Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

$B(C_6F_5)_3$-Catalyzed Transfer Hydrogenations of Imines with Hantzsch Ester

Qiaotian Wang,[a,b] Jingjing Chen,[a,b] Xiangqing Feng,[a,b*] and Haifeng Du [a,b,*]

[a] *Beijing National Laboratory of Molecular Sciences, CAS Key Laboratory of Molecular Recognition and Function, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China.*

[b] *University of Chinese Academy of Sciences, Beijing 100049, P. R. China*

Supporting Information

General consideration

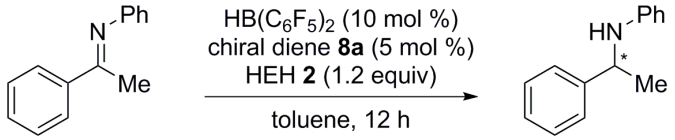
All air-sensitive compounds were handled under an atmosphere of argon or in a nitrogen-filled glovebox. ^{1}H NMR and ^{13}C NMR spectra were recorded on Bruker AV 400 at ambient temperature with $CDCl_3$ as solvent and TMS as internal standard. Chemical shifts (δ) were given in ppm, referenced to the residual proton resonance of TMS (0) or to the carbon resonance of the $CDCl_3$ (77.23). Coupling constants (*J*) were given in Hertz (Hz). All solvents were purified by conventional methods, distilled before use. Commercially available reagents were used without further purification. All the substrates were synthesized according to reported method.

General procedure for the metal-free catalytic transfer hydrogenation of imine (Scheme 3): Dissolving $B(C_6F_5)_3$ (0.0010 g, 0.002 mmol) in *n*-hexane (10 mL) to give a solution of catalyst (0.0002 M). Then to a sealed-tube were added imine **5** (0.6 mmol), Hantzsch Ester (0.1820 g, 0.72 mmol) and the solution of *n*-hexane with dissolved catalyst (0.0002 M, 3.0 mL, 0.0006 mmol) in a nitrogen atmosphere glovebox. After being sealed, the resulting mixture was stirred for 48 h at 120 °C. The reaction mixture was cooled to room temperature, and the solvent was removed under reduced pressure. The crude residue was purified by flash chromatography on silica gel using *n*-hexane/DCM (20/1-50/1) as the fluent to give the desired product **7**.

General procedure for the asymmetric transfer hydrogenation of imine (Scheme 5): To a sealed-tube were added $HB(C_6F_5)_2$ (0.0104 g, 0.03 mmol), chiral diene **8**

(0.0102 g, 0.015 mmol) and dry toluene (1.5 mL). The resulting mixture was stirred for 5 min at room temperature, and substrate imine **5** (0.3 mmol) and Hantzsch Ester (0.0911 g, 0.36 mmol) was added in a nitrogen atmosphere glovebox. After being sealed, the resulting mixture was stirred for 12 h at 40 °C. The reaction mixture was cooled to room temperature, and the solvent was removed under reduced pressure, and the crude residue was purified by flash chromatography on silica gel using *n*-hexane/DCM (20/1-50/1) as the fluent to give the desired product **7.**

Table S1. Optimization of reaction conditions for asymmetric transfer hydrogenations of imine **5a**. [a]

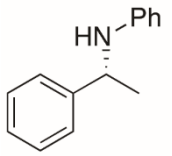


5a **7a**

Entry	Solvent	Temp. (°C)	Conv. (%)[b]	Ee (%)[c]
1	toluene	0	16	*rac.*
2	toluene	25	83	13
3	**toluene**	**40**	**100**	**38**
4	toluene	50	100	36
5	toluene	60	100	33
6	toluene	80	100	29
7	DCM	40	100	11
8	*n*-hexane	40	100	9
9	cyclohexane	40	100	24
10	*n*-pentane	40	100	32
11	*n*-heptane	40	100	27

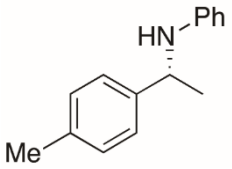
[a] All the reactions were carried out with chiral diene (5 mol %), $HB(C_6F_5)_2$ (10 mol %), imine **5a** (0.1 mmol) and Hantzsch ester **1** (0.12 mmol) in solvent (1.0 mL) unless otherwise noted. [b] Determined by crude ^1H NMR. [c] Determined by chiral HPLC.

Characterization of products



(*R*)-*N*-(1-Phenylethyl)aniline (7a): Colorless oil; $[\alpha]_D^{20}$ = -6.8 (*c* 0.84, MeOH) (38% ee) [lit.: $[\alpha]_D^{20}$ = -4.3 (*c* 1.1, $CHCl_3$) (78% ee for *R*-isomer)]; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.35 (d, *J* = 7.6 Hz, 2H), 7.29 (dd, *J* = 7.6, 7.2 Hz, 2H), 7.24-7.17 (m, 1H), 7.07 (dd, *J* = 7.6, 7.6 Hz, 2H), 6.65-6.60 (m, 1H), 6.49 (d, *J* = 8.0 Hz, 2H), 4.46 (q, *J* = 6.8 Hz, 1H), 3.99 (brs, 1H), 1.49 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 147.6, 145.5, 129.4, 128.9, 127.1, 126.1, 117.5, 113.6, 53.7, 25.3.

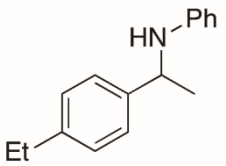
W. Li, G. Hou, M, Chang and X. Zhang, *Adv. Synth. Catal.,* 2009, **351**, 3123.



(*R*)-*N*-(1-(*p*-Tolyl)ethyl)aniline (7b): Yellow oil; $[\alpha]_D^{20}$ = +1.3 (*c* 0.99, MeOH) (37% ee); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.25 (d, *J* = 8.0 Hz, 2H), 7.11 (d, *J* = 8.0 Hz, 2H),7.09 (dd, *J* = 8.4, 7.6 Hz, 2H), 6.65-6.60 (m, 1H), 6.50 (d, *J* = 8.4 Hz, 2H), 4.45

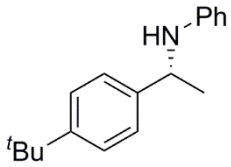
(q, J = 6.8 Hz, 1H), 3.98 (brs, 1H), 2.31 (s, 3H), 1.48 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 147.6, 142.5, 136.6, 129.6, 129.3, 126.0, 117.4, 113.5, 53.4, 25.3, 21.3.

K. Ye, X. Wang, C. G. Daniliuc, G. Kehr and G. Erker, *Eur. J. Inorg. Chem.*, 2016, 368.



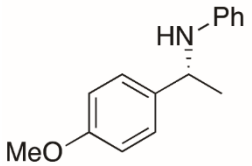
***N*-(1-(4-Ethylphenyl)ethyl)aniline (7c):** Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.26 (d, J = 7.6 Hz, 2H), 7.13 (d, J = 7.6 Hz, 2H), 7.08 (dd, J = 7.6, 7.6 Hz, 2H), 6.66-6.59 (m, J = 7.2 Hz, 1H), 6.50 (d, J = 8.0 Hz, 2H), 4.45 (q, J = 6.4 Hz, 1H), 3.97 (brs, 1H), 2.61 (q, J = 7.6 Hz, 2H), 1.48 (d, J = 6.8 Hz, 3H), 1.21 (t, J = 7.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 147.7, 143.0, 142.7, 129.4, 128.4, 126.1, 117.4, 113.56, 53.4, 28.7, 25.2, 15.8.

Y. Liu and H. Du, *J. Am. Chem. Soc*., 2013, **135**, 6810.



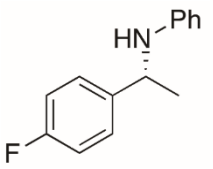
(*R*)-*N*-(1-(4-(*tert*-Butyl)phenyl)ethyl)aniline (7d): Yellow solid, m.p. 60-62°C; $[\alpha]_D^{20}$ = +2.1 (*c* 0.99, CH_2Cl_2) (20% ee) [lit.: $[\alpha]_D^{20}$ = +5.0 (*c* 0.50, CH_2Cl_2) (85% ee for *R*-isomer)]; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.29 (dd, *J* = 8.2, 8.2 Hz, 4H), 7.08 (dd, *J* = 8.0, 7.6 Hz, 2H), 6.66-6.60 (m, 1H), 6.52 (d, *J* = 8.0 Hz, 2H), 4.46 (q, *J* = 6.8 Hz, 1H), 3.98 (brs, 1H), 1.49 (d, *J* = 6.4 Hz, 3H), 1.29 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 149.9, 147.7, 142.3, 129.4, 125.8, 125.8, 117.4, 113.5, 53.2, 34.7, 31.7, 25.0.

E. Kumaran and W. K. Leong, *Organometallics*, 2012, **31**, 1068.



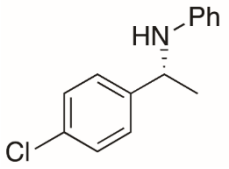
(*R*)-*N*-(1-(4-Methoxyphenyl)ethyl)aniline (7e): Yellow oil; $[\alpha]_D^{20}$ = -2.8 (*c* 0.99, MeOH) (24% ee) [lit.: $[\alpha]_D^{20}$ = -6.2 (*c* 0.55, MeOH) (84% ee for *R*-isomer); ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.24 (d, *J* = 7.6 Hz, 2H), 7.11 (d, *J* = 8.0 Hz, 2H), 7.08 (dd, *J* = 8.4, 7.6 Hz, 2H), 6.66-6.59 (m, 1H), 6.51 (d, *J* = 8.4 Hz, 2H), 4.44 (q, *J* = 6.8 Hz, 1H), 3.97 (brs, 1H), 3.77 (s, 3H), 1.48 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 158.7, 147.6, 137.5, 129.3, 127.1, 117.4, 114.2, 113.5, 55.5, 53.1, 25.2.

A. V. Malkov, S. Stončius, K. N. MacDougall, A. Mariani, G. D. MacGeoch and P. Kočovský, *Tetrahedron,* 2005, **62**, 264.



(*R*)-*N*-(1-(4-Fluorophenyl)ethyl)aniline (7f): Yellow oil; $[\alpha]_D^{20}$ = -11.8 (*c* 1.01, MeOH) (37% ee); ^{1}H NMR (300 MHz, $CDCl_3$, ppm) δ 7.38-7.28 (m, 2H), 7.13-7.05 (m, 2H), 7.04-6.94 (m, 2H), 6.69-6.61 (m, 1H), 6.48 (d, *J* = 7.8 Hz, 2H), 4.46 (q, *J* = 6.6 Hz, 1H), 4.00 (brs, 1H), 1.49 (d, *J* = 6.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 162.0 (d, *J* = 240.0 Hz), 147.3, 141.2 (d, *J* = 3.0 Hz), 141.2, 129.3, 127.6 (d, *J* = 8.0 Hz), 117.7, 115.7 (d, *J* = 21.0 Hz), 113.6, 53.1, 25.4.

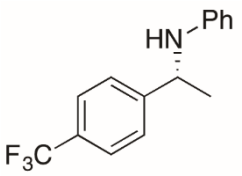
W. Pan, Y. Deng, J. He, B. Bai and H. Zhu, *Tetrahedron*, 2013, **69**, 7253.



(*R*)-*N*-(1-(4-Chlorophenyl)ethyl)aniline (7g): Yellow oil; $[\alpha]_D^{20}$ = +0.7 (*c* 0.83, MeOH) (36% ee); ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.38-7.27 (m, 4H), 7.18-7.10 (m, 2H), 6.74-6.66 (m, 1H), 6.51 (d, *J* = 8.0 Hz, 2H), 4.47 (q, *J* = 6.8 Hz, 1H), 4.02

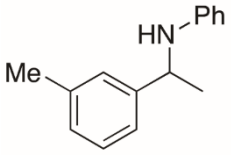
(brs, 1H), 1.50 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 147.3, 144.12, 132.7, 129.5, 129.1, 127.6, 117.8, 113.6, 53.3, 25.4.

W. Pan, Y. Deng, J. He, B. Bai and H. Zhu, *Tetrahedron*, 2013, **69**, 7253.



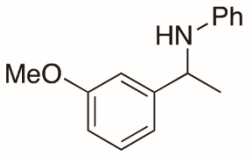
(*R*)-*N*-(1-(4-(Trifluoromethyl)phenyl)ethyl)aniline (7h): Yellow oil; $[\alpha]_D^{20}$ = -11.1 (c 0.98, CH_2Cl_2) (33% ee) [lit.: $[\alpha]_D^{20}$ = -23.1 (c 0.59, CH_2Cl_2) (85% ee for *R*-isomer)]; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.57 (d, J = 8.0 Hz, 2H), 7.48 (d, J = 8.4 Hz, 2H), 7.12-7.05 (m, 2H), 6.70-6.64 (m, 1H), 6.47 (d, J = 7.6 Hz, 2H), 4.52 (q, J = 6.8 Hz, 1H), 4.04 (brs, 1H), 1.52 (d, J = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 149.7, 147.0, 129.6, 129.4, 129.2, 126.4, 125.9 (q, J = 4.0 Hz), 123.1, 117.9, 113.5, 53.5, 29.9, 25.3, 1.2.

M. Rueping, E. Sugiono, C. Azap, T. Theissmann and M. Bolte, *Org. Lett*., 2005, **7**, 3781.



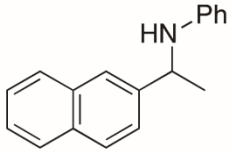
***N*-(1-(*m*-Tolyl)ethyl)aniline (7i):** Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.24-7.12 (m, 3H), 7.08 (dd, *J* = 7.6, 7.6 Hz, 2H), 7.03 (d, *J* = 7.2 Hz, 1H), 6.66-6.61 (m, 1H), 6.51 (d, *J* = 8.0 Hz, 2H), 4.44 (q, *J* = 6.8 Hz, 1H), 3.98 (brs, 1H), 2.33 (s, 3H), 1.49 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 147.6, 145.5, 138.4, 129.3, 128.7, 127.9, 126.8, 123.1, 117.4, 113.5, 53.7, 25.2, 21.8.

A. Lefranc, Z.-W. Qu, S. Grimme and M. Oestreich, *Chem. Eur. J*., 2016, **22**, 10009.



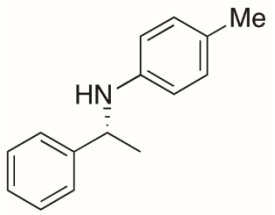
***N*-(1-(3-Methoxyphenyl)ethyl)aniline (7j):** Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.13 (dd, *J* = 8.0, 7.6 Hz, 1H), 6.98 (dd, *J* = 7.6, 7.2 Hz, 2H), 6.88-6.81 (m, 2H), 6.69-6.63 (m, 1H), 6.54 (dd, *J* = 7.6, 7.2 Hz, 1H), 6.41 (d, *J* = 8.4 Hz, 2H), 4.34 (q, *J* = 6.8 Hz, 1H), 3.90 (s, 1H), 3.65 (s, 3H), 1.39 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 160.2, 147.6, 147.45, 130.0, 129.4, 118.5, 117.6, 113.6, 112.3, 112.0, 55.4, 53.8, 25.3.

A. Lefranc, Z.-W. Qu, S. Grimme and M. Oestreich, *Chem. Eur. J*., 2016, **22**, 10009.



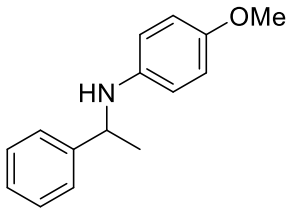
***N*-(1-(Naphthalen-2-yl)ethyl)aniline (7k):** Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.83-7.74 (m, 4H), 7.50-7.45 (m, 1H), 7.45-7.36 (m, 2H), 7.10-7.02 (m, 2H), 6.66-6.58 (m, 1H), 6.53 (d, *J* = 8.0 Hz, 2H), 4.61 (q, *J* = 6.8 Hz, 1H), 4.08 (brs, 1H), 1.55 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 147.6, 143.1, 133.9, 133.0, 129.4, 128.8, 128.1, 128.0, 126.3, 125.8, 124.7, 124.5, 117.6, 113.7, 54.0, 25.3.

S. Guizzetti, M. Benaglia, F. Cozzi and R. Annunziata, *Tetrahedron*, 2009, **65**, 6354.



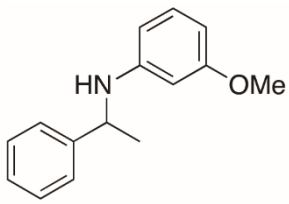
(*R*)-4-Methyl-*N*-(1-phenylethyl)aniline (7l): Yellow oil; $[\alpha]_D^{20}$ = -4.0 (*c* 1.0, EtOAc) (16% ee) [lit.: $[\alpha]_D^{25}$ = +27.3 (*c* 0.7, EtOAc) (91% ee for *S*-isomer)]; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.40-7.25 (m, 4H), 7.24-7.16 (m, 1H), 6.89 (d, *J* = 8.0 Hz, 2H), 6.42 (d, *J* = 8.0 Hz, 2H), 4.44 (q, *J* = 6.4 Hz, 1H), 3.86 (brs, 1H), 2.17 (s, 3H), 1.48 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 145.7, 145.3, 129.9, 128.9, 128.5, 127.1, 126.6, 126.1, 113.7, 53.9, 25.3, 20.6.

D. Pei, Z. Wang, S. Wei, Y. Zhang and J. Sun, *Org. Lett.,* 2006, **8**, 5913.



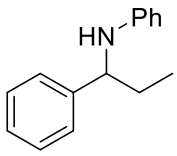
4-Methoxy-*N*-(1-phenylethyl)aniline (7m): Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.35 (d, *J* = 7.5 Hz, 2H), 7.33-7.26 (m, 2H), 7.21 (d, *J* = 6.0 Hz, 1H), 6.68 (d, *J* = 9.0 Hz, 2H), 6.46 (d, *J* = 9.0 Hz, 2H), 4.40 (q, *J* = 7.0 Hz, 1H), 3.77 (brs, 1H), 3.67 (s, 3H), 1.48 (d, *J* = 6.5 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$, ppm) δ 150.8, 144.5, 140.5, 127.6, 125.8, 124.8, 113.7, 113.5, 54.7, 53.2, 24.1.

I. Chatterjee and M. Oestreich, *Angew. Chem., Int. Ed.*, 2015, **54**, 1965.



3-Methoxy-*N*-(1-phenylethyl)aniline (7n): Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$, ppm) δ 7.37-7.24 (m, 4H), 7.23-7.14 (m, 1H), 6.97 (dd, *J* = 8.0, 8.0 Hz, 1H), 6.20 (d, *J* = 8.0 Hz, 1H), 6.13 (d, *J* = 7.6 Hz, 1H), 6.05 (s, 1H), 4.45 (q, *J* = 6.4 Hz, 1H), 4.03 (brs, 1H), 3.65 (s, 3H), 1.47 (d, *J* = 6.8 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$, ppm) δ 161.0, 149.0, 145.5, 130.1, 128.9, 127.2, 126.1, 106.8, 102.7, 99.7, 55.2, 53.8, 25.2.

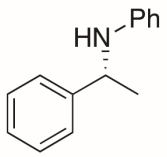
X.-Y. Liu and C.-M. Che, *Org. Lett.*, 2009, **11**, 4204.



***N*-(1-Phenylpropyl)aniline (7o)**: Yellow oil; ^{1}H NMR (500 MHz, $CDCl_3$, ppm) δ 7.37-7.24 (m, 4H), 7.23-7.17 (m, 1H), 7.10-7.02 (t, *J* = 7.5 Hz, 2H), 6.65-6.58 (m, 1H), 6.50 (d, *J* = 8.0 Hz, 2H), 4.21 (t, *J* = 6.7 Hz, 1H), 4.03 (brs, 1H), 1.80 (m, 2H), 0.94 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (126 MHz, $CDCl_3$, ppm) δ 146.5, 142.9, 128.0, 127.4, 125.83, 125.4, 116.1, 112.2, 58.7, 30.6, 9.8.

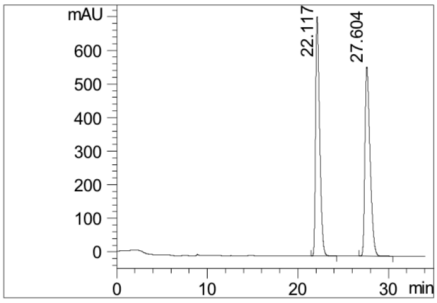
I. Chatterjee and M. Oestreich, *Angew. Chem., Int. Ed.*, 2015, **54**, 1965.

The chromatography for the determination of enantiomeric excess



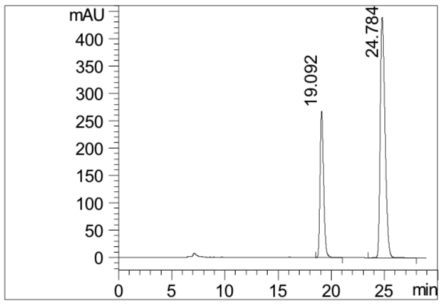
HPLC Conditions: Column: Chiralcel OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (98/2); **Flow rate:** 0.5 mL/min; **Detection:** UV 254 nm

Racemic

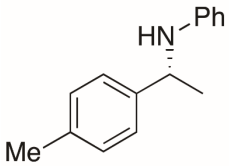


Peak #	RT [min]	Area %	Area
1	22.117	49.897	2.212e4
2	27.604	50.103	2.221e4

Chiral

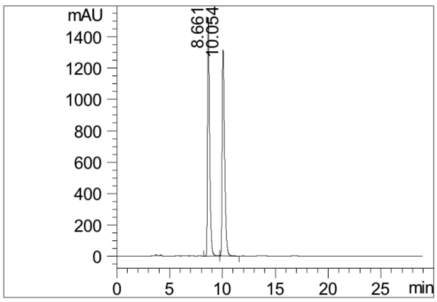


Peak #	RT [min]	Area %	Area
1	19.092	31.085	6.205e3
2	24.784	68.915	1.376e4



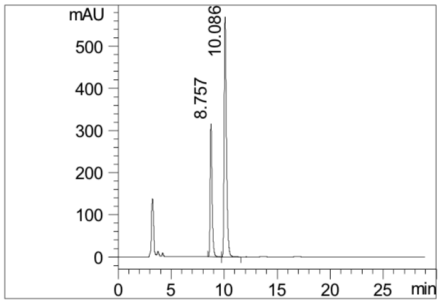
HPLC Conditions: Column: Chiralcel OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (99/1); **Flow rate:** 1.0 mL/min; **Detection:** UV 254 nm

Racemic

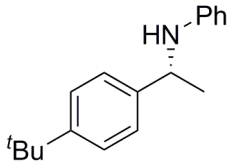


Peak #	RT [min]	Area %	Area
1	8.661	49.661	2.084e4
2	10.054	50.339	2.112e4

Chiral

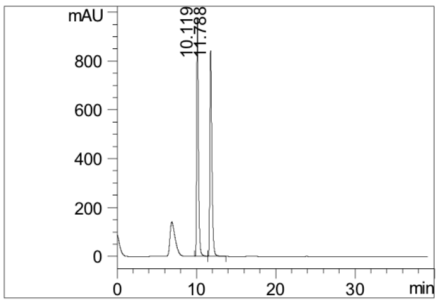


Peak #	RT [min]	Area %	Area
1	8.757	31.789	3.980e3
2	10.086	68.211	8.541e3



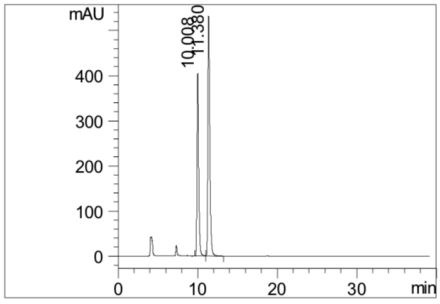
HPLC Conditions: Column: Chiralcel OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (98/2); **Flow rate:** 0.8 mL/min; **Detection:** UV 254 nm

Racemic

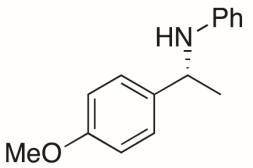


Peak #	RT [min]	Area %	Area
1	10.119	49.825	1.488e4
2	11.788	50.175	1.499e4

Chiral

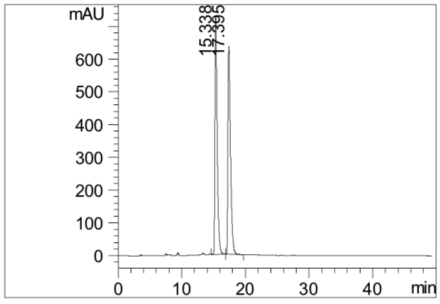


Peak #	RT [min]	Area %	Area
1	10.008	39.932	5.900e3
2	11.380	60.068	8.875e3



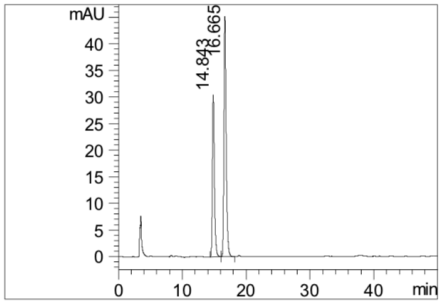
HPLC Conditions: Column: Chiralcel OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (99/1); **Flow rate:** 0.8 mL/min; **Detection:** UV 254 nm

Racemic

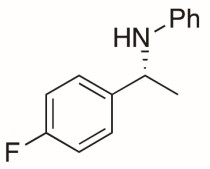


Peak #	RT [min]	Area %	Area
1	15.338	50.021	1.799e4
2	17.395	49.979	1.798e4

Chiral

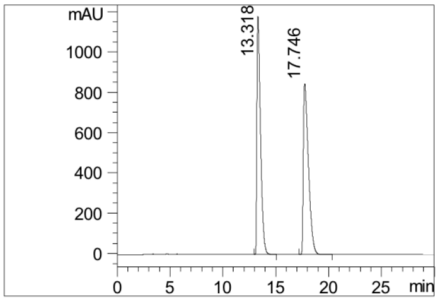


Peak #	RT [min]	Area %	Area
1	14.843	38.115	673.712
2	16.665	61.885	1.094e3



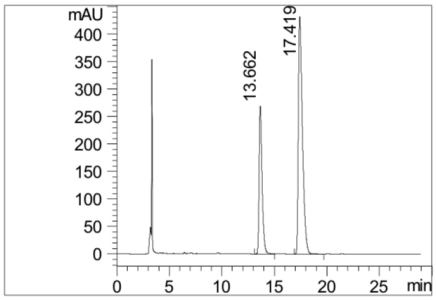
HPLC Conditions: Column: Chiralcel OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (99/1); **Flow rate:** 1.0 mL/min; **Detection:** UV 254 nm

Racemic

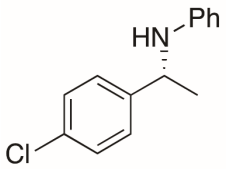


Peak #	RT [min]	Area %	Area
1	13.318	49.676	2.815e4
2	17.746	50.324	2.851e4

Chiral

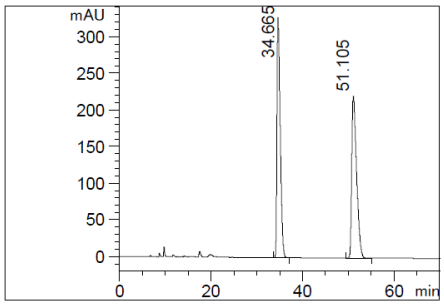


Peak #	RT [min]	Area %	Area
1	13.662	31.294	5.321e3
2	17.419	68.706	1.168e4



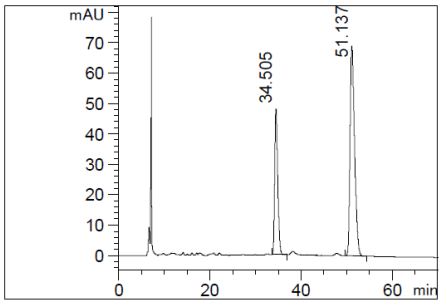
HPLC Conditions: Column: Chiralcel OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (98/2); **Flow rate:** 0.5 mL/min; **Detection:** UV 254 nm

Racemic

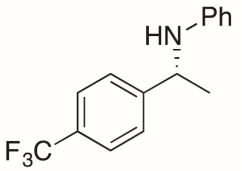


Peak #	RT [min]	Area %	Area
1	34.665	49.866	1.624e4
2	51.105	50.134	1.632e4

Chiral

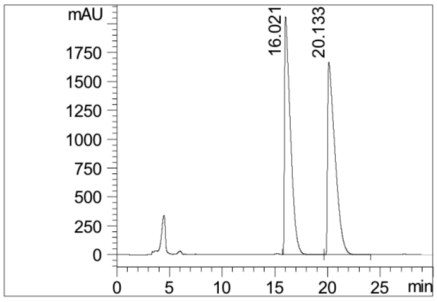


Peak #	RT [min]	Area %	Area
1	34.505	31.839	2.235e3
2	51.137	68.161	4.785e3



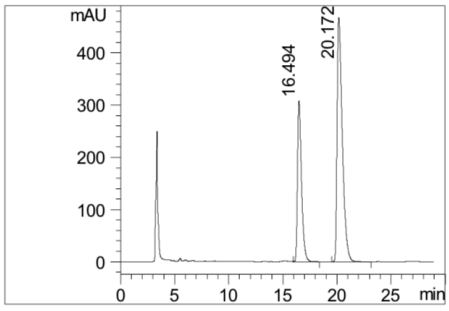
HPLC Conditions: Column: Chiralcel OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (98/2); **Flow rate:** 0.6 mL/min; **Detection:** UV 254 nm

Racemic

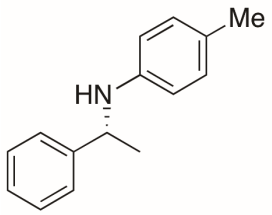


Peak #	RT [min]	Area %	Area
1	16.021	49.578	8.049e4
2	20.133	50.422	8.185e4

Chiral

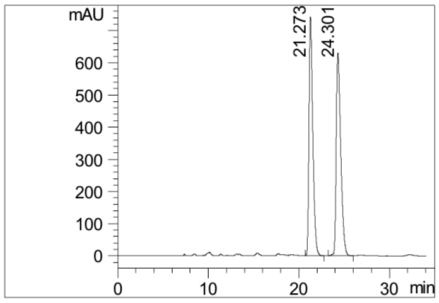


Peak #	RT [min]	Area %	Area
1	16.494	33.668	7.972e3
2	20.172	66.332	1.571e4



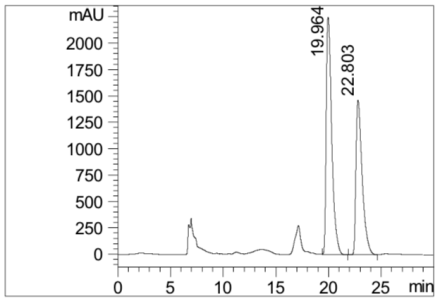
HPLC Conditions: Column: Chiralcel OD-H, Daicel Chemical Industries, Ltd., **Eluent:** Hexanes/IPA (98/2); **Flow rate:** 0.5 mL/min; **Detection:** UV 254 nm

Racemic

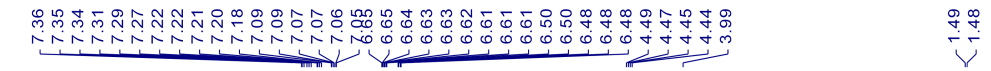


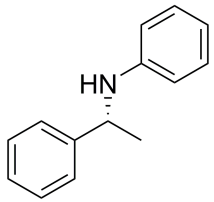
Peak #	RT [min]	Area %	Area
1	21.273	49.887	2.181e4
2	24.301	50.113	2.191e4

Chiral

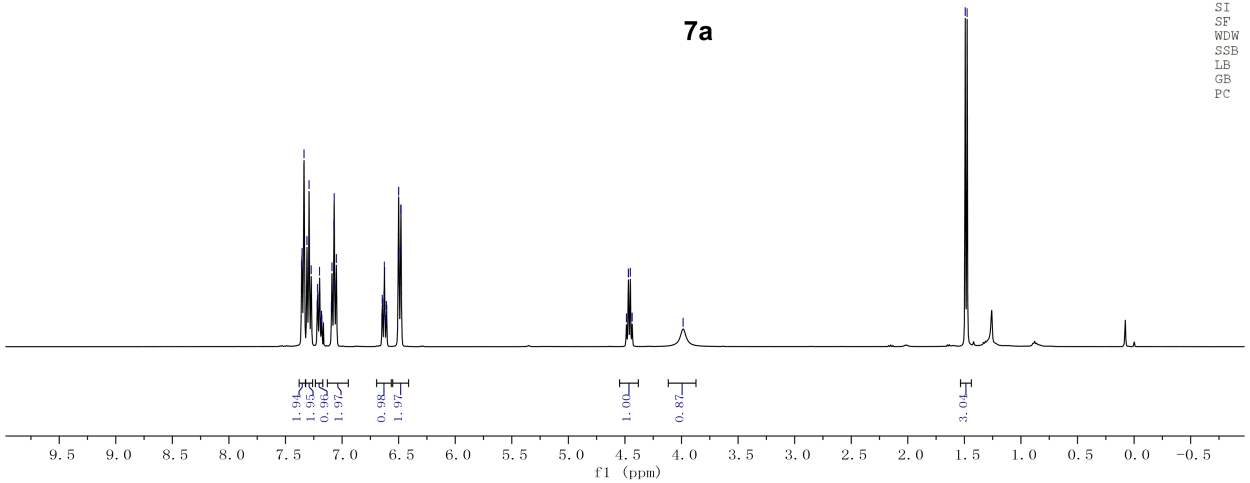


Peak #	RT [min]	Area %	Area
1	19.964	57.782	8.256e4
2	22.803	42.218	6.032e4





7a

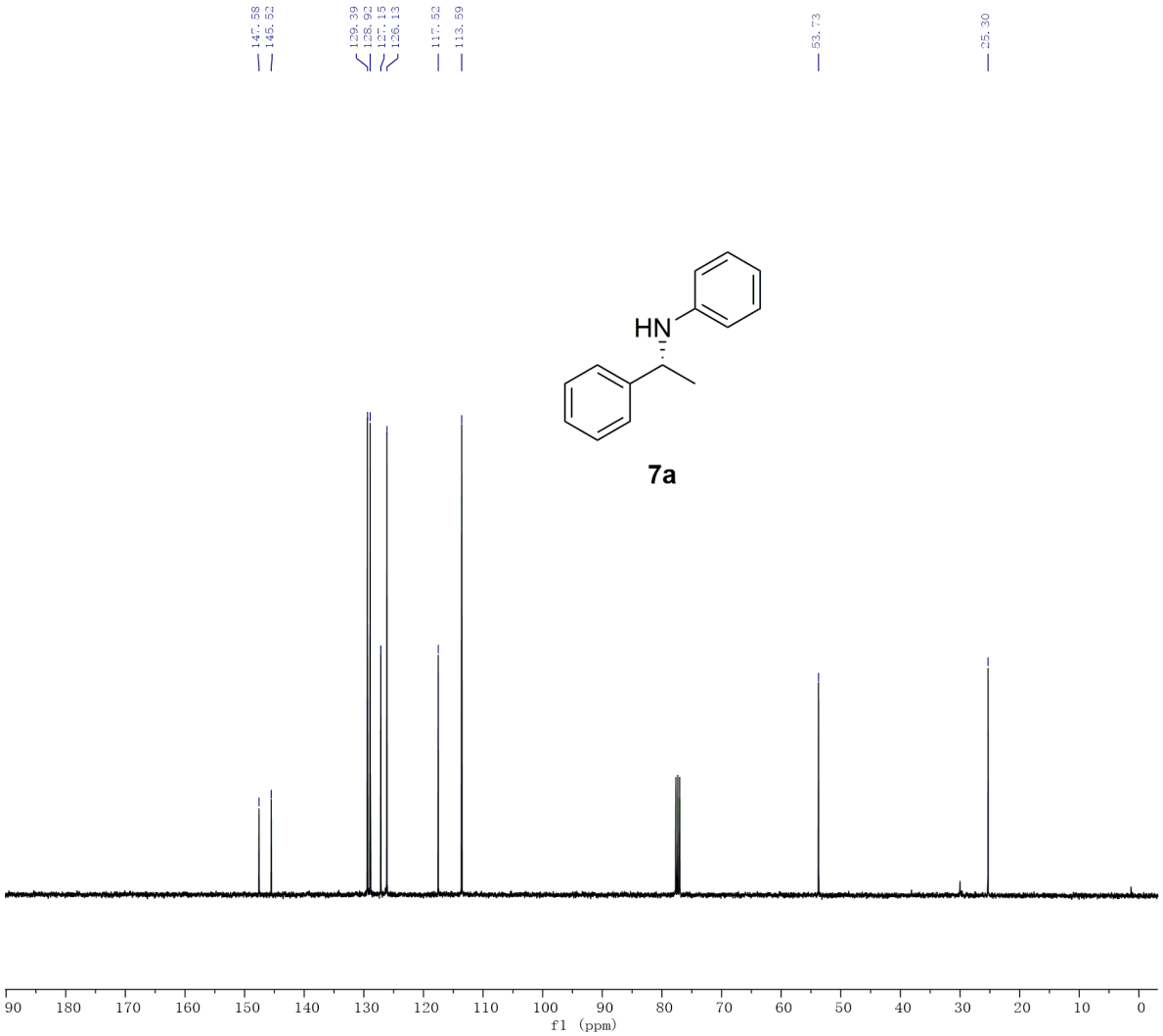



```
Current Data Parameters
NAME       Product-rac-H
EXPNO                 54
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170506
Time                8.20
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES             0.122266 Hz
AQ              4.0894465 sec
RG                    57
DW                 62.400 usec
DE                  6.50 usec
TE                298.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 12.00 usec
PLW1         13.06000042 W

F2 - Processing parameters
SI                 65536
SF           400.1300476 MHz
WDW                   EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```



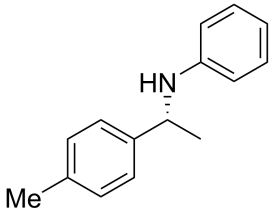

```
Current Data Parameters
NAME       Product-rac-C
EXPNO                 9
PROCNO                1

F2 - Acquisition Parameters
Date_          20170506
Time               8.12
INSTRUM           spect
PROBHD   5 mm PADUL 13C
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  104
DS                    0
SWH           25252.525 Hz
FIDRES         0.770646 Hz
AQ             0.6488064 sec
RG                  203
DW               19.800 usec
DE                6.50 usec
TE                298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                 9.40 usec
PLW1        43.63899994 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        13.06000042 W
PLW12        0.25598001 W
PLW13        0.20734000 W

F2 - Processing parameters
SI                 32768
SF          100.6127487 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



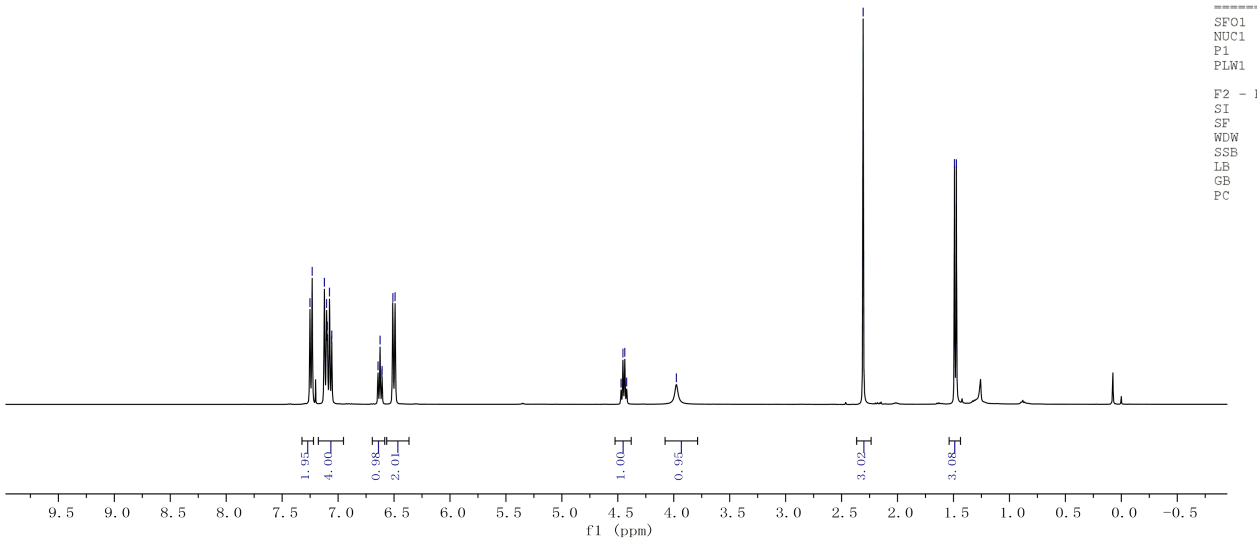
7b

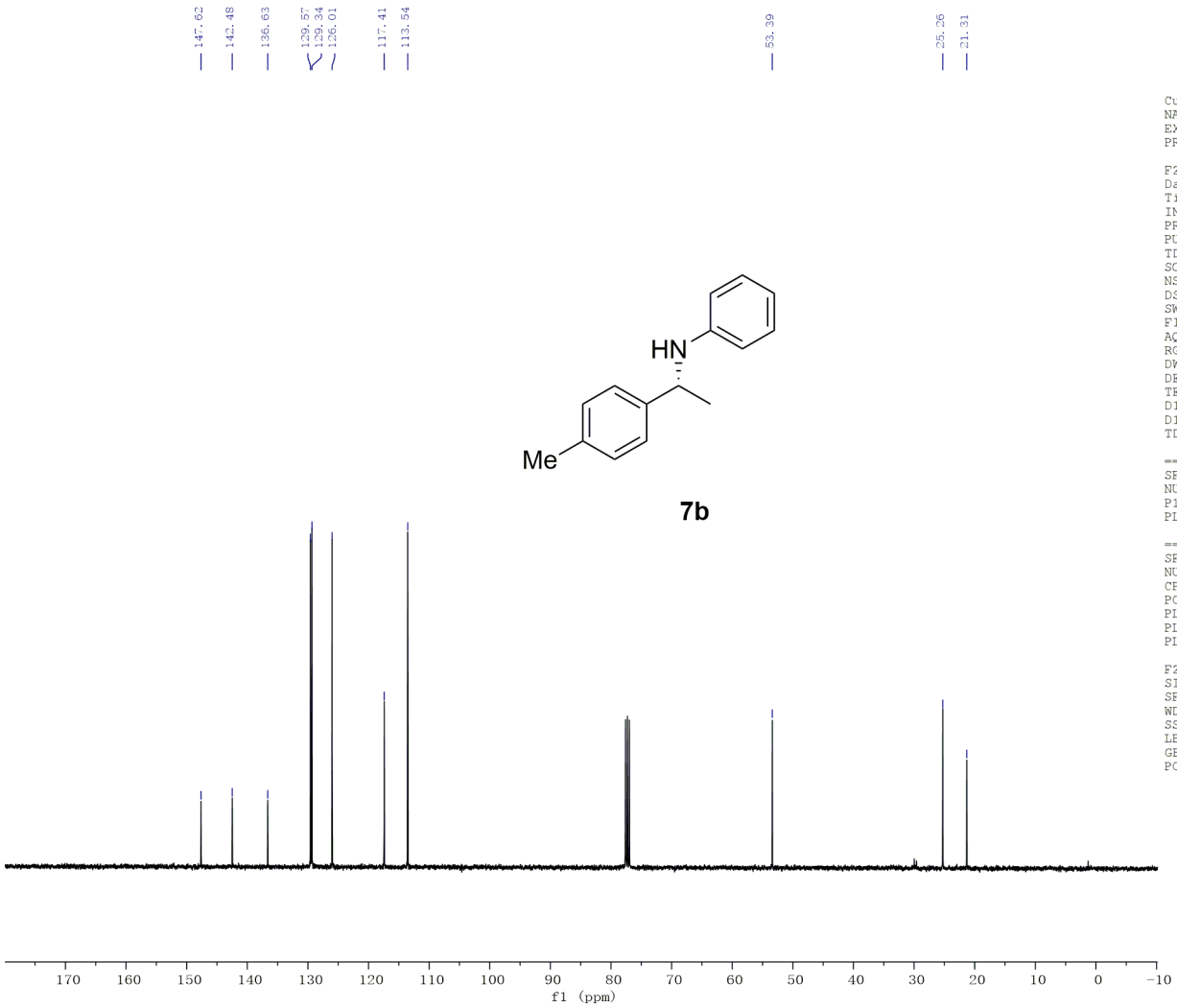
```
Current Data Parameters
NAME       Product-rac-H
EXPNO                 55
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170506
Time                8.26
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES             0.122266 Hz
AQ              4.0894465 sec
RG                    57
DW                62.400 usec
DE                 6.50 usec
TE                298.1 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                  1H
P1                 12.00 usec
PLW1          13.06000042 W

F2 - Processing parameters
SI                 65536
SF            400.1300332 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```





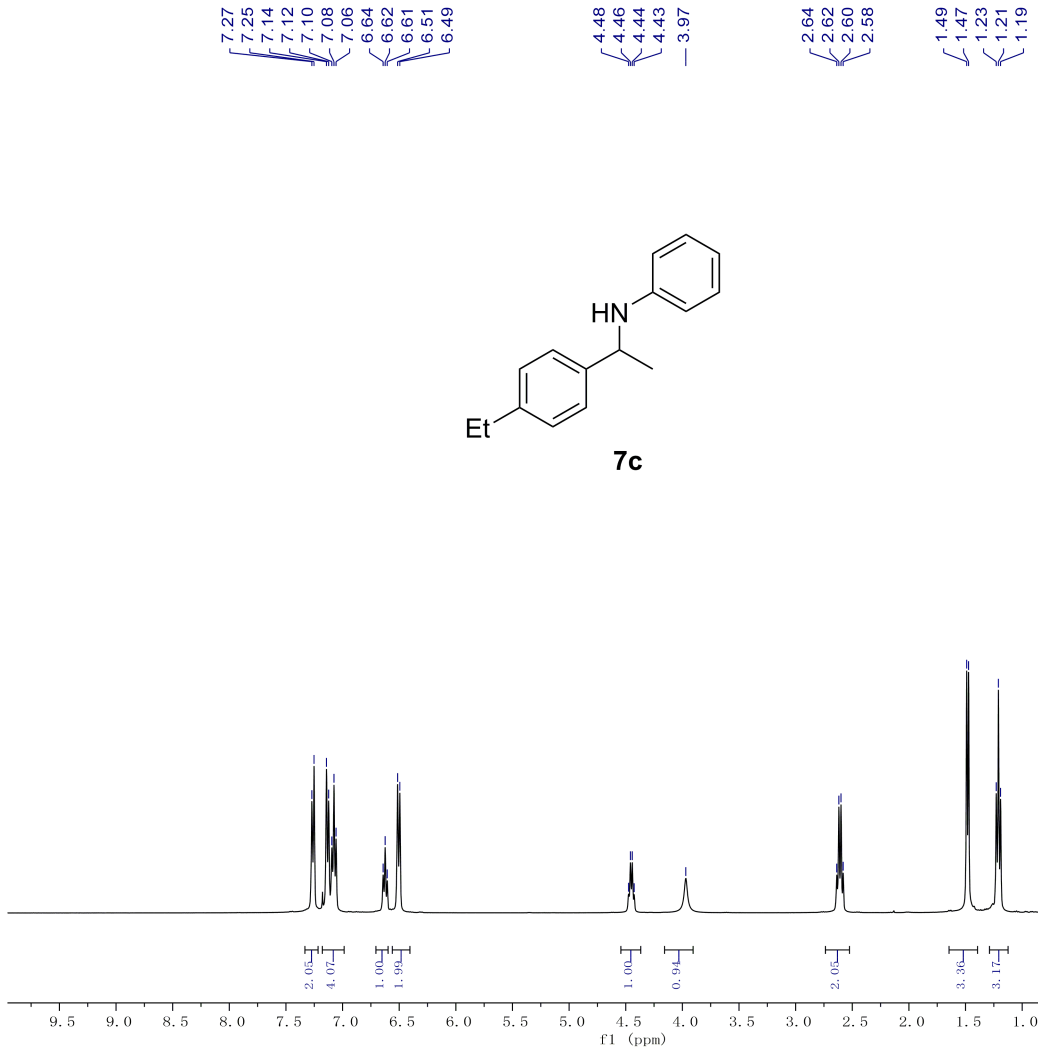

```
Current Data Parameters
NAME      Product-rac-C
EXPNO                10
PROCNO                1

F2 - Acquisition Parameters
Date_          20170506
Time               8.32
INSTRUM           spect
PROBHD   5 mm PADUL 13C
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  188
DS                    0
SWH           25252.525 Hz
FIDRES         0.770646 Hz
AQ             0.6488064 sec
RG                  203
DW               19.800 usec
DE                6.50 usec
TE                298.3 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                13C
P1                 9.40 usec
PLW1         43.63899994 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.06000042 W
PLW12         0.25598001 W
PLW13         0.20734000 W

F2 - Processing parameters
SI                 32768
SF           100.6127487 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

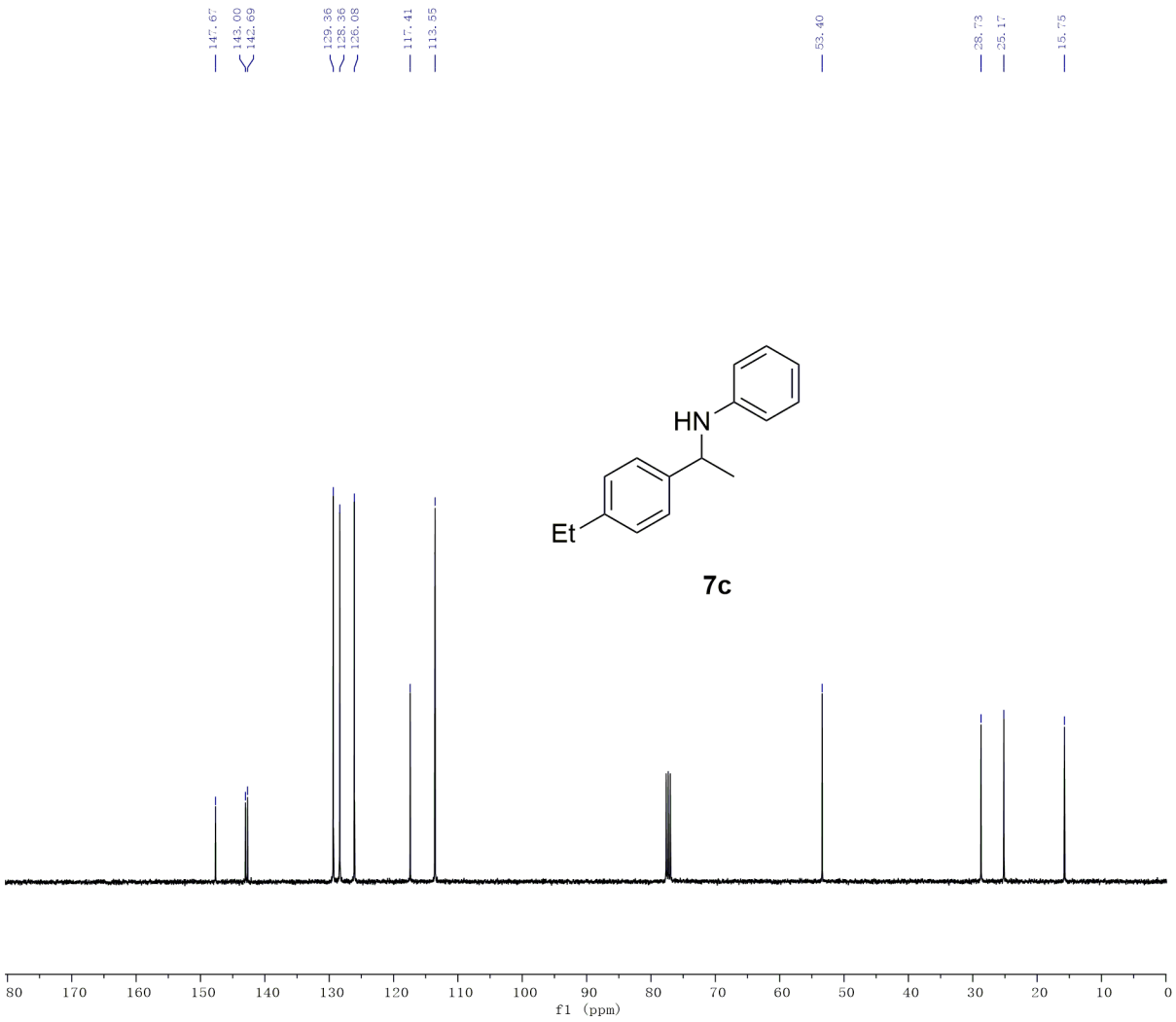



```
Current Data Parameters
NAME      Product-rac-H
EXPNO                86
PROCNO                1

F2 - Acquisition Parameters
Date_          20170726
Time               9.46
INSTRUM           spect
PROBHD   5 mm PADUL 13C
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894465 sec
RG                   57
DW               62.400 usec
DE                6.50 usec
TE               673.2 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1               1H
P1                12.00 usec
PLW1         13.06000042 W

F2 - Processing parameters
SI                65536
SF           400.1300424 MHz
WDW                EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



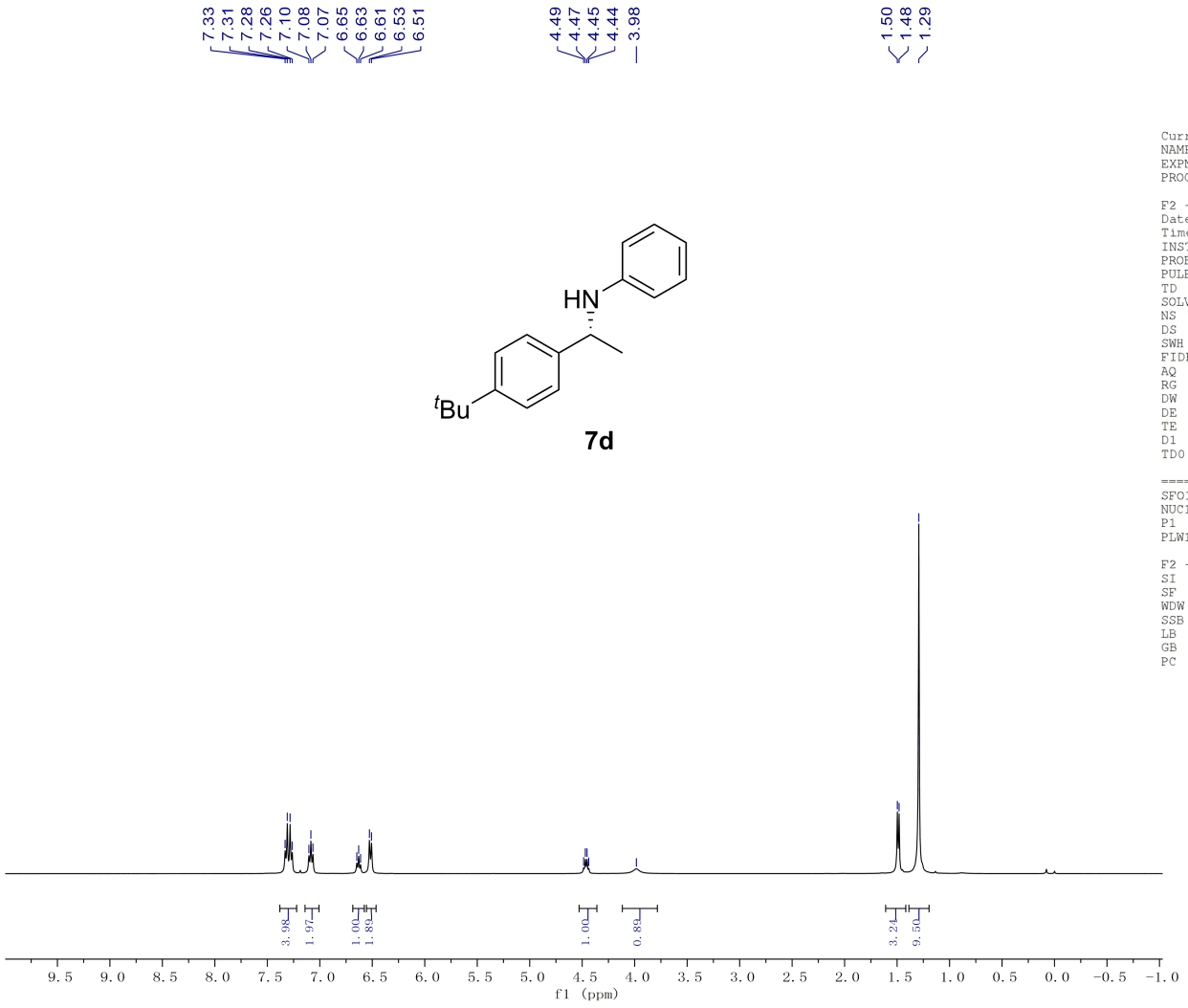

```
Current Data Parameters
NAME      Product-rac-C
EXPNO                25
PROCNO                1

F2 - Acquisition Parameters
Date_          20170726
Time               9.51
INSTRUM           spect
PROBHD   5 mm PADUL 13C
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  206
DS                    0
SWH           25252.525 Hz
FIDRES         0.770646 Hz
AQ            0.6488064 sec
RG                  161
DW               19.800 usec
DE                6.50 usec
TE                673.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1               13C
P1                9.40 usec
PLW1         43.63899994 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.06000042 W
PLW12         0.25598001 W
PLW13         0.20734000 W

F2 - Processing parameters
SI                32768
SF          100.6127487 MHz
WDW                EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```




```
Current Data Parameters
NAME      Product-rac-H
EXPNO                67
PROCNO                1

F2 - Acquisition Parameters
Date_          20170512
Time               3.21
INSTRUM           spect
PROBHD   5 mm PADUL 13C
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES             0.122266 Hz
AQ              4.0894465 sec
RG                    57
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                 1H
P1                12.00 usec
PLW1         13.06000042 W

F2 - Processing parameters
SI                 65536
SF           400.1300387 MHz
WDW                  EM
SSB      0
LB                0.30 Hz
GB       0
PC                1.00
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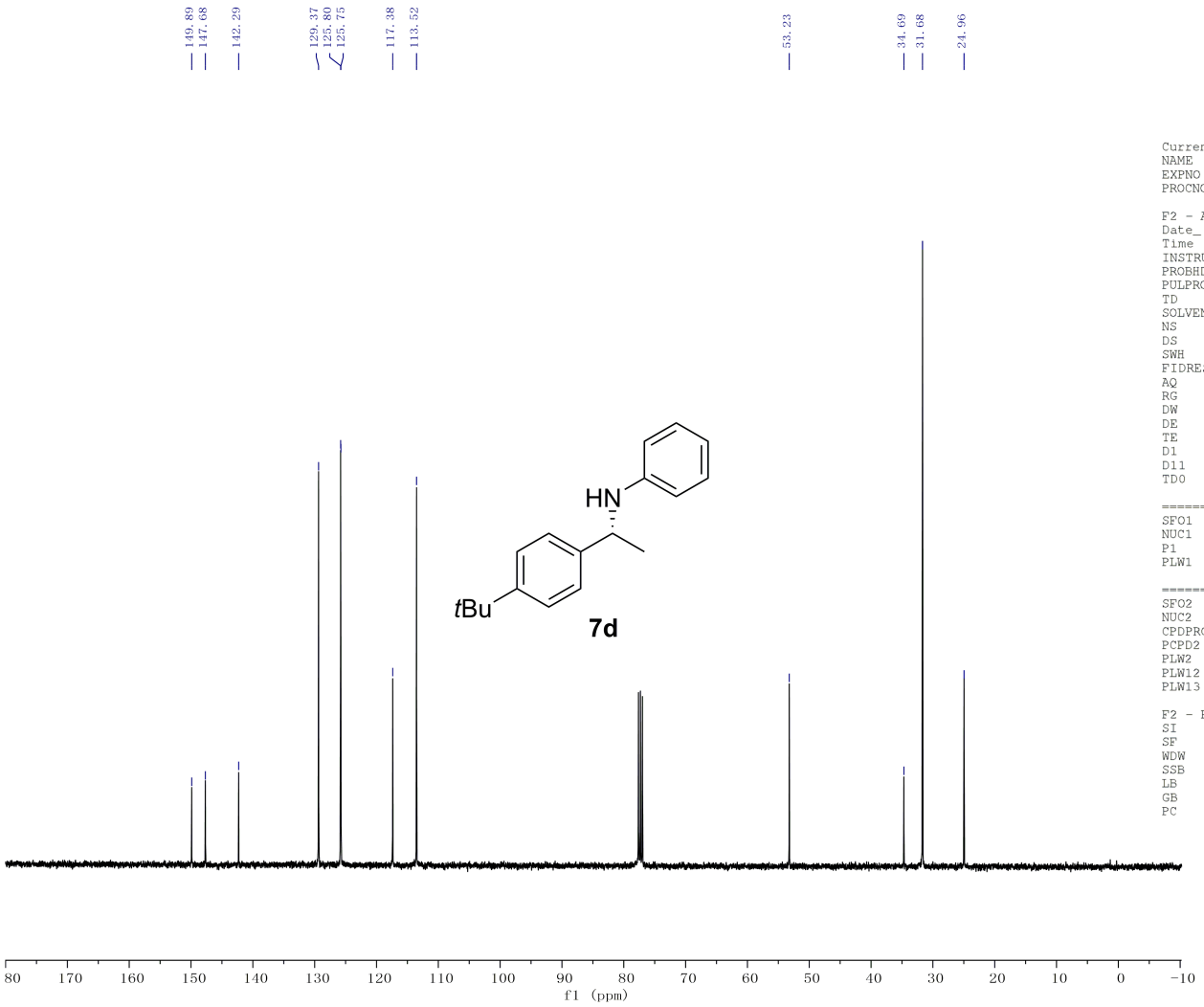


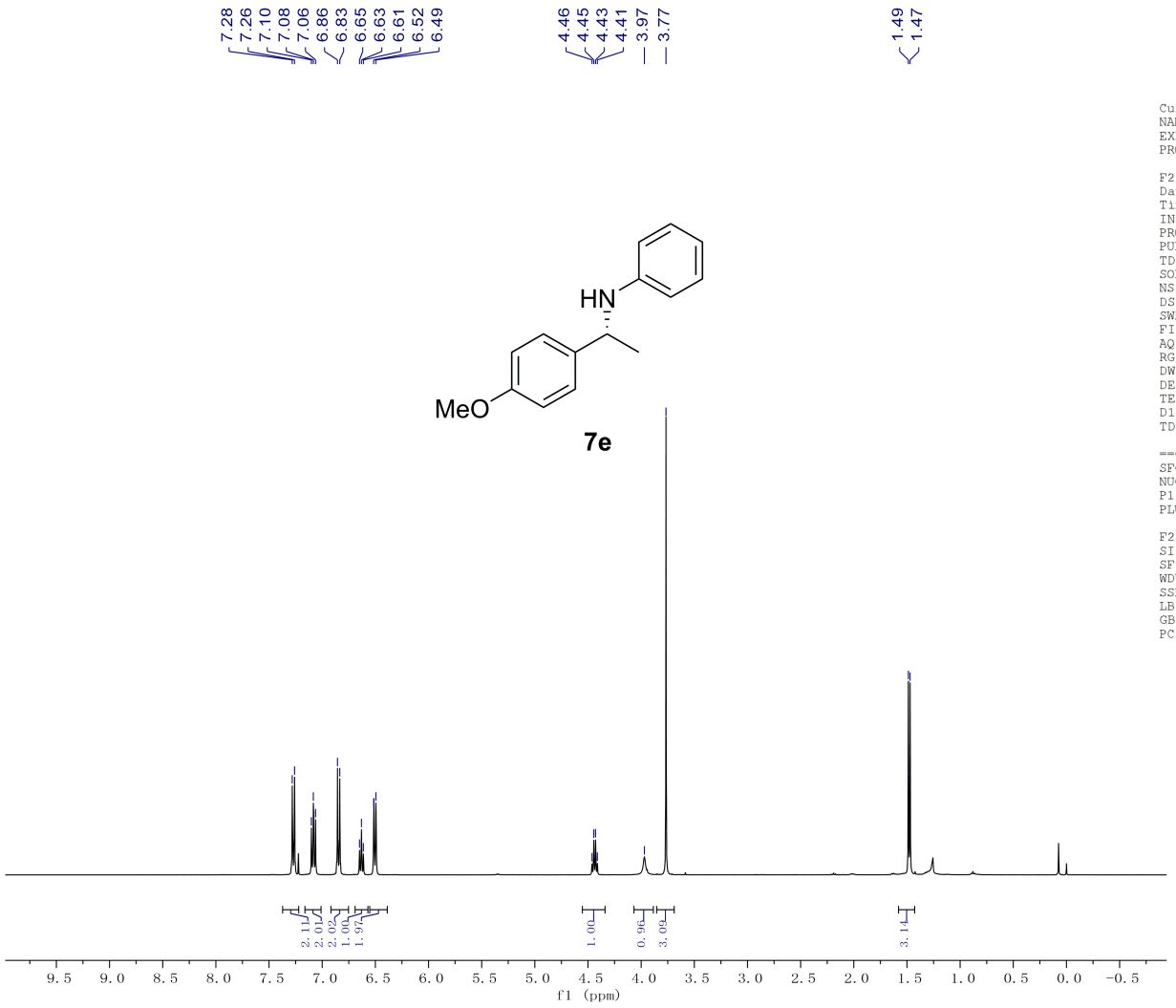

```
Current Data Parameters
NAME       Product-rac-C
EXPNO                 20
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170512
Time                3.28
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  156
DS                    0
SWH           25252.525 Hz
FIDRES         0.770646 Hz
AQ             0.6488064 sec
RG                  161
DW               19.800 usec
DE                6.50 usec
TE                298.7 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                  9.40 usec
PLW1         43.63899994 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2         13.06000042 W
PLW12         0.25598001 W
PLW13         0.20734000 W

F2 - Processing parameters
SI                  32768
SF           100.6127487 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

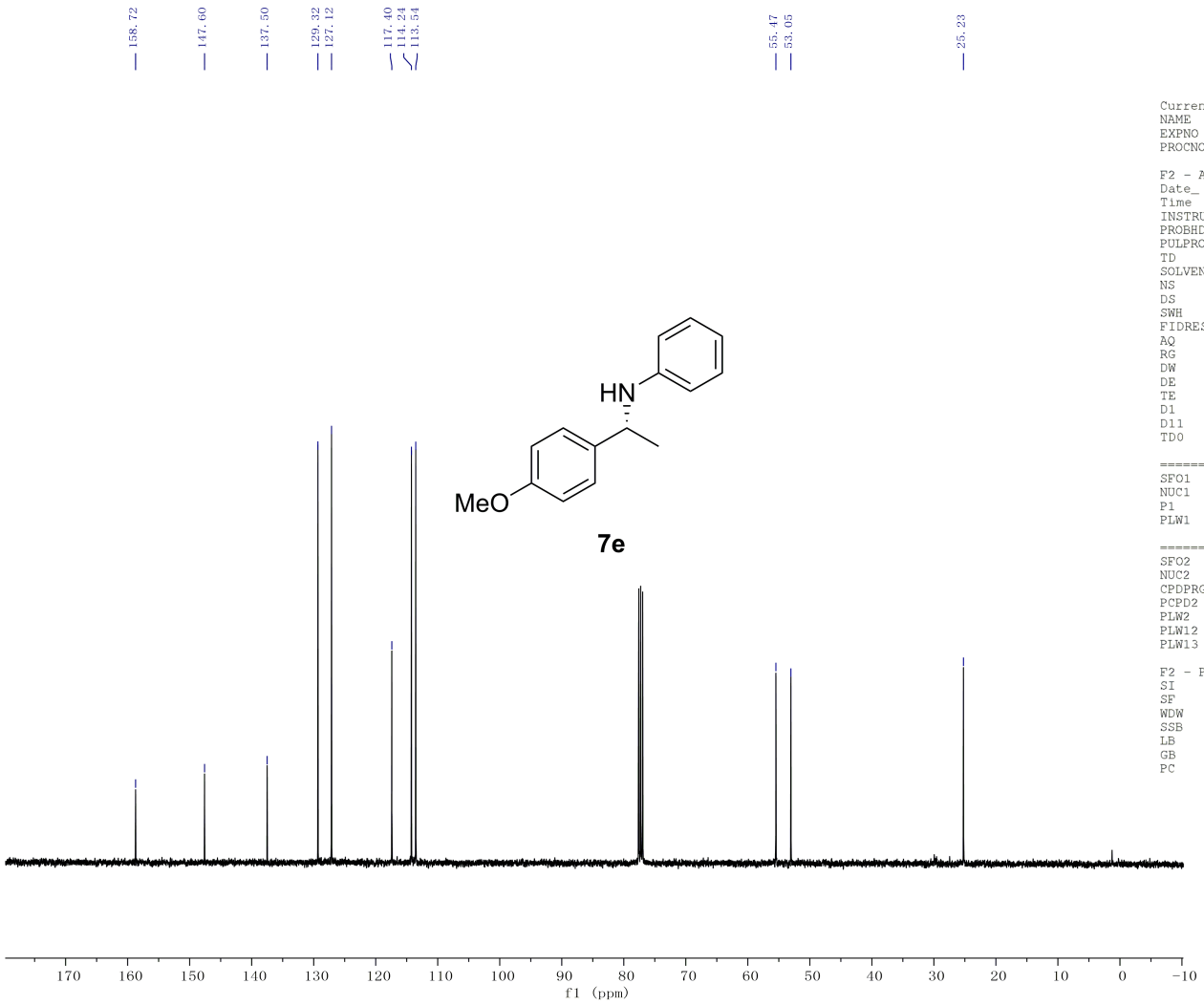



```
Current Data Parameters
NAME      Product-rac-H
EXPNO                56
PROCNO                1

F2 - Acquisition Parameters
Date_          20170506
Time               8.47
INSTRUM           spect
PROBHD   5 mm PADUL 13C
PULPROG             zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES            0.122266 Hz
AQ             4.0894465 sec
RG                  101
DW                62.400 usec
DE                 6.50 usec
TE                298.2 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                 1H
P1                12.00 usec
PLW1         13.06000042 W

F2 - Processing parameters
SI                65536
SF           400.1300243 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



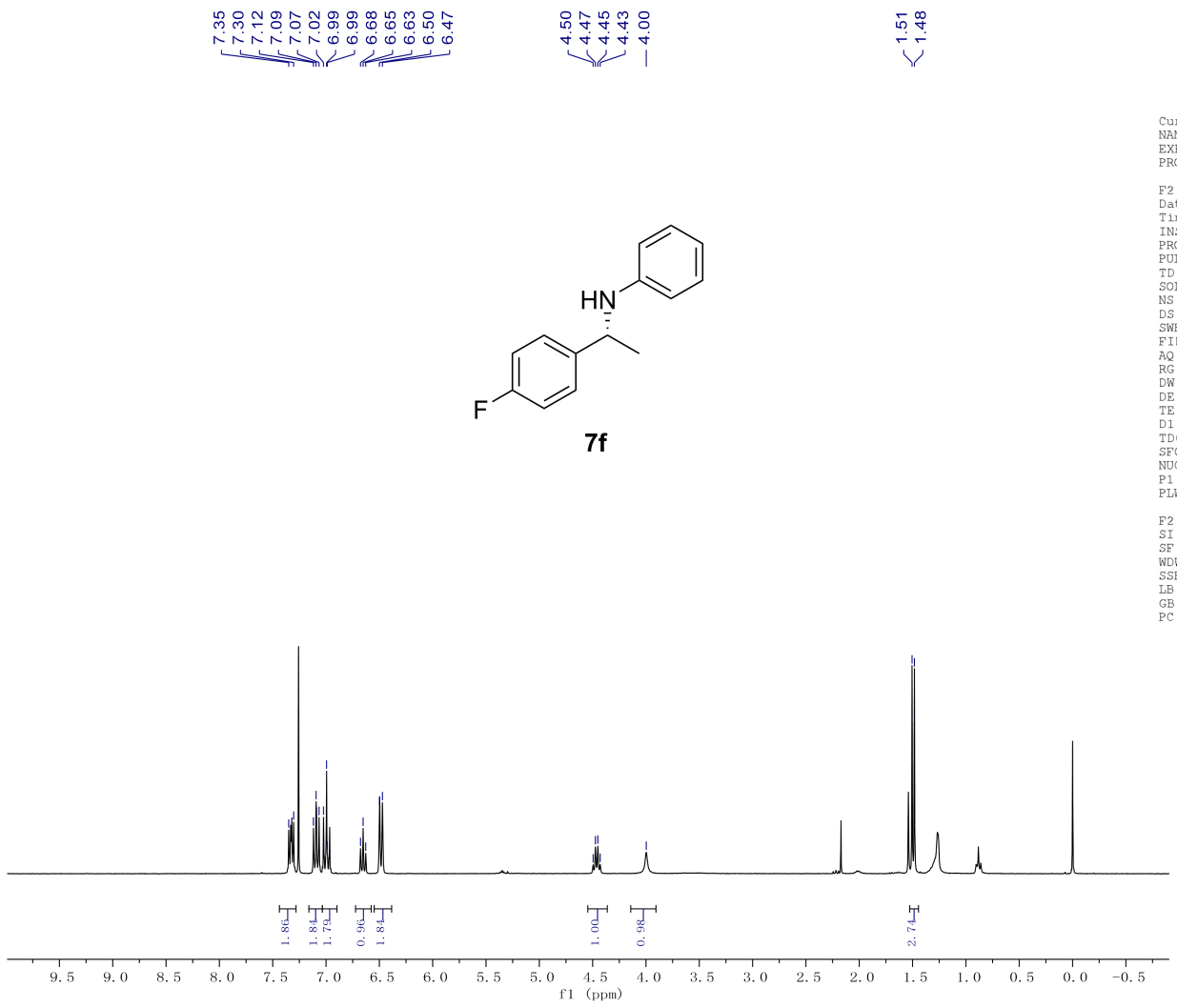

```
Current Data Parameters
NAME       Product-rac-C
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170506
Time                8.54
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  228
DS                    0
SWH           25252.525 Hz
FIDRES         0.770646 Hz
AQ            0.6488064 sec
RG                  203
DW               19.800 usec
DE                6.50 usec
TE                298.8 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                 9.40 usec
PLW1        43.63899994 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        13.06000042 W
PLW12        0.25598001 W
PLW13        0.20734000 W

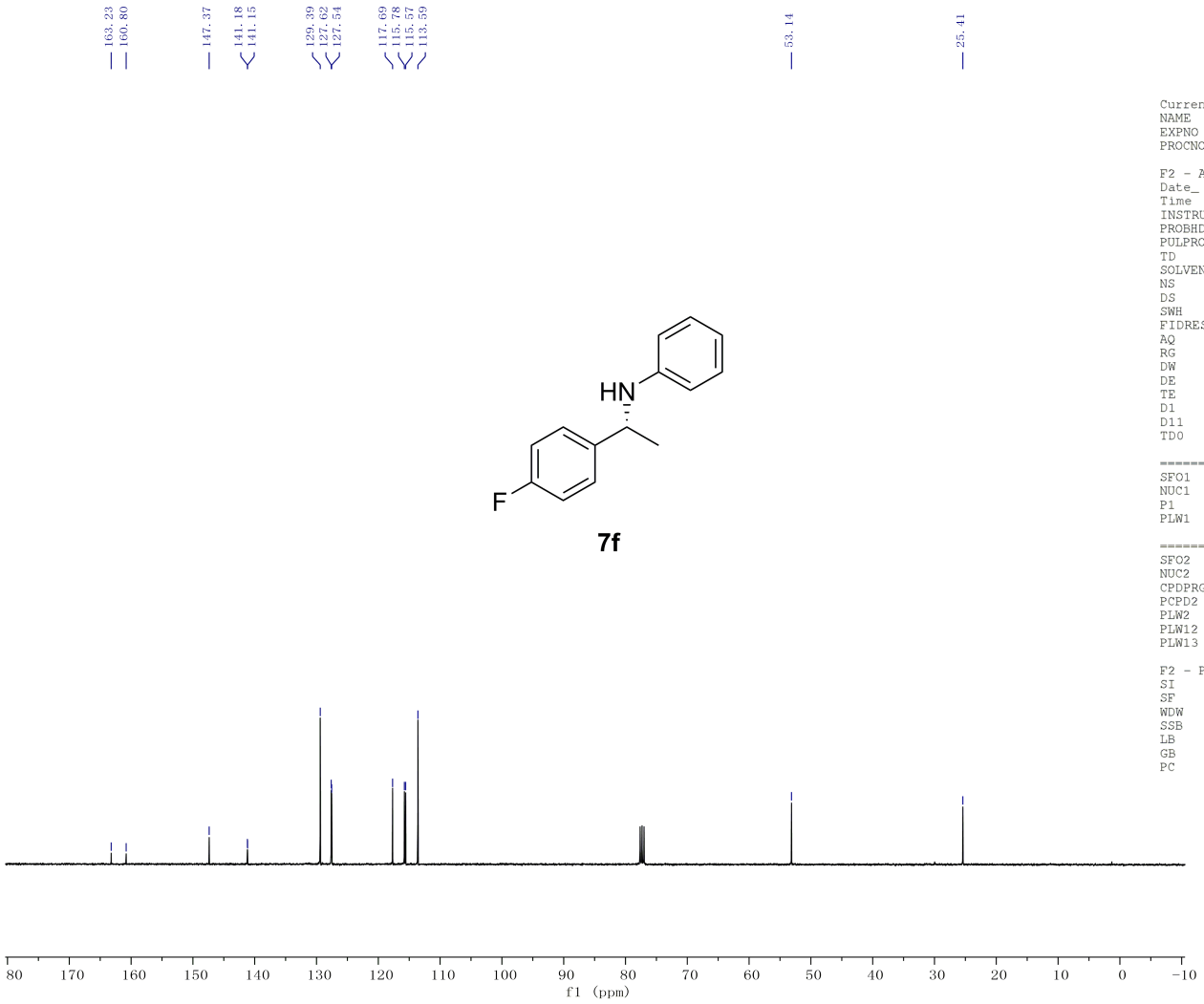
F2 - Processing parameters
SI                32768
SF          100.6127487 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```




```
Current Data Parameters
NAME       Product-rac-H
EXPNO               338
PROCNO                1

F2 - Acquisition Parameters
Date_          20170428
Time              17.25
INSTRUM           spect
PROBHD   5 mm DUL 13C-1
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            6009.615 Hz
FIDRES          0.091699 Hz
AQ             5.4525952 sec
RG                209.09
DW                83.200 usec
DE                 6.50 usec
TE        0 K
D1           1.00000000 sec
TD0                   1
SFO1         300.1318534 MHz
NUC1                 1H
P1                8.00 usec
PLW1         18.00000000 W

F2 - Processing parameters
SI                65536
SF           300.1300080 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



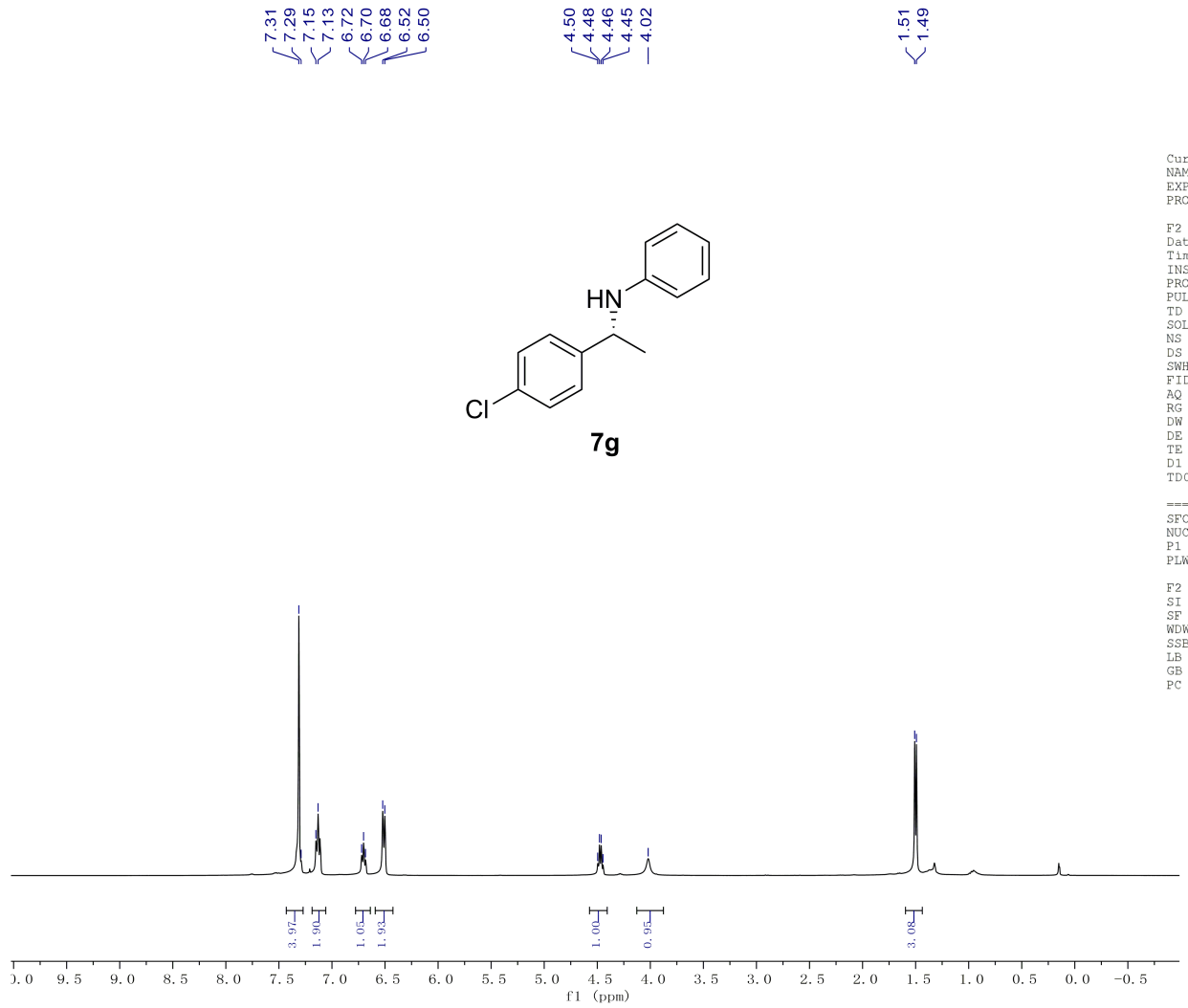

```
Current Data Parameters
NAME       Product-rac-C
EXPNO                 15
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170507
Time                3.04
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                   98
DS                    0
SWH           25252.525 Hz
FIDRES         0.770646 Hz
AQ             0.6488064 sec
RG                  181
DW                19.800 usec
DE                 6.50 usec
TE                299.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                 9.40 usec
PLW1        43.63899994 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2        13.06000042 W
PLW12        0.25598001 W
PLW13        0.20734000 W

F2 - Processing parameters
SI                32768
SF          100.6127487 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

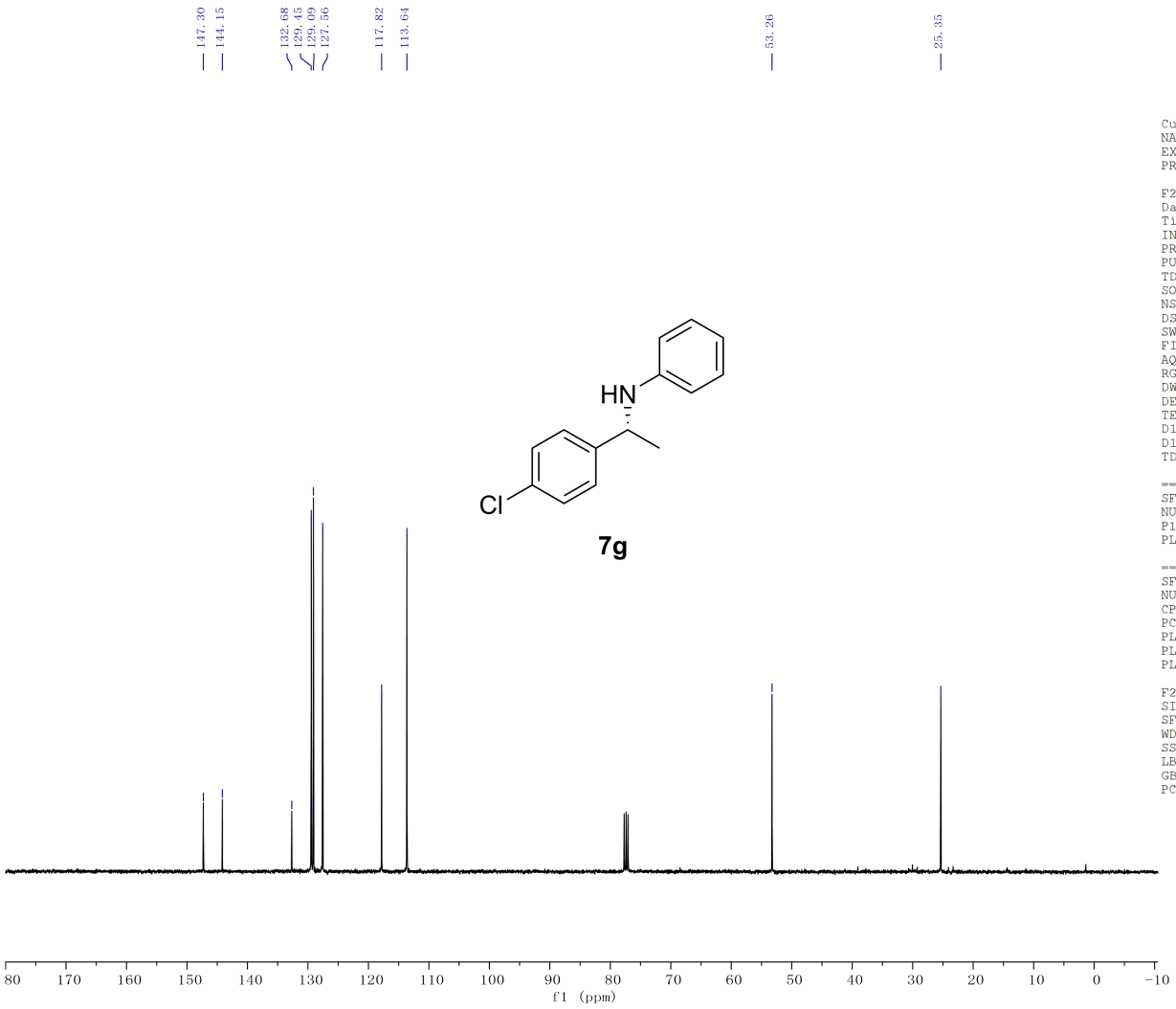



```
Current Data Parameters
NAME       Product-rac-H
EXPNO                 65
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170507
Time                3.54
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES             0.122266 Hz
AQ              4.0894465 sec
RG                  40.3
DW                62.400 usec
DE                 6.50 usec
TE                298.0 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                  1H
P1                 12.00 usec
PLW1          13.06000042 W

F2 - Processing parameters
SI                 65536
SF            400.1300295 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



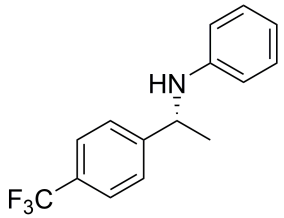

```
Current Data Parameters
NAME       Product-rac-C
EXPNO                 14
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170507
Time                2.50
INSTRUM            spect
PROBHD   5 mm PADUL 13C
PULPROG          zgpg30
TD                 32768
SOLVENT            CDC13
NS                    84
DS                     0
SWH            25252.525 Hz
FIDRES          0.770646 Hz
AQ              0.6488064 sec
RG                   181
DW                19.800 usec
DE                 6.50 usec
TE                298.9 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                  9.40 usec
PLW1         43.63899994 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         13.06000042 W
PLW12         0.25598001 W
PLW13         0.20734000 W

F2 - Processing parameters
SI                 32768
SF           100.6127487 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

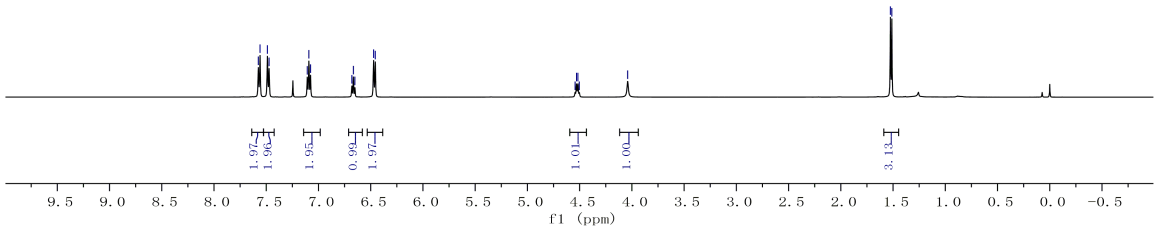


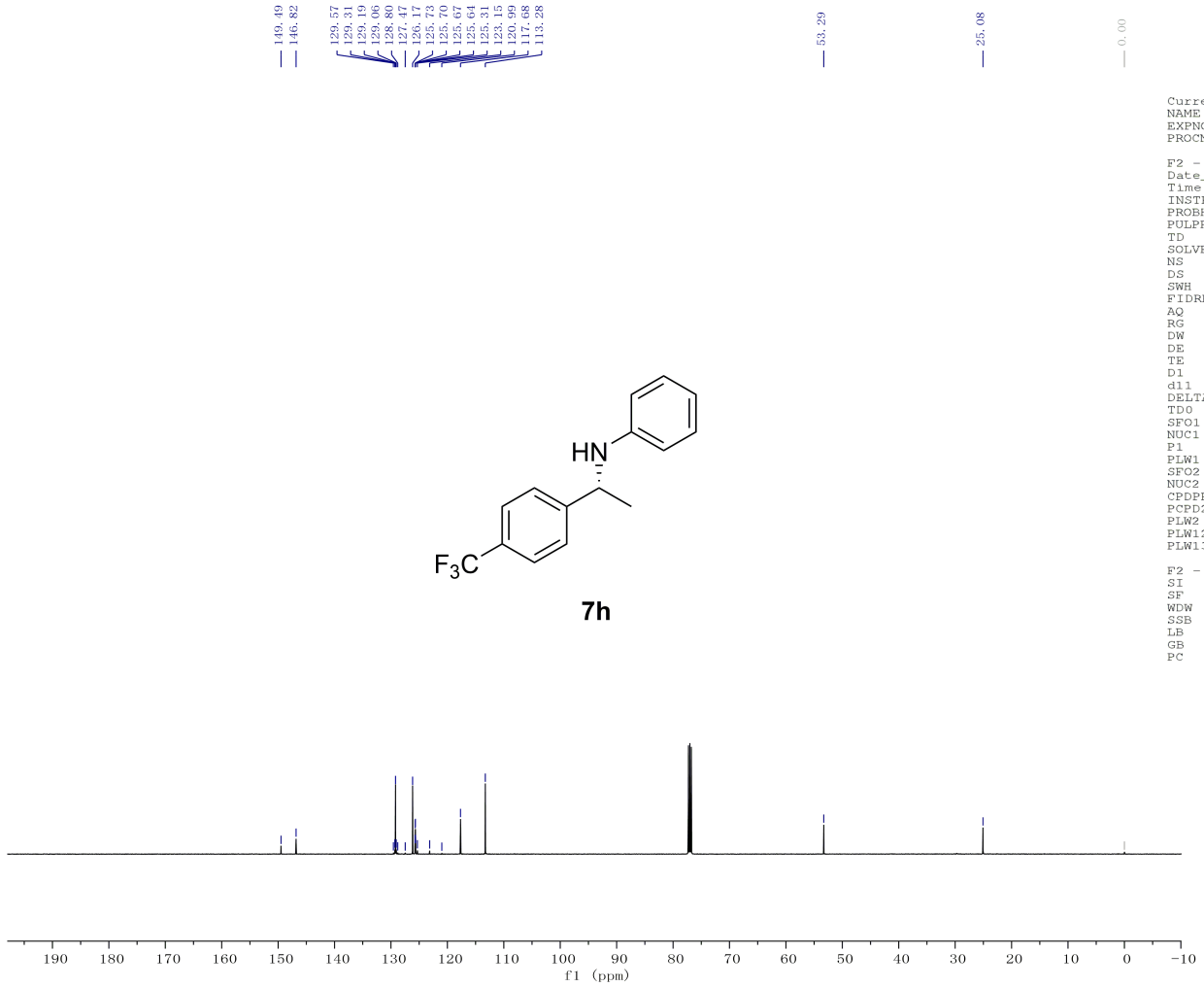
7h

```
Current Data Parameters
NAME       500MHz-H-2018
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180129
Time               14.28
INSTRUM            spect
PROBHD   5 mm CPPBBO BB
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10000.000 Hz
FIDRES             0.152588 Hz
AQ             3.2767999 sec
RG                 31.72
DW                 50.000 usec
DE                  6.50 usec
TE                298.1 K
D1             1.00000000 sec
TD0                    1
SFO1          500.1330885 MHz
NUC1                  1H
P1                 11.50 usec
PLW1          20.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.1300199 MHz
WDW                   EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

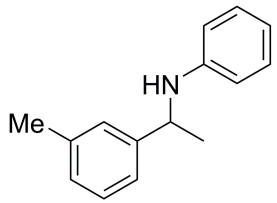





```
Current Data Parameters
NAME       500MHz-C-2018
EXPNO                  9
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180129
Time               14.30
INSTRUM            spect
PROBHD   5 mm CPPBBO BB
PULPROG          zgpg30
TD                65536
SOLVENT            CDC13
NS                   417
DS                     4
SWH            29761.904 Hz
FIDRES          0.454131 Hz
AQ              1.1010048 sec
RG                 192.89
DW                16.800 usec
DE                18.00 usec
TE                298.1 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1
SFO1         125.7703637 MHz
NUC1                13C
P1                 9.80 usec
PLW1          57.00000000 W
SFO2         500.1320005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2             80.00 usec
PLW2          20.00000000 W
PLW12          0.35778001 W
PLW13          0.22898000 W

F2 - Processing parameters
SI                 32768
SF           125.7577907 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



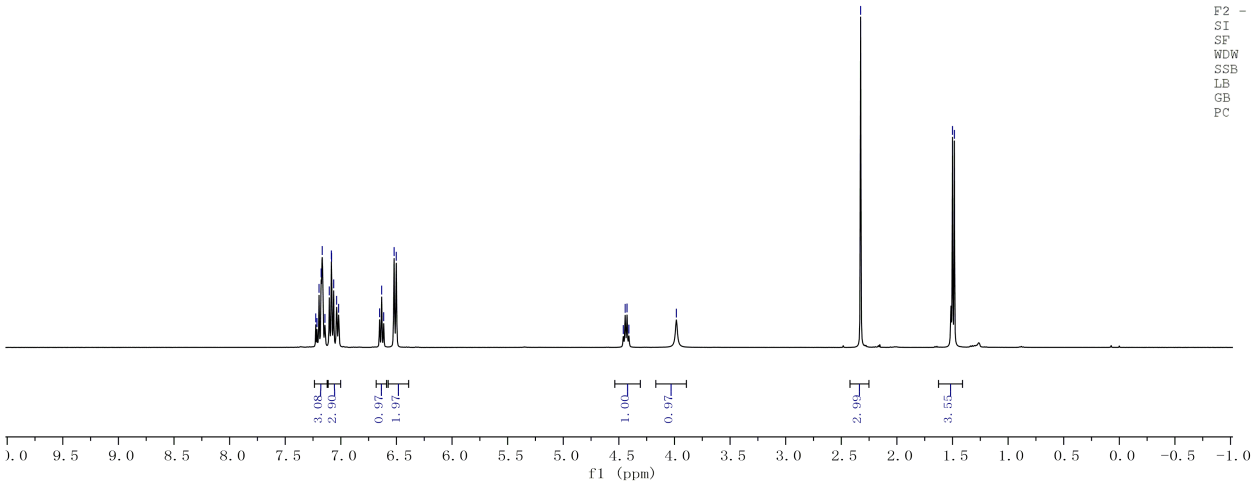
7i

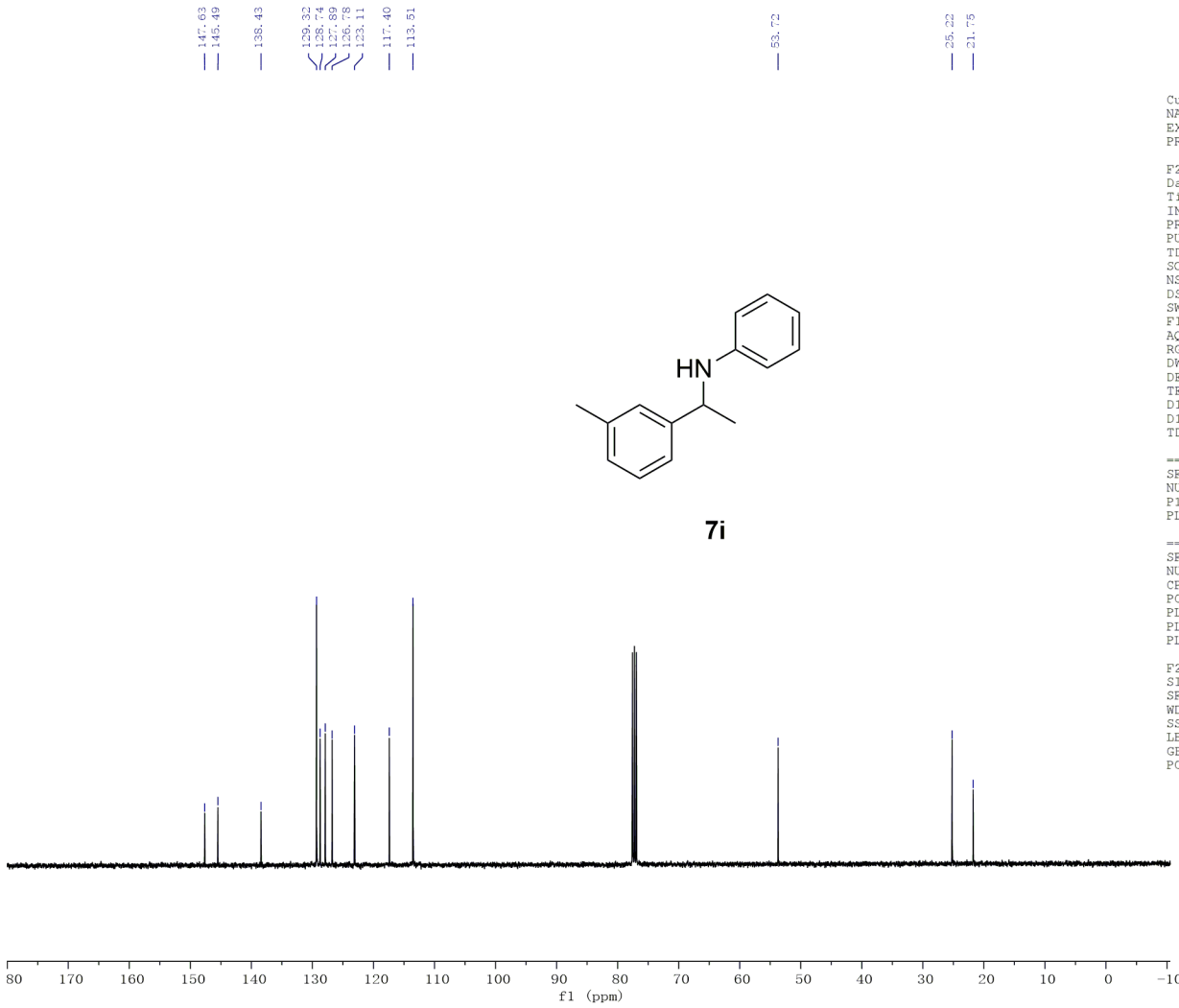
```
Current Data Parameters
NAME       Product-rac-H
EXPNO                 87
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170726
Time              10.10
INSTRUM           spect
PROBHD   5 mm PADUL 13C
PULPROG             zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894465 sec
RG                  161
DW                62.400 usec
DE                 6.50 usec
TE                673.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1               1H
P1                12.00 usec
PLW1         13.06000042 W

F2 - Processing parameters
SI                65536
SF           400.1300232 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```





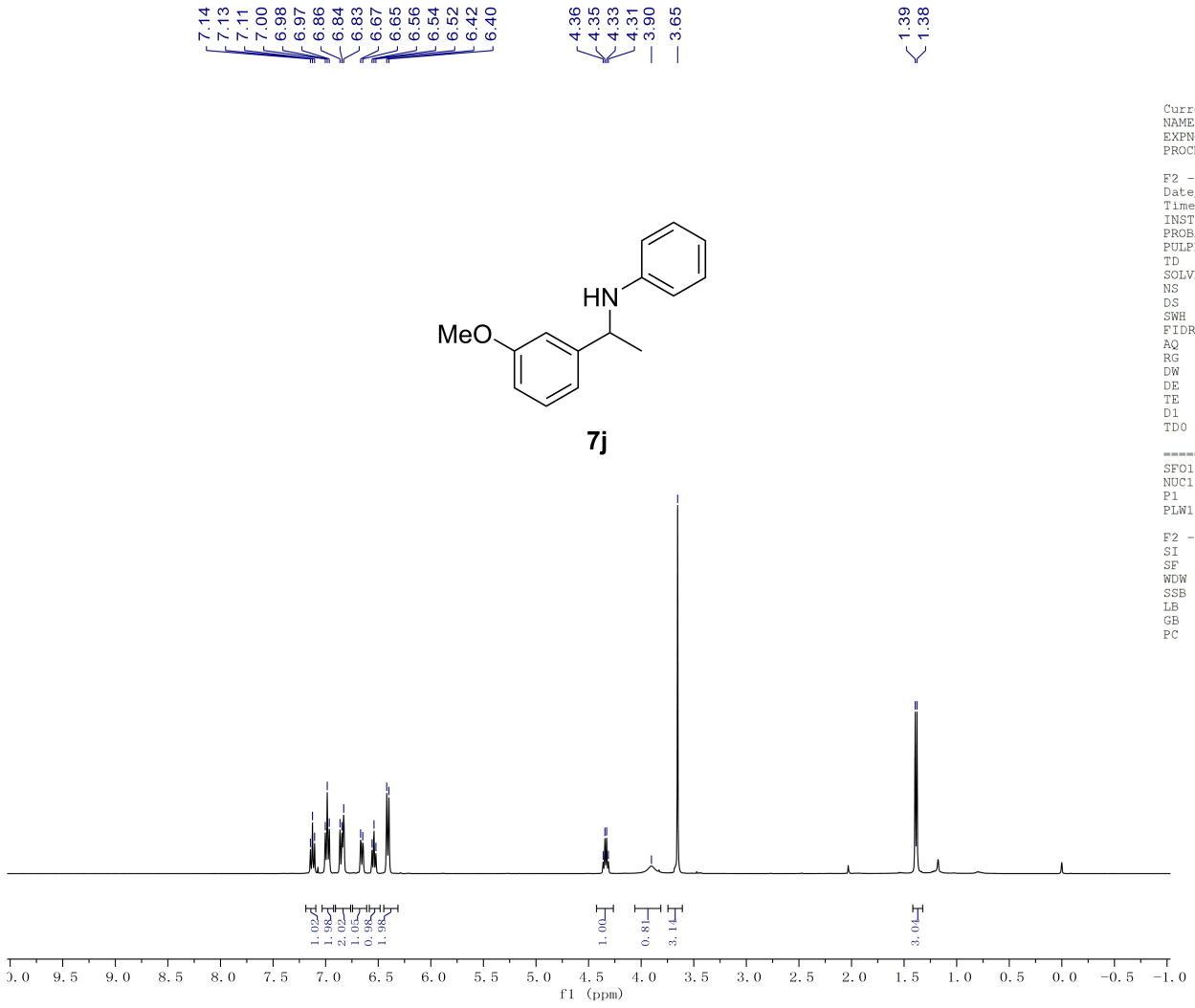

```
Current Data Parameters
NAME      Product-rac-C
EXPNO                26
PROCNO                1

F2 - Acquisition Parameters
Date_          20170726
Time              10.13
INSTRUM           spect
PROBHD   5 mm PADUL 13C
PULPROG         zgpg30
TD              32768
SOLVENT          CDCl3
NS                 273
DS                   0
SWH          25252.525 Hz
FIDRES        0.770646 Hz
AQ            0.6488064 sec
RG                 161
DW              19.800 usec
DE               6.50 usec
TE              673.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1               13C
P1                9.40 usec
PLW1        43.63899994 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2               1H
CPDPRG[2        waltz16
PCPD2            90.00 usec
PLW2        13.06000042 W
PLW12        0.25598001 W
PLW13        0.20734000 W

F2 - Processing parameters
SI                32768
SF          100.6127487 MHz
WDW                EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.40
```

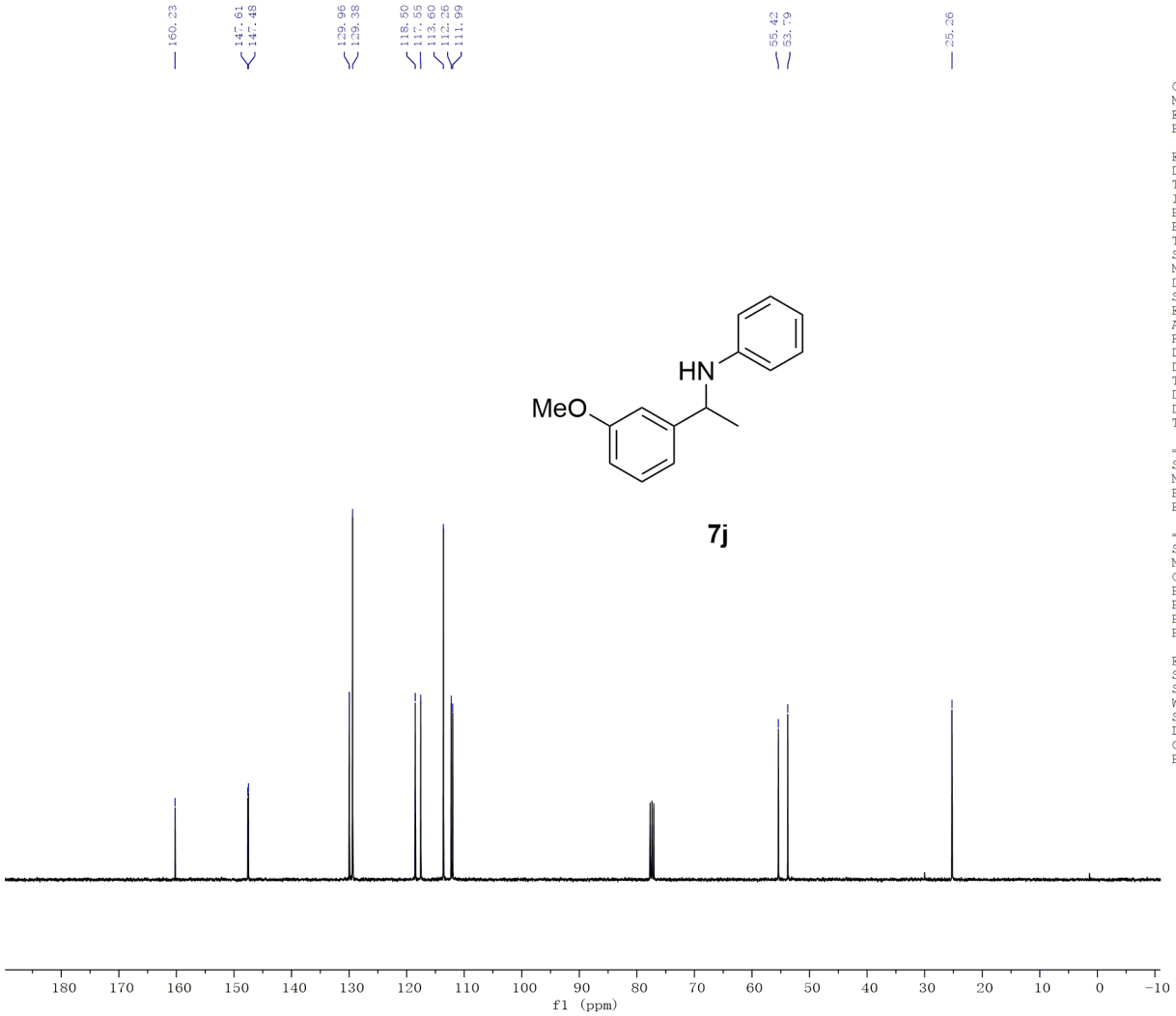



```
Current Data Parameters
NAME      Product-rac-H
EXPNO                85
PROCNO                1

F2 - Acquisition Parameters
Date_          20170726
Time               9.33
INSTRUM           spect
PROBHD   5 mm PADUL 13C
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8012.820 Hz
FIDRES             0.122266 Hz
AQ              4.0894465 sec
RG                    57
DW                62.400 usec
DE                 6.50 usec
TE                673.2 K
D1             1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 12.00 usec
PLW1         13.06000042 W

F2 - Processing parameters
SI                 65536
SF           400.1300836 MHz
WDW                   EM
SSB      0
LB                 0.30 Hz
GB       0
PC                 1.00
```



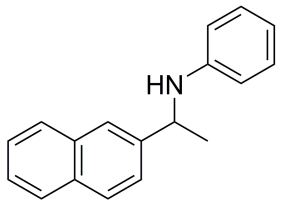

```
Current Data Parameters
NAME      Product-rac-C
EXPNO                24
PROCNO                1

F2 - Acquisition Parameters
Date_          20170726
Time               9.36
INSTRUM           spect
PROBHD   5 mm PADUL 13C
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  106
DS                    0
SWH           25252.525 Hz
FIDRES        0.770646 Hz
AQ            0.6488064 sec
RG                  161
DW               19.800 usec
DE                6.50 usec
TE               673.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

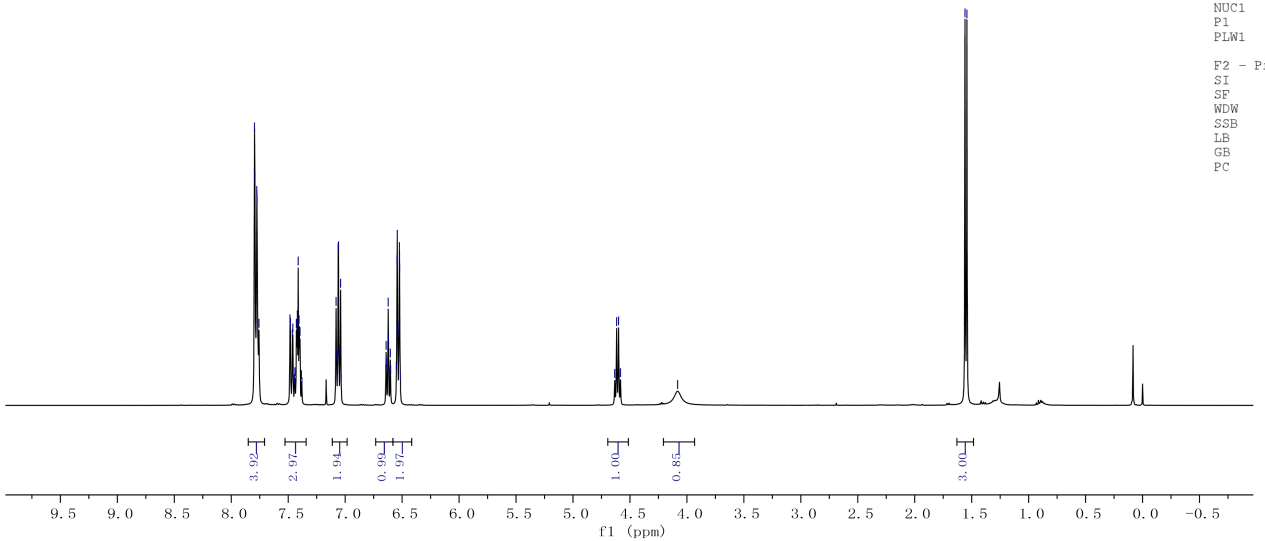
======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                9.40 usec
PLW1         43.63899994 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.06000042 W
PLW12         0.25598001 W
PLW13         0.20734000 W

F2 - Processing parameters
SI                32768
SF           100.6127487 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



7k

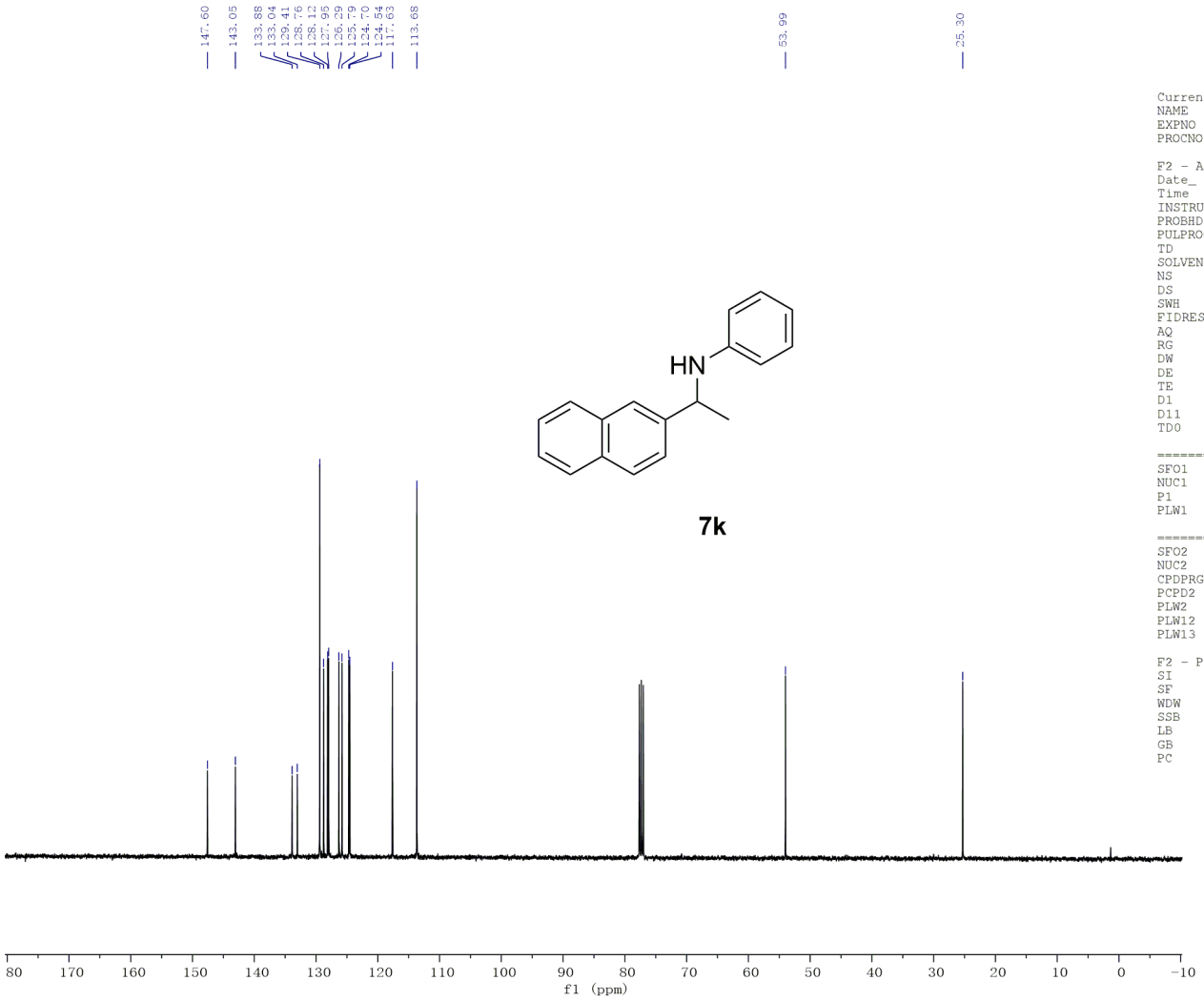



```
Current Data Parameters
NAME      Product-rac-H
EXPNO                66
PROCNO                1

F2 - Acquisition Parameters
Date_          20170512
Time               3.37
INSTRUM           spect
PROBHD   5 mm PADUL 13C
PULPROG             zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894465 sec
RG                   57
DW                62.400 usec
DE                 6.50 usec
TE                298.2 K
D1             1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                 1H
P1                12.00 usec
PLW1         13.06000042 W

F2 - Processing parameters
SI                65536
SF           400.1300467 MHz
WDW                  EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



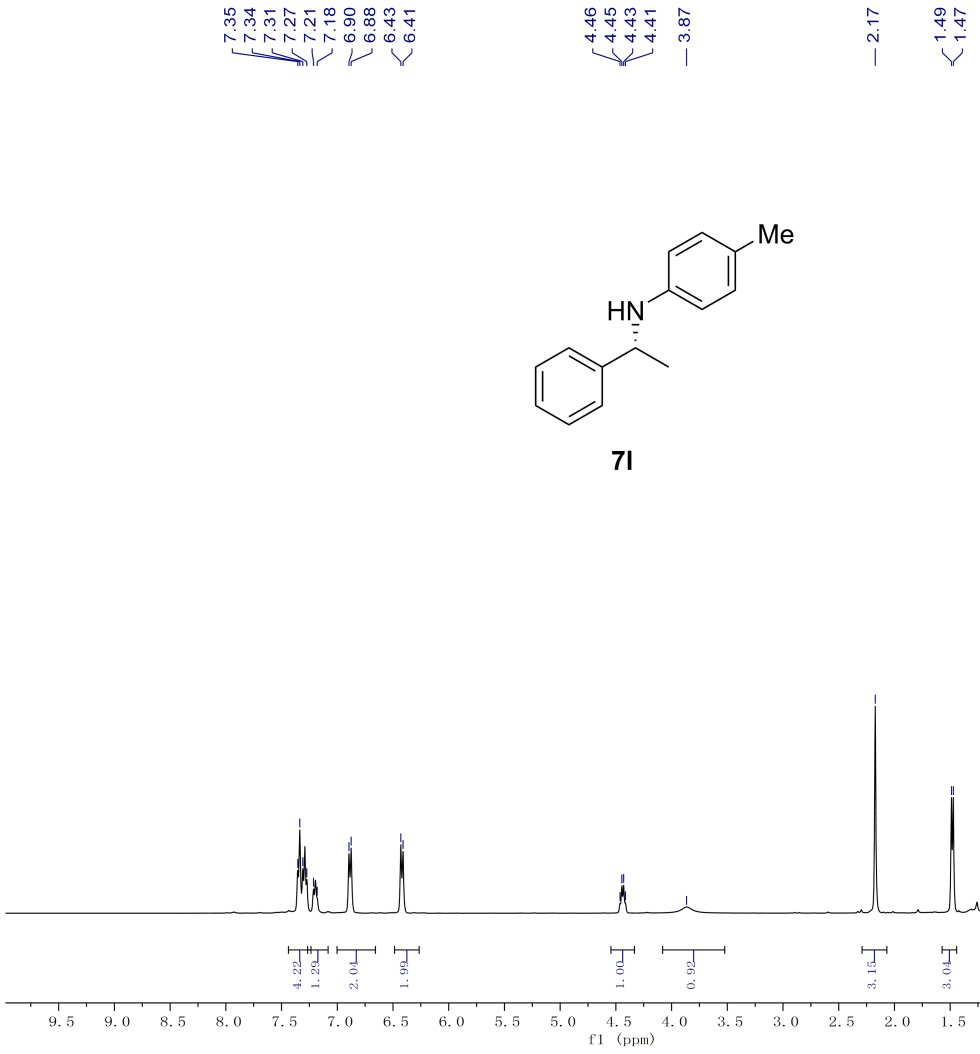

```
Current Data Parameters
NAME      Product-rac-C
EXPNO                21
PROCNO                1

F2 - Acquisition Parameters
Date_          20170512
Time               3.43
INSTRUM           spect
PROBHD   5 mm PADUL 13C
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  204
DS                    0
SWH           25252.525 Hz
FIDRES         0.770646 Hz
AQ            0.6488064 sec
RG                  161
DW               19.800 usec
DE                6.50 usec
TE                298.7 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                13C
P1                9.40 usec
PLW1         43.63899994 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.06000042 W
PLW12         0.25598001 W
PLW13         0.20734000 W

F2 - Processing parameters
SI                 32768
SF           100.6127487 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



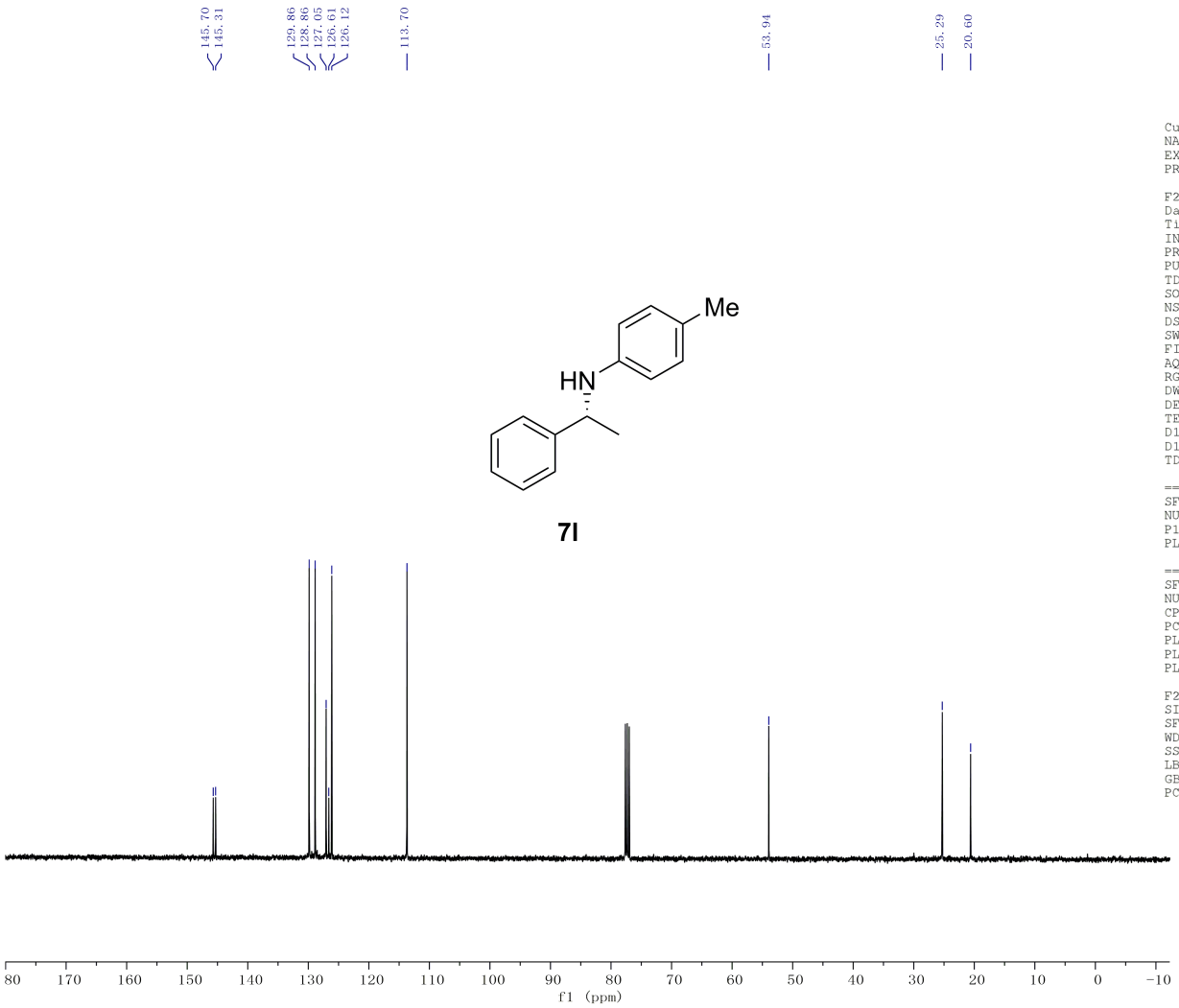
7l

```
Current Data Parameters
NAME      Product-rac-H
EXPNO               77
PROCNO               1

F2 - Acquisition Parameters
Date_          20170616
Time              11.38
INSTRUM           spect
PROBHD   5 mm PADUL 13C
PULPROG             zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES            0.122266 Hz
AQ             4.0894465 sec
RG                   57
DW               62.400 usec
DE                6.50 usec
TE                673.2 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1               1H
P1                12.00 usec
PLW1         13.06000042 W

F2 - Processing parameters
SI                65536
SF           400.1300384 MHz
WDW                EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



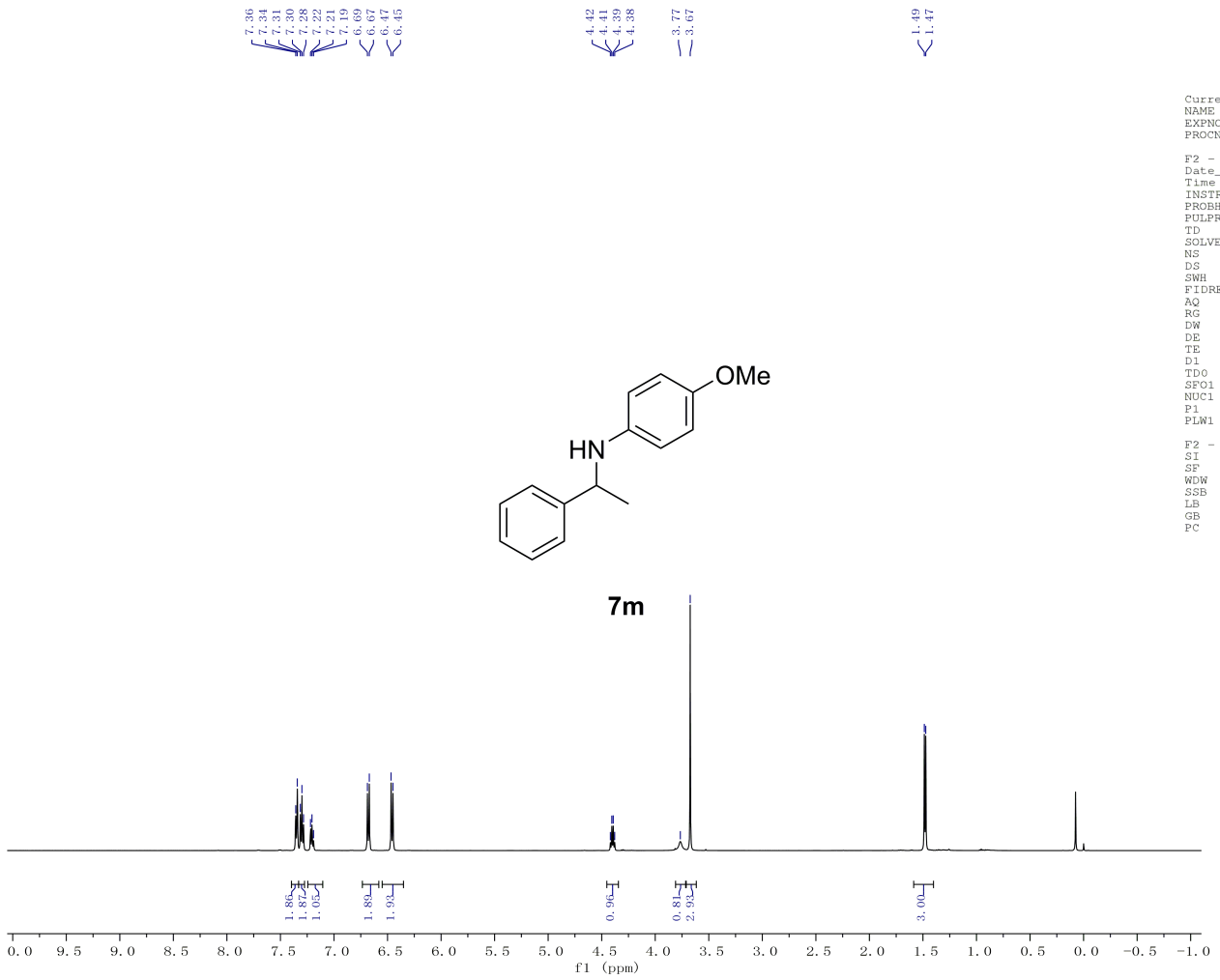

```
Current Data Parameters
NAME      Product-rac-C
EXPNO                22
PROCNO                1

F2 - Acquisition Parameters
Date_          20170616
Time              11.44
INSTRUM           spect
PROBHD   5 mm PADUL 13C
PULPROG         zgpg30
TD                32768
SOLVENT           CDCl3
NS                  138
DS                    0
SWH           25252.525 Hz
FIDRES         0.770646 Hz
AQ             0.6488064 sec
RG                  161
DW               19.800 usec
DE                6.50 usec
TE                673.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         100.6228298 MHz
NUC1                 13C
P1                  9.40 usec
PLW1         43.63899994 W

======== CHANNEL f2 ========
SFO2         400.1316005 MHz
NUC2                 1H
CPDPRG[2         waltz16
PCPD2              90.00 usec
PLW2         13.06000042 W
PLW12         0.25598001 W
PLW13         0.20734000 W

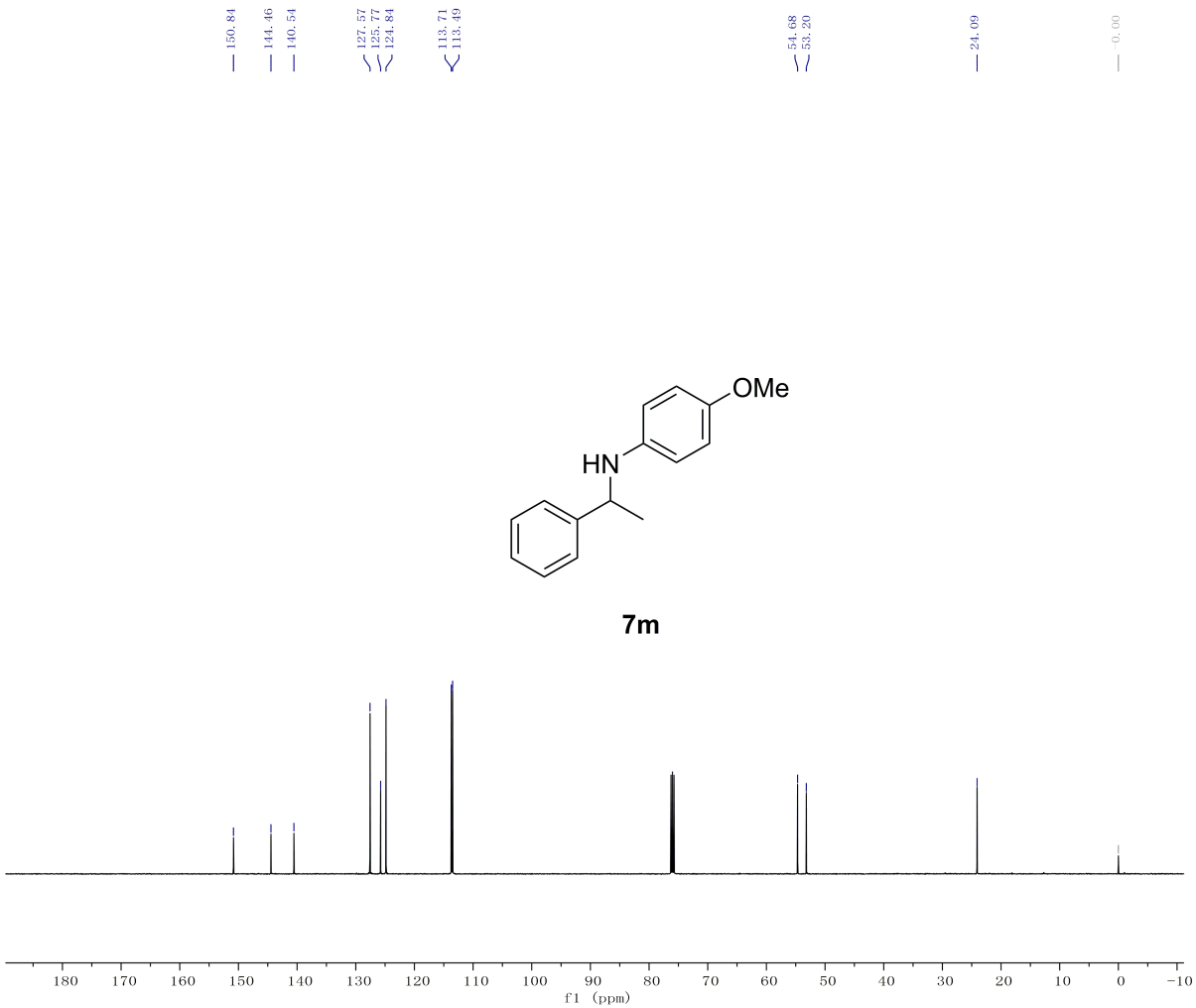
F2 - Processing parameters
SI                32768
SF           100.6127487 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```




```
Current Data Parameters
NAME       500MHz-H-2018
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180129
Time               9.23
INSTRUM            spect
PROBHD   5 mm CPPBBO BB
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10000.000 Hz
FIDRES         0.152588 Hz
AQ             3.2767999 sec
RG                 31.72
DW                50.000 usec
DE                 6.50 usec
TE                298.1 K
D1             1.00000000 sec
TD0                    1
SFO1          500.1330885 MHz
NUC1                  1H
P1                11.50 usec
PLW1          20.00000000 W

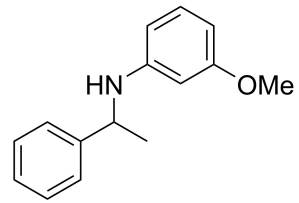
F2 - Processing parameters
SI                 65536
SF            500.1300332 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```




```
Current Data Parameters
NAME       500MHz-C-2018
EXPNO                  8
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180129
Time               9.43
INSTRUM           spect
PROBHD   5 mm CPPBBO BB
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  100
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                192.89
DW                16.800 usec
DE                18.00 usec
TE                298.2 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   1
SFO1         125.7703637 MHz
NUC1                 13C
P1                 9.80 usec
PLW1         57.00000000 W
SFO2         500.1320005 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             80.00 usec
PLW2         20.00000000 W
PLW12         0.35778001 W
PLW13         0.22898000 W

F2 - Processing parameters
SI                 32768
SF           125.7579251 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```



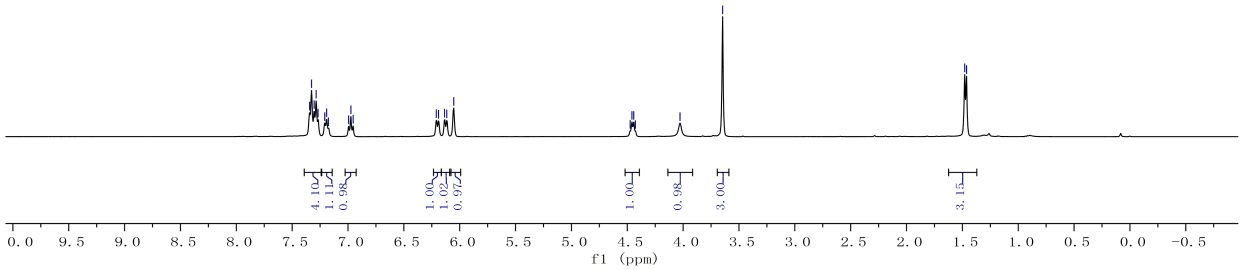
7n

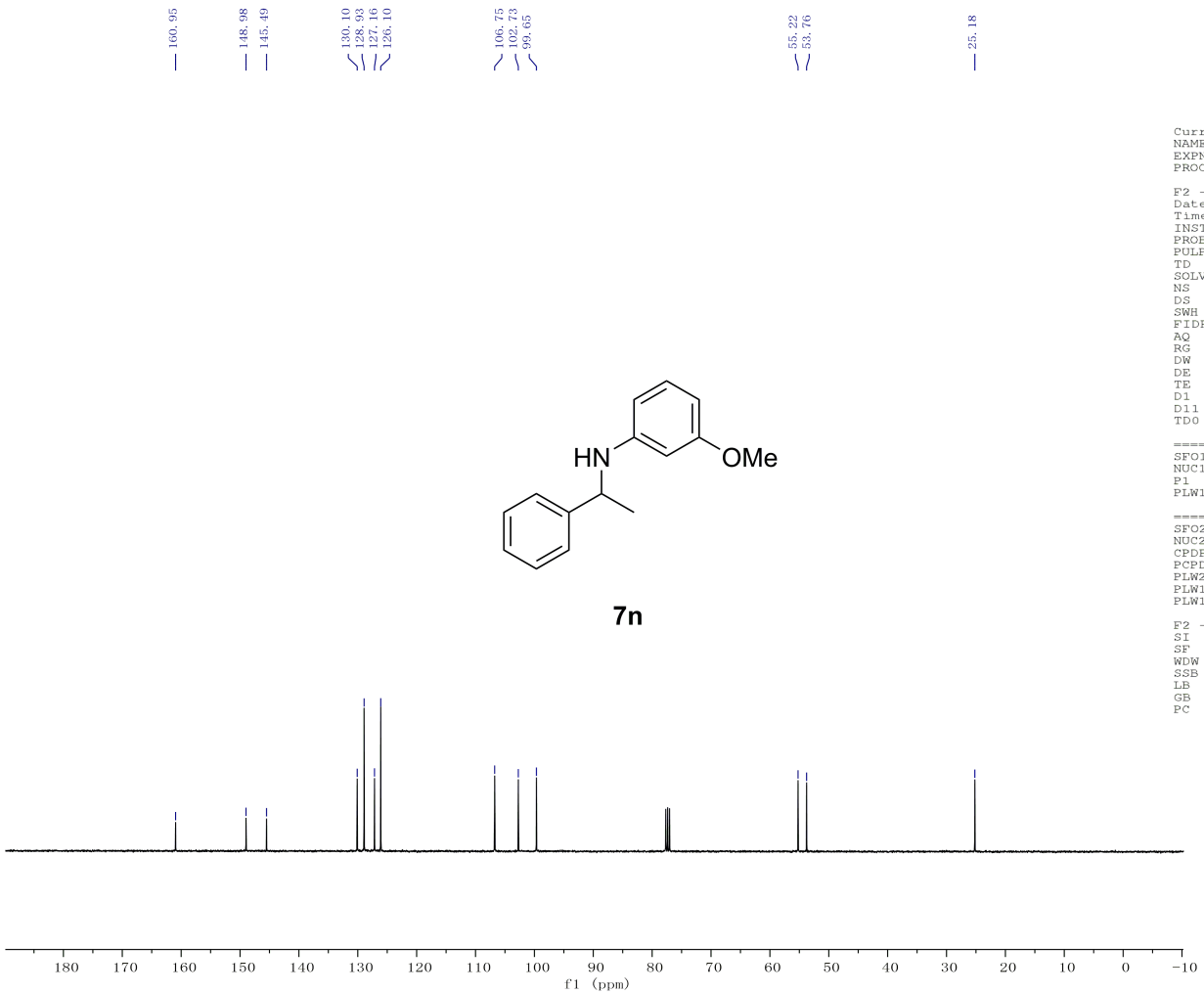
```
Current Data Parameters
NAME       Product-rac-H
EXPNO                 78
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170616
Time              11.51
INSTRUM           spect
PROBHD   5 mm PADUL 13C
PULPROG             zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8012.820 Hz
FIDRES         0.122266 Hz
AQ             4.0894465 sec
RG                   57
DW                62.400 usec
DE                 6.50 usec
TE                673.2 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                 1H
P1                12.00 usec
PLW1         13.06000042 W

F2 - Processing parameters
SI                65536
SF           400.1300457 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```





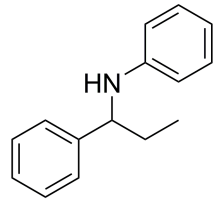

```
Current Data Parameters
NAME       Product-rac-C
EXPNO                 23
PROCNO                 1

F2 - Acquisition Parameters
Date_           20170616
Time               11.55
INSTRUM             spect
PROBHD   5 mm PADUL 13C
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  101
DS                    0
SWH           25252.525 Hz
FIDRES         0.770646 Hz
AQ            0.6488064 sec
RG                  161
DW               19.800 usec
DE                6.50 usec
TE               673.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                 9.40 usec
PLW1         43.63899994 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             90.00 usec
PLW2         13.06000042 W
PLW12         0.25598001 W
PLW13         0.20734000 W

F2 - Processing parameters
SI                32768
SF          100.6127487 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

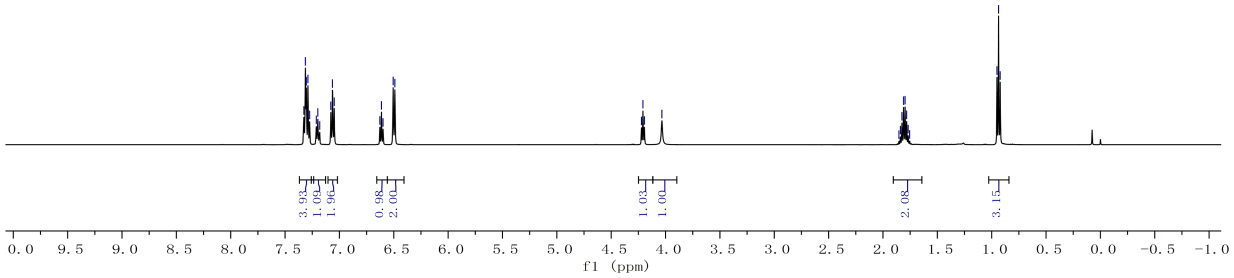


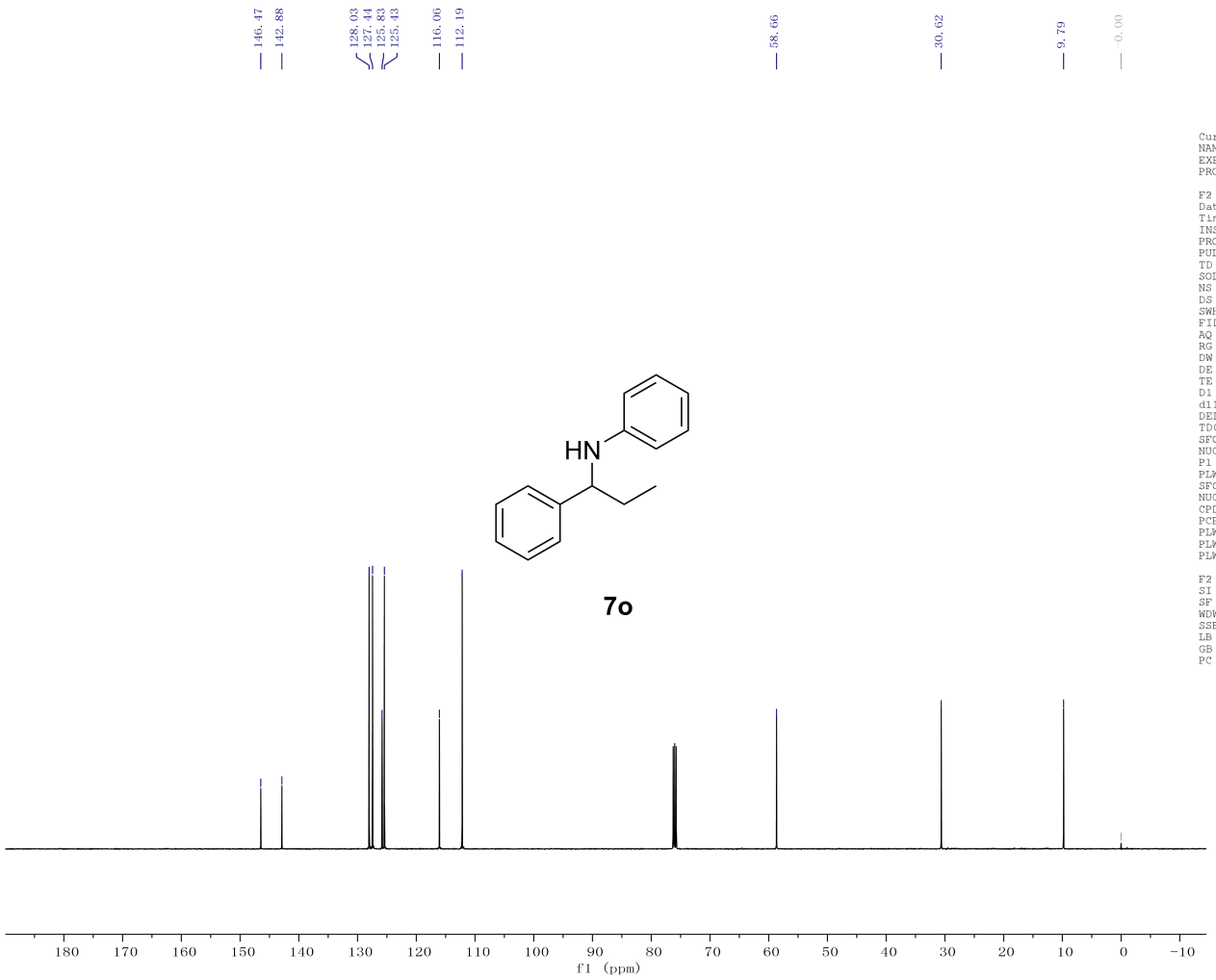
7o

```
Current Data Parameters
NAME       500MHz-H-2018
EXPNO                  9
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180129
Time                9.20
INSTRUM             spect
PROBHD   5 mm CPPBBO BB
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10000.000 Hz
FIDRES             0.152588 Hz
AQ             3.2767999 sec
RG                 25.06
DW                50.000 usec
DE                 6.50 usec
TE                298.1 K
D1             1.00000000 sec
TD0                    1
SFO1           500.1330885 MHz
NUC1                   1H
P1                11.50 usec
PLW1          20.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.1300513 MHz
WDW                    EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```






```
Current Data Parameters
NAME       500MHz-C-2018
EXPNO                 7
PROCNO                1

F2 - Acquisition Parameters
Date_          20180129
Time               9.36
INSTRUM           spect
PROBHD    5 mm CPPBBO BB
PULPROG         zgpg30
TD               65536
SOLVENT           CDCl3
NS                   83
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG               192.89
DW              16.800 usec
DE              18.00 usec
TE              298.1 K
D1           2.00000000 sec
d11          0.03000000 sec
DELTA        1.89999998 sec
TD0                   1
SFO1        125.7703637 MHz
NUC1                13C
P1               9.80 usec
PLW1        57.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2        waltz16
PCPD2           80.00 usec
PLW2        20.00000000 W
PLW12        0.35778001 W
PLW13        0.22898000 W

F2 - Processing parameters
SI                32768
SF          125.7579304 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```