Supporting Information for:

Alkoxide-Functionalized Imidazolium Betaine for CO_2 Activation and Catalytic Transformation

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Contents:

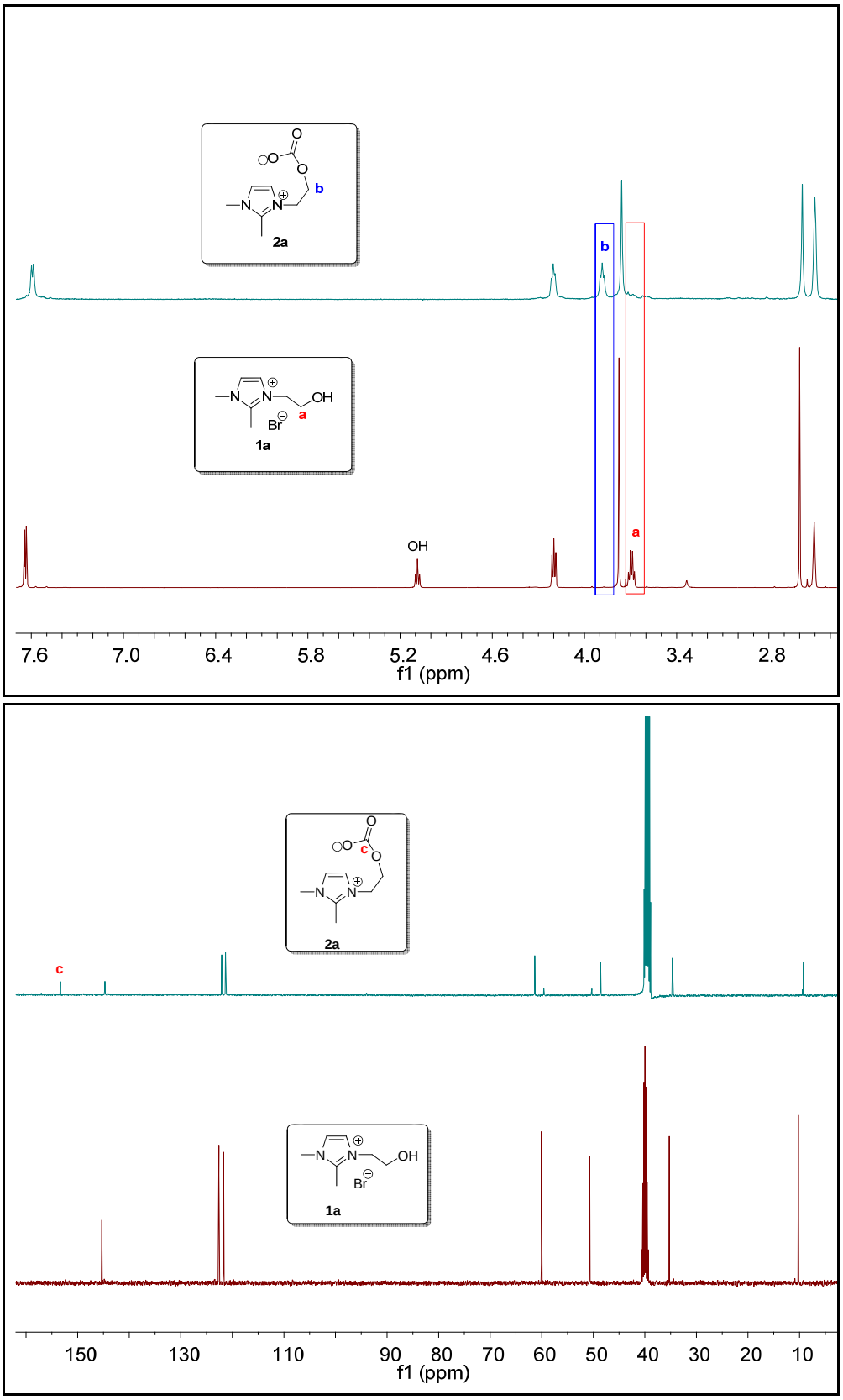
1. Crystallography

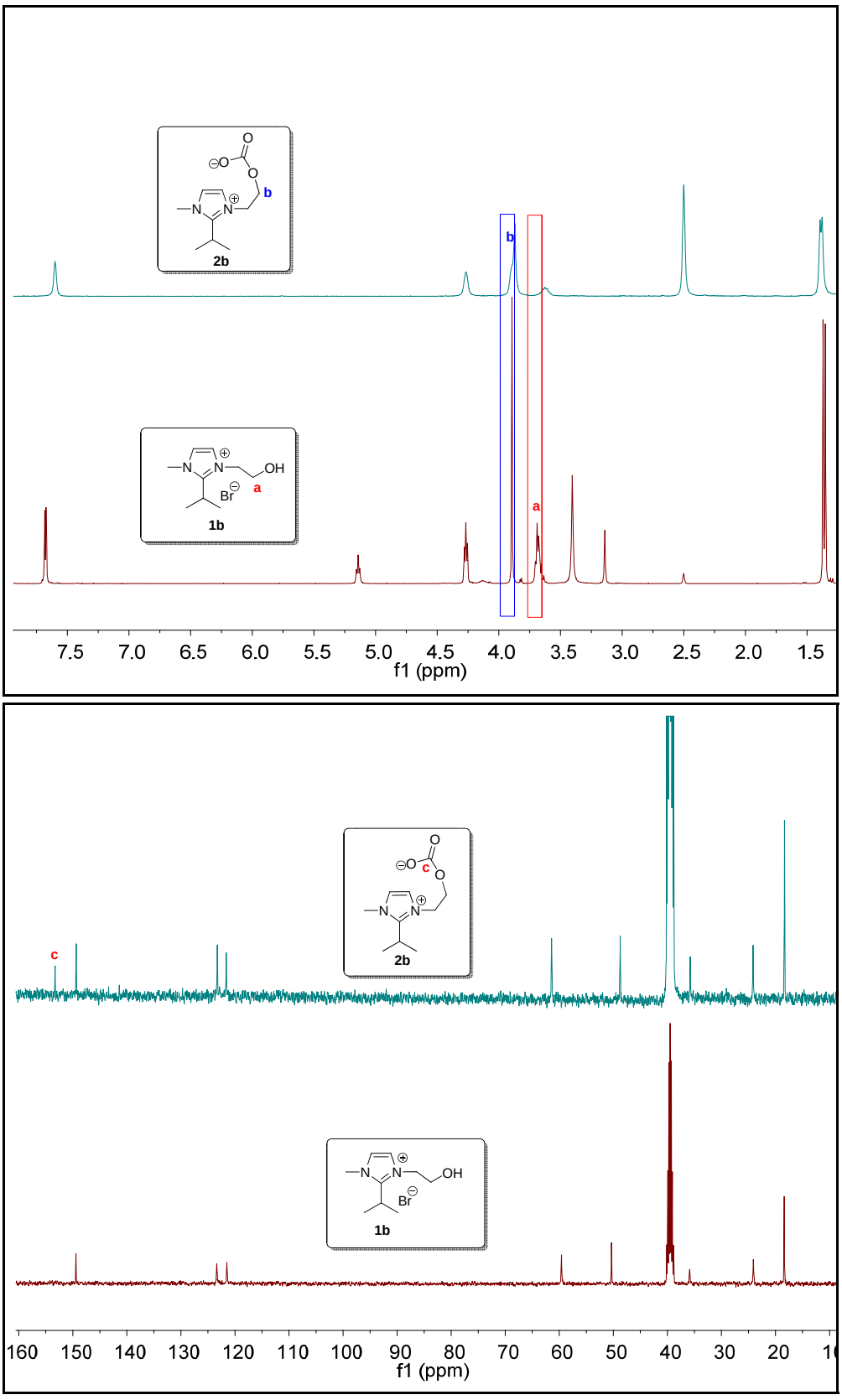
Single crystals of complexe **3c** suitable for X-ray structural analysis were obtained from a CH_2Cl_2/hexane solution at -30°C. Single crystals of complexes **4b** and **4c** suitable for X-ray structural analysis were obtained from a CH_3OH/H_2O solution at -10 °C. Diffraction datas were collected at 220 K on a Bruker SMART-CCD diffractometer using graphite-monochromated Mo Kα radiation (λ = 0.71073 Å). The structures were solved by direct methods and refined by full-matrix least squares on F^2. All nonhydrogen atoms were refined anisotropically, and the hydrogen atoms were included in idealized positions. All calculations were performed using the SHELXTL crystallographic software packages. Details of the crystal data, data collections, and structure refinements are summarized in Table S1. CCDC-971545 (**3c**), CCDC-971543 (**4b**), and CCDC-971544 (**4c**) contain supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

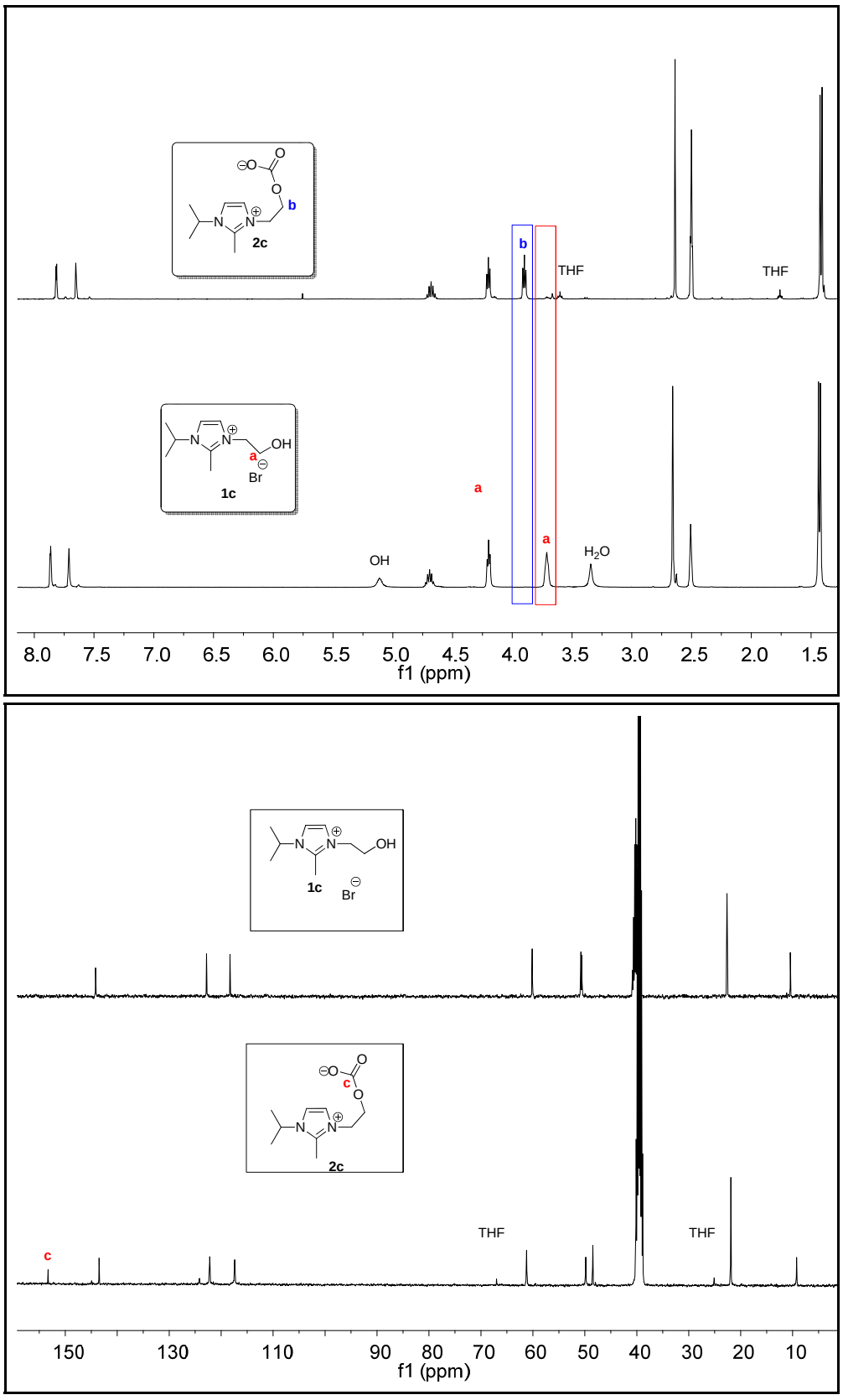
Table S1. Crystal data and structural refinement details for complexes **3c**, **4b and 4c**

	3c	**4b**	**4c**
mol formula	$C_{10}H_{19}N_2O_5$	$C_{10}H_{16}N_2OS_2$	$C_{10}H_{16}N_2OS_2$
mol wt	247.27	244.37	244.37
cryst syst	Orthorhombic	Monoclinic	Monoclinic
space group	Pbcn	P2(1)/c	P2(1)/n
a/Å	12.1669(7)	10.7382(3)	7.0242(4)
b/Å	12.0650(7)	10.2853(3)	15.4761(9)
c/Å	19.281(1)	11.9959(3)	11.2508(7)
α/deg	90.00	90.00	90.00
β/deg	90.00	114.837 (1)	92.082 (1)
γ/deg	90.00	90.00	90.00
V/Å^3	2830.3(3)	1202.35(6)	1222.2 (1)
Z	8	4	4
R_{int}	0.0309	0.0267	0.0533
R1 (I > 2σ)	0.108	0.0345	0.0518
wR2 (I > 2σ)	0.405	0.1000	0.1340
GOF	0.933	1.051	1.028

2, Representative ^{1}H NMR and ^{13}C NMR comparison for 1 and 2, 2 and 3.






2c
b
THF
THF
1c
a
Br
OH
a
OH
H_2O
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
f1 (ppm)
1c
OH
Br
2c
c
THF
THF
c
150 130 110 90 80 70 60 50 40 30 20 10
f1 (ppm)

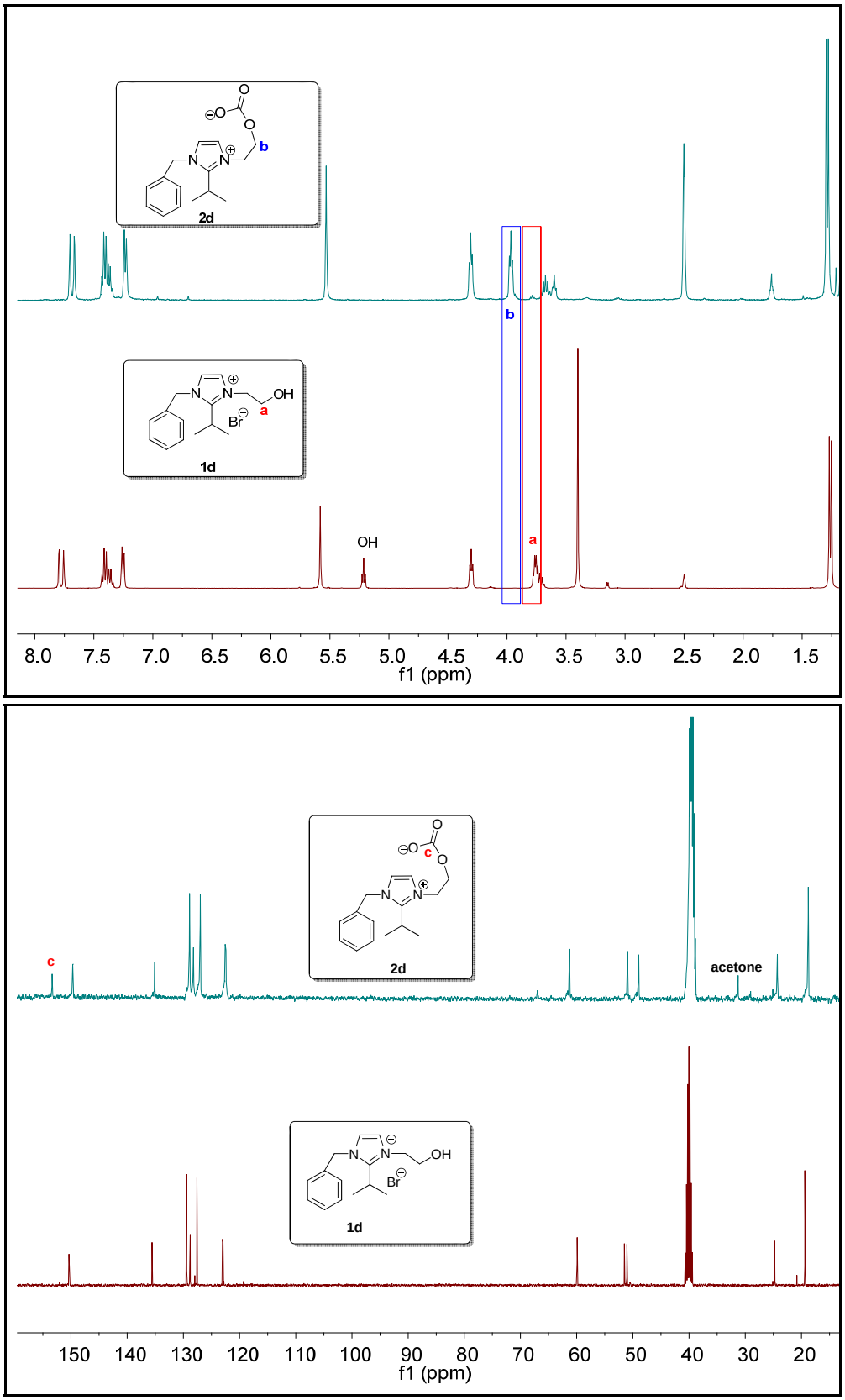


Figure S1 ^{1}H NMR and ^{13}C NMR comparison for **1** and **2**

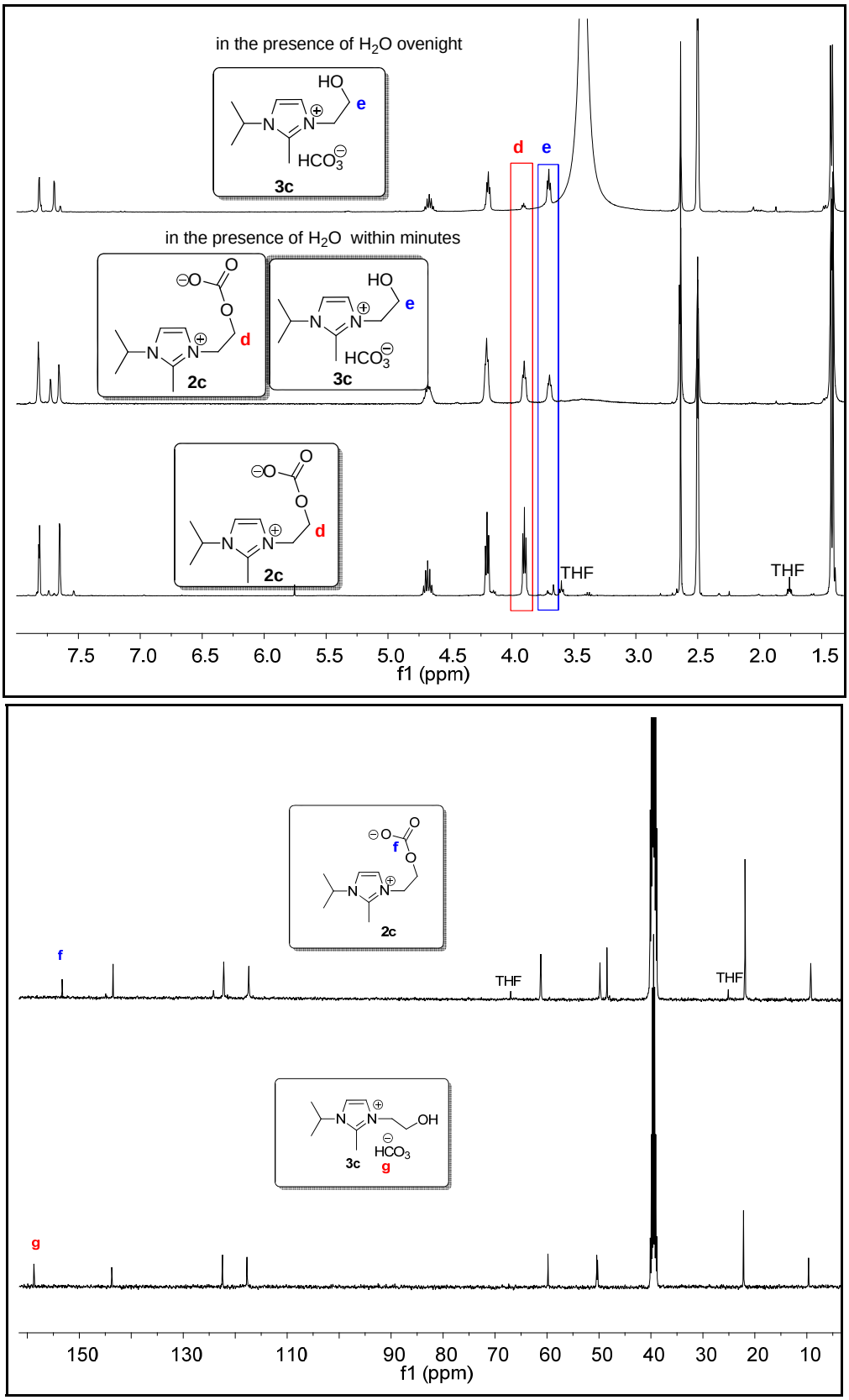
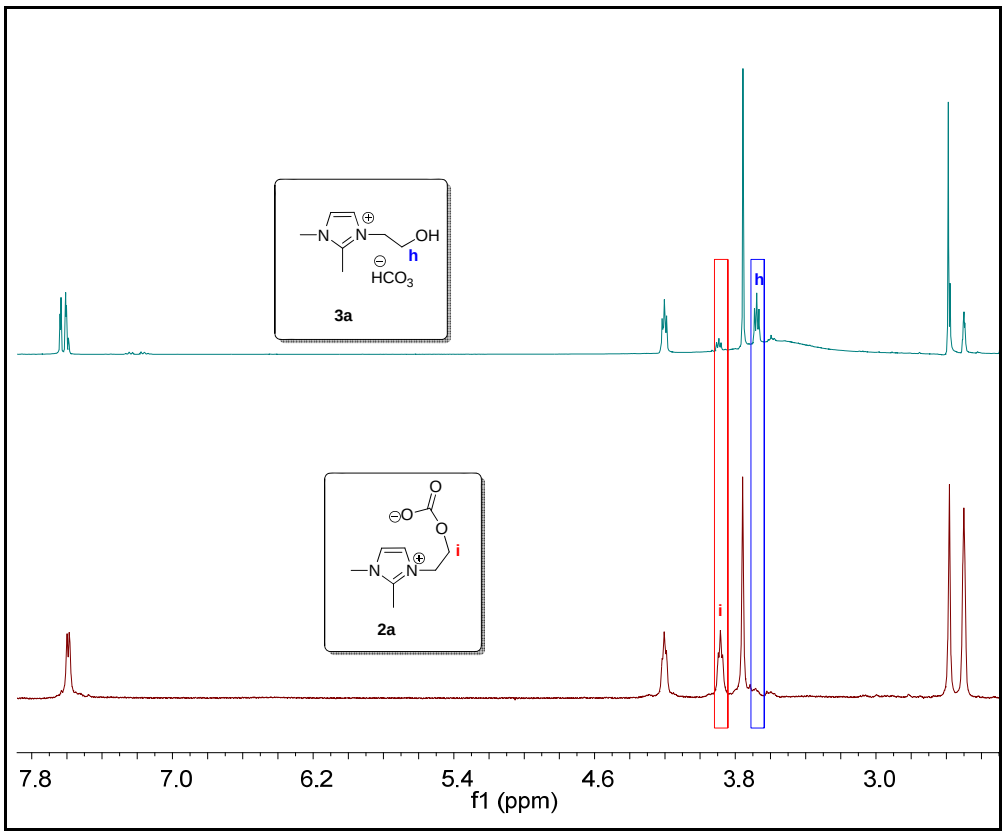
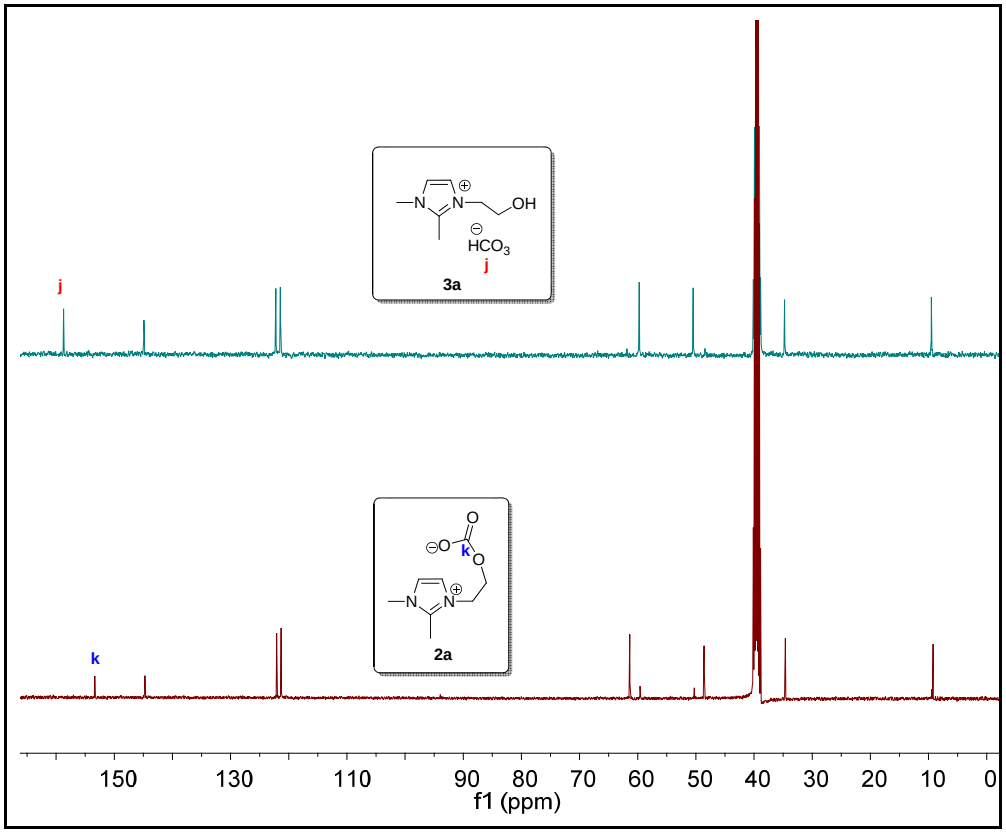
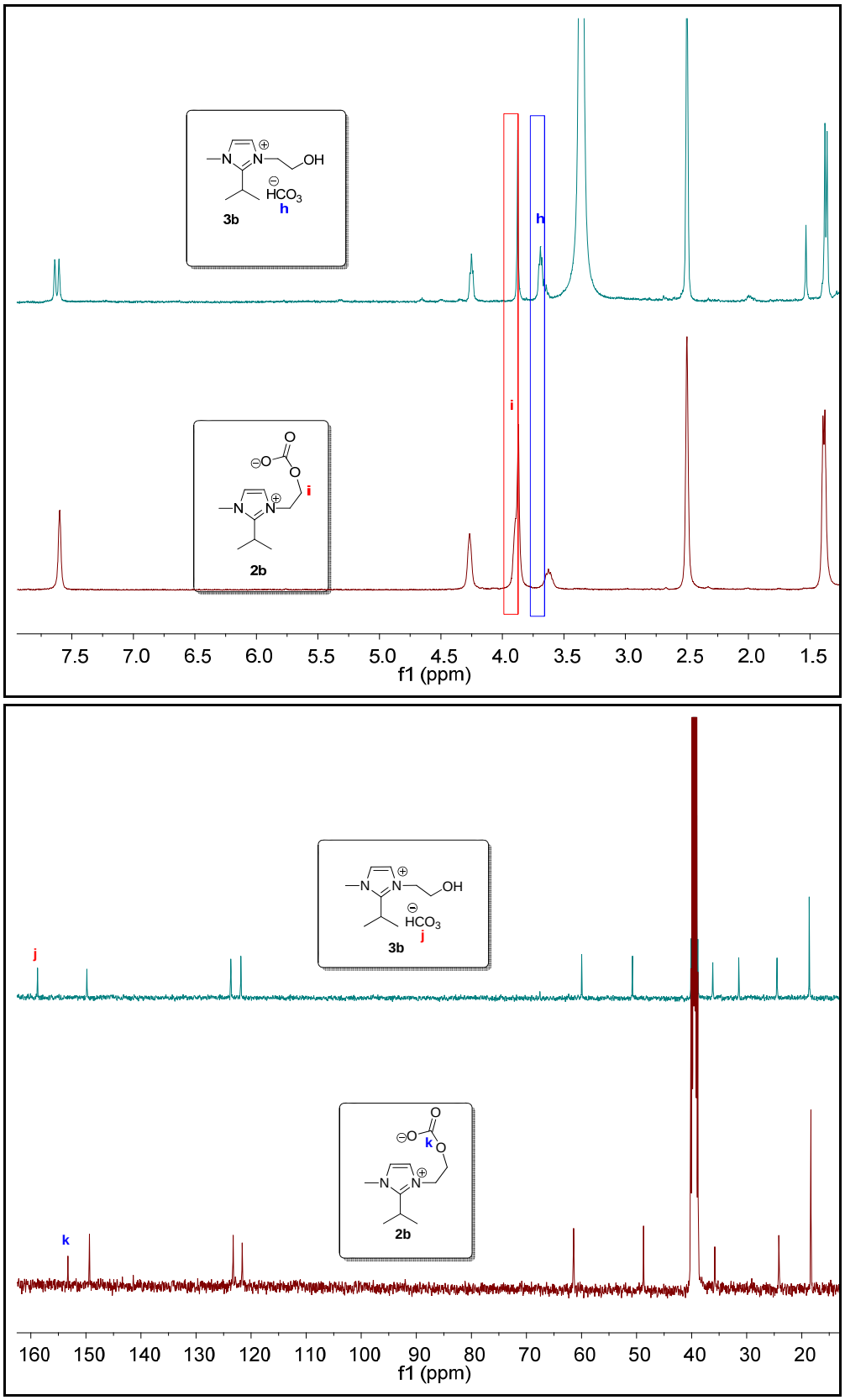


Figure S2 ^{1}H NMR and ^{13}C NMR comparison for **2c** and **3c**







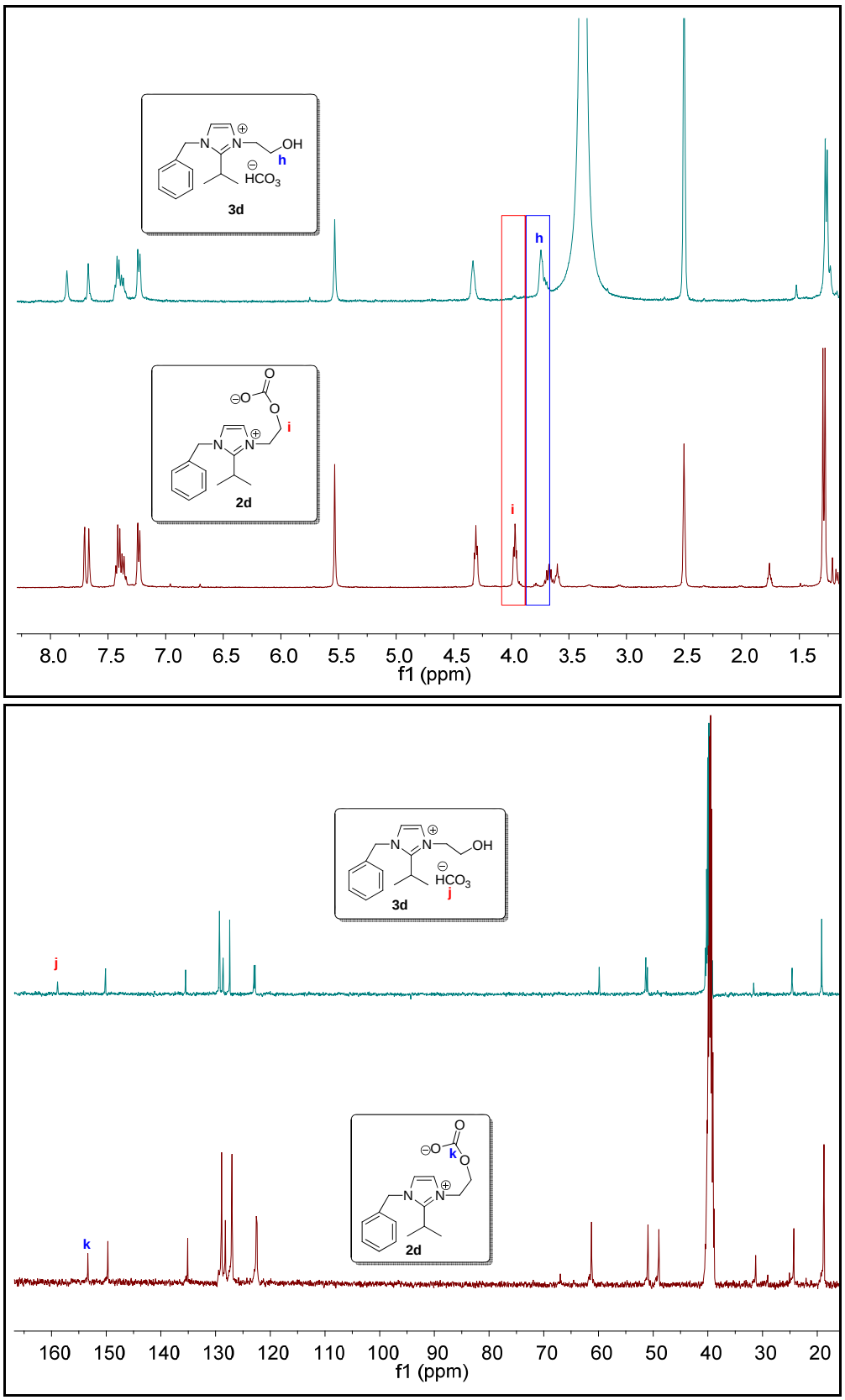
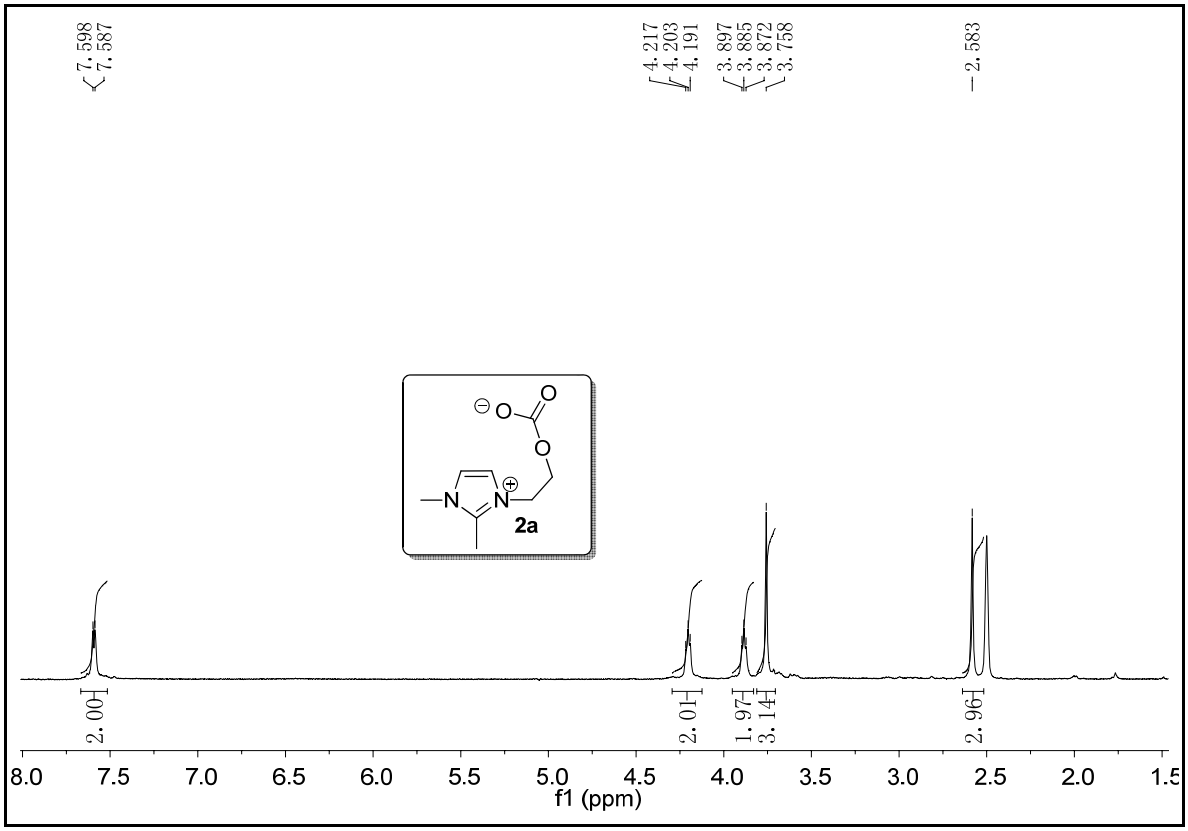
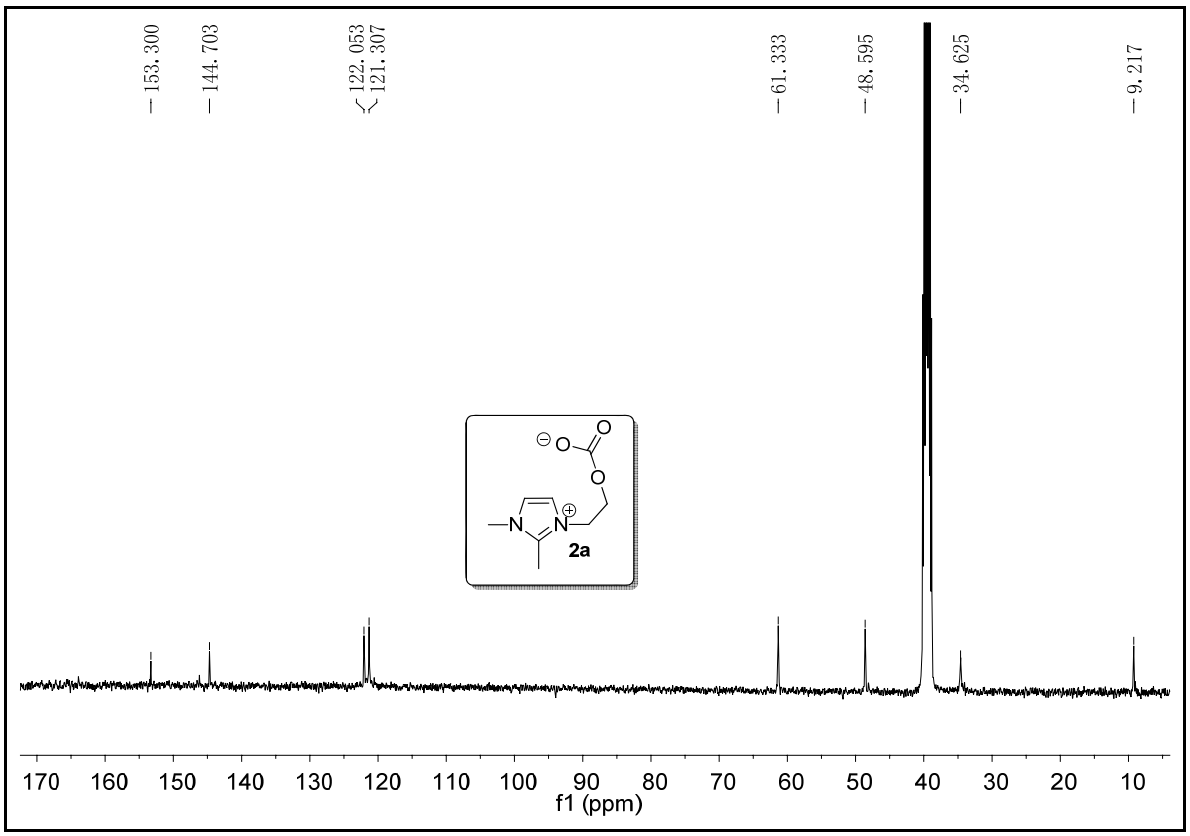
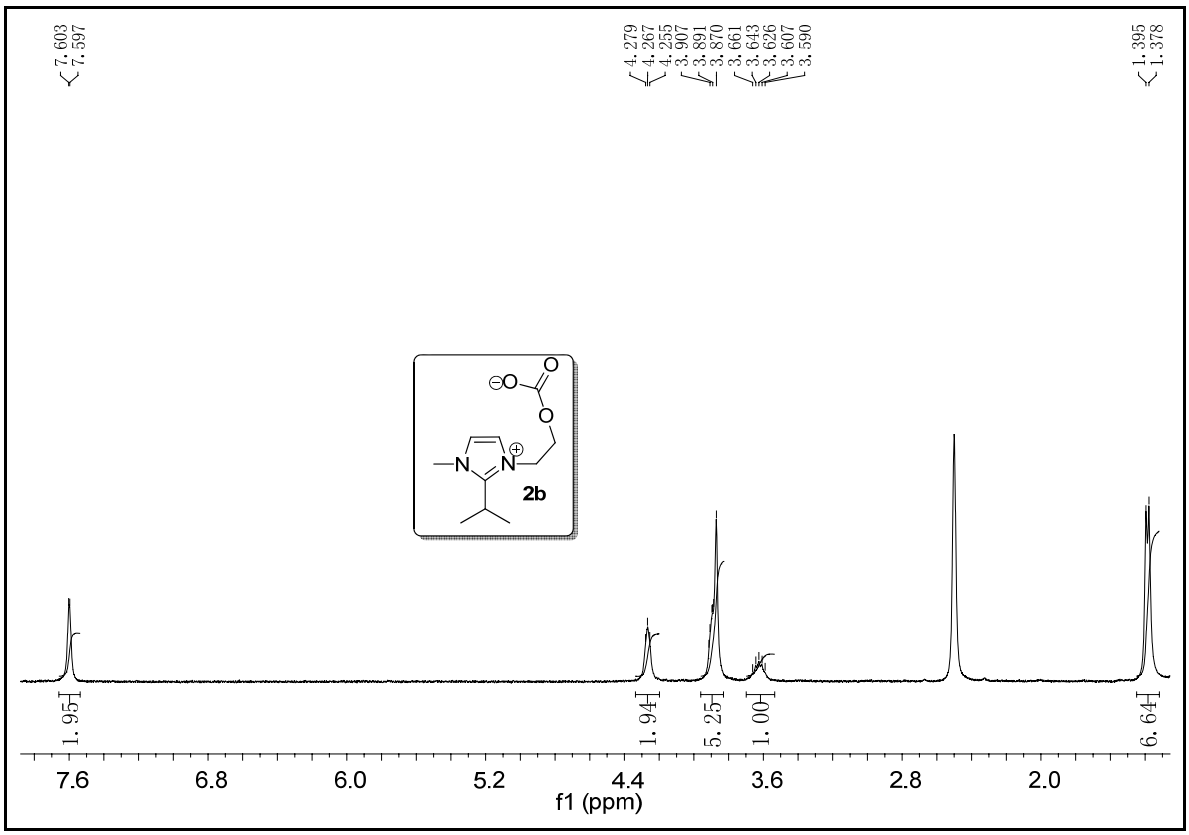


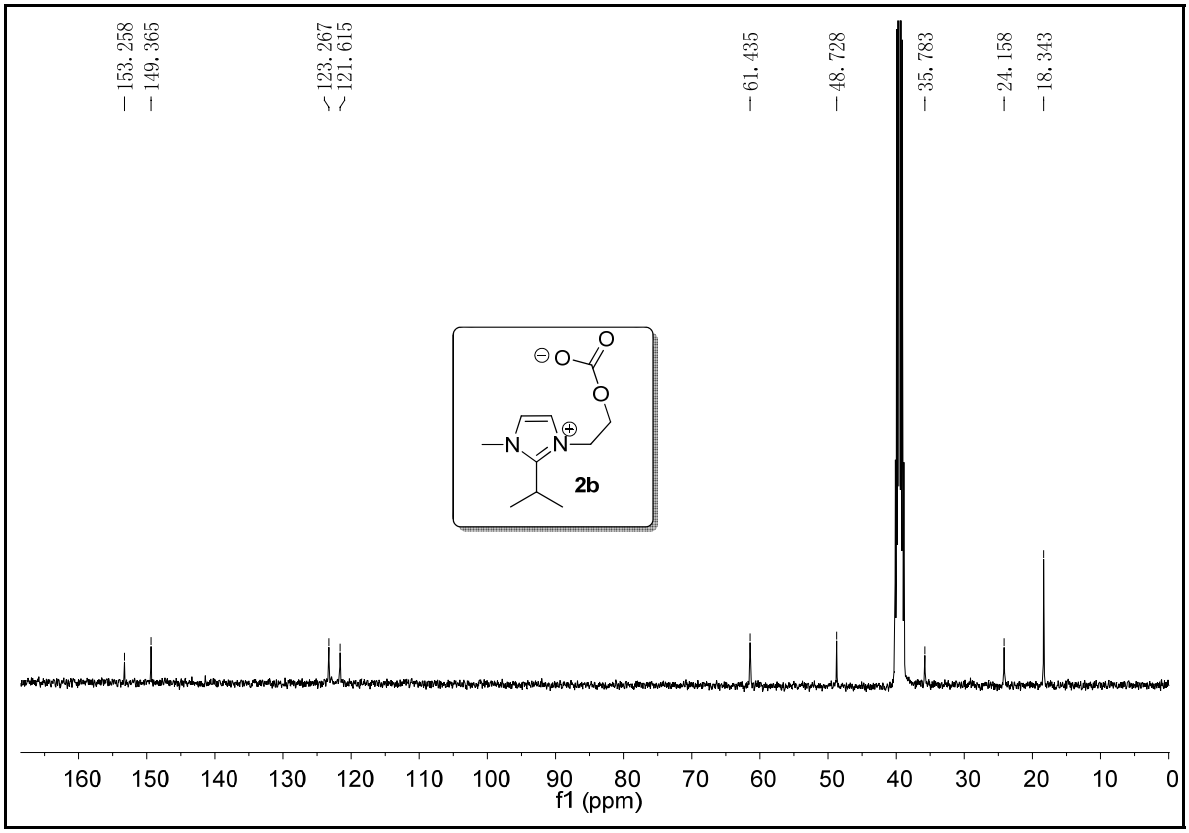
Figure S3 ^{1}H NMR and ^{13}C NMR comparison for **2a-2b, 2d** and **3a-3b, 3d.**

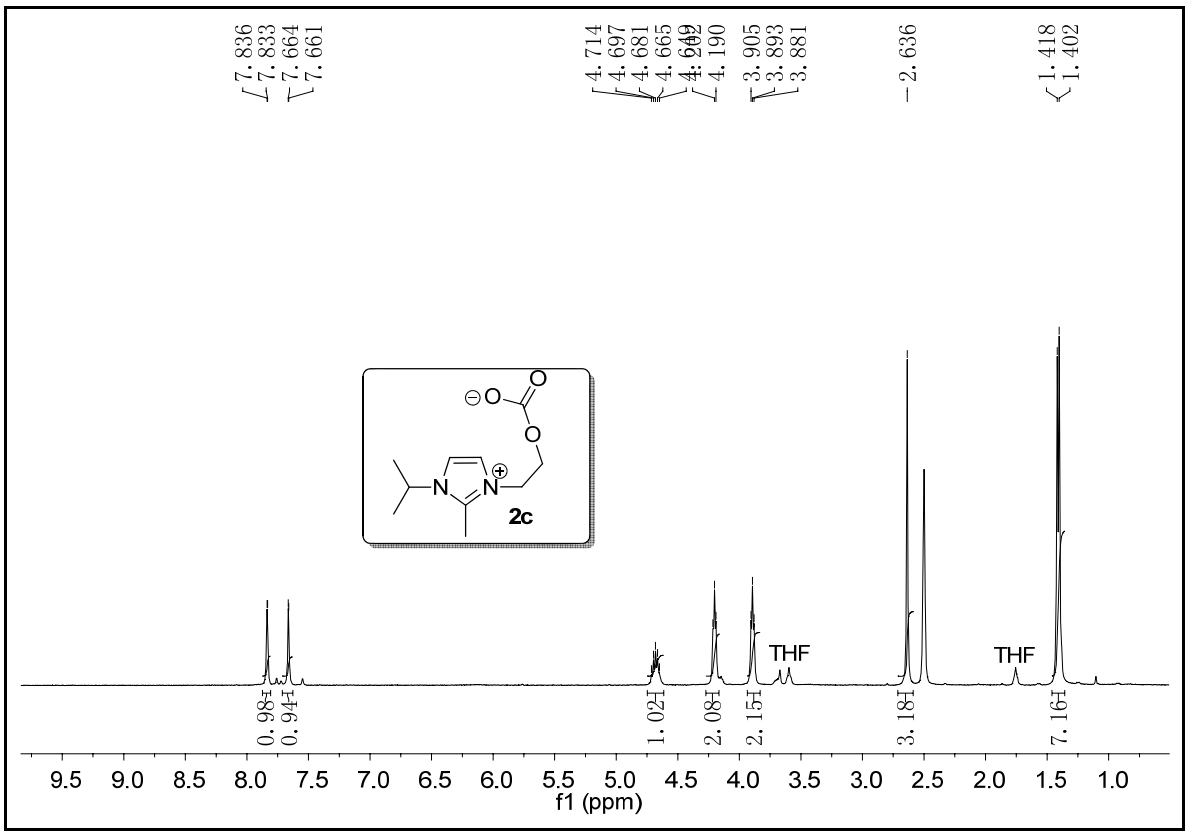
3. ^{1}H NMR and ^{13}C NMR spectra of 2a-2d, 4a-4d and alkylidene cyclic carbonates (6a-6i)







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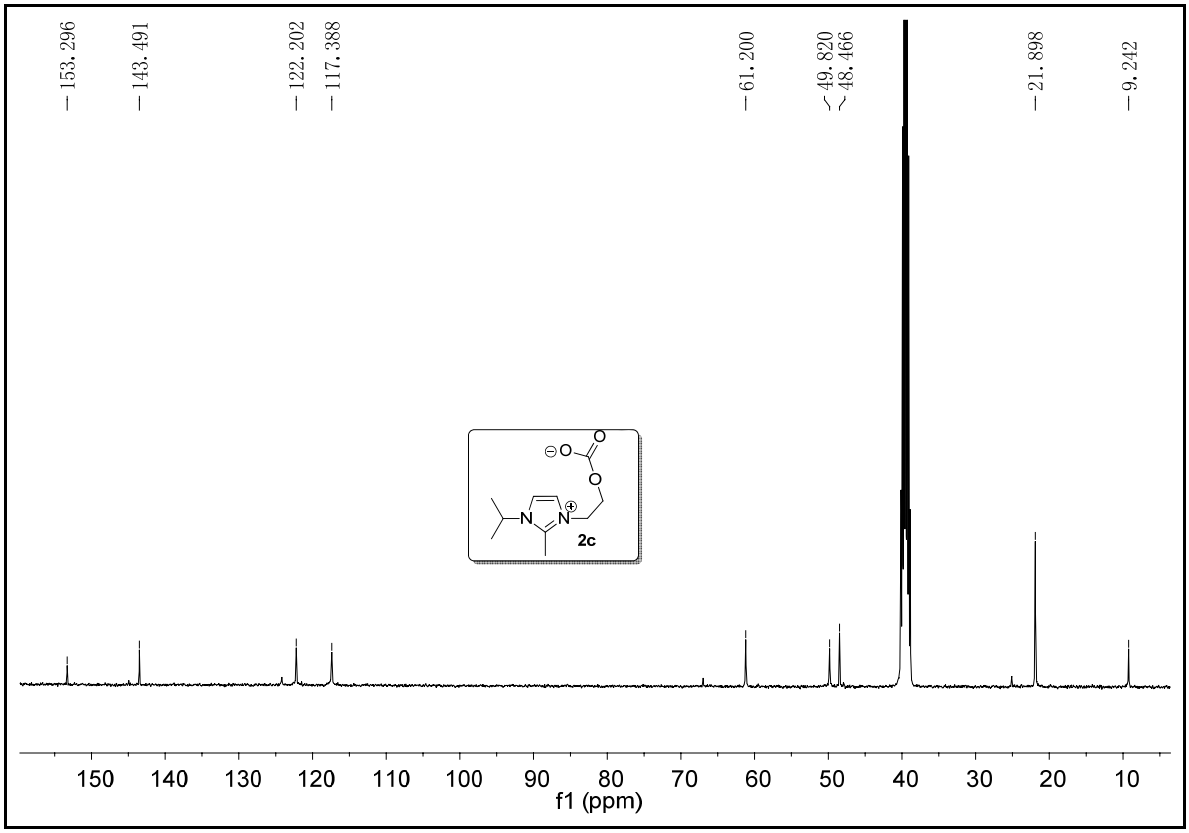
7.664
7.661
4.714
4.697
4.681
4.665
4.190
3.905
3.893
3.881
2.636
1.418
1.402
2c
THF
THF
0.98
0.94
1.02
2.08
2.15
3.18
7.16
f1 (ppm)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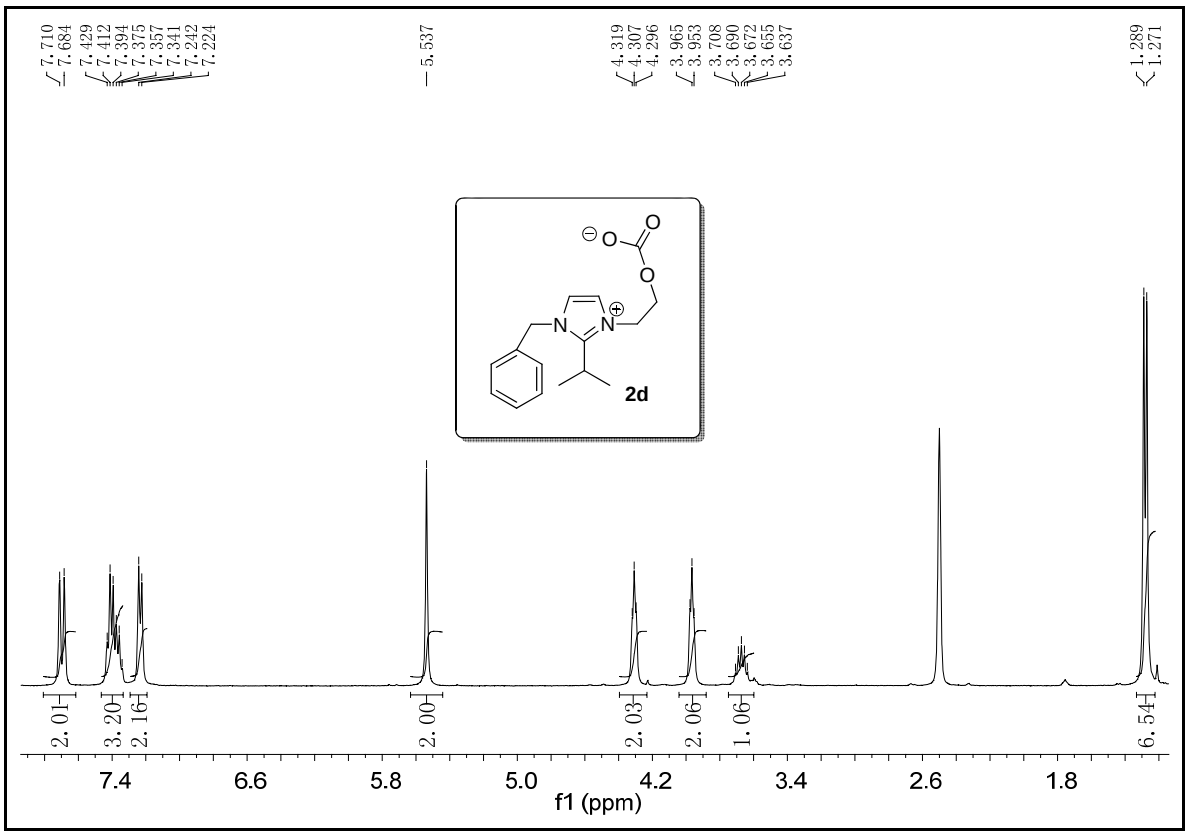
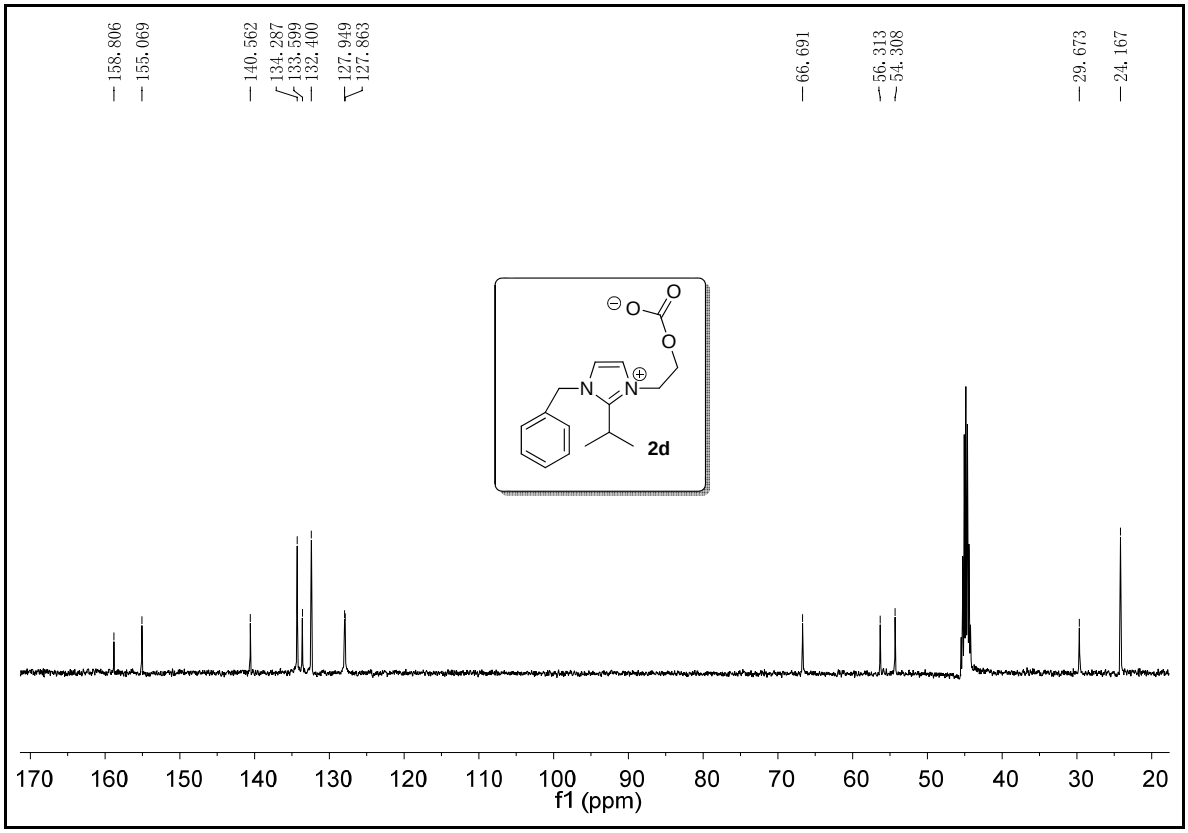
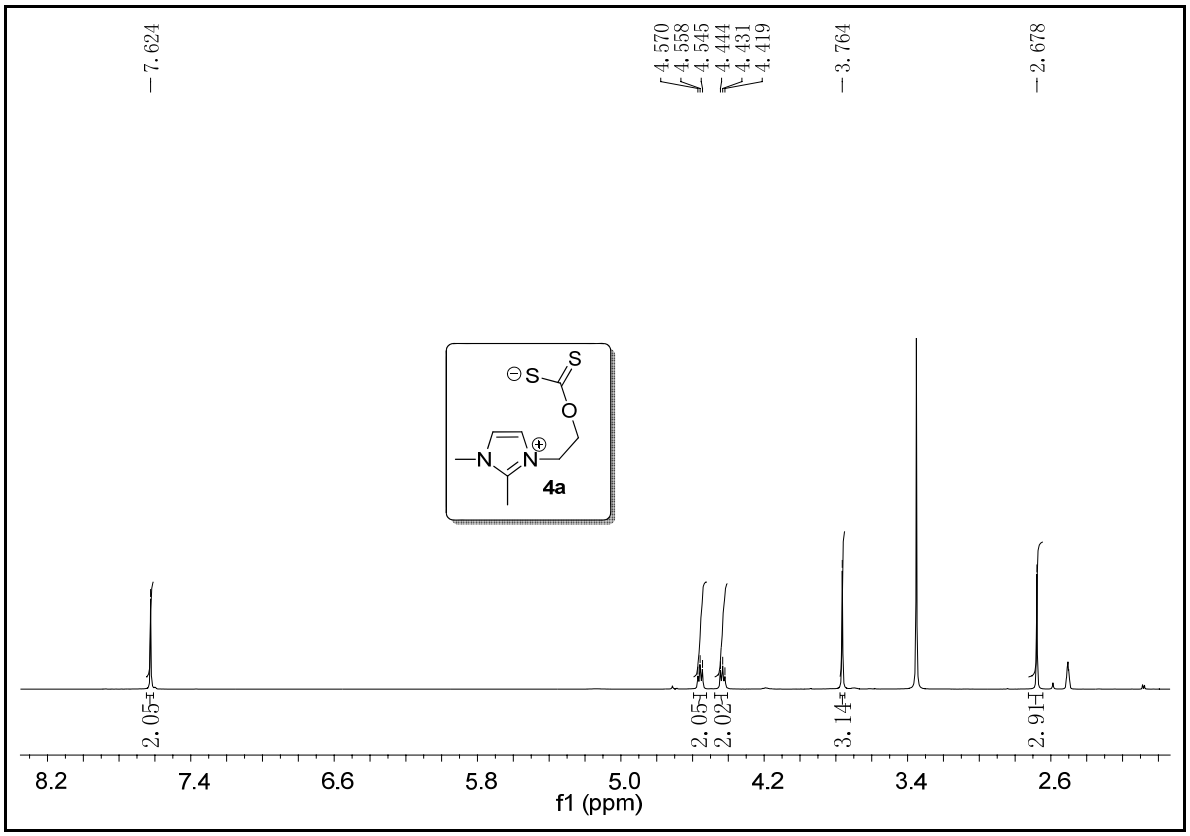
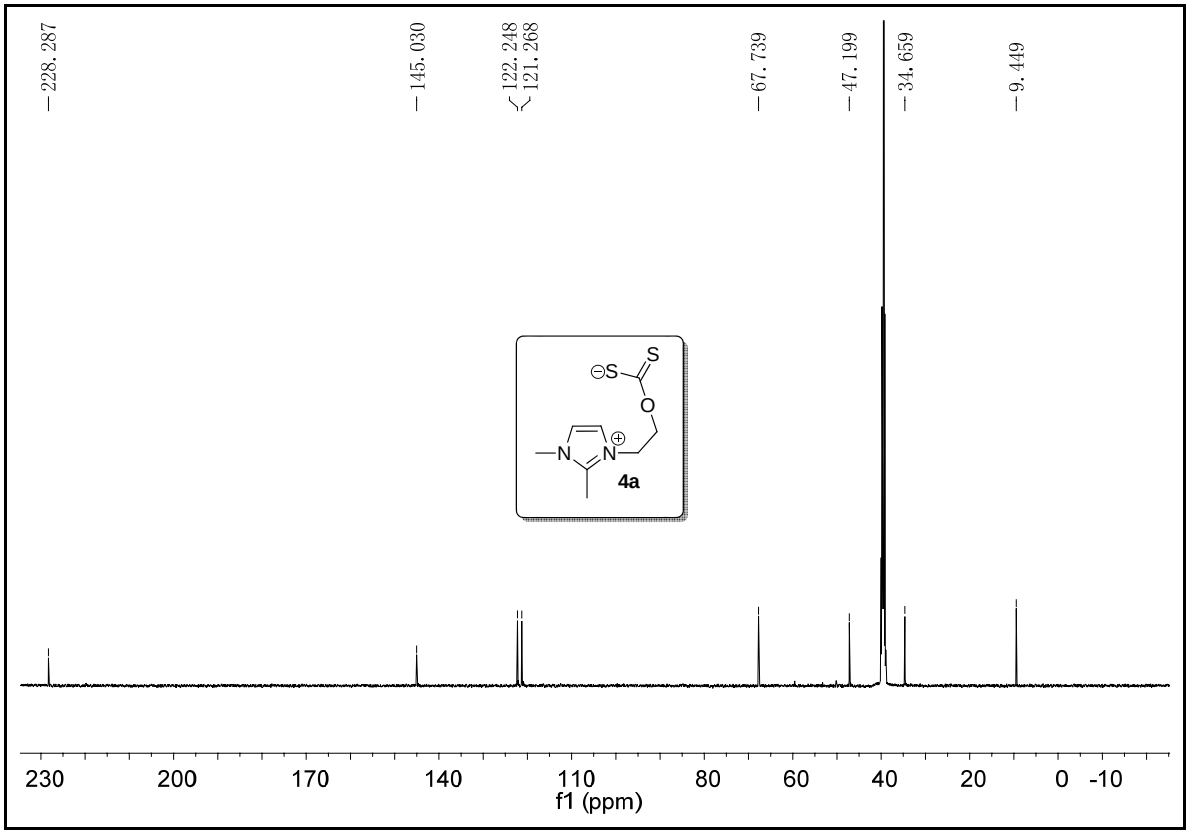
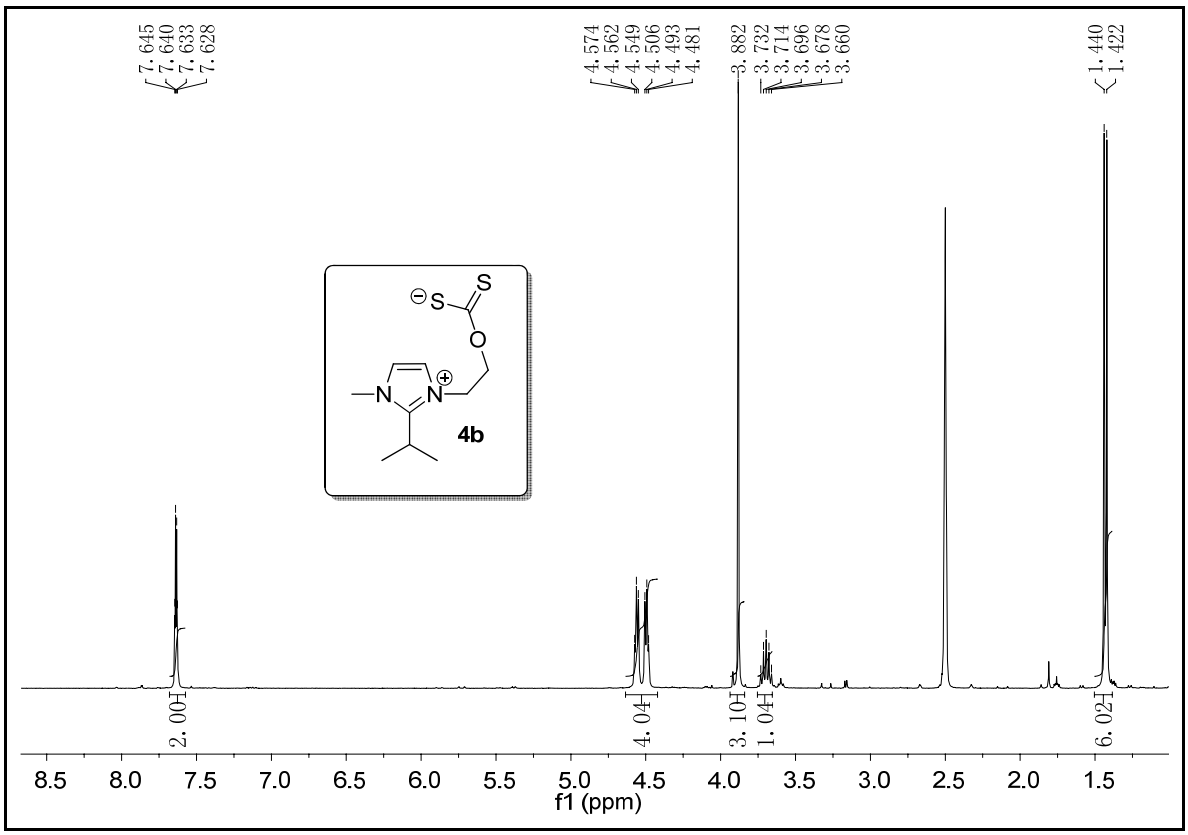
117.388
61.200
49.820
48.466
21.898
9.242
2c
f1 (ppm)

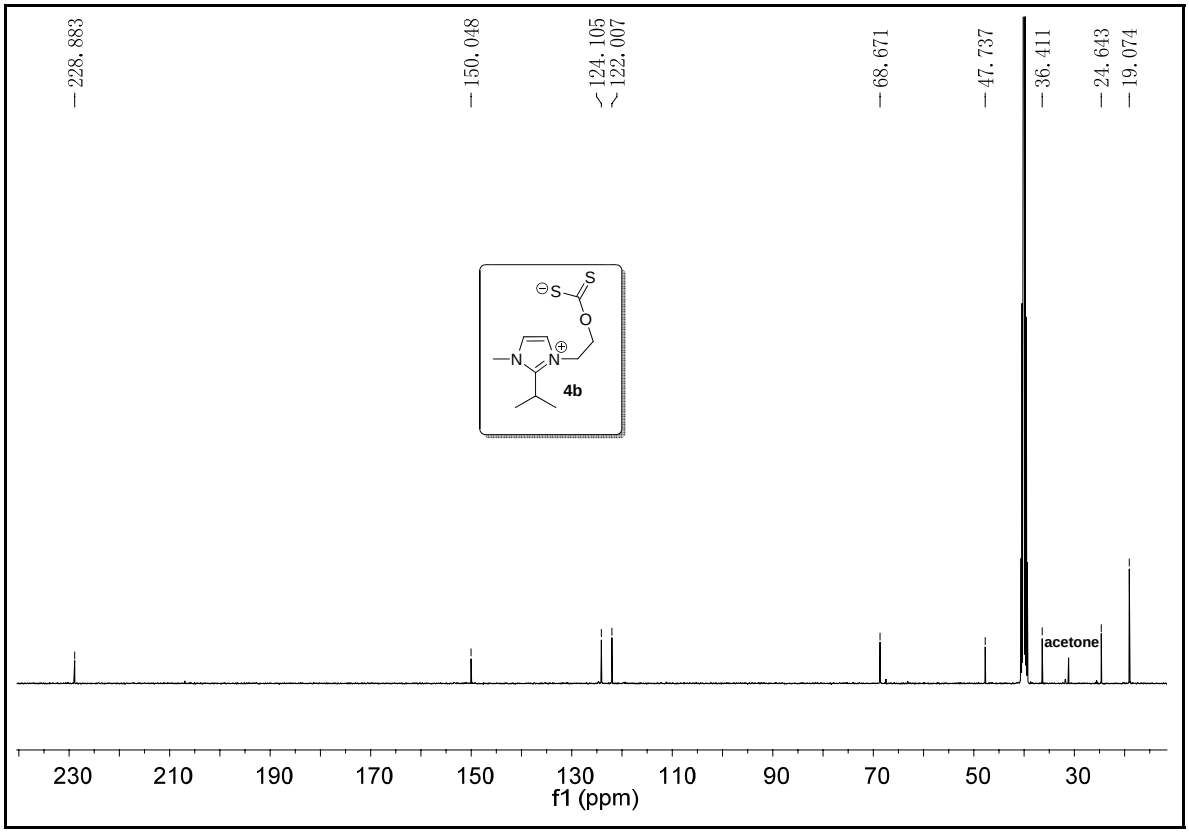


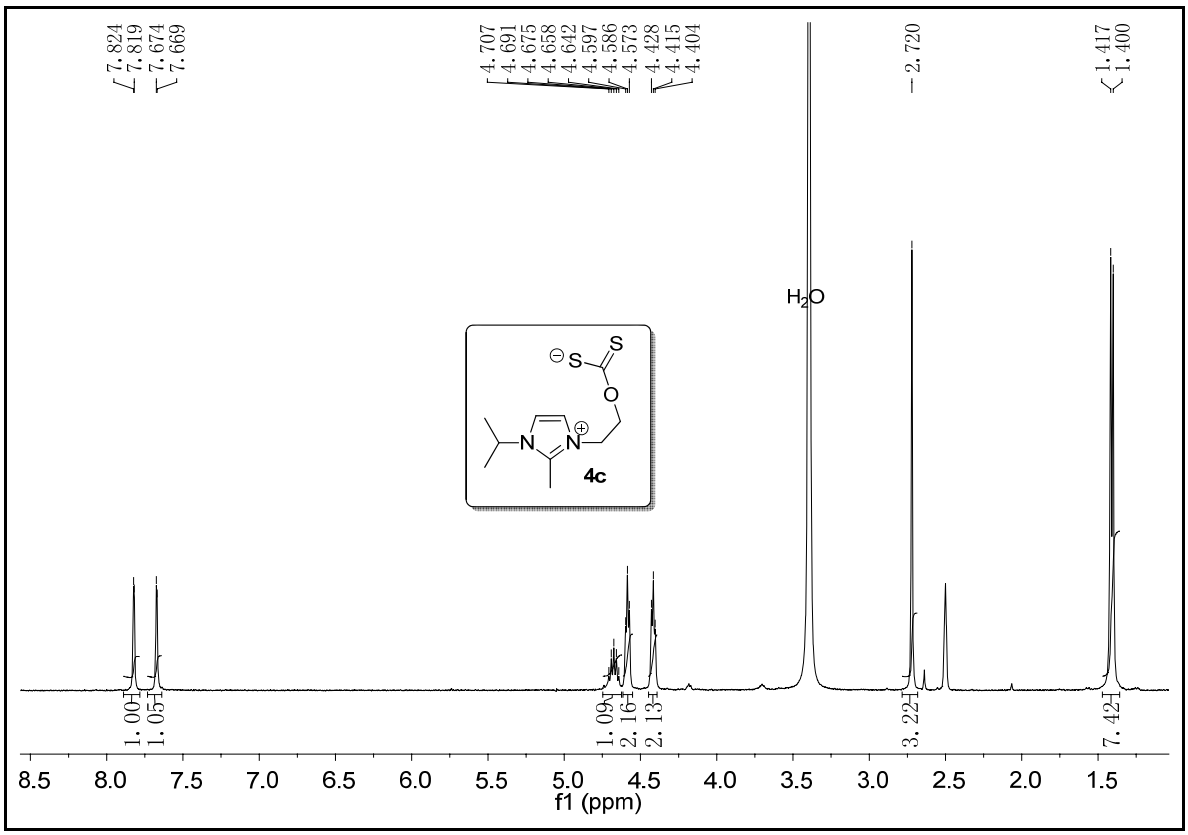








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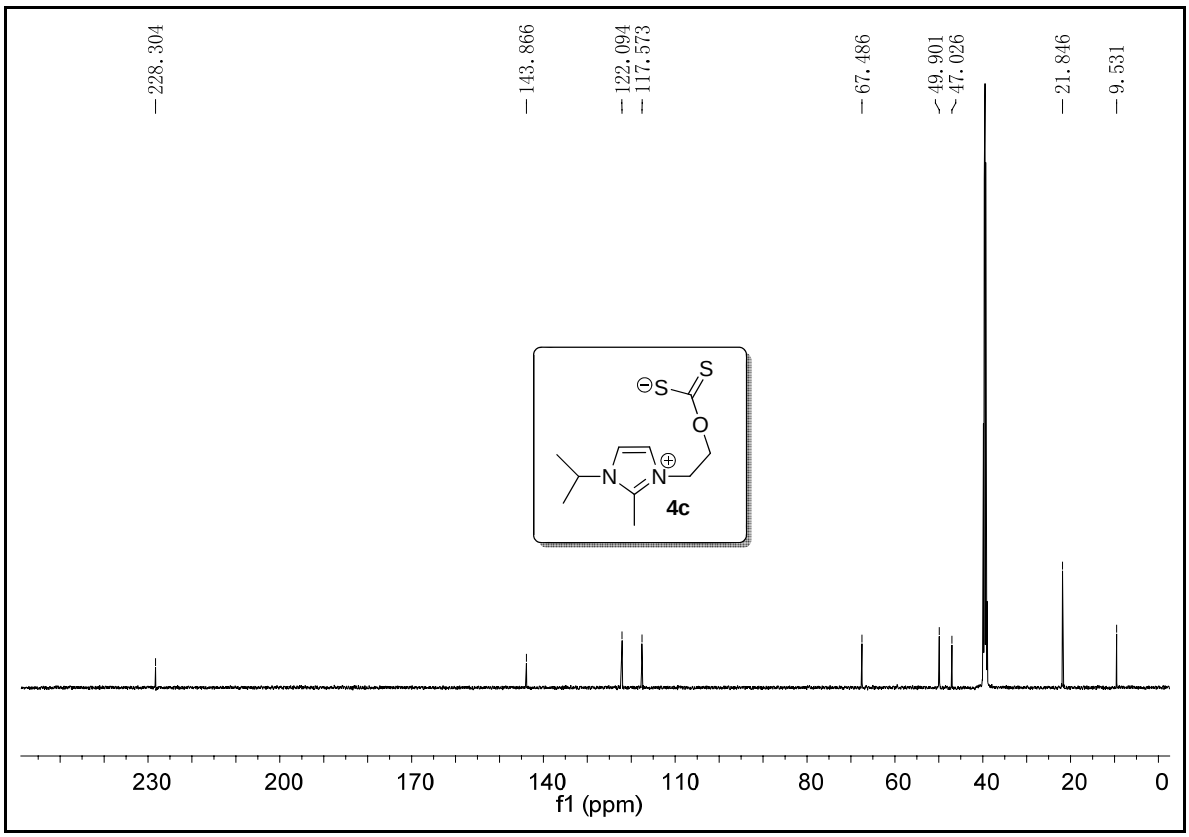
7.669
4.707
4.691
4.675
4.658
4.642
4.597
4.586
4.573
4.428
4.415
4.404
2.720
1.417
1.400
H2O
4c
1.00
1.05
1.09
2.16
2.13
3.22
7.42
f1 (ppm)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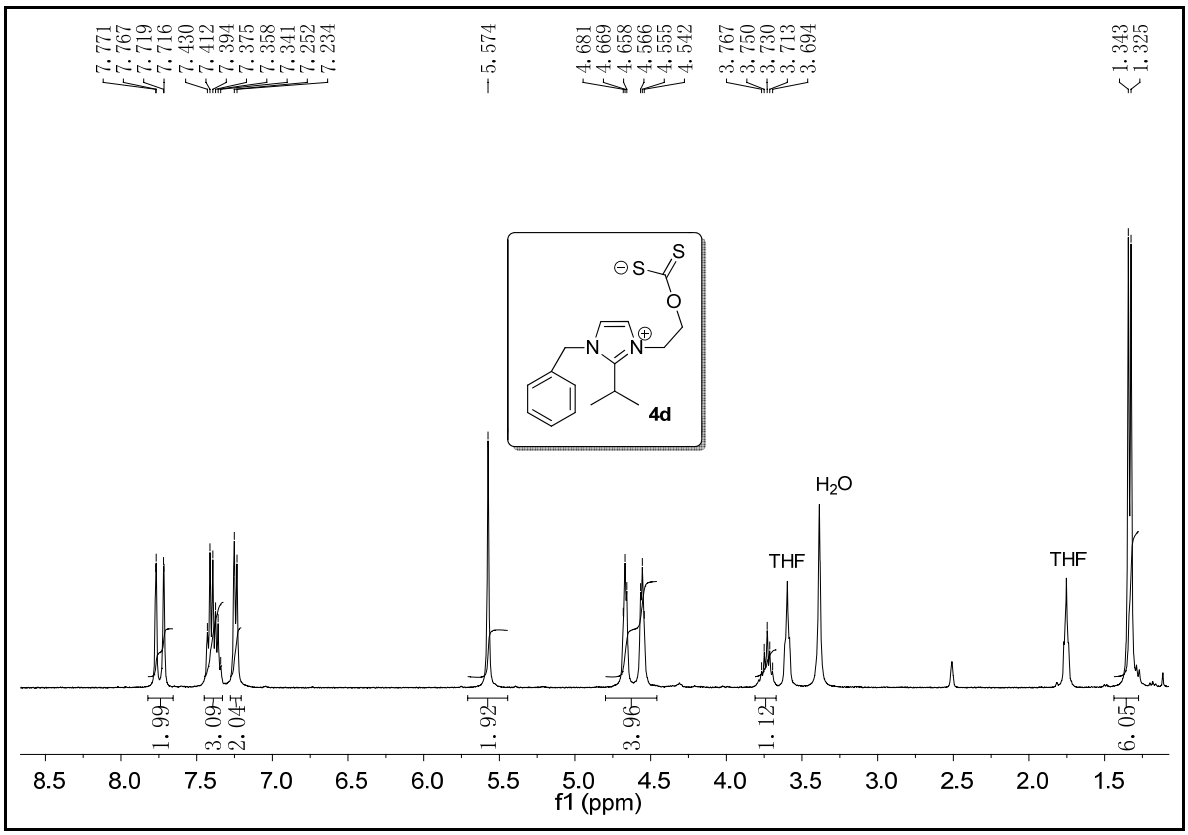
122.094
117.573
67.486
49.901
47.026
21.846
9.531
4c
f1 (ppm)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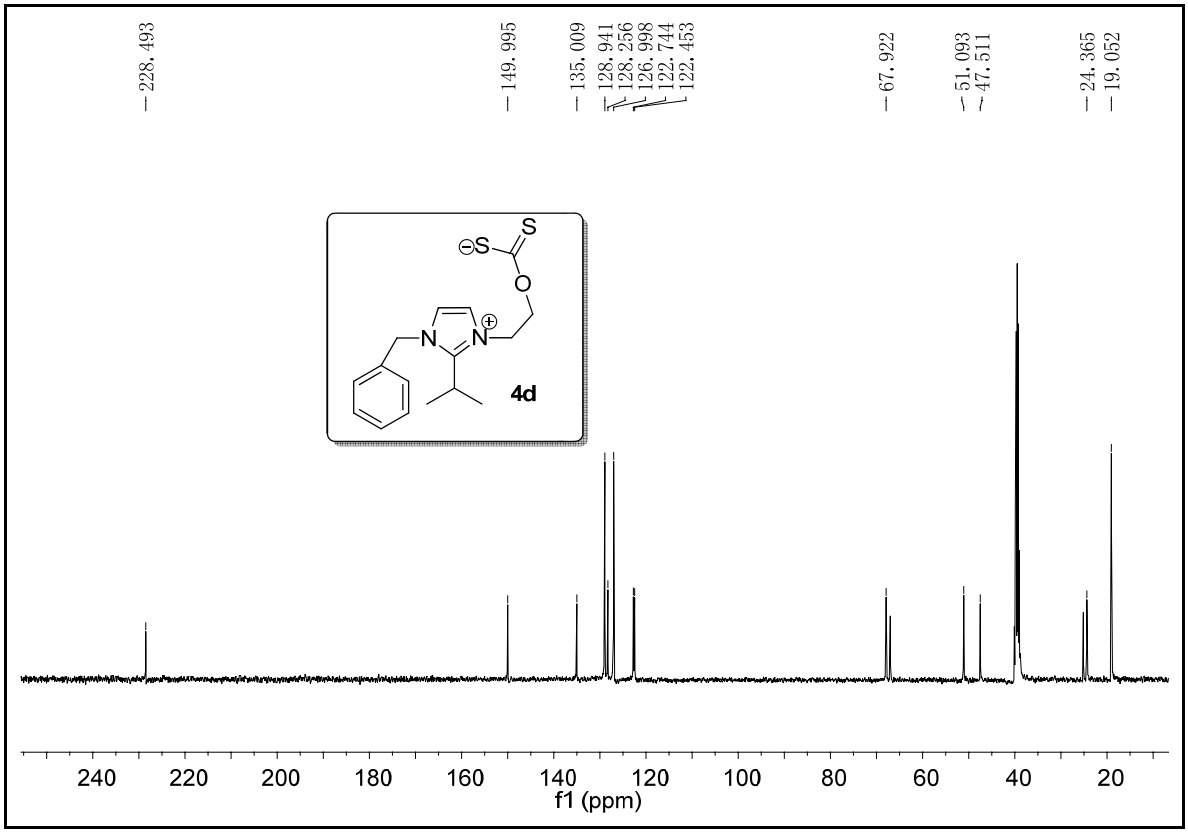
7.719
7.716
7.430
7.412
7.394
7.375
7.358
7.341
7.252
7.234
5.574
4.681
4.669
4.658
4.566
4.555
4.542
3.767
3.750
3.730
3.713
3.694
1.343
1.325
4d
H2O
THF
THF
1.99
3.09
2.04
1.92
3.96
1.12
6.05
f1 (ppm)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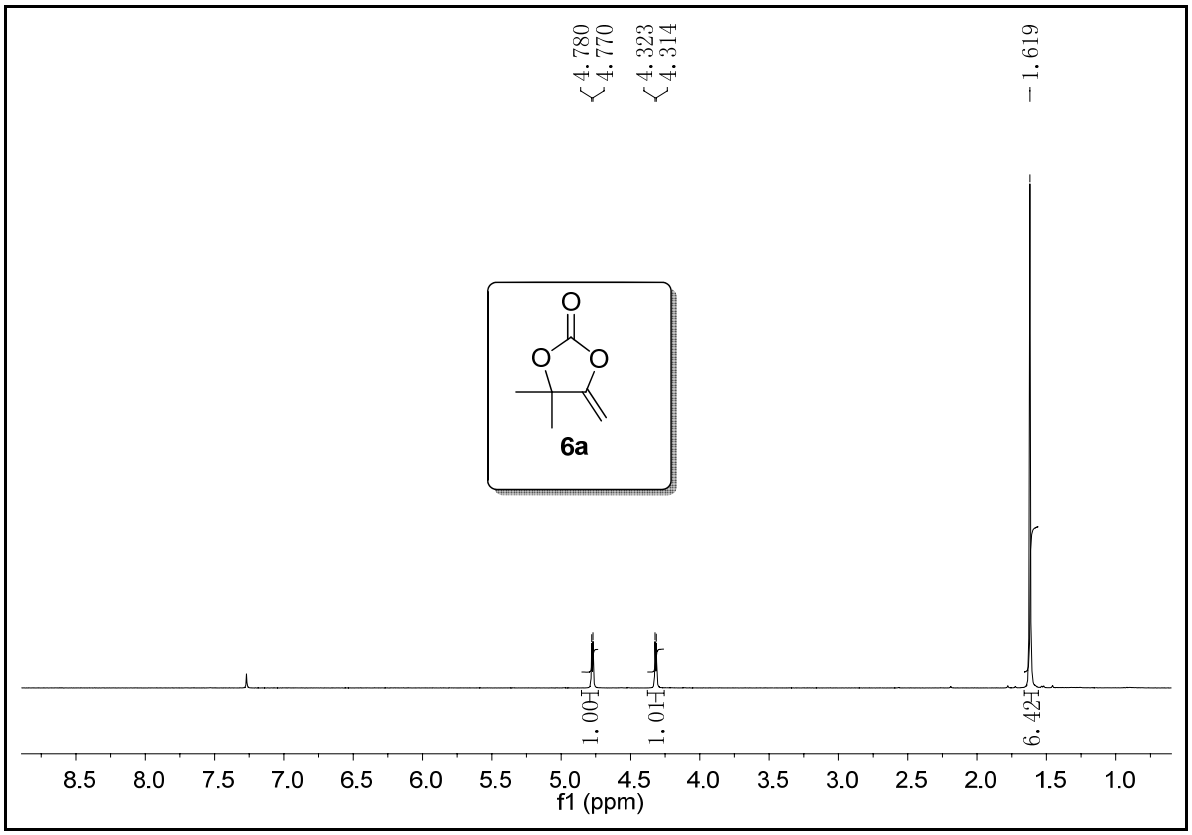
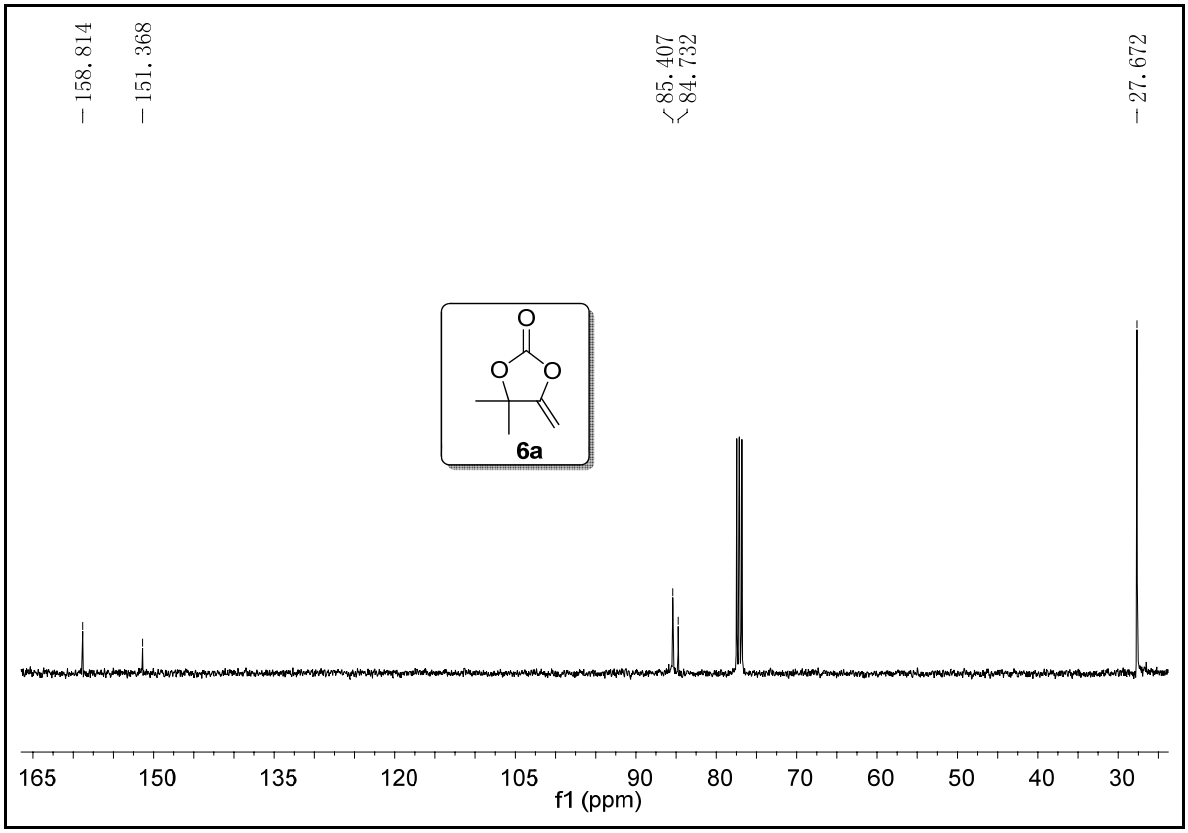
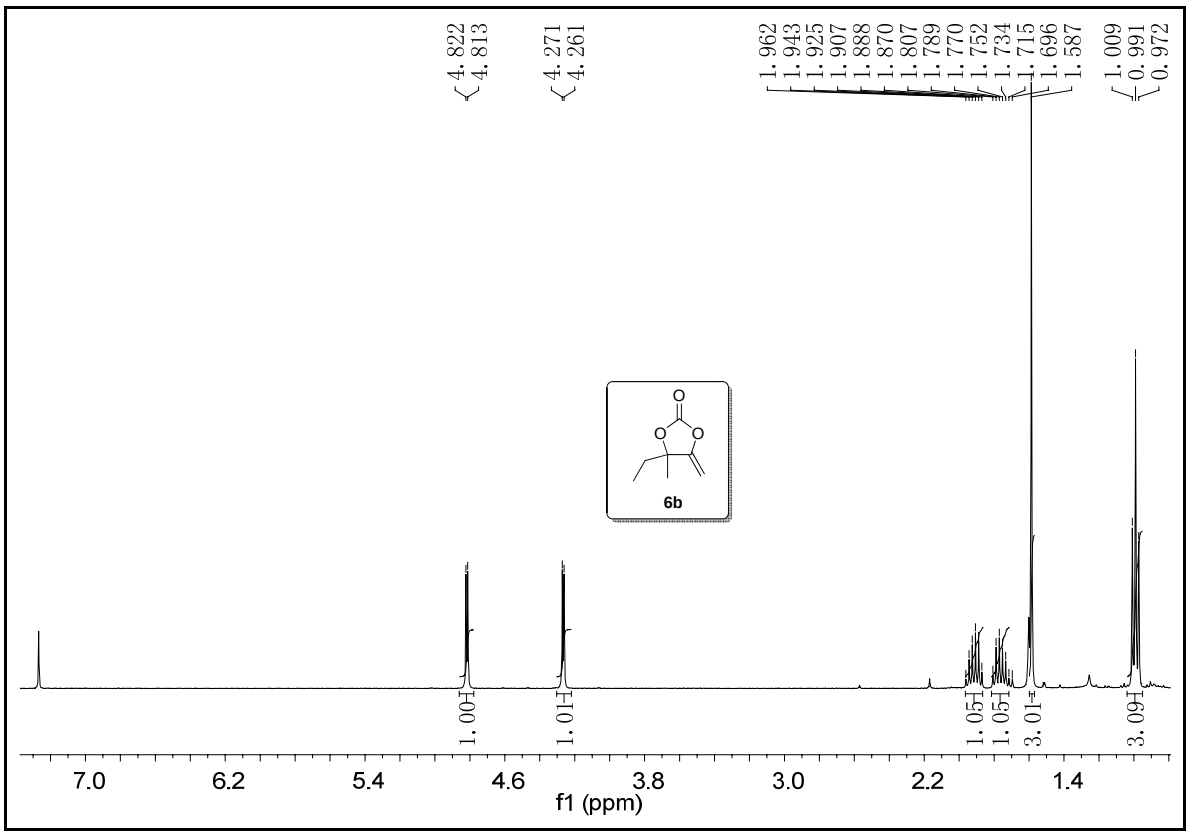
135.009
128.941
128.256
126.998
122.744
122.453
67.922
51.093
47.511
24.365
19.052
4d
f1 (ppm)



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1.943
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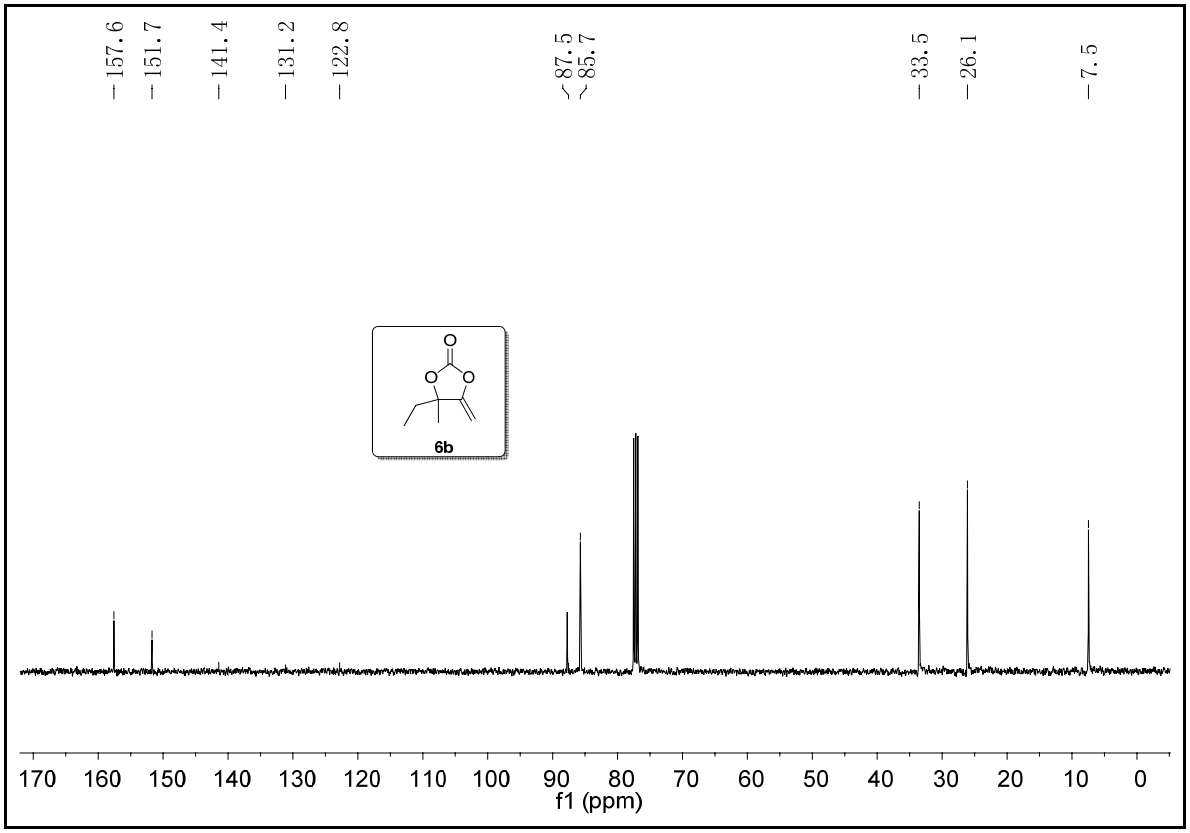
1.907
1.888
1.870
1.807
1.789
1.770
1.752
1.734
1.715
1.696
1.587
1.009
0.991
0.972
6b
1.00
1.01
1.05
1.05
3.01
3.09
7.0
6.2
5.4
4.6
3.8
3.0
2.2
1.4
f1 (ppm)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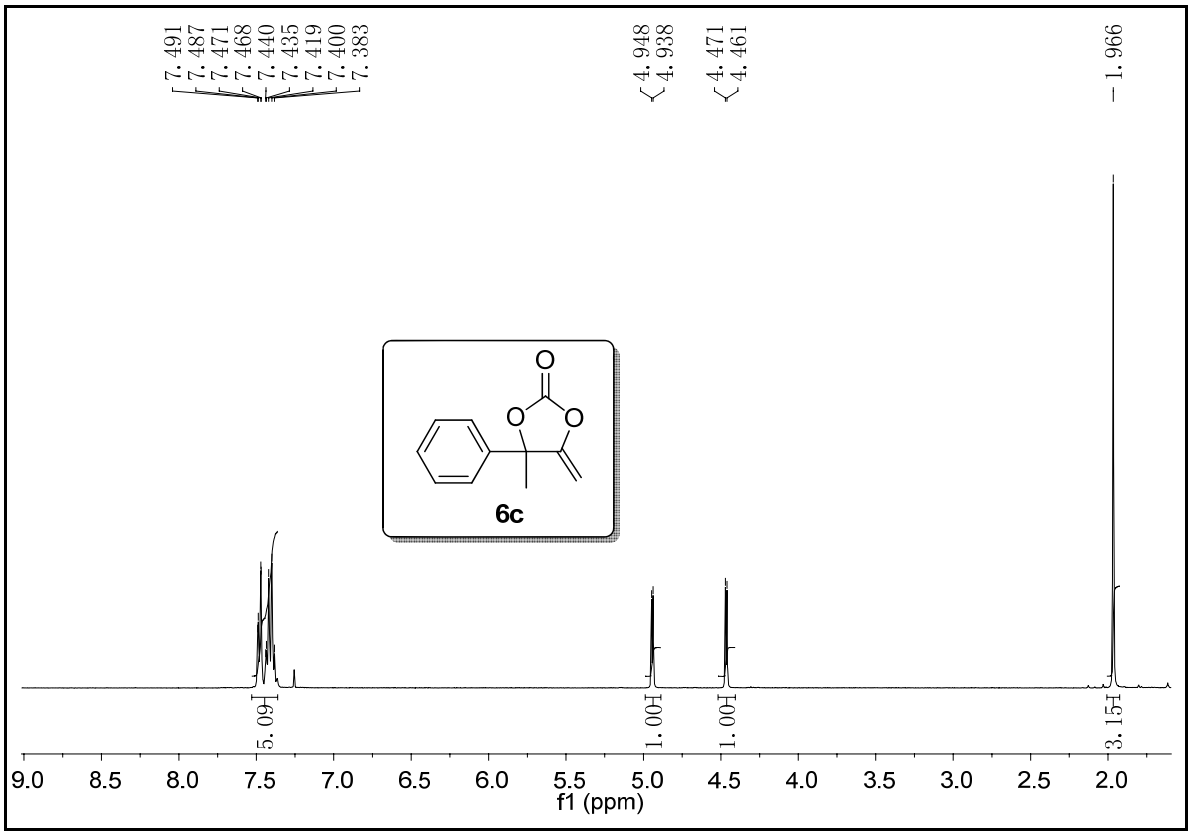
151.7
141.4
131.2
122.8
87.5
85.7
33.5
26.1
7.5
6b
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.471
7.468
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7.435
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7.400
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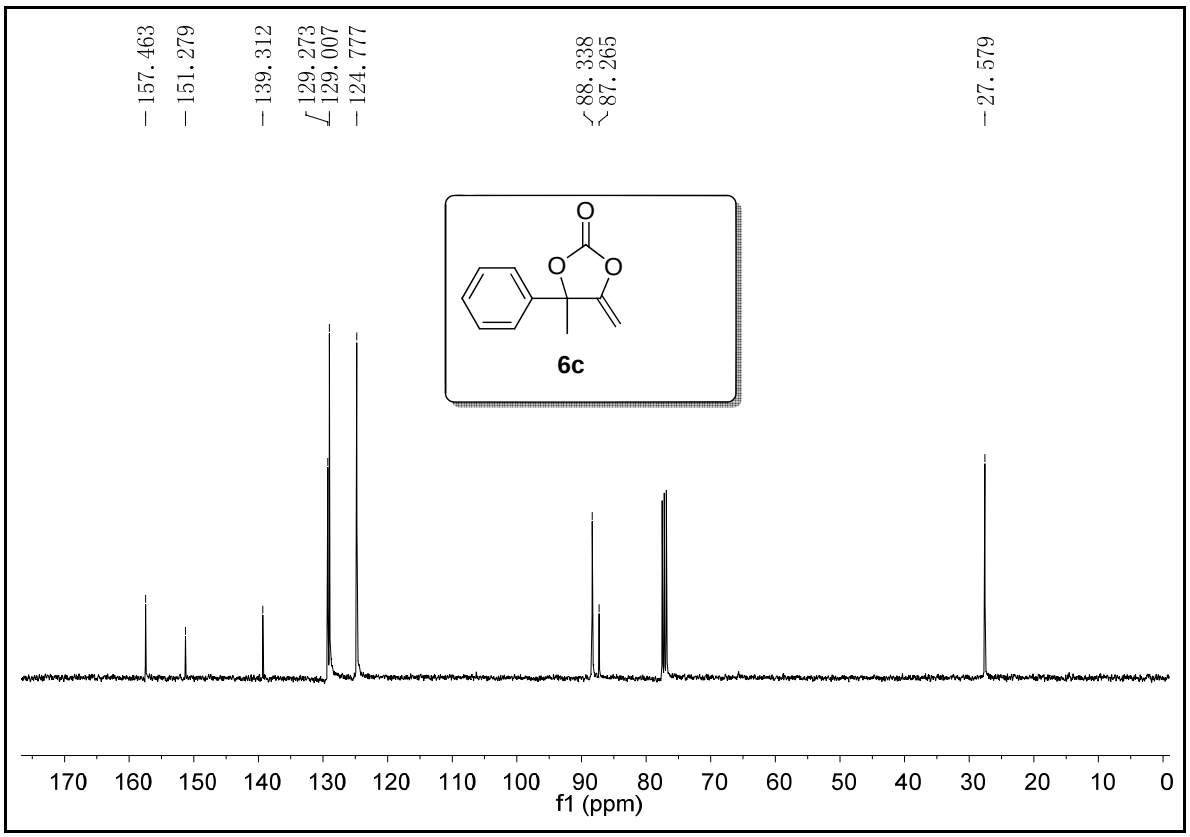
4.461
1.966
6c
5.09
1.00
1.00
3.15
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
f1 (ppm)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87.265
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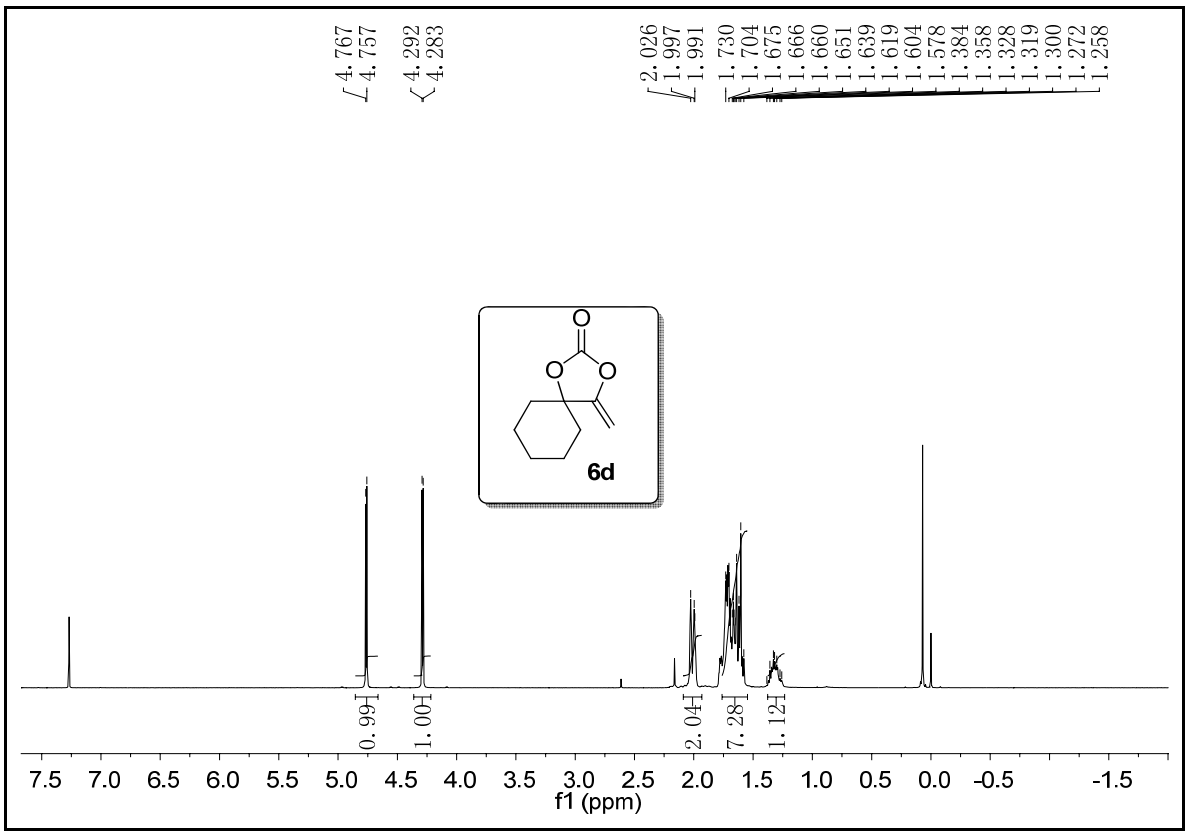
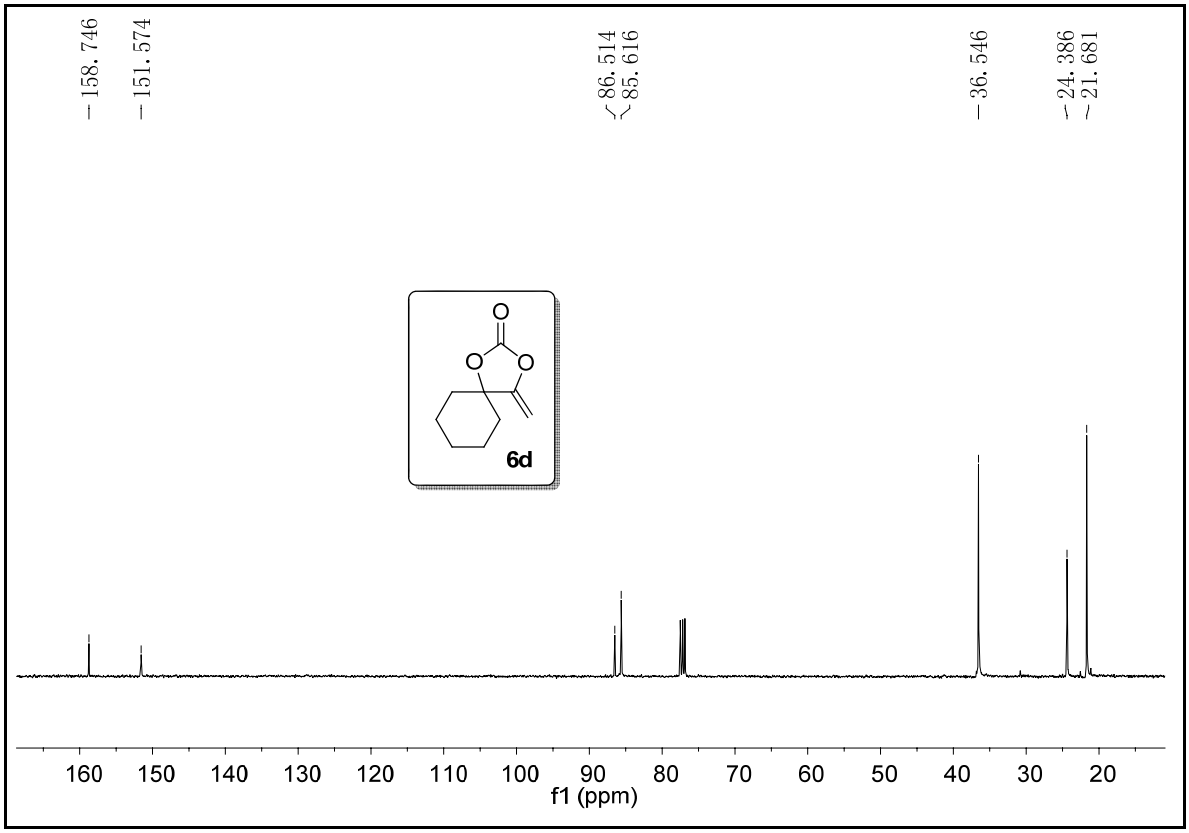
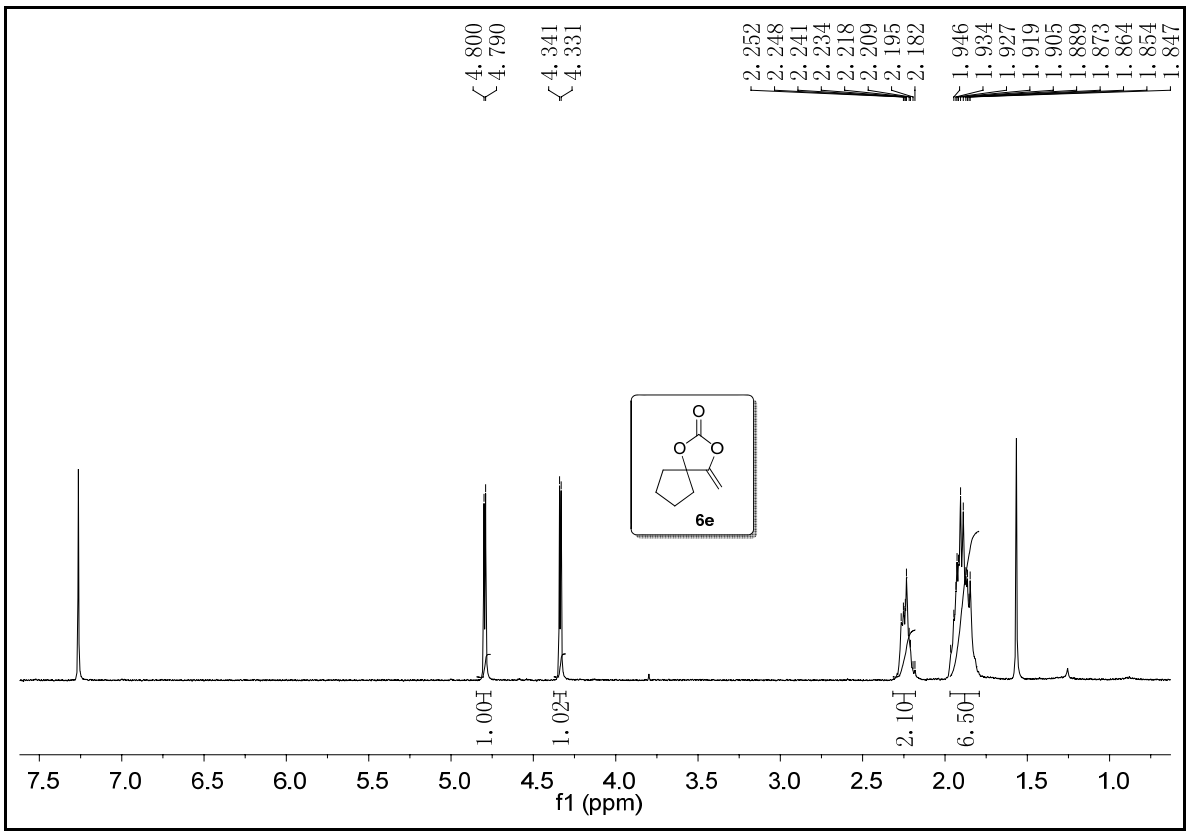
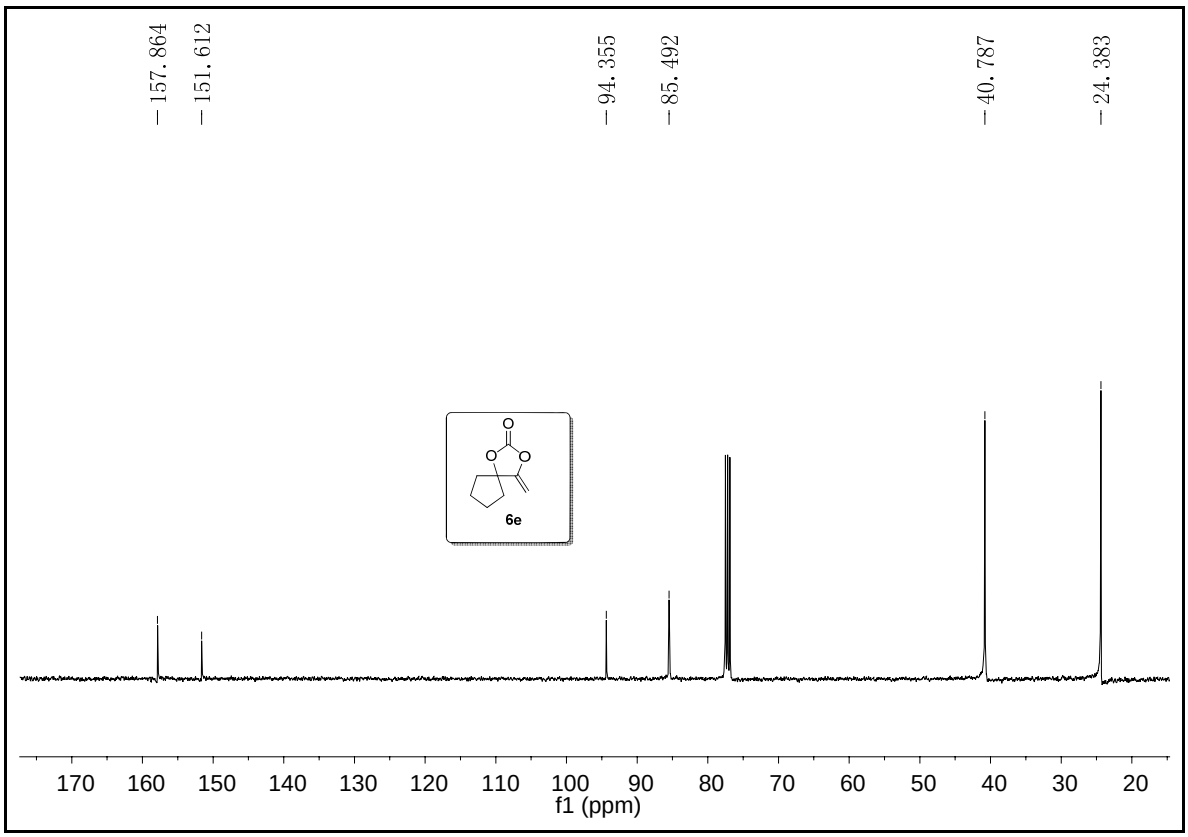
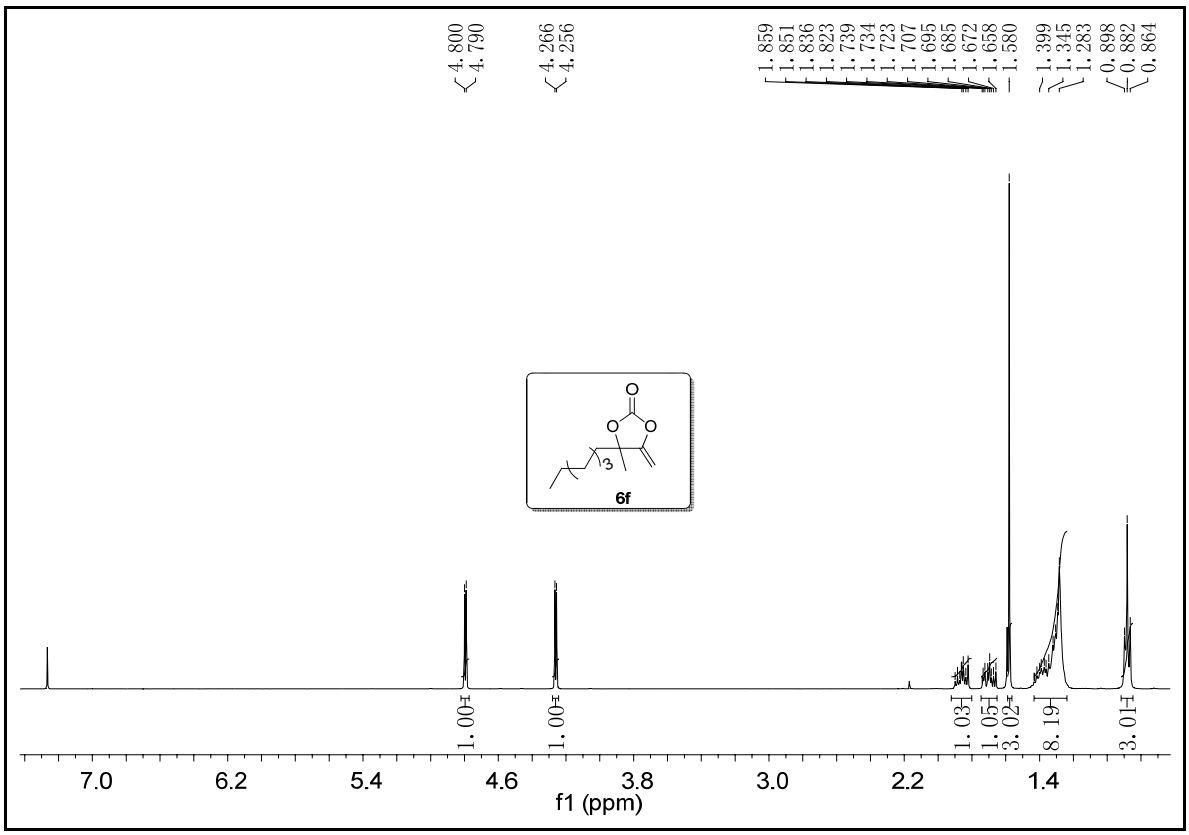
6c
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)







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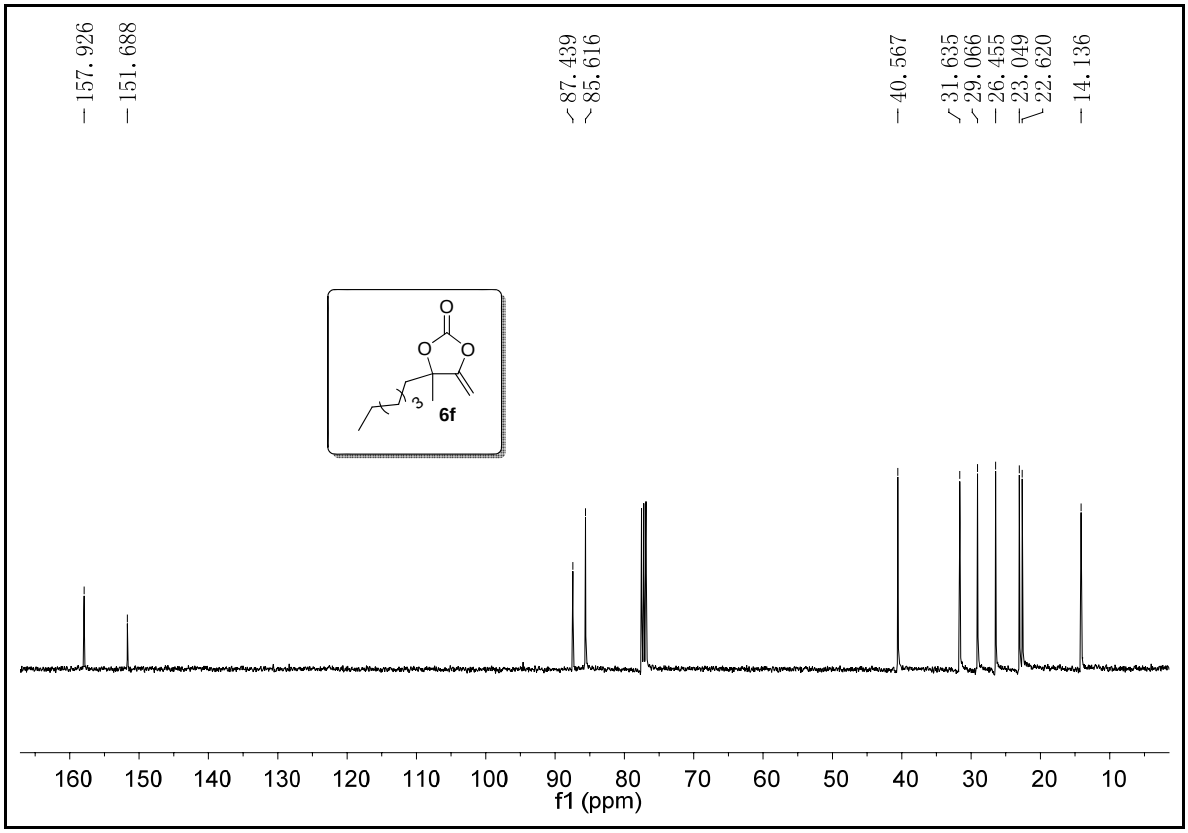
4.790
4.266
4.256
1.859
1.851
1.836
1.823
1.739
1.734
1.723
1.707
1.695
1.685
1.672
1.658
1.580
1.399
1.345
1.283
0.898
0.882
0.864
6f
1.00
1.00
1.03
1.05
3.02
8.19
3.01
7.0
6.2
5.4
4.6
3.8
3.0
2.2
1.4
f1 (ppm)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85.616
40.567
31.635
29.066
26.455
23.049
22.620
14.136
6f
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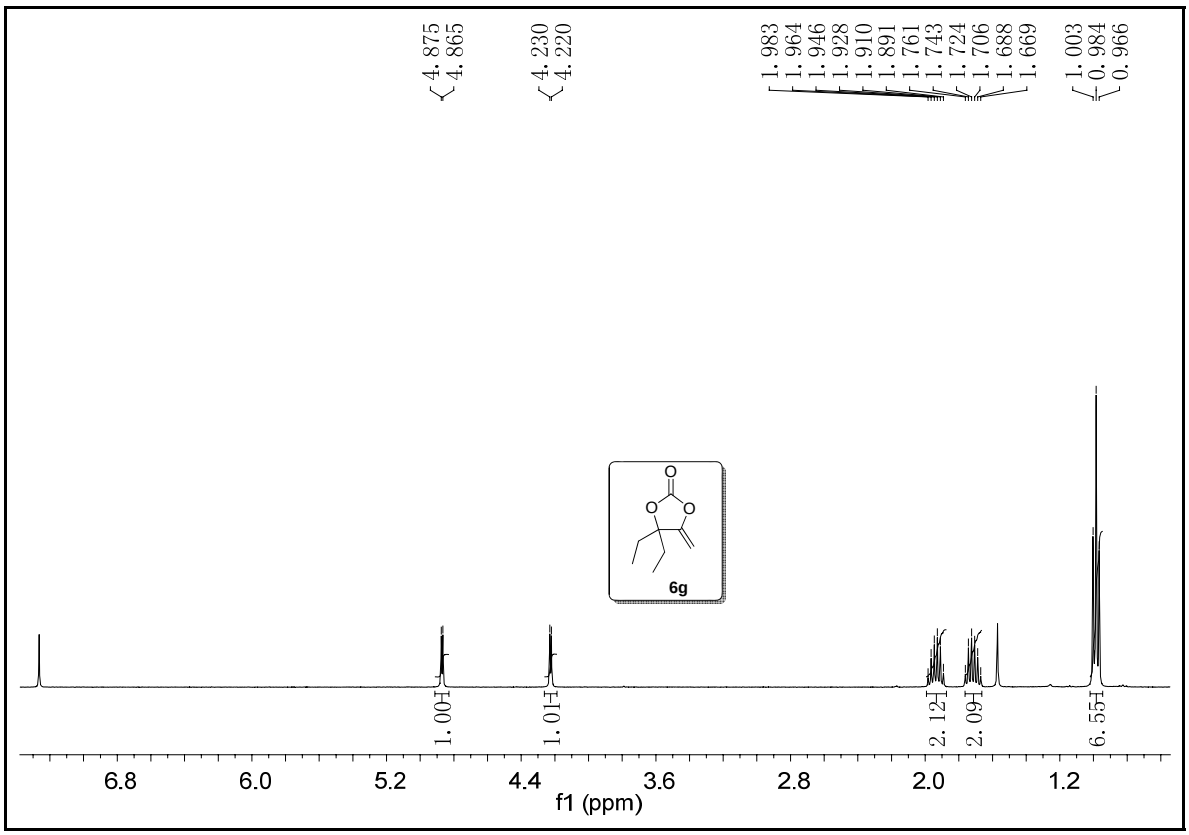
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)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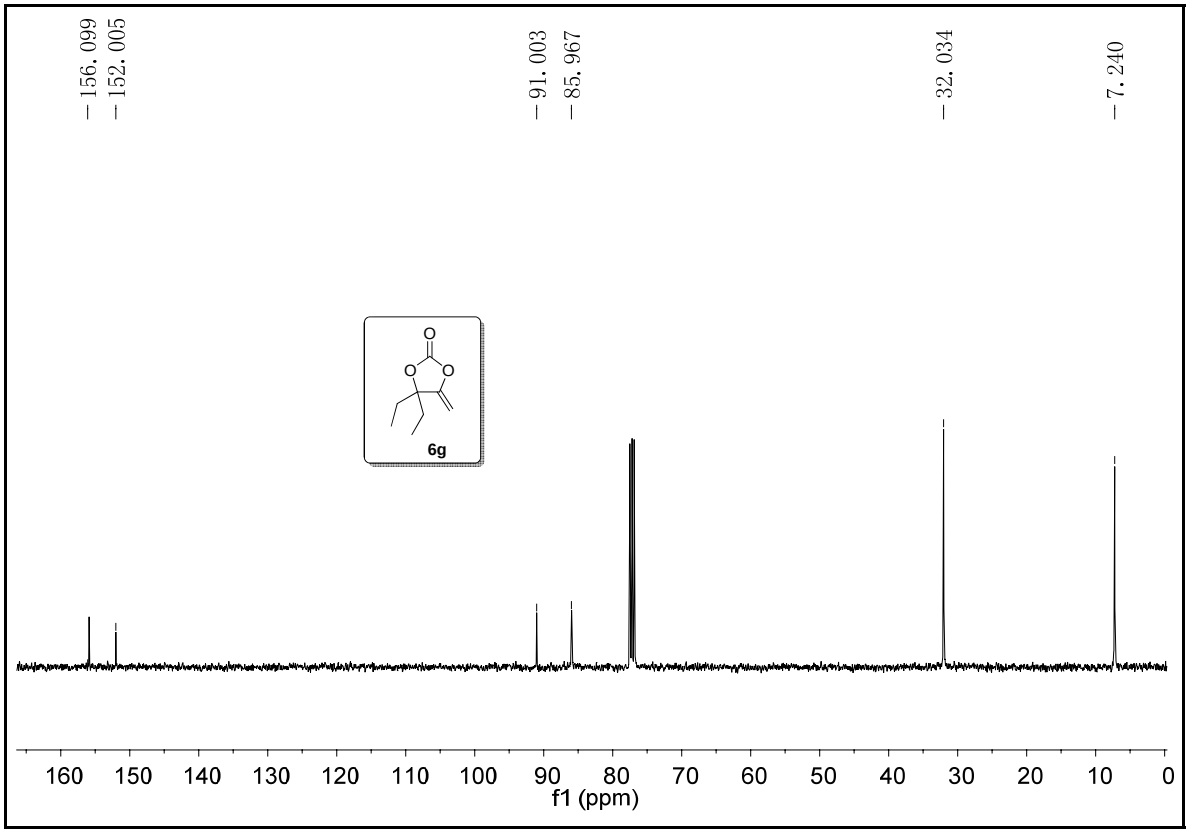
4.865
4.230
4.220
1.983
1.964
1.946
1.928
1.910
1.891
1.761
1.743
1.724
1.706
1.688
1.669
1.003
0.984
0.966
6g
1.00
1.01
2.12
2.09
6.55
6.8
6.0
5.2
4.4
3.6
2.8
2.0
1.2
f1 (ppm)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152.005
91.003
85.967
32.034
7.240
6g
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)