Supporting Information for:

A ppm level Rh based composites as ecofriendly catalyst for transfer hydrogenation of Nitriles: Triple guarantee of selectivity for primary amine

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Contents

Experimental section

Preparation of Fe_3O_4@nSiO_2-NH_2. Firstly, Fe_3O_4 nanosphere purchased from Aladdin Reagent Co., Ltd., China. (0.2 g) was activated with 0.1 mol/L HCl solution (60 mL) in ultrasonic vibrator for 30 minutes. After washing the magnetite three times with deionized water, it was redispersed in the mixed solution that contained deionized H_2O (40 mL), ethanol (160 mL), and 25% $NH_3 \cdot H_2O$ (4 mL). When one milliliter of TEOS was added dropwise, the mixture was stirred vigorously for 6 hours under ambient temperature accompanied by multiple ultrasounds. After magnetic separation from the suspension the solid were functionalized with $–NH_2$ through reaction with APTES (0.5 mL) in isopropanol (200 mL) at 80 ^oC for 3 h. Then the Fe_3O_4@nSiO_2-NH_2 nanocomposite was successfully fabricated after isolation by an external magnet and washing with ethanol.

Preparation of Fe_3O_4@nSiO_2-NH_2-RhCu@mSiO_2. The obtained Fe_3O_4@nSiO_2-NH_2 was stirred vigorously in the homogeneous solution that contains $RhCl_3 \cdot 3H_2O$ (1 mg), $Cu(NO_3)_2 \cdot 6H_2O$ (1 mmol), H_2O (100 mL), ethanol (90 mL) for 1 hour. Subsequently, 10 mL methanol solution of 0.2 g $NaBH_4$ was quickly added under Ar atmosphere. After continuous stirring for 1 h, the resulting solid was redispersed in 80 mL H_2O. Meanwhile, 2.5 mL $NH_3 \cdot H_2O$ were injected to the transparent solution of CTAB (0.32 g) and 60 mL ethanol. This solution was then added into the above suspension and the mixture were stirred for 30 min. When 1.5 mL TEOS were dropped in, the system was vigorously stirred for 6 h under ambient temperature. Then the collected solid via magnetic separation were stirred vigorously in 150 mL boiling ethanol for 3 h and three times in succession to remove CTAB. The ultimate material was obtained through washing with ethanol and drying.

Typical procedure for the synthesis of benzylamine: FS-NH_2-RhCu@mSiO_2(10 mg), benzonitrile (1 mmol) and HCOOH-NEt_3 (20:1, 2 mL) were successively added to a tube (15 mL) and the reactor was immediately sealed and heated at 40 ^oC for 3 hour. After the tube was cooled with ice water to quench the reaction, the conversion and selectivity were acquired by GC with toluene as the internal standard. The reaction liquid was firstly extracted with H_2O (30 mL) and CH_2Cl_2 (10 mL). The aqueous phase was adjusted to alkaline by adding sodium hydroxide and subsequently extracted with H_2O (10 mL) and CH_2Cl_2 (30 mL). The organic phase was concentrated in vacuum after desiccation with anhydrous Na_2SO_4. The residue was purified by flash column chromatography on silica gel (SiO_2, petroleum ether/EtOAc, 2:1) to afford the benzylamine.

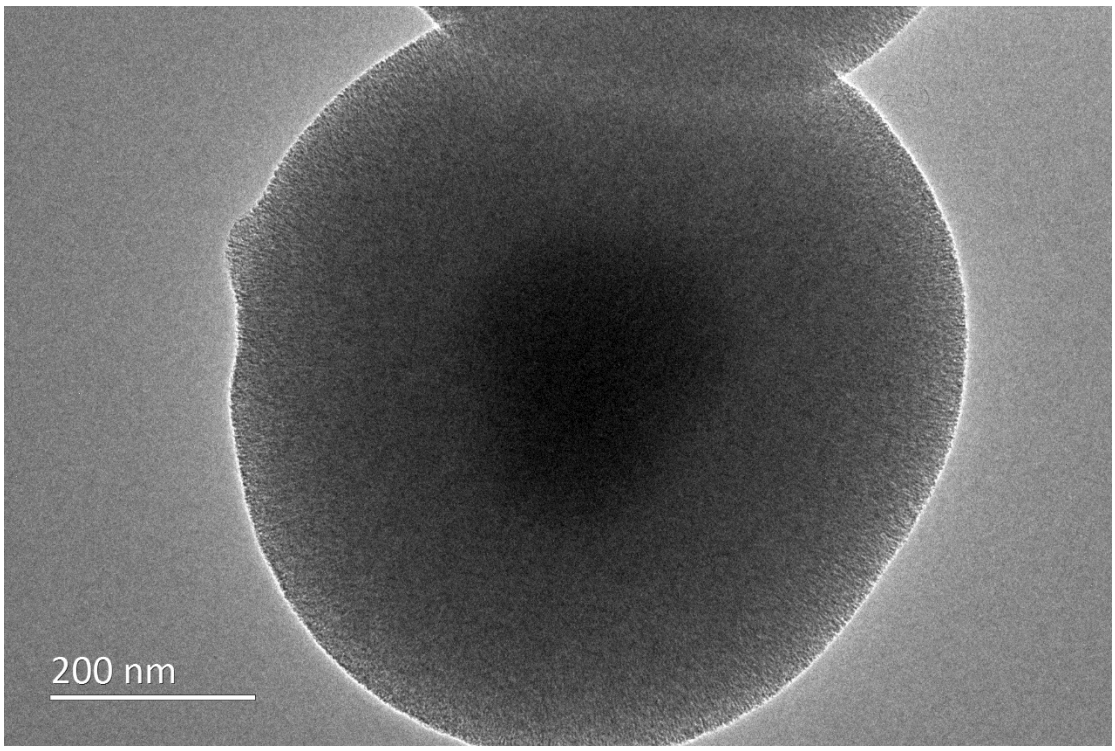


Figure S1. The regular pore structure of the catalyst in HRTEM image.

We can easily distinguish the pore structure of the material, which is significant to the mass transfer process.

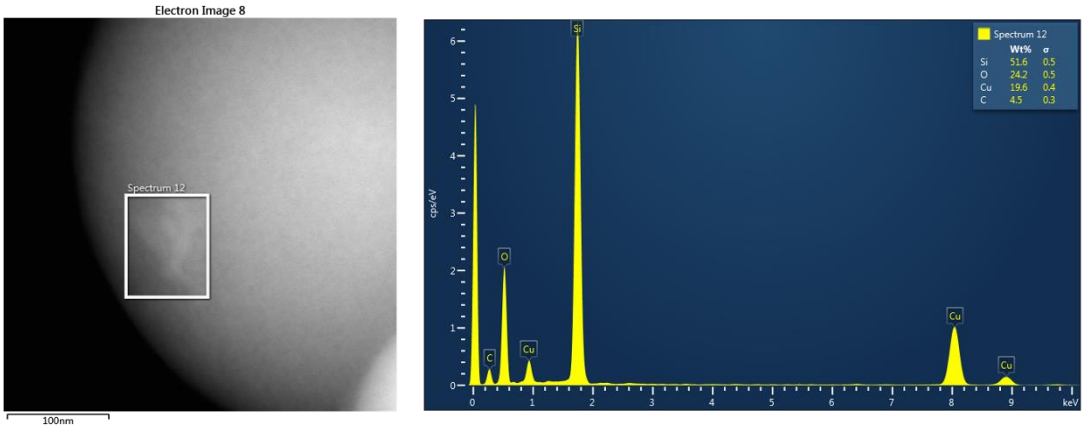


Figure S2. The EDX characterization of the catalyst.

We characterized the metal particle we struggled to find with EDX system. The results showed only the presence of copper element. The possible reasons are as follows: the level of rhodium belows the detection limit of this system (the existence of rhodium is verified according to SAED and ICP-MS characterization), and most of the active sites may exist as ultra-small particles because it's hard to find another metal particle in HRTEM. And the thickness of the silicon shell is also a factor.

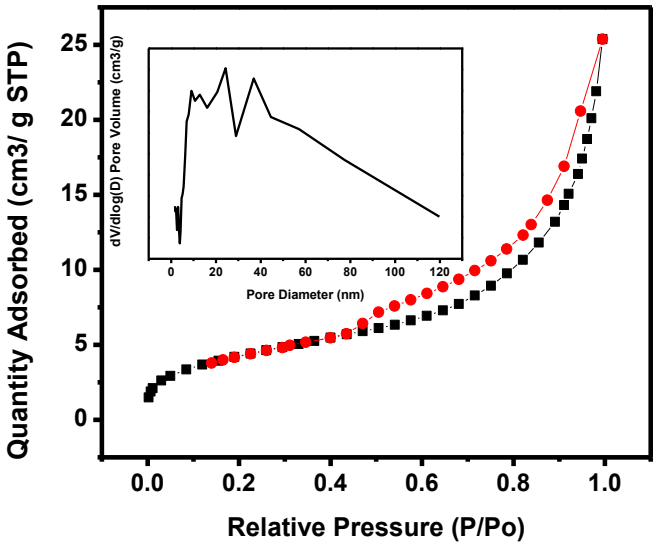


Figure S3. The N_2-adsorption-desorption isotherm of the analogous catalyst fabricated by etching.

The N_2-adsorption-desorption isotherm of the analogous catalyst belongs to a type IV classification coupling with a H3 hysteresis loop, indicating mesoporous structure with an average pore diameter of 10.7 nm calculated by the Barrett- Joyner-Halenda model. Under the same reaction conditions, the selectivity was reduced by 9 percent, indicating that the pore structure affected the reaction selectivity.

Characterization data of products

Benzylamine **(1a)**[1]

^{1}H NMR (600 MHz, CHLOROFORM-D) δ 7.30 – 7.25 (m, 5H), 3.83 (s, 2H), 2.03 (s, active H).

^{13}C NMR (151 MHz, CHLOROFORM-D) δ 129.0, 128.8, 128.63, 127.79, 45.40.

GC-MS: m/z(%) 51(11), 79(49), 106(100), HRMS Calcd. (ESI) m/z for C_7H_9N: $[M+H]^+$ 108.0808, found 108.0803

IR (KBr) cm^{-1}: 880, 1460, 1520, 2851, 2930, 3040, 3300, 3380.

p-tolylmethanamine **(2a)**[2]

^{1}H NMR (600 MHz, CHLOROFORM-D) δ 7.20 (d, *J* = 7.9 Hz, 2H), 7.14 (d, *J* = 7.8 Hz, 2H), 3.82 (s, 2H), 2.34 (s, 3H), 1.74 (s, active H).

^{13}C NMR (151 MHz, CHLOROFORM-D) δ 140.03, 136.46, 129.23, 127.09, 46.16, 21.06.

GC-MS: m/z(%) 65(30), 77(45), 104(100), 120(65), HRMS Calcd. (ESI) m/z for $C_8H_{11}N$: $[M+H]^+$ 122.0964, found 122.0960

IR (KBr) cm^{-1}: 870, 1450, 1515, 2850, 2930, 3030, 3310, 3390.

m-tolylmethanamine **(3a)**[2]

^{1}H NMR (600 MHz, CHLOROFORM-D) δ 7.23 (t, *J* = 7.4 Hz, 1H), 7.14 – 7.09 (m, 2H), 7.07 (d, *J* = 6.8 Hz, 1H), 3.83 (s, 2H), 2.35 (s, 3H), 1.98 (s, 2H).

^{13}C NMR (151 MHz, CHLOROFORM-D) δ 138.24, 131.57, 128.50, 127.98, 127.66, 124.20, 46.31, 21.39.

GC-MS: m/z(%) 65(30), 77(45), 104(100), 120(65), HRMS Calcd. (ESI) m/z for $C_8H_{11}N$: $[M+H]^+$ 122.0964, found 122..0969

IR (KBr) cm^{-1}: 850, 1450, 1495, 2861, 2920, 3030, 3310, 3390.

o-tolylmethanamine **(4a)**[2]

^{1}H NMR (600 MHz, CHLOROFORM-D) δ 7.31 (d, *J* = 7.2 Hz, 1H), 7.22 (d, *J* = 7.5 Hz, 1H), 7.19 (s, 1H), 7.17 (d, *J* = 2.1 Hz, 1H), 3.87 (s, 2H), 2.34 (s, 3H), 1.89 (s, 2H).

^{13}C NMR (151 MHz, CHLOROFORM-D) δ 140.50, 135.55, 130.32, 127.15, 126.96, 126.22, 43.91, 18.83.

GC-MS: m/z(%) 65(30), 77(45), 104(100), 120(65), HRMS Calcd. (ESI) m/z for $C_8H_{11}N$: $[M+H]^+$ 122.0964, found 122.0959

IR (KBr) cm^{-1}: 860, 1456, 1505, 2850, 2930, 3030, 3310, 3390.

(3,5-dimethylphenyl)methanamine **(5a)**

^{1}H NMR (600 MHz, CHLOROFORM-D) δ 6.90 (s, 2H), 6.87 (s, 1H), 3.75 (s, 2H), 2.30 (s, 6H), 1.97 (s, 2H).

^{13}C NMR (151 MHz, CHLOROFORM-D) δ 143.04, 138.08, 128.43, 124.93, 46.31, 21.25.

GC-MS: m/z(%) 65(20), 77(35), 91(65), 118(100), HRMS Calcd. (ESI) m/z for $C_9H_{13}N$: $[M+H]^+$ 136.1121, found 136.1117

IR (KBr) cm^{-1}: 860, 1453, 1513, 2860, 2940, 3033, 3311, 3385.

(4-methoxyphenyl)methanamine **(6a)**[2]

^{1}H NMR (600 MHz, CHLOROFORM-D) δ 7.21 (d, *J* = 8.6 Hz, 2H), 6.86 (d, *J* = 8.6 Hz, 2H), 3.78 (s, 3H), 3.78 (s, 2H), 1.83 (s, 2H).

^{13}C NMR (151 MHz, CHLOROFORM-D) δ 158.52, 135.37, 128.29, 113.92, 55.27, 45.81.

GC-MS: m/z(%) 65(30), 77(55), 106(70), 136(100), 137(65), HRMS Calcd. (ESI) m/z for $C_8H_{11}NO$: $[M+H]^+$ 138.0913, found 138.0916

IR (KBr) cm^{-1}: 820, 1450, 1520, 2851, 2933, 3050, 3308, 3391.

(3-methoxyphenyl)methanamine **(7a)**[2]

^{1}H NMR (600 MHz, CHLOROFORM-D) δ 7.23 (t, *J* = 7.8 Hz, 1H), 6.90 – 6.84 (m, 2H), 6.77 (d, *J* = 10.3 Hz, 1H), 3.81 (s, 2H), 3.79 (s, 3H), 1.76 (s, 2H).

^{13}C NMR (151 MHz, CHLOROFORM-D) δ 159.83, 144.89, 129.53, 119.32, 112.60, 112.22, 55.16, 46.40.

GC-MS: m/z(%) 65(30), 77(55), 106(70), 136(100), 137(65), HRMS Calcd. (ESI) m/z for $C_8H_{11}NO$: $[M+H]^+$ 138.0913, found 138.0909

IR (KBr) cm^{-1}: 850, 1460, 1600, 2839, 2950, 3010, 3290, 3390.

(3,5-dimethoxyphenyl)methanamine **(8a)**

^{1}H NMR (600 MHz, CHLOROFORM-D) δ 6.45 (s, 2H), 6.32 (s, 1H), 3.76 (s, 2H), 3.75 (s, 6H), 1.94 (s, 2H).

^{13}C NMR (151 MHz, CHLOROFORM-D) δ 161.01, 145.73, 104.94, 98.76, 55.26, 46.53.

HRMS Calcd. (ESI) m/z for $C_9H_{13}NO_2$: $[M+H]^+$ 168.1019, found 168.1015

IR (KBr) cm^{-1}: 860, 1455, 1590, 2841, 2951, 3013, 3294, 3391.

(4-chlorophenyl)methanamine **(9a)**[3]

^{1}H NMR (600 MHz, CHLOROFORM-D) δ 7.30 (d, *J* = 9.2 Hz, 2H), 7.25 (d, *J* = 8.4 Hz, 2H), 3.84 (s, 2H), 1.73 (s, active H).

^{13}C NMR (151 MHz, CHLOROFORM-D) δ 141.56, 132.59, 128.70, 128.56, 45.82.

GC-MS: m/z(%) 51(25), 77(45), 106(100), 125(10), 140(35), HRMS Calcd. (ESI) m/z for C_7H_8ClN: $[M+H]^+$ 142.0418, found 142.0414

IR (KBr) cm^{-1}: 800, 1490, 1600, 2850, 2900, 3030, 3290, 3370.

(2-chlorophenyl)methanamine **(10a)**[1]

^{1}H NMR (600 MHz, CHLOROFORM-D) δ 7.38 (d, *J* = 7.7 Hz, 1H), 7.35 (d, *J* = 7.6 Hz, 1H), 7.24 (d, *J* = 7.3 Hz, 1H), 7.20 (t, *J* = 7.6 Hz, 1H), 3.94 (s, 2H), 2.29 (s, 2H).

^{13}C NMR (151 MHz, CHLOROFORM-D) δ 139.86, 133.40, 129.58, 129.15, 128.39, 127.13, 44.33.

GC-MS: m/z(%) 51(25), 77(45), 106(100), 125(10), 140(35), HRMS Calcd. (ESI) m/z for C_7H_8ClN: $[M+H]^+$ 142.0418, found 142.0420

IR (KBr) cm^{-1}: 750, 1490, 1610, 2860, 2900, 3050, 3300, 3390.

(3,4-difluorophenyl)methanamine **(11a)**

^{1}H NMR (600 MHz, CHLOROFORM-D) δ 7.14 (d, *J* = 9.4 Hz, 1H), 7.10 (d, *J* = 10.2 Hz, 1H), 7.03 (s, 1H), 3.84 (s, 2H), 1.71 (s, active H).

^{13}C NMR (151 MHz, CHLOROFORM-D) δ 150.37 (dd, J=250 Hz, 12 Hz), 149.27 (dd, J=249 Hz, 12 Hz), 140.10 (dd, *J* = 6 Hz, 4 Hz), 122.83 (dd, J=7 Hz, 4Hz), 117.33 (d, J= 18 Hz), 116.19 (d, J=17 Hz), 45.44.

GC-MS: m/z(%) 63(40), 75(20), 95(15), 123(100), 142(65), HRMS Calcd. (ESI) m/z for $C_7H_7F_2N$: $[M+H]^+$ 144.0619, found 144.0615

IR (KBr) cm^{-1}: 790, 1460, 1610, 2850, 2930, 3010, 3310, 3380.

(4-(trifluoromethyl)phenyl)methanamine **(12a)**[1]

^{1}H NMR (600 MHz, CHLOROFORM-D) δ 7.59 (d, *J* = 8.0 Hz, 2H), 7.44 (d, *J* = 8.0 Hz, 2H), 3.94 (s, 2H), 1.76 (s, 2H).

^{13}C NMR (151 MHz, CHLOROFORM-D) δ 146.93 (s), 128.35 (q, J=37.9 Hz), 127.36 (s), 125.48 (q, *J* = 2.6Hz), 124.02 (q, *J* = 165.7Hz), 45.96 (s).

GC-MS: m/z(%) 51(30), 77(30), 106(100), 127(65), 156(20), 174(90), HRMS Calcd. (ESI) m/z for $C_8H_8F_3N$: $[M+H]^+$ 176.0682, found 176.0688

IR (KBr) cm^{-1}: 810, 1440, 1610, 2870, 2950, 3000, 3300, 3391.

4-(aminomethyl)aniline **(13a)**[2]

^{1}H NMR (600 MHz, CHLOROFORM-D) δ 7.41 (d, *J* = 8.6 Hz, 2H), 6.65 (d, *J* = 8.6 Hz, 2H), 4.17 (s, 2H), 3.81 (s, 2H), 1.62 (s, 1H).

^{13}C NMR (151 MHz, CHLOROFORM-D) δ 151.22 (s), 133.81 (s), 120.74 (s), 114.51 (s), 99.10 (s).

GC-MS: m/z(%) 66(35), 78(10), 93(100), 122(95), HRMS Calcd. (ESI) m/z for $C_7H_{10}N_2$: $[M+2H]^{2+}$ 124.0990, found 124.0985

IR (KBr) cm^{-1}: 890, 1512, 1539, 2860, 2940, 3050, 3328, 3423.

3-(aminomethyl)aniline **(14a)**[2]

^{1}H NMR (600 MHz, CHLOROFORM-D) δ 7.09 (t, *J* = 7.7 Hz, 1H), 6.73 – 6.67 (m, 2H), 6.57 (d, *J* = 7.9 Hz, 1H), 3.71 (s, 2H), 3.57 (s, 2H), 1.25 (s, 1H).

^{13}C NMR (151 MHz, CHLOROFORM-D) δ 146.63 (s), 140.31 (s), 129.35 (s), 118.59 (s), 114.99 (s), 114.00 (s), 52.68 (s).

GC-MS: m/z(%) 66(35), 78(10), 93(100), 122(95), HRMS Calcd. (ESI) m/z for $C_7H_{10}N_2$: $[M+2H]^{2+}$ 124.0990, found 124.0993

IR (KBr) cm^{-1}: 900, 1510, 1540, 2870, 2940, 3050, 3340, 3450.

(4-(aminomethyl)phenyl)methanol **(15a)**

^{1}H NMR (600 MHz, CHLOROFORM-D) δ 7.30 (s, 4H), 4.64 (s, 2H), 3.77 (s, 2H), 2.11 (s, 2H), 2.04 (s, 1H).

^{13}C NMR (151 MHz, CHLOROFORM-D) δ 139.84 (s), 139.08 (s), 128.45 (s), 127.17 (s), 65.04 (s), 52.66 (s).

HRMS Calcd. (ESI) m/z for $C_8H_{11}NO$: $[M+H]^+$ 138.0913, found 138.0909.

IR (KBr) cm^{-1}: 870, 1450, 1520, 2850, 2930, 3030, 3310, 3390, 3650.

Phenethylamine **(16a)**[1]

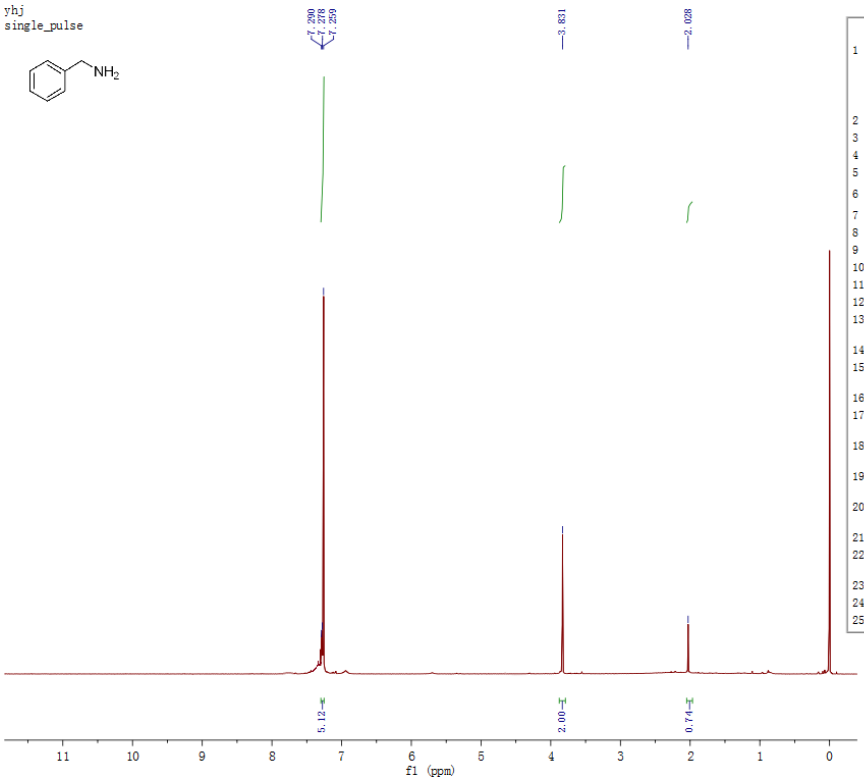
^{1}H NMR (600 MHz, CHLOROFORM-D) δ 7.31 (d, *J* = 7.8 Hz, 2H), 7.26 (s, 2H), 7.20 (s, 1H), 3.52 (dd, *J* = 13.0, 6.8 Hz, 2H), 2.82 (d, *J* = 6.9 Hz, 2H), 2.28 (s, 2H).

^{13}C NMR (151 MHz, CHLOROFORM-D) δ 138.87, 128.71 (d, *J* = 13.0 Hz), 126.54, 40.64, 35.63.

GC-MS: m/z(%) 65(70), 77(20), 91(100), 121(20), HRMS Calcd. (ESI) m/z for $C_8H_{11}N$: $[M+H]^+$ 122.0964, found 122.0966

IR (KBr) cm^{-1}: 850, 1440, 1500, 2850, 2920, 3040, 3290, 3400.

Copies of 1H and 13C NMR spectrums



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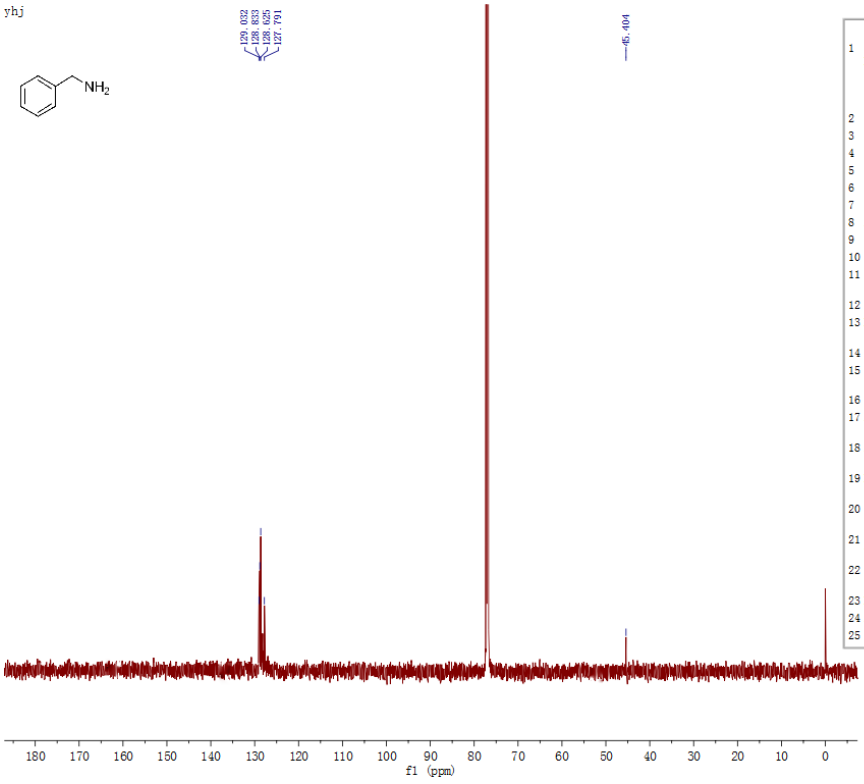

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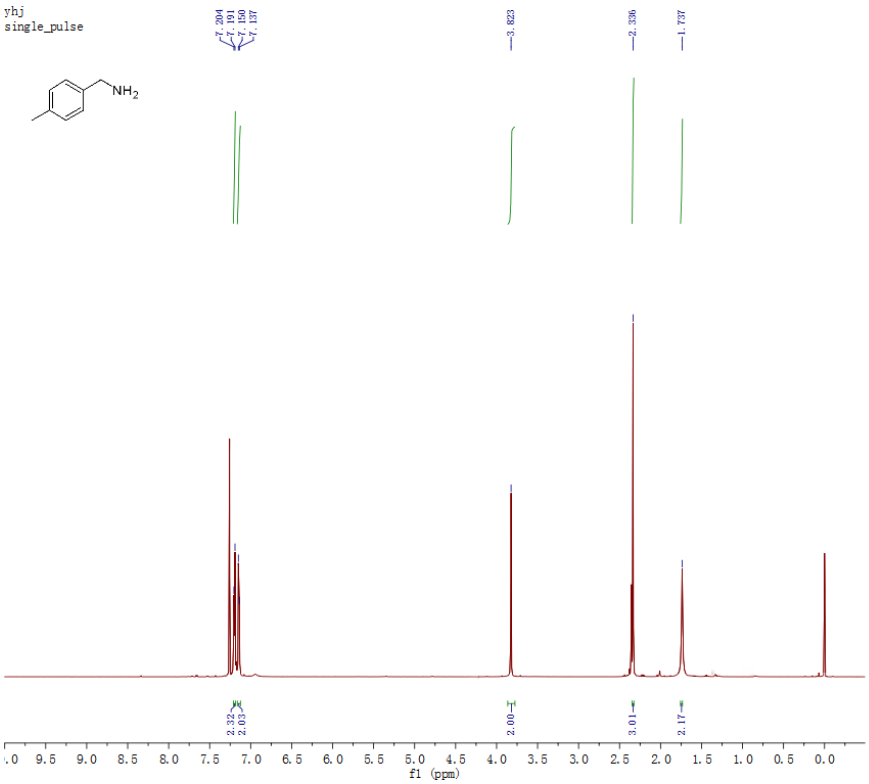

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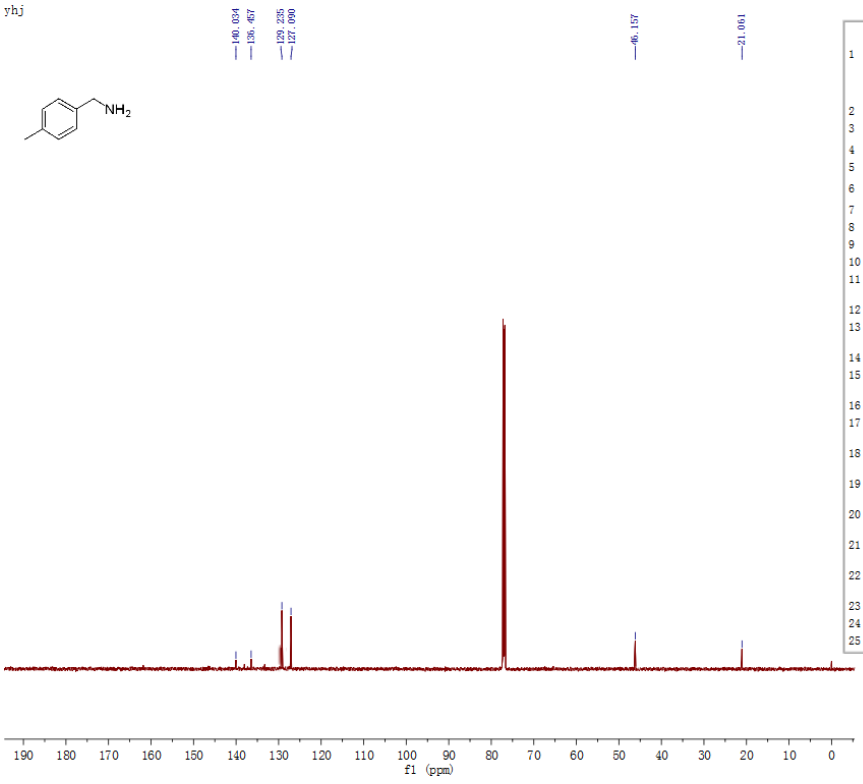

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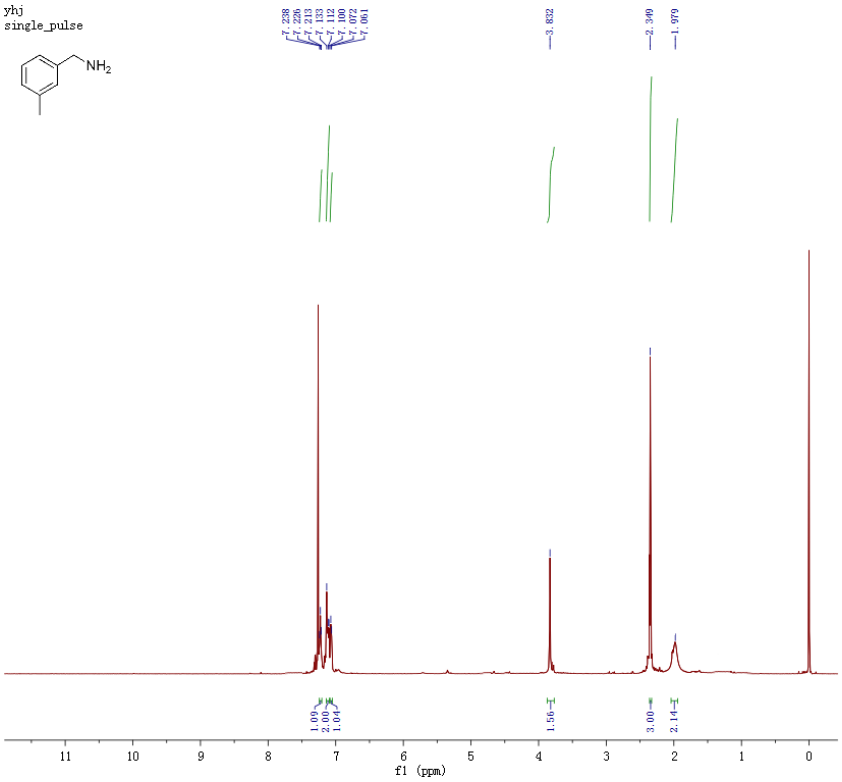

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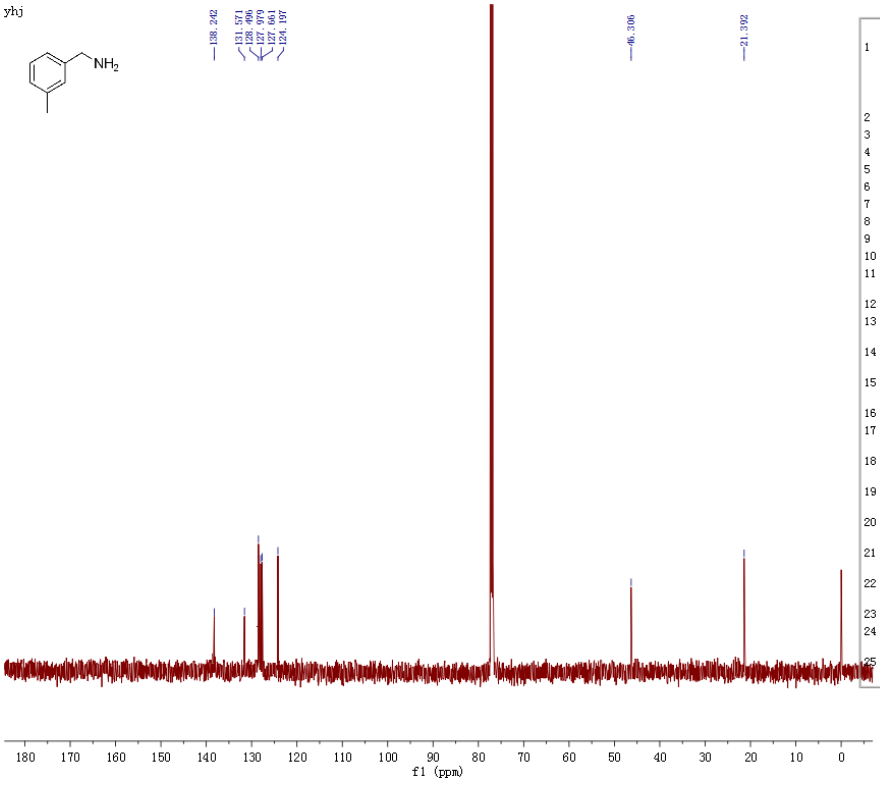

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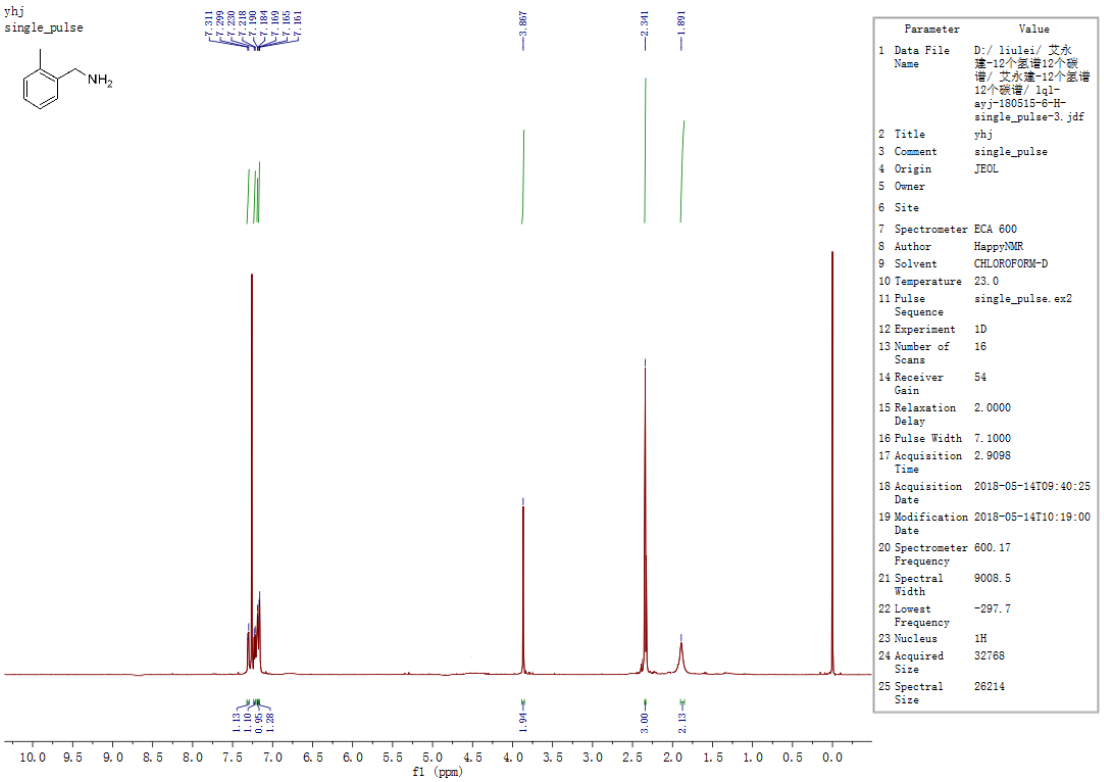
2	Title	yhj
3	Comment	
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	ECA 600
8	Author	HappyNMR
9	Solvent	CHLOROFORM-D
10	Temperature	24.7
11	Pulse Sequence	single_pulse_dec
12	Experiment	1D
13	Number of Scans	1024
14	Receiver Gain	58
15	Relaxation Delay	2.0000
16	Pulse Width	4.0633
17	Acquisition Time	0.6921
18	Acquisition Date	2018-05-21T12:49:26
19	Modification Date	2018-05-21T13:05:04
20	Spectrometer Frequency	150.91
21	Spectral Width	37876.8
22	Lowest Frequency	-3859.4
23	Nucleus	13C
24	Acquired Size	32768
25	Spectral Size	26214



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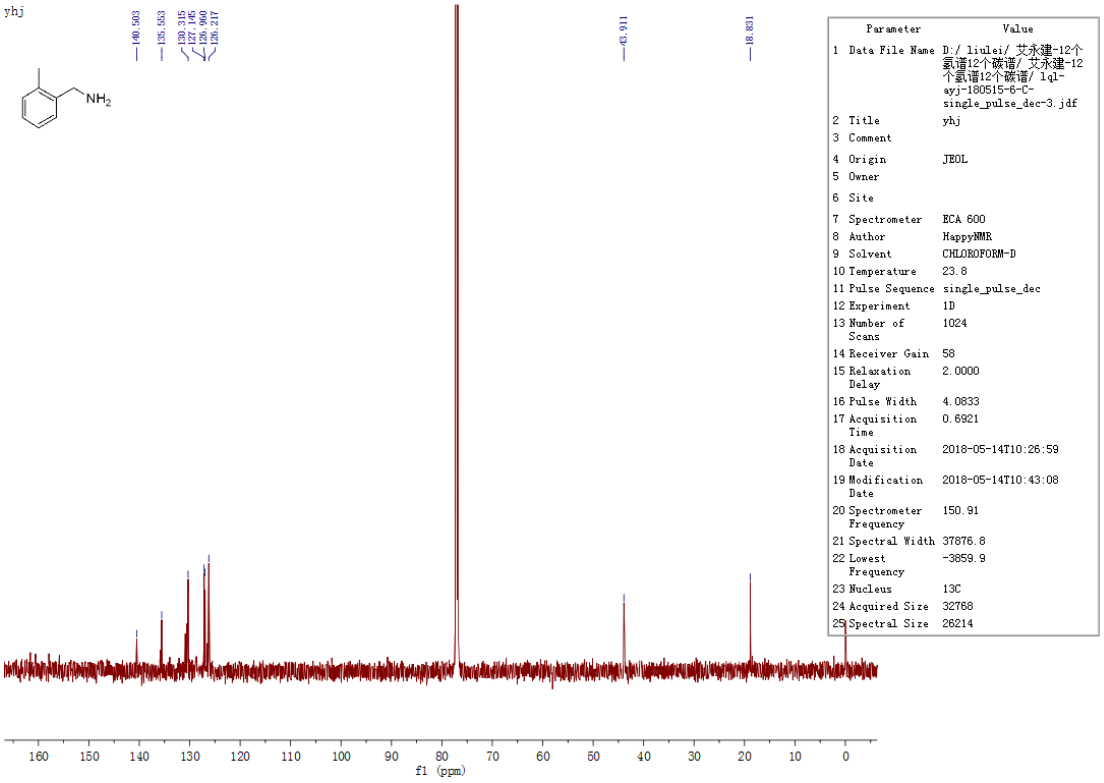
2	Title	yhj
3	Comment	single_pulse
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	ECA 600
8	Author	HappyNMR
9	Solvent	CHLOROFORM-D
10	Temperature	23.0
11	Pulse Sequence	single_pulse.ex2
12	Experiment	1D
13	Number of Scans	16
14	Receiver Gain	54
15	Relaxation Delay	2.0000
16	Pulse Width	7.1000
17	Acquisition Time	2.9098
18	Acquisition Date	2018-05-14T09:40:25
19	Modification Date	2018-05-14T10:19:00
20	Spectrometer Frequency	600.17
21	Spectral Width	9008.5
22	Lowest Frequency	-297.7
23	Nucleus	1H
24	Acquired Size	32768
25	Spectral Size	26214



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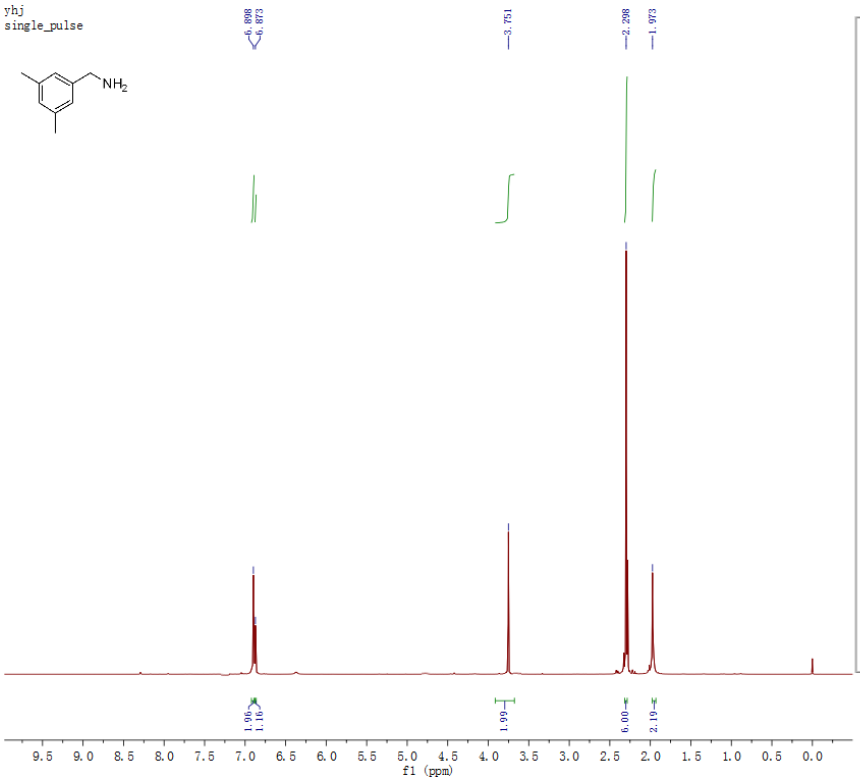
2	Title	yhj
3	Comment	
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	ECA 600
8	Author	HappyNMR
9	Solvent	CHLOROFORM-D
10	Temperature	23.8
11	Pulse Sequence	single_pulse_dec
12	Experiment	1D
13	Number of Scans	1024
14	Receiver Gain	58
15	Relaxation Delay	2.0000
16	Pulse Width	4.0833
17	Acquisition Time	0.6921
18	Acquisition Date	2018-05-14T10:26:59
19	Modification Date	2018-05-14T10:43:08
20	Spectrometer Frequency	150.91
21	Spectral Width	37876.8
22	Lowest Frequency	-3859.9
23	Nucleus	13C
24	Acquired Size	32768
25	Spectral Size	26214



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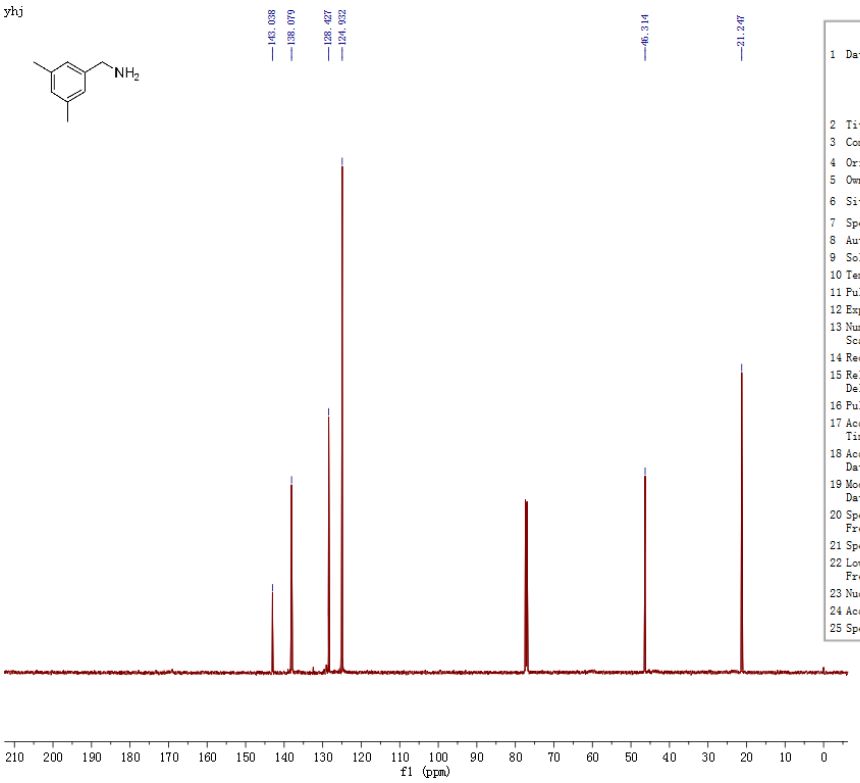
2	Title	yhj
3	Comment	single_pulse
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	ECA 600
8	Author	HappyNMR
9	Solvent	CHLOROFORM-D
10	Temperature	23.8
11	Pulse Sequence	single_pulse.ex2
12	Experiment	1D
13	Number of Scans	16
14	Receiver Gain	26
15	Relaxation Delay	2.0000
16	Pulse Width	7.1000
17	Acquisition Time	2.9098
18	Acquisition Date	2018-05-18T15:17:13
19	Modification Date	2018-05-18T15:34:36
20	Spectrometer Frequency	600.17
21	Spectral Width	9008.5
22	Lowest Frequency	-307.3
23	Nucleus	1H
24	Acquired Size	32768
25	Spectral Size	26214



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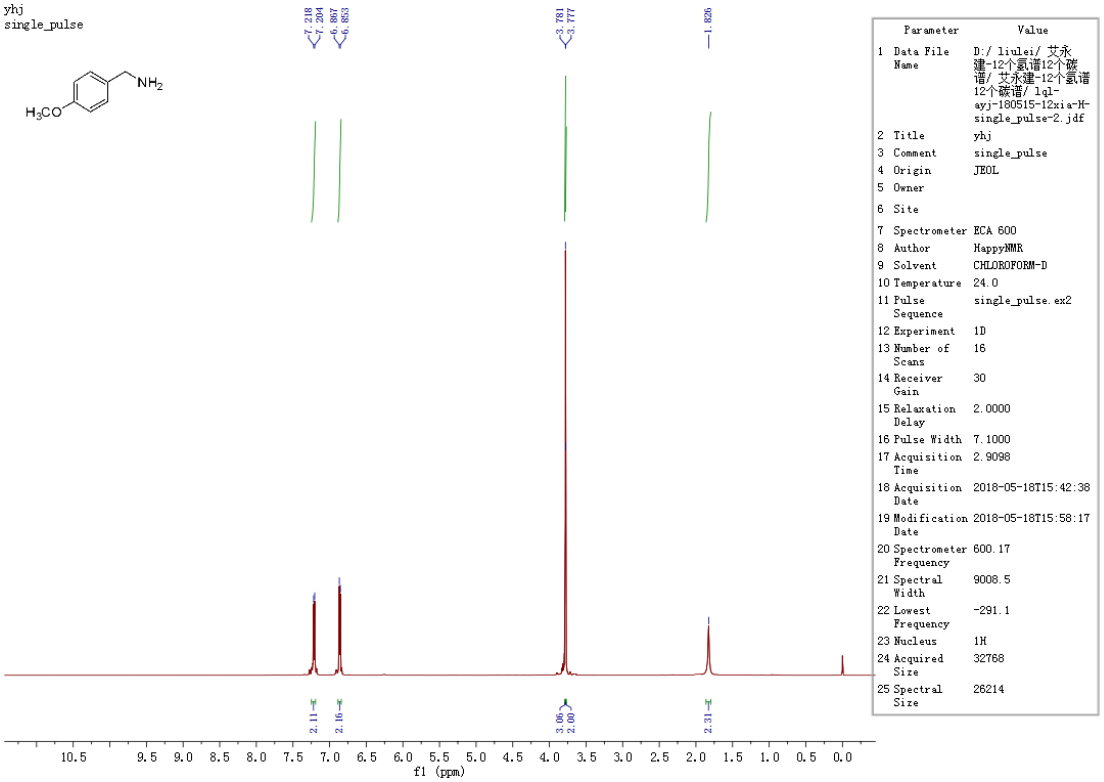
2	Title	yhj
3	Comment	
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	ECA 600
8	Author	HappyNMR
9	Solvent	CHLOROFORM-D
10	Temperature	25.0
11	Pulse Sequence	single_pulse_dec
12	Experiment	1D
13	Number of Scans	247
14	Receiver Gain	58
15	Relaxation Delay	2.0000
16	Pulse Width	4.0833
17	Acquisition Time	0.6921
18	Acquisition Date	2018-05-18T15:30:25
19	Modification Date	2018-05-18T15:47:15
20	Spectrometer Frequency	150.91
21	Spectral Width	37876.8
22	Lowest Frequency	-3861.5
23	Nucleus	13C
24	Acquired Size	32768
25	Spectral Size	26214



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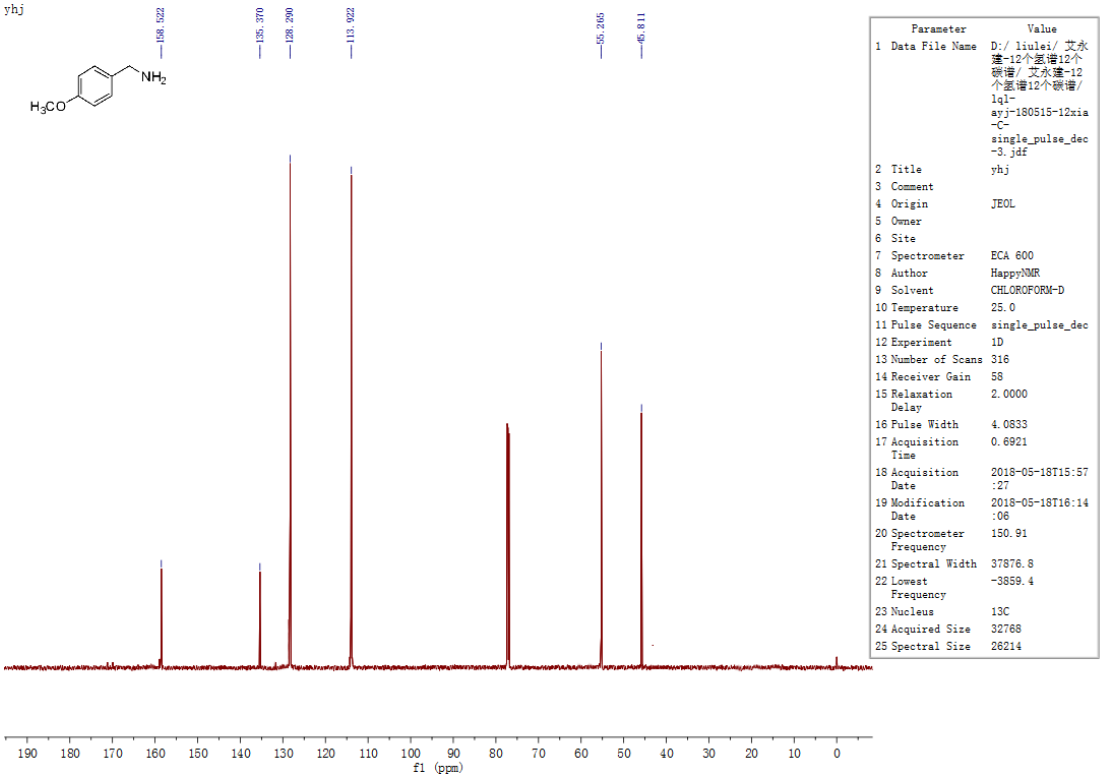
2	Title	yhj
3	Comment	single_pulse
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	ECA 600
8	Author	HappyNMR
9	Solvent	CHLOROFORM-D
10	Temperature	24.0
11	Pulse Sequence	single_pulse.ex2
12	Experiment	1D
13	Number of Scans	16
14	Receiver Gain	30
15	Relaxation Delay	2.0000
16	Pulse Width	7.1000
17	Acquisition Time	2.9098
18	Acquisition Date	2018-05-18T15:42:38
19	Modification Date	2018-05-18T15:58:17
20	Spectrometer Frequency	600.17
21	Spectral Width	9008.5
22	Lowest Frequency	-291.1
23	Nucleus	1H
24	Acquired Size	32768
25	Spectral Size	26214



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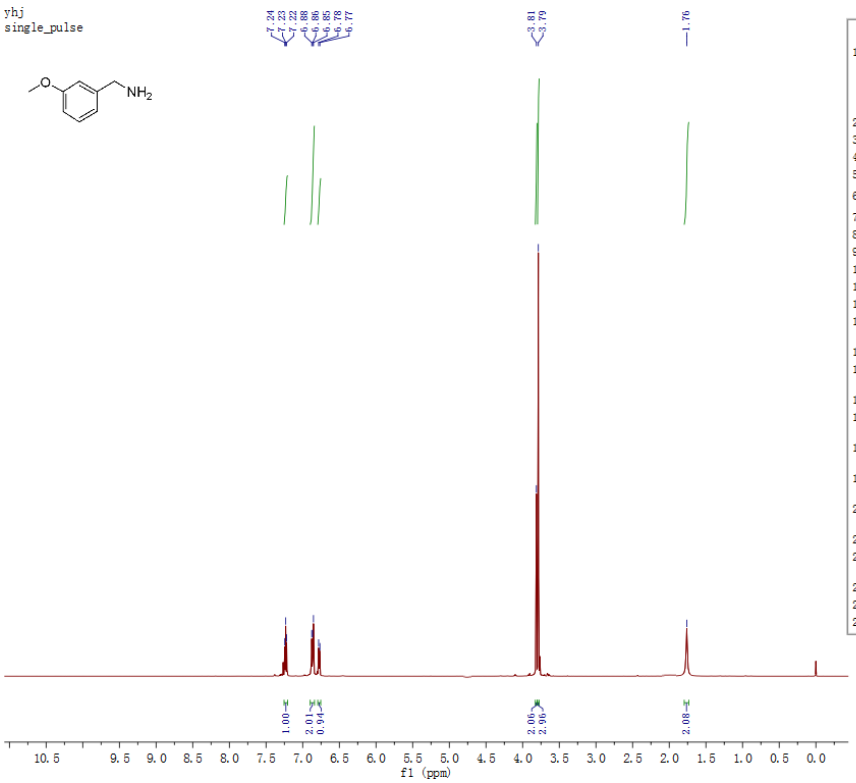
2	Title	yhj
3	Comment	
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	ECA 600
8	Author	HappyNMR
9	Solvent	CHLOROFORM-D
10	Temperature	25.0
11	Pulse Sequence	single_pulse_dec
12	Experiment	1D
13	Number of Scans	316
14	Receiver Gain	58
15	Relaxation Delay	2.0000
16	Pulse Width	4.0833
17	Acquisition Time	0.6921
18	Acquisition Date	2018-05-18T15:57:27
19	Modification Date	2018-05-18T16:14:06
20	Spectrometer Frequency	150.91
21	Spectral Width	37876.8
22	Lowest Frequency	-3859.4
23	Nucleus	13C
24	Acquired Size	32768
25	Spectral Size	26214



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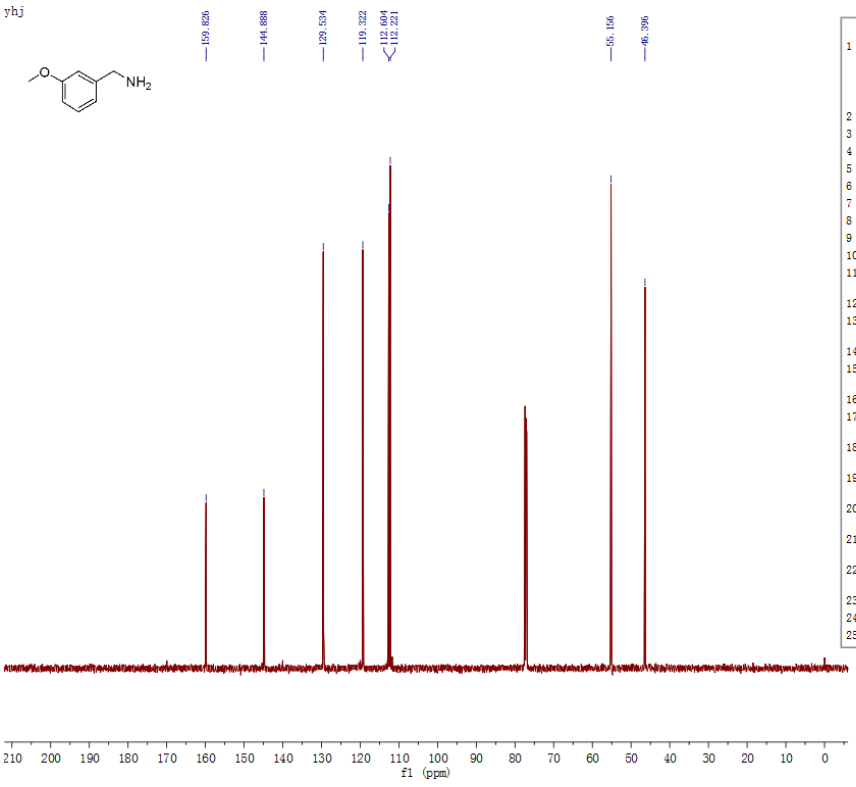
2	Title	yhj
3	Comment	single_pulse
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	ECA 600
8	Author	HappyNMR
9	Solvent	CHLOROFORM-D
10	Temperature	24.0
11	Pulse Sequence	single_pulse.ex2
12	Experiment	1D
13	Number of Scans	16
14	Receiver Gain	28
15	Relaxation Delay	2.0000
16	Pulse Width	7.1000
17	Acquisition Time	2.9098
18	Acquisition Date	2018-05-18T16:34:51
19	Modification Date	2018-05-18T16:50:30
20	Spectrometer Frequency	600.17
21	Spectral Width	9008.5
22	Lowest Frequency	-293.5
23	Nucleus	1H
24	Acquired Size	32768
25	Spectral Size	26214



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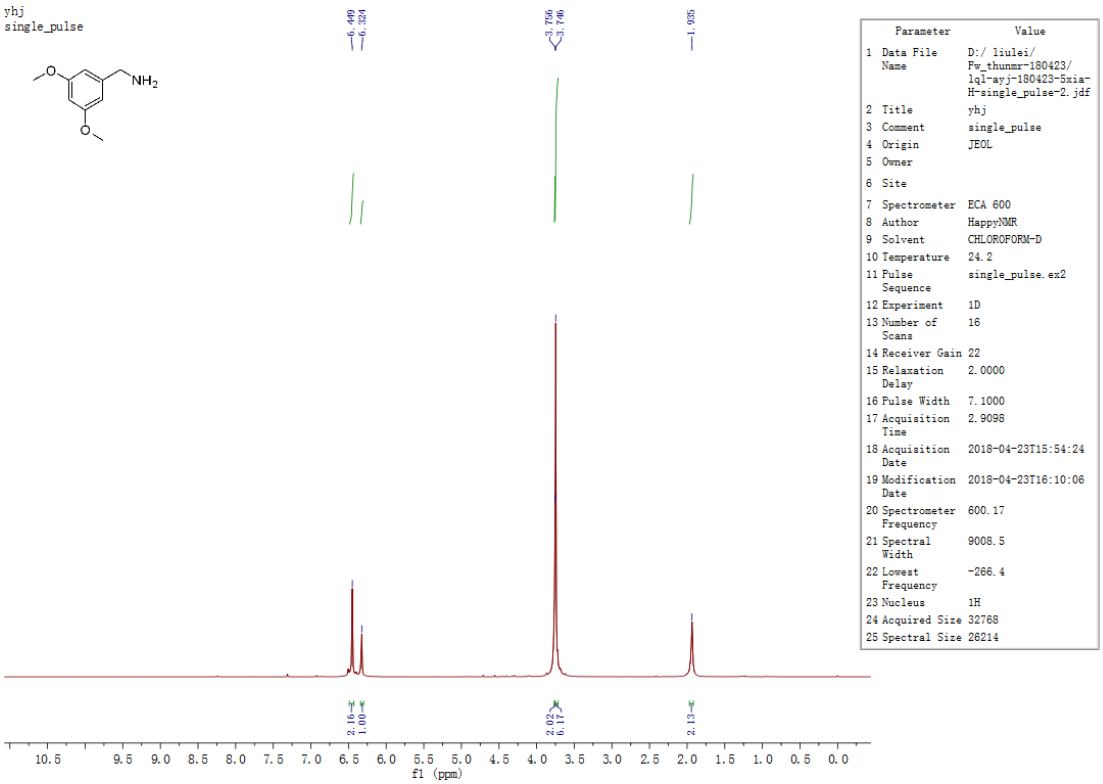
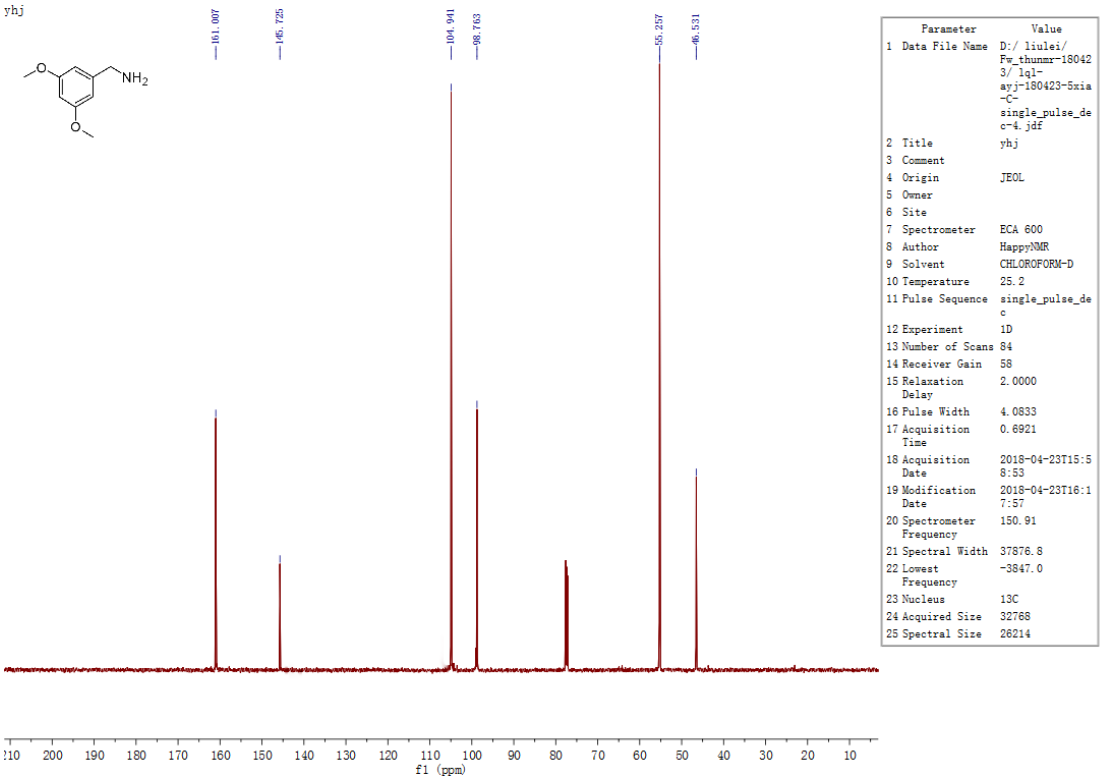
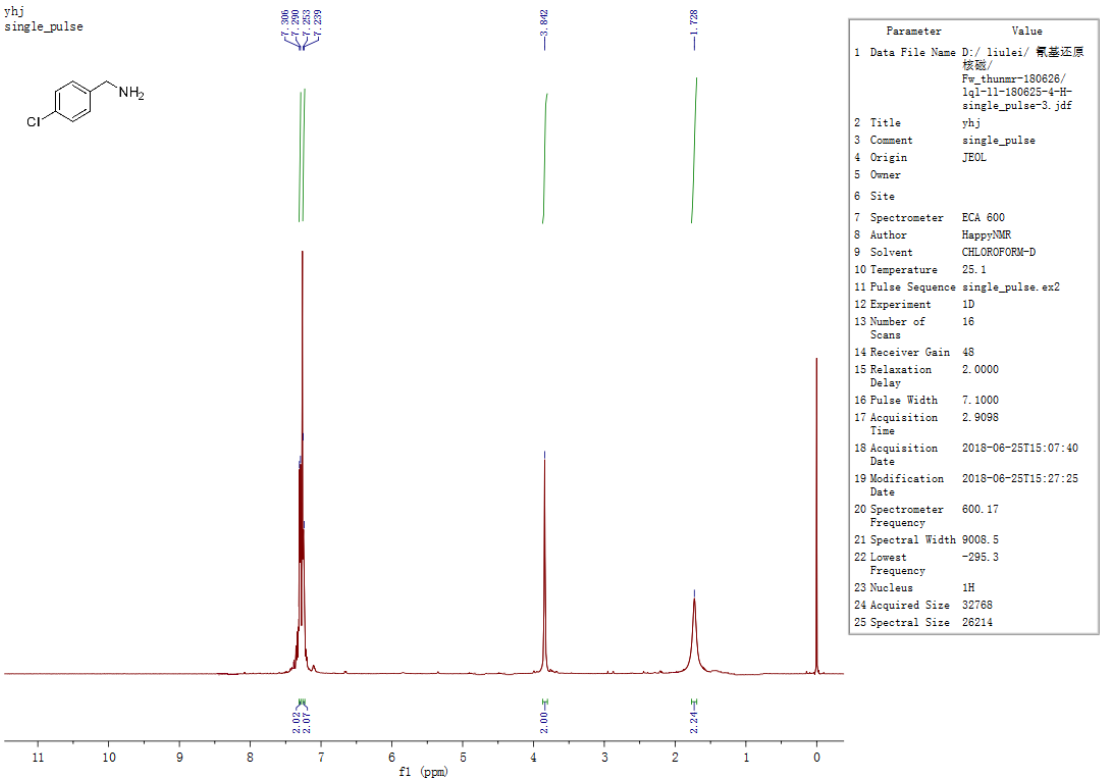
2	Title	yhj
3	Comment	
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	ECA 600
8	Author	HappyNMR
9	Solvent	CHLOROFORM-D
10	Temperature	25.0
11	Pulse Sequence	single_pulse_dec
12	Experiment	1D
13	Number of Scans	112
14	Receiver Gain	58
15	Relaxation Delay	2.0000
16	Pulse Width	4.0833
17	Acquisition Time	0.6921
18	Acquisition Date	2018-05-18T16:40:30
19	Modification Date	2018-05-18T16:57:06
20	Spectrometer Frequency	150.91
21	Spectral Width	37876.8
22	Lowest Frequency	-3860.9
23	Nucleus	13C
24	Acquired Size	32768
25	Spectral Size	26214



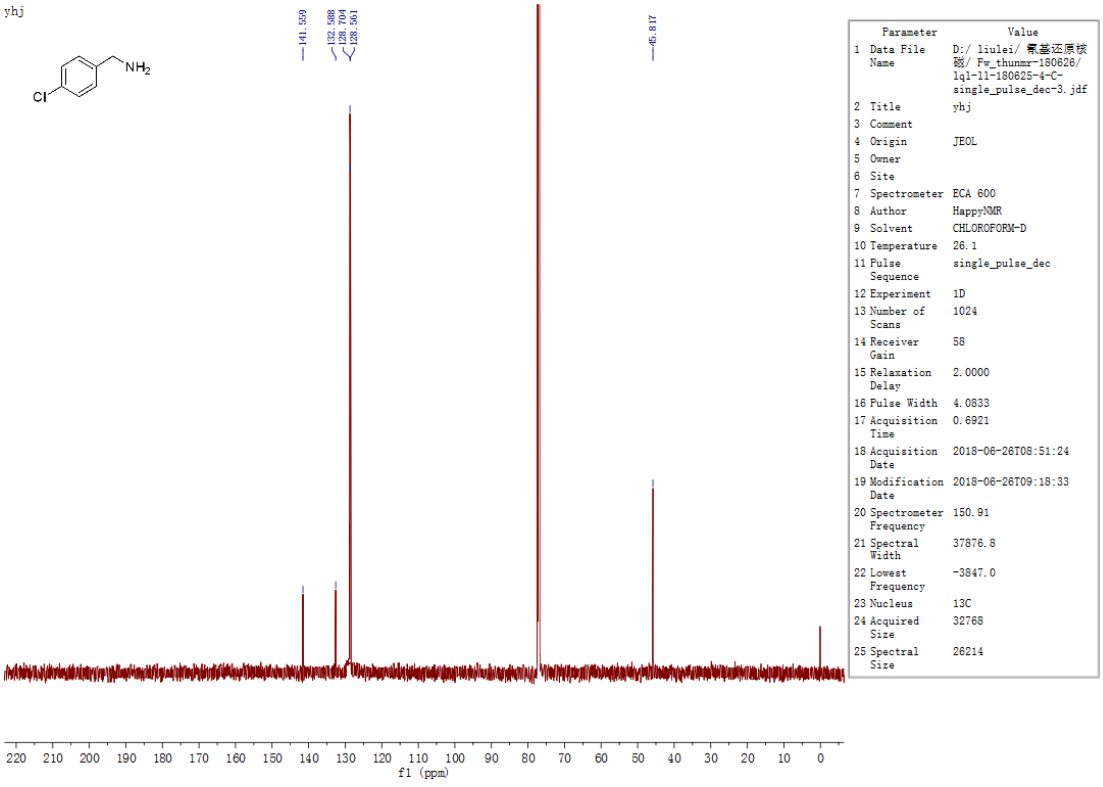
	Parameter	Value
1	Data File Name	D:/ liulei/ Fw_thunmr-180423/ lql-ayj-180423-5xia-H-single_pulse-2.jdf
2	Title	yhj
3	Comment	single_pulse
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	ECA 600
8	Author	HappyNMR
9	Solvent	CHLOROFORM-D
10	Temperature	24.2
11	Pulse Sequence	single_pulse.ex2
12	Experiment	1D
13	Number of Scans	16
14	Receiver Gain	22
15	Relaxation Delay	2.0000
16	Pulse Width	7.1000
17	Acquisition Time	2.9098
18	Acquisition Date	2018-04-23T15:54:24
19	Modification Date	2018-04-23T16:10:06
20	Spectrometer Frequency	600.17
21	Spectral Width	9008.5
22	Lowest Frequency	-266.4
23	Nucleus	1H
24	Acquired Size	32768
25	Spectral Size	26214



	Parameter	Value
1	Data File Name	D:/ liulei/ Fw_thunmr-18042 3/ lql-ayj-180423-5xia -C-single_pulse_dec-4.jdf
2	Title	yhj
3	Comment	
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	ECA 600
8	Author	HappyNMR
9	Solvent	CHLOROFORM-D
10	Temperature	25.2
11	Pulse Sequence	single_pulse_dec
12	Experiment	1D
13	Number of Scans	84
14	Receiver Gain	58
15	Relaxation Delay	2.0000
16	Pulse Width	4.0833
17	Acquisition Time	0.6921
18	Acquisition Date	2018-04-23T15:58:53
19	Modification Date	2018-04-23T16:17:57
20	Spectrometer Frequency	150.91
21	Spectral Width	37876.8
22	Lowest Frequency	-3847.0
23	Nucleus	13C
24	Acquired Size	32768
25	Spectral Size	26214



	Parameter	Value
1	Data File Name	D:/ liulei/ 氧基还原核磁/ Fw_thunmr-180626/ lql-ll-180625-4-H-single_pulse-3.jdf
2	Title	yhj
3	Comment	single_pulse
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	ECA 600
8	Author	HappyNMR
9	Solvent	CHLOROFORM-D
10	Temperature	25.1
11	Pulse Sequence	single_pulse.ex2
12	Experiment	1D
13	Number of Scans	16
14	Receiver Gain	48
15	Relaxation Delay	2.0000
16	Pulse Width	7.1000
17	Acquisition Time	2.9098
18	Acquisition Date	2018-06-25T15:07:40
19	Modification Date	2018-06-25T15:27:25
20	Spectrometer Frequency	600.17
21	Spectral Width	9008.5
22	Lowest Frequency	-295.3
23	Nucleus	1H
24	Acquired Size	32768
25	Spectral Size	26214



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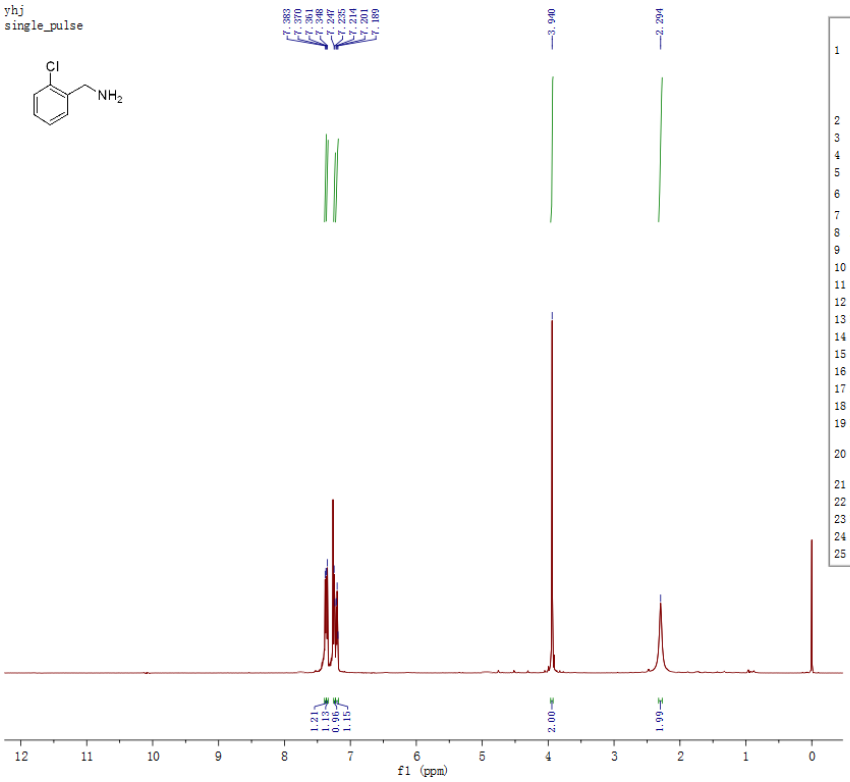
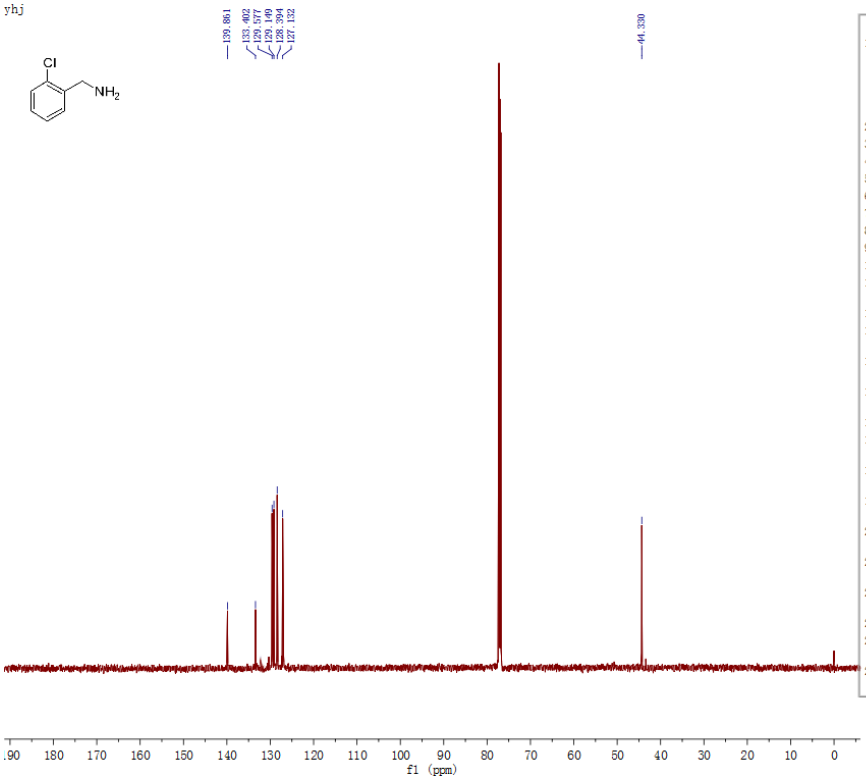
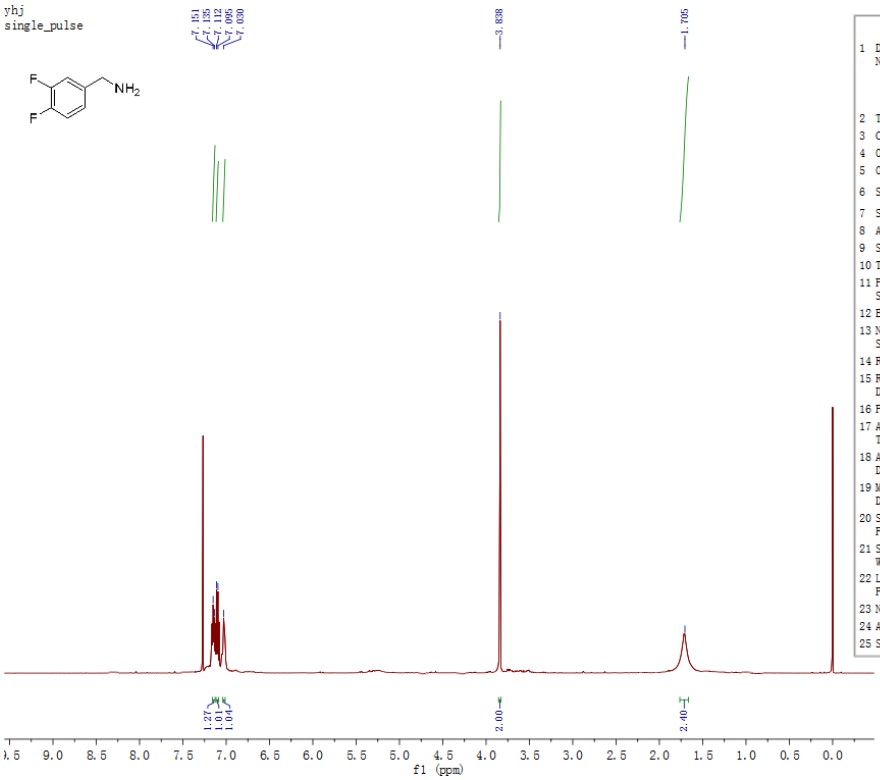
3	Comment	
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	ECA 600
8	Author	HappyNMR
9	Solvent	CHLOROFORM-D
10	Temperature	26.1
11	Pulse Sequence	single_pulse_dec
12	Experiment	1D
13	Number of Scans	1024
14	Receiver Gain	58
15	Relaxation Delay	2.0000
16	Pulse Width	4.0833
17	Acquisition Time	0.6921
18	Acquisition Date	2018-06-26T08:51:24
19	Modification Date	2018-06-26T09:18:33
20	Spectrometer Frequency	150.91
21	Spectral Width	37876.8
22	Lowest Frequency	-3847.0
23	Nucleus	13C
24	Acquired Size	32768
25	Spectral Size	26214



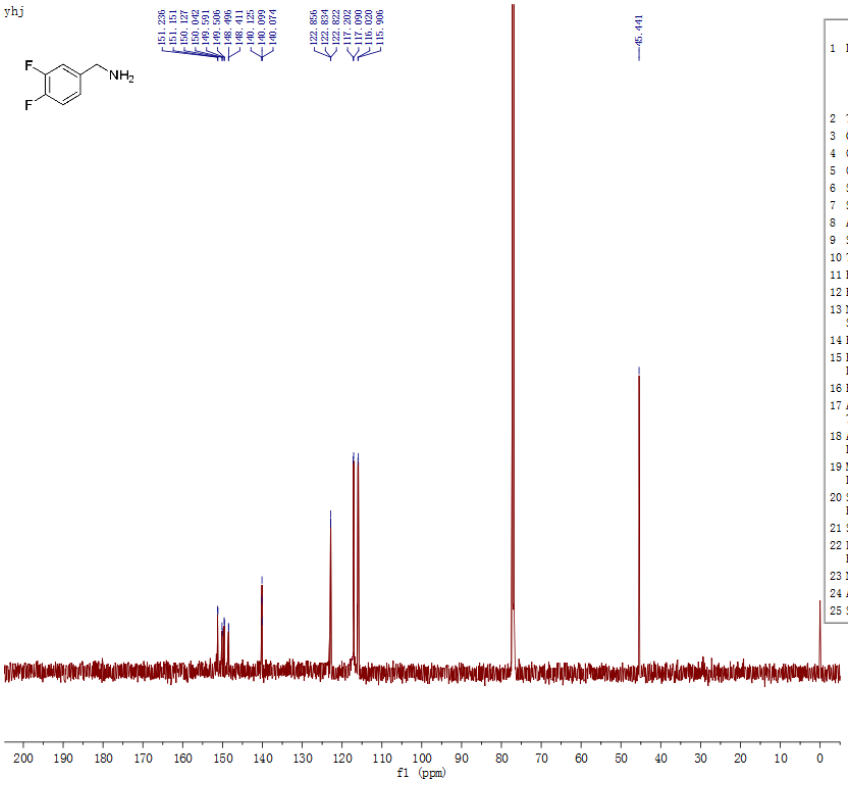
	Parameter	Value
1	Data File Name	D:/ liulei/ 艾永建-12个氢谱12个碳谱/ 艾永建-12个氢谱12个碳谱/ lql-ayj-180515-11xia-H-single_pulse-3.jdf
2	Title	yhj
3	Comment	single_pulse
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	ECA 600
8	Author	HappyNMR
9	Solvent	CHLOROFORM-D
10	Temperature	24.1
11	Pulse Sequence	single_pulse.ex2
12	Experiment	1D
13	Number of Scans	16
14	Receiver Gain	42
15	Relaxation Delay	2.0000
16	Pulse Width	7.1000
17	Acquisition Time	2.9098
18	Acquisition Date	2018-05-18T12:14:11
19	Modification Date	2018-05-18T12:30:42
20	Spectrometer Frequency	600.17
21	Spectral Width	9008.5
22	Lowest Frequency	-294.7
23	Nucleus	1H
24	Acquired Size	32768
25	Spectral Size	26214



	Parameter	Value
1	Data File Name	D:/ liulei/ 艾永建-12个氢谱12个碳谱/ 艾永建-12个氢谱12个碳谱/ lql-ayj-180515-11xia-C-single_pulse_dec-3.jdf
2	Title	yhj
3	Comment	
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	ECA 600
8	Author	HappyNMR
9	Solvent	CHLOROFORM-D
10	Temperature	25.1
11	Pulse Sequence	single_pulse_dec
12	Experiment	1D
13	Number of Scans	728
14	Receiver Gain	58
15	Relaxation Delay	2.0000
16	Pulse Width	4.0833
17	Acquisition Time	0.6921
18	Acquisition Date	2018-05-18T12:47:28
19	Modification Date	2018-05-18T13:03:20
20	Spectrometer Frequency	150.91
21	Spectral Width	37876.8
22	Lowest Frequency	-3859.3
23	Nucleus	13C
24	Acquired Size	32768
25	Spectral Size	26214



	Parameter	Value
1	Data File Name	D:/ liulei/ 刘磊-12个氢谱12个碳谱/ 刘磊-12个氢谱12个碳谱/ lql-ll-180521-17xia-H-single_pulse-3.jdf
2	Title	yhj
3	Comment	single_pulse
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	ECA 600
8	Author	HappyNMR
9	Solvent	CHLOROFORM-D
10	Temperature	23.7
11	Pulse Sequence	single_pulse.ex2
12	Experiment	1D
13	Number of Scans	16
14	Receiver Gain	42
15	Relaxation Delay	2.0000
16	Pulse Width	7.1000
17	Acquisition Time	2.9098
18	Acquisition Date	2018-05-24T14:48:14
19	Modification Date	2018-05-24T15:04:32
20	Spectrometer Frequency	600.17
21	Spectral Width	9008.5
22	Lowest Frequency	-292.3
23	Nucleus	1H
24	Acquired Size	32768
25	Spectral Size	26214



	Parameter	Value
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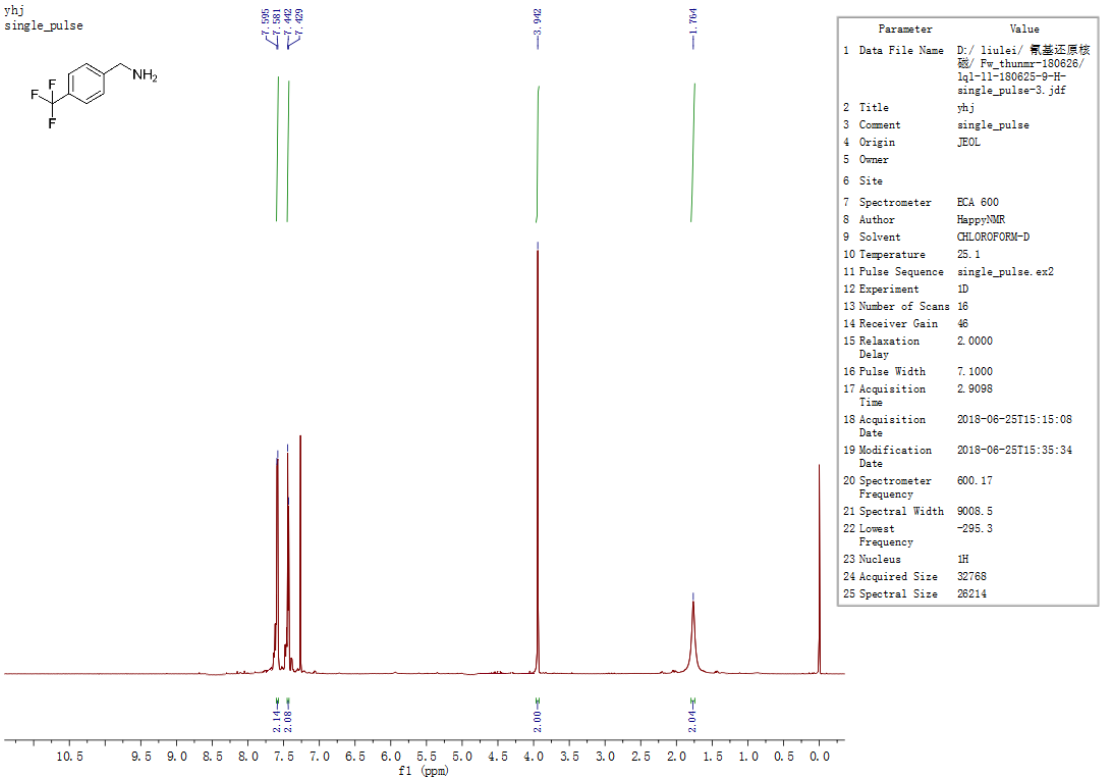
2	Title	yhj
3	Comment	
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	ECA 600
8	Author	HappyNMR
9	Solvent	CHLOROFORM-D
10	Temperature	24.7
11	Pulse Sequence	single_pulse_dec
12	Experiment	1D
13	Number of Scans	1024
14	Receiver Gain	58
15	Relaxation Delay	2.0000
16	Pulse Width	4.0833
17	Acquisition Time	0.6921
18	Acquisition Date	2018-05-24T15:35:18
19	Modification Date	2018-05-24T15:52:26
20	Spectrometer Frequency	150.91
21	Spectral Width	37876.8
22	Lowest Frequency	-3855.3
23	Nucleus	13C
24	Acquired Size	32768
25	Spectral Size	26214



	Parameter	Value
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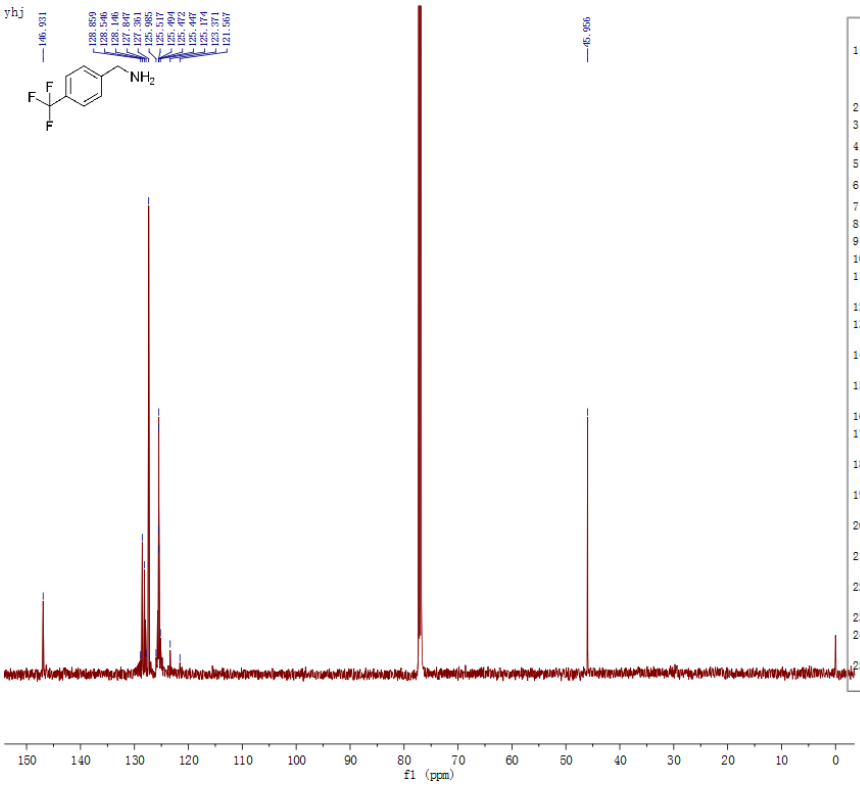
2	Title	yhj
3	Comment	single_pulse
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	ECA 600
8	Author	HappyNMR
9	Solvent	CHLOROFORM-D
10	Temperature	25.1
11	Pulse Sequence	single_pulse.ex2
12	Experiment	1D
13	Number of Scans	16
14	Receiver Gain	46
15	Relaxation Delay	2.0000
16	Pulse Width	7.1000
17	Acquisition Time	2.9098
18	Acquisition Date	2018-06-25T15:15:08
19	Modification Date	2018-06-25T15:35:34
20	Spectrometer Frequency	600.17
21	Spectral Width	9008.5
22	Lowest Frequency	-295.3
23	Nucleus	1H
24	Acquired Size	32768
25	Spectral Size	26214



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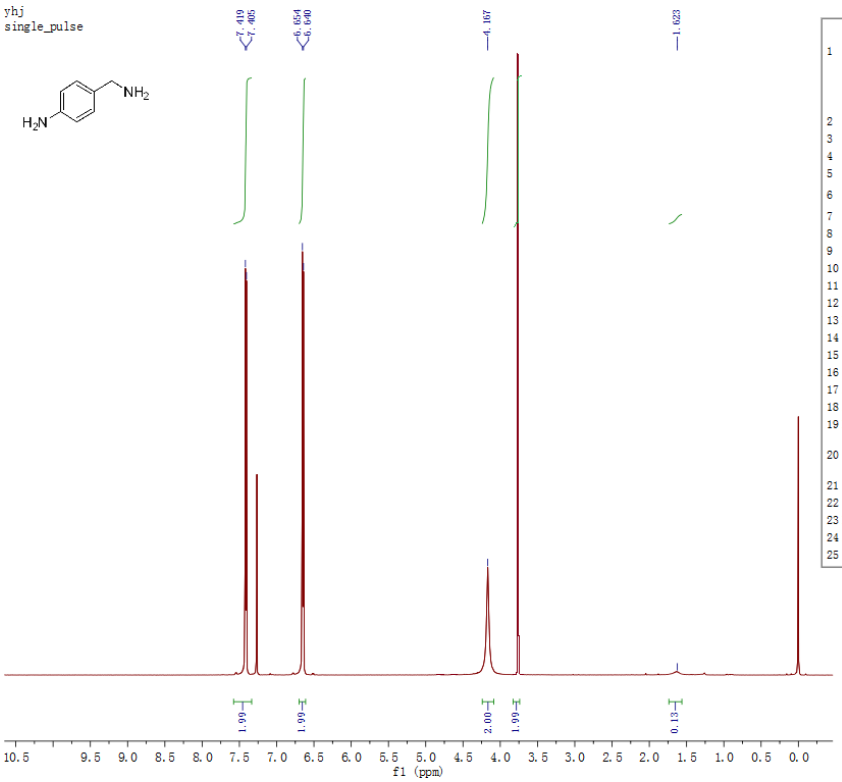
2	Title	yhj
3	Comment	
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	ECA 600
8	Author	HappyNMR
9	Solvent	CHLOROFORM-D
10	Temperature	26.7
11	Pulse Sequence	single_pulse_dec
12	Experiment	1D
13	Number of Scans	1024
14	Receiver Gain	56
15	Relaxation Delay	2.0000
16	Pulse Width	4.0833
17	Acquisition Time	0.6921
18	Acquisition Date	2018-06-25T16:09:08
19	Modification Date	2018-06-25T16:28:54
20	Spectrometer Frequency	150.91
21	Spectral Width	37876.8
22	Lowest Frequency	-3853.7
23	Nucleus	13C
24	Acquired Size	32768
25	Spectral Size	26214



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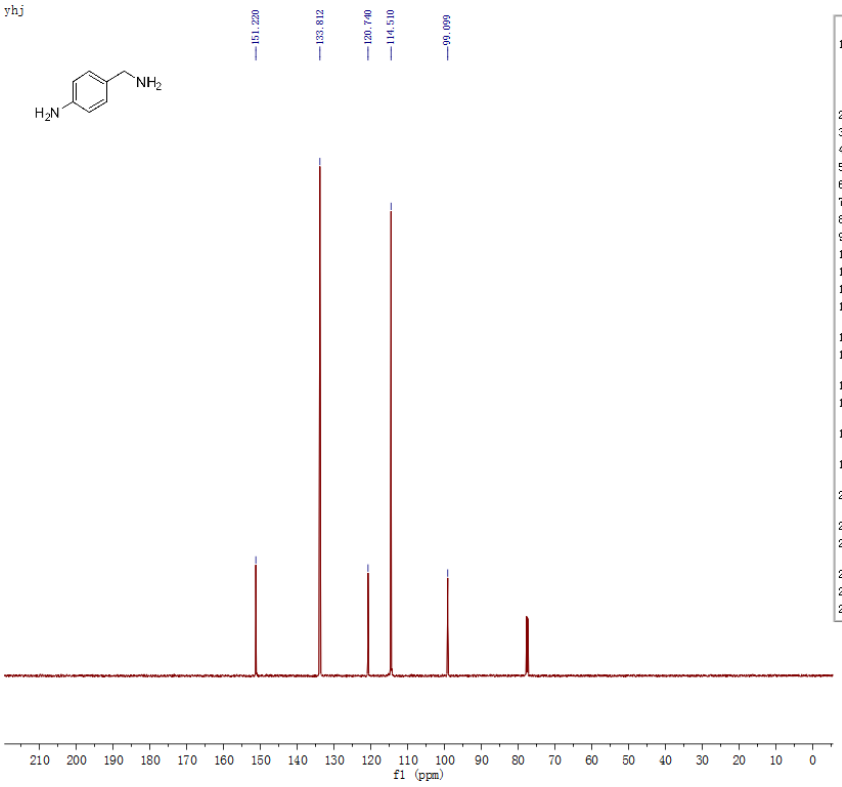
1 Data File Name	D:/ liulei/ 艾永建-12个氢谱12个碳谱/ 艾永建-12个氢谱12个碳谱/ lql-ayj-180515-15xia-H-single_pulse-3.jdf
2 Title	yhj
3 Comment	single_pulse
4 Origin	JEOL
5 Owner	
6 Site	
7 Spectrometer	ECA 600
8 Author	HappyNMR
9 Solvent	CHLOROFORM-D
10 Temperature	23.7
11 Pulse Sequence	single_pulse.ex2
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	46
15 Relaxation Delay	2.0000
16 Pulse Width	7.1000
17 Acquisition Time	2.9098
18 Acquisition Date	2018-05-17T13:50:33
19 Modification Date	2018-05-17T14:08:04
20 Spectrometer Frequency	600.17
21 Spectral Width	9008.5
22 Lowest Frequency	-294.1
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	26214



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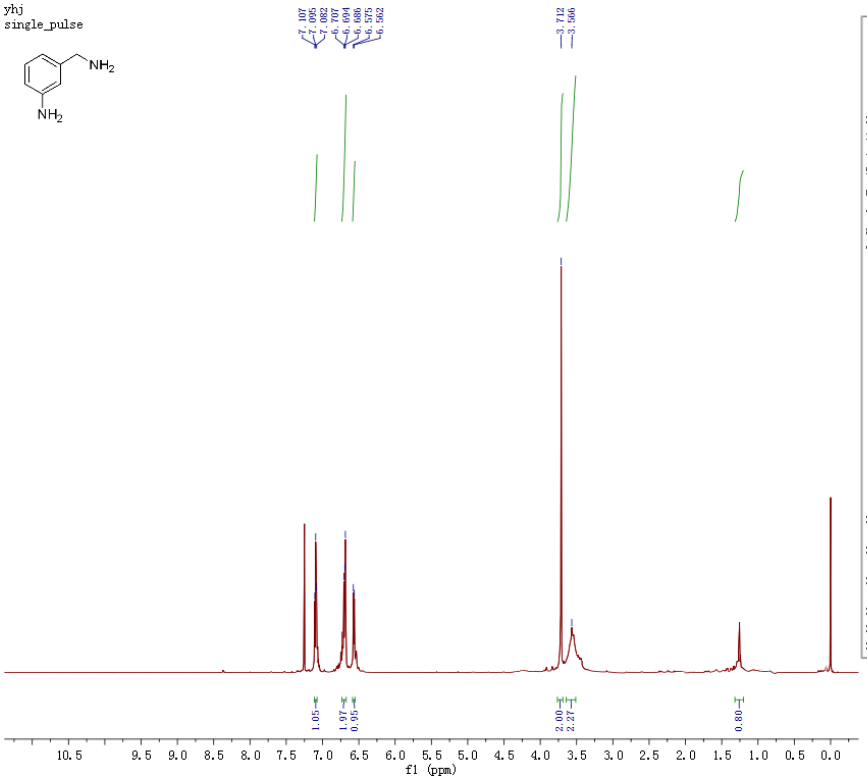
2 Title	yhj
3 Comment	
4 Origin	JEOL
5 Owner	
6 Site	
7 Spectrometer	ECA 600
8 Author	HappyNMR
9 Solvent	CHLOROFORM-D
10 Temperature	24.9
11 Pulse Sequence	single_pulse_dec
12 Experiment	1D
13 Number of Scans	211
14 Receiver Gain	56
15 Relaxation Delay	2.0000
16 Pulse Width	4.0833
17 Acquisition Time	0.6921
18 Acquisition Date	2018-05-17T14:02:37
19 Modification Date	2018-05-17T14:18:16
20 Spectrometer Frequency	150.91
21 Spectral Width	37876.8
22 Lowest Frequency	-3847.0
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	26214

yhj
single_pulse



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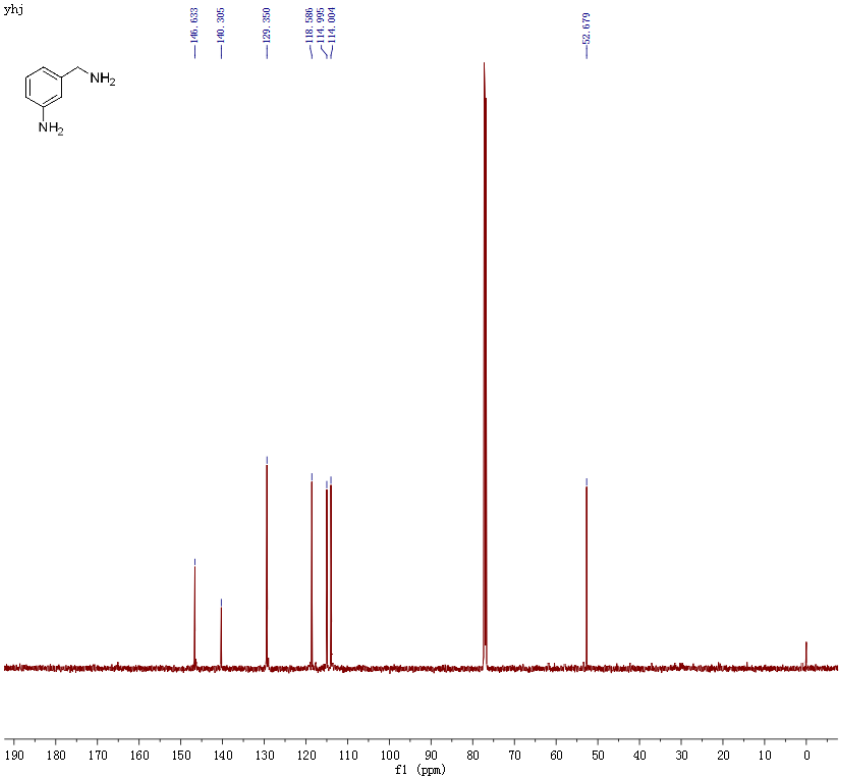
3	Comment	single_pulse
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	ECA 600
8	Author	HappyNMR
9	Solvent	CHLOROFORM-D
10	Temperature	23.6
11	Pulse Sequence	single_pulse.ex2
12	Experiment	1D
13	Number of Scans	16
14	Receiver Gain	38
15	Relaxation Delay	2.0000
16	Pulse Width	7.1000
17	Acquisition Time	2.9098
18	Acquisition Date	2018-05-22T12:04:52
19	Modification Date	2018-05-22T13:16:27
20	Spectrometer Frequency	600.17
21	Spectral Width	9008.5
22	Lowest Frequency	-303.1
23	Nucleus	1H
24	Acquired Size	32768
25	Spectral Size	26214

yhj



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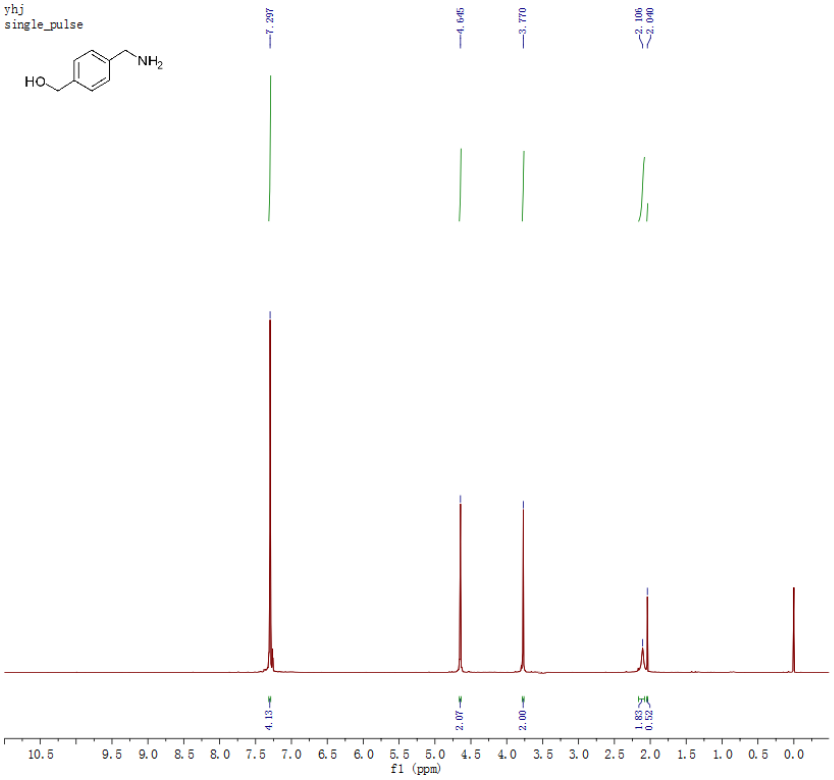
2	Title	yhj
3	Comment	
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	ECA 600
8	Author	HappyNMR
9	Solvent	CHLOROFORM-D
10	Temperature	24.3
11	Pulse Sequence	single_pulse_dec
12	Experiment	1D
13	Number of Scans	1024
14	Receiver Gain	58
15	Relaxation Delay	2.0000
16	Pulse Width	4.0833
17	Acquisition Time	0.6921
18	Acquisition Date	2018-05-22T12:02:53
19	Modification Date	2018-05-22T13:16:34
20	Spectrometer Frequency	150.91
21	Spectral Width	37876.8
22	Lowest Frequency	-3862.4
23	Nucleus	13C
24	Acquired Size	32768
25	Spectral Size	26214

yhj
single_pulse



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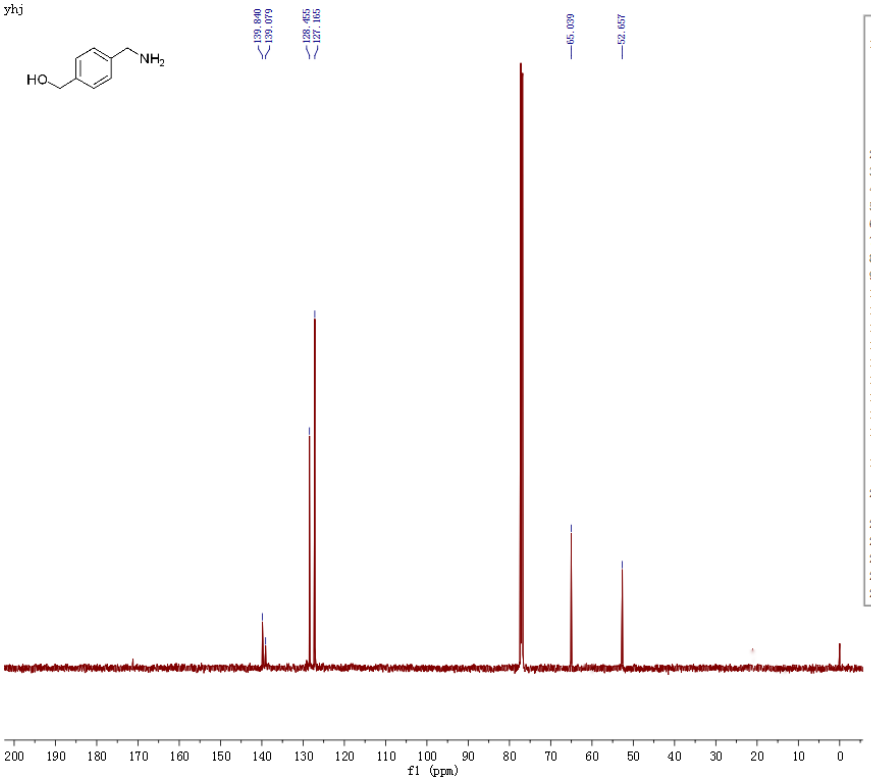
2 Title	yhj
3 Comment	single_pulse
4 Origin	JEOL
5 Owner	
6 Site	
7 Spectrometer	ECA 600
8 Author	HappyNMR
9 Solvent	CHLOROFORM-D
10 Temperature	23.6
11 Pulse Sequence	single_pulse.ex2
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	42
15 Relaxation Delay	2.0000
16 Pulse Width	7.1000
17 Acquisition Time	2.9098
18 Acquisition Date	2018-05-25T08:09:24
19 Modification Date	2018-05-25T08:26:06
20 Spectrometer Frequency	600.17
21 Spectral Width	9008.5
22 Lowest Frequency	-297.7
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	26214

yhj



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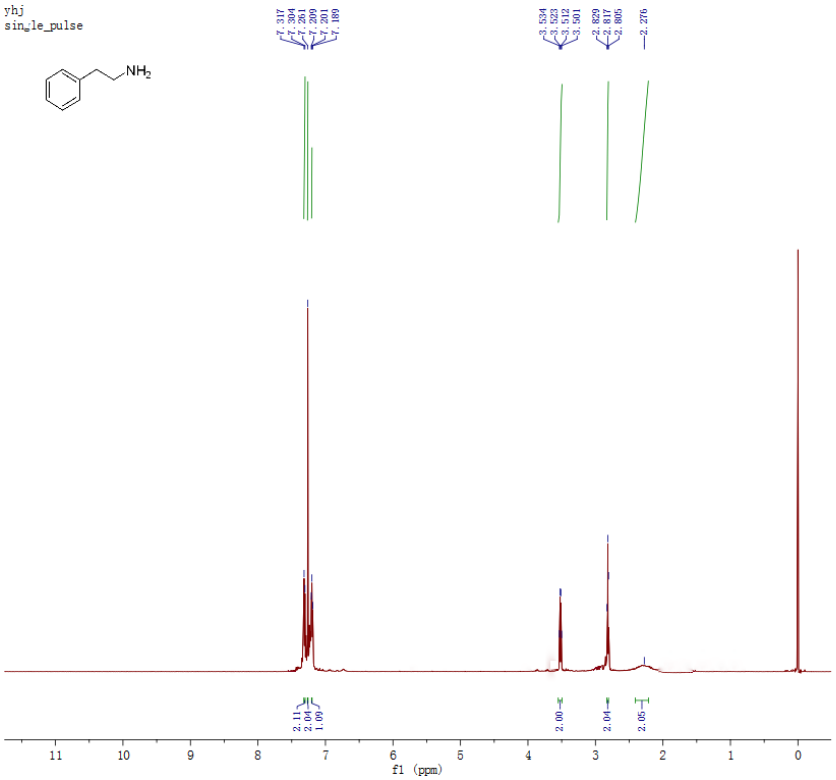
2 Title	yhj
3 Comment	
4 Origin	JEOL
5 Owner	
6 Site	
7 Spectrometer	ECA 600
8 Author	HappyNMR
9 Solvent	CHLOROFORM-D
10 Temperature	25.0
11 Pulse Sequence	single_pulse_dec
12 Experiment	1D
13 Number of Scans	813
14 Receiver Gain	58
15 Relaxation Delay	2.0000
16 Pulse Width	4.0833
17 Acquisition Time	0.6921
18 Acquisition Date	2018-05-25T08:46:30
19 Modification Date	2018-05-25T09:02:56
20 Spectrometer Frequency	150.91
21 Spectral Width	37876.8
22 Lowest Frequency	-3859.6
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	26214



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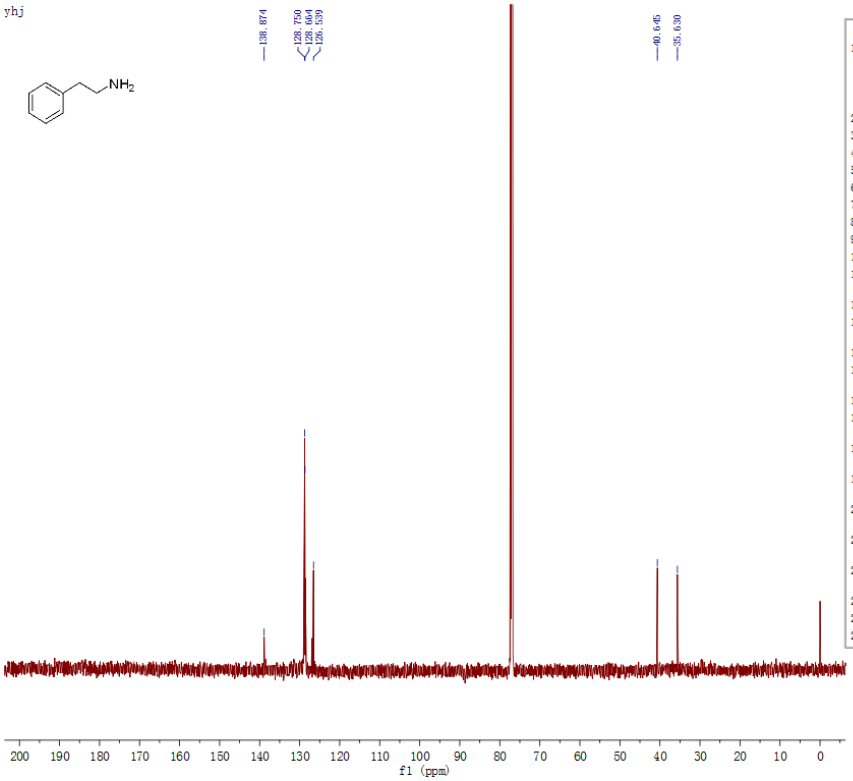
1	Data File Name	D:/ liulei/ 刘磊-12个氢谱12个碳谱/ 刘磊-12个氢谱12个碳谱/ lql-11-180521-16xia-H-single_pulse-3.jdf
2	Title	yhj
3	Comment	single_pulse
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	ECA 600
8	Author	HappyNMR
9	Solvent	CHLOROFORM-D
10	Temperature	23.1
11	Pulse Sequence	single_pulse.ex2
12	Experiment	1D
13	Number of Scans	16
14	Receiver Gain	44
15	Relaxation Delay	2.0000
16	Pulse Width	7.1000
17	Acquisition Time	2.9098
18	Acquisition Date	2018-05-23T12:53:32
19	Modification Date	2018-05-23T13:17:17
20	Spectrometer Frequency	600.17
21	Spectral Width	9008.5
22	Lowest Frequency	-296.5
23	Nucleus	1H
24	Acquired Size	32768
25	Spectral Size	26214



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2	Title	yhj
3	Comment	
4	Origin	JEOL
5	Owner	
6	Site	
7	Spectrometer	ECA 600
8	Author	HappyNMR
9	Solvent	CHLOROFORM-D
10	Temperature	24.5
11	Pulse Sequence	single_pulse_dec
12	Experiment	1D
13	Number of Scans	1024
14	Receiver Gain	58
15	Relaxation Delay	2.0000
16	Pulse Width	4.0833
17	Acquisition Time	0.6921
18	Acquisition Date	2018-05-23T13:40:06
19	Modification Date	2018-05-23T13:56:50
20	Spectrometer Frequency	150.91
21	Spectral Width	37876.8
22	Lowest Frequency	-3859.1
23	Nucleus	13C
24	Acquired Size	32768
25	Spectral Size	26214

Reference

1. R. Adam, C. B. Bheeter, J. R. Cabrero-Antonino, K. Junge, R. Jackstell and M. Beller, *Chemsuschem*, 2017, **10**, 842-846.
2. K. Tokmic, B. J. Jackson, A. Salazar, T. J. Woods and A. R. Fout, *J. Am. Chem. Soc.*, 2017, **139**, 13554-13561.
3. R. Adam, E. Alberico, W. Baumann, H.-J. Drexler, R. Jackstell, H. Junge and M. Beller, *Chem. Eur. J.*, 2016, **22**, 4991-5002.