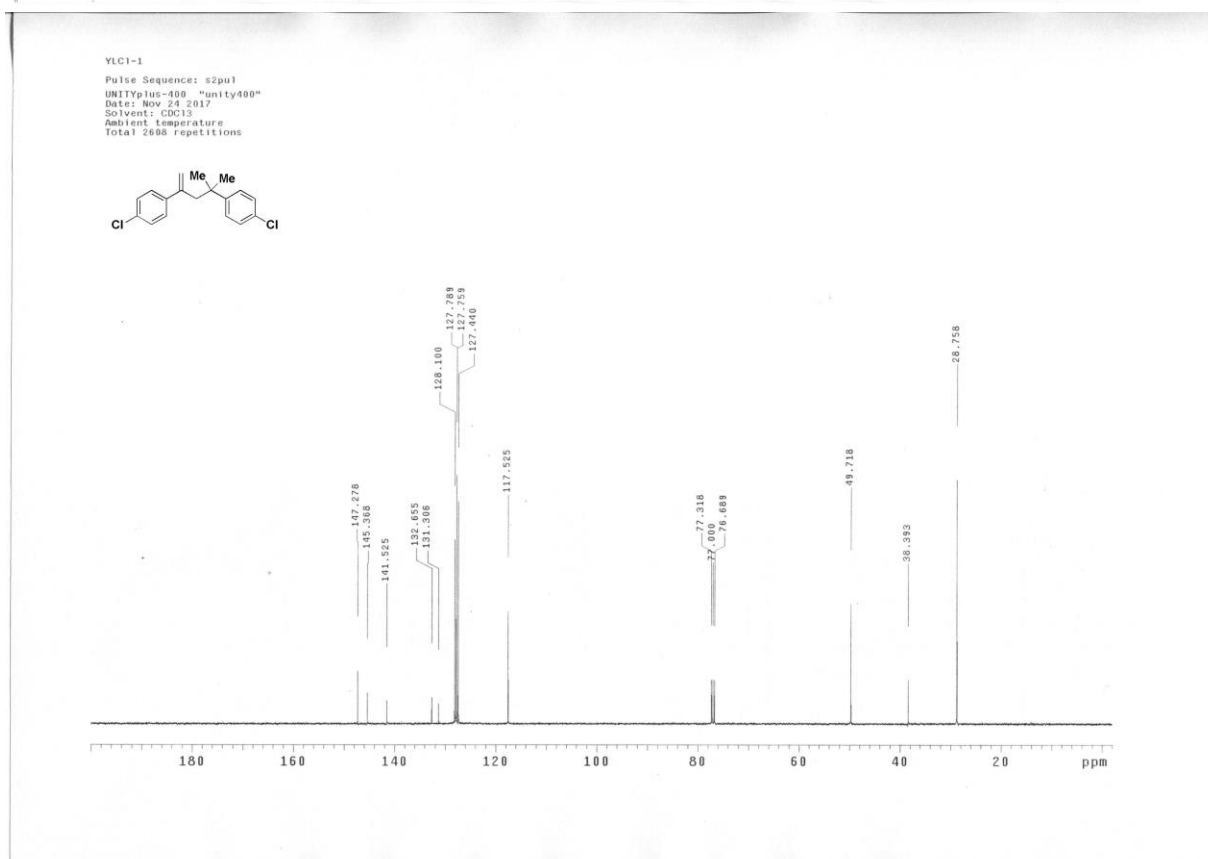
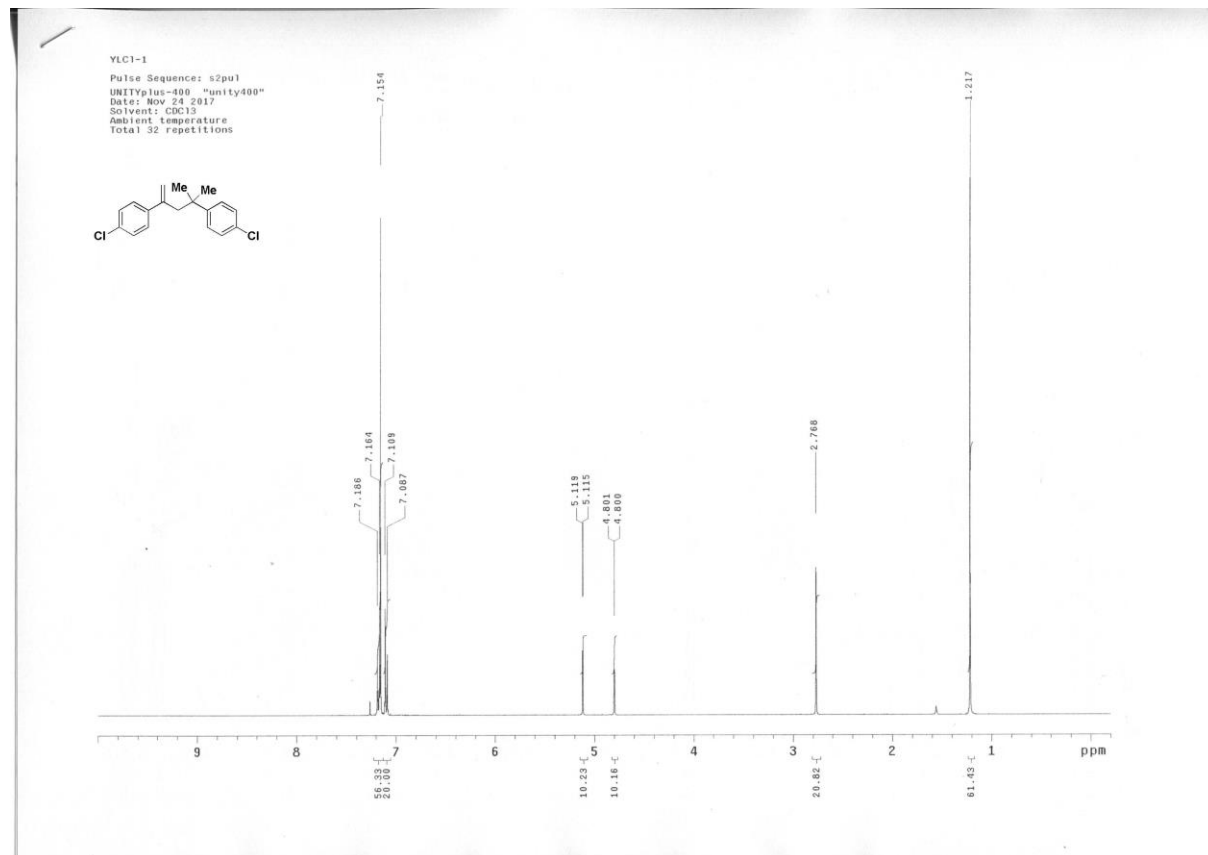
YL4C1  
 Pulse Sequence: s2pul  
 UNITYplus-400 "unity400"  
 Date: Mar 22 2018  
 Solvent: CDCl3  
 Ambient temperature  
 Total 32 Repetitions



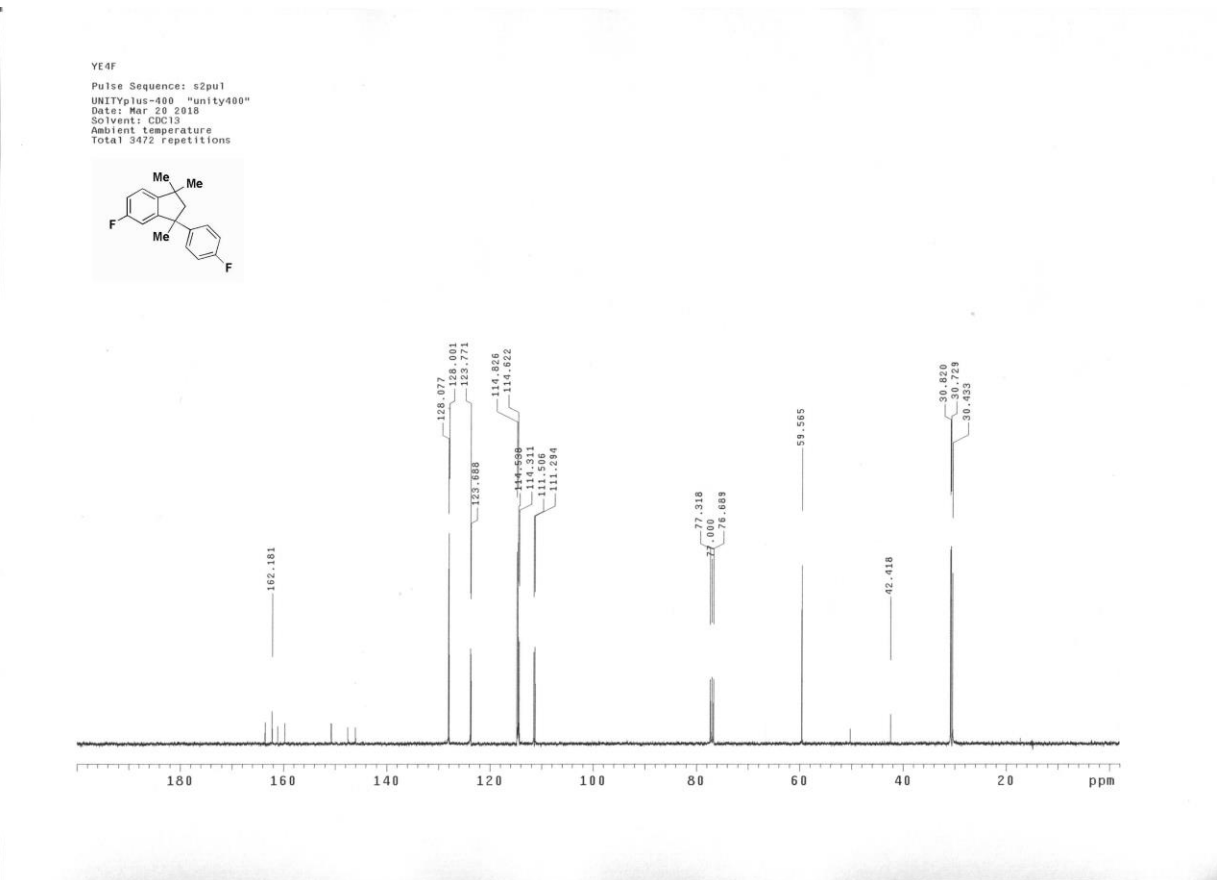
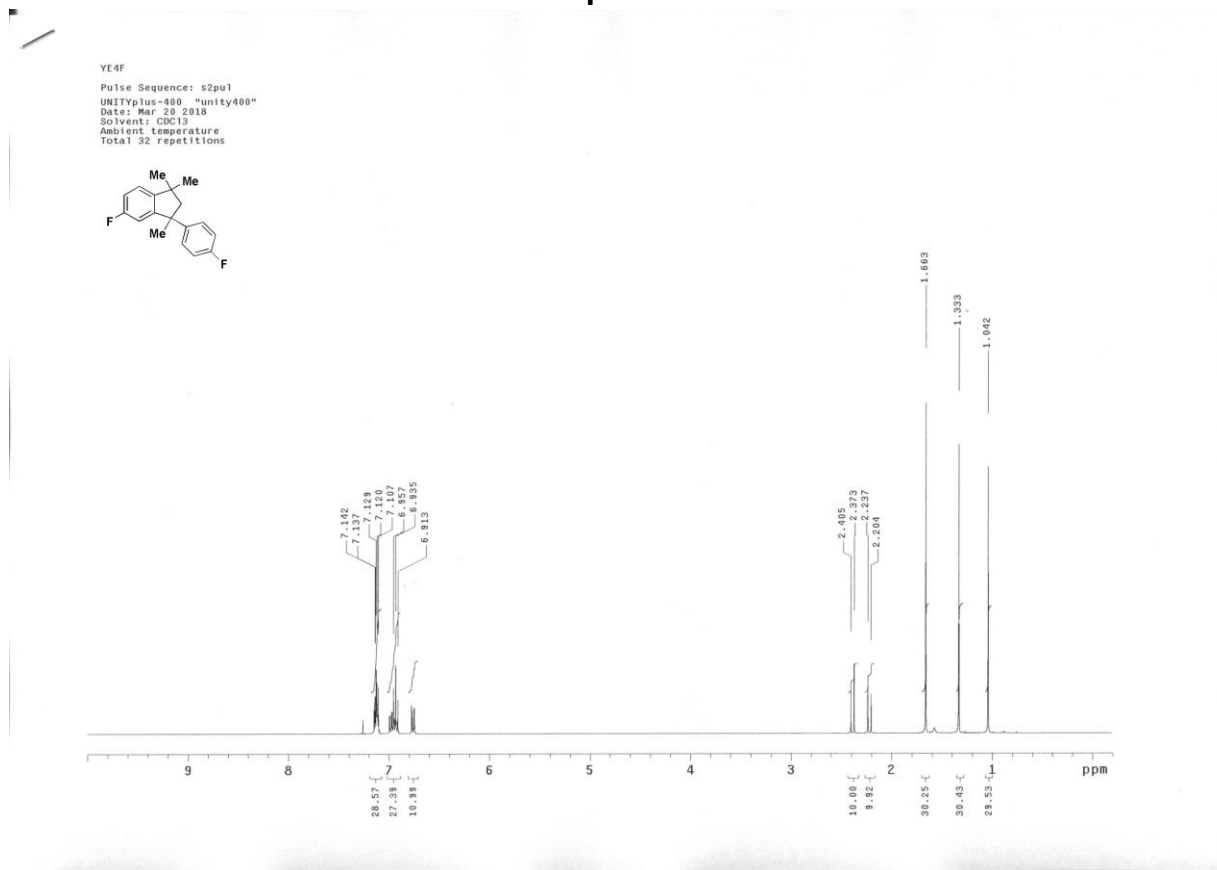
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 Solvent: CDCl3  
 Ambient temperature  
 Total 2800 repetitions



## Compound 4e-1

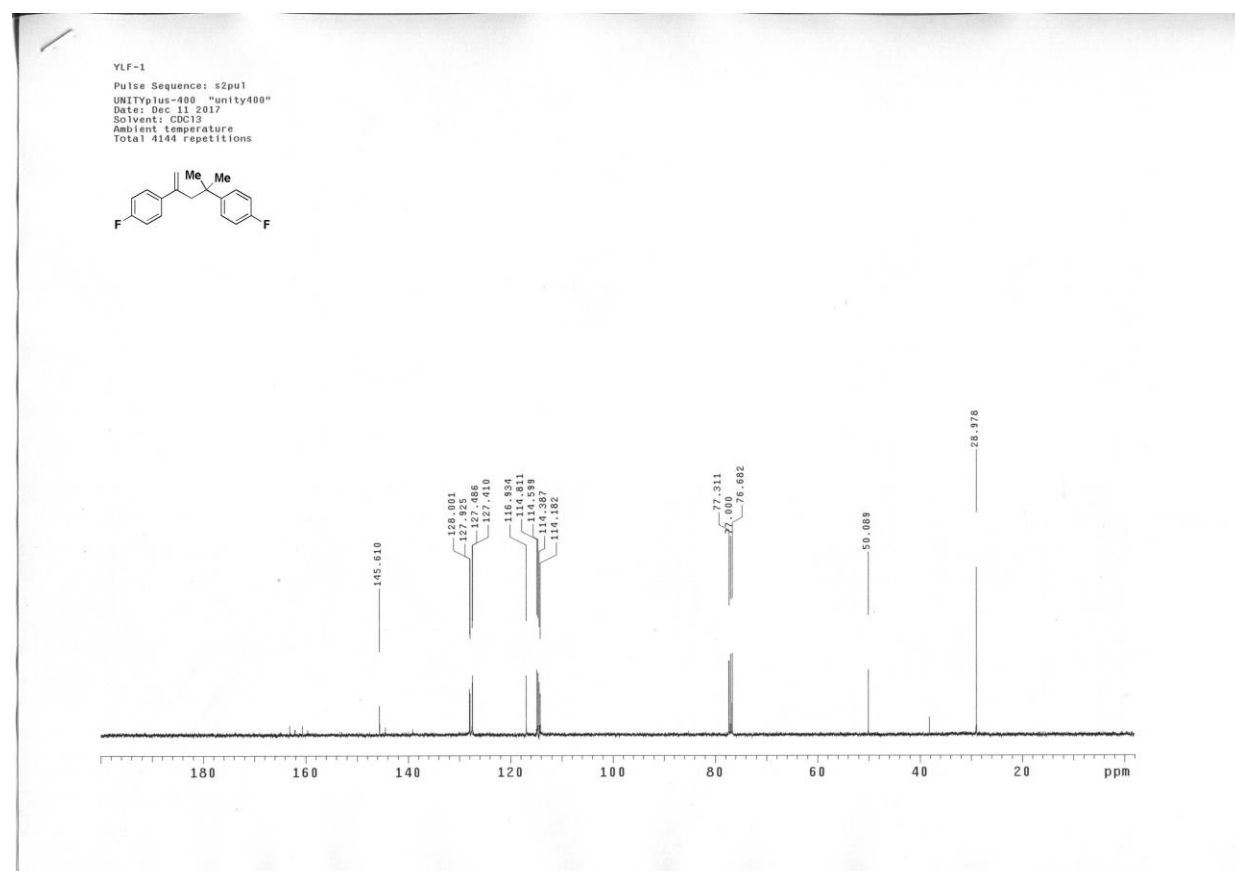
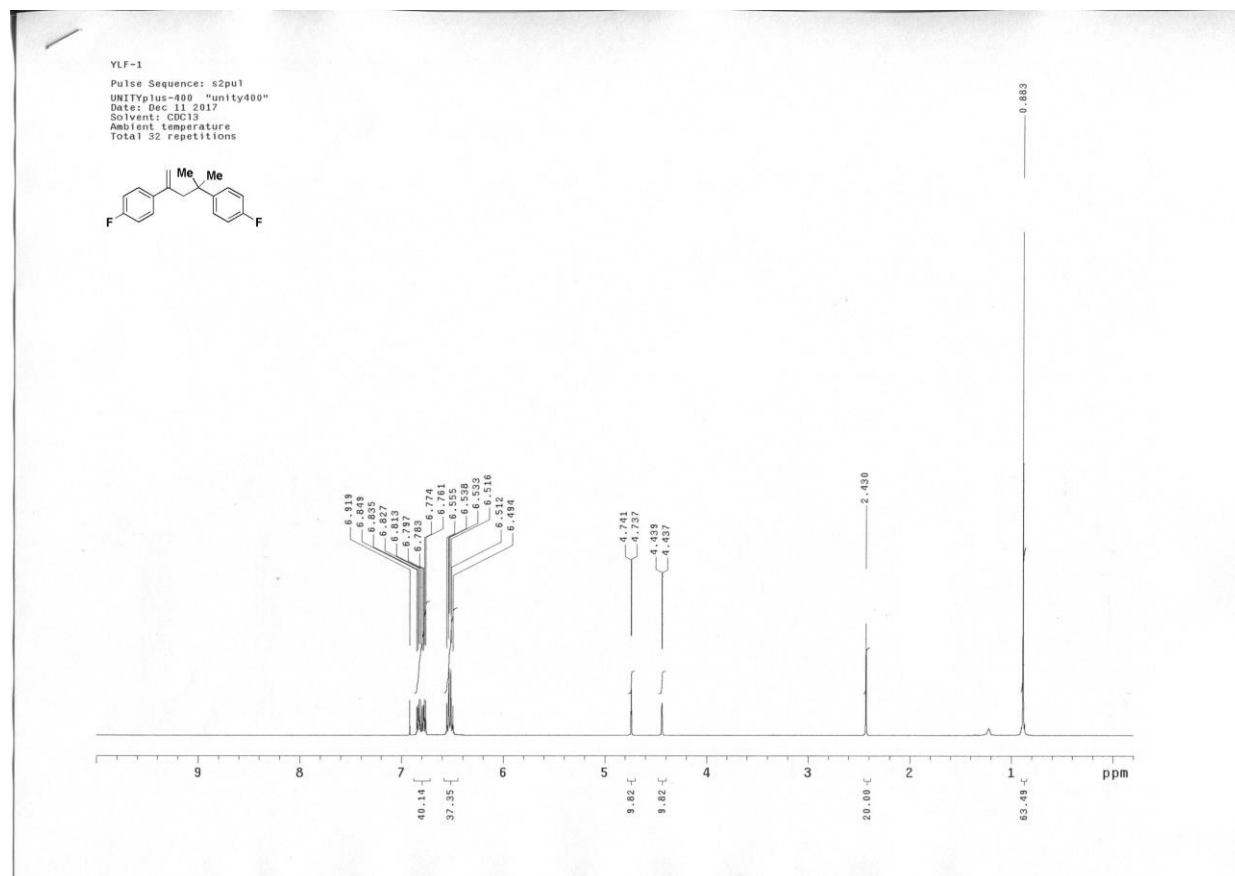


## Compound 4f

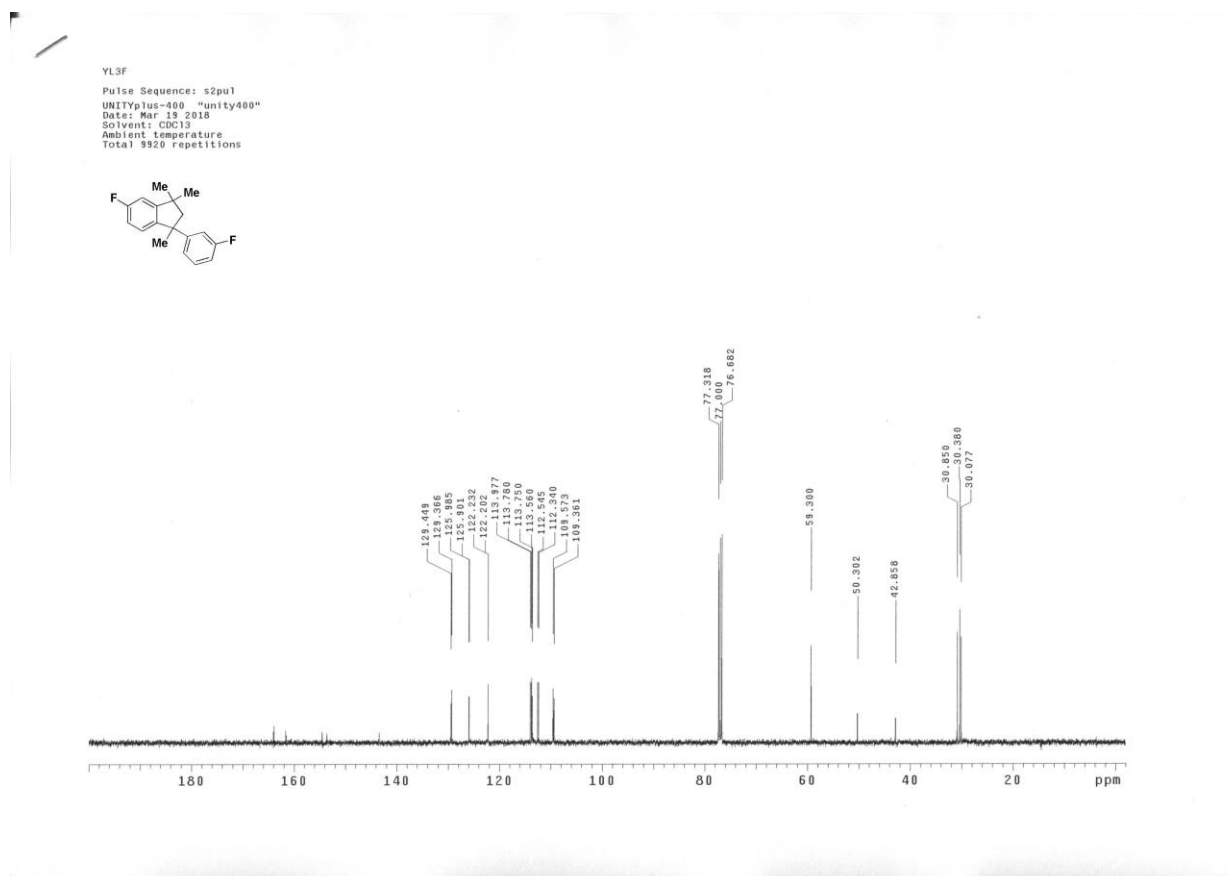
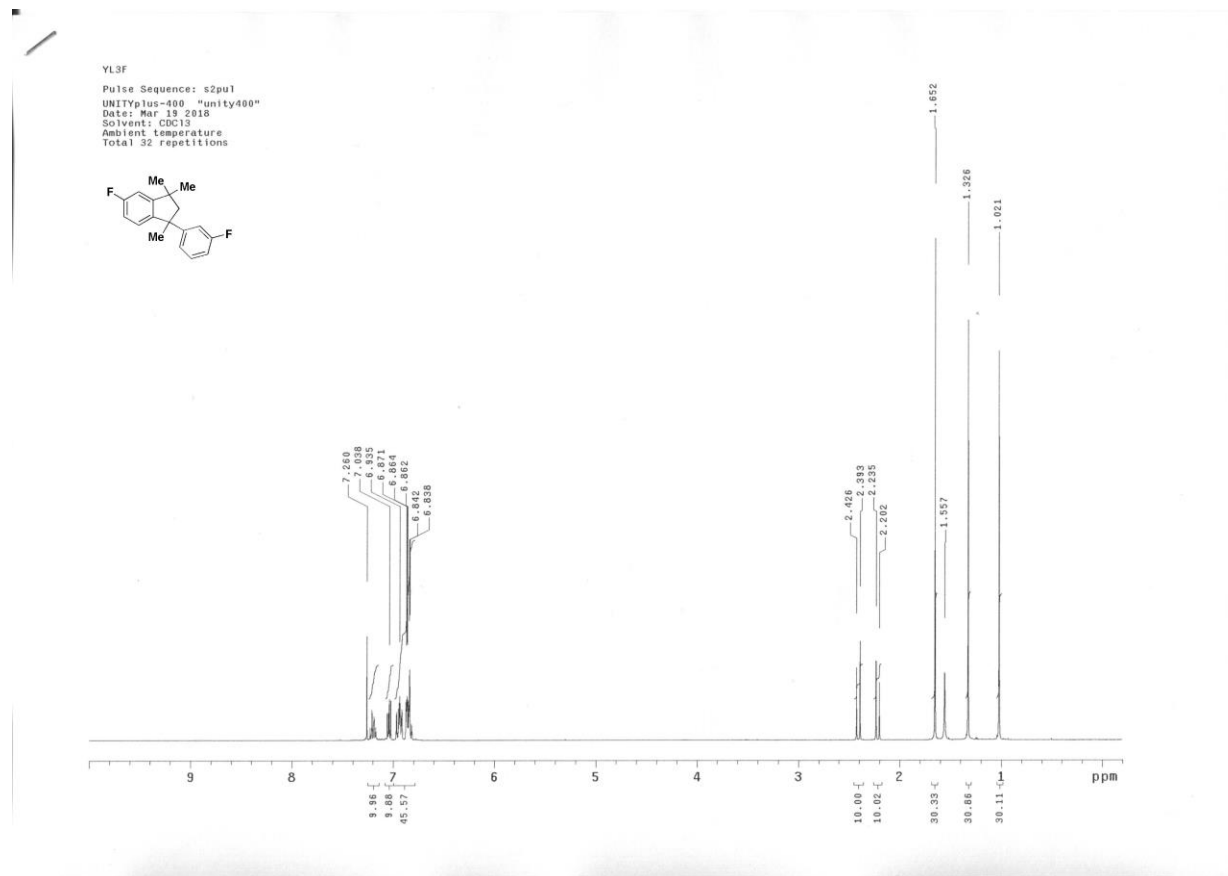




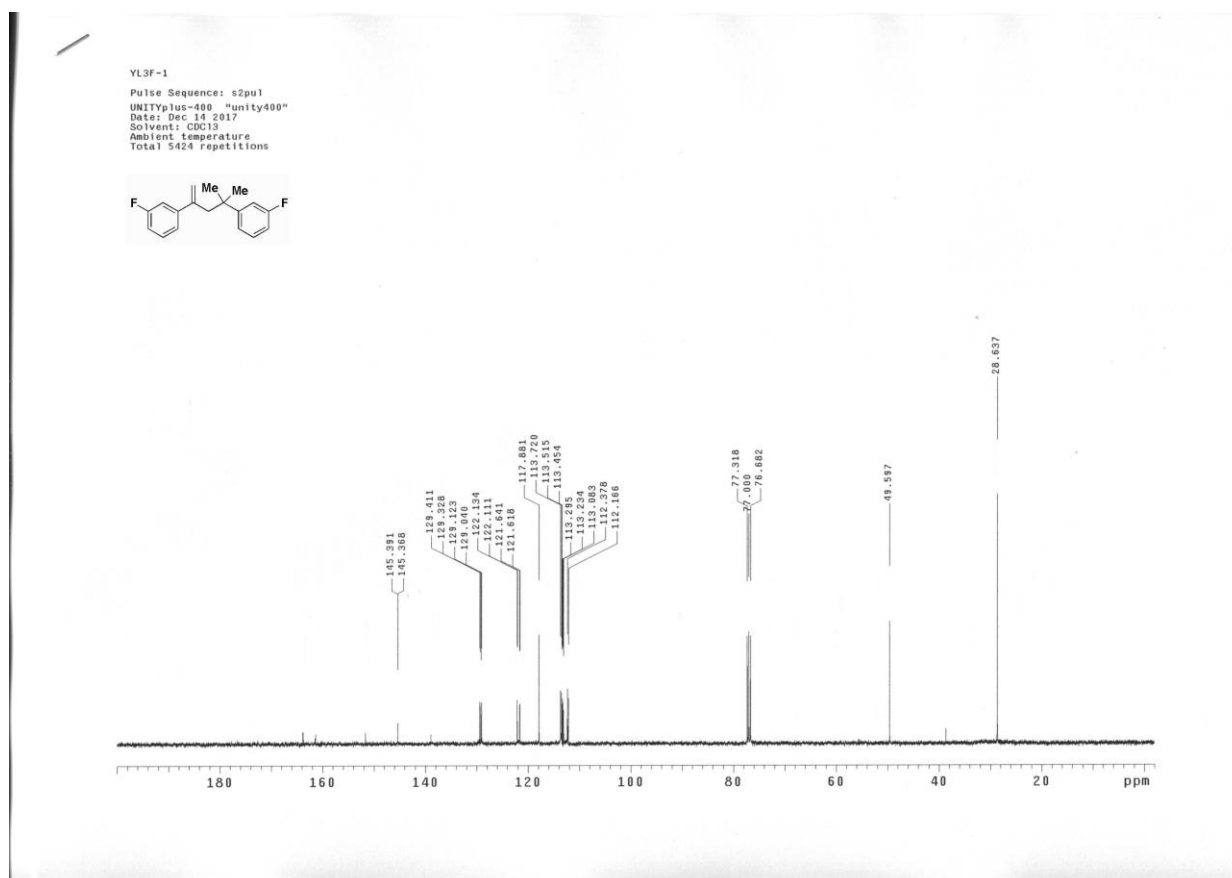
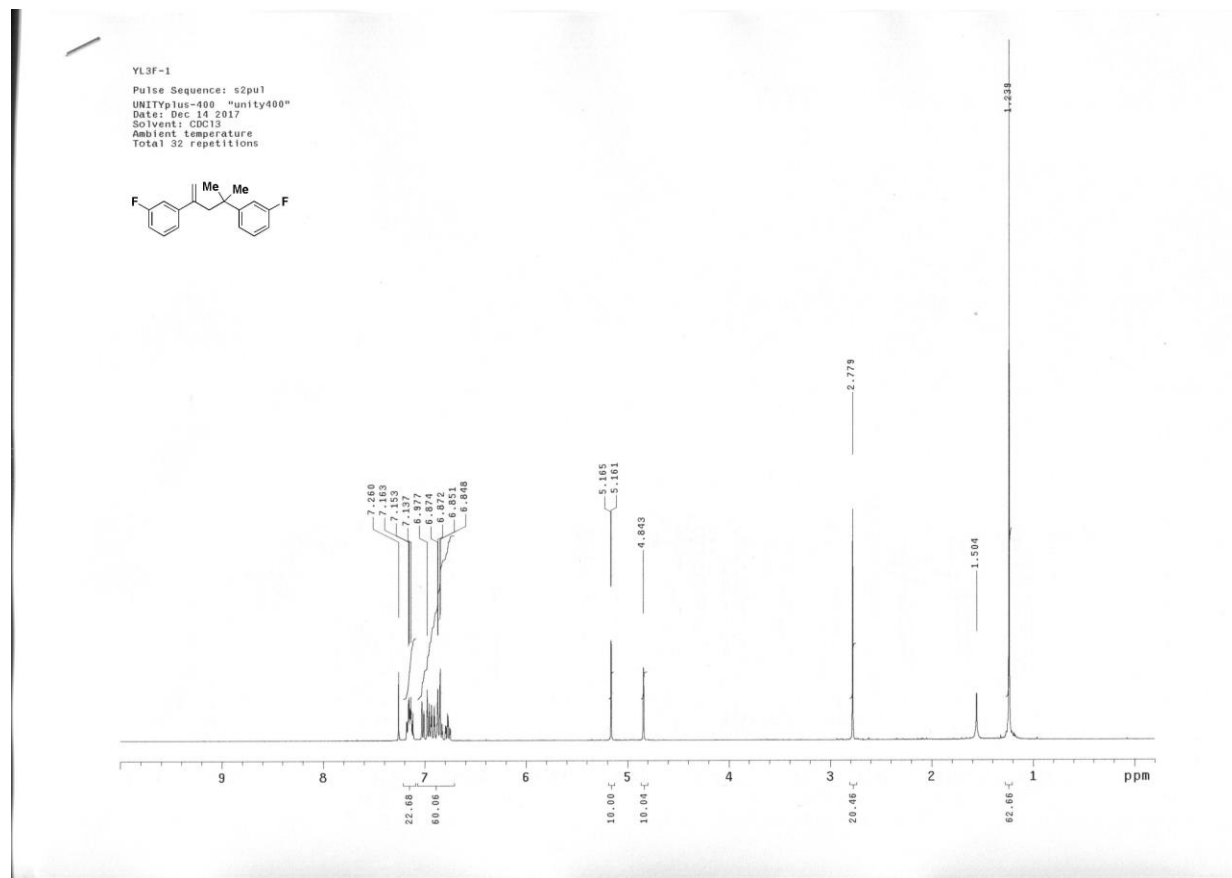
## Compound 4f-1



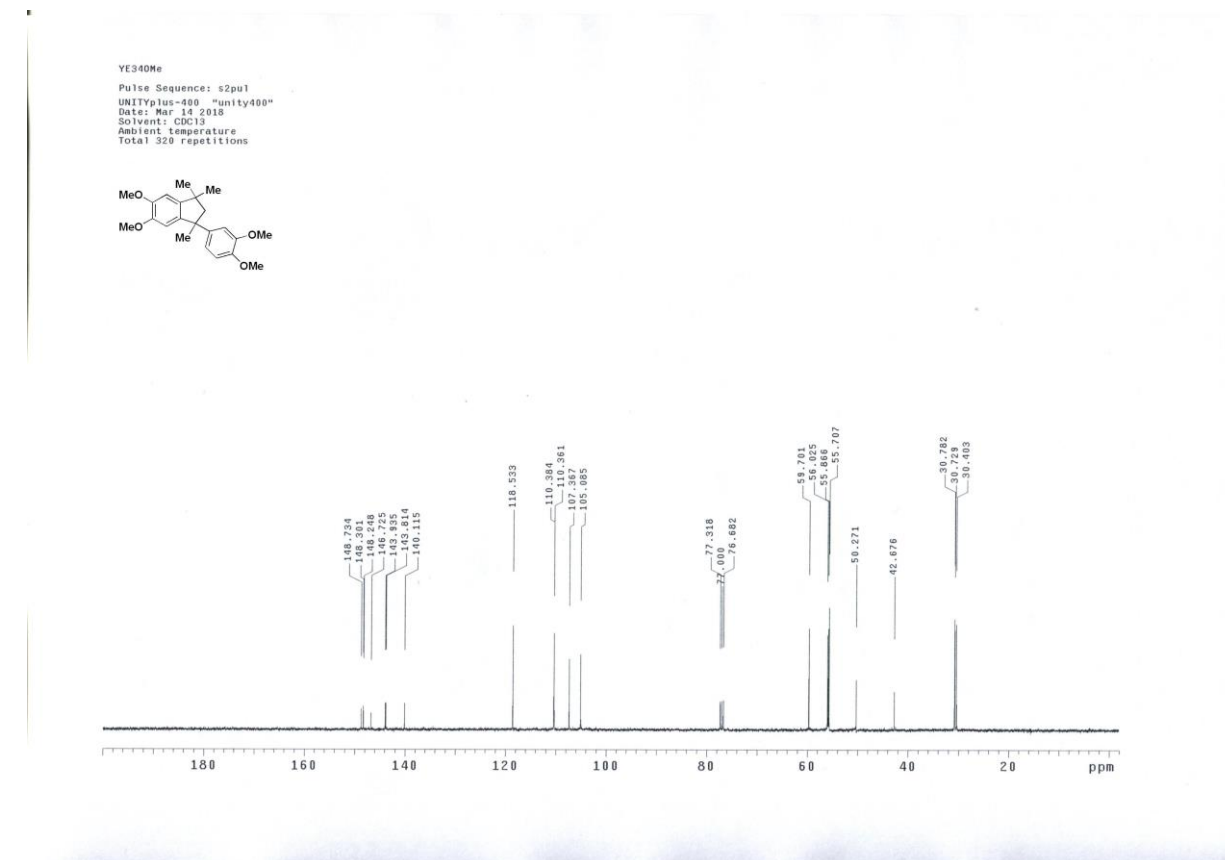
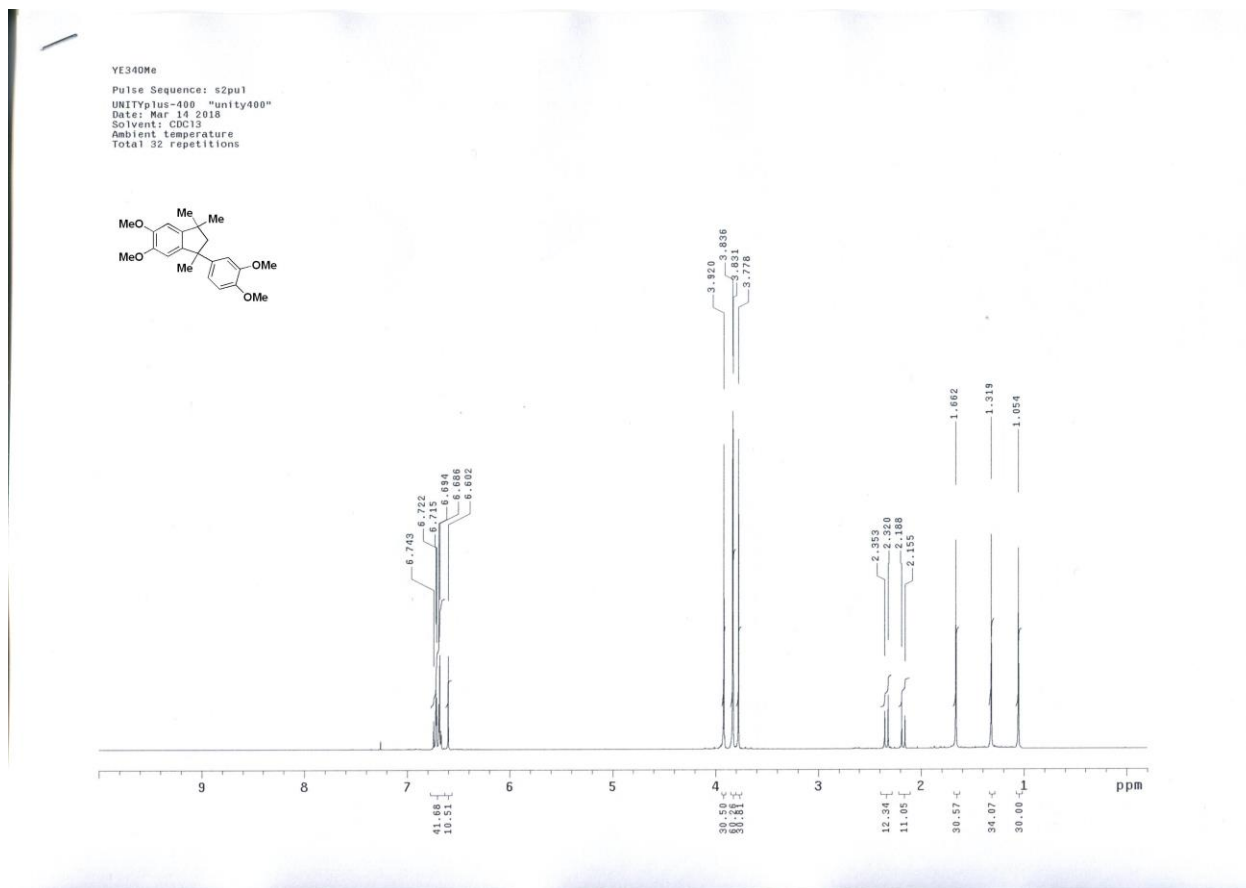
## Compound 4g



## Compound 4g-1

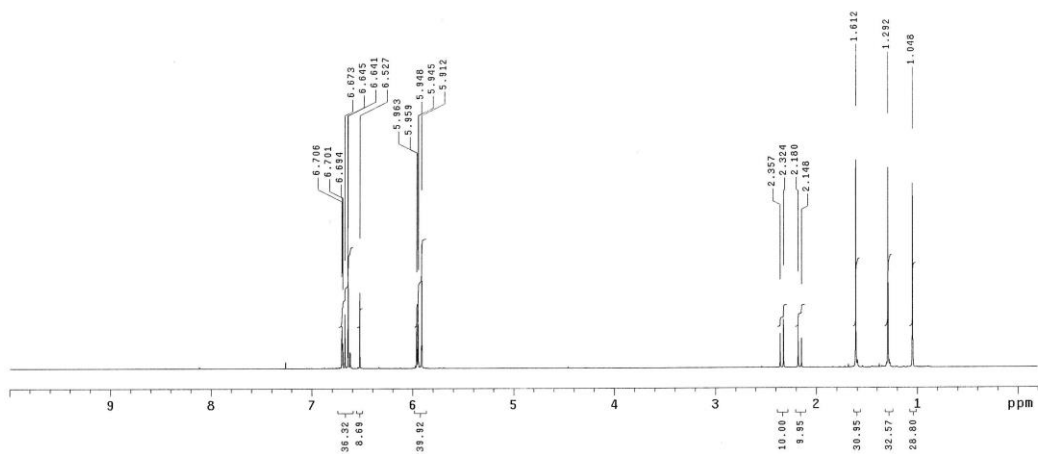
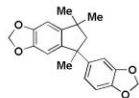


Compound 4h

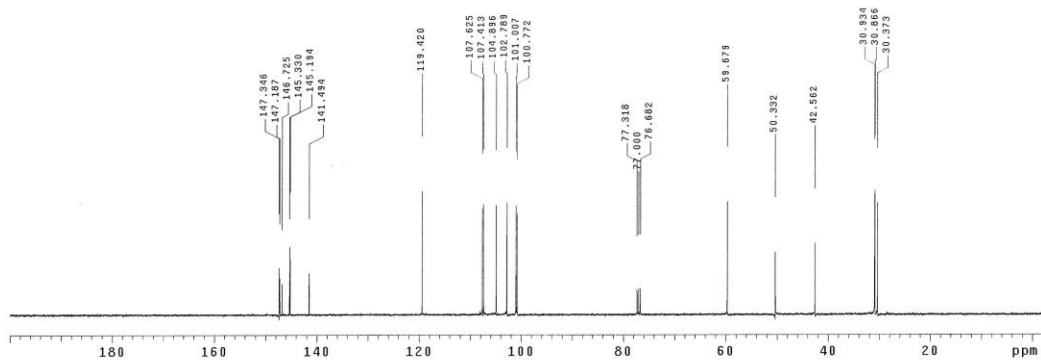
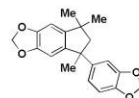


## Compound 4i

NC1060301  
Pulse Sequence: s2pu1  
UNITYplus-400 "unity400"  
Date: Mar 2 2017  
Solvent: CDCl3  
Ambient temperature  
Total 18 repetitions

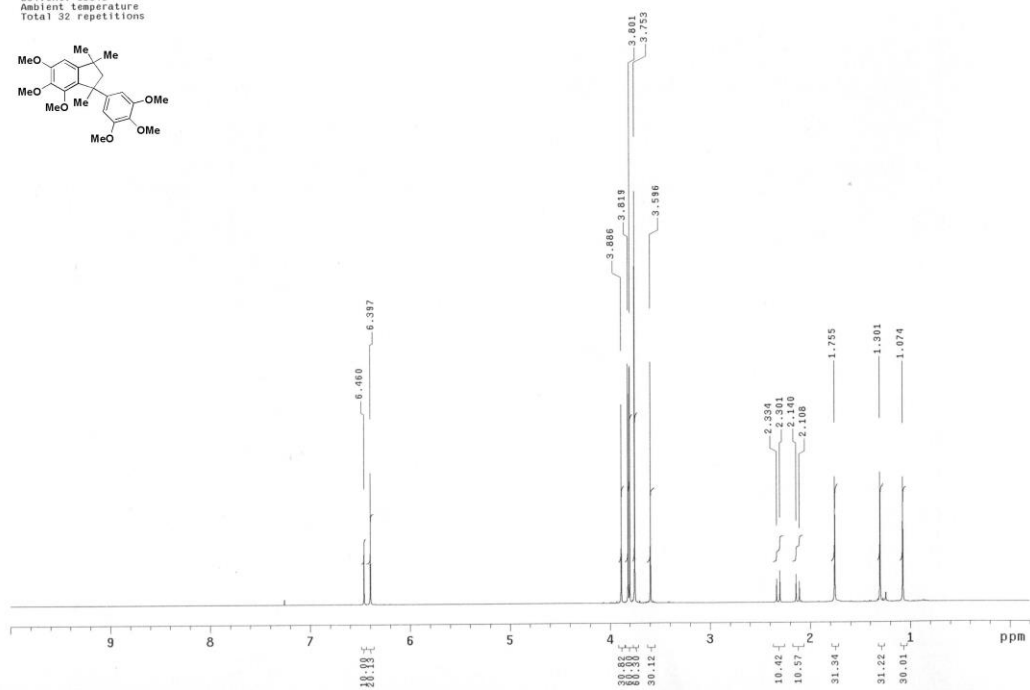
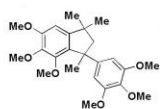


NC1060301  
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UNITYplus-400 "unity400"  
Date: Mar 2 2017  
Solvent: CDCl3  
Ambient temperature  
Total 1104 repetitions

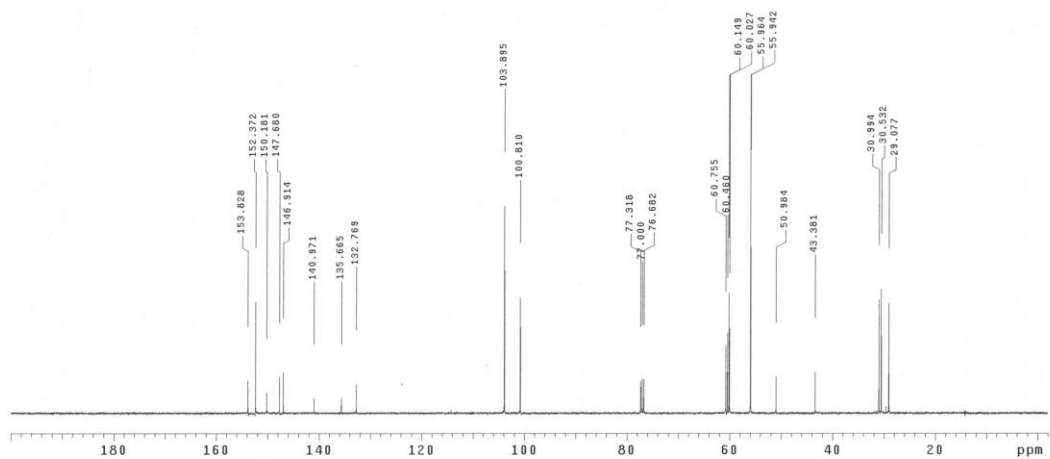
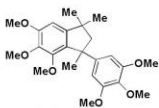


## Compound 4j

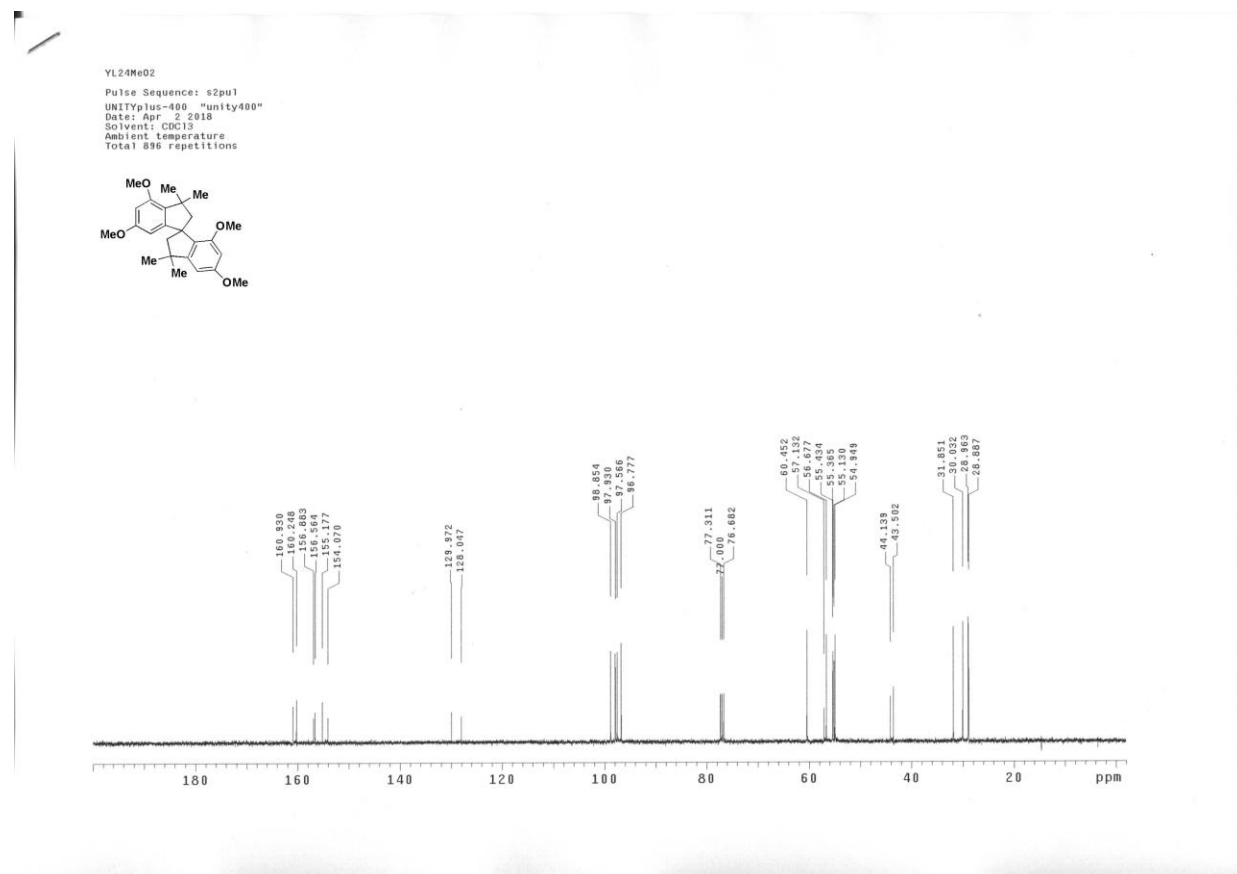
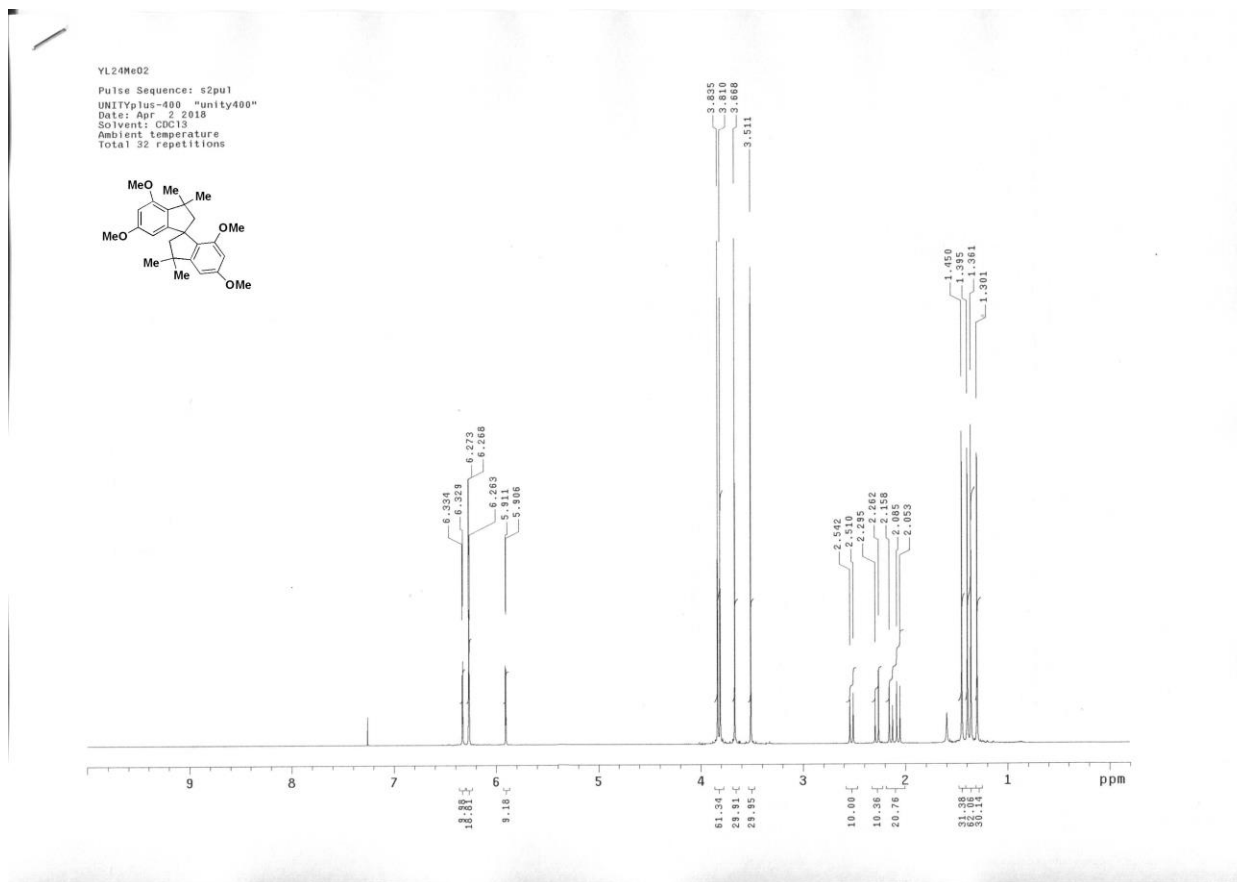
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 Solvent: CDCl3  
 Ambient temperature  
 Total 32 repetitions



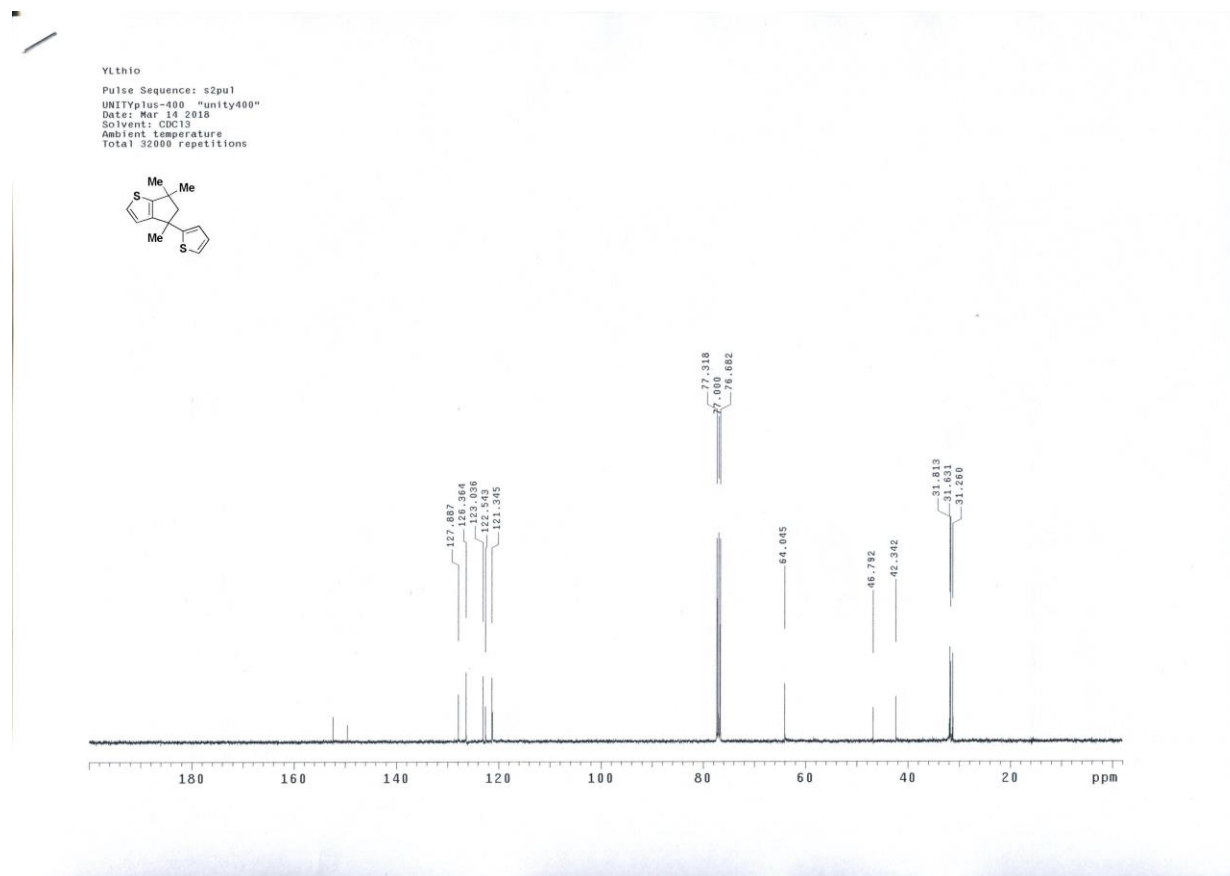
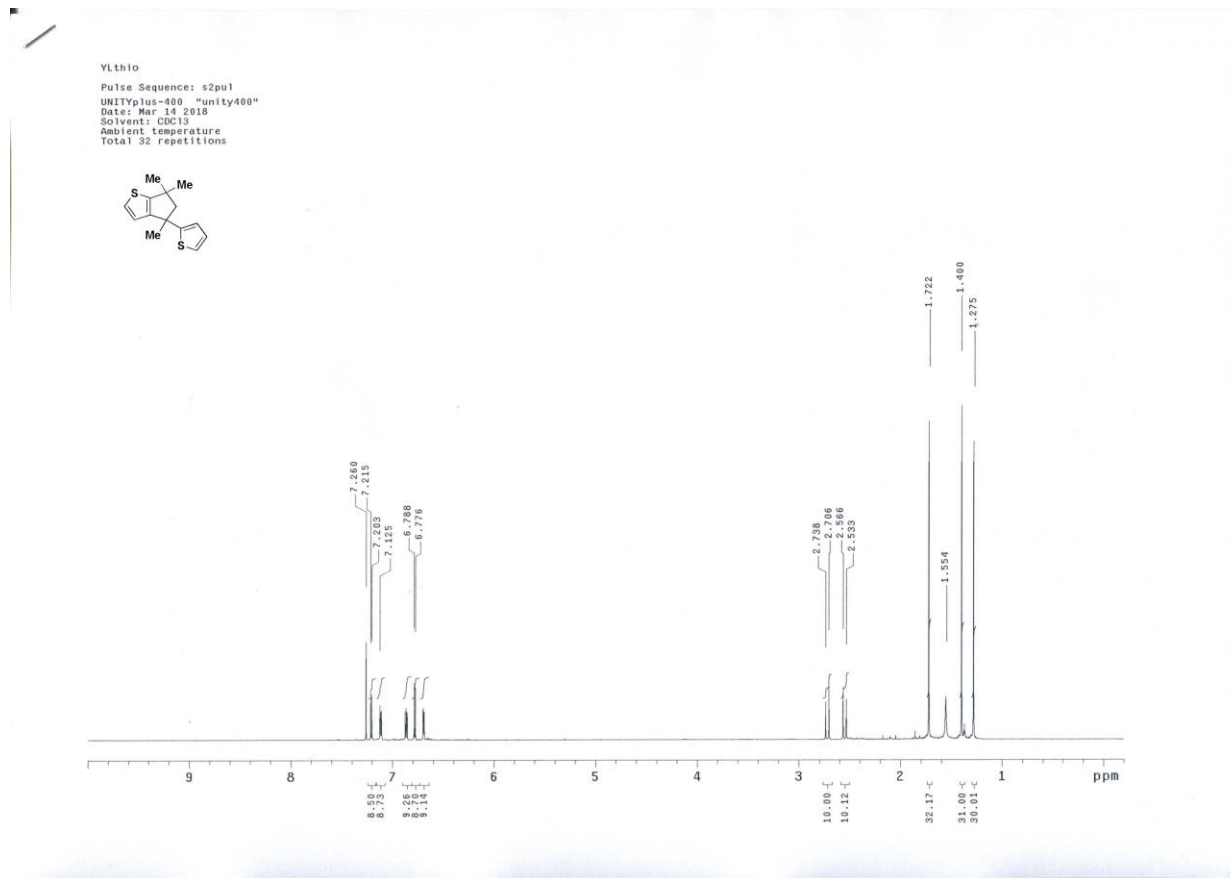
YL30Me  
 Pulse Sequence: s2pul  
 UNIFIplus-400 "unity400"  
 Date: Mar 5 2018  
 Solvent: CDCl3  
 Ambient temperature  
 Total 1792 repetitions



## Compound 4k

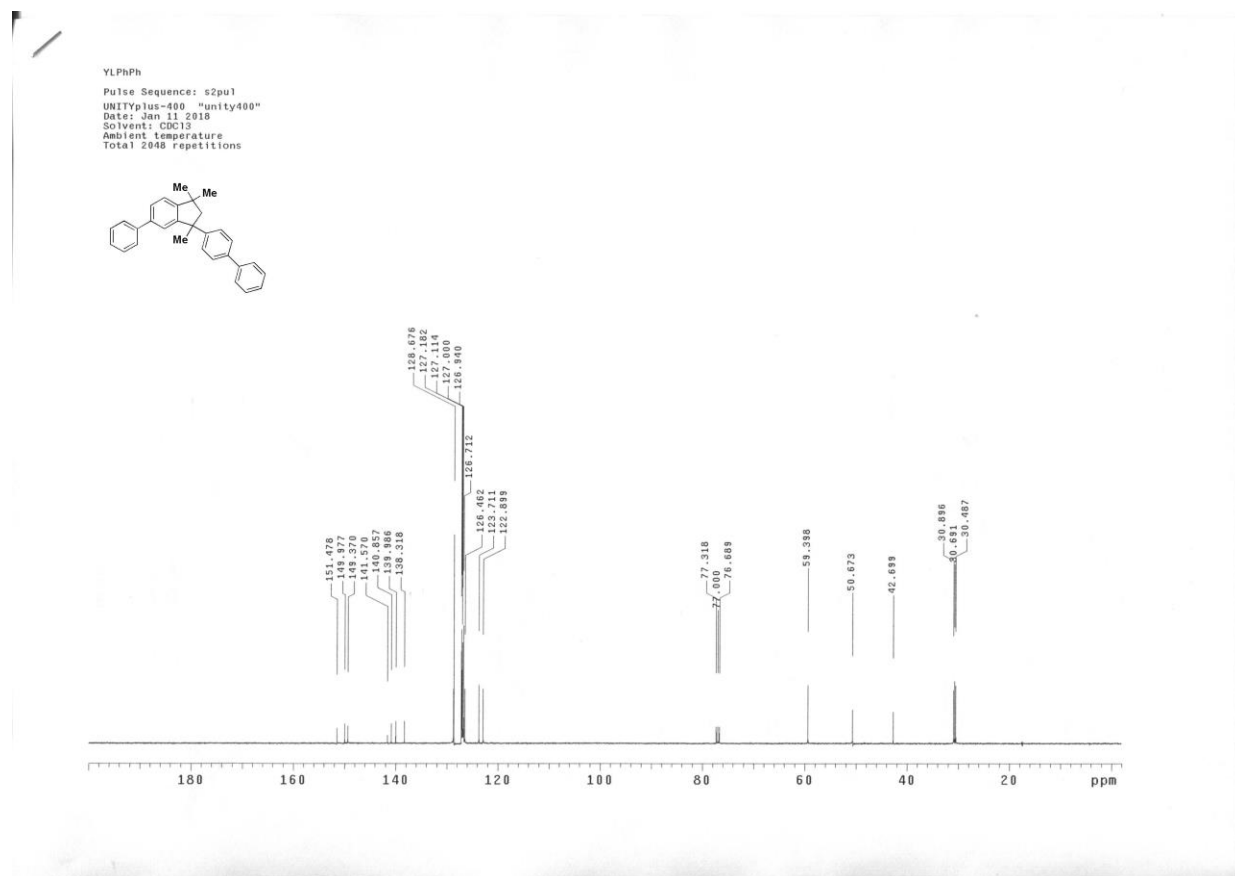
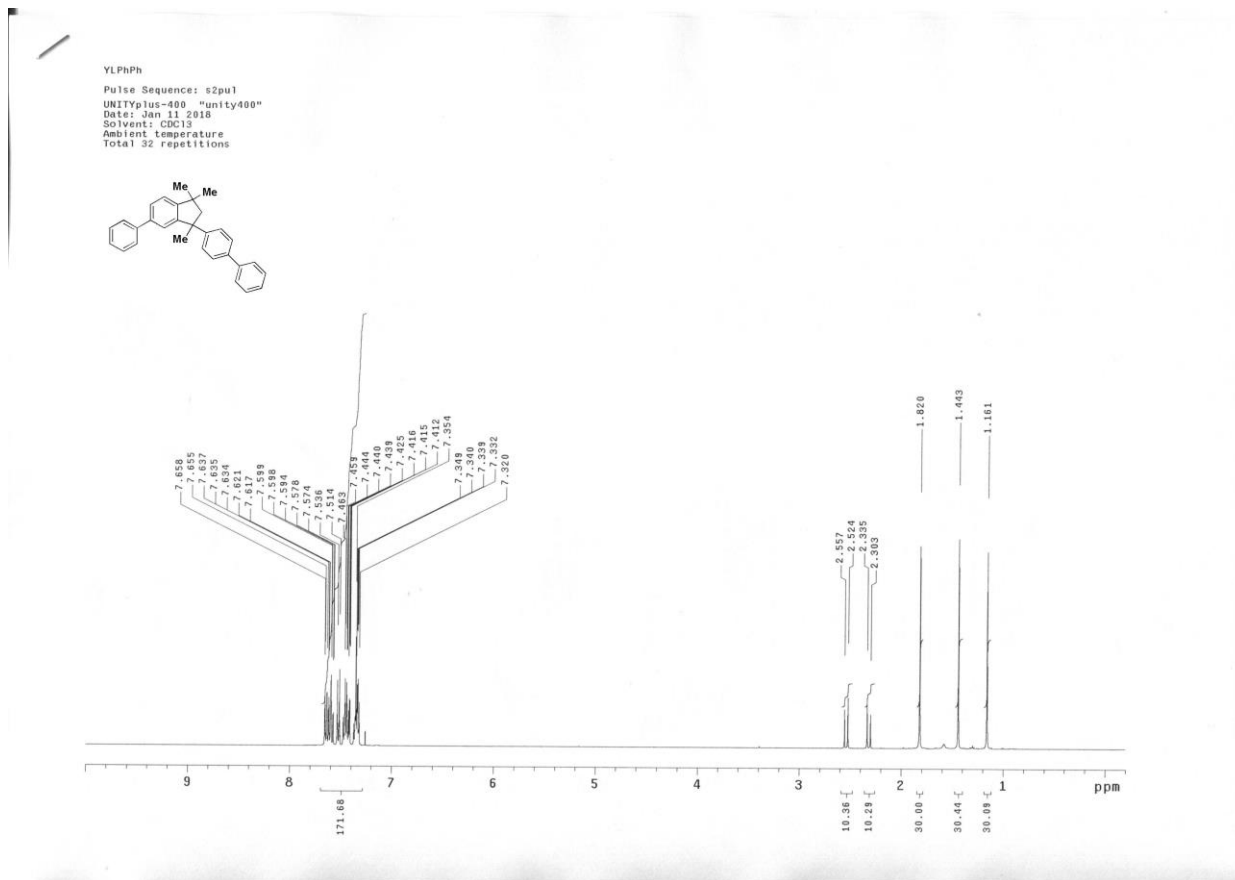


## Compound 4l

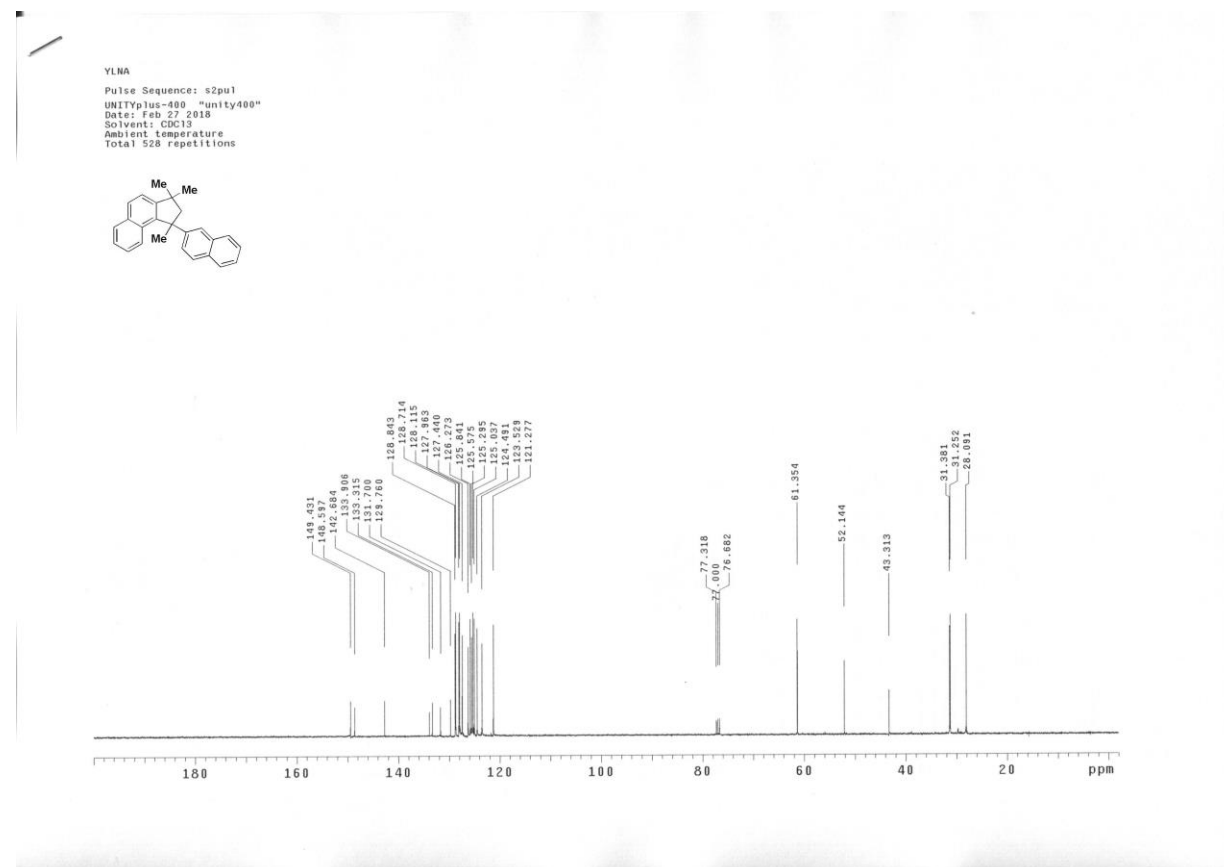
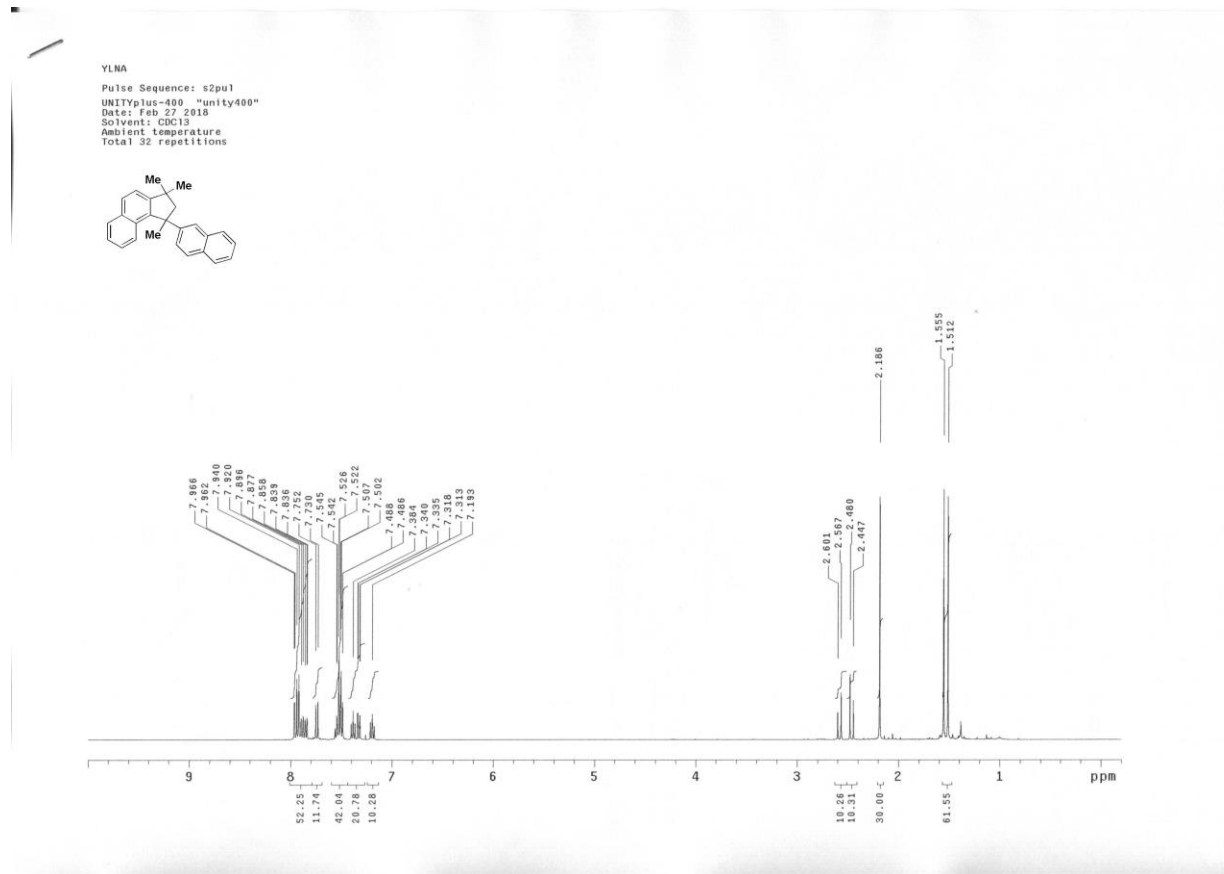




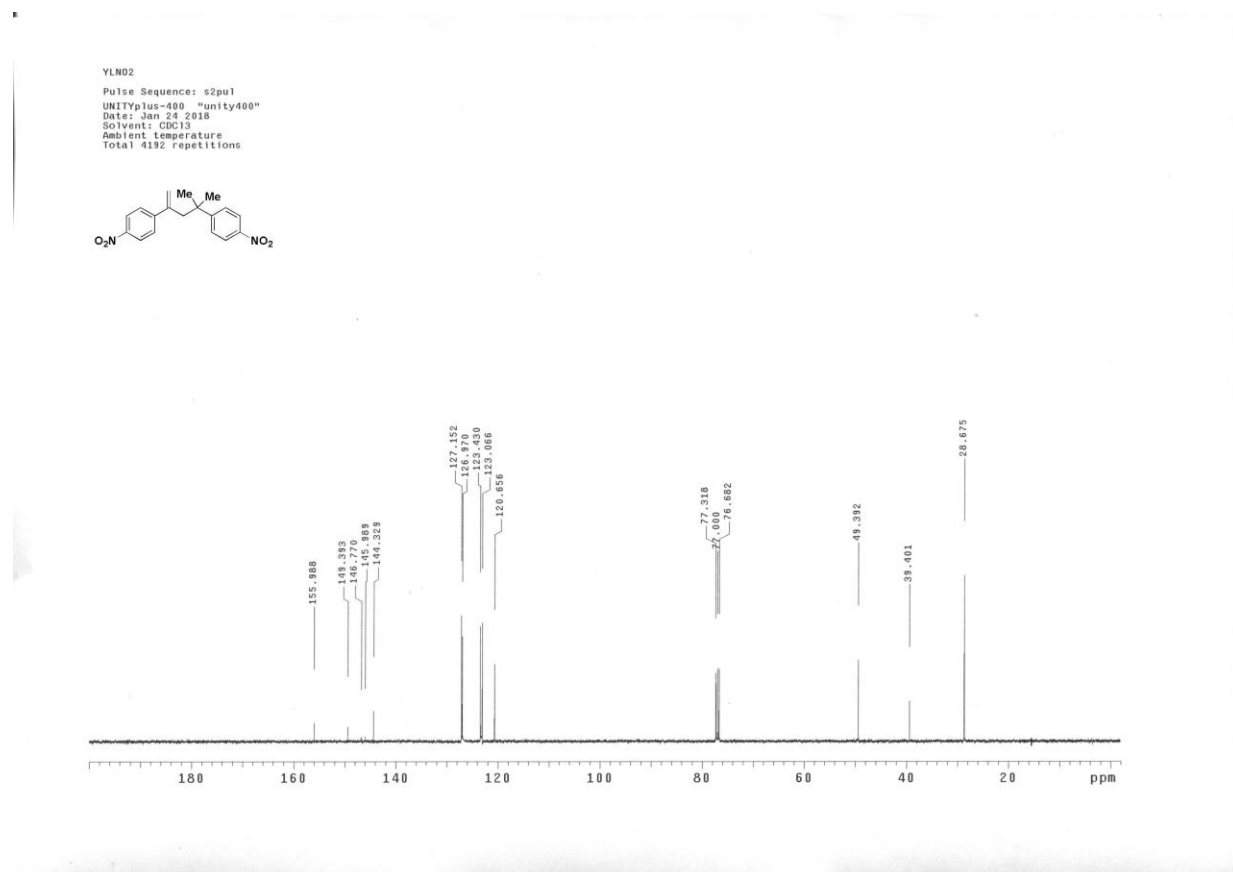
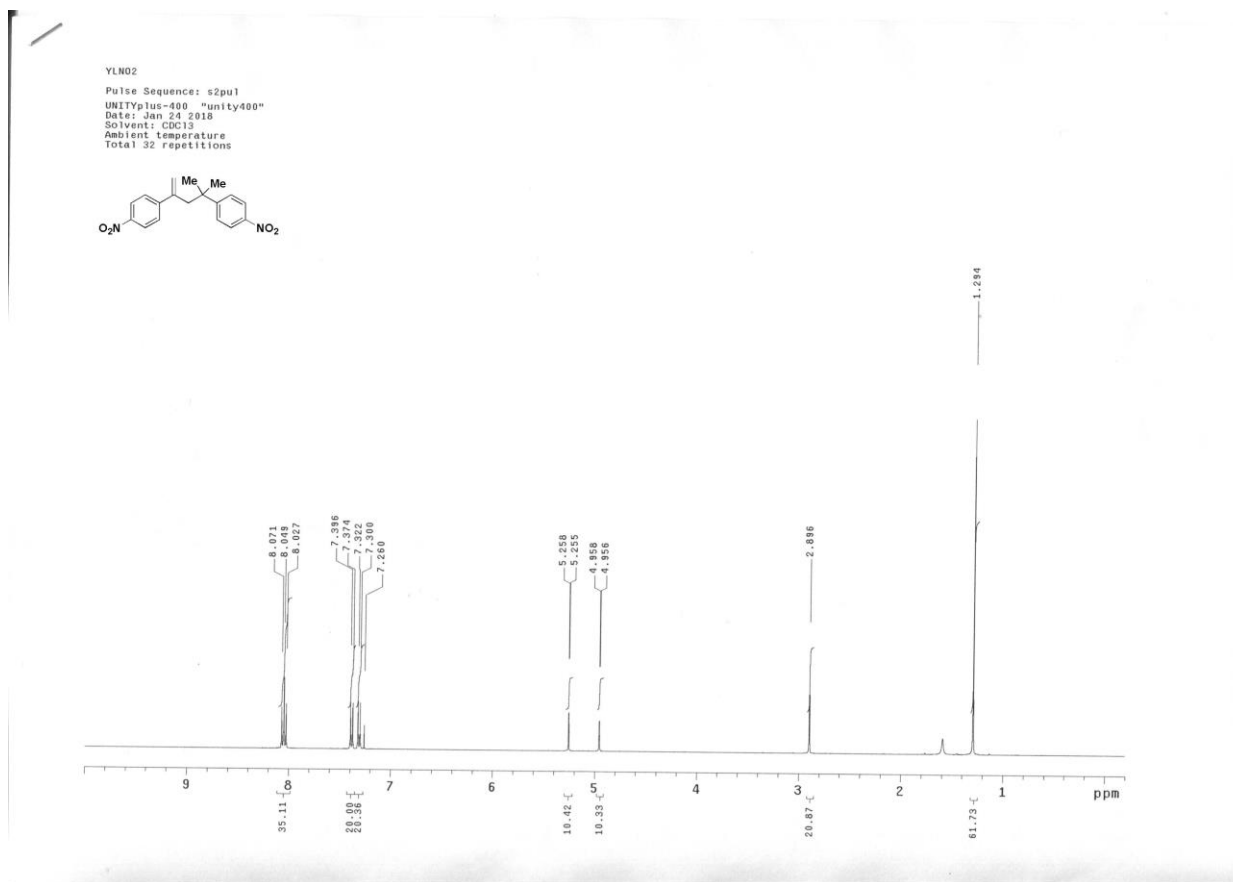
## Compound 4m



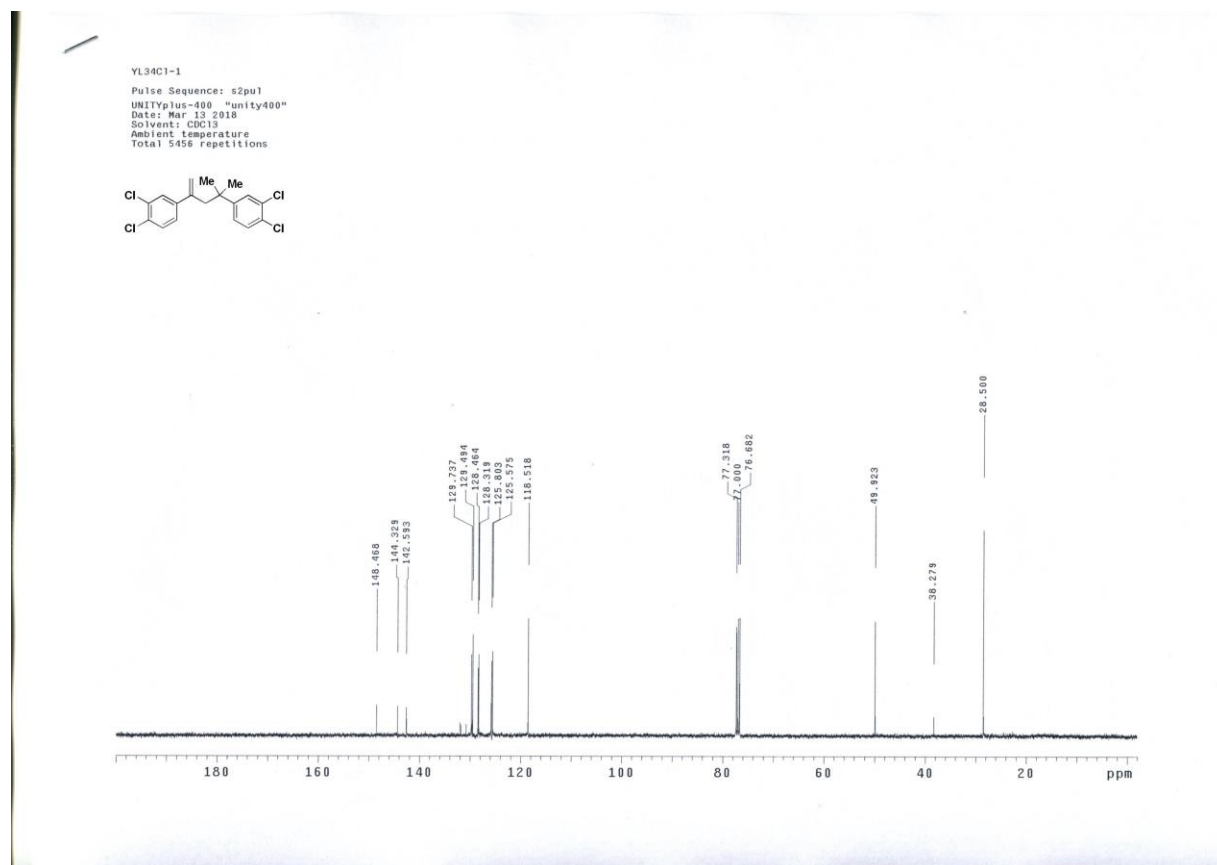
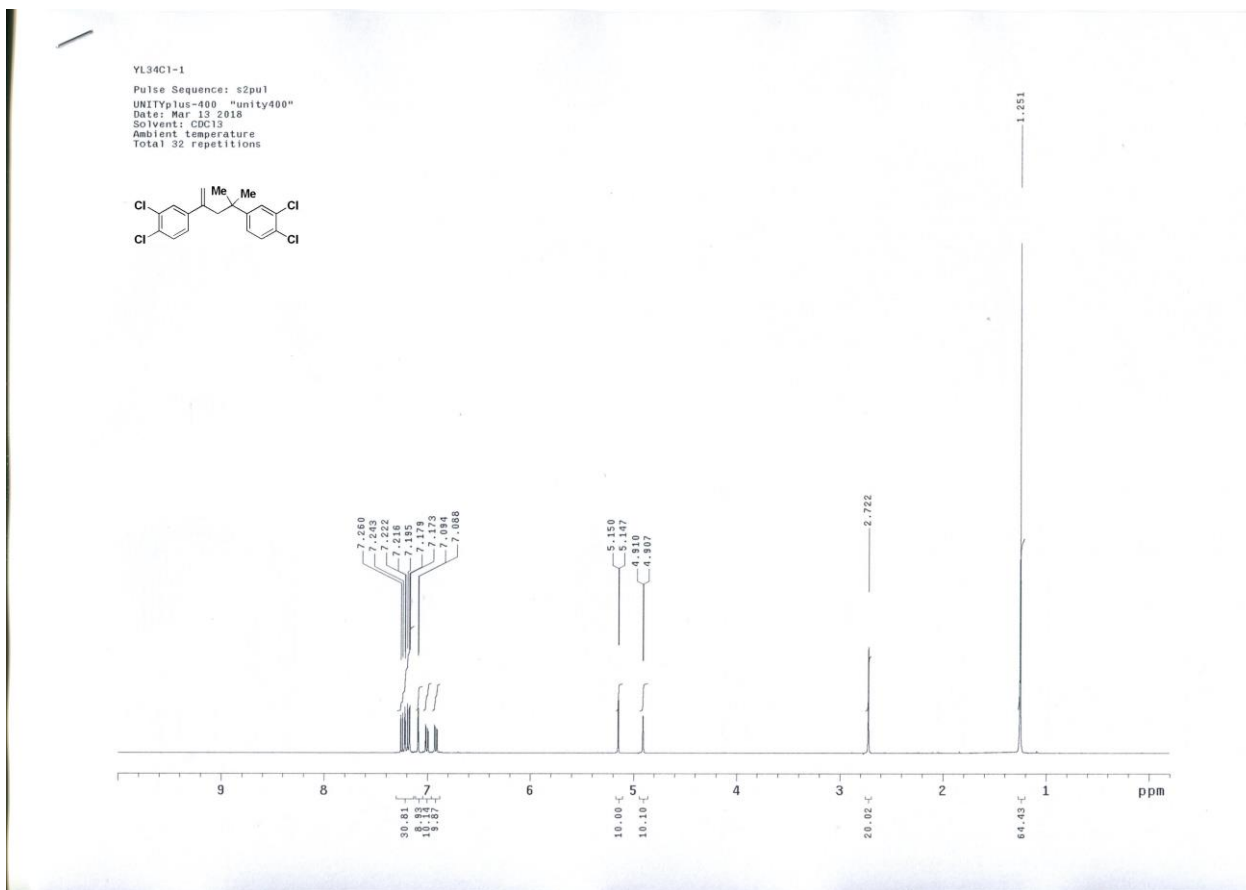
## Compound 4n



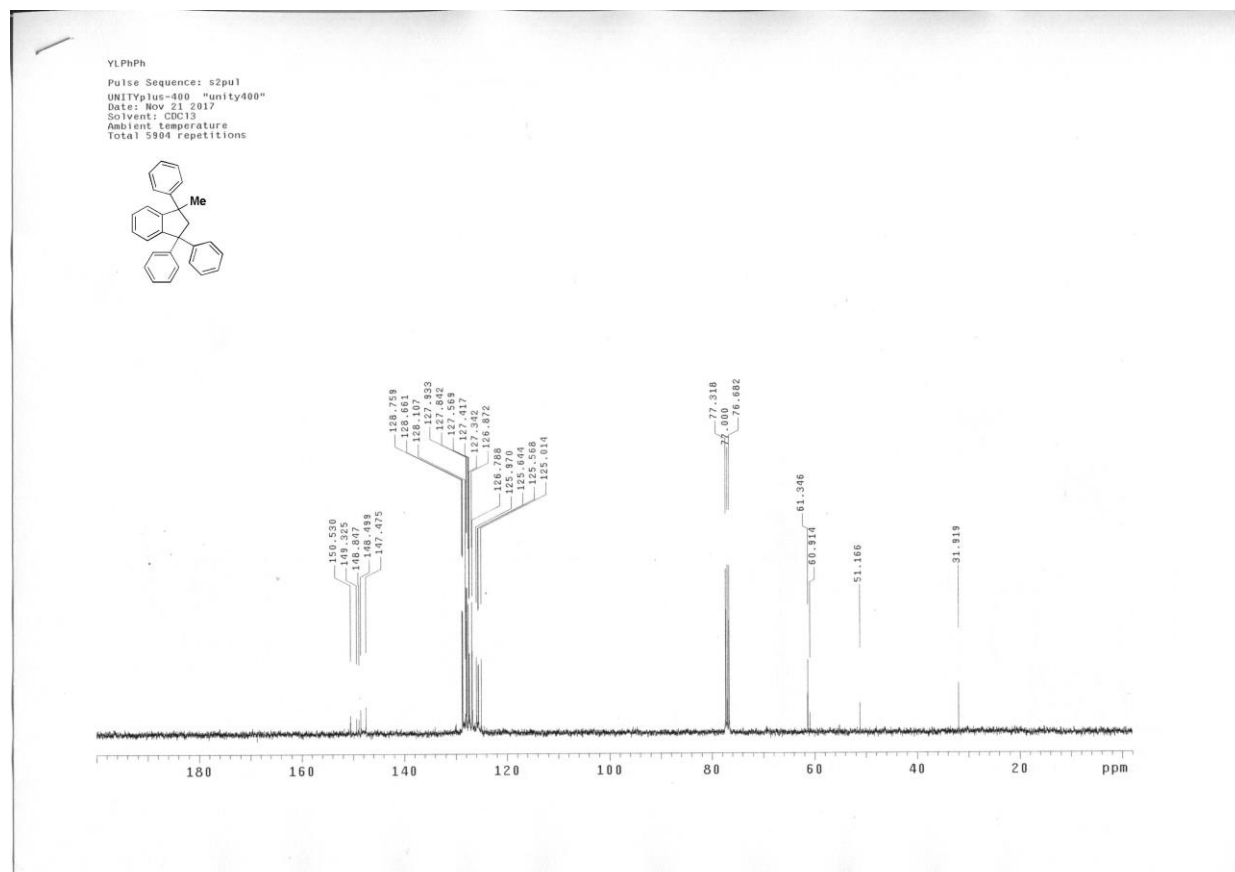
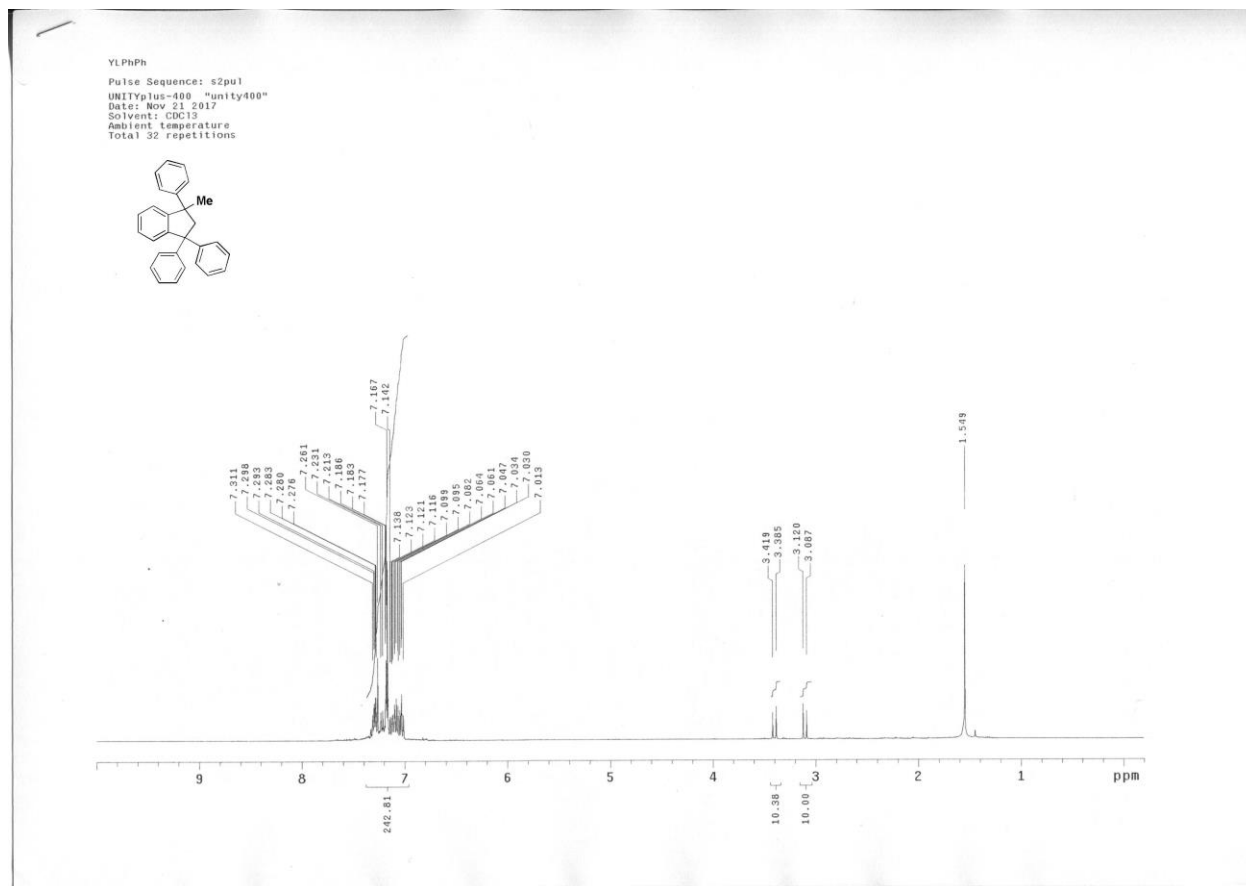
## Compound 4o-1



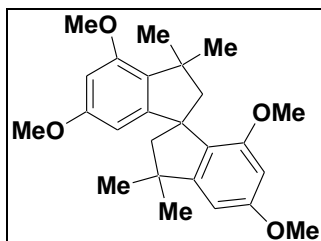
## Compound 4p-1



Compound 4q



## X-ray crystal data of compound 4k



Empirical formula	C <sub>50</sub> H <sub>64</sub> O <sub>8</sub>
Formula weight	793.01
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P -1
Unit cell dimensions	a = 9.4024(3) Å      α = 98.783(2)°. b = 15.5199(5) Å      β = 105.756(2)°. c = 16.4035(6) Å      γ = 104.7270(10)°.
Volume	2163.91(13) Å <sup>3</sup>
Z	2
Density (calculated)	1.217 Mg/m <sup>3</sup>
Absorption coefficient	0.081 mm <sup>-1</sup>
F(000)	856
Crystal size	0.18 x 0.15 x 0.05 mm <sup>3</sup>
Theta range for data collection	1.328 to 26.411°.
Index ranges	-11 ≤ h ≤ 11, -19 ≤ k ≤ 19, -20 ≤ l ≤ 20
Reflections collected	31205
Independent reflections	8872 [R(int) = 0.0374]
Completeness to theta = 25.242°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9485 and 0.9042
Refinement method	Full-matrix least-squares on F <sup>2</sup>
Data / restraints / parameters	8872 / 0 / 539
Goodness-of-fit on F <sup>2</sup>	1.059
Final R indices [I > 2σ(I)]	R1 = 0.0771, wR2 = 0.1993
R indices (all data)	R1 = 0.0976, wR2 = 0.2137
Extinction coefficient	n/a
Largest diff. peak and hole	1.290 and -0.428 e.Å <sup>-3</sup>

**checkCIF/PLATON report**

Structure factors have been supplied for datablock(s) 180413LT\_0m

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No syntax errors found. CIF dictionary Interpreting this report

**Datablock: 180413LT\_0m**

Bond precision: C-C = 0.0042 Å Wavelength=0.71073

Cell: a=9.4024 (3) b=15.5199 (5) c=16.4035 (6)  
 alpha=98.783 (2) beta=105.756 (2) gamma=104.727 (1)  
 Temperature: 100 K

	Calculated	Reported
Volume	2163.92 (13)	2163.91 (13)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C25 H32 O4	?
Sum formula	C25 H32 O4	C50 H64 O8
Mr	396.51	793.01
Dx, g cm <sup>-3</sup>	1.217	1.217
Z	4	2
Mu (mm <sup>-1</sup> )	0.081	0.081
F000	856.0	856.0
F000'	856.40	
h, k, lmax	11, 19, 20	11, 19, 20
Nref	8898	8872
Tmin, Tmax	0.986, 0.996	0.904, 0.948
Tmin'	0.986	

Correction method= # Reported T Limits: Tmin=0.904 Tmax=0.948  
 AbsCorr = MULTI-SCAN

Data completeness= 0.997 Theta (max)= 26.411

R(reflections)= 0.0771 ( 6827) wR2(reflections)= 0.2137 ( 8872)

S = 1.059 Npar= 539

The following ALERTS were generated. Each ALERT has the format  
**test-name\_ALERT\_alert-type\_alert-level**.  
 Click on the hyperlinks for more details of the test.

## The thermal ellipsoid was drawn at the 50% probability level

