Supporting Information:

$Ru_3(CO)_{12}$-Catalyzed Reactions of Catechols with Alkynes: An Atom-Economic Process for Synthesis of 2,2-Disubstituted 1,3-Benzodioxoles from Double Addition of O-H Bond Across a Triple Bond

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1. Experimental section and characterization of products

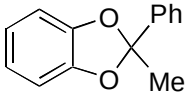
(1) General method

All organic starting materials are analytically pure and used without further purification. $Ru_3(CO)_{12}$ was prepared by the reaction of $RuCl_3 \cdot 3H_2O$ with CO in methanol (Bruce, M. I.; Jensen, C. M.; Jones, N. L. *Inorg. Synth*. **1989**, *26*, 259). ^{1}H NMR (300 MHz) chemical shifts (δ) were referenced to TMS, and ^{13}C NMR (75 MHz) chemical shifts (δ) were referenced to internal solvent resonance.

(2) Typical Experimental Procedure for Addition of Phenylacetylene (2a) with 1,2-Benzenediol (2a) To Afford 3a (Table 1, entry 7): A mixture of phenylacetylene (**1a**) (112.3 mg, 1.1 mmol), catechol (**2a**) (110.0 mg, 1mmol), $Ru_3(CO)_{12}$ (12.7 mg, 0.02 mmol), and toluene (1.0 mL) under nitrogen in a screw-capped tube was heated with stirring at 80 ^{o}C for 12 h. After cooling, the reaction mixture was diluted with CH_2Cl_2 to 3.0 mL, and *n*-octadecane (38.1 mg, 0.1 mmol) was added as internal standard material for GC analysis. After GC and GC-MS analyses, solvents and volatiles were removed under vacuum, and the residue was then purified by column chromatography (silica gel, eluted with petroleum ether) to afford **3a** (179.0 mg, 0.84 mmol, 84.0%) as yellow oil. GC analysis of the reaction mixture disclosed that **3a** was formed in 90% yield.

(3) Characterization of products

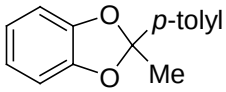
3b, **3d**, **3f**, **3g**, **3i**, **3i'**, **3j**, **3j'**, **3l**, **3m** and **3n** are new compounds, which were characterized by ^{1}H, ^{13}C-NMR, mass spectra and elemental analysis. Other products are known compounds and were characterized by ^{1}H, ^{13}C-NMR and mass spectra.



3a

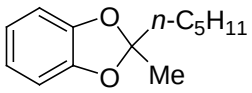
2-Methyl-2-phenyl-1,3-benzodioxole **3a**[1]: yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.61-7.58 (m, 2H), 7.38-7.32 (m, 3H), 6.80-6.76 (m, 4H), 1.98 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 147.3, 141.3, 129.0, 128.5, 125.1, 121.5, 116.7, 108.8, 27.2; GCMS *m/z* (% relative intensity): 212 (M^+, 68), 197 (100), 166 (2), 151 (3), 135 (12), 110 (67), 103 (69),

91 (4), 77 (27).



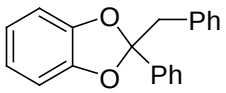
3b

2-Methyl-2-*p*-tolyl-1,3-benzodioxole **3b**: yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.47 (d, 2H, *J* = 7.8 Hz), 7.16 (d, 2H, *J* = 7.8 Hz), 6.80-6.75 (m, 4H), 2.32 (s, 3H), 1.96 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 147.4, 138.8, 138.4, 129.1, 125.0, 121.4, 116.9, 108.7, 27.1, 21.3; GCMS *m/z* (% relative intensity): 226 (M^+, 61), 211 (90), 135 (10), 117 (100), 110 (39), 91 (28), 149 (23). Anal. Calcd for $C_{15}H_{14}O_2$: C, 79.65; H, 6.19. Found: C, 79.73; H, 6.24.



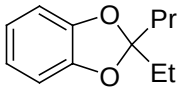
3c

2-Methyl-2-*n*-pentyl-1,3-benzodioxole **3c**[1]: yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 6.76-6.73 (m, 4H), 1.90 (t, 2H, *J* = 7.6Hz), 1.60 (s, 3H), 1.45-1.50 (m, 2H), 1.32-1.30 (m, 4H), 0.88 (t, 3H, *J* = 6.7 Hz); ^{13}C NMR (75 MHz, $CDCl_3$) δ 146.9, 120.2, 118.4, 107.5, 38.5, 31.1, 23.5, 22.1, 21.8, 13.3; GCMS *m/z* (% relative intensity): 206 (M^+, 18), 191 (9), 163 (1), 151 (2), 135 (100), 110 (17), 91 (2), 81 (3).



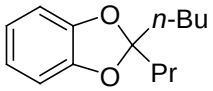
3d

2-Benzyl-2-phenyl-1,3-benzodioxole **3d**: yellow solid; m.p. 83-84 ^{o}C (recrystallization with CH_2Cl_2/cyclohexane); ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.47-7.44 (m, 2H), 7.29-7.27 (m, 3H), 7.16-7.09 (m, 5H), 6.78-6.69 (m, 4H), 3.47 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 147.2, 140.0, 133.9, 130.8, 128.7, 128.0, 127.8, 126.8, 125.5, 121.2, 117.3, 108.5, 46.6; GCMS *m/z* (% relative intensity): 288 (M^+, 1), 211 (1), 197 (100), 178 (8), 152 (2), 110 (1), 105 (10), 77 (8). Anal. Calcd for $C_{20}H_{16}O_2$: C, 83.33; H, 5.55. Found: C, 83.03; H, 5.41.



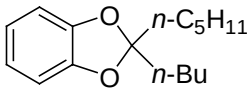
3e

2-Ethyl-2-propyl-1,3-benzodioxole **3e**[2]: yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 6.75-6.68 (m, 4H), 1.92-1.82 (m, 4H), 1.52-1.40 (m, 2H), 1.00-0.88 (m, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 148.4, 121.0, 108.5, 108.1, 39.8, 31.0, 16.4, 14.4, 7.35; GCMS *m/z* (% relative intensity): 192 (M^+, 45), 163 (93), 149 (100), 134 (8), 121 (8), 110 (36), 92 (2), 81 (3).



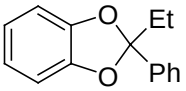
3f

2-*n*-Butyl-2-propyl-1,3-benzodioxole **3f**: yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 6.78-6.65 (m, 4H), 1.90-1.82 (m, 4H), 1.53-1.26 (m, 6H), 0.99-0.86 (m, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 148.2, 120.9, 120.7, 108.0, 40.1, 37.7, 25.0, 22.9, 16.3, 14.3, 14.1; GCMS *m/z* (% relative intensity): 220 (M^+, 27), 177 (94), 163 (100), 147 (5), 135 (10), 121 (9), 110 (23), 91 (1), 81 (3), 77 (1). Anal. Calcd for $C_{14}H_{20}O_2$: C, 76.36; H, 9.09. Found: C, 75.92; H, 8.83.



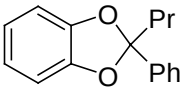
3g

2-*n*-Butyl-2-*n*-pentyl-1,3-benzodioxole **3g**: yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 6.77-6.69 (m, 4H), 1.90-1.85 (m, 4H), 1.45-1.26 (m, 10H), 0.94-0.85 (m, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 148.1, 120.8, 120.7, 108.0, 37.8, 37.5, 31.9, 24.9, 22.8, 22.6, 22.5, 14.1, 14.0; GCMS *m/z* (% relative intensity): 248 (M^+, 23), 191 (83), 177 (100), 147 (7), 135 (14), 121 (9), 110 (20), 81 (4); Anal. Calcd for $C_{16}H_{24}O_2$: C, 77.42; H, 9.68. Found: C, 77.33; H, 9.75.



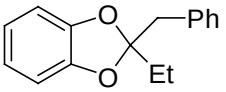
3h

2-Ethyl-2-phenyl-1,3-benzodioxole **3h**[3]: yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.58-7.55 (m, 2H), 7.38-7.28 (m, 3H), 6.82-6.74 (m, 4H), 2.24 (q, 2H, *J* = 7.4Hz), 0.99 (t, 3H, *J* = 7.4Hz); ^{13}C NMR (75 MHz, $CDCl_3$) δ 147.5, 140.6, 128.6, 128.2, 125.3, 121.2, 118.5, 108.4, 33.4, 7.4; GCMS *m/z* (% relative intensity): 226 (M^+, 18), 197 (100), 149 (2), 135 (57), 115 (19), 110 (19), 115 (22), 91 (11).



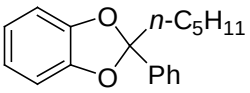
3i

2-Propyl-2-phenyl-1,3-benzodioxole **3i**: yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.57-7.51 (m, 2H), 7.38-7.33 (m, 3H), 6.81-6.74 (m, 4H), 2.19 (t, 2H, *J* = 8.0 Hz), 1.49 (m, 2H), 0.91 (t, 3H, *J* = 7.4Hz); ^{13}C NMR (75 MHz, $CDCl_3$) δ 147.4, 140.9, 128.6, 128.2, 125.2, 121.2, 118.2, 108.4, 42.5, 16.5, 13.9; GCMS *m/z* (% relative intensity): 240 (M^+, 14), 197 (100), 149 (55), 181 (7), 115 (7), 110 (5), 105 (8), 91 (12), 77 (11).



3i'

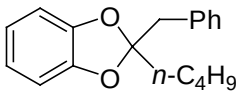
2-Benzyl-2-ethyl-1,3-benzodioxole **3i'**: yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.27-7.19 (m, 5H), 6.72 (s, 4H), 3.15 (s, 2H), 1.88 (q, 2H, *J* = 7.4Hz), 0.98 (t, 3H, *J* = 7.4Hz); ^{13}C NMR (75 MHz, $CDCl_3$) δ 147.8, 134.8, 130.5, 128.1, 126.8, 120.9, 119.7, 108.1, 43.6, 29.9, 6.84; GCMS *m/z* (% relative intensity): 240 (M^+, 7), 211 (2), 149 (100), 134 (4), 115 (3), 110 (1), 91 (12), 77 (2). Anal. Calcd for $C_{16}H_{16}O_2$ (a mixture of **3i** and **3i'**): C, 80.00; H, 6.67. Found: C, 79.83; H, 6.24.



3j

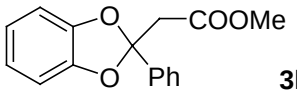
2-*n*-Pentyl-2-phenyl-1,3-benzodioxole **3j**: yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ

7.57-7.54 (m, 2H), 7.40-7.30 (m, 3H), 6.80-6.75 (m, 4H), 2.20 (t, 2H, J = 8.1 Hz), 1.43-1.26 (m, 4H), 1.18-1.00 (m, 2H), 0.84 (t, 3H, J = 7.1 Hz); GCMS *m/z* (% relative intensity): 268 (M^+, 11), 197 (100), 177 (30), 115 (6), 105 (7), 91 (8), 77 (7).



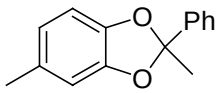
3j'

2-Benzyl-2-*n*-butyl-1,3-benzodioxole **3j'**: yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.20-7.08 (m, 5H), 6.61 (s, 4H), 3.04 (s, 2H), 1.75 (t, 2H, J = 7.4 Hz), 1.41-1.23 (m, 2H), 1.23-1.14 (m, 2H), 0.74 (t, 3H, J = 7.2 Hz); ^{13}C NMR (75 MHz, $CDCl_3$) δ 147.9, 134.9, 130.7, 128.2, 126.9, 121.1, 119.6, 108.2, 44.0, 36.7, 24.7, 22.7, 14.1; GCMS *m/z* (% relative intensity): 268 (M^+, 5), 211 (4), 177 (100), 147 (3), 135 (13), 121 (8), 115 (7), 91 (17). Anal. Calcd for $C_{18}H_{20}O_2$ (a mixture of **3j** and **3j'**): C, 80.60; H, 7.46. Found: C, 80.65; H, 7.45.



3k

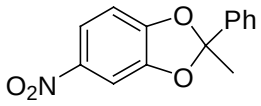
(2-Phenylbenzo[1,3]dioxol-2-yl)acetic acid methyl ester **3k**[4]: yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.62-7.59 (m, 2H), 7.40-7.33 (m, 3H), 6.86-6.78 (m, 4H), 3.55 (s, 3H), 3.30 (s, 2H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 167.9, 146.9, 139.4, 129.2, 128.3, 125.2, 121.7, 114.7, 108.8, 51.9, 44.9; GCMS *m/z* (% relative intensity): 270 (M^+, 24), 197 (100), 161 (7), 129 (4), 115 (4), 110 (6), 105 (15), 91 (4).



3l

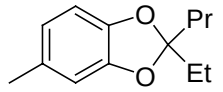
2,5-Dimethyl-2-phenyl-1,3-benzodioxole **3l**: yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.57 (m, 2H), 7.28-7.36 (m, 3H), 6.68-6.62 (m, 2H), 6.55 (d, 1H, J = 7.9 Hz), 2.22 (s, 3H), 1.94 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 147.4, 145.2, 141.5, 131.2, 128.9, 128.4, 125.1, 121.4, 116.7, 109.7, 108.1, 27.1, 21.3; GCMS *m/z* (% relative intensity): 226 (M^+,81), 211 (77), 149 (10), 124 (100), 103 (63), 77 (36). Anal. Calcd for $C_{15}H_{14}O_2$: C, 79.62; H, 6.24.

Found: C, 79.73; H, 6.24.



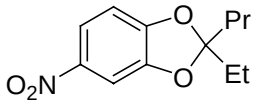
3m

2-Methyl-5-nitro-2-phenyl-1,3-benzodioxole **3m**: yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.84 (dd, 1H, *J* = 8.6Hz, *J* = 2.1Hz), 7.64 (d, 1H, *J* = 2.1Hz), 7.54-7.57 (m, 2H), 7.37-7.42 (m, 3H), 6.82 (d, 1H, *J* = 8.6Hz), 2.03 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 152.8, 147.9, 142.8, 139.7, 129.6, 128.6, 124.8, 120.4, 119.7, 107.6, 104.6, 21.2; GCMS *m/z* (% relative intensity): 257 (M^+, 20), 242 (34), 196 (8), 180 (5), 134 (4), 103 (100), 91 (3), 77 (25). Anal. Calcd for $C_{14}H_{11}NO_4$: C, 65.37; H, 4.31; N, 5.44. Found: C, 65.78; H, 4.62; N, 5.42.



3n

2-Ethyl-5-methyl-2-propyl-1,3-benzodioxole **3n**: yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 6.54-6.60 (m, 3H), 2.24 (s, 3H), 1.82-1.93 (m, 4H), 1.44-1.51(m, 2H), 0.91-0.98 (m, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 148.3, 146.2, 130.5, 120.9, 120.7, 108.8, 107.3, 39.7, 30.9, 21.3, 16.3, 14.3, 7.2; GCMS *m/z* (% relative intensity): 206 (M^+, 37), 177 (87), 163 (100), 148 (6), 135 (7), 124 (41), 106 (6), 77 (7). Anal. Calcd for $C_{13}H_{18}O_2$: C, 75.69; H, 8.80. Found: C, 75.87; H, 9.00.



3o

2-Ethyl-5-nitro-2-propyl-1,3-benzodioxole **3o**[5]: yellow oil; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.83 (dd, 1H, *J* = 8.6 Hz, *J* = 2.1 Hz),7.56 (d, 1H, *J* = 2.4Hz), 6.75 (d, 1H, *J* = 8.6 Hz), 1.89-1.99 (m, 4H), 1.44-1.50 (m, 2H), 0.94-0.99 (m, 6H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 154.0, 148.9, 142.4, 124.8, 119.4, 106.8, 103.7, 39.7, 31.0, 16.0, 14.1, 9.7; GCMS *m/z* (% relative intensity): 237 (M^+, 13), 208 (69), 194 (100), 162 (32), 148 (45), 125 (6), 92 (22), 79 (18), 77(4).

References for known products:

[1] Li, T.-S.; Li, L.-J.; Lu, B.; Yang, F. *J. Chem. Soc., Perkin Trans. 1*, **1998**, 3561-3564.

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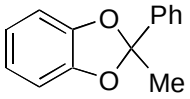
[3] Napolitano, E.; Fiaschi, R.; Mastrorilli, E. *Synthesis* **1986**, 122-125.

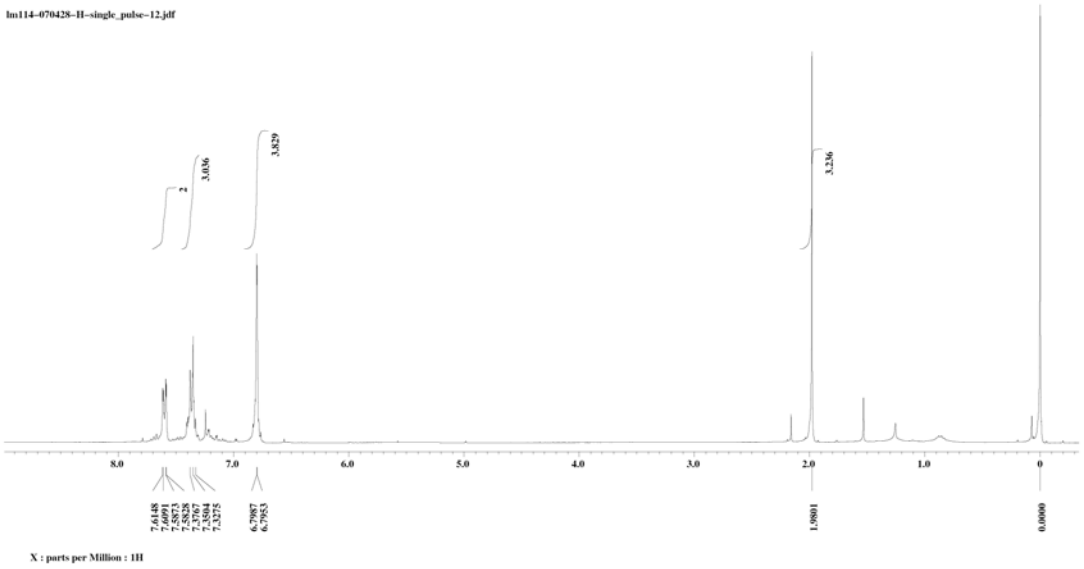
[4] Rosnati, V.; Sannicolo, F.; Pagani, G. *Gazz. Chim. Ital.* **1968**, *98*, 1069-1084.

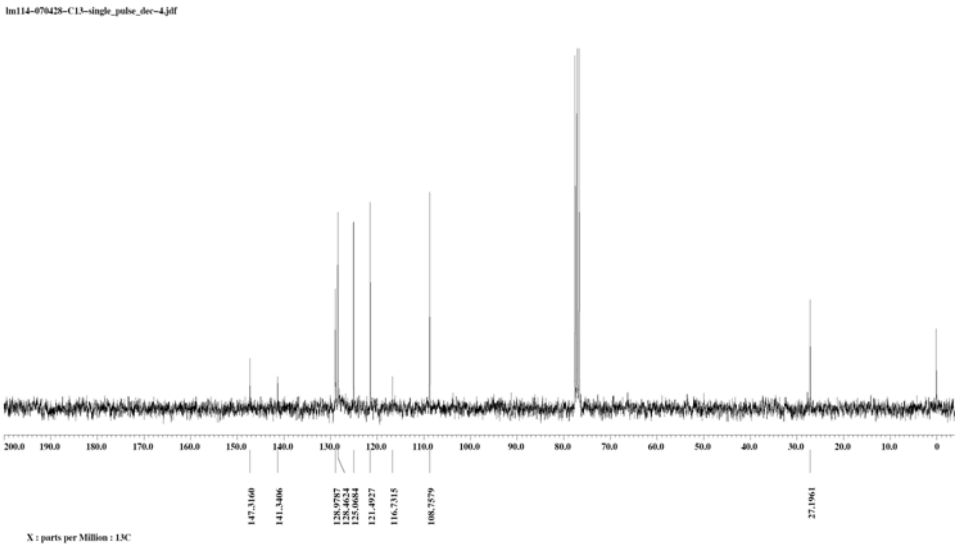
[5] Isobe, T.; Seino, H. *Bokin Bobai* **1989**, *17*, 365-369.

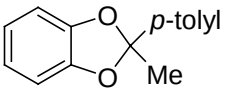
2. ^{1}H, and ^{13}C-NMR charts of products



3a



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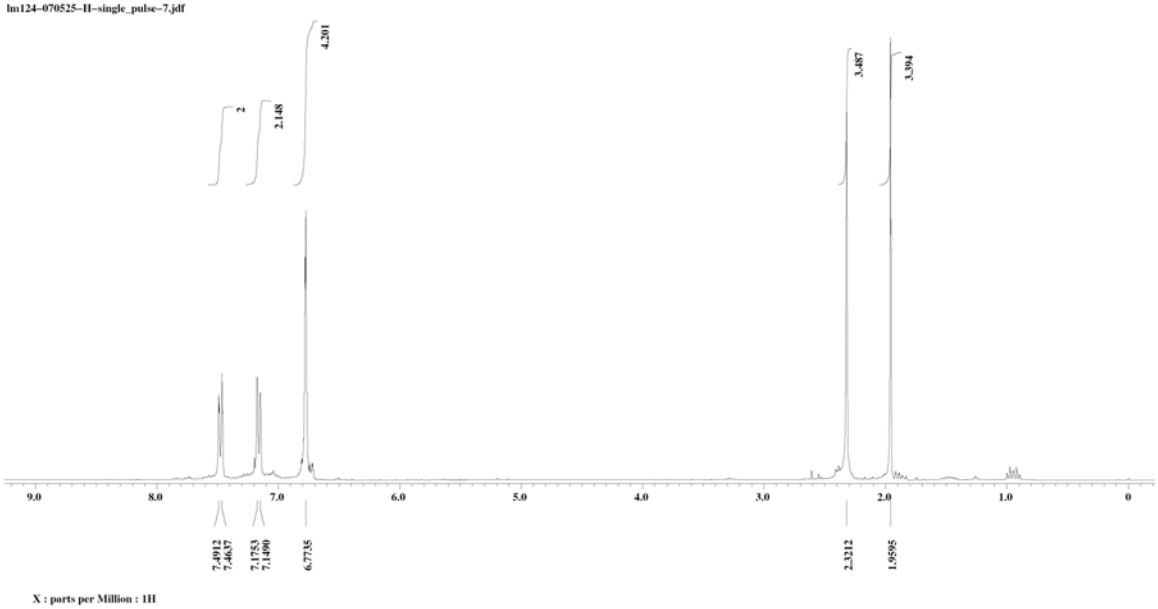
O
O
p-tolyl
Me

3b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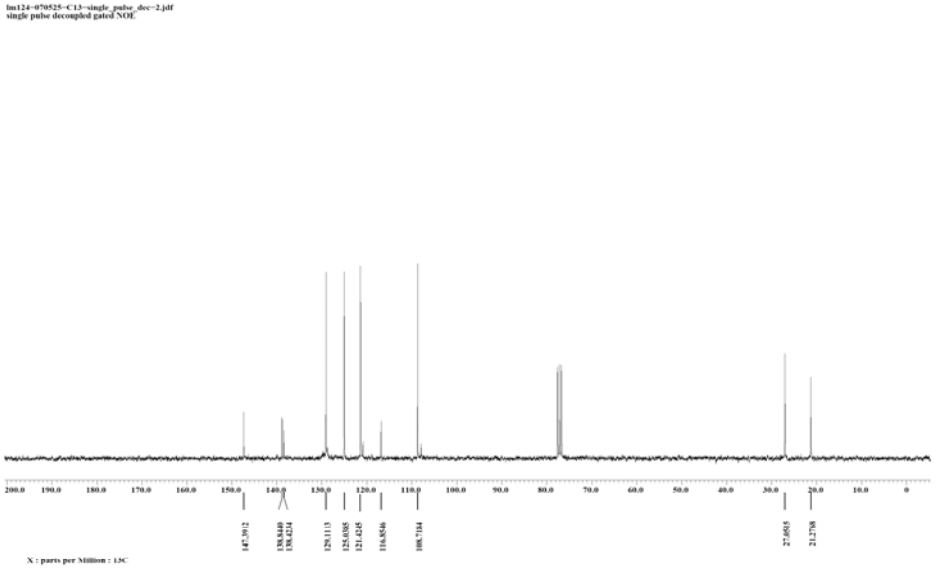
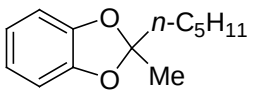
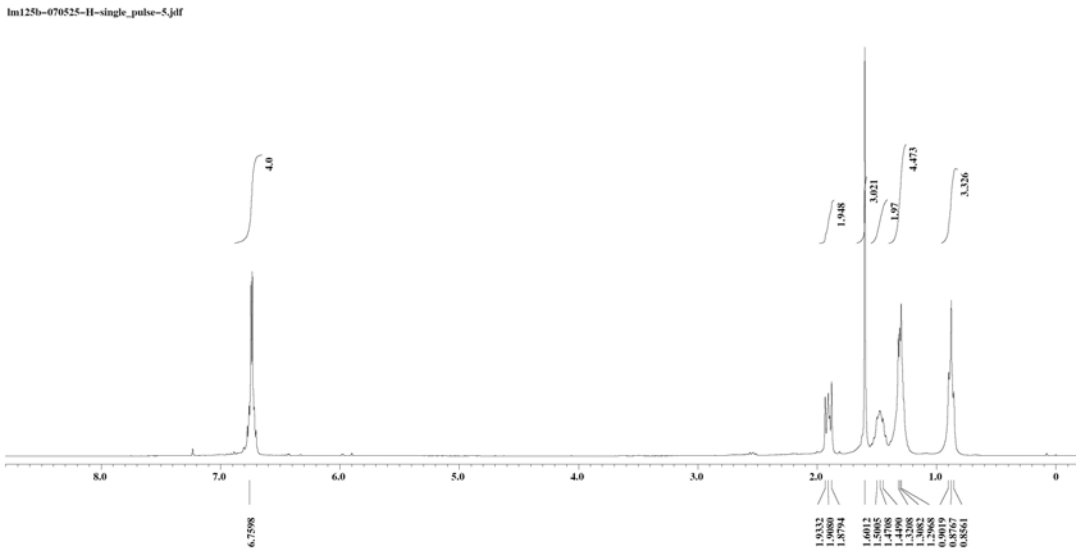
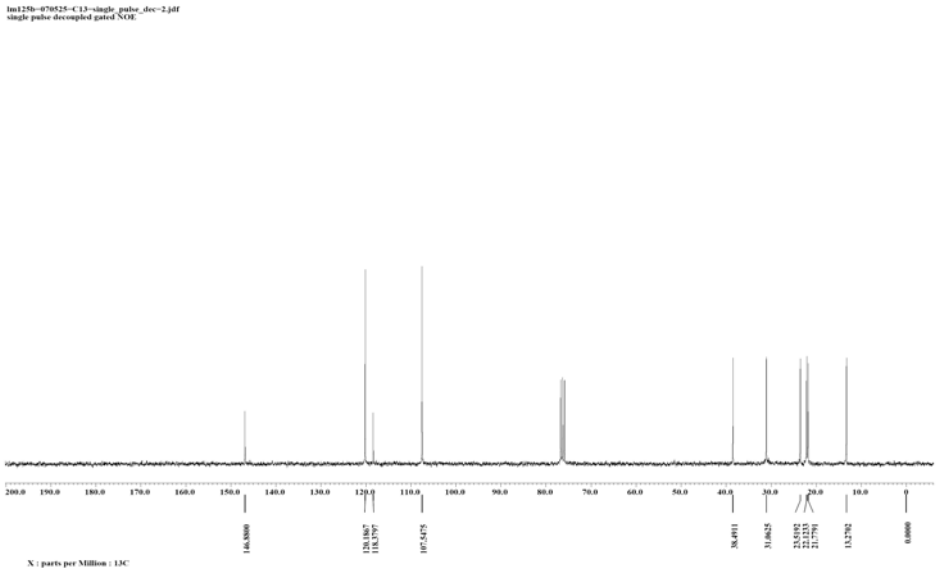
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.4912
7.4637
7.1753
7.1490
6.7735
2.3212
1.9595
X : parts per Million : 1H

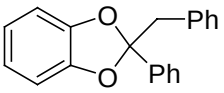

lm124-070525-C13-single_pulse_dec-2.jdf
single pulse decoupled gated NOE
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
147.3912
138.8440
138.4234
129.1113
125.6305
121.4245
116.8546
108.7104
27.6925
21.2708
X : parts per Million : 13C


O
n-C5H11
O
Me

3c


lm125b~070525~H~single_pulse~5.jdf
4.0
1.948
3.021
1.97
4.473
3.326
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
6.7598
1.9332
1.9080
1.8794
1.6012
1.5985
1.4708
1.4490
1.3208
1.2882
1.2698
0.9019
0.8767
0.8561
X : parts per Million : 1H

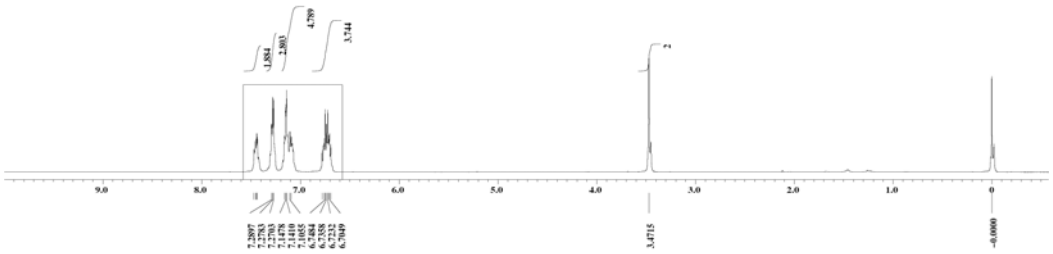

lm125b~070525~C13~single_pulse_dec~2.jdf
single pulse decoupled gated NOE
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
146.8800
120.1867
118.3797
107.5475
38.4911
31.0625
23.8535
22.1335
21.7791
13.2782
0.0000
X : parts per Million : 13C



3d

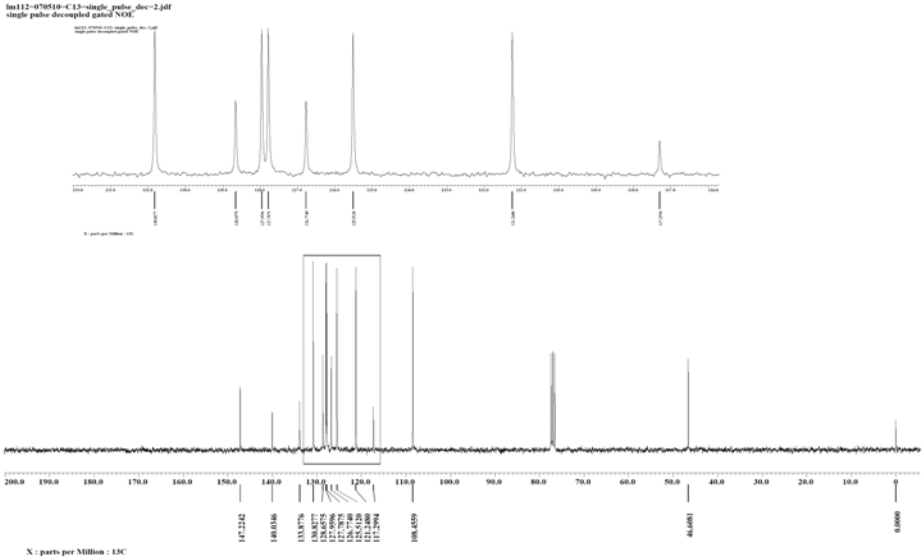
```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
```

lm112-070510-H-single_pulse-3.jdf

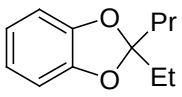


X : parts per Million : 1H

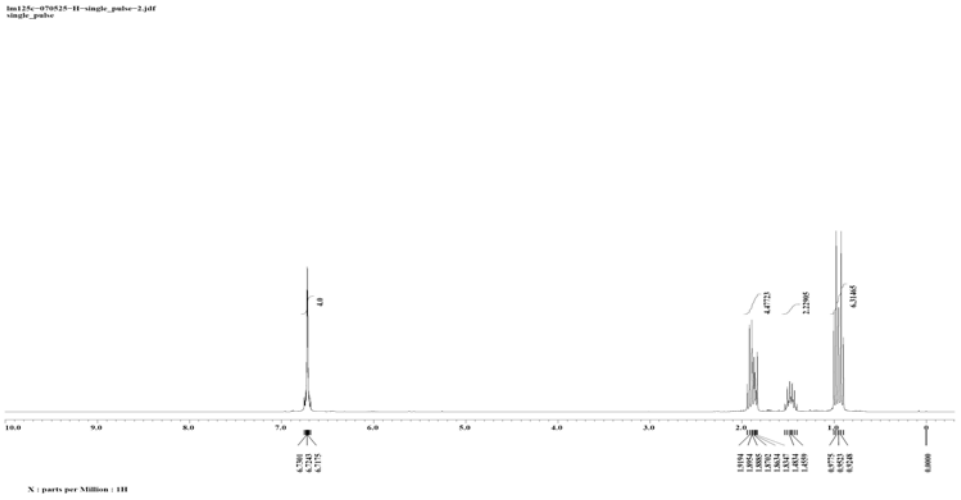
lm112-070510-C13-single_pulse_dec-2.jdf
single pulse decoupled gated NOE

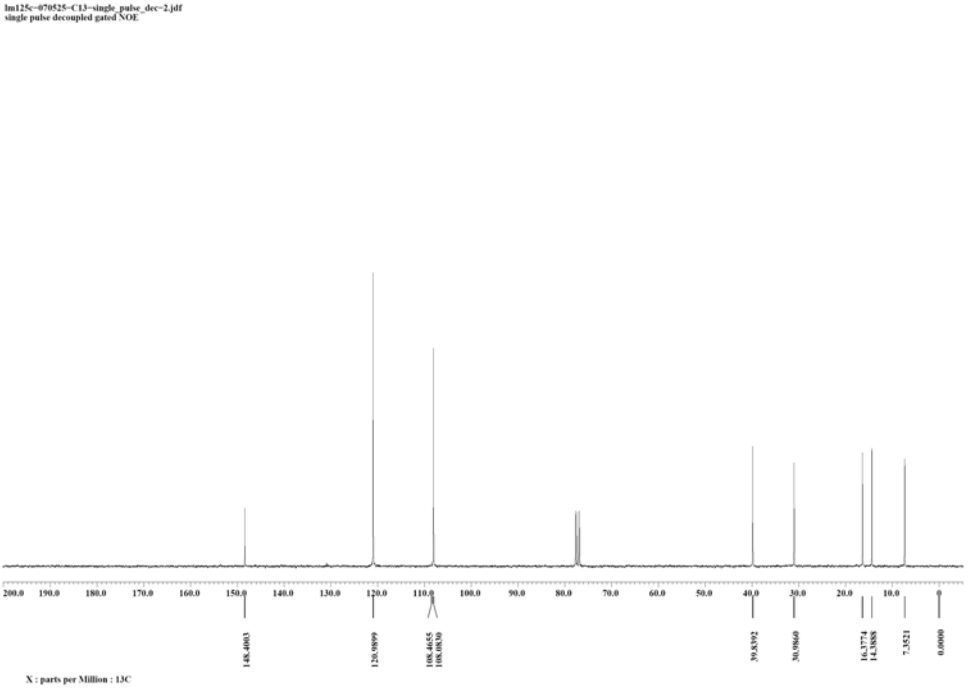


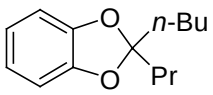
X : parts per Million : 13C


O
Pr
O
Et

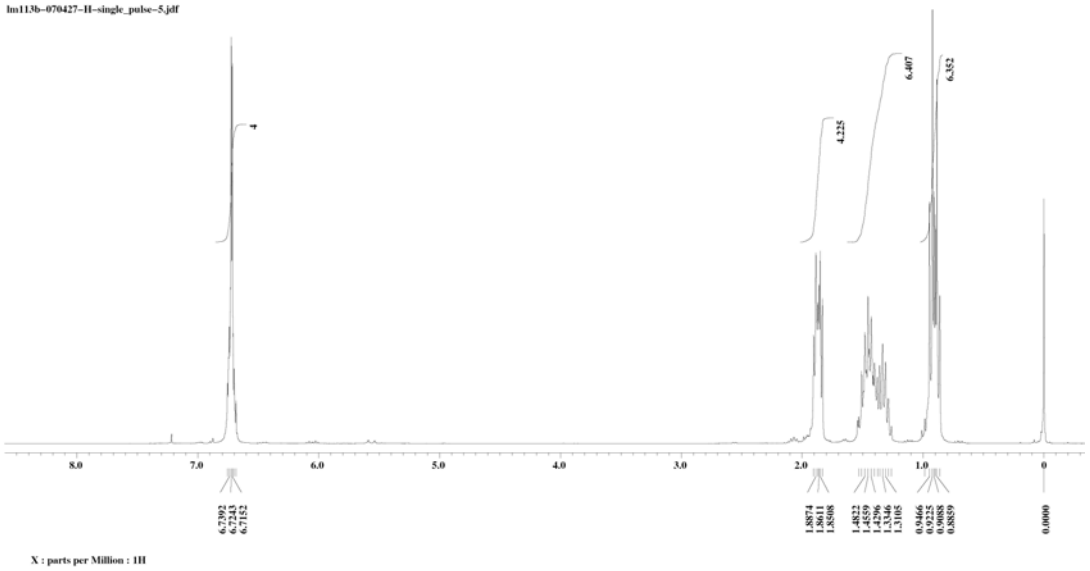
3e

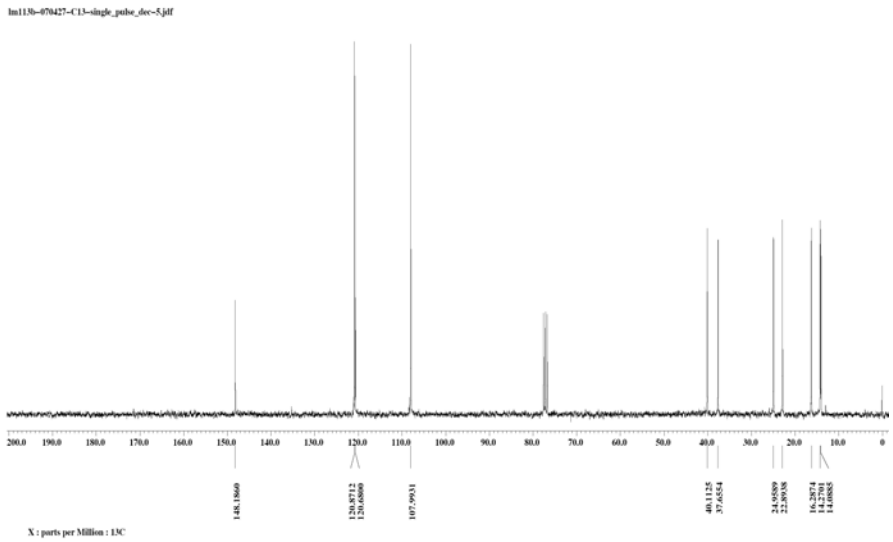

lm125c-070528-H-single_pulse-2.jdf
single_pulse
4.0
4.4733
2.2305
6.3165
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
6.7301
6.7243
6.7175
1.9194
1.8954
1.8804
1.8702
1.8634
1.8347
1.8054
1.4589
0.8775
0.8523
0.8268
0.000
X : parts per Million : 1H

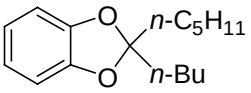

lm125c-070525-C13-single_pulse_dec-2.jdf
single pulse decoupled gated NOE
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
148.4003
120.9899
108.4655
108.0830
39.8392
30.9860
16.3774
14.3888
7.3521
0.0000
X : parts per Million : 13C


O
n-Bu
O
Pr

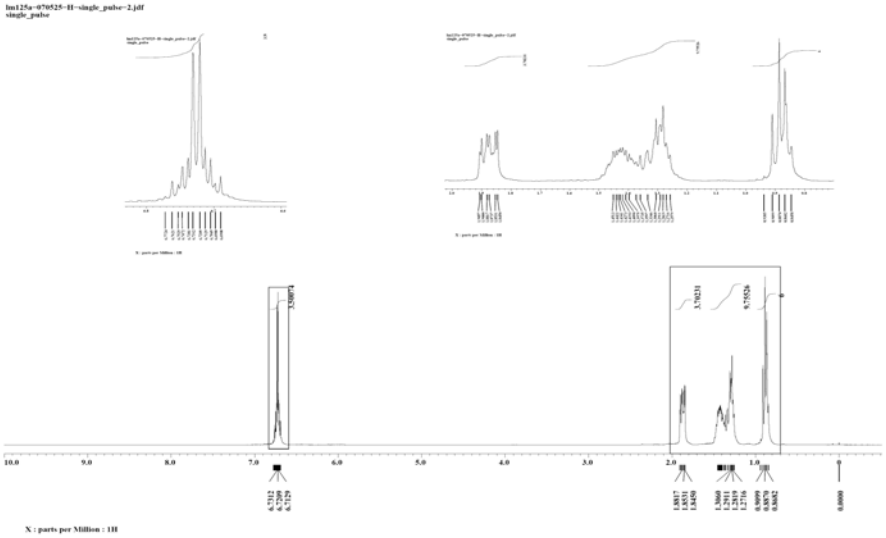
3f

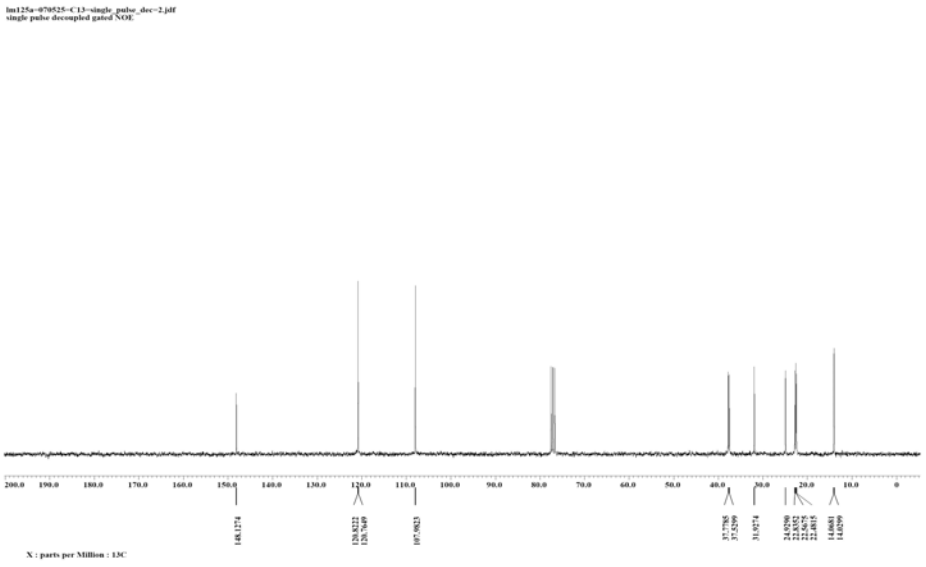

lm113b-070427-H-single_pulse-5.jdf
4
4.225
6.407
6.352
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
6.7392
6.7243
6.7152
1.8874
1.8611
1.8508
1.4822
1.4559
1.4296
1.3346
1.3105
0.9466
0.9225
0.8984
0.8859
0.0000
X : parts per Million : 1H

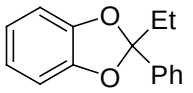

lm113b-070427-C13-single_pulse_dec-5.jdf
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
148.1860
120.8712
120.6800
107.9931
40.1125
37.6854
24.9509
22.9938
16.2874
14.2701
14.0065
X : parts per Million : 13C


O
O
O
n-C5H11
n-Bu

3g


lm125a~070525~H~single_pulse~2.jdf
single_pulse
X : parts per Million : 1H

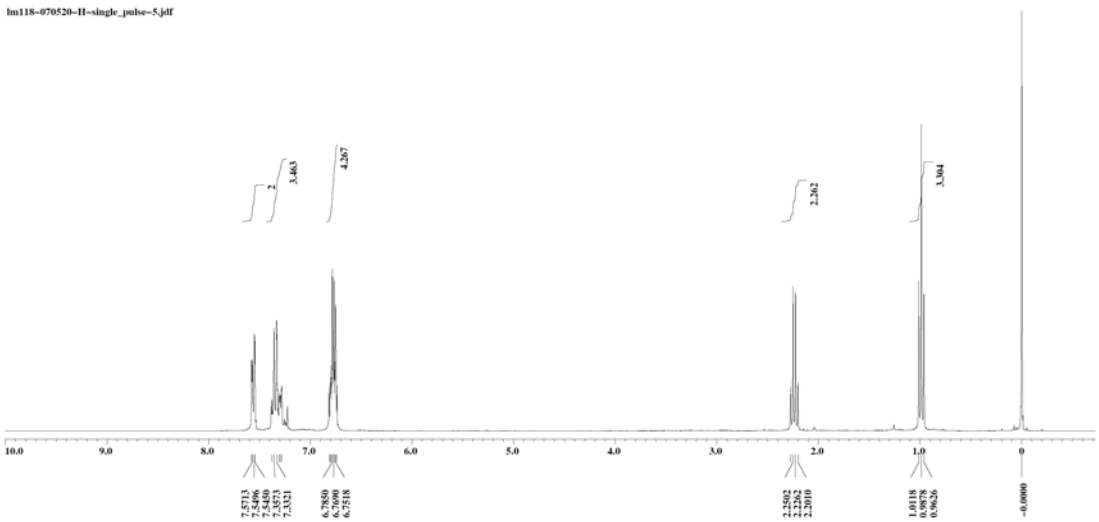

lm125a~070525~C13~single_pulse_dec~2.jdf
single pulse decoupled gated NOE
X : parts per Million : 13C



3h

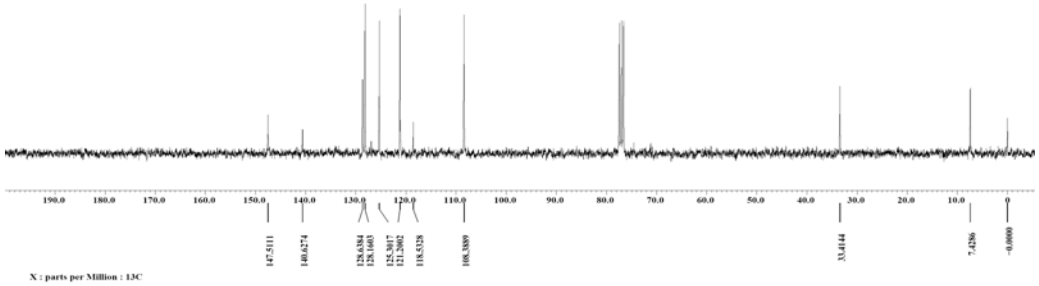
```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
```

lm118-070520-H-single_pulse-5.jdf

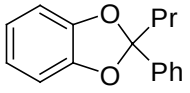


X : parts per Million : 1H

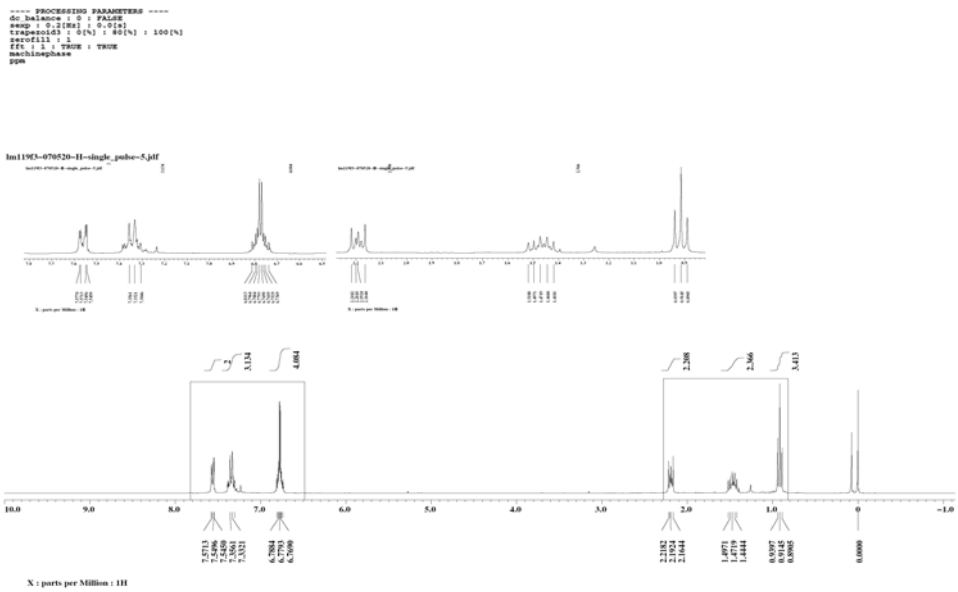
lm118-070520-C13-single_pulse_dec-2.jdf
single pulse decoupled gated NOE

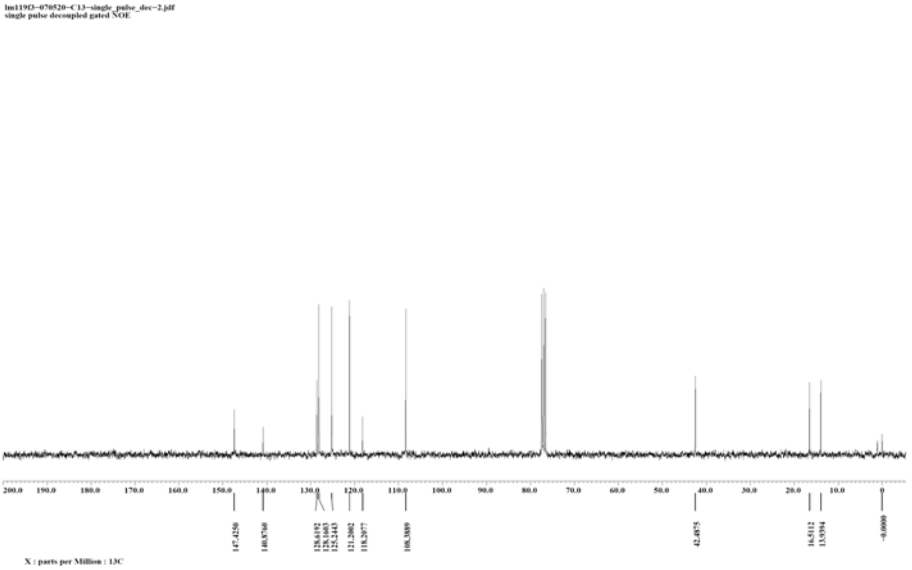


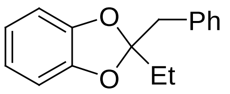
X : parts per Million : 13C


O
Pr
Ph
O

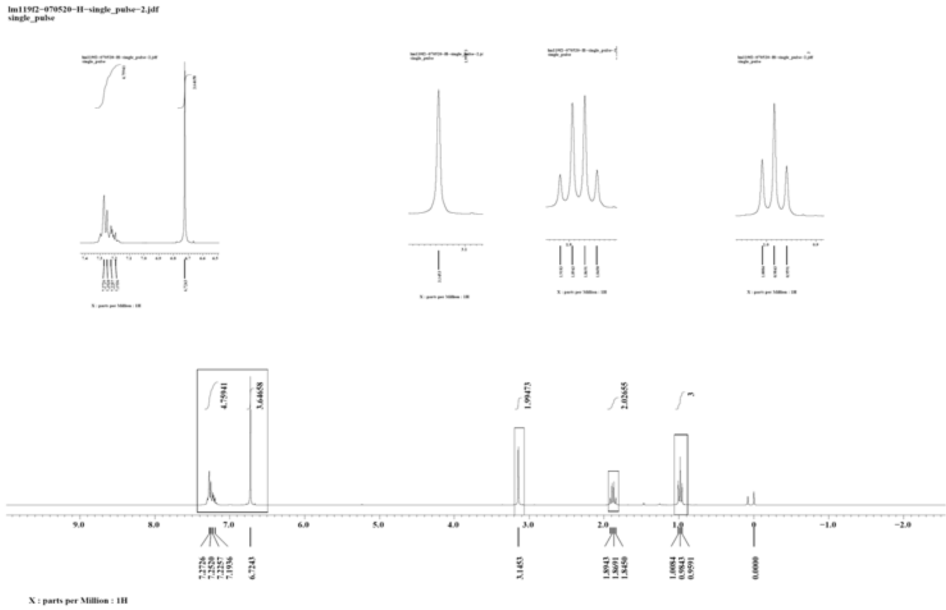
3i

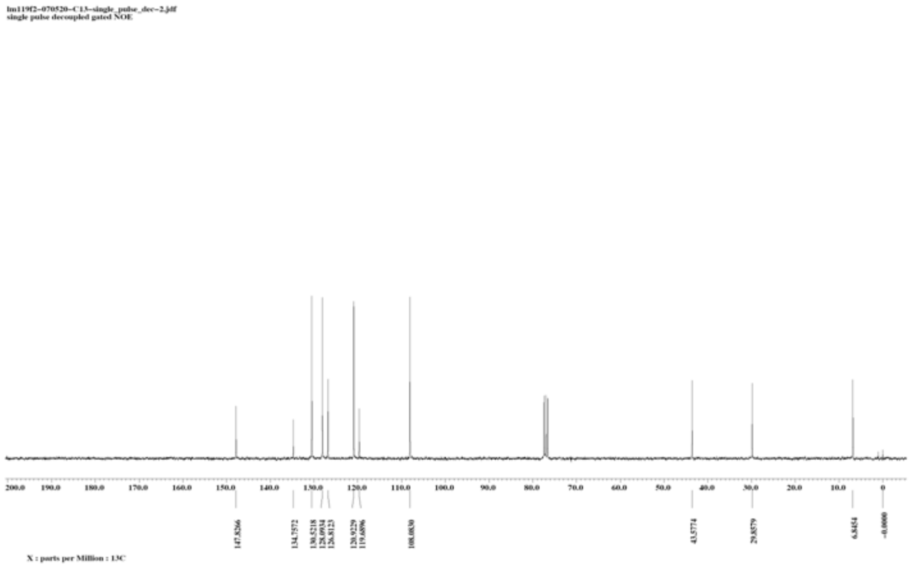

===== PROCESSING PARAMETERS =====
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
lm11903-070520-H-single_pulse-5.jdf
3.134
4.084
2.308
2.366
3.413
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
7.5713
7.5546
7.5458
7.3561
7.3531
6.7984
6.7793
6.7699
2.2182
2.1924
2.1644
1.4971
1.4779
1.4444
0.9397
0.9145
0.8965
0.0000
X : parts per Million : 1H

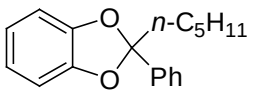

lm11903-070520-C13-single_pulse_dec-2.jdf
single pulse decoupled gated NOE
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
147.4250
140.8760
128.6192
128.1683
125.2243
121.3062
118.3277
108.3889
42.4875
16.5112
13.5594
-0.0000
X : parts per Million : 13C


O
Ph
O
Et

3i'


lm119f2-070520-H-single_pulse-2.jdf
single_pulse
4.75941
3.64658
1.99473
2.02655
3
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
-1.0
-2.0
7.2726
7.2520
7.2257
7.1936
6.7243
3.1453
1.8943
1.8691
1.8450
1.0084
0.9841
0.9591
0.0000
X : parts per Million : 1H

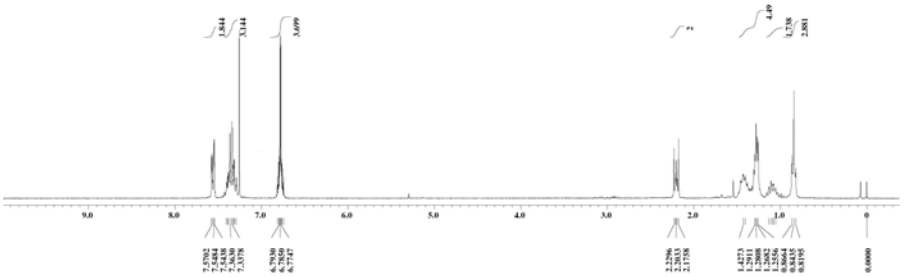

lm119f2-070520-C13-single_pulse_dec-2.jdf
single pulse decoupled gated NOE
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
147.8266
134.7572
130.5218
128.0934
126.8123
120.9229
119.6096
108.0830
43.5774
29.8579
6.8454
-0.0000
X : parts per Million : 13C



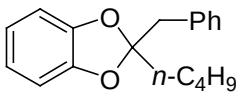
3j

```
---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid3 : 0[%] : 80[%] : 100[%]
zerofill : 1
fft : 1 : TRUE : TRUE
machinephase
ppm
```

lm125df2~080108~H~single_pulse~4.jdf

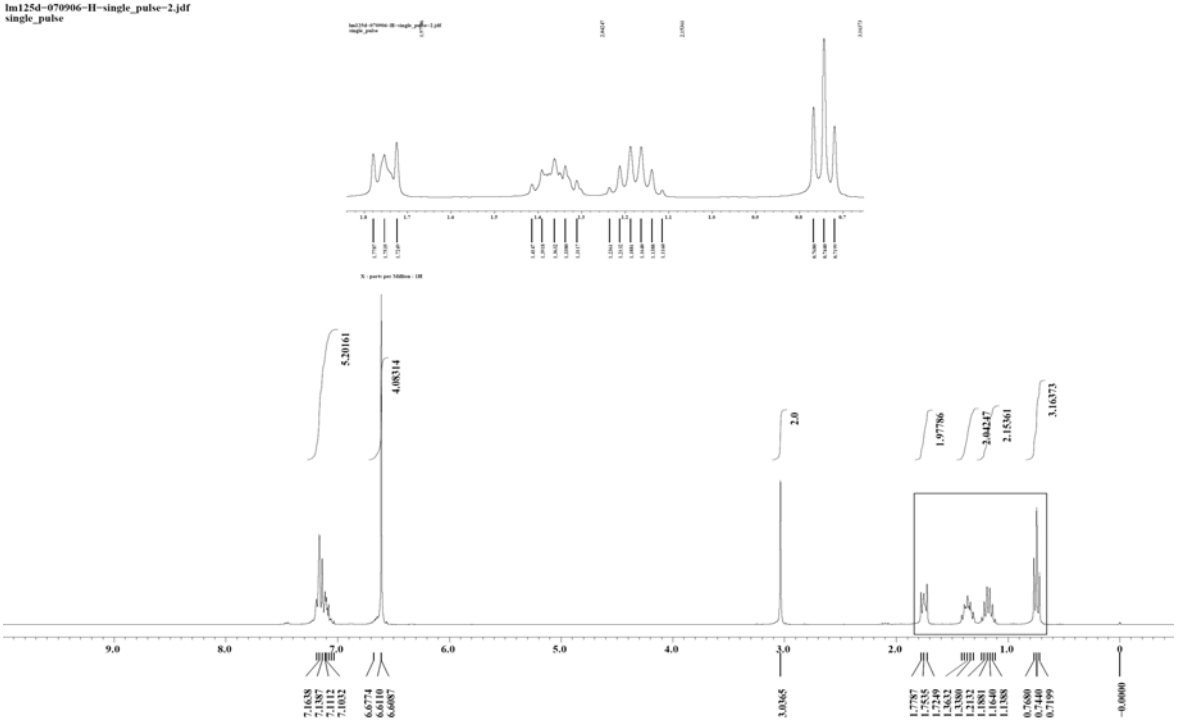


X : parts per Million : 1H



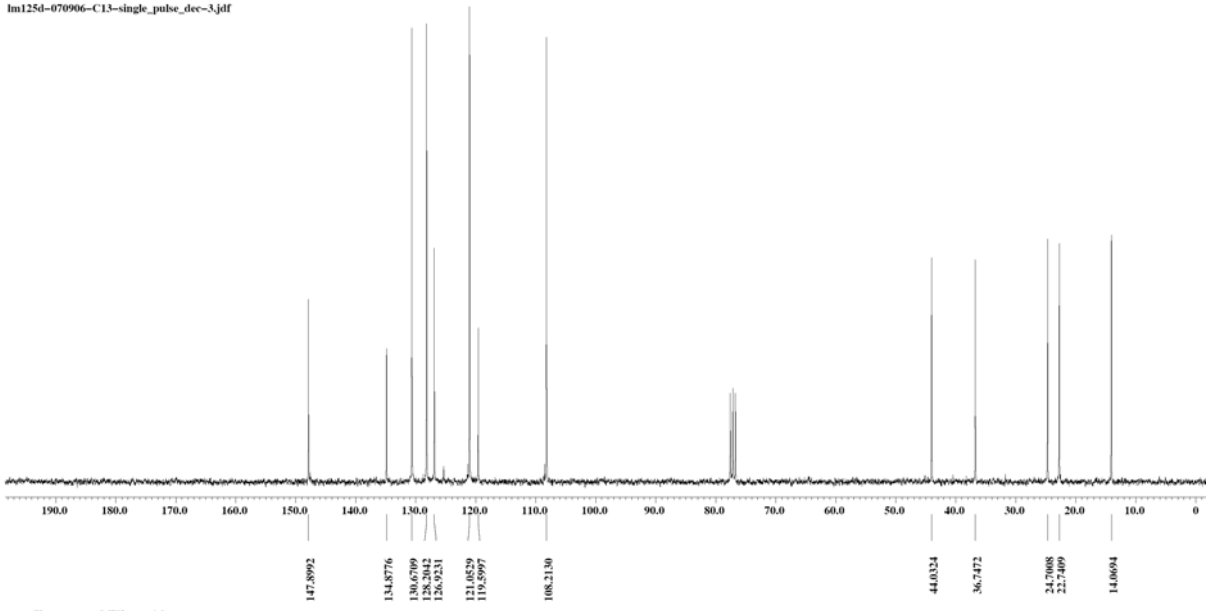
3j'

lm125d~070906~H~single_pulse~2.jdf
single_pulse

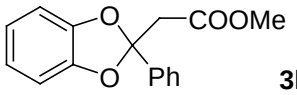


X : parts per Million : 1H

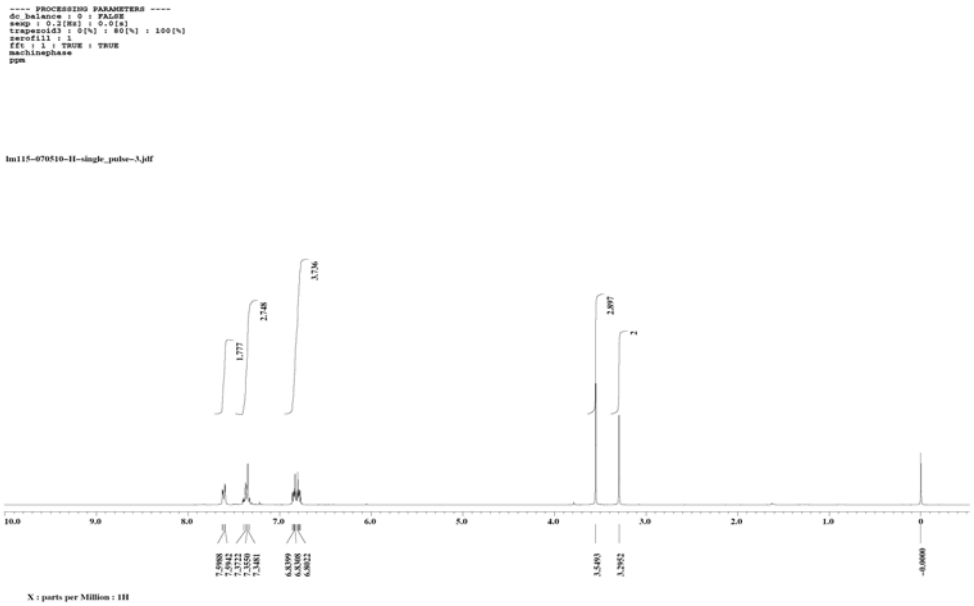
lm125d~070906~C13~single_pulse_dec~3.jdf

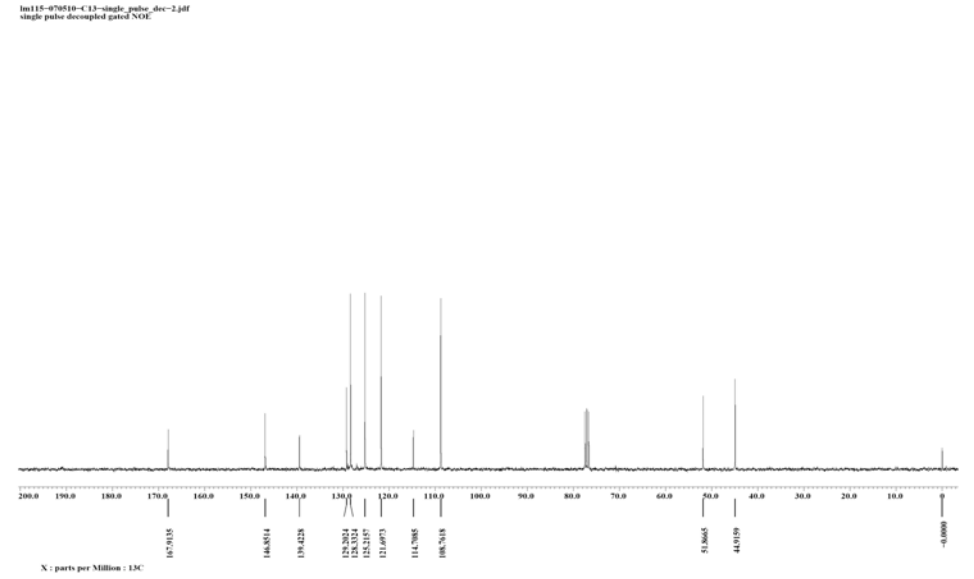


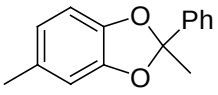
X : parts per Million : 13C


O
COOMe
O
Ph

3k

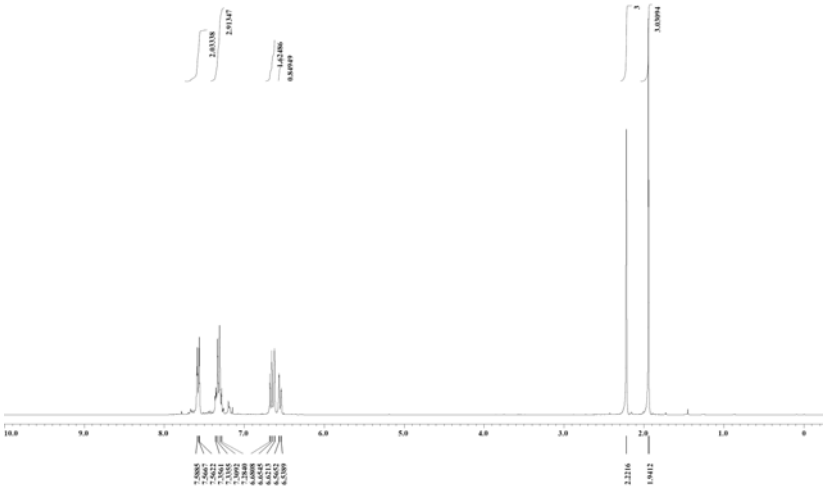

---- PROCESSING PARAMETERS ----
dc_balance : 0 : FALSE
sexp : 0.2[Hz] : 0.0[s]
trapezoid2 : 0[%] : 80[%] : 100[%]
zerofill : 1
ff% : 1 : TRUE : TRUE
machinephase
ppm
lm115-070510-H-single_pulse-3.jdf
1.777
2.748
3.736
2.897
2
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0
7.5988
7.5942
7.3722
7.3550
7.3481
6.8399
6.8308
6.8032
3.5493
3.2952
-0.0000
X : parts per Million : 1H


lm115-070510-C13-single_pulse_dec-2.jdf
single pulse decoupled gated NOE
200.0
190.0
180.0
170.0
160.0
150.0
140.0
130.0
120.0
110.0
100.0
90.0
80.0
70.0
60.0
50.0
40.0
30.0
20.0
10.0
0
167.9135
146.8514
139.4228
129.2024
128.3324
125.2157
121.6973
114.7085
108.7618
51.8665
44.9159
-0.0000
X : parts per Million : 13C



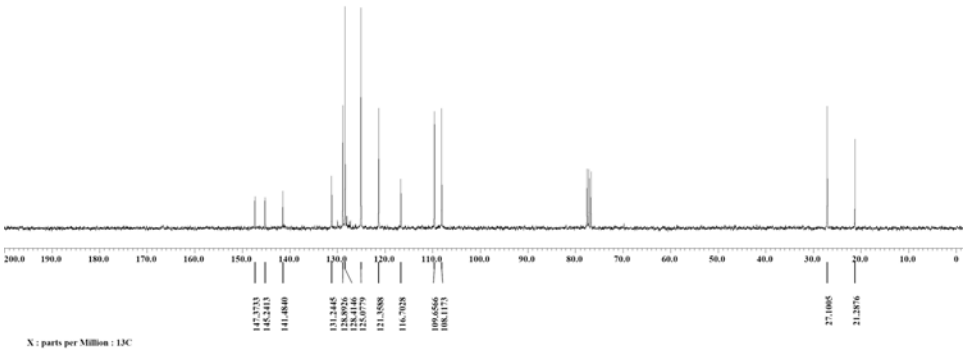
3l

lm~Aa~080508~H~single_pulse~2.jdf
single_pulse

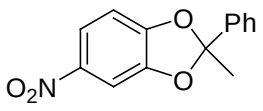


X : parts per Million : 1H

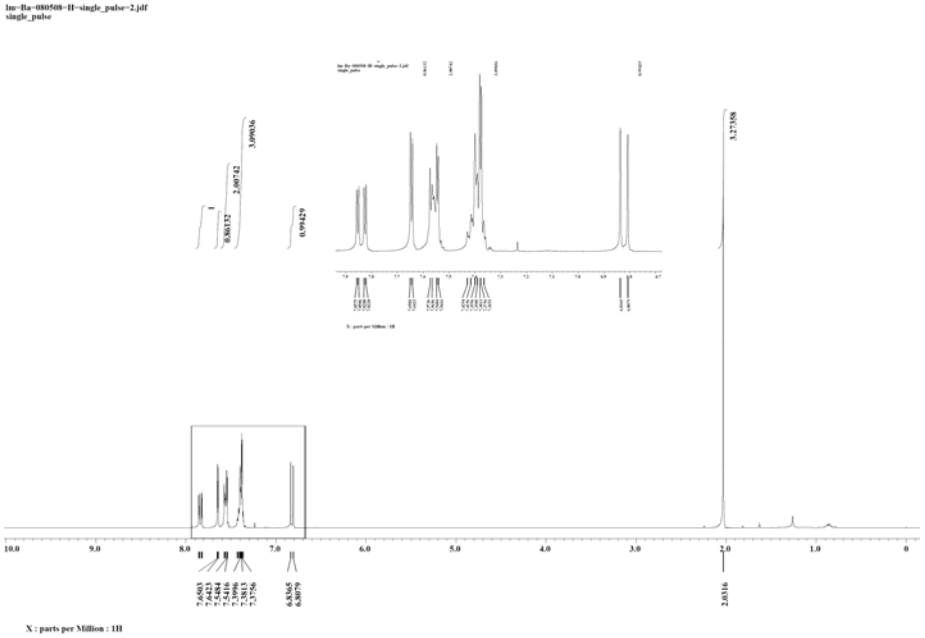
lm~Aa~080508~C13~single_pulse_dec~2.jdf
single pulse decoupled gated NOE

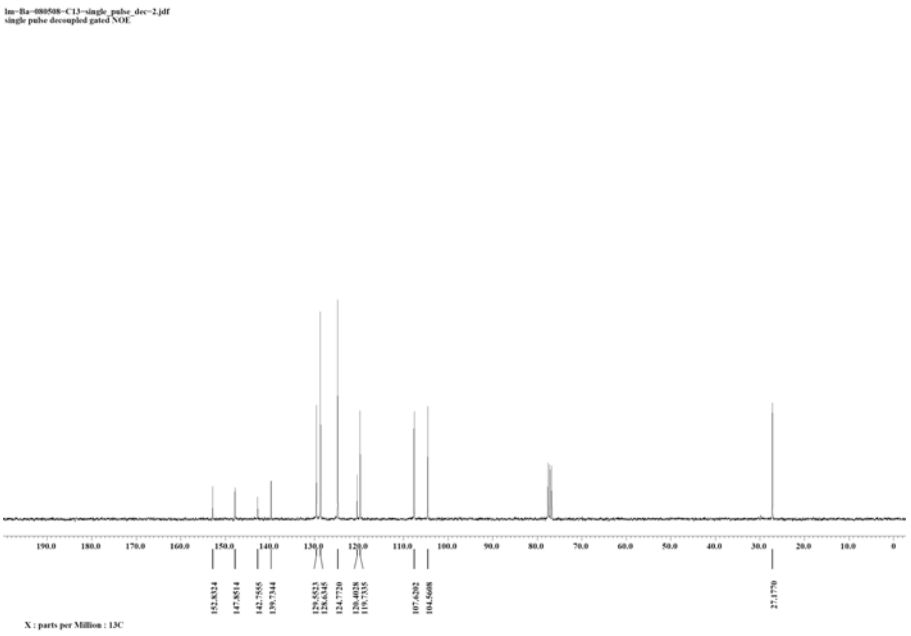


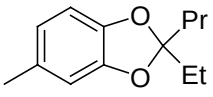
X : parts per Million : 13C


O
Ph
O
O2N

3m

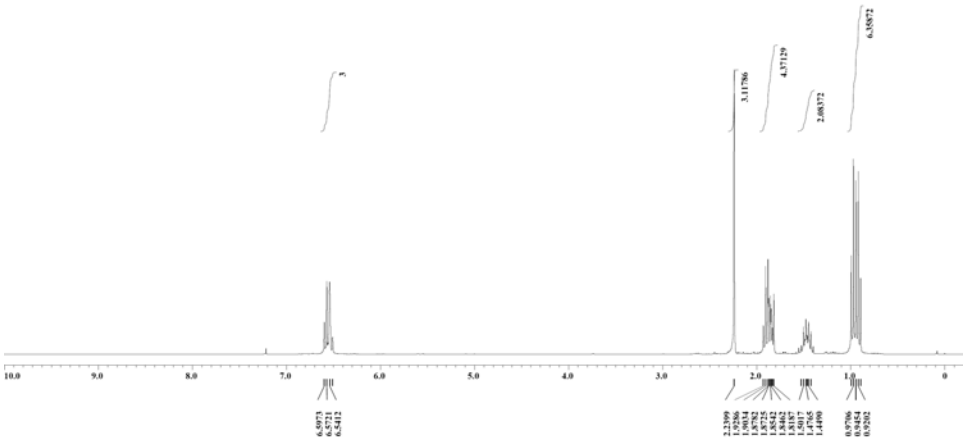

lm~Ba~080508~H~single_pulse~2.jdf
single_pulse
3.09036
2.09742
0.80132
0.99429
3.27558
2.0316
X : parts per Million : 1H


lm~Ba~080508~C13~single_pulse_dec~2.jdf
single pulse decoupled gated NOE
X : parts per Million : 13C



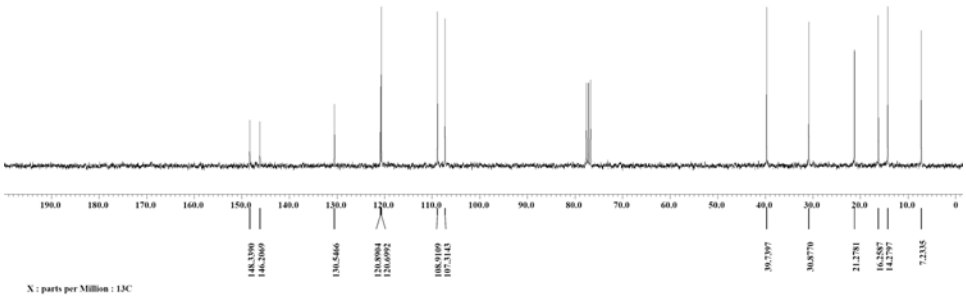
3n

lm~Ab~080508~H~single_pulse~2.jdf
single_pulse

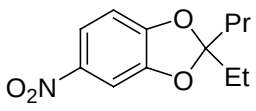


X : parts per Million : 1H

lm~Ab~080508~C13~single_pulse_dec~2.jdf
single pulse decoupled gated NOE

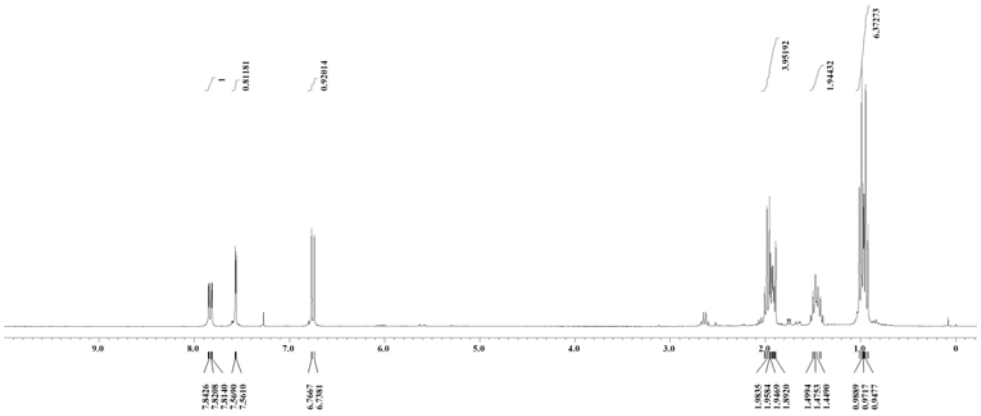


X : parts per Million : 13C



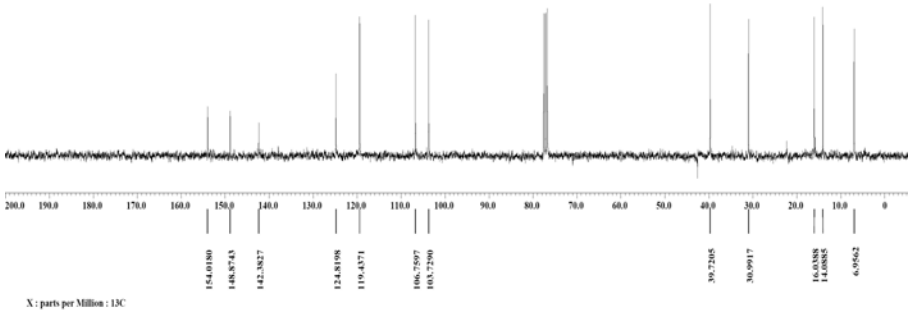
3o

lmBb~080513~H~single_pulse~2.jdf
single_pulse



X : parts per Million : 1H

lmBb~080513~C13~single_pulse_dec~3.jdf
single pulse decoupled gated NOE



X : parts per Million : 13C