Supporting Information

CuI-Mediated Sequential Iodination/Cycloetherification of *o*-Arylphenols: Synthesis of 2- or 4-Iododibenzofurans and Mechanistic Studies

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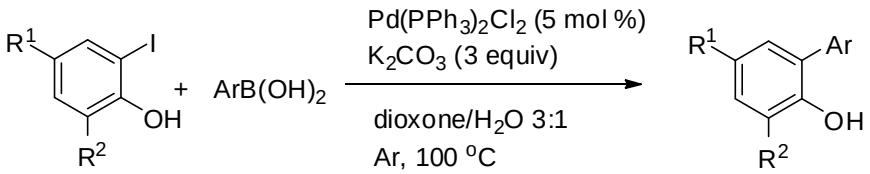
1. General information

DMSO was distilled under reduced pressure before use. Reactions were monitored using thin-layer chromatography (TLC) on commercial silica gel plates (GF 254). Visualization of the developed plates was performed under UV lights (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) were 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 were 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 s = broad singlet, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Coupling constant, *J*, was reported in Hertz unit (Hz). High resolution mass spectra (HRMS) were obtained on an ESI-LC-MS/MS spectrometer.

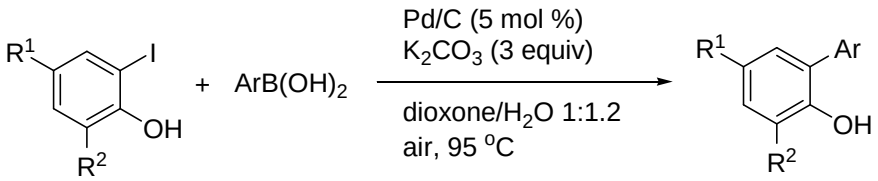
2. Synthesis of substrates

2.1 General procedures

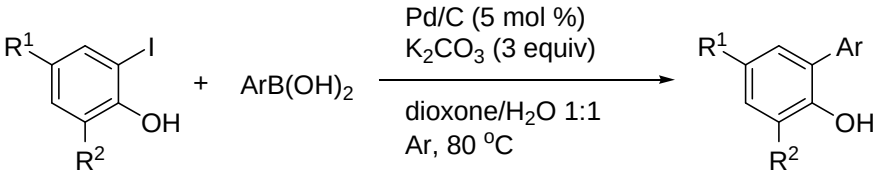
Except for compounds **1a**, **1b** and **1q**, substrates **1** were synthesized according to the general procedures **A** to **C**.



Procedure A: A mixture of substituted 2-iodophenol (2 mmol), arylboronic acid (3 mmol, 1.5 equiv), $Pd(Ph_3P)_2Cl_2$ (70 mg, 0.1 mmol, 5 mol %) and potassium carbonate (828 mg, 6 mmol, 3 equiv) in dioxone/H_2O (6/2 mL) was stirred at 100 °C under argon atmosphere until the starting material was consumed (typically 20 h). HCl aqueous solution (10%, 4 mL) was added to acidify the solution with vigorous stirring. The mixture was then extracted with EtOAc (15 mL × 2), and the organic layers were combined, washed with brine, and dried over Na_2SO_4. The concentrated crude product was purified by column chromatography to afford 2-arylphenol **1**.



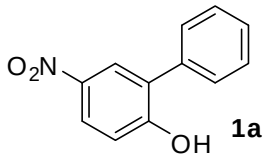
Procedure B[1]: A solution of substituted 2-iodophenol (1 mmol), arylboronic acid (2 mmol, 2 equiv), Pd/C (10%, 53 mg, 0.05 mmol, 0.05 equiv), potassium carbonate (414 mg, 3 mmol, 3 equiv) in dioxone/water (4/4.8 mL) was stirred at 95 °C under air. The reaction was monitored by TLC until the staring material was consumed (typically 10 h). HCl aqueous solution (10%, 4 mL) was added to the reaction mixture to acidify the solution with vigorous stirring. The mixture was then extracted with EtOAc (15 mL × 2) and the organic layers were combined, washed with brine, dried over Na_2SO_4. The concentrated crude product was purified by flash column chromatography to afford 2-arylphenol **1**.



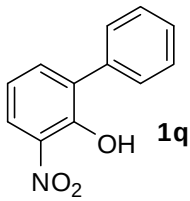
Procedure C[2]: A solution of substituted 2-iodophenol (1 mmol), arylboronic acid (2 mmol, 1.5 equiv), Pd/C (10%, 53 mg, 0.05 mmol, 0.05 equiv) and potassium carbonate (414 mg, 3 mmol, 3 equiv) in dioxone/H_2O (3/3 mL) was stirred at 80 °C under argon atmosphere until the starting material was consumed (typically 5-8 h). HCl aqueous solution (10%, 4 mL) was added to the reaction mixture to acidify the solution with vigorous stirring. The mixture was then extracted with EtOAc (15 mL × 2) and the organic layers were combined, washed with brine, dried over Na_2SO_4. The concentrated crude product was purified by flash column chromatography to afford 2-arylphenol **1**.

2.2 Characterization of substrates

4-nitro-2-phenylphenol (1a)[3] and **2-nitro-6-phenylphenol (1q)**



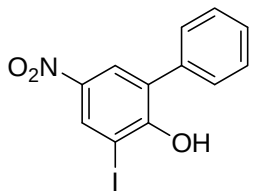
1a



1q

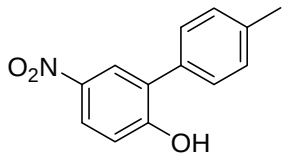
A 500 mL round-bottom flask was charged with 2-phenylphenol (4.01 g, 23.6 mmol) and AcOH (50 mL). The solution was stirred at 15 °C while a solution of concentrated HNO_3 (1.2 mL, 23.6 mmol, 1 equiv) in AcOH (20 mL) was added from a dropping funnel slowly. The addition rate was controlled at about 6 drops per minute, and the temperature was maintained at 15 to 20 °C. Upon completion of addition, the reaction mixture was transferred into a beaker and saturated $NaHCO_3$ aqueous solution (400 mL) was poured into the mixture slowly with vigorous stirring. The mixture was extracted with dichloromethane (200 mL) for three times. The organic layers were combined, and dried over Na_2SO_4. The concentrated crude product was purified by column chromatography to afford 1.80 g of **1a** as a yellow solid (34%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17-8.20 (m, 2H), 7.54-7.58 (m, 2H), 7.46-7.51 (m, 3H), 7.08 (d, J = 8.8 Hz, 1H), 5.96 (br s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.1, 141.9, 134.7, 129.7, 129.1, 128.9, 128.8, 126.2, 125.2, 116.3. And 1.58 g of **1q** was also obtained as a yellow solid (30%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 11.13 (s, 1H), 8.14 (dd, J = 8.4, 1.6 Hz, 1H), 7.64 (dd, J = 7.2, 1.4 Hz, 1H), 7.58-7.55 (m, 2H), 7.49-7.46 (m, 2H), 7.43-7.40 (m, 1H), 7.08-7.04 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 152.8, 138.4, 135.8, 134.1, 133.1, 129.3, 128.3, 128.1, 124.3, 119.8.

2-iodo-4-nitro-6-phenylphenol (1b)



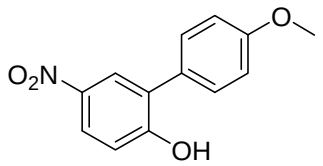
A mixture of **1a** (215 mg, 1 mmol) and iodine (508 mg, 2 mmol) in 5 mL of DMSO was stirred at 110 °C. The reaction was monitored by TLC until the starting material was consumed. The mixture was diluted with EtOAc, and it was washed with aqueous solution of sodium hydrosulfite and brine, successively. The organic layer was dried over Na_2SO_4 and concentrated under vacuum. The crude product was purified by column chromatography to provide 283 mg of **1b** as a yellow solid (83%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.60 (d, J = 2.6 Hz, 1H), 8.19 (d, J = 2.6 Hz, 1H), 7.45-7.55 (m, 5H), 6.24 (br s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.1, 142.2, 135.0, 133.7, 129.3, 129.1, 129.0, 128.5, 126.4, 84.5.

2-(4-methylphenyl)-4-nitrophenol (1c)



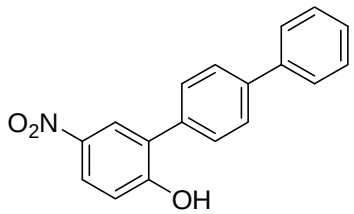
Following the general method **A**, 2-iodo-4-nitrophenol and 4-methylphenylboronic acid were used. Yellow solid, yield: 76%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.15-8.17 (m, 2H), 7.36 (s, 4H), 7.06 (d, *J* = 8.0 Hz, 1H), 5.94 (s, 1H), 2.44 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.2, 141.8, 139.2, 131.6, 130.5, 128.8, 126.1, 125.0, 116.2, 21.2.

2-(4-methoxyphenyl)-4-nitrophenol (1d)



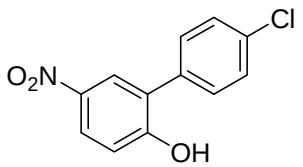
Following the general method **A**, 2-iodo-4-nitrophenol and 4-methoxyphenylboronic acid were used. Yellow solid, yield: 71%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.14-8.16 (m, 2H), 7.39 (d, *J* = 8.8 Hz, 2H), 7.04-7.08 (m, 3H), 5.94 (s, 1H), 3.88 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 160.2, 158.2, 141.6, 130.2, 128.4, 126.5, 126.2, 124.9, 116.1, 115.2, 55.4.

4-nitro-2-(4-phenylphenyl)phenol (1e)



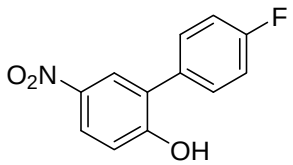
Following the general method **A**, 2-iodo-4-nitrophenol and 4-phenylphenylboronic acid were used. Yellow solid, yield: 82%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.25 (d, *J* = 2.8 Hz, 1H), 8.20 (dd, *J* = 8.8, 2.8 Hz, 1H), 7.78 (d, *J* = 8.4 Hz, 2H), 7.64-7.66 (m, 2H), 7.56 (d, *J* = 8.4 Hz, 2H), 7.48-7.51 (m, 2H), 7.39-7.43 (m, 1H), 7.10 (d, *J* = 8.8 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 158.1, 142.1, 141.8, 140.0, 133.3, 129.3, 129.0, 128.4, 128.3, 127.9, 127.1, 126.2, 125.2, 116.4.

2-(4-chlorophenyl)-4-nitrophenol (1f)



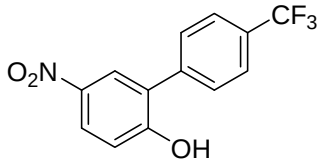
Following the general method **A**, 2-iodo-4-nitrophenol and 4-chlorophenylboronic acid were used. Yellow solid, yield: 85%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.16-8.19 (m, 2H), 7.52 (d, *J* = 8.4 Hz, 2H), 7.44 (d, *J* = 8.4 Hz, 2H), 7.05-7.07 (m, 1H), 5.92 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.9, 141.8, 135.2, 133.1, 130.4, 129.8, 127.6, 126.3, 125.4, 116.5.

2-(4-fluorophenyl)-4-nitrophenol (1g)



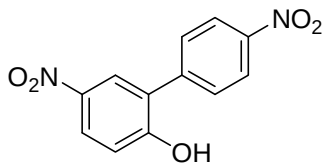
Following the general method **A**, 2-iodo-4-nitrophenol and 4-fluorophenylboronic acid were used. Yellow solid, yield: 78%. ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.33 (br s, 1H), 8.11-8.14 (m, 2H), 7.64 (dd, *J* = 8.6, 5.6 Hz, 2H), 7.28 (t, *J* = 8.8 Hz, 2H), 7.12 (d, *J* = 8.6 Hz, 1H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 162.6, 160.8, 160.7, 139.8, 132.5, 132.5, 131.2, 131.1, 127.3, 126.0, 124.9, 116.3, 115.1, 115.0.

4-nitro-2-(4-trifluoromethylphenyl)phenol (1h)



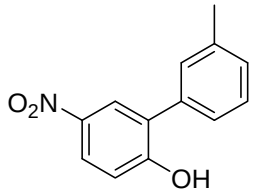
Following the general method **A**, 2-iodo-4-nitrophenol and 4-trifluoromethylphenylboronic acid were used. Yellow solid, yield: 58%. ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.51 (br s, 1H), 8.17-8.18 (m, 2H), 7.80-7.85 (m, 4H), 7.15-7.17 (m, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 160.7, 140.3, 139.9, 129.8, 128.4, 128.2, 128.1, 127.8, 127.5, 126.7, 126.0, 125.5, 125.3, 124.9, 124.9, 124.8, 124.8, 122.8, 120.1, 116.4.

4-nitro-2-(4-nitrophenyl)phenol (1i)



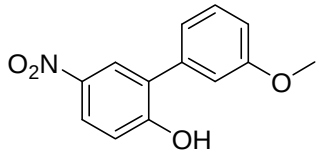
Following the general method **C**, 2-iodo-4-nitrophenol and 4-nitrophenylboronic acid were used. Yellow solid, yield: 75%. ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.67 (br s, 1H), 8.30 (d, *J* = 8.8 Hz, 2H), 8.19-8.22 (m, 2H), 7.91 (d, *J* = 8.8 Hz, 2H), 7.17 (d, *J* = 8.8 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 160.9, 146.6, 142.9, 139.9, 130.4, 126.2, 126.0, 125.9, 123.2, 116.6.

2-(3-methylphenyl)-4-nitrophenol (1j)



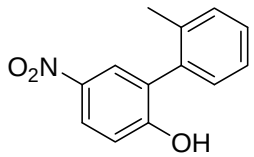
Following the general method **A**, 2-iodo-4-nitrophenol and 3-methylphenylboronic acid were used. Yellow solid, yield: 72%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.16-8.18 (m, 2H), 7.44 (t, *J* = 7.6 Hz, 1H), 7.25-7.31 (m, 3H), 7.07 (d, *J* = 7.6 Hz, 1H), 6.00 (s, 1H), 2.44 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 158.1, 141.6, 139.9, 134.4, 129.9, 129.7, 129.5, 128.7, 126.1, 125.8, 125.1, 116.2, 21.5.

2-(3-methoxyphenyl)-4-nitrophenol (1k)



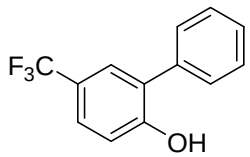
Following the general method **A**, 2-iodo-4-nitrophenol and 3-methoxyphenylboronic acid were used. Yellow solid, yield: 55%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.17-8.20 (m, 2H), 7.47 (t, *J* = 8.0 Hz, 1H), 7.08 (d, *J* = 8.4 Hz, 1H), 7.01-7.04 (m, 2H), 6.97 (d, *J* = 1.6 Hz, 1H), 6.02 (s, 1H), 3.87 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 160.7, 158.1, 141.6, 135.8, 131.0, 128.4, 126.0, 125.3, 120.8, 116.3, 114.7, 114.5, 55.4.

2-(2-methylphenyl)-4-nitrophenol (1l)



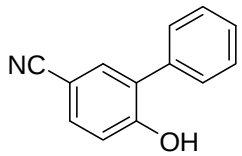
Following the general method **B**, 2-iodo-4-nitrophenol and 2-methylphenylboronic acid were used. Yellow solid, yield: 48%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21 (dd, *J* = 9.0, 2.8 Hz, 1H), 8.09 (d, *J* = 2.8 Hz, 1H), 7.32-7.43 (m, 3H), 7.23 (d, *J* = 7.8 Hz, 1H), 7.08 (d, *J* = 9.0 Hz, 1H), 5.57 (br s, 1H), 2.17 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.3, 141.6, 137.3, 133.2, 131.2, 130.3, 129.6, 128.4, 126.9, 126.3, 125.4, 115.9, 19.6.

2-phenyl-4-trifluoromethylphenol (1m)



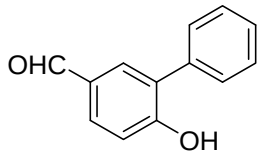
Following the general method **C**, 2-iodo-4-trifluoromethylphenol and phenylboronic acid were used. White solid, yield: 83%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.52-7.58 (m, 4H), 7.42-7.49 (m, 3H), 7.06 (d, *J* = 9.2 Hz, 1H), 5.80 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 156.3, 134.6, 134.4, 133.3, 129.7, 129.3, 128.9, 128.9, 119.0, 116.9, 104.3.

4-cyano-2-phenylphenol (1n)



Following the general method **A**, 2-iodo-4-cyanophenol and phenylboronic acid were used. White solid, yield: 81%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.52-7.58 (m, 4H), 7.42-7.49 (m, 3H), 7.06 (d, *J* = 9.0 Hz, 1H), 5.79 (s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 156.3, 134.6, 134.4, 133.3, 129.7, 129.3, 129.0, 128.9, 119.0, 116.9, 104.4.

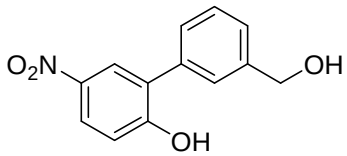
4-formyl-2-phenylphenol (1o)



Following the general method **A**, 2-iodo-4-formylphenol and phenylboronic acid were used. White solid, yield: 69%. ^{1}H NMR (400 MHz, DMSO-d_6): δ 10.80 (s, 1H), 9.86 (s,

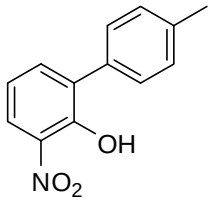
1H), 7.82 (d, J = 2.0 Hz, 1H), 7.75 (dd, J = 8.4, 2.0 Hz, 1H), 7.57-7.59 (m, 2H), 7.42-7.45 (m, 2H), 7.33-7.37 (m, 1H), 7.12 (d, J = 8.4 Hz, 1H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 191.1, 160.2, 137.2, 133.0, 130.2, 129.0, 128.7, 128.3, 128.1, 127.1, 116.5.

2-(3-hydroxymethylphenyl)-4-nitrophenol (1p)



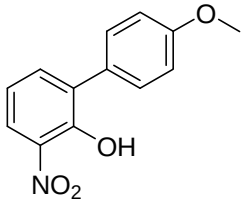
Following the general method **A**, 2-iodo-4-nitrophenol and 3-hydroxymethylphenylboronic acid were used. Yellow solid, yield: 65%. ^{1}H NMR (400 MHz, DMSO-d_6): δ 11.21 (br s, 1H), 8.09-8.13 (m, 2H), 7.52 (s, 1H), 7.47 (d, J = 7.6 Hz, 1H), 7.40 (t, J = 7.6 Hz, 1H), 7.33 (d, J = 7.6 Hz, 1H), 7.13 (d, J = 8.8 Hz, 1H), 5.21 (t, J = 5.6 Hz, 1H), 4.56 (d, J = 5.2 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 160.7, 142.4, 139.8, 135.9, 128.5, 127.7, 127.2, 126.9, 125.8, 125.6, 124.4, 116.2, 62.7.

6-(4-methylphenyl)-2-nitrophenol (1r)



Following the general method **B**, 2-iodo-6-nitriphenol and 4-methylphenylboronic acid were used. Yellow solid, yield: 65%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 11.12 (s, 1H), 8.11 (d, J = 7.8 Hz, 1H), 7.63 (d, J = 7.8 Hz, 1H), 7.45 (d, J = 8.0 Hz, 2H), 7.28 (d, J = 8.0 Hz, 2H), 7.06-7.02 (m, 1H), 2.42 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 152.8, 138.2, 138.0, 134.1, 133.1, 132.9, 129.2, 129.1, 124.0, 119.7, 21.2.

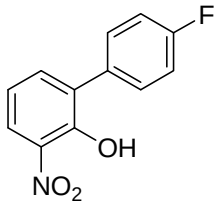
6-(4-methoxyphenyl)-2-nitrophenol (1s)



Following the general method **B**, 2-iodo-6-nitriphenol and 4-methoxyphenylboronic

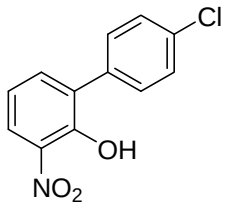
acid were used. Yellow solid, yield: 63%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 11.14 (s, 1H), 8.10 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.62 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.50 (d, *J* = 8.8 Hz, 2H), 7.06-6.99 (m, 3H), 3.87 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 159.5, 152.8, 138.1, 134.2, 132.8, 130.5, 128.1, 123.8, 119.7, 113.8, 55.3.

6-(4-fluorophenyl)-2-nitrophenol (1t)



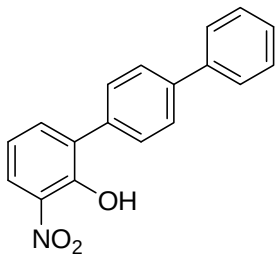
Following the general method **B**, 2-iodo-6-nitriphenol and 4-fluorophenylboronic acid were used. Yellow solid, yield: 88 %. ^{1}H NMR (400 MHz, $CDCl_3$): δ 11.14 (s, 1H), 8.14 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.61 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.55-7.52 (m, 2H), 7.18-7.13 (m, 2H), 7.08-7.04 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 163.6, 161.6, 152.7, 138.2, 134.2, 132.0, 131.71, 131.69, 131.1, 131.0, 124.4, 119.8, 115.4, 115.3.

6-(4-chlorophenyl)-2-nitrophenol (1u)



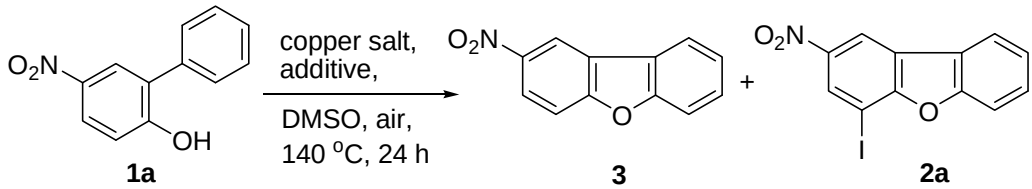
Following the general method **B**, 2-iodo-6-nitriphenol and 4-chlorophenylboronic acid were used. Yellow solid, yield: 78 %. ^{1}H NMR (400 MHz, $CDCl_3$): δ 11.14 (s, 1H), 8.15 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.61 (dd, *J* = 7.6, 1.6 Hz, 1H), 7.51-7.49 (m, 2H), 7.45-7.43 (m, 2H), 7.09-7.04 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 152.6, 147.1, 138.1, 134.21, 134.15, 131.8, 130.6, 128.6, 125.4, 124.6, 121.6, 119.8.

2-nitro-6-(4-phenylphenyl)phenol (1v)



Following the general method **B**, 2-iodo-6-nitriphenol and 4-phenylphenylboronic acid were used. Yellow solid, yield: 83 %. ^{1}H NMR (400 MHz, $CDCl_3$): δ 11.19 (s, 1H), 8.15 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.73-7.64 (m, 7H), 7.49-7.45 (m, 2H), 7.38 (t, *J* = 7.4 Hz, 1H), 7.10-7.06 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 152.8, 141.0, 140.5, 138.2, 134.7, 134.2, 132.6, 129.7, 128.8, 127.5, 127.10, 127.06, 124.3, 119.8.

3. Optimization of the reaction conditions



entry	Cu salt (equiv)	additive (equiv)	yield (%)[b] **3**	**2a**
1[c]	$Cu(OAc)_2$ (1.0)	--	0	0
2[d]	$Cu(OAc)_2$ (1.0)	--	0	0
3[e]	$Cu(OAc)_2$ (1.0)	--	0	0
4[f]	$Cu(OAc)_2$ (1.0)	--	14	0
5	$Cu(OAc)_2$ (1.0)	--	39	0
6	$Cu(TFA)_2$ (1.0)	--	trace	0
7	$Cu(OTf)_2$ (1.0)	--	7	0
8	CuCl (1.0)	--	0	0
9	CuI (1.0)	--	0	55
10	CuI (1.5)	--	0	63
11	CuI (2.0)	--	0	63
12[g]	CuI (1.5)	--	0	60
13[h]	CuI (1.5)	--	0	9
14[i]	CuI (0.2)	I_2 (1.0)	0	0
15[i]	CuI (0.5)	I_2 (1.0)	0	0
16	CuI (0.5)	LiI (1.0)	0	0
17	CuI (0.5)	NaI (1.0)	0	0
18	CuI (0.5)	KI (1.0)	0	0
19	CuI (0.5)	*n*-Bu_4NI (1.0)	0	0
20	CuI (1.5)	AcOH (1.0)	0	79
21	CuI (1.5)	PivOH (1.0)	0	82
22	CuI (1.5)	PivOH (2.0)	0	82
23[j]	CuI (1.5)	PivOH (1.0)	0	81

[a]The reactions were carried out at 0.2 mmol scale in 1 mL of solvent. [b]Isolated yield. [c]The reaction was performed in *o*-dichlorobenzene at 140 °C. [d]The reaction was performed in toluene under reflux. [e]The reaction was performed in acetic acid under reflux. [f]The reaction was performed in DMF at 140 °C. [g]The reaction was performed under balloon pressure of O_2. [h]The reaction was performed under balloon pressure of Ar. [i]**1b** was formed in 80% yield. [j]The reaction time was 12 h.

4. General procedures and product characterization

4.1 General procedures

A reaction tube was charged with 2-arylphenol substrate **1** (0.2 mmol), CuI (57 mg, 0.3 mmol, 1.5 equiv), PivOH (22.5 μL, 0.2 mmol, 1 equiv) and DMSO (1 mL). The mixture was stirred open to air at temperatures described in procedures **A** to **D**.

Procedure **A**: the reaction mixture was stirred at 110 °C for 10 h and then at 140 °C for another 10 h (for **2k**, 26 h).

Procedure **B**: the reaction mixture was stirred at 140 °C for 10 h (for **2q-2v**, 24 h).

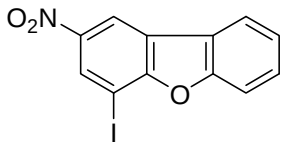
Procedure **C**: the reaction mixture was stirred at 60 °C for 90 h and at 80 °C for another 40 h.

Procedure **D**: CuBr (1.5 equiv) was used instead of CuI; the reaction mixture was stirred at 100 °C for 24 h and at 140 °C for another 10 h.

After the completion of the reaction, EtOAc (25 mL) was added to the cooled reaction mixture. The solution was washed with concentrated NH_4OH (15 mL) and brine (15 mL), successively. The organic layer was dried over Na_2SO_4, and concentrated under vacuum. The residue was purified by column chromatography to give the corresponding products.

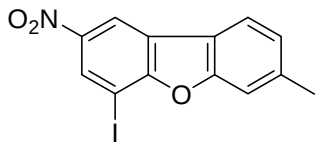
4.2 Product characterization

4-iodo-2-nitrodibenzofuran (2a)



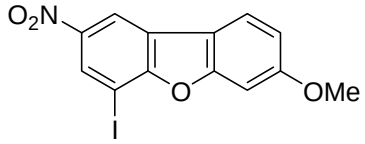
Following the general procedure **B**; white solid, yield: 82%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.83 (d, *J* = 2.0 Hz, 1H), 8.75 (d, *J* = 2.0 Hz, 1H), 8.01 (d, *J* = 8.0 Hz, 1H), 7.72 (d, *J* = 8.4 Hz, 1H), 7.61 (t, *J* = 7.8 Hz, 1H), 7.48 (t, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.7, 157.1, 144.4, 131.4, 129.4, 124.4, 124.4, 123.7, 121.8, 116.6, 112.6, 74.8; HRMS (ESI): Exact mass calcd for $C_{12}H_{16}INNaO_3$ $[M+Na]^+$ 361.9285, found 361.9285.

4-iodo-7-methyl-2-nitrodibenzofuran (2b)



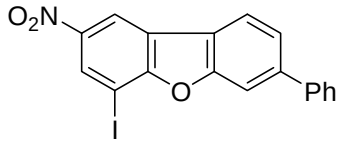
Following the general procedure **A**; white solid, yield: 76%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.77 (d, *J* = 2.0 Hz, 1H), 8.71 (d, *J* = 2.0 Hz, 1H), 7.87 (d, *J* = 8.0 Hz, 1H), 7.52 (s, 1H), 7.29 (d, *J* = 8.0 Hz, 1H), 2.57 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.7, 157.5, 144.4, 140.5, 130.8, 125.7, 124.6, 121.2, 121.0, 116.2, 112.7, 74.6, 22.1; HRMS (ESI): Exact mass calcd for $C_{13}H_8INNaO_3$ $[M+Na]^+$ 375.9441, found 375.9444.

4-iodo-7-methoxy-2-nitrodibenzofuran (2c)



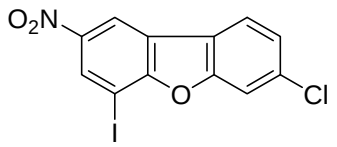
Following general procedure **A**; white solid, yield: 70%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.71 (d, *J* = 2.2 Hz, 1H), 8.65 (d, *J* = 2.2 Hz, 1H), 7.86 (d, *J* = 8.8 Hz, 1H), 7.22 (d, *J* = 2.0 Hz, 1H), 7.05 (dd, *J* = 8.8, 2.2 Hz, 1H), 3.93 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 161.7, 159.8, 158.6, 144.5, 129.9, 124.7, 122.1, 116.4, 115.5, 113.1, 97.0, 74.2, 55.9; HRMS (ESI): Exact mass calcd for $C_{13}H_8INNaO_4$ $[M+Na]^+$ 391.9390, found 391.9400.

4-iodo-2-nitro-7-phenyldibenzofuran (2d)



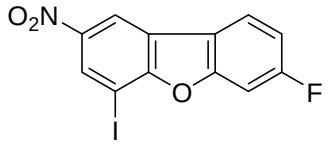
Following the general procedure **A**; white solid, yield: 67%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.84 (d, *J* = 2.0 Hz, 1H), 8.75 (d, *J* = 2.0 Hz, 1H), 8.05 (d, *J* = 8.0 Hz, 1H), 7.94 (s, 1H), 7.68-7.73 (m, 3H), 7.52 (t, *J* = 7.2 Hz, 2H), 7.43 (t, *J* = 7.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.1, 157.7, 144.5, 143.2, 140.1, 131.2, 129.1, 128.2, 127.4, 124.3, 123.8, 122.5, 121.8, 116.5, 110.9, 74.7; HRMS (ESI): Exact mass calcd for $C_{18}H_{10}INNaO_3$ $[M+Na]^+$ 437.9598, found 437.9594.

7-chloro-4-iodo-2-nitrodibenzofuran (2e)



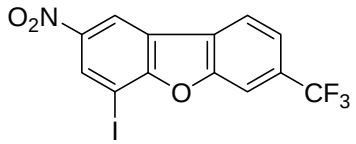
Following the general procedure **B**; white solid, yield: 70%. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.16 (d, *J* = 2.0 Hz, 1H), 8.66 (d, *J* = 2.0 Hz, 1H), 8.36 (d, *J* = 8.4 Hz, 1H), 8.07 (d, *J* = 1.2 Hz, 1H), 7.56 (dd, *J* = 8.4, 1.4 Hz, 1H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 159.5, 156.3, 144.4, 133.7, 131.0, 124.8, 123.9, 123.1, 122.3, 117.6, 112.7, 76.7; HRMS (ESI): Exact mass calcd for $C_{12}H_5ClINNaO_3$ $[M+Na]^+$ 395.8895, found 395.8893.

7-fluoro-4-iodo-2-nitrodibenzofuran (2f)



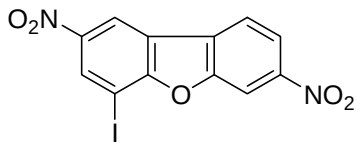
Following the general procedure **B**; white solid, yield: 74%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.77 (d, *J* = 2.0 Hz, 1H), 8.72 (d, *J* = 2.0 Hz, 1H), 7.96 (dd, *J* = 8.6, 5.2 Hz, 1H), 7.43 (dd, *J* = 8.4, 2.2 Hz, 1H), 7.20-7.25 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 164.7, 162.2, 160.3, 157.5, 157.4, 144.7, 131.1, 124.0, 122.7, 122.6, 120.0, 120.0, 116.3, 113.0, 112.7, 100.9, 100.6, 74.7; HRMS (ESI): Exact mass calcd for $C_{12}H_5FINNaO_3$ $[M+Na]^+$ 379.9190, found 379.9193.

4-iodo-2-nitro-7-trifluoromethyldibenzofuran (2g)



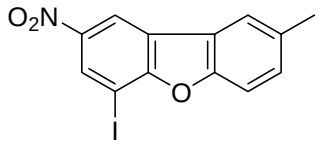
Following the general procedure **B**; white solid, yield: 67%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.90 (d, *J* = 2.0 Hz, 1H), 8.83 (d, *J* = 2.0 Hz, 1H), 8.14 (d, *J* = 8.0 Hz, 1H), 8.02 (s, 1H), 7.76 (d, *J* = 8.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 160.5, 156.2, 144.8, 132.6, 132.0, 131.7, 131.4, 131.1, 127.7, 126.8, 125.0, 123.2, 122.4, 122.3, 121.4, 121.4, 121.4, 121.3, 119.6, 117.3, 110.4, 110.4, 110.3, 110.3, 75.2.

2,7-dinitro-4-iodo-dibenzofuran (2h)



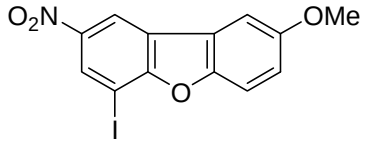
Following the general procedure **A**; pale yellow solid, yield: 67%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.94 (d, *J* = 2.0 Hz, 1H), 8.88 (d, *J* = 2.0 Hz, 1H), 8.64 (d, *J* = 1.8 Hz, 1H), 8.42 (dd, *J* = 8.4, 1.8 Hz, 1H), 8.18 (d, *J* = 8.4 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 161.4, 155.9, 148.2, 144.9, 133.4, 129.3, 122.6, 122.2, 119.9, 117.8, 109.0, 75.6; HRMS (ESI): Exact mass calcd for $C_{12}H_5IN_2NaO_5$ $[M+Na]^+$ 406.9135, found 406.9136.

4-iodo-8-methyl-2-nitrodibenzofuran (2i)



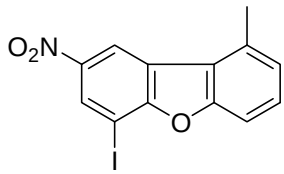
Following the general procedure in **A**; white solid, yield: 81%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.79 (d, *J* = 2.2 Hz, 1H), 8.73 (d, *J* = 2.2 Hz, 1H), 7.80 (s, 1H), 7.59 (d, *J* = 8.4 Hz, 1H), 7.41 (d, *J* = 7.6 Hz, 1H), 2.55 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 159.9, 155.4, 144.3, 134.2, 131.1, 130.6, 124.4, 123.6, 121.5, 116.5, 112.1, 74.7, 21.3; HRMS (ESI): Exact mass calcd for $C_{13}H_8INNaO_3$ $[M+Na]^+$ 375.9441, found 375.9441.

4-iodo-8-methoxy-2-nitrodibenzofuran (2j)[9]



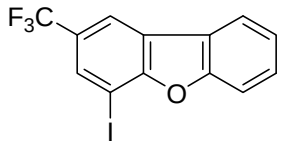
Following the general procedure **A**; pale yellow solid, yield: 65% (13% of the regioisomer). ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.21 (d, *J* = 2.2 Hz, 1H), 8.67 (d, *J* = 2.2 Hz, 1H), 8.03 (d, *J* = 2.4 Hz, 1H), 7.80 (d, *J* = 9.2 Hz, 1H), 7.23 (dd, *J* = 9.2, 2.6 Hz, 1H), 3.88 (s, 3H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 159.7, 156.4, 150.8, 143.8, 130.5, 124.0, 123.8, 117.7, 117.5, 112.8, 105.4, 76.7, 55.8; HRMS (ESI): Exact mass calcd for $C_{13}H_8INNaO_4$ $[M+Na]^+$ 391.9390, found 391.9393.

6-iodo-1-methyl-8-nitrodibenzofuran (2k)



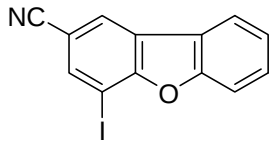
Following the general procedure **A**, the reaction was performed at 140 °C for 26 h. White solid, yield: 26%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.85 (d, *J* = 2.2 Hz, 1H), 8.75 (d, *J* = 2.2 Hz, 1H), 7.56 (d, *J* = 8.2 Hz, 1H), 7.49 (t, *J* = 7.8 Hz, 1H), 7.24 (d, *J* = 7.2 Hz, 1H), 2.84 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 159.6, 157.0, 144.2, 134.8, 130.9, 129.2, 125.5, 124.8, 122.3, 118.0, 109.9, 74.7, 19.7; HRMS (ESI): Exact mass calcd for $C_{13}H_8INNaO_3$ $[M+Na]^+$ 375.9441, found 375.9446.

4-iodo-2-trifluoromethyldibenzofuran (2l)



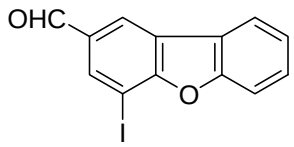
Following the general procedure **A**; white solid, yield: 71%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.22 (d, *J* = 1.4 Hz, 1H), 8.08 (d, *J* = 1.4 Hz, 1H), 7.96 (d, *J* = 7.4 Hz, 1H), 7.70 (d, *J* = 8.4 Hz, 1H), 7.57-7.61 (m, 1H), 7.44-7.47 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 158.6, 156.3, 138.8, 129.3, 124.9, 124.8, 124.2, 123.0, 121.6, 117.7, 112.5, 108.3, 75.9.

2-cyano-4-iododibenzofuran (2m)



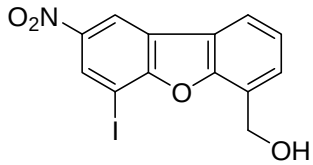
Following the general procedure **B**; white solid, yield: 43%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.23 (d, *J* = 1.4 Hz, 1H), 8.09 (d, *J* = 1.4 Hz, 1H), 7.96 (d, *J* = 7.8 Hz, 1H), 7.71 (d, *J* = 8.4 Hz, 1H), 7.58-7.62 (m, 1H), 7.44-7.48 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.6, 156.4, 138.9, 129.3, 124.9, 124.8, 124.2, 123.1, 121.6, 117.6, 112.5, 108.4, 75.9; HRMS (ESI): Exact mass calcd for $C_{13}H_6INNaO$ $[M+Na]^+$ 341.9386, found 341.9383.

2-formyl-4-iododibenzofuran (2n)



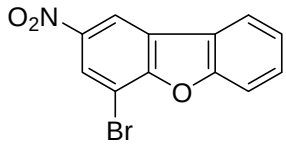
Following the general procedure **B**; white solid, yield: 35%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 10.04 (s, 1H), 8.43 (d, *J* = 1.4 Hz, 1H), 8.34 (d, *J* = 1.4 Hz, 1H), 7.98 (d, *J* = 7.6 Hz, 1H), 7.69 (d, *J* = 8.4 Hz, 1H), 7.54-7.59 (m, 1H), 7.42-7.46 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 189.9, 159.9, 156.5, 137.7, 133.6, 128.8, 125.1, 124.0, 123.9, 122.5, 121.5, 112.4, 76.1; HRMS (ESI): Exact mass calcd for $C_{13}H_7INaO_2$ $[M+Na]^+$ 344.9383, found 344.9382.

6-hydroxymethyl-4-iodo-2-nitrodibenzofuran (2o)



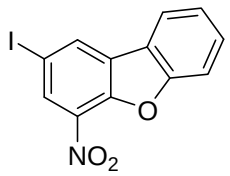
Following the general procedure **C**; white solid, yield: 54%. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.18 (d, *J* = 2.2 Hz, 1H), 8.68 (d, *J* = 2.2 Hz, 1H), 8.27 (d, *J* = 7.6 Hz, 1H), 7.69 (d, *J* = 7.4 Hz, 1H), 7.51 (t, *J* = 7.6 Hz, 1H), 5.50 (t, *J* = 5.6 Hz, 1H), 4.90 (d, *J* = 5.6 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 159.0, 153.5, 144.1, 130.6, 127.8, 126.8, 124.2, 123.8, 122.8, 121.2, 117.4, 76.7, 57.1; HRMS (ESI): Exact mass calcd for $C_{13}H_8INNaO_4$ $[M+Na]^+$ 391.9390, found 391.9391.

4-bromo-2-nitrodibenzofuran (2p)



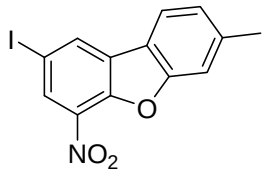
Following the general procedure **D**; white solid, yield: 63%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.79 (d, *J* = 2.0 Hz, 1H), 8.56 (d, *J* = 2.0 Hz, 1H), 8.01 (d, *J* = 7.6 Hz, 1H), 7.71 (d, *J* = 8.4 Hz, 1H), 7.59-7.64 (m, 1H), 7.46-7.50 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.4, 156.6, 144.4, 129.6, 125.8, 125.7, 124.5, 123.4, 121.7, 115.8, 112.6, 104.8; HRMS (ESI): Exact mass calcd for $C_{12}H_6BrNNaO_3$ $[M+Na]^+$ 313.9423, found 313.9425.

2-iodo-4-nitrodibenzofuran (2q)



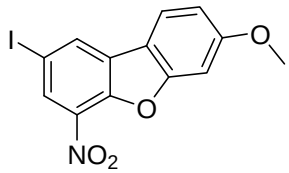
Following the general procedure **B**; pale yellow solid, yield: 50%. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.05 (d, *J* = 1.6 Hz, 1H), 8.51 (d, *J* = 1.6 Hz, 1H), 8.30 (d, *J* = 7.6 Hz, 1H), 7.89 (d, *J* = 8.4 Hz, 1H), 7.67 (t, *J* = 7.4 Hz, 1H), 7.53 (t, *J* = 7.4 Hz, 1H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 156.1, 147.4, 136.2, 134.0, 130.4, 129.9, 129.7, 124.5, 122.1, 120.8, 112.1, 85.7; HRMS (ESI): Exact mass calcd for $C_{12}H_7INO_3[M+H]^+$ 339.9465, found 339.9464.

2-iodo-7-methyl-4-nitrodibenzofuran (2r)



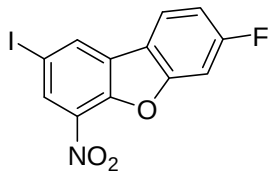
Following the general procedure **B**; pale yellow solid, yield: 42%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.49 (d, *J* = 1.6 Hz, 1H), 8.46 (d, *J* = 1.6 Hz, 1H), 7.79 (d, *J* = 8.0 Hz, 1H), 7.52 (s, 1H), 7.27-7.25 (m, 1H), 2.56 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.4, 148.2, 140.7, 134.9, 134.3, 130.7, 130.4, 125.8, 120.5, 118.4, 112.7, 83.7, 22.1; HRMS (ESI): Exact mass calcd for $C_{13}H_9INO_3[M+H]^+$ 353.9622, found 353.9622.

2-iodo-7-methoxy-4-nitrodibenzofuran (2s)



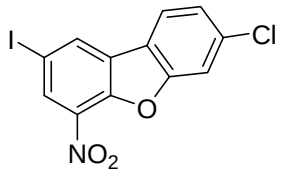
Following the general procedure **B**; pale yellow solid, yield: 32%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.46 (d, *J* = 1.6 Hz, 1H), 8.42 (d, *J* = 1.6 Hz, 1H), 7.80 (d, *J* = 8.8 Hz, 1H), 7.25-7.24 (m, 1H), 7.04 (dd, *J* = 8.8, 2.2 Hz, 1H), 3.93 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 161.7, 158.6, 148.4, 134.3, 134.2, 130.8, 129.4, 121.4, 113.9, 113.4, 96.8, 84.0, 55.9; HRMS (ESI): Exact mass calcd for $C_{13}H_9INO_4[M+H]^+$ 369.9571, found 369.9569.

7-fluoro-2-iodo-4-nitrodibenzofuran (2t)



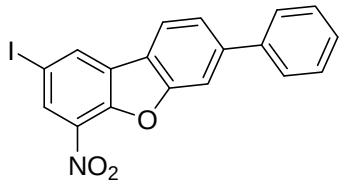
Following the general procedure **B**; pale yellow solid, yield: 75%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.53 (d, *J* = 1.6 Hz, 1H), 8.50 (d, *J* = 1.6 Hz, 1H), 7.91 (dd, *J* = 8.4, 5.2 Hz, 1H), 7.46 (dd, *J* = 8.4, 2.2 Hz, 1H), 7.25-7.20 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 164.5, 162.5, 157.5, 157.4, 148.8, 135.0, 134.4, 130.7, 129.9, 121.9, 121.8, 117.44, 117.43, 113.0, 112.8, 100.9, 100.7, 84.4; HRMS (ESI): Exact mass calcd for $C_{12}H_6FINO_3[M+H]^+$ 357.9371, found 357.9370.

7-chloro-2-iodo-4-nitrodibenzofuran (2u)



Following the general procedure **B**; pale yellow solid, yield: 45%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.56 (d, *J* = 1.6 Hz, 1H), 8.51 (d, *J* = 1.6 Hz, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.76 (d, *J* = 1.6 Hz, 1H), 7.45 (d, *J* = 8.4 Hz, J = 1.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.2, 148.5, 135.5, 135.2, 134.7, 131.3, 129.8, 125.3, 121.5, 119.8, 113.3, 84.2; HRMS (ESI): Exact mass calcd for $C_{12}H_6ClINO_3[M+H]^+$ 373.9075, found 373.9084.

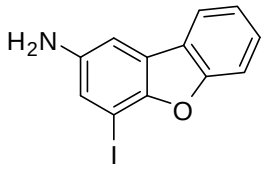
2-iodo-4-nitro-7-phenyldibenzofuran (2v)



Following the general procedure **B**; pale yellow solid, yield: 56%. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.56-8.55 (m, 2H), 8.01-7.97 (m, 2H), 7.73-7.68 (m, 3H), 7.53-7.49 (m, 2H), 7.45-7.41 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.8, 148.7, 143.5, 140.1, 135.2, 134.6, 130.9, 130.5, 129.1, 128.2, 127.4, 123.9, 121.1, 120.0, 110.9, 83.9; HRMS (ESI): Exact mass calcd for $C_{18}H_{11}INO_3[M+H]^+$ 415.9778, found 415.9778.

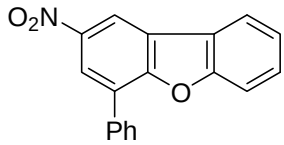
5. Diversification of 2a

2-amino-4-iododibenzofuran (4)



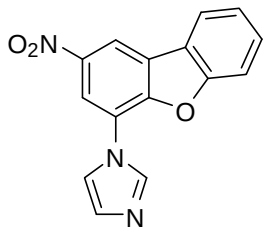
A mixture of **2a** (34 mg, 0.1 mmol), iron powder (28 mg, 0.5 mmol, 5 equiv), 10% HCl aqueous solution (1 mL) in THF (2 mL) was stirred at 85 °C under argon atmosphere for 6 h, then another 2.5 equiv of iron powder (14 mg), 0.5 mL of 10% HCl aqueous solution and 1mL THF were added. The reaction mixture was stired for another 6 h. The mixture was diluted by EtOAc (20 mL), washed with concentrated NH_4OH (15 mL) and brine (15 mL), and dried over Na_2SO_4. The concentrated residue was purified by column chromatography to give **4** as a pink solid in 63% yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 (d, *J* = 7.6 Hz, 1H), 7.59 (d, *J* = 8.4 Hz, 1H), 7.47-7.43 (m, 1H), 7.33-7.29 (m, 1H), 7.21-7.19 (m, 2H), 3.70 (br s, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 156.4, 150.9, 143.4, 127.5, 124.9, 124.8, 124.0, 122.7, 121.0, 112.1, 106.1, 75.2; HRMS (ESI): Exact mass calcd for $C_{12}H_9INO[M+H]^+$ 309.9723, found 309.9726.

2-nitro-4-phenyldibenzofuran (5)



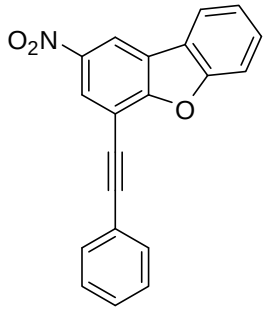
Following the general procedure for the synthesis of substrate **1**, **2a** and phenylboronic acid were used. Compound **5** was isolated in 91% yield as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.84 (d, *J* = 2.4 Hz, 1H), 8.55 (d, *J* = 2.4 Hz, 1H), 8.07 (d, *J* = 7.6 Hz, 1H), 7.93-7.95 (m, 2H), 7.67 (d, *J* = 8.2 Hz, 1H), 7.56-7.61 (m, 3H), 7.47-7.53 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 157.3, 156.3, 144.2, 134.2, 129.0, 128.9, 128.8, 126.5, 125.7, 124.0, 123.2, 122.1, 121.2, 115.4, 112.3; HRMS (ESI): Exact mass calcd for $C_{18}H_{11}NNaO_3$ $[M+Na]^+$ 312.0631, found 312.0631.

1-(2-nitrodibenzo[*b*,*d*]furan-4-yl)-1*H*-imidazole (6)



Substrate **1a** (22 mg, 0.1 mmol) was subjected to the standard iodocyclization condition (procedure **B**). When **1a** was completely converted to **2a**, imidazole (28 mg, 0.4 mmol, 4 equiv) and KOH (17 mg, 0.3 mmol, 3 equiv) were added to the reaction mixture. The mixture was stirred at 140 °C for 20 h in argon. The cooled reaction mixture was diluted with EtOAc (20 mL), washed with concentrated NH_4OH (15 mL) and brine (15 mL), and dried over Na_2SO_4. The concentrated residue was purified by column chromatography to give **6** in 36% yield as a yellow solid. ^{1}H NMR (400 MHz, DMSO-d_6): δ 9.19 (d, *J* = 2.2 Hz, 1H), 8.63 (d, *J* = 2.2 Hz, 1H), 8.56 (s, 1H), 8.45 (d, *J* = 7.4 Hz, 1H), 8.06 (s, 1H), 7.89 (d, *J* = 8.4 Hz, 1H), 7.71-7.67 (m, 1H), 7.57-7.53 (m, 1H), 7.27 (s, 1H); ^{13}C NMR (125 MHz, DMSO-d_6): δ 156.8, 149.9, 144.0, 137.4, 129.9, 129.8, 126.6, 124.7, 122.62, 122.58, 122.4, 119.7, 115.9, 115.8, 112.6. HRMS (ESI): Exact mass calcd for $C_{15}H_{10}N_3O_3[M+H]^+$ 280.0717, found 280.0718.

2-nitro-4-(phenylethynyl)dibenzofuran (7)



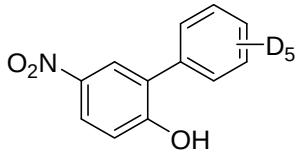
A mixture of **2a** (44 mg, 0.2 mmol), phenylacetylene (28.5 μL, 0.26 mmol, 1.3 equiv), $Pd(PPh_3)_2Cl_2$ (2.8 mg, 0.004 mmol, 2 mol %), CuI (1.5 mg, 0.008 mmol, 4 mol %), Et_2NH (164 μL, 1.6 mmol, 8 equiv) in DMF (2 mL) was stirred at room temperature in Ar for 3 h. The mixture was diluted with EtOAc (20 mL), washed with brine (15 mL), and dried over Na_2SO_4. The concentrated residue was purified by column chromatography to give **7** in 75% yield as a white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.78 (d, *J* = 2.4 Hz, 1H), 8.52 (d, *J* = 2.4 Hz, 1H), 8.02 (d, *J* = 7.4 Hz, 1H), 7.72-7.67 (m, 3H), 7.62-7.58 (m, 1H), 7.48-7.42 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 158.8, 157.4, 143.7, 132.0, 129.3, 129.2, 128.5, 125.7, 125.1, 124.2, 123.0, 122.1,

121.4, 116.4, 112.5, 108.9, 96.4, 81.6; HRMS (ESI): Exact mass calcd for $C_{20}H_{12}NO_3[M+H]^+$ 314.0812, found 314.0813.

6. Mechanistic studies

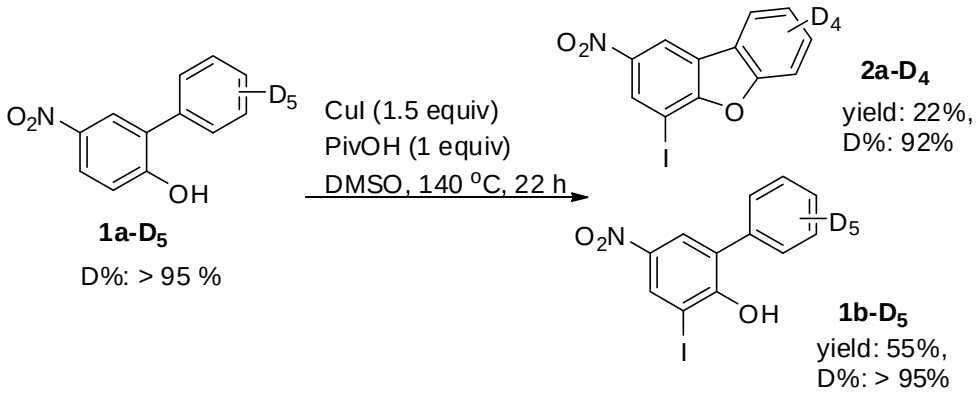
Synthesis and characterization of deuterated substrate 1a-D_5

4-nitro-2-pentadeuteriumphenylphenol (1a-D_5)



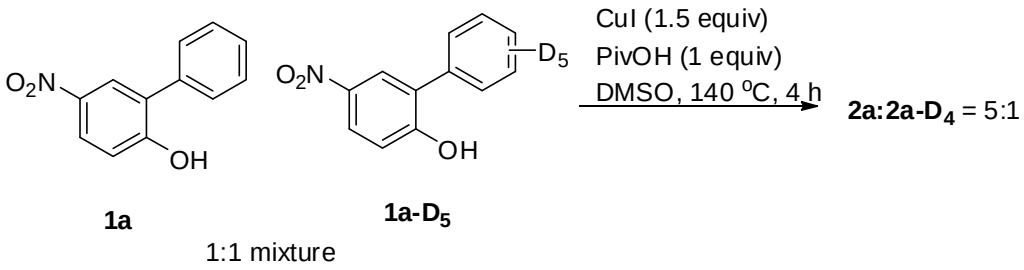
Following the method **A** for the synthesis of substrate **1**, 2-iodo-4-nitrophenol and pentadeuteriumphenylboronic acid were used. **1a-D_5** was obtained in 83% yield as a yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.20-8.17 (m, 2H), 7.08 (d, J = 8.4 Hz, 1H), 5.90 (s, 1H).

H/D Exchange experiment



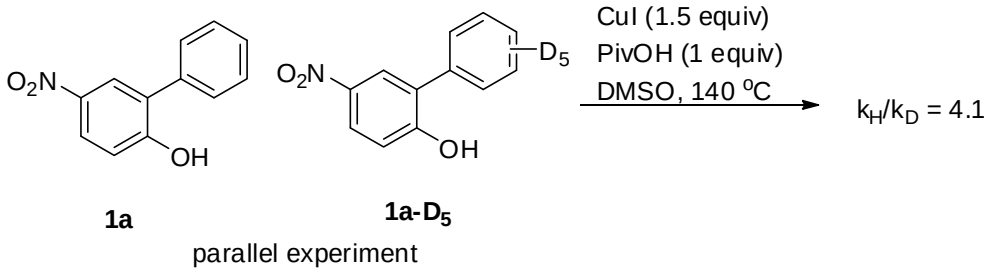
A mixture of **1a-D_5** (44 mg, 0.2 mmol, the deuterium rate is over 95%), CuI (57 mg, 0.3 mmol, 1.5 equiv), PivOH (22.5 μL, 0.2 mmol, 1 equiv) in DMSO was stirred at 140 °C in air for 22 h. The mixture was diluted with EtOAc (20 mL), washed with concentrated NH_4OH (15 mL) and brine (15 mL), and dried over Na_2SO_4. The concentrated residue was purified by column chromatography to give **2a-D_4** (D% was about 92%) in 22% yield. The iodinated intermediate **1b-D_5** (D% was over 95%) was obtained in 55% yield.

Intermolecular competition reaction of a mixture of 1a and 1a-D_5

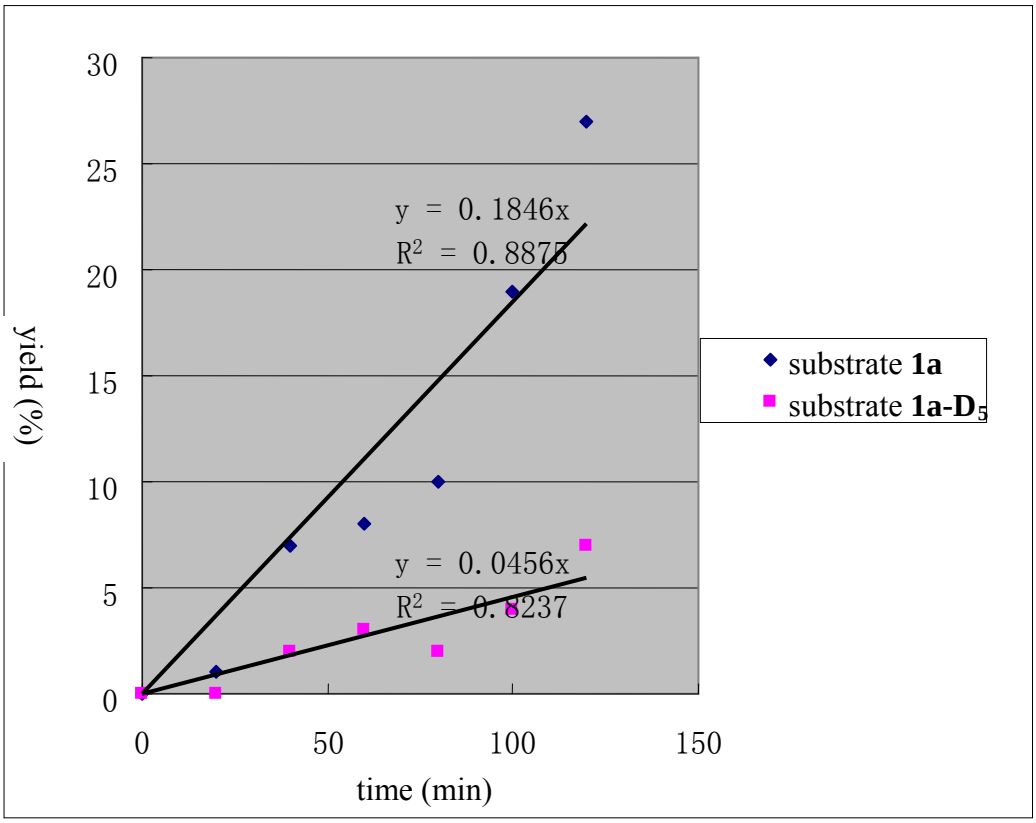


A mixture of **1a** (11 mg, 0.05 mmol, 0.5 equiv), **1a-D$_5$** (11mg, 0.05mmol, 0.5 equiv), PivOH (11.2 μL, 0.1 mmol, 1 equiv) and CuI (29mg, 0.15 mmol, 1.5 equiv) in DMSO (0.5 mL) was stirred at 140 °C for in air 4 h. The mixture was diluted with EtOAc (20 mL), washed with concentrated NH_4OH (15 mL) and brine (15 mL), and dried over Na_2SO_4. The concentrated residue was purified by column chromatography to give a mixture of **2a** and **2a-D$_4$** in a total yield of 59% in a ratio of 5:1 as determined by ^{1}H NMR.

Parallel competition reactions of 1a and 1a-D$_5$ in separate tubes



Six identical reactions were set side-by-side. Each reaction tube was charged with **1a** (22 mg, 0.1 mmol), PivOH (11.2 μL, 0.1 mmol, 1 equiv) and CuI (29 mg, 0.15 mmol, 1.5 equiv) in DMSO (0.5 mL). The reactions were stirred at 140 °C in air and stopped in 20, 40, 60, 80, 100 and 120 min, respectively. In a parallel experiment, the same six reactions were performed using **1a-D$_5$** (22 mg, 0.1mmol) as a substrate under otherwise identical conditions. Each of the reaction was worked up following procedures mentioned above. The crude reaction mixture was analyzed by ^{1}H NMR using 4-iodoanisole as an internal standard. The yields of **2a** and **2a-D$_4$** of the 12 reactions were plotted against reaction time. The ratio of product formation was determined to be 4.1 by comparing the slopes.



7. DFT calculations

Molecular geometries of the complex were optimized at the Becke3LYP level of density functional theory.[4] Frequency calculations at the same level of theory were also performed to identify all the stationary points as minima (zero imaginary frequencies) or transition states (one imaginary frequency) and to provide free energies at 298.15 K. Intrinsic reaction coordinate (IRC)[5] analysis was executed to confirm that all stationary points were smoothly connected to each other. The Hay and Wadt effective core potential (ECP) with double-valence basis set (LANL2DZ)[6] was used to describe I atom in Becke3LYP calculations. Polarization functions were added for the O atom (ζ_d=1.154).[7] Polarization functions were also added for the C atom (ζ_d=0.600) and for the H atom (ζ_p=1.100) involved in the C−H bond-breaking process.[7] The 6-311G* basis set was used for the Cu atom, while the 6-31G basis set was used for other atoms. All calculations were performed with the Gaussian 03 packages.[8]

For the S_EAr mechanism, a metal–carbon bond will be formed resulting in a

Wheland intermediate. Our DFT calculations showed that the Wheland intermediate is higher in energy by 25.8 kcal/mol than **A**, indicate that such a S_EAr mechanism has a higher barrier than the CMD mechanism and can be ruled out. As shown in Figure S1, the SET mechanism can be summarized in two main elementary steps. The first one is the breaking of a Cu-O bond and the formation of a new O-C bond with an energy barrier of 37.8 kcal/mol; then elimination of the aromatic proton yields **D**. The SET mechanism is also excluded because the calculated activation energy for the SET mechanism was 37.8 kcal/mol, which is higher than the value of 21.9 kcal/mol for the CMD mechanism.

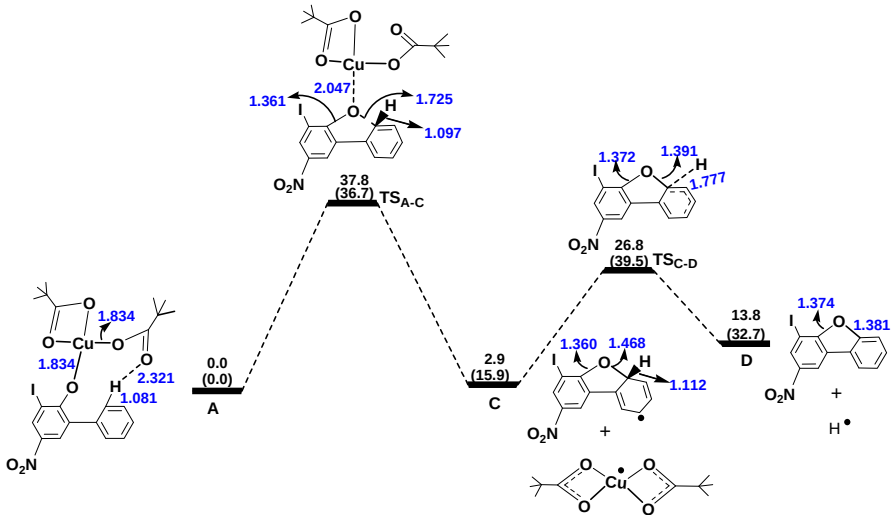


Figure S1. Energy profiles of the SET mechanism for the C-H cycloetherification step with the Cu(III) catalyst. The calculated relative free energies and electronic energies (in parentheses) are given in kcal/mol. Selected bond distances (Å) calculated for species are shown in blue.

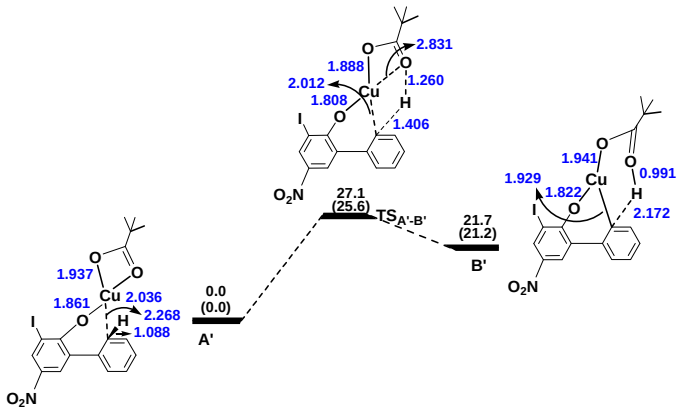


Figure S2. Energy profiles of the CMD mechanism for the C−H cycloetherification step with the Cu(II) catalyst. The calculated relative free energies and electronic

energies (in parentheses) are given in kcal/mol. Selected bond distances (Å) calculated for species are shown in blue.

8. References

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(2) Xu, F.; Huang, D.; Han, C.; Shen, W.; Lin, X.; Wang, Y. *J. Org. Chem.* **2010**, *75*, 8677.

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9. Cartesian coordinates for all the species calculated in this study

A

E=-3085.811241au

C	-3.898395	-0.859434	-0.271069
C	-3.588821	0.452169	-0.614478
C	-2.267366	0.822809	-0.899955
C	-1.239119	-0.190710	-0.832788
C	-1.623356	-1.530200	-0.499376
C	-2.933298	-1.870206	-0.211149
H	-4.381716	1.187093	-0.630763
H	-3.228373	-2.877019	0.048382
C	-1.986017	2.215702	-1.323461
C	-2.917023	2.881151	-2.152852
C	-0.838063	2.920699	-0.906726
C	-2.712597	4.203449	-2.547182
H	-3.791200	2.347973	-2.512283
C	-0.643549	4.248453	-1.293789
H	-0.106556	2.449722	-0.264146
C	-1.574566	4.894826	-2.115034
H	-3.435383	4.690000	-3.193974
H	0.238134	4.777040	-0.945591
H	-1.414655	5.924750	-2.417767
N	-5.300644	-1.205355	0.044995
O	-5.546775	-2.378129	0.354653
O	-6.144233	-0.302409	-0.020674
I	-0.138685	-3.065671	-0.487918
O	-0.006451	0.096516	-1.174679
Cu	1.459679	0.076101	-0.072731
O	3.262159	-0.062624	0.618639
O	0.492473	0.033398	1.484936
C	3.714901	-0.009064	-0.589092
O	2.797725	0.072529	-1.486754
C	5.194599	-0.036703	-0.892713
C	5.845424	1.187870	-0.192040
H	6.926729	1.170594	-0.366053
H	5.449522	2.128194	-0.591251

H	5.662415	1.165237	0.886157
C	5.781242	-1.346513	-0.299193
H	5.595901	-1.406362	0.777228
H	5.342699	-2.229137	-0.778387
H	6.862817	-1.367954	-0.470428
C	5.425435	0.021865	-2.415030
H	4.959291	-0.828894	-2.921811
H	5.007641	0.936988	-2.845752
H	6.501046	0.001183	-2.621521
C	0.633186	1.186521	2.135729
O	1.201560	2.155683	1.630042
C	0.026921	1.178493	3.554397
C	0.160759	2.586854	4.164051
H	-0.377054	3.329062	3.565907
H	-0.254675	2.588670	5.178523
H	1.208559	2.897238	4.213219
C	0.807408	0.144993	4.407443
H	0.721314	-0.858653	3.981316
H	1.870283	0.406077	4.466800
H	0.402966	0.129384	5.426303
C	-1.464012	0.767596	3.469597
H	-1.902369	0.766369	4.474420
H	-2.034232	1.472632	2.853254
H	-1.572787	-0.232523	3.041104

$TS_{A\text{-}B}$

E=-3085.779783au

C	-4.090308	0.842259	-0.035689
C	-3.157623	1.865650	0.038082
C	-1.821875	1.607670	-0.301284
C	-1.443818	0.292086	-0.751748
C	-2.440009	-0.734724	-0.781115
C	-3.750920	-0.460284	-0.439905
H	-3.469103	2.839528	0.391255
H	-4.521144	-1.218367	-0.472744
C	-0.791712	2.636913	-0.206614
C	-1.096848	3.984748	-0.498833
C	0.537586	2.307358	0.231600
C	-0.120766	4.971436	-0.406306
H	-2.090825	4.243478	-0.846579
C	1.515637	3.335014	0.293942
H	0.540146	1.510522	1.142191
C	1.191993	4.650671	-0.007629
H	-0.371226	5.996026	-0.661720

H	2.518709	3.076547	0.613789
H	1.940371	5.431681	0.072226
N	-5.489292	1.122336	0.342297
O	-6.300673	0.190515	0.274096
O	-5.768166	2.274843	0.699209
I	-1.893482	-2.684860	-1.430023
O	-0.251523	0.061603	-1.226325
Cu	1.331772	0.538418	-0.497724
O	3.141371	0.957268	-0.154604
O	1.313098	-0.955137	0.997057
C	3.592724	0.044293	-0.978160
O	2.715303	-0.545801	-1.669127
C	0.869002	-0.574168	2.126040
O	0.398169	0.600911	2.333289
C	5.074552	-0.273990	-1.015031
C	0.863737	-1.553339	3.315184
C	5.874894	1.047392	-1.126627
H	5.649999	1.569218	-2.064079
H	5.643734	1.718018	-0.293791
H	6.948177	0.828077	-1.109573
C	5.423941	-0.986510	0.322667
H	4.849331	-1.912150	0.434358
H	6.490652	-1.236594	0.332577
H	5.206863	-0.339584	1.178013
C	5.378040	-1.199271	-2.209547
H	6.445334	-1.447014	-2.219953
H	4.803712	-2.127780	-2.145120
H	5.126378	-0.716459	-3.159692
C	1.589896	-0.879822	4.506478
H	1.550208	-1.532509	5.386822
H	2.644545	-0.693254	4.269794
H	1.119236	0.075705	4.754367
C	1.563156	-2.872004	2.937819
H	1.546071	-3.560145	3.791865
H	1.068008	-3.354319	2.090045
H	2.606532	-2.697491	2.654806
C	-0.615744	-1.821826	3.698679
H	-0.661523	-2.488298	4.568325
H	-1.125457	-0.886108	3.947855
H	-1.154394	-2.302556	2.873329

B

E= -2738.998926au

C	-3.767708	0.743786	0.577704

C	-2.816193	1.742156	0.398608
C	-1.534683	1.418374	-0.058422
C	-1.210102	0.047801	-0.300390
C	-2.213282	-0.938847	-0.114041
C	-3.486330	-0.601518	0.316756
H	-3.094389	2.760721	0.631034
H	-4.255250	-1.346519	0.465921
C	-0.505397	2.442332	-0.319271
C	-0.861035	3.805554	-0.480427
C	0.859216	2.145552	-0.456061
C	0.088730	4.782922	-0.764247
H	-1.905694	4.088063	-0.418854
C	1.826535	3.099279	-0.764331
C	1.435669	4.437466	-0.909793
H	-0.226213	5.813843	-0.886859
H	2.872365	2.828300	-0.847088
H	2.182550	5.194047	-1.126591
N	-5.105971	1.110123	1.062561
O	-5.936904	0.203004	1.210164
O	-5.329459	2.307807	1.295170
I	-1.735109	-2.981261	-0.515861
O	-0.014377	-0.327209	-0.728188
Cu	1.543633	0.396001	-0.249253
O	3.330943	0.826577	0.206153
C	3.650172	-0.435146	0.327122
O	2.706499	-1.251715	0.096839
C	5.056542	-0.833607	0.726801
C	6.047570	-0.212962	-0.293635
H	7.073324	-0.465684	-0.004037
H	5.873317	-0.604455	-1.302368
H	5.951111	0.876381	-0.322098
C	5.334062	-0.251116	2.139860
H	5.224748	0.837458	2.143527
H	4.647553	-0.673192	2.882498
H	6.356929	-0.501689	2.441650
C	5.183548	-2.368962	0.740320
H	4.478892	-2.819310	1.445815
H	4.980164	-2.792593	-0.248095
H	6.200314	-2.649503	1.036179

PivOH

E= -346.813834au

O	-1.529000	1.258732	-0.000035
C	-0.944306	0.193607	-0.000049

O	-1.625661	-0.997094	-0.000029
C	0.573590	-0.010128	-0.000009
C	0.972377	-0.810874	-1.267775
H	2.058396	-0.957949	-1.280249
H	0.487772	-1.791230	-1.284318
H	0.693018	-0.270374	-2.179595
C	1.262367	1.367726	-0.000282
H	0.980692	1.950001	0.882570
H	2.350396	1.238002	-0.000229
H	0.980744	1.949624	-0.883403
C	0.972294	-0.810319	1.268147
H	0.487643	-1.790646	1.285109
H	2.058305	-0.957440	1.280729
H	0.692922	-0.269384	2.179704
H	-2.570540	-0.773773	-0.000002

$TS_{A\text{-}C}$

E= -3085.752697au

C	-3.995948	-1.091492	0.357965
C	-3.635612	-0.107810	1.267729
C	-2.269343	0.092435	1.501985
C	-1.295128	-0.669594	0.784012
C	-1.697549	-1.656400	-0.132992
C	-3.056402	-1.869489	-0.340402
H	-4.398818	0.464586	1.777921
H	-3.411341	-2.626030	-1.026393
C	-1.584996	1.062154	2.313926
C	-1.984431	2.357304	2.643573
C	-0.179036	0.650391	2.473685
C	-1.017618	3.309737	2.979353
H	-3.024821	2.648332	2.539867
C	0.807603	1.705311	2.660323
C	0.365287	2.983007	2.936087
H	-1.319890	4.323755	3.216368
H	1.851438	1.419838	2.694443
H	1.093165	3.758745	3.151502
N	-5.433554	-1.342628	0.112840
O	-5.733045	-2.225733	-0.699284
O	-6.248719	-0.650662	0.735335
I	-0.263501	-2.806866	-1.201468
O	-0.007837	-0.321001	1.057873
H	-0.008823	-0.234488	3.099941
C	0.087207	3.876151	-2.133850
C	0.604411	2.597670	-1.491370

O	-0.180969	1.902426	-0.719796
O	1.781729	2.159576	-1.650496
Cu	1.173464	0.607815	-0.331984
O	2.584253	-0.570896	-0.286124
C	3.298968	-0.717658	0.805320
O	3.051315	-0.168056	1.885736
C	4.536210	-1.632846	0.615400
C	1.154895	4.467735	-3.073402
H	0.778876	5.392996	-3.524842
H	2.077459	4.693489	-2.530251
H	1.406365	3.767144	-3.875787
C	-1.204659	3.539447	-2.922374
H	-0.995976	2.838403	-3.738813
H	-1.956477	3.090900	-2.266611
H	-1.619153	4.455225	-3.358909
C	-0.246079	4.879616	-0.996611
H	-0.977896	4.453547	-0.303757
H	0.654671	5.143910	-0.430311
H	-0.659639	5.798858	-1.426729
C	5.211048	-1.877897	1.977809
H	4.530276	-2.385723	2.669094
H	6.102242	-2.503419	1.844887
H	5.509404	-0.934219	2.443404
C	5.516525	-0.906332	-0.342610
H	5.040356	-0.709825	-1.307734
H	5.843800	0.050056	0.082347
H	6.405824	-1.526883	-0.508210
C	4.099350	-2.976253	-0.014344
H	4.974118	-3.622905	-0.156087
H	3.389678	-3.504464	0.633676
H	3.623096	-2.812530	-0.984768

C

E= -752.828371au

C	-0.737471	2.258556	0.016343
C	0.651484	2.172782	0.134981
C	1.212775	0.897372	0.220747
C	0.373672	-0.254314	0.163573
C	-1.009887	-0.142999	0.034440
C	-1.572580	1.133661	-0.034936
H	1.246720	3.075382	0.163903
H	-2.640341	1.276677	-0.126566
C	2.568576	0.405187	0.273121
C	3.798482	0.964831	-0.033379

C	2.451530	-1.074025	0.558259
C	4.886833	0.114852	-0.307253
H	3.904209	2.037951	-0.160018
C	3.508283	-1.904205	-0.095851
C	4.697057	-1.303550	-0.412961
H	5.852589	0.539797	-0.556315
H	3.349449	-2.972347	-0.194979
H	5.518251	-1.906095	-0.788815
N	-1.360423	3.594318	-0.057979
O	-2.592561	3.654946	-0.162845
O	-0.611114	4.579698	-0.011584
I	-2.228003	-1.888090	-0.057559
O	1.066051	-1.423580	0.219485
H	2.504697	-1.240235	1.656338

$Cu(PivO)_2$

E=-2332.957469au

Cu	0.000001	-0.000053	-0.000765
O	-1.654026	-1.069854	0.000074
O	1.653979	1.069803	0.000123
C	-2.328793	0.026083	-0.000253
O	-1.638983	1.108473	-0.000824
C	-3.847662	0.012378	0.000236
C	-4.318474	-0.755354	-1.263643
H	-5.412107	-0.822913	-1.265428
H	-4.008250	-0.237279	-2.178472
H	-3.903531	-1.767326	-1.280392
C	-4.317274	-0.747670	1.269299
H	-3.902582	-1.759644	1.291675
H	-4.005956	-0.224107	2.180623
H	-5.410918	-0.814972	1.272633
C	-4.399733	1.450122	-0.003770
H	-4.064435	2.005660	0.877549
H	-4.065467	2.000308	-0.888847
H	-5.495311	1.424493	-0.003088
C	2.328794	-0.026107	-0.000090
O	1.639038	-1.108528	-0.000762
C	3.847661	-0.012324	0.000322
C	4.317456	0.750117	1.267840
H	4.006398	0.228229	2.180214
H	5.411092	0.817558	1.270825
H	3.902629	1.762071	1.288438
C	4.318212	0.753070	-1.265112
H	4.007743	0.233307	-2.178899

H	3.903337	1.765043	-1.283616
H	5.411848	0.820566	-1.267269
C	4.399800	-1.450047	-0.001164
H	5.495377	-1.424363	-0.000791
H	4.064762	-2.003956	0.881284
H	4.065329	-2.001900	-0.885119

$TS_{C\text{-}D}$

E= -752.790753au

C	-0.770249	2.250856	0.001125
C	0.622246	2.185331	0.030180
C	1.200155	0.914980	0.048578
C	0.368441	-0.235126	0.032375
C	-1.021641	-0.152425	0.003847
C	-1.598596	1.117047	-0.011696
H	1.206026	3.095757	0.039579
H	-2.671081	1.251232	-0.033106
C	2.560012	0.412362	0.061742
C	3.834125	0.982747	-0.016948
C	2.434597	-1.007873	0.154027
C	4.941341	0.132892	-0.101464
H	3.962430	2.059526	-0.043431
C	3.530421	-1.869268	-0.070986
C	4.785276	-1.271324	-0.151052
H	5.937000	0.557283	-0.168060
H	3.392938	-2.942387	-0.120941
H	5.663753	-1.896662	-0.269313
N	-1.413840	3.582838	-0.015722
O	-2.649882	3.627125	-0.040208
O	-0.675225	4.575964	-0.004846
I	-2.218891	-1.911997	-0.019461
O	1.103507	-1.393619	0.036374
H	2.463080	-1.105740	1.927824

D

E=-752.301378au

C	-0.738136	2.250305	-0.000047
C	0.654603	2.173667	0.000012
C	1.221875	0.899451	0.000035
C	0.380424	-0.242179	-0.000007
C	-1.008969	-0.150144	-0.000072
C	-1.576016	1.123475	-0.000087
H	1.245557	3.079571	0.000038
H	-2.647551	1.266397	-0.000129

C	2.579703	0.377431	0.000092
C	3.863864	0.939670	0.000146
C	2.440575	-1.025389	0.000083
C	4.964537	0.079581	0.000194
H	4.002230	2.015514	0.000154
C	3.521118	-1.901182	0.000128
C	4.794382	-1.319077	0.000186
H	5.967223	0.492758	0.000239
H	3.378758	-2.974986	0.000120
H	5.669109	-1.960708	0.000223
N	-1.371251	3.587278	-0.000071
O	-2.607264	3.641602	0.000142
O	-0.624546	4.574579	0.000218
I	-2.219868	-1.901030	-0.000136
O	1.112891	-1.404750	0.000024

H·

E= -0.500273au

H	0.000000	0.000000	0.000000

A’

E=-2739.616198au

C	3.488930	1.437972	0.541206
C	2.291897	2.113962	0.301942
C	1.172329	1.401848	-0.121924
C	1.228859	-0.025196	-0.281471
C	2.479044	-0.661154	-0.048182
C	3.594396	0.052661	0.359741
H	2.260721	3.189434	0.422328
H	4.542365	-0.432497	0.547668
C	-0.103224	2.095950	-0.437033
C	-0.631810	3.096694	0.406331
C	-0.789672	1.811508	-1.655451
C	-1.778958	3.803662	0.043741
H	-0.131465	3.313237	1.344205
C	-1.938162	2.544949	-2.015533
H	-0.318868	1.156172	-2.385076
C	-2.437268	3.530140	-1.165824
H	-2.166535	4.570100	0.706689
H	-2.427015	2.339081	-2.962269
H	-3.327717	4.085887	-1.437207
N	4.662581	2.192774	0.979521
O	5.718727	1.570338	1.170709
O	4.537934	3.418795	1.138896

I	2.605410	-2.776865	-0.316448
O	0.166739	-0.720778	-0.622222
Cu	-1.520845	0.042807	-0.438498
O	-3.365217	0.521129	-0.091220
C	-3.612089	-0.669954	0.355130
O	-2.626472	-1.479795	0.340078
C	-4.994039	-1.041468	0.861288
C	-5.022053	-2.515622	1.306895
H	-4.299898	-2.701734	2.107643
H	-6.022449	-2.770116	1.674275
H	-4.776591	-3.185297	0.476842
C	-6.008603	-0.800475	-0.287893
H	-7.021411	-1.021476	0.066696
H	-5.974635	0.239036	-0.627064
H	-5.798480	-1.453190	-1.143005
C	-5.331242	-0.106030	2.053672
H	-4.630320	-0.255611	2.882897
H	-5.291313	0.944120	1.749437
H	-6.340395	-0.328322	2.417728

TS $_{A'-B'}$

E= -2739.575457au

C	-3.116064	1.502036	1.005215
C	-1.949465	2.129868	0.574613
C	-1.002118	1.425221	-0.173094
C	-1.235175	0.039655	-0.486151
C	-2.449823	-0.547623	-0.037118
C	-3.383413	0.162374	0.699465
H	-1.786843	3.166749	0.838888
H	-4.301976	-0.289371	1.047735
C	0.193943	2.115939	-0.717816
C	0.043265	3.411889	-1.252514
C	1.478793	1.498310	-0.774468
C	1.109444	4.072165	-1.866359
H	-0.932231	3.885844	-1.226430
C	2.529152	2.172069	-1.441678
H	2.128303	0.976772	0.358544
C	2.358445	3.448450	-1.977994
H	0.958106	5.064974	-2.278009
H	3.506607	1.698586	-1.499605
H	3.183401	3.954740	-2.468397
N	-4.088607	2.259171	1.799178
O	-5.119472	1.675557	2.166742
O	-3.828269	3.444750	2.058749

I	-2.817008	-2.600832	-0.517454
O	-0.384400	-0.669923	-1.204742
Cu	1.388613	-0.508355	-0.889395
O	3.120949	-1.050138	-0.369224
C	3.565458	-0.463754	0.683845
O	2.989898	0.568378	1.182213
C	4.834361	-1.015559	1.336853
C	5.183897	-0.223670	2.610710
H	4.380957	-0.286626	3.351634
H	6.097331	-0.633516	3.055461
H	5.350485	0.834768	2.389767
C	5.982190	-0.899878	0.296692
H	6.899856	-1.321426	0.721136
H	5.737167	-1.445731	-0.618838
H	6.178750	0.147594	0.039709
C	4.591518	-2.509525	1.676908
H	3.781901	-2.622798	2.407177
H	4.332744	-3.078397	0.779499
H	5.501244	-2.936770	2.112452

B’

E= -2739.582418 6au

C	-3.338081	1.425363	0.881489
C	-2.172657	2.079101	0.488194
C	-1.157143	1.401930	-0.195877
C	-1.315867	-0.012415	-0.441765
C	-2.538926	-0.624688	-0.043163
C	-3.542715	0.068238	0.609042
H	-2.069816	3.125924	0.739302
H	-4.461429	-0.407758	0.921966
C	0.036938	2.150714	-0.684781
C	-0.087620	3.527601	-0.979039
C	1.298749	1.536080	-0.897313
C	0.991216	4.278621	-1.449919
H	-1.051326	4.013052	-0.871590
C	2.366360	2.299728	-1.399215
H	2.768735	1.149437	0.654726
C	2.228966	3.669328	-1.665296
H	0.854495	5.332962	-1.668426
H	3.323940	1.822485	-1.603957
H	3.068339	4.241146	-2.048972
N	-4.370597	2.170321	1.602987
O	-5.401864	1.564480	1.935667
O	-4.162292	3.371052	1.845062

I	-2.797260	-2.713078	-0.451982
O	-0.396629	-0.747002	-1.033052
Cu	1.370679	-0.387381	-0.773617
O	3.160611	-0.963340	-0.291525
C	3.868894	-0.416184	0.580707
O	3.561421	0.762737	1.107893
C	5.156214	-1.034871	1.105483
C	5.064534	-1.134297	2.653222
H	4.239273	-1.785791	2.961623
H	5.995645	-1.563647	3.037046
H	4.921169	-0.150700	3.108418
C	6.332320	-0.095591	0.711969
H	7.267536	-0.521143	1.090228
H	6.418247	-0.002467	-0.376512
H	6.204712	0.901995	1.141289
C	5.356907	-2.431197	0.486885
H	4.533869	-3.104800	0.745150
H	5.419663	-2.379645	-0.604081
H	6.287732	-2.864319	0.866713

Wheland Im

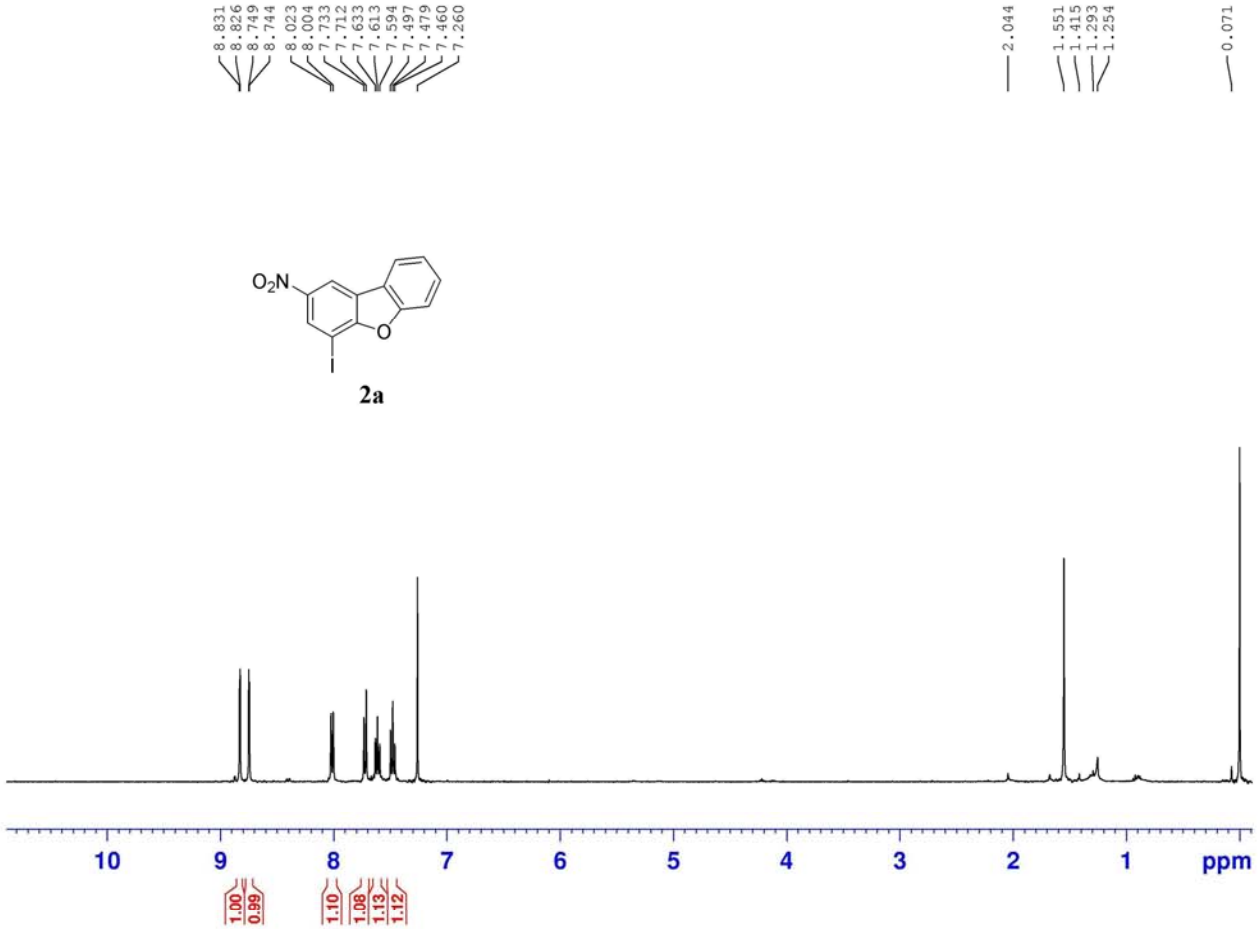
E= -3085.772804au

C	4.294603	1.354149	-0.288747
C	3.273201	2.218367	0.093777
C	1.987260	1.708452	0.284334
C	1.735434	0.296820	0.142955
C	2.816039	-0.541294	-0.272094
C	4.082674	-0.018178	-0.481444
H	3.483040	3.273729	0.210544
H	4.912398	-0.640474	-0.787767
C	0.861168	2.559600	0.685050
C	0.965065	3.443851	1.772341
C	-0.383402	2.476069	-0.012475
C	-0.131411	4.210926	2.171012
H	1.896749	3.498825	2.324351
C	-1.476214	3.282036	0.389222
C	-1.356534	4.127110	1.486647
H	-0.037345	4.871237	3.026873
H	-2.396589	3.235787	-0.176833
H	-2.199018	4.730033	1.805329
N	5.645225	1.902113	-0.515324
O	6.534766	1.115994	-0.863987
O	5.807670	3.117476	-0.338984
I	2.466593	-2.620768	-0.525864

O	0.588087	-0.212702	0.524773
H	-0.363503	2.134780	-1.052899
C	-4.909410	1.003350	-1.438813
C	-3.705873	0.836121	-0.479624
O	-2.533464	0.917267	-1.092558
O	-3.827734	0.643507	0.729840
Cu	-1.032241	0.335235	-0.179352
O	-1.494188	-1.418357	-0.546981
C	-1.589359	-2.527107	0.194049
C	-1.958263	-2.533281	1.690834
O	-1.497632	-3.578411	-0.436858
C	-1.239159	-3.733947	2.350980
H	-1.466419	-4.662802	1.821272
H	-0.152337	-3.593972	2.344471
H	-1.566748	-3.832227	3.392150
C	-1.602857	-1.235466	2.439874
H	-0.528851	-1.033673	2.409122
H	-2.160122	-0.379532	2.046758
H	-1.893786	-1.347070	3.491256
C	-3.499434	-2.755507	1.748007
H	-3.811381	-2.853811	2.794375
H	-4.032521	-1.905201	1.311601
H	-3.778653	-3.669715	1.214232
C	-4.945014	-0.240490	-2.365474
H	-4.020246	-0.325568	-2.942869
H	-5.070627	-1.160613	-1.784066
H	-5.789120	-0.157923	-3.060640
C	-4.725876	2.282126	-2.290965
H	-4.685678	3.178603	-1.658654
H	-3.807770	2.232208	-2.882896
H	-5.575102	2.396422	-2.974747
C	-6.206888	1.093754	-0.613870
H	-6.191142	1.959107	0.057143
H	-7.066691	1.191795	-1.287045
H	-6.344082	0.201230	0.002804

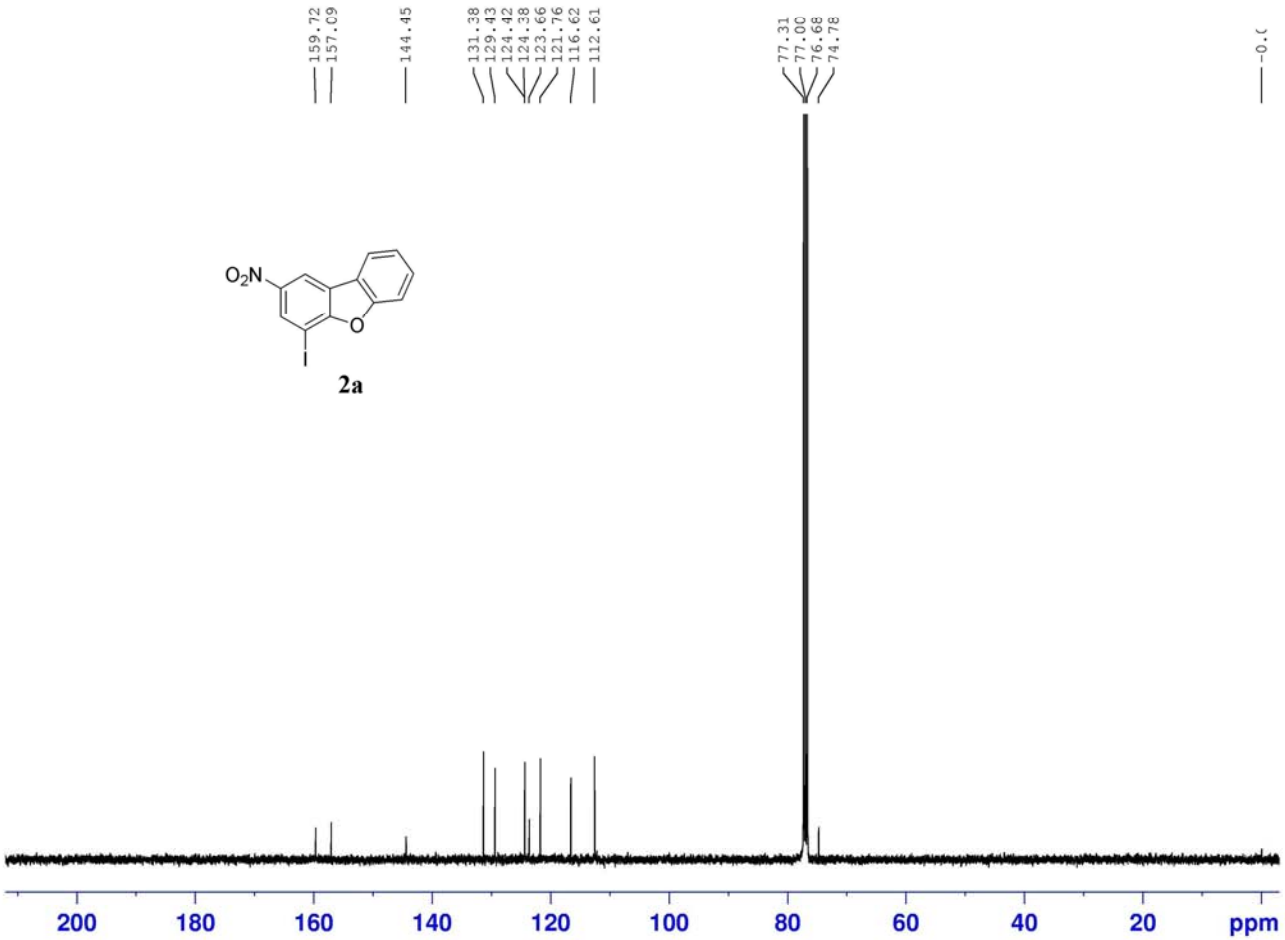
10. Copies of ^{1}H NMR and ^{13}C NMR

131654



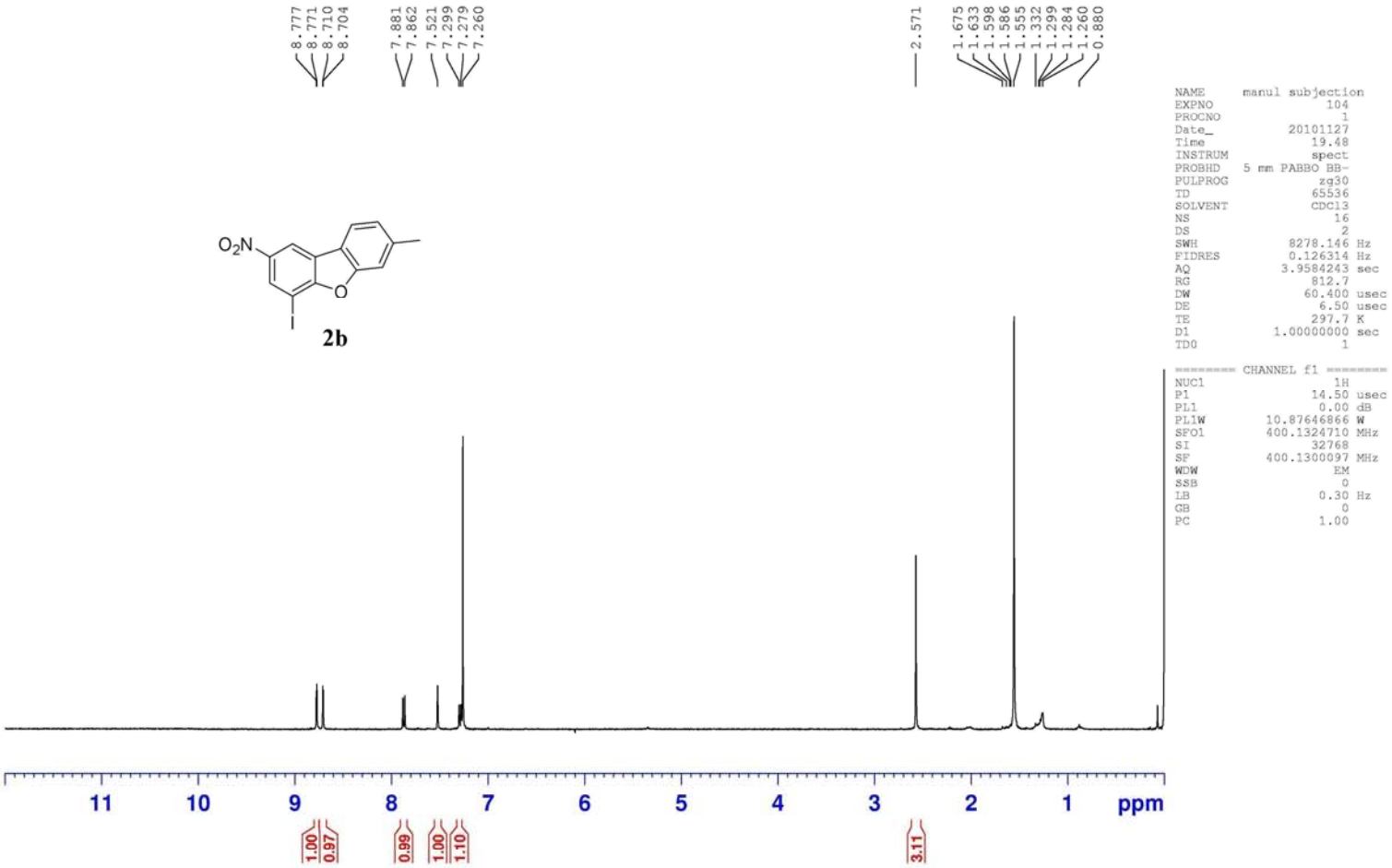
NAME	11.09
EXPNO	26
PROCNO	1
Date_	20101109
Time	16.19
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	812.7
DW	60.400 usec
DE	6.50 usec
TE	298.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.00 dB
PL1W	10.87646866 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300097 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

131654-c

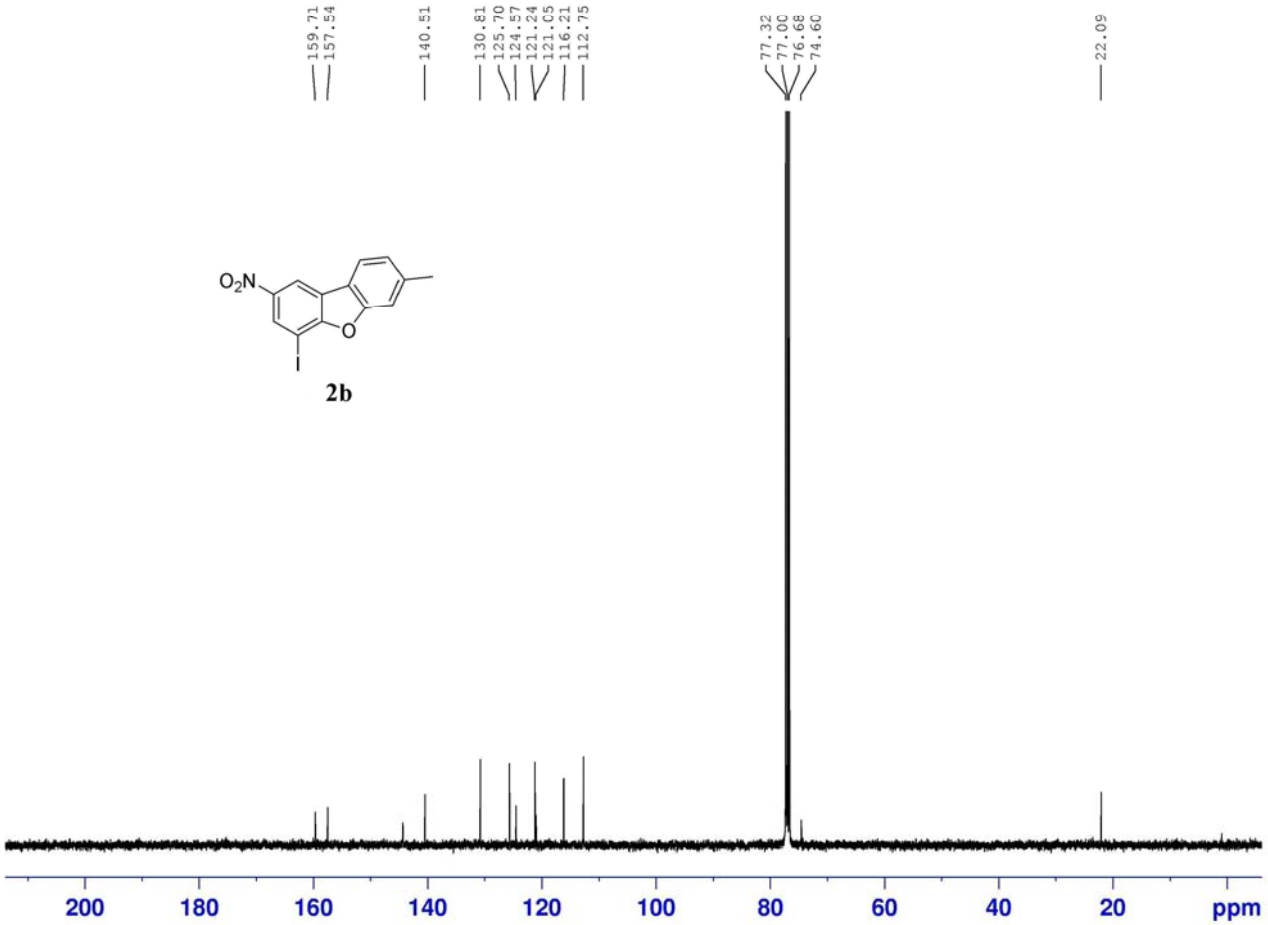



```
NAME        manul subjection
EXPNO                     97
PROCNO                     1
Date_               20101109
Time                   19.13
INSTRUM                spect
PROBHD     5 mm PABBO BB-
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       656
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                      302.1 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                 100.6127659 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```

131685

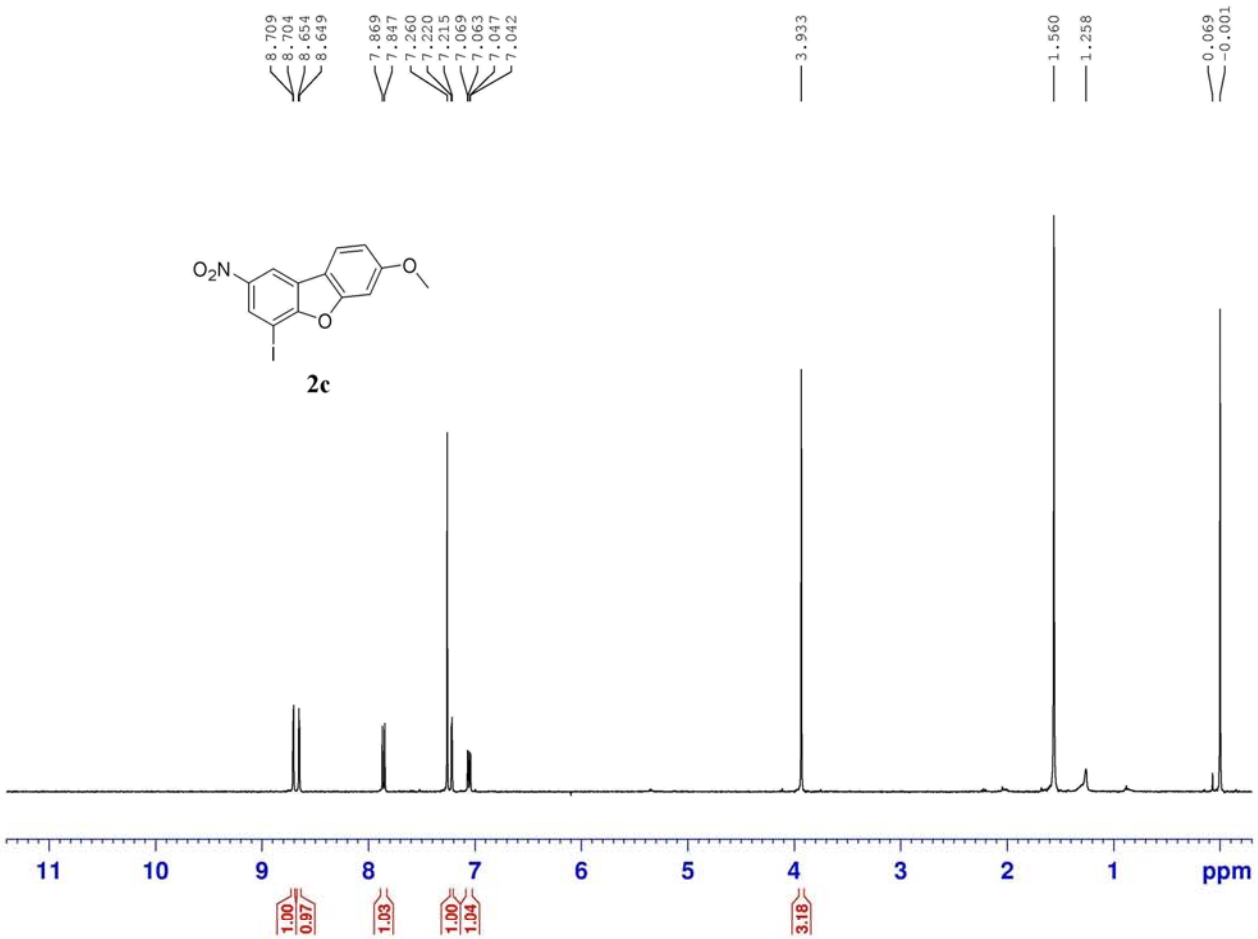

8.777
8.771
8.710
8.704
7.881
7.862
7.521
7.299
7.279
7.260
2.571
1.675
1.633
1.598
1.586
1.555
1.332
1.299
1.284
1.260
0.880
O_2N
O
I
2b
11
10
9
8
7
6
5
4
3
2
1
ppm
1.00
0.97
0.99
1.00
1.10
3.11
NAME manul subjection
EXPNO 104
PROCNO 1
Date_ 20101127
Time 19.48
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 812.7
DW 60.400 usec
DE 6.50 usec
TE 297.7 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 400.1300097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

131685-c



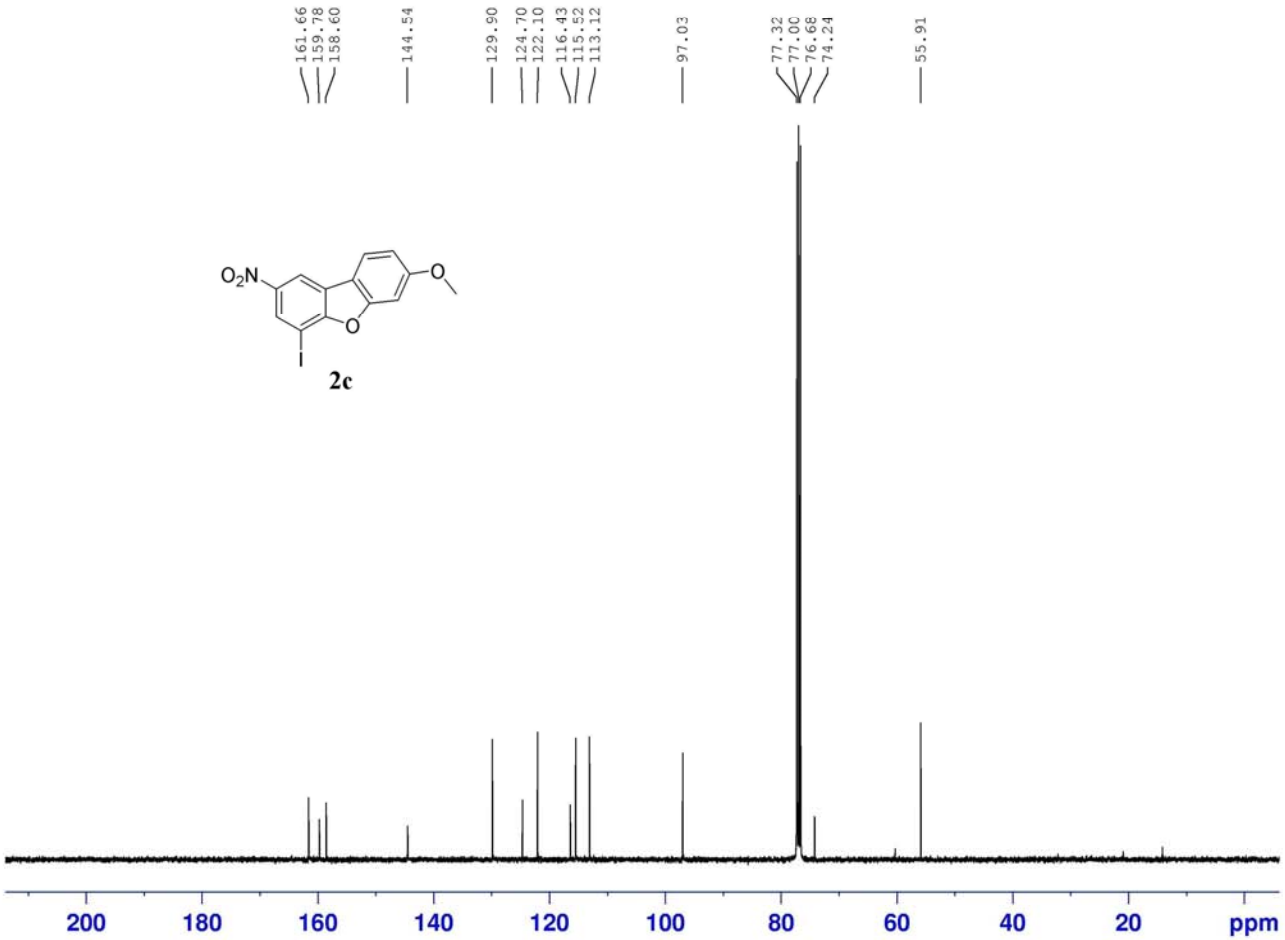

```
NAME        manul subjection
EXPNO                    105
PROCNO                     1
Date_               20101127
Time                   20.22
INSTRUM                spect
PROBHD     5 mm PABBO BB-
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       656
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                      303.3 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                 100.6127660 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```

131689



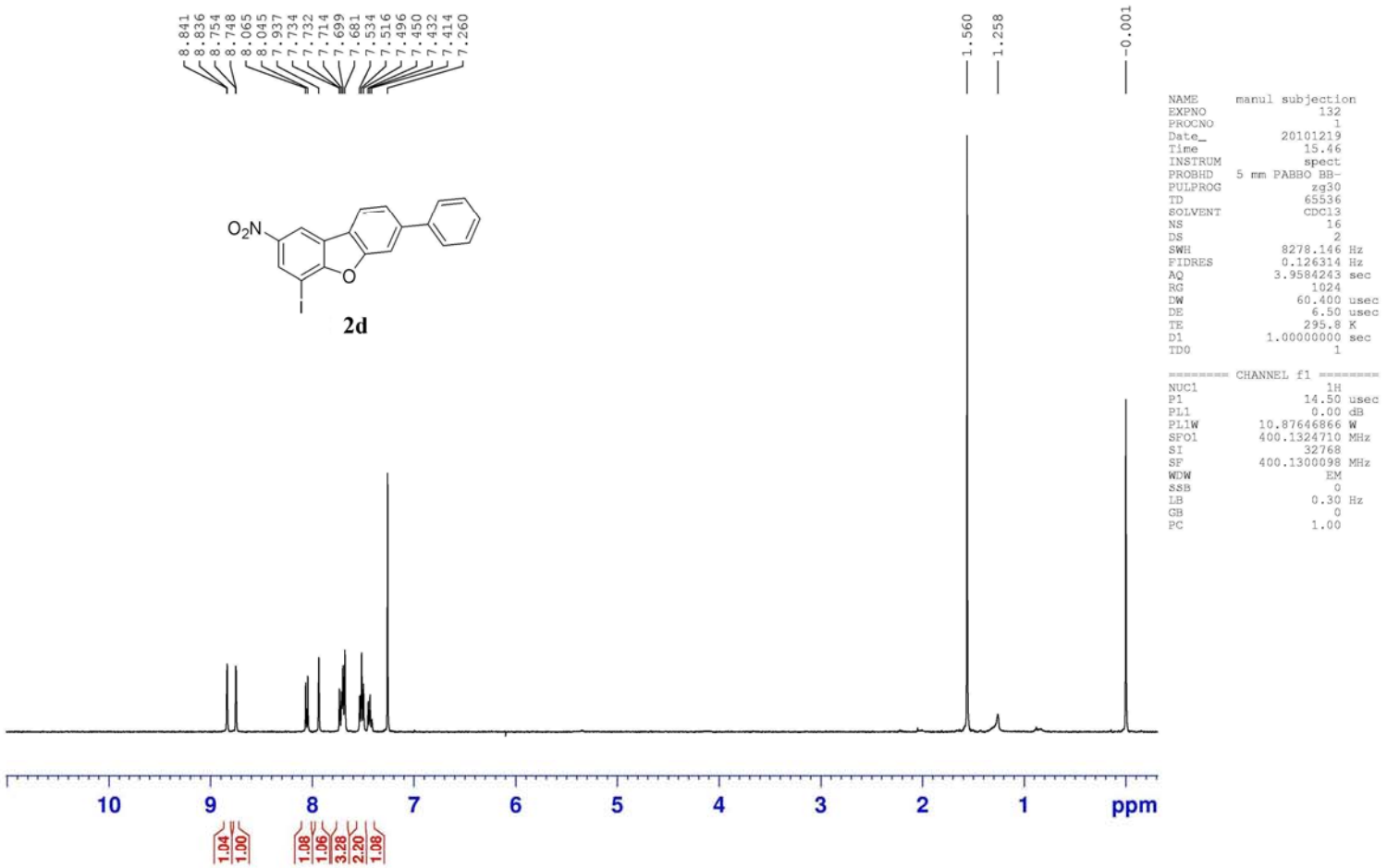

```
NAME        manul subjection
EXPNO                    109
PROCNO                     1
Date_               20101129
Time                   19.21
INSTRUM                spect
PROBHD     5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 8278.146 Hz
FIDRES              0.126314 Hz
AQ                3.9584243 sec
RG                    812.7
DW                   60.400 usec
DE                     6.50 usec
TE                    297.8 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              400.1300098 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.00
```

131689-C



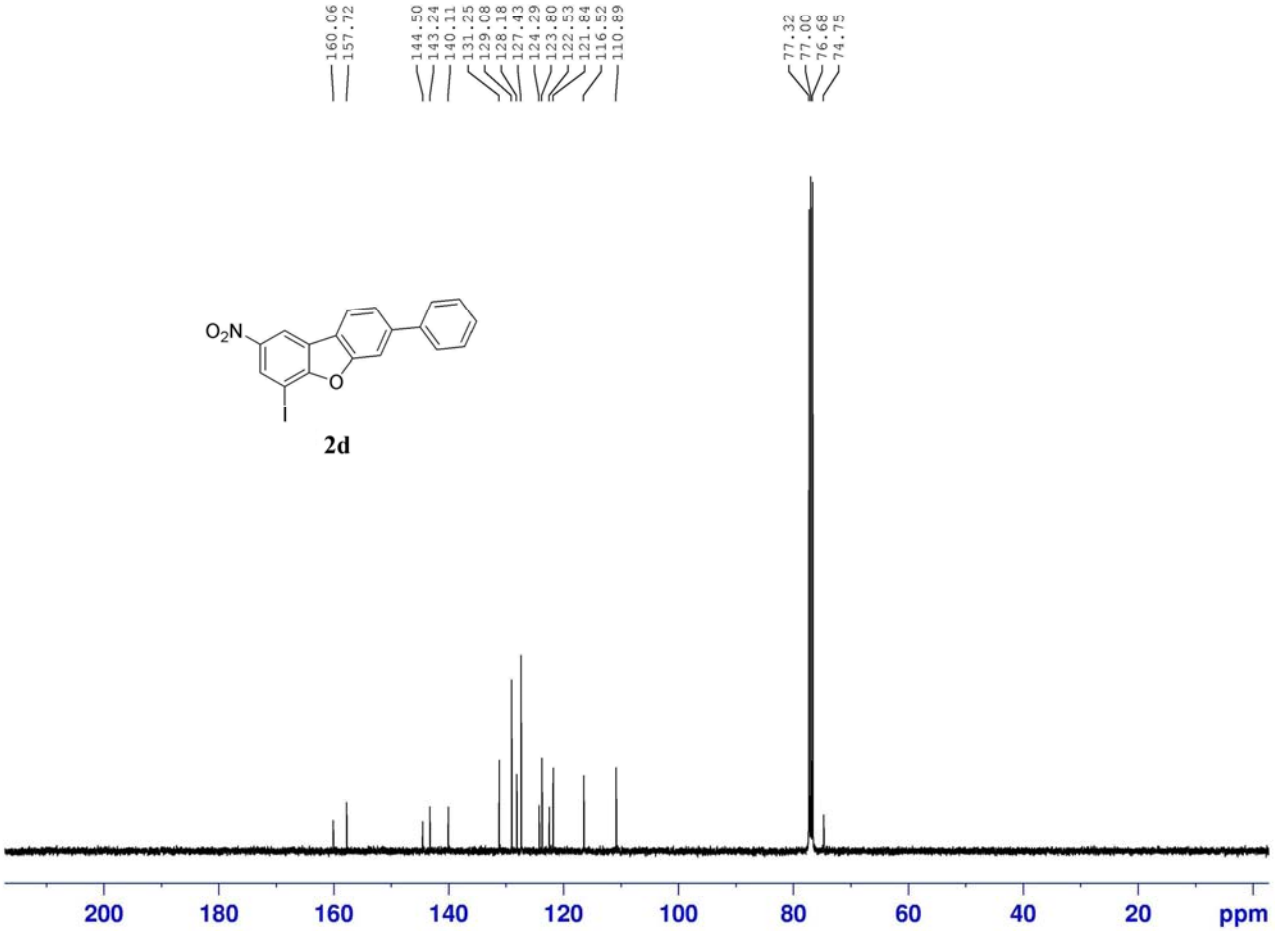

```
NAME        manul subjection
EXPNO                    110
PROCNO                     1
Date_           20101129
Time                   21.53
INSTRUM                spect
PROBHD    5 mm PABBO BB-
PULPROG              zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      1964
DS                         4
SWH                23980.814 Hz
FIDRES              0.365918 Hz
AQ                 1.3664756 sec
RG                     574.7
DW                    20.850 usec
DE                      6.50 usec
TE                     303.2 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             100.6127653 MHz
WDW                       EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
```

131709-2



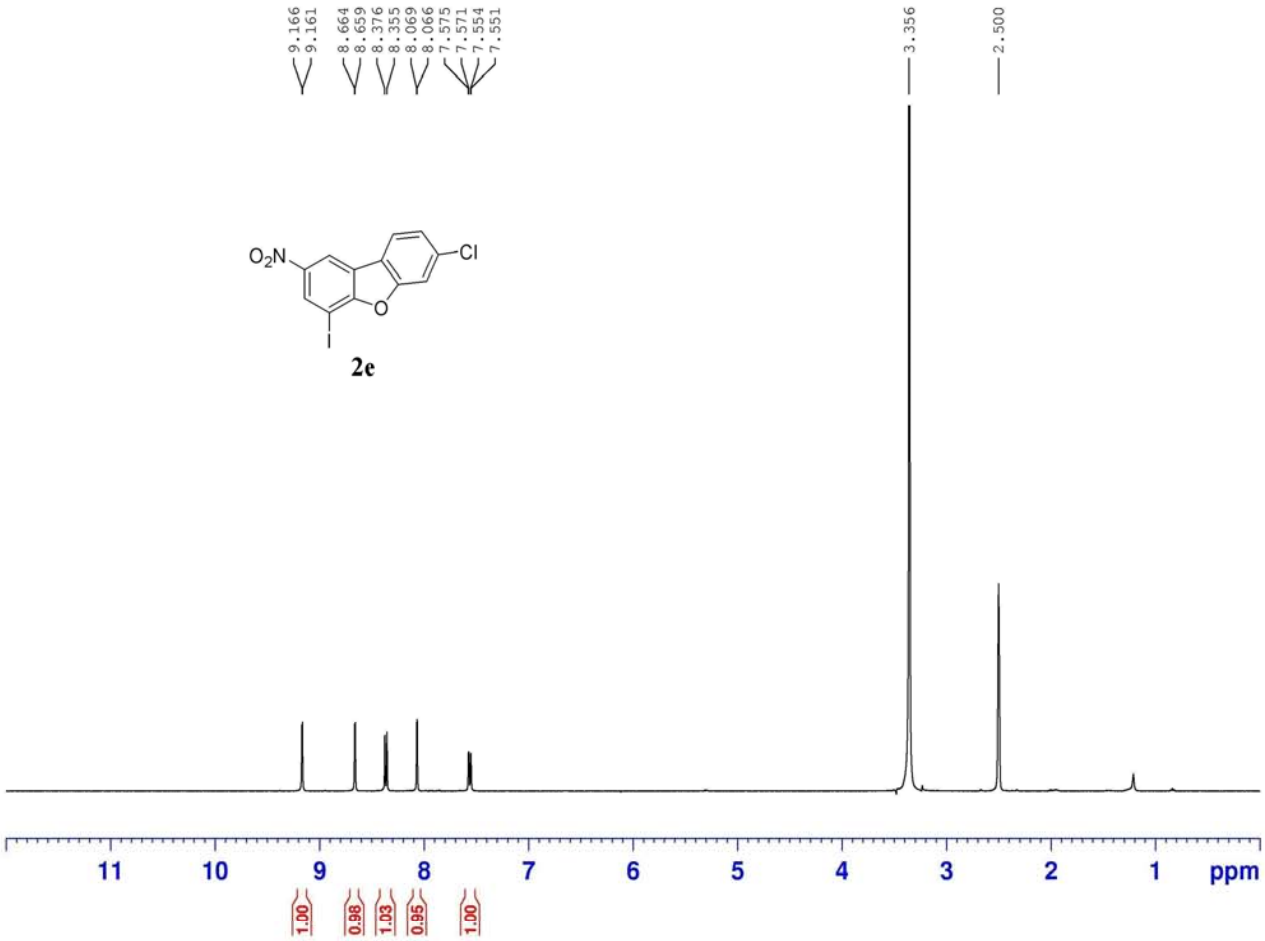
NAME	manul subjection
EXPNO	132
PROCNO	1
Date_	20101219
Time	15.46
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	1024
DW	60.400 usec
DE	6.50 usec
TE	295.8 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.00 dB
PL1W	10.87646866 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300098 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

131709-2C



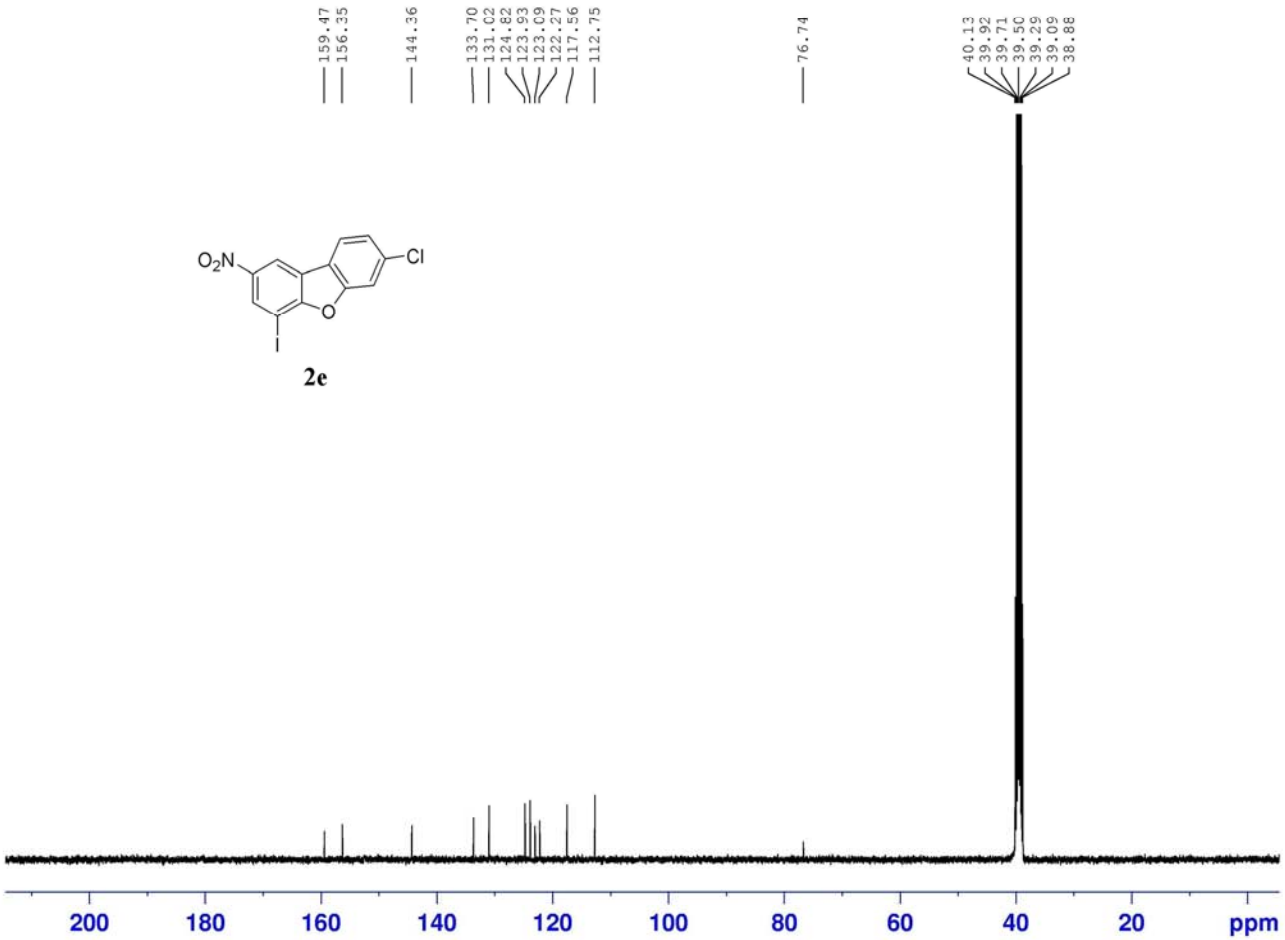

```
NAME        manul subjection
EXPNO                    133
PROCNO                     1
Date_               20101219
Time                   22.35
INSTRUM                spect
PROBHD     5 mm PABBO BB-
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       843
DS                         4
SWH                 23980.814 Hz
FIDRES               0.365918 Hz
AQ                  1.3664756 sec
RG                      574.7
DW                     20.850 usec
DE                       6.50 usec
TE                      301.4 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             100.6127674 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```

131702-2



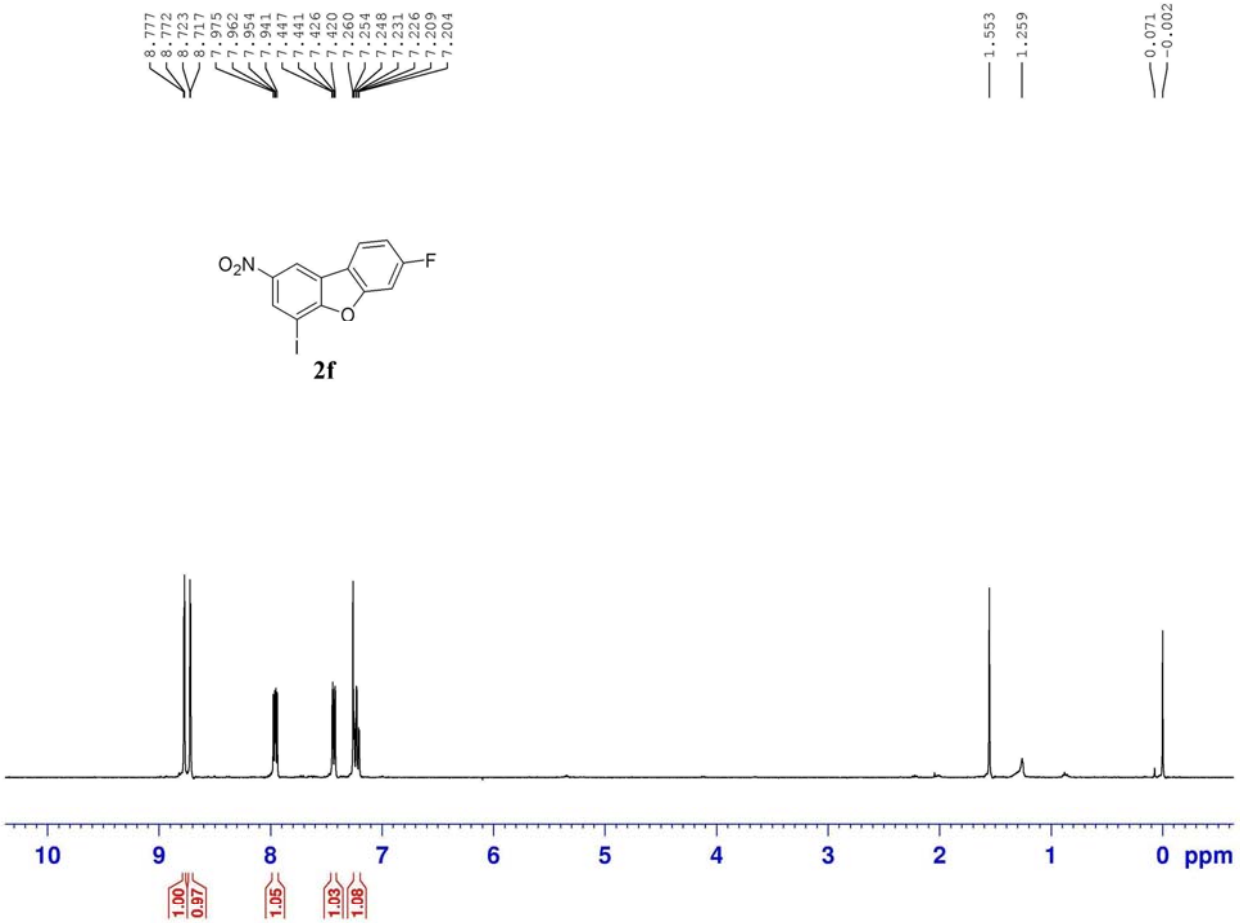

```
NAME        manul subjection
EXPNO                    119
PROCNO                     1
Date_               20101211
Time                     0.04
INSTRUM                 spect
PROBHD     5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                 DMSO
NS                        16
DS                         2
SWH                 8278.146 Hz
FIDRES              0.126314 Hz
AQ                  3.9584243 sec
RG                      322.5
DW                     60.400 usec
DE                       6.50 usec
TE                      298.1 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                 400.1300035 MHz
WDW                        EM
SSB                         0
LB                       0.30 Hz
GB                          0
PC                       1.00
```

131702-2C



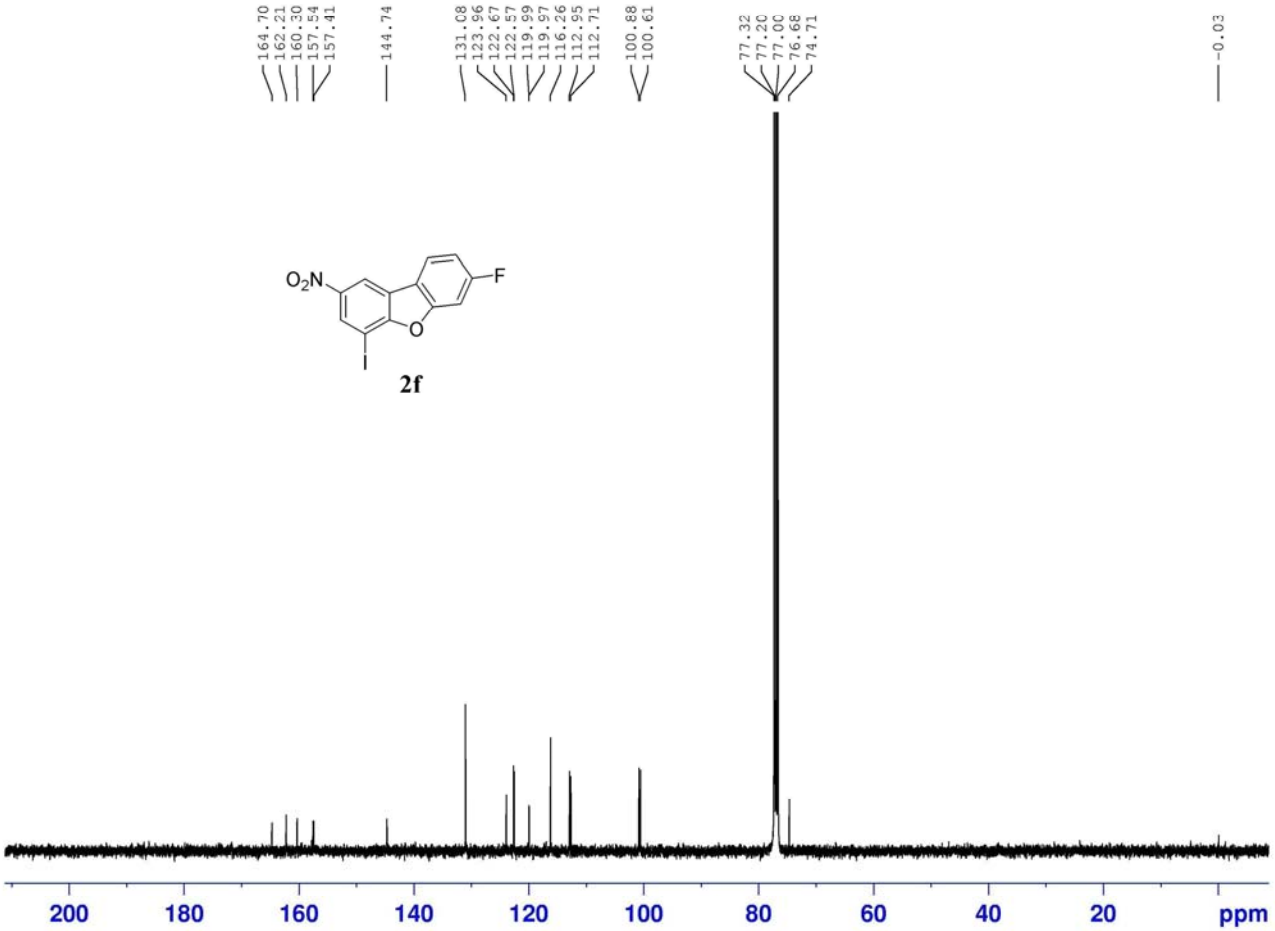

```
NAME        manul subjection
EXPNO                    120
PROCNO                     1
Date_               20101211
Time                    0.09
INSTRUM                spect
PROBHD     5 mm PABBO BB-
PULPROG               zgpg30
TD                     65536
SOLVENT                 DMSO
NS                      2048
DS                         4
SWH                 23980.814 Hz
FIDRES               0.365918 Hz
AQ                  1.3664756 sec
RG                      645.1
DW                     20.850 usec
DE                       6.50 usec
TE                      300.5 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               100.6128286 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```

131687-2



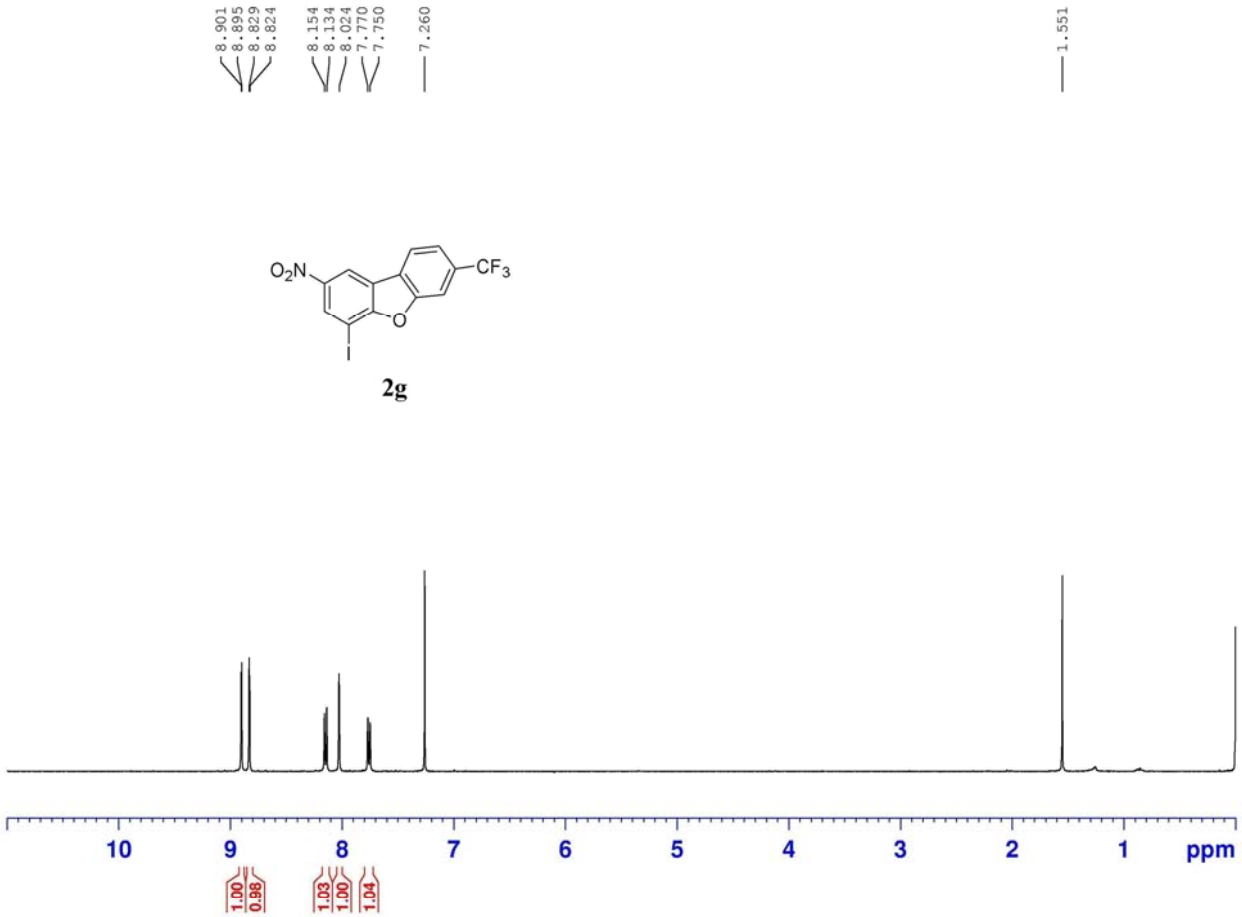
NAME	manul subjection
EXPNO	107
PROCNO	1
Date_	20101128
Time	23.26
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	812.7
DW	60.400 usec
DE	6.50 usec
TE	297.7 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.00 dB
PL1W	10.87646866 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300098 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

131687-2C



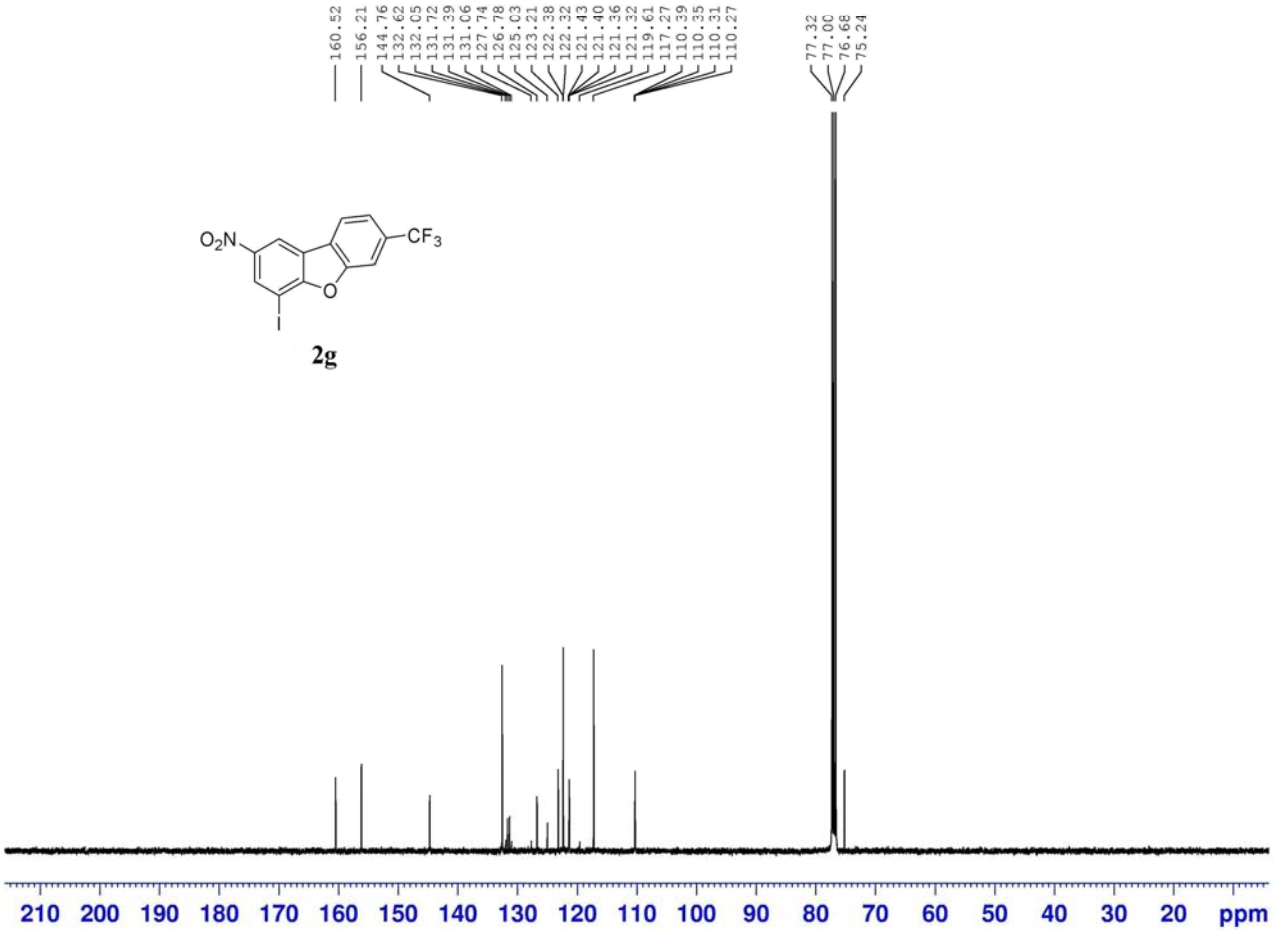

```
NAME        manul subjection
EXPNO                    108
PROCNO                     1
Date_               20101128
Time                   23.31
INSTRUM                spect
PROBHD     5 mm PABBO BB-
PULPROG              zgpg30
TD                     65536
SOLVENT                CDCl3
NS                      2048
DS                         4
SWH                 23980.814 Hz
FIDRES               0.365918 Hz
AQ                  1.3664756 sec
RG                      645.1
DW                     20.850 usec
DE                      6.50 usec
TE                     302.2 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              100.6127653 MHz
WDW                        EM
SSB                         0
LB                       1.00 Hz
GB                          0
PC                       1.40
```

131728-2



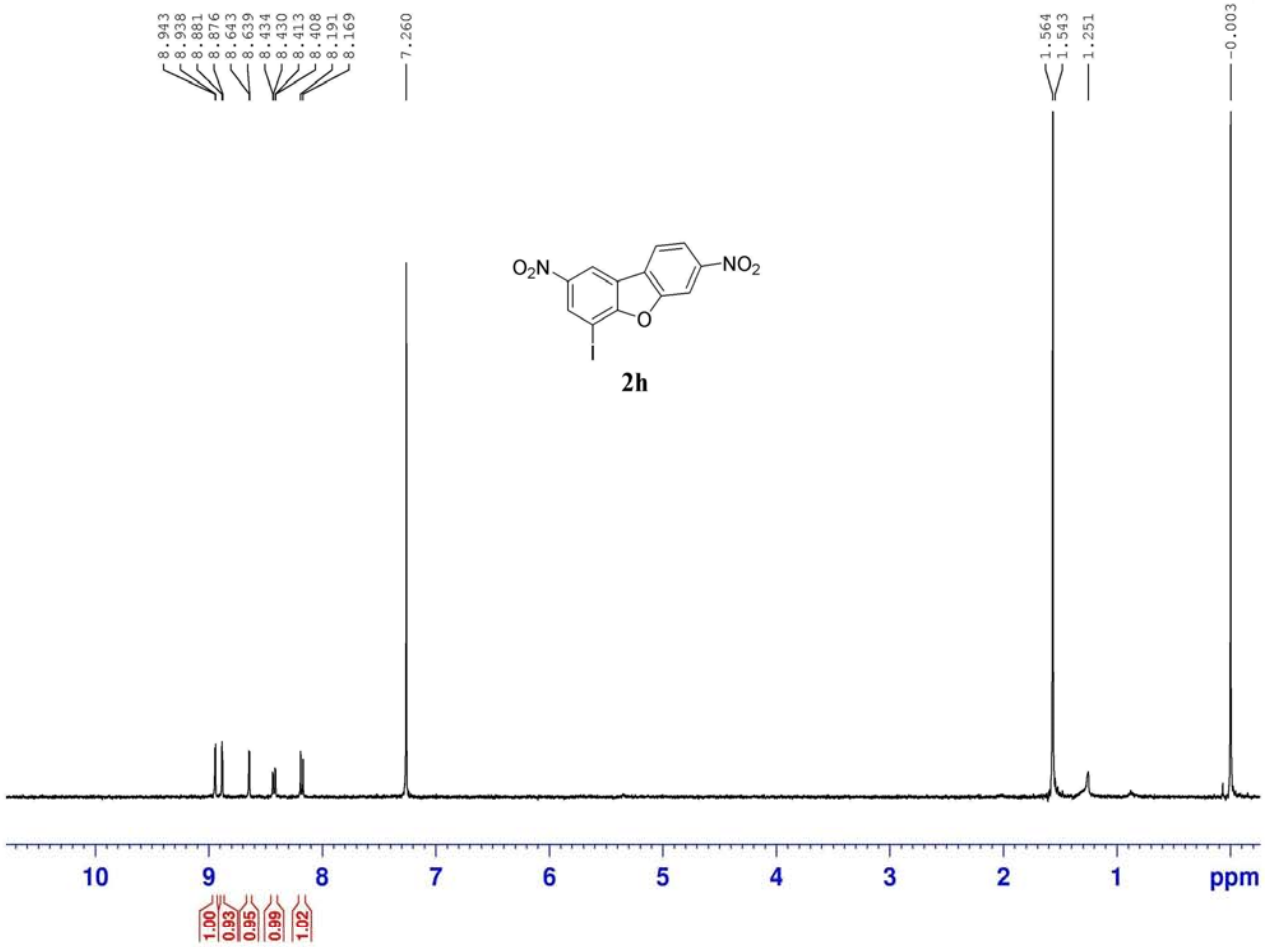

```
NAME          2011manual
EXPNO              153
PROCNO               1
Date_         20110109
Time             19.33
INSTRUM          spect
PROBHD   5 mm PABBO BB-
PULPROG          zg30
TD              65536
SOLVENT         CDCl3
NS                  16
DS                   2
SWH           8278.146 Hz
FIDRES        0.126314 Hz
AQ           3.9584243 sec
RG              1149.4
DW              60.400 usec
DE               6.50 usec
TE              295.8 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          400.1300098 MHz
WDW                EM
SSB                 0
LB               0.30 Hz
GB                  0
PC               1.00
```

131728-2C



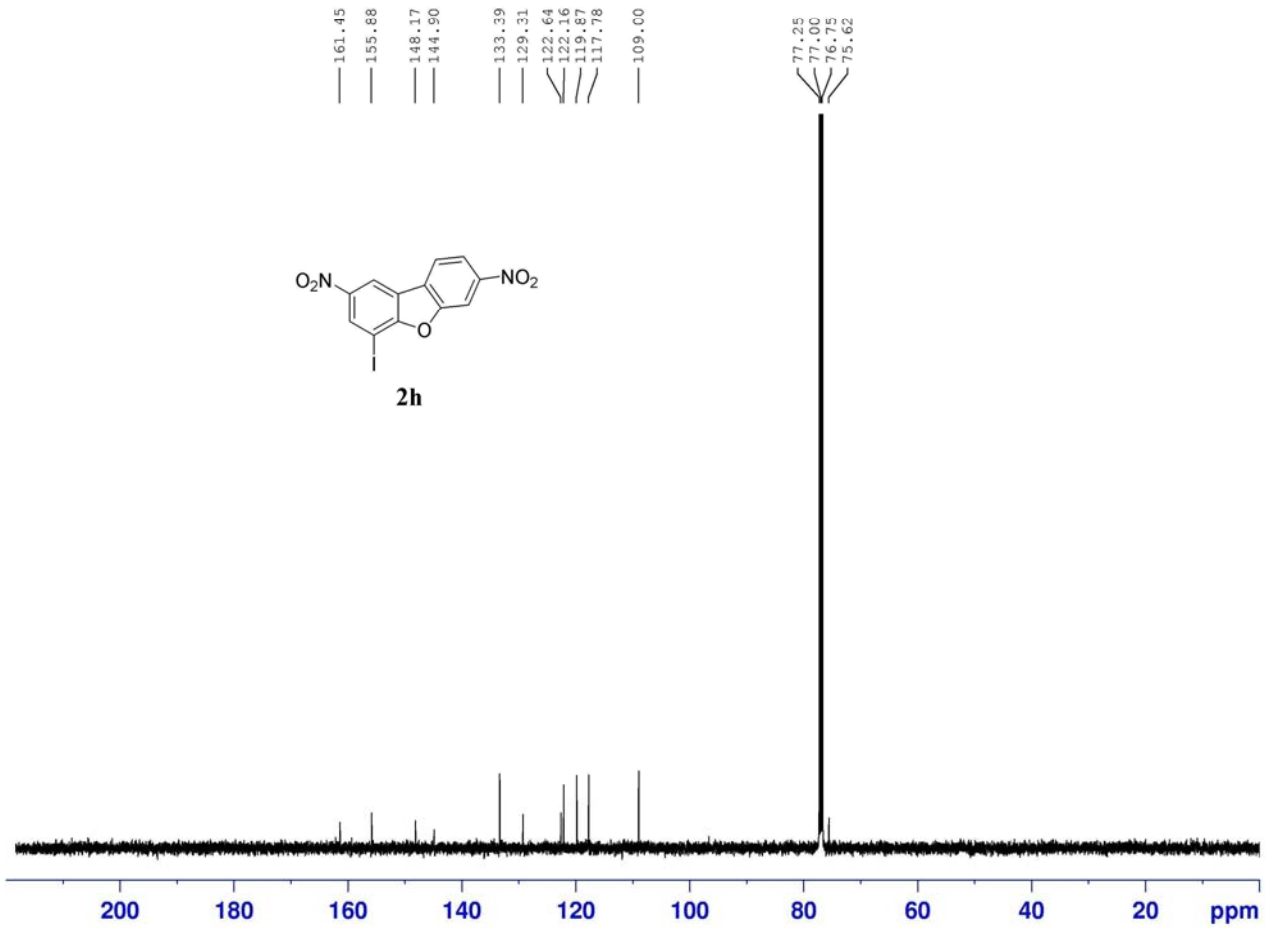

```
NAME          2011manual
EXPNO              155
PROCNO               1
Date_         20110110
Time              0.43
INSTRUM          spect
PROBHD   5 mm PABBO BB-
PULPROG        zgpg30
TD              65536
SOLVENT          CDCl3
NS                2048
DS                   4
SWH          23980.814 Hz
FIDRES        0.365918 Hz
AQ           1.3664756 sec
RG               574.7
DW              20.850 usec
DE               6.50 usec
TE              305.3 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         100.6127667 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```

181804



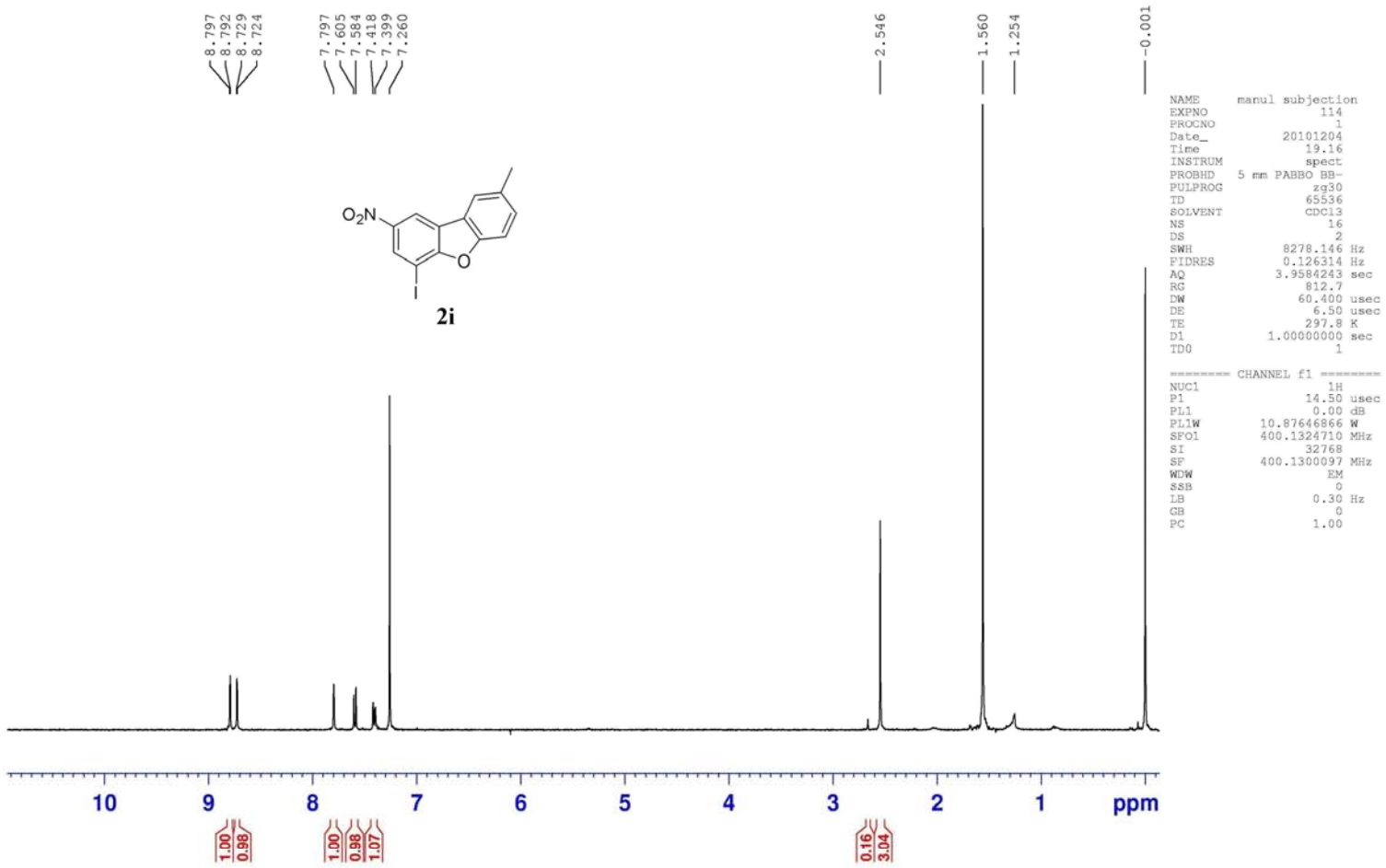

```
NAME          2011manual
EXPNO               198
PROCNO                1
Date_          20110404
Time              19.49
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8278.146 Hz
FIDRES         0.126314 Hz
AQ           3.9584243 sec
RG              1625.5
DW              60.400 usec
DE               6.50 usec
TE              294.5 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          400.1300098 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```

zjj181804-C

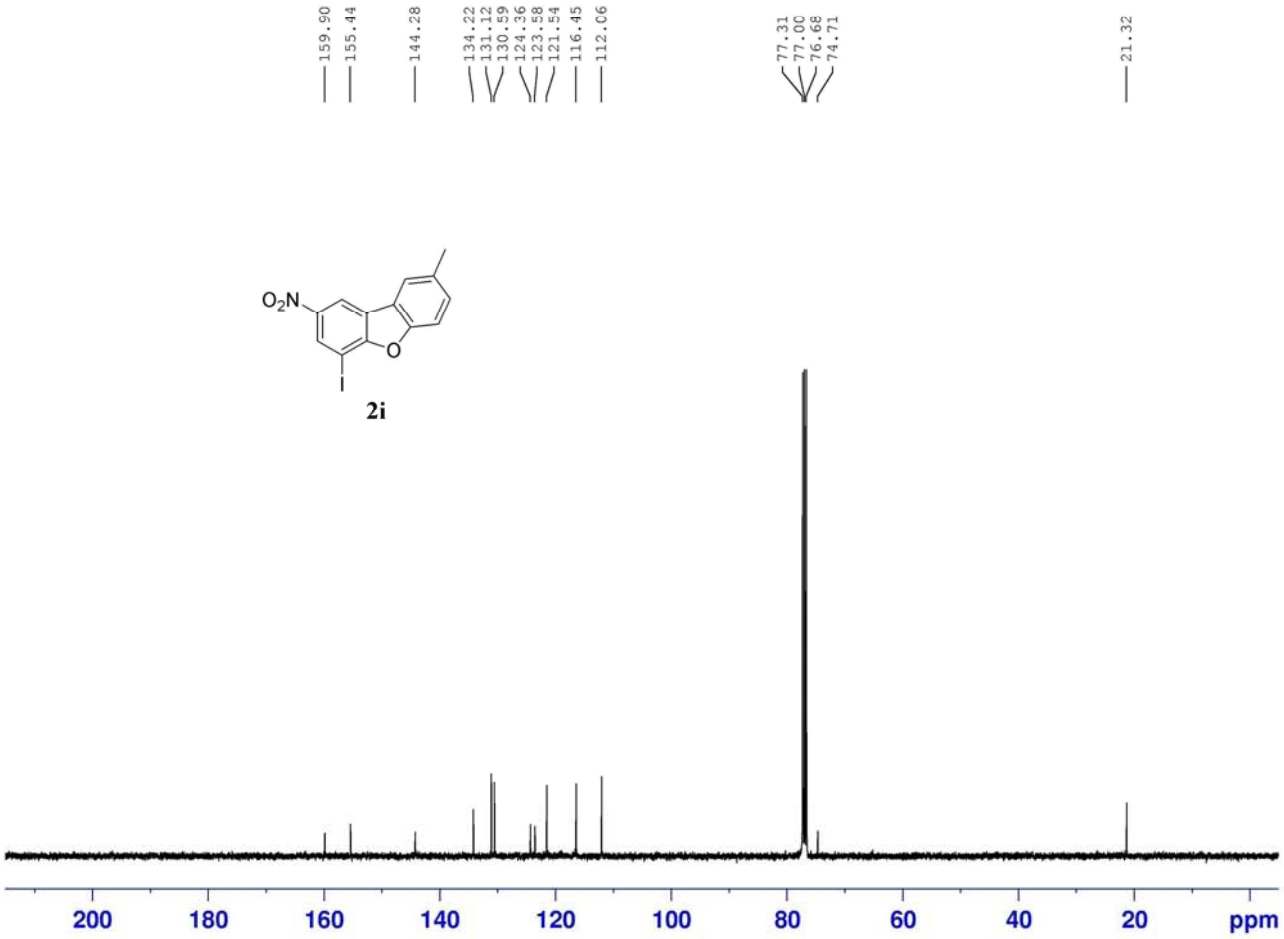



```
NAME            181804-c
EXPNO                  1
PROCNO                 1
Date_           20110407
Time               15.55
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  398
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ            1.1010548 sec
RG                  203
DW               16.800 usec
DE                 6.50 usec
TE                294.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.70 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         125.7577946 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```

131697

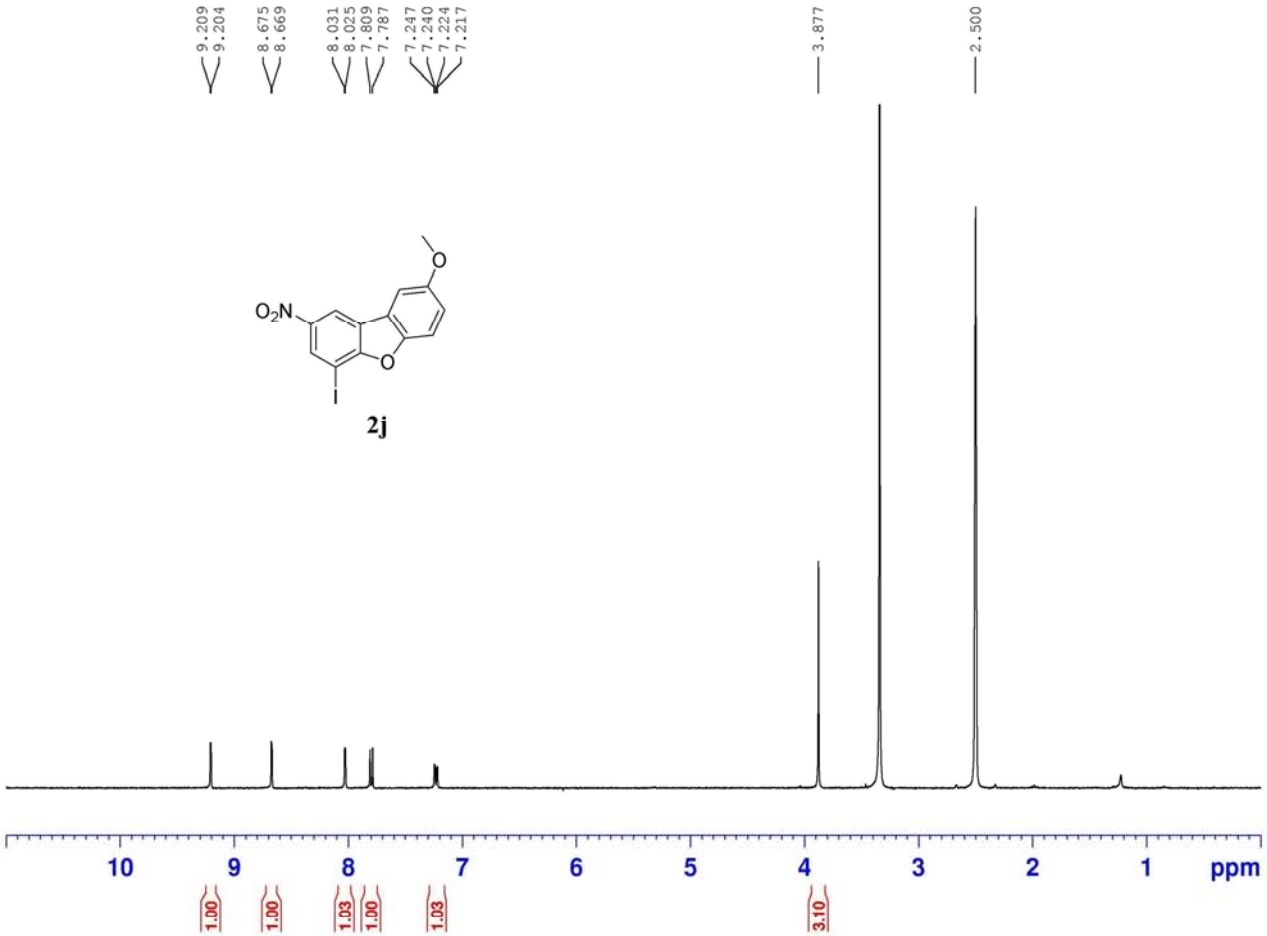

8.797
8.792
8.729
8.724
7.797
7.605
7.584
7.418
7.399
7.260
2.546
1.560
1.254
-0.001
O_2N
O
I
2i
NAME manul subjection
EXPNO 114
PROCNO 1
Date_ 20101204
Time 19.16
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 812.7
DW 60.400 usec
DE 6.50 usec
TE 297.8 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 400.1300097 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
10
9
8
7
6
5
4
3
2
1
ppm
1.00
0.98
1.00
0.98
1.07
0.16
3.04

131697-c



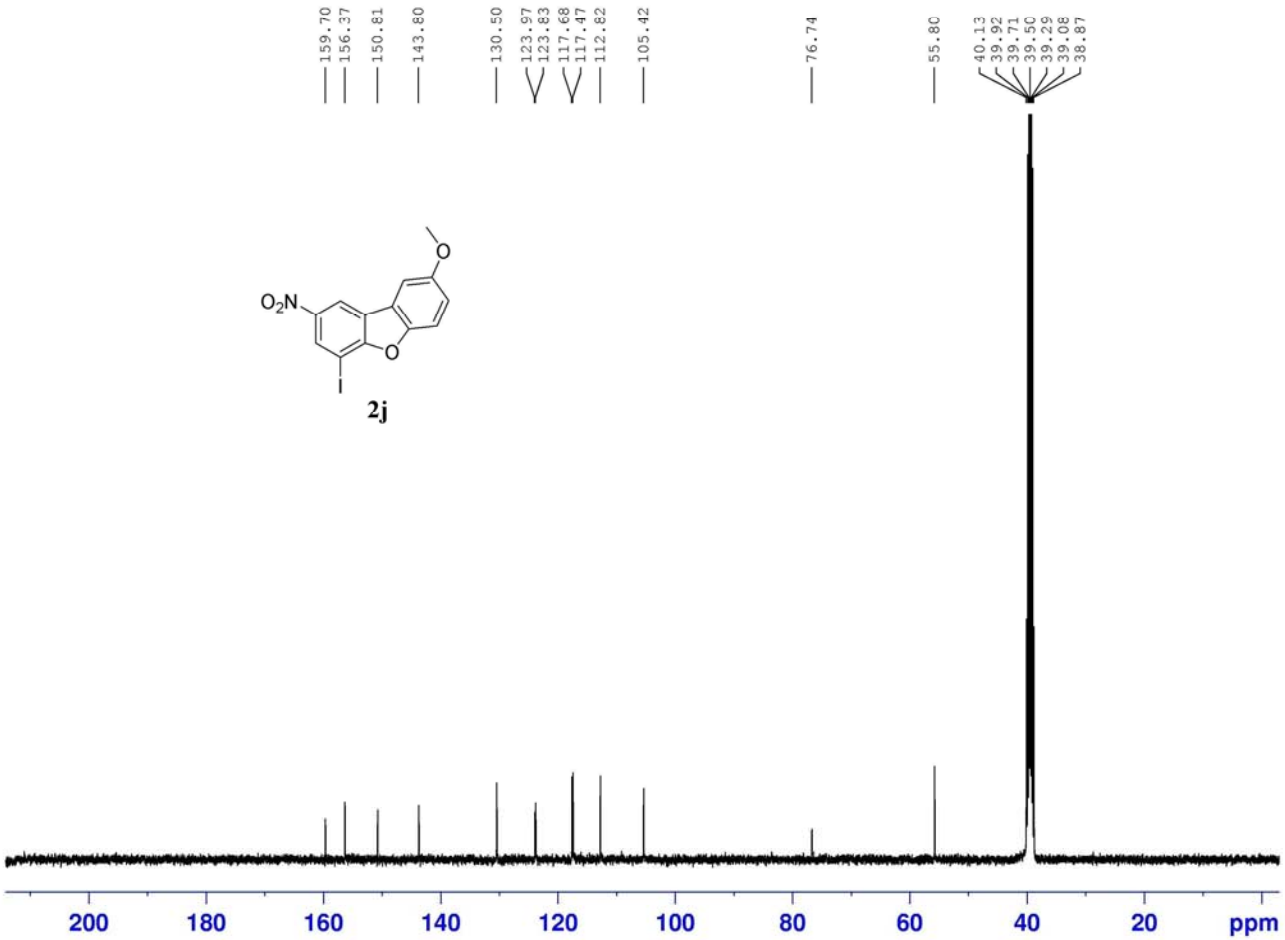

```
NAME        manul subjection
EXPNO                    115
PROCNO                     1
Date_               20101204
Time                   20.00
INSTRUM                spect
PROBHD     5 mm PABBO BB-
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       650
DS                         4
SWH                 23980.814 Hz
FIDRES               0.365918 Hz
AQ                  1.3664756 sec
RG                      645.1
DW                     20.850 usec
DE                       6.50 usec
TE                      301.4 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              100.6127667 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```

131729-2



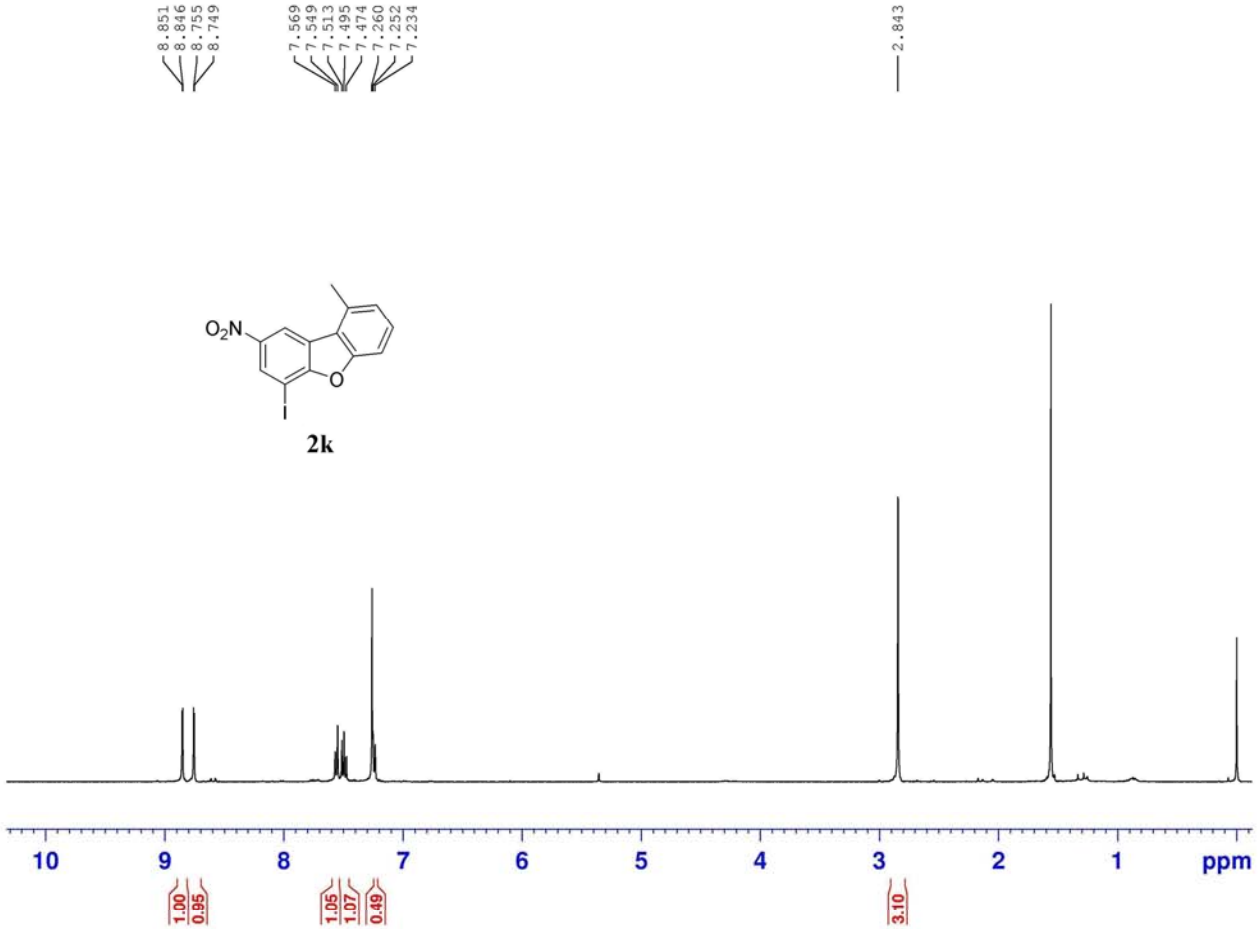

```
NAME          2011manual
EXPNO              156
PROCNO               1
Date_          20110110
Time              19.12
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT            DMSO
NS                    16
DS                     2
SWH            8278.146 Hz
FIDRES         0.126314 Hz
AQ             3.9584243 sec
RG              1149.4
DW              60.400 usec
DE               6.50 usec
TE              293.9 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          400.1300034 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

131729-2C



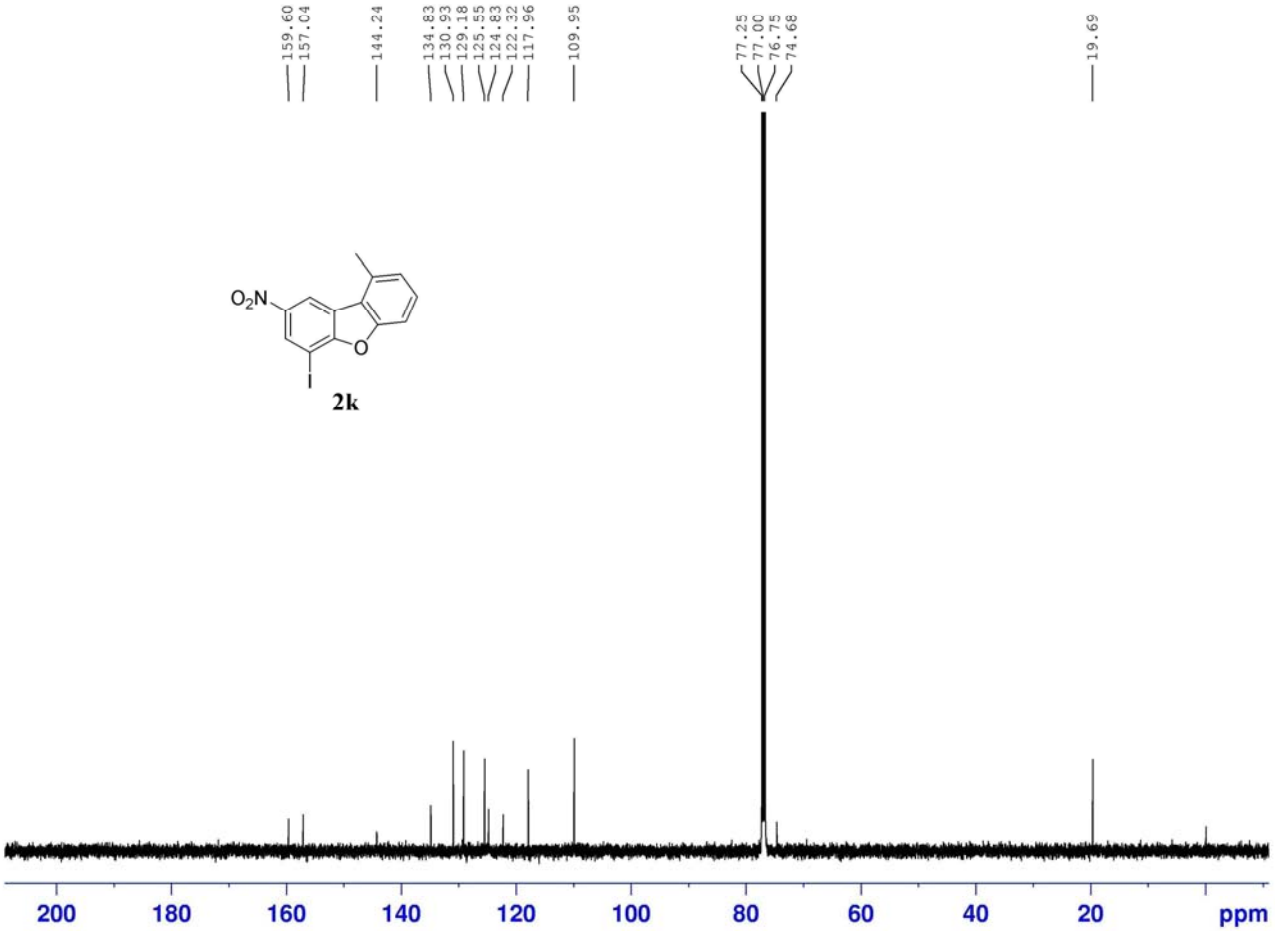

```
NAME          2011manual
EXPNO                159
PROCNO                 1
Date_           20110111
Time                0.10
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 1284
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ            1.3664756 sec
RG                645.1
DW                20.850 usec
DE                 6.50 usec
TE                301.4 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         100.6128234 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```

181997-3



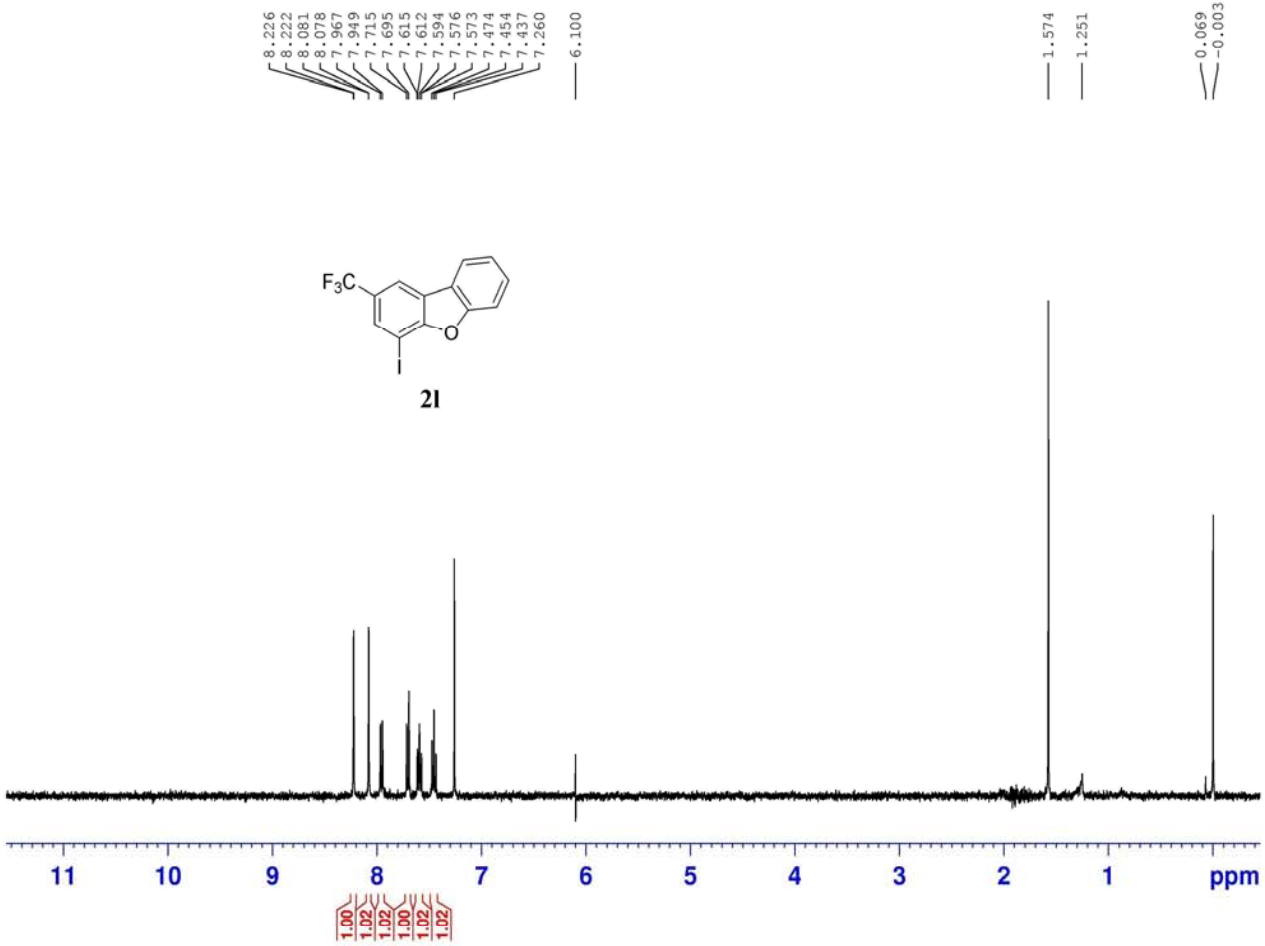

```
NAME            20110906
EXPNO                  2
PROCNO                 1
Date_           20110906
Time                9.53
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ             3.9584243 sec
RG                   512
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           400.1300093 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

181997-3



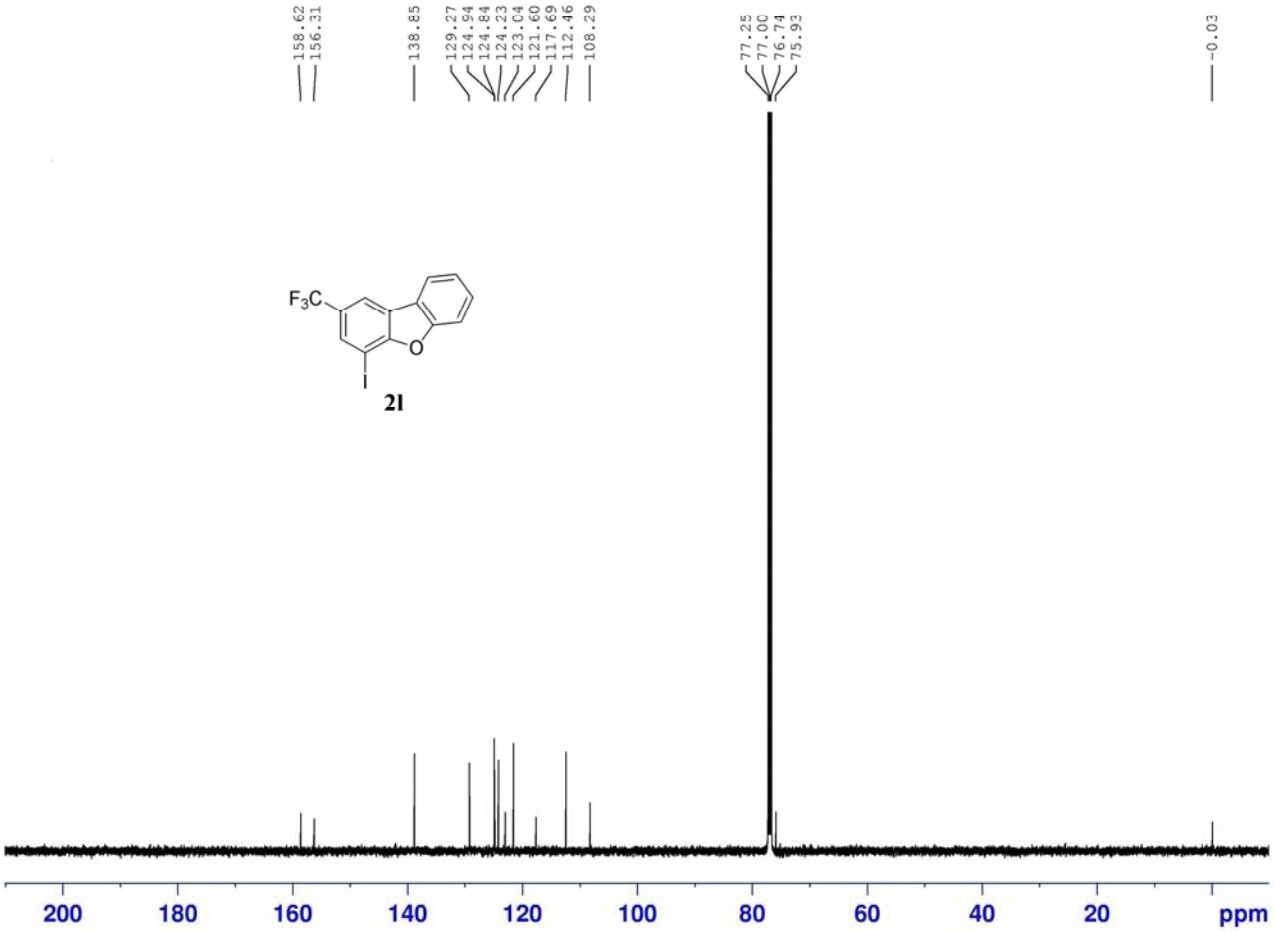
NAME	181997-3
EXPNO	1
PROCNO	1
Date_	20110906
Time	23.55
INSTRUM	Spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	298.8 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL 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	125.7577922 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

181815




```
NAME          2011manual
EXPNO              204
PROCNO               1
Date_          20110410
Time              10.24
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              9195.2
DW               60.400 usec
DE                6.50 usec
TE               294.9 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          400.1300098 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

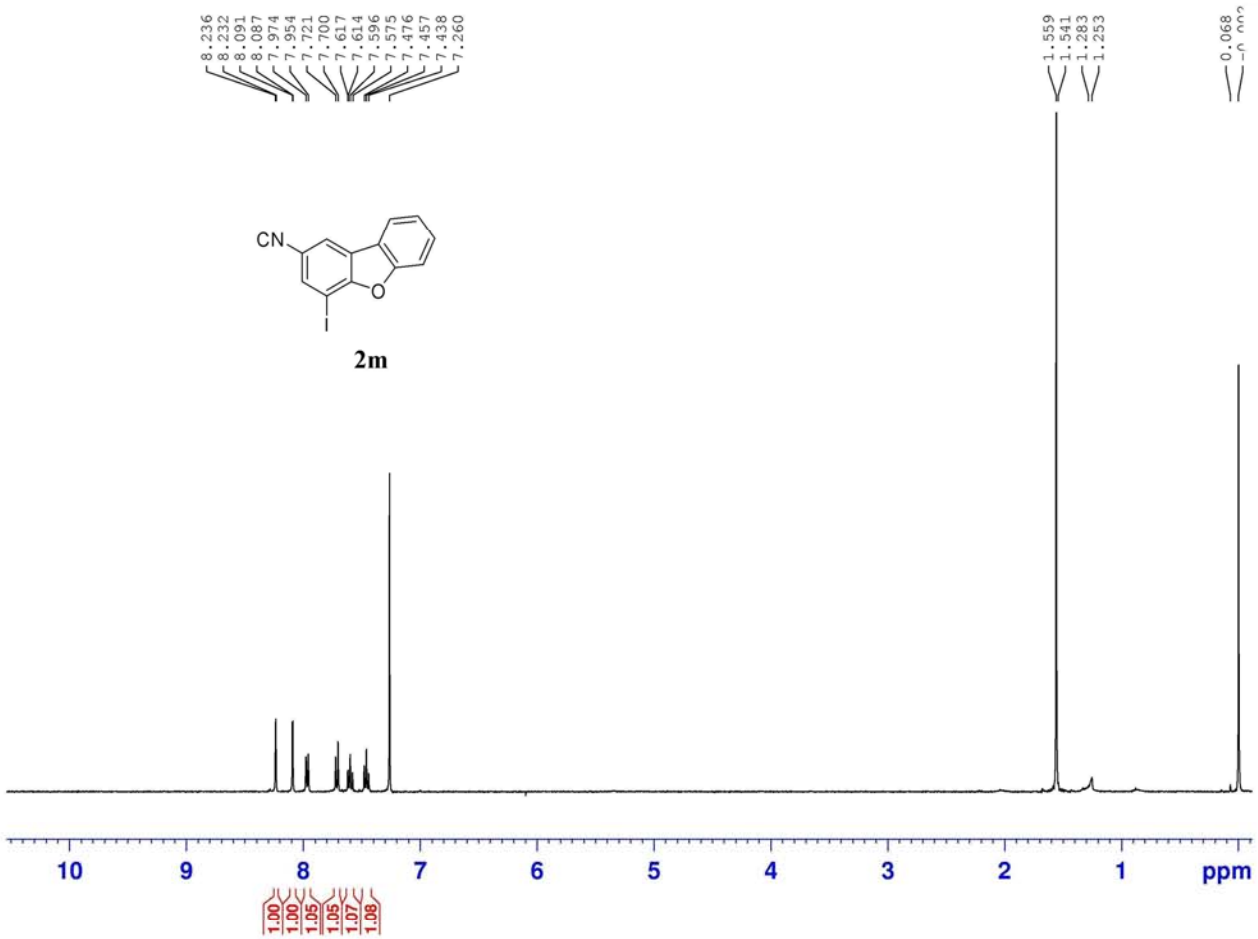
181815



2l

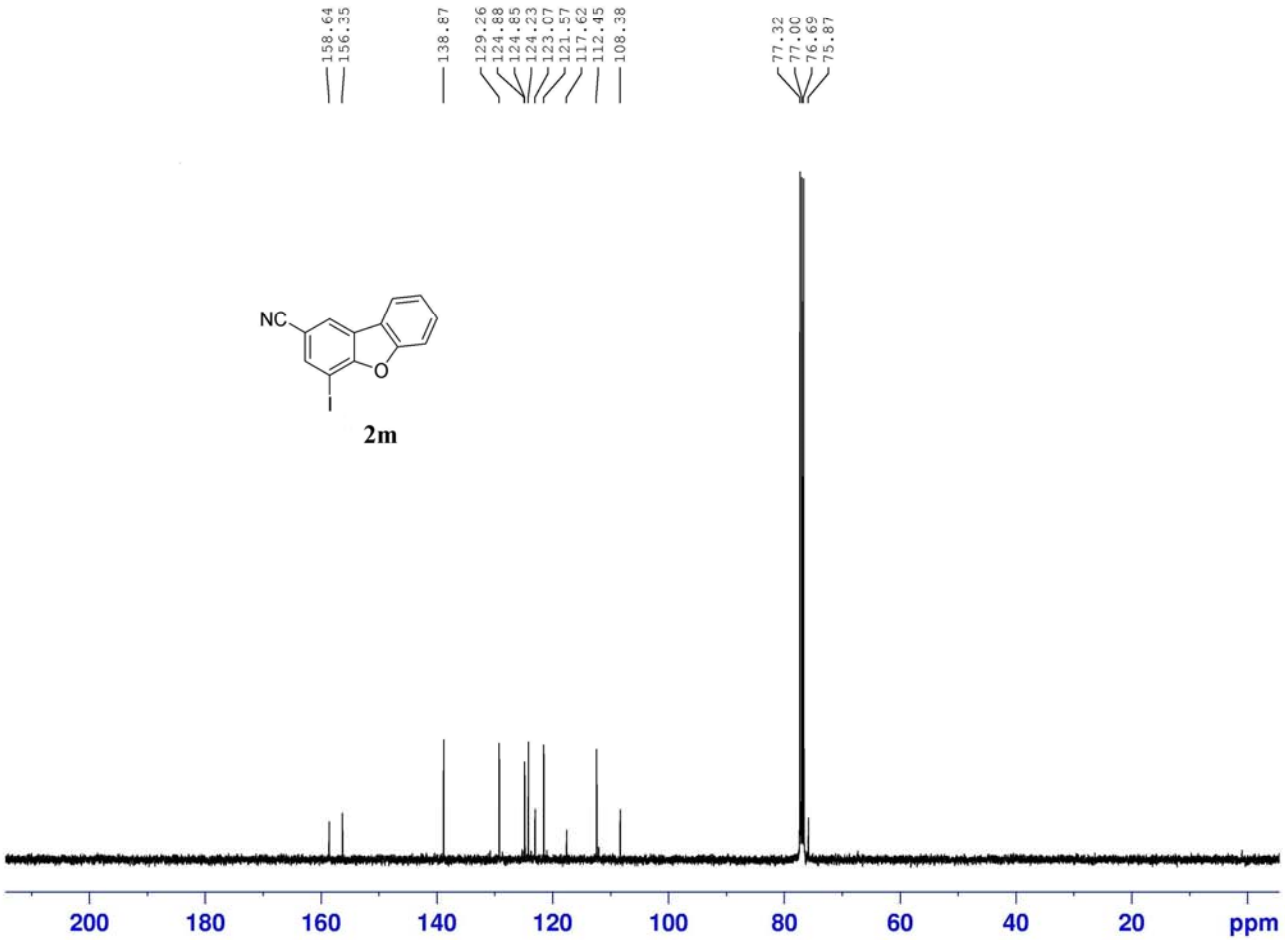
```
NAME              181815
EXPNO                  1
PROCNO                 1
Date_           20110410
Time               16.39
INSTRUM            Spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ            1.1010548 sec
RG                  203
DW                16.800 usec
DE                 6.50 usec
TE                297.4 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.70 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         125.7577940 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```

131700



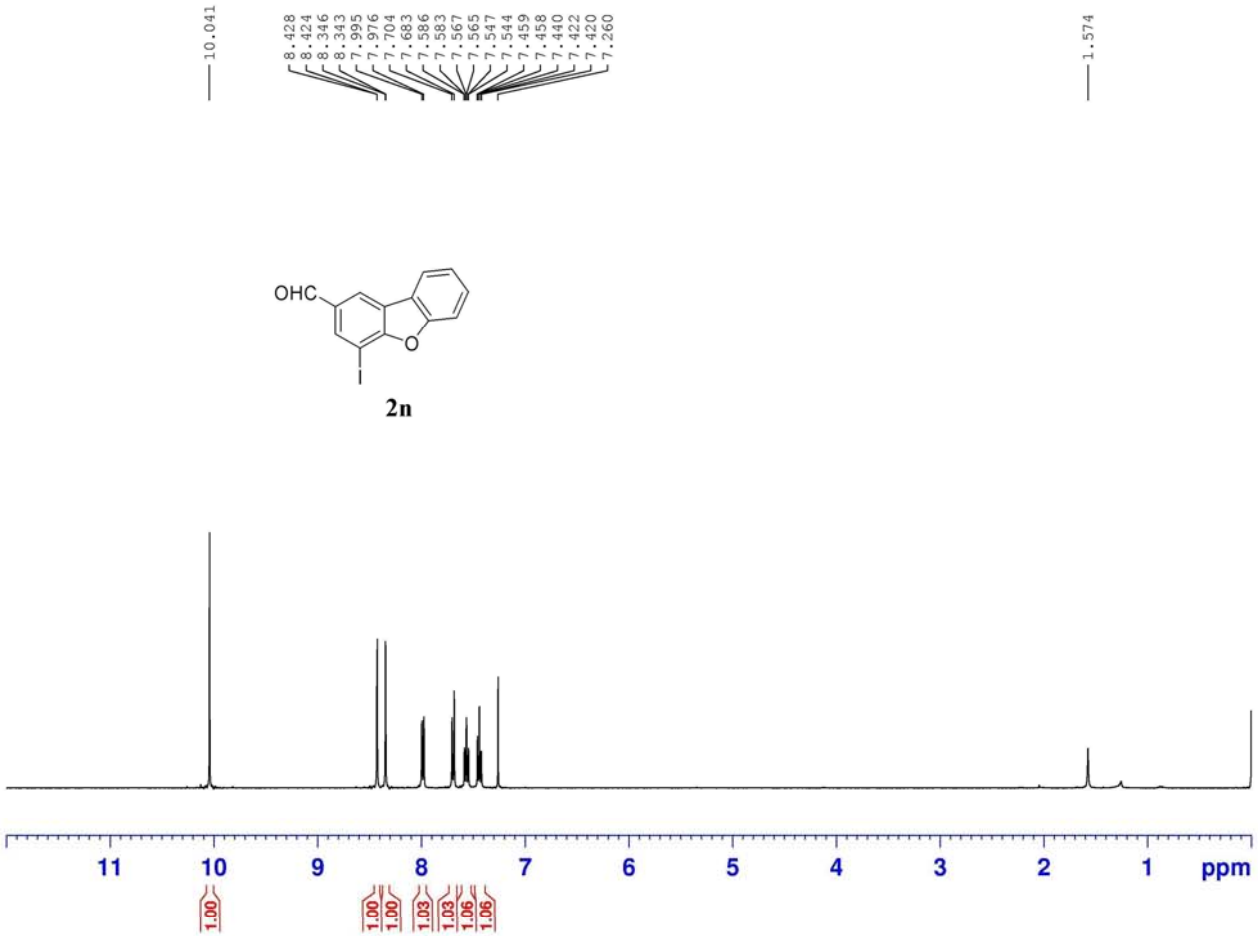

```
NAME                12.06
EXPNO                  57
PROCNO                  1
Date_            20101206
Time                17.15
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8278.146 Hz
FIDRES           0.126314 Hz
AQ             3.9584243 sec
RG                  812.7
DW                 60.400 usec
DE                   6.50 usec
TE                  297.6 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          400.1300100 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

131700



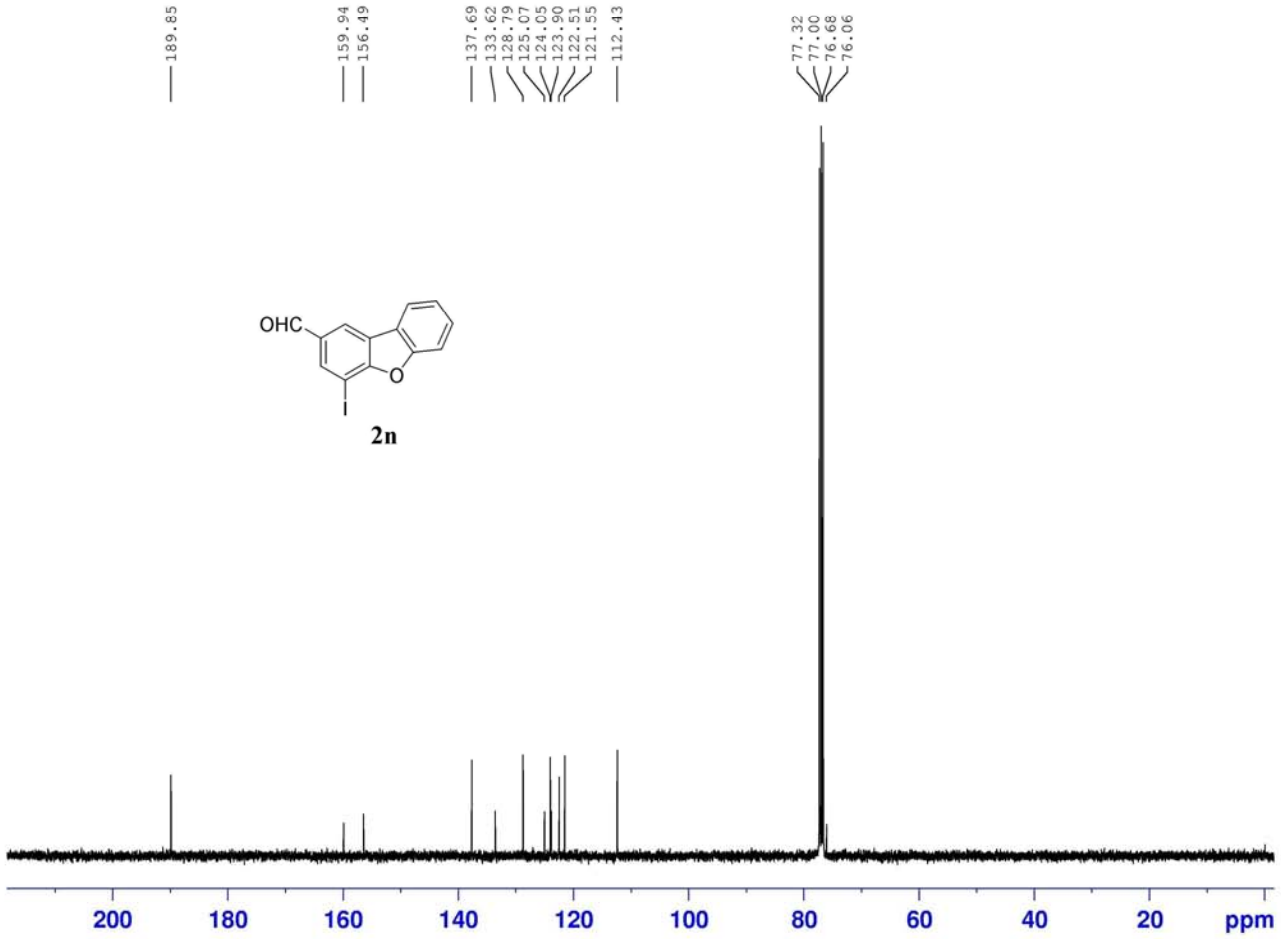

```
NAME        manul subjection
EXPNO                    117
PROCNO                     1
Date_               20101206
Time                   17.48
INSTRUM                spect
PROBHD     5 mm PABBO BB-
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       573
DS                         4
SWH                 23980.814 Hz
FIDRES               0.365918 Hz
AQ                  1.3664756 sec
RG                      574.7
DW                     20.850 usec
DE                       6.50 usec
TE                      301.4 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              100.6127675 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```

131718-2



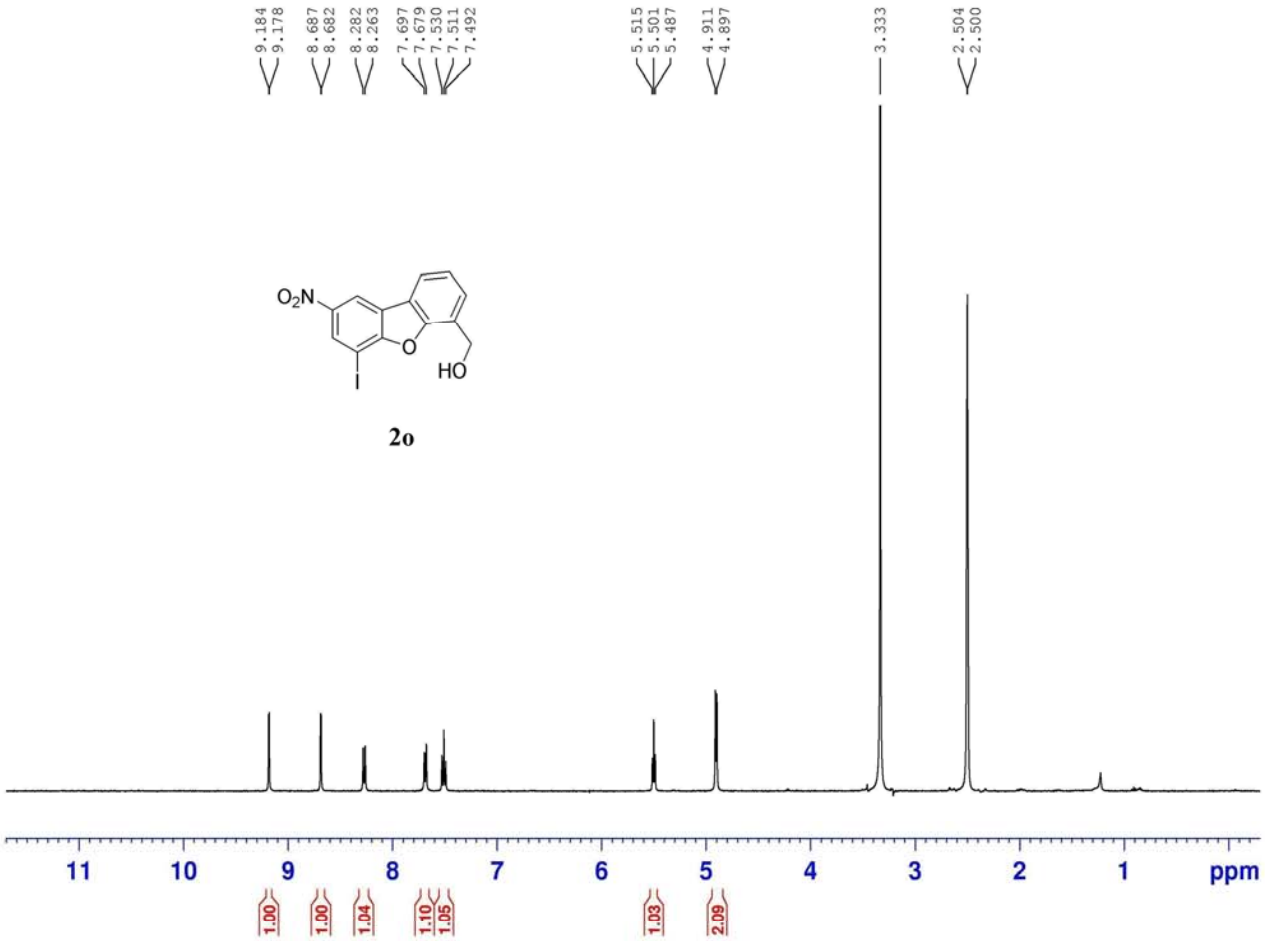

```
NAME        manul subjection
EXPNO                    137
PROCNO                     1
Date_               20101224
Time                   20.35
INSTRUM                spect
PROBHD     5 mm PABBO BB-
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        16
DS                         2
SWH                 8278.146 Hz
FIDRES              0.126314 Hz
AQ                 3.9584243 sec
RG                     812.7
DW                    60.400 usec
DE                      6.50 usec
TE                     297.8 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               400.1300097 MHz
WDW                       EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
```

131718-2C



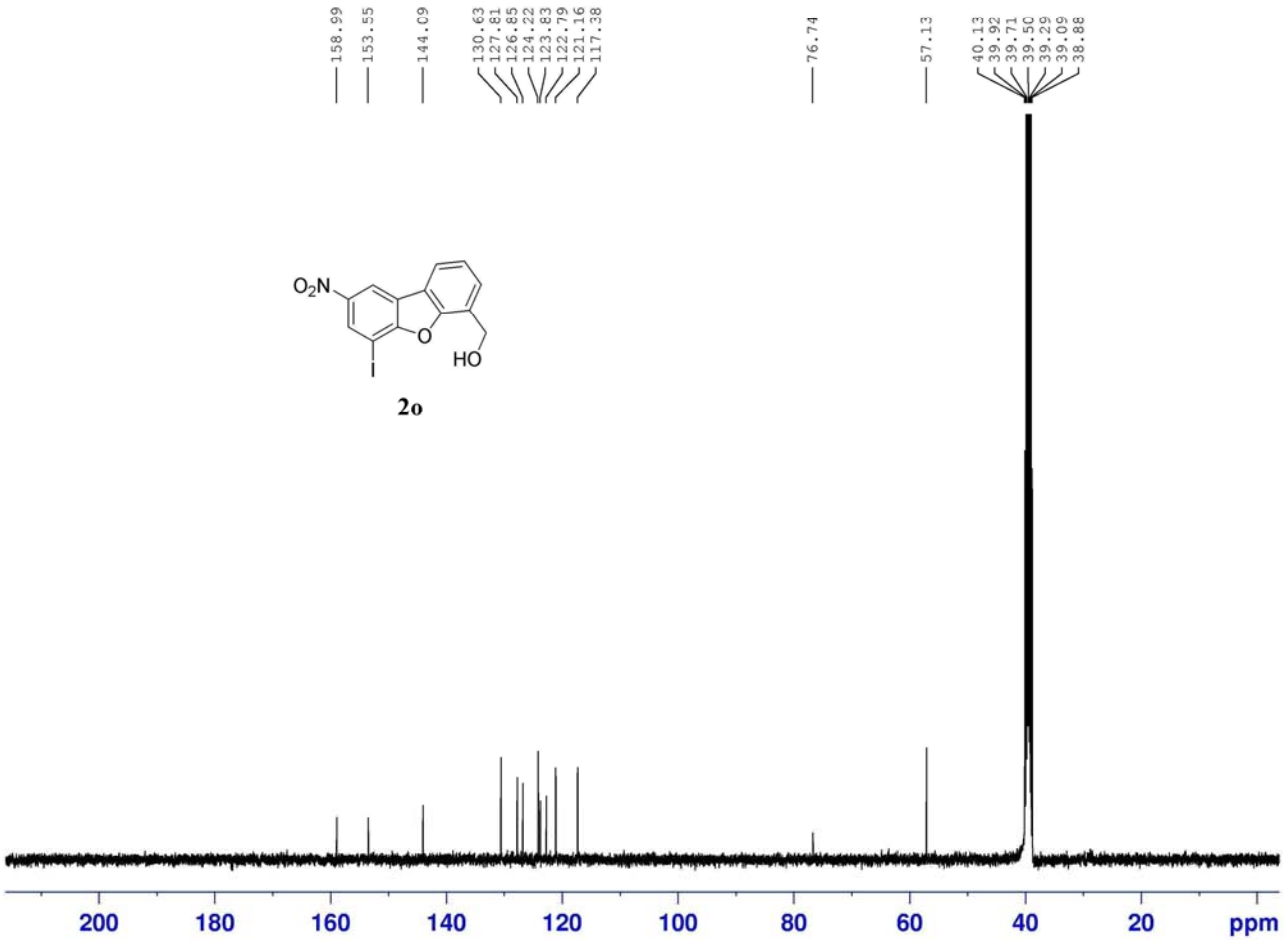

```
NAME        manul subjection
EXPNO                    138
PROCNO                     1
Date_               20101224
Time                   20.45
INSTRUM                spect
PROBHD     5 mm PABBO BB-
PULPROG               zgpg30
TD                     65536
SOLVENT                CDCl3
NS                       474
DS                         4
SWH                 23980.814 Hz
FIDRES               0.365918 Hz
AQ                  1.36664756 sec
RG                       574.7
DW                      20.850 usec
DE                        6.50 usec
TE                       300.6 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             100.6127675 MHz
WDW                         EM
SSB                          0
LB                        1.00 Hz
GB                           0
PC                        1.40
```

131724



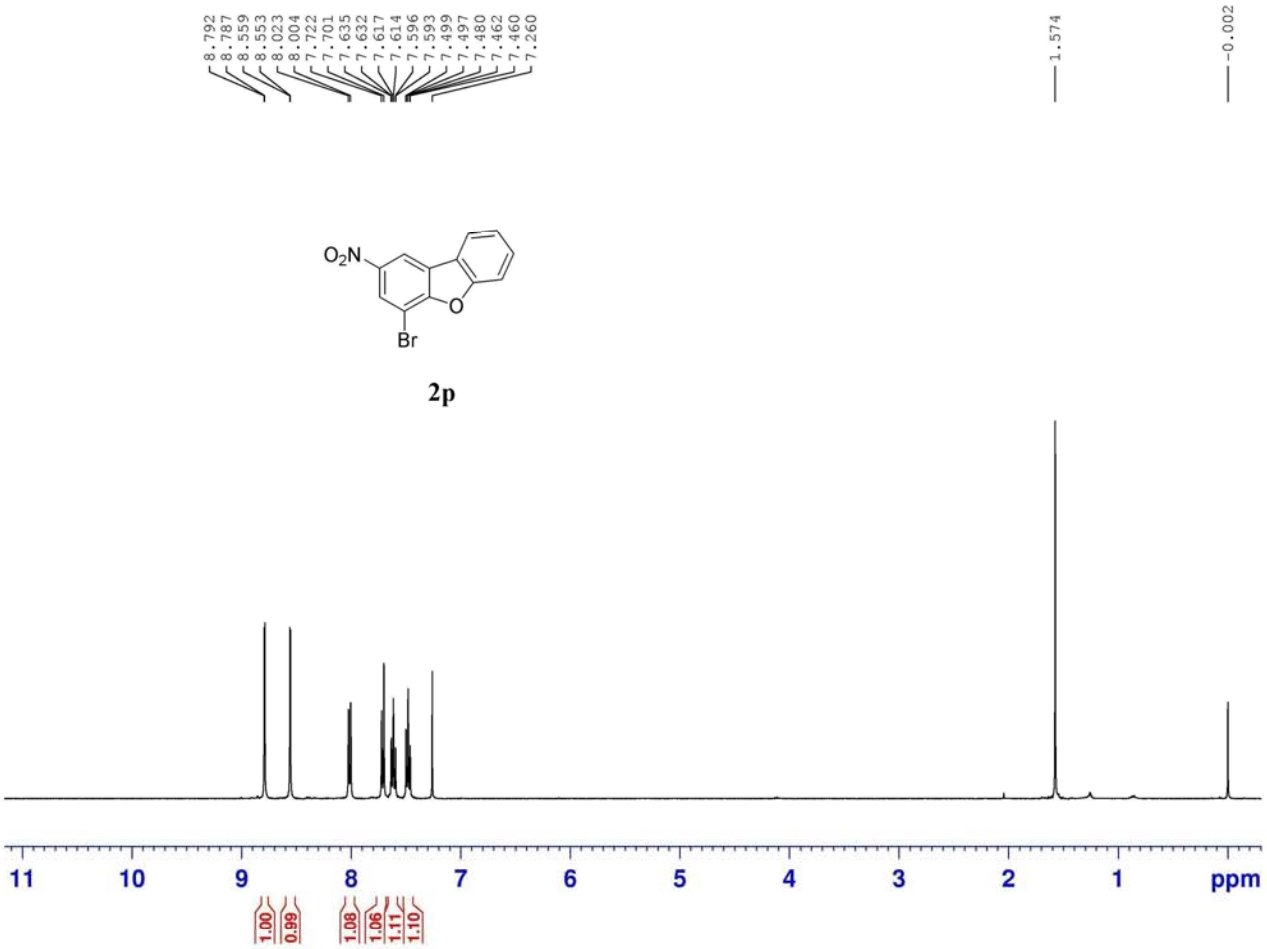

```
NAME          2011manual
EXPNO              152
PROCNO               1
Date_         20110109
Time             16.11
INSTRUM          spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               65536
SOLVENT           DMSO
NS                  16
DS                   2
SWH           8278.146 Hz
FIDRES        0.126314 Hz
AQ           3.9584243 sec
RG               812.7
DW              60.400 usec
DE               6.50 usec
TE              296.1 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         400.1300035 MHz
WDW                 EM
SSB                  0
LB                0.30 Hz
GB                   0
PC                1.00
```

131724-C



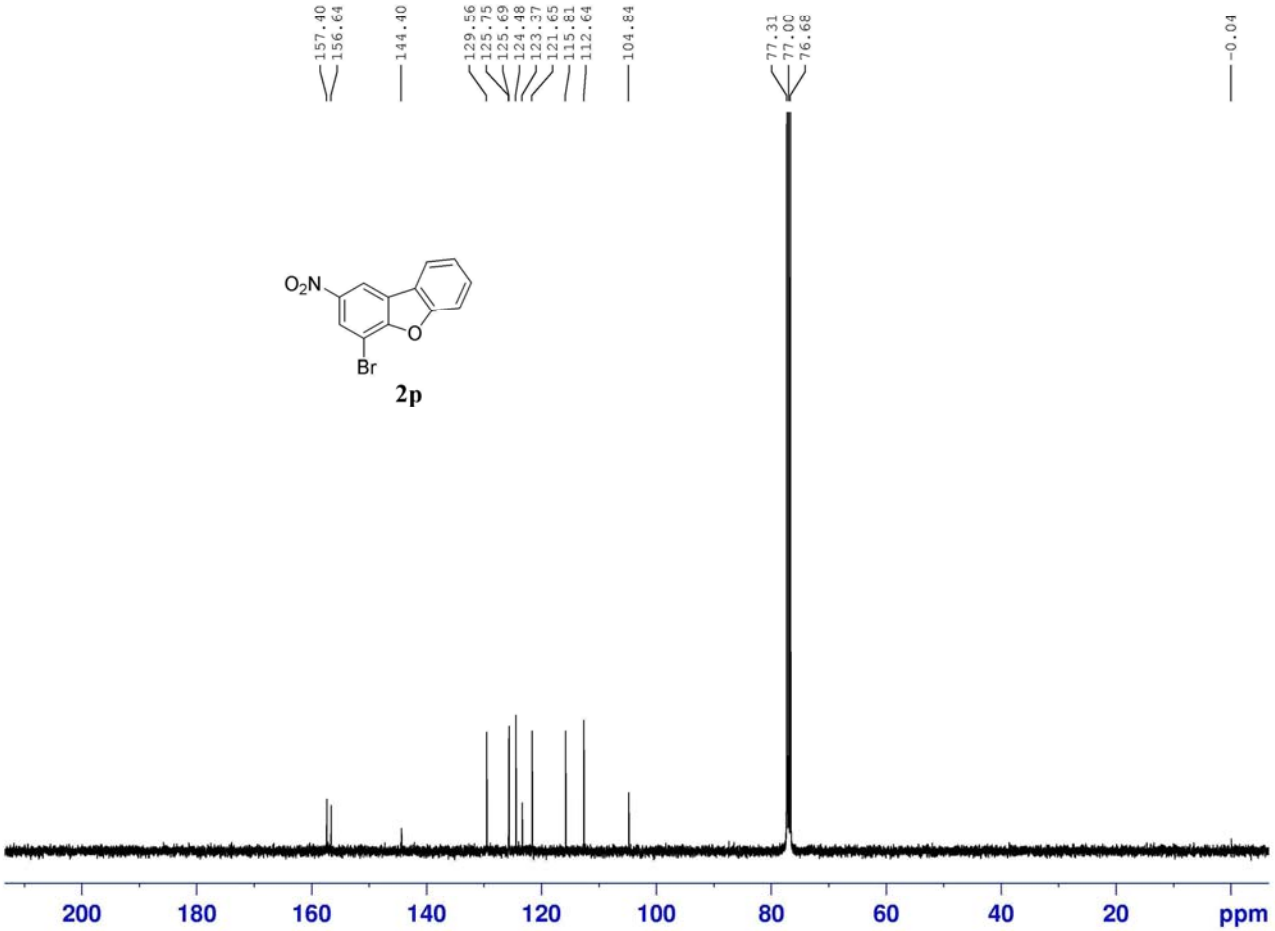

```
NAME          2011manual
EXPNO                154
PROCNO                 1
Date_           20110109
Time               22.44
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 1917
DS                    4
SWH           23980.814 Hz
FIDRES         0.365918 Hz
AQ            1.3664756 sec
RG                574.7
DW               20.850 usec
DE                 6.50 usec
TE                304.8 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         100.6128286 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40
```

181919-3

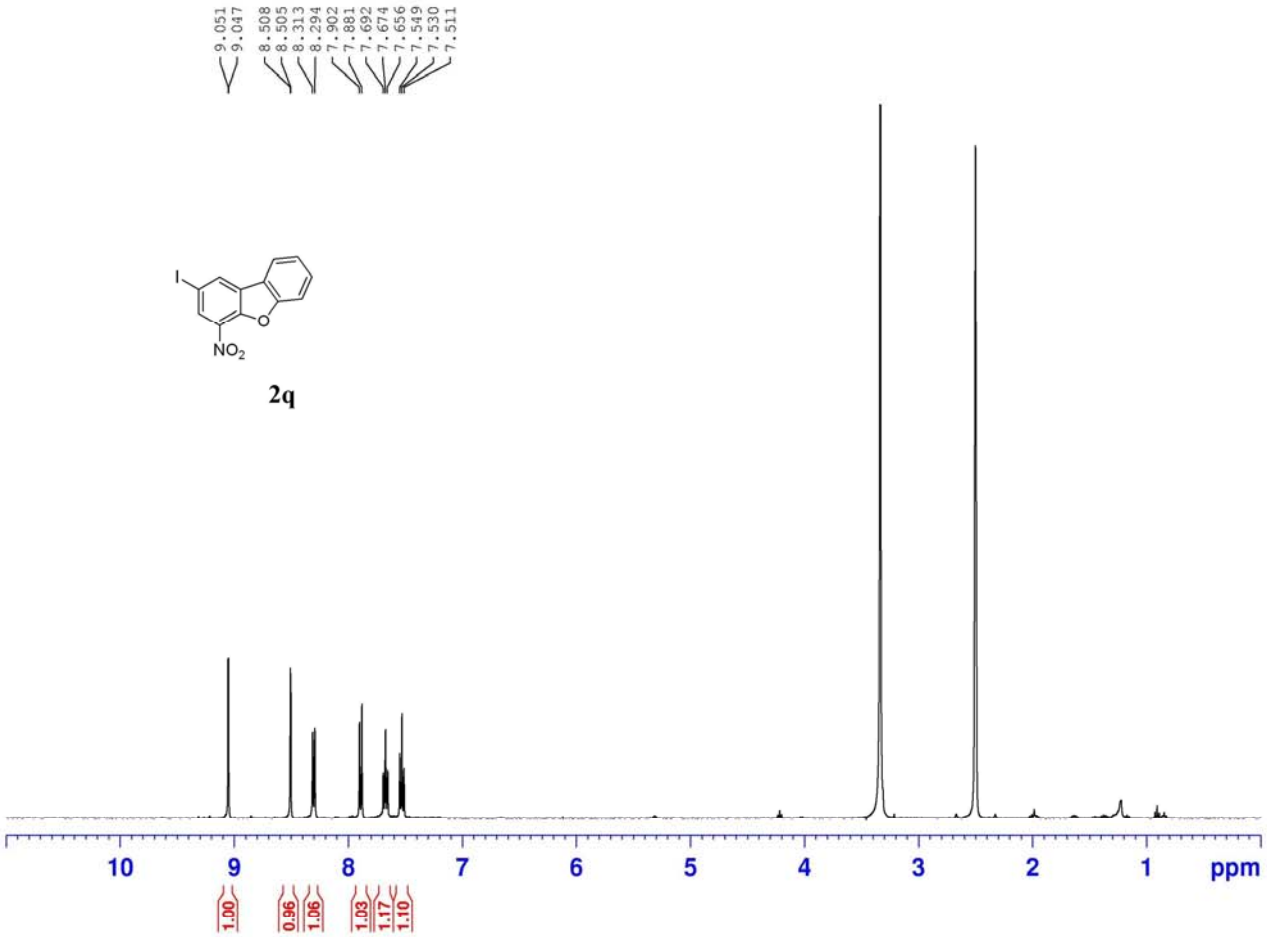


NAME	2011manual
EXPNO	263
PROCNO	1
Date_	20110703
Time	19.09
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	322.5
DW	60.400 usec
DE	6.50 usec
TE	298.4 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.00 dB
PL1W	10.87646866 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300092 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

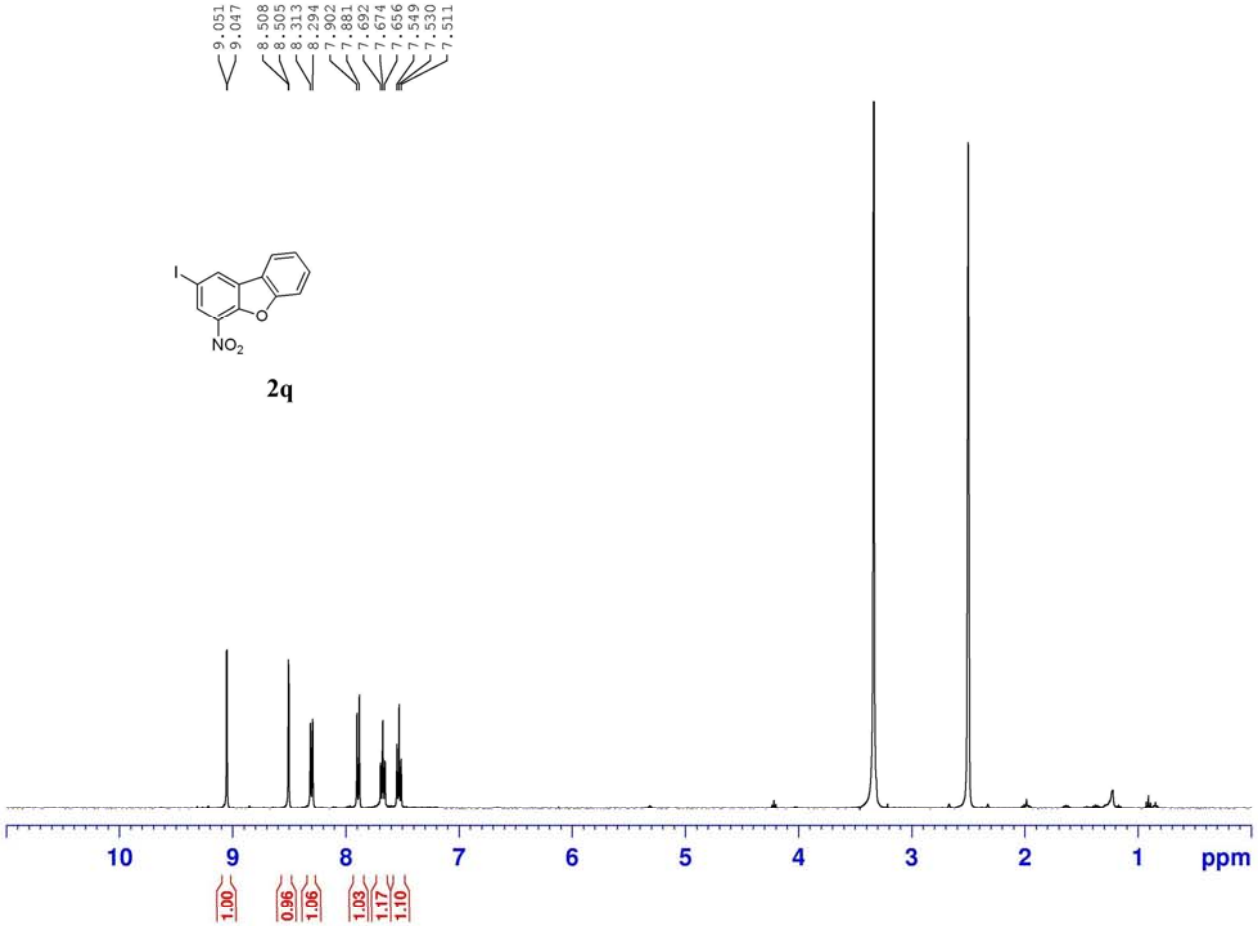
181919-3C




```
NAME          2011manual
EXPNO              264
PROCNO               1
Date_         20110703
Time             19.15
INSTRUM          spect
PROBHD   5 mm PABBO BB-
PULPROG        zgpg30
TD             65536
SOLVENT        CDCl3
NS              1101
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             305.9 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        100.6127630 MHz
WDW               EM
SSB                0
LB              1.00 Hz
GB                 0
PC              1.40
```

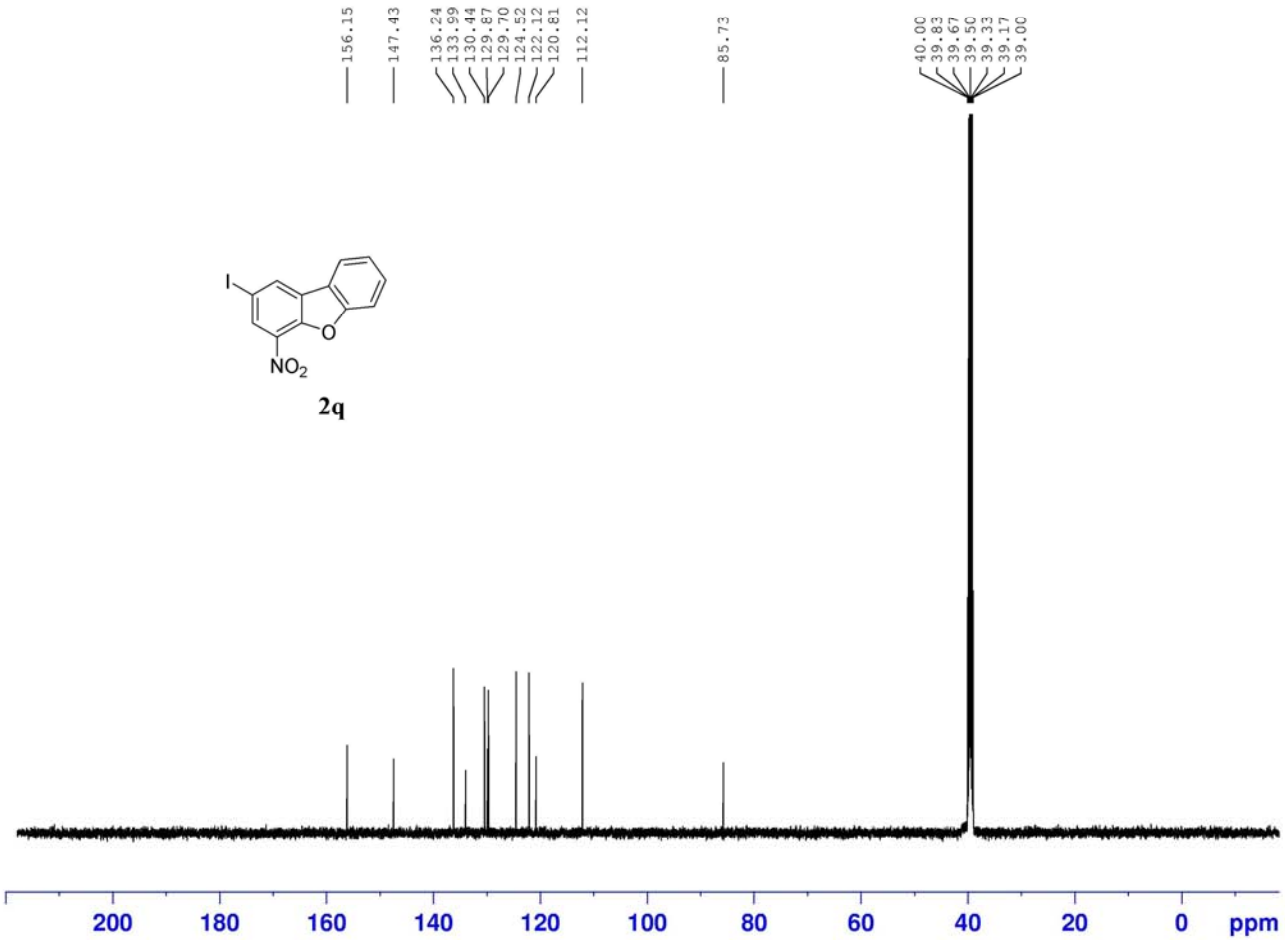



```
NAME            20120314
EXPNO                67
PROCNO                1
Date_          20120314
Time              16.52
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT            DMSO
NS                    16
DS                     2
SWH            8278.146 Hz
FIDRES         0.126314 Hz
AQ            3.9584243 sec
RG                  362
DW               60.400 usec
DE                6.50 usec
TE               296.7 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         400.1300020 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

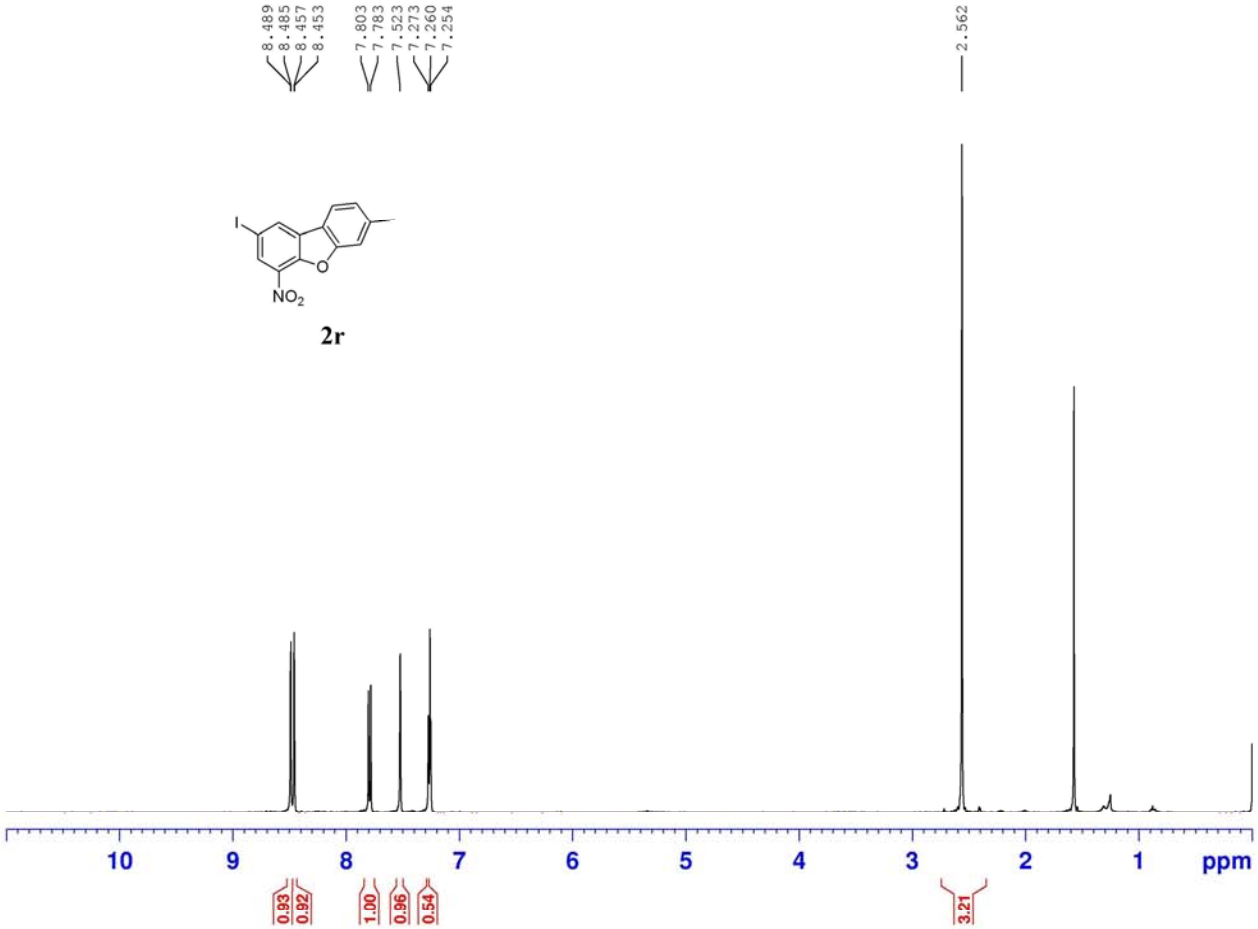


NAME	20120314
EXPNO	67
PROCNO	1
Date_	20120314
Time	16.52
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	362
DW	60.400 usec
DE	6.50 usec
TE	296.7 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.00 dB
PL1W	10.87646866 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300020 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

153995-C

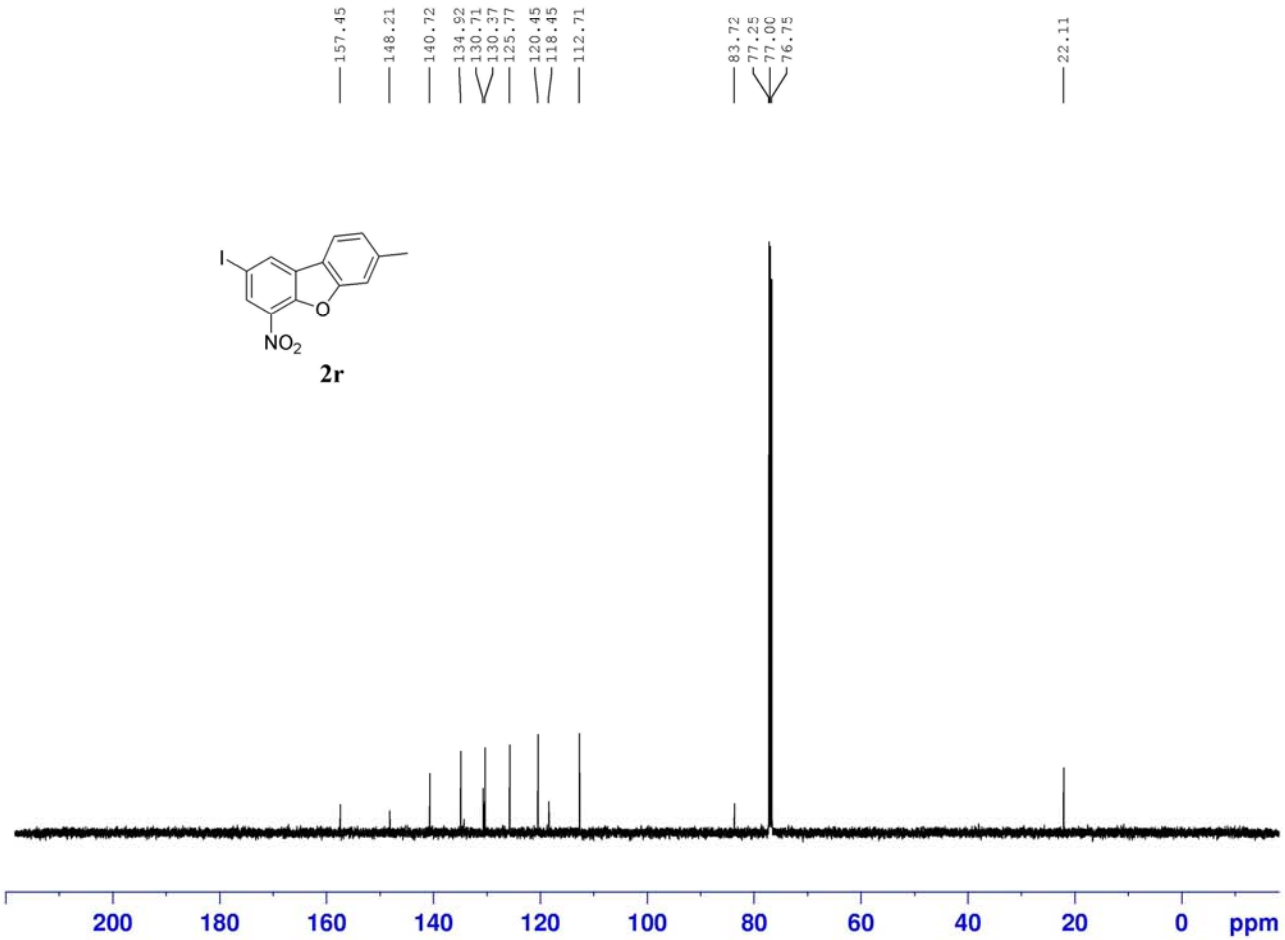



```
NAME            153995-c
EXPNO                  1
PROCNO                 1
Date_           20120315
Time               18.56
INSTRUM            Spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                   581
DS                     4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ            1.1010548 sec
RG                   203
DW                16.800 usec
DE                 6.50 usec
TE                297.2 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         125.7578536 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```

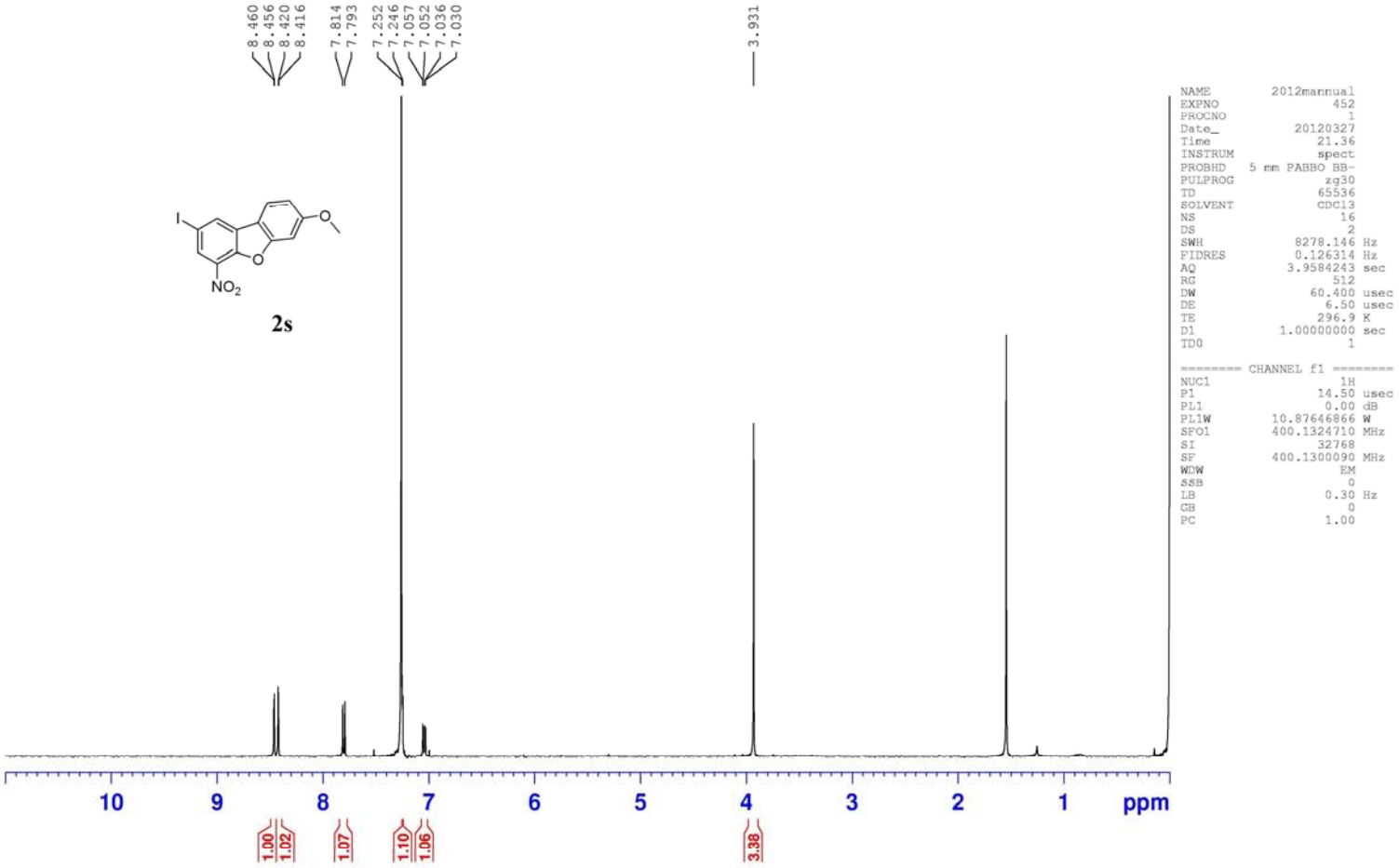


NAME	2012mannual
EXPNO	449
PROCNO	1
Date_	20120317
Time	15.10
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	322.5
DW	60.400 usec
DE	6.50 usec
TE	297.3 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	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

45202-C

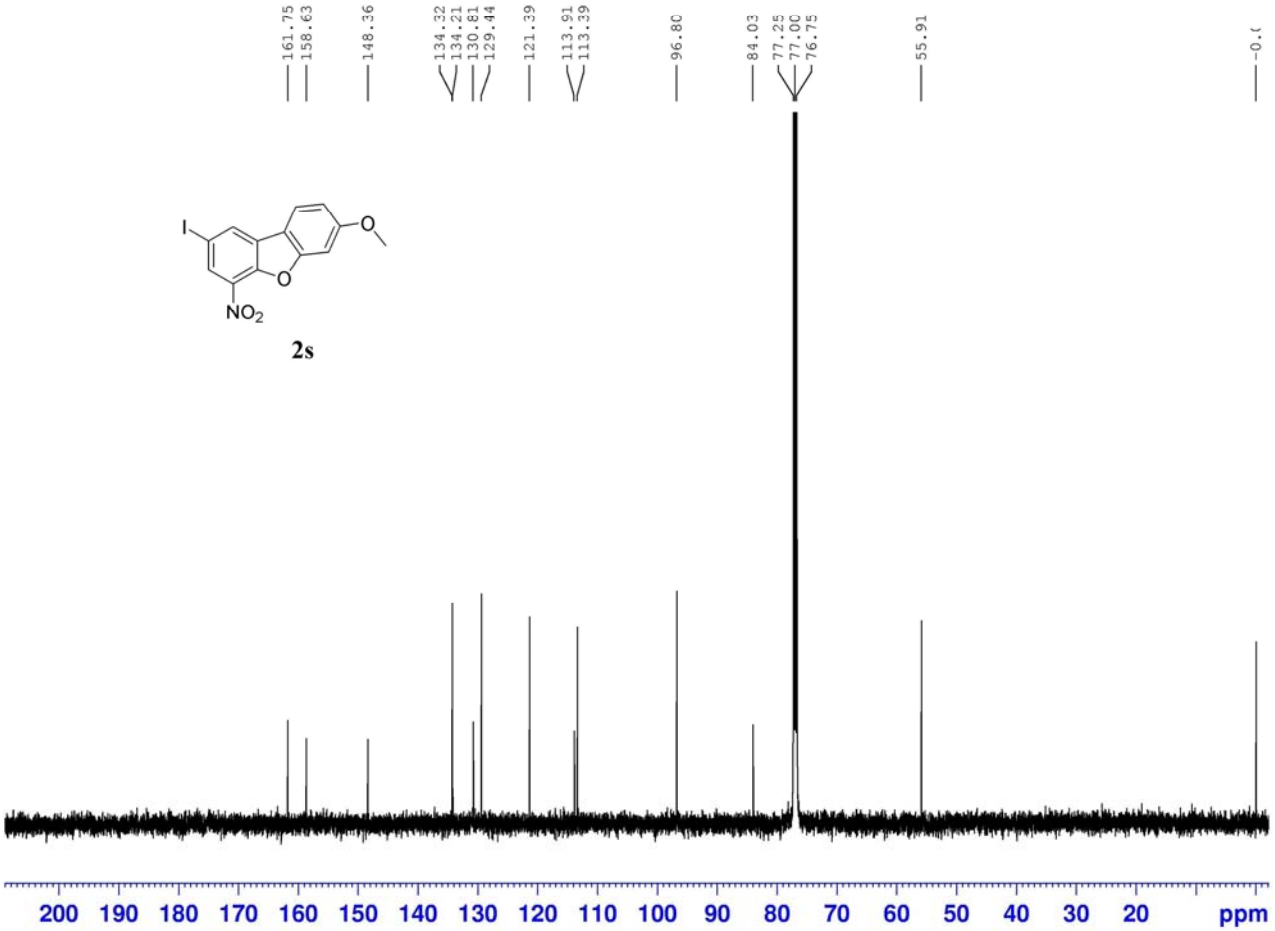



```
NAME            45202-c
EXPNO                 1
PROCNO                1
Date_          20120321
Time              22.59
INSTRUM           Spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  160
DS                    4
SWH           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          125.7577948 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```

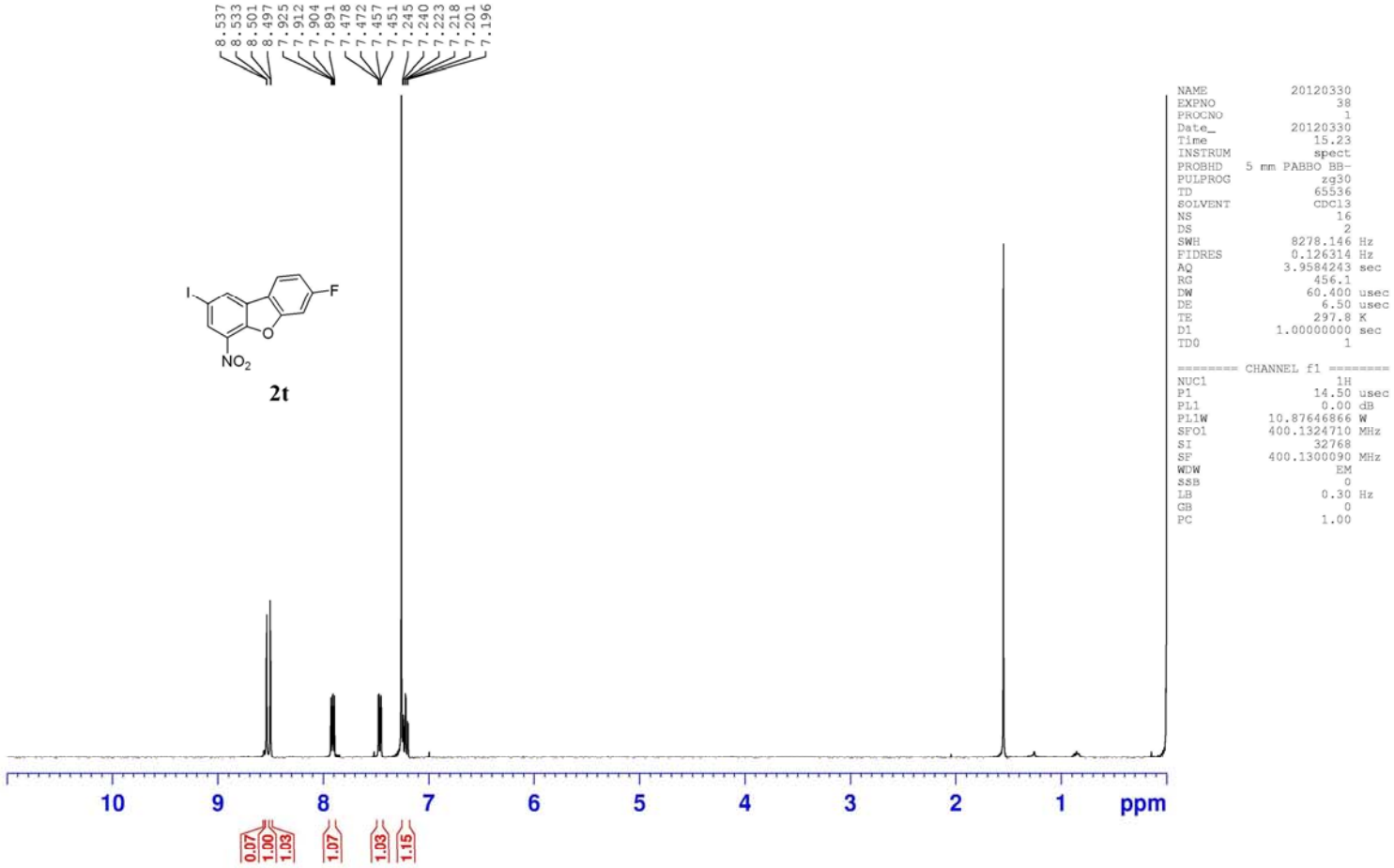



```
NAME          2012mannual
EXPNO               452
PROCNO                1
Date_          20120327
Time              21.36
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8278.146 Hz
FIDRES         0.126314 Hz
AQ           3.9584243 sec
RG                  512
DW               60.400 usec
DE                6.50 usec
TE               296.9 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
```

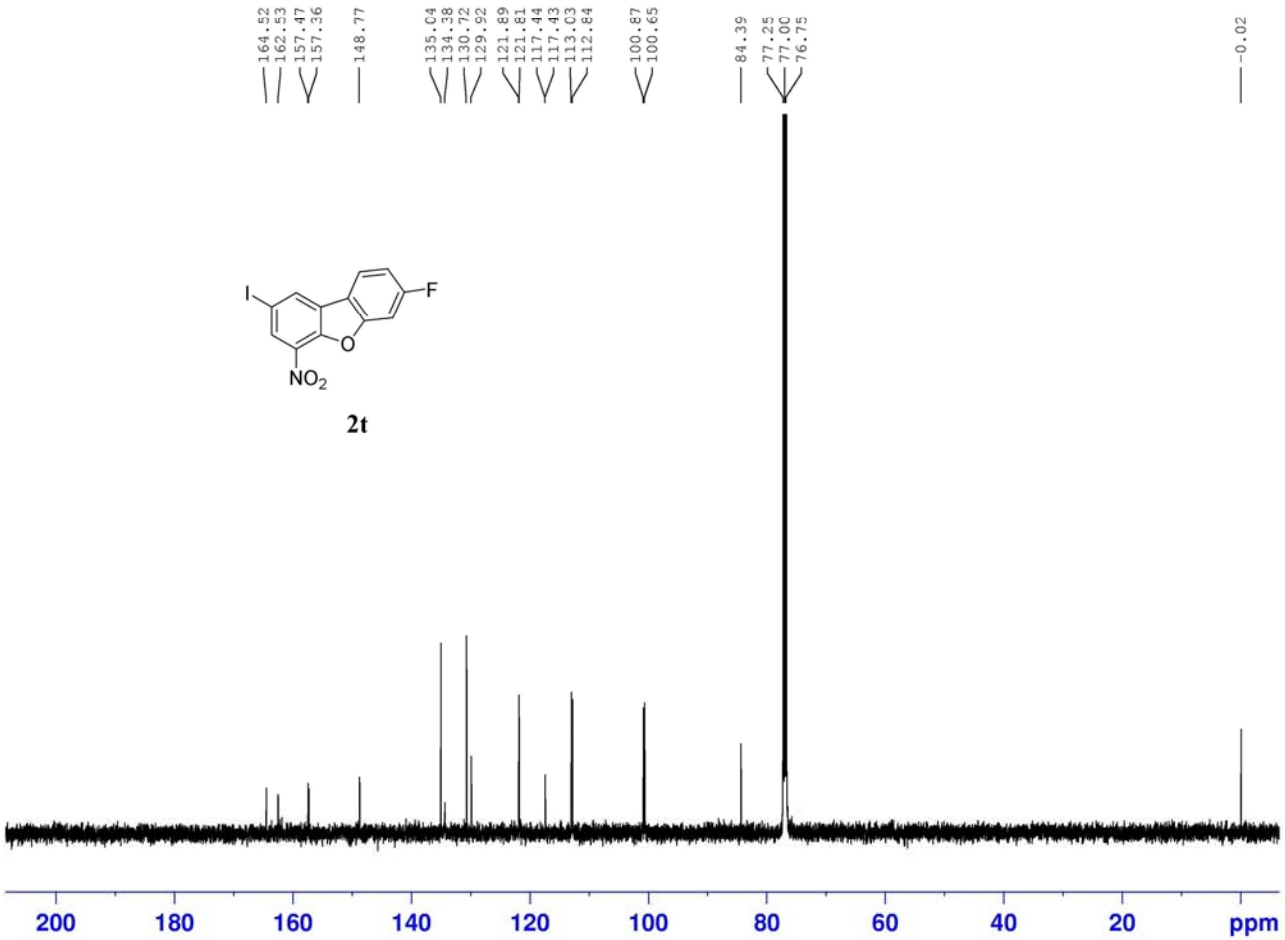
45204-C



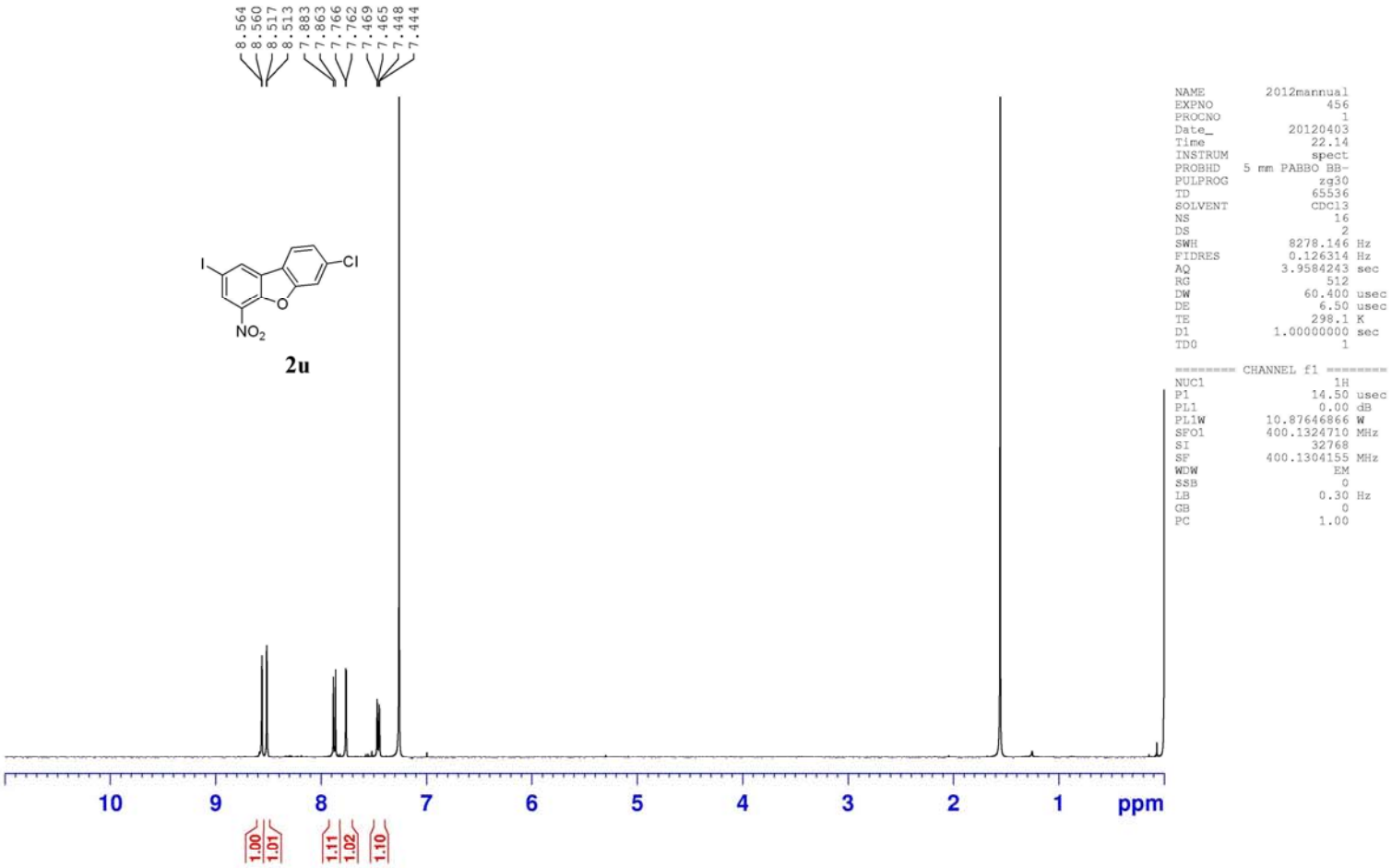

```
NAME            45204-c
EXPNO                 1
PROCNO                1
Date_          20120328
Time              19.30
INSTRUM           Spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 2497
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ            1.1010548 sec
RG                  203
DW               16.800 usec
DE                6.50 usec
TE               295.5 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         125.7577931 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```


8.537
8.533
8.501
8.497
7.925
7.912
7.904
7.891
7.478
7.472
7.457
7.451
7.245
7.240
7.223
7.218
7.201
7.196
I
F
O
NO2
2t
10
9
8
7
6
5
4
3
2
1
ppm
0.07
1.00
1.03
1.07
1.03
1.15
NAME 20120330
EXPNO 38
PROCNO 1
Date_ 20120330
Time 15.23
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 456.1
DW 60.400 usec
DE 6.50 usec
TE 297.8 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 400.1300090 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

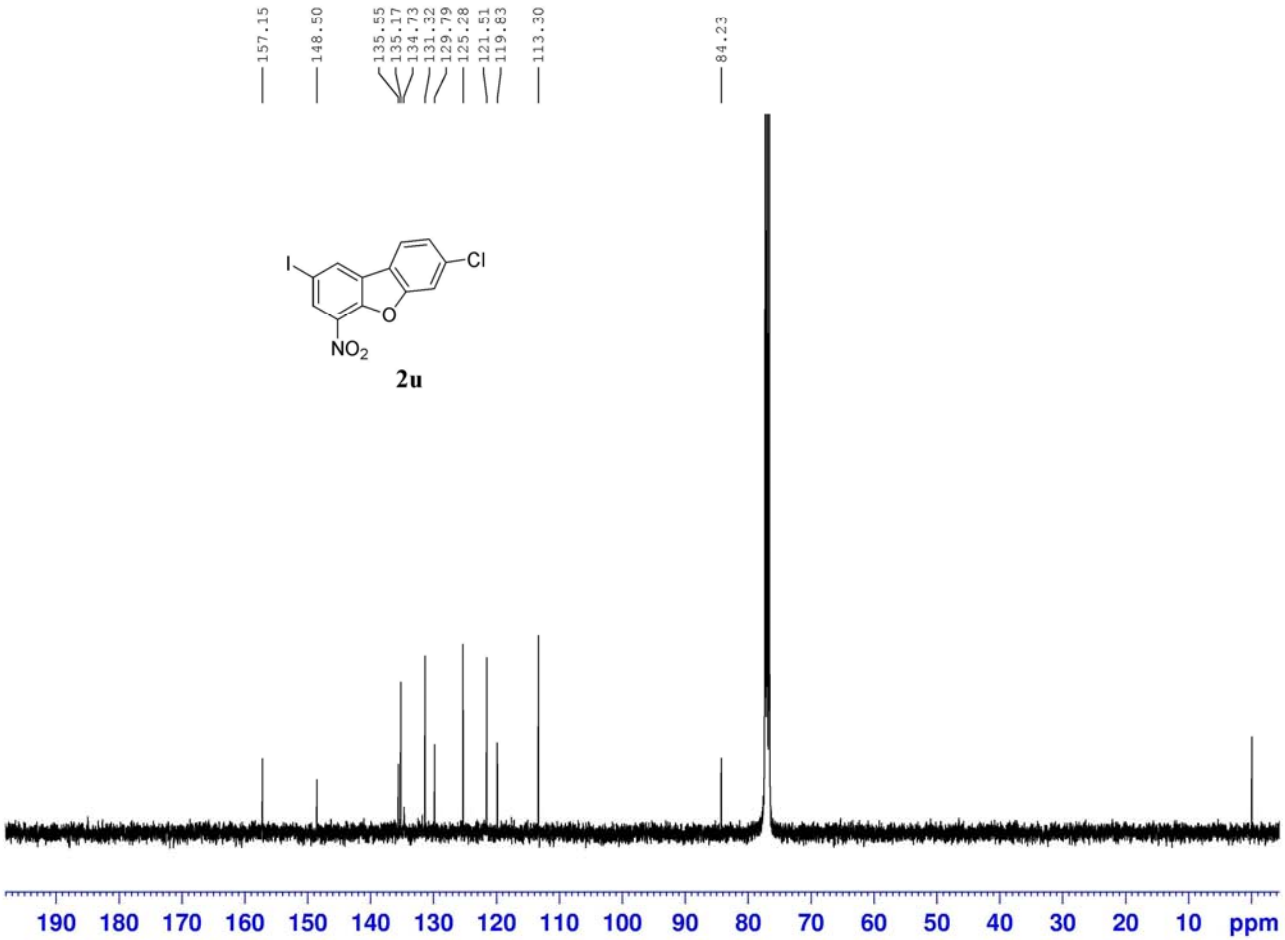
45203-4C



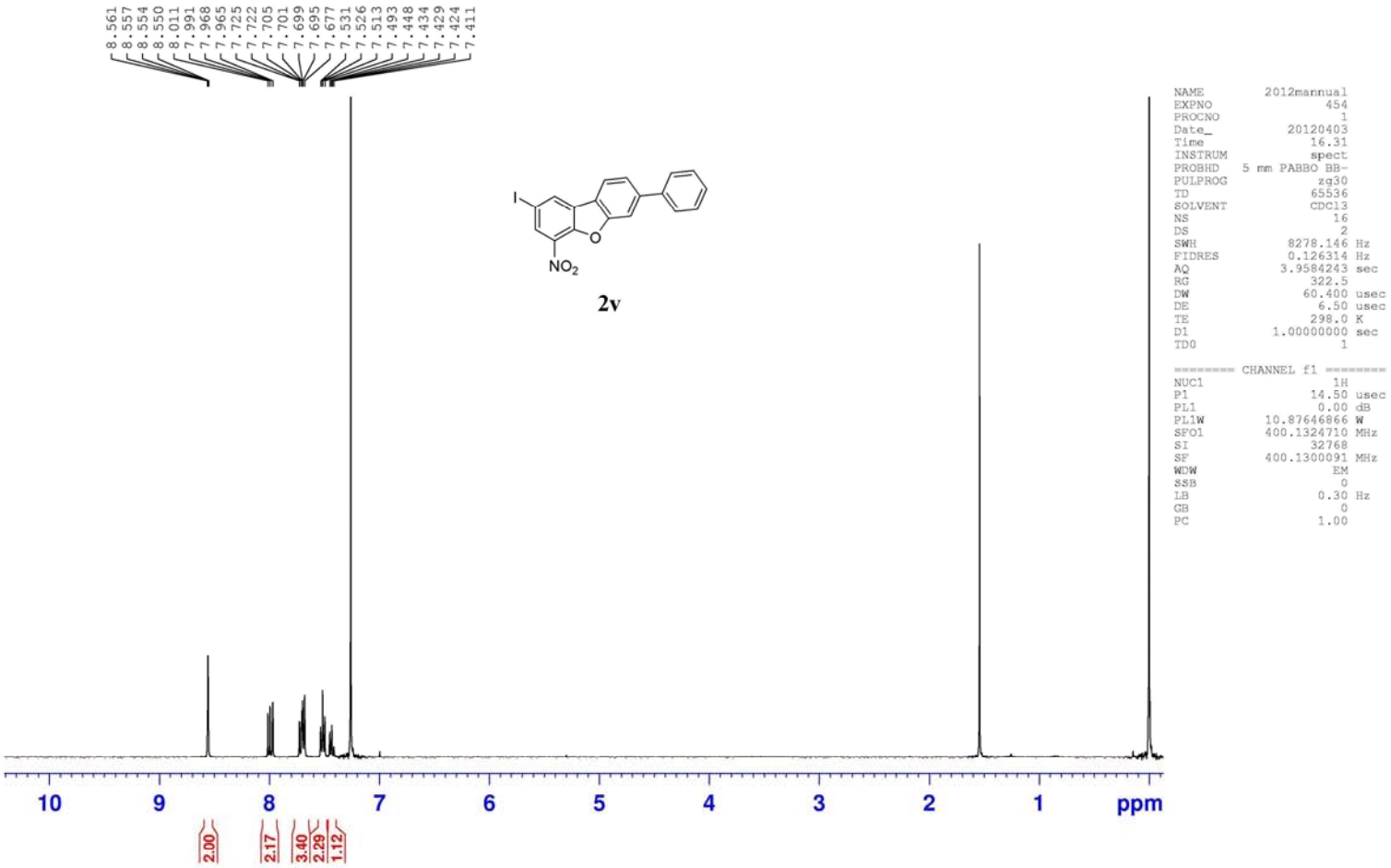

```
NAME            45203-4c
EXPNO                  1
PROCNO                 1
Date_           20120331
Time                1.14
INSTRUM            Spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           29761.904 Hz
FIDRES         0.454131 Hz
AQ            1.1010548 sec
RG                  203
DW               16.800 usec
DE                6.50 usec
TE                297.4 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          125.7577931 MHz
WDW                  EM
SSB                   0
LB                 1.00 Hz
GB                    0
PC                 1.40
```


8.564
8.560
8.517
8.513
7.883
7.863
7.766
7.762
7.469
7.465
7.448
7.444
I
Cl
O
NO2
2u
10
9
8
7
6
5
4
3
2
1
ppm
1.00
1.01
1.11
1.02
1.10
NAME 2012mannual
EXPNO 456
PROCNO 1
Date_ 20120403
Time 22.14
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 512
DW 60.400 usec
DE 6.50 usec
TE 298.1 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 400.1304155 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

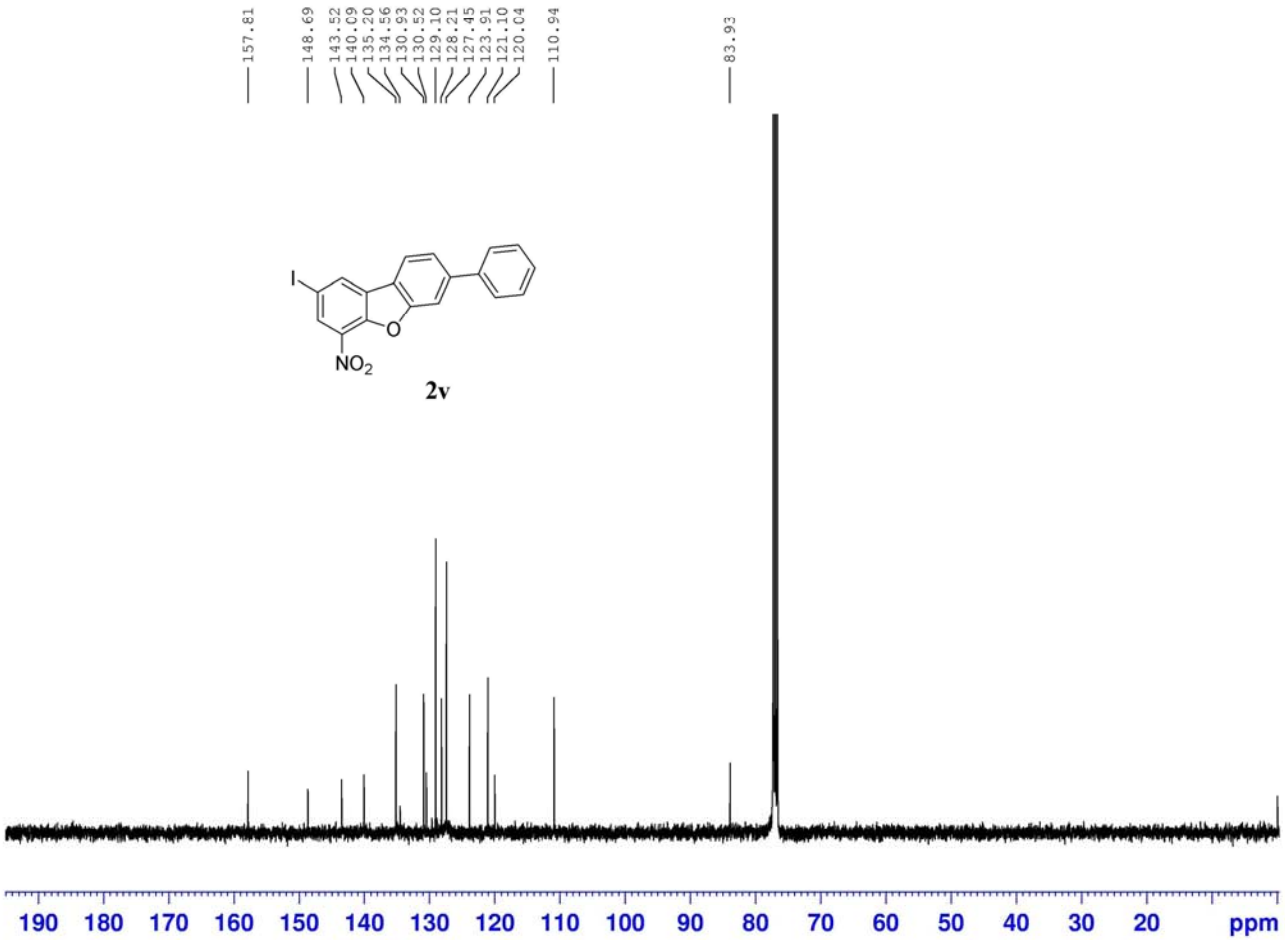
45211-2C




```
NAME          2012mannual
EXPNO                 459
PROCNO                  1
Date_            20120404
Time                 0.10
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   6144
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                   309.1 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           100.6127609 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
```

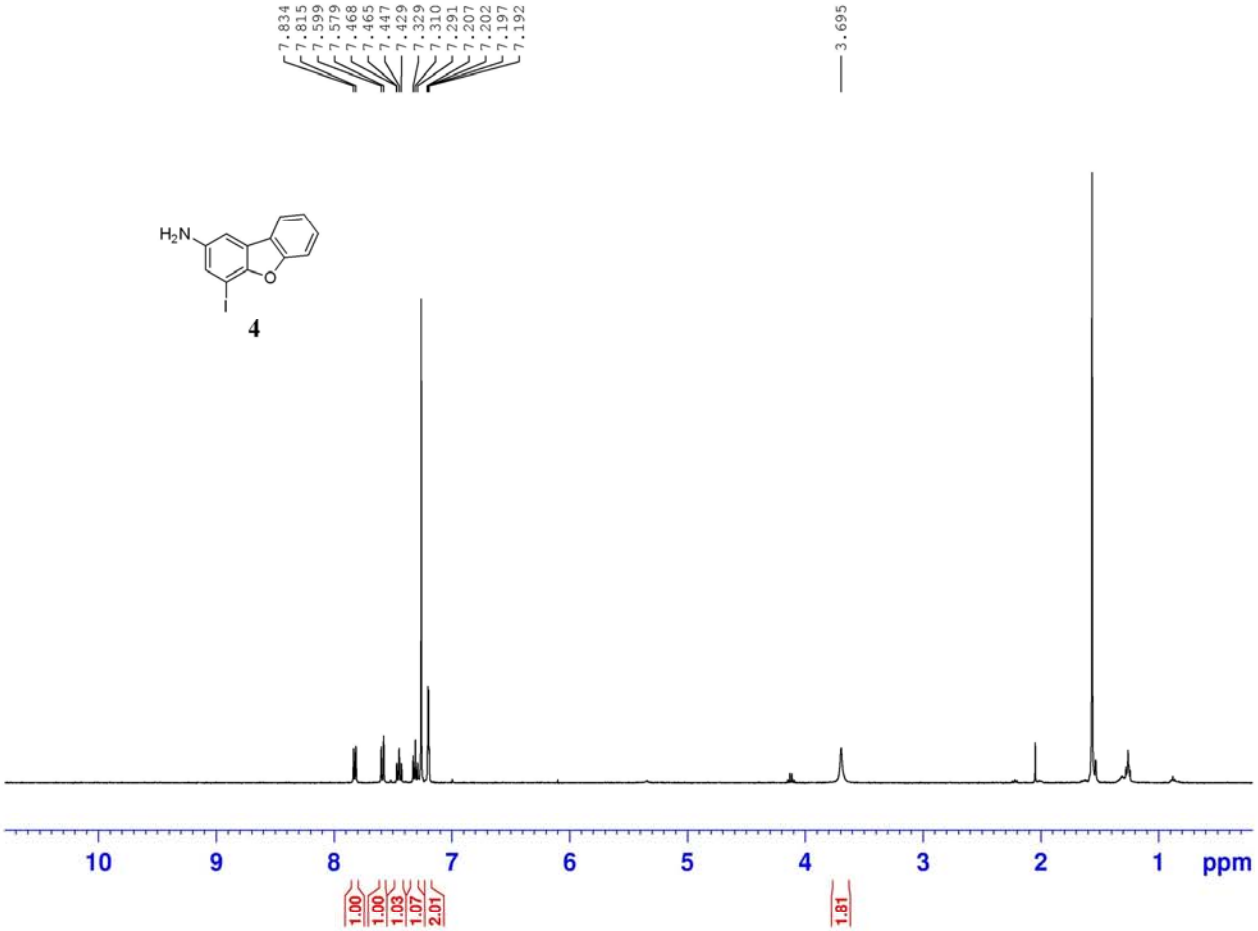

8.561
8.557
8.554
8.550
8.011
7.991
7.968
7.965
7.725
7.722
7.705
7.701
7.699
7.695
7.677
7.531
7.526
7.513
7.493
7.448
7.434
7.429
7.424
7.411
I
O
NO2
2v
10
9
8
7
6
5
4
3
2
1
ppm
2.00
2.17
3.40
2.29
1.12
NAME 2012mannual
EXPNO 454
PROCNO 1
Date_ 20120403
Time 16.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
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 298.0 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 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

45219-c



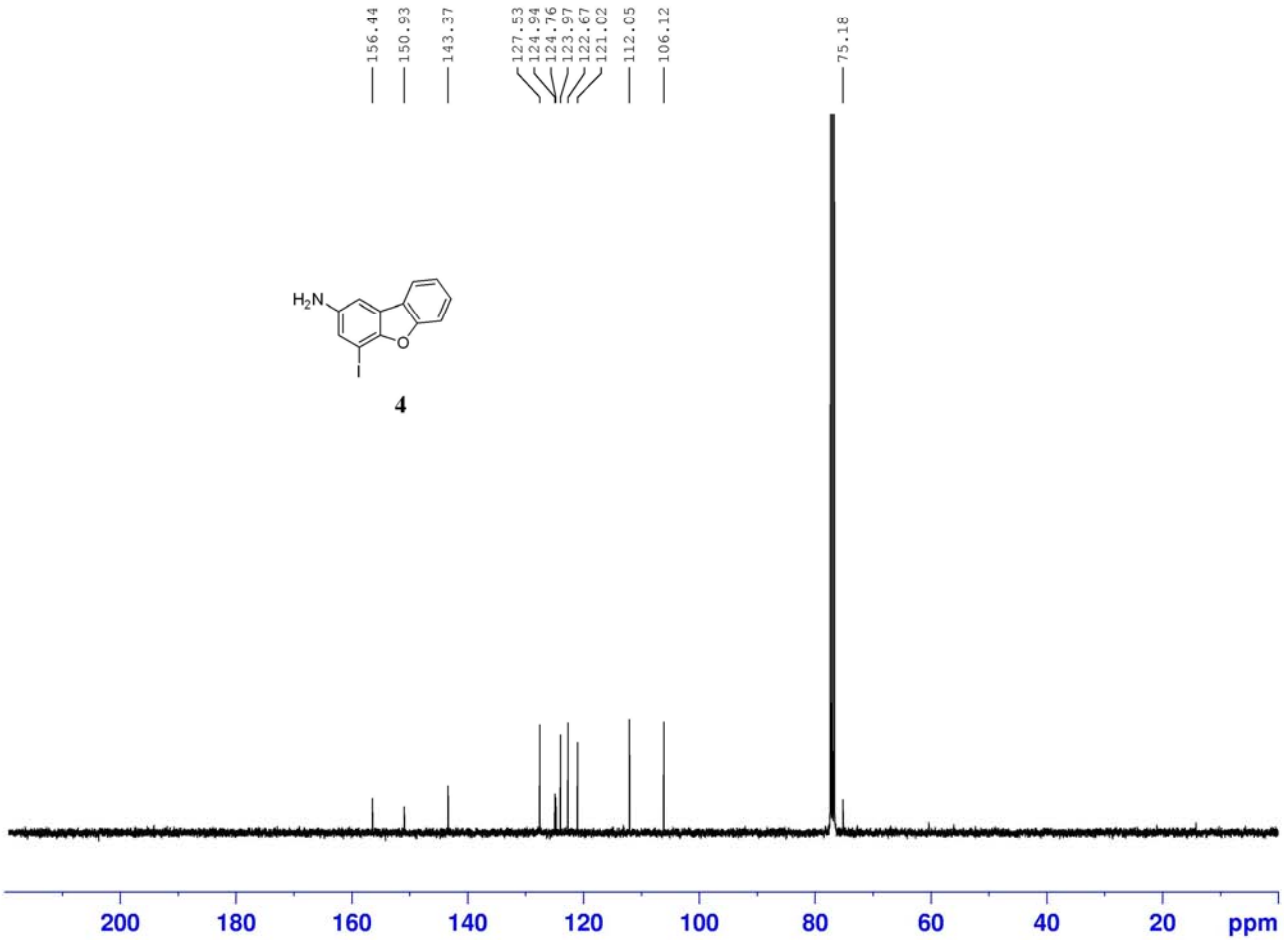

```
NAME          2012mannual
EXPNO                 455
PROCNO                  1
Date_            20120403
Time                19.24
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     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                  305.8 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         100.6128730 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```

153961



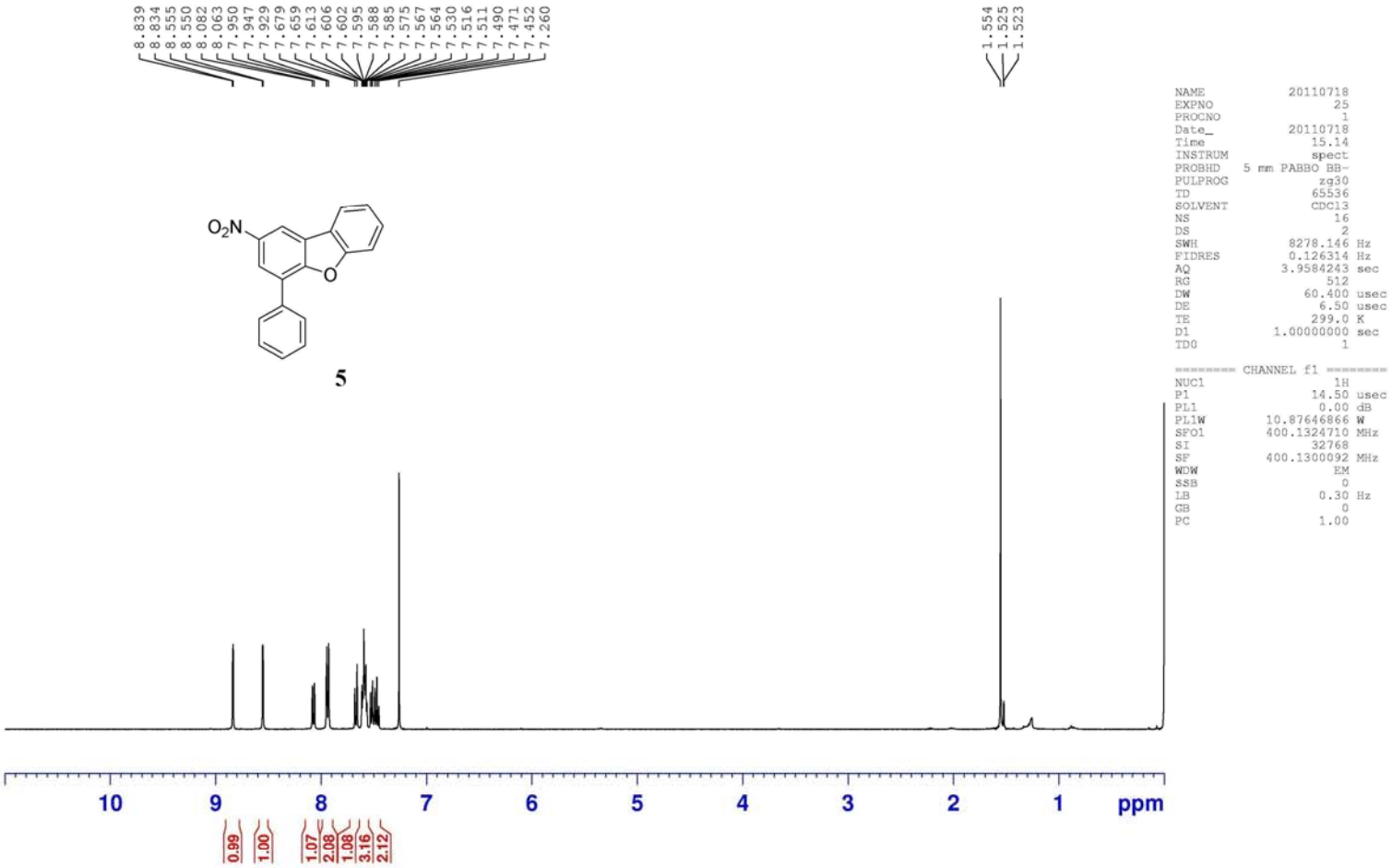
NAME	2012mannual
EXPNO	432
PROCNO	1
Date_	20120211
Time	17.27
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	512
DW	60.400 usec
DE	6.50 usec
TE	294.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.00 dB
PL1W	10.87646866 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300090 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

153961-C



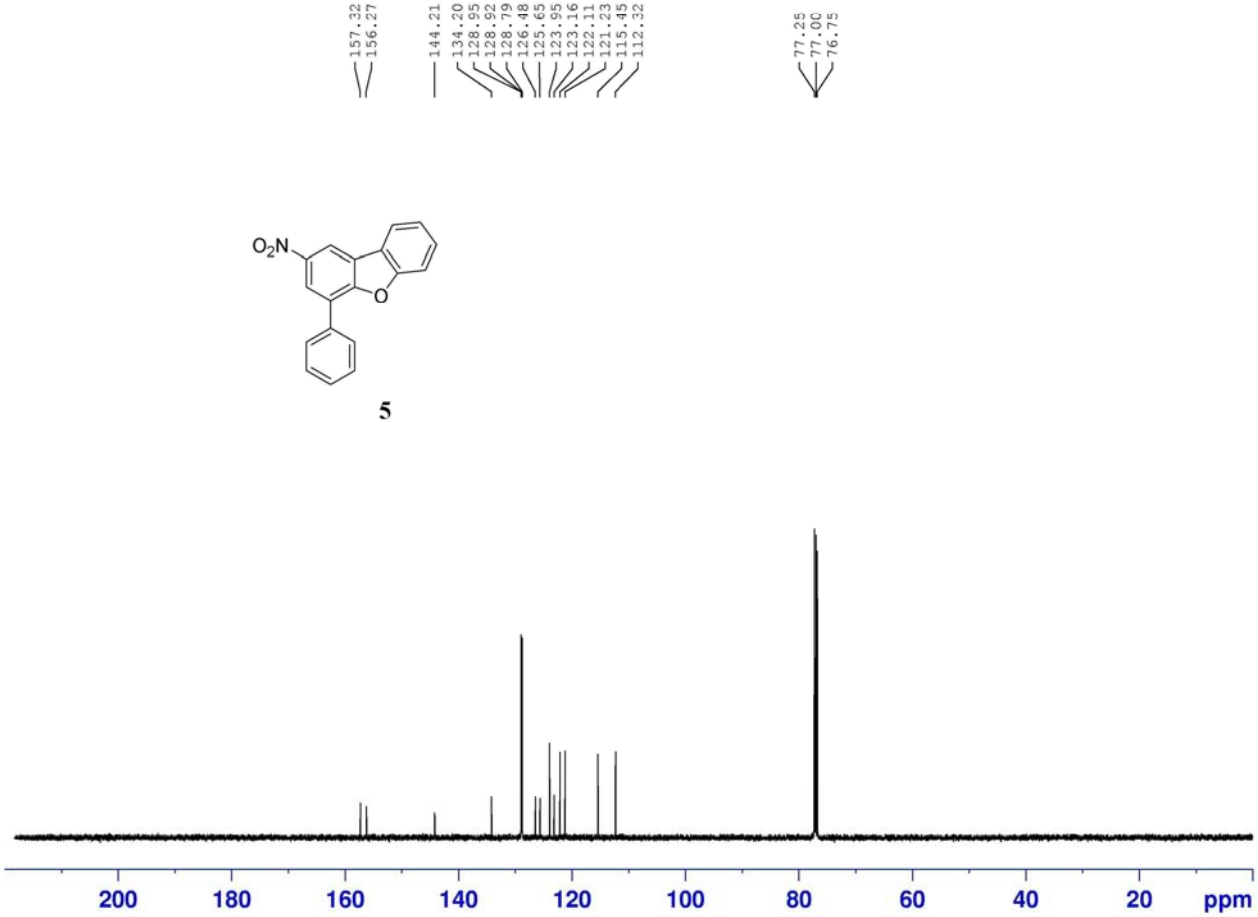

```
NAME          2012mannual
EXPNO                 433
PROCNO                  1
Date_            20120211
Time               21.05
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH            23980.814 Hz
FIDRES          0.365918 Hz
AQ             1.3664756 sec
RG                2298.8
DW                20.850 usec
DE                  6.50 usec
TE                 299.4 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         100.6127653 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```

181940



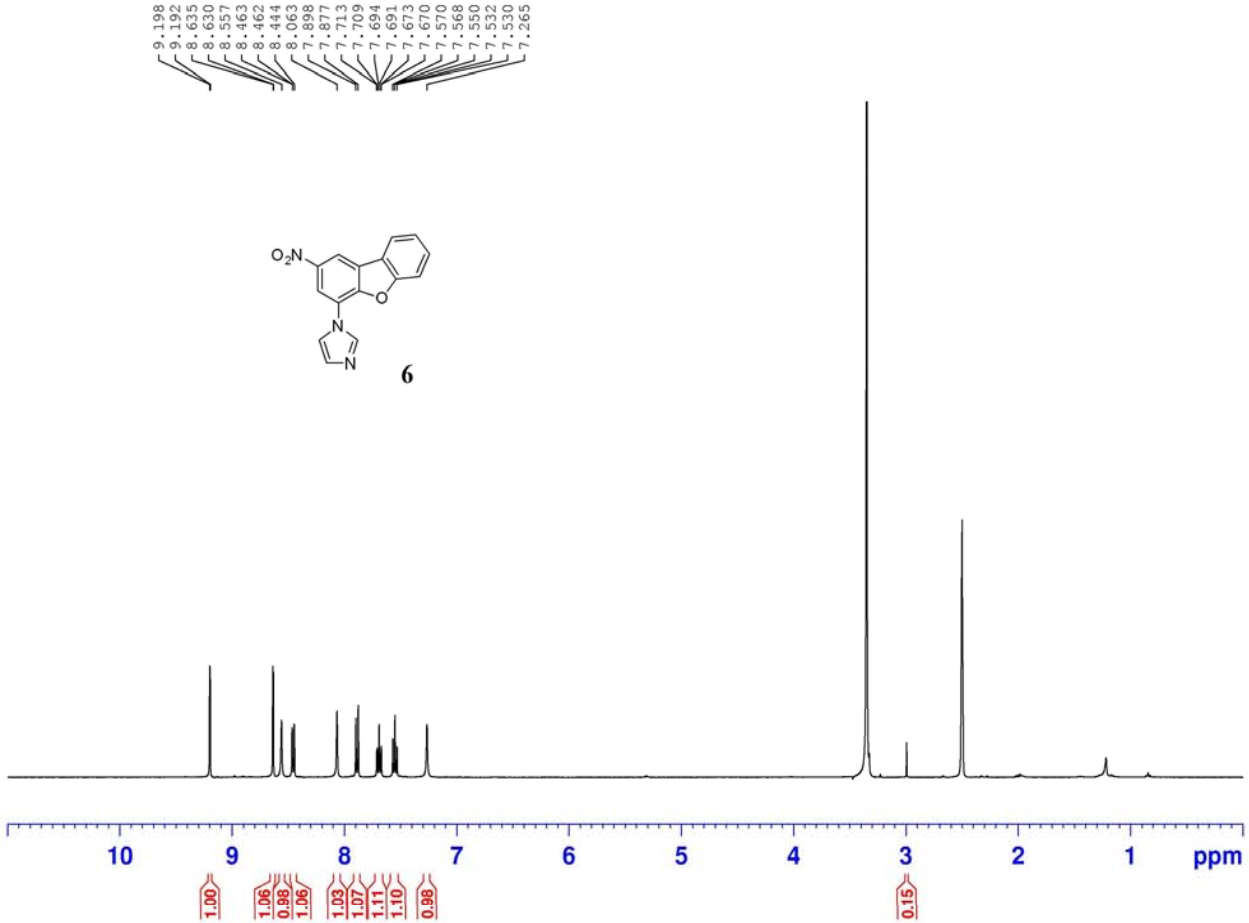
NAME	20110718
EXPNO	25
PROCNO	1
Date_	20110718
Time	15.14
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	512
DW	60.400 usec
DE	6.50 usec
TE	299.0 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
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

181940-C



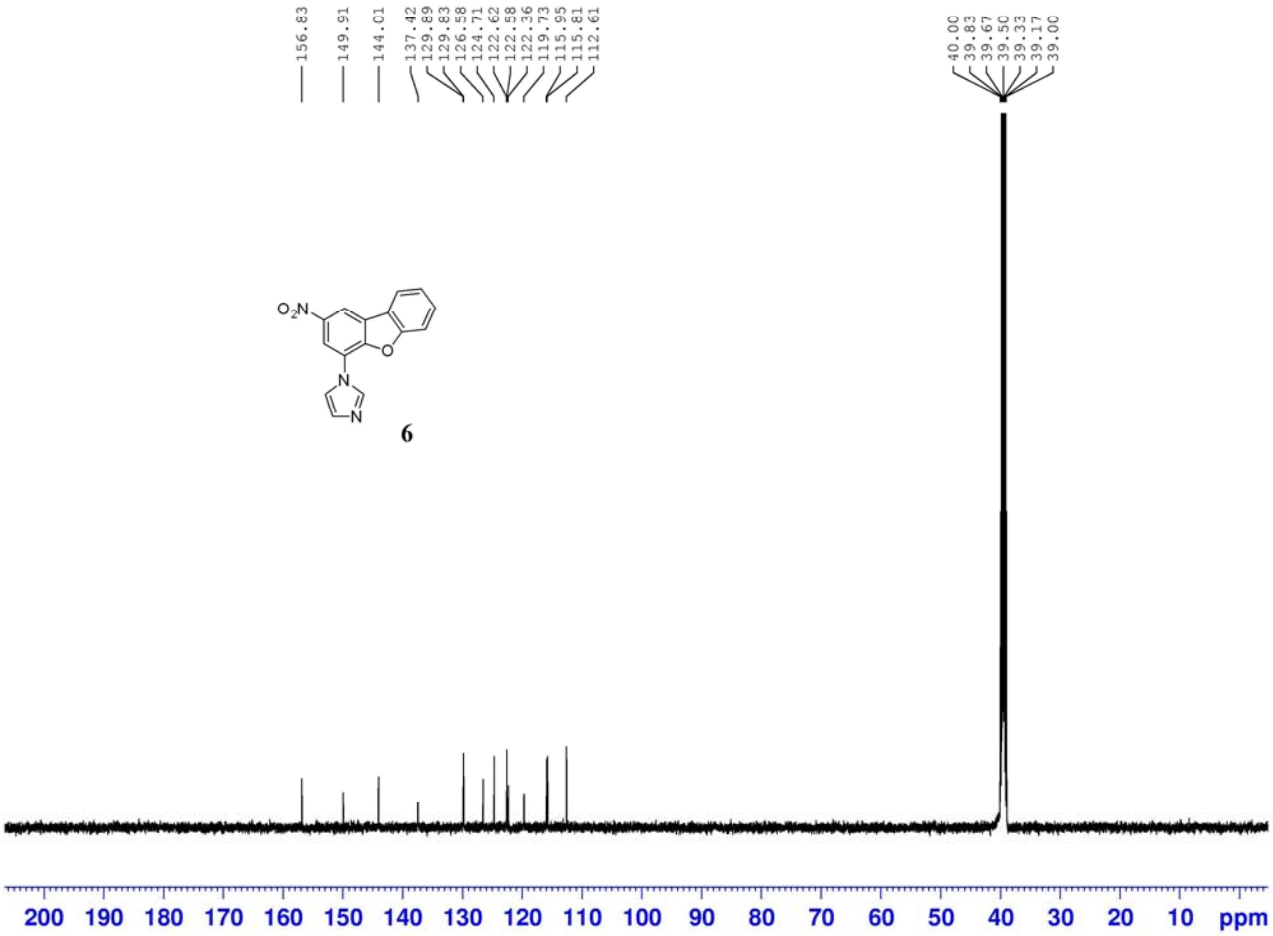

```
NAME            181940-c
EXPNO                  1
PROCNO                 1
Date_           20110803
Time               15.02
INSTRUM            Spect
PROBHD   5 mm PABBO BB-
PULPROG            zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   167
DS                     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         125.7577965 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```

153941-A




```
NAME            20120110
EXPNO                15
PROCNO                1
Date_           20120110
Time               10.45
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                 161.3
DW                60.400 usec
DE                 6.50 usec
TE                 297.1 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          400.1300024 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

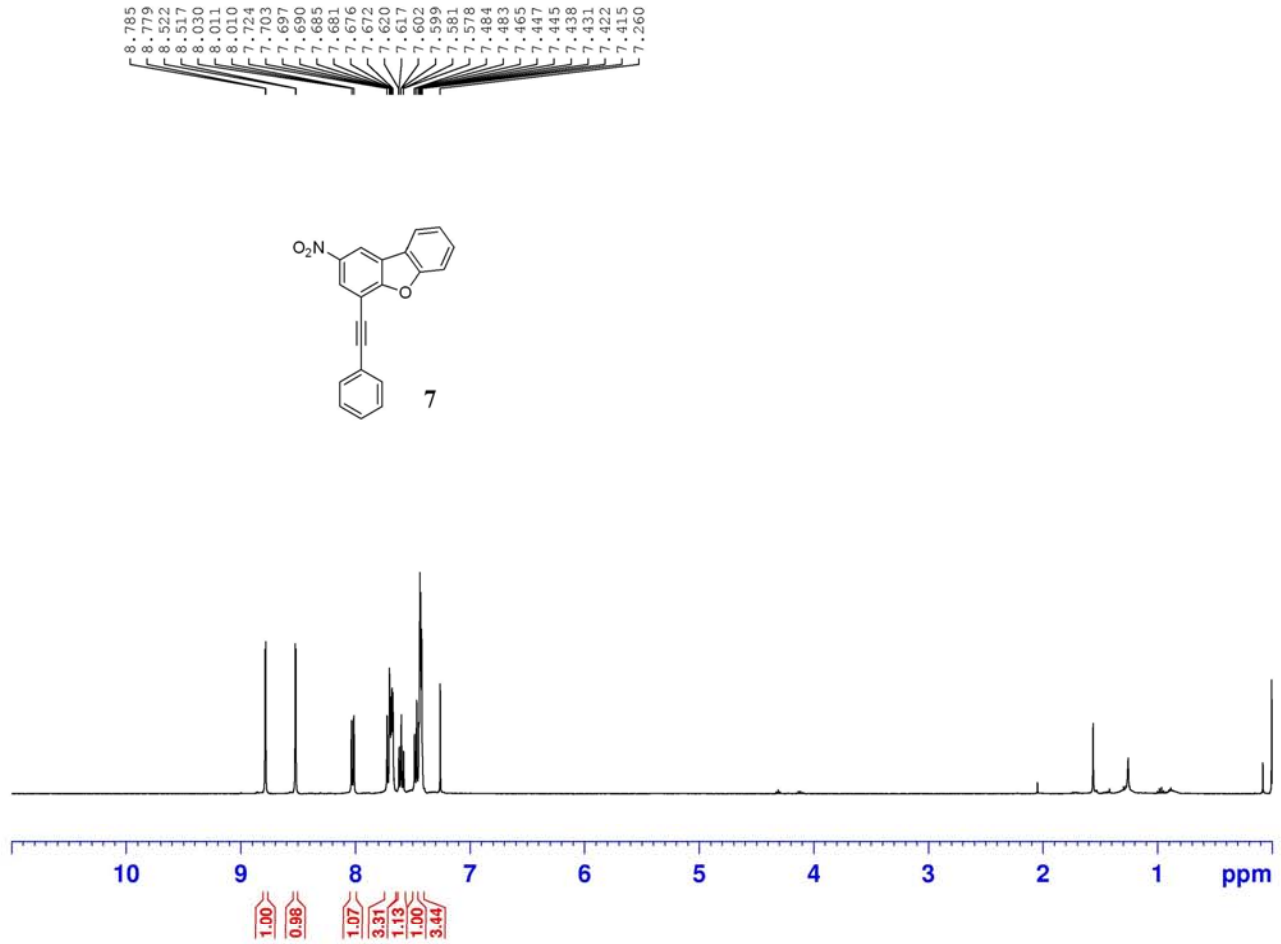
153941



6

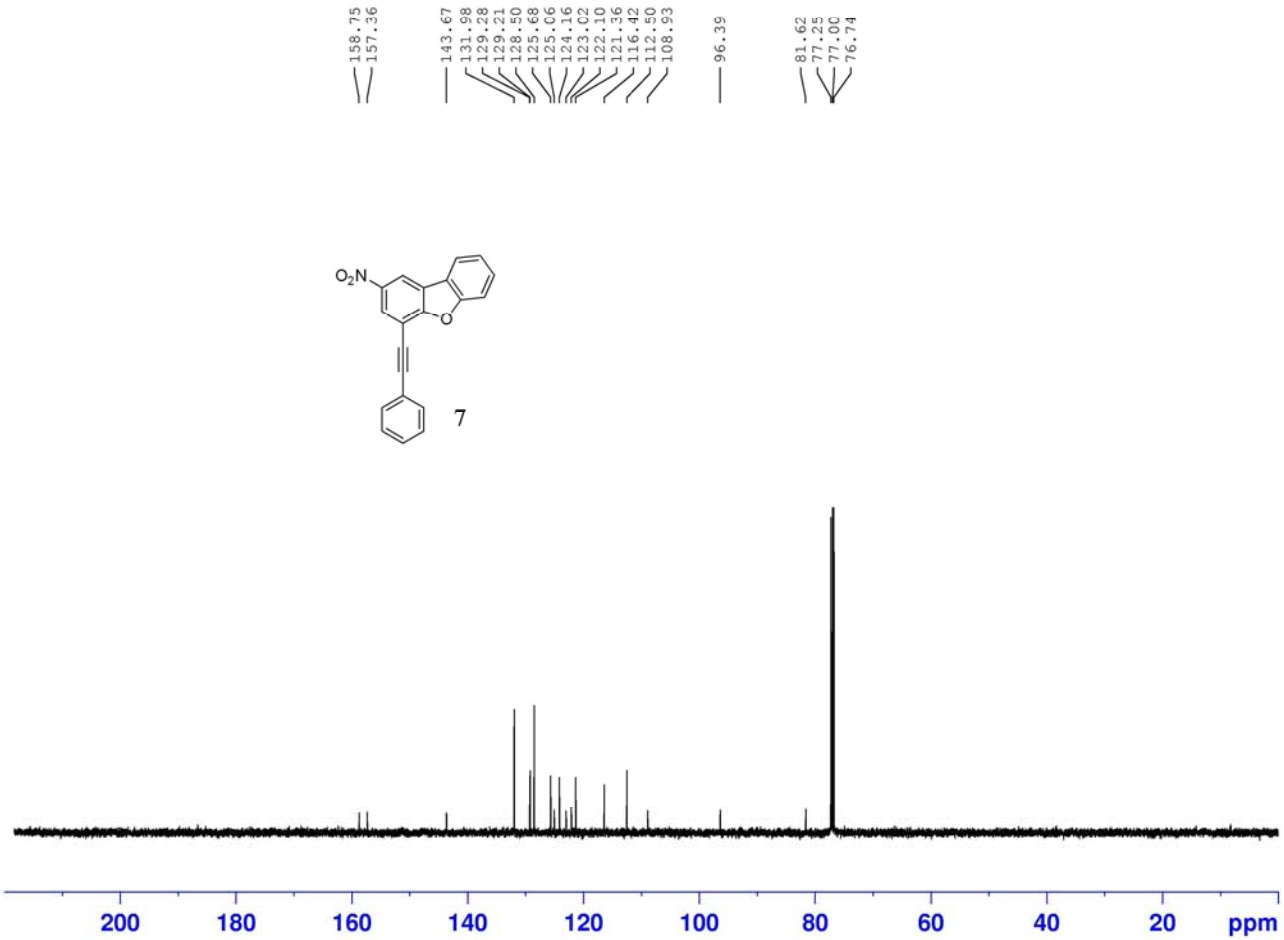
NAME	153941
EXPNO	1
PROCNO	1
Date_	20120111
Time	20.53
INSTRUM	Spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	958
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	297.1 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
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	125.7578379 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

wy111221-1

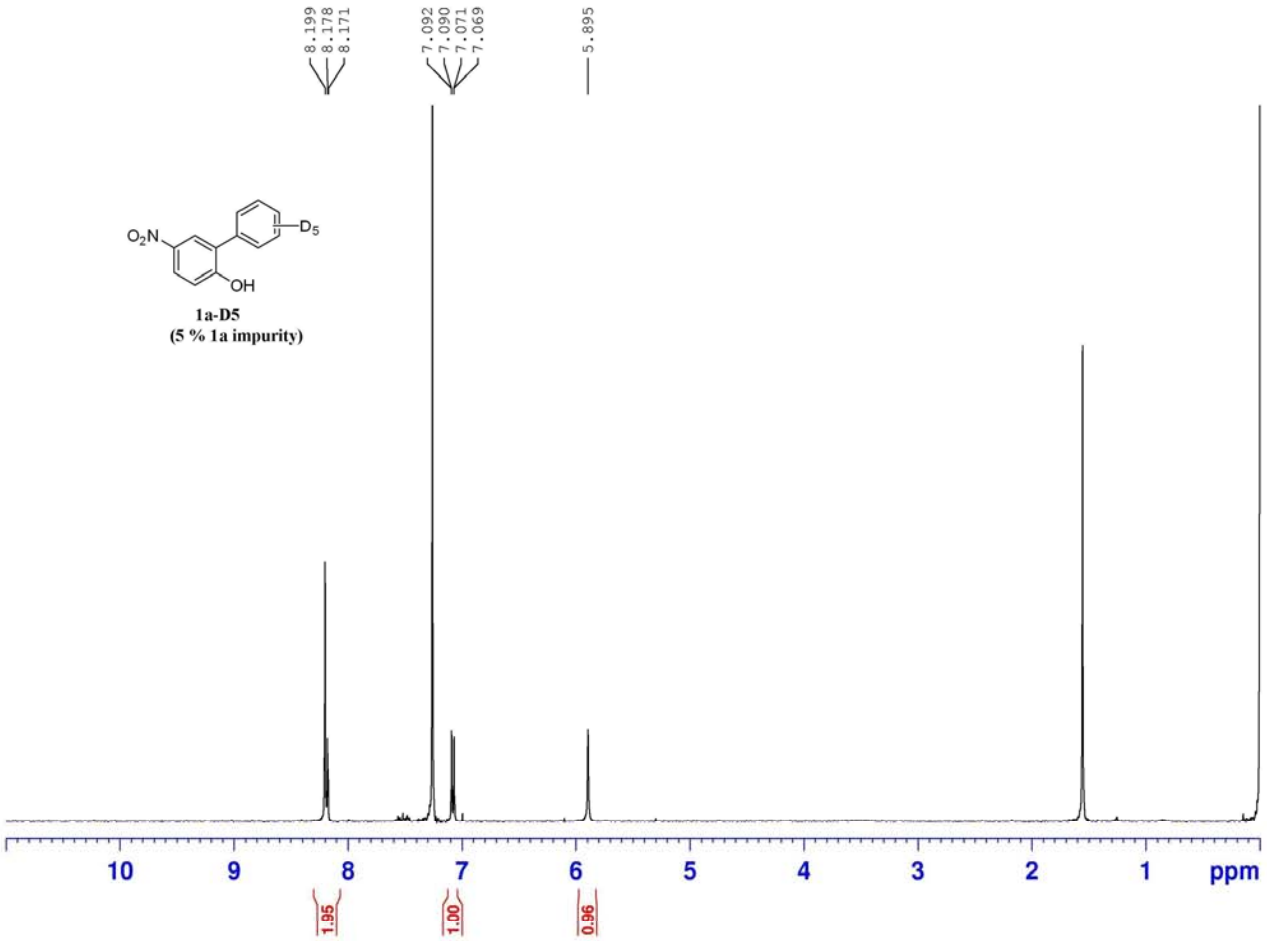


NAME	20111223
EXPNO	25
PROCNO	1
Date_	20111223
Time	11.34
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	256
DW	60.400 usec
DE	6.50 usec
TE	297.7 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.00 dB
PL1W	10.87646866 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300093 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

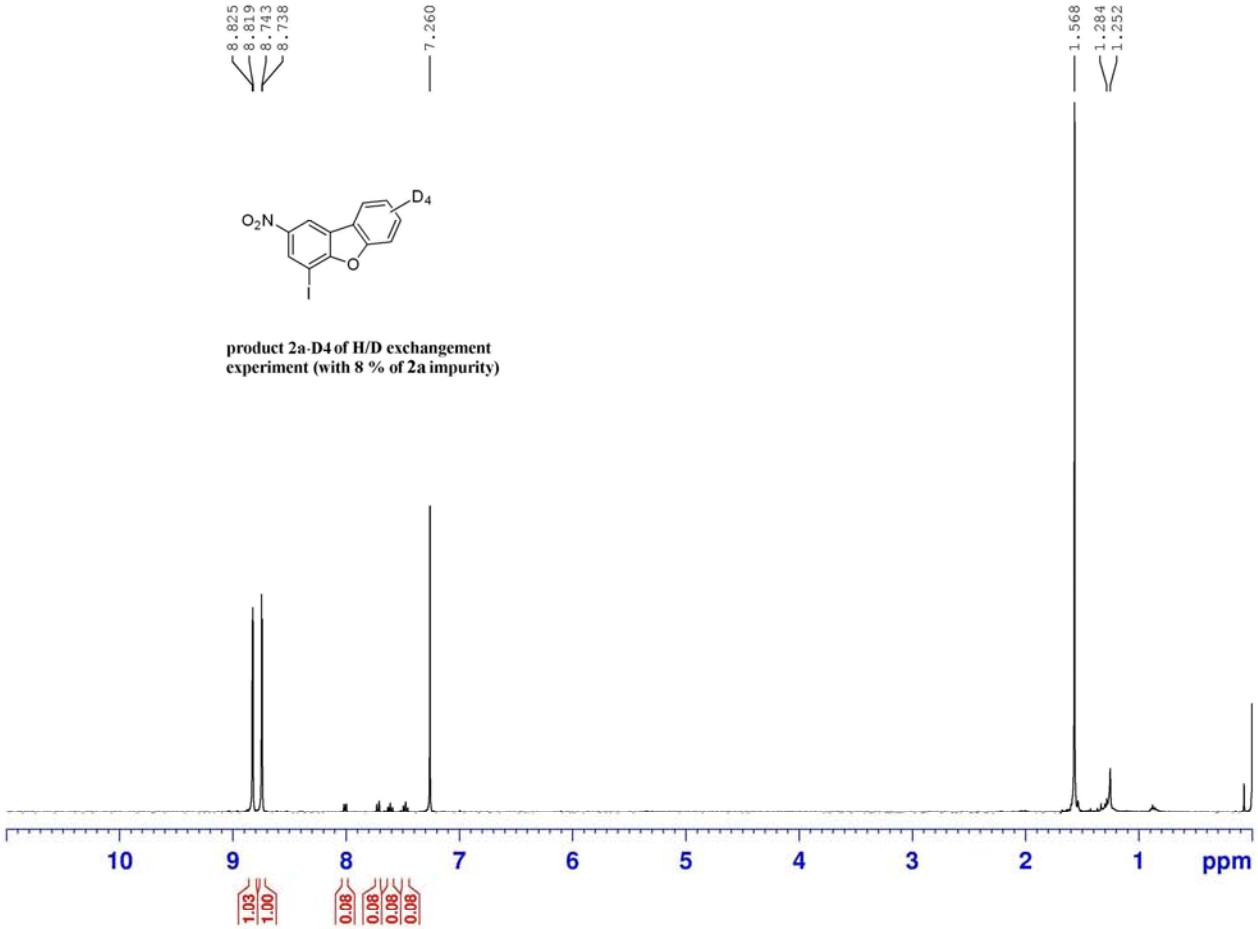
wy111221-1




```
NAME            111221-1
EXPNO                  1
PROCNO                 1
Date_           20111226
Time              21.48
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                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         125.7577954 MHz
WDW                 EM
SSB                  0
LB                1.00 Hz
GB                   0
PC                1.40
```

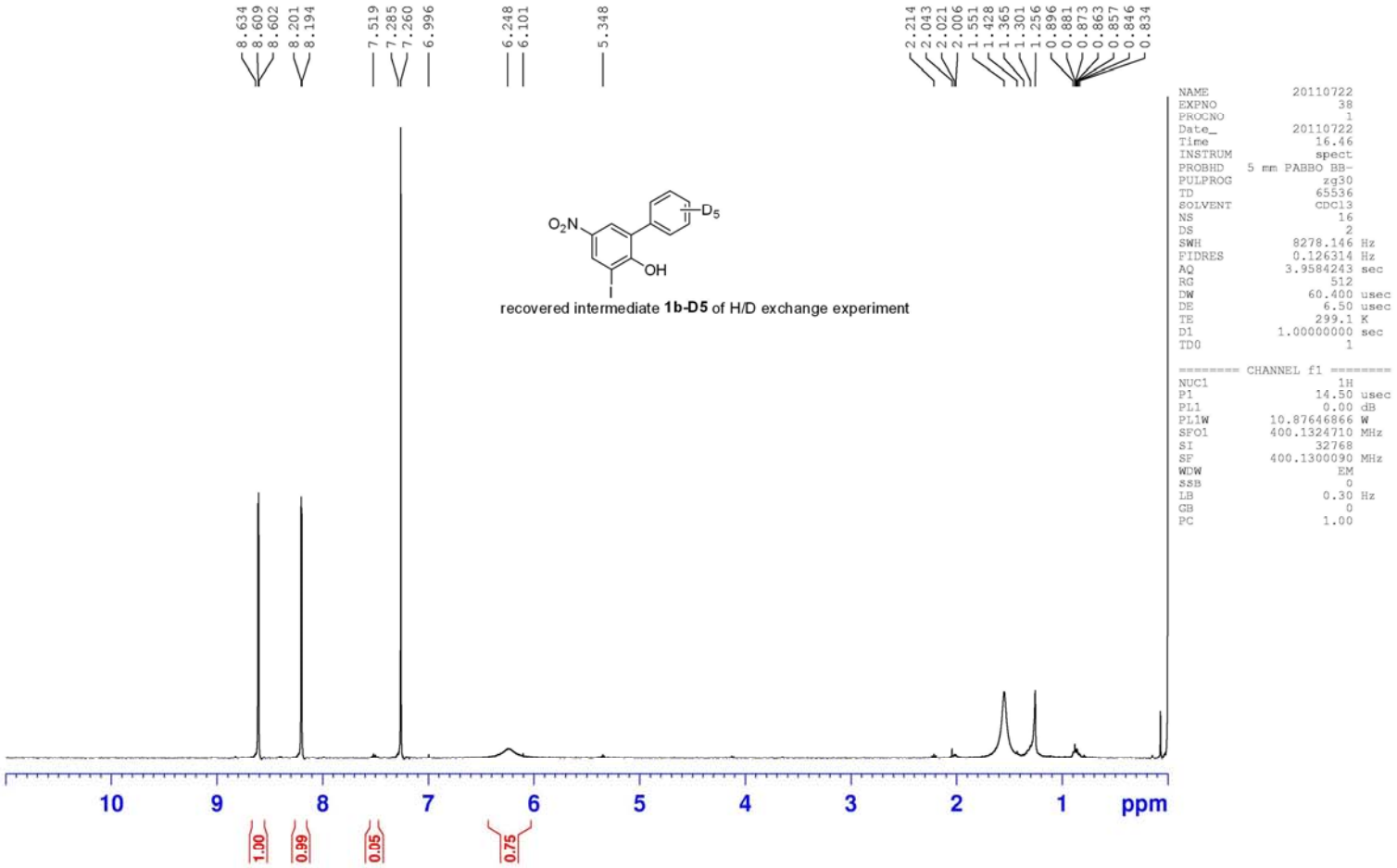



```
NAME            20120420
EXPNO                30
PROCNO                1
Date_           20120420
Time               15.23
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ             3.9584243 sec
RG                   512
DW                60.400 usec
DE                 6.50 usec
TE                673.2 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          400.1300090 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

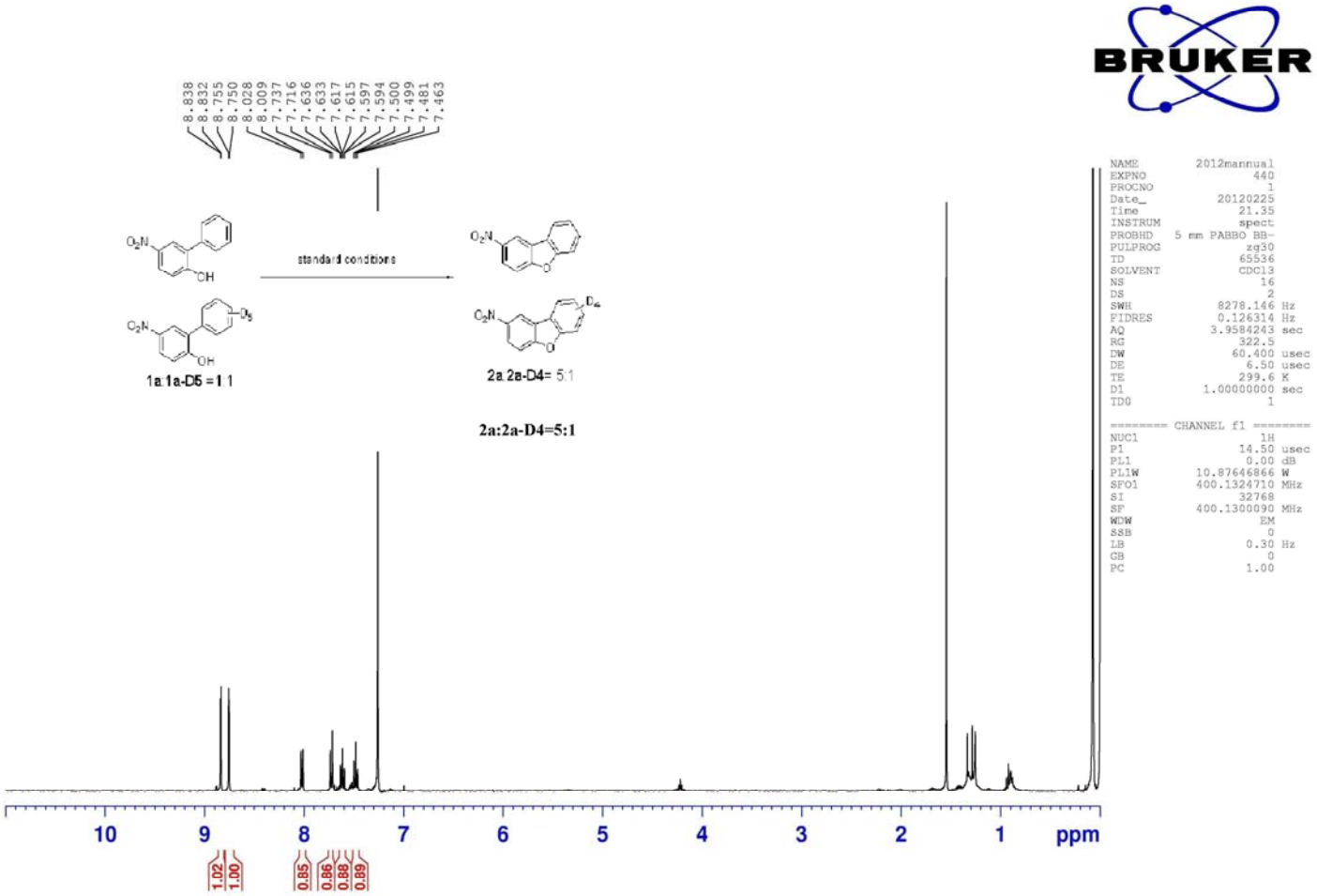


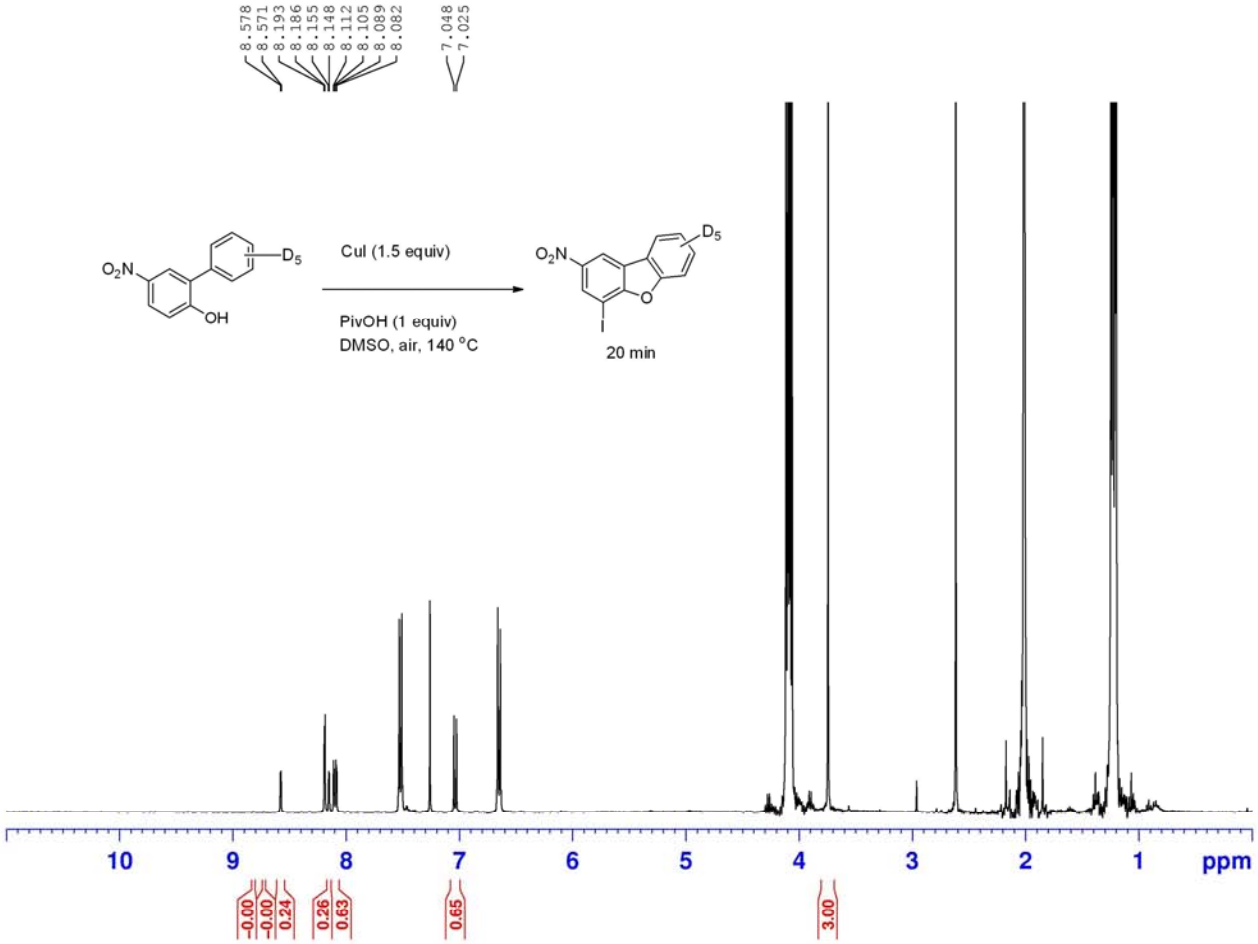
product 2a-D4 of H/D exchangement experiment (with 8 % of 2a impurity)

NAME	20110722
EXPNO	6
PROCNO	1
Date_	20110722
Time	10.47
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	512
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	400.1300091 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

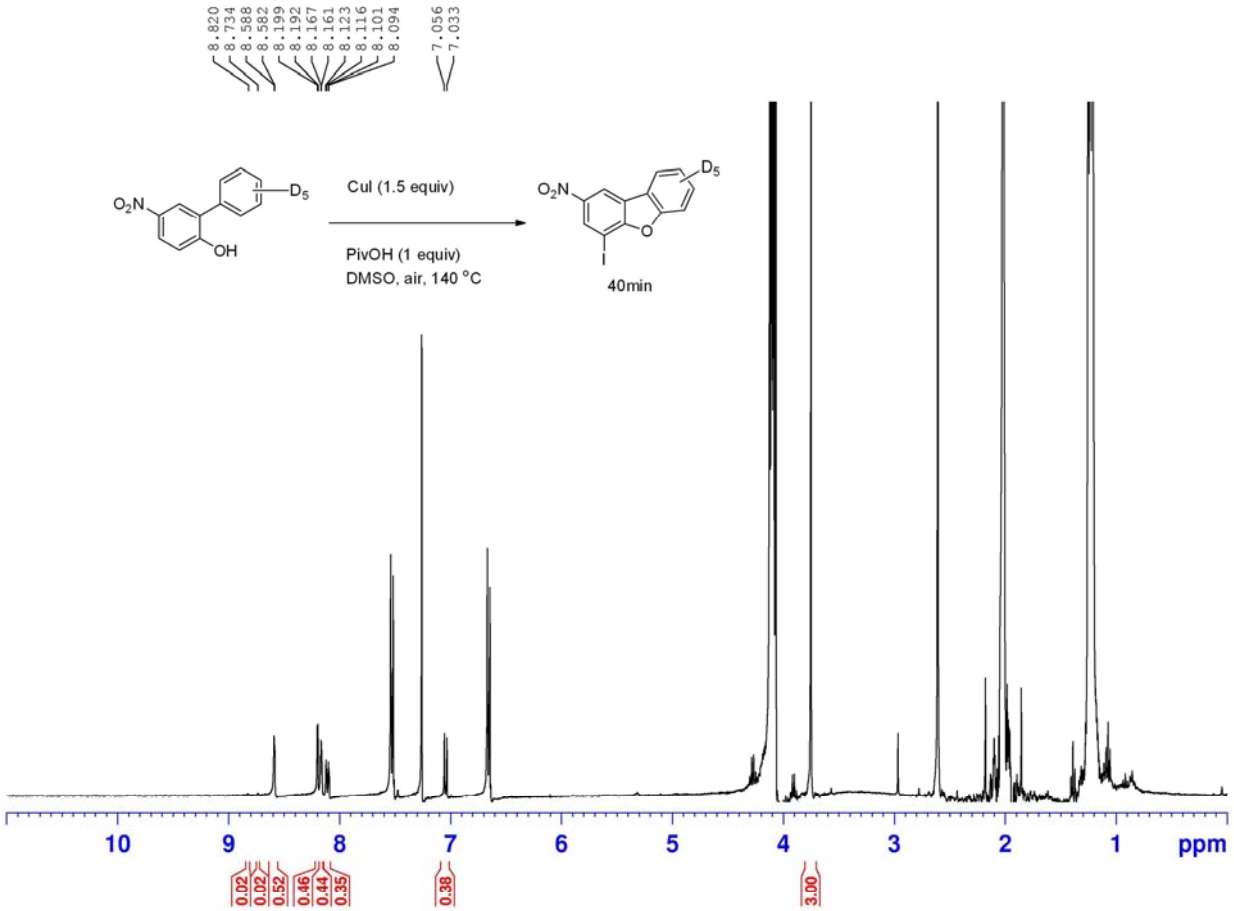



```
NAME            20110722
EXPNO                38
PROCNO                1
Date_           20110722
Time              16.46
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8278.146 Hz
FIDRES         0.126314 Hz
AQ           3.9584243 sec
RG                  512
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          400.1300090 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```

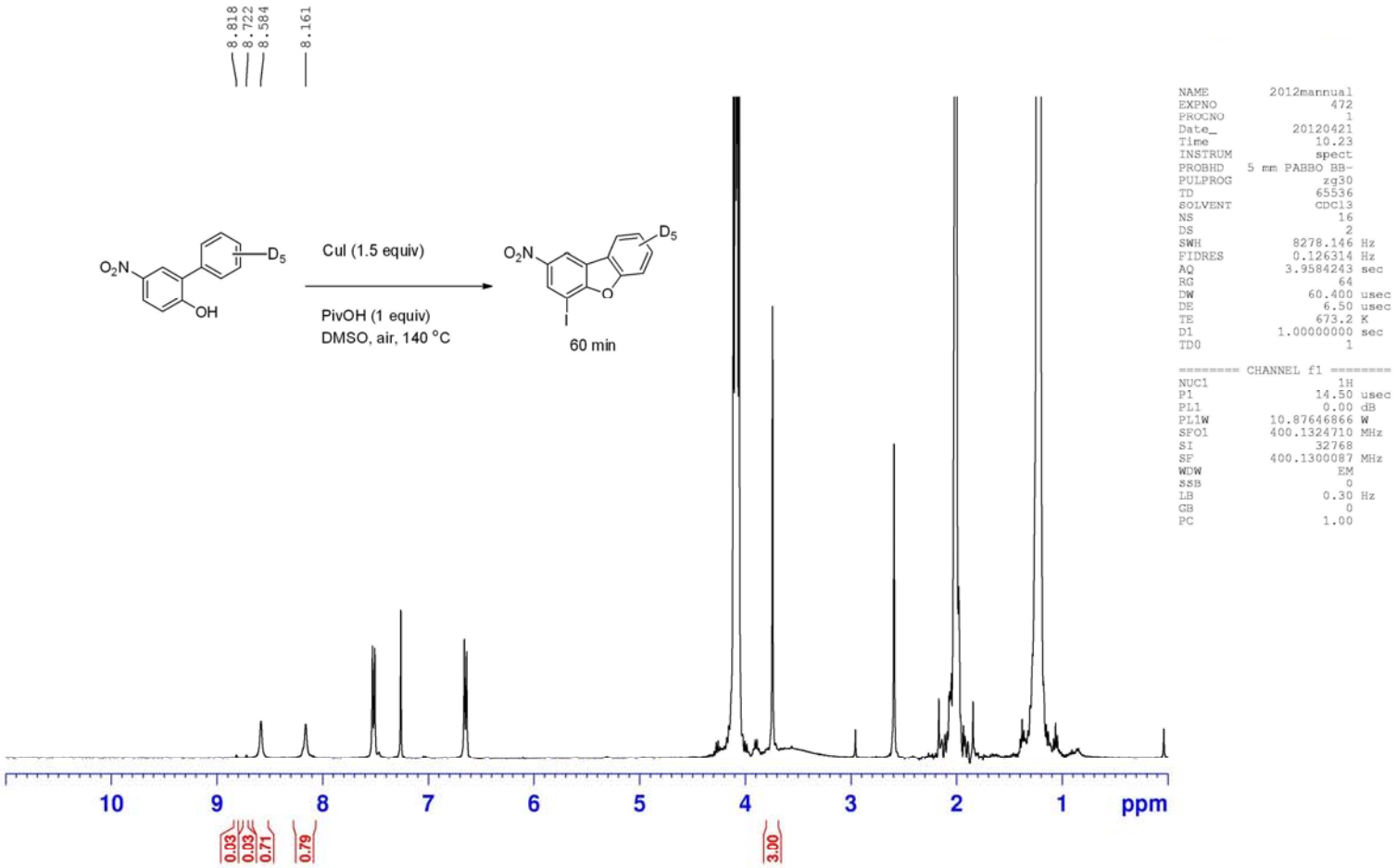

8.838
8.832
8.755
8.750
8.028
8.009
7.737
7.716
7.636
7.633
7.617
7.615
7.597
7.594
7.500
7.499
7.481
7.463
standard conditions
1a:1a-D5 = 1:1
2a:2a-D4= 5:1
2a:2a-D4=5:1
10
9
8
7
6
5
4
3
2
1
ppm
1.02
1.00
0.85
0.86
0.86
0.89
NAME 2012mannual
EXPNO 440
PROCNO 1
Date_ 20120225
Time 21.35
INSTRUM spect
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 299.6 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



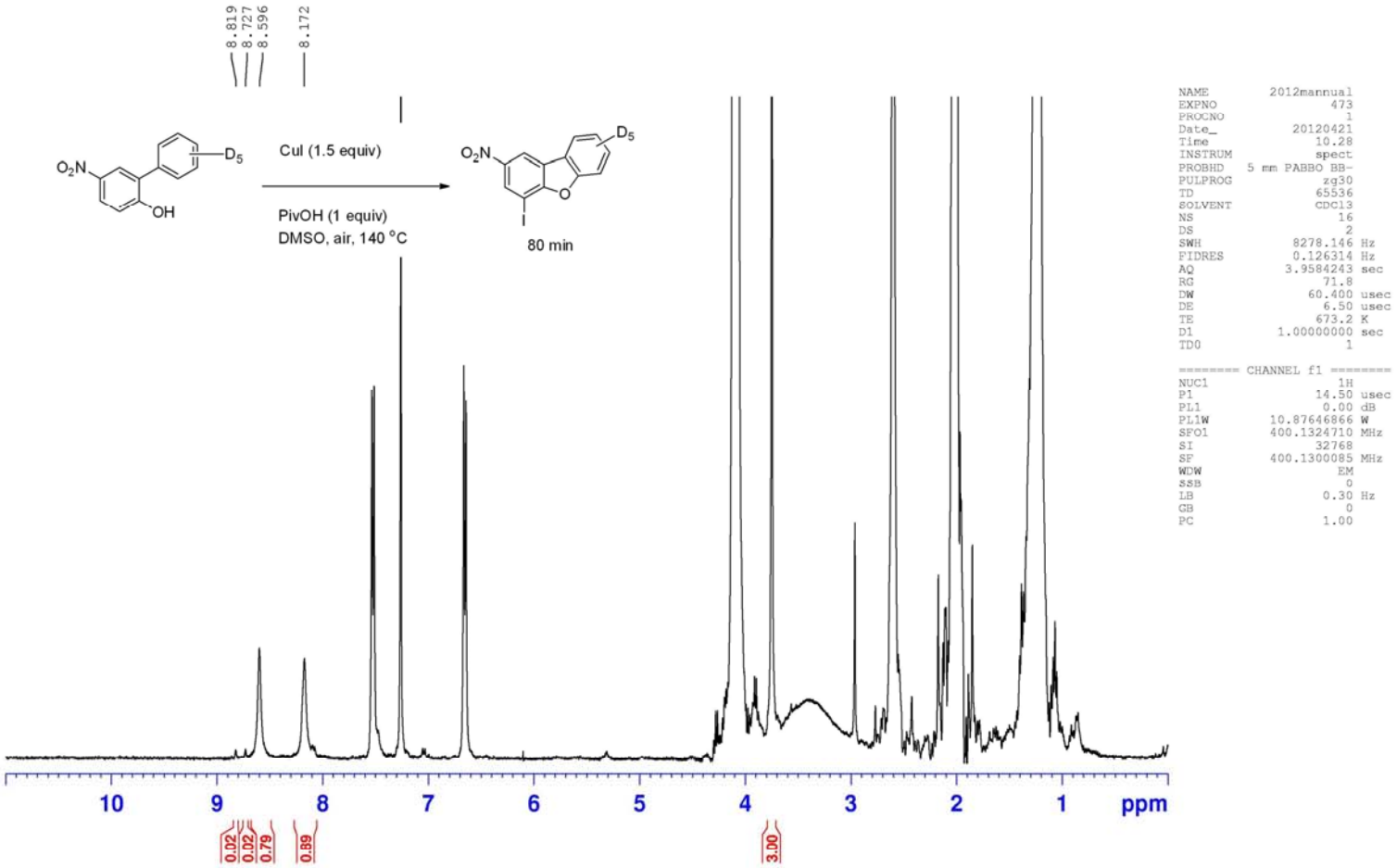

```
NAME          2012mannual
EXPNO                 470
PROCNO                  1
Date_            20120421
Time                10.13
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH               8278.146 Hz
FIDRES            0.126314 Hz
AQ               3.9584243 sec
RG                     64
DW                 60.400 usec
DE                  6.50 usec
TE                 673.2 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            400.1300088 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



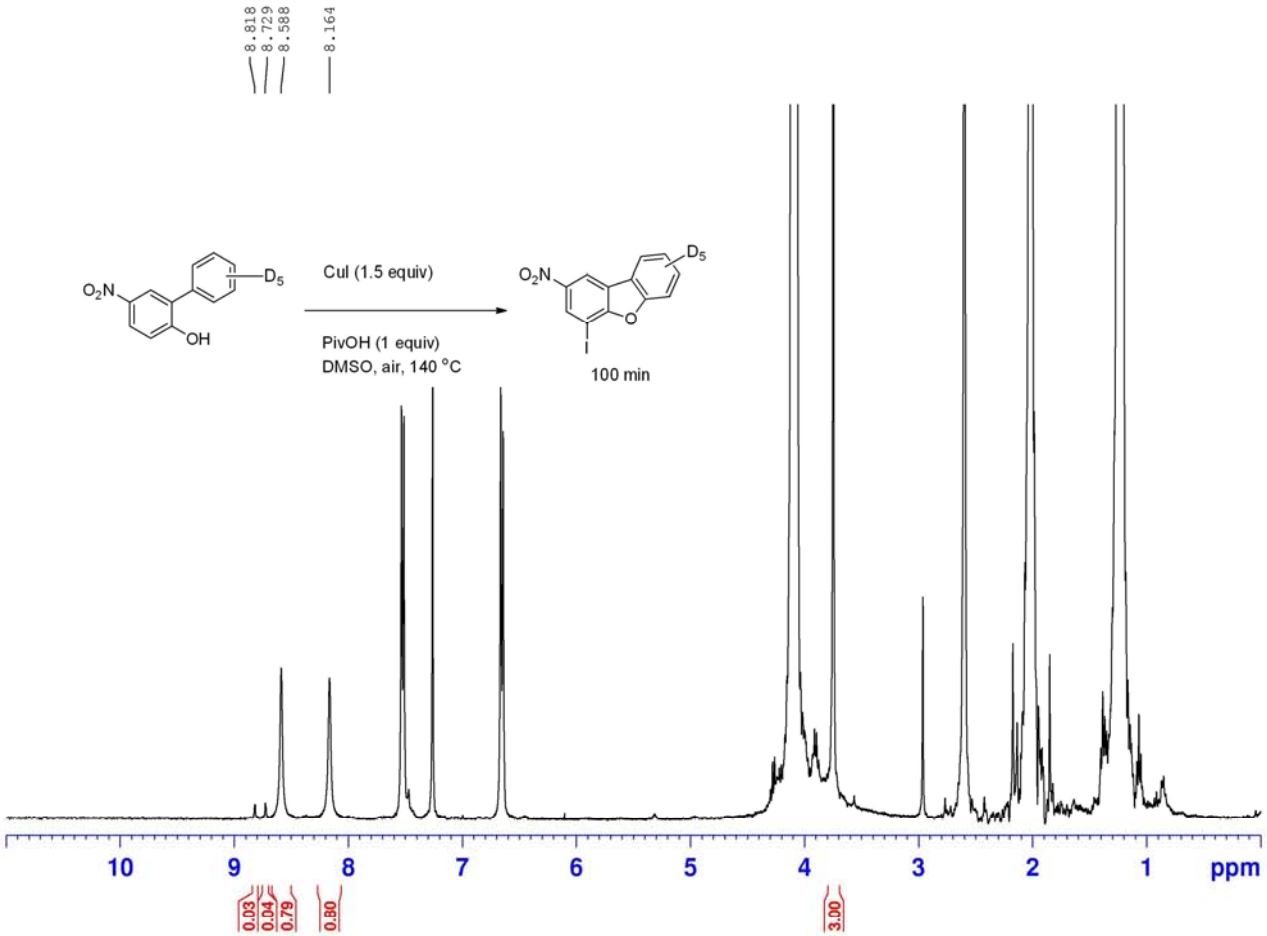

```
NAME          2012mannual
EXPNO                 471
PROCNO                  1
Date_            20120421
Time                10.18
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      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                673.2 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          400.1300090 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```



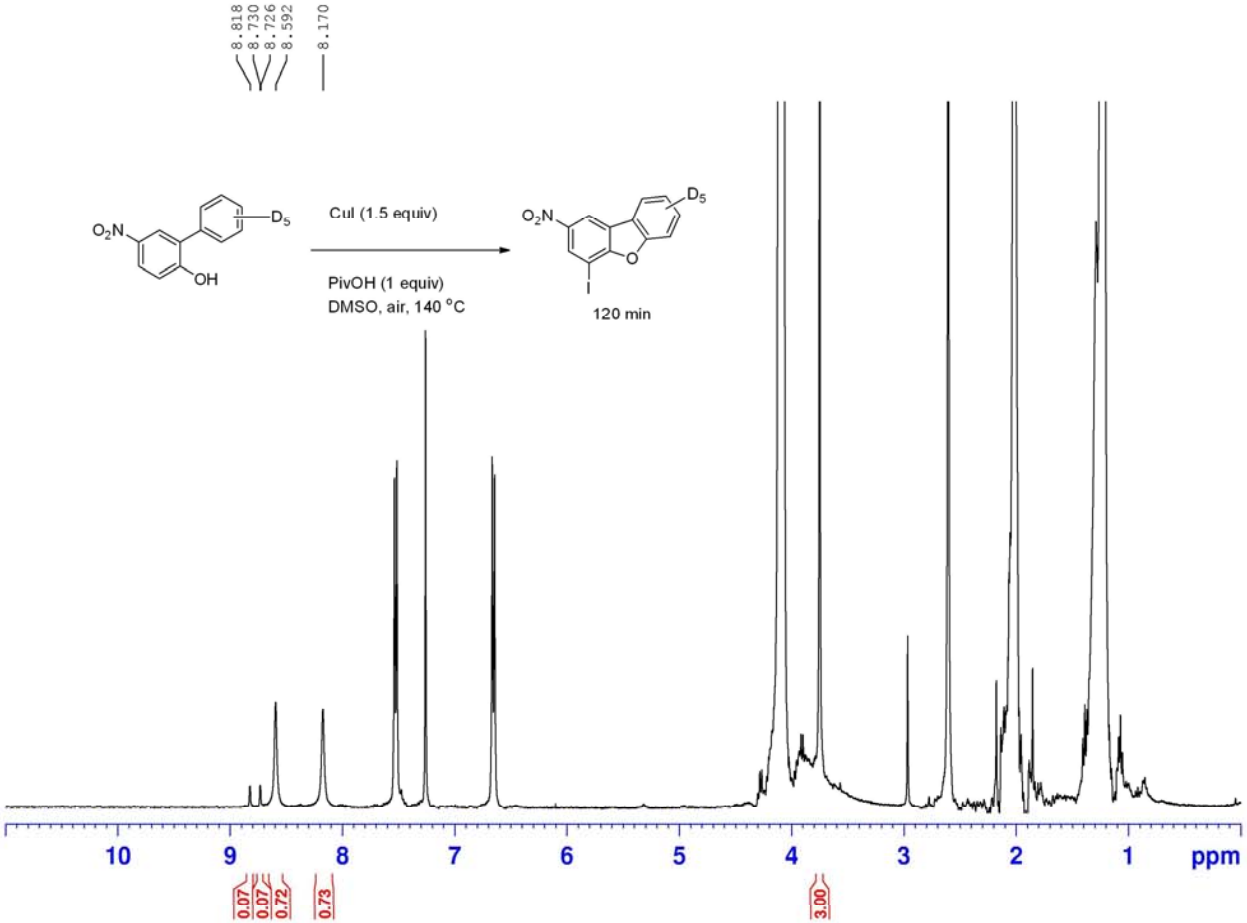

```
NAME          2012mannual
EXPNO                 472
PROCNO                  1
Date_            20120421
Time                10.23
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       2
SWH               8278.146 Hz
FIDRES            0.126314 Hz
AQ               3.9584243 sec
RG                      64
DW                  60.400 usec
DE                   6.50 usec
TE                  673.2 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            400.1300087 MHz
WDW                      EM
SSB                       0
LB                     0.30 Hz
GB                        0
PC                     1.00
```



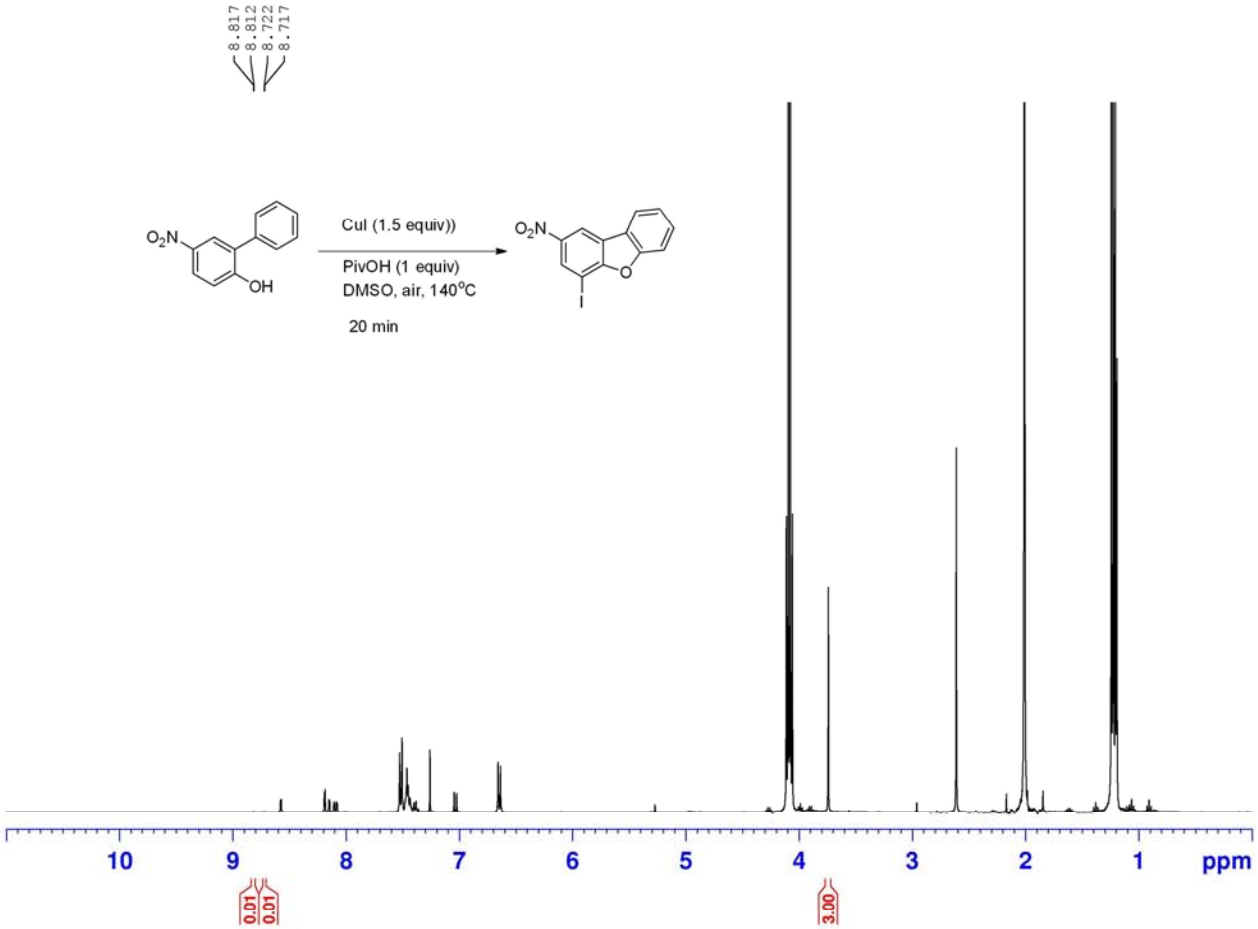

```
NAME          2012mannual
EXPNO                 473
PROCNO                  1
Date_            20120421
Time                10.28
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      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                673.2 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          400.1300085 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



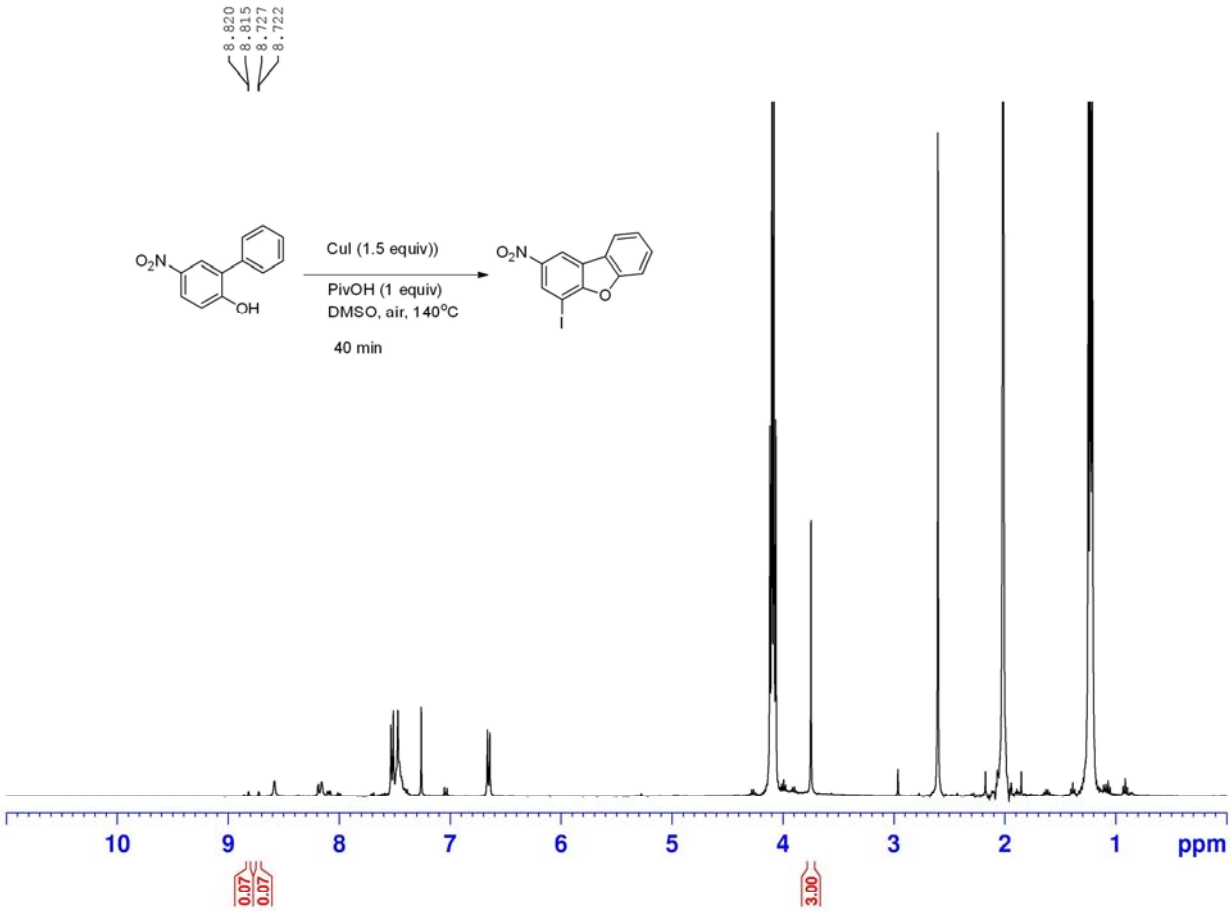

```
NAME          2012mannual
EXPNO                 474
PROCNO                  1
Date_            20120421
Time                10.33
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      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                673.2 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           400.1300085 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```



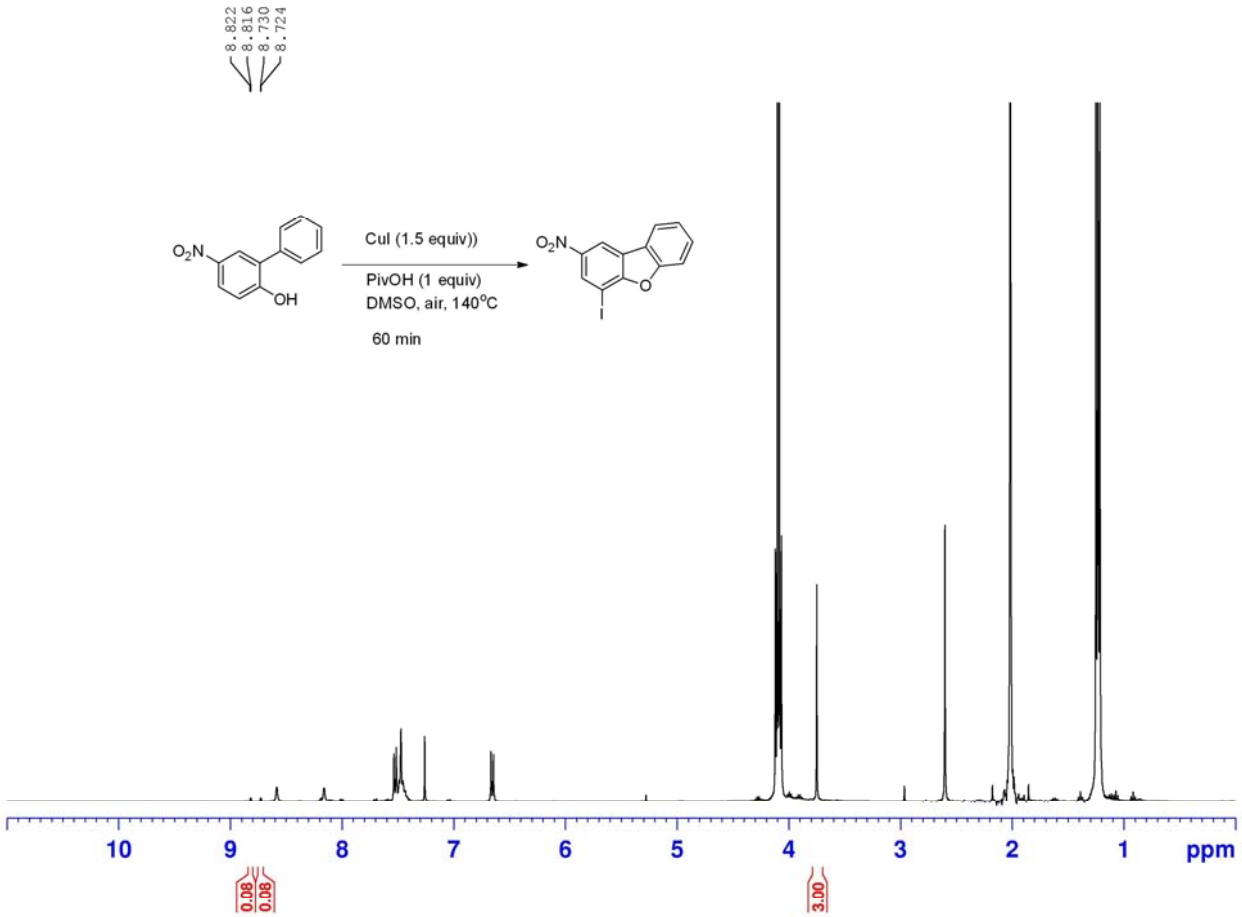

```
NAME          2012mannual
EXPNO                 475
PROCNO                  1
Date_            20120421
Time                10.38
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                      16
DS                       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                   673.2 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            400.1300087 MHz
WDW                     EM
SSB                      0
LB                    0.30 Hz
GB                       0
PC                    1.00
```



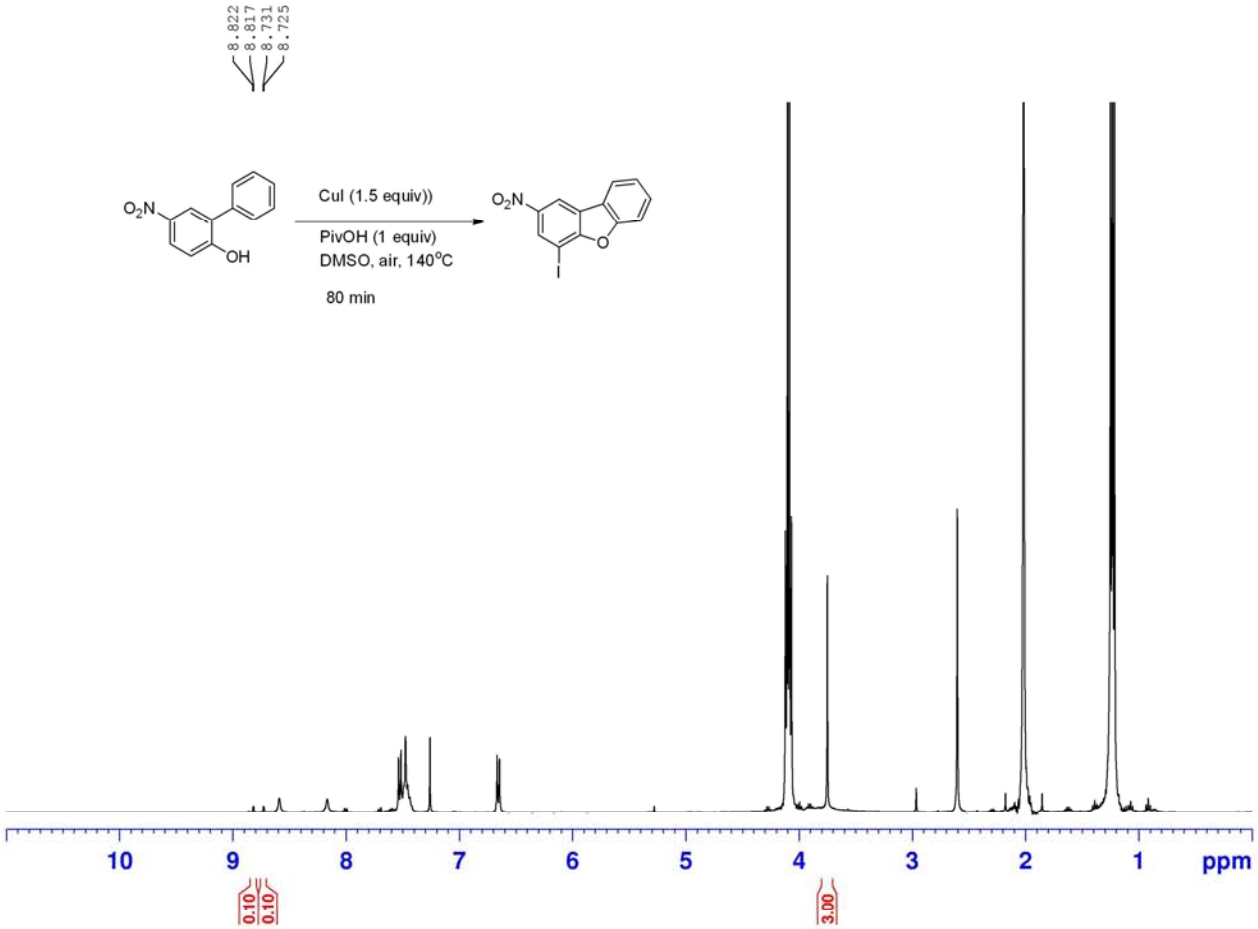

```
NAME            20120420
EXPNO                  1
PROCNO                 1
Date_           20120420
Time                9.37
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ             3.9584243 sec
RG                  45.3
DW                60.400 usec
DE                 6.50 usec
TE                673.2 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          400.1300088 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



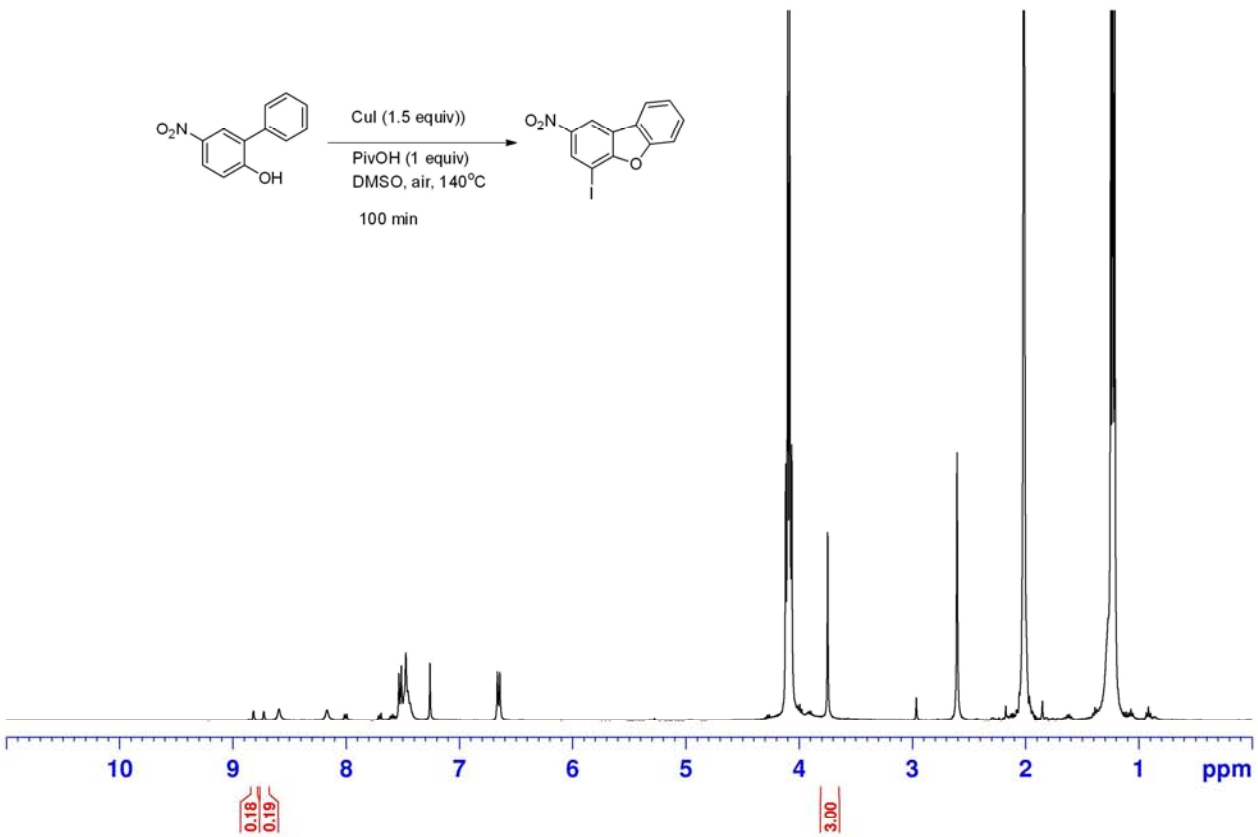

```
NAME            20120420
EXPNO                  2
PROCNO                 1
Date_           20120420
Time                9.44
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            8278.146 Hz
FIDRES         0.126314 Hz
AQ           3.9584243 sec
RG                    64
DW               60.400 usec
DE                 6.50 usec
TE                673.2 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          400.1300088 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```



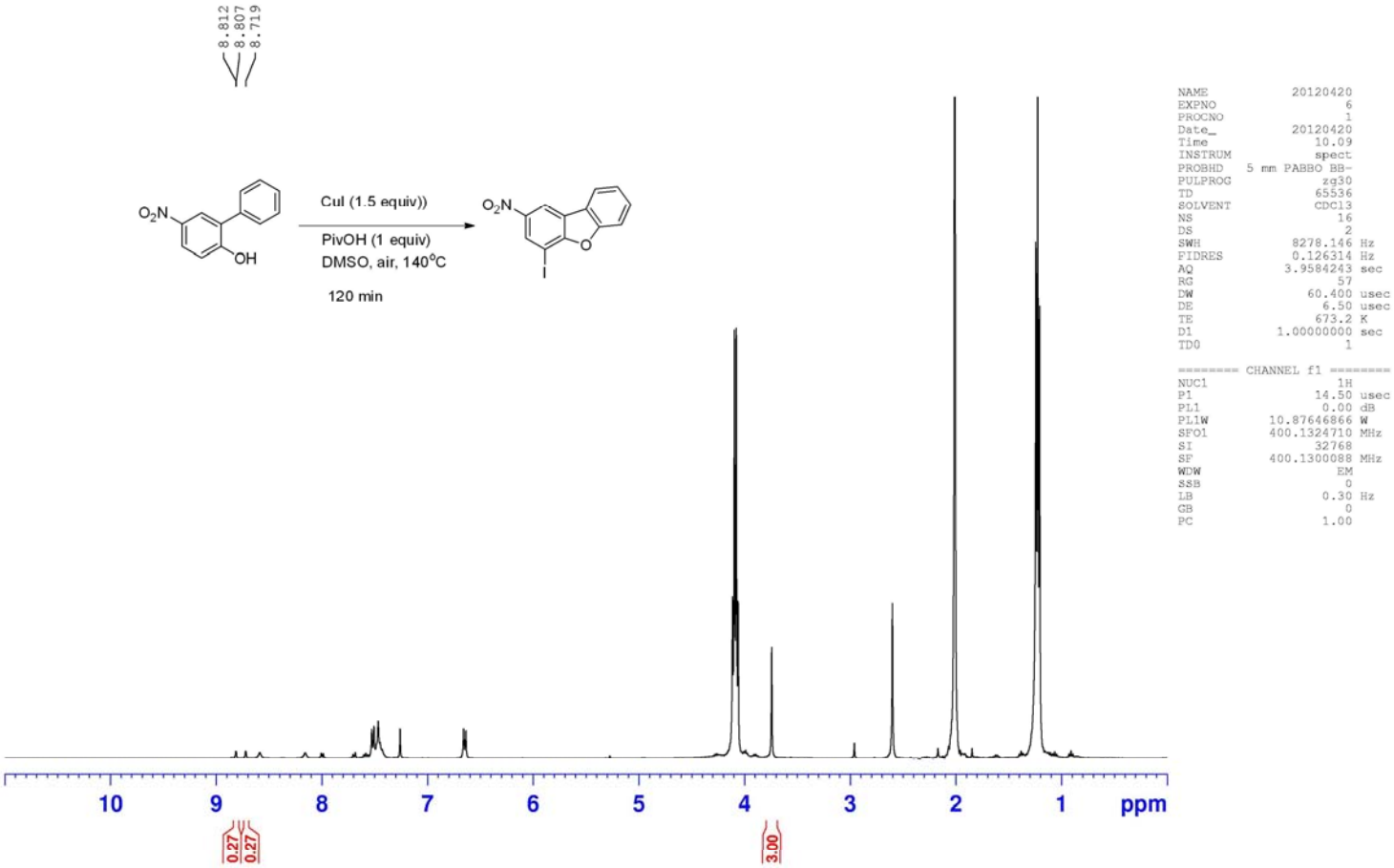

```
NAME            20120420
EXPNO                  3
PROCNO                 1
Date_           20120420
Time                9.50
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    16
DS                     2
SWH             8278.146 Hz
FIDRES          0.126314 Hz
AQ            3.9584243 sec
RG                    64
DW                60.400 usec
DE                 6.50 usec
TE                673.2 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           400.1300088 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
NAME            20120420
EXPNO                  4
PROCNO                 1
Date_           20120420
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                    64
DW                60.400 usec
DE                 6.50 usec
TE                673.2 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          400.1300089 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```




```
NAME            20120420
EXPNO                  5
PROCNO                 1
Date_           20120420
Time               10.03
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                    64
DW                60.400 usec
DE                 6.50 usec
TE                673.2 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          400.1300087 MHz
WDW                  EM
SSB                   0
LB                 0.30 Hz
GB                    0
PC                 1.00
```


8.812
8.807
8.719
O_2N
OH
CuI (1.5 equiv))
PivOH (1 equiv)
DMSO, air, 140°C
120 min
O_2N
O
I
10
9
8
7
6
5
4
3
2
1
ppm
0.27
0.27
3.00
NAME 20120420
EXPNO 6
PROCNO 1
Date_ 20120420
Time 10.09
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 57
DW 60.400 usec
DE 6.50 usec
TE 673.2 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 400.1300088 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00