

## Supplementary Information

### **New method for C-H arylation/alkylation at $\alpha$ -position of cyclic aliphatic ethers by iron-oxide mediated reaction**

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## 1.0 Tables

### 1.1 Table 5: containing chemical shift value of CH-Ar & CH-Alkyl

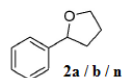
S. No.	Entry	$\delta$ CH-Ar & CH-Alkyl ( $^1\text{H}$ NMR)	C-Ar & CH-Alkyl $^{13}\text{C}$ NMR	C-Ar & CH-Alkyl DEPT
1	2a, b & n	4.70-4.72 (t)	74.27	74.29
2	2c, d & o	4.66-4.70 (dd)	73.72	73.41
3	2e	4.92-4.95 (t)	70.28	70.27
4	2f	4.69-4.72 (t)	74.20	74.19
5	2g & p	4.65-4.68 (t)	73.99	73.99
6	2h & q	4.70-4.73 (t)	74.12	74.15
7	2i	4.70-4.73 (t)	73.32	73.37
8	2j	4.70-4.73 (dd)	73.45	73.45
9	2k	4.68-4.70 (t)	73.02	73.03
10	2l	5.46 (brn),	71.38	69.91
11	2m	4.72-4.74 (m)	70.51	70.52
12	2r	3.62-3.64 (m, signal merged with other peak)	71.97	71.93
13	2s	3.62-3.64 (m, signal merged with other peak)	71.96	71.94
14	2t	3.68-3.77 (m, signal merged with other peak)	71.97	71.98
15	2u	3.47-3.58 (m)	75.08	75.11
16	6/7a & e	4.68-4.75 (m) for <b>6a/e</b>	73.83 ( <b>6a/e</b> ), 74.18 ( <b>7a/e</b> )	73.90 ( <b>6a/e</b> )
17	6/7b & f	4.62-4.69 (m) for <b>6b/f</b>	73.59 ( <b>6b/f</b> ), 73.93 ( <b>7b/f</b> )	73.59 ( <b>6b/f</b> )
18	6/7c & g	5.47-5.54 (m) for <b>6c/g</b>	70.47 ( <b>6c/g</b> ), 75.81 ( <b>7c/g</b> )	70.47 ( <b>6c/g</b> )
19	6/7d & h	4.68-4.71 (m) for <b>6d/h</b>	73.24 ( <b>6d/h</b> ), 73.86 ( <b>7d/h</b> )	73.24 ( <b>6d/h</b> )
20	4a & e	4.66-4.69 (t)	74.29	74.31
21	4b & f	4.59-4.63 (m)	73.92	73.67
22	4c & g	5.42-5.45 (m)	71.50	71.60
23	4d & h	4.60-4.64 (t)	73.65	73.66
24	1l	4.61-4.88 (q)	69.86	69.87

Table 5: Chemical shift value of CH-Ar & CH-Alkyl

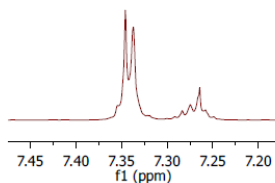
## 2.1 Scanned spectra of compounds:

### <sup>1</sup>H NMR for tetrahydro-2-phenylfuran in CDCl<sub>3</sub> (Table 2, entry a, b and n)

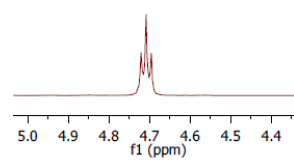
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BER



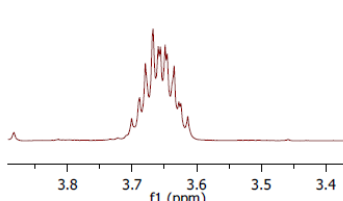
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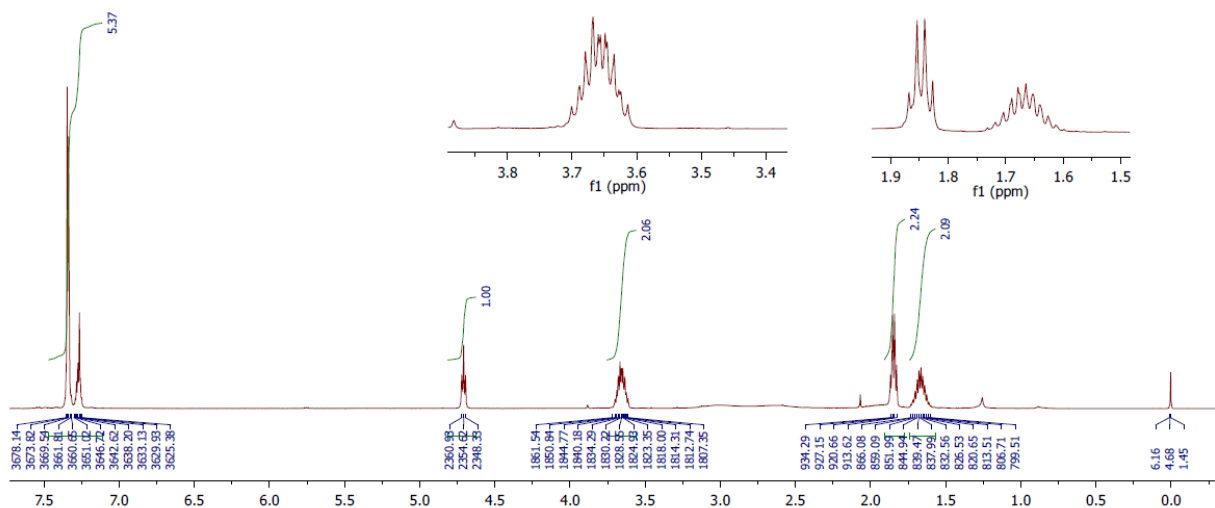
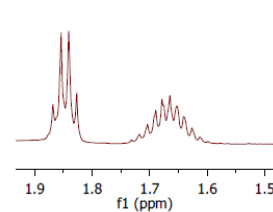
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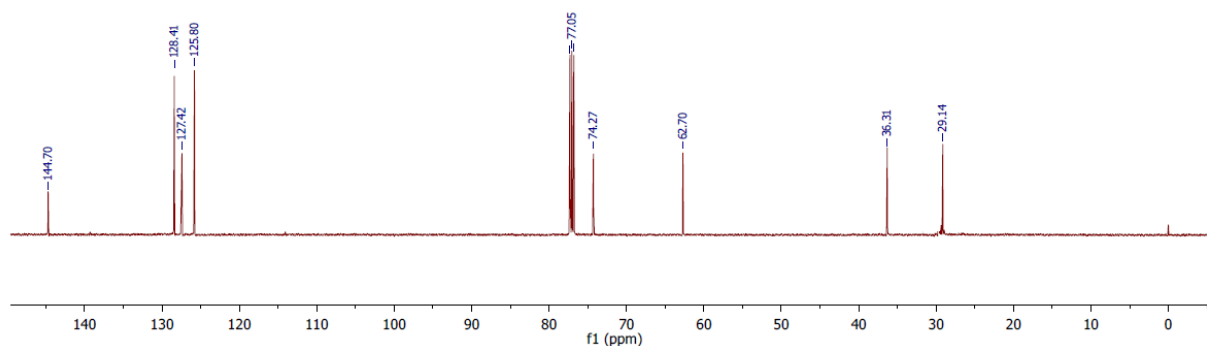
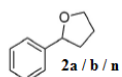


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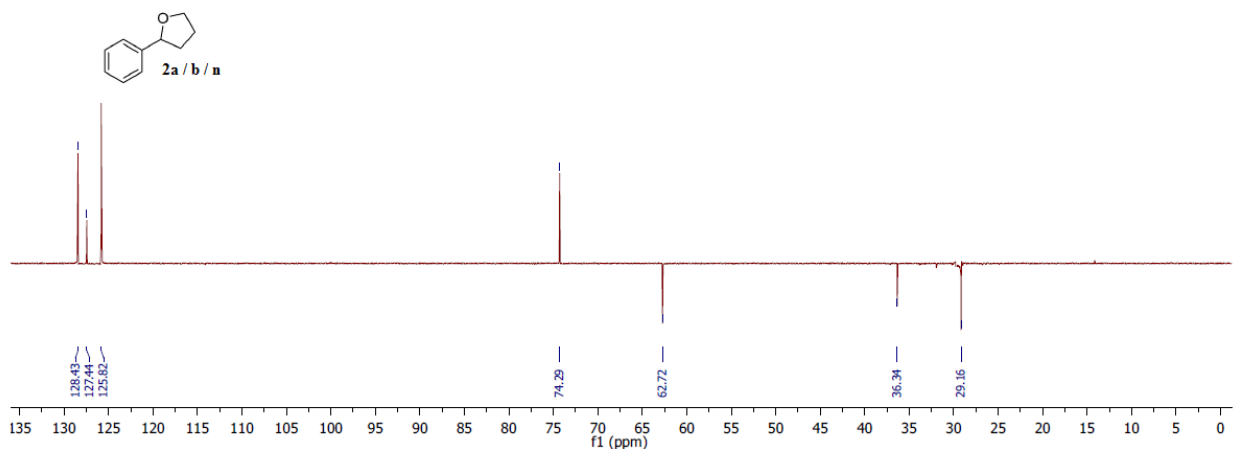
### <sup>13</sup>C NMR for tetrahydro-2-phenylfuran in CDCl<sub>3</sub> (Table 2, entry a, b and n)

Oct19-2010-purnima  
Br

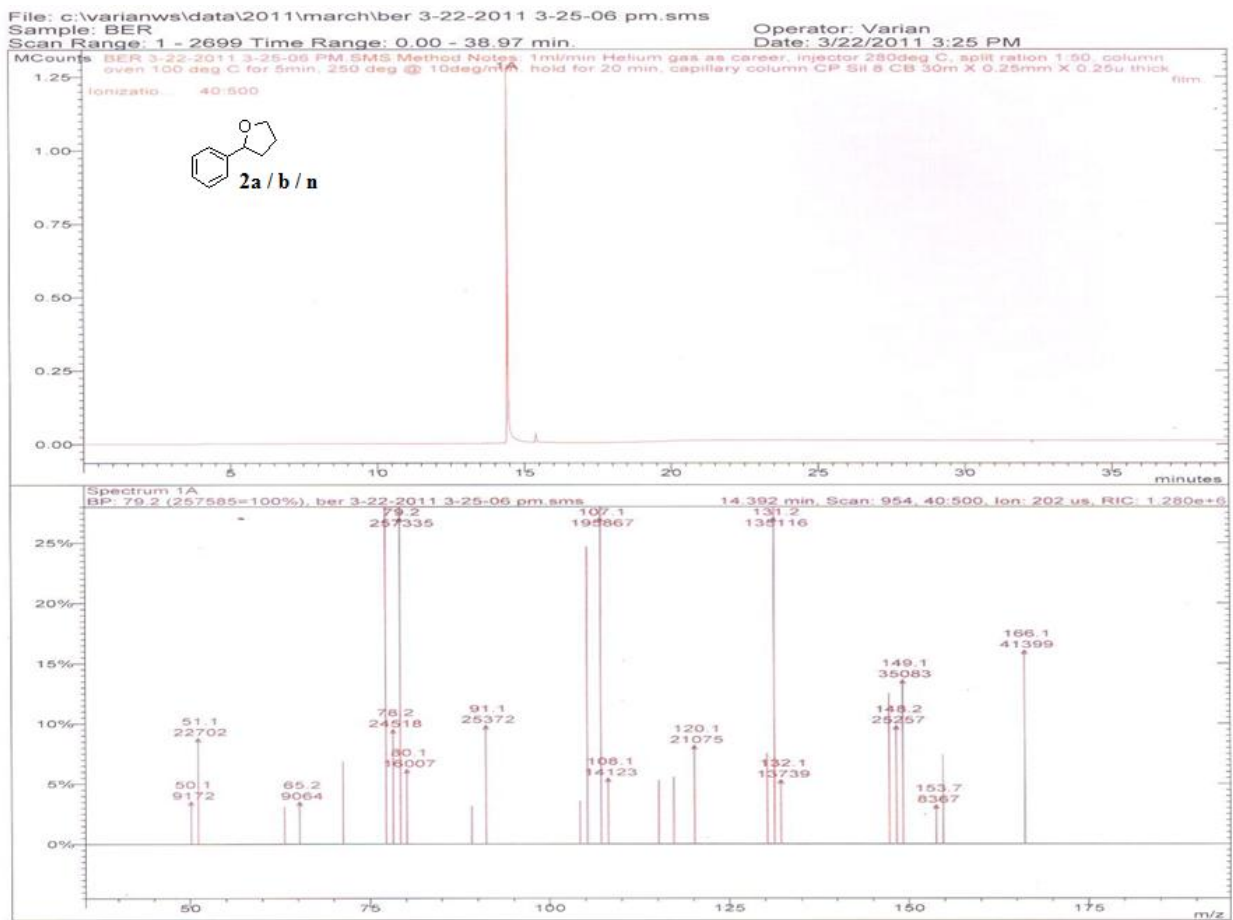


## DEPT at 135 for tetrahydro-2-phenylfuran in CDCl<sub>3</sub> (Table 2, entry a, b and n)

Oct19-2010-purnima  
3r



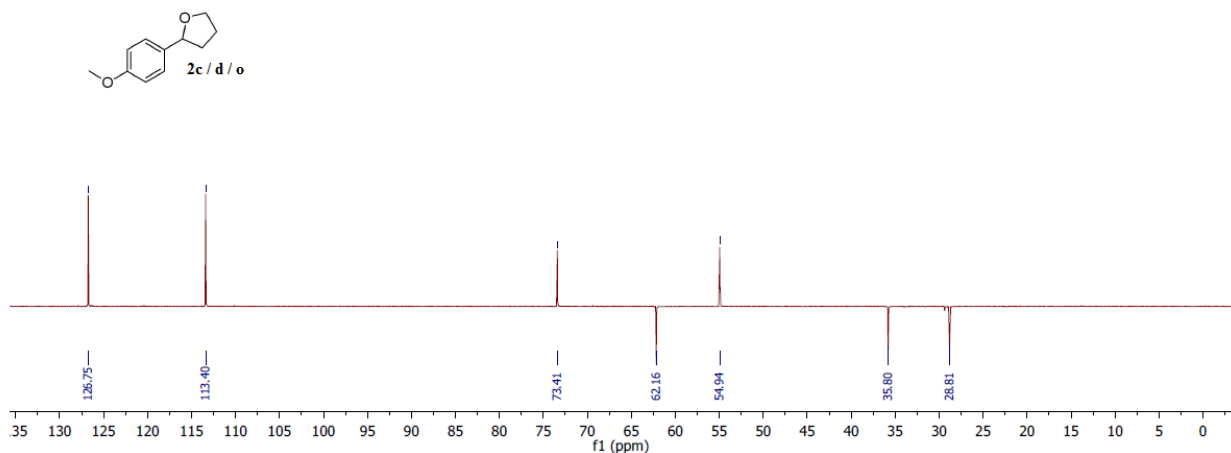
## GCMS for tetrahydro-2-phenylfuran (Table 2, entry a, b and n)



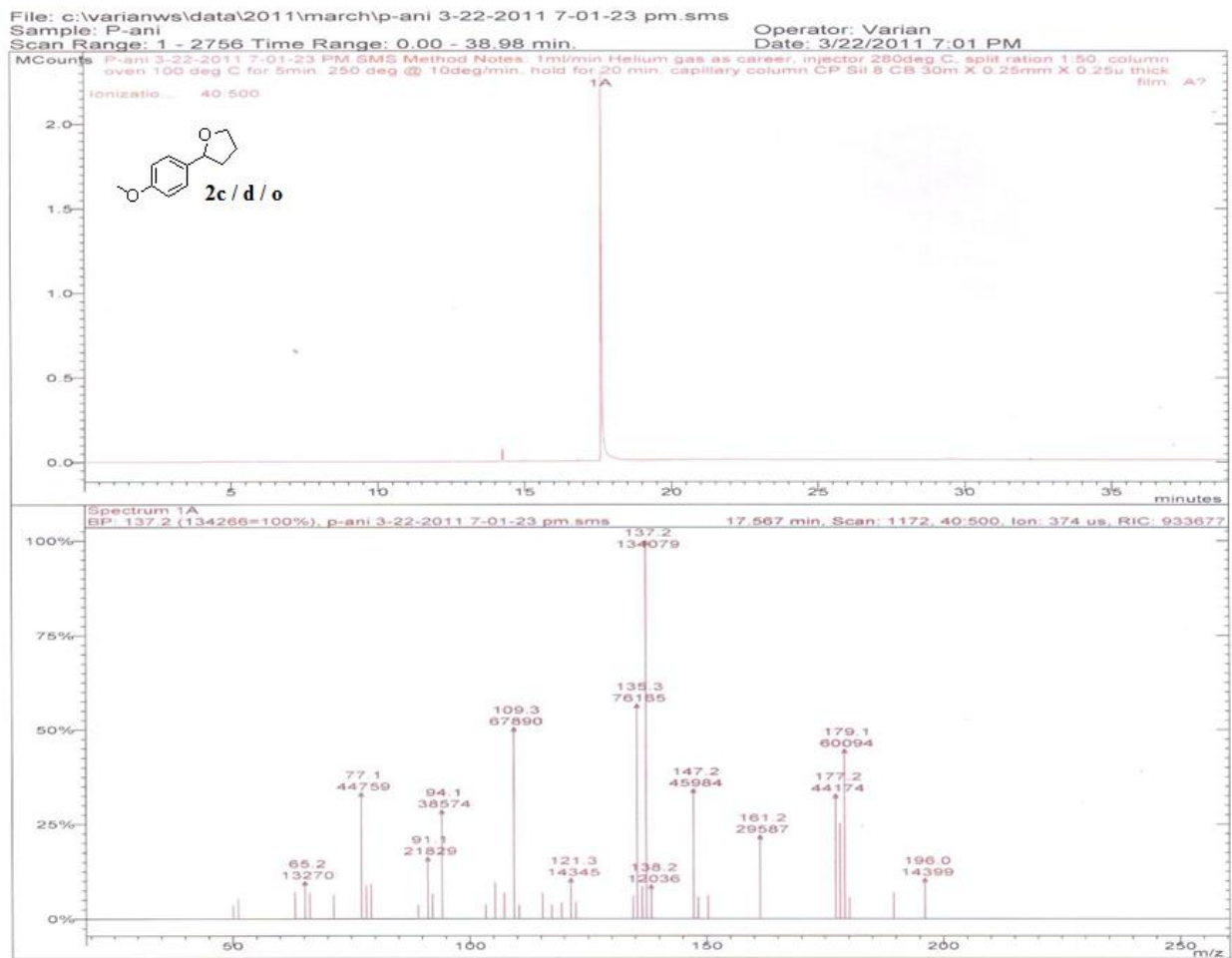


## DEPT at 135 for tetrahydro-2-(4-methoxyphenyl)furan in CDCl<sub>3</sub> (Table 2, entry c, d and o)

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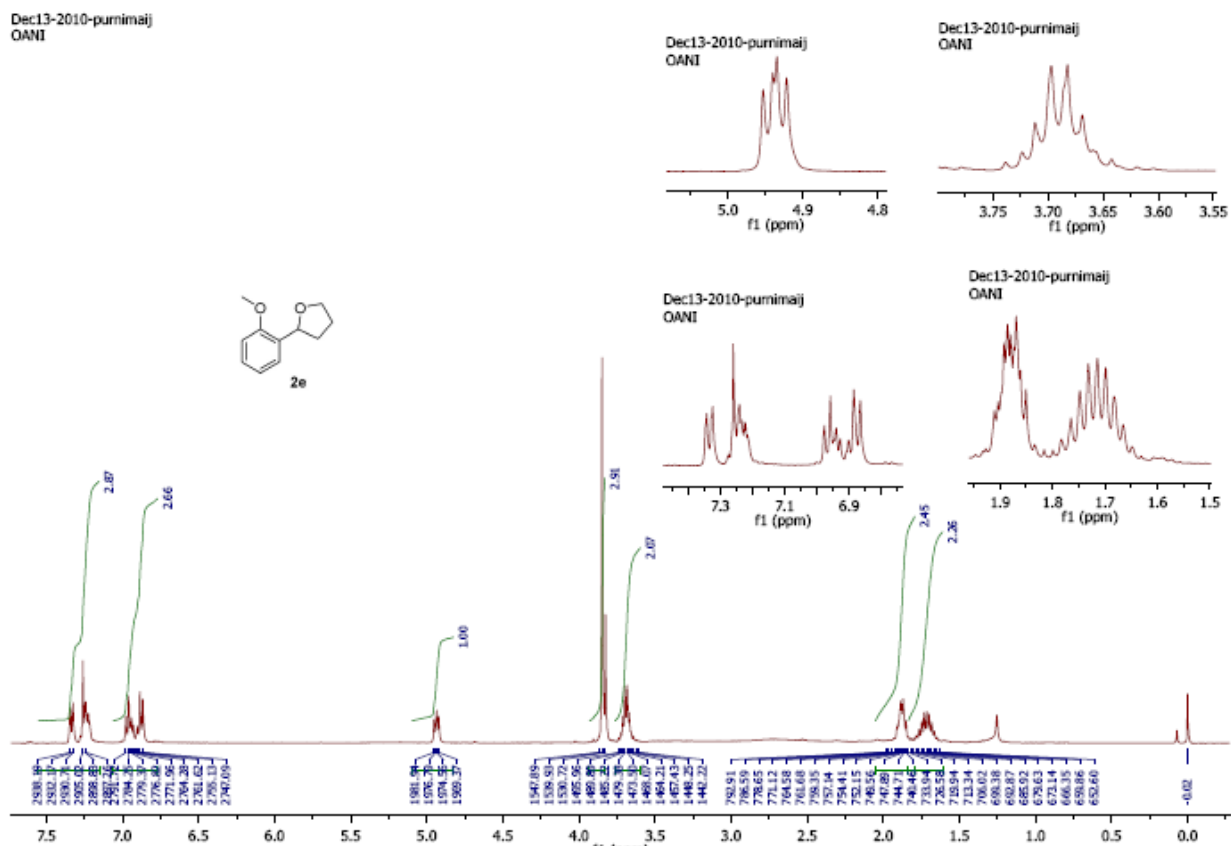


## GCMS for tetrahydro-2-(4-methoxyphenyl)furan (Table 2, entry c, d and o)



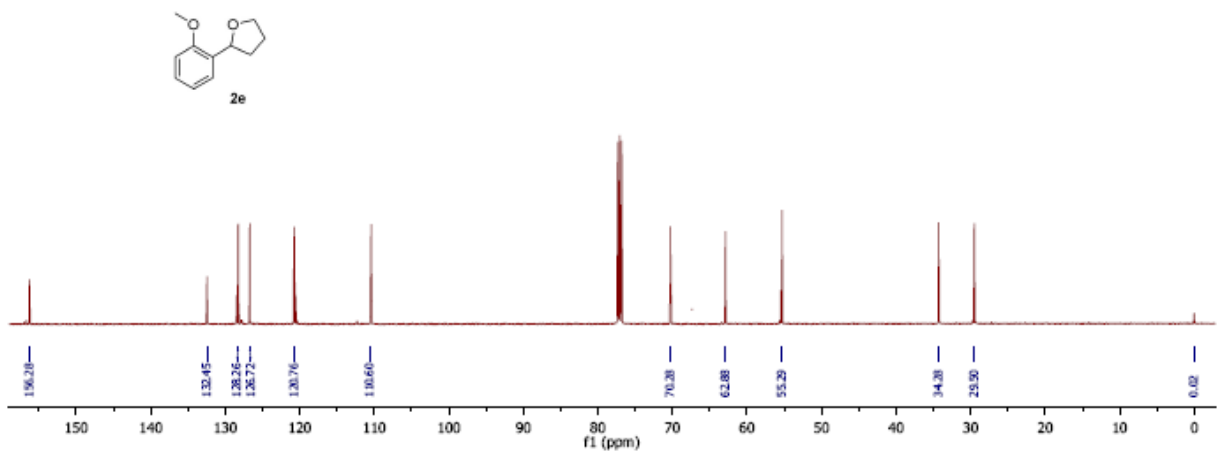
# **<sup>1</sup>H NMR for tetrahydro-2-(2-methoxyphenyl)furan in CDCl<sub>3</sub> (Table 2, entry e)**

Dec13-2010-pumimaj  
OANI



# **<sup>13</sup>C NMR for tetrahydro-2-(2-methoxyphenyl)furan in CDCl<sub>3</sub> (Table 2, entry e)**

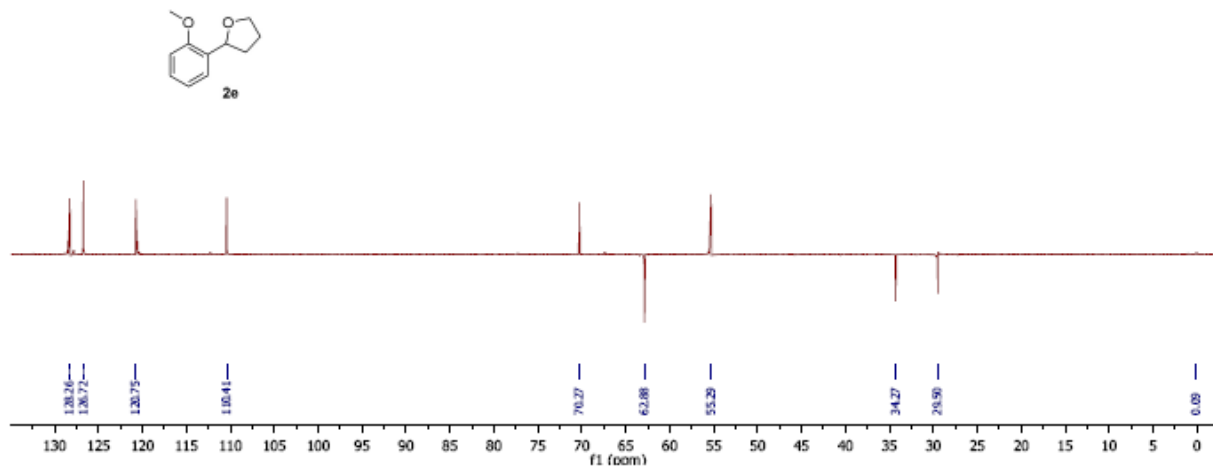
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OANI





## DEPT at 135 for tetrahydro-2-(2-methoxyphenyl)furan in CDCl<sub>3</sub> (Table 2, entry e)

Jan28-2011-pumima  
QANI



## GCMS for tetrahydro-2-(2-methoxyphenyl)furan (Table 2, entry e)

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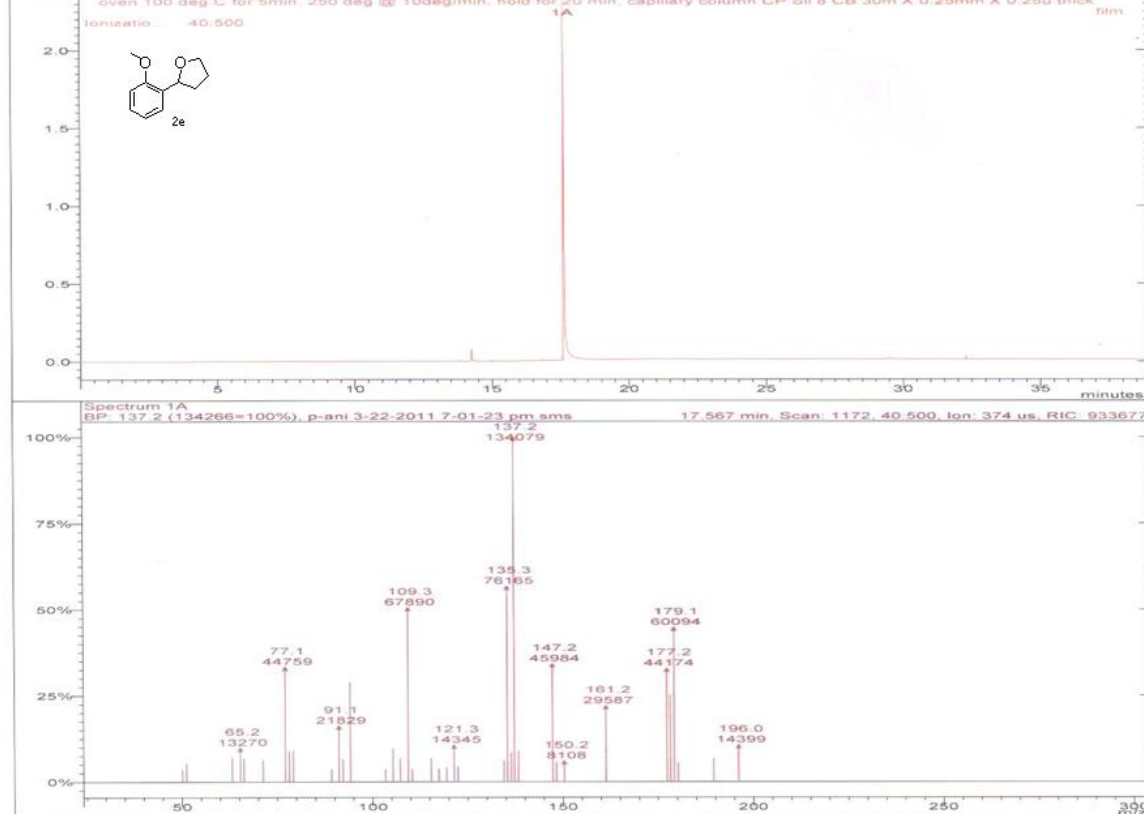
Sample: 6-ani

Operator: Varian

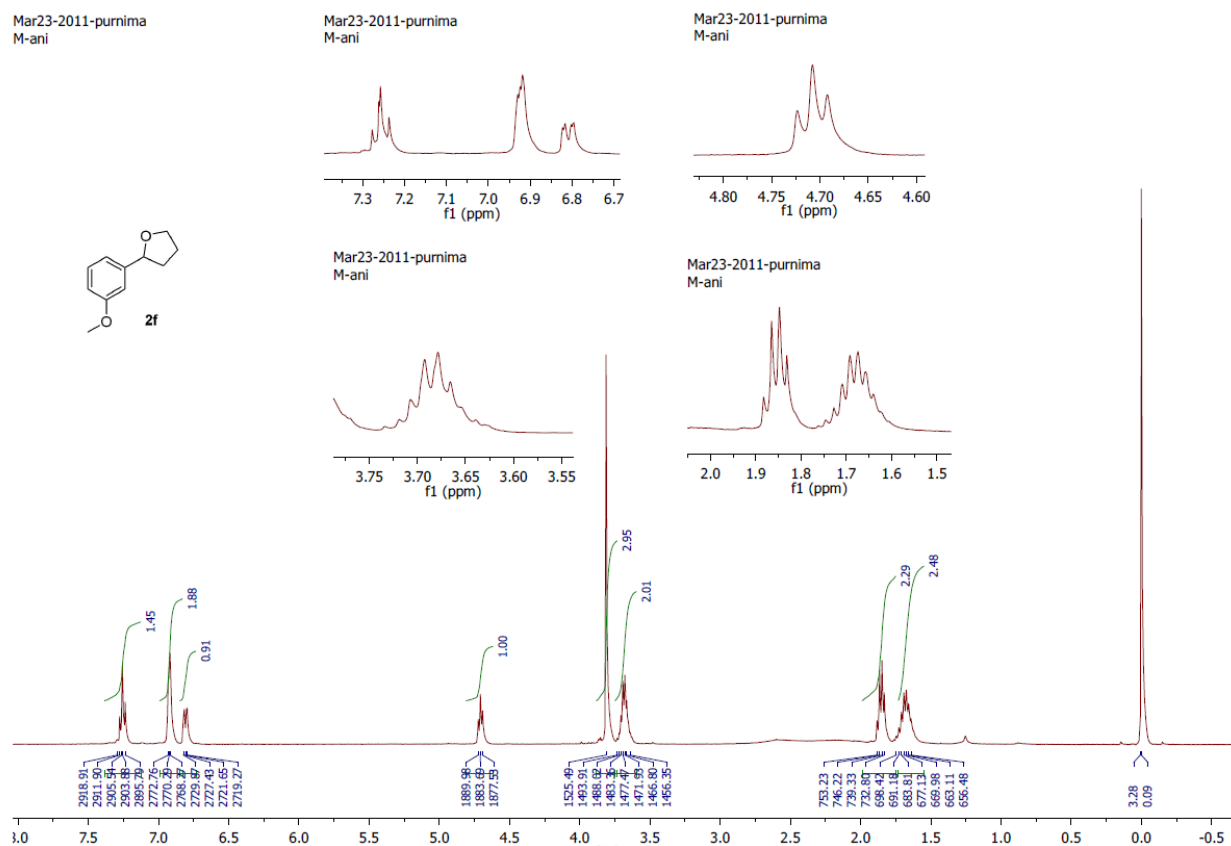
Date: 3/22/2011 7:01 PM

Scan Range: 1 - 2756 Time Range: 0.00 - 38.98 min.

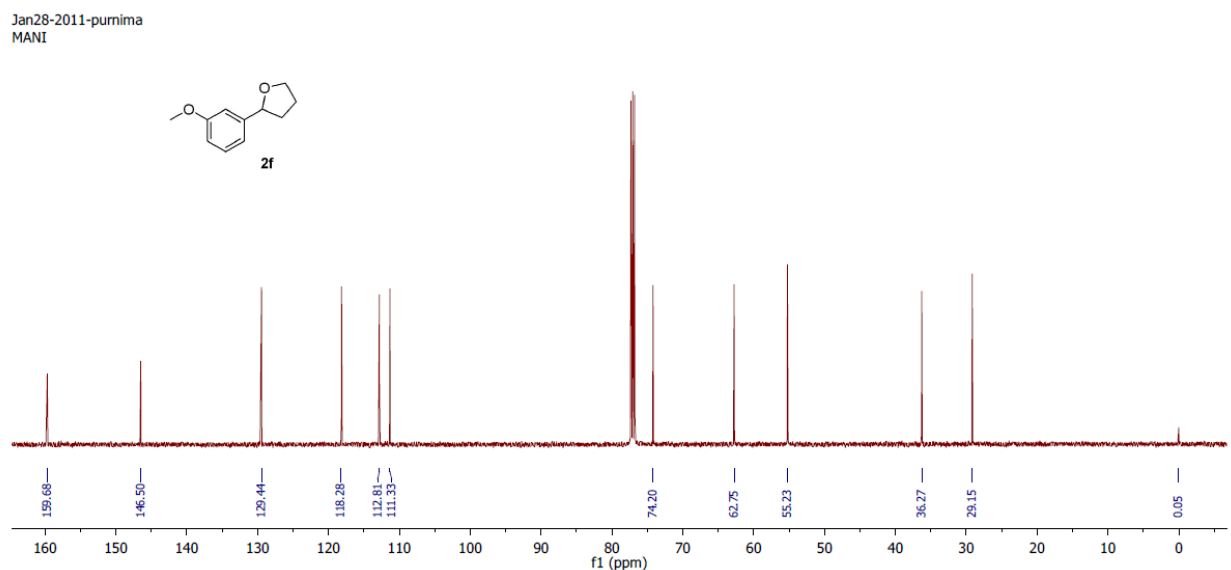
Method: P-ani 3-22-2011 7-01-23 PM SMS Method Notes: 1ml/min Helium gas as carrier, injector 250deg C, split ratio 1:50, column oven 100 deg C for 5min, 250 deg @ 10deg/min, hold for 20 min, capillary column CP Sil 8 CB 30m X 0.25mm X 0.25u thick.



# <sup>1</sup>H NMR for tetrahydro-2-(3-methoxyphenyl)furan in CDCl<sub>3</sub> (Table 2, entry f)

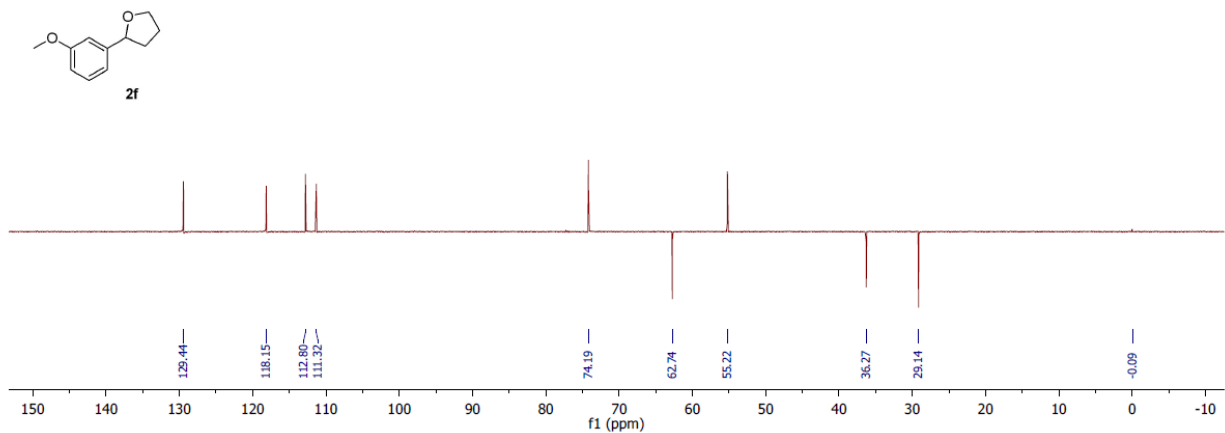


# <sup>13</sup>C NMR for tetrahydro-2-(3-methoxyphenyl)furan in CDCl<sub>3</sub> (Table 2, entry f)

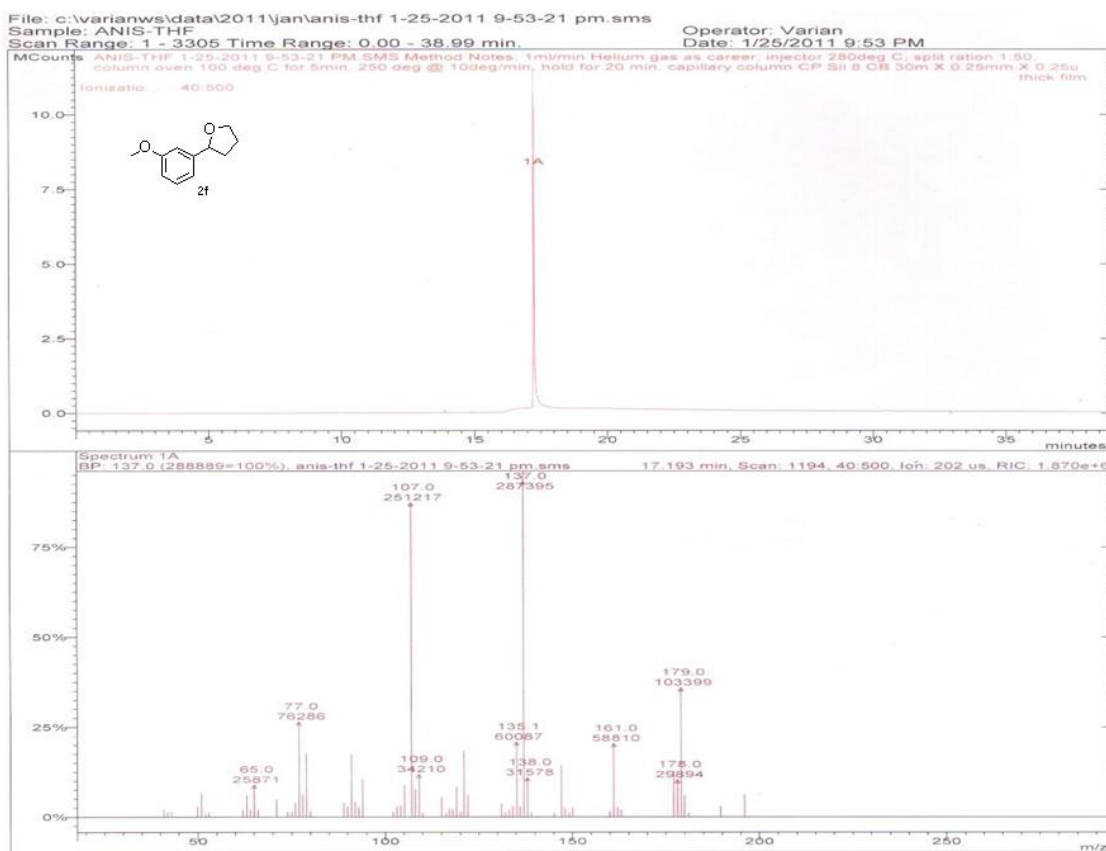


## DEPT at 135 for tetrahydro-2-(3-methoxyphenyl)furan in CDCl<sub>3</sub> (Table 2, entry f)

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MANI

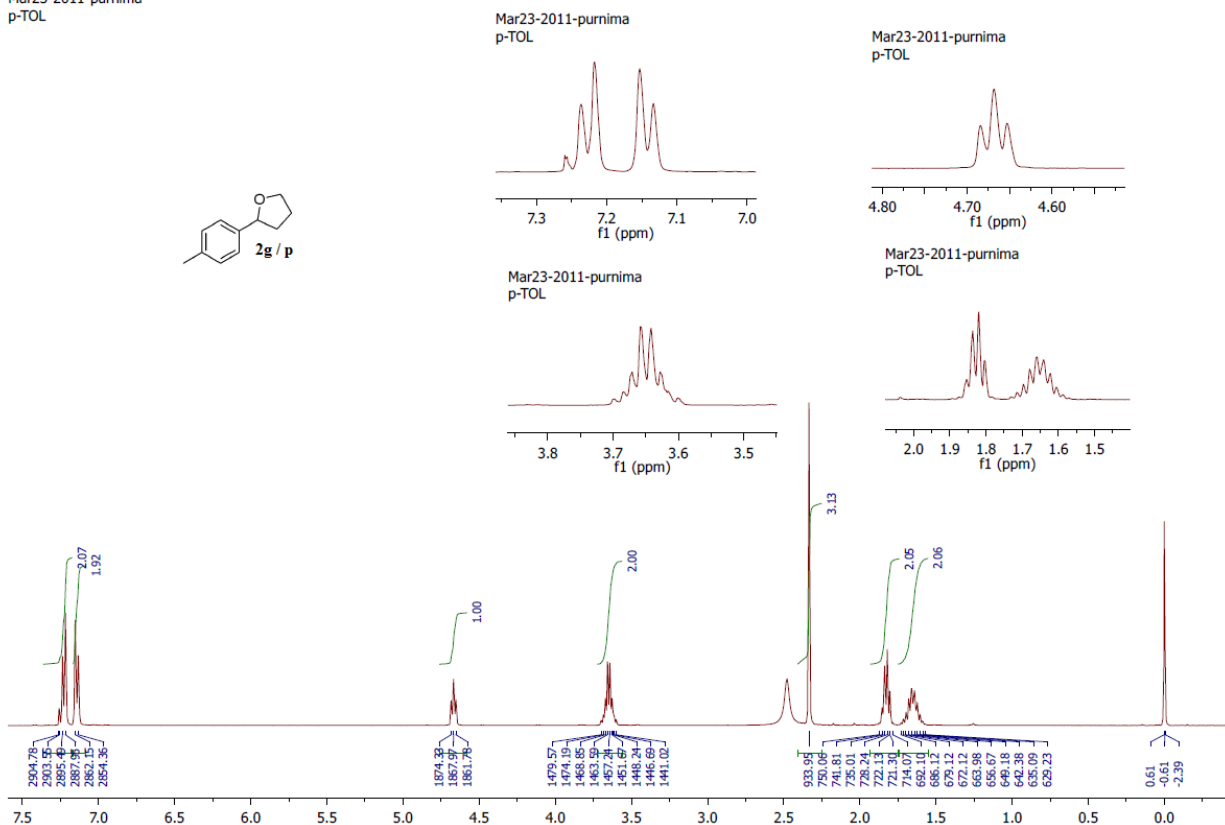
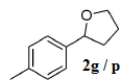


## GCMS for tetrahydro-2-(3-methoxyphenyl)furan (Table 2, entry f)



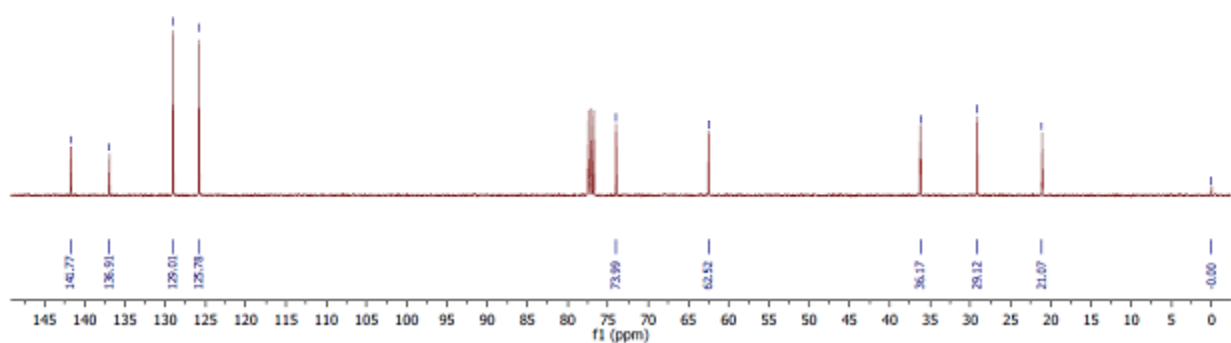
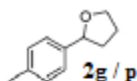
# <sup>1</sup>H NMR for tetrahydro-2-*p*-tolylfuran in CDCl<sub>3</sub> (Table 2, entry g and p)

Mar23-2011-purnima  
p-TOL



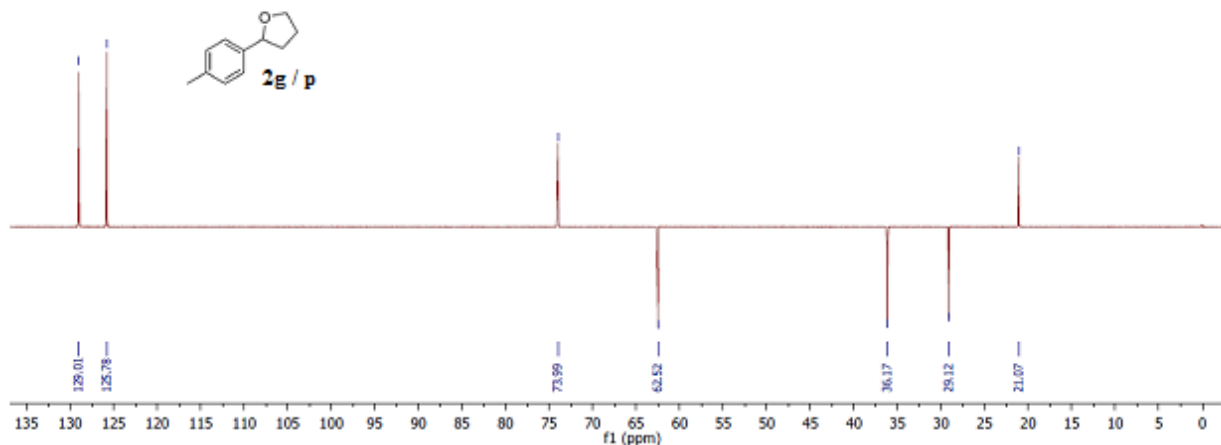
# <sup>13</sup>C NMR for tetrahydro-2-*p*-tolylfuran in CDCl<sub>3</sub> (Table 2, entry g and p)

Mar23-2011-purnima  
p-TOL

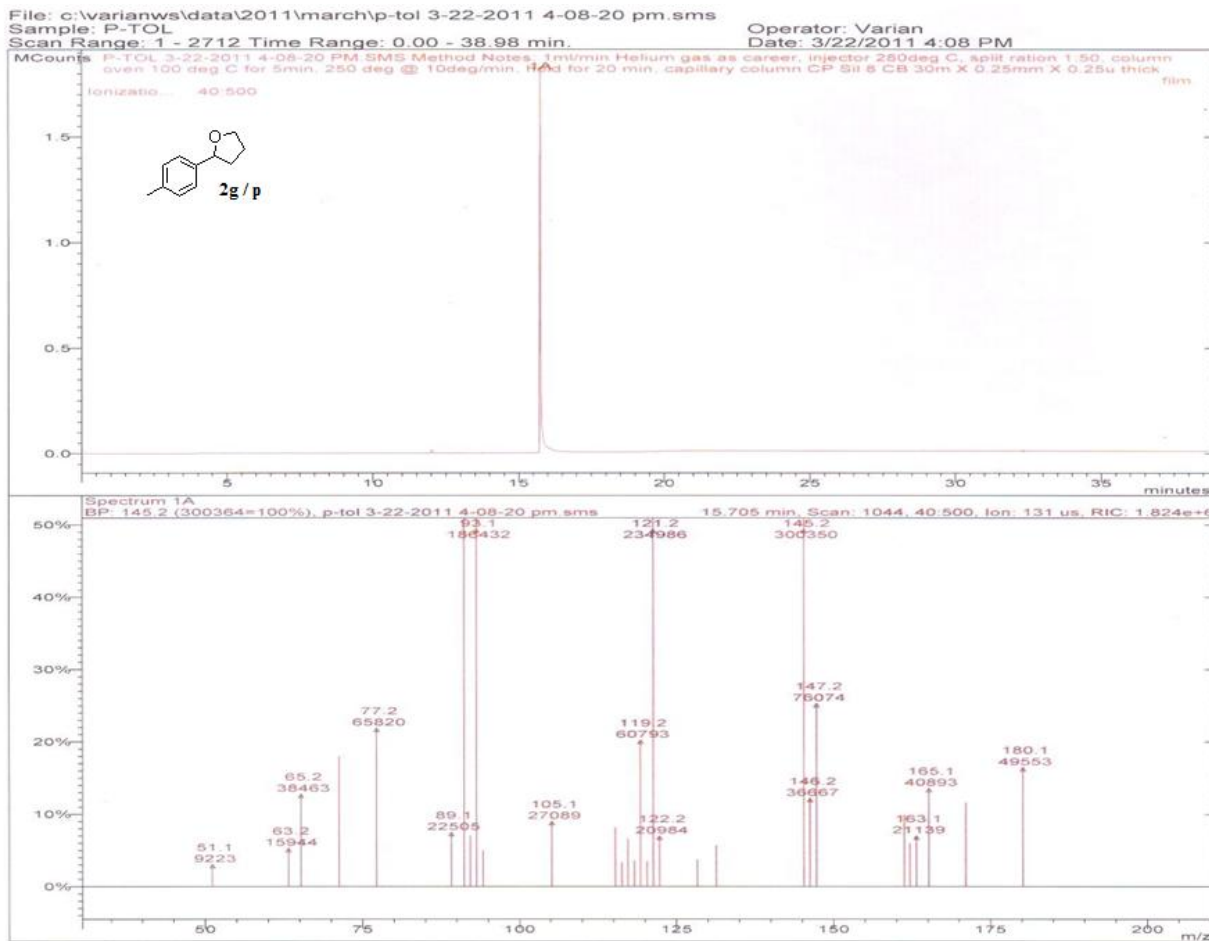


# DEPT at 135 for tetrahydro-2-*p*-tolylfuran in CDCl<sub>3</sub> (Table 2, entry g and p)

Mar23-2011-pumima  
p-TOL

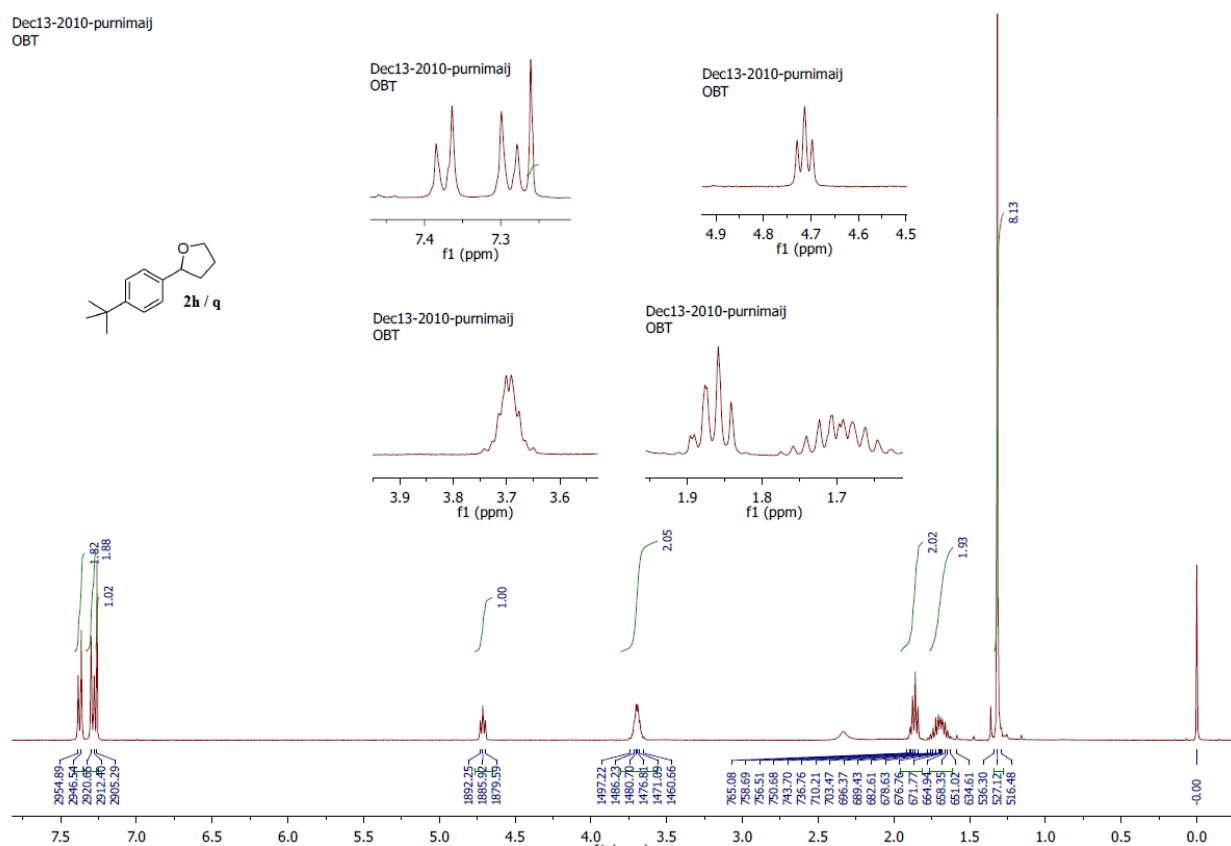


# GCMS for tetrahydro-2-*p*-tolylfuran (Table 2, entry g and p)



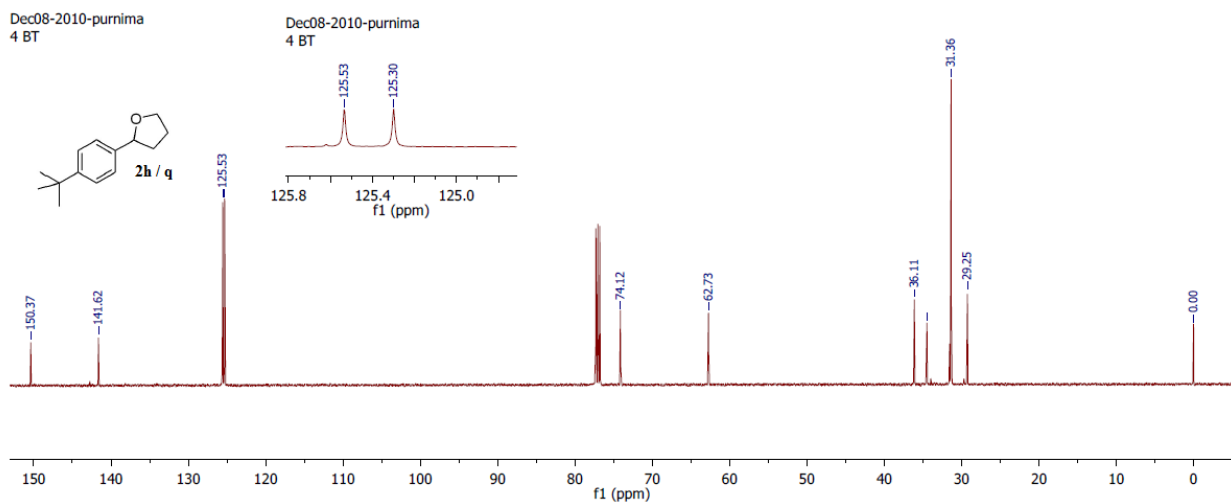
# **<sup>1</sup>H NMR for 2-(4-*tert*-butylphenyl)-tetrahydrofuran in CDCl<sub>3</sub> (Table 2, entry h and q)**

Dec13-2010-purnimaij  
OBT



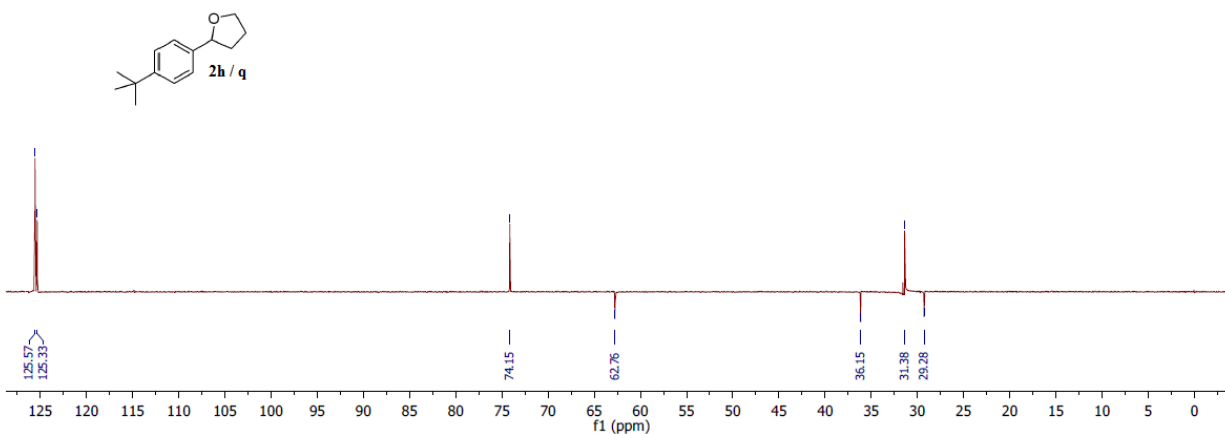
# **<sup>13</sup>C NMR for 2-(4-*tert*-butylphenyl)-tetrahydrofuran in CDCl<sub>3</sub> (Table 2, entry h and q)**

Dec08-2010-purnima  
4 BT

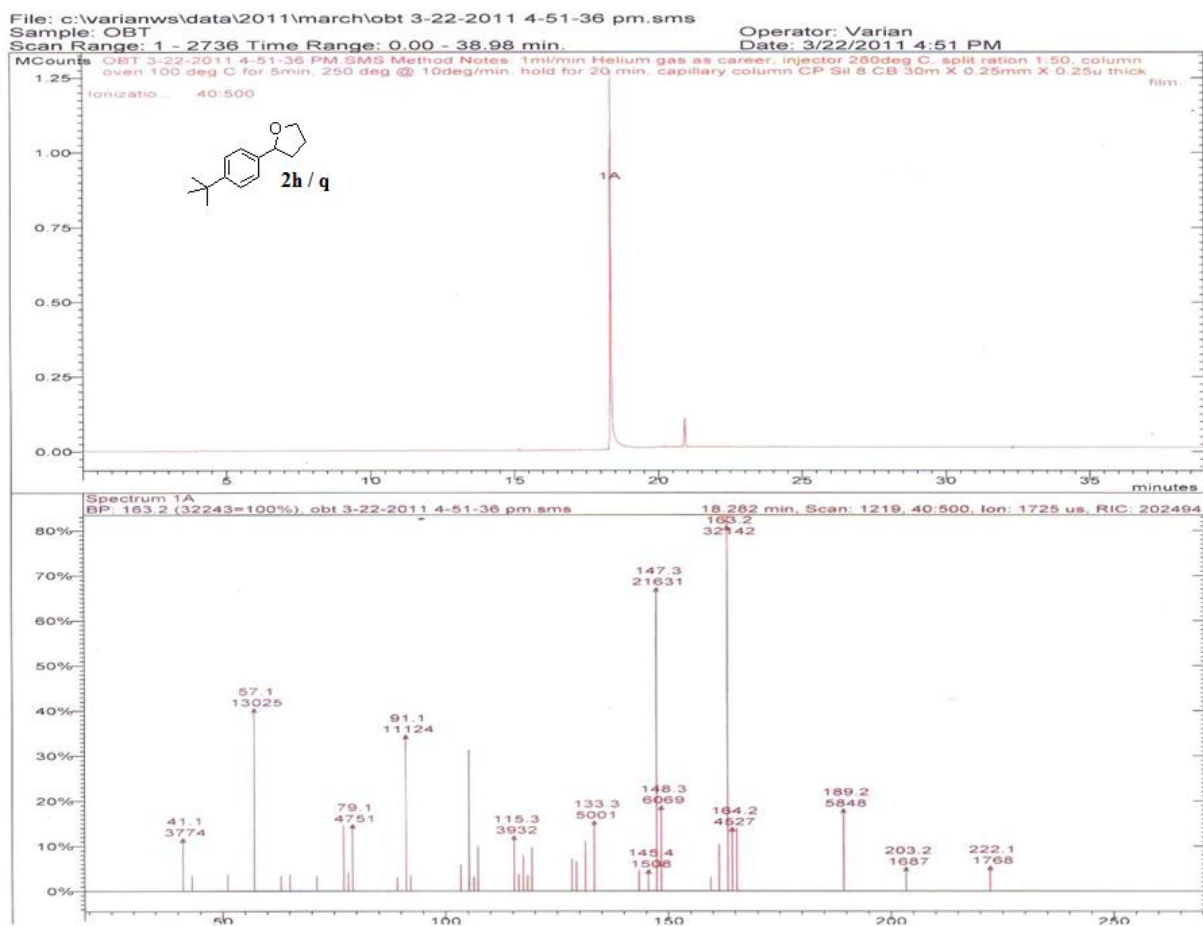


# DEPT at 135 for 2-(4-*tert*-butylphenyl)-tetrahydrofuran in CDCl<sub>3</sub> (Table 2, entry h and q)

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4 BT

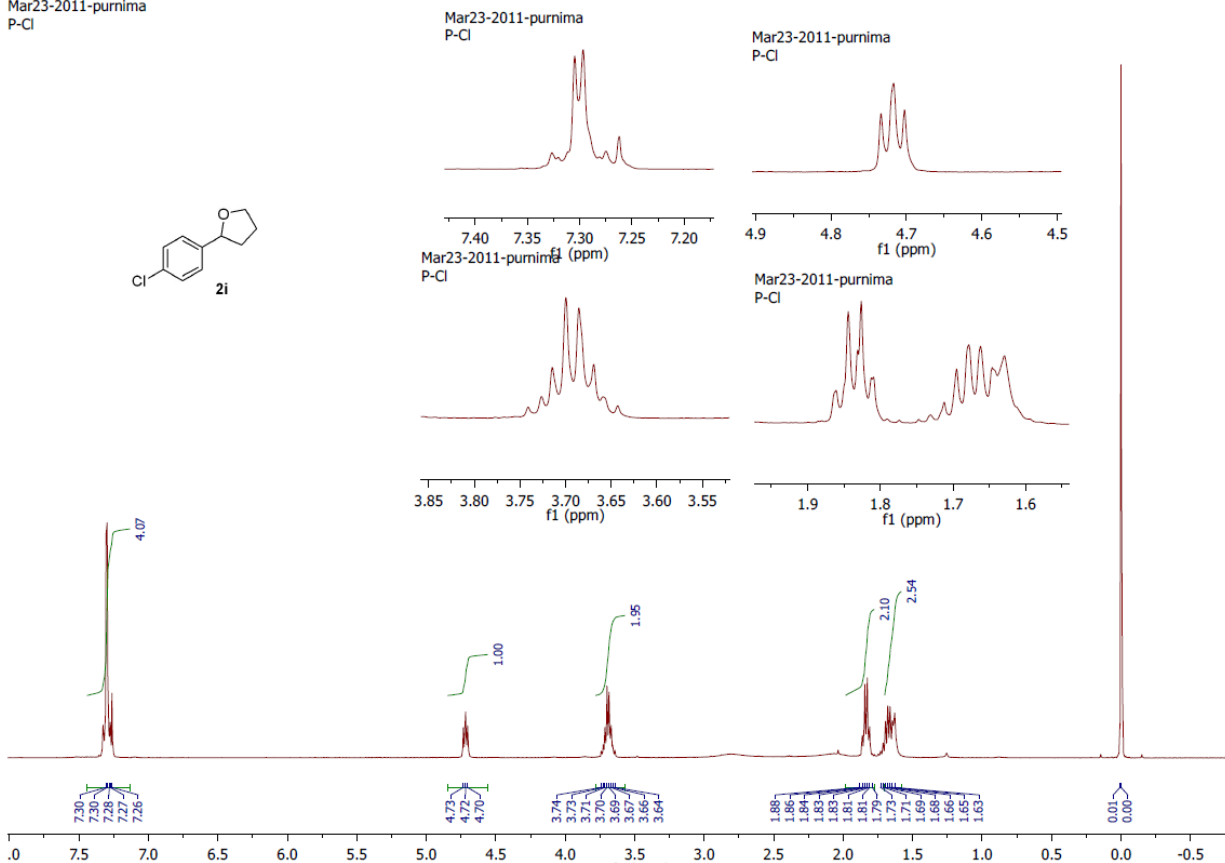


# GCMS for 2-(4-*tert*-butylphenyl)-tetrahydrofuran (Table 2, entry h and q)



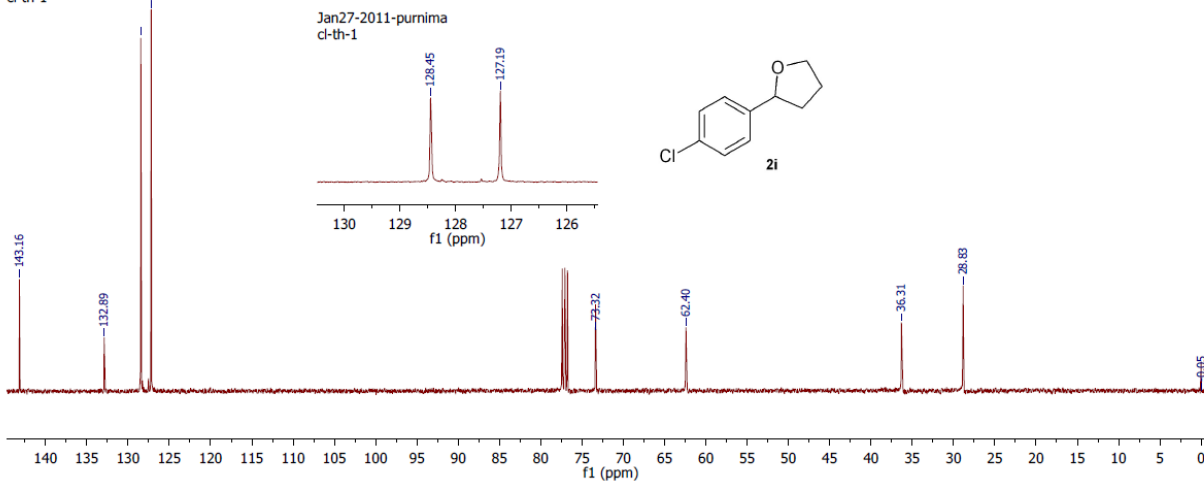
# **<sup>1</sup>H NMR for 2-(4-chlorophenyl)-tetrahydrofuran in CDCl<sub>3</sub> (Table 2, entry i)**

Mar23-2011-purnima  
P-Cl



# **<sup>13</sup>C NMR for 2-(4-chlorophenyl)-tetrahydrofuran in CDCl<sub>3</sub> (Table 2, entry i)**

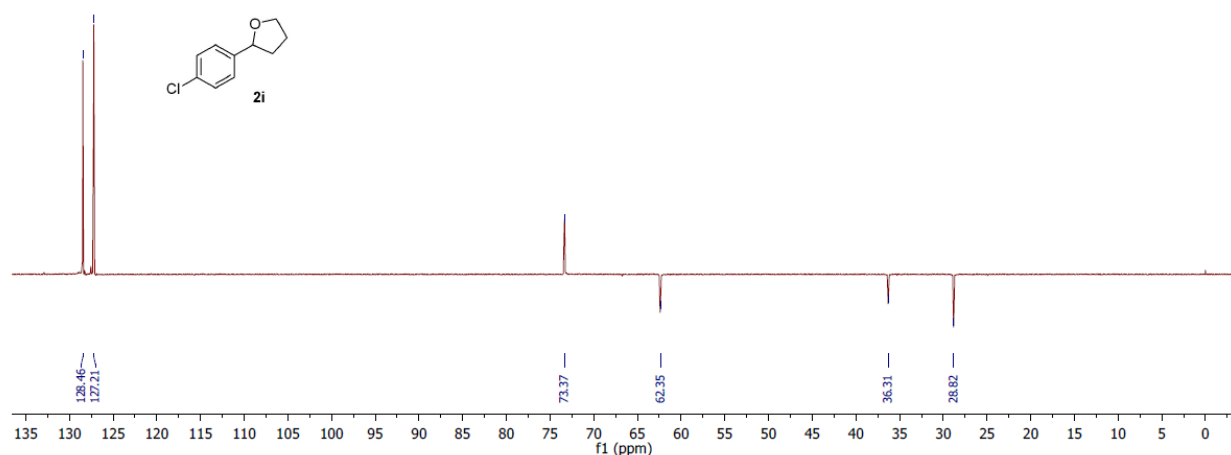
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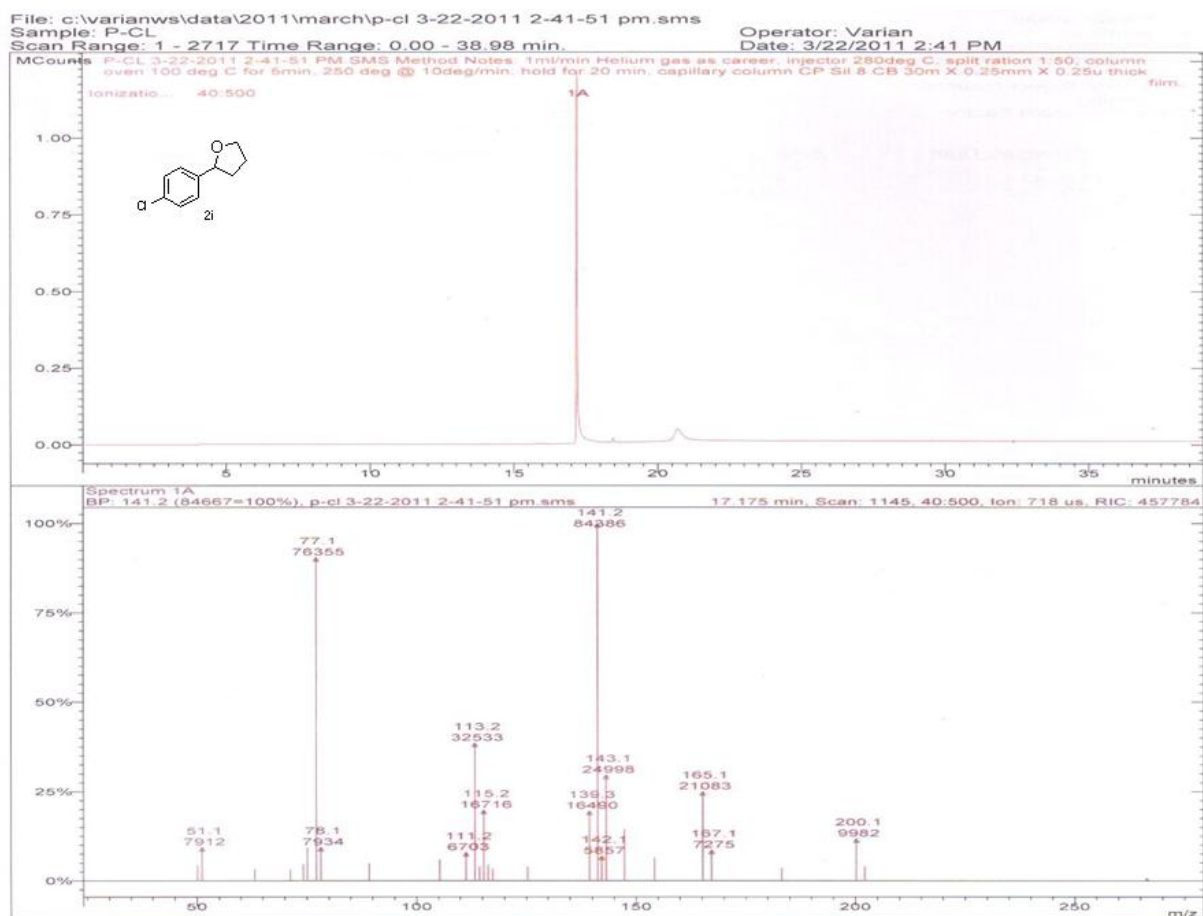


## DEPT at 135 for 2-(4-chlorophenyl)-tetrahydrofuran in CDCl<sub>3</sub> (Table 2, entry i)

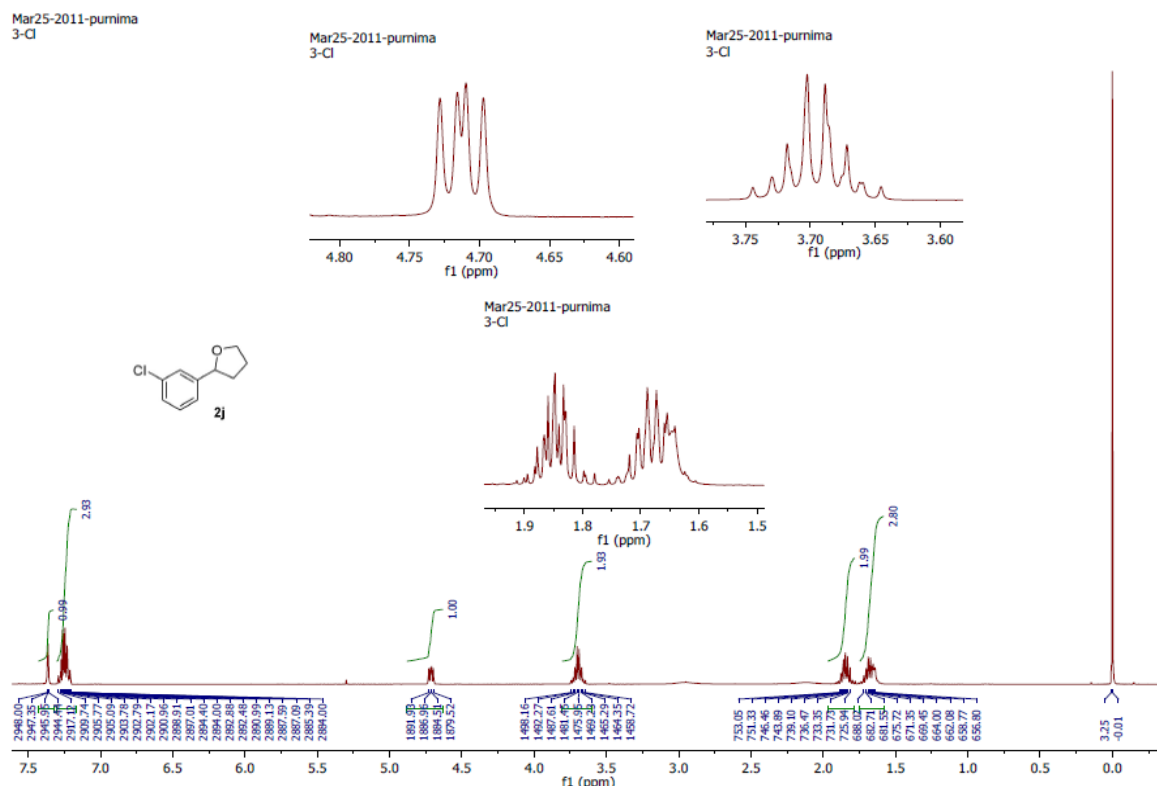
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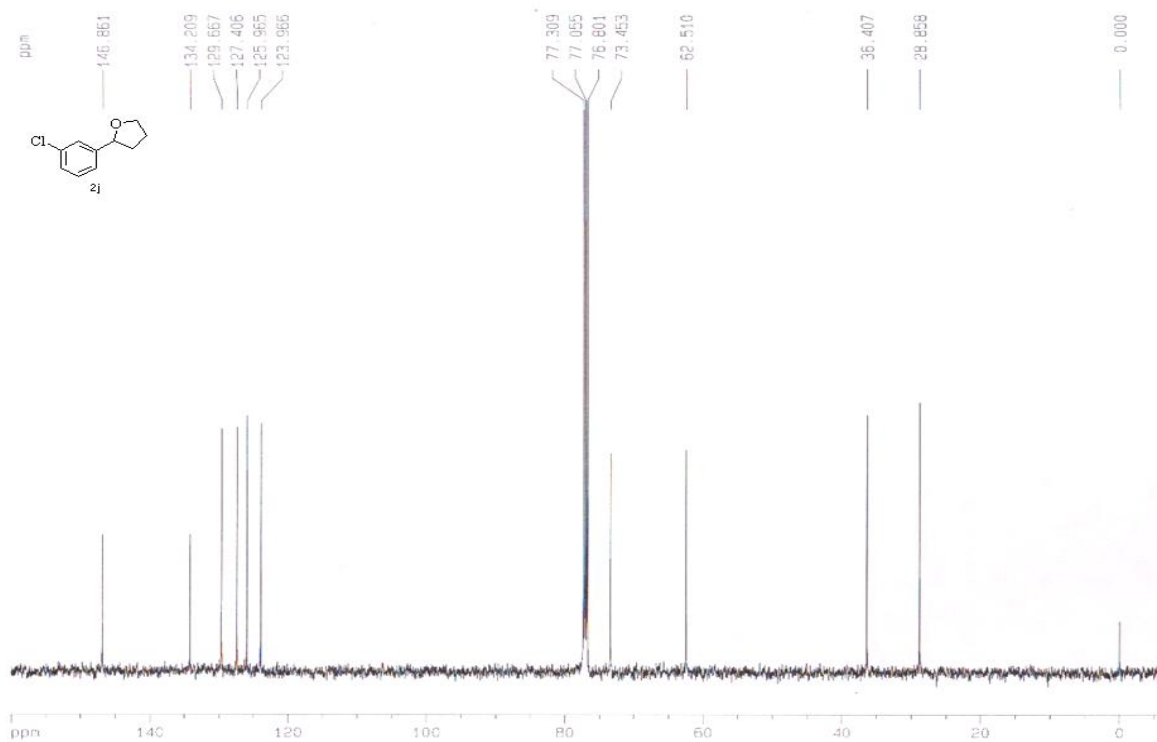
## GCMS for 2-(4-chlorophenyl)-tetrahydrofuran (Table 2, entry i)



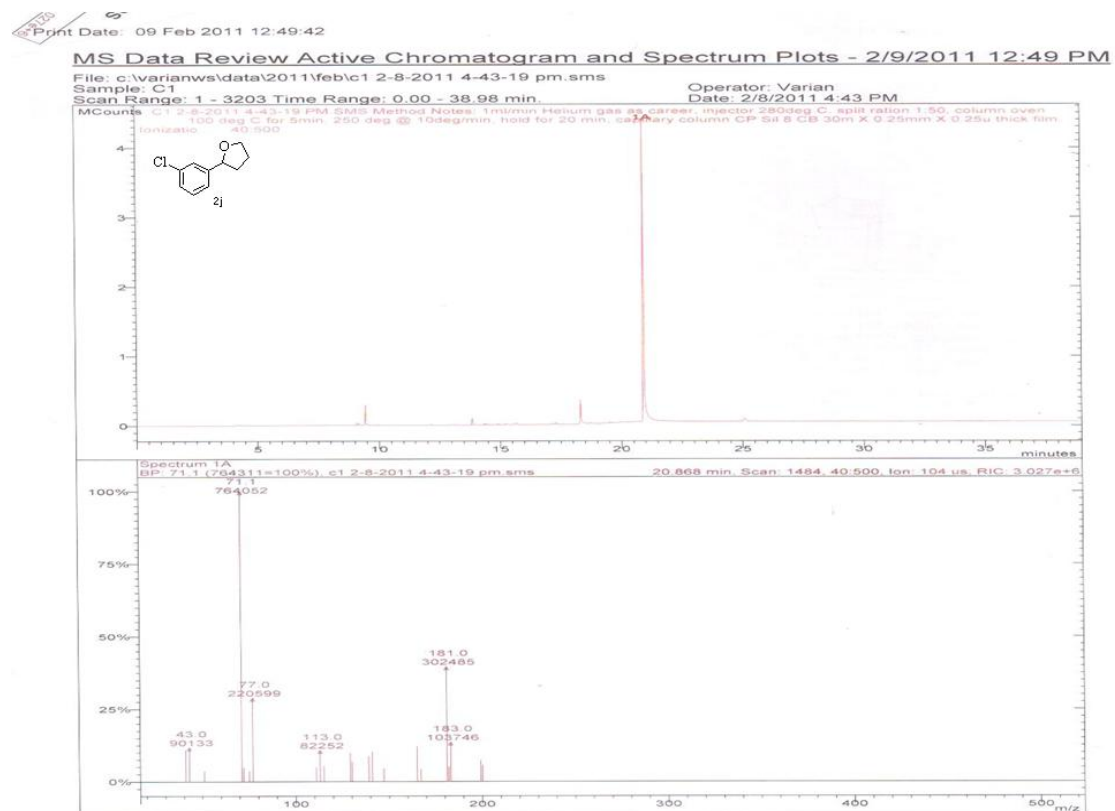
# <sup>1</sup>H NMR for 2-(3-Chlorophenyl)-tetrahydrofuran in CDCl<sub>3</sub> (Table 2, entry j)



# <sup>13</sup>C NMR for 2-(3-Chlorophenyl)-tetrahydrofuran in CDCl<sub>3</sub> (Table 2, entry j)

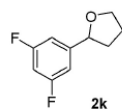


# GCMS for 2-(3-Chlorophenyl)-tetrahydrofuran (Table 2, entry j)

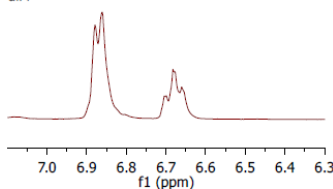


# **<sup>1</sup>H NMR for 2-(3,5-difluorophenyl)-tetrahydrofuran in CDCl<sub>3</sub> (Table 2, entry k)**

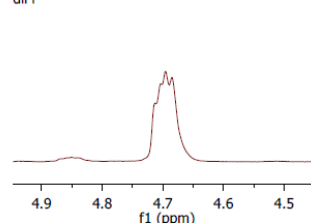
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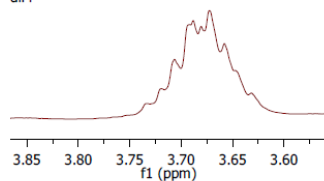
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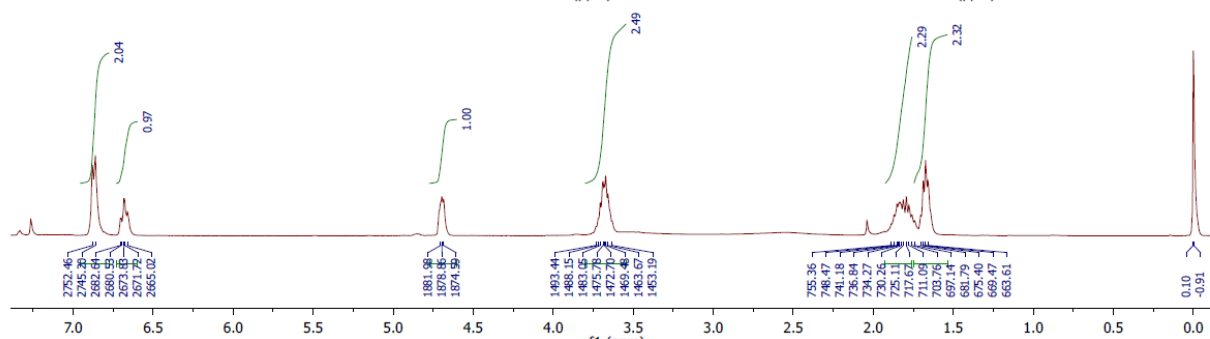
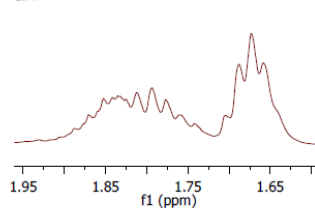
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Mar23-2011-purnima  
dIFI

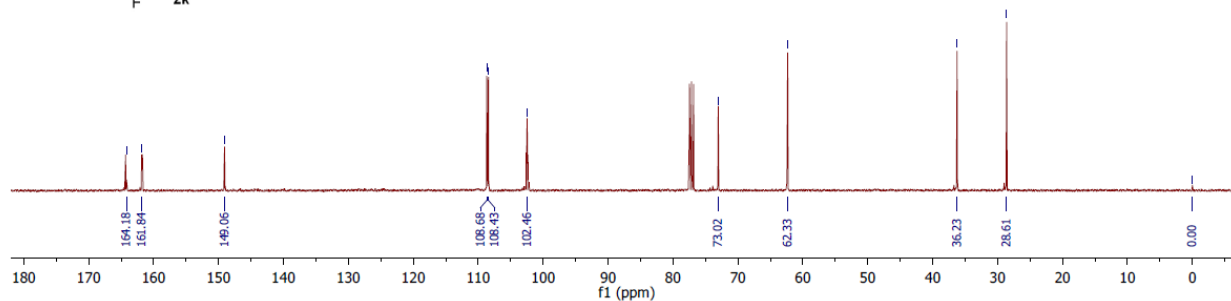
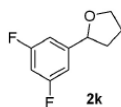


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dIFI



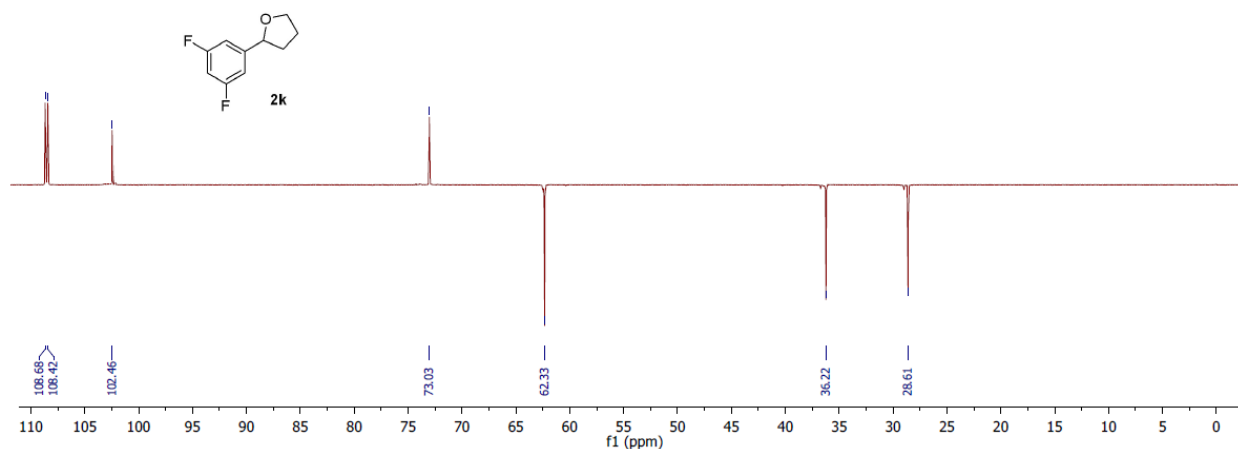
# **<sup>13</sup>C NMR for 2-(3,5-difluorophenyl)-tetrahydrofuran in CDCl<sub>3</sub> (Table 2, entry k)**

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DIFL

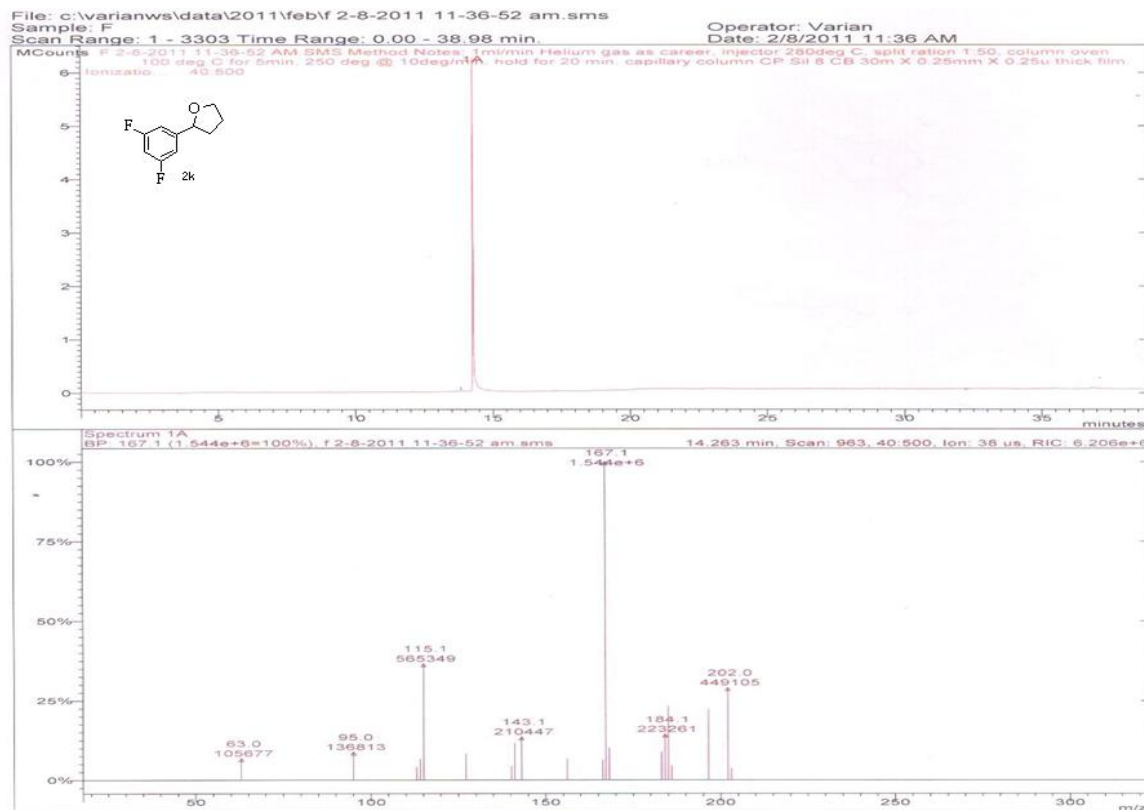


# DEPT at 135 for 2-(3,5-difluorophenyl)-tetrahydrofuran in CDCl<sub>3</sub> (Table 2, entry k)

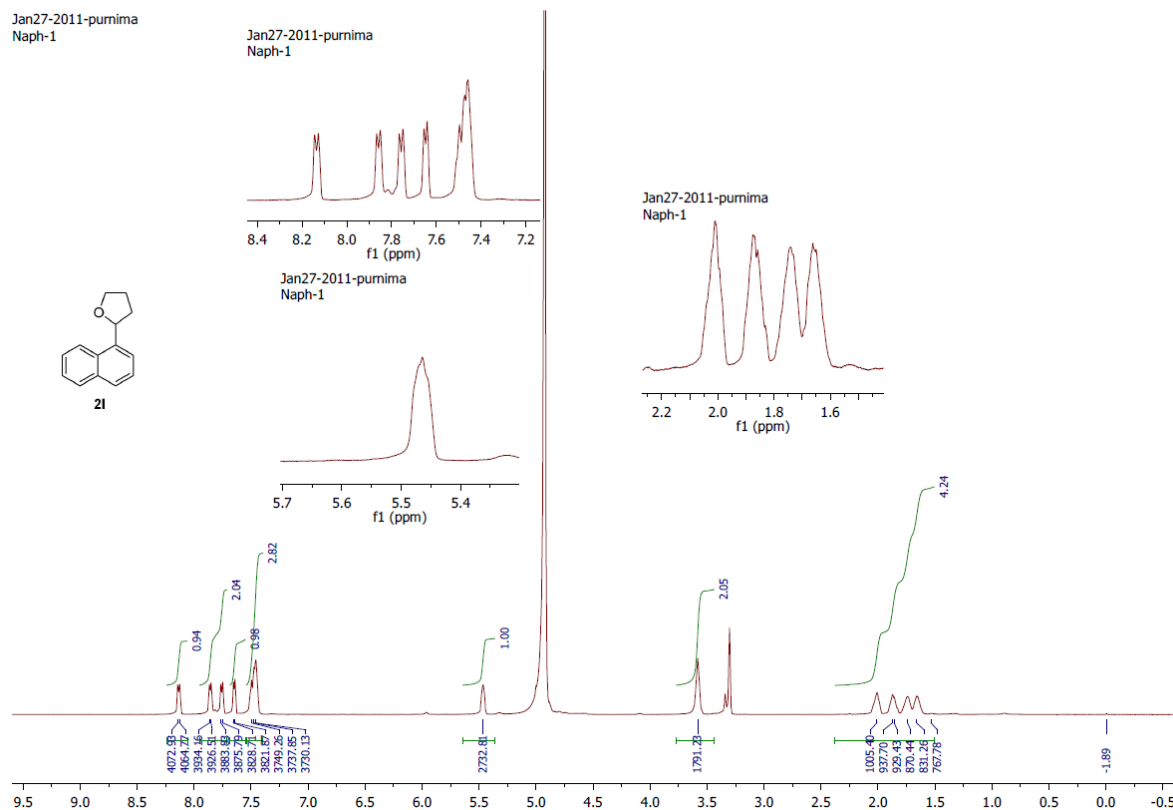
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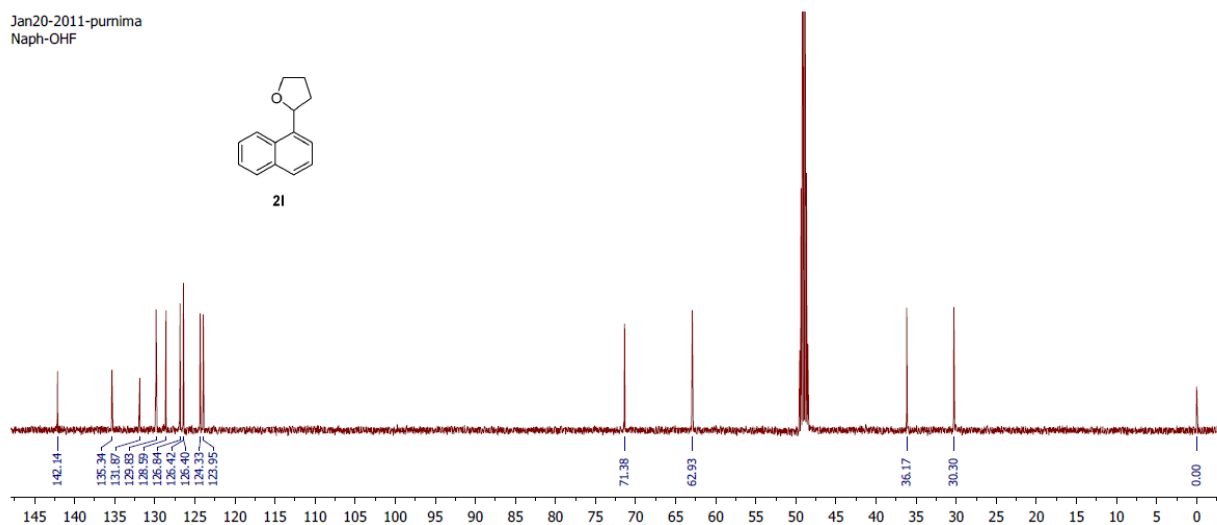
# GCMS for 2-(3,5-difluorophenyl)-tetrahydrofuran (Table 2, entry k)



# **<sup>1</sup>H NMR for tetrahydro-2-(naphthalen-4-yl)furan in CD<sub>3</sub>OD (Table 2, entry 1)**

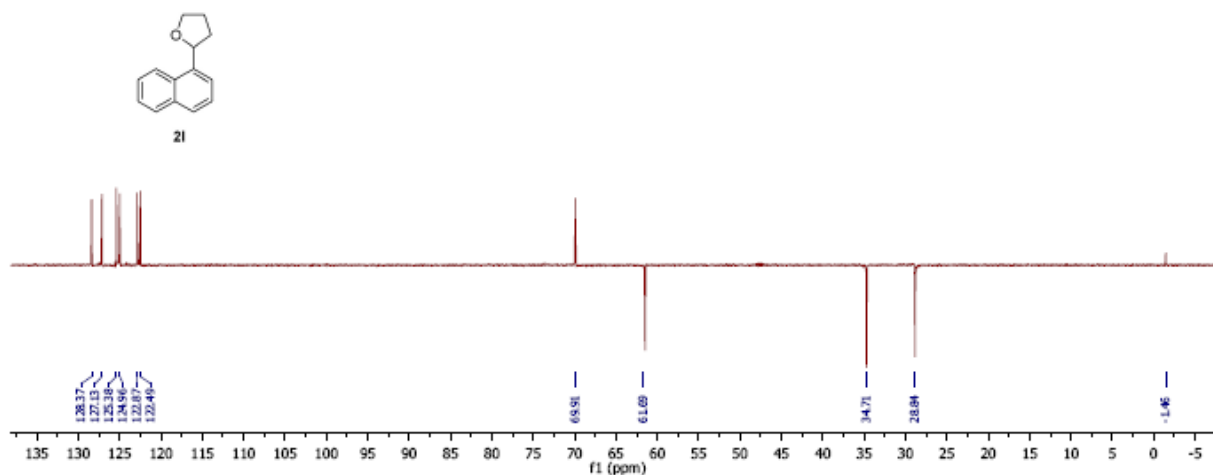


# **<sup>13</sup>C NMR for tetrahydro-2-(naphthalen-4-yl)furan in CD<sub>3</sub>OD (Table 2, entry 1)**

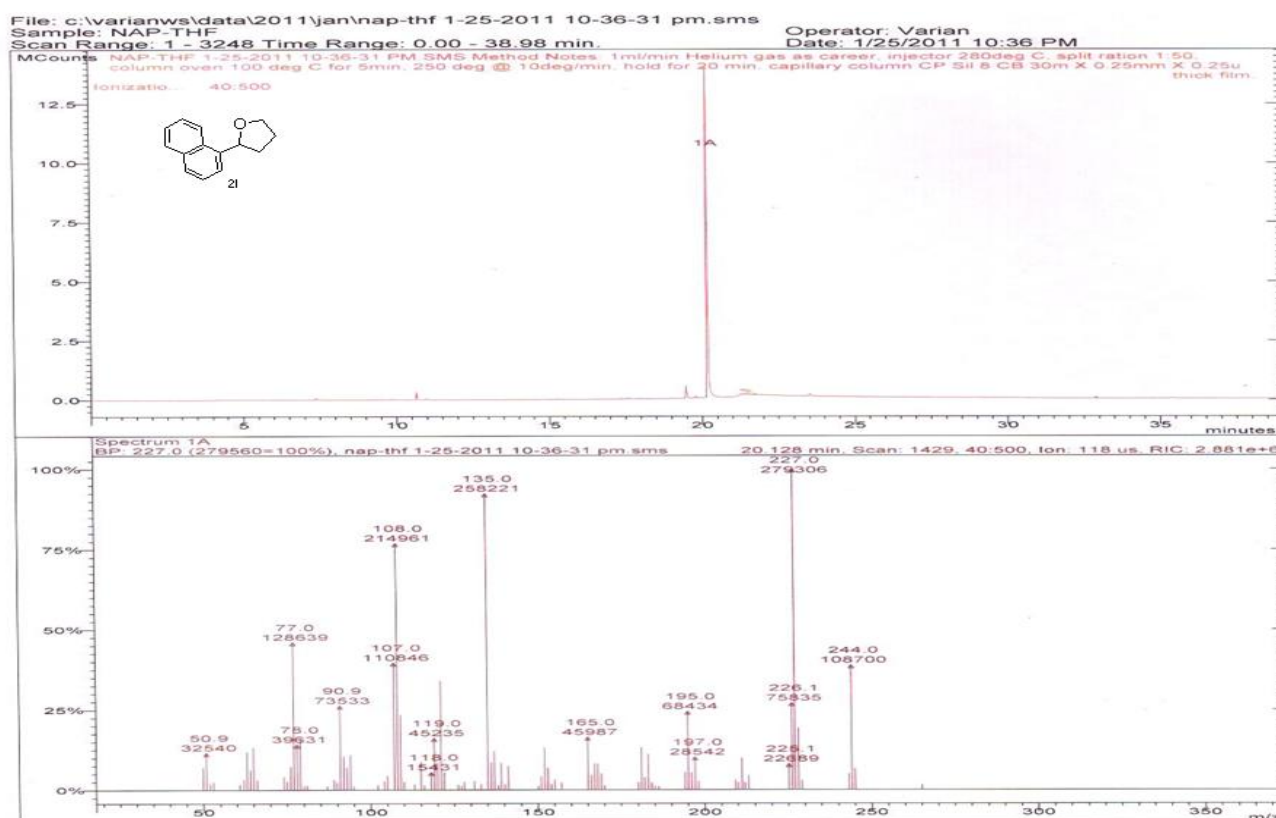


# DEPT at 135 for tetrahydro-2-(naphthalen-4-yl)furan in CD<sub>3</sub>OD (Table 2, entry I)

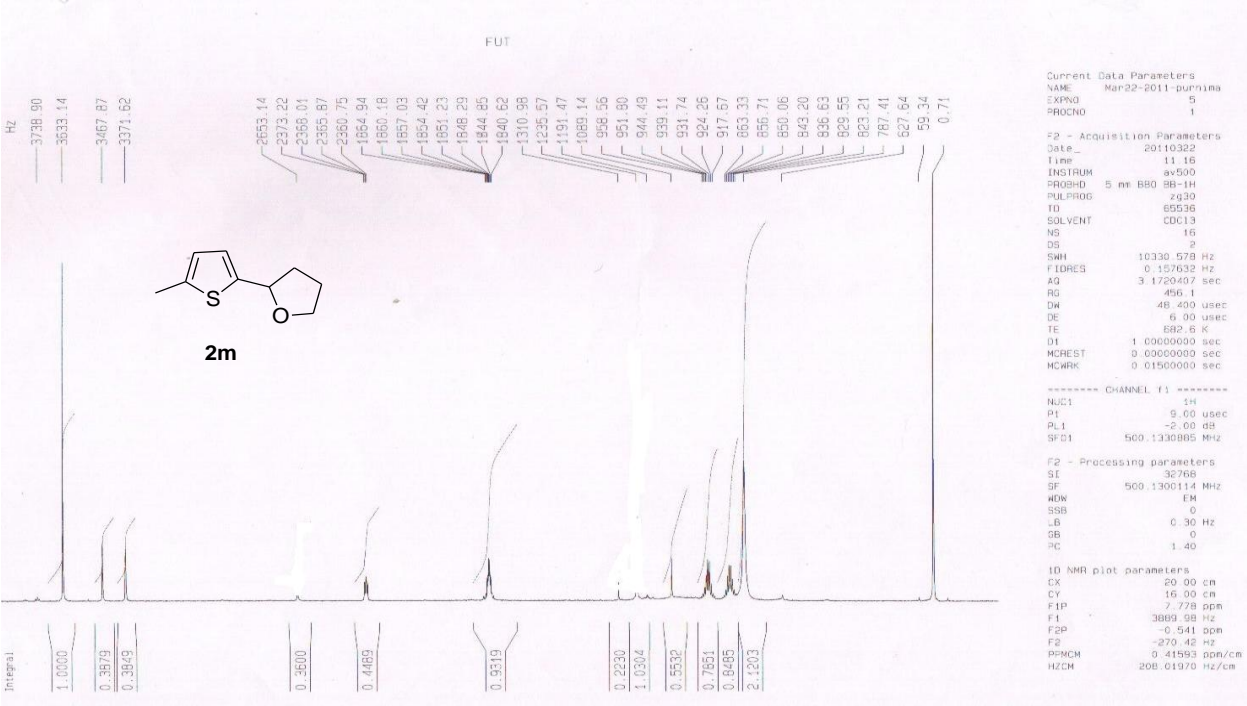
Jan20-2011-purnima  
Naph-CHF



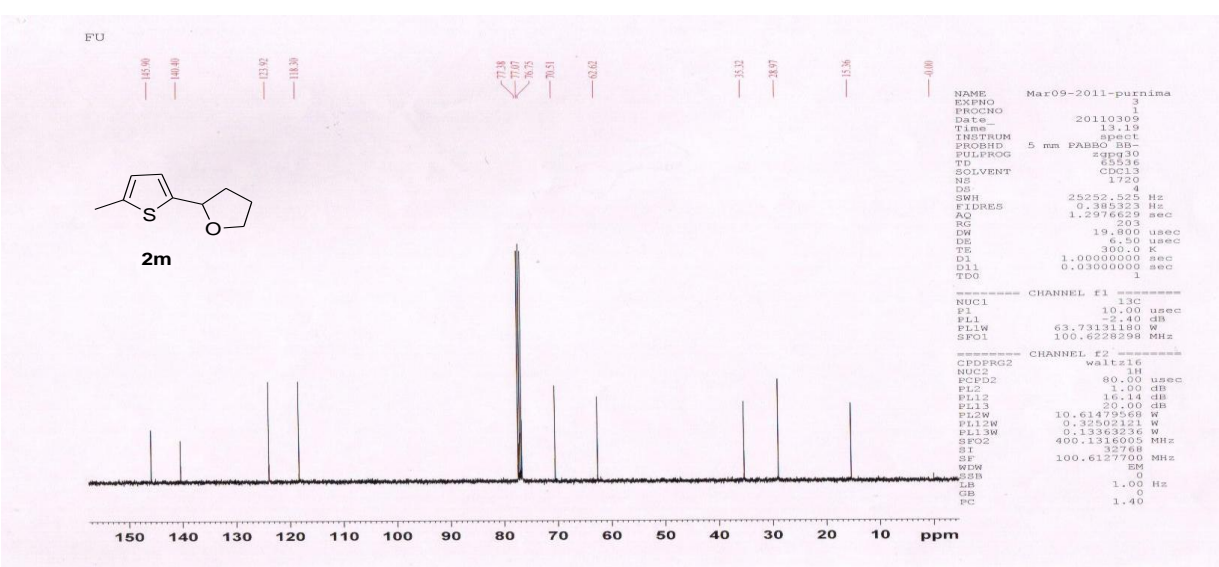
# GCMS for tetrahydro-2-(naphthalen-4-yl)-furan (Table 2, entry I)



<sup>1</sup>H NMR for 2-(thiophen-2-yl)-tetrahydrofuran in CDCl<sub>3</sub> (Table 2, entry m)

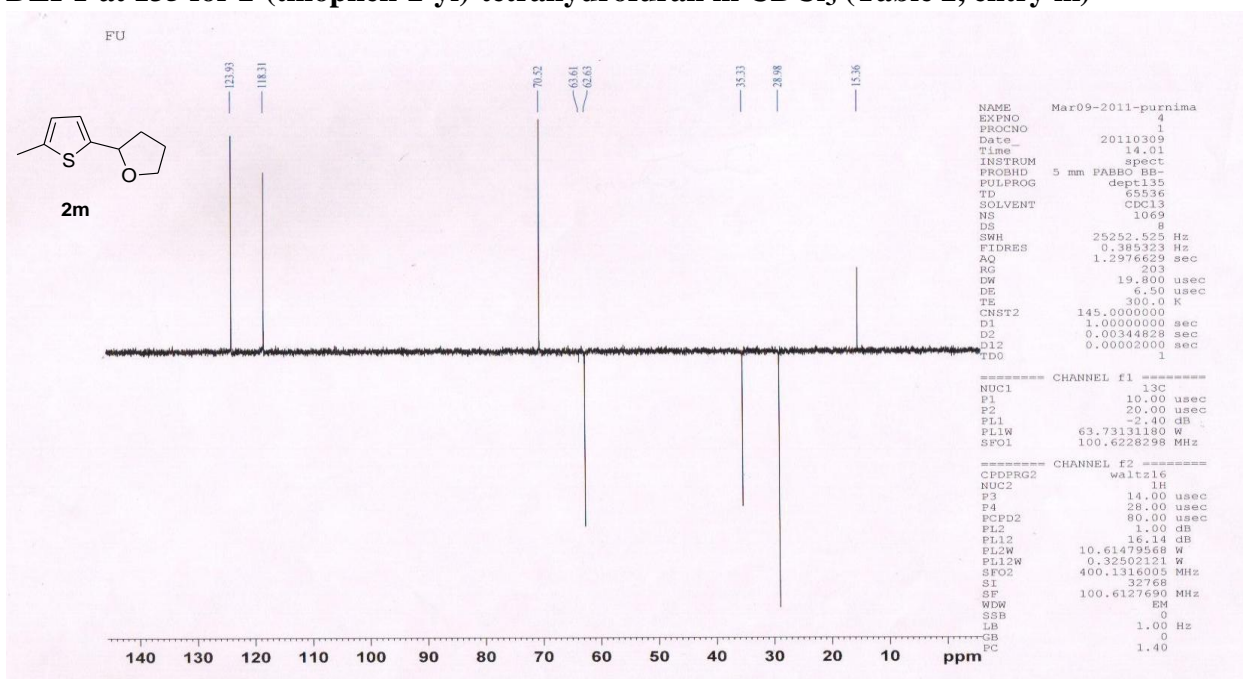


<sup>13</sup>C NMR for 2-(thiophen-2-yl)-tetrahydrofuran in CDCl<sub>3</sub> (Table 2, entry m)

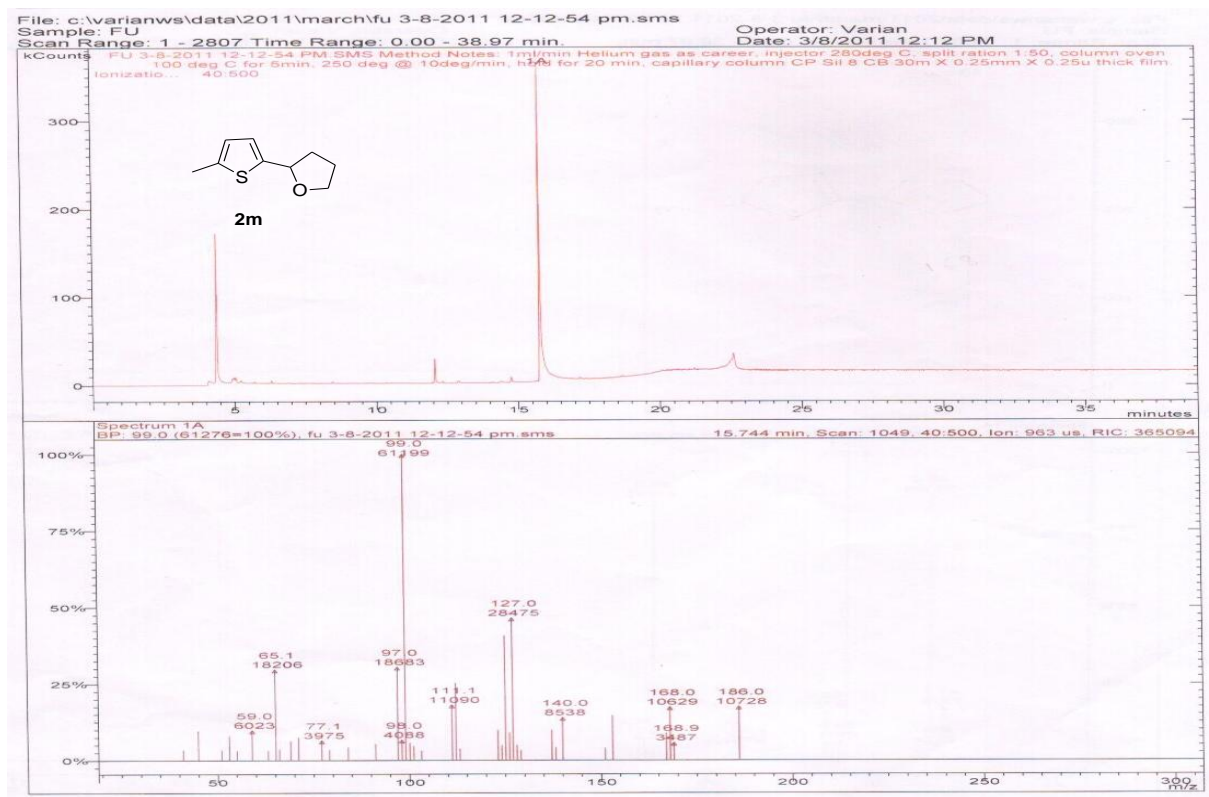




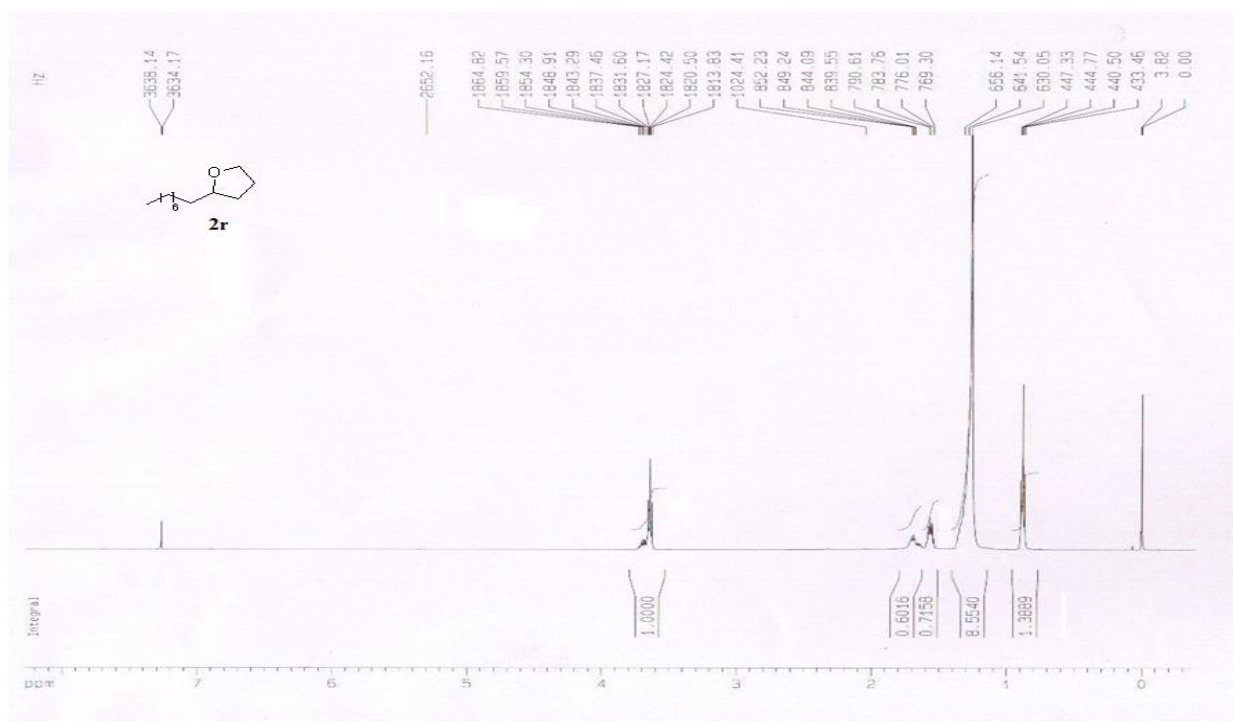
### DEPT at 135 for 2-(thiophen-2-yl)-tetrahydrofuran in CDCl<sub>3</sub> (Table 2, entry m)



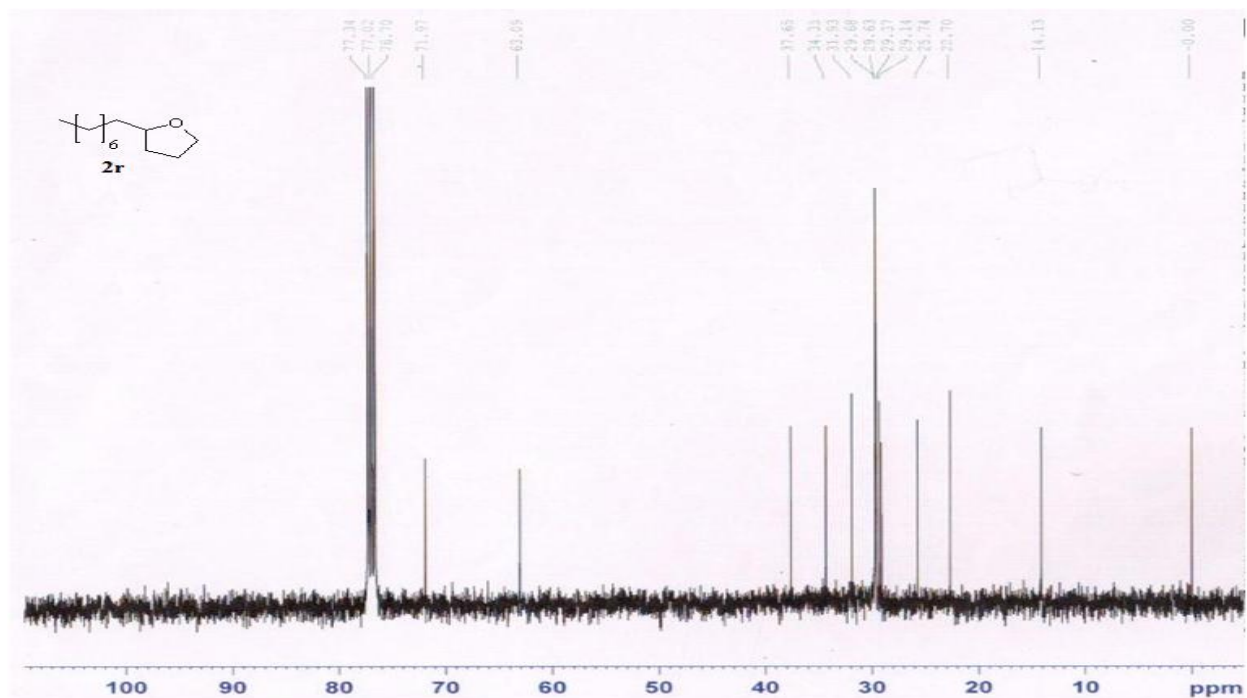
### GC-MS for 2-(thiophen-2-yl)-tetrahydrofuran (Table 2, entry m)



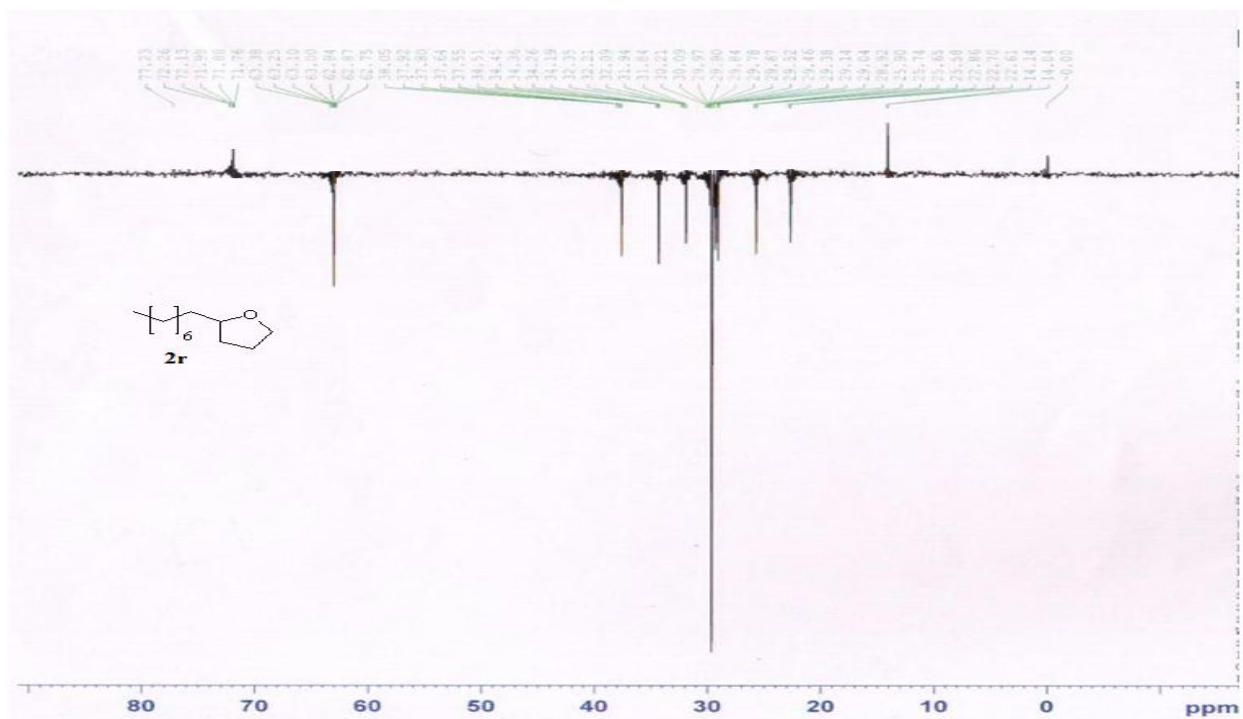
**<sup>1</sup>H NMR for 2-octyl-tetrahydrofuran in CDCl<sub>3</sub> (Table 2, entry r)**



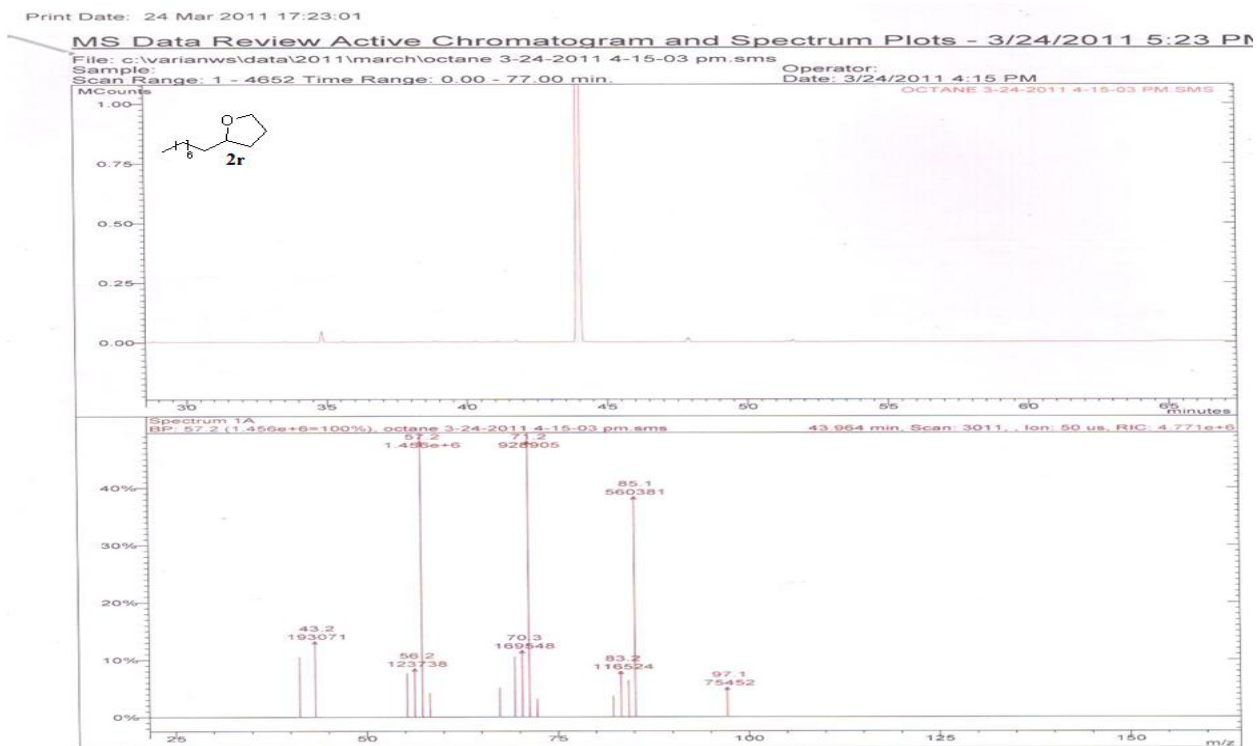
**<sup>13</sup>C NMR for 2-octyl-tetrahydrofuran in CDCl<sub>3</sub> (Table 2, entry r)**



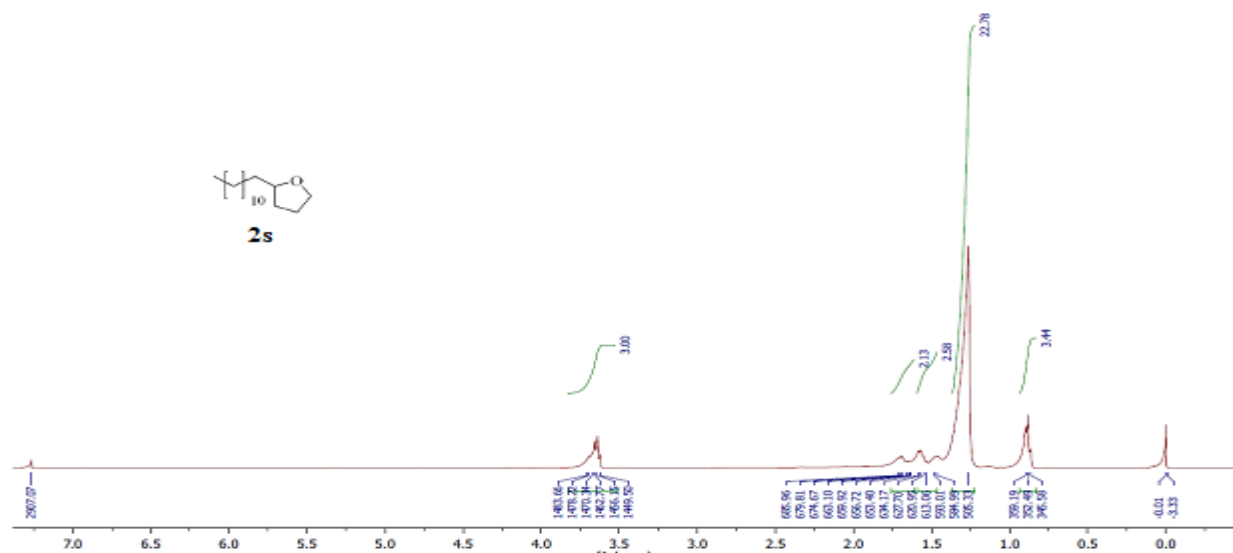
DEPT at 135 for 2-octyl-tetrahydrofuran in CDCl<sub>3</sub> (Table 2, entry r)



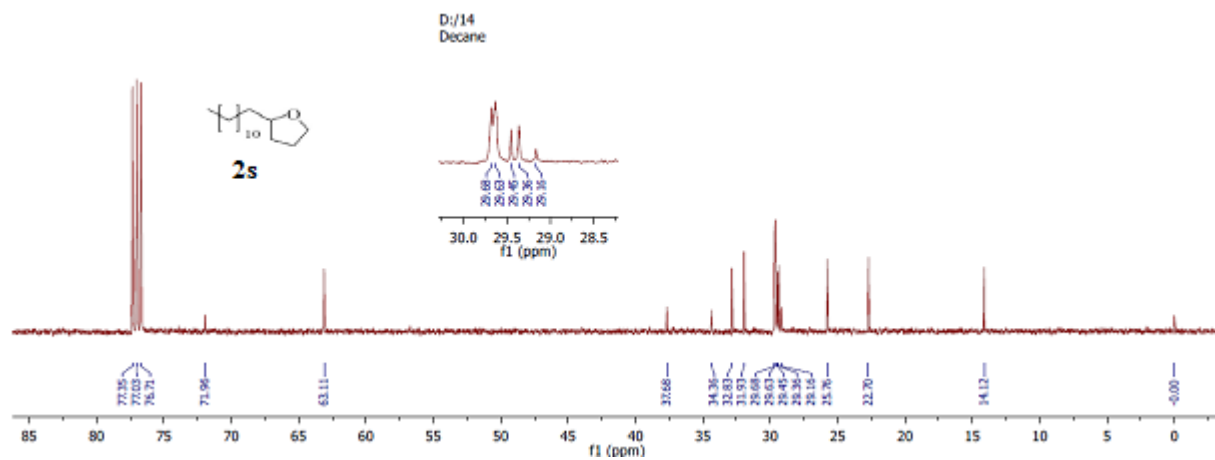
GCMS for 2-octyl-tetrahydrofuran (Table 2, entry r)



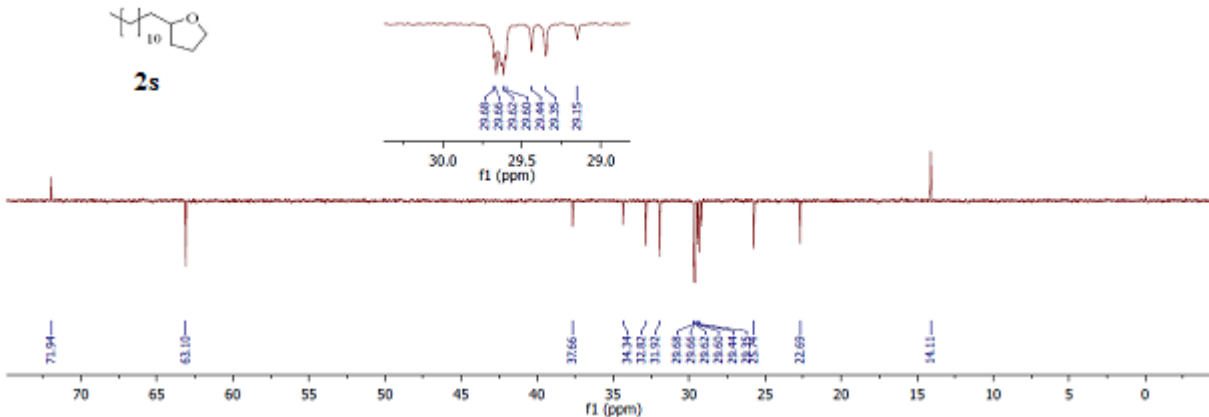
**<sup>1</sup>H NMR for 2-dodecyl-tetrahydrofuran in CDCl<sub>3</sub> (Table 2, entry s)**



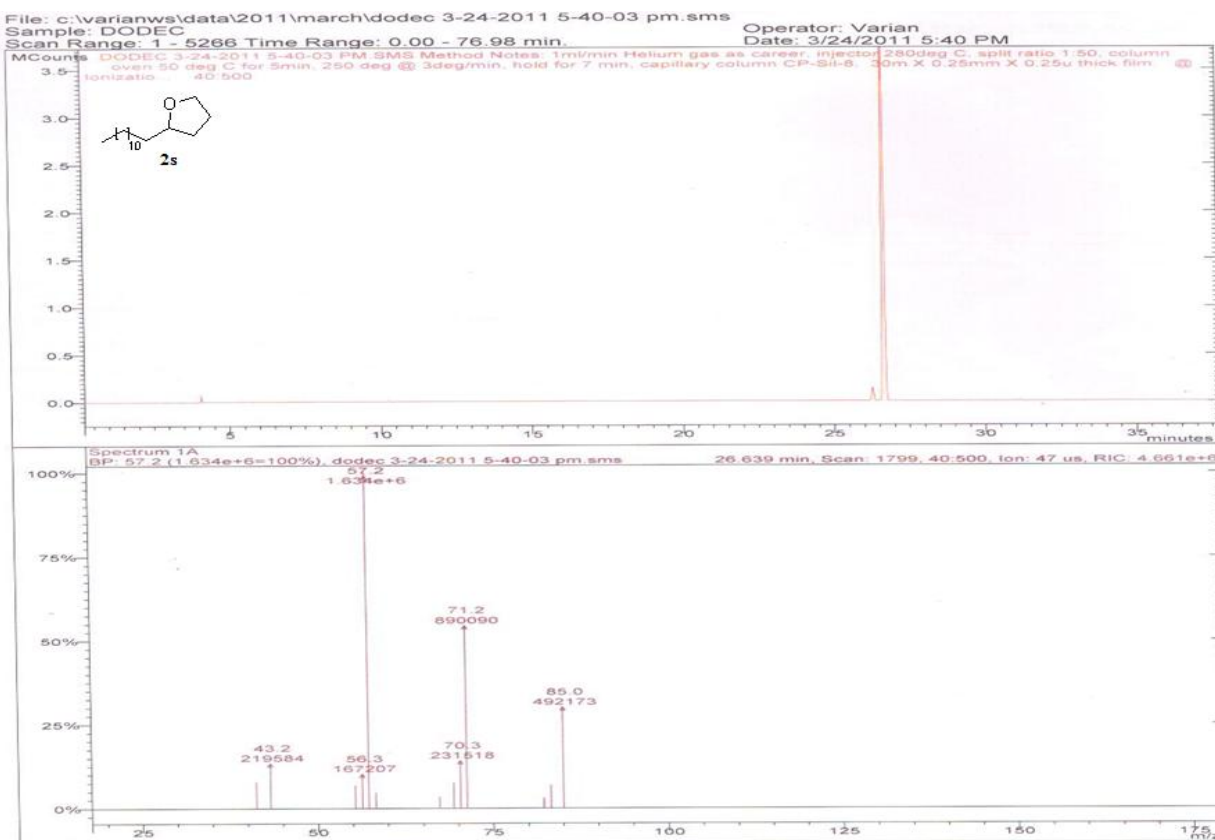
**<sup>13</sup>C NMR for 2-dodecyl-tetrahydrofuran in CDCl<sub>3</sub> (Table 2, entry s)**



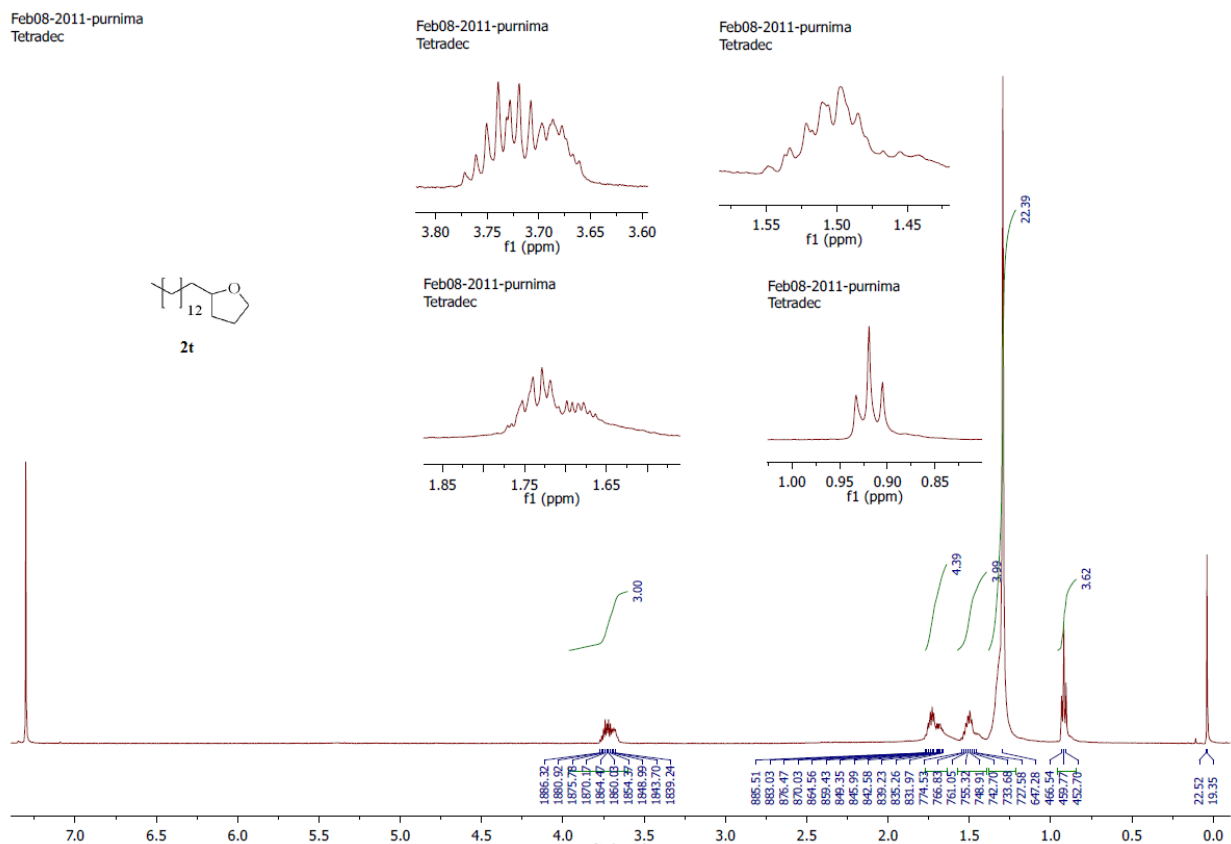
### DEPT at 135 for 2-dodecyl-tetrahydrofuran in CDCl<sub>3</sub> (Table 2, entry s)



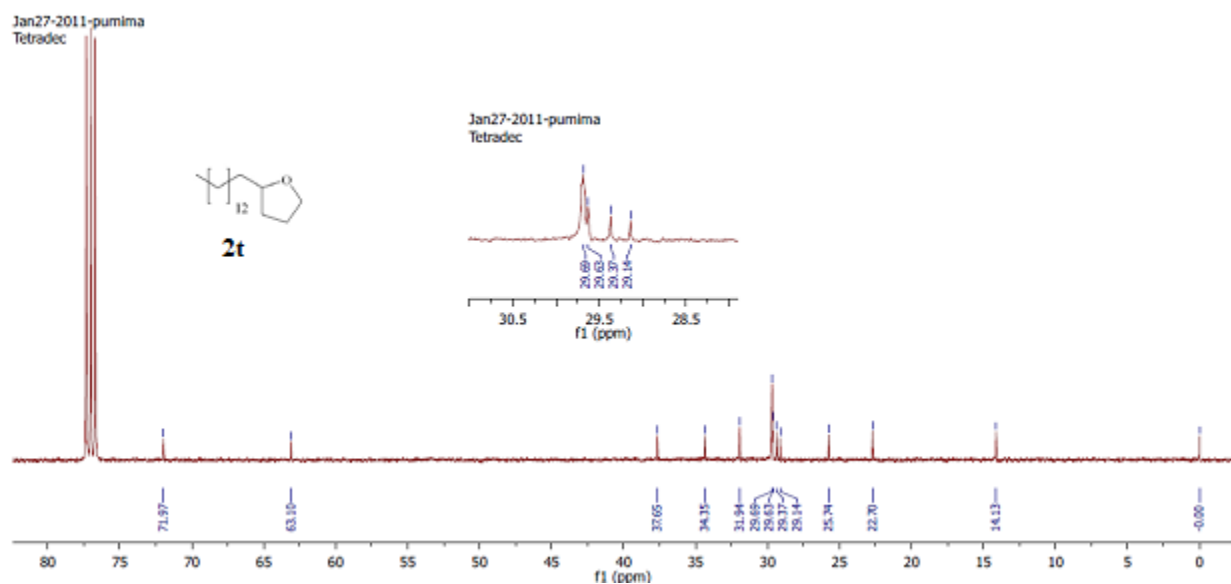
### GCMS for 2-dodecyl-tetrahydrofuran (Table 2, entry s)



# **<sup>1</sup>H NMR for tetrahydro-2-tetradecylfuran in CDCl<sub>3</sub> (Table 2, entry t)**

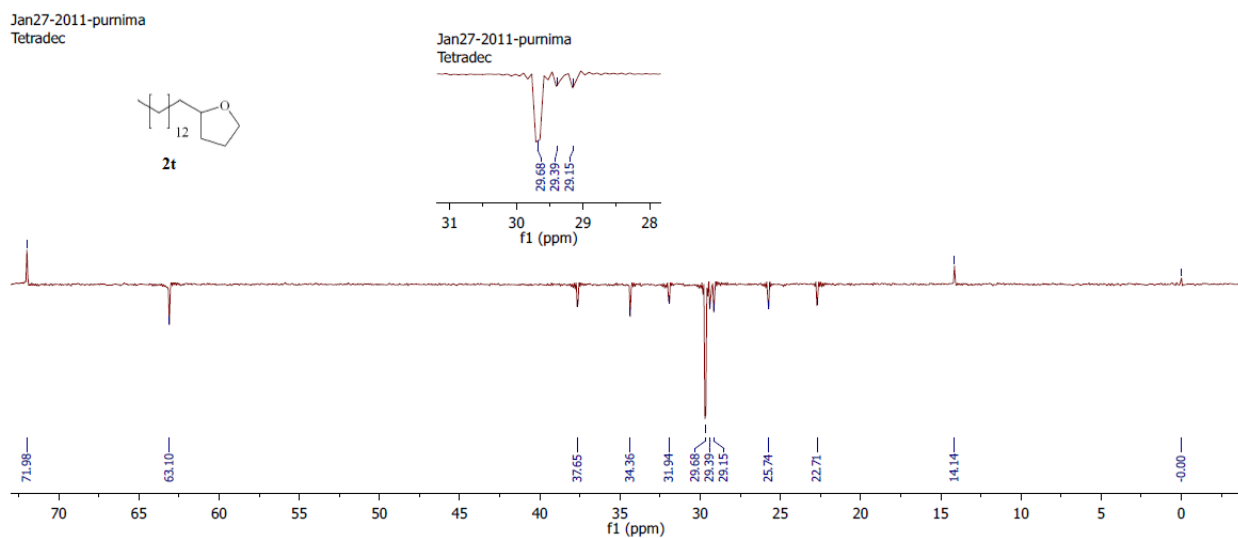


# **<sup>13</sup>C NMR for tetrahydro-2-tetradecylfuran in CDCl<sub>3</sub> (Table 2, entry t)**

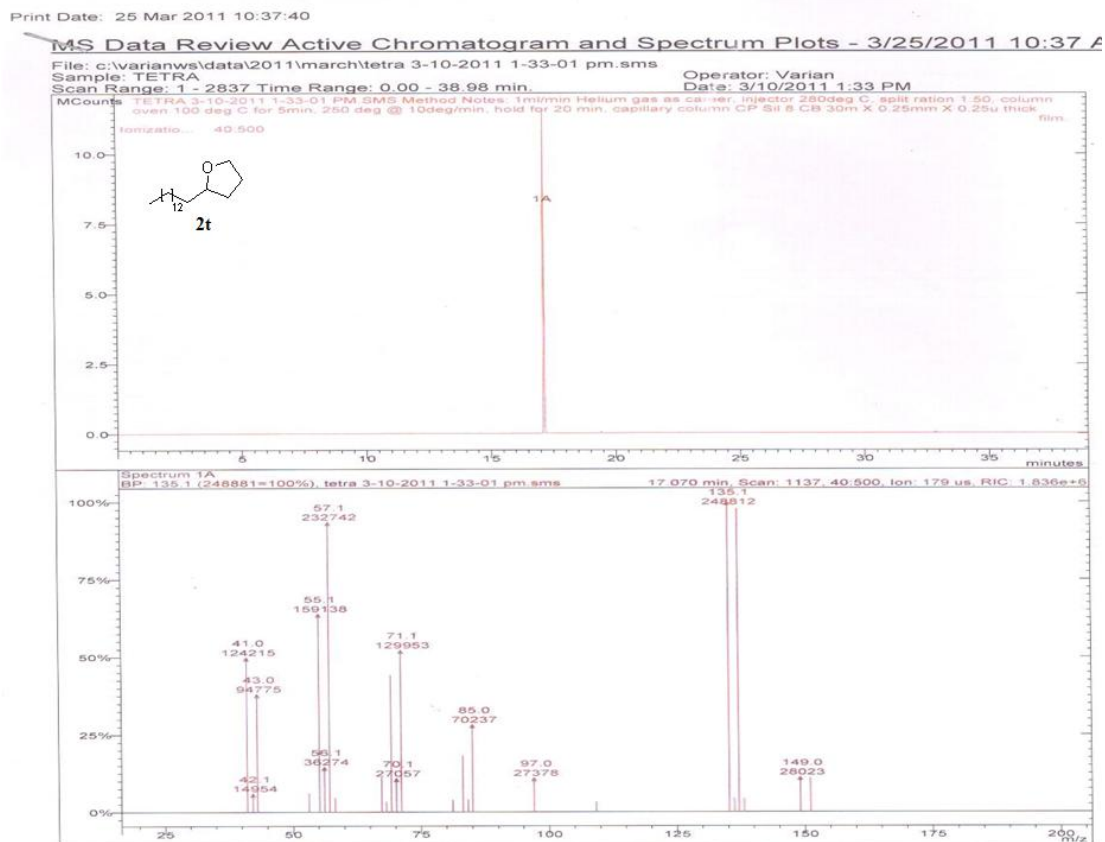




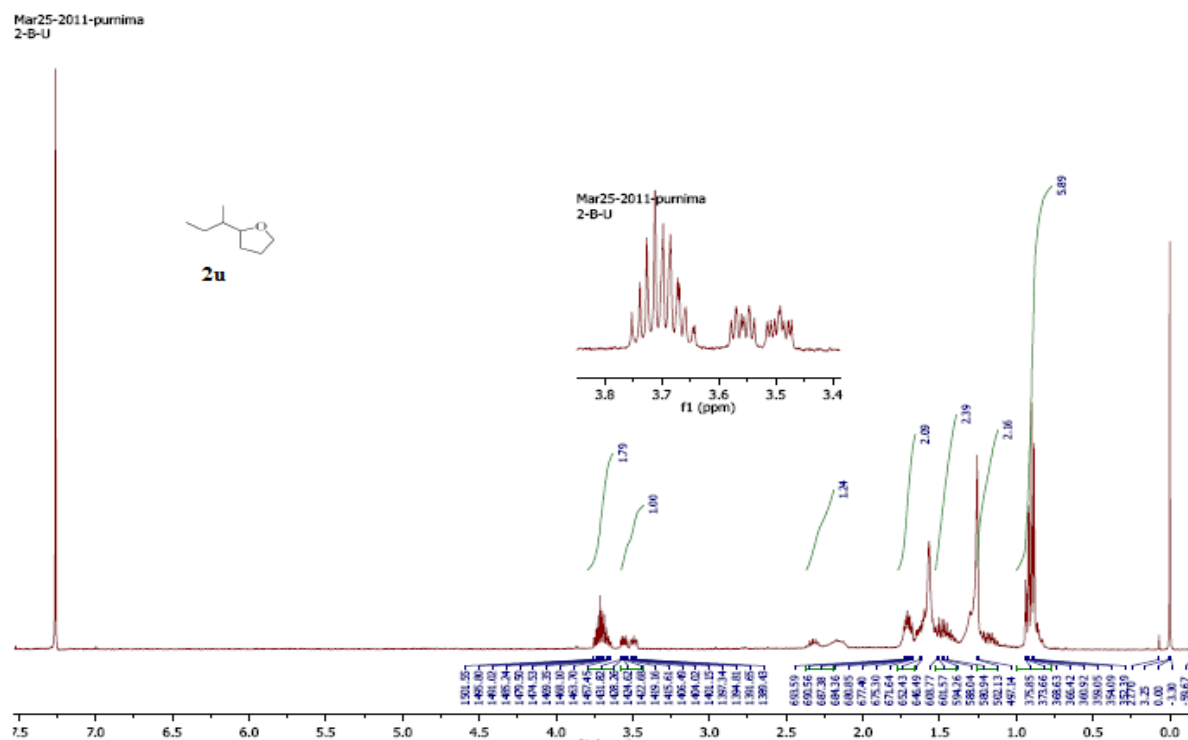
## DEPT at 135 for tetrahydro-2-tetradecylfuran in CDCl<sub>3</sub> (Table 2, entry t)



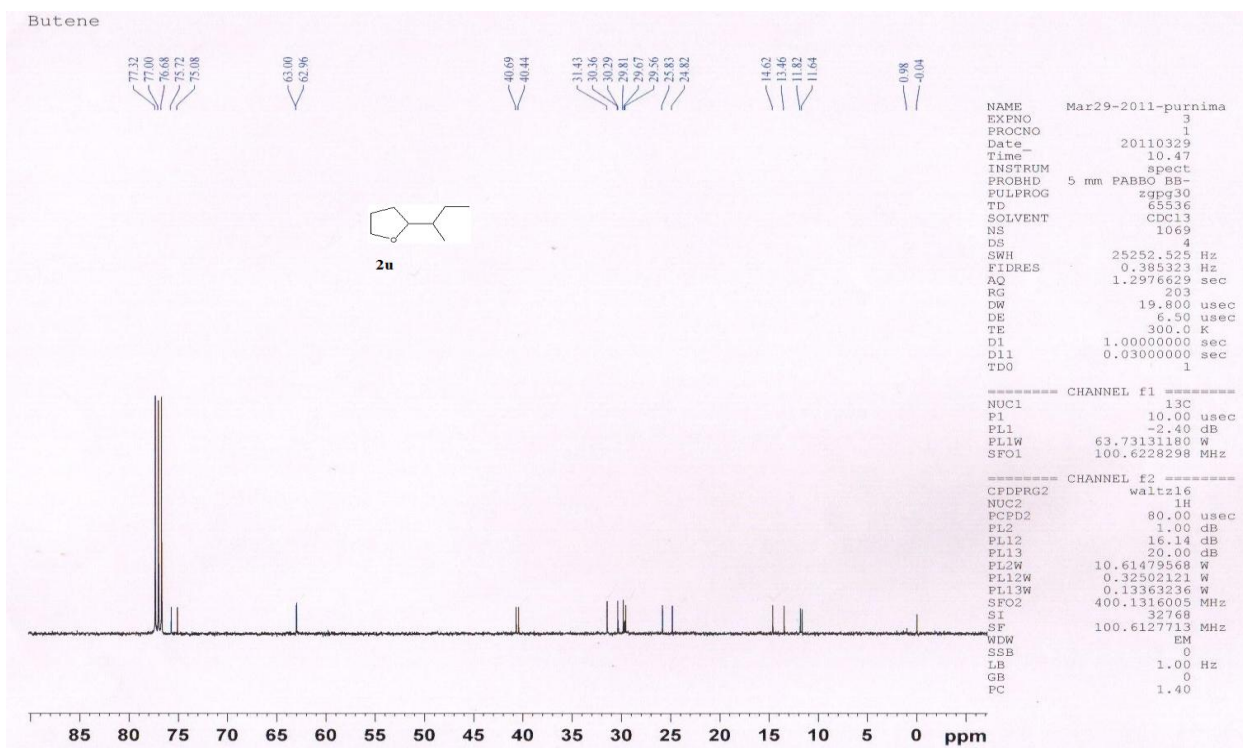
## GCMS for tetrahydro-2-tetradecylfuran (Table 2, entry t)



# <sup>1</sup>H NMR for 2-sec-butyl-tetrahydrofuran in CDCl<sub>3</sub> (Table 2, entry u)

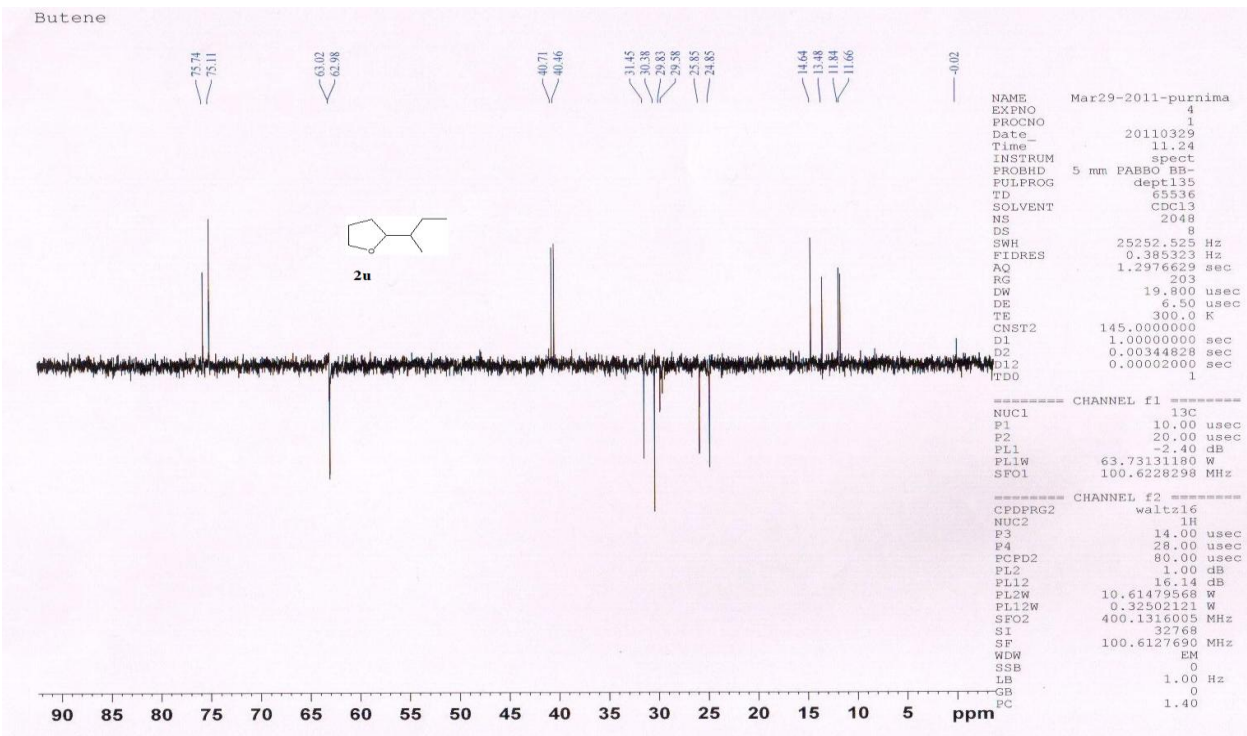


# <sup>13</sup>C NMR for 2-sec-butyl-tetrahydrofuran in CDCl<sub>3</sub> (Table 2, entry u)

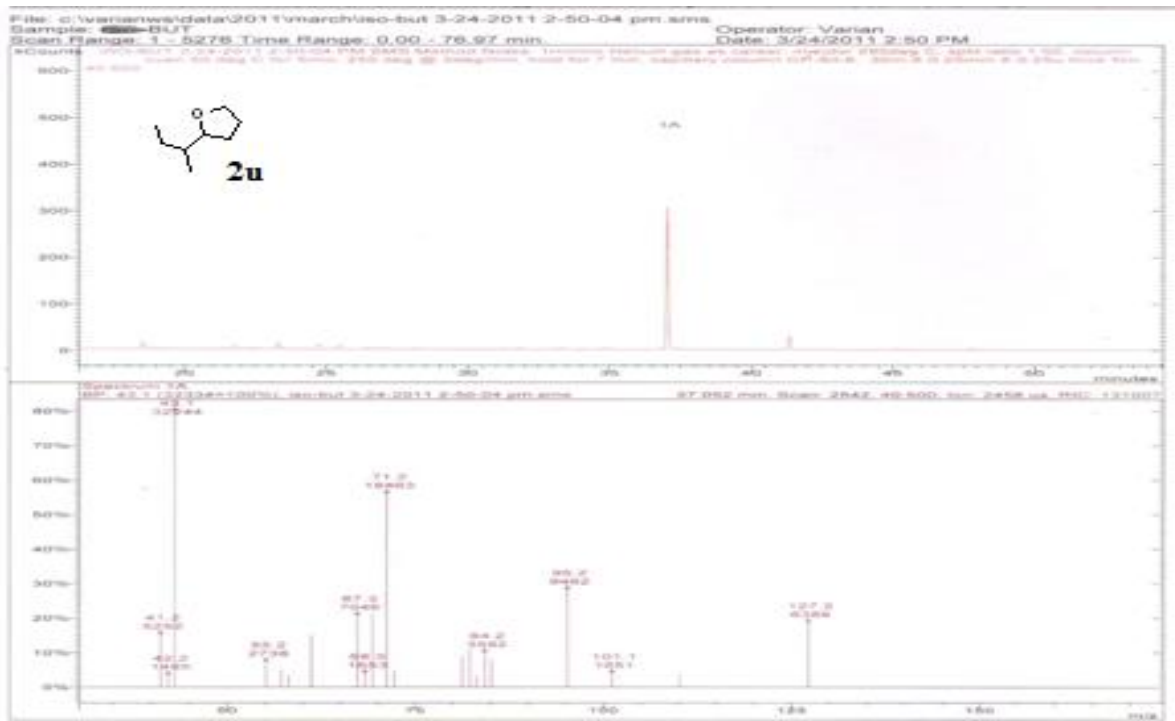




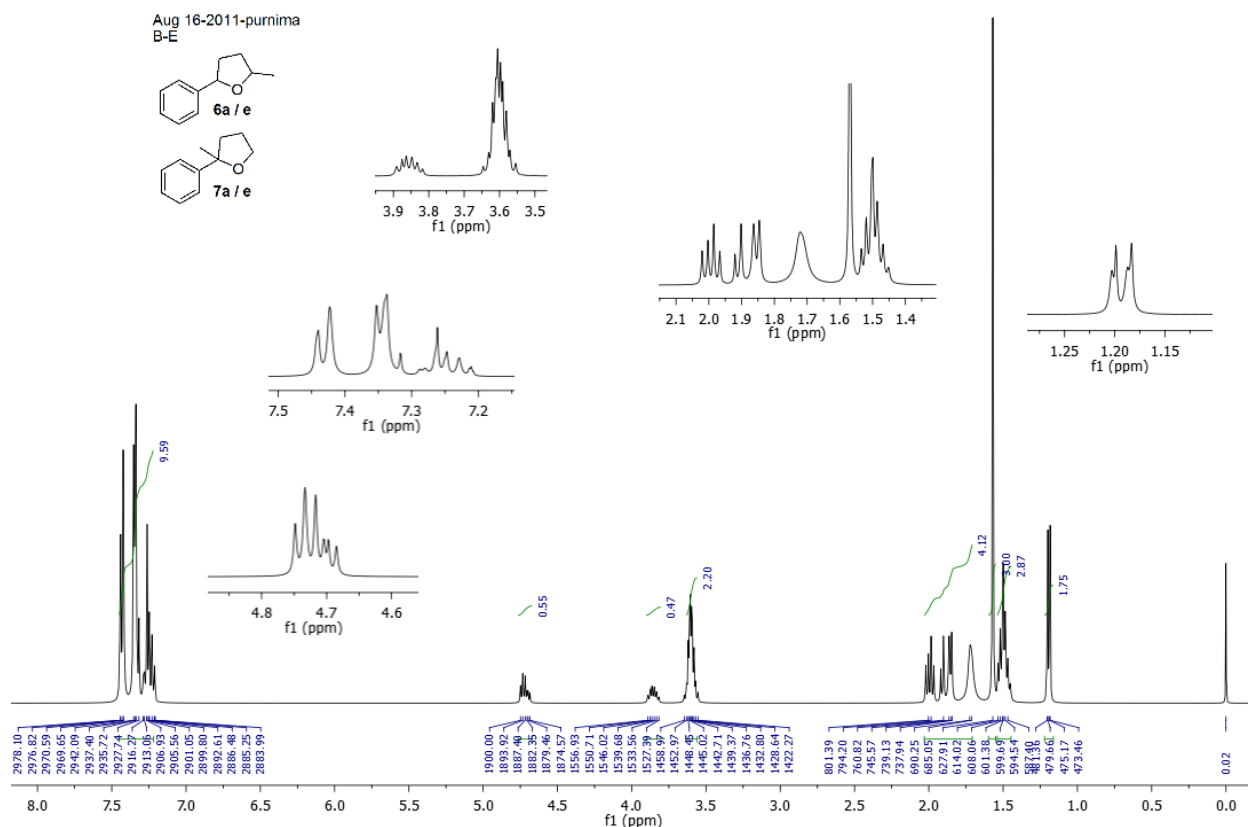
DEPT at 135 for 2-sec-butyl-tetrahydrofuran in CDCl<sub>3</sub> (Table 2, entry u)



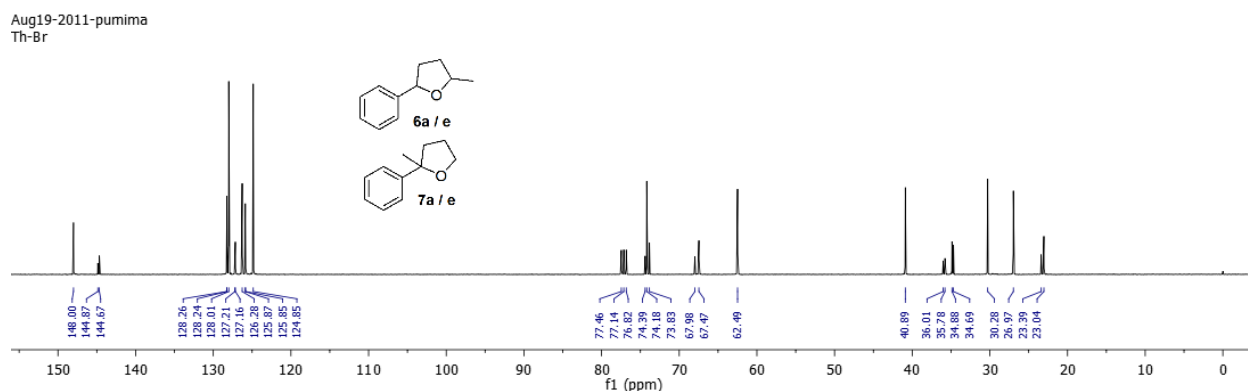
GCMS for 2-sec-butyl-tetrahydrofuran (Table 2, entry u)



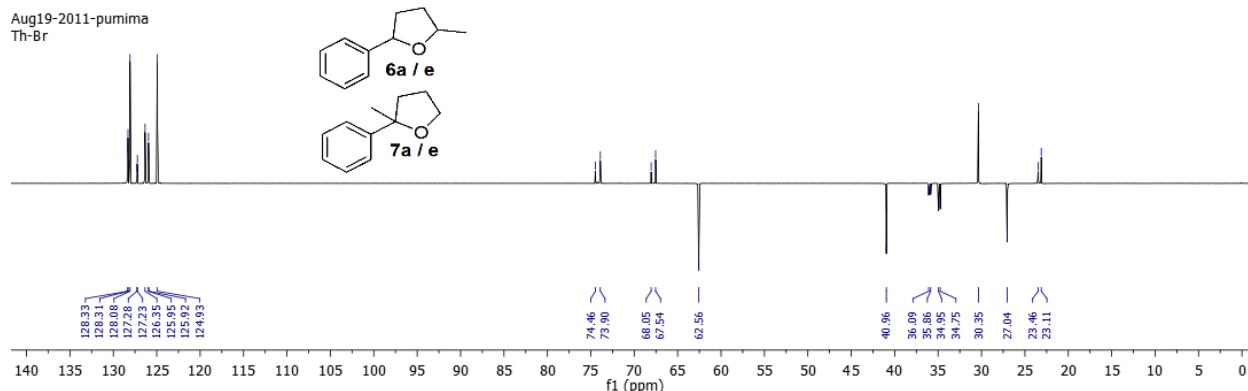
**<sup>1</sup>H NMR for 2-methyl-5-phenyl-tetrahydrofuran and 2-methyl-2-phenyl-tetrahydrofuran in CDCl<sub>3</sub> (Table 3, entry a and e)**



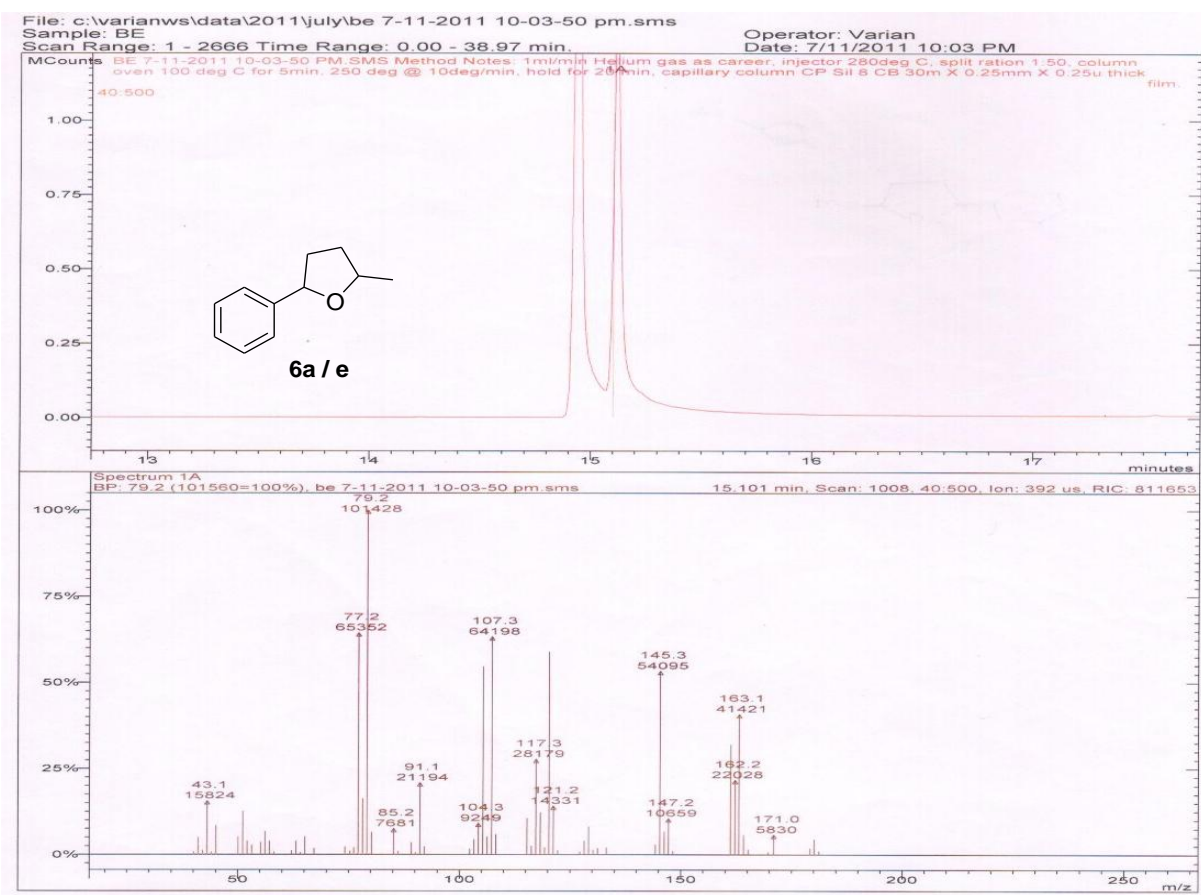
**<sup>13</sup>C NMR for 2-methyl-5-phenyl-tetrahydrofuran and 2-methyl-2-phenyl-tetrahydrofuran in CDCl<sub>3</sub> (Table 3, entry a and e)**



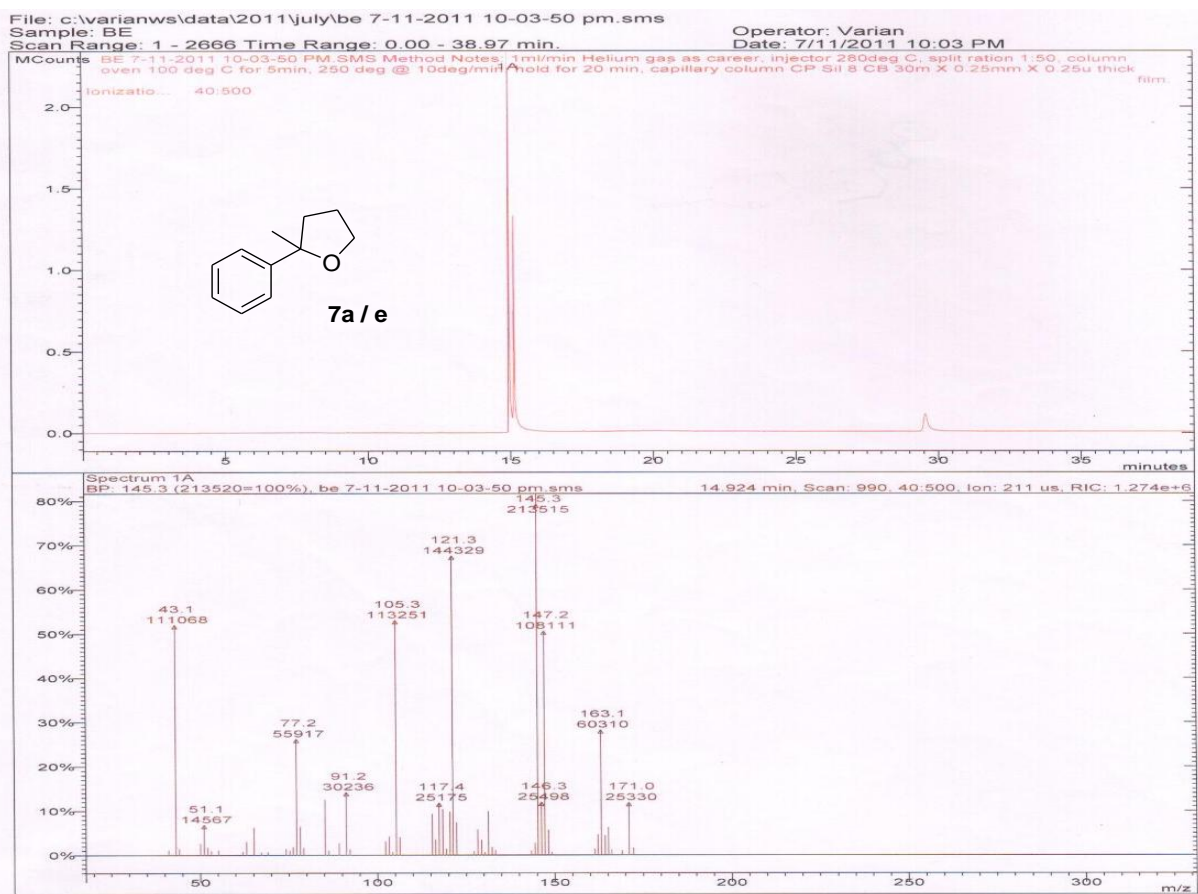
# DEPT at 135 for 2-methyl-5-phenyl-tetrahydrofuran and 2-methyl-2-phenyl-tetrahydrofuran in CDCl<sub>3</sub> (Table 3, entry a and e)



## GCMS for 2-methyl-5-phenyl-tetrahydrofuran (Table 3, entry a and e)

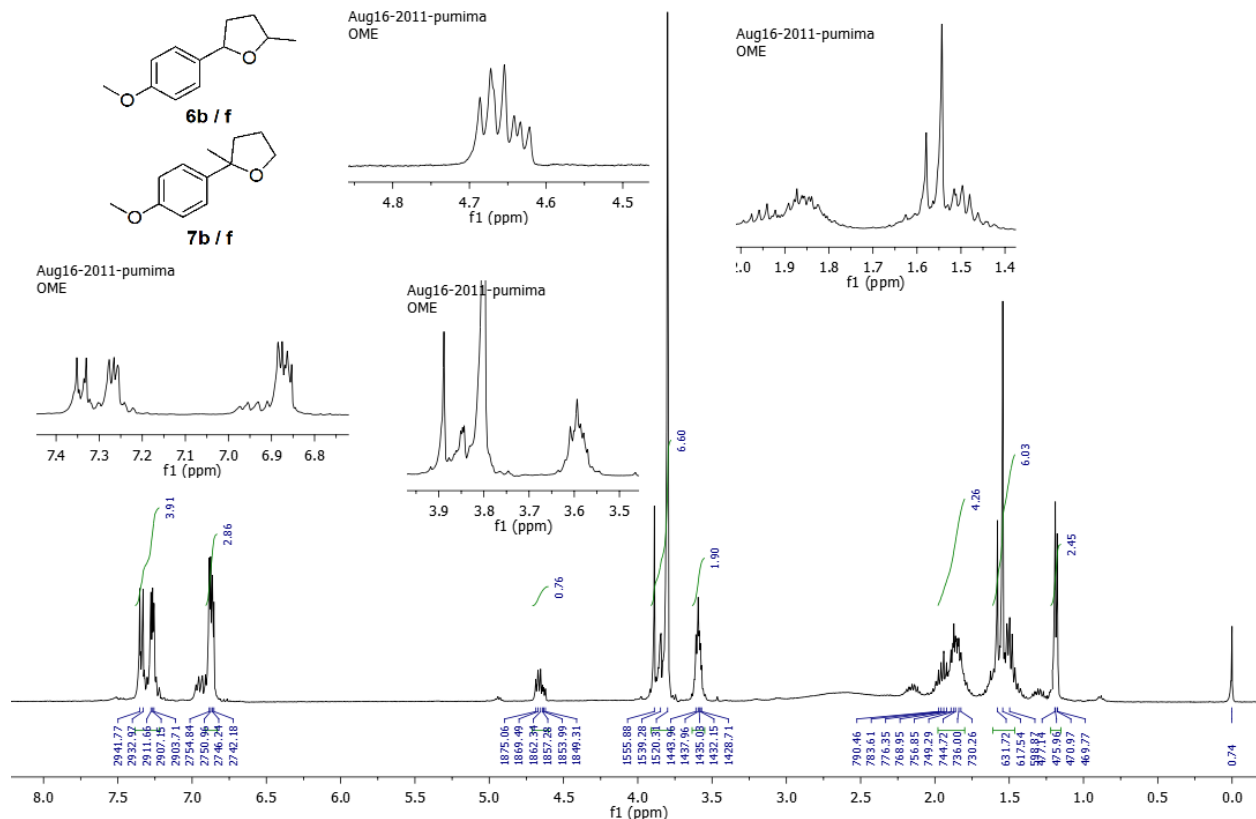


# GCMS for 2-methyl-2-phenyl-tetrahydrofuran (Table 3, entry a and e)



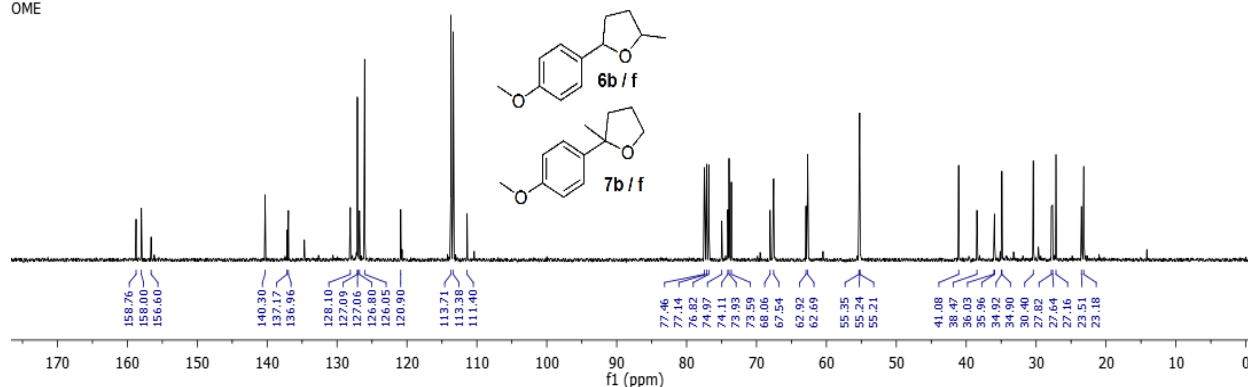
# **<sup>1</sup>H NMR for 2-(4-methoxyphenyl)-5-methyl-tetrahydrofuran and 2-(4-methoxyphenyl)-2-methyl-tetrahydrofuran in CDCl<sub>3</sub> (Table 3, entry b and f)**

Aug16-2011-pumima  
OME



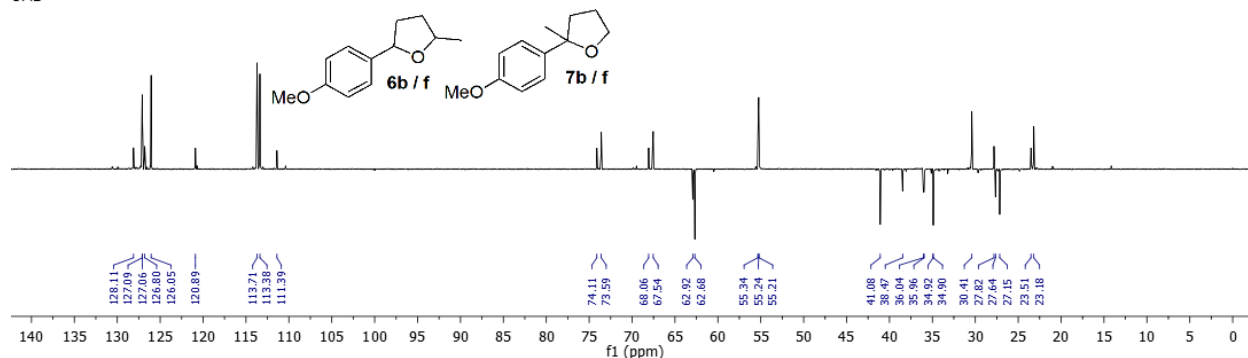
# **<sup>13</sup>C NMR for 2-(4-methoxyphenyl)-5-methyl-tetrahydrofuran and 2-(4-methoxyphenyl)-2-methyl-tetrahydrofuran in CDCl<sub>3</sub> (Table 3, entry b and f)**

Aug17-2011-pumima  
OME

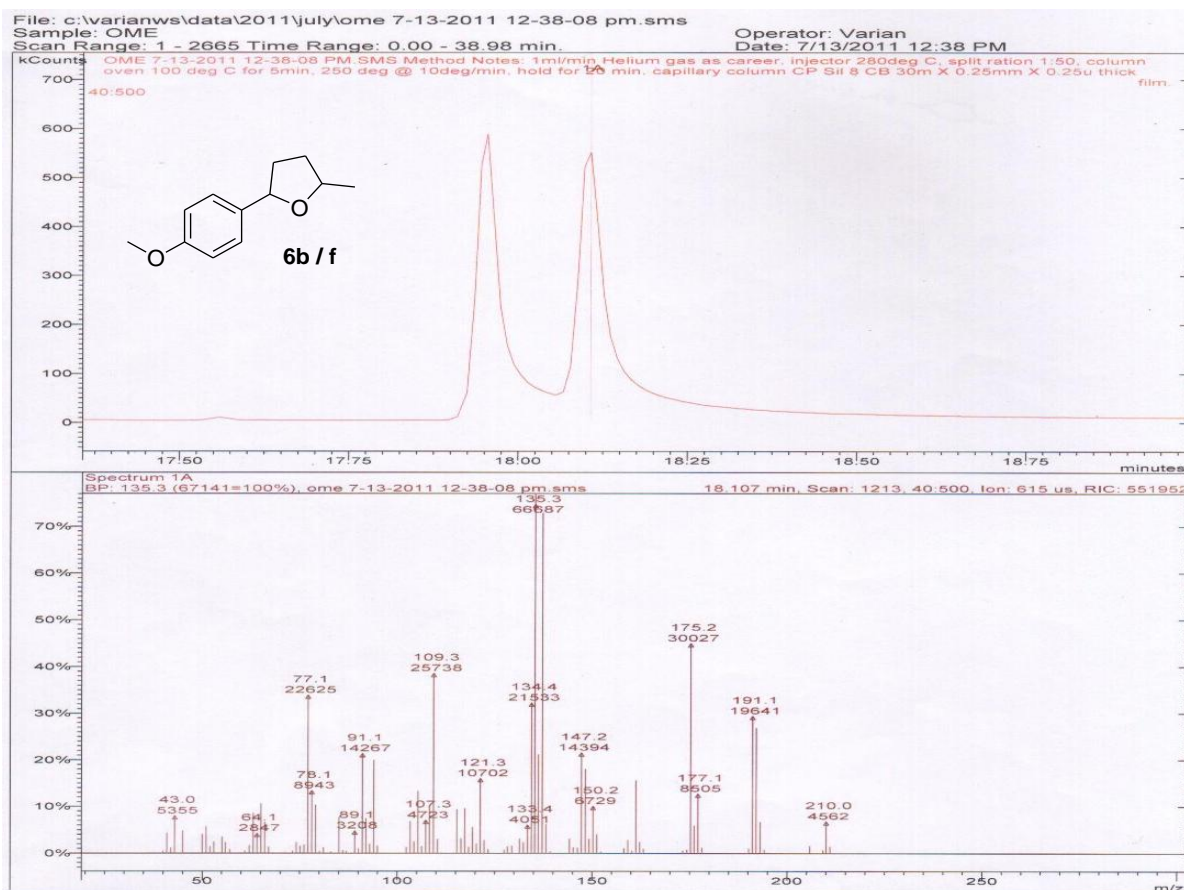


# **DEPT at 135 for 2-(4-methoxyphenyl)-5-methyl-tetrahydrofuran and 2-(4-methoxyphenyl)-2-methyl-tetrahydrofuran in CDCl<sub>3</sub> (Table 3, entry b and f)**

Aug17-2011-pumima  
OME

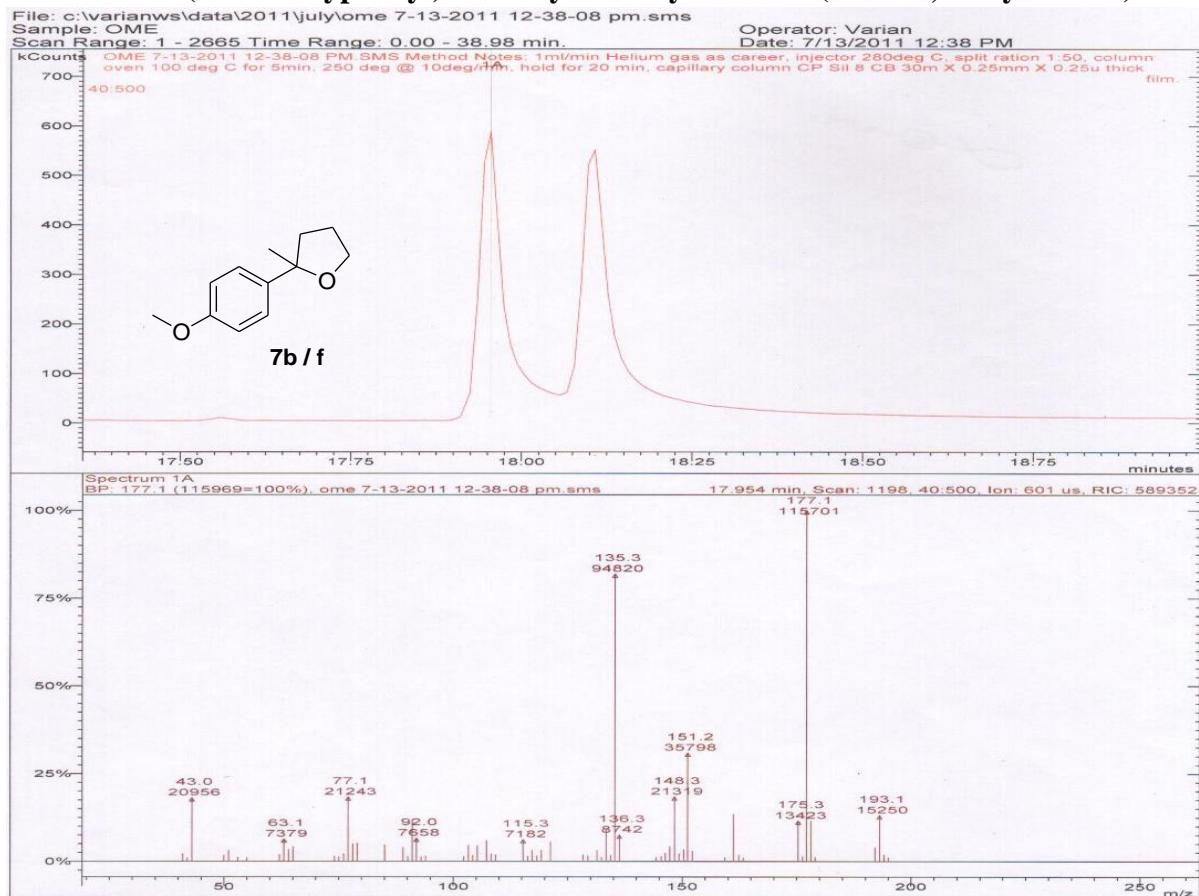


## **GCMS for 2-(4-methoxyphenyl)-5-methyl-tetrahydrofuran (Table 3, entry b and f)**





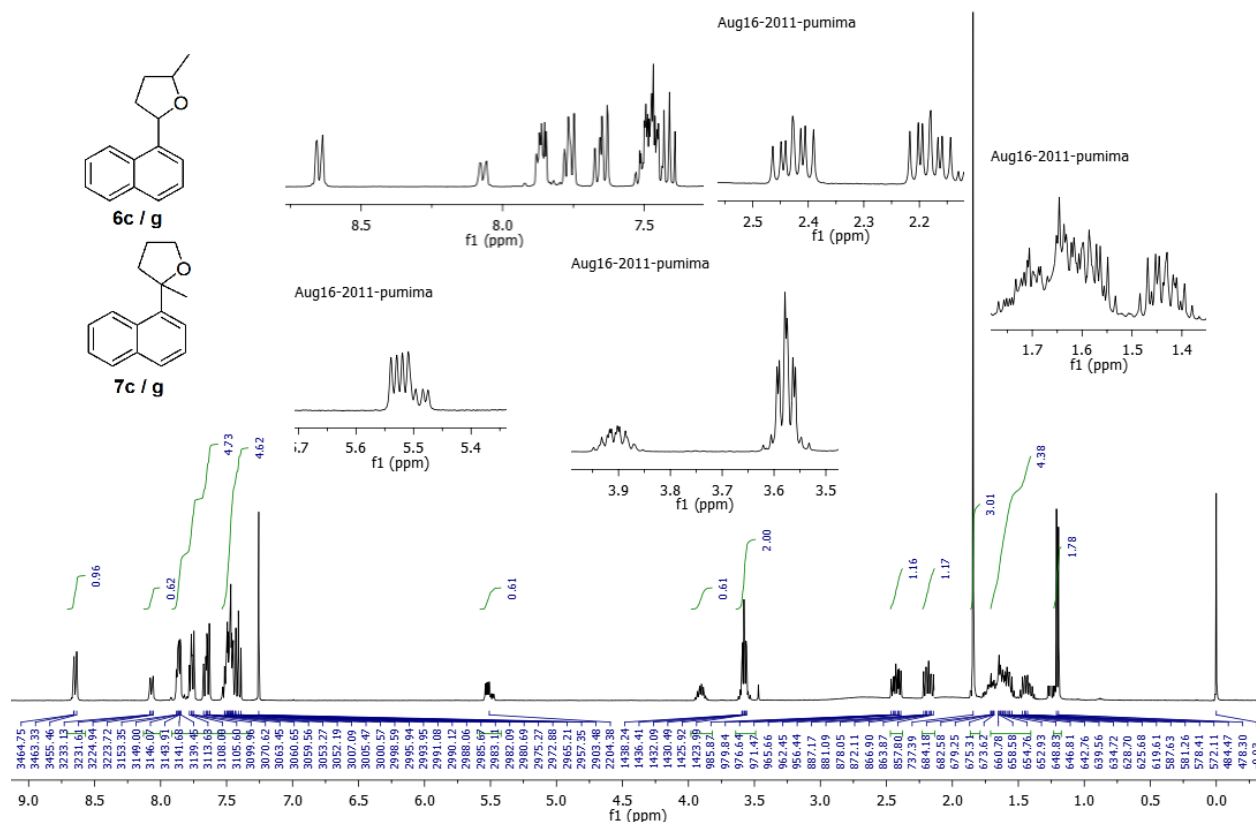
# GCMS for 2-(4-methoxyphenyl)-2-methyl-tetrahydrofuran (Table 3, entry b and f)



# **<sup>1</sup>H NMR for 2-methyl-5-(naphthalen-1-yl)-tetrahydrofuran and 2-methyl-2-(naphthalen-1-yl)-tetrahydrofuran in CDCl<sub>3</sub> (Table 3, entry c and g)**

Aug16-2011-pumima

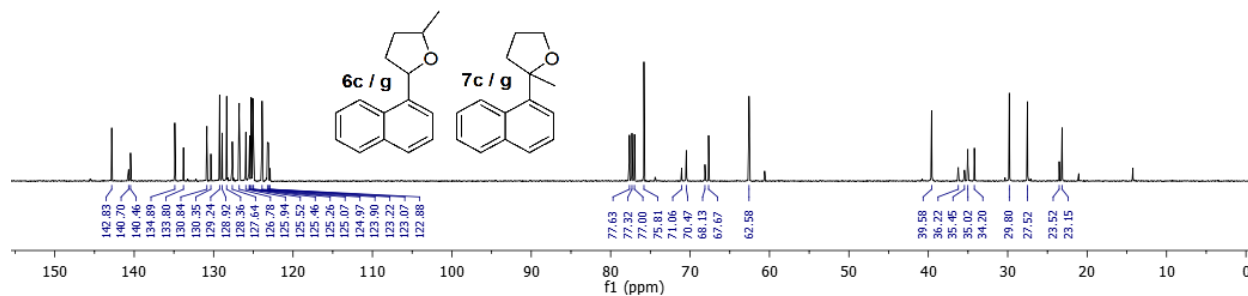
Aug16-2011-pumima



# **<sup>13</sup>C NMR for 2-methyl-5-(naphthalen-1-yl)-tetrahydrofuran and 2-methyl-2-(naphthalen-1-yl)-tetrahydrofuran in CDCl<sub>3</sub> (Table 3, entry c and g)**

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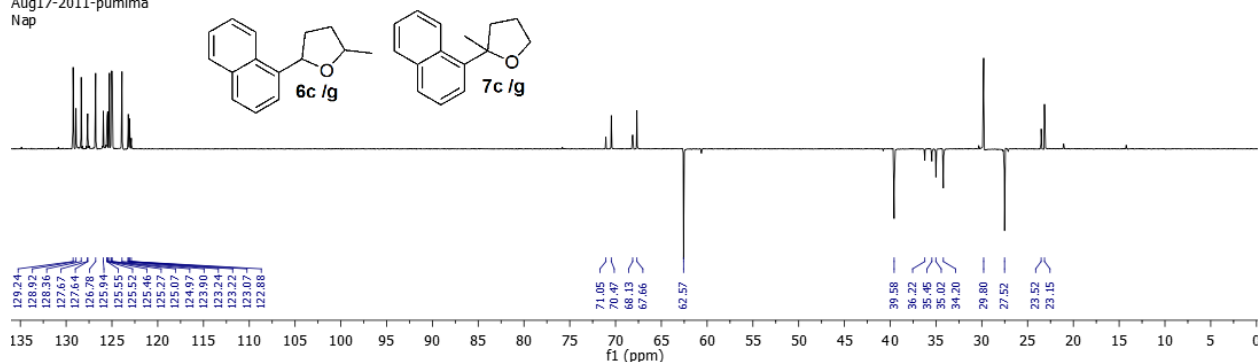
Nap



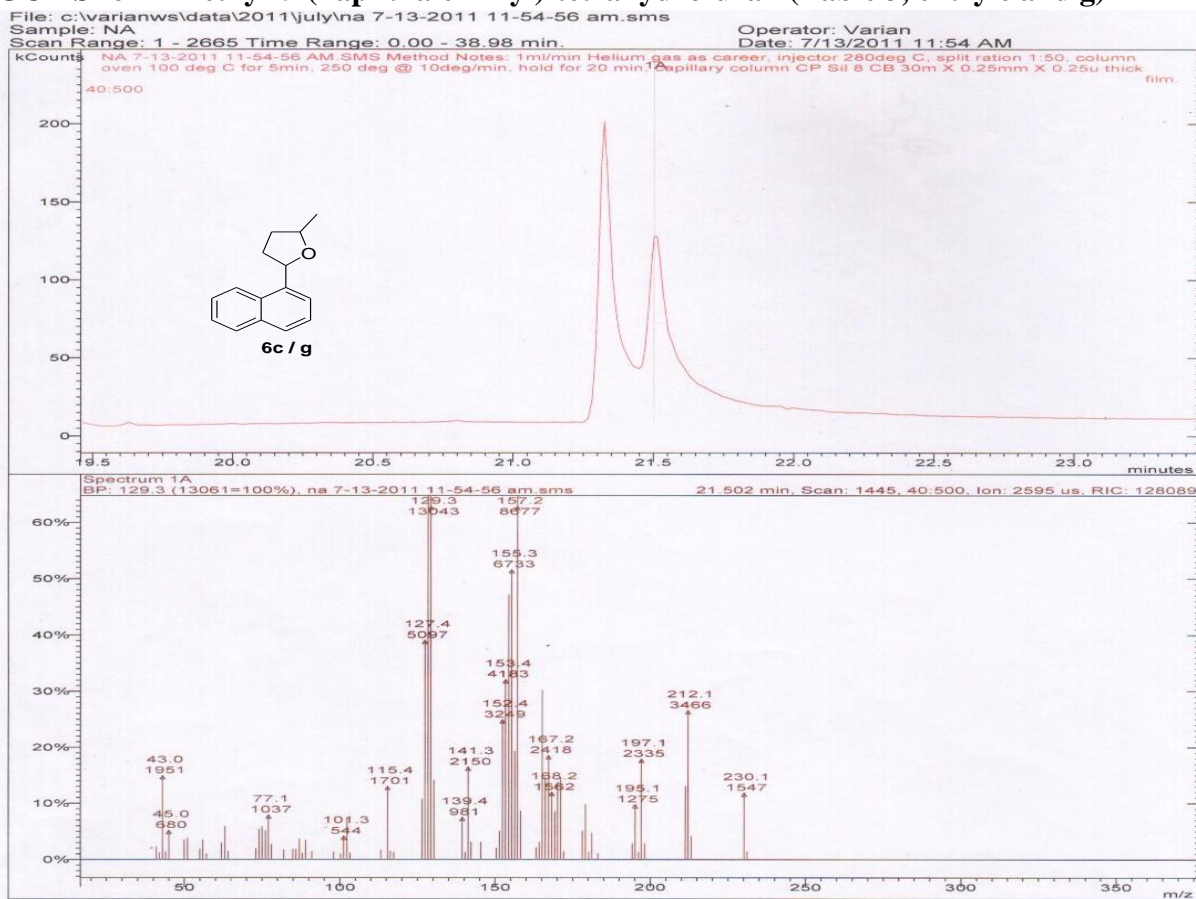


# **DEPT at 135 for 2-methyl-5-(naphthalen-1-yl)-tetrahydrofuran and 2-methyl-2-(naphthalen-1-yl)-tetrahydrofuran in CDCl<sub>3</sub> (Table 3, entry c and g)**

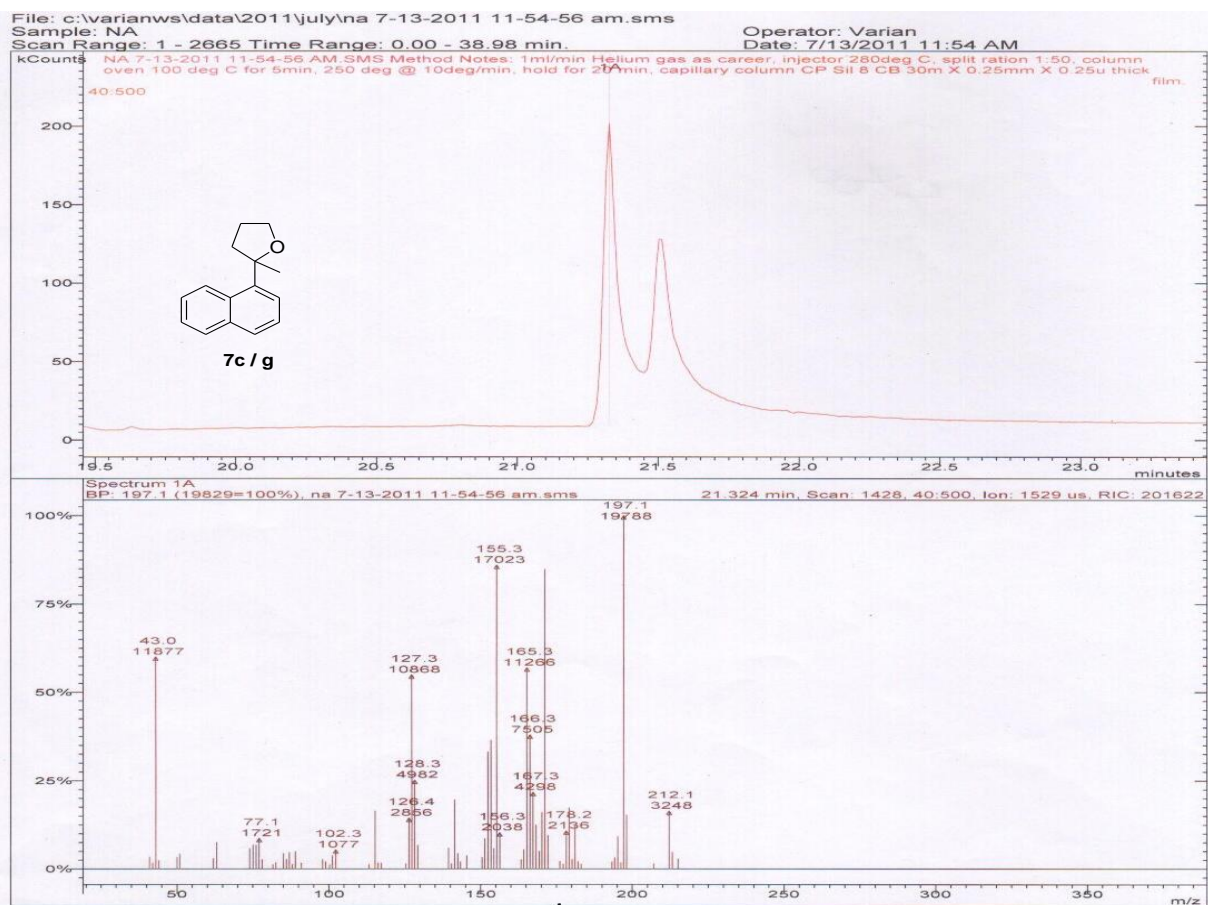
Aug17-2011-pumima  
Nap



## **GCMS for 2-methyl-5-(naphthalen-1-yl)-tetrahydrofuran (Table 3, entry c and g)**



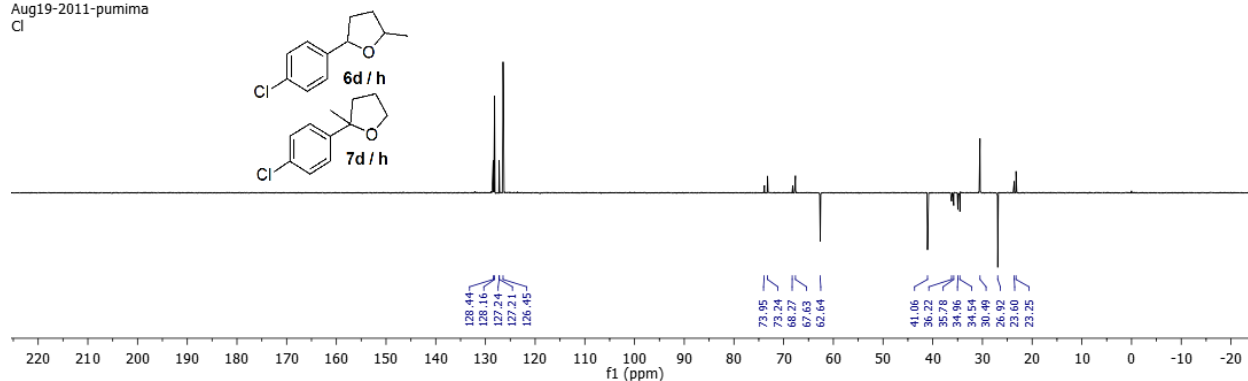
# GCMS for 2-methyl-2-(naphthalen-1-yl)-tetrahydrofuran (Table 3, entry c and g)



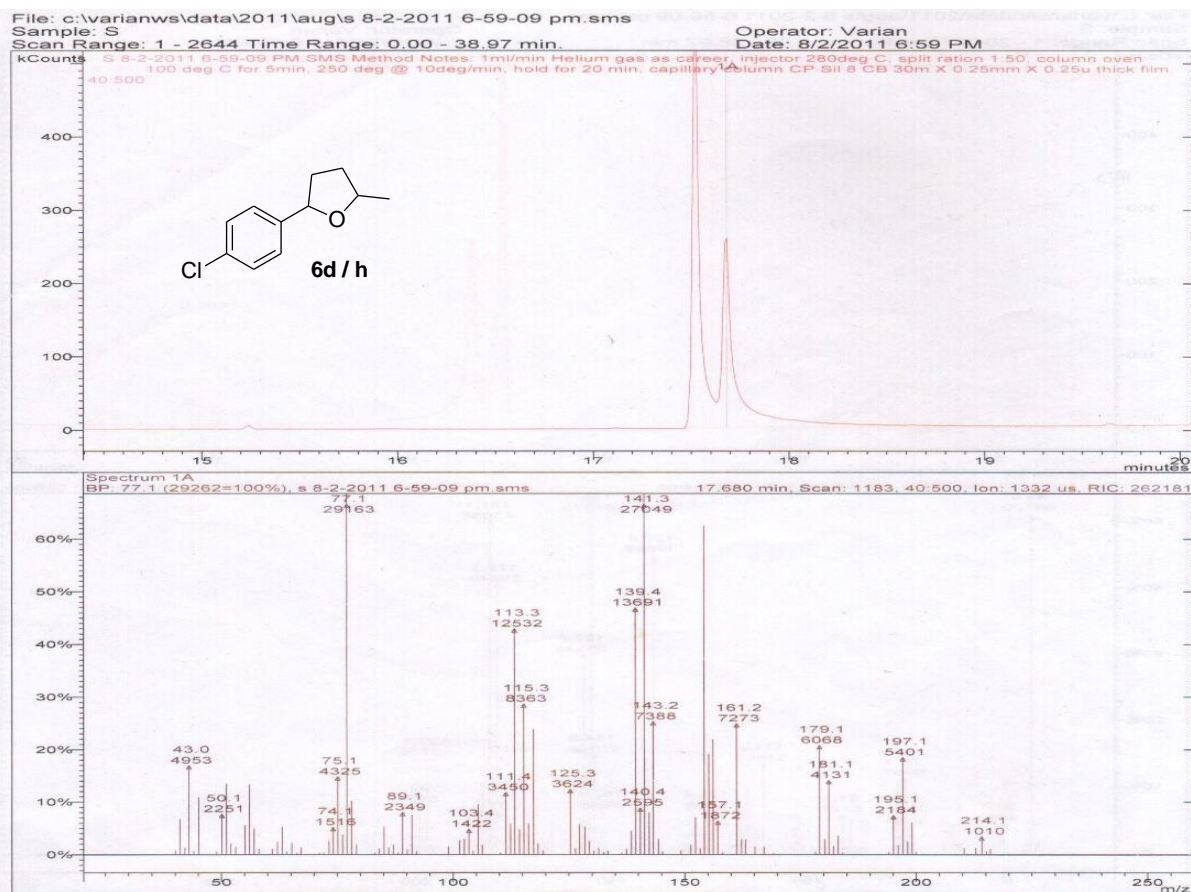


# DEPT at 135 for 2-(4-chlorophenyl)-5-methyl-tetrahydrofuran and 2-(4-chlorophenyl)-2-methyl-tetrahydrofuran in CDCl<sub>3</sub> (Table 3, entry d and h)

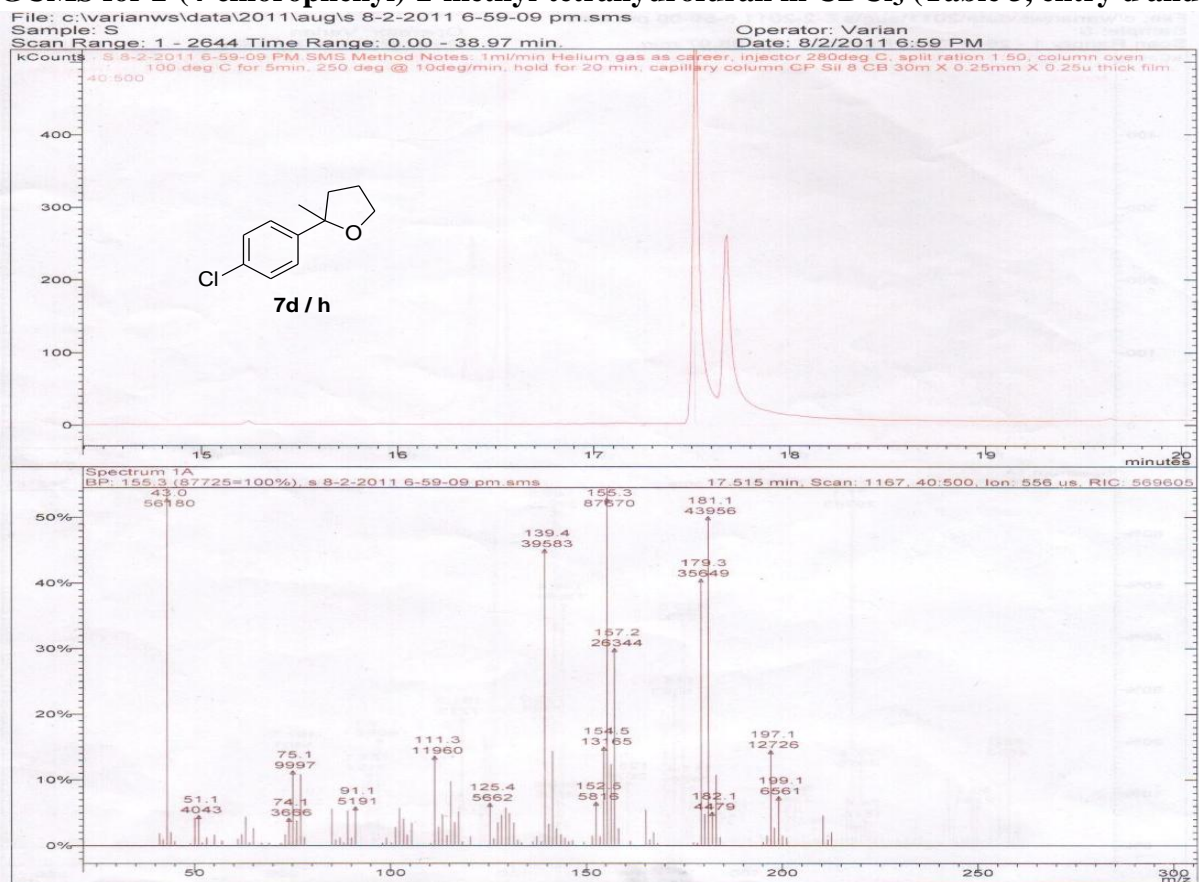
Aug19-2011-pumima  
Cl



## GCMS for 2-(4-chlorophenyl)-5-methyl-tetrahydrofuran (Table 3, entry d and h)

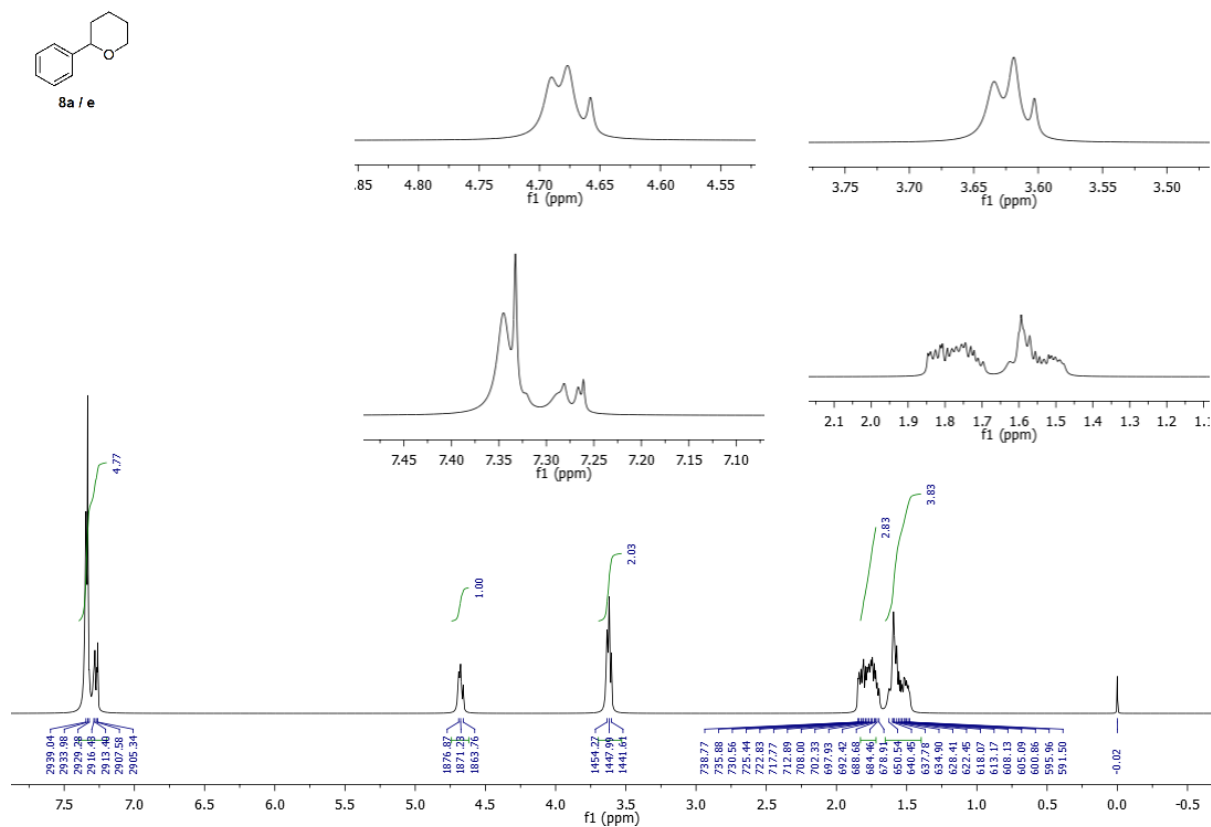


# GCMS for 2-(4-chlorophenyl)-2-methyl-tetrahydrofuran in CDCl<sub>3</sub> (Table 3, entry d and h)

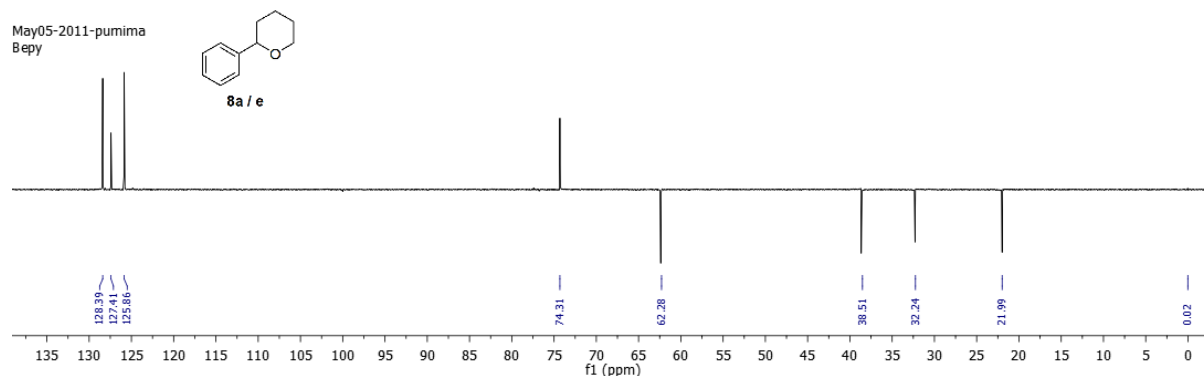




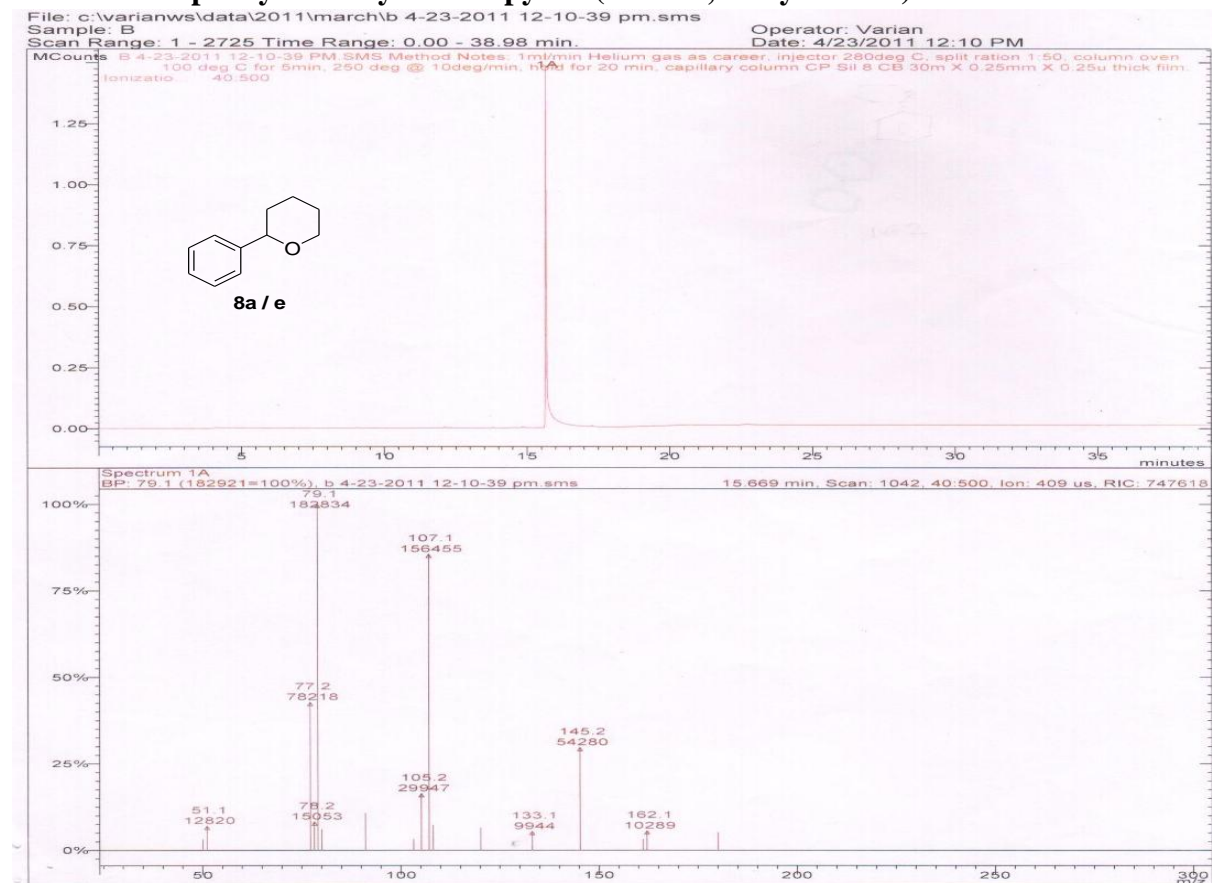
# **<sup>1</sup>H NMR for 2-phenyl-tetrahydro-2H-pyran in CDCl<sub>3</sub> (Table 4, entry a and e)**



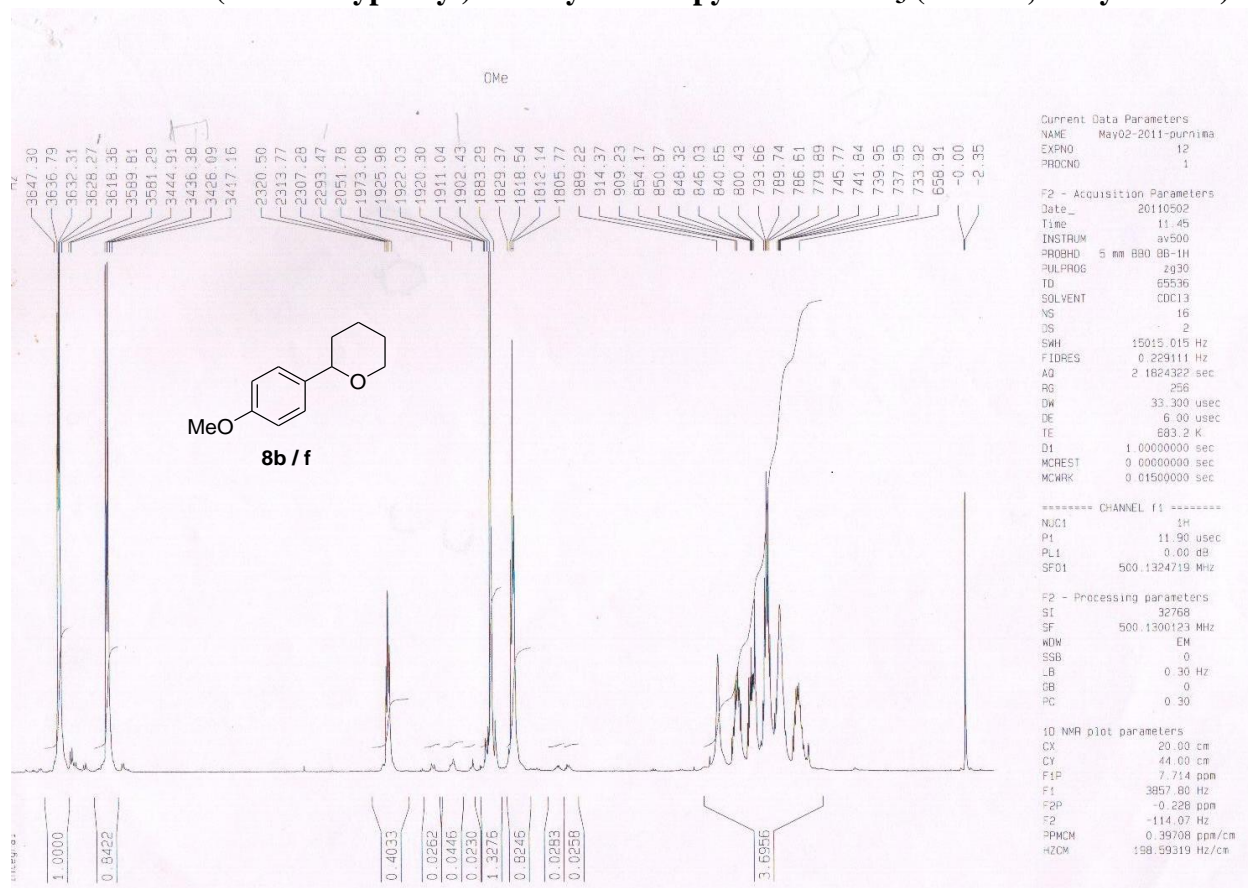
# DEPT at 135 for 2-phenyl-tetrahydro-2H-pyran in CDCl<sub>3</sub> (Table 4, entry a and e)



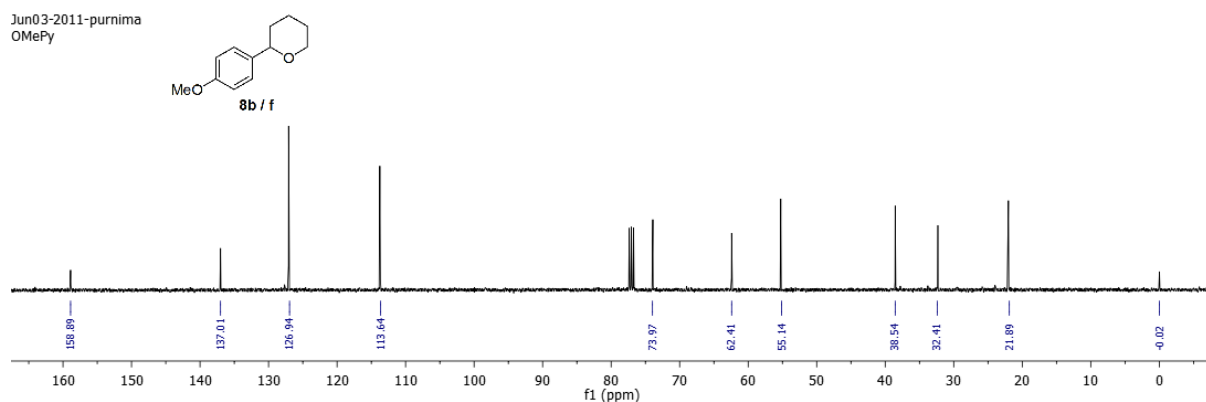
# GCMS for 2-phenyl-tetrahydro-2H-pyran (Table 4, entry a and e)



# **<sup>1</sup>H NMR for 2-(4-methoxyphenyl)-tetrahydro-2H-pyran in CDCl<sub>3</sub> (Table 4, entry b and f)**

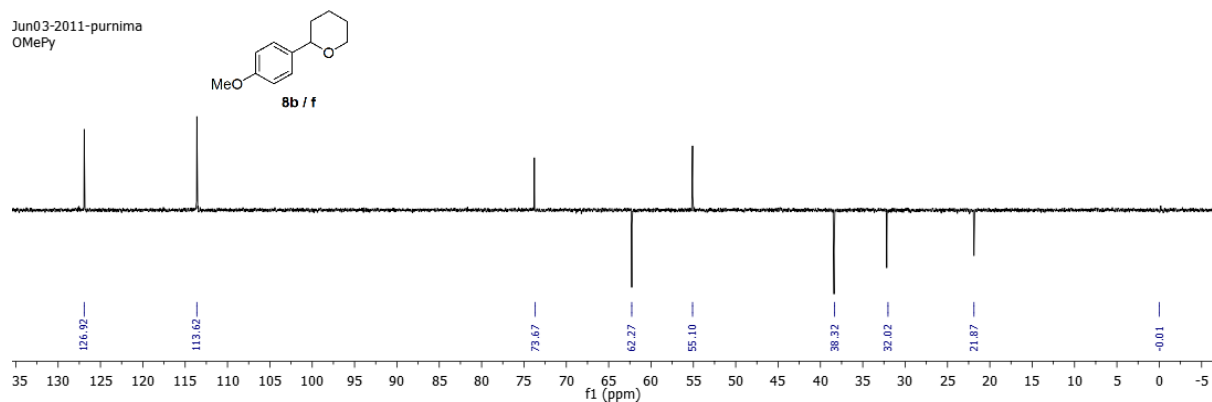


# **<sup>13</sup>C NMR for 2-(4-methoxyphenyl)-tetrahydro-2H-pyran in CDCl<sub>3</sub> (Table 4, entry b and f)**

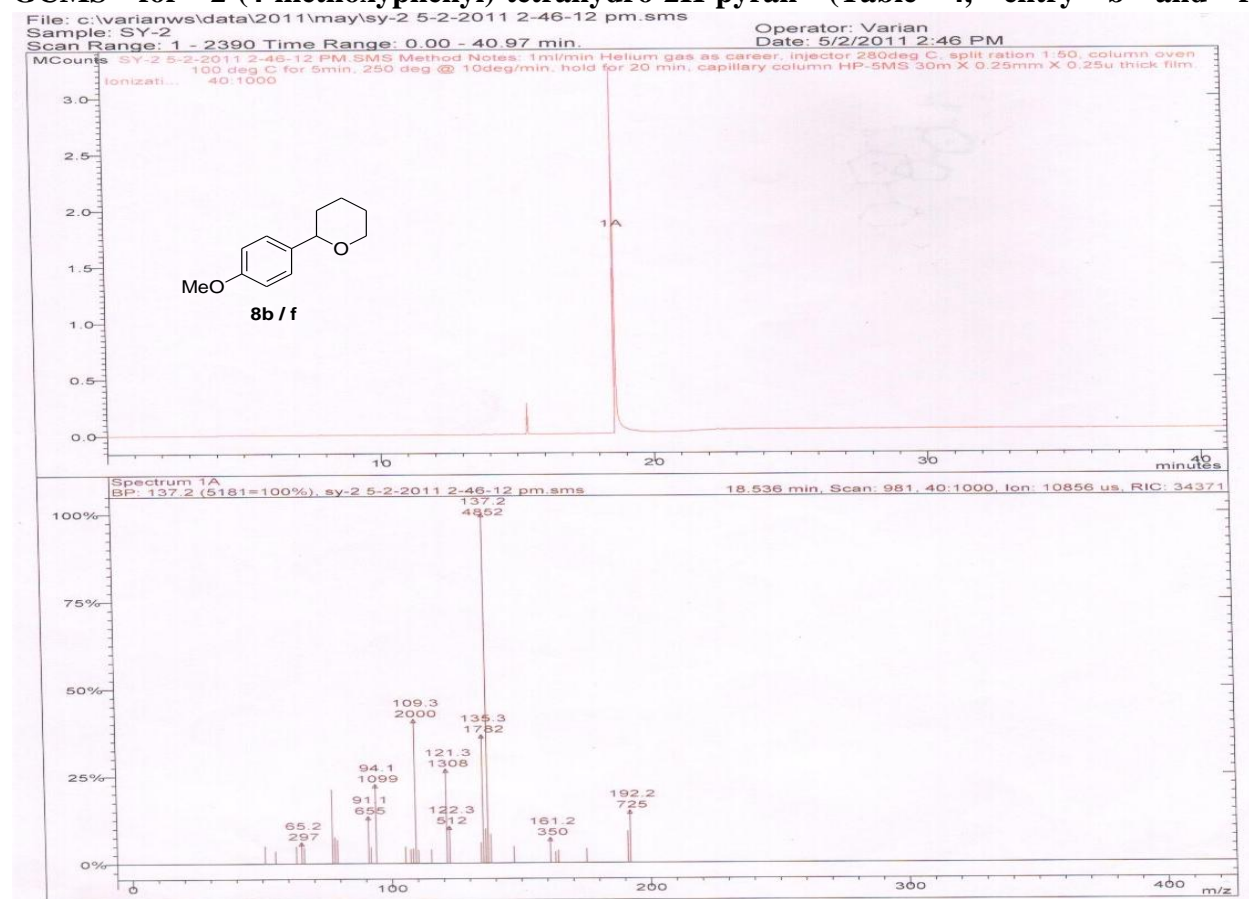




# DEPT at 135 for 2-(4-methoxyphenyl)-tetrahydro-2H-pyran in CDCl<sub>3</sub> (Table 4, entry b and f)

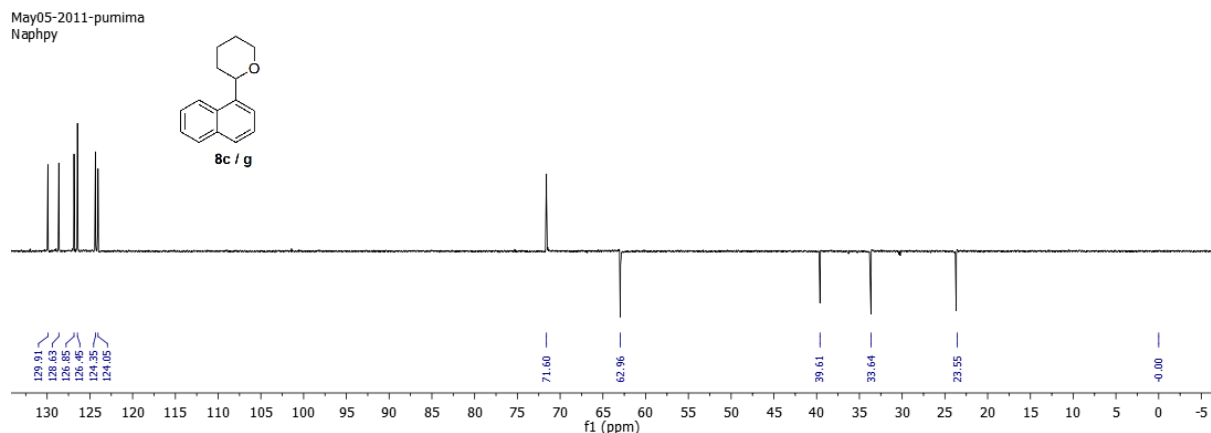


# GCMS for 2-(4-methoxyphenyl)-tetrahydro-2H-pyran (Table 4, entry b and f)

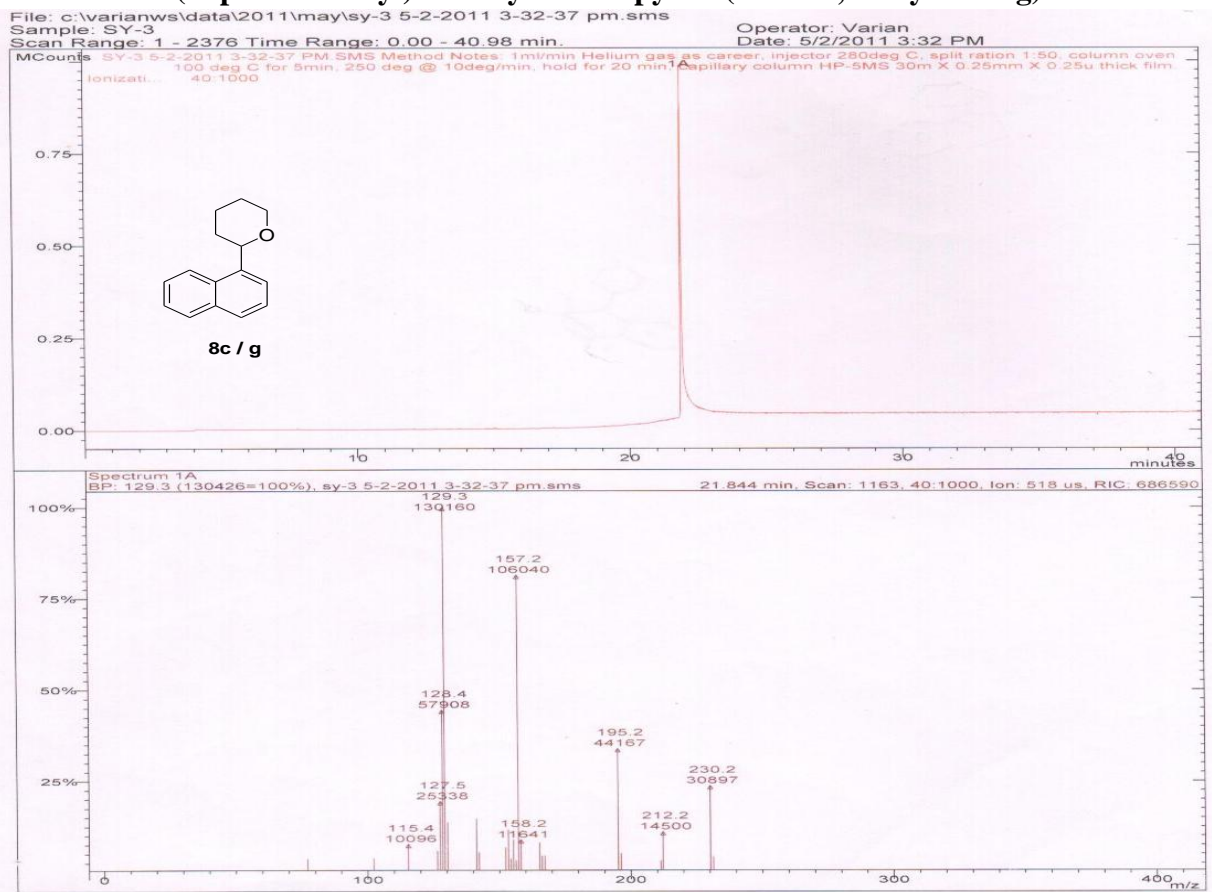




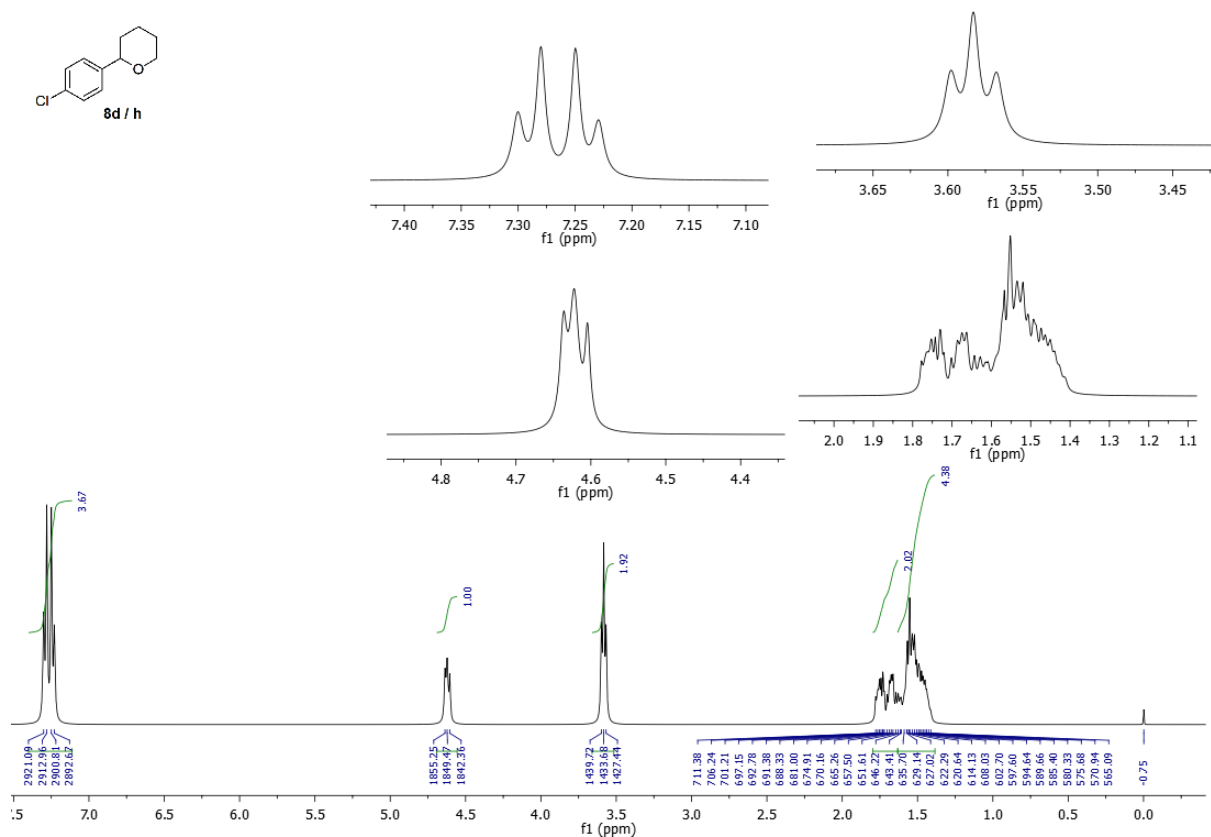
**DEPT at 135 for 2-(naphthalen-1-yl)-tetrahydro-2H-pyran in CD<sub>3</sub>OD (Table 4, entry c and g)**



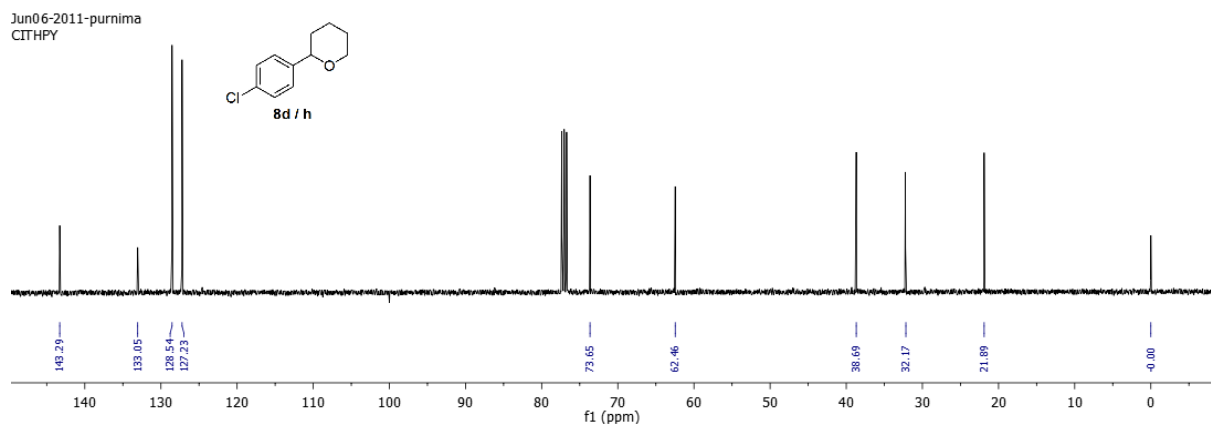
**GCMS for 2-(naphthalen-1-yl)-tetrahydro-2H-pyran (Table 4, entry c and g)**



**<sup>1</sup>H NMR for 2-(4-chlorophenyl)-tetrahydro-2H-pyran in CDCl<sub>3</sub> (Table 4, entry d and h)**

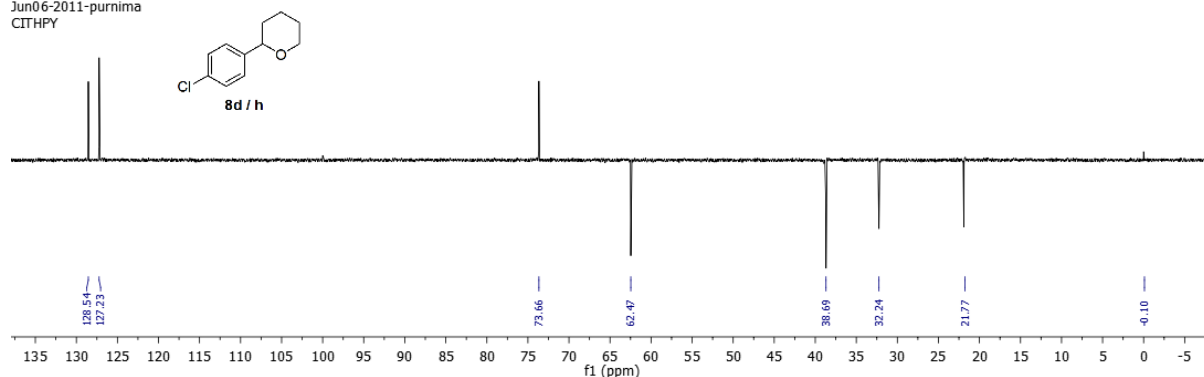


**<sup>13</sup>C NMR for 2-(4-chlorophenyl)-tetrahydro-2H-pyran in CDCl<sub>3</sub> (Table 4, entry d and h)**

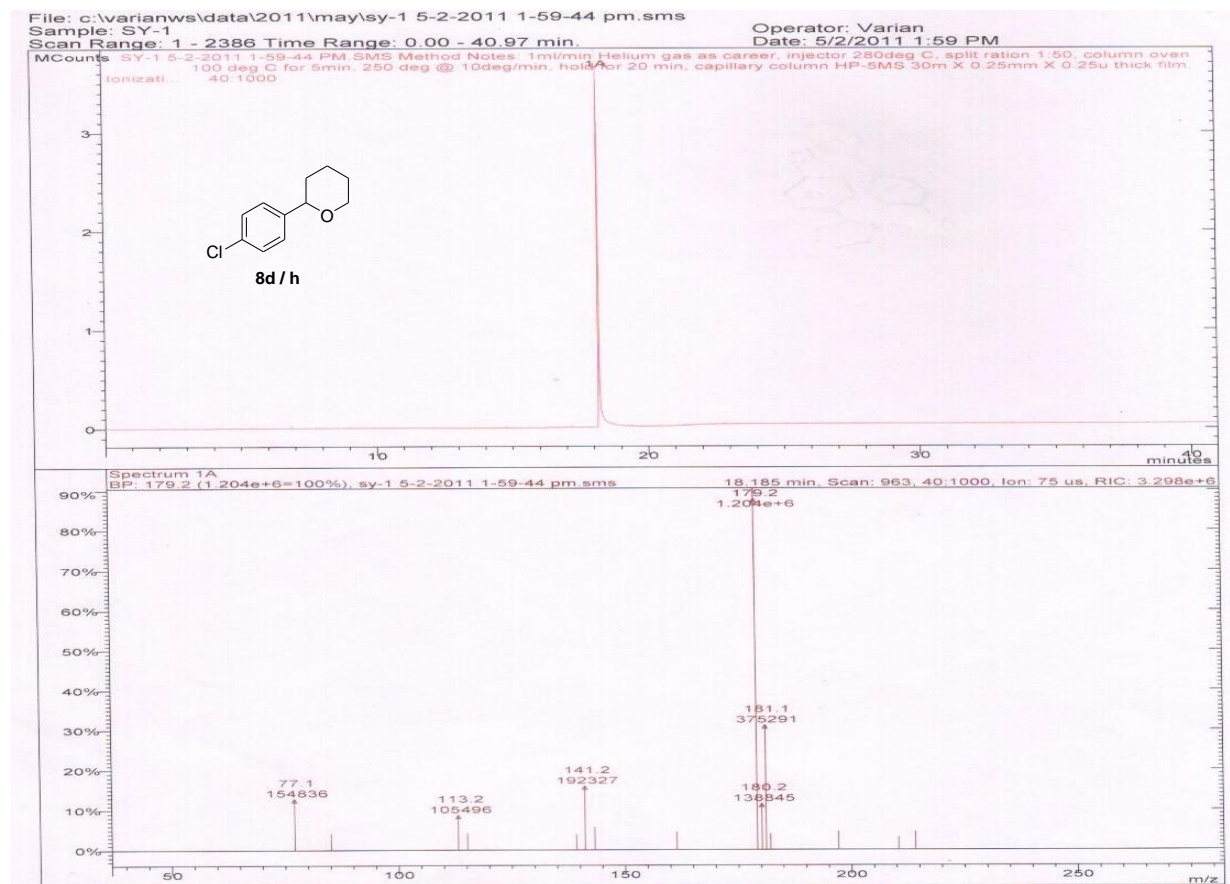


### DEPT at 135 for 2-(4-chlorophenyl)-tetrahydro-2H-pyran (Table 4, entry d and h)

Jun06-2011-purnima  
CITHPY



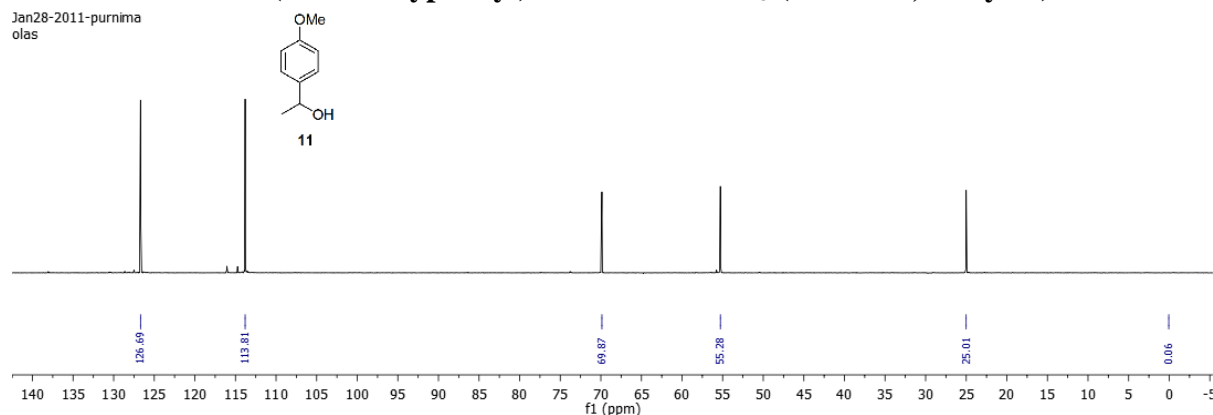
### GCMS for 2-(4-chlorophenyl)-tetrahydro-2H-pyran (Table 4, entry d and h)





# DEPT at 135 for 1-(4-methoxyphenyl) ethanol in CDCl<sub>3</sub> (scheme 2, entry 11)

Jan28-2011-purnima  
olas



# GCMS for 1-(4-methoxyphenyl) ethanol (scheme 2, entry 11)

