Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Supplementary Information

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

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1.0 Tables

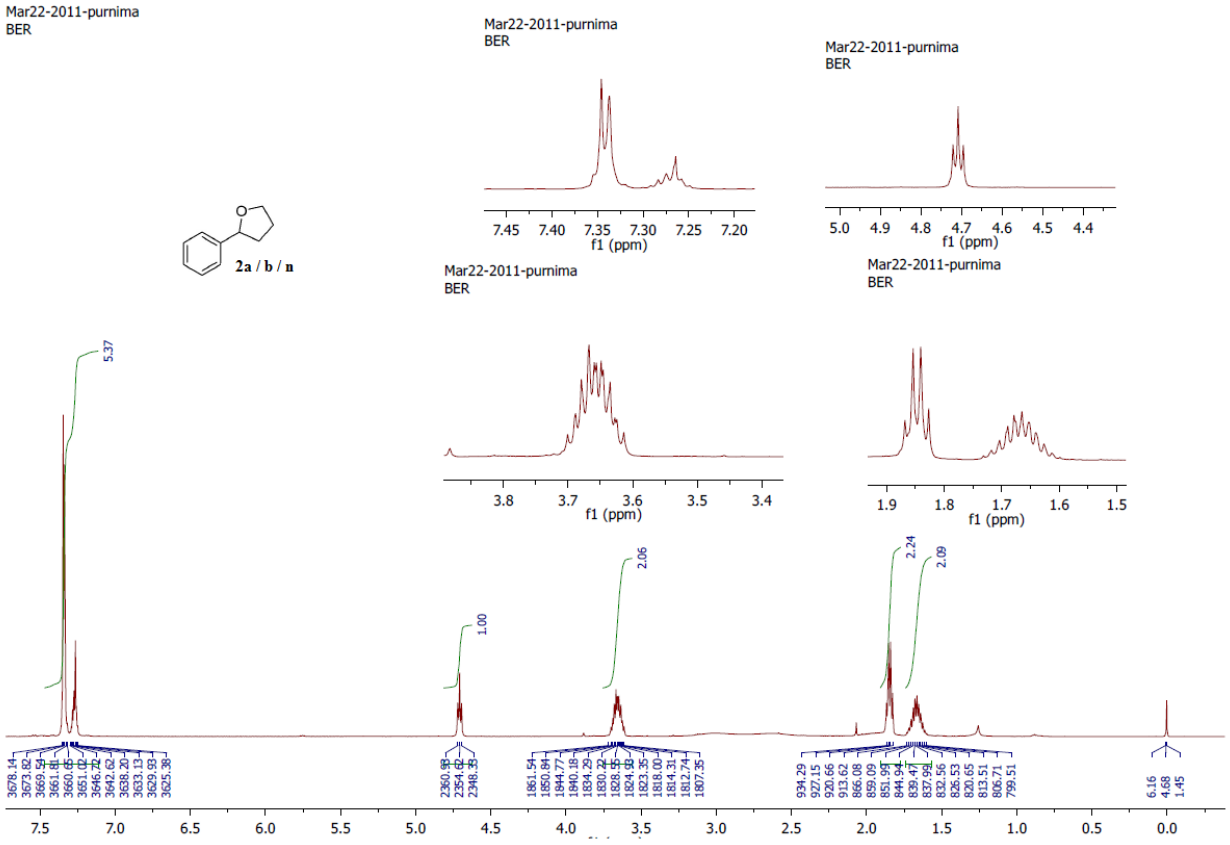
1.1 Table 5: containing chemical shift value of CH-Ar & CH-Alkyl

S. No.	Entry	δ CH-Ar & CH-Alkyl (^{1}H NMR)	C-Ar & CH-Alkyl ^{13}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 (brm),	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 **6a/e**	73.83 **(6a/e)**, 74.18 **(7a/e)**	73.90 **(6a/e)**
17	6/7b & f	4.62-4.69 (m) for **6b/f**	73.59 **(6b/f)**, 73.93 **(7b/f)**	73.59 **(6b/f)**
18	6/7c & g	5.47-5.54 (m) for **6c/g**	70.47 **(6c/g)**, 75.81 **(7c/g)**	70.47 **(6c/g)**
19	6/7d & h	4.68-4.71 (m) for **6d/h**	73.24 **(6d/h)**, 73.86 **(7d/h)**	73.24 **(6d/h)**
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	11	4.61-4.88 (q)	69.86	69.87

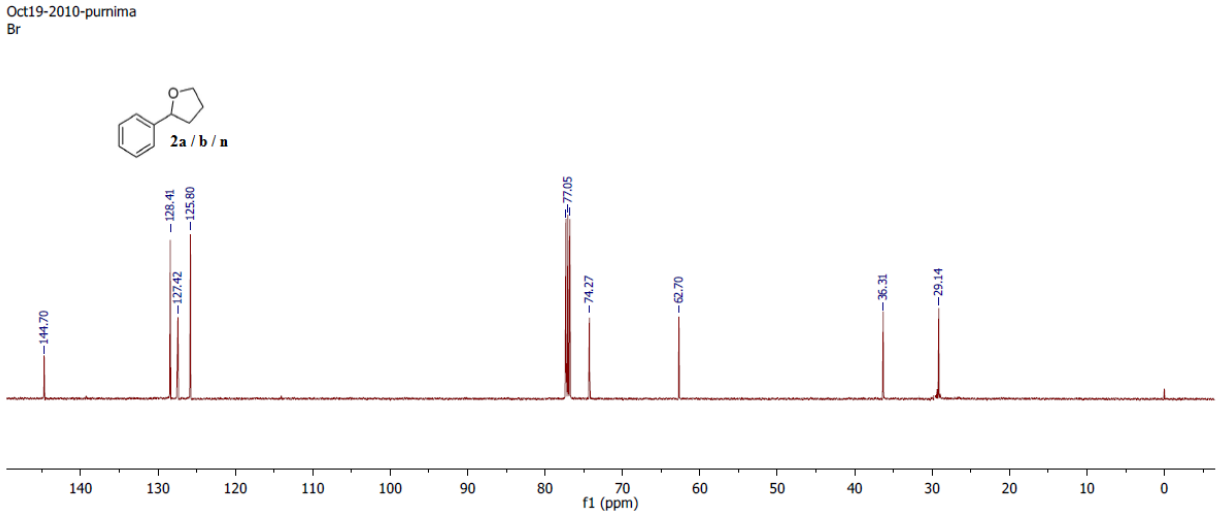
Table 5: Chemical shift value of CH-Ar & CH-Alkyl

2.1 Scanned spectra of compounds:

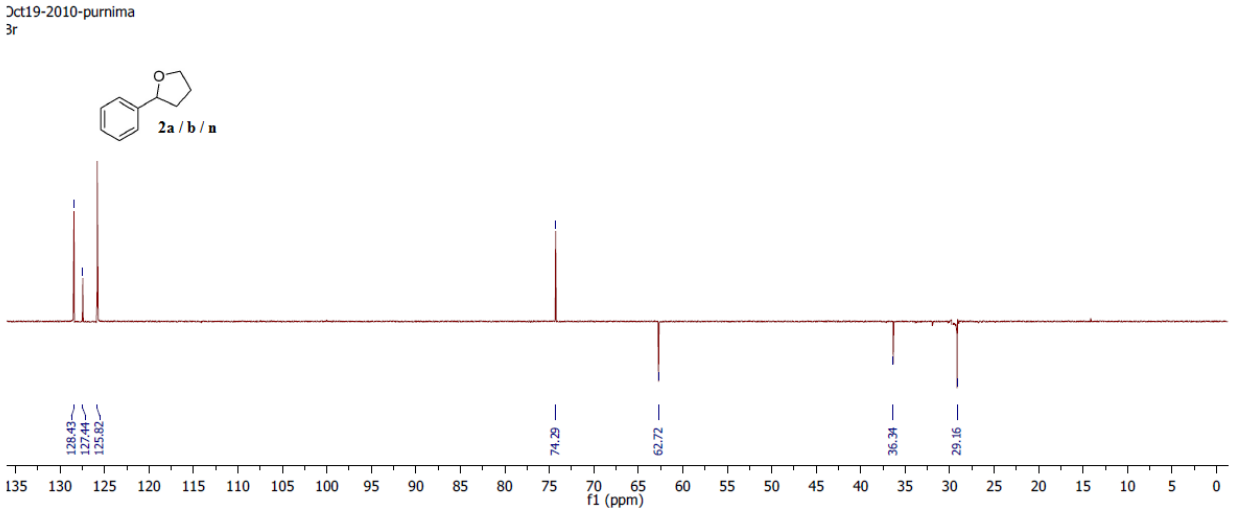
^{1}H NMR for tetrahydro-2-phenylfuran in $CDCl_3$ (Table 2, entry a, b and n)



^{13}C NMR for tetrahydro-2-phenylfuran in $CDCl_3$ (Table 2, entry a, b and n)

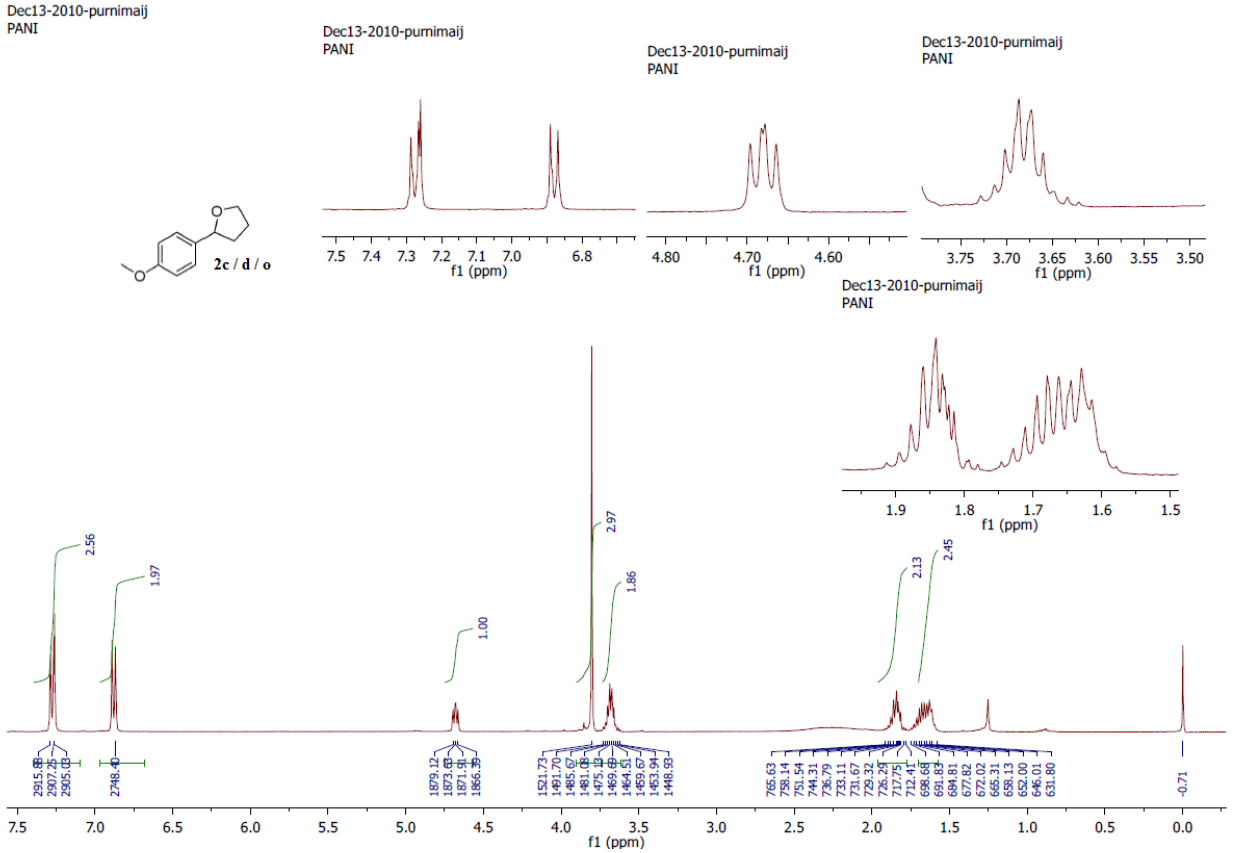


DEPT at 135 for tetrahydro-2-phenylfuran in $CDCl_3$ (Table 2, entry a, b and n)

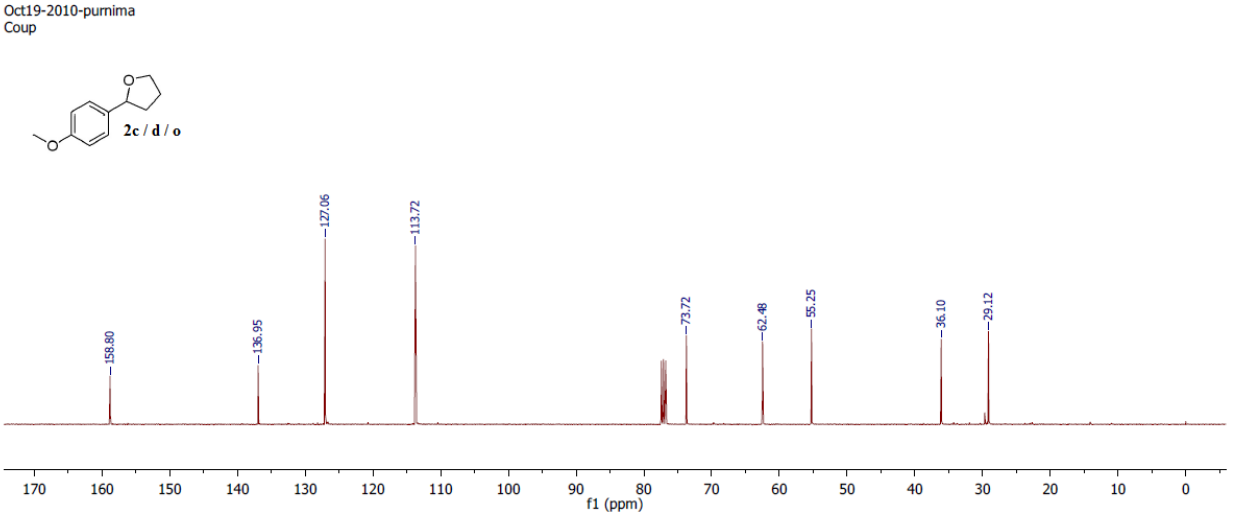


GCMS for tetrahydro-2-phenylfuran (Table 2, entry a, b and n)

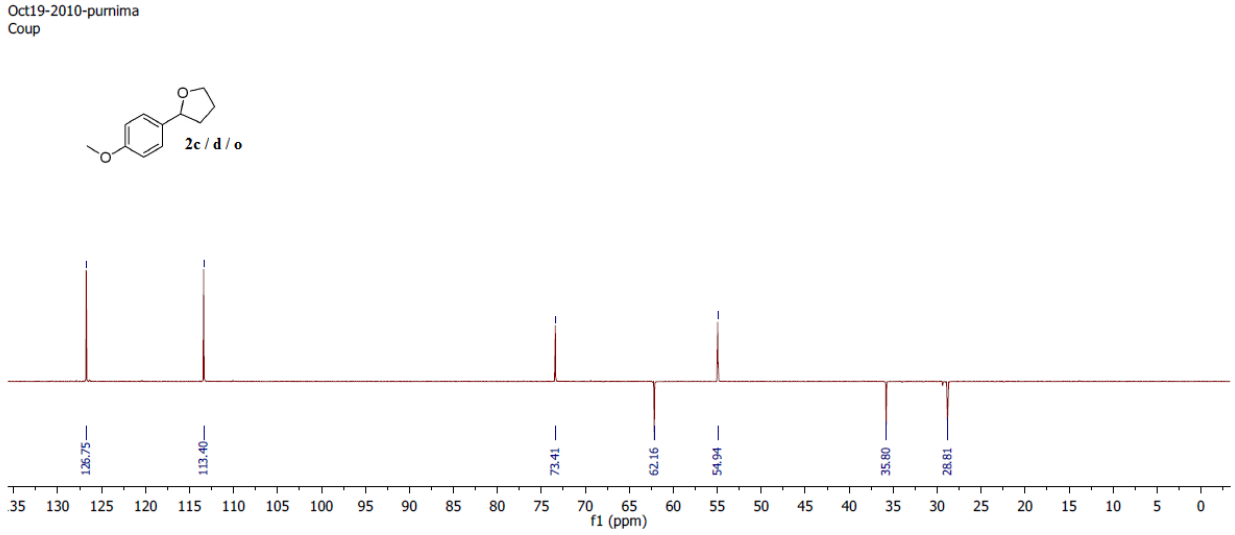
^{1}H NMR for tetrahydro-2-(4-methoxyphenyl)furan in $CDCl_3$ (Table 2, entry c, d and o)



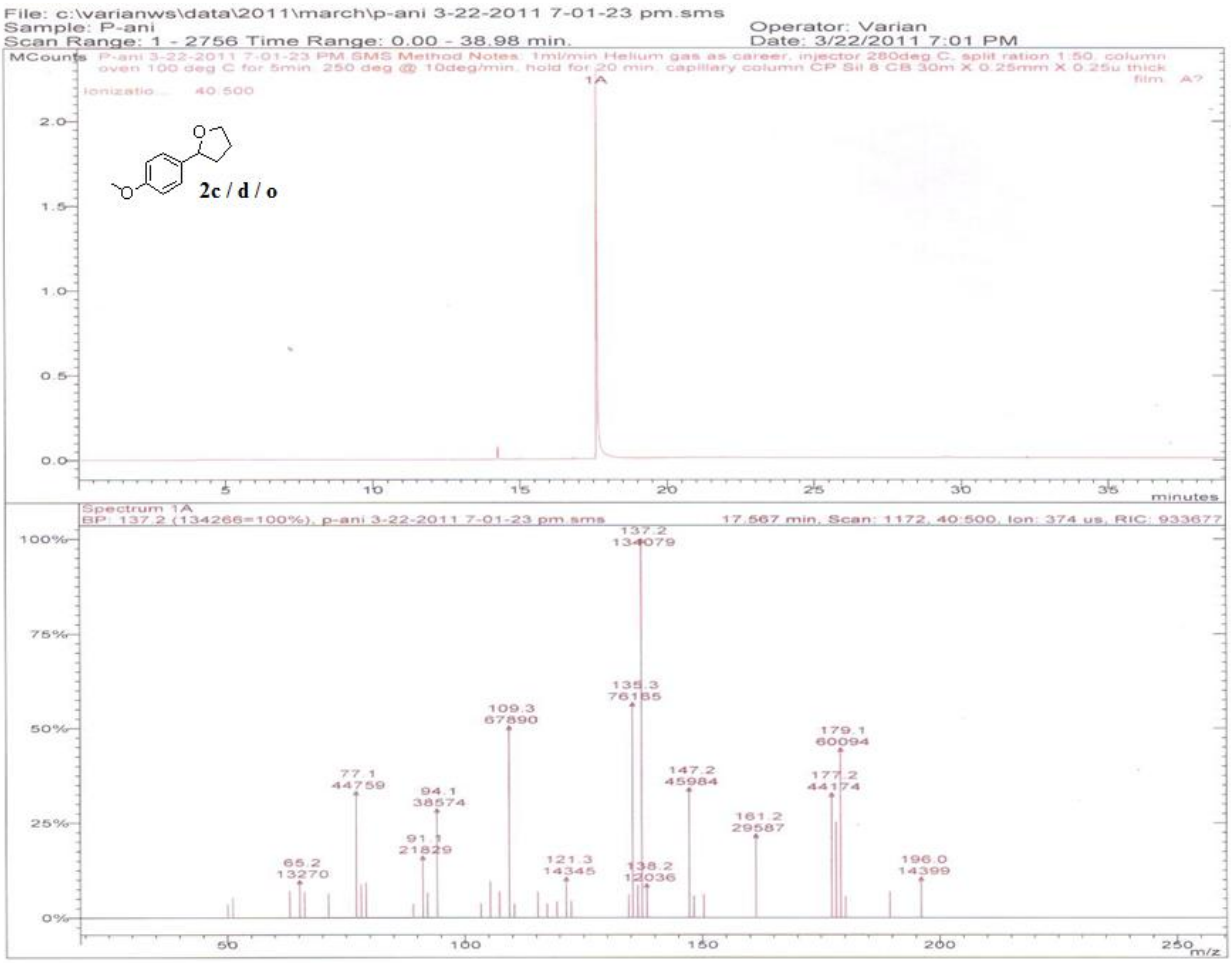
^{13}C NMR for tetrahydro-2-(4-methoxyphenyl)furan in $CDCl_3$ (Table 2, entry c, d and o)



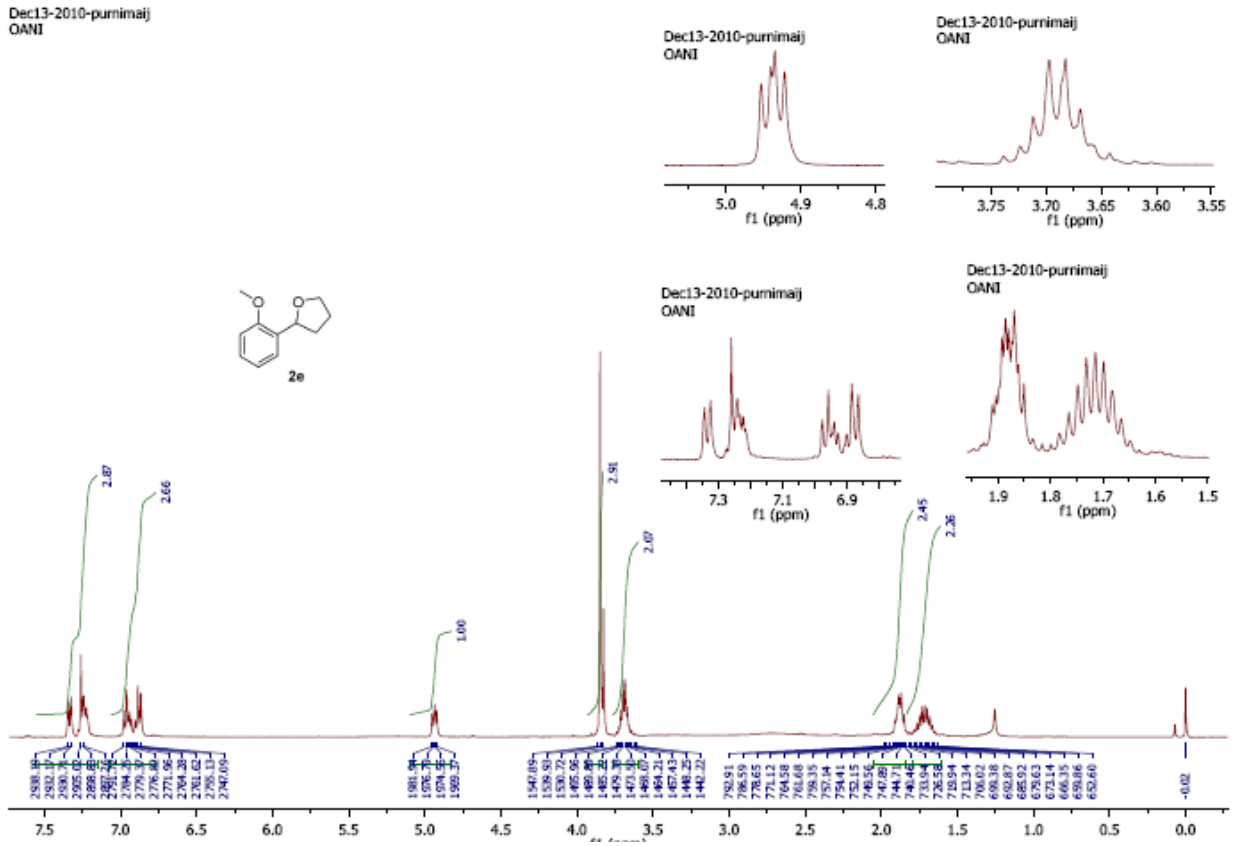
DEPT at 135 for tetrahydro-2-(4-methoxyphenyl)furan in $CDCl_3$ (Table 2, entry c, d and o)



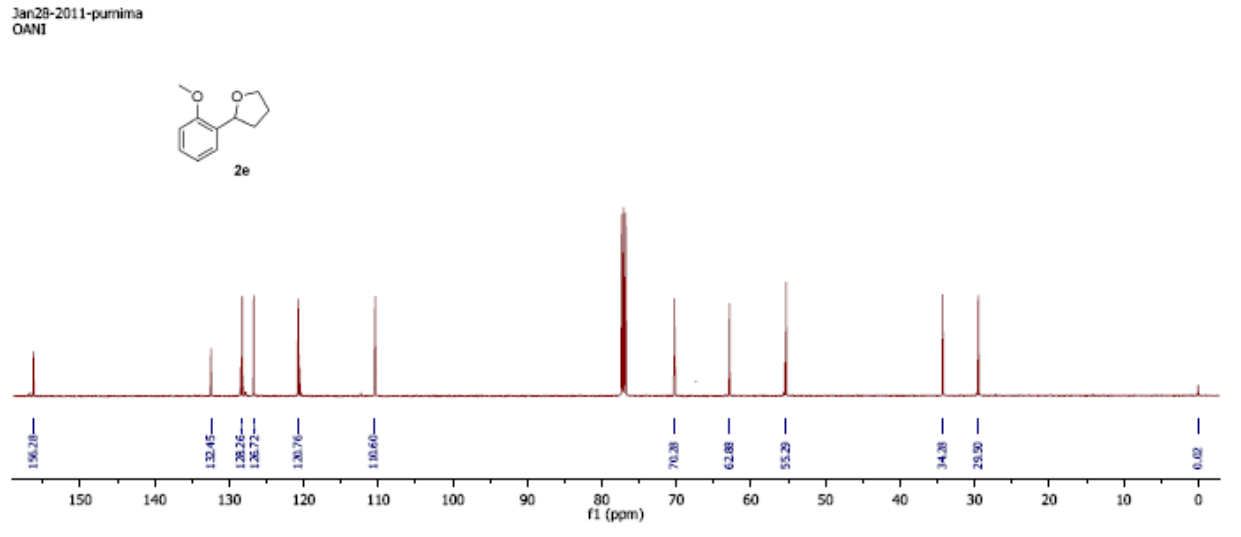
GCMS for tetrahydro-2-(4-methoxyphenyl)furan (Table 2, entry c, d and o)



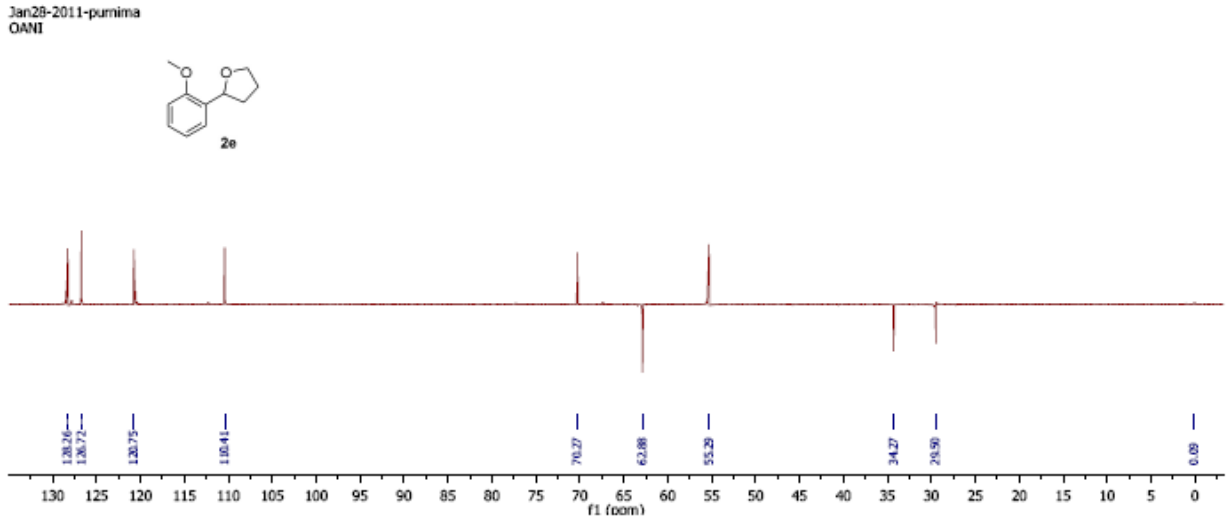
^{1}H NMR for tetrahydro-2-(2-methoxyphenyl)furan in $CDCl_3$ (Table 2, entry e)



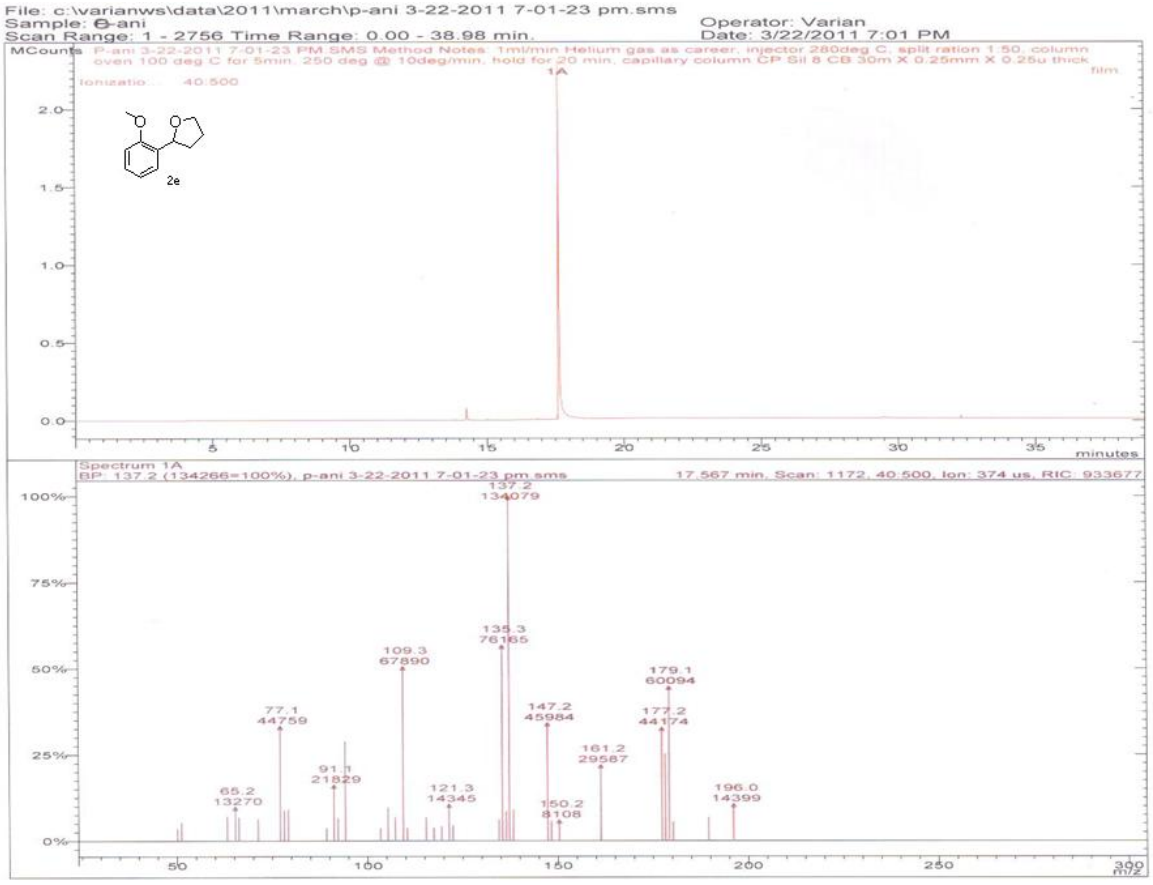
^{13}C NMR for tetrahydro-2-(2-methoxyphenyl)furan in $CDCl_3$ (Table 2, entry e)



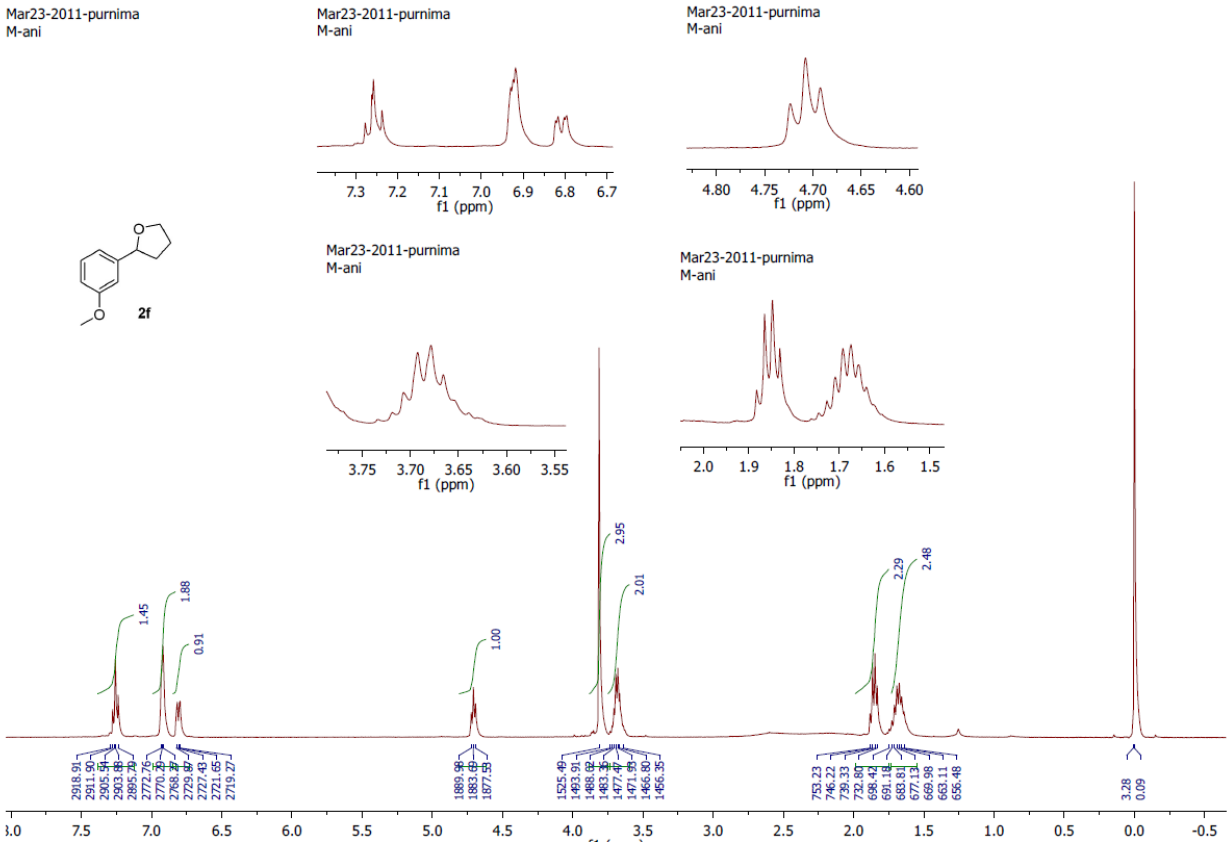
DEPT at 135 for tetrahydro-2-(2-methoxyphenyl)furan in $CDCl_3$ (Table 2, entry e)



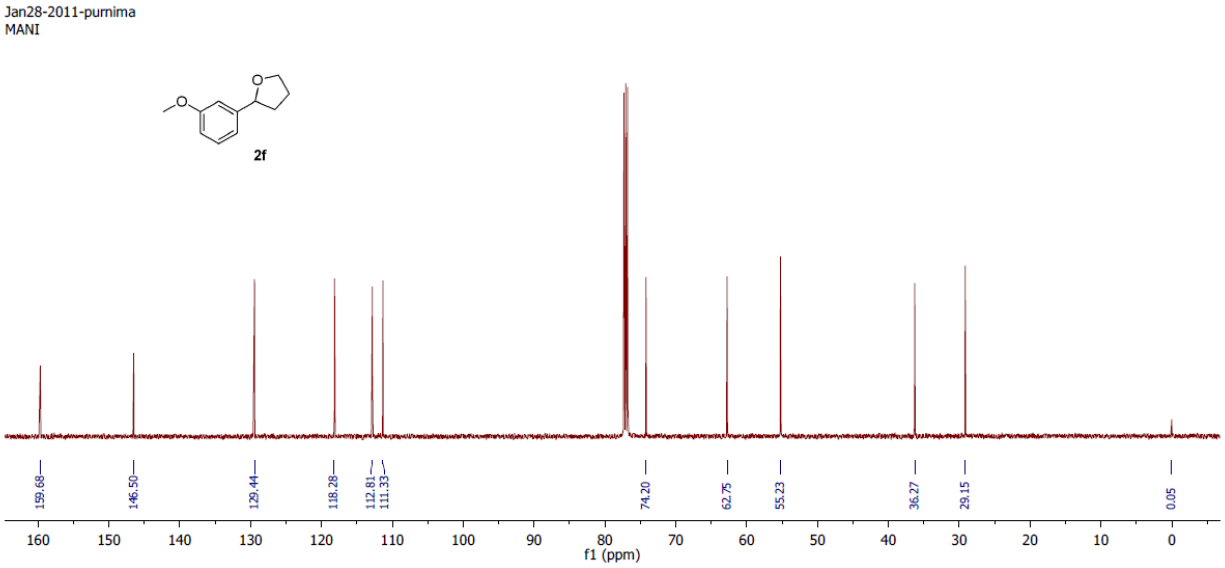
GCMS for tetrahydro-2-(2-methoxyphenyl)furan (Table 2, entry e)



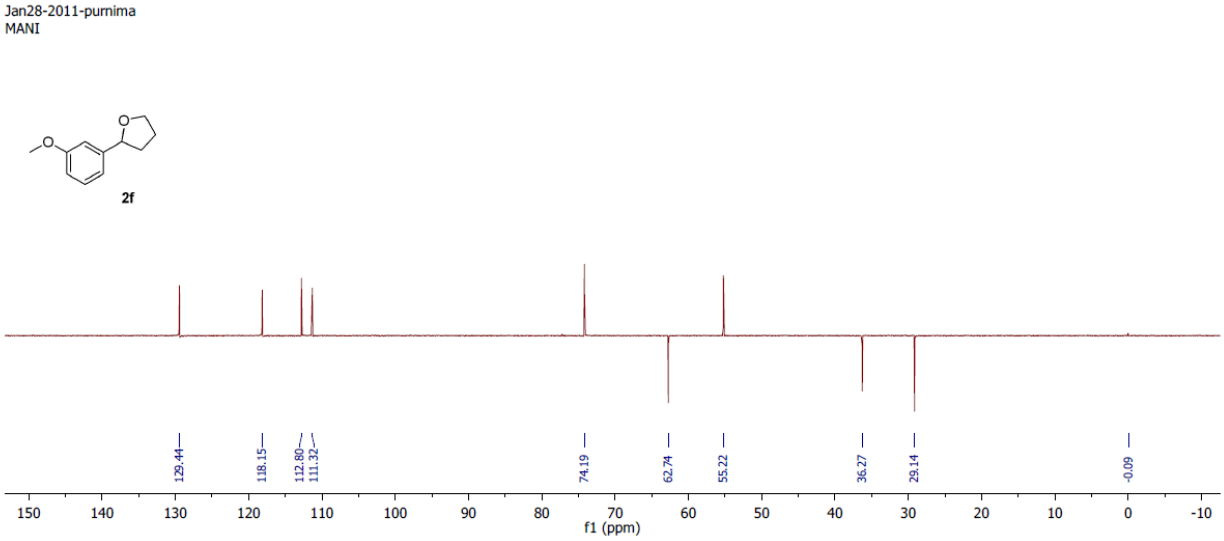
^{1}H NMR for tetrahydro-2-(3-methoxyphenyl)furan in $CDCl_3$ (Table 2, entry f)



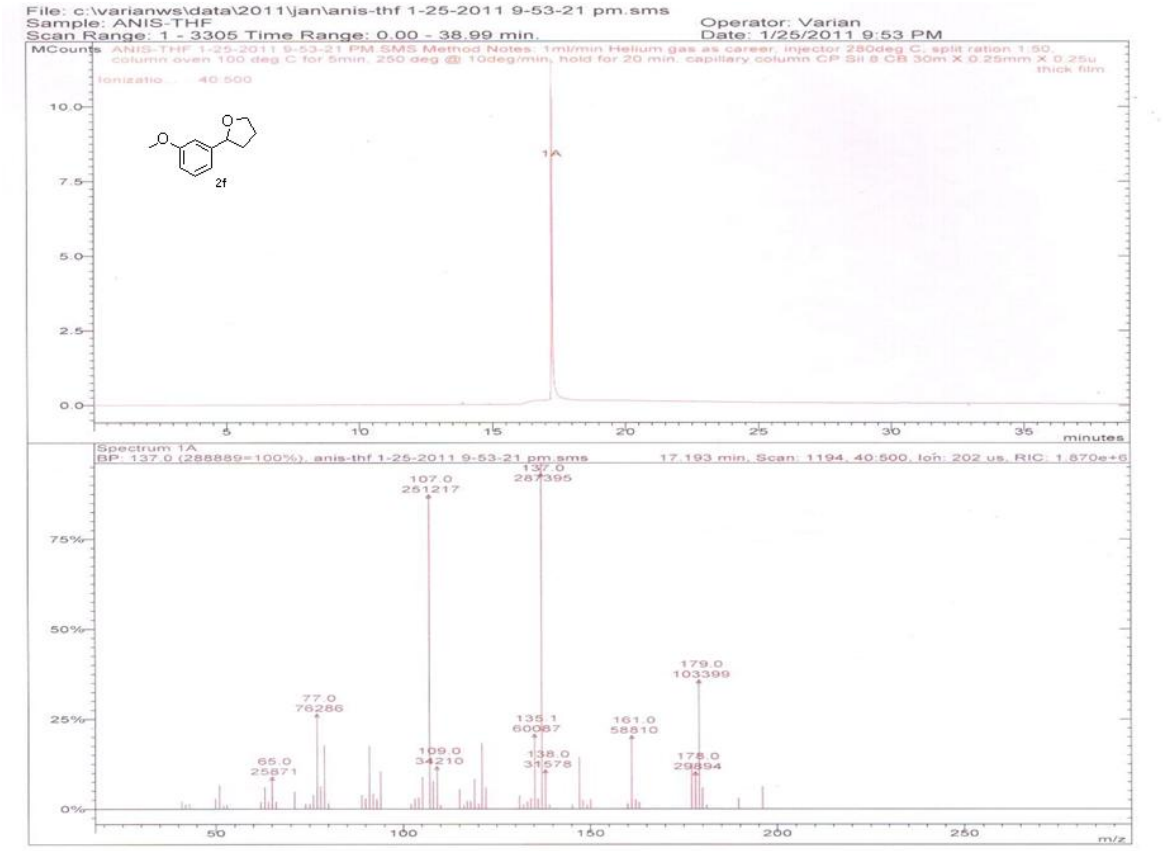
^{13}C NMR for tetrahydro-2-(3-methoxyphenyl)furan in $CDCl_3$ (Table 2, entry f)



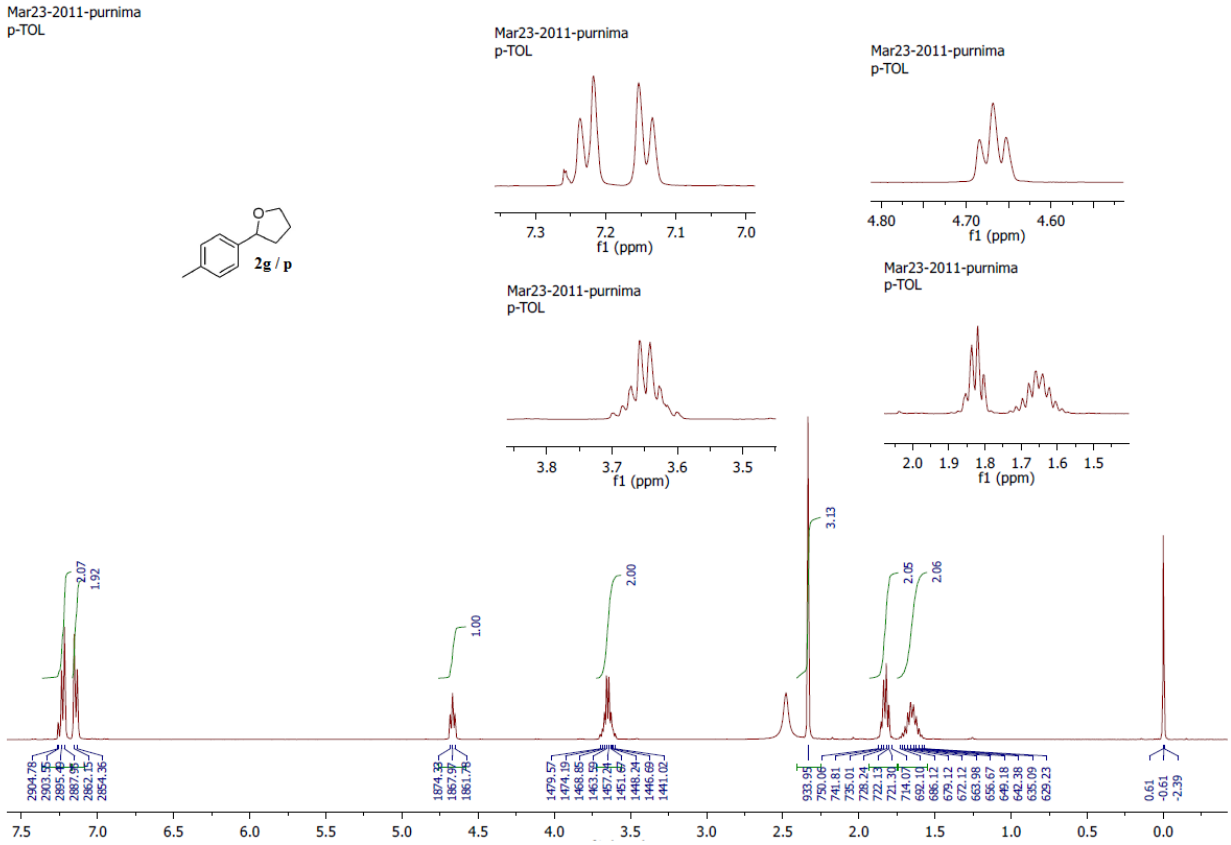
DEPT at 135 for tetrahydro-2-(3-methoxyphenyl)furan in $CDCl_3$ (Table 2, entry f)



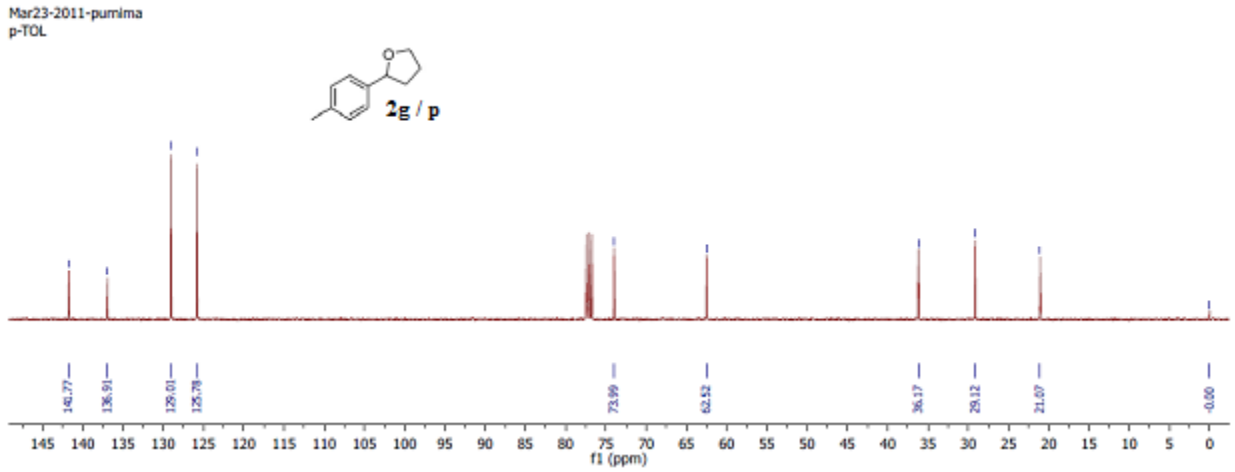
GCMS for tetrahydro-2-(3-methoxyphenyl)furan (Table 2, entry f)



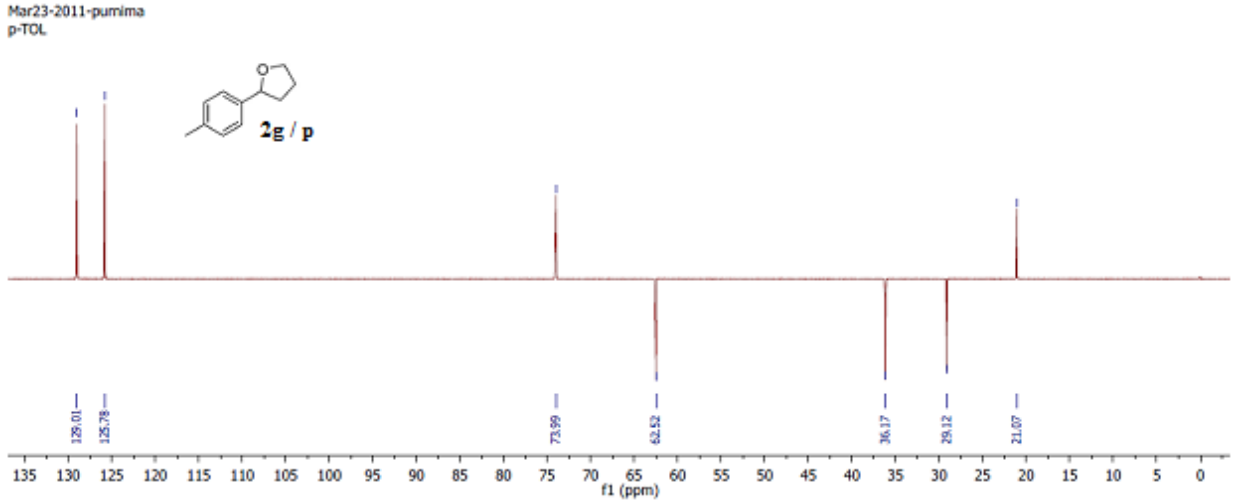
^{1}H NMR for tetrahydro-2-*p*-tolylfuran in $CDCl_3$ (Table 2, entry g and p)



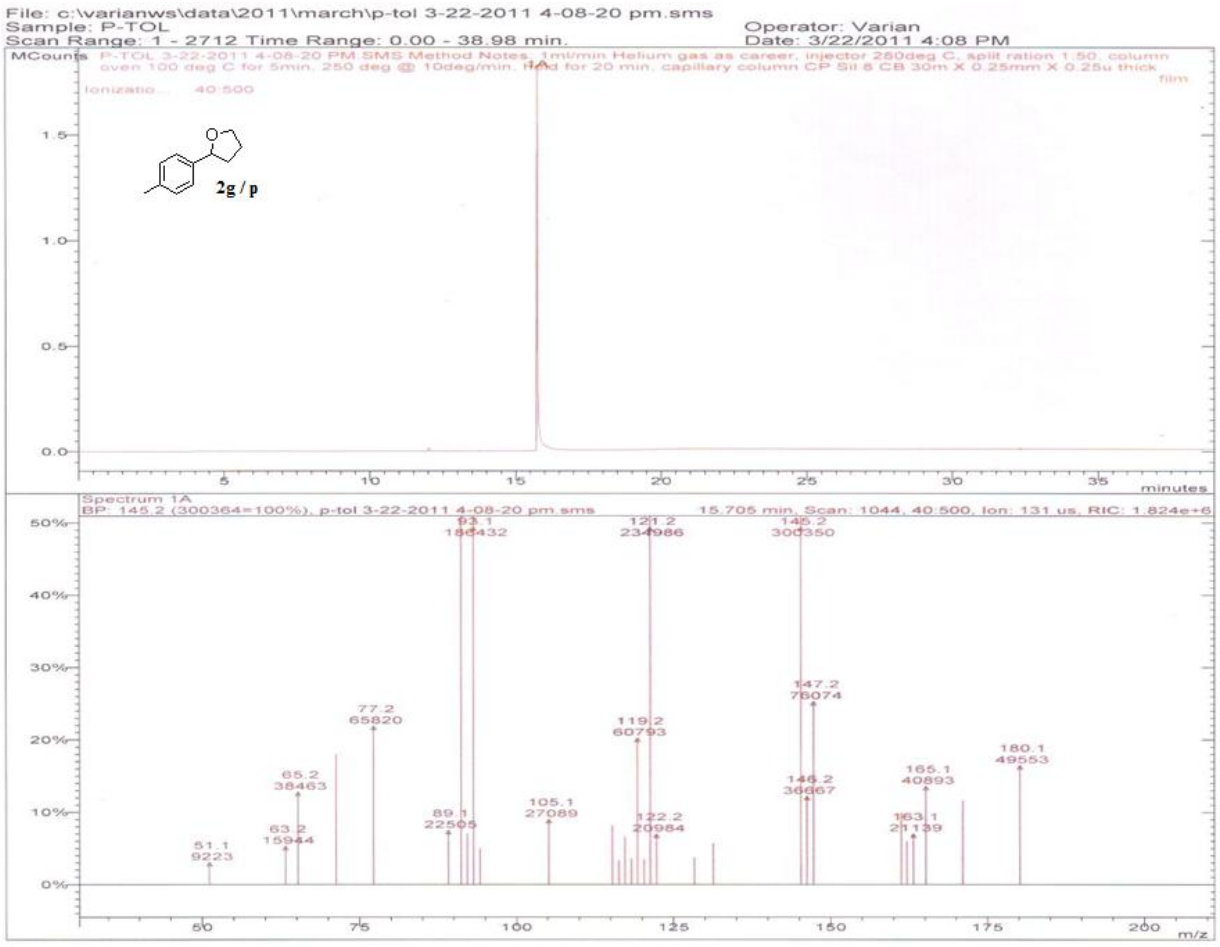
^{13}C NMR for tetrahydro-2-*p*-tolylfuran in $CDCl_3$ (Table 2, entry g and p)



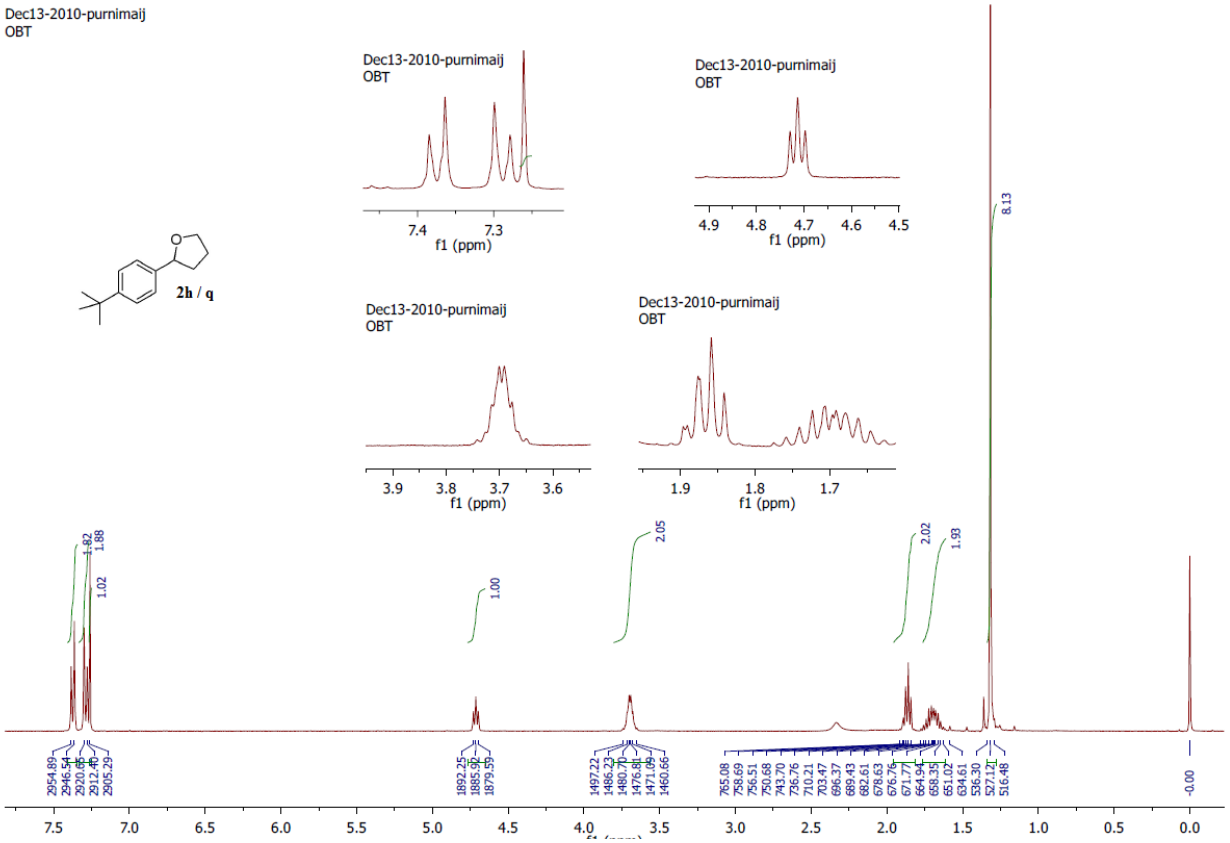
DEPT at 135 for tetrahydro-2-*p*-tolylfuran in $CDCl_3$ (Table 2, entry g and p)



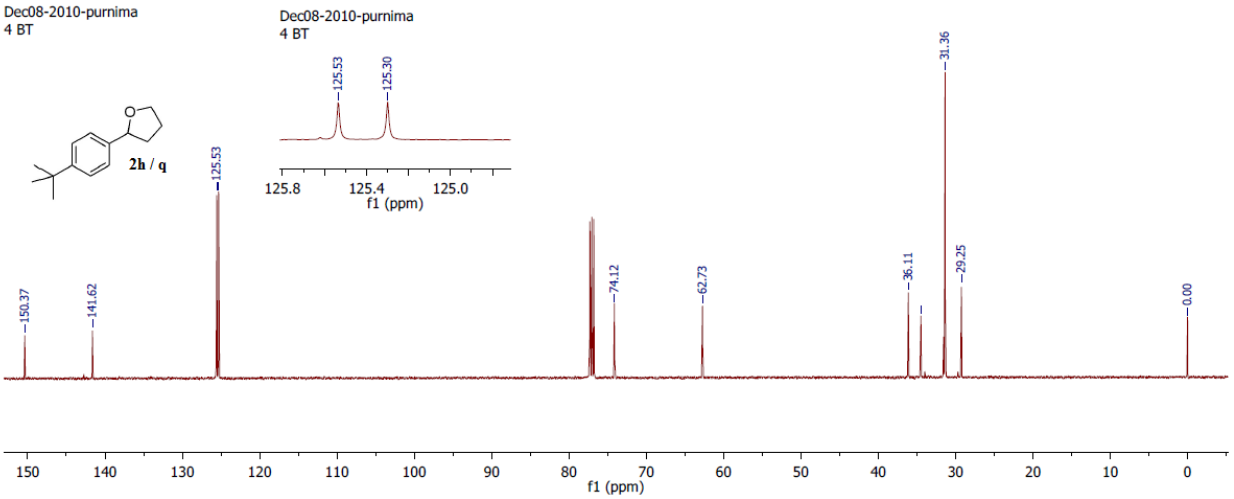
GCMS for tetrahydro-2-*p*-tolylfuran (Table 2, entry g and p)



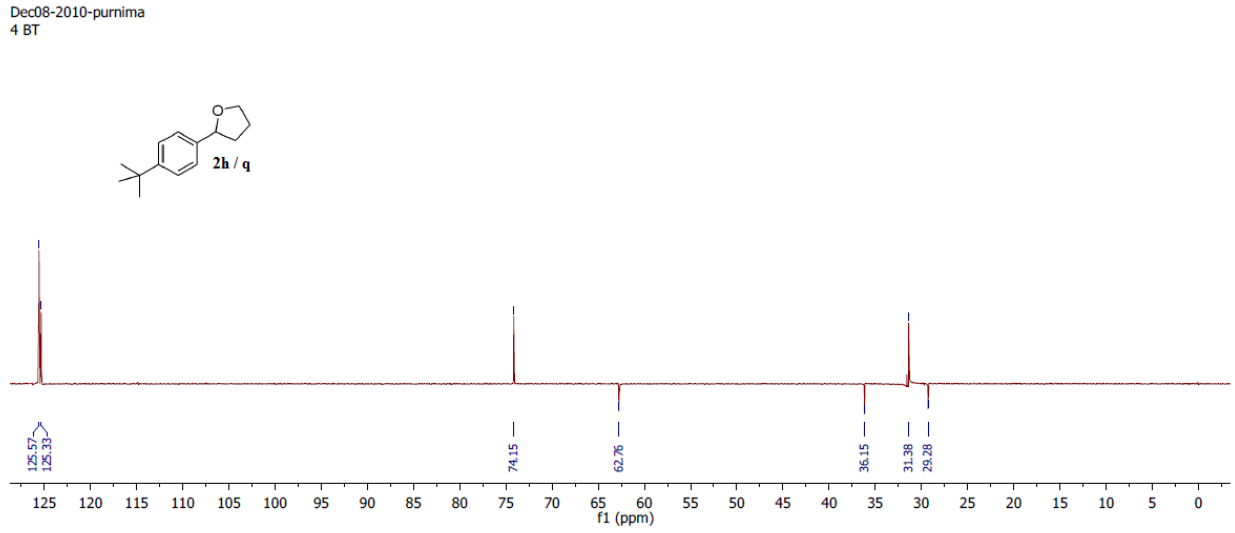
^{1}H NMR for 2-(4-*tert*-butylphenyl)-tetrahydrofuran in $CDCl_3$ (Table 2, entry h and q)



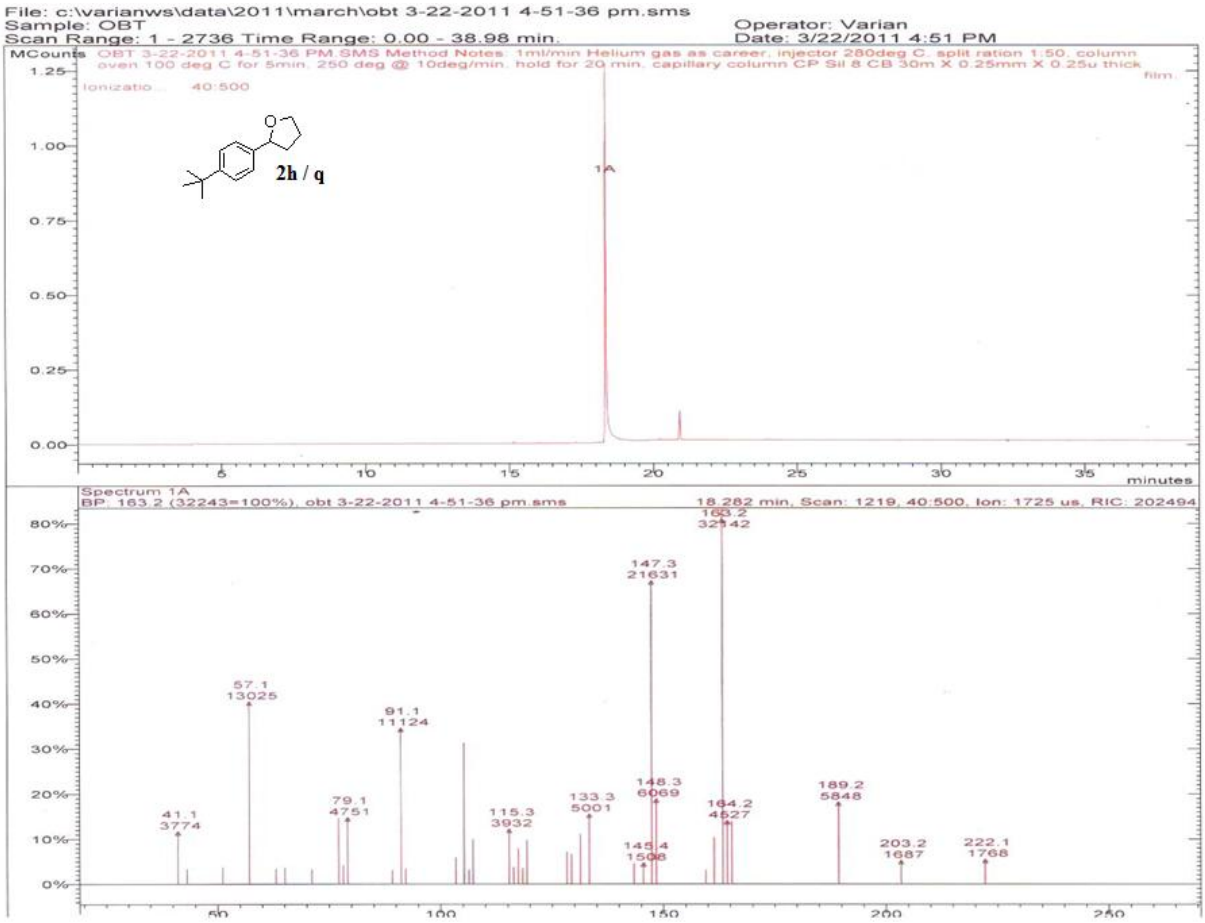
^{13}C NMR for 2-(4-*tert*-butylphenyl)-tetrahydrofuran in $CDCl_3$ (Table 2, entry h and q)



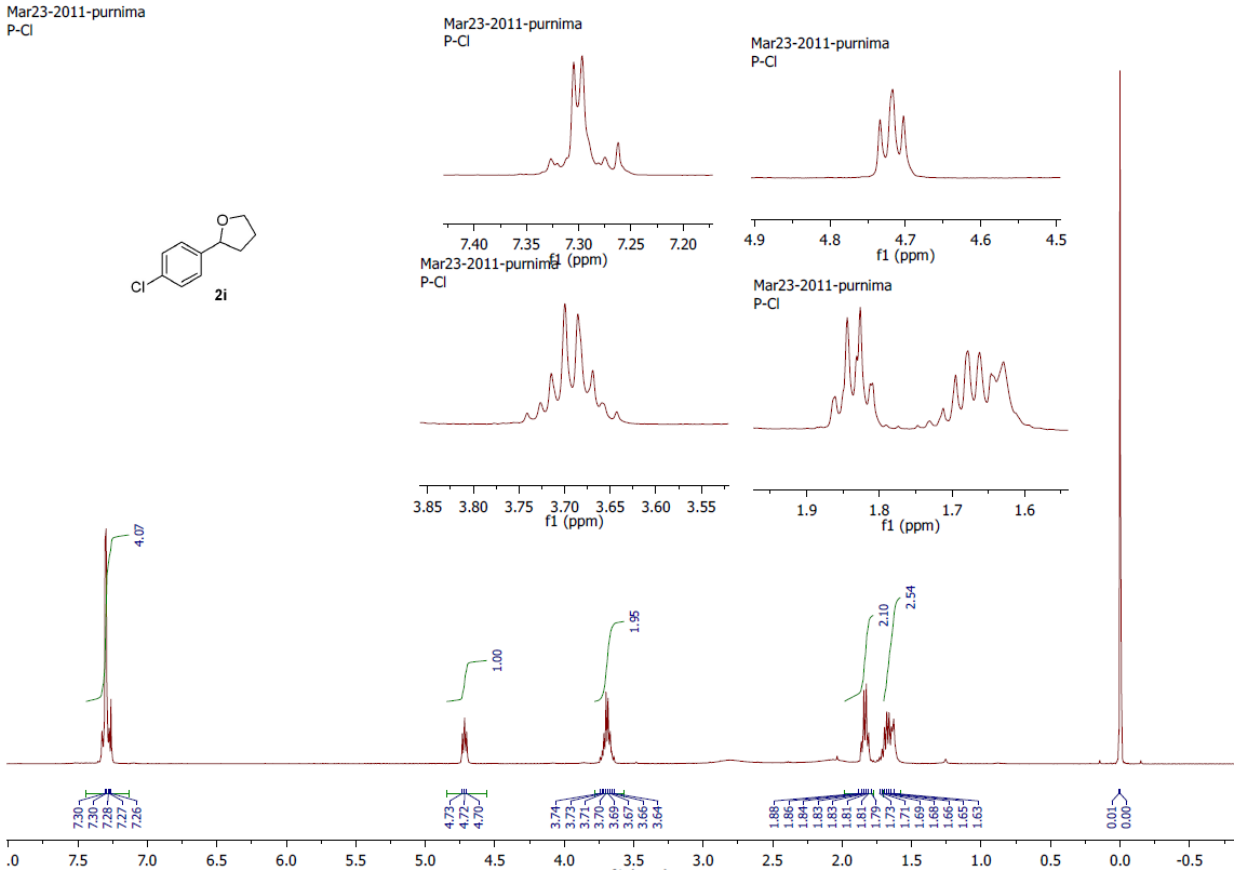
DEPT at 135 for 2-(4-*tert*-butylphenyl)-tetrahydrofuran in $CDCl_3$ (Table 2, entry h and q)



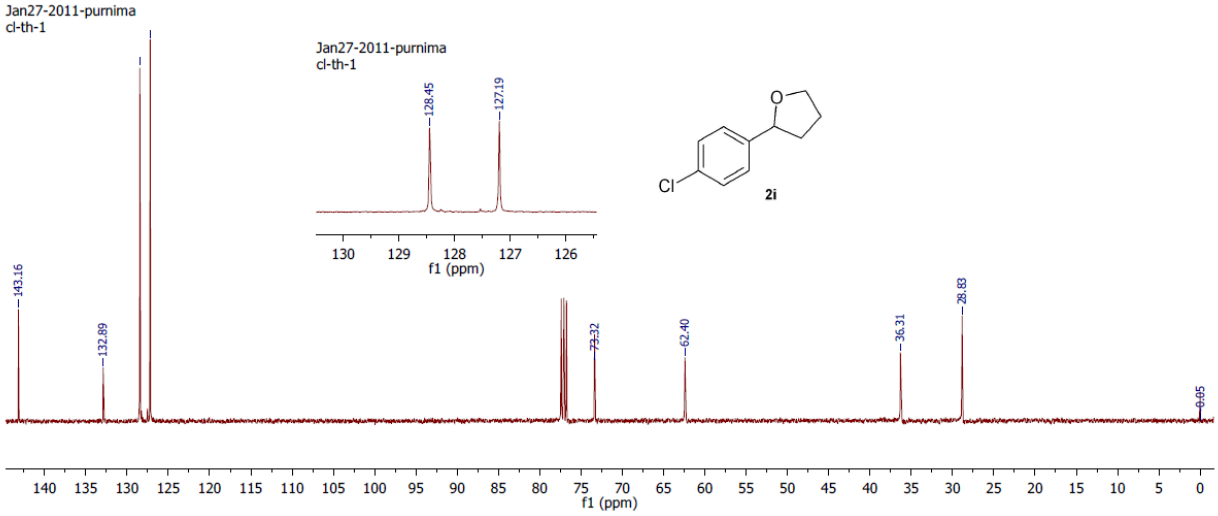
GCMS for 2-(4-*tert*-butylphenyl)-tetrahydrofuran (Table 2, entry h and q)



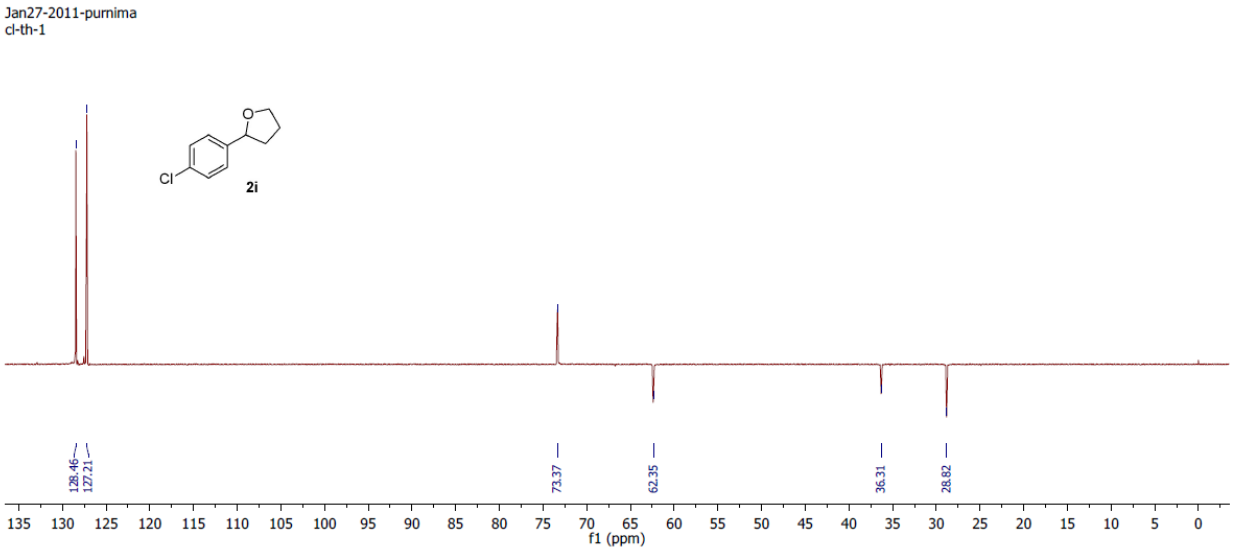
^{1}H NMR for 2-(4-chlorophenyl)-tetrahydrofuran in $CDCl_3$ (Table 2, entry i)



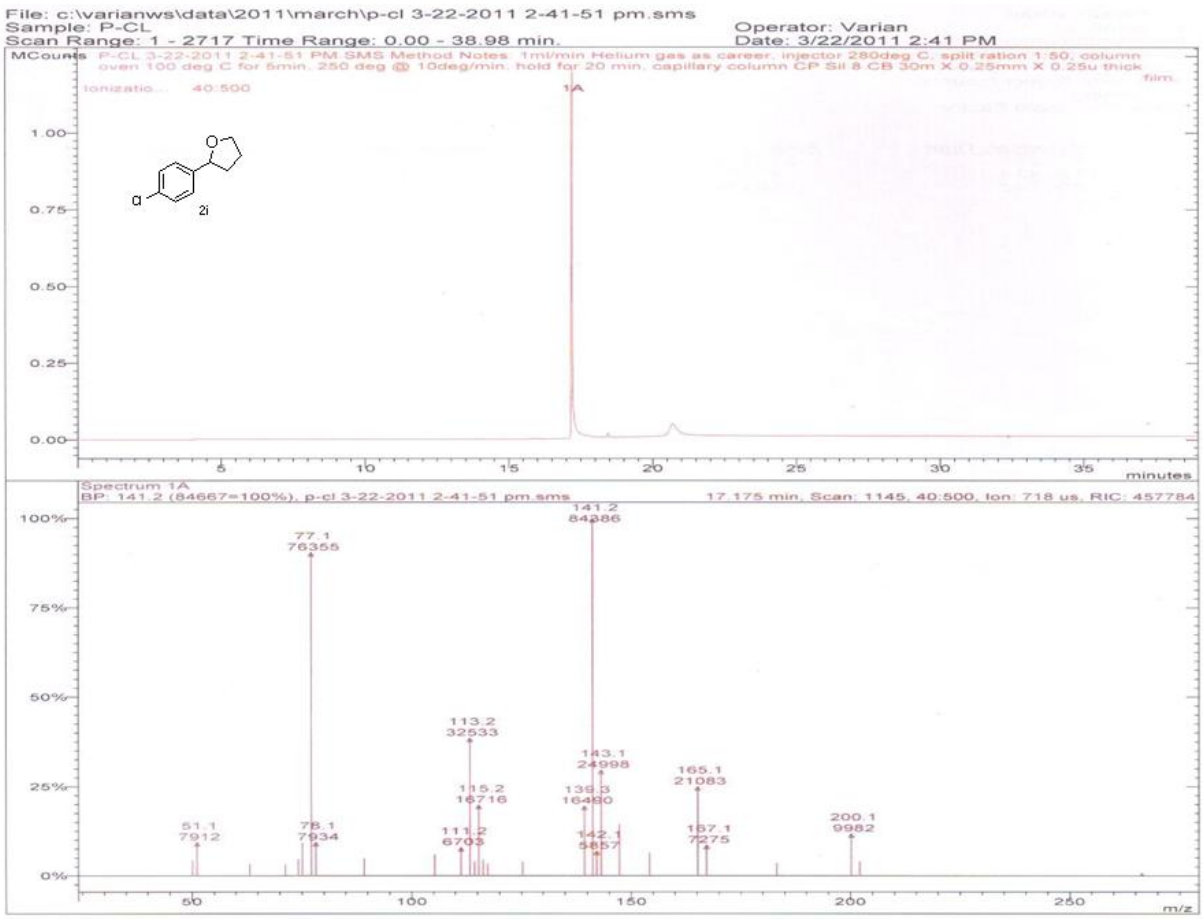
^{13}C NMR for 2-(4-chlorophenyl)-tetrahydrofuran in $CDCl_3$ (Table 2, entry i)



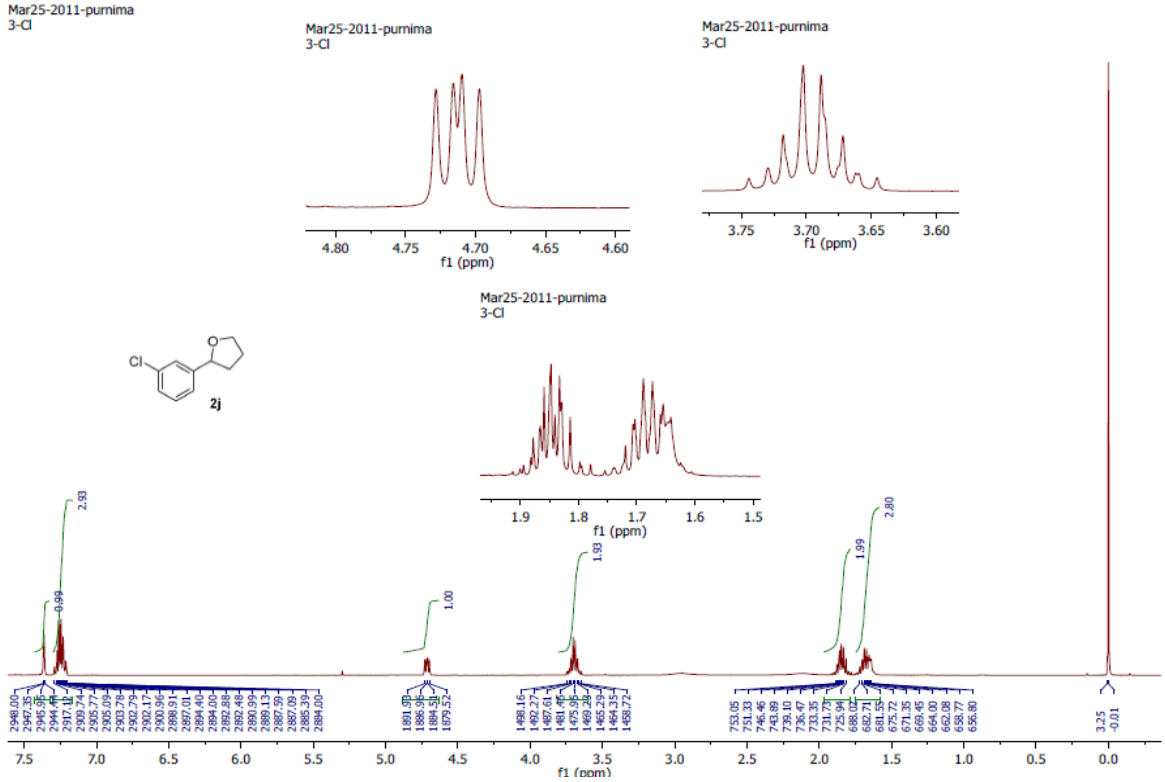
DEPT at 135 for 2-(4-chlorophenyl)-tetrahydrofuran in $CDCl_3$ (Table 2, entry i)



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



^{1}H NMR for 2-(3-Chlorophenyl)-tetrahydrofuran in $CDCl_3$ (Table 2, entry j)



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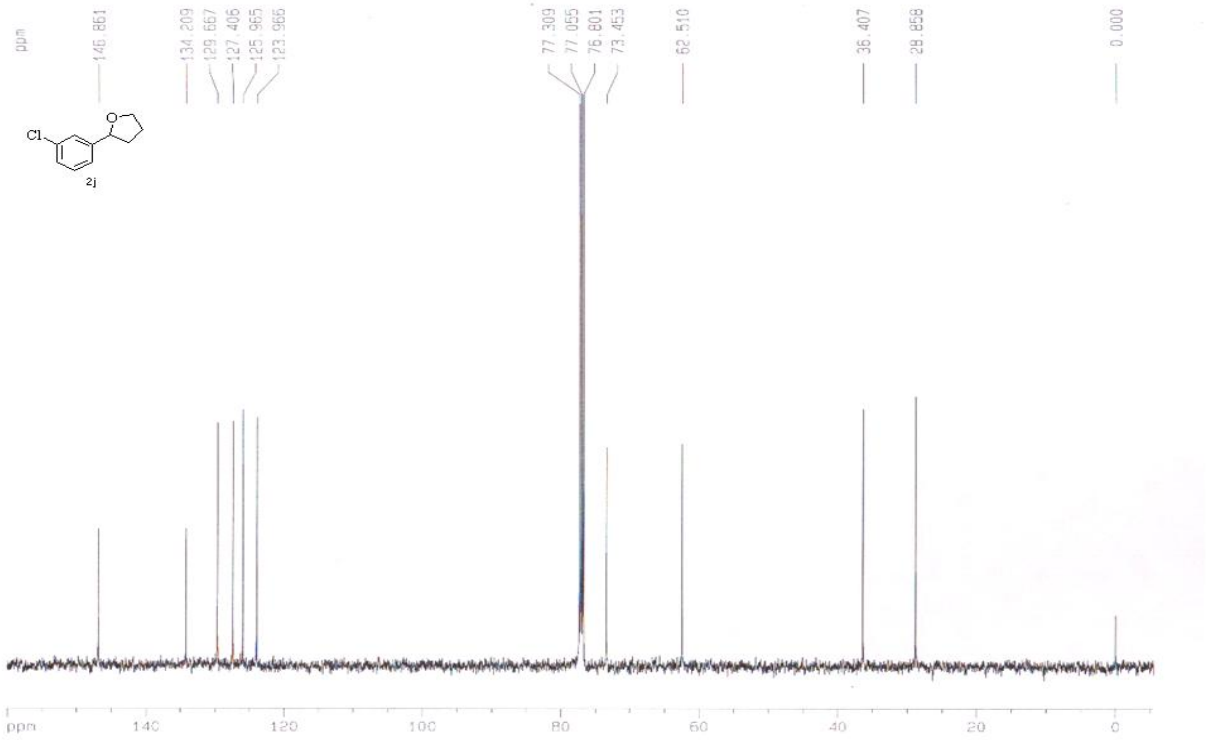
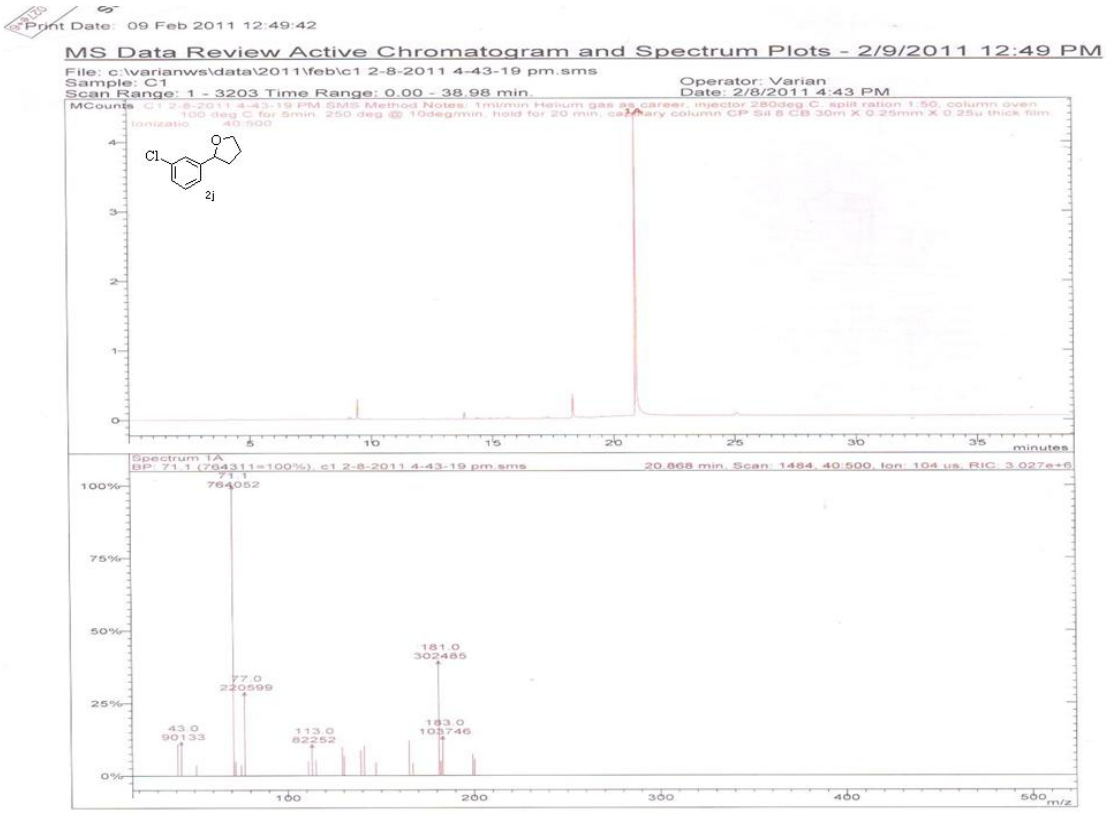
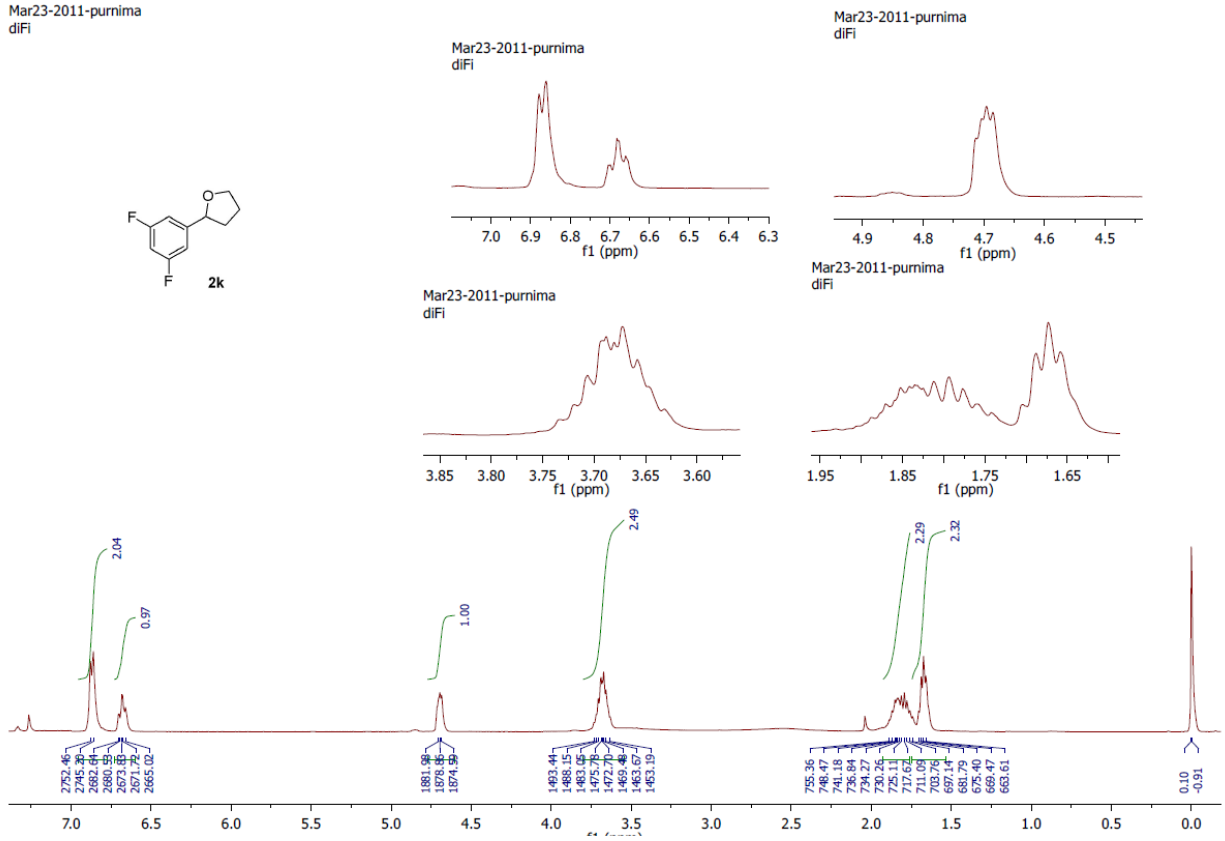


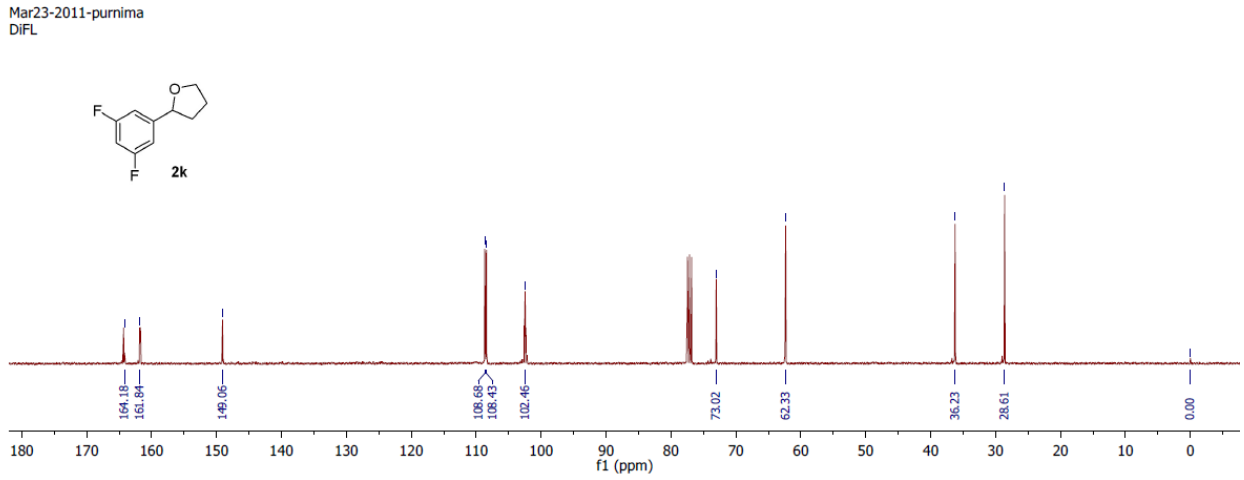
GCMS for 2-(3-Chlorophenyl)-tetrahydrofuran (Table 2, entry j)



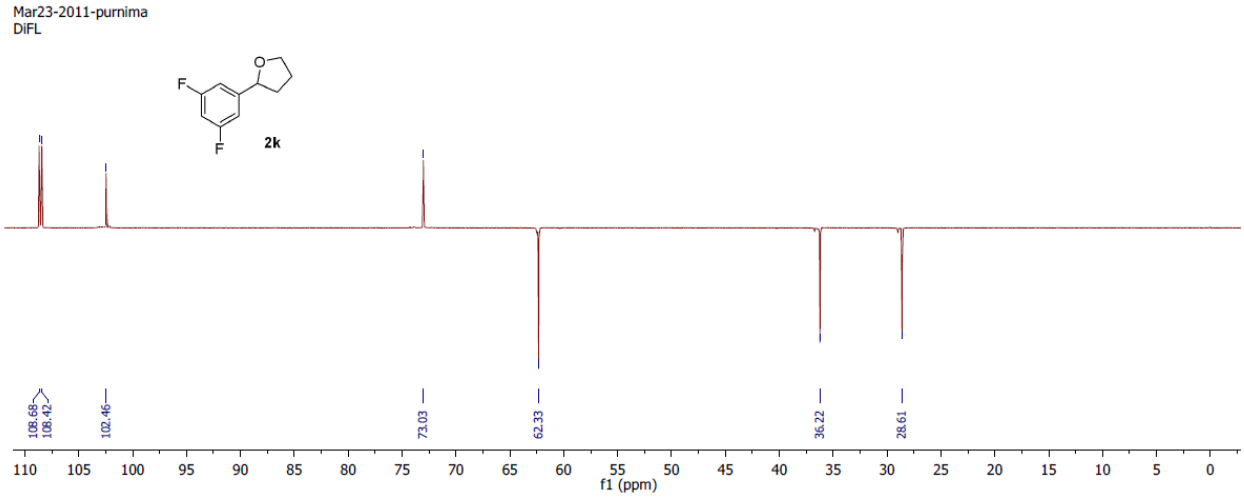
^{1}H NMR for 2-(3,5-difluorophenyl)-tetrahydrofuran in $CDCl_3$ (Table 2, entry k)



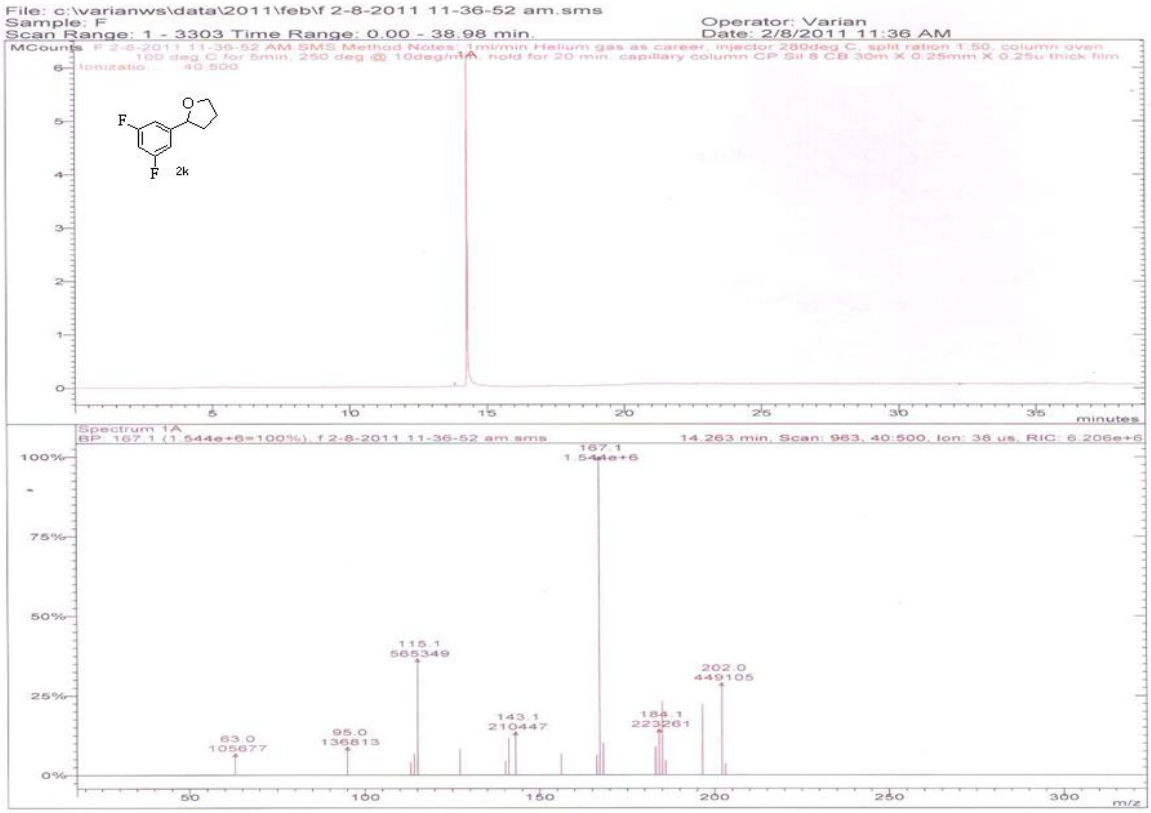
^{13}C NMR for 2-(3,5-difluorophenyl)-tetrahydrofuran in $CDCl_3$ (Table 2, entry k)



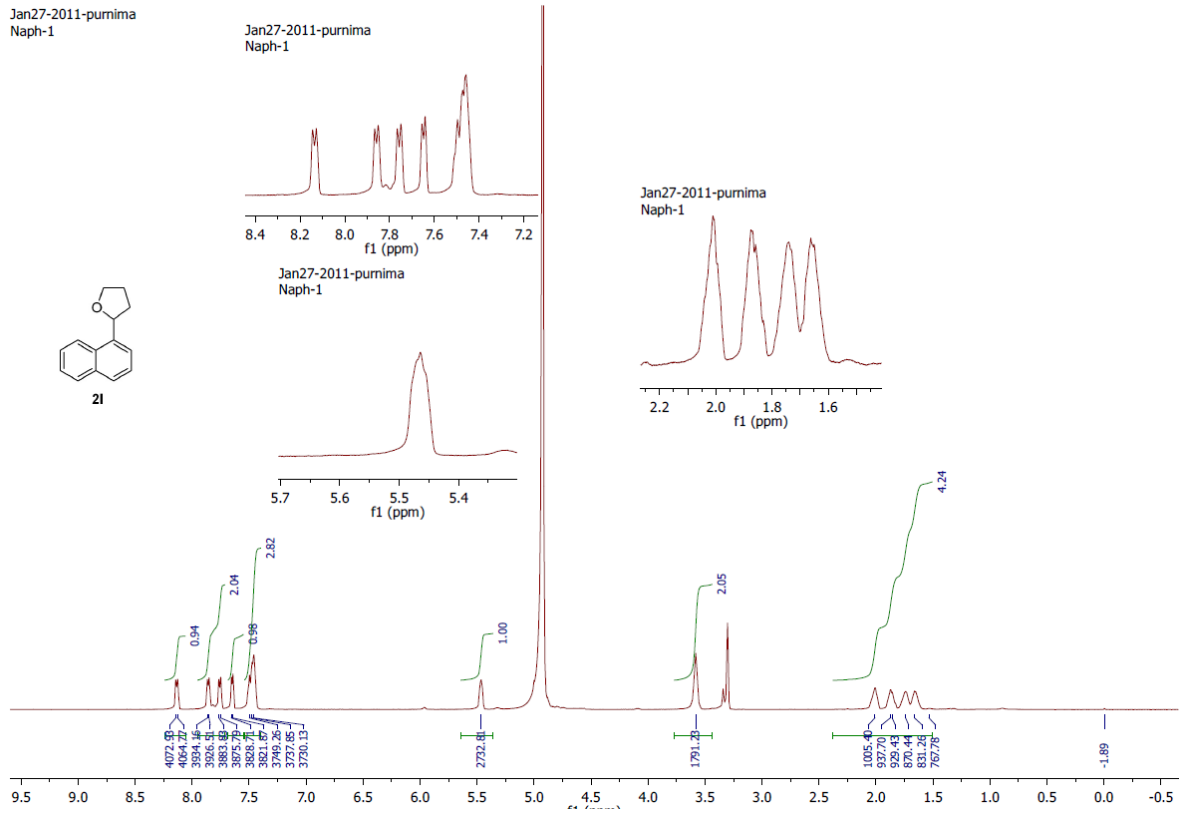
DEPT at 135 for 2-(3,5-difluorophenyl)-tetrahydrofuran in $CDCl_3$ (Table 2, entry k)



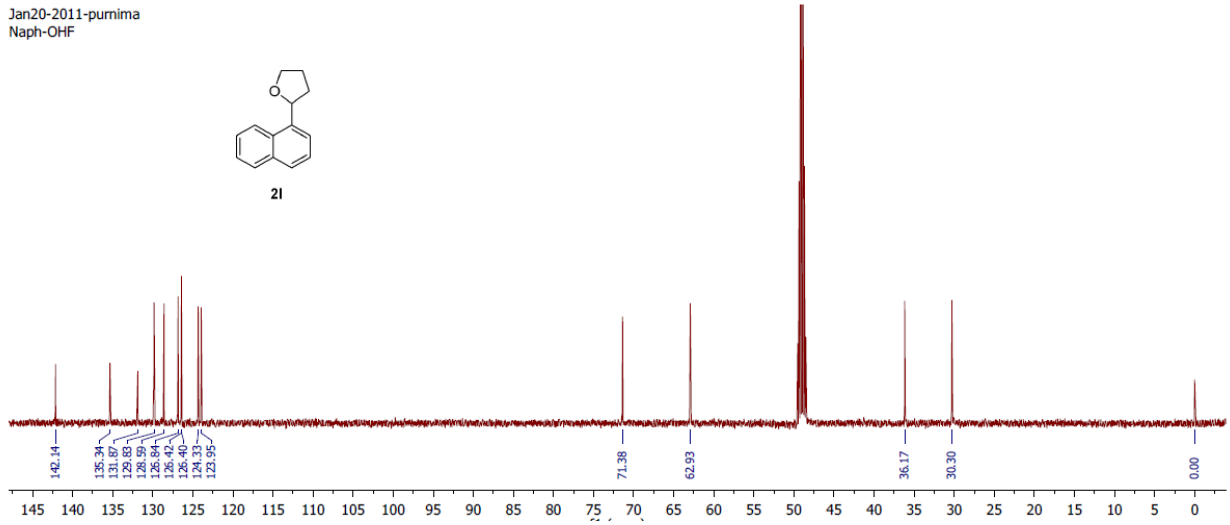
GCMS for 2-(3,5-difluorophenyl)-tetrahydrofuran (Table 2, entry k)



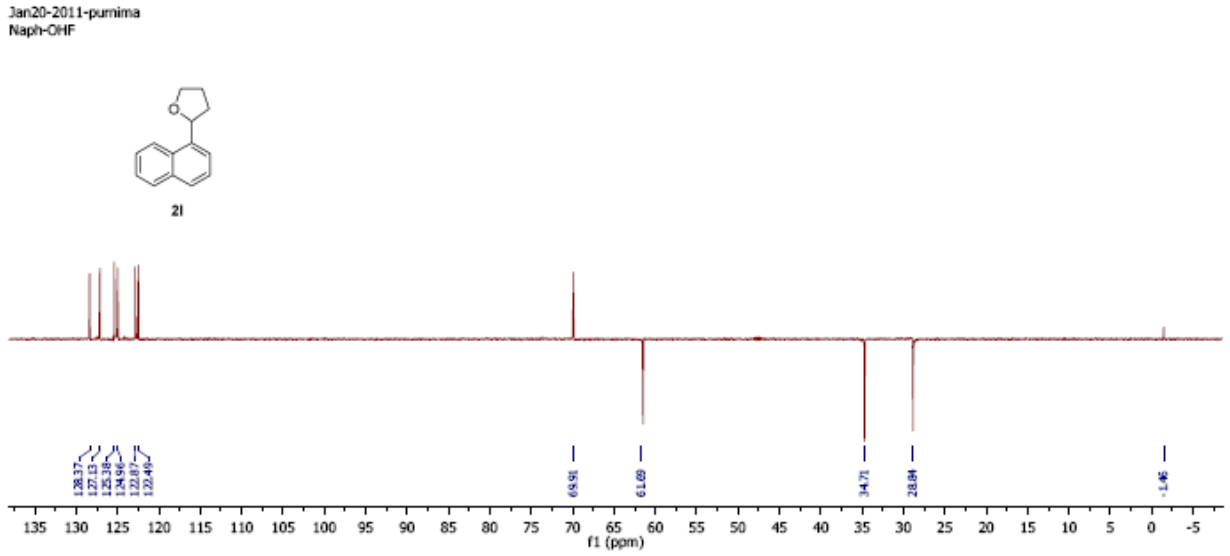
^{1}H NMR for tetrahydro-2-(naphthalen-4-yl)furan in CD_3OD (Table 2, entry l)



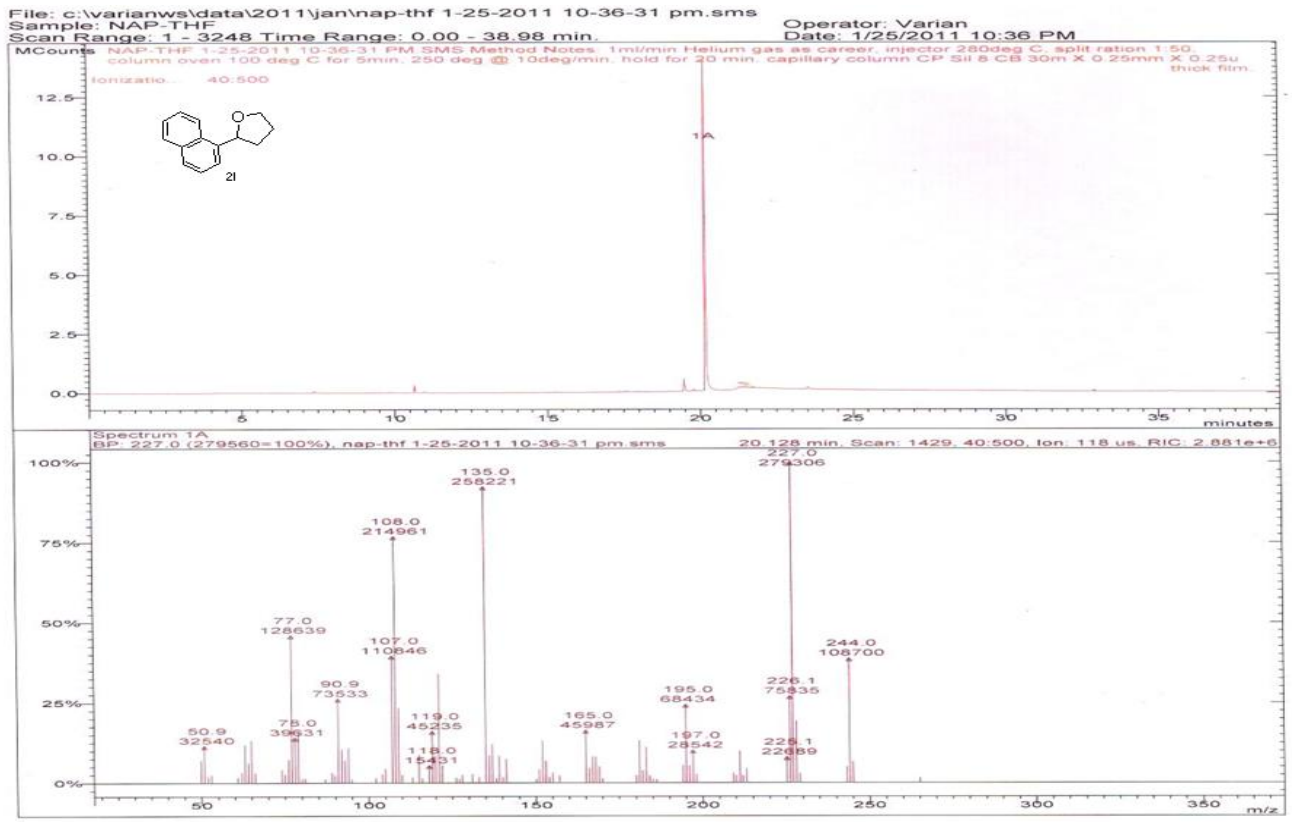
^{13}C NMR for tetrahydro-2-(naphthalen-4-yl)furan in CD_3OD (Table 2, entry l)



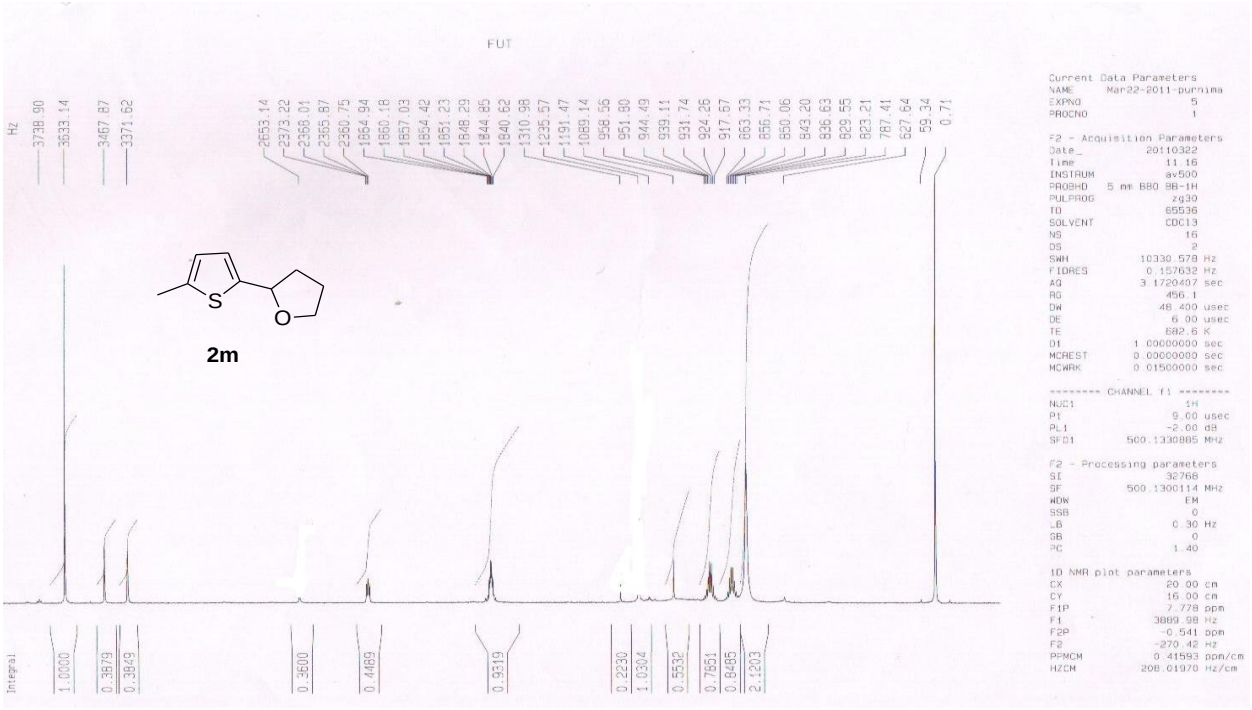
DEPT at 135 for tetrahydro-2-(naphthalen-4-yl)furan in CD_3OD (Table 2, entry l)



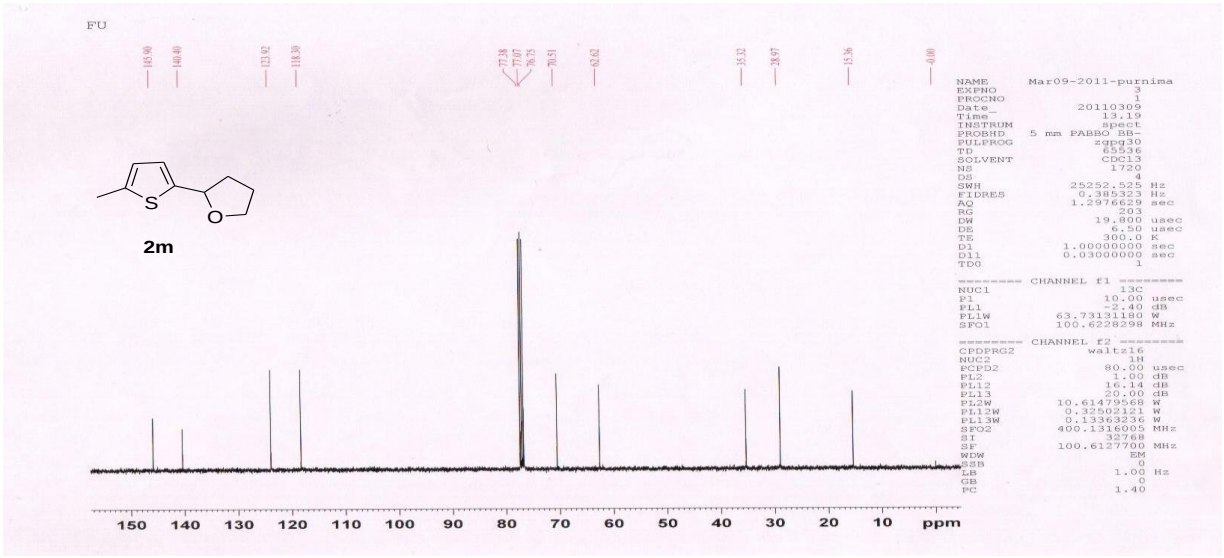
GCMS for tetrahydro-2-(naphthalen-4-yl)-furan (Table 2, entry l)



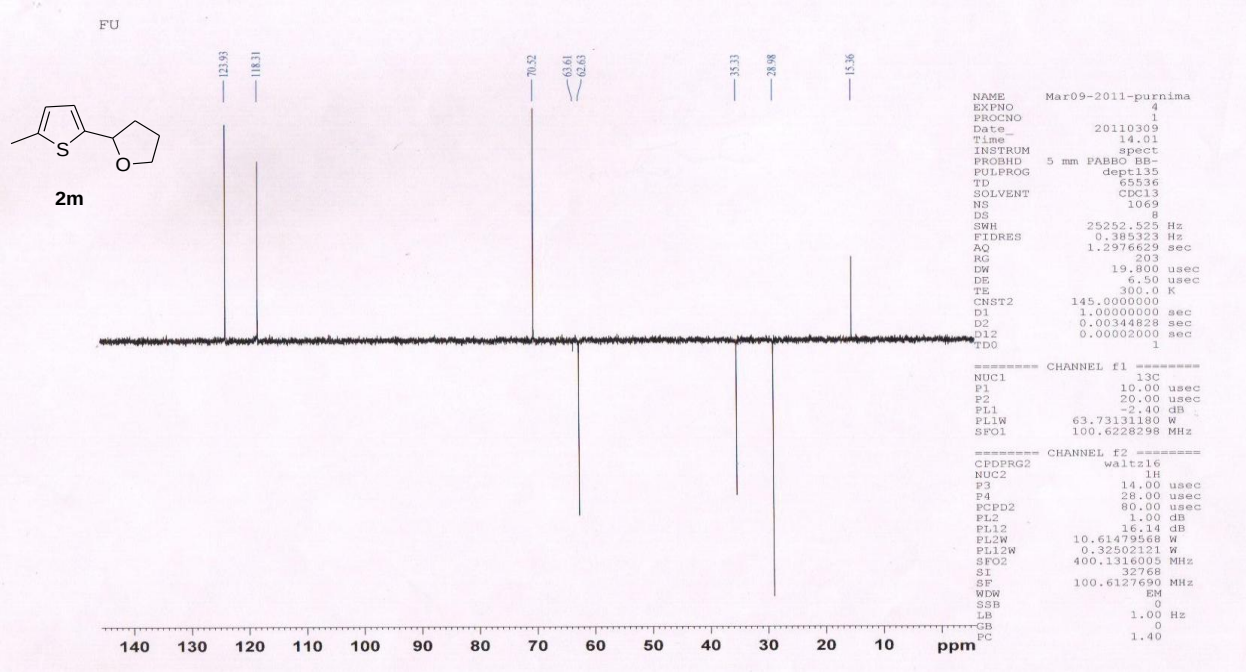
^{1}H NMR for 2-(thiophen-2-yl)-tetrahydrofuran in $CDCl_3$ (Table 2, entry m)



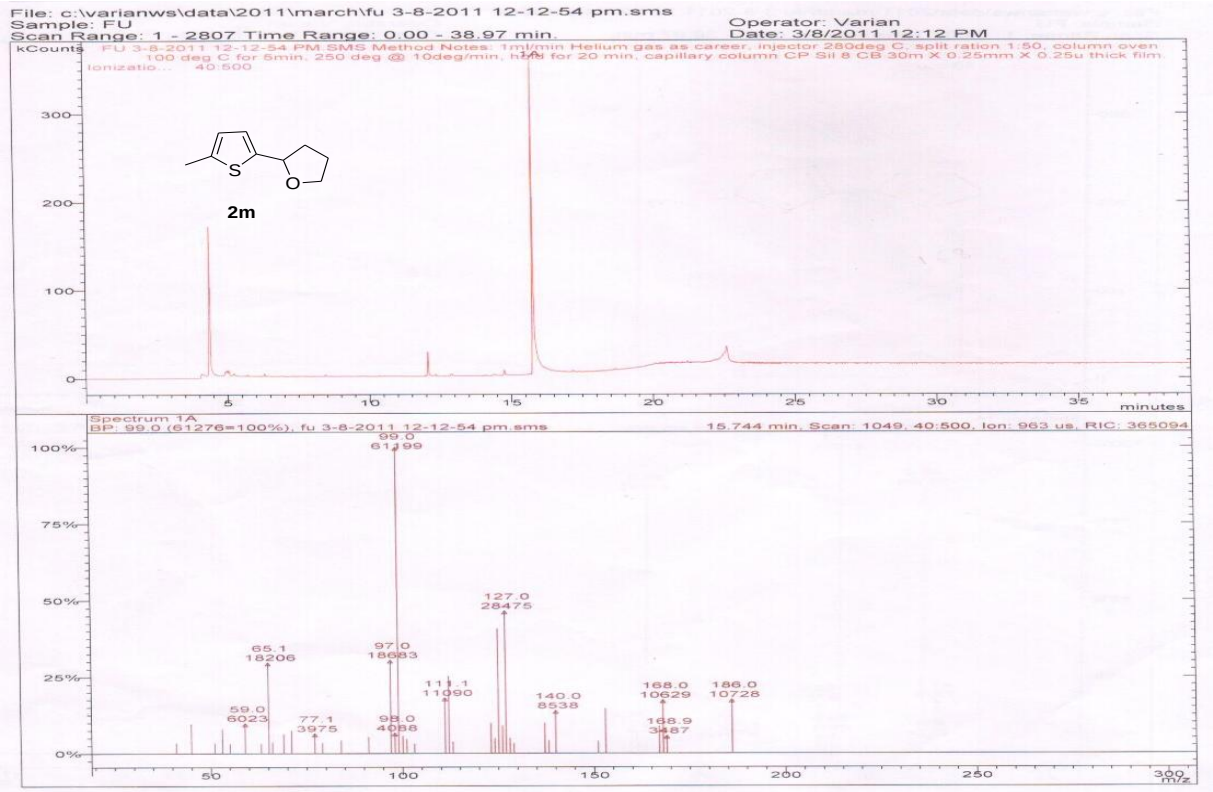
^{13}C NMR for 2-(thiophen-2-yl)-tetrahydrofuran in $CDCl_3$ (Table 2, entry m)



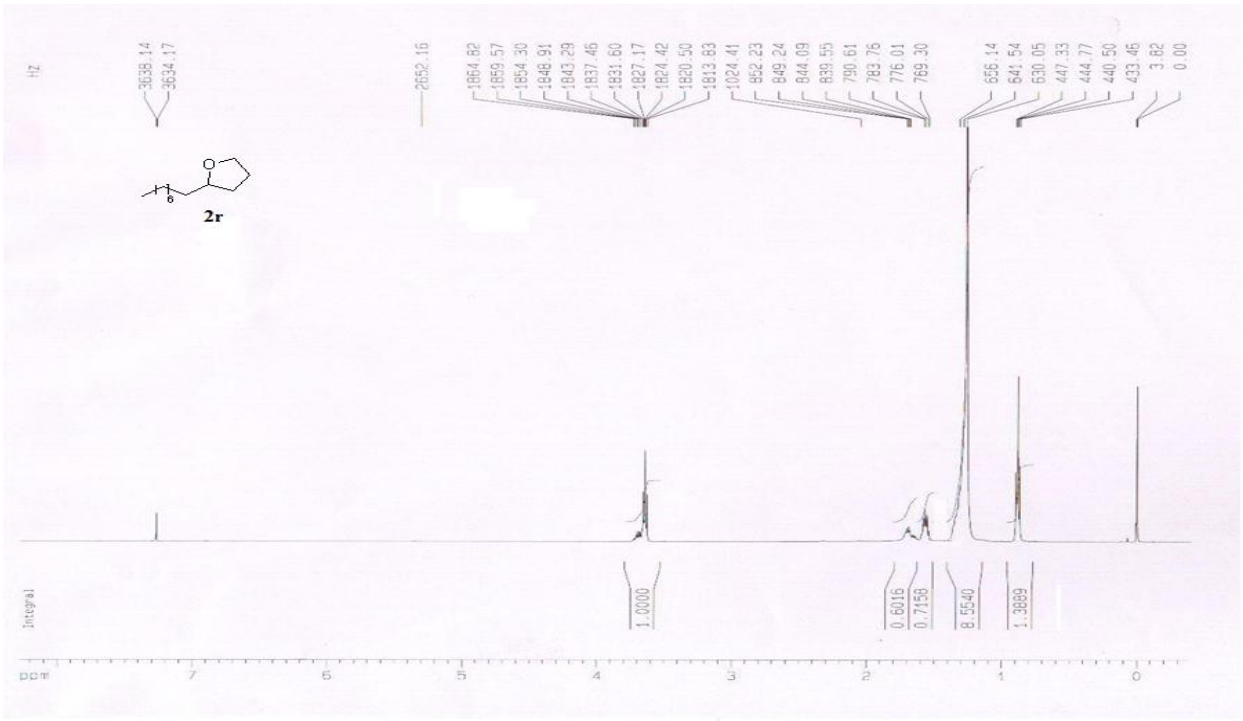
DEPT at 135 for 2-(thiophen-2-yl)-tetrahydrofuran in $CDCl_3$ (Table 2, entry m)



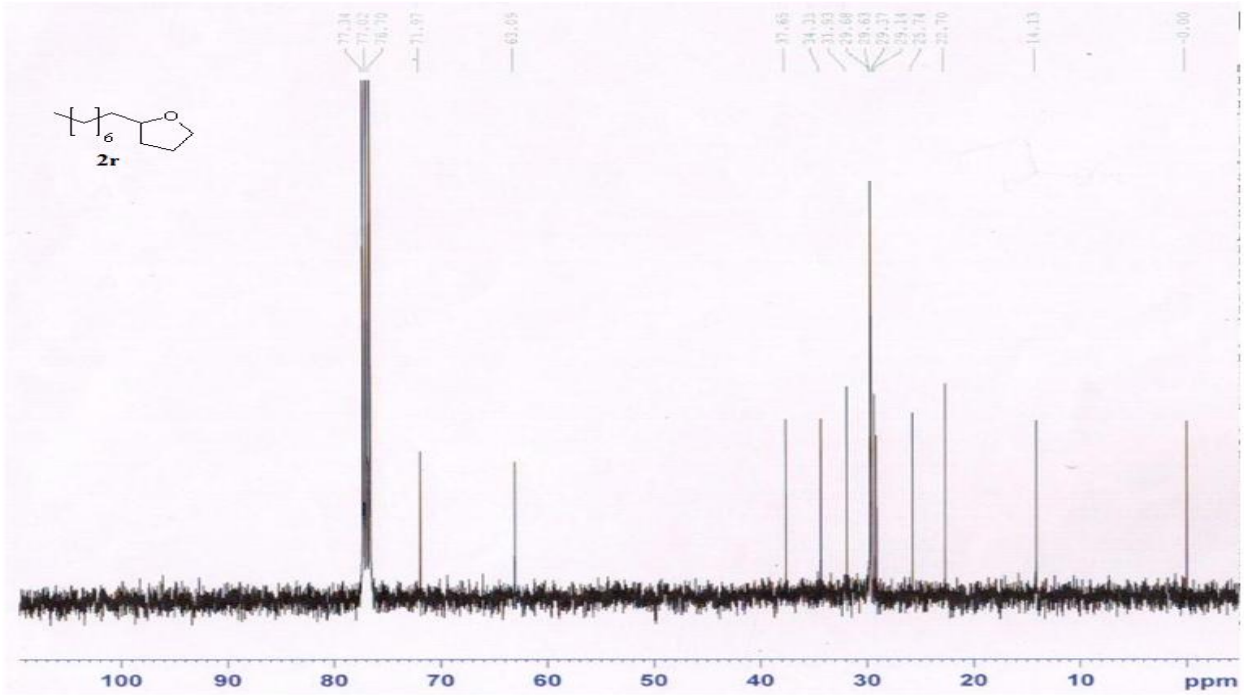
GC-MS for 2-(thiophen-2-yl)-tetrahydrofuran (Table 2, entry m)



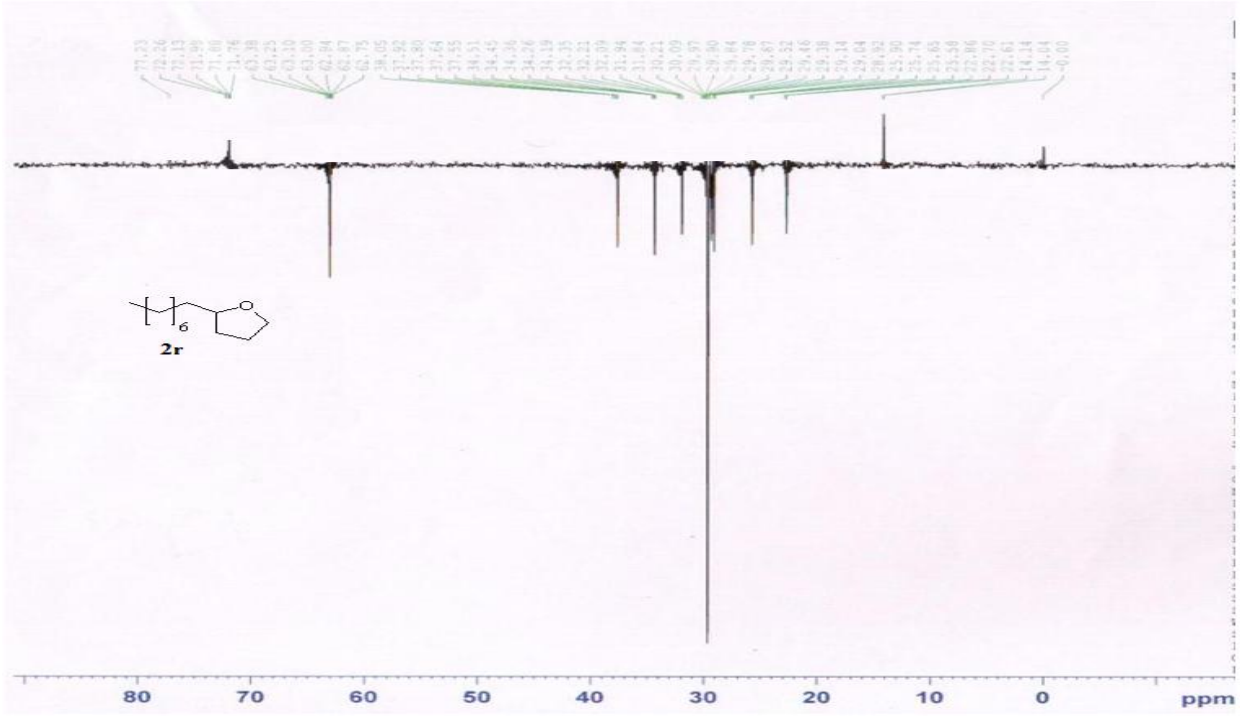
^{1}H NMR for 2-octyl-tetrahydrofuran in $CDCl_3$ (Table 2, entry r)



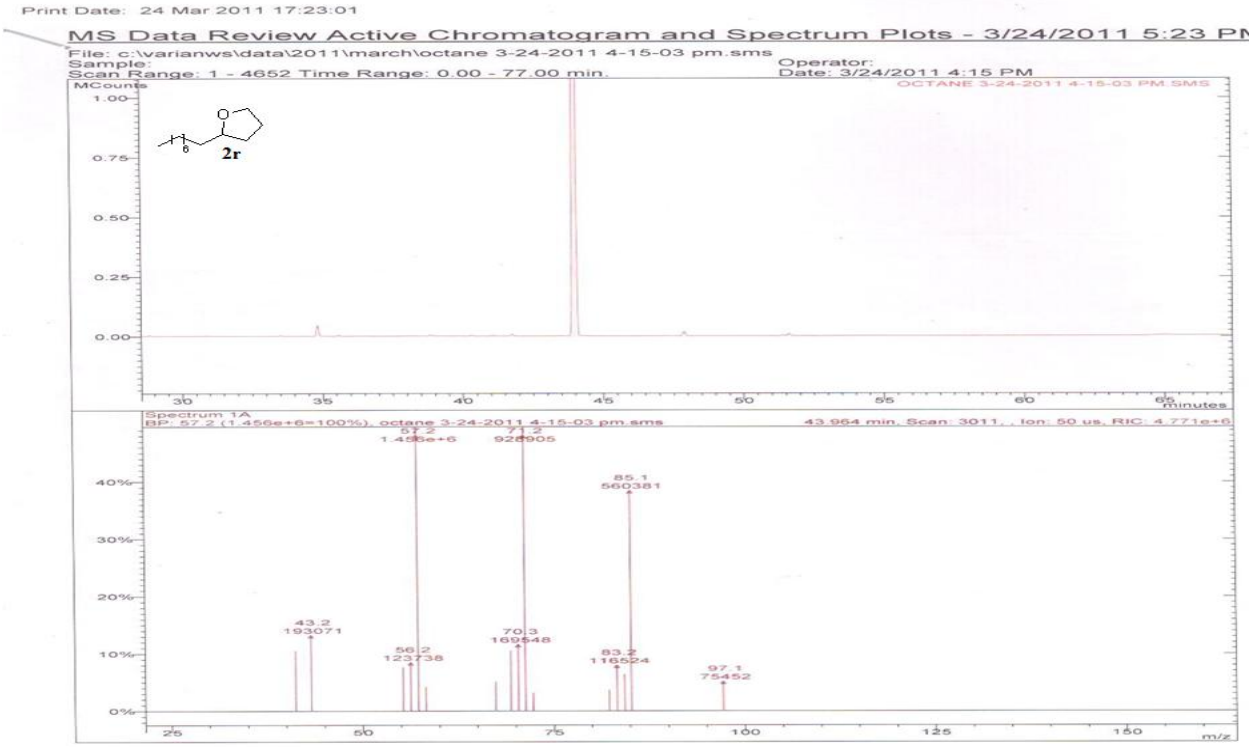
^{13}C NMR for 2-octyl-tetrahydrofuran in $CDCl_3$ (Table 2, entry r)



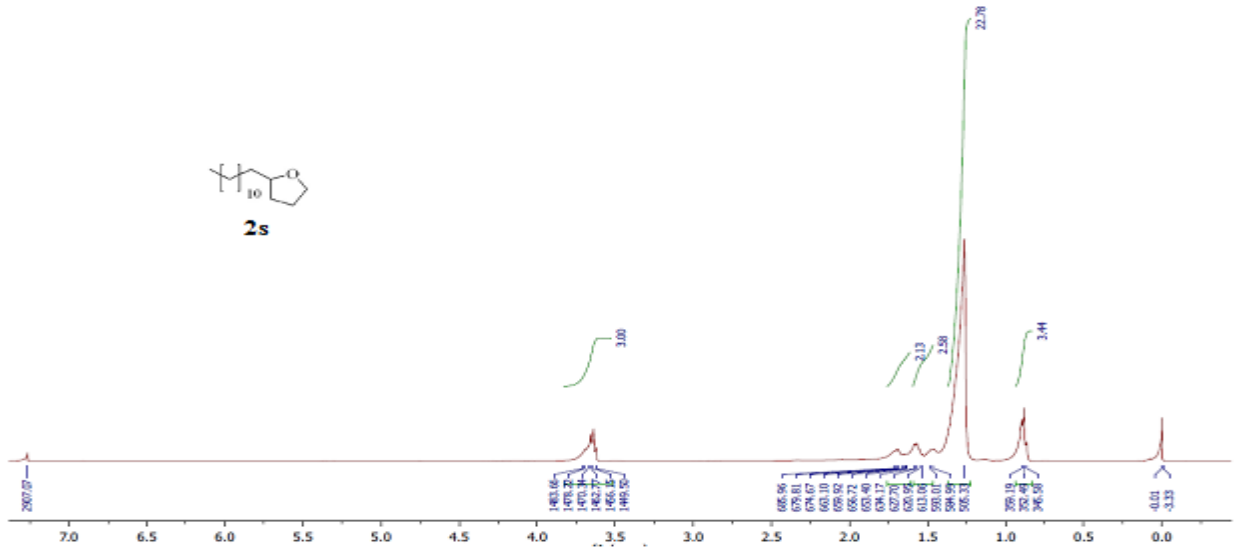
DEPT at 135 for 2-octyl-tetrahydrofuran in $CDCl_3$ (Table 2, entry r)



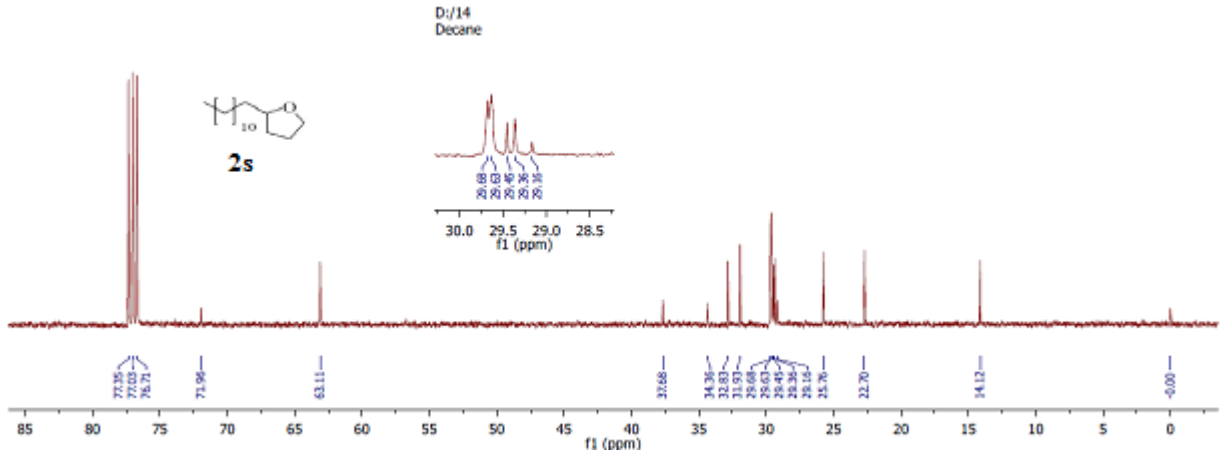
GCMS for 2-octyl-tetrahydrofuran (Table 2, entry r)



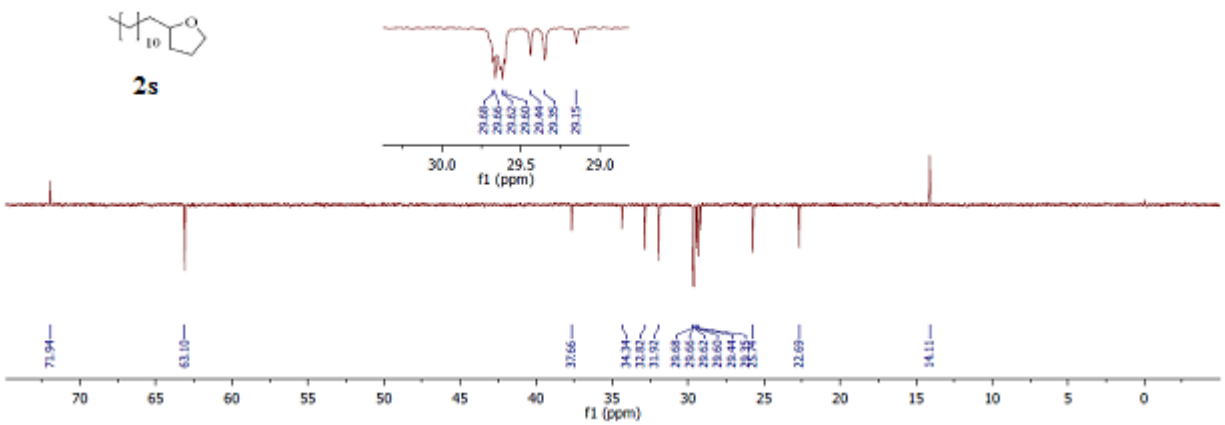
^{1}H NMR for 2-dodecyl-tetrahydrofuran in $CDCl_3$ (Table 2, entry s)



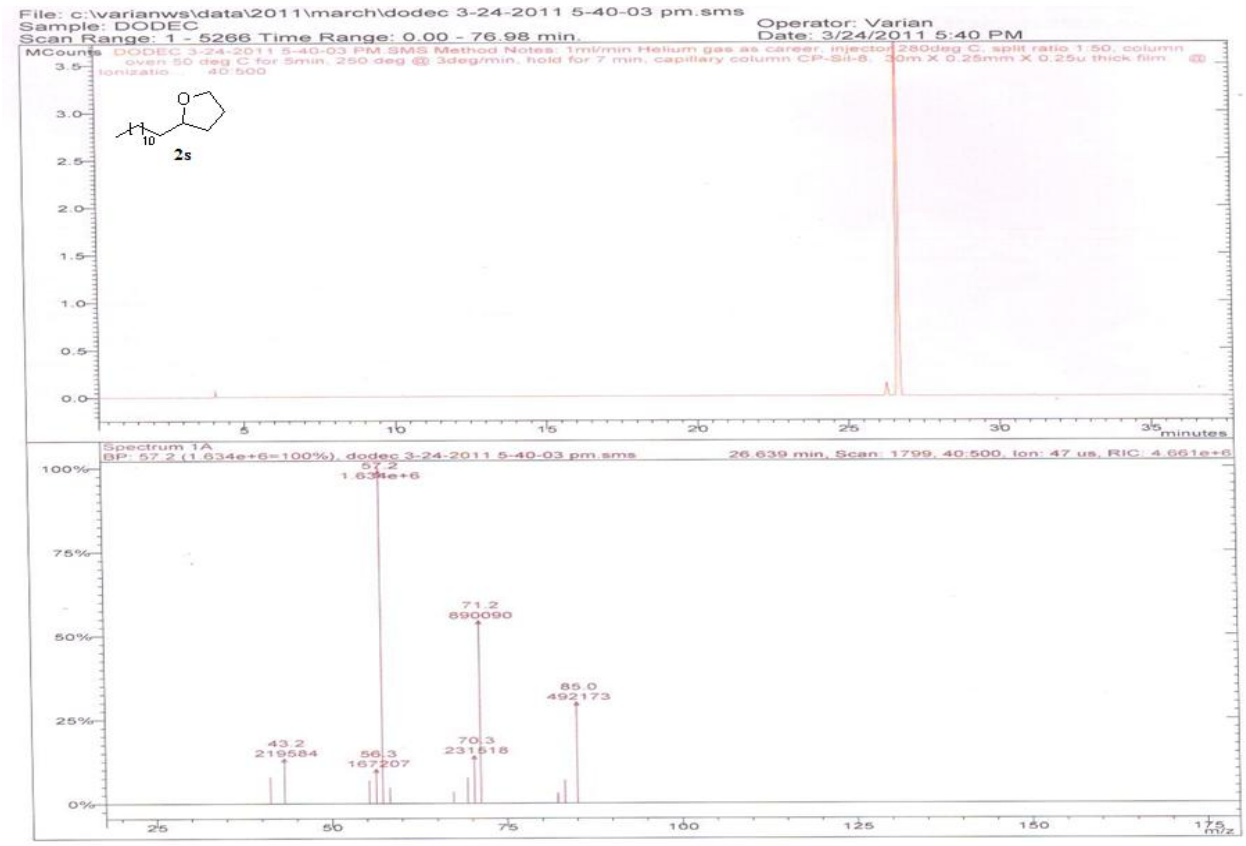
^{13}C NMR for 2-dodecyl-tetrahydrofuran in $CDCl_3$ (Table 2, entry s)



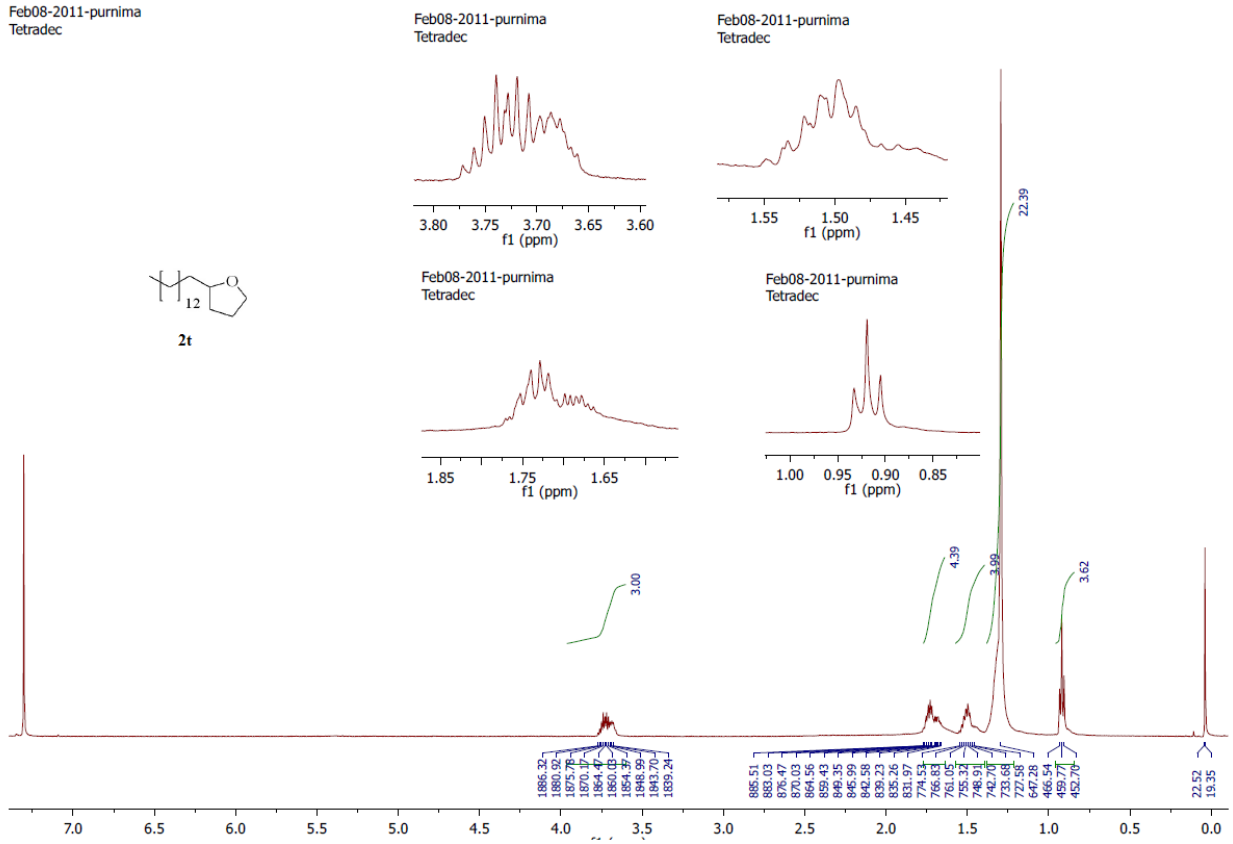
DEPT at 135 for 2-dodecyl-tetrahydrofuran in $CDCl_3$ (Table 2, entry s)



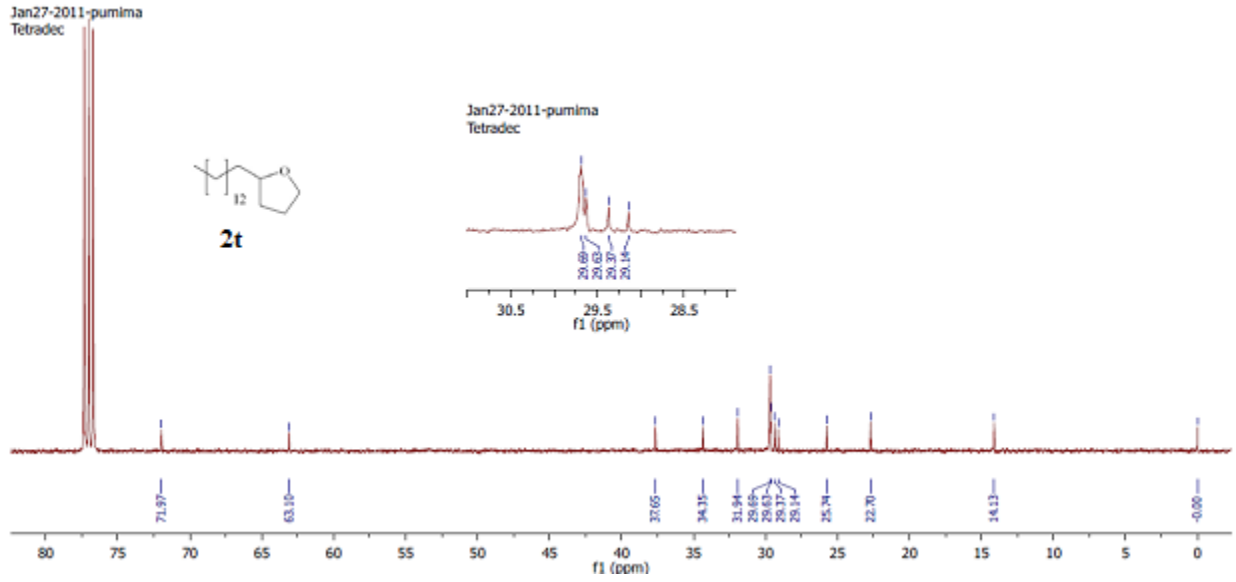
GCMS for 2-dodecyl-tetrahydrofuran (Table 2, entry s)



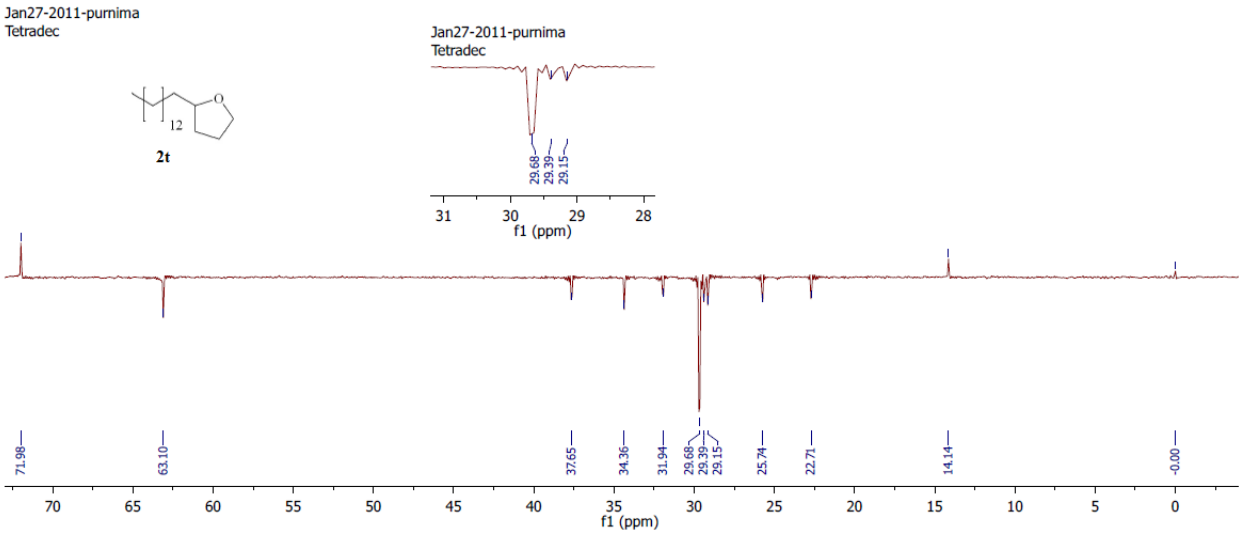
^{1}H NMR for tetrahydro-2-tetradecylfuran in $CDCl_3$ (Table 2, entry t)



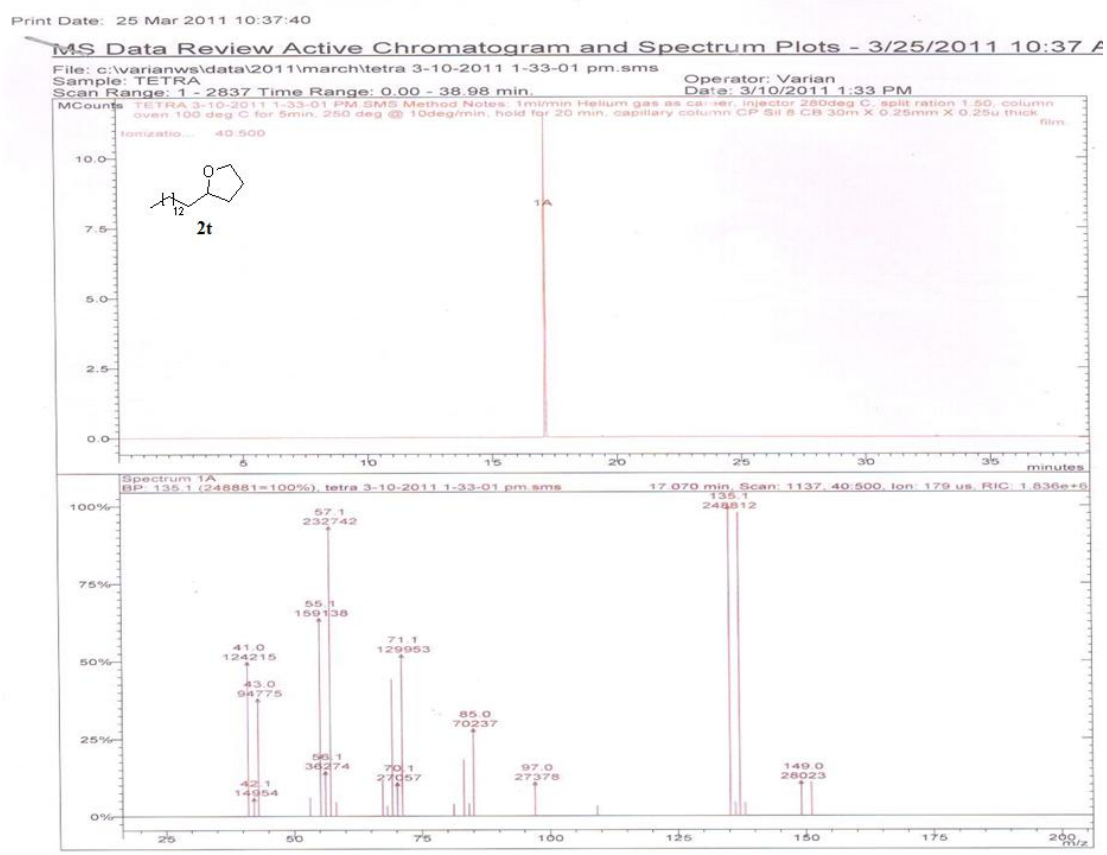
^{13}C NMR for tetrahydro-2-tetradecylfuran in $CDCl_3$ (Table 2, entry t)



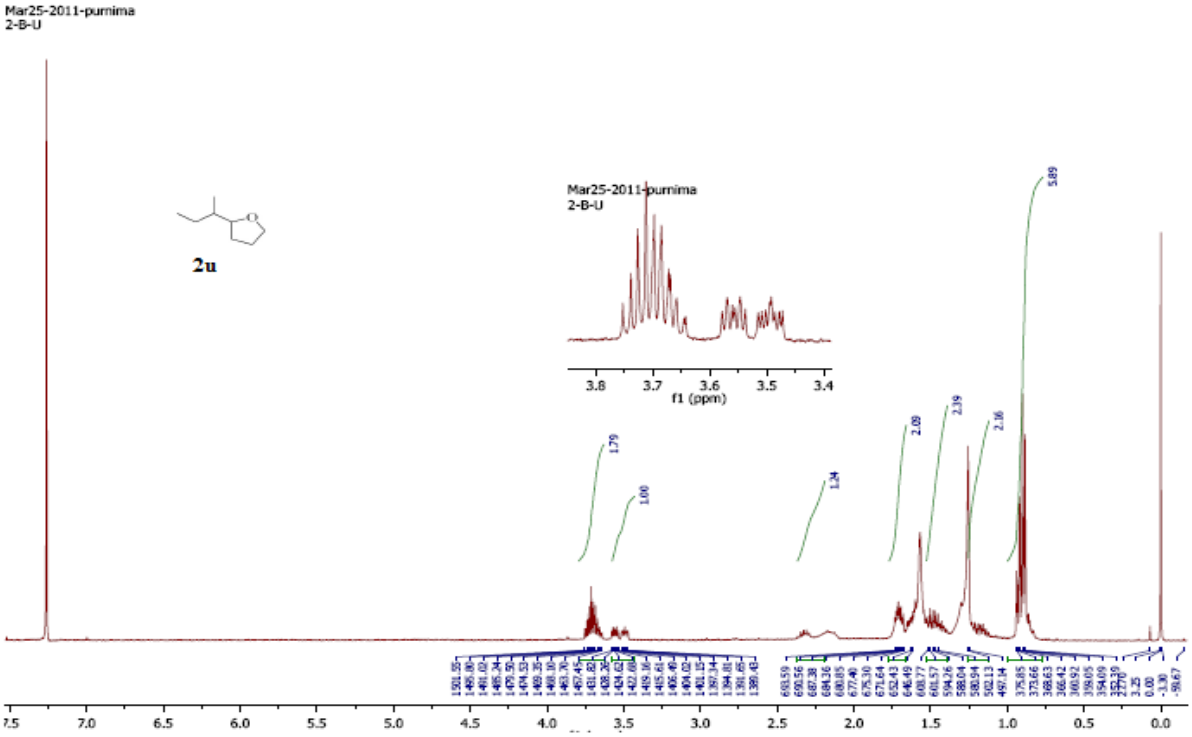
DEPT at 135 for tetrahydro-2-tetradecylfuran in $CDCl_3$ (Table 2, entry t)



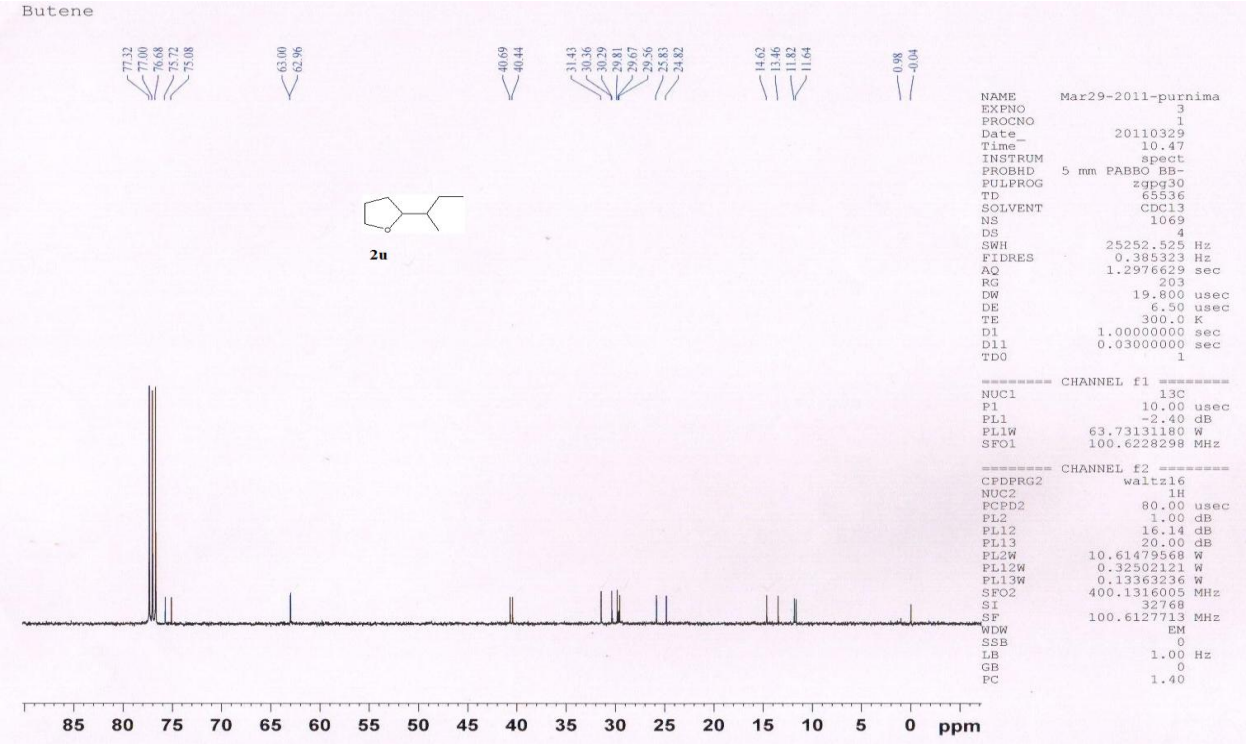
GCMS for tetrahydro-2-tetradecylfuran (Table 2, entry t)



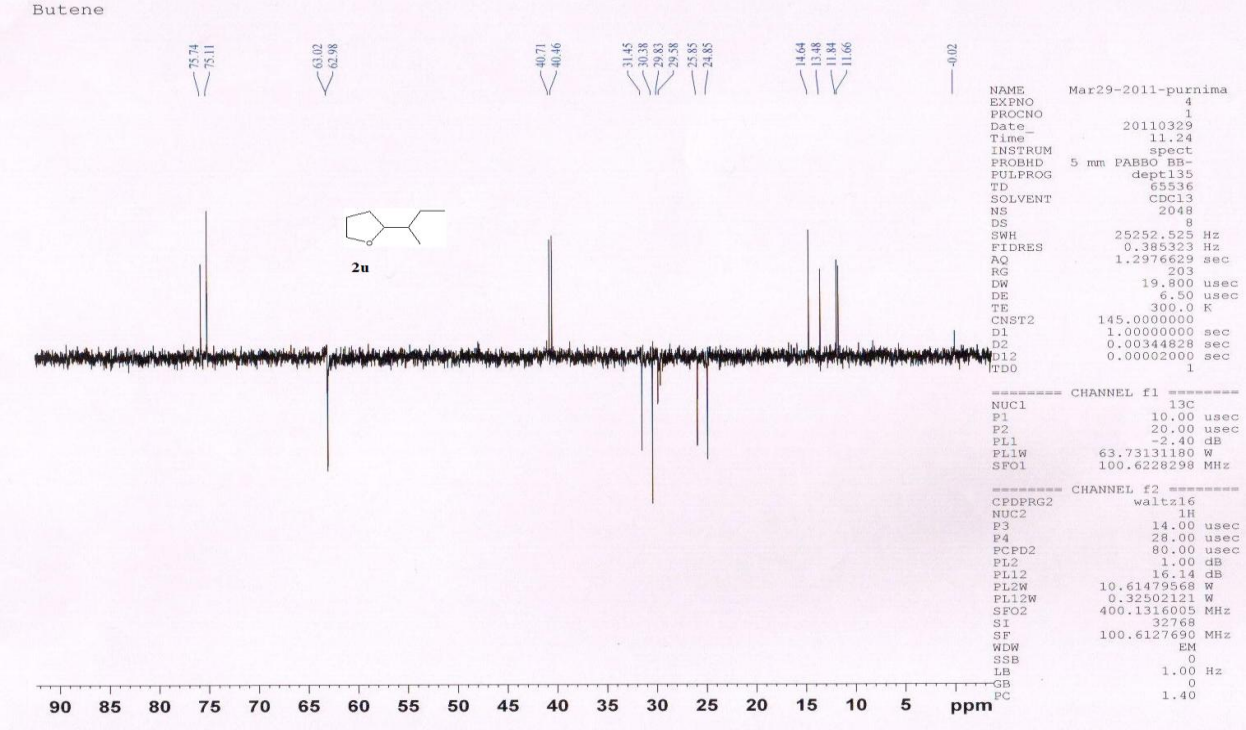
^{1}H NMR for 2-*sec*-butyl-tetrahydrofuran in $CDCl_3$ (Table 2, entry u)



^{13}C NMR for 2-*sec*-butyl-tetrahydrofuran in $CDCl_3$ (Table 2, entry u)

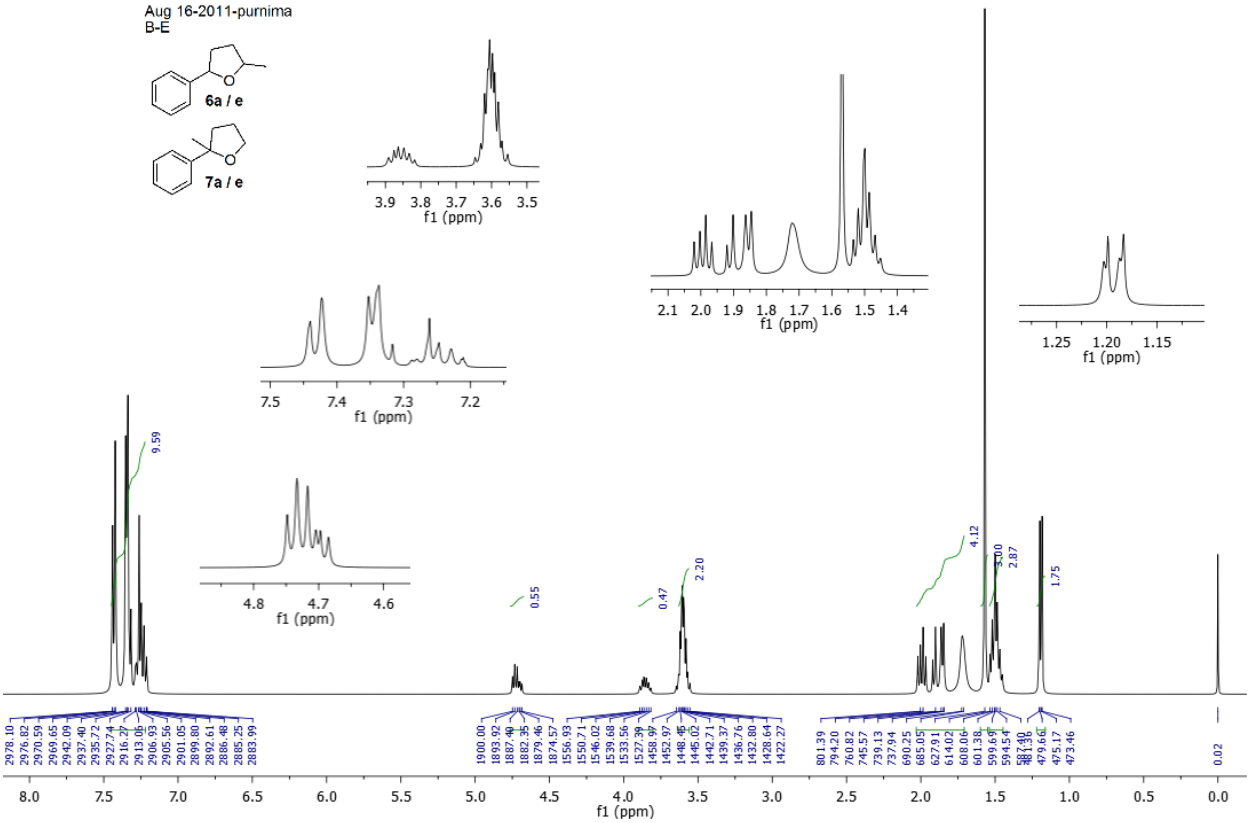


DEPT at 135 for 2-*sec*-butyl-tetrahydrofuran in $CDCl_3$ (Table 2, entry u)

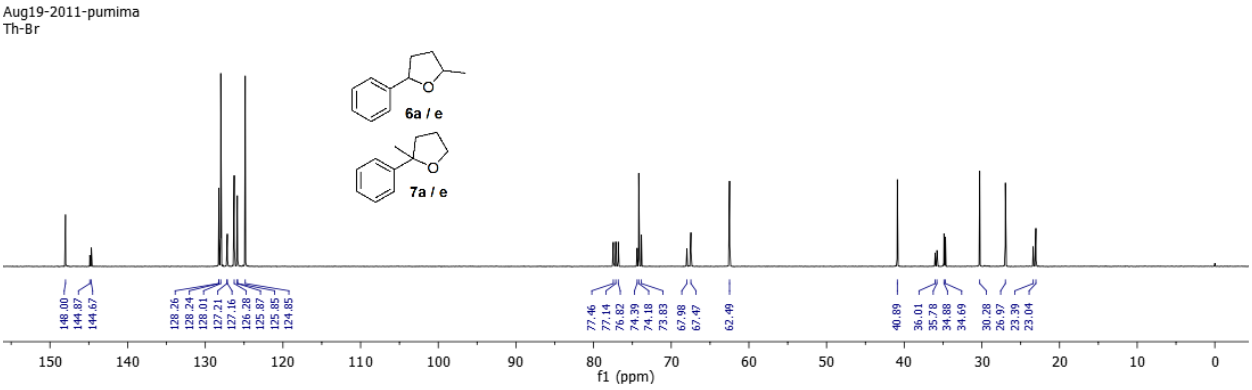


GCMS for 2-*sec*-butyl-tetrahydrofuran (Table 2, entry u)

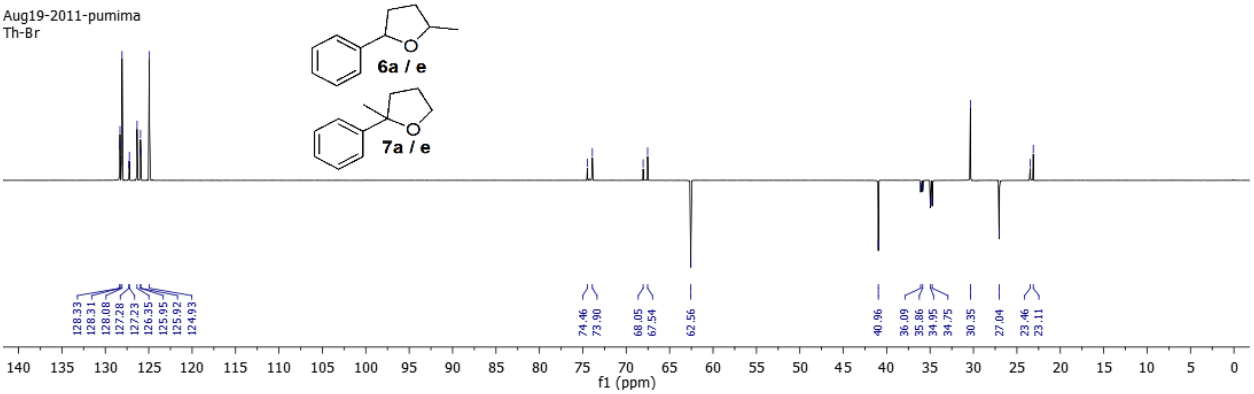
^{1}H NMR for 2-methyl-5-phenyl-tetrahydrofuran and 2-methyl-2-phenyl-tetrahydrofuran in $CDCl_3$ (Table 3, entry a and e)



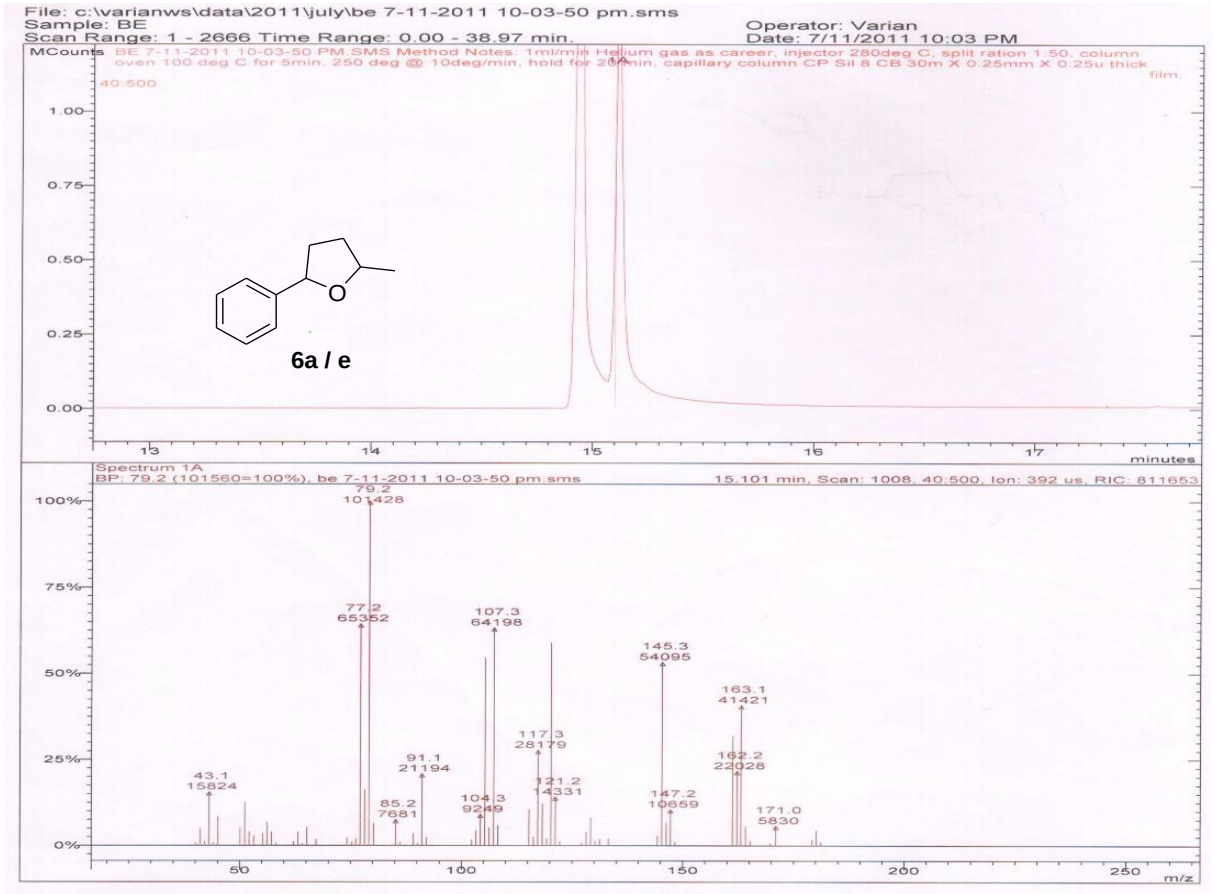
^{13}C NMR for 2-methyl-5-phenyl-tetrahydrofuran and 2-methyl-2-phenyl-tetrahydrofuran in $CDCl_3$ (Table 3, entry a and e)



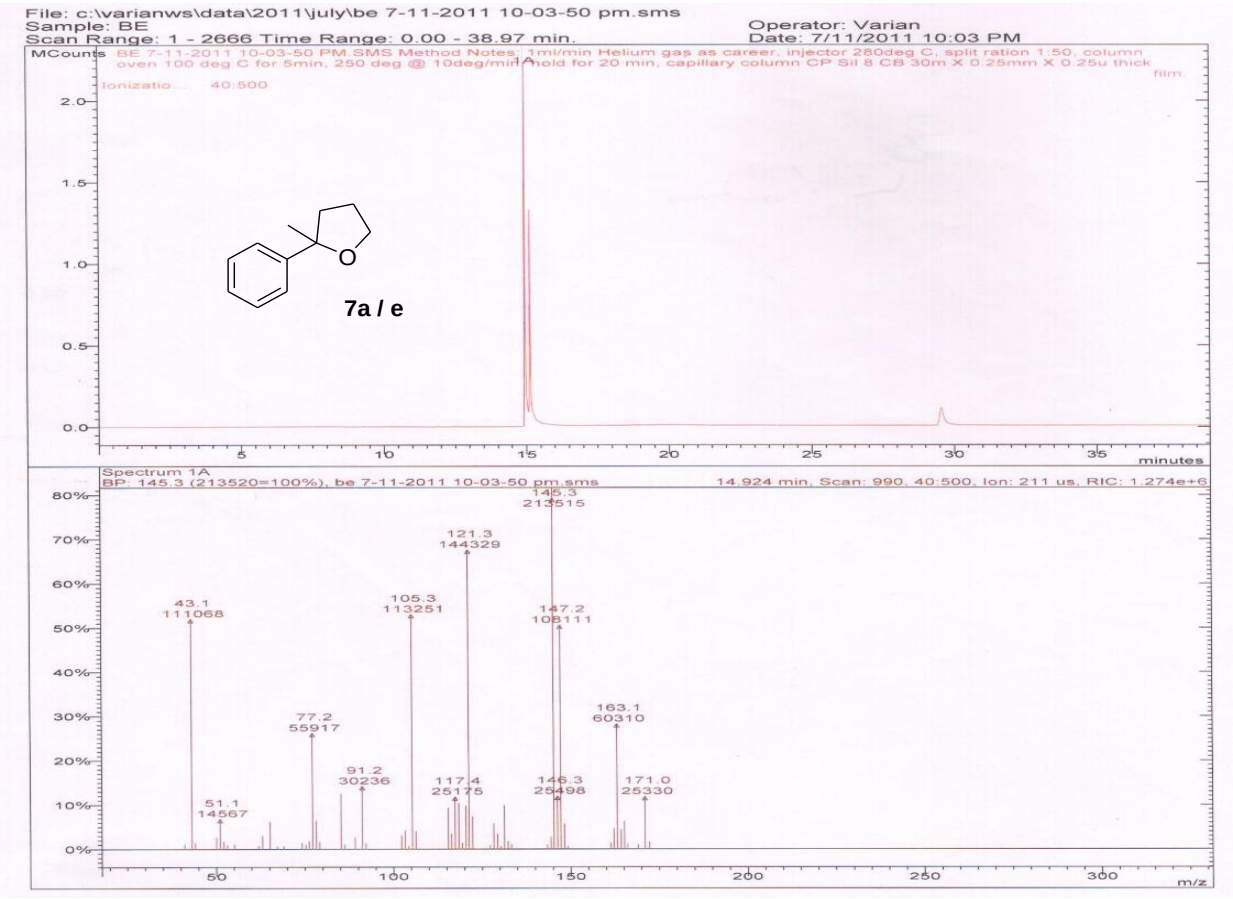
DEPT at 135 for 2-methyl-5-phenyl-tetrahydrofuran and 2-methyl-2-phenyl-tetrahydrofuran in $CDCl_3$ (Table 3, entry a and e)



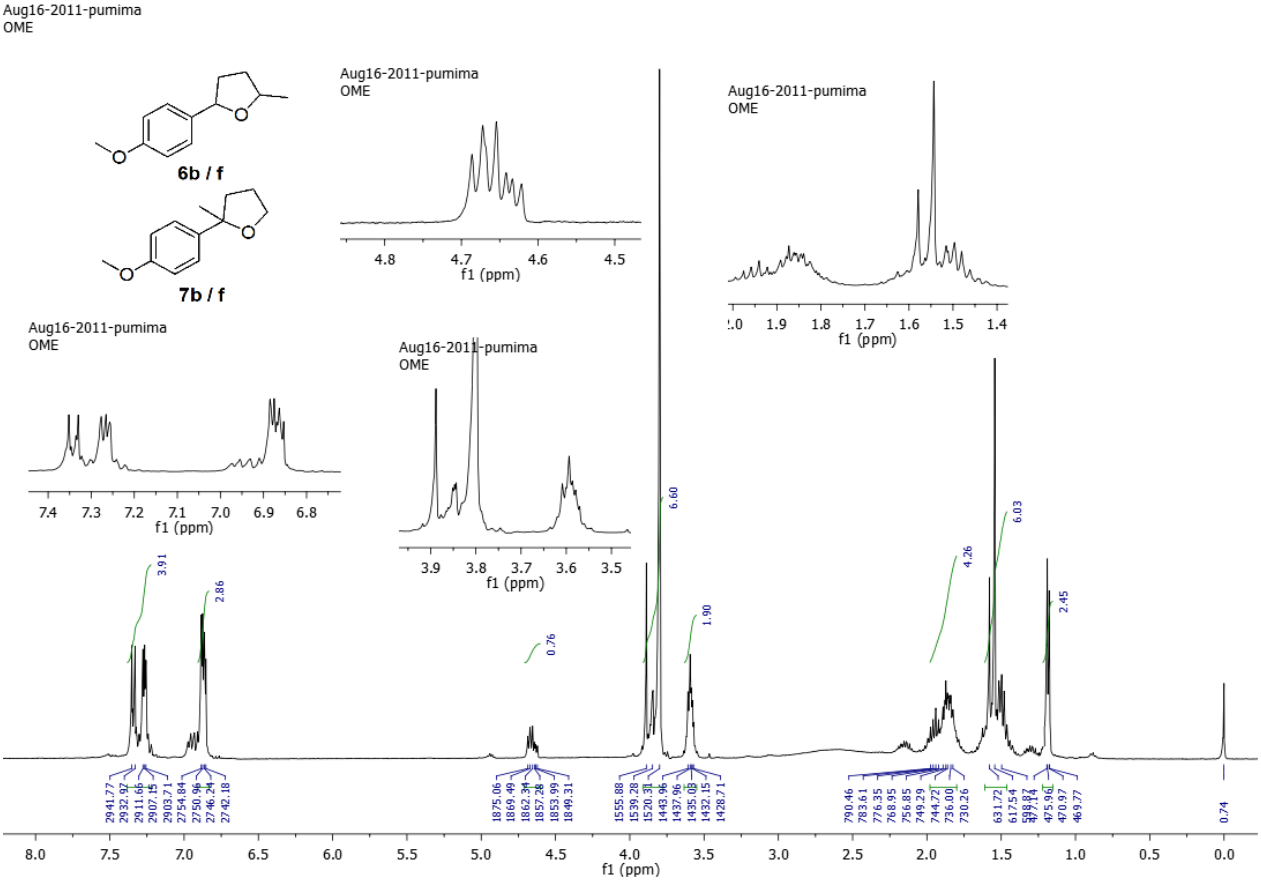
GCMS for 2-methyl-5-phenyl-tetrahydrofuran (Table 3, entry a and e)



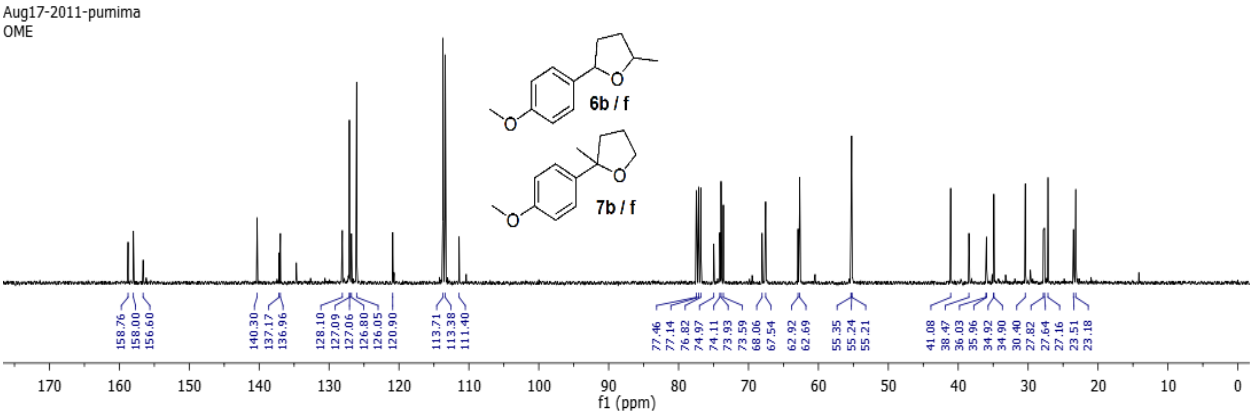
GCMS for 2-methyl-2-phenyl-tetrahydrofuran (Table 3, entry a and e)



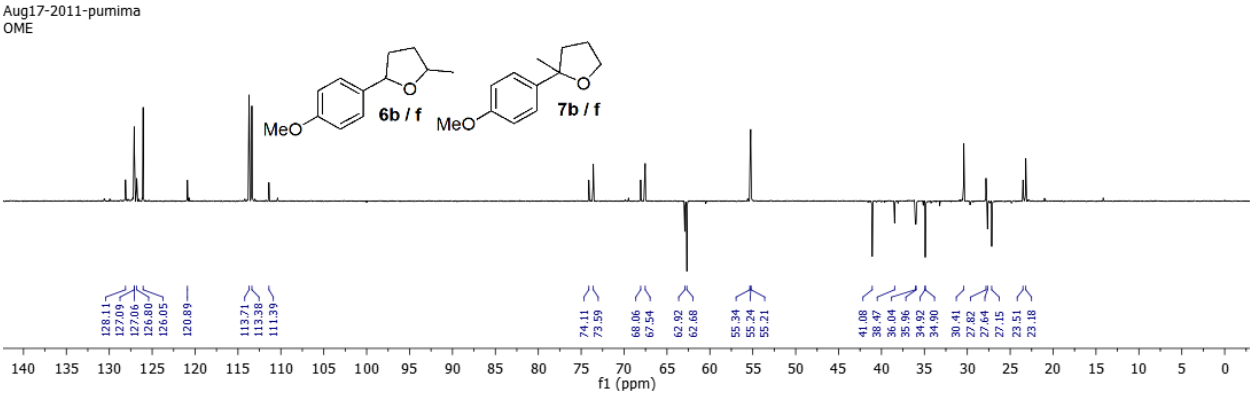
^{1}H NMR for 2-(4-methoxyphenyl)-5-methyl-tetrahydrofuran and 2-(4-methoxyphenyl)-2-methyl-tetrahydrofuran in $CDCl_3$ (Table 3, entry b and f)



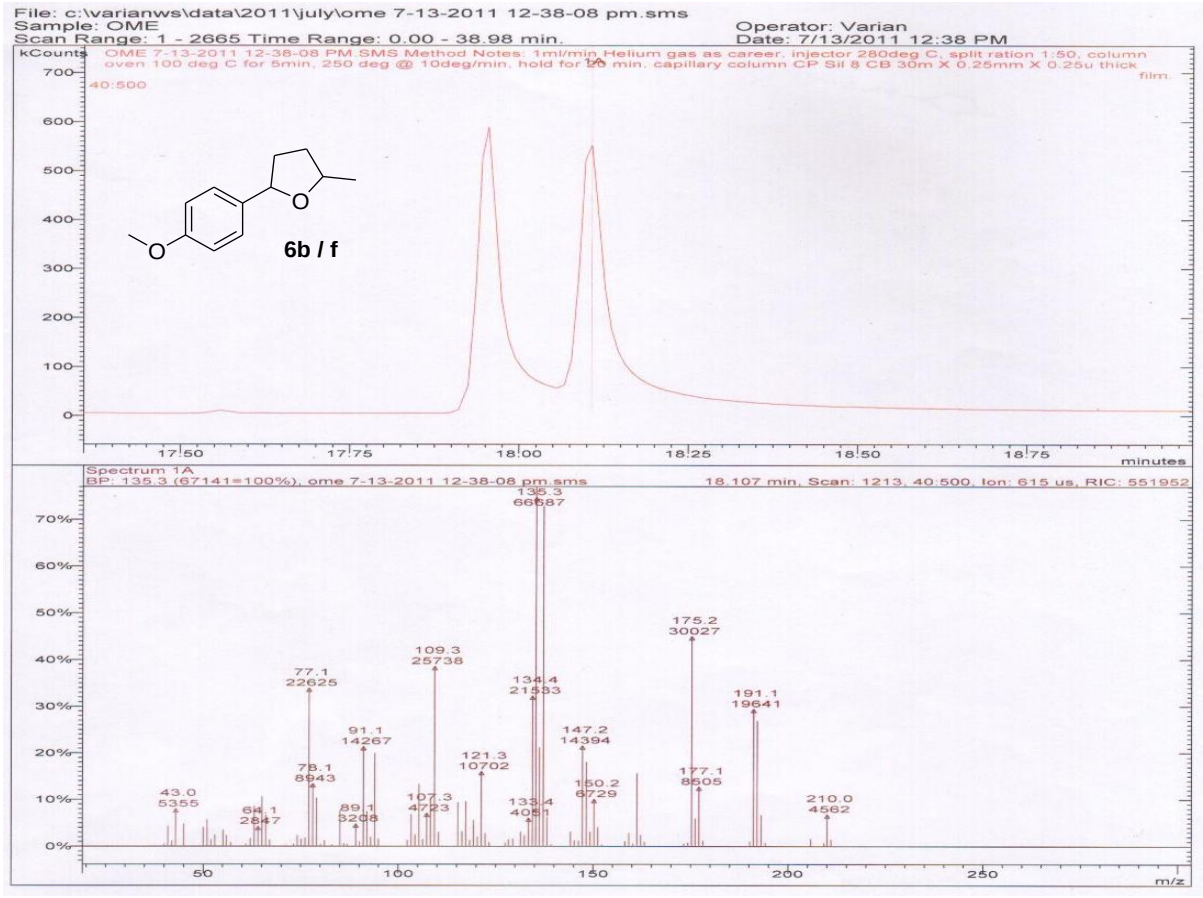
^{13}C NMR for 2-(4-methoxyphenyl)-5-methyl-tetrahydrofuran and 2-(4-methoxyphenyl)-2-methyl-tetrahydrofuran in $CDCl_3$ (Table 3, entry b and f)



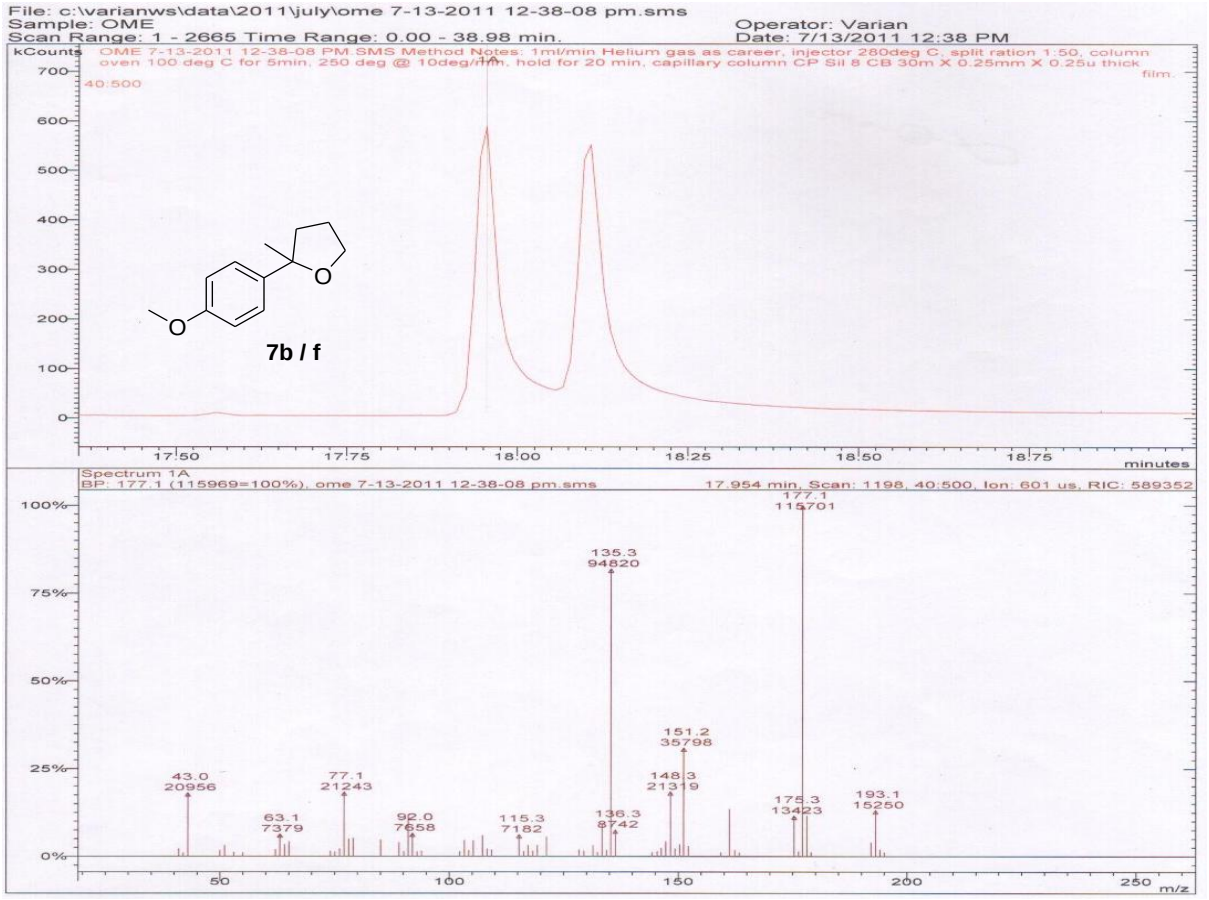
DEPT at 135 for 2-(4-methoxyphenyl)-5-methyl-tetrahydrofuran and 2-(4-methoxyphenyl)-2-methyl-tetrahydrofuran in $CDCl_3$ (Table 3, entry b and f)



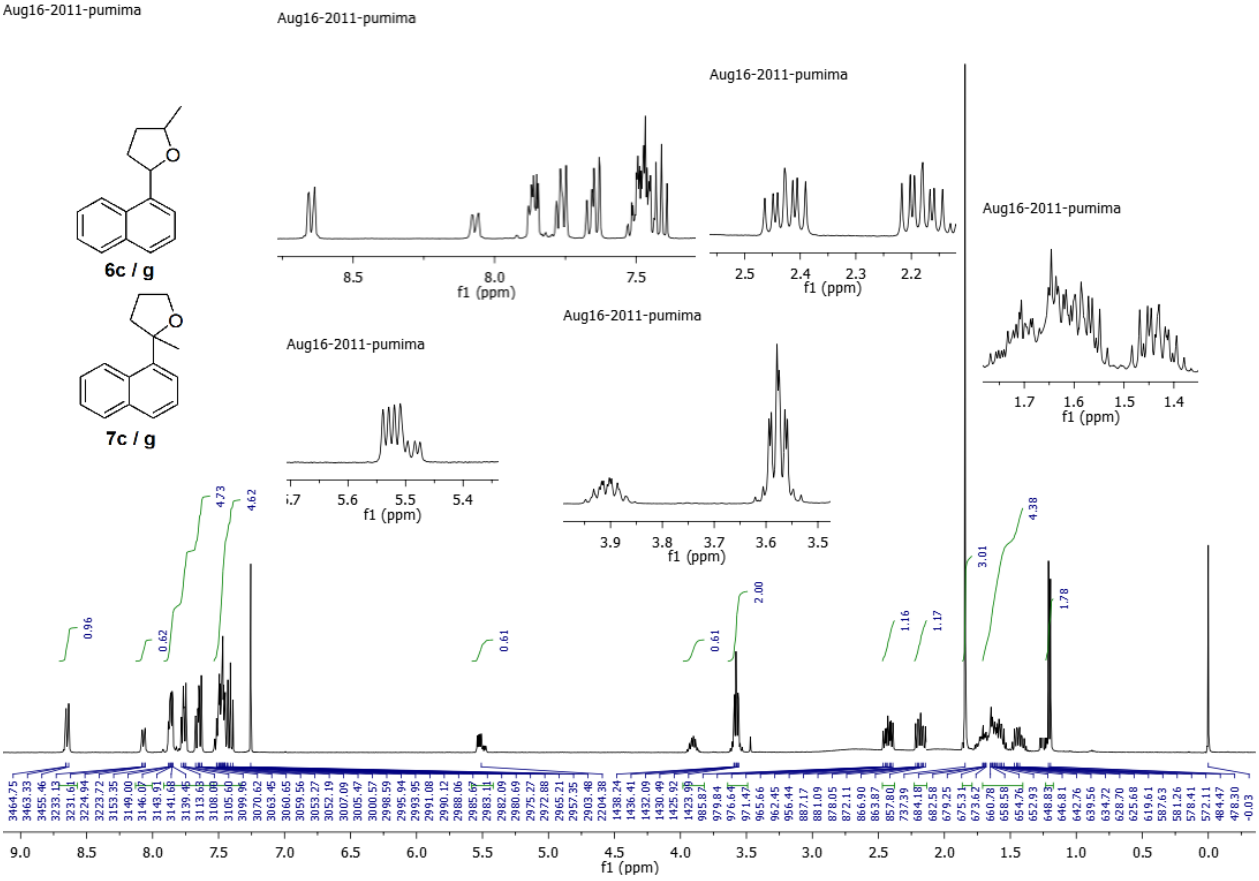
GCMS for 2-(4-methoxyphenyl)-5-methyl-tetrahydrofuran (Table 3, entry b and f)



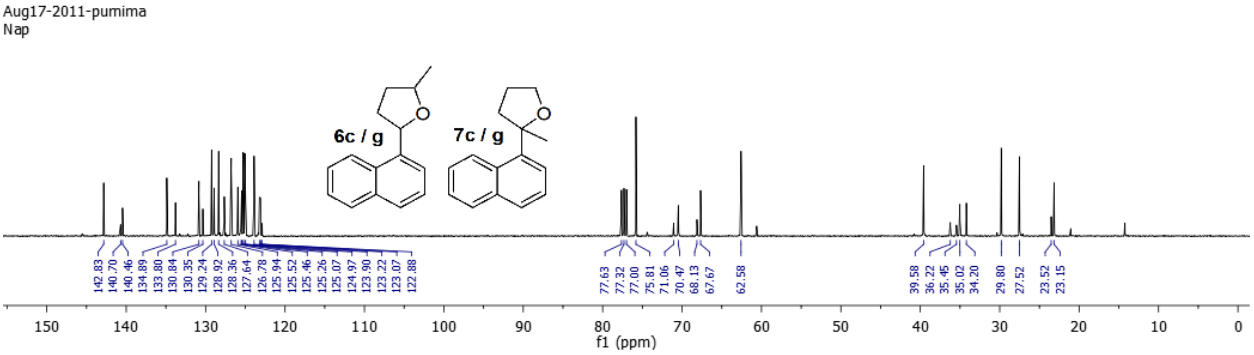
GCMS for 2-(4-methoxyphenyl)-2-methyl-tetrahydrofuran (Table 3, entry b and f)



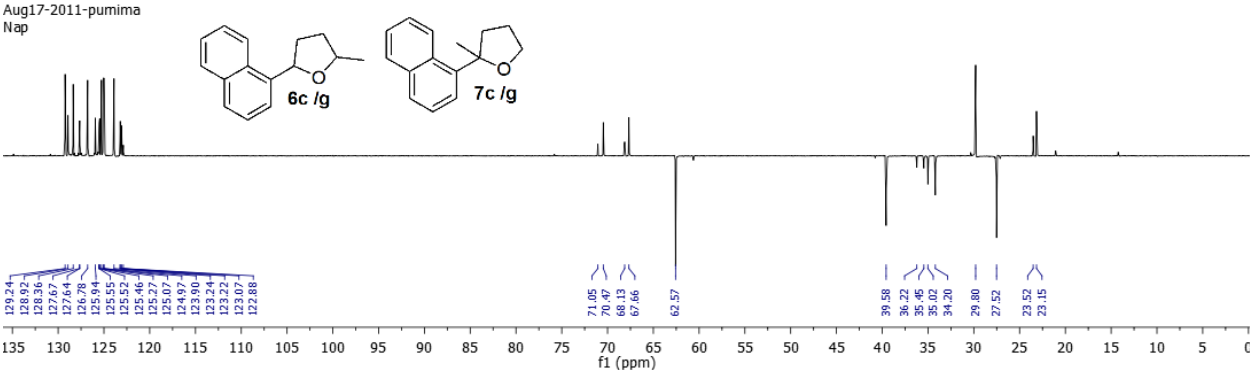
^{1}H NMR for 2-methyl-5-(naphthalen-1-yl)-tetrahydrofuran and 2-methyl-2-(naphthalen-1-yl)-tetrahydrofuran in $CDCl_3$ (Table 3, entry c and g)



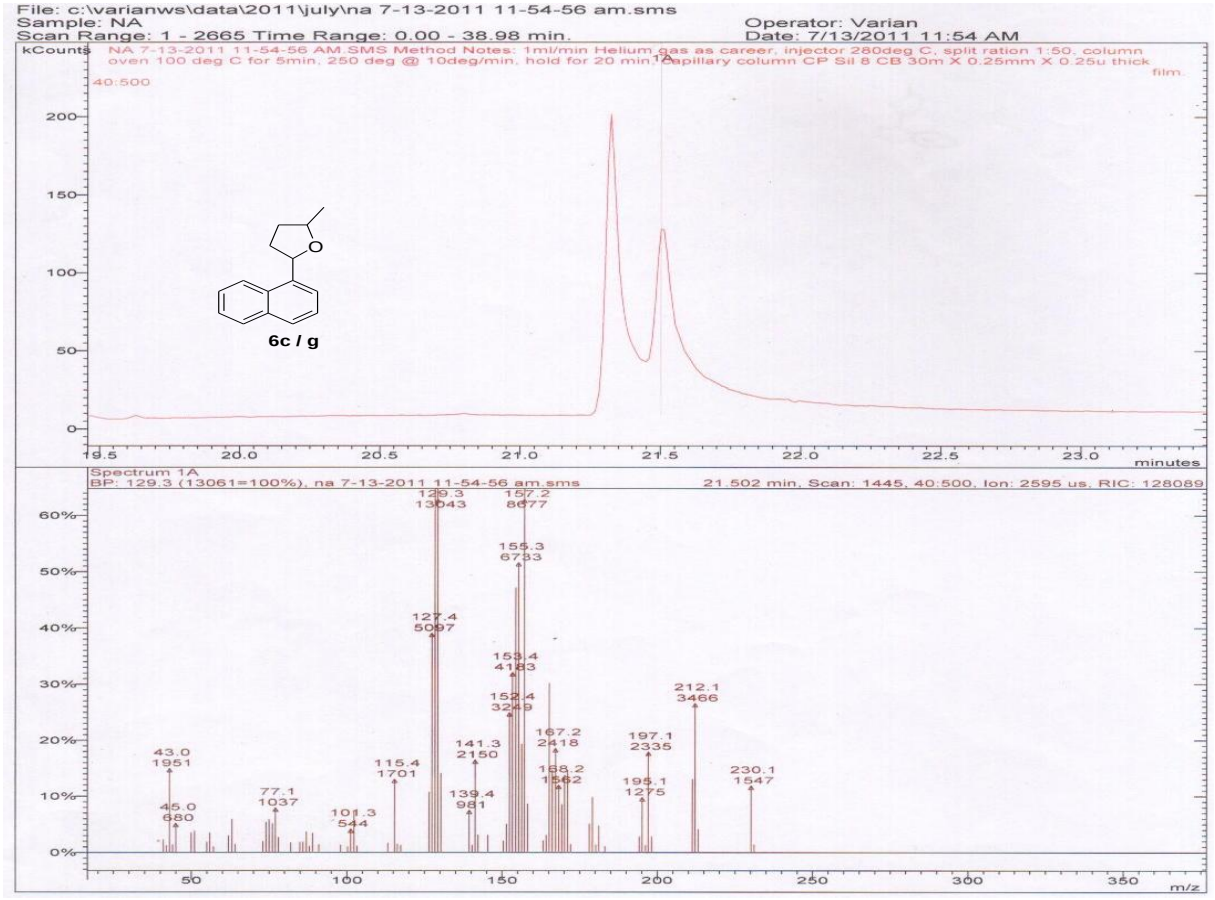
^{13}C NMR for 2-methyl-5-(naphthalen-1-yl)-tetrahydrofuran and 2-methyl-2-(naphthalen-1-yl)-tetrahydrofuran in $CDCl_3$ (Table 3, entry c and g)



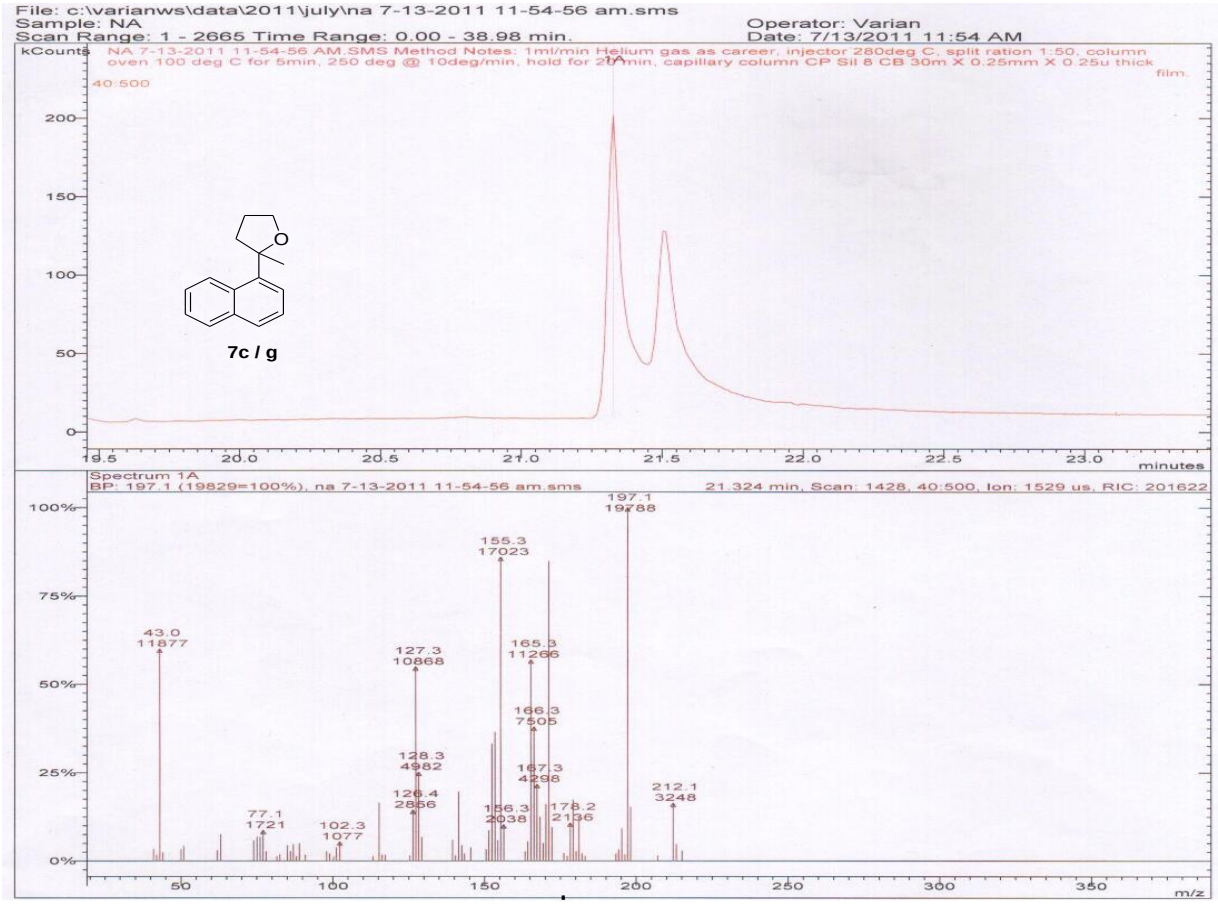
DEPT at 135 for 2-methyl-5-(naphthalen-1-yl)-tetrahydrofuran and 2-methyl-2-(naphthalen-1-yl)-tetrahydrofuran in $CDCl_3$ (Table 3, entry c and g)



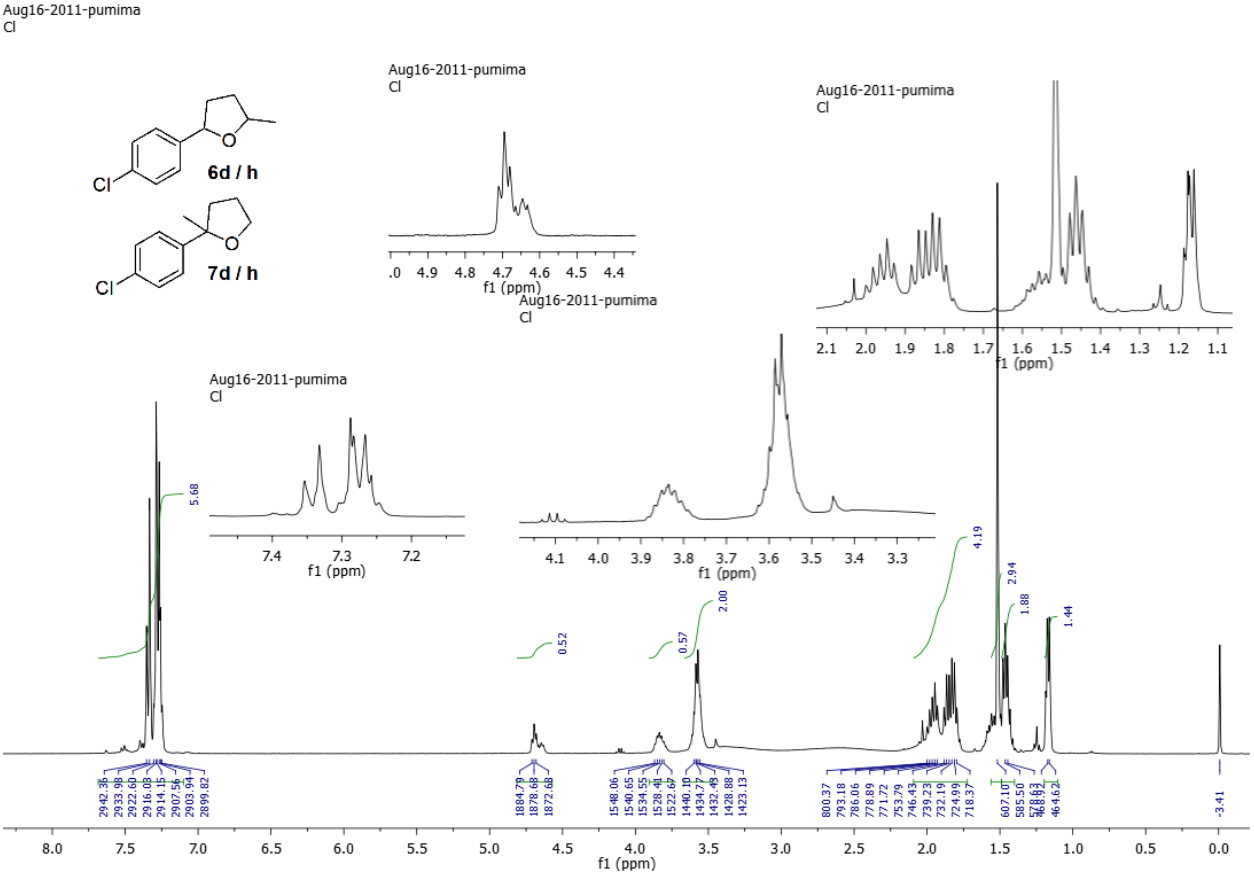
GCMS for 2-methyl-5-(naphthalen-1-yl)-tetrahydrofuran (Table 3, entry c and g)



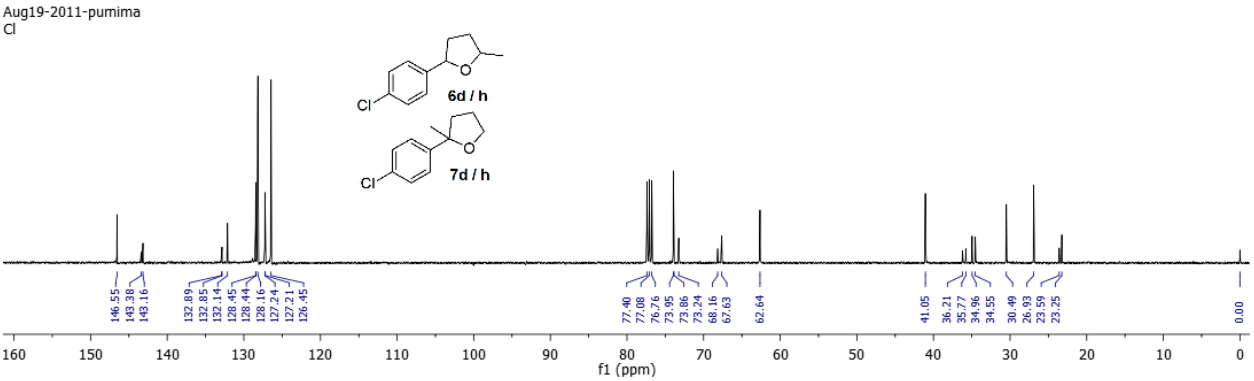
GCMS for 2-methyl-2-(naphthalen-1-yl)-tetrahydrofuran (Table 3, entry c and g)



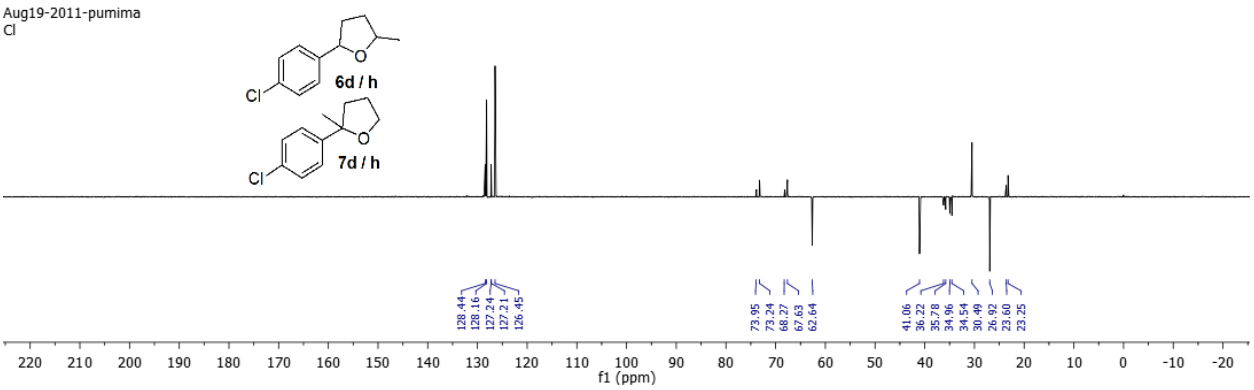
^{1}H NMR for 2-(4-chlorophenyl)-5-methyl-tetrahydrofuran and 2-(4-chlorophenyl)-2-methyl-tetrahydrofuran in $CDCl_3$ (Table 3, entry d and h)



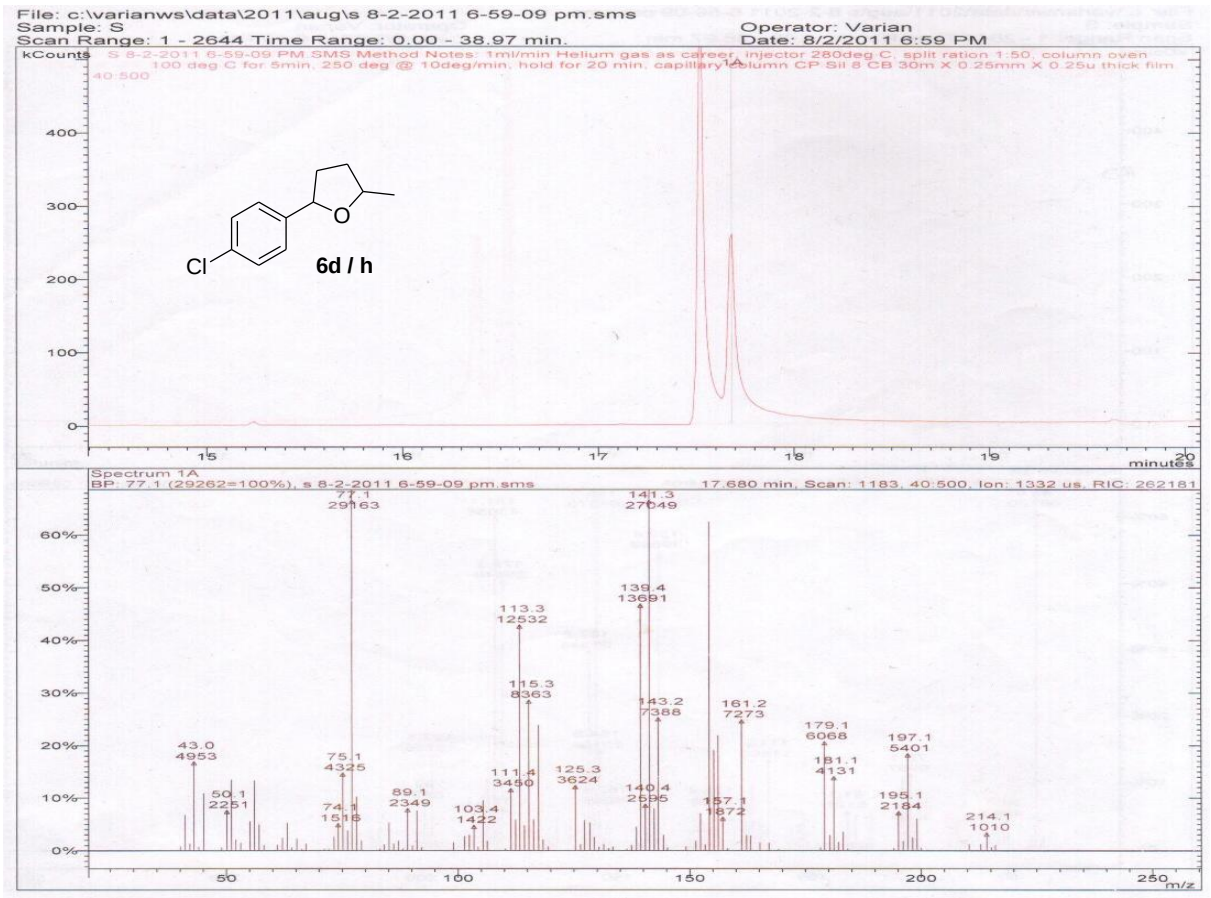
^{13}C NMR for 2-(4-chlorophenyl)-5-methyl-tetrahydrofuran and 2-(4-chlorophenyl)-2-methyl-tetrahydrofuran in $CDCl_3$ (Table 3, entry d and h)



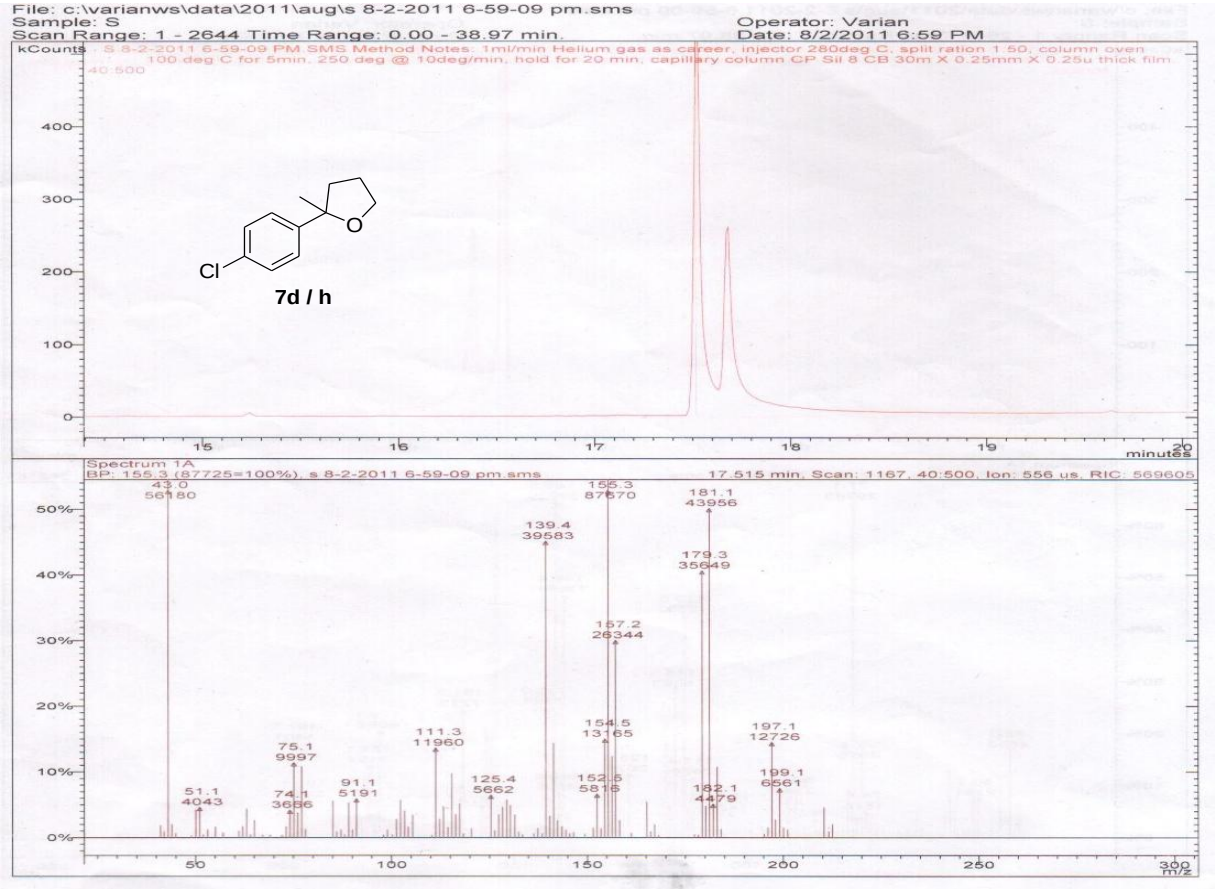
DEPT at 135 for 2-(4-chlorophenyl)-5-methyl-tetrahydrofuran and 2-(4-chlorophenyl)-2-methyl-tetrahydrofuran in $CDCl_3$ (Table 3, entry d and h)



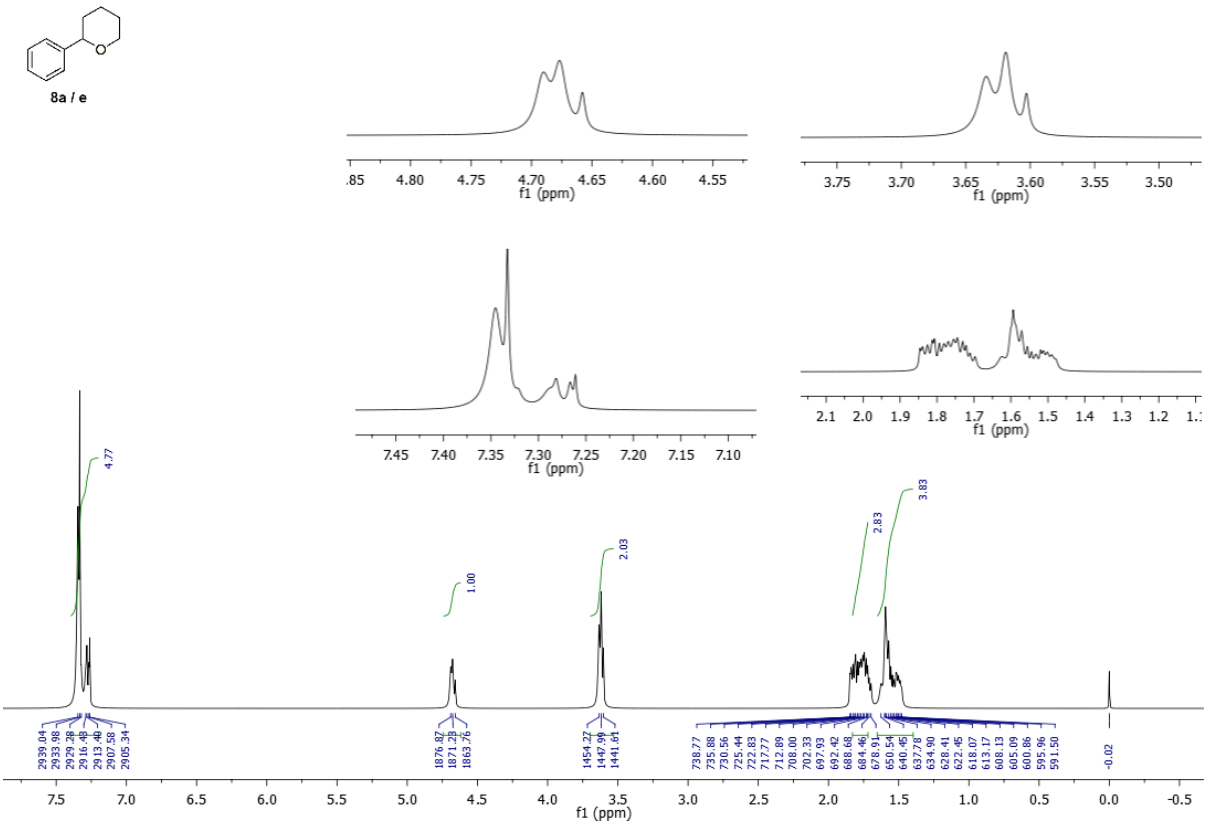
GCMS for 2-(4-chlorophenyl)-5-methyl-tetrahydrofuran (Table 3, entry d and h)



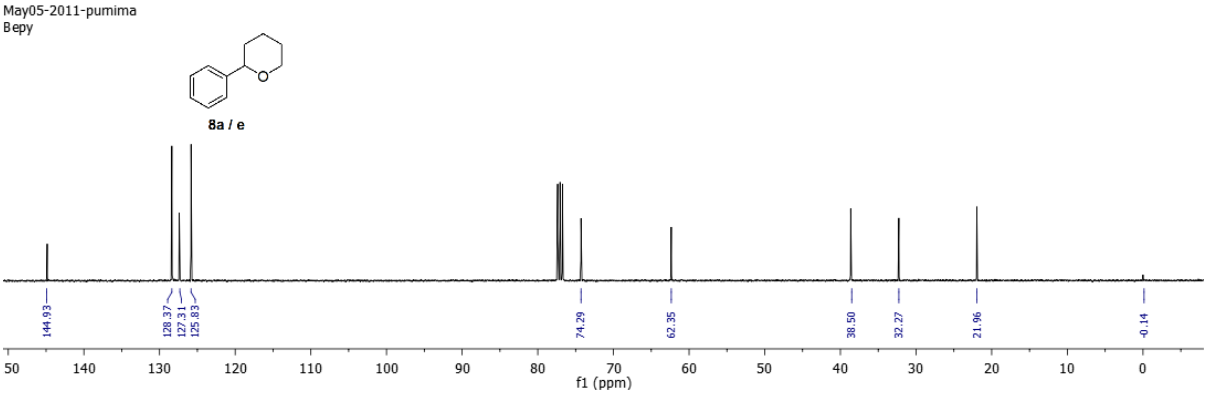
GCMS for 2-(4-chlorophenyl)-2-methyl-tetrahydrofuran in $CDCl_3$ (Table 3, entry d and h)



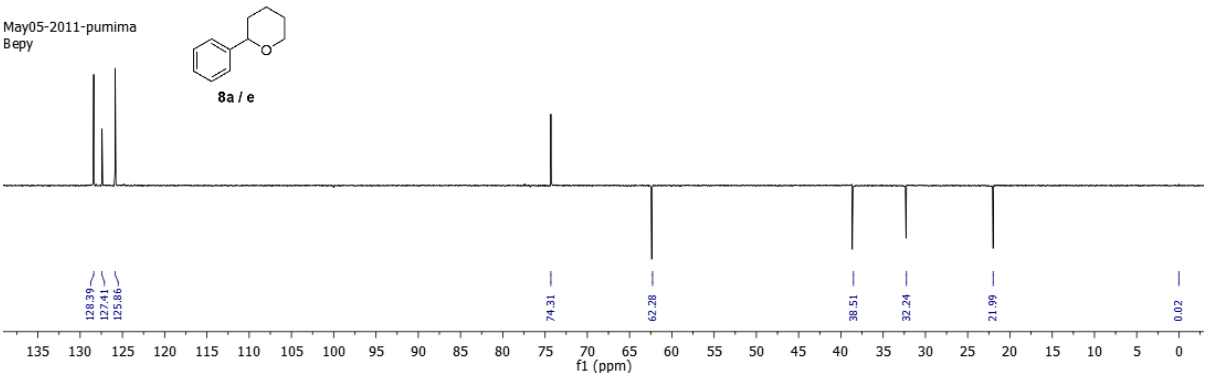
^{1}H NMR for 2-phenyl-tetrahydro-2H-pyran in $CDCl_3$ (Table 4, entry a and e)



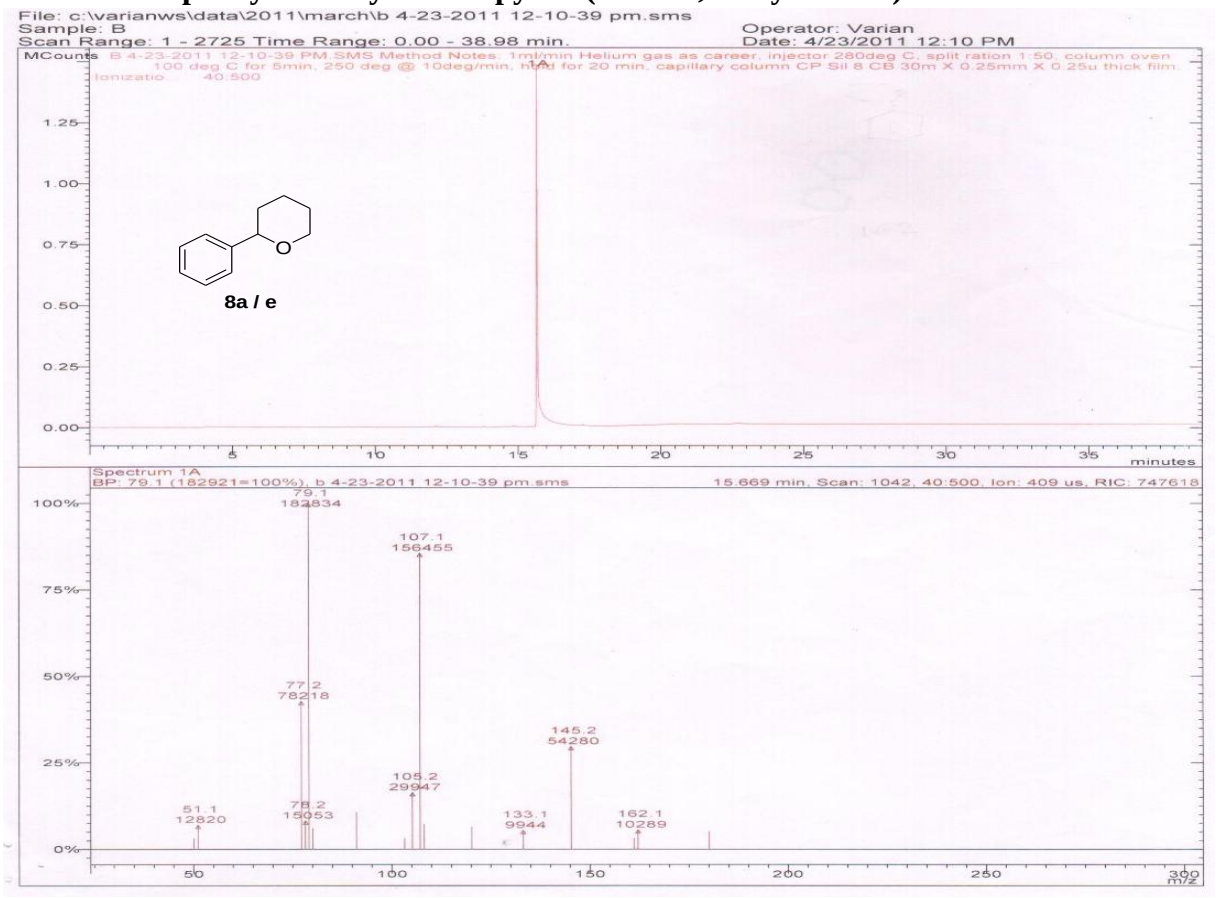
^{13}C NMR for 2-phenyl-tetrahydro-2H-pyran in $CDCl_3$ (Table 4, entry a and e)



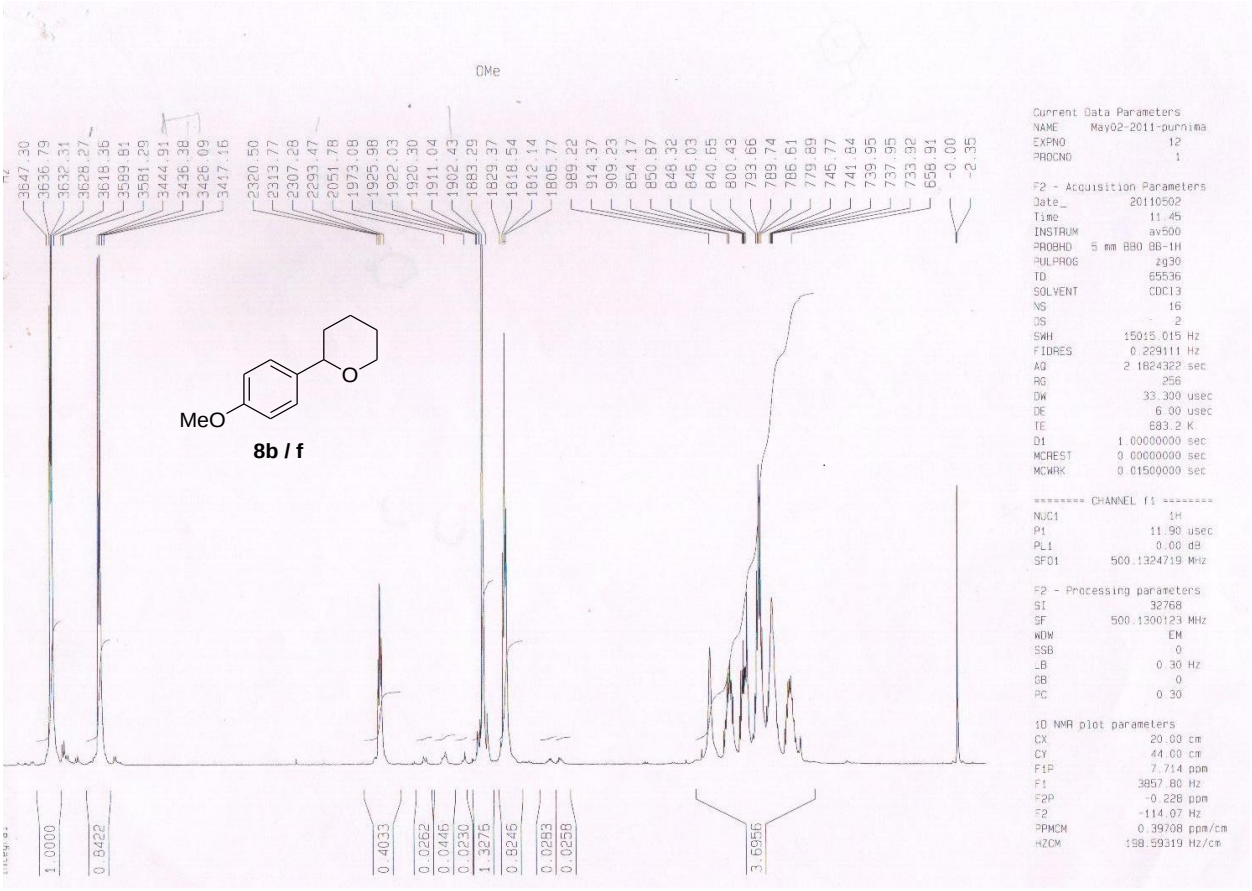
DEPT at 135 for 2-phenyl-tetrahydro-2H-pyran in $CDCl_3$ (Table 4, entry a and e)



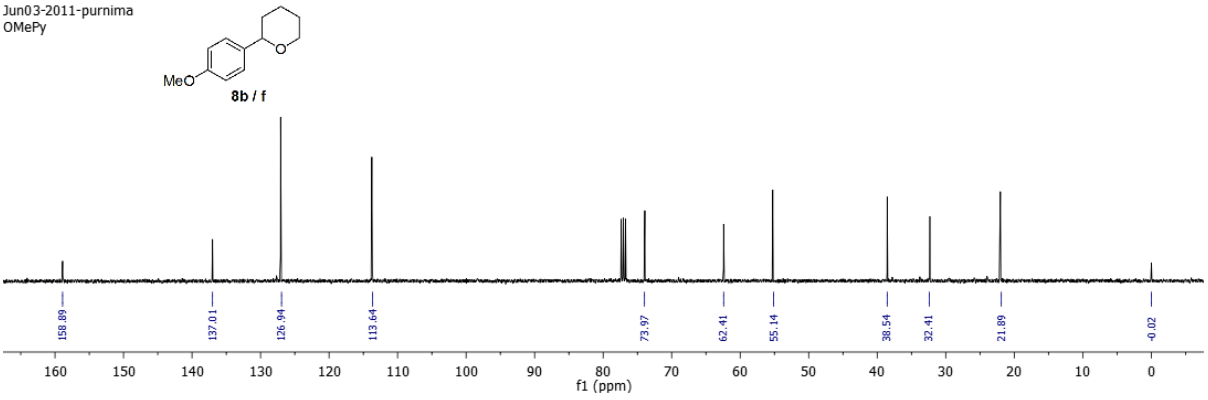
GCMS for 2-phenyl-tetrahydro-2H-pyran (Table 4, entry a and e)



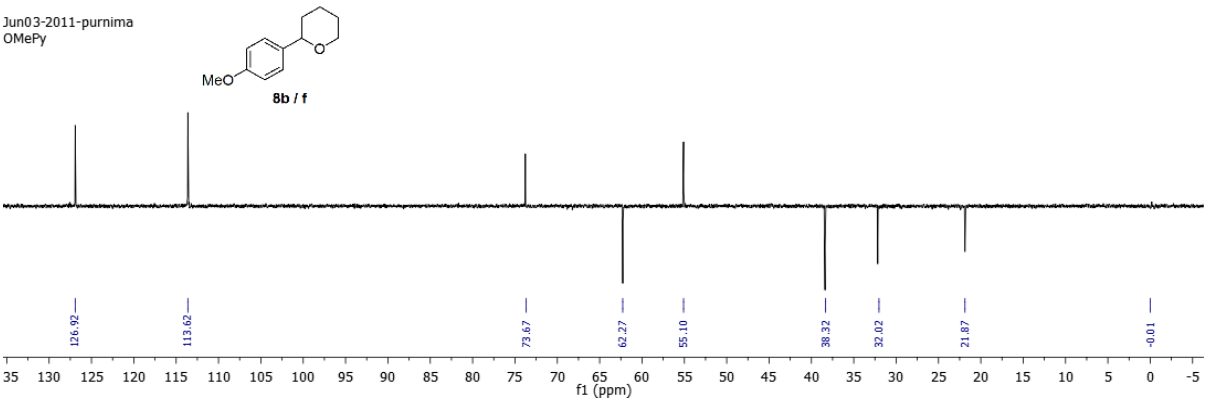
^{1}H NMR for 2-(4-methoxyphenyl)-tetrahydro-2H-pyran in $CDCl_3$ (Table 4, entry b and f)



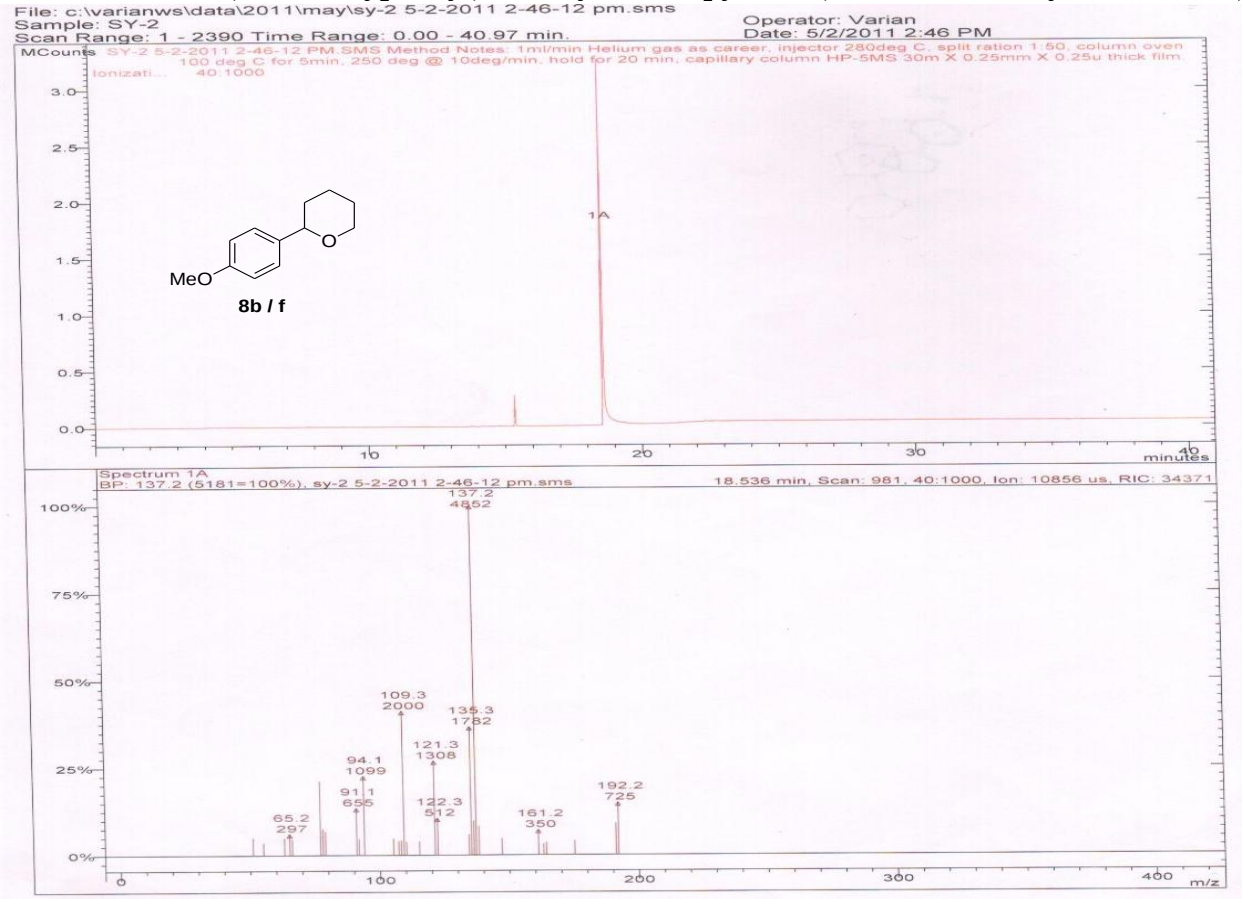
^{13}C NMR for 2-(4-methoxyphenyl)-tetrahydro-2H-pyran in $CDCl_3$ (Table 4, entry b and f)



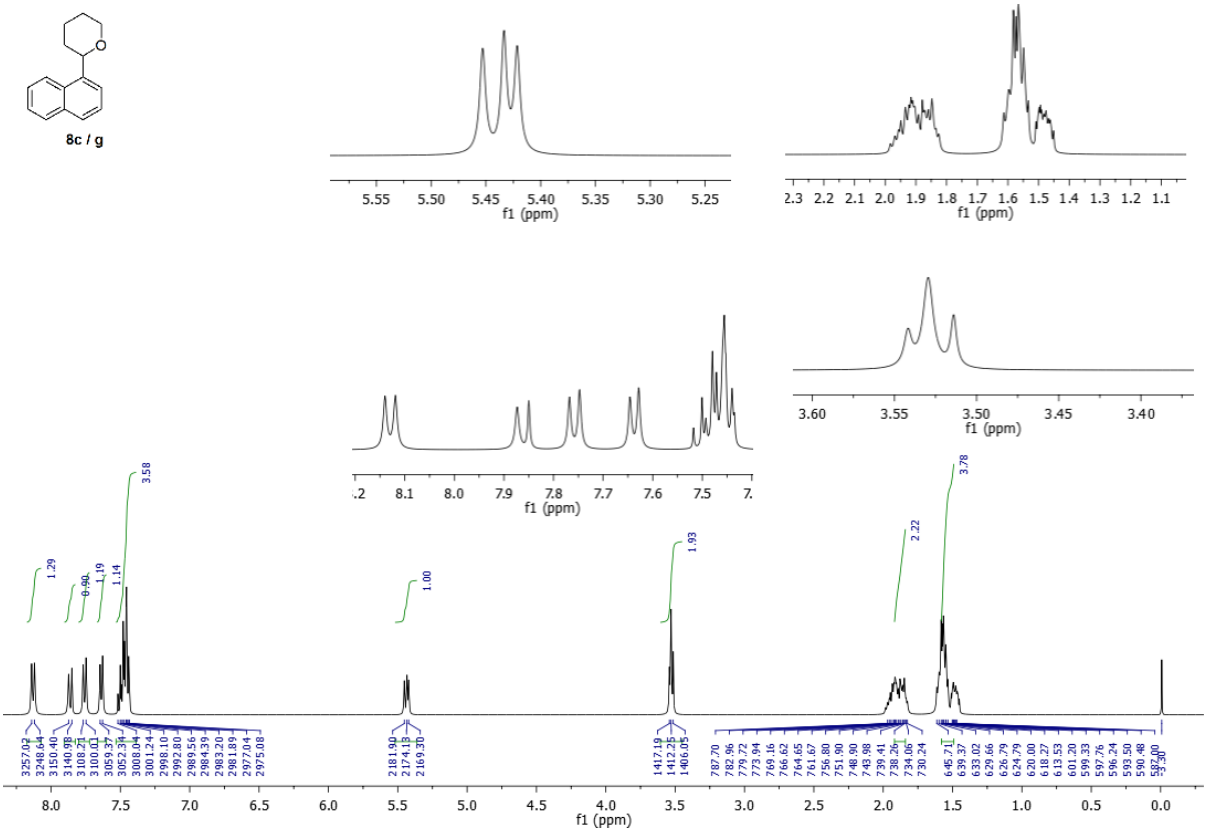
DEPT at 135 for 2-(4-methoxyphenyl)-tetrahydro-2H-pyran in $CDCl_3$ (Table 4, entry b and f)



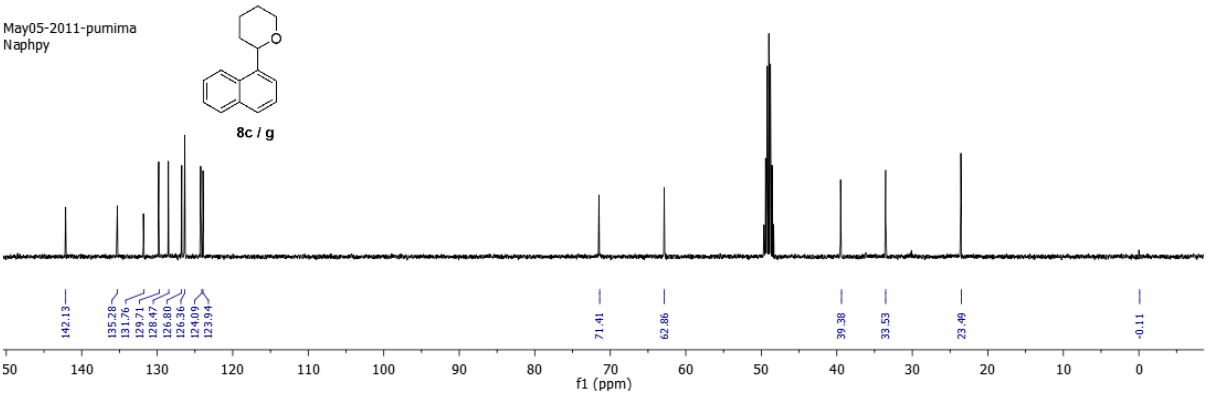
GCMS for 2-(4-methoxyphenyl)-tetrahydro-2H-pyran (Table 4, entry b and f)



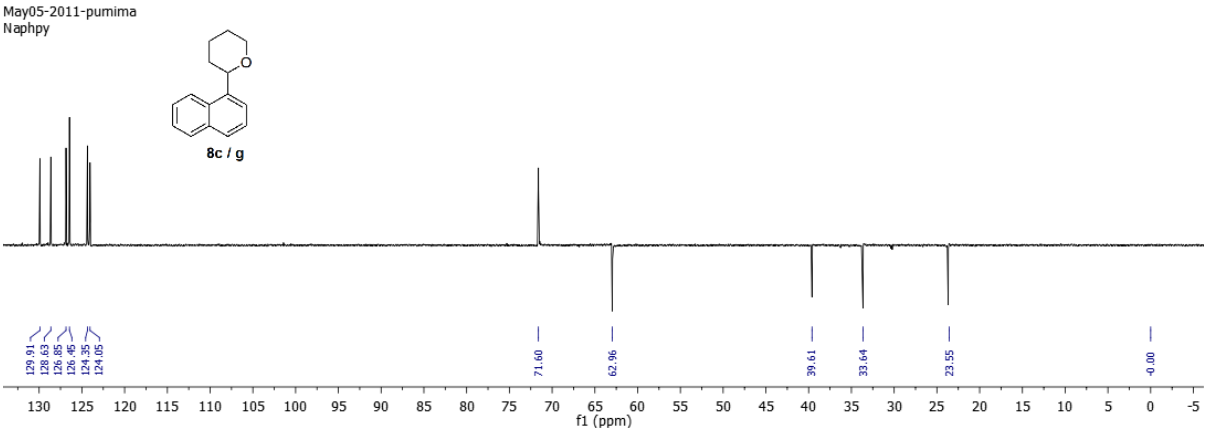
^{1}H NMR for 2-(naphthalen-1-yl)-tetrahydro-2H-pyran in CD_3OD (Table 4, entry c and g)



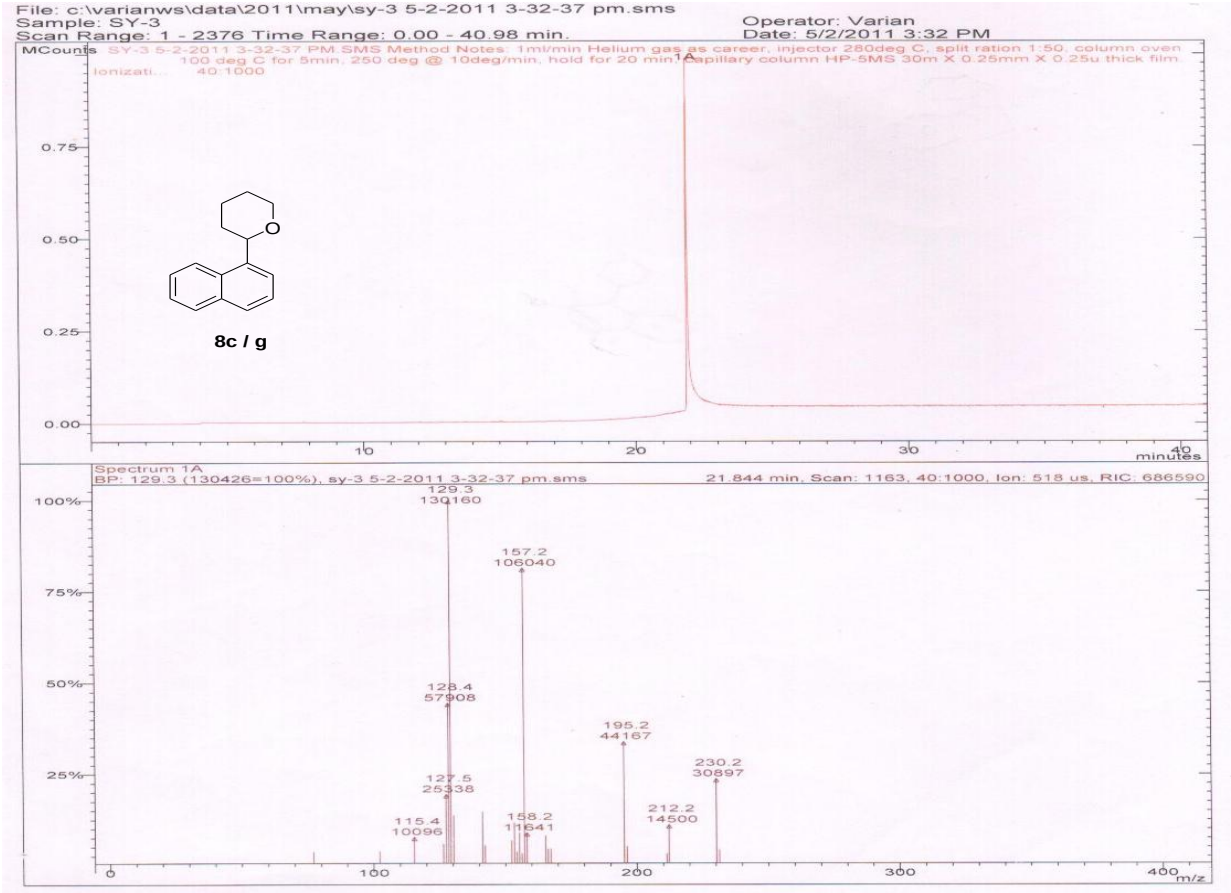
^{13}C NMR for 2-(naphthalen-1-yl)-tetrahydro-2H-pyran in CD_3OD (Table 4, entry c and g)



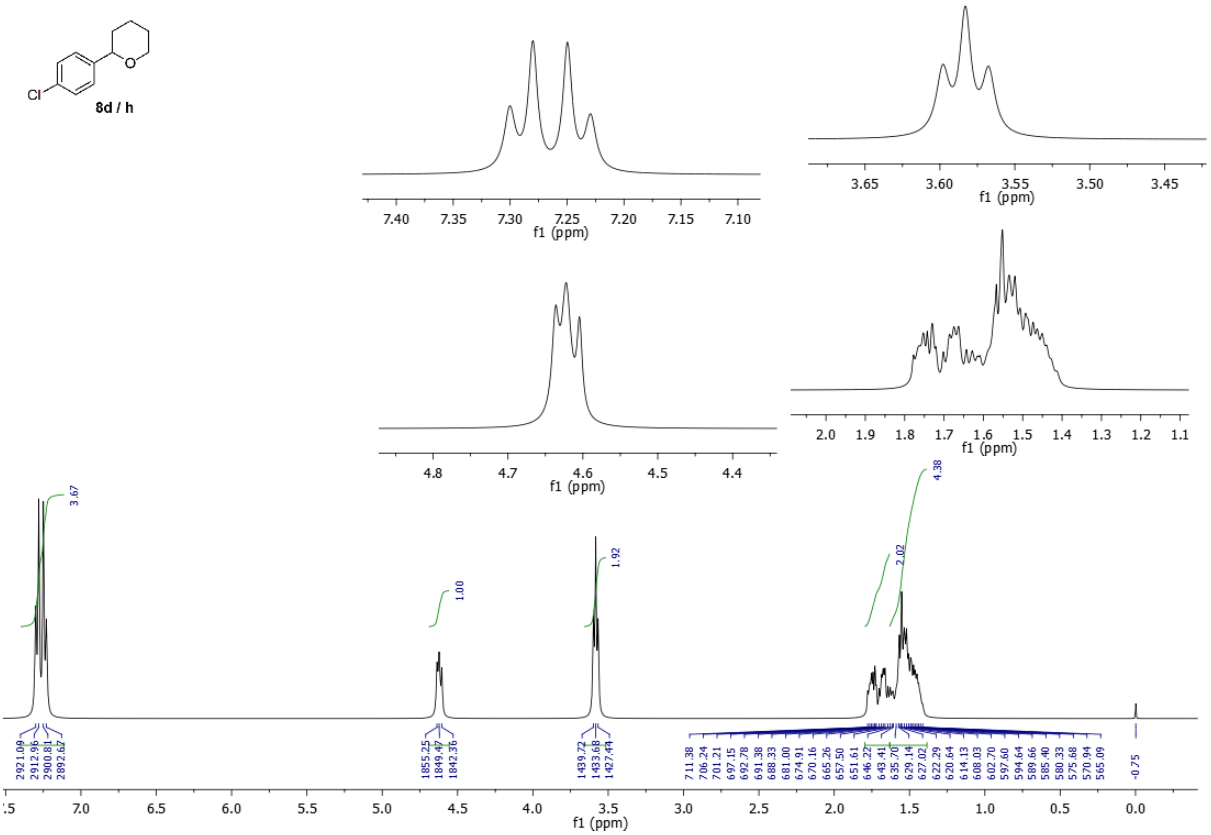
DEPT at 135 for 2-(naphthalen-1-yl)-tetrahydro-2H-pyran in CD_3OD (Table 4, entry c and g)



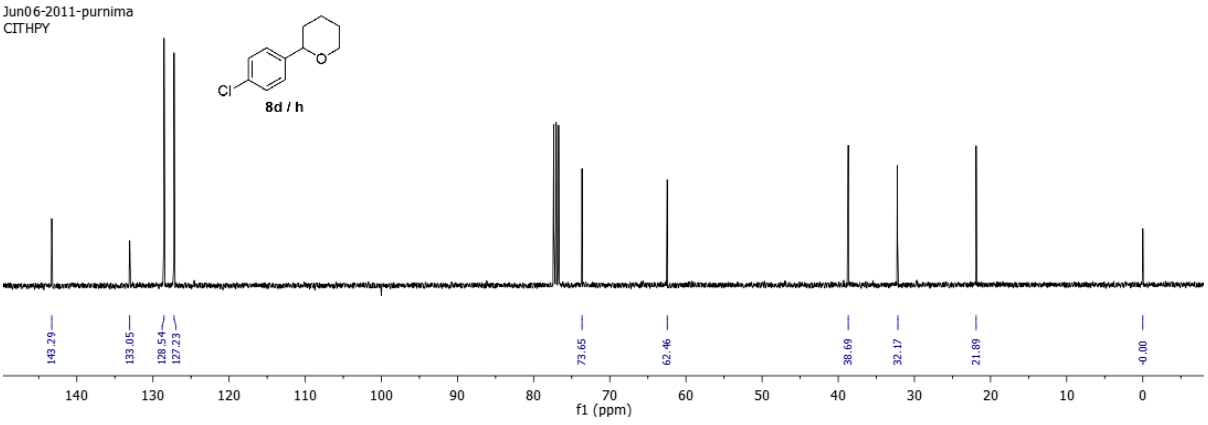
GCMS for 2-(naphthalen-1-yl)-tetrahydro-2H-pyran (Table 4, entry c and g)



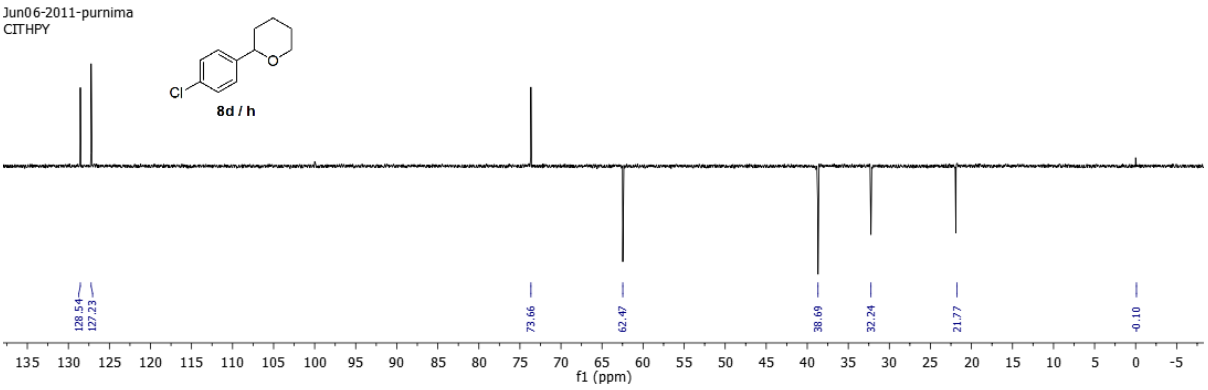
^{1}H NMR for 2-(4-chlorophenyl)-tetrahydro-2H-pyran in $CDCl_3$ (Table 4, entry d and h)



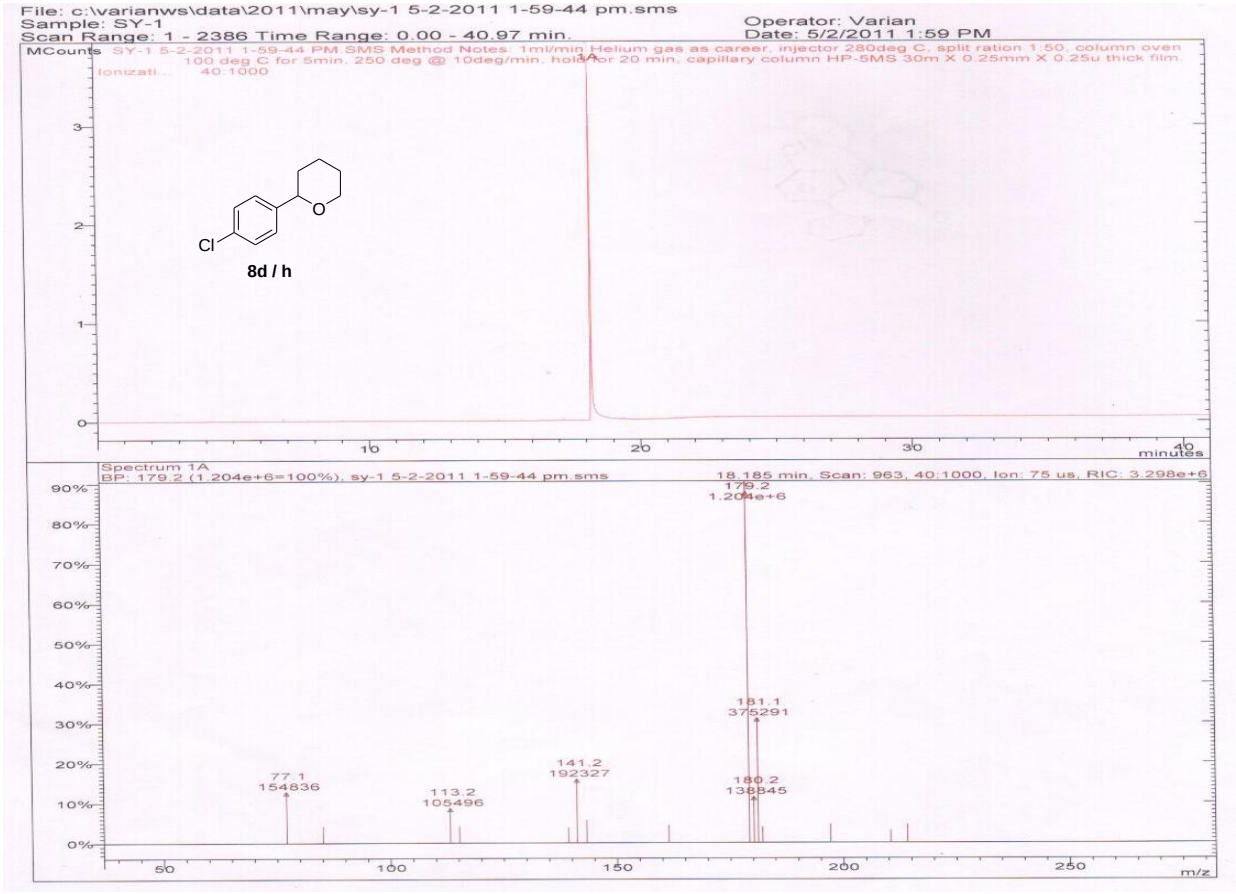
^{13}C NMR for 2-(4-chlorophenyl)-tetrahydro-2H-pyran in $CDCl_3$ (Table 4, entry d and h)



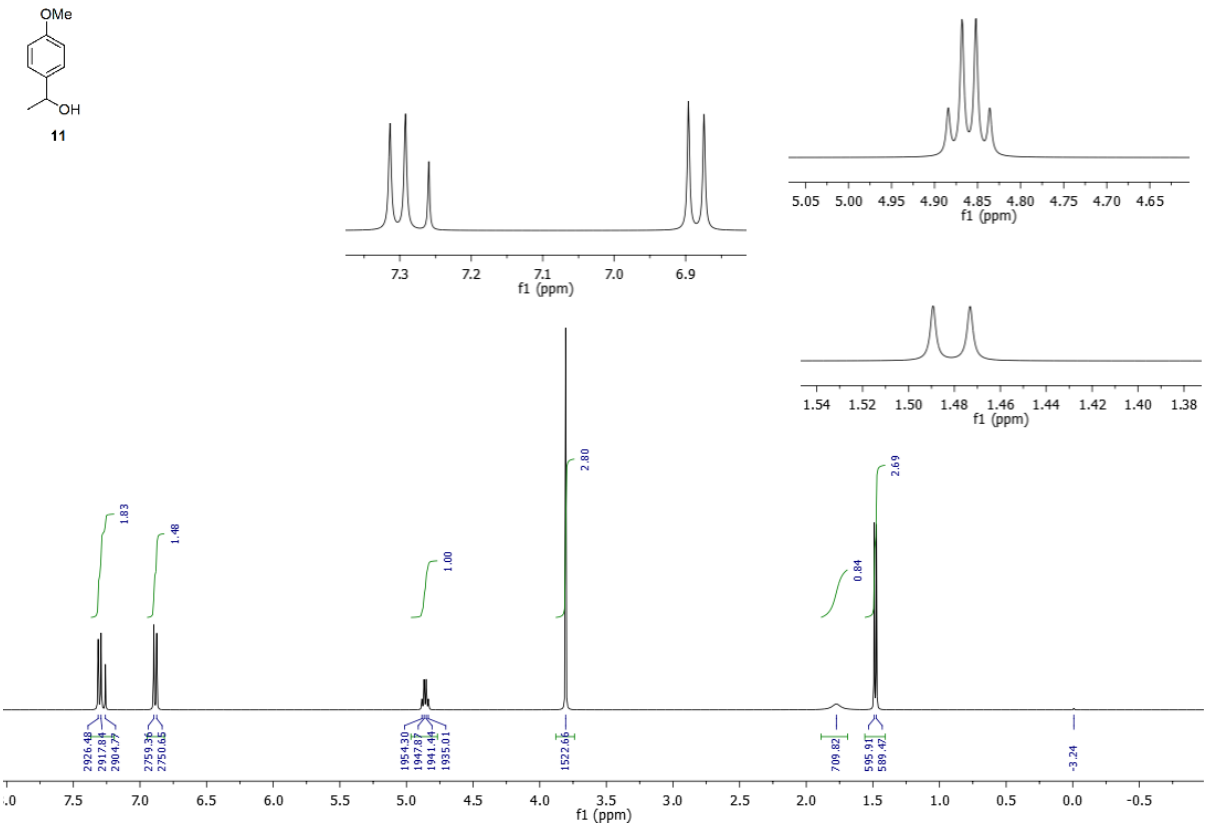
DEPT at 135 for 2-(4-chlorophenyl)-tetrahydro-2H-pyran (Table 4, entry d and h)



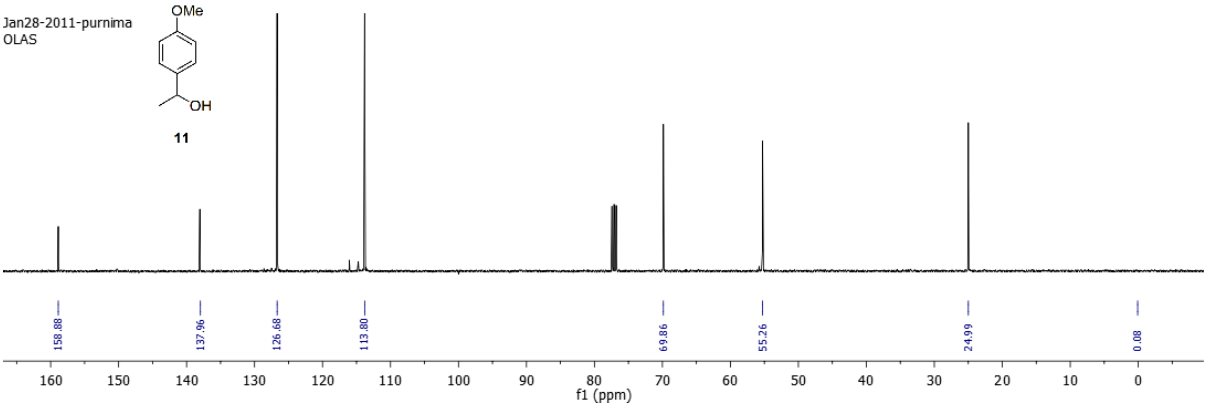
GCMS for 2-(4-chlorophenyl)-tetrahydro-2H-pyran (Table 4, entry d and h)



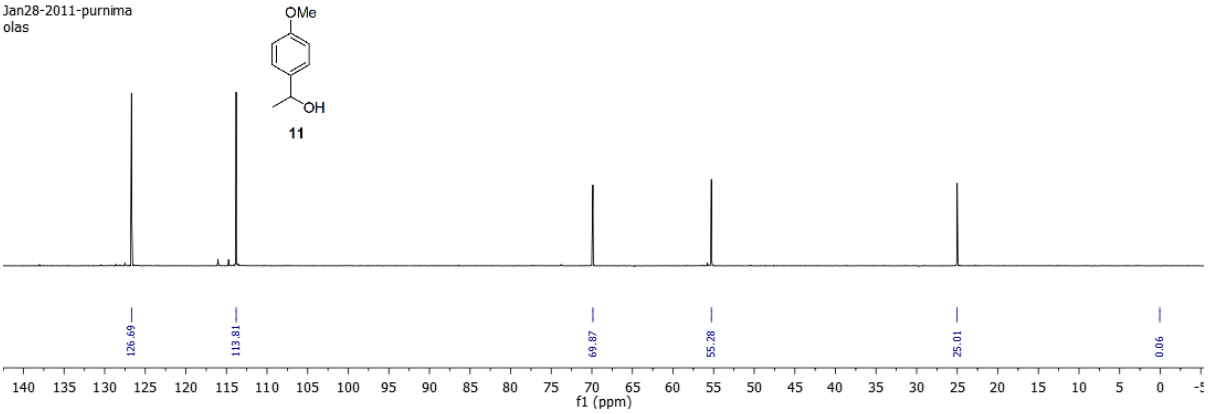
^{1}H NMR for 1-(4-methoxyphenyl) ethanol in $CDCl_3$ (scheme 2, entry 11)



^{13}C NMR for 1-(4-methoxyphenyl) ethanol in $CDCl_3$ (scheme 2, entry 11)



DEPT at 135 for 1-(4-methoxyphenyl) ethanol in $CDCl_3$ (scheme 2, entry 11)



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