

Nickel-Catalyzed Cross-Coupling of Allyl Alcohols with Aryl- or Alkenylzinc Reagents

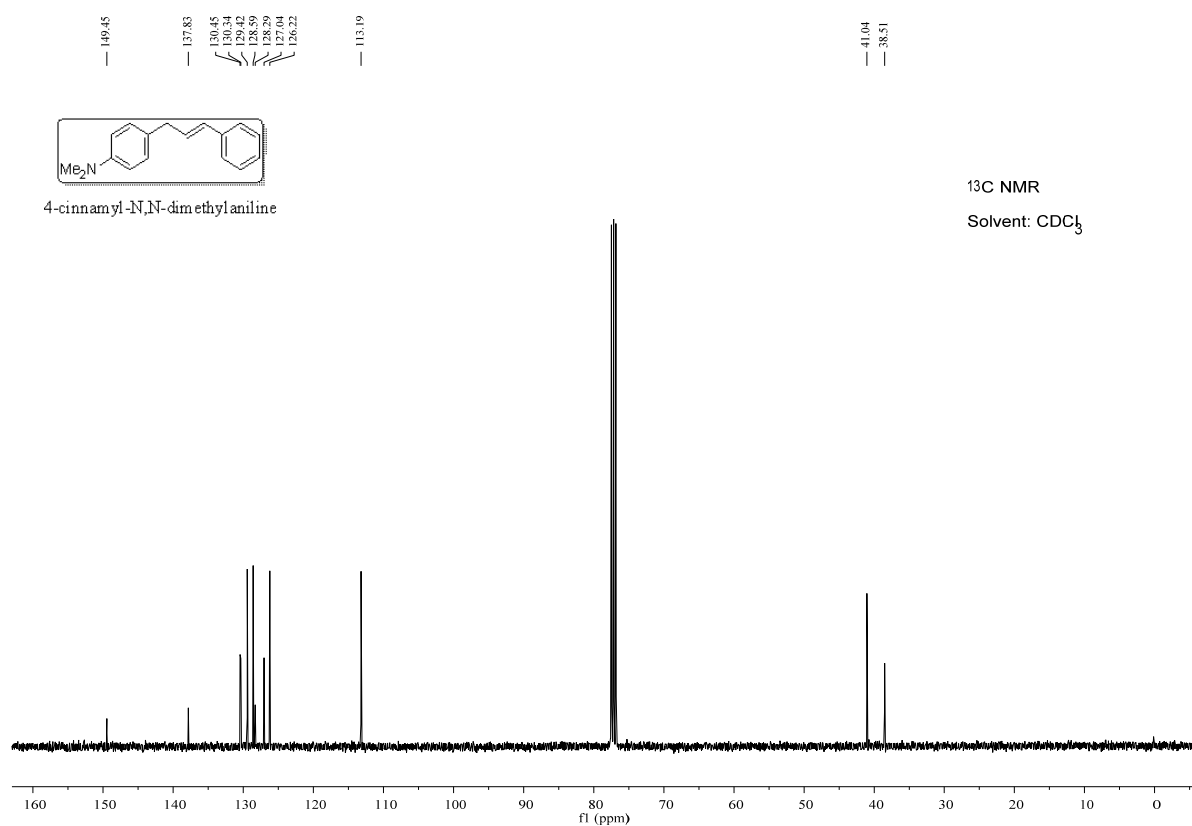
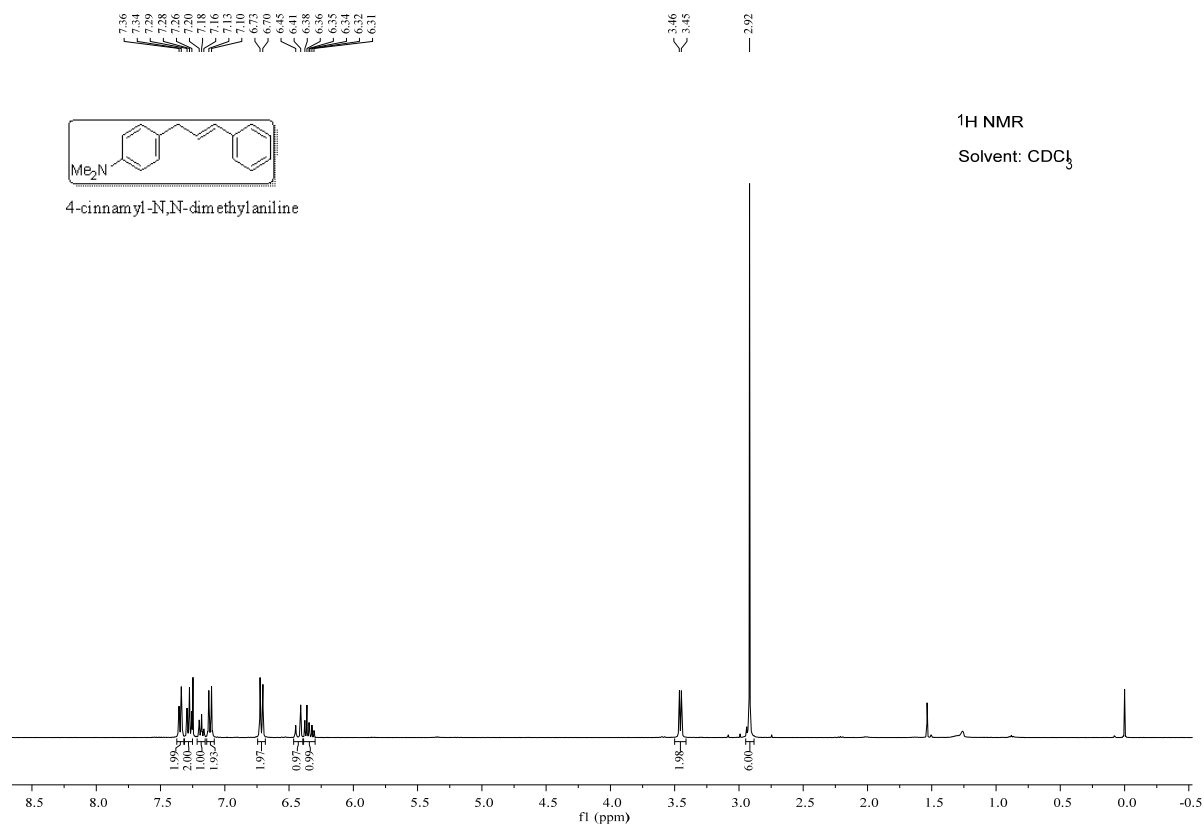
Bo Yang, and Zhong-Xia Wang*

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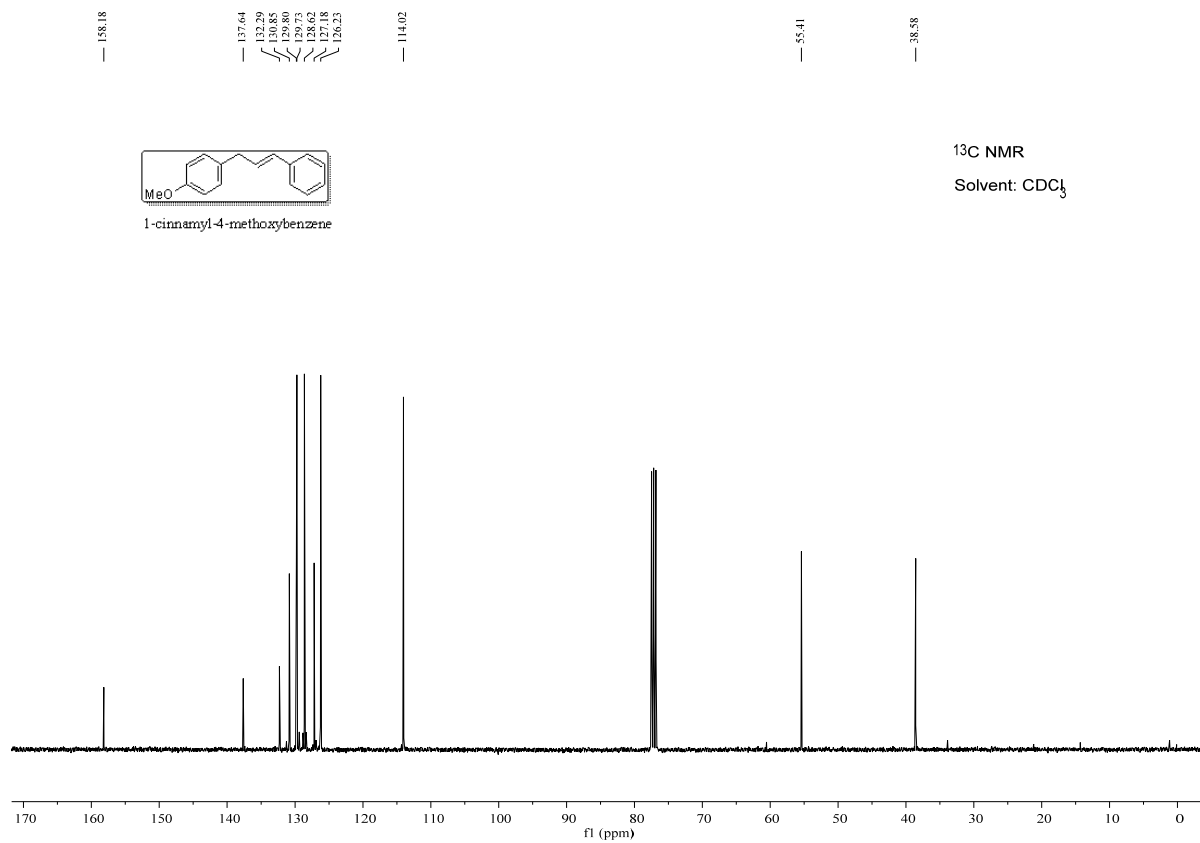
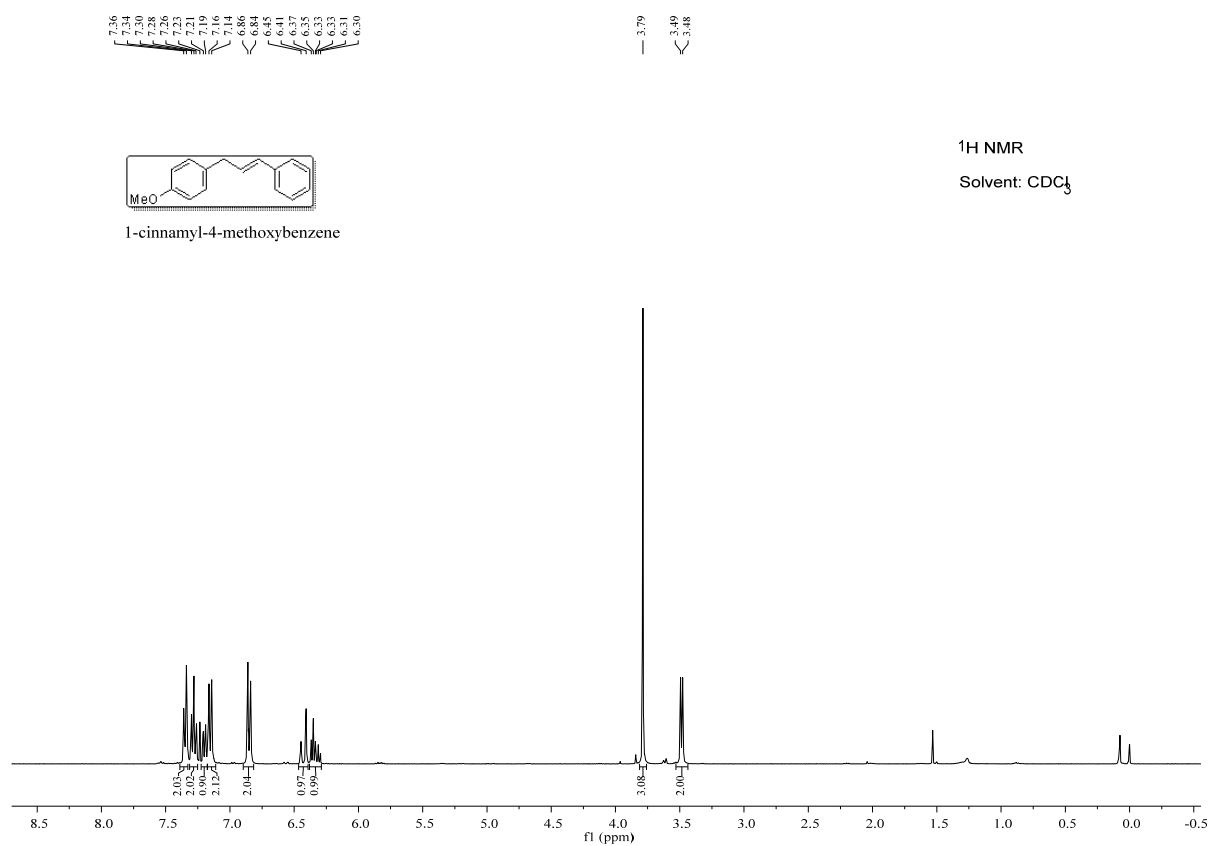
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5-cinnamylbenzo[d][1,3]dioxole (3c)	4
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Copies of NMR spectra of the cross-coupling products

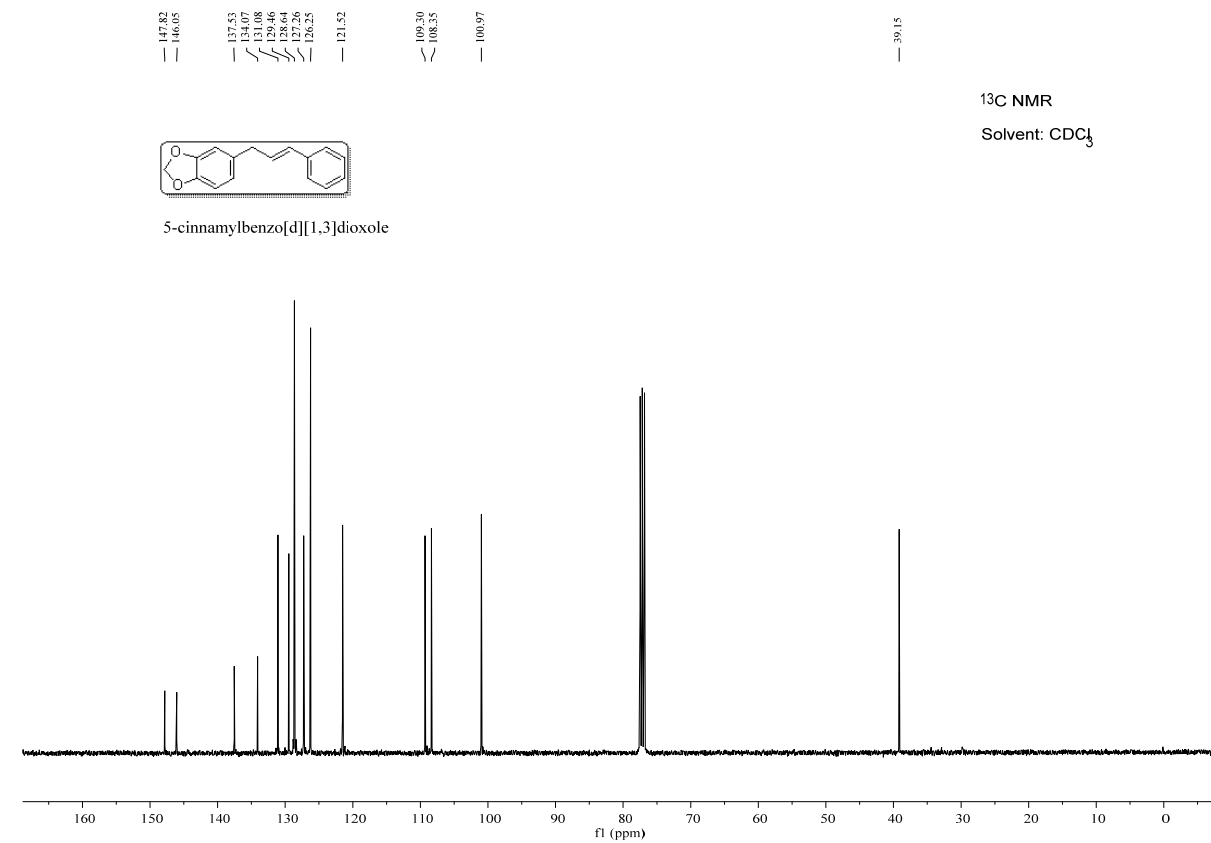
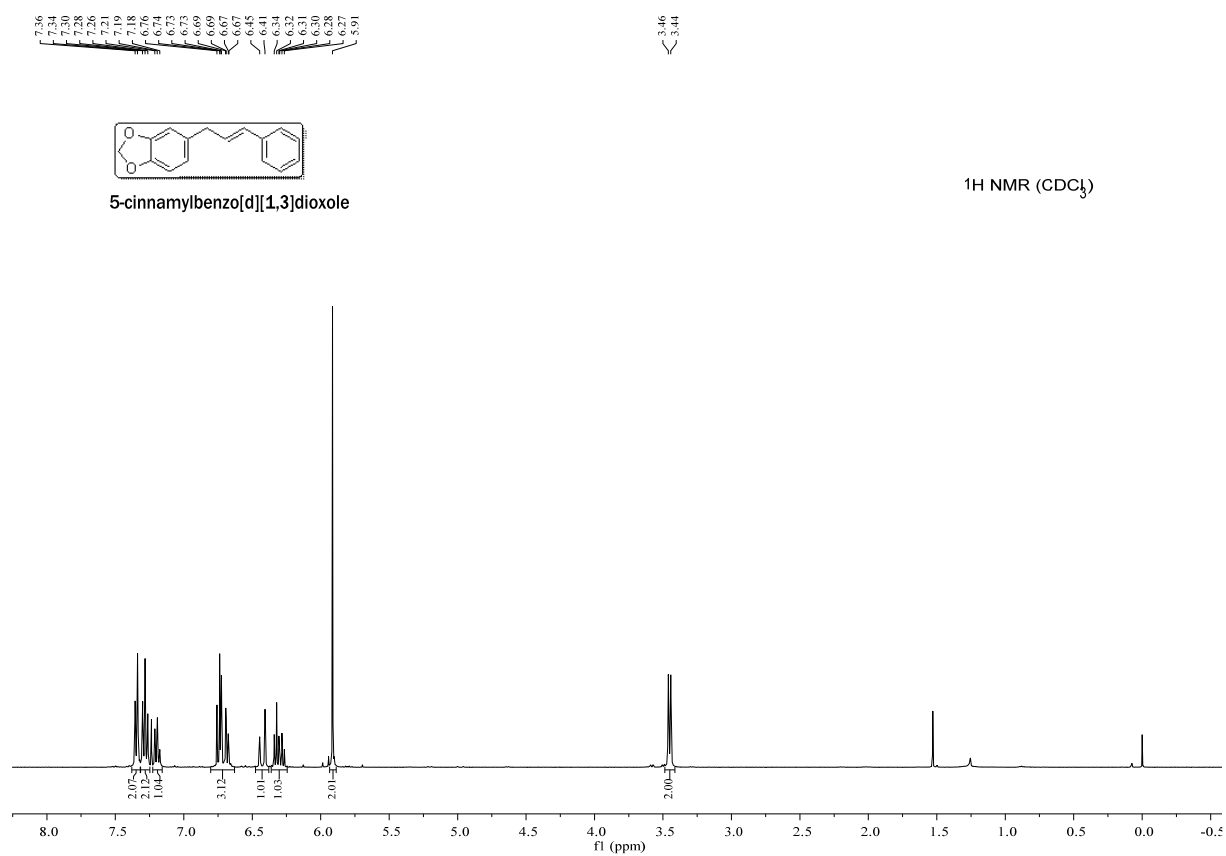
(1) 4-cinnamyl-*N,N*-dimethylaniline (**3a**)



(2) 1-cinnamyl-4-methoxybenzene (**3b**)



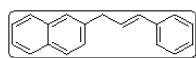
(3) 5-cinnamylbenzo[d][1,3]dioxole (3c)



(4) 2-cinnamyl naphthalene (3d)

7.81
7.79
7.77
7.66
7.46
7.44
7.42
7.41
7.40
7.35
7.30
7.28
7.26
7.21
7.18
7.15
6.46
6.44
6.42
6.41
6.40
6.38

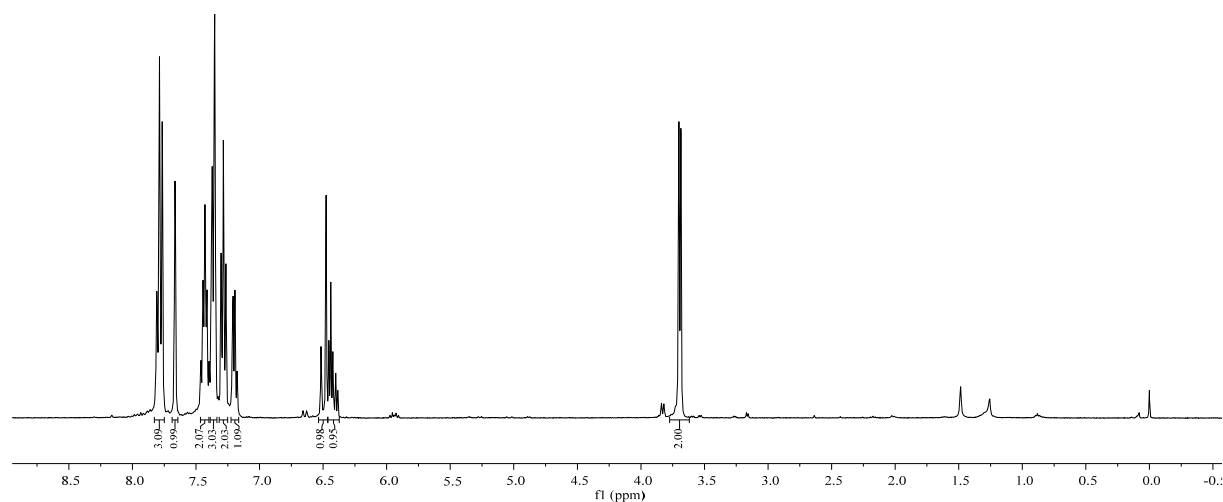
3.70
3.69



2-cinnamyl naphthalene

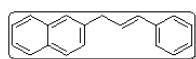
¹H NMR

Solvent: CDCl₃



137.79
137.61
137.44
133.82
132.33
131.47
129.20
128.66
128.18
127.78
127.65
127.59
127.50
126.89
126.30
126.13
125.47

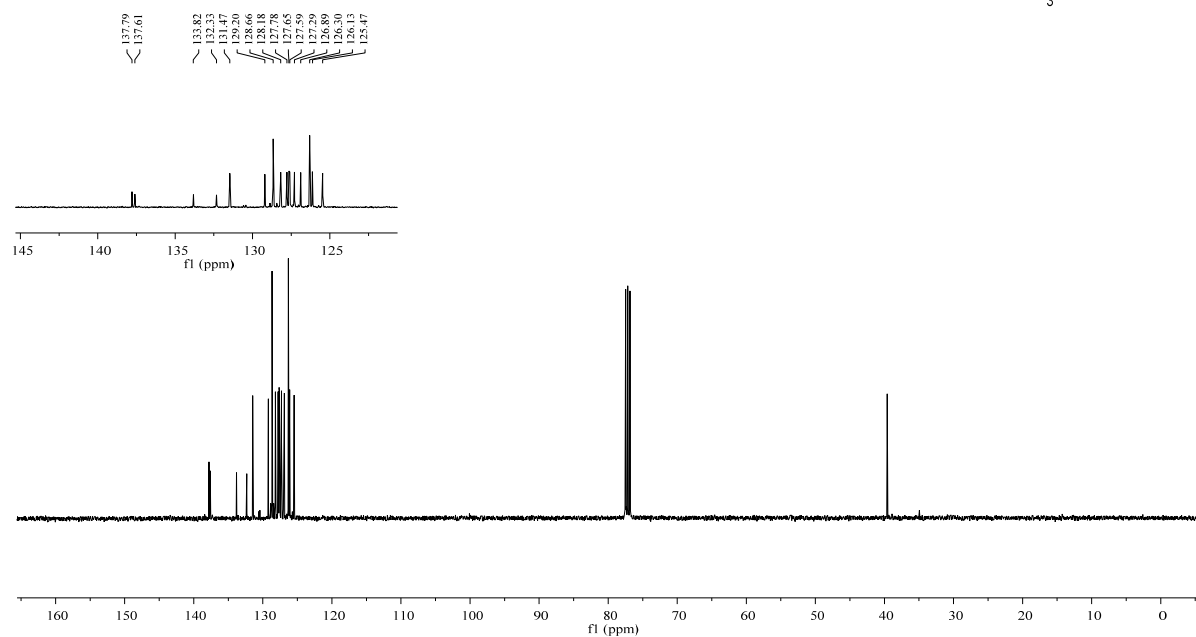
39.60



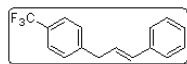
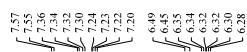
2-cinnamyl naphthalene

¹³C NMR

Solvent: CDCl₃



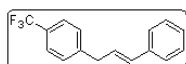
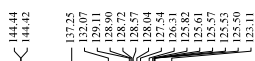
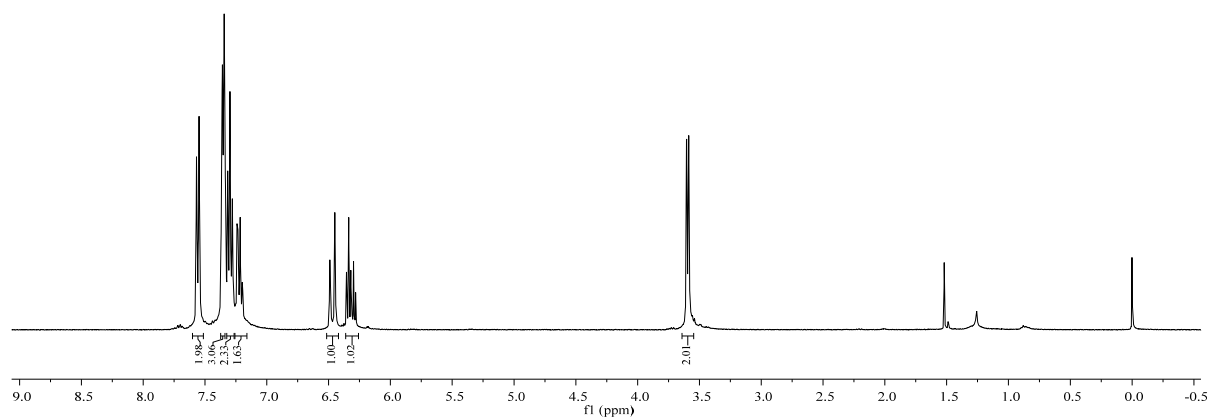
(5) 1-cinnamyl-4-(trifluoromethyl)benzene (**3e**)



1-cinnamyl-4-(trifluoromethyl)benzene

¹H NMR

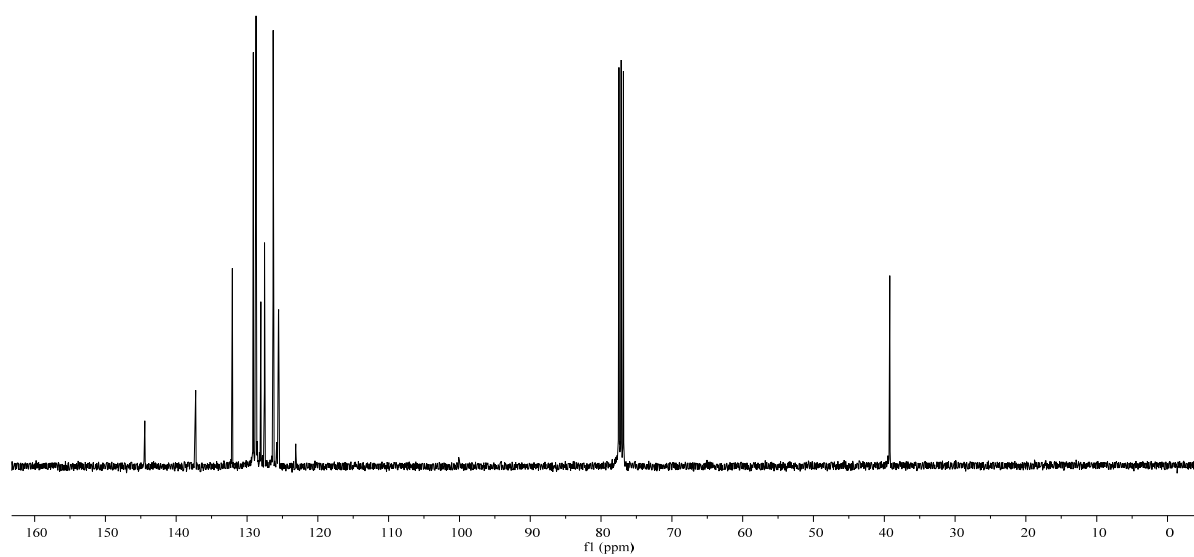
Solvent: CDCl₃

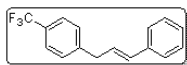


1-cinnamyl-4-(trifluoromethyl)benzene

¹³C NMR

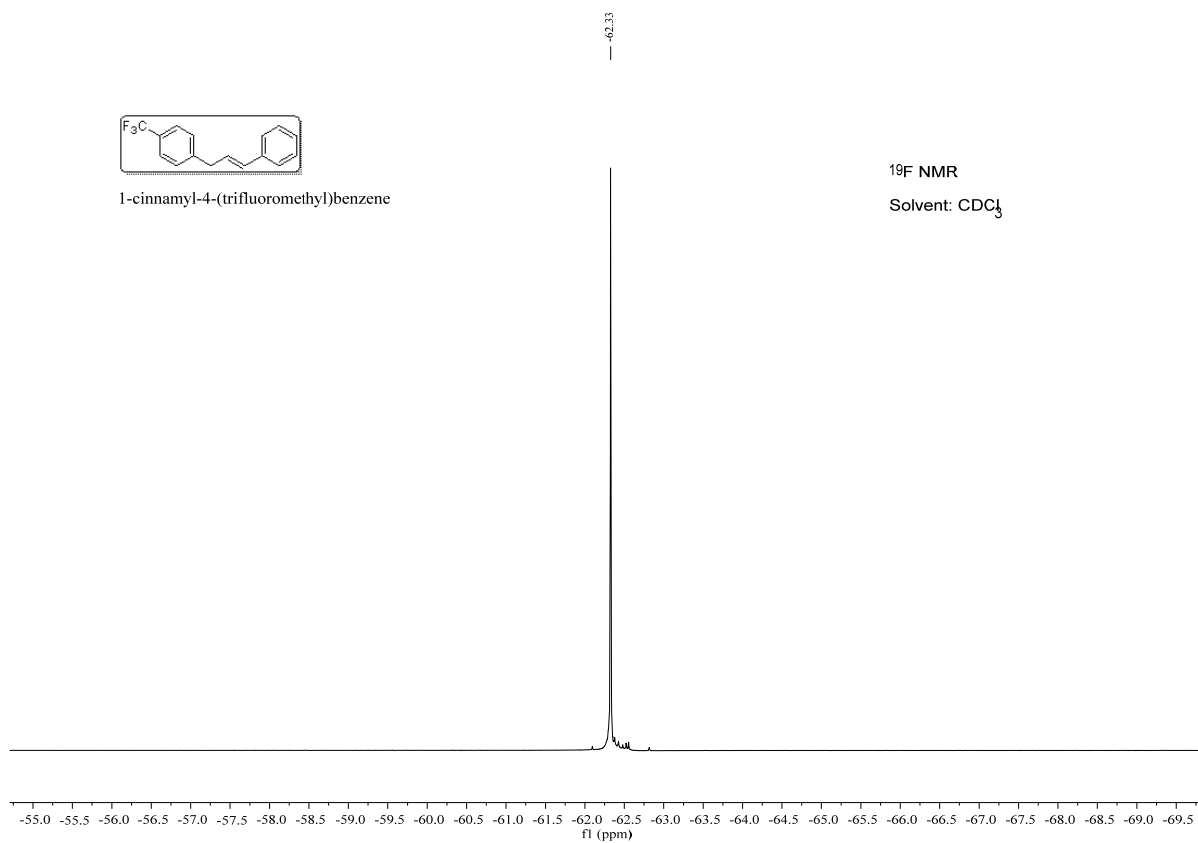
Solvent: CDCl₃



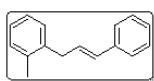


1-cinnamyl-4-(trifluoromethyl)benzene

^{19}F NMR
Solvent: CDCl_3



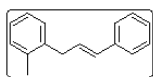
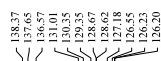
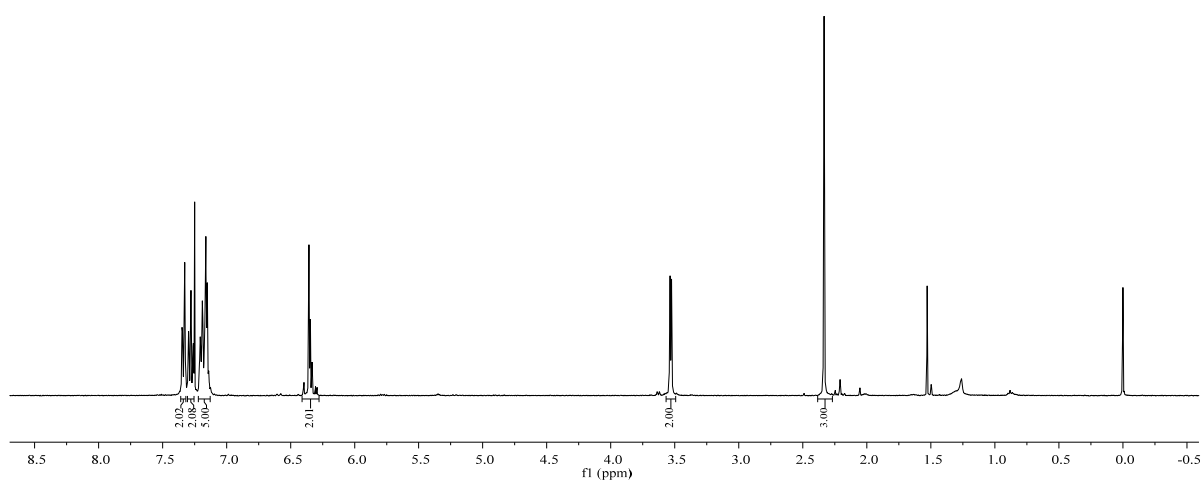
(6) 1-cinnamyl-2-methylbenzene (**3f**)



1-cinnamyl-2-methylbenzene

¹H NMR

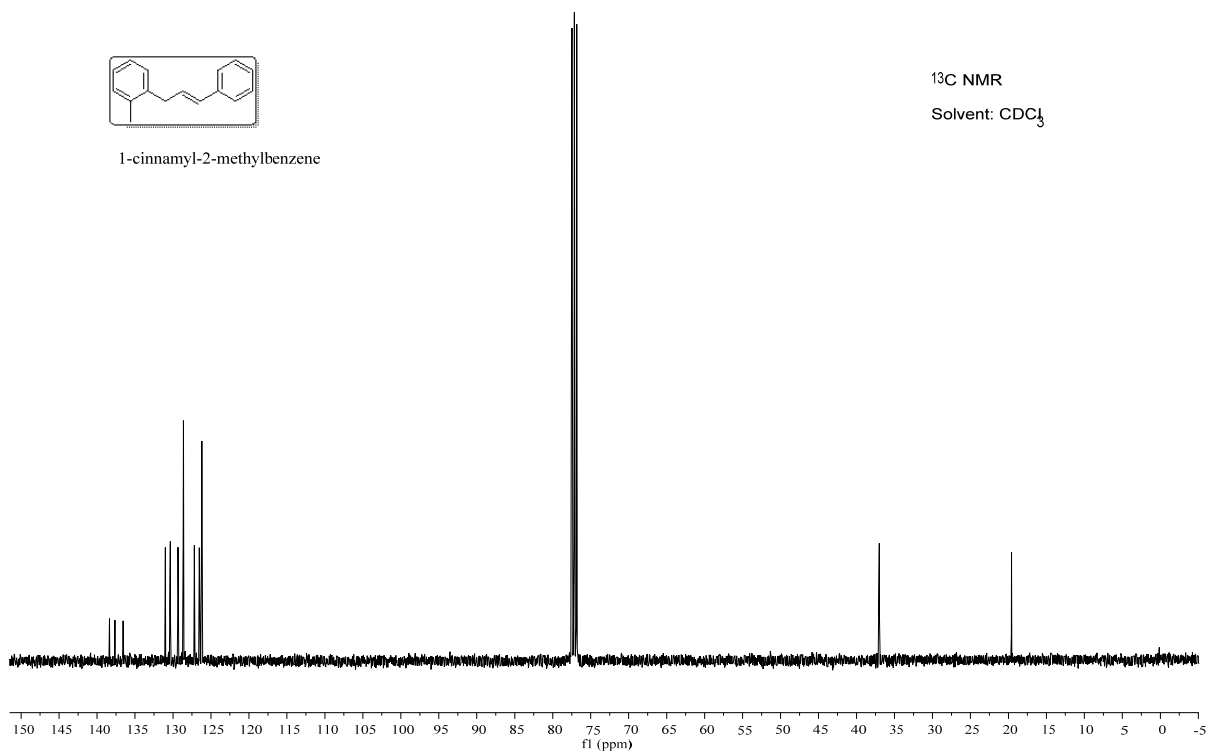
Solvent: CDCl₃



1-cinnamyl-2-methylbenzene

¹³C NMR

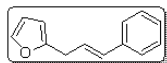
Solvent: CDCl₃



(7) 2-cinnamylfuran (**3g**)

7.36
7.36
7.34
7.33
7.30
7.30
7.28
7.27
7.21
7.19
7.18
6.63
6.63
6.32
6.30
6.29
6.28
6.26
6.05

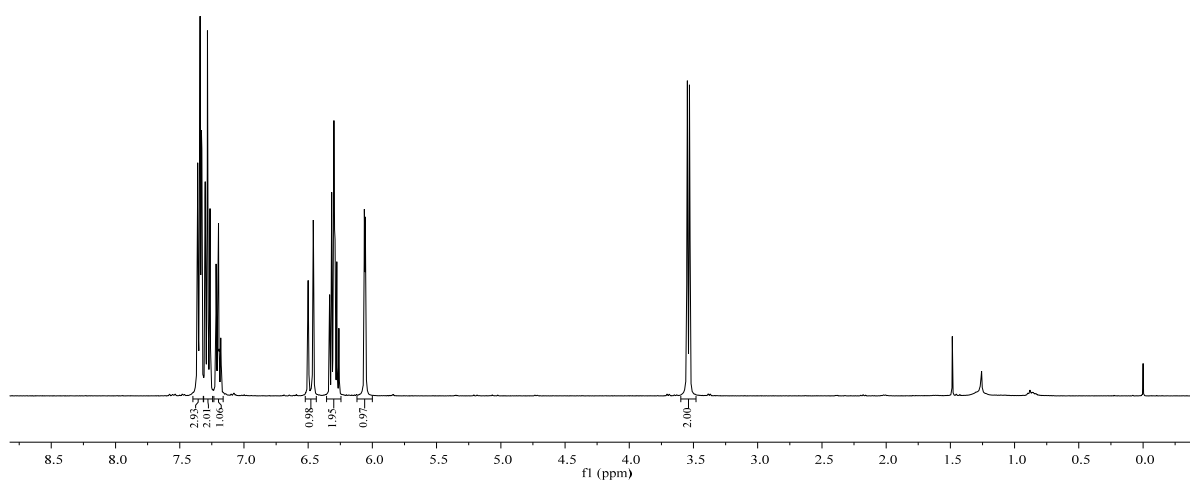
3.55
3.53



2-cinnamylfuran

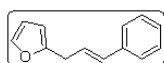
¹H NMR

Solvent: CDCl₃



153.99
141.48
137.32
128.63
127.42
126.32
125.67
110.43
105.76

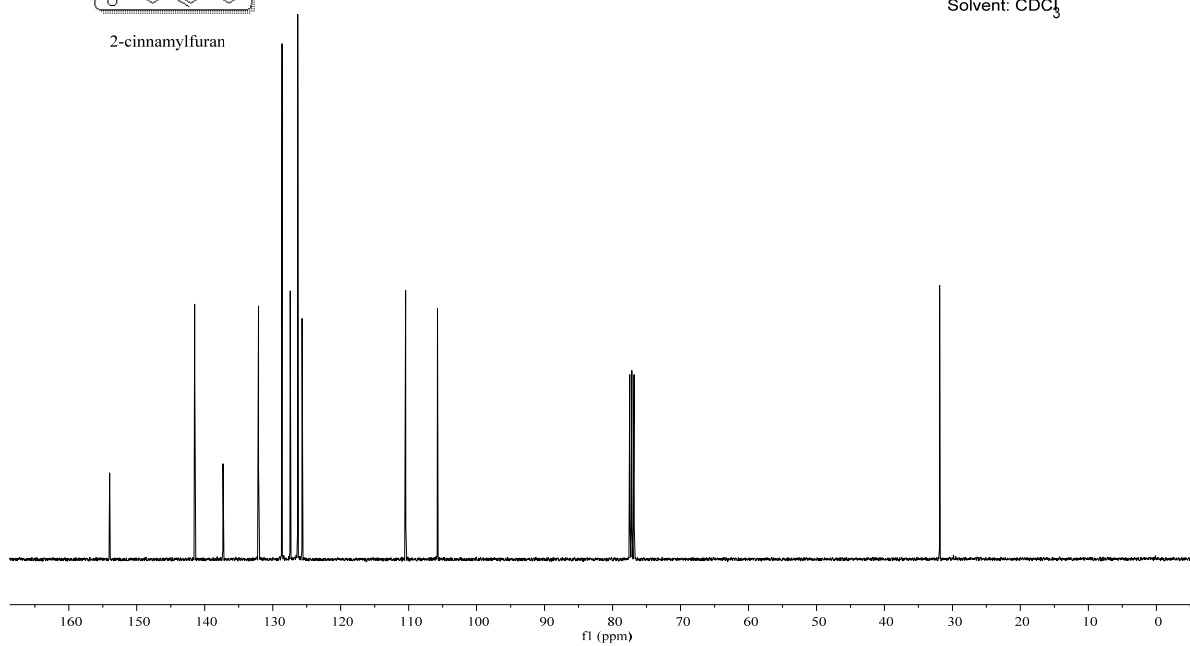
31.88



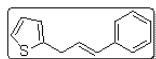
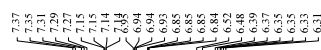
2-cinnamylfuran

¹³C NMR

Solvent: CDCl₃



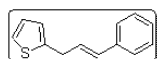
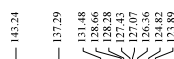
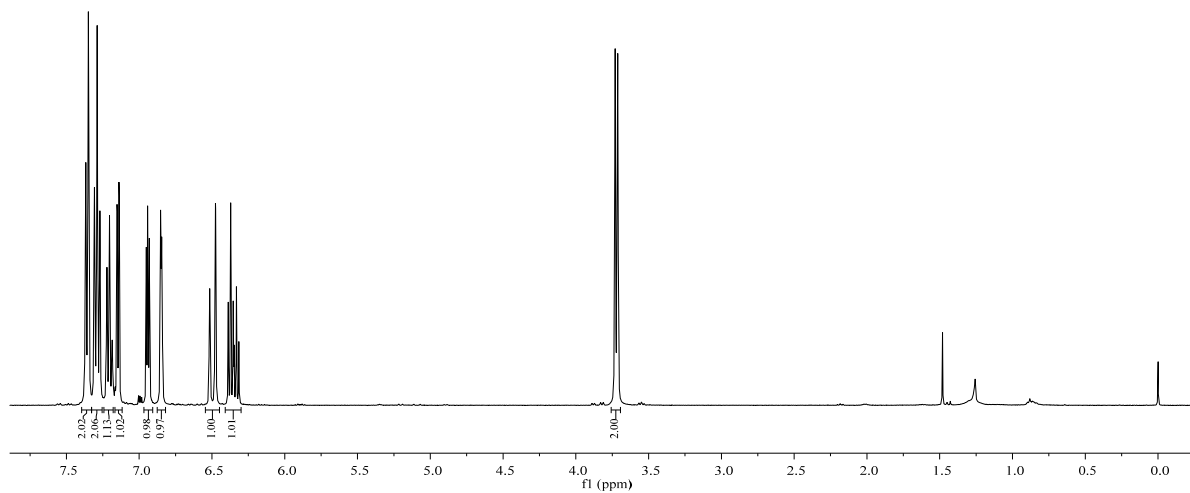
(8) 2-cinnamylthiophene (**3h**)



2-cinnamylthiophene

¹H NMR

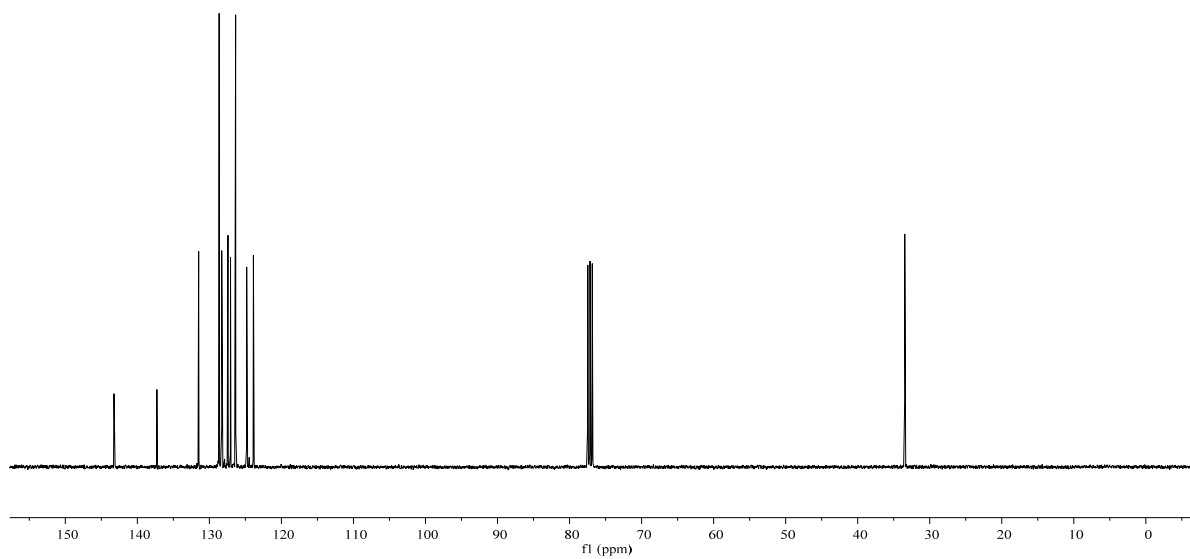
Solvent: CDCl₃



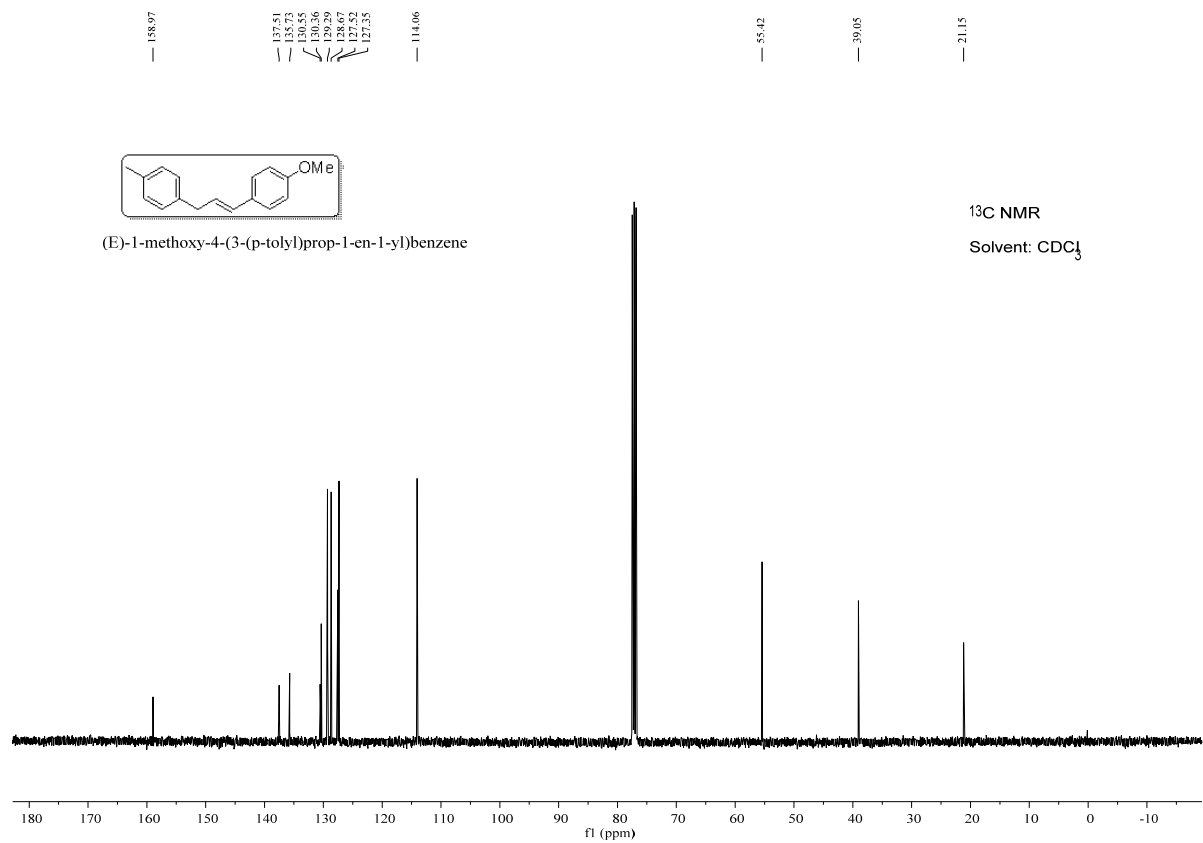
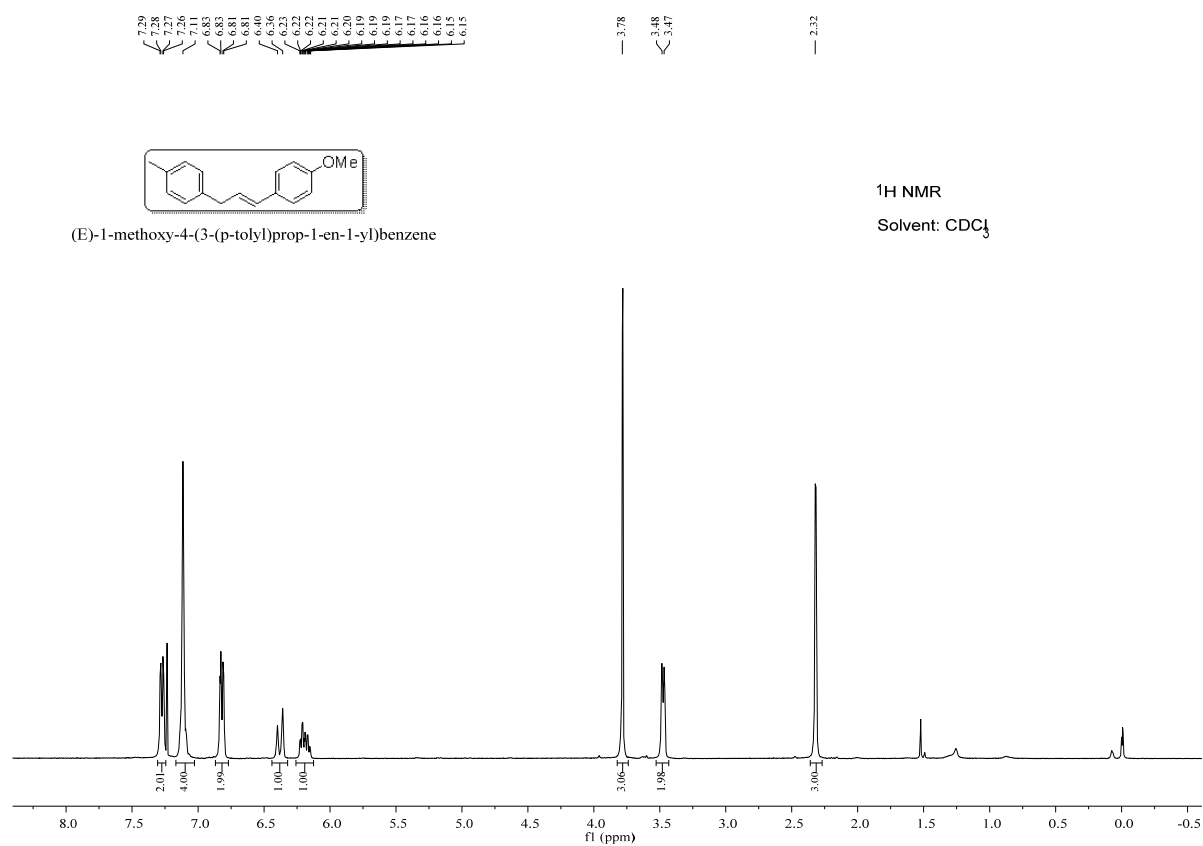
2-cinnamylthiophene

¹³C NMR

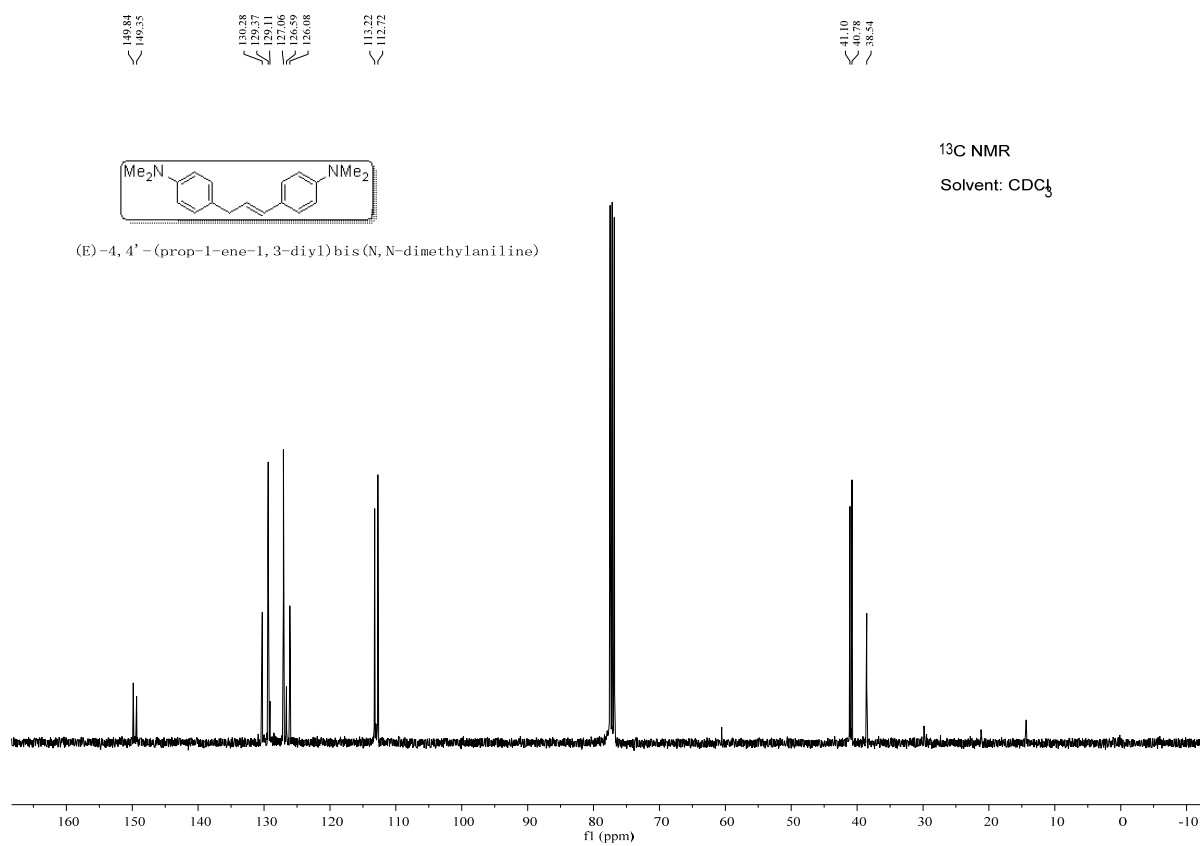
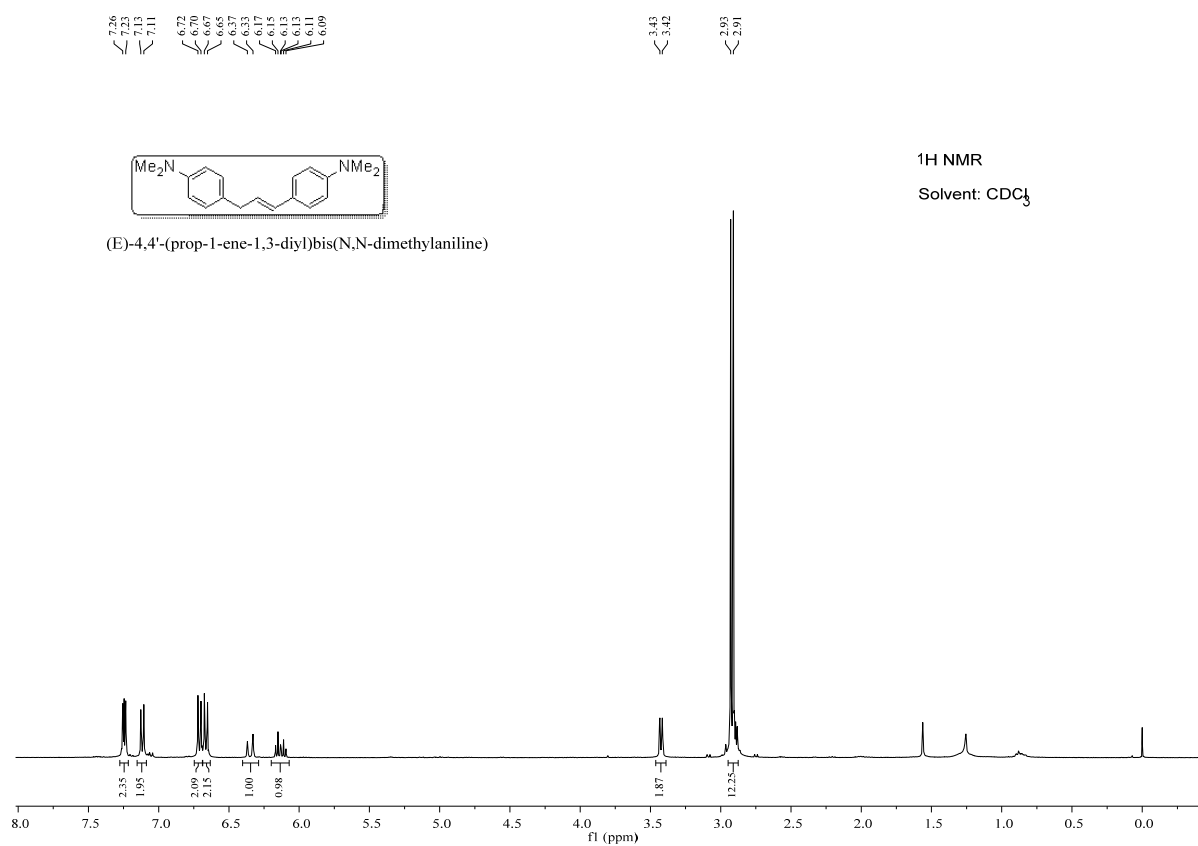
Solvent: CDCl₃



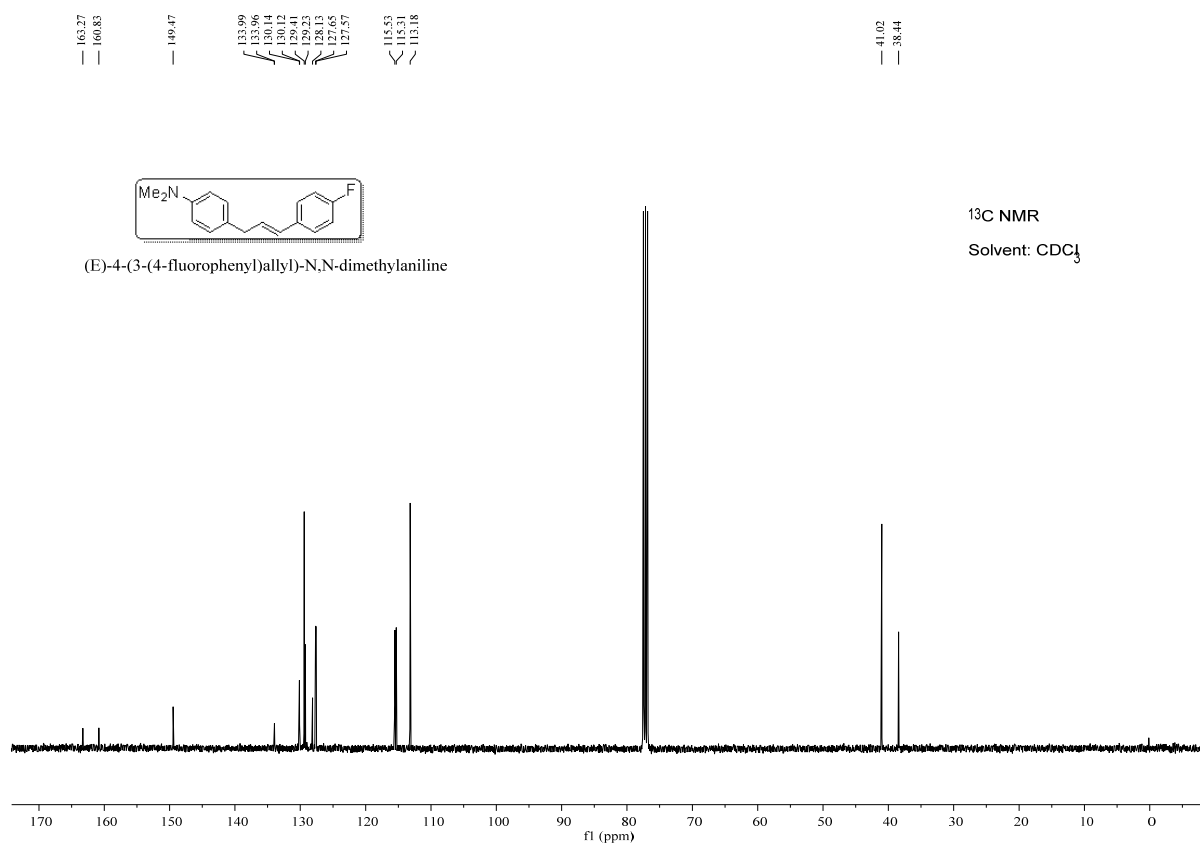
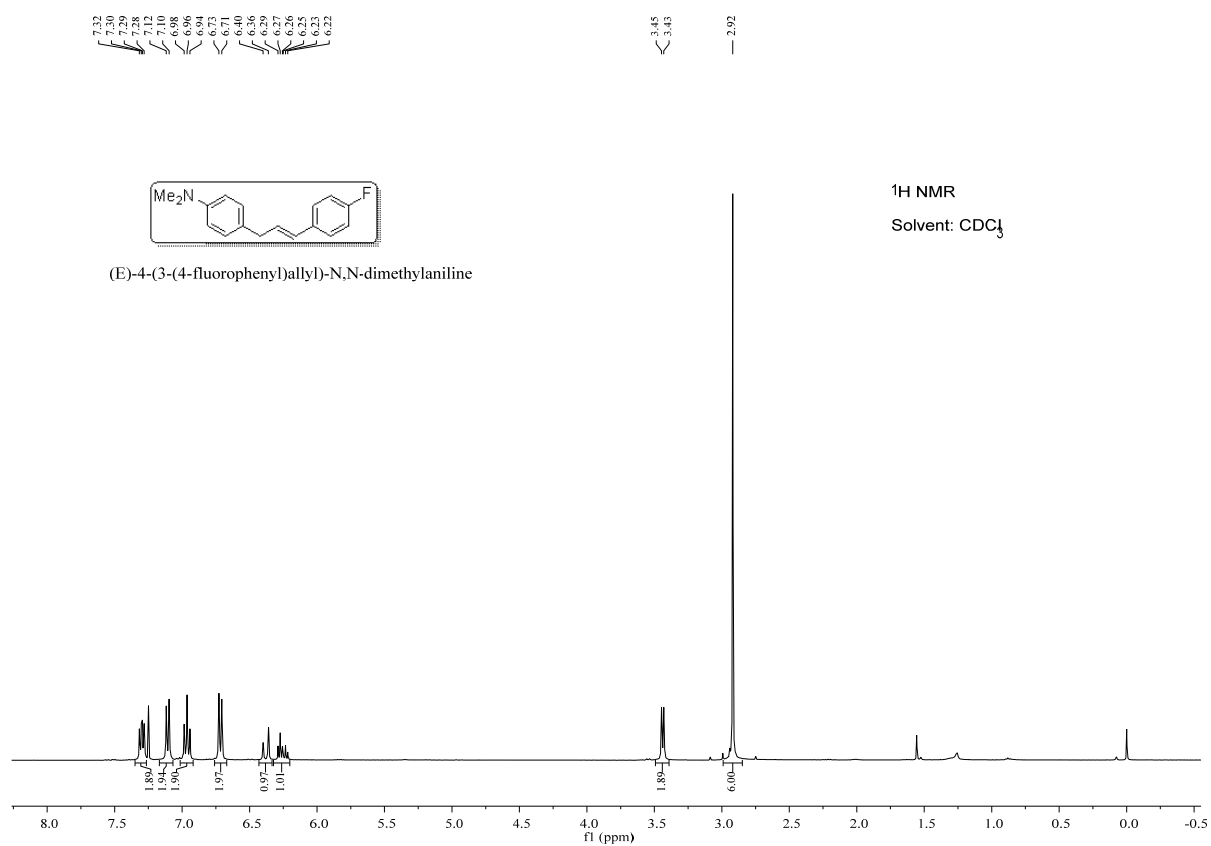
(9) (*E*)-1-methoxy-4-(3-(*p*-tolyl)prop-1-en-1-yl)benzene (**3i**)



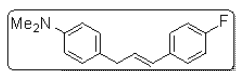
(10) (*E*)-4,4'-(prop-1-ene-1,3-diyl)bis(*N,N*-dimethylaniline) (**3j**)



(11) (*E*)-4-(3-(4-fluorophenyl)allyl)-*N,N*-dimethylaniline (**3k**)



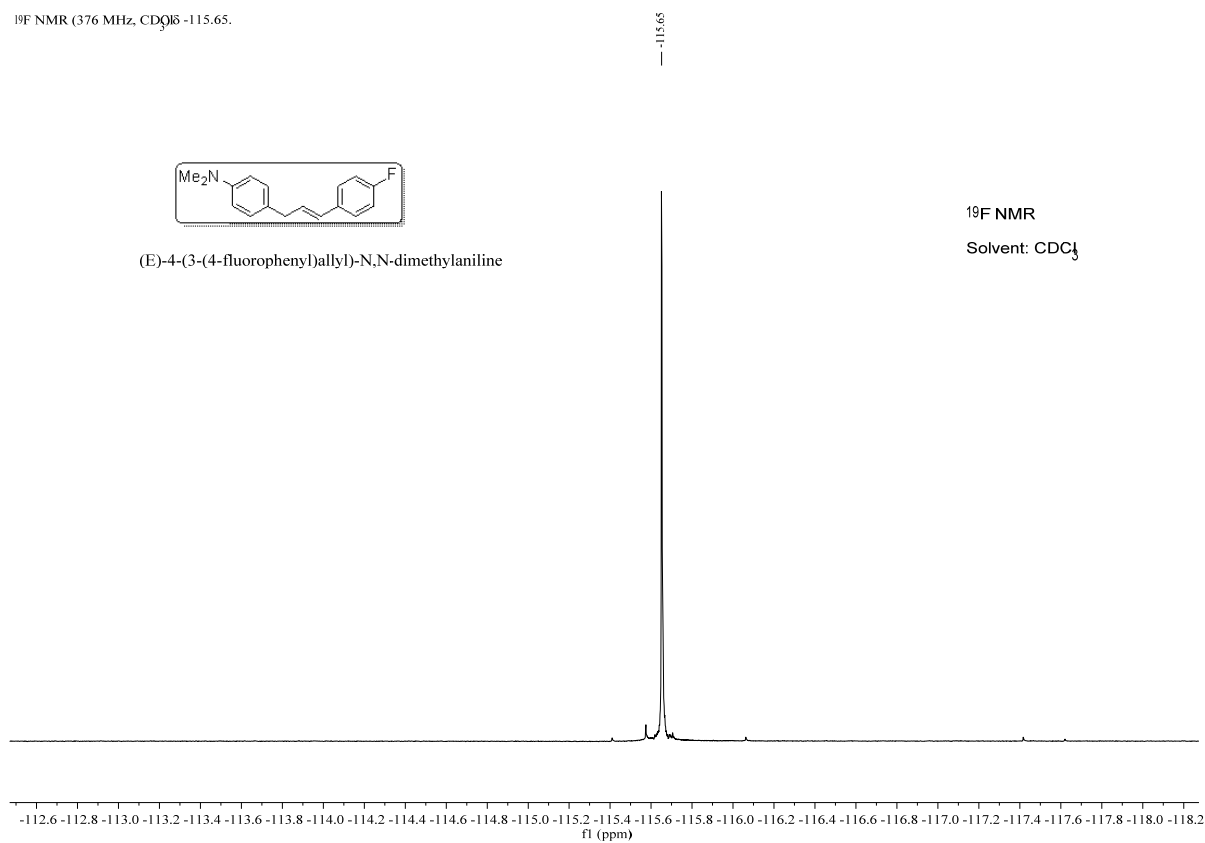
^{19}F NMR (376 MHz, CDCl_3) δ -115.65.



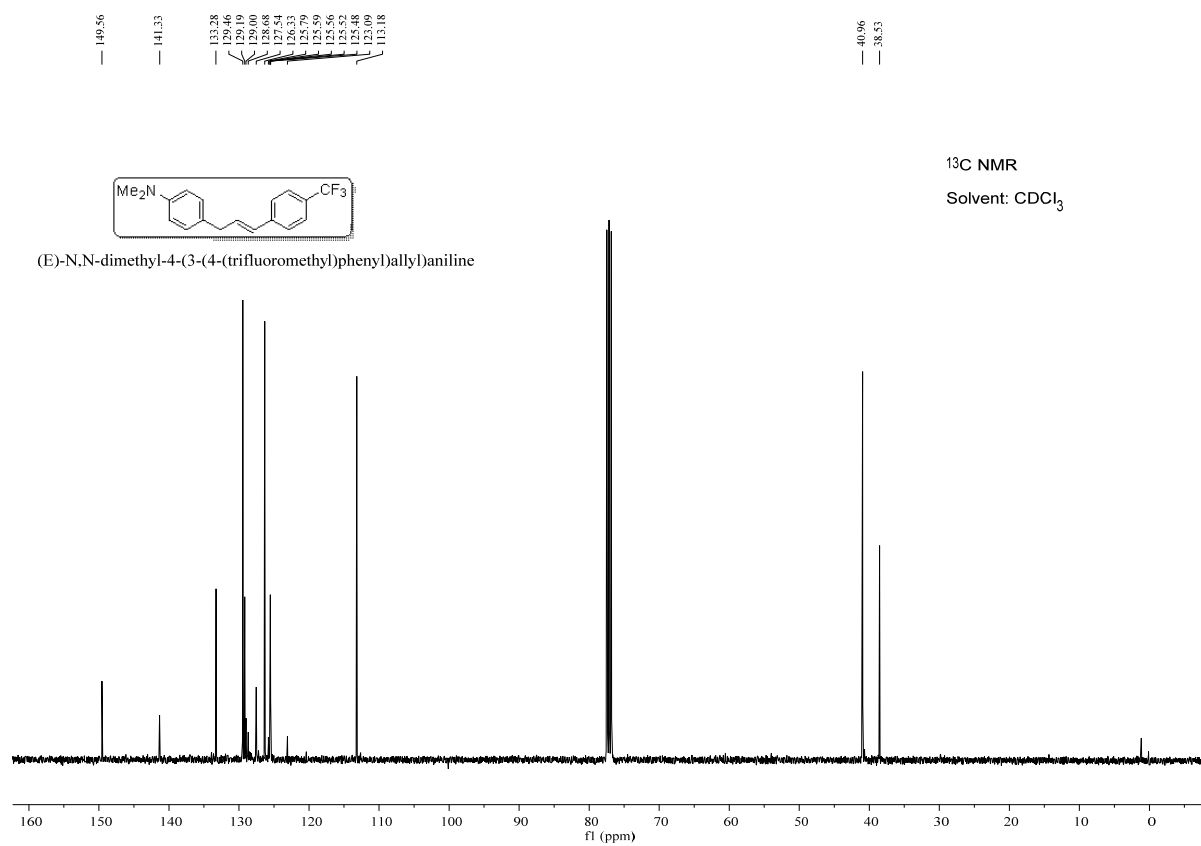
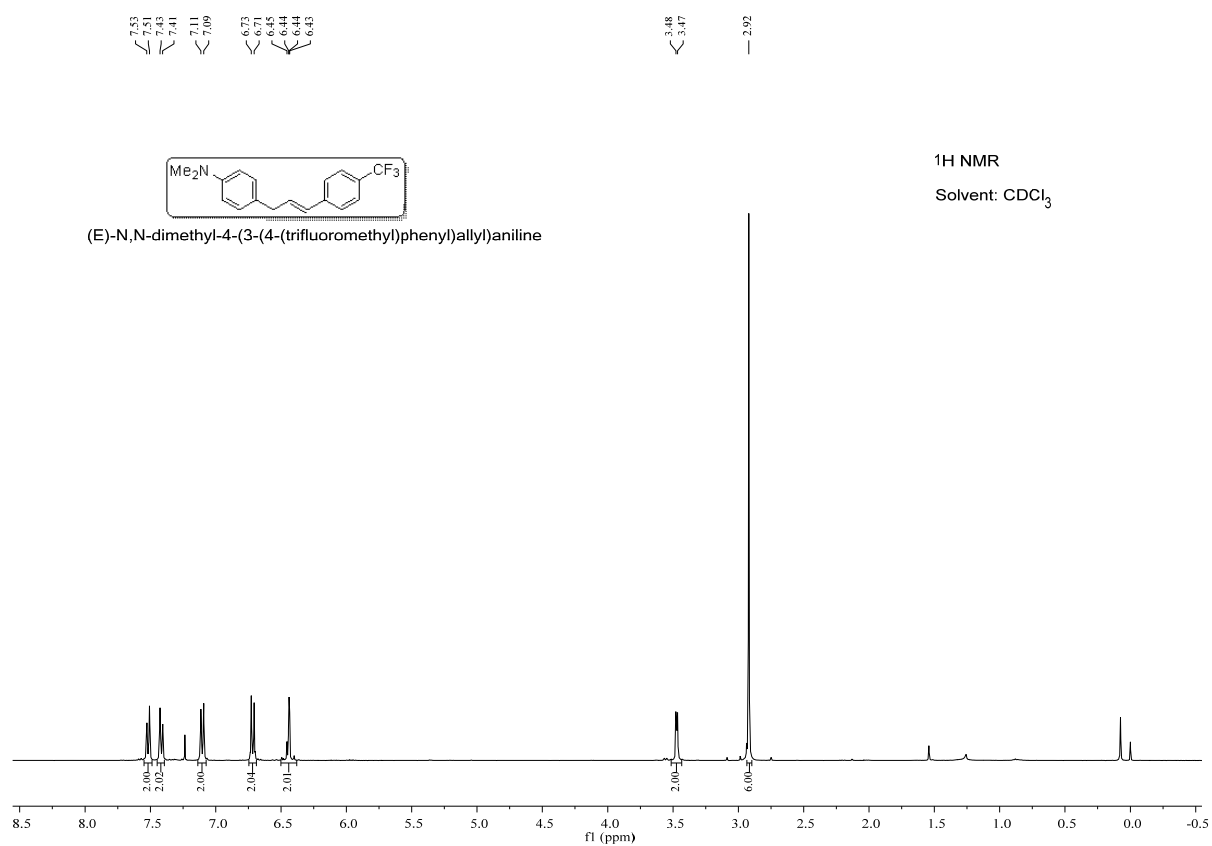
(E)-4-(3-(4-fluorophenyl)allyl)-N,N-dimethylaniline

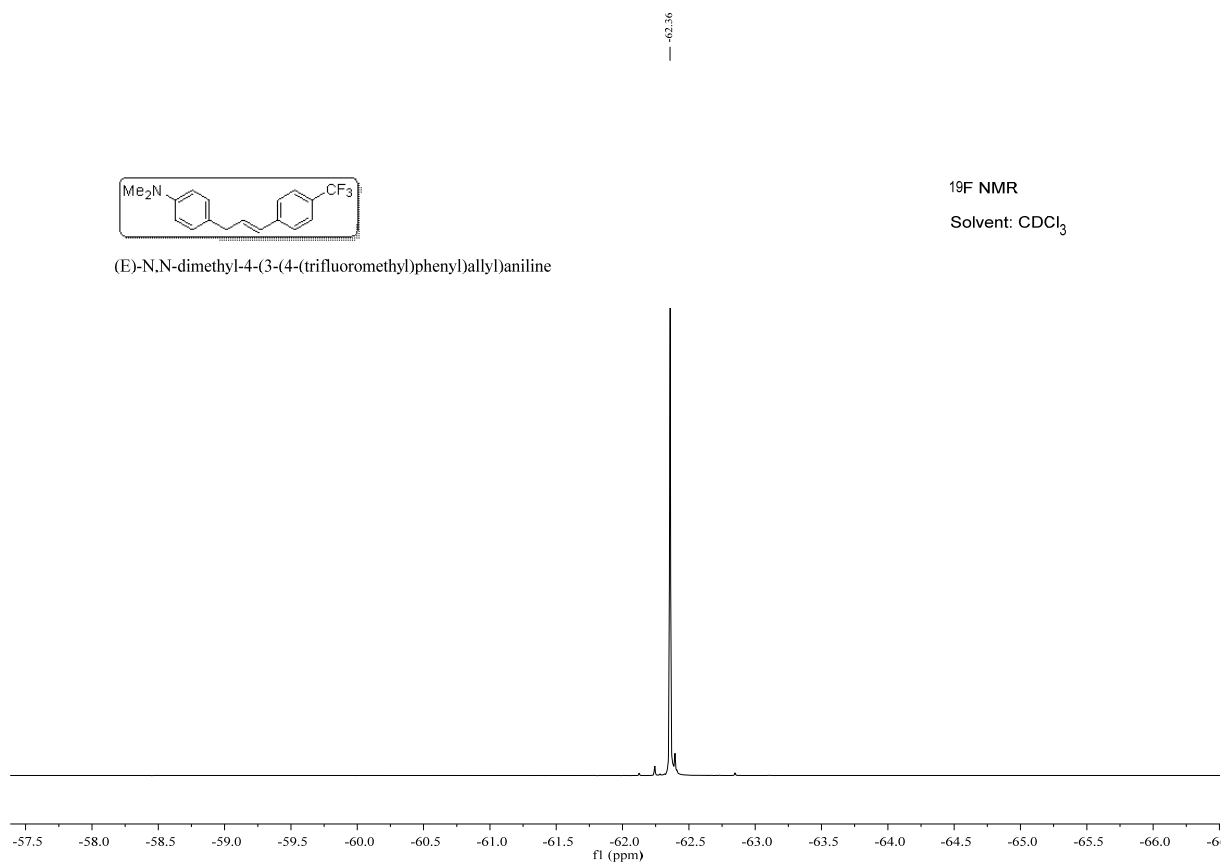
^{19}F NMR

Solvent: CDCl_3



(12) (*E*)-*N,N*-dimethyl-4-(3-(4-(trifluoromethyl)phenyl)allyl)aniline (**3l**)



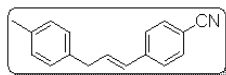


(13) (*E*)-4-(3-(*p*-tolyl)prop-1-en-1-yl)benzonitrile (**3m**)

7.52
7.51
7.42
7.40
7.15
7.13
7.10
6.53
6.50
6.49
6.48
6.46
6.44
6.40

3.54
3.53

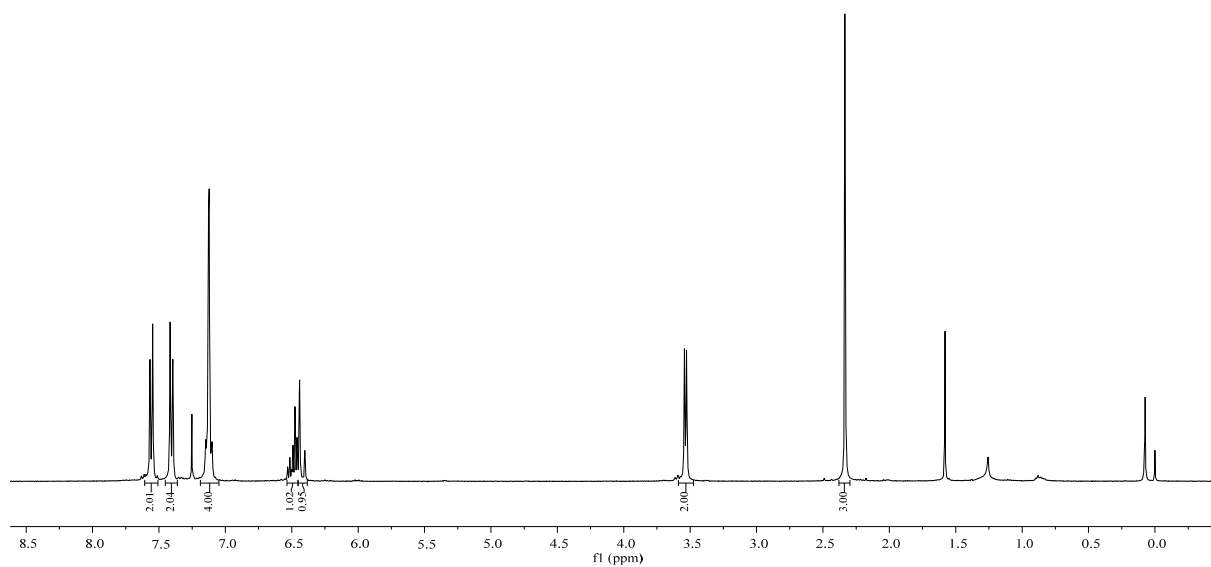
2.33



(*E*)-4-(3-(*p*-tolyl)prop-1-en-1-yl)benzonitrile

¹H NMR

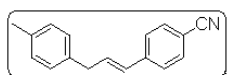
Solvent: CDCl₃



142.16
136.20
136.18
134.04
132.47
128.65
128.70
119.20
110.36
100.11

39.09

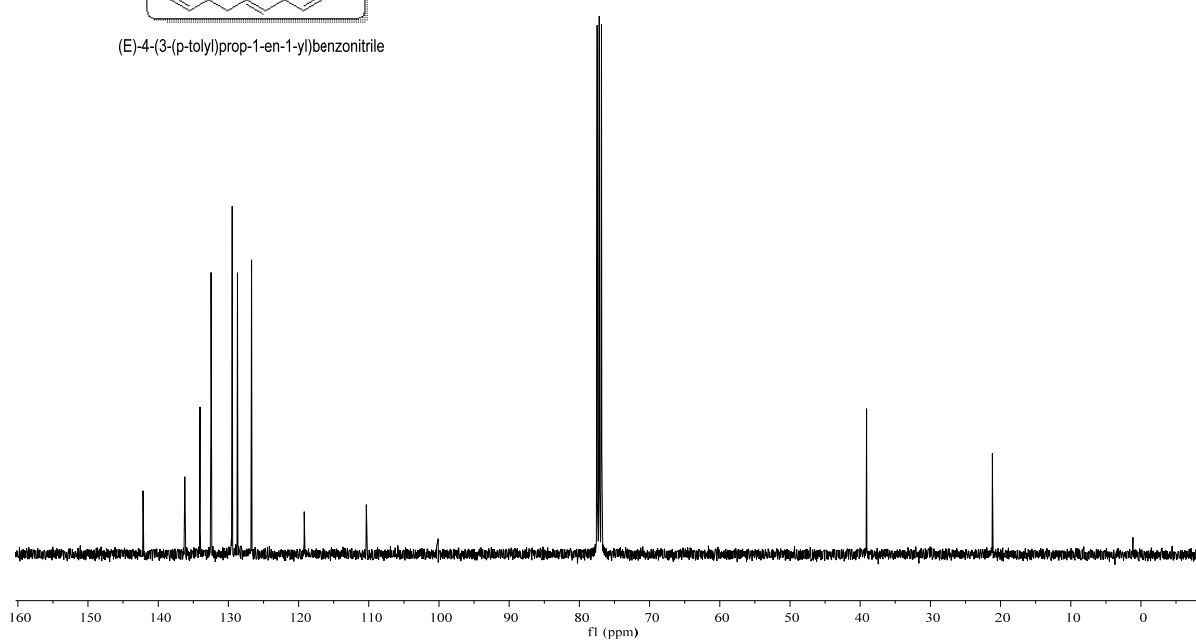
21.16



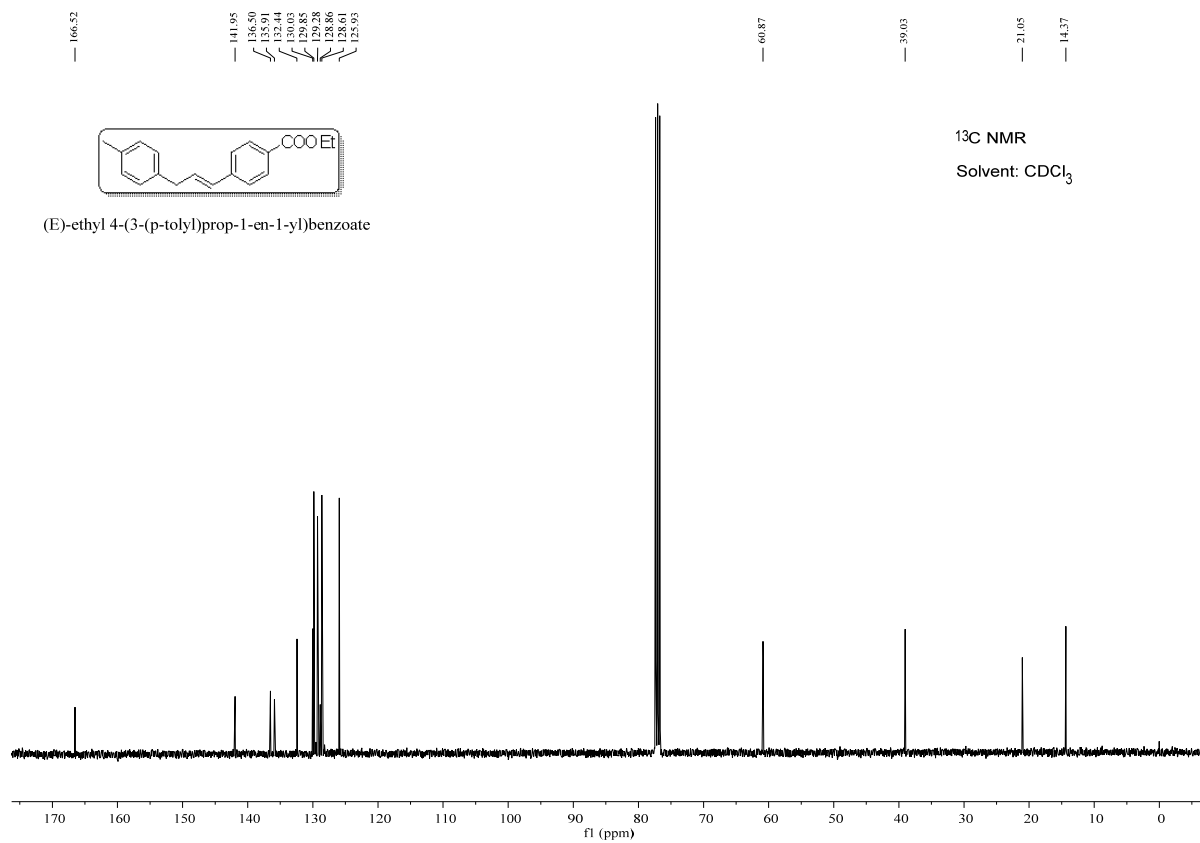
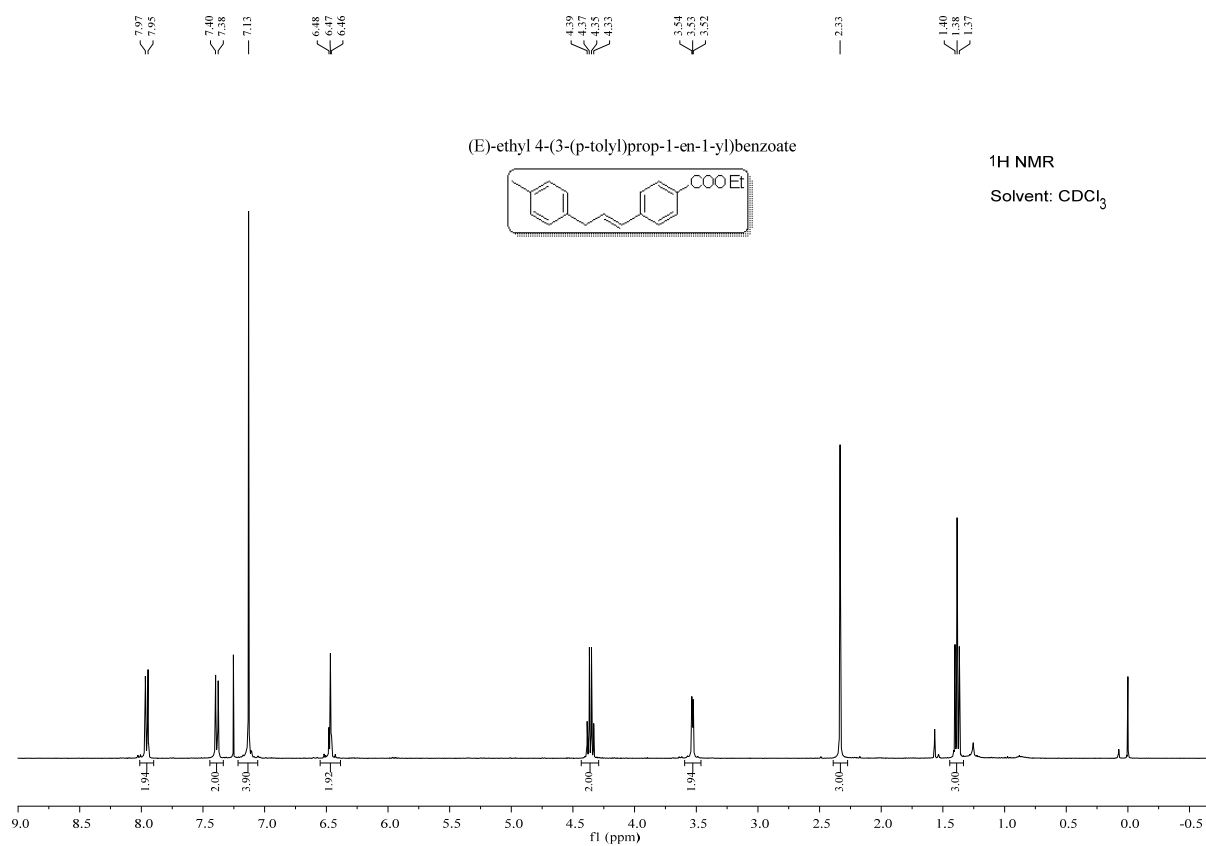
(*E*)-4-(3-(*p*-tolyl)prop-1-en-1-yl)benzonitrile

¹³C NMR

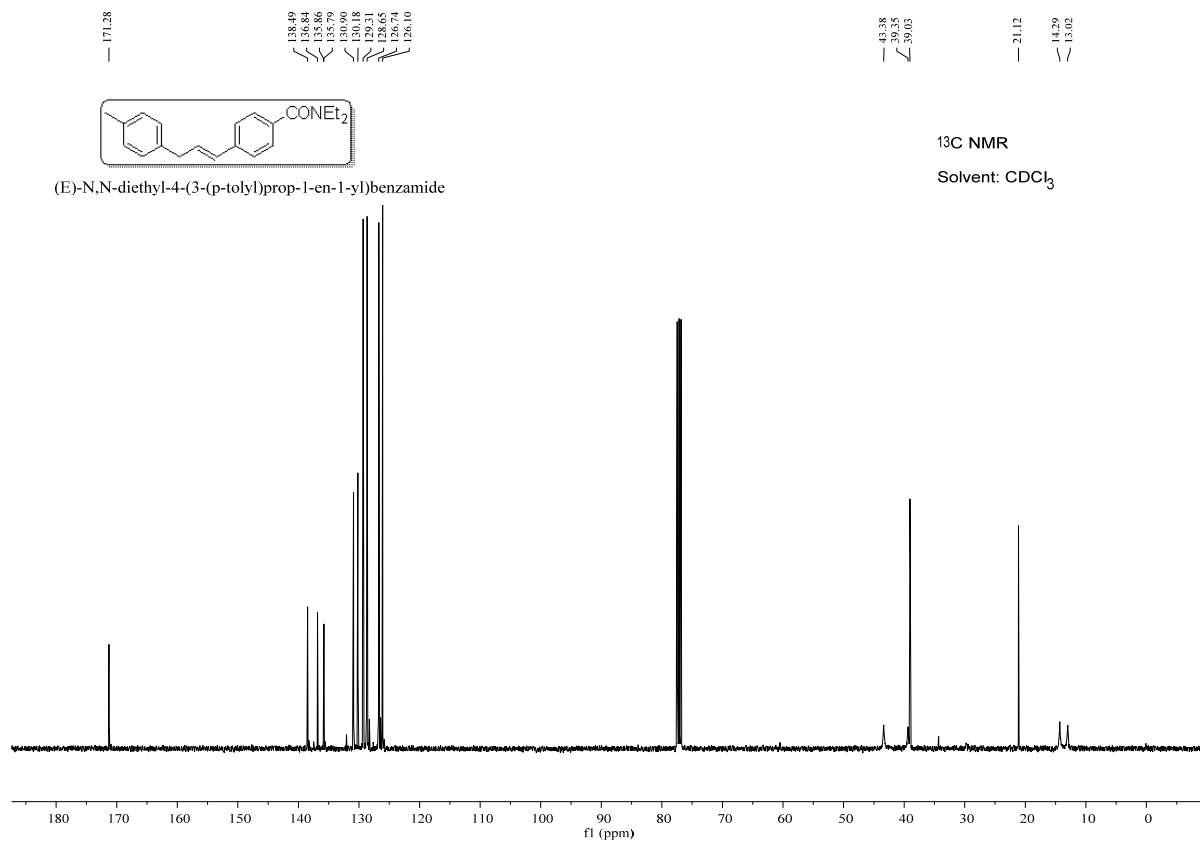
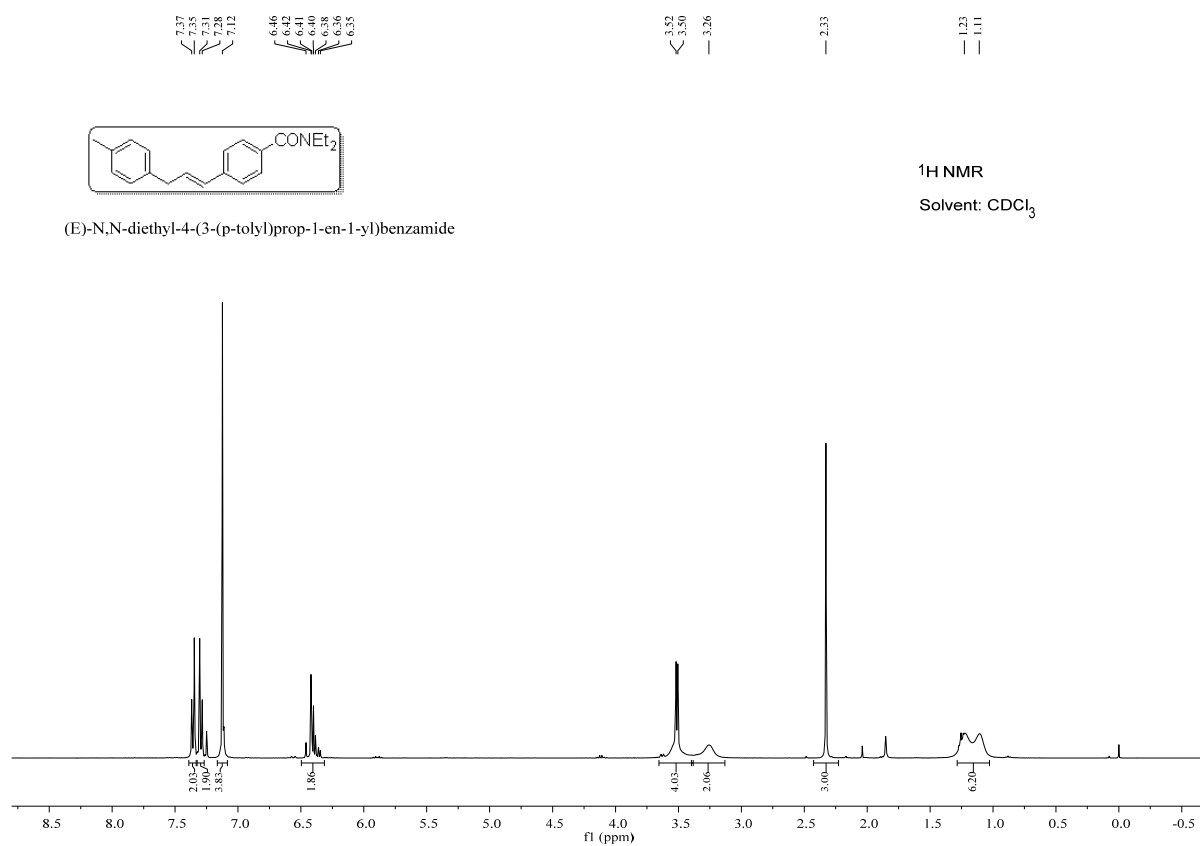
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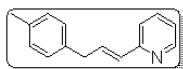
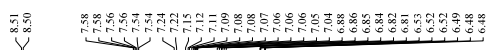
(14) (E)-ethyl 4-(3-(p-tolyl)prop-1-en-1-yl)benzoate (**3n**)



(15) (*E*)-*N,N*-diethyl-4-(3-(*p*-tolyl)prop-1-en-1-yl)benzamide (**3o**)



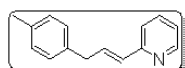
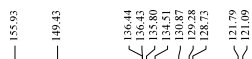
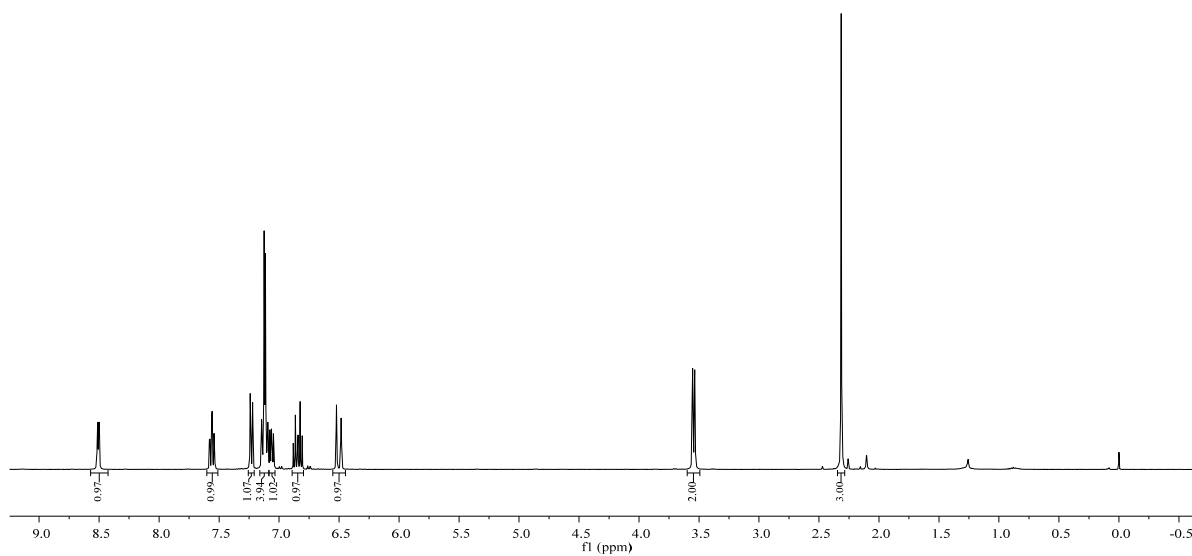
(16) (E)-2-(3-(p-tolyl)prop-1-en-1-yl)pyridine (**3p**)



(E)-2-(3-(p-tolyl)prop-1-en-1-yl)pyridine

¹H NMR

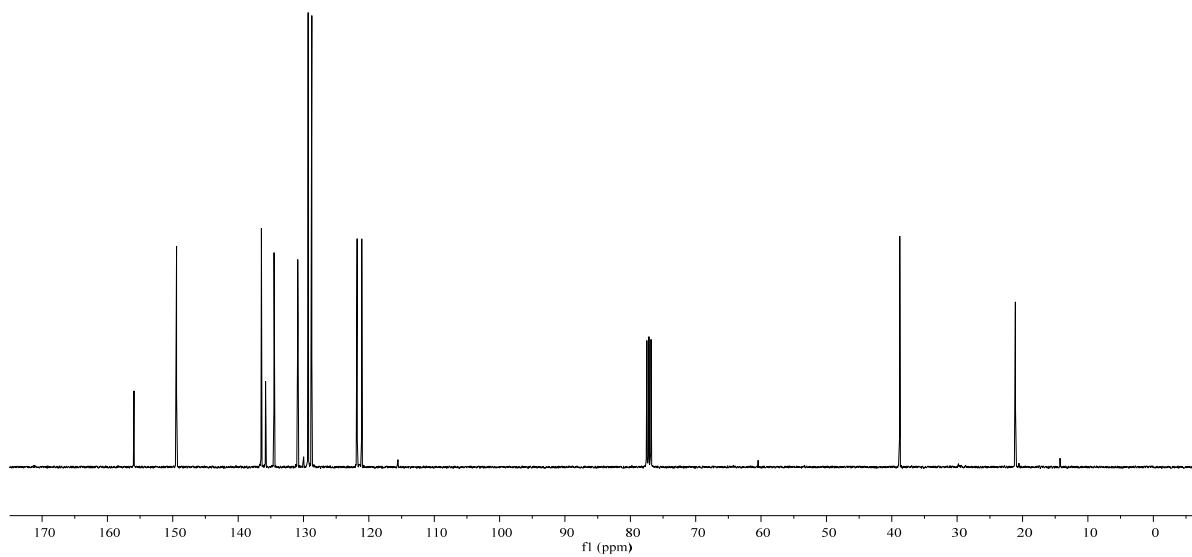
Solvent: CDCl₃



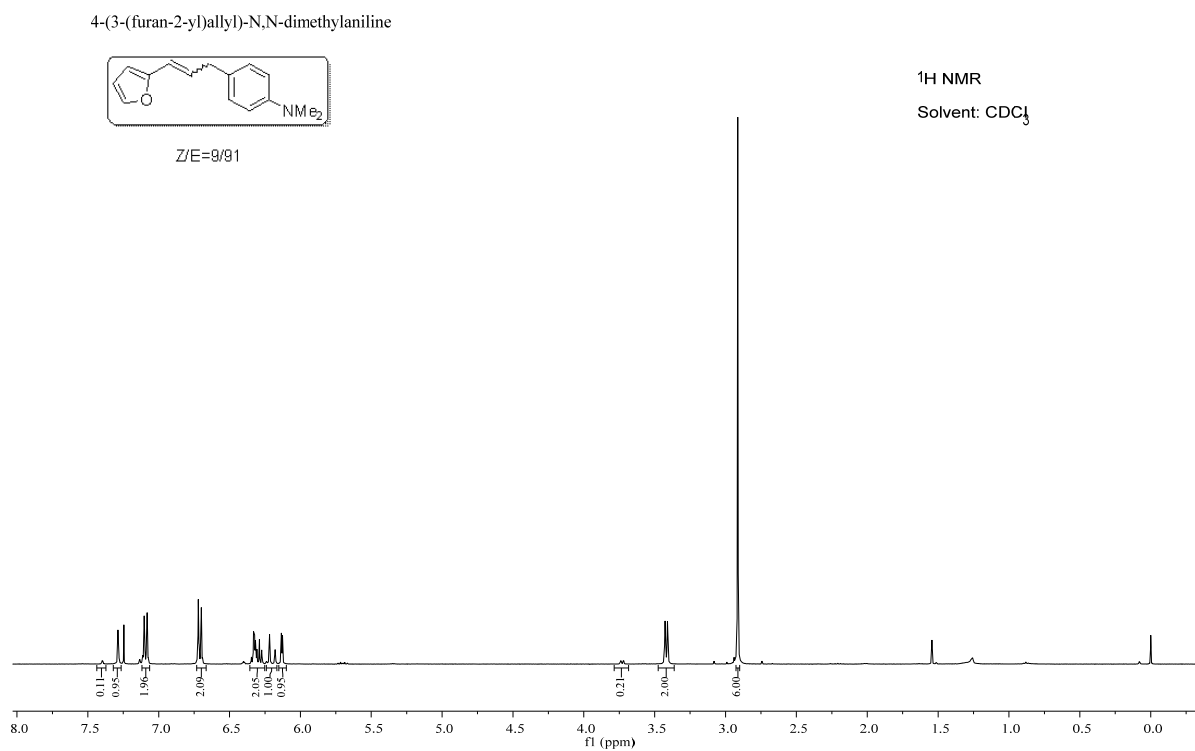
(E)-2-(3-(p-tolyl)prop-1-en-1-yl)pyridine

¹³C NMR

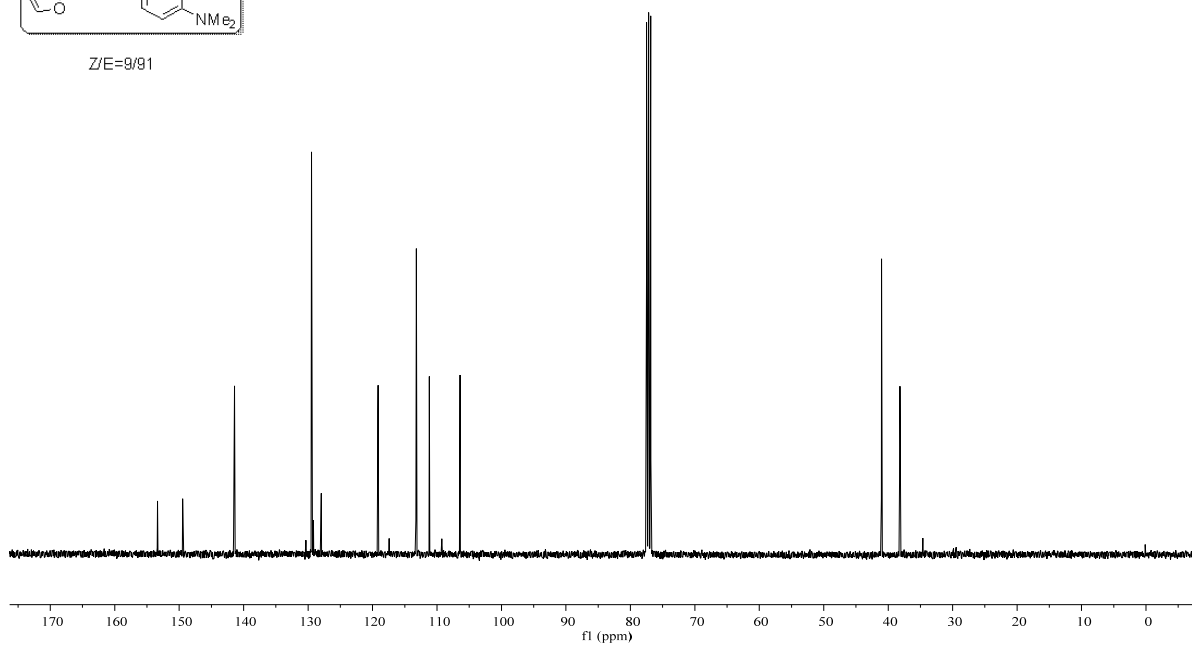
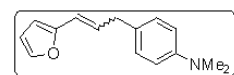
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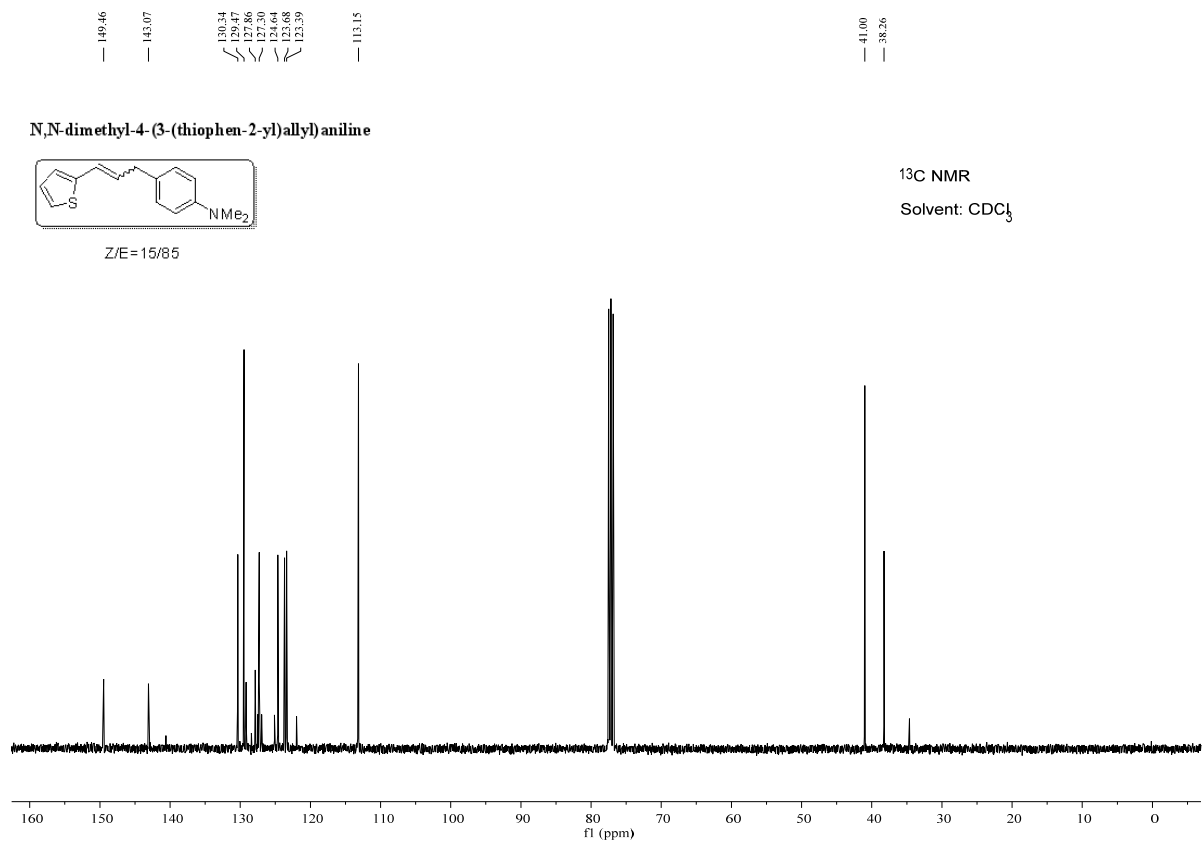
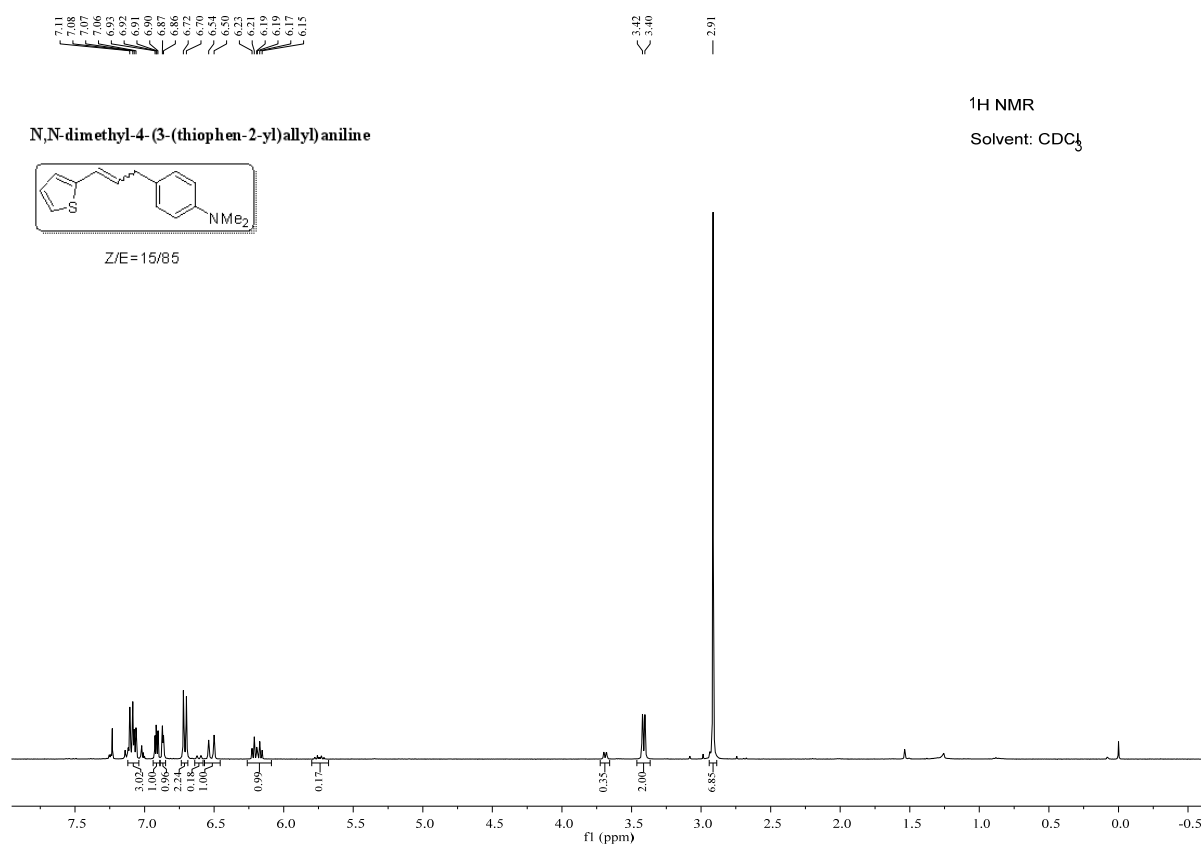
(17) 4-(3-(furan-2-yl)allyl)-*N,N*-dimethylaniline (**3q**)



4-(3-(furan-2-yl)allyl)-*N,N*-dimethylaniline

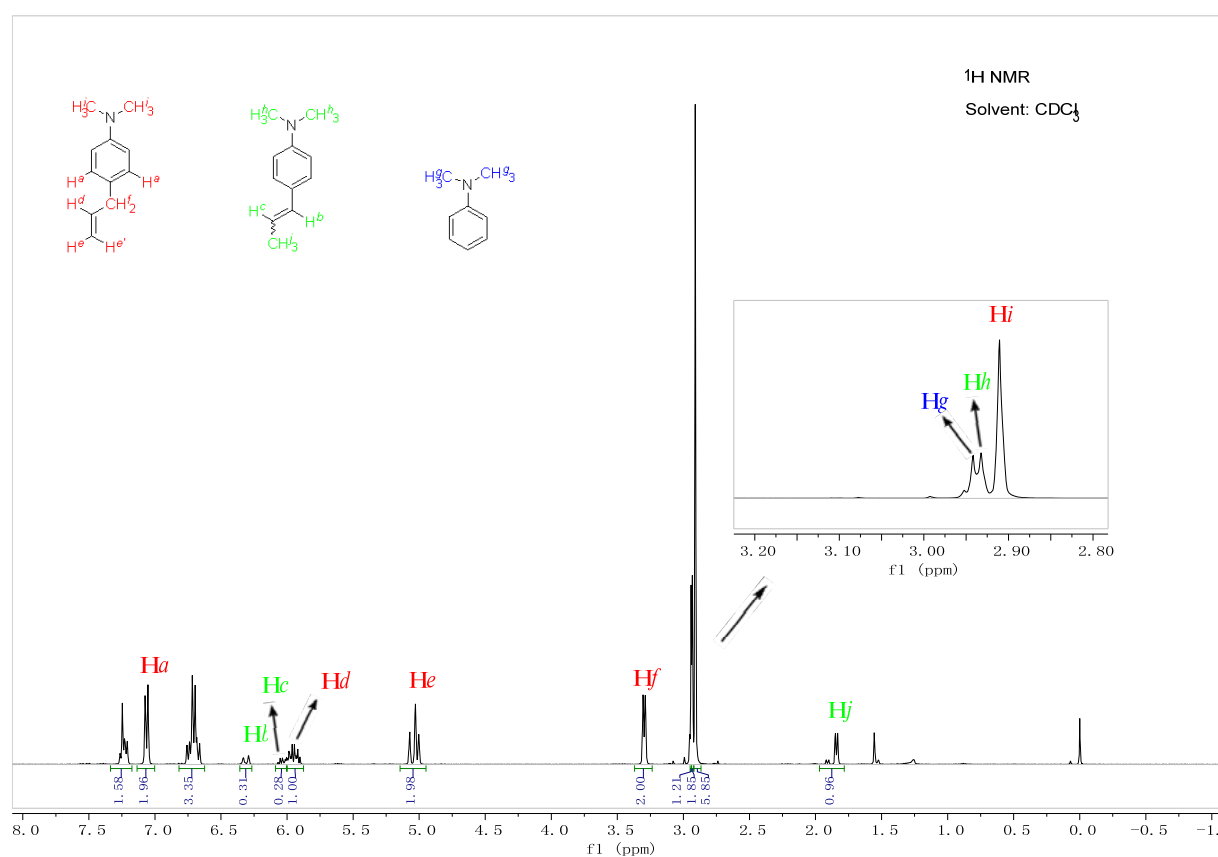


(18) *N,N*-dimethyl-4-(3-(thiophen-2-yl)allyl)aniline (**3r**)

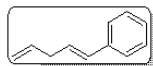
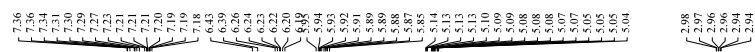


(19) A mixture of 4-allyl-*N,N*-dimethylaniline (**3s**), *N,N*-dimethyl-4-(prop-1-en-1-yl) aniline (**3t**), and *N,N*-dimethylaniline

After the reaction completed, a mixture of 4-allyl-*N,N*-dimethylaniline (**3s**), *N,N*-dimethyl-4-(prop-1-en-1-yl) aniline (**3t**), and *N,N*-dimethylaniline was isolated by column chromatography. *N,N*-Dimethylaniline was formed by hydrolysis of excess (4-(dimethylamino)phenyl)zinc chloride. The proportion of the components was calculated through the integration of the ^1H NMR spectrum.



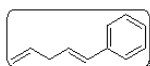
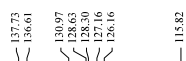
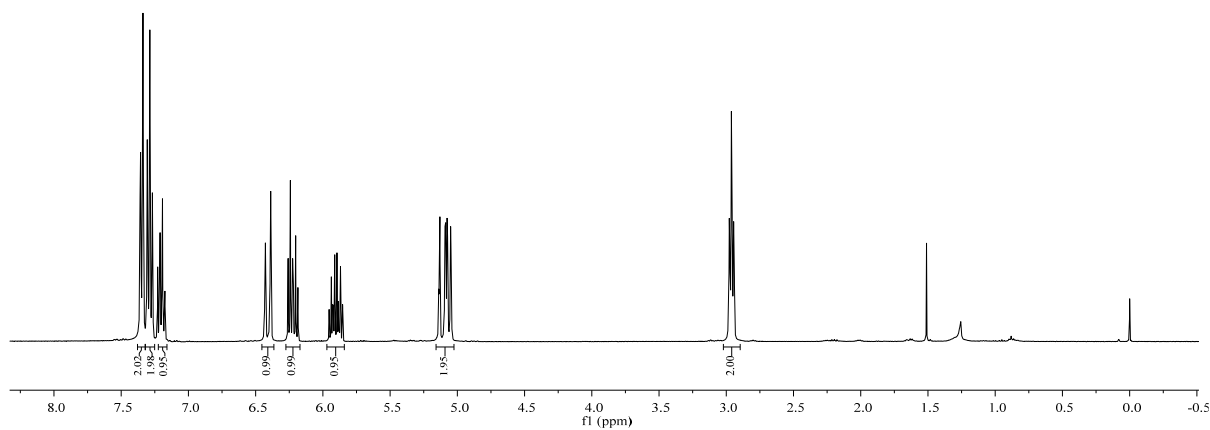
(20) (E)-penta-1,4-dien-1-ylbenzene (5a)



(E)-penta-1,4-dien-1-ylbenzene

¹H NMR

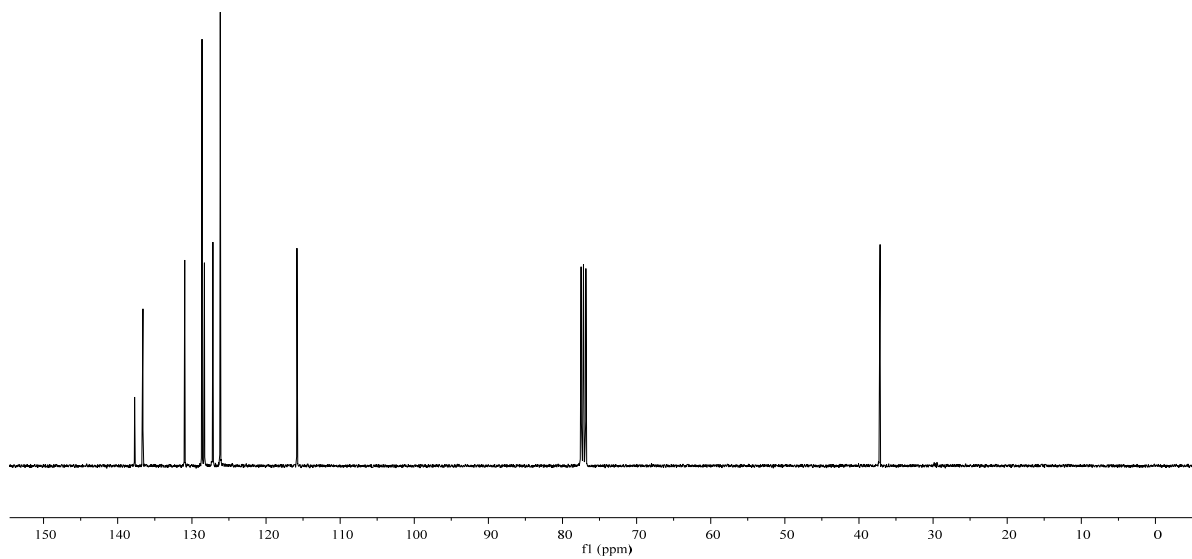
Solvent: CDCl₃



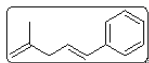
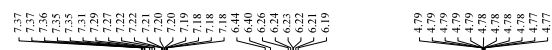
(E)-penta-1,4-dien-1-ylbenzene

¹³C NMR

Solvent: CDCl₃



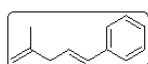
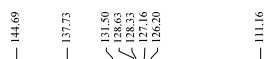
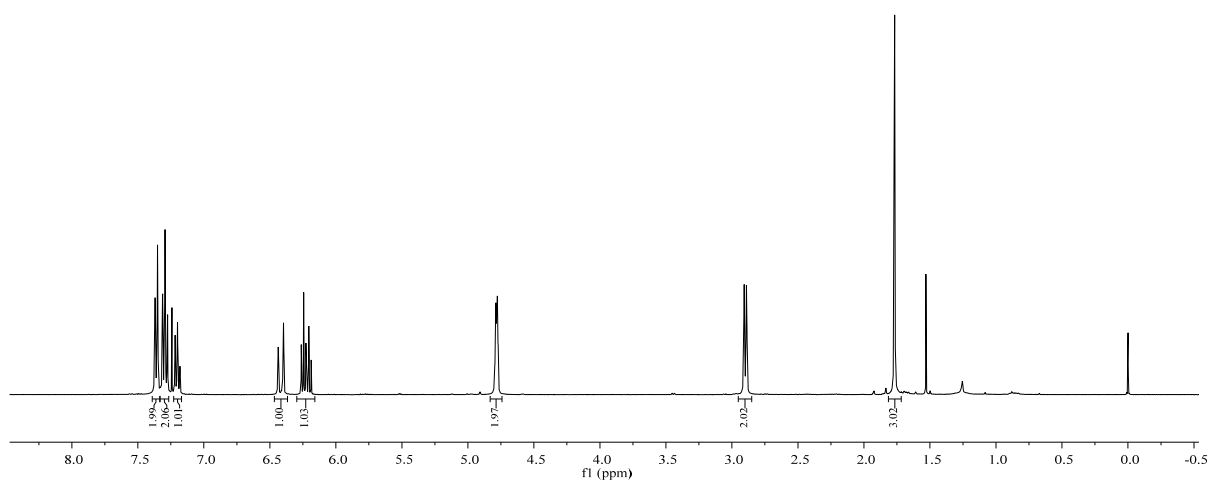
(21) (*E*)-(4-methylpenta-1,4-dien-1-yl)benzene (**5b**)



(*E*)-(4-methylpenta-1,4-dien-1-yl)benzene

¹H NMR

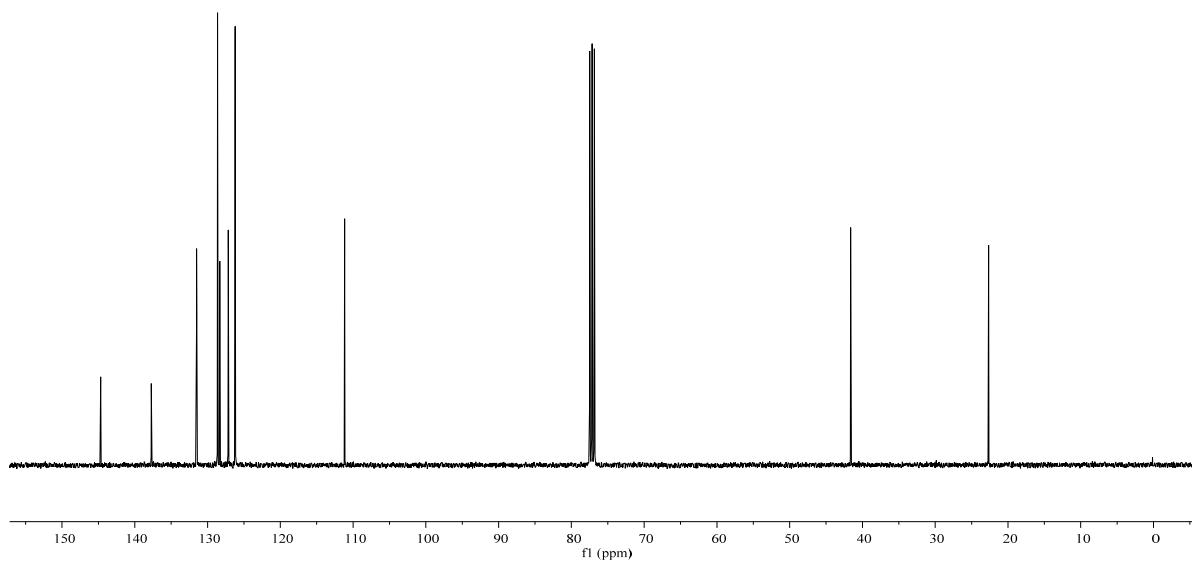
Solvent: CDCl₃



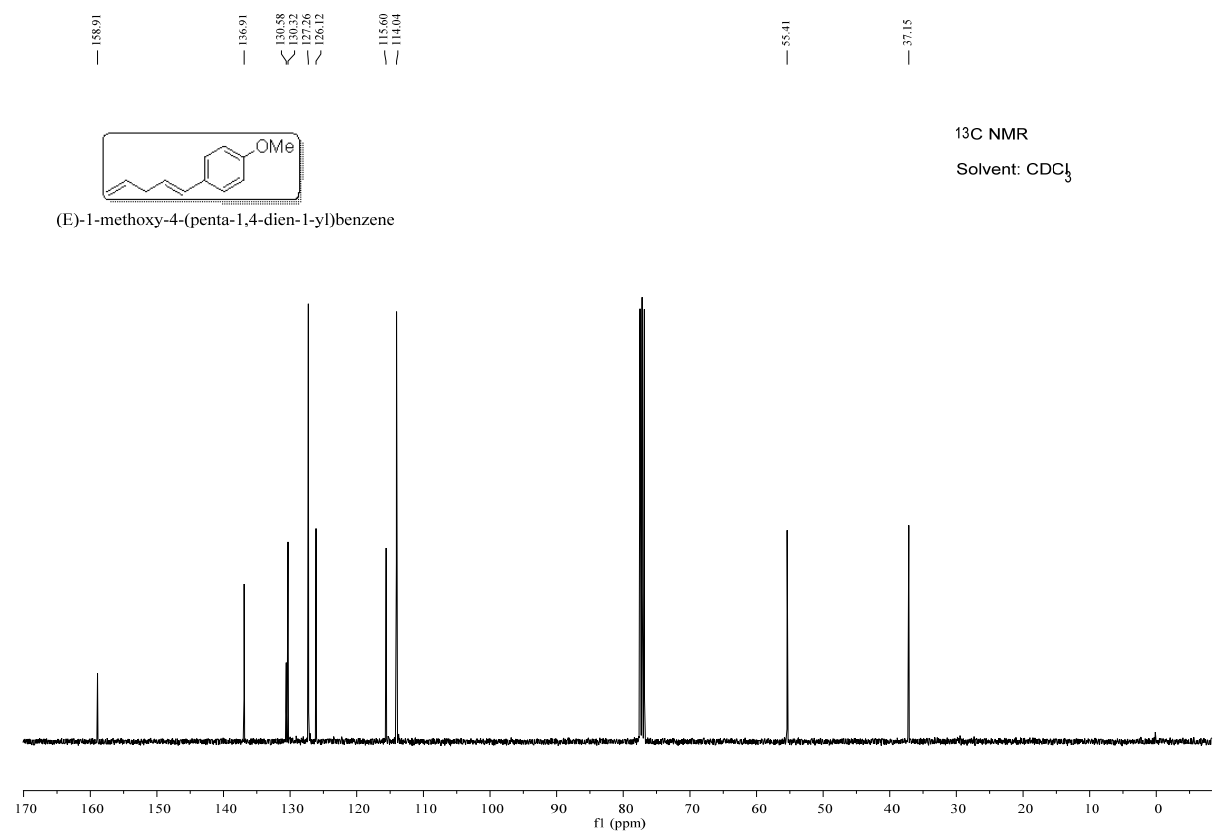
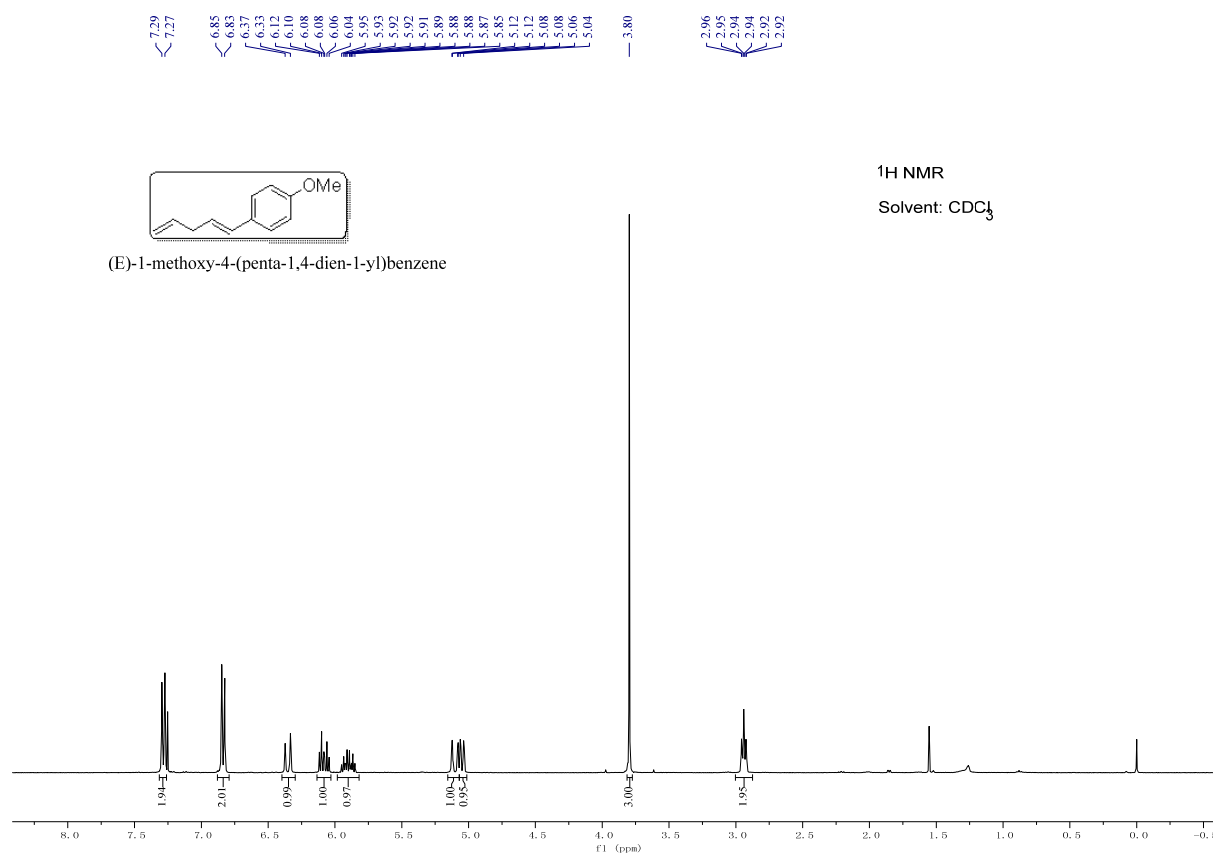
(*E*)-(4-methylpenta-1,4-dien-1-yl)benzene

¹³C NMR

Solvent: CDCl₃



(22) (E)-1-methoxy-4-(penta-1,4-dien-1-yl)benzene (5c)



(23) (*E*)-1-methoxy-4-(4-methylpenta-1,4-dien-1-yl)benzene (**5d**)

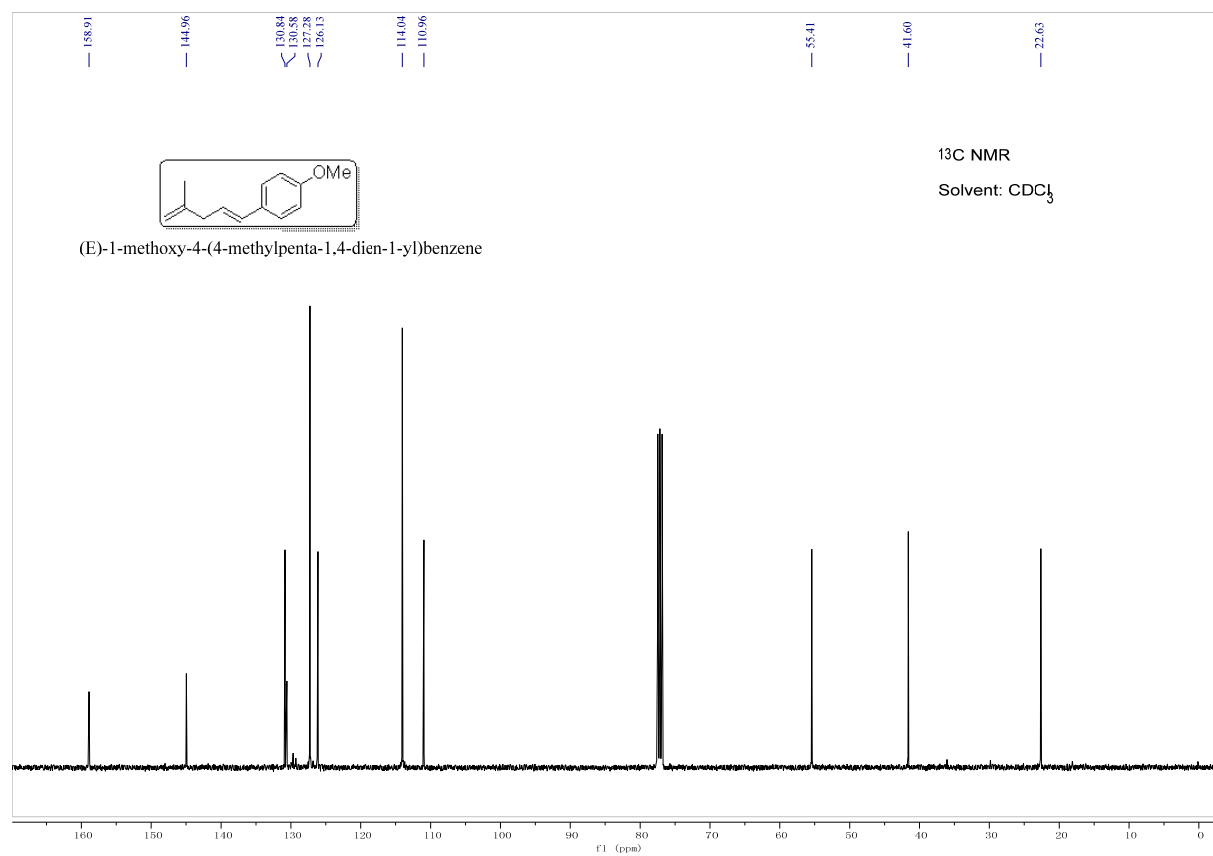
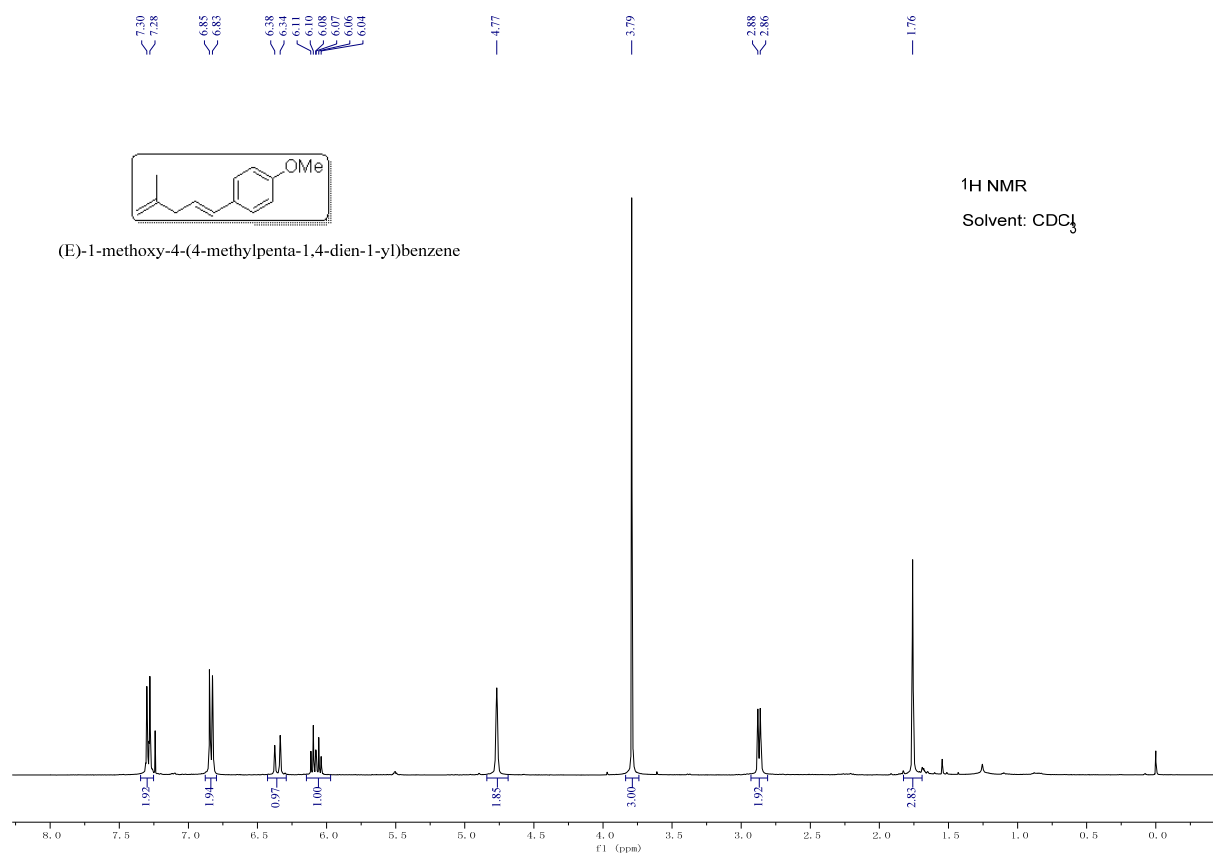
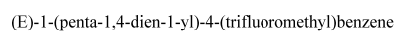
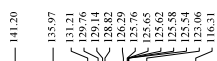


Figure 1 is a dendrogram illustrating the hierarchical clustering of 18 variables. The variables are grouped into three main clusters. The first cluster on the left contains variables 1-10, the middle cluster contains variables 11-17, and the right cluster contains variable 18. The dendrogram shows the distance between variables, with a scale from 0 to 100 on the x-axis.

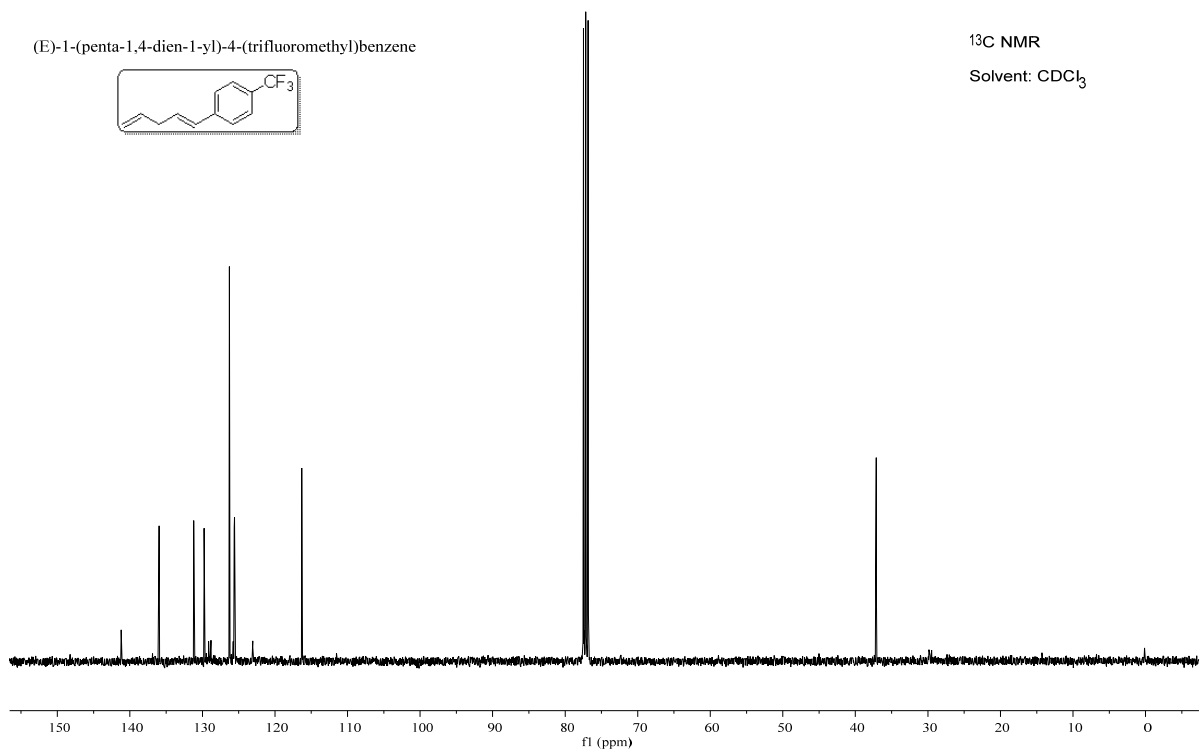
Variable	Cluster	Distance
1	1-10	7.55
2	1-10	7.53
3	1-10	7.44
4	1-10	7.42
5	1-10	6.46
6	1-10	6.42
7	1-10	6.37
8	1-10	6.35
9	1-10	6.34
10	1-10	6.33
11	11-17	6.31
12	11-17	6.30
13	11-17	5.95
14	11-17	5.94
15	11-17	5.93
16	11-17	5.92
17	11-17	5.91
18	18	5.89
19	18	5.88
20	18	5.88
21	18	5.87
22	18	5.85
23	18	5.15
24	18	5.15
25	18	5.14
26	18	5.14
27	18	5.11
28	18	5.10
29	18	5.09
30	18	5.08
31	18	5.08
32	18	5.08
33	18	3.01
34	18	3.01
35	18	2.99
36	18	2.99
37	18	2.98
38	18	2.97

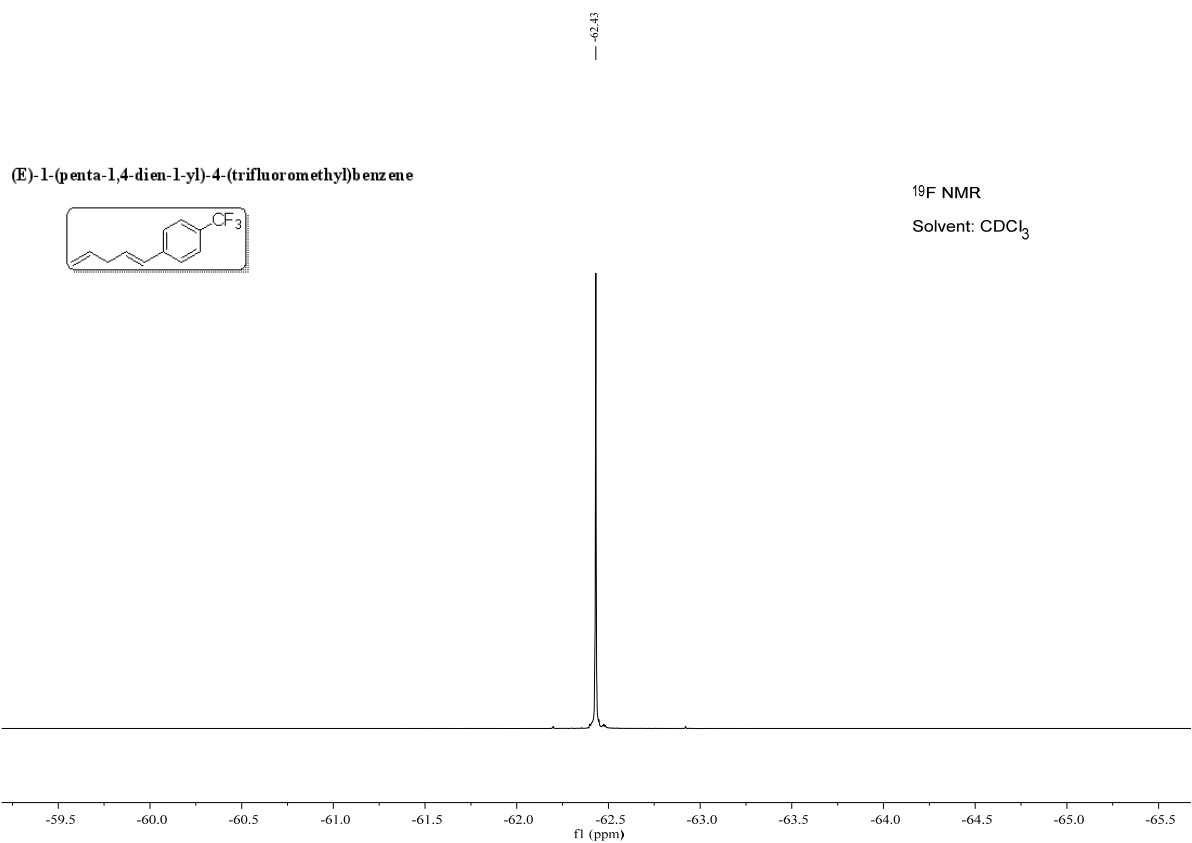


Solvent: CDCl_3

C=CC=Cc1ccc(C(F)(F)F)cc1

Solvent: CDCl₃

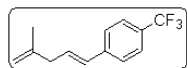




(25) (*E*)-1-(4-methylpenta-1,4-dien-1-yl)-4-(trifluoromethyl)benzene (**5f**)

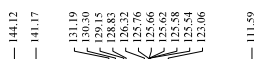
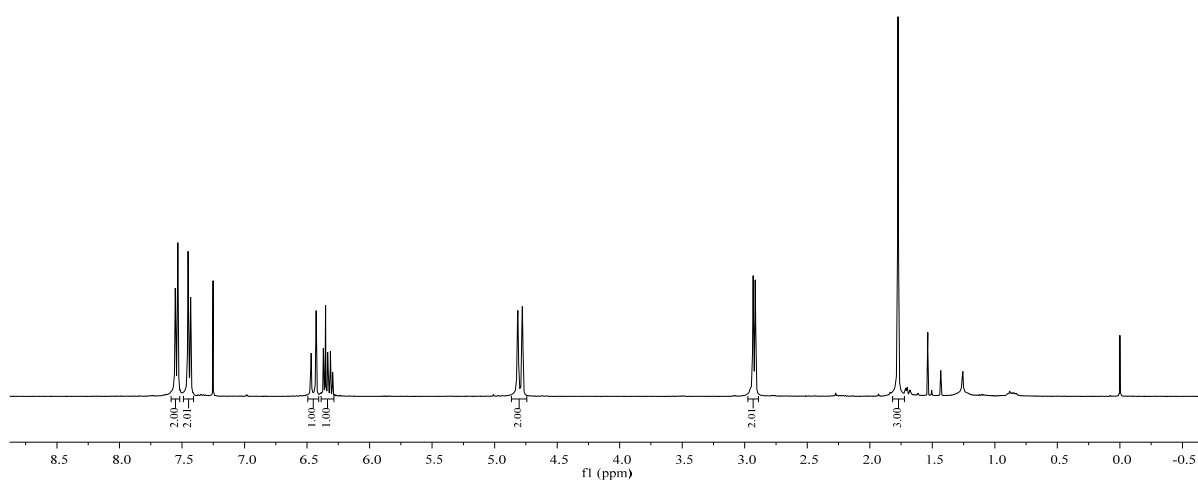


(*E*)-1-(4-methylpenta-1,4-dien-1-yl)-4-(trifluoromethyl)benzene

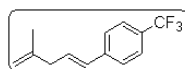


¹H NMR

Solvent: CDCl₃

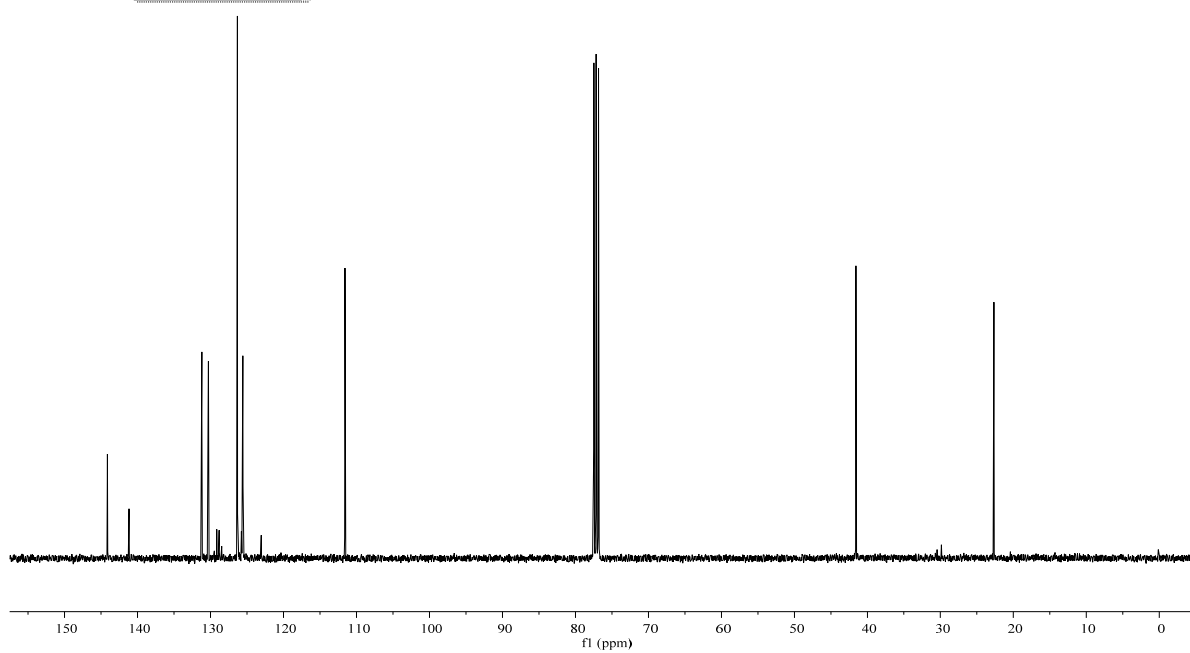


(*E*)-1-(4-methylpenta-1,4-dien-1-yl)-4-(trifluoromethyl)benzene

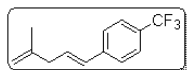


¹³C NMR

Solvent: CDCl₃

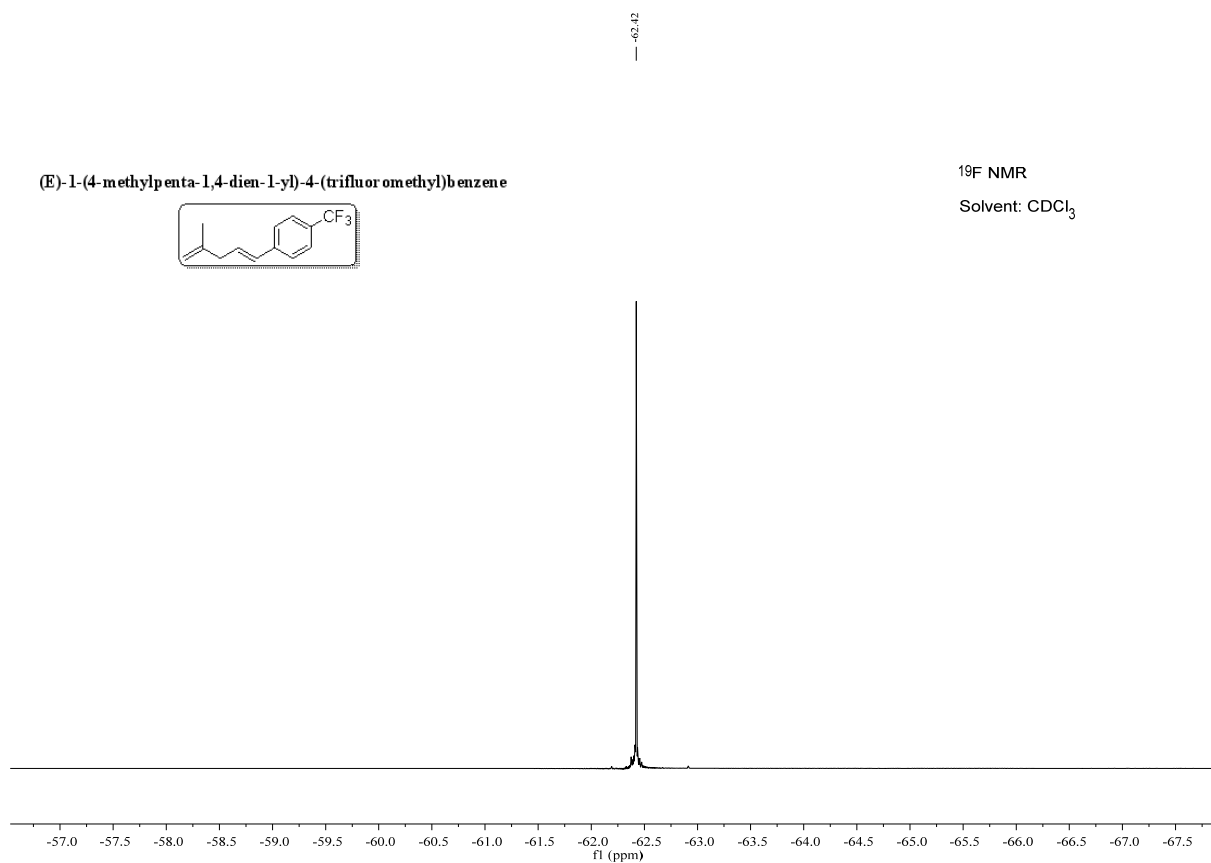


(E)-1-(4-methylpenta-1,4-dien-1-yl)-4-(trifluoromethyl)benzene

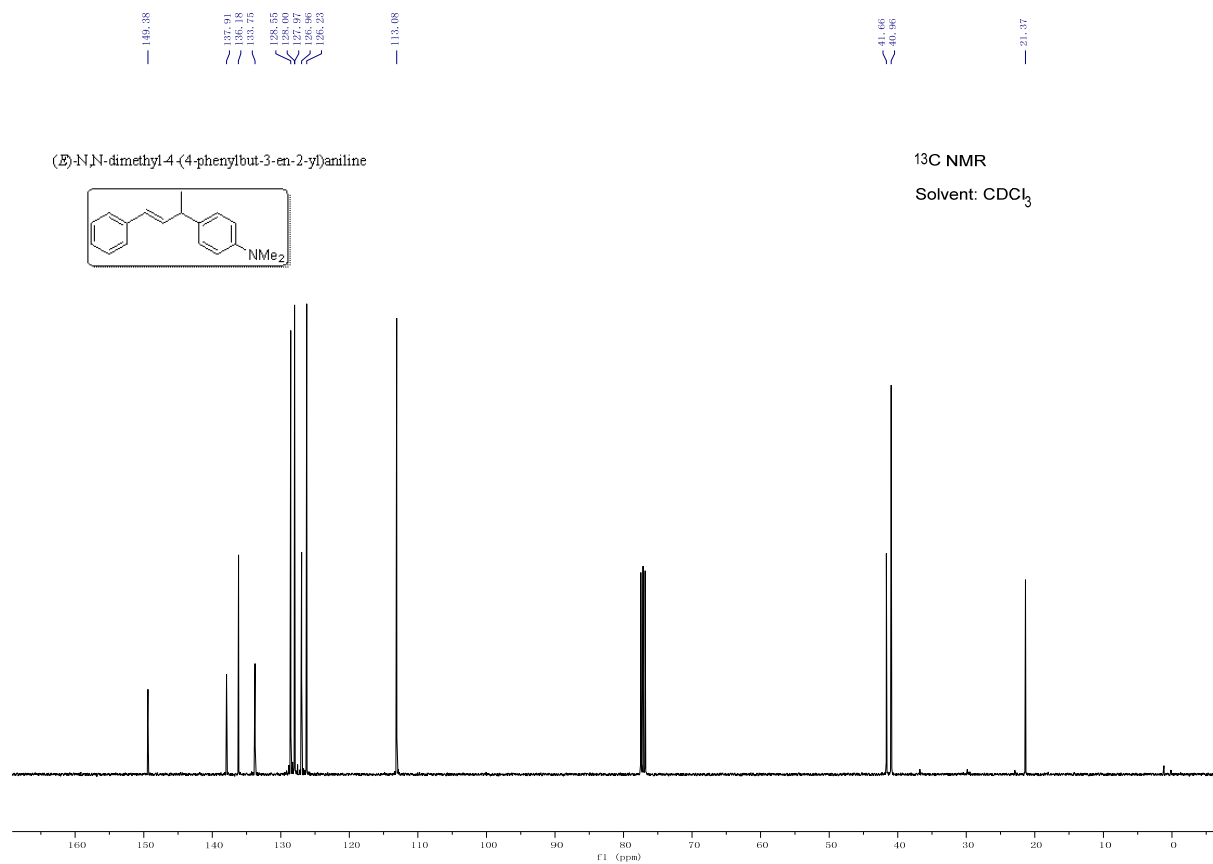
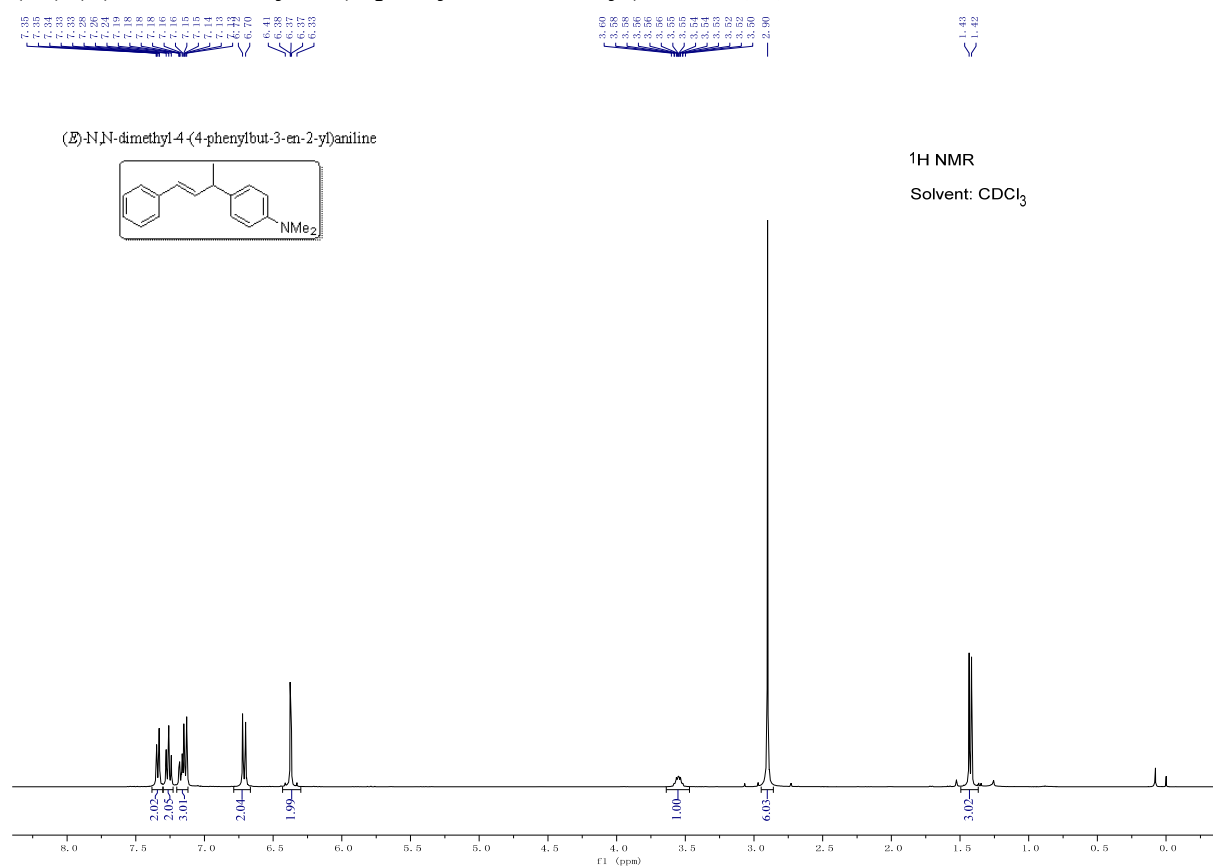


^{19}F NMR

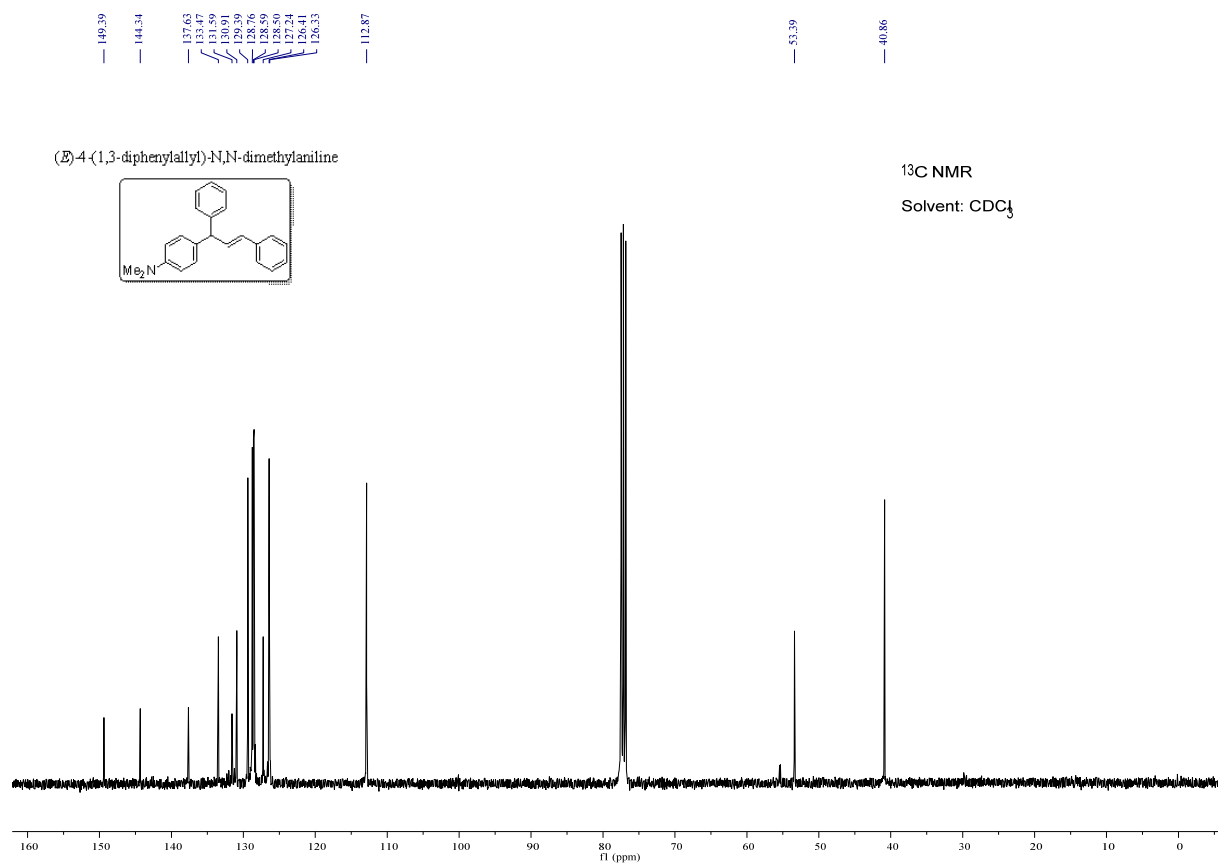
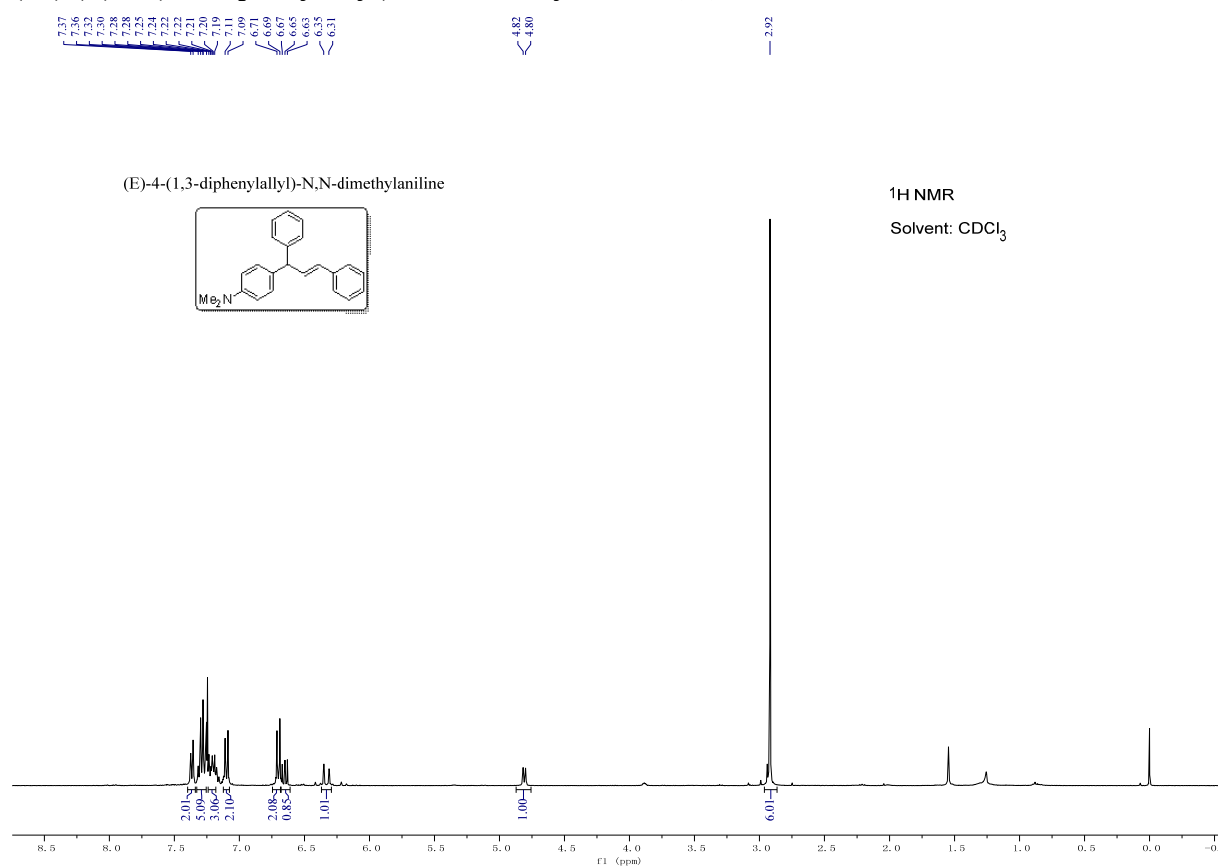
Solvent: CDCl_3



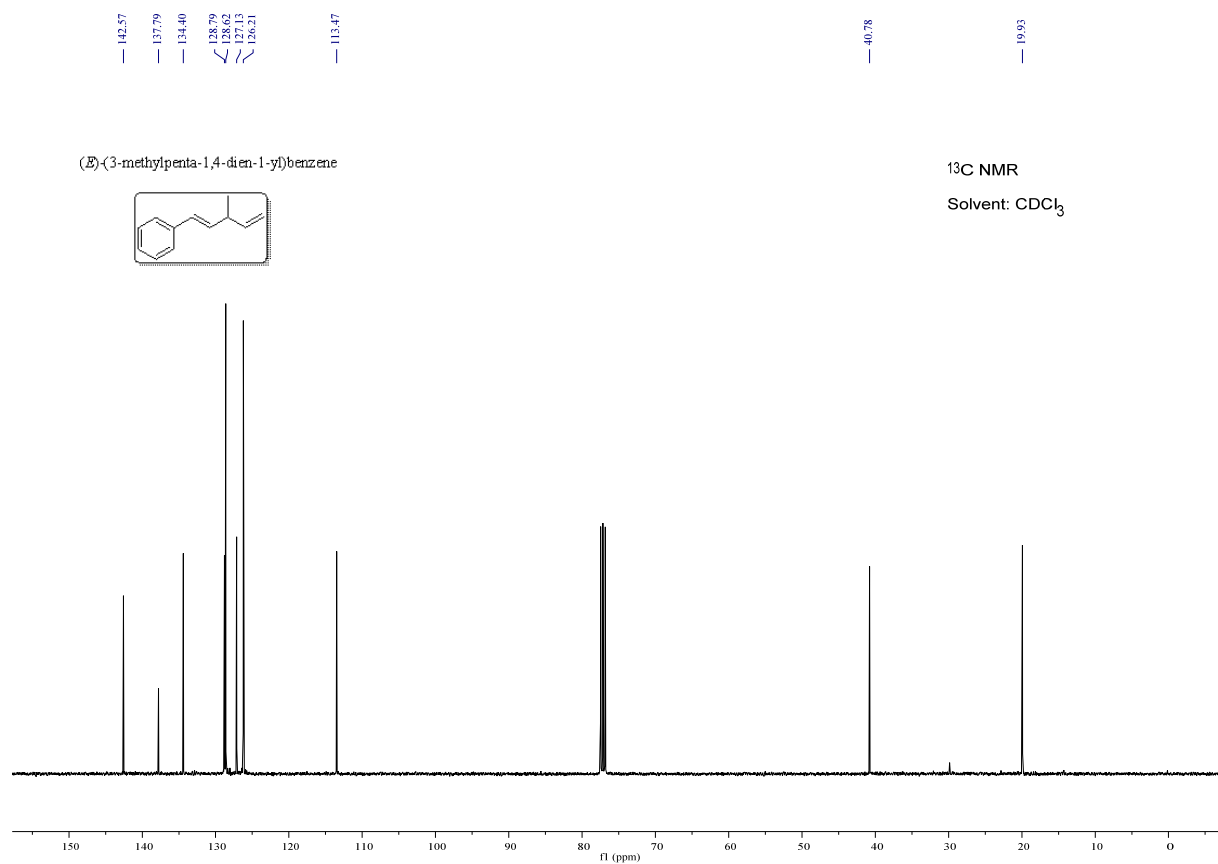
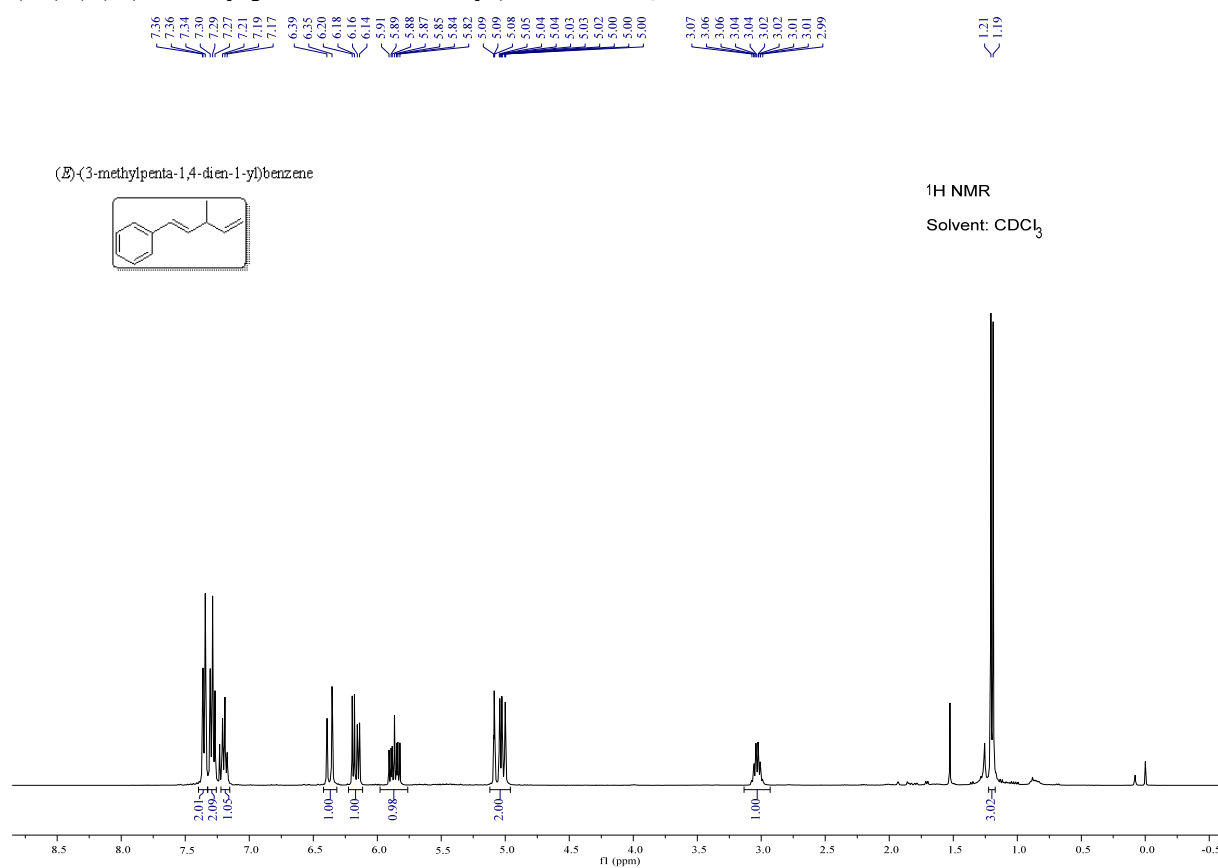
(26) (*E*)-*N,N*-dimethyl-4-(4-phenylbut-3-en-2-yl)aniline (**3u**)



(27) (E)-4-(1,3-diphenylallyl)-N,N-dimethylaniline (**3v**)



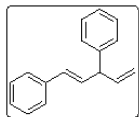
(28) (*E*)-(3-methylpenta-1,4-dien-1-yl)benzene (5g)



(29) (*E*)-penta-1,4-diene-1,3-diyl dibenzene (5h)

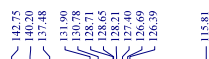
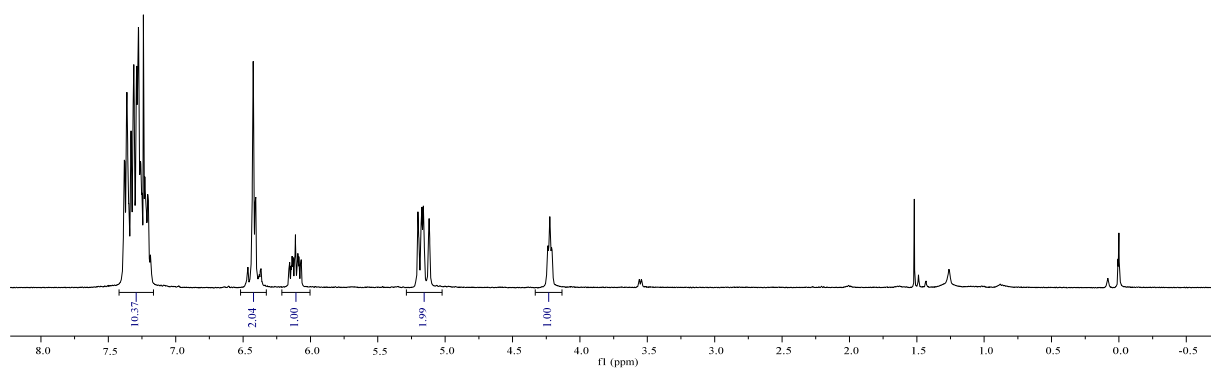


(*E*)-penta-1,4-diene-1,3-diyl dibenzene

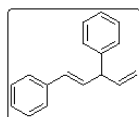


¹H NMR

Solvent: CDCl₃



(*E*)-penta-1,4-diene-1,3-diyl dibenzene



¹³C NMR

Solvent: CDCl₃

