Electronic Supplementary Information (ESI)

Direct carboxamidation of indoles by palladium-catalyzed C−H activation and isocyanide insertion

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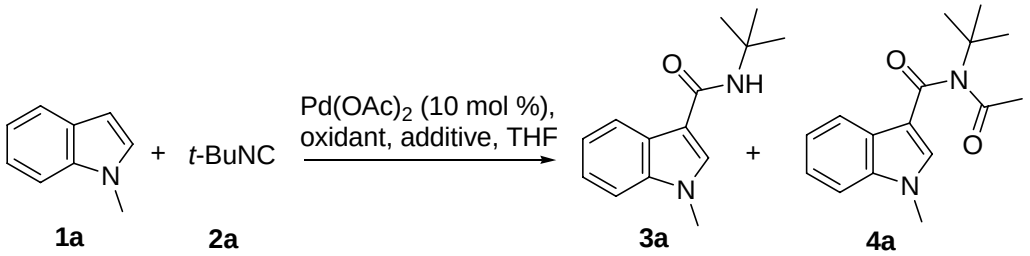
Table of Contents

I. General information

All reagents were purchased without further purification unless otherwise noted. Reactions were monitored using thin-layer chromatography (TLC) on commercial silica gel plates (GF254). Visualization of the developed plates was performed under UV light (254 nm). Flash column chromatography was performed on silica gel (200-300 mesh). ^{1}H and ^{13}C NMR spectra were recorded on a 400 or 500 MHz spectrometer. Chemical shifts (δ) are reported in ppm referenced to an internal tetramethylsilane standard or the DMSO-d_6 residual peak (δ 2.50) for ^{1}H NMR. Chemical shifts of ^{13}C NMR are reported relative to $CDCl_3$ (δ 77.0) or DMSO-d_6 (δ 39.5). The following abbreviations were used to describe peak splitting patterns when appropriate: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Coupling constants, *J*, were reported in Hertz unit (Hz). High resolution mass spectra (HRMS) were obtained on an ESI-LC-MS/MS spectrometer.

II. Screening of the reaction conditions



1a **2a** **3a** **4a**

entry	oxidant (equiv)	additive (equiv)	solvent	T/°C	yield (%)[b]	
					3a	**4a**
1	$Cu(OAc)_2$ (1)	--	AcOH	110	54	n.d.
2	$Cu(OAc)_2$ (1)	--	Toluene	110	n.d.	67
3	$Cu(OAc)_2$ (1)	--	THF	110	4	82
4	$AgOA_C$ (1)	--	AcOH	110	37	n.d.
5	CuO (1)	--	AcOH	110	n.r.	n.r.
6	O_2	--	AcOH	110	10[c]	n.d.
7	BQ (1)	--	AcOH	110	26	n.d.
8	$K_2S_2O_8$ (1)	--	AcOH	110	19	n.d.

9	$PhI(OAc)_2$ (1)	--	AcOH	110	n.d.	n.d.
10	Oxone (1)	--	AcOH	110	n.d.	n.d.
11[e]	$Cu(OAc)_2$ (1)	*p*-TsOH (2)	Toluene	110	23	35
12	$Cu(OAc)_2$ (1)	PivOH (2)	Toluene	110	n.d.	n.d.
13	$Cu(OAc)_2$ (1)	AcOH (2)	Toluene	110	10	68
14	$Cu(OAc)_2$ (1)	TFA (2)	Toluene	110	59	n.d.
15	$Cu(OAc)_2$ (1)	TFA (2)	Toluene	90	68	n.d.
16	$Cu(OAc)_2$ (1)	TFA (1)	Toluene	90	65	5
17	$Cu(OAc)_2$ (1)	TFA (0.5)	Toluene	90	21	37
18	$Cu(OAc)_2$ (1)	TFA (0.2)	Toluene	90	7	53
19	$Cu(OAc)_2$ (1)	TFA (1)	Toluene	70	69	5
20	$Cu(OAc)_2$ (1)	TFA (1)	DCE	70	72	n.d.
21	$Cu(OAc)_2$ (1)	TFA (1)	*t*-BuOH	70	87	n.d.
22	$Cu(OAc)_2$ (1)	TFA (1)	THF	70	89	5
23	$Cu(OAc)_2$ (1)	TFA (1.2)	THF	70	**94**	n.d.
24[d]	**$Cu(OAc)_2$ (1)**	**TFA (1.2)**	**THF**	**70**	**89**	**n.d.**

Reaction conditions: [a] **1a** (0.2 mmol), **2a** (0.24 mmol), $Pd(OAc)_2$ (10 mol %), oxidant (1.0 equiv), H_2O (5 equiv), solvent (1 mL), 1.5 h. [b] Isolated yield. [c] 30 h. [d] 5 mol % of $Pd(OAc)_2$.

III. General procedures and characterization of the products

General procedures

General procedure for the synthesis of 3

A mixture of substrate **1** (0.4 mmol), isocyanide **2** (0.48 mmol, 1.2 equiv), $Pd(OAc)_2$ (4.5 mg, 0.02 mmol, 5 mol %), $Cu(OAc)_2$ (73.2 mg, 0.4 mmol, 1 equiv), TFA (0.48 mmol, 1.2 equiv), H_2O (36 mg, 2 mmol, 5 equiv) in THF (2.0 mL) was stirred in a sealed tube under air atmosphere at 70 ^oC. The reaction was cooled down to room temperature after complete consumption of the starting material as being monitored by TLC. Saturated NH_4OH (10 mL) and EtOAc (10 mL) were added to the reaction mixture successively. The organic phase was separated, and the aqueous phase was further extracted with EtOAc (2 × 10 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated. The residue was purified by flash chromatography to provide the desired product **3**.

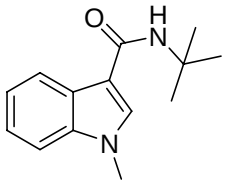
General procedure for the synthesis of 4

A mixture of substrate **1** (0.4 mmol), isocyanide **2** (0.48 mmol, 1.2 equiv), $Pd(OAc)_2$ (9 mg, 0.04 mmol, 10 mol %), $Cu(OAc)_2$ (73.2 mg, 0.4 mmol, 1 equiv), in

THF (2.0 mL) was stirred in a sealed tube under air atmosphere at 90 °C. The reaction was cooled down to room temperature after complete consumption of the starting material as being monitored by TLC. Saturated aqueous NH_4OH (10 mL) and EtOAc (10 mL) were added to the reaction mixture successively. The organic phase was separated, and the aqueous phase was further extracted with EtOAc (2 × 10 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and concentrated. The residue was purified by flash chromatography to provide the products **4** (major) and **3** (minor).

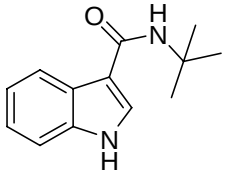
Characterization of the products

***N-tert*-butyl-1-methyl-1*H*-indole-3-carboxamide (3a)**



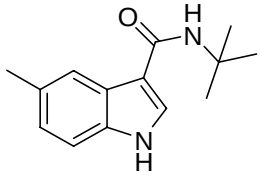
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.87-7.89 (m, 1H), 7.61 (s, 1H), 7.34 (d, *J* = 7.2 Hz, 1H), 7.23-7.32 (m, 1H), 5.88 (br, 1H), 3.78 (s, 1H), 1.51(s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.6, 137.2, 132.2, 125.1, 122.3, 121.2, 119.7, 112.1, 110.0, 51.3, 33.1, 29.2; HRMS (ESI): Exact mass calcd for $C_{14}H_{19}N_2O$ $[M+H]^+$ 231.1492, Found 231.1495.

***N-tert*-butyl-1*H*-indole-3-carboxamide (3b)[1]**



^{1}H NMR (400 MHz, $CDCl_3$) δ 10.24 (br, 1H), 7.83-7.85 (m, 1H), 7.62 (d, *J* = 2.8 Hz, 1H), 7.42-7.44 (m, 1H), 7.20-7.23 (m, 2H), 5.79 (s, 1H), 1.55 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.7, 136.7, 128.6, 124.3, 122.5, 121.2, 119.0, 112.8, 112.5, 51.5, 29.3; HRMS (ESI): Exact mass calcd for $C_{13}H_{17}N_2O$ $[M+H]^+$ 217.1335, Found 217.1337.

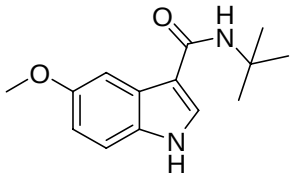
***N-tert*-butyl-5-methyl-1*H*-indole-3-carboxamide (3c)**



^{1}H NMR (400 MHz, $CDCl_3$) δ 10.13 (br, 1H), 7.65 (s, 1H), 7.54 (d, *J* = 2.8 Hz, 1H), 7.29 (d, *J* = 8 Hz 1H), 7.02 (dd, *J* = 8, 0.8 Hz, 1H), 5.94 (br, 1H), 2.45 (s, 3H), 1.54 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.8, 135.0, 130.5, 128.4, 124.6, 118.9, 112.1, 51.4, 29.2; HRMS (ESI): Exact mass

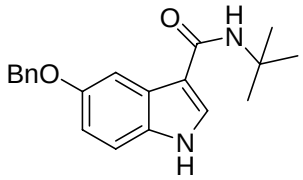
calcd for $C_{14}H_{18}N_2ONa$ $[M+Na]^+$ 253.1311, Found 253.1313.

***N-tert*-butyl-5-methoxy-1*H*-indole-3-carboxamide (3d)**



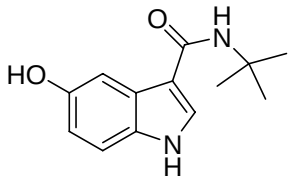
^{1}H NMR (400 MHz, DMSO-d_6) δ 11.33 (br, 1H), 8.02 (d, *J* = 2.8 Hz, 1H), 7.65 (d, *J* = 2.4 Hz, 1H), 7.28 (d, *J* = 8.8 Hz, 1H), 7.09 (br, 1H), 6.76 (dd, *J* = 8.8, 2.4 Hz, 1H), 3.76 (s, 3H), 1.40 (s, 9H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 164.6, 154.1, 130.1, 127.8, 126.8, 112.0, 111.7, 111.1, 102.7, 55.1, 50.0, 28.9; HRMS (ESI): Exact mass calcd for $C_{14}H_{19}N_2O_2$ $[M+H]^+$ 247.1441, Found 247.1440.

***N-tert*-butyl-5-(benzyloxy)-1*H*-indole-3-carboxamide (3e)**



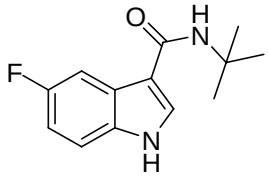
^{1}H NMR (400 MHz, DMSO-d_6) δ 11.38 (br, 1H), 8.05 (d, *J* = 2.8 Hz, 1H), 7.77 (d, *J* = 2.0 Hz, 1H), 7.48 (d, *J* = 7.6 Hz, 2H), 7.39 (t, *J* = 7.2 Hz, 2H), 7.32 (t, *J* = 8.8 Hz, 2H), 7.12 (s, 1H), 6.85 (dd, *J* = 8.8, 2.0 Hz, 1H), 5.09 (s, 1H), 1.40 (s, 9H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 164.6, 153.2, 137.6, 131.2, 128.1, 127.9, 127.3, 127.3, 126.8, 112.3, 112.1, 111.2, 104.3, 69.7, 50.0, 28.9; HRMS (ESI): Exact mass calcd for $C_{20}H_{23}N_2O_2$ $[M+H]^+$ 323.1754, Found 323.1756.

***N-tert*-butyl-5-hydroxy-1*H*-indole-3-carboxamide (3f)**



^{1}H NMR (400 MHz, DMSO-d_6) δ 11.12 (br, 1H), 8.37 (s, 1H), 7.92 (d, *J* = 3.2 Hz, 1H), 7.49 (d, *J* = 2.4 Hz, 1H), 7.17 (d, *J* = 8.8 Hz, 1H), 6.98 (br, 1H), 6.62 (dd, *J* = 8.4, 2.4 Hz, 1H), 1.38 (s, 9H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 164.8, 151.6, 130.4, 127.8, 127.2, 111.9, 111.8, 110.7, 105.2, 50.1, 29.1; HRMS (ESI): Exact mass calcd for $C_{13}H_{17}N_2O_2$ $[M+H]^+$ 233.1285, Found 233.1286.

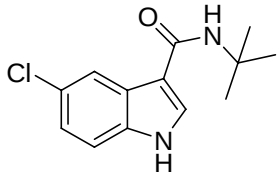
***N-tert*-butyl-5-fluoro-1*H*-indole-3-carboxamide (3g)**



^{1}H NMR (400 MHz, DMSO-d_6) δ 11.60 (br, 1H), 8.16 (d, *J* = 2.8 Hz), 7.82 (dd, *J* = 10.4, 2.4 Hz,

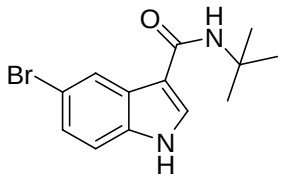
1H), 7.40 (dd, *J* = 8.8, 4.4 Hz, 1H), 7.22 (br, 1H), 6.95-7.00 (m, 1H), 1.39 (s, 9H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 164.2, 158.7, 156.4, 132.6, 129.2, 126.8, 126.7, 112.5, 112.4, 11.6, 111.6, 109.8, 109.5, 105.7, 105.4, 50.1, 28.9; HRMS (ESI): Exact mass calcd for $C_{13}H_{15}FN_2ONa$ $[M+Na]^+$ 257.1061, Found 257.1062.

N-tert-butyl-5-chloro-1_H_-indole-3-carboxamide (3h)



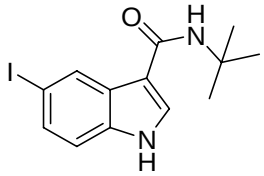
^{1}H NMR (400 MHz, DMSO-d_6) δ 11.67 (br, 1H), 8.14 (d, *J* = 8.8 Hz, 1H), 8.13 (d, *J* = 2.0 Hz, 1H), 7.41 (d, *J* = 8.8 Hz, 1H), 7.26 (br, 1H), 7.13 (dd, *J* = 8.4, 2.0 Hz, 1H), 1.39, (s, 9H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 164.0, 134.4, 128.9, 127.4, 124.8, 121.5, 120.1, 113.0, 111.2, 50.1, 28.8; HRMS (ESI): Exact mass calcd for $C_{13}H_{16}ClN_2O$ $[M+H]^+$ 251.0946, Found 251.0945.

N-tert-butyl-5-bromo-1_H_-indole-3-carboxamide (3i)



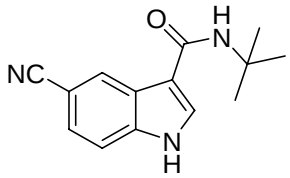
^{1}H NMR (400 MHz, DMSO-d_6) δ 11.67 (br, 1H), 8.29 (d, 1.6 Hz, 1H), 8.12 (d, *J* = 2.8 Hz, 1H), 7.37 (d, *J* = 8.8 Hz, 1H), 7.23-7.26 (m, 2H), 1.39 (s, 9H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 164.0, 134.6, 128.7, 128.1, 124.0, 123.2, 113.5, 112.8, 111.0, 50.1, 40.1, 28.8; HRMS (ESI): Exact mass calcd for $C_{13}H_{16}BrN_2O$ $[M+H]^+$ 295.0441, Found 295.0442.

N-tert-butyl-5-iodo-1_H_-indole-3-carboxamide (3j)



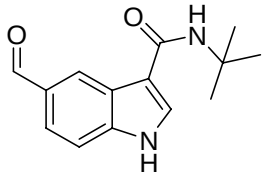
^{1}H NMR (400 MHz, DMSO-D_6) δ 11.64 (br, 1H), 8.50 (d, *J* = 2.8 Hz, 1H), 8.07 (d, *J* = 2.4 Hz, 1H), 7.39 (dd, *J* = 8.4, 2.0 Hz, 1H), 7.24-7.27 (m, 2H), 1.39 (s, 9H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 164.0,135.0, 129.5, 129.4, 128.2, 113.9, 110.7, 84.1, 50.1, 40.1, 28.8; HRMS (ESI): Exact mass calcd for $C_{13}H_{16}IN_2O$ $[M+H]^+$ 343.0302, Found 343.0301.

N-tert-butyl-5-cyano-1_H_-indole-3-carboxamide (3k)



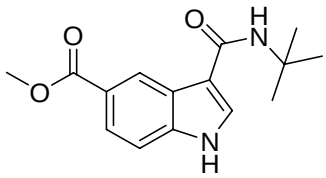
^{1}H NMR (400 MHz, DMSO-d_6) δ 12.02(br, 1H), 8.54 (d, *J* = 0.8 Hz, 1H), 8.28 (d, *J* = 2.4 Hz), 7.58 (d, 8.4 Hz, 1H), 7.48 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.40 (br, 1H), 1.40 (s, 9H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 164.2, 138.3, 130.5, 127.0, 126.7, 124.9, 120.9, 112.6, 112.2, 103.0, 50.9, 29.4; HRMS (ESI): Exact mass calcd for $C_{14}H_{15}N_3ONa$ $[M+Na]^+$ 264.1107, Found 264.1108.

N-tert-butyl-5-formyl-1_H_-indole-3-carboxamide (3l)



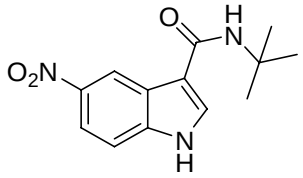
^{1}H NMR (400 MHz, DMSO-d_6) δ 11.94 (br, 1H), 10.01 (s, 1H), 8.74 (d, *J* = 1.2 Hz, 1H), 8.20 (d, *J* = 2.4 Hz, 1H), 7.67 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.56 (d, *J* = 8.4 Hz, 1H), 7.38 (br, 1H), 1.41 (s, 9H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 192.6, 163.9, 139.3, 129.8, 129.3, 126.5, 126.2, 121.4, 113.1, 112.3, 50.3, 28.9; HRMS (ESI): Exact mass calcd for $C_{14}H_{16}N_2O_2Na$ $[M+Na]^+$ 267.1104, Found 267.1106.

methyl 3-(_tert_-butylcarbamoyl)-1_H_-indole-5-carboxylate (3m)



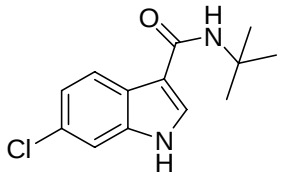
^{1}H NMR (400 MHz, DMSO-d_6) δ 11.81(br, 1H), 8.88 (d, *J* = 1.2 Hz, 1H), 8.19 (d, *J* = 2.8 Hz, 1H), 7.76 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.49 (d, *J* = 8.8 Hz, 1H), 7.31 (br, 1H), 3.86 (s, 3H), 1.41 (s, 9H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 167.1, 163.9, 138.5, 128.9, 125.9, 123.7, 122.5, 121.6, 112.6, 111.4, 51.4, 50.2, 38.9, 25.8; HRMS (ESI): Exact mass calcd for $C_{15}H_{19}N_2O_3$ $[M+H]^+$ 275.1390, Found 275.1391.

N-tert-butyl-5-nitro-1_H_-indole-3-carboxamide (3n)



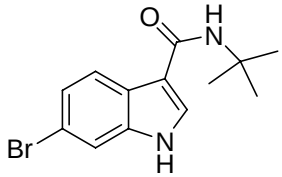
^{1}H NMR (400 MHz, DMSO-d_6) δ 12.15 (br, 1H), 9.08 (d, *J* = 2.0 Hz, 1H), 8.33 (d, *J* = 0.8 Hz, 1H), 8.03 (dd, *J* = 7.2, 1.6 Hz, 1H), 7.60 (d, *J* = 7.2 Hz, 1H), 7.48 (br, 1H), 1.41 (s, 9H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 163.5, 141.6, 139.1, 125.9, 118.0, 117.1, 113.4, 112.3, 50.5, 28.9; HRMS (ESI): Exact mass calcd for $C_{13}H_{16}N_3O_3$ $[M+H]^+$ 262.1186, Found 262.1188.

N-tert-butyl-6-chloro-1_H_-indole-3-carboxamide (3o)



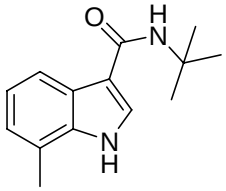
^{1}H NMR (400 MHz, DMSO-d_6) δ 11.58 (br, 1H), 8.09-8.12 (m, 1H), 7.45 (d, *J* = 1.6 Hz, 1H), 7.23 (br, 1H), 7.08 (dd, *J* = 8.4, 1.6 Hz, 1H), 1.39 (s, 9H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 164.0, 136.3, 128.3, 126.2, 125.0, 122.2, 120.2 11.7, 111.1, 50.1, 40.1, 28.8; HRMS (ESI): Exact mass calcd for $C_{13}H_{16}ClN_2O$ $[M+H]^+$ 251.0947, Found 251.0946.

N-tert-butyl-6-bromo-1_H_-indole-3-carboxamide (3p)



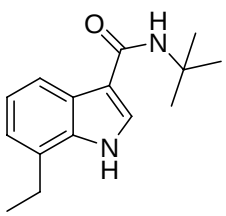
^{1}H NMR (400 MHz, DMSO-d_6) δ 11.59 (br, 1H), 8.09 (d, *J* = 2.8 Hz, 1H), 8.08 (d, *J* = 8.8 Hz, 1H), 7.60 (d, *J* = 1.6 Hz, 1H), 7.25 (s, 1H), 7.22 (dd, *J* = 8.8, 1.6 Hz, 1H), 3.34 (s, 1H), 1.39 (s, 9H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 164.1, 136.9, 128.5, 125.4, 123.0, 122.9, 114.4, 114.2, 111.7, 50.3, 29.0; HRMS (ESI): Exact mass calcd for $C_{13}H_{16}BrN_2O$ $[M+H]^+$ 295.0441, Found 295.0444.

N-tert-butyl-7-methyl-1_H_-indole-3-carboxamide (3q)



^{1}H NMR (400 MHz, DMSO-d_6) δ 11.43 (br, 1H), 8.06 (d, *J* = 2.8 Hz, 1H), 7.94 (d, *J* = 7.6 Hz, 1H), 7.12 (br, 1H), 6.97 (t, *J* = 8.0 Hz, 1H), 6.91 (d, *J* = 6.8 Hz, 1H), 2.46 (s, 3H), 1.39 (s, 9H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 164.5, 135.4, 127.2, 125.8, 121.9, 120.5, 120.1, 118.5, 111.9, 50.0, 28.9, 16.4; HRMS (ESI): Exact mass calcd for $C_{14}H_{19}N_2O$ $[M+H]^+$ 231.1492, Found 231.1492.

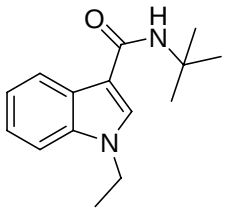
N-tert-butyl-7-ethyl-1_H_-indole-3-carboxamide (3r)



^{1}H NMR (400 MHz, $CDCl_3$) δ 10.09 (br, 1H), 7.69 (d, *J* = 2.8 Hz, 1H), 7.56 (d, *J* = 4.0 Hz, 1H), 7.19 (t, *J* = 7.6 Hz, 1H), 7.07 (d, *J* = 7.2 Hz, 1H), 5.98 (br, 1H), 2.91 (dd, *J* = 14.8, 7.2 Hz, 2H), 1.53 (s, 9H), 1.32 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.6, 135.5, 128.4, 124.0,

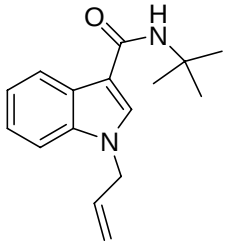
121.6, 121.1, 116.6, 113.5, 51.4, 29.2, 23.9, 13.9; HRMS (ESI): Exact mass calcd for $C_{15}H_{21}N_2O$ $[M+H]^+$ 245.1648, Found 245.1649.

***N-tert*-butyl-1-ethyl-1*H*-indole-3-carboxamide (3s)[2]**



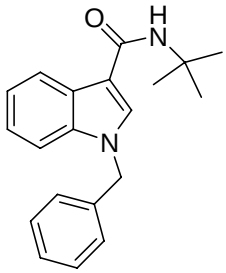
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.13 (d, *J* = 8.0 Hz, 1H), 8.10 (s, 1H), 7.76(dd, *J* = 8.4, 1.6 Hz, 1H), 7.49(d, *J* = 8.8 Hz, 1H), 7.31 (br, 1H), 3.86 (s, 3H), 1.41 (s, 9H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 164.1, 135.6, 129.8, 126.6, 121.5, 121.2, 120.1, 110.7, 109.8, 50.1, 28.9, 14.9; HRMS (ESI): Exact mass calcd for $C_{15}H_{21}N_2O$ $[M+H]^+$ 245.1648, Found 245.1649.

***N-tert*-butyl-1-allyl-1*H*-indole-3-carboxamide (3t)**



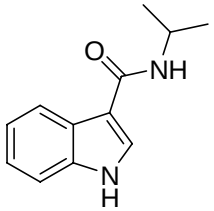
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88-7.90 (m, 1H), 7.66 (s, 1H), 7.33-7.36 (m, 1H), 7.23-7.28(m, 2H), 5.93-6.02 (m, 1H), 5.83 (br, 1H), 5.24 (dd, *J* = 10.4, 1.2 Hz, 1H), 5.13 (dd, *J* = 16.8, 1.2 Hz, 1H) 4.74 (t, *J* = 1.6 Hz, 1H), 1.52 (s, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.6, 136.6, 132.3, 131.2, 125.3, 122.2, 121.3, 119.9, 118.2, 112.5, 110.5, 51.3, 49.1, 29.3; HRMS (ESI): Exact mass calcd for $C_{16}H_{20}N_2ONa$ $[M+Na]^+$ 279.1468, Found 279.1466.

***N-tert*-butyl-1-benzyl-1*H*-indole-3-carboxamide (3u)**



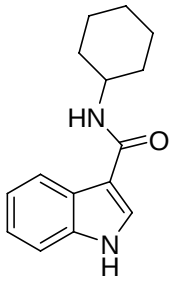
^{1}H NMR (400 MHz, DMSO-d_6) δ 8.13 (d, *J* = 8.0 Hz, 1H), 8.10 (s, 1H), 7.76(dd, *J* = 8.4, 1.6 Hz, 1H), 7.49(d, *J* = 8.8 Hz, 1H), 7.31 (br, 1H), 3.86 (s, 3H), 1.41 (s, 9H); ^{13}C NMR (100 MHz, DMSO-d_6) δ 164.2, 137.6, 136.0, 131.1, 128.6, 127.5, 127.0, 126.8, 121.9, 121.4, 120.5, 111.2, 110.4, 50.3, 49.4, 29.0; HRMS (ESI): Exact mass calcd for $C_{20}H_{22}N_2ONa$ $[M+Na]^+$ 329.1624, Found 329.1627.

***N*-isopropyl-1*H*-indole-3-carboxamide (3v)**



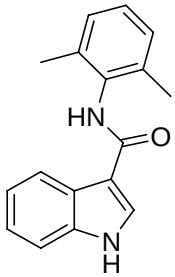
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.74(br, 1H), 7.89-7.91 (m, 1H), 7.65 (d, *J* = 2.8 Hz, 1H), 7.41-7.43 (m, 1H), 7.20-7.26 (m, 2H), 5.90 (d, *J* = 3.6 Hz, 1H), 4.34-4.42 (m, 1H), 1.30 (d, *J* = 2.8 Hz, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 165.1, 136.6, 128.3, 122.7, 121.4, 119.5, 112.3, 112.2, 41.4, 23.1; HRMS (ESI): Exact mass calcd for $C_{12}H_{14}N_2ONa$ $[M+Na]^+$ 225.0998, Found 225.0998.

_N_-cyclohexyl-1_H_-indole-3-carboxamide (3w)[3]



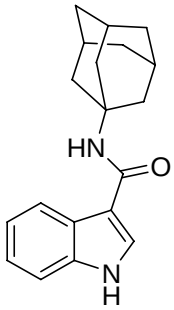
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.31 (br, 1H), 7.88-7.91 (m, 1H), 7.69 (d, *J* = 2.8 Hz, 1H), 7.41-7.43 (m, 1H), 7.23-7.25 (m, 2H), 5.91 (d, *J* = 8.0 Hz, 1H), 4.04-4.11 (m, 1H), 2.05-2.10 (m, 2H), 1.74-1.79 (m, 2H), 1.63-1.67 (m, 1H), 1.40-1.50 (m, 2H), 1.22-1.35 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.5, 136.4, 127.8, 124.6, 122.9, 121.5, 119.7, 113.1, 112.0, 48.1, 33.5, 25.7, 24.9; HRMS (ESI): Exact mass calcd for $C_{15}H_{19}N_2O$ $[M+H]^+$ 243.1492, Found 243.1493.

_N_-(2, 6-dimethylphenyl)-1_H_-indole-3-carboxamide (3x)



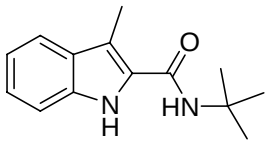
^{1}H NMR (400 MHz, $CDCl_3$) δ 11.66 (br, 1H), 9.20 (br, 1H), 8.24 (d, *J* = 2.4 Hz, 1H), 8.16 (d, *J* = 8.0 Hz, 1H), 7.47 (d, *J* = 8.0 Hz, 1H), 7.11-7.20 (m, 5H), 2.22 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 163.1, 136.2, 135.9, 135.7, 128.2, 128.1, 127.6, 127.6, 126.3, 126.2, 122.0, 121.1, 121.0, 120.4, 111.8, 110.3, 18.2; HRMS (ESI): Exact mass calcd for $C_{17}H_{16}N_2ONa$ $[M+Na]^+$ 287.1155, Found 287.1154.

_N_- (1-Ad)-1_H_-indole-3-carboxamide (3y)



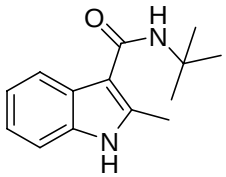
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.82 (br, 1H), 7.84-7.87 (m, 1H), 7.62 (d, *J* = 4.0 Hz, 1H), 7.40-7.44 (m, 1H), 7.19-7.24 (m, 2H), 5.81 (br, 1H), 2.20-2.21 (m, 6H), 2.14 (s, 3H), 1.75-1.78 (m, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 165.1, 136.6, 128.3, 124.4, 122.5, 121.3, 119.3, 113.2, 112.3, 50.2, 42.2, 36.5, 29.6; HRMS (ESI): Exact mass calcd for $C_{19}H_{22}N_2ONa$ $[M+Na]^+$ 317.1624, Found 317.1623.

N-tert-butyl-3-methyl-1_H_-indole-2-carboxamide (3z)[4]



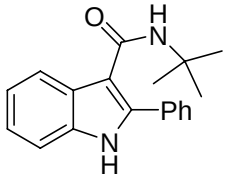
^{1}H NMR (400 MHz, $CDCl_3$) δ 9.45 (br, 1H), 7.61(d, *J* = 8.0 Hz, 1H), 7.40 (d, *J* = 8.0 Hz, 1H), 7.25-7.29 (m, 1H), 7.11-7.15 (m, 1H), 5.95 (br, 1H), 2.55 (s, 3H), 1.54 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 162.0, 135.0, 128.7, 128.4, 124.3, 119.8, 119.6, 111.7, 110.5, 51.7, 29.1, 10.2; HRMS (ESI): Exact mass calcd for $C_{14}H_{18}N_2ONa$ $[M+Na]^+$ 253.1311, Found 253.1312.

N-tert-butyl-2-methyl-1_H_-indole-3-carboxamide (3aa)[5]



^{1}H NMR (400 MHz, DMSO-d_6) δ 11.32 (br, 1H), 7.66-7.68 (m, 1H), 7.29-7.32 (m, 1H), 7.02-7.08 (m, 2H), 6.78 (s, 1H), 2.55 (s, 3H), 1.41 (s, 9H); ^{13}C NMR (125 MHz, DMSO-d_6) δ 165.2, 138.5, 134.5, 126.3, 120.8, 119.7, 110.8, 109.1, 50.3, 28.9, 13.1; HRMS (ESI): Exact mass calcd for $C_{14}H_{19}N_2O$ $[M+H]^+$ 231.1492, Found 231.1493.

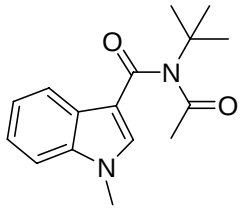
N-tert-butyl-2-phenyl-1_H_-indole-3-carboxamide (3ab)



^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (br, 1H), 8.12-8.14 (m, 1H), 7.59-7.61 (m, 1H), 7.42-7.47 (m, 3H), 7.18-7.24 (m, 2H), 5.38 (br, 1H), 1.28 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 164.8, 137.9, 135.3, 121.7, 129.3, 128.9, 127.8, 123.1, 121.5, 121.4, 110.8, 51.0, 28.8; HRMS (ESI): Exact mass

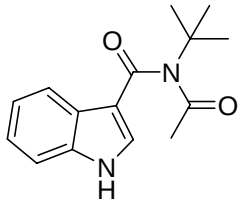
calcd for $C_{19}H_{20}N_2ONa$ $[M+Na]^+$ 315.1468, Found 315.1466.

_N_-acetyl-_N-tert_-butyl-1-methyl-1_H_-indole-3-carboxamide (4a)



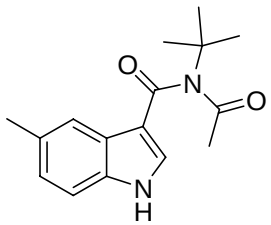
^1H NMR (400 MHz, $CDCl_3$) δ 8.29-8.31 (m, 1H), 7.86 (s, 1H), 7.36-7.41(m, 3H), 3.89 (s, 3H), 1.99 (s, 3H), 1.54 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.5, 169.0, 138.0, 137.9, 126.5, 124.1, 123.3, 122.0, 115.2, 110.2, 57.7, 33.8, 25.5, 25.3; HRMS (ESI): Exact mass calcd for $C_{16}H_{20}N_2O_2Na$ $[M+Na]^+$ 295.1417, Found 295.1420.

_N_-acetyl-_N-tert_-butyl-1_H_-indole-3-carboxamide (4b)



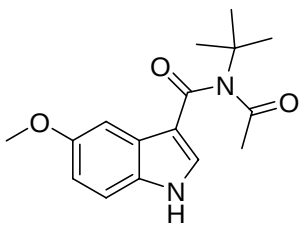
^1H NMR (400 MHz, $CDCl_3$) δ 10.81 (br, 1H), 8.31-8.33 (m, 1H), 7.87 (d, J = 3.2 Hz, 1H), 7.52-7.55(m, 1H), 7.34-7.39 (m, 2H), 2.07 (s, 3H), 1.59 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.6, 169.7, 137.3, 134.8, 125.8, 124.4, 123.2, 121.6, 116.1, 112.3, 58.0, 25.5, 25.3; HRMS (ESI): Exact mass calcd for $C_{15}H_{18}N_2O_2Na$ $[M+Na]^+$ 281.1260, Found 281.1261.

_N_-acetyl-_N-tert_-butyl-5-methyl-1_H_-indole-3-carboxamide (4c)



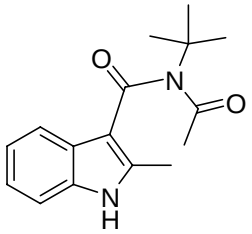
^1H NMR (400 MHz, $CDCl_3$) δ 10.26 (br, 1H), 8.13 (s, 1H), 7.78 (d, J = 3.2 Hz, 1H), 7.39 (d, J = 8.0 Hz, 1H), 2.50 (s, 3H), 2.04 (s, 3H), 1.57 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.6, 169.6, 135.4, 134.6, 133.1, 126.0, 126.0, 121.4, 111.8, 57.9, 28.5, 25.3, 21.6; HRMS (ESI): Exact mass calcd for $C_{16}H_{20}N_2O_2$ Na $[M+Na]^+$ 295.1417, Found 295.1413.

_N_-acetyl-_N-tert_-butyl-5-methoxy-1_H_-indole-3-carboxamide (4d)



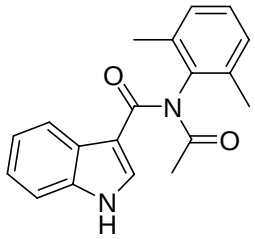
^{1}H NMR (400 MHz, $CDCl_3$) δ 10.39 (br, 1H), 7.77-7.79 (m, 2H), 7.79 (d, *J* = 8.8 Hz, 1H), 6.98 (dd, *J* = 8.8, 2.4 Hz, 1H), 3.90 (s, 3H), 2.04 (s, 3H), 1.57 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.6, 169.6, 156.8, 134.6, 131.9, 126.7, 116.0, 114.9, 113.1, 120.9, 57.9, 55.7, 28.4, 25.3; HRMS (ESI): Exact mass calcd for $C_{16}H_{20}N_2O_3Na$ $[M+Na]^+$ 311.1366, Found 311.1369.

_N_-acetyl-_N_-_tert_-butyl-2-methyl-1_H_-indole-3-carboxamide (4aa)



^{1}H NMR (400 MHz, $CDCl_3$) δ 12.31 (br, 1H), 7.83-7.85 (m, 1H), 7.42-7.44 (m, 1H), 7.18-7.23(m, 2H), 2.69 (s, 3H), 1.81 (s, 3H), 1.43 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 170.9, 169.4, 135.8, 133.8, 127.6, 125.6, 123.6, 123.2, 119.5, 117.1, 57.9, 28.5, 25.4, 23.9, 10.0; HRMS (ESI): Exact mass calcd for $C_{16}H_{20}N_2O_2Na$ $[M+Na]^+$ 295.1417, Found 295.1418.

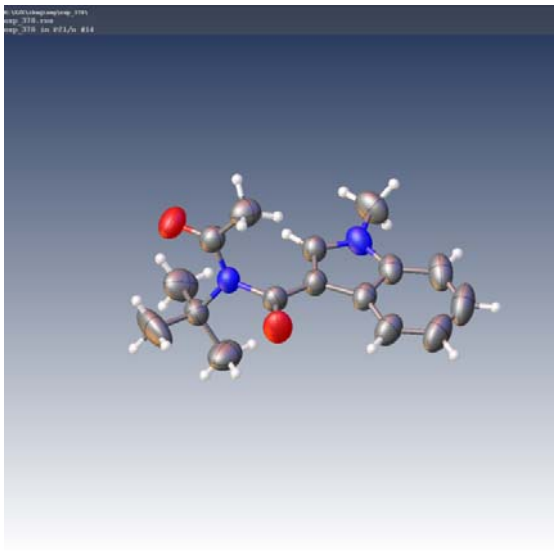
_N_-acetyl-_N_-(2, 6-dimetylphenyl)-1_H_-indole-3-carboxamide (4x)



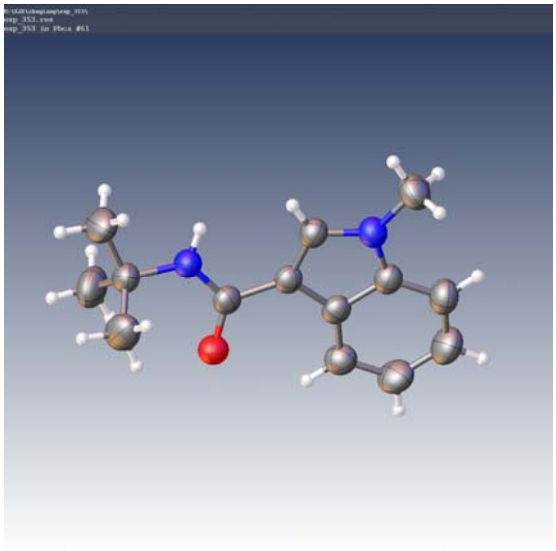
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62 (br, 1H), 8.42 (d, *J* = 8.0 Hz, 1H), 7.19-7.31(m, 4H), 7.11 (d, *J* = 7.6 Hz, 2H), 6.25 (d, *J* = 3.2 Hz, 1H), 2.68 (s, 3H), 2.17 (s, 6H); ^{13}C NMR (125 MHz, $CDCl_3$) δ 174.2, 166.5, 138.4, 136.8, 135.3, 130.0, 129.0, 128.8, 127.6, 123.6, 122.5, 122.5, 122.2, 111.4, 110.5, 26.6, 18.2; HRMS (ESI): Exact mass calcd for $C_{19}H_{18}N_2O_2$ $[M+Na]^+$ 329.1266, Found 329.1260.

IV. X-ray Structures of 4a and 3a

4a: The deposition number at the Cambridge Crystallographic Data Centre is CCDC 858032.



3a: The deposition number at the Cambridge Crystallographic Data Centre is CCDC 862590.



V. References

(1) H. L. Hassinger, R. M. Soll and G. W. Gribble, *Tetrahedron Lett.,* 1998, **39**, 3095.
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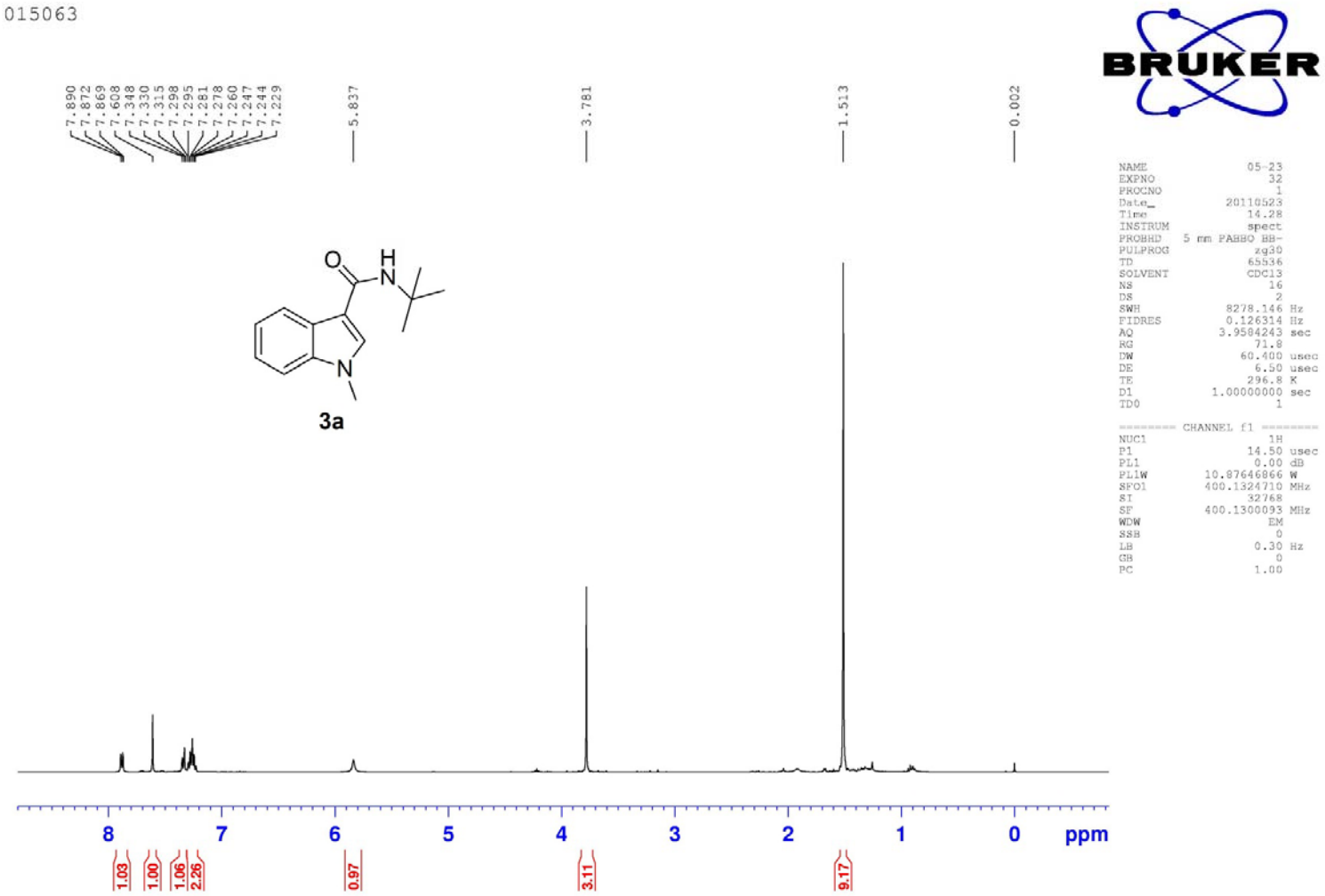
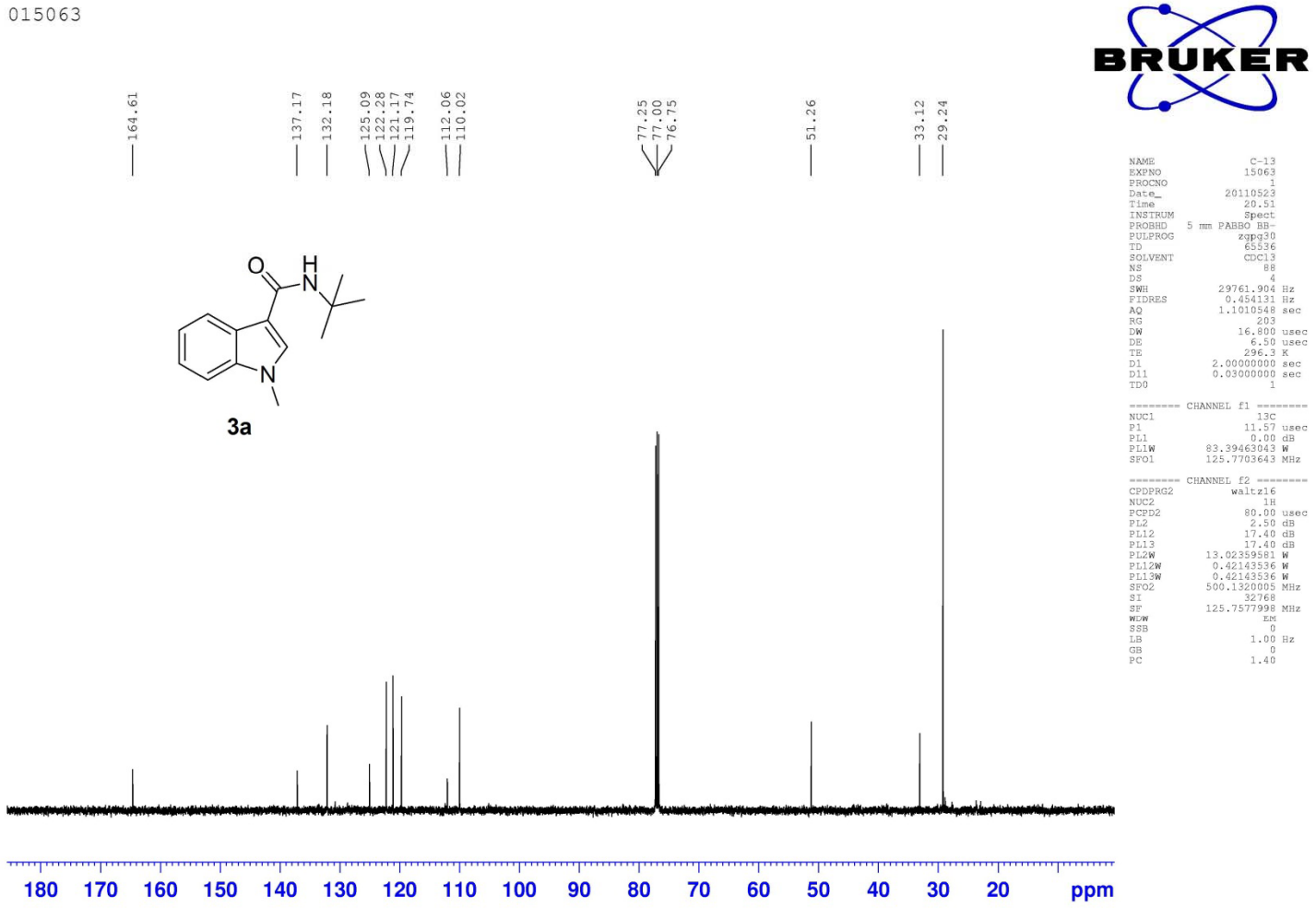
(3) P. Y. Choy, C. P. Lau and F. Y. Kwong, *J. Org. Chem.,* 2011, **76**, 80.
(4) H. Person, D. A. M. Pardo and A. Foucaud, *Tetrahedron Lett.,* 1980, **21**, 281.
(5) (a) S. Denison and S. T. Hilton, *Synlett*, 2004, 2806; (b) A. R. Katritzky, K. Akutagawa, R. A. Jones, *Synth. Commun.*, 1988, **18**, 1151; (c) B. Zeeh, *Tetrahedron Lett.*, 1967, 3881.

VI. Copies of ^{1}H NMR and ^{13}C NMR Spectra

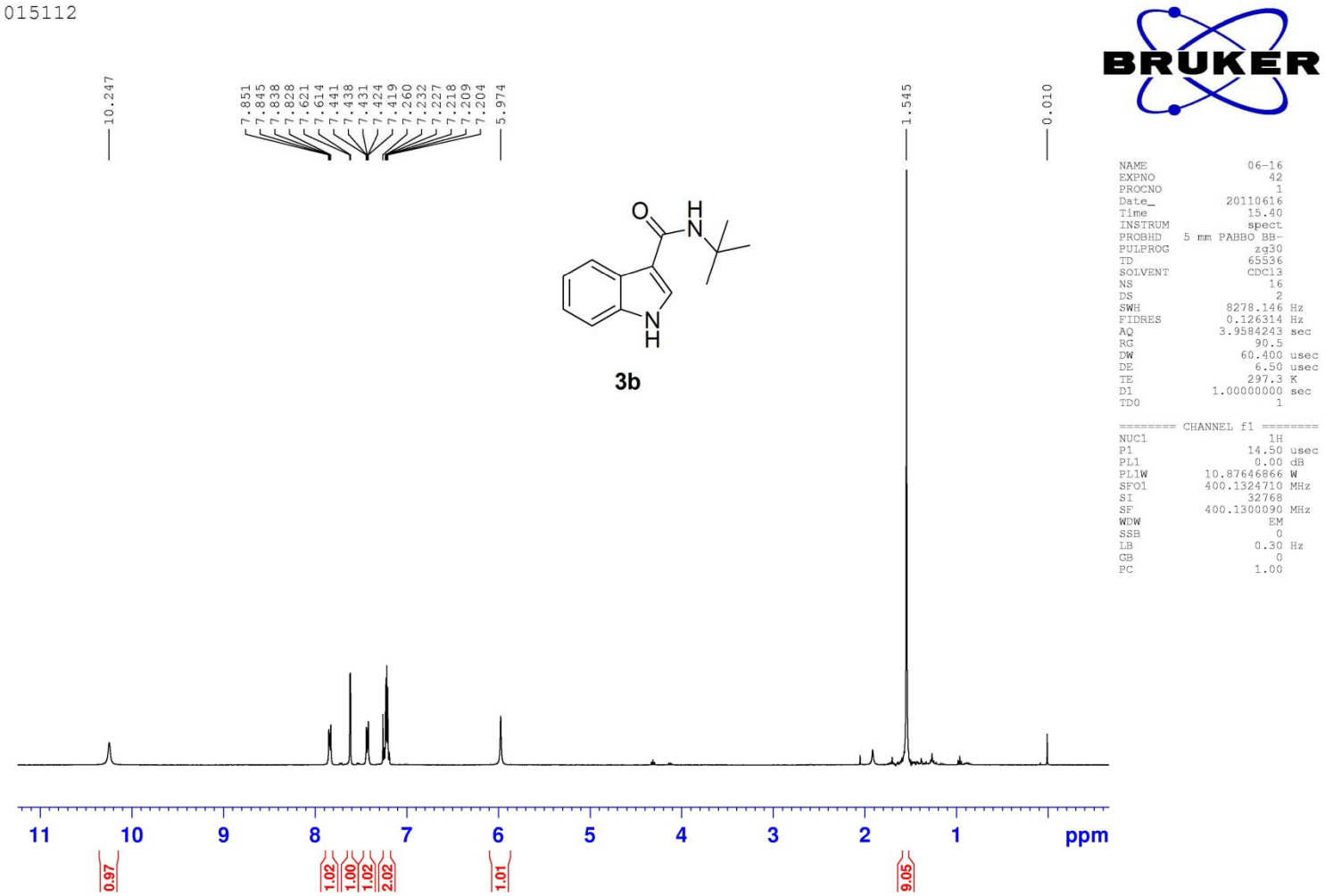


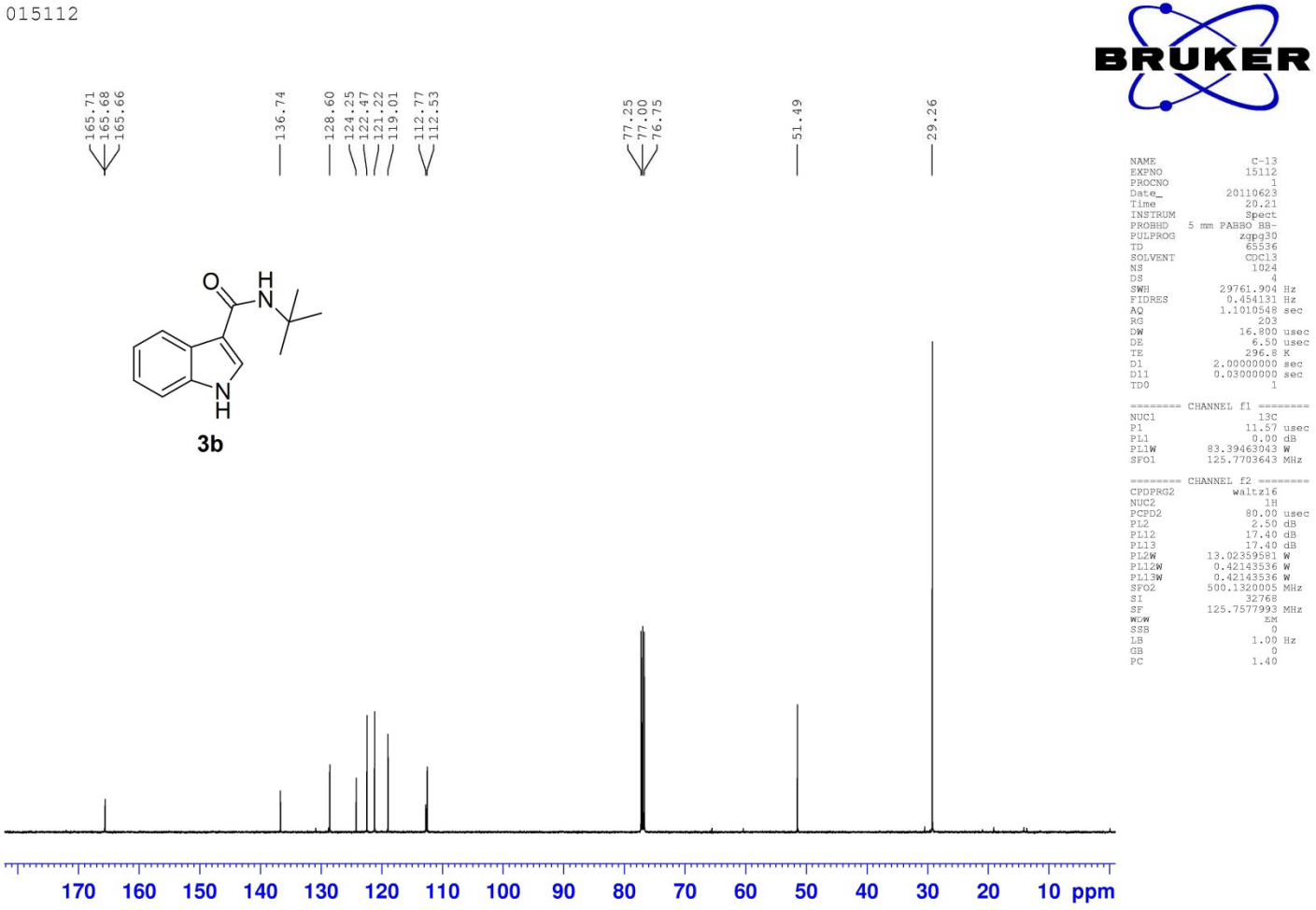
NAME	05-23
EXPNO	32
PROCNO	1
Date_	20110523
Time	14.28
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	71.8
DW	60.400 usec
DE	6.50 usec
TE	296.8 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.00 dB
PL1W	10.87646866 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300093 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



BRUKER

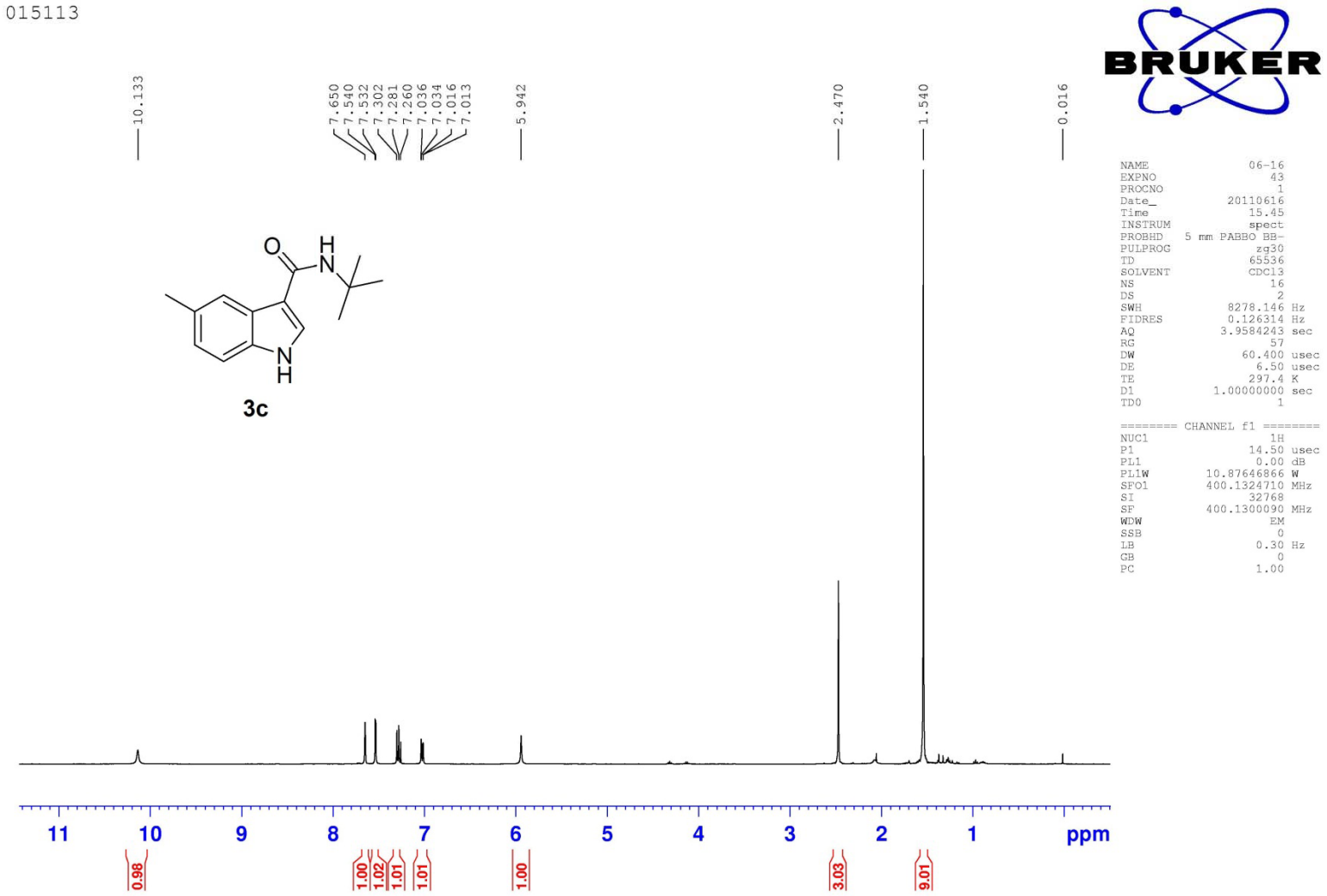
NAME	C-13
EXPNO	15063
PROCNO	1
Date_	20110523
Time	20.51
INSTRUM	Spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	88
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	296.3 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	11.57 usec
PL1	0.00 dB
PL1W	83.39463043 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.50 dB
PL12	17.40 dB
PL13	17.40 dB
PL2W	13.02359581 W
PL12W	0.42143536 W
PL13W	0.42143536 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7577998 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

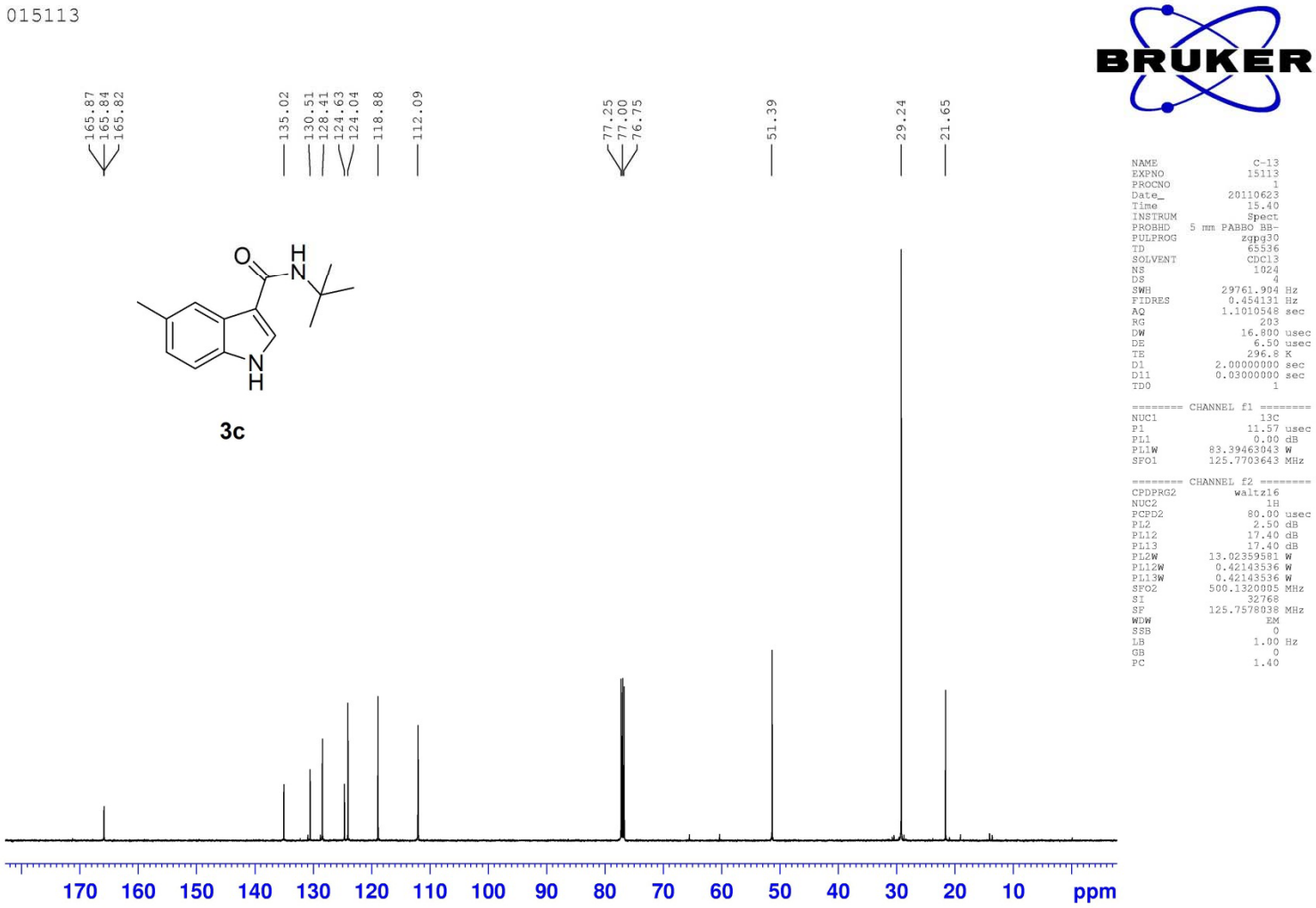

015112
10.247
7.851
7.845
7.838
7.828
7.621
7.614
7.441
7.438
7.431
7.424
7.419
7.260
7.232
7.227
7.218
7.209
7.204
5.974
1.545
0.010
O
H
N
N
H
3b
11
10
9
8
7
6
5
4
3
2
1
ppm
0.97
1.02
1.00
1.02
2.02
1.01
9.05
NAME 06-16
EXPNO 42
PROCNO 1
Date_ 20110616
Time 15.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 90.5
DW 60.400 usec
DE 6.50 usec
TE 297.3 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.50 usec
PL1 0.00 dB
PL1W 10.87646866 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300090 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



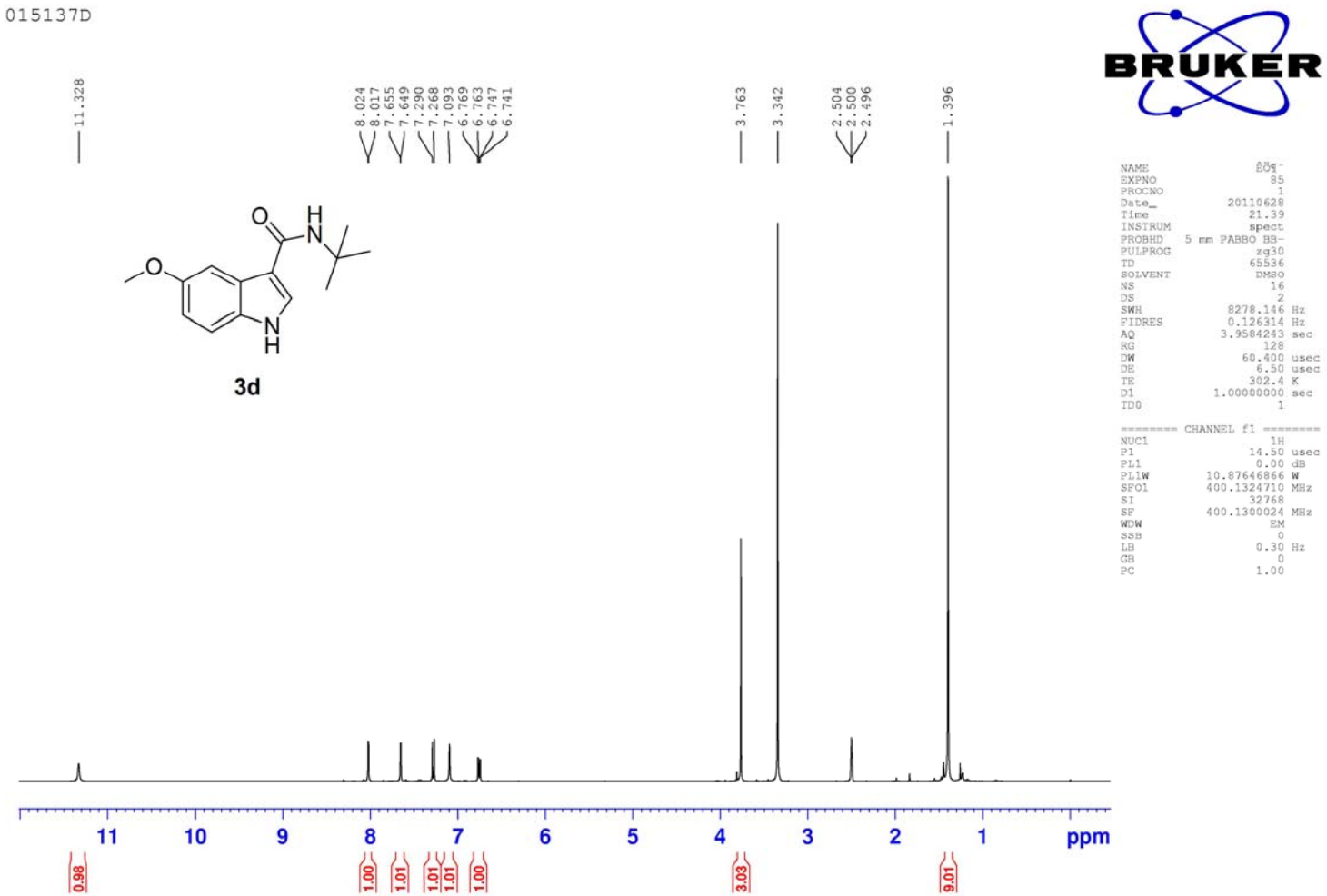
BRUKER

NAME	C-13
EXPNO	15112
PROCNO	1
Date_	20110623
Time	20.21
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	296.8 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	11.57 usec
PL1	0.00 dB
PL1W	83.39463043 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.50 dB
PL12	17.40 dB
PL13	17.40 dB
PL2W	13.02359581 W
PL12W	0.42143536 W
PL13W	0.42143536 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7577993 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

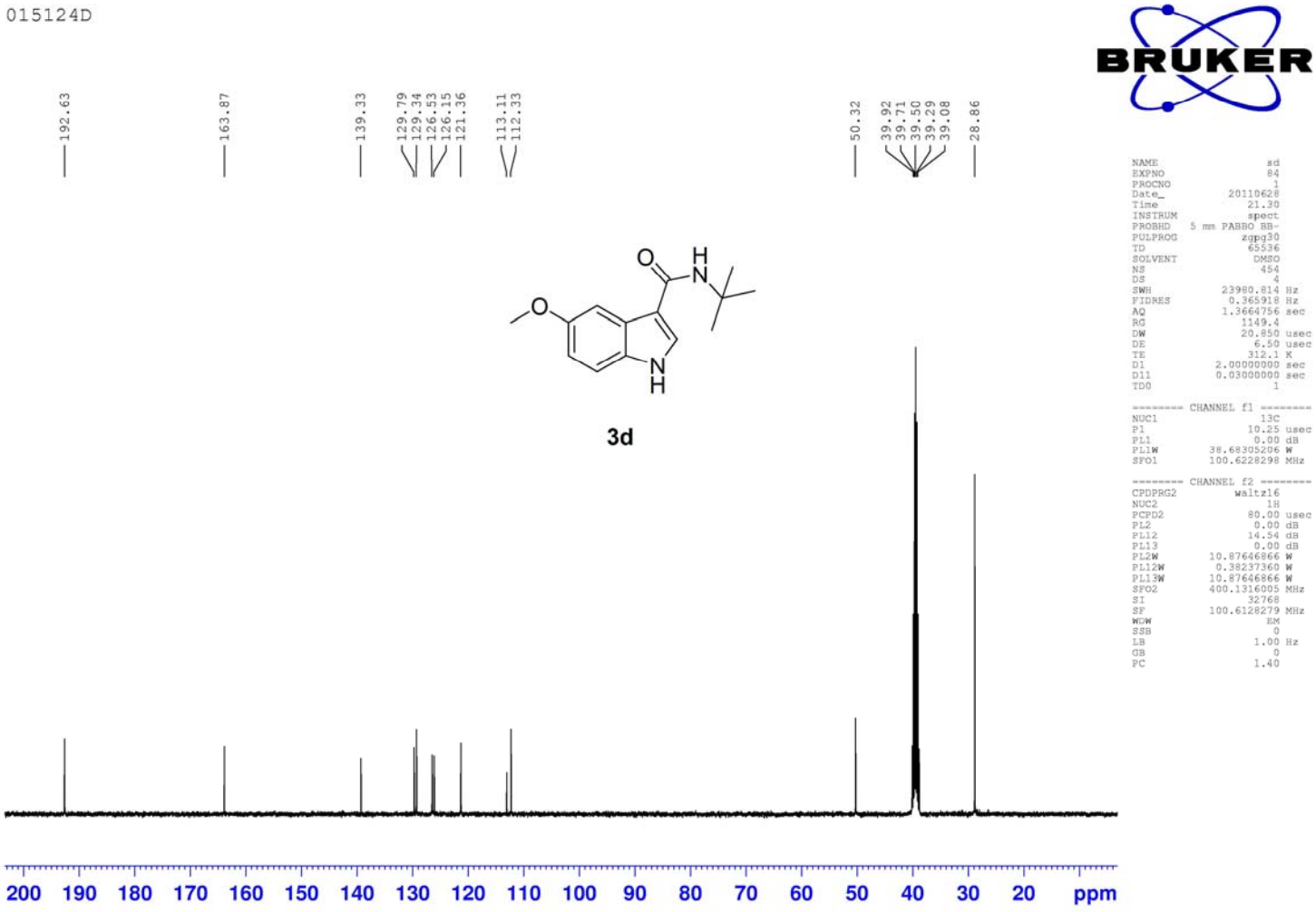




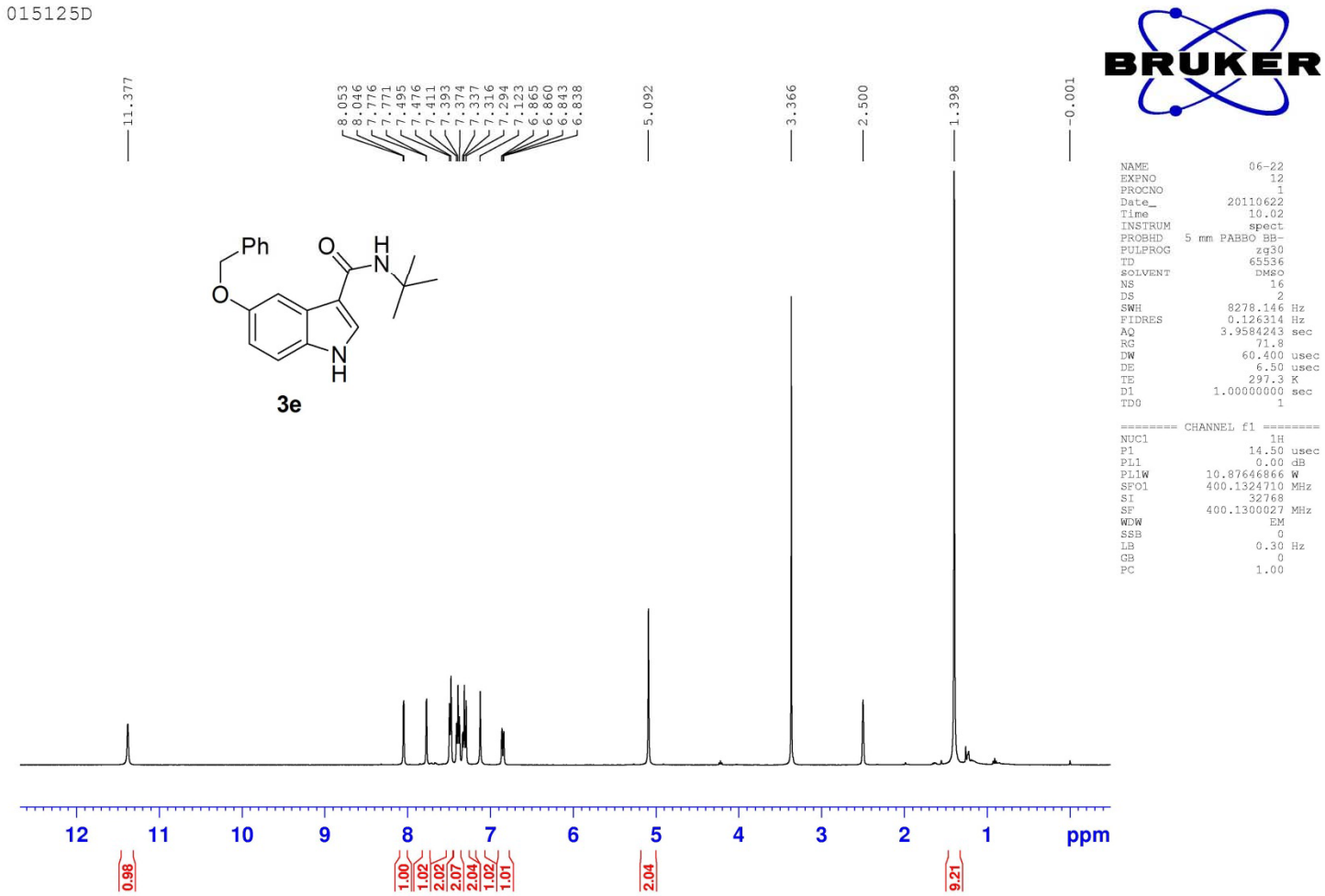
NAME	C-13
EXPNO	15113
PROCNO	1
Date_	20110623
Time	15.40
INSTRUM	Spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	296.8 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	11.57 usec
PL1	0.00 dB
PL1W	83.39463043 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.50 dB
PL12	17.40 dB
PL13	17.40 dB
PL2W	13.02359581 W
PL12W	0.42143536 W
PL13W	0.42143536 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7578038 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

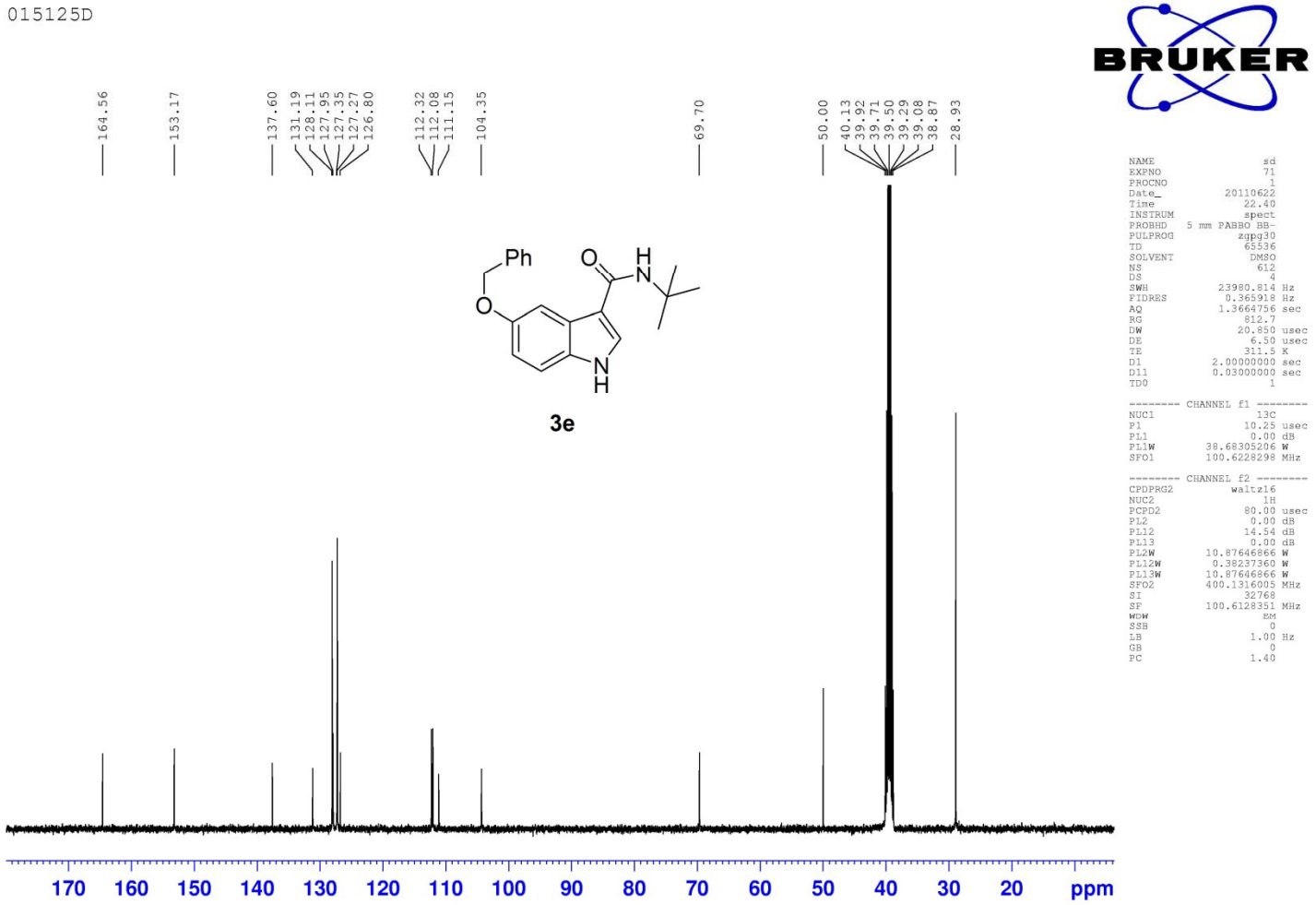


NAME	
EXPNO	85
PROCNO	1
Date_	20110628
Time	21.39
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	128
DW	60.400 usec
DE	6.50 usec
TE	302.4 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.00 dB
PL1W	10.87646866 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300024 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



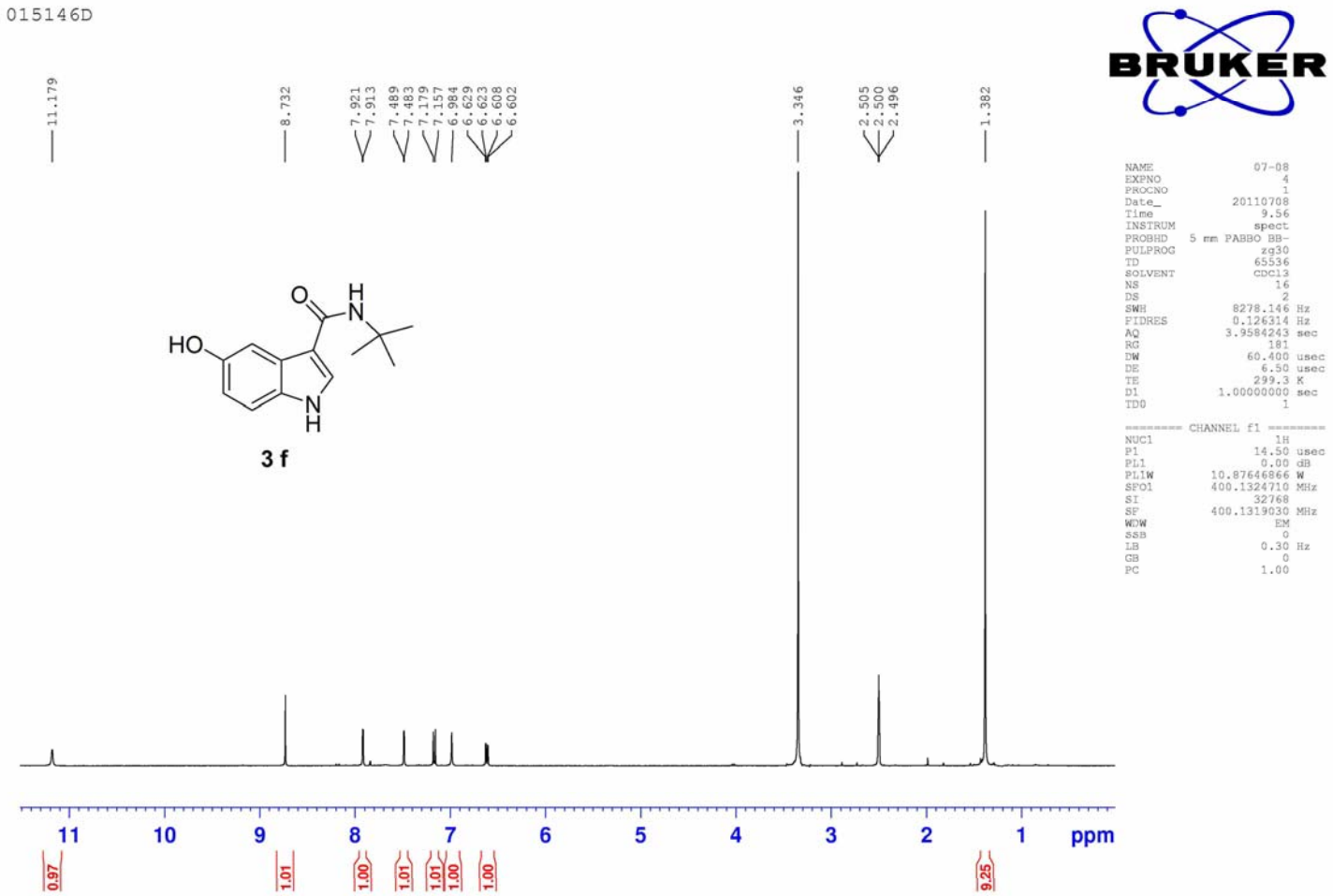
NAME	sd
EXPNO	84
PROCNO	1
Date_	20110628
Time	21.30
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	454
DS	4
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	1149.4
DW	20.850 usec
DE	6.50 usec
TE	312.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.25 usec
PL1	0.00 dB
PL1W	38.68305206 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	14.54 dB
PL13	0.00 dB
PL2W	10.87646866 W
PL12W	0.38237360 W
PL13W	10.87646866 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6128279 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

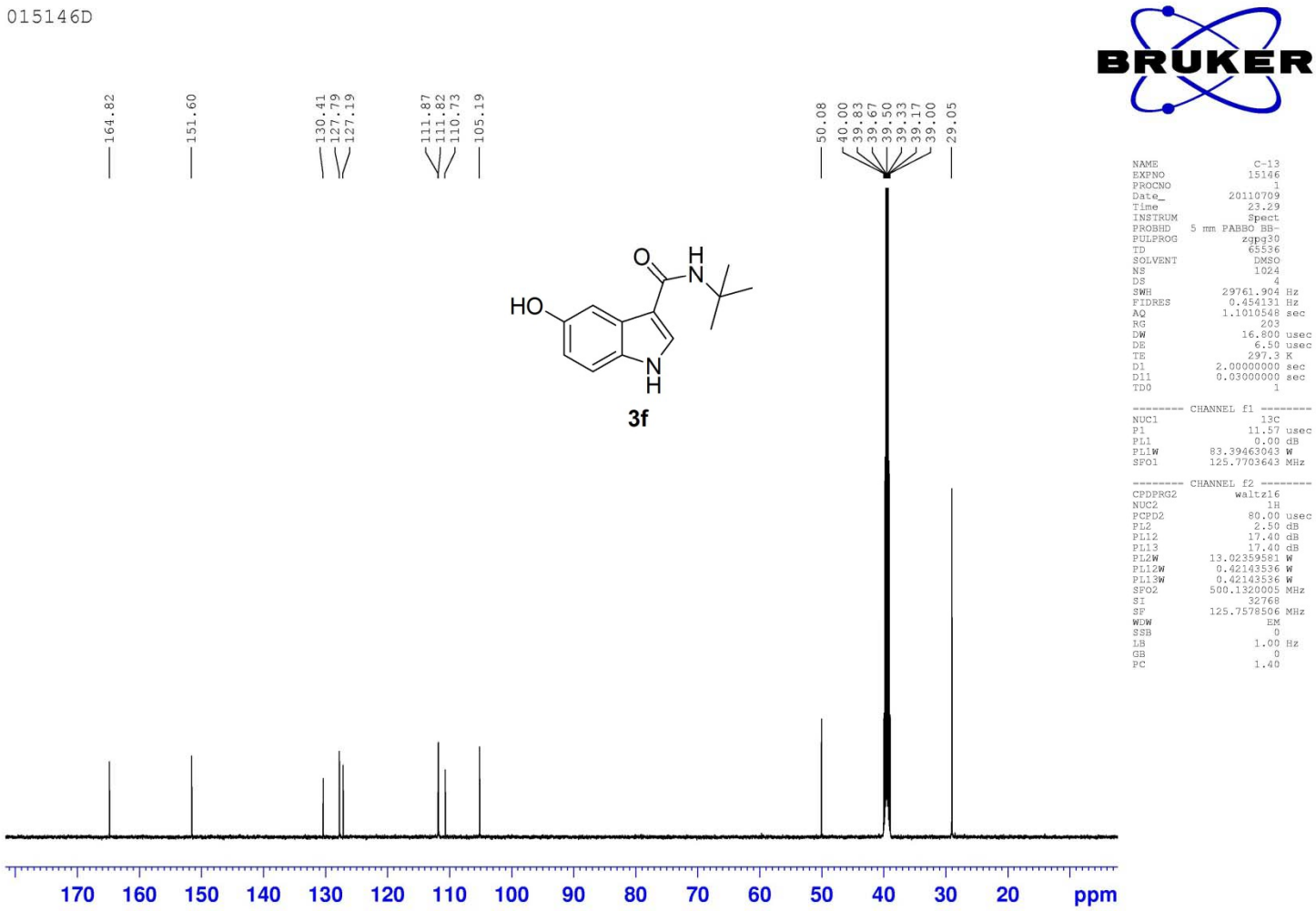




BRUKER

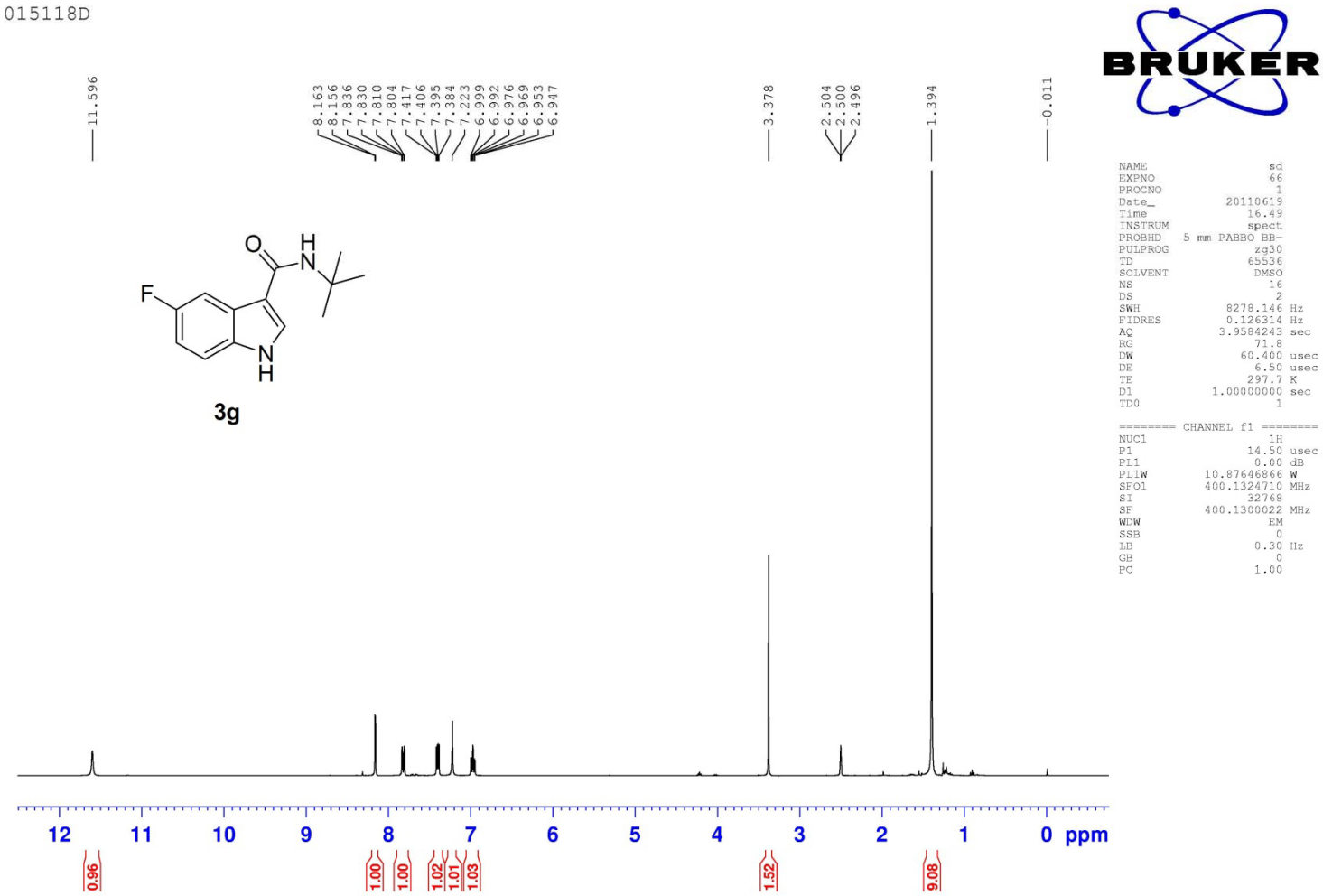
NAME	sd
EXPNO	71
PROCNO	1
Date_	20110622
Time	22.40
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	612
DS	4
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	812.7
DW	20.850 usec
DE	6.50 usec
TE	311.5 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.25 usec
PL1	0.00 dB
PL1W	38.68305206 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	14.54 dB
PL13	0.00 dB
PL2W	10.87646866 W
PL12W	0.38237360 W
PL13W	10.87646866 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6128351 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

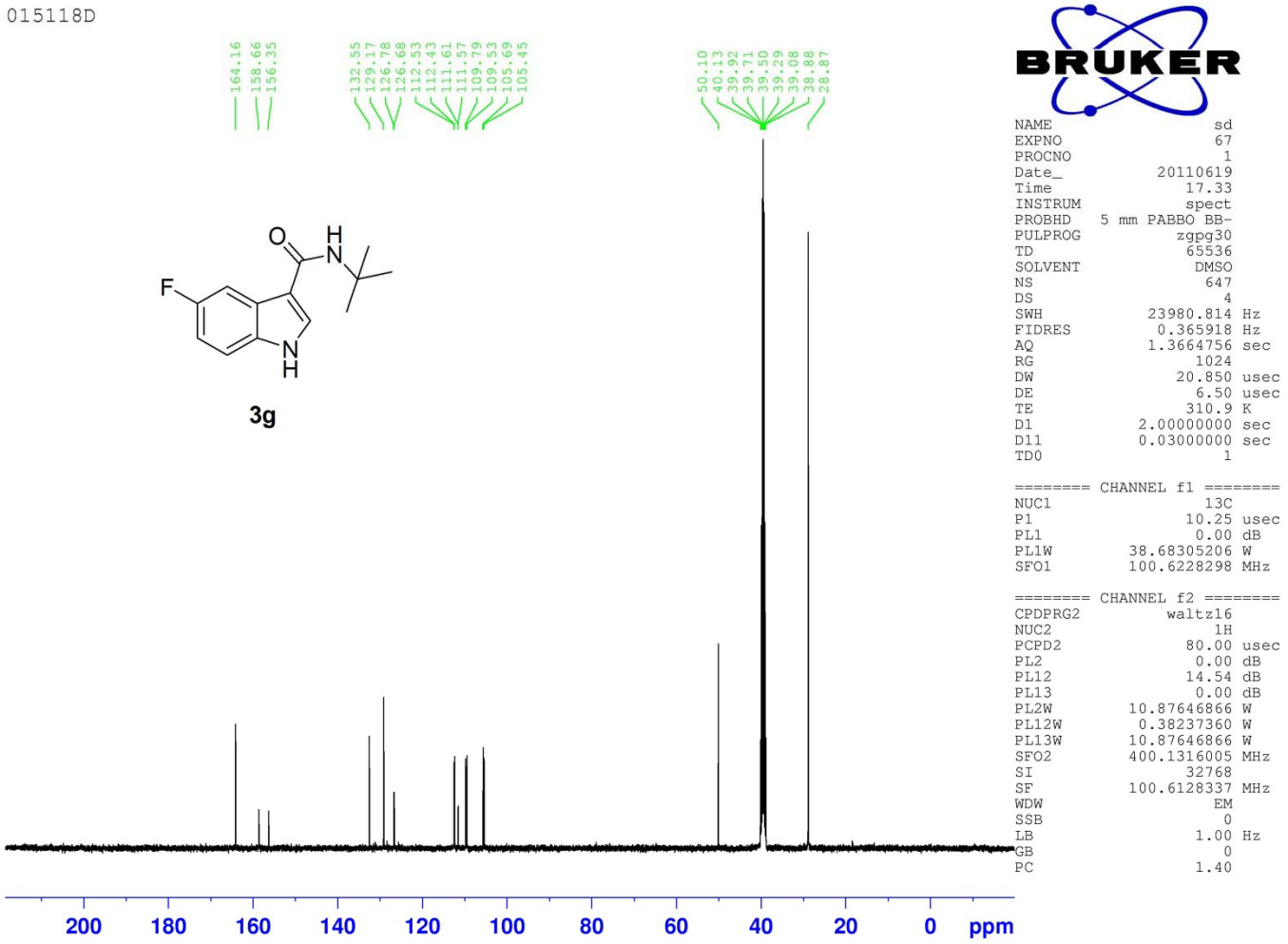

015146D
11.179
8.732
7.921
7.913
7.489
7.483
7.179
7.157
6.984
6.629
6.623
6.608
6.602
3.346
2.505
2.500
2.496
1.382
HO
O
H
N
N
H
3 f
11
10
9
8
7
6
5
4
3
2
1
ppm
0.97
1.01
1.00
1.01
1.01
1.00
1.00
9.25
NAME 07-08
EXPNO 4
PROCNO 1
Date_ 20110708
Time 9.56
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 181
DW 60.400 usec
DE 6.50 usec
TE 299.3 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 14.50 usec
PL1 0.00 dB
PL1W 10.87646866 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1319030 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



BRUKER

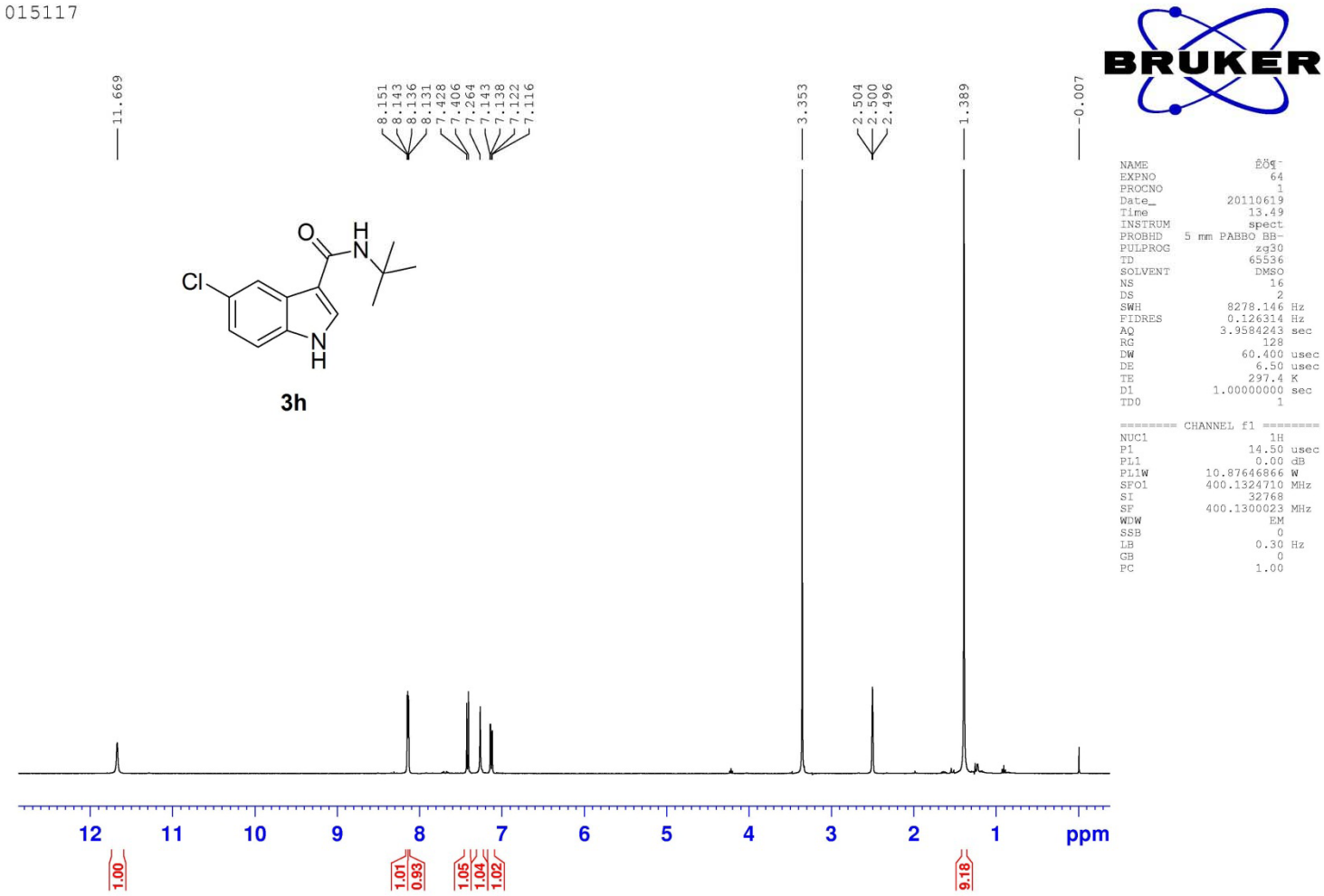
NAME	C-13
EXPNO	15146
PROCNO	1
Date_	20110709
Time	23.29
INSTRUM	Spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	1024
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	297.3 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	11.57 usec
PL1	0.00 dB
PL1W	83.39463043 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.50 dB
PL12	17.40 dB
PL13	17.40 dB
PL2W	13.02359581 W
PL12W	0.42143536 W
PL13W	0.42143536 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7578506 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

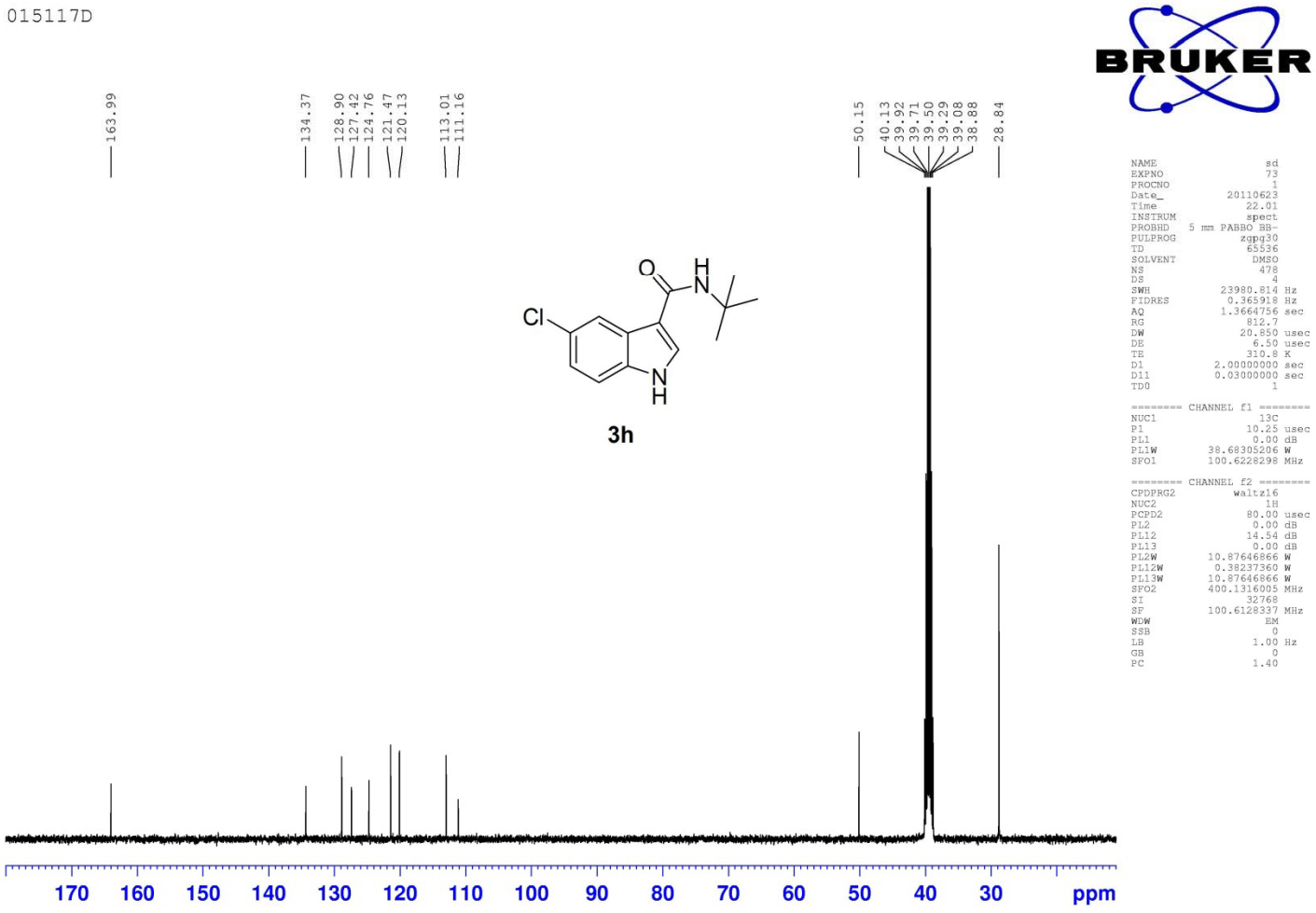


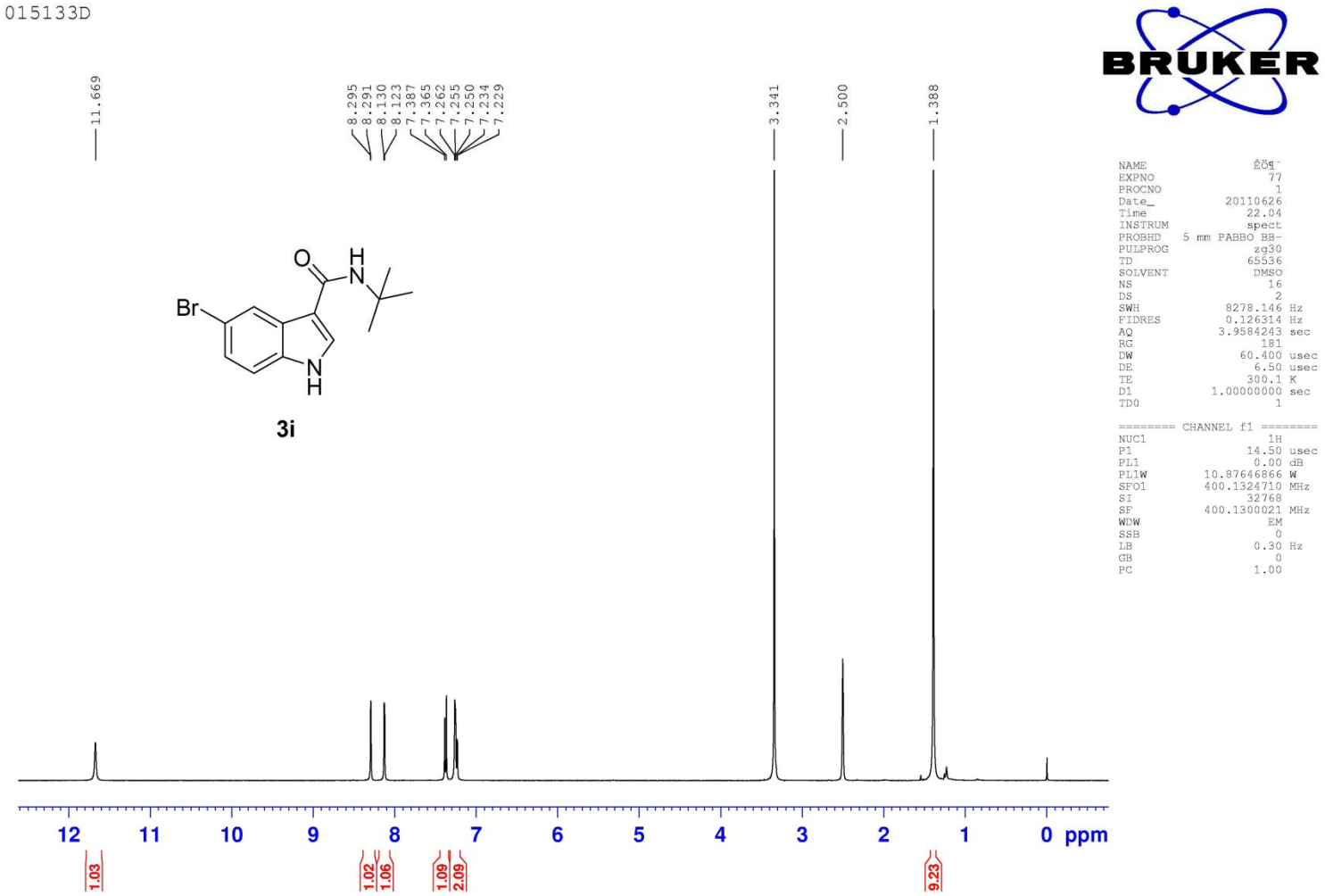


BRUKER

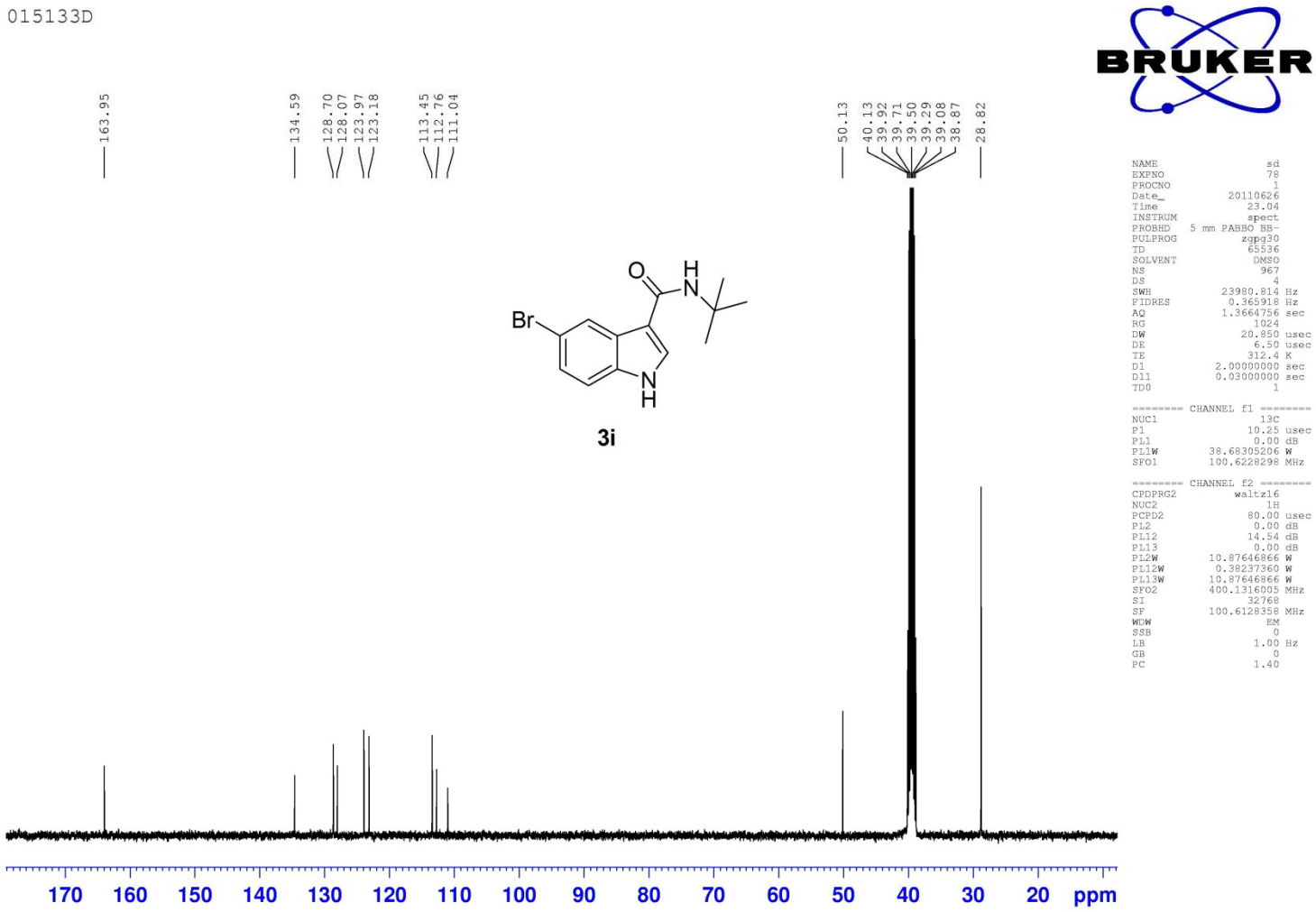
NAME	sd
EXPNO	67
PROCNO	1
Date_	20110619
Time	17.33
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	647
DS	4
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	1024
DW	20.850 usec
DE	6.50 usec
TE	310.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.25 usec
PL1	0.00 dB
PL1W	38.68305206 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	14.54 dB
PL13	0.00 dB
PL2W	10.87646866 W
PL12W	0.38237360 W
PL13W	10.87646866 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6128337 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40


015117
11.669
8.151
8.143
8.136
8.131
7.428
7.406
7.264
7.143
7.138
7.122
7.116
3.353
2.504
2.500
2.496
1.389
-0.007
BRUKER
Cl
O
H
N
N
H
3h
NAME
EXPNO 64
PROCNO 1
Date_ 20110619
Time 13.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 128
DW 60.400 usec
DE 6.50 usec
TE 297.4 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.50 usec
PL1 0.00 dB
PL1W 10.87646866 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300023 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.01
0.93
1.05
1.04
1.02
9.18


015117D
163.99
134.37
128.90
127.42
124.76
121.47
120.13
113.01
111.16
50.15
40.13
39.92
39.71
39.50
39.29
39.08
38.88
28.84
Cl
O
H
N
N
H
3h
BRUKER
NAME sd
EXPNO 73
PROCNO 1
Date_ 20110623
Time 22.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 478
DS 4
SWH 23980.814 Hz
FIDRES 0.365918 Hz
AQ 1.3664756 sec
RG 812.7
DW 20.850 usec
DE 6.50 usec
TE 310.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 10.25 usec
PL1 0.00 dB
PL1W 38.68305206 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 0.00 dB
PL12 14.54 dB
PL13 0.00 dB
PL2W 10.87646866 W
PL12W 0.38237360 W
PL13W 10.87646866 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6128337 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 ppm

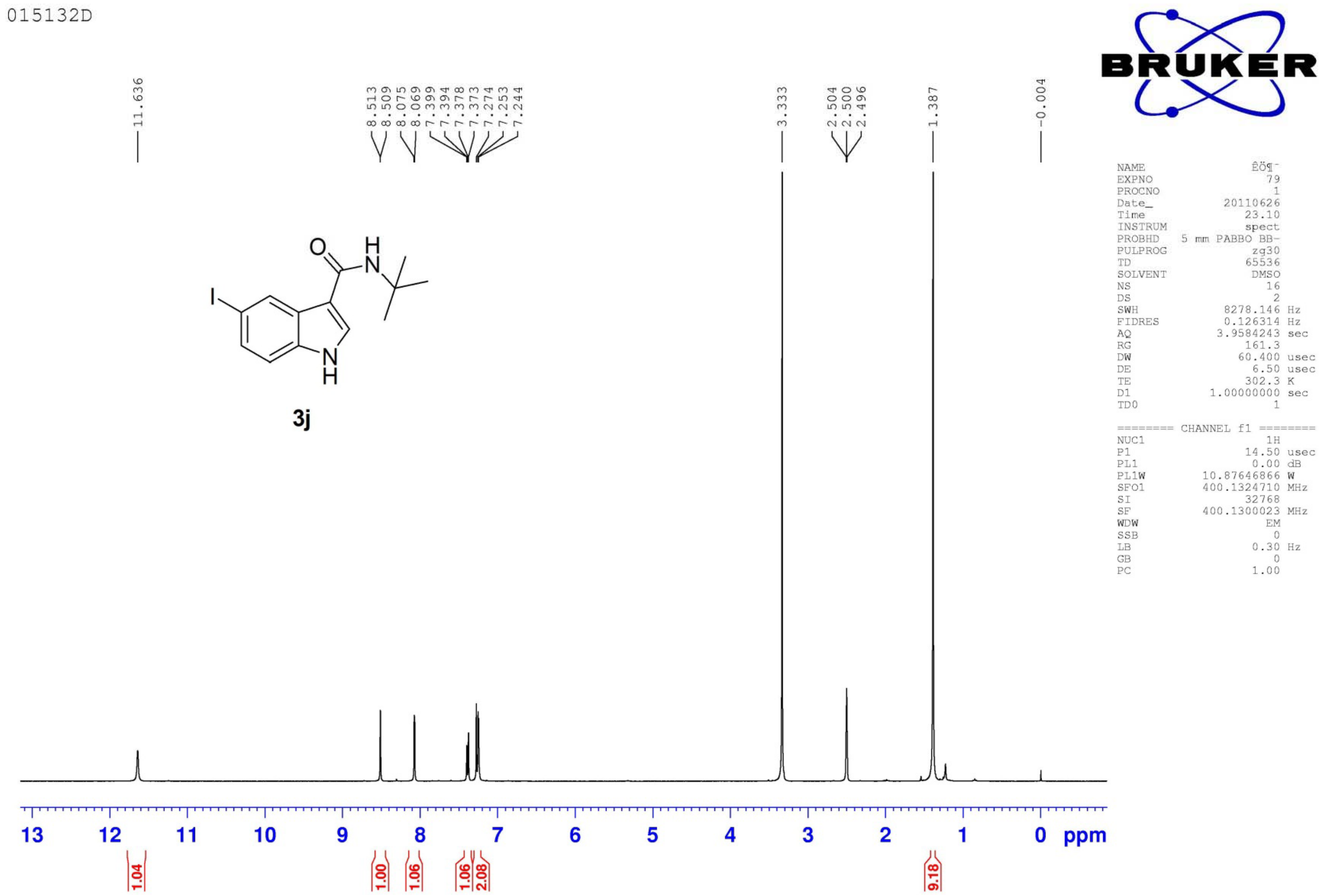


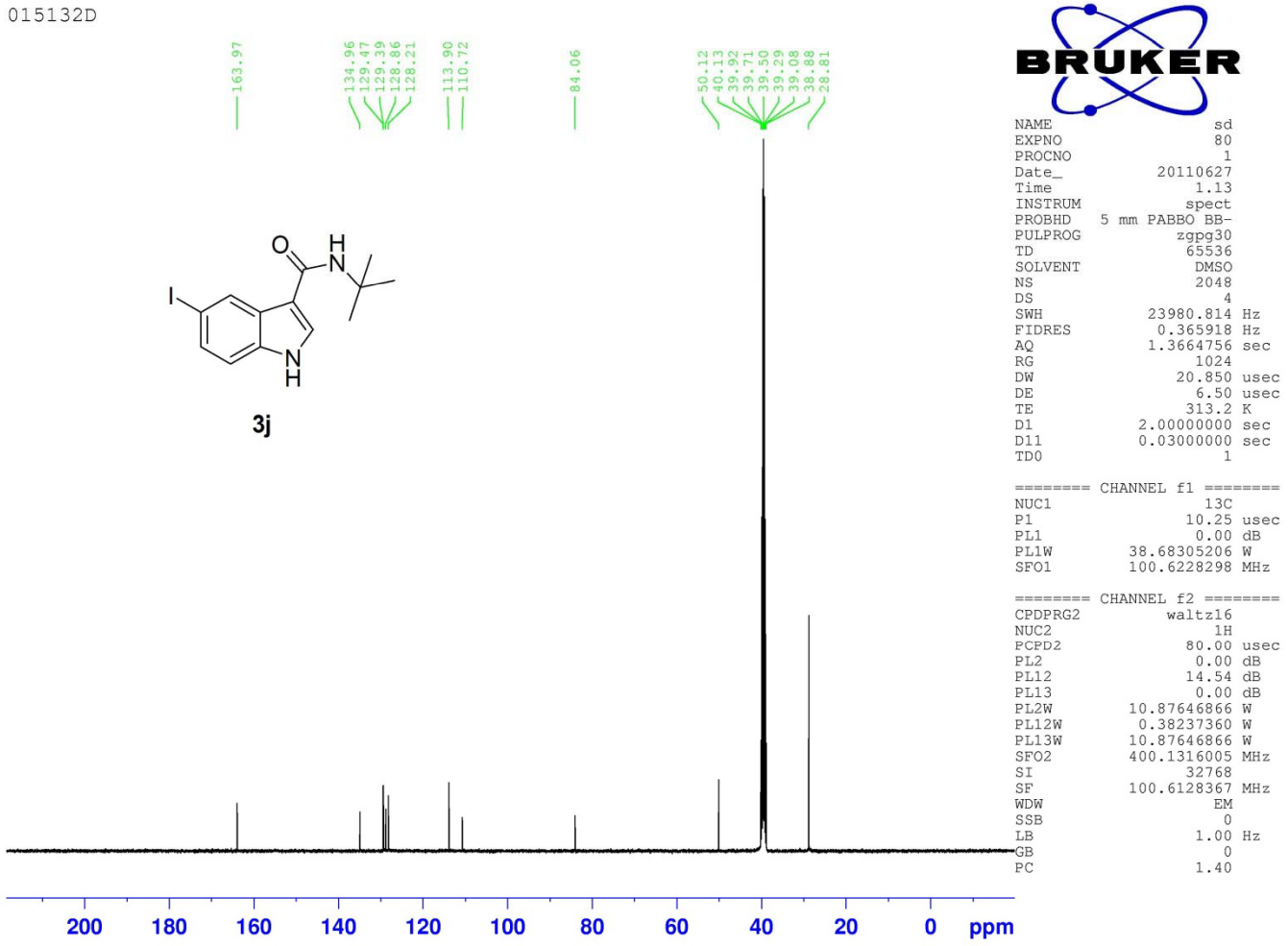
NAME	ÊÖ¶¯
EXPNO	77
PROCNO	1
Date_	20110626
Time	22.04
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	181
DW	60.400 usec
DE	6.50 usec
TE	300.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.00 dB
PL1W	10.87646866 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300021 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

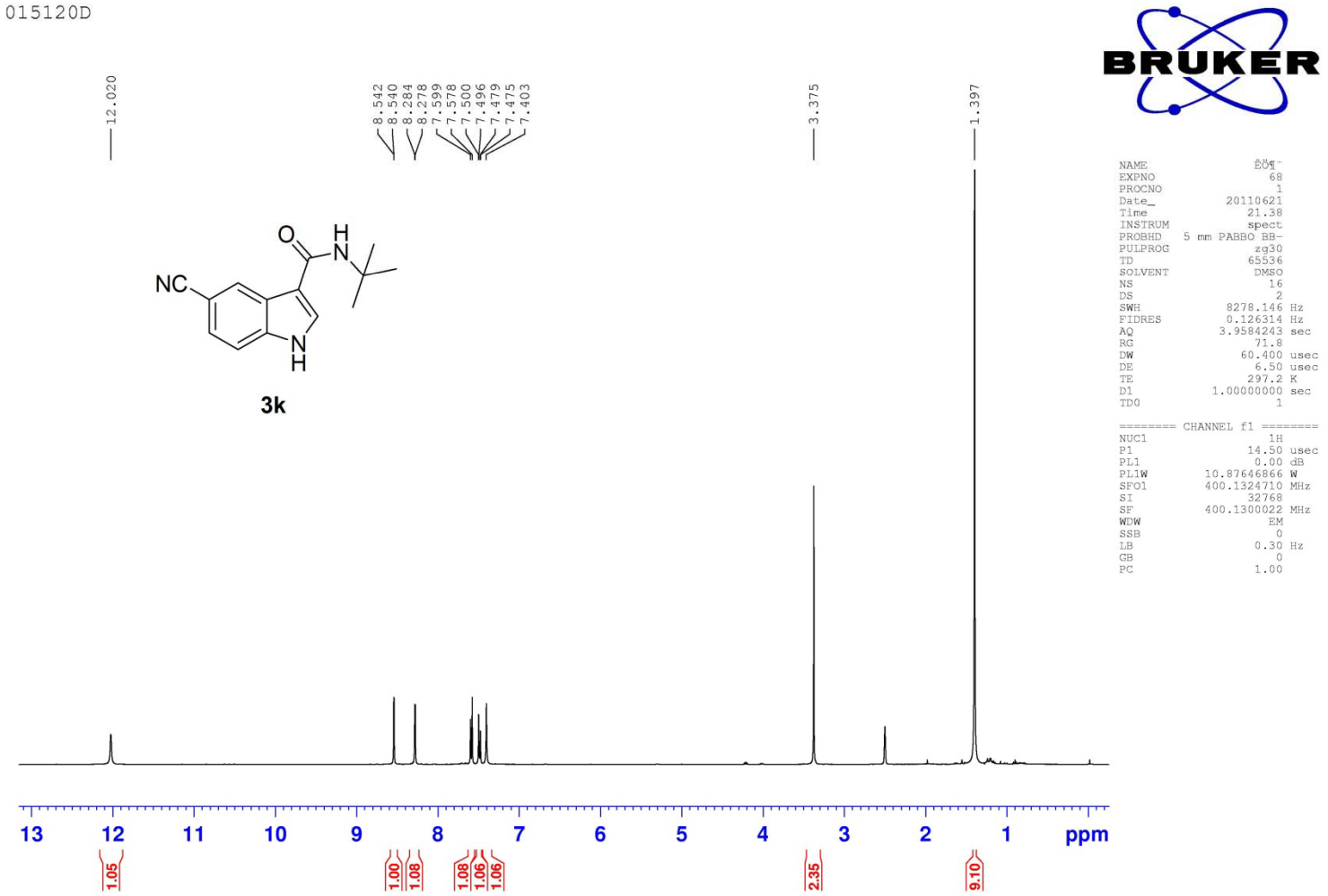


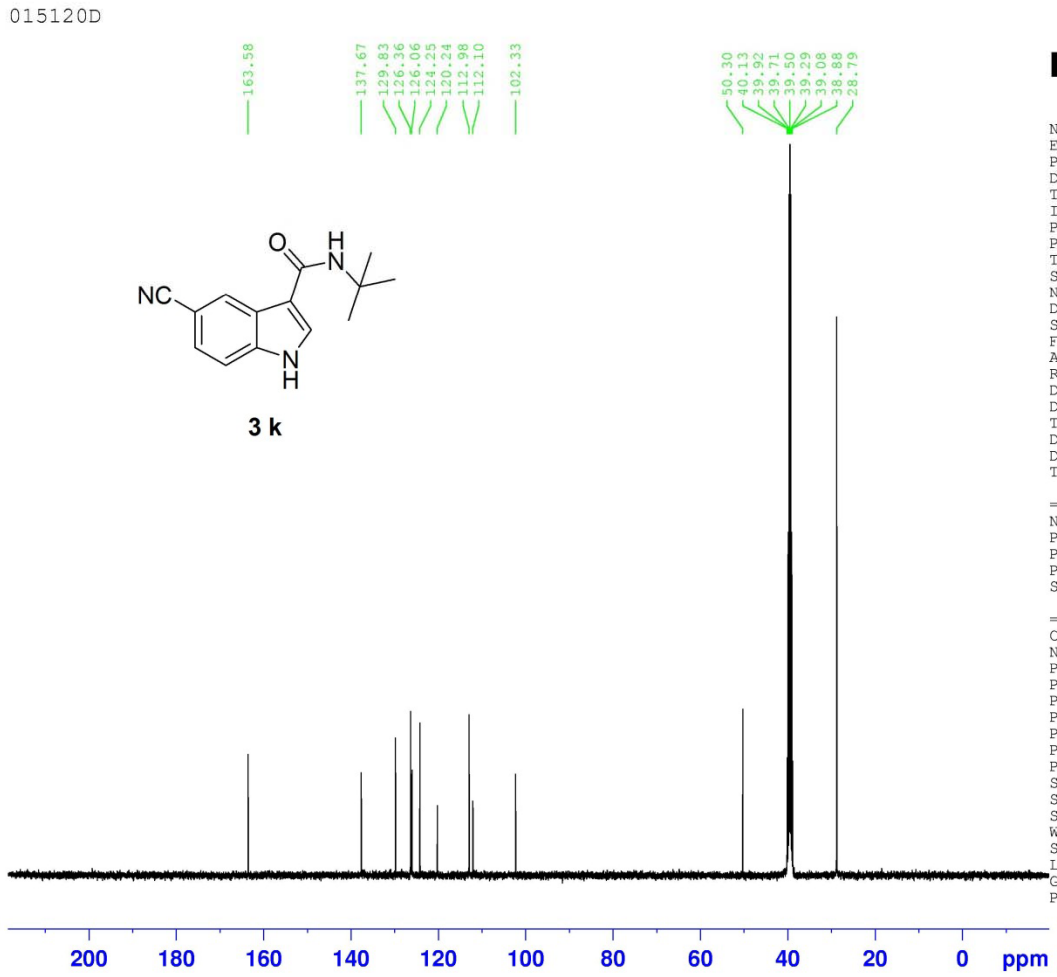
NAME	sd
EXPNO	78
PROCNO	1
Date_	20110626
Time	23.04
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	967
DS	4
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	1024
DW	20.850 usec
DE	6.50 usec
TE	312.4 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.25 usec
PL1	0.00 dB
PL1W	38.68305206 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	14.54 dB
PL13	0.00 dB
PL2W	10.87646866 W
PL12W	0.38237360 W
PL13W	10.87646866 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6128358 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

Electronic Supplementary Material (ESI) for Chemical Communications



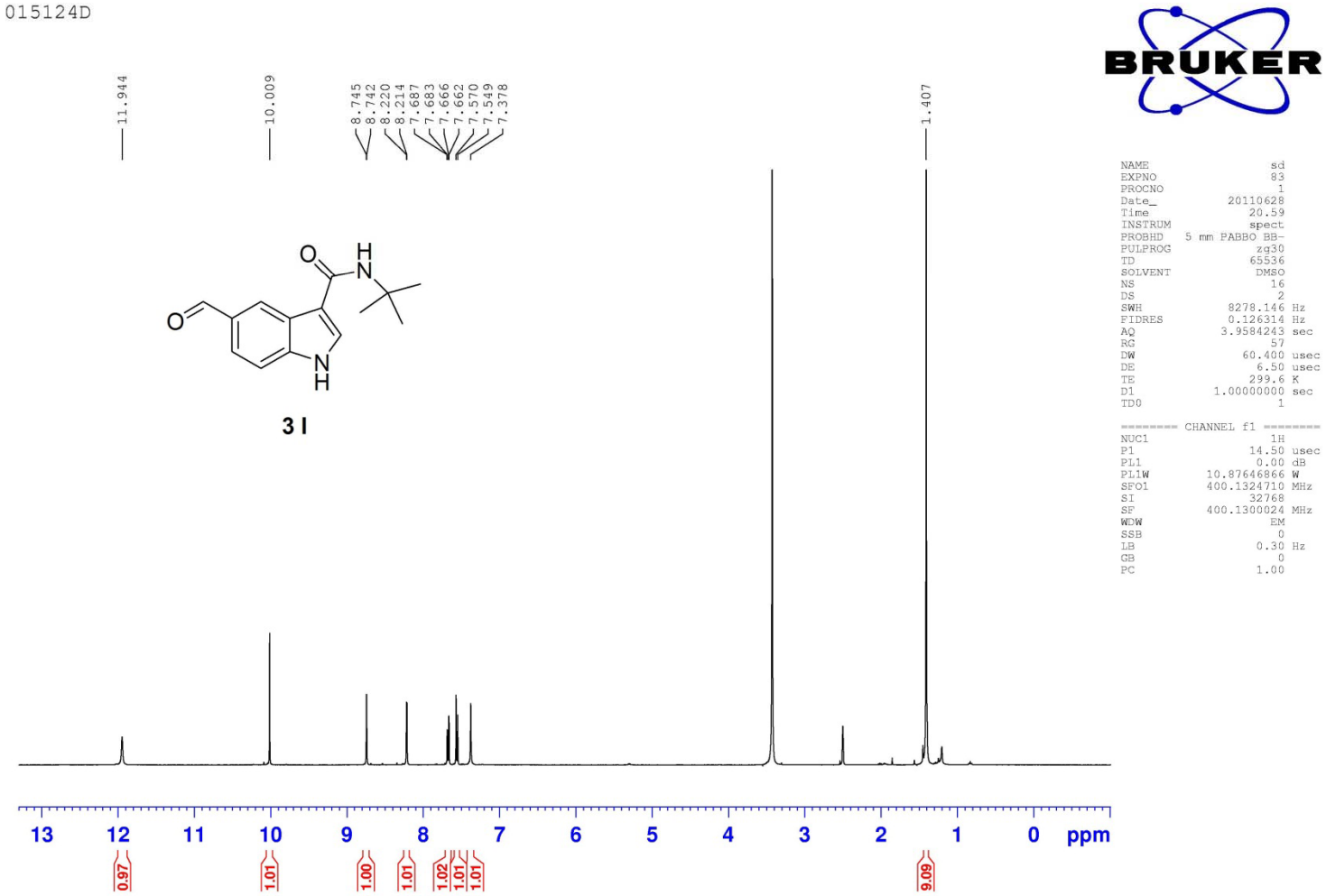


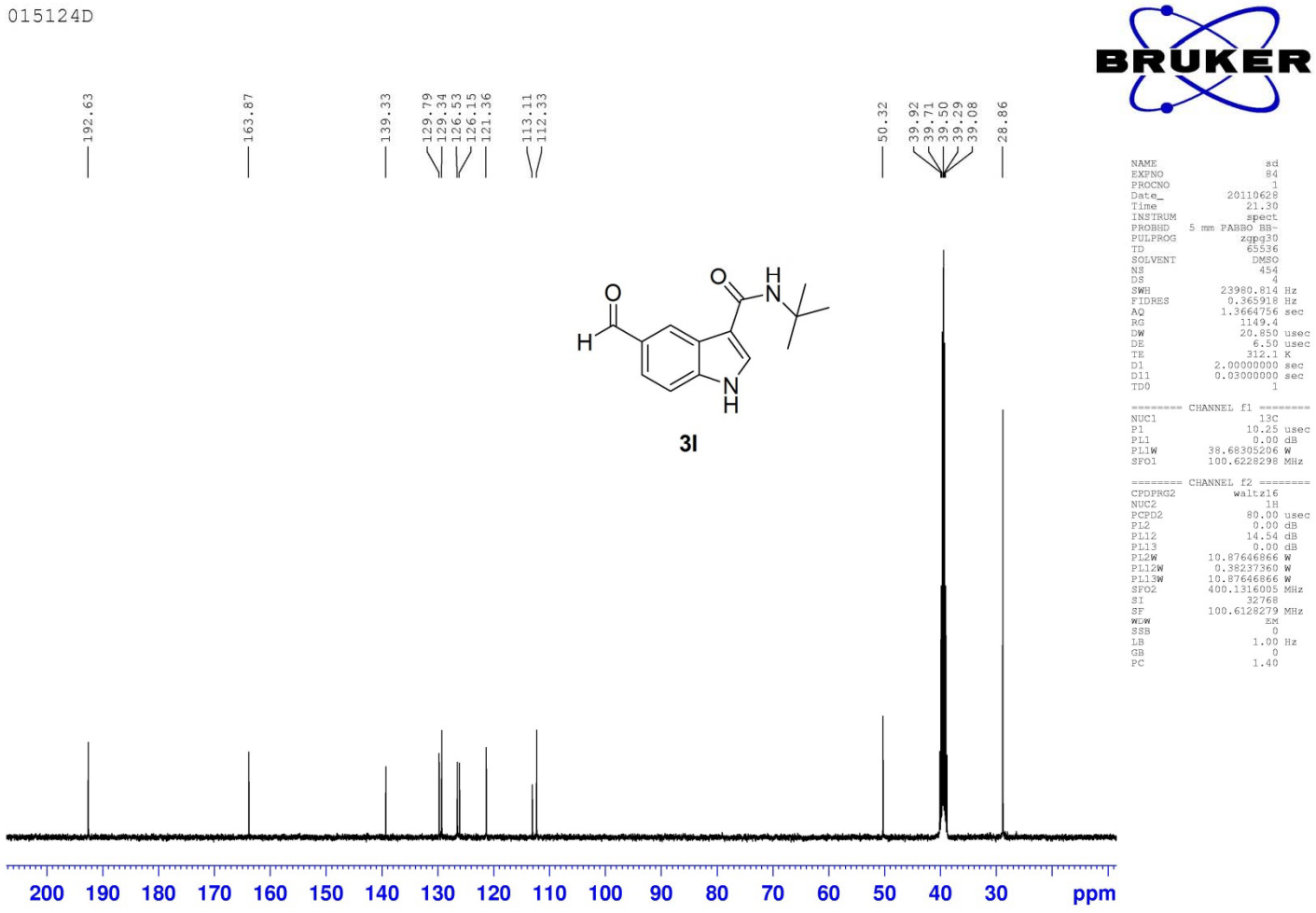

015120D
12.020
8.542
8.540
8.284
8.278
7.599
7.578
7.500
7.496
7.479
7.475
7.403
3.375
1.397
NC
O
H
N
N
H
3k
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.05
1.00
1.08
1.08
1.06
1.06
2.35
9.10
NAME ÊÖ¶¯
EXPNO 68
PROCNO 1
Date_ 20110621
Time 21.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 71.8
DW 60.400 usec
DE 6.50 usec
TE 297.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.50 usec
PL1 0.00 dB
PL1W 10.87668866 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300022 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



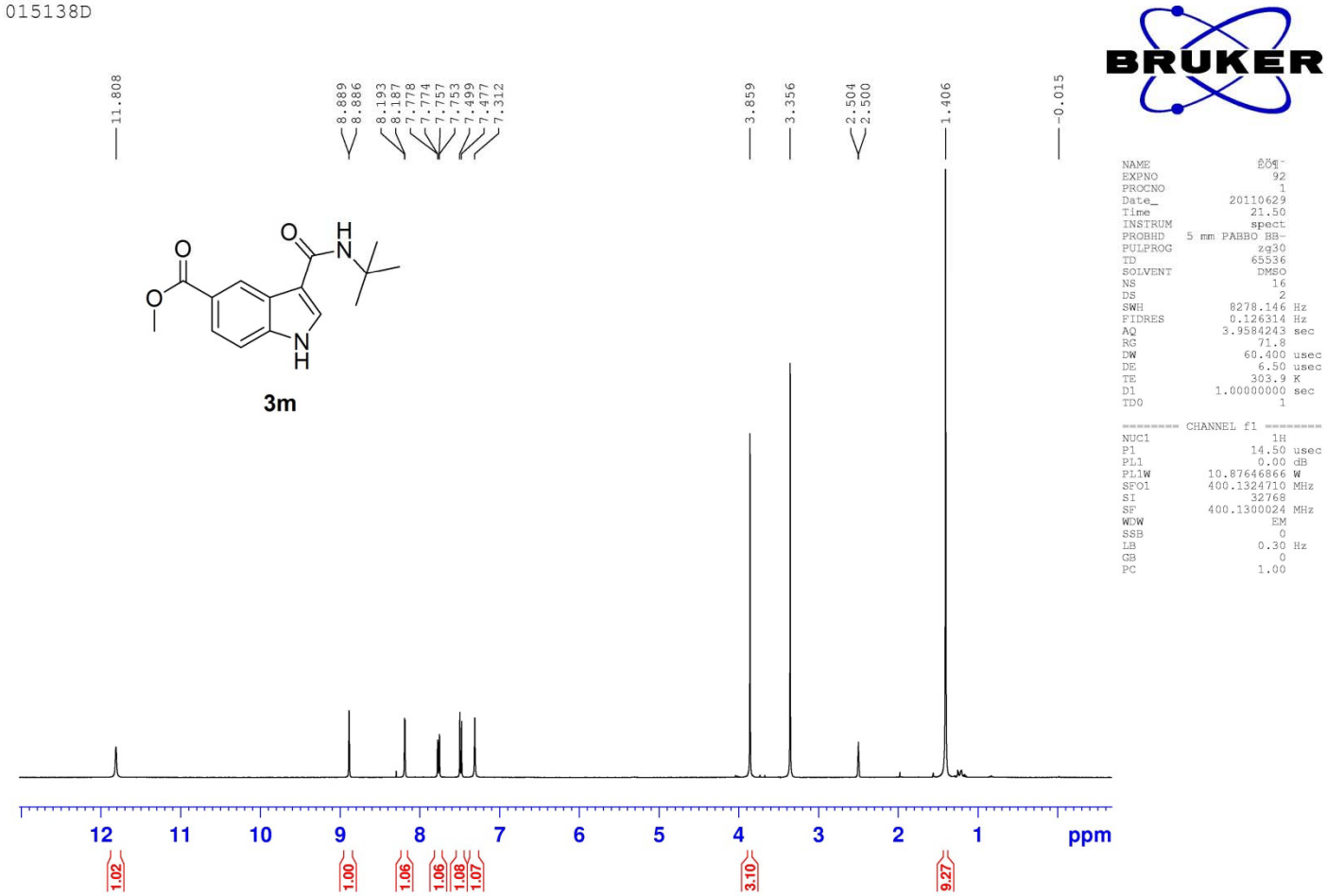
BRUKER

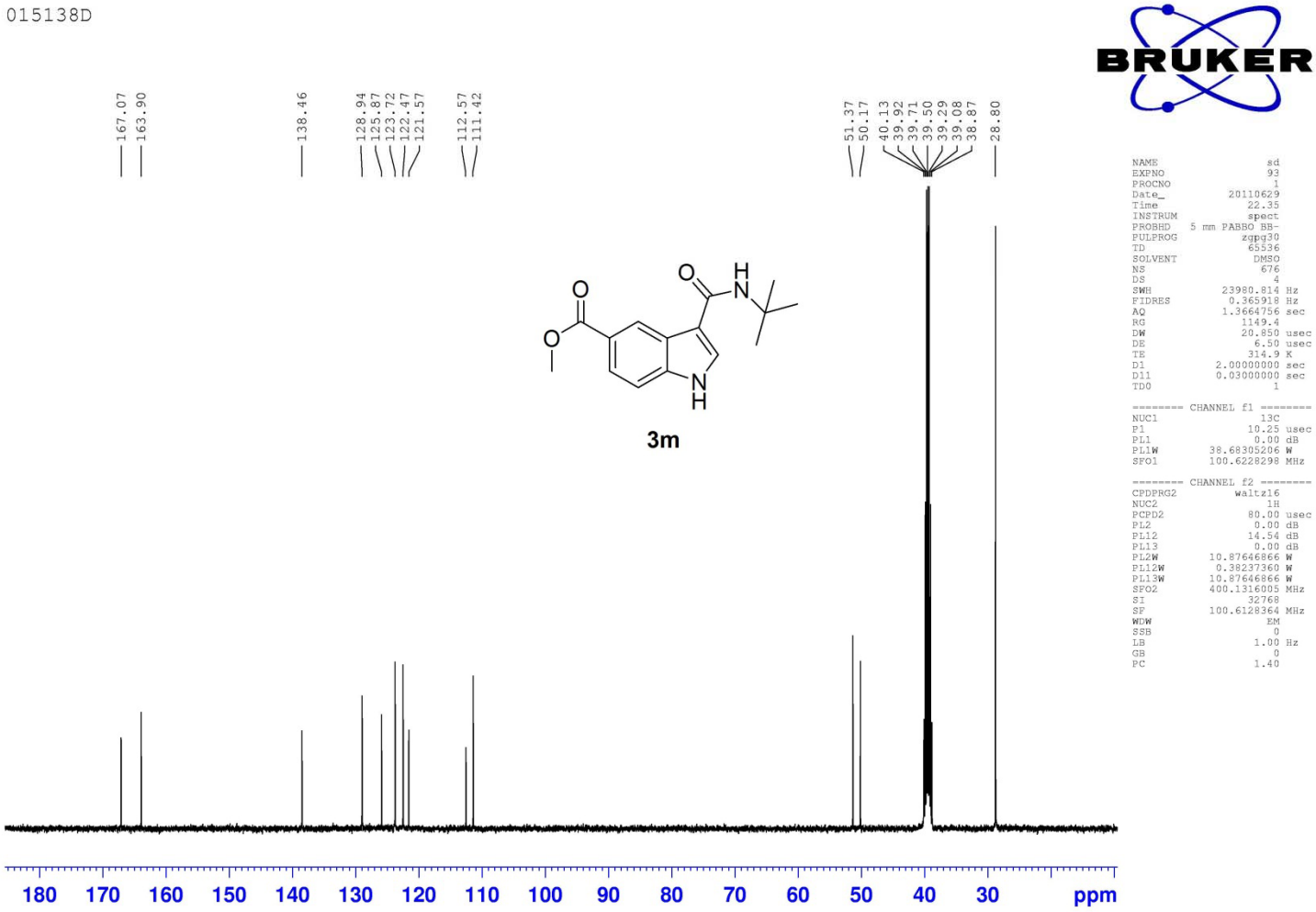
NAME	sd
EXPNO	69
PROCNO	1
Date_	20110621
Time	22.12
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	440
DS	4
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	1149.4
DW	20.850 usec
DE	6.50 usec
TE	309.7 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.25 usec
PL1	0.00 dB
PL1W	38.68305206 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	14.54 dB
PL13	0.00 dB
PL2W	10.87646866 W
PL12W	0.38237360 W
PL13W	10.87646866 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6128324 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



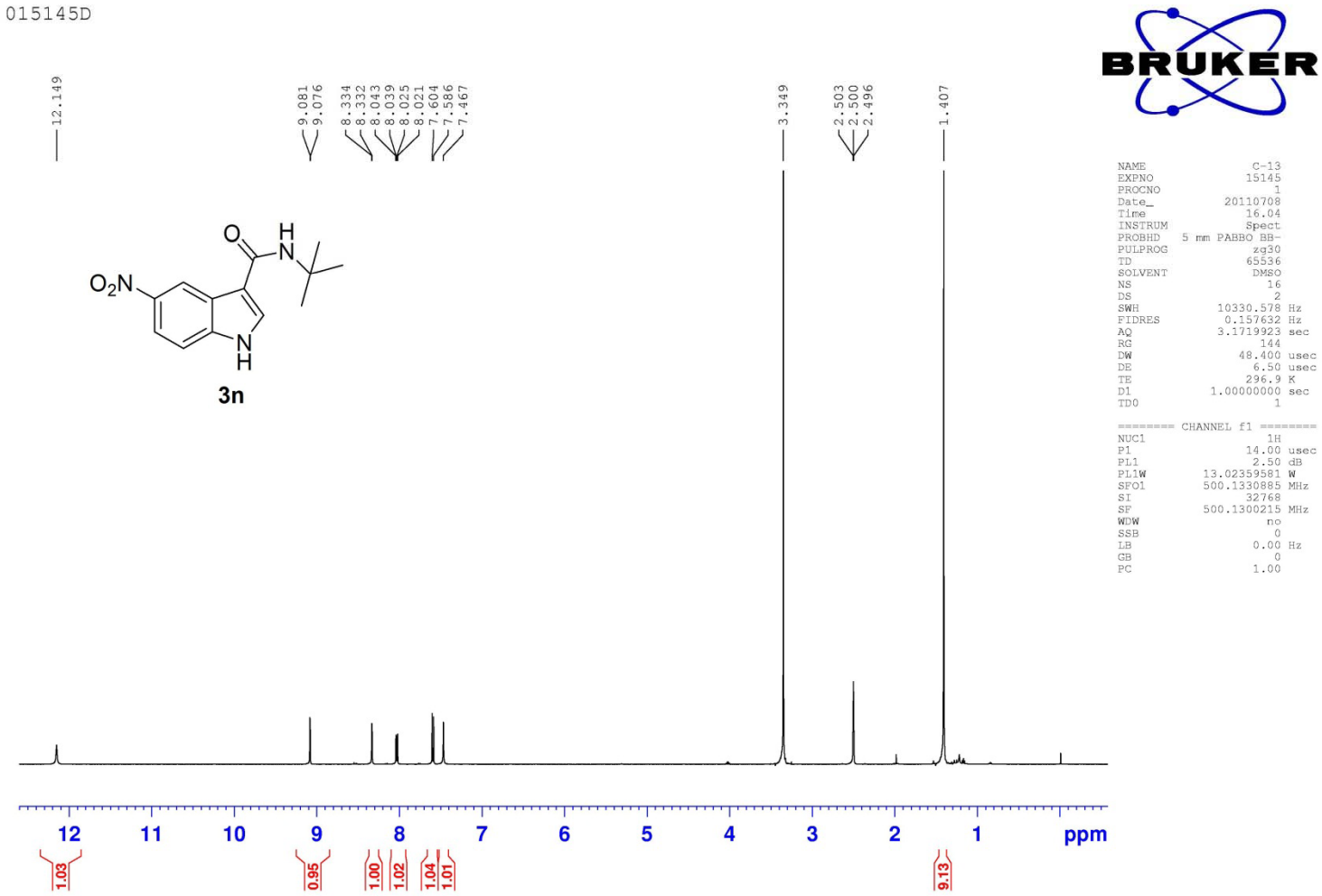


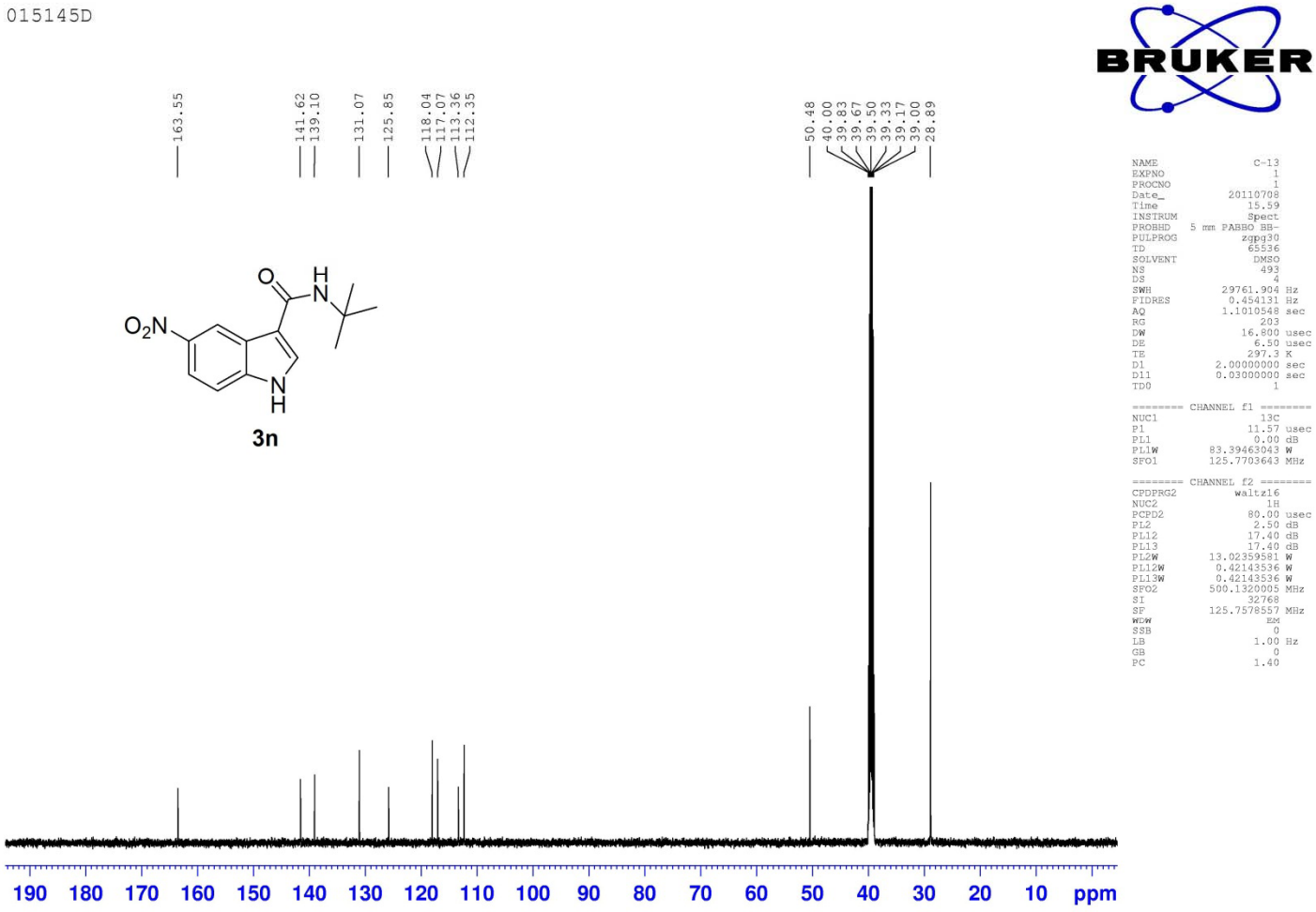

```
NAME                  sd
EXPNO                 84
PROCNO                 1
Date_           20110628
Time               21.30
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                   454
DS                     4
SWH          23980.814 Hz
FIDRES        0.365918 Hz
AQ            1.3664756 sec
RG               1149.4
DW              20.850 usec
DE               6.50 usec
TE              312.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                10.25 usec
PL1                0.00 dB
PL1W        38.68305206 W
SFO1       100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2                0.00 dB
PL12              14.54 dB
PL13               0.00 dB
PL2W        10.87646866 W
PL12W        0.38237360 W
PL13W       10.87646866 W
SFO2       400.1316005 MHz
SI                 32768
SF         100.6128279 MHz
WDW                   EM
SSB                    0
LB                1.00 Hz
GB                     0
PC                 1.40
```

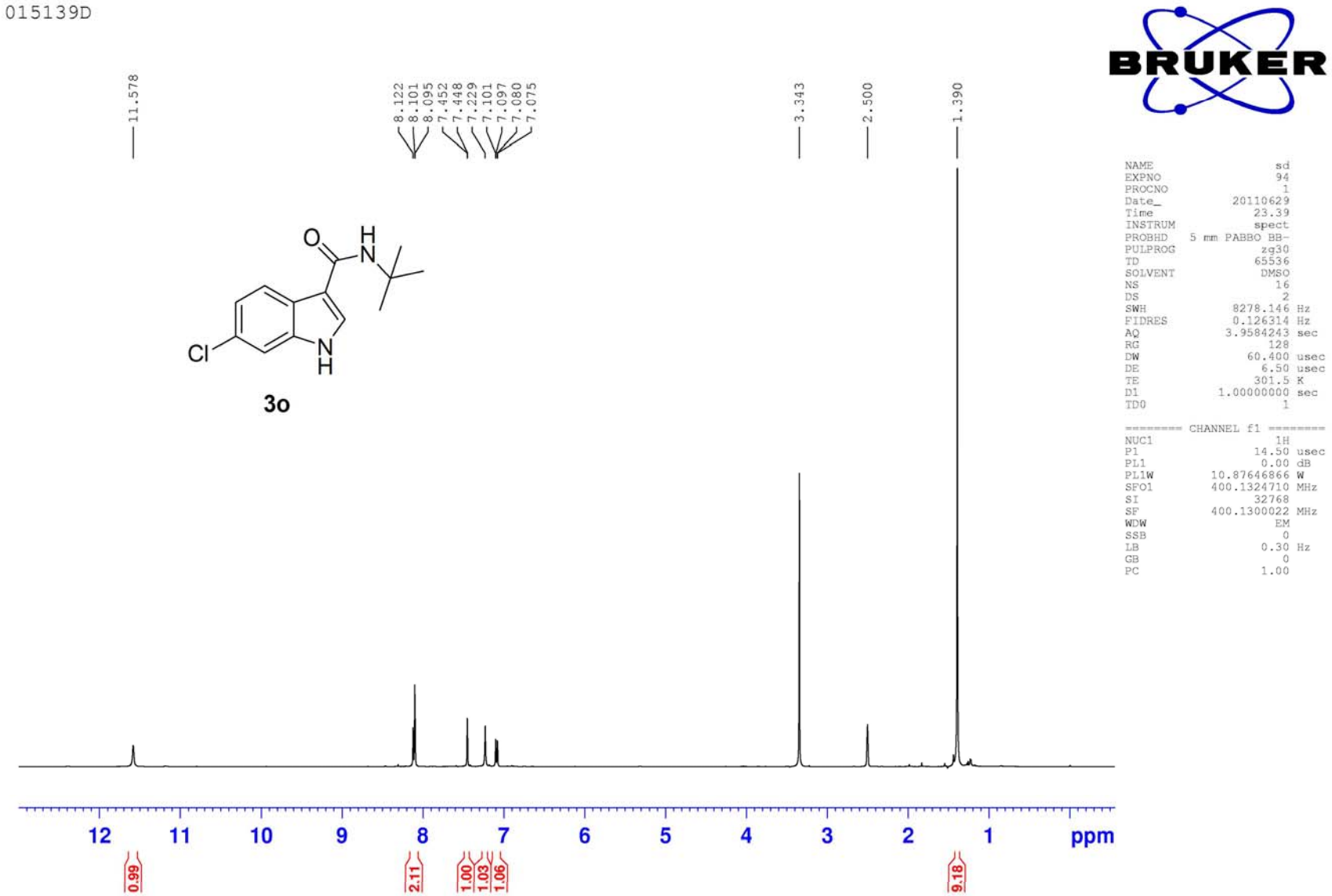

015138D
11.808
8.889
8.886
8.193
8.187
7.778
7.774
7.757
7.753
7.499
7.477
7.312
3.859
3.356
2.504
2.500
1.406
-0.015
3m
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.02
1.00
1.06
1.06
1.08
1.07
3.10
9.27
NAME EO4
EXPNO 92
PROCNO 1
Date_ 20110629
Time 21.50
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 71.8
DW 60.400 usec
DE 6.50 usec
TE 303.9 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 14.50 usec
PL1 0.00 dB
PL1W 10.87646866 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300024 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

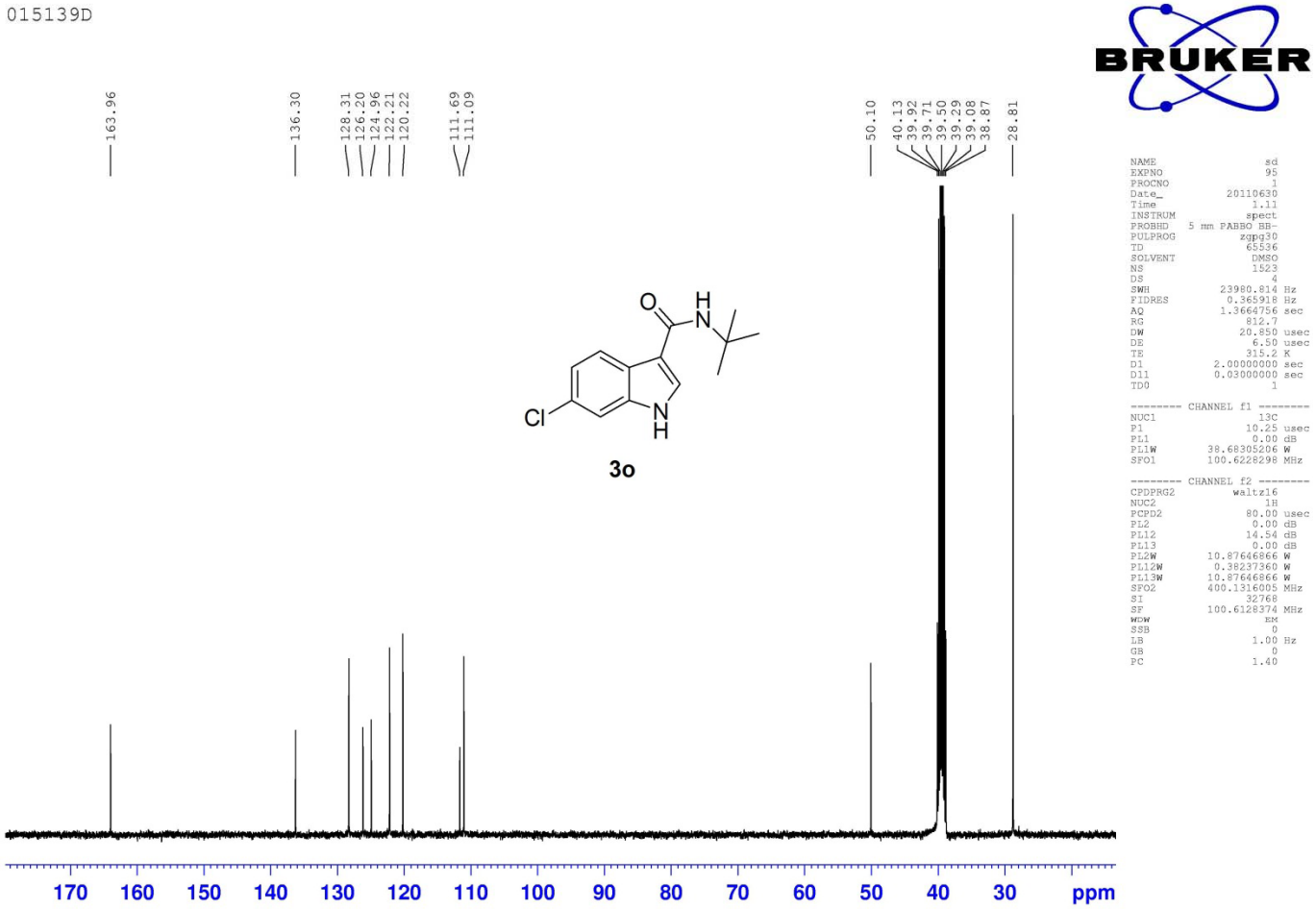


NAME	sd
EXPNO	93
PROCNO	1
Date_	20110629
Time	22.35
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	676
DS	4
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	1149.4
DW	20.850 usec
DE	6.50 usec
TE	314.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.25 usec
PL1	0.00 dB
PL1W	38.68305206 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	14.54 dB
PL13	0.00 dB
PL2W	10.87646866 W
PL12W	0.38237360 W
PL13W	10.87646866 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6128364 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

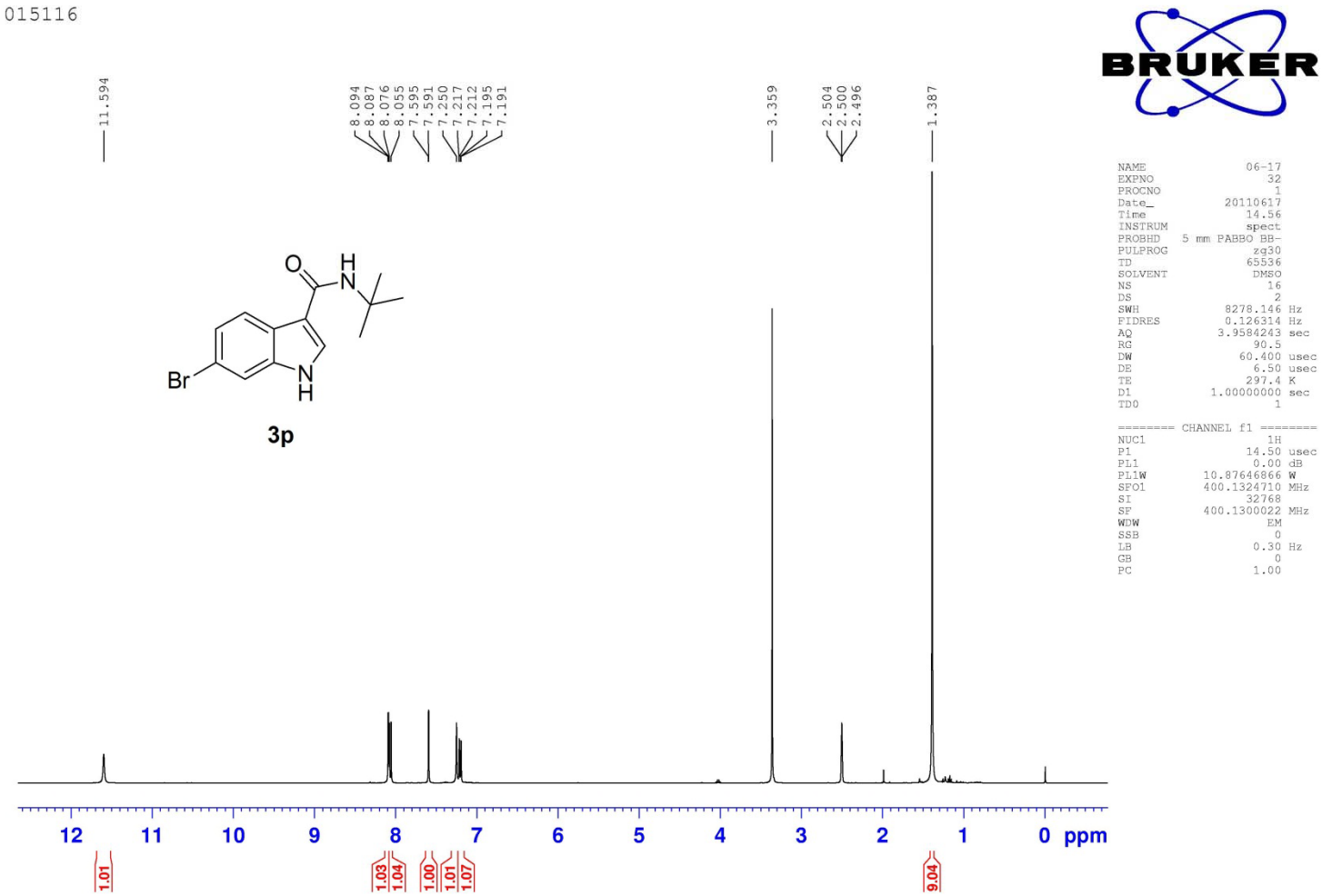

015145D
12.149
9.081
9.076
8.334
8.332
8.043
8.039
8.025
8.021
7.604
7.586
7.467
3.349
2.503
2.500
2.496
1.407
O2N
O
H
N
N
H
3n
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.03
0.95
1.00
1.02
1.04
1.01
9.13
BRUKER
NAME C-13
EXPNO 15145
PROCNO 1
Date_ 20110708
Time 16.04
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 10330.578 Hz
FIDRES 0.157632 Hz
AQ 3.1719923 sec
RG 144
DW 48.400 usec
DE 6.50 usec
TE 296.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.00 usec
PL1 2.50 dB
PL1W 13.02359581 W
SFO1 500.1330885 MHz
SI 32768
SF 500.1300215 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00


015145D
163.55
141.62
139.10
131.07
125.85
118.04
117.07
113.36
112.35
50.48
40.00
39.83
39.67
39.50
39.33
39.17
39.00
28.89
O
H
N
O2N
N
H
3n
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm
NAME C-13
EXPNO 1
PROCNO 1
Date_ 20110708
Time 15.59
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 493
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 297.3 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 11.57 usec
PL1 0.00 dB
PL1W 83.39463043 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7578557 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

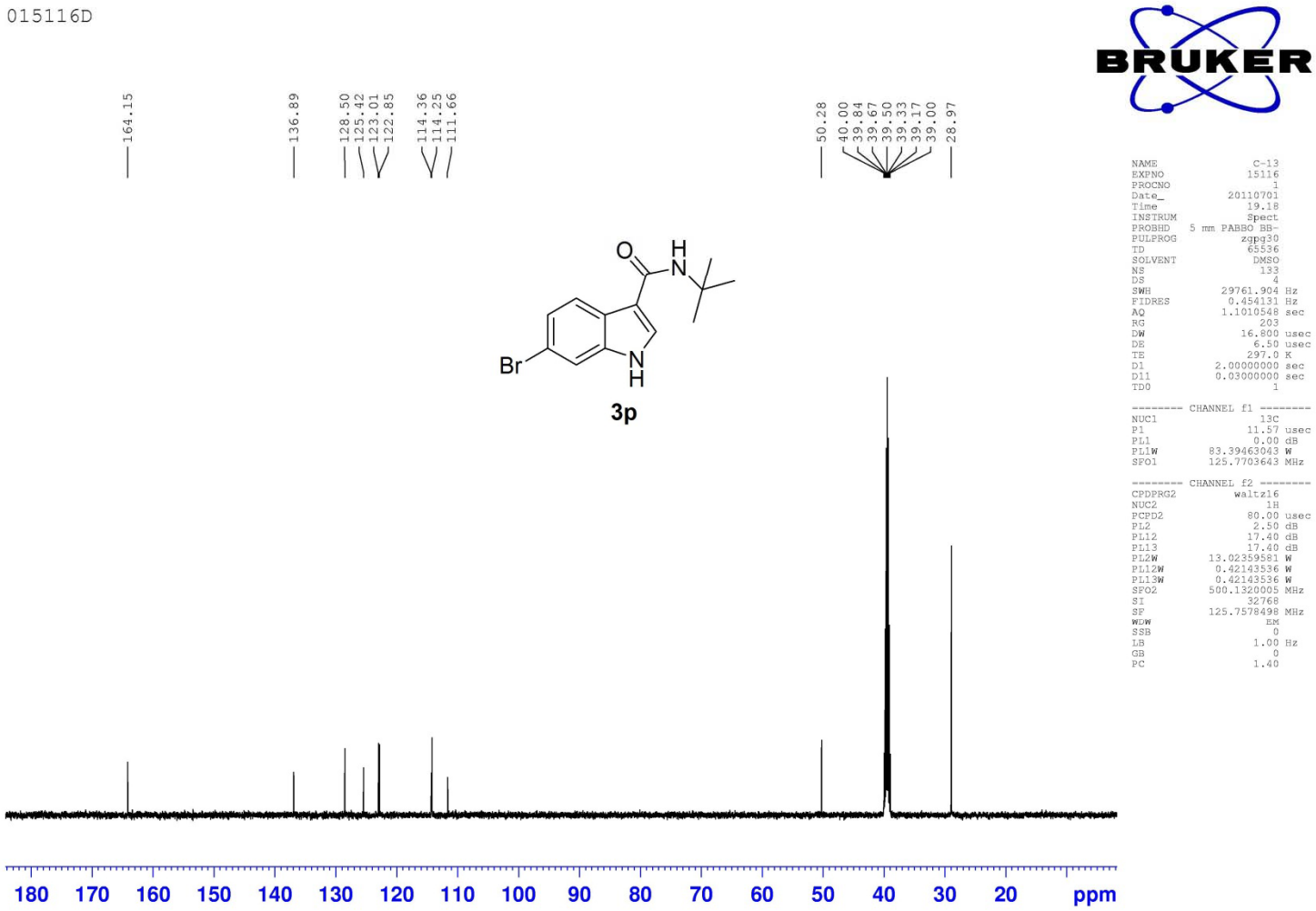


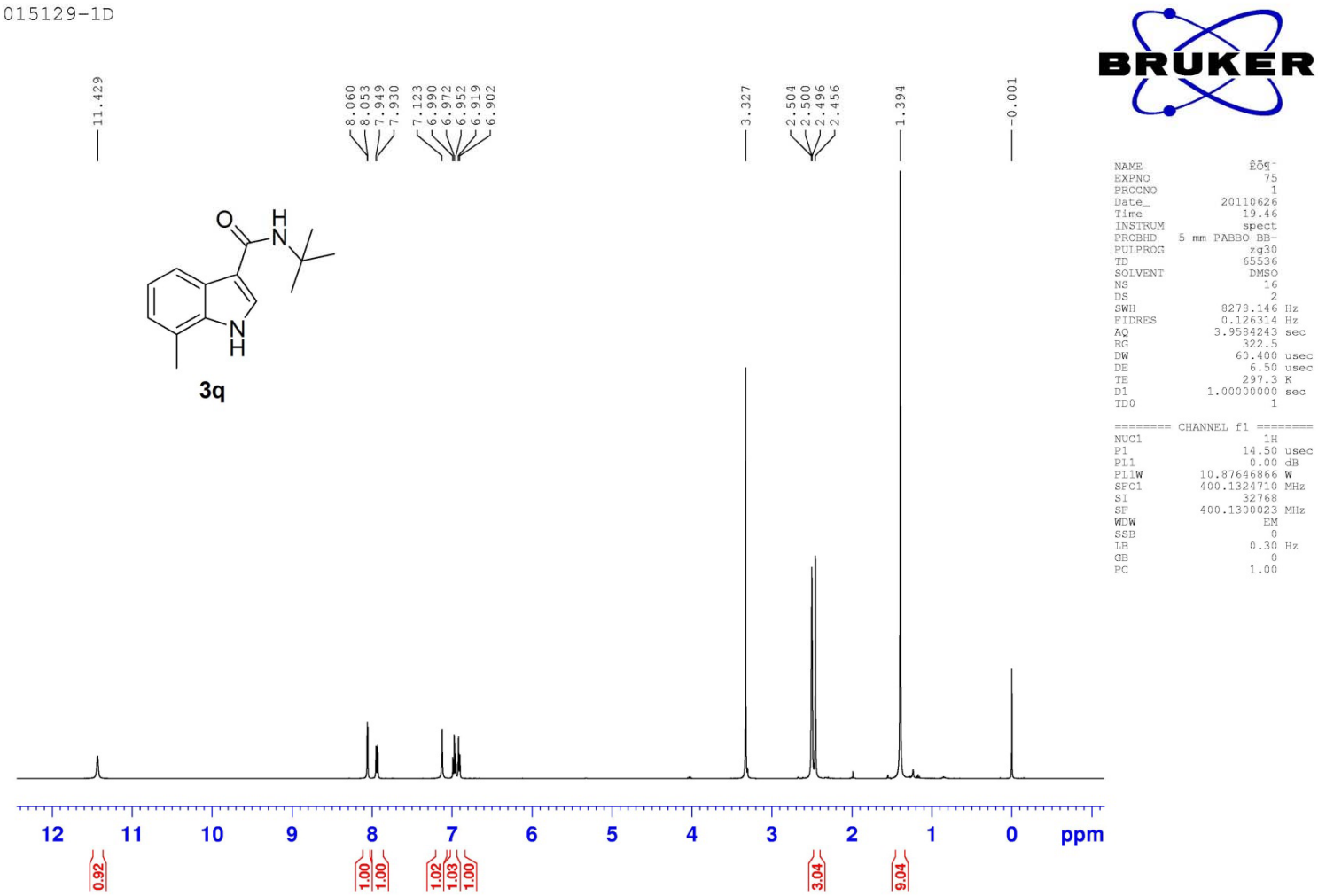


NAME	sd
EXPNO	95
PROCNO	1
Date_	20110630
Time	1.11
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	1523
DS	4
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	812.7
DW	20.850 usec
DE	6.50 usec
TE	315.2 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.25 usec
PL1	0.00 dB
PL1W	38.68305206 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	14.54 dB
PL13	0.00 dB
PL2W	10.87646866 W
PL12W	0.38237360 W
PL13W	10.87646866 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6128374 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

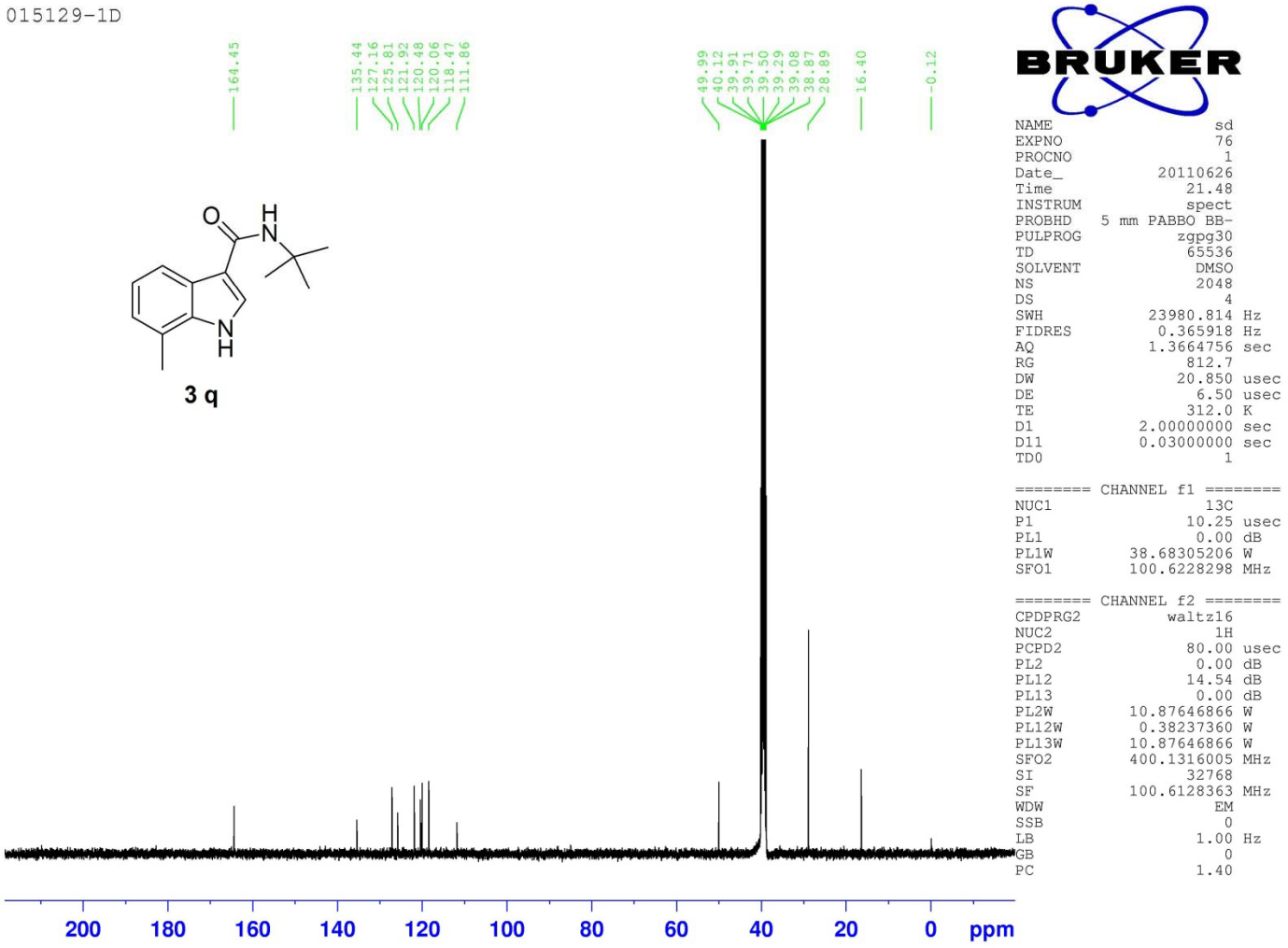


NAME	06-17
EXPNO	32
PROCNO	1
Date_	20110617
Time	14.56
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	90.5
DW	60.400 usec
DE	6.50 usec
TE	297.4 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.00 dB
PL1W	10.87646866 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300022 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

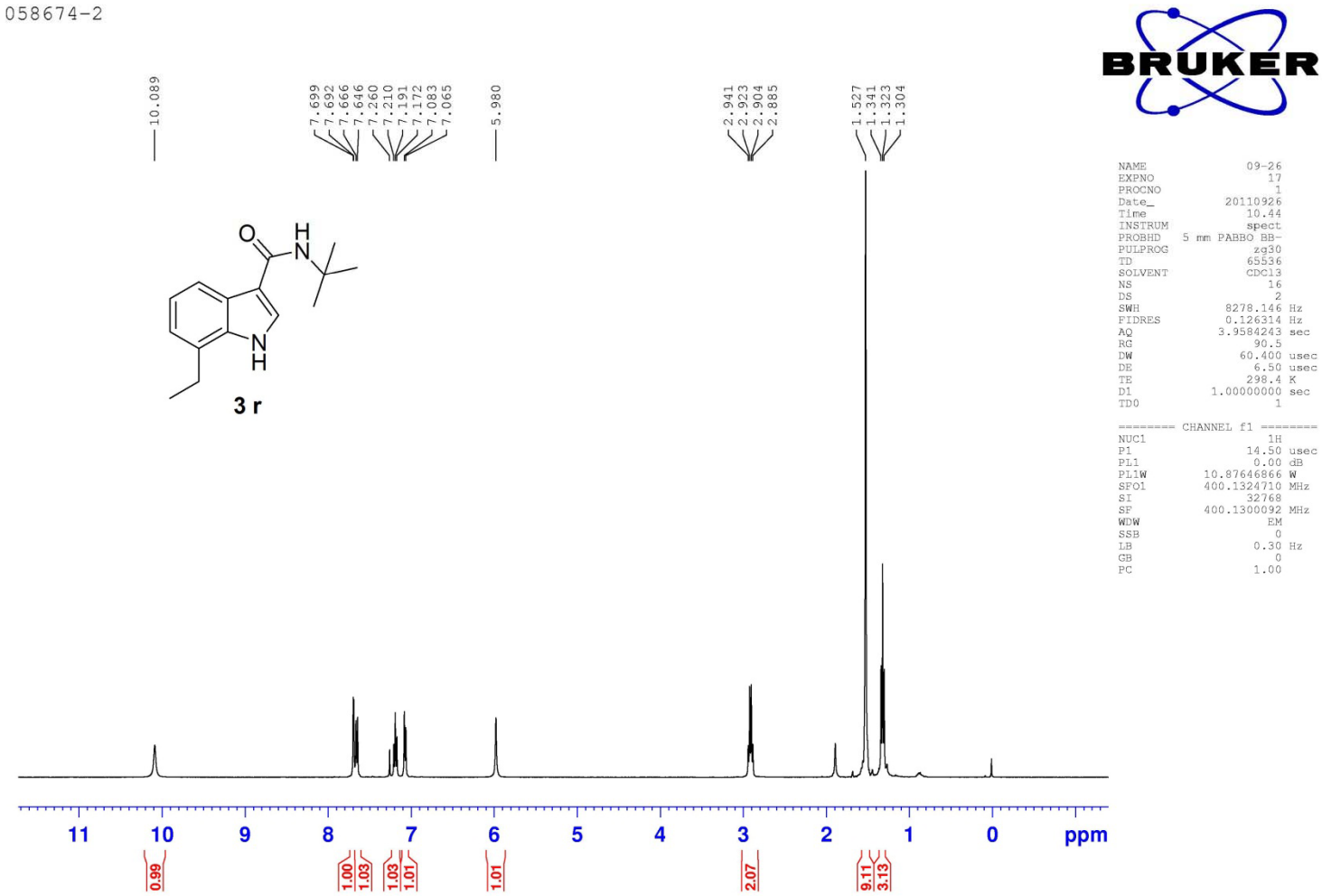

015116D
164.15
136.89
128.50
125.42
123.01
122.85
114.36
114.25
111.66
50.28
40.00
39.84
39.67
39.50
39.33
39.17
39.00
28.97
O
H
N
Br
N
H
3p
BRUKER
NAME C-13
EXPNO 15116
PROCNO 1
Date_ 20110701
Time 19.18
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 133
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 297.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 11.57 usec
PL1 0.00 dB
PL1W 83.39463043 W
SFO1 125.7703643 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7578498 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 ppm



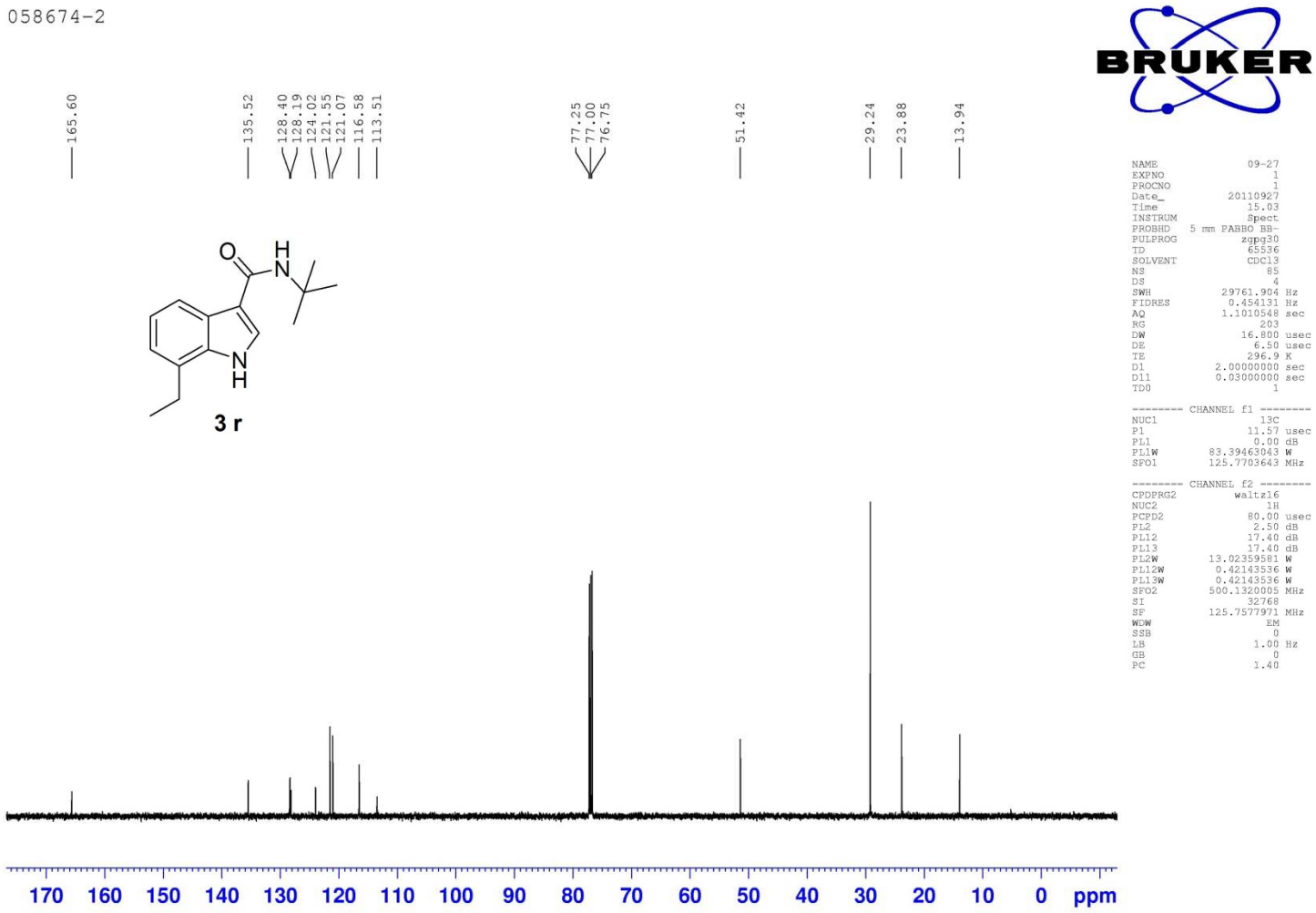

```
NAME                 ÊÖ¶¯
EXPNO                   75
PROCNO                   1
Date_             20110626
Time                 19.46
INSTRUM              spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                      16
DS                       2
SWH              8278.146 Hz
FIDRES           0.126314 Hz
AQ               3.9584243 sec
RG                   322.5
DW                  60.400 usec
DE                   6.50 usec
TE                  297.3 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    1H
P1                   14.50 usec
PL1                   0.00 dB
PL1W          10.87646866 W
SFO1          400.1324710 MHz
SI                   32768
SF            400.1300023 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```

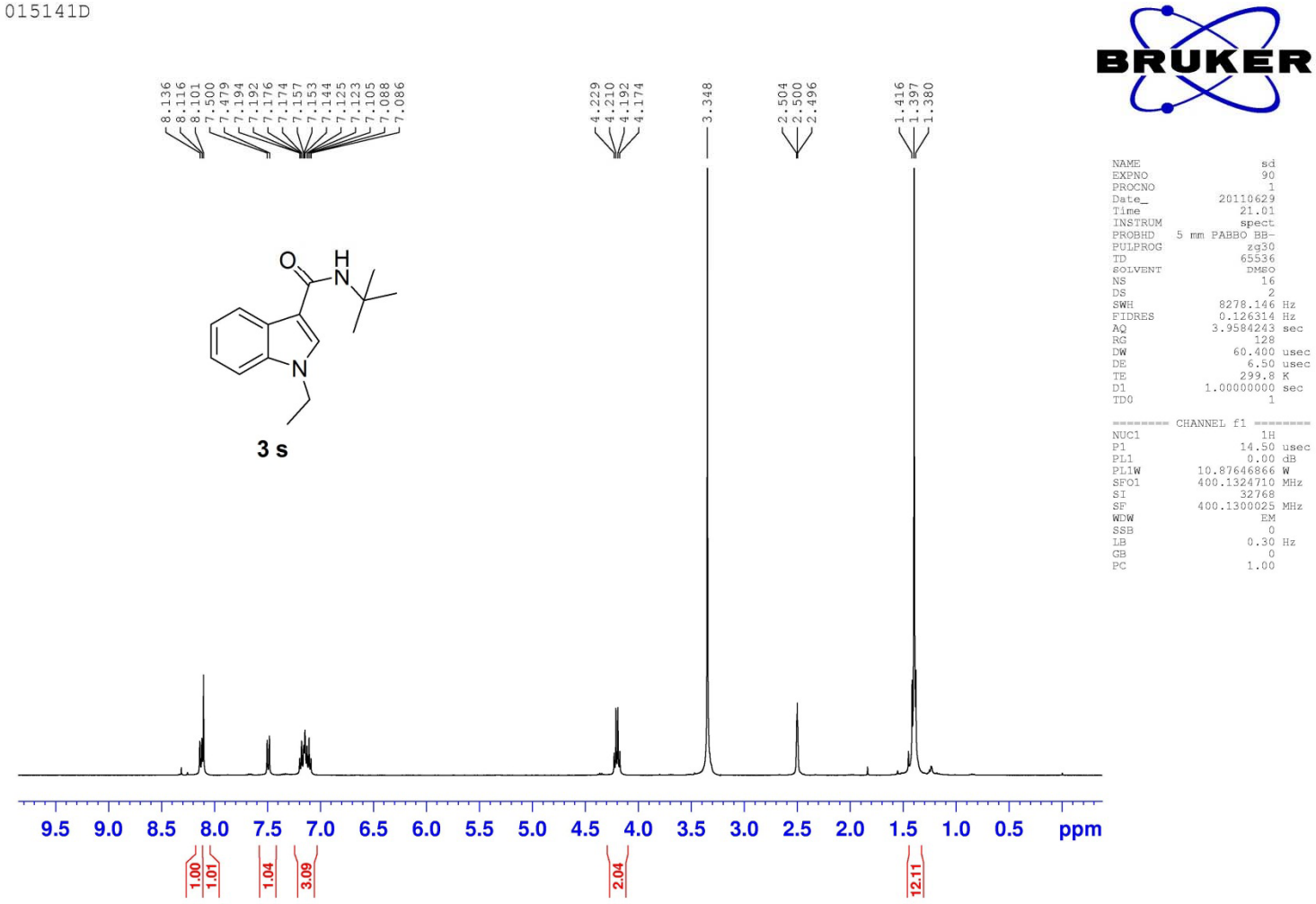


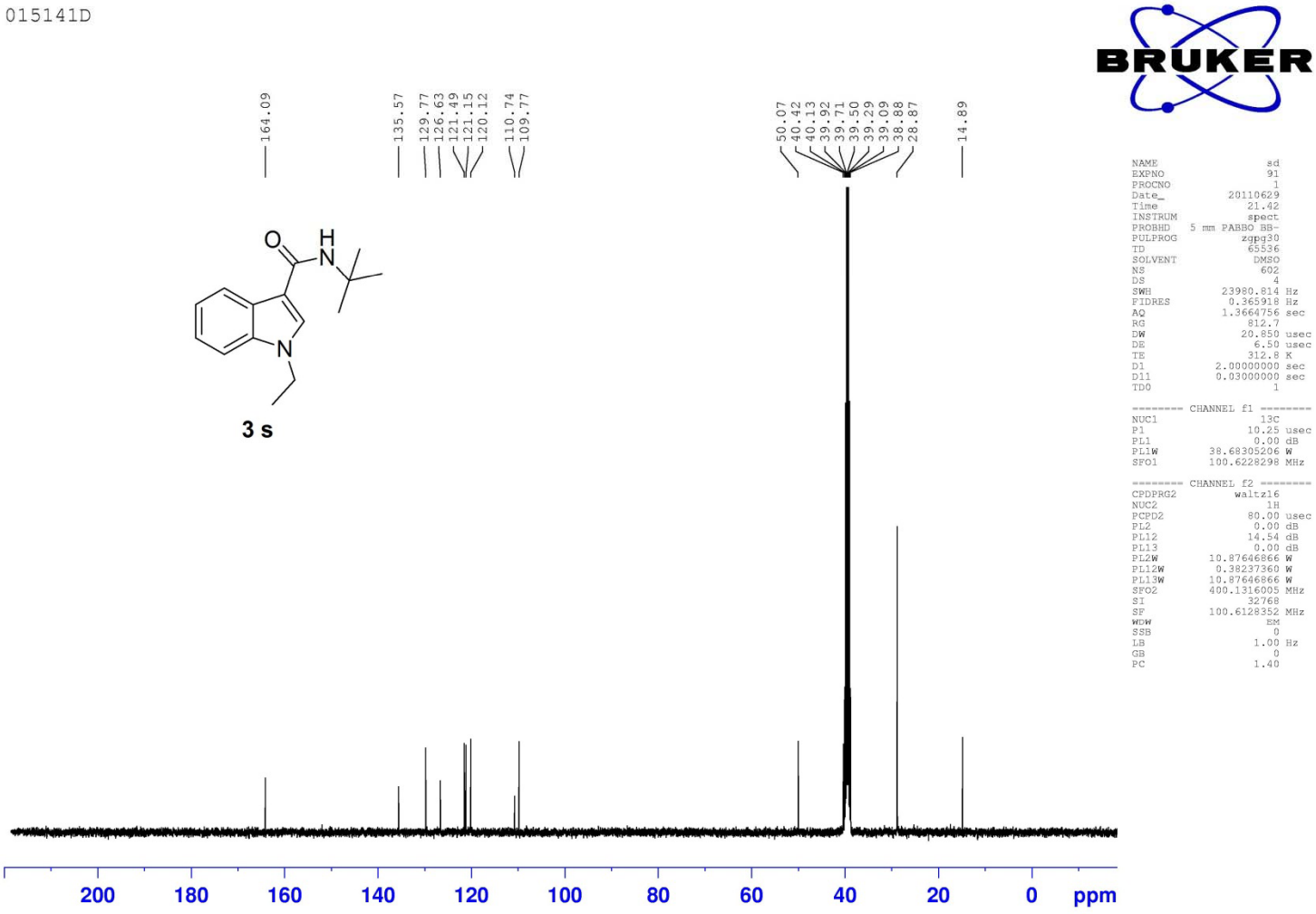

```
NAME                  sd
EXPNO                 76
PROCNO                 1
Date_           20110626
Time               21.48
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT             DMSO
NS                  2048
DS                     4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ            1.3664756 sec
RG                812.7
DW               20.850 usec
DE                6.50 usec
TE                312.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                 10.25 usec
PL1                 0.00 dB
PL1W         38.68305206 W
SFO1        100.6228298 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2              80.00 usec
PL2                 0.00 dB
PL12               14.54 dB
PL13                0.00 dB
PL2W         10.87646866 W
PL12W         0.38237360 W
PL13W        10.87646866 W
SFO2        400.1316005 MHz
SI                 32768
SF          100.6128363 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```



NAME	09-26
EXPNO	17
PROCNO	1
Date_	20110926
Time	10.44
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	90.5
DW	60.400 usec
DE	6.50 usec
TE	298.4 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.00 dB
PL1W	10.87646966 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300092 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

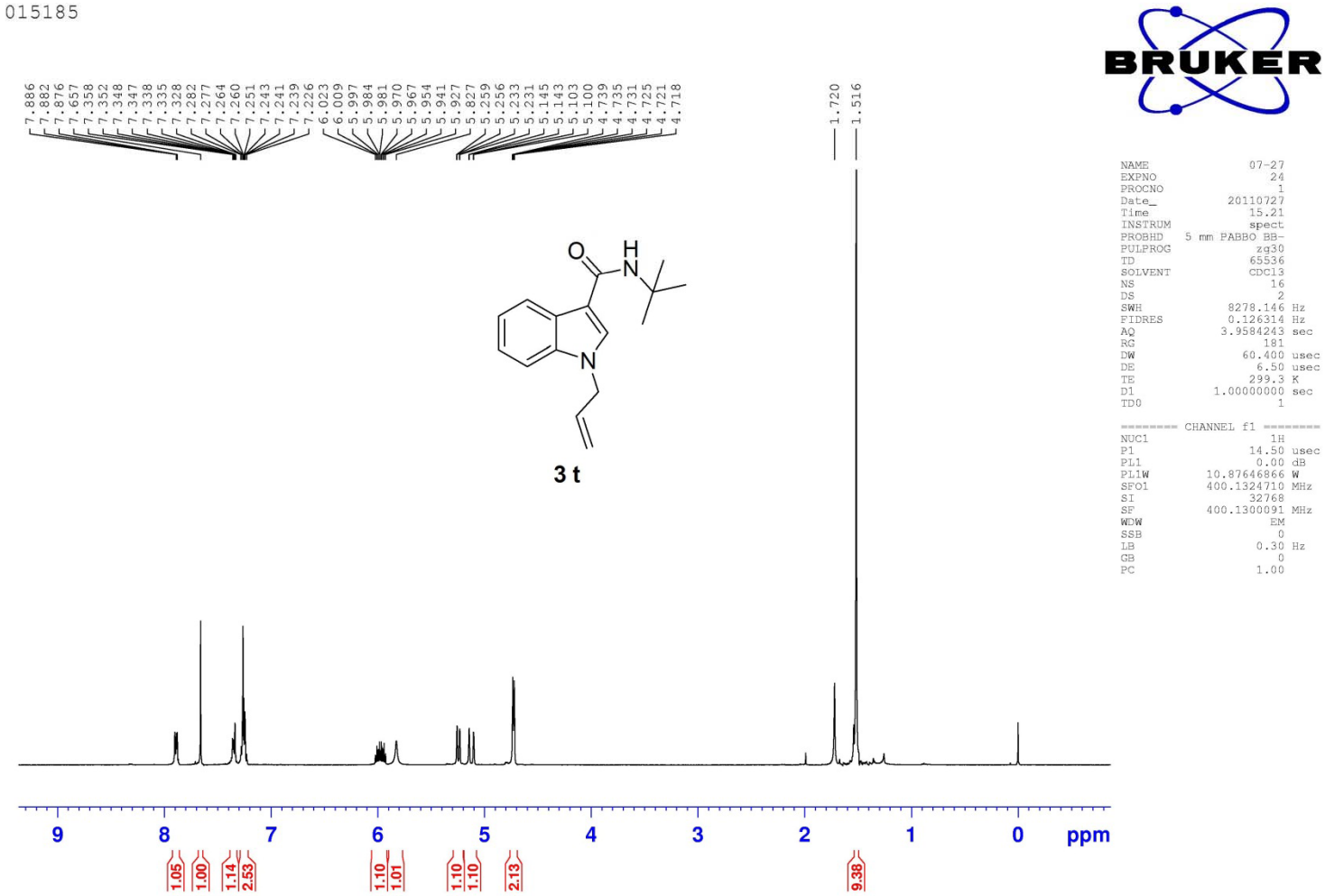

058674-2
165.60
135.52
128.40
128.19
124.02
121.55
121.07
116.58
113.51
77.25
77.00
76.75
51.42
29.24
23.88
13.94
3 r
NAME 09-27
EXPNO 1
PROCNO 1
Date_ 20110927
Time 15.03
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 85
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 296.9 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 11.57 usec
PL1 0.00 dB
PL1W 83.39463043 W
SFO1 125.7703643 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577971 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


015141D
8.136
8.116
8.101
7.500
7.479
7.194
7.192
7.176
7.174
7.157
7.153
7.144
7.125
7.123
7.105
7.088
7.086
4.229
4.210
4.192
4.174
3.348
2.504
2.500
2.496
1.416
1.397
1.380
O
H
N
N
3 s
BRUKER
NAME sd
EXPNO 90
PROCNO 1
Date_ 20110629
Time 21.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 128
DW 60.400 usec
DE 6.50 usec
TE 299.8 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 14.50 usec
PL1 0.00 dB
PL1W 10.87646866 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300025 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
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 ppm
1.00
1.01
1.04
3.09
2.04
12.11



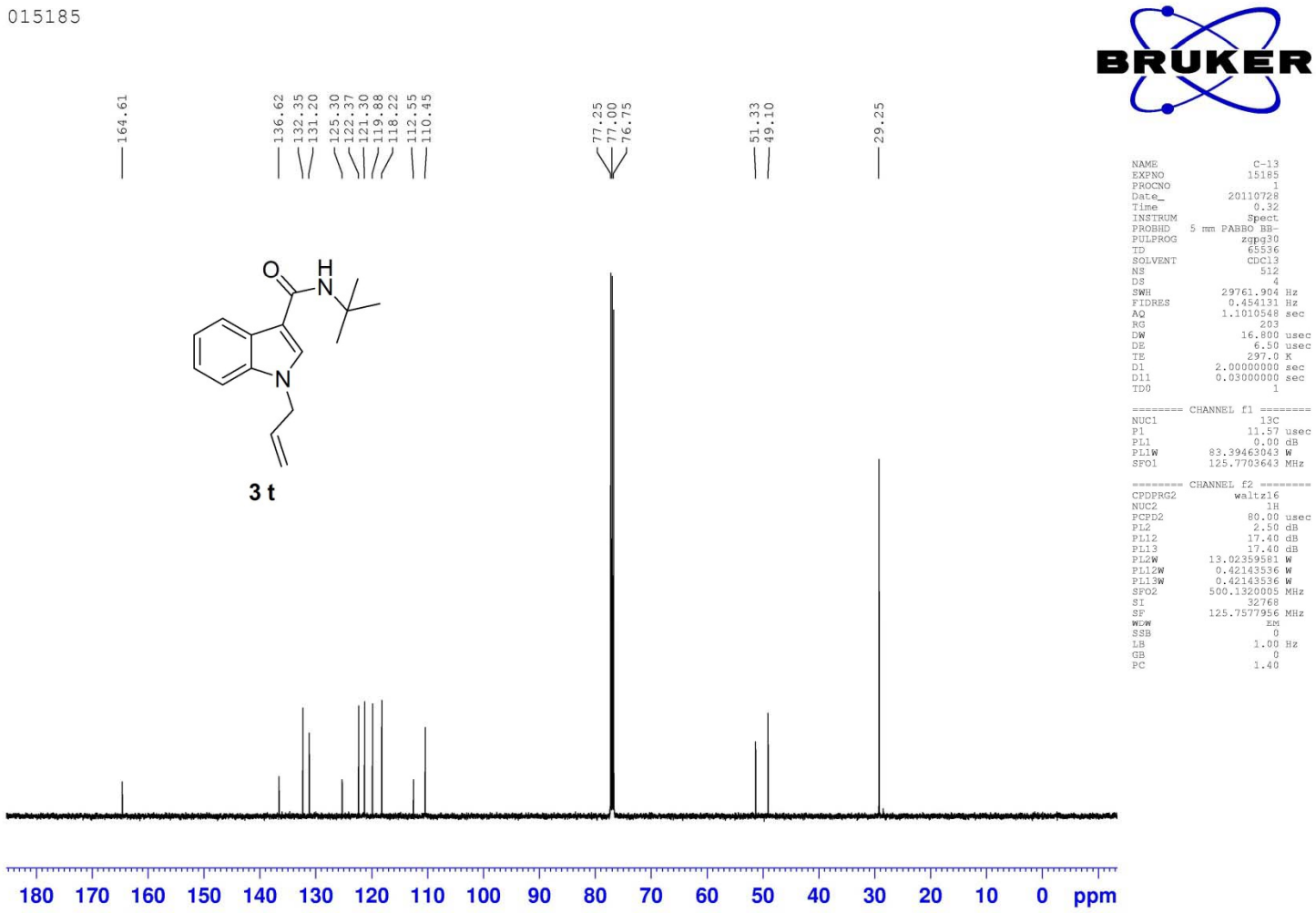
BRUKER

NAME	sd
EXPNO	91
PROCNO	1
Date_	20110629
Time	21.42
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	602
DS	4
SWH	23980.814 Hz
FIDRES	0.365918 Hz
AQ	1.3664756 sec
RG	812.7
DW	20.850 usec
DE	6.50 usec
TE	312.8 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	10.25 usec
PL1	0.00 dB
PL1W	38.68305206 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	0.00 dB
PL12	14.54 dB
PL13	0.00 dB
PL2W	10.87646866 W
PL12W	0.38237360 W
PL13W	10.87646866 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6128352 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



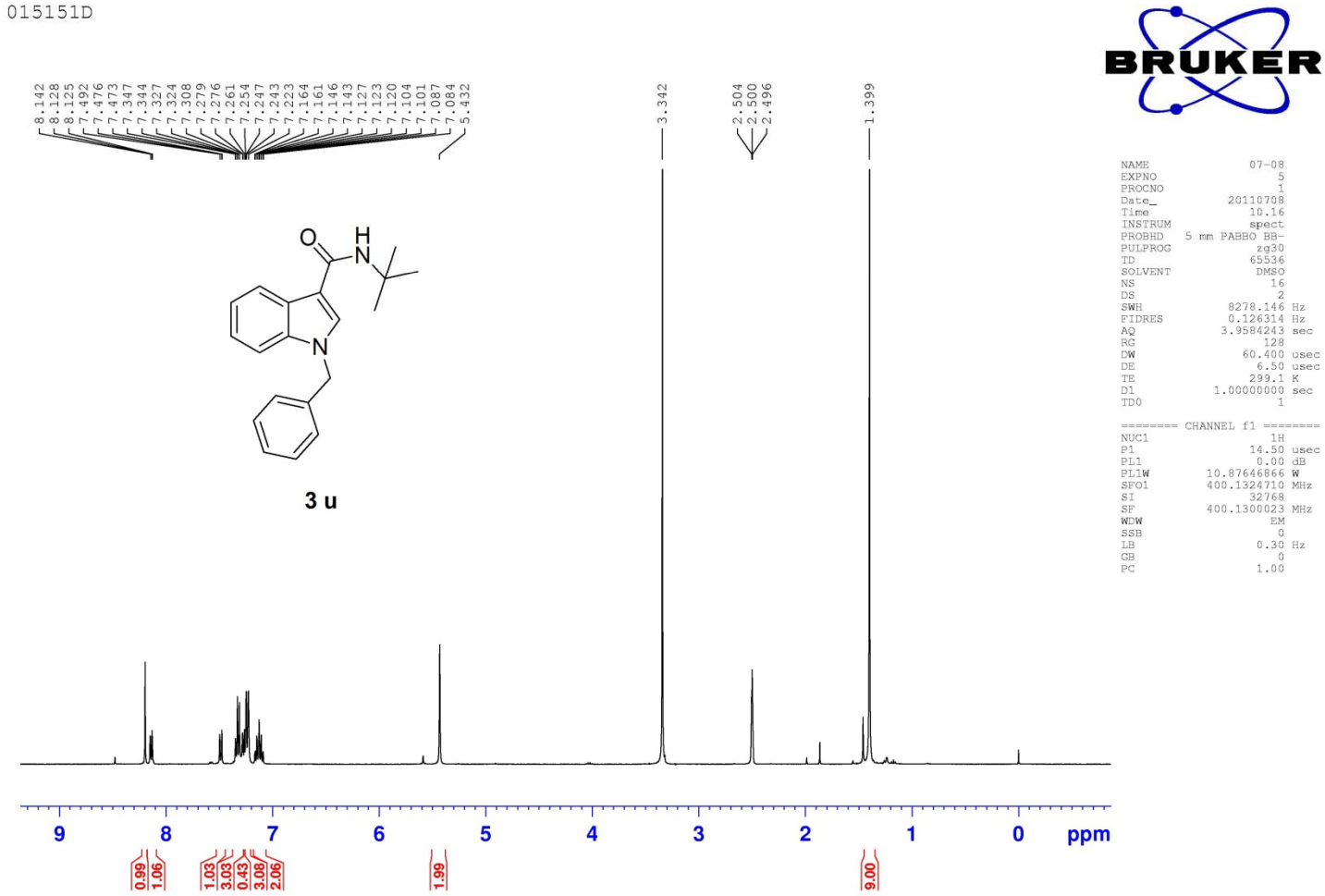
BRUKER

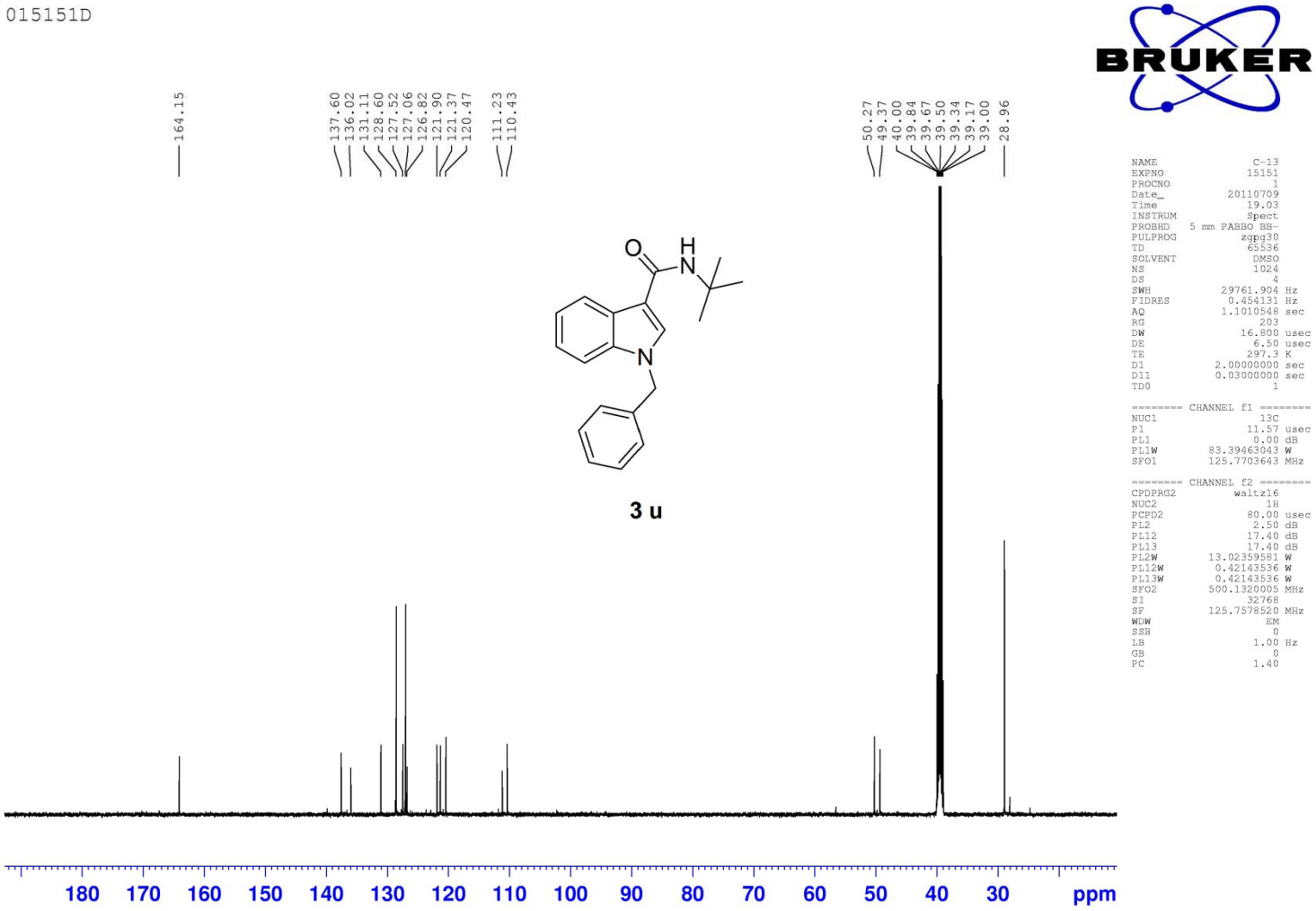
NAME	07-27
EXPNO	24
PROCNO	1
Date_	20110727
Time	15.21
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	181
DW	60.400 usec
DE	6.50 usec
TE	299.3 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.00 dB
PL1W	10.87646866 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300091 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



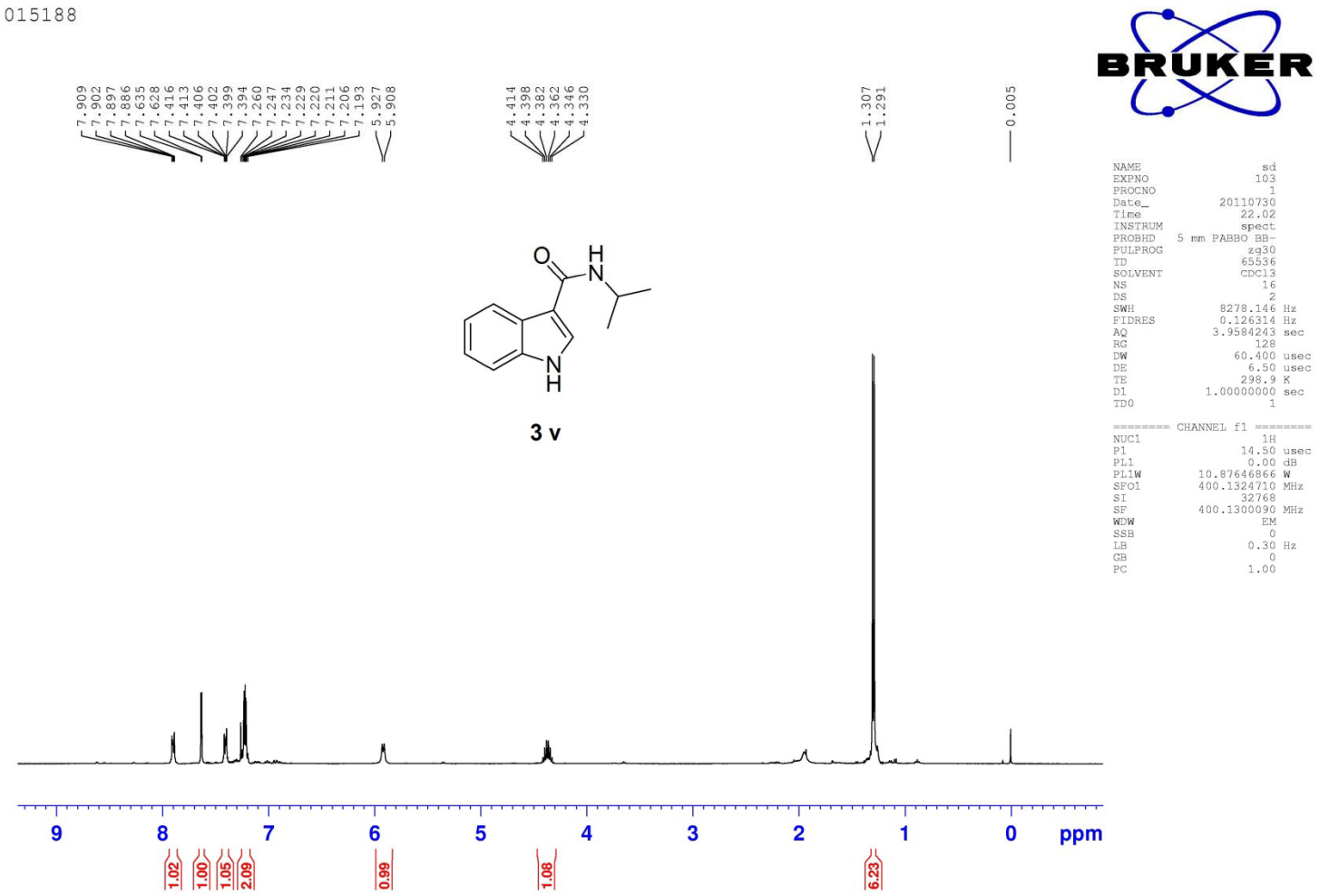
BRUKER

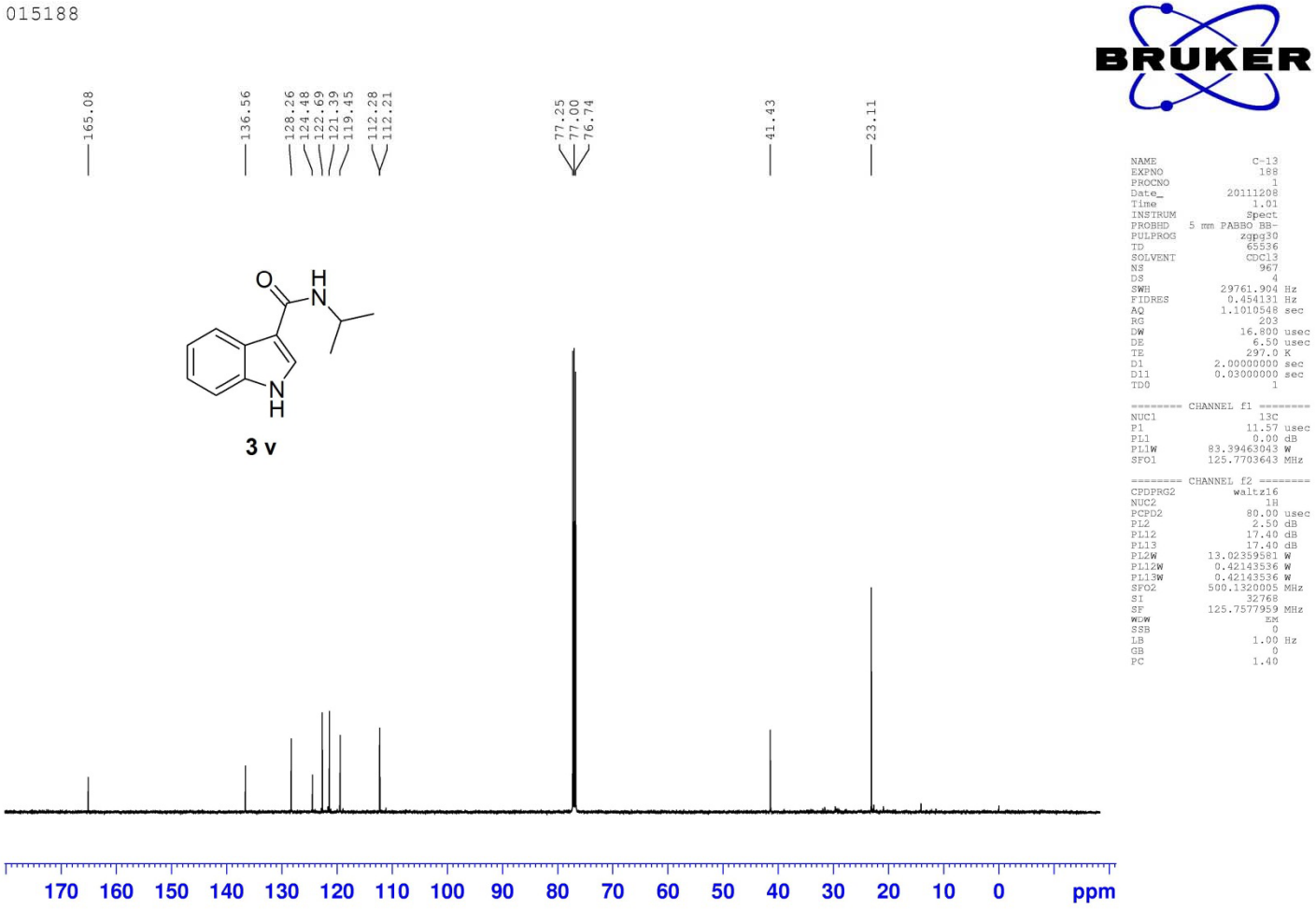
NAME	C-13
EXPNO	15185
PROCNO	1
Date_	20110728
Time	0.32
INSTRUM	Spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	512
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	297.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	11.57 usec
PL1	0.00 dB
PL1W	83.39463043 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.50 dB
PL12	17.40 dB
PL13	17.40 dB
PL2W	13.02359581 W
PL12W	0.42143536 W
PL13W	0.42143536 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7577956 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

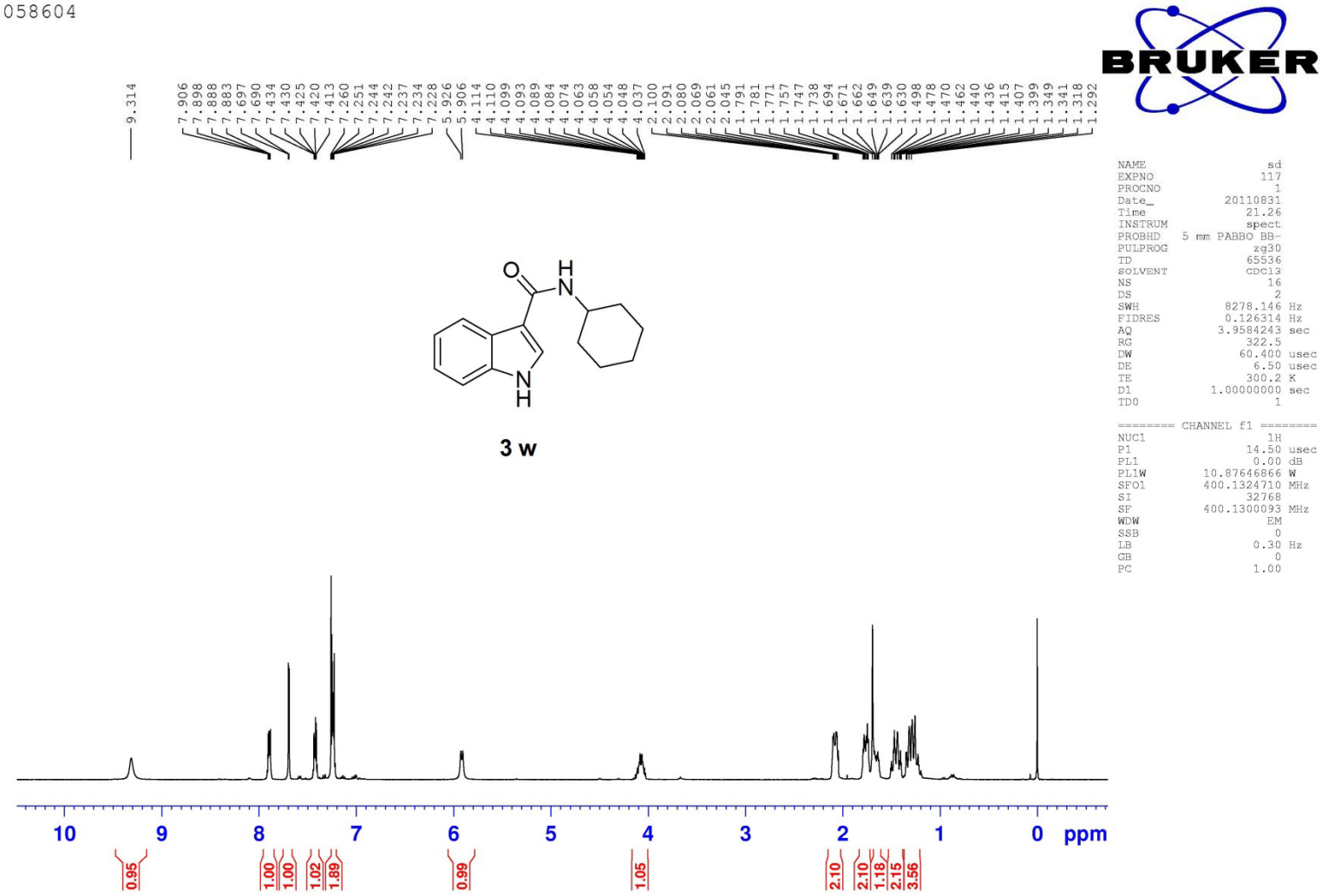

015151D
8.142
8.128
8.125
7.492
7.476
7.473
7.347
7.344
7.327
7.324
7.308
7.279
7.276
7.261
7.254
7.247
7.243
7.223
7.164
7.161
7.146
7.143
7.127
7.123
7.120
7.104
7.101
7.087
7.084
5.432
3.342
2.504
2.500
2.496
1.399
O
H
N
N
3 u
NAME 07-08
EXPNO 5
PROCNO 1
Date_ 20110708
Time 10.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 128
DW 60.400 usec
DE 6.50 usec
TE 299.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.50 usec
PL1 0.00 dB
PL1W 10.87646866 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300023 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
0.99
1.06
1.03
3.03
0.43
3.08
2.06
1.99
9.00

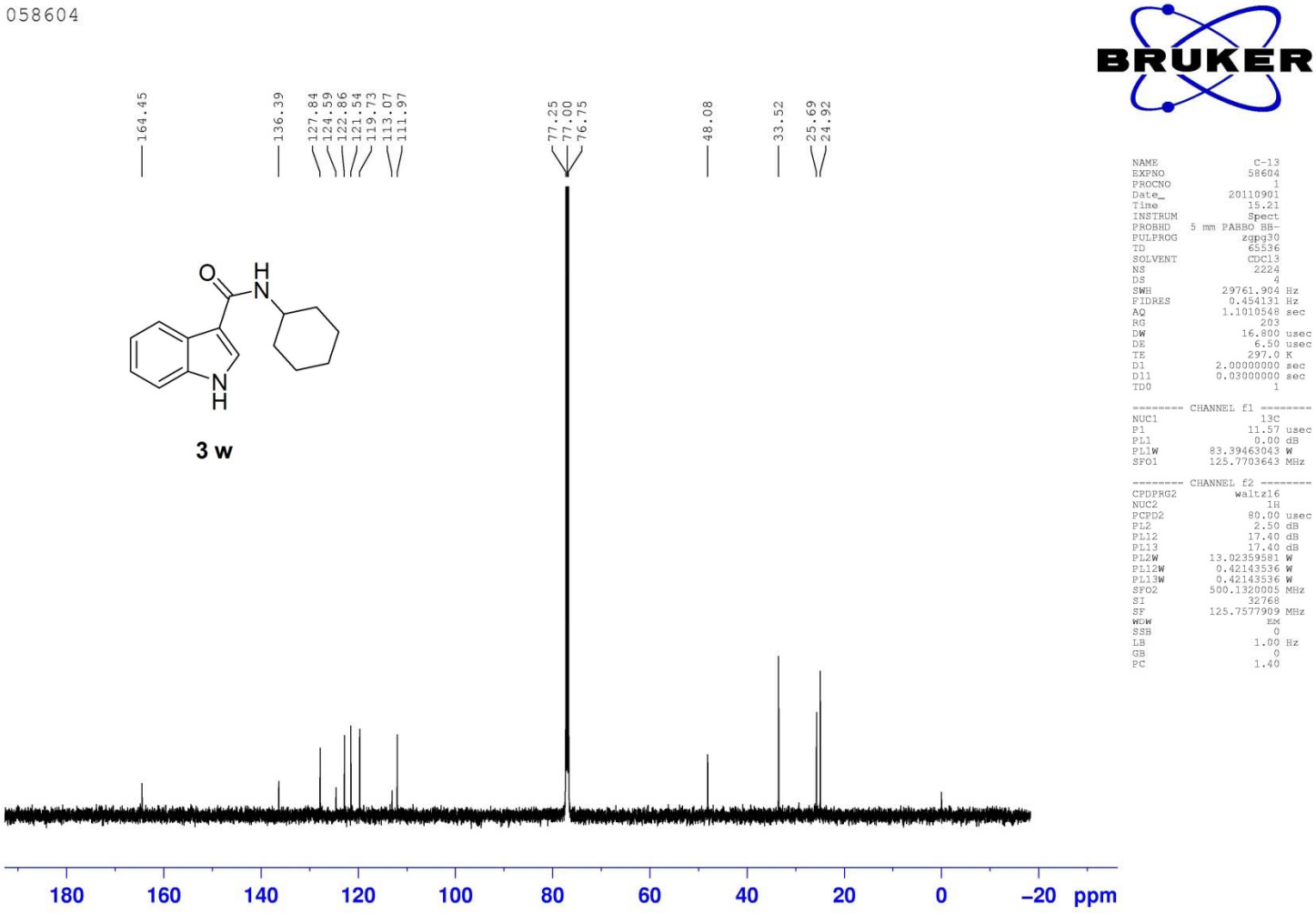


NAME	C-13
EXPNO	15151
PROCNO	1
Date_	20110709
Time	19.03
INSTRUM	Spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	1024
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	297.3 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	11.57 usec
PL1	0.00 dB
PL1W	83.39463043 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.50 dB
PL12	17.40 dB
PL13	17.40 dB
PL2W	13.02359581 W
PL12W	0.42143536 W
PL13W	0.42143536 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7578520 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

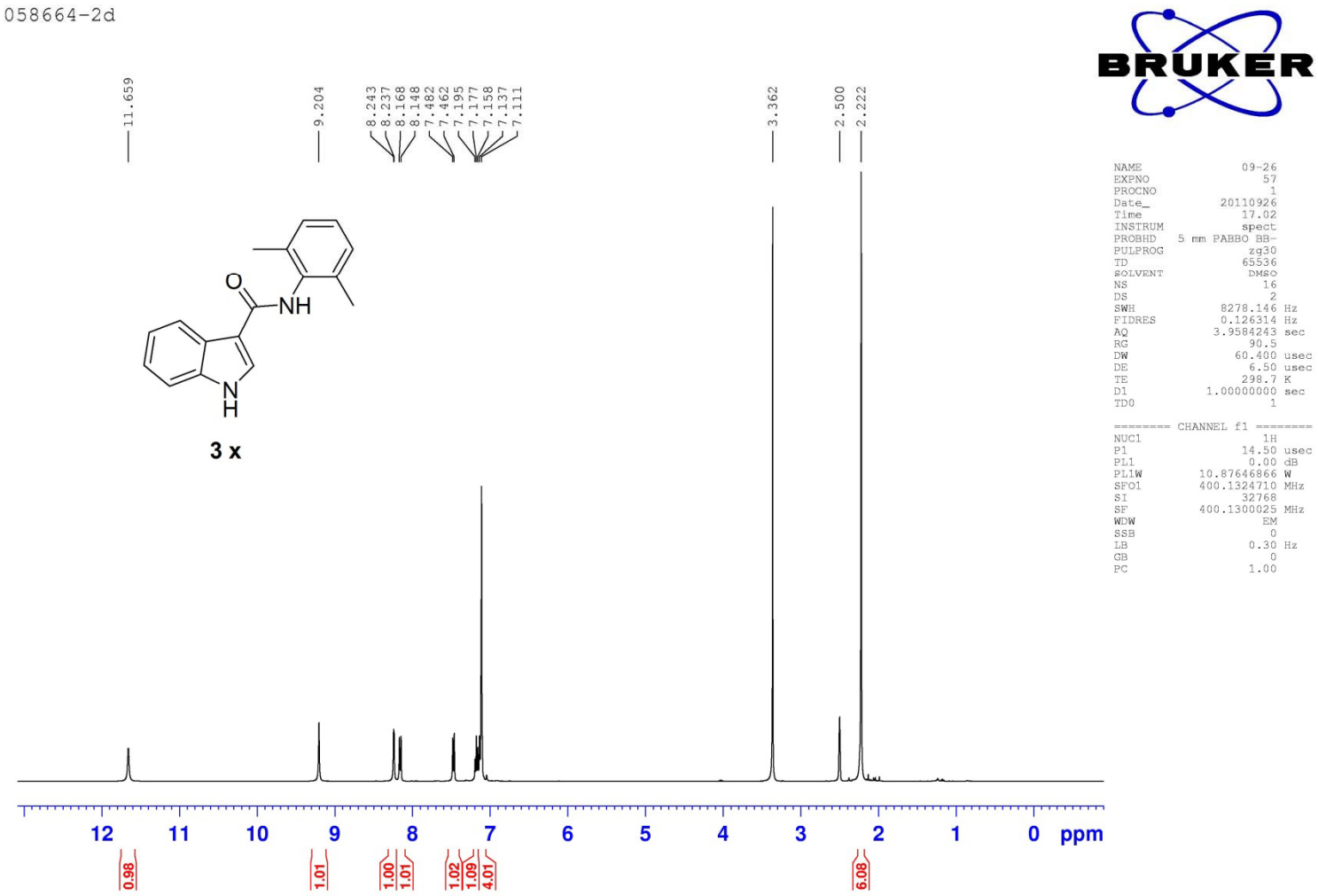

015188
7.909
7.902
7.897
7.886
7.635
7.628
7.416
7.413
7.406
7.402
7.399
7.394
7.260
7.247
7.234
7.229
7.220
7.211
7.206
7.193
5.927
5.908
4.414
4.398
4.382
4.362
4.346
4.330
1.307
1.291
0.005
3 v
NAME sd
EXPNO 103
PROCNO 1
Date_ 20110730
Time 22.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 128
DW 60.400 usec
DE 6.50 usec
TE 298.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.50 usec
PL1 0.00 dB
PL1W 10.87646866 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300090 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
1.02
1.00
1.05
2.09
0.99
1.08
6.23

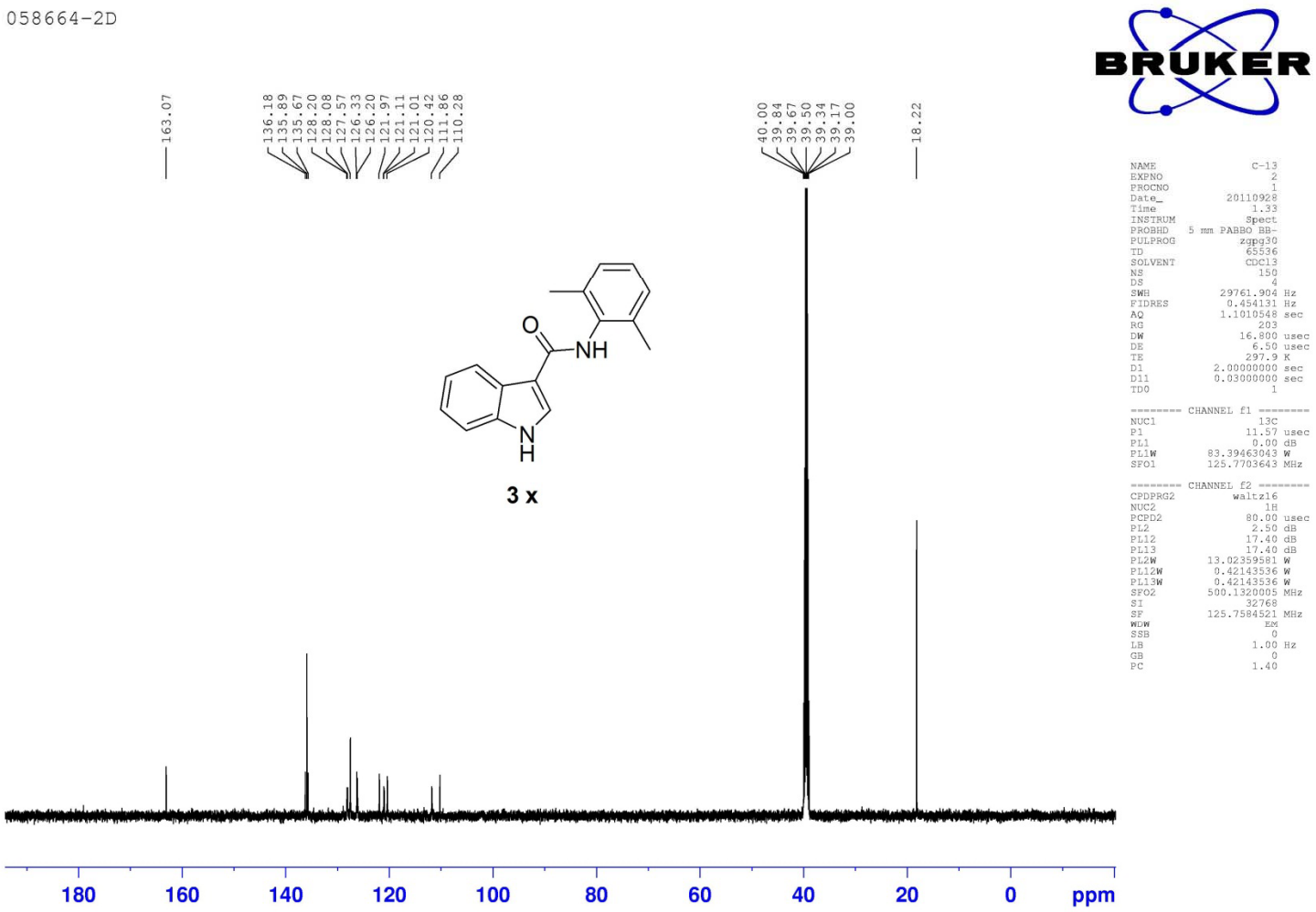

015188
165.08
136.56
128.26
124.48
122.69
121.39
119.45
112.28
112.21
77.25
77.00
76.74
41.43
23.11
O
H
N
N
H
3 v
BRUKER
NAME C-13
EXPNO 188
PROCNO 1
Date_ 20111208
Time 1.01
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 967
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 297.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 11.57 usec
PL1 0.00 dB
PL1W 83.39463043 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577959 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


058604
9.314
7.906
7.898
7.888
7.883
7.697
7.690
7.434
7.430
7.425
7.420
7.413
7.260
7.251
7.244
7.242
7.237
7.234
7.228
5.926
5.906
4.114
4.110
4.099
4.093
4.089
4.084
4.074
4.063
4.058
4.054
4.048
4.037
2.100
2.091
2.080
2.069
2.061
2.045
1.791
1.781
1.771
1.757
1.747
1.738
1.694
1.671
1.662
1.649
1.639
1.630
1.498
1.478
1.470
1.462
1.440
1.436
1.415
1.407
1.399
1.349
1.341
1.318
1.292
BRUKER
NAME sd
EXPNO 117
PROCNO 1
Date_ 20110831
Time 21.26
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 322.5
DW 60.400 usec
DE 6.50 usec
TE 300.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.50 usec
PL1 0.00 dB
PL1W 10.87646866 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
3 w
10
9
8
7
6
5
4
3
2
1
0
ppm
0.95
1.00
1.00
1.02
1.89
0.99
1.05
2.10
2.10
1.18
2.15
3.56



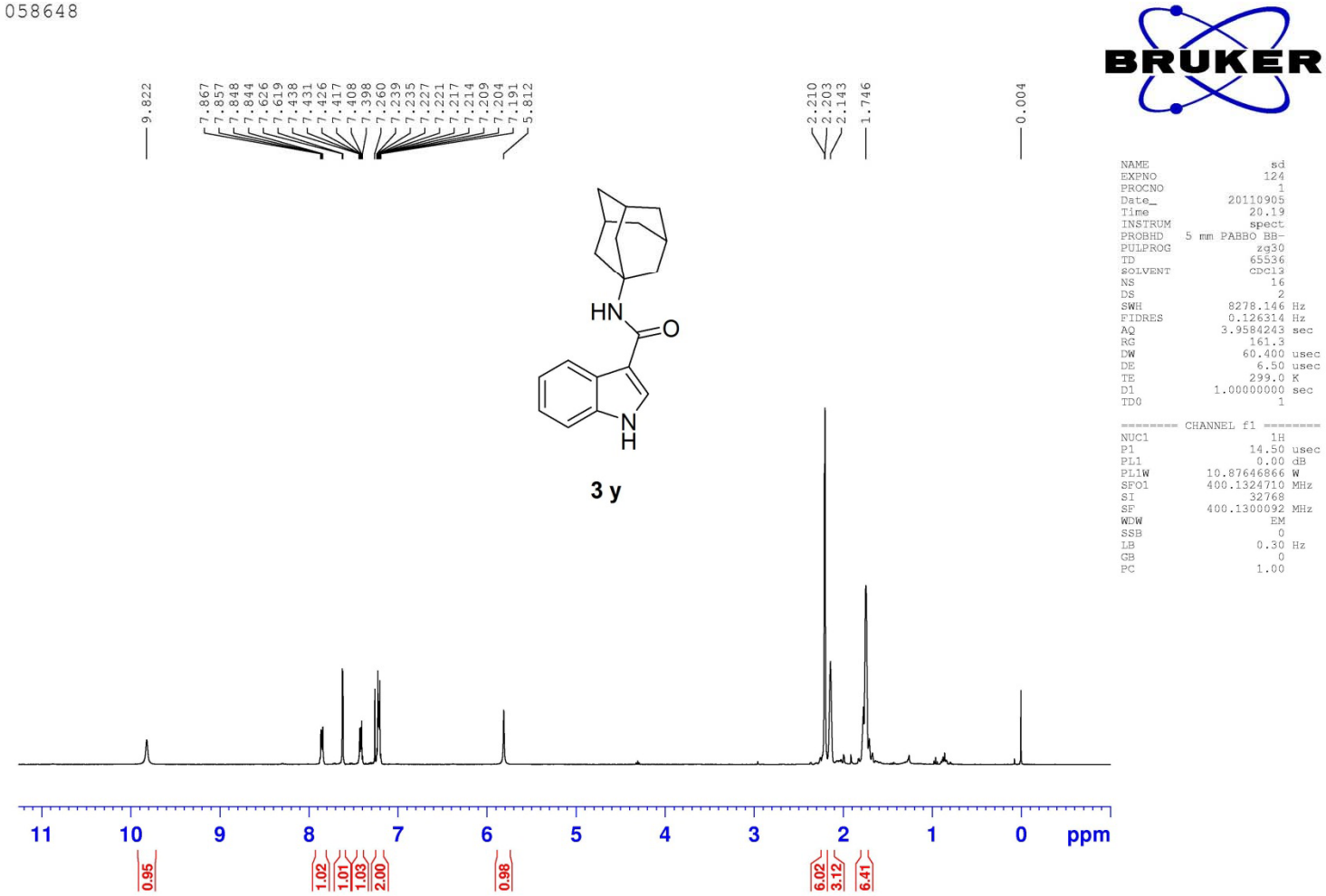
NAME	C-13
EXPNO	58604
PROCNO	1
Date_	20110901
Time	15.21
INSTRUM	Spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	2224
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	297.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	11.57 usec
PL1	0.00 dB
PL1W	83.39463043 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.50 dB
PL12	17.40 dB
PL13	17.40 dB
PL2W	13.02359581 W
PL12W	0.42143536 W
PL13W	0.42143536 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7577909 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

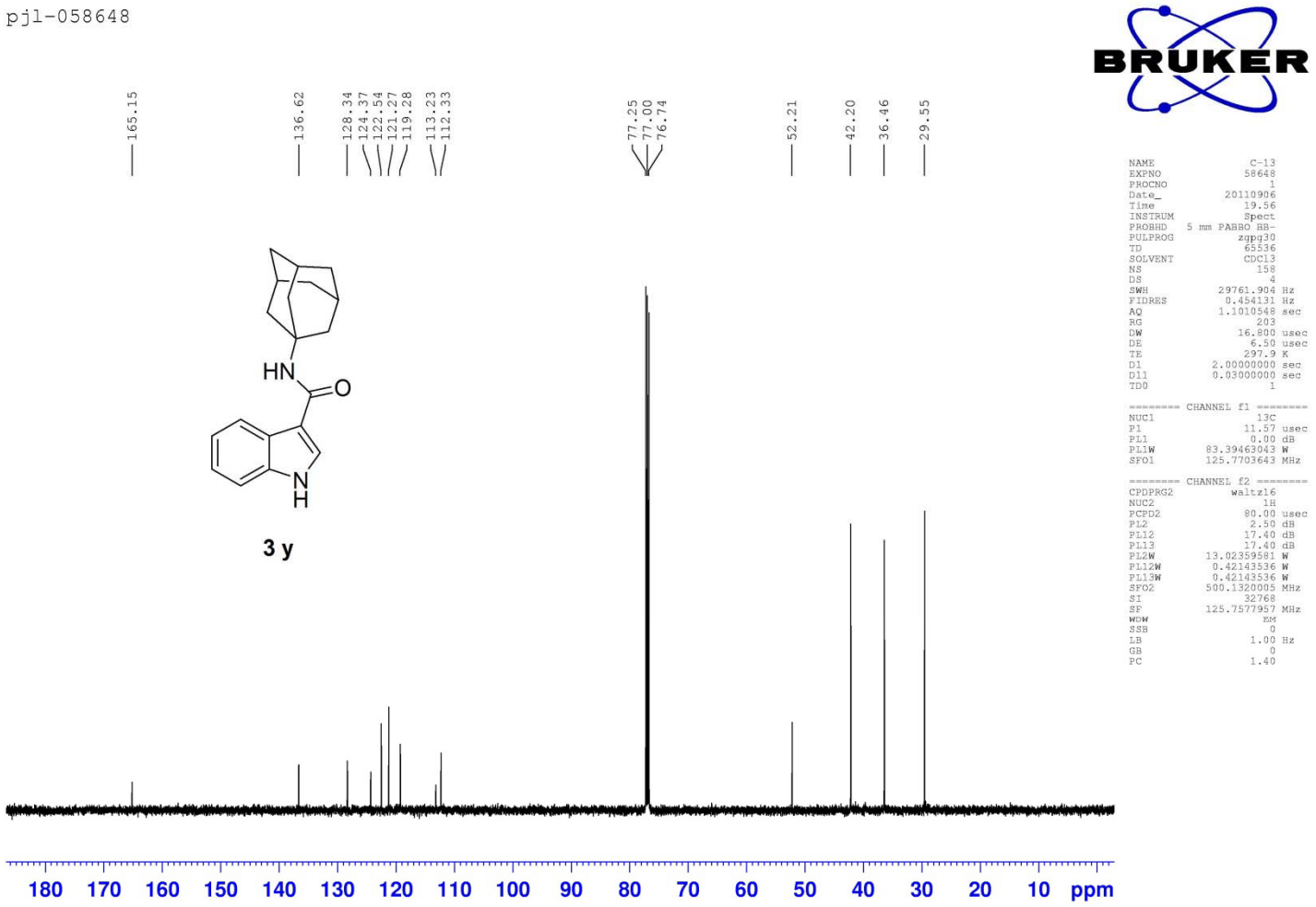

058664-2d
11.659
9.204
8.243
8.237
8.168
8.148
7.482
7.462
7.195
7.177
7.158
7.137
7.111
3.362
2.500
2.222
O
NH
N
H
3 x
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.98
1.01
1.00
1.01
1.02
1.09
4.01
6.08
BRUKER
NAME 09-26
EXPNO 57
PROCNO 1
Date_ 20110926
Time 17.02
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 90.5
DW 60.400 usec
DE 6.50 usec
TE 298.7 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.50 usec
PL1 0.00 dB
PL1W 10.87646866 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300025 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00



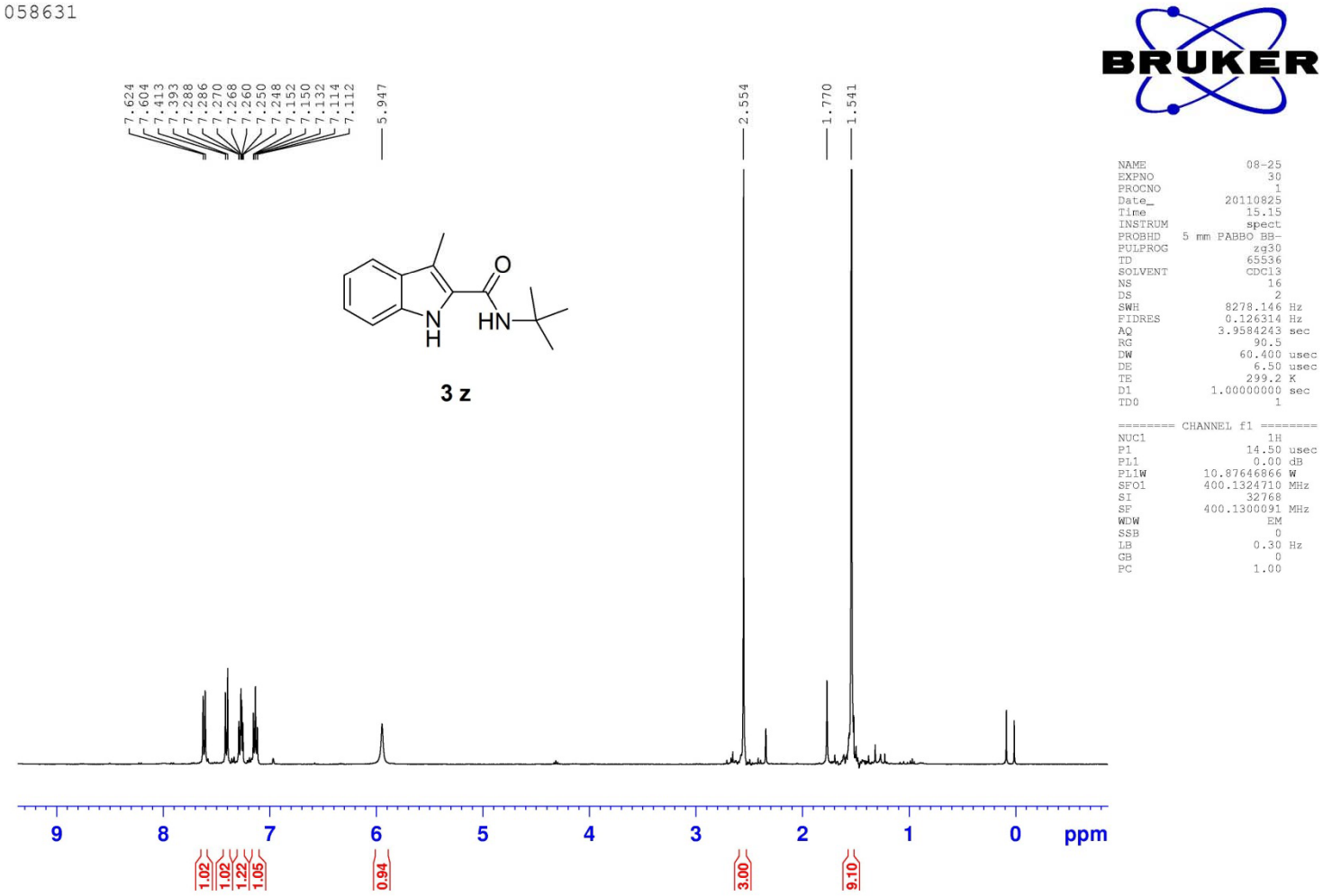
BRUKER

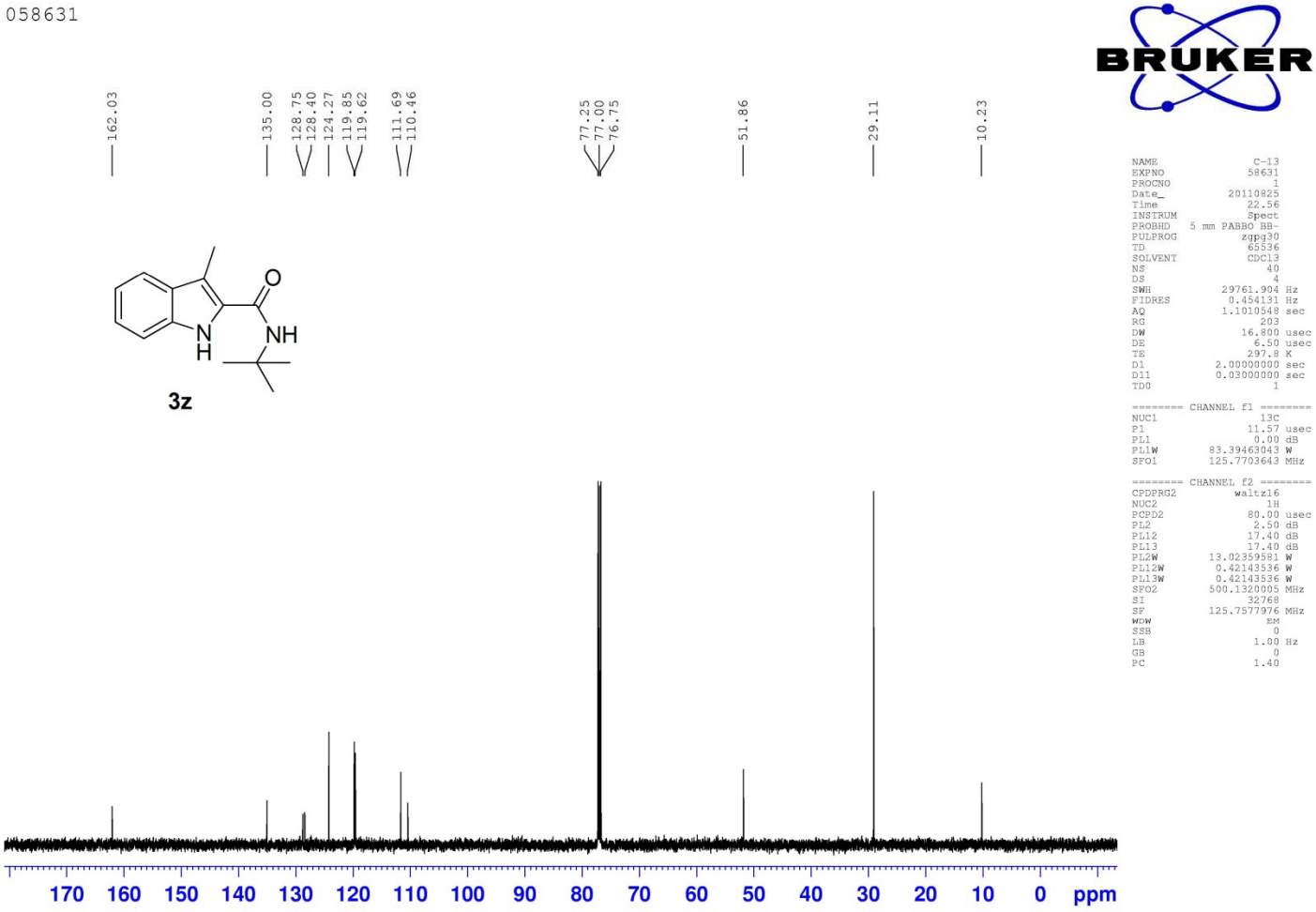
NAME	C-13
EXPNO	2
PROCNO	1
Date_	20110928
Time	1.33
INSTRUM	Spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	150
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	297.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	11.57 usec
PL1	0.00 dB
PL1W	83.39463043 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.50 dB
PL12	17.40 dB
PL13	17.40 dB
PL2W	13.02359581 W
PL12W	0.42143536 W
PL13W	0.42143536 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7584521 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

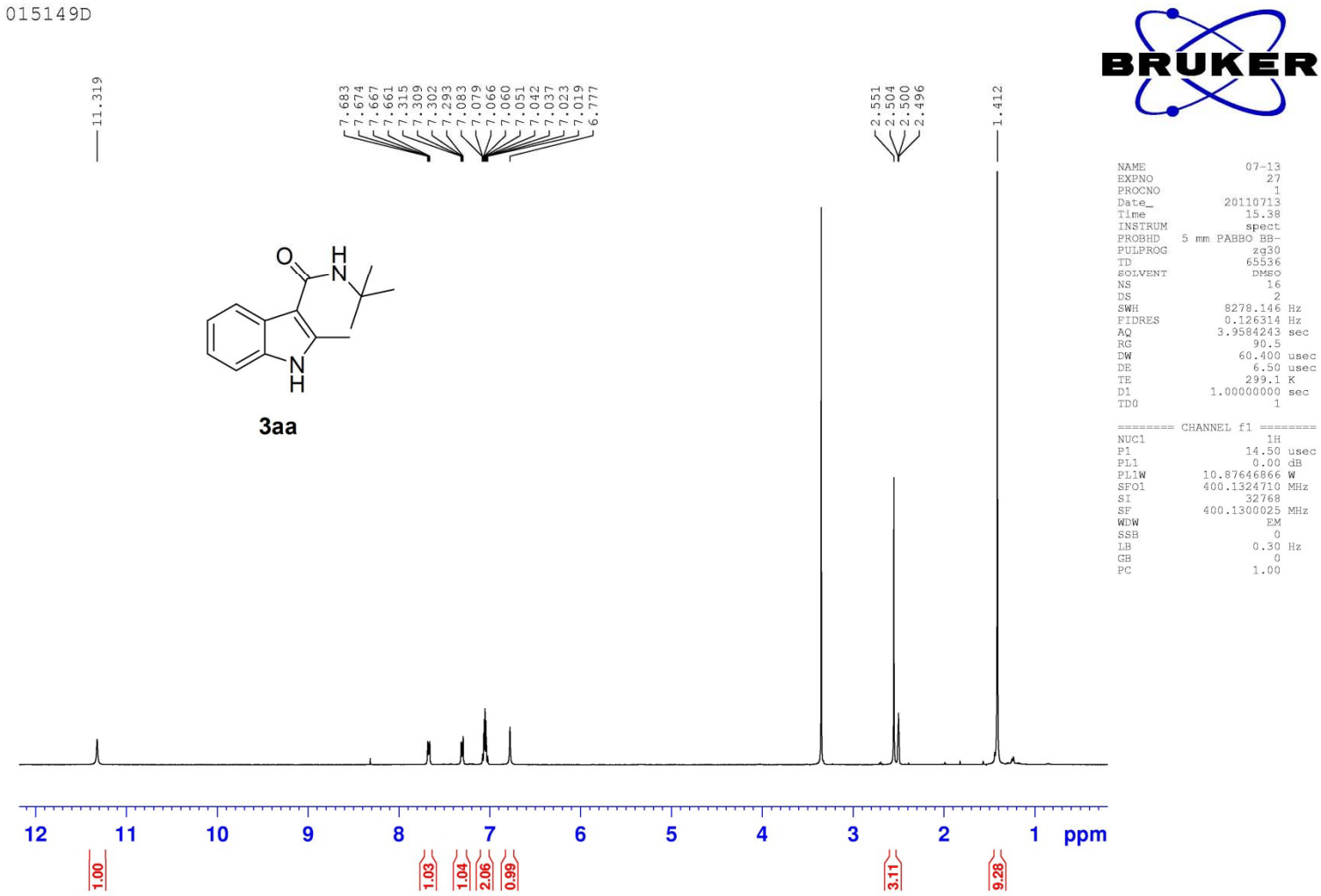

058648
9.822
7.867
7.857
7.848
7.844
7.626
7.619
7.438
7.431
7.426
7.417
7.408
7.398
7.260
7.239
7.235
7.227
7.221
7.217
7.214
7.209
7.204
7.191
5.812
2.210
2.203
2.143
1.746
0.004
HN
O
N
H
3 y
NAME sd
EXPNO 124
PROCNO 1
Date_ 20110905
Time 20.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 161.3
DW 60.400 usec
DE 6.50 usec
TE 299.0 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.50 usec
PL1 0.00 dB
PL1W 10.87646866 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300092 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.95
1.02
1.01
1.03
2.00
0.98
6.02
3.12
6.41

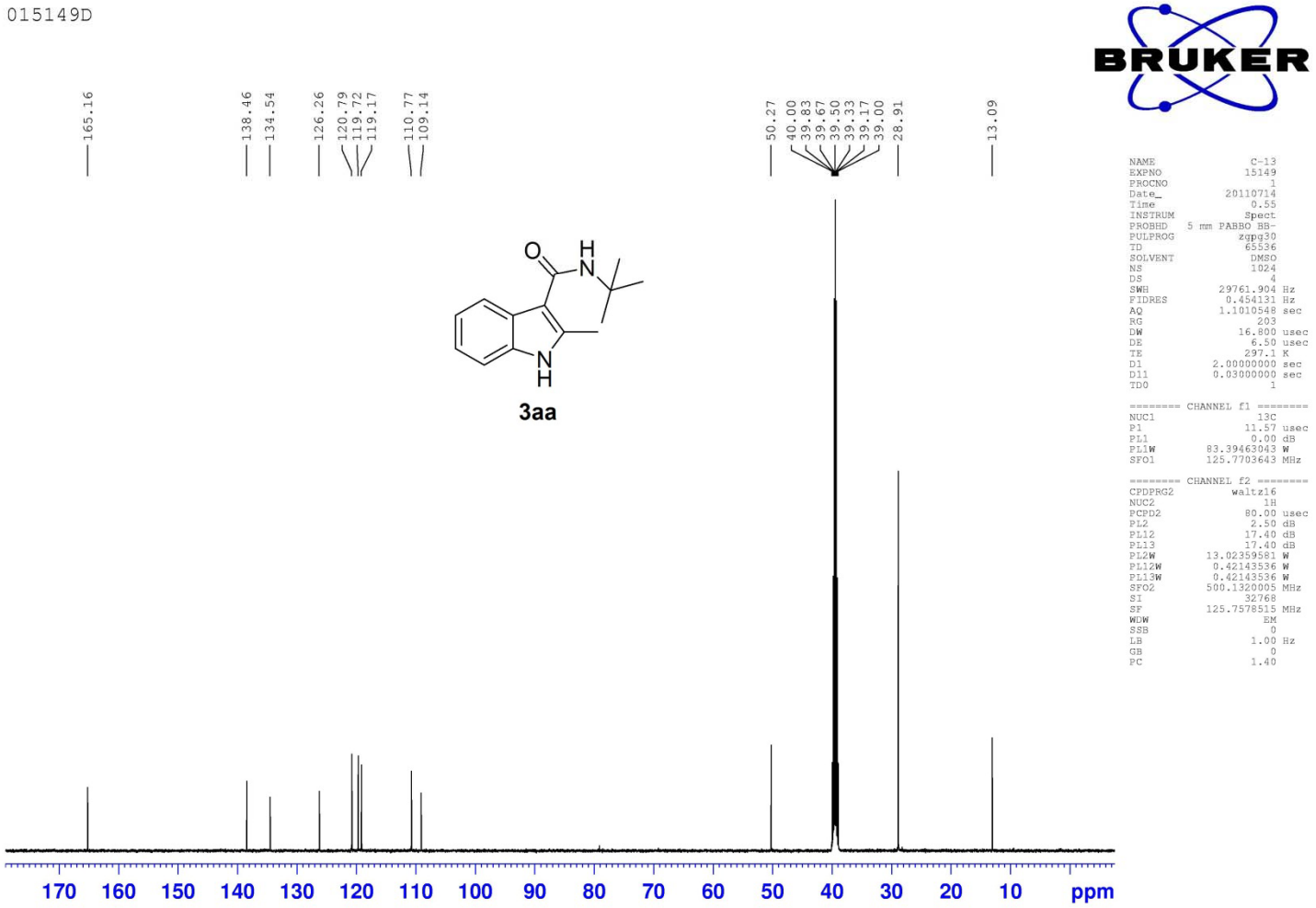


NAME	C-13
EXPNO	58648
PROCNO	1
Date_	20110906
Time	19.56
INSTRUM	Spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	158
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	297.9 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	11.57 usec
PL1	0.00 dB
PL1W	83.39463043 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.50 dB
PL12	17.40 dB
PL13	17.40 dB
PL2W	13.02359581 W
PL12W	0.42143536 W
PL13W	0.42143536 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7577957 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

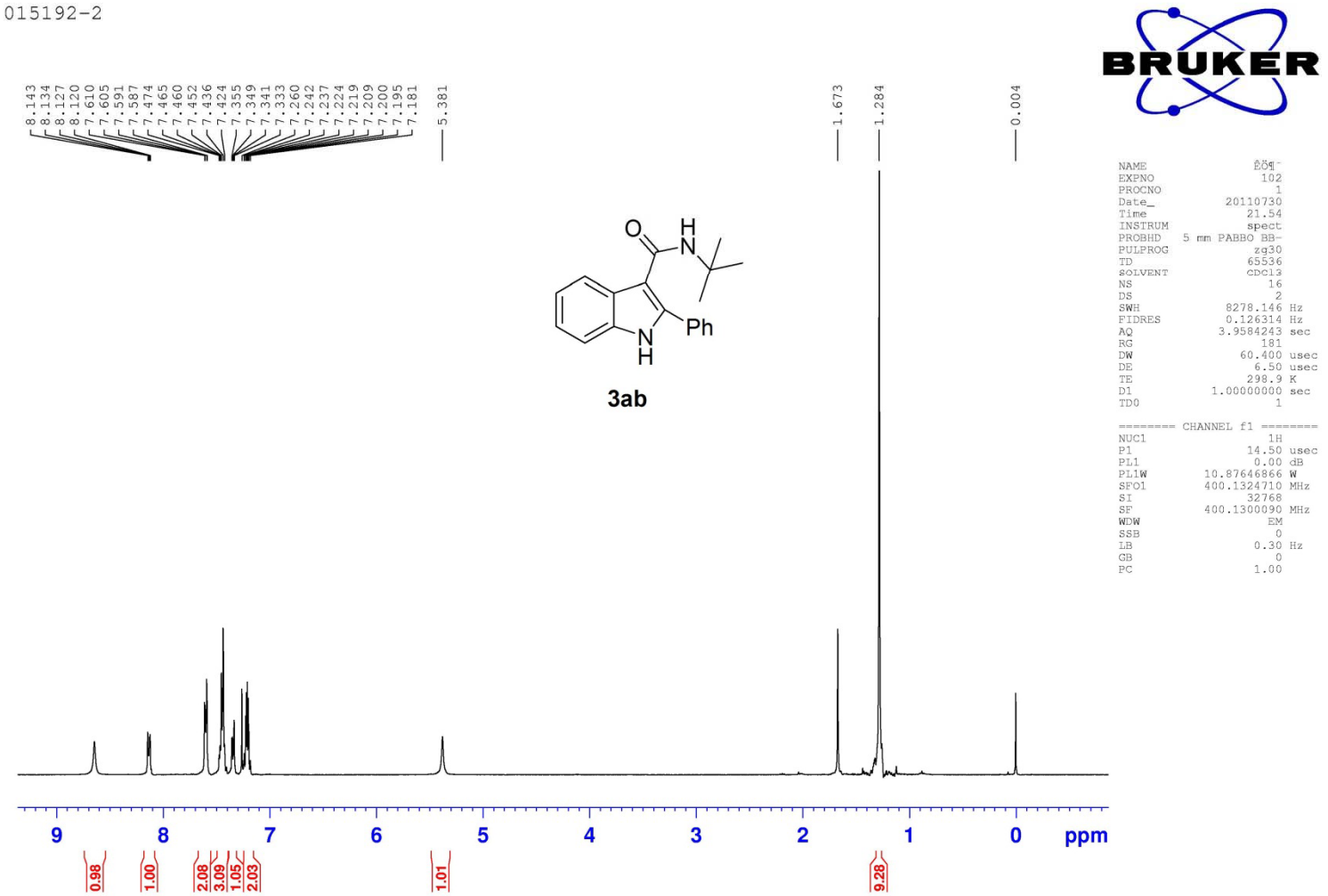


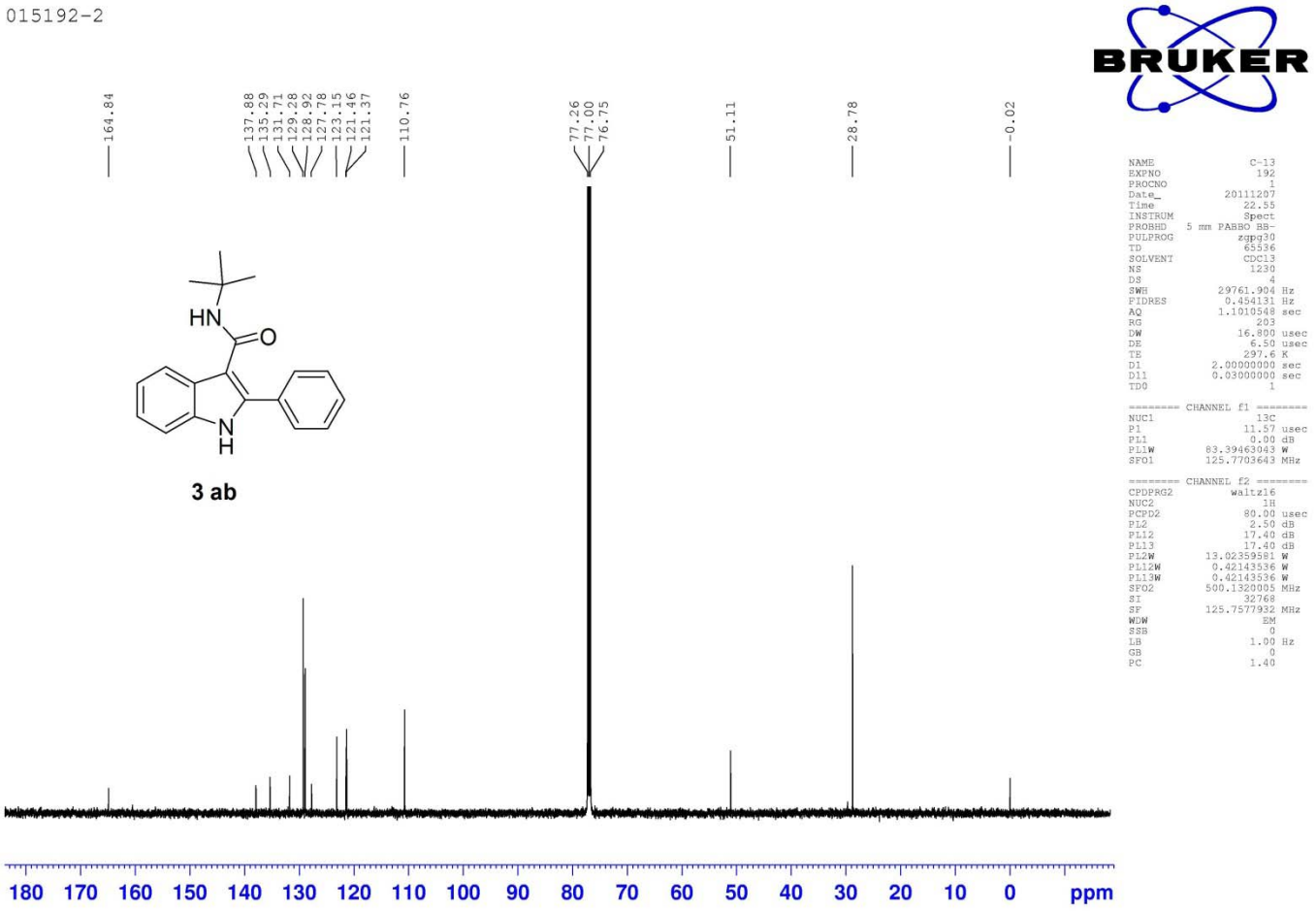

058631
162.03
135.00
128.75
128.40
124.27
119.85
119.62
111.69
110.46
77.25
77.00
76.75
51.86
29.11
10.23
O
NH
N
H
3z
NAME C-13
EXPNO 58631
PROCNO 1
Date_ 20110825
Time 22.56
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 40
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 297.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 11.57 usec
PL1 0.00 dB
PL1W 83.39463043 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577976 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


015149D
11.319
7.683
7.674
7.667
7.661
7.315
7.309
7.302
7.293
7.083
7.079
7.066
7.060
7.051
7.042
7.037
7.023
7.019
6.777
2.551
2.504
2.500
2.496
1.412
3aa
NAME 07-13
EXPNO 27
PROCNO 1
Date_ 20110713
Time 15.38
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 90.5
DW 60.400 usec
DE 6.50 usec
TE 299.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.50 usec
PL1 0.00 dB
PL1W 10.87646866 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300025 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
12
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.03
1.04
2.06
0.99
3.11
9.28

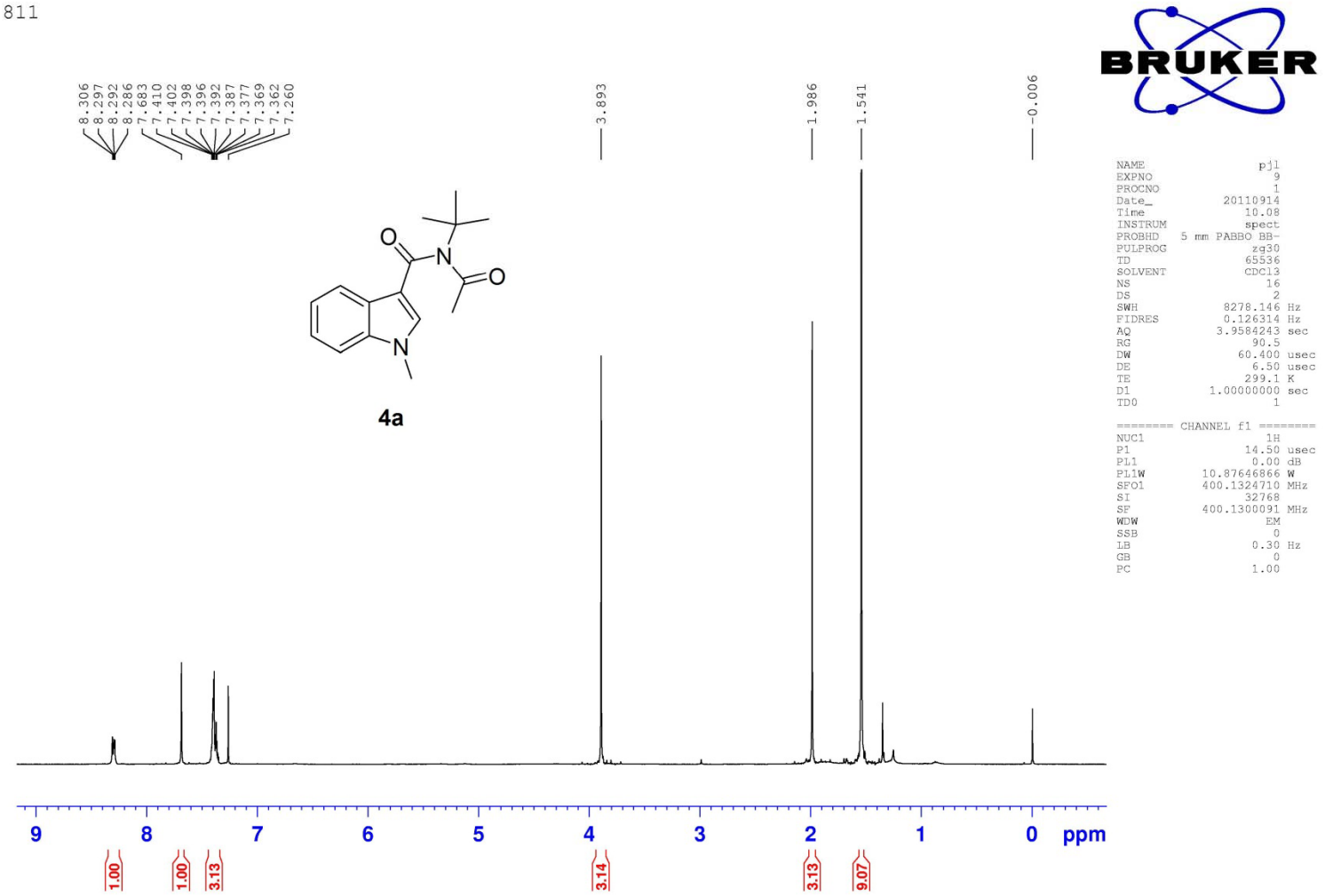


NAME	C-13
EXPNO	15149
PROCNO	1
Date_	20110714
Time	0.55
INSTRUM	Spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	1024
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	297.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	11.57 usec
PL1	0.00 dB
PL1W	83.39463043 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.50 dB
PL12	17.40 dB
PL13	17.40 dB
PL2W	13.02359581 W
PL12W	0.42143536 W
PL13W	0.42143536 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7578515 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

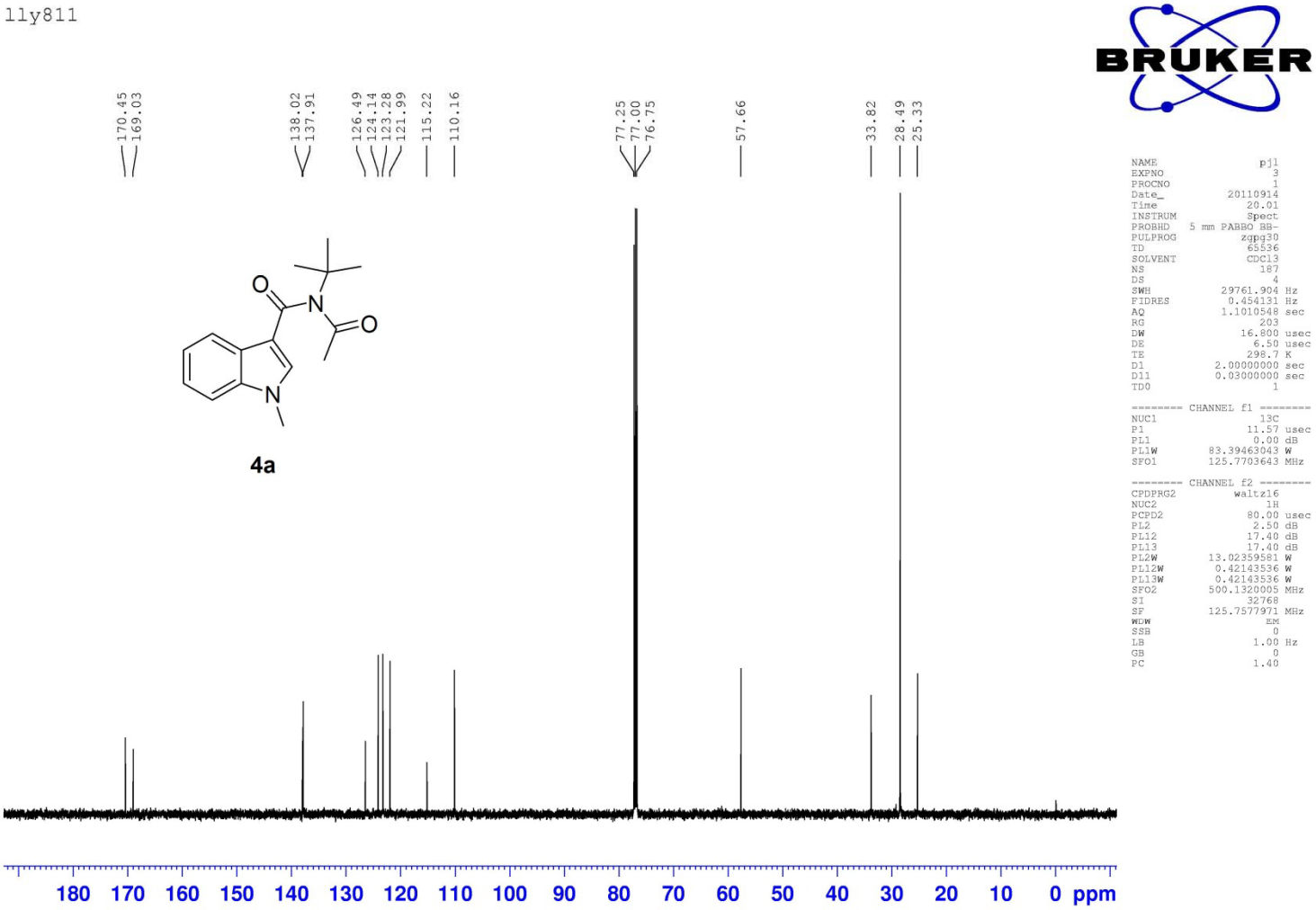

015192-2
8.143
8.134
8.127
8.120
7.610
7.605
7.591
7.587
7.474
7.465
7.460
7.452
7.436
7.424
7.355
7.349
7.341
7.333
7.260
7.242
7.237
7.224
7.219
7.209
7.200
7.195
7.181
5.381
1.673
1.284
0.004
O
H
N
Ph
N
H
3ab
NAME
EXPNO 102
PROCNO 1
Date_ 20110730
Time 21.54
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 181
DW 60.400 usec
DE 6.50 usec
TE 298.9 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.50 usec
PL1 0.00 dB
PL1W 10.87646866 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300090 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
0.98
1.00
2.08
3.09
1.05
2.03
1.01
9.28

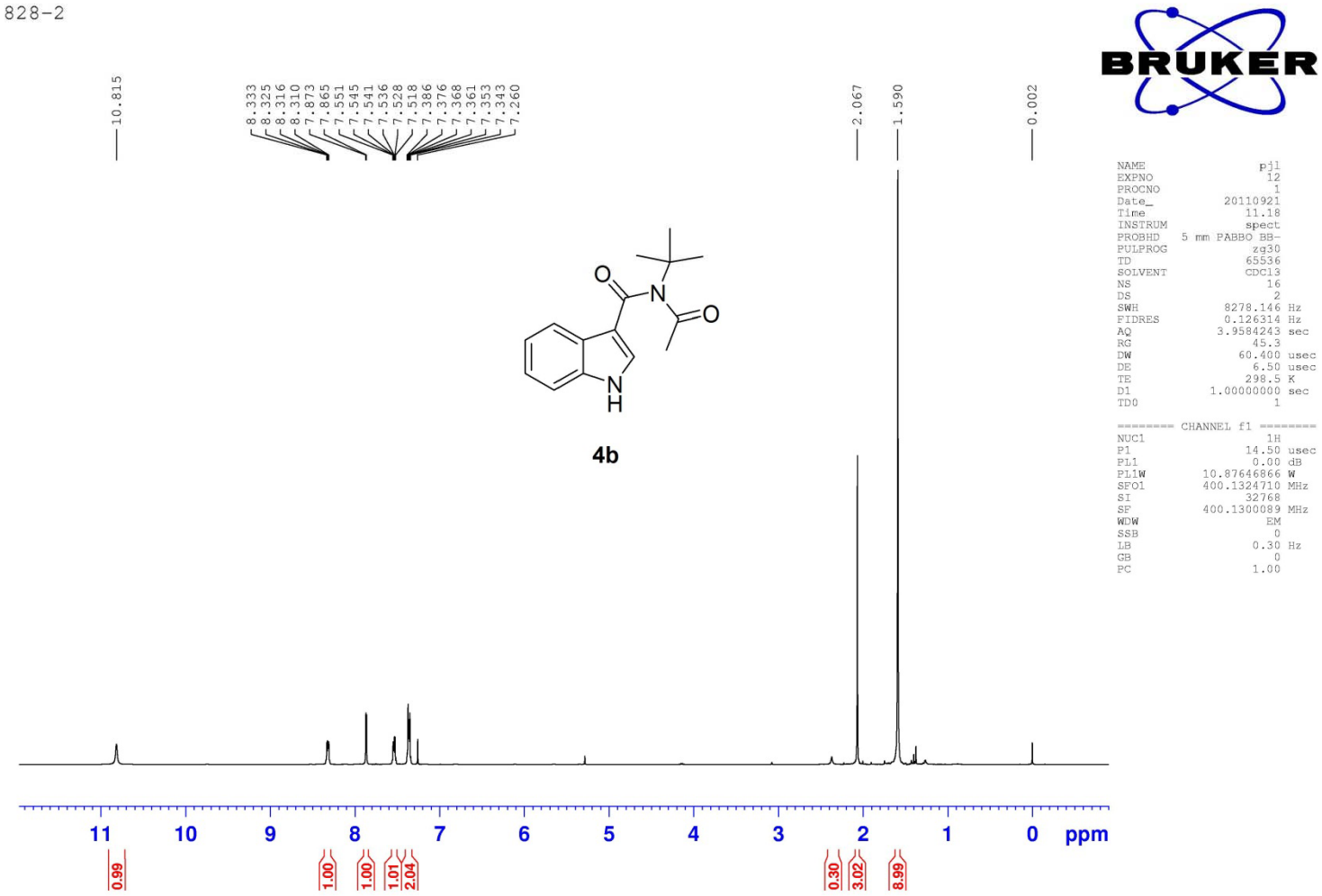


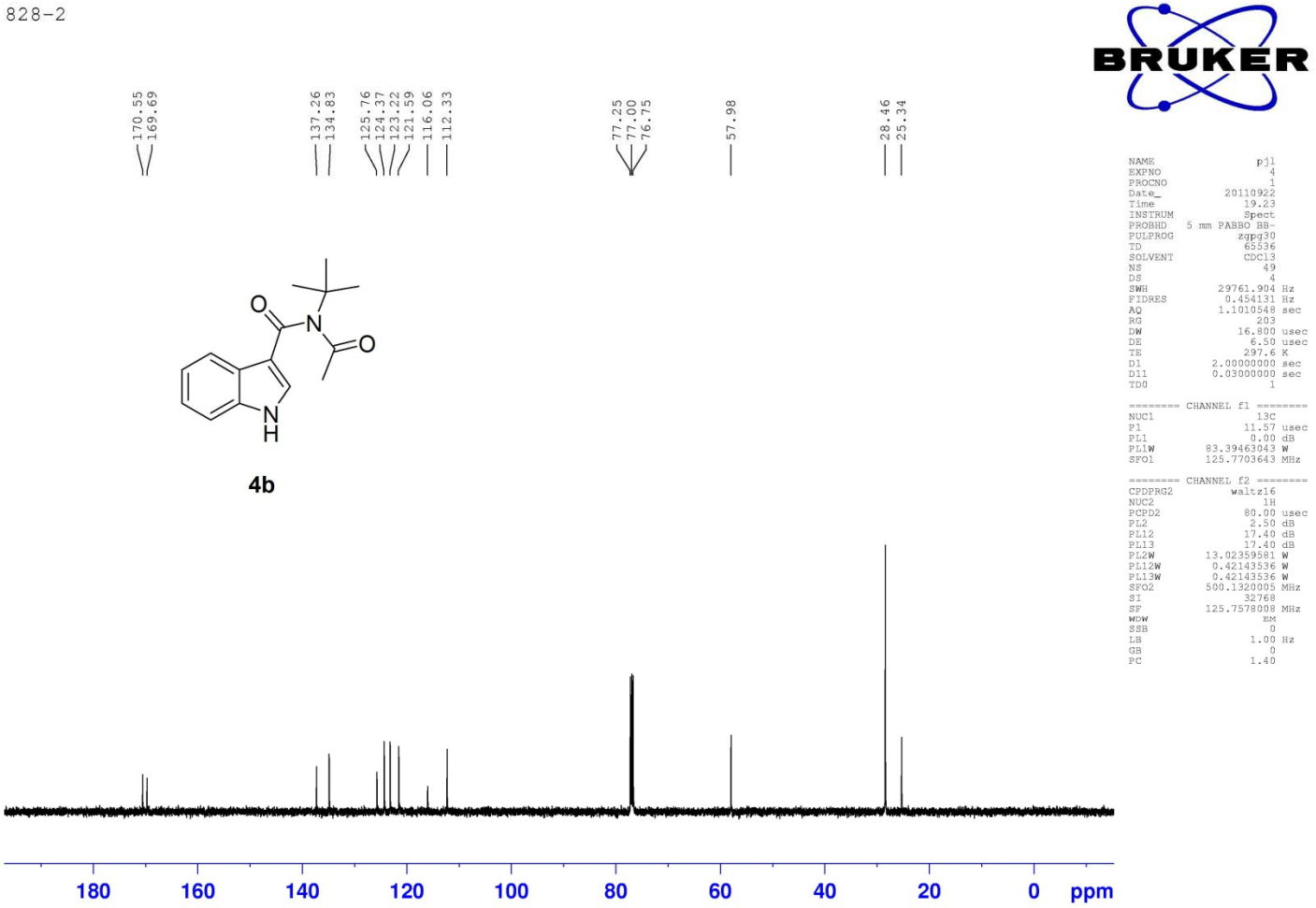
NAME	C-13
EXPNO	192
PROCNO	1
Date_	20111207
Time	22.55
INSTRUM	Spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1230
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	297.6 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	11.57 usec
PL1	0.00 dB
PL1W	83.39463043 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.50 dB
PL12	17.40 dB
PL13	17.40 dB
PL2W	13.02359581 W
PL12W	0.42143536 W
PL13W	0.42143536 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7577932 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

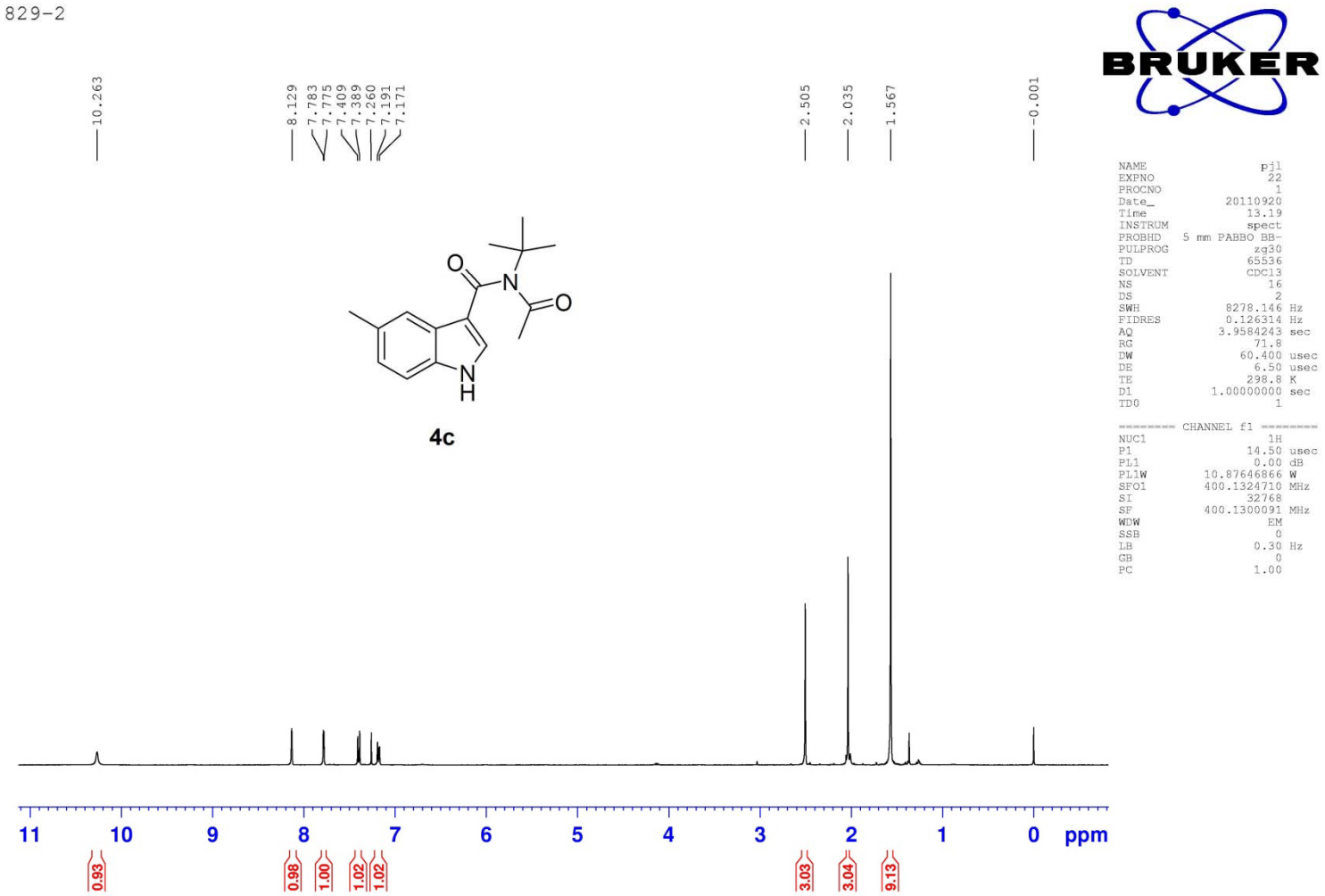


NAME	pjl
EXPNO	9
PROCNO	1
Date_	20110914
Time	10.08
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	90.5
DW	60.400 usec
DE	6.50 usec
TE	299.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.00 dB
PL1W	10.87646866 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300091 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

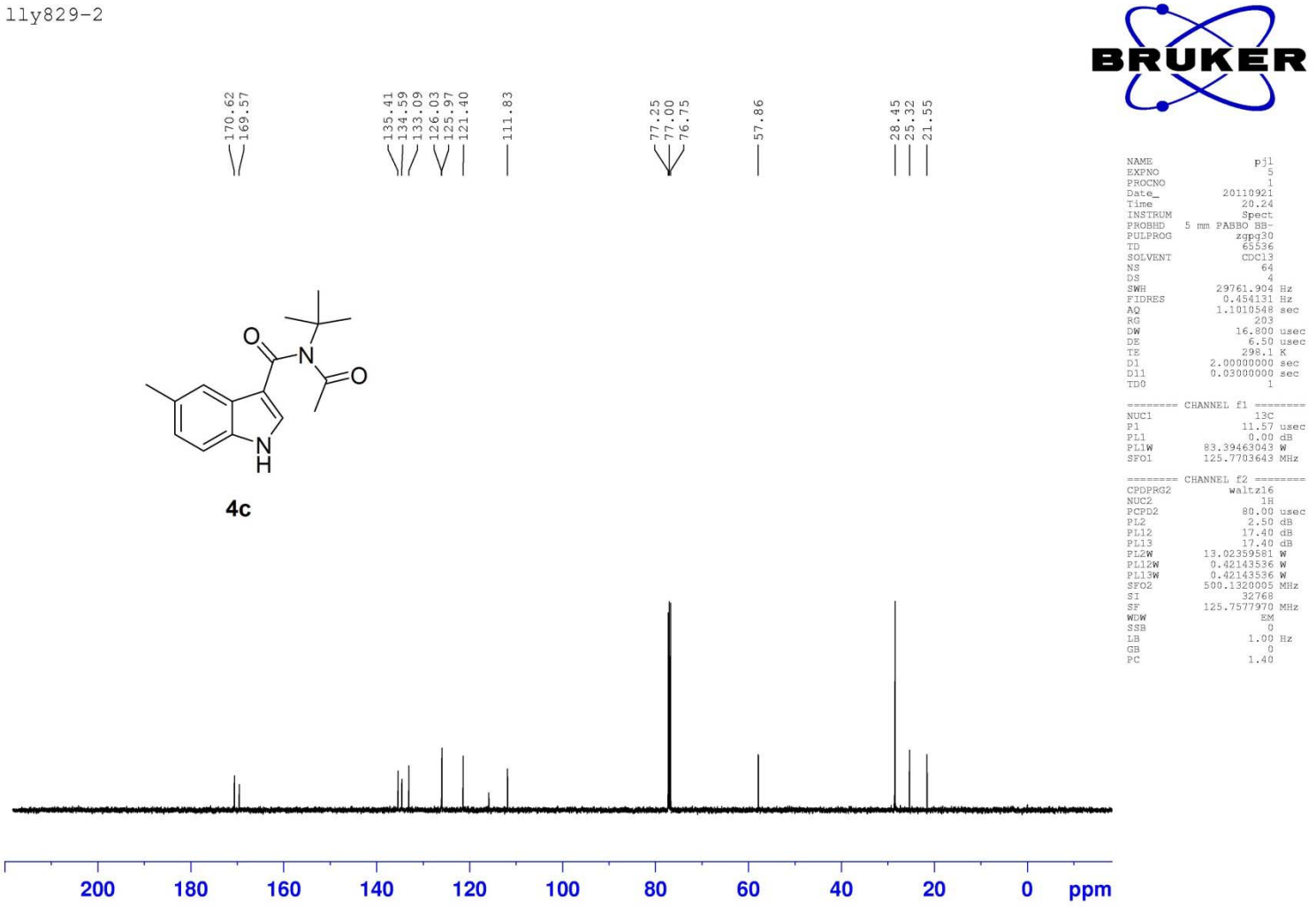

lly811
170.45
169.03
138.02
137.91
126.49
124.14
123.28
121.99
115.22
110.16
77.25
77.00
76.75
57.66
33.82
28.49
25.33
4a
NAME pj1
EXPNO 3
PROCNO 1
Date_ 20110914
Time 20.01
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 187
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 298.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 11.57 usec
PL1 0.00 dB
PL1W 83.39463043 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577971 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



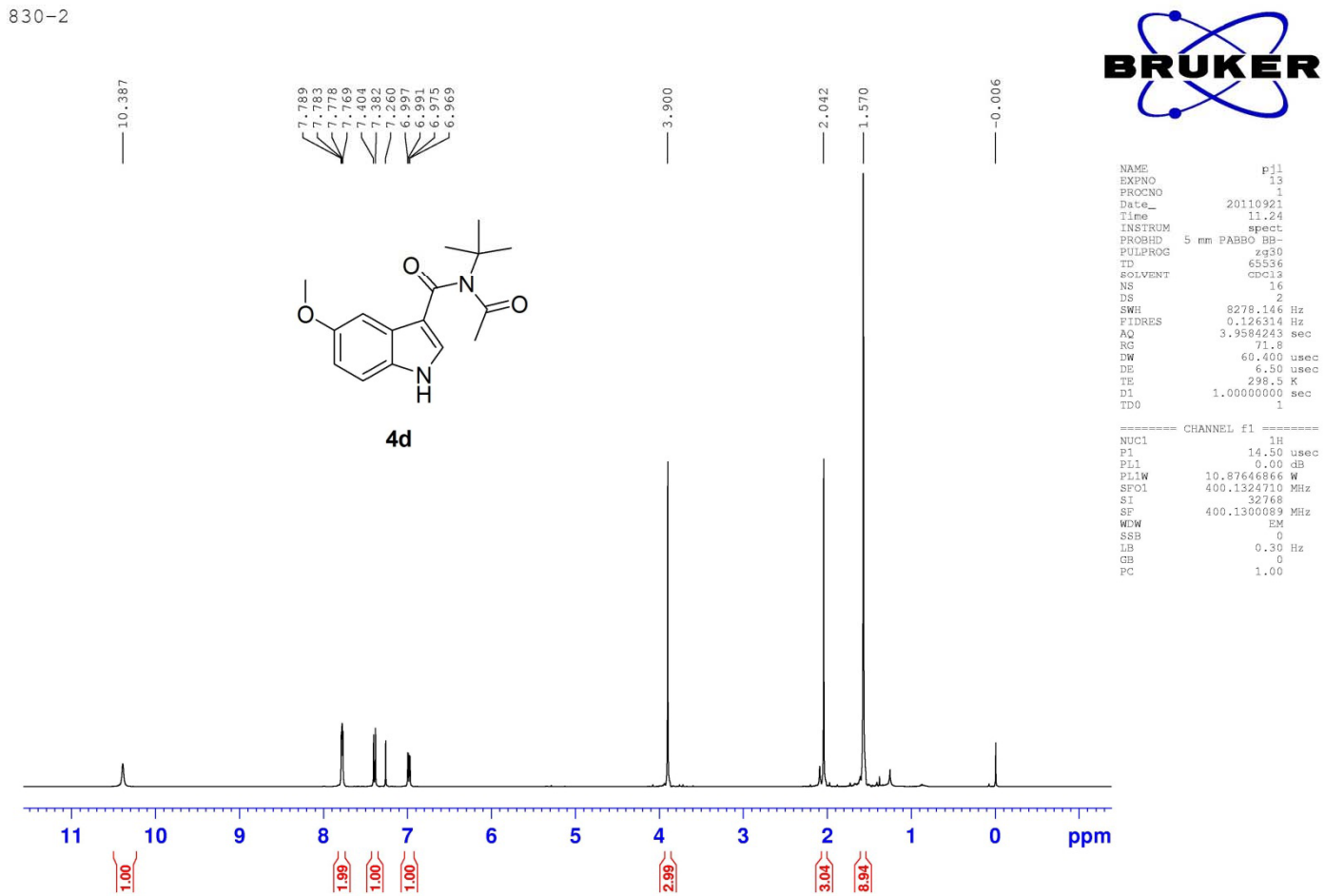

828-2
170.55
169.69
137.26
134.83
125.76
124.37
123.22
121.59
116.06
112.33
77.25
77.00
76.75
57.98
28.46
25.34
4b
NAME pj1
EXPNO 4
PROCNO 1
Date_ 20110922
Time 19.23
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 49
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 297.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 11.57 usec
PL1 0.00 dB
PL1W 83.39463043 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7578008 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180
160
140
120
100
80
60
40
20
0
ppm



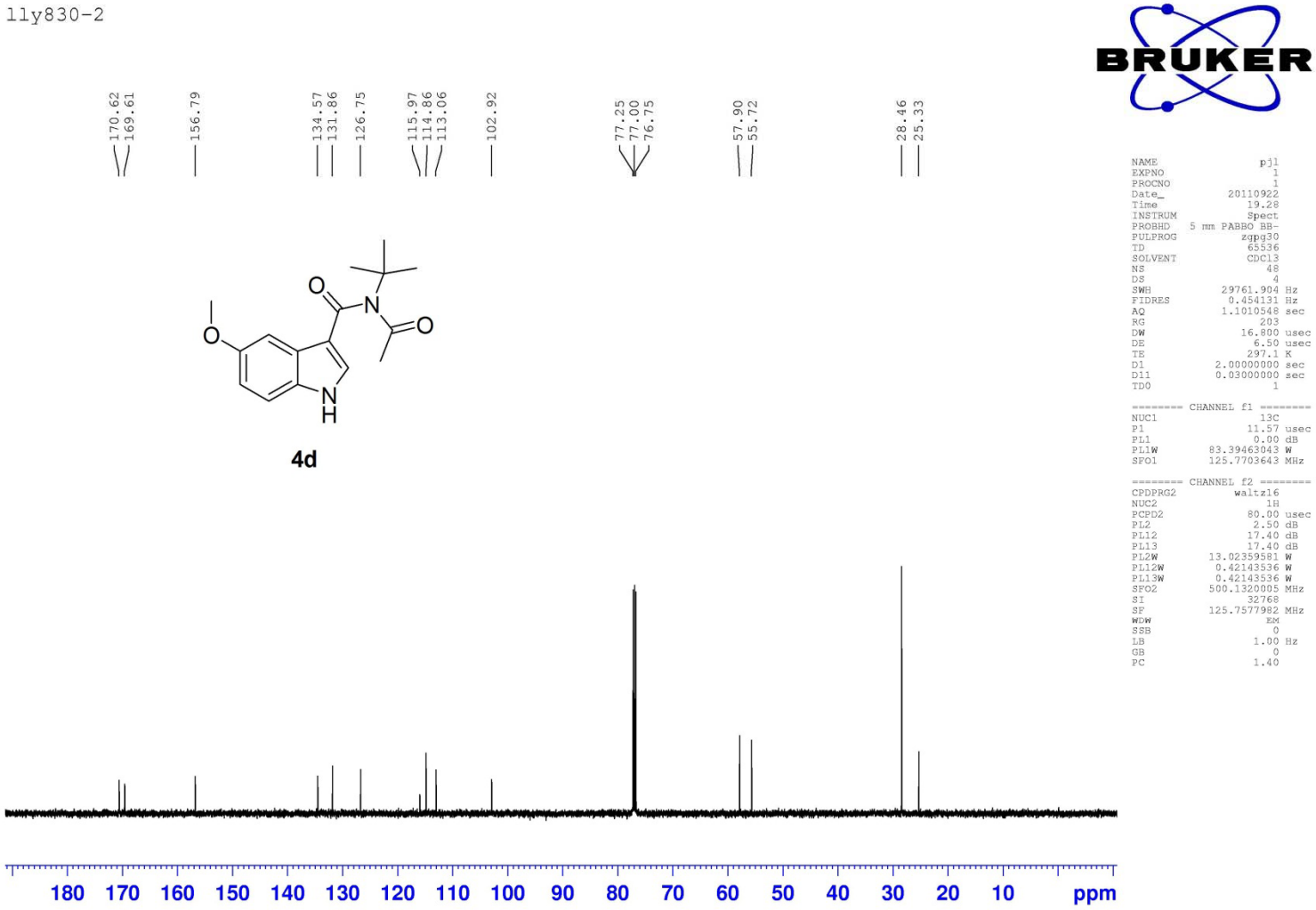
NAME	pj1
EXPNO	22
PROCNO	1
Date_	20110920
Time	13.19
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	71.8
DW	60.400 usec
DE	6.50 usec
TE	298.8 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.00 dB
PL1W	10.87646866 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300091 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

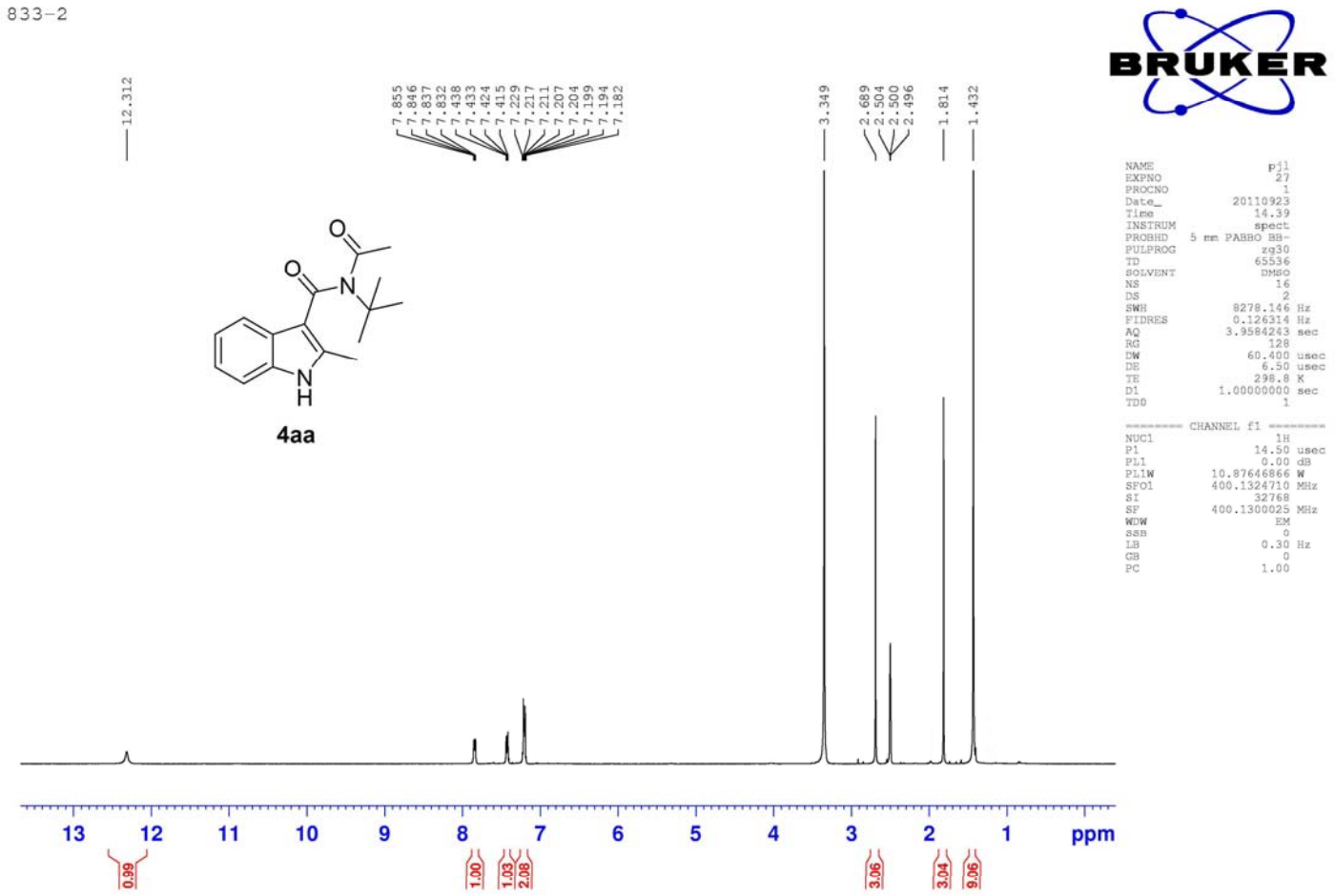


NAME	pjl
EXPNO	5
PROCNO	1
Date_	20110921
Time	20.24
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	64
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	298.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	11.57 usec
PL1	0.00 dB
PL1W	83.39463043 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.50 dB
PL12	17.40 dB
PL13	17.40 dB
PL2W	13.02359581 W
PL12W	0.42143536 W
PL13W	0.42143536 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7577970 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



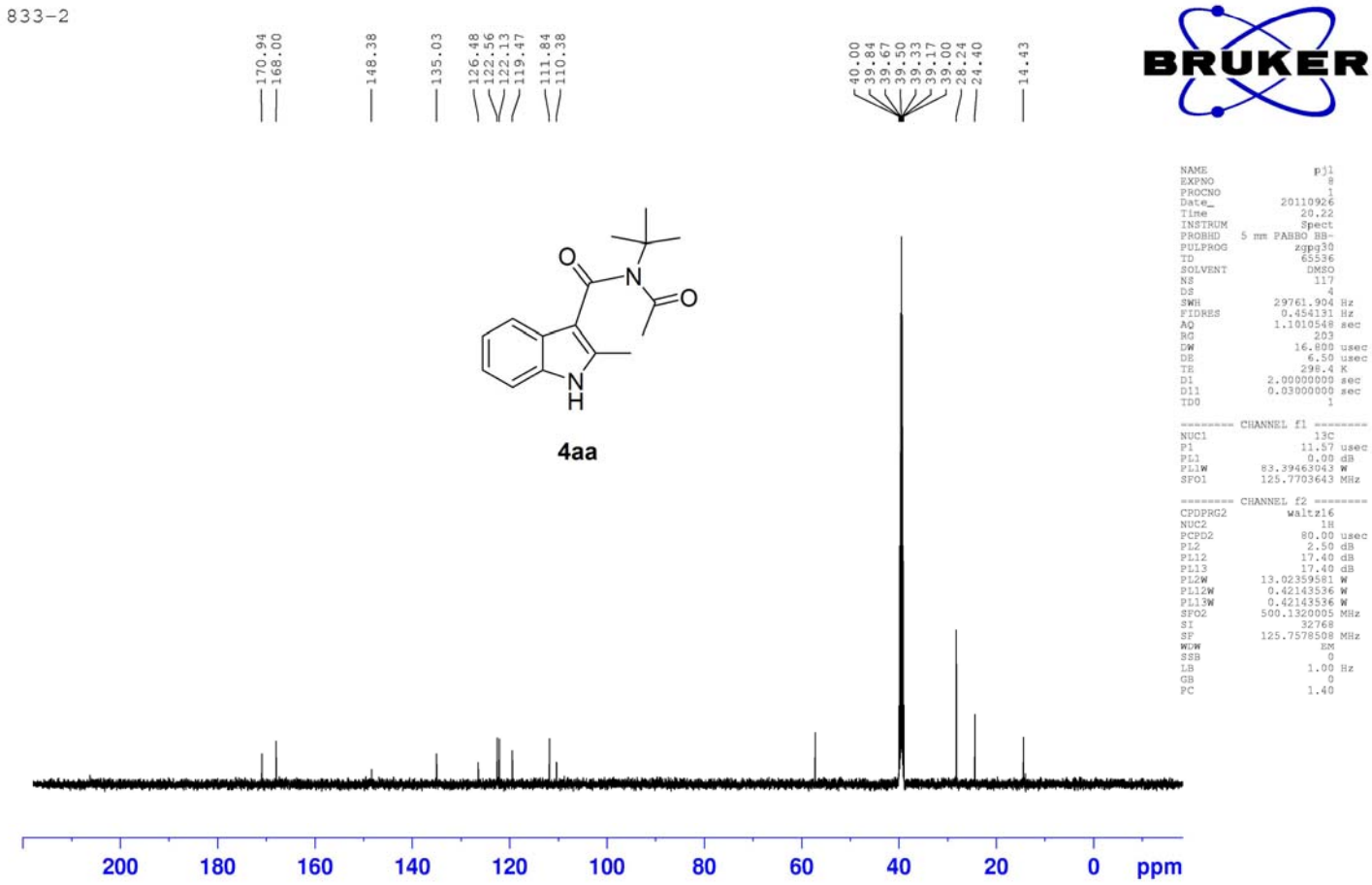
NAME	p11
EXPNO	13
PROCNO	1
Date_	20110921
Time	11.24
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	71.8
DW	60.400 usec
DE	6.50 usec
TE	298.5 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.00 dB
PL1W	10.87646866 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300089 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

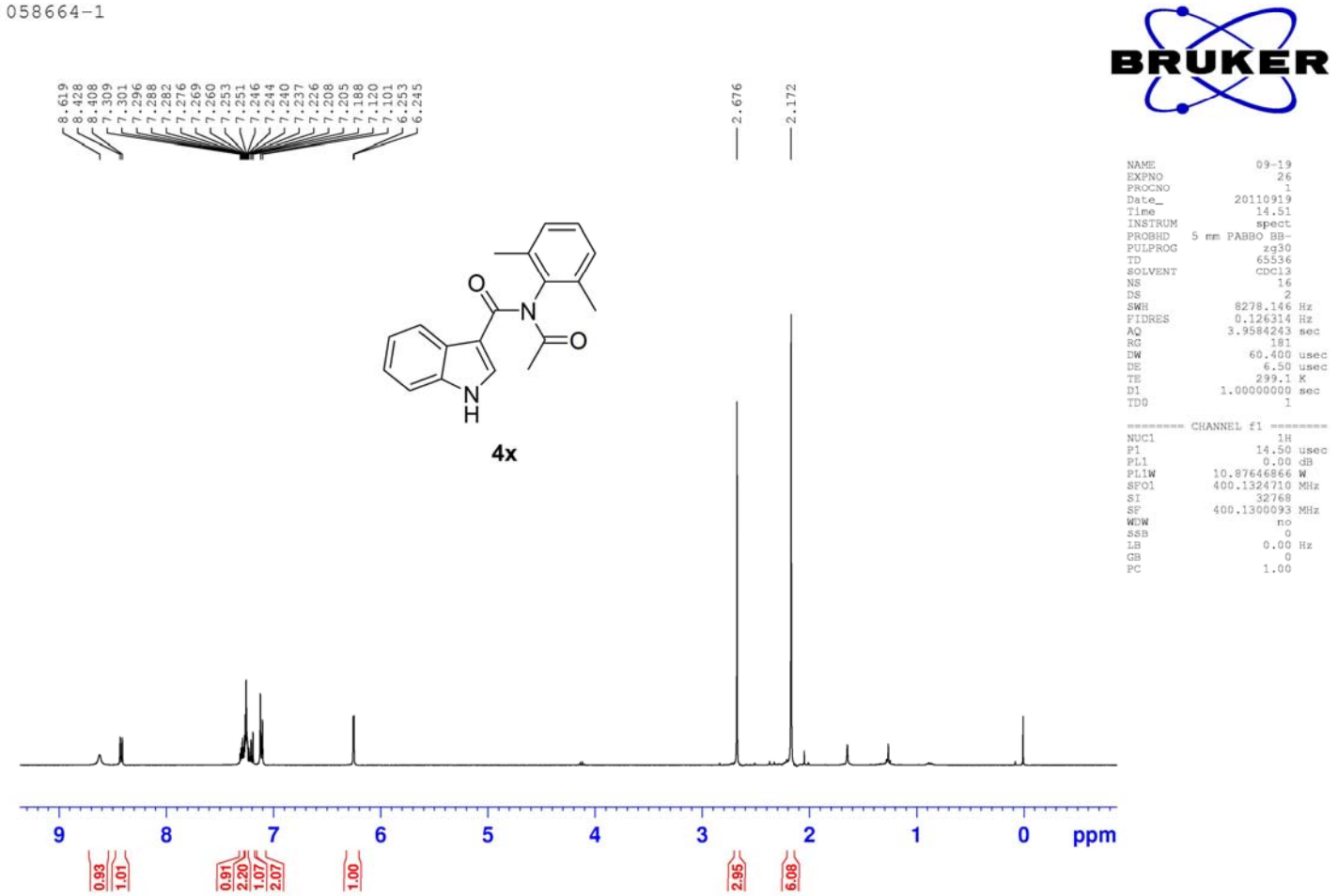

lly830-2
170.62
169.61
156.79
134.57
131.86
126.75
115.97
114.86
113.06
102.92
77.25
77.00
76.75
57.90
55.72
28.46
25.33
O
N
O
O
N
H
4d
NAME pjl
EXPNO 1
PROCNO 1
Date_ 20110922
Time 19.28
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 48
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 297.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 11.57 usec
PL1 0.00 dB
PL1W 83.39463043 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577982 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

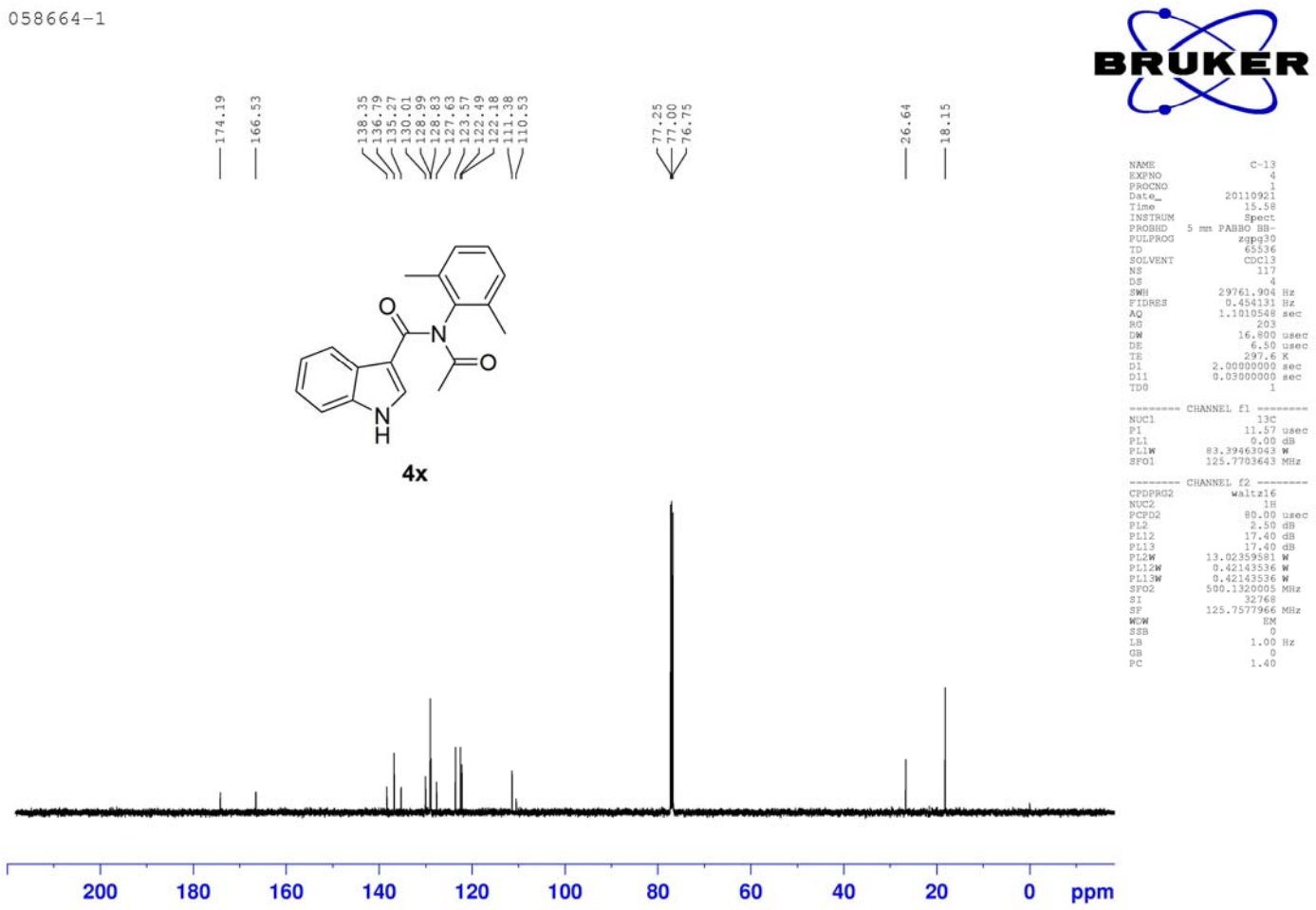


BRUKER

NAME	pjl
EXPNO	27
PROCNO	1
Date_	20110923
Time	14.39
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	128
DW	60.400 usec
DE	6.50 usec
TE	298.8 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.00 dB
PL1W	10.87646866 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300025 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00


833-2
170.94
168.00
148.38
135.03
126.48
122.56
122.13
119.47
111.84
110.38
40.00
39.84
39.67
39.50
39.33
39.17
39.00
28.24
24.40
14.43
BRUKER
4aa
NAME pj1
EXPNO 8
PROCNO 1
Date_ 20110926
Time 20.22
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 117
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 298.4 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 11.57 usec
PL1 0.00 dB
PL1W 83.39463043 W
SFO1 125.7703643 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7578508 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm


058664-1
8.619
8.428
8.408
7.309
7.301
7.296
7.288
7.282
7.276
7.269
7.260
7.253
7.251
7.246
7.244
7.240
7.237
7.226
7.208
7.205
7.188
7.120
7.101
6.253
6.245
2.676
2.172
4x
NAME 09-19
EXPNO 26
PROCNO 1
Date_ 20110919
Time 14.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 181
DW 60.400 usec
DE 6.50 usec
TE 299.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.50 usec
PL1 0.00 dB
PL1W 10.87646866 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300093 MHz
WDW no
SSB 0
LB 0.00 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
0.93
1.01
0.91
2.20
1.07
2.07
1.00
2.95
6.08



NAME	C-13
EXPNO	4
PROCNO	1
Date_	20110921
Time	15.58
INSTRUM	Spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	117
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	297.6 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	11.57 usec
PL1	0.00 dB
PL1W	83.39463043 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.50 dB
PL12	17.40 dB
PL13	17.40 dB
PL2W	13.02359581 W
PL12W	0.42143536 W
PL13W	0.42143536 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7577966 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40