Supplementary Material (ESI) for Green Chemistry


# Electronic Supplementary Information

## A $CO_2/H_2O_2$-tunable reaction: direct conversion of styrene into styrene carbonate or phenacyl benzoate catalyzed by sodium phosphotungstate/n-$Bu_4NBr$

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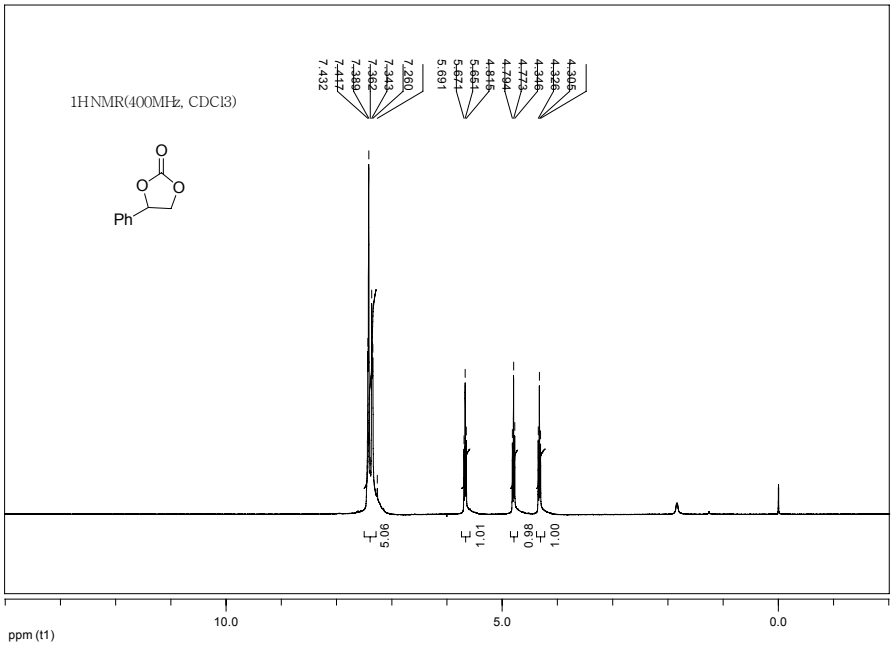
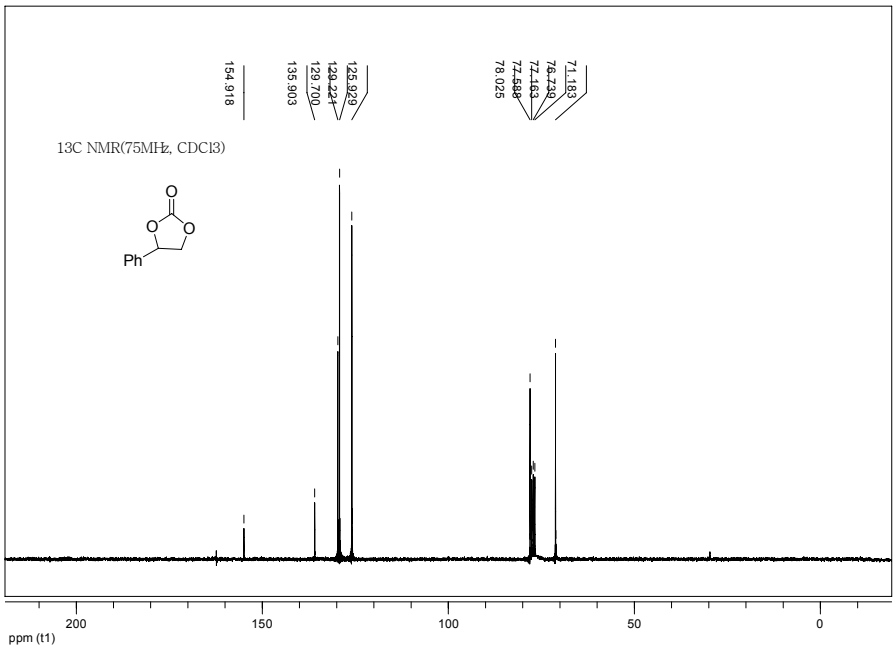
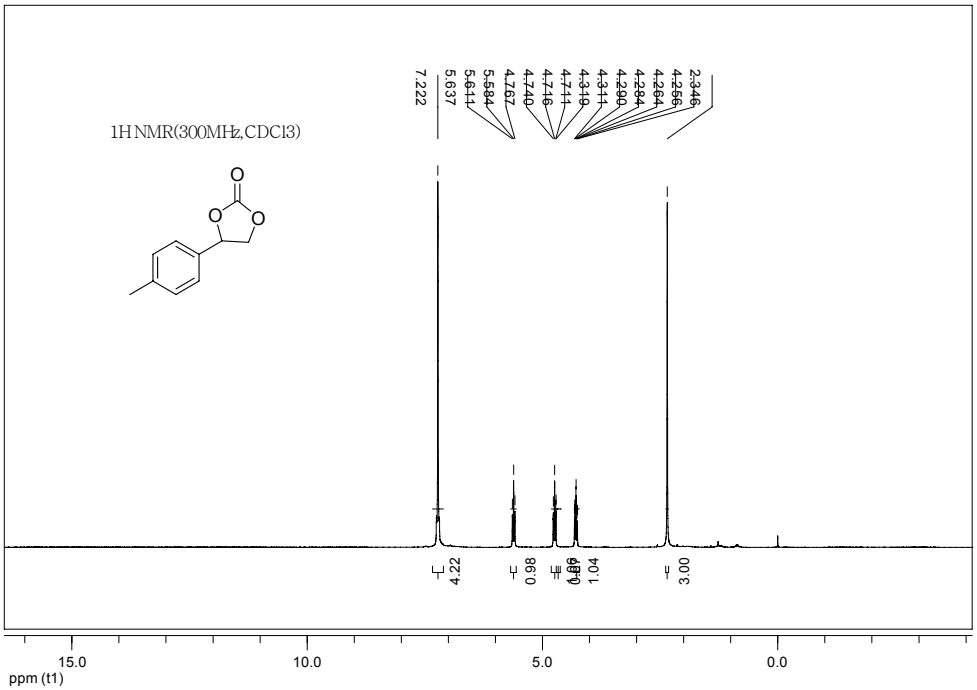
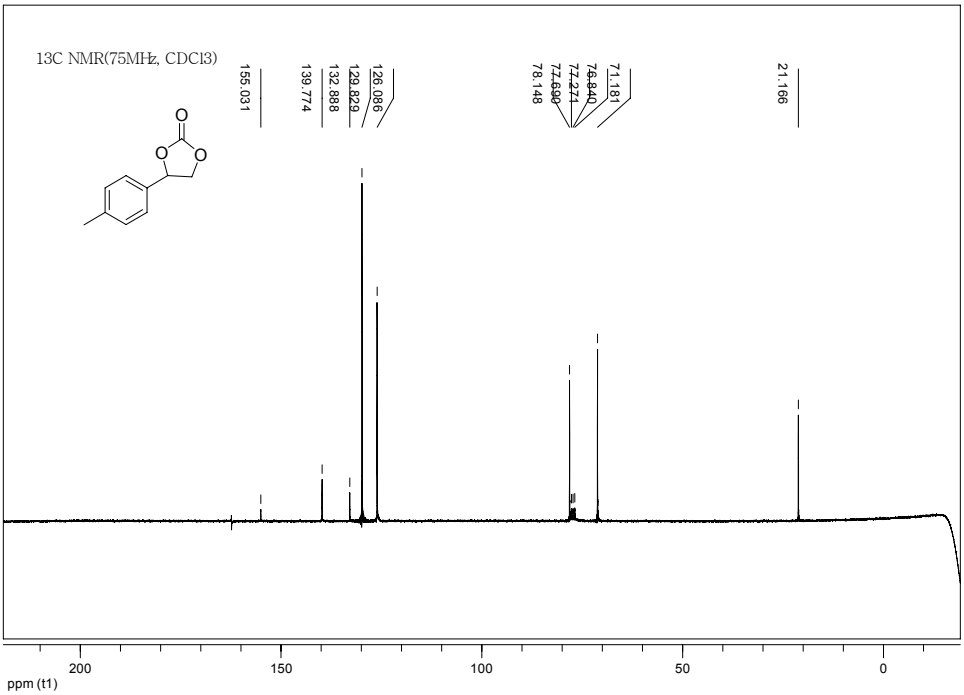
## (1) The $^{1}H$ NMR and $^{13}C$ NMR charts for products



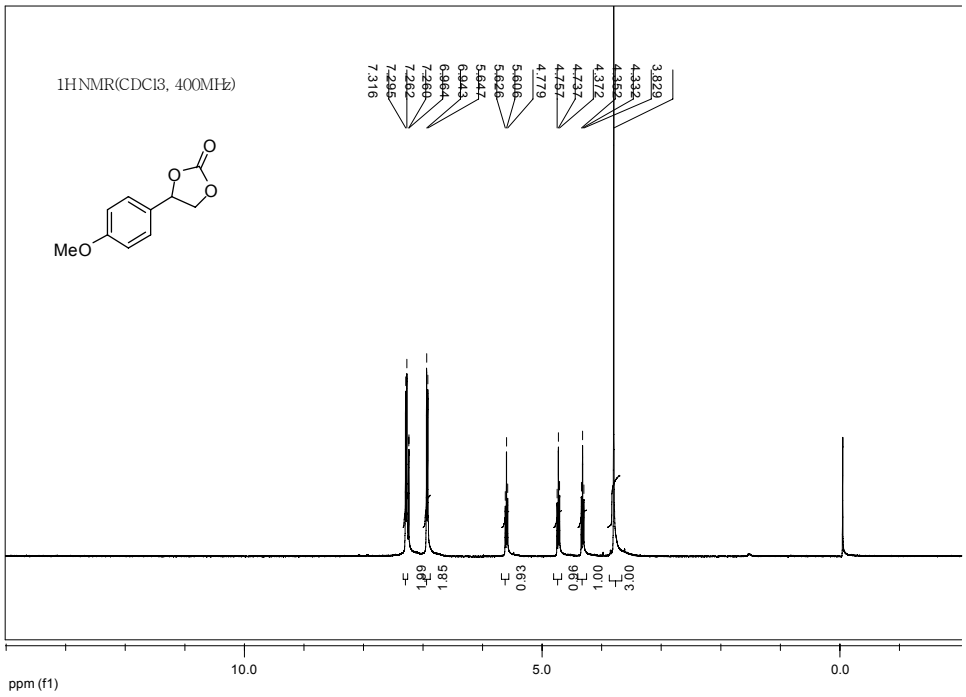



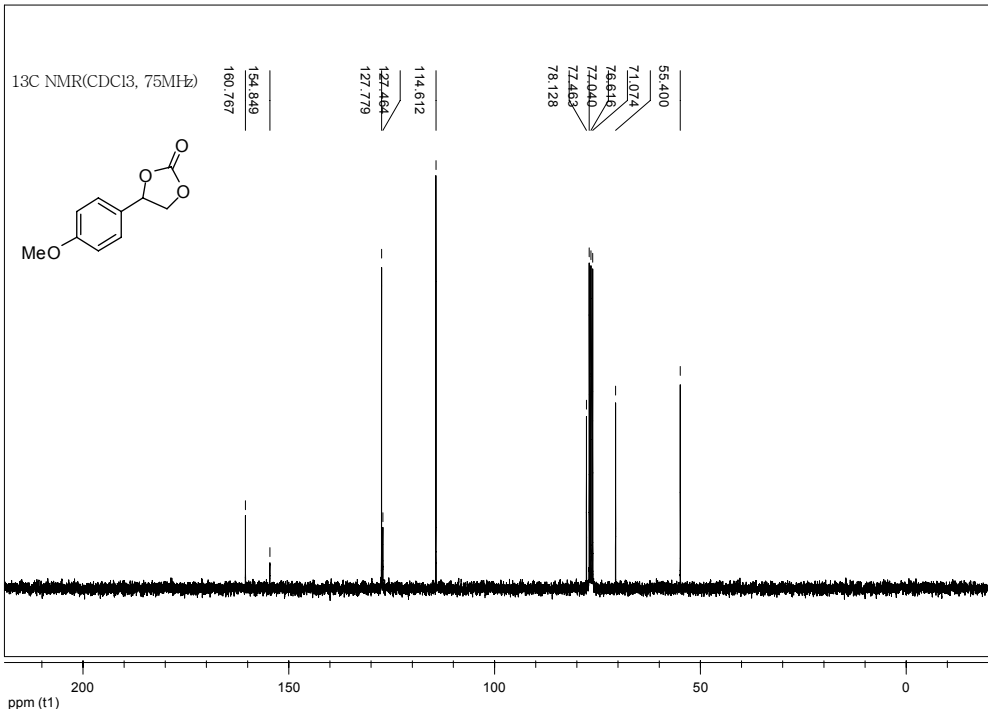

Product **1a**


1H NMR(300MHz,CDCl3)
7.222
5.637
5.611
5.594
4.767
4.740
4.716
4.711
4.319
4.311
4.290
4.284
4.264
4.256
2.346
4.22
0.98
3.00
15.0
10.0
5.0
0.0
ppm (t1)

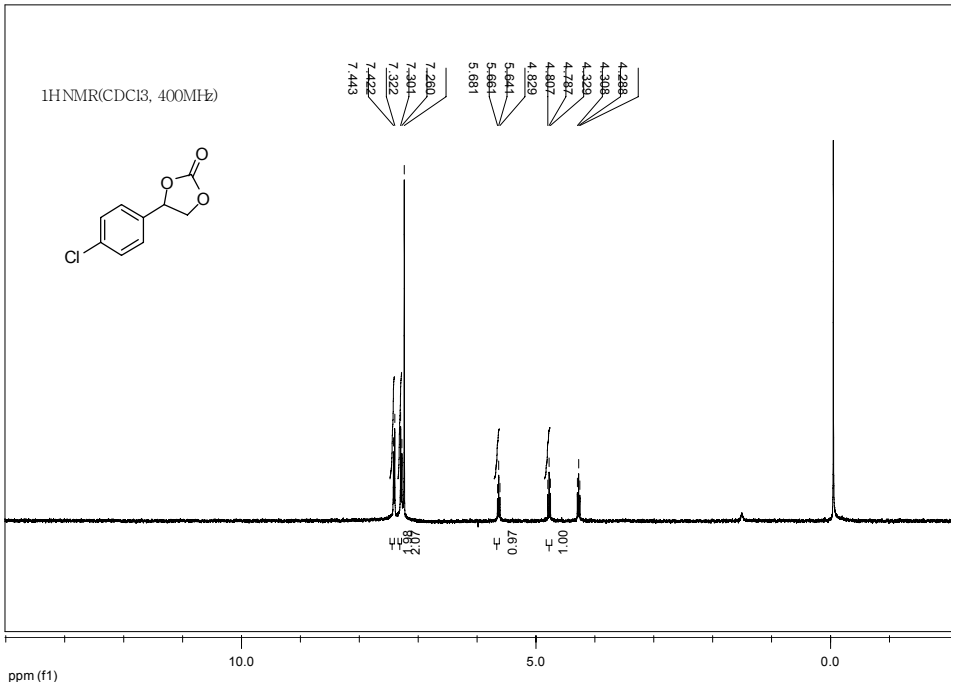

13C NMR(75MHz, CDCl3)
155.031
139.774
132.888
129.829
126.086
78.148
77.690
77.271
76.840
71.181
21.166
200
150
100
50
0
ppm (t1)

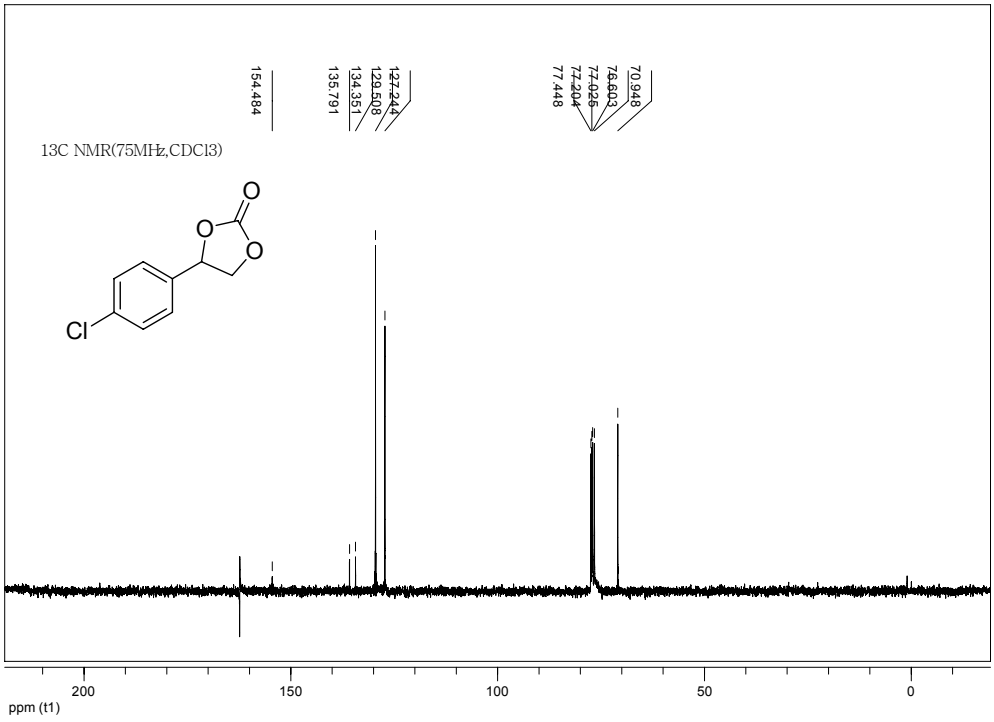
Product **2a**


1H NMR(CDCl3, 400MHz)
7.316
7.295
7.262
7.260
6.964
6.943
5.647
5.626
5.606
4.779
4.757
4.737
4.372
4.352
4.332
3.829
MeO
1.89
1.86
0.93
0.98
1.00
3.00
10.0
5.0
0.0
ppm (f1)


13C NMR(CDCl3, 75MHz)
160.767
154.849
127.779
127.484
114.612
78.128
77.463
77.040
76.616
71.074
55.400
MeO
200
150
100
50
0
ppm (t1)

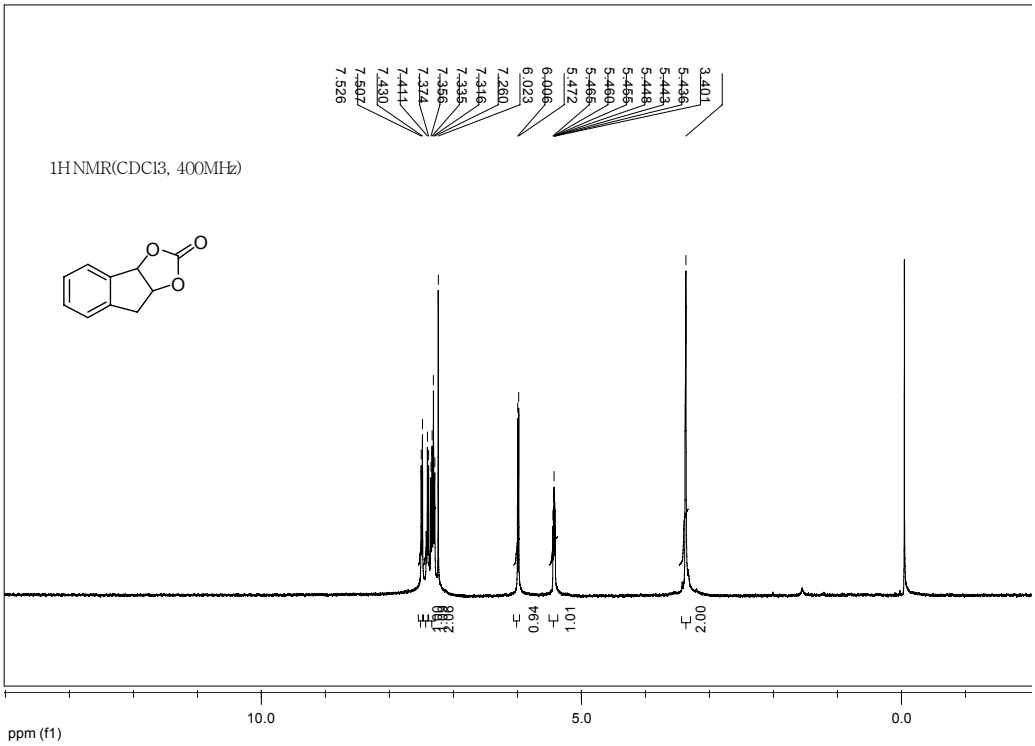
Product **3a**

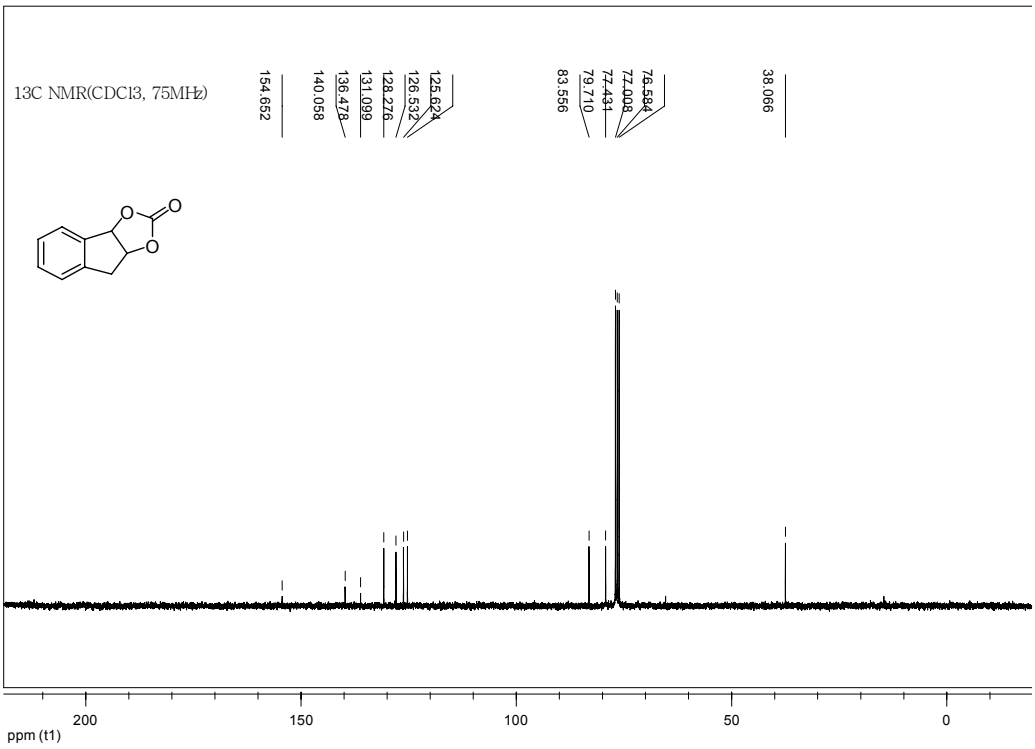

1H NMR(CDCl3, 400MHz)
7.443
7.422
7.322
7.301
7.280
5.681
5.661
5.641
4.829
4.807
4.787
4.329
4.308
4.288
2.07
1.98
0.97
1.00
Cl
10.0
5.0
0.0
ppm (f1)


154.484
135.791
134.351
129.508
127.244
77.448
77.204
77.025
76.603
70.948
13C NMR(75MHz,CDCl3)
Cl
200
150
100
50
0
ppm (t1)

Product **4a**

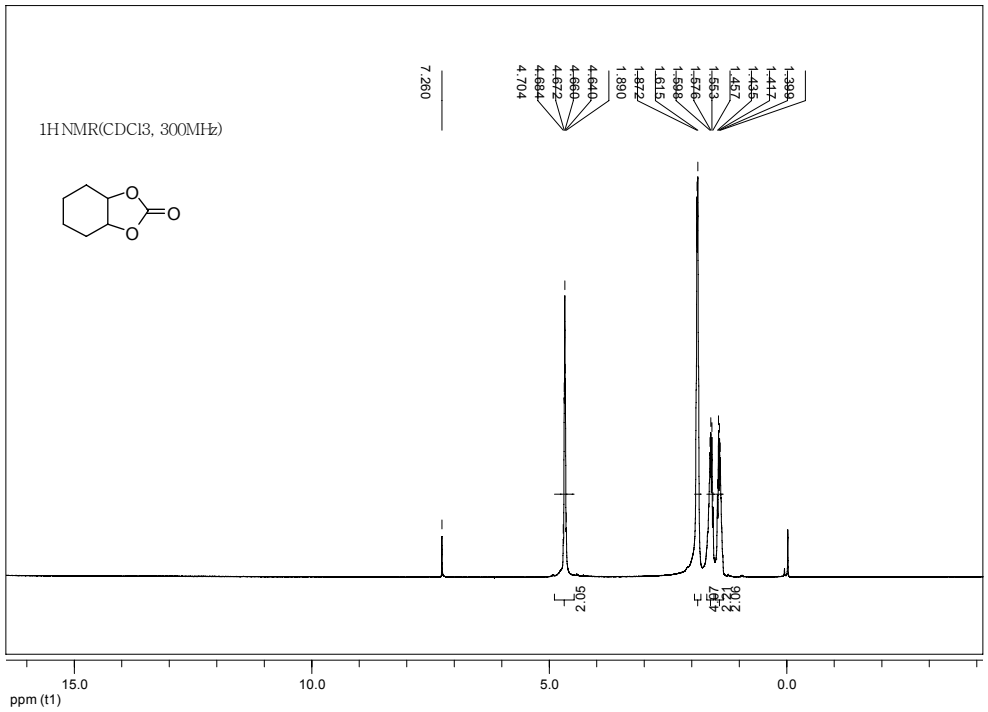
**S5**

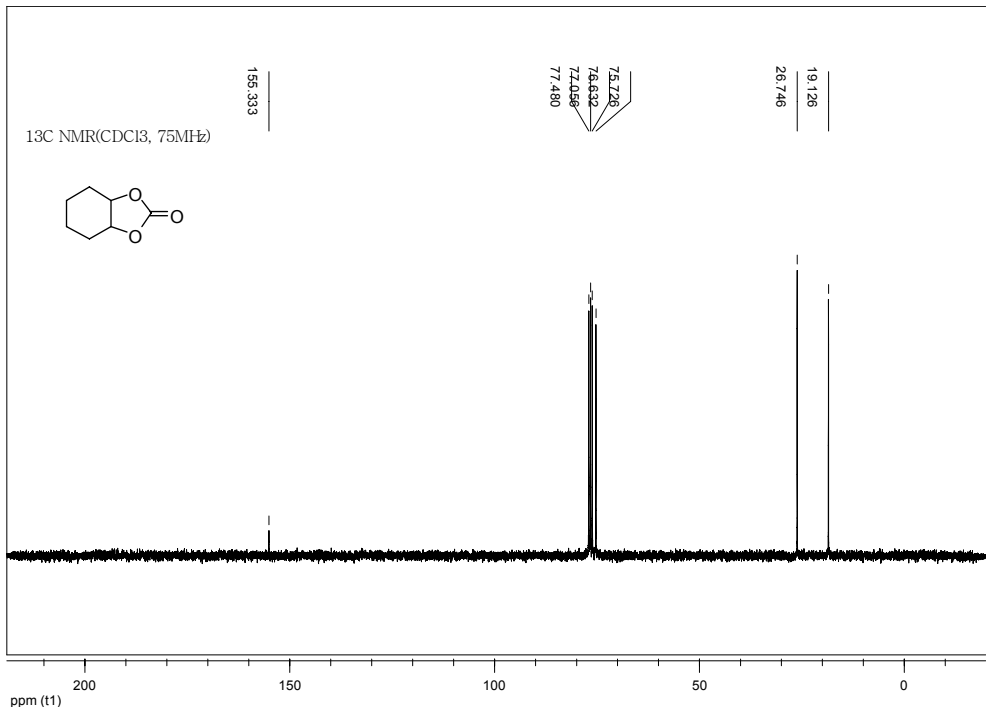

1H NMR(CDCl3, 400MHz)
7.526
7.507
7.430
7.411
7.374
7.356
7.335
7.316
7.260
6.023
6.006
5.472
5.465
5.460
5.455
5.448
5.443
5.436
3.401
0.94
1.01
2.00
10.0
5.0
0.0
ppm (f1)


13C NMR(CDCl3, 75MHz)
154.652
140.058
136.478
131.099
128.276
126.532
125.624
83.556
79.710
77.431
77.008
76.584
38.066
200
150
100
50
0
ppm (t1)

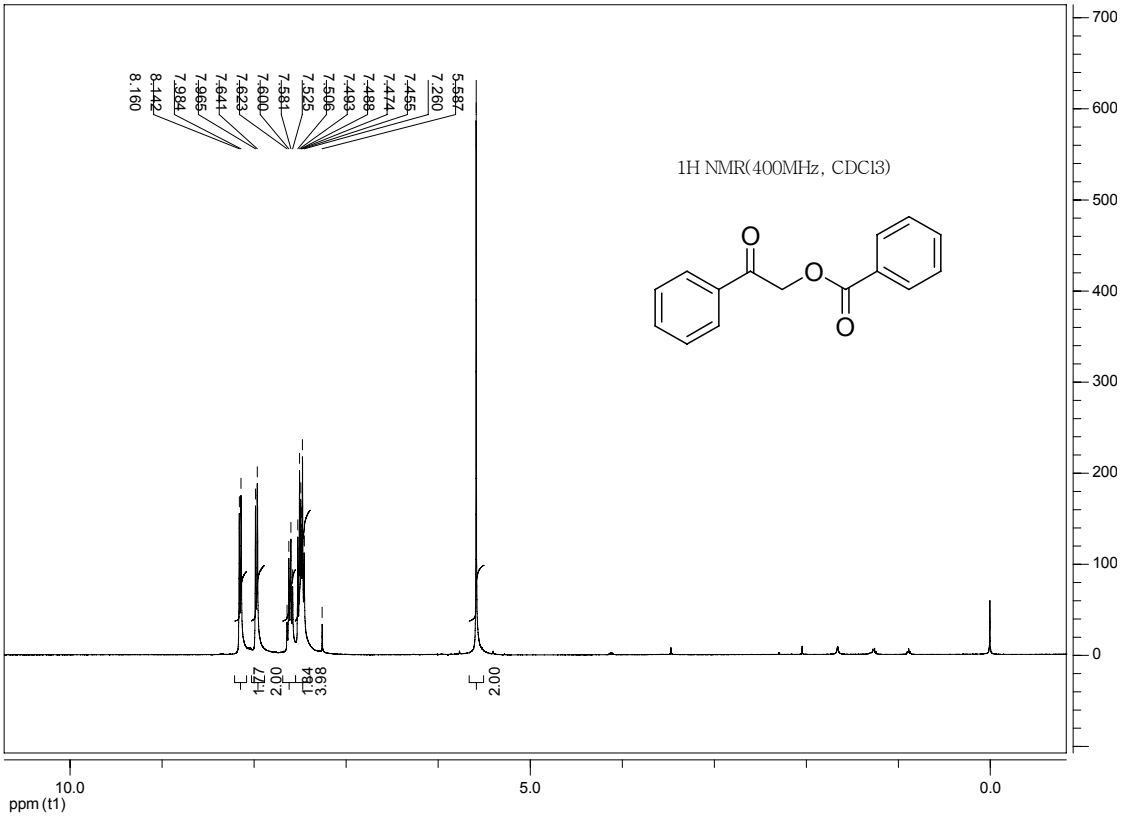
Product **5a**

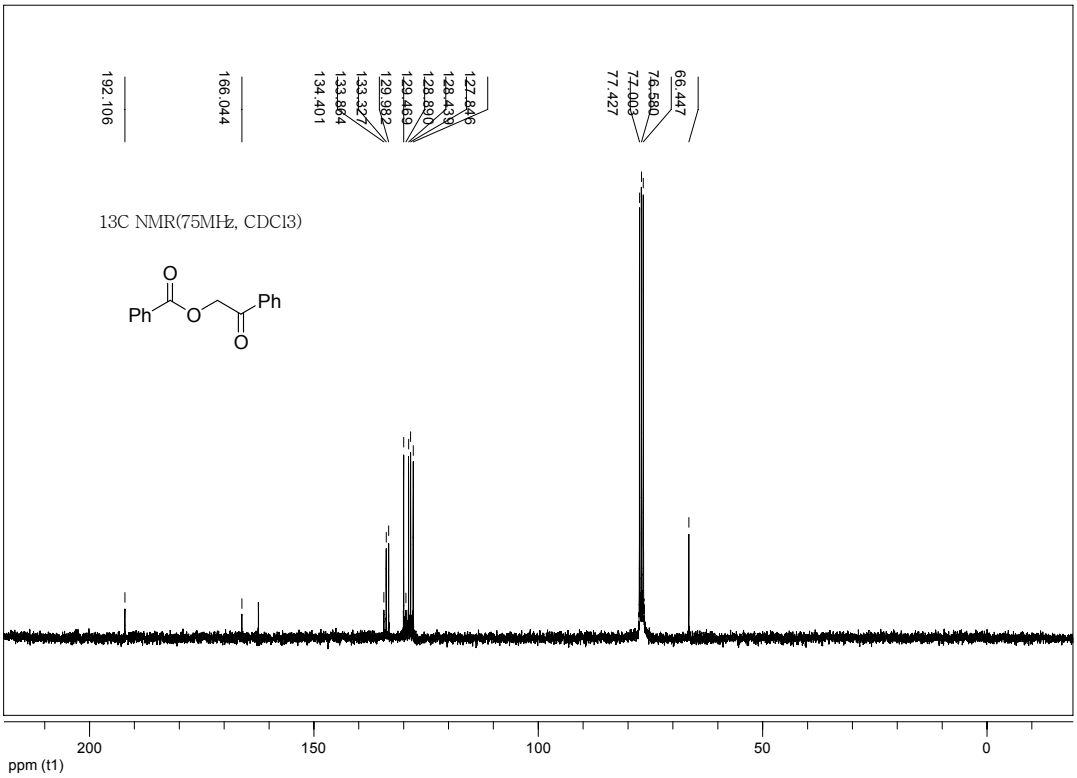




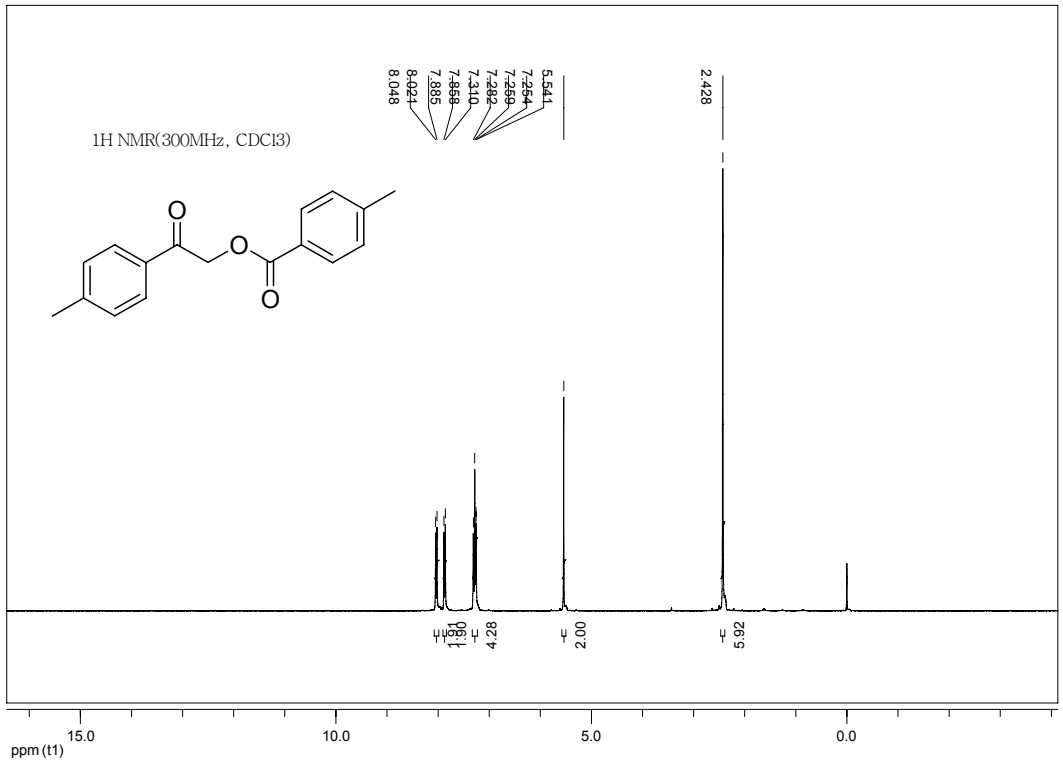

Product **6a**

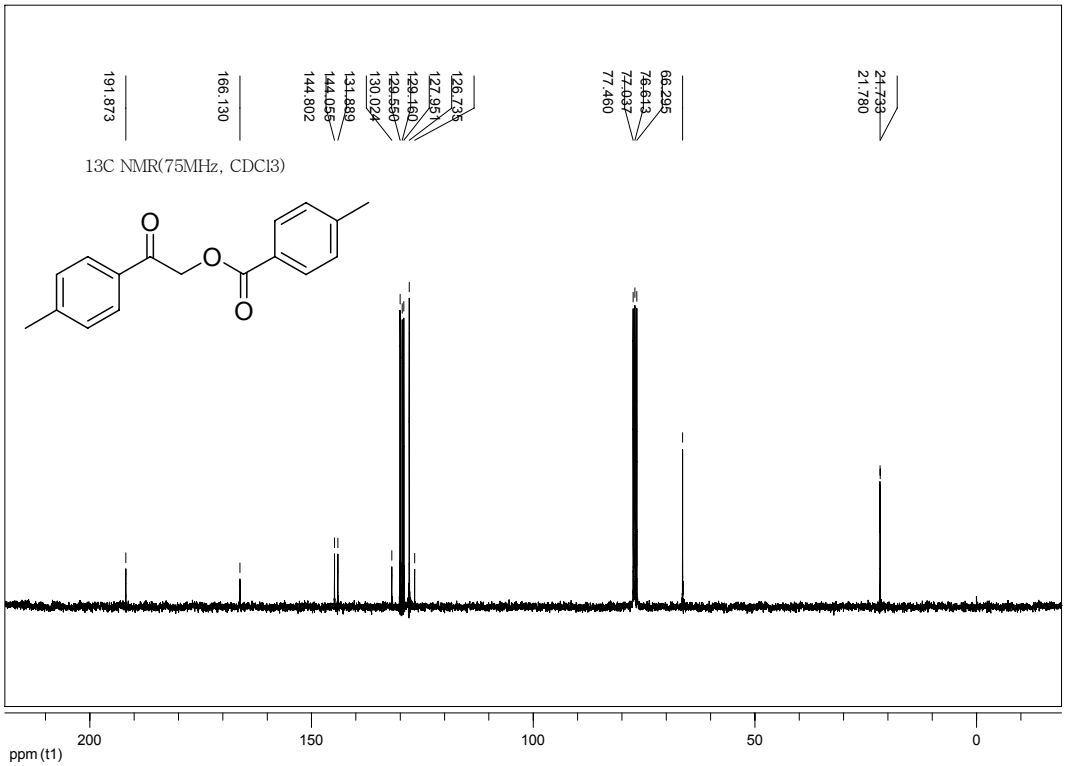

8.160
8.142
7.984
7.965
7.641
7.623
7.600
7.581
7.525
7.506
7.493
7.488
7.474
7.455
7.260
5.587
1H NMR(400MHz, CDCl3)
O
O
O
1.77
2.00
1.84
3.98
2.00
700
600
500
400
300
200
100
0
10.0
5.0
0.0
ppm (t1)


192.106
166.044
134.401
133.864
133.327
129.982
129.469
128.890
128.439
127.846
77.427
77.003
76.580
66.447
13C NMR(75MHz, CDCl3)
O
Ph
O
Ph
O
200
150
100
50
0
ppm (t1)

Product **1b**

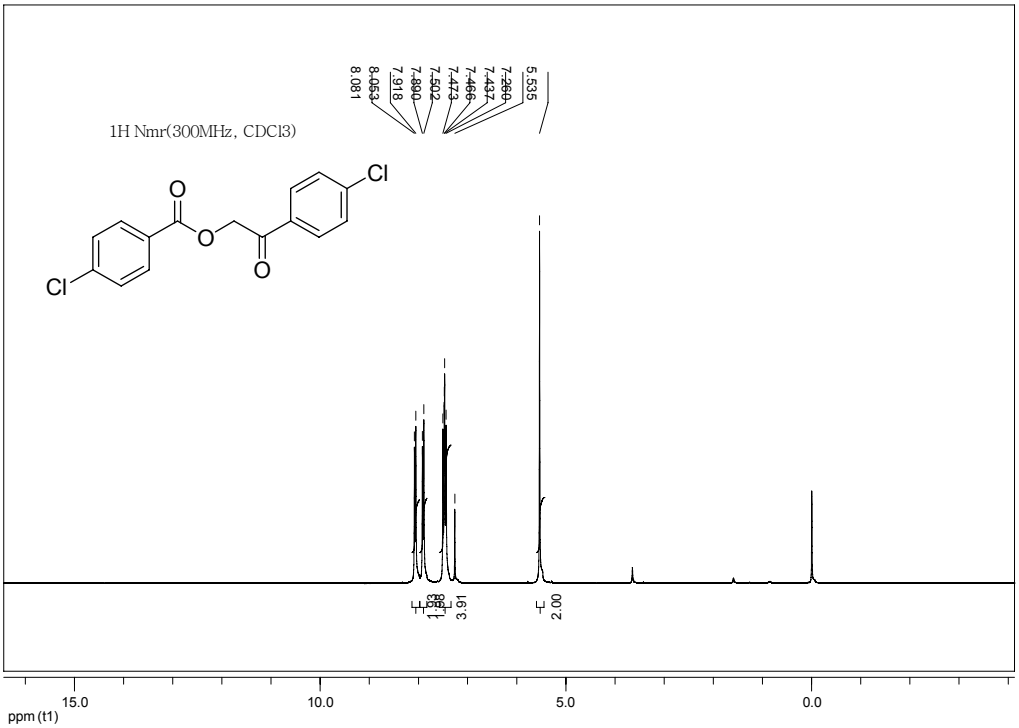


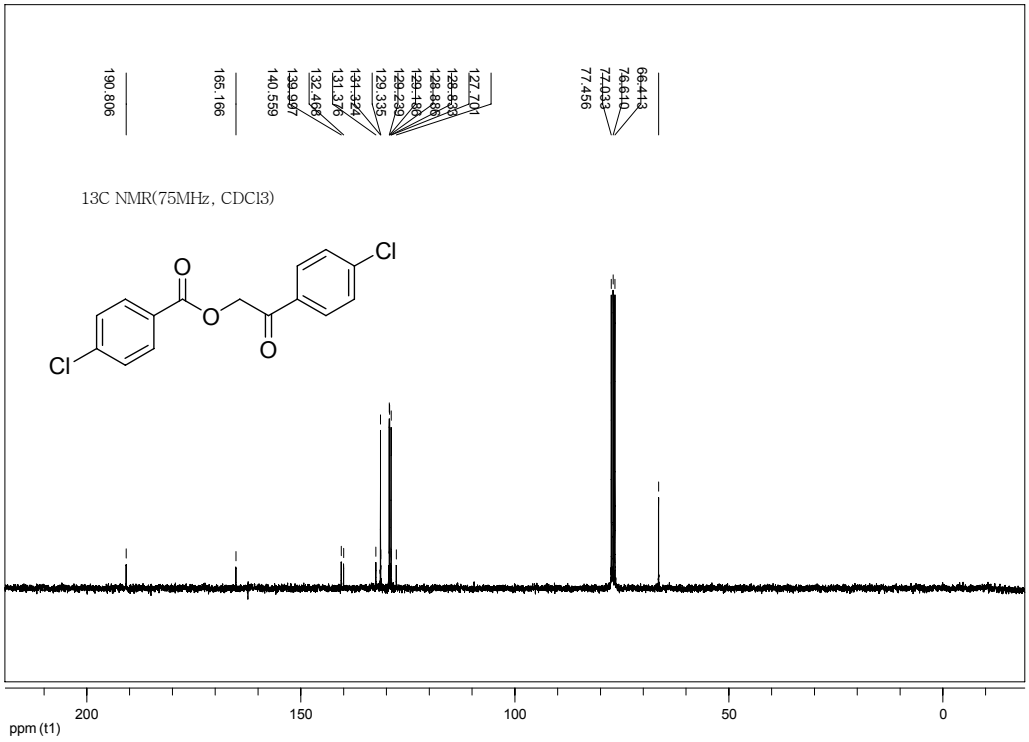

8.048
8.021
7.885
7.868
7.310
7.282
7.259
7.254
5.541
2.428
1H NMR(300MHz, CDCl3)
O
O
O
1.00
1.61
4.28
2.00
5.92
15.0
10.0
5.0
0.0
ppm (t1)


191.873
166.130
144.802
144.056
131.889
130.024
129.550
129.160
127.951
126.735
77.460
77.037
76.613
66.295
21.780
21.733
13C NMR(75MHz, CDCl3)
O
O
O
200
150
100
50
0
ppm (t1)

Product **2b**



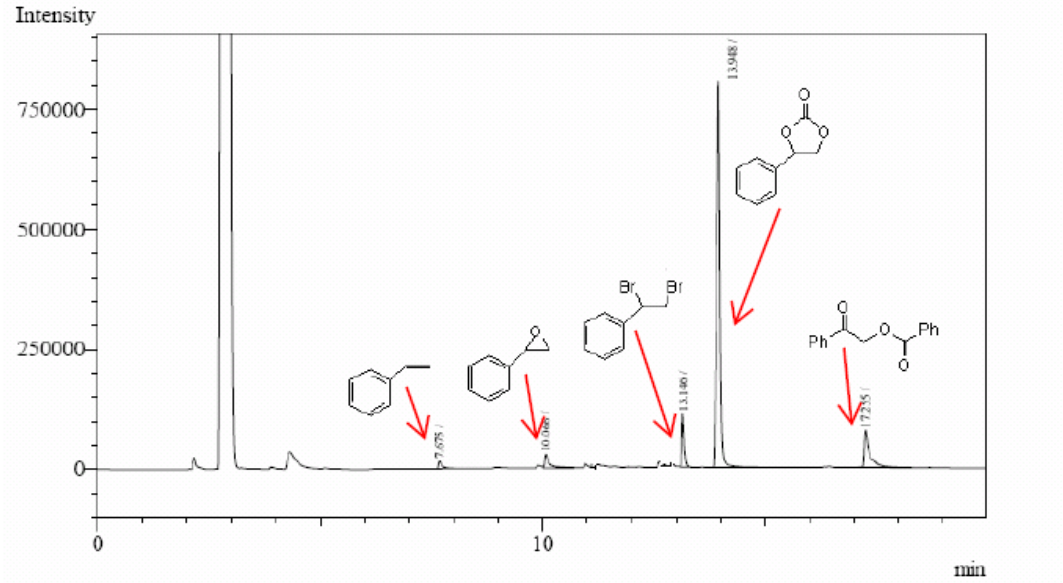

8.081
8.053
7.918
7.890
7.502
7.473
7.466
7.437
7.260
5.535
1H Nmr(300MHz, CDCl3)
Cl
Cl
O
O
O
3.91
2.00
15.0
10.0
5.0
0.0
ppm (t1)




Product **4b**

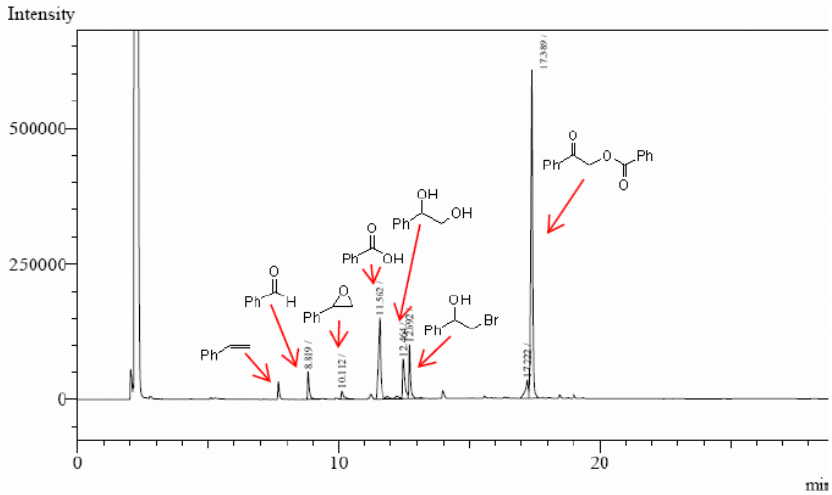


**(2) Typical GC chart of the reaction mixture for producing 1a**




| Peak# | Ret.Time | Area | Height | Conc. | Unit | Mark | ID# | Cmpd Name | Height% | Area% |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 7.675 | 90246 | 14551 | 0.000 | | | | | 1.4128 | 1.6066 |
| 2 | 10.066 | 238725 | 28583 | 0.000 | | V | | | 2.7751 | 4.2499 |
| 3 | 13.146 | 369083 | 108453 | 0.000 | | | | | 10.5297 | 6.5706 |
| 4 | 13.948 | 4256732 | 801254 | 0.000 | | | | | 77.7933 | 75.7800 |
| 5 | 17.255 | 662435 | 77137 | 0.000 | | V | | | 7.4892 | 11.7929 |
| **Total** | | 5617221 | 1029978 | | | | | | 100.0000 | 100.0000 |

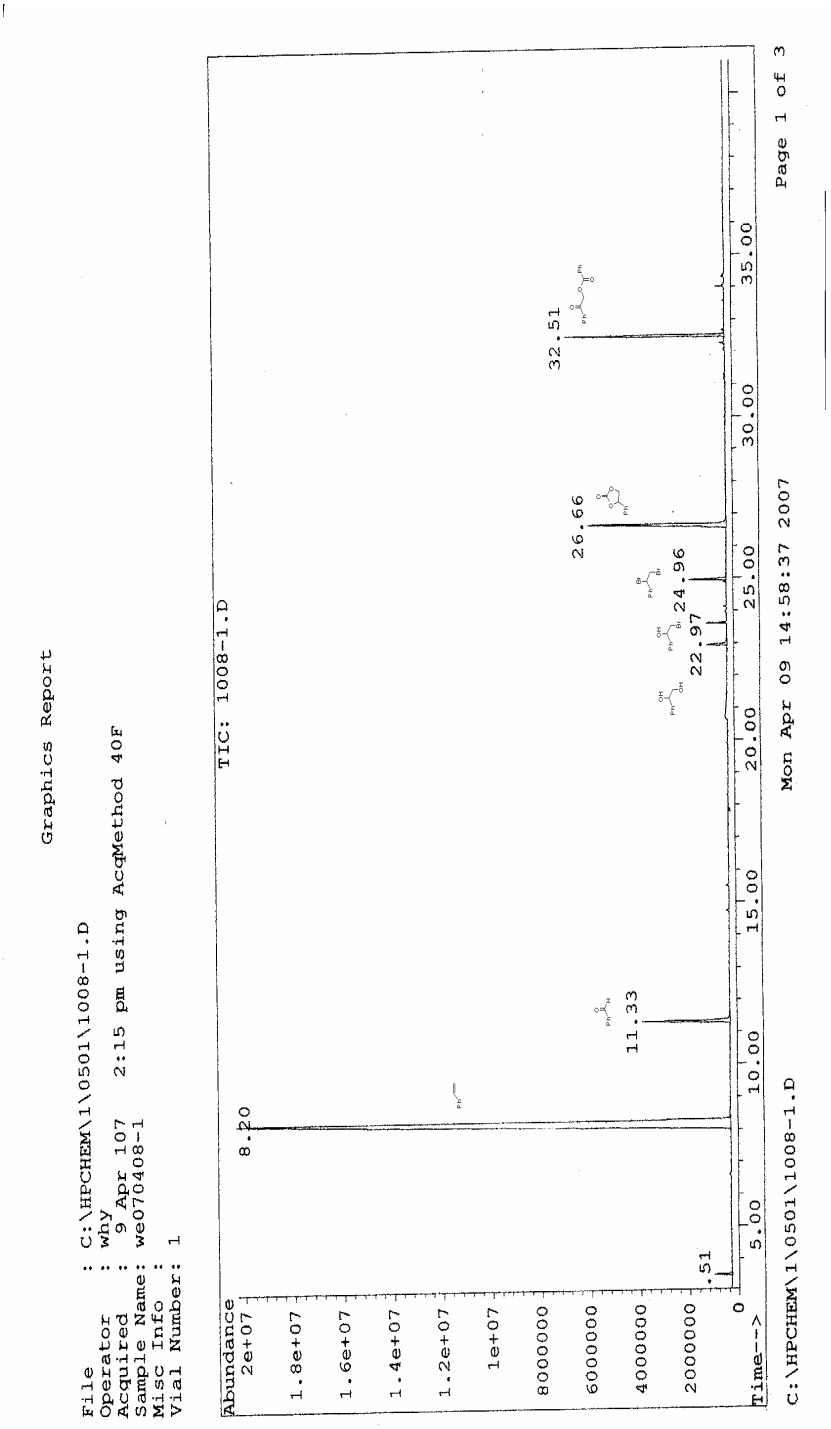
## (3) Typical GC chart of the reaction mixture for producing 1b

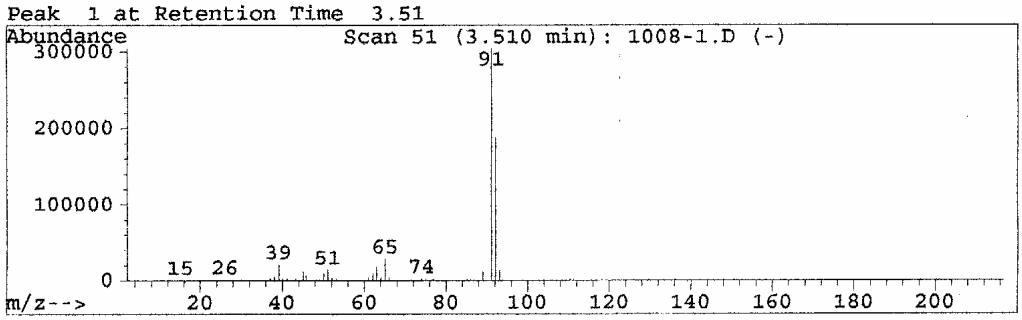


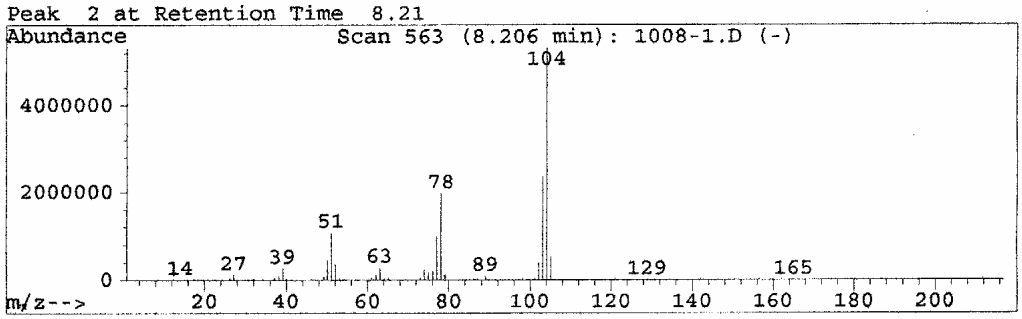

| Peak# | Ret.Time | Area | Height | Conc. | Unit | Mark | ID# | Cmpd Name | Area% |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 8.819 | 222307 | 50906 | 0.000 | | S | | | 4.1665 |
| 2 | 10.112 | 103535 | 16486 | 0.000 | | V | | | 1.9405 |
| 3 | 11.562 | 994508 | 150169 | 0.000 | | S | | | 18.6391 |
| 4 | 12.464 | 441379 | 74642 | 0.000 | | V | | | 8.2723 |
| 5 | 12.692 | 415735 | 99758 | 0.000 | | SV | | | 7.7917 |
| 6 | 17.222 | 271018 | 34396 | 0.000 | | | | | 5.0794 |
| 7 | 17.389 | 2887124 | 600703 | 0.000 | | V | | | 54.1105 |
| **Total** | | 5335606 | 1027060 | | | | | | 100.0000 |

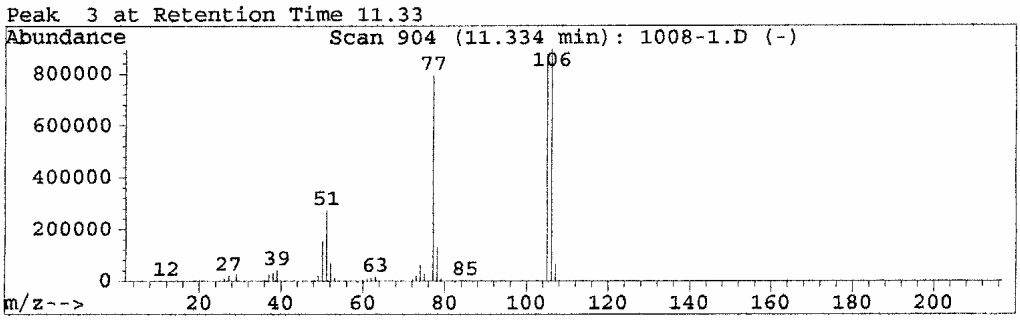


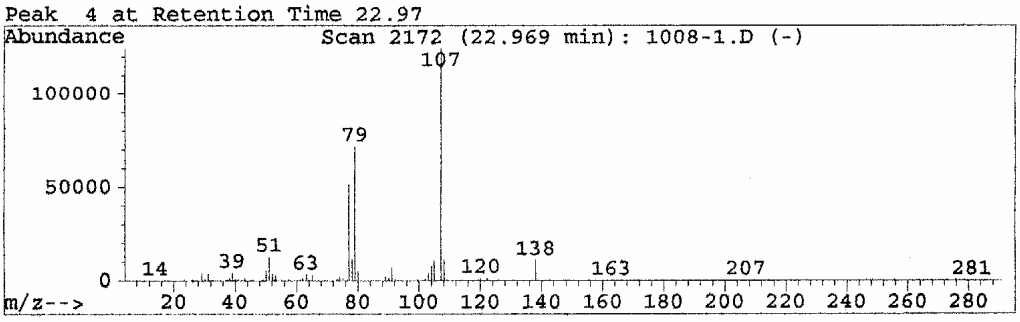
## (4) GC-MS charts of the reaction mixture

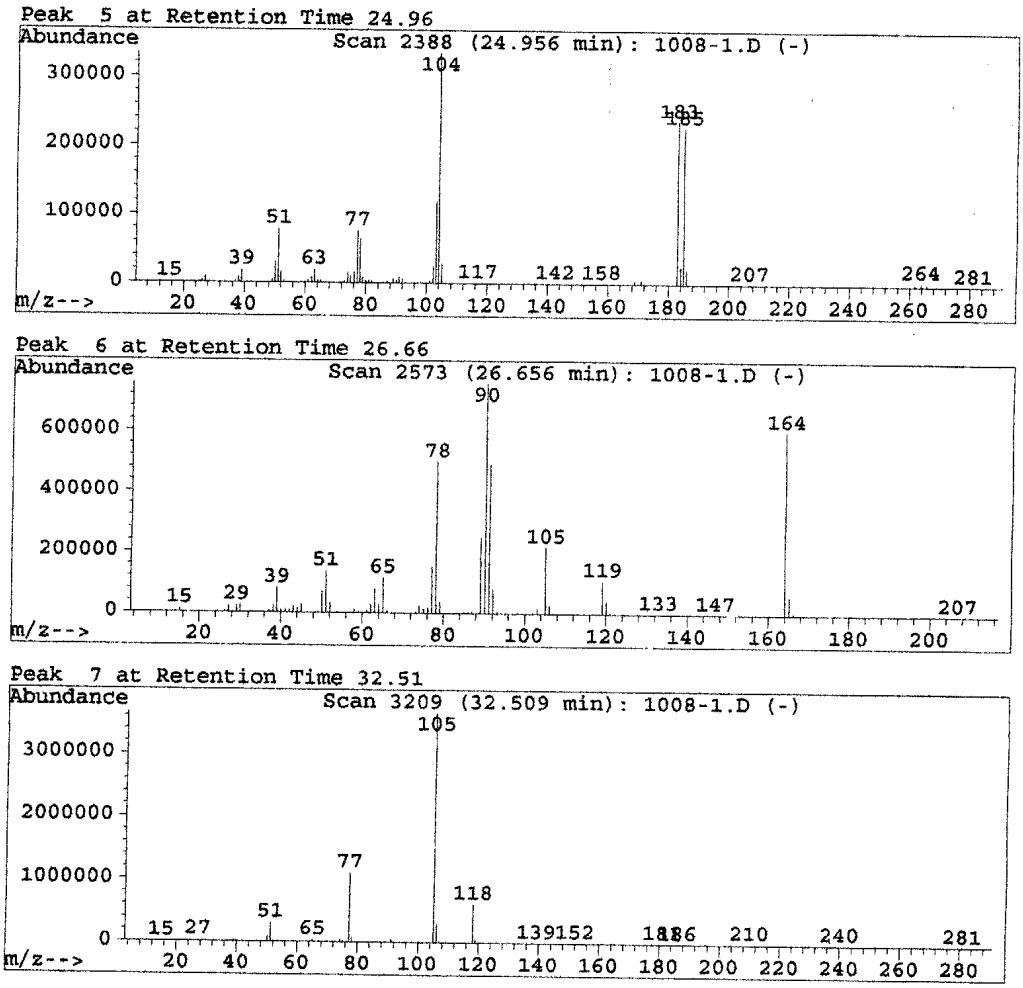

Graphics Report
File : C:\HPCHEM\1\0501\1008-1.D
Operator : why
Acquired : 9 Apr 107 2:15 pm using AcqMethod 40F
Sample Name: we070408-1
Misc Info :
Vial Number: 1
TIC: 1008-1.D
Abundance
8.20
11.33
22.97
24.96
26.66
32.51
Time-->
C:\HPCHEM\1\0501\1008-1.D
Mon Apr 09 14:58:37 2007
Page 1 of 3


Peak 1 at Retention Time 3.51
Abundance
Scan 51 (3.510 min): 1008-1.D (-)
300000
200000
100000
0
91
15 26 39 51 65 74
m/z-->
20 40 60 80 100 120 140 160 180 200


Peak 2 at Retention Time 8.21
Abundance
Scan 563 (8.206 min): 1008-1.D (-)
4000000
2000000
0
104
78
51
14 27 39 63 89 129 165
m/z-->
20 40 60 80 100 120 140 160 180 200


Peak 3 at Retention Time 11.33
Abundance
Scan 904 (11.334 min): 1008-1.D (-)
800000
600000
400000
200000
0
77
106
51
12 27 39 63 85
m/z-->
20 40 60 80 100 120 140 160 180 200


Peak 4 at Retention Time 22.97
Abundance
Scan 2172 (22.969 min): 1008-1.D (-)
100000
50000
0
107
79
51
14 39 63 120 138 163 207 281
m/z-->
20 40 60 80 100 120 140 160 180 200 220 240 260 280




C:\HPCHEM\1\0501\1008-1.D Mon Apr 09 14:58:41 2007 Page 3 of 3