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A highly efficient catalyst for Suzuki–Miyaura Coupling Reaction of Benzyl chloride under mild conditions

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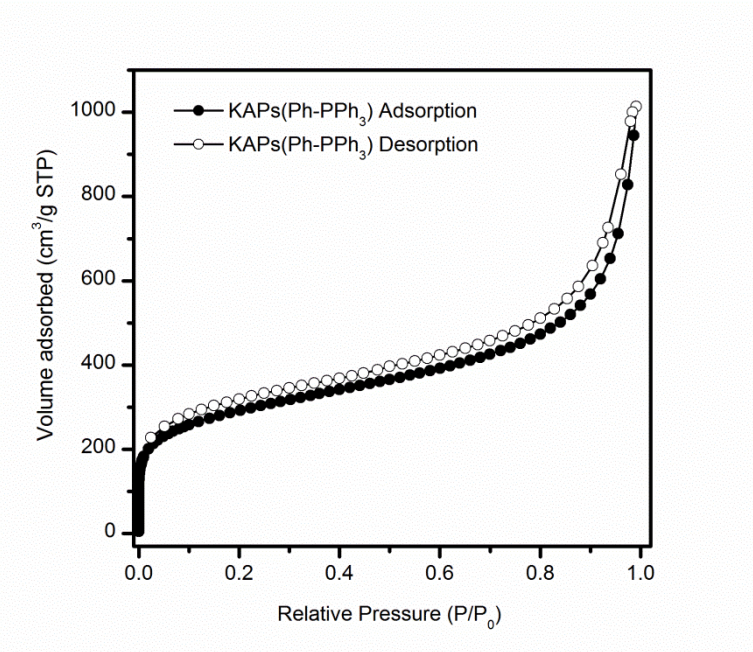


Fig. S1 Nitrogen adsorption (solid) and desorption (open) isotherms of KAPs(Ph-PPh_3).

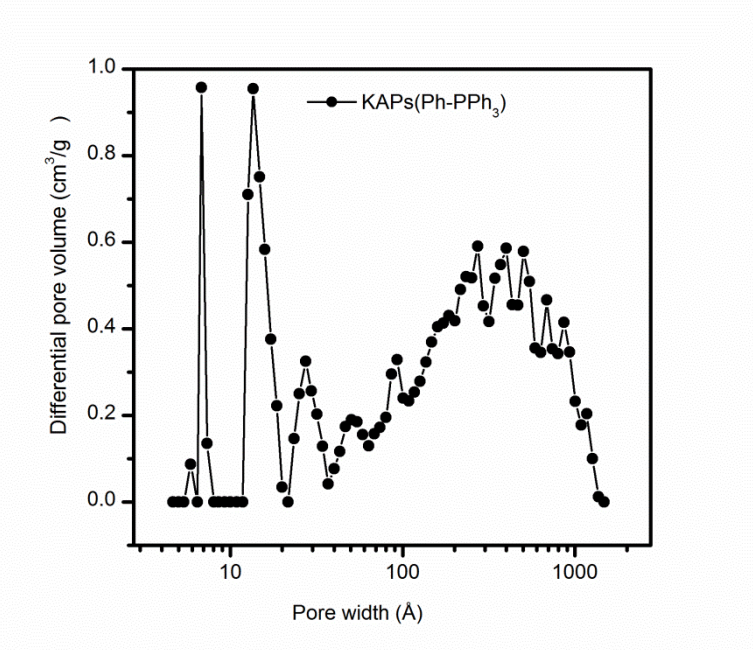


Fig. S2 Pore size distributions calculated using DFT methods (slit pore models, differential pore volumes. pore width) of KAPs(Ph-PPh_3).

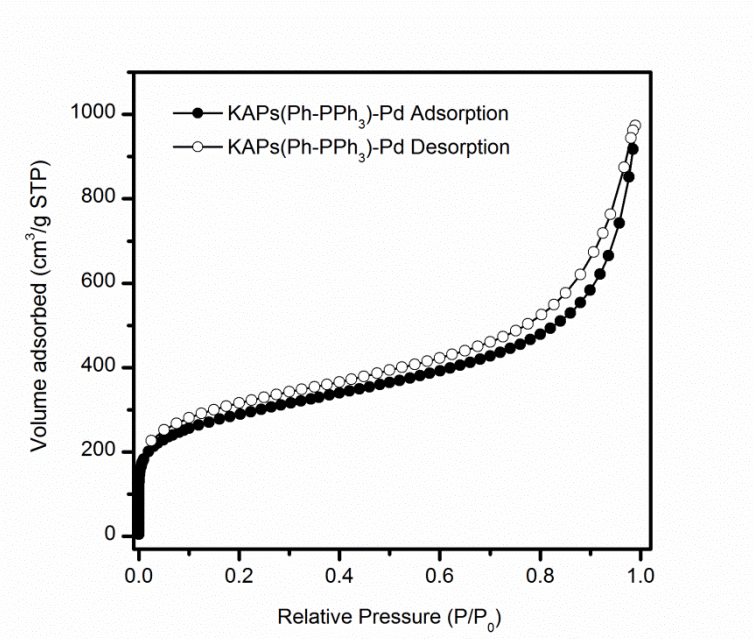


Fig. S3 Nitrogen adsorption (solid) and desorption (open) isotherms of KAPs(Ph-PPh_3)-Pd.

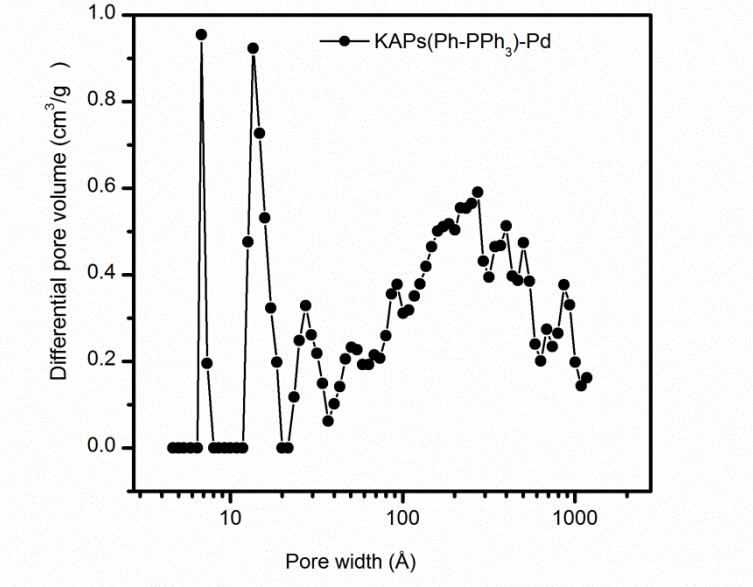


Fig. S4 Pore size distributions calculated using DFT methods (slit pore models, differential pore volumes. pore width) of KAPs(Ph-PPh_3)-Pd.

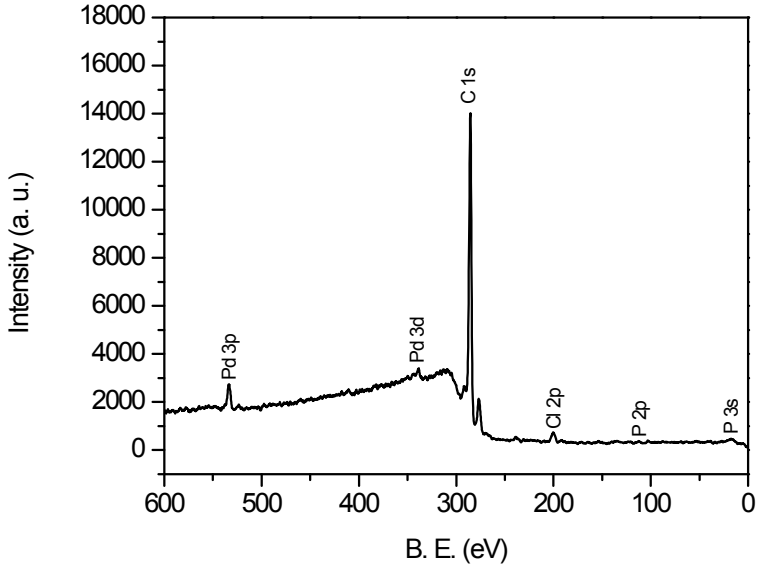


Fig. S5 XPS spectra of KAPs(Ph-PPh_3)-Pd (elemental scan).

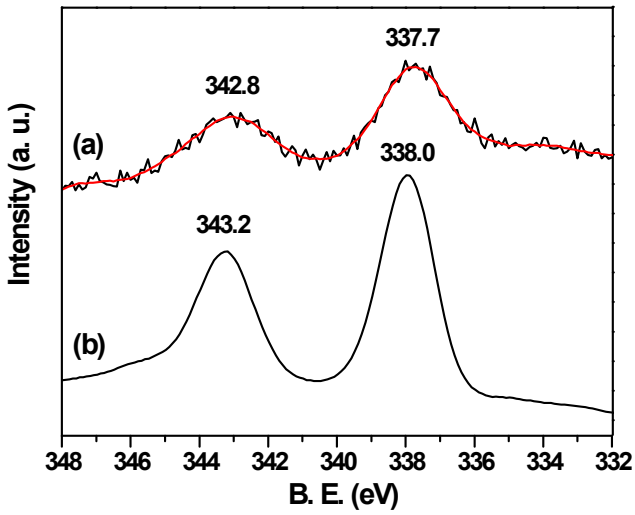


Figure S6 XPS spectra for Pd on fresh KAPs(Ph-PPh_3)-Pd (a) and pure $PdCl_2$ compound (b).

Table S1 Suzuki coupling reactions by fresh and recovered catalyst.

Run	Time (min)	Yield (%) [b]
1st	5	99
2nd	5	99

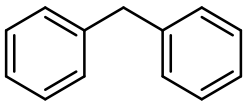
3rd	5	97
4th	20	84

[a] Reaction conditions: 0.5 mol% of Pd, 0.5 mmol of benzyl chloride, 0.75 mmol of phenyl boronic acid, 1 mmol of $K_3PO_4 \cdot 3H_2O$, 2 ml of EtOH, 80 °C, 5 min, in air.

[b] GC yield (naphthaline as internal standard).

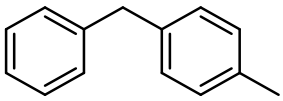
^{1}HNMR

Diphenylmethane



^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.26 (t, *J* = 7.2 Hz, 4H), 7.18 (m, 6H), 3.97 (s, 2H).

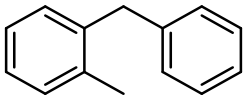
Benzyl-4-methylbenzene



^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.39 (d, *J* = 8.0 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 3H), 4.21 (s, 4H), 4.06 (s, 2H), 2.44 (s, 3H).

^{13}C NMR (400 MHz, $CDCl_3$, δ): 141.51, 138.18, 135.61, 129.25, 128.97, 128.53, 126.08, 41.62, 21.12.

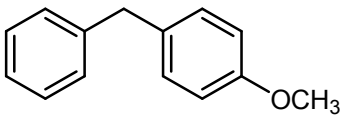
Benzyl-2-methylbenzene



^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.42 (m, 2H), 7.31 (m, 7H), 4.14 (s, 2H), 2.40 (s, 3H).

^{13}C NMR (400 MHz, $CDCl_3$, δ): 140.53, 139.06, 136.75, 130.43, 130.10, 128.89, 128.53, 126.15, 126.06, 39.61, 19.82.

Benzyl-4-methoxybenzene

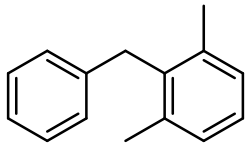


^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.36 (t, *J* = 8.0 Hz, 2H), 7.27 (m, 3H), 7.19 (d, *J* = 8.0 Hz, 2H),

6.91 (d, J = 8.0 Hz, 2H), 4.01 (s, 2H), 3.85 (s, 3H).

^{13}C NMR (400 MHz, $CDCl_3$, δ): 158.02, 141.65, 133.30, 129.93, 128.87, 128.49, 126.04, 113.93, 55.29, 41.10.

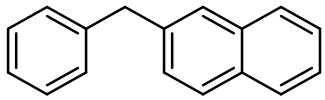
Benzyl-1,3-dimethylbenzene



^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.29 (m, 2H), 7.22 (d, J = 8.0 Hz, 1H), 7.13 (s, 3H), 7.07 (d, J = 8.0 Hz, 2H), 4.12 (s, 2H), 2.30 (s, 6H).

^{13}C NMR (400 MHz, $CDCl_3$, δ): 139.82, 137.20, 136.89, 128.40, 128.15, 127.90, 126.35, 125.75, 35.08, 20.27.

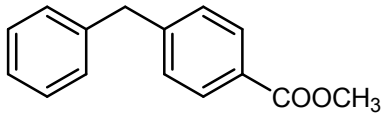
2-Benzylnaphthalene



^{1}H NMR (400 MHz, $CDCl_3$, δ): 8.04 (m, 1H), 7.94 (m, 1H), 7.84 (d, J = 8.0 Hz, 1H), 7.53 (m, 4H), 7.33 (m, 5H), 4.53 (s, 2H).

^{13}C NMR (400 MHz, $CDCl_3$, δ): 140.69, 136.68, 134.00, 132.20, 128.80, 128.72, 128.51, 127.39, 127.21, 126.11, 126.03, 125.61, 124.34, 39.11.

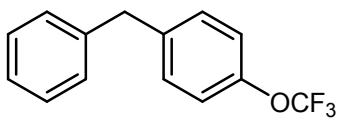
Methyl 4-benzylbenzoate



^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.97 (d, J = 8.0 Hz, 2H), 7.31 (m, 4H), 7.21 (m, 3H), 4.04 (s, 2H), 3.90 (s, 3H).

^{13}C NMR (400 MHz, $CDCl_3$, δ): 167.05, 146.53, 140.13, 129.83, 128.96, 128.62, 126.39, 52.01, 41.93.

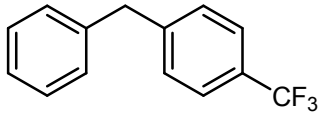
Benzyl-4-(trifluoromethoxy)benzene



^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.36 (t, *J* = 8.0 Hz, 2H), 7.29 (d, *J* = 8.0 Hz, 1H), 7.24 (t, *J* = 8.0 Hz, 4H), 7.18 (d, *J* = 8.0 Hz, 2H), 4.03 (s, 2H).

^{13}C NMR (400 MHz, $CDCl_3$, δ): 147.61, 140.45, 139.91, 130.14, 128.92, 128.63, 126.38, 121.03, 41.22.

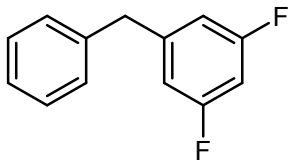
Benzyl-4-(trifluoromethyl)benzene



^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.61 (d, *J* = 8.0 Hz, 2H), 7.37 (m, 4H), 7.30 (t, *J* = 8.0 Hz, 1H), 7.25 (d, *J* = 8.0 Hz, 2H), 4.10 (s, 2H).

^{13}C NMR (400 MHz, $CDCl_3$, δ): 145.27, 140.02, 129.23, 128.98, 128.70, 121.51, 125.45, 125.41, 41.75.

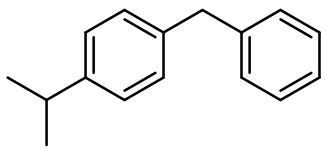
Benzyl-3,5-difluorobenzene



^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.38 (t, *J* = 8.0 Hz, 2H), 7.31 (m, 1H), 7.24 (d, *J* = 8.0 Hz, 2H), 6.66 (d, *J* = 8.0 Hz, 2H), 6.70 (m, 1H), 4.00 (s, 2H).

^{13}C NMR (400 MHz, $CDCl_3$, δ): 164.39, 164.26, 161.92, 161.80, 145.11, 139.46, 128.97, 128.75, 126.67, 111.81, 111.57, 101.61, 41.62.

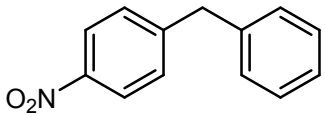
Benzyl-4-isopropylbenzene



^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.35 (m, 2H), 7.23 (m, 7H), 4.03 (s, 2H), 2.95 (m, 1H), 1.31 (d, *J* = 4.0 Hz, 6H).

^{13}C NMR (400 MHz, $CDCl_3$, δ): 146.62, 141.40, 138.90, 129.00, 128.85, 128.47, 126.54, 126.03, 41.61, 33.75, 24.09.

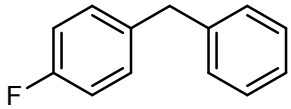
Benzyl-4-nitrobenzene



^{1}H NMR (400 MHz, $CDCl_3$, δ): 8.17 (m, 2H), 7.34 (t, *J* = 8.0 Hz, 4H), 7.29 (m, 1H), 7.22 (d, *J* = 8.0 Hz, 2H), 4.11 (s, 2H).

^{13}C NMR (400 MHz, $CDCl_3$, δ): 148.92, 146.52, 139.23, 129.67, 128.99, 128.84, 126.77, 123.76, 41.74.

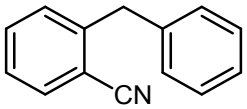
Benzyl-4-fluorobenzene



^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.32 (t, *J* = 8.0 Hz, 2H), 7.21 (m, 5H), 7.00 (m, 2H), 3.98 (s, 2H).

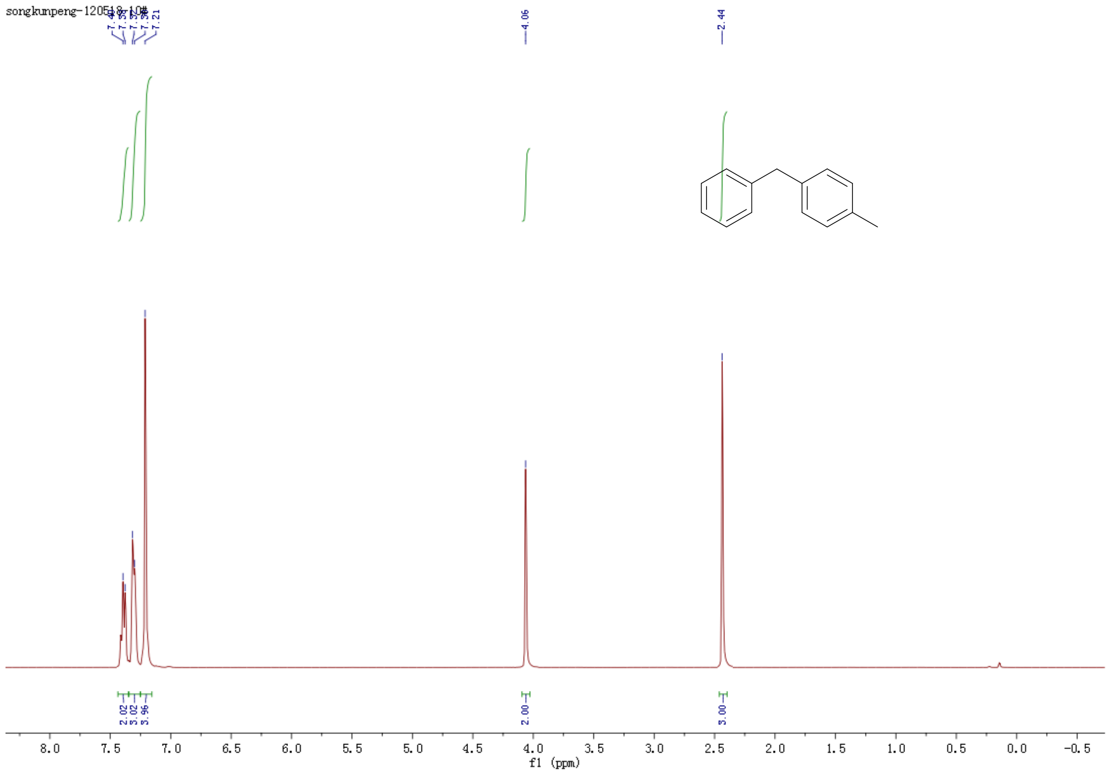
^{13}C NMR (400 MHz, $CDCl_3$, δ): 162.67, 160.25, 140.98, 136.82, 130.36, 130.28, 128.87, 128.57, 126.24, 115.34, 115.13, 41.11.

2-Benzylbenzonitrile



^{1}H NMR (400 MHz, $CDCl_3$, δ): 7.65 (d, *J* = 8.0 Hz, 1H), 7.52 (m, 1H), 7.29 (m, 7H), 4.24 (s, 2H).

^{13}C NMR (400 MHz, $CDCl_3$, δ): 144.96, 138.81, 132.90, 130.07, 128.98, 128.73, 126.82, 126.72, 118.17, 112.60, 40.21.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3.00
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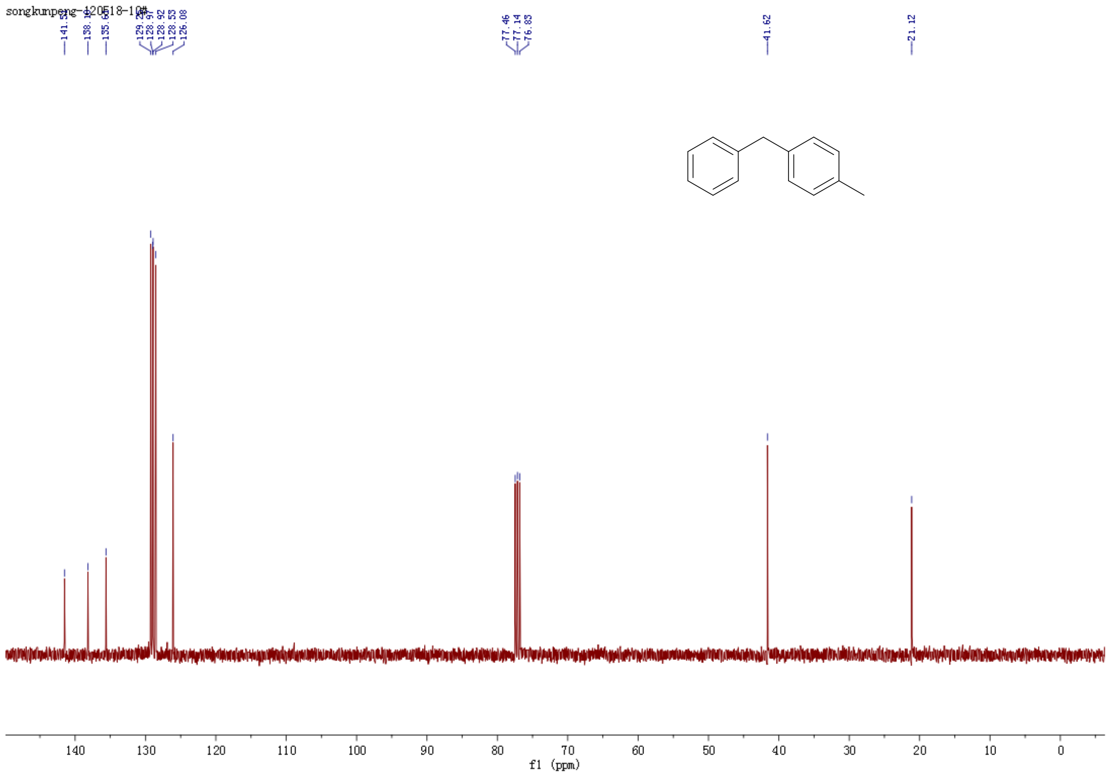
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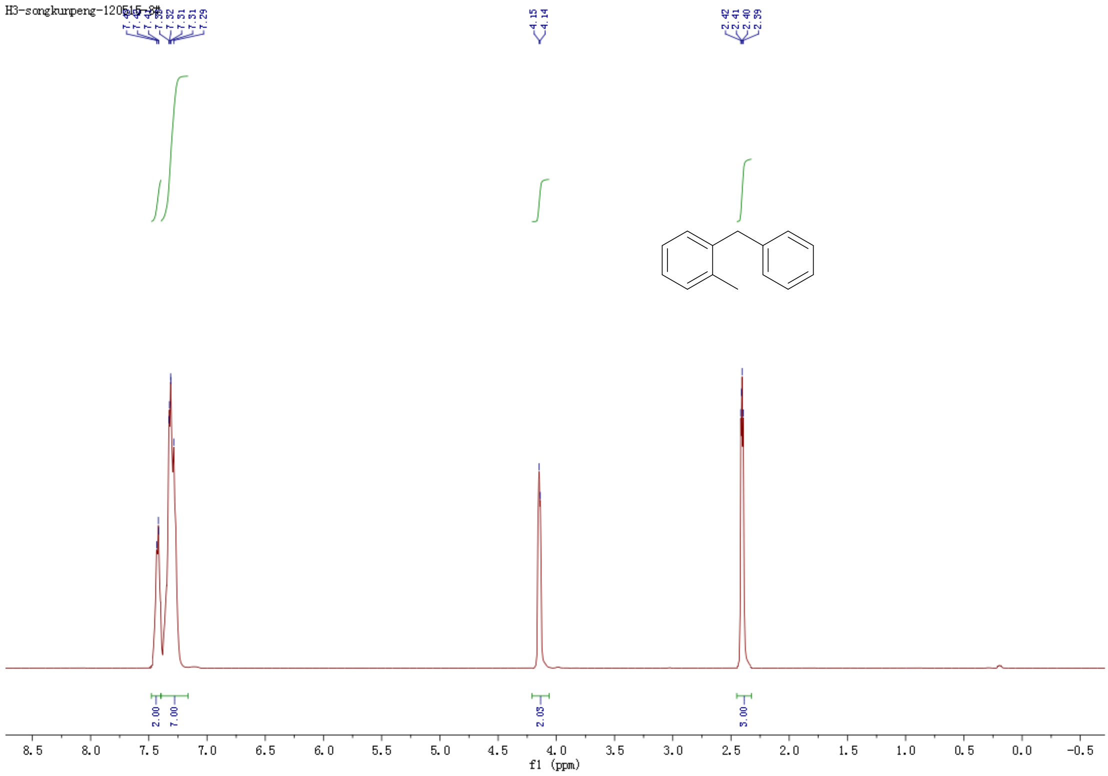

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3.00
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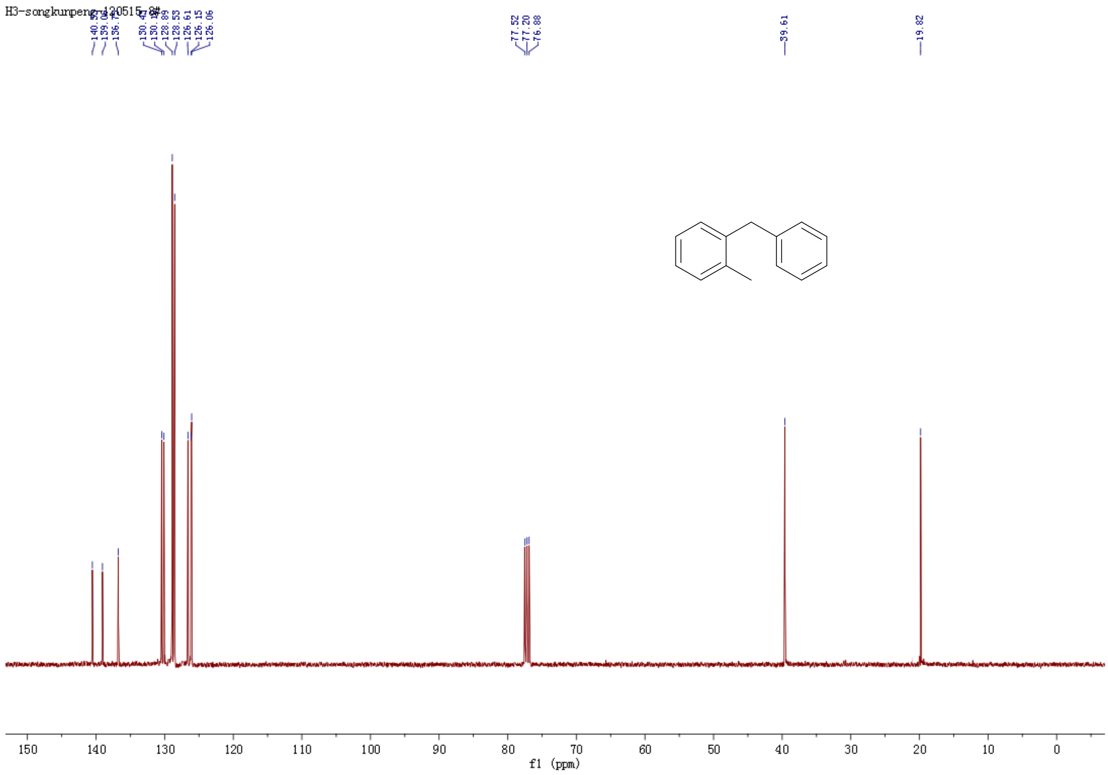

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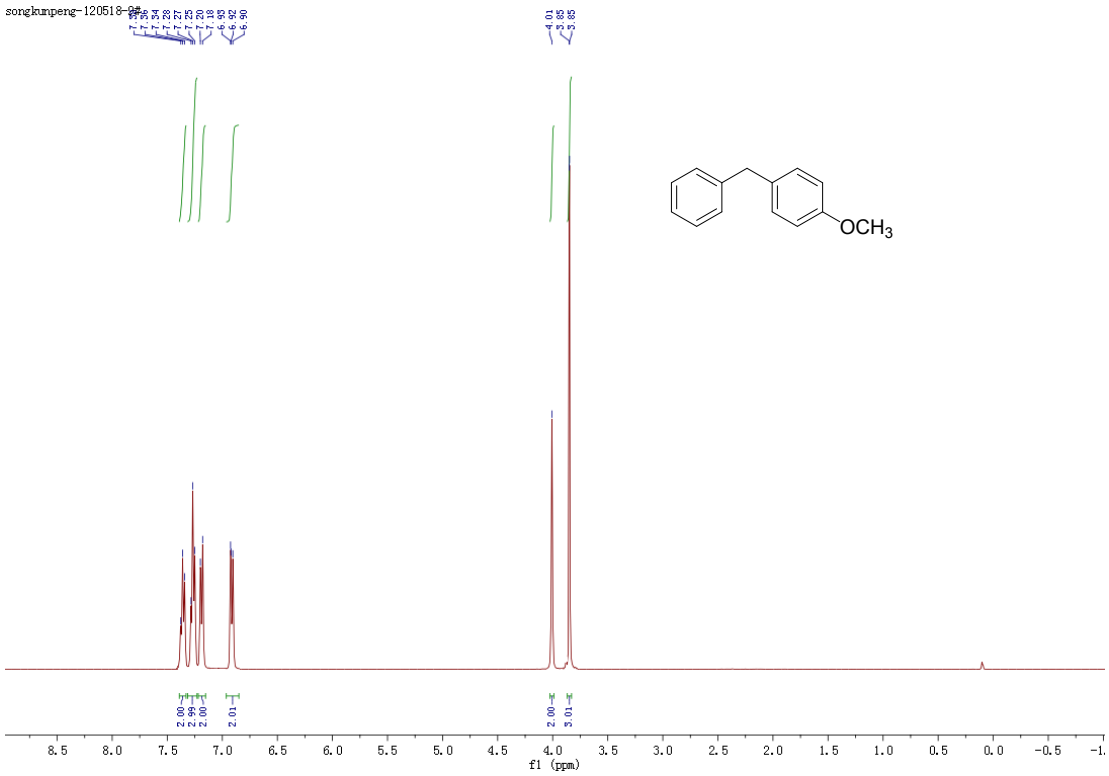
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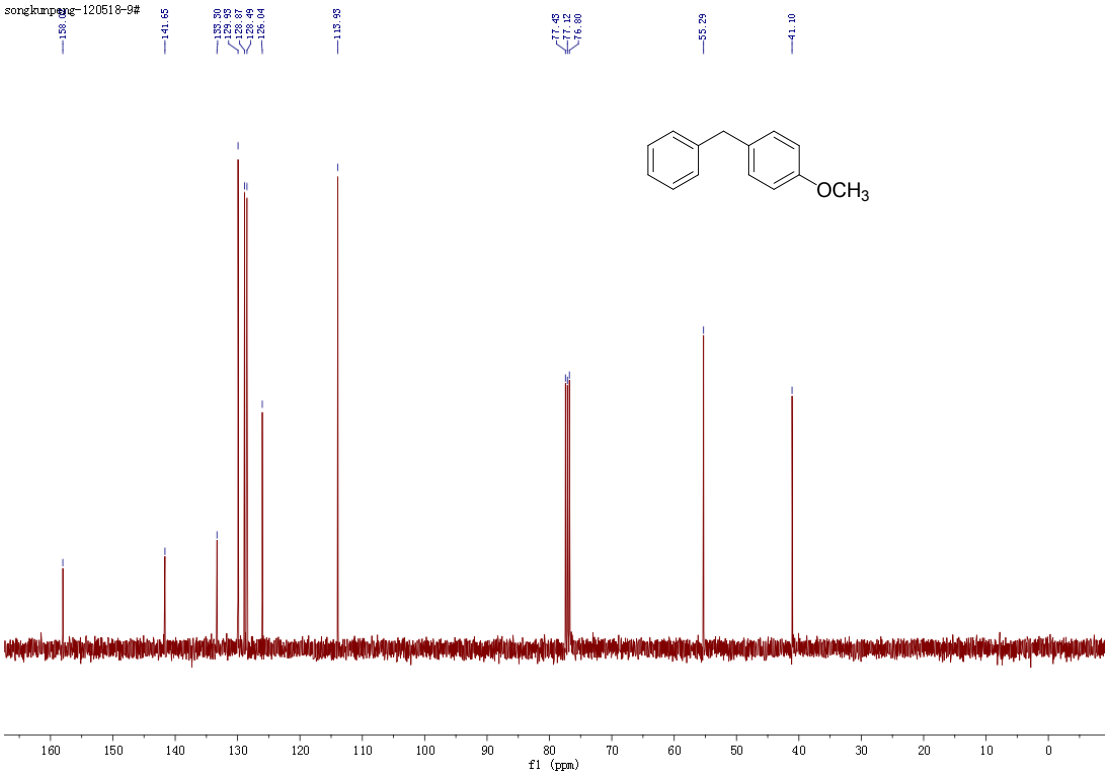
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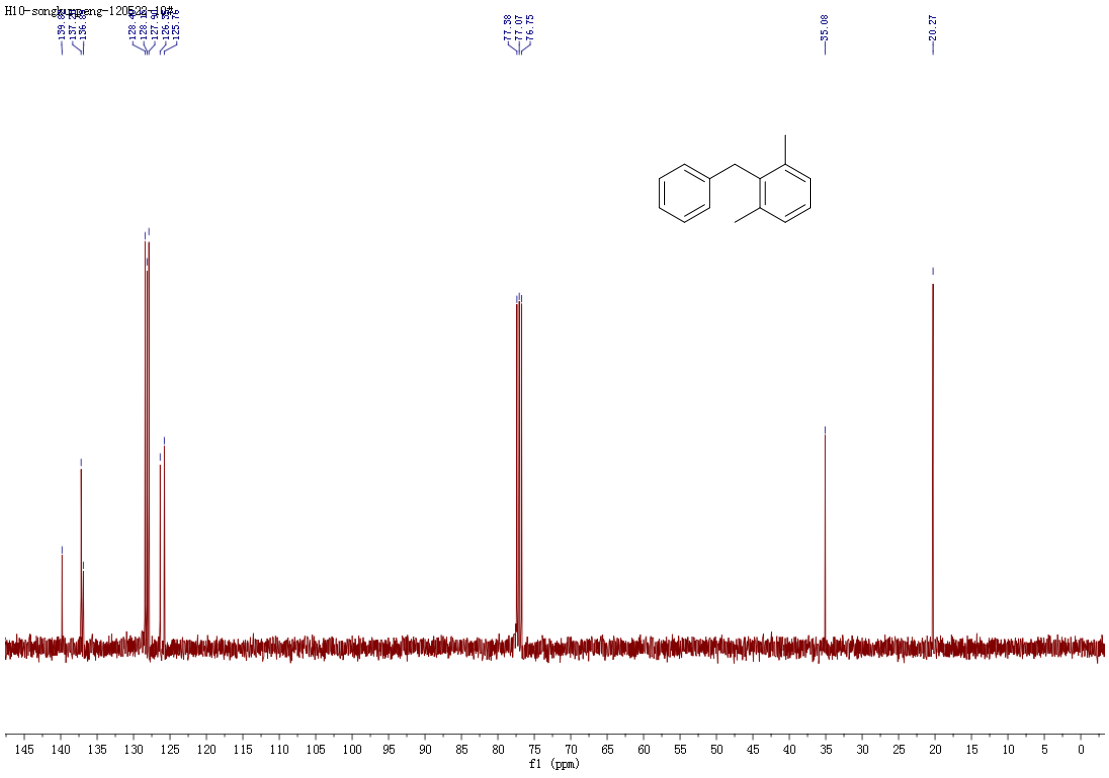
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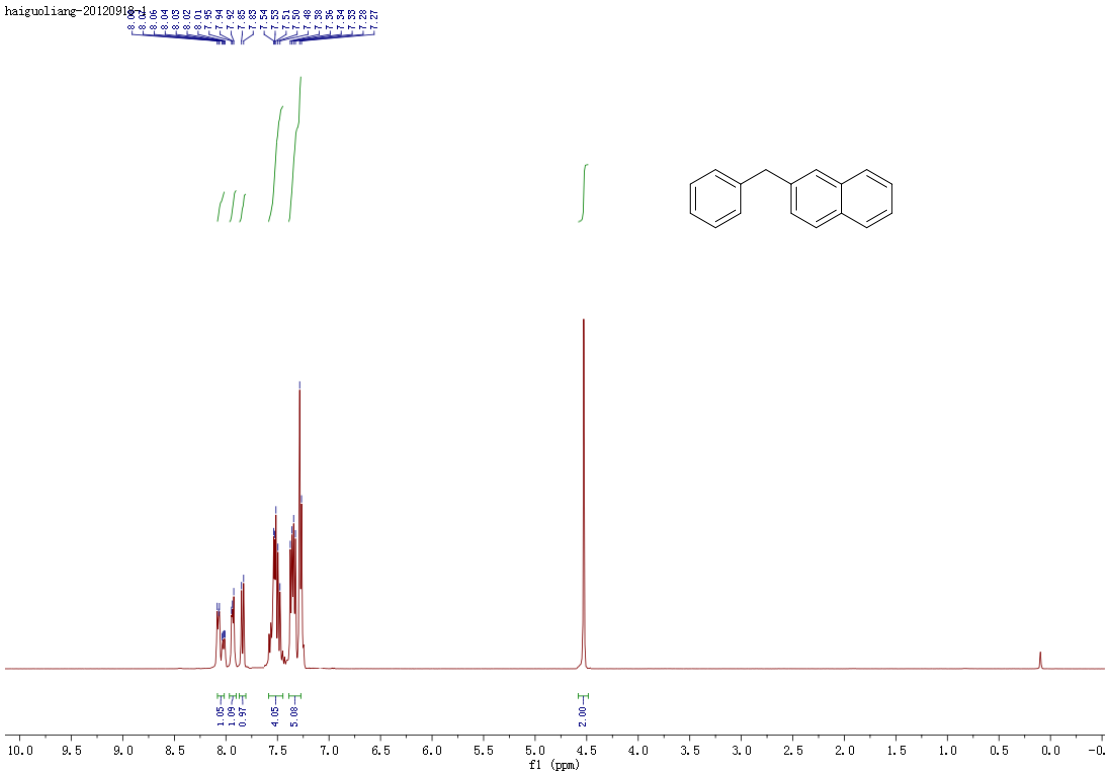

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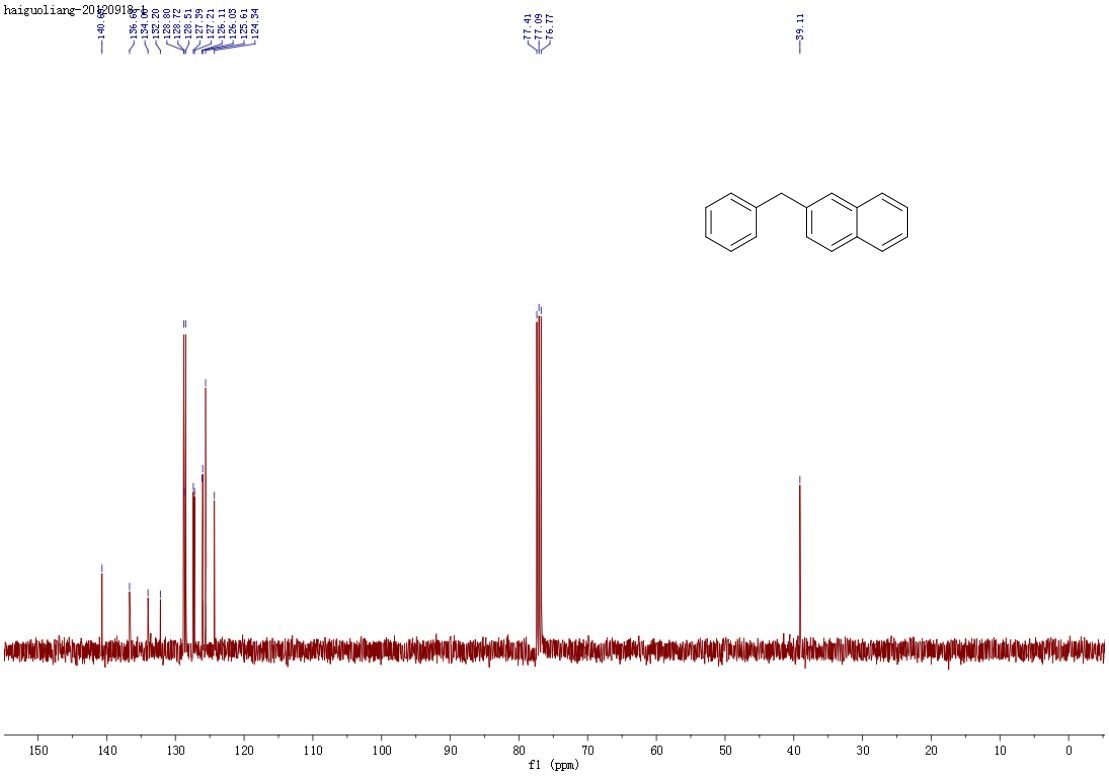

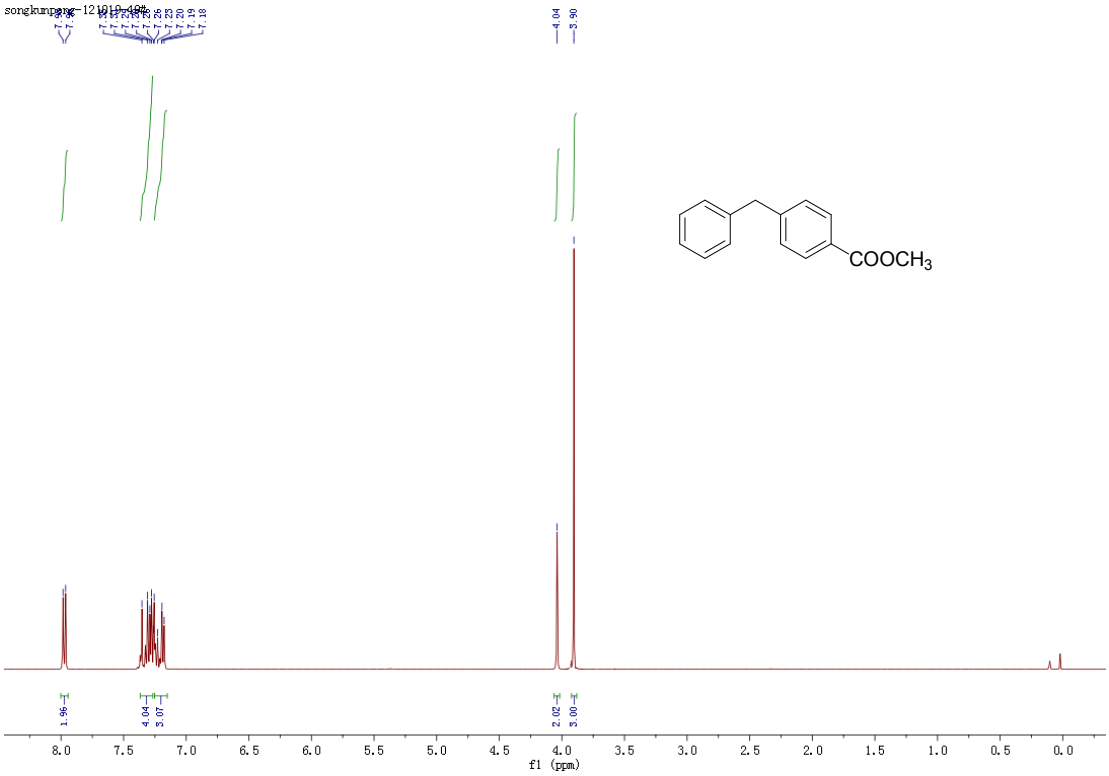
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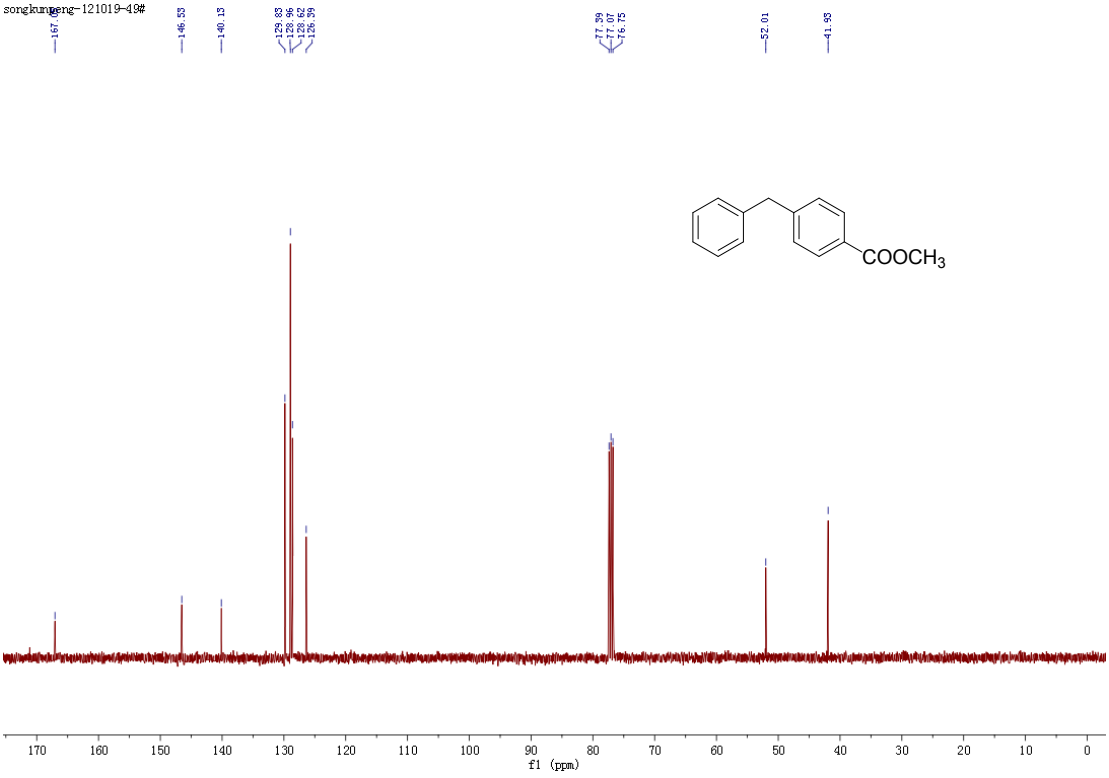
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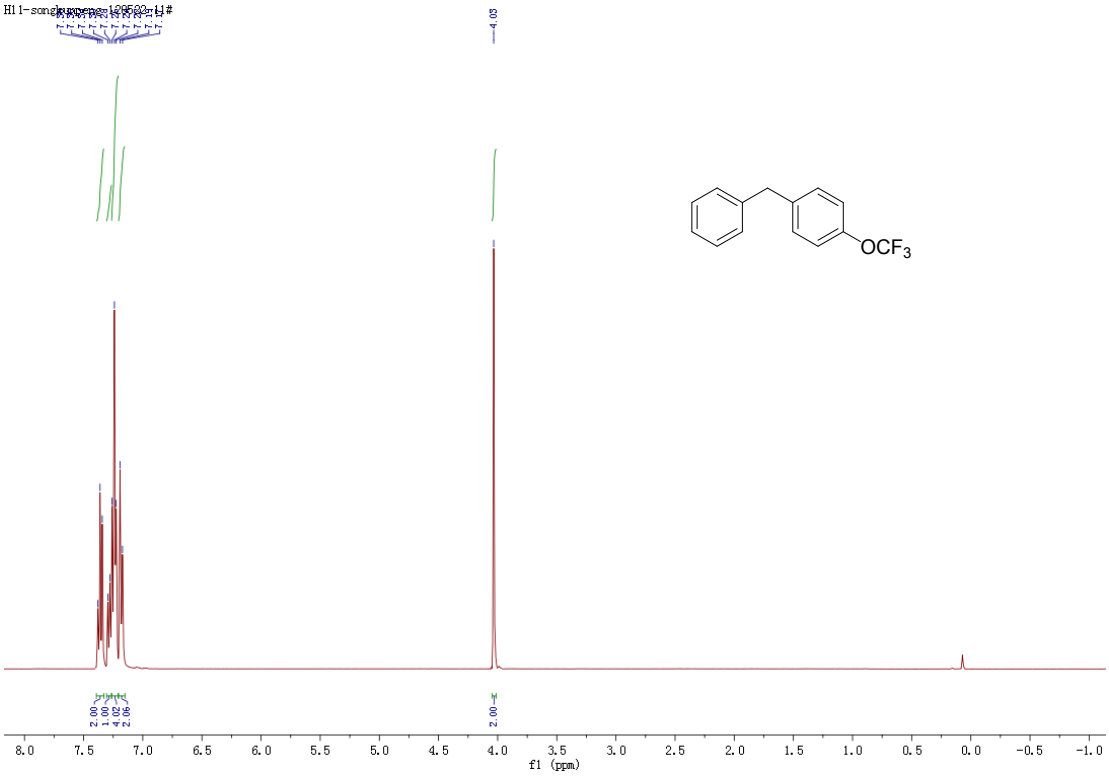
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5.0
4.5
4.0
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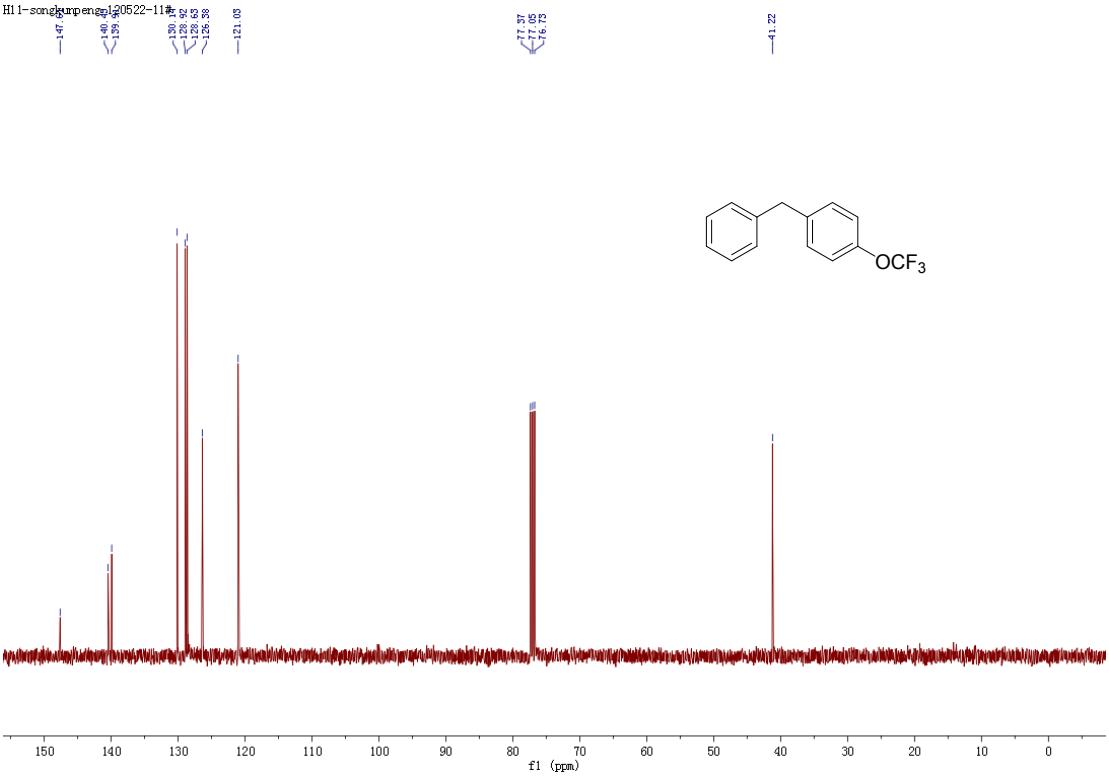
f1 (ppm)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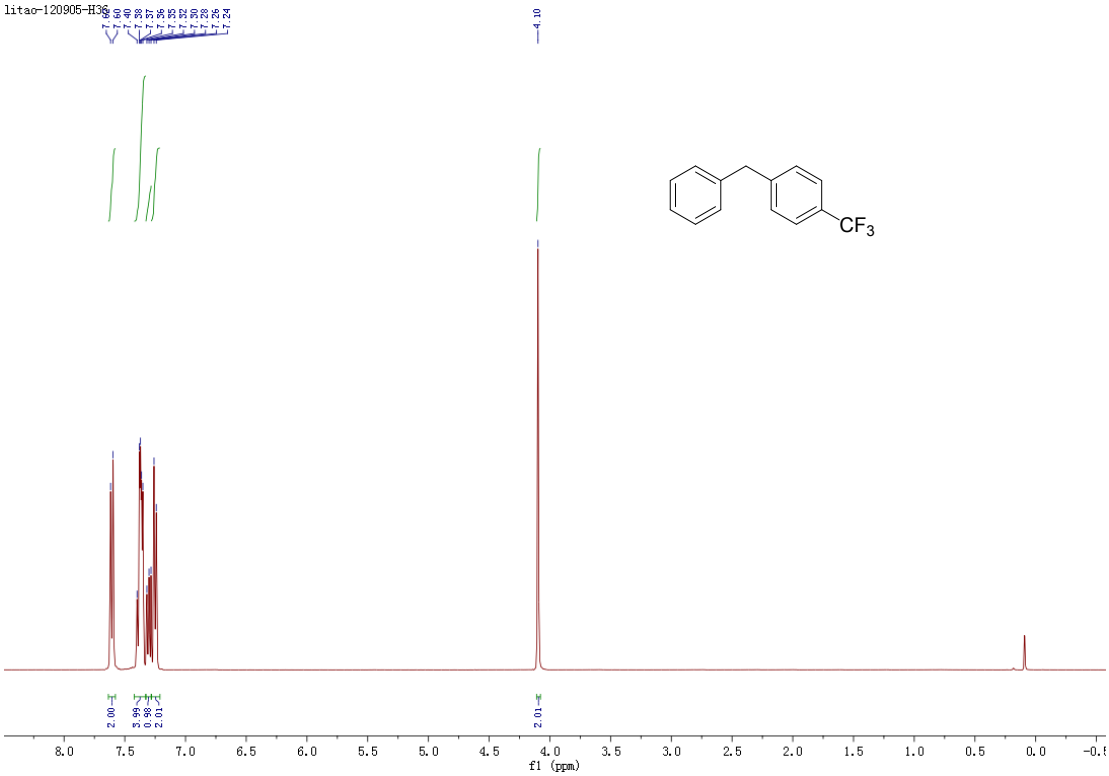
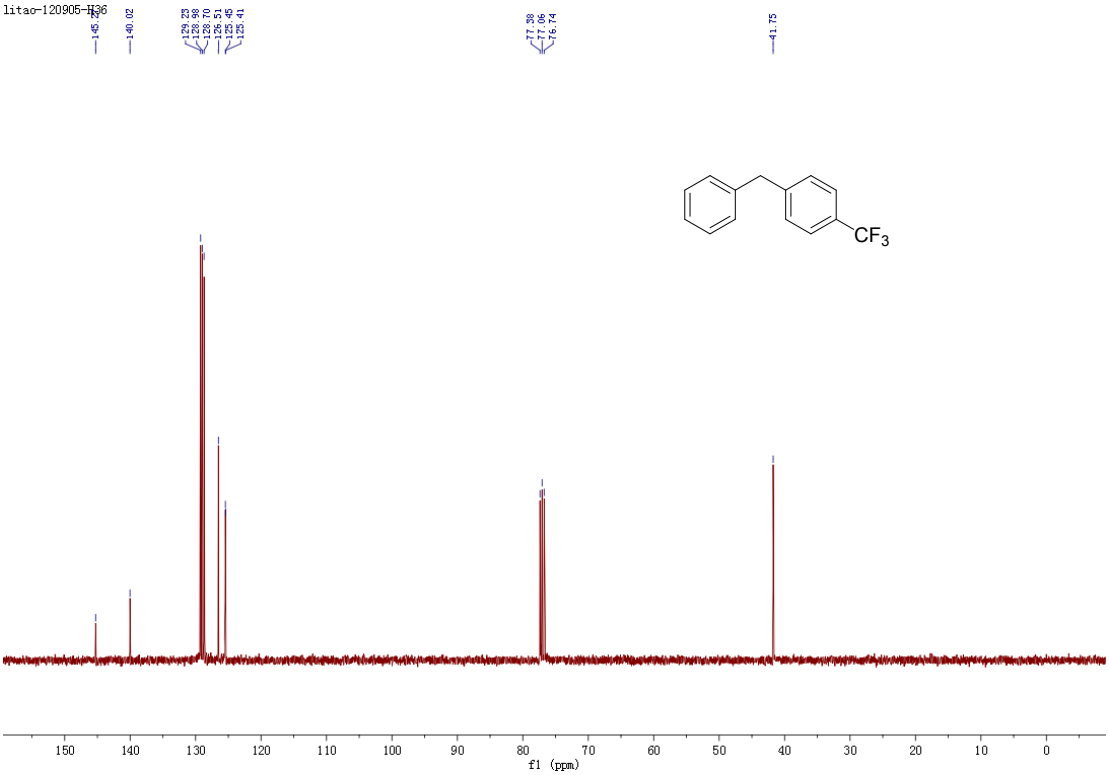
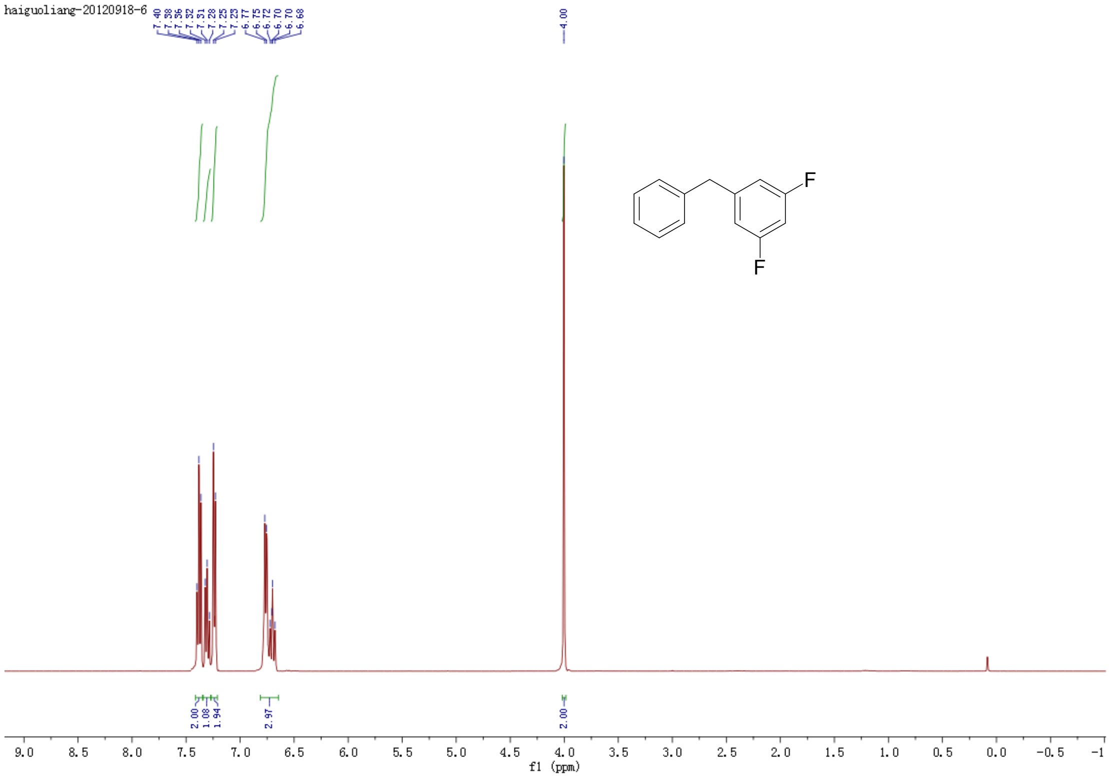
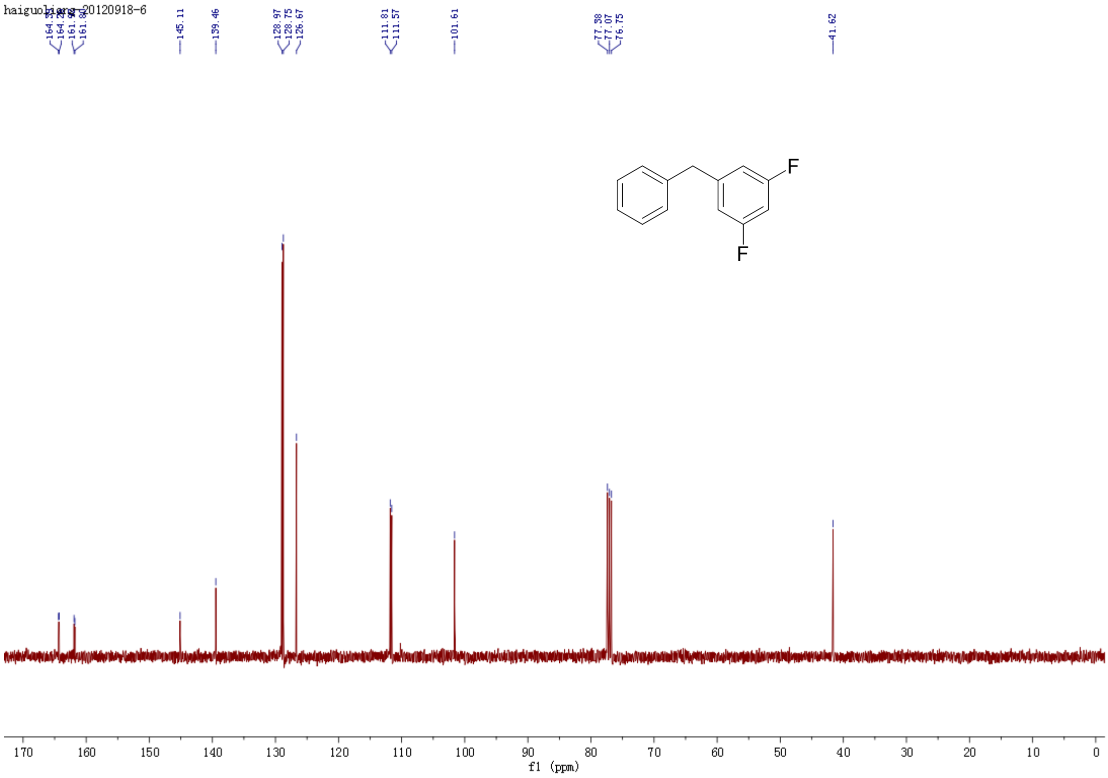
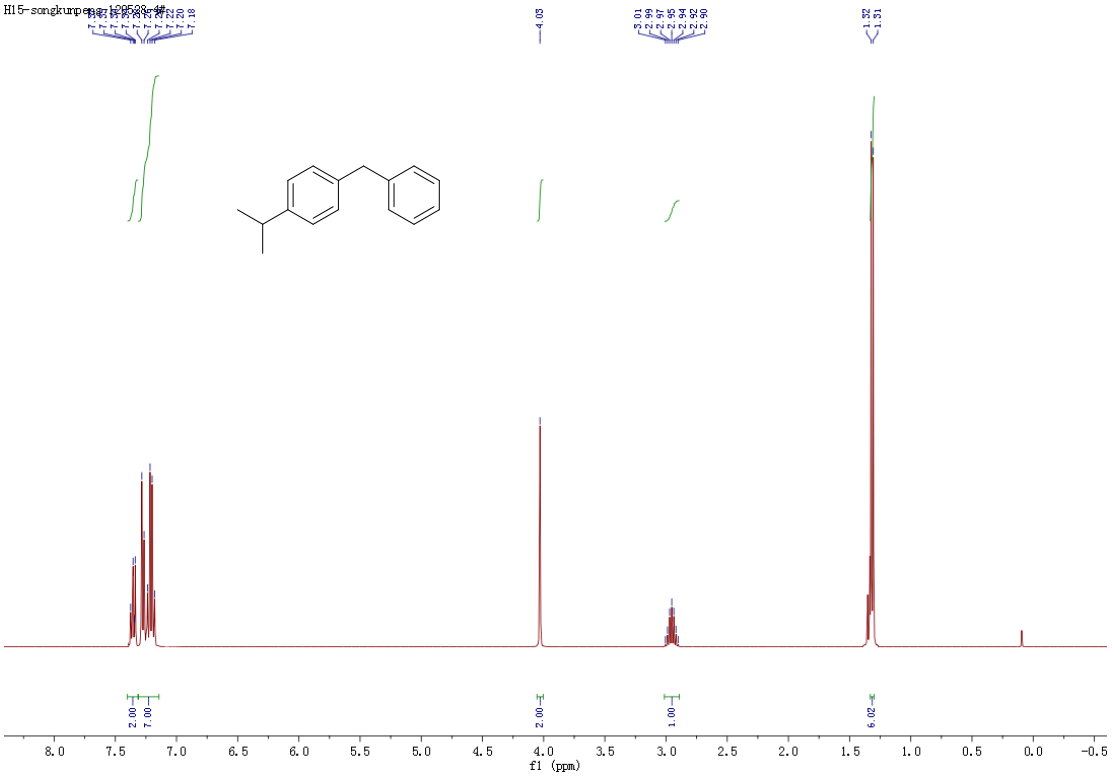
147.
140.
139.
130.14
128.92
128.53
126.38
121.03
77.37
77.05
76.73
41.22
OCF3
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

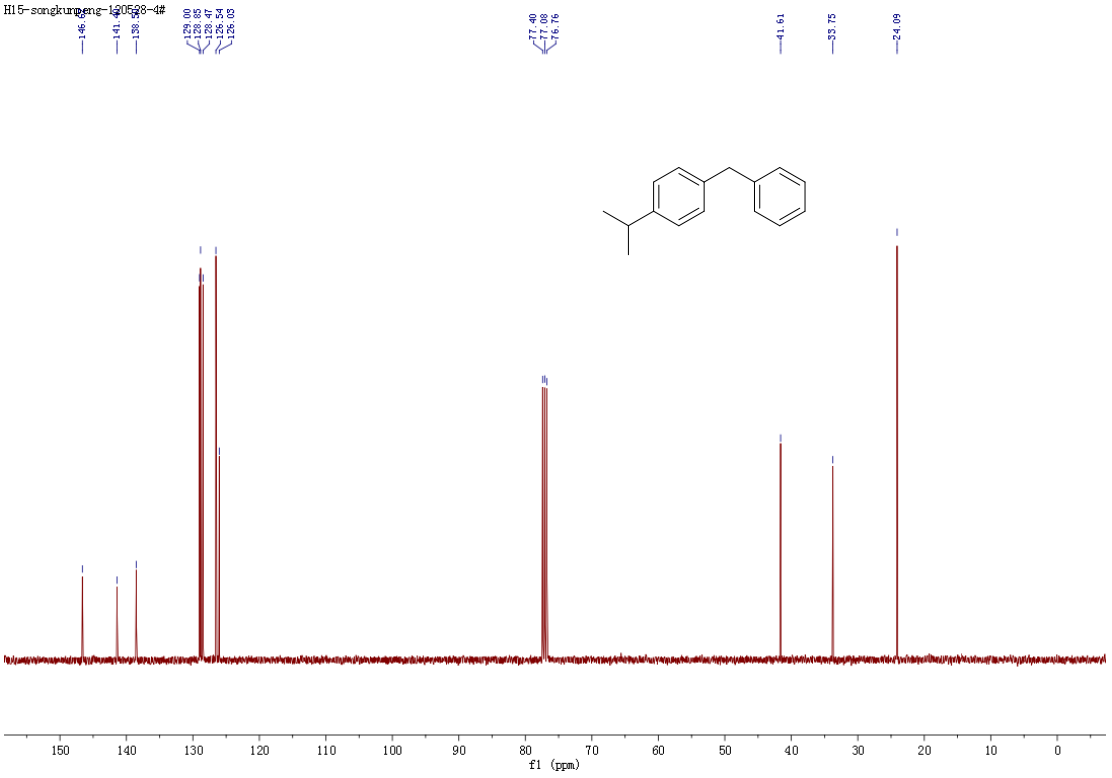

litao-120905-H36
7.60
7.40
7.39
7.37
7.36
7.35
7.32
7.30
7.28
7.26
7.24
4.10
CF3
2.00
3.99
0.98
2.01
2.01
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

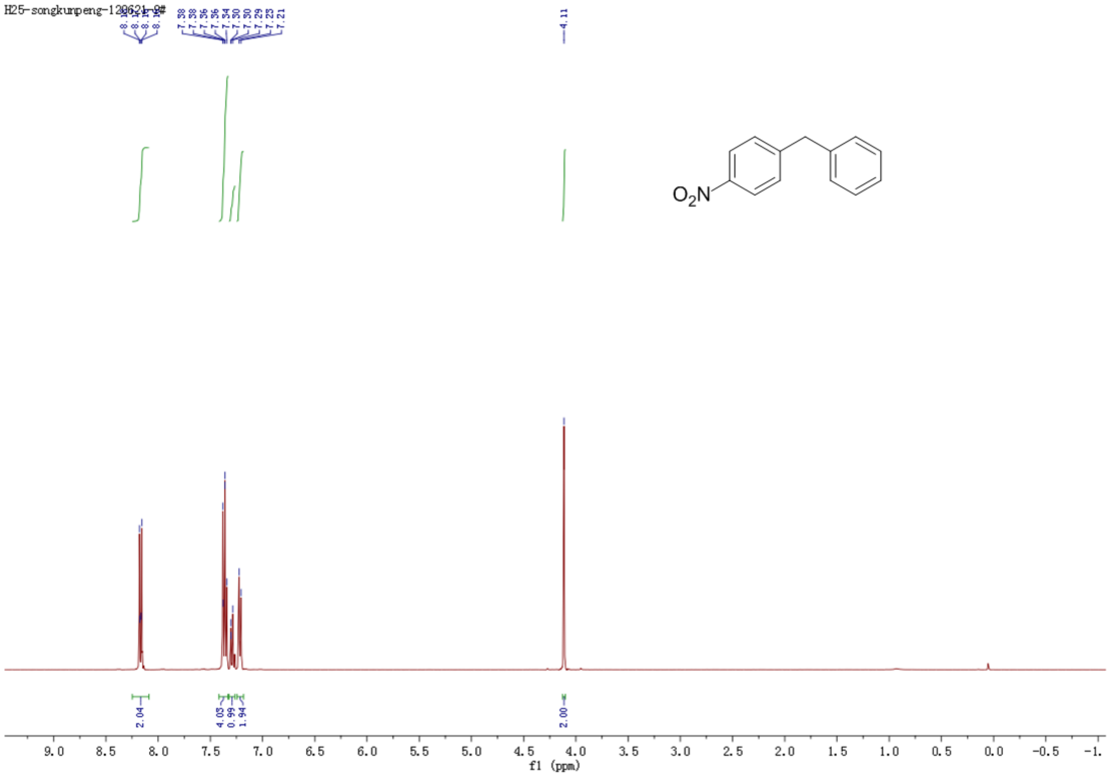

litao-120905-H36
145.42
140.02
129.23
128.98
128.70
126.51
125.45
125.41
77.38
77.06
76.74
41.75
CF3
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

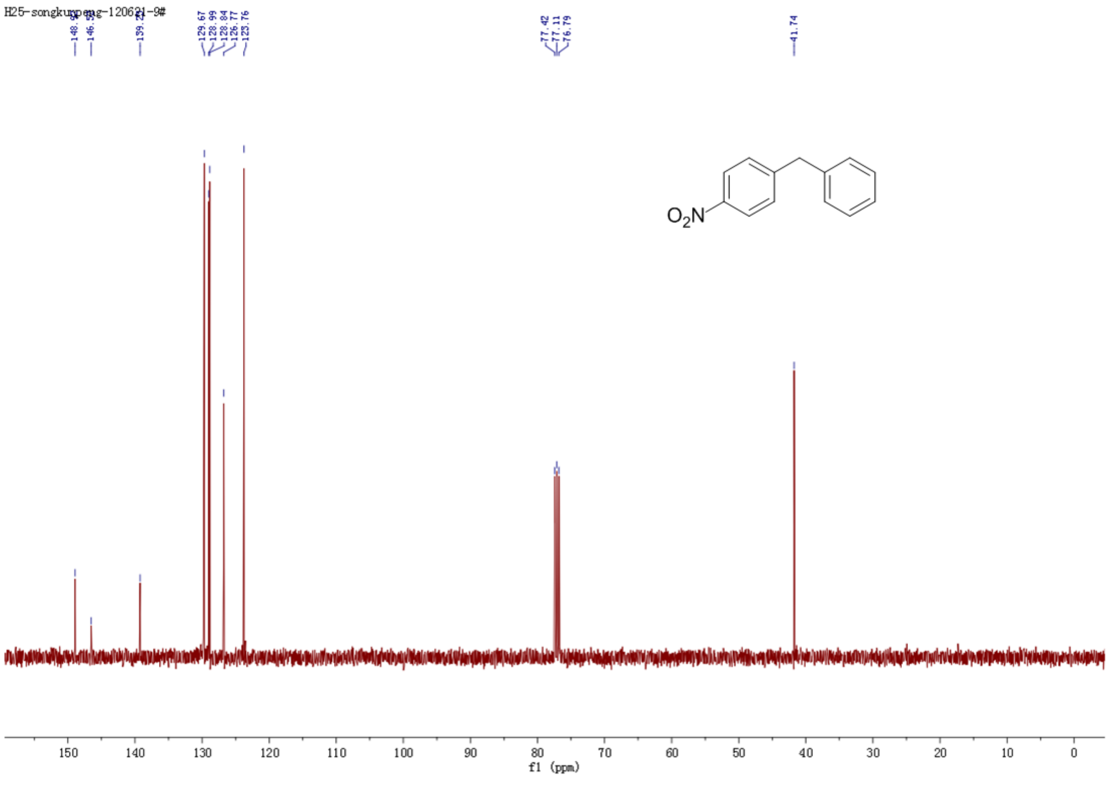

haiguoliang-20120918-6
7.40
7.38
7.36
7.32
7.31
7.28
7.25
7.23
6.77
6.75
6.72
6.70
6.70
6.68
4.00
F
F
2.00
1.08
1.94
2.97
2.00
f1 (ppm)

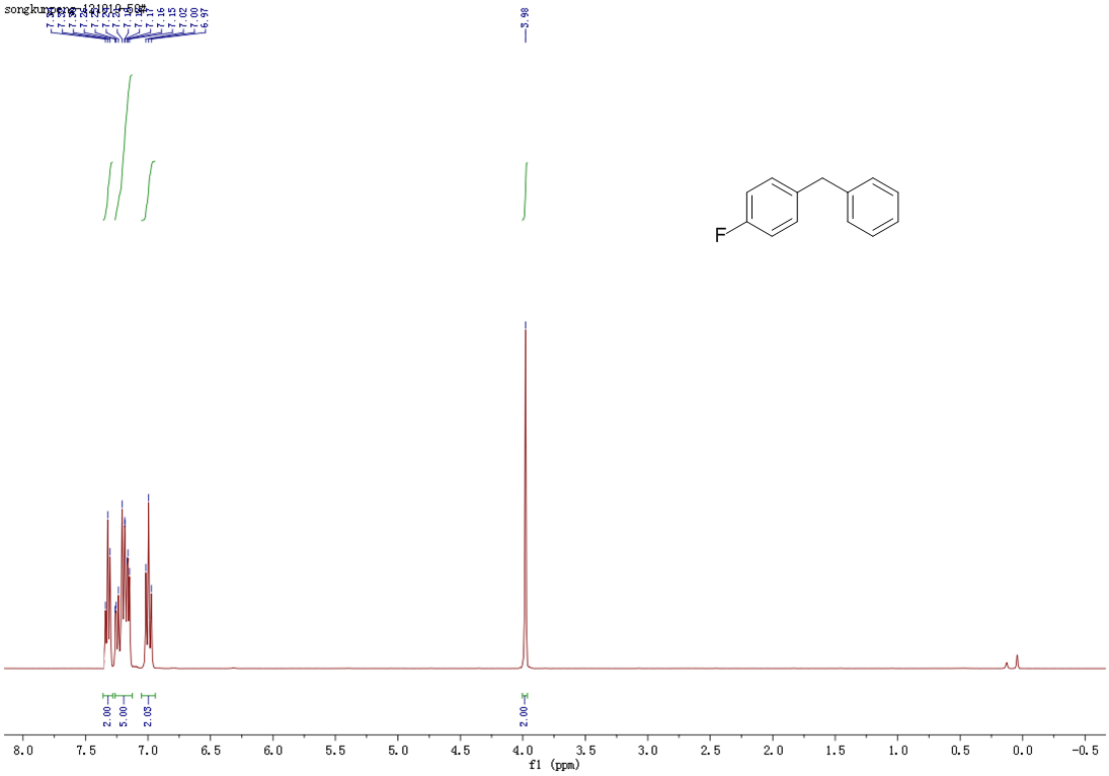

haiguoliang-20120918-6
145.11
139.46
128.97
128.75
126.67
111.81
111.57
101.61
77.38
77.07
76.75
41.62
F
F
f1 (ppm)

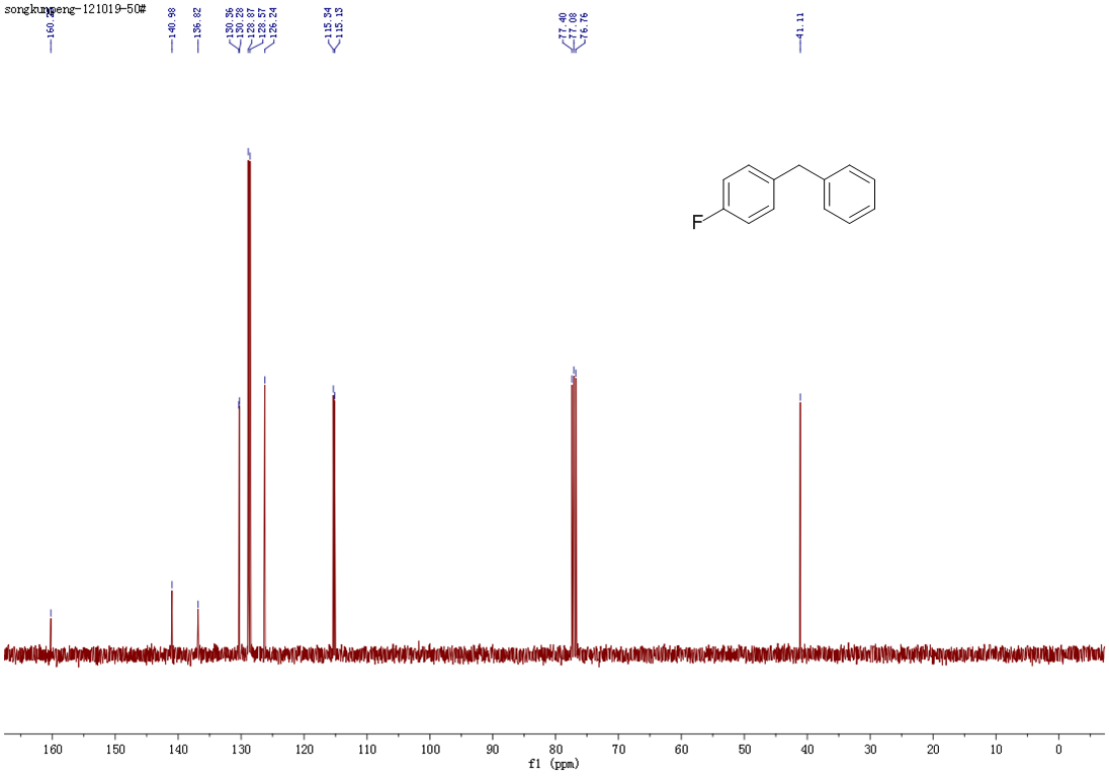

H15-songkunpeng-120528-4#
4.03
3.01
2.99
2.97
2.95
2.94
2.92
2.90
1.32
1.31
2.00
7.00
2.00
1.00
6.02
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


H15-songkunpeng-120528-4#
146.
141.
138.
129.00
128.65
128.47
126.54
126.03
77.40
77.08
76.76
41.61
33.75
24.09
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

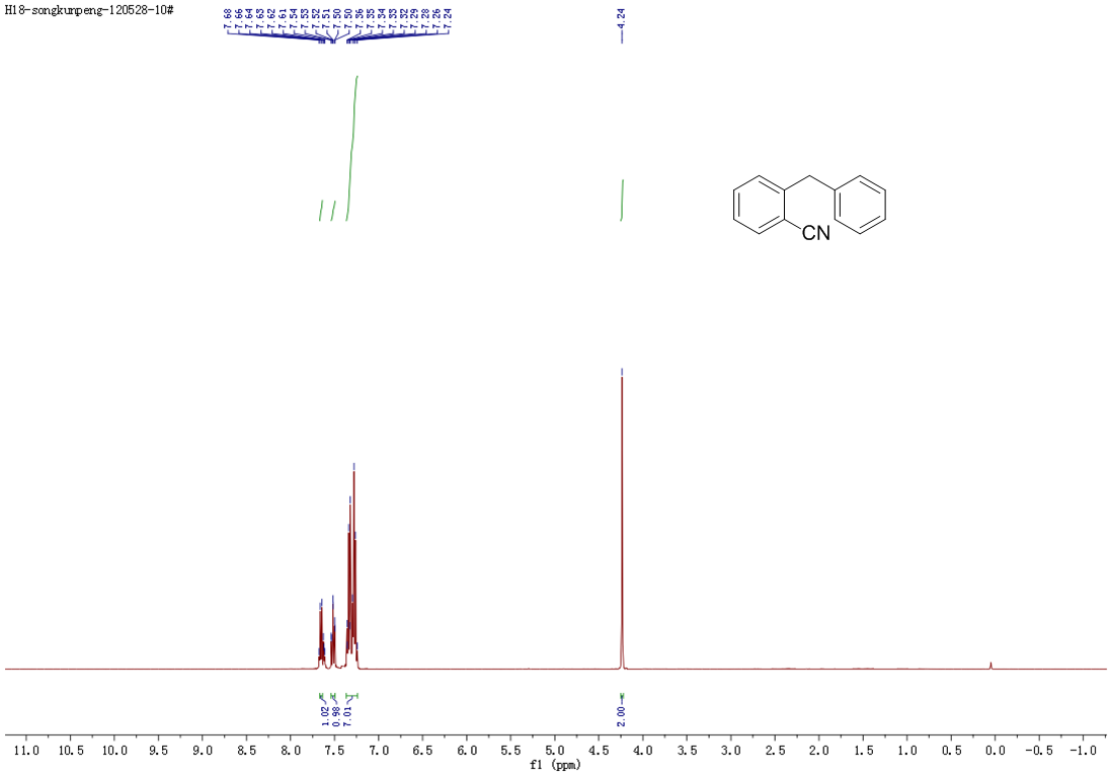

H25-songkunpeng-120621-9#
4.11
2.04
4.03
0.99
1.94
2.00
O2N
f1 (ppm)


H25-songkunpeng-120621-9#
129.67
128.99
128.84
126.77
123.76
77.42
77.11
76.79
41.74
O2N
f1 (ppm)


F
2.00
5.00
2.03
2.00
f1 (ppm)


F
f1 (ppm)

H18-songkunpeng-120528-10#



H18-songkunpeng-120528-10#