Supporting Information:

Synthesis of Ethers via Reaction of Carbanions and Monoperoxyacetals

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Table of Contents

Optimized Coordinates and Energies for Calculated Structures in Scheme 5

	R = t-Bu, M = Li	R = THP, M = Li	R = t-Bu, M = Na	R = THP, M = Na
$ROOCH_3$	page 5	Page 9	Page 13	Page 17
CH_3M	page 5	Page 9	Page 14	Page 18
Intermediate II	page 6	Page 10	Page 14	Page 18
TS III	page 6	Page 11	Page 15	Page 19
Intermediate IV	page 7	Page 11	Page 16	Page 20
ROM	page 8	Page 12	Page 16	Page 21
CH_3OCH_3	Page 8	Page 13	Page 17	Page 21

Thermal analyses (DSC/TGA)

2-(10-Phenyldecylperoxy) tetrahydro-2H-pyran (**10b**) 22

10-(*tert*-Butylperoxy)decylbenzene (**10a**) 23

NMR spectra: hydroperoxides

2-Tetrahydropyranyl OOH (**2**) (^{1}H and ^{13}C) 24

2-Methoxyprop-2-yl OOH (**3**) ^{1}H and ^{13}C) 25

dimethyloctenyl OOH (**4**)(^{1}H and ^{13}C) 26

1-methylhydroperoxide (**5**) (^{1}H and ^{13}C) 27

3-Phenylpropyl hydroperoxide (**6**) (^{1}H and ^{13}C) 28

3-Phenylpropyl hydroperoxide (**7**) (^{1}H and ^{13}C) 29

NMR spectra: peroxides and peroxyacetals

8-(*tert*-Butylperoxy)-2,6-dimethyloct-2-ene (**8a**) (^{1}H and ^{13}C) 30

2-(3,7-Dimethyloct-6-ene-1-yl)peroxy)-tetrahydro-2H-pyran (**8b**): (^{1}H and ^{13}C) 31

8-((2-Methoxypropan-2-yl) peroxy)-2,6-dimethyloct-2-ene (**8c**): (^{1}H and ^{13}C) 32

t-Butyldimethylsilyl 3,7-dimethyl-6-octenyl peroxide (**8d**): (^{1}H and ^{13}C) 33
3-*tert*-Butylperoxypropyl benzene (**9a**) (^{1}H and ^{13}C) 34
2-(3-Phenylpropylperoxy)tetrahydro-2H-pyran (**9b**) (^{1}H and ^{13}C) 35
3-(2-Methoxyethylperoxy)propyl benzene (**9e**): (^{1}H and ^{13}C) 36
10-(*tert*-Butylperoxy)decylbenzene (**10a**): (^{1}H and ^{13}C) 37
2-(10-Phenyldecylperoxy) tetrahydro-2H-pyran (**10b**) (^{1}H and ^{13}C) 38
t-Butyldimethylsilyl 10-phenyldecyl peroxide (**10d**): (^{1}H and ^{13}C) 39
tert-Butylperoxy octane (**11a**) (^{1}H and ^{13}C) 40
2-(Decylperoxy)-tetrahydro-2H-pyran (**12b**) (^{1}H and ^{13}C) 41
2-(2-Octylperoxy)-tetrahydro-2H-pyran (**13b**) (^{1}H and ^{13}C) 42
2-(1-Methylcyclohexylperoxy)-tetrahydro-2H-pyran (**15b**) (^{1}H and ^{13}C) 43
bis-(Tetrahydro-2H-pyranyl) peroxide (**14b**) (^{1}H and ^{13}C) 44
(*E,Z*)-2-(Undec-2-en-1-yl peroxy) tetrahydro-2H-pyran (**16b**): (^{1}H and ^{13}C) 45

Ethers:

8-Butoxy-2,6-dimethyloct-2-ene (**17a**) (^{1}H and ^{13}C) 46
8-Hexyloxy-2,6-dimethyl-2-octene (**17b**): (^{1}H and ^{13}C) 47
8-Allyloxy-2,6-dimethyloct-2-ene (**17c**) (^{1}H and ^{13}C) 48
8-*tert*-Butoxy-2,6-dimethyl-2-octene (**17d**) (^{1}H and ^{13}C) 49
3-Phenylpropyl trimethylsilylmethyl ether (**17e**): (^{1}H and ^{13}C) 50
2-Butoxy octane (**17f**) (^{1}H and ^{13}C) 51
2-Hexyloxy octane (**17g**) (^{1}H and ^{13}C) 52
2-Butoxy-tetrahydro-2H-pyran (**17h**) (^{1}H and ^{13}C) 53
2-Hexyloxy-tetrahydro-*2H*-pyran (**17i**): (^{1}H and ^{13}C) 54
1-Butoxy-1-methyl cyclohexane (**17j**): (^{1}H and ^{13}C) 55
1-Hexyloxy 1-methyl cyclohexane (**17k**): (^{1}H and ^{13}C) 56
(E/Z)-1-Butoxyundec-2-ene (**17l**): (^{1}H and ^{13}C) 57
(E/Z)-Hexyl 2-undecenyl ether (**17m**): (^{1}H and ^{13}C) 58

Reactions of peroxides with sp^2 organometallics:

3,7-Dimethyl-6-octen-1-yl phenyl ether (**18a**) (^{1}H and ^{13}C) 59
2-Methylprop-1-en-1-yl 3-phenylpropyl ether (**18b**): (^{1}H and ^{13}C) 60
3,7-Dimethyl-6-octen-1-yl vinyl ether (**18c**): (^{1}H and ^{13}C) 61
2-(3,7-Dimethyloct-6-en-1-oxy)-thiophene (**18d**) (^{1}H and ^{13}C) 62

2-(Decyloxy)-thiophene (**18e**): (^{1}H and ^{13}C) 63

Reaction with lithiated dithianes:

3,3-Difluoro-3-((10-phenyldecyl)oxy)propyl)benzene (**19**): (^{1}H and ^{13}C) 64

Synthesis of mixed acetals:

Tributyl(1-(methoxymethoxy)-3-phenylpropyl)stannane (**20**) (^{1}H and ^{13}C) 65

Benzene, 3-methoxymethoxy-3-octyloxypropyl (**21a**): (^{1}H and ^{13}C) 66

3-Methoxymethoxy-3-phenylpropoxy propylbenzene (**21b**) ^{1}H and ^{13}C) 67

3-Decyloxy-3-methoxymethoxy propyl benzene (**21c**) (^{1}H and ^{13}C) 68

3-((3,7-Dimethyloct-6-en-1-yl)oxy)-3-(methoxymethoxy)propylbenzene (**21d**): (^{1}H,^{13}C) 69

3-methoxymethyloxy-2-methyl-5-phenylpentan-2-ol (**22**) (^{1}H and ^{13}C) 70

3-methoxymethoxypropyl benzene (^{1}H and ^{13}C) 71

Synthesis of cyclopropyl ethers:

3,7-Dimethyloct-6-en-1-yl cyclopropyl ether (**23a**): (^{1}H and ^{13}C) 72

Cyclopropyl 3-phenylpropyl ether (**23b**): (^{1}H and ^{13}C) 73

Cyclopropyl decyl ether (**23c**) (^{1}H and ^{13}C) 74

Cyclopropyl 2-octyl ether (**23d**) (^{1}H and ^{13}C) 75

Synthesis of radical probes

1,1-dimethyl-2-phenylethyl hydroperoxide (^{1}H and ^{13}C) 76

t-Butyl 1,1-dimethyl-2-phenylethyl peroxide (**24a**) (^{1}H and ^{13}C) 77

2-((2-Methyl-3-phenylpropan-1-yl)tetrahydro-2*H*-pyranyl peroxide (**24b**): (^{1}H and ^{13}C) 78

Triethylsilyl (2-methyl-1-phenylpropan-2-yl) peroxide (**24d**) (^{1}H and ^{13}C) 79

Reactions of organometallics with radical probes

2-Butoxy-2-methylpropyl)benzene (**25a**) (^{1}H and ^{13}C) 80

(2-Hexyloxy-2-methylpropyl)benzene (**25b**): (^{1}H and ^{13}C) 81

2-Methyl-1-phenylpropan-2-ol (**26**) (^{1}H and ^{13}C) 82

Pentylbenzene (^{1}H and ^{13}C) 83

Triethylsilanol (^{1}H and ^{13}C) 84

Competition reactions:

Butyl decyl ether (**27**): (^{1}H and ^{13}C) 85
3-butoxypropyl benzene (**28**) (^{1}H and ^{13}C) 86
3-Phenoxy propyl benzene (**29)** (^{1}H and ^{13}C) 87
Biphenyl (^{1}H and ^{13}C) 88

B3LYP/6-31+G(d,p) Optimized Coordinates, Electronic Energy (hartree), and Zero-Point Energy (Z-PE, hartree) of All Structures Labeled in Scheme 5.

Series: M = Li, R = t-Bu

$ROOCH_3$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.533651
3	6	0	1.423955	0.000000	2.103459
4	1	0	1.984956	0.868284	1.749504
5	1	0	1.396243	0.028408	3.197064
6	1	0	1.955483	-0.905414	1.791292
7	6	0	-0.817725	-1.173097	2.088728
8	1	0	-0.364067	-2.118132	1.773747
9	1	0	-0.841334	-1.146448	3.182119
10	1	0	-1.846235	-1.141483	1.716564
11	8	0	-0.739335	1.140197	2.037959
12	8	0	-0.042567	2.366366	1.625158
13	6	0	-1.069365	3.320219	1.419849
14	1	0	-1.656388	3.472614	2.333568
15	1	0	-0.540194	4.243903	1.165260
16	1	0	-1.731204	3.026437	0.595988
17	1	0	0.526324	0.876300	-0.386601
18	1	0	0.500662	-0.896810	-0.380359
19	1	0	-1.025594	0.010110	-0.382996

Electronic Energy = -348.144760513 Zero-Point Energy = 0.166644

CH_3M (M = Li, R = t-Bu)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	1	0	0.000000	0.000000	1.101519
3	3	0	1.838809	0.000000	-0.751486
4	1	0	-0.578614	-0.883046	-0.314291
5	1	0	-0.578614	0.883046	-0.314291

Electronic Energy = -47.4099503490 Zero-Point Energy = 0.033322

II (M = Li, R = t-Bu)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.268834	-1.433332	0.092589
2	8	0	0.276686	-0.398672	0.918117
3	8	0	1.461319	-0.963484	1.596175
4	6	0	2.646619	-0.125536	1.340567
5	6	0	2.398490	1.296127	1.850536
6	1	0	1.600044	1.784565	1.285924
7	1	0	2.130424	1.293291	2.912563
8	1	0	3.308302	1.893450	1.734629
9	6	0	2.981160	-0.155879	-0.150770
10	1	0	2.183264	0.302724	-0.741143
11	1	0	3.900341	0.408782	-0.334988
12	1	0	3.136854	-1.182976	-0.494701
13	6	0	3.704264	-0.852513	2.178697
14	1	0	4.658982	-0.326939	2.080854
15	1	0	3.425673	-0.866991	3.236130
16	1	0	3.839054	-1.881887	1.834638
17	3	0	0.069583	-0.462888	2.975303
18	6	0	-0.763128	-0.245003	4.779472
19	1	0	-1.109523	0.784936	4.974447
20	1	0	-1.649894	-0.888407	4.916852
21	1	0	-0.081459	-0.496199	5.610725
22	1	0	0.418870	-1.683438	-0.719550
23	1	0	-0.506132	-2.323159	0.683247
24	1	0	-1.187856	-0.994725	-0.306401

Electronic Energy = -395.58520113 Zero-Point Energy = 0.201671

TS III (M = Li, R = t-Bu)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.081949	0.009900	0.049293
2	8	0	-1.167976	0.263292	-0.805253
3	3	0	-3.026125	-0.093124	-0.400788
4	8	0	-2.533263	1.521970	0.002439
5	6	0	-5.074297	-0.128577	0.387009
6	1	0	-5.643516	0.198322	-0.482398
7	1	0	-5.119374	-1.198688	0.598396
8	1	0	-5.148486	0.516874	1.256641
9	6	0	-2.469086	2.755352	-0.640655

10	1	0	-3.378043	3.313593	-0.357550
11	1	0	-1.602759	3.348063	-0.318139
12	1	0	-2.463594	2.655213	-1.736074
13	6	0	0.794505	-1.003200	-0.738680
14	1	0	1.676438	-1.268005	-0.143581
15	1	0	0.229468	-1.915262	-0.952462
16	1	0	1.122461	-0.564661	-1.684855
17	6	0	0.715581	1.299185	0.306816
18	1	0	1.618241	1.094377	0.893131
19	1	0	1.011783	1.757559	-0.641926
20	1	0	0.099546	2.012794	0.861844
21	6	0	-0.548408	-0.619094	1.375590
22	1	0	0.297604	-0.839603	2.035912
23	1	0	-1.221832	0.068932	1.896866
24	1	0	-1.080116	-1.560111	1.188185

Electronic Energy = -395.56562573 Zero-Point Energy = 0.198141

IV (M = Li, R = t-Bu)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.004639	-0.010878	0.011409
2	8	0	1.386255	-0.071420	0.060408
3	3	0	3.007872	-0.146105	0.111409
4	8	0	4.918394	-0.052501	0.045223
5	6	0	5.581843	1.029789	-0.616312
6	1	0	6.215537	1.578867	0.090816
7	1	0	6.193545	0.653489	-1.445356
8	1	0	4.809532	1.695206	-1.006146
9	6	0	5.821579	-1.007999	0.607490
10	1	0	6.442111	-1.456698	-0.177956
11	1	0	6.464560	-0.531617	1.357773
12	1	0	5.220221	-1.784277	1.083874
13	6	0	-0.564884	0.202263	1.434700
14	1	0	-1.661361	0.258350	1.443502
15	1	0	-0.255077	-0.623850	2.085377
16	1	0	-0.166744	1.132385	1.856783
17	6	0	-0.438547	1.166601	-0.890311
18	1	0	-1.530801	1.255795	-0.957595
19	1	0	-0.038084	2.106723	-0.493182
20	1	0	-0.039643	1.028795	-1.902138
21	6	0	-0.559813	-1.330660	-0.567260
22	1	0	-1.656148	-1.328420	-0.626300
23	1	0	-0.158634	-1.494178	-1.574310

24	1	0	-0.248735	-2.173076	0.061517

Electronic Energy = -395.72907068 Zero-Point Energy = 0.206463

ROM (M = Li, R = t-Bu)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000108	-0.000049	0.000140
2	6	0	-0.520399	-0.061786	1.454236
3	1	0	-0.152660	-0.971458	1.942752
4	1	0	-0.148219	0.800713	2.019009
5	1	0	-1.616705	-0.061284	1.504072
6	6	0	-0.518833	-1.228560	-0.781132
7	1	0	-1.615027	-1.271383	-0.809216
8	1	0	-0.147662	-1.197103	-1.811984
9	1	0	-0.148731	-2.148990	-0.315067
10	6	0	-0.519337	1.290515	-0.673581
11	1	0	-0.148095	2.168059	-0.131835
12	1	0	-0.150192	1.346630	-1.704089
13	1	0	-1.615594	1.335829	-0.695909
14	8	0	1.389658	-0.000138	0.000930
15	3	0	2.994254	-0.000488	0.001449

Electronic Energy = -240.65654517 Zero-Point Energy = 0.125188

CH_3OCH_3 (M = Li, R = t-Bu)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.016461	0.006851	0.010759
2	8	0	-0.018126	-0.001046	1.425528
3	6	0	1.272169	-0.001710	2.004672
4	1	0	1.141321	-0.006315	3.089283
5	1	0	1.846278	-0.893950	1.708405
6	1	0	1.844066	0.894414	1.715772
7	1	0	0.528625	-0.885043	-0.383383
8	1	0	-1.019064	0.005979	-0.336842
9	1	0	0.525163	0.904382	-0.374824

Electronic Energy = -155.04131200 Zero-Point Energy = 0.079631

Series: M = Li, R = THP

$ROOCH_3$ (M = Li, R = THP)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.538238
3	6	0	1.443195	0.000000	2.064687
4	6	0	2.243814	1.124958	1.406899
5	8	0	2.193538	1.048803	-0.022713
6	6	0	0.878986	1.133757	-0.521975
7	1	0	0.441286	2.119197	-0.281792
8	8	0	1.079012	1.063406	-1.935128
9	8	0	-0.176339	1.505777	-2.534268
10	6	0	0.174651	2.551588	-3.431510
11	1	0	0.874452	2.193484	-4.194314
12	1	0	-0.772403	2.836844	-3.899927
13	1	0	0.604952	3.407745	-2.898942
14	1	0	1.860097	2.107252	1.731543
15	1	0	3.305307	1.073602	1.661277
16	1	0	1.923987	-0.959395	1.835684
17	1	0	1.466405	0.126712	3.154289
18	1	0	-0.523456	0.894165	1.906732
19	1	0	-0.554508	-0.864727	1.919055
20	1	0	0.413134	-0.939954	-0.385184
21	1	0	-1.012035	0.112306	-0.401841

Electronic Energy = -461.45919003 Zero-Point Energy = 0.181506

CH_3M (M = Li, R = THP)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	1	0	0.000000	0.000000	1.101519
3	3	0	1.838809	0.000000	-0.751486
4	1	0	-0.578614	-0.883046	-0.314291
5	1	0	-0.578614	0.883046	-0.314291

Electronic Energy = -47.4099503490 Zero-Point Energy = 0.033322

II (M = Li, R = THP)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.259545	0.550608	1.487799
2	3	0	1.079965	-0.314965	2.720402
3	8	0	3.107629	-0.472275	2.529756
4	6	0	3.732987	-0.713343	1.269323
5	1	0	3.480389	0.170877	0.679541
6	1	0	4.816227	-0.801666	1.394043
7	1	0	3.317028	-1.607639	0.796225
8	8	0	3.365630	-1.684142	3.347854
9	6	0	2.868285	-1.386341	4.618381
10	6	0	3.155821	-2.584285	5.516333
11	6	0	2.458316	-2.391180	6.875762
12	6	0	0.967225	-2.072999	6.685238
13	6	0	0.789442	-0.897782	5.728572
14	8	0	1.459136	-1.161872	4.476388
15	1	0	-0.255535	-0.725655	5.464838
16	1	0	1.195633	0.029064	6.161179
17	1	0	0.445304	-2.947023	6.277027
18	1	0	0.496762	-1.829926	7.645132
19	1	0	2.942277	-1.570064	7.422389
20	1	0	2.587078	-3.291910	7.484641
21	1	0	2.777747	-3.482862	5.015886
22	1	0	4.238230	-2.692440	5.637506
23	1	0	3.329796	-0.460902	4.998504
24	1	0	-1.283965	0.562373	1.900067
25	1	0	-0.020620	1.602611	1.251243
26	1	0	-0.337643	0.033838	0.514372

Electronic Energy = -508.91668091 Zero-Point Energy = 0.217024

III (M = Li, R = THP)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.654434	0.065428	0.083312
2	3	0	-0.340521	-0.269998	1.905763
3	8	0	1.213878	-0.146847	2.776682
4	6	0	2.557853	-0.577634	2.739845
5	1	0	2.908711	-0.377371	1.721896
6	1	0	3.164270	-0.010403	3.454064
7	1	0	2.634963	-1.651642	2.945803

8	8	0	0.718985	-0.503367	4.398825
9	6	0	-0.327613	0.342602	4.584075
10	6	0	-0.925179	0.101509	5.975265
11	6	0	-2.204038	0.933176	6.172831
12	6	0	-3.196221	0.685935	5.028578
13	6	0	-2.515114	0.902342	3.679608
14	8	0	-1.347692	0.068998	3.551842
15	1	0	-3.169417	0.633251	2.846076
16	1	0	-2.221818	1.957172	3.558382
17	1	0	-3.575264	-0.342701	5.075216
18	1	0	-4.060041	1.357162	5.107889
19	1	0	-1.946090	2.000706	6.208772
20	1	0	-2.659356	0.687852	7.138717
21	1	0	-1.141124	-0.968907	6.064855
22	1	0	-0.169411	0.355061	6.725254
23	1	0	-0.041422	1.400867	4.448454
24	1	0	-0.165825	0.263697	-0.619686
25	1	0	1.347378	0.910188	0.108017
26	1	0	1.174039	-0.861943	-0.181870

Electronic Energy = -508.91047097 Zero-Point Energy = 0.215297

IV (M = Li, R = THP)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.220352	0.406320	0.215110
2	8	0	-1.253307	-0.567636	0.111164
3	6	0	-0.766565	-1.914109	-0.017160
4	1	0	-0.156082	-2.007782	-0.923987
5	1	0	-0.166270	-2.181460	0.861422
6	1	0	-1.645372	-2.557917	-0.084874
7	3	0	-3.156587	-0.566635	0.080950
8	8	0	-4.054472	-2.112087	-0.082103
9	6	0	-5.236868	-1.529253	-0.031399
10	6	0	-6.142065	-1.685687	-1.258028
11	6	0	-7.394825	-0.796607	-1.189934
12	6	0	-7.019531	0.680311	-0.993003
13	6	0	-6.087654	0.842699	0.209965
14	8	0	-4.940572	0.015427	0.081877
15	1	0	-5.736882	1.877286	0.307592
16	1	0	-6.625922	0.584525	1.138289
17	1	0	-6.508821	1.056346	-1.889779
18	1	0	-7.916999	1.295918	-0.846254
19	1	0	-8.028059	-1.120984	-0.350943

20	1	0	-7.999202	-0.917910	-2.097290
21	1	0	-5.539721	-1.446427	-2.143935
22	1	0	-6.418759	-2.744784	-1.331534
23	1	0	-5.820193	-1.716813	0.899110
24	1	0	0.399315	0.219429	1.101849
25	1	0	0.414663	0.393898	-0.680370
26	1	0	-0.698287	1.383774	0.306622

Electronic Energy = -509.07220251 Zero-Point Energy = 0.221195

ROM (M = Li, R = THP)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	-0.941288	1.055419	0.582653
3	8	0	-2.291065	0.784194	0.227006
4	6	0	-2.850381	-0.630952	0.708065
5	6	0	-1.911832	-1.668454	0.089811
6	6	0	-0.433928	-1.410182	0.428004
7	1	0	0.201968	-2.164659	-0.050509
8	1	0	-0.282151	-1.520279	1.511720
9	1	0	-2.073557	-1.656144	-0.995659
10	1	0	-2.228947	-2.654307	0.451654
11	1	0	-2.690712	-0.565688	1.806616
12	8	0	-4.111646	-0.653143	0.321108
13	3	0	-4.023980	0.968303	-0.351621
14	1	0	-0.850256	1.075172	1.681687
15	1	0	-0.698495	2.058243	0.211559
16	1	0	-0.014481	0.077194	-1.095493
17	1	0	1.027083	0.208212	0.327240

Electronic Energy = -354.00163109 Zero-Point Energy = 0.139566

CH_3OCH_3 (M = Li, R = THP)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.016461	0.006851	0.010759
2	8	0	-0.018126	-0.001046	1.425528
3	6	0	1.272169	-0.001710	2.004672
4	1	0	1.141321	-0.006315	3.089283
5	1	0	1.846278	-0.893950	1.708405
6	1	0	1.844066	0.894414	1.715772

7	1	0	0.528625	-0.885043	-0.383383
8	1	0	-1.019064	0.005979	-0.336842
9	1	0	0.525163	0.904382	-0.374824

Electronic Energy = -155.04131200
Zero-Point Energy = 0.079631

Series: M = Na, R = t-Bu

$ROOCH_3$ (M = Na, R = t-Bu)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.533651
3	6	0	1.423955	0.000000	2.103459
4	1	0	1.984956	0.868284	1.749504
5	1	0	1.396243	0.028408	3.197064
6	1	0	1.955483	-0.905414	1.791292
7	6	0	-0.817725	-1.173097	2.088728
8	1	0	-0.364067	-2.118132	1.773747
9	1	0	-0.841334	-1.146448	3.182119
10	1	0	-1.846235	-1.141483	1.716564
11	8	0	-0.739335	1.140197	2.037959
12	8	0	-0.042567	2.366366	1.625158
13	6	0	-1.069365	3.320219	1.419849
14	1	0	-1.656388	3.472614	2.333568
15	1	0	-0.540194	4.243903	1.165260
16	1	0	-1.731204	3.026437	0.595988
17	1	0	0.526324	0.876300	-0.386601
18	1	0	0.500662	-0.896810	-0.380359
19	1	0	-1.025594	0.010110	-0.382996

Electronic Energy = -348.144760513 Zero-Point Energy = 0.166644

CH_3M (M = Na, R = t-Bu)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.085127	0.000000	0.034790
2	1	0	-0.039438	0.000000	1.130289
3	11	0	2.054754	0.000000	-0.839739
4	1	0	-0.624698	-0.893189	-0.301783

5	1	0	-0.624698	0.893189	-0.301784

Electronic Energy = -202.17683220 Zero-Point Energy = 0.032840

II (M = Na, R = t-Bu)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.182554	-0.982199	0.605849
2	8	0	0.892206	0.200236	0.980799
3	8	0	1.746186	-0.157554	2.125536
4	6	0	3.153329	0.126035	1.817272
5	6	0	3.831361	-0.271704	3.133424
6	1	0	3.663021	-1.329047	3.356999
7	1	0	4.909198	-0.103171	3.048698
8	1	0	3.455417	0.328572	3.966991
9	6	0	3.622857	-0.750268	0.654285
10	1	0	3.089640	-0.499466	-0.266779
11	1	0	4.690837	-0.588901	0.477068
12	1	0	3.470884	-1.810376	0.879218
13	6	0	3.333549	1.616903	1.518059
14	1	0	2.775997	1.908731	0.624377
15	1	0	2.999779	2.231381	2.361127
16	1	0	4.391625	1.836531	1.343888
17	11	0	0.177193	1.502179	2.955131
18	6	0	-0.838495	3.003668	4.432762
19	1	0	-1.930931	3.017145	4.305052
20	1	0	-0.630965	2.736680	5.479617
21	1	0	-0.474674	4.029697	4.273737
22	1	0	-0.493304	-0.648692	-0.187194
23	1	0	0.865069	-1.746747	0.224277
24	1	0	-0.396931	-1.377572	1.446605

Electronic Energy = -550.33903279 Zero-Point Energy = 0.200395

TS III (M = Na, R = t-Bu)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.026613	-0.007895	-0.000337
2	8	0	-1.039230	0.177320	-0.972338
3	11	0	-3.234551	-0.912223	-0.373817
4	8	0	-2.481124	1.025989	-0.212803
5	6	0	-5.021817	0.529652	0.640100

6	1	0	-5.440768	1.051575	-0.222649
7	1	0	-5.683804	-0.252821	1.025738
8	1	0	-4.679359	1.206284	1.420594
9	6	0	-2.576355	2.285635	-0.827443
10	1	0	-3.493328	2.751443	-0.438156
11	1	0	-1.726623	2.930028	-0.571568
12	1	0	-2.660999	2.203975	-1.919868
13	6	0	1.095727	-0.742648	-0.769759
14	1	0	1.939639	-0.948699	-0.100607
15	1	0	0.730784	-1.692907	-1.172376
16	1	0	1.449734	-0.128344	-1.602301
17	6	0	0.491242	1.338381	0.531960
18	1	0	1.336187	1.192715	1.214376
19	1	0	0.822532	1.969943	-0.298377
20	1	0	-0.301918	1.860639	1.074143
21	6	0	-0.529767	-0.885781	1.162529
22	1	0	0.255796	-1.066143	1.904511
23	1	0	-1.366305	-0.393317	1.670097
24	1	0	-0.852277	-1.867698	0.788114

Electronic Energy = -550.31657606 Zero-Point Energy = 0.197889

IV (M = Na, R = t-Bu)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.063148	0.188185	-0.070970
2	8	0	1.299189	0.431278	-0.089643
3	11	0	3.251493	0.114061	-0.484811
4	8	0	4.422853	1.884881	0.298575
5	6	0	3.411857	2.741932	0.867931
6	1	0	3.608989	2.890878	1.937498
7	1	0	3.415415	3.713121	0.356299
8	1	0	2.449857	2.235430	0.721776
9	6	0	5.735927	2.418196	0.413208
10	1	0	5.813138	3.380644	-0.110704
11	1	0	6.007826	2.562096	1.467766
12	1	0	6.426327	1.704110	-0.042225
13	6	0	-0.824792	1.388786	-0.688274
14	1	0	-1.913571	1.243091	-0.695710
15	1	0	-0.602574	2.298885	-0.118576
16	1	0	-0.488598	1.546859	-1.719924
17	6	0	-0.400182	-1.085338	-0.888909
18	1	0	-1.474563	-1.314336	-0.900554
19	1	0	-0.065786	-0.956834	-1.926019

20	1	0	0.129359	-1.947390	-0.463869
21	6	0	-0.547774	-0.015834	1.386960
22	1	0	-1.627406	-0.207720	1.452941
23	1	0	-0.016840	-0.863149	1.837129
24	1	0	-0.318470	0.877723	1.979402

Electronic Energy = -550.47205043 Zero-Point Energy = 0.204825

ROM (M = Na, R = t-Bu)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.013684	0.000123	-0.000009
2	6	0	-0.545472	1.069671	0.986226
3	1	0	-0.174542	0.856973	1.995982
4	1	0	-0.175871	2.059041	0.691290
5	1	0	-1.642771	1.105861	1.020739
6	6	0	-0.543916	-1.389254	0.433617
7	1	0	-1.641113	-1.438235	0.449978
8	1	0	-0.173877	-2.156929	-0.256454
9	1	0	-0.172080	-1.628478	1.437081
10	6	0	-0.545340	0.319063	-1.419531
11	1	0	-0.174990	1.300305	-1.739571
12	1	0	-0.174798	-0.430525	-2.128925
13	1	0	-1.642595	0.329998	-1.468696
14	8	0	1.370234	0.000760	-0.000403
15	11	0	3.334788	0.000057	-0.001577

Electronic Energy = -395.40630130 Zero-Point Energy = 0.123470

CH_3OCH_3 (M = Na, R = t-Bu)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.016461	0.006851	0.010759
2	8	0	-0.018126	-0.001046	1.425528
3	6	0	1.272169	-0.001710	2.004672
4	1	0	1.141321	-0.006315	3.089283
5	1	0	1.846278	-0.893950	1.708405
6	1	0	1.844066	0.894414	1.715772
7	1	0	0.528625	-0.885043	-0.383383
8	1	0	-1.019064	0.005979	-0.336842
9	1	0	0.525163	0.904382	-0.374824

Electronic Energy = -155.04131200
Zero-Point Energy = 0.079631

Series: M = Na, R = THP

$ROOCH_3$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.000000	0.000000
2	6	0	0.000000	0.000000	1.538238
3	6	0	1.443195	0.000000	2.064687
4	6	0	2.243814	1.124958	1.406899
5	8	0	2.193538	1.048803	-0.022713
6	6	0	0.878986	1.133757	-0.521975
7	1	0	0.441286	2.119197	-0.281792
8	8	0	1.079012	1.063406	-1.935128
9	8	0	-0.176339	1.505777	-2.534268
10	6	0	0.174651	2.551588	-3.431510
11	1	0	0.874452	2.193484	-4.194314
12	1	0	-0.772403	2.836844	-3.899927
13	1	0	0.604952	3.407745	-2.898942
14	1	0	1.860097	2.107252	1.731543
15	1	0	3.305307	1.073602	1.661277
16	1	0	1.923987	-0.959395	1.835684
17	1	0	1.466405	0.126712	3.154289
18	1	0	-0.523456	0.894165	1.906732
19	1	0	-0.554508	-0.864727	1.919055
20	1	0	0.413134	-0.939954	-0.385184
21	1	0	-1.012035	0.112306	-0.401841

Electronic Energy = -461.45919003 Zero-Point Energy = 0.181506

CH_3M (M = Na, R = THP)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.085127	0.000000	0.034790
2	1	0	-0.039438	0.000000	1.130289
3	11	0	2.054754	0.000000	-0.839739
4	1	0	-0.624698	-0.893189	-0.301783
5	1	0	-0.624698	0.893189	-0.301784

Electronic Energy = -202.17683220 Zero-Point Energy = 0.032840

II (M = Na, R = THP)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.078589	0.483870	-1.312338
2	11	0	0.555145	-0.164415	0.859604
3	8	0	2.589378	-0.266647	2.226775
4	6	0	3.914491	-0.609503	1.827476
5	1	0	4.197469	0.187763	1.134968
6	1	0	4.587448	-0.623374	2.690391
7	1	0	3.928327	-1.573869	1.309813
8	8	0	2.145340	-1.363019	3.115466
9	6	0	1.160200	-0.828330	3.951706
10	6	0	0.830280	-1.893995	4.993504
11	6	0	-0.372765	-1.438171	5.839988
12	6	0	-1.548007	-1.022711	4.942235
13	6	0	-1.087402	-0.004645	3.902279
14	8	0	0.023021	-0.521689	3.141822
15	1	0	-1.864331	0.219546	3.168118
16	1	0	-0.784337	0.938487	4.383053
17	1	0	-1.955724	-1.900136	4.425441
18	1	0	-2.358639	-0.589287	5.539777
19	1	0	-0.074832	-0.588918	6.470340
20	1	0	-0.669892	-2.243488	6.519700
21	1	0	0.596014	-2.825169	4.465180
22	1	0	1.710322	-2.071491	5.619764
23	1	0	1.525856	0.103215	4.411745
24	1	0	-1.169949	0.435387	-1.449246
25	1	0	0.232282	1.517101	-1.531710
26	1	0	0.374350	-0.163497	-2.079069

Electronic Energy = -663.66769749 Zero-Point Energy = 0.215318

TS III (M = Na, R = THP)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.000203	0.000129	-0.000160
2	11	0	2.215520	-0.073720	-1.064186
3	8	0	1.964042	1.950541	-0.408240
4	6	0	1.156844	3.073983	-0.143994
5	1	0	0.190687	2.681230	0.196376
6	1	0	1.589989	3.696745	0.648649

7	1	0	1.000578	3.674610	-1.048663
8	8	0	3.462774	2.642075	-0.987116
9	6	0	4.434618	1.972975	-0.319376
10	6	0	5.793670	2.602057	-0.661436
11	6	0	6.947687	1.801491	-0.034526
12	6	0	6.846149	0.317005	-0.408905
13	6	0	5.451983	-0.213913	-0.081001
14	8	0	4.433614	0.558714	-0.735143
15	1	0	5.322909	-1.244293	-0.426704
16	1	0	5.281427	-0.196746	1.008087
17	1	0	7.032418	0.186777	-1.482502
18	1	0	7.596832	-0.275403	0.128716
19	1	0	6.914186	1.904753	1.059109
20	1	0	7.908342	2.217446	-0.358829
21	1	0	5.885654	2.623540	-1.753210
22	1	0	5.793594	3.637311	-0.306039
23	1	0	4.264848	1.967386	0.772624
24	1	0	-0.298261	-1.055024	-0.000101
25	1	0	0.059527	0.396753	1.014979
26	1	0	-0.651887	0.600631	-0.639880

Electronic Energy = -663.65869534 Zero-Point Energy = 0.213483

IV (M = Na, R = THP)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.891654	-0.110436	-0.151961
2	8	0	-0.716602	1.188639	0.442981
3	6	0	-1.736313	2.109266	0.078043
4	1	0	-1.753062	2.263794	-1.009638
5	1	0	-2.722479	1.750406	0.403478
6	1	0	-1.518493	3.059249	0.572110
7	11	0	1.161756	1.070764	1.738666
8	8	0	1.744438	-0.980617	1.505247
9	6	0	2.916269	-0.927660	2.092728
10	6	0	3.099089	-1.809990	3.336791
11	6	0	4.438704	-1.575304	4.053150
12	6	0	4.618082	-0.095838	4.424075
13	6	0	4.401133	0.792589	3.196507
14	8	0	3.130414	0.560157	2.606599
15	1	0	4.452414	1.856145	3.463090
16	1	0	5.196841	0.599293	2.454922
17	1	0	3.889514	0.184811	5.197043
18	1	0	5.619211	0.085961	4.838116

19	1	0	5.263214	-1.880970	3.392191
20	1	0	4.511269	-2.205850	4.948335
21	1	0	2.255432	-1.607544	4.009685
22	1	0	3.009791	-2.854735	3.013601
23	1	0	3.794800	-1.043832	1.414068
24	1	0	-1.847735	-0.543968	0.169300
25	1	0	-0.879858	-0.024587	-1.246469
26	1	0	-0.060414	-0.733076	0.188784

Electronic Energy = -663.81927375 Zero-Point Energy = 0.219280

ROM (M = Na, R = THP)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.015367	0.008300	0.005048
2	6	0	0.935219	-1.037997	0.591535
3	8	0	2.282242	-0.777199	0.222815
4	6	0	2.838285	0.642344	0.725460
5	6	0	1.893399	1.676236	0.099242
6	6	0	0.413491	1.421355	0.426733
7	1	0	-0.220603	2.173669	-0.058806
8	1	0	0.255012	1.535961	1.509199
9	1	0	2.061913	1.662105	-0.985617
10	1	0	2.206194	2.664025	0.459965
11	1	0	2.644234	0.557382	1.820199
12	8	0	4.100836	0.716480	0.382812
13	11	0	4.291474	-1.179094	-0.516043
14	1	0	0.845992	-1.044151	1.692294
15	1	0	0.682798	-2.045598	0.236717
16	1	0	0.000686	-0.073302	-1.090430
17	1	0	-1.042135	-0.203445	0.332716

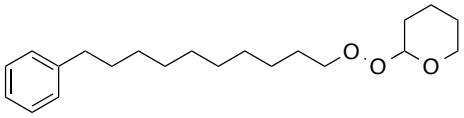
Electronic Energy = -508.75507622 Zero-Point Energy = 0.137994

CH_3OCH_3 (M = Na, R = THP)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.016461	0.006851	0.010759
2	8	0	-0.018126	-0.001046	1.425528
3	6	0	1.272169	-0.001710	2.004672
4	1	0	1.141321	-0.006315	3.089283
5	1	0	1.846278	-0.893950	1.708405

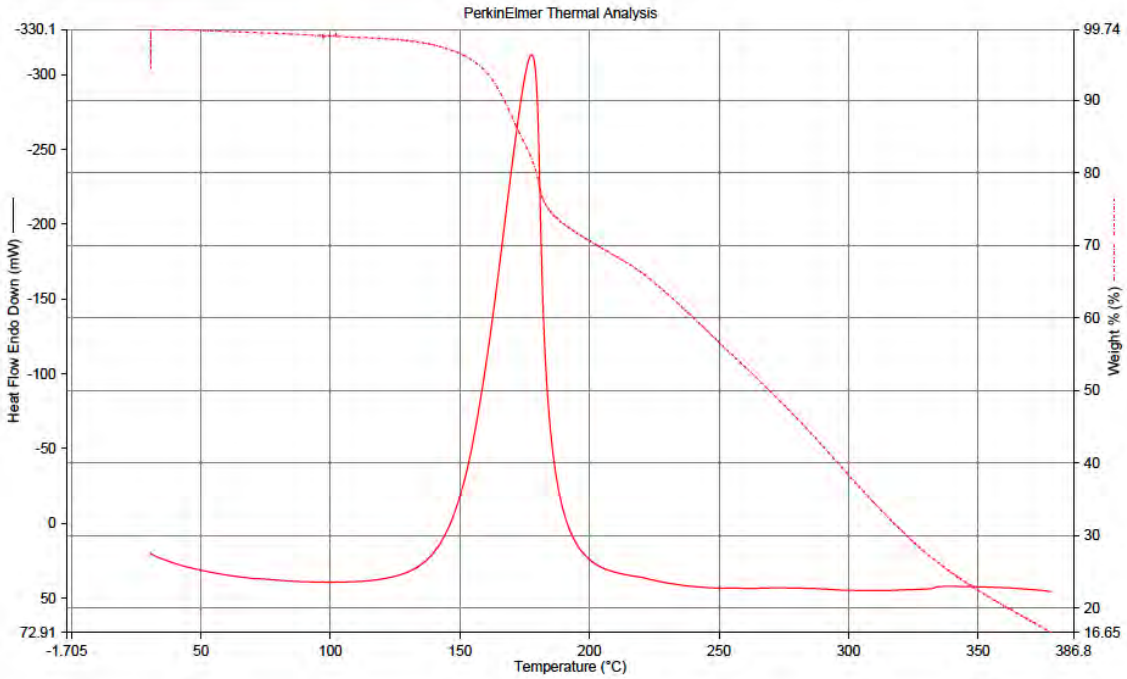
6	1	0	1.844066	0.894414	1.715772
7	1	0	0.528625	-0.885043	-0.383383
8	1	0	-1.019064	0.005979	-0.336842
9	1	0	0.525163	0.904382	-0.374824

Electronic Energy = -155.04131200
Zero-Point Energy = 0.079631



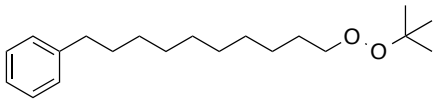
10b

Filename: c:\program files\pyris\dat...\ksk08-65.stad
Operator ID:
Sample ID: ksk08-65
Sample Weight: 18.923 mg
Comment:

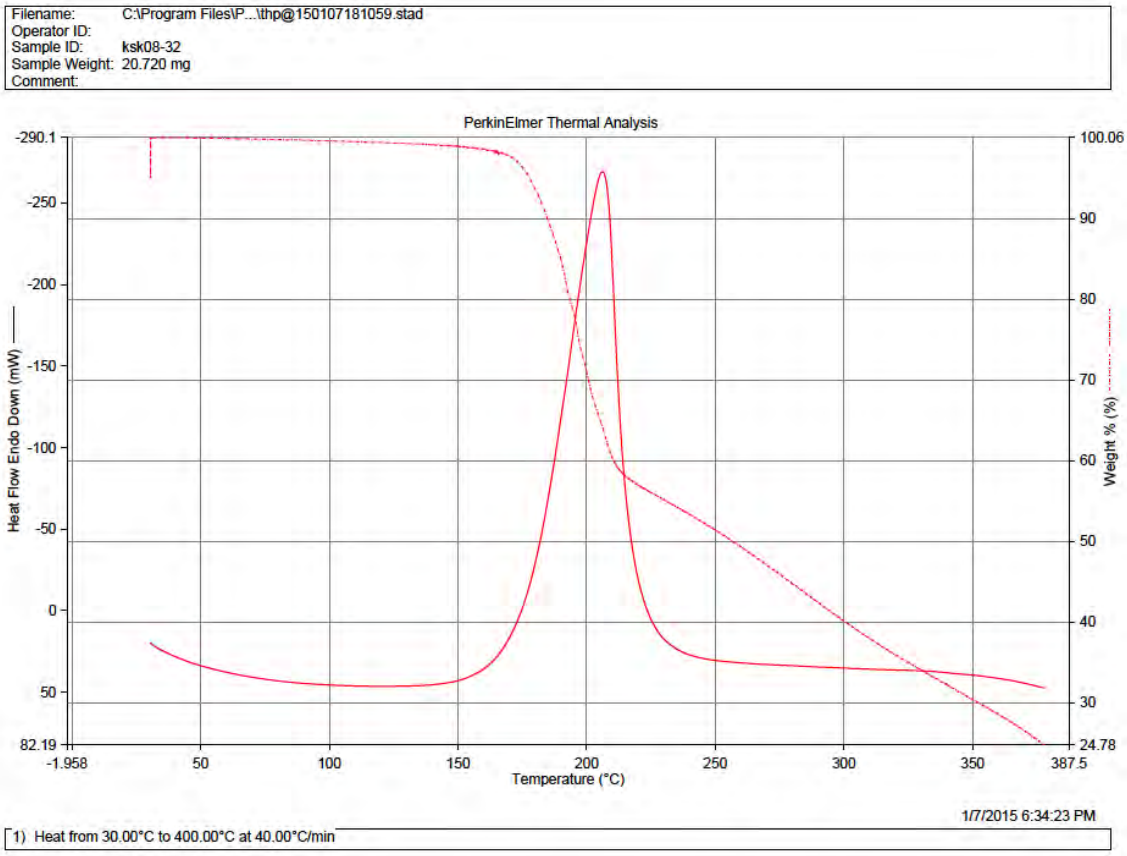


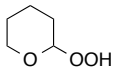
1/7/2015 5:54:19 PM

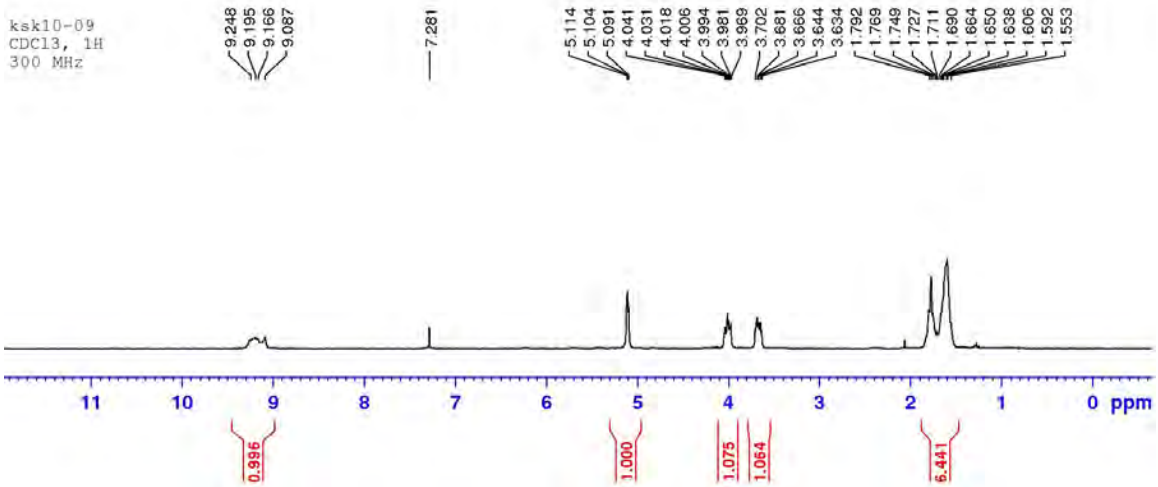
1) Heat from 30.00°C to 400.00°C at 40.00°C/min

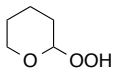


10a

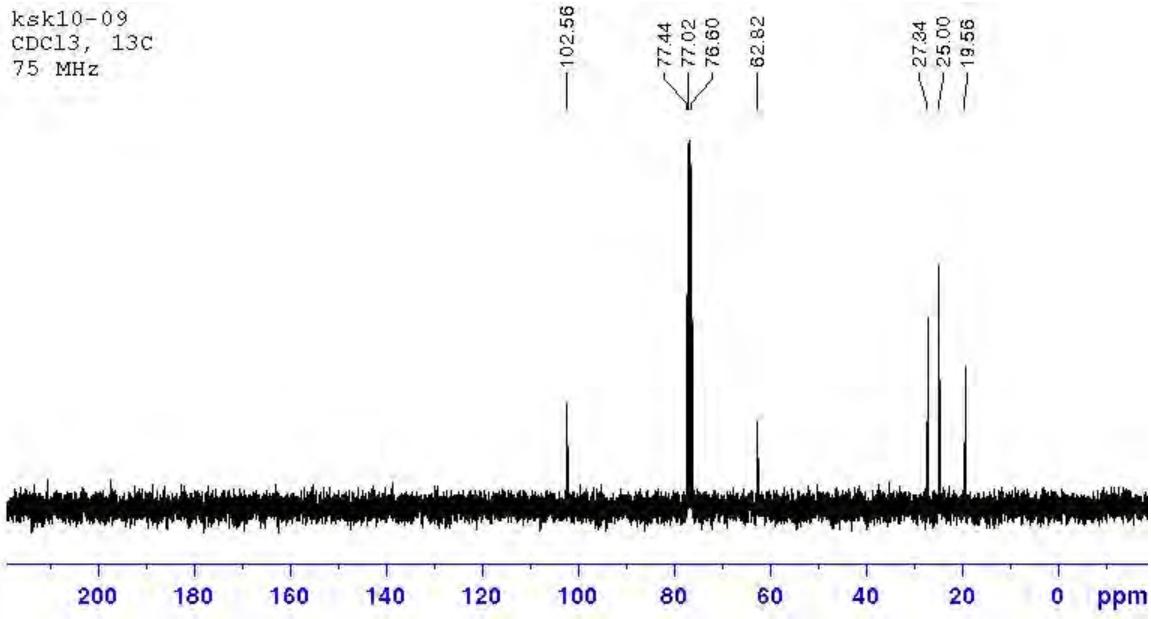

Filename: C:\Program Files\P...\thp@150107181059.stad
Operator ID:
Sample ID: ksk08-32
Sample Weight: 20.720 mg
Comment:
PerkinElmer Thermal Analysis
Heat Flow Endo Down (mW)
Weight % (%)
Temperature (°C)
-290.1
-250
-200
-150
-100
-50
0
50
82.19
100.06
90
80
70
60
50
40
30
24.78
-1.958
50
100
150
200
250
300
350
387.5
1/7/2015 6:34:23 PM
1) Heat from 30.00°C to 400.00°C at 40.00°C/min

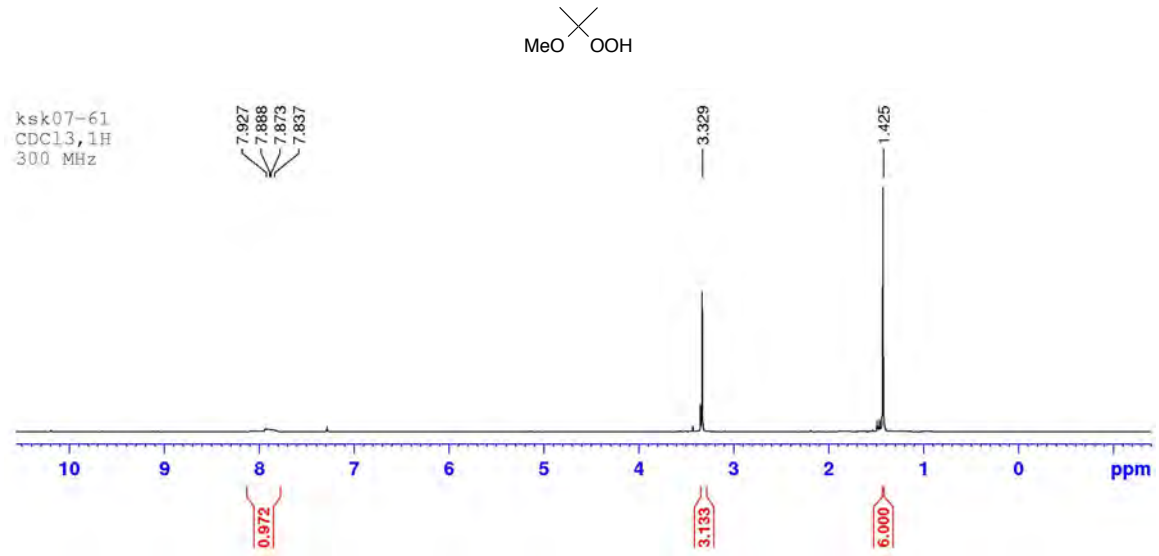

O
OOH

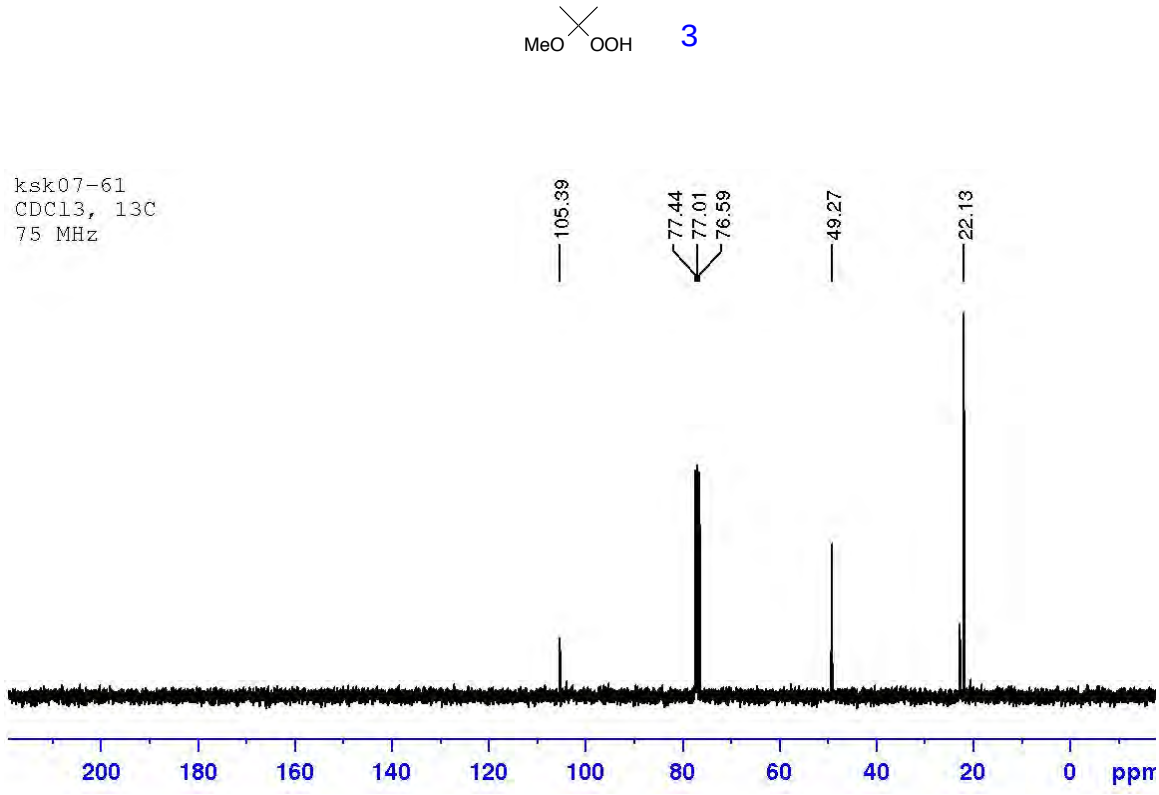

ksk10-09
CDCl3, 1H
300 MHz
9.248
9.195
9.166
9.087
7.281
5.114
5.104
5.091
4.041
4.031
4.018
4.006
3.994
3.981
3.969
3.702
3.681
3.666
3.644
3.634
1.792
1.769
1.749
1.727
1.711
1.690
1.664
1.650
1.638
1.606
1.592
1.553
11
10
9
8
7
6
5
4
3
2
1
0 ppm
0.996
1.000
1.075
1.064
6.441


O
OOH

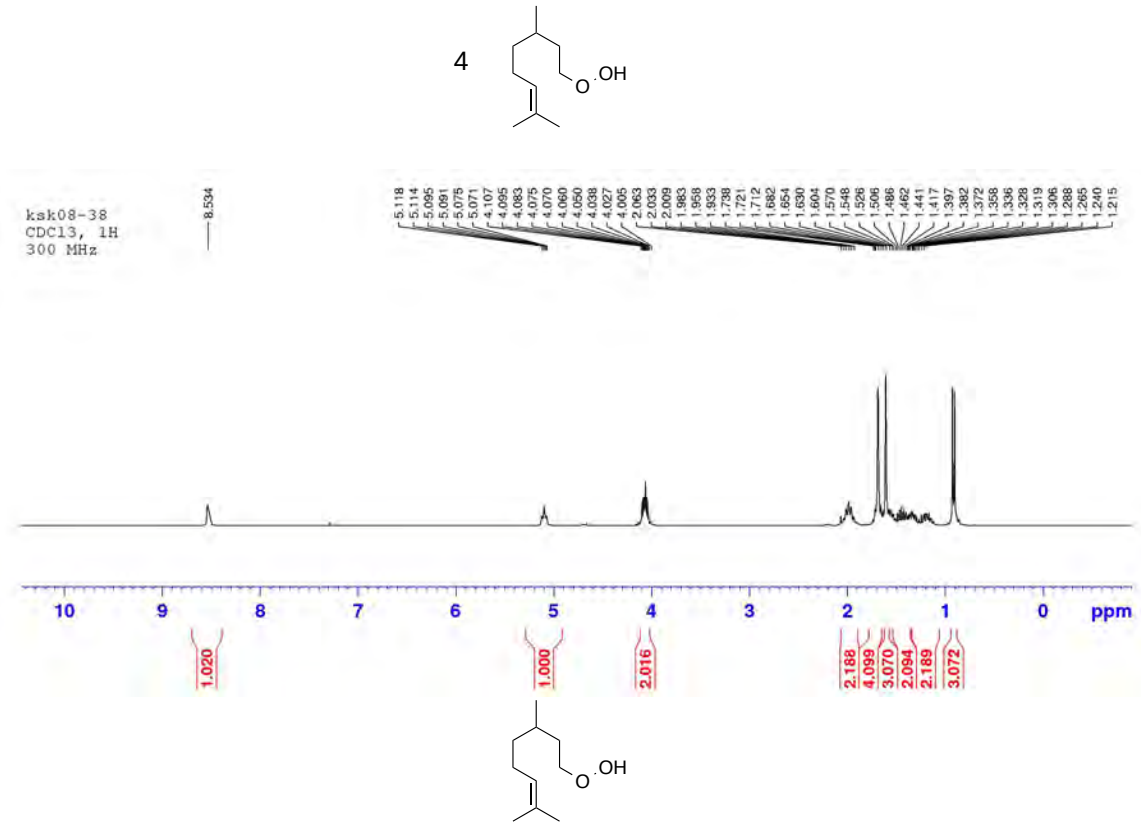
2

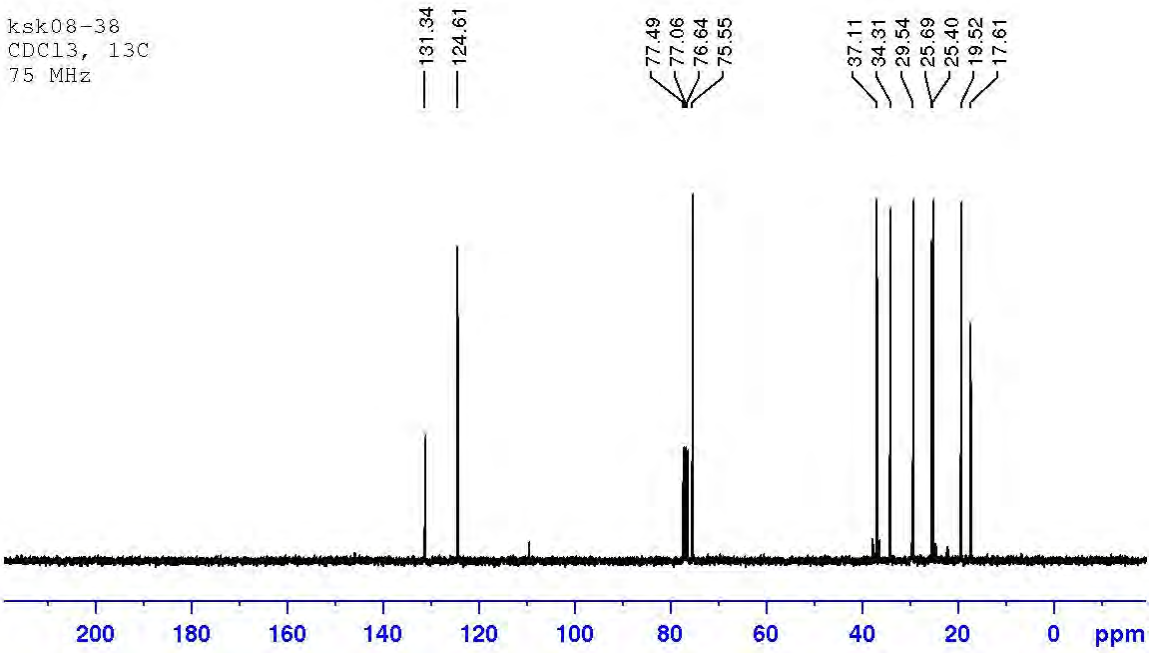

ksk10-09
CDCl3, 13C
75 MHz
102.56
77.44
77.02
76.60
62.82
27.34
25.00
19.56
200
180
160
140
120
100
80
60
40
20
0 ppm


MeO
OOH
ksk07-61
CDCl3,1H
300 MHz
7.927
7.888
7.873
7.837
3.329
1.425
10
9
8
7
6
5
4
3
2
1
0
ppm
0.972
3.133
6.000


MeO
OOH
3
ksk07-61
CDCl3, 13C
75 MHz
105.39
77.44
77.01
76.59
49.27
22.13
200
180
160
140
120
100
80
60
40
20
0
ppm

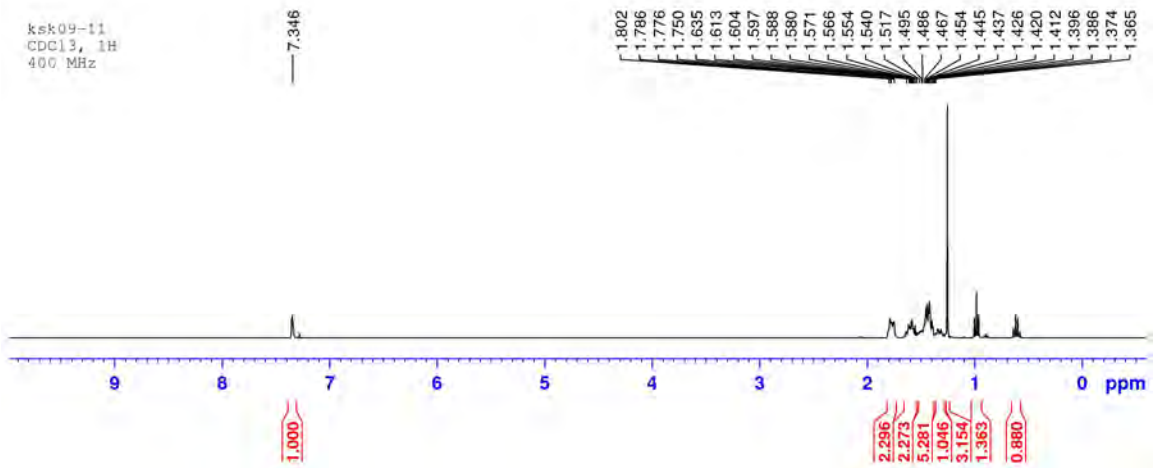
4


ksk08-38
CDCl3, 1H
300 MHz
8.534
5.118
5.114
5.095
5.091
5.075
5.071
4.107
4.095
4.083
4.075
4.070
4.060
4.050
4.038
4.027
4.005
2.063
2.033
2.009
1.983
1.958
1.933
1.738
1.721
1.712
1.682
1.654
1.630
1.604
1.570
1.548
1.526
1.506
1.486
1.462
1.441
1.417
1.397
1.382
1.372
1.358
1.336
1.328
1.319
1.306
1.288
1.265
1.240
1.215
10
9
8
7
6
5
4
3
2
1
0
ppm
1.020
1.000
2.016
2.188
4.099
3.070
2.094
2.189
3.072

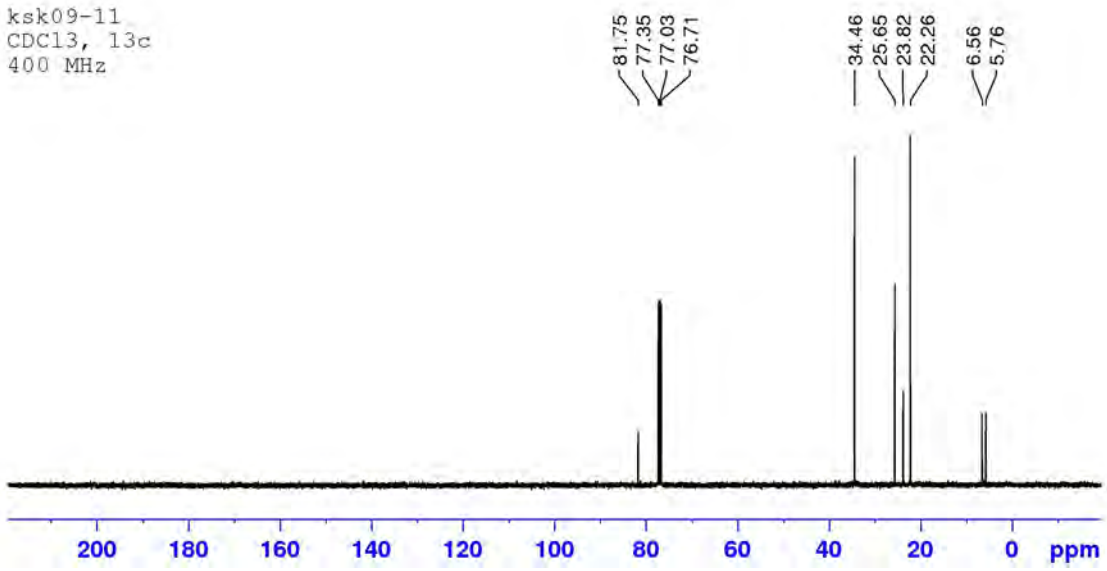

ksk08-38
CDCl3, 13C
75 MHz
131.34
124.61
77.49
77.06
76.64
75.55
37.11
34.31
29.54
25.69
25.40
19.52
17.61
200
180
160
140
120
100
80
60
40
20
0
ppm

5

OOH

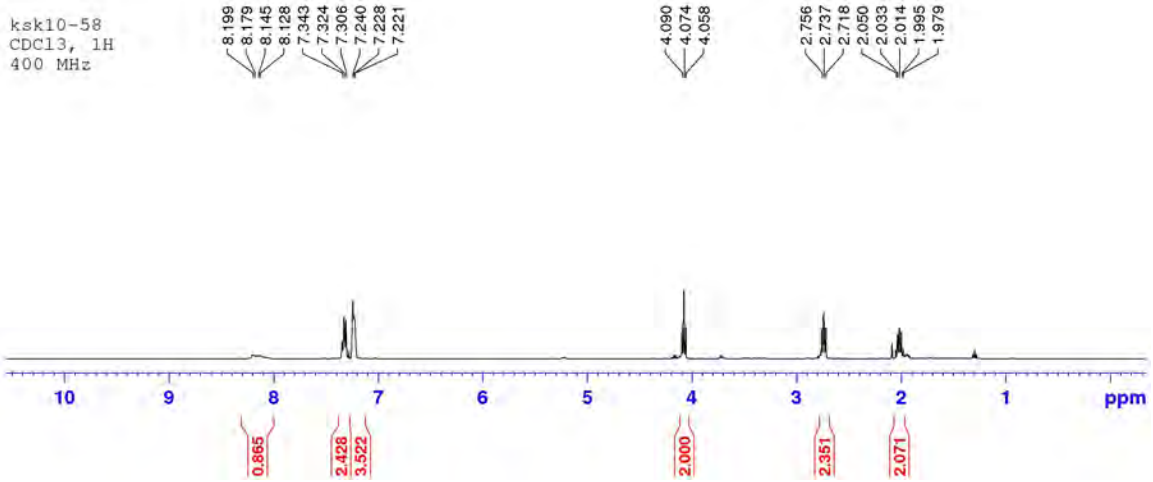

ksk09-11
CDCl3, 1H
400 MHz
7.346
1.802
1.786
1.776
1.750
1.635
1.613
1.604
1.597
1.588
1.580
1.571
1.566
1.554
1.540
1.517
1.495
1.486
1.467
1.454
1.445
1.437
1.426
1.420
1.412
1.396
1.386
1.374
1.365
9
8
7
6
5
4
3
2
1
0 ppm
1.000
2.296
2.273
5.281
1.046
3.154
1.363
0.880

OOH

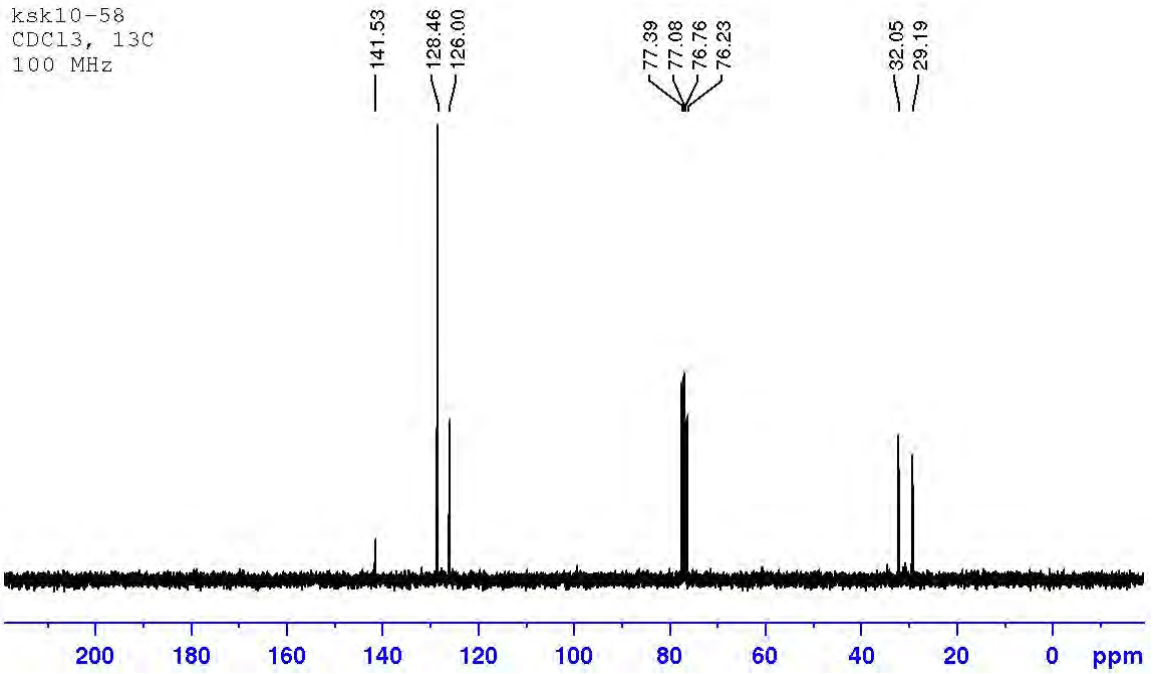

ksk09-11
CDCl3, 13c
400 MHz
81.75
77.35
77.03
76.71
34.46
25.65
23.82
22.26
6.56
5.76
200
180
160
140
120
100
80
60
40
20
0 ppm

6

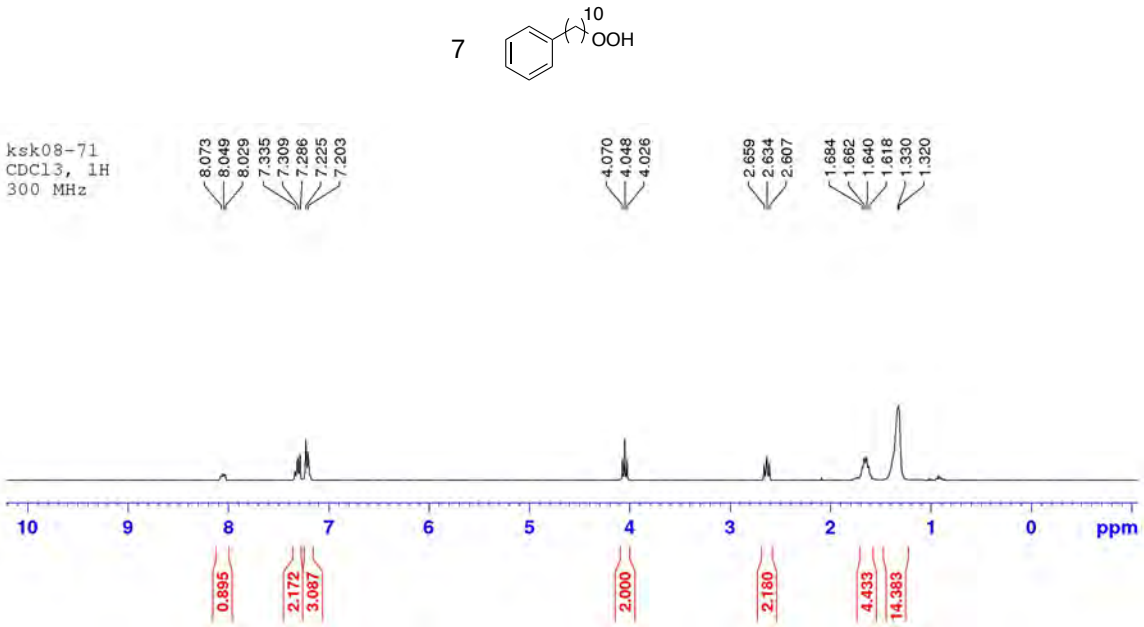
3
OOH

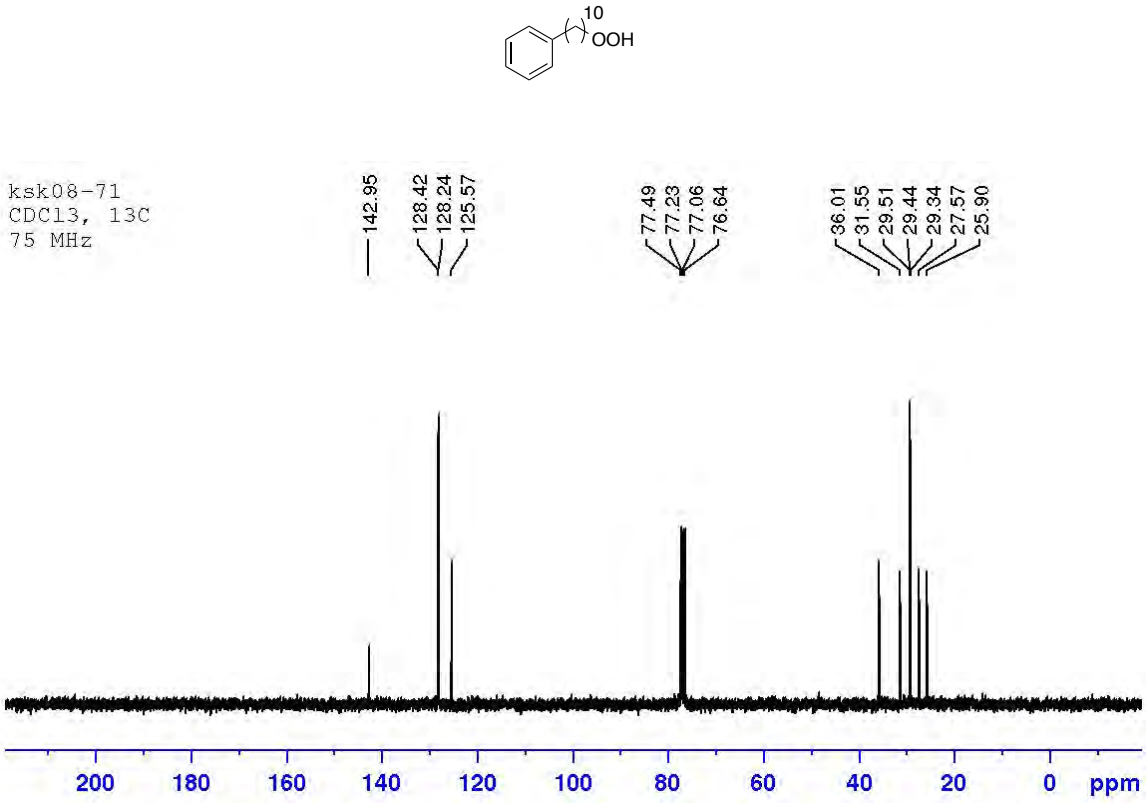

ksk10-58
CDCl3, 1H
400 MHz
8.199
8.179
8.145
8.128
7.343
7.324
7.306
7.240
7.228
7.221
4.090
4.074
4.058
2.756
2.737
2.718
2.050
2.033
2.014
1.995
1.979
10
9
8
7
6
5
4
3
2
1
ppm
0.865
2.426
3.522
2.000
2.351
2.071

3
OOH

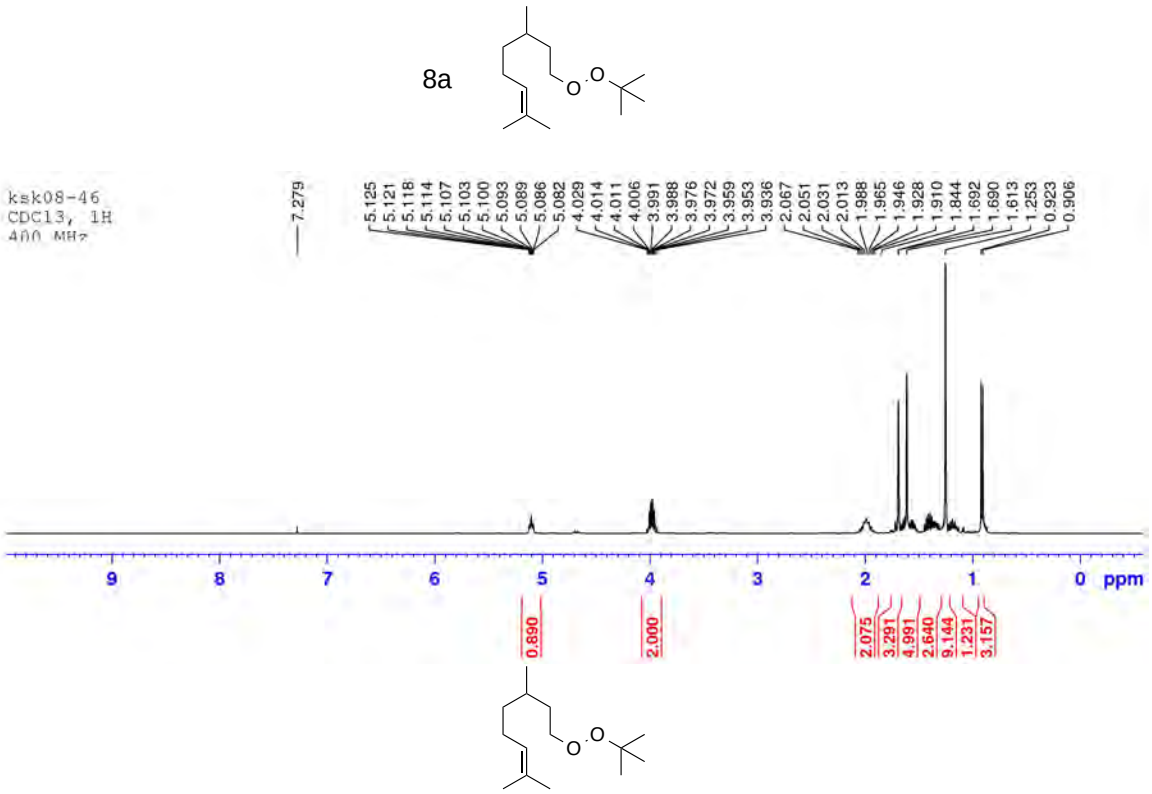

ksk10-58
CDCl3, 13C
100 MHz
141.53
128.46
126.00
77.39
77.08
76.76
76.23
32.05
29.19
200
180
160
140
120
100
80
60
40
20
0
ppm

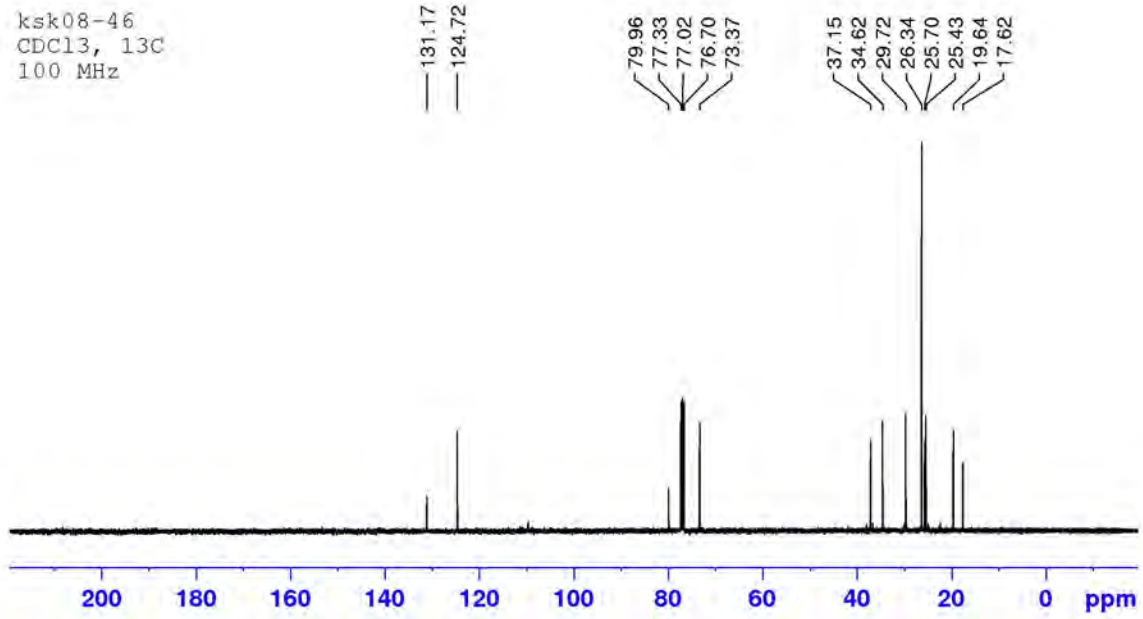
7


ksk08-71
CDCl3, 1H
300 MHz
8.073
8.049
8.029
7.335
7.309
7.286
7.225
7.203
4.070
4.048
4.026
2.659
2.634
2.607
1.684
1.662
1.640
1.618
1.330
1.320
10
OOH
10
9
8
7
6
5
4
3
2
1
0
ppm
0.895
2.172
3.087
2.000
2.180
4.433
14.383

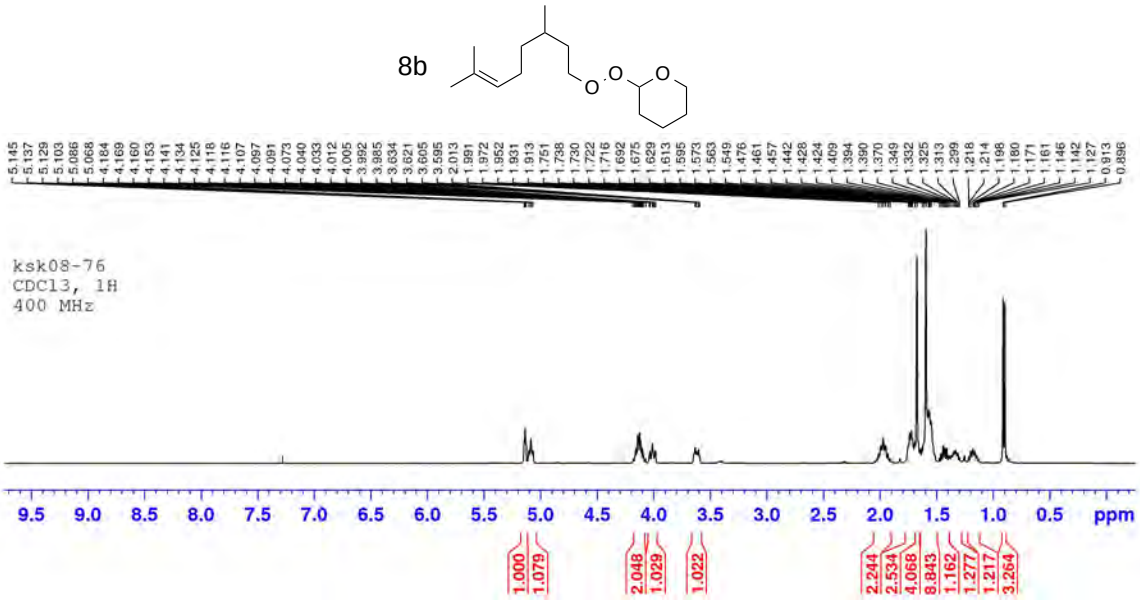

10
OOH
ksk08-71
CDCl3, 13C
75 MHz
142.95
128.42
128.24
125.57
77.49
77.23
77.06
76.64
36.01
31.55
29.51
29.44
29.34
27.57
25.90
200
180
160
140
120
100
80
60
40
20
0
ppm

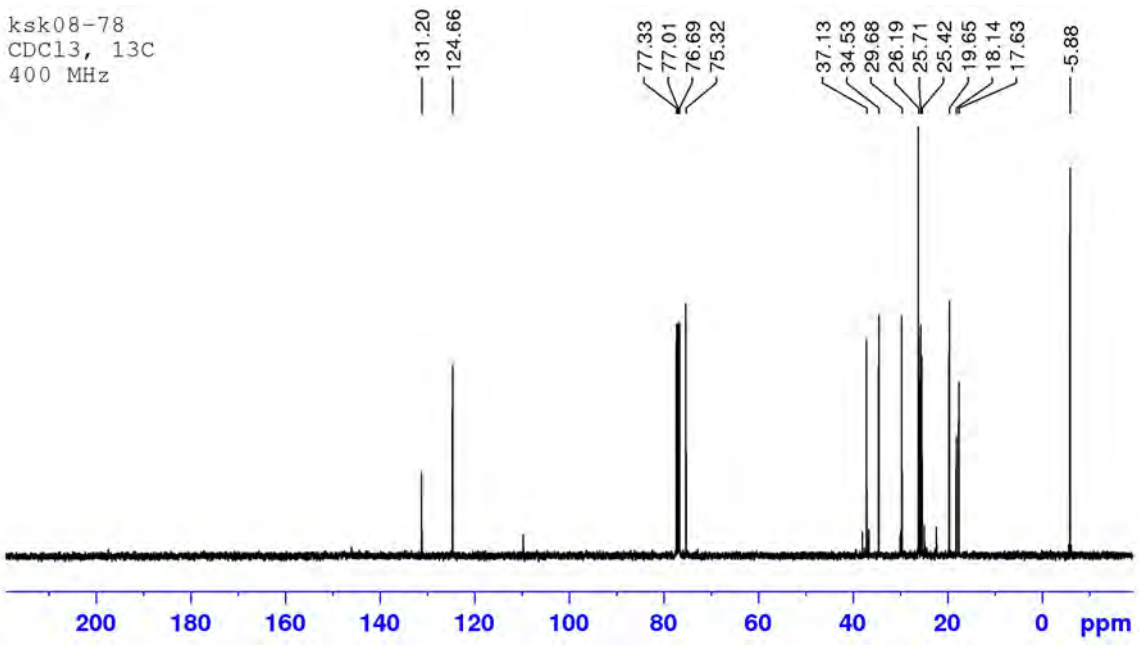
8a


ksk08-46
CDCl3, 1H
400 MHz
7.279
5.125
5.121
5.118
5.114
5.107
5.103
5.100
5.093
5.089
5.086
5.082
4.029
4.014
4.011
4.006
3.991
3.988
3.976
3.972
3.959
3.953
3.936
2.067
2.051
2.031
2.013
1.988
1.965
1.946
1.928
1.910
1.844
1.692
1.690
1.613
1.253
0.923
0.906
9
8
7
6
5
4
3
2
1
0 ppm
0.890
2.000
2.075
3.291
4.991
2.640
9.144
1.231
3.157

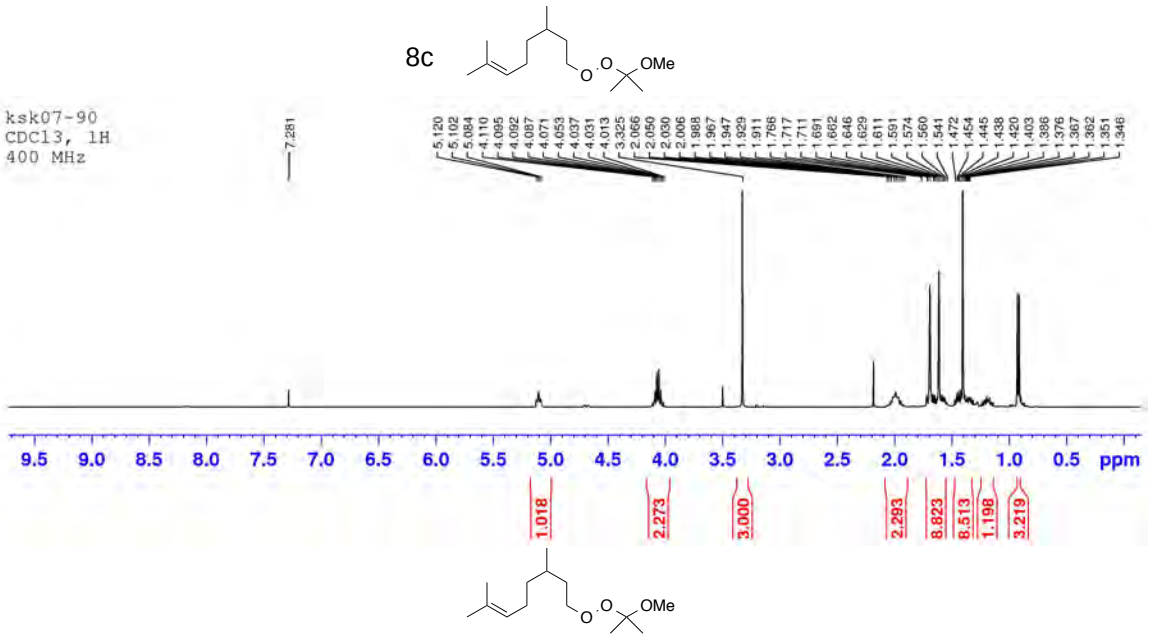

ksk08-46
CDCl3, 13C
100 MHz
131.17
124.72
79.96
77.33
77.02
76.70
73.37
37.15
34.62
29.72
26.34
25.70
25.43
19.64
17.62
200
180
160
140
120
100
80
60
40
20
0 ppm

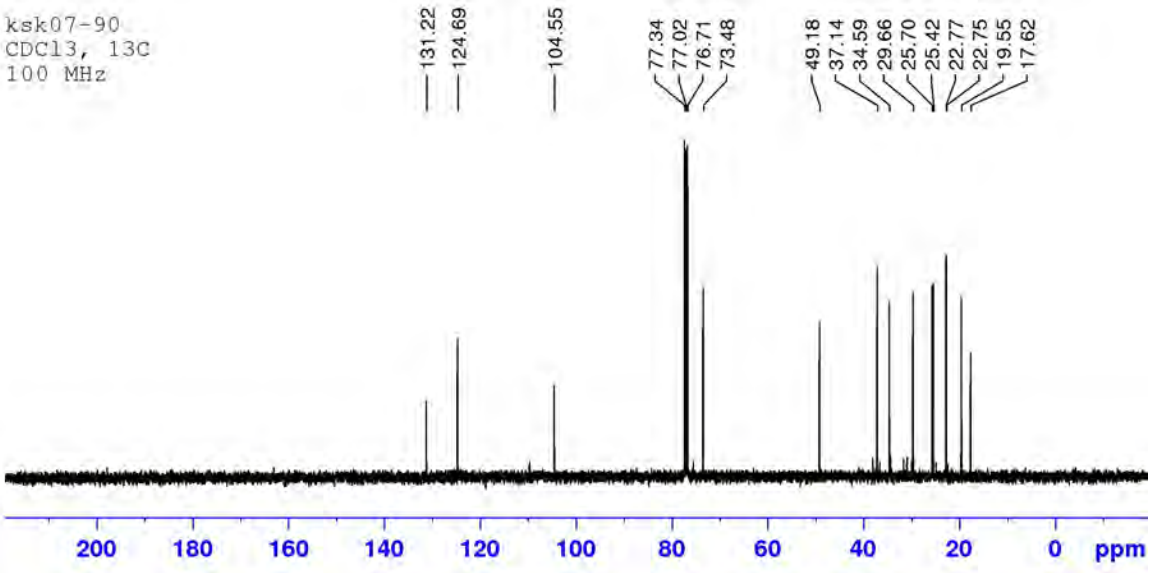
8b


ksk08-76
CDCl3, 1H
400 MHz
9.5 9.0 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 ppm
1.000 1.079 2.048 1.029 1.022 2.244 2.534 4.068 8.843 1.162 1.277 1.217 3.264


ksk08-78
CDCl3, 13C
400 MHz
131.20 124.66 77.33 77.01 76.69 75.32 37.13 34.53 29.68 26.19 25.71 25.42 19.65 18.14 17.63 -5.88
200 180 160 140 120 100 80 60 40 20 0 ppm

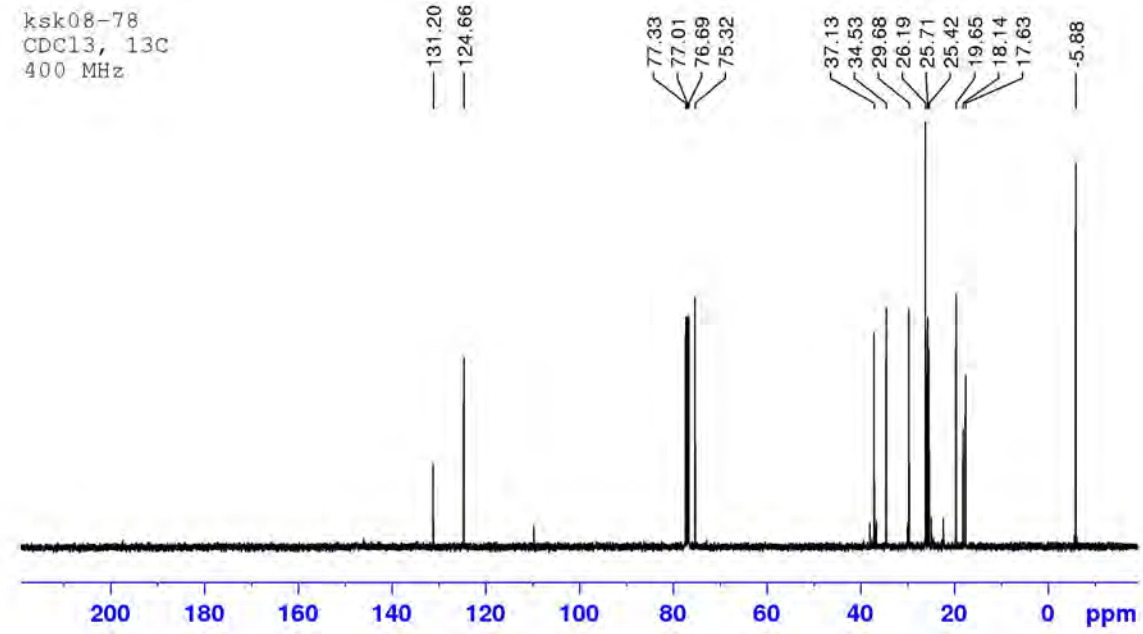
8c

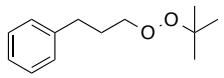

ksk07-90
CDCl3, 1H
400 MHz
7.281
5.120
5.102
5.084
4.110
4.095
4.092
4.087
4.071
4.053
4.037
4.031
4.013
3.325
2.066
2.050
2.030
2.006
1.988
1.967
1.947
1.929
1.911
1.766
1.717
1.711
1.691
1.662
1.646
1.629
1.611
1.591
1.574
1.560
1.541
1.472
1.454
1.445
1.438
1.420
1.403
1.398
1.376
1.367
1.362
1.351
1.346
9.5 9.0 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 ppm
1.018
2.273
3.000
2.293
8.823
8.513
1.198
3.219

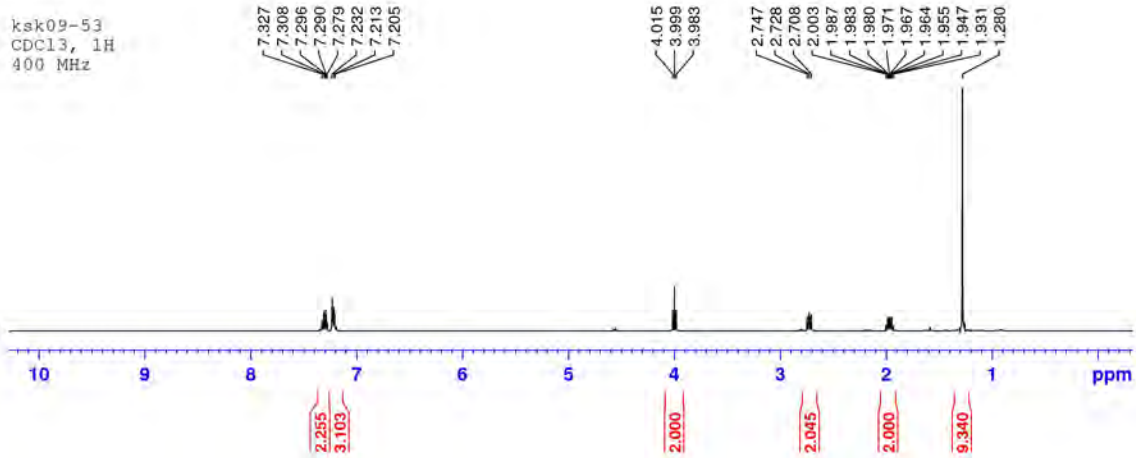

ksk07-90
CDCl3, 13C
100 MHz
131.22
124.69
104.55
77.34
77.02
76.71
73.48
49.18
37.14
34.59
29.66
25.70
25.42
22.77
22.75
19.55
17.62
200 180 160 140 120 100 80 60 40 20 0 ppm

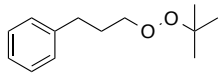
8d

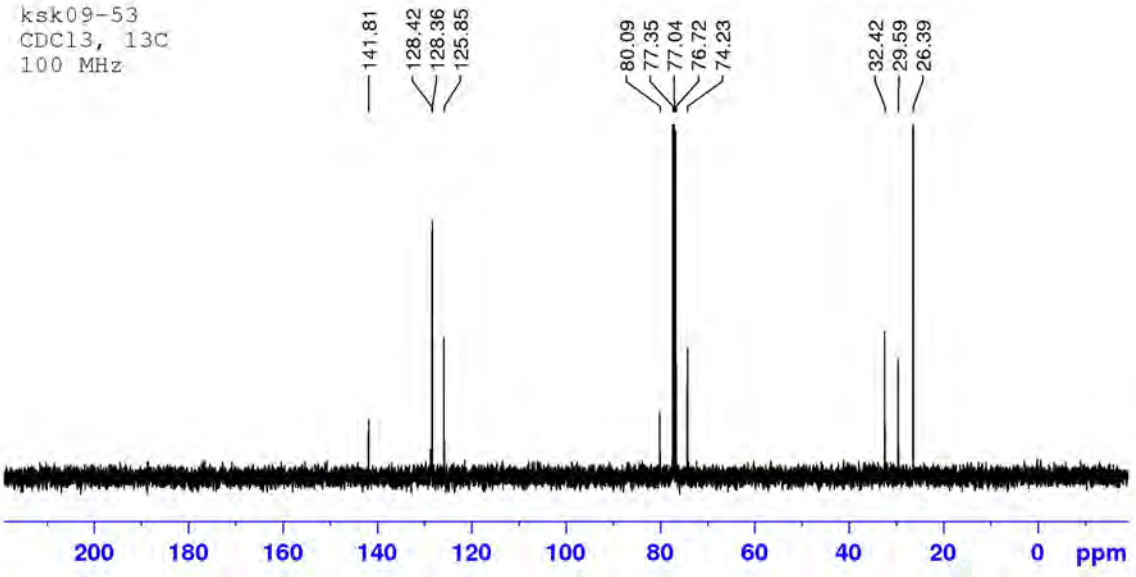
ksk08-78
CDCl3, 1H
400 MHz
9
8
7
6
5
4
3
2
1
0
ppm
0.916
2.161
2.090
3.169
4.000
1.019
2.479
1.247
9.364
3.169
6.181


ksk08-78
CDCl3, 13C
400 MHz
131.20
124.66
77.33
77.01
76.69
75.32
37.13
34.53
29.68
26.19
25.71
25.42
19.65
18.14
17.63
-5.88
200
180
160
140
120
100
80
60
40
20
0
ppm

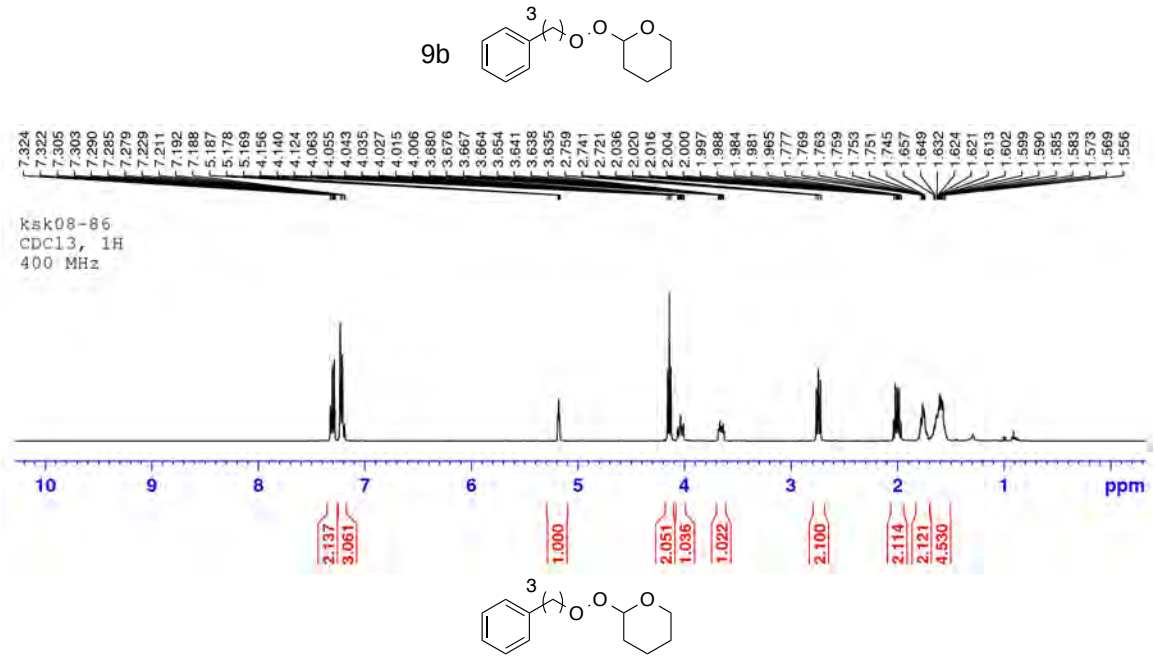
9a 

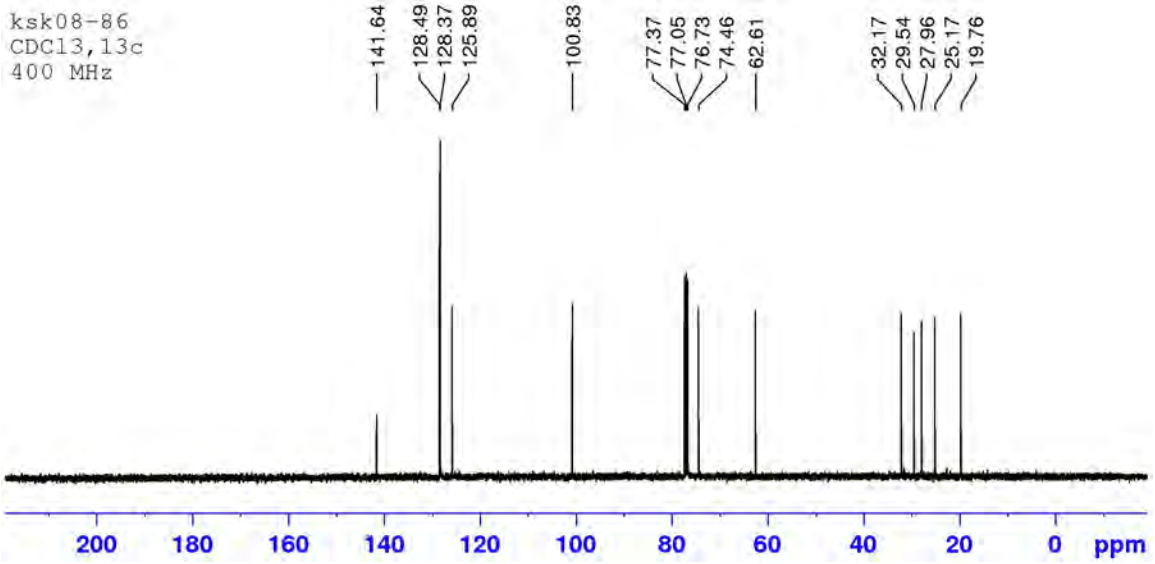

ksk09-53
CDCl3, 1H
400 MHz
7.327
7.308
7.296
7.290
7.279
7.232
7.213
7.205
4.015
3.999
3.983
2.747
2.728
2.708
2.003
1.987
1.983
1.980
1.971
1.967
1.964
1.955
1.947
1.931
1.280
10
9
8
7
6
5
4
3
2
1
ppm
2.255
3.103
2.000
2.045
2.000
9.340



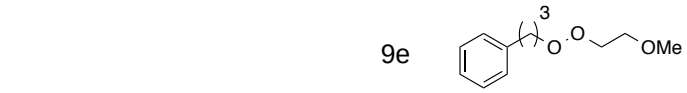

ksk09-53
CDCl3, 13C
100 MHz
141.81
128.42
128.36
125.85
80.09
77.35
77.04
76.72
74.23
32.42
29.59
26.39
200
180
160
140
120
100
80
60
40
20
0
ppm

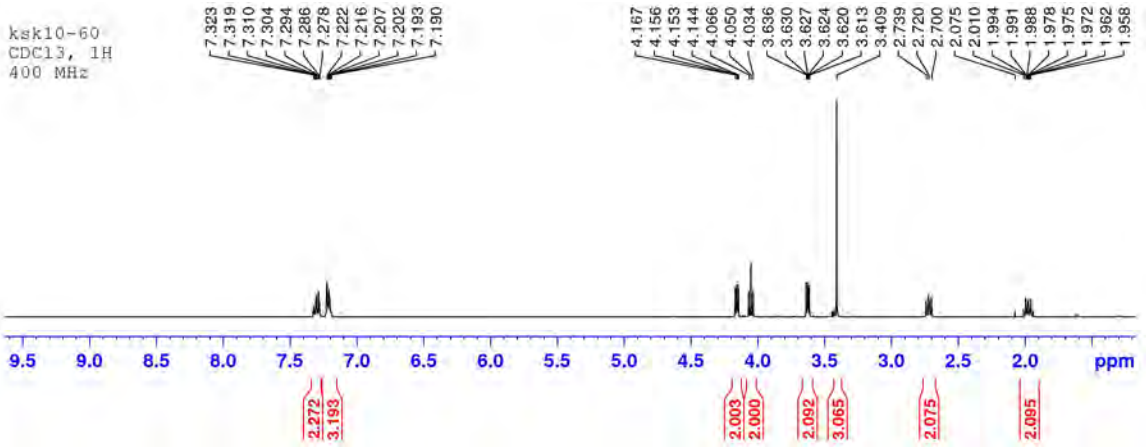
9b



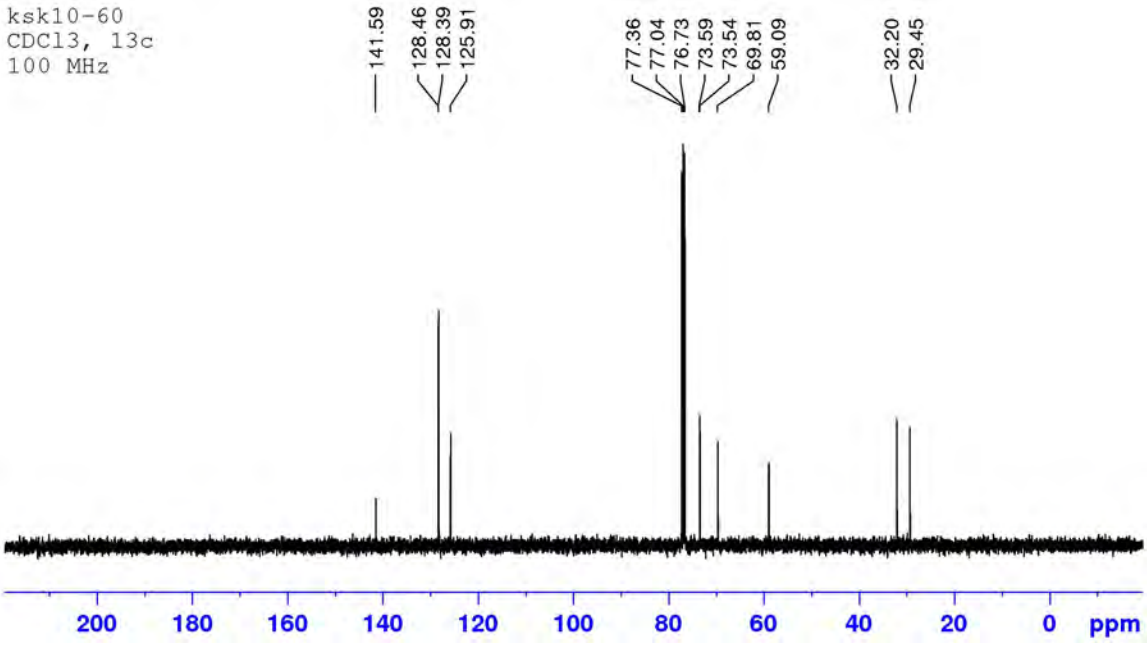


9e

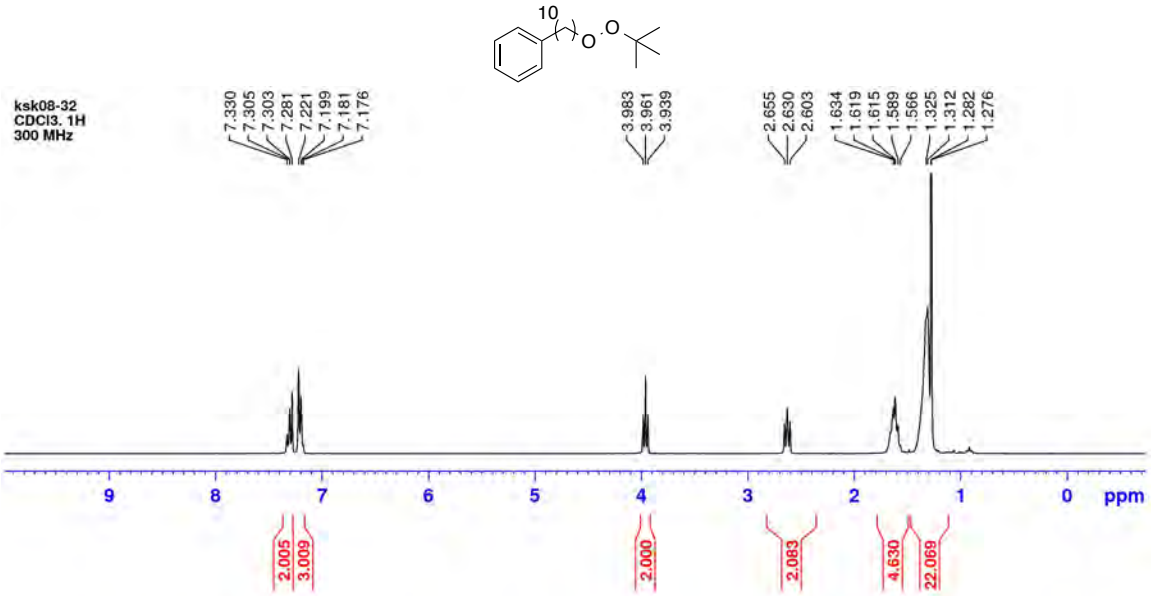

3
O
O
OMe

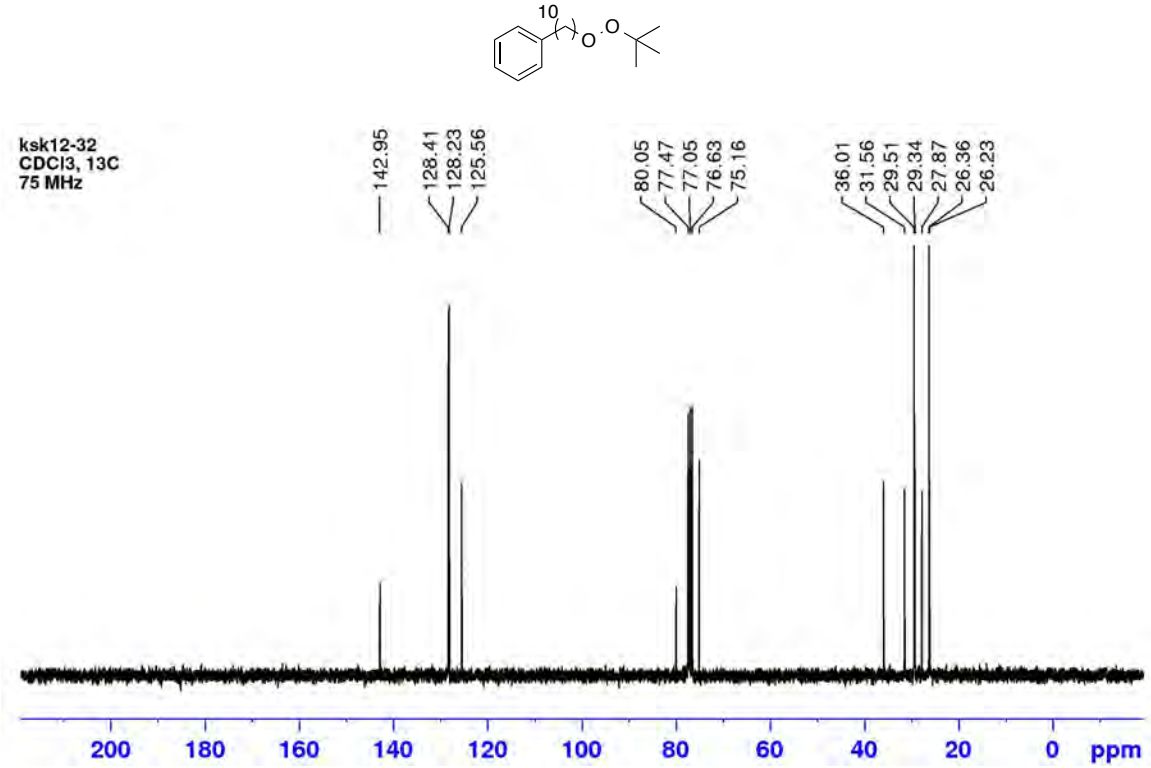

ksk10-60
CDCl3, 1H
400 MHz
7.323
7.319
7.310
7.304
7.294
7.286
7.278
7.222
7.216
7.207
7.202
7.193
7.190
4.167
4.156
4.153
4.144
4.066
4.050
4.034
3.636
3.630
3.627
3.624
3.620
3.613
3.409
2.739
2.720
2.700
2.075
2.010
1.994
1.991
1.988
1.978
1.975
1.972
1.962
1.958
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
ppm
2.272
3.193
2.003
2.000
2.092
3.065
2.075
2.095

3
O
O
OMe

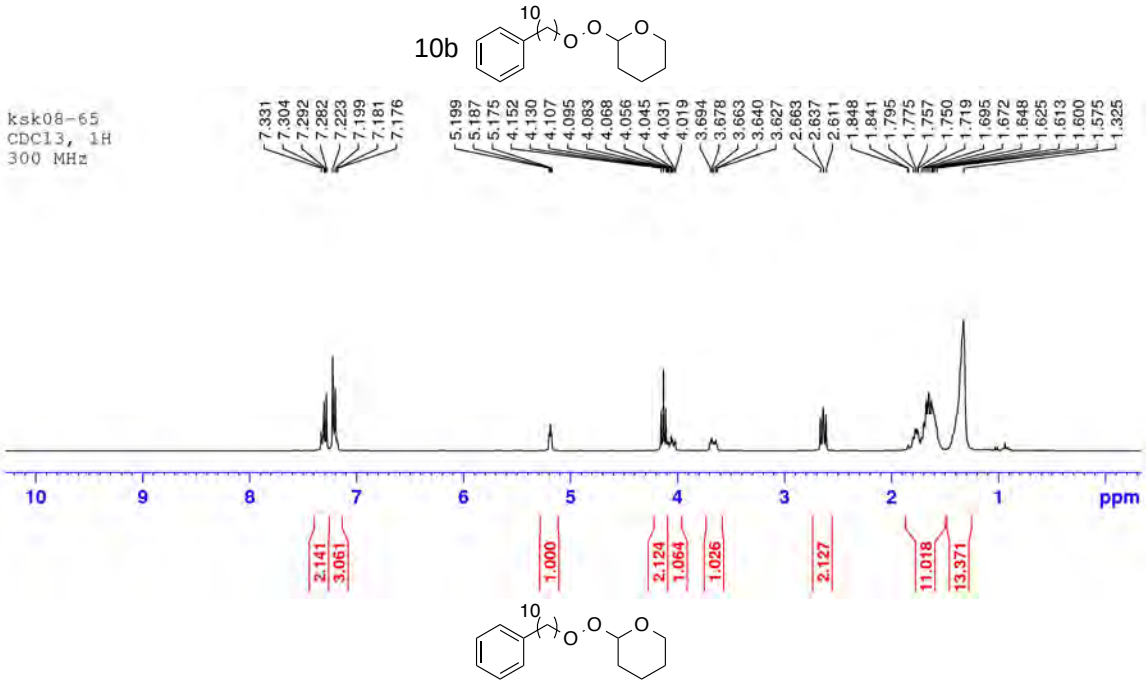

ksk10-60
CDCl3, 13c
100 MHz
141.59
128.46
128.39
125.91
77.36
77.04
76.73
73.59
73.54
69.81
59.09
32.20
29.45
200
180
160
140
120
100
80
60
40
20
0
ppm

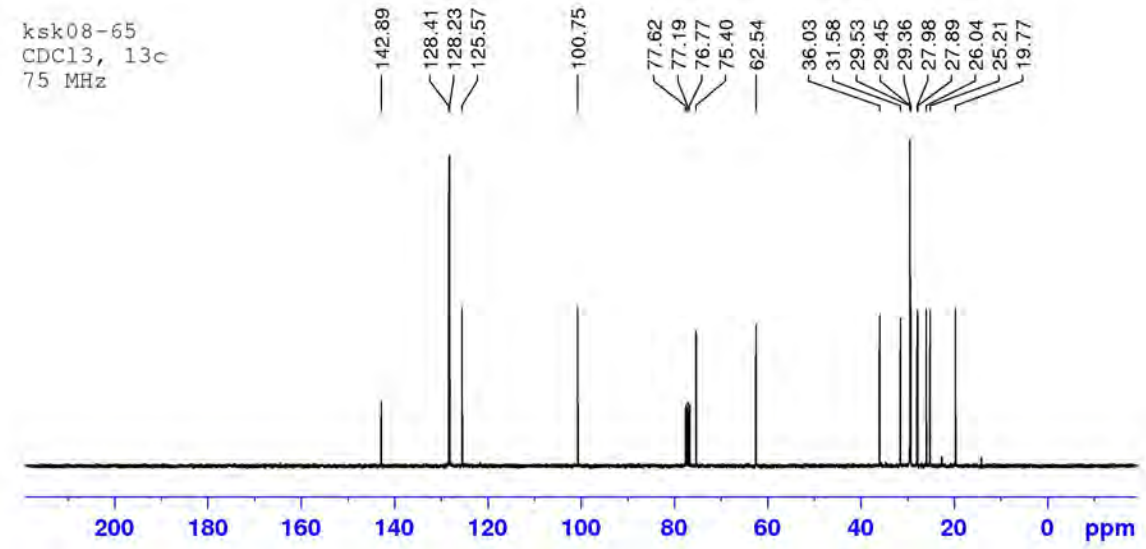
10a


ksk08-32
CDCl3. 1H
300 MHz
7.330
7.305
7.303
7.281
7.221
7.199
7.181
7.176
3.983
3.961
3.939
2.655
2.630
2.603
1.634
1.619
1.615
1.589
1.566
1.325
1.312
1.282
1.276
9
8
7
6
5
4
3
2
1
0
ppm
2.005
3.009
2.000
2.083
4.630
22.069

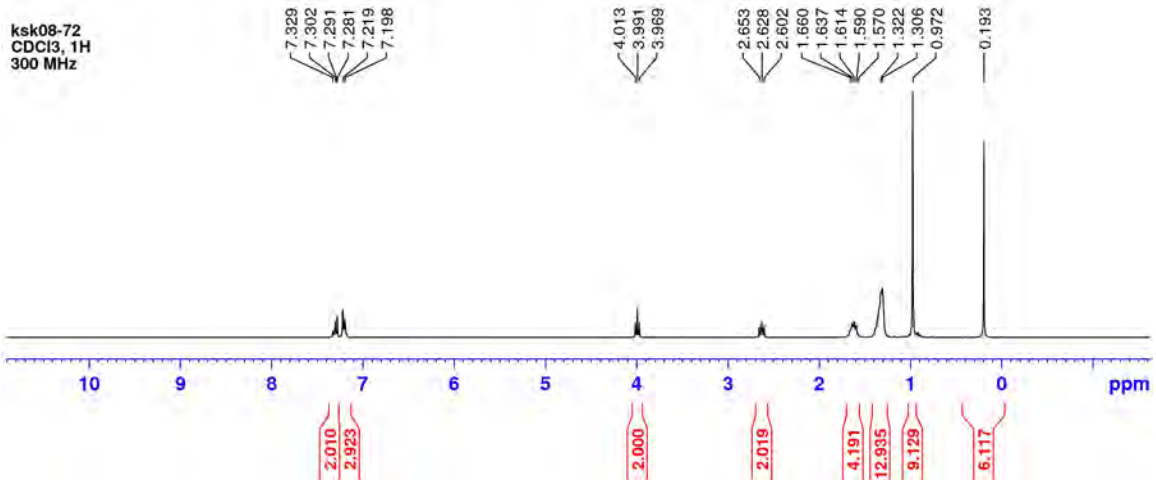

ksk12-32
CDCl3, 13C
75 MHz
142.95
128.41
128.23
125.56
80.05
77.47
77.05
76.63
75.16
36.01
31.56
29.51
29.34
27.87
26.36
26.23
200
180
160
140
120
100
80
60
40
20
0
ppm

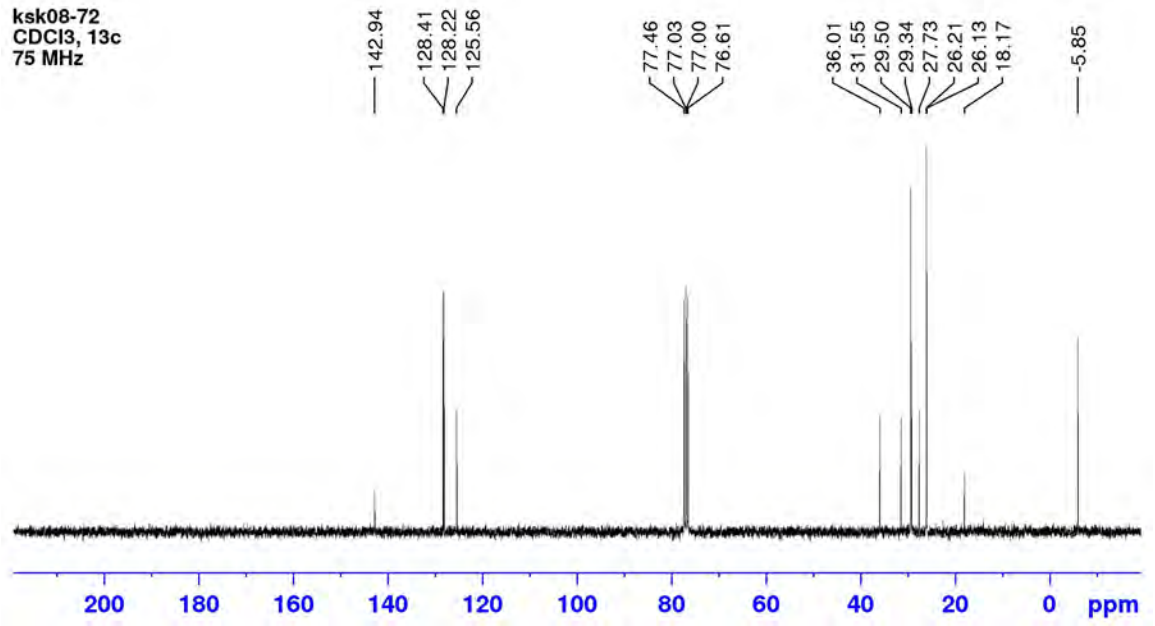
10b


ksk08-65
CDCl3, 1H
300 MHz
7.331
7.304
7.292
7.282
7.223
7.199
7.181
7.176
5.199
5.187
5.175
5.152
4.130
4.107
4.095
4.083
4.068
4.056
4.045
4.031
4.019
3.694
3.678
3.663
3.640
3.627
2.663
2.637
2.611
1.848
1.841
1.795
1.775
1.757
1.750
1.719
1.695
1.672
1.648
1.625
1.613
1.600
1.575
1.325
10
9
8
7
6
5
4
3
2
1
ppm
2.141
3.061
1.000
2.124
1.064
1.026
2.127
11.018
13.371

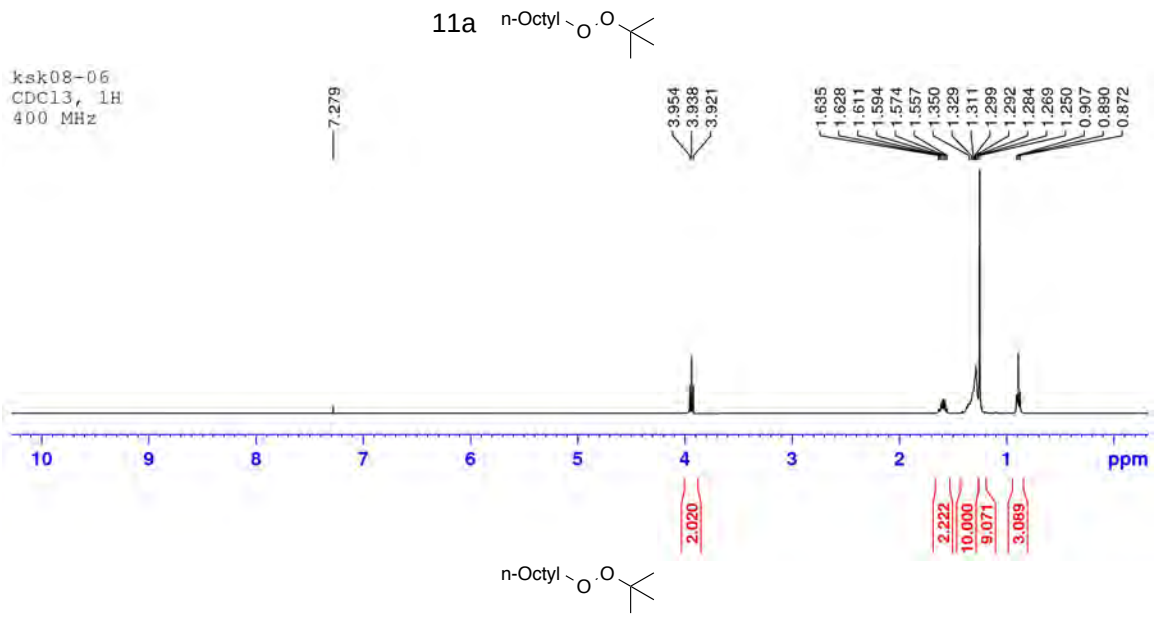

ksk08-65
CDCl3, 13c
75 MHz
142.89
128.41
128.23
125.57
100.75
77.62
77.19
76.77
75.40
62.54
36.03
31.58
29.53
29.45
29.36
27.98
27.89
26.04
25.21
19.77
200
180
160
140
120
100
80
60
40
20
0
ppm

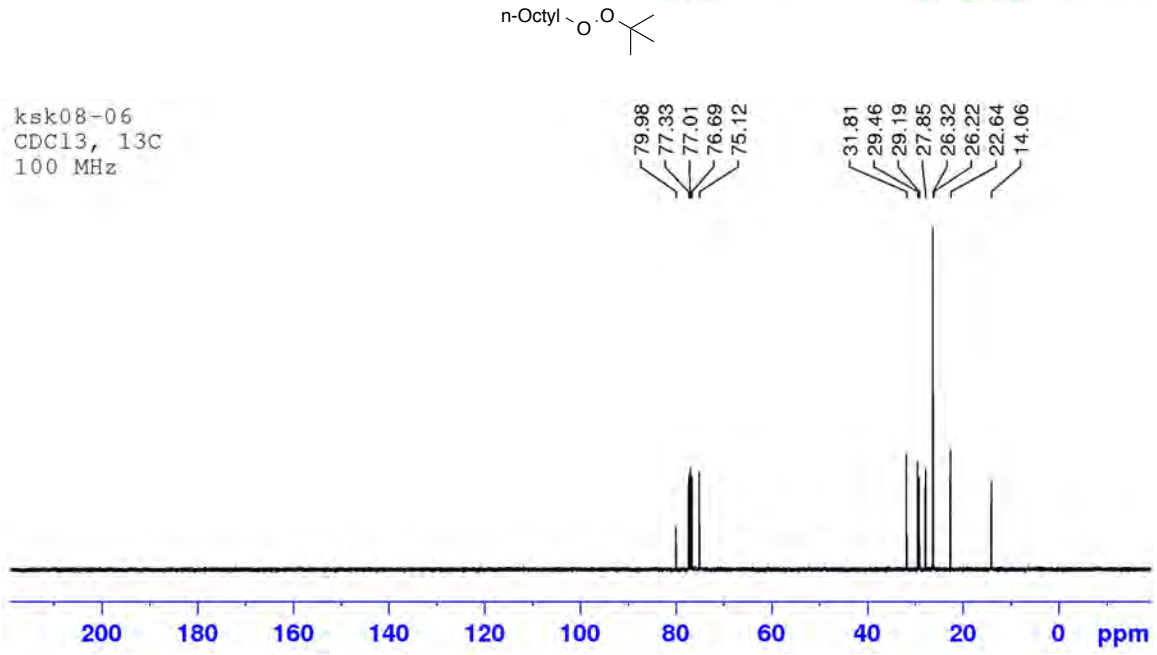
10d

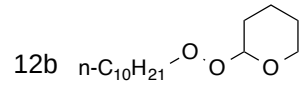

ksk08-72
CDCl3, 1H
300 MHz
7.329
7.302
7.291
7.281
7.219
7.198
4.013
3.991
3.969
2.653
2.628
2.602
1.660
1.637
1.614
1.590
1.570
1.322
1.306
0.972
0.193
10
9
8
7
6
5
4
3
2
1
0
ppm
2.010
2.923
2.000
2.019
4.191
12.935
9.129
6.117

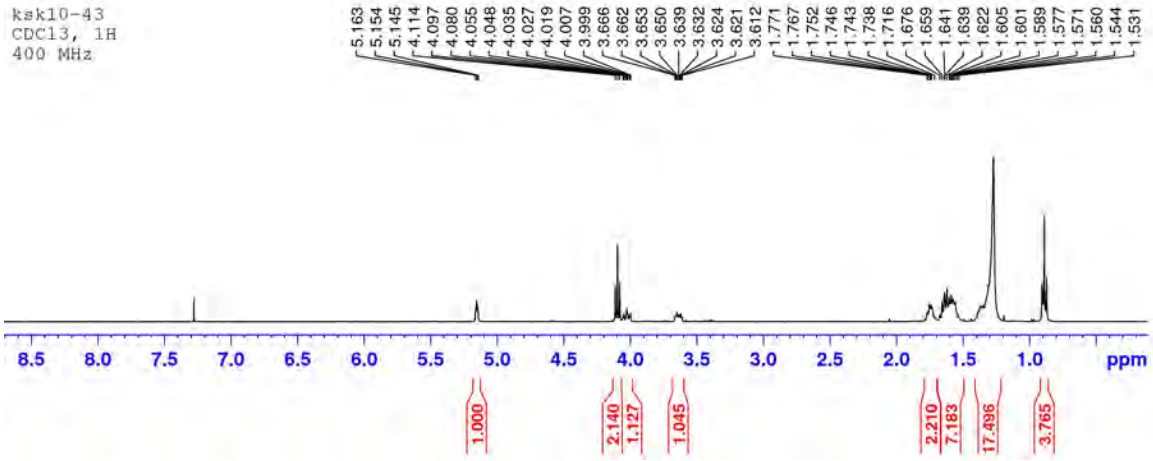

ksk08-72
CDCl3, 13c
75 MHz
142.94
128.41
128.22
125.56
77.46
77.03
77.00
76.61
36.01
31.55
29.50
29.34
27.73
26.21
26.13
18.17
-5.85
200
180
160
140
120
100
80
60
40
20
0
ppm

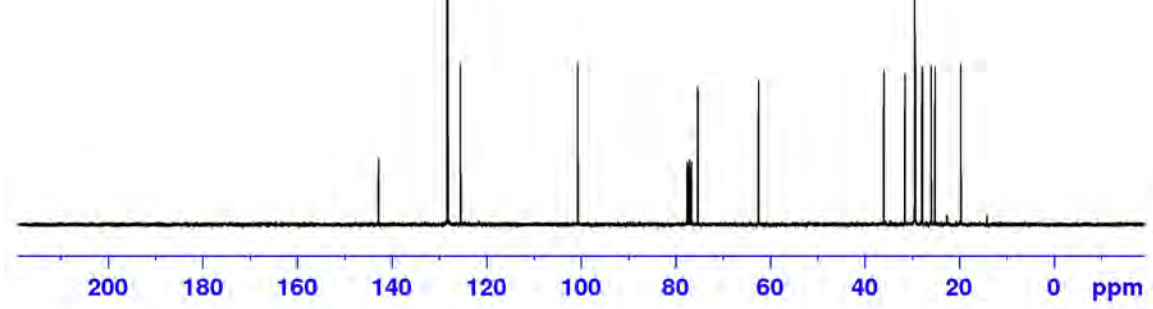
11a

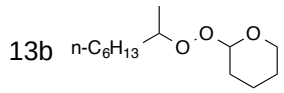

n-Octyl
O
O
ksk08-06
CDCl3, 1H
400 MHz
7.279
3.954
3.938
3.921
1.635
1.628
1.611
1.594
1.574
1.557
1.350
1.329
1.311
1.299
1.292
1.284
1.269
1.250
0.907
0.890
0.872
10
9
8
7
6
5
4
3
2
1
ppm
2.020
2.222
10.000
9.071
3.089

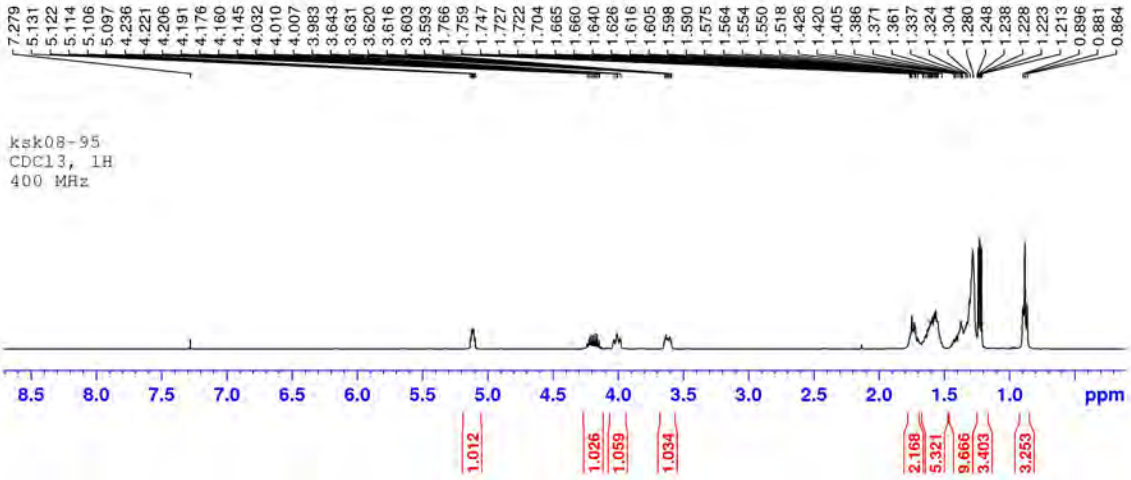

n-Octyl
O
O
ksk08-06
CDCl3, 13C
100 MHz
79.98
77.33
77.01
76.69
75.12
31.81
29.46
29.19
27.85
26.32
26.22
22.64
14.06
200
180
160
140
120
100
80
60
40
20
0
ppm

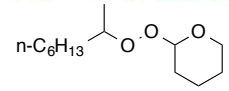
12b 

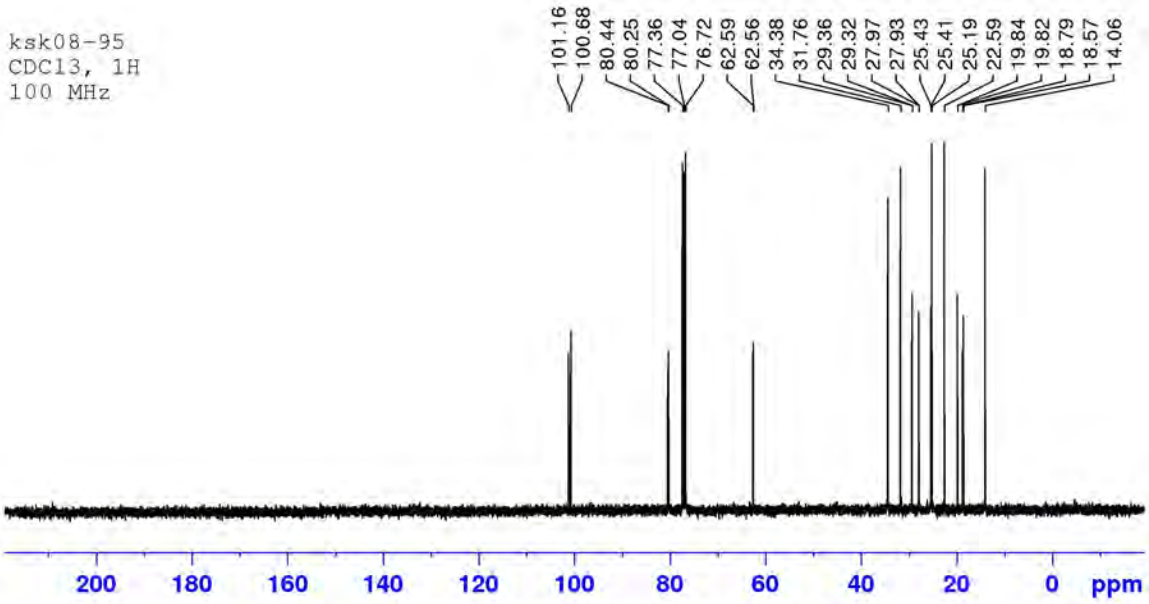

ksk10-43
CDCl3, 1H
400 MHz
5.163
5.154
5.145
4.114
4.097
4.080
4.055
4.048
4.035
4.027
4.019
4.007
3.999
3.666
3.662
3.653
3.650
3.639
3.632
3.624
3.621
3.612
1.771
1.767
1.752
1.746
1.743
1.738
1.716
1.676
1.659
1.641
1.639
1.622
1.605
1.601
1.589
1.577
1.571
1.560
1.544
1.531
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.000
2.140
1.127
1.045
2.210
7.183
17.496
3.765

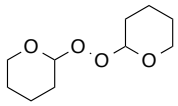

ksk08-65
CDCl3, 13c
75 MHz
142.89
128.41
128.23
125.57
100.75
77.62
77.19
76.77
75.40
62.54
36.03
31.58
29.53
29.45
29.36
27.98
27.89
26.04
25.21
19.77
200
180
160
140
120
100
80
60
40
20
0
ppm

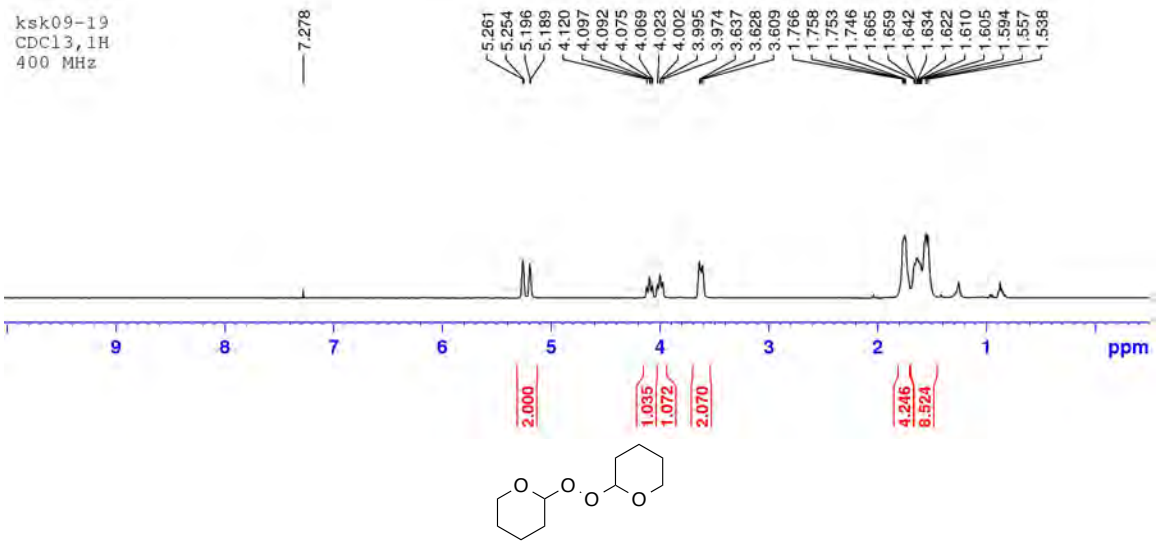
13b 
n-C6H13
O
O
O

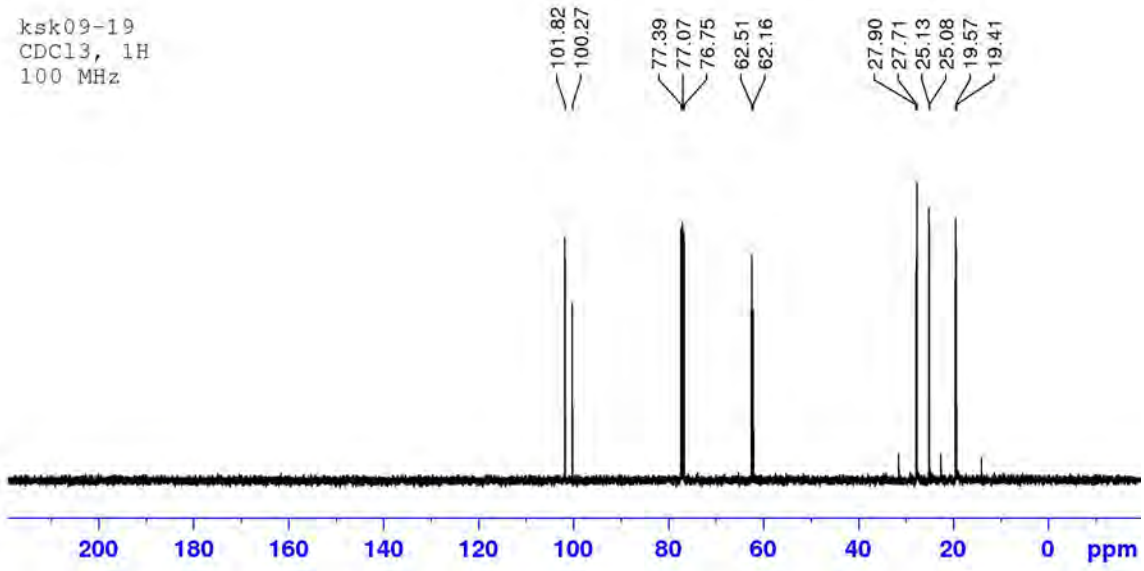

7.279
5.131
5.122
5.114
5.106
5.097
4.236
4.221
4.206
4.191
4.176
4.160
4.145
4.032
4.010
4.007
3.983
3.643
3.631
3.620
3.616
3.603
3.593
1.766
1.759
1.747
1.727
1.722
1.704
1.665
1.660
1.640
1.626
1.616
1.605
1.598
1.590
1.575
1.564
1.554
1.550
1.518
1.426
1.420
1.405
1.386
1.371
1.361
1.337
1.324
1.304
1.280
1.248
1.238
1.228
1.223
1.213
0.896
0.881
0.864
ksk08-95
CDCl3, 1H
400 MHz
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
ppm
1.012
1.026
1.059
1.034
2.168
5.321
9.666
3.403
3.253

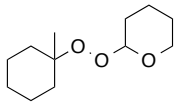

n-C6H13
O
O
O

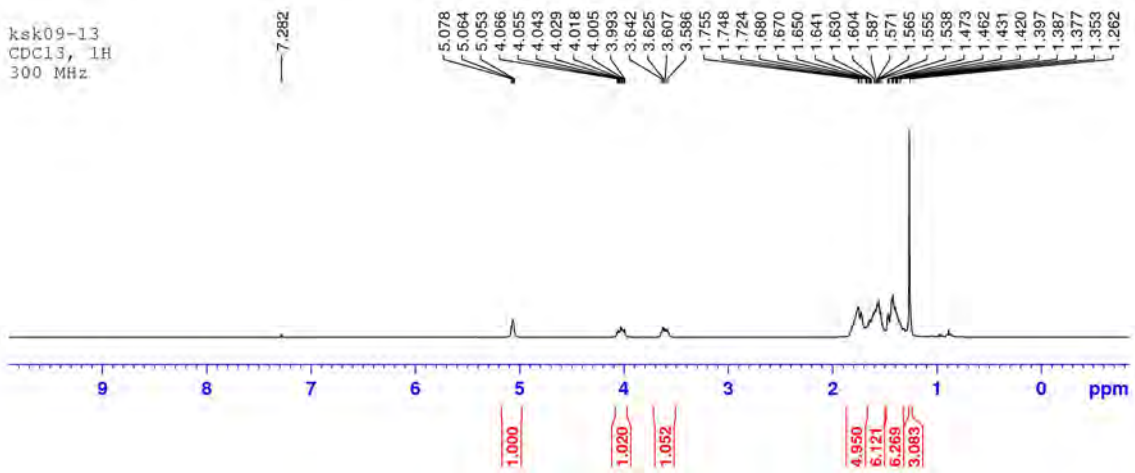

ksk08-95
CDCl3, 1H
100 MHz
101.16
100.68
80.44
80.25
77.36
77.04
76.72
62.59
62.56
34.38
31.76
29.36
29.32
27.97
27.93
25.43
25.41
25.19
22.59
19.84
19.82
18.79
18.57
14.06
200
180
160
140
120
100
80
60
40
20
0
ppm

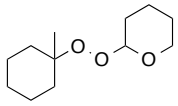
14b 

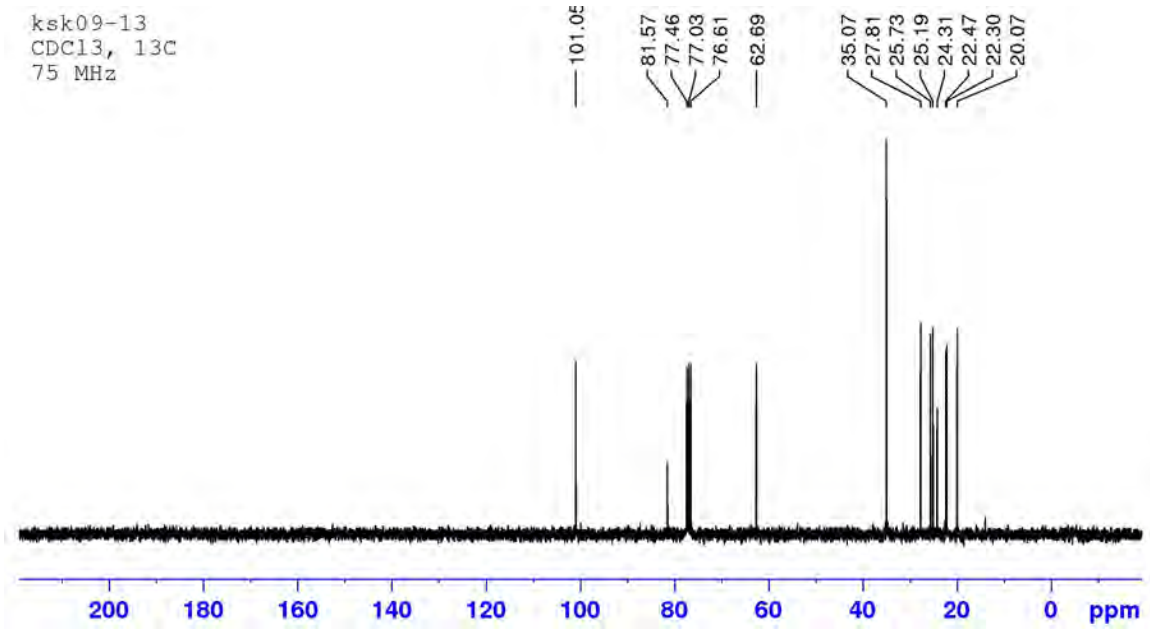

ksk09-19
CDCl3,1H
400 MHz
7.278
5.261
5.254
5.196
5.189
4.120
4.097
4.092
4.075
4.069
4.023
4.002
3.995
3.974
3.637
3.628
3.609
1.766
1.758
1.753
1.746
1.665
1.659
1.642
1.634
1.622
1.610
1.605
1.594
1.557
1.538
9
8
7
6
5
4
3
2
1
ppm
2.000
1.035
1.072
2.070
4.246
8.524

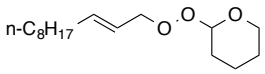

ksk09-19
CDCl3, 1H
100 MHz
101.82
100.27
77.39
77.07
76.75
62.51
62.16
27.90
27.71
25.13
25.08
19.57
19.41
200
180
160
140
120
100
80
60
40
20
0
ppm

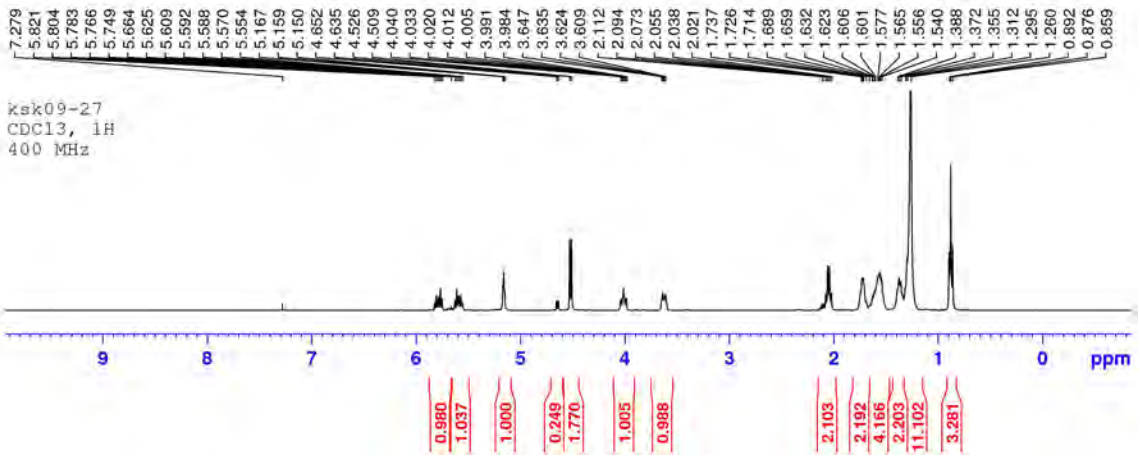
15b 

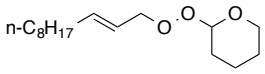

ksk09-13
CDCl3, 1H
300 MHz
7.282
5.078
5.064
5.053
4.086
4.055
4.043
4.029
4.018
4.005
3.993
3.642
3.625
3.607
3.586
1.755
1.748
1.724
1.680
1.670
1.650
1.641
1.630
1.604
1.587
1.571
1.565
1.555
1.538
1.473
1.462
1.431
1.420
1.397
1.387
1.377
1.353
1.262
9
8
7
6
5
4
3
2
1
0
ppm
1.000
1.020
1.052
4.950
6.121
6.269
3.083

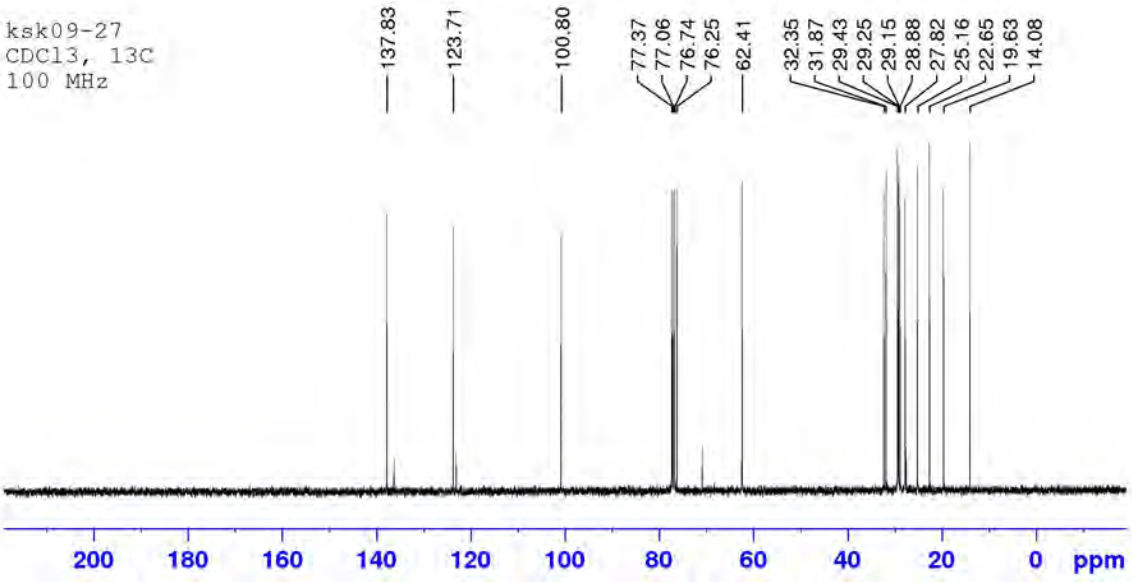



ksk09-13
CDCl3, 13C
75 MHz
101.05
81.57
77.46
77.03
76.61
62.69
35.07
27.81
25.73
25.19
24.31
22.47
22.30
20.07
200
180
160
140
120
100
80
60
40
20
0
ppm

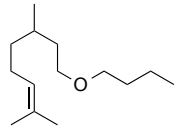
16b 
n-C8H17
O
O
O

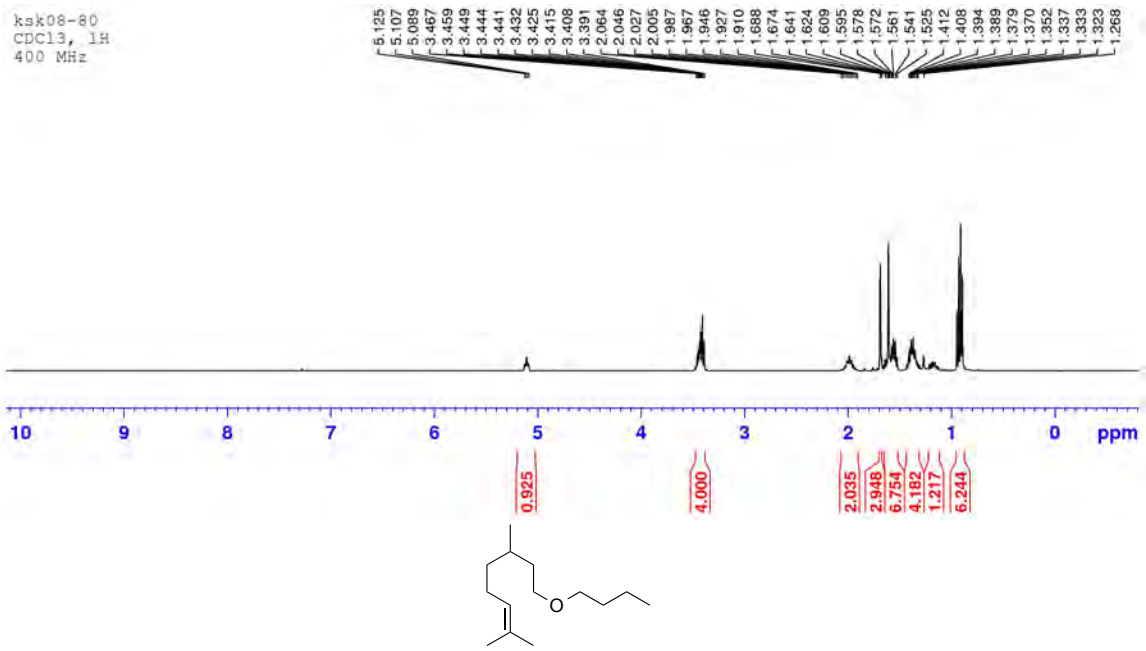

7.279
5.821
5.804
5.783
5.766
5.749
5.664
5.625
5.609
5.592
5.588
5.570
5.554
5.167
5.159
5.150
4.652
4.635
4.526
4.509
4.040
4.033
4.020
4.012
4.005
3.991
3.984
3.647
3.635
3.624
3.609
2.112
2.094
2.073
2.055
2.038
2.021
1.737
1.726
1.714
1.689
1.659
1.632
1.623
1.606
1.601
1.577
1.565
1.556
1.540
1.388
1.372
1.355
1.312
1.295
1.260
0.892
0.876
0.859
ksk09-27
CDCl3, 1H
400 MHz
9
8
7
6
5
4
3
2
1
0
ppm
0.980
1.037
1.000
0.249
1.770
1.005
0.988
2.103
2.192
4.166
2.203
11.102
3.281

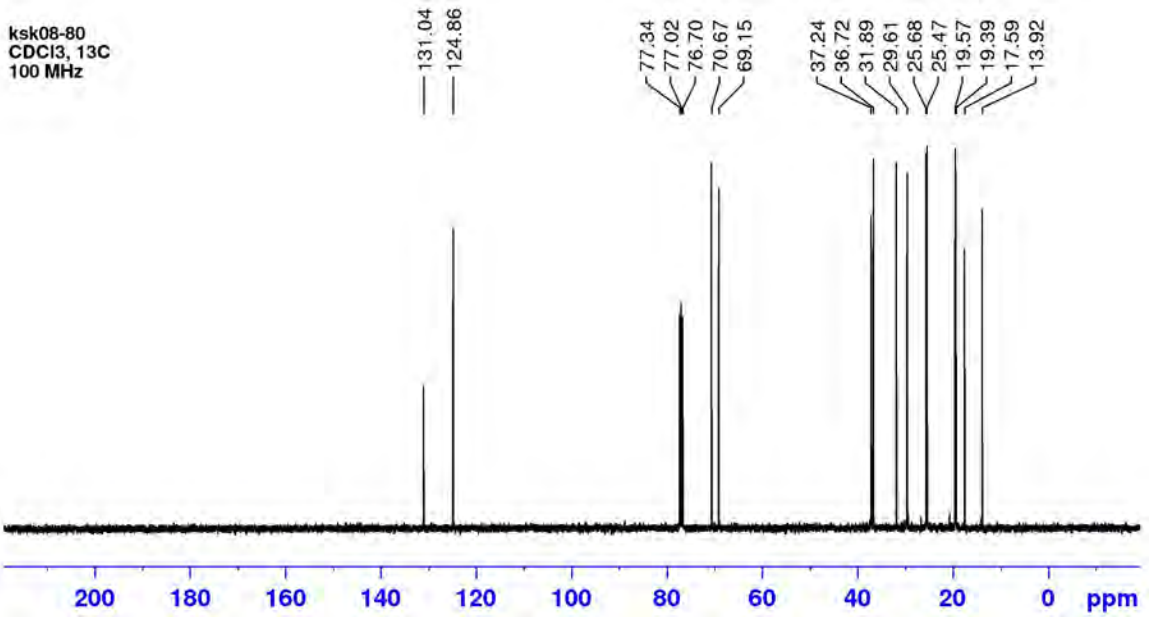

n-C8H17
O
O
O


ksk09-27
CDCl3, 13C
100 MHz
137.83
123.71
100.80
77.37
77.06
76.74
76.25
62.41
32.35
31.87
29.43
29.25
29.15
28.88
27.82
25.16
22.65
19.63
14.08
200
180
160
140
120
100
80
60
40
20
0
ppm

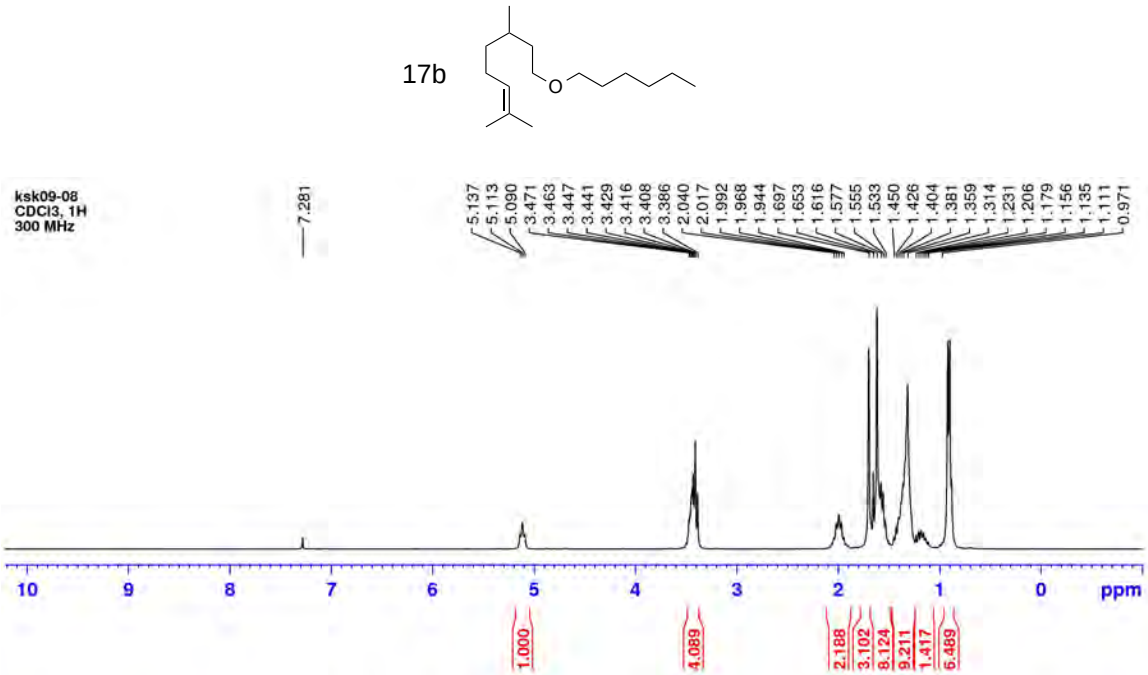
17a

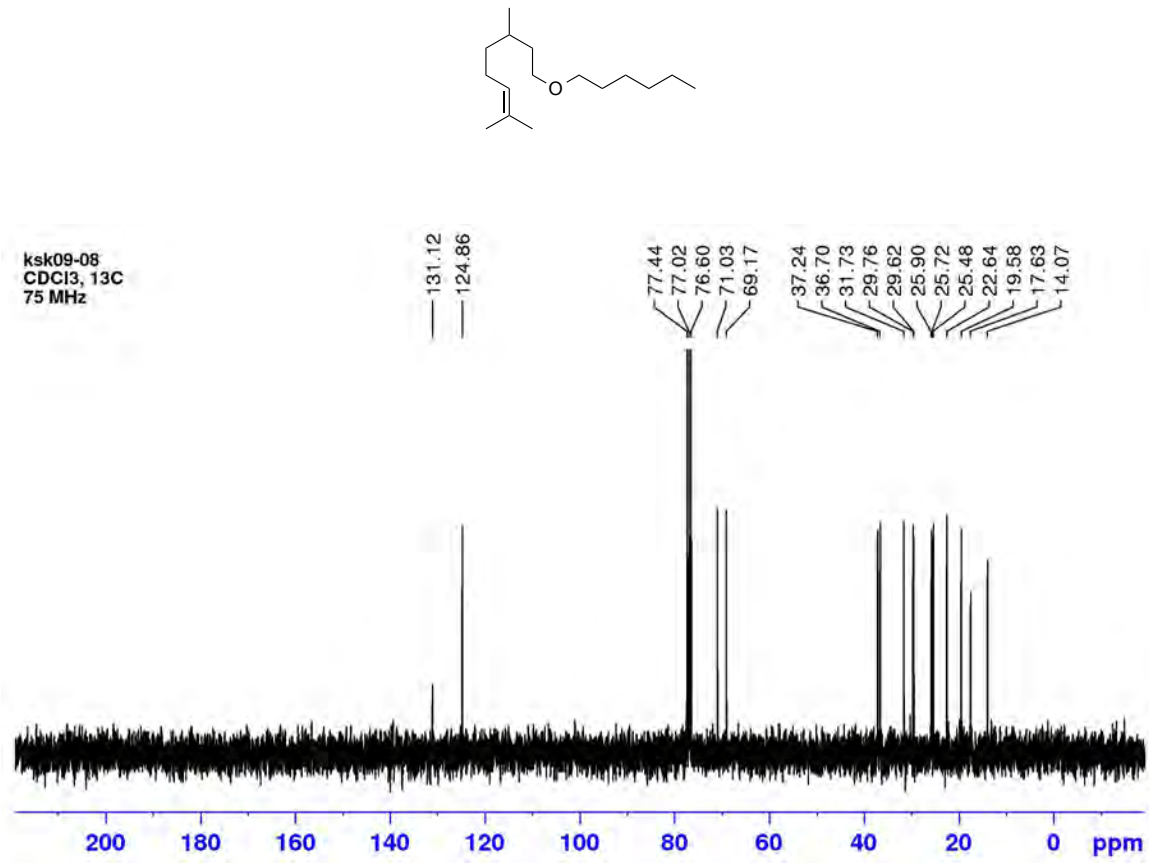



ksk08-80
CDCl3, 1H
400 MHz
5.125
5.107
5.089
3.467
3.459
3.449
3.444
3.441
3.432
3.425
3.415
3.408
3.391
2.064
2.046
2.027
2.005
1.987
1.967
1.946
1.927
1.910
1.688
1.674
1.641
1.624
1.609
1.595
1.578
1.572
1.561
1.541
1.525
1.412
1.408
1.394
1.389
1.379
1.370
1.352
1.337
1.333
1.323
1.268
10
9
8
7
6
5
4
3
2
1
0
ppm
0.925
4.000
2.035
2.948
6.754
4.182
1.217
6.244

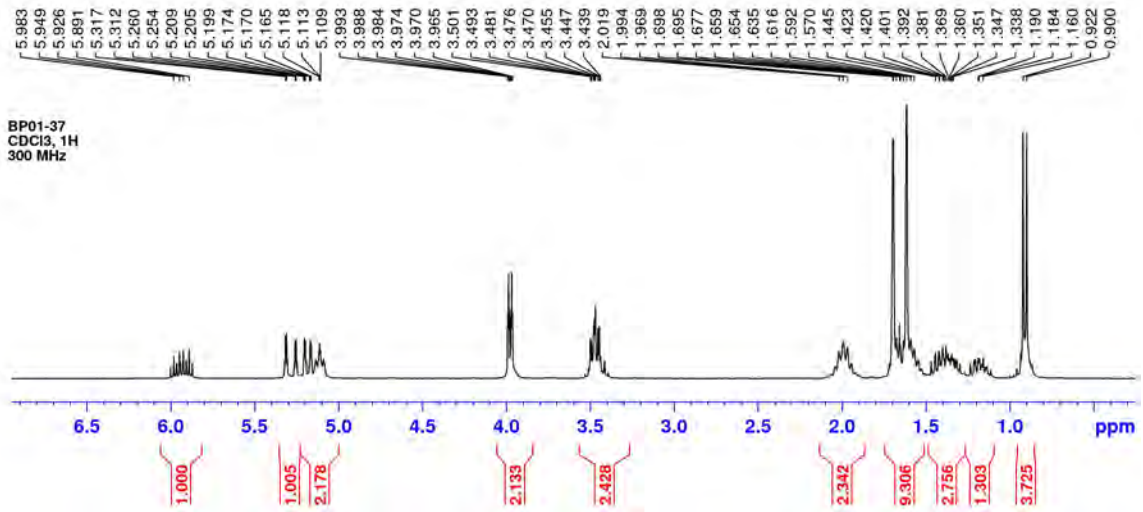

ksk08-80
CDCl3, 13C
100 MHz
131.04
124.86
77.34
77.02
76.70
70.67
69.15
37.24
36.72
31.89
29.61
25.68
25.47
19.57
19.39
17.59
13.92
200
180
160
140
120
100
80
60
40
20
0
ppm

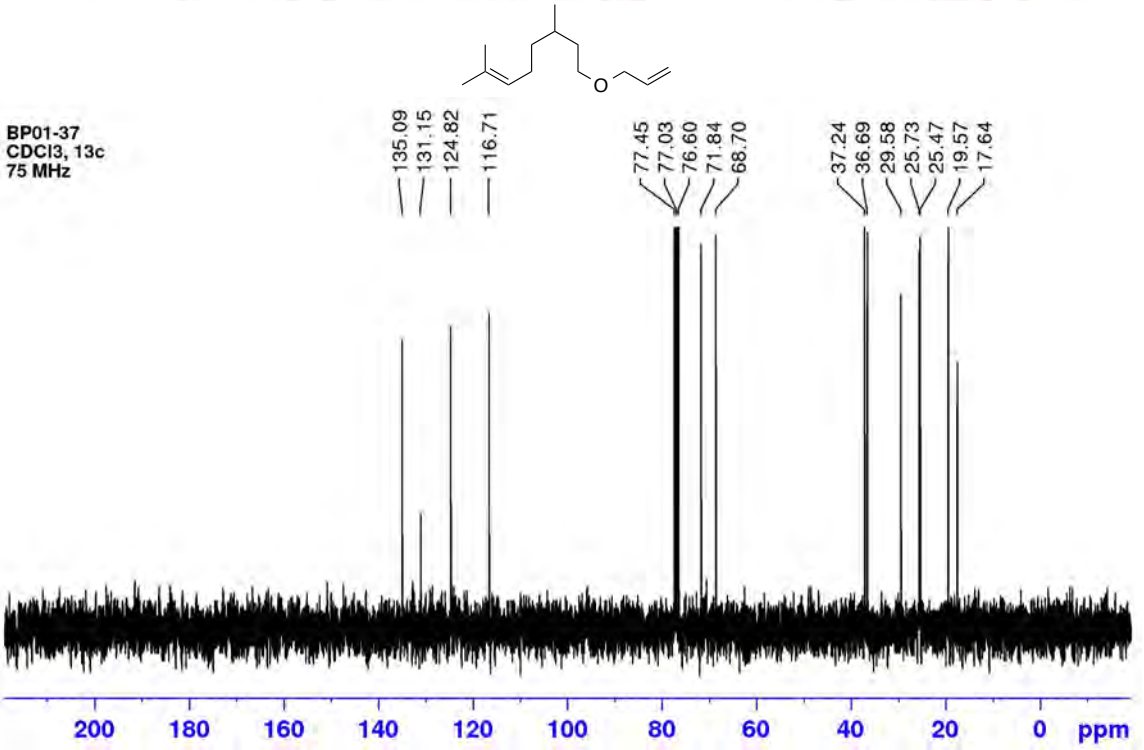
17b


ksk09-08
CDCl3, 1H
300 MHz
7.281
5.137
5.113
5.090
3.471
3.463
3.447
3.441
3.429
3.416
3.408
3.386
2.040
2.017
1.992
1.968
1.944
1.697
1.653
1.616
1.577
1.555
1.533
1.450
1.426
1.404
1.381
1.359
1.314
1.231
1.206
1.179
1.156
1.135
1.111
0.971
10
9
8
7
6
5
4
3
2
1
0
ppm
1.000
4.089
2.188
3.102
8.124
9.211
1.417
6.489

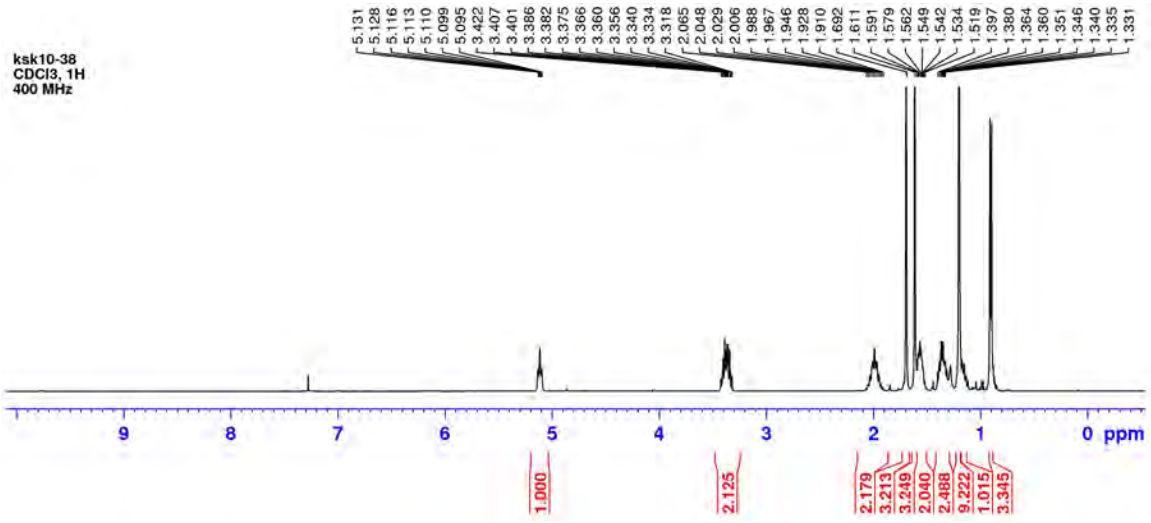

ksk09-08
CDCl3, 13C
75 MHz
131.12
124.86
77.44
77.02
76.60
71.03
69.17
37.24
36.70
31.73
29.76
29.62
25.90
25.72
25.48
22.64
19.58
17.63
14.07
200
180
160
140
120
100
80
60
40
20
0
ppm

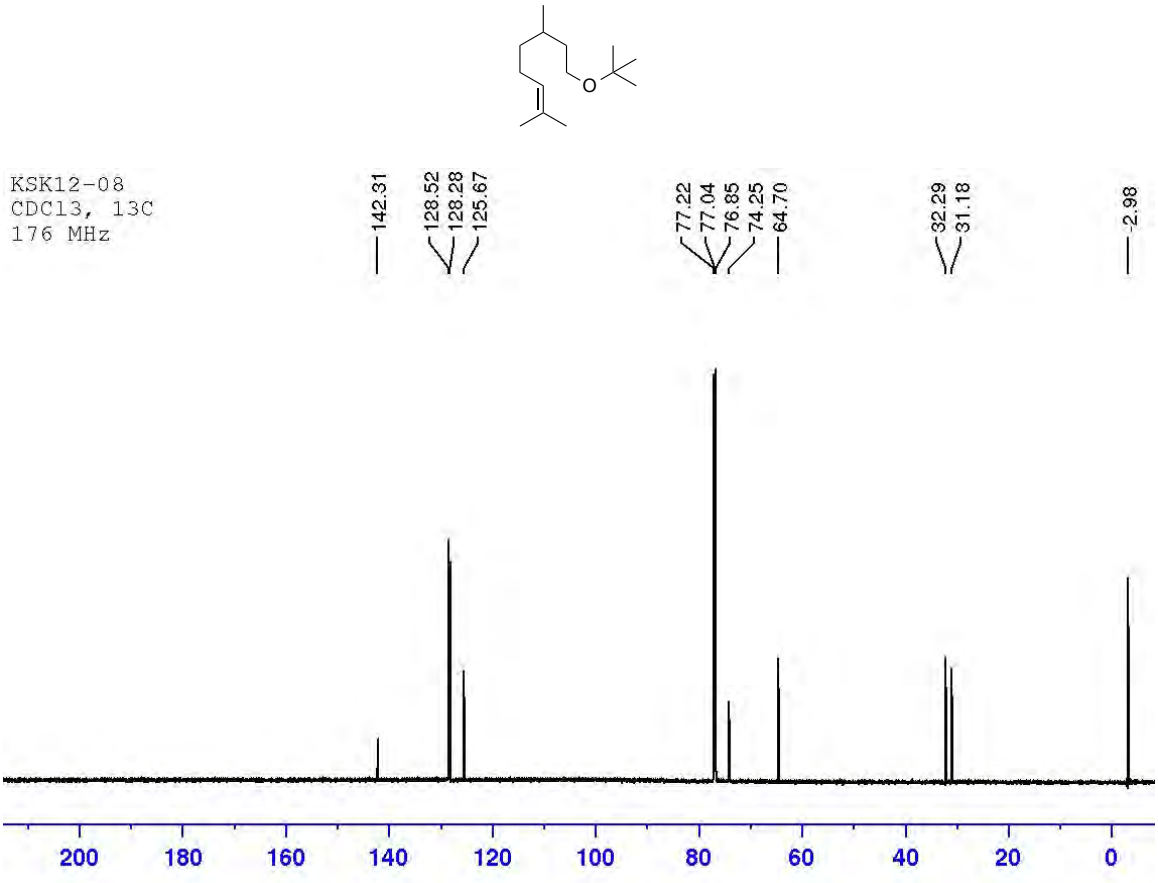
17c

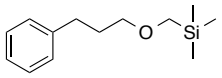

5.983
5.949
5.926
5.891
5.317
5.312
5.260
5.254
5.209
5.205
5.199
5.174
5.170
5.165
5.118
5.113
5.109
3.993
3.988
3.984
3.974
3.970
3.965
3.501
3.493
3.481
3.476
3.470
3.455
3.447
3.439
2.019
1.994
1.969
1.698
1.695
1.677
1.659
1.654
1.635
1.616
1.592
1.570
1.445
1.423
1.420
1.401
1.392
1.381
1.369
1.360
1.351
1.347
1.338
1.190
1.184
1.160
0.922
0.900
BP01-37
CDCl3, 1H
300 MHz
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.000
1.005
2.178
2.133
2.428
2.342
9.306
2.756
1.303
3.725

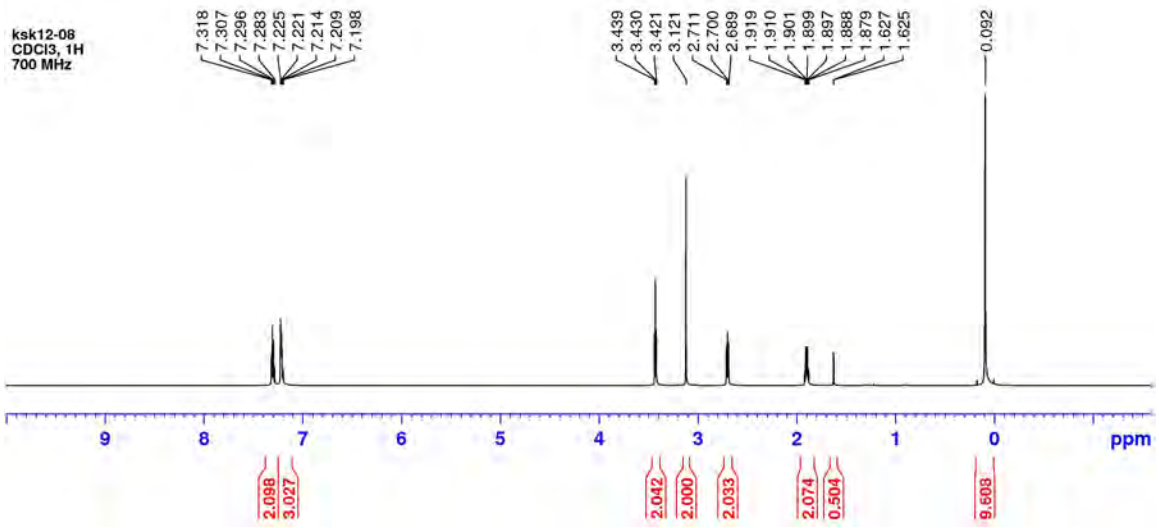

BP01-37
CDCl3, 13c
75 MHz
135.09
131.15
124.82
116.71
77.45
77.03
76.60
71.84
68.70
37.24
36.69
29.58
25.73
25.47
19.57
17.64
200
180
160
140
120
100
80
60
40
20
0
ppm

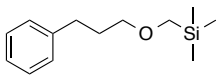
17d

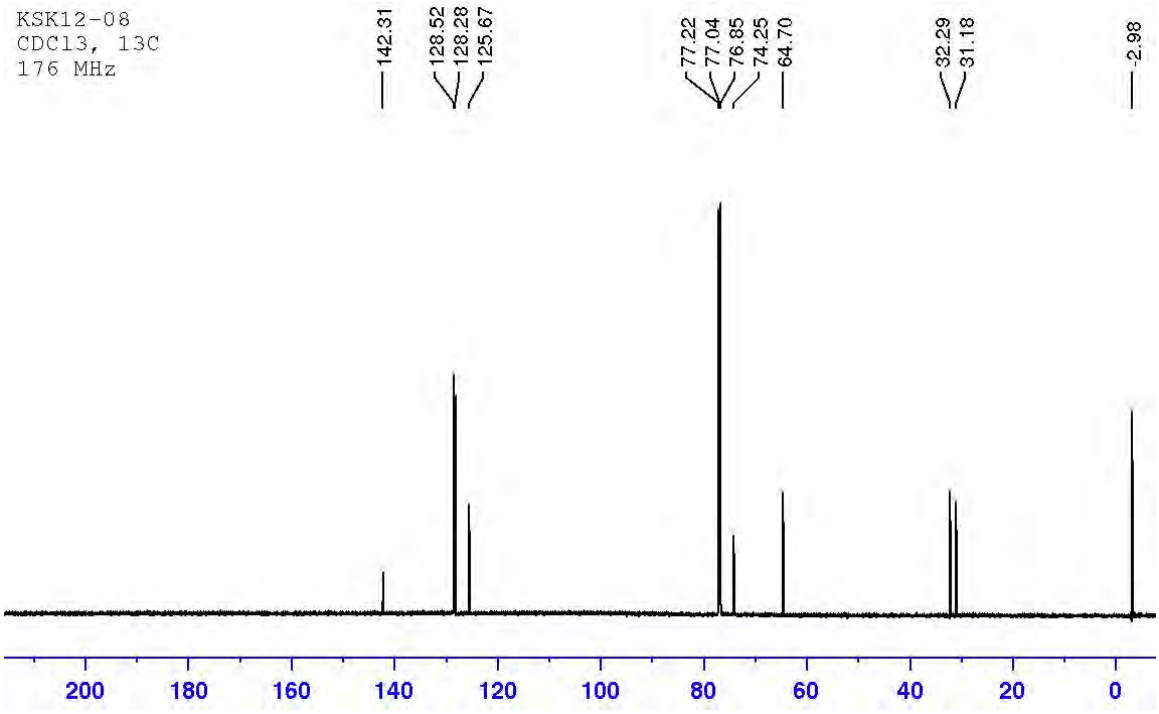

ksk10-38
CDCl3, 1H
400 MHz
5.131
5.128
5.116
5.113
5.110
5.099
5.095
3.422
3.407
3.401
3.386
3.382
3.375
3.366
3.360
3.356
3.340
3.334
3.318
2.065
2.048
2.029
2.006
1.988
1.967
1.946
1.928
1.910
1.692
1.611
1.591
1.579
1.562
1.549
1.542
1.534
1.519
1.397
1.380
1.364
1.360
1.351
1.346
1.340
1.335
1.331
9
8
7
6
5
4
3
2
1
0 ppm
1.000
2.125
2.179
3.213
3.249
2.040
2.488
9.222
1.015
3.345

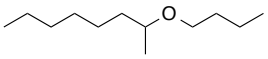

KSK12-08
CDCl3, 13C
176 MHz
142.31
128.52
128.28
125.67
77.22
77.04
76.85
74.25
64.70
32.29
31.18
-2.98
200
180
160
140
120
100
80
60
40
20
0

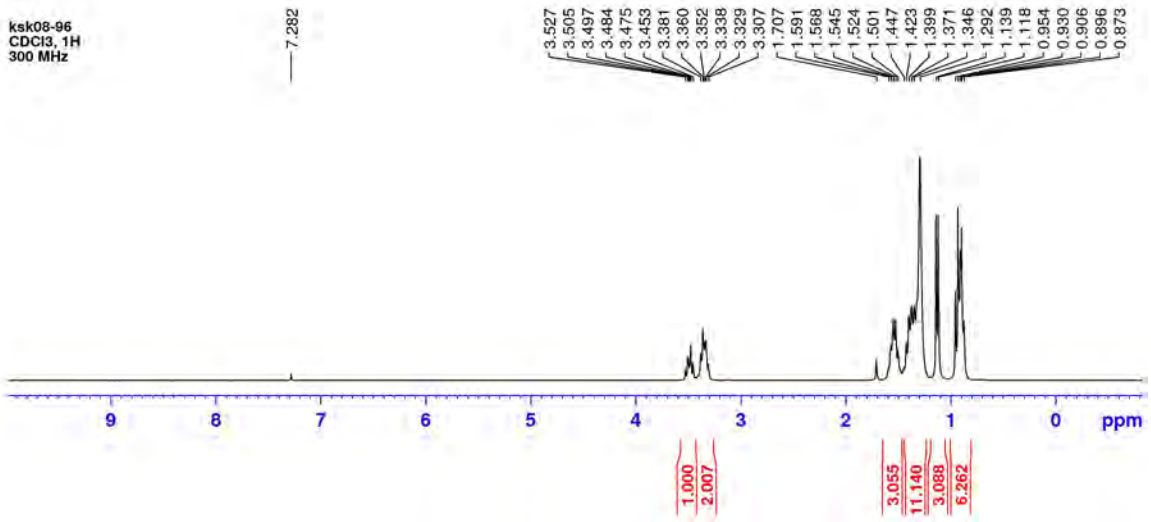
17e 
O
Si

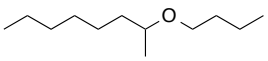

ksk12-08
CDCl3, 1H
700 MHz
7.318
7.307
7.296
7.283
7.225
7.221
7.214
7.209
7.198
3.439
3.430
3.421
3.121
2.711
2.700
2.689
1.919
1.910
1.901
1.899
1.897
1.888
1.879
1.627
1.625
0.092
9
8
7
6
5
4
3
2
1
0
ppm
2.098
3.027
2.042
2.000
2.033
2.074
0.504
9.608

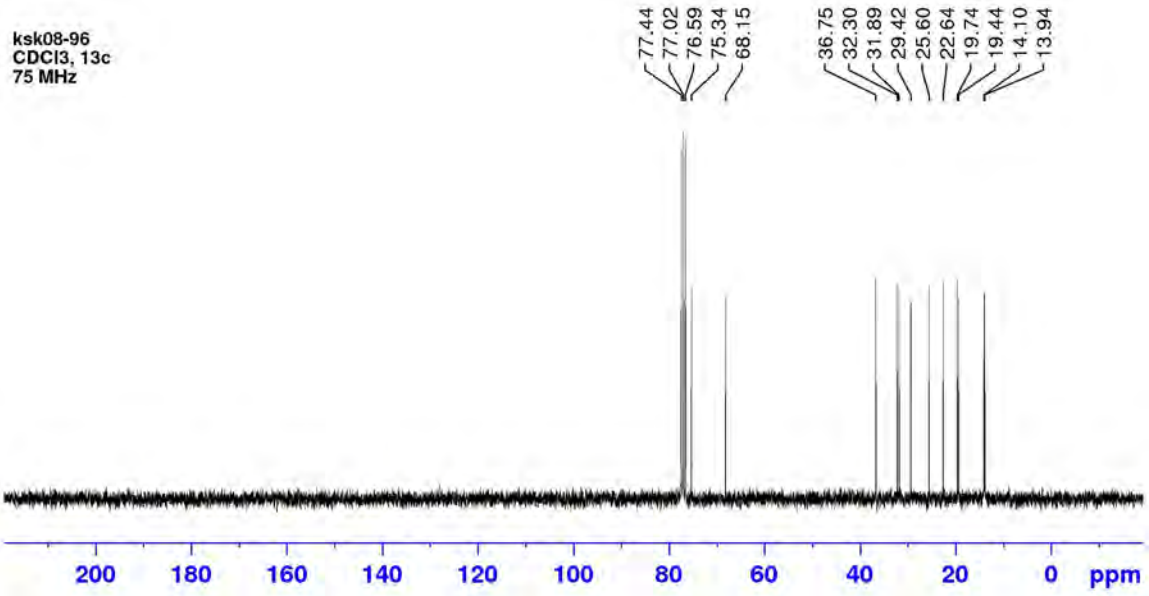

O
Si

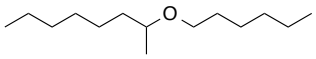

KSK12-08
CDCl3, 13C
176 MHz
142.31
128.52
128.28
125.67
77.22
77.04
76.85
74.25
64.70
32.29
31.18
-2.98
200
180
160
140
120
100
80
60
40
20
0

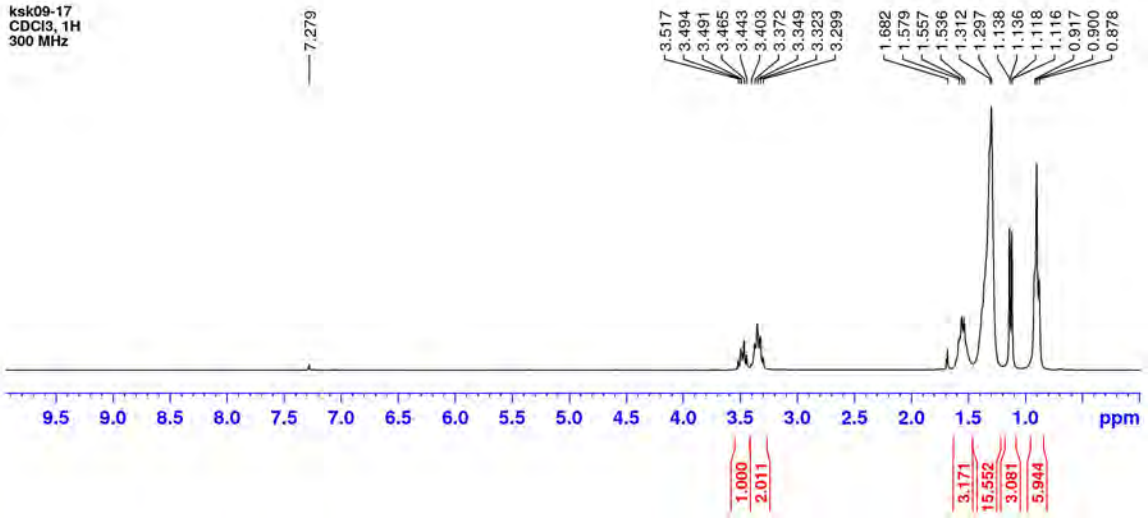
17f 

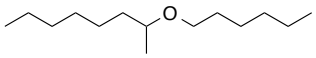

ksk08-96
CDCl3, 1H
300 MHz
7.282
3.527
3.505
3.497
3.484
3.475
3.453
3.381
3.360
3.352
3.338
3.329
3.307
1.707
1.591
1.568
1.545
1.524
1.501
1.447
1.423
1.399
1.371
1.346
1.292
1.139
1.118
0.954
0.930
0.906
0.896
0.873
9
8
7
6
5
4
3
2
1
0
ppm
1.000
2.007
3.055
11.140
3.088
6.262

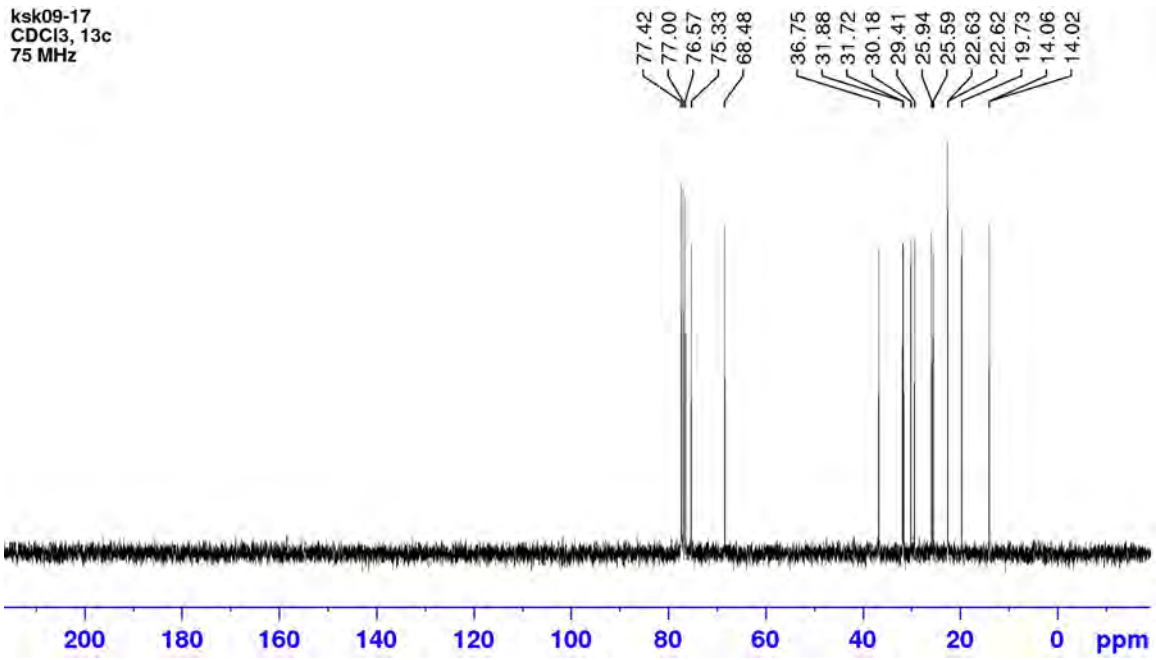


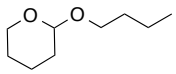

ksk08-96
CDCl3, 13c
75 MHz
77.44
77.02
76.59
75.34
68.15
36.75
32.30
31.89
29.42
25.60
22.64
19.74
19.44
14.10
13.94
200
180
160
140
120
100
80
60
40
20
0
ppm

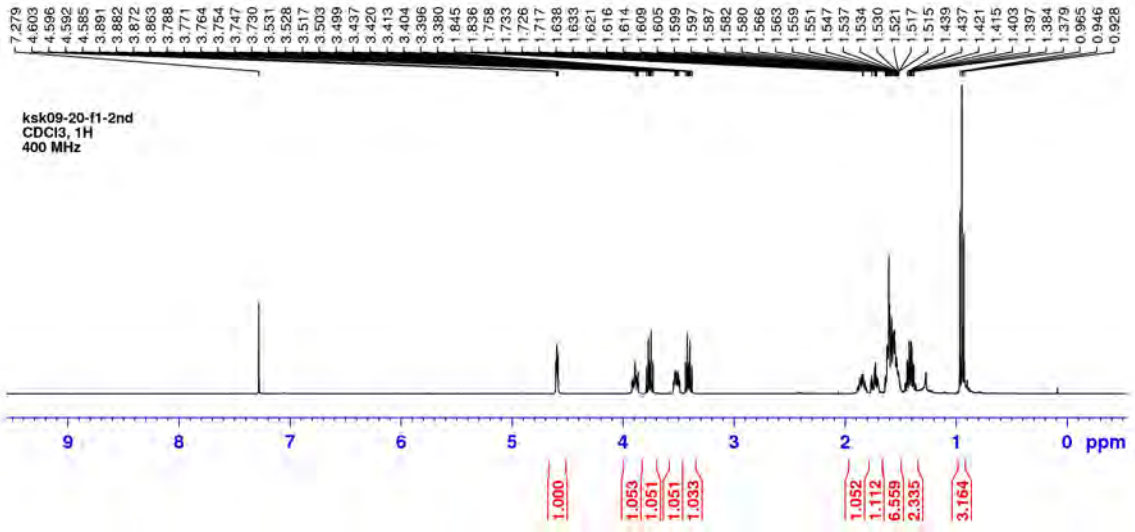
17g 

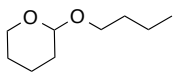

ksk09-17
CDCl3, 1H
300 MHz
7.279
3.517
3.494
3.491
3.465
3.443
3.403
3.372
3.349
3.323
3.299
1.682
1.579
1.557
1.536
1.312
1.297
1.138
1.136
1.118
1.116
0.917
0.900
0.878
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.000
2.011
3.171
15.552
3.081
5.944

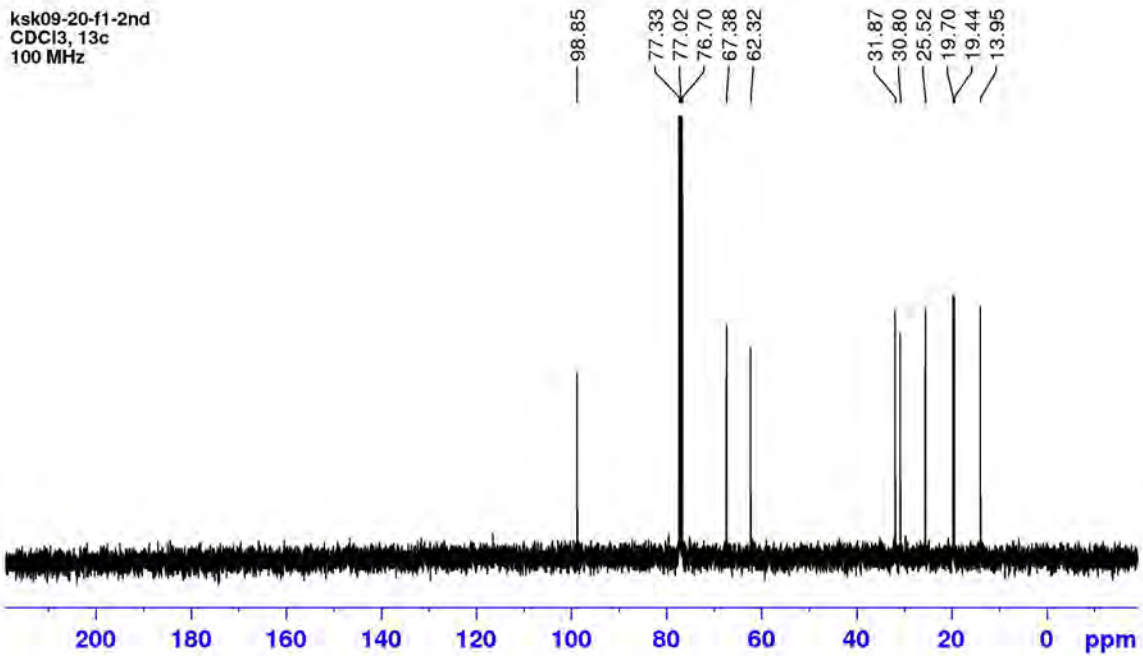


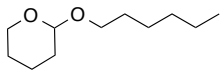

ksk09-17
CDCl3, 13c
75 MHz
77.42
77.00
76.57
75.33
68.48
36.75
31.88
31.72
30.18
29.41
25.94
25.59
22.63
22.62
19.73
14.06
14.02
200 180 160 140 120 100 80 60 40 20 0 ppm

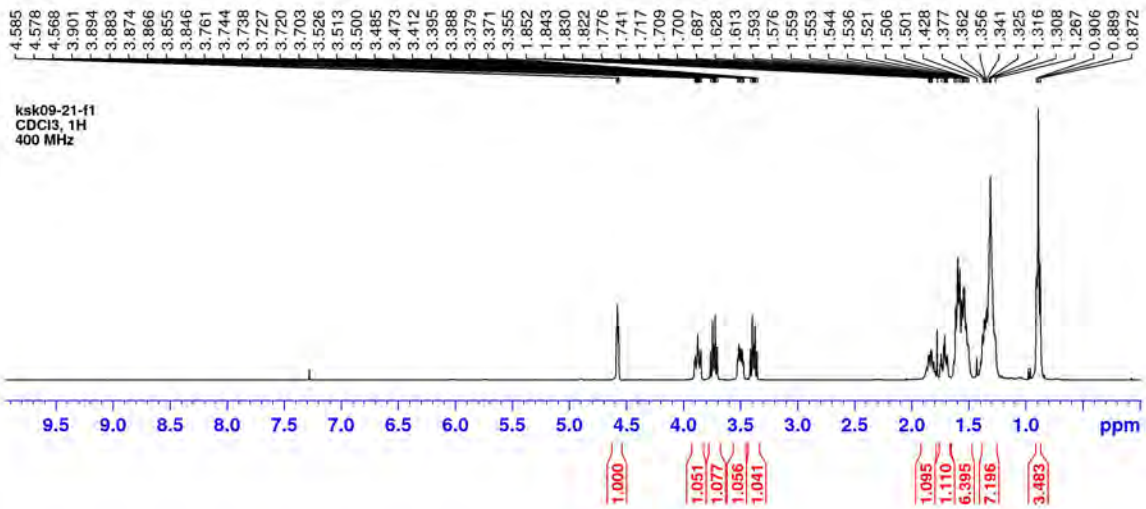
17h 

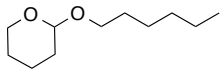

7.279
4.603
4.596
4.592
4.585
3.891
3.882
3.872
3.863
3.788
3.771
3.764
3.754
3.747
3.730
3.531
3.528
3.517
3.503
3.499
3.437
3.420
3.413
3.404
3.396
3.380
1.845
1.836
1.758
1.733
1.726
1.717
1.638
1.633
1.621
1.616
1.614
1.609
1.605
1.599
1.597
1.587
1.582
1.580
1.566
1.563
1.559
1.551
1.547
1.537
1.534
1.530
1.521
1.517
1.515
1.439
1.437
1.421
1.415
1.403
1.397
1.384
1.379
0.965
0.946
0.928
ksk09-20-f1-2nd
CDCl3, 1H
400 MHz
9
8
7
6
5
4
3
2
1
0 ppm
1.000
1.053
1.051
1.051
1.033
1.052
1.112
6.559
2.335
3.164

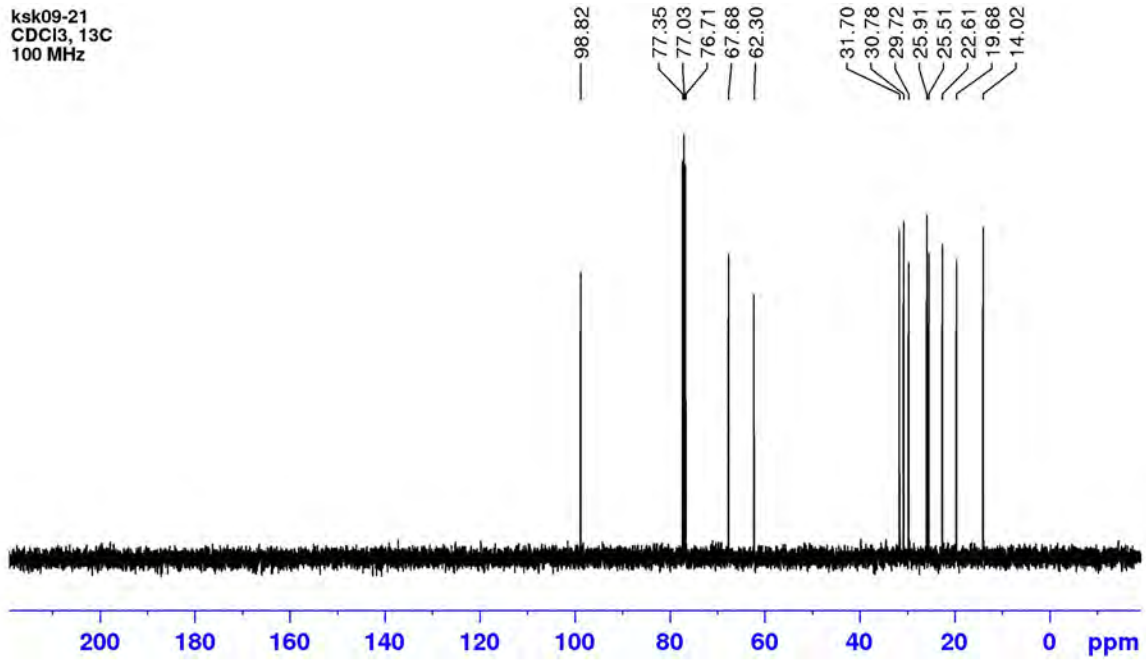



ksk09-20-f1-2nd
CDCl3, 13c
100 MHz
98.85
77.33
77.02
76.70
67.38
62.32
31.87
30.80
25.52
19.70
19.44
13.95
200
180
160
140
120
100
80
60
40
20
0 ppm

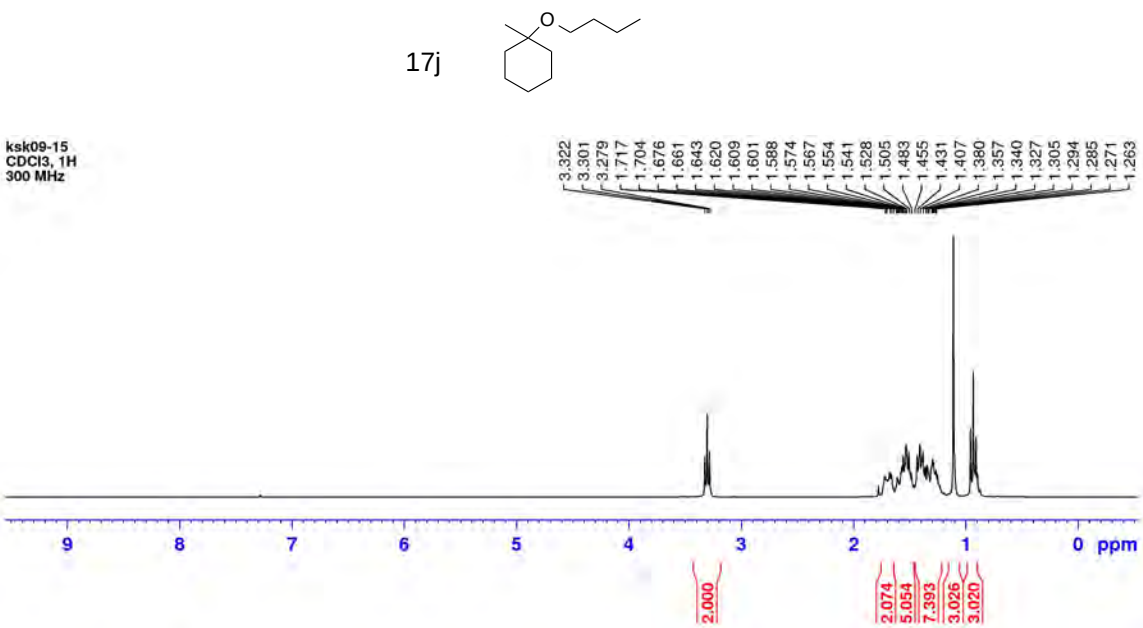
17i 

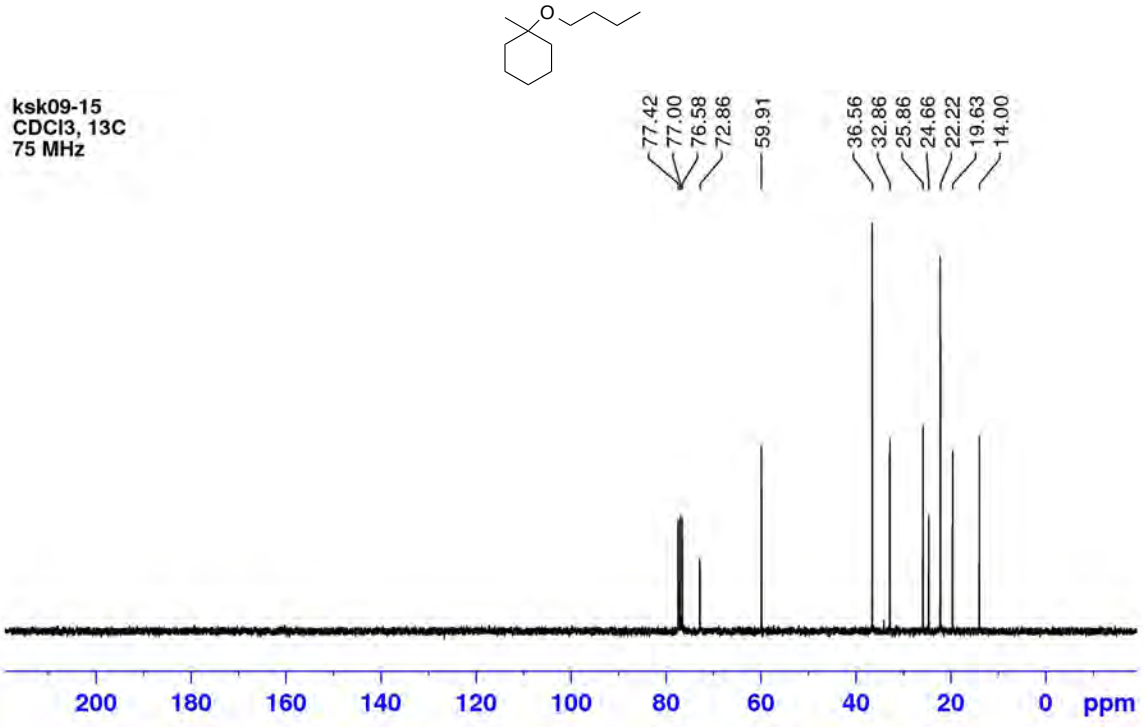

4.585
4.578
4.568
3.901
3.894
3.883
3.874
3.866
3.855
3.846
3.761
3.744
3.738
3.727
3.720
3.703
3.526
3.513
3.500
3.485
3.473
3.412
3.395
3.388
3.379
3.371
3.355
1.852
1.843
1.830
1.822
1.776
1.741
1.717
1.709
1.700
1.687
1.628
1.613
1.593
1.576
1.559
1.553
1.544
1.536
1.521
1.506
1.501
1.428
1.377
1.362
1.356
1.341
1.325
1.316
1.308
1.267
0.906
0.889
0.872
ksk09-21-f1
CDCl3, 1H
400 MHz
9.5 9.0 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 ppm
1.000
1.051
1.077
1.056
1.041
1.095
1.110
6.395
7.196
3.483



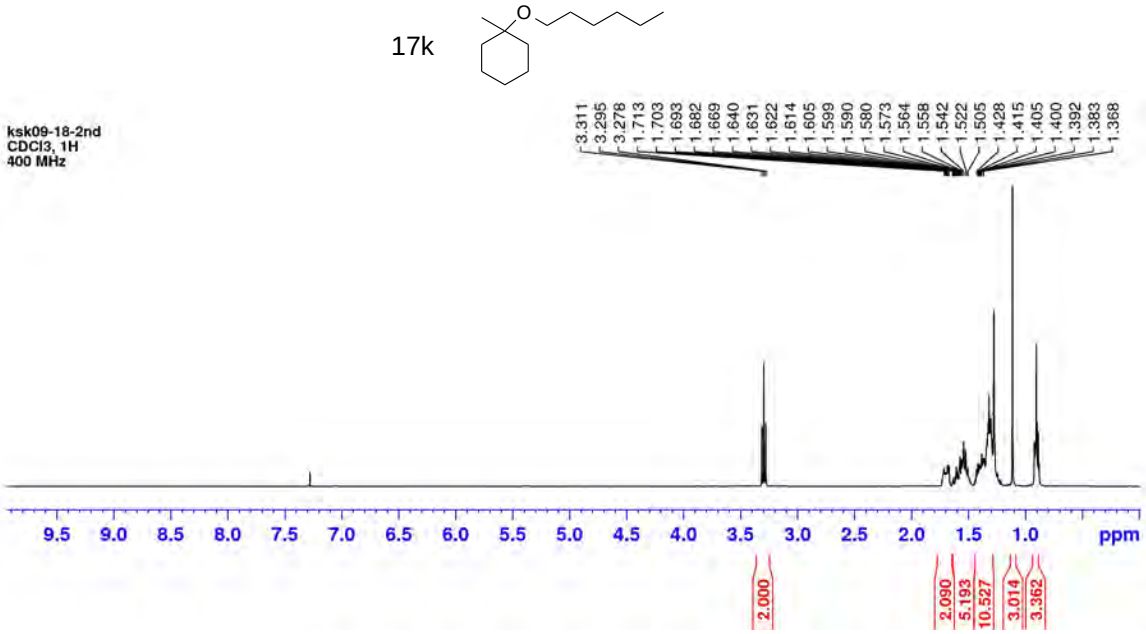

ksk09-21
CDCl3, 13C
100 MHz
98.82
77.35
77.03
76.71
67.68
62.30
31.70
30.78
29.72
25.91
25.51
22.61
19.68
14.02
200 180 160 140 120 100 80 60 40 20 0 ppm

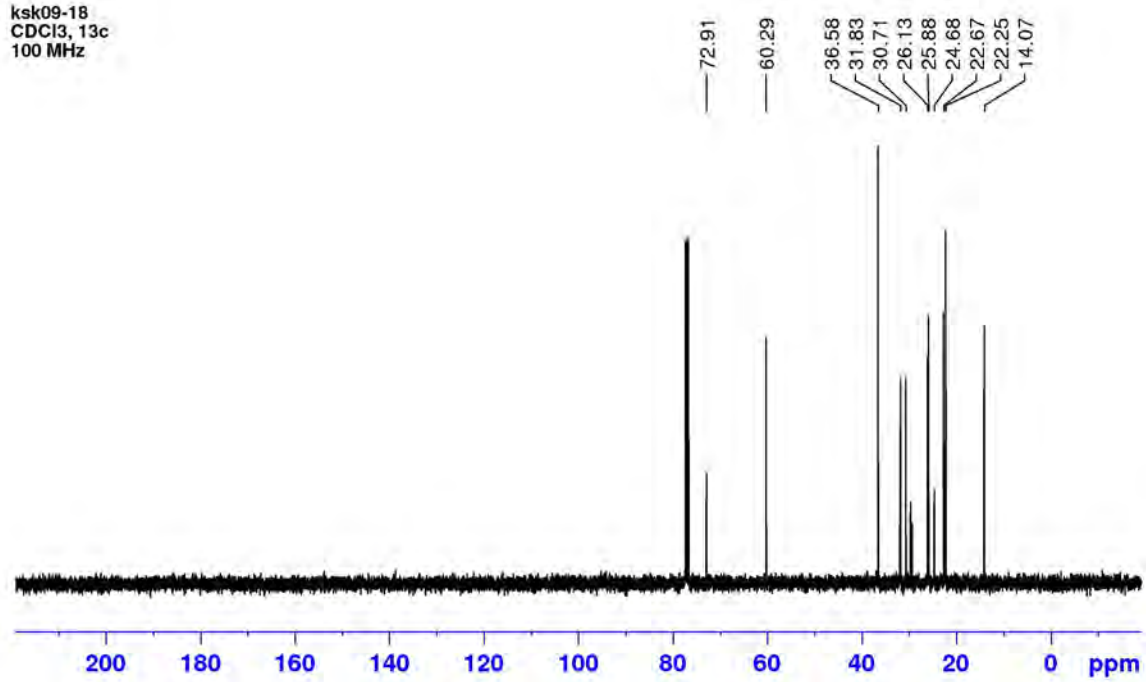
17j

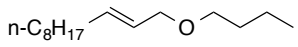

ksk09-15
CDCl3, 1H
300 MHz
3.322
3.301
3.279
1.717
1.704
1.676
1.661
1.643
1.620
1.609
1.601
1.588
1.574
1.567
1.554
1.541
1.528
1.505
1.483
1.455
1.431
1.407
1.380
1.357
1.340
1.327
1.305
1.294
1.285
1.271
1.263
9
8
7
6
5
4
3
2
1
0 ppm
2.000
2.074
5.054
7.393
3.026
3.020

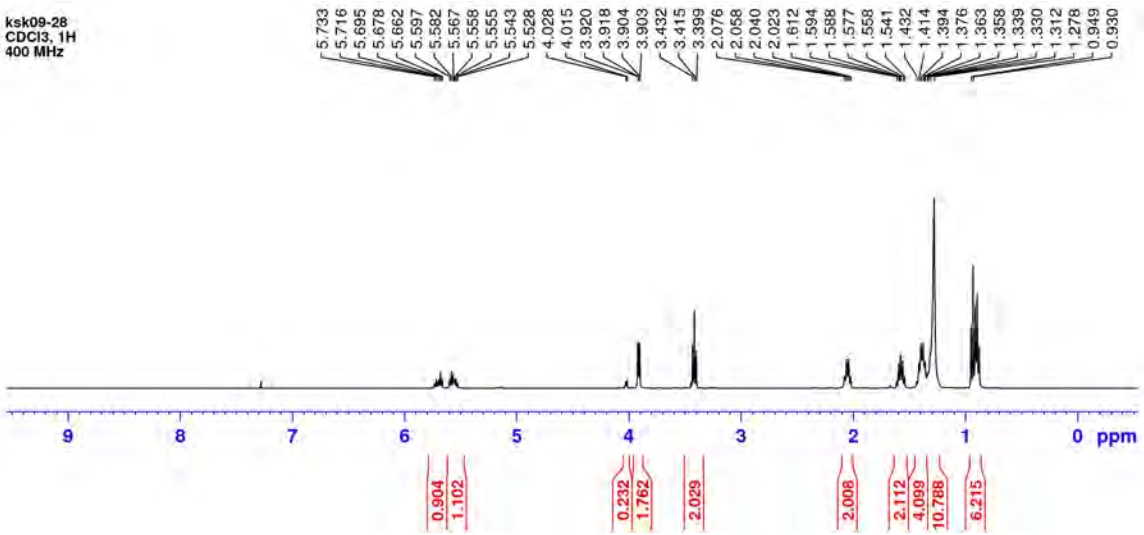

ksk09-15
CDCl3, 13C
75 MHz
77.42
77.00
76.58
72.86
59.91
36.56
32.86
25.86
24.66
22.22
19.63
14.00
200
180
160
140
120
100
80
60
40
20
0 ppm

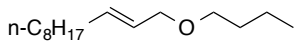
17k

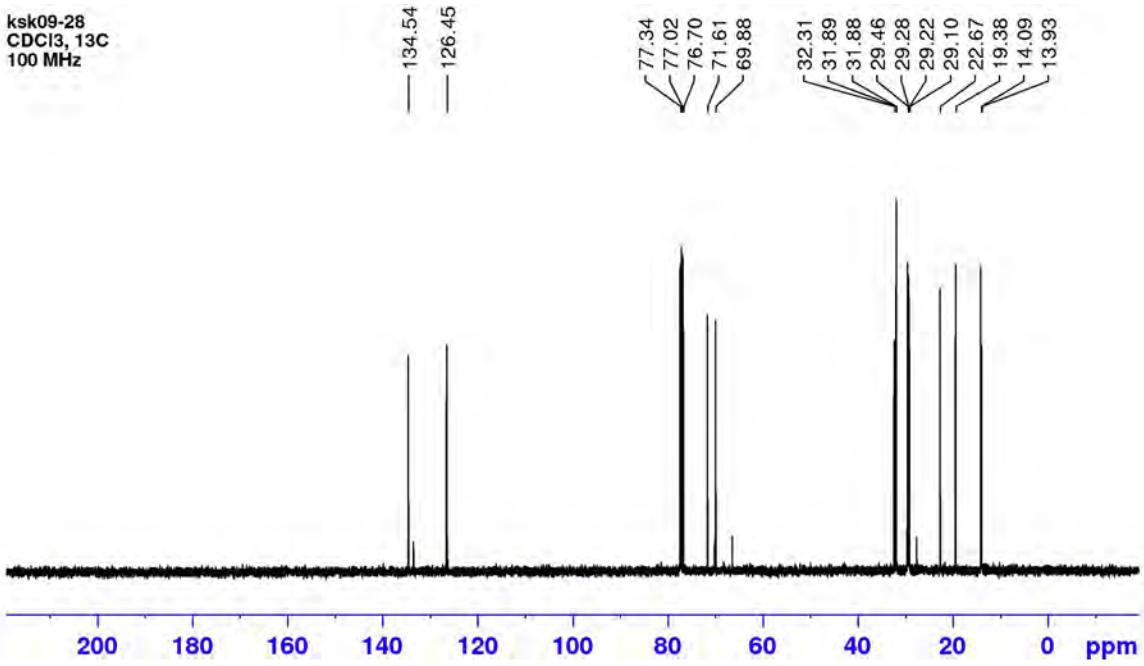

ksk09-18-2nd
CDCl3, 1H
400 MHz
3.311
3.295
3.278
1.713
1.703
1.693
1.682
1.669
1.640
1.631
1.622
1.614
1.605
1.599
1.590
1.580
1.573
1.564
1.558
1.542
1.522
1.505
1.428
1.415
1.405
1.400
1.392
1.383
1.368
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
2.000
2.090
5.193
10.527
3.014
3.362

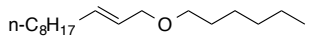

ksk09-18
CDCl3, 13c
100 MHz
72.91
60.29
36.58
31.83
30.71
26.13
25.88
24.68
22.67
22.25
14.07
200 180 160 140 120 100 80 60 40 20 0 ppm

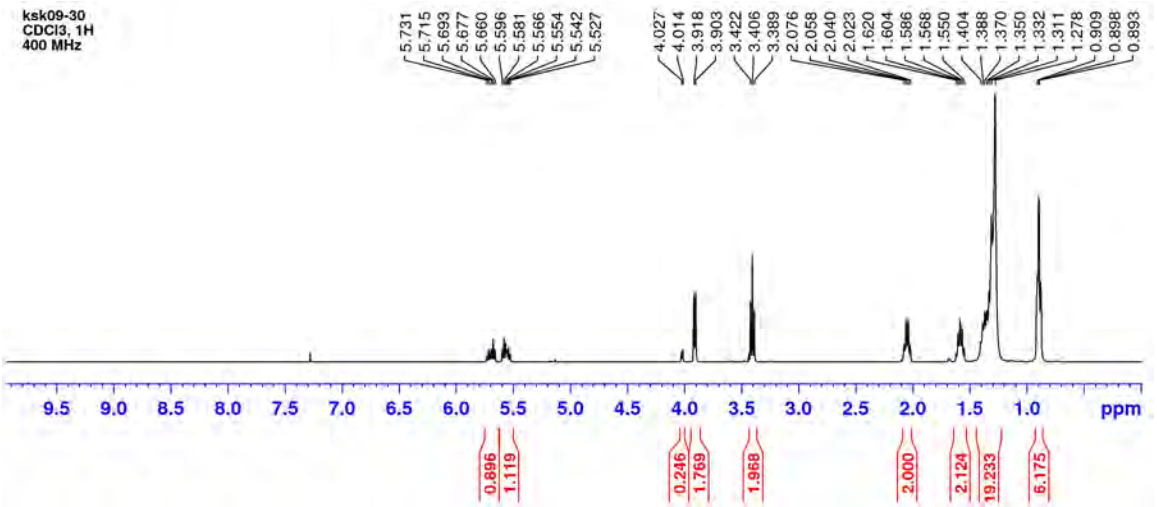
17l 

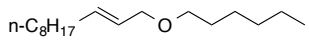

ksk09-28
CDCl3, 1H
400 MHz
5.733
5.716
5.695
5.678
5.662
5.597
5.582
5.567
5.558
5.555
5.543
5.528
4.028
4.015
3.920
3.918
3.904
3.903
3.432
3.415
3.399
2.076
2.058
2.040
2.023
1.612
1.594
1.588
1.577
1.558
1.541
1.432
1.414
1.394
1.376
1.363
1.358
1.339
1.330
1.312
1.278
0.949
0.930
9
8
7
6
5
4
3
2
1
0 ppm
0.904
1.102
0.232
1.762
2.029
2.008
2.112
4.099
10.788
6.215

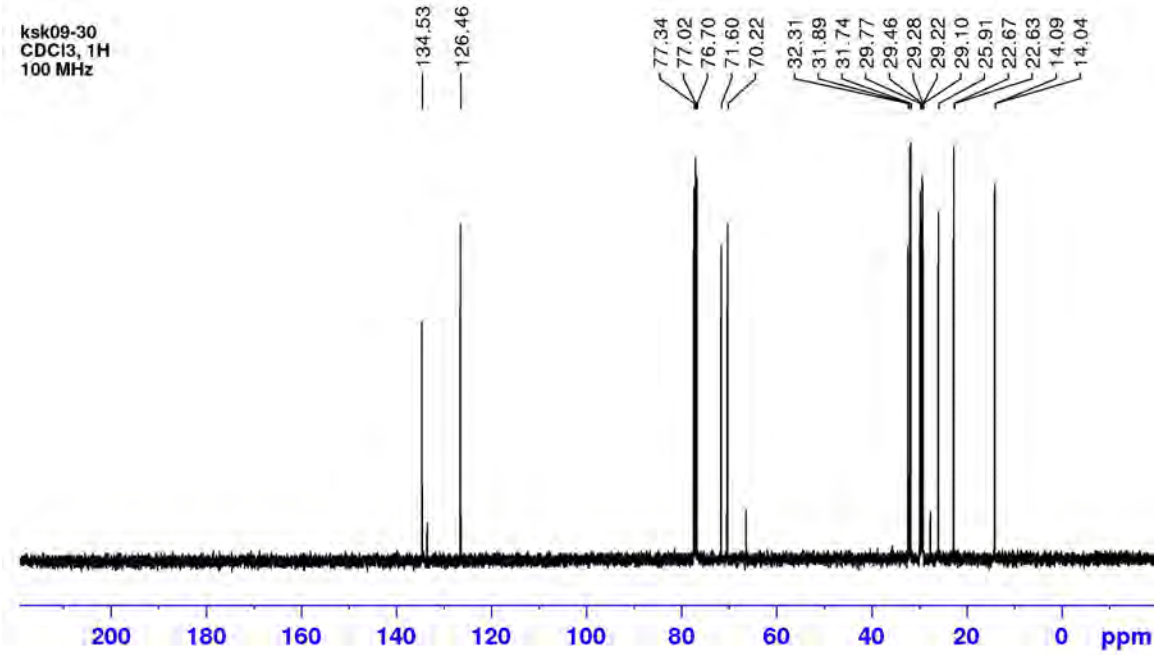



ksk09-28
CDCl3, 13C
100 MHz
134.54
126.45
77.34
77.02
76.70
71.61
69.88
32.31
31.89
31.88
29.46
29.28
29.22
29.10
22.67
19.38
14.09
13.93
200
180
160
140
120
100
80
60
40
20
0 ppm

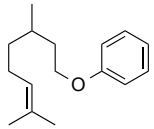
17m 
n-C8H17
O

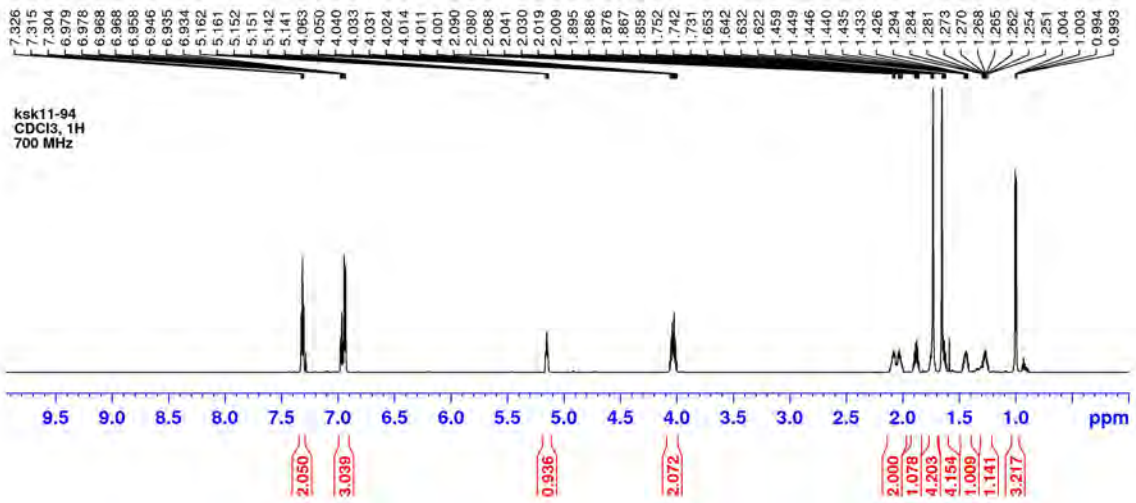

ksk09-30
CDCl3, 1H
400 MHz
5.731
5.715
5.693
5.677
5.660
5.596
5.581
5.566
5.554
5.542
5.527
4.027
4.014
3.918
3.903
3.422
3.406
3.389
2.076
2.058
2.040
2.023
1.620
1.604
1.586
1.568
1.550
1.404
1.388
1.370
1.350
1.332
1.311
1.278
0.909
0.898
0.893
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
0.896
1.119
0.246
1.769
1.968
2.000
2.124
19.233
6.175

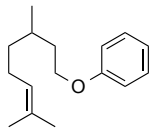

n-C8H17
O

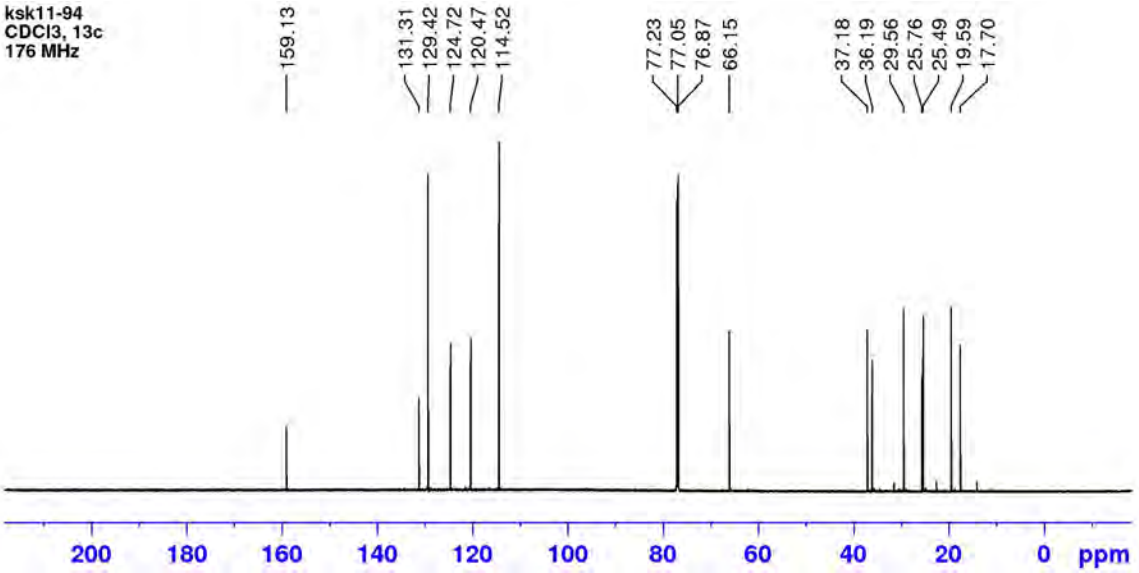

ksk09-30
CDCl3, 1H
100 MHz
134.53
126.46
77.34
77.02
76.70
71.60
70.22
32.31
31.89
31.74
29.77
29.46
29.28
29.22
29.10
25.91
22.67
22.63
14.09
14.04
200 180 160 140 120 100 80 60 40 20 0 ppm

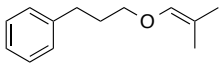
18a

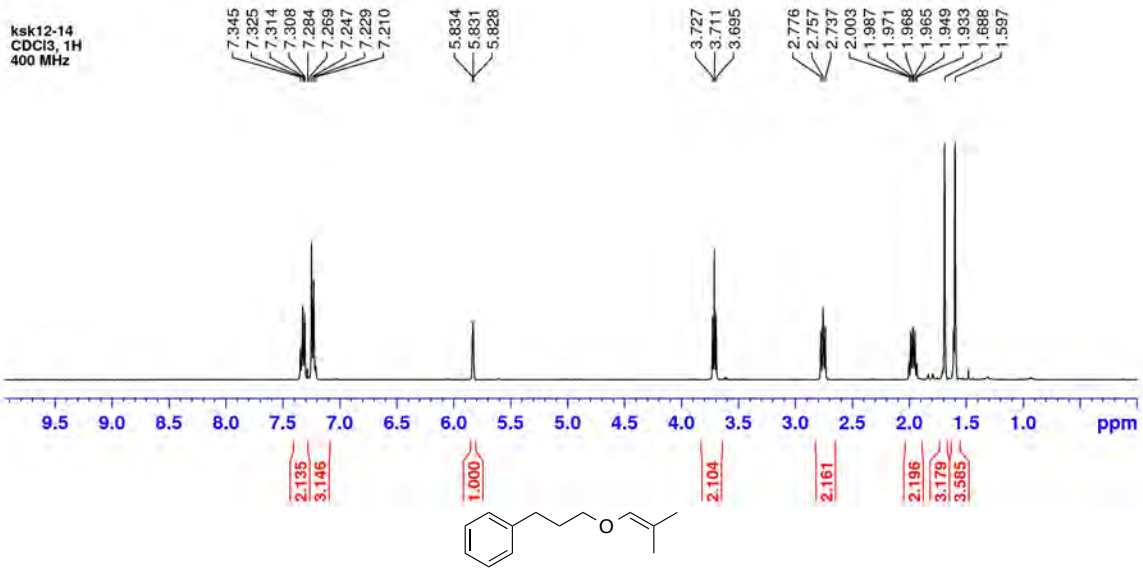


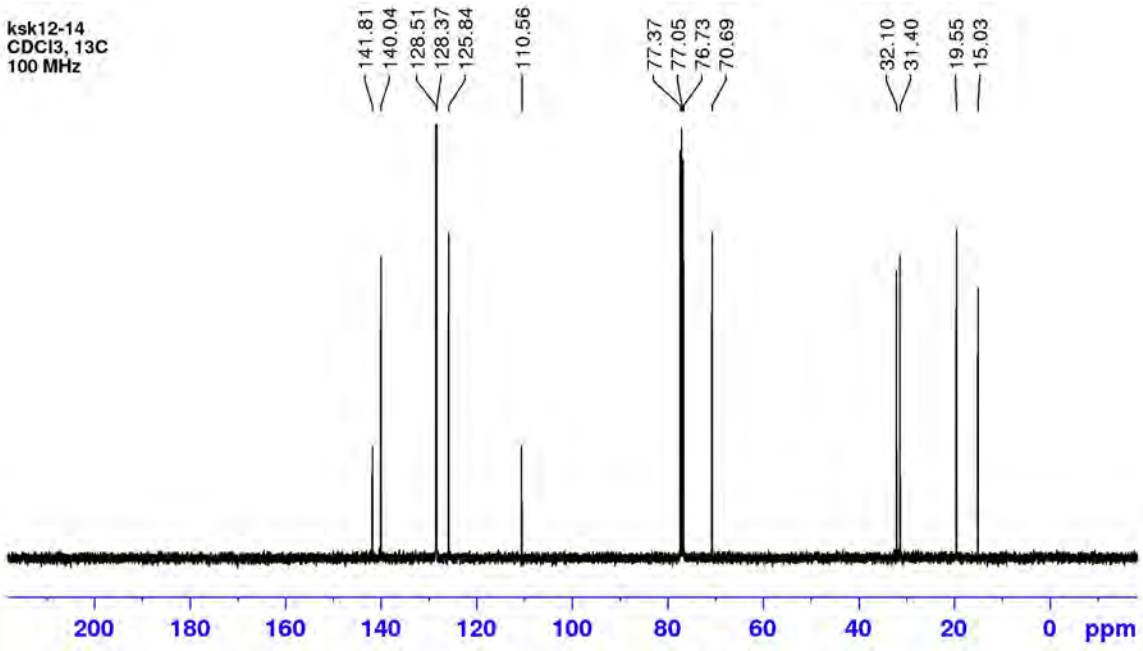




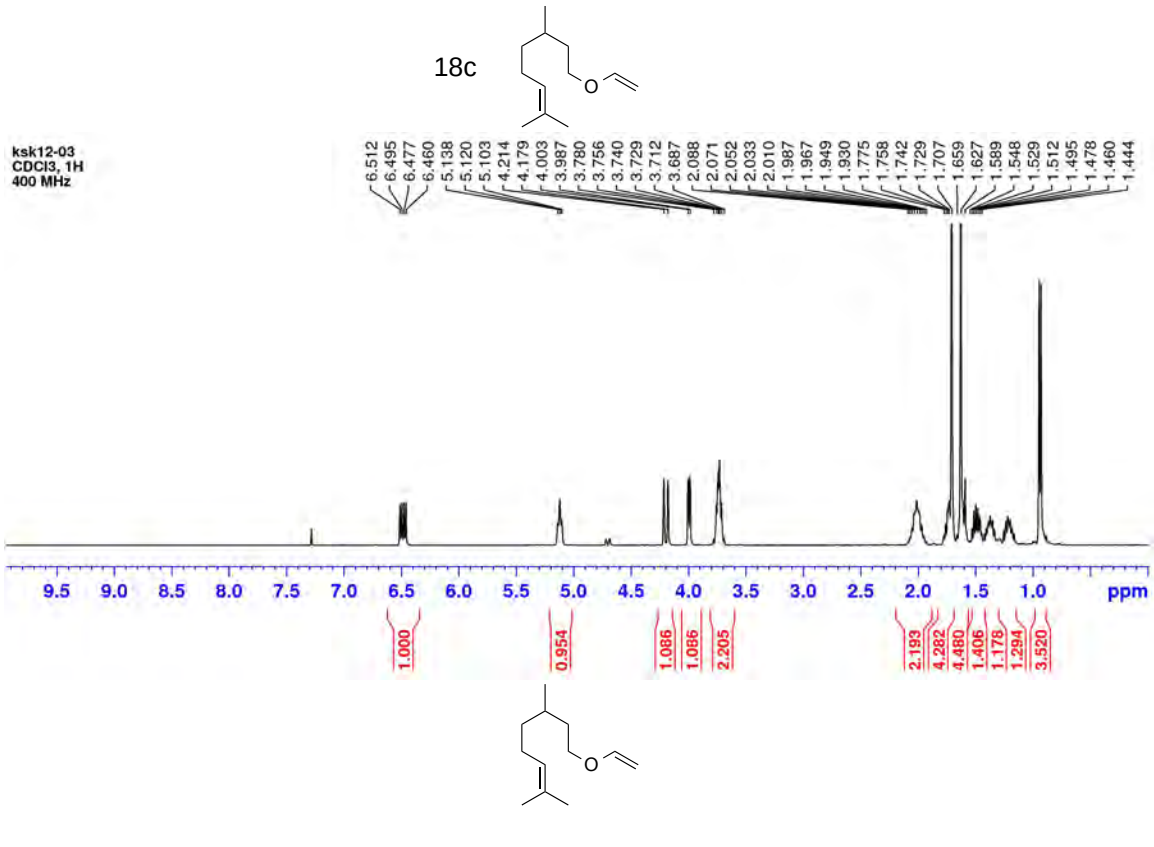


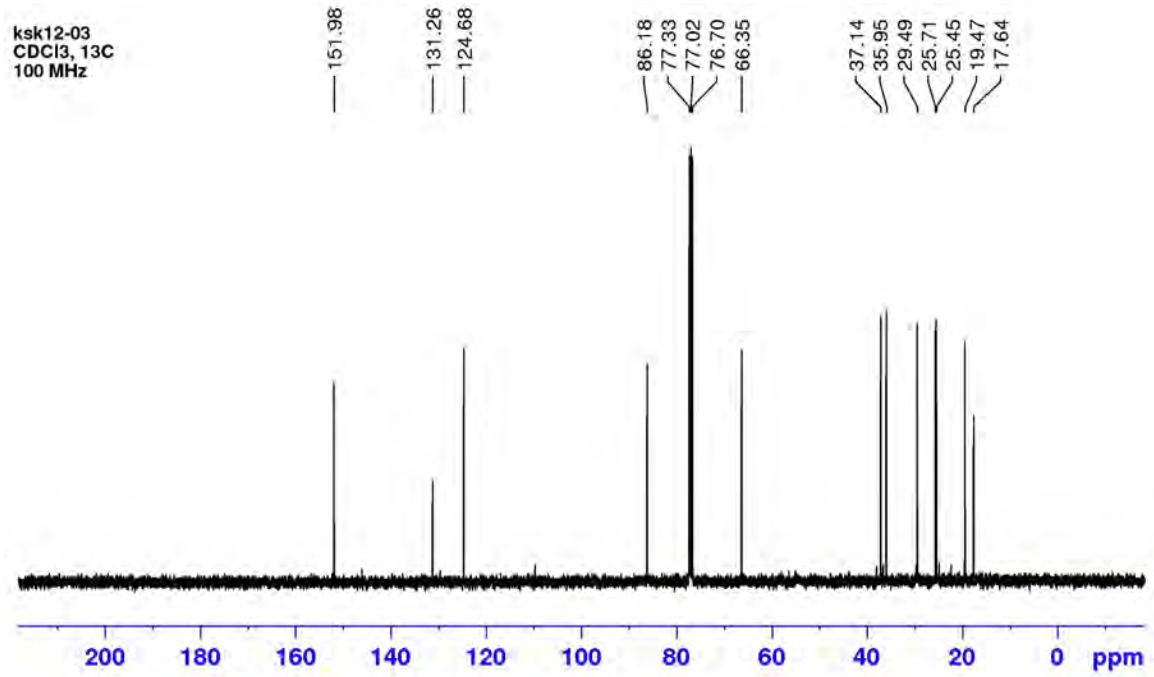
18b 


ksk12-14
CDCl3, 1H
400 MHz
7.345
7.325
7.314
7.308
7.284
7.269
7.247
7.229
7.210
5.834
5.831
5.828
3.727
3.711
3.695
2.776
2.757
2.737
2.003
1.987
1.971
1.968
1.965
1.949
1.933
1.688
1.597
9.5 9.0 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 ppm
2.135
3.146
1.000
2.104
2.161
2.196
3.179
3.585

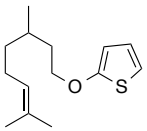

ksk12-14
CDCl3, 13C
100 MHz
141.81
140.04
128.51
128.37
125.84
110.56
77.37
77.05
76.73
70.69
32.10
31.40
19.55
15.03
200 180 160 140 120 100 80 60 40 20 0 ppm

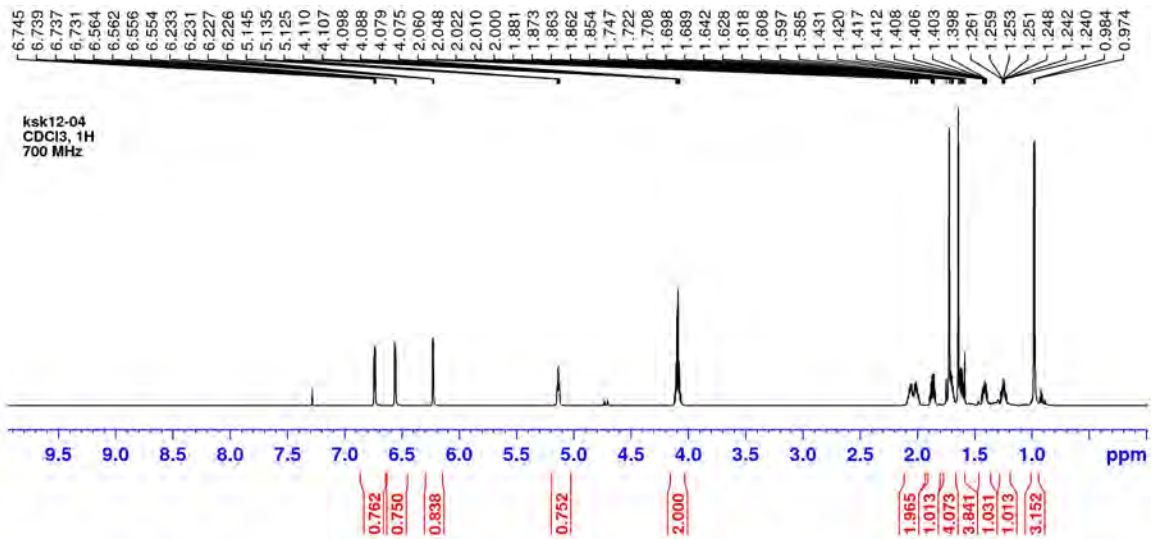
18c

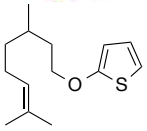

ksk12-03
CDCl3, 1H
400 MHz
6.512
6.495
6.477
6.460
5.138
5.120
5.103
4.214
4.179
4.003
3.987
3.780
3.756
3.740
3.729
3.712
3.687
2.088
2.071
2.052
2.033
2.010
1.987
1.967
1.949
1.930
1.775
1.758
1.742
1.729
1.707
1.659
1.627
1.589
1.548
1.529
1.512
1.495
1.478
1.460
1.444
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.000
0.954
1.086
1.086
2.205
2.193
4.282
4.480
1.406
1.178
1.294
3.520

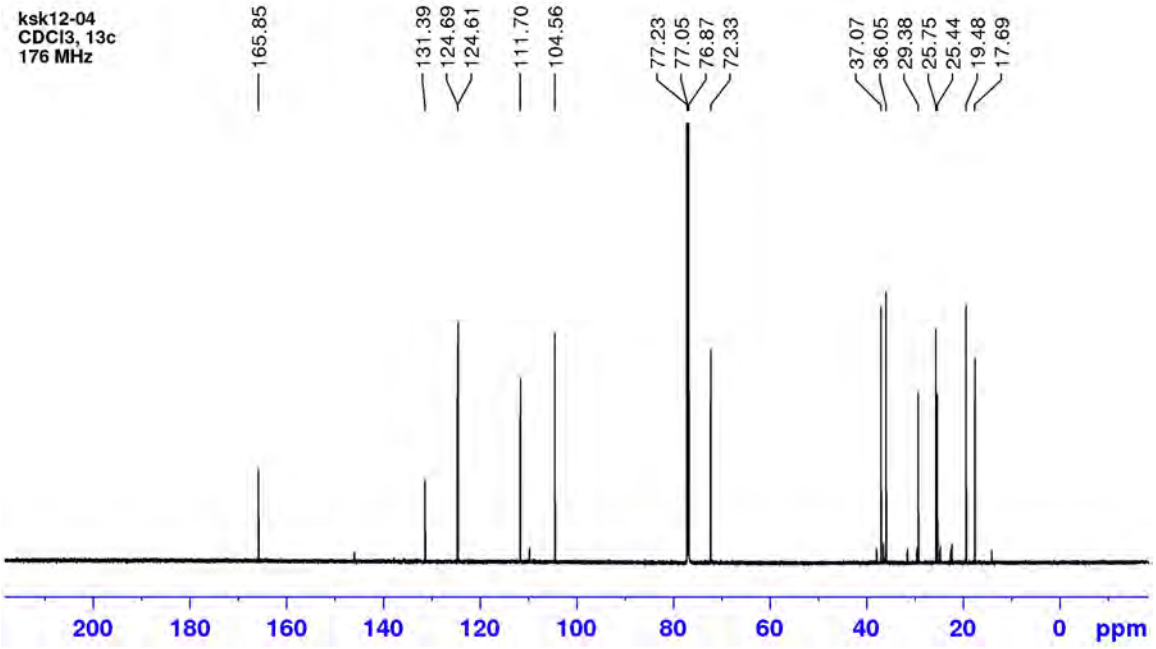

ksk12-03
CDCl3, 13C
100 MHz
151.98
131.26
124.68
86.18
77.33
77.02
76.70
66.35
37.14
35.95
29.49
25.71
25.45
19.47
17.64
200 180 160 140 120 100 80 60 40 20 0 ppm

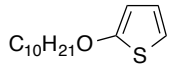
18d

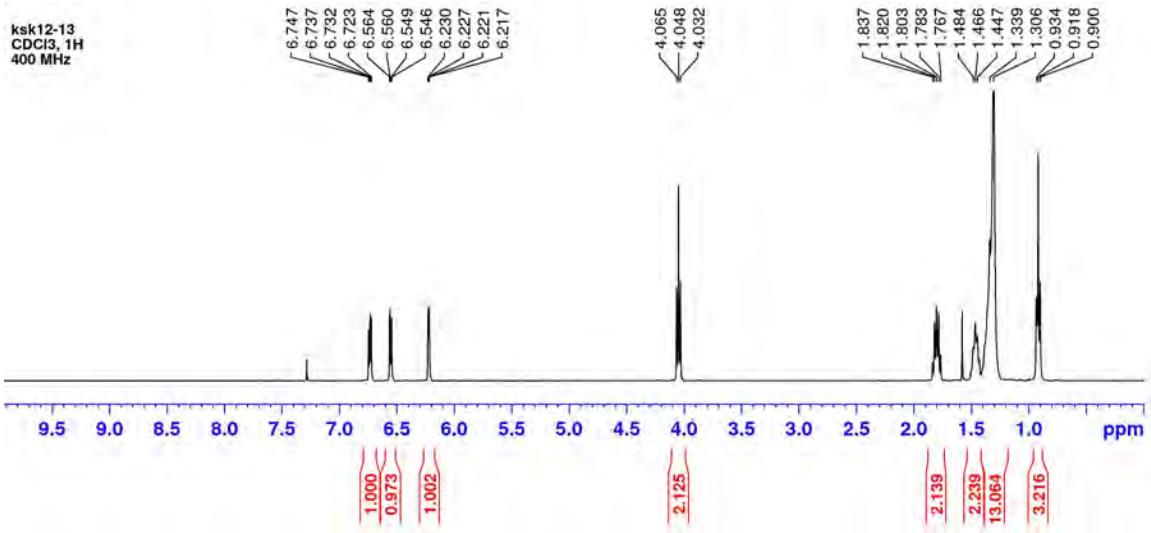

O
S

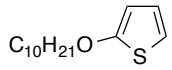

6.745
6.739
6.737
6.731
6.564
6.562
6.556
6.554
6.233
6.231
6.227
6.226
5.145
5.135
5.125
4.110
4.107
4.098
4.088
4.079
4.075
2.060
2.048
2.022
2.010
2.000
1.881
1.873
1.863
1.862
1.854
1.747
1.722
1.708
1.698
1.689
1.642
1.628
1.618
1.608
1.597
1.585
1.431
1.420
1.417
1.412
1.408
1.406
1.403
1.398
1.261
1.259
1.253
1.251
1.248
1.242
1.240
0.984
0.974
ksk12-04
CDCl3, 1H
700 MHz
9.5
9.0
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
ppm
0.762
0.750
0.838
0.752
2.000
1.965
1.013
4.073
3.841
1.031
1.013
3.152

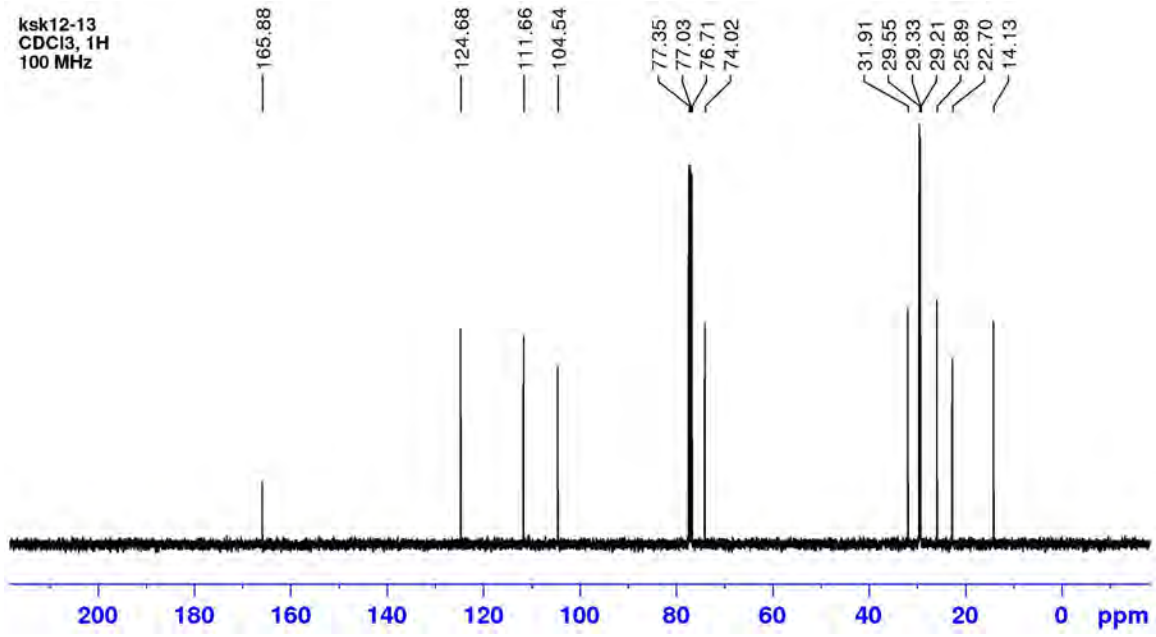

O
S


ksk12-04
CDCl3, 13c
176 MHz
165.85
131.39
124.69
124.61
111.70
104.56
77.23
77.05
76.87
72.33
37.07
36.05
29.38
25.75
25.44
19.48
17.69
200
180
160
140
120
100
80
60
40
20
0
ppm

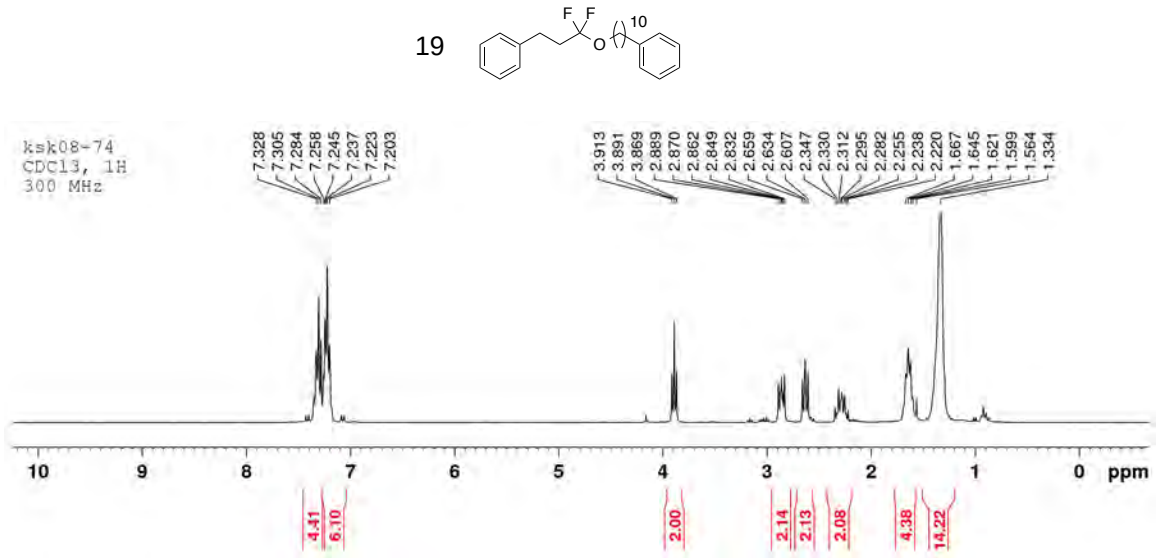
18e 
$C_{10}H_{21}O$
S

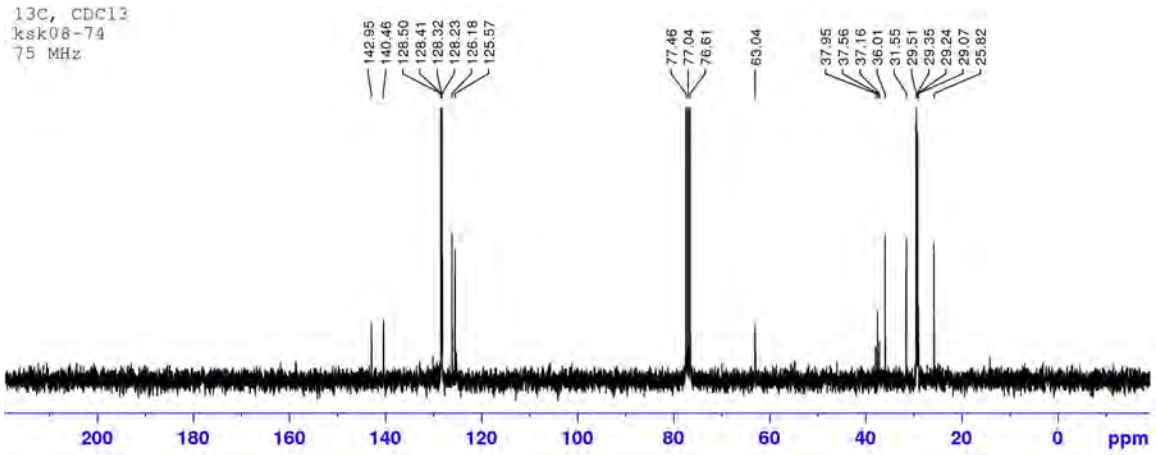

ksk12-13
CDCl3, 1H
400 MHz
6.747
6.737
6.732
6.723
6.564
6.560
6.549
6.546
6.230
6.227
6.221
6.217
4.065
4.048
4.032
1.837
1.820
1.803
1.783
1.767
1.484
1.466
1.447
1.339
1.306
0.934
0.918
0.900
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.000
0.973
1.002
2.125
2.139
2.239
13.064
3.216

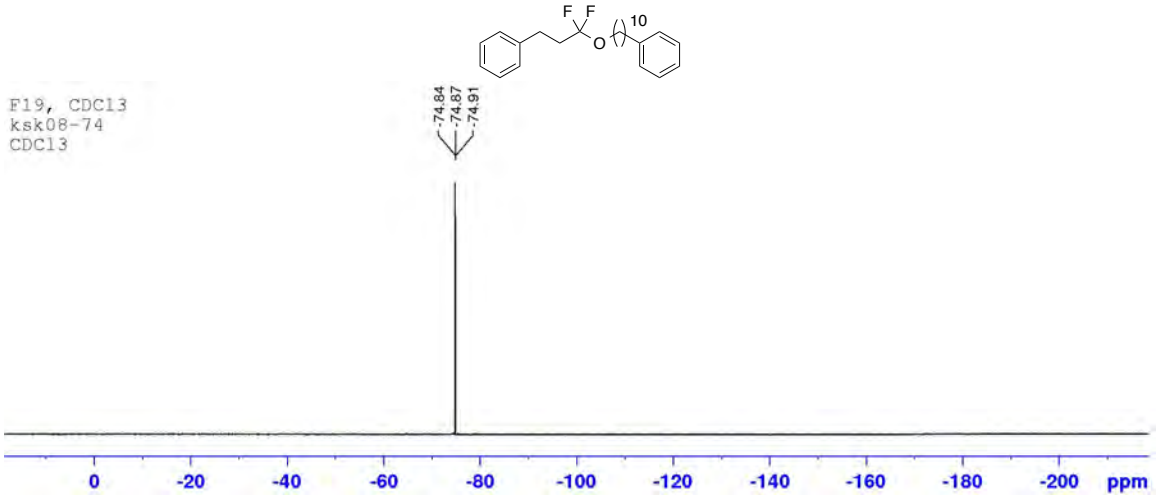

$C_{10}H_{21}O$
S


ksk12-13
CDCl3, 1H
100 MHz
165.88
124.68
111.66
104.54
77.35
77.03
76.71
74.02
31.91
29.55
29.33
29.21
25.89
22.70
14.13
200 180 160 140 120 100 80 60 40 20 0 ppm

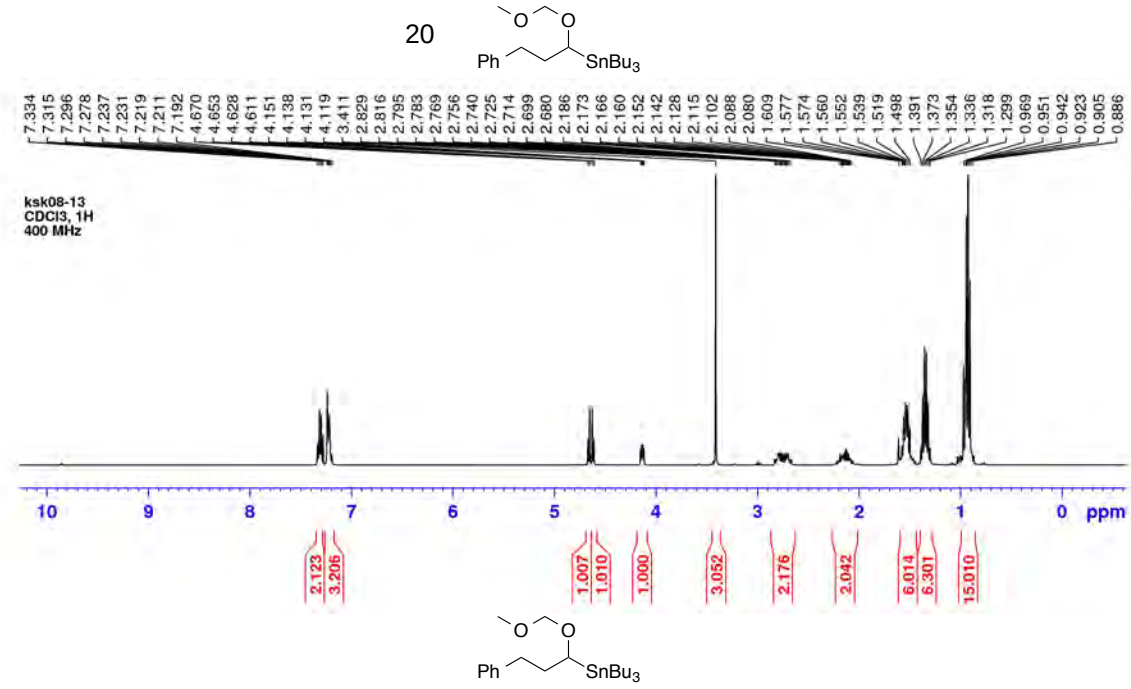
19

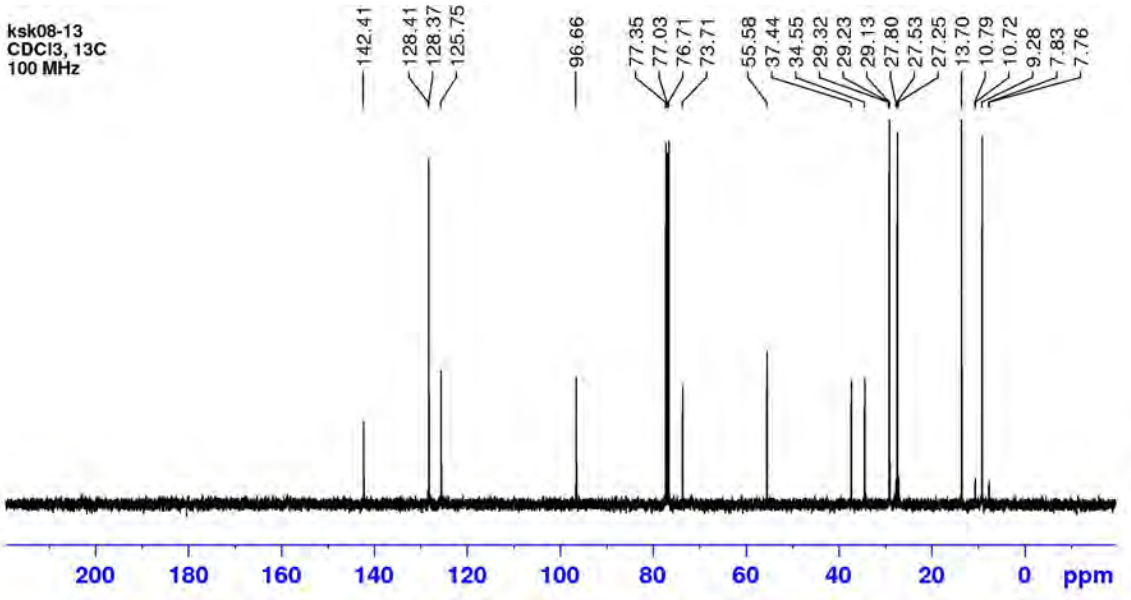

ksk08-74
CDCl3, 1H
300 MHz
7.328
7.305
7.284
7.258
7.245
7.237
7.223
7.203
3.913
3.891
3.869
2.889
2.870
2.862
2.849
2.832
2.659
2.634
2.607
2.347
2.330
2.312
2.295
2.282
2.255
2.238
2.220
1.667
1.645
1.621
1.599
1.564
1.334
10 9 8 7 6 5 4 3 2 1 0 ppm
4.41
6.10
2.00
2.14
2.13
2.08
4.38
14.22


13C, CDCl3
ksk08-74
75 MHz
142.95
140.46
128.50
128.41
128.32
128.23
126.18
125.57
77.46
77.04
76.61
63.04
37.95
37.56
37.16
36.01
31.55
29.51
29.35
29.24
29.07
25.82
200 180 160 140 120 100 80 60 40 20 0 ppm

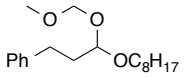

F19, CDCl3
ksk08-74
CDCl3
-74.84
-74.87
-74.91
0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 ppm

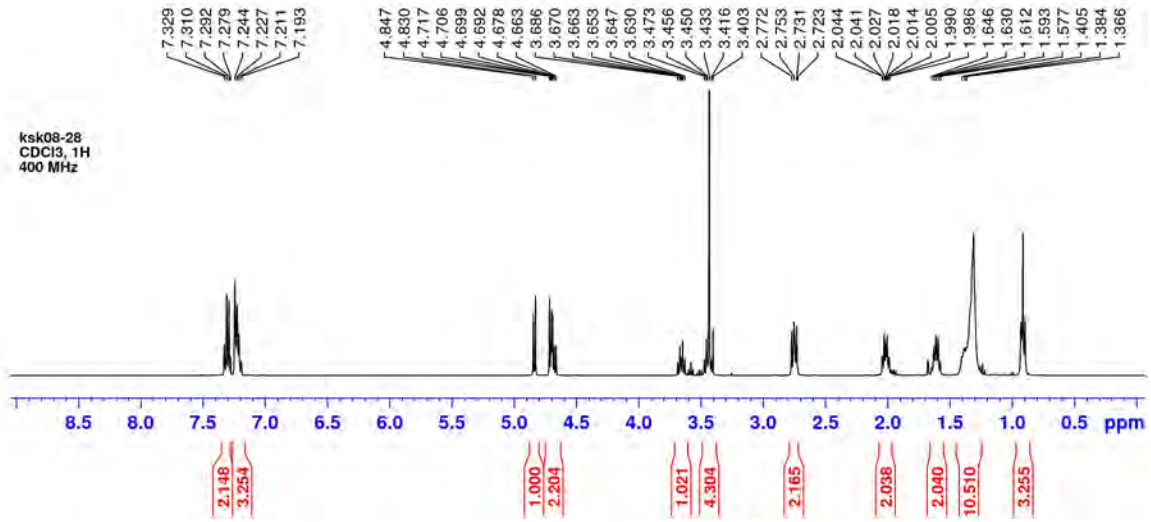
20

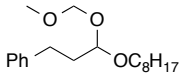

ksk08-13
CDCl3, 1H
400 MHz
7.334
7.315
7.296
7.278
7.237
7.231
7.219
7.211
7.192
4.670
4.653
4.628
4.611
4.151
4.138
4.131
4.119
3.411
2.829
2.816
2.795
2.783
2.769
2.756
2.740
2.725
2.714
2.699
2.680
2.186
2.173
2.166
2.160
2.152
2.142
2.128
2.115
2.102
2.088
2.080
1.609
1.577
1.574
1.560
1.552
1.539
1.519
1.498
1.391
1.373
1.354
1.336
1.318
1.299
0.969
0.951
0.942
0.923
0.905
0.886
10
9
8
7
6
5
4
3
2
1
0
ppm
2.123
3.206
1.007
1.010
1.000
3.052
2.176
2.042
6.014
6.301
15.010

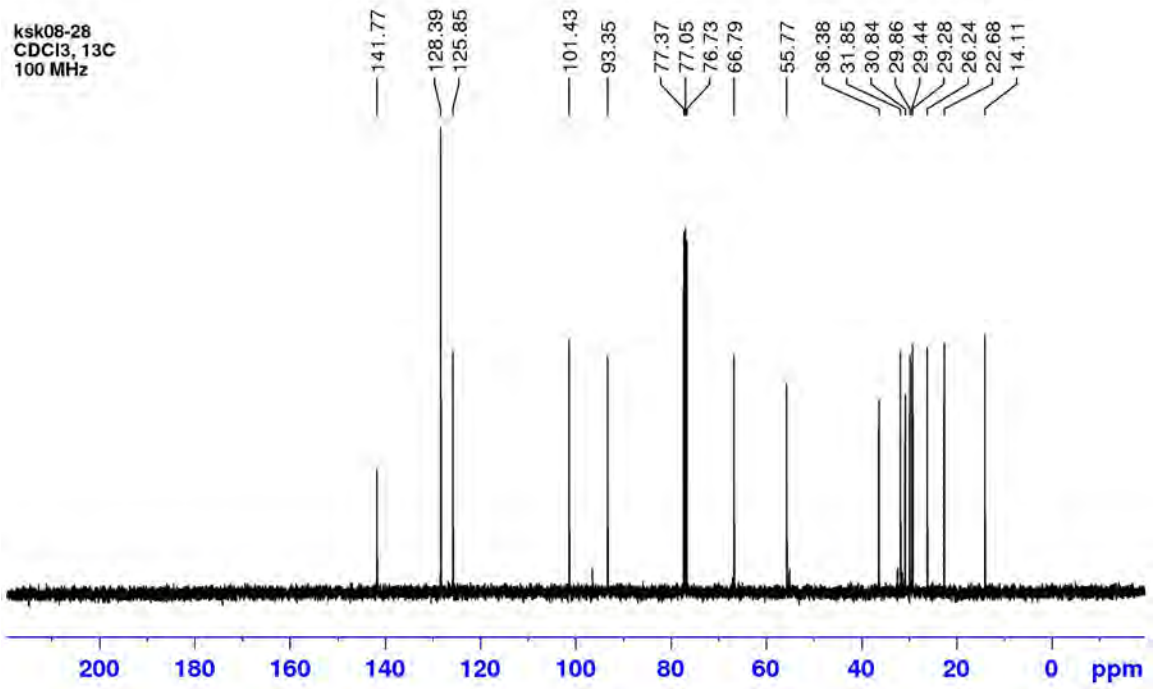

ksk08-13
CDCl3, 13C
100 MHz
142.41
128.41
128.37
125.75
96.66
77.35
77.03
76.71
73.71
55.58
37.44
34.55
29.32
29.23
29.13
27.80
27.53
27.25
13.70
10.79
10.72
9.28
7.83
7.76
200
180
160
140
120
100
80
60
40
20
0
ppm

21a

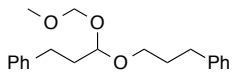

O
O
Ph
OC8H17

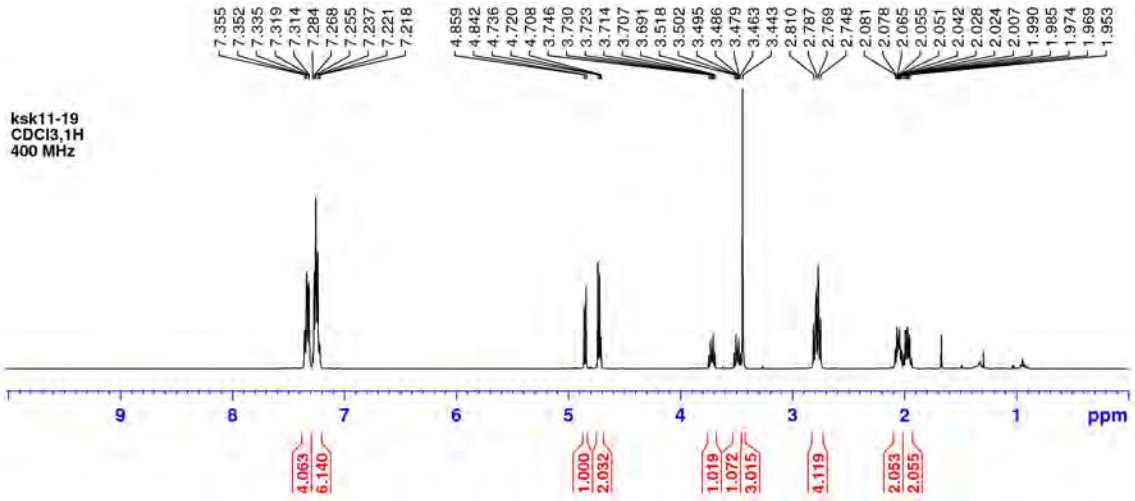

ksk08-28
CDCl3, 1H
400 MHz
7.329
7.310
7.292
7.279
7.244
7.227
7.211
7.193
4.847
4.830
4.717
4.706
4.699
4.692
4.678
4.663
3.686
3.670
3.663
3.653
3.647
3.630
3.473
3.456
3.450
3.433
3.416
3.403
2.772
2.753
2.731
2.723
2.044
2.041
2.027
2.018
2.014
2.005
1.990
1.986
1.646
1.630
1.612
1.593
1.577
1.405
1.384
1.366
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
ppm
2.148
3.254
1.000
2.204
1.021
4.304
2.165
2.038
2.040
10.510
3.255

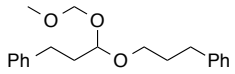

O
O
Ph
OC8H17

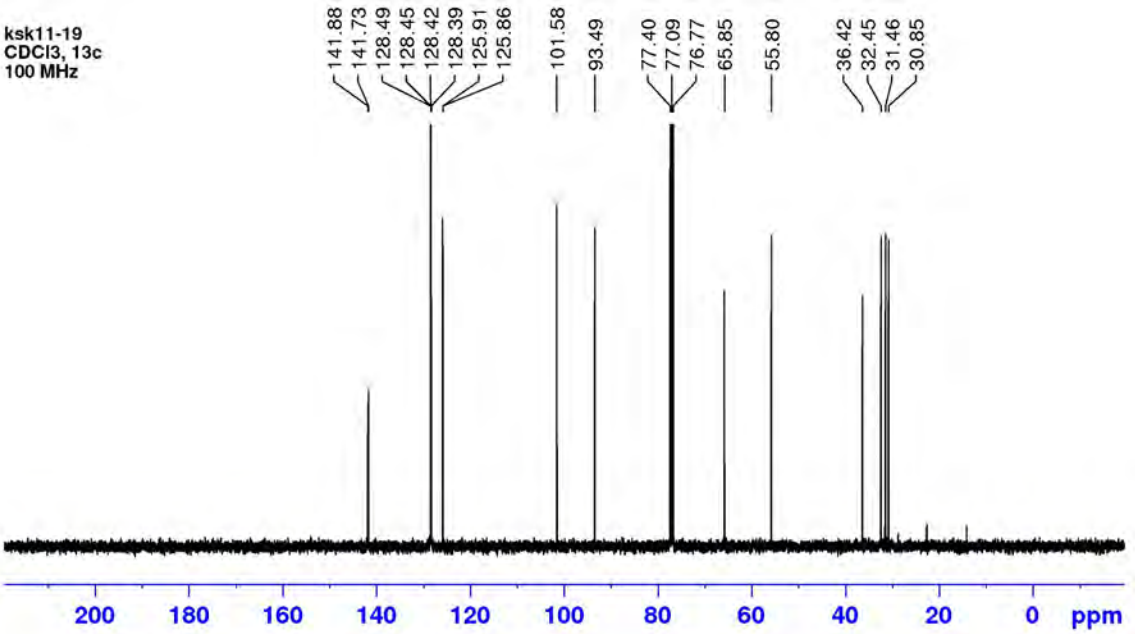

ksk08-28
CDCl3, 13C
100 MHz
141.77
128.39
125.85
101.43
93.35
77.37
77.05
76.73
66.79
55.77
36.38
31.85
30.84
29.86
29.44
29.28
26.24
22.68
14.11
200
180
160
140
120
100
80
60
40
20
0
ppm

21b

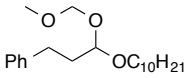

O
O
Ph
O
Ph

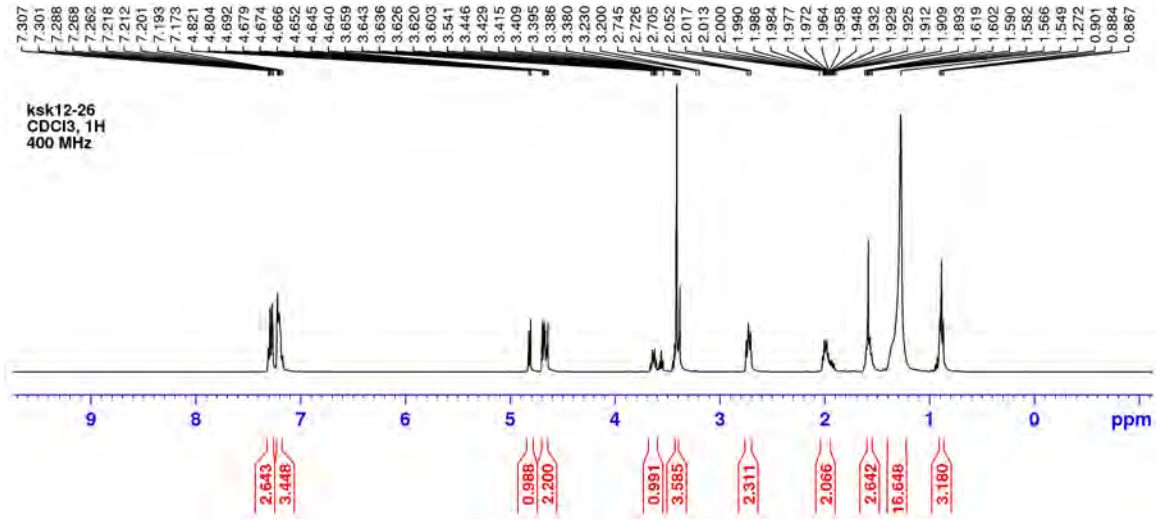

7.355
7.352
7.335
7.319
7.314
7.284
7.268
7.255
7.237
7.221
7.218
4.859
4.842
4.736
4.720
4.708
3.746
3.730
3.723
3.714
3.707
3.691
3.518
3.502
3.495
3.486
3.479
3.463
3.443
2.810
2.787
2.769
2.748
2.081
2.078
2.065
2.055
2.051
2.042
2.028
2.024
2.007
1.990
1.985
1.974
1.969
1.953
ksk11-19
CDCl3,1H
400 MHz
9
8
7
6
5
4
3
2
1
ppm
4.063
6.140
1.000
2.032
1.019
1.072
3.015
4.119
2.053
2.055

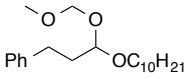

O
O
Ph
O
Ph

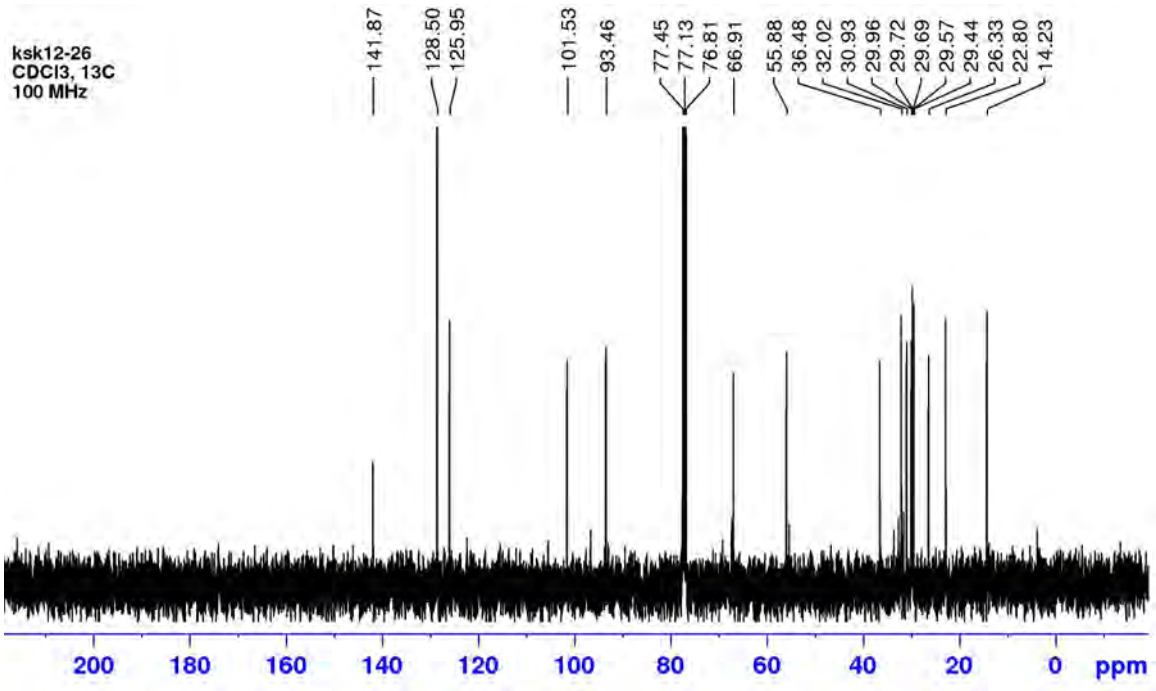

141.88
141.73
128.49
128.45
128.42
128.39
125.91
125.86
101.58
93.49
77.40
77.09
76.77
65.85
55.80
36.42
32.45
31.46
30.85
ksk11-19
CDCl3, 13c
100 MHz
200
180
160
140
120
100
80
60
40
20
0
ppm

21c

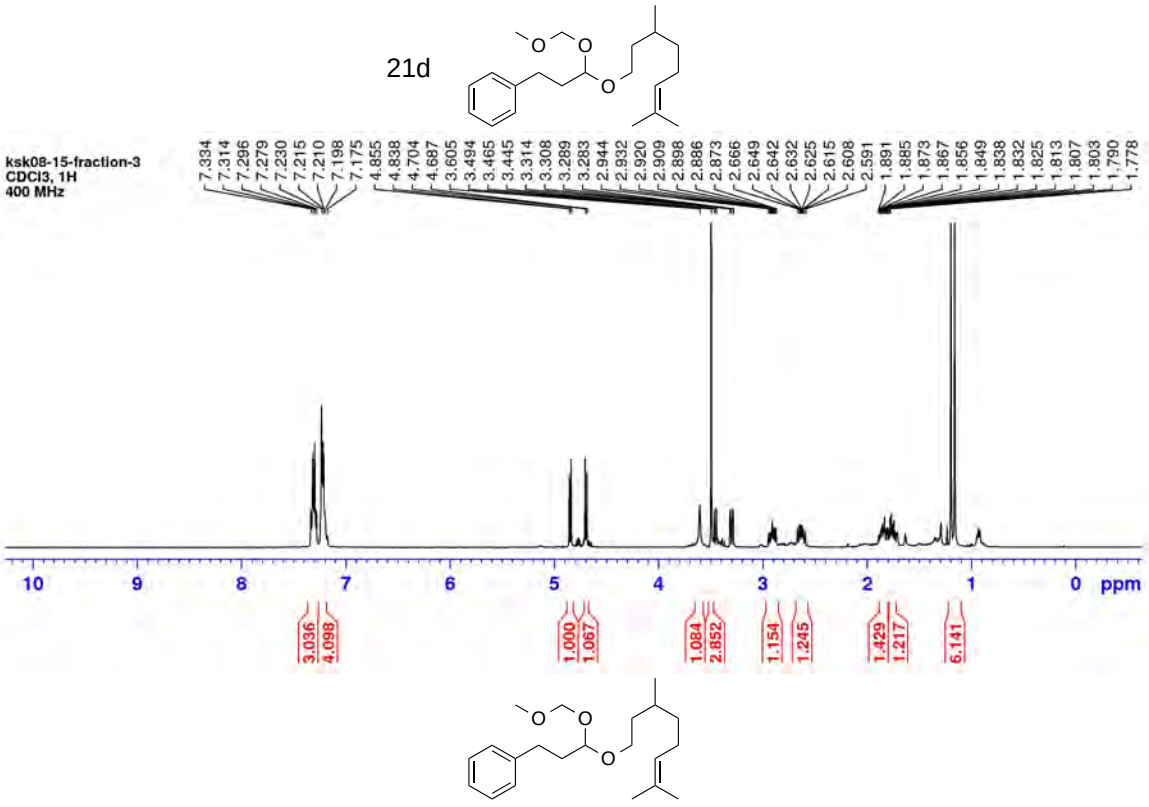

O
O
Ph
$OC_{10}H_{21}$

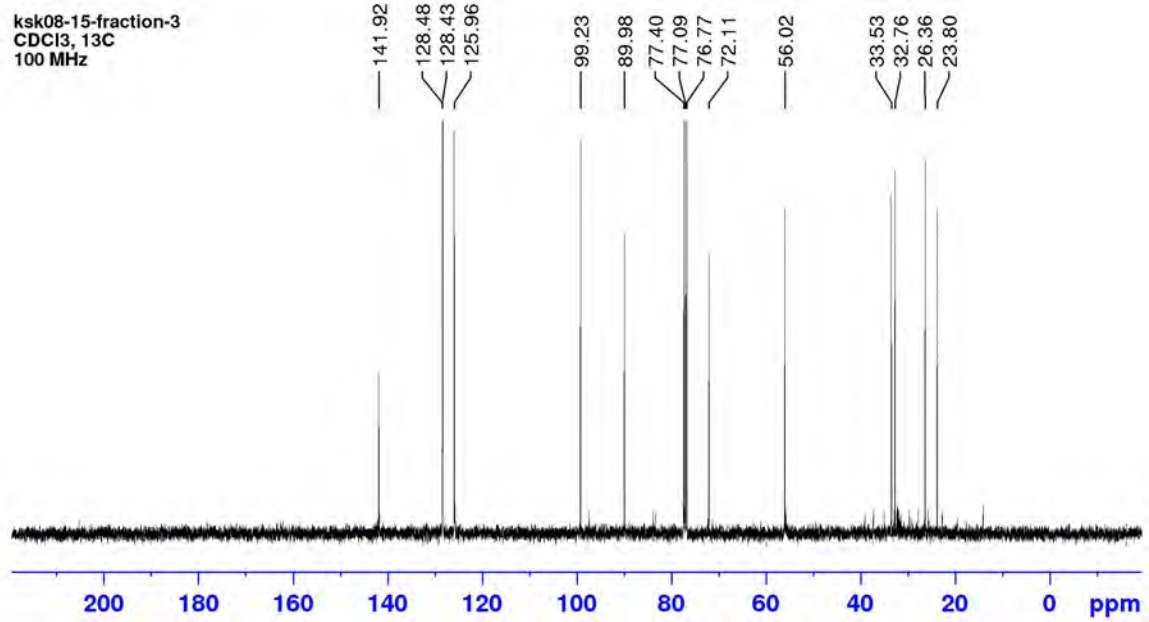

7.307
7.301
7.288
7.268
7.262
7.218
7.212
7.201
7.193
7.173
4.821
4.804
4.692
4.679
4.674
4.666
4.652
4.645
4.640
3.659
3.643
3.636
3.626
3.620
3.603
3.541
3.446
3.429
3.415
3.409
3.395
3.386
3.380
3.230
3.200
2.745
2.726
2.705
2.052
2.017
2.013
2.000
1.990
1.986
1.984
1.977
1.972
1.964
1.958
1.948
1.932
1.929
1.925
1.912
1.909
1.893
1.619
1.602
1.590
1.582
1.566
1.549
1.272
0.901
0.884
0.867
ksk12-26
CDCl3, 1H
400 MHz
9
8
7
6
5
4
3
2
1
0
ppm
2.643
3.448
0.988
2.200
0.991
3.585
2.311
2.066
2.642
16.648
3.180


O
O
Ph
$OC_{10}H_{21}$

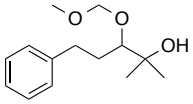

ksk12-26
CDCl3, 13C
100 MHz
141.87
128.50
125.95
101.53
93.46
77.45
77.13
76.81
66.91
55.88
36.48
32.02
30.93
29.96
29.72
29.69
29.57
29.44
26.33
22.80
14.23
200
180
160
140
120
100
80
60
40
20
0
ppm

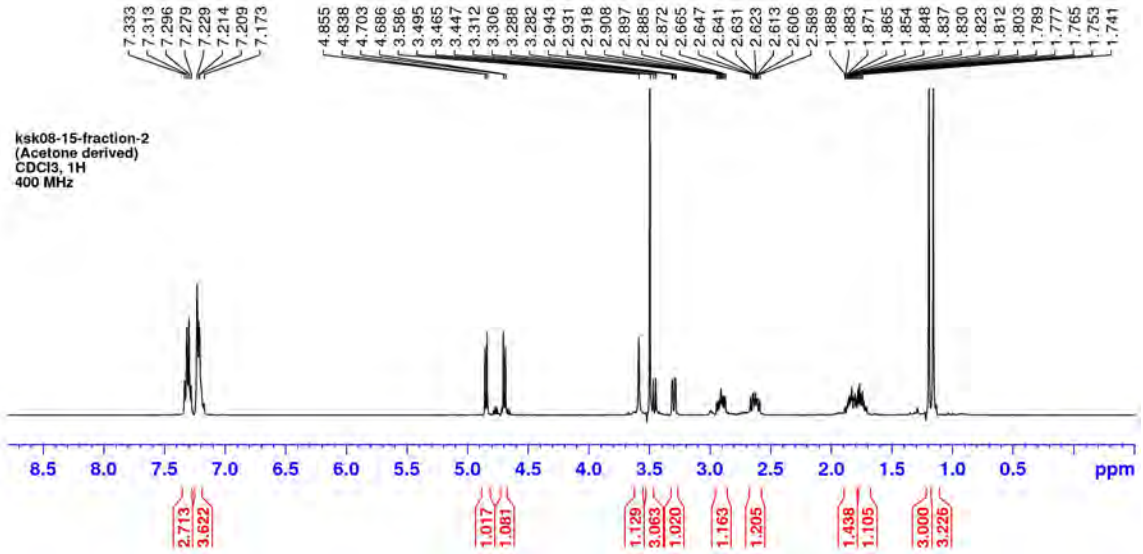
21d

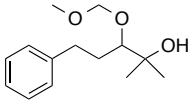

ksk08-15-fraction-3
CDCl3, 1H
400 MHz
7.334
7.314
7.296
7.279
7.230
7.215
7.210
7.198
7.175
4.855
4.838
4.704
4.687
3.605
3.494
3.465
3.445
3.314
3.308
3.289
3.283
2.944
2.932
2.920
2.909
2.898
2.886
2.873
2.666
2.649
2.642
2.632
2.625
2.615
2.608
2.591
1.891
1.885
1.873
1.867
1.856
1.849
1.838
1.832
1.825
1.813
1.807
1.803
1.790
1.778
10
9
8
7
6
5
4
3
2
1
0
ppm
3.036
4.098
1.000
1.067
1.084
2.852
1.154
1.245
1.429
1.217
6.141

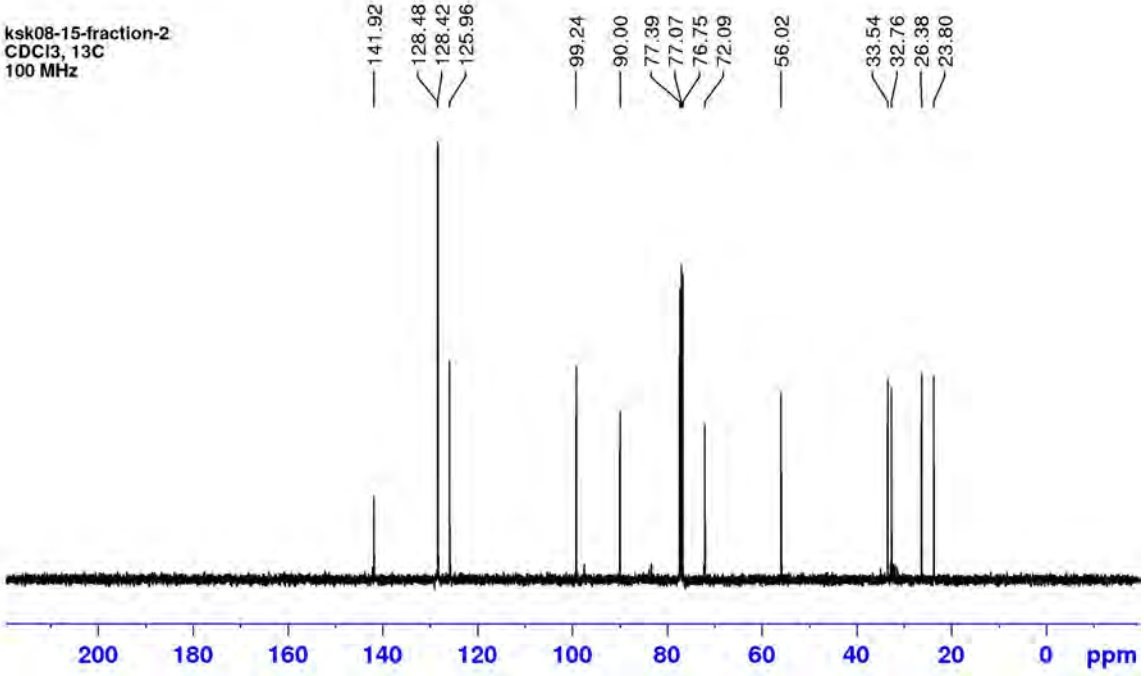

ksk08-15-fraction-3
CDCl3, 13C
100 MHz
141.92
128.48
128.43
125.96
99.23
89.98
77.40
77.09
76.77
72.11
56.02
33.53
32.76
26.36
23.80
200
180
160
140
120
100
80
60
40
20
0
ppm

22

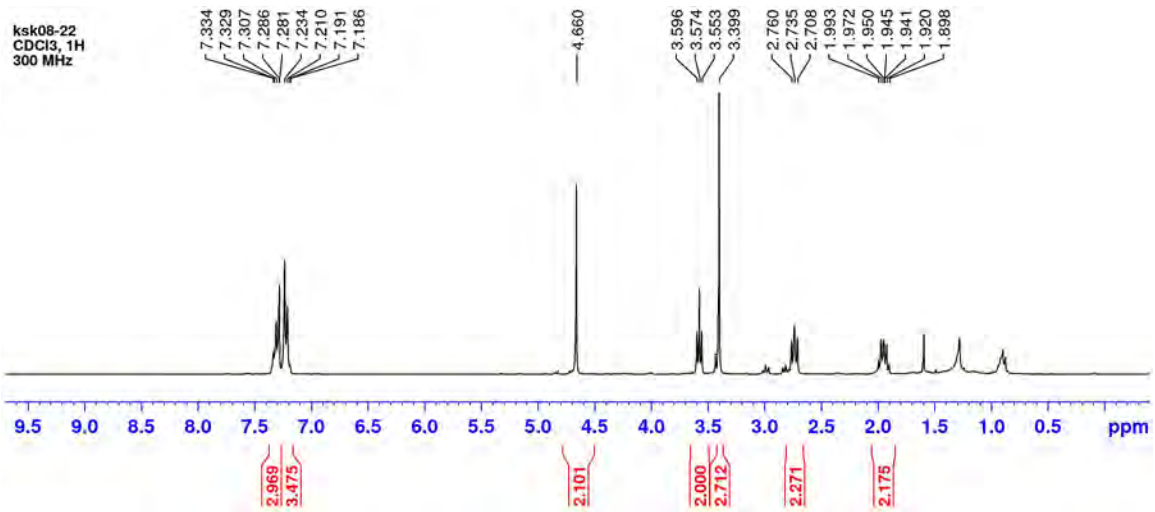

O
O
OH

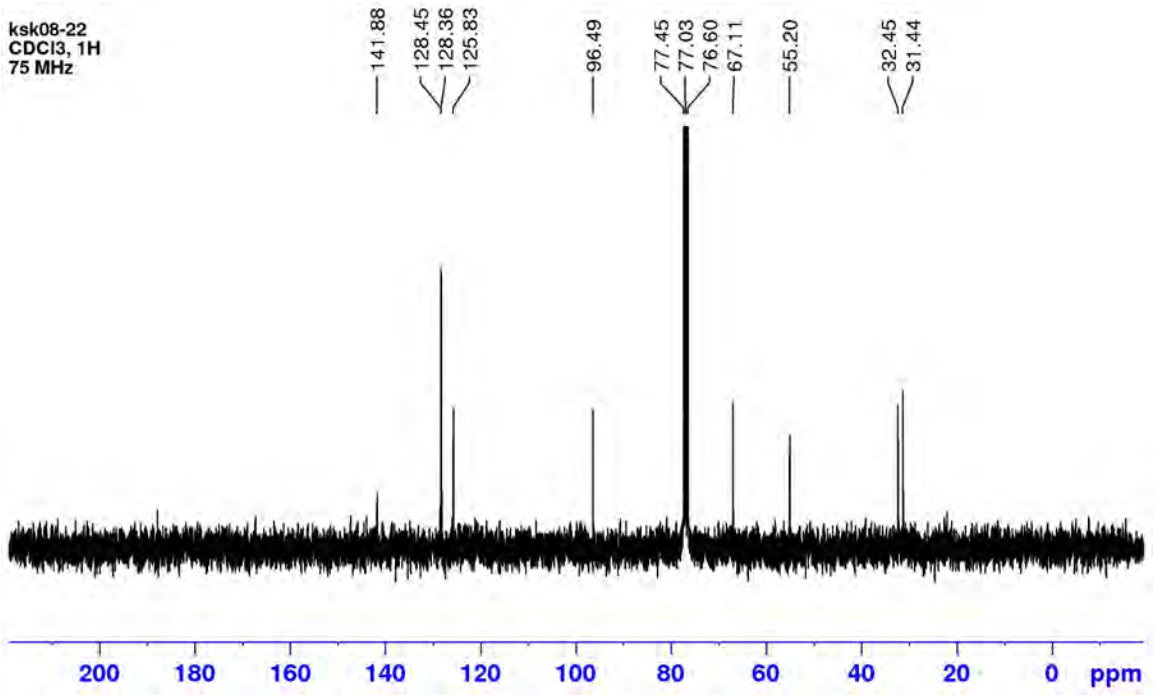

ksk08-15-fraction-2
(Acetone derived)
CDCl3, 1H
400 MHz
ppm


O
O
OH

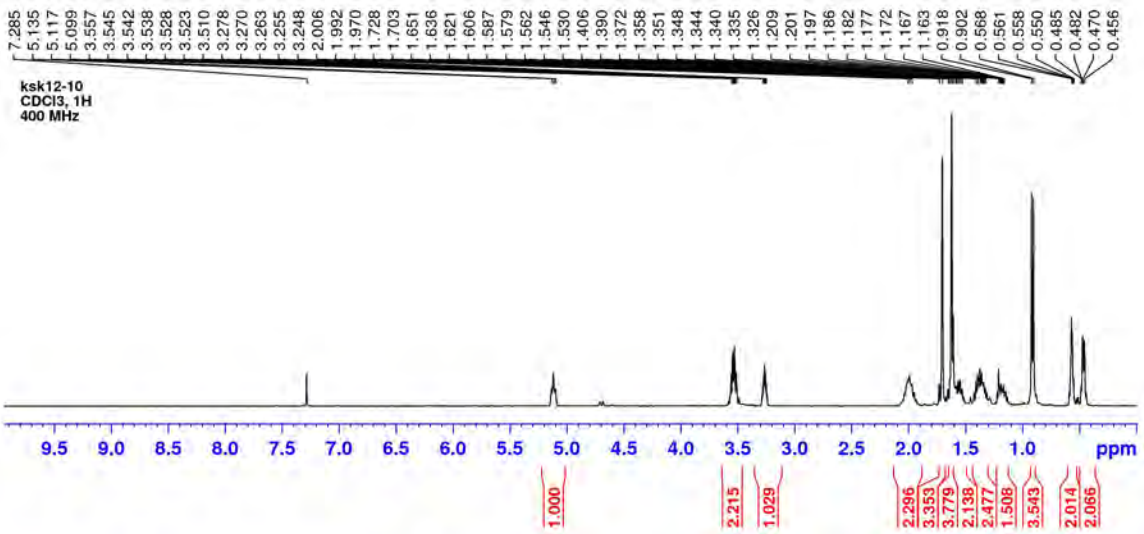

ksk08-15-fraction-2
CDCl3, 13C
100 MHz
ppm

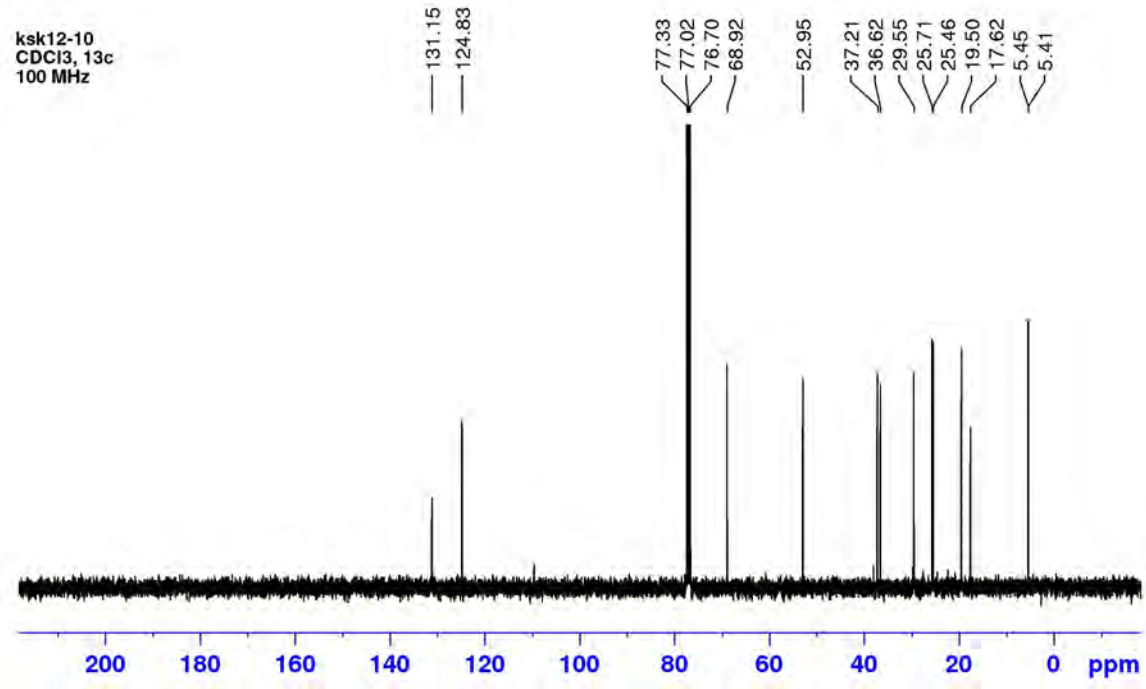
PhCH2CH2CH2OCH2OMe



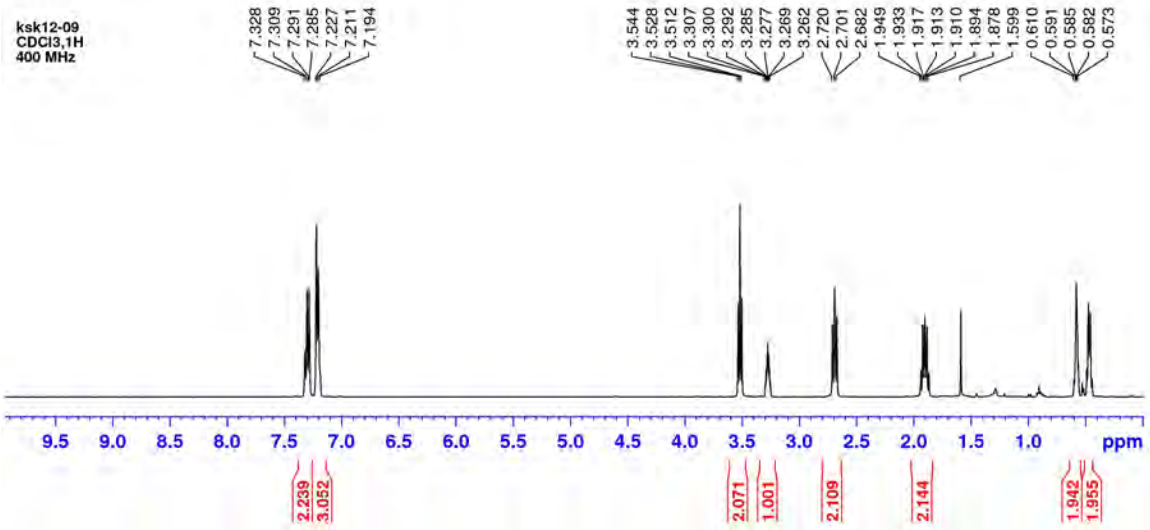


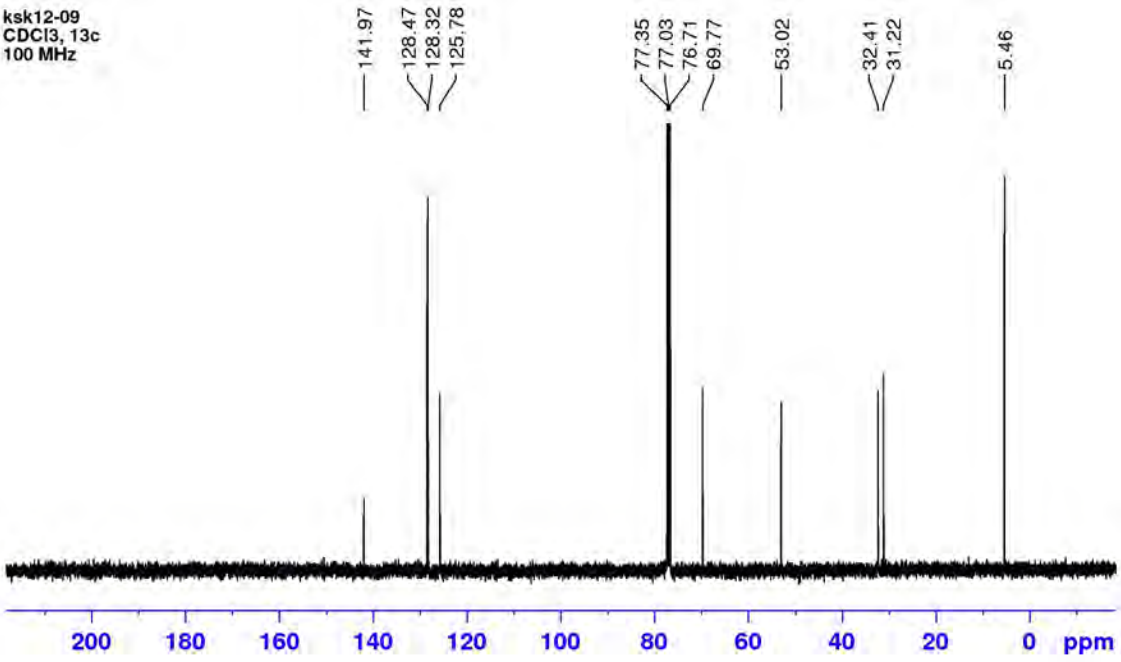
23a

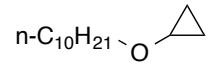

ksk12-10
CDCl3, 1H
400 MHz
7.285
5.135
5.117
5.099
3.557
3.545
3.542
3.538
3.528
3.523
3.510
3.278
3.270
3.263
3.255
3.248
2.006
1.992
1.970
1.728
1.703
1.651
1.636
1.621
1.606
1.587
1.579
1.562
1.546
1.530
1.406
1.390
1.372
1.358
1.351
1.348
1.344
1.340
1.335
1.326
1.209
1.201
1.197
1.186
1.182
1.177
1.172
1.167
1.163
0.918
0.902
0.568
0.561
0.558
0.550
0.485
0.482
0.470
0.456
9.5 9.0 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 ppm
1.000
2.215
1.029
2.296
3.353
3.779
2.138
2.477
1.508
3.543
2.014
2.066

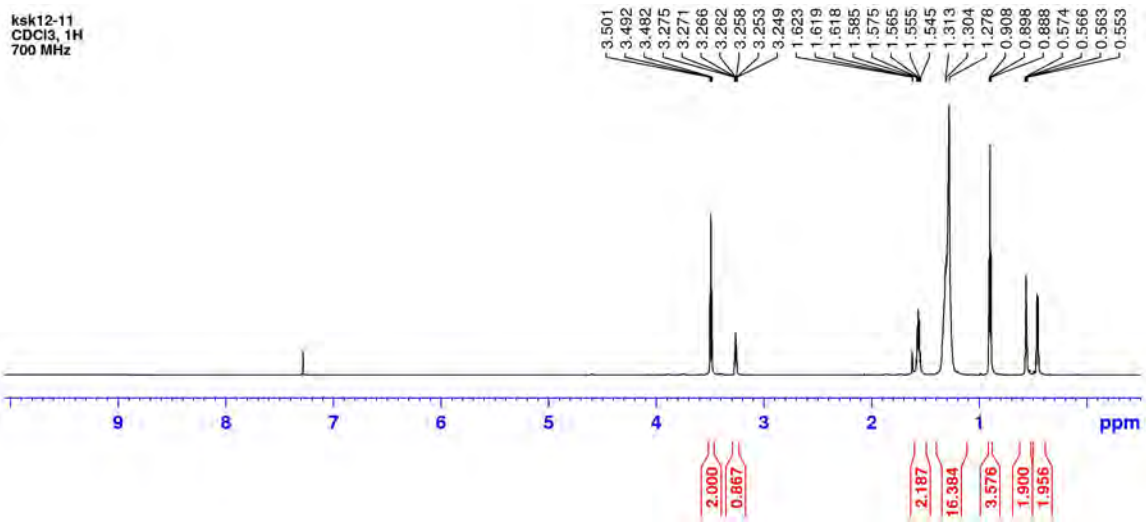

ksk12-10
CDCl3, 13c
100 MHz
131.15
124.83
77.33
77.02
76.70
68.92
52.95
37.21
36.62
29.55
25.71
25.46
19.50
17.62
5.45
5.41
200 180 160 140 120 100 80 60 40 20 0 ppm

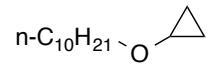
23b

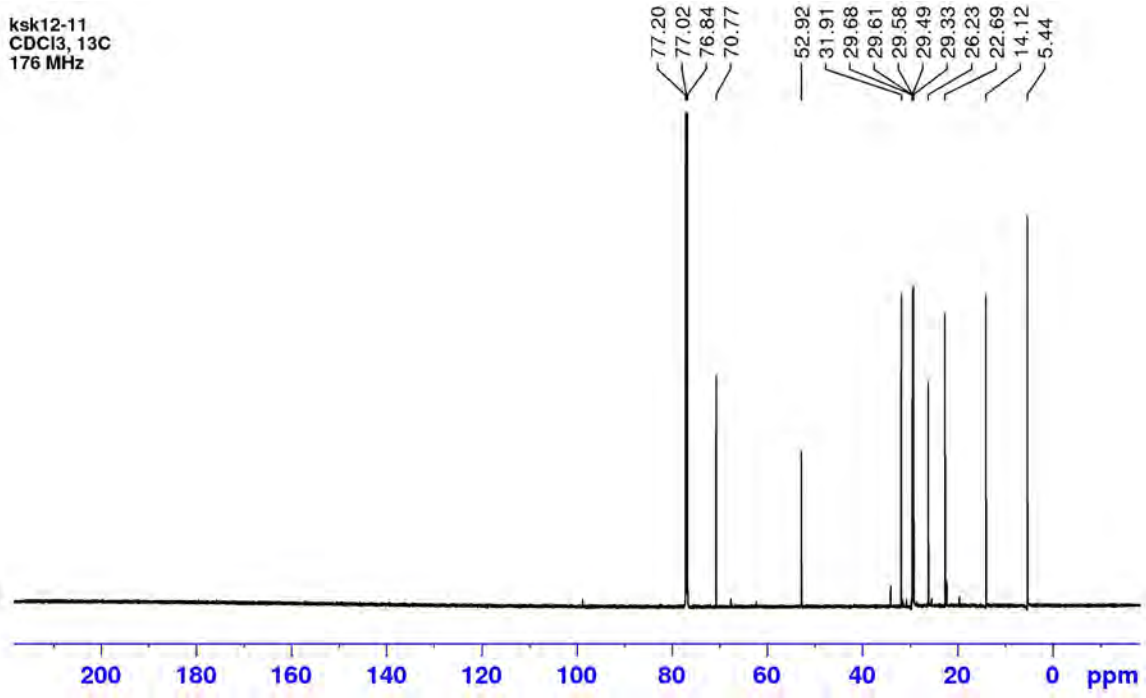

ksk12-09
CDCl3,1H
400 MHz
7.328
7.309
7.291
7.285
7.227
7.211
7.194
3.544
3.528
3.512
3.307
3.300
3.292
3.285
3.277
3.269
3.262
2.720
2.701
2.682
1.949
1.933
1.917
1.913
1.910
1.894
1.878
1.599
0.610
0.591
0.585
0.582
0.573
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
2.239
3.052
2.071
1.001
2.109
2.144
1.942
1.955

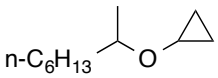

ksk12-09
CDCl3, 13c
100 MHz
141.97
128.47
128.32
125.78
77.35
77.03
76.71
69.77
53.02
32.41
31.22
5.46
200 180 160 140 120 100 80 60 40 20 0 ppm

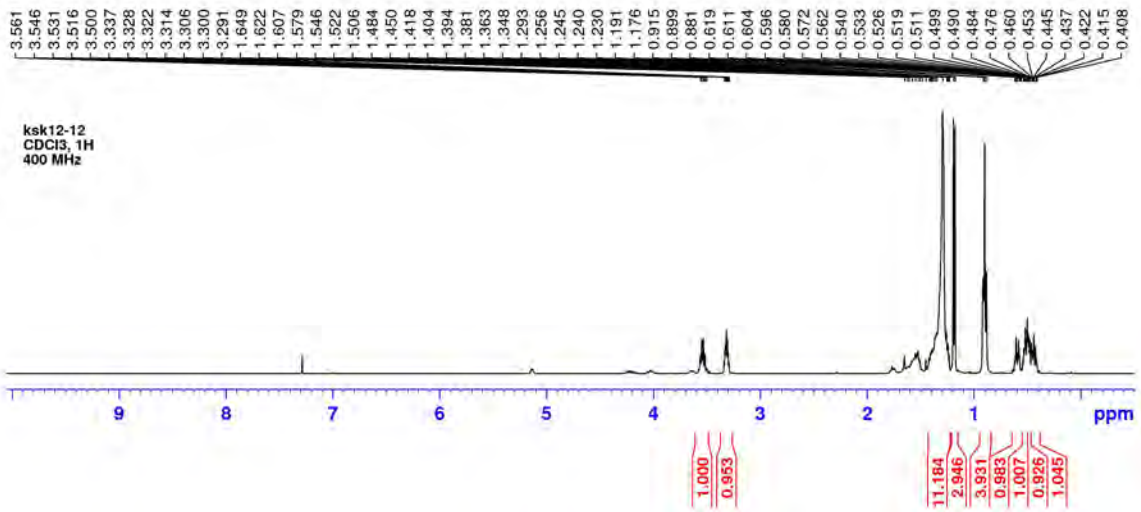
23c 

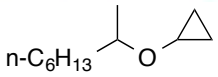

ksk12-11
CDCl3, 1H
700 MHz
3.501
3.492
3.482
3.275
3.271
3.266
3.262
3.258
3.253
3.249
1.623
1.619
1.618
1.585
1.575
1.565
1.555
1.545
1.313
1.304
1.278
0.908
0.898
0.888
0.574
0.566
0.563
0.553
9
8
7
6
5
4
3
2
1
ppm
2.000
0.867
2.187
16.384
3.578
1.900
1.956

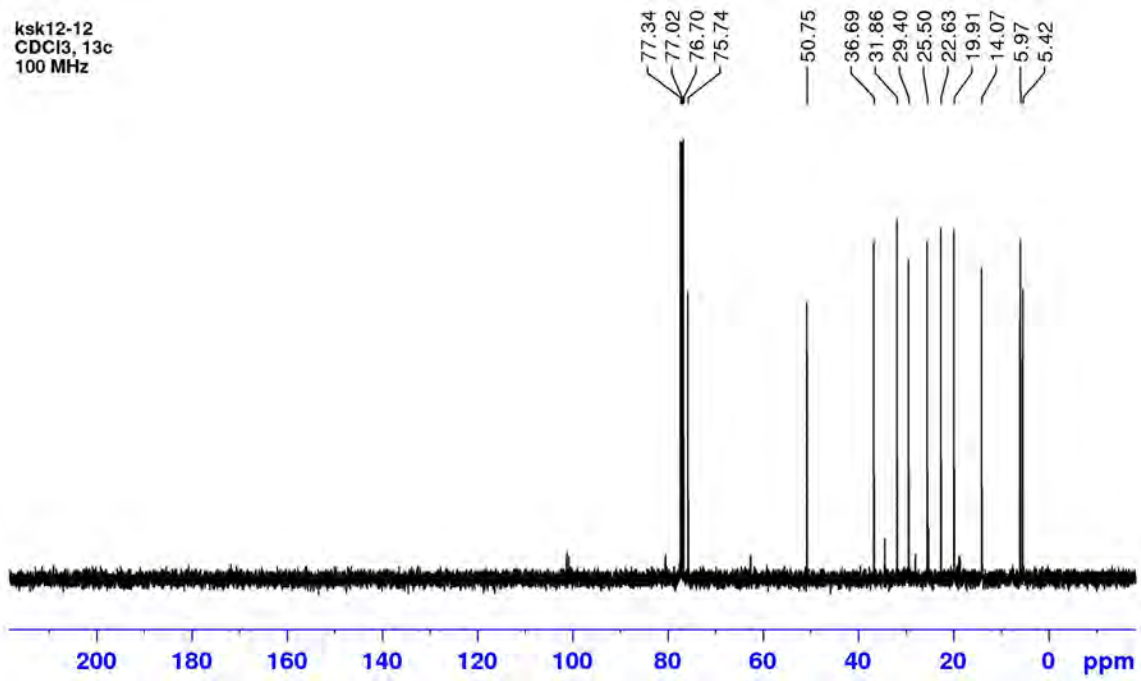


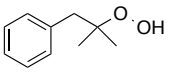

ksk12-11
CDCl3, 13C
176 MHz
77.20
77.02
76.84
70.77
52.92
31.91
29.68
29.61
29.58
29.49
29.33
26.23
22.69
14.12
5.44
200
180
160
140
120
100
80
60
40
20
0
ppm

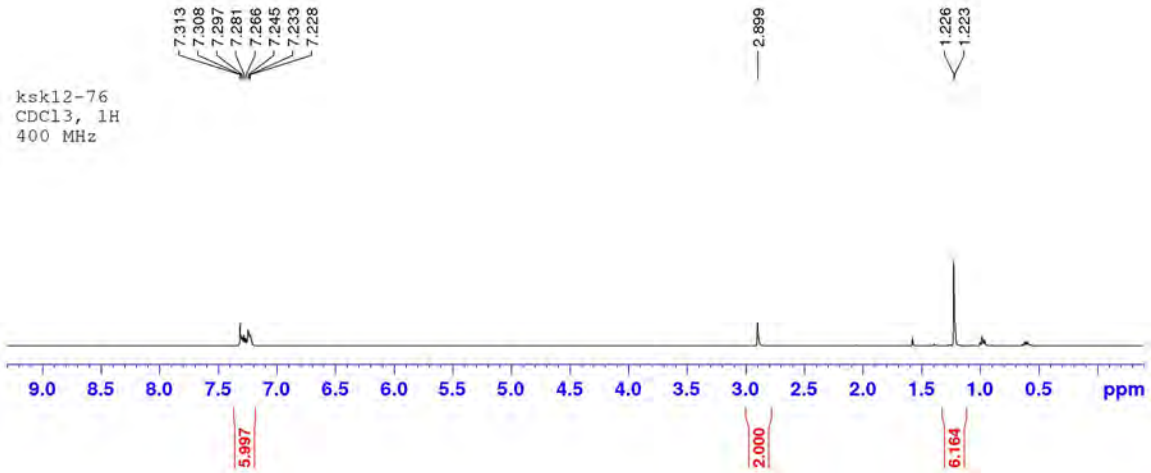
23d 
n-C6H13
O

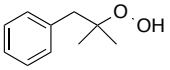

3.561
3.546
3.531
3.516
3.500
3.337
3.328
3.322
3.314
3.306
3.300
3.291
1.649
1.622
1.607
1.579
1.546
1.522
1.506
1.484
1.450
1.418
1.404
1.394
1.381
1.363
1.348
1.293
1.256
1.245
1.240
1.230
1.191
1.176
0.915
0.899
0.881
0.619
0.611
0.604
0.596
0.580
0.572
0.562
0.540
0.533
0.526
0.519
0.511
0.499
0.490
0.484
0.476
0.460
0.453
0.445
0.437
0.422
0.415
0.408
ksk12-12
CDCl3, 1H
400 MHz
9
8
7
6
5
4
3
2
1
ppm
1.000
0.953
11.184
2.946
3.931
0.983
1.007
0.926
1.045

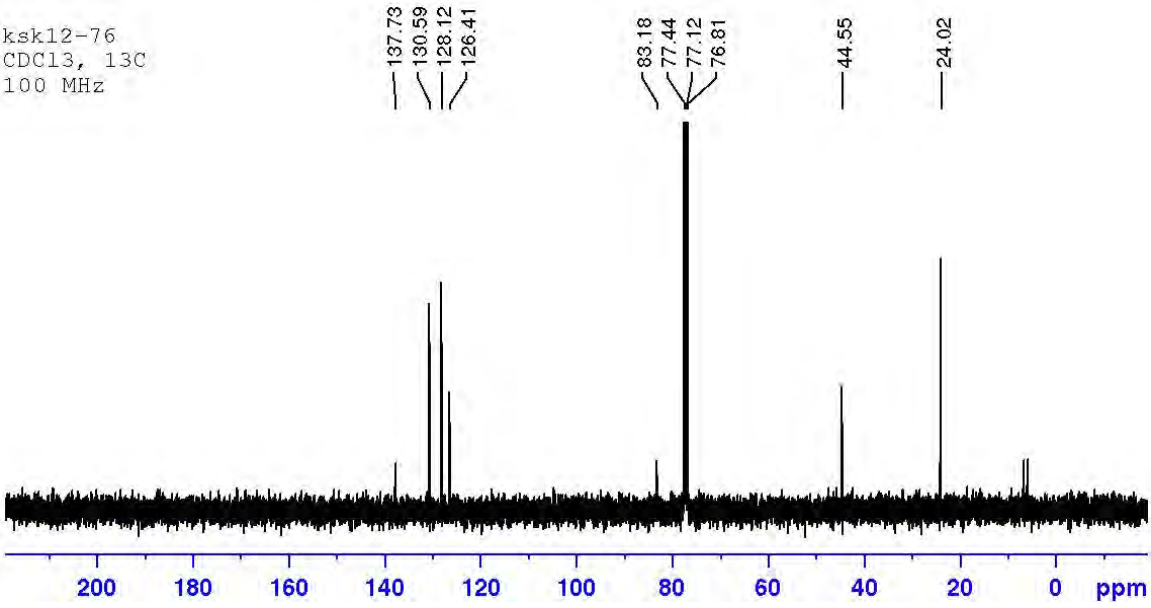

n-C6H13
O

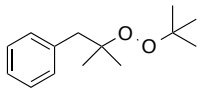

ksk12-12
CDCl3, 13c
100 MHz
77.34
77.02
76.70
75.74
50.75
36.69
31.86
29.40
25.50
22.63
19.91
14.07
5.97
5.42
200
180
160
140
120
100
80
60
40
20
0
ppm

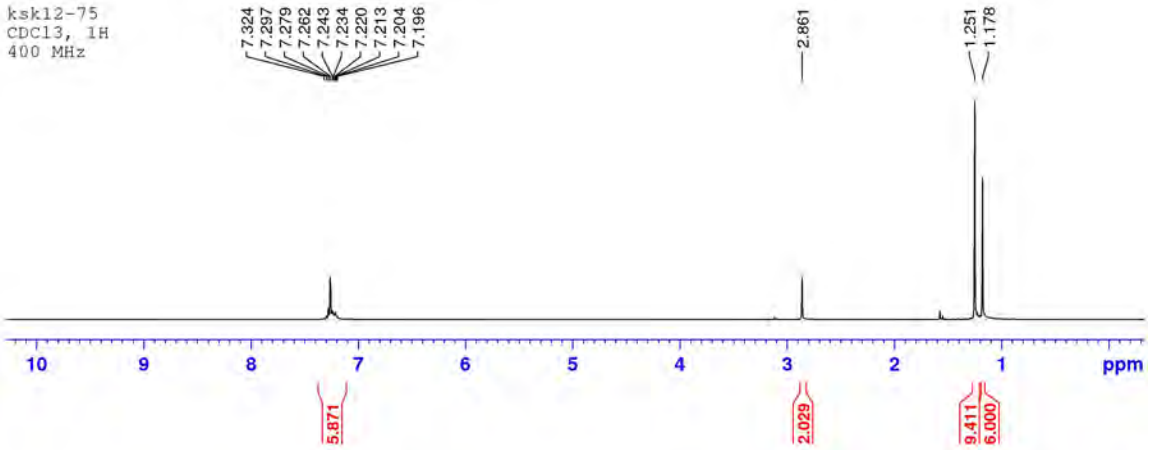

O
OH

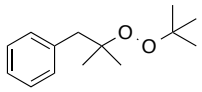

7.313
7.308
7.297
7.281
7.266
7.245
7.233
7.228
2.899
1.226
1.223
ksk12-76
CDCl3, 1H
400 MHz
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
5.997
2.000
6.164

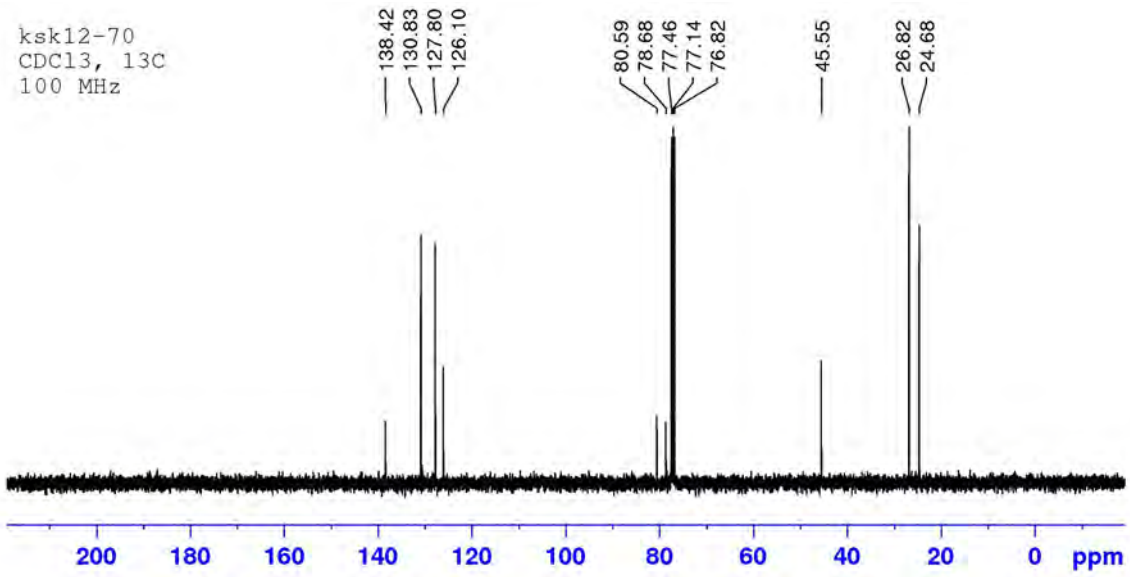

O
OH


ksk12-76
CDCl3, 13C
100 MHz
137.73
130.59
128.12
126.41
83.18
77.44
77.12
76.81
44.55
24.02
200
180
160
140
120
100
80
60
40
20
0
ppm

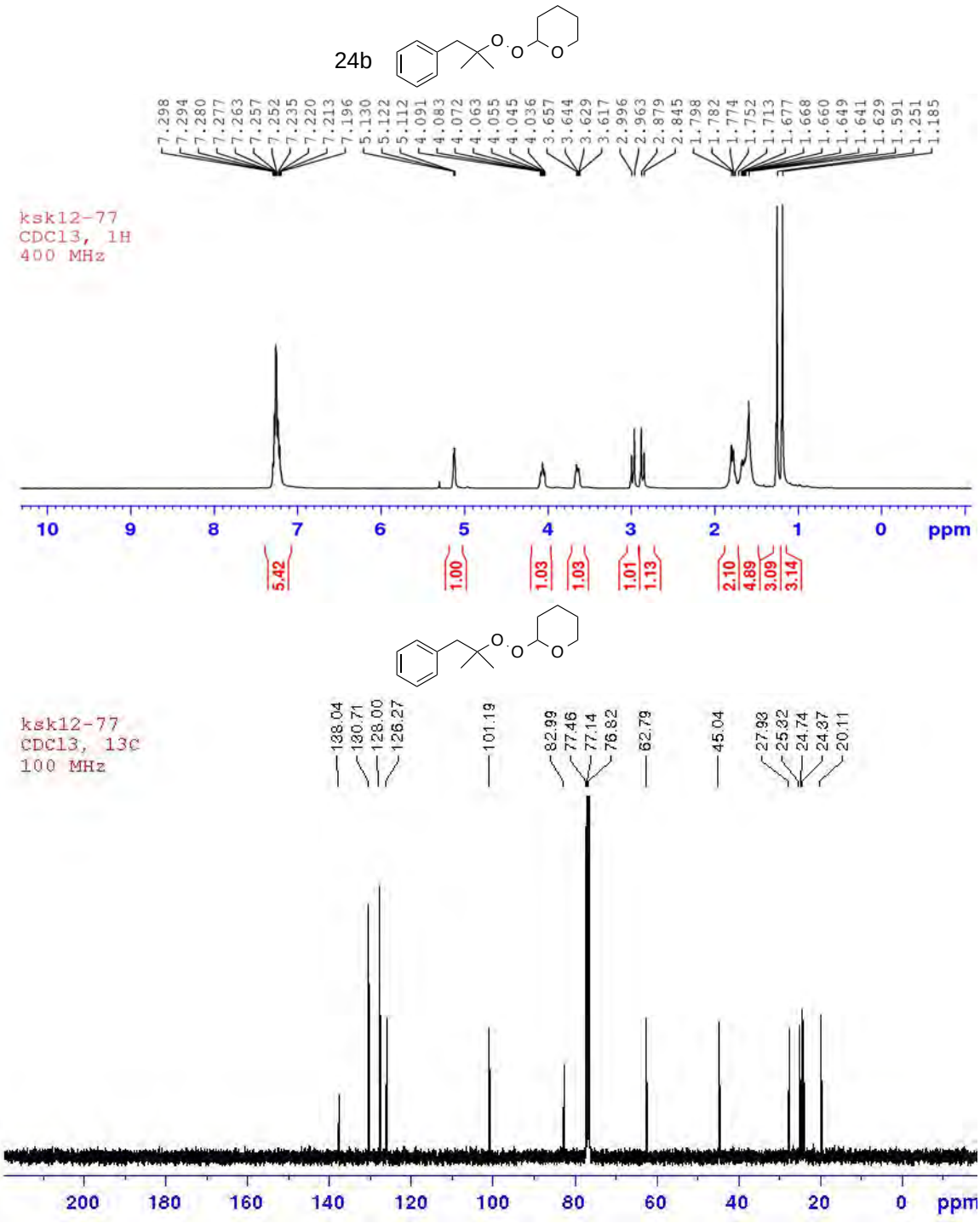
24a 


ksk12-75
CDCl3, 1H
400 MHz
7.324
7.297
7.279
7.262
7.243
7.234
7.220
7.213
7.204
7.196
2.861
1.251
1.178
10
9
8
7
6
5
4
3
2
1
ppm
5.871
2.029
9.411
6.000

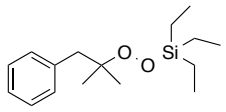



ksk12-70
CDCl3, 13C
100 MHz
138.42
130.83
127.80
126.10
80.59
78.68
77.46
77.14
76.82
45.55
26.82
24.68
200
180
160
140
120
100
80
60
40
20
0
ppm

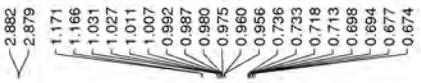
24b

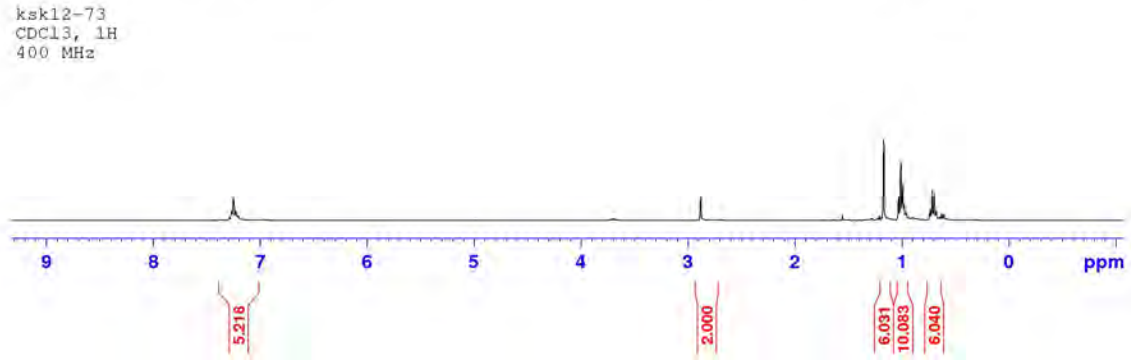

7.298
7.294
7.280
7.277
7.263
7.257
7.252
7.235
7.220
7.213
7.196
5.130
5.122
5.112
4.091
4.083
4.072
4.063
4.055
4.045
4.036
3.657
3.644
3.629
3.617
2.996
2.963
2.879
2.845
1.798
1.782
1.774
1.752
1.713
1.677
1.668
1.660
1.649
1.641
1.629
1.591
1.251
1.185
ksk12-77
CDCl3, 1H
400 MHz
10
9
8
7
6
5
4
3
2
1
0
ppm
5.42
1.00
1.03
1.03
1.01
1.13
2.10
4.89
3.09
3.14
ksk12-77
CDCl3, 13C
100 MHz
138.04
130.71
128.00
126.27
101.19
82.99
77.46
77.14
76.82
62.79
45.04
27.93
25.32
24.74
24.37
20.11
200
180
160
140
120
100
80
60
40
20
0
ppm

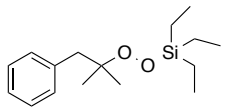
24d

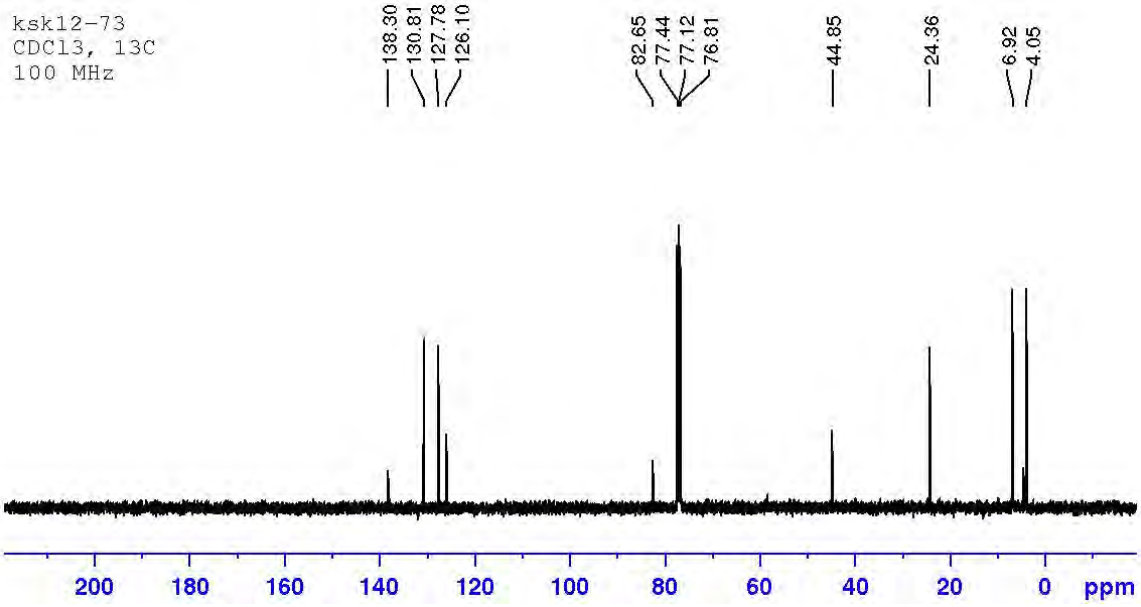

O
O
Si

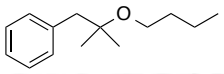
7.290
7.286
7.269
7.267
7.249
7.244
7.231
7.227
7.210
7.206
7.197
7.194
7.189

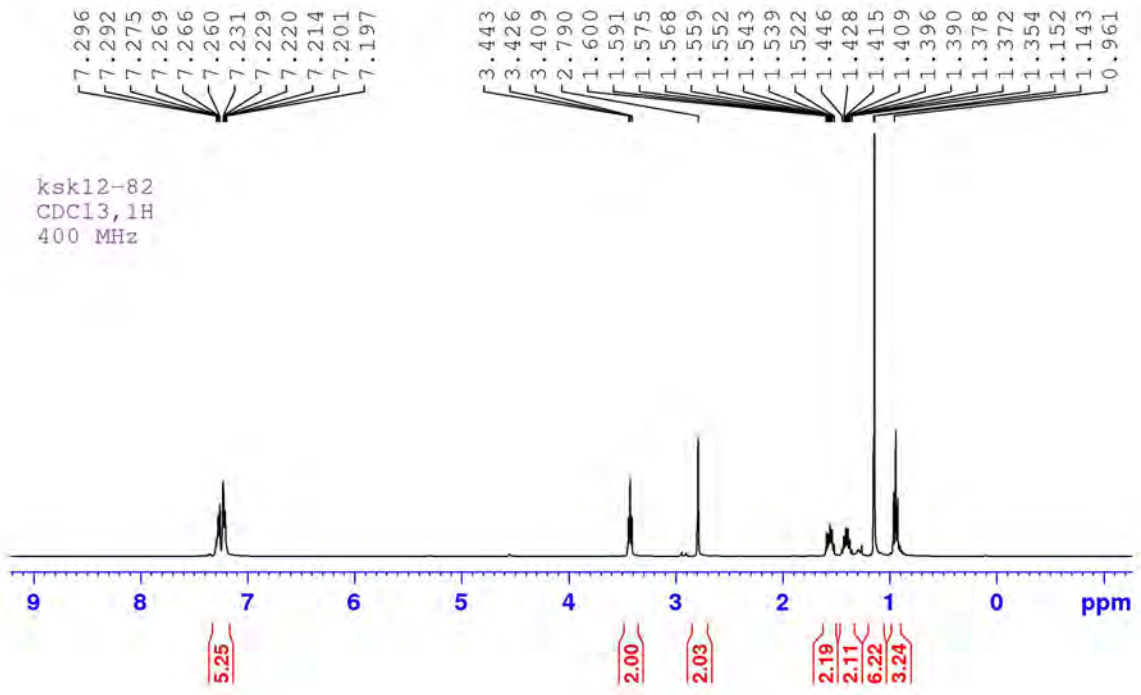

2.882
2.879
1.171
1.166
1.031
1.027
1.011
1.007
0.992
0.987
0.980
0.975
0.960
0.956
0.736
0.733
0.718
0.713
0.698
0.694
0.677
0.674

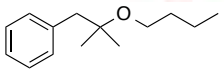

ksk12-73
CDCl3, 1H
400 MHz
9
8
7
6
5
4
3
2
1
0
ppm
5.218
2.000
6.031
10.083
6.040

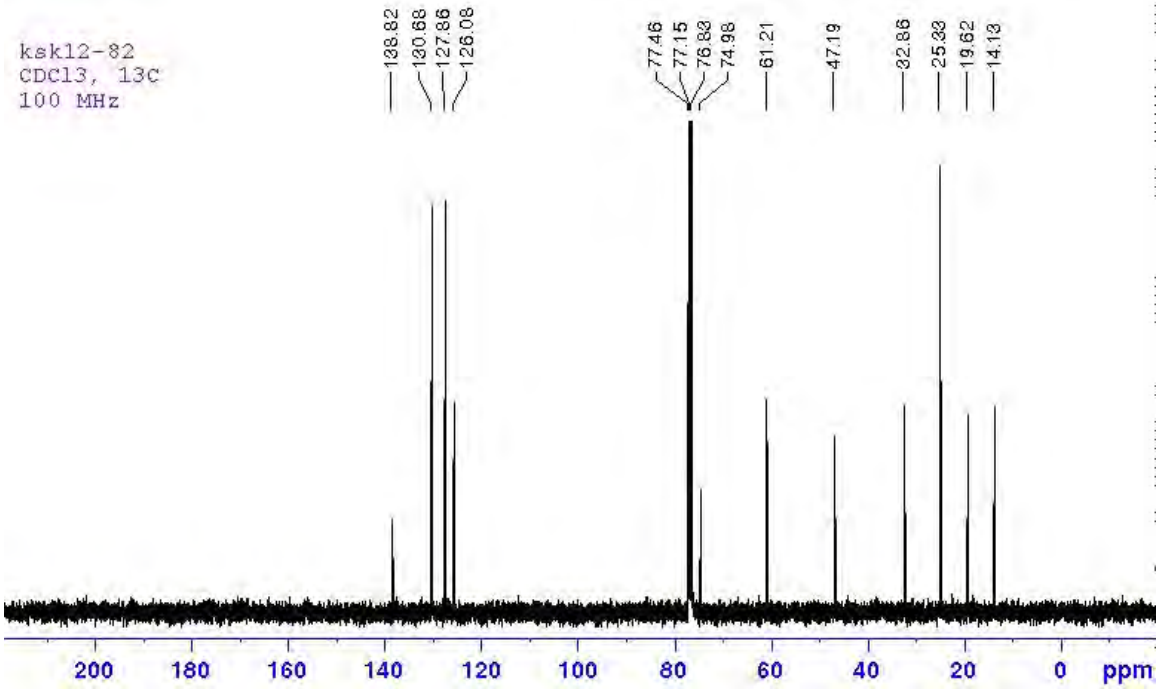

O
O
Si


ksk12-73
CDCl3, 13C
100 MHz
138.30
130.81
127.78
126.10
82.65
77.44
77.12
76.81
44.85
24.36
6.92
4.05
200
180
160
140
120
100
80
60
40
20
0
ppm

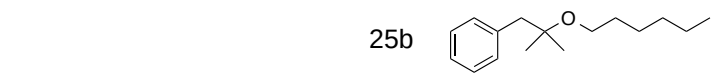
25a 

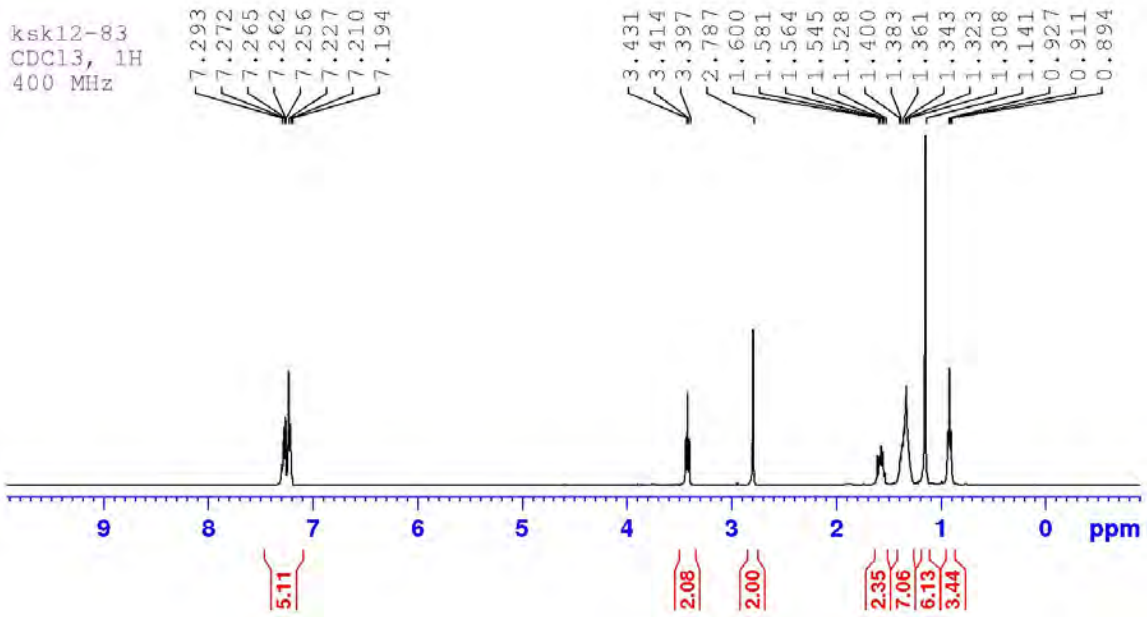

7.296
7.292
7.275
7.269
7.266
7.260
7.231
7.229
7.220
7.214
7.201
7.197
3.443
3.426
3.409
2.790
1.600
1.591
1.575
1.568
1.559
1.552
1.543
1.539
1.522
1.446
1.428
1.415
1.409
1.396
1.390
1.378
1.372
1.354
1.152
1.143
0.961
ksk12-82
CDCl3,1H
400 MHz
9
8
7
6
5
4
3
2
1
0
ppm
5.25
2.00
2.03
2.19
2.11
6.22
3.24

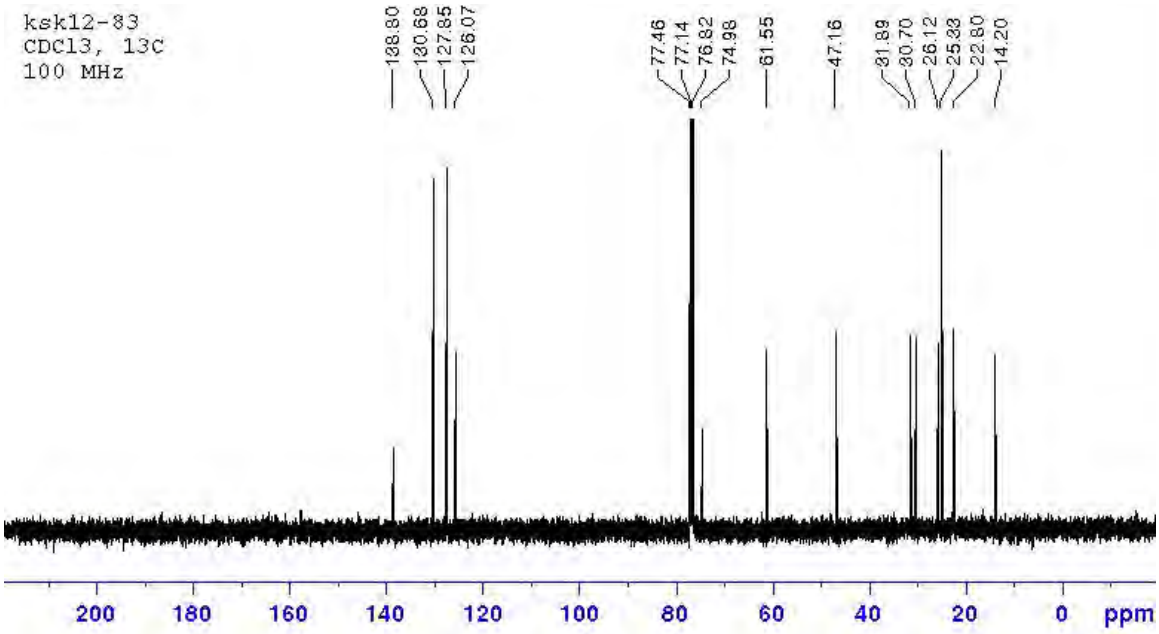



ksk12-82
CDCl3, 13C
100 MHz
138.82
130.68
127.86
126.08
77.46
77.15
76.83
74.98
61.21
47.19
32.86
25.33
19.62
14.13
200
180
160
140
120
100
80
60
40
20
0
ppm

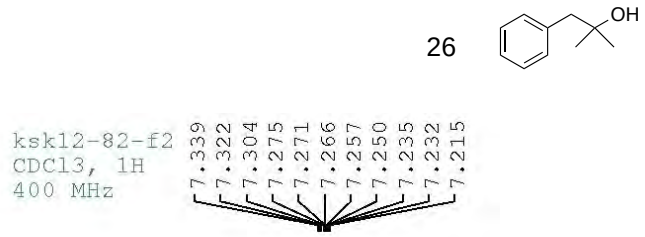
25b

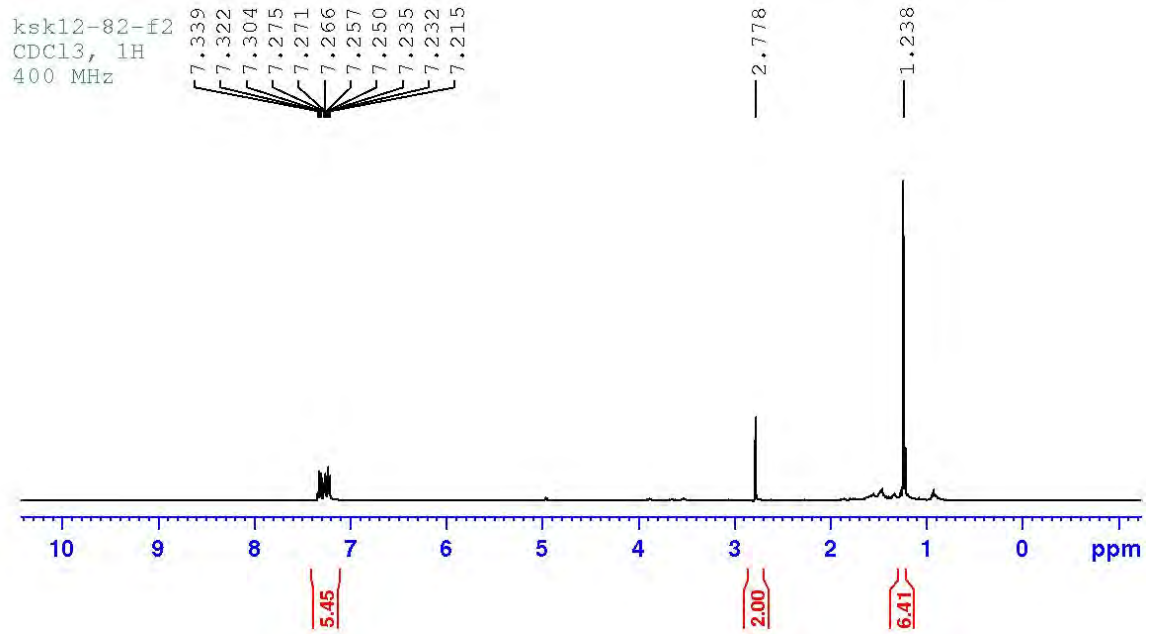



ksk12-83
CDCl3, 1H
400 MHz
7.293
7.272
7.265
7.262
7.256
7.227
7.210
7.194
3.431
3.414
3.397
2.787
1.600
1.581
1.564
1.545
1.528
1.400
1.383
1.361
1.343
1.323
1.308
1.141
0.927
0.911
0.894
9
8
7
6
5
4
3
2
1
0
ppm
5.11
2.08
2.00
2.35
7.06
6.13
3.44

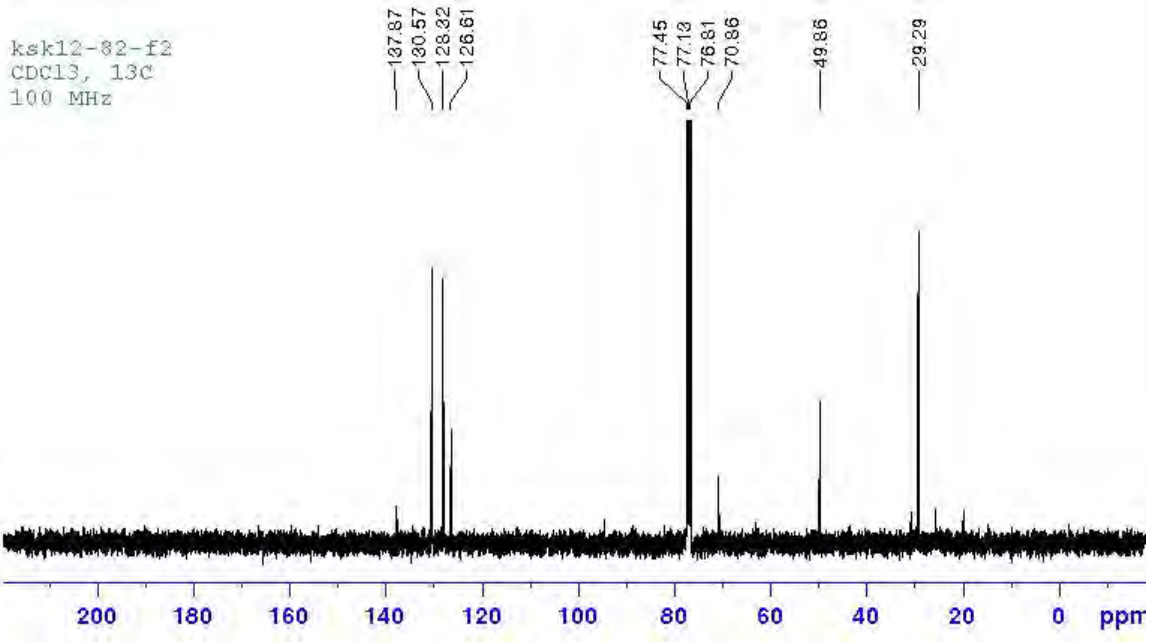

ksk12-83
CDCl3, 13C
100 MHz
138.80
130.68
127.85
126.07
77.46
77.14
76.82
74.98
61.55
47.16
31.89
30.70
26.12
25.38
22.80
14.20
200
180
160
140
120
100
80
60
40
20
0
ppm

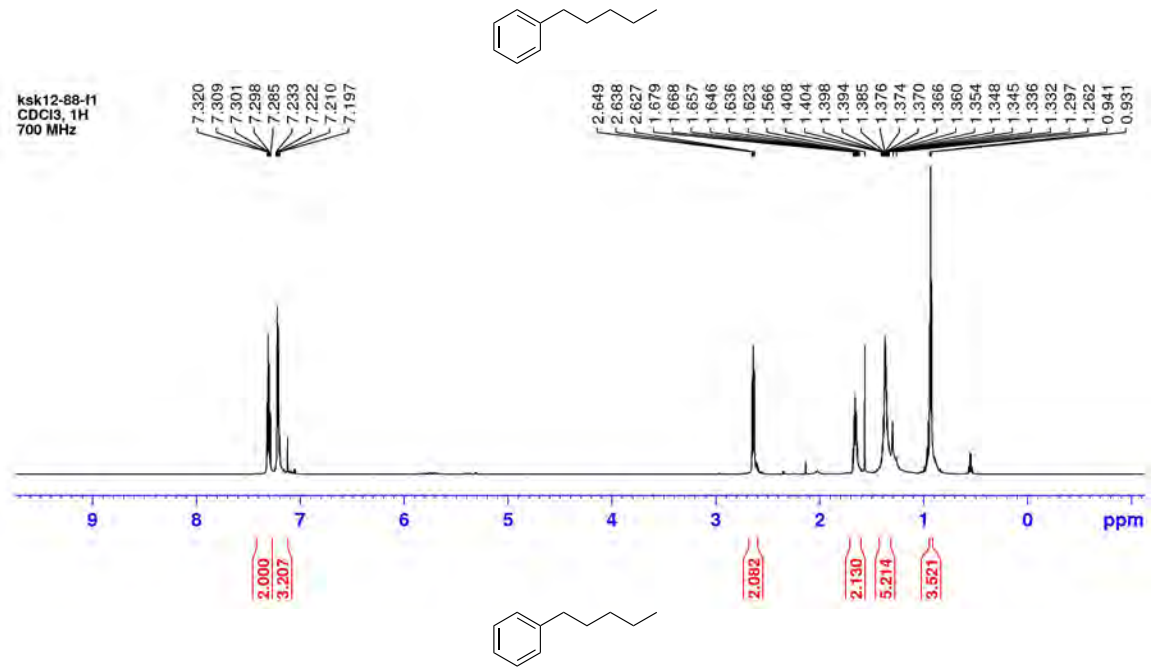
26

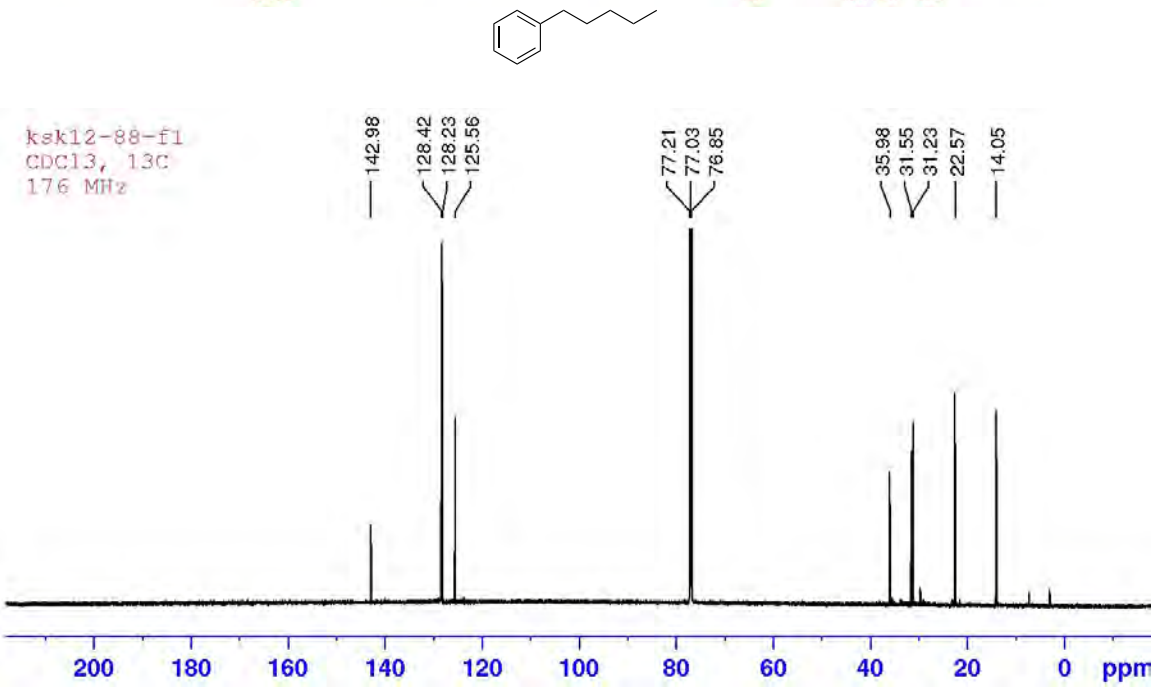

OH

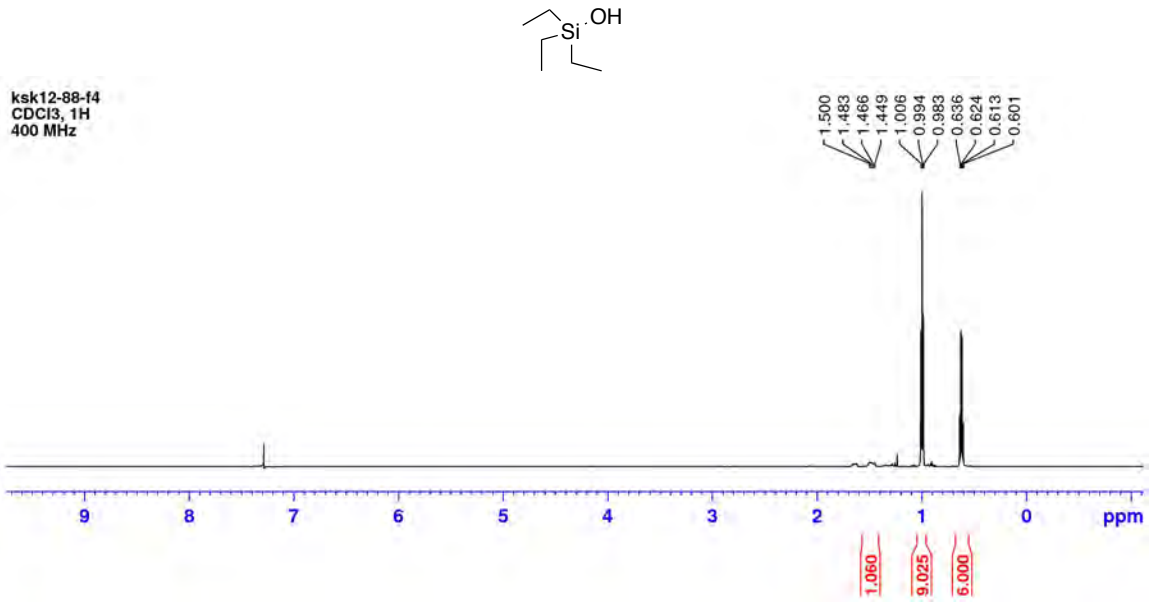

ksk12-82-f2
CDCl3, 1H
400 MHz
7.339
7.322
7.304
7.275
7.271
7.266
7.257
7.250
7.235
7.232
7.215
2.778
1.238
10
9
8
7
6
5
4
3
2
1
0
ppm
5.45
2.00
6.41

OH


ksk12-82-f2
CDCl3, 13C
100 MHz
137.87
130.57
128.32
126.61
77.45
77.13
76.81
70.86
49.86
29.29
200
180
160
140
120
100
80
60
40
20
0
ppm

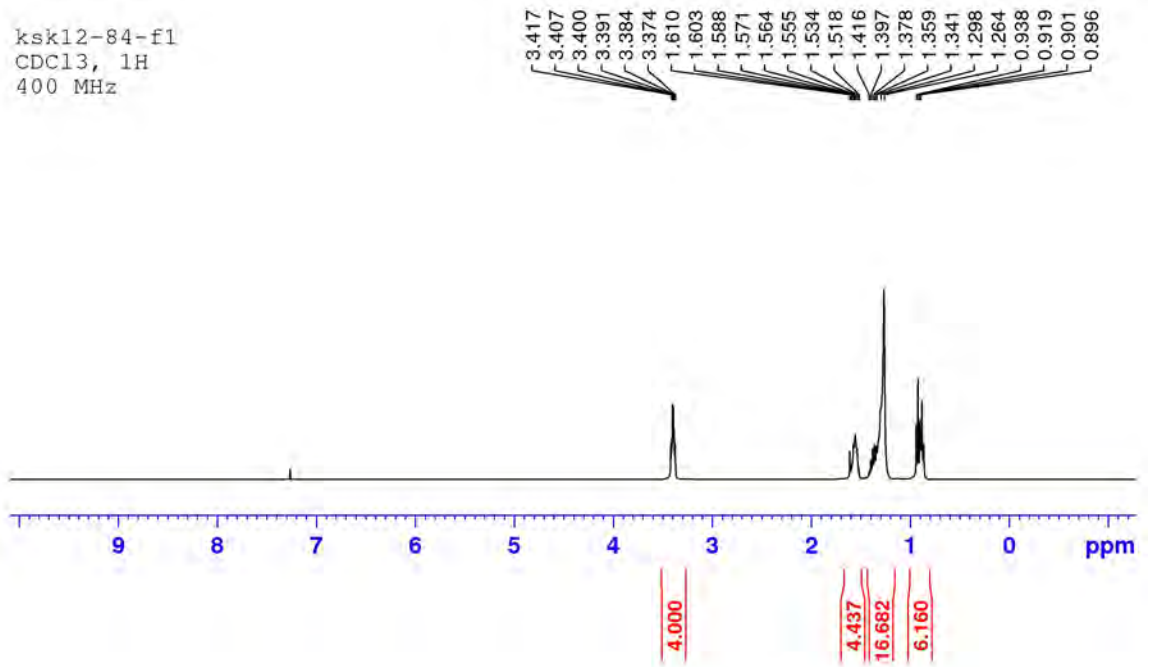

ksk12-88-f1
CDCl3, 1H
700 MHz
7.320
7.309
7.301
7.298
7.285
7.233
7.222
7.210
7.197
2.649
2.638
2.627
1.679
1.668
1.657
1.646
1.636
1.623
1.566
1.408
1.404
1.398
1.394
1.385
1.376
1.374
1.370
1.366
1.360
1.354
1.348
1.345
1.336
1.332
1.297
1.262
0.941
0.931
9
8
7
6
5
4
3
2
1
0
ppm
2.000
3.207
2.082
2.130
5.214
3.521


ksk12-88-f1
CDCl3, 13C
176 MHz
142.98
128.42
128.23
125.56
77.21
77.03
76.85
35.98
31.55
31.23
22.57
14.05
200
180
160
140
120
100
80
60
40
20
0
ppm

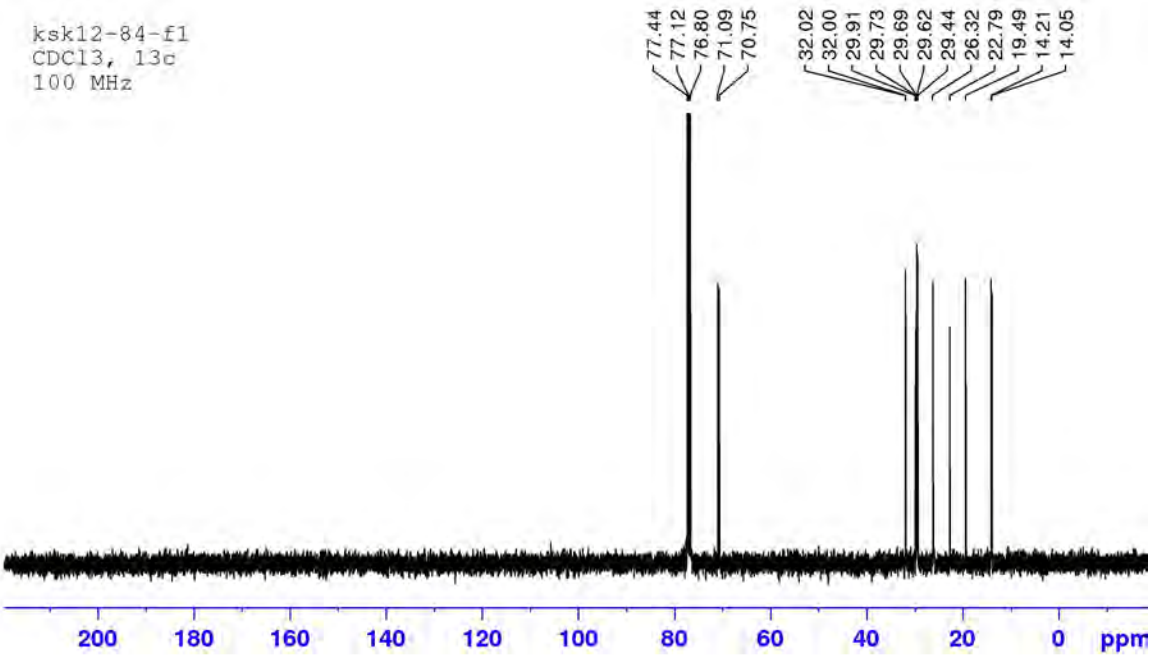

Si
OH
ksk12-88-f4
CDCl3, 1H
400 MHz
1.500
1.483
1.466
1.449
1.006
0.994
0.983
0.636
0.624
0.613
0.601
9
8
7
6
5
4
3
2
1
0
ppm
1.060
9.025
6.000

Si
OH
ksk12-88-f4
CDCl3, 13c
176 MHz
77.20
77.02
76.84
6.58
5.80
200
180
160
140
120
100
80
60
40
20
0
ppm

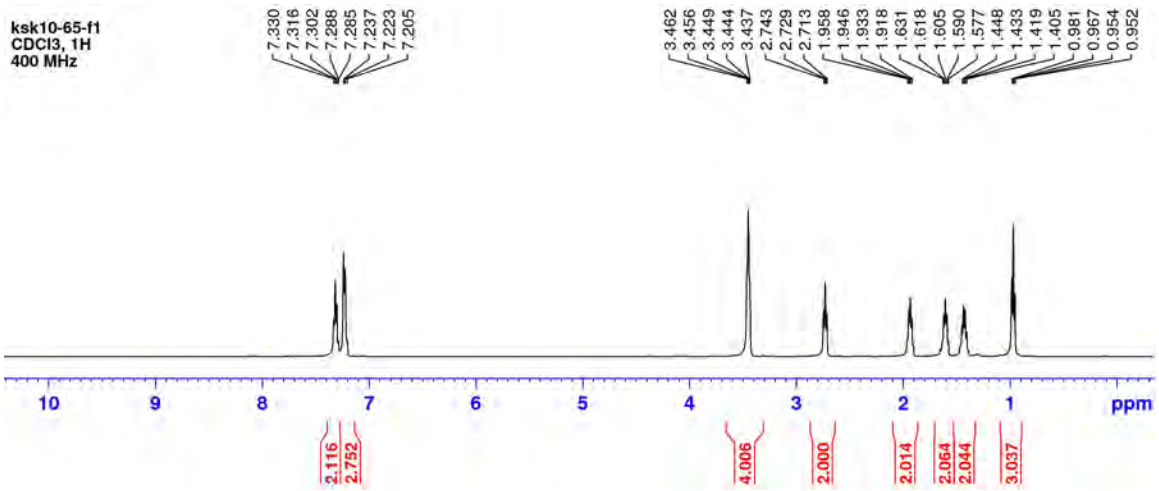
27 $n\text{-}C_{10}H_{11}$–O–$n\text{-}C_4H_9$

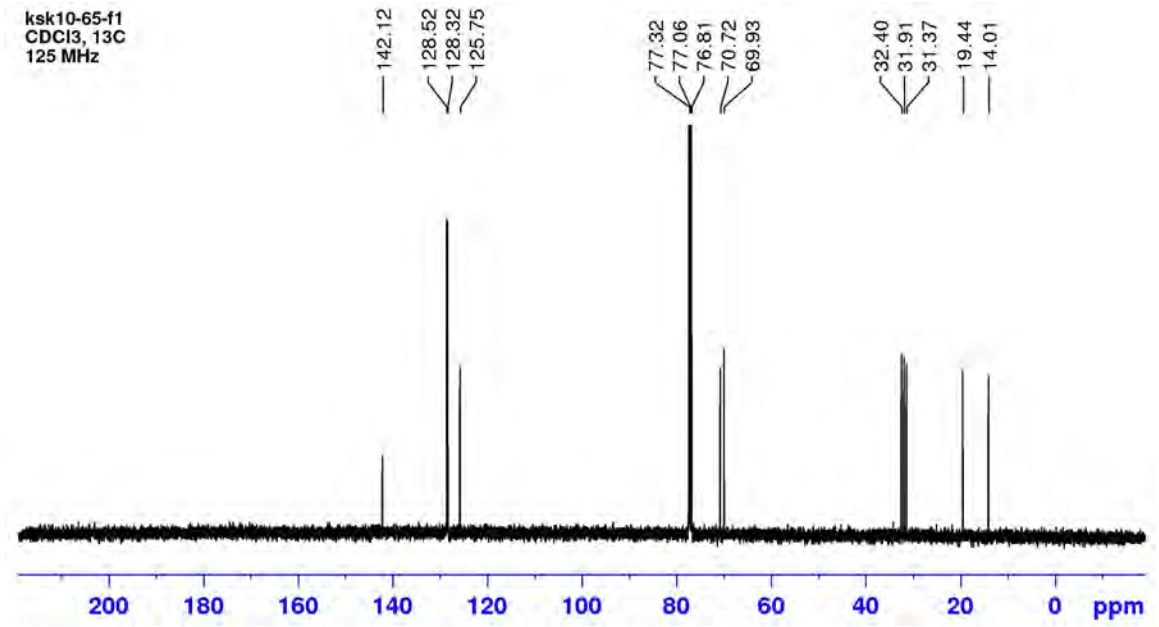


$n\text{-}C_{10}H_{11}$–O–$n\text{-}C_4H_9$

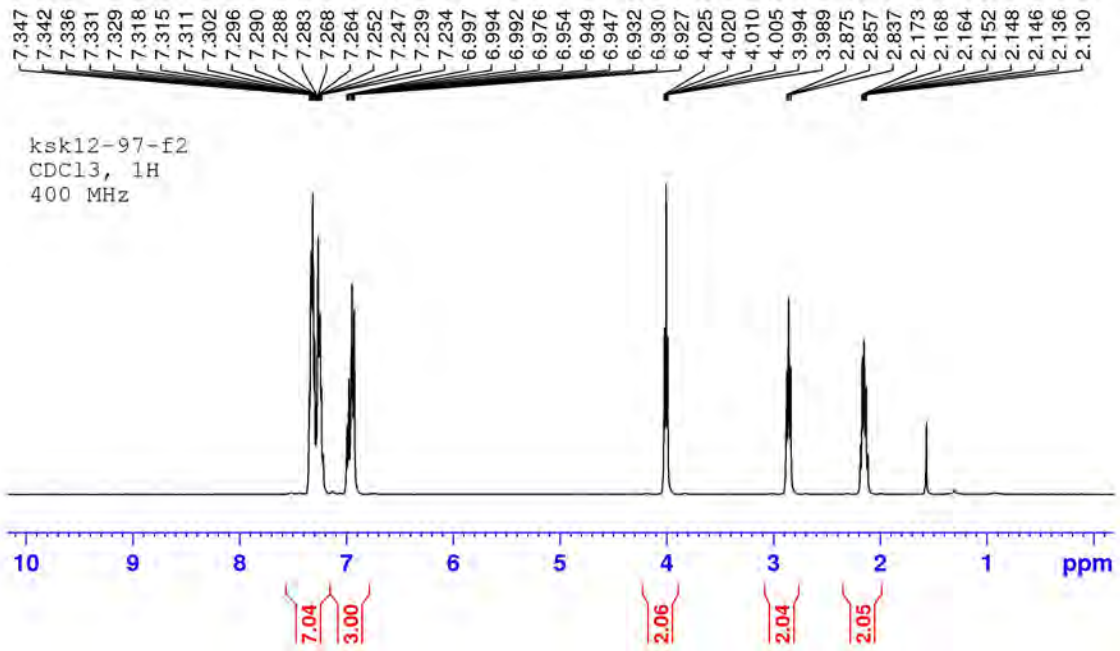


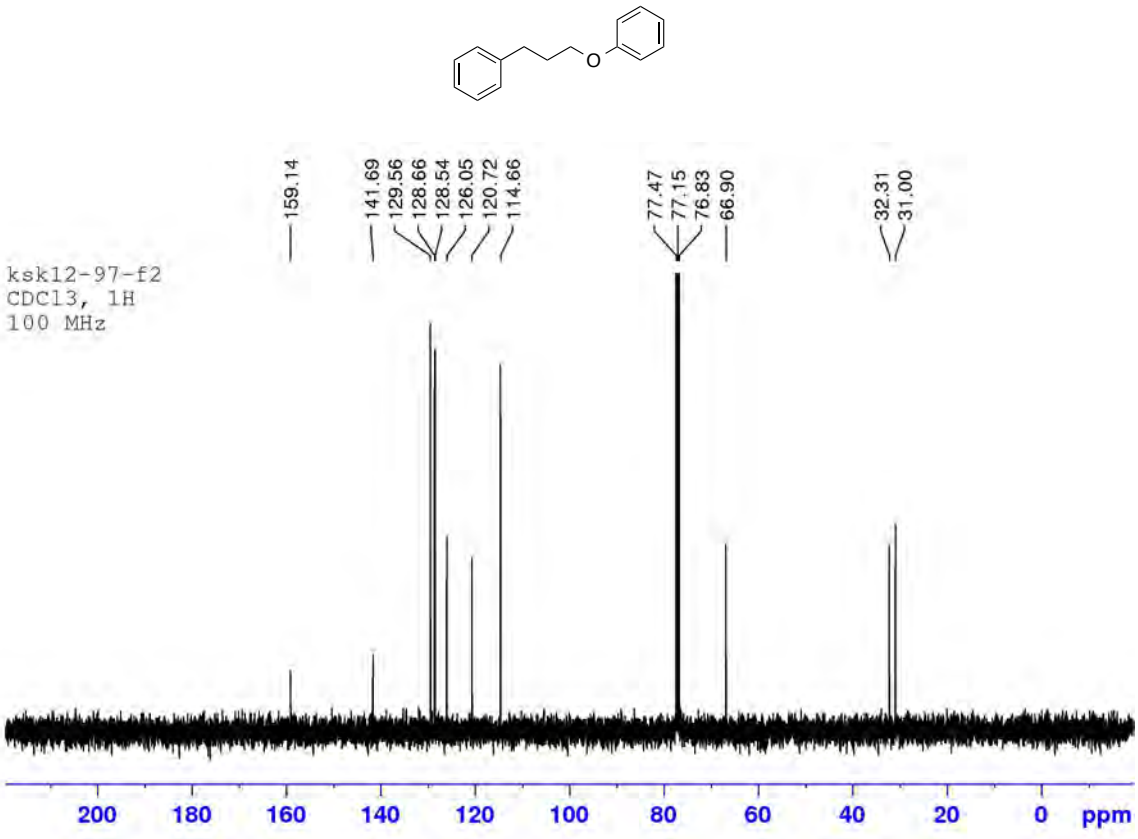
28

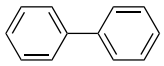

ksk10-65-f1
CDCl3, 1H
400 MHz
7.330
7.316
7.302
7.288
7.285
7.237
7.223
7.205
3.462
3.456
3.449
3.444
3.437
2.743
2.729
2.713
1.958
1.946
1.933
1.918
1.631
1.618
1.605
1.590
1.577
1.448
1.433
1.419
1.405
0.981
0.967
0.954
0.952
10
9
8
7
6
5
4
3
2
1
ppm
2.116
2.752
4.006
2.000
2.014
2.064
2.044
3.037

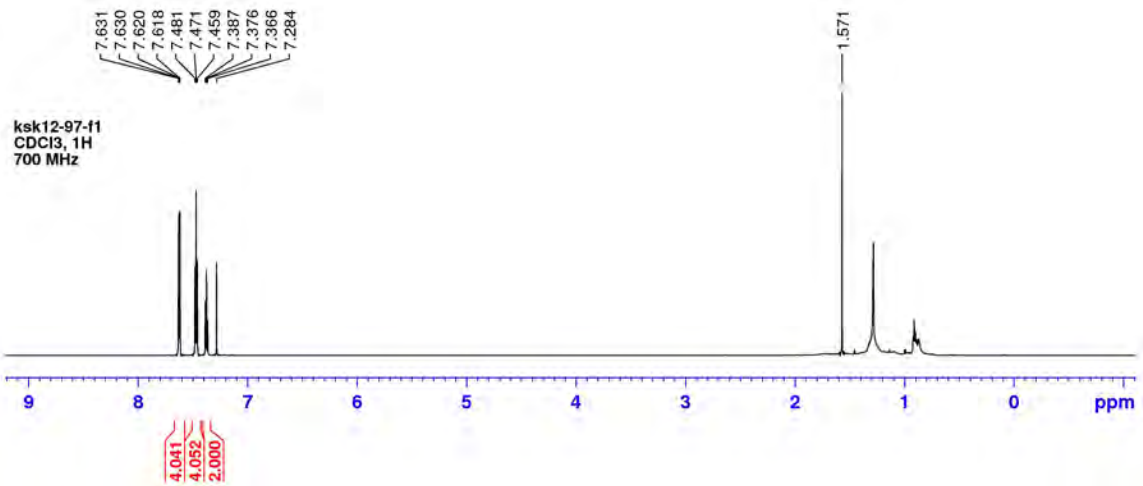

ksk10-65-f1
CDCl3, 13C
125 MHz
142.12
128.52
128.32
125.75
77.32
77.06
76.81
70.72
69.93
32.40
31.91
31.37
19.44
14.01
200
180
160
140
120
100
80
60
40
20
0
ppm

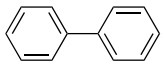
29

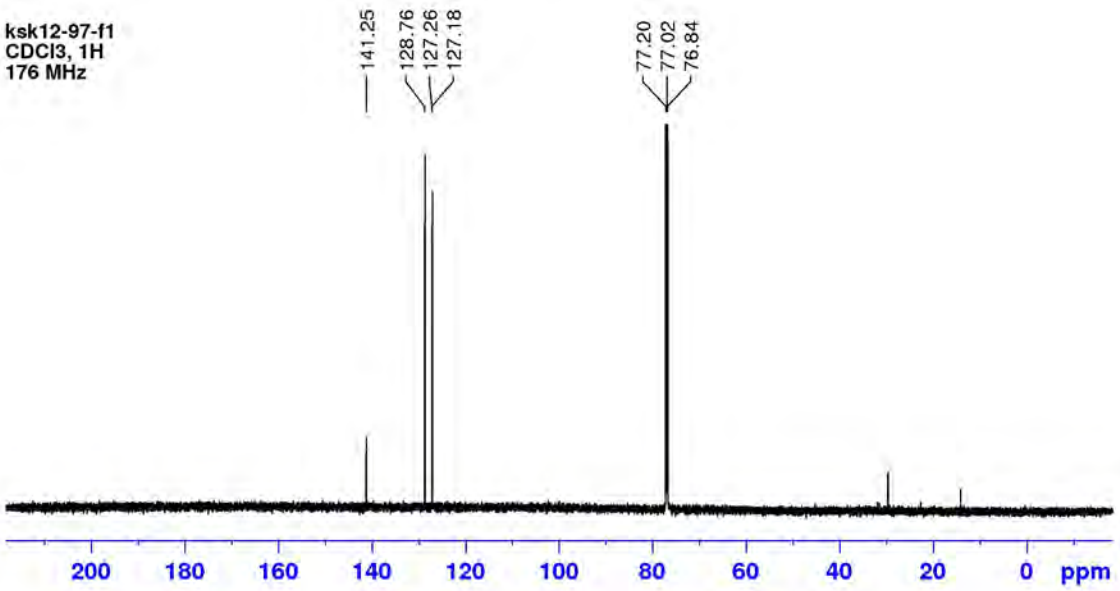

7.347
7.342
7.336
7.331
7.329
7.318
7.315
7.311
7.302
7.296
7.290
7.288
7.283
7.268
7.264
7.252
7.247
7.239
7.234
6.997
6.994
6.992
6.976
6.954
6.949
6.947
6.932
6.930
6.927
4.025
4.020
4.010
4.005
3.994
3.989
2.875
2.857
2.837
2.173
2.168
2.164
2.152
2.148
2.146
2.136
2.130
ksk12-97-f2
CDCl3, 1H
400 MHz
10
9
8
7
6
5
4
3
2
1
ppm
7.04
3.00
2.06
2.04
2.05


159.14
141.69
129.56
128.66
128.54
126.05
120.72
114.66
77.47
77.15
76.83
66.90
32.31
31.00
ksk12-97-f2
CDCl3, 1H
100 MHz
200
180
160
140
120
100
80
60
40
20
0
ppm




7.631
7.630
7.620
7.618
7.481
7.471
7.459
7.387
7.376
7.366
7.284
1.571
ksk12-97-f1
CDCl3, 1H
700 MHz
9
8
7
6
5
4
3
2
1
0
ppm
4.041
4.052
2.000




ksk12-97-f1
CDCl3, 1H
176 MHz
141.25
128.76
127.26
127.18
77.20
77.02
76.84
200
180
160
140
120
100
80
60
40
20
0
ppm