Supporting Materials to

An operationally simple approach to (*E*)-α-halo vinyl sulfides and their applications for accessing stereodefined trisubstituted alkenes

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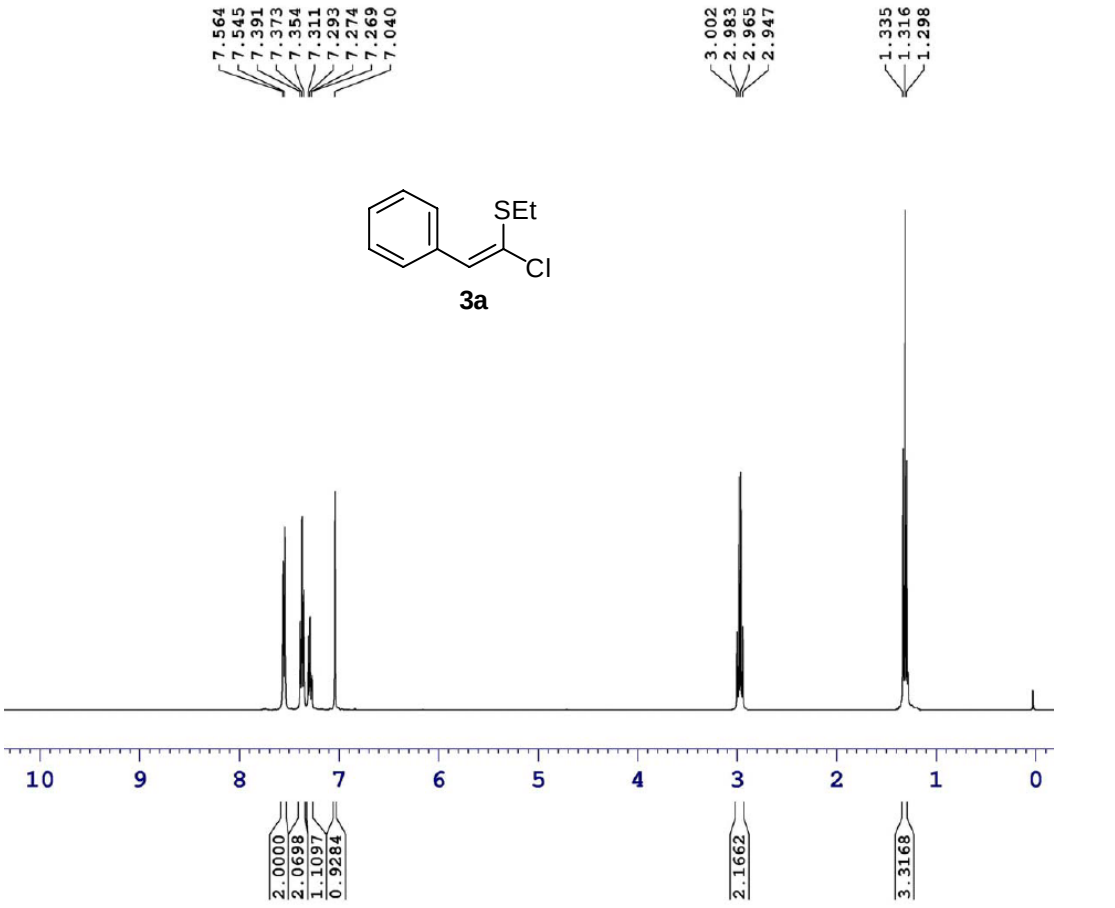

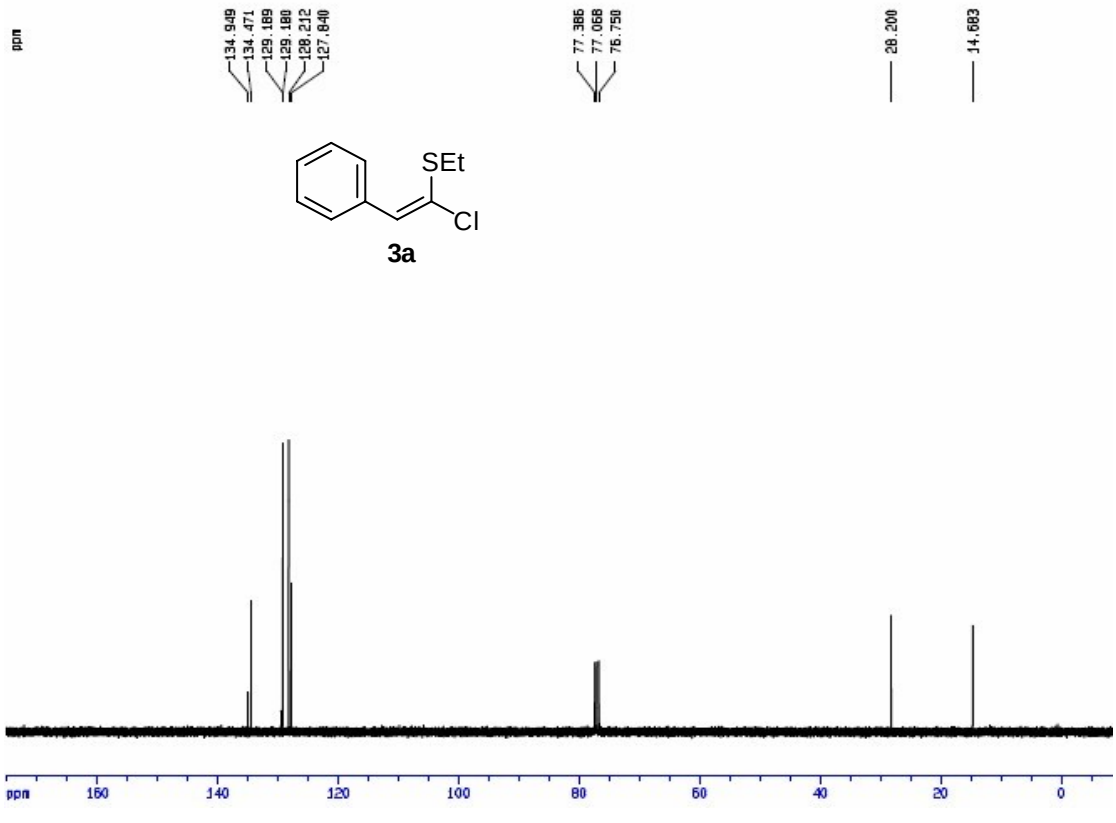

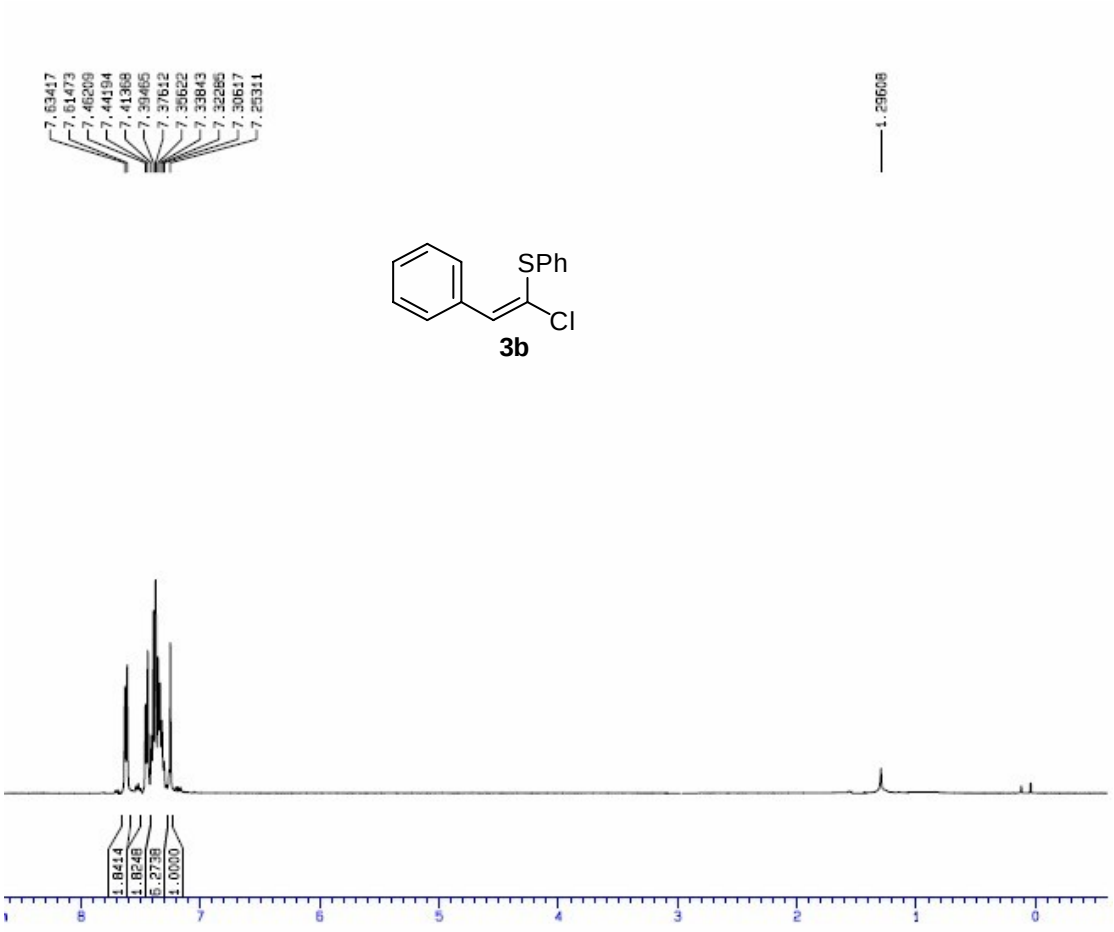

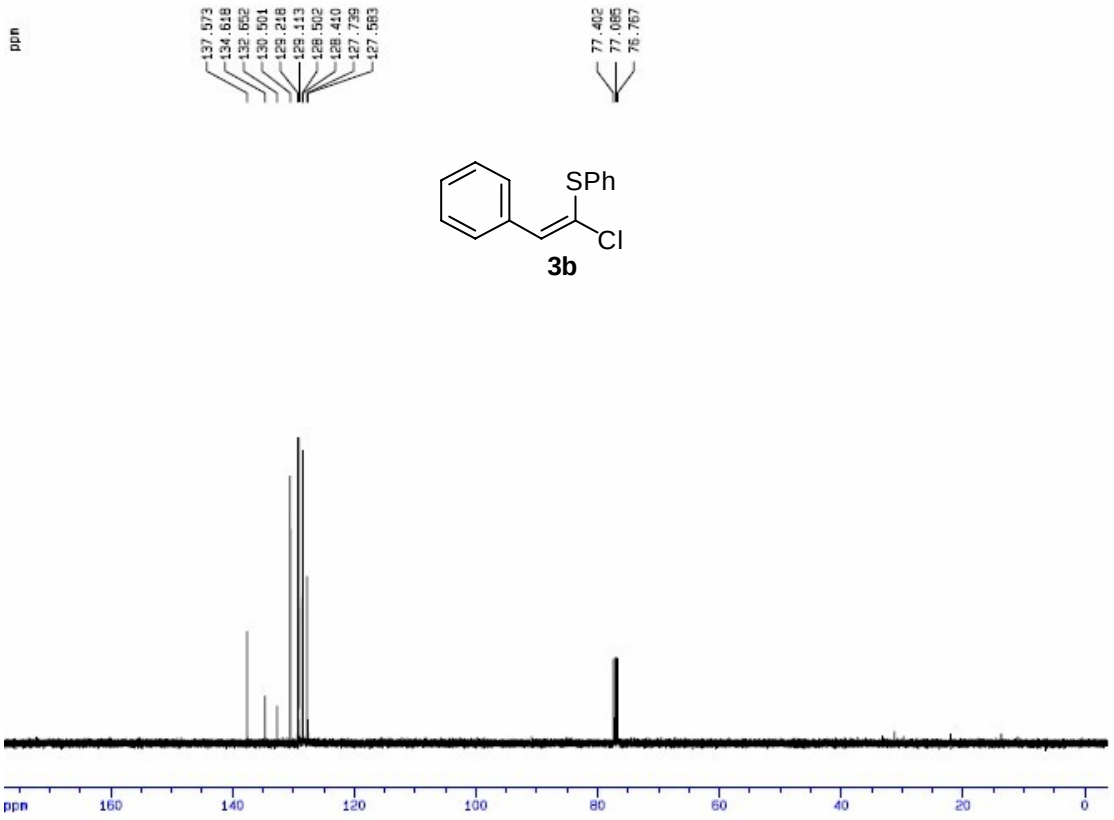

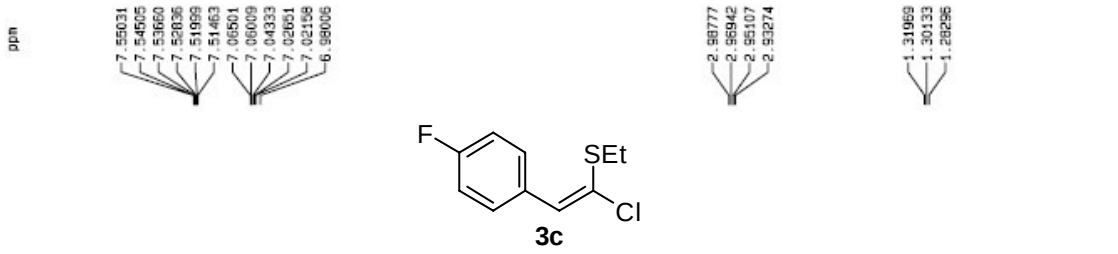

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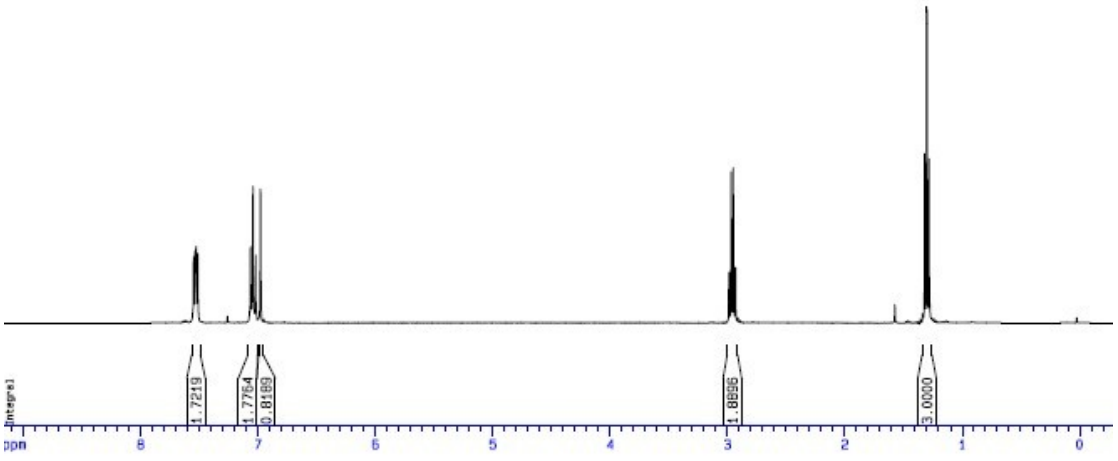

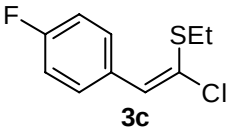

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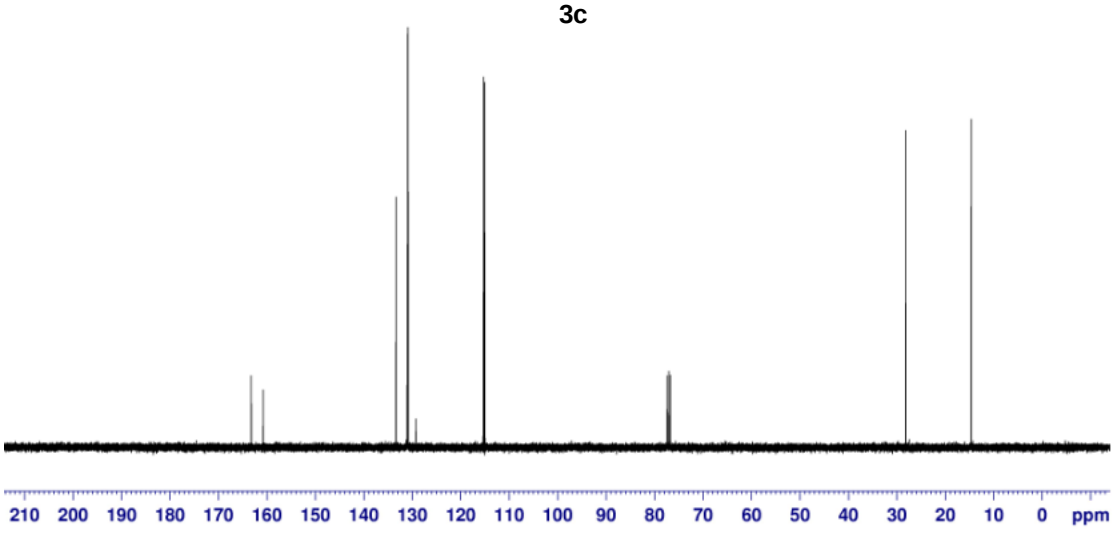

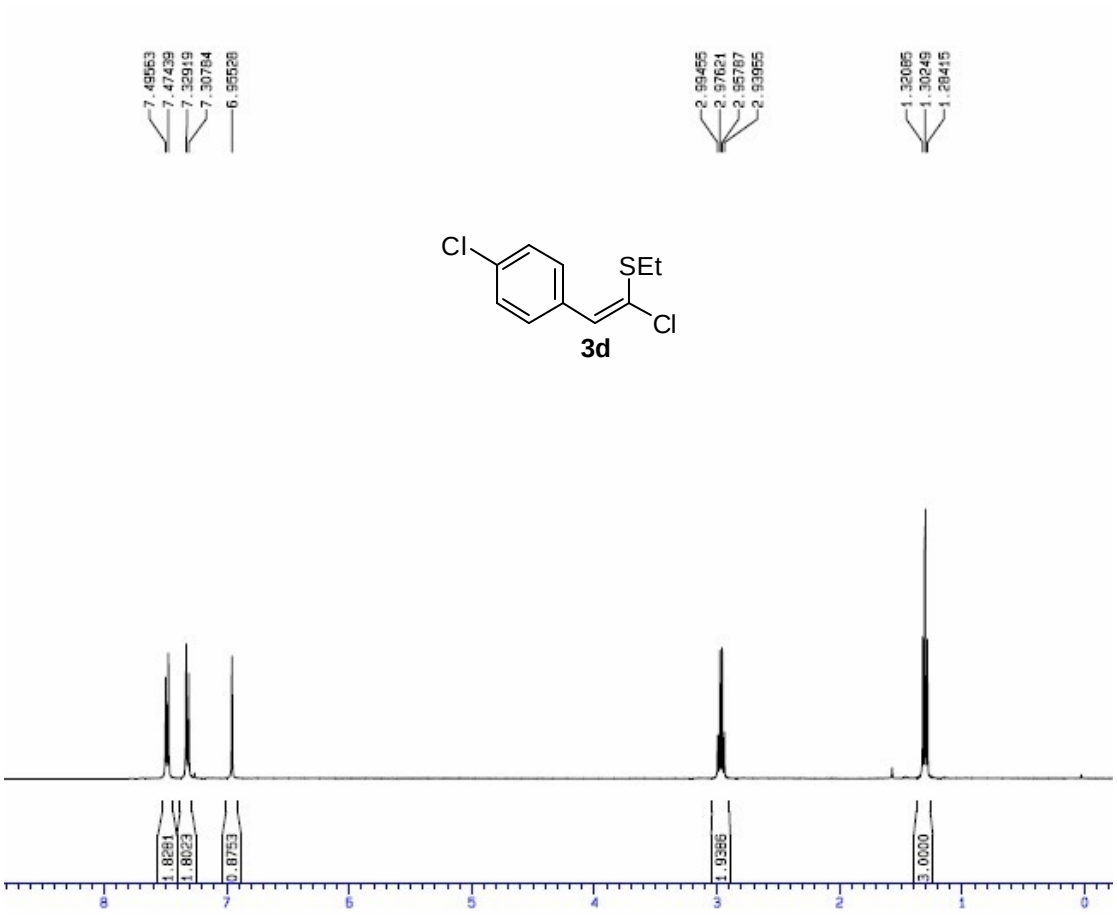

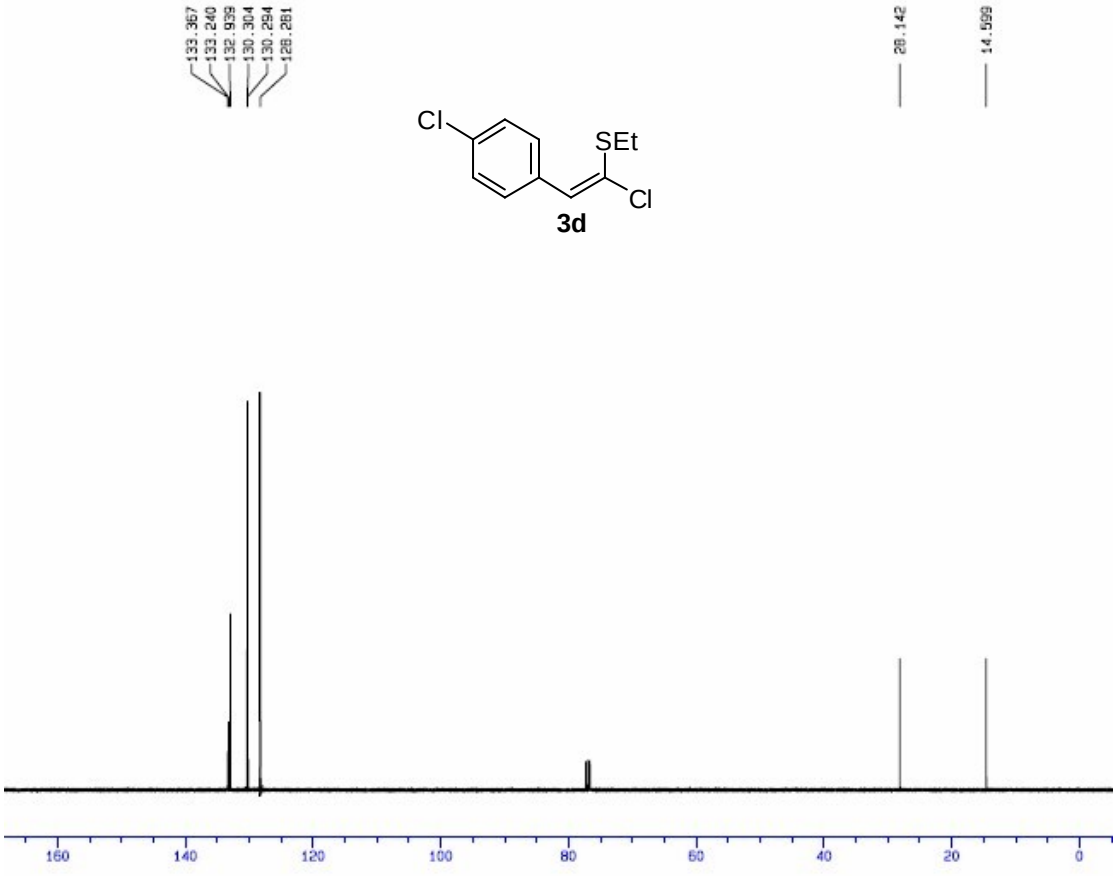

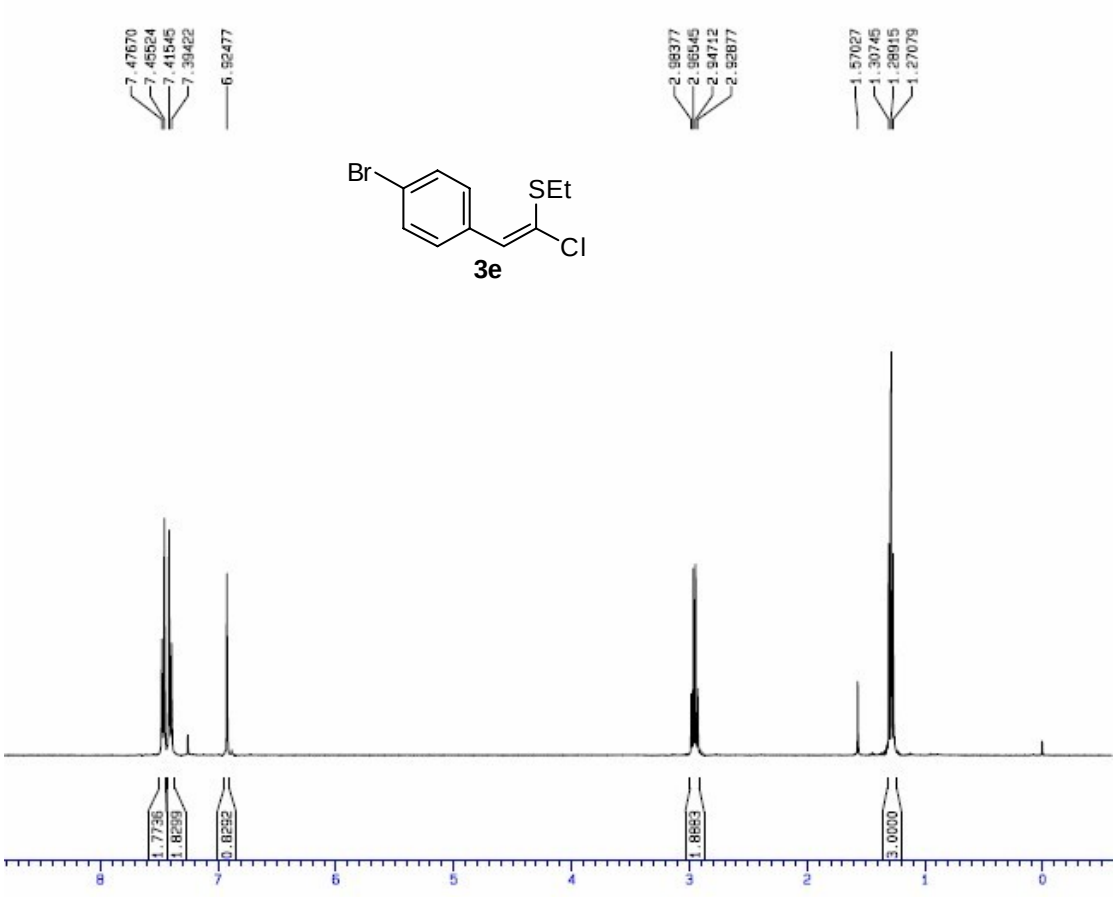

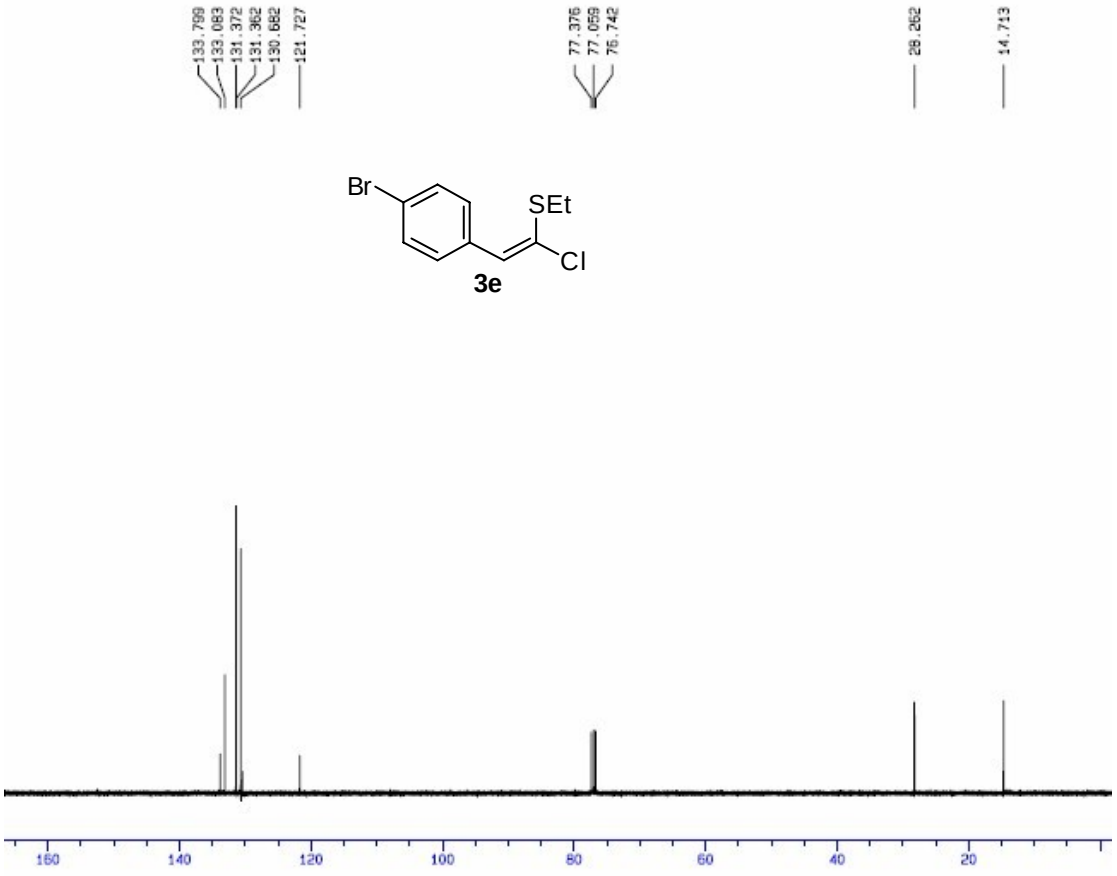

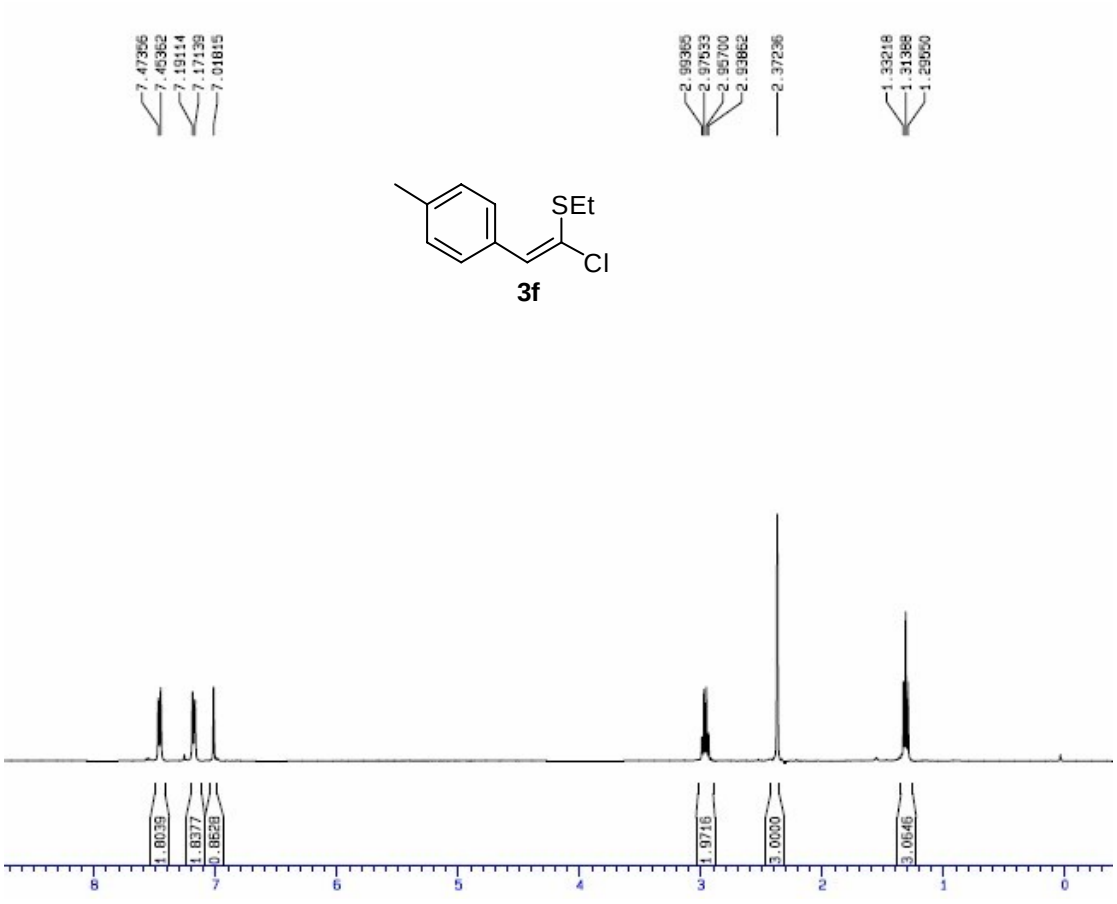

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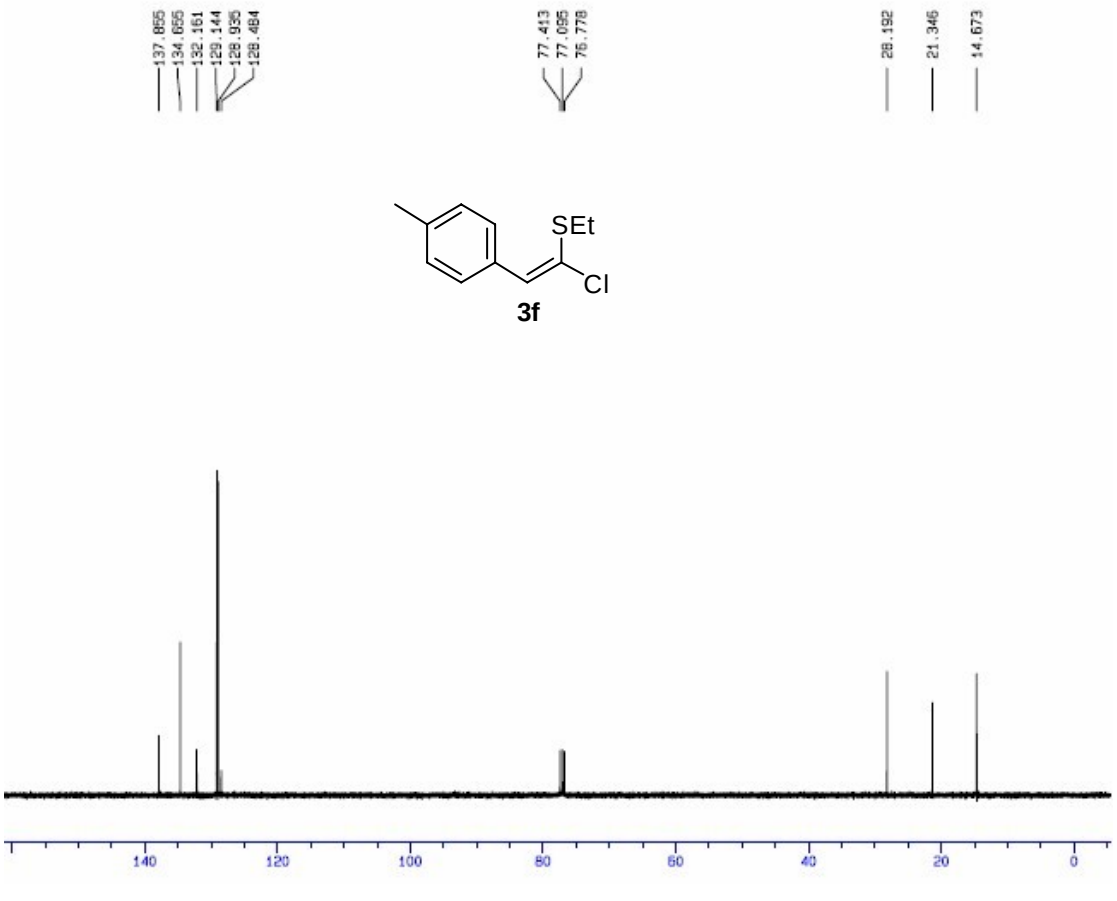

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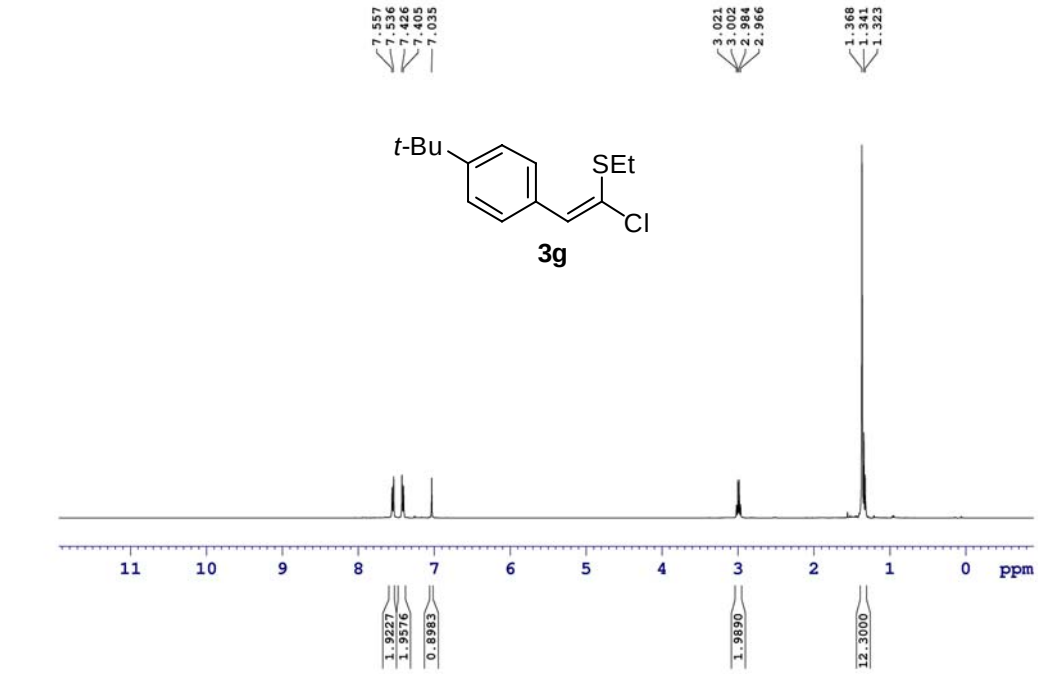

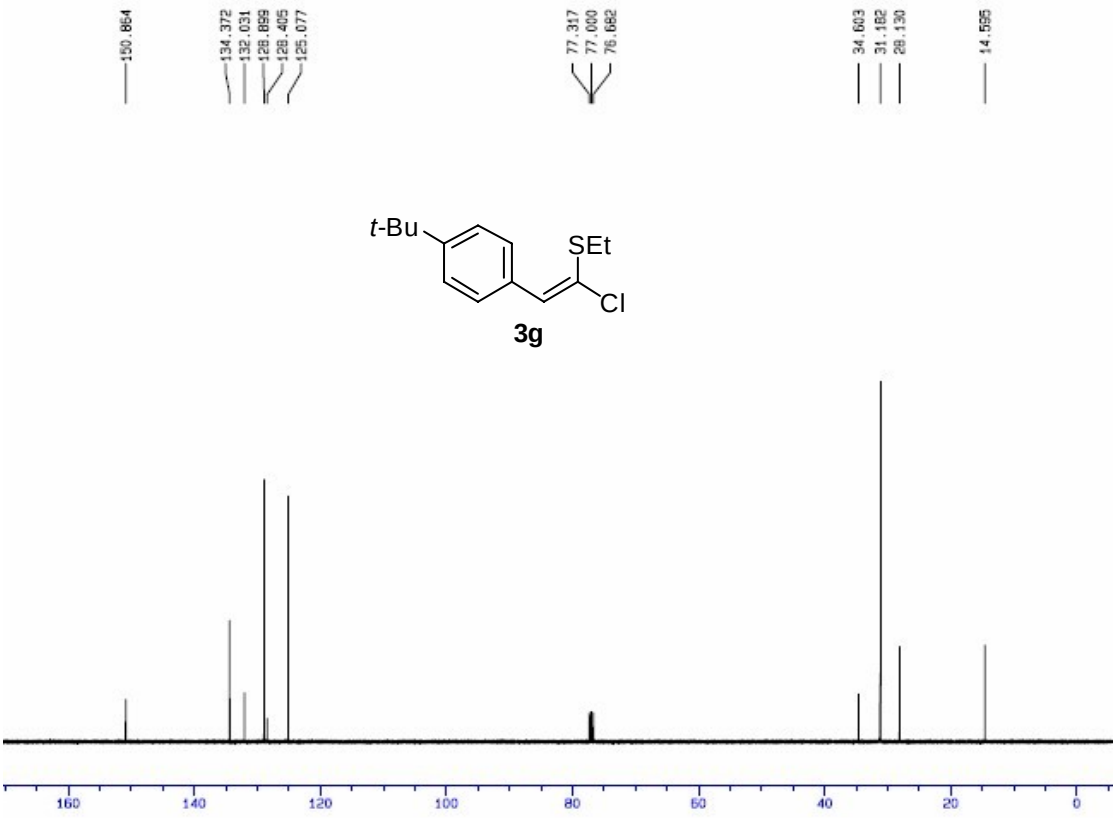

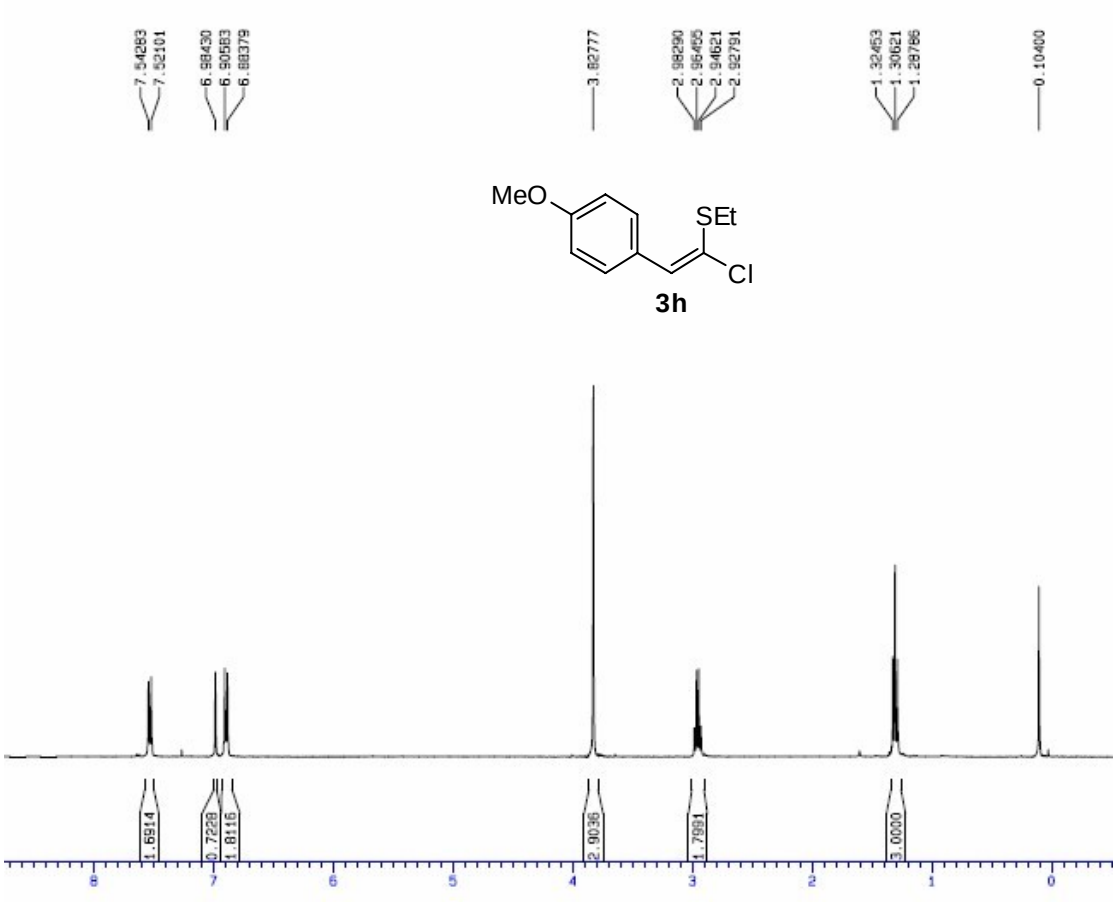

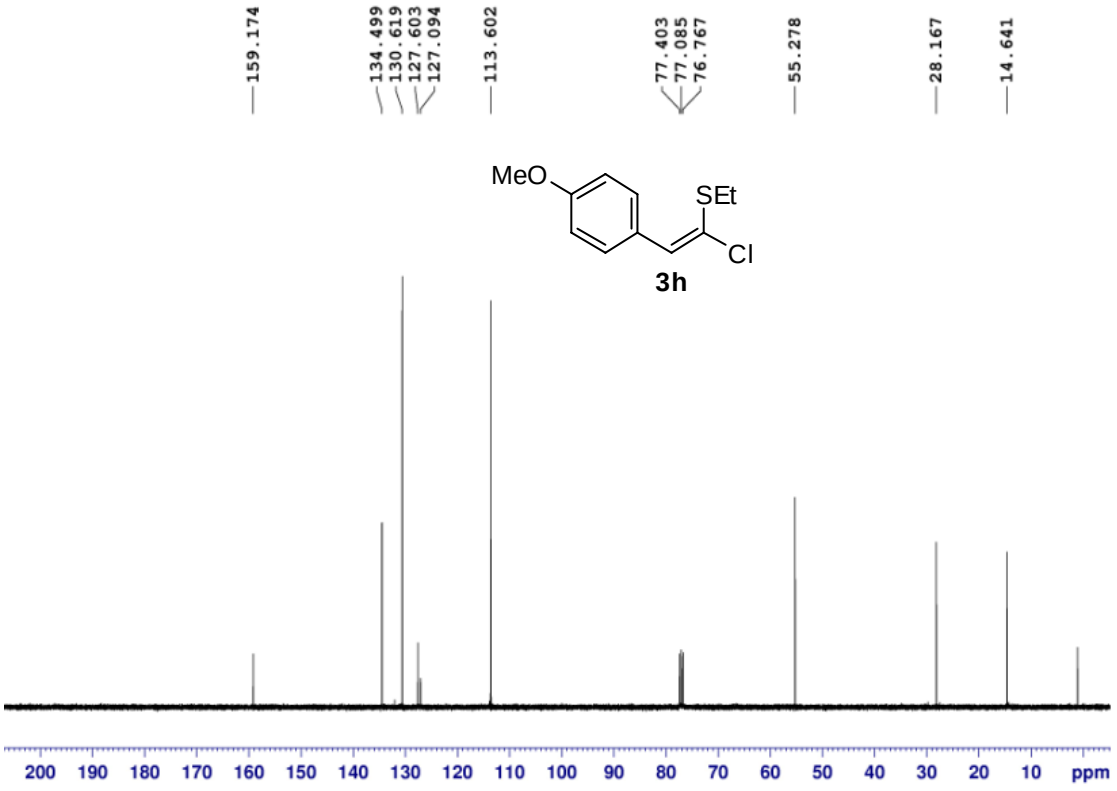

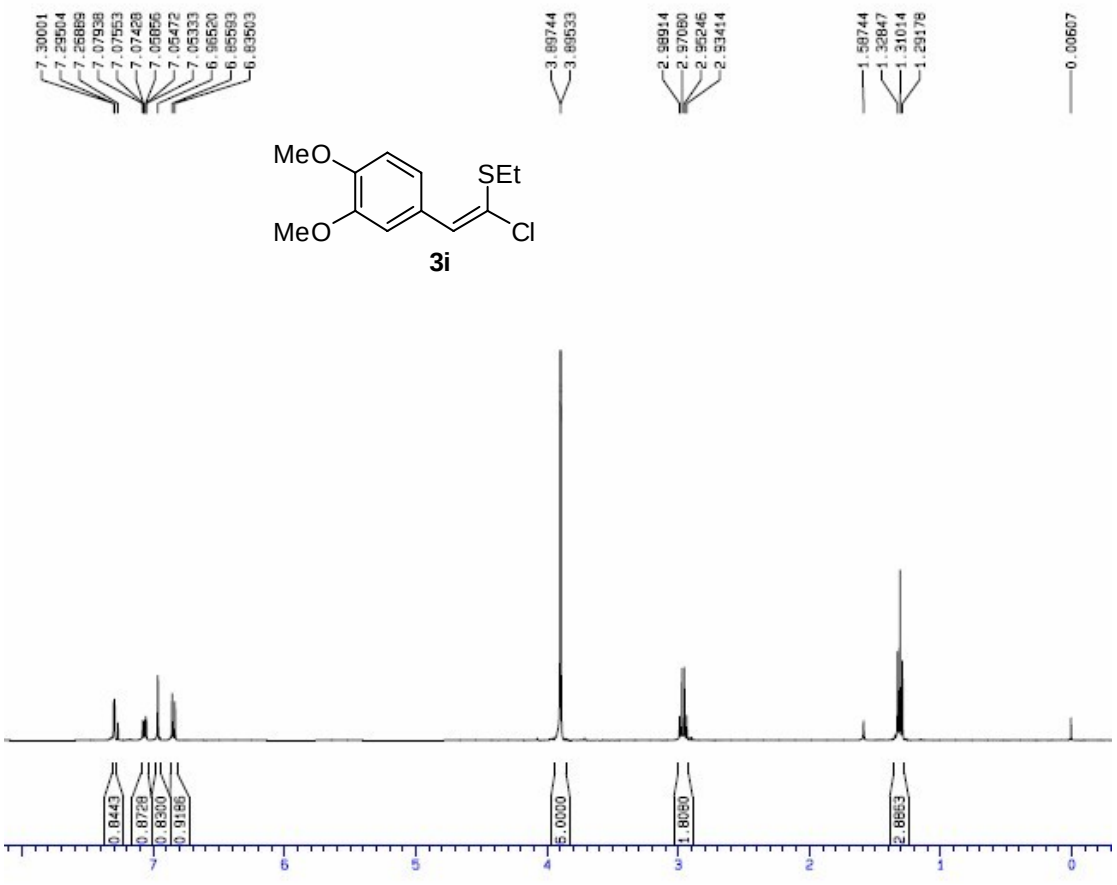

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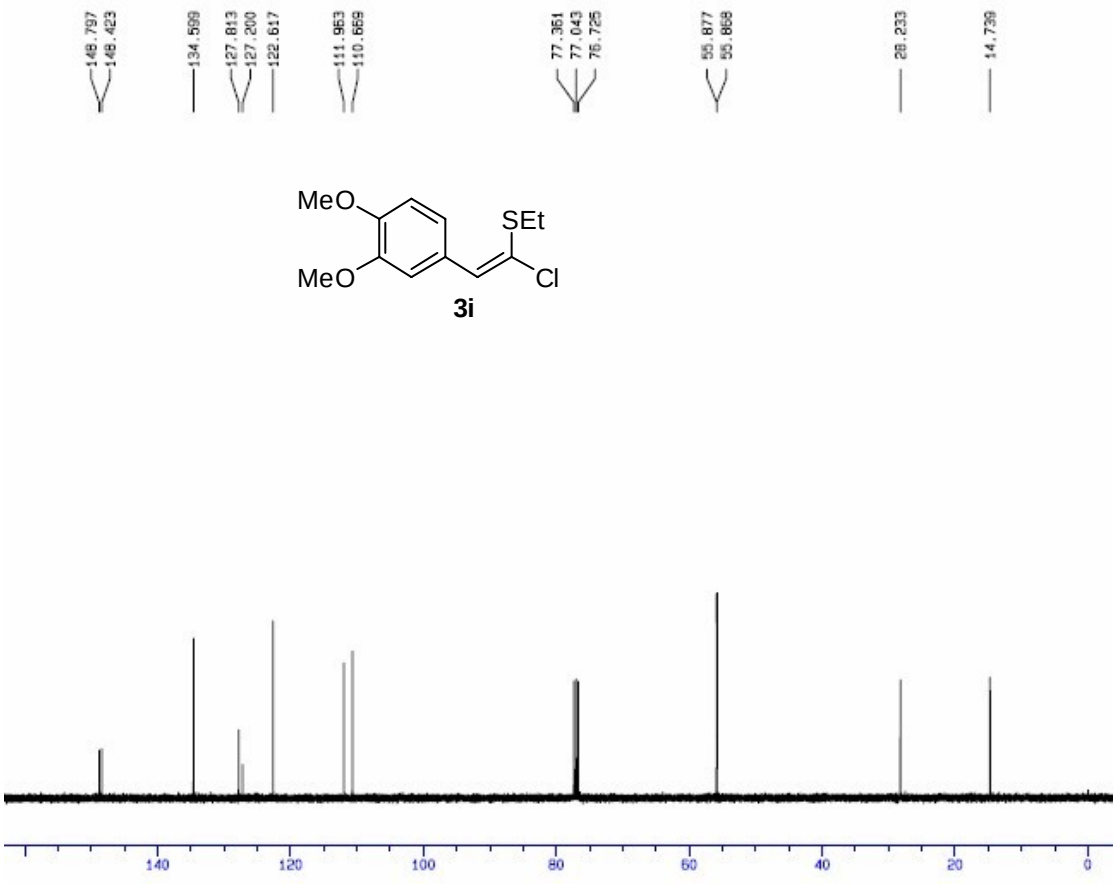

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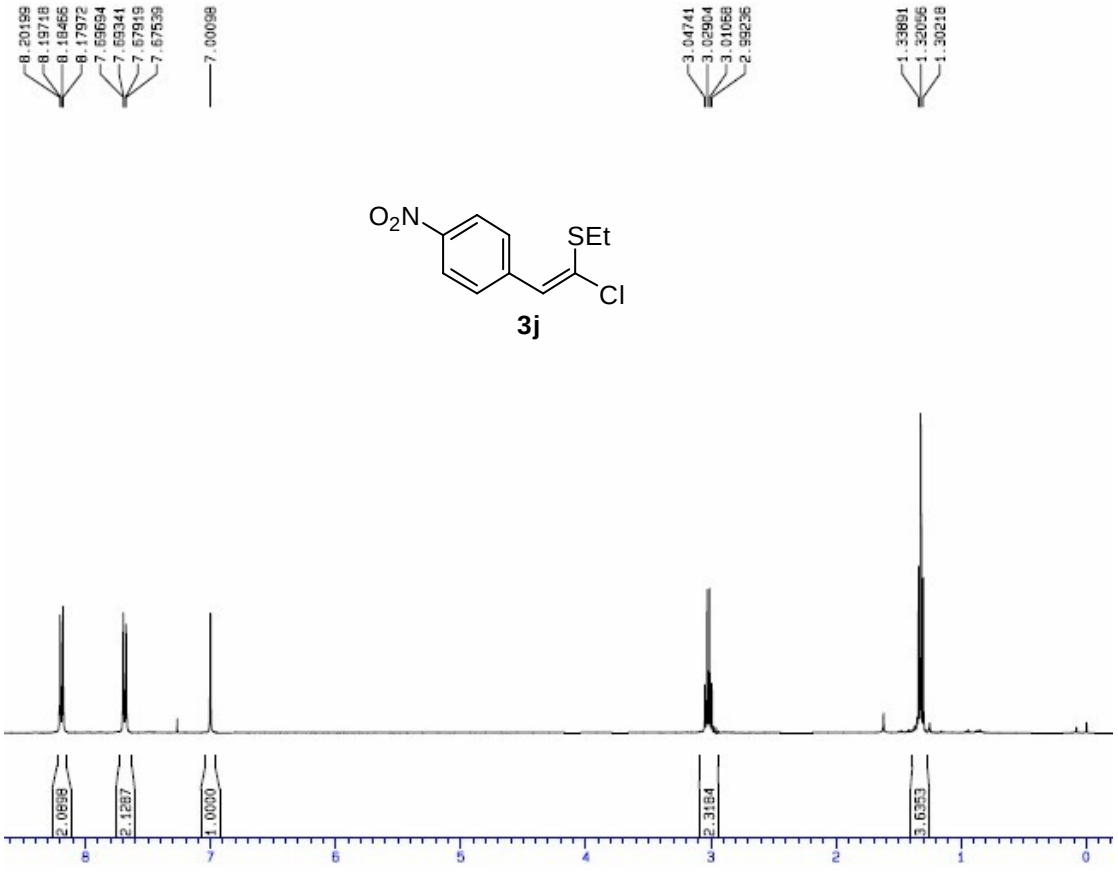

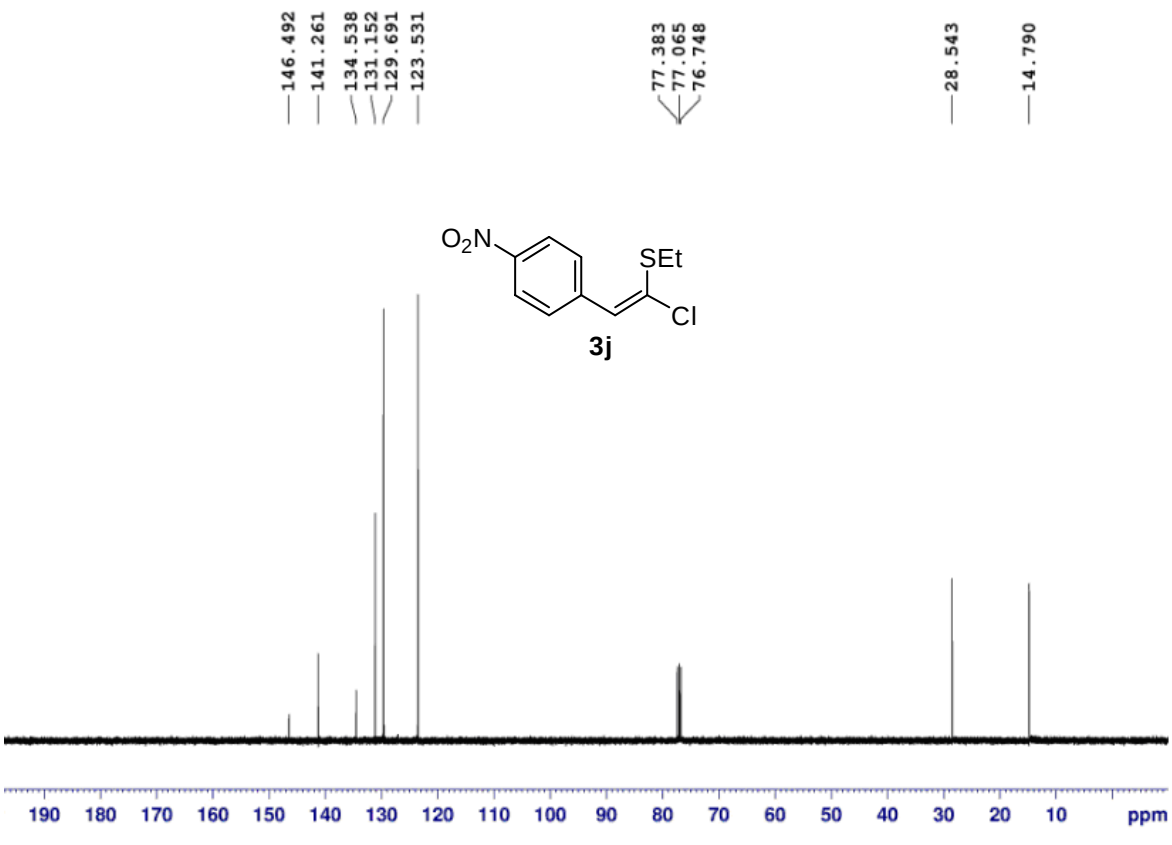

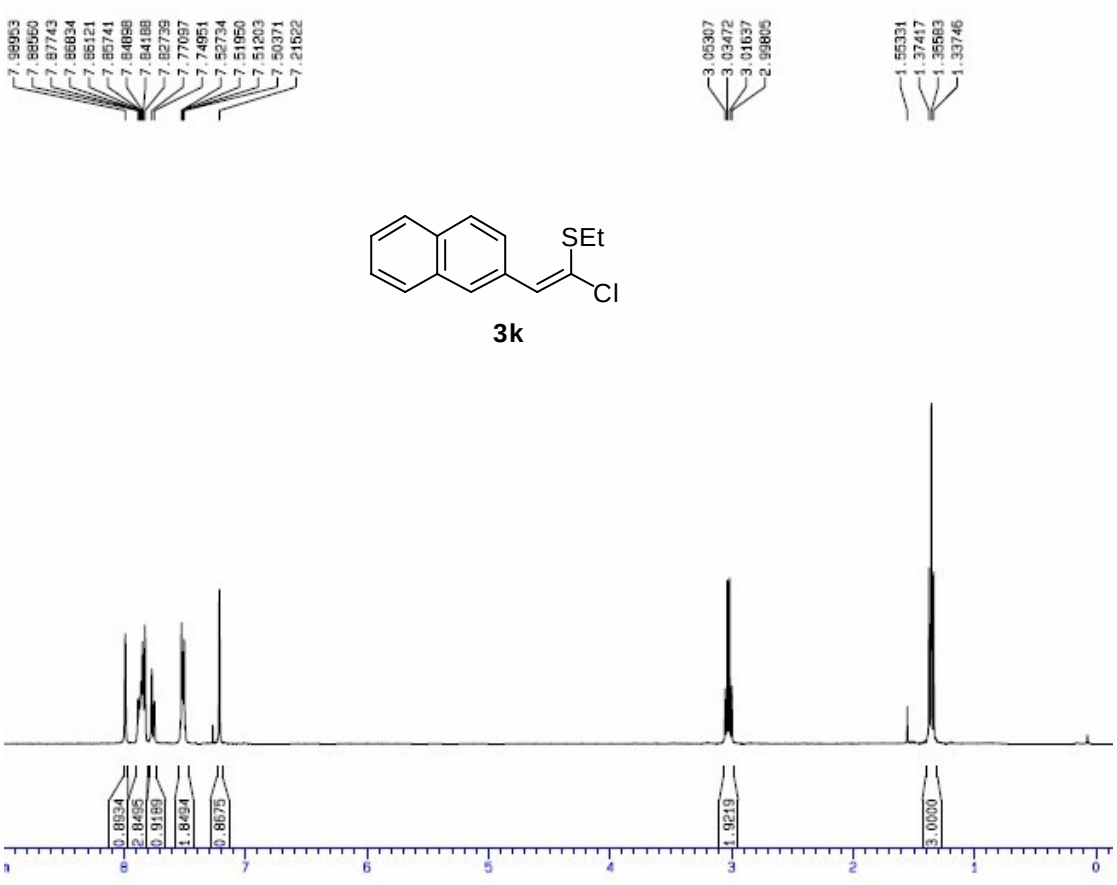

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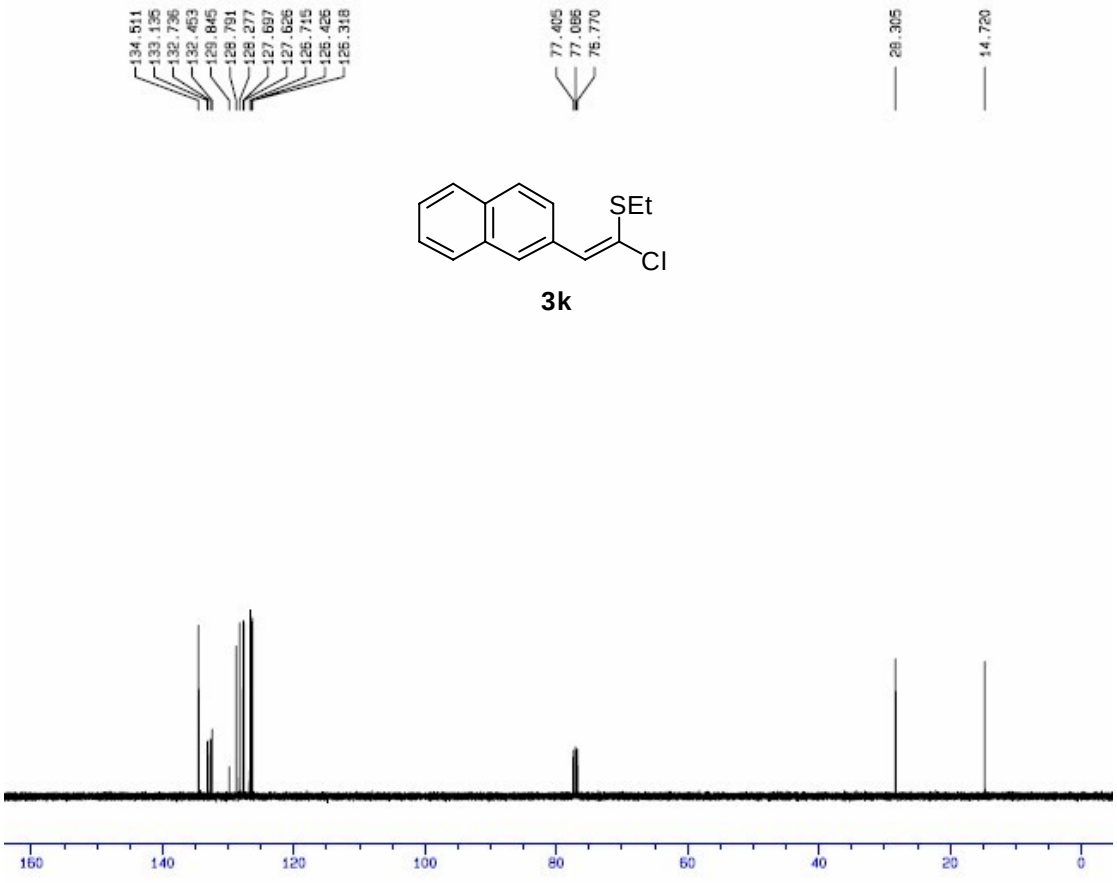

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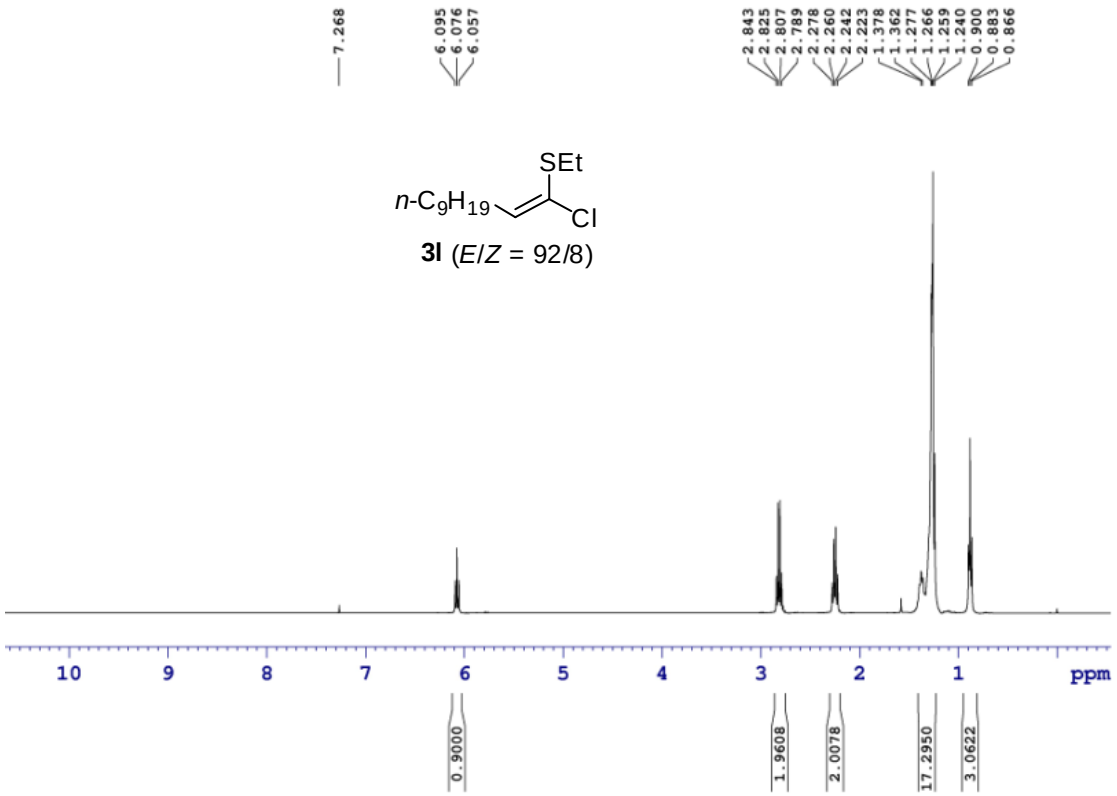

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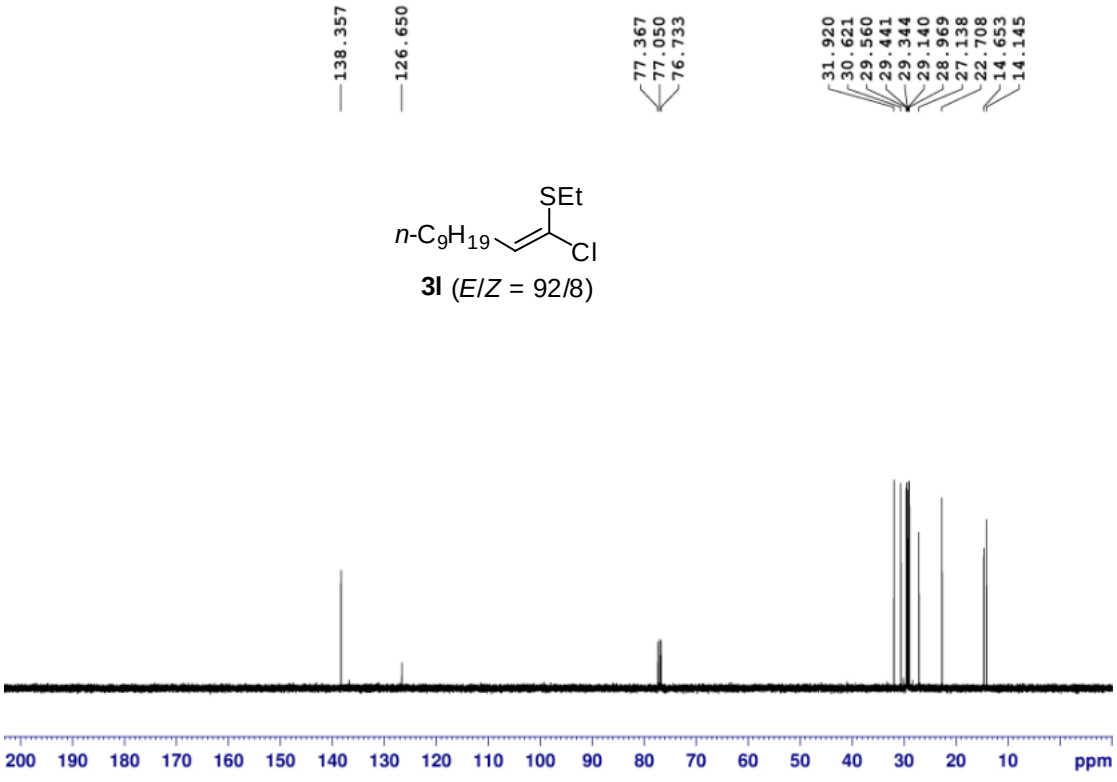

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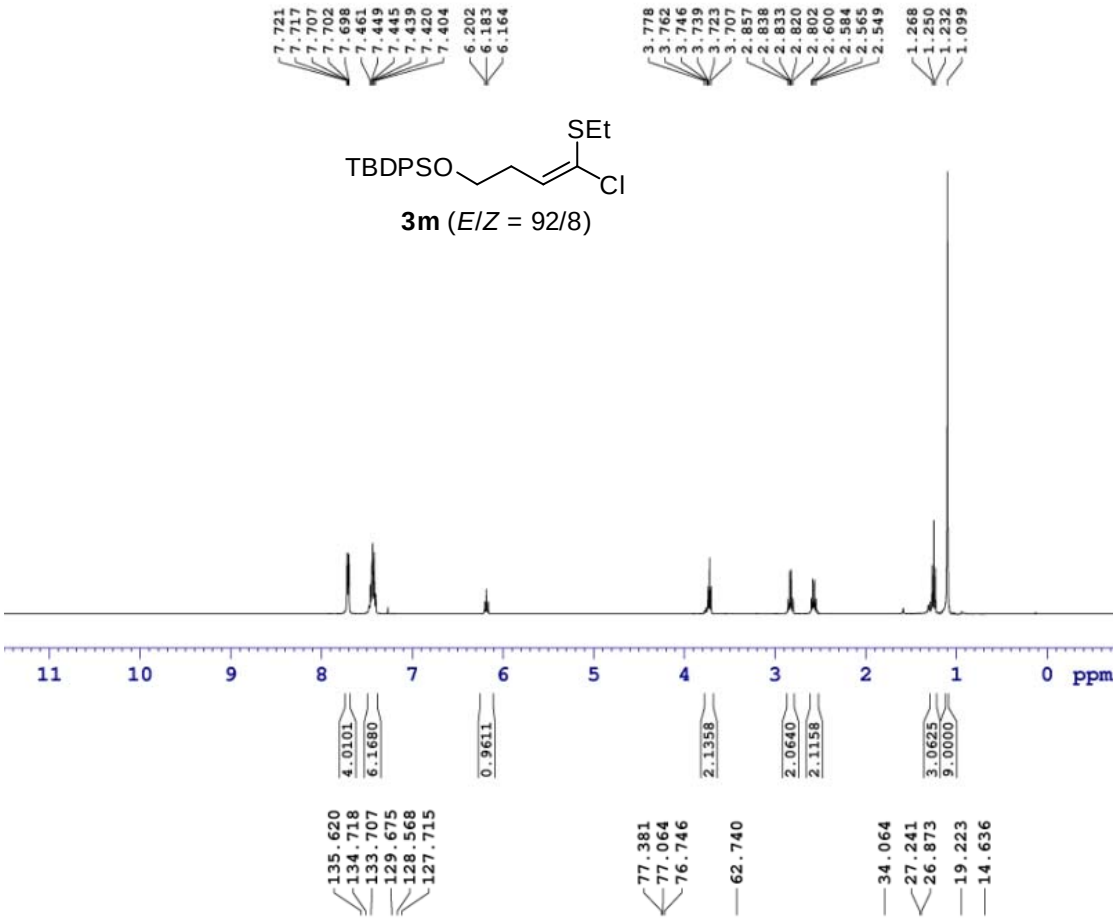

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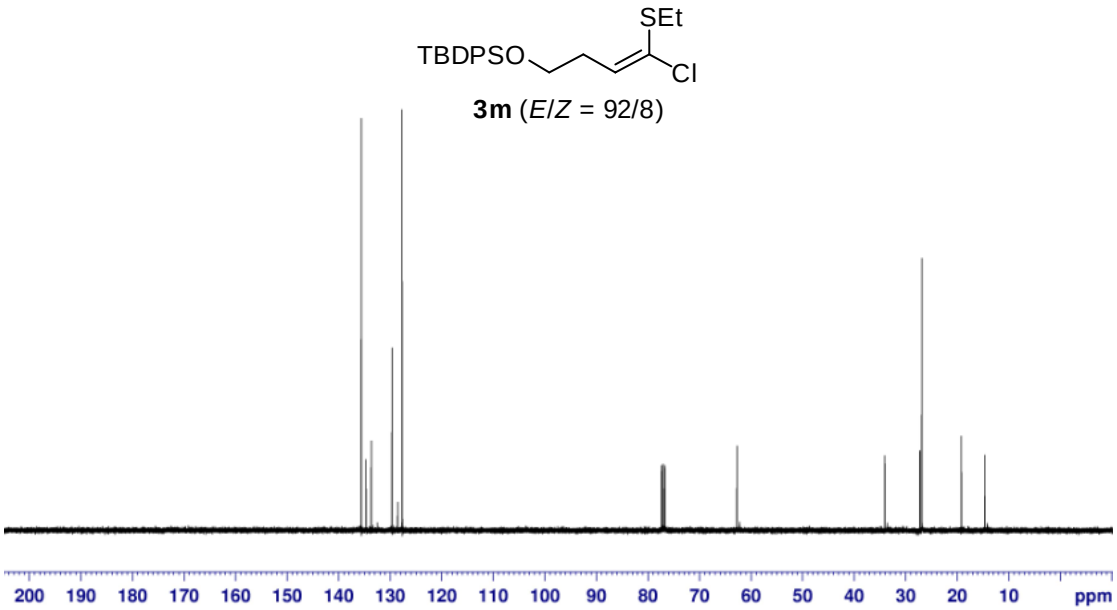

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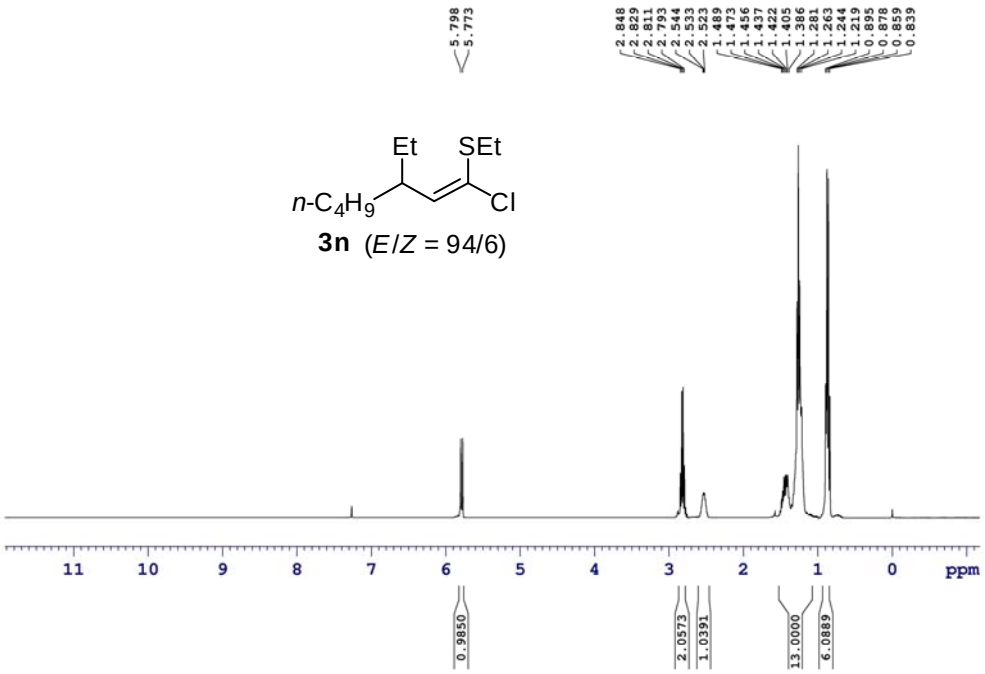

Et SEt
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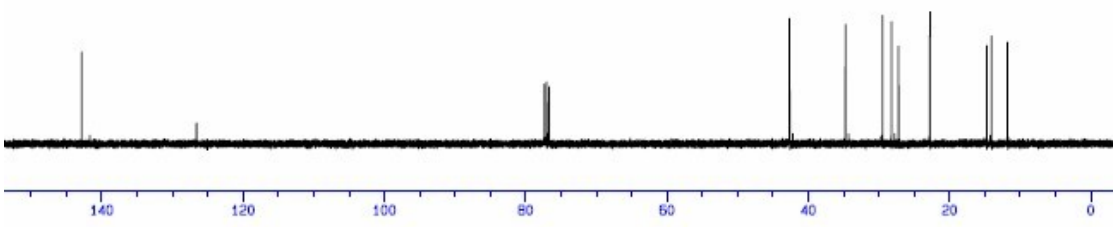
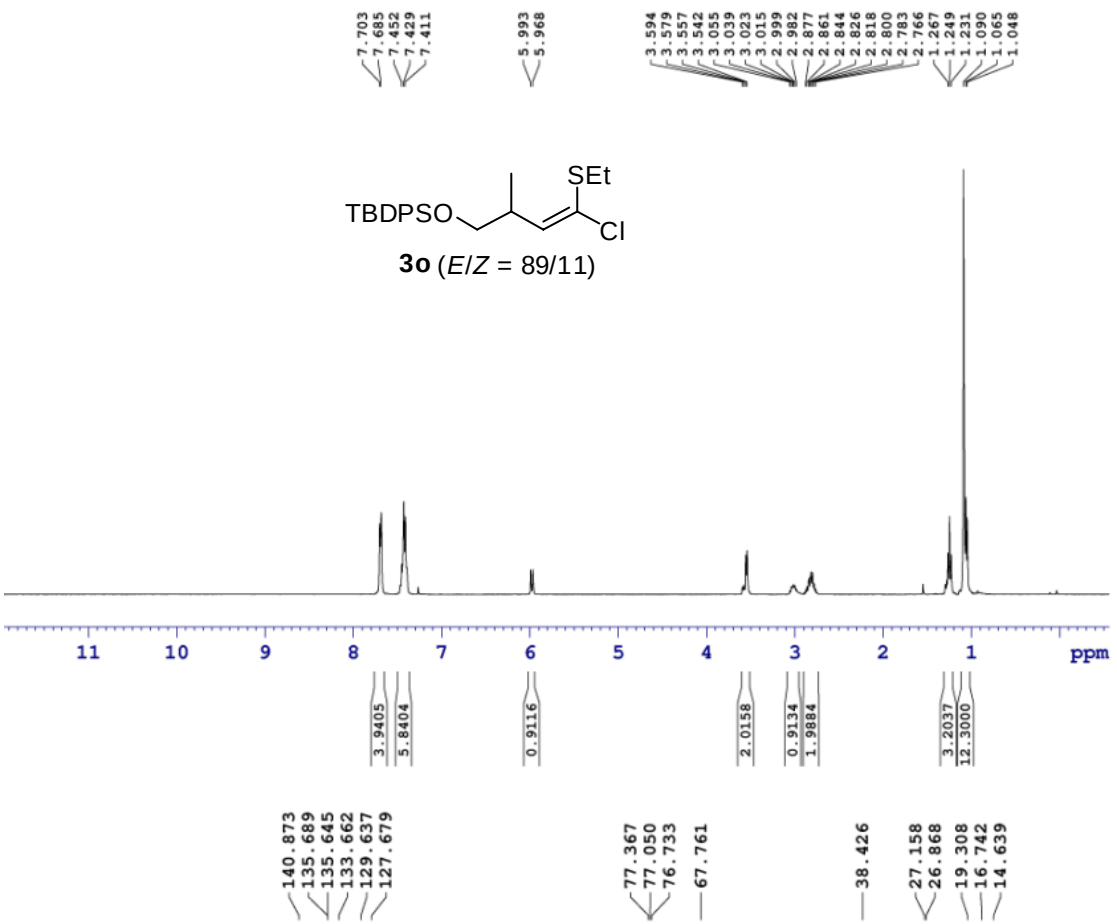
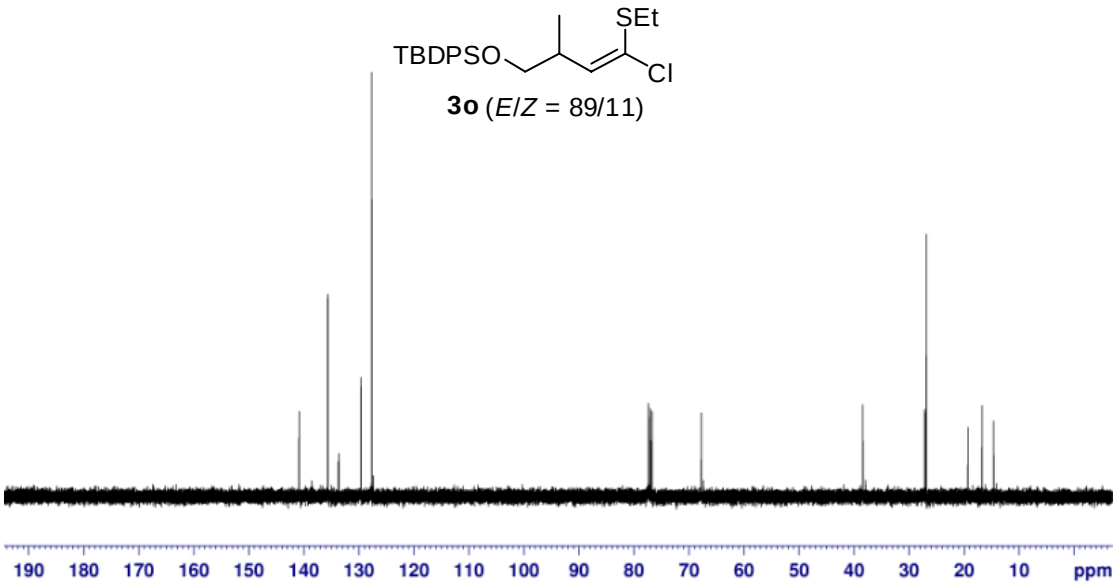
3n (*E*/*Z* = 94/6)

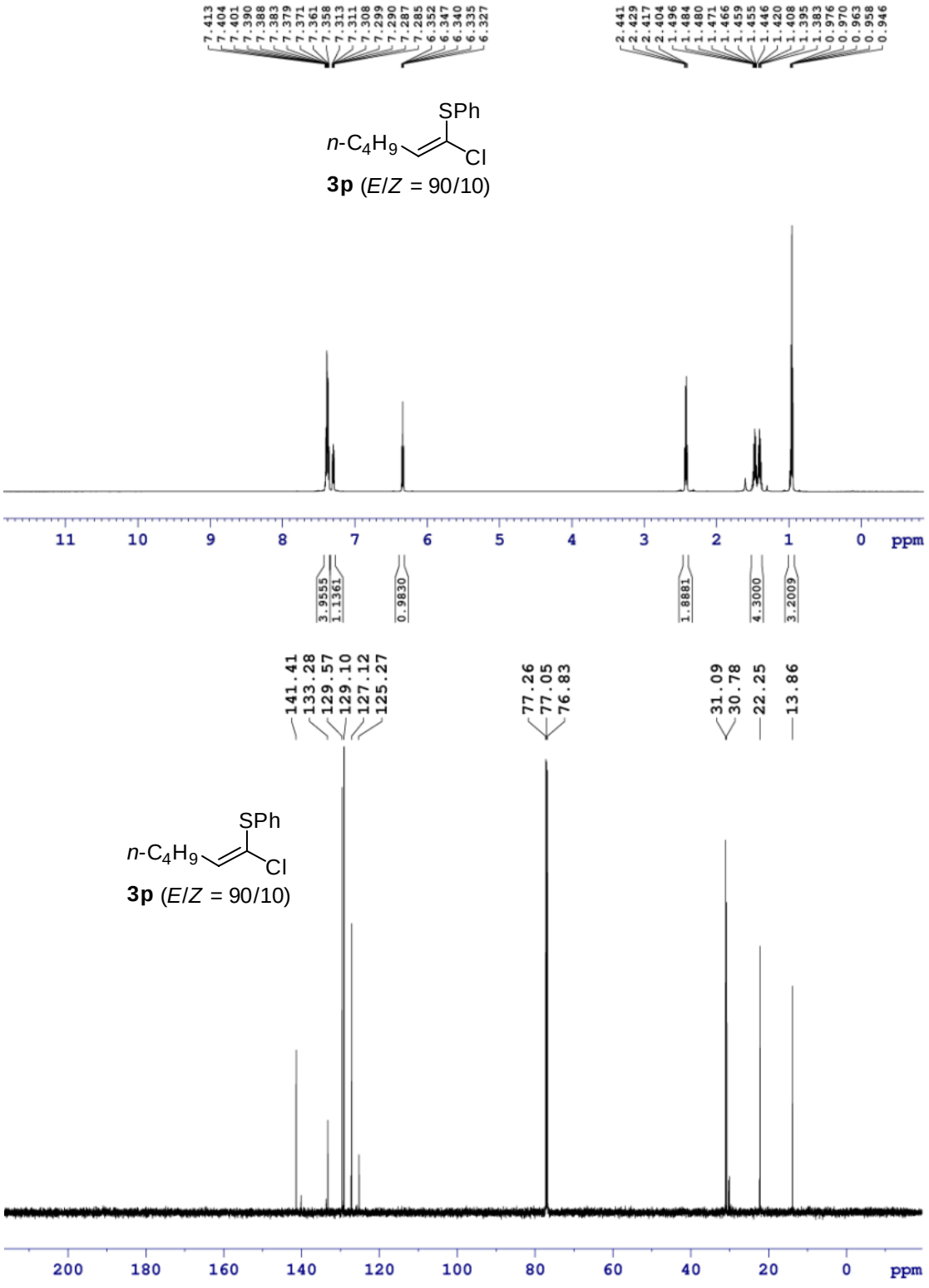
Et SEt
n-C_4H_9 Cl

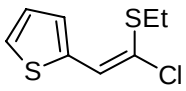
3n (*E*/*Z* = 94/6)











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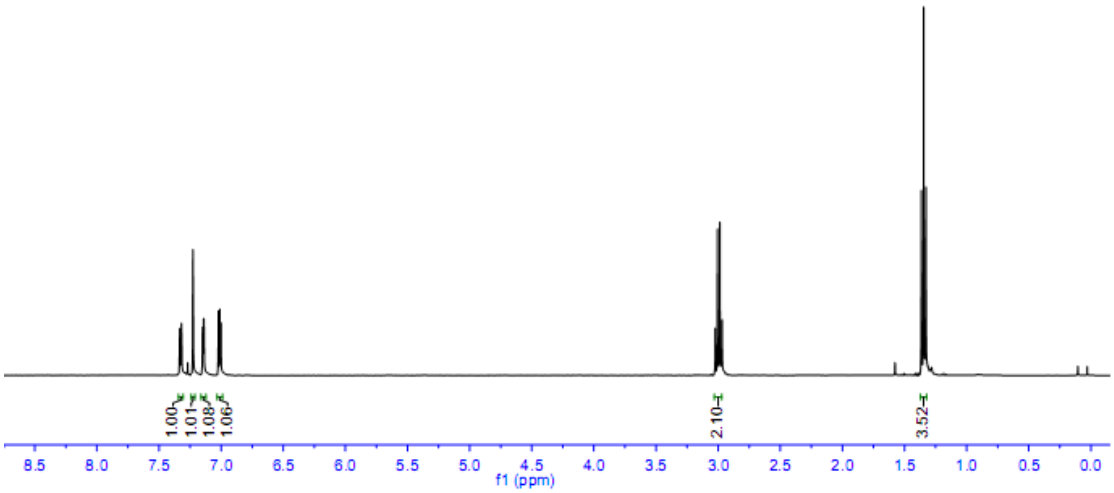

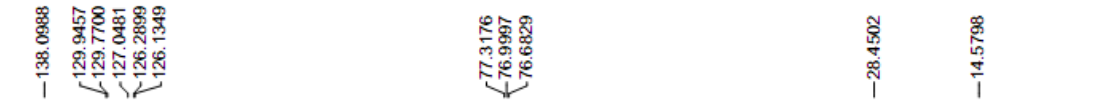

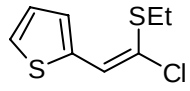

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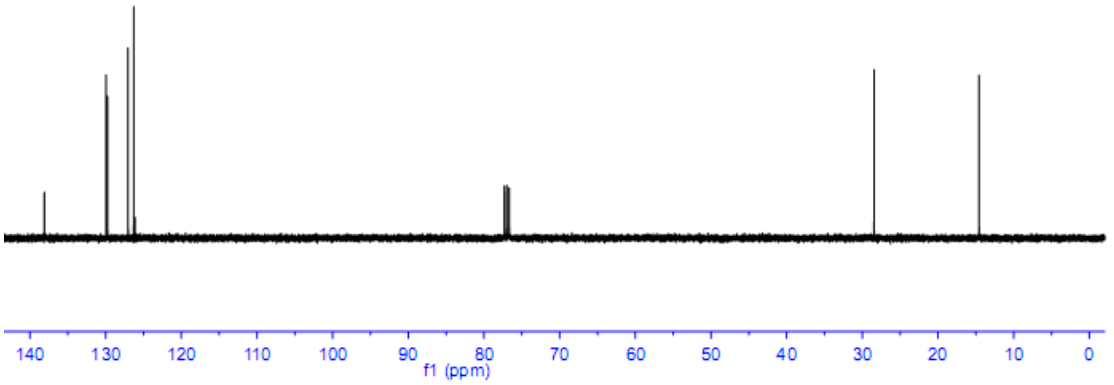

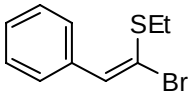

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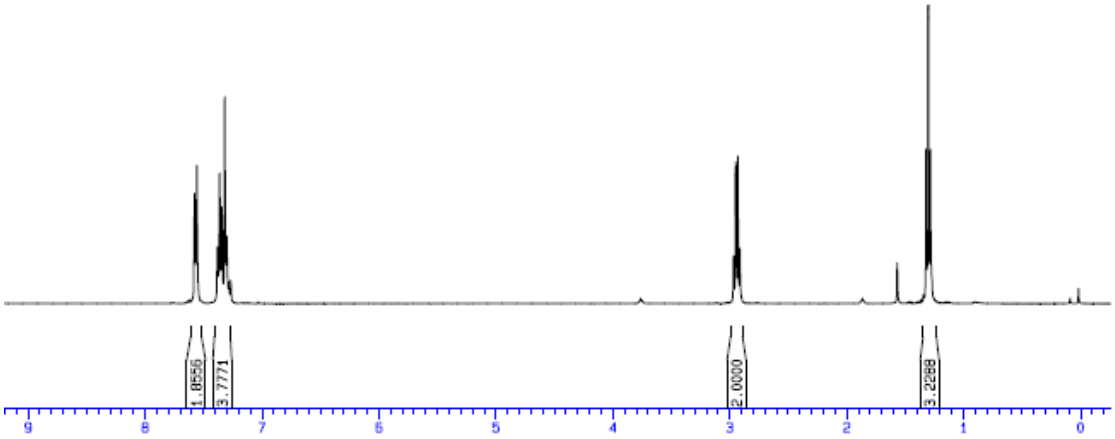

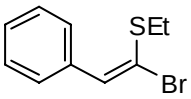

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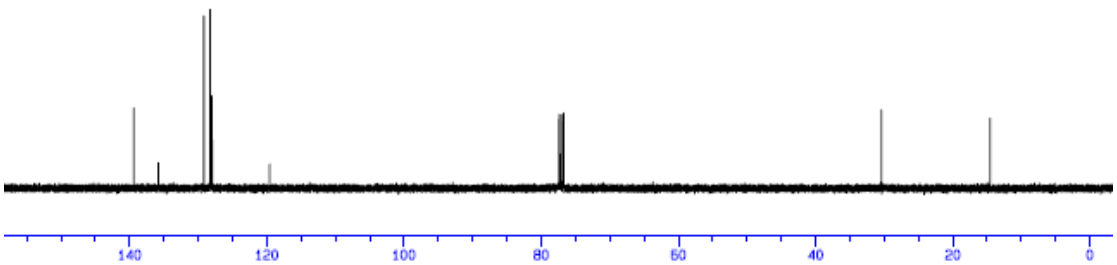

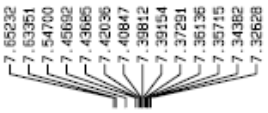
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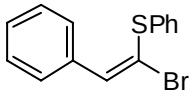
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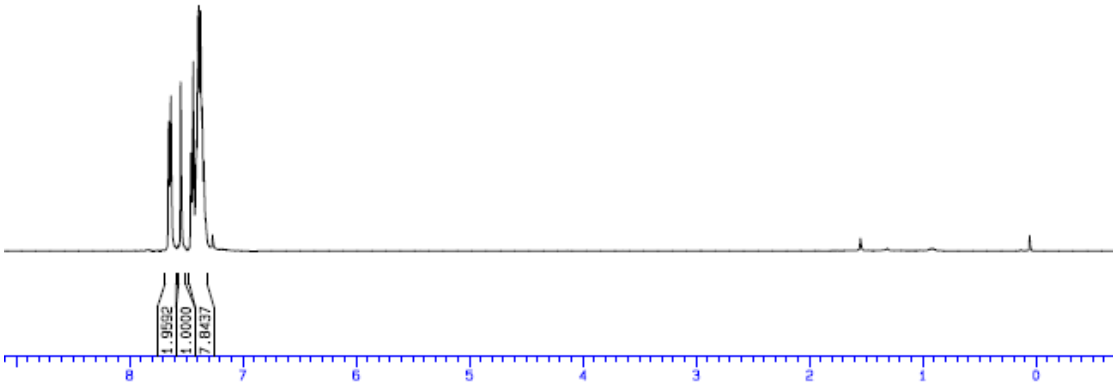
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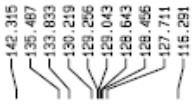
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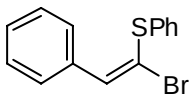
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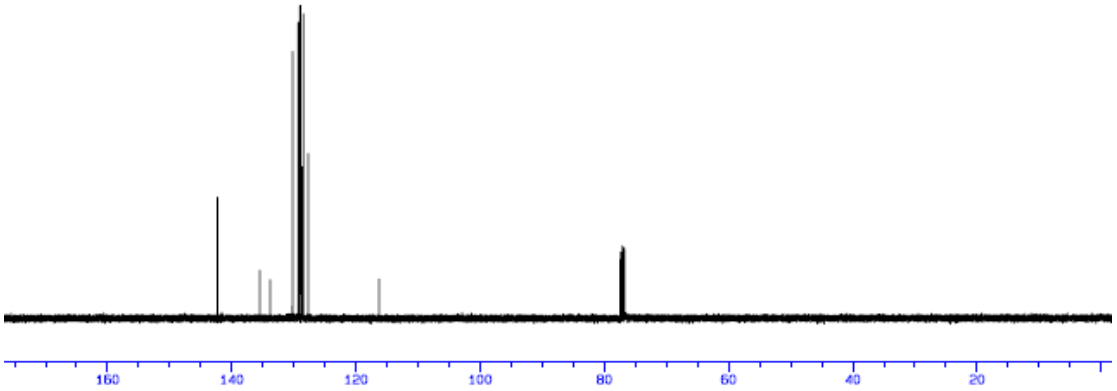
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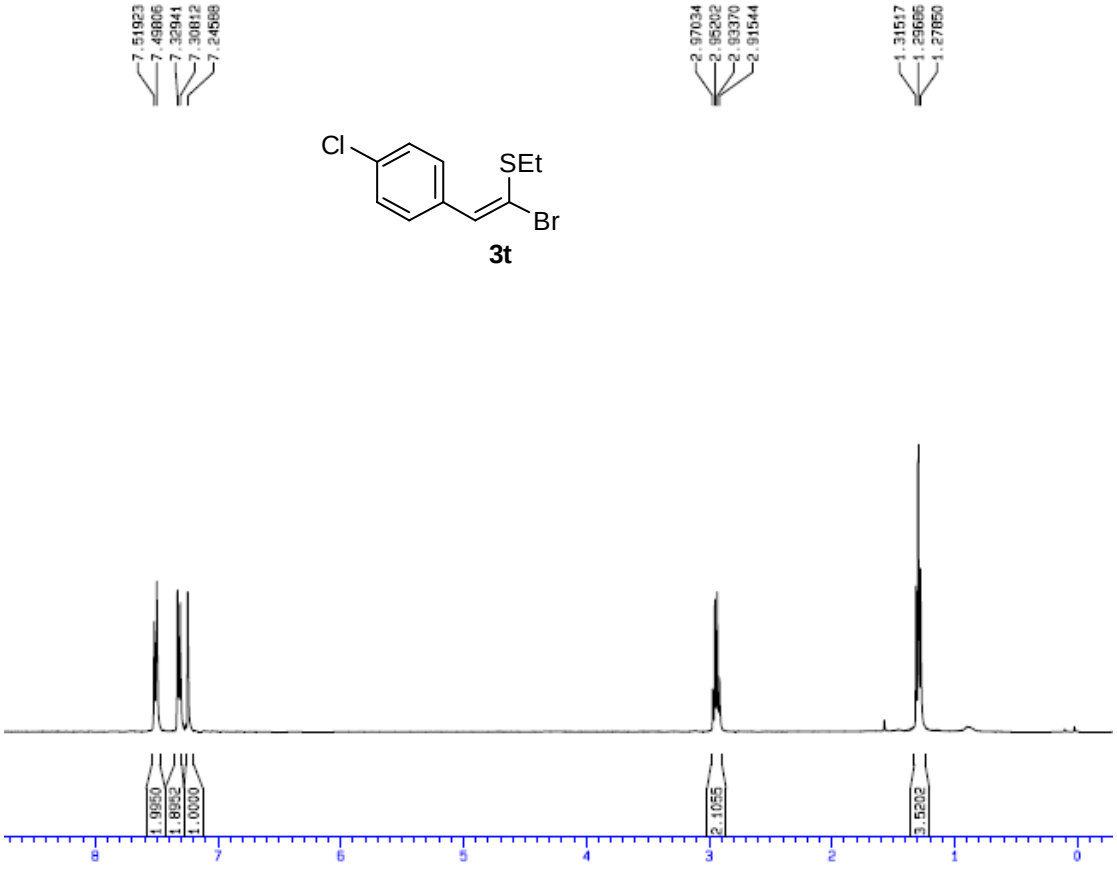

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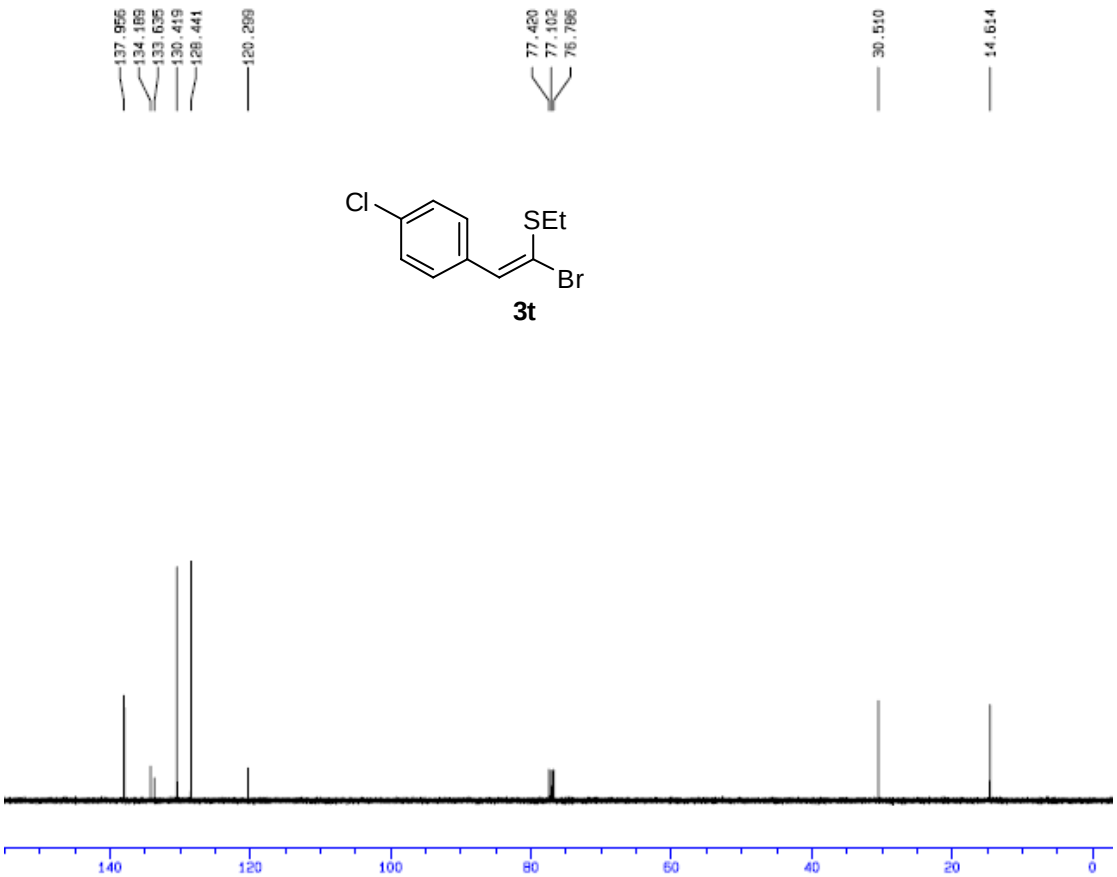

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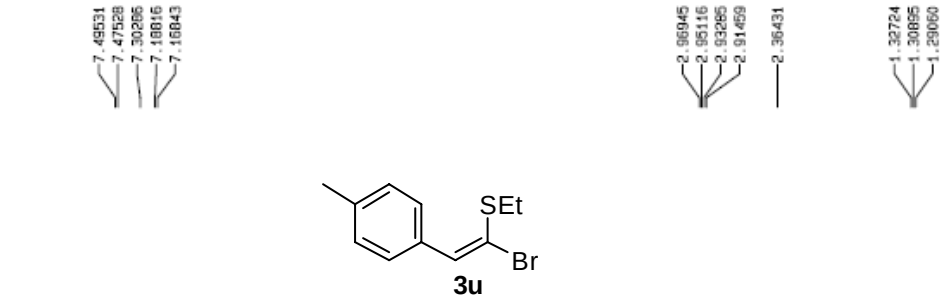

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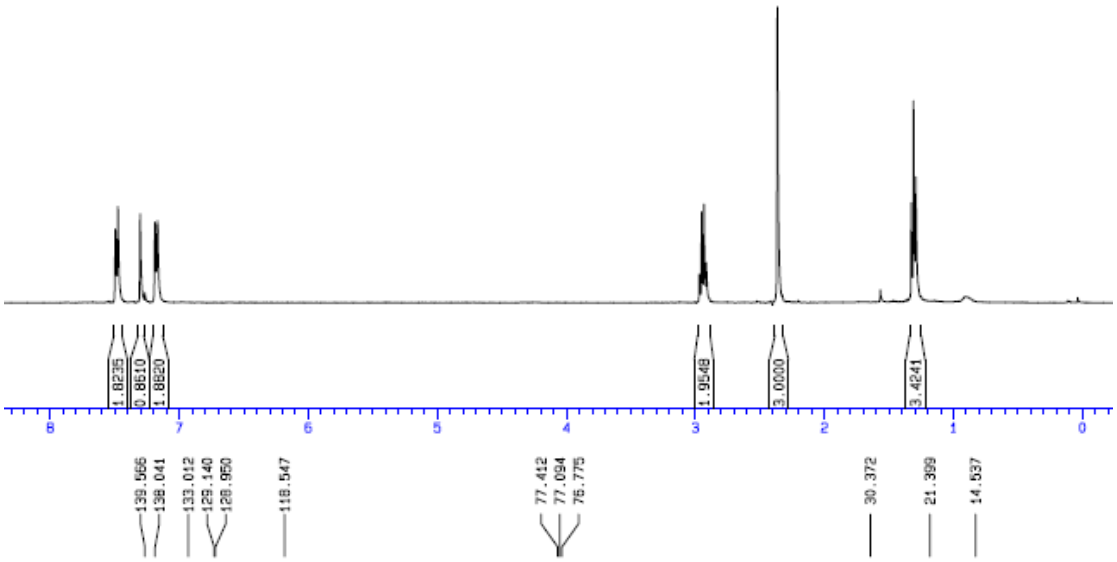

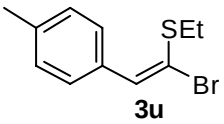

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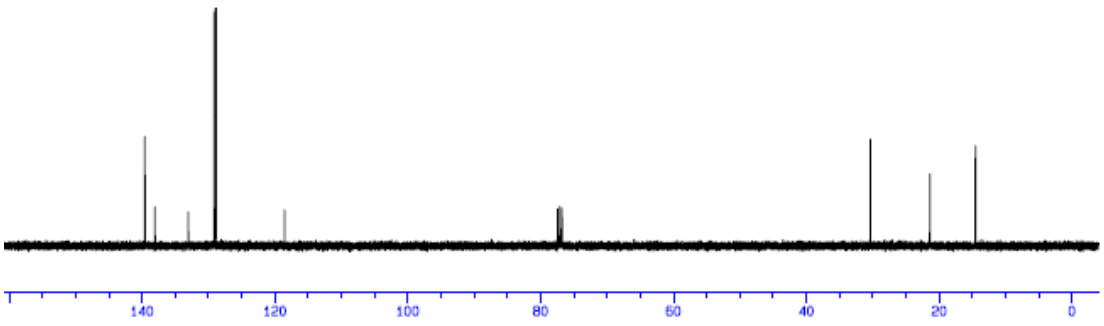
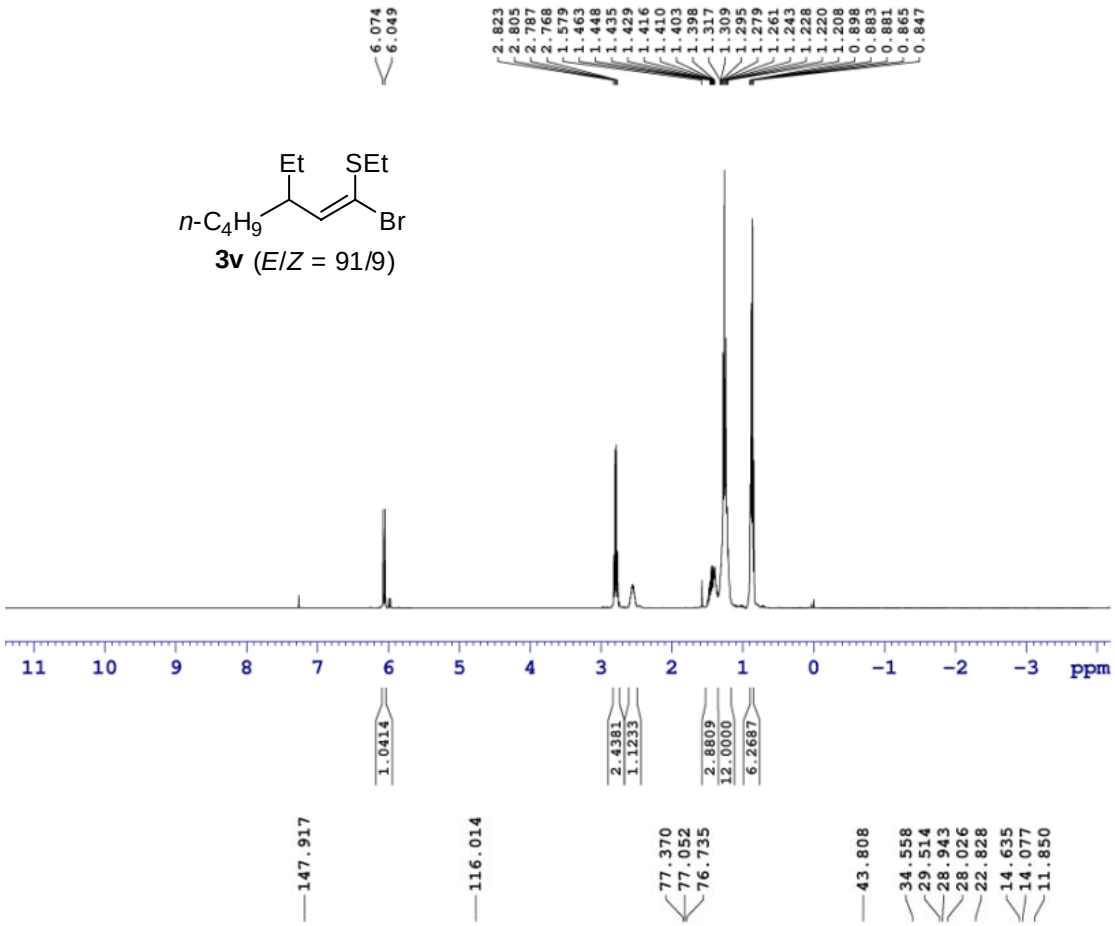
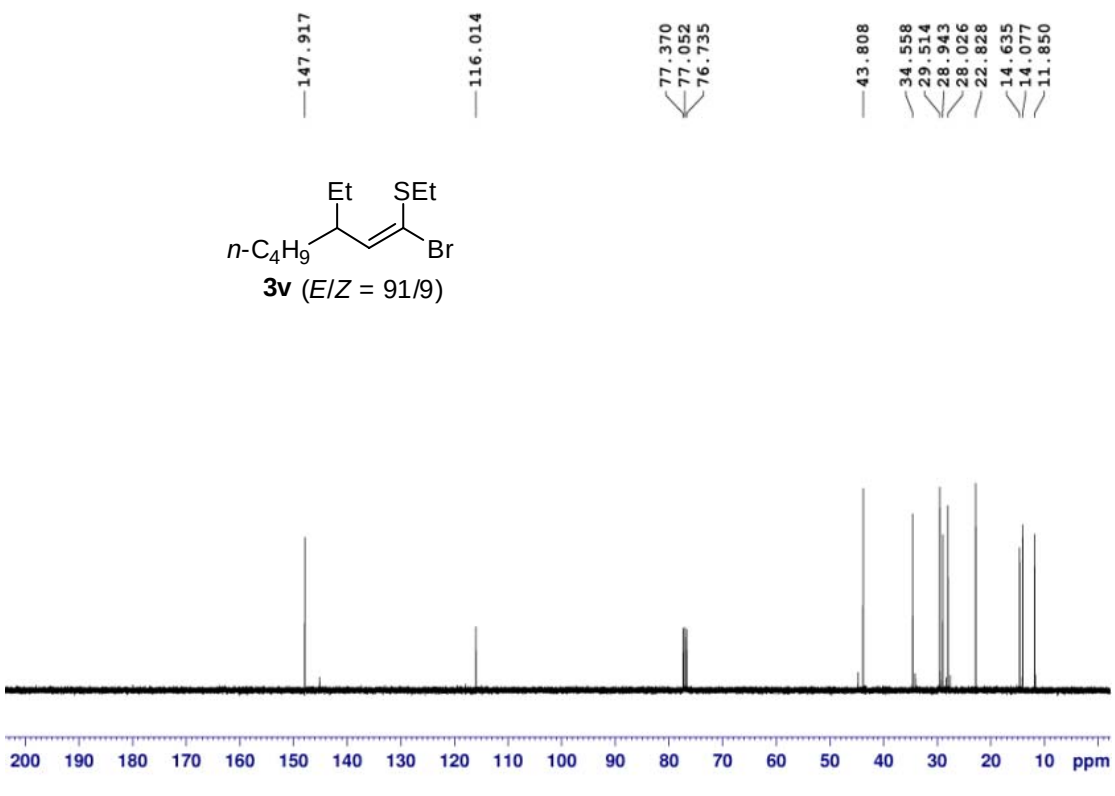
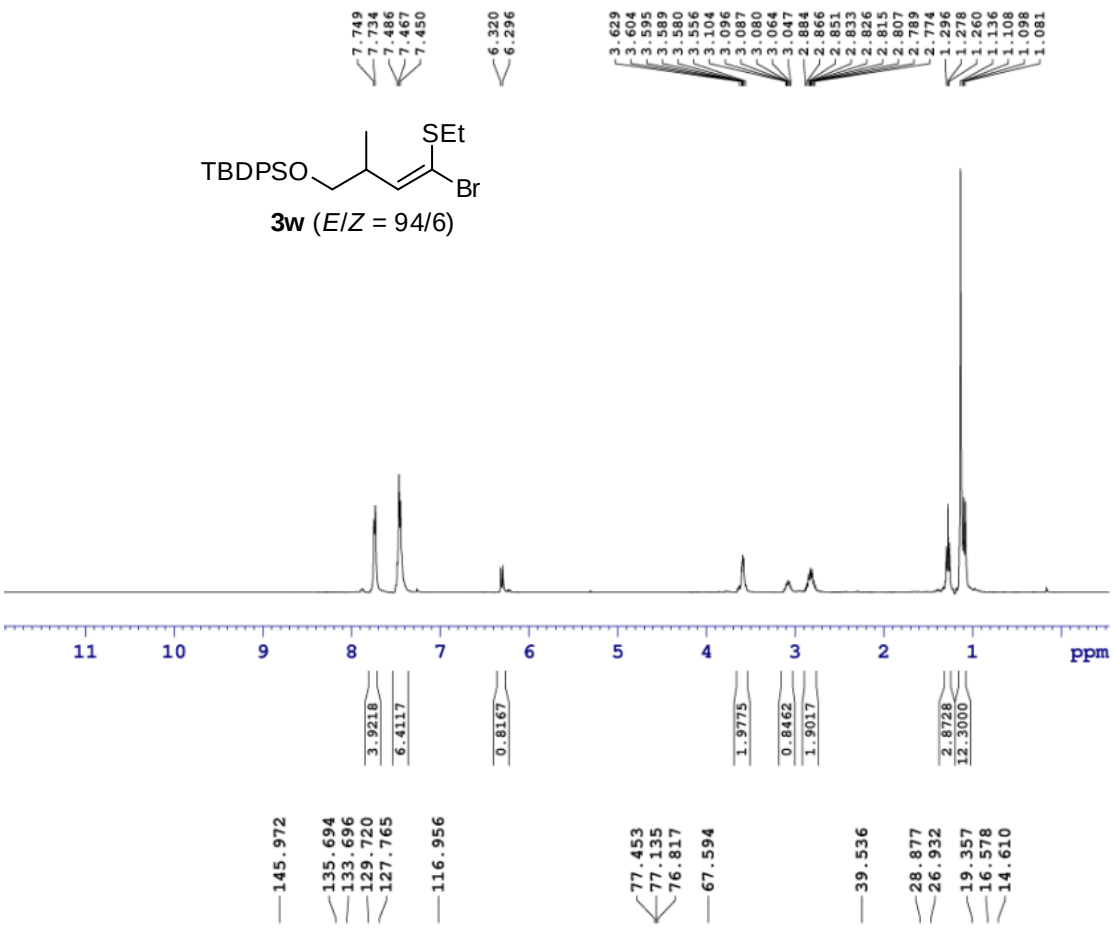
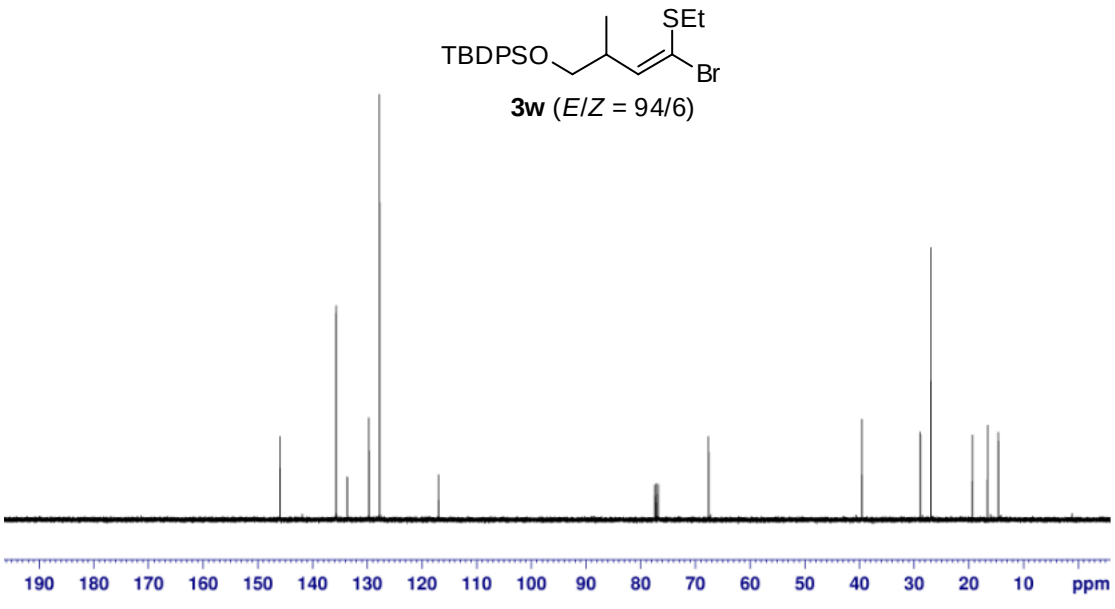




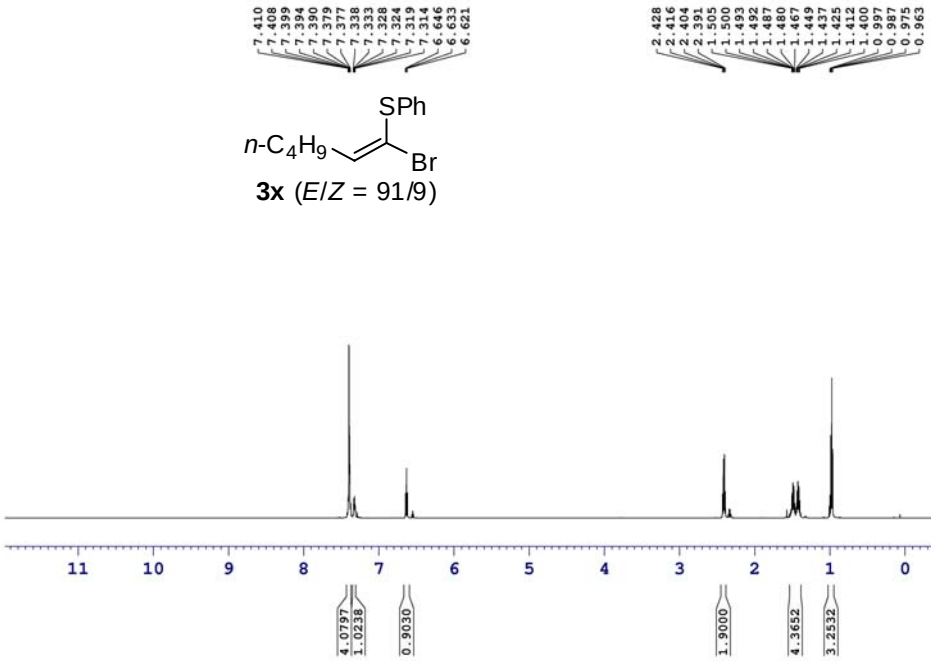




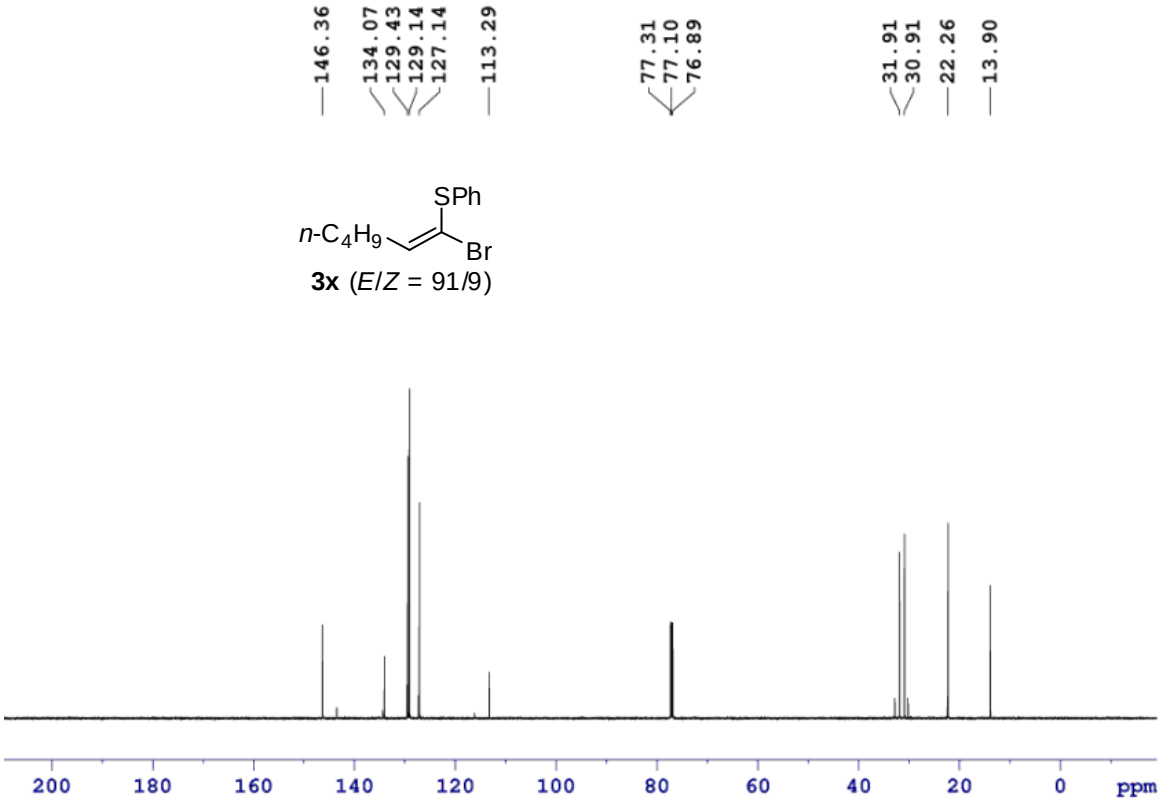
3w (*E*/*Z* = 94/6)



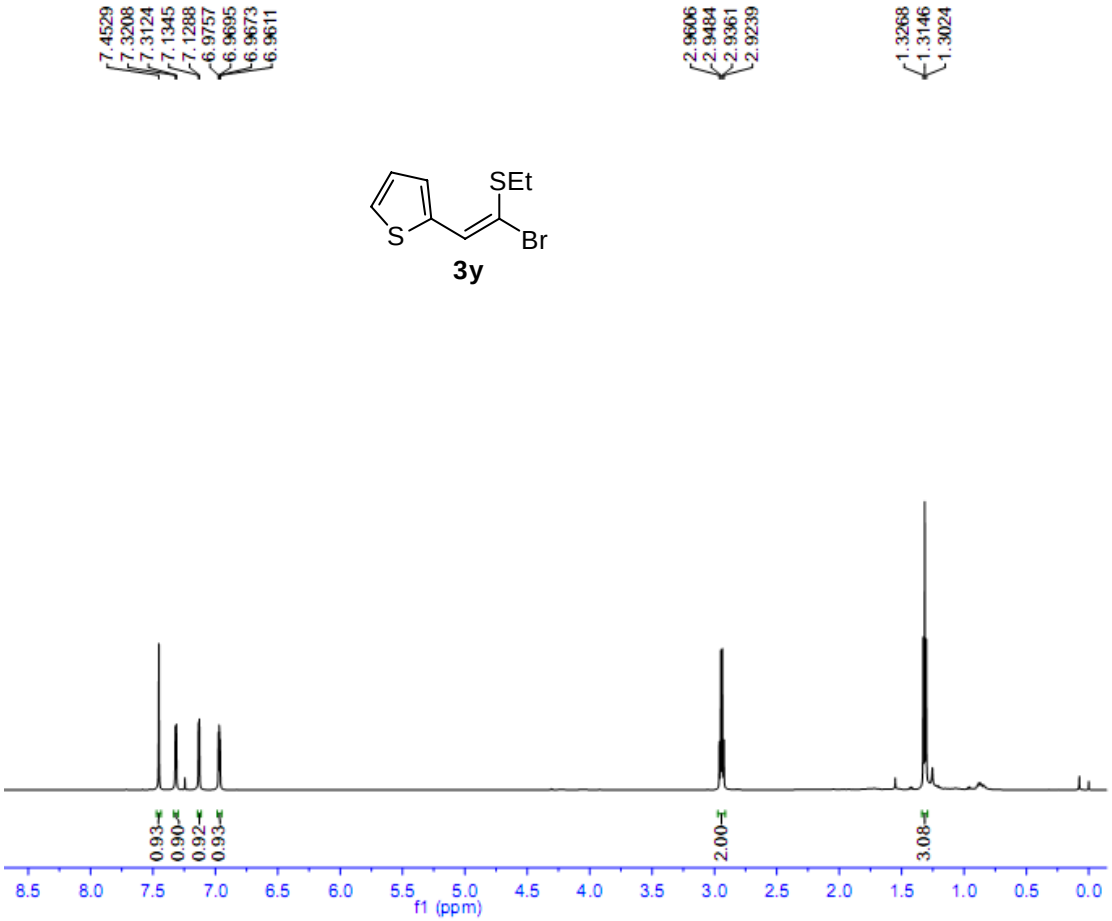
3w (*E*/*Z* = 94/6)

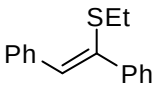


3x (*E*/*Z* = 91/9)



3x (*E*/*Z* = 91/9)





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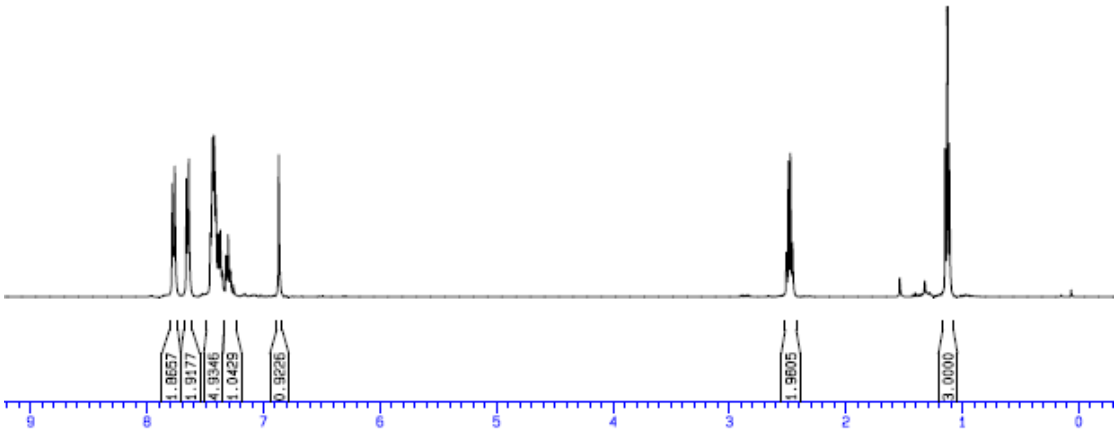

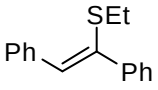

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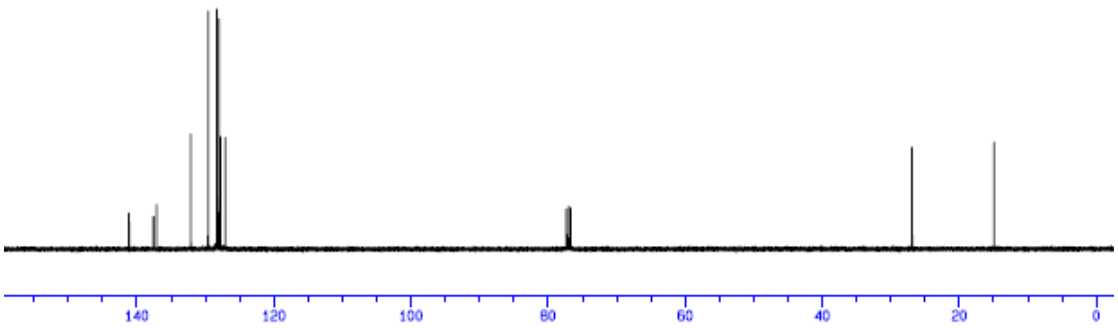

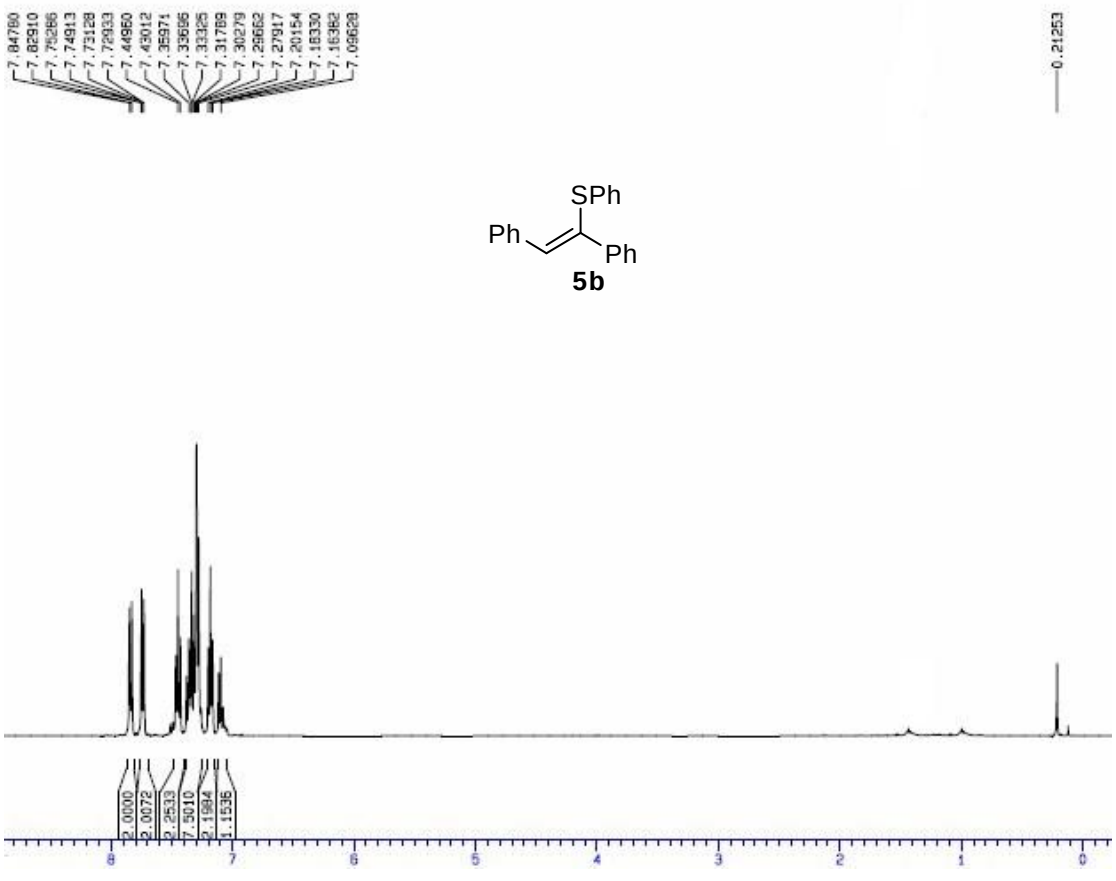

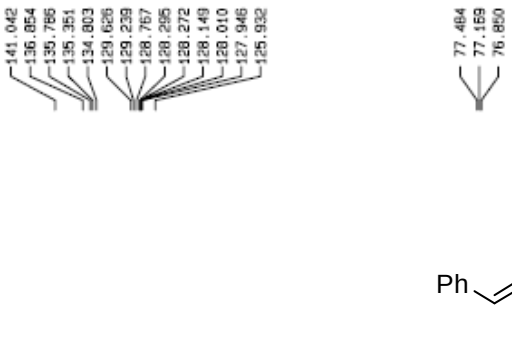

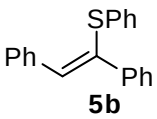

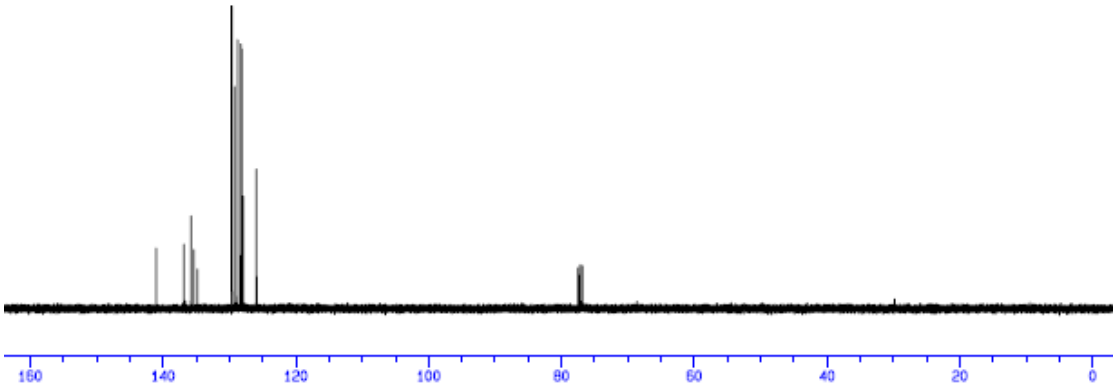

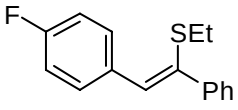

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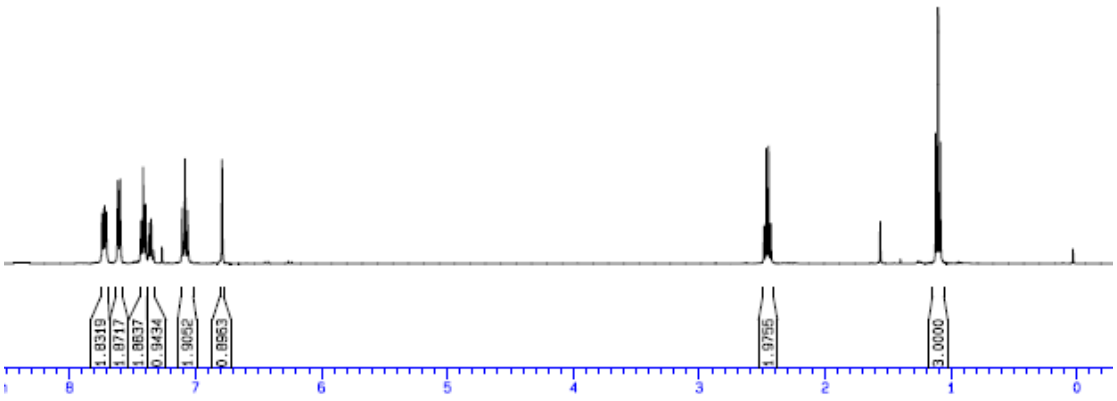

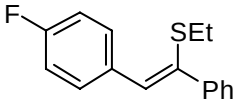

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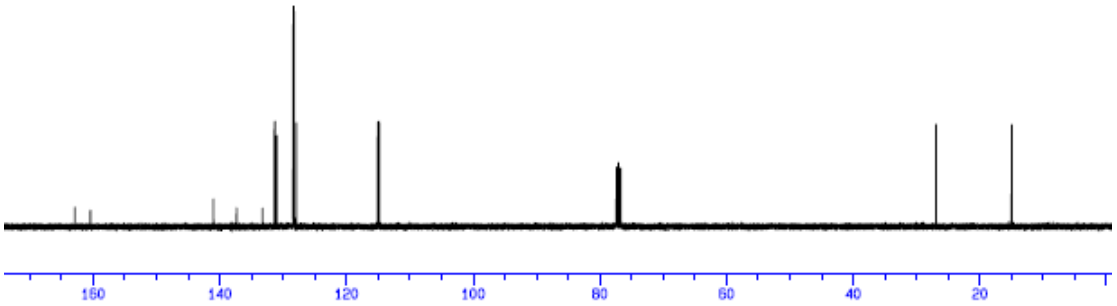

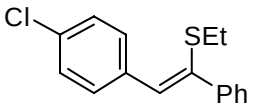

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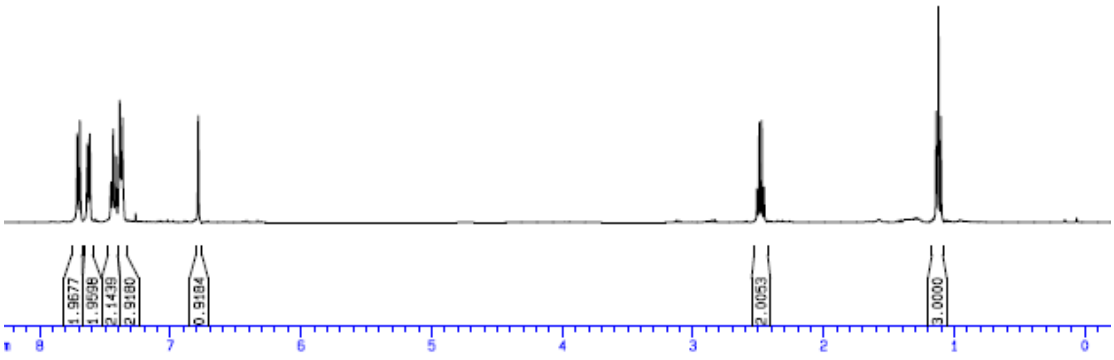

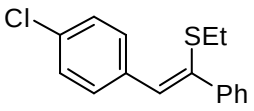

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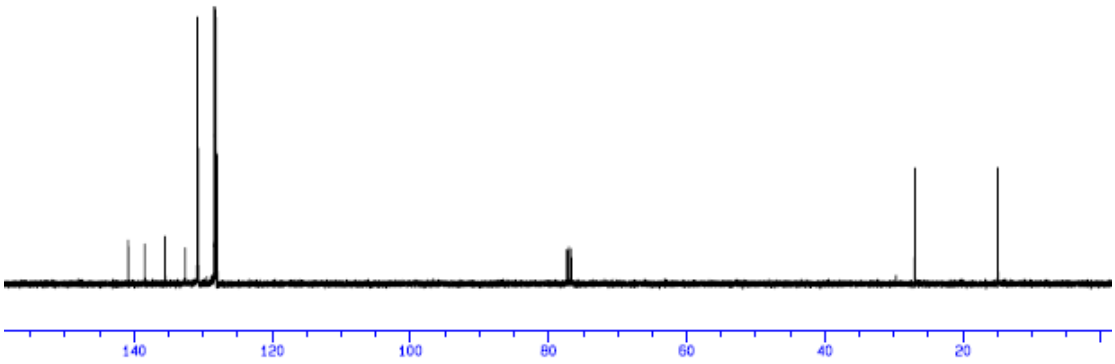

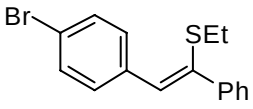

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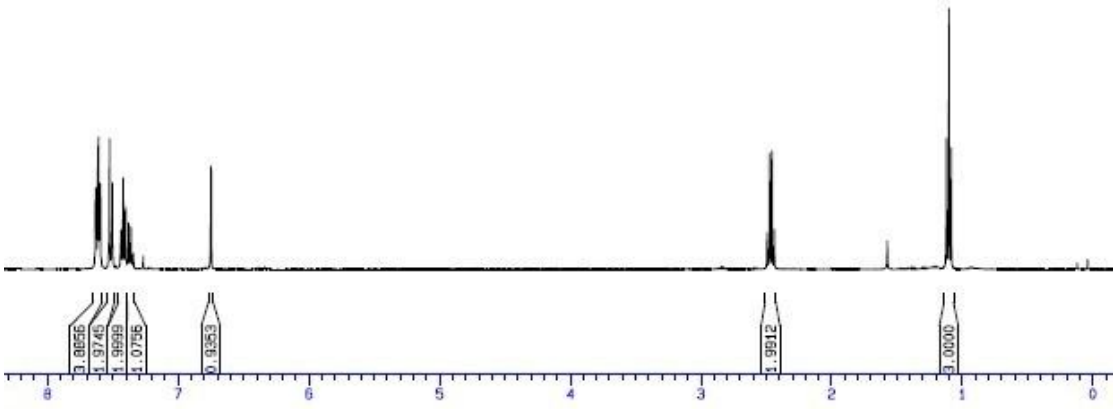

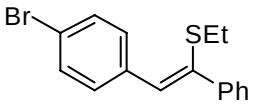

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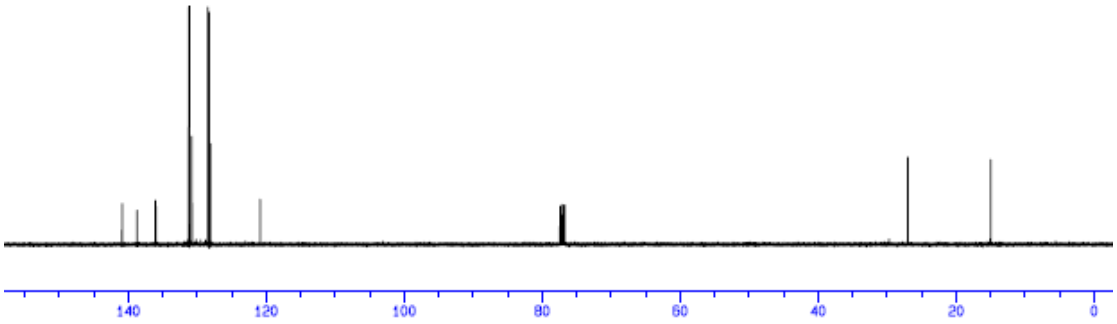

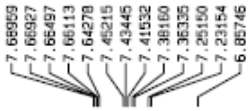

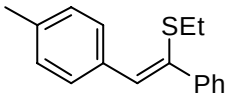

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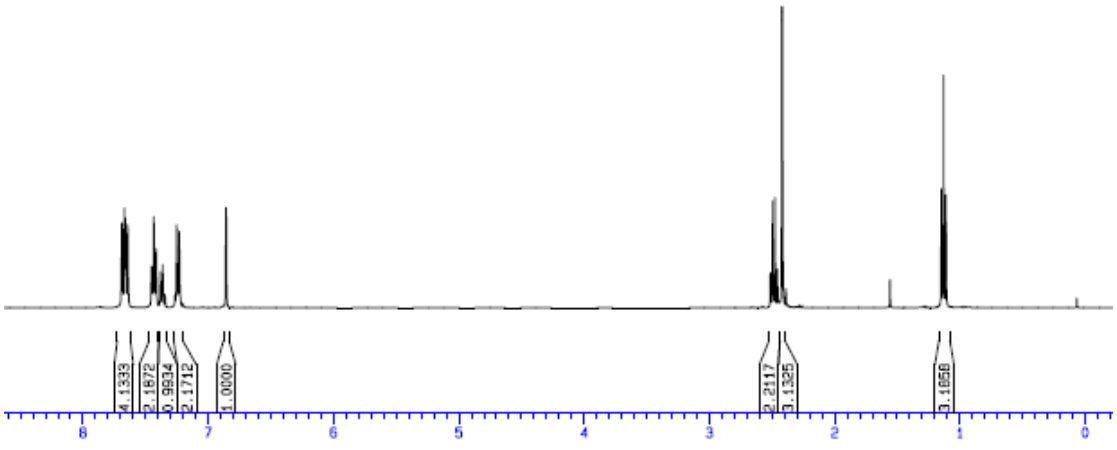

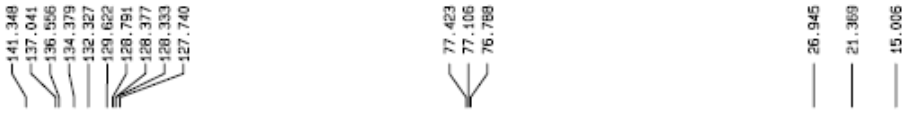

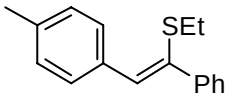

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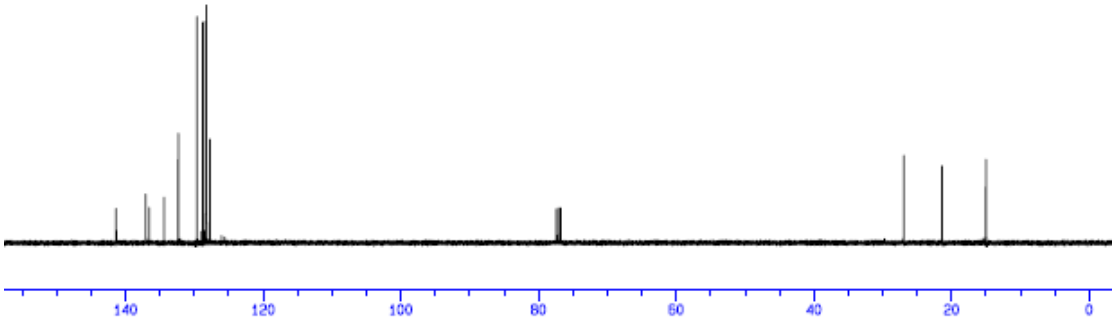

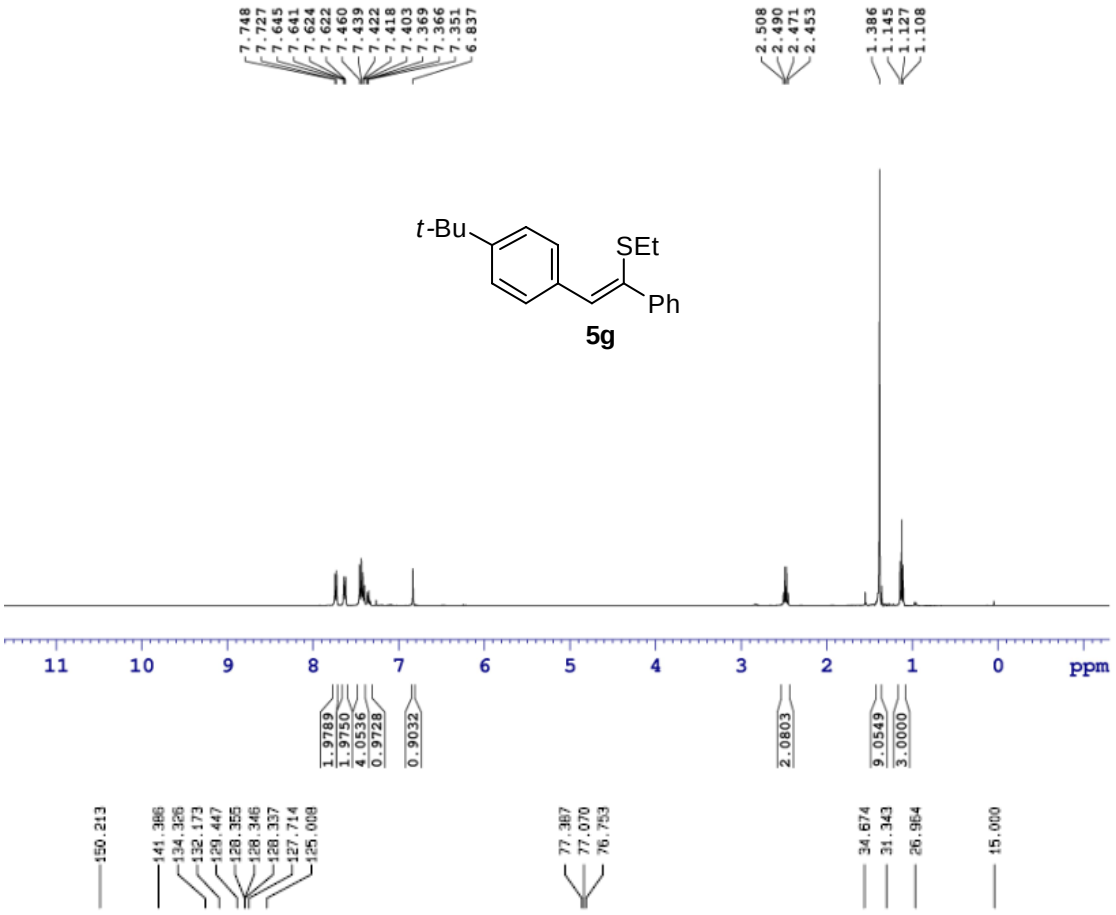

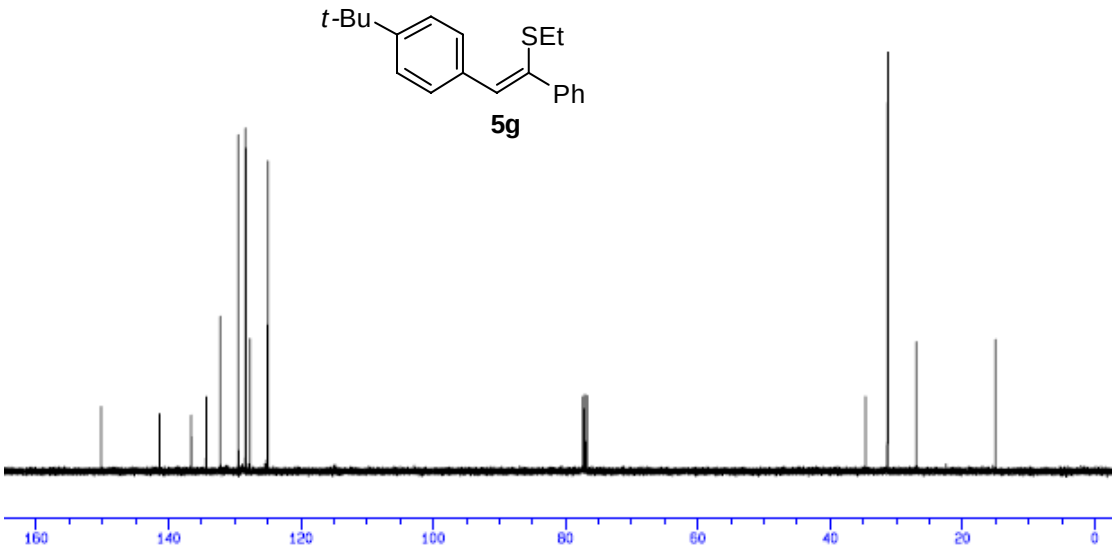

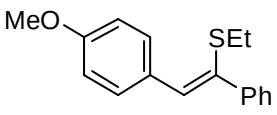

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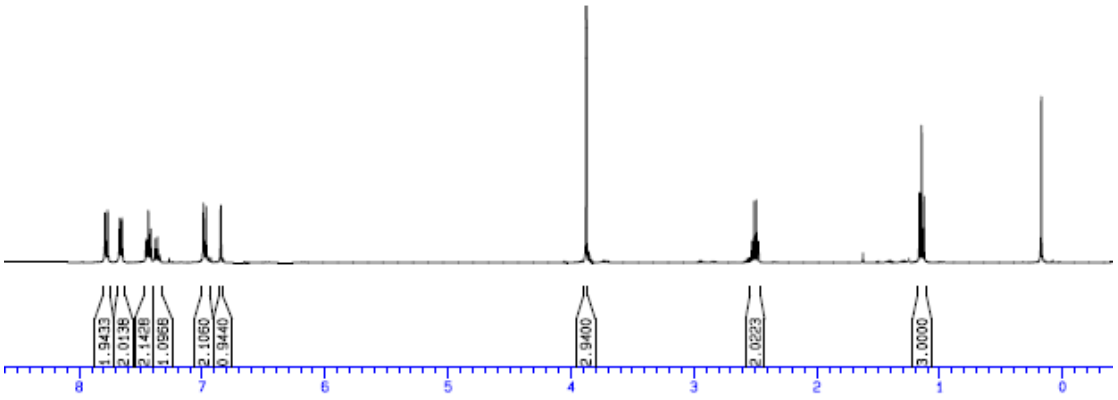

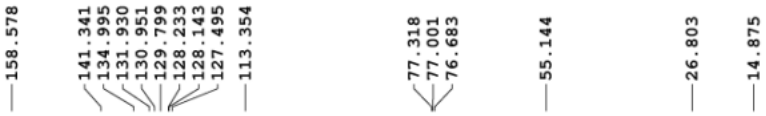

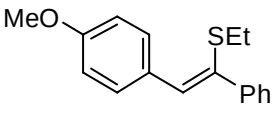

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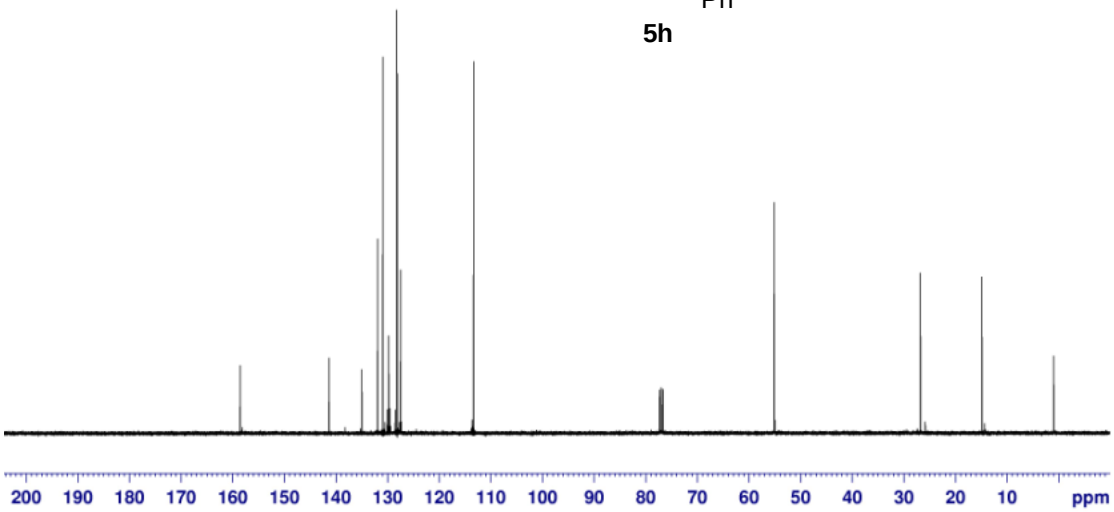

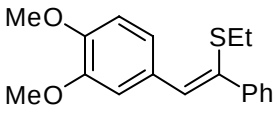

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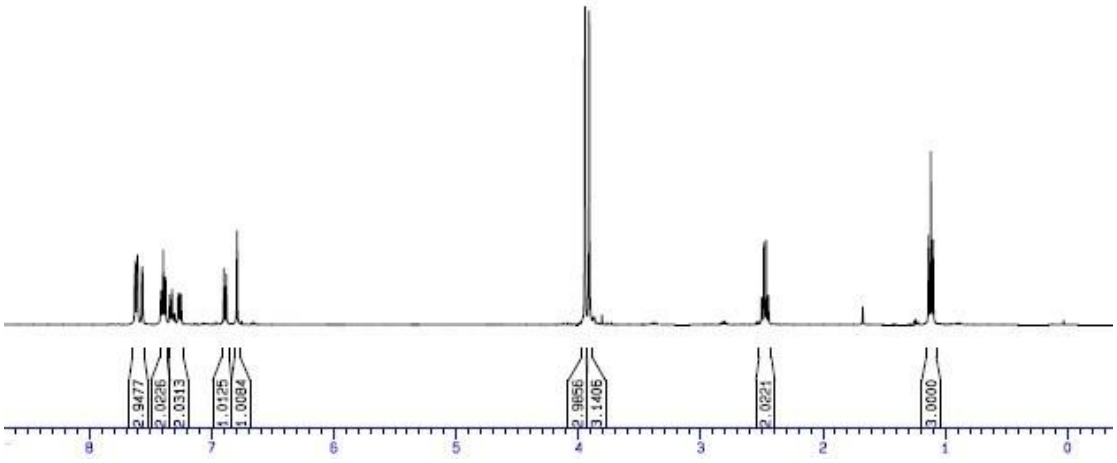

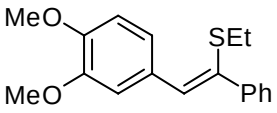

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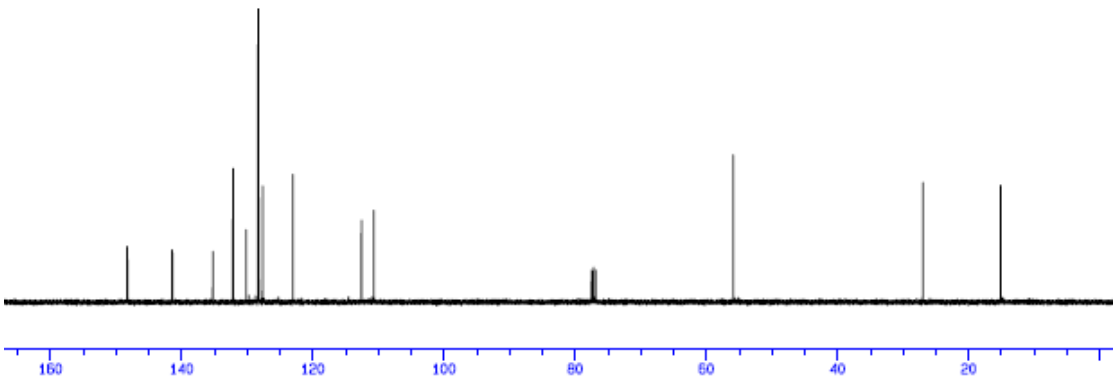

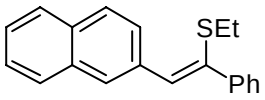

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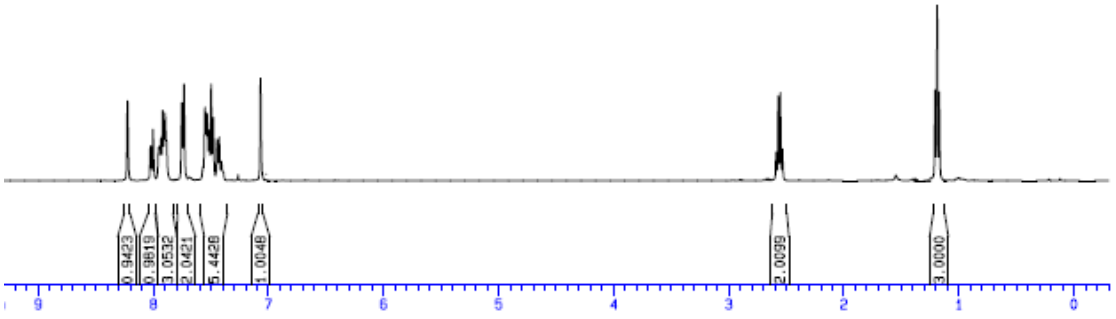

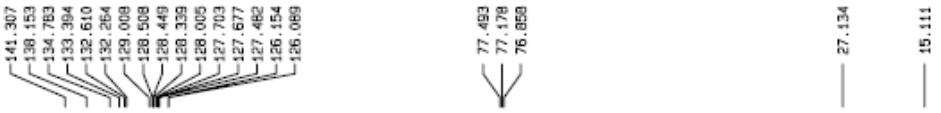

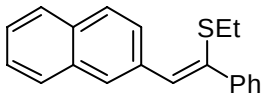

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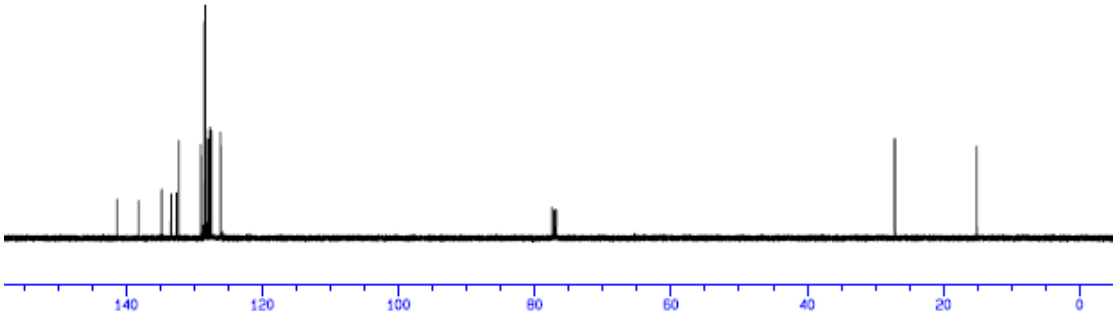
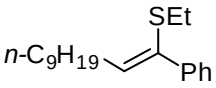
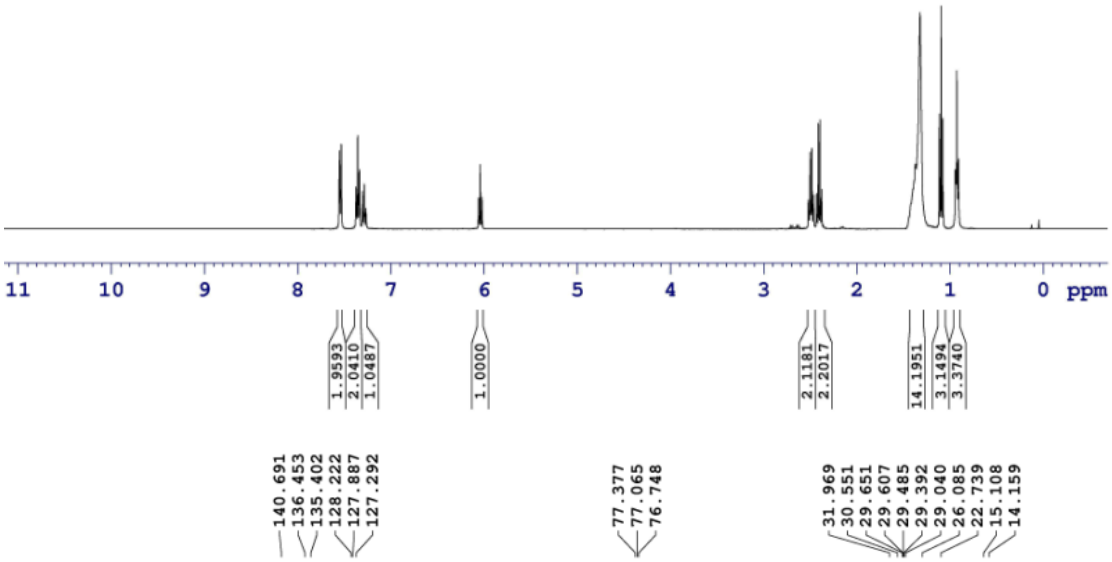
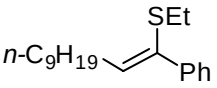




5k (*Z*/*E* > 95/5)





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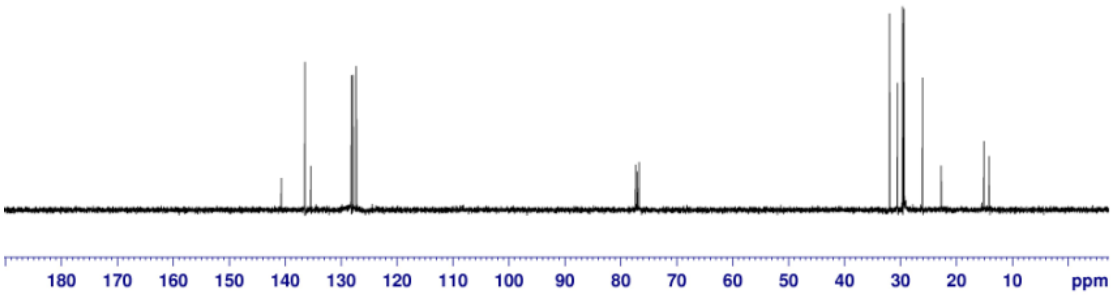
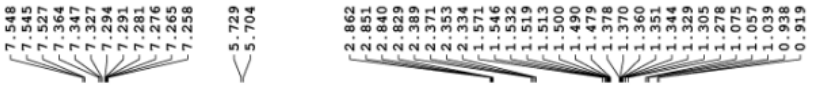
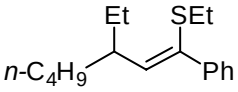
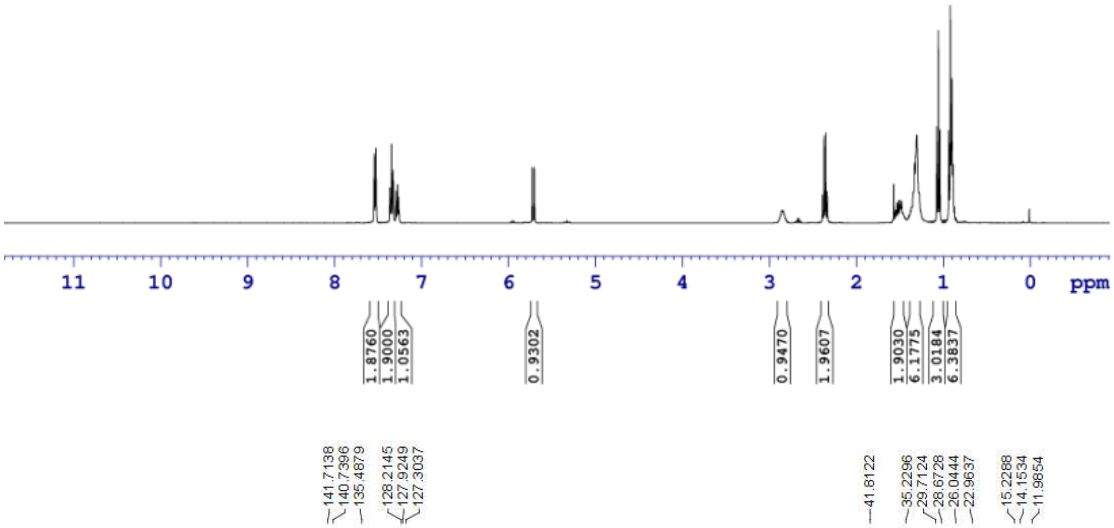
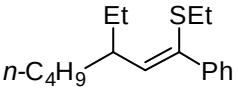






5l (*Z*/*E* > 95/5)





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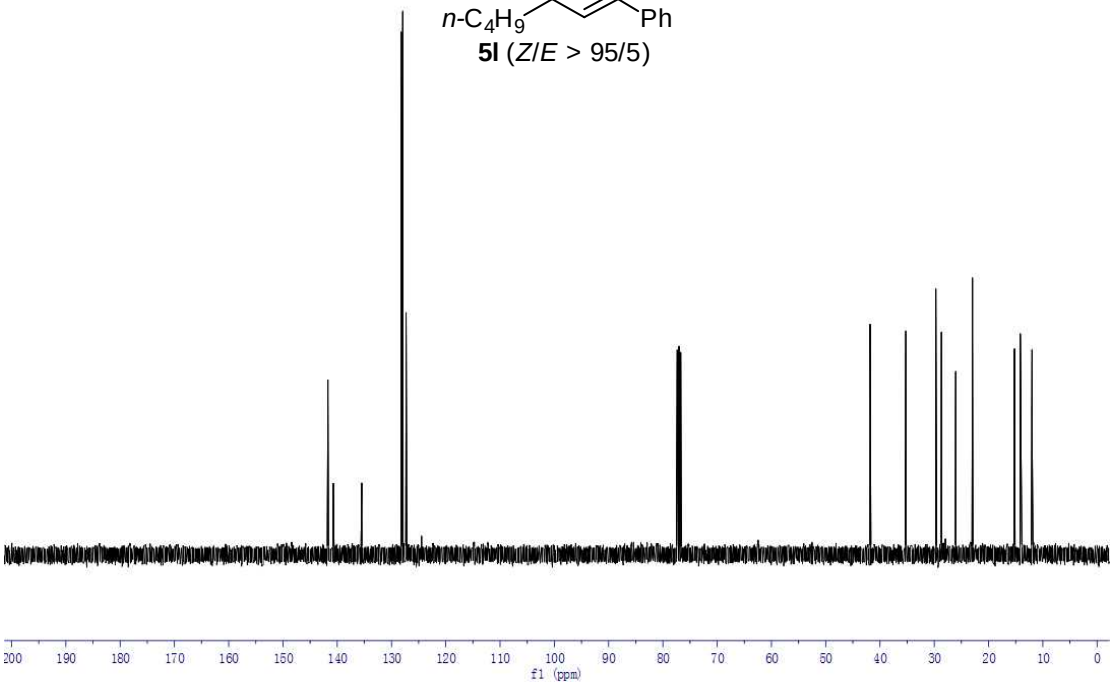

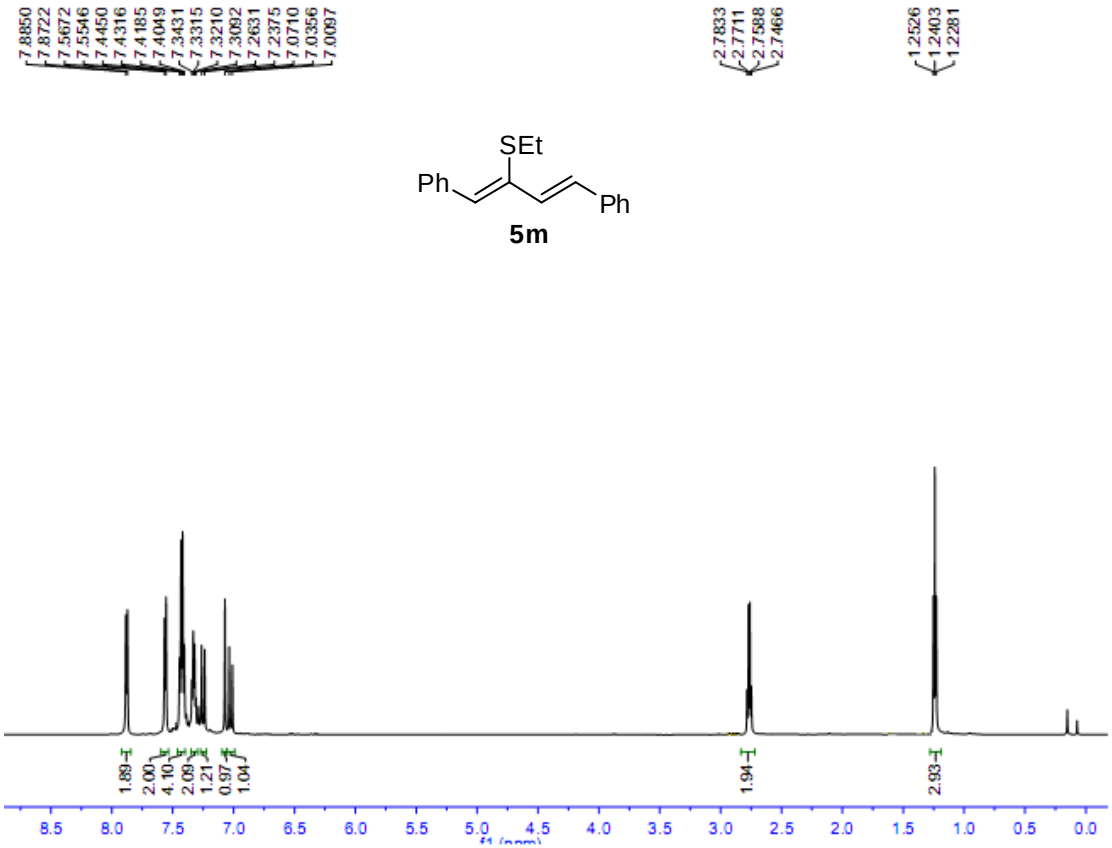
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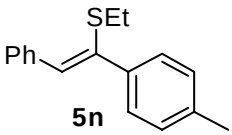

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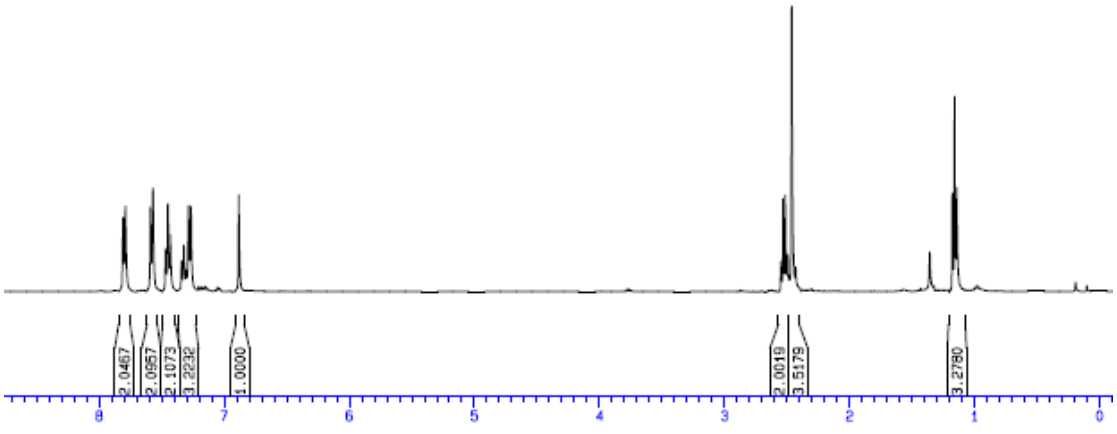

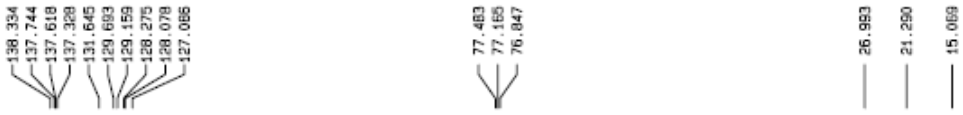

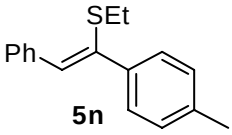

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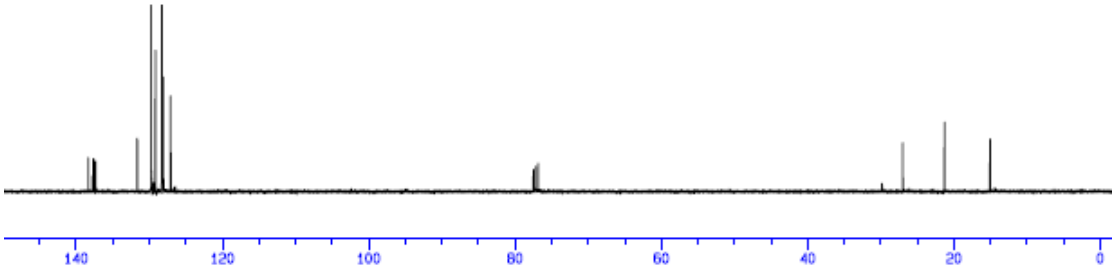

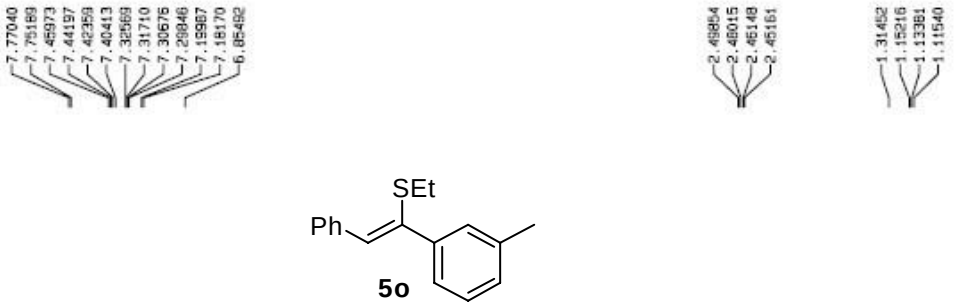

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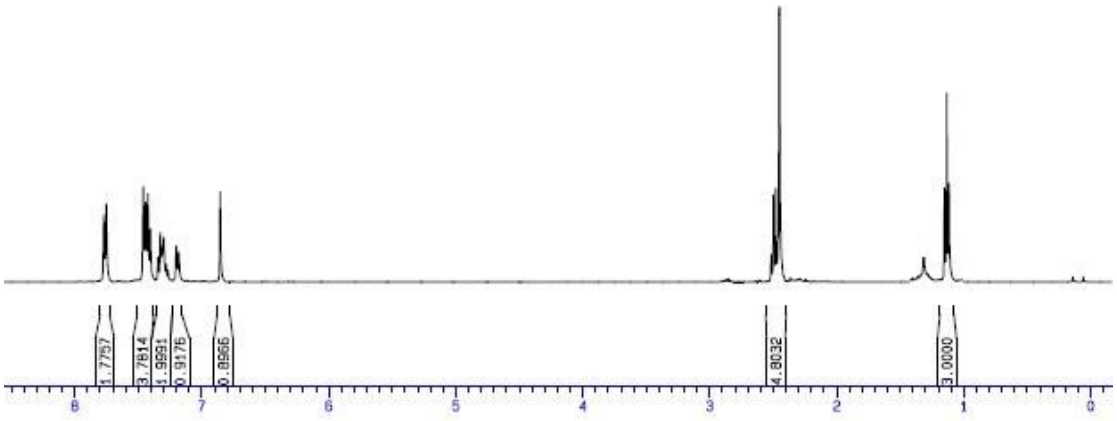

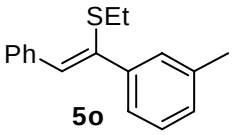

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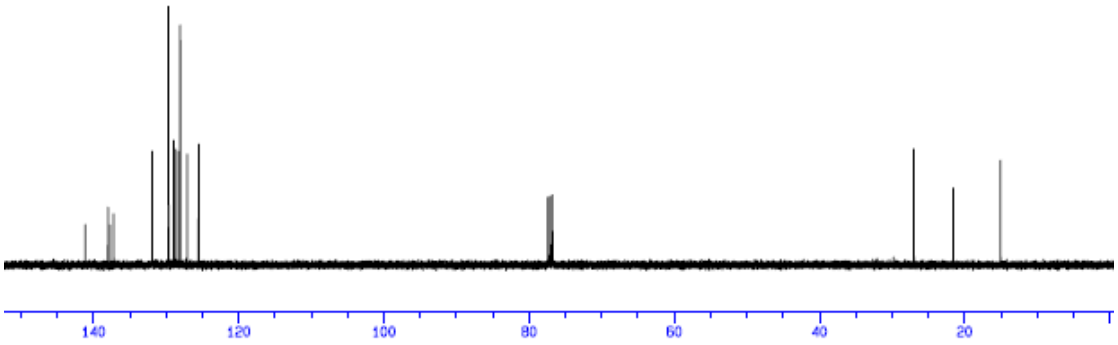

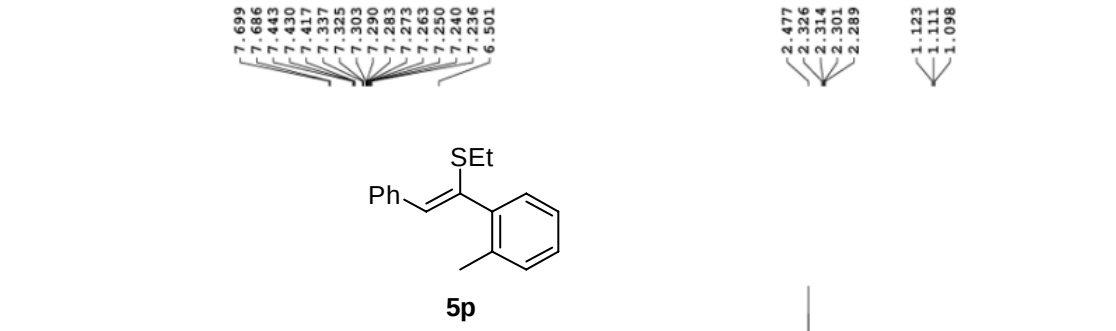

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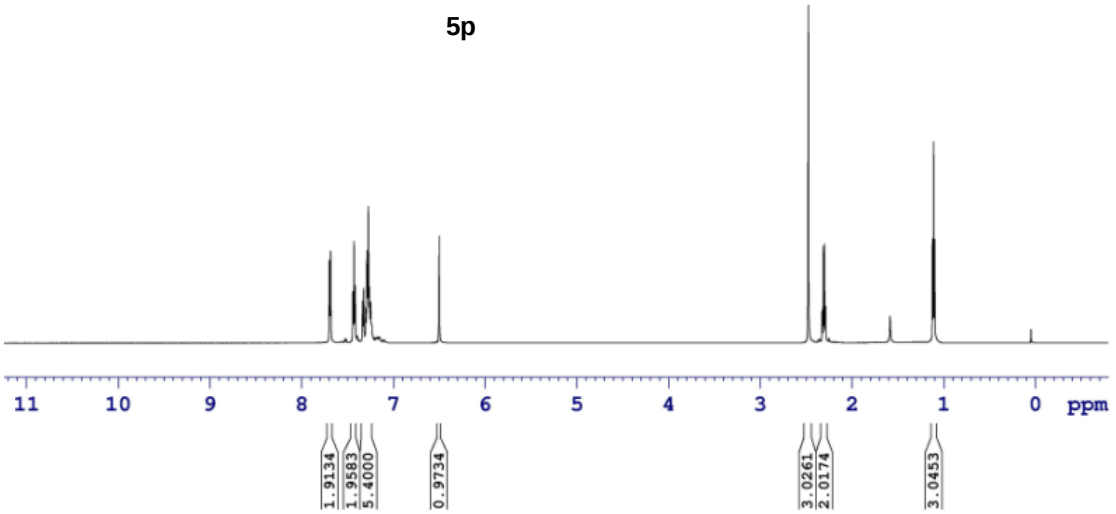

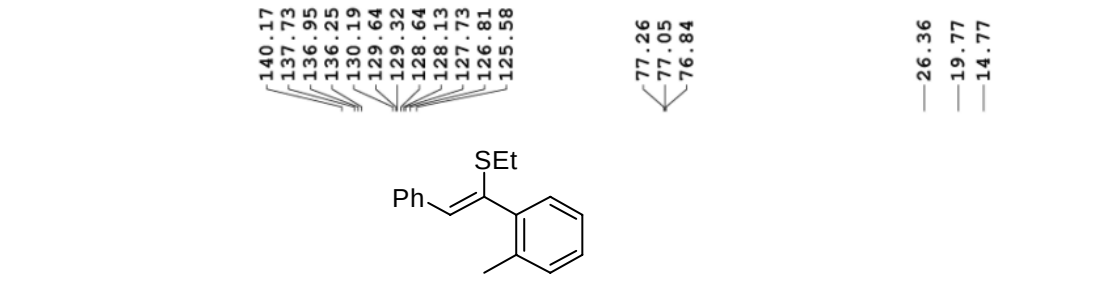

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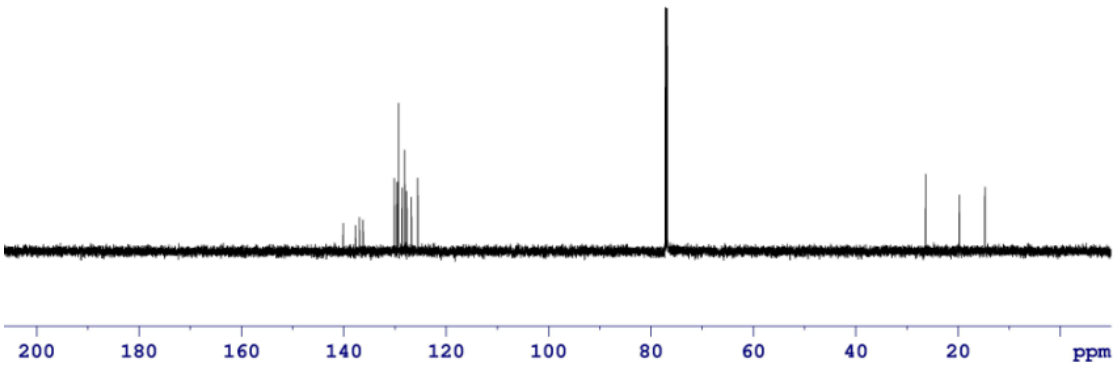

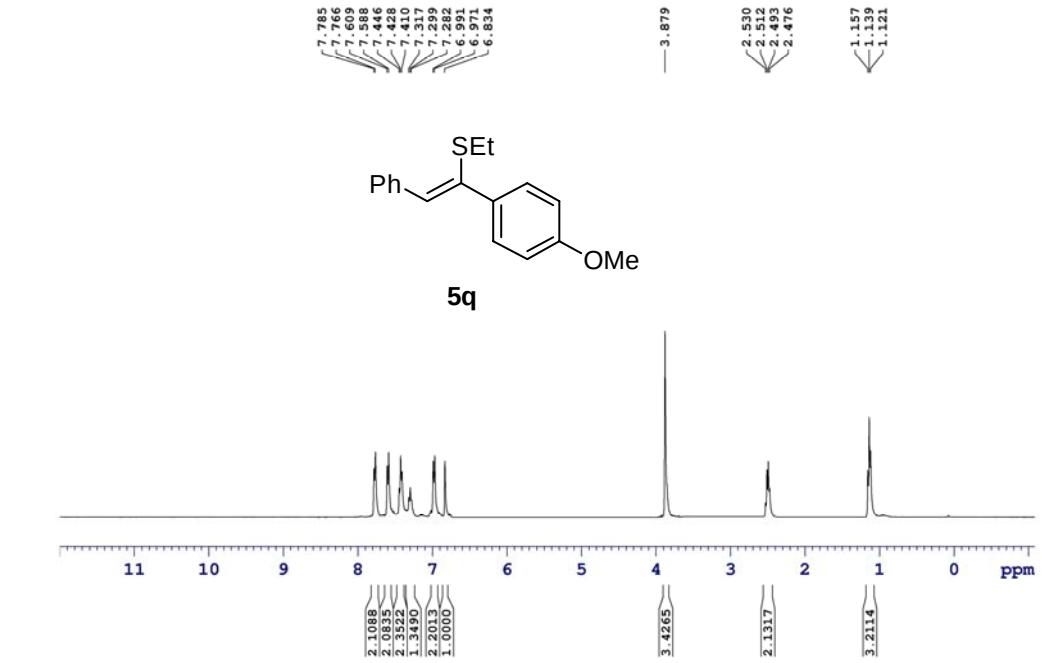

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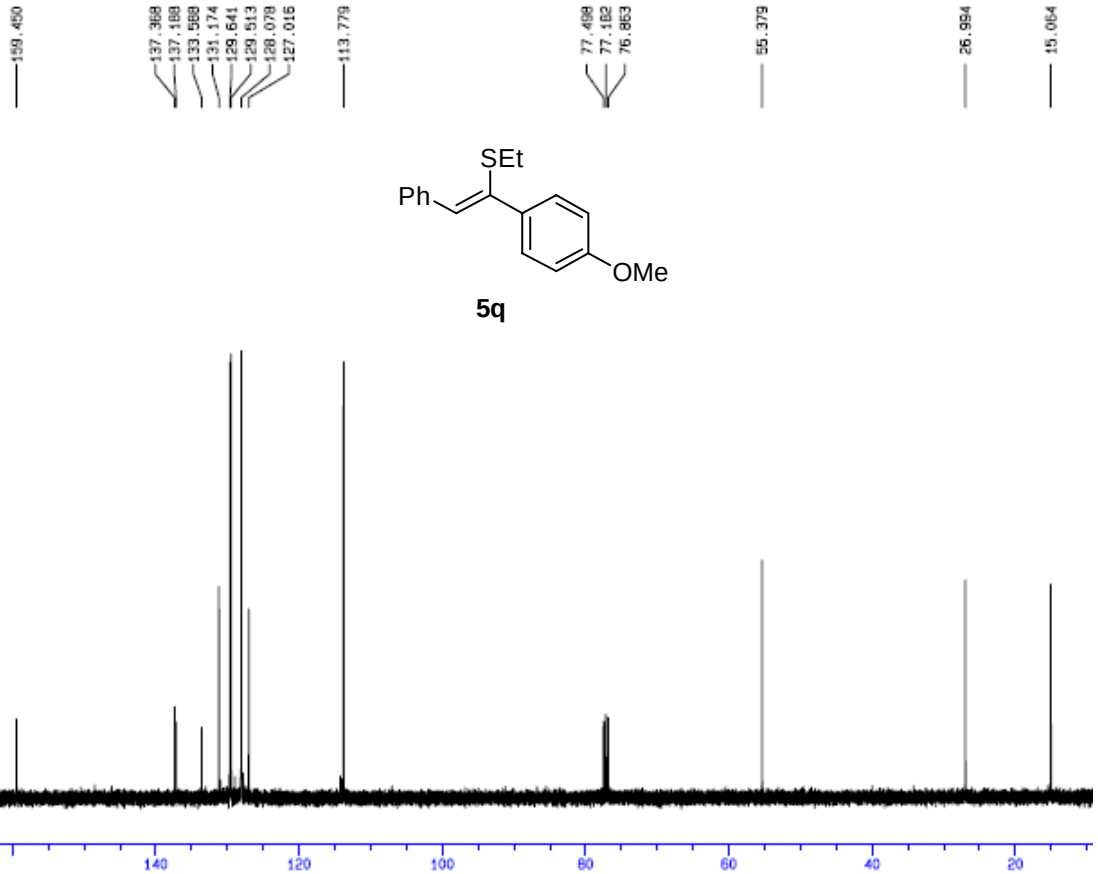

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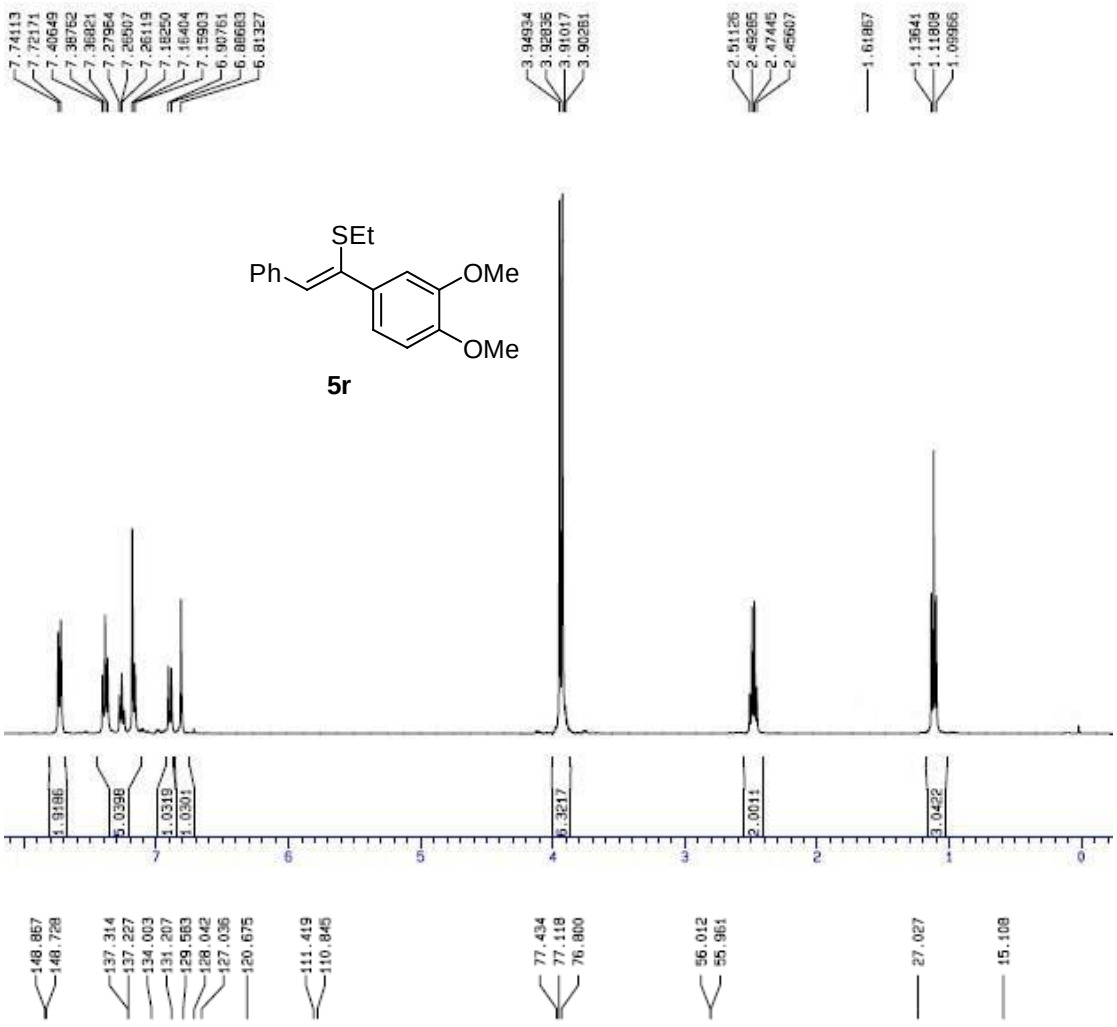

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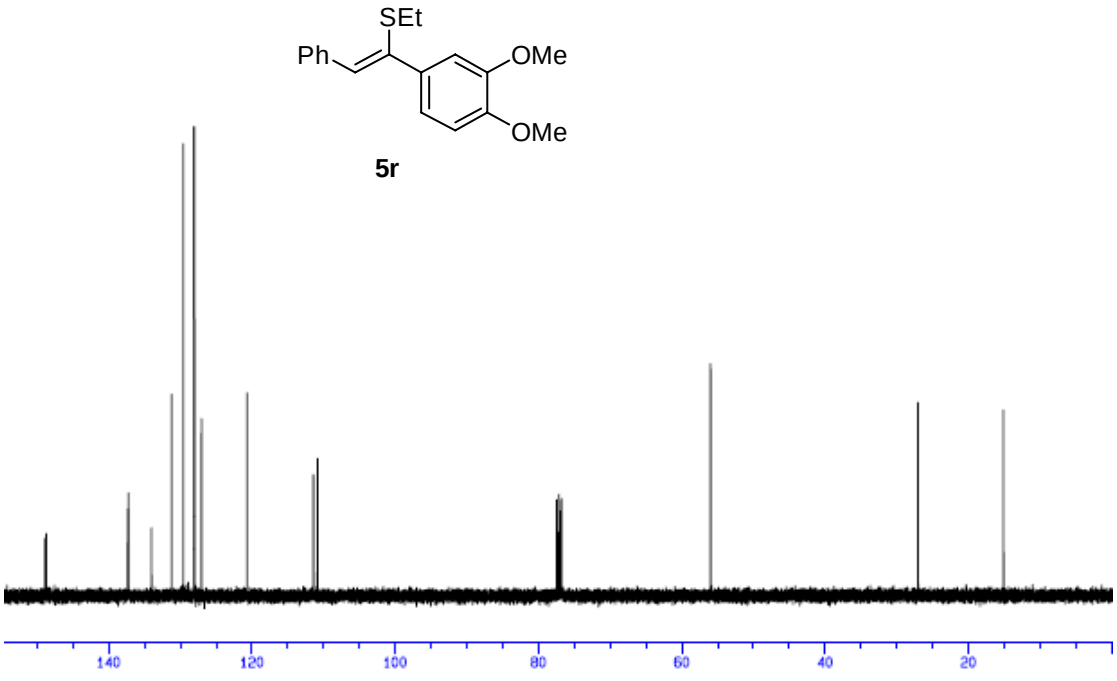

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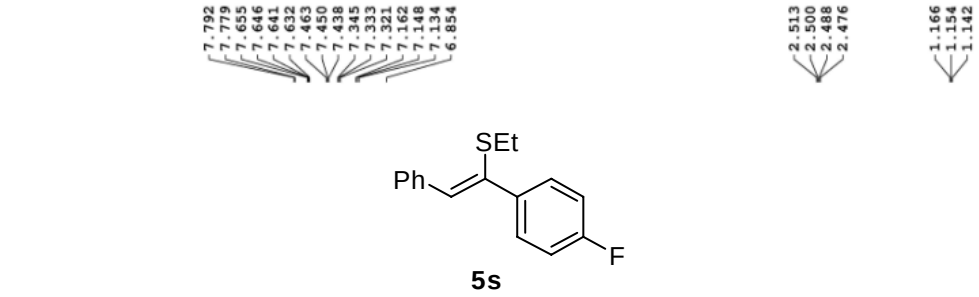
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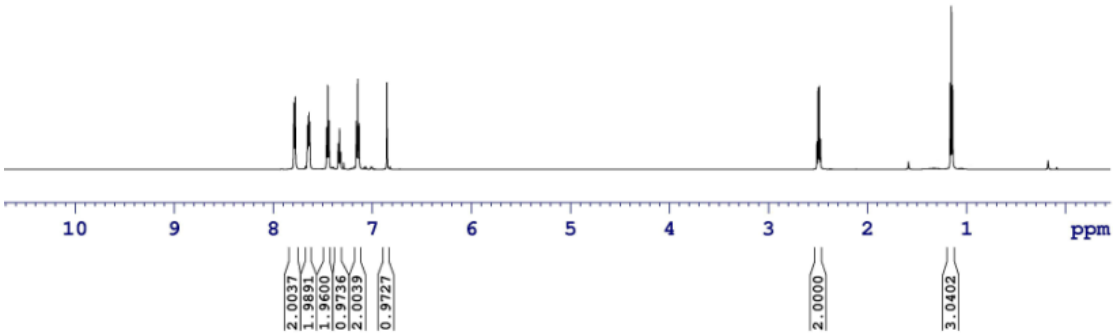
2.500
2.488
2.476
1.166
1.154
1.142

SEt
Ph
F

5s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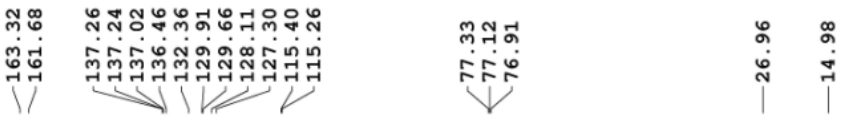
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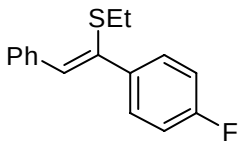
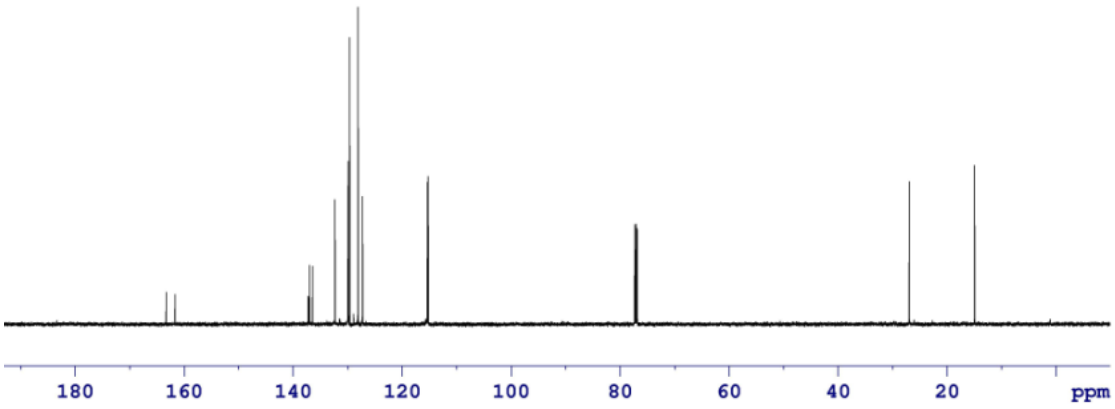
26.96
14.98


SEt
Ph
F

5s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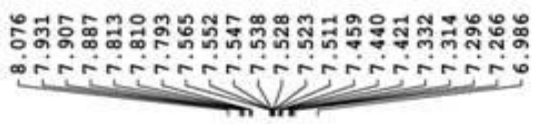
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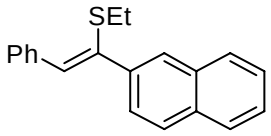
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Ph

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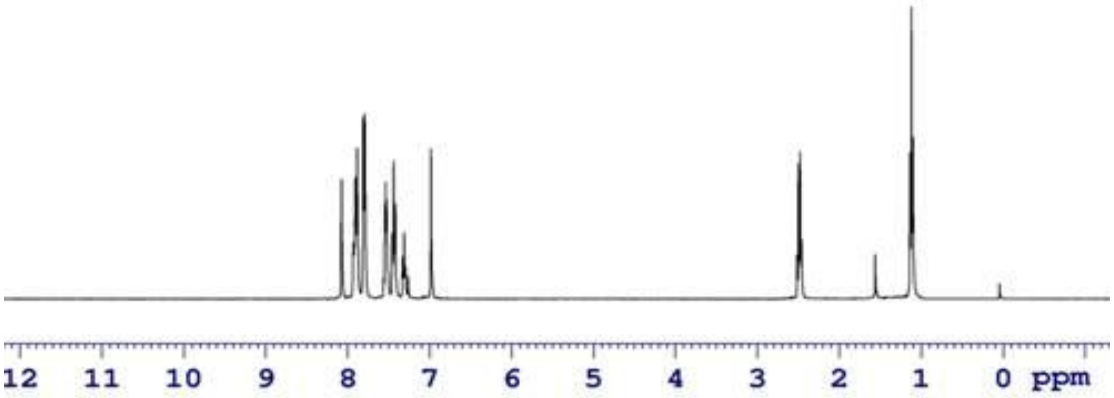
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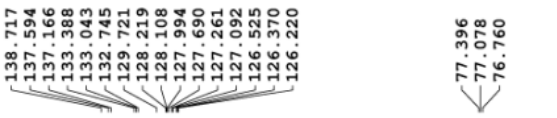
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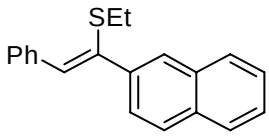
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Ph

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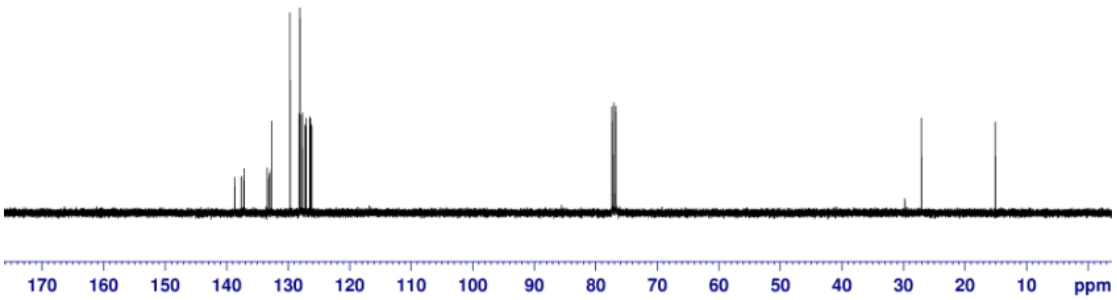
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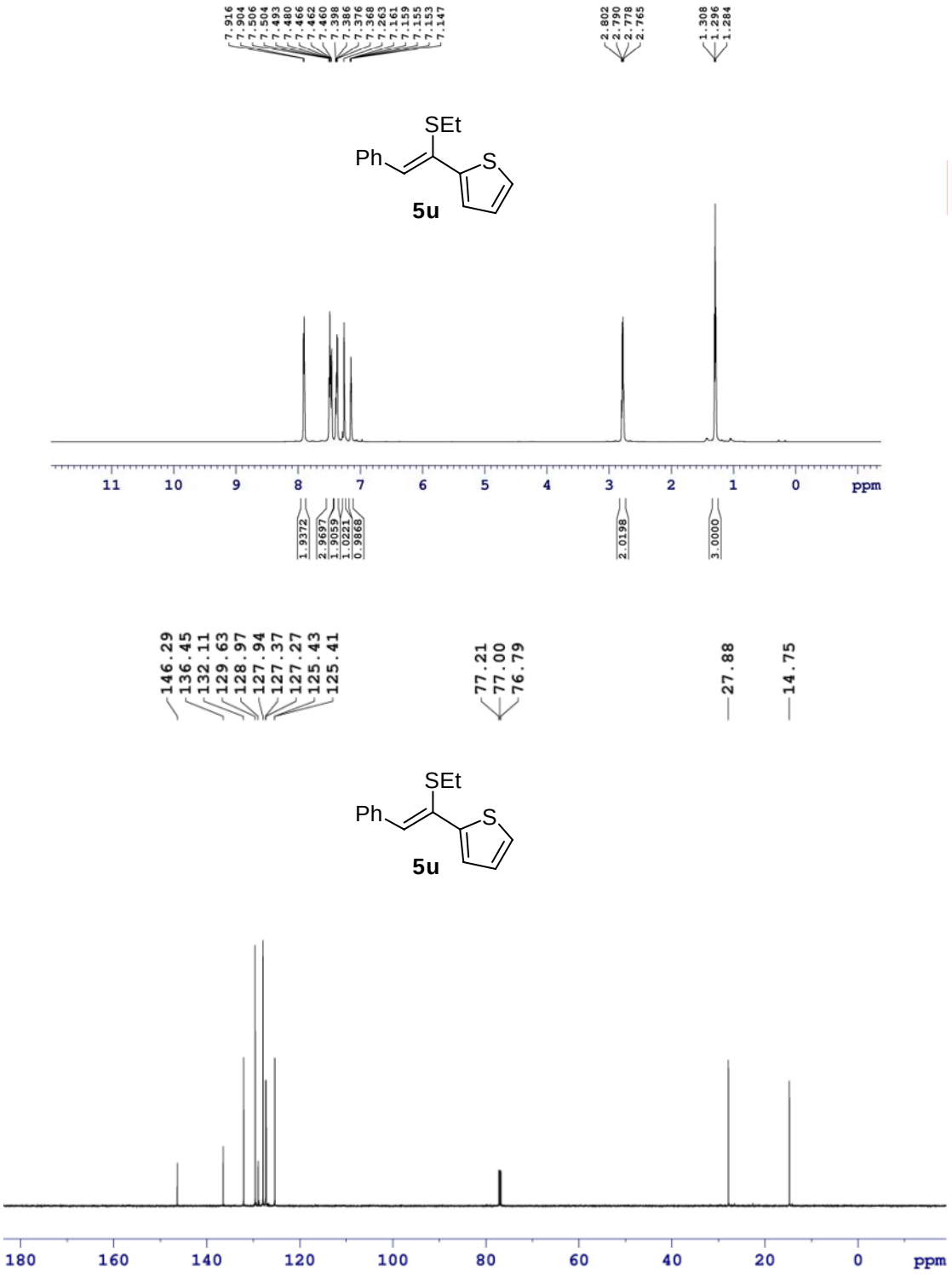
ppm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7.263
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7.155
7.153
7.147
2.802
2.790
2.778
2.765
1.308
1.296
1.284
SEt
Ph
S
5u
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10
9
8
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6
5
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3
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ppm
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127.37
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77.21
77.00
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Ph
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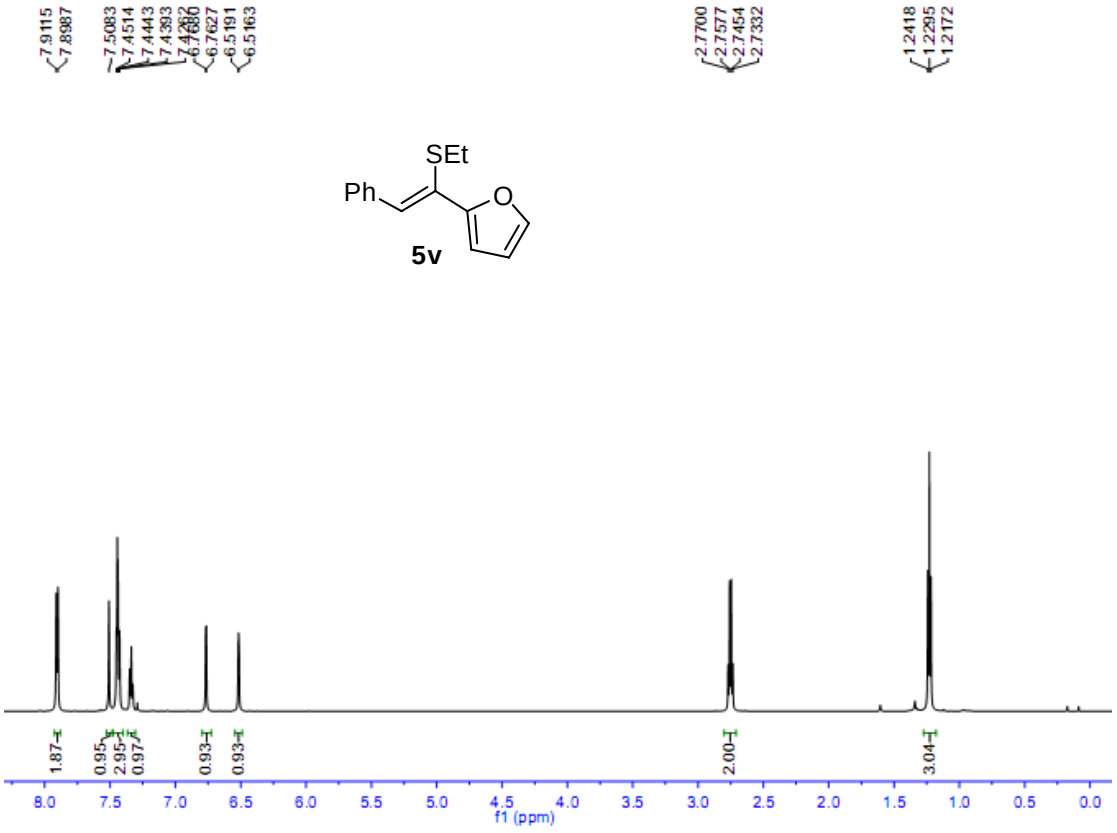

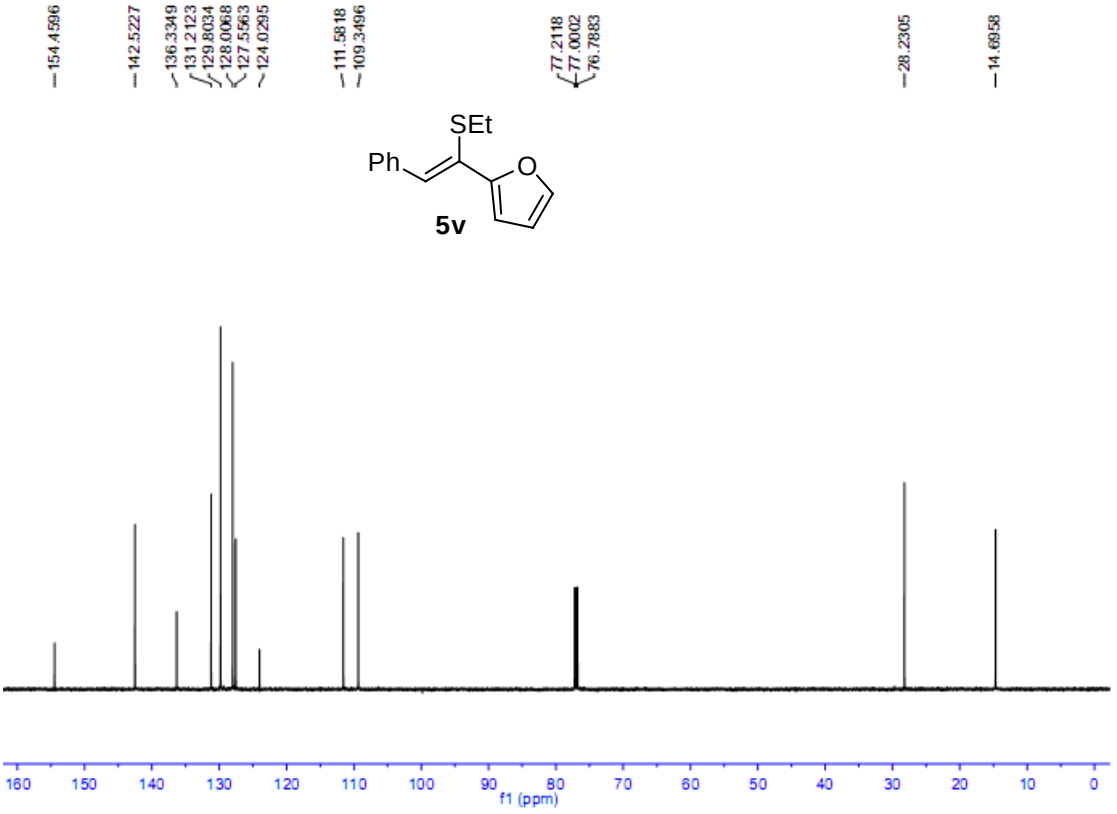

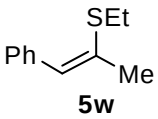

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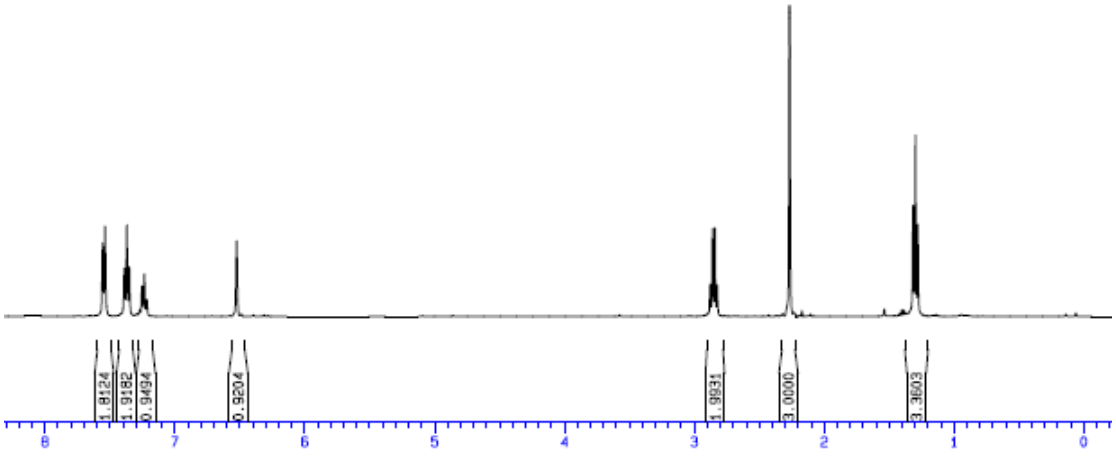

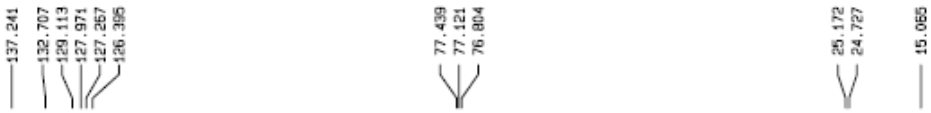

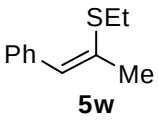

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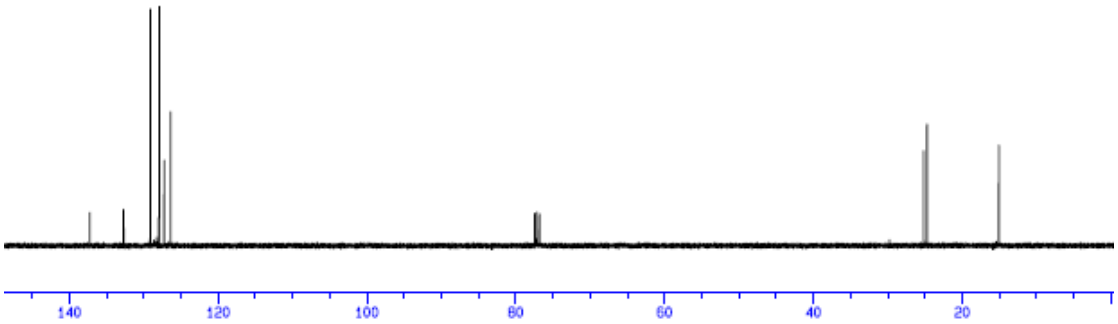

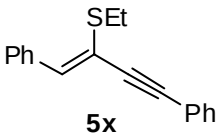

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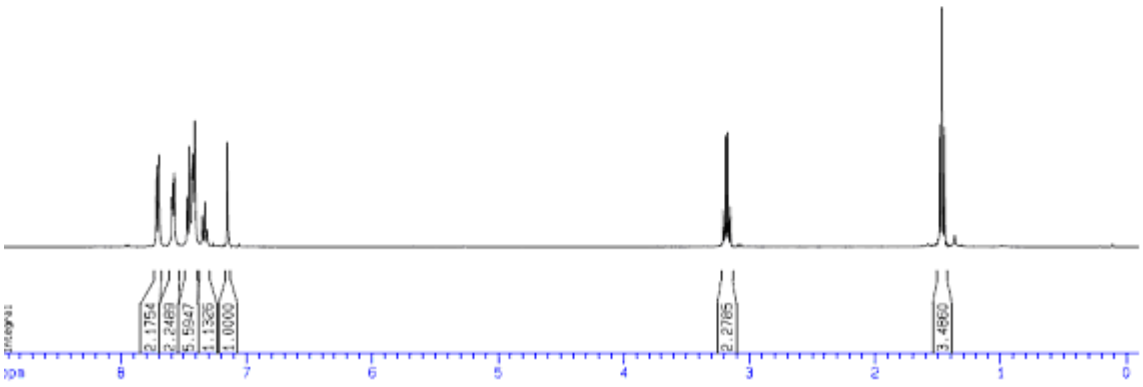

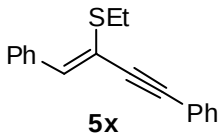

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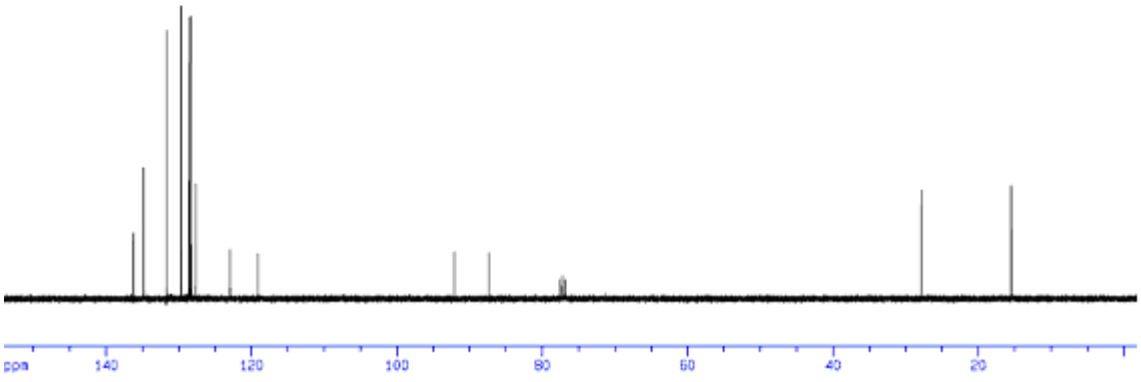

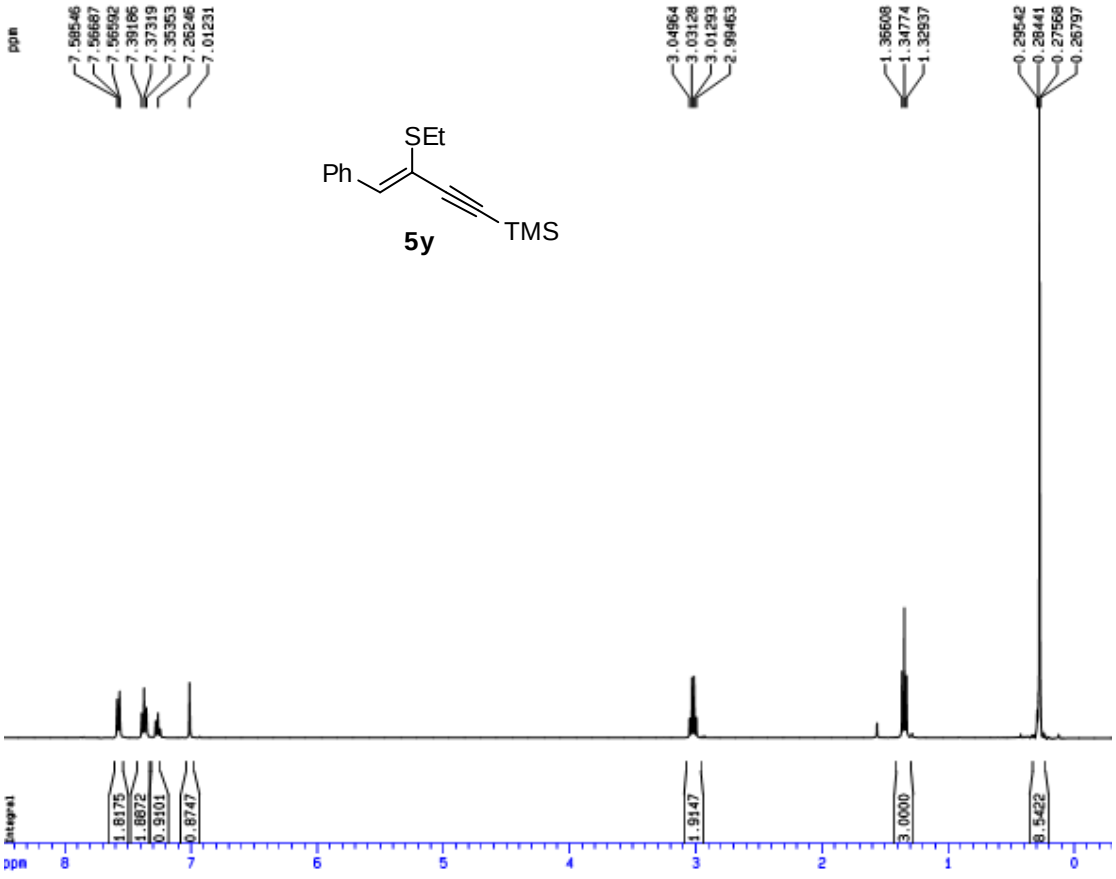

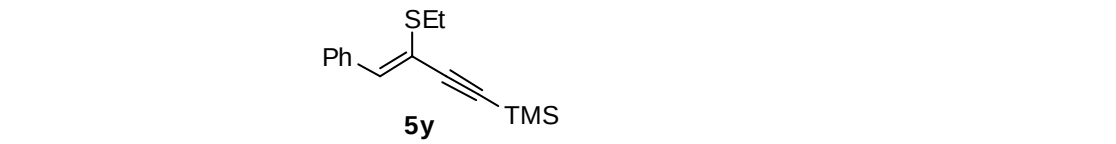

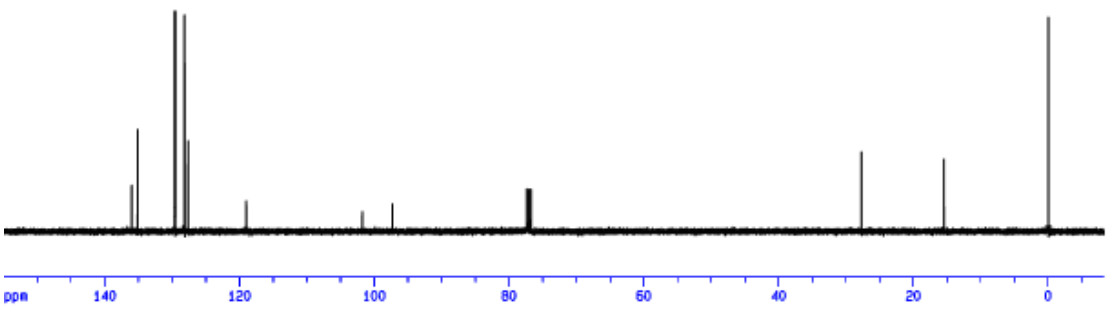

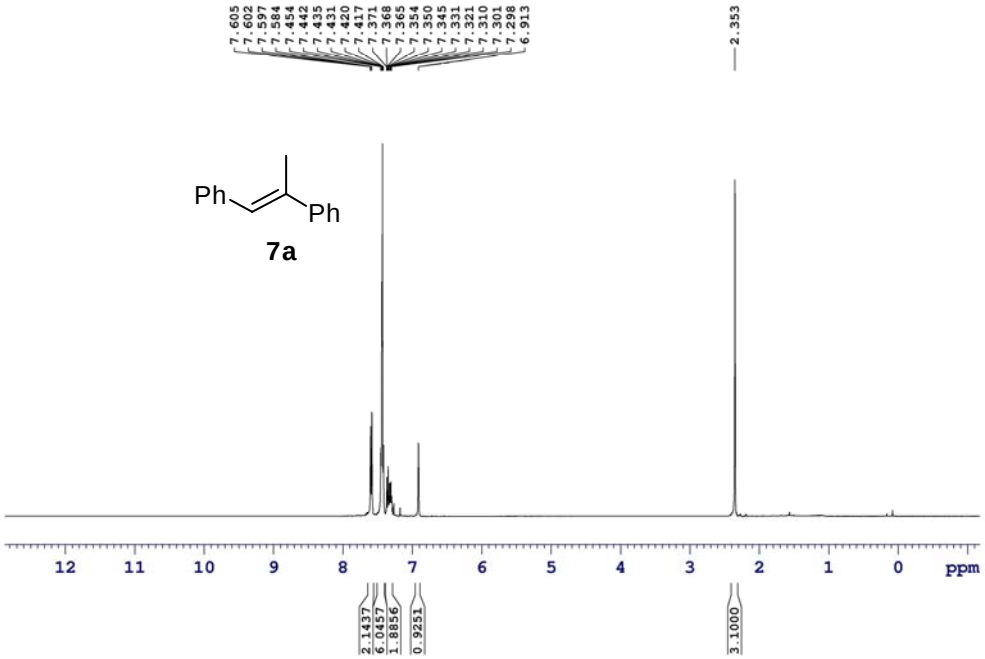

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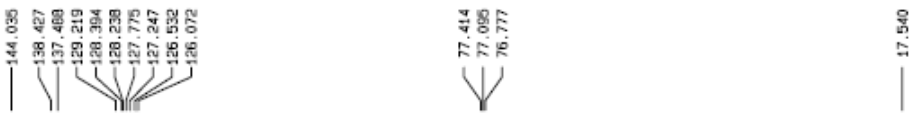

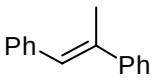

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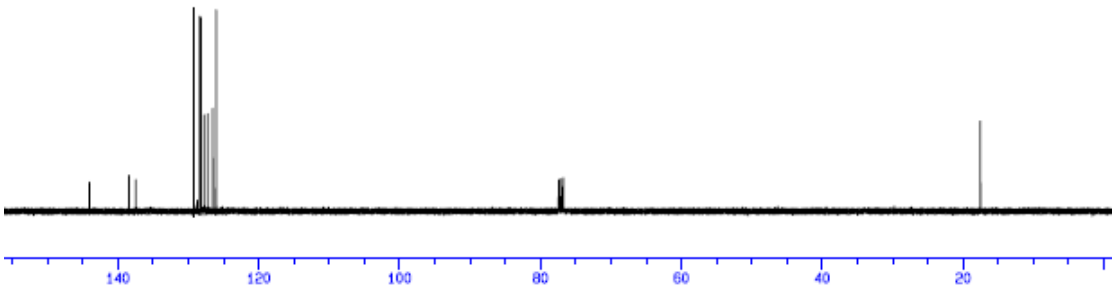

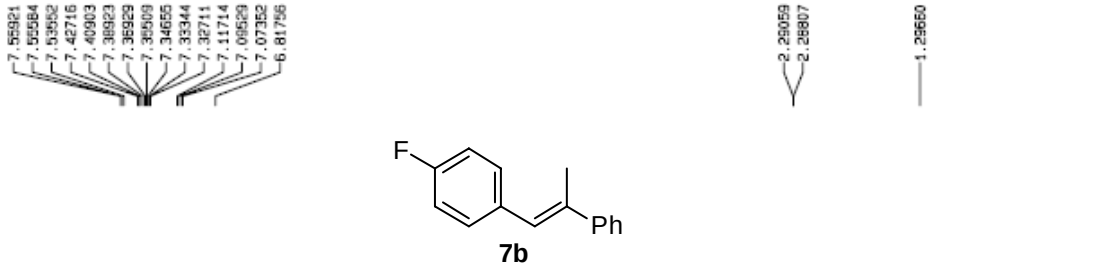

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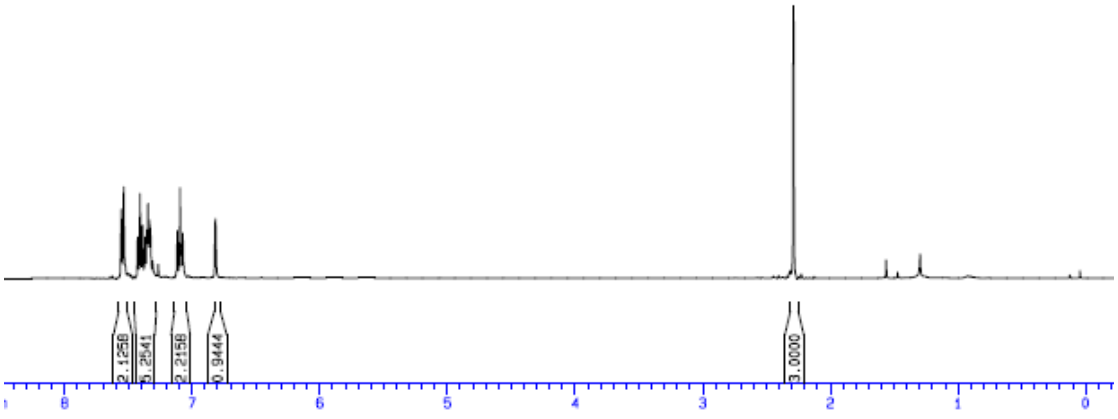

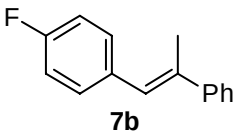

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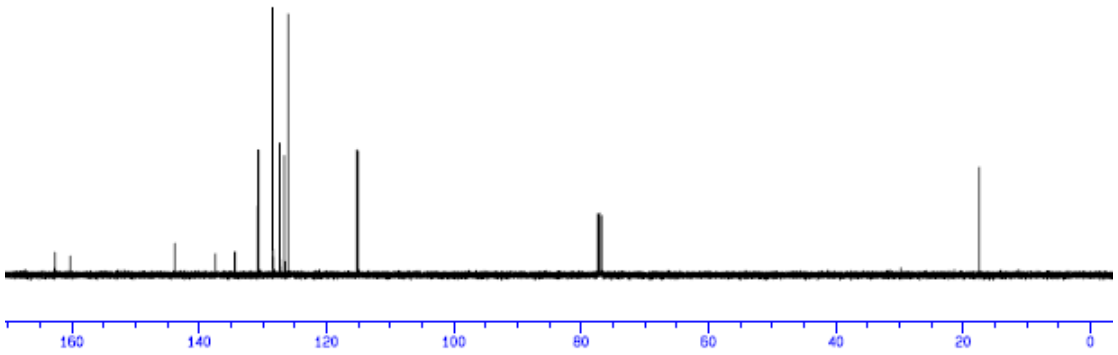

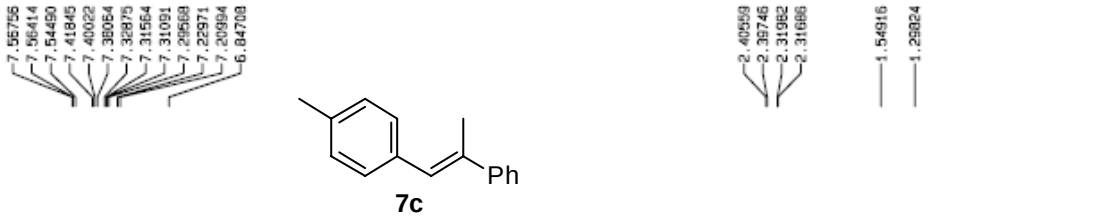

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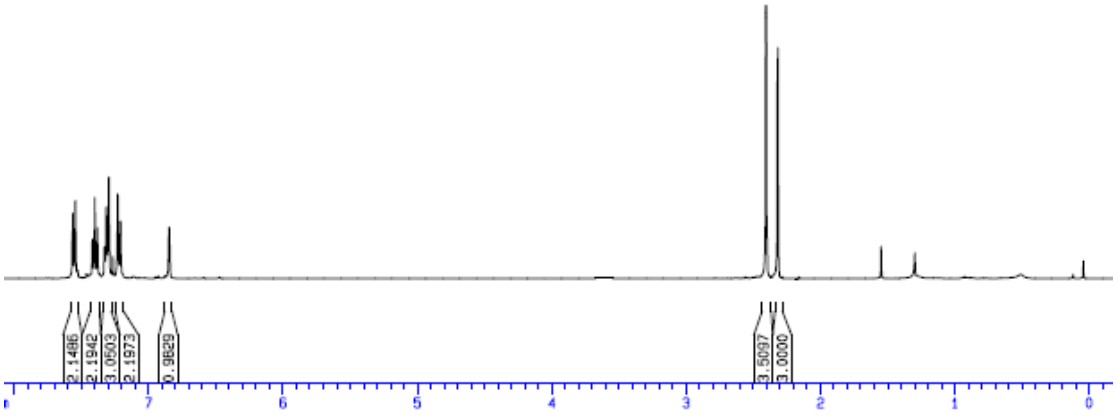

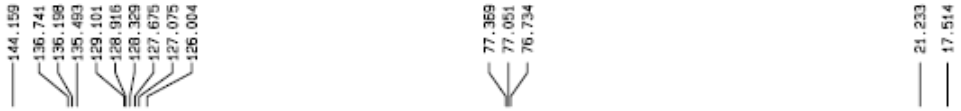

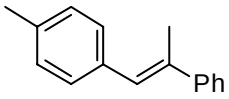

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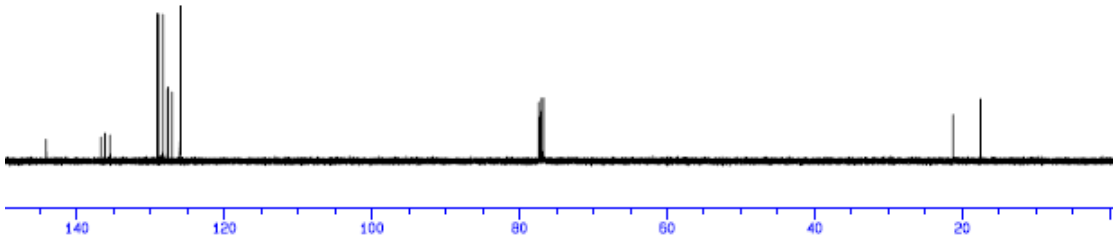

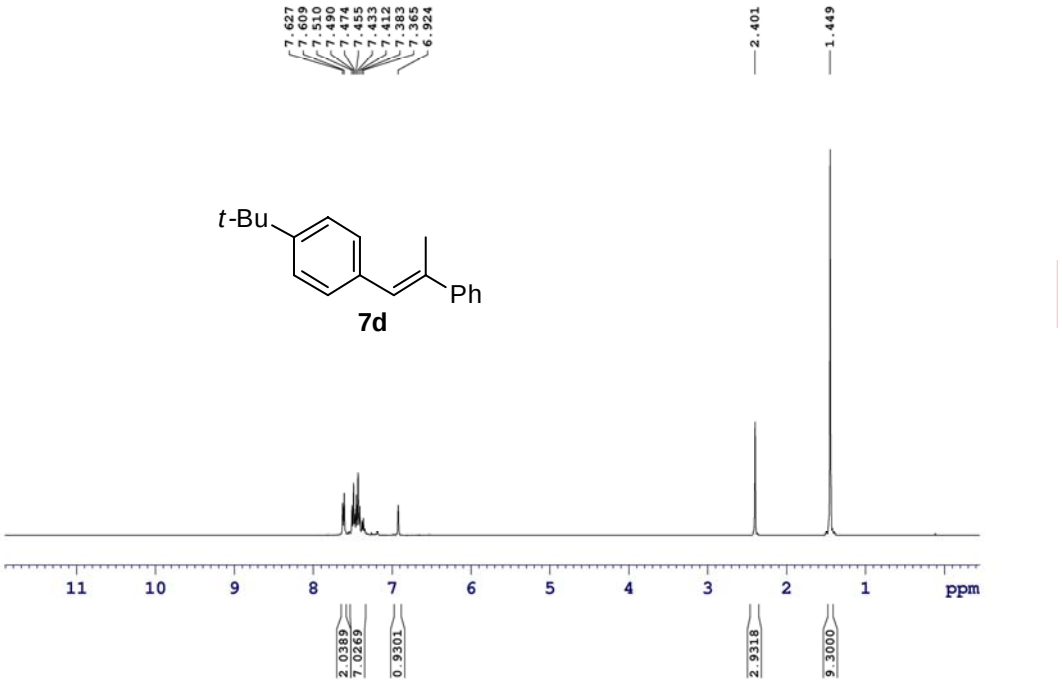

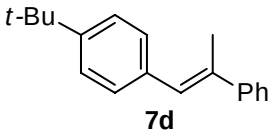

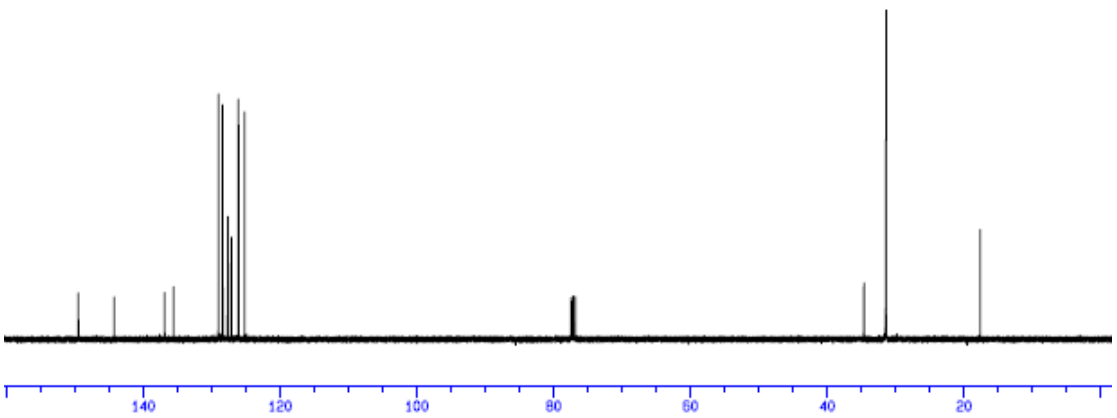

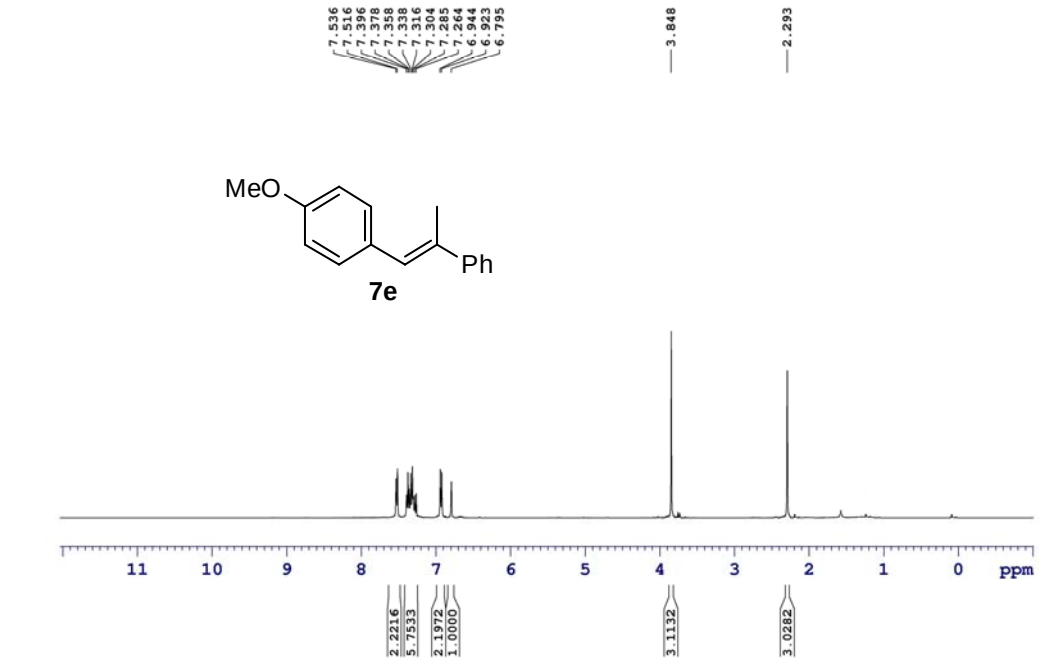

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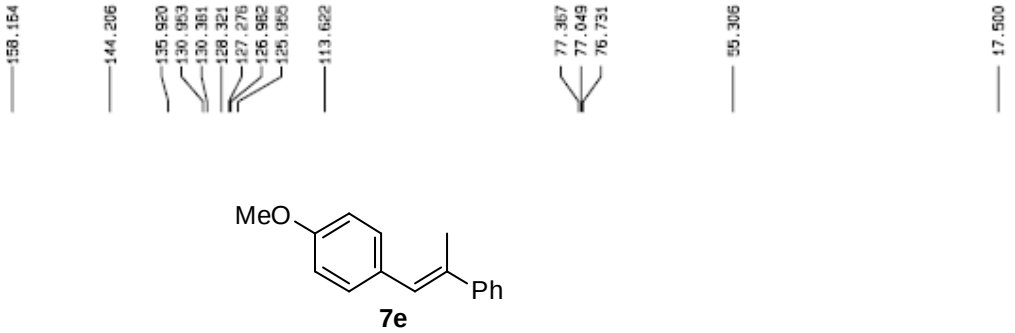

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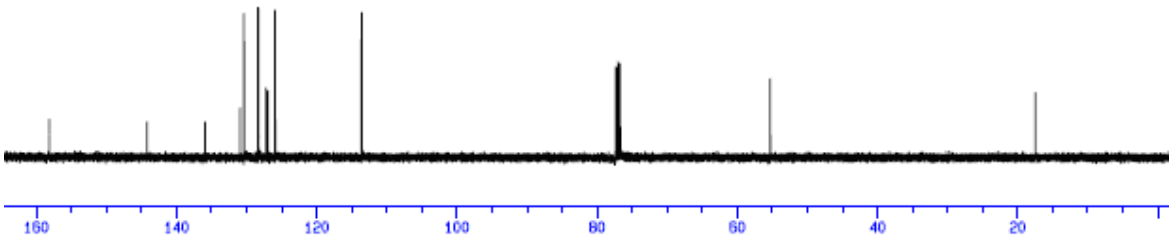
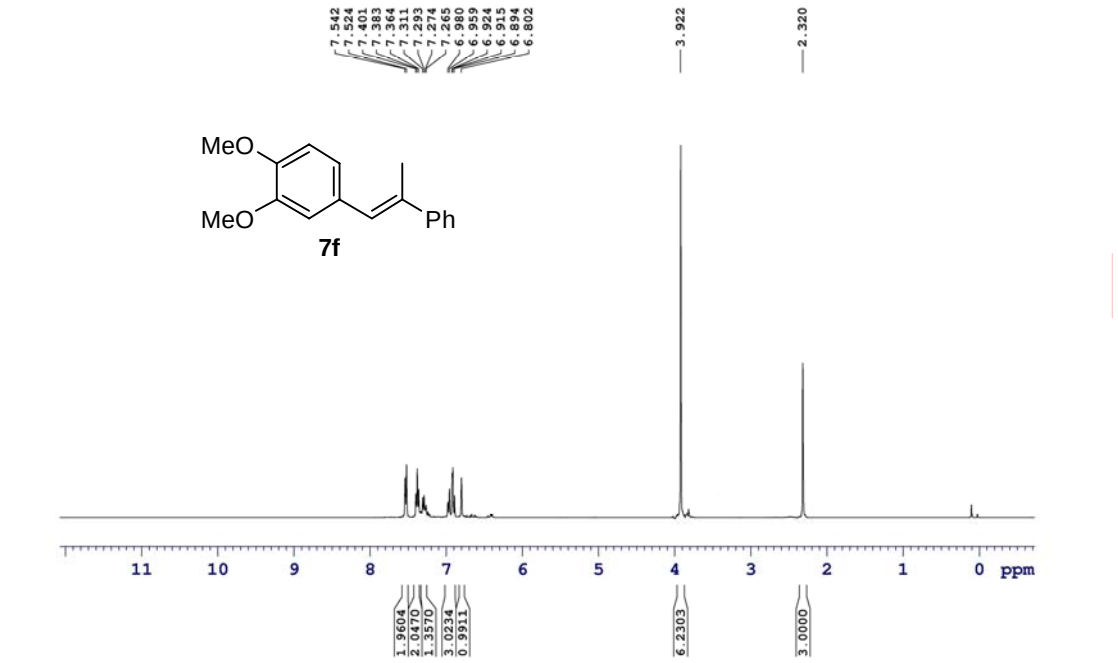
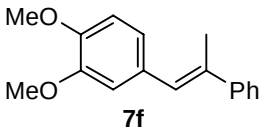
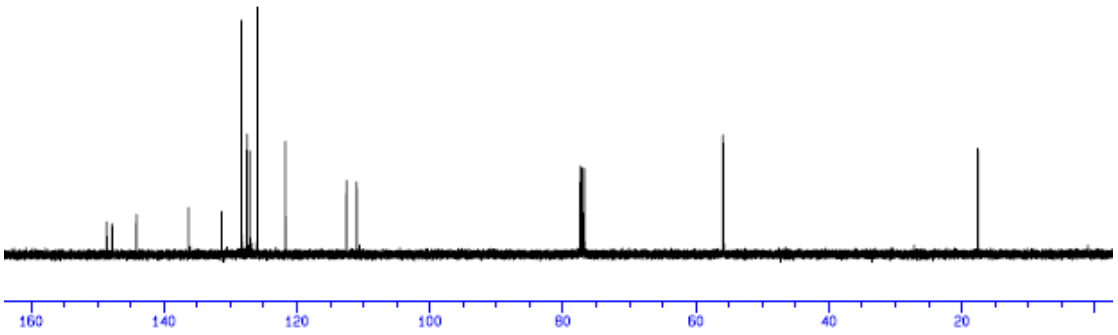
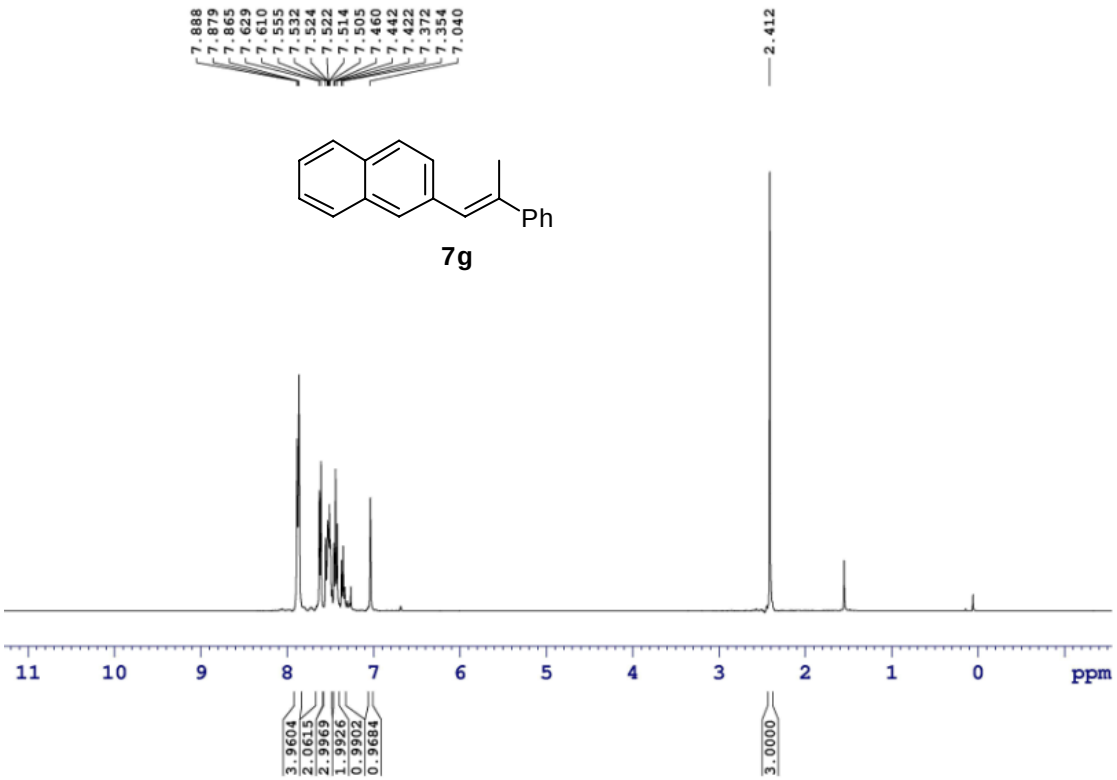


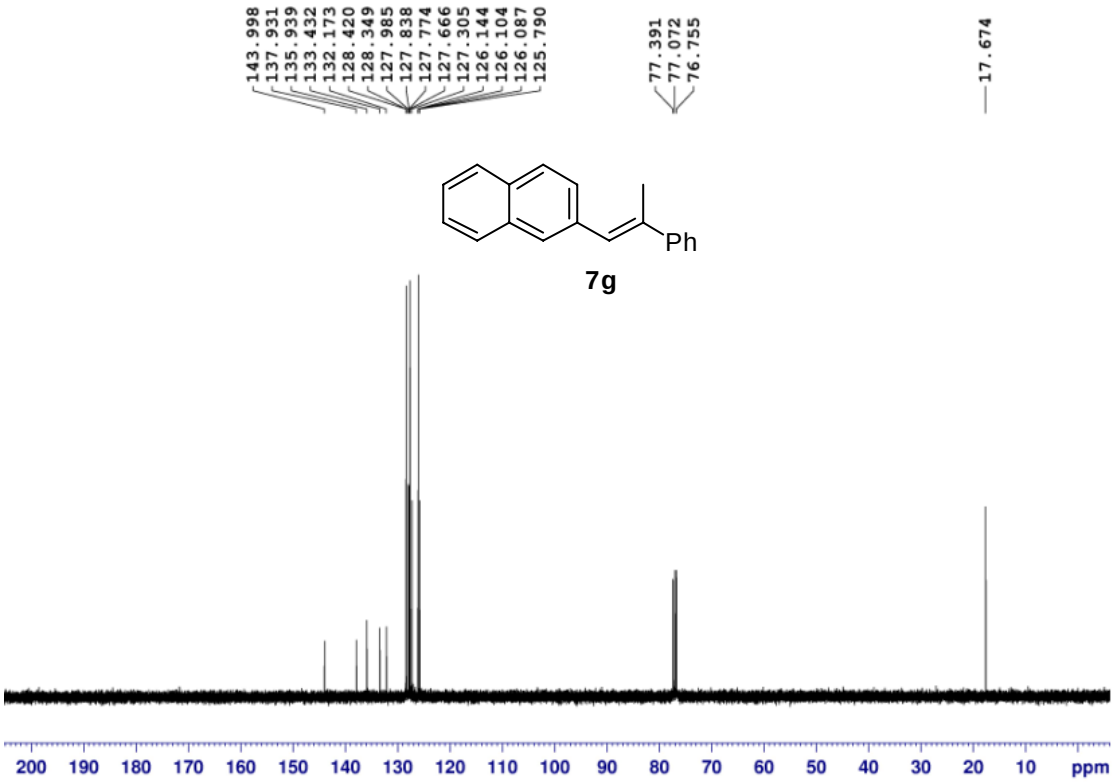








7g



7g


7.414
7.412
7.400
7.398
7.339
7.327
7.314
7.288
7.248
7.246
7.244
7.237
7.234
7.231
7.224
7.222
7.220
5.823
5.820
5.811
5.808
5.798
5.796
2.234
2.222
2.210
2.198
2.056
1.496
1.485
1.473
1.460
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1.375
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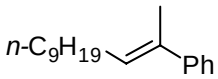
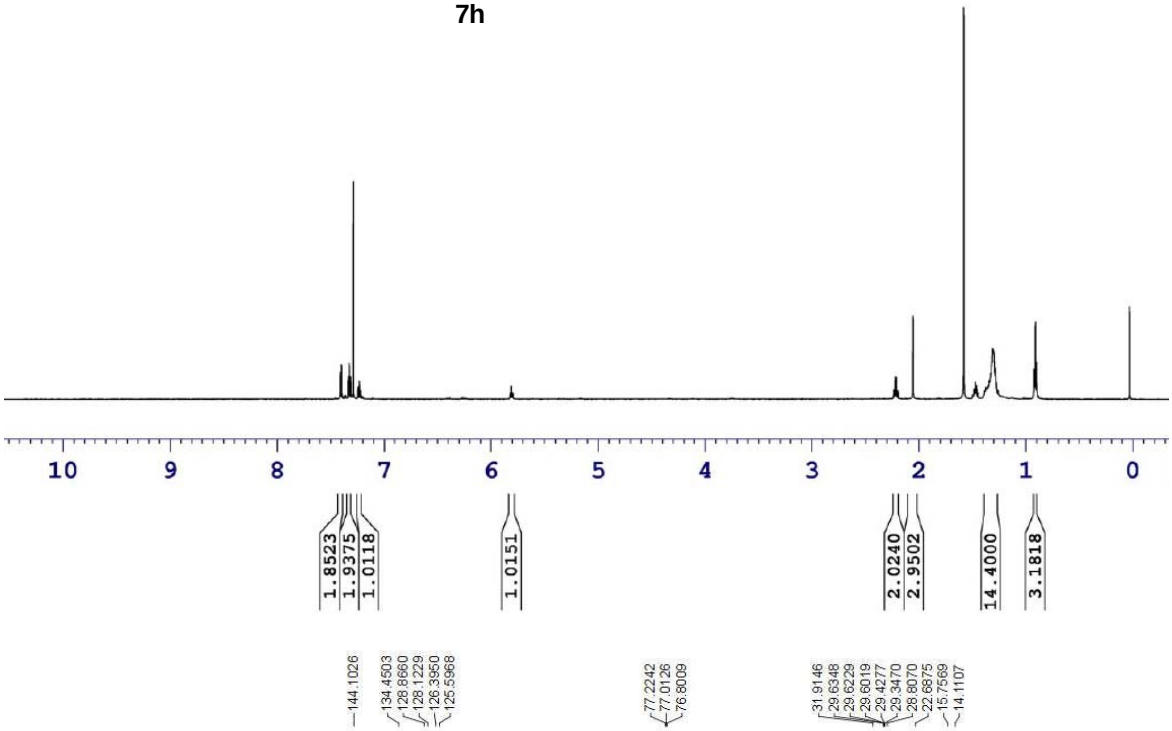
1.359
1.342
1.330
1.309
1.302
1.285
1.273
1.261
0.922


n-C9H19
Ph

7h


10
9
8
7
6
5
4
3
2
1
0
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1.9375
1.0118
1.0151
2.0240
2.9502
14.4000
3.1818

144.1026
134.4503
128.8660
128.1229
126.3950
125.5968
77.2242
77.0126
76.8009
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29.6229
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29.4277
29.3470
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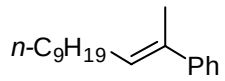
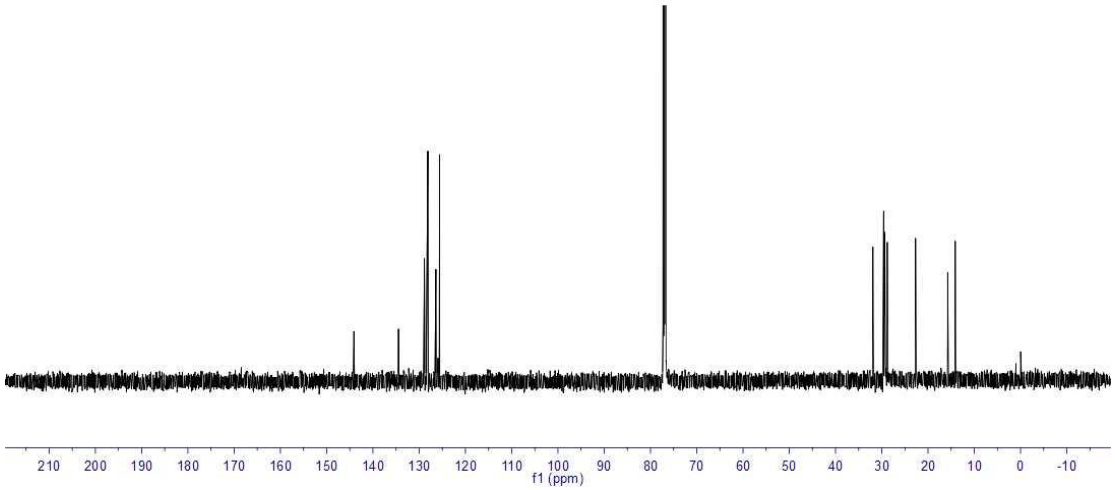
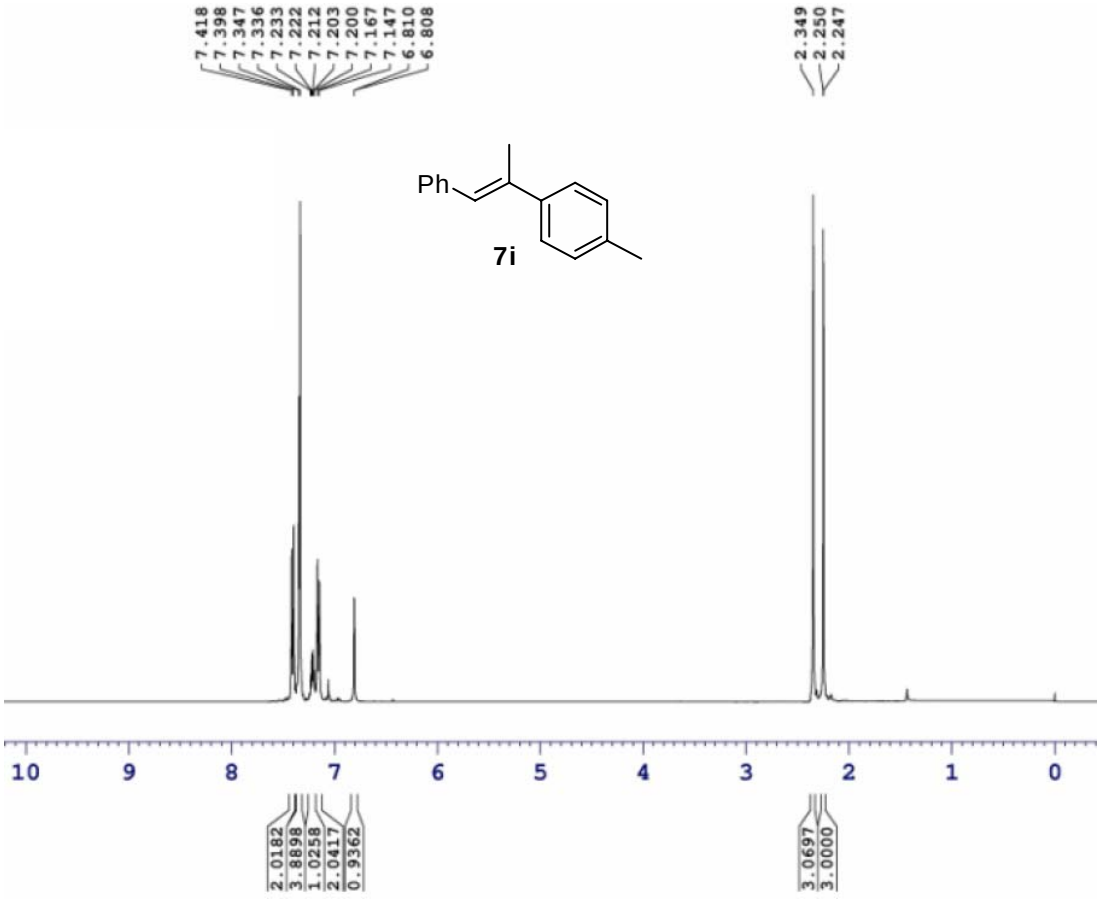
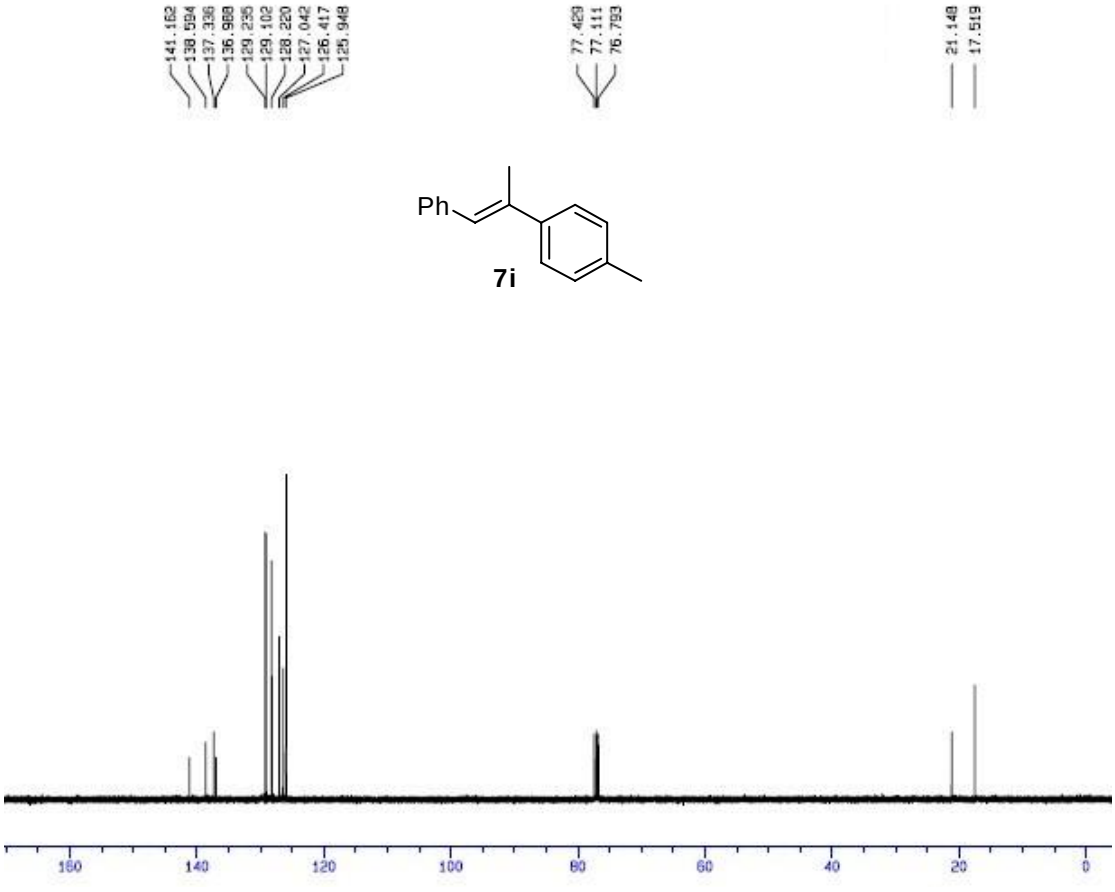
15.7569
14.1107

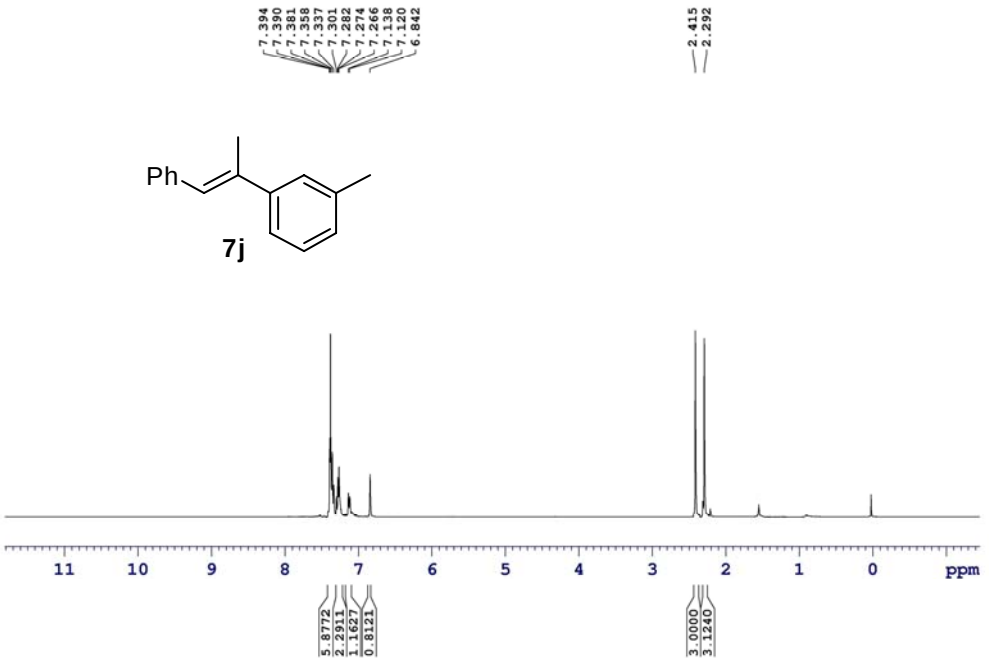

n-C9H19
Ph

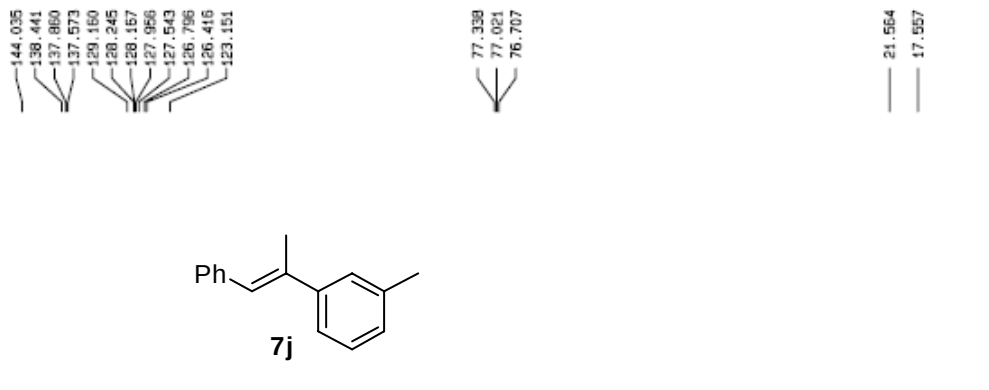
7h

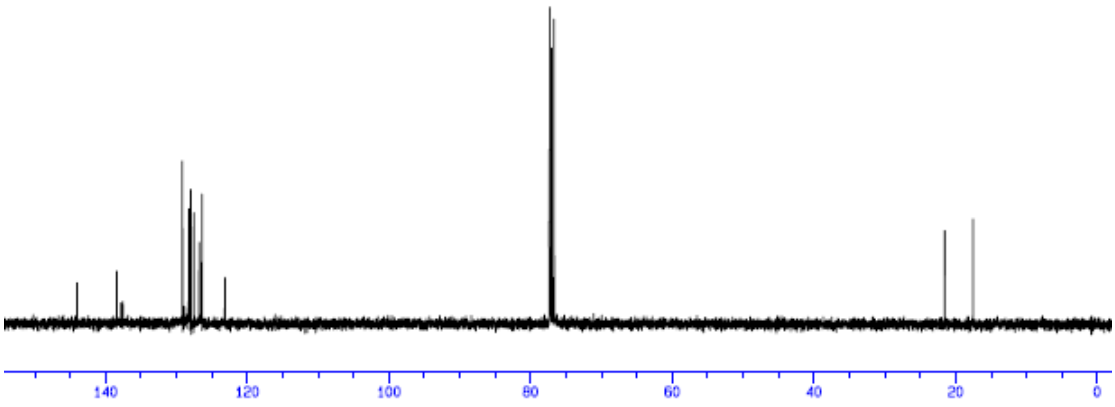

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

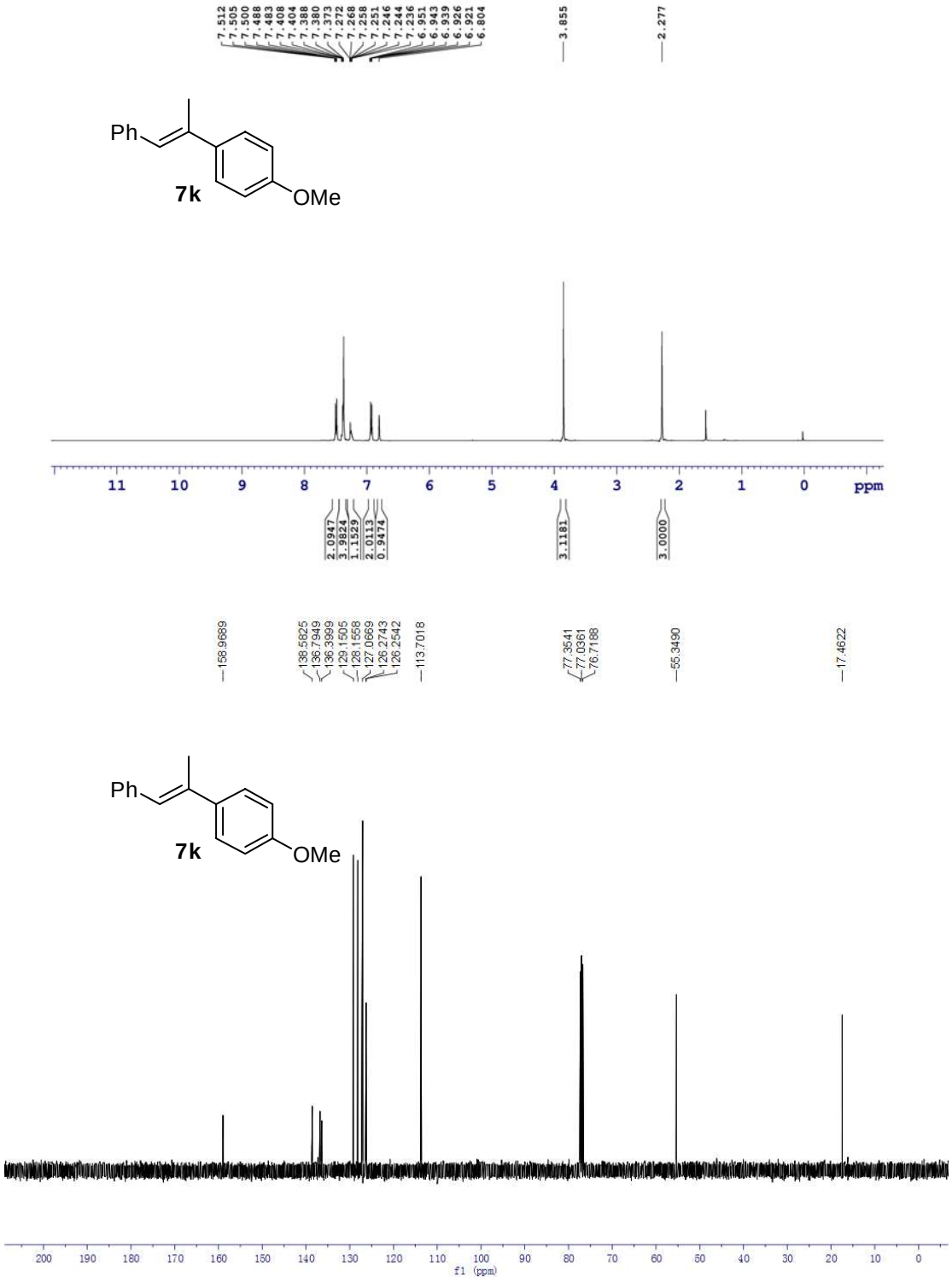








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7.272
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7.251
7.246
7.244
7.236
6.951
6.943
6.939
6.926
6.921
6.804
3.855
2.277
Ph
7k
OMe
11
10
9
8
7
6
5
4
3
2
1
0
ppm
2.0947
3.9824
1.1529
2.0113
0.9474
3.1181
3.0000
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136.3999
129.1505
128.1558
127.0669
126.2743
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77.0361
76.7188
55.3490
17.4622
Ph
7k
OMe
200
190
180
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160
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140
130
120
110
100
90
80
70
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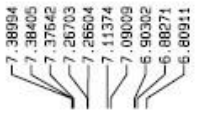
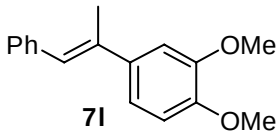
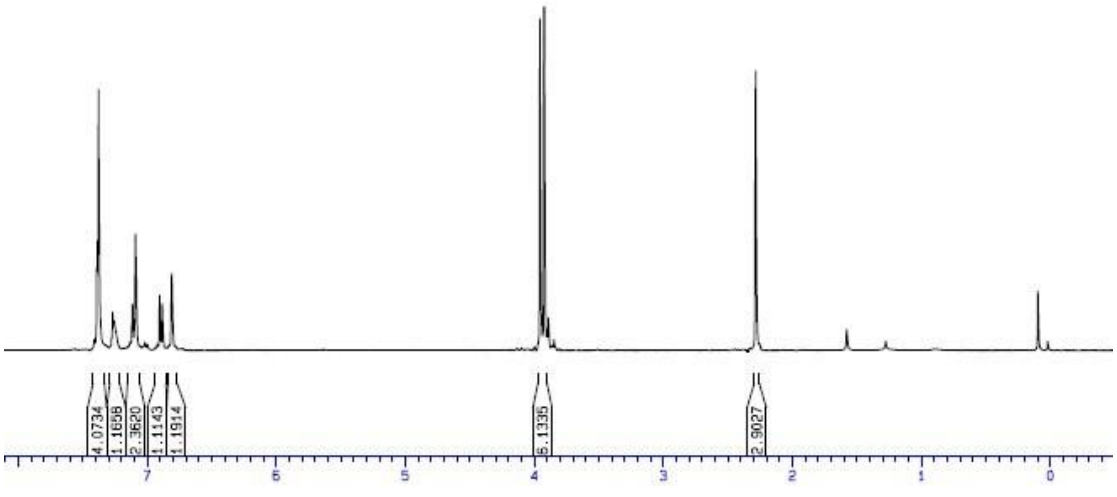
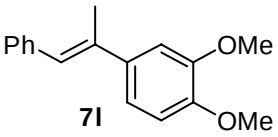
50
40
30
20
10
0
f1 (ppm)



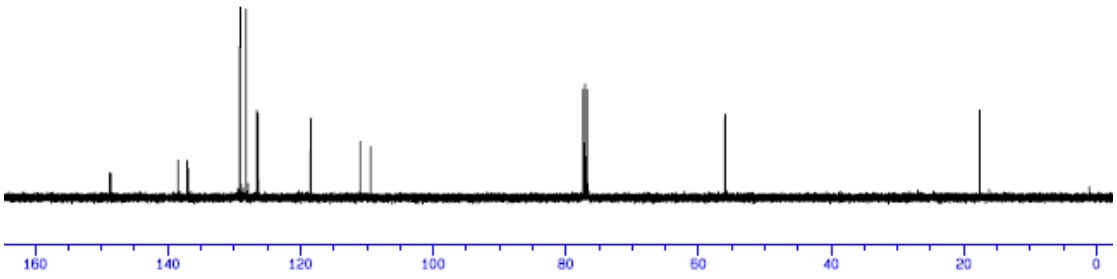


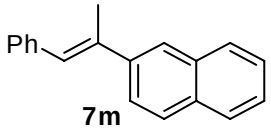
7l



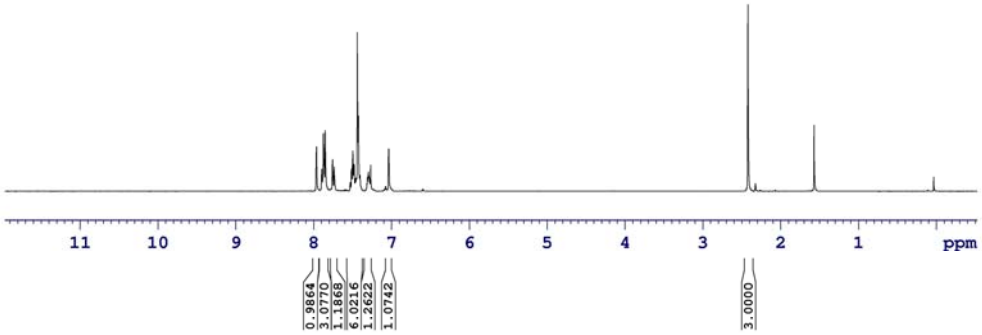


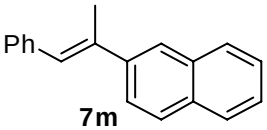
7l



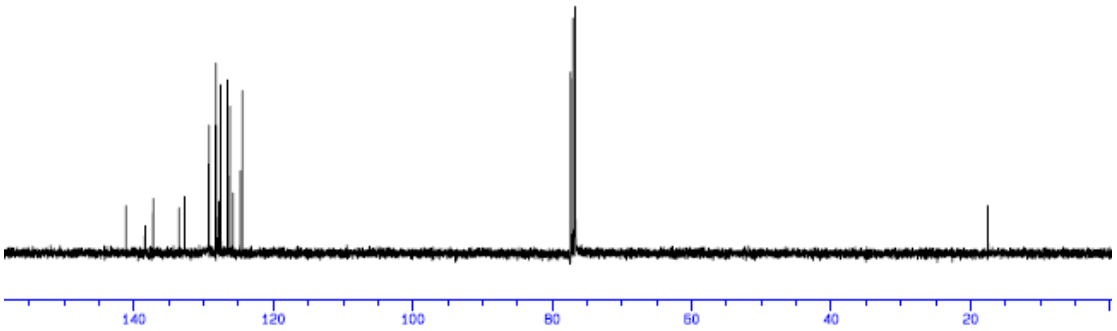


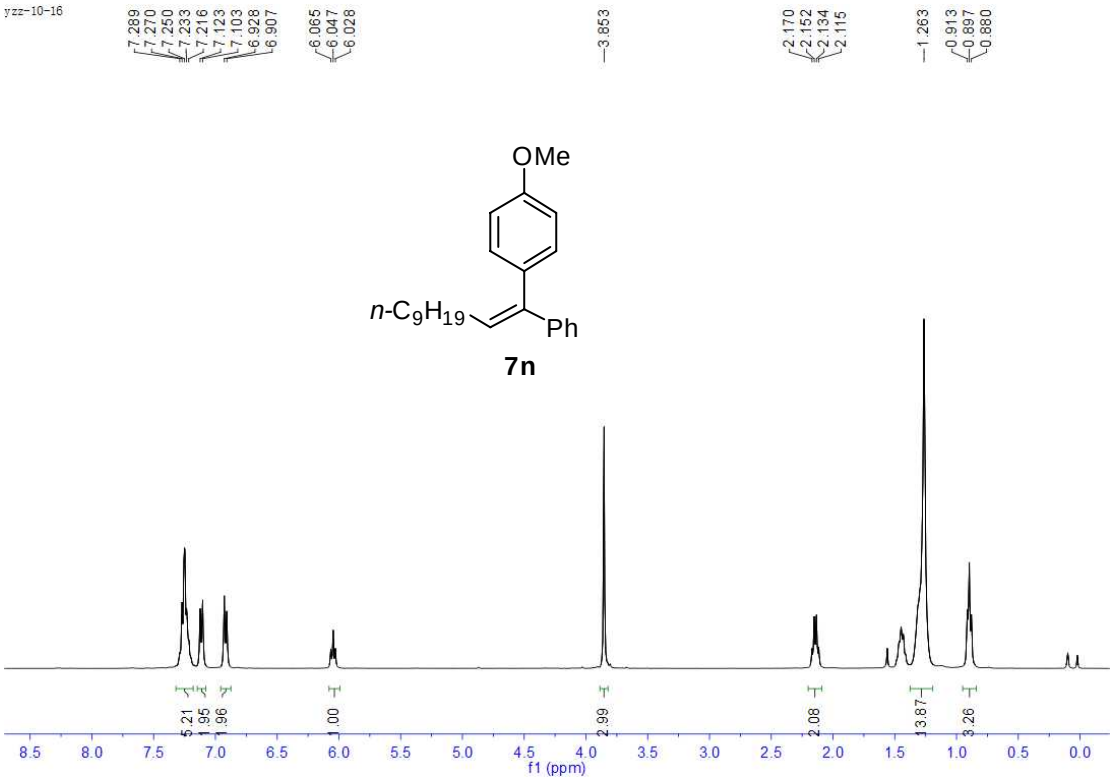
7m





7m

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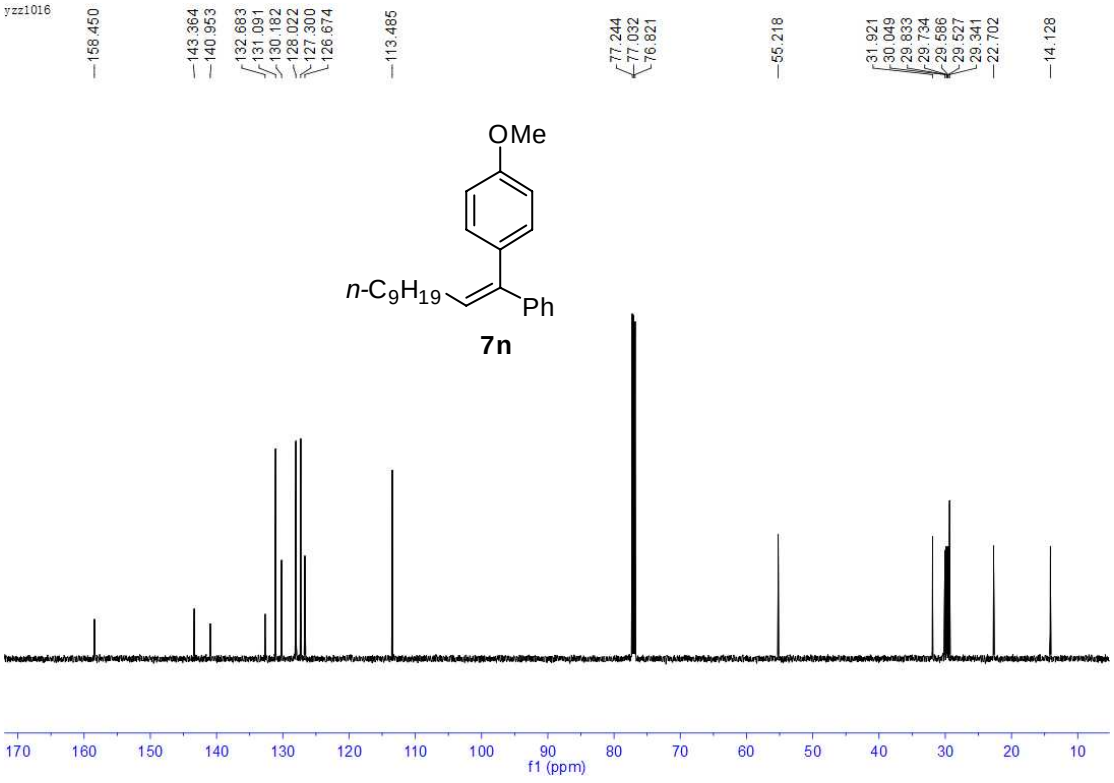
7.270
7.250
7.233
7.216
7.123
7.103
6.928
6.907
6.065
6.047
6.028
3.853
2.170
2.152
2.134
2.115
1.263
0.913
0.897
0.880
OMe
n-C9H19
Ph
7n
5.21
1.95
1.96
1.00
2.99
2.08
13.87
3.26
f1 (ppm)


yzz1016
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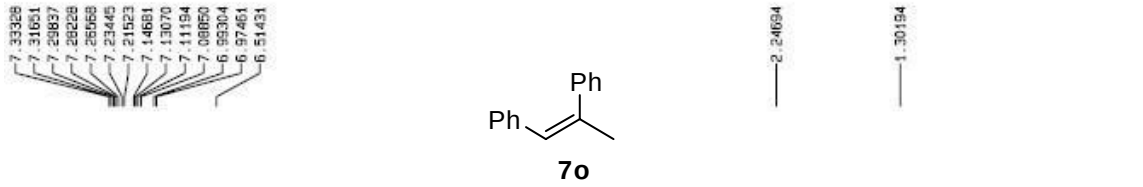
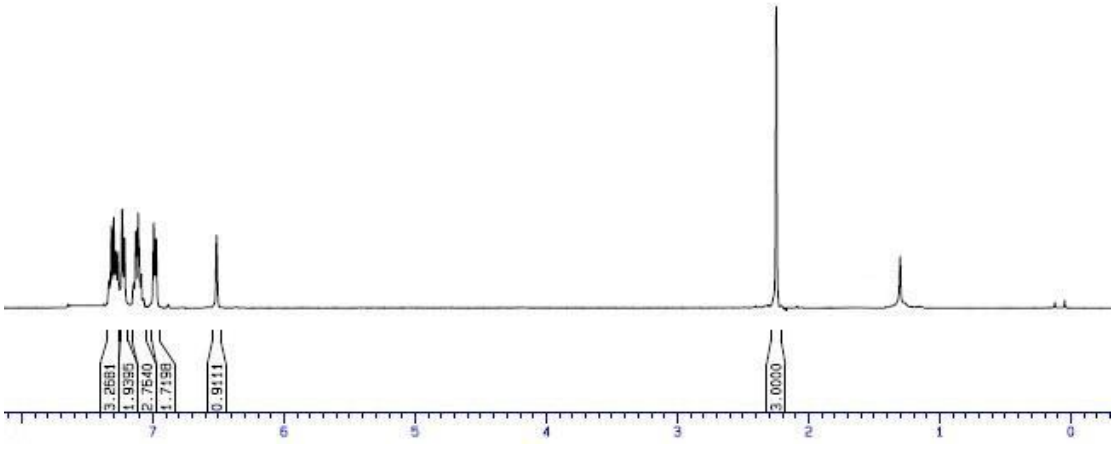
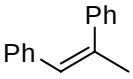
140.953
132.683
131.091
130.182
128.022
127.300
126.674
113.485
77.244
77.032
76.821
55.218
31.921
30.049
29.833
29.734
29.586
29.527
29.341
22.702
14.128
OMe
n-C9H19
Ph
7n
f1 (ppm)

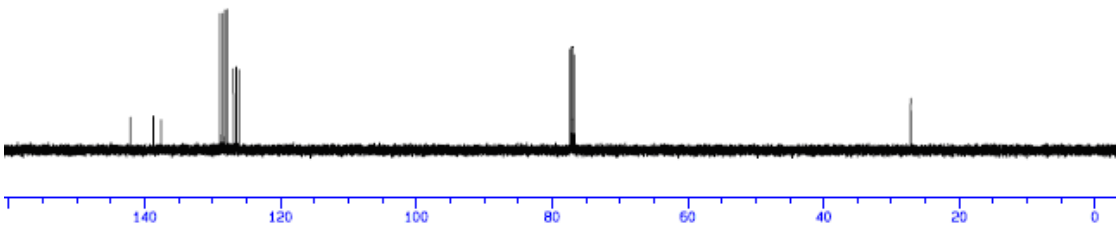


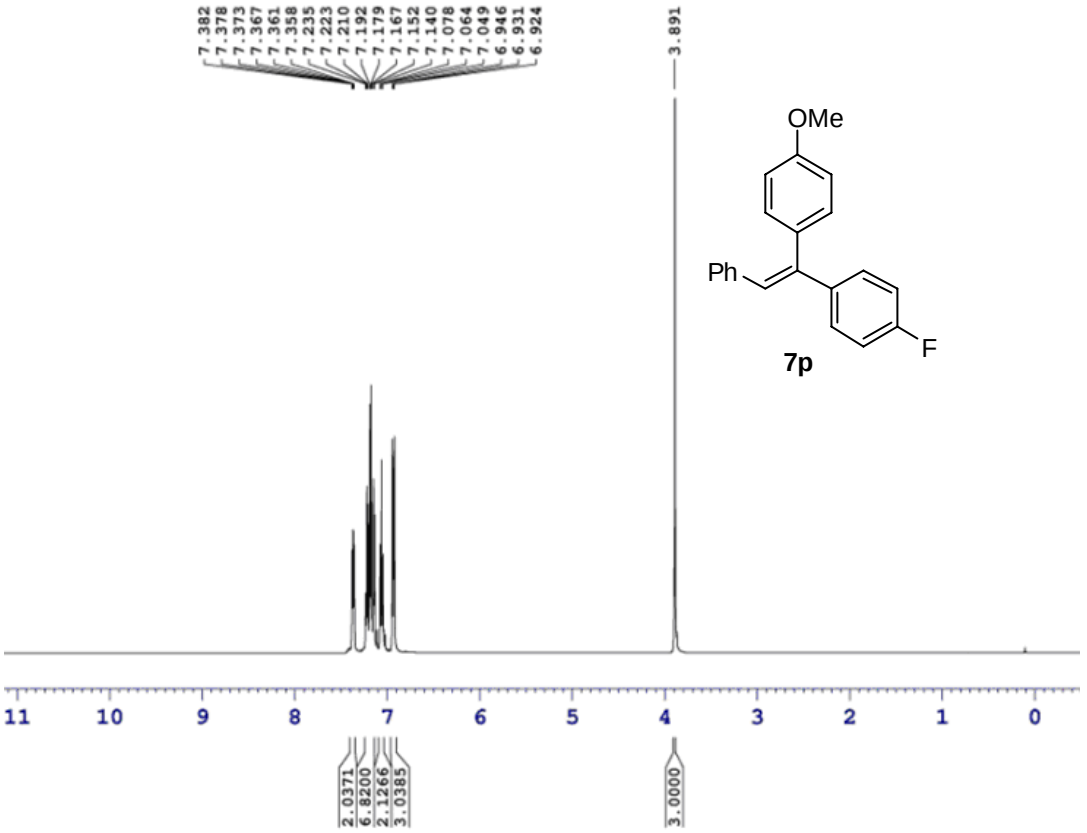
7o

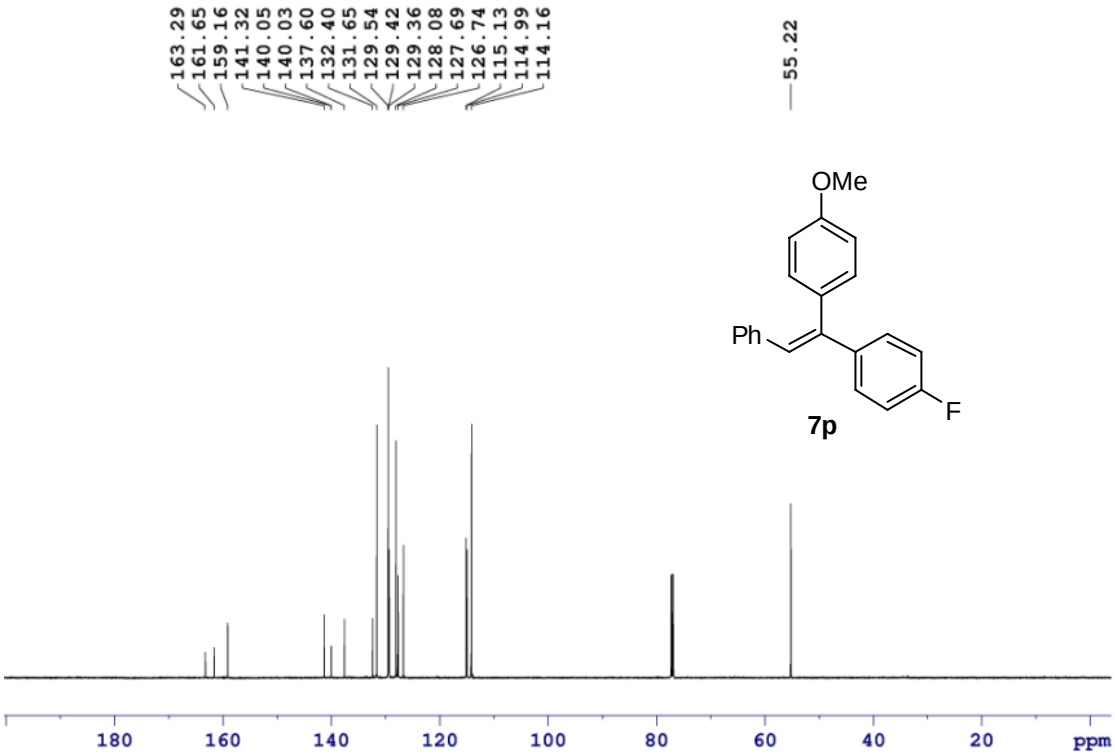


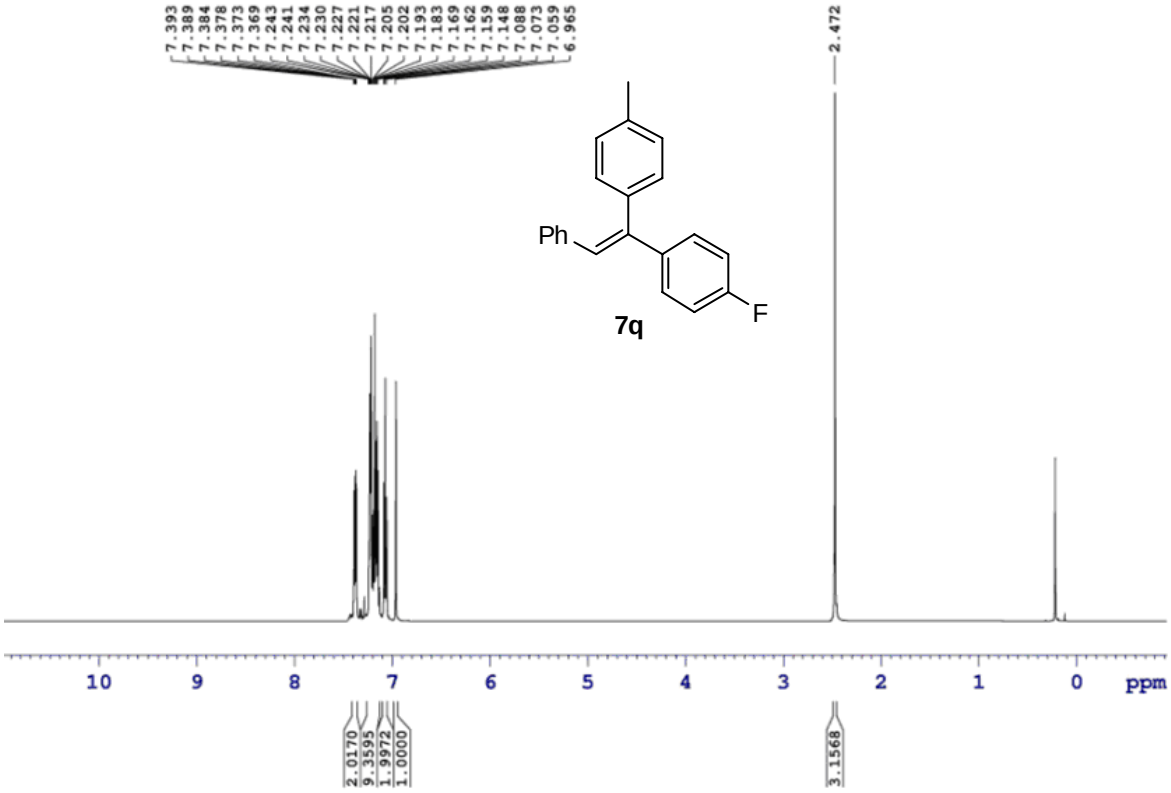


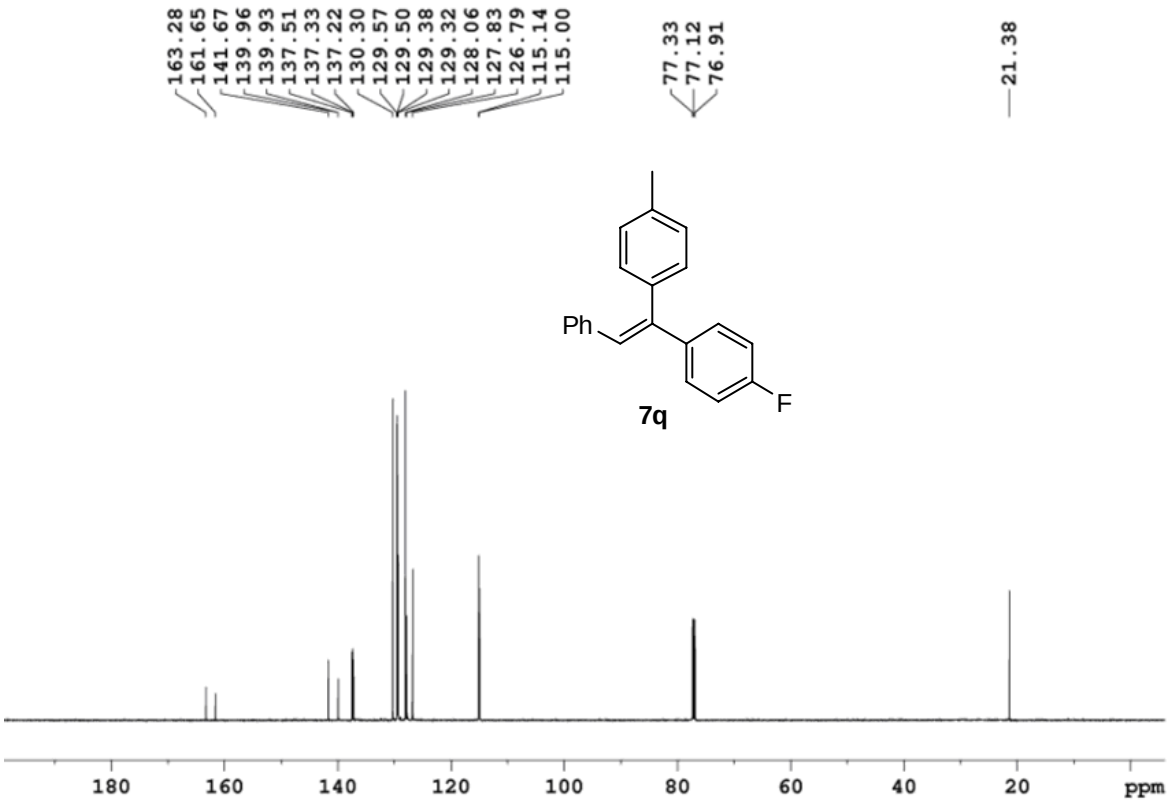
7o

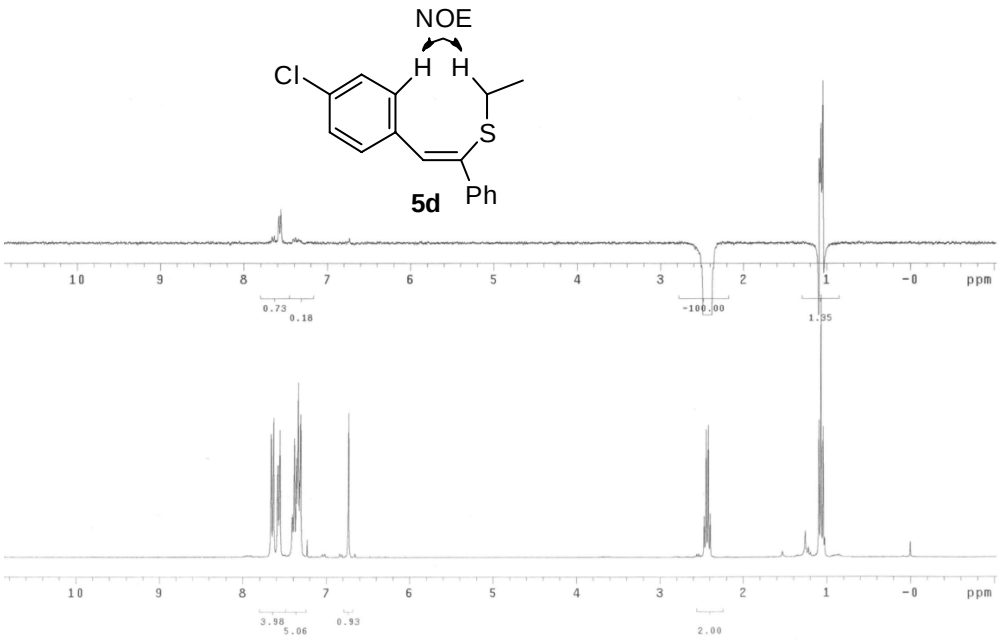


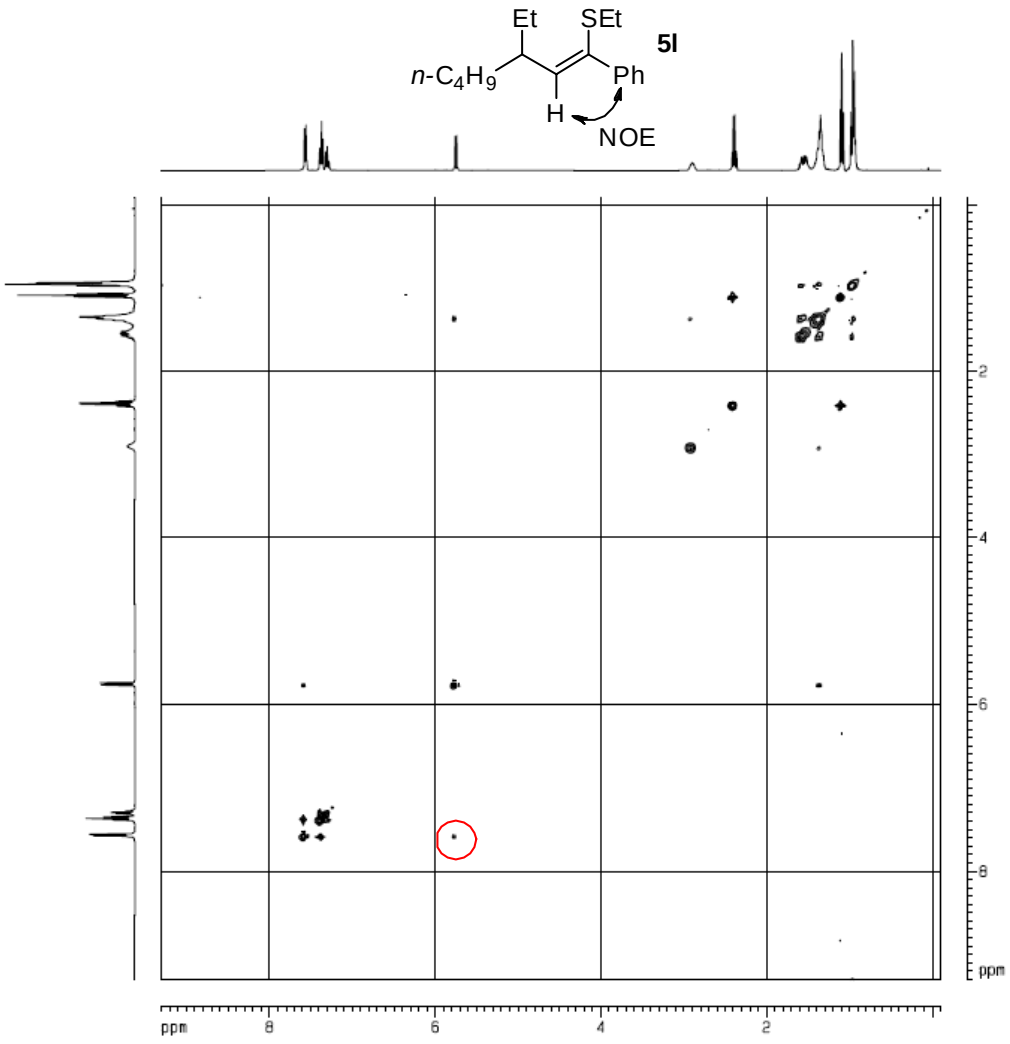


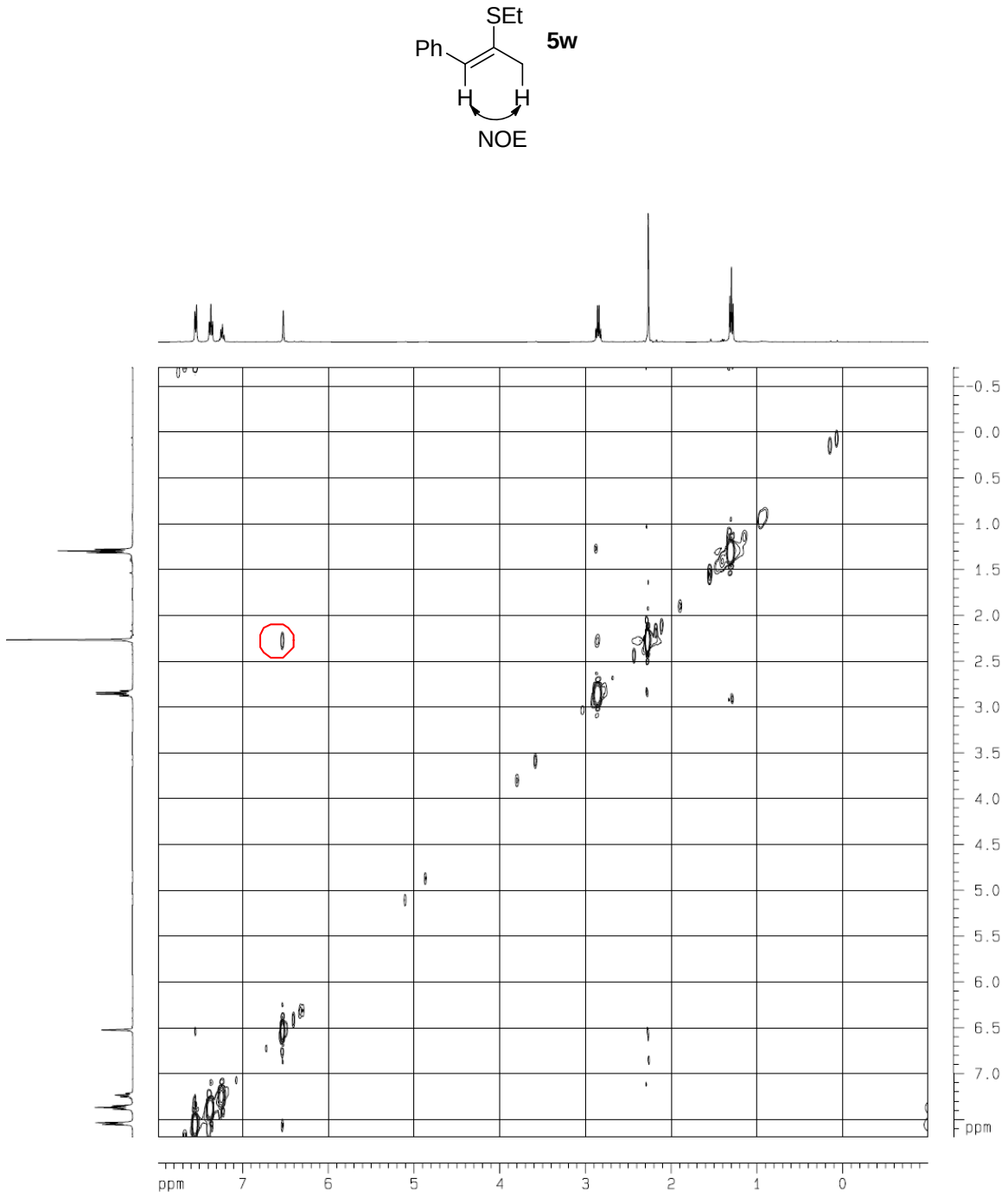


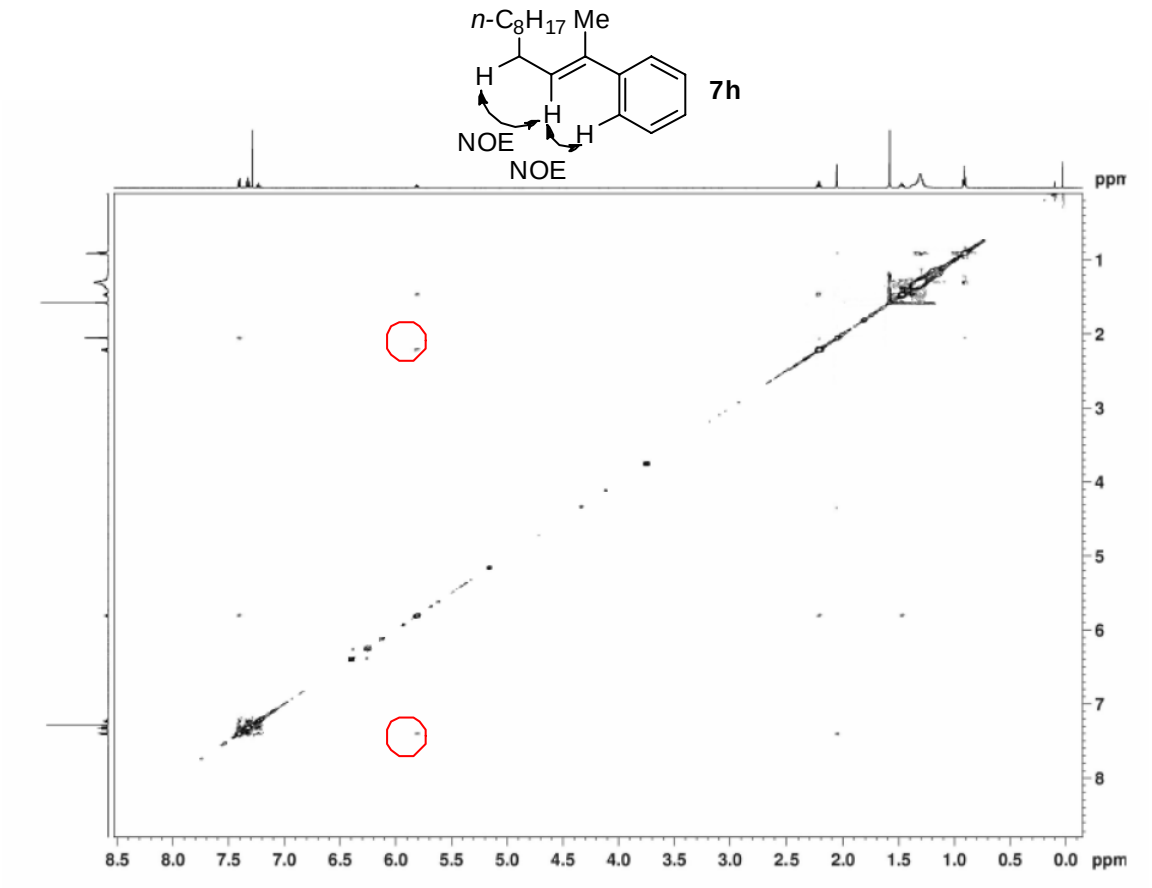


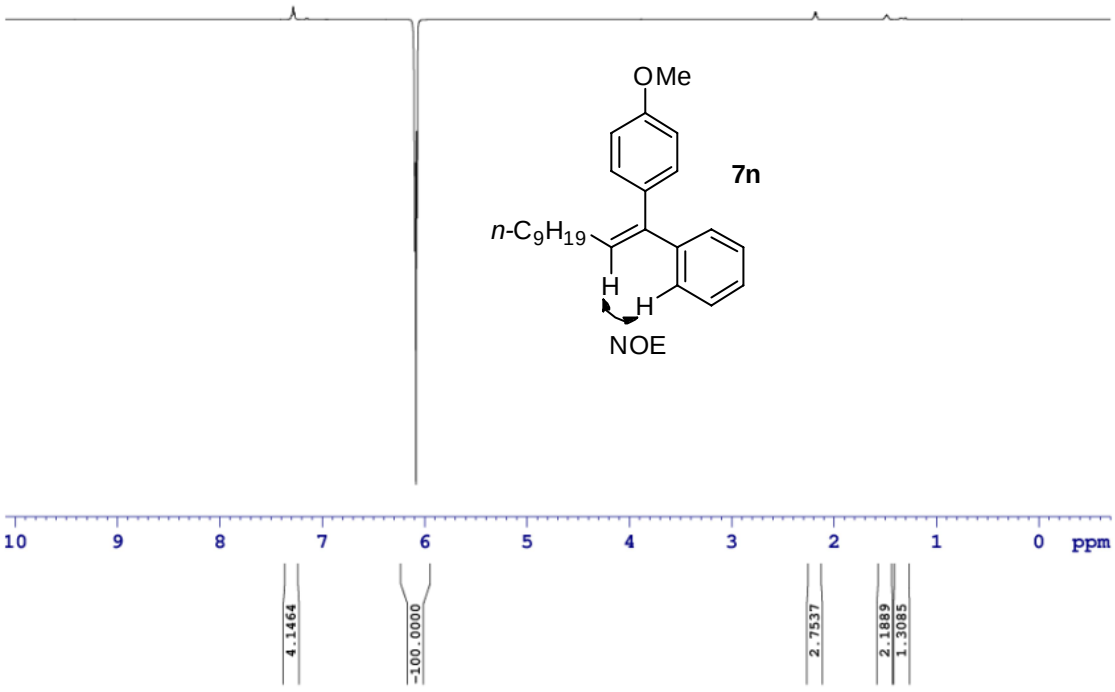









n-C8H17 Me
H
H
H
NOE
NOE
7h
ppm
1
2
3
4
5
6
7
8
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm


OMe
7n
n-C9H19
H
H
NOE
10 9 8 7 6 5 4 3 2 1 0 ppm
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-100.0000
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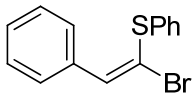
2.1889
1.3085



3s

Crystal data for **3s** ($C_{14}H_{11}BrS$, 291.20) orthorhombic, space group *P*2(1)2(1)2(1), *a* = 6.0206(4) Å, *b* =10.2488(7) Å, *c* = 20.3688(13) Å, volume = 1256.83(14) $Å^3$, *Z* = 4, specimen 0.403 × 0.204 × 0.057 mm^3, *T* = 296(2) K, SIEMENS P4 diffractometer, absorption coefficient 3.405 mm^{-1}, reflections collected 8909, independent reflections 2206 [R(int) = 0.0350], refinement by full-matrix least-squares on F^2, data/restraints/parameters 2206/0/145, goodness-of-fit on F^2 = 1.059, final *R* indices [$I>2\sigma(I)$] R1 = 0.0353, wR2 =0.0740, *R* indices (all data) R1 = 0.0682, wR2 = 0.0815, largest diff peak and hole 0.573 and –0.371 $eÅ^{-3}$. CCDC 902936 (**3s**) contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre viawww.ccdc.cam.ac.uk/data_request/cif.

checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

No syntax errors found. CIF dictionary Interpreting this report

Datablock: a

Bond precision: C-C = 0.0072 A Wavelength=0.71073

Cell: a=6.0206(4) b=10.2488(7) c=20.3688(13)
alpha=90 beta=90 gamma=90
Temperature: 296 K

	Calculated	Reported
Volume	1256.84(14)	1256.83(14)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C14 H11 Br S	C14 H11 Br S
Sum formula	C14 H11 Br S	C14 H11 Br S
Mr	291.20	291.20
Dx,g cm-3	1.539	1.539
Z	4	4
Mu (mm-1)	3.405	3.405
F000	584.0	584.0
F000'	583.54	
h,k,lmax	7,12,24	7,12,24
Nref	1312[2206]	2206
Tmin,Tmax	0.439,0.824	0.924,0.970
Tmin'	0.251	

Correction method= EMPIRICAL

Data completeness= 1.68/1.00 Theta(max)= 24.980

R(reflections)= 0.0353(1546) wR2(reflections)= 0.0815(2206)

S = 1.059 Npar= 145

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.

Alert level C

PLAT241_ALERT_2_C Check High Ueq as Compared to Neighbors for S2
PLAT242_ALERT_2_C Check Low Ueq as Compared to Neighbors for C9
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.0072 Ang

Datablock a - ellipsoid plot