Supporting Information for:

Aryl-Palladium-NHC complex: Efficient Phosphine-free Catalyst Precursors for the Carbonylation of Aryl Iodides with Amines or Alkynes

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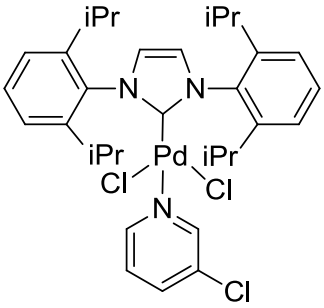
CONTENTS

1. General methods

All non-aqueous reactions and manipulations were using standard Schlenk techniques. All solvents were purchased from Alfa Aesar, and before use were dried and degassed by standard methods and stored under argon atmosphere. Aryl iodides were obtained from Alfa Aesar. Carbon monoxide (CO) with a purity of 99.99% was commercially available. All reactions were monitored by TLC with silica gel-coated plates. NMR spectra were recorded on BRUKER Avance III 400 MHz spectrometers. Chemical shifts were reported in parts per million (ppm) down field from TMS with the solvent resonance as the internal standard. Coupling constants (J) were reported in Hz and refered to apparent peak multiplications. High resolution mass spectra (HRMS) were recorded on Bruker MicroTOF-QII mass instrument (ESI) or Waters GCT Premier mass spectrometer (EI).

2. Synthesis of NHC palladium complexes

2.1 Synthesis of Pd(IPr)(3-Cl-pyridinyl)Cl_2 complex[1]

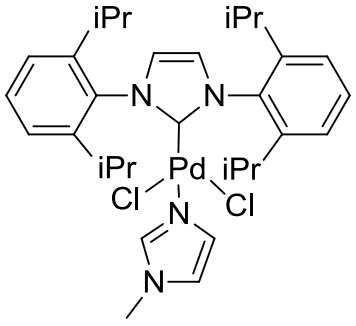


Under argon atmosphere, a mixture of $PdCl_2$ (1.0 mmol), IPr·HCl (1.2 mmol), and K_2CO_3 (5 mmol) and 3-Chloropyridine (6 mL) was stirred at 80 ℃ for 16 h. The solvent was removed under reduced pressure. **Pd(IPr)(3-Cl-pyridinyl)Cl_2** was obtained as a off-white crystalline solid (82% yield) after crystallization from DCM and pentane and drying in vacuum.

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.11 (d, *J* = 1.12, 12H), 1.47 (d, *J* = 1.42, 12H), 3.12-3.19 (m, 4H), 7.01-7.04 (m, 1H), 7.14 (s, 2H), 7.34-7.52 (m, 7H), 8.49-8.58 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 23.3, 26.4, 28.8, 124.1, 124.1, 124.4, 125.2, 130.4, 132.0, 135.0, 137.5, 146.7, 149.4, 150.4, 153.4.

2.2 Synthesis of IPr-Pd-Im-Cl_2 complex[2]



Under argon atmosphere, a mixture of compound IPr•HCl (1.1 mmol), $PdCl_2$ (1

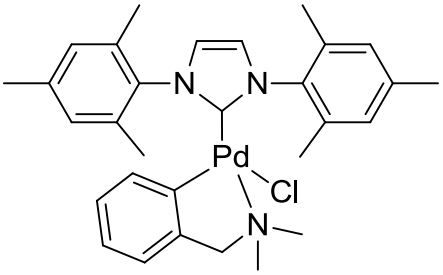
[1] O'Brien, C. J.; Kantchev, E. A. B.; Valente, C.; Hadei, N.;Chass, G. A.; Lough, A.; Hopkinson, A. C.; Organ, M. G. *Chem.−Eur. J.* 2006, **12**, 4743.
[2] L. Zhu, T. Gao, L.-X. Shao, *Tetrahedron* 2011, **67**, 5150.

mmol), K_2CO_3 (1.5 mmol), and 1-methylimidazole (4.0 ml) was stirred in anhydrous THF (5.0 mL) under reflux for 20 h. The solvent was removed under reduced pressure, and the residue was purified by aflash chromatography on silica gel (PE:EA=1:1). **IPr-Pd-Im-Cl$_2$** was obtained as a yellow crystalline solid (84% yield) .

^{1}H NMR (400 MHz, CDCl$_3$) δ 1.10 (d, *J* = 2.88, 12H), 1.46 (d, *J* = 6.64, 12H), 3.14-3.21 (m, 4H), 3.41 (s, 3H), 6.51 (s, 1H), 7.09-7.16 (m, 3H), 7.31-7.48 (m, 6H), 7.66 (s, 1H).

^{13}C NMR (100 MHz, CDCl$_3$) δ 23.2, 26.2, 28.6, 33.9, 119.0, 123.9, 124.8, 128.4, 130.0, 135.2, 138.3, 146.7, 156.5

2.3 Synthesis of IMes-Pd-dmba-Cl complex[3]



Under argon atmosphere, a mixture of compound $PdCl_2$ (1.0 mmol), *N*,*N*-dimethylbenzylamine (1.2 mmol) was stirred in CH_3CN (5 mL) under reflux until a clear, dark orange solution was formed and $PdCl_2$ was dissolved completely. Finely powdered K_2CO_3(2.5 mmol) was added in one portion, and the mixture was stirred until the solution changed color to bright canary yellow. IMes·HCl (1.1 mmol) was added in one portion, and the reflux continued for another 18 h. After cooling, the mixture was diluted DCM, the solvent was removed under reduced pressure. **IMes-Pd-dmba-Cl** was obtained as a white crystalline solid (67% yield).

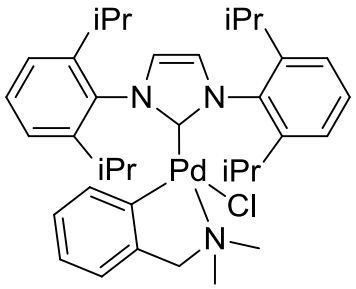
^{1}H NMR (400 MHz, CDCl$_3$) δ 2.21 (s, 6H), 2.27 (s, 6H), 2.42 (d, *J* = 2.43, 6H), 3.51

[3] G.-R. Peh, E. Assen, B. Kantchev, C. Zhang, J. Y. Ying, *Org. Biomol. Chem.*, 2009, **7**, 2110.

(s, 2H), 6.56-6.58 (m, 1H), 6.67-6.71 (m, 1H), 6.75-6.83 (m, 4H), 6.97 (s, 2H), 7.08 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 19.8, 20.3, 21.1, 50.0, 72.3, 121.2, 122.9, 123.2, 123.9, 128.7, 129.4, 133.9, 136.2, 137.4, 138.3, 138.3, 147.6, 149.3, 175.7.

2.4 Synthesis of IPr-Pd-dmba-Cl complex[4]



Under argon atmosphere, a mixture of compound $PdCl_2$ (1.0 mmol), *N*,*N*-dimethylbenzylamine (1.2 mmol) was stirred in CH_3CN (5 mL) under reflux until a clear, dark orange solution was formed and $PdCl_2$ was dissolved completely. Finely powdered K_2CO_3(2.5 mmol) was added in one portion, and the mixture was stirred until the solution changed color to bright canary yellow. IPr·HCl (1.1 mmol) was added in one portion, and the reflux continued for another 18 h. After cooling, the mixture was diluted DCM, the solvent was removed under reduced pressure. **IPr-Pd-dmba-Cl** was obtained as a white crystalline solid (78% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ 0.80 (d, *J* = 0.81, 6H), 1.01 (d, *J* = 1.02, 6H), 1.17 (d, *J* = 1.17, 6H), 1.48 (d, *J* = 1.48, 6H), 2.38 (s, 6H), 3.12-3.19 (m, 2H), 3.32-3.39 (m, 2H), 3.45 (s, 2H), 6.52-6.79 (m, 4H), 7.14-7.20 (m, 4H),7.29-7.41 (m, 4H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 23.2, 23.3, 26.2, 26.4, 28.3, 29.0, 49.8, 72.6, 121.5, 122.6, 123.7, 124.0, 124.5, 125.4, 129.7, 136.2, 136.2, 144.7, 147.8, 147.8, 150.6, 177.6.

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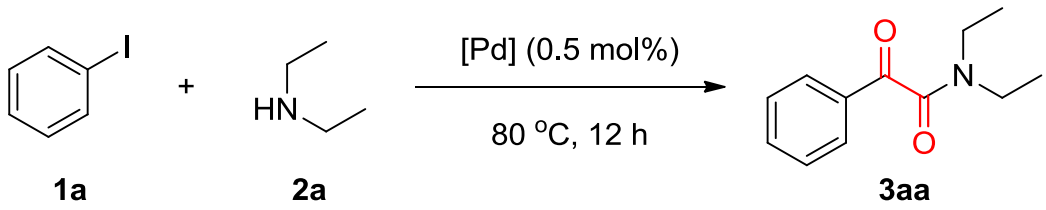
[4] E. Assen, B. Kantchev, J. Y. Ying, *Organometallics* 2009, **28**, 289.

3. General procedure for the carbonylation reaction

3.1 Screening Optimal Conditions



1a **2a** **3aa**

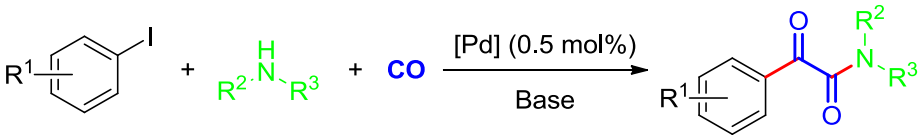
Entry	P_{CO} (MPa)	**1a**:**2a**	Base	Solvent	Yield (%)
1	0.1	1:5	K_2CO_3	dioxane	19
2	1	1:5	K_2CO_3	dioxane	27
3	2	1:5	K_2CO_3	dioxane	46
4	3	1:5	K_2CO_3	dioxane	81
5	4	1:5	K_2CO_3	dioxane	91 (0)[b]
6	**4**	**1:2**	**K_2CO_3**	**dioxane**	**92** (0)[c]
7	4	1:2	$NaHCO_3$	dioxane	17
8	4	1:2	$CsCO_3$	dioxane	88
9	4	1:2	DBU	dioxane	30
10	4	1:2	KO*t*Bu	dioxane	43
11	4	1:2	K_2CO_3	DMSO	76
12	4	1:2	K_2CO_3	toluene	21
13	4	1:2	K_2CO_3	EA	47
14	4	1:2	K_2CO_3	CH_3CN	45
15	4	1:2	K_2CO_3	THF	60
16	4	1:2	K_2CO_3	*t*-AmOH	52

[a] Reaction condition: **1a** (1.0 mmol), **2a**, [Pd] (0.5 mol%), Base (2.0 equiv), solvent (5.0 mL), CO, 80 °C, 12 h. Isolated yield.
[b] No IPr-Pd(dmba)Cl. [c] No K_2CO_3.

All carbonylation experiments were carried out in a 75 mL autoclave equipped with magnetic stirring and automatic temperature control. In a typical experiment, aryl iodides (1.0 mmol), IPr-Pd-dmba-Cl (0.5 mol%), base (2.0 mmol), amine and solvent (5.0 ml) were charged into the reactor in the presence of air. Then the autoclave was purged three times with carbon monoxide, pressurized with carbon monoxide to a pressure of 0.1 - 4.0 MPa. The autoclave was placed in an oil bath pre-heated at 80℃, and the whole reaction mixture was stirred for 12 hours. After

the reaction, the autoclave was cooled, and excess CO was discharged slowly at room temperature. The reaction mixture was qualitatively and quantitatively analyzed by GC-MS. The crude product was purified by column chromatography on silica gel to give the desired product.

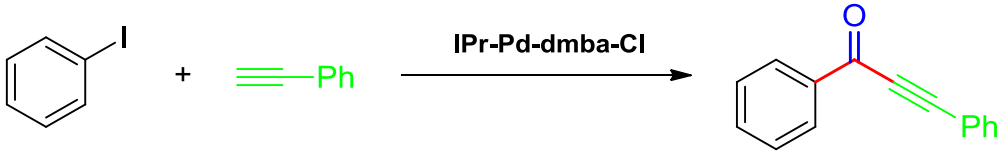
3.2 General procedure for the double carbonylation reaction



All carbonylation experiments were carried out in a 75 mL autoclave equipped with magnetic stirring and automatic temperature control. In a typical experiment, aryl iodides (1.0 mmol), IPr-Pd-dmba-Cl (0.5 mol%), K_2CO_3 (2.0 mmol), amine (2.0 mmmol) and 1,4-dioxane (5.0 ml) were charged into the reactor in the presence of air. Then the autoclave was purged three times with carbon monoxide, pressurized with carbon monoxide to a pressure of 4.0 MPa. The autoclave was placed in an oil bath pre-heated at 80℃, and the whole reaction mixture was stirred for 12 hours. After the reaction, the autoclave was cooled, and excess CO was discharged slowly at room temperature. The reaction mixture was qualitatively and quantitatively analyzed by GC-MS. The crude product was purified by column chromatography on silica gel to give the desired product.

3.3 Screening Optimal Conditions

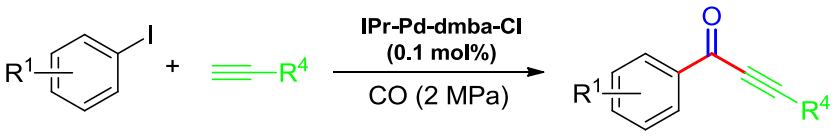
All carbonylation experiments were carried out in a 75 mL autoclave equipped with magnetic stirring and automatic temperature control. In a typical experiment, aryl iodides (1.0 mmol), alkynes (1.2 mmol), IPr-Pd-dmba-Cl, base (2.0 mmol) and solvent (5.0 ml) were charged into the reactor in the presence of air. Then the autoclave was purged three times with carbon monoxide, pressurized with carbon monoxide to a pressure of 1.0 – 4.0 MPa. The autoclave was placed in an oil bath pre-heated at 100 ℃, and the whole reaction mixture was stirred for 4 - 18 hours. After the reaction, the autoclave was cooled, and excess CO was discharged slowly at room temperature. The reaction mixture was qualitatively and quantitatively analyzed by GC-MS. The crude product was purified by column chromatography on silica gel to give the desired product.



Entry	P_{CO} (MPa)	[Pd]	t/h	Base (2 eq.)	Solvent (5 ml)	Yield (%)
1	1	0.2%	4	TEA	toluene	28
2	1	0.2%	6	TEA	toluene	35
3	1	0.2%	12	TEA	toluene	57
4	1	0.2%	14	TEA	toluene	76
5	1	0.2%	16	TEA	toluene	83
6	1	0.2%	18	TEA	toluene	88
7	2	0.2%	16	TEA	toluene	>99
8	3	0.2%	16	TEA	toluene	58
9	4	0.2%	16	TEA	toluene	38
10	2	0.1%	16	TEA	toluene	85
11	2	0.05%	16	TEA	toluene	57
12	**2**	**0.1%**	**18**	**TEA**	**toluene**	**98**
13	2	0.1%	18	DBU	toluene	42
14	2	0.1%	18	K_2CO_3	toluene	10
15	2	0.1%	18	$CsCO_3$	toluene	4
16	2	0.1%	18	CH_3COONa	toluene	23
17	2	0.1%	18	KO*t*Bu	toluene	37

18	2	0.1%	18	$NaHCO_3$	toluene	7
19	2	0.1%	18	DABCO	toluene	25
20	2	0.1%	18	TEA	CH3OH	NR
21	2	0.1%	18	TEA	CH3CN	96
22	2	0.1%	18	TEA	THF	68
23	2	0.1%	18	TEA	dioxane	84
24	2	0.1%	18	TEA	DMSO	5.5
25	2	0.1%	18	TEA	anisole	75
26	2	0.1%	18	TEA	EA	10
27	2	0.1%	18	TEA	DCM	20

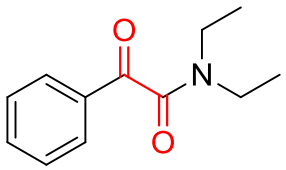
3.4 General procedure for the carbonylation reaction



All carbonylation experiments were carried out in a 75 mL autoclave equipped with magnetic stirring and automatic temperature control. In a typical experiment, aryl iodides (1.0 mmol), alkynes (1.2 mmol), IPr-Pd-dmba-Cl (0.1 mol%), Et_3N (2.0 mmol) and toluene (5.0 ml) were charged into the reactor in the presence of air. Then the autoclave was purged three times with carbon monoxide, pressurized with carbon monoxide to a pressure of 2.0 MPa. The autoclave was placed in an oil bath pre-heated at 100 ℃, and the whole reaction mixture was stirred for 18 hours. After the reaction, the autoclave was cooled, and excess CO was discharged slowly at room temperature. The reaction mixture was qualitatively and quantitatively analyzed by GC-MS. The crude product was purified by column chromatography on silica gel to give the desired product.

4. Experimental characterization data of products

N,N-diethyl-2-oxo-2-phenylacetamide (3aa):



3aa

Yellow oil, 92% yield.

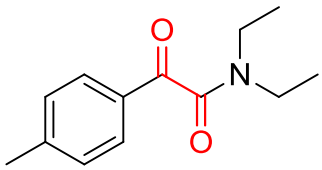
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.03 (t, *J* = 7.12, 3H), 1.17 (t, *J* = 7.16, 3H), 3.11 (dd, J_1 = 14.2, J_2 = 7.08, 2H), 3.43 (dd, J_1 = 14.3, J_2 = 7.16, 2H), 7.37-7.41 (m, 2H), 7.50-7.54 (m, 1H), 7.81-7.83 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 12.6, 13.8, 38.5, 41.9, 128.7, 129.3, 133.0, 134.4, 166.5, 191.4.

HRMS (ESI) calcd. for $C_{12}H_{15}NO_2$ [M+H]: 206.1176, found: 206.1177.

IR (KBr, cm^{-1}) 2977, 2362, 1638, 1443, 1240, 855, 725.

N,N-diethyl-2-oxo-2-(p-tolyl)acetamide (3ba):



3ba

Yellow oil, 79% yield.

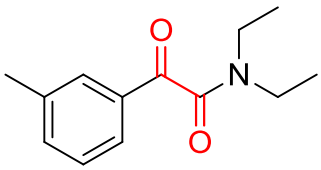
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.12-1.16 (m, 3H), 1.26-1.30 (m, 3H), 2.42 (s, 3H), 3.20-3.24 (m, 2H), 3.52-3.58 (m, 2H), 7.29 (d, *J* = 7.36, 2H), 7.81-7.84 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 12.5, 13.8, 21.5, 38.4, 41.8, 76.7, 77.0, 77.3, 129.4, 129.4, 130.5, 145.5, 166.7, 191.1.

HRMS (ESI) calcd. for $C_{13}H_{17}NO_2$ [M+H]: 220.1332, found: 220.1326.

IR (KBr, cm^{-1}) 2970, 1638, 1435, 1246, 868, 737.

N,N-diethyl-2-oxo-2-(m-tolyl)acetamide (3ca):



3ca

Yellow oil, 73% yield.

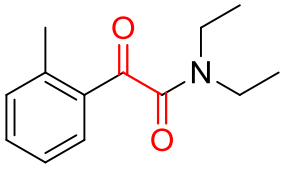
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.04 (t, *J* = 7.12, 3H), 1.83 (t, *J* = 7.16, 3H), 2.30 (s, 3H), 3.10 (dd, J_1 = 14.2, J_2 = 7.28, 2H), 3.43 (dd, J_1 = 14.3, J_2 = 7.16, 2H), 7.27-7.35 (m, 2H), 7.61-7.65 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 12.8, 14.0, 21.2, 38.7, 42.1, 126.9, 128.8, 129.8, 133.2, 135.4, 138.8, 166.8, 191.8.

HRMS (ESI) calcd. for $C_{13}H_{17}NO_2$ [M+Na]: 242.1151, found: 242.1161.

IR (KBr, cm^{-1}) 2936, 2349, 1638, 1442, 1207, 959, 718.

N,N-diethyl-2-oxo-2-(o-tolyl)acetamide (3da):



3da

Yellow oil, 95% yield.

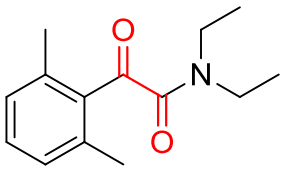
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.01-1.05 (m, 3H), 1.12-1.16 (m, 3H), 2.53 (s, 3H), 3.10 (dd, J_1 = 14.1, J_2 = 7.04, 2H), 3.39 (dd, J_1 = 14.3, J_2 = 7.12, 2H), 7.15-7.10 (m, 2H), 7.31-7.36 (m, 1H), 7.57 (d, *J* = 7.68, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 12.2, 13.4, 21.3, 38.3, 41.7, 125.7, 131.2, 132.1, 133.1, 140.8, 167, 119.3.

HRMS (ESI) calcd. for $C_{13}H_{17}NO_2$ [M+Na]: 242.1151, found: 242.1156.

IR (KBr, cm^{-1}) 2970, 2342, 1645, 1456, 1220, 868, 737.

2-(2,6-dimethylphenyl)-N,N-diethyl-2-oxoacetamide (3ea):



3ea

Yellow oil, 12% yield

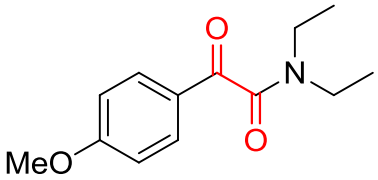
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.21 (t, *J* = 7.16, 3H), 1.32 (t, *J* = 7.04, 3H), 2.34 (s, 6H), 3.44-3.51 (m, 4H), 7.03 (d, *J* = 7.56, 2H), 7.20-7.26 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ12.0, 13.9, 20.1, 39.7, 42.3, 128.6, 130.6, 136.7, 166.1, 195.1.

HRMS (ESI) calcd. for $C_{14}H_{19}NO_2$ [M+Na]: 256.1308, found: 256.1310.

IR (KBr, cm^{-1}) 2963, 1638, 1475, 1220, 868, 776.

N,N-diethyl-2-(4-methoxyphenyl)-2-oxoacetamide (3fa):



3fa

Yellow oil, 78% yield.

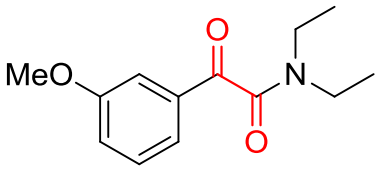
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.10 (t, *J* = 7.12, 3H), 1.23 (t, *J* = 7.16, 3H), 3.17 (dd, J_1 = 14.2, J_2 = 7.08, 2H), 3.48 (dd, J_1 = 14.4, J_2 = 7.20, 2H), 3.83 (s, 3H), 6.92-6.94 (m, 2H), 7.84-7.87 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 12.7, 14.0, 38.6, 42.0, 55.5, 76.7, 77.0, 77.3, 114.1, 126.2, 131.9, 164.6, 167.0, 190.3.

HRMS (ESI) calcd. for C13H17NO3 [M+Na]: 270.1107 found: 270.1103.

IR (KBr, cm^{-1}) 2930, 2349, 1638, 1384, 1285, 1142, 679.

N,N-diethyl-2-(3-methoxyphenyl)-2-oxoacetamide (3ga):



3ga

Yellow oil, 70% yield.

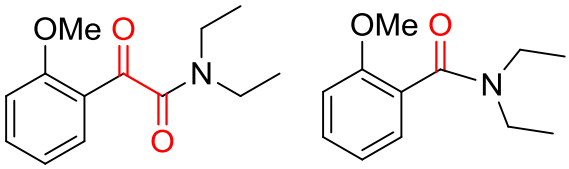
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.07 (t, *J* = 7.12, 3H), 1.21 (t, *J* = 7.16, 3H), 3.13 (dd, J_1 = 14.2, J_2 = 7.08, 2H), 3.45 (dd, J_1 = 14.3, J_2 = 7.16, 2H), 3.77 (s, 3H), 7.09-7.11 (m, 1H), 7.31 (d, *J* = 8.00, 1H), 7.35-7.41 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 12.7, 14.0, 38.7, 42.1, 55.4, 112.8, 121.4, 122.6, 130.0, 134.5, 156.0, 166.7, 191.5.

HRMS (ESI) calcd. for $C_{13}H_{17}NO_3$ [M+Na]: 258.1101, found: 258.1111.

IR (KBr, cm^{-1}) 2982, 2362, 1638, 1500, 1240, 868, 607.

N,N-diethyl-2-(2-methoxyphenyl)-2-oxoacetamide (3ha):



3ha **3ha'**

Yellow oil, 98% yield (10:1).

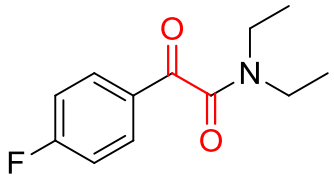
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.07 (t, *J* = 7.12, 3H), 1.21 (t, *J* = 7.16, 3H), 3.13 (dd, J_1 = 14.2, J_2 = 7.08, 2H), 3.45 (dd, J_1 = 14.3, J_2 = 7.16, 2H), 3.77 (s, 3H), 7.09-7.11 (m, 1H), 7.31 (d, *J* = 8.00, 1H), 7.35-7.41 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 12.7, 14.0, 38.7, 42.1, 55.4, 112.8, 121.4, 122.6, 130.0, 134.5, 156.0, 166.7, 191.5.

HRMS (ESI) calcd. for $C_{13}H_{17}NO_3$ [M+Na]: 258.1101, found: 258.1100.

IR (KBr, cm^{-1}) 2989, 2356, 1645, 1442, 1285, 1024, 764.

N,N-diethyl-2-(4-fluorophenyl)-2-oxoacetamide (3ia):



3ia

Yellow solid , 95% yield, M.P. 98℃.

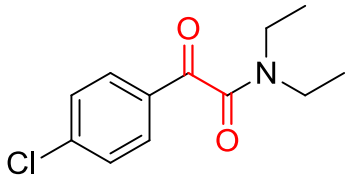
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.14 (t, *J* = 7.12, 3H), 1.28 (t, *J* = 7.16, 3H), 3.22 (dd, J_1 = 14.2, J_2 = 7.08, 2H), 3.53 (dd, J_1 = 14.3, J_2 = 7.16, 2H), 7.18-7.22 (m, 2H), 7.97-7.80 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 12.4, 13.7, 38.5, 41.8, 115.8, 116.0, 129.4, 129.5, 132.0, 132.1, 164.9, 166.1, 167.4, 189.6..

HRMS (ESI) calcd. for $C_{12}H_{14}FNO_2$ [M+Na]: 246.0901, found: 246.0905.

IR(KBr, cm^{-1}) 2982, 1625, 1505, 1234, 875, 620.

2-(4-chlorophenyl)-N,N-diethyl-2-oxoacetamide (3ja):



3ja

Yellow oil, 97% yield.

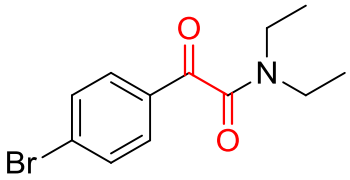
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.02 (t, *J* = 7.08, 3H), 1.15 (t, *J* = 7.4, 3H), 3.10 (dd, J_1 = 14.16, J_2 = 7.08, 2H), 3.42 (dd, J_1 = 14.32, J_2 = 7.16, 2H), 7.37-7.39 (m, 2H), 7.77-7.79 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 12.5, 13.8, 38.6, 41.8, 76.7, 77.0, 77.3, 129.0, 130.6, 131.3, 140.7, 165.9, 189.8.

HRMS (ESI) calcd. for $C_{12}H_{14}ClNO_2$ [M+Na]: 262.0605, found: 262.0610.

IR (KBr, cm^{-1}) 3334, 1651, 1442, 1312, 1063, 692.

2-(4-bromophenyl)-N,N-diethyl-2-oxoacetamide (3ka):



3ka

Yellow solid, 87% yield.

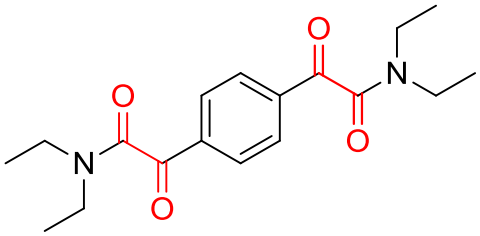
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.09-1.13 (m, 3H), 1.22-1.26 (m, 3H), 3.16-3.22 (m, 2H), 3.48-3.54 (m, 2H), 7.60-7.63 (m, 2H), 7.75-7.78 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 12.7, 14.1, 38.8, 42.0, 129.9, 130.9, 131.9, 132.2, 166.0, 190.2.

HRMS (ESI) calcd. for $C_{12}H_{14}BrNO_2$ [M+Na]: 284.0281, found: 284.0279.

IR (KBr, cm^{-1}) 2982, 1638, 1579, 1227, 1070, 764.

2,2'-(1,4-phenylene)bis(N,N-diethyl-2-oxoacetamide) (3ka'):



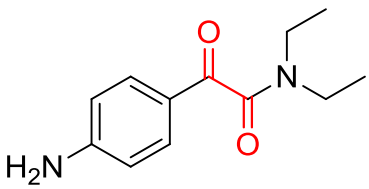
3ka'

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.13-1.13(m, 12H), 3.22 (dd, J_1 = 15.04, J_2 = 5.24, 4H), 3.55 (dd, J_1 = 15.04, J_2 = 5.24, 4H), 8.07 (s, 4H),

^{13}C NMR (100 MHz, $CDCl_3$) δ 12.8, 14.2, 39.1, 42.2, 130.0, 137.3, 165.9, 190.3.

12.8, 14.2, 39.1, 42.2, 130.0, 137.3, 165.9, 190.3.

2-(4-aminophenyl)-N,N-diethyl-2-oxoacetamide (3ma):



3ma

Yellow solid , 16% yield, M.P. 38℃.

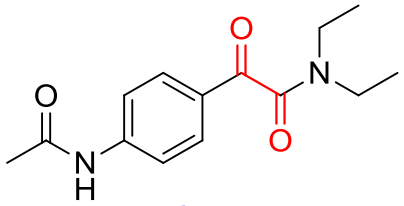
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.12 (t, J = 7.12, 3H), 1.25 (t, J = 7.16, 3H), 3.21 (dd, J_1 = 14.16, J_2 = 7.08, 2H), 3.51 (dd, J_1 = 14.32, J_2 = 7.16, 2H), 4.37 (s, 2H), 6.63 (d, J = 8.72, 2H), 7.72 (d, J = 8.60, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ12.9, 14.1, 38.6, 42.1, 113.9, 123.5, 132.3, 152.6, 167.6, 190.0.

HRMS (ESI) calcd. for $C_{12}H_{16}N_2O_2$ [M+H]: 221.1285, found: 221.1281.

IR (KBr, cm^{-1}) 3354, 2936, 1579, 1253, 1148, 750, 620.

2-(4-acetamidophenyl)-N,N-diethyl-2-oxoacetamide (3oa):



3oa

Yellow solid , 47% yield, M.P. 42℃.

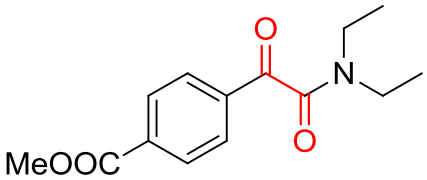
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.13 (t, J = 7.12, 3H), 1.26 (t, J = 7.20, 3H), 3.22 (dd, J_1 = 14.16, J_2 = 7.08, 2H), 3.52 (dd, J_1 = 14.72, J_2 = 7.2, 2H), 3.88 (s, 3H), 6.96 dd, J_1 = 7.00, J_2 = 1.88, 2H), 7.89 (dd, J_1 = 6.96, J_2 = 1.88, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 12.7, 14.0, 38.6, 42.0, 55.5, 114.1, 126.2, 131.9, 164.6, 166.9, 190.3.

HRMS (ESI) calcd. for $C_{14}H_{18}N_2O_3$ [M+Na]: 285.1210, found: 285.1214.

IR (KBr, cm^{-1}) 2963, 1592, 1468, 1267, 1070, 750.

methyl 4-(2-(diethylamino)-2-oxoacetyl)benzoate (3pa):



3pa

Pale yellow solid , 98% yield, M.P. 48℃.

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.13 (t, J = 7.04, 3H), 1.26 (t, J = 6.44, 3H), 3.20 (dd,

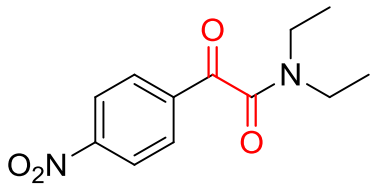
J_1 = 14.16, J_2 = 7.04, 2H), 3.53 (dd, J_1 = 14.28, J_2 = 7.12, 2H), 3.94 (s, 3H), 7.98 (d, J = 8.04, 2H), 8.13 (d, J = 8.2, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 12.8, 14.1, 38.9, 42.1, 52.5, 129.5, 130.0, 135.0, 136.4, 165.9, 166.1, 190.6.

HRMS (ESI) calcd. for $C_{18}H_{18}NO_4$ [M+Na]: 286.1047, found: 286.1050.

IR (KBr, cm^{-1}) 2982, 1722, 1632, 1468, 1285, 1102, 725.

N,N-diethyl-2-(4-nitrophenyl)-2-oxoacetamide (3oa):



3qa

Pale red oil, 58% yield.

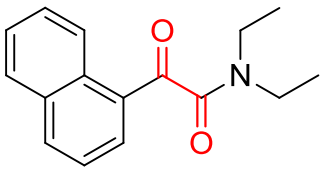
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.16 (t, J = 7.08, 3H), 1.27 (t, J = 7.2, 3H), 3.23 (dd, J_1 = 14.16, J_2 = 7.08, 2H), 3.55 (dd, J_1 = 14.36, J_2 = 6.64, 2H), 8.10-8.14 (m, 2H), 8.32-8.36 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 12.8, 14.3, 39.3, 42.3, 124.1, 130.7, 137.7, 151.0, 165.4, 189.1.

HRMS (ESI) calcd. for $C_{11}H_{15}N_2O_3$ [M+Na]: 245.0908, found: 245.0897.

IR (KBr, cm^{-1}) 2976, 1632, 1449, 1240, 848, 711.

N,N-diethyl-2-(naphthalen-1-yl)-2-oxoacetamide (3pa):



3ra

Yellow oil, 92% yield.

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.09 (t, J = 7.08, 3H), 1.25 (t, J = 7.2, 3H), 3.22 (dd, J_1 = 14.16, J_2 = 7.08, 2H), 3.51 (dd, J_1 = 14.32, J_2 = 7.16, 2H), 7.47-7.66 (m, 3H),

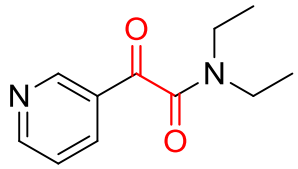
7.84-8.05 (m, 3H), 9.30 (d, *J* = 8.6, 3H),.

^{13}C NMR (100 MHz, $CDCl_3$) δ 12.5, 13.7, 38.6, 42.0, 124.3, 125.5, 126.7, 128.3, 128.5, 128.9, 130.7, 133.8, 134.0, 135.5, 167.0, 193.9.

HRMS (ESI) calcd. for $C_{16}H_{17}NO_2$ [M+Na]: 278.1151, found: 278.1156.

IR (KBr, cm^{-1}) 3334, 2930, 1625, 1442, 1213, 1018, 750.

N,N-diethyl-2-oxo-2-(pyridin-3-yl)acetamide (3qa):



3sa

Yellow oil, 92% yield.

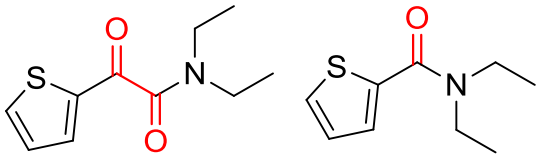
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.06-1.10 (m, 3H), 1.16-1.20 (m, 3H), 3.15-3.21 (m, 2H), 3.44-3.50 (m, 2H), 7.38-7.42 (m, 1H), 8.13 (t, *J* = 1.56, 1H), 8.73 (t, *J* = 8.08, 1H), 9.01 (s, 1H),.

^{13}C NMR (100 MHz, $CDCl_3$) δ 12.4, 13.8, 38.7, 41.8,123.5, 128.4, 136.2, 150.7, 154.2, 165.2, 189.6.

HRMS (ESI) calcd. for $C_{11}H_{14}N_2O_2$ [M+Na]: 229.0945, found:229.0947.

IR (KBr, cm^{-1}) 2976, 1632, 1423, 1018, 855, 692

N,N-diethyl-2-oxo-2-(thiophen-2-yl)acetamide (3ra):



3ua **3ua'**

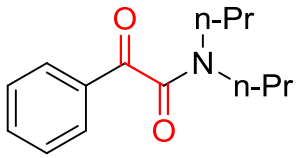
Yellow oil, >99% yield (9:1).

^{1}H NMR (400 MHz, $CDCl_3$) δ 1.16-1.28 (m, 7.68H), 3.29-3.50 (m, 2.12H), 3.51-3.57 (m, 2.93H), 7.03-7.05 (m, 0.17H), 7.17-7.19 (m, 1H), 7.32 (d, *J* = 1.56, 0.18H), 7.42 (d, *J* = 8.08, 0.16H), 7.76-7.81 (m, 1.94H),.

^{13}C NMR (100 MHz, $CDCl_3$) δ 12.4, 13.9, 38.9, 42.1 126.5, 127.6, 127.9, 128.4, 135.7, 136.0, 138.0, 140.2, 163.5, 165.4, 183.5.

HRMS (ESI) calcd. for $C_{14}H_{18}N_2O_3$ [M+Na]: 285.1210, found: 285.1214.

2-oxo-2-phenyl-N,N-dipropylacetamide (3ab):



3ab

Yellow oil, 85% yield .

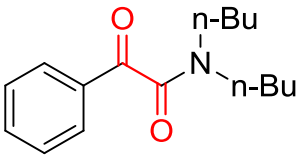
^{1}H NMR (400 MHz, $CDCl_3$) δ 0.66 (t, *J* = 7.44, 3H), 0.88 (t, *J* = 7.44, 3H), 1.45 (t, *J* = 7.52, 2H), 1.59 (t, *J* = 7.52, 2H), 3.00-3.05 (m, 2H), 3.35-3.90 (m, 2H), 7.38-7.42 (m, 2H), 7.50-7.55 (m, 1H), 7.83-7.85 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 10.7, 11.1, 20.3, 21.5, 45.5, 49.0, 128.7, 129.3, 133.1, 134.3, 166.9, 191.3.

HRMS (ESI) calcd. for $C_{14}H_{19}NO_2$ [M+Na]: 256.1308, found: 256.1321.

IR (KBr, cm^{-1}) 2963, 2356, 1638, 1442, 1213, 847, 725.

N,N-dibutyl-2-oxo-2-phenylacetamide (3ac):



3ac

Yellow oil, 84% yield .

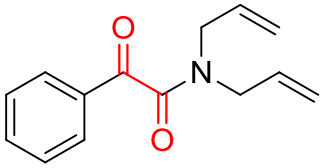
^{1}H NMR (400 MHz, $CDCl_3$) δ 0.79 (t, *J* = 7.4, 3H), 0.92 (t, *J* = 7.4, 3H), 1.14-1.123 (m, 2H), 1.37-1.46 (m, 2H), 1.50-1.58 (m, 2H), 1.66-1.69 (m, 2H), 7.48-7.52 (m, 2H), 7.61-7.64 (m, 1H), 7.92-7.95 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 13.3, 13.6, 19.5, 20.0, 29.2, 30.4, 43.8, 47.2, 128.7, 129.3, 133.1, 134.3, 166.9, 191.4.

HRMS (ESI) calcd. for $C_{12}H_{16}NO_2$ [M+Na]: 228.1006, found: 228.0995.

IR (KBr, cm^{-1}) 2956, 2349, 1638, 1449, 1213, 947, 725.

N,N-diallyl-2-oxo-2-phenylacetamide (3ad):



3ad

Yellow oil, 82% yield .

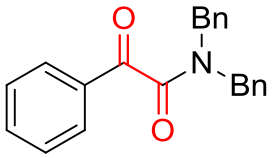
^{1}H NMR (400 MHz, $CDCl_3$) δ 3.80-3.82 (m, 2H), 4.13-4.16 (m, 2H), 5.14-5.30 (m, 4H), 5.67-5.90 (m, 2H), 7.49-7.53 (m, 2H), 7.62-7.66 (m, 1H), 7.94-7.96 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 45.9, 49.4, 118.7, 119.4, 129.0, 129.7, 131.8, 132.1, 133.1, 134.7, 167.0, 191.2.

HRMS (ESI) calcd. for $C_{14}H_{15}NO_2$ [M+Na]: 229.1110, found:229.1114.

IR (KBr, cm^{-1}) 2917, 2356, 1651, 1442, 1201, 933, 731.

N,N-dibenzyl-2-oxo-2-phenylacetamide (3ae):



3ae

Yellow oil, 63% yield.

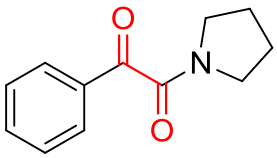
^{1}H NMR (400 MHz, $CDCl_3$) δ 4.28 (s, 2H), 4.62 (s, 2H), 7.24-7.41 (m, 10H), 7.49-7.53 (m, 2H), 7.62-7.64 (m, 1H), 7.98-8.01 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 46.0, 50.1, 127.9, 128.2, 128.3, 128.7, 128.8, 128.9, 129.0, 129.8, 133.3, 134.7, 134.8, 135.9, 167.5, 191.3.

HRMS (ESI) calcd. for $C_{22}H_{19}N_3O_4$ [M+Na]: 352.1308, found: 352.1308.

IR (KBr, cm^{-1}) 2924, 2342, 1971, 1632, 1449, 1207, 947, 698.

1-phenyl-2-(pyrrolidin-1-yl)ethane-1,2-dione (3af):



3af

Yellow oil, 69% yield.

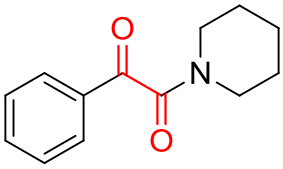
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.91-1.96 (m, 4H), 3.39 (t, *J* = 6.6, 2H), 3.62 (t, *J* = 6.6, 2H), 7.48-7.52 (m, 2H), 7.61-7.65 (m, 1H), 7.97-7.80 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 23.6, 25.5, 44.9, 46.3, 128.6, 129.5, 132.5, 134.3, 164.6, 191.3.

HRMS (ESI) $C_{12}H_{14}NO_2$ [M+Na]: 226.0850, found: 226.0838.

IR (KBr, cm^{-1}) 2911, 2632, 1632, 1449, 1246, 731, 658.

1-phenyl-2-(piperidin-1-yl)ethane-1,2-dione (3ag):



3ag

Yellow oil, 48% yield.

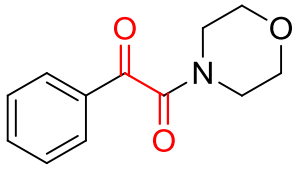
^{1}H NMR (400 MHz, $CDCl_3$) δ 1.45 (s, 2H), 1.60-1.61 (m, 4H), 3.19 (t, *J* = 5.56, 2H), 3.62 (s, 2H), 7.41-7.45 (m, 2H), 7.5-7.58 (m, 1H), 7.86 (d, *J* = 7.24, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 24.1, 25.2, 25.9, 41.8, 46.7, 128.8, 129.2, 132.9, 134.4, 165.2, 191.7.

HRMS (ESI) calcd. for $C_{13}H_{16}NO_2$ [M+Na]: 240.1003, found: 240.0995.

IR (KBr, cm^{-1}) 2943, 1652, 1449, 1220, 972, 718.

1-morpholino-2-phenylethane-1,2-dione (3ah):



3ah

Yellow oil, 92% yield.

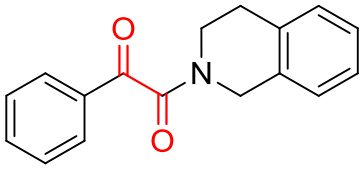
^{1}H NMR (400 MHz, $CDCl_3$) δ 3.24-3.26 (m, 2H), 3.50-3.53 (m, 2H), 3.66 (s, 4H), 7.39-7.43 (m, 2H), 7.52-7.56 (m, 1H), 7.83-7.85 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 41.2, 45.8, 66.2, 66.3, 128.7, 129.2, 132.6, 134.6, 165.0, 190.8.

HRMS (ESI) calcd. for $C_{12}H_{14}NO_3$ [M+Na]: 242.0791, found: 242.0788.

IR (KBr, cm^{-1}) 2851, 1651, 1456, 1227, 1116, 992, 711.

1-(3,4-dihydroisoquinolin-2(1H)-yl)-2-phenylethane-1,2-dione (3ai):



3ai

Yellow oil, 66% yield.

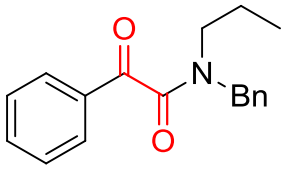
^{1}H NMR (400 MHz, $CDCl_3$) δ 2.85-2.88 (m, 1.3H), 2.99-3.02 (m, 0.73H), 3.62-3.64 (m, 1.29H), 3.98-4.01 (m, 0.73H), 4.54 (s, 0.70H), 4.92 (s, 1.28H), 6.93-6.95 (m, 0.36H), 7.11-7.26 (m, 3.87H), 7.54-7.47 (m, 1.96H), 7.61-7.68 (m, 0.98H), 7.94-7.99 (m, 1.88H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 126.1, 126.6, 126.7, 126.9, 126.9, 127.3, 128.9, 129.0, 129.1, 129.1, 129.7, 129.8, 131.6, 131.8, 133.1, 133.1, 133.4, 134.2, 134.8, 134.9, 165.8, 166.1, 191.4, 191.5.

HRMS (ESI) calcd. for $C_{17}H_{16}NO_2$ [M+Na]: 288.0999, found: 288.0995.

IR (KBr, cm^{-1}) 2911, 1645, 1442, 1207, 901, 725.

N-benzyl-2-oxo-2-phenyl-N-propylacetamide (3aj):



3aj

Yellow oil, 53% yield.

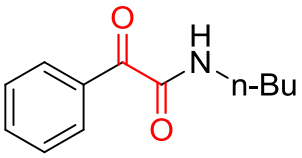
^{1}H NMR (400 MHz, $CDCl_3$) δ 0.72-0.76 (m, 1.75H), 0.93-0.97 (m,1.39H), 1.53-1.69 (m, 2.13H), 3.05-3.09 (m, 1.17H), 3.39-3.41 (m, 0.93H), 4.39 (s, 0.93H), 4.76 (s, 1.18H), 7.26-7.38 (m, 5.06H), 7.48-7.52 (m, 2.06H), 7.60-7.65 (m, 1.03H), 7.95-7.99 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 11.0, 11.4, 20.2, 21.3, 45.3, 46.9, 48.6, 51.1, 127.8, 127.9, 128.1, 128.3, 128.8, 128.8, 129.0, 129.0, 129.7, 129.7, 133.3, 134.6, 134.7, 135.3, 136.4, 167.3, 167.5, 191.3, 191.6.

HRMS (ESI) calcd. for $C_{18}H_{20}NO_2$ [M+Na]: 304.1311, found: 304.1308.

IR (KBr, cm^{-1}) 2969, 2362, 1651, 1442, 1220, 958, 731.

***N*-butyl-2-oxo-2-phenylacetamide (3ak):**



3ak

Yellow oil, 83% yield.

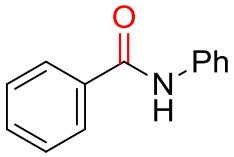
^{1}H NMR (400 MHz, $CDCl_3$) δ 0.91 (t, J = 7.32, 3H), 1.35 (dd, J_1 = 15.04, J_2 = 5.24, 2H), 1.53-1.58 (m, 2H), 3.34 (dd, J_1 = 13.44, J_2 = 7.04, 2H), 7.31 (br, 1H), 7.42-7.50 (m, 2H), 7.56-7.60 (m, 1H), 8.28-8.30 (m, 2H),

^{13}C NMR (100 MHz, $CDCl_3$) δ 13.7, 20.0, 31.3, 39.1, 128.4, 131.0, 133.4, 134.3, 162.1, 188.1.

HRMS (ESI) calcd. for $C_{14}H_{18}N_2O_3$ [M+Na]: 199.1210, found: 199.1214.

IR (KBr, cm^{-1}) 2963, 2356, 1631, 1449, 1207, 947, 725.

***N*-phenylbenzamide (3al):**



3al

Yellow solid, 31% yield, M.P. 52℃.

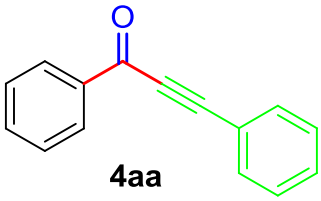
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.06-7.19 m, 1H), 7.27-7.23 (m, 2H), 7.45-7.49 (m, 3H), 7.56-7.58 (m, 2H), 7.78-7.81 (m, 3H),

^{13}C NMR (100 MHz, $CDCl_3$) δ 120.2, 124.6, 127.0, 128.8, 129.1, 131.8, 135.0, 137.9, 165.8.

HRMS (ESI) calcd. for $C_{13}H_{11}NO$ [M+Na]: 220.0743, found: 220.0733.

IR (KBr, cm^{-1}) 3348, 1664, 1442, 1318, 1024, 685.

1,3-diphenylprop-2-yn-1-one (4aa):



4aa

White solid, 98% yield, M.P. 43℃.

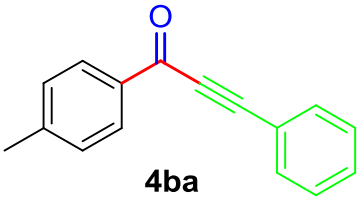
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22-8.24(m, 2H), 7.61-7.70 (m, 3H), 7.26-7.54 (m, 5H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 86.9, 93.1, 120.1, 128.6, 128.7, 129.6, 130.8, 133.1, 134.1, 136.9, 178.0.

HRMS (ESI) calcd. for $C_{15}H_{11}O$ [M+H]: 207.0804, found: 207.0804.

IR (KBr, cm^{-1}) 2203, 1644, 1254, 1002, 755.

3-phenyl-1-(p-tolyl)prop-2-yn-1-one (4ba):



4ba

Yellow oil, 82% yield .

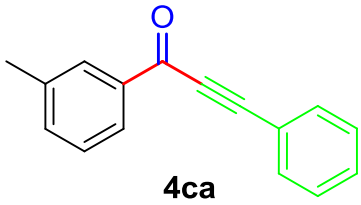
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (t, 2H), 7.59-7.62 (m, 2H), 7.31-7.42 (m, 3H), 7.18-7.24 (m, 2H), 2.36 (s, 3H),

^{13}C NMR (100 MHz, $CDCl_3$) δ 20.8, 85.9, 91.6, 119.2, 127.6, 128.3, 128.7, 129.6, 132.0, 144.2, 176.7.

HRMS (ESI) calcd. for $C_{16}H_{13}O$ [M+H]: 221.0961, found: 221.0953.

IR (KBr, cm^{-1}) 2913, 2203, 1637, 1288, 1009, 765.

3-phenyl-1-(m-tolyl)prop-2-yn-1-one (4ca):



4ca

White solid, 96% yield, M.P. 56℃.

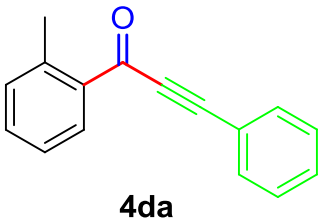
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93-7.96 (m, 2H), 7.58-7.61 (m, 2H), 7.17-7.42 (m, 5H), 2.36 (s, 3H),

^{13}C NMR (100 MHz, $CDCl_3$) δ 20.3, 86.0, 91.8, 119.2, 126.1, 127.5, 127.6, 128.7, 129.7, 132.0, 133.9, 135.9, 137.5,

HRMS (ESI) calcd. for $C_{16}H_{13}O$ [M+H]: 221.0961, found: 221.0961.

IR (KBr, cm^{-1}) 2926, 2210, 1637, 1308, 1159, 725.

3-phenyl-1-(o-tolyl)prop-2-yn-1-one (4da):



4da

Yellow oil, 63% yield .

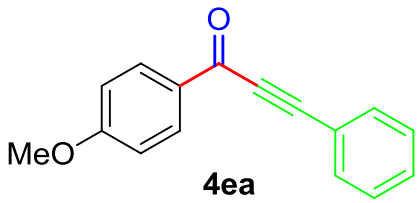
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22-8.26 (m, 1H), 7.58-7.60 (m, 2H), 7.29-7.40 (m, 5H), 7.19-7.22 (m, 1H), 2.60 (s, 3H),

^{13}C NMR (100 MHz, $CDCl_3$) δ 22.0, 88.4, 91.8, 120.4, 125.9, 128.6, 130.6, 132.2, 132.9, 132.9, 133.2, 135.8, 140.5,

HRMS (ESI) calcd. for $C_{16}H_{13}O$ [M+H]: 221.0961, found: 221.0961.

IR (KBr, cm^{-1}) 2934, 2203, 1642, 1321, 1004, 725.

1-(4-methoxyphenyl)-3-phenylprop-2-yn-1-one (4ea):



4ea

White solid, 60% yield, M.P. 96℃.

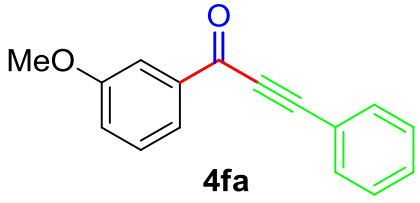
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18 (d, *J* = 8.84, 2H), 7.66-7.68 (m, 2H), 7.40-7.49 (m, 3H), 6.98 (d, *J* = 8.84, 2H), 3.90 (s, 3H),

^{13}C NMR (100 MHz, $CDCl_3$) δ 55.6, 86.9, 92.3, 113.9, 120.4, 128.7, 130.3, 130.6, 132.0, 133.0, 164.5, 176.7.

HRMS (ESI) calcd. for $C_{17}H_{15}O_2$ [M+H]: 251.1073, found: 251.1076.

IR (KBr, cm^{-1}) 2203, 1630, 1487, 1254, 1004, 750.

1-(3-methoxyphenyl)-3-phenylprop-2-yn-1-one (4fa):



4fa

Yellow oil, 83% yield .

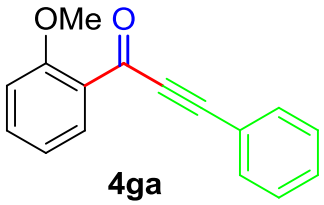
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.85-7.87 (m, 1H), 7.67-7.71 (m, 3H), 7.40-7.48 (m, 4H), 7.18-7.19 (m, 1H), 3.88 (s, 3H),

^{13}C NMR (100 MHz, $CDCl_3$) δ 55.5, 87.0, 93.0, 112.9, 120.1, 121.0, 122.9, 128.7, 129.7, 130.8, 133.1, 138.3, 159.8,

HRMS (ESI) calcd. for $C_{17}H_{15}O_2$ [M+H]: 251.1073, found: 251.1076.

IR (KBr, cm^{-1}) 2203, 1634, 1521, 1302, 1159, 757.

1-(2-methoxyphenyl)-3-phenylprop-2-yn-1-one (4ga):



4ga

Yellow oil, 71% yield .

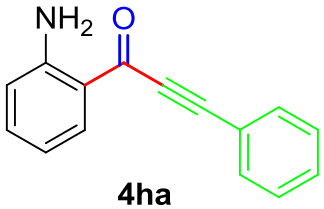
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.07-8.09 (m, 1H), 7.37-7.63 (m, 6H), 7.00-7.07 (m, 2H), 3.96 (s, 3H),

^{13}C NMR (100 MHz, $CDCl_3$) δ 56.0, 89.2, 91.6, 112.3, 120.3, 120.7, 126.8, 128.6, 130.5, 132.6, 133.0, 135.1, 159.8.

HRMS (ESI) calcd. for $C_{17}H_{15}O_2$ [M+H]: 251.1073, found: 251.1076.

IR (KBr, cm^{-1}) 2203, 1630, 1268, 1016, 757.

1-(2-aminophenyl)-3-phenylprop-2-yn-1-one (4ha):



4ha

Yellowish solid, 90% yield, M.P. 65℃.

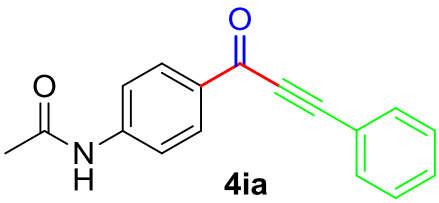
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17-8.19 (m, 1H), 7.65 (d, *J* = 6.72, 2H), 7.40-7.42 (m, 4H), 6.65-6.74 (m, 2H), 6.39 (br, 2H),

^{13}C NMR (100 MHz, $CDCl_3$) δ 87.2, 92.3, 116.1, 116.8, 118.9, 120.6, 128.6, 130.4, 132.8, 134.5, 135.3, 151.1, 179.5.

HRMS (ESI) calcd. for $C_{15}H_{12}NO$ [M+H]: 222.0913, found: 222.0911.

IR (KBr, cm^{-1}) 3431, 3329, 2196, 1618, 1220, 743.

N-(4-(3-phenylpropioloyl)phenyl)acetamide (4ia):



4ia

White solid, 39% yield, M.P. 169℃.

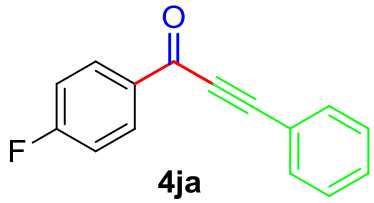
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05-8.12 (m, 3H), 7.56-7.67 (m, 4H), 7.19-7.42 (m, 3H), 2.17 (s, 3H),

^{13}C NMR (100 MHz, $CDCl_3$) δ 23.8, 85.8, 92.2, 117.8, 119.0, 127.7, 129.8, 130.1, 131.6, 132.0, 142.6, 167.9, 175.9.

HRMS (ESI) calcd. for $C_{17}H_{14}NO_2$ [M+H]: 264.1019, found: 264.1024.

IR (KBr, cm^{-1}) 2947, 2210, 1609, 1426, 1241, 1036, 750, 538.

1-(4-fluorophenyl)-3-phenylprop-2-yn-1-one (4ja):



4ja

Yellow solid, 78% yield, M.P. 45℃.

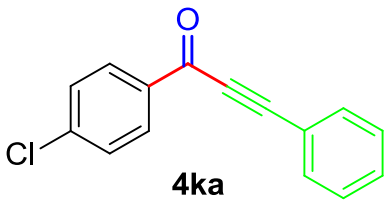
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.23-8.28 (m, 2H), 7.67-7.70 (m, 2H), 7.41-7.56 (m, 3H), 7.17-7.22 (m, 2H),

^{13}C NMR (100 MHz, $CDCl_3$) δ 86.6, 93.4, 115.7, 115.9, 119.9, 128.7, 130.9, 132.2, 132.3, 133.0, 133.4, 133.4, 165.2, 167.7, 176.3.

HRMS (ESI) calcd. for $C_{15}H_{10}FO$ [M+H]: 225.0710, found: 225.0705.

IR (KBr, cm^{-1}) 2210, 1630, 1222, 1028, 845, 730.

1-(4-fluorophenyl)-3-phenylprop-2-yn-1-one (4ka):



4ka

White solid, 68% yield, M.P. 105℃.

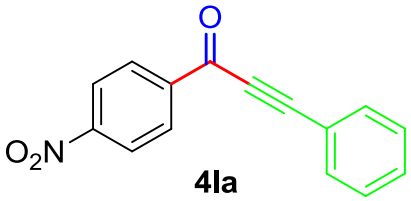
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15-8.17 (m, 2H), 7.68-7.70 (m, 3H), 7.42-7.7.51 (m, 5H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 86.6, 93.6, 12.0, 128.7, 129.0, 130.9, 131.0, 133.1, 135.3, 140.7 176.7.

HRMS (ESI) calcd. for $C_{15}H_{10}ClO$ [M+H]: 241.0415, found: 241.0407.

IR (KBr, cm^{-1}) 2203, 1657, 1213, 1002, 743, 675.

1-(4-nitrophenyl)-3-phenylprop-2-yn-1-one (4la):



4la

Yellowish solid, 92% yield, M.P. 134℃.

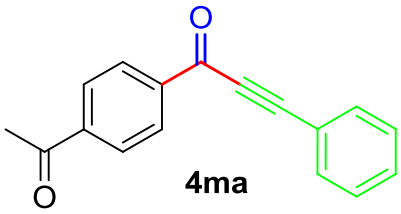
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.30 (s, 4H), 7.63-7.66 (m, 2H), 7.37-7.47 (m, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 85.5, 94.4, 118.4, 122.9, 127.9, 129.4, 130.4, 132.3, 140.0, 149.9, 174.9.

HRMS (ESI) calcd. for $C_{15}H_9NO_3$ [M+H]: 251.0543, found: 251.0533.

IR (KBr, cm^{-1}) 2203, 1630, 1288, 1097, 764.

1-(4-acetylphenyl)-3-phenylprop-2-yn-1-one (4ma):



4ma

White solid, 38% yield, M.P. 82℃.

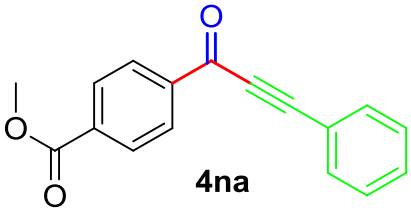
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.27-8.29 (m, 2H), 8.17-8.19 (m, 2H), 7.70-7.72 (m, 2H), 7.43-7.54 (m, 3H), 3.97 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 52.5, 86.8, 94.2, 119.8, 128.8, 129.4, 129.8, 131.1, 133.2, 134.7, 139.9, 166.1, 177.2.

HRMS (ESI) calcd. for $C_{17}H_{12}NaO_2$ [M+Na]: 271.0730, found: 271.0726.

IR (KBr, cm^{-1}) 2203, 1623, 1288, 1207, 1014, 757.

methyl 4-(3-phenylpropioloyl)benzoate (4na):



4na

White solid, 47% yield, M.P. 79℃.

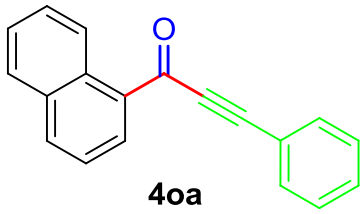
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (d, *J* = 8.48, 2H), 8.10 (d, *J* = 8.48, 2H), 7.70-7.72 (m, 2H), 7.43-7.54 (m, 3H), 2.68 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 27.0, 86.8, 94.3, 119.8, 128.5, 128.8, 129.7, 131.1, 133.2, 139.9, 140.8, 177.1, 197.4.

HRMS (ESI) calcd. for $C_{17}H_{12}NaO_3$ [M+Na]: 287.0679, found: 287.0680.

IR (KBr, cm^{-1}) 2210, 1734, 1637, 1281, 1111, 702.

1-(naphthalen-1-yl)-3-phenylprop-2-yn-1-one (4oa):



4oa

Yellow solid, 82% yield, M.P. 54℃.

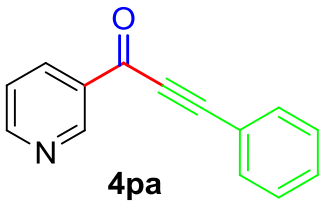
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.15 (d, *J* = 8.68, 1H), 8.57 (d, *J* = 1.12, 1H), 8.01 (d, *J* = 8.16, 1H), 7.83 (d, *J* = 8.12, 1H), 7.18-7.63 (m, 8H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 88.5, 91.7, 120.4, 124.5, 126.0, 126.8, 128.6, 128.7, 129.0, 130.6, 130.8, 133.0, 133.0.

HRMS (ESI) calcd. for $C_{19}H_{13}O$ [M+Na]: 257.0961, found: 257.0951.

IR (KBr, cm^{-1}) 2196, 1657, 1268, 1077, 804.

3-phenyl-1-(pyridin-3-yl)prop-2-yn-1-one (4pa):



4pa

White solid, 50% yield, M.P. 71℃.

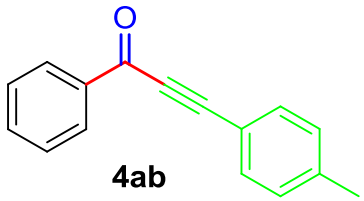
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.37 (d, *J* = 1.64, 1H), 8.77 (t, *J* = 1.52, 1H), 8.35 (d, *J* = 7.96, 1H), 7.44-7.46 (m, 2H), 7.34-7.44 (m, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 86.3, 94.8, 119.6, 123.6, 128.8 131.3, 132.2, 133.5, 136.2 151.4, 154.2, 176.4.

HRMS (ESI) calcd. for $C_{14}H_9NNaO$ [M+Na]: 230.0576, found: 230.0578.

IR (KBr, cm^{-1}) 2203, 1650, 1302, 1220, 1036, 716.

1-phenyl-3-(p-tolyl)prop-2-yn-1-one (4ab):



4ab

Yellow solid, 97% yield, M.P. 38℃.

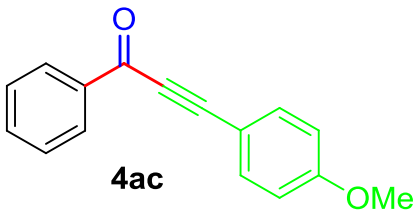
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14-8.17(m, 2H), 7.43-7.58 (m, 5H), 7.15-7.19 (m, 2H), 2.33 (s, 3H),

^{13}C NMR (100 MHz, $CDCl_3$) δ 20.8, 85.8, 92.8, 116.0, 127.6, 128.5, 128.5, 132.1, 133.0, 136.0, 140.5, 177.1.

HRMS (ESI) calcd. for $C_{16}H_{13}O$ [M+H]: 221.0961, found: 221.0953.

IR (KBr, cm^{-1}) 2203, 1637, 1275, 1008, 811, 702.

3-(4-methoxyphenyl)-1-phenylprop-2-yn-1-one (4ac):



4ac

White solid, 93% yield, M.P. 64℃.

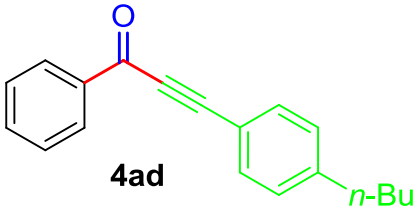
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.21-8.23 (m, 2H), 7.50-7.66 (m, 5H), 6.92-9.94 (m, 2H), 3.86 (s, 3H), 1.63 (J_1 = 9.44, J_2 = 7.64, 2H), 1.33-1.38 (m, 2H), 0.93 (*J* = 7.32, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 55.5, 86.9, 94.3, 111.9, 114.4, 128.6, 129.5, 133.9, 135.2, 137.1, 161.8, 178.1.

HRMS (ESI) calcd. for $C_{16}H_{13}O_2$ [M+H]: 237.0910, found: 237.0906.

IR (KBr, cm^{-1}) 2920, 2203, 1657, 1288, 1002, 839, 689.

3-(4-butylphenyl)-1-phenylprop-2-yn-1-one (4ad):



Yellowish solid, 65% yield, M.P. 53℃.

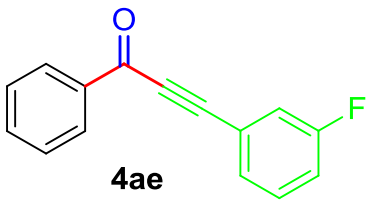
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.2.1-8.24 (m, 2H), 7.49-7.64 (m, 5H), 7.22-7.25 (m, 2H), 2.65 (t, J = 7.84, 2H), 1.63 (J_1 = 9.44, J_2 = 7.64, 2H), 1.33-1.38 (m, 2H), 0.93 (J = 7.32, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 13.9, 22.3, 33.2 35.8, 86.8, 93.9, 117.2, 128.6, 128.9, 129.6, 133.2, 134.0, 137.0, 146.5.

HRMS (ESI) calcd. for $C_{19}H_{19}O$ [M+H]: 263.1430, found: 263.1440.

IR (KBr, cm^{-1}) 2926, 2203, 1644, 1288, 1009, 695.

3-(3-fluorophenyl)-1-phenylprop-2-yn-1-one (4ae):



White solid, 95% yield, M.P. 48℃.

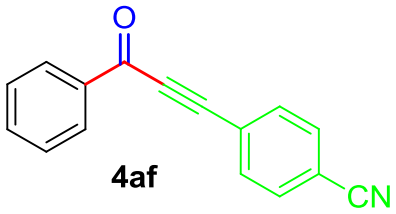
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12-8.15 (m, 2H), 7.28-7.59 (m, 6H), 7.12-7.15 (m, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 86.1, 90.0, 90.1, 117.1, 117.3, 118.5, 118.8, 120.9, 121.0, 127.7, 127.9, 127.9, 128.6, 129.4, 129.5, 133.3, 135.7, 160.0, 162.5, 176.7.

HRMS (ESI) calcd. for $C_{15}H_{10}FO$ [M+Na]: 225.0710, found: 225.0709.

IR (KBr, cm^{-1}) 2933,2203, 1657, 1234, 1018, 784, 685.

4-(3-oxo-3-phenylprop-1-yn-1-yl)benzonitrile (4af):



4af

Yellowish solid, 96% yield, M.P. 137℃.

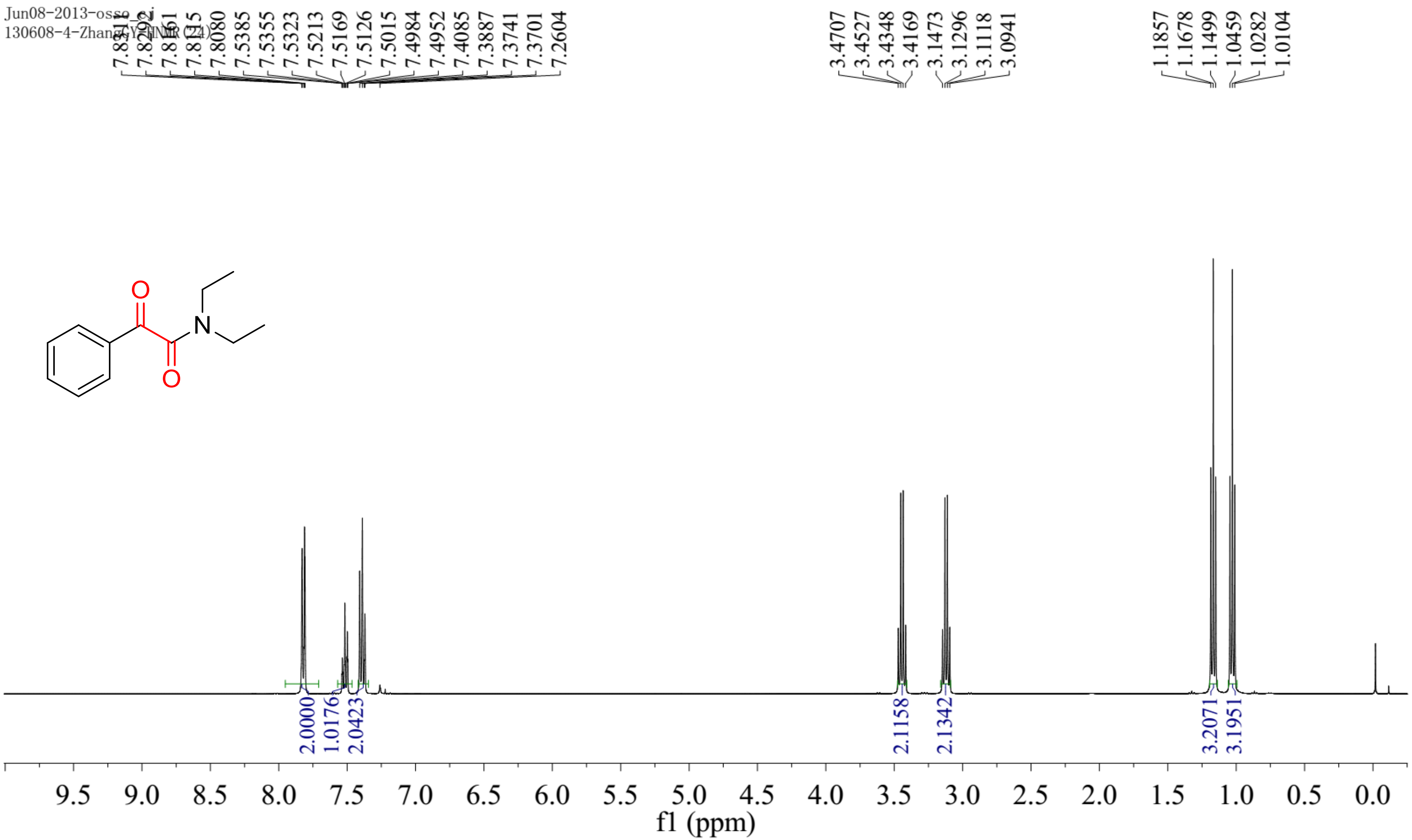
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.8.19-8.21 (m, 2H), 7.65-7.79 (m, 5H), 7.52-7.56 (m, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 89.4, 89.6, 114.1, 117.9, 125.0, 128.8, 129.6, 132.3, 133.3, 134.6, 136.5, 177.5.

HRMS (ESI) calcd. for $C_{16}H_{19}NO$ [M+Na]: 254.0720; found: 254.0721.

IR (KBr, cm^{-1}) 2830, 2183, 1603, 1254, 1029, 825, 702.

4. Copies for ^{1}H NMR and ^{13}C NMR of the Compounds and Products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7.5015
7.4984
7.4952
7.4085
7.3887
7.3741
7.3701
7.2604
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3.4527
3.4348
3.4169
3.1473
3.1296
3.1118
3.0941
1.1857
1.1678
1.1499
1.0459
1.0282
1.0104
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N
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2.0423
2.1158
2.1342
3.2071
3.1951
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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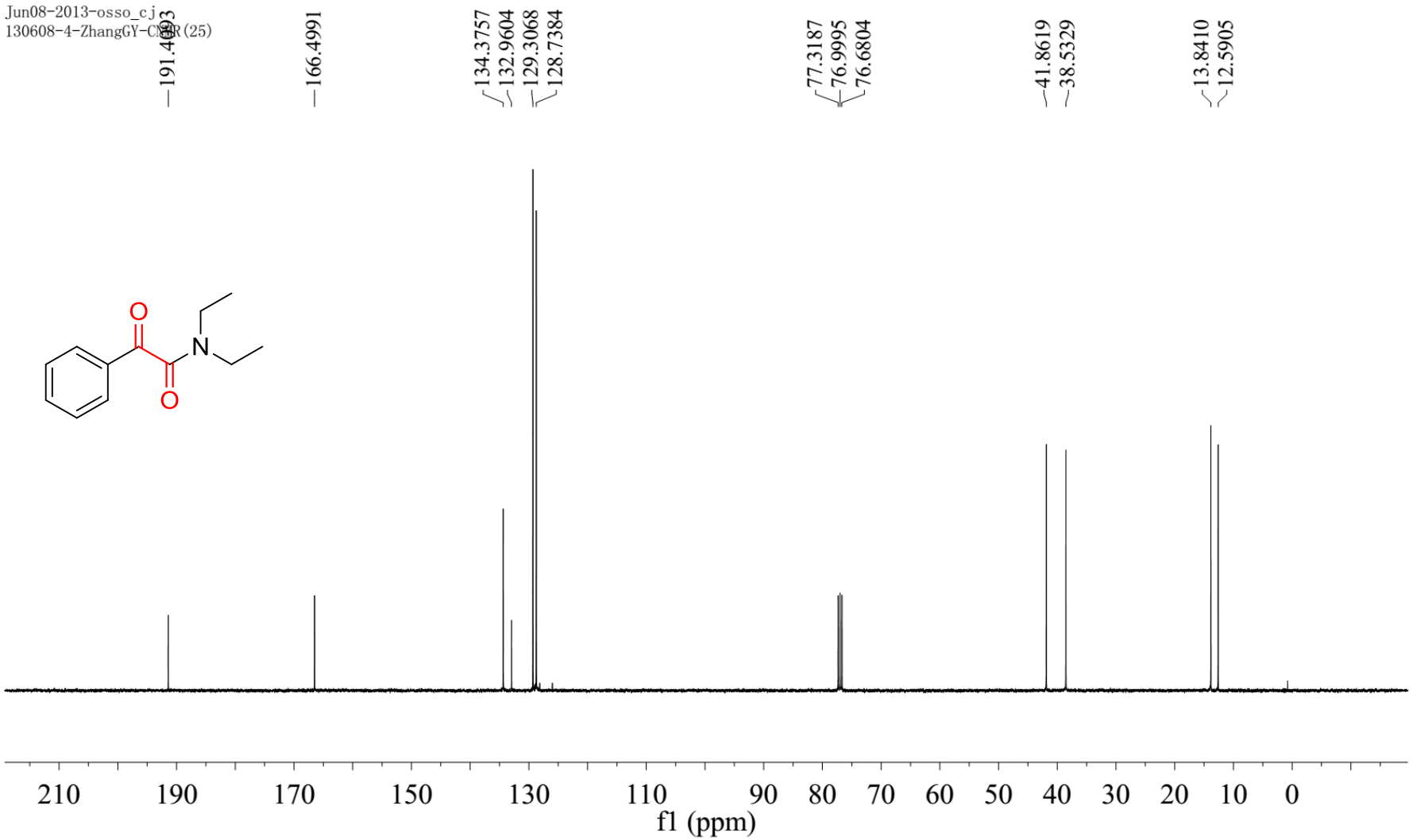
f1 (ppm)


Jun08-2013-osso_cj
130608-4-ZhangGY-CMR(25)
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13.8410
12.5905
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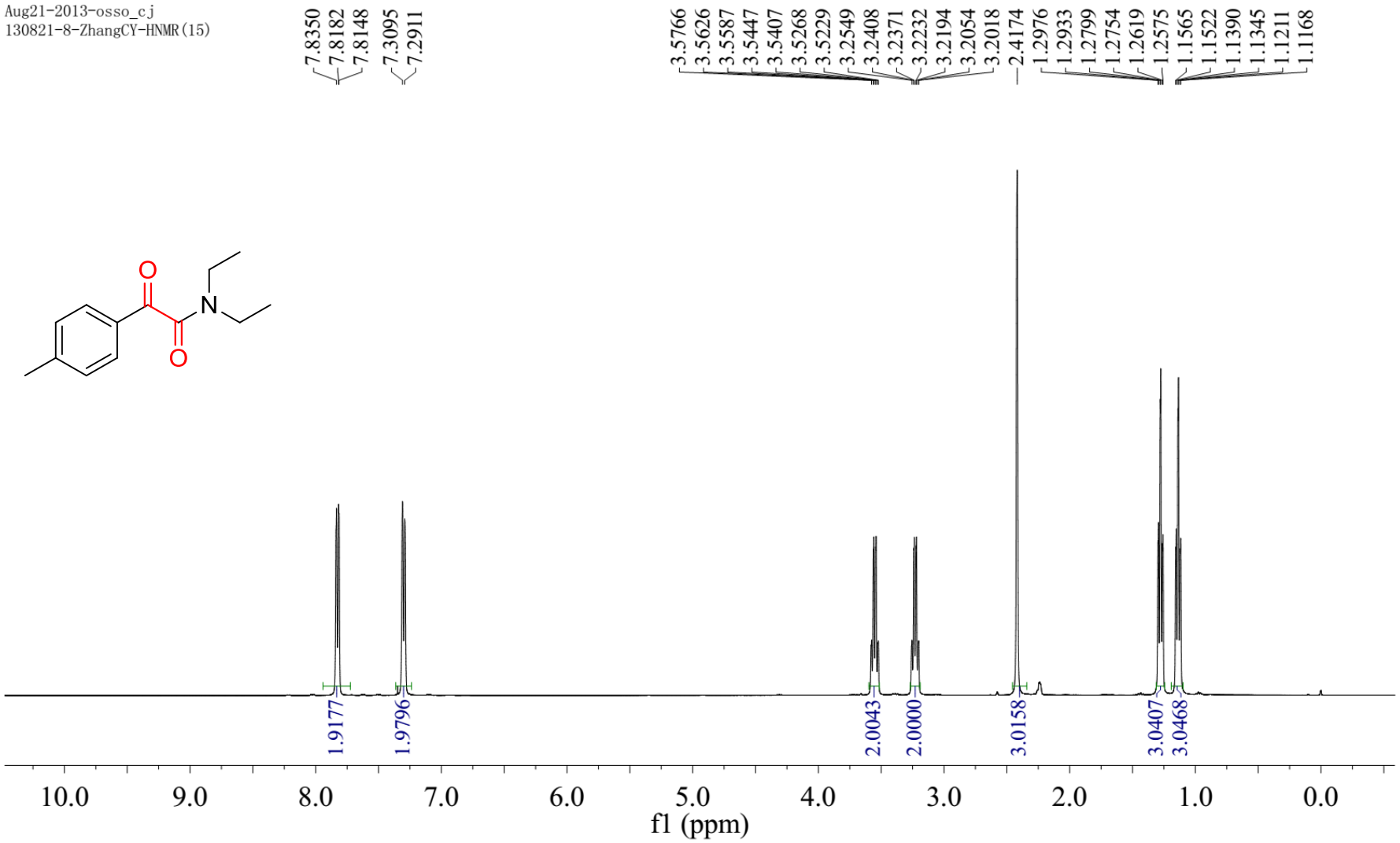
f1 (ppm)


Aug21-2013-osso_cj
130821-8-ZhangCY-HNMR(15)
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3.5229
3.2549
3.2408
3.2371
3.2232
3.2194
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3.2018
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1.2933
1.2799
1.2754
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1.1565
1.1522
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1.1345
1.1211
1.1168
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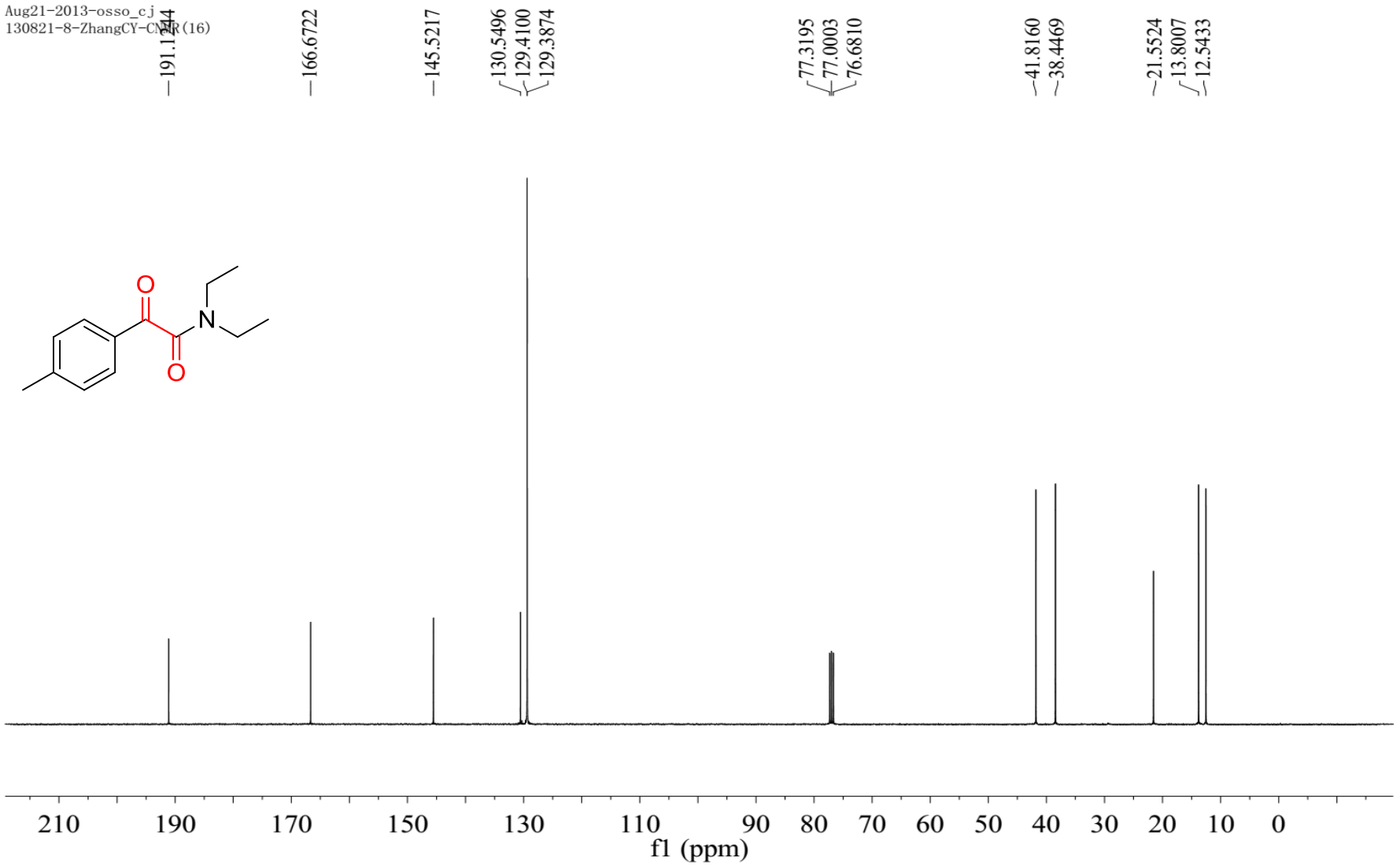
Aug21-2013-osso_cj
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21.5524
13.8007
12.5433
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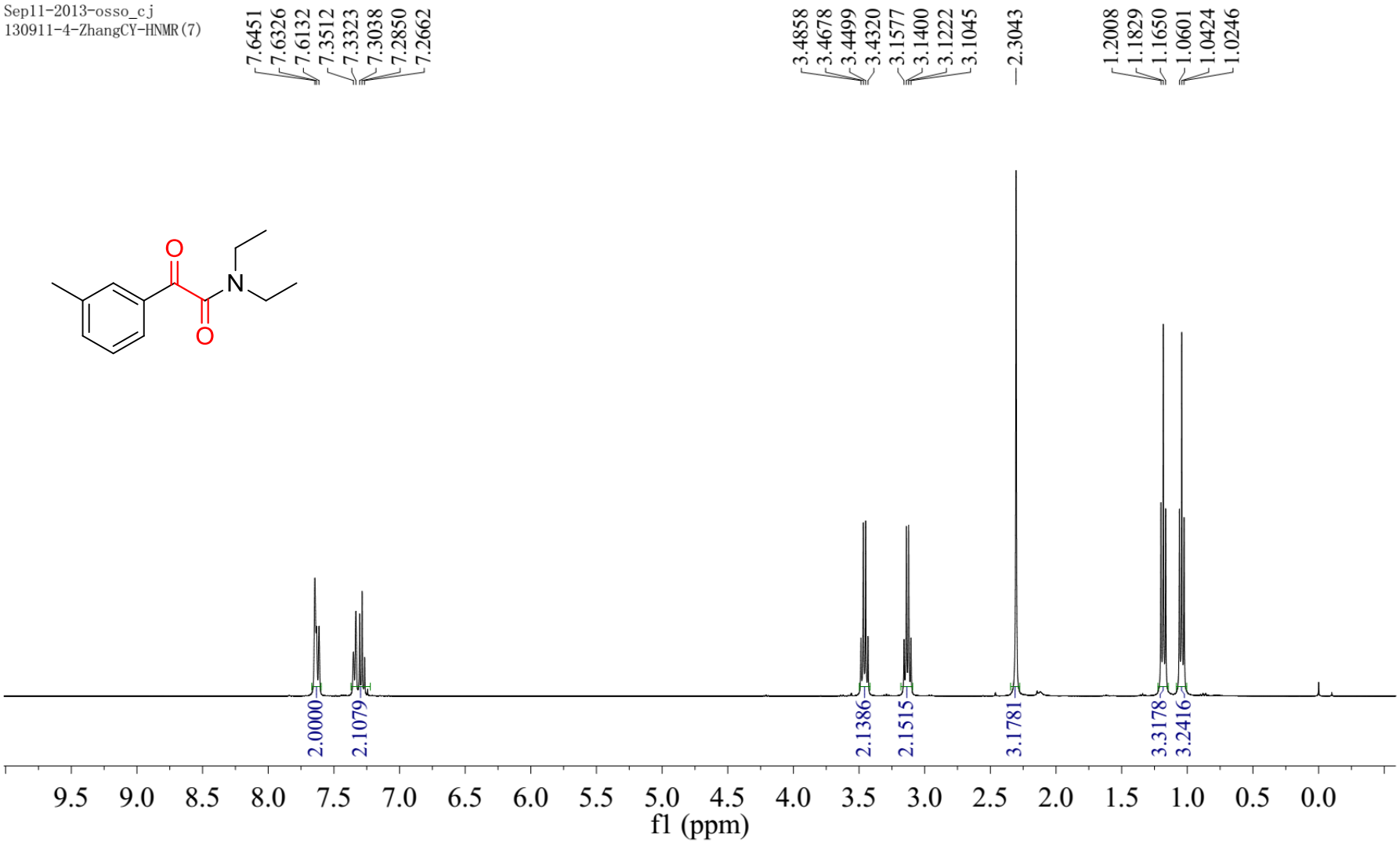
f1 (ppm)


Sep11-2013-osso_cj
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3.1045
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1.1650
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1.0424
1.0246
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3.3178
3.2416
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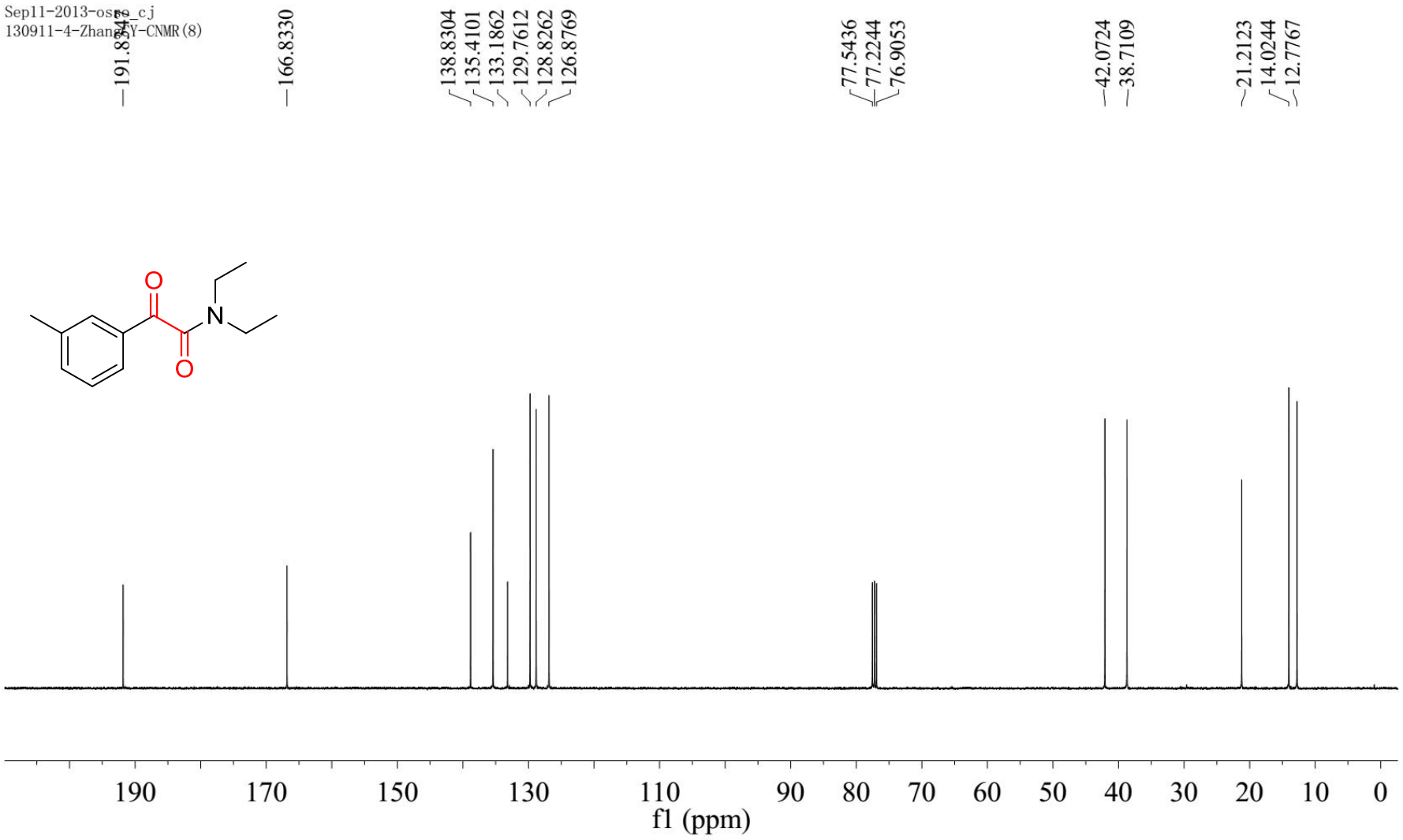
f1 (ppm)


Sep11-2013-osse_cj
130911-4-ZhangSY-CNMR(8)
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77.2244
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42.0724
38.7109
21.2123
14.0244
12.7767
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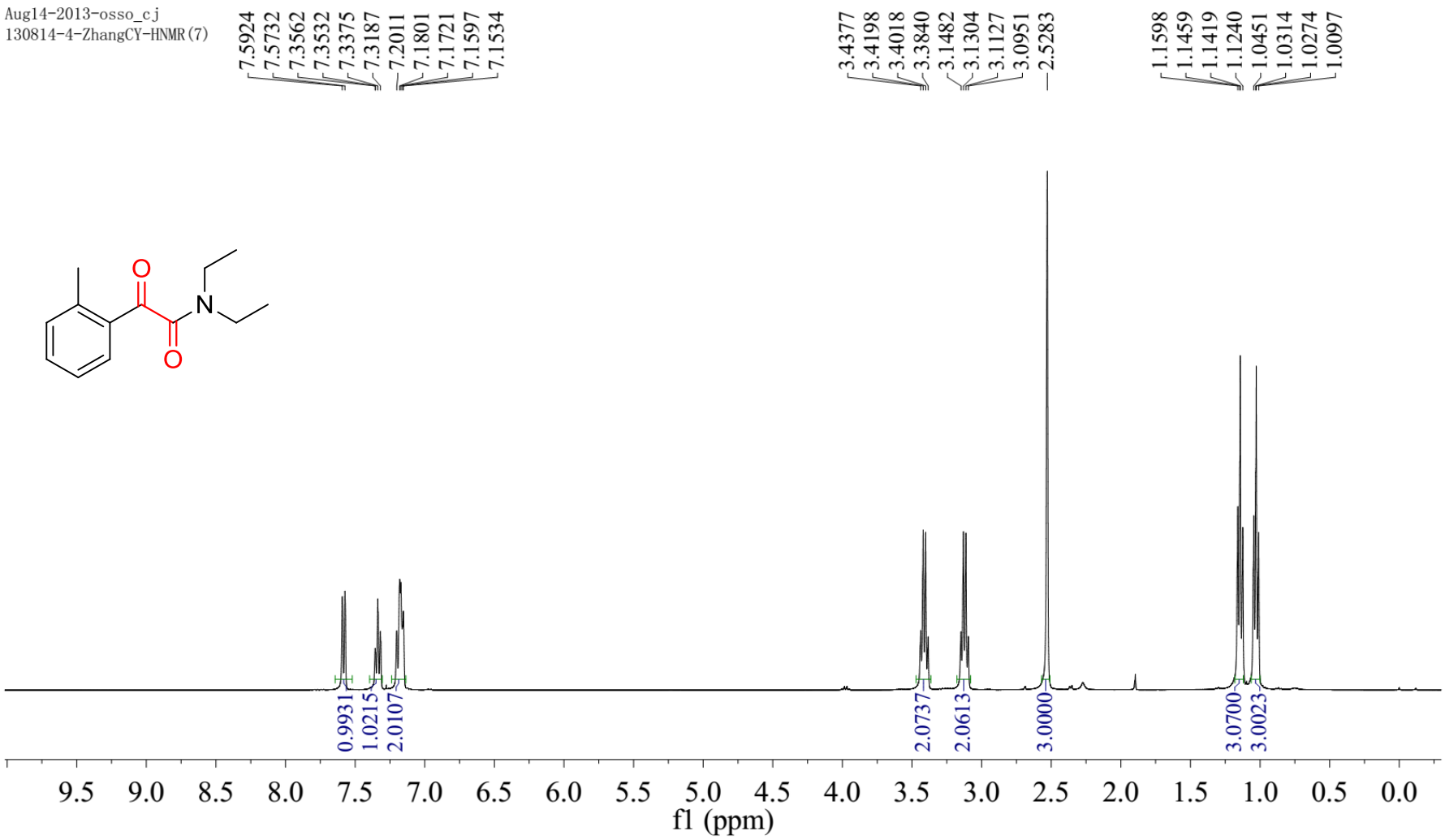
f1 (ppm)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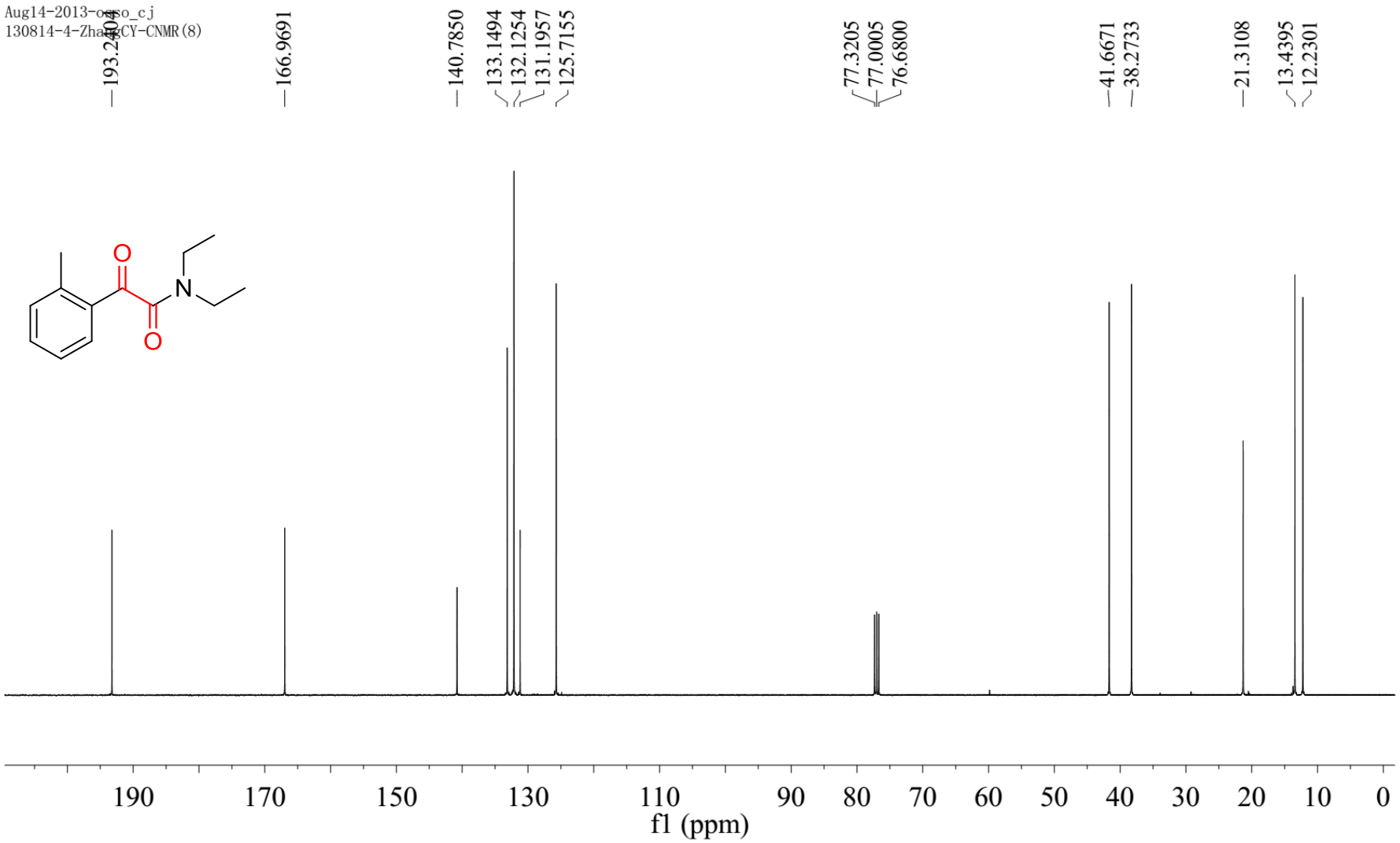
f1 (ppm)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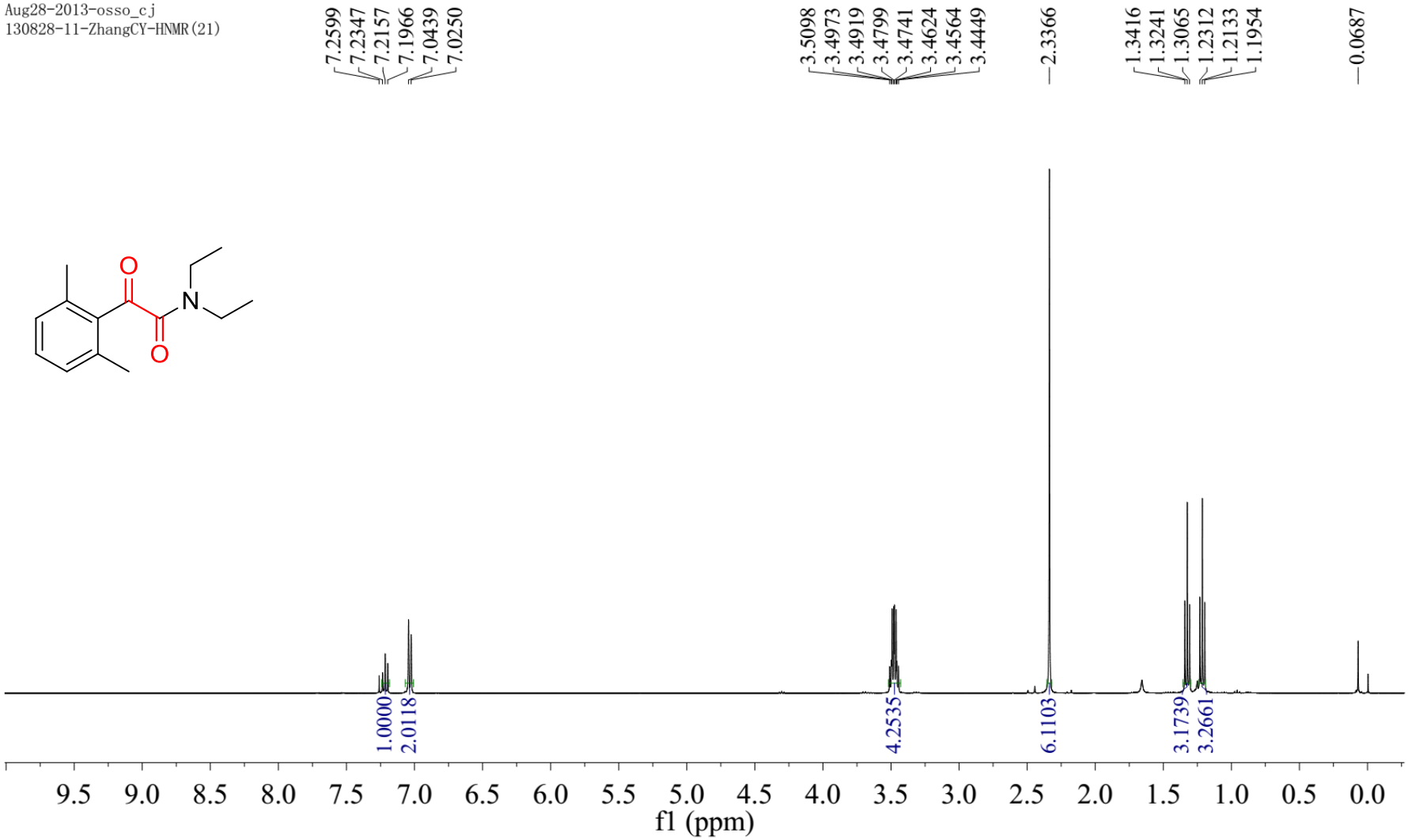
Aug28-2013-osso_cj
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3.4741
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3.4449
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1.3241
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1.2312
1.2133
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3.2661
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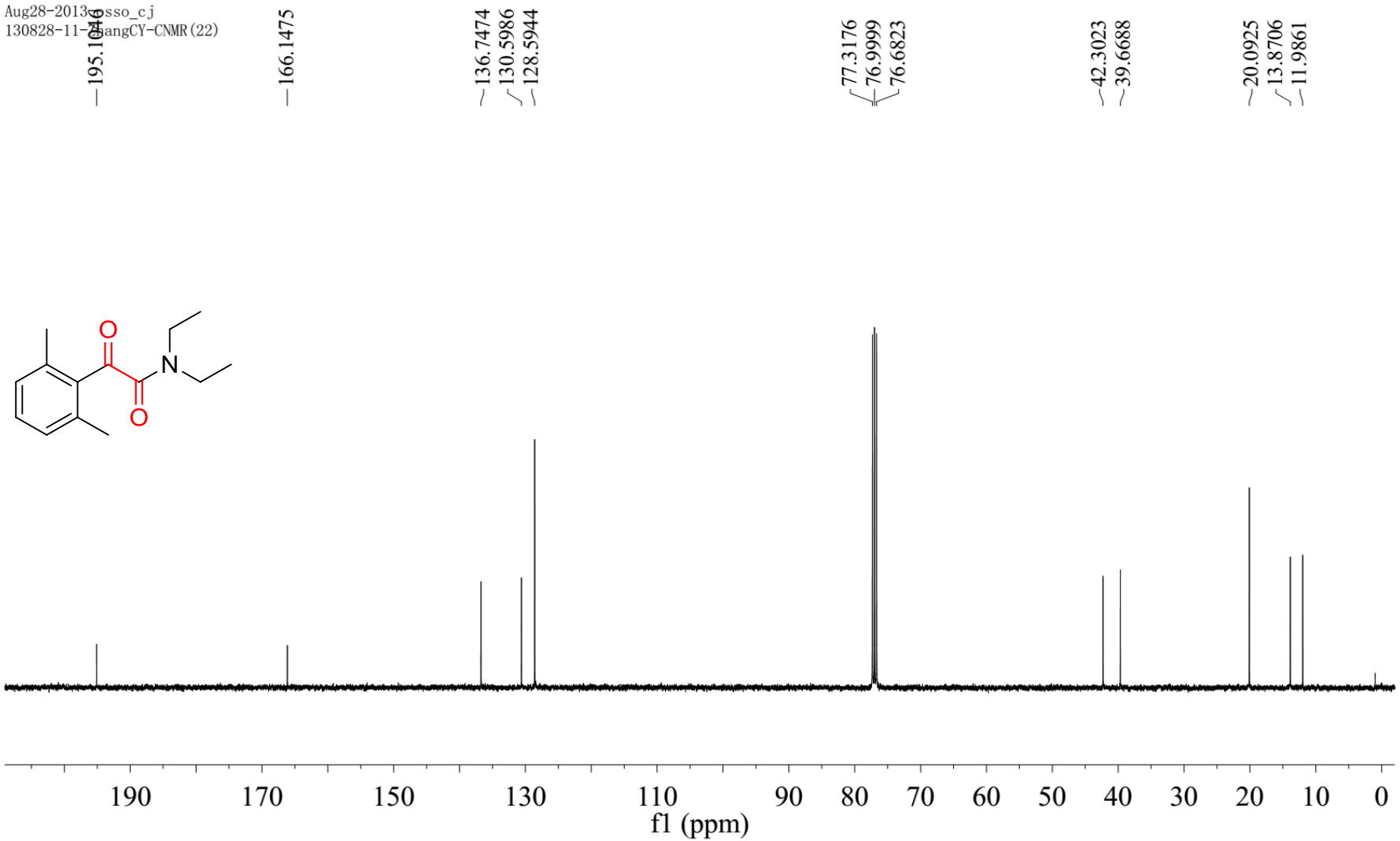
f1 (ppm)


Aug28-2013-osso_cj
130828-11-ZhangCY-CNMR(22)
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42.3023
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13.8706
11.9861
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90
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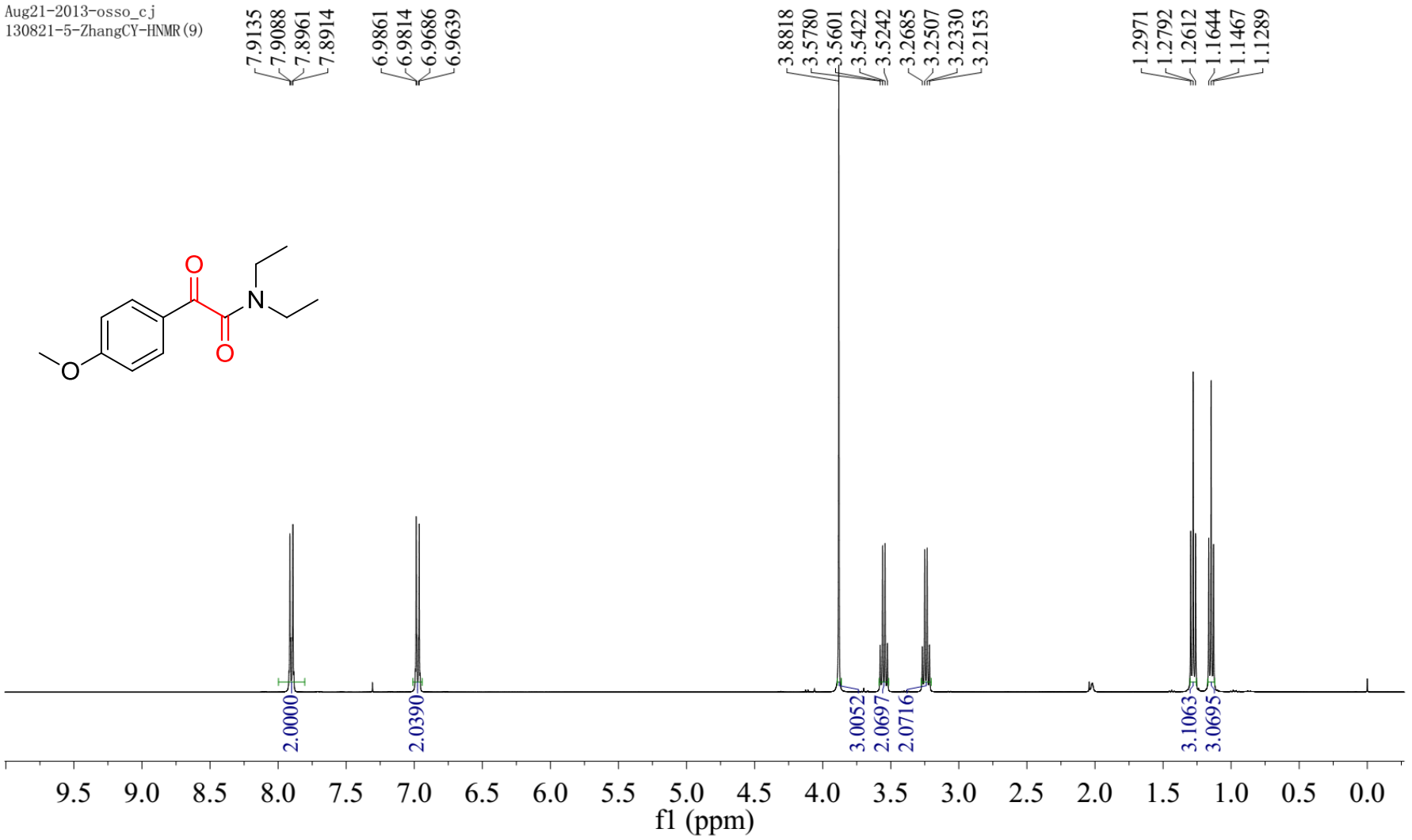
Aug21-2013-osso_cj
130821-5-ZhangCY-HNMR(9)
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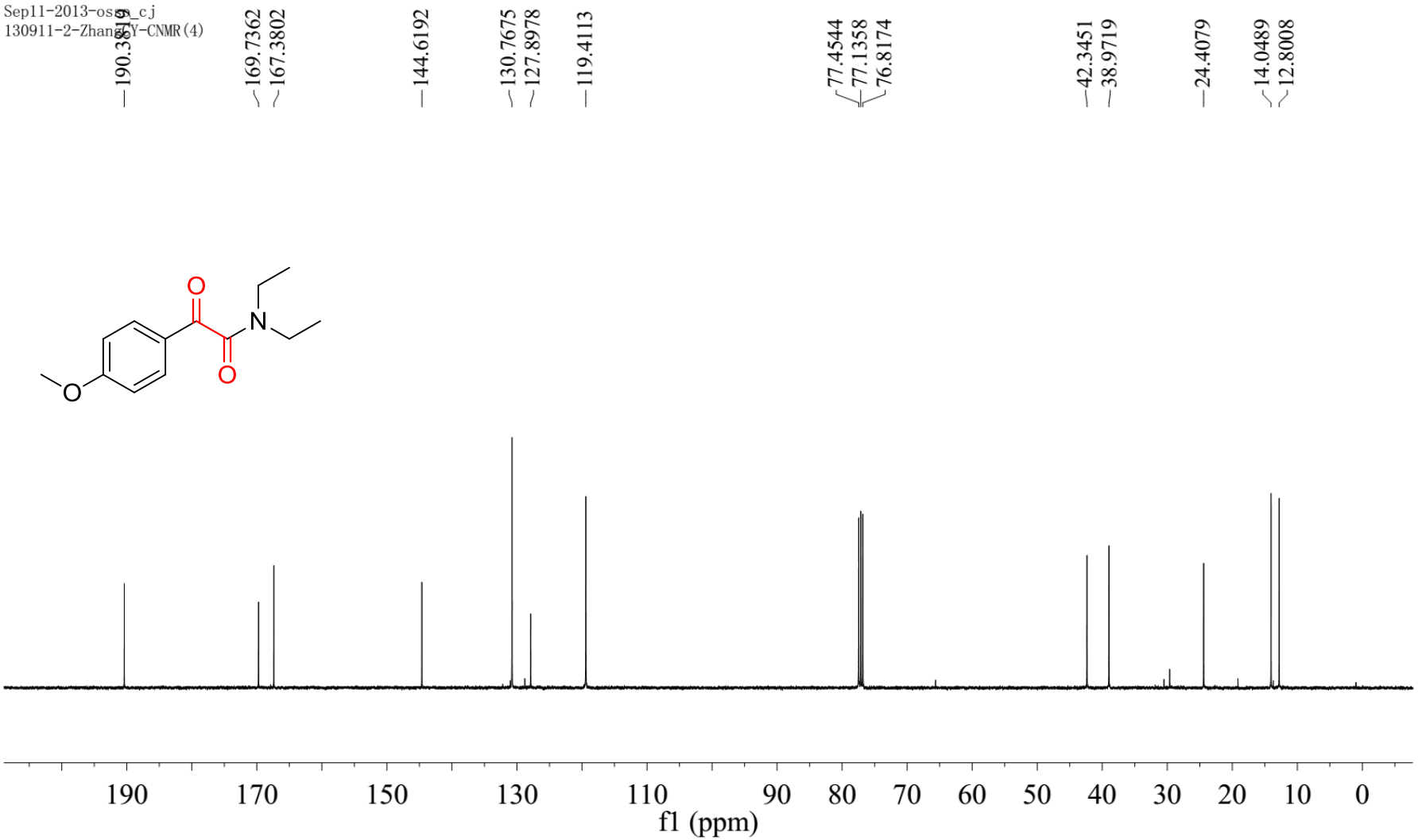
Sep11-2013-osa_cj
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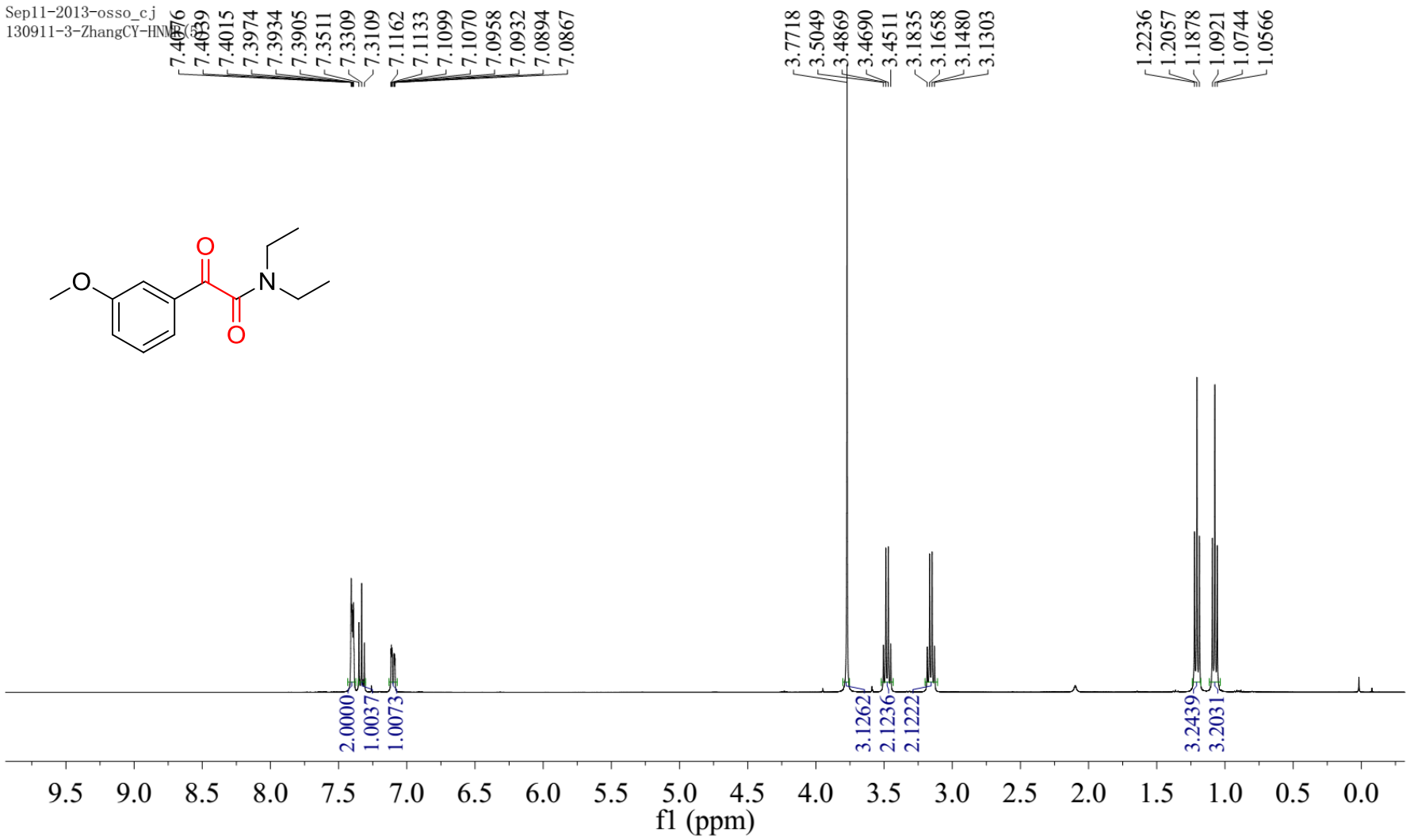
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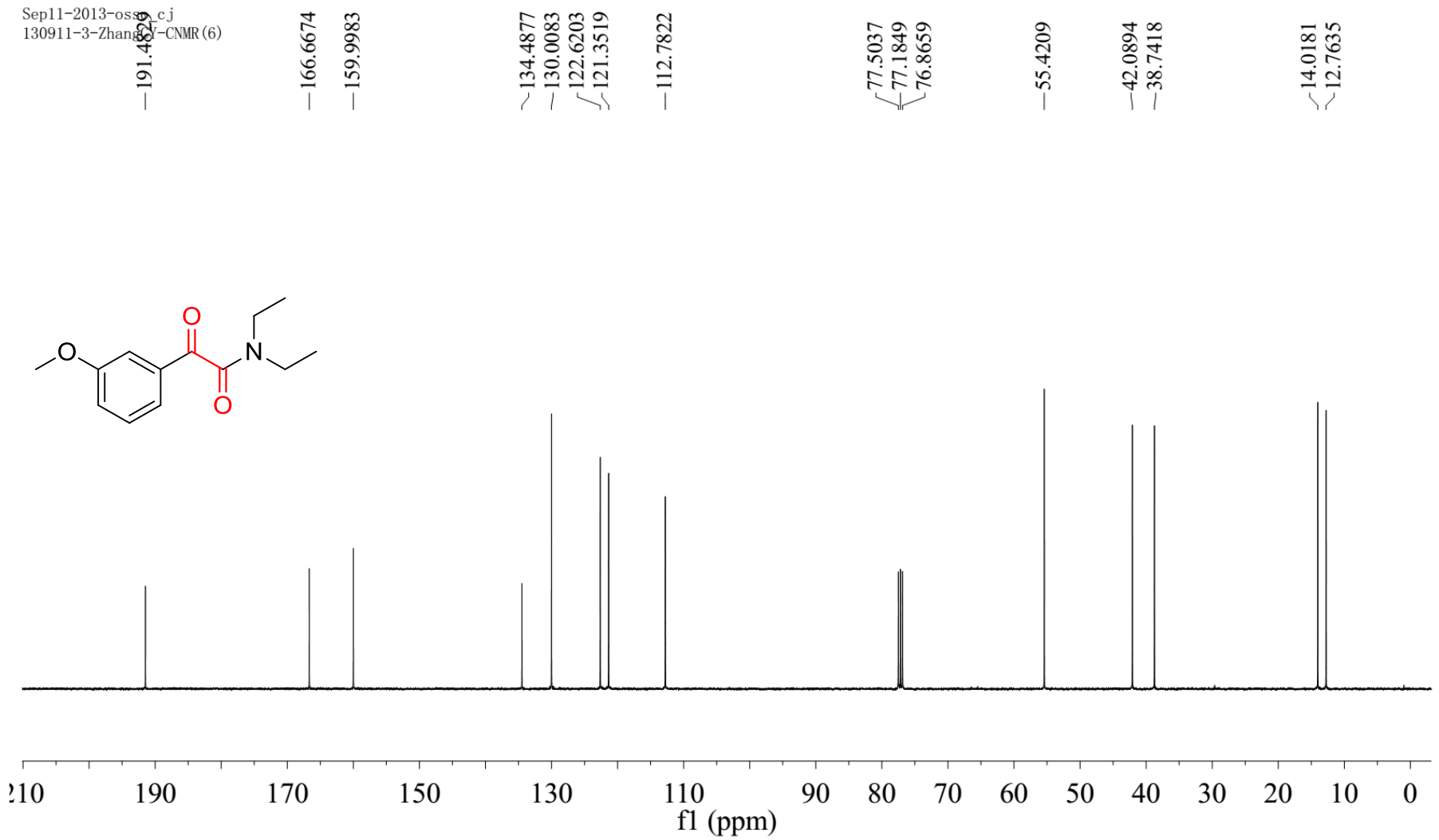
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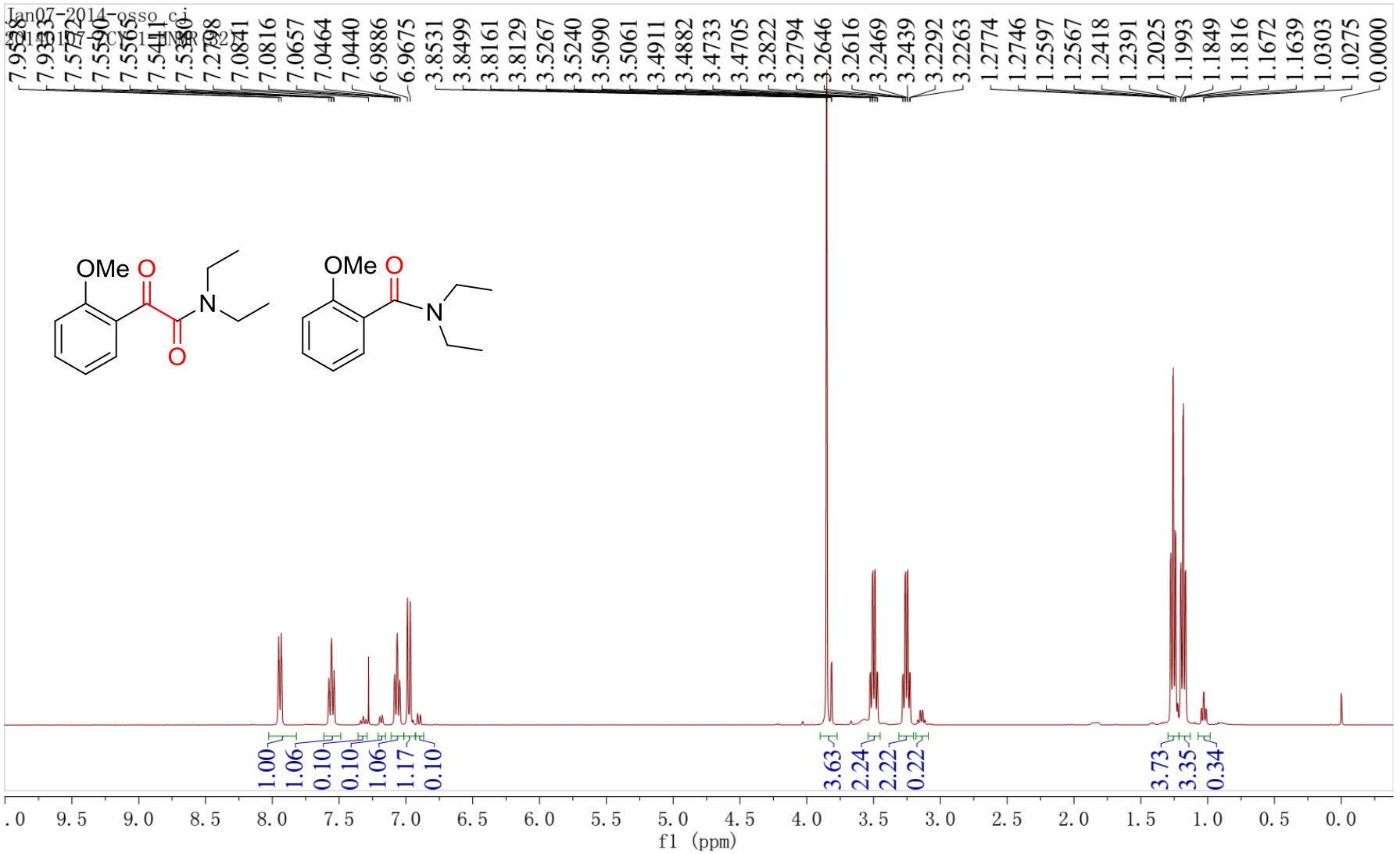
Jan07-2014-osso_cj
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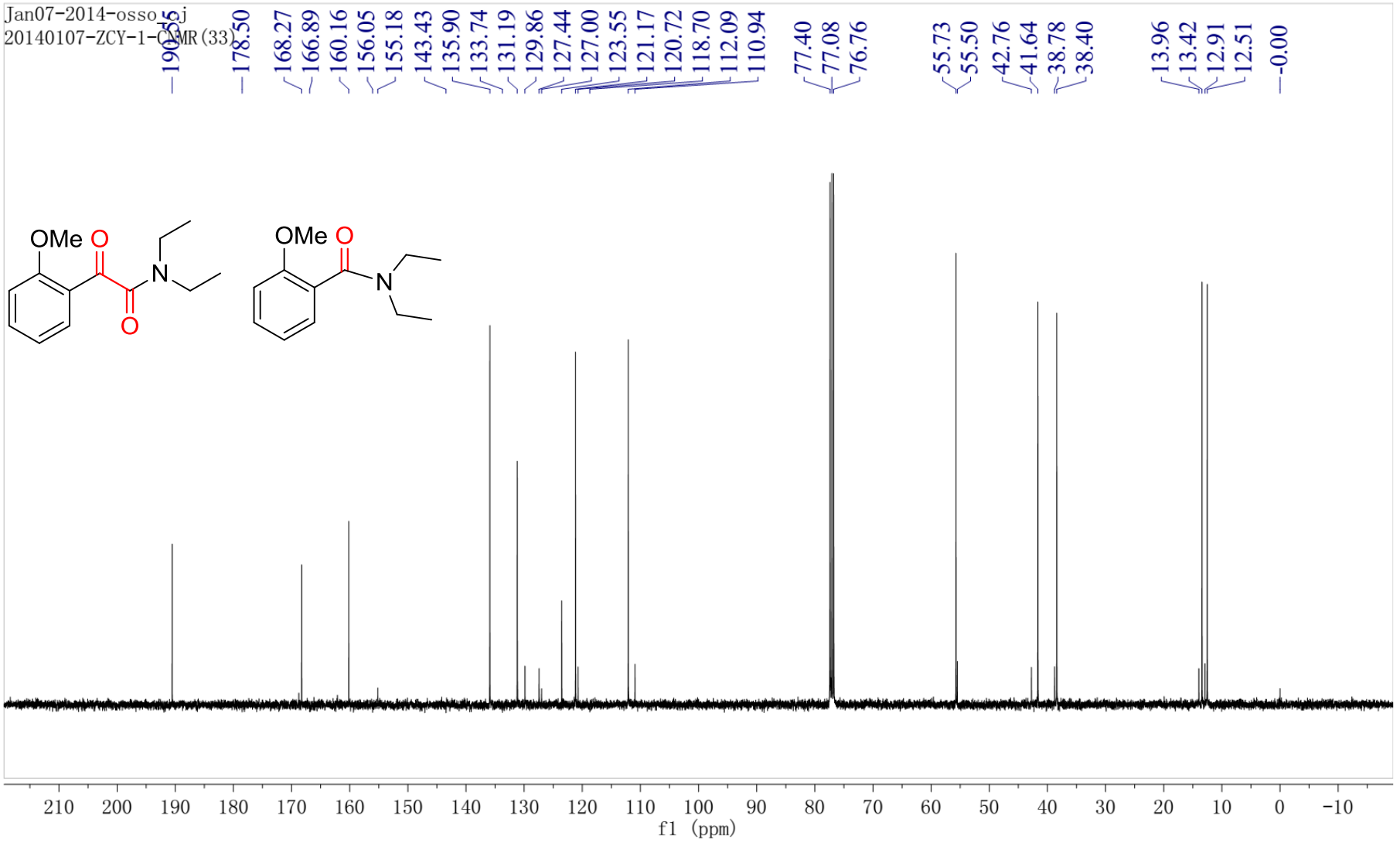
Jan07-2014-osso_j
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160.16
156.05
155.18
143.43
135.90
133.74
131.19
129.86
127.44
127.00
123.55
121.17
120.72
118.70
112.09
110.94
77.40
77.08
76.76
55.73
55.50
42.76
41.64
38.78
38.40
13.96
13.42
12.91
12.51
-0.00
OMe
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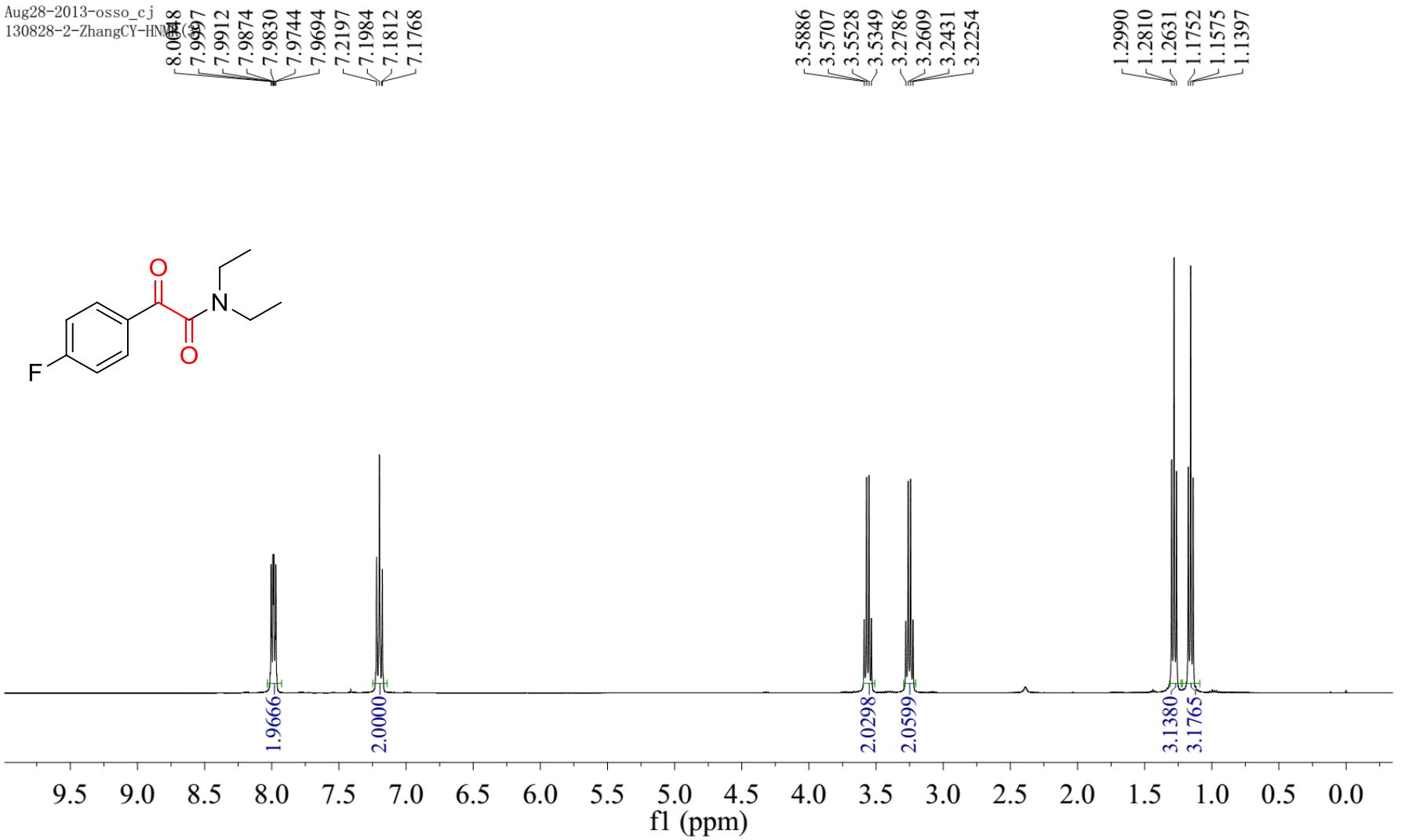
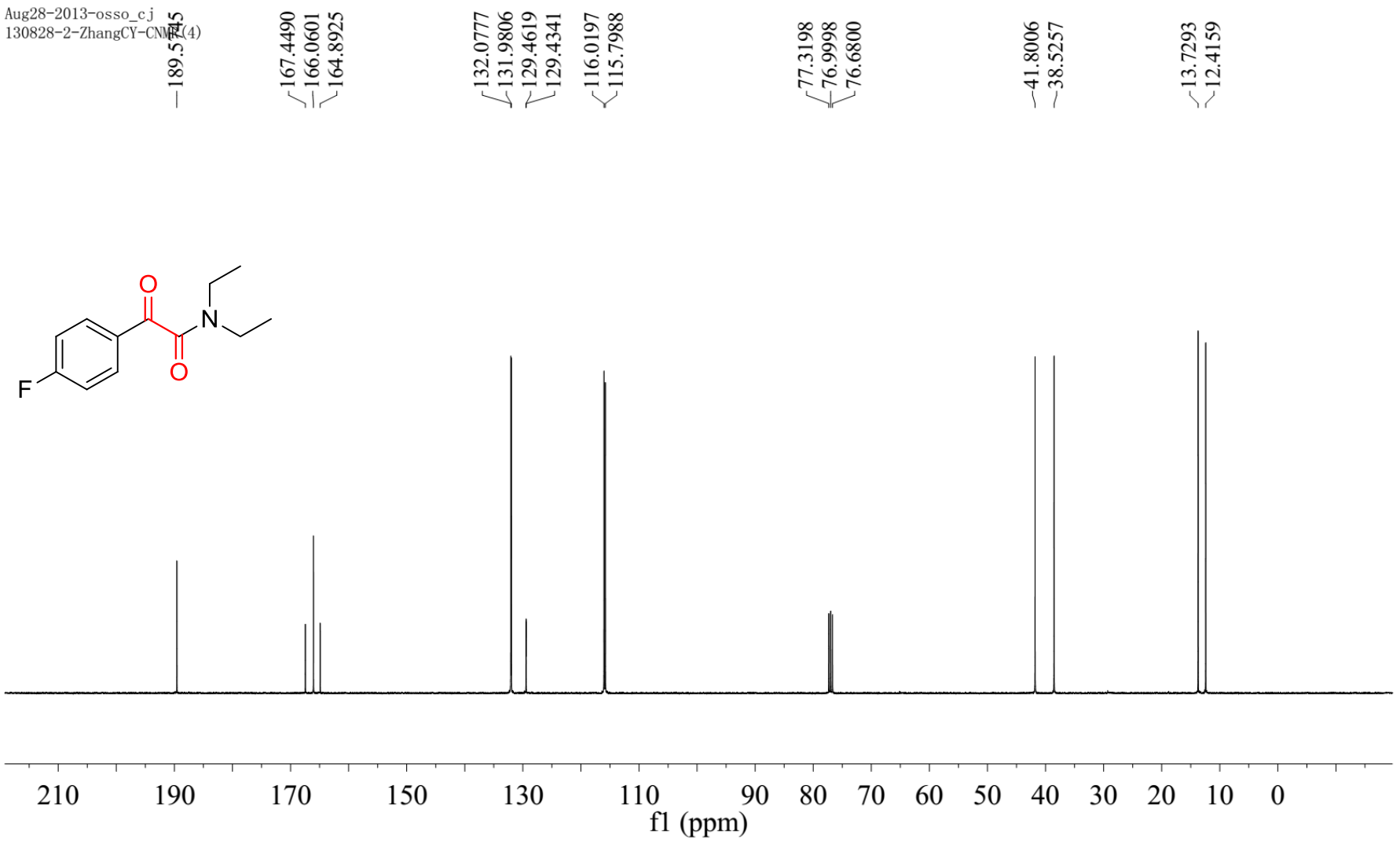
N
O
OMe
O
N
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


Aug28-2013-osso_cj
130828-2-ZhangCY-HNMR(3)
8.0048
7.9997
7.9912
7.9874
7.9830
7.9744
7.9694
7.2197
7.1984
7.1812
7.1768
3.5886
3.5707
3.5528
3.5349
3.2786
3.2609
3.2431
3.2254
1.2990
1.2810
1.2631
1.1752
1.1575
1.1397
O
N
O
F
1.9666
2.0000
2.0298
2.0599
3.1380
3.1765
9.5 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 1.5 1.0 0.5 0.0
f1 (ppm)


Aug28-2013-osso_cj
130828-2-ZhangCY-CNMR(4)
189.5745
167.4490
166.0601
164.8925
132.0777
131.9806
129.4619
129.4341
116.0197
115.7988
77.3198
76.9998
76.6800
41.8006
38.5257
13.7293
12.4159
O
N
O
F
210
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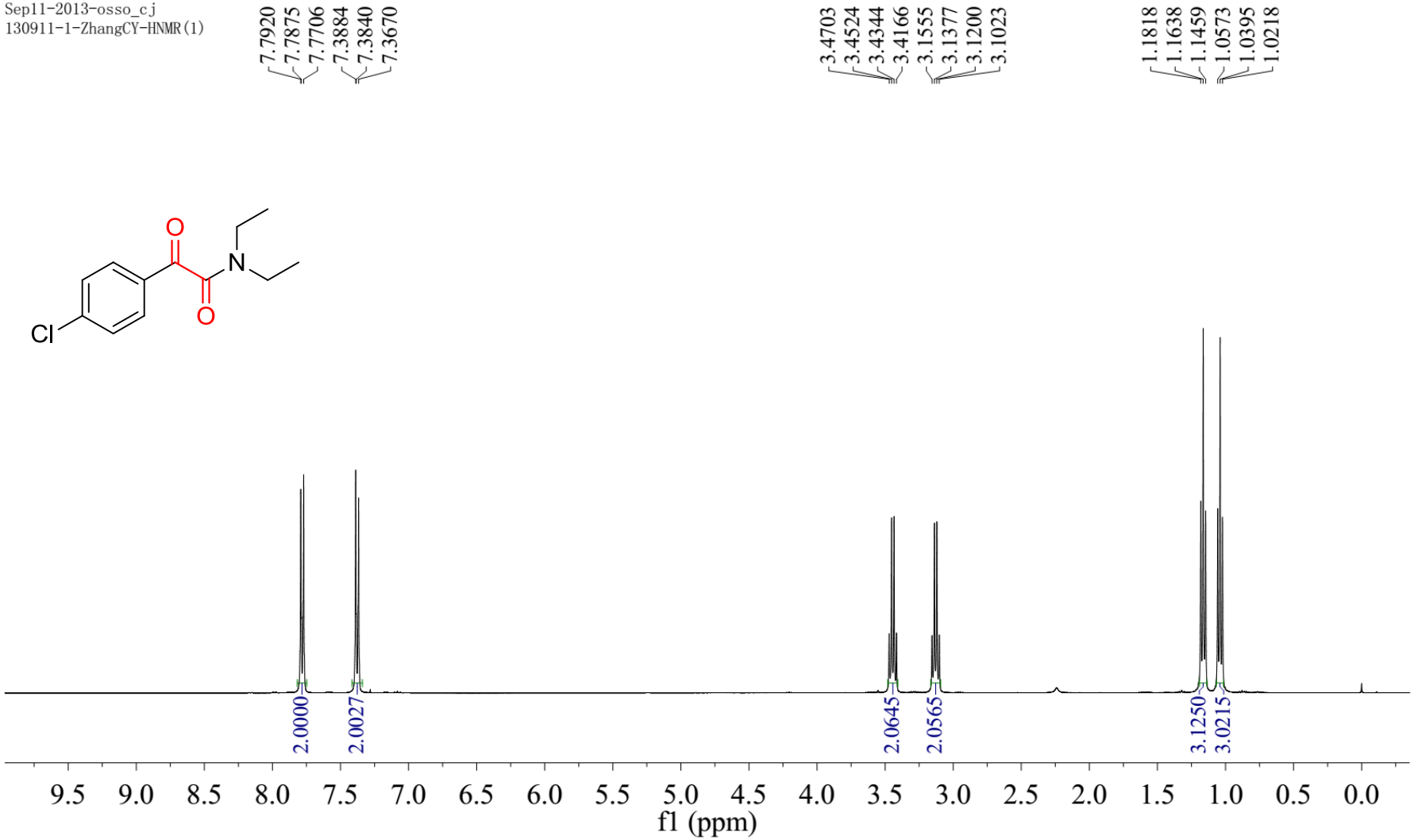
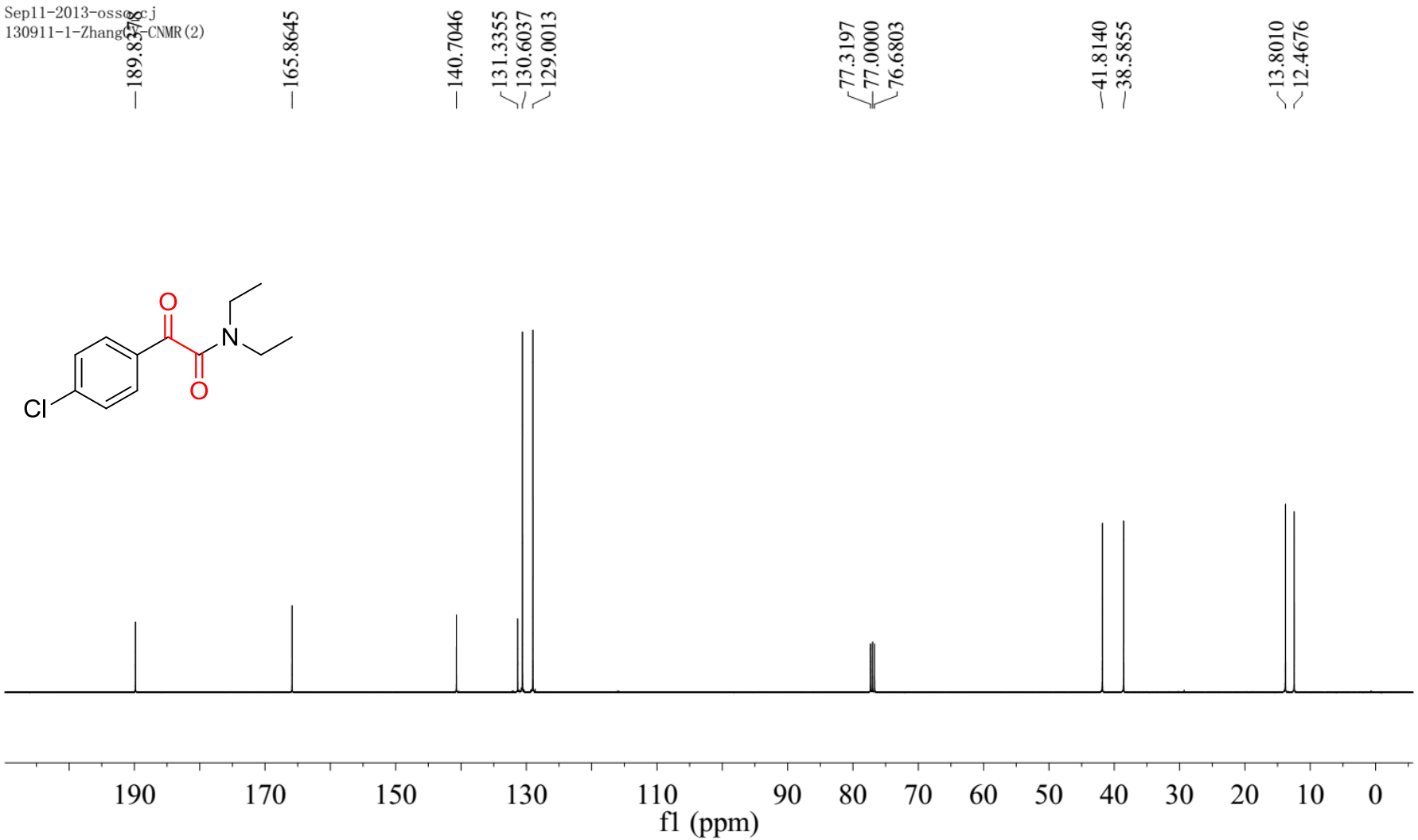
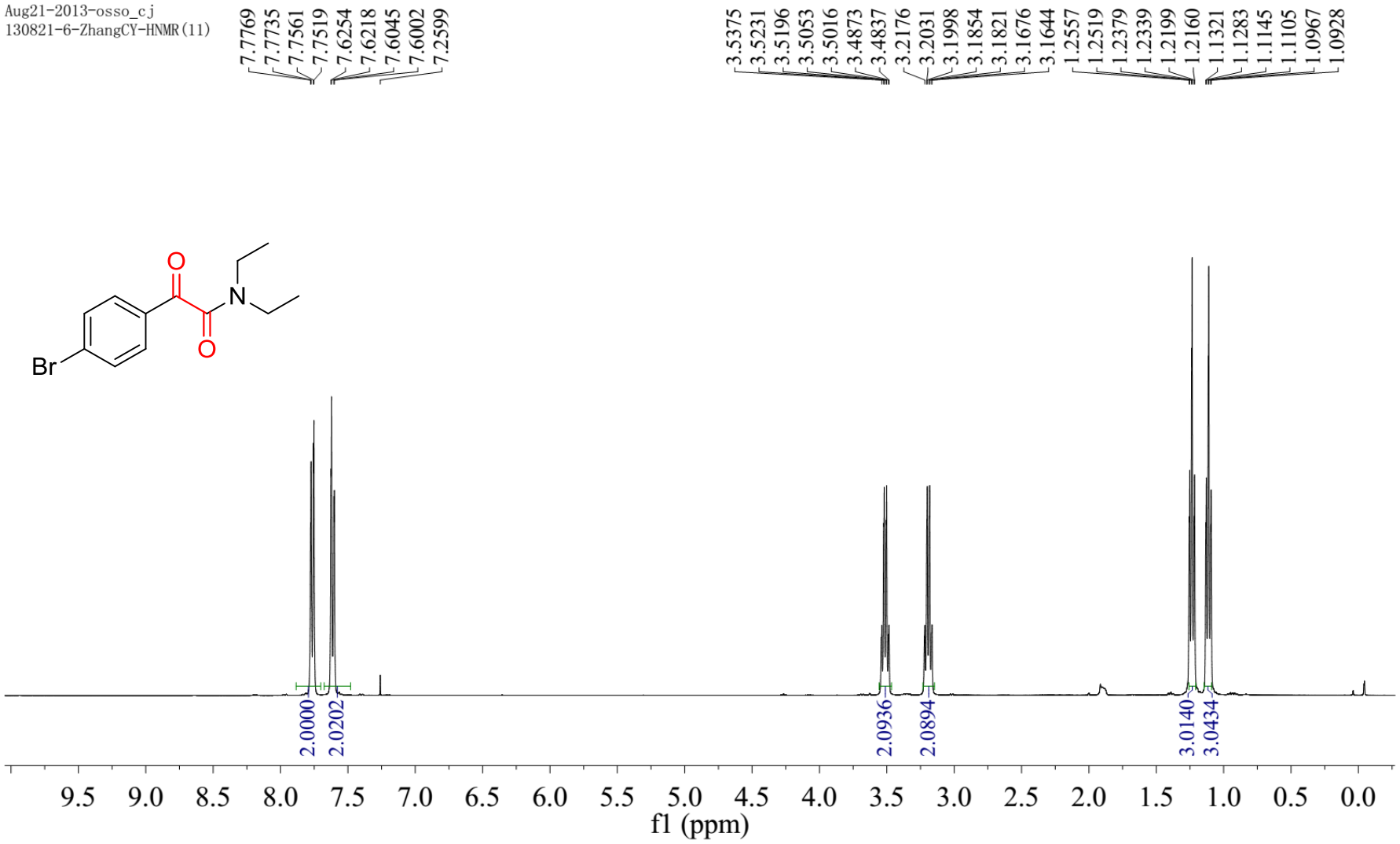
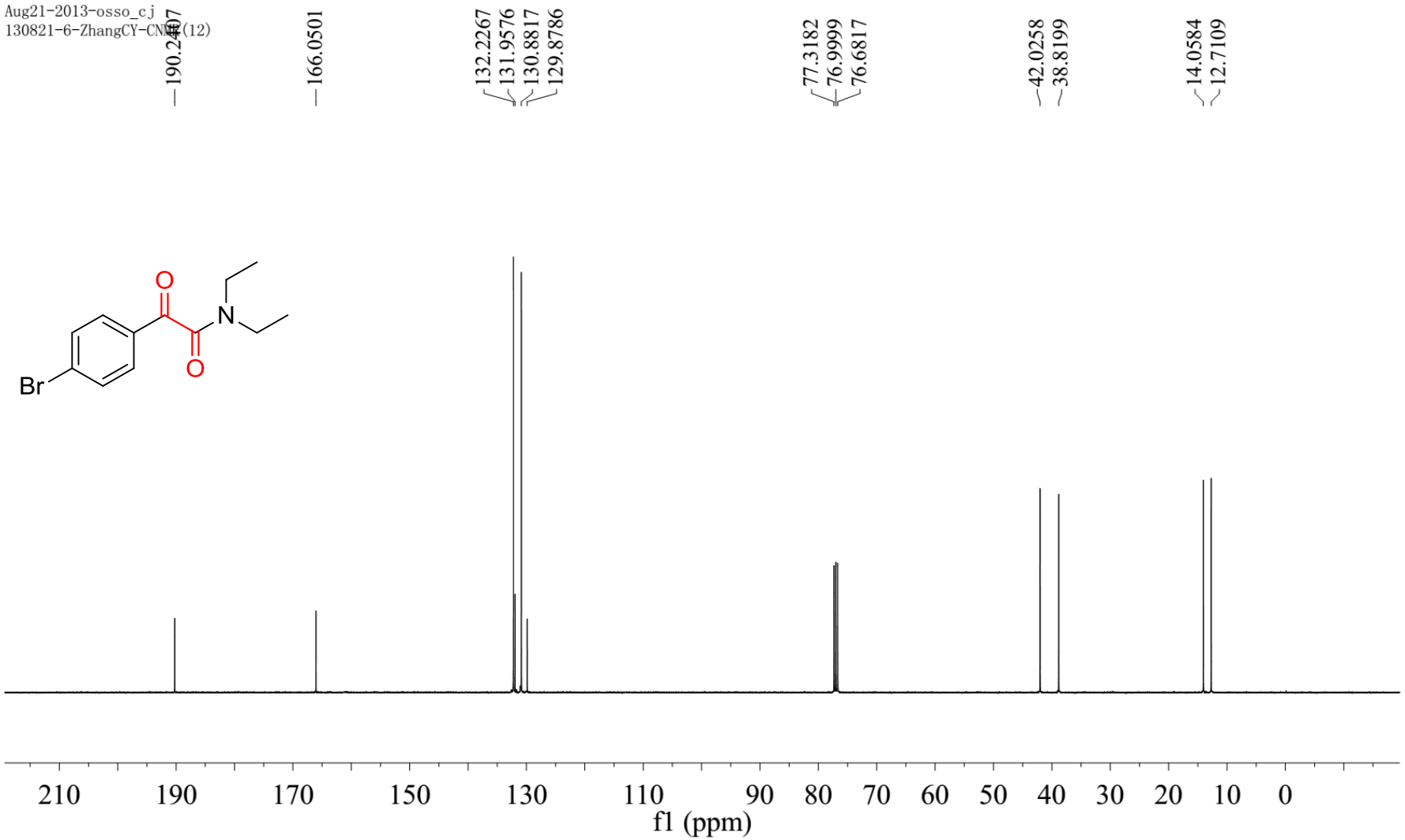
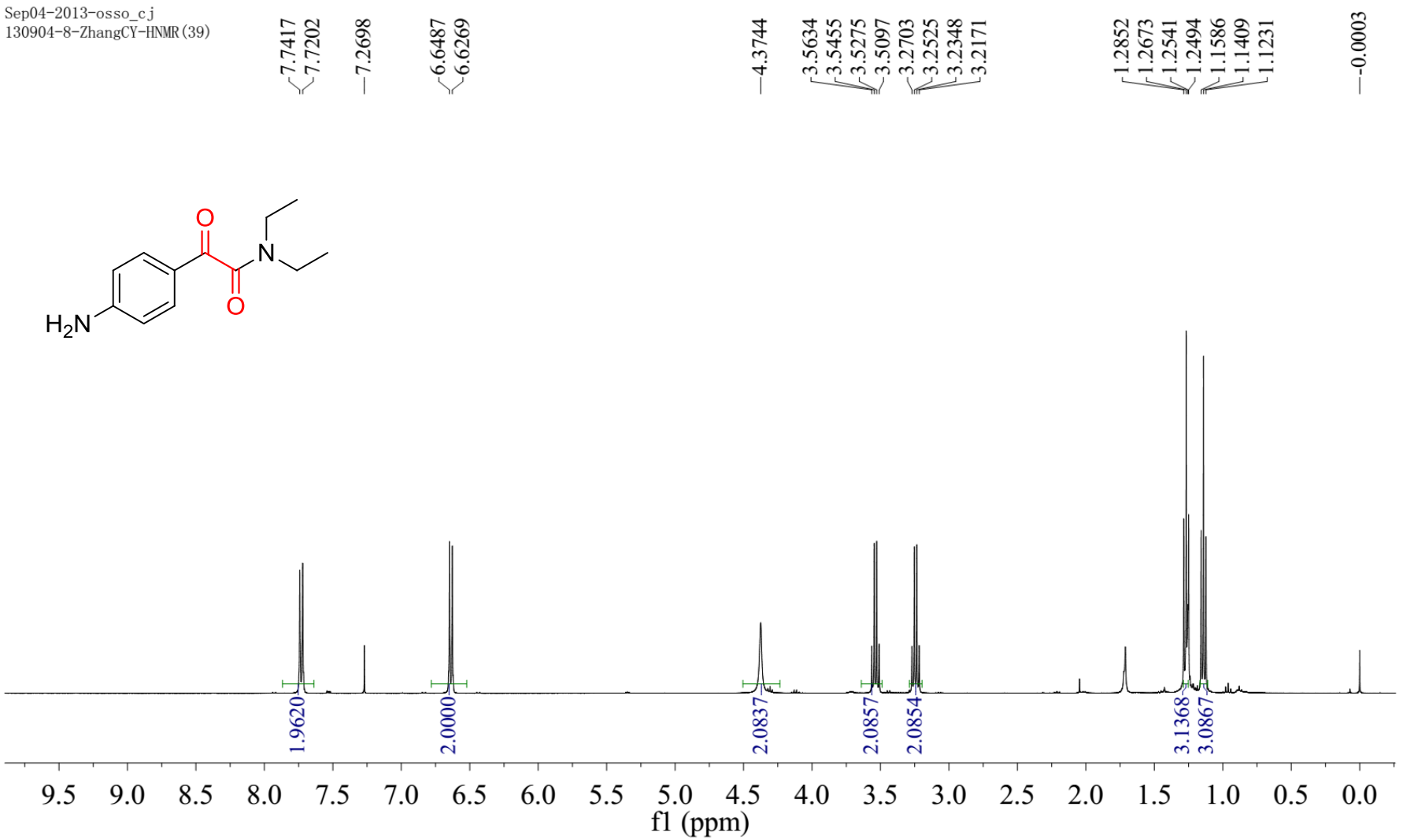
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

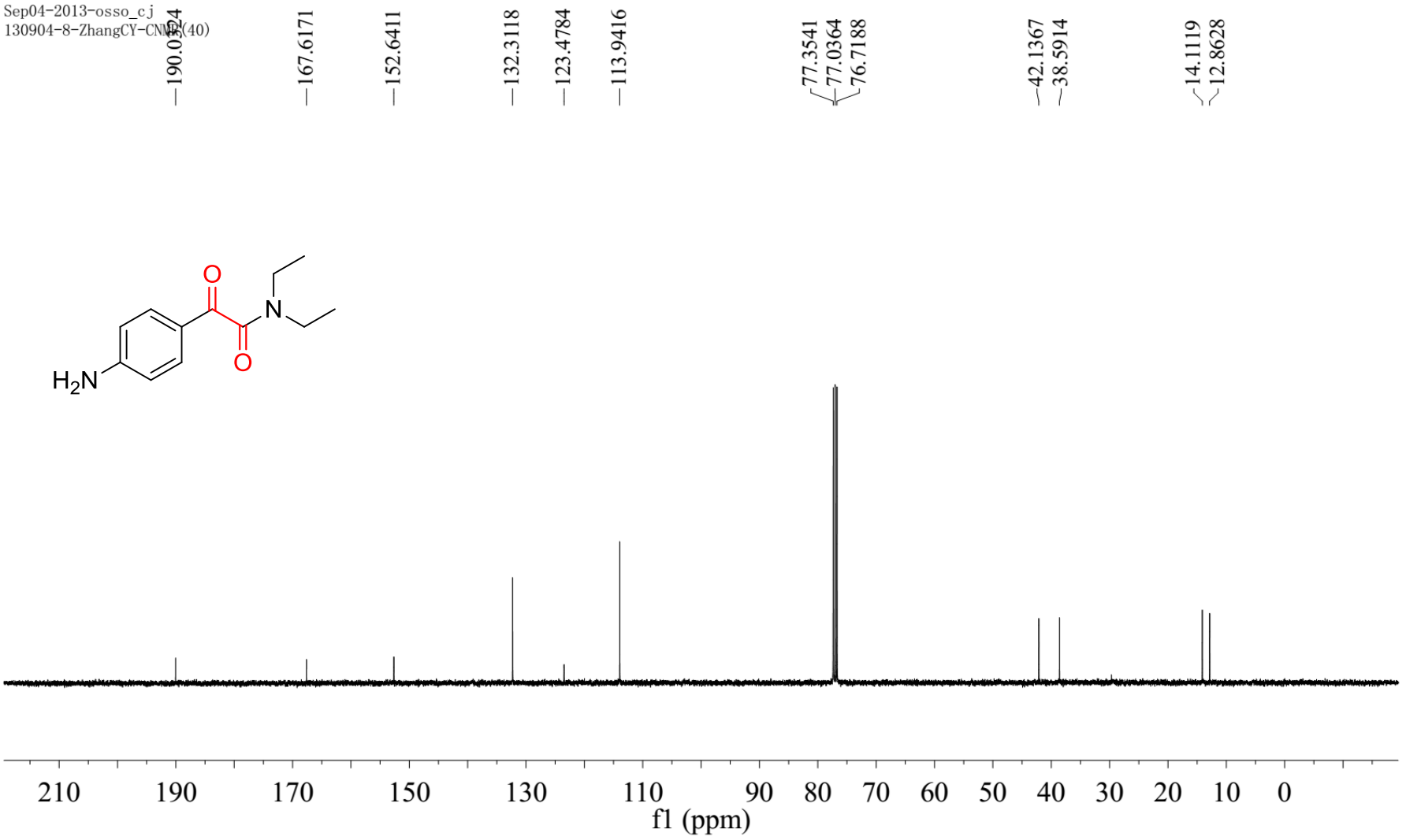

Sep11-2013-osso_cj
130911-1-ZhangCY-HNMR(1)
7.7920
7.7875
7.7706
7.3884
7.3840
7.3670
3.4703
3.4524
3.4344
3.4166
3.1555
3.1377
3.1200
3.1023
1.1818
1.1638
1.1459
1.0573
1.0395
1.0218
O
N
O
Cl
2.0000
2.0027
2.0645
2.0565
3.1250
3.0215
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

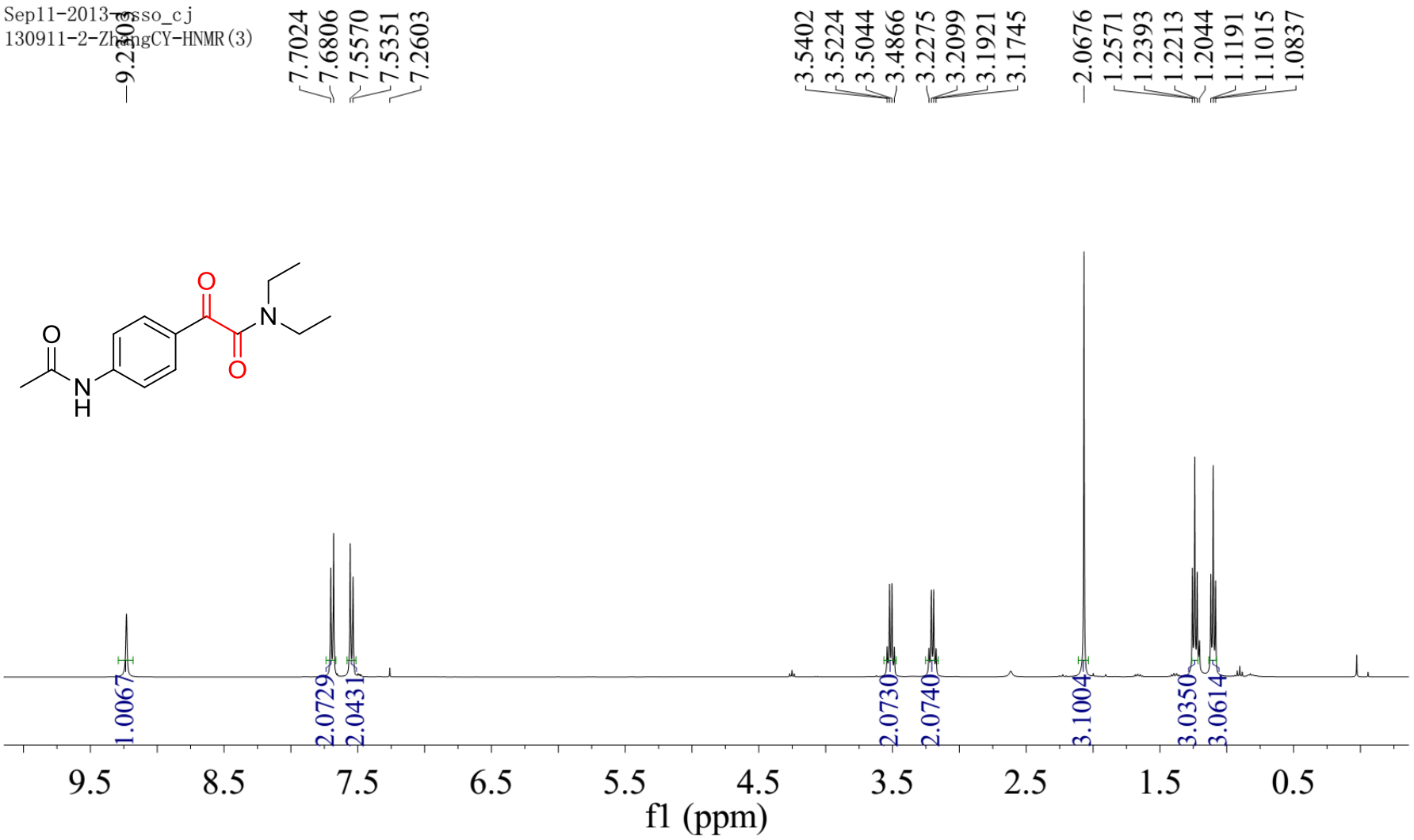

Sep11-2013-ossc.cj
130911-1-Zhang-13-CNMR(2)
189.8378
165.8645
140.7046
131.3355
130.6037
129.0013
77.3197
77.0000
76.6803
41.8140
38.5855
13.8010
12.4676
O
N
O
Cl
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

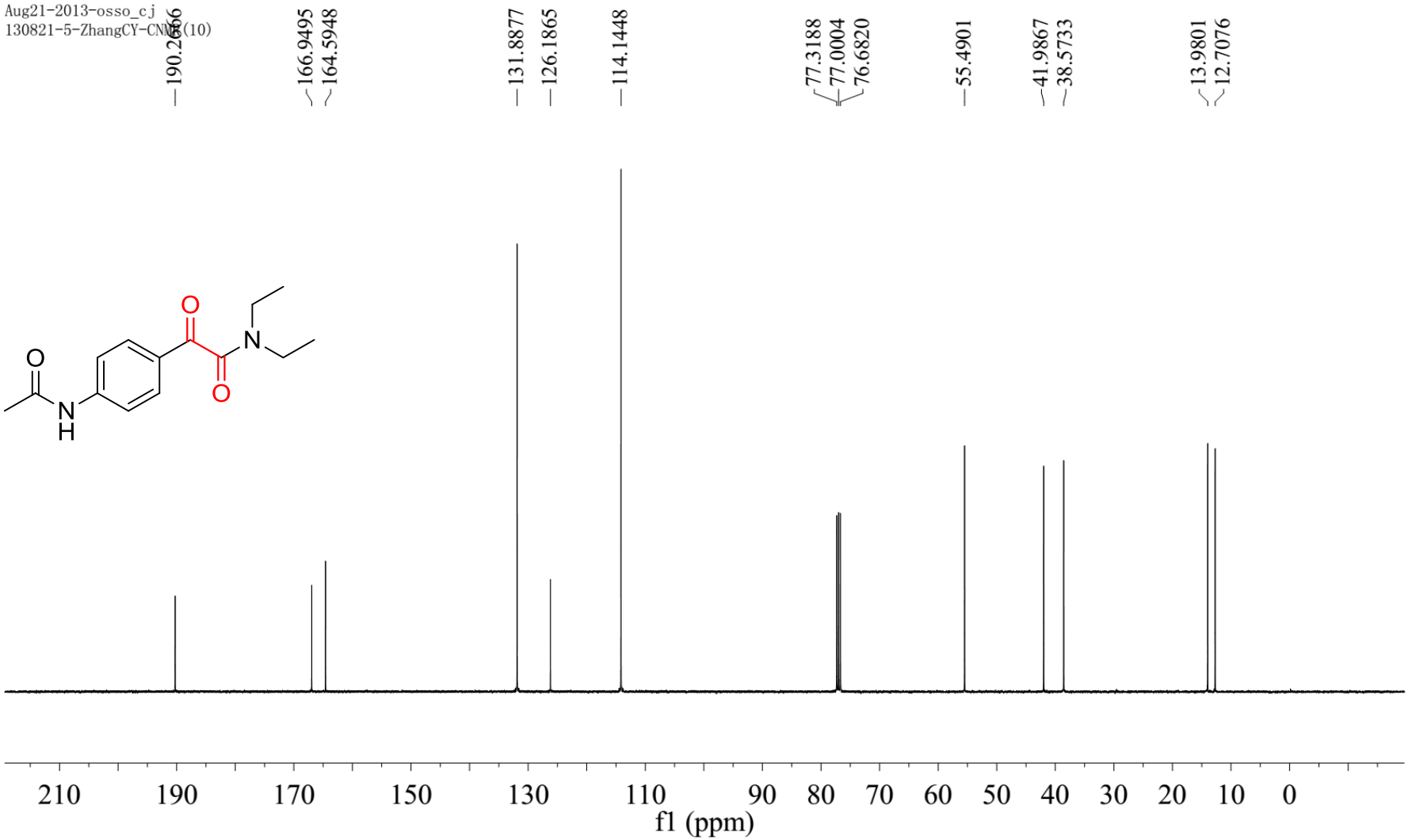

Aug21-2013-osso_cj
130821-6-ZhangCY-HNMR(11)
7.7769
7.7735
7.7561
7.7519
7.6254
7.6218
7.6045
7.6002
7.2599
3.5375
3.5231
3.5196
3.5053
3.5016
3.4873
3.4837
3.2176
3.2031
3.1998
3.1854
3.1821
3.1676
3.1644
1.2557
1.2519
1.2379
1.2339
1.2199
1.2160
1.1321
1.1283
1.1145
1.1105
1.0967
1.0928
O
N
O
Br
2.0000
2.0202
2.0936
2.0894
3.0140
3.0434
9.5 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 1.5 1.0 0.5 0.0
f1 (ppm)

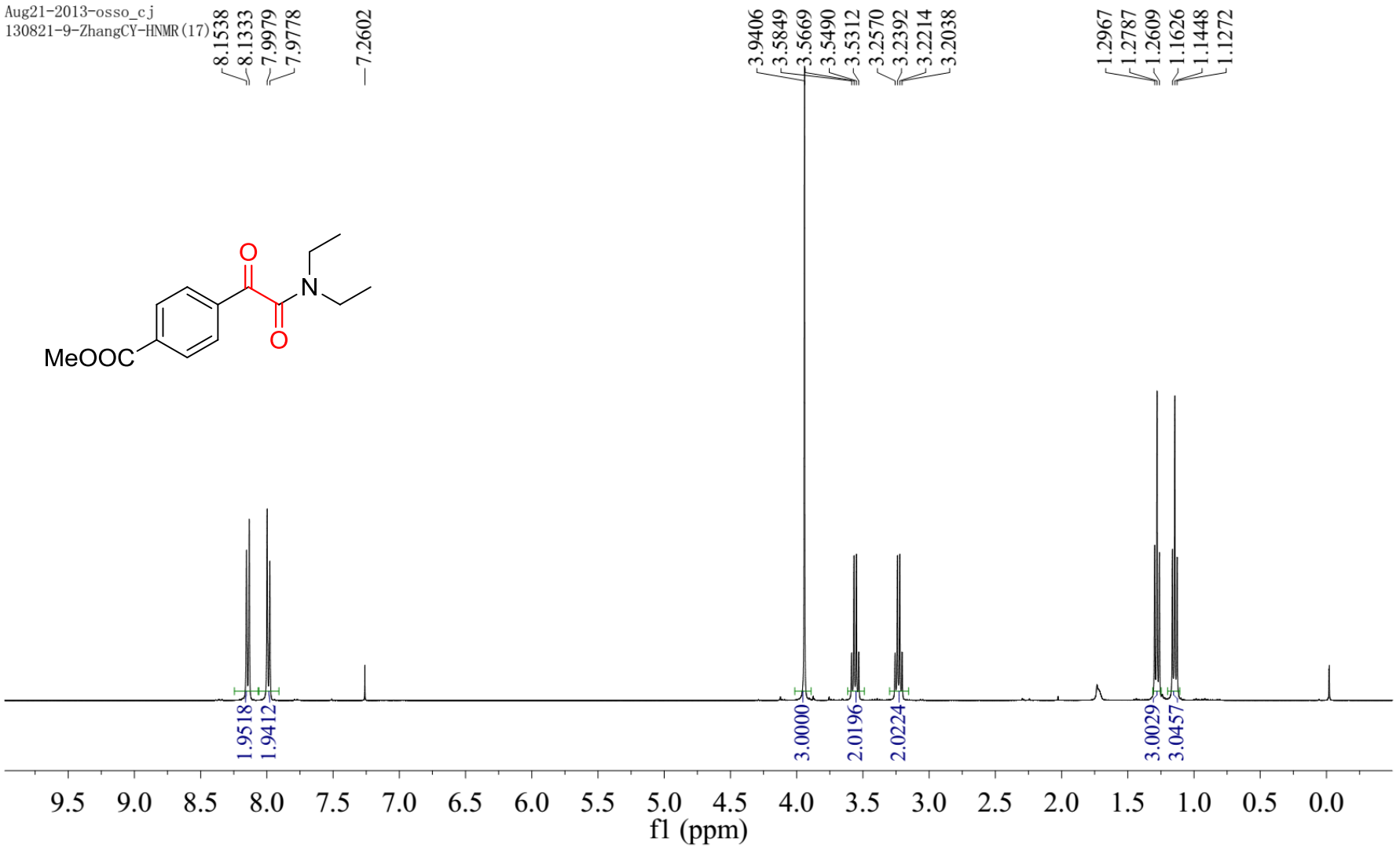

Aug21-2013-osso_cj
130821-6-ZhangCY-CNDF(12)
190.2407
166.0501
132.2267
131.9576
130.8817
129.8786
77.3182
76.9999
76.6817
42.0258
38.8199
14.0584
12.7109
O
N
O
Br
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

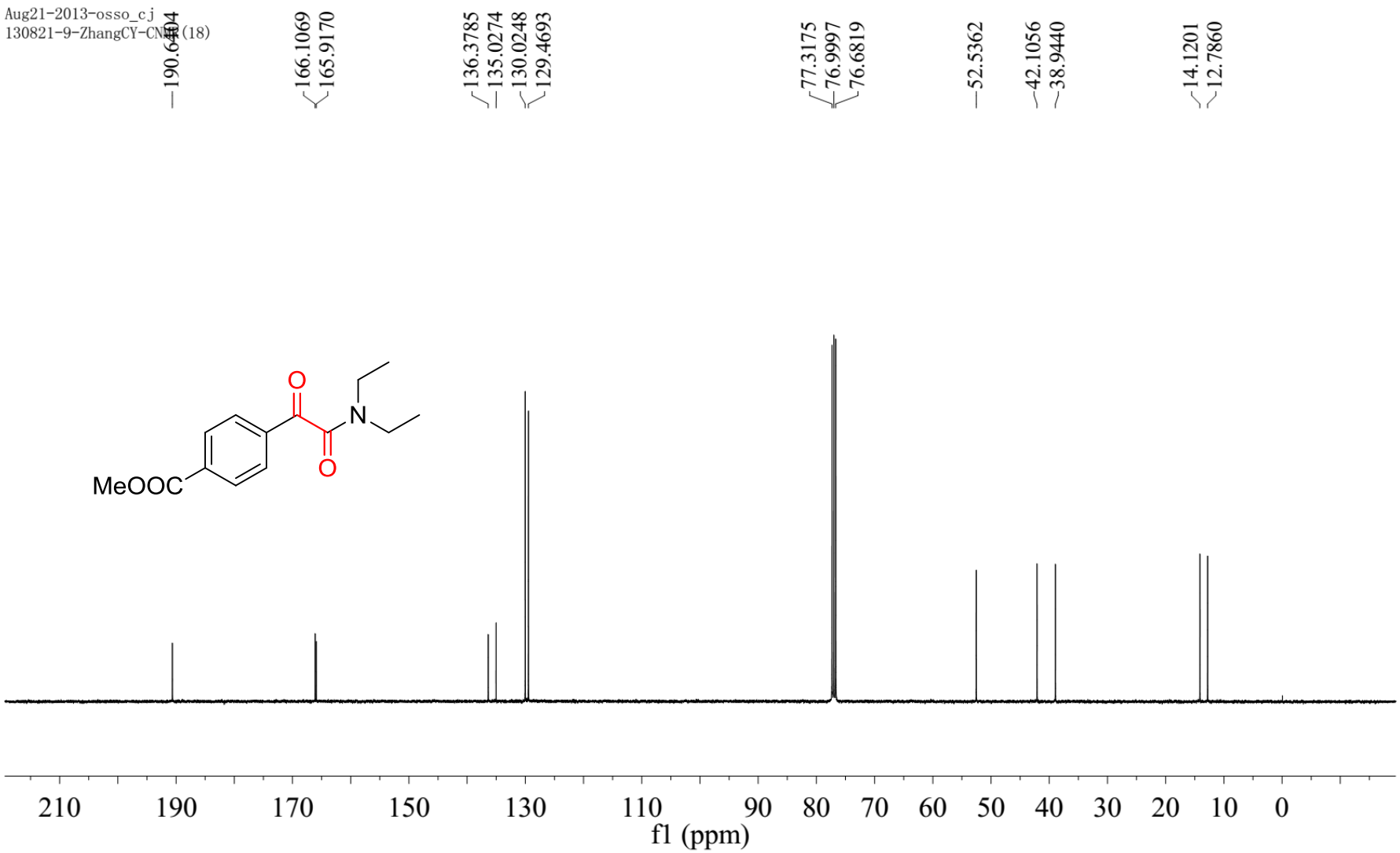

Sep04-2013-osso_cj
130904-8-ZhangCY-HNMR(39)
7.7417
7.7202
7.2698
6.6487
6.6269
4.3744
3.5634
3.5455
3.5275
3.5097
3.2703
3.2525
3.2348
3.2171
1.2852
1.2673
1.2541
1.2494
1.1586
1.1409
1.1231
-0.0003
O
N
O
H2N
1.9620
2.0000
2.0837
2.0857
2.0854
3.1368
3.0867
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

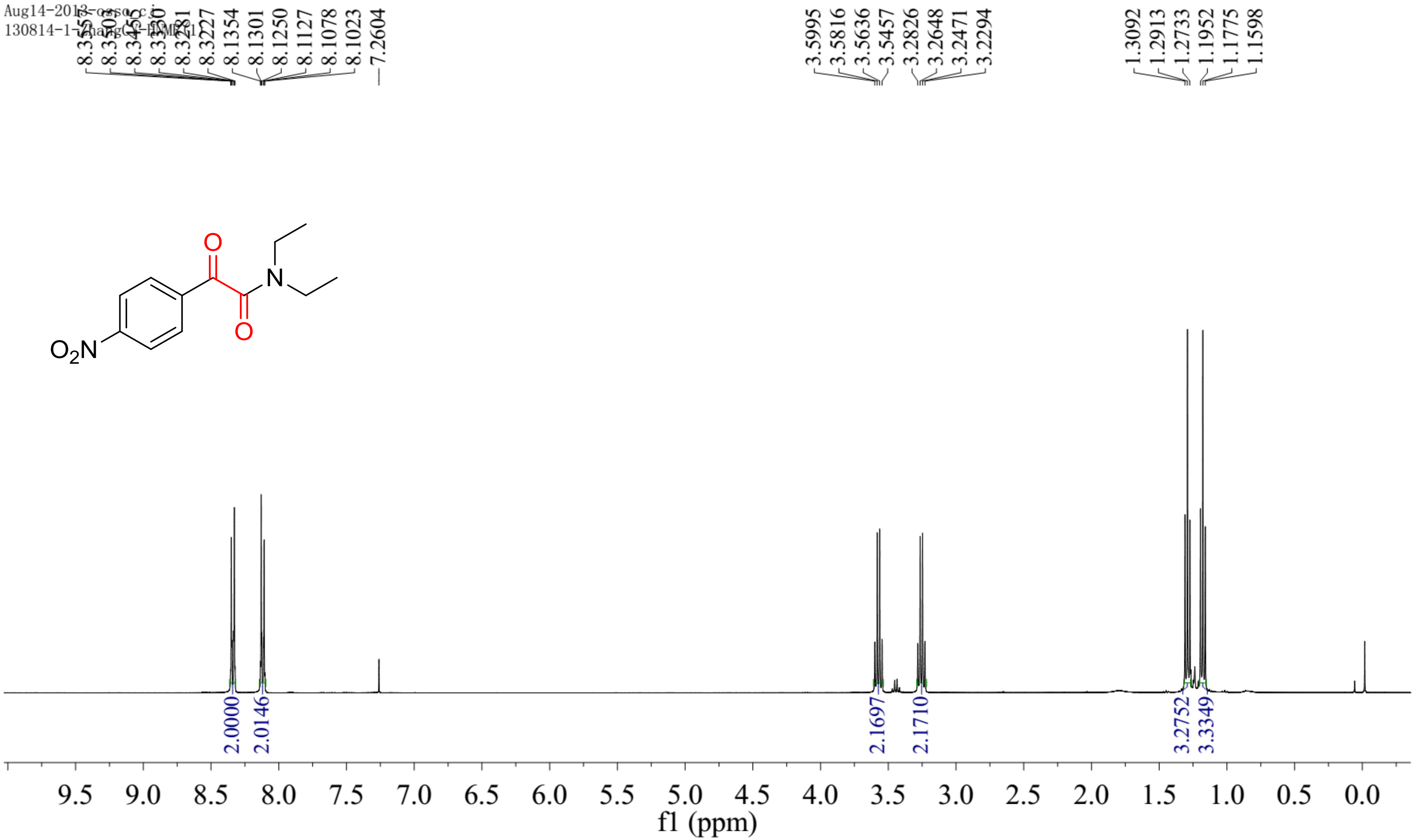

Sep04-2013-osso_cj
130904-8-ZhangCY-CNMR(40)
190.0324
167.6171
152.6411
132.3118
123.4784
113.9416
77.3541
77.0364
76.7188
42.1367
38.5914
14.1119
12.8628
O
N
O
H2N
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Sep11-2013-asso_cj
130911-2-ZhangCY-HNMR(3)
9.2303
7.7024
7.6806
7.5570
7.5351
7.2603
3.5402
3.5224
3.5044
3.4866
3.2275
3.2099
3.1921
3.1745
2.0676
1.2571
1.2393
1.2213
1.2044
1.1191
1.1015
1.0837
O
N
H
O
O
N
1.0067
2.0729
2.0431
2.0730
2.0740
3.1004
3.0350
3.0614
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)

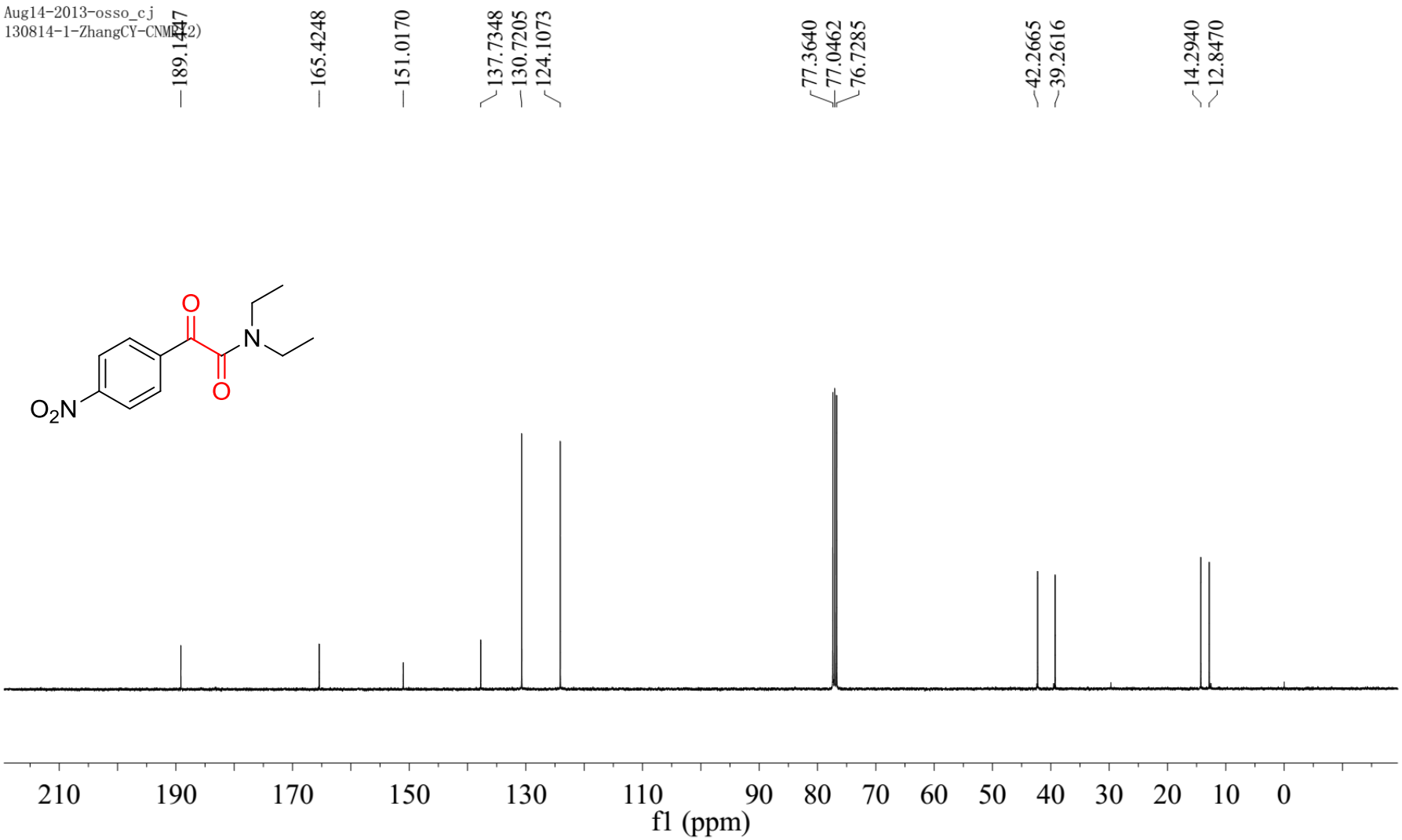

Aug21-2013-osso_cj
130821-5-ZhangCY-CNMR(10)
190.2666
166.9495
164.5948
131.8877
126.1865
114.1448
77.3188
77.0004
76.6820
55.4901
41.9867
38.5733
13.9801
12.7076
O
N
H
O
O
N
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

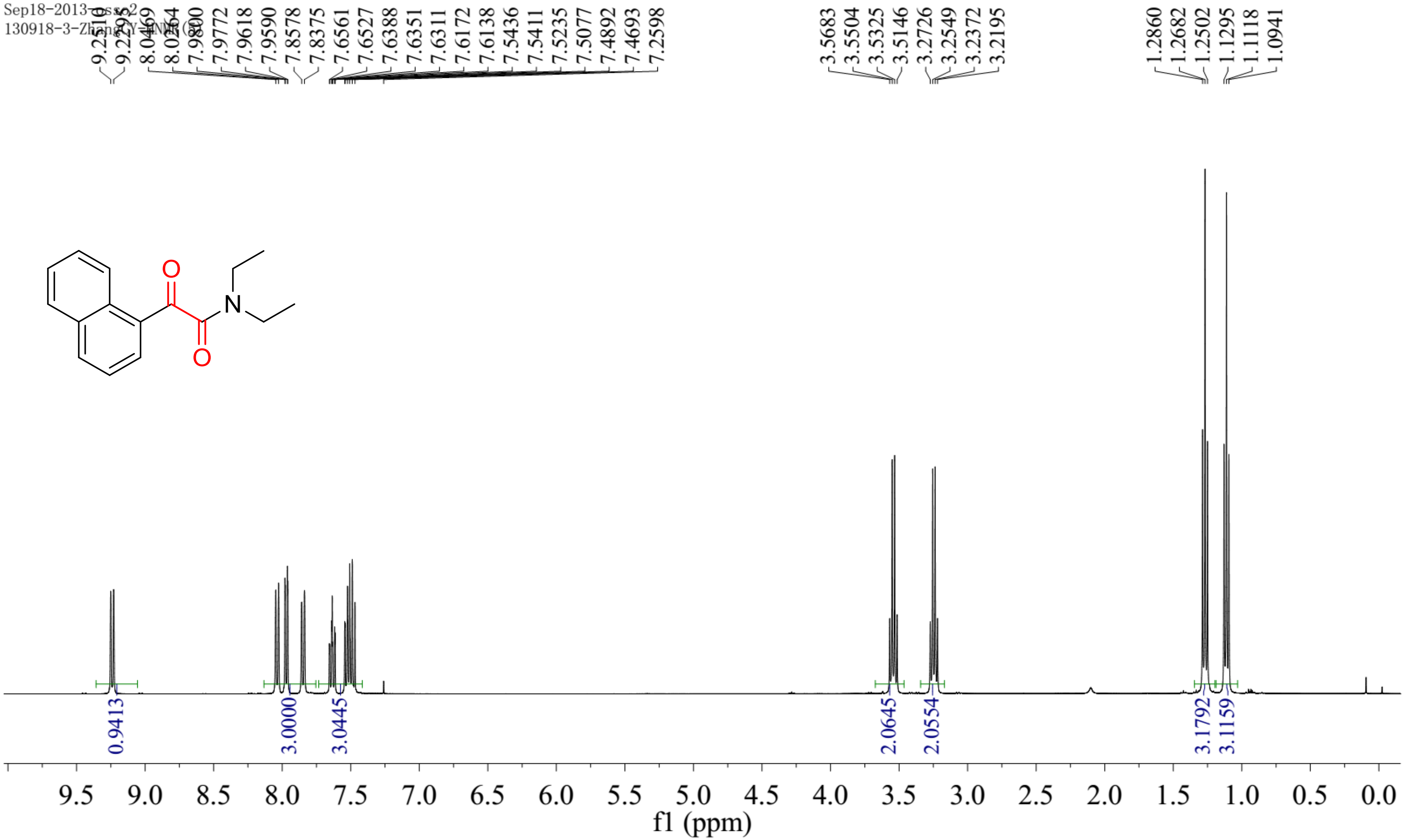

Aug21-2013-osso_cj
130821-9-ZhangCY-HNMR(17)
8.1538
8.1333
7.9979
7.9778
7.2602
3.9406
3.5849
3.5669
3.5490
3.5312
3.2570
3.2392
3.2214
3.2038
1.2967
1.2787
1.2609
1.1626
1.1448
1.1272
O
N
O
MeOOC
1.9518
1.9412
3.0000
2.0196
2.0224
3.0029
3.0457
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

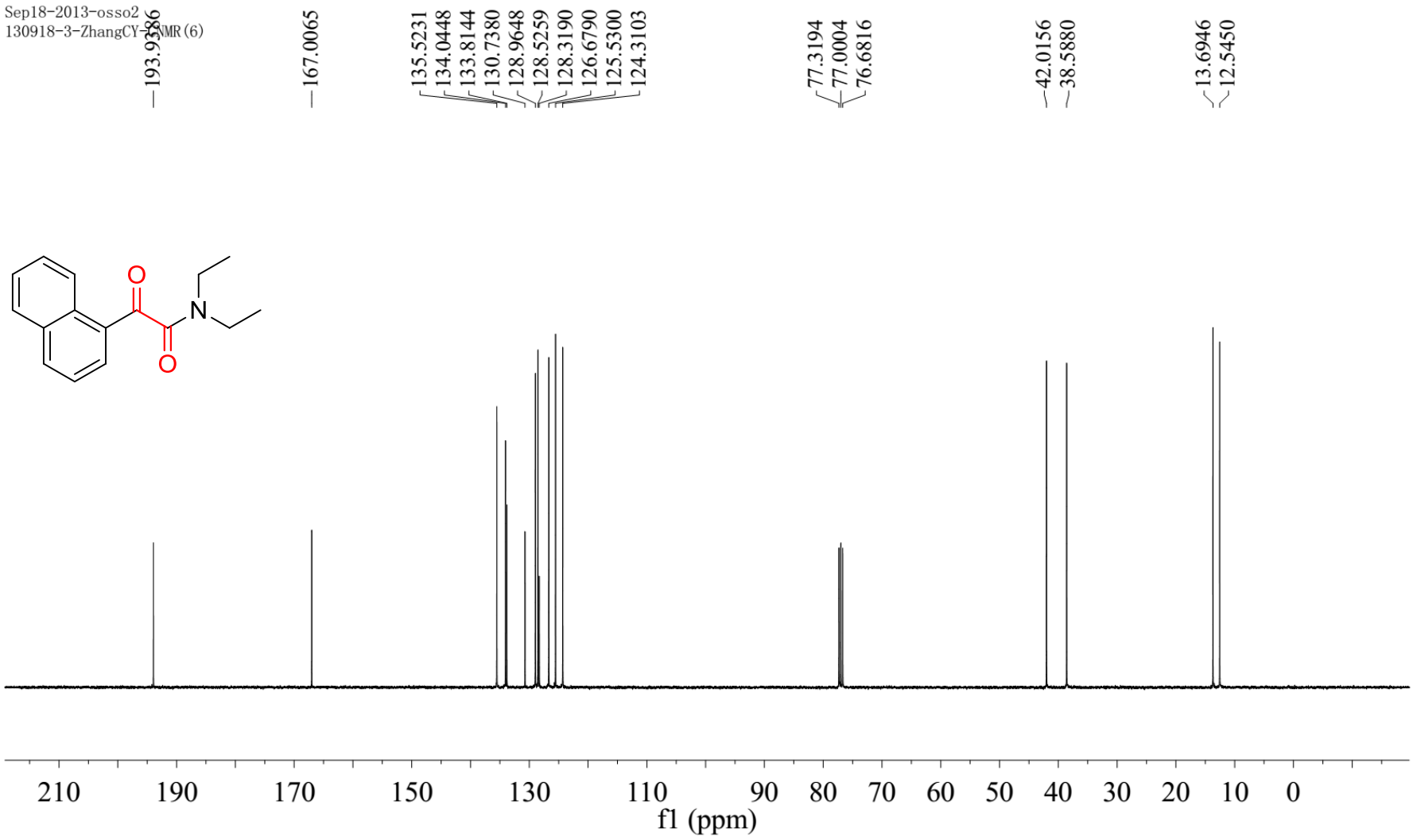

Aug21-2013-osso_cj
130821-9-ZhangCY-CNMR(18)
190.6404
166.1069
165.9170
136.3785
135.0274
130.0248
129.4693
77.3175
76.9997
76.6819
52.5362
42.1056
38.9440
14.1201
12.7860
O
N
O
MeOOC
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



8.1354
8.1301
8.1250
8.1127
8.1078
8.1023
7.2604
3.5995
3.5816
3.5636
3.5457
3.2826
3.2648
3.2471
3.2294
1.3092
1.2913
1.2733
1.1952
1.1775
1.1598
O
N
O
O₂N
2.0000
2.0146
2.1697
2.1710
3.2752
3.3349
9.5
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
1.5
1.0
0.5
0.0
f1 (ppm)


Aug14-2013-osso_cj
130814-1-ZhangCY-CNMR(2)
189.1447
165.4248
151.0170
137.7348
130.7205
124.1073
77.3640
77.0462
76.7285
42.2665
39.2616
14.2940
12.8470
O
N
O
O2N
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Sep18-2013-ssss2
130918-3-ZhangY-HNMR(5)
9.2510
9.2295
8.0469
8.0264
7.9800
7.9772
7.9618
7.9590
7.8578
7.8375
7.6561
7.6527
7.6388
7.6351
7.6311
7.6172
7.6138
7.5436
7.5411
7.5235
7.5077
7.4892
7.4693
7.2598
3.5683
3.5504
3.5325
3.5146
3.2726
3.2549
3.2372
3.2195
1.2860
1.2682
1.2502
1.1295
1.1118
1.0941
O
N
O
0.9413
3.0000
3.0445
2.0645
2.0554
3.1792
3.1159
9.5 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 1.5 1.0 0.5 0.0
f1 (ppm)


Sep18-2013-osso2
130918-3-ZhangCY-13CNMR(6)
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135.5231
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133.8144
130.7380
128.9648
128.5259
128.3190
126.6790
125.5300
124.3103
77.3194
77.0004
76.6816
42.0156
38.5880
13.6946
12.5450
O
N
O
210
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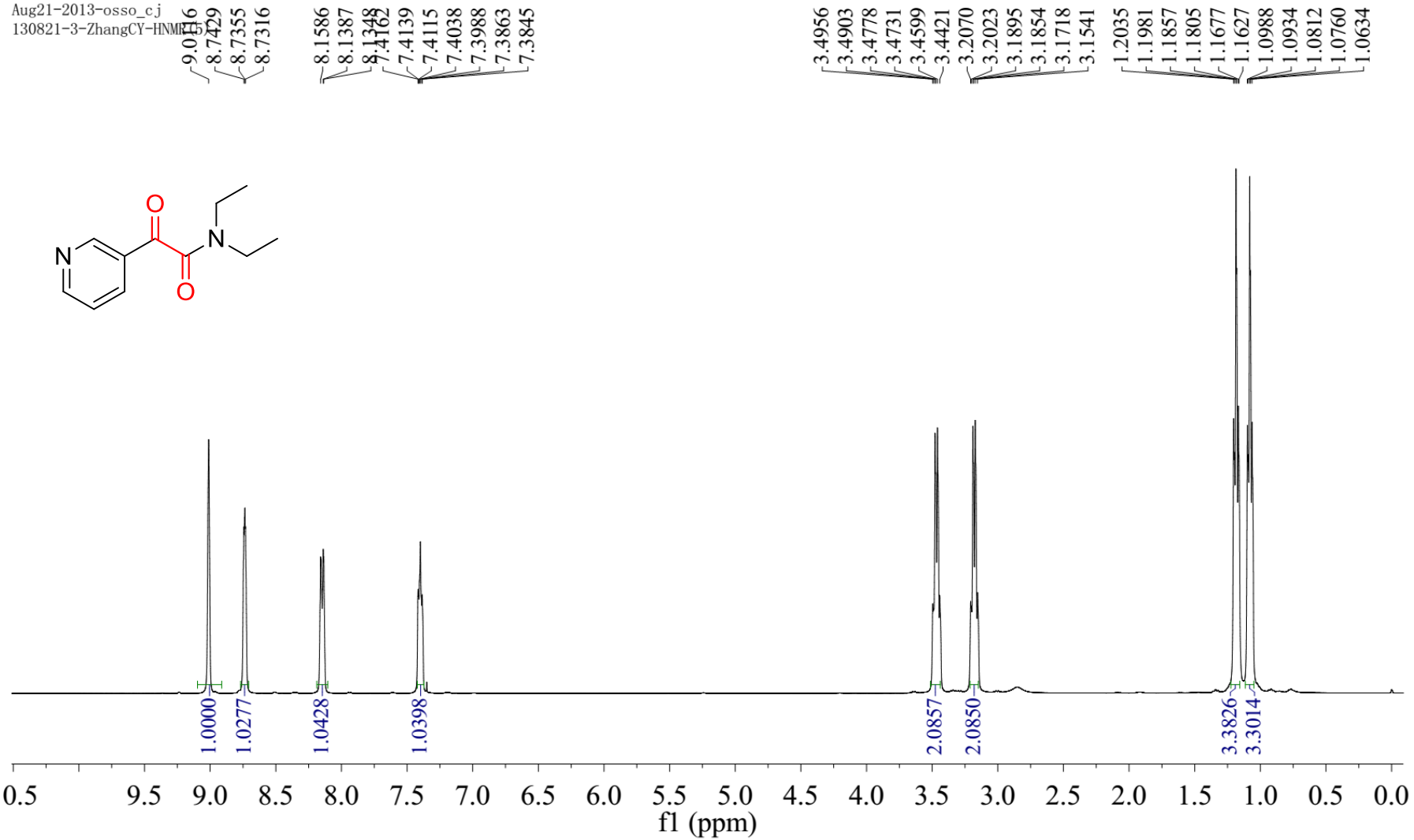
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Aug21-2013-osso_cj
130821-3-ZhangCY-HNMR-15
9.0116
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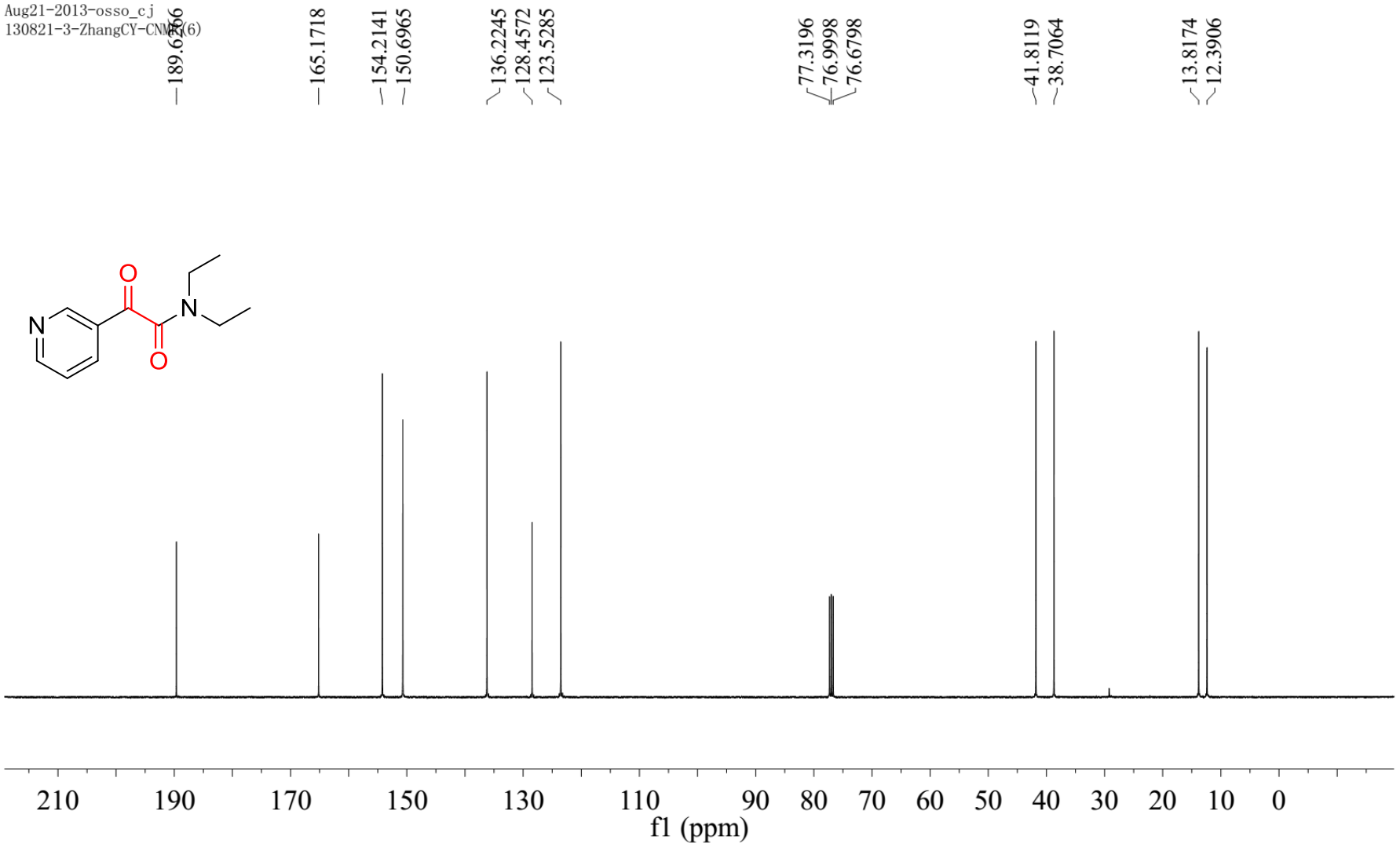
8.7355
8.7316
8.1586
8.1387
8.1348
7.4162
7.4139
7.4115
7.4038
7.3988
7.3863
7.3845
3.4956
3.4903
3.4778
3.4731
3.4599
3.4421
3.2070
3.2023
3.1895
3.1854
3.1718
3.1541
1.2035
1.1981
1.1857
1.1805
1.1677
1.1627
1.0988
1.0934
1.0812
1.0760
1.0634
O
N
O
N
1.0000
1.0277
1.0428
1.0398
2.0857
2.0850
3.3826
3.3014
0.5
9.5
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
1.5
1.0
0.5
0.0
f1 (ppm)


Aug21-2013-osso_cj
130821-3-ZhangCY-CNMR(6)
189.6266
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154.2141
150.6965
136.2245
128.4572
123.5285
77.3196
76.9998
76.6798
41.8119
38.7064
13.8174
12.3906
O
N
O
N
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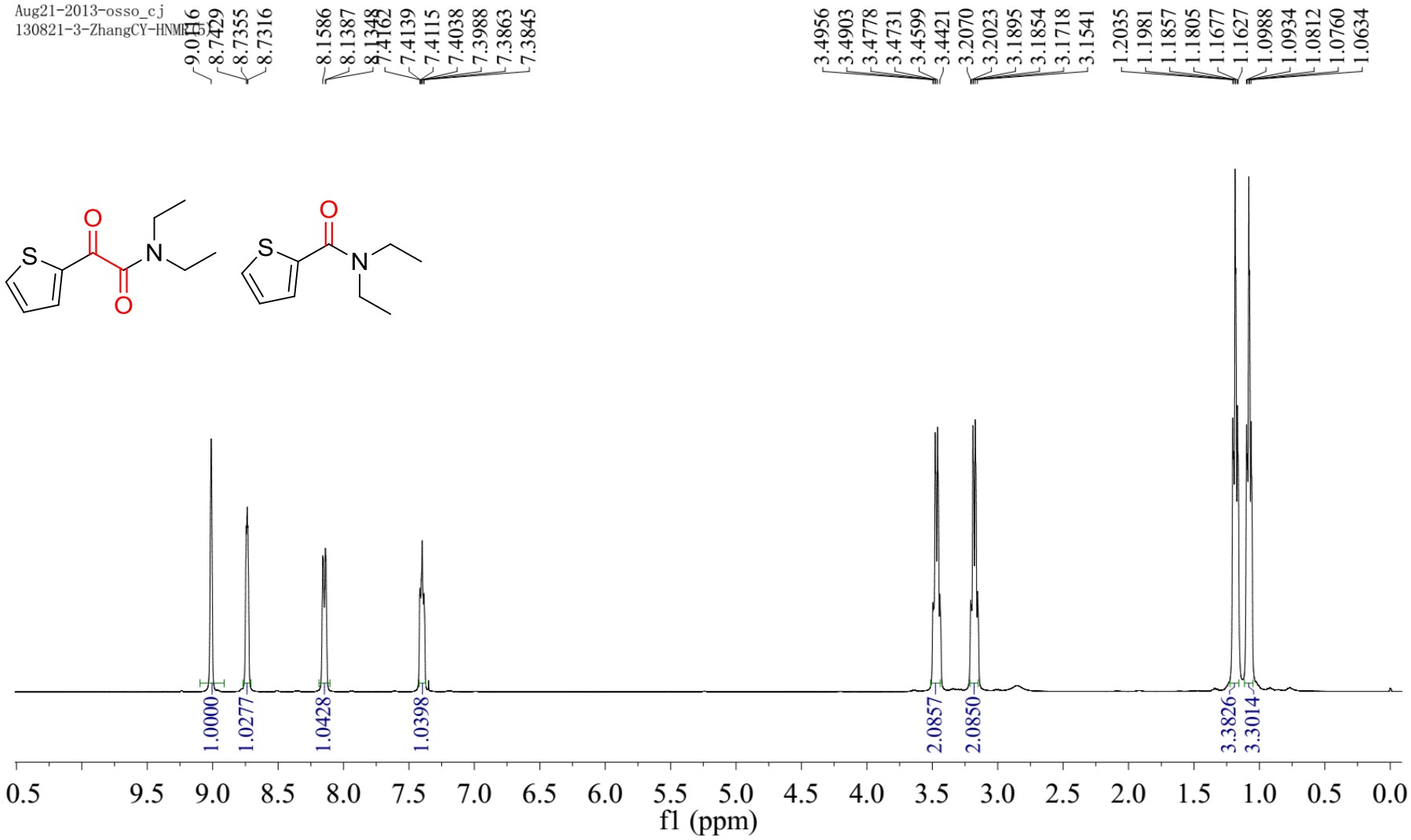
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Aug21-2013-osso_cj
130821-3-ZhangCY-HNMR-5
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8.7316
8.1586
8.1387
8.1348
7.4162
7.4139
7.4115
7.4038
7.3988
7.3863
7.3845
3.4956
3.4903
3.4778
3.4731
3.4599
3.4421
3.2070
3.2023
3.1895
3.1854
3.1718
3.1541
1.2035
1.1981
1.1857
1.1805
1.1677
1.1627
1.0988
1.0934
1.0812
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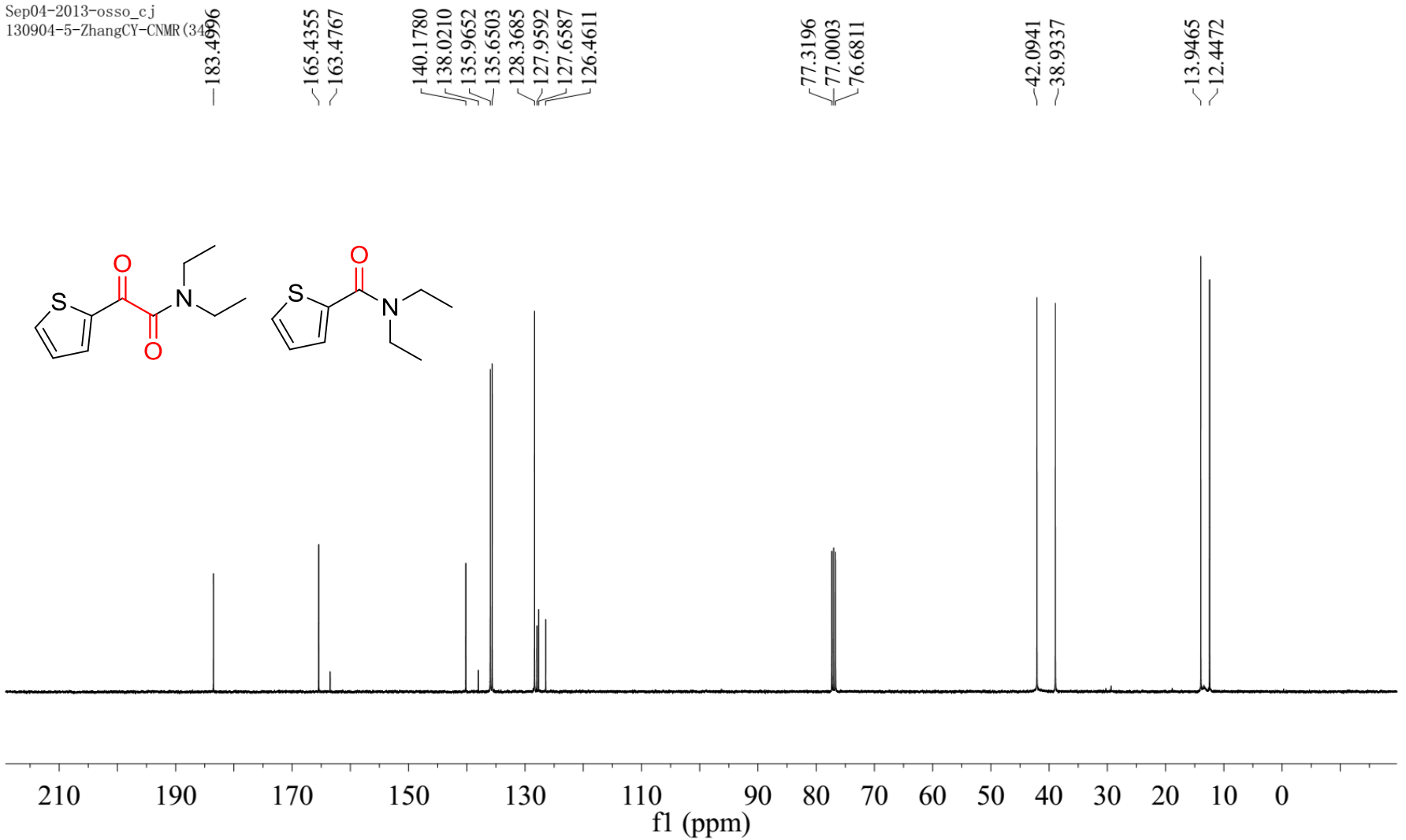
N
O
O
S
N
1.0000
1.0277
1.0428
1.0398
2.0857
2.0850
3.3826
3.3014
0.5
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


Sep04-2013-osso_cj
130904-5-ZhangCY-CNMR(34
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140.1780
138.0210
135.9652
135.6503
128.3685
127.9592
127.6587
126.4611
77.3196
77.0003
76.6811
42.0941
38.9337
13.9465
12.4472
O
S
N
O
O
S
N
210
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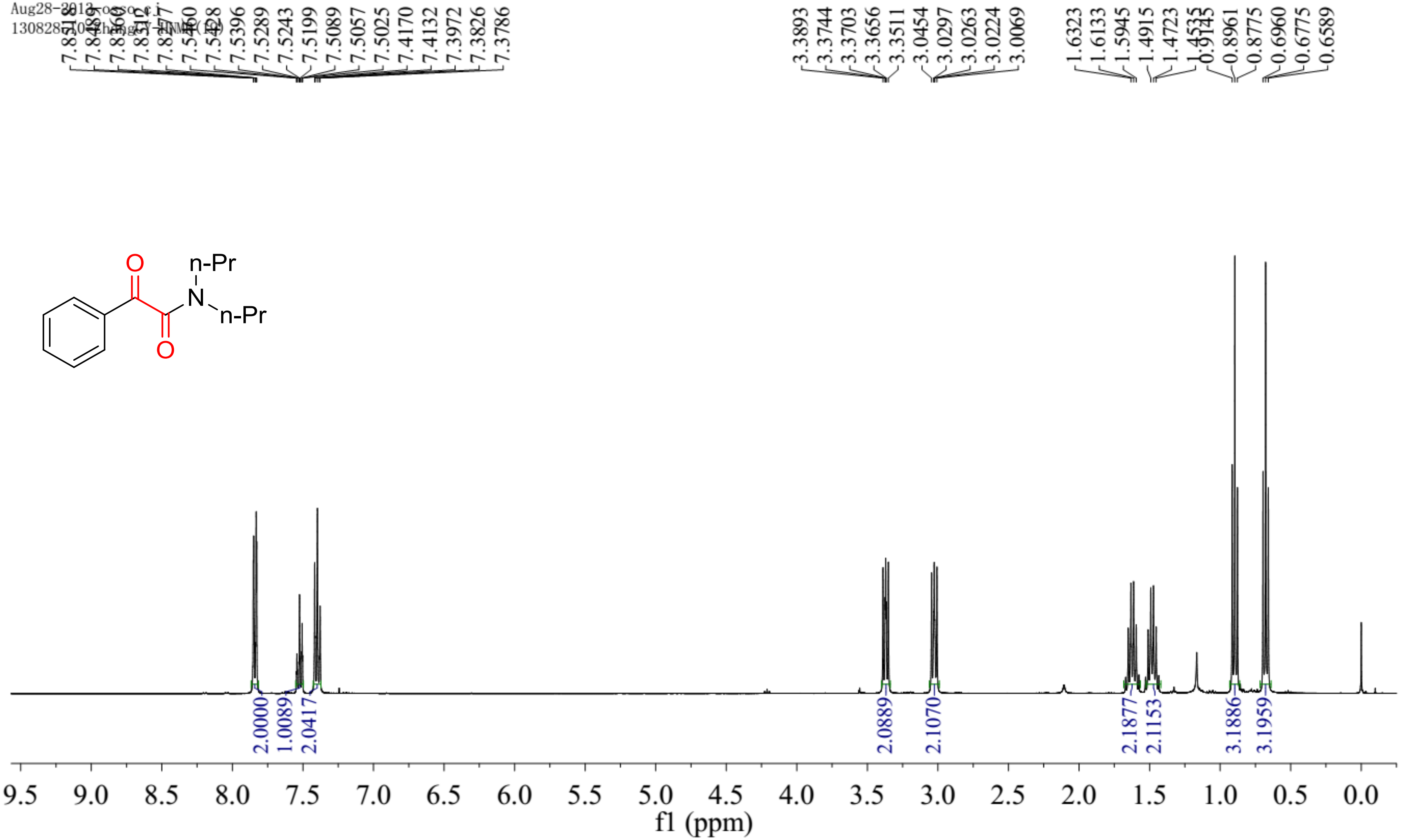
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


O
n-Pr
N
n-Pr
O
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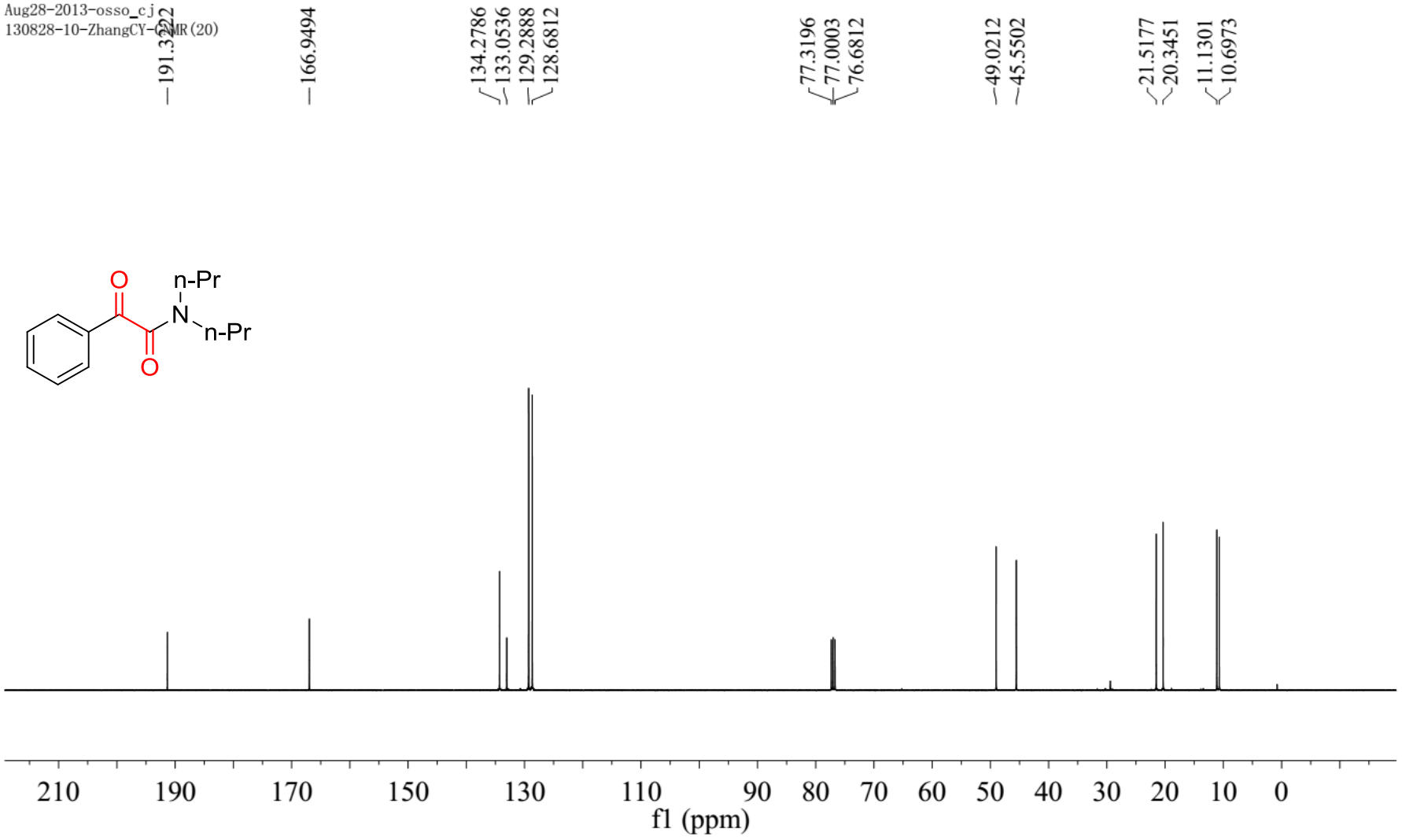
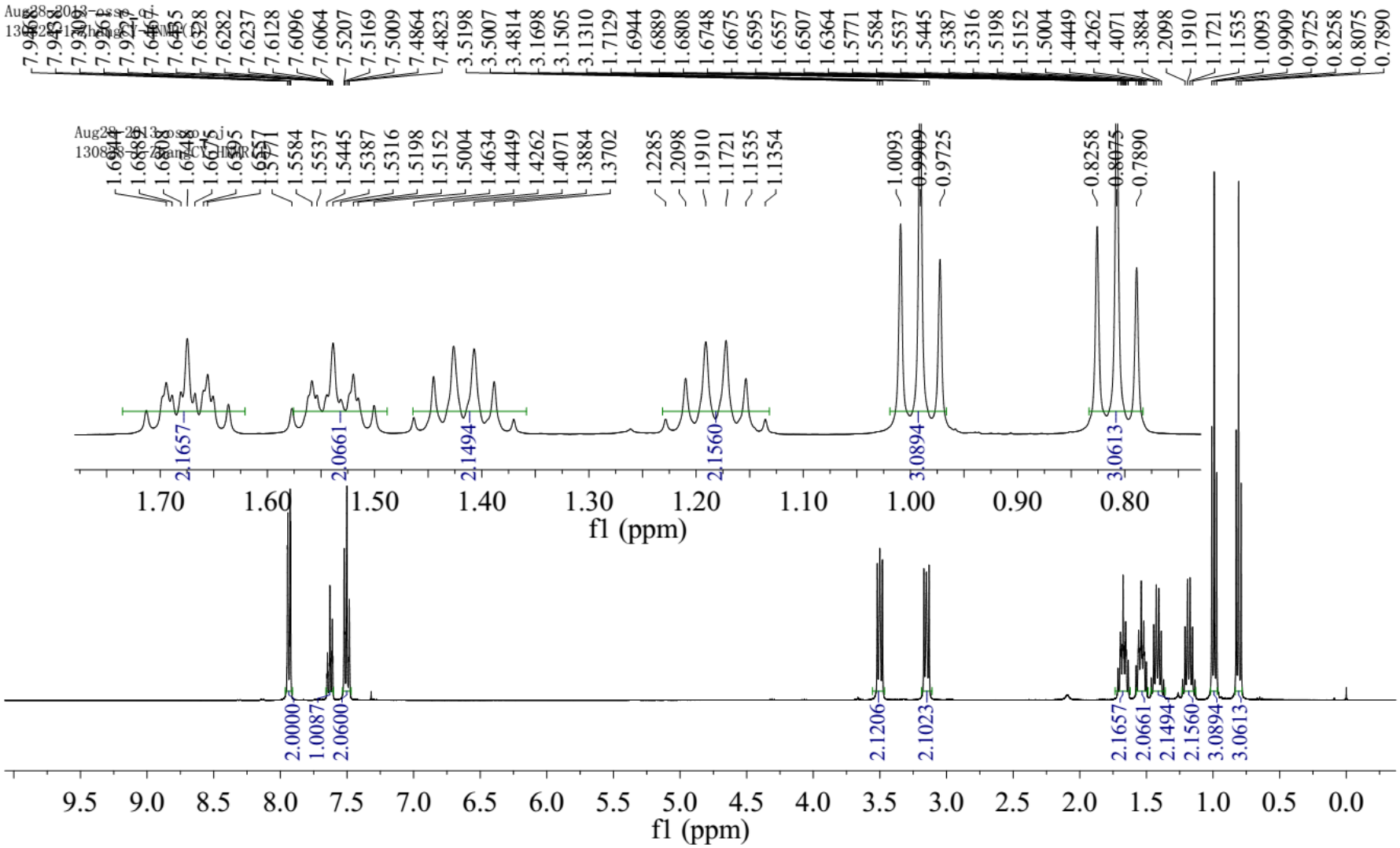
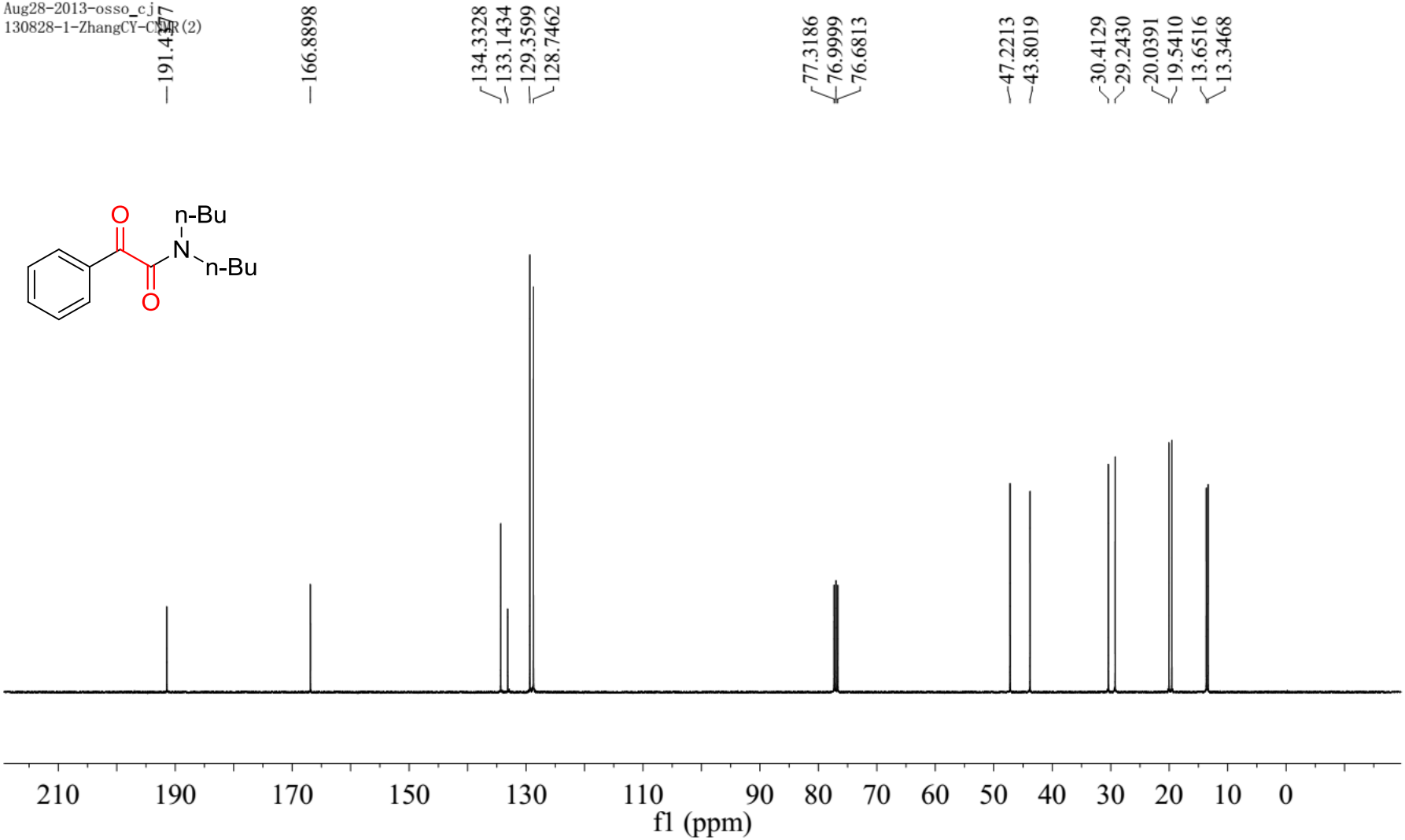
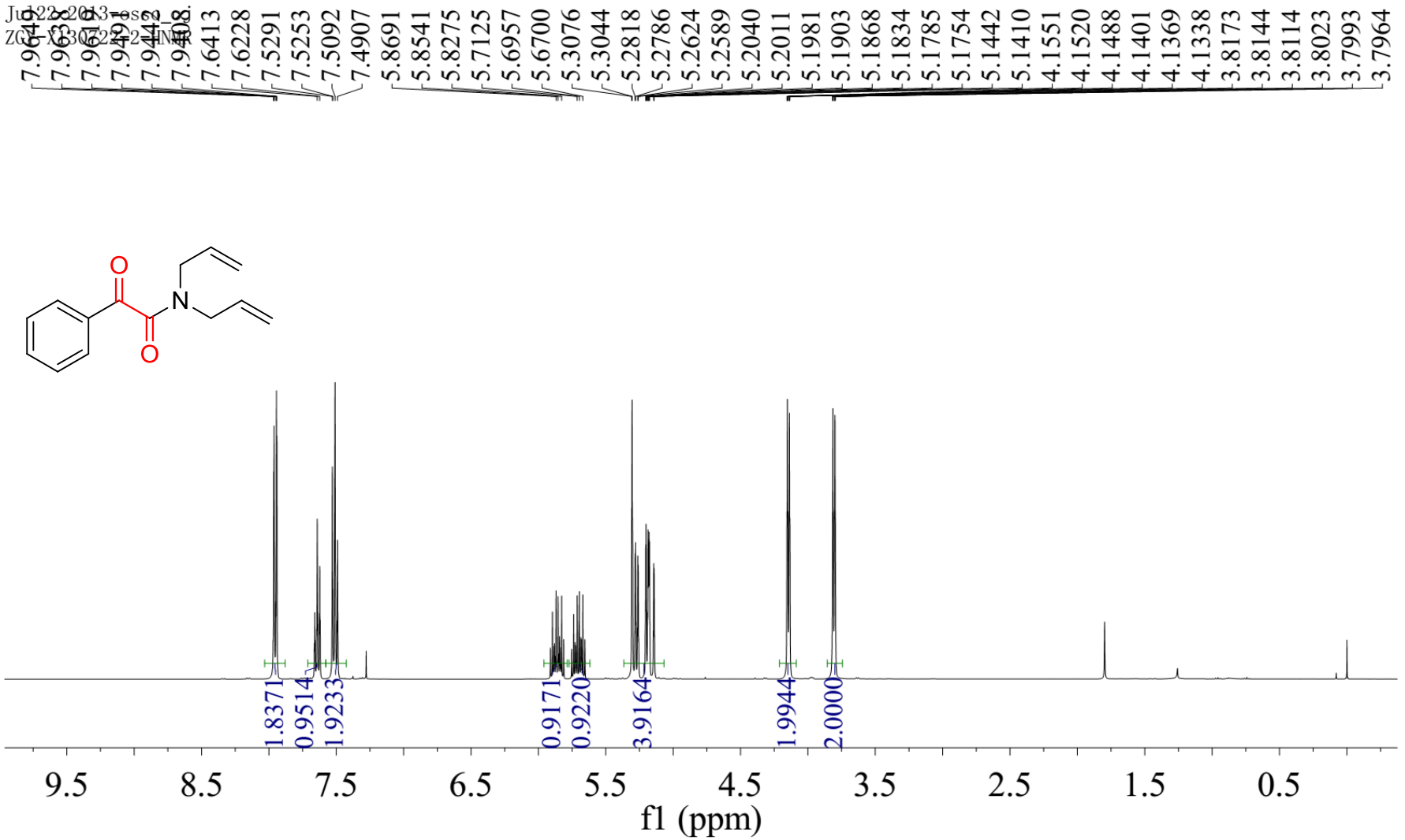
1.0089
2.0417
2.0889
2.1070
2.1877
2.1153
3.1886
3.1959
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


Aug28-2013-osso_cj
130828-10-ZhangCY-C13MR(20)
191.3222
166.9494
134.2786
133.0536
129.2888
128.6812
77.3196
77.0003
76.6812
49.0212
45.5502
21.5177
20.3451
11.1301
10.6973
O
n-Pr
N
n-Pr
O
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


fl (ppm)
fl (ppm)


Aug28-2013-osso_cj
130828-1-ZhangCY-CNMR(2)
191.4177
166.8898
134.3328
133.1434
129.3599
128.7462
77.3186
76.9999
76.6813
47.2213
43.8019
30.4129
29.2430
20.0391
19.5410
13.6516
13.3468
O
n-Bu
N
n-Bu
O
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.5291
7.5253
7.5092
7.4907
5.8691
5.8541
5.8275
5.7125
5.6957
5.6700
5.3076
5.3044
5.2818
5.2786
5.2624
5.2589
5.2040
5.2011
5.1981
5.1903
5.1868
5.1834
5.1785
5.1754
5.1442
5.1410
4.1551
4.1520
4.1488
4.1401
4.1369
4.1338
3.8173
3.8144
3.8114
3.8023
3.7993
3.7964
O
N
O
1.8371
0.9514
1.9233
0.9171
0.9220
3.9164
1.9944
2.0000
9.5
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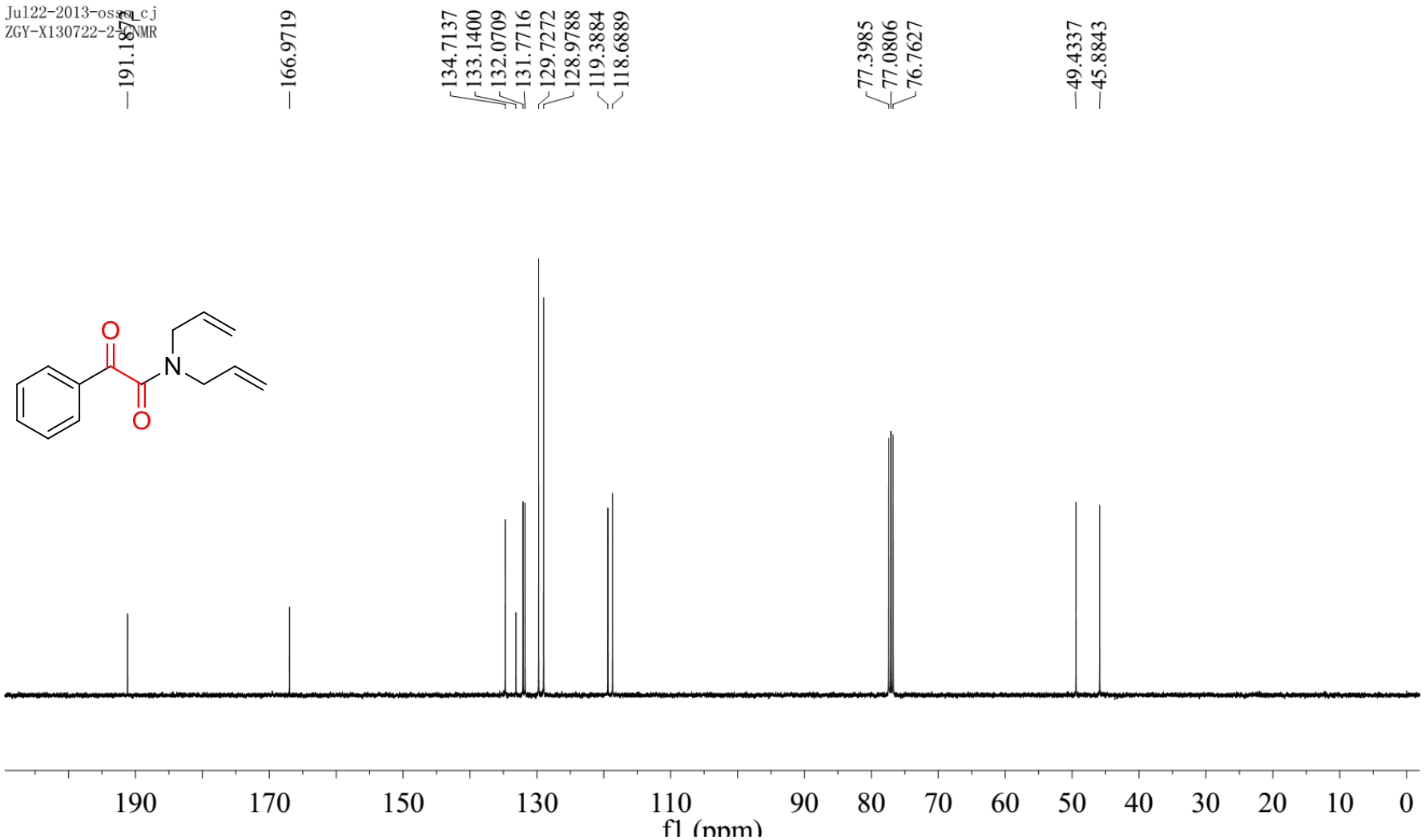
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
f1 (ppm)


Jul22-2013-ossa_cj
ZGY-X130722-2-13CNMR
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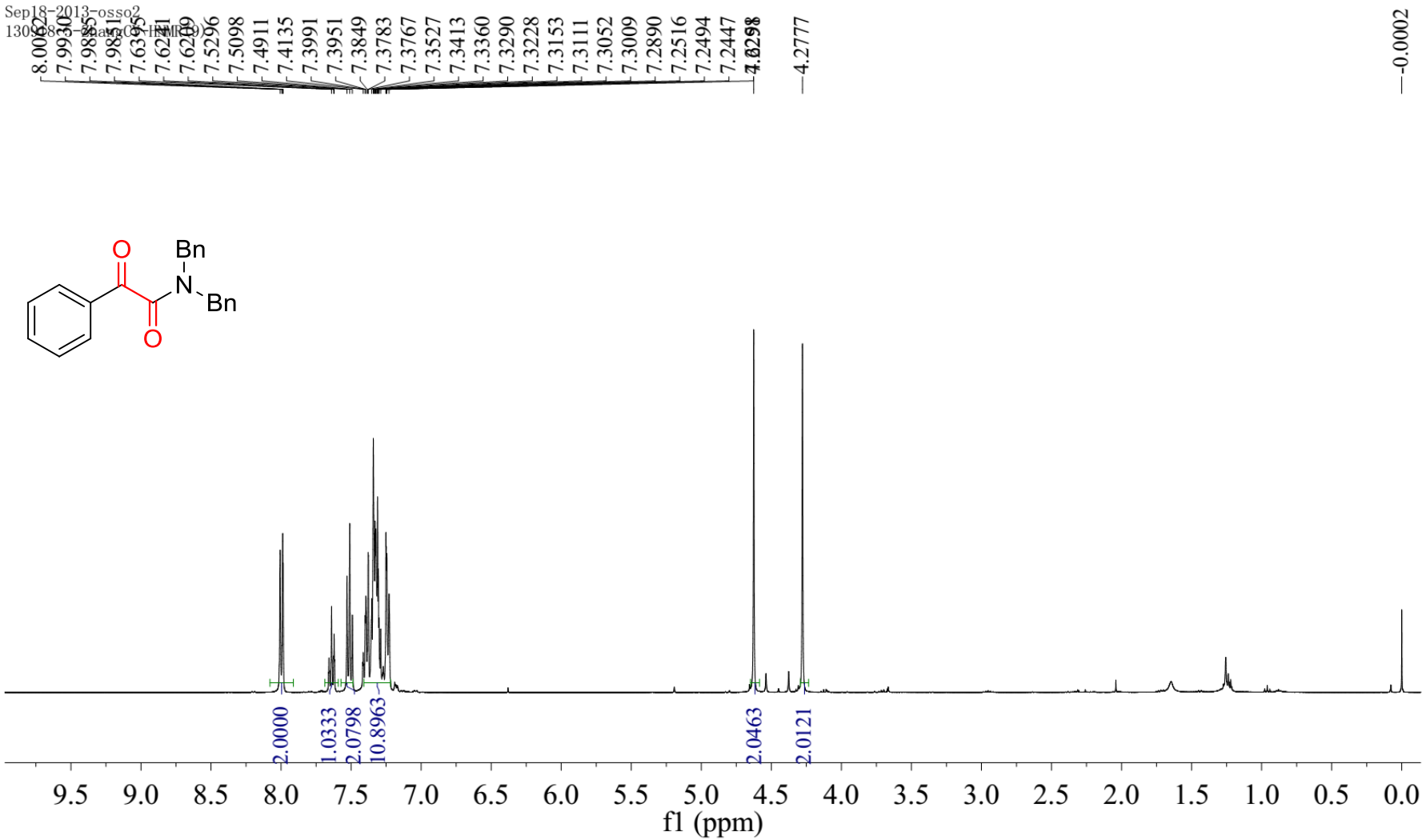
132.0709
131.7716
129.7272
128.9788
119.3884
118.6889
77.3985
77.0806
76.7627
49.4337
45.8843
O
N
O
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Sep18-2013-osso2
8.0016
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7.6395
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7.5296
7.5098
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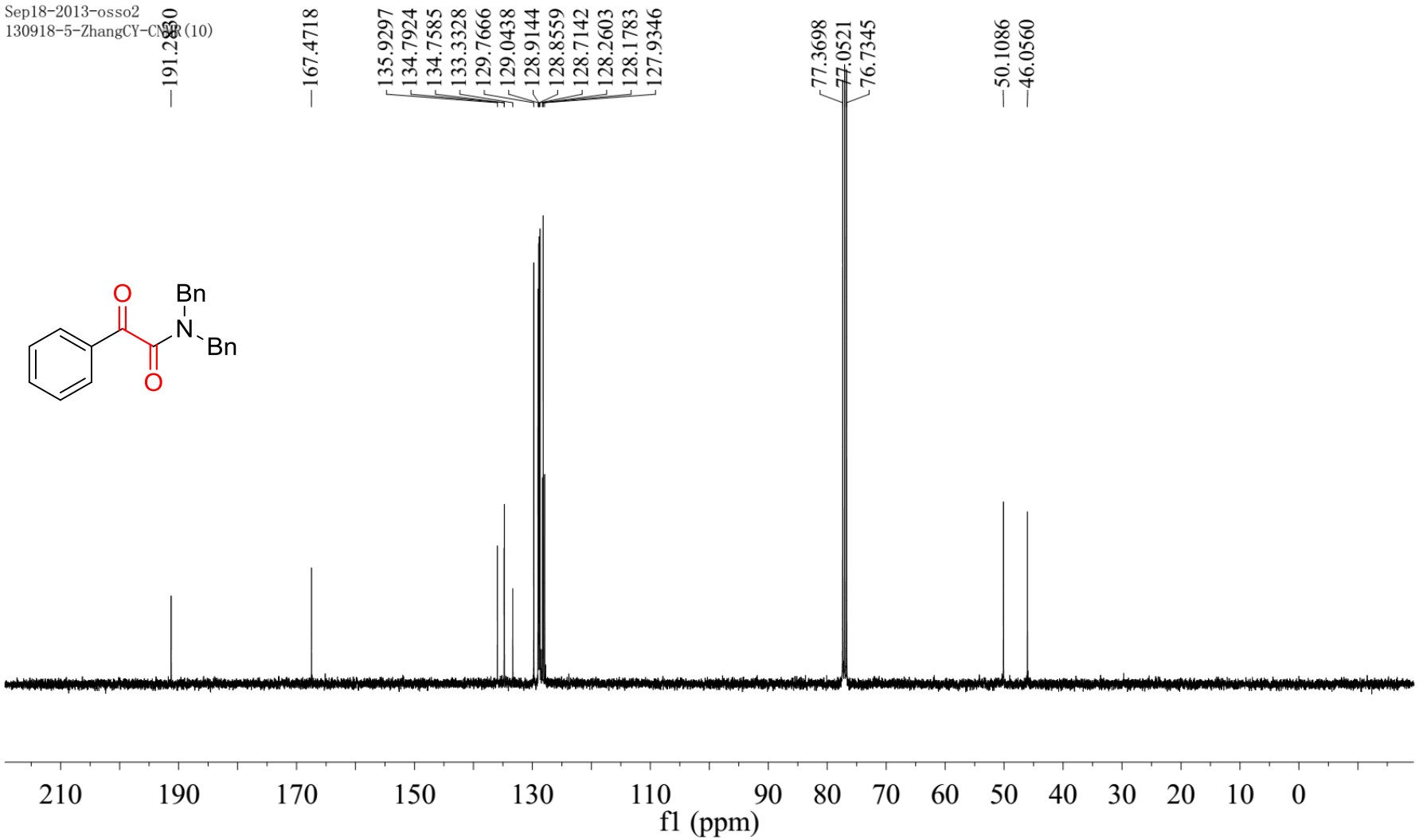
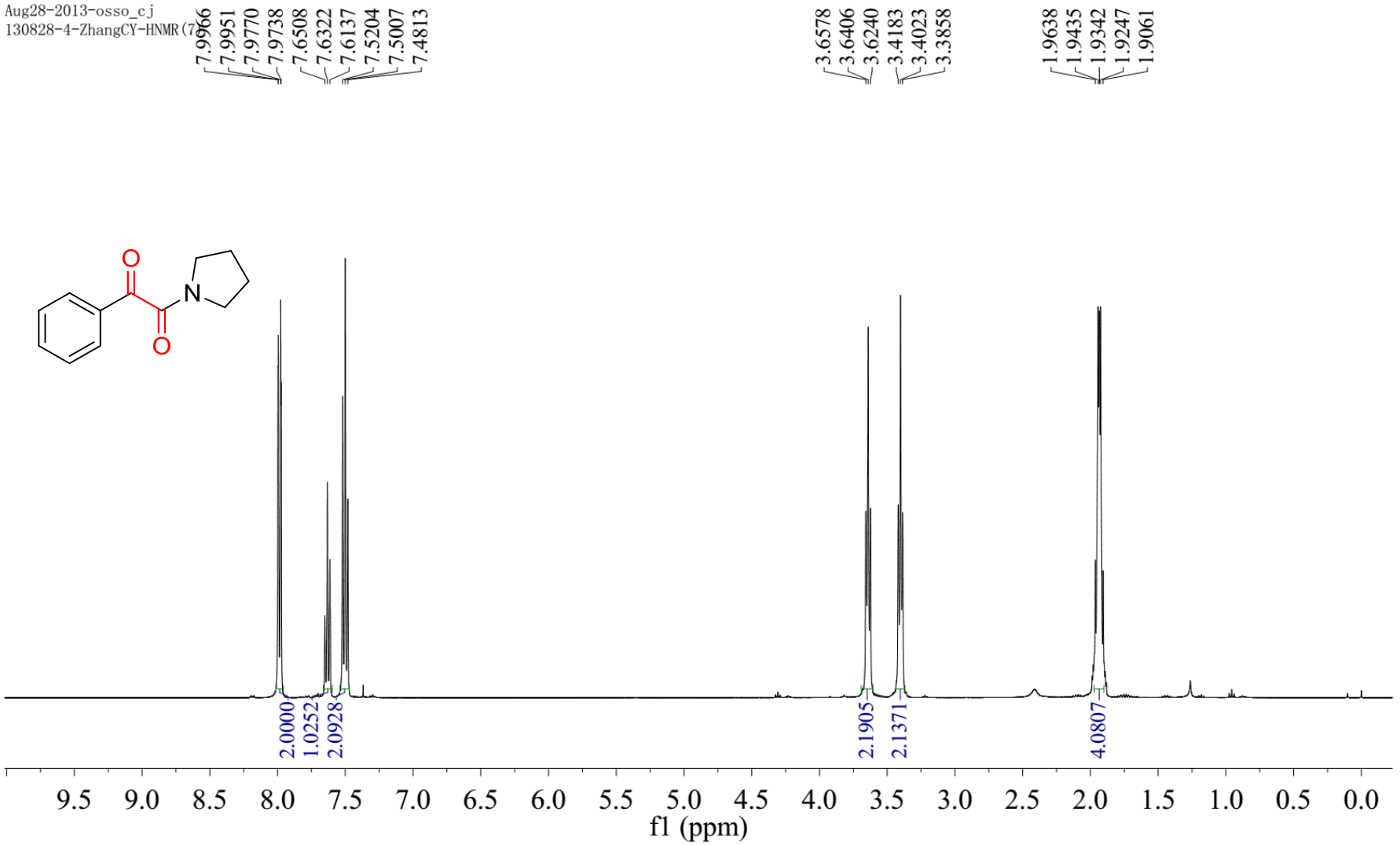
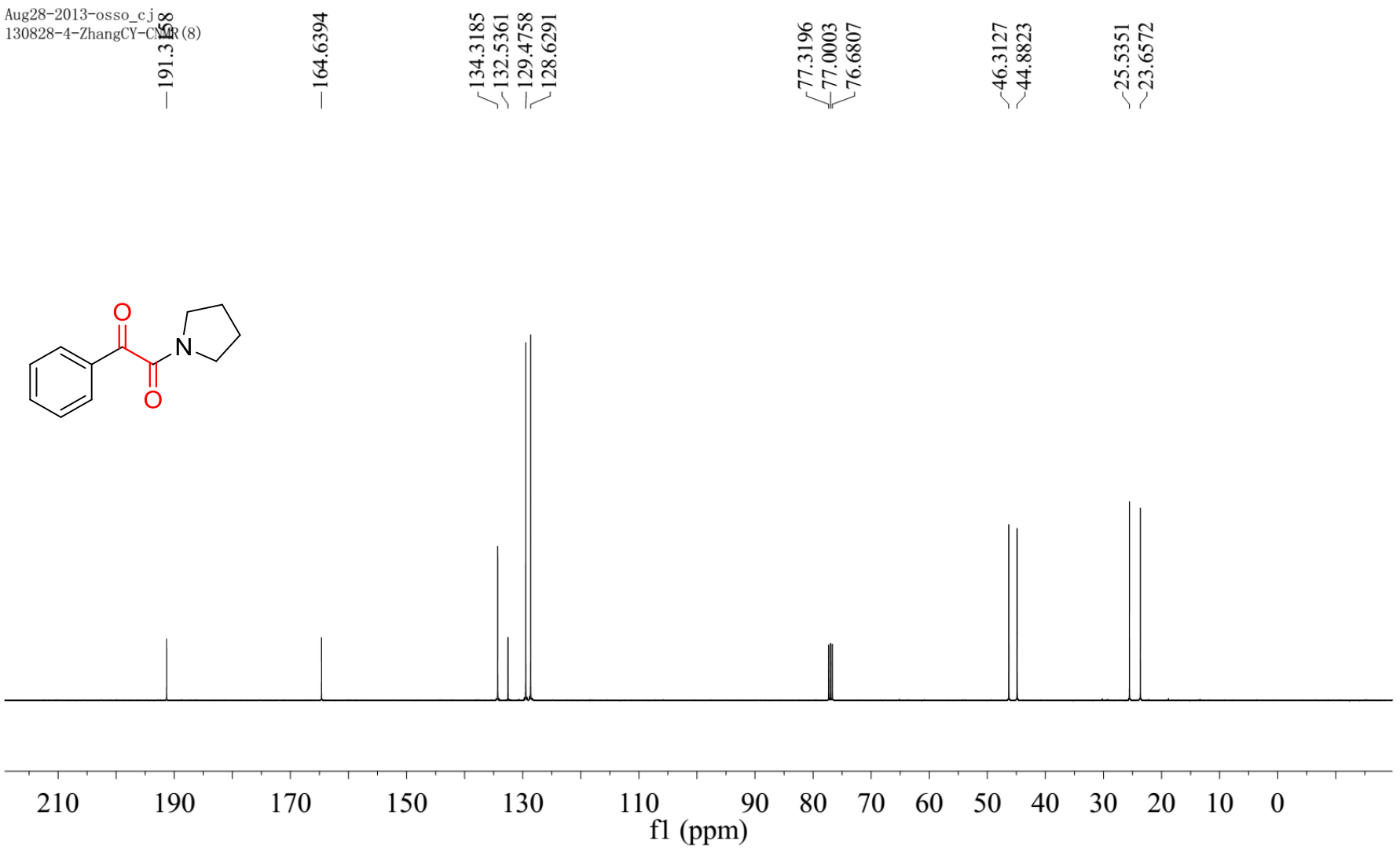
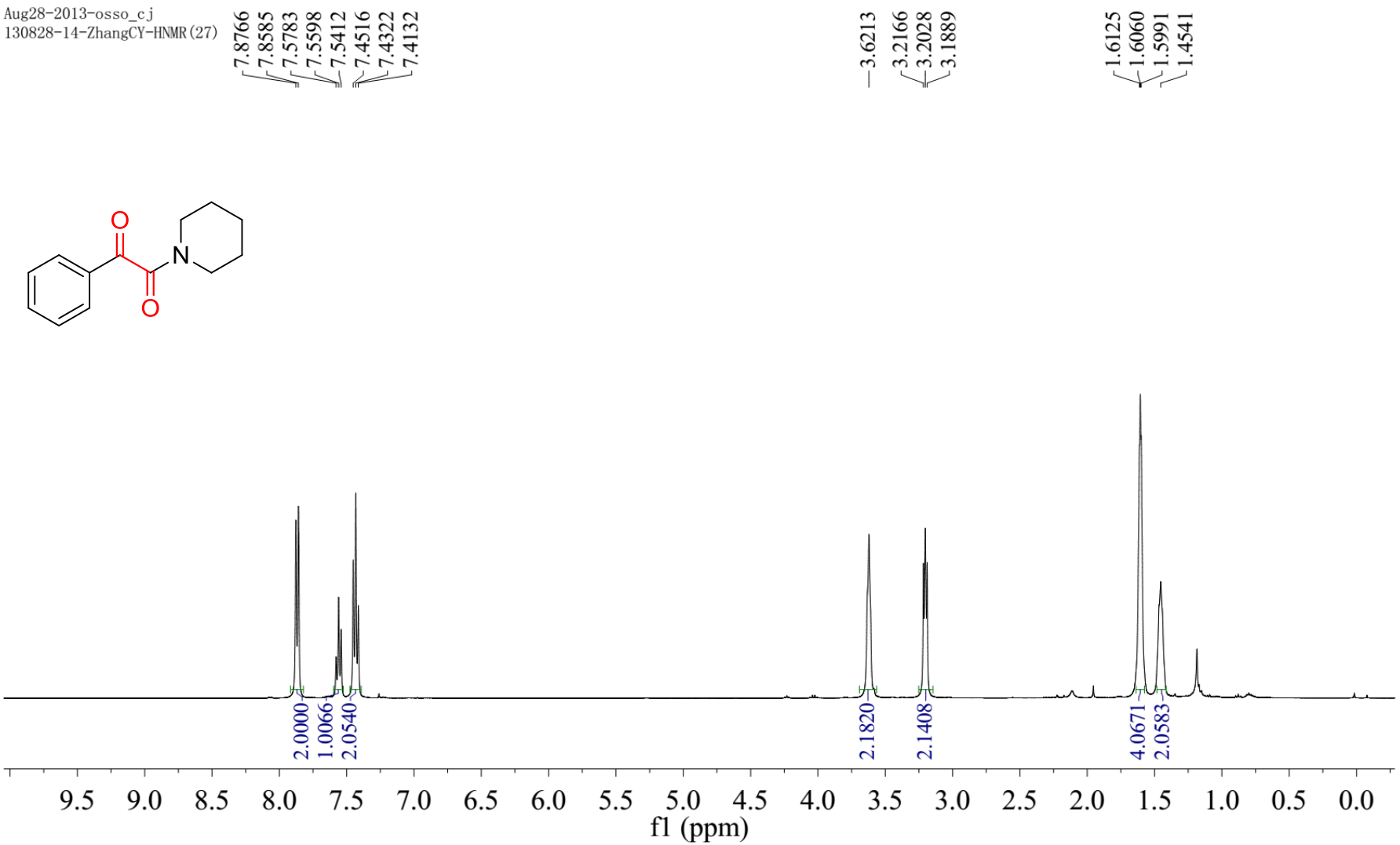
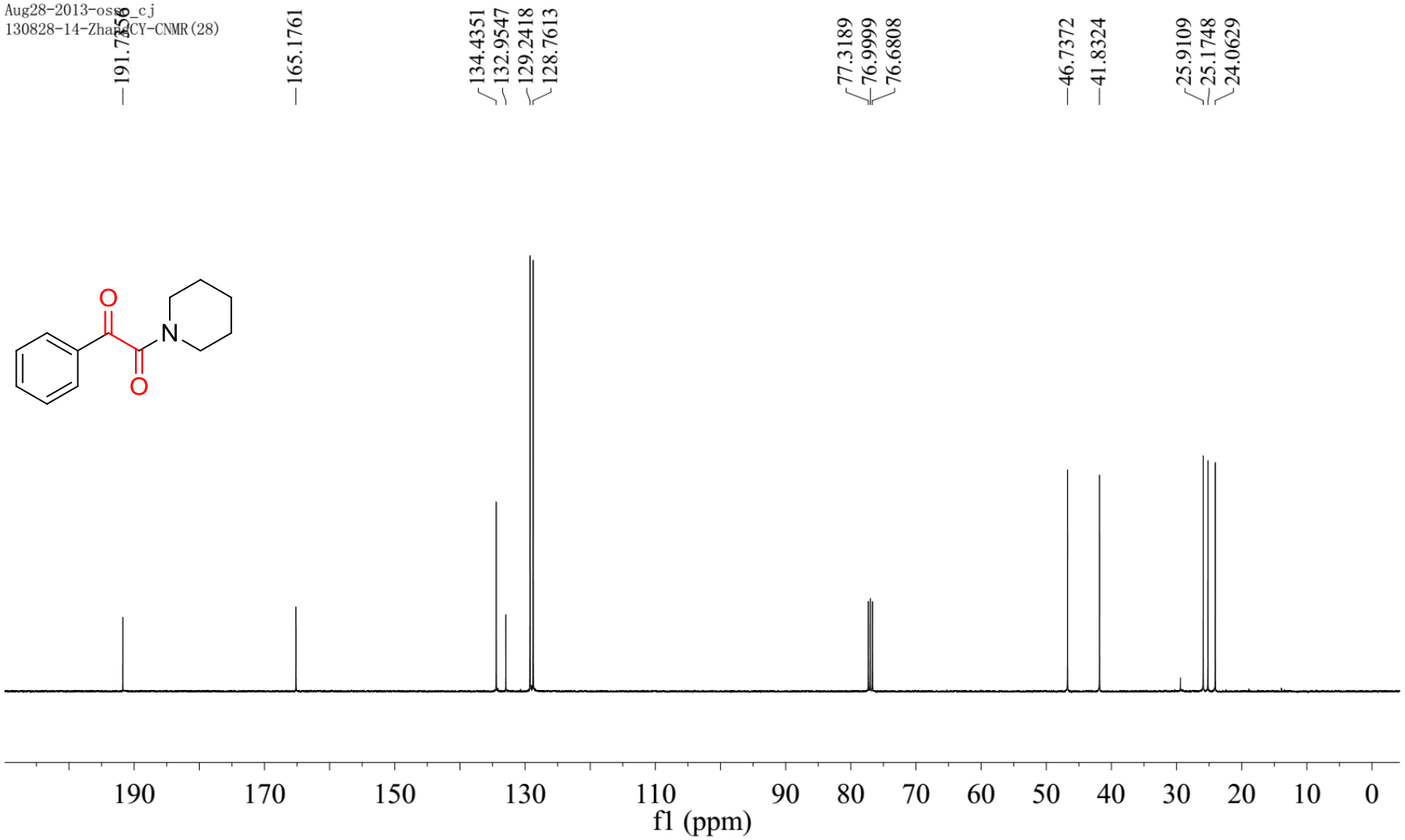
7.4135
7.3991
7.3951
7.3849
7.3783
7.3767
7.3527
7.3413
7.3360
7.3290
7.3228
7.3153
7.3111
7.3052
7.3009
7.2890
7.2516
7.2494
7.2447
4.2777
-0.0002
O
Bn
N
Bn
O
2.0000
1.0333
2.0798
10.8963
2.0463
2.0121
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

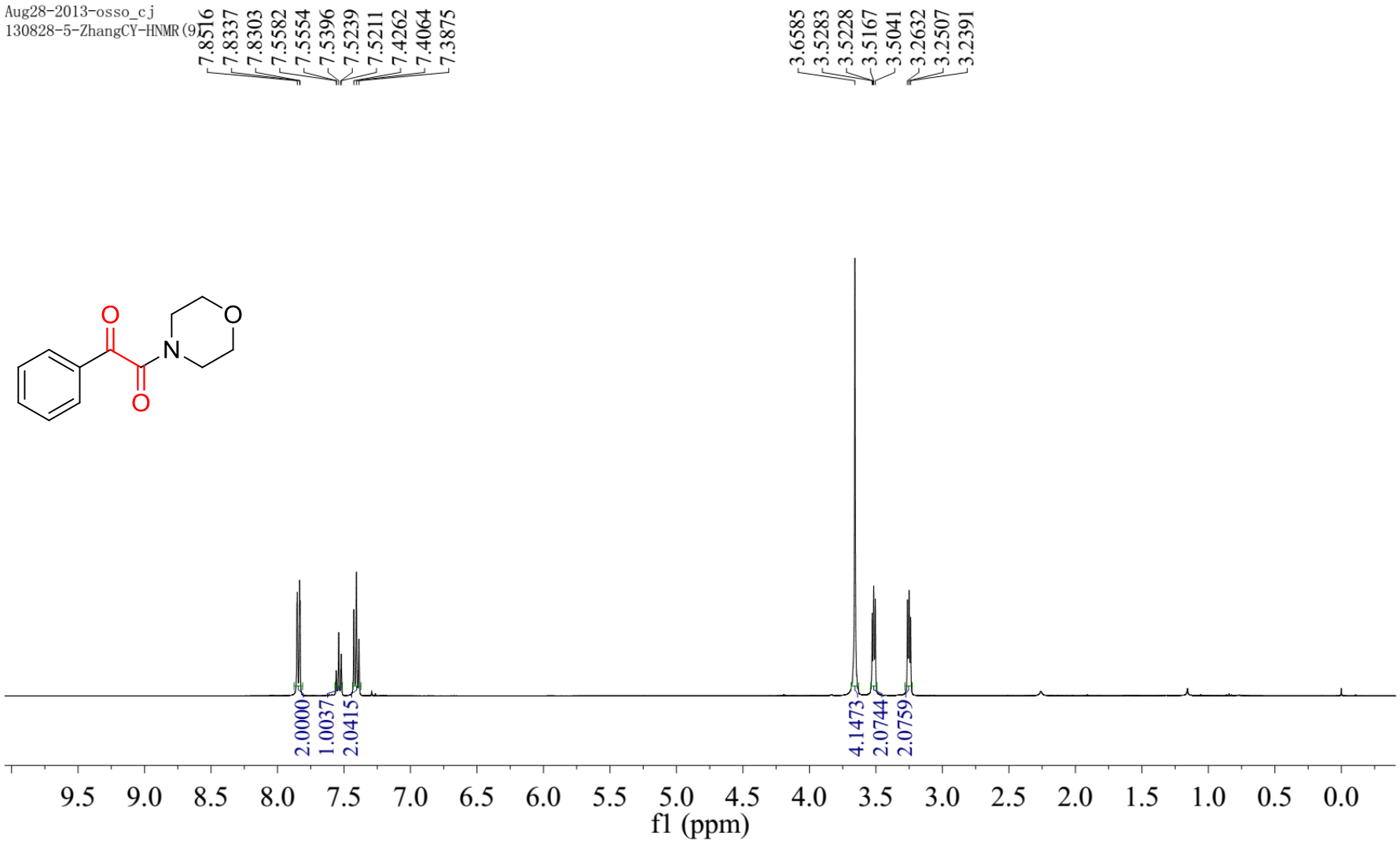

Sep18-2013-osso2
130918-5-ZhangCY-CMR(10)
191.2330
167.4718
135.9297
134.7924
134.7585
133.3328
129.7666
129.0438
128.9144
128.8559
128.7142
128.2603
128.1783
127.9346
77.3698
77.0521
76.7345
50.1086
46.0560
O
Bn
N
Bn
O
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

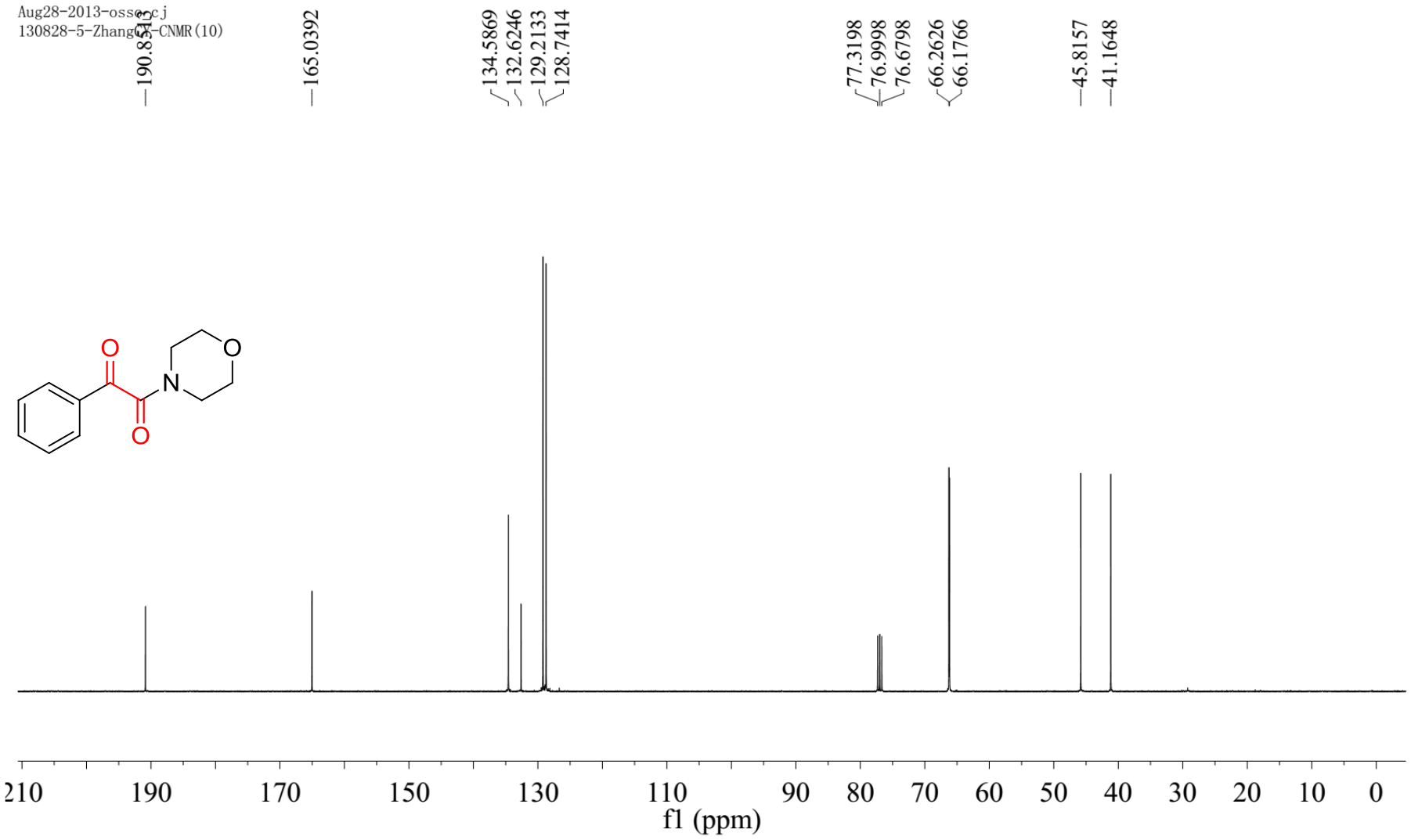

Aug28-2013-osso_cj
130828-4-ZhangCY-HNMR(7)
7.9966
7.9951
7.9770
7.9738
7.6508
7.6322
7.6137
7.5204
7.5007
7.4813
3.6578
3.6406
3.6240
3.4183
3.4023
3.3858
1.9638
1.9435
1.9342
1.9247
1.9061
O
O
N
2.0000
1.0252
2.0928
2.1905
2.1371
4.0807
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

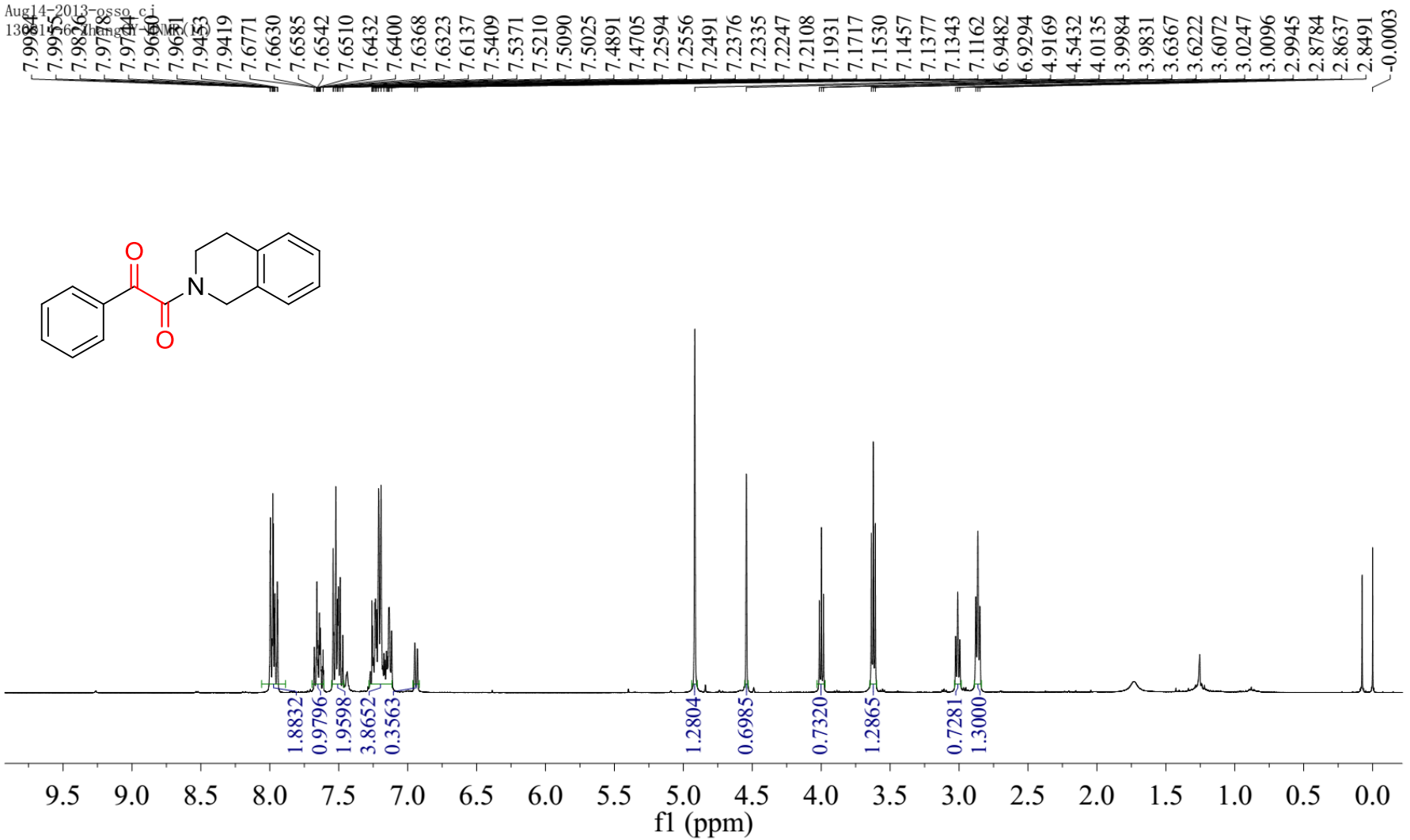

Aug28-2013-osso_cj
130828-4-ZhangCY-CMR(8)
191.3158
164.6394
134.3185
132.5361
129.4758
128.6291
77.3196
77.0003
76.6807
46.3127
44.8823
25.5351
23.6572
O
O
N
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Aug28-2013-osso_cj
130828-14-ZhangCY-HNMR(27)
7.8766
7.8585
7.5783
7.5598
7.5412
7.4516
7.4322
7.4132
3.6213
3.2166
3.2028
3.1889
1.6125
1.6060
1.5991
1.4541
O
O
N
2.0000
1.0066
2.0540
2.1820
2.1408
4.0671
2.0583
9.5 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 1.5 1.0 0.5 0.0
f1 (ppm)


Aug28-2013-oss_cj
130828-14-Zhao-CY-CNMR(28)
191.7256
165.1761
134.4351
132.9547
129.2418
128.7613
77.3189
76.9999
76.6808
46.7372
41.8324
25.9109
25.1748
24.0629
O
N
O
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Aug28-2013-osso_cj
130828-5-ZhangCY-HNMR(9)
7.8516
7.8337
7.8303
7.5582
7.5554
7.5396
7.5239
7.5211
7.4262
7.4064
7.3875
3.6585
3.5283
3.5228
3.5167
3.5041
3.2632
3.2507
3.2391
O
O
N
O
2.0000
1.0037
2.0415
4.1473
2.0744
2.0759
9.5 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 1.5 1.0 0.5 0.0
f1 (ppm)


Aug28-2013-ossscj
130828-5-ZhangGJ-CNMR(10)
190.8543
165.0392
134.5869
132.6246
129.2133
128.7414
77.3198
76.9998
76.6798
66.2626
66.1766
45.8157
41.1648
O
N
O
O
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Aug14-2013-osso ci
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7.9788
7.9744
7.9600
7.9581
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7.9419
7.6771
7.6630
7.6585
7.6542
7.6510
7.6432
7.6400
7.6368
7.6323
7.6137
7.5409
7.5371
7.5210
7.5090
7.5025
7.4891
7.4705
7.2594
7.2556
7.2491
7.2376
7.2335
7.2247
7.2108
7.1931
7.1717
7.1530
7.1457
7.1377
7.1343
7.1162
6.9482
6.9294
4.9169
4.5432
4.0135
3.9984
3.9831
3.6367
3.6222
3.6072
3.0247
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-0.0003
O
O
N
1.8832
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0.3563
1.2804
0.6985
0.7320
1.2865
0.7281
1.3000
9.5
9.0
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8.0
7.5
7.0
6.5
6.0
5.5
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3.5
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2.5
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1.0
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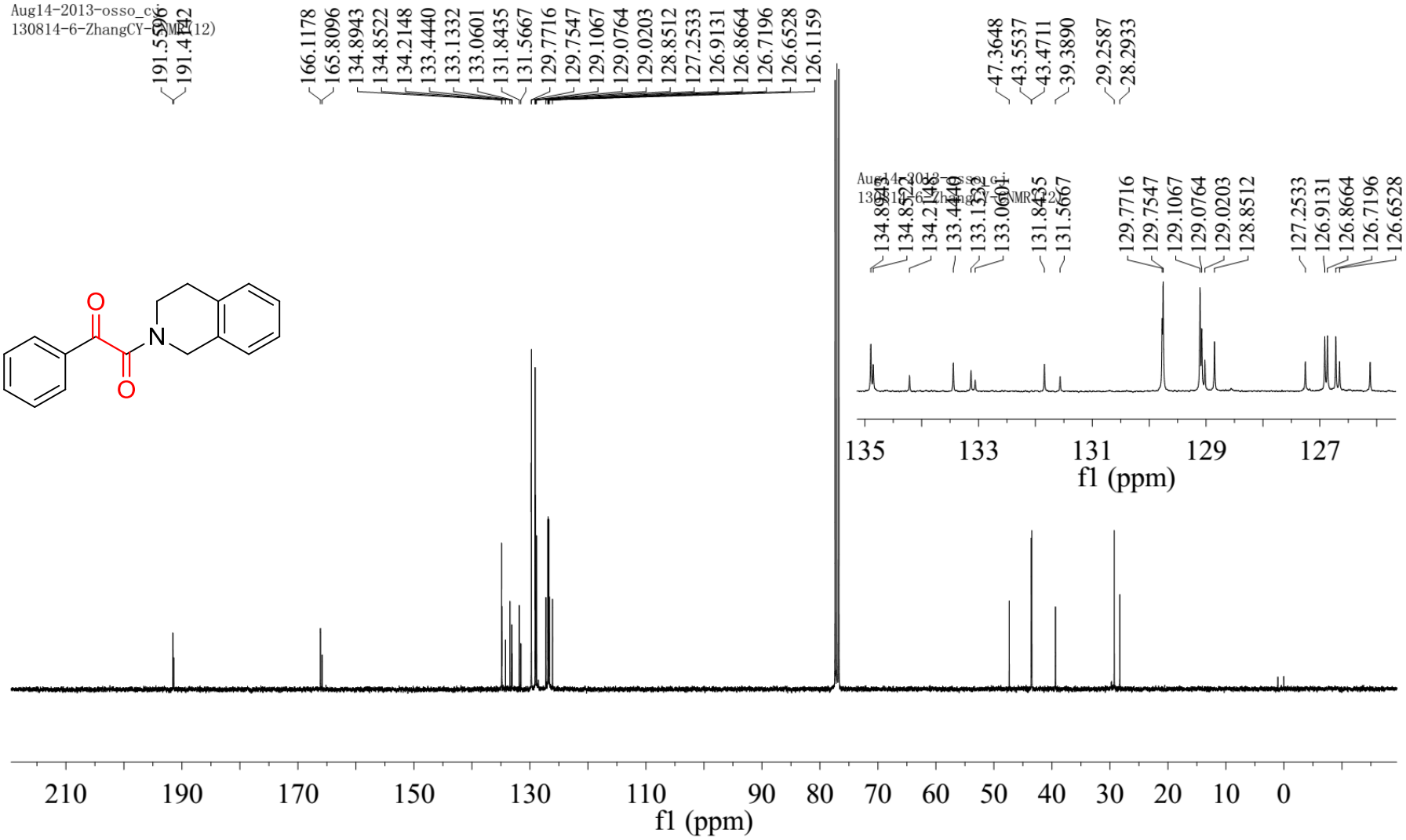
0.0
f1 (ppm)


Aug14-2013-osso_cy
130814-6-ZhangCY-1HNMR-12)
191.5506
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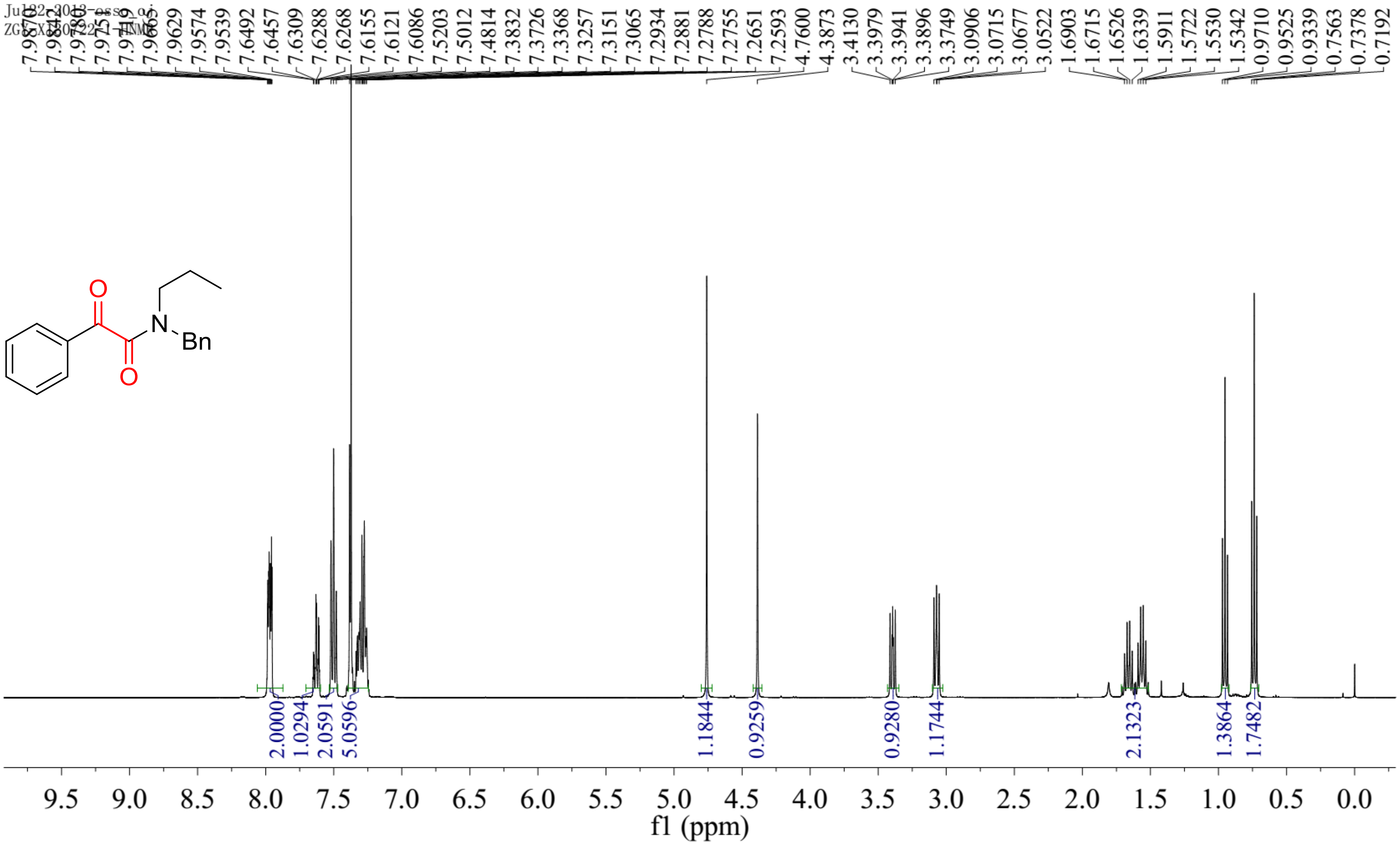
165.8096
134.8943
134.8522
134.2148
133.4440
133.1332
133.0601
131.8435
131.5667
129.7716
129.7547
129.1067
129.0764
129.0203
128.8512
127.2533
126.9131
126.8664
126.7196
126.6528
126.1159
47.3648
43.5537
43.4711
39.3890
29.2587
28.2933
O
O
N
135
133
131
129
127
f1 (ppm)
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.6086
7.5203
7.5012
7.4814
7.3832
7.3726
7.3368
7.3257
7.3151
7.3065
7.2934
7.2881
7.2788
7.2755
7.2651
7.2593
4.7600
4.3873
3.4130
3.3979
3.3941
3.3896
3.3749
3.0906
3.0715
3.0677
3.0522
1.6903
1.6715
1.6526
1.6339
1.5911
1.5722
1.5530
1.5342
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0.9525
0.9339
0.7563
0.7378
0.7192
O
N
Bn
O
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5.0596
1.1844
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0.9280
1.1744
2.1323
1.3864
1.7482
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9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.5
3.0
2.5
2.0
1.5
1.0
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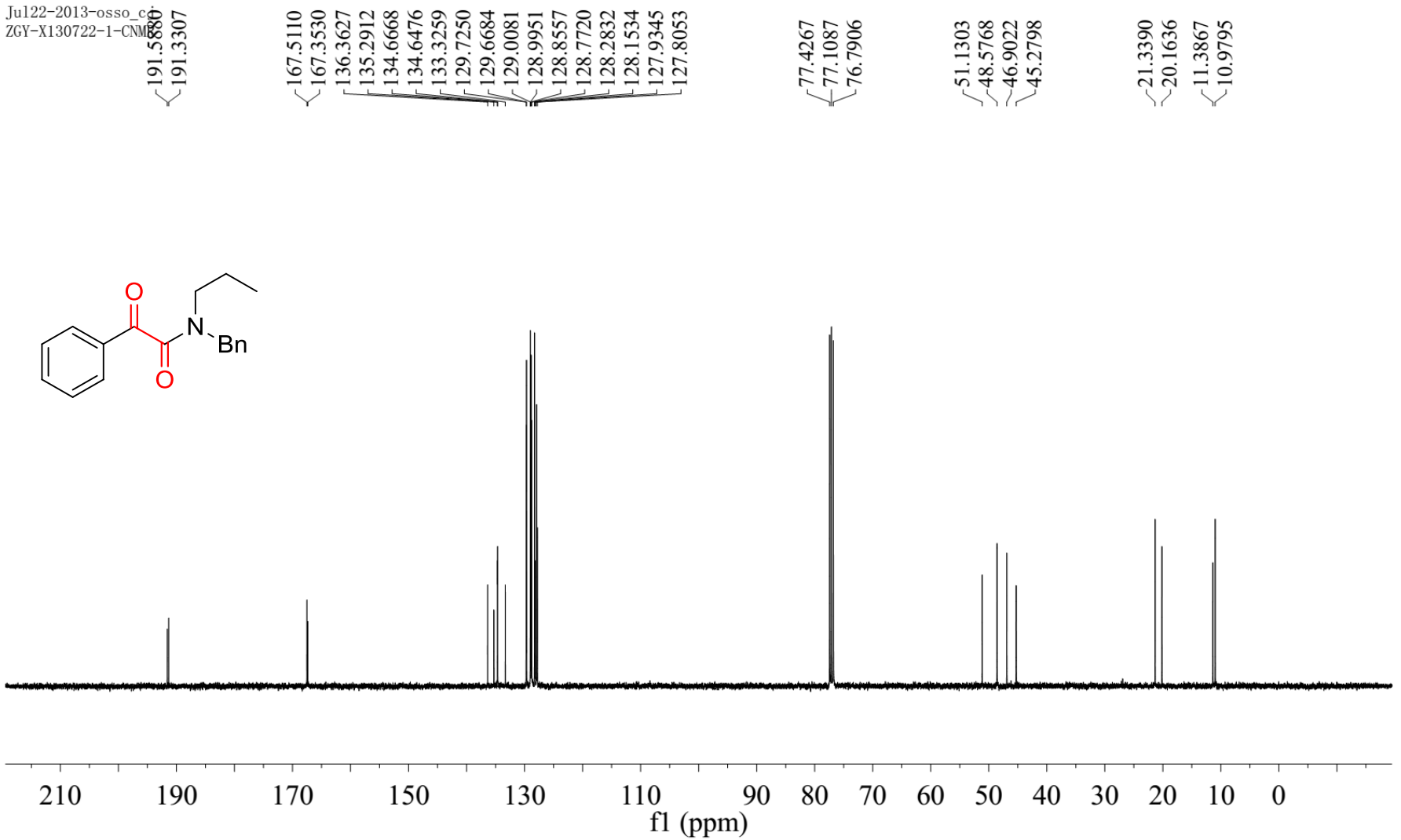
0.0
f1 (ppm)


Jul22-2013-osso_cq
ZGY-X130722-1-CNMR
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167.3530
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135.2912
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134.6476
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128.9951
128.8557
128.7720
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128.1534
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77.4267
77.1087
76.7906
51.1303
48.5768
46.9022
45.2798
21.3390
20.1636
11.3867
10.9795
O
O
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150
130
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90
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50
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20
10
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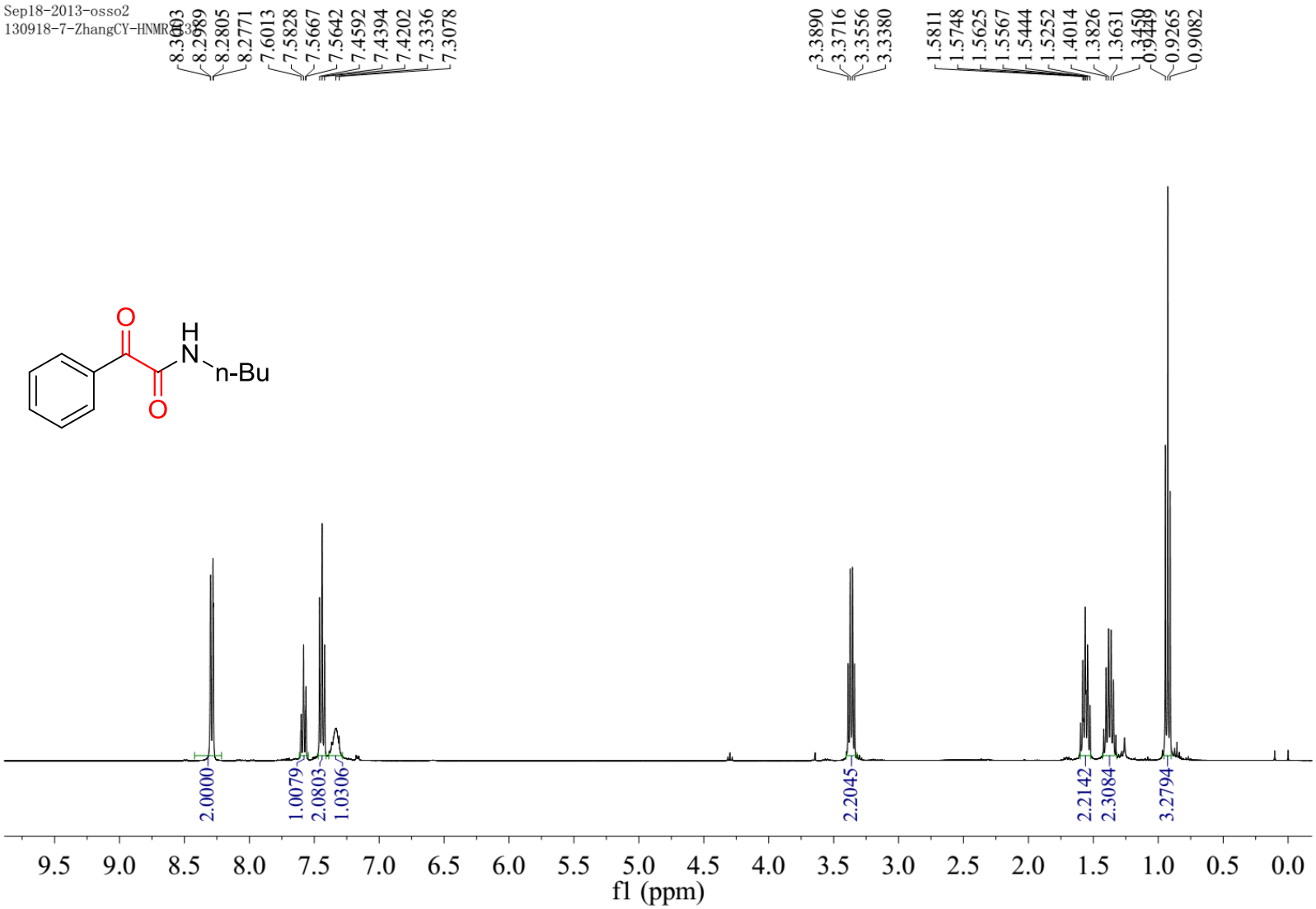
f1 (ppm)


Sep18-2013-osso2
130918-7-ZhangCY-HNMR-3
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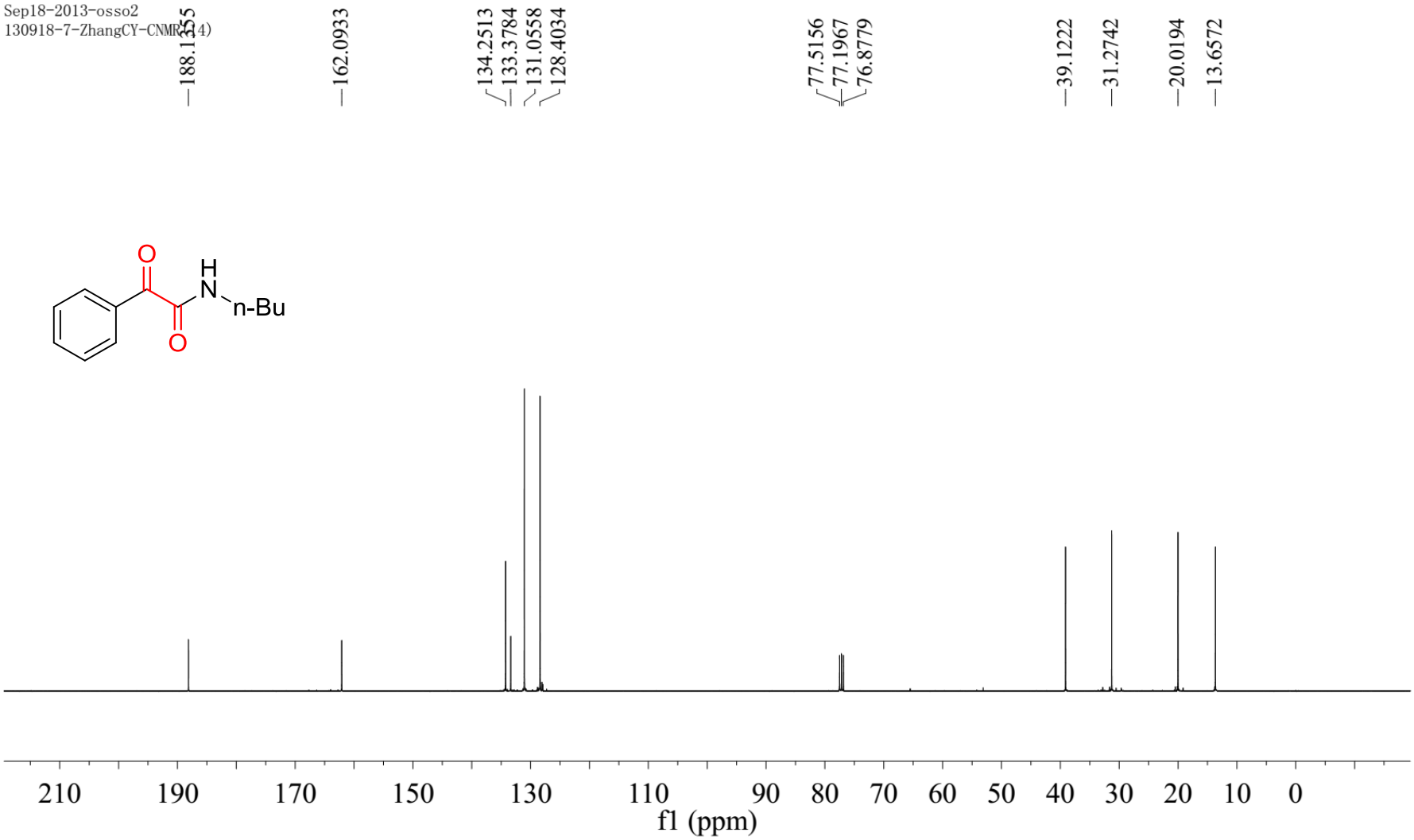
8.2771
7.6013
7.5828
7.5667
7.5642
7.4592
7.4394
7.4202
7.3336
7.3078
3.3890
3.3716
3.3556
3.3380
1.5811
1.5748
1.5625
1.5567
1.5444
1.5252
1.4014
1.3826
1.3631
1.3450
0.9449
0.9265
0.9082
O
H
N
n-Bu
O
2.0000
1.0079
2.0803
1.0306
2.2045
2.2142
2.3084
3.2794
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


Sep18-2013-osso2
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134.2513
133.3784
131.0558
128.4034
77.5156
77.1967
76.8779
39.1222
31.2742
20.0194
13.6572
O
H
N
n-Bu
O
210
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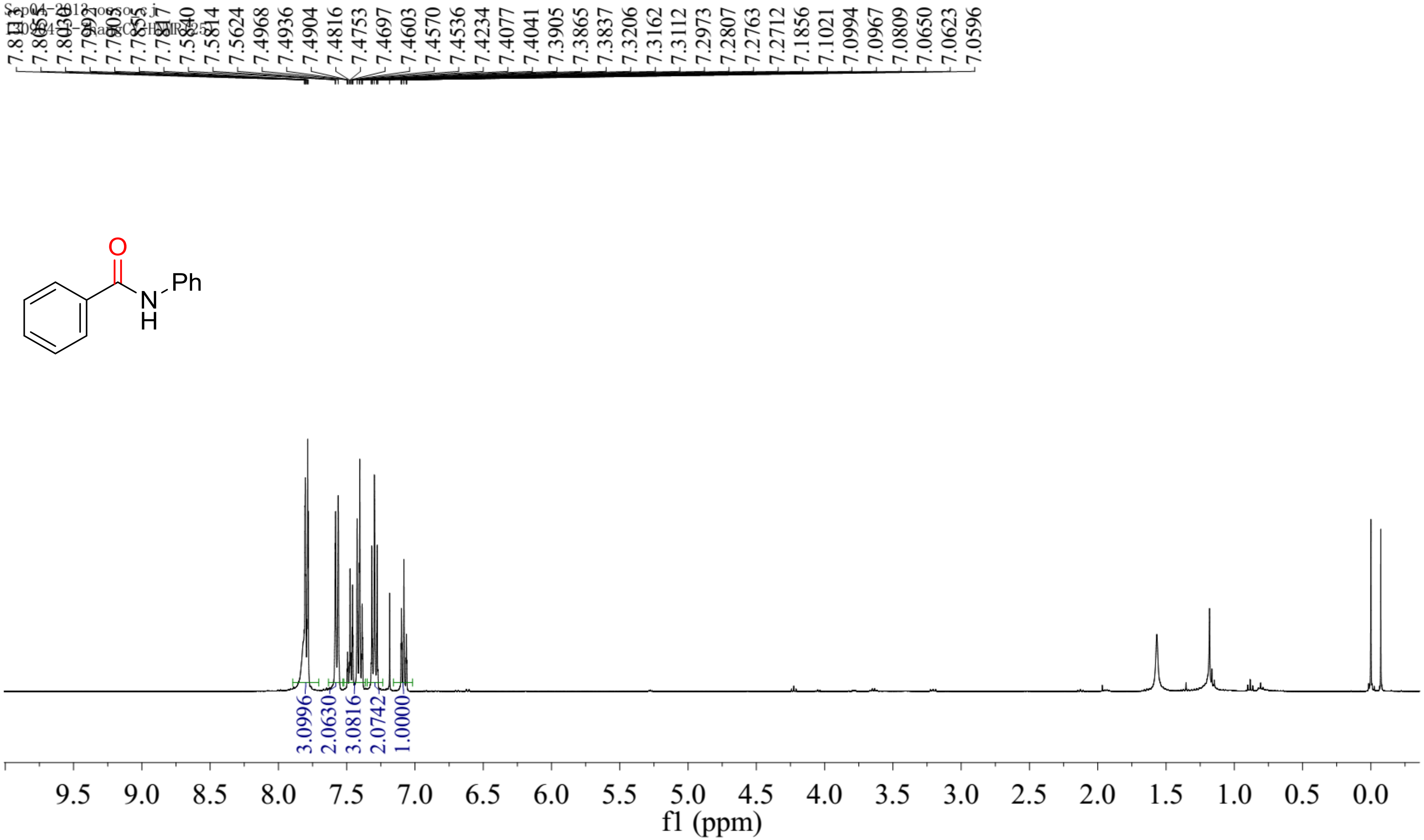
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)



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7.4816
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7.4570
7.4536
7.4234
7.4077
7.4041
7.3905
7.3865
7.3837
7.3206
7.3162
7.3112
7.2973
7.2807
7.2763
7.2712
7.1856
7.1021
7.0994
7.0967
7.0809
7.0650
7.0623
7.0596
O
N
H
Ph
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2.0630
3.0816
2.0742
1.0000
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8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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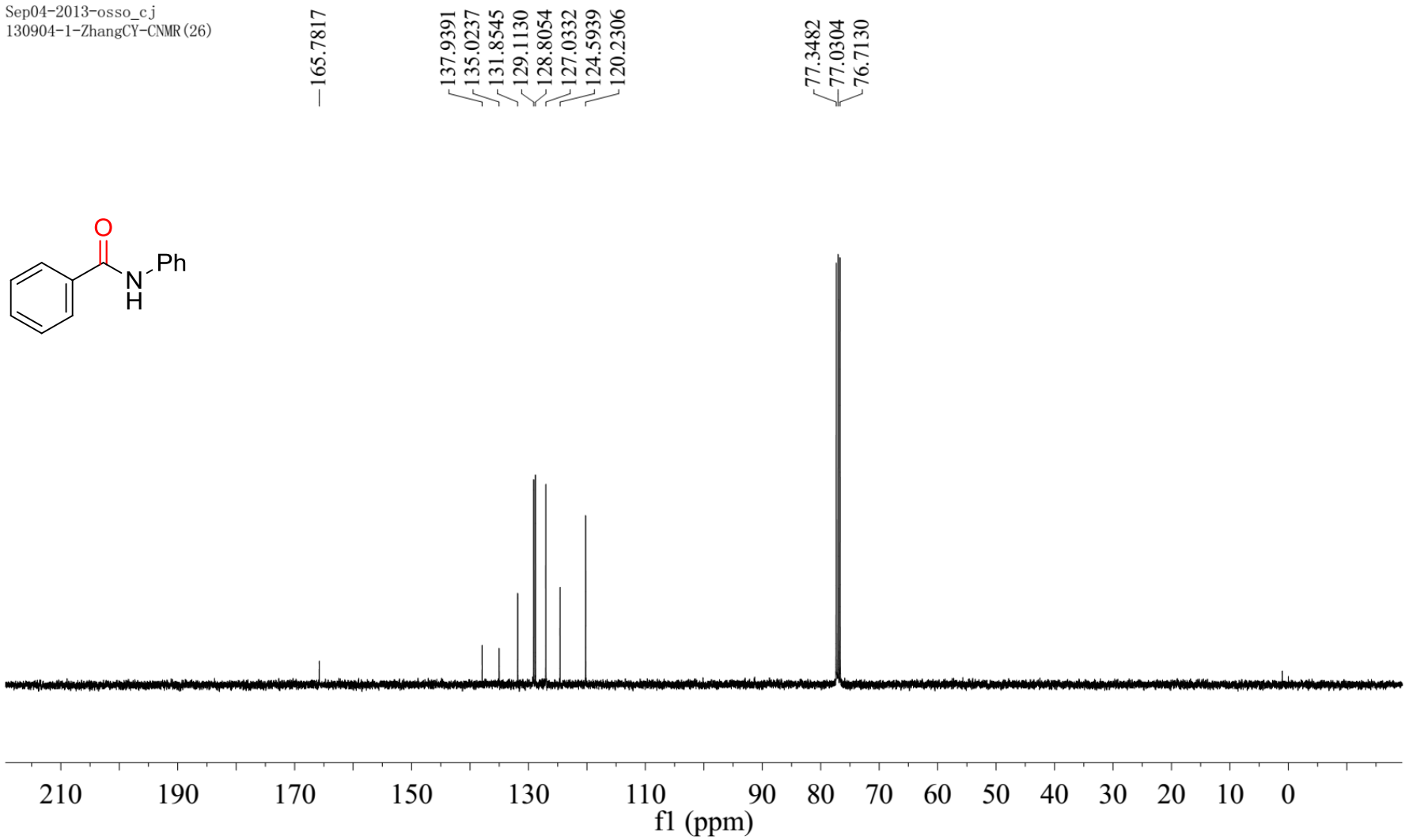
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


Sep04-2013-osso_cj
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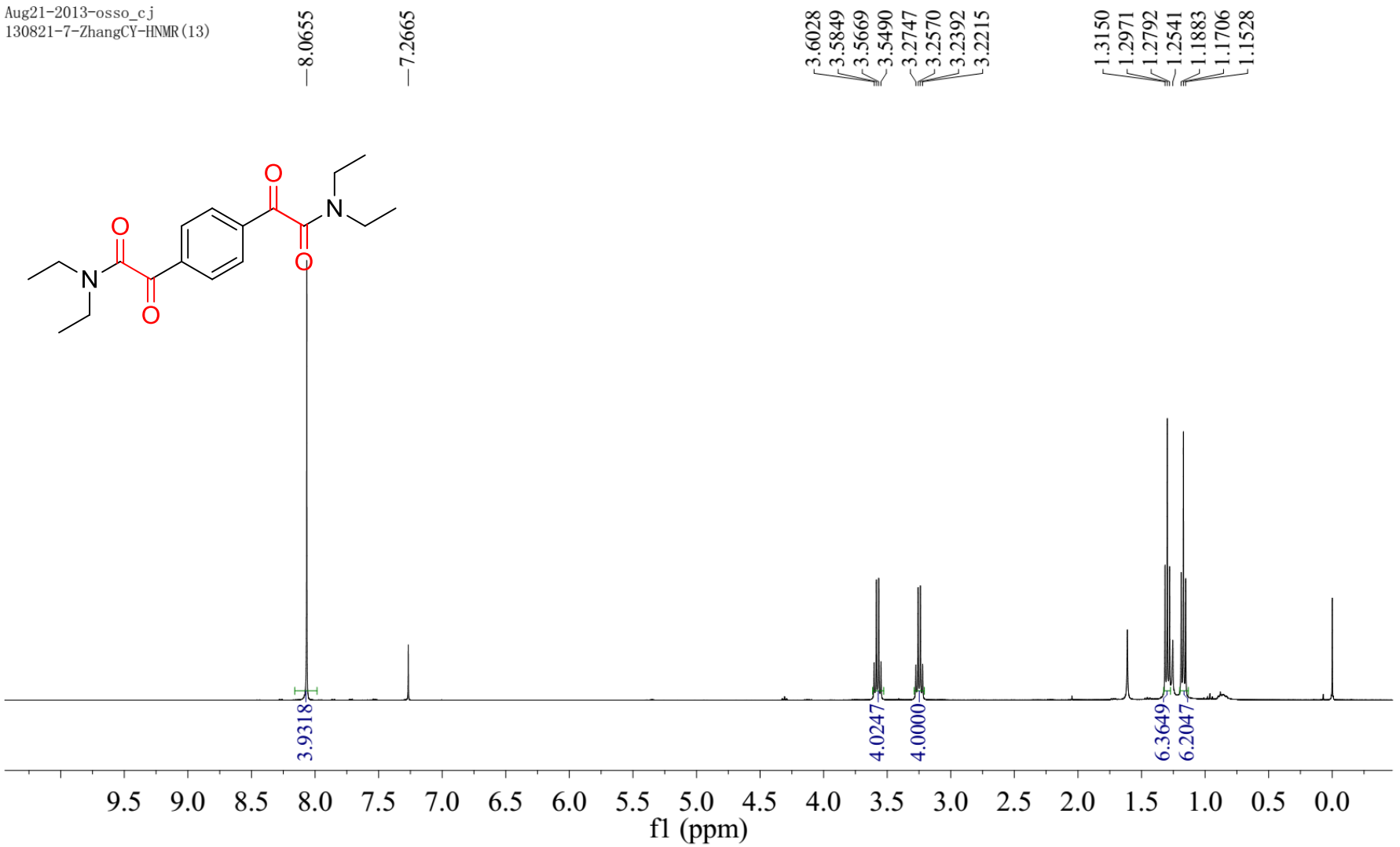
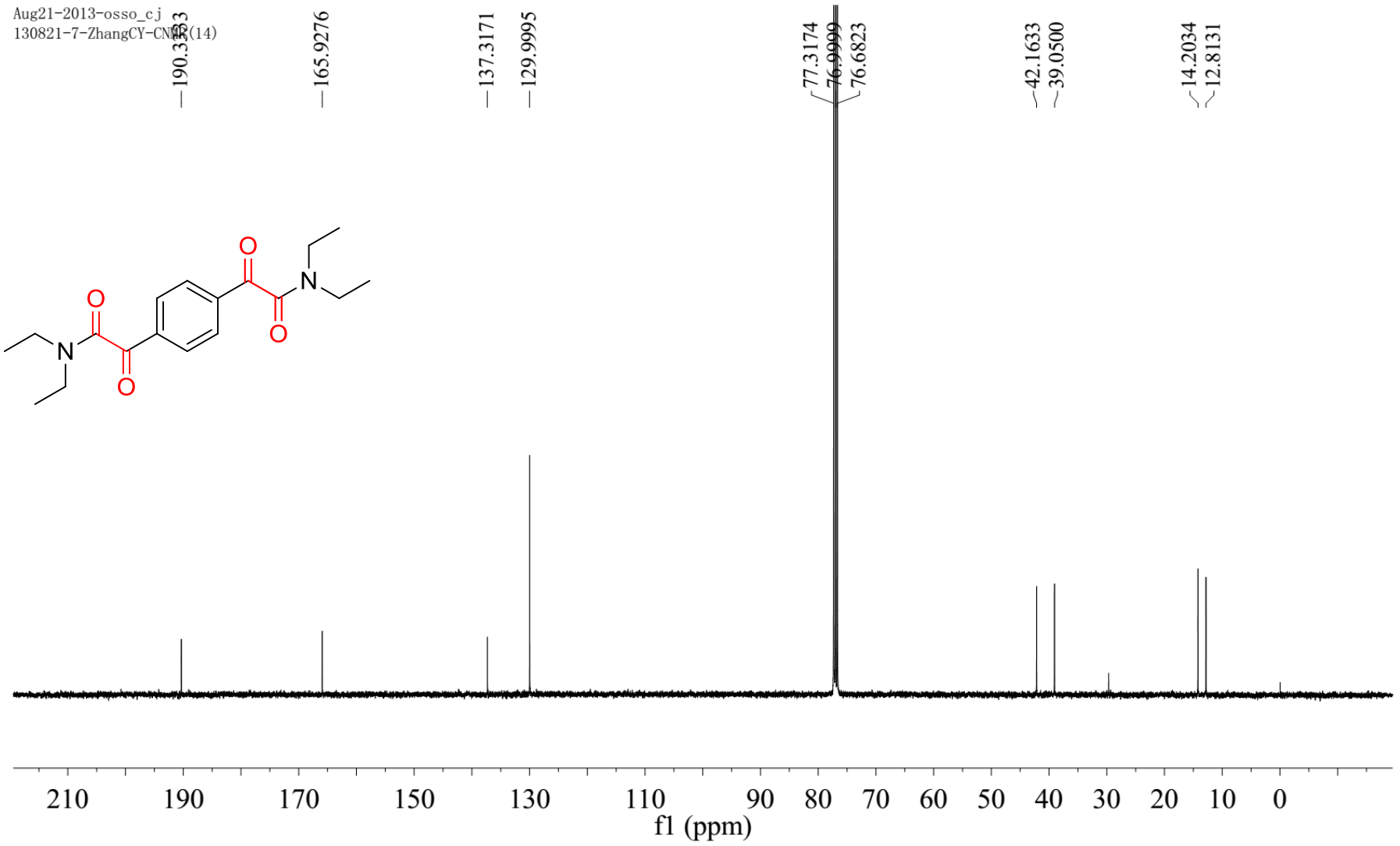
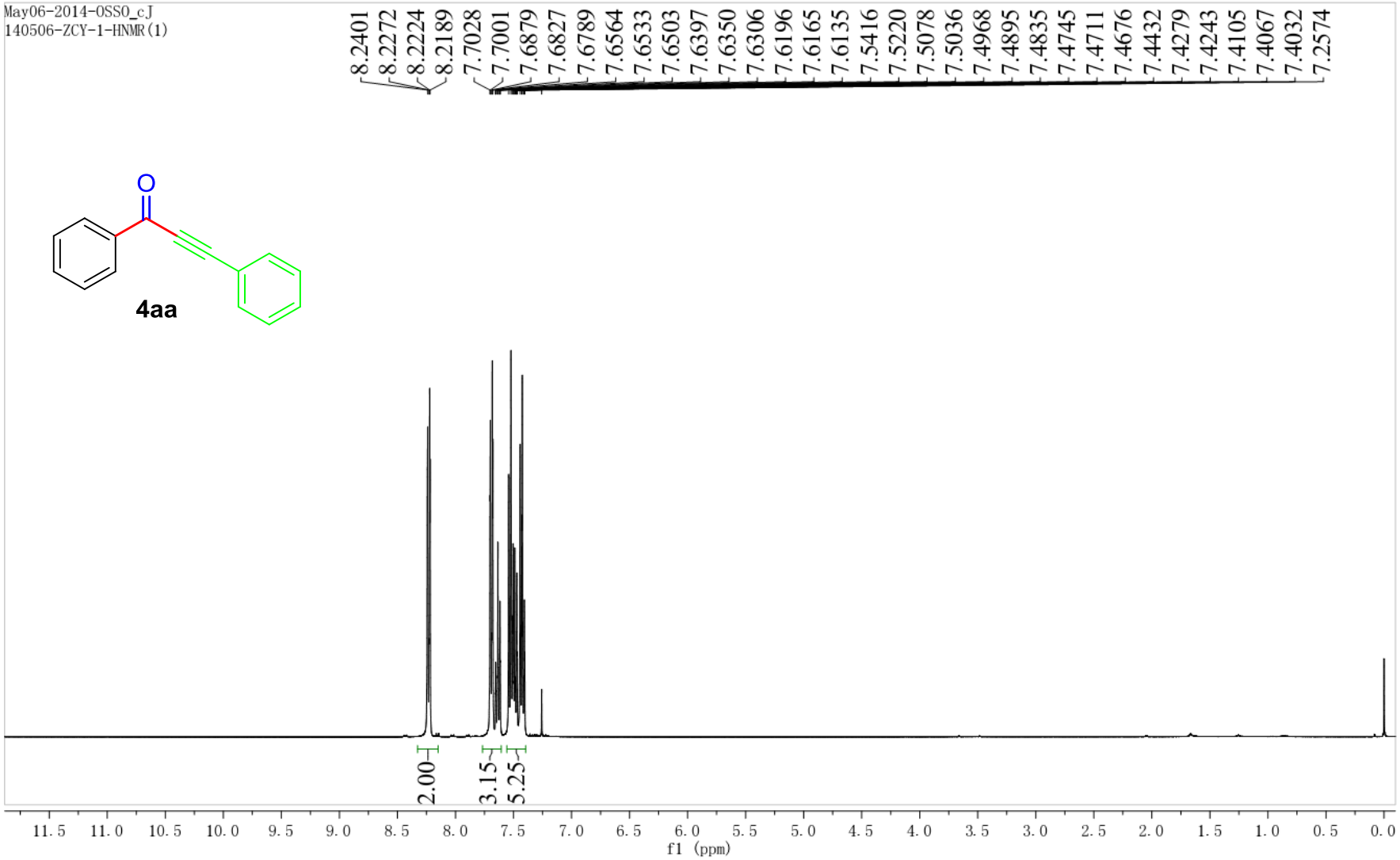
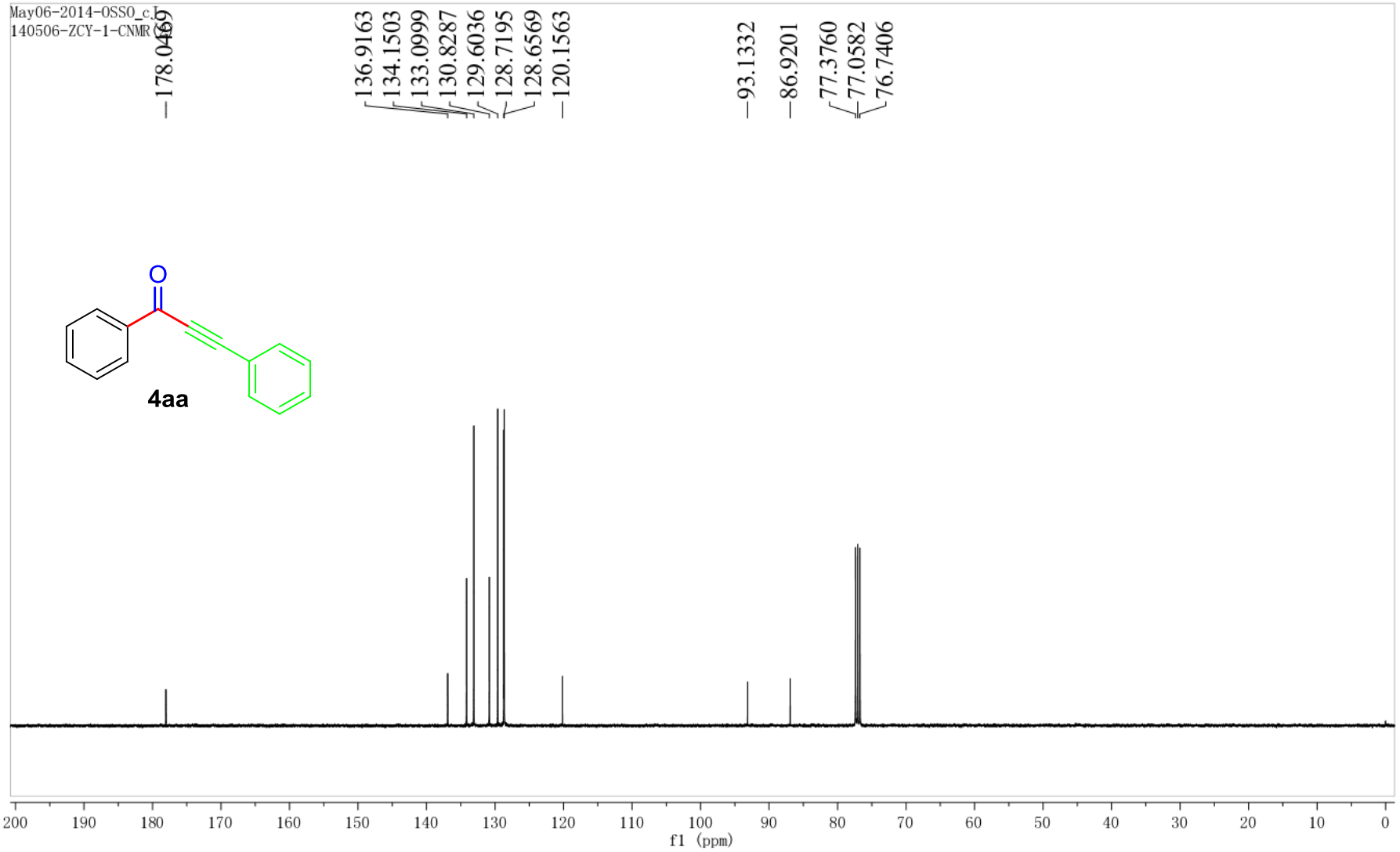
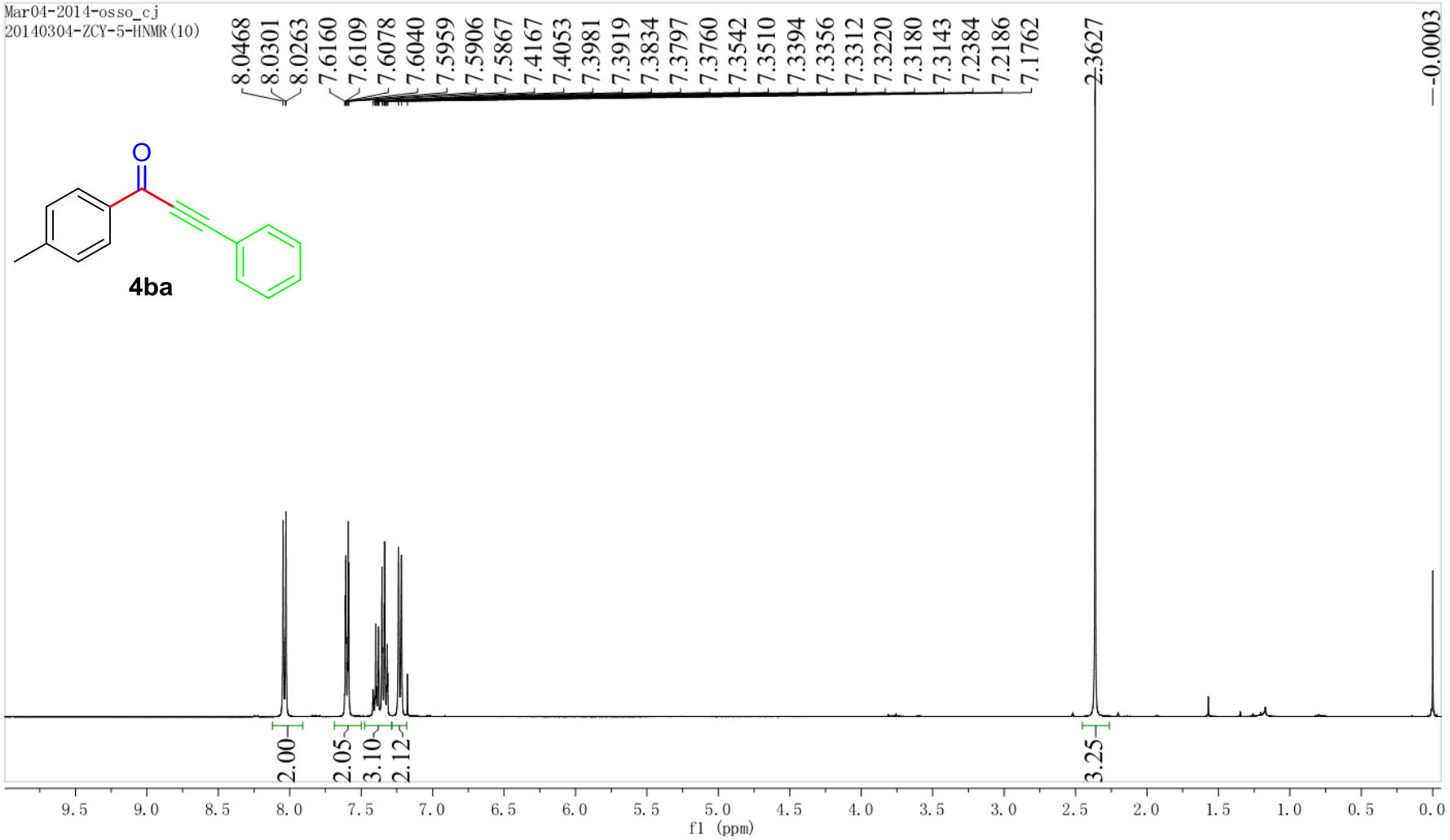
135.0237
131.8545
129.1130
128.8054
127.0332
124.5939
120.2306
77.3482
77.0304
76.7130
O
N
H
Ph
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

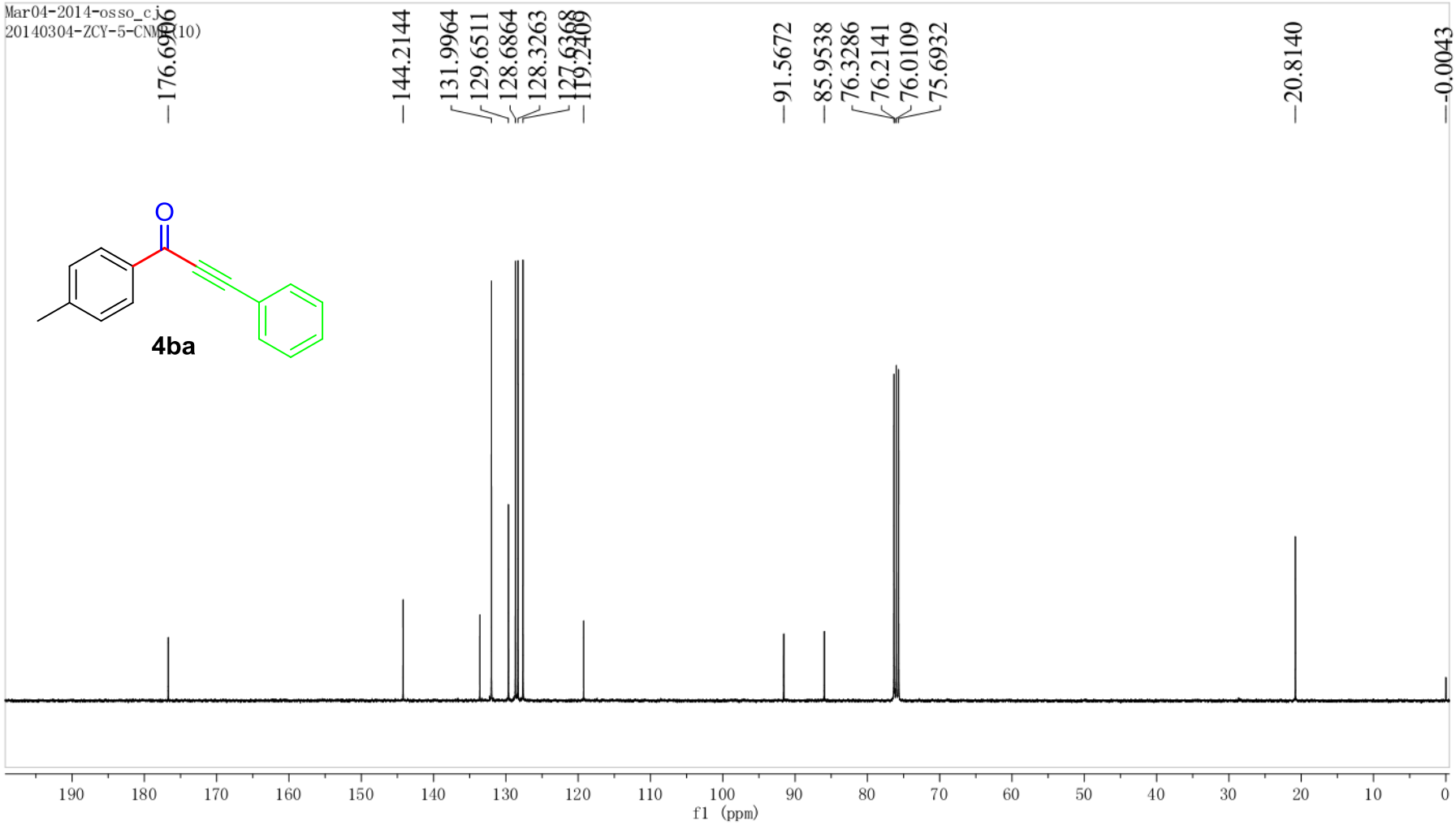

Aug21-2013-osso_cj
130821-7-ZhangCY-HNMR(13)
8.0655
7.2665
3.6028
3.5849
3.5669
3.5490
3.2747
3.2570
3.2392
3.2215
1.3150
1.2971
1.2792
1.2541
1.1883
1.1706
1.1528
O
N
O
O
N
O
3.9318
4.0247
4.0000
6.3649
6.2047
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

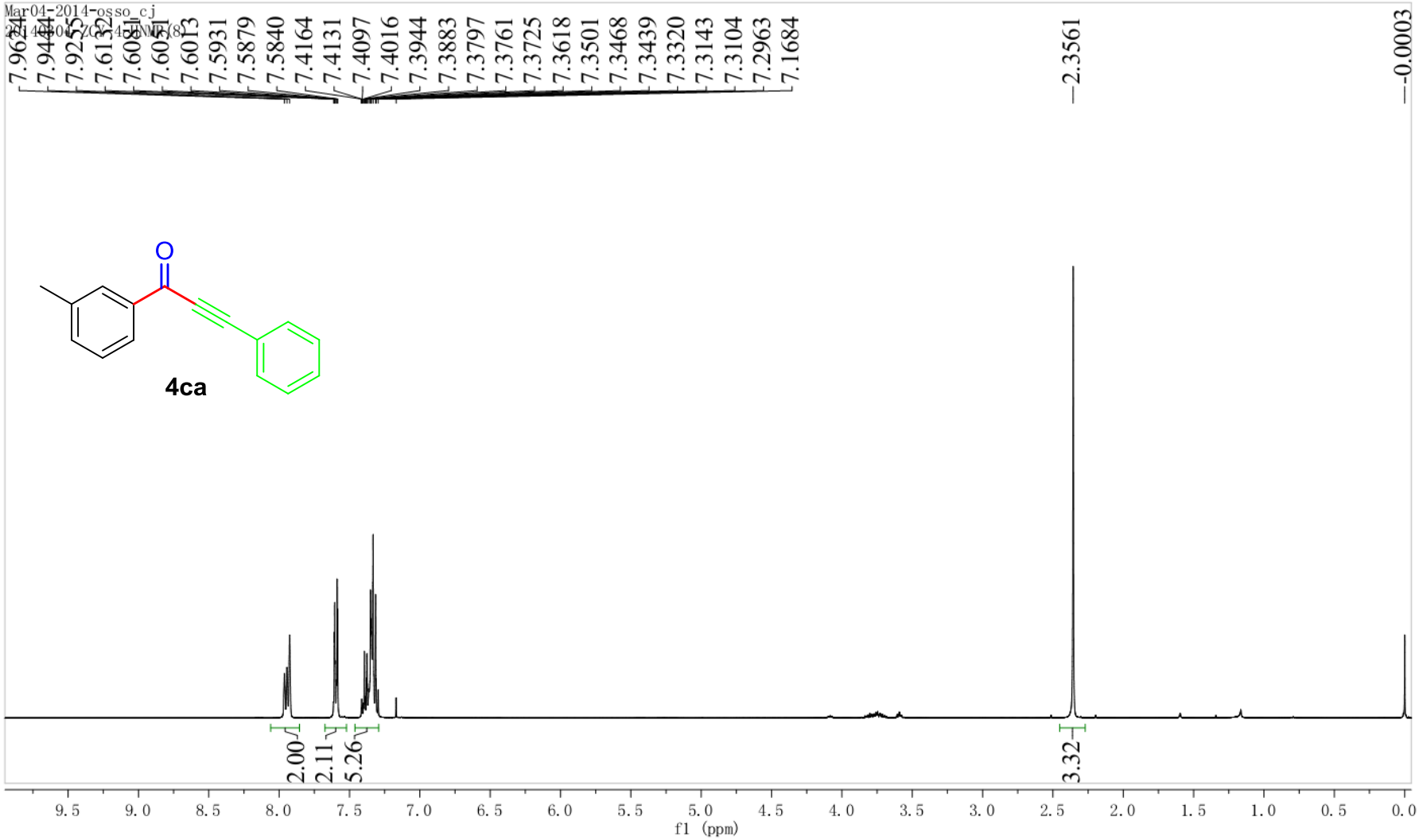

Aug21-2013-osso_cj
130821-7-ZhangCY-CNDS(14)
190.3353
165.9276
137.3171
129.9995
77.3174
76.9999
76.6823
42.1633
39.0500
14.2034
12.8131
O
O
O
O
N
N
210
190
170
150
130
110
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

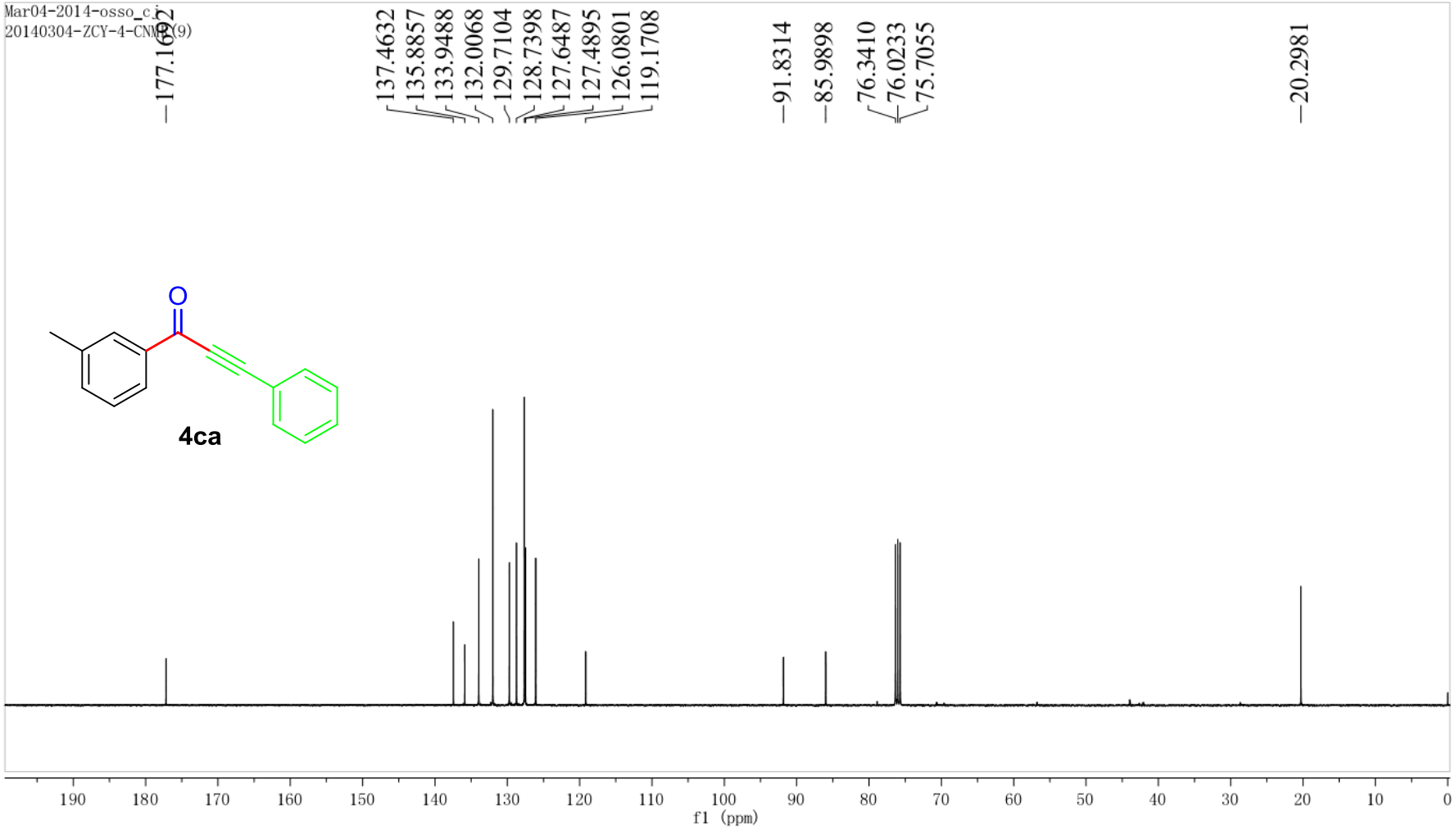

May06-2014-OSSO_c.J
140506-ZCY-1-HNMR(1)
8.2401
8.2272
8.2224
8.2189
7.7028
7.7001
7.6879
7.6827
7.6789
7.6564
7.6533
7.6503
7.6397
7.6350
7.6306
7.6196
7.6165
7.6135
7.5416
7.5220
7.5078
7.5036
7.4968
7.4895
7.4835
7.4745
7.4711
7.4676
7.4432
7.4279
7.4243
7.4105
7.4067
7.4032
7.2574
O
4aa
2.00
3.15
5.25
11.5 11.0 10.5 10.0 9.5 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 1.5 1.0 0.5 0.0
f1 (ppm)

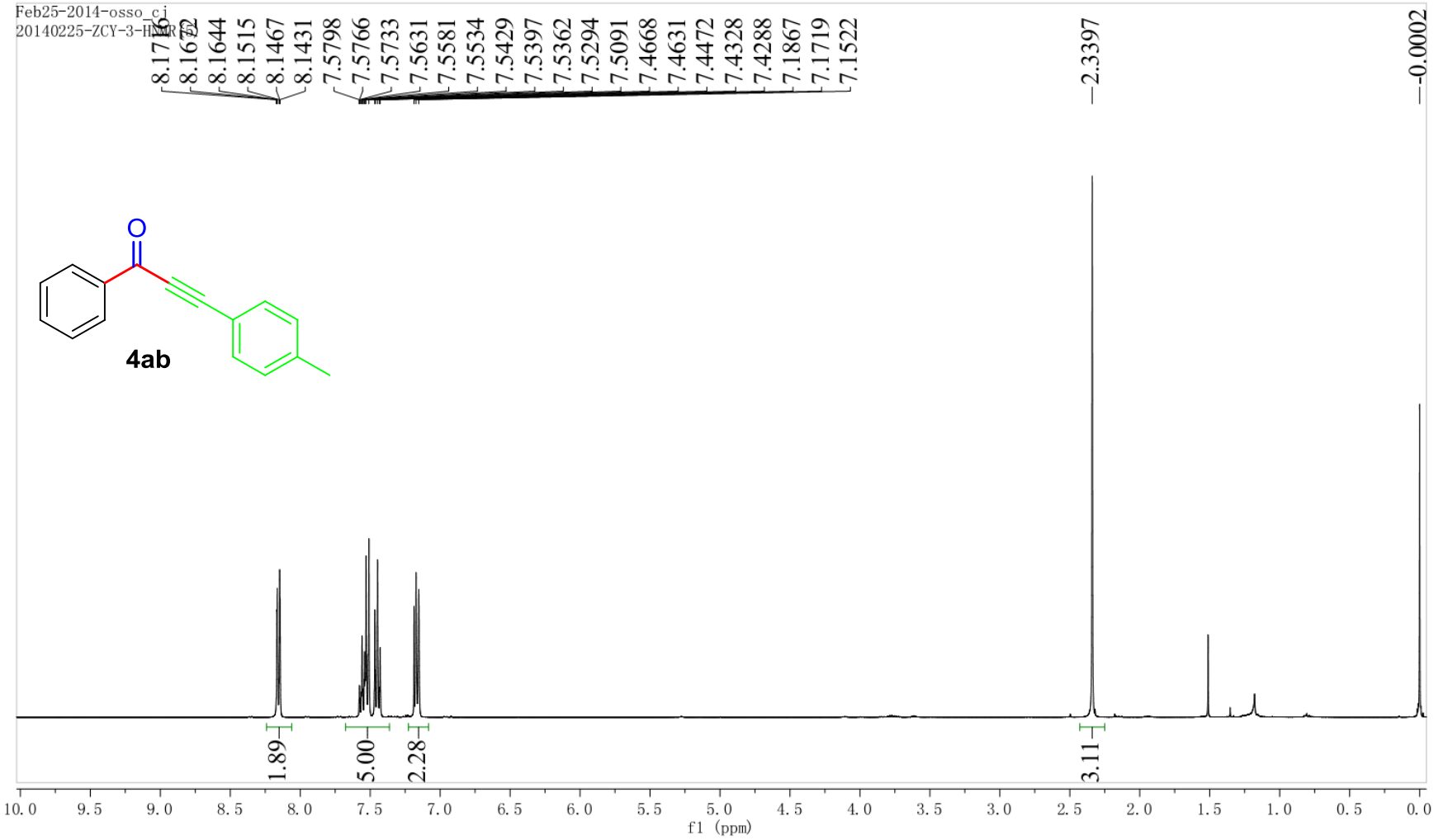

May06-2014-OSSO_c.1
140506-ZCY-1-CNMR
178.0469
136.9163
134.1503
133.0999
130.8287
129.6036
128.7195
128.6569
120.1563
93.1332
86.9201
77.3760
77.0582
76.7406
O
4aa
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

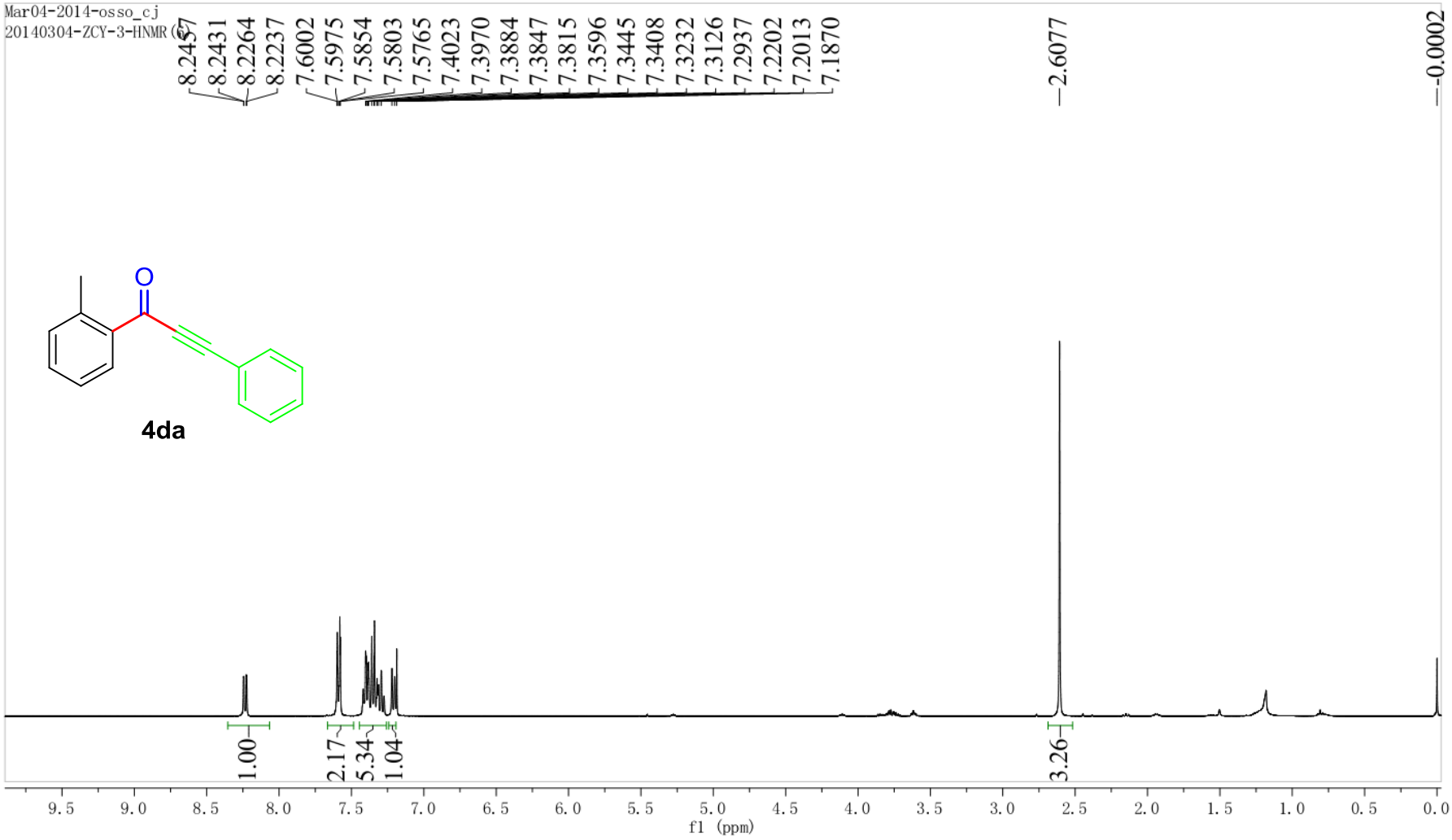

Mar04-2014-osso_cj
20140304-ZCY-5-HNMR(10)
8.0468
8.0301
8.0263
7.6160
7.6109
7.6078
7.6040
7.5959
7.5906
7.5867
7.4167
7.4053
7.3981
7.3919
7.3834
7.3797
7.3760
7.3542
7.3510
7.3394
7.3356
7.3312
7.3220
7.3180
7.3143
7.2384
7.2186
7.1762
2.3627
-0.0003
O
4ba
2.00
2.05
3.10
2.12
3.25
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

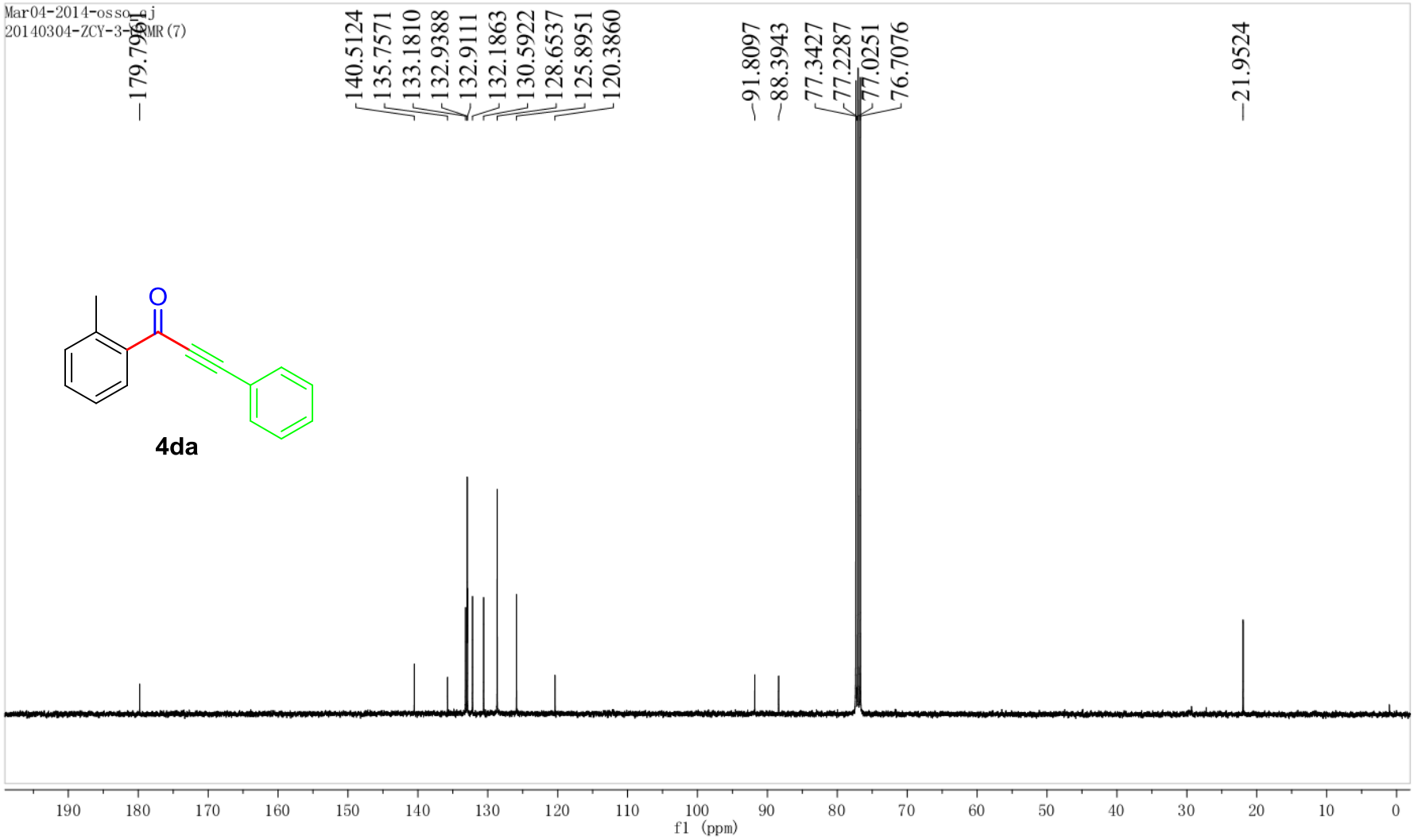

Mar04-2014-osso_cj
20140304-ZCY-5-CNMR(10)
176.6916
144.2144
131.9964
129.6511
128.6864
128.3263
127.6368
119.2409
91.5672
85.9538
76.3286
76.2141
76.0109
75.6932
20.8140
-0.0043
O
4ba
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

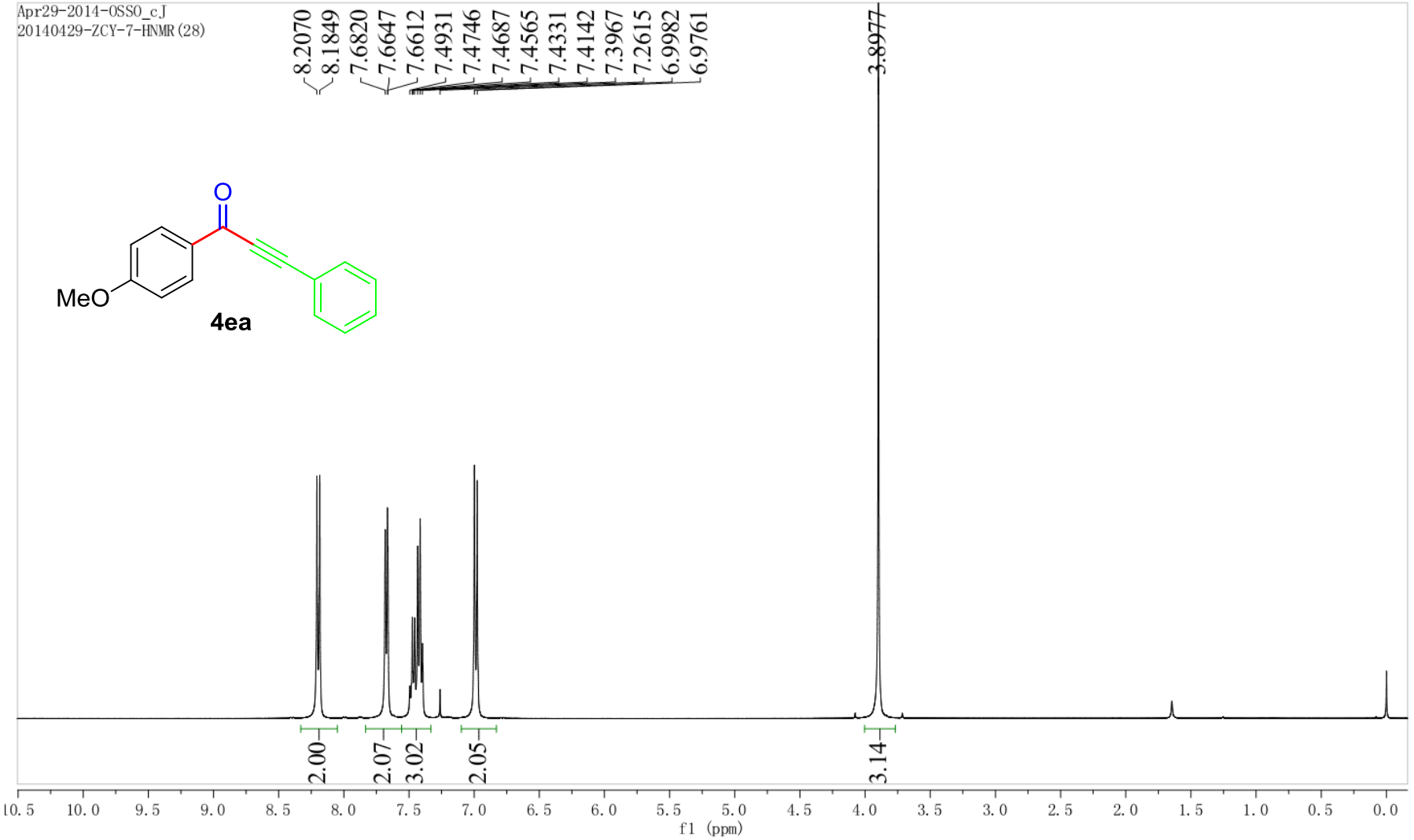

Mar04-2014-osso_cj
7.9624
7.9440
7.9252
7.6132
7.6088
7.6053
7.6013
7.5931
7.5879
7.5840
7.4164
7.4131
7.4097
7.4016
7.3944
7.3883
7.3797
7.3761
7.3725
7.3618
7.3501
7.3468
7.3439
7.3320
7.3143
7.3104
7.2963
7.1684
2.3561
-0.0003
4ca
2.00
2.11
5.26
3.32
f1 (ppm)

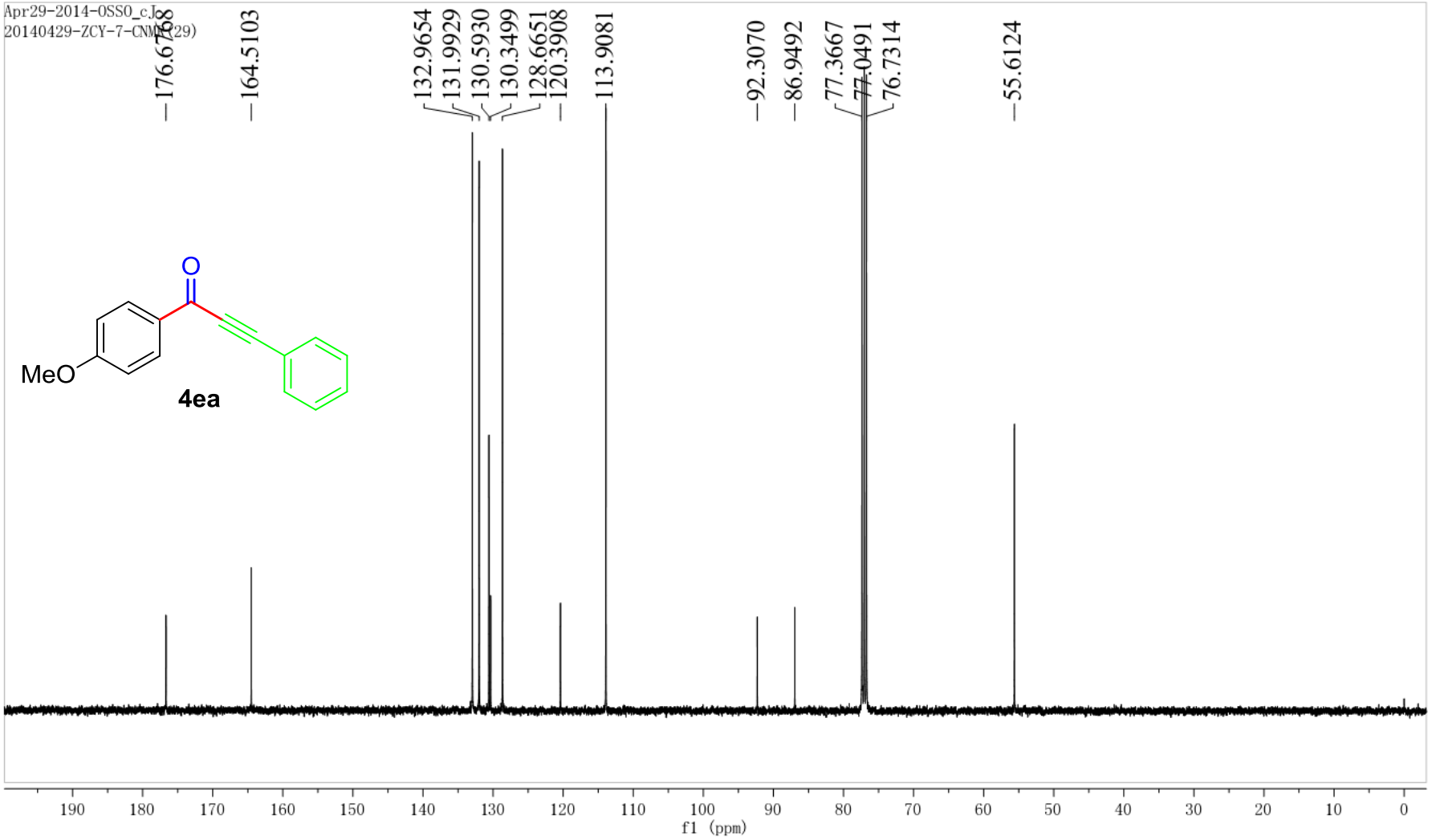

Mar04-2014-osso_c_i
20140304-ZCY-4-CNMR(9)
177.1692
137.4632
135.8857
133.9488
132.0068
129.7104
128.7398
127.6487
127.4895
126.0801
119.1708
91.8314
85.9898
76.3410
76.0233
75.7055
20.2981
O
4ca
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

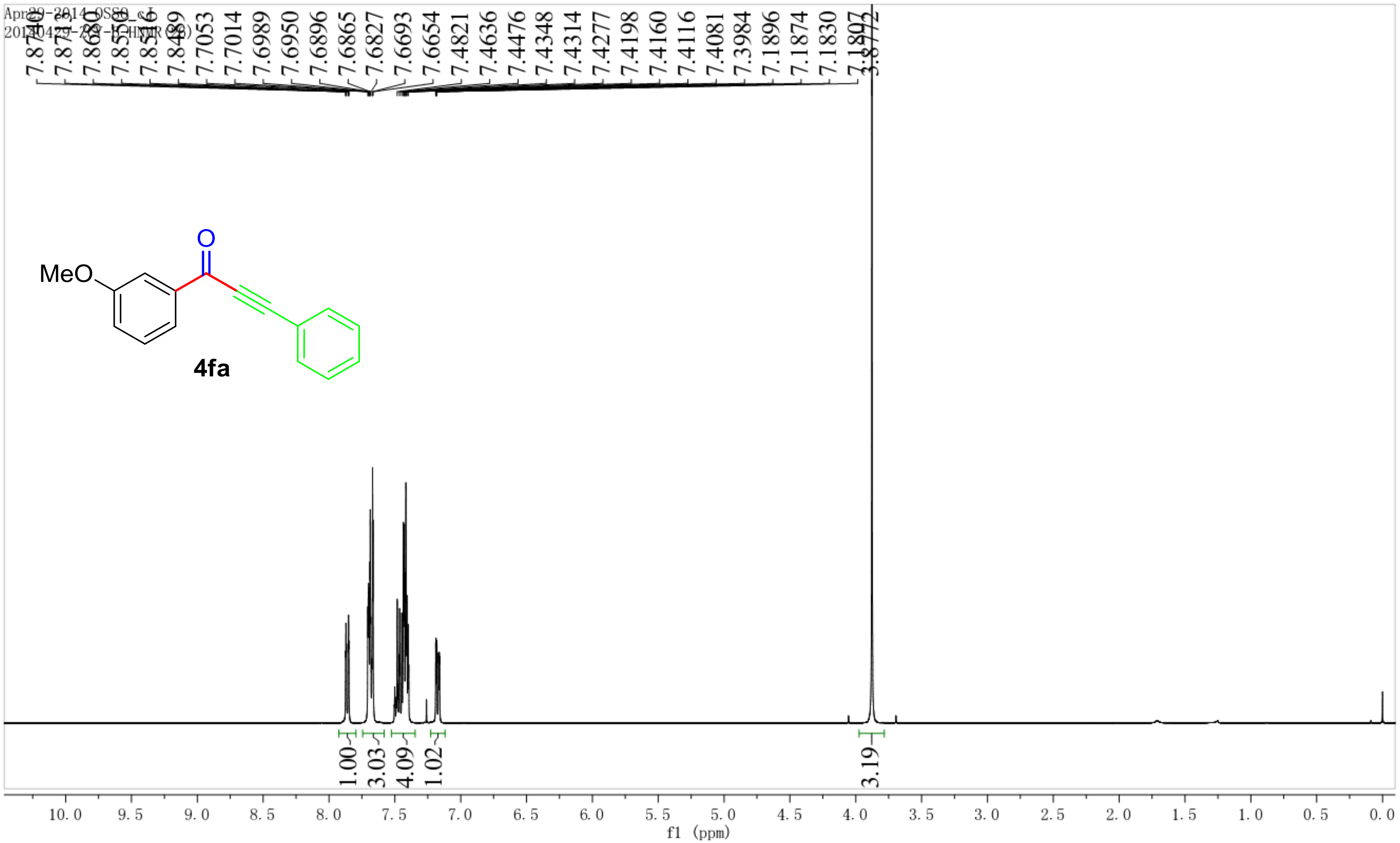

Feb25-2014-osso_cj
20140225-ZCY-3-HMR-22
8.1716
8.1672
8.1644
8.1515
8.1467
8.1431
7.5798
7.5766
7.5733
7.5631
7.5581
7.5534
7.5429
7.5397
7.5362
7.5294
7.5091
7.4668
7.4631
7.4472
7.4328
7.4288
7.1867
7.1719
7.1522
2.3397
0.0002
O
4ab
1.89
5.00
2.28
3.11
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

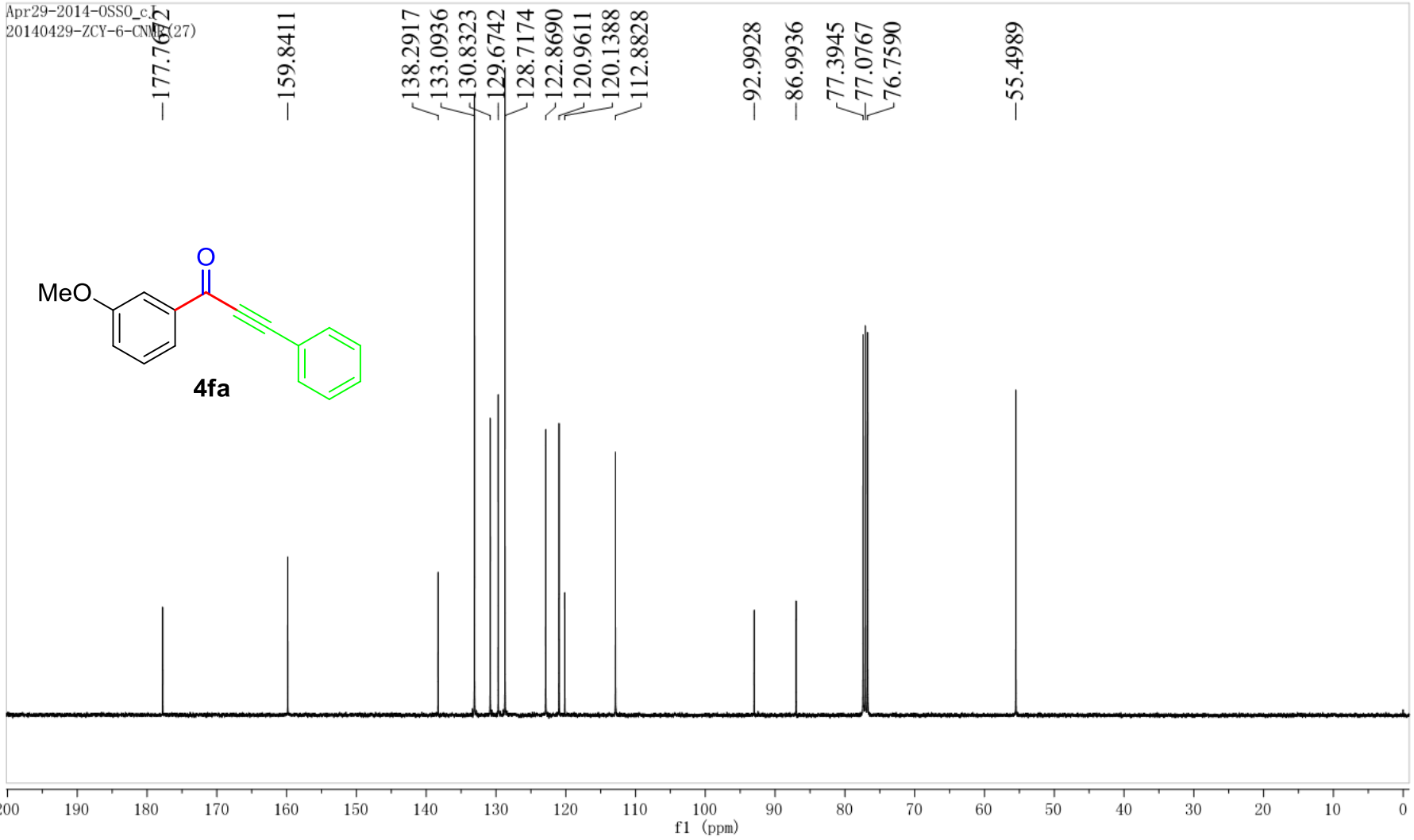

Mar04-2014-osso_cj
20140304-ZCY-3-HNMR(C
8.2457
8.2431
8.2264
8.2237
7.6002
7.5975
7.5854
7.5803
7.5765
7.4023
7.3970
7.3884
7.3847
7.3815
7.3596
7.3445
7.3408
7.3232
7.3126
7.2937
7.2202
7.2013
7.1870
2.6077
-0.0002
O
4da
1.00
2.17
5.34
1.04
3.26
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

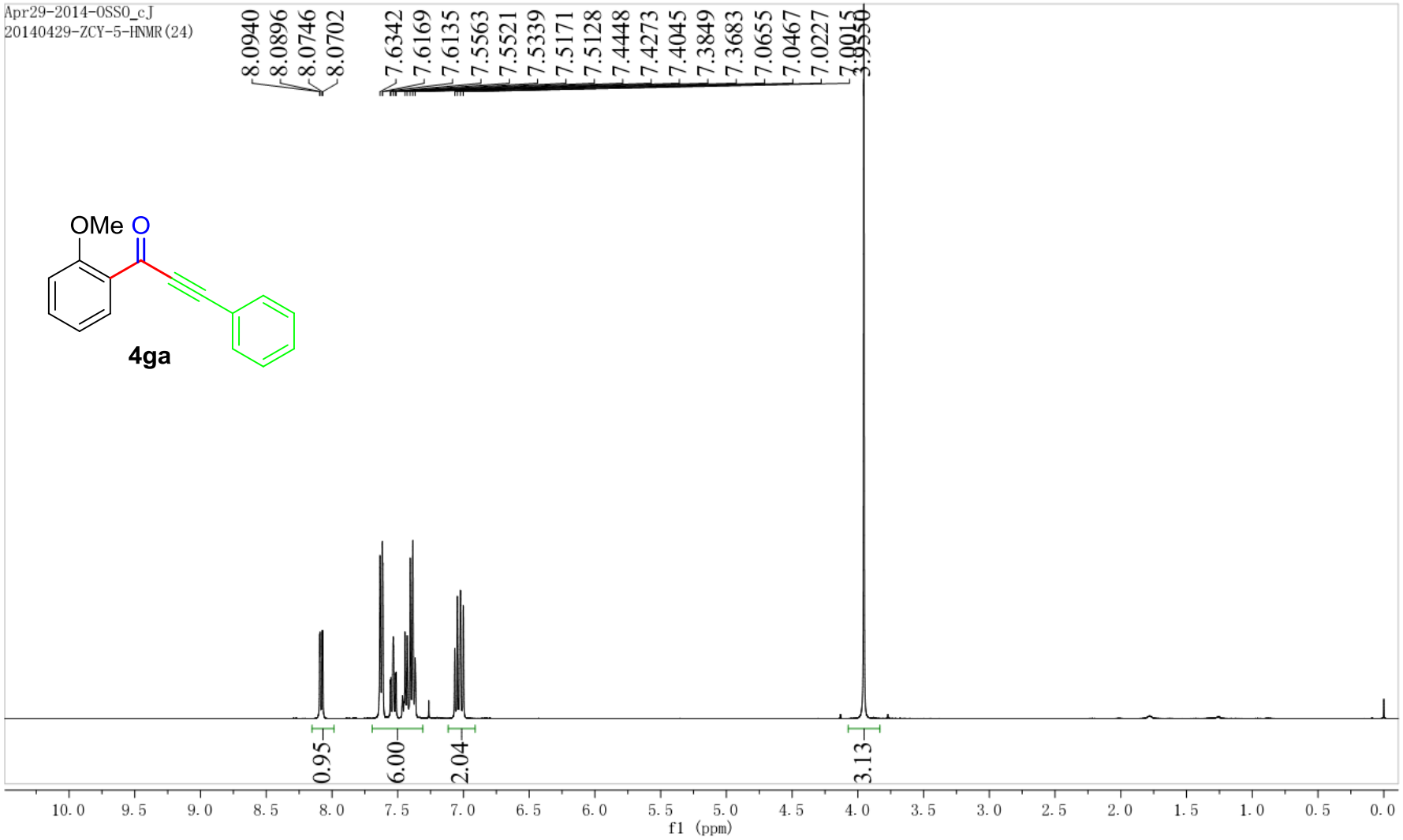

Mar04-2014-osso_ej
20140304-ZCY-3-1 1HMR(7)
179.7966
140.5124
135.7571
133.1810
132.9388
132.9111
132.1863
130.5922
128.6537
125.8951
120.3860
91.8097
88.3943
77.3427
77.2287
77.0251
76.7076
21.9524
O
4da
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

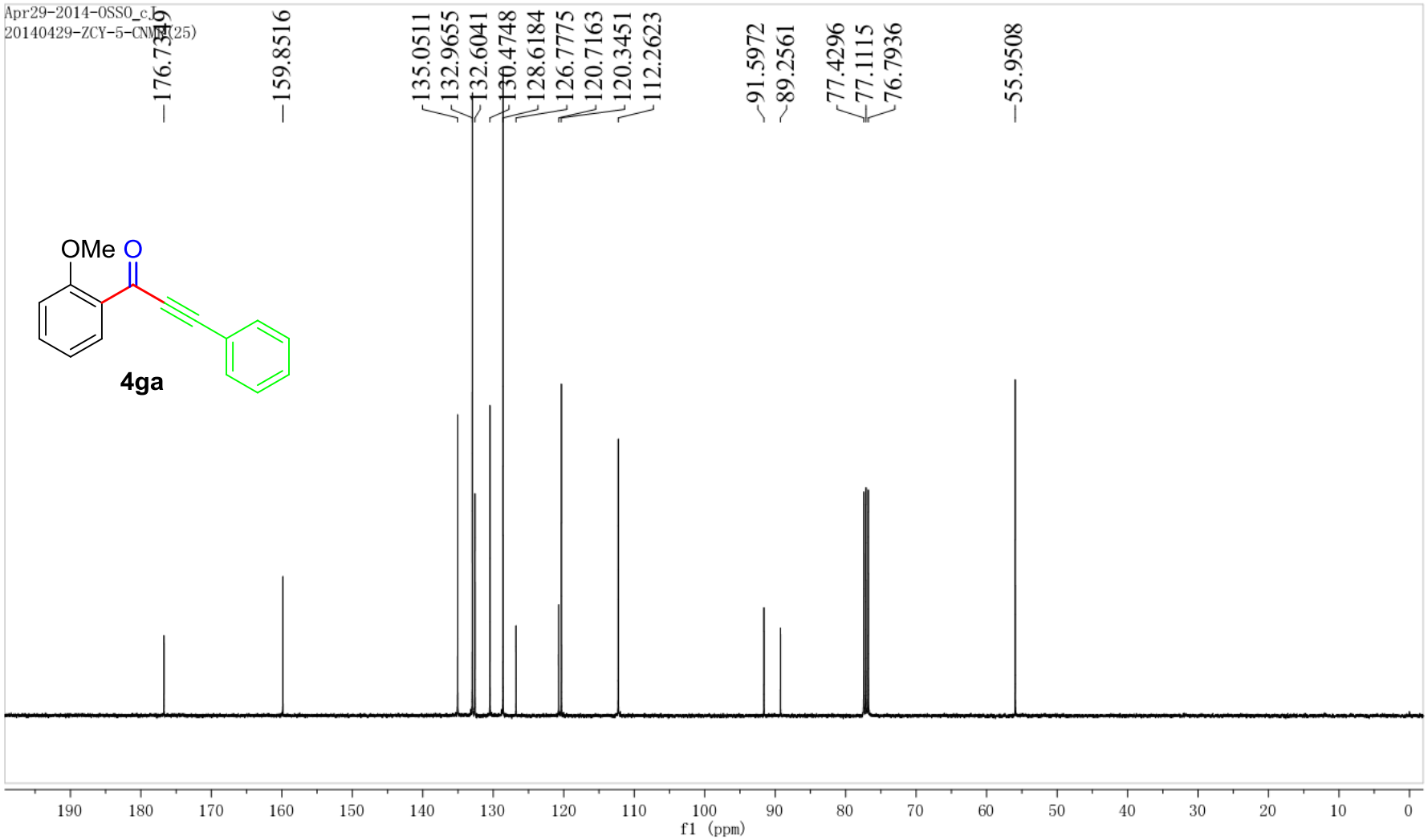

Apr29-2014-OSSO_cJ
20140429-ZCY-7-HNMR(28)
8.2070
8.1849
7.6820
7.6647
7.6612
7.4931
7.4746
7.4687
7.4565
7.4331
7.4142
7.3967
7.2615
6.9982
6.9761
3.8977
O
MeO
4ea
2.00
2.07
3.02
2.05
3.14
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

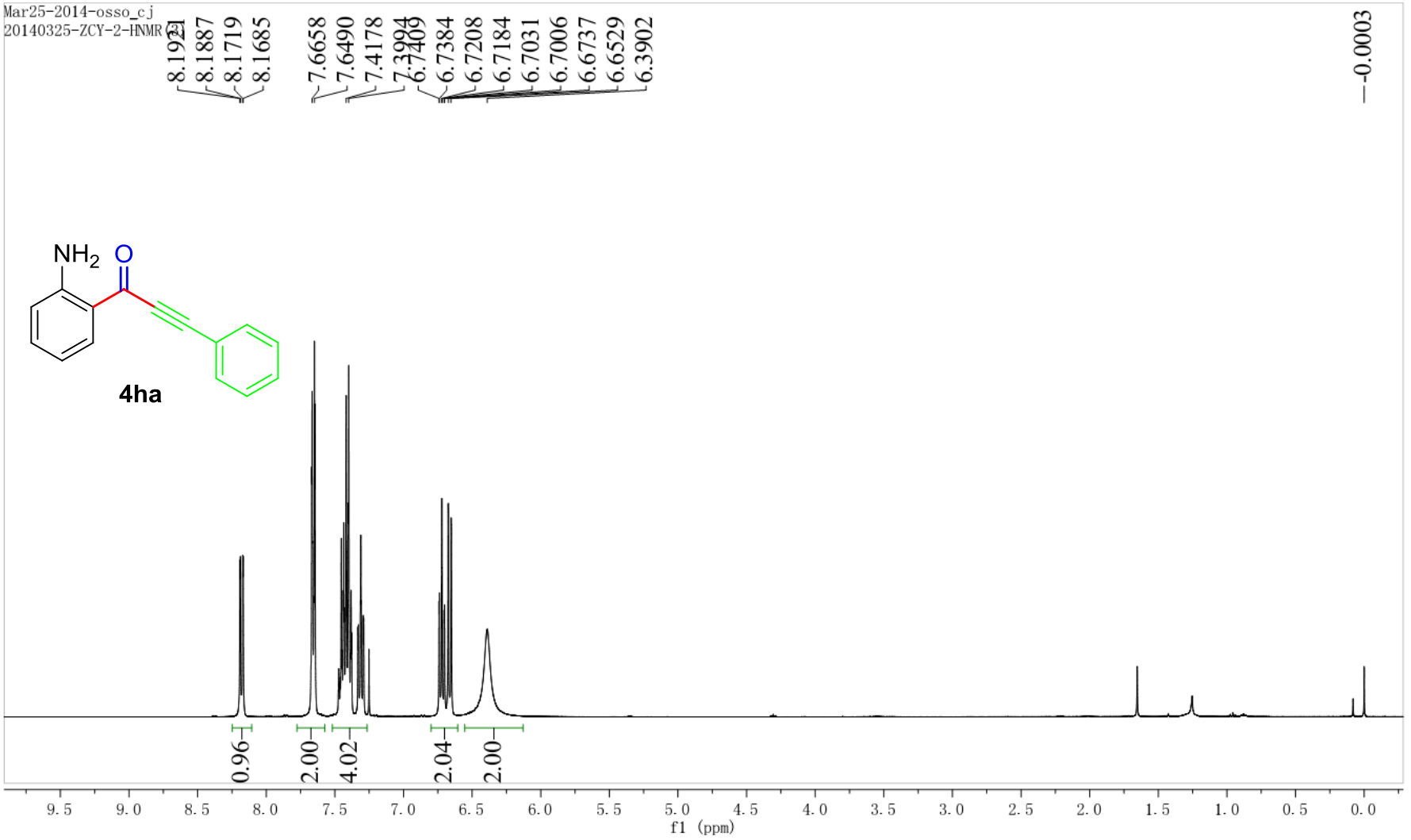

Apr29-2014-OSSO_cJ
20140429-ZCY-7-CNM
176.6768
164.5103
132.9654
131.9929
130.5930
130.3499
128.6651
120.3908
113.9081
92.3070
86.9492
77.3667
77.0491
76.7314
55.6124
O
MeO
4ea
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

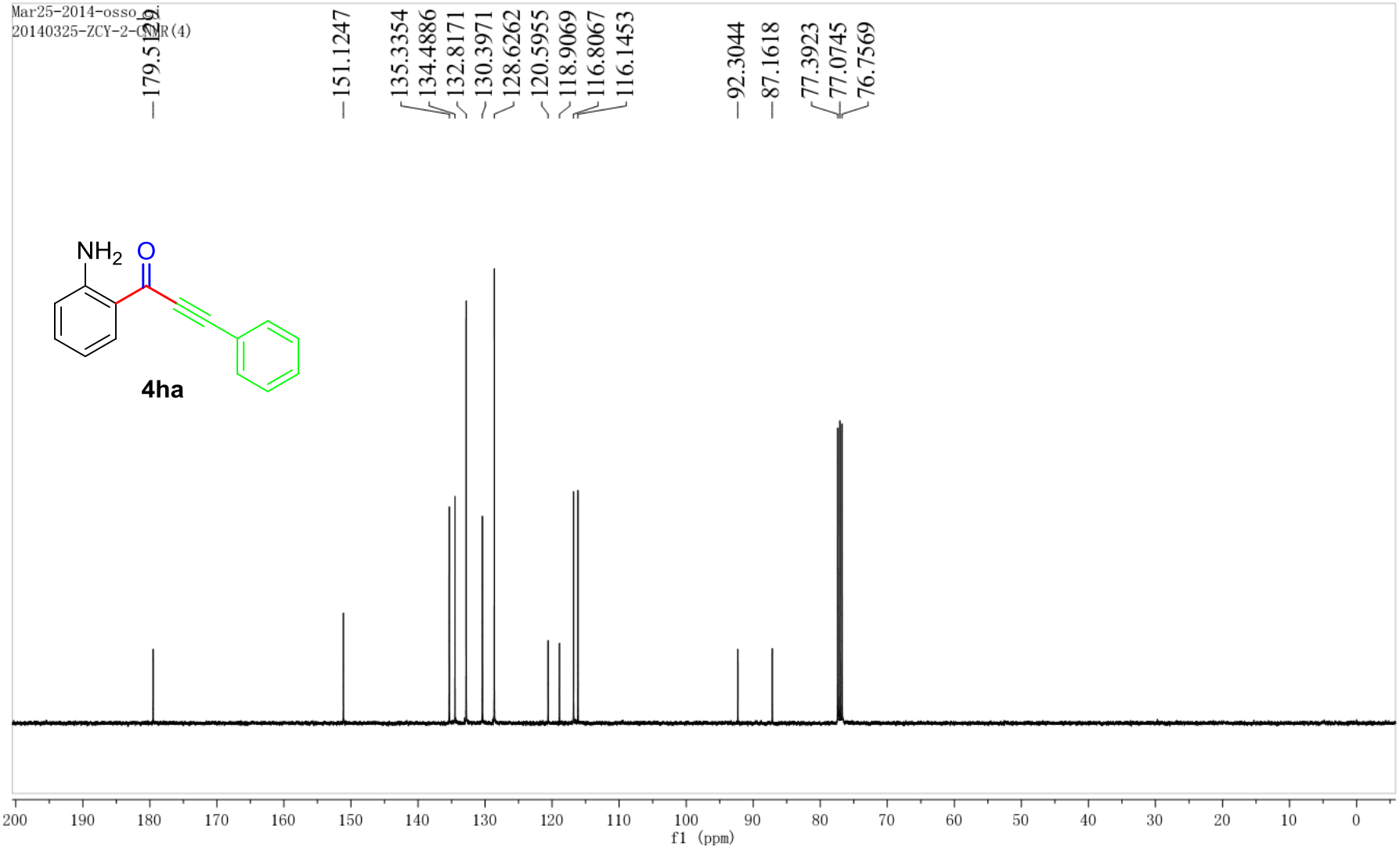

7.8740
7.8713
7.8680
7.8550
7.8516
7.8489
7.7053
7.7014
7.6989
7.6950
7.6896
7.6865
7.6827
7.6693
7.6654
7.4821
7.4636
7.4476
7.4348
7.4314
7.4277
7.4198
7.4160
7.4116
7.4081
7.3984
7.1896
7.1874
7.1830
7.1807
3.8772
MeO
O
4fa
1.00
3.03
4.09
1.02
3.19
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

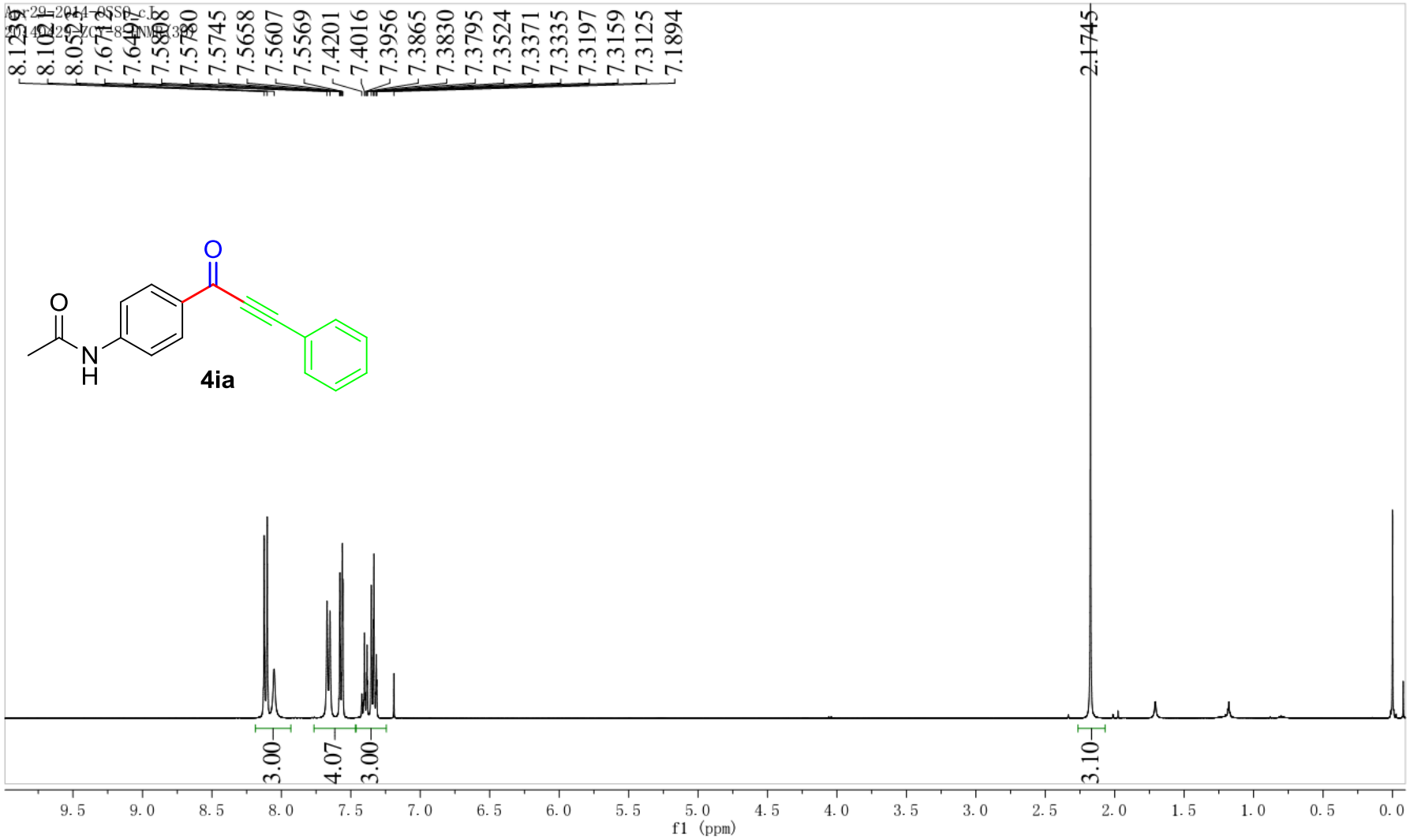

Apr29-2014-OSSO_c_1
20140429-ZCY-6-CNMR(27)
177.7672
159.8411
138.2917
133.0936
130.8323
129.6742
128.7174
122.8690
120.9611
120.1388
112.8828
92.9928
86.9936
77.3945
77.0767
76.7590
55.4989
MeO
O
4fa
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

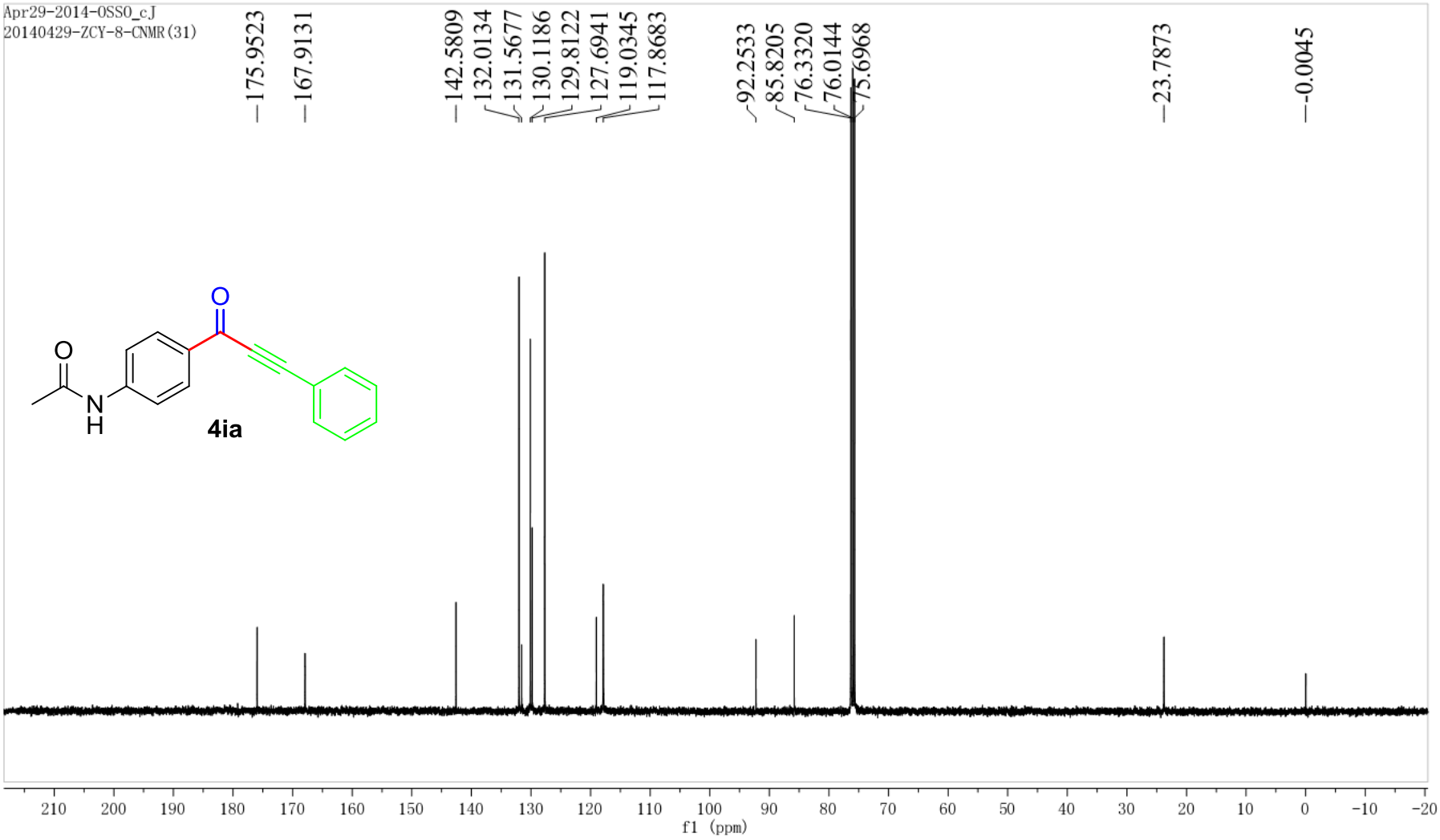

Apr29-2014-OSSO_cJ
20140429-ZCY-5-HNMR(24)
8.0940
8.0896
8.0746
8.0702
7.6342
7.6169
7.6135
7.5563
7.5521
7.5339
7.5171
7.5128
7.4448
7.4273
7.4045
7.3849
7.3683
7.0655
7.0467
7.0227
7.0015
3.9550
OMe
O
4ga
0.95
6.00
2.04
3.13
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

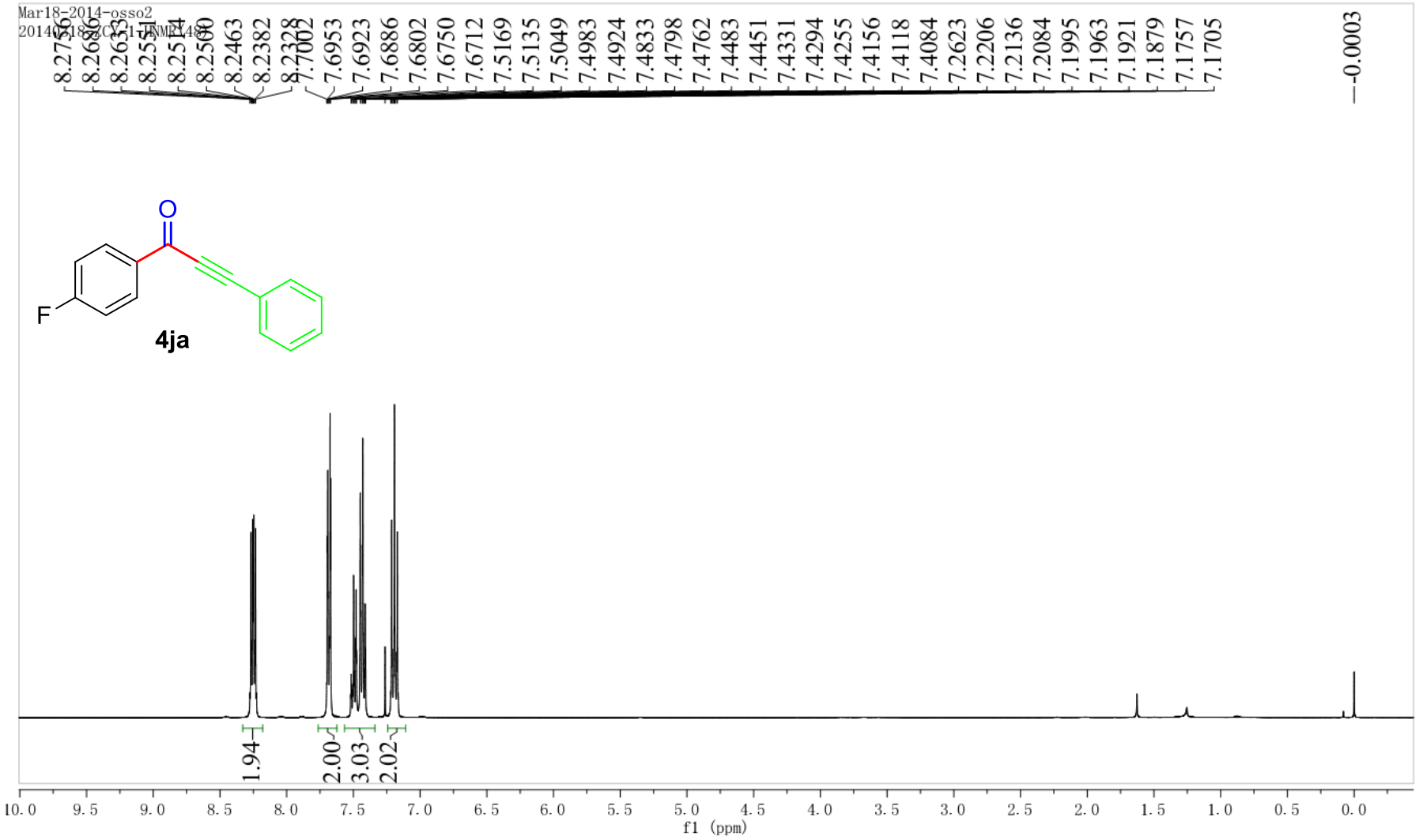

Apr29-2014-OSSO_c.1
20140429-ZCY-5-CNMR(25)
176.7349
159.8516
135.0511
132.9655
132.6041
130.4748
128.6184
126.7775
120.7163
120.3451
112.2623
91.5972
89.2561
77.4296
77.1115
76.7936
55.9508
OMe
O
4ga
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Mar25-2014-osso_cj
20140325-ZCY-2-HNMR
8.1921
8.1887
8.1719
8.1685
7.6658
7.6490
7.4178
7.3994
7.3409
6.7384
6.7208
6.7184
6.7031
6.7006
6.6737
6.6529
6.3902
-0.0003
NH2
O
4ha
0.96
2.00
4.02
2.04
2.00
9.5
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
1.5
1.0
0.5
0.0
f1 (ppm)


Mar25-2014-osso_si
20140325-ZCY-2-CNMR(4)
179.5129
151.1247
135.3354
134.4886
132.8171
130.3971
128.6262
120.5955
118.9069
116.8067
116.1453
92.3044
87.1618
77.3923
77.0745
76.7569
NH2
O
4ha
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.1239
8.1021
8.0521
7.6713
7.6497
7.5898
7.5780
7.5745
7.5658
7.5607
7.5569
7.4201
7.4016
7.3956
7.3865
7.3830
7.3795
7.3524
7.3371
7.3335
7.3197
7.3159
7.3125
7.1894
2.1745
O
O
N
H
4ia
3.00
4.07
3.00
3.10
9.5
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
1.5
1.0
0.5
0.0
f1 (ppm)


Apr29-2014-OSSO_cJ
20140429-ZCY-8-CNMR(31)
175.9523
167.9131
142.5809
132.0134
131.5677
130.1186
129.8122
127.6941
119.0345
117.8683
92.2533
85.8205
76.3320
76.0144
75.6968
23.7873
-0.0045
O
O
N
H
4ia
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


Mar18-2014-osso2
8.2750
8.2686
8.2633
8.2551
8.2514
8.2500
8.2463
8.2382
8.2328
8.2302
7.6953
7.6923
7.6886
7.6802
7.6750
7.6712
7.5169
7.5135
7.5049
7.4983
7.4924
7.4833
7.4798
7.4762
7.4483
7.4451
7.4331
7.4294
7.4255
7.4156
7.4118
7.4084
7.2623
7.2206
7.2136
7.2084
7.1995
7.1963
7.1921
7.1879
7.1757
7.1705
-0.0003
O
F
4ja
1.94
2.00
3.03
2.02
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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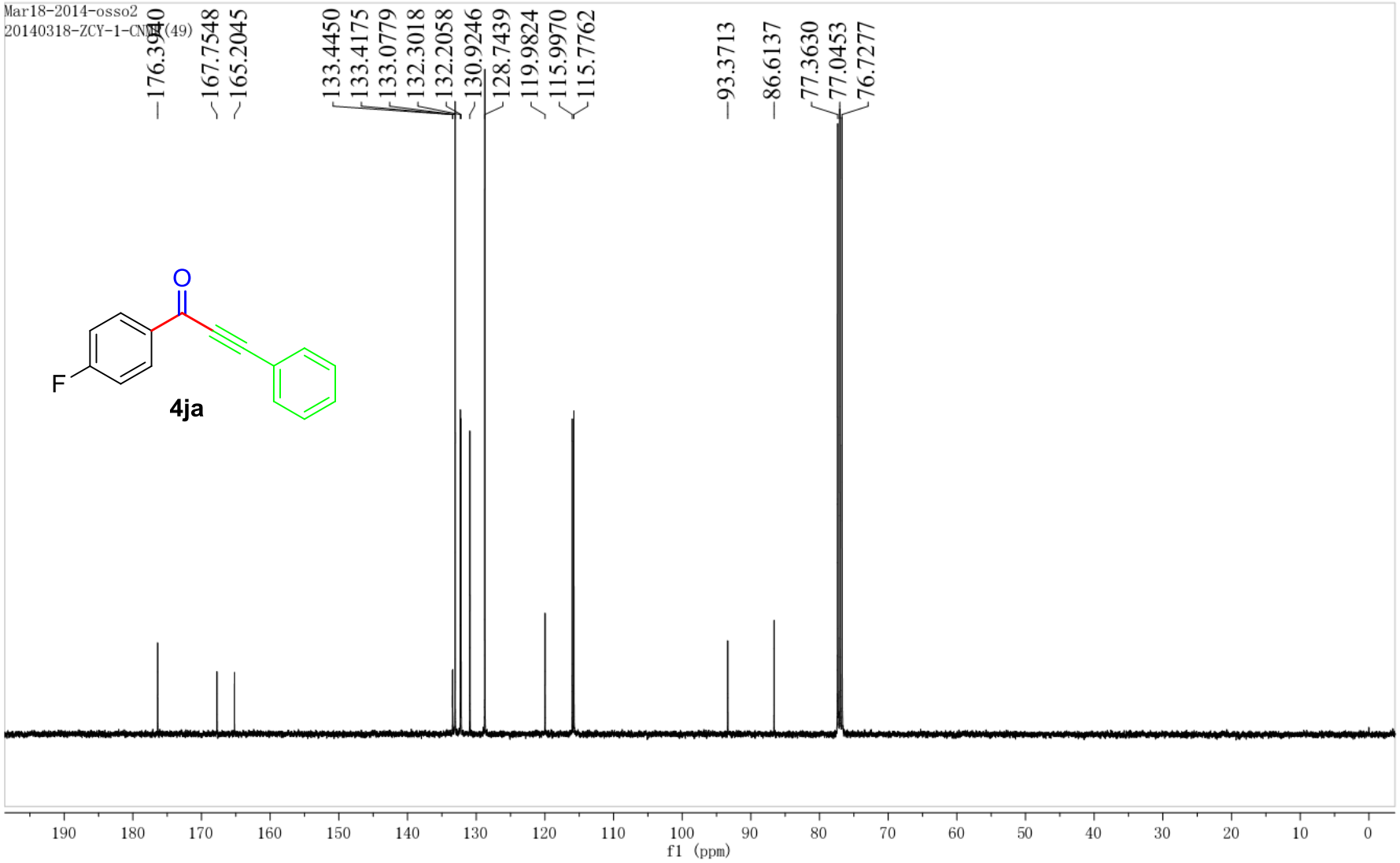
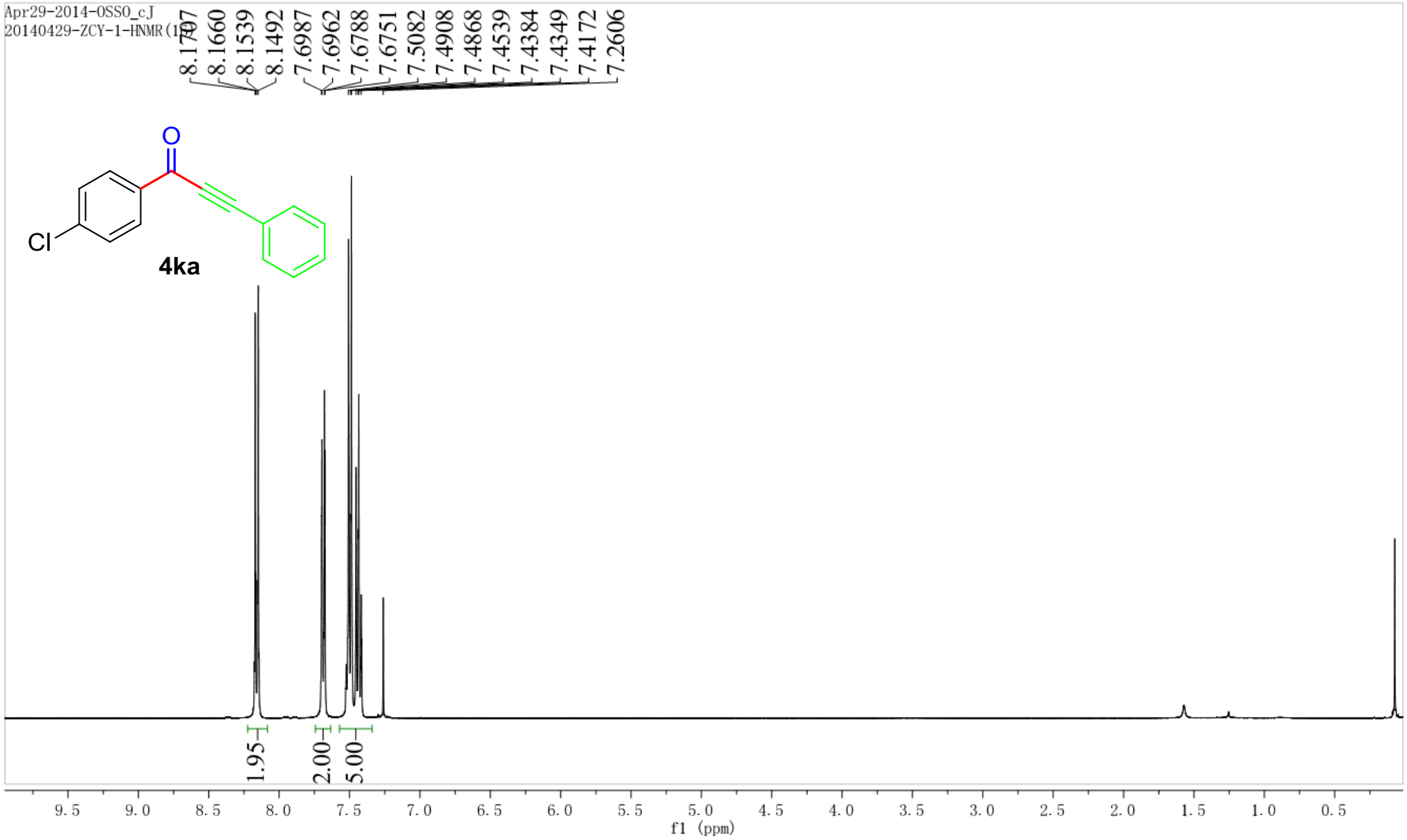
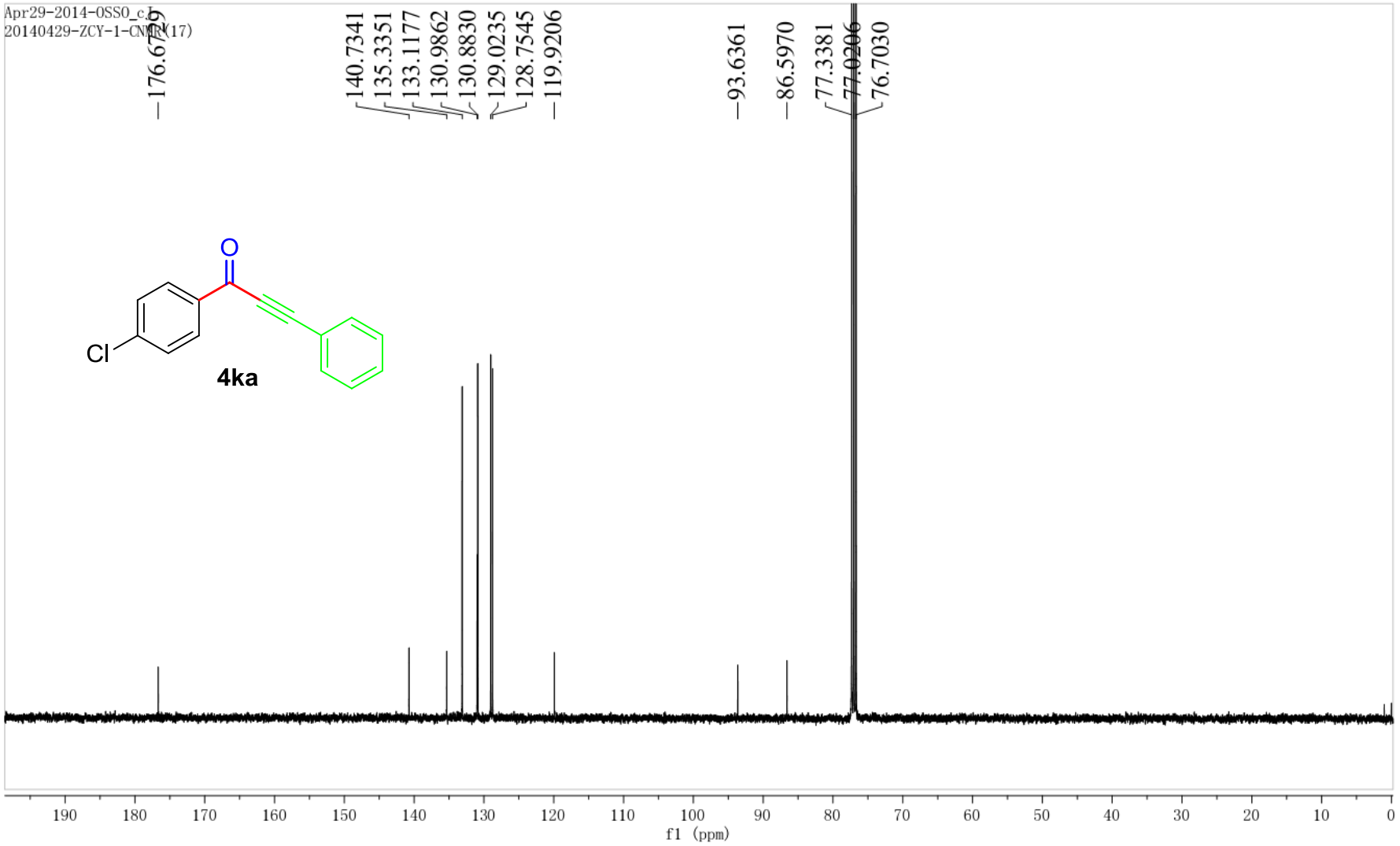
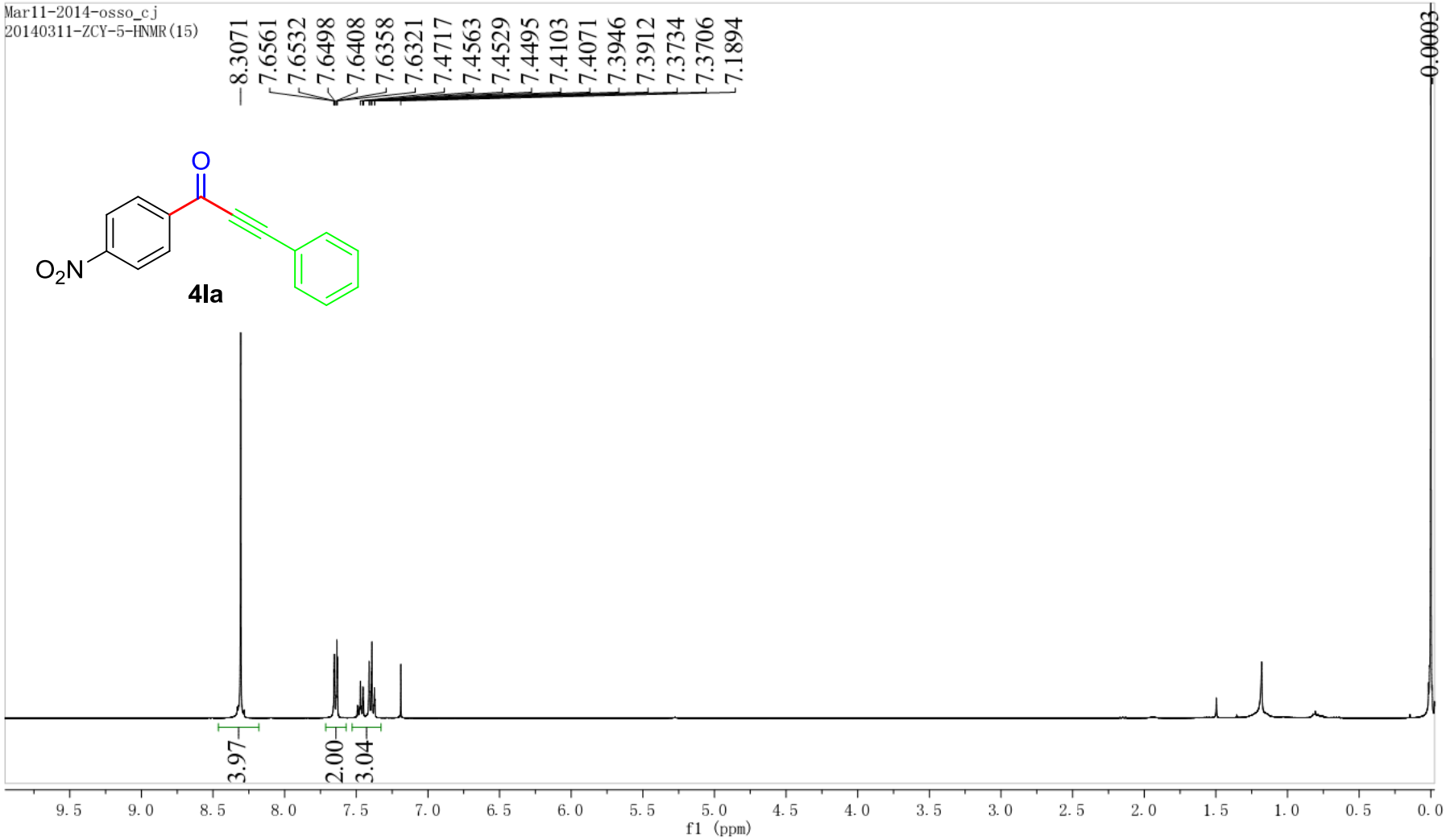
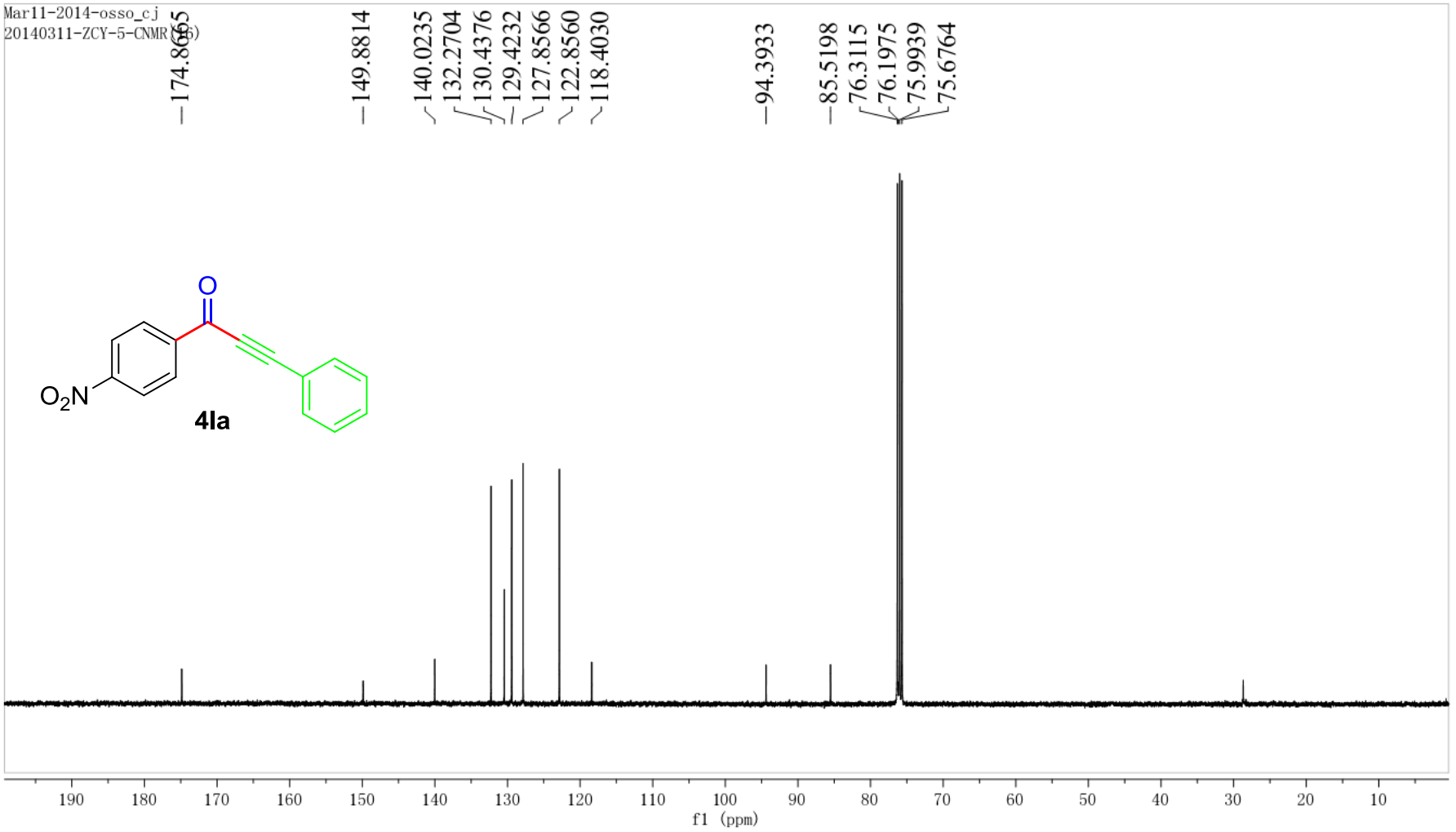
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

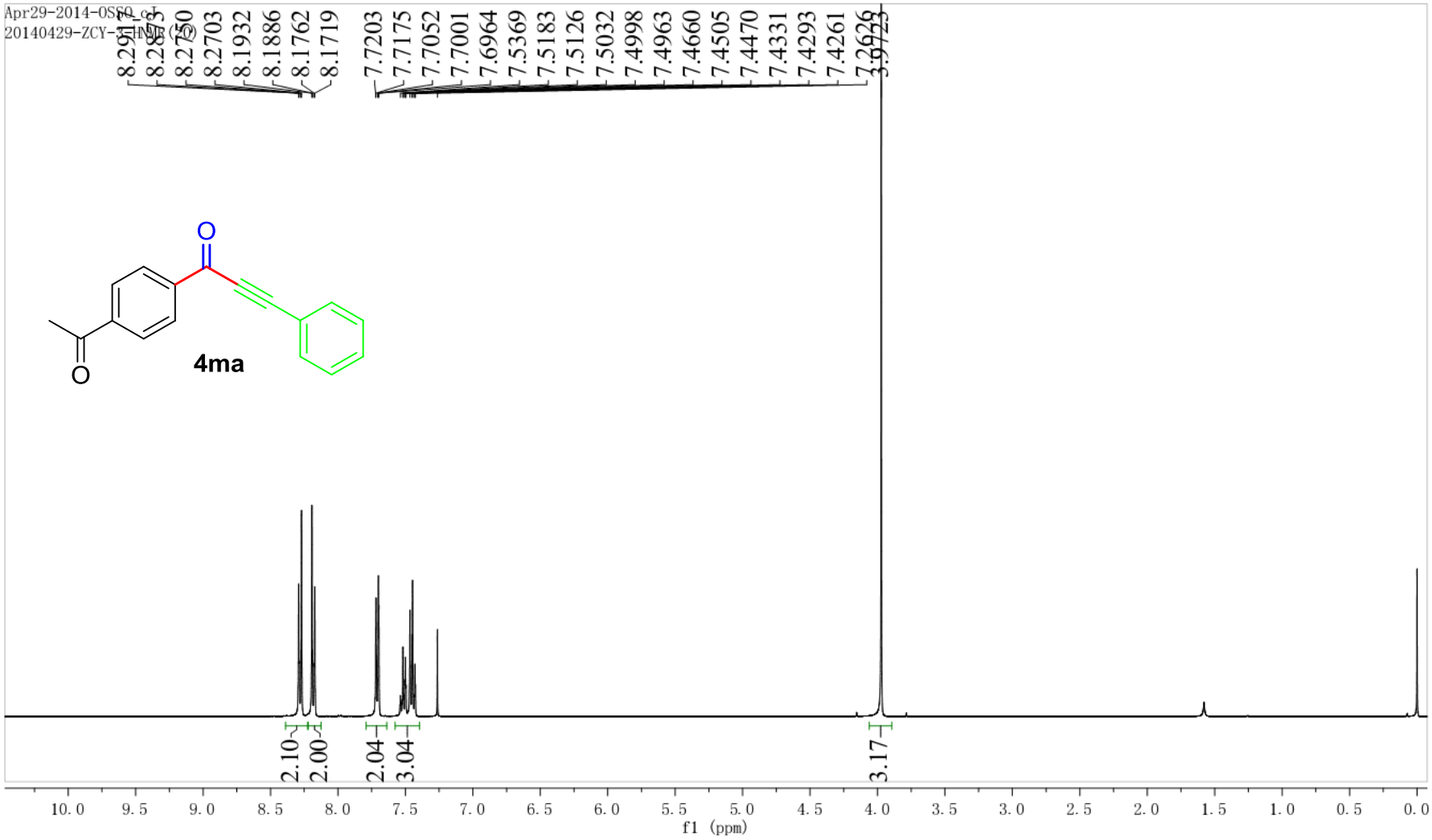

Mar18-2014-osso2
20140318-ZCY-1-CNMR(49)
176.3940
167.7548
165.2045
133.4450
133.4175
133.0779
132.3018
132.2058
130.9246
128.7439
119.9824
115.9970
115.7762
93.3713
86.6137
77.3630
77.0453
76.7277
O
F
4ja
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

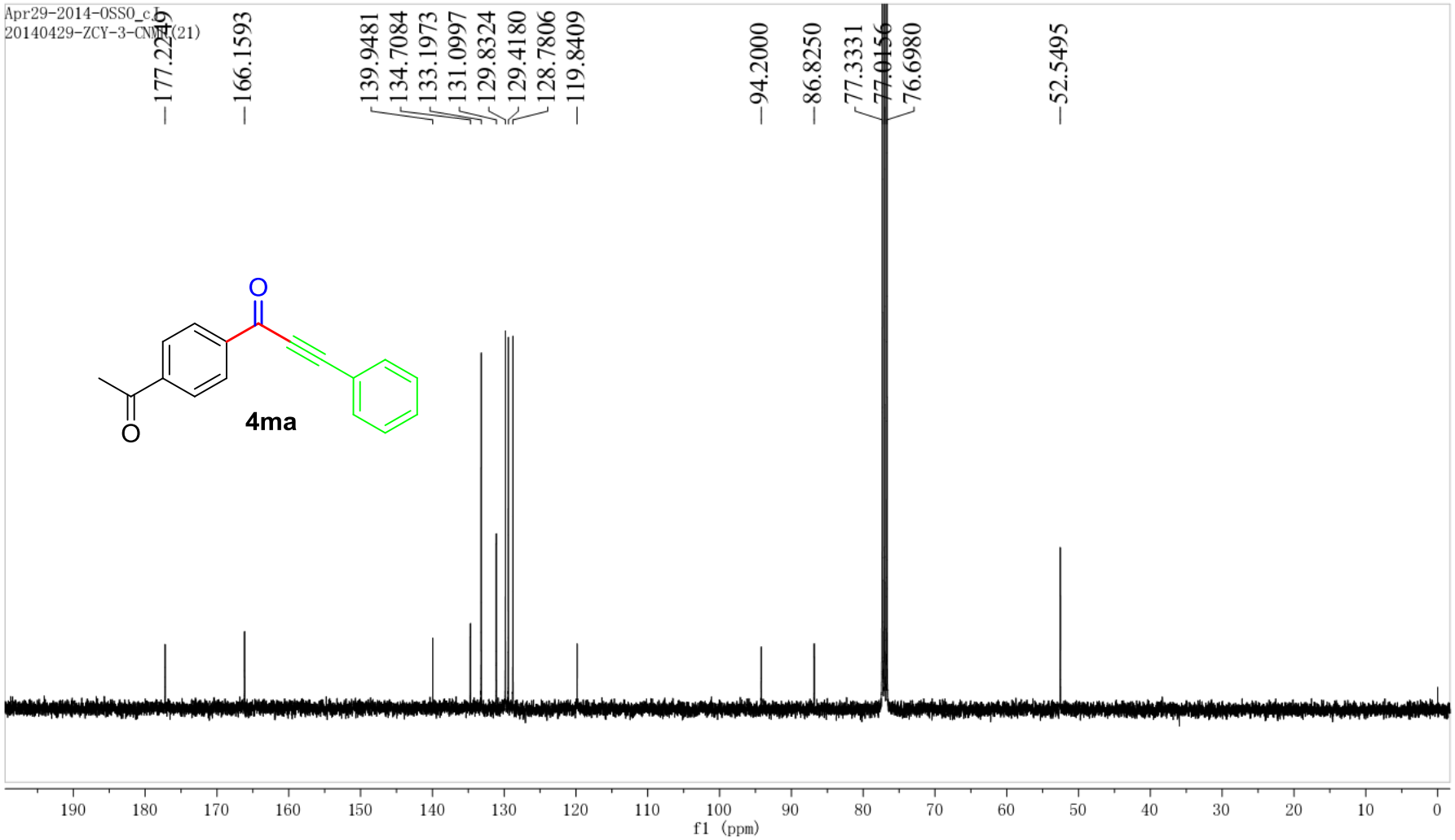

Apr29-2014-OSSO_cJ
20140429-ZCY-1-HNMR(1
8.1707
8.1660
8.1539
8.1492
7.6987
7.6962
7.6788
7.6751
7.5082
7.4908
7.4868
7.4539
7.4384
7.4349
7.4172
7.2606
O
Cl
4ka
1.95
2.00
5.00
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

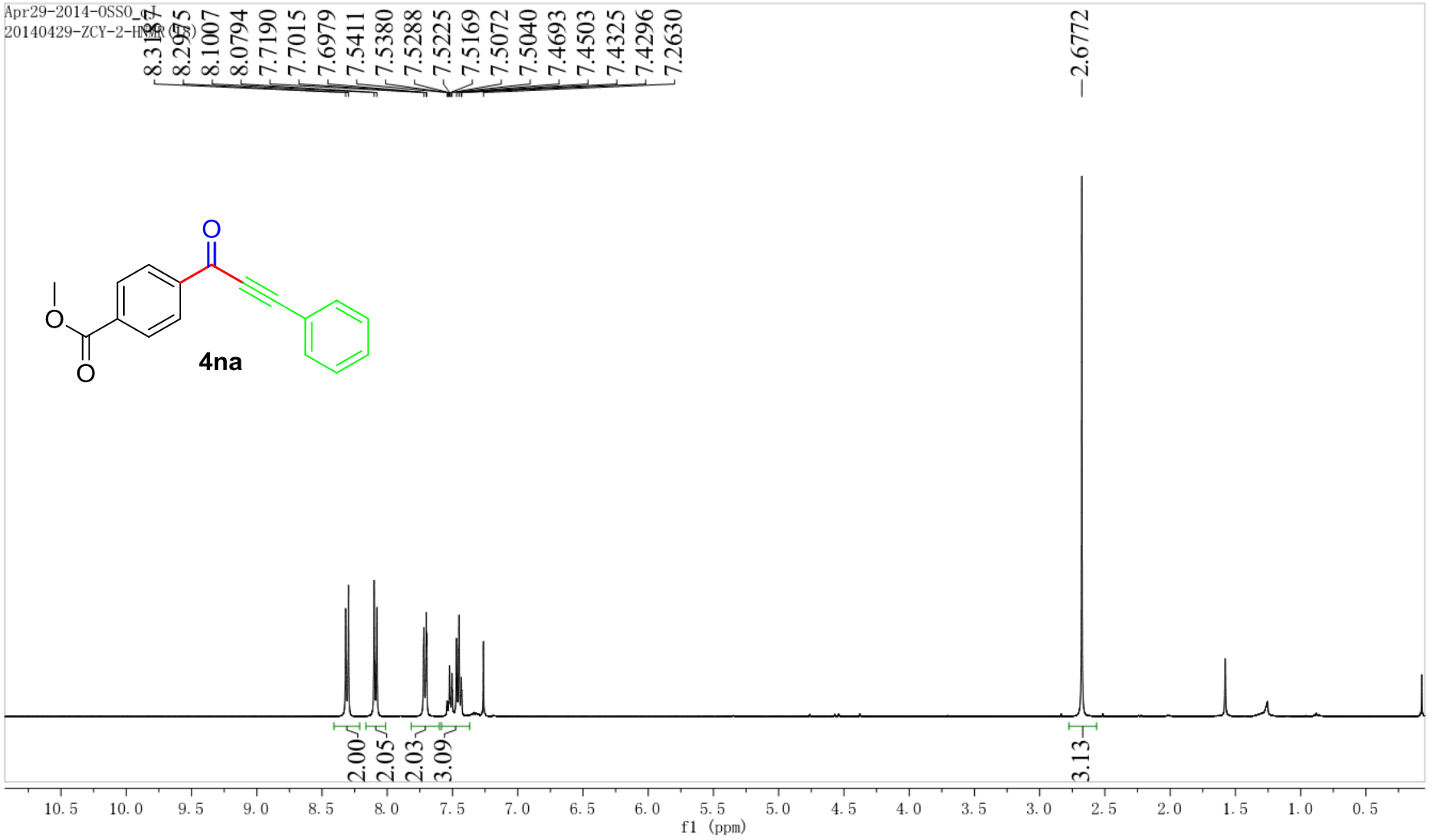

Apr29-2014-OSSO_c.1
20140429-ZCY-1-CNMR(17)
176.6739
140.7341
135.3351
133.1177
130.9862
130.8830
129.0235
128.7545
119.9206
93.6361
86.5970
77.3381
77.0206
76.7030
O
Cl
4ka
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

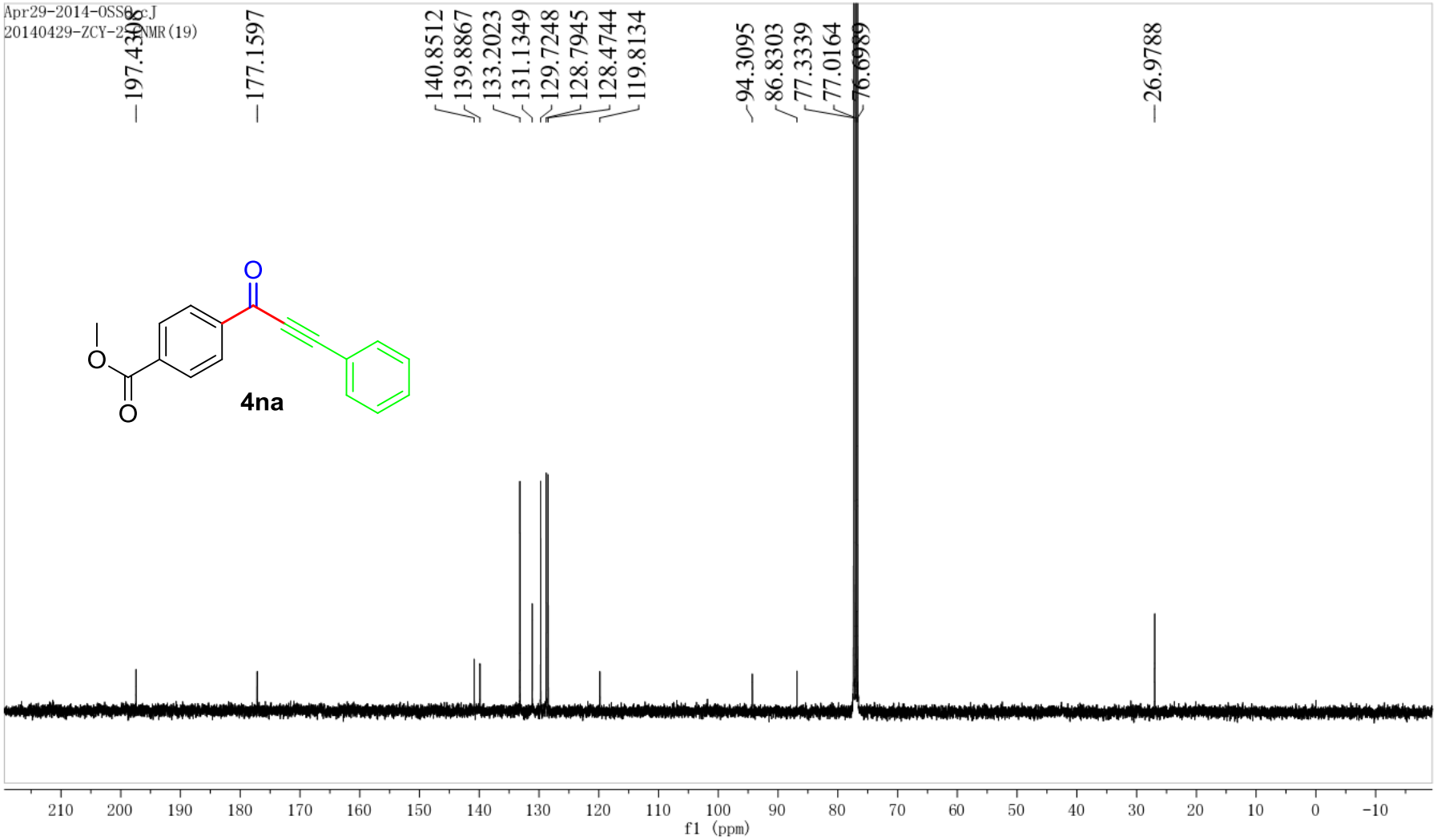

Mar11-2014-osso_cj
20140311-ZCY-5-HNMR(15)
8.3071
7.6561
7.6532
7.6498
7.6408
7.6358
7.6321
7.4717
7.4563
7.4529
7.4495
7.4103
7.4071
7.3946
7.3912
7.3734
7.3706
7.1894
0.0003
O
O2N
4la
3.97
2.00
3.04
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)

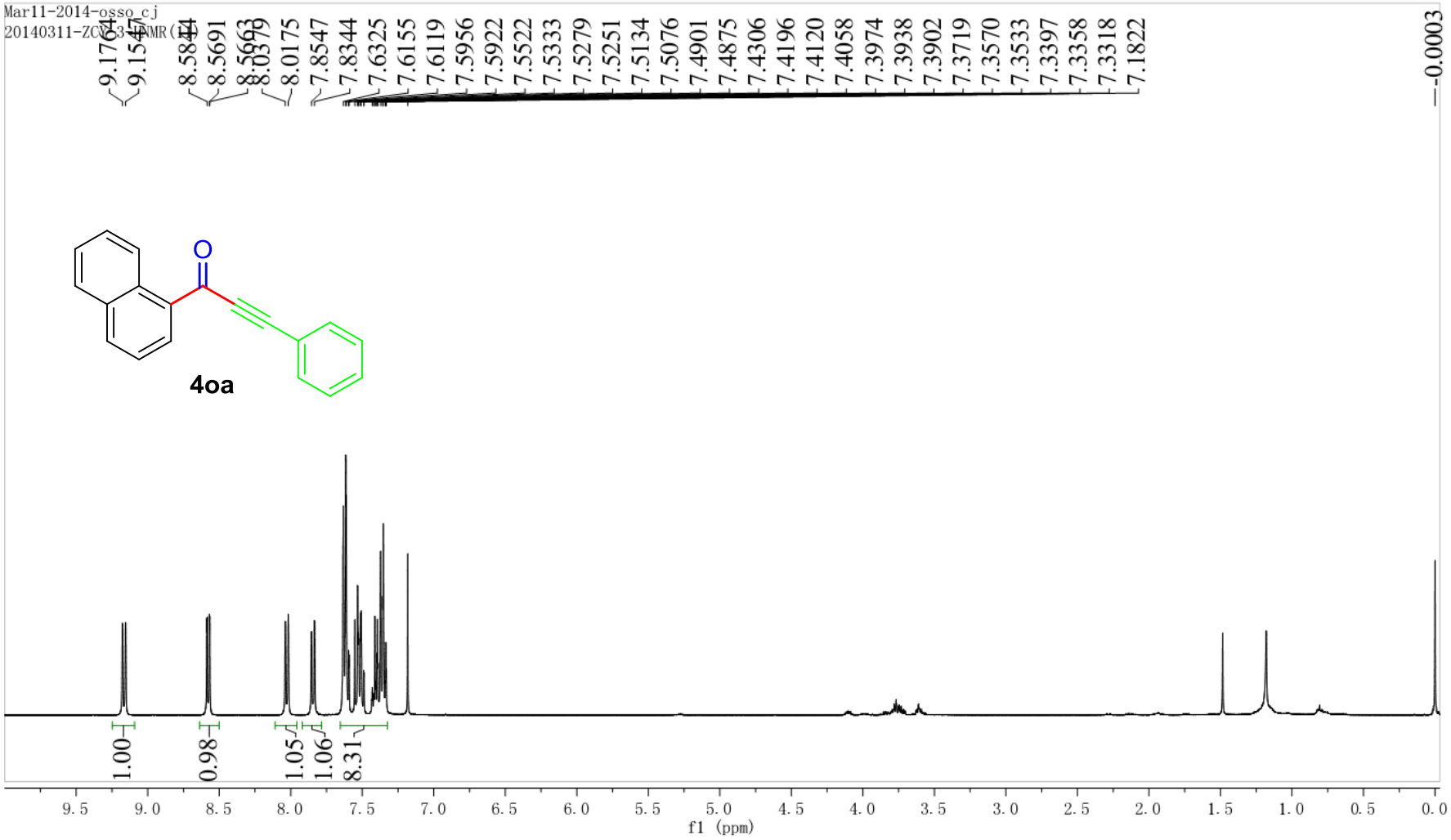

Mar11-2014-osso_cj
20140311-ZCY-5-CNMR(16)
174.8665
149.8814
140.0235
132.2704
130.4376
129.4232
127.8566
122.8560
118.4030
94.3933
85.5198
76.3115
76.1975
75.9939
75.6764
O
O2N
4la
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

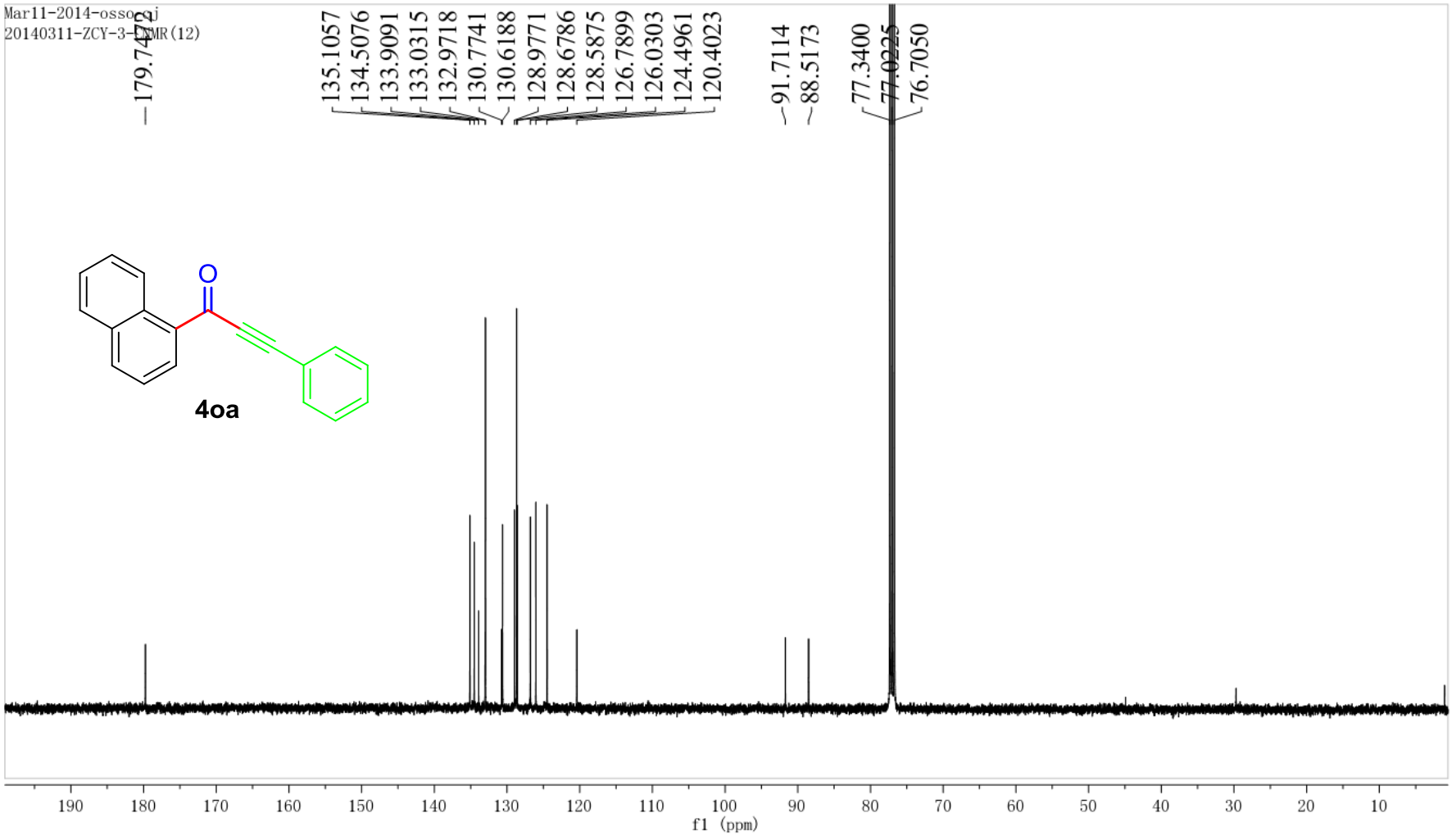

Apr29-2014-OSSO_cl
20140429-ZCY-1HNMR(2)
8.2913
8.2853
8.2750
8.2703
8.1932
8.1886
8.1762
8.1719
7.7203
7.7175
7.7052
7.7001
7.6964
7.5369
7.5183
7.5126
7.5032
7.4998
7.4963
7.4660
7.4505
7.4470
7.4331
7.4293
7.4261
7.2626
3.9723
O
O
4ma
2.10
2.00
2.04
3.04
3.17
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

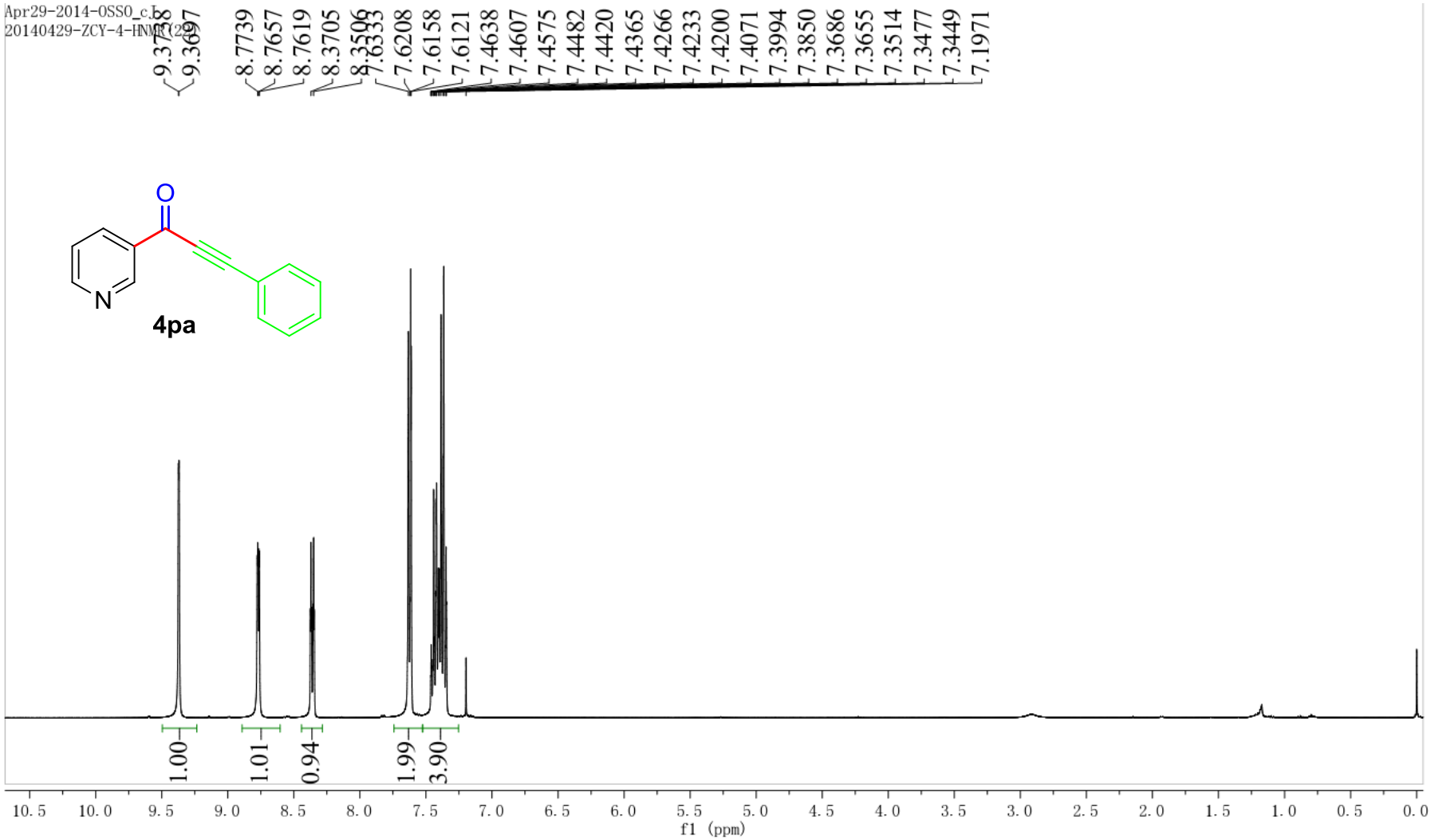

Apr29-2014-OSSO_c
20140429-ZCY-3-CNMR(21)
177.2249
166.1593
139.9481
134.7084
133.1973
131.0997
129.8324
129.4180
128.7806
119.8409
94.2000
86.8250
77.3331
77.0156
76.6980
52.5495
O
O
4ma
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

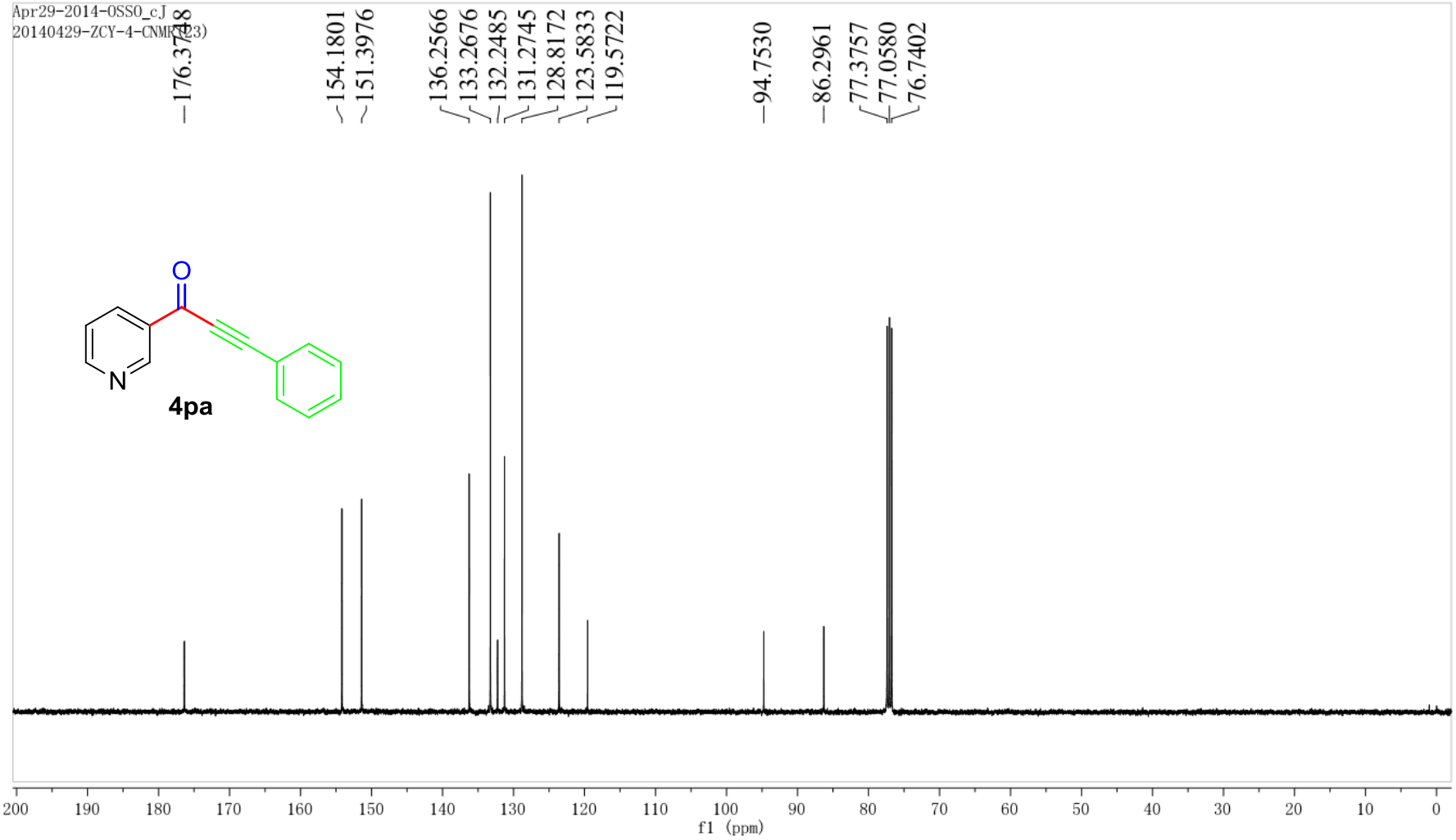

Apr29-2014-OSSO_cl
20140429-ZCY-2-HNMR(CS)
8.3187
8.2975
8.1007
8.0794
7.7190
7.7015
7.6979
7.5411
7.5380
7.5288
7.5225
7.5169
7.5072
7.5040
7.4693
7.4503
7.4325
7.4296
7.2630
2.6772
O
O
O
4na
2.00
2.05
2.03
3.09
3.13
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

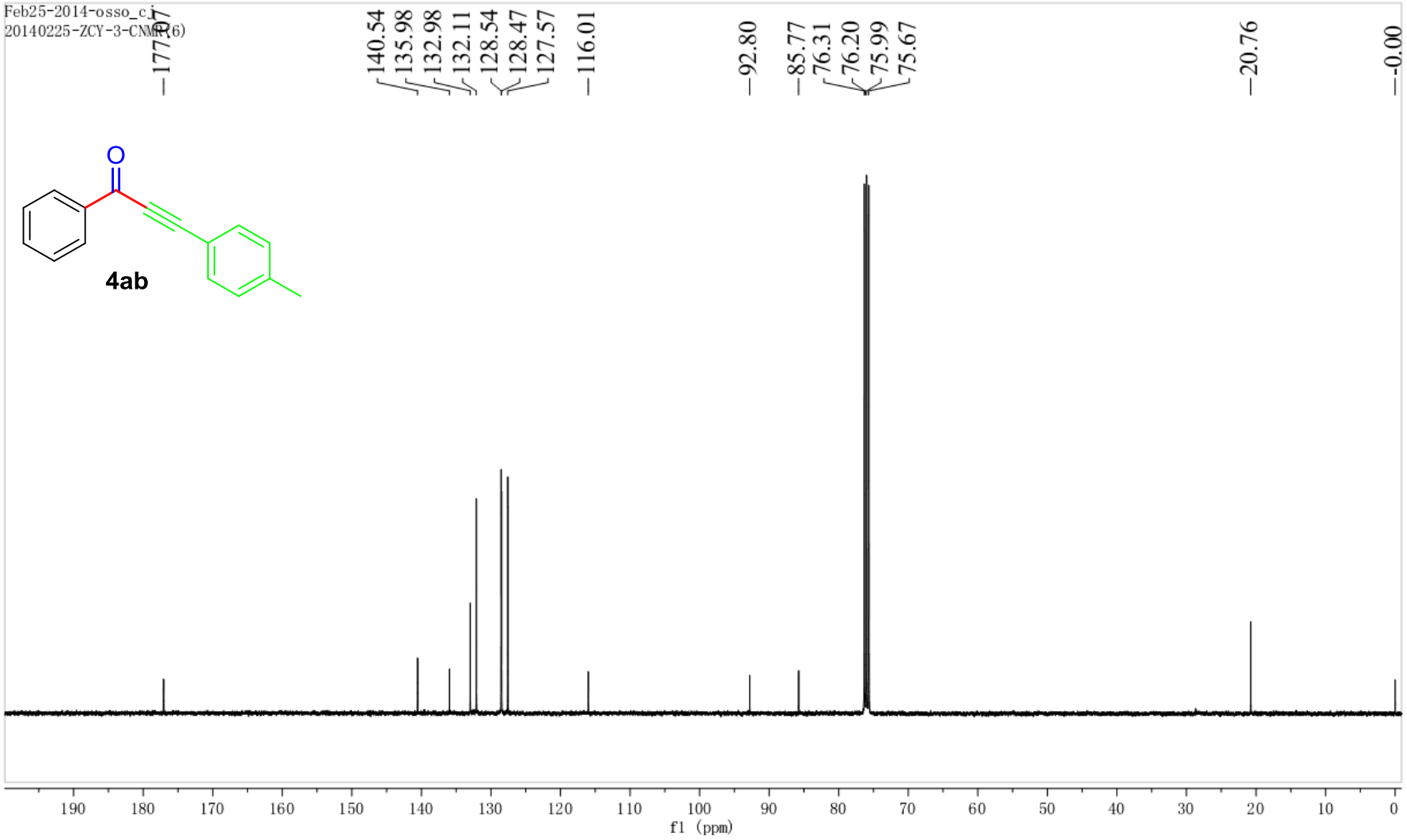

Apr29-2014-OSS8.cJ
20140429-ZCY-2 13CNMR(19)
197.4308
177.1597
140.8512
139.8867
133.2023
131.1349
129.7248
128.7945
128.4744
119.8134
94.3095
86.8303
77.3339
77.0164
76.6989
26.9788
O
O
O
4na
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

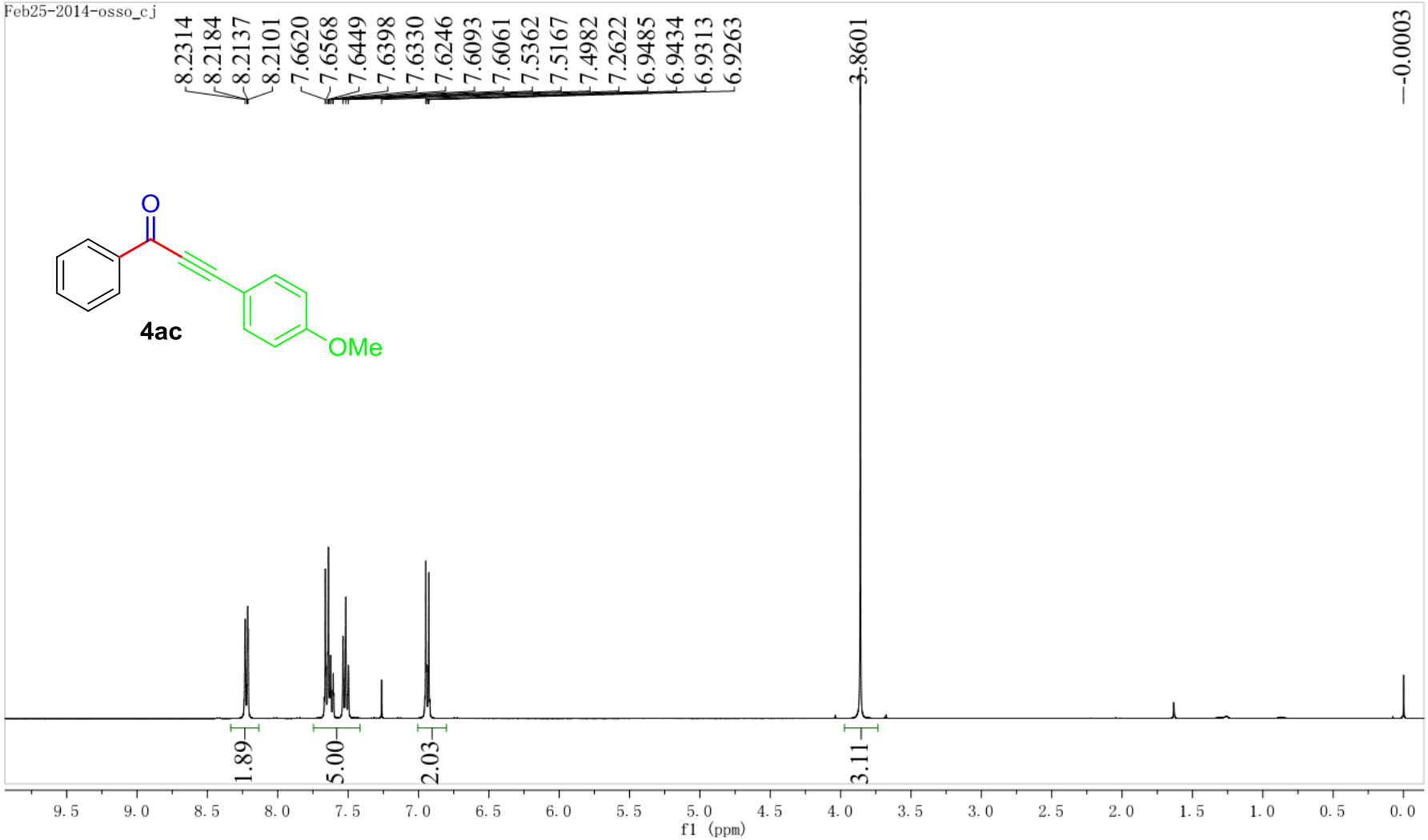

Mar11-2014-osso_cj
20140311-ZCX-3-1HNMR(1)
9.1764
9.1547
8.5844
8.5691
8.5663
8.0379
8.0175
7.8547
7.8344
7.6325
7.6155
7.6119
7.5956
7.5922
7.5522
7.5333
7.5279
7.5251
7.5134
7.5076
7.4901
7.4875
7.4306
7.4196
7.4120
7.4058
7.3974
7.3938
7.3902
7.3719
7.3570
7.3533
7.3397
7.3358
7.3318
7.1822
-0.0003
O
4oa
1.00
0.98
1.05
1.06
8.31
9.5
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
1.5
1.0
0.5
0.0
f1 (ppm)

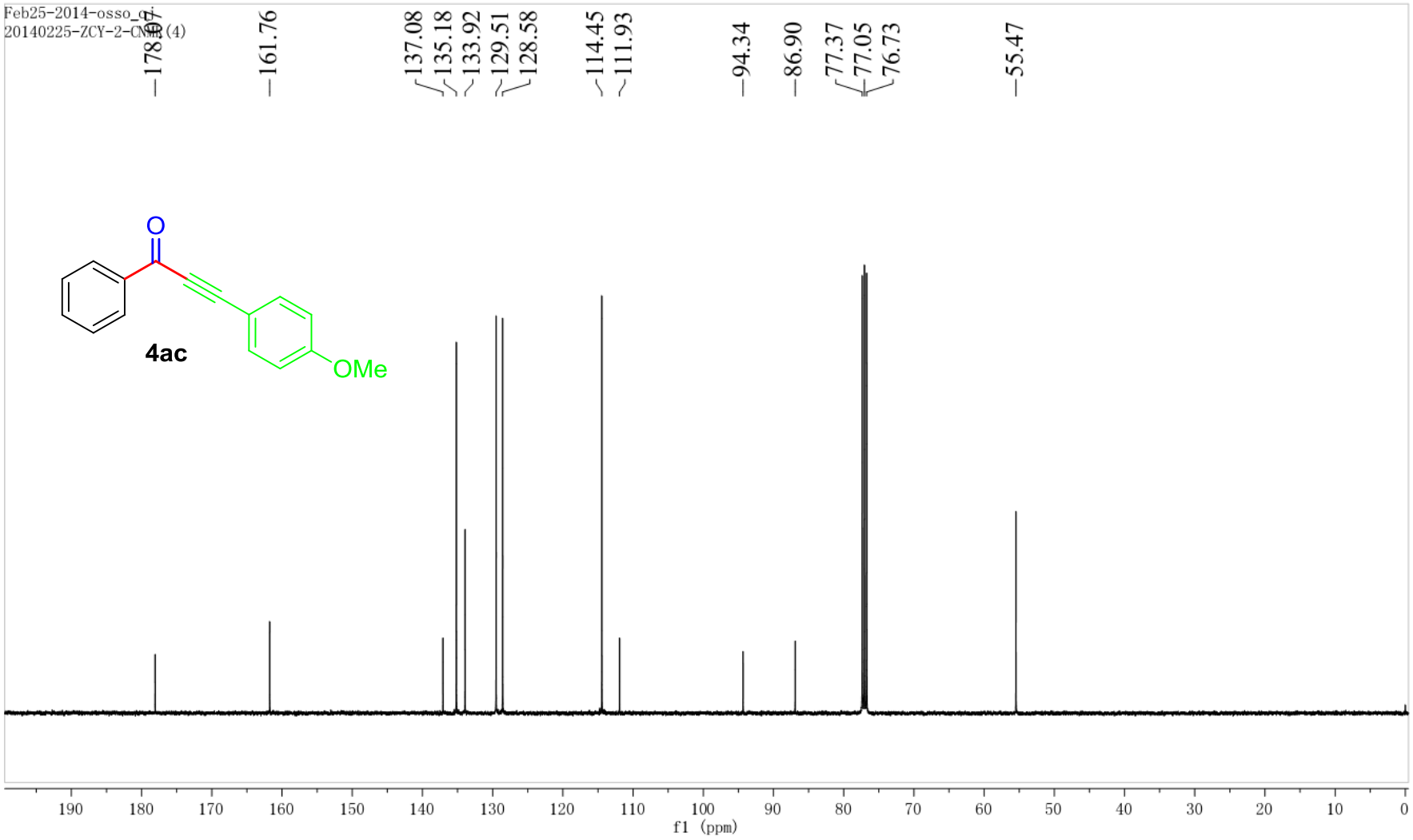

Mar11-2014-ossocj
20140311-ZCY-3-13CNMR(12)
179.7422
135.1057
134.5076
133.9091
133.0315
132.9718
130.7741
130.6188
128.9771
128.6786
128.5875
126.7899
126.0303
124.4961
120.4023
91.7114
88.5173
77.3400
77.0225
76.7050
O
4oa
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

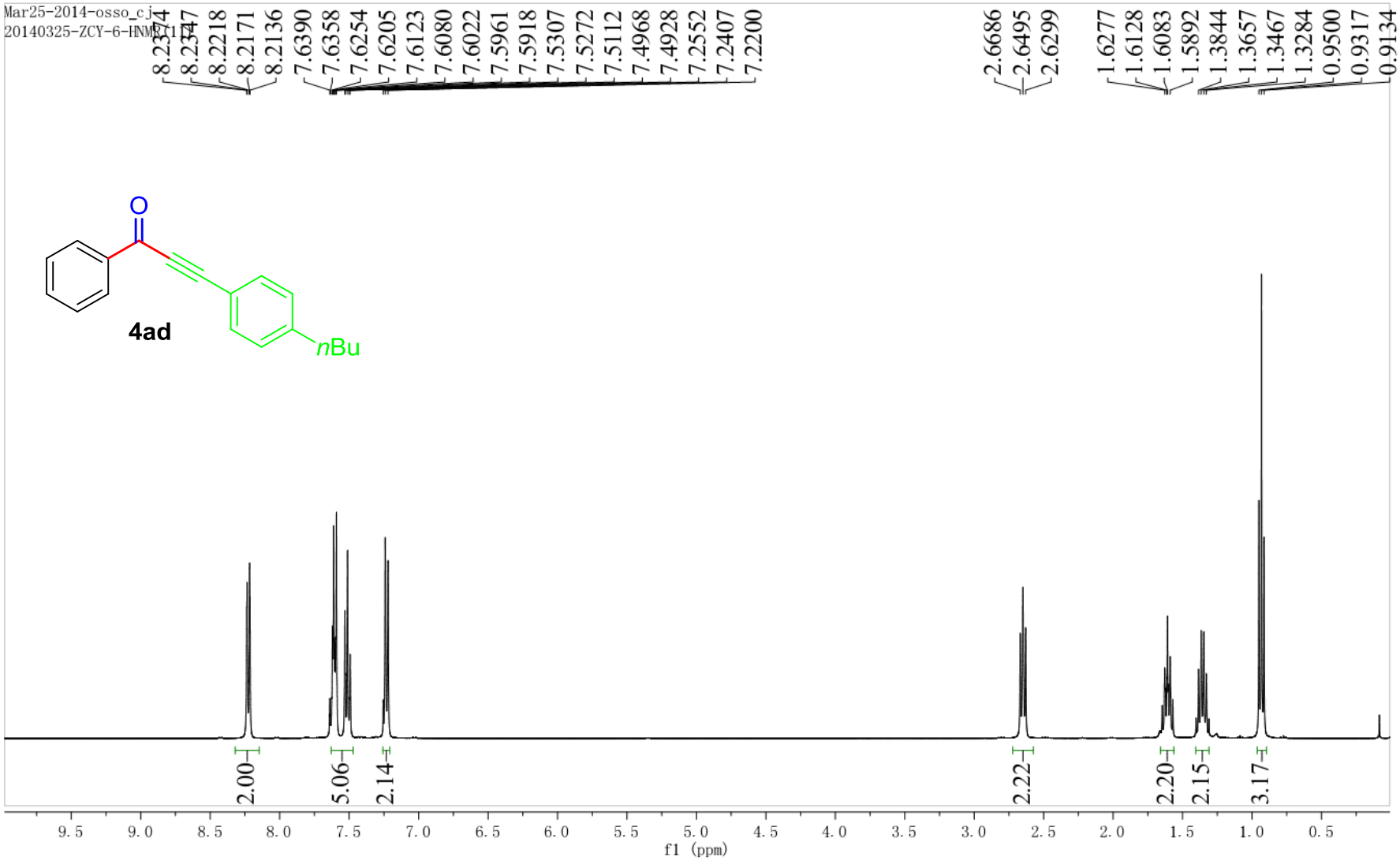

Apr29-2014-OSSO_c.1
20140429-ZCY-4-HNMR(2)
9.3758
9.3697
8.7739
8.7657
8.7619
8.3705
8.3506
8.3333
7.6208
7.6158
7.6121
7.4638
7.4607
7.4575
7.4482
7.4420
7.4365
7.4266
7.4233
7.4200
7.4071
7.3994
7.3850
7.3686
7.3655
7.3514
7.3477
7.3449
7.1971
O
N
4pa
1.00
1.01
0.94
1.99
3.90
10.5
10.0
9.5
9.0
8.5
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
1.5
1.0
0.5
0.0
f1 (ppm)

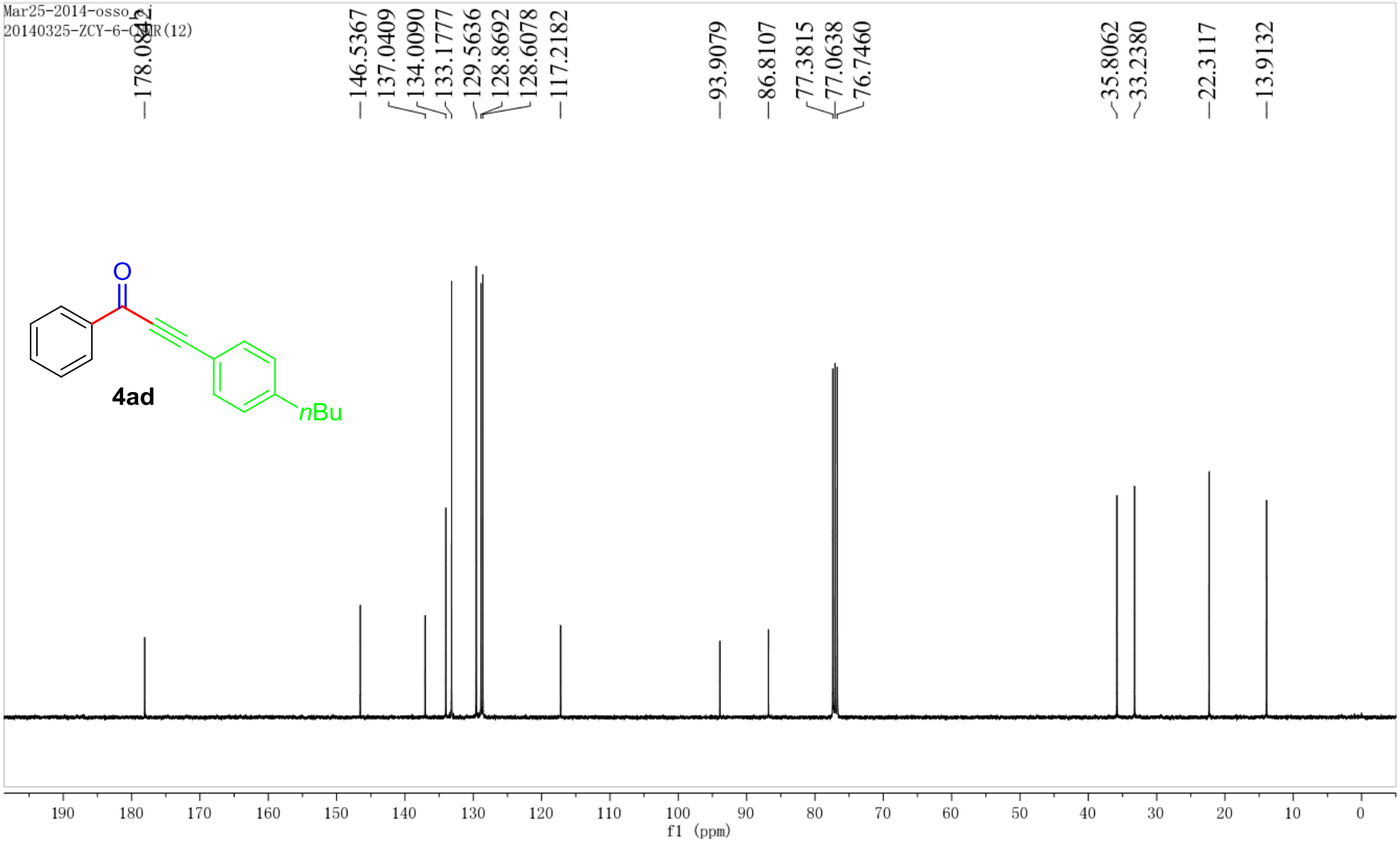

Apr29-2014-OSSO_cJ
20140429-ZCY-4-CNMR(23)
176.3718
154.1801
151.3976
136.2566
133.2676
132.2485
131.2745
128.8172
123.5833
119.5722
94.7530
86.2961
77.3757
77.0580
76.7402
O
N
4pa
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

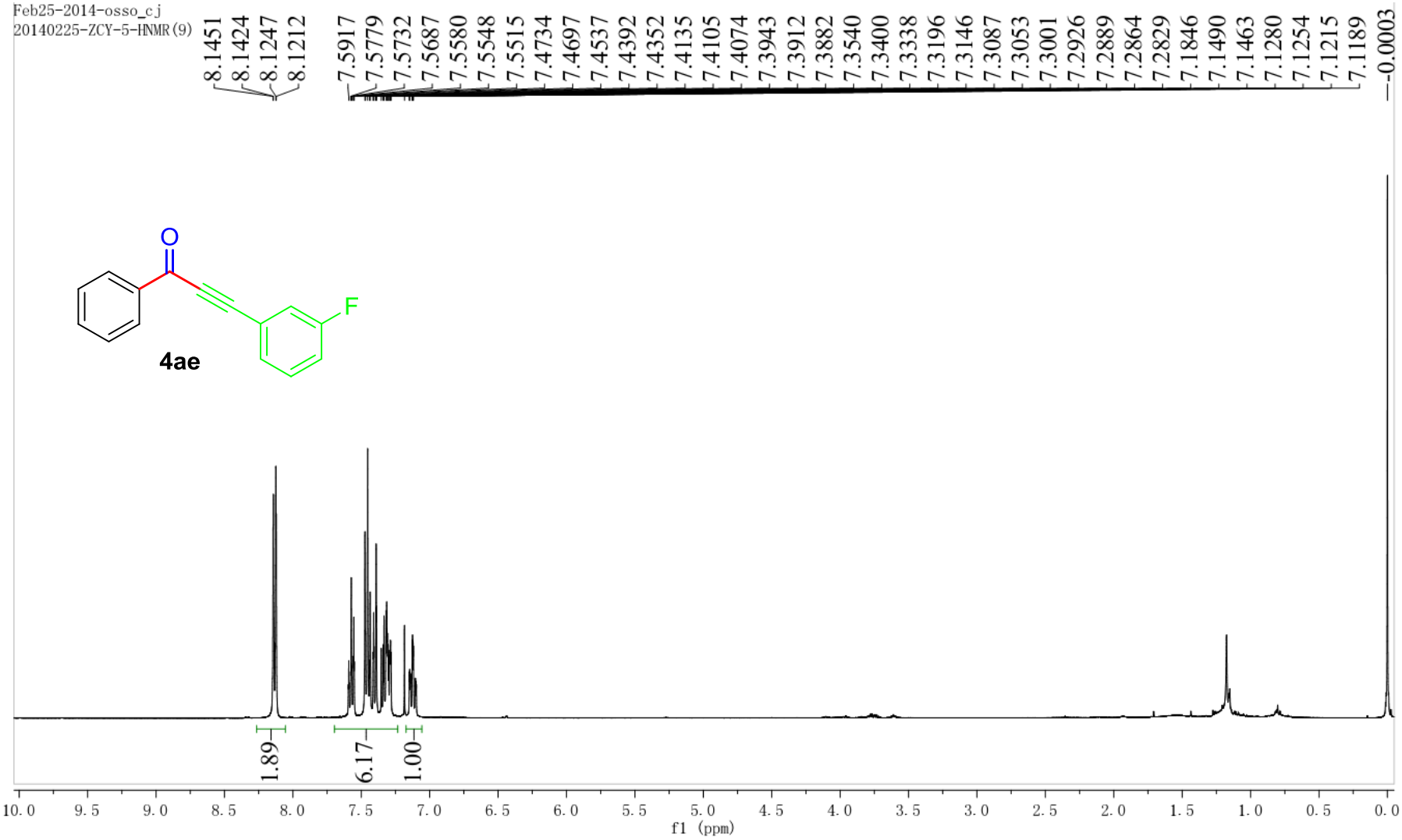

Feb25-2014-osso_c.i
20140225-ZCY-3-CMR(6)
177.07
140.54
135.98
132.98
132.11
128.54
128.47
127.57
116.01
92.80
85.77
76.31
76.20
75.99
75.67
20.76
-0.00
O
4ab
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Feb25-2014-osso_cj
8.2314
8.2184
8.2137
8.2101
7.6620
7.6568
7.6449
7.6398
7.6330
7.6246
7.6093
7.6061
7.5362
7.5167
7.4982
7.2622
6.9485
6.9434
6.9313
6.9263
3.8601
-0.0003
O
4ac
OMe
1.89
5.00
2.03
3.11
9.5
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
1.5
1.0
0.5
0.0
f1 (ppm)


Feb25-2014-osso_c
20140225-ZCY-2-CNMR(4)
178.07
161.76
137.08
135.18
133.92
129.51
128.58
114.45
111.93
94.34
86.90
77.37
77.05
76.73
55.47
O
4ac
OMe
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Mar25-2014-osso_cj
20140325-ZCY-6-HNMR1H
8.2374
8.2347
8.2218
8.2171
8.2136
7.6390
7.6358
7.6254
7.6205
7.6123
7.6080
7.6022
7.5961
7.5918
7.5307
7.5272
7.5112
7.4968
7.4928
7.2552
7.2407
7.2200
2.6686
2.6495
2.6299
1.6277
1.6128
1.6083
1.5892
1.3844
1.3657
1.3467
1.3284
0.9500
0.9317
0.9134
O
4ad
nBu
2.00
5.06
2.14
2.22
2.20
2.15
3.17
9.5
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
1.5
1.0
0.5
f1 (ppm)


Mar25-2014-osso_cj
20140325-ZCY-6-CNMR(12)
178.0854
146.5367
137.0409
134.0090
133.1777
129.5636
128.8692
128.6078
117.2182
93.9079
86.8107
77.3815
77.0638
76.7460
35.8062
33.2380
22.3117
13.9132
O
4ad
nBu
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Feb25-2014-osso_cj
20140225-ZCY-5-HNMR(9)
8.1451
8.1424
8.1247
8.1212
7.5917
7.5779
7.5732
7.5687
7.5580
7.5548
7.5515
7.4734
7.4697
7.4537
7.4392
7.4352
7.4135
7.4105
7.4074
7.3943
7.3912
7.3882
7.3540
7.3400
7.3338
7.3196
7.3146
7.3087
7.3053
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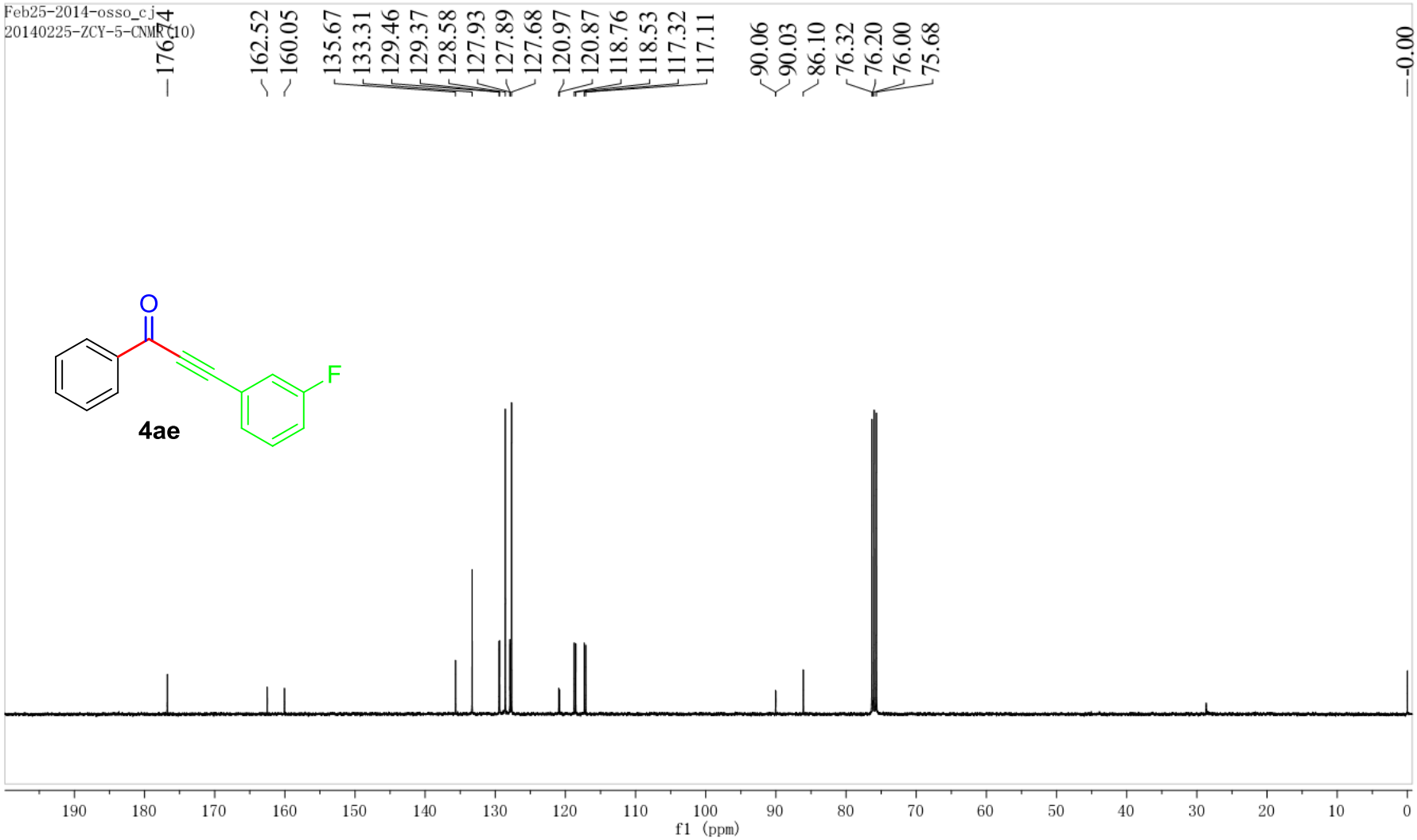
7.2926
7.2889
7.2864
7.2829
7.1846
7.1490
7.1463
7.1280
7.1254
7.1215
7.1189
-0.0003
O
F
4ae
1.89
6.17
1.00
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


Feb25-2014-osso_cj
20140225-ZCY-5-CNMR(10)
176.24
162.52
160.05
135.67
133.31
129.46
129.37
128.58
127.93
127.89
127.68
120.97
120.87
118.76
118.53
117.32
117.11
90.06
90.03
86.10
76.32
76.20
76.00
75.68
-0.00
O
F
4ae
190
180
170
160
150
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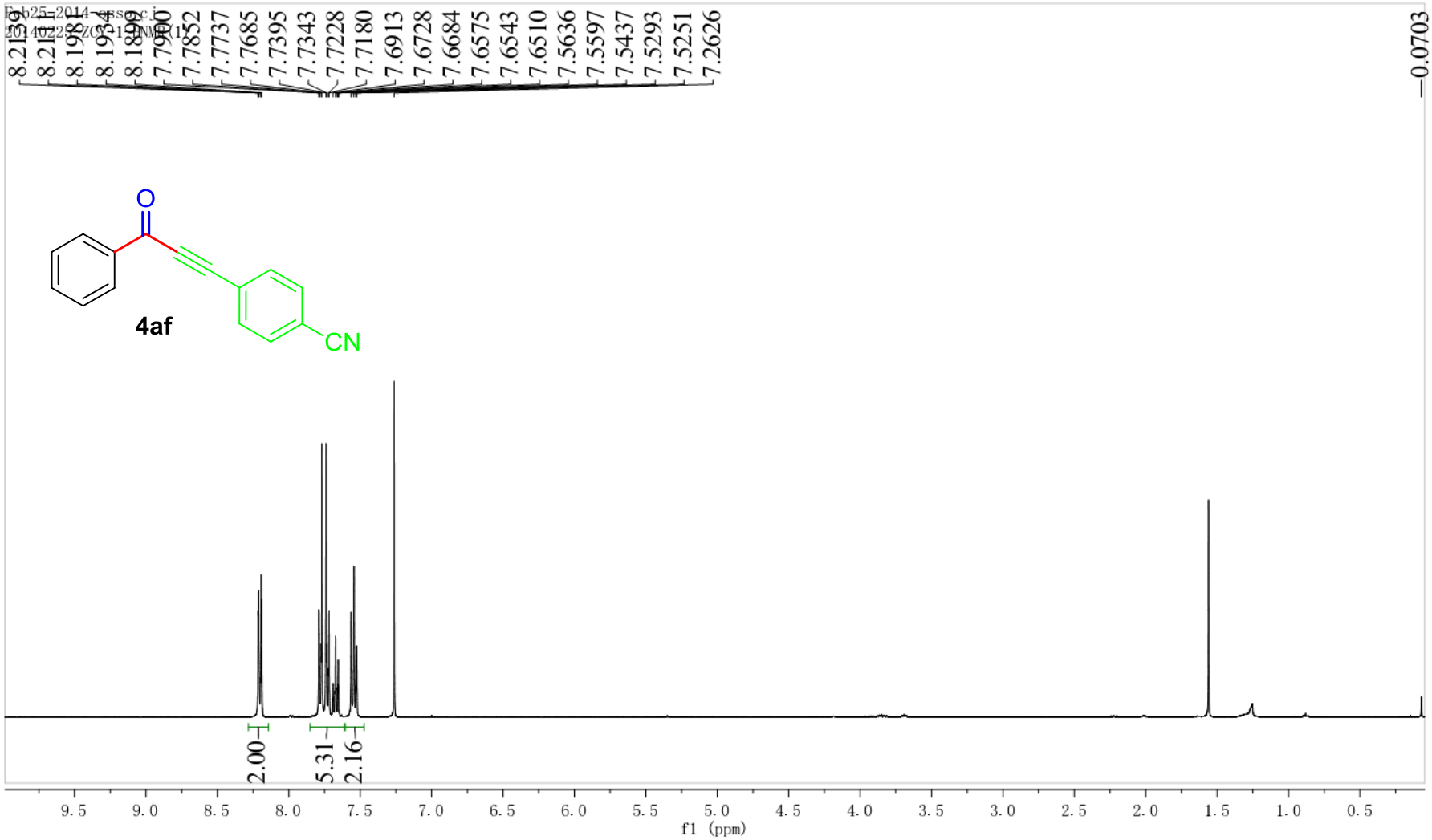
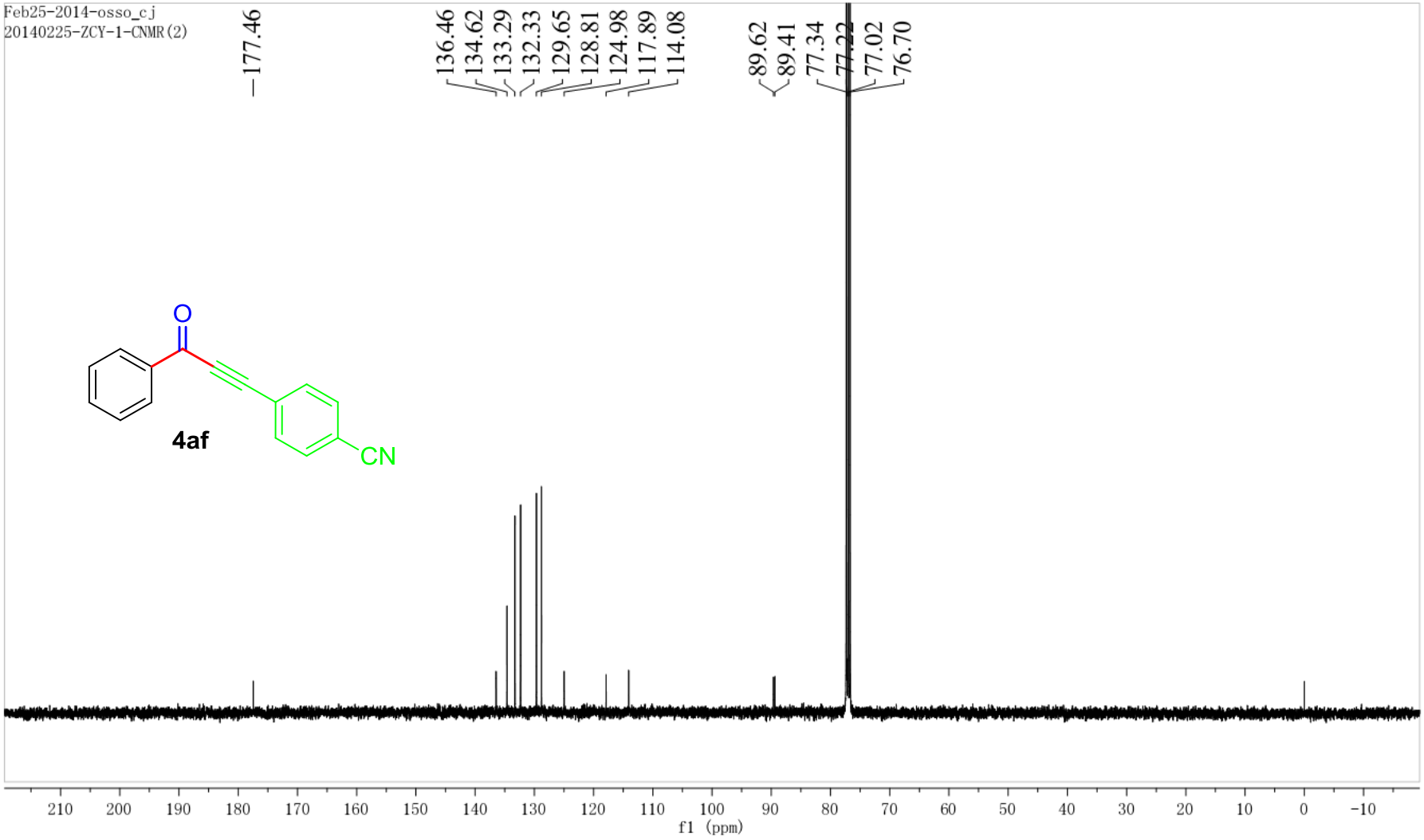
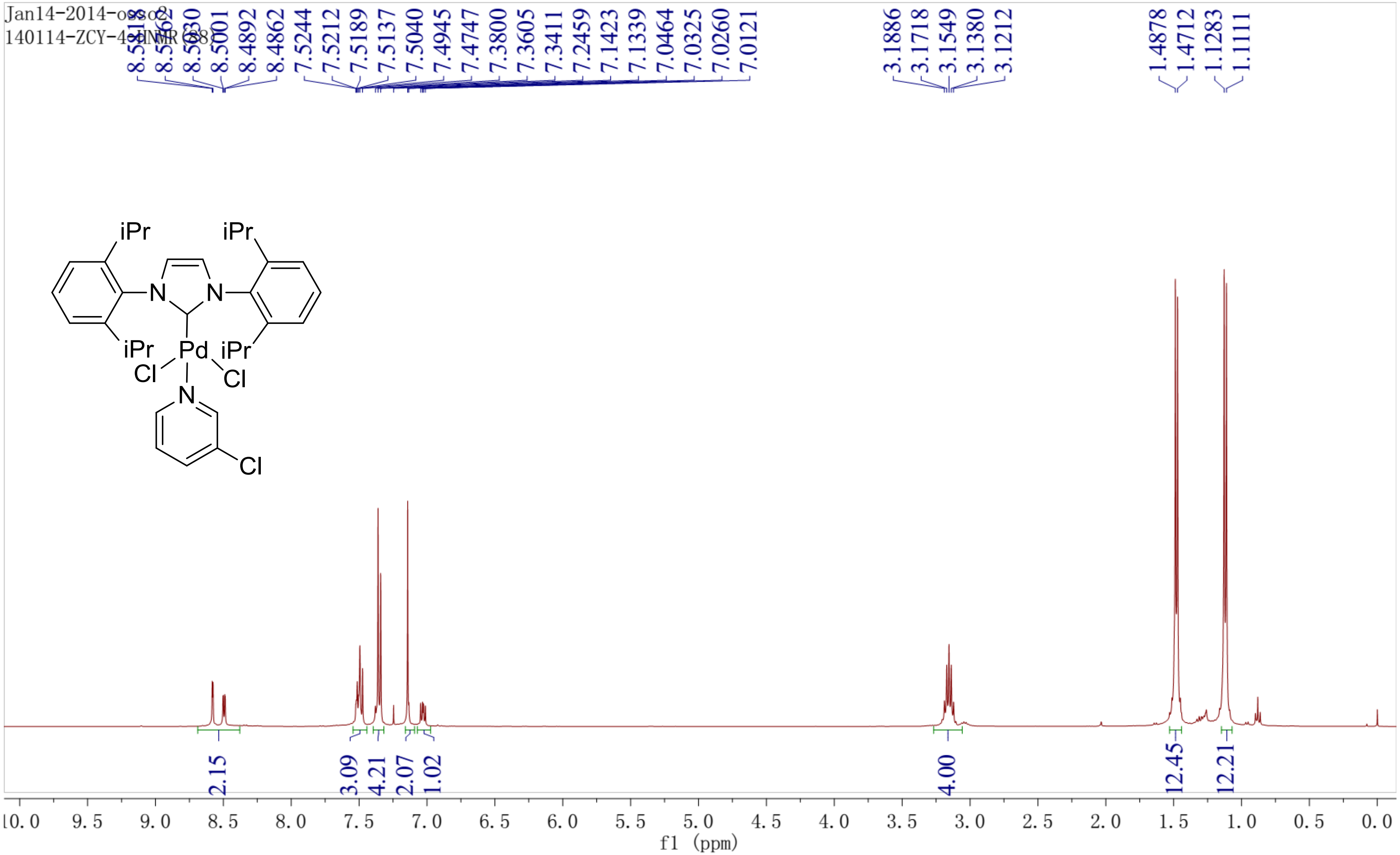
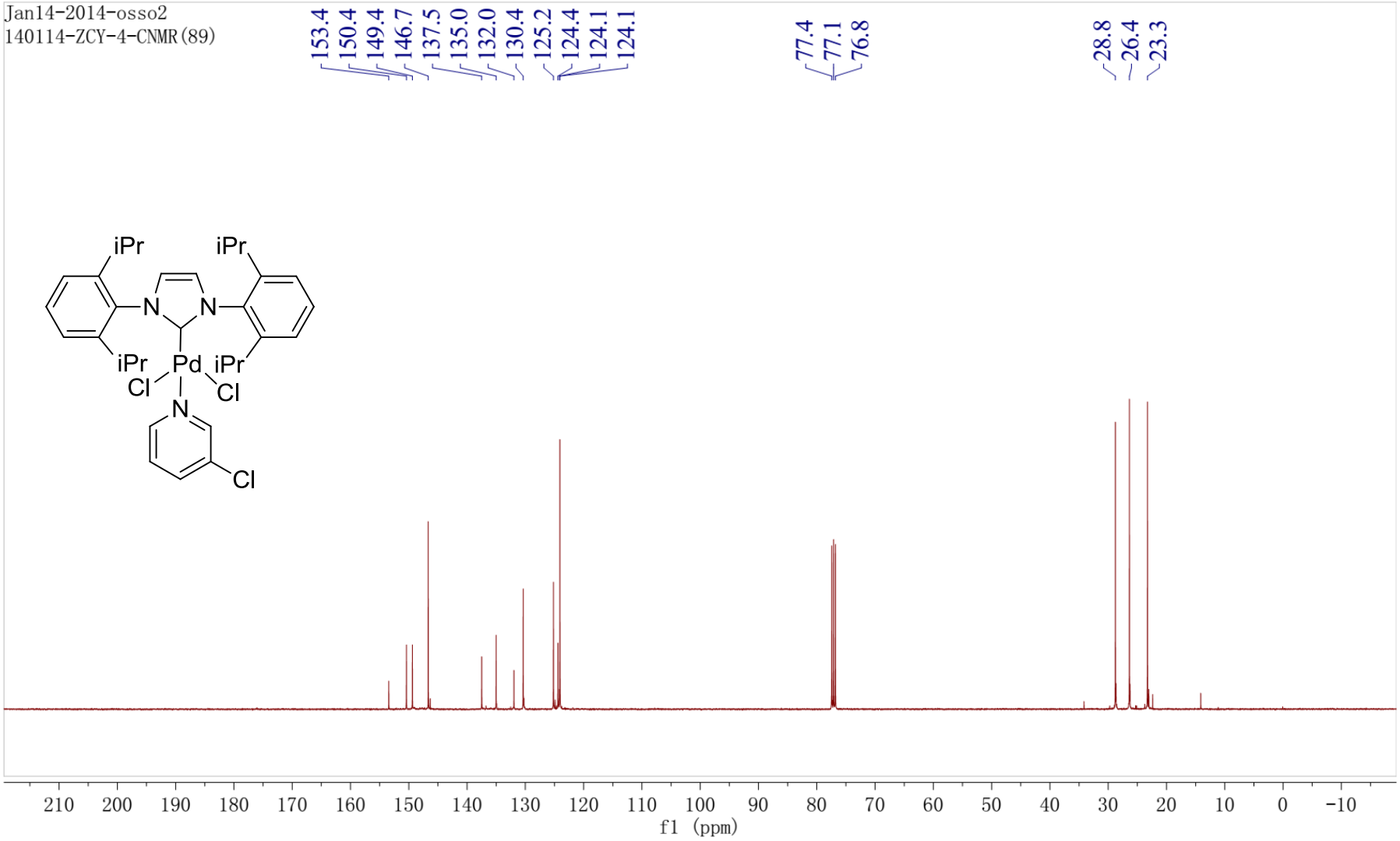
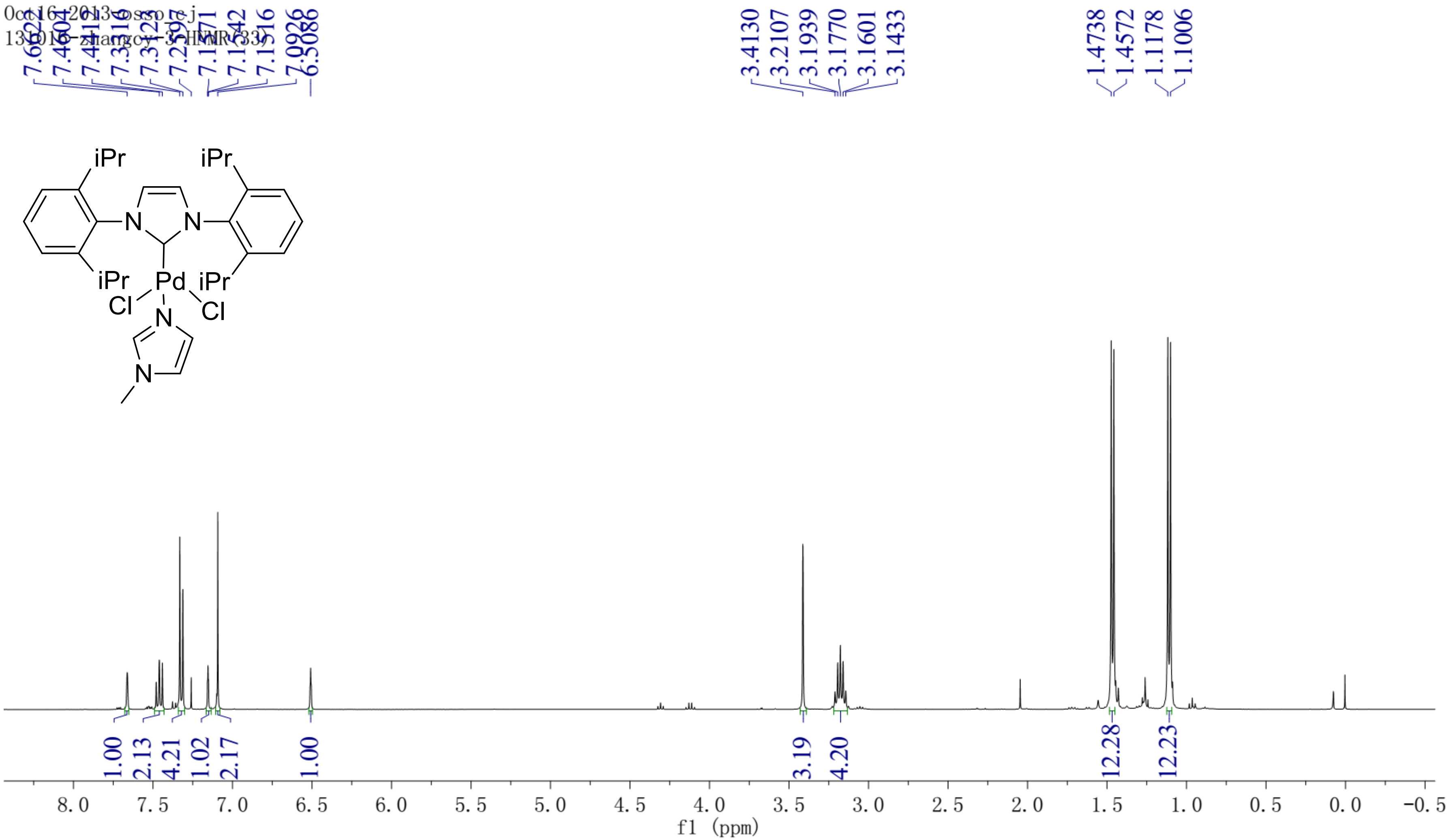
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

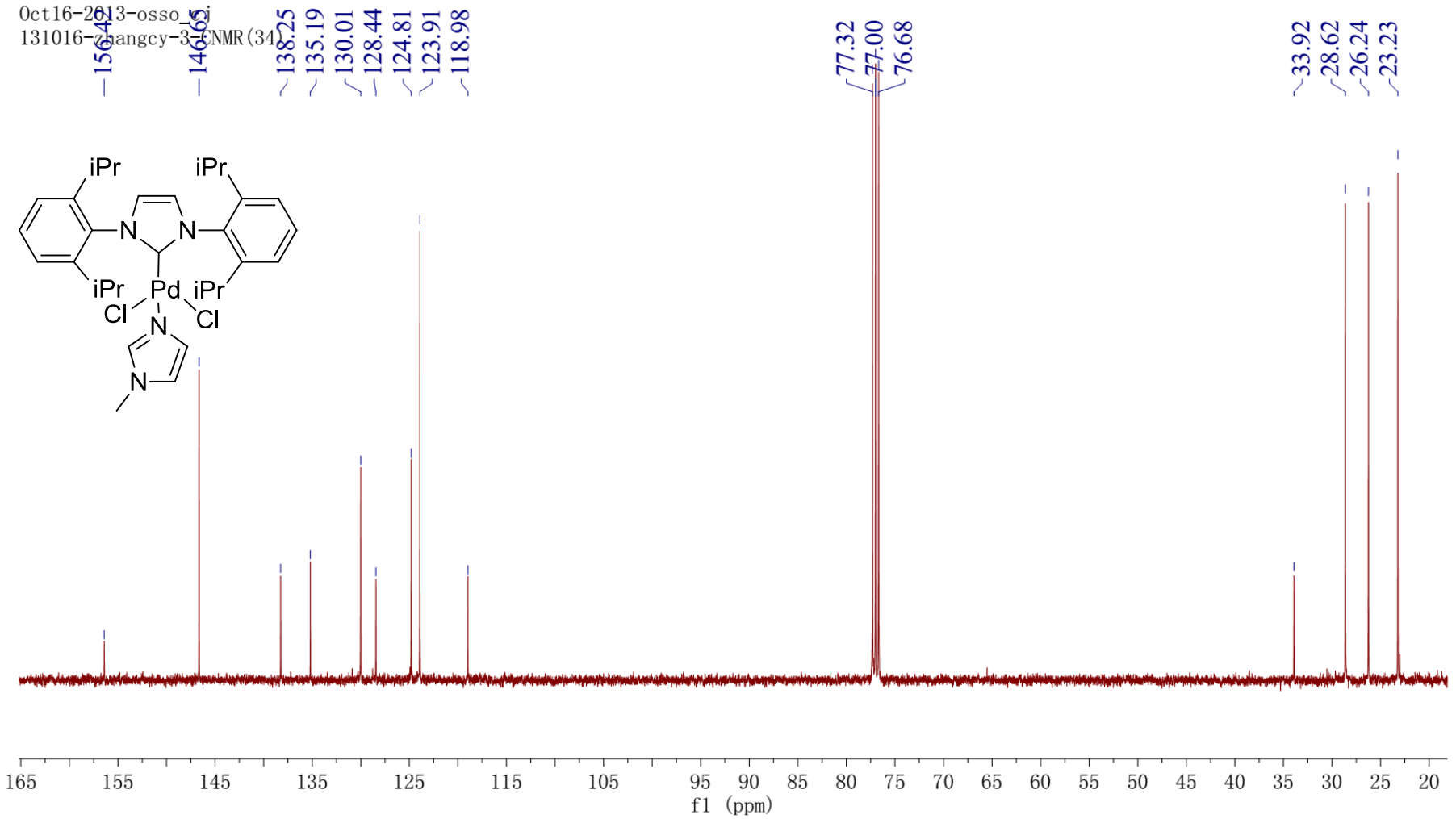

8.2139
8.2111
8.1981
8.1934
8.1899
7.7900
7.7852
7.7737
7.7685
7.7395
7.7343
7.7228
7.7180
7.6913
7.6728
7.6684
7.6575
7.6543
7.6510
7.5636
7.5597
7.5437
7.5293
7.5251
7.2626
0.0703
O
4af
CN
2.00
5.31
2.16
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

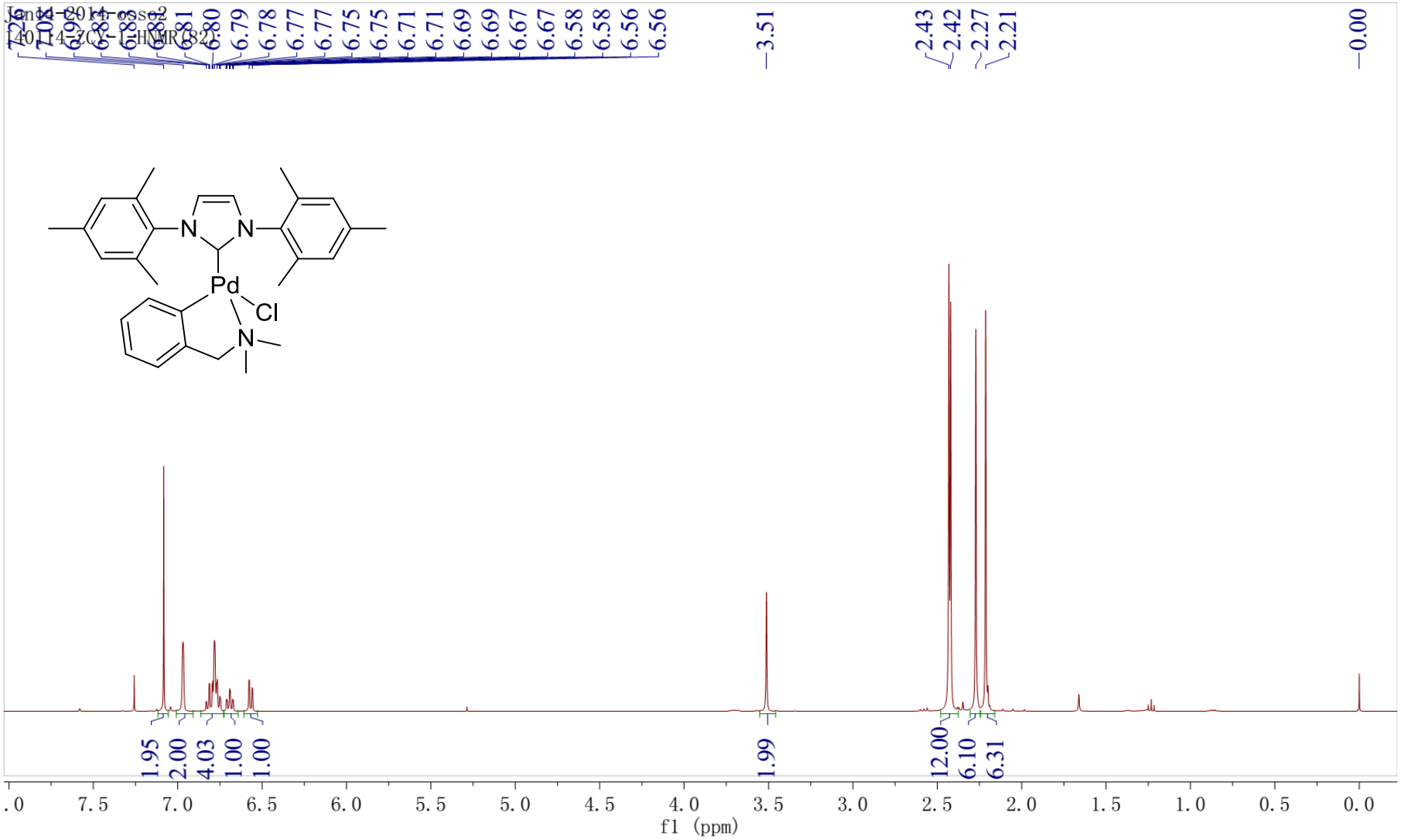

Feb25-2014-osso_cj
20140225-ZCY-1-CNMR(2)
177.46
136.46
134.62
133.29
132.33
129.65
128.81
124.98
117.89
114.08
89.62
89.41
77.34
77.22
77.02
76.70
O
CN
4af
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

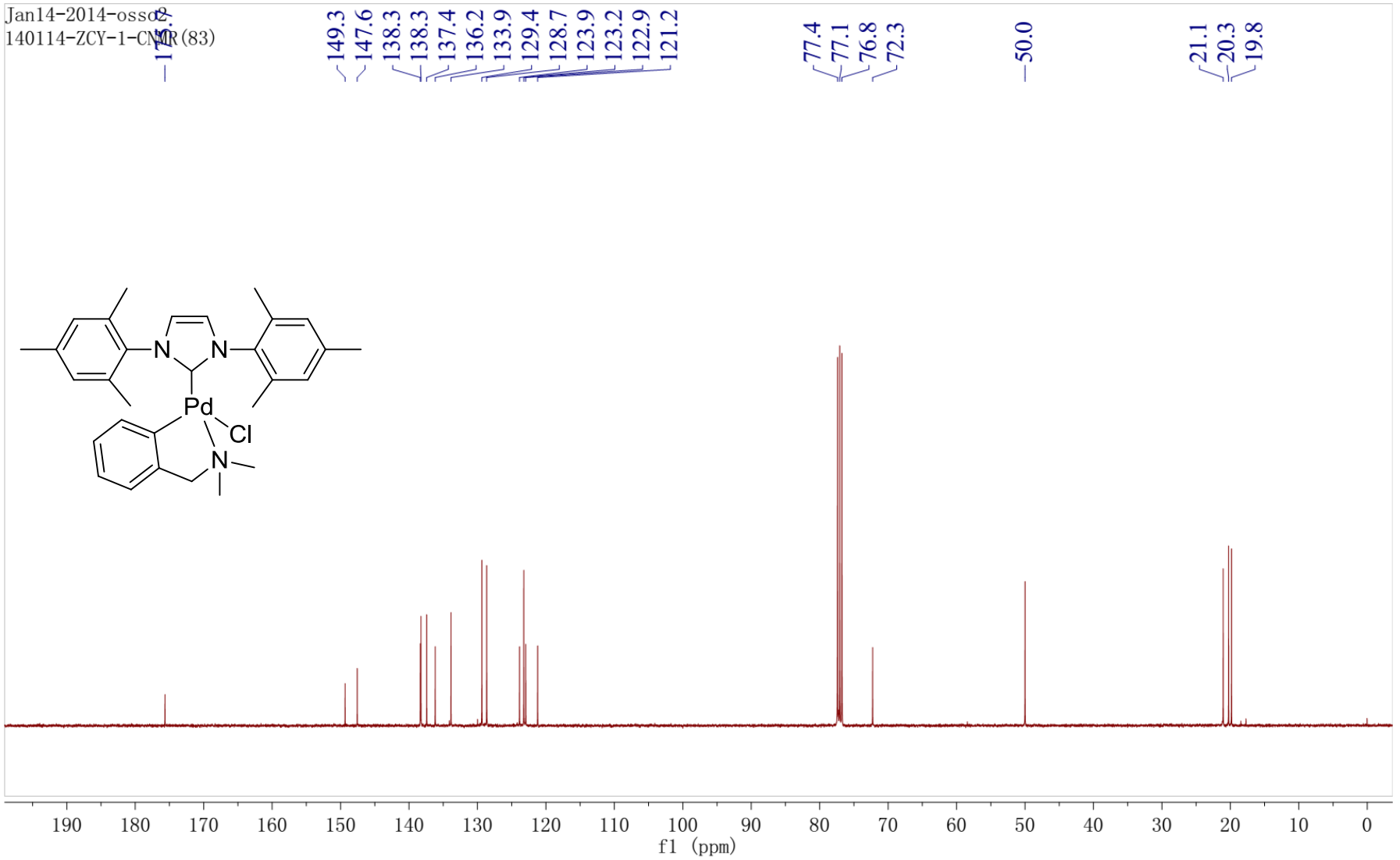

8.5018
8.5030
8.5001
8.4892
8.4862
7.5244
7.5212
7.5189
7.5137
7.5040
7.4945
7.4747
7.3800
7.3605
7.3411
7.2459
7.1423
7.1339
7.0464
7.0325
7.0260
7.0121
3.1886
3.1718
3.1549
3.1380
3.1212
1.4878
1.4712
1.1283
1.1111
iPr
iPr
N
N
iPr
Pd
iPr
Cl
Cl
N
Cl
2.15
3.09
4.21
2.07
1.02
4.00
12.45
12.21
10.0 9.5 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 1.5 1.0 0.5 0.0
f1 (ppm)

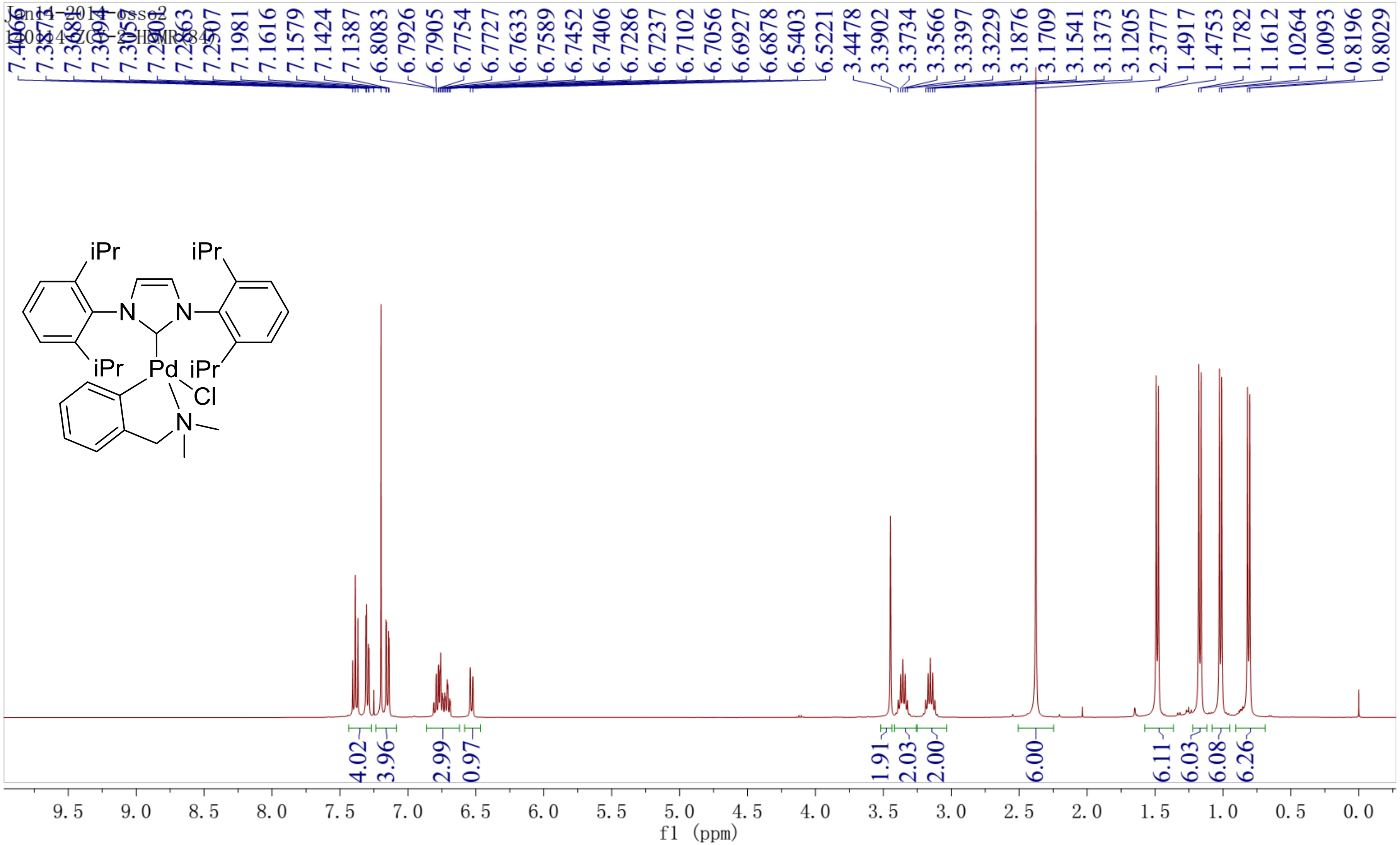

Jan14-2014-osso2
140114-ZCY-4-CNMR(89)
153.4
150.4
149.4
146.7
137.5
135.0
132.0
130.4
125.2
124.4
124.1
124.1
77.4
77.1
76.8
28.8
26.4
23.3
iPr
iPr
N
N
iPr
Pd
iPr
Cl
Cl
N
Cl
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

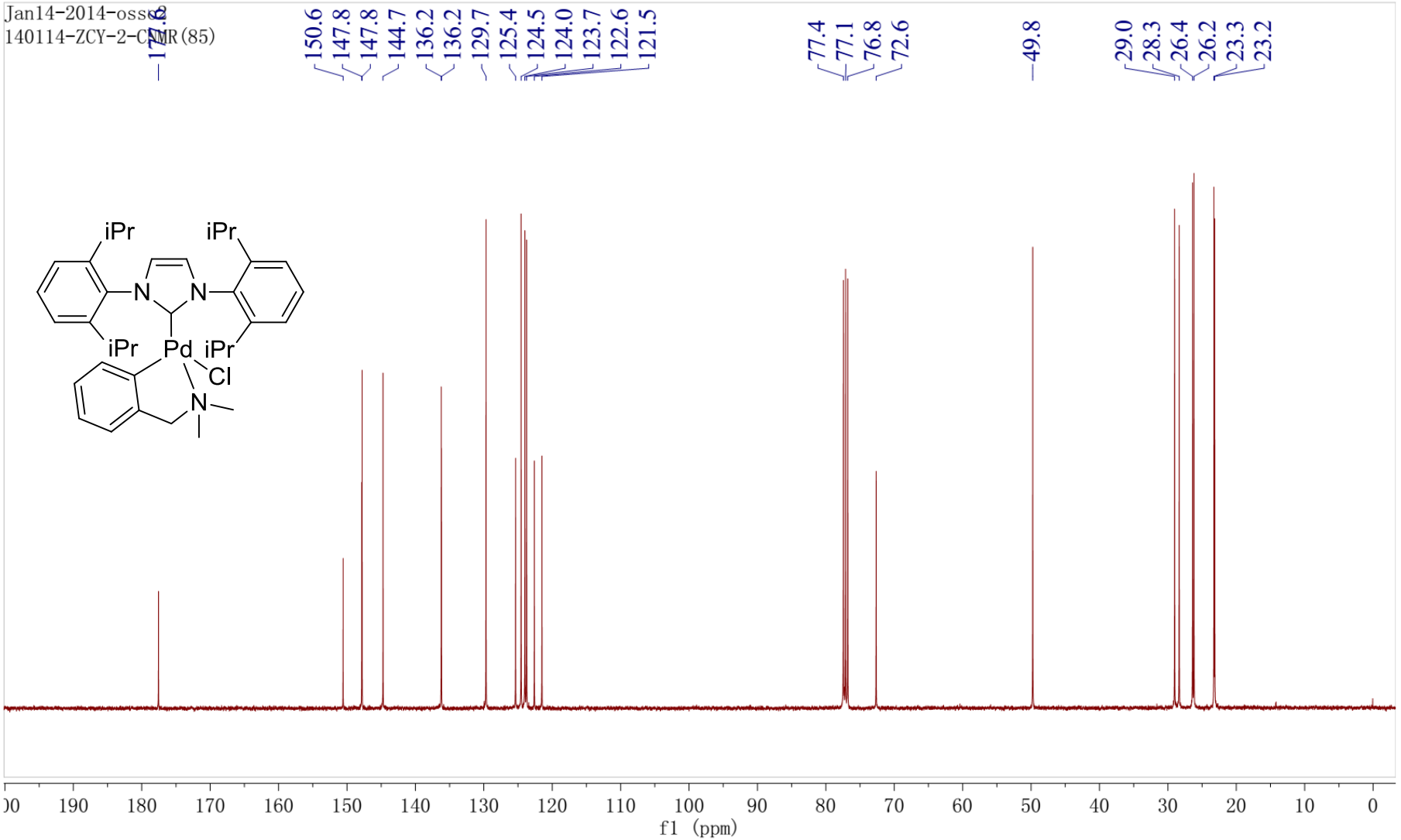

Oct16-2013-osso rej
131016-zhangcy-3-HNMR(33)
7.6627
7.4604
7.4412
7.3316
7.3129
7.2897
7.1571
7.1242
7.1016
7.0926
6.5086
3.4130
3.2107
3.1939
3.1770
3.1601
3.1433
1.4738
1.4572
1.1178
1.1006
iPr
iPr
N
N
iPr
Pd
iPr
Cl
Cl
N
N
1.00
2.13
4.21
1.02
2.17
1.00
3.19
4.20
12.28
12.23
8.0
7.5
7.0
6.5
6.0
5.5
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)


Oct16-2013-osso_j
131016-zhangcy-3-CNMR(34)
156.42
146.65
138.25
135.19
130.01
128.44
124.81
123.91
118.98
77.32
77.00
76.68
33.92
28.62
26.24
23.23
iPr
iPr
iPr
iPr
N
N
Pd
Cl
Cl
N
N
165
155
145
135
125
115
105
95
90
85
80
75
70
65
60
55
50
45
40
35
30
25
20
f1 (ppm)


Jan14-2014-osse2
140114-ZCY-1-1HNMR-82
7.26
7.04
6.99
6.84
6.83
6.82
6.81
6.80
6.79
6.78
6.77
6.77
6.75
6.75
6.71
6.71
6.69
6.69
6.67
6.67
6.58
6.58
6.56
6.56
3.51
2.43
2.42
2.27
2.21
0.00
N
N
Pd
Cl
N
1.95
2.00
4.03
1.00
1.00
1.99
12.00
6.10
6.31
.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)


Jan14-2014-ossc2
140114-ZCY-1-CNMR(83)
175.1
149.3
147.6
138.3
138.3
137.4
136.2
133.9
129.4
128.7
123.9
123.2
122.9
121.2
77.4
77.1
76.8
72.3
50.0
21.1
20.3
19.8
N
N
Pd
Cl
N
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


Jan14-2014-osso2
140114-ZCY-2-HNMR(84)
iPr
iPr
iPr
iPr
N
N
Pd
Cl
N
7.4066
7.3877
7.3588
7.3394
7.3355
7.2902
7.2863
7.2507
7.1981
7.1616
7.1579
7.1424
7.1387
6.8083
6.7926
6.7905
6.7754
6.7727
6.7633
6.7589
6.7452
6.7406
6.7286
6.7237
6.7102
6.7056
6.6927
6.6878
6.5403
6.5221
3.4478
3.3902
3.3734
3.3566
3.3397
3.3229
3.1876
3.1709
3.1541
3.1373
3.1205
2.3777
1.4917
1.4753
1.1782
1.1612
1.0264
1.0093
0.8196
0.8029
4.02
3.96
2.99
0.97
1.91
2.03
2.00
6.00
6.11
6.03
6.08
6.26
9.5
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
1.5
1.0
0.5
0.0
f1 (ppm)


Jan14-2014-osss2
140114-ZCY-2-CNMR(85)
177.2
150.6
147.8
147.8
144.7
136.2
136.2
129.7
125.4
124.5
124.0
123.7
122.6
121.5
77.4
77.1
76.8
72.6
49.8
29.0
28.3
26.4
26.2
23.3
23.2
iPr
iPr
iPr
iPr
N
N
Pd
Cl
N
f1 (ppm)