Electronic Supplementary Material (ESI) for Chemical Communications
This journal is © The Royal Society of Chemistry 2011

Supplementary Material (ESI) for Chemical Communications
This journal is (c) The Royal Society of Chemistry 2011

Supporting Information

Potassium *tert*-Butoxide Mediated Heck-Type Cyclization/Isomerization Reaction for the Synthesis of Benzofurans

Magnus Rueping*, Matthias Leiendecker, Arindam Das, Thomas Poisson, Lan Bui

Institute of Organic Chemistry
RWTH Aachen University
Landoltweg 1
52074 Aachen, Germany

Correspondence should be addressed to Magnus.Rueping@rwth-aachen.de

Contents

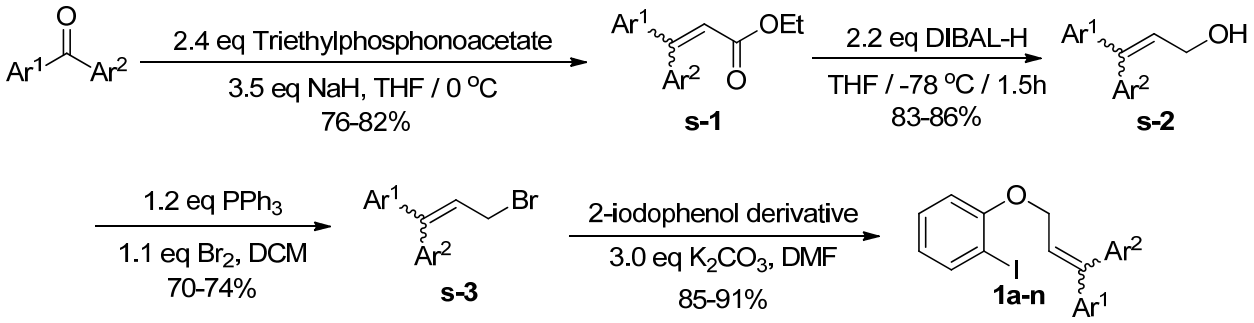
Electronic Supplementary Material (ESI) for Chemical Communications
This journal is © The Royal Society of Chemistry 2011

(I) General Methods

Unless otherwise noted, all commercially available compounds were used as provided without further purification. Solvents used in reactions were p.A. grade and dried before use. Solvents for chromatography were technical grade and distilled prior to use. Potassium *tert*-butoxide was purchased from Aldrich (99.999%) or Acros (97%, sublimated before use) and stored and handled inside a glove box. Analytical thin-layer chromatography (TLC) was performed on Merck silica gel aluminium plates with F-254 indicator, visualized by irradiation with UV light. Column chromatography was performed using silica gel Merck 60 (particle size 0.63 – 0.2 mm). Solvent mixtures are understood as volume/volume. ^{1}H-NMR and ^{13}C-NMR were recorded on a Varian VNMR 600 or 400 MHz and Mercury 300 MHz spectrometer in $CDCl_3$. Data are reported in the following order: chemical shift (δ) in ppm; multiplicities are indicated br (broad singlet), s (singlet), d (doublet), dd (doublet of doublet), t (triplet), q (quartet), m (multiplet); coupling constants (*J*) are in Hertz (Hz). Mass spectra (MS-EI, 70 eV) were conducted on a Finnigan MAT SSQ 700 spectrometer. IR spectra were recorded on a Perkin Elmer Spectrum 100 spectrometer and are reported in terms of frequency of absorption (cm^{-1}). Yields refer to the isolated product after preparative thin layer or column chromatography.

Supplementary Material (ESI) for Chemical Communications
This journal is (c) The Royal Society of Chemistry 2011

(II) Experimental procedure for the synthesis of starting materials:



In a typical procedure, Triethyl phosphonoacetate (7.4 g, 32.9 mmol) was slowly added to a suspension of NaH (60% in oil, 1.9 g, 47.5 mmol) in THF (30 ml) at 0 °C. The mixture was stirred at room temperature for 30 min. For the synthesis of **1a**, a solution of benzophenone (2.5 g, 13.7 mmol) in THF (10 ml) was added. The resulting mixture was stirred at room temperature for 7h, and then treated with saturated NH_4Cl solution. The aqueous phase was extracted with ethylacetate and the combined organic layer was washed with brine, dried over Na_2SO_4, filtered and evaporated under reduced pressure. The residue was eluted through a silica column to obtain compound **s-1a** (2.7 g, 78%) as a yellow liquid.

DIBAL-H (1.5 M, 8.1 ml, 12.21 mmol) was slowly added to a stirred solution of ester **s-1a** (1.4 g, 5.55 mmol) in THF (20 ml) at −78 °C. The reaction mixture was stirred for one hour at −78 °C and for another 30 minutes at room temperature. After completion, the reaction mixture was poured into cold diluted HCl (0.5 N), and extracted with ethyl acetate. The combined organic layers were dried over Na_2SO_4, and evaporated under reduced pressure to obtain compound **s-2** (1.0 g, 86%) as a yellow liquid.

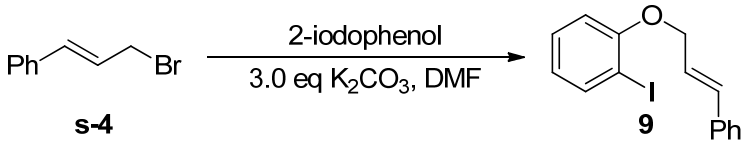
To a stirred solution of triphenyl phosphine (1.8 g, 6.86 mmol) in dry DCM was added Br_2 (1.0 g, 6.29 mmol) at 0 °C and stirred for 15 min. After the bromine color was dispersed, a solution of alcohol **s-2a** (1.2 g, 5.72 mmol) in DCM was added at 0 °C. Full conversion was obtained after 15 min and the reaction was quenched with water. The product was extracted with dichloromethane. The combined organic layer was washed with sodium thiosulfate, brine and dried over Na_2SO_4. The solvent was removed under reduced pressure and the product was purified by a short column chromatography to obtain compound **s-3a** (1.14 g, 73%) as a yellow liquid.

The bromo compound **s-3a** (0.8 g, 2.93 mmol) was added to a solution of 2-iodophenol (0.54 g,

Electronic Supplementary Material (ESI) for Chemical Communications
This journal is © The Royal Society of Chemistry 2011

2.44 mmol) and anhydrous K_2CO_3 (1.01 g, 7.29 mmol) in DMF at room temperature. The reaction mixture was stirred at room temperature overnight then it was poured into cold water and extracted with ethyl acetate. The combined organic extracts were washed with water, aqueous KOH solution (10%), $Na_2S_2O_3$ solution (10%) and brine. Then it was dried over Na_2SO_4, filtered and concentrated under reduced pressure. The residue was eluted through a silica column to obtain compound **1a** (0.9 g, 89%) as yellow liquid.

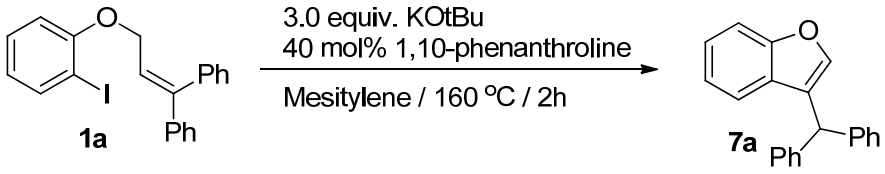
(III) Experimental procedure for the synthesis of substrate (9)



s-4 **9**

Cinnamyl bromide (3.55 g, 18 mmol) was added to a solution of 2-iodophenol (3.3 g, 15 mmol) and anhydrous K_2CO_3 (6.2 g, 45 mmol) in DMF at room temperature. The reaction mixture was stirred at room temperature overnight, then poured into cold water and extracted with pentane. The combined organic extracts were washed with water, aqueous KOH (10 %), anqueous $Na_2S_2O_3$ solution (10%) and brine. Then it was dried over Na_2SO_4, filtered and concentrated under reduced pressure to obtain compound **s-4** (4.49 g, 89%) as yellow liquid.

(IV) Standard procedure for the potassium *tert*-butoxide mediated cycloisomerization of (3-(2-iodophenoxy)prop-1-ene-1,1-diyl)dibenzene



1a **7a**

Potassium *tert*-butoxide (3.0 equiv.) and 1,10-phenanthroline (40 mol%) were transferred into a dried Schlenk tube. The sealed tube was evacuated and filled with argon three times. A solution of the starting compound **1a** (0.2 mmol) in 2 mL mesitylene (anhydrous and degassed) was added via syringe and the mixture was stirred for 5 seconds at room temperature. The tube was placed in a preheated oil bath at 160 °C and it was stirred for 2 hours. After cooling down, the reaction mixture was filtered through a short silica plug and the silica was washed with ethyl acetate. The organic solvents were evaporated under reduced pressure and the product was purified by preparative thin layer or column chromatography.

Supplementary Material (ESI) for Chemical Communications
This journal is (c) The Royal Society of Chemistry 2011

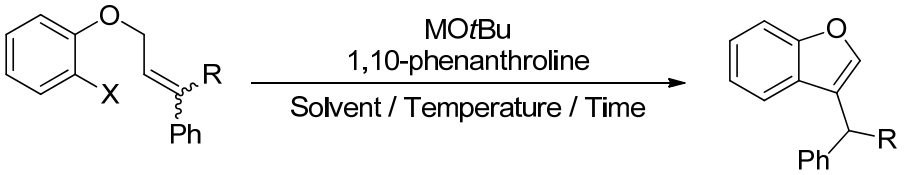
(V) ICP-MS measurements

Chemical	Source	Ag	Au	Co	Cu	Fe	Ni	Pd	Pt
1,10-Phenantholine	Acros	n. d.	n. d.	n. d.	0.34 ppm	n. d.	n. d.	n. d.	n. d.
KO*t*Bu	Sigma-Aldrich 99.999%	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.
KO*t*Bu	Acros 97% sublimated in our lab	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.	n. d.

n.d. = not detected

Supplementary Material (ESI) for Chemical Communications
This journal is (c) The Royal Society of Chemistry 2011

(VI) Table S-1: Selected Experiments for the Optimization of the Reaction Conditions



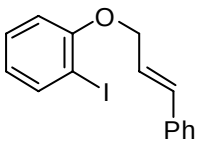
Entry	Solvent	T (°C)	R	X	M	MO*t*Bu (equiv.)	Additive (equiv.)	Time (h)	Metal salt (5 mol%)	Yield[a]
1	toluene	110	H	I	K	3	Phen (0.4)	14	-	28
2	dioxane	110	H	I	K	3	Phen (0.4)	14	-	30
3	dioxane	110	H	Br	K	3	Phen (0.4)	14	-	0
4	dioxane	110	H	Cl	K	3	Phen (0.4)	14	-	0
5	dioxane	110	H	I	Na	3	Phen (0.4)	14	-	0
6	dioxane	110	H	I	Li	3	Phen (0.4)	14	-	0
7	DMF	110	H	I	K	3	Phen (0.4)	14	-	0
8	DMF	80	H	I	K	3	EtOH (0.2)	14	-	0
9	DMSO	110	H	I	K	3	Phen (0.4)	14	-	0
10	mesitylene	150	H	I	K	3	Phen (0.4)	14	-	29
11	mesitylene	150	H	I	K	3	Phen (0.4)	2	-	38
12	mesitylene	150	H	I	K	3	-	2	-	0
13	pyridine	120	H	I	K	3	Phen (0.4)	2	-	18[b]
14	pyridine	120	H	I	K	3	-	2	-	10[b]
15	pyridine	160[e]	H	I	K	3	Phen (0.4)	2	-	21[b]
16	mesitylene	80	Ph	I	K	3	Phen (0.4)	2	-	16[b]
17	mesitylene	120	Ph	I	K	3	Phen (0.4)	2	-	25
18	mesitylene	160	Ph	I	K	3	Phen (0.4)	1.5	-	63
19	mesitylene	170	Ph	I	K	3	Phen (0.4)	2	-	58
20	mesitylene	150	Ph	I	K	-	Phen (0.4)	2	-	0
21	mesitylene	160	Ph	I	K	3	Phen (0.2)	1.5	-	39[b]
22	mesitylene	160	Ph	I	K	3	Phen (0.8)	1.5	-	49[b]
23	mesitylene	150	Ph	I	K	1.5	Phen (0.4)	2	-	23[b]
24	mesitylene	150	Ph	I	K	5	Phen (0.4)	2	-	43
25	mesitylene	155[e]	Ph	I	K	3	Phen (0.4)	0.25	-	46
26	mesitylene	160	Ph	I	K	3	Phen-Me_2[c] (0.4)	1.5	-	33[b]
27	mesitylene	160	Ph	I	K	3	DMEDA[d] (0.4)	1.5	-	40[b]
28	mesitylene	170	Ph	I	K	3	Phen (0.4)	2	CuCl	32
29	mesitylene	170	Ph	I	K	3	Phen (0.4)	2	$CuCl_2$	25
30	mesitylene	170	Ph	I	K	3	Phen (0.4)	2	CuI	46

[a] Yield of isolated product. [b] Determined by ^{1}H-NMR (internal standard: 1,3,5-trimethoxybenzene). [c] 4,7-Dimethyl-1,10-phenanthroline. [d] N,N'-Dimethylethylenediamine [e] Microwave reaction.

Electronic Supplementary Material (ESI) for Chemical Communications
This journal is © The Royal Society of Chemistry 2011

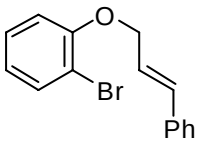
(VII) Spectral data

Spectral data for 1-(cinnamyloxy)-2-iodobenzene:



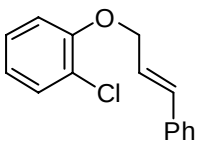
1H NMR (400 MHz, CDCl3): δ 7.79 (dd, *J* = 1.6, 8.0 Hz, 1H), 7.42 (s, 1H), 7.41 (s, 1H), 7.34 – 7.24 (m, 4H), 6.86 (d, *J* = 8.4 Hz, 1H), 6.81 (d, *J* = 16 Hz, 1H), 6.72 (td, *J* = 1.2, 7.2 Hz, 1H), 6.41 (dt, *J* = 5.2, 16 Hz, 1H), 4.76 (dd, *J* = 1.6, 5.6 Hz, 1H); 13C NMR (100 MHz, CDCl3): δ 157.56, 139.90, 136.78, 133.24, 129.76, 128.93 (2C), 128.24, 126.95 (2C), 124.27, 123.11, 113.10, 87.20, 70.09; IR (neat): ν = 3036, 2925, 1563, 1481, 1241, 974, 732 cm^{-1} EI-MS: m/z = 337(M^++1, 1%), 336(7%), 118(19%), 117 (100%), 115 (37%), 91(15%).

Spectral data for 1-(cinnamyloxy)-2-bromobenzene:



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.59 (dd, *J* = 1.6, 7.6 Hz, 1H), 7.44 (s, 1H), 7.42 (s, 1H), 7.37 – 7.24 (m, 4H), 6.96 (d, *J* = 8.0 Hz, 1H), 6.86 (td, *J* = 1.2, 7.6 Hz, 1H), 6.80 (d, *J* = 16 Hz, 1H), 6.43 (dt, *J* = 5.6, 16 Hz, 1H), 4.76 (dd, *J* = 1.2, 5.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.29, 136.64, 133.72, 133.29, 128.87 (2C), 128.71, 128.21, 126.90 (2C), 124.18, 122.37, 114.10, 112.70, 69.94; IR (neat): ν = 3030, 2937, 1578, 1475, 1238, 996, 744 cm^{-1}; EI-MS: m/z = 290(M^++2, 3%), 288(2%), 118(19%), 117(100%), 115(48%), 91(16%).

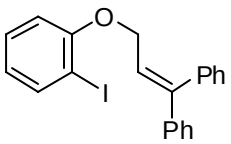
Spectral data for 1-(cinnamyloxy)-2-chlorobenzene:



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.44 – 7.20 (m, 7H), 6.99 (d, *J* = 8.0 Hz, 1H), 6.92 (t, *J* = 8.0 Hz, 1H), 6.79 (d, *J* = 16 Hz, 1H), 6.44 (dt, *J* = 5.6, 16 Hz, 1H), 4.78 (dd, *J* = 1.2, 6.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.45, 136.63, 133.43, 130.66, 128.88 (2C), 128.25, 127.97, 126.92 (2C), 124.20, 123.41, 121,90, 113.27, 69,94; IR (neat): ν = 3027, 2941, 1568, 1481, 1246, 952, 768 cm^{-1} EI-MS: m/z = 244(M^+, 3%), 118(17%), 117(100%), 115(51%), 91(17%).

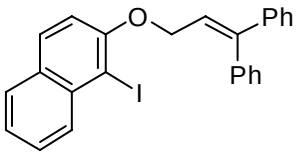
Supplementary Material (ESI) for Chemical Communications
This journal is (c) The Royal Society of Chemistry 2011

Spectral data for (3-(2-iodophenoxy)prop-1-ene-1,1-diyl)dibenzene:



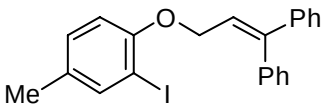
^{1}H NMR (300 MHz, $CDCl_3$): δ 7.84 (dd, *J* = 7.7, 1.7 Hz, 1H), 7.47-7.23 (m, 11H), 6.78-6.69 (m, 2H), 6.44 (t, *J* = 6.7 Hz, 1H), 4.72 (d, *J* = 6.7 Hz, 2H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 157.3, 146.0, 141.5, 139.6, 138.9, 129.8 (2C), 129.4, 128.5 (2C), 128.3 (2C), 128.0 (2C), 127.8 (2C), 123.5, 122.7, 112.9, 87.1, 67.4; IR (neat): ν = 3043, 2928, 1574, 1464, 1232, 985, 757 cm^{-1}; CI-MS: m/z = 413(M^++1, 2%), 194(16%), 193 (100%).

Spectral data for 2-(3,3-diphenylallyloxy)-1-iodonaphthalene:



^{1}H NMR (600 MHz, $CDCl_3$): δ 8.26 (d, *J* = 8.4 Hz, 1H), 7.75 (t, *J* = 8.9 Hz, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.50- 7.42 (m, 5H), 7.37-7.31(m, 6H), 7.05 (d, *J* = 8.9 Hz, 1H), 6.53 (t, *J* = 6.4 Hz, 1H), 4.88 (d, *J* = 6.4 Hz, 2H); 13C NMR (150 MHz, CDCl3): δ 156.0, 146.1, 141.5, 139.0, 135.8, 131.5, 130.2, 130.1, 129.9 (2C), 128.5 (2C), 128.3 (2C), 128.2, 128.1, 128.0, 127.9, 127.8 (2C), 124.5, 123.7, 115.0, 89.3, 68.5; IR (neat): ν = 3056, 2923, 1593, 1499, 1263, 804, 759 cm^{-1}; EI-MS: m/z = 463(M^++1, 1.2%), 462(4%), 194(36%), 193(100%), 115(69%), 91(24%).

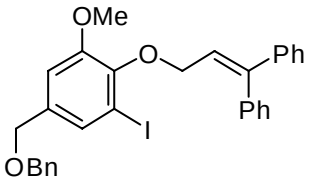
Spectral data for (3-(2-iodo-4-methylphenoxy)prop-1-ene-1,1-diyl)dibenzene:



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.64 (d, *J* = 1.7 Hz, 1H), 7.45-7.36 (m, 3H), 7.34-7.26 (m, 7H), 7.02 (dd, *J* = 8.6, 1.3 Hz, 1H), 6.59 (d, *J* = 8.6 Hz, 1H), 6.40 (t, *J* = 6.6 Hz, 1H), 4.66 (d, *J* = 6.6 Hz, 2H), 2.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.3, 145.8, 141.5, 139.8, 139.0, 132.3, 129.9, 129.8 (2C), 128.4 (2C), 128.3 (2C), 127.9 (2C), 127.8 (2C), 123.7, 112.8, 86.9, 67.6, 20.0; IR (neat): ν = 3027, 2921, 1598, 1486, 1240, 997, 764 cm^{-1}; EI-MS: m/z = 426(M^+, 1.3%), 194(33%), 193(100%), 115(81%), 91(31%).

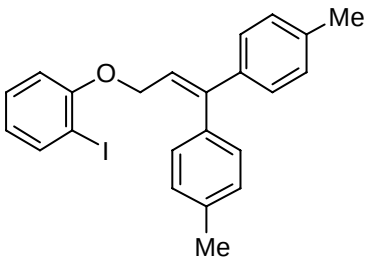
Electronic Supplementary Material (ESI) for Chemical Communications
This journal is © The Royal Society of Chemistry 2011

Spectral data for (3-(4-(benzyloxymethyl)-2-iodo-6-methoxyphenoxy)prop-1-ene-1,1-diyl)dibenzene:



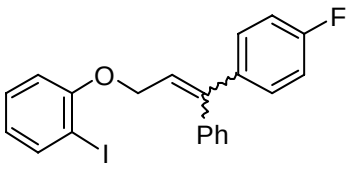
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.36-7.27 (m, 14H), 7.15-7.12 (m, 2H), 6.83 (s, 1H), 6.54-6.49 (m, 1H), 4.65-4.62 (m, 2H), 4.54 (s, 2H), 4.44 (s, 2H), 3.68 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.6, 147.1, 145.4, 141.8, 139.0, 137.9, 136.2, 129.9 (2C), 129.5, 128.4 (2C), 128.1 (2C), 128.0 (2C), 127.8 (2C), 127.7 (3C), 127.6, 127.4, 124.4, 112.0, 93.3, 72.2, 71.0, 70.6, 55.7; IR (neat): ν = 3057, 3026, 2934, 2855, 1563, 1460, 1272, 965, 756 cm^{-1}; EI-MS: m/z = 434(M^+-128, 1%), 194(14%), 193(100%), 115(39%), 91(56%).

Spectral data for 4,4'-(3-(2-iodophenoxy)prop-1-ene-1,1-diyl)bis(methylbenzene):



^{1}H NMR (300 MHz, $CDCl_3$): δ 7.68 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.17-7.00 (m, 9H), 6.62-6.56 (m, 2H), 6.20 (t, *J* = 6.7 Hz, 1H), 4.57 (d, *J* = 6.7 Hz, 2H), 2.31 (s, 3H), 2.23 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 157.3, 145.8, 138.9, 138.3, 137.7, 137.5, 136.0, 129.7 (2C), 129.3, 129.0 (2C), 128.9 (2C), 127.7 (2C), 122.5, 122.3, 112.8, 86.9, 67.4, 21.3, 21.1; IR (neat): ν = 3025, 2921, 1577, 1467, 1278, 1015, 819 cm^{-1}; CI-MS: m/z = 441(M^++1, 6%), 359(28%), 331(24%), 222(19%), 221(100%).

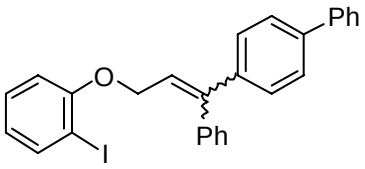
Spectral data for 1-(3-(4-fluorophenyl)-3-phenylallyloxy)-2-iodobenzene:



Obtained as a 1:0.92 mixture of E:Z isomers .^{1}H NMR (300 MHz, $CDCl_3$): δ 7.79-7.76 (m, 2H), 7.43-7.36 (m, 3H), 7.31-7.20 (m, 13H), 7.11-7.07 (m, 2H), 7.00-6.96 (m, 2H), 6.72-6.64 (m, 4H), 6.37 (t, *J* = 6.4 Hz, 1H), 6.30 (t, *J* = 6.4 Hz, 1H), 4.64-4.61 (m, 4H); ^{13}C NMR (75 MHz, $CDCl_3$): δ 162.6 (J_{CF} = 246.1 Hz), 162.4 (J_{CF} = 246.0 Hz), 157.2 (2C), 145.2, 144.9, 141.3, 139.6, 139.5, 138.6, 137.6 (d, J_{CF} = 3.2 Hz), 134.7 (J_{CF} = 3.3 Hz), 131.5 (J_{CF} = 7.9 Hz, 2C), 129.6 (2C), 129.5, 129.4 (2C), 129.3, 128.4 (2C), 128.3 (2C), 128.0 (2C), 127.7 (2C), 123.6, 123.3, 123.2, 122.7 (J_{CF} = 6.4 Hz, 2C), 115.4 (J_{CF} = 21.2 Hz, 2C), 115.1 (J_{CF} = 21.4 Hz, 2C), 112.8, 87.0, 86.9, 67.3, 67.2. IR (neat): ν = 3057, 2938, 1583, 1479, 1271, 814, 756 cm^{-1}; EI-MS: m/z = 430(M^+ 0.88%), 212(45%), 211(100%), 133(45%), 115(37%).

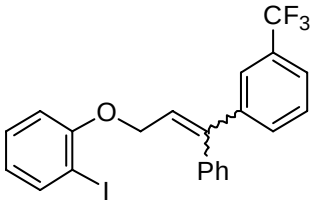
Supplementary Material (ESI) for Chemical Communications
This journal is (c) The Royal Society of Chemistry 2011

Spectral data for 4-(3-(2-iodophenoxy)-1-phenylprop-1-enyl)biphenyl:



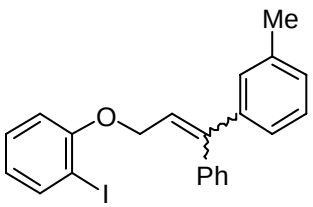
Obtained as a 1:1 mixture of E:Z isomers .^{1}H NMR (400 MHz, $CDCl_3$): δ 7.89 (d, *J* = 8.0 Hz, 2H), 7.76-7.73 (m, 4H), 7.69 (d, *J* = 7.3 Hz, 2H), 7.63 (d, *J* = 8.6, Hz, 2H), 7.55-7.37 (m, 20H), 7.29 (dt, *J* = 7.6, 1.6 Hz, 2H), 6.79-6.74 (m, 4H), 6.55 (t, *J* = 6.6 Hz, 1H), 6.51 (t, *J* = 6.6 Hz, 1H), 4.80 (d, *J* = 6.6 Hz, 2H), 4.76 (d, *J* = 6.6 Hz, 2H), ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.3 (2C), 145.8, 145.6, 141.6, 140.7 (2C), 140.6, 140.5, 140.4, 139.7, 138.9, 137.9, 130.4 (2C), 129.9 (2C), 129.5, 129.4, 129.0 (2C), 128.9 (3C), 128.6 (2C), 128.4 (2C), 128.3 (2C), 128.1 (2C), 128.0 (2C), 127.7, 127.6, 127.3 (2C), 127.2 (2C), 127.1 (2C), 127.0 (2C), 123.7, 123.5, 122.8 (2C), 112.9 (2C), 87.2 (2C), 67.5 (2C); IR (neat): ν = 3029, 2923, 1576, 1467, 1234, 990, 752 cm^{-1}; EI-MS: m/z = 488(M^+, 0.66%), 270(44%), 269(100%), 91(70%).

Spectral data for 1-iodo-2-(3-phenyl-3-(3-(trifluoromethyl)phenyl)allyloxy)benzene:



Obtained as a 1.4:1 mixture of E:Z isomers .^{1}H NMR (600 MHz, $CDCl_3$): δ 7.82 (d, *J* = 7.9 Hz, 2H), 7.68 (d, *J* = 7.4 Hz, 1H), 7.61-7.56 (m, 4H), 7.52-7.53 (m, 5H), 7.37-7.36 (m, 4H), 7.31-7.23 (m, 6H), 6.75-6.70 (m, 4H), 6.51 (t, *J* = 6.4 Hz, 1H), 6.47 (t, *J* = 6.4 Hz, 1H), 4.71 (d, *J* = 6.4 Hz, 2H), 4.64 (d, *J* = 6.4 Hz, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 157.2, 157.1, 144.9, 144.8, 142.3, 140.7, 139.7, 139.6, 138.0, 133.2, 131.1, 131.0, 130.8 (d, *J* = 2.5 Hz), 130.6 (d, *J* = 2.7 Hz), 129.7, 129.4, 129.0, 128.8, 128.7, 128.5, 128.4, 128.3, 127.7, 126.4 (q, *J* = 3.6 Hz), 125.1, 124.8 (q, *J* = 3.6 Hz), 124.6 (q, *J* = 3.6 Hz), 124.5, 124.3 (q, *J* = 3.7 Hz), 124.1 (d, *J* = 271.1 Hz), 123.0, 122.9, 112.9, 112.8, 87.1, 87.0, 67.3, 67.1 IR (neat): ν = 3062, 2924, 1578, 1468, 1322, 1009, 753 cm^{-1}; EI-MS: m/z = 480(M^+, 1.8%), 262(40%), 261(100%), 183(29%), 91 (14%).

Spectral data for 1-iodo-2-(3-phenyl-3-m-tolylallyloxy)benzene:

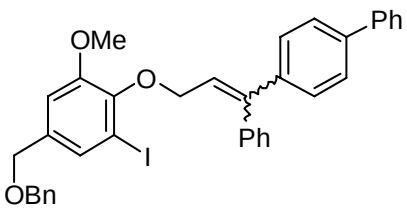


Obtained as a 1:1 mixture of E:Z isomers .^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82-7.80 (m, 2H), 7.46-7.39 (m, 4H), 7.33-7.08 (m, 16H), 6.73-6.68 (m, 4H), 6.42-6.38 (m, 2H), 4.70 (d, *J* = 3.0, Hz, 2H), 4.68 (d, *J* = 3.0 Hz, 2H), 2.39 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (100 MHz,

Electronic Supplementary Material (ESI) for Chemical Communications
This journal is © The Royal Society of Chemistry 2011

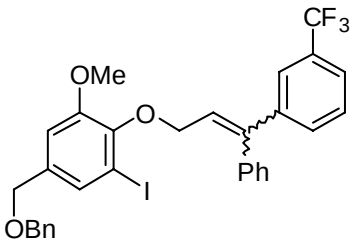
$CDCl_3$): δ 157.3 (2C), 146.2, 146.1, 141.6, 141.5, 139.5 (2C), 139.0, 138.8, 138.0, 137.8, 130.3, 129.8 (2C), 129.4, 129.3, 128.7, 128.6, 128.4 (3C), 128.3 (3C), 128.2, 127.9, (2C), 127.8 (2C), 126.8, 125.0, 123.4, 123.3, 122.6 (2C), 112.9, 112.8, 87.1, 87.0, 67.5, 67.4, 21.5 (2C). IR (neat): ν = 3053, 2921, 1579, 1468, 1236, 1010, 751 cm^{-1}; EI-MS: m/z = 427(M^++1, 0.66%), 426(3%), 208 (31%), 207(100%), 115(50%).

Spectral data for 4-(3-(4-(benzyloxymethyl)-2-iodo-6-methoxyphenoxy)-1-phenylprop-1-enyl)biphenyl:



Obtained as a 1.7:1 mixture of E:Z isomers .^{1}H NMR (400 MHz, $CDCl_3$): δ 7.63-7.16 (m, 40H), 6.83 (d, *J* = 1.3 Hz, 1H), 6.82 (d, *J* = 1.7 Hz, 1H), 6.58 (t, *J* = 7.3 Hz, 1H), 6.53 (t, *J* = 7.0 Hz, 1H), 4.70 (d, *J* = 7.3 Hz, 2H), 4.65 (d, *J* = 7.0 Hz, 2H), 4.54 (s, 4H), 4.44 (s, 4H), 3.68 (s, 3H), 3.67 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.6 (2C), 147.1, 145.3, 145.0, 141.8, 140.7, 140.6 (2C), 140.4, 140.2, 138.9 (2C), 137.9 (2C), 136.2 (3C), 130.4 (2C), 129.9 (2C), 129.5(2C), 128.8 (2C), 128.7 (2C), 128.4 (3C), 128.2 (2C), 128.1 (2C), 128.0 (2C), 127.9 (2C), 127.8 (3C), 127.7 (2C), 127.6, 127.5 (2C), 127.4, 127.3 (2C), 127.0 (2C), 126.9 (2C), 126.8 (2C), 126.7 (2C), 124.6, 124.4, 112.0, 11.9, 93.3 (2C), 72.2 (2C), 71.0 (2C), 70.6, 70.5, 55.7 (2C); IR (neat): ν = 3068, 3029, 2926, 2863, 1578, 1469, 1327, 1123, 987 cm^{-1}; EI-MS: m/z = 285(M^+-128, 2%), 370(12%), 270(12%), 269(48%), 91(100%).

Spectral data for 5-(benzyloxymethyl)-1-iodo-3-methoxy-2-(3-phenyl-3-(3-(trifluoro-methyl)phenyl)allyloxy)benzene:

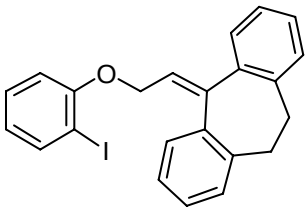


Obtained as a 1.56:1 mixture of E:Z isomers . ^{1}H NMR (400 MHz, $CDCl_3$): δ 7.60-7.59 (m, 2H), 7.53-7.25 (m, 26H), 7.15-7.12 (m, 2H), 6.85 (d, *J* = 1.7 Hz, 1H), 6.84 (d, *J* = 1.7 Hz, 1H), 6.61 (t, *J* = 7.3 Hz, 1H), 6.57 (t, *J* = 7.0 Hz, 1H), 4.66 (d, *J* = 7.0 Hz, 2H), 4.61 (d, *J* = 7.3 Hz, 2H), 4.55 (s, 4H), 4.45 (s, 2H), 4.44 (s, 2H), 3.70 (s, 3H), 3.68 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.6, 152.5, 147.0, 146.8, 144.2, 142.6, 140.9, 139.8, 138.1, 137.9, 136.4, 133.4, 131.2, 131.1, 130.8 (d, *J* = 3.6 Hz), 130.4 (d, *J* = 3.7 Hz), 129.8, 129.6, 129.5, 128.7, 128.6, 128.5, 128.4, 128.3, 128.0, 127.9, 127.8, 127.7, 127.6, 126.4 (q, *J* = 3.8 Hz), 126.2, 125.5, 124.3 (q, *J* = 3.7 Hz), 124.2, 112.0, 111.9, 93.2, 72.3, 72.2,

Electronic Supplementary Material (ESI) for Chemical Communications
This journal is © The Royal Society of Chemistry 2011

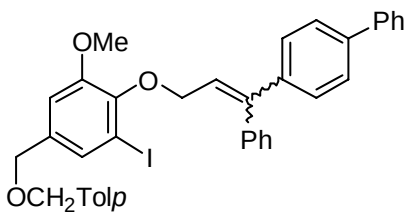
71.0, 70.9, 70.3, 70.0, 55.7, 55.6; IR (neat): ν = 3061, 3031, 2935, 2857, 1564, 1464, 1321, 1128, 968 cm^{-1}; EI-MS: m/z = 631(M^++1, 0.69 %), 630(2%), 262(49%), 261(100%), 91(36%).

Spectral data for 5-(2-(2-iodophenoxy)ethylidene)-10,11-dihydro-5H-dibenzo[a,d]-[7]annulene



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.85 (dd, *J* = 7.6, 1.3 Hz, 1H), 7.49-7.46 (m, 1H), 7.37-7.21 (m, 7H), 7.17-7.13 (m, 1H), 6.73 (t, *J* = 8.3 Hz, 1H), 6.67 (t, *J* = 8.3 Hz, 1H), 6.29 (t, *J* = 6.6 Hz, 1H), 4.79-4.78 (br, 2H), 3.50-3.29 (m, 2H), 3.15-3.06 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 157.2, 147.4, 140.3, 139.6, 139.2, 138.8, 137.5, 130.2, 129.3, 128.7, 128.6, 128.5, 128.4, 127.9, 126.4, 126.1, 126.0, 122.7, 112.8, 87.1, 67.1, 33.7, 32.2; IR (neat): ν = 3014, 2921, 1578, 1469, 1219, 1014, 753 cm^{-1}; CI-MS: m/z = 439(M^++1, 2%), 438(7%), 359(80%), 331(75%), 235(31%), 219(100%).

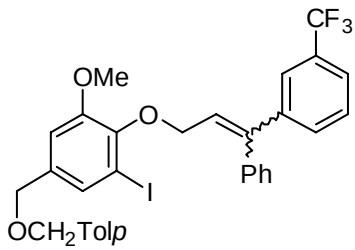
Spectral data for 4-(3-(2-iodo-6-methoxy-4-((4-methylbenzyloxy)methyl)phenoxy)-1-phenylprop-1-enyl)biphenyl:



Obtained as a 1:1 mixture of E:Z isomers .^{1}H NMR (400 MHz, $CDCl_3$): δ 7.53-7.41 (m, 9H), 7.37-7.17 (m, 18H), 7.15-7.05 (m, 11H), 6.73-6.72 (m, 2H), 6.49 (dt, *J* = 7.2, 2.0 Hz, 1H), 6.44 (dt, *J* = 7.2, 2.0 Hz, 1H), 4.61 (dd, *J* = 7.2, 2.0 Hz, 2H), 4.56 (dd, *J* = 7.2, 2.0 Hz, 2H), 4.40 (s, 4H), 4.31 (s, 4H), 3.58 (s, 3H), 3.56 (s, 3H), 2.25 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.7, 152.6, 147.1, 147.0, 145.3, 145.0, 141.8, 140.8, 140.7, 140.6, 140.4, 140.2, 138.9, 138.0, 137.5 (2C), 136.3 (2C), 134.9 (2C), 130.4 (2C), 129.9 (2C), 129.5 (2C), 129.2 (4C), 128.9 (2C), 128.8 (2C), 128.3 (2C), 128.2 (2C), 128.1 (2C), 128.0 (4C), 127.9 (2C), 127.7, 127.5, 127.4, 127.3, 127.1 (2C), 127.0 (2C), 126.8 (2C), 126.7 (2C), 124.6, 124.4, 112.0, 111.9, 93.3 (2C), 72.1 (2C), 70.9 (2C), 70.6, 70.5, 55.7 (2C), 21.2 (2C); IR (neat): ν = 3027, 2931, 2857, 1563, 1463, 1272, 965, 843 cm^{-1}; CI-MS: m/z = 524(M^+-128, 1%), 279(23%), 263(100%), 121(39%), 105(38%).

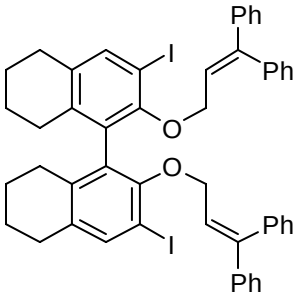
Supplementary Material (ESI) for Chemical Communications
This journal is (c) The Royal Society of Chemistry 2011

Spectral data for 1-iodo-3-methoxy-5-((4-methylbenzyloxy)methyl)-2-(3-phenyl-3-(3-(trifluoromethyl)phenyl)allyloxy)benzene:



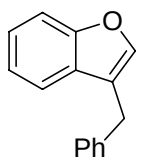
Obtained as a 1.7:1 mixture of E:Z isomers .^{1}H NMR (400 MHz, $CDCl_3$): δ 7.55 (s, 1H), 7.53 (s, 1H), 7.47- 7.40 (m, 3H), 7.36-7.28 (m, 6H), 7.26-7.24 (m, 5H), 7.20-7.17 (m, 7H), 7.12-7.10 (m, 3H), 7.08-7.05 (m, 2H), 6.78 (d, *J* = 1.6 Hz, 1H), 6.76 (d, *J* = 1.6 Hz, 1H), 6.54 (t, *J* = 7.2 Hz, 1H), 6.49 (t, *J* = 7.2 Hz, 1H), 4.58 (d, *J* = 7.2 Hz, 2H), 4.53 (d, *J* = 7.2 Hz, 2H), 4.44 (s, 4H), 4.35 (s, 4H), 3.64 (s, 3H), 3.61 (s, 3H), 2.30 (6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 152.6, 152.5, 146.9, 146.8, 144.1, 142.6, 140.9, 139.7, 138.0, 137.5, 136.5, 134.8, 133.4, 131.1, 129.8, 129.5, 129.1, 128.6, 128.5, 128.3, 128.2, 127.9, 127.8, 127.6, 126.4 (q, *J* = 3.7 Hz), 126.1, 125.5, 124.4, 124.3, 124.2, 124.1, 124.0, 111.9, 93.1, 72.2, 72.1, 70.8, 70.3, 70.0, 55.7, 55.6, 21.2; IR (neat): ν = 3015, 2925, 2854, 1565, 1464, 1321, 1131, 758 cm^{-1}; EI-MS: m/z = 645(M^{+}+1, 0.78%), 644(3%), 262(36%), 261(100%), 105(32%).

Spectral data for 2,2'-bis(3,3-diphenylallyloxy)-3,3'-diiodo-5,5',6,6',7,7',8,8'-octahydro-1,1'-binaphthyl:



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.50 (s, 2H), 7.29-7.23 (m, 12H), 7.21-7.18 (m, 4H), 6.99-6.96 (m, 4H), 6.12 (t, *J* = 6.6 Hz, 2H), 4.17 (ddab, *J* = 11.6, 6.6 Hz, 2H), 4.10 (ddab, *J* = 11.6, 6.6 Hz, 2H), 2.73-2.58 (m, 4H), 2.30-2.22 (m, 2H), 2.06-1.99 (m, 2H), 1.72-1.48 (m, 8H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.9 (2C), 143.9 (2C), 141.7 (2C), 139.2 (2C), 138.9 (2C), 137.4 (2C), 135.4 (2C), 131.3 (2C), 129.4 (4C), 128.1 (4C), 128.0 (4C), 127.6 (4C), 127.5 (2C), 127.4 (2C), 125.2 (2C), 89.1 (2C), 71.3 (2C), 29.1 (2C), 27.4 (2C), 22.7 (2C), 22.6 (2C); IR (neat): ν = 3066, 3056, 2941, 2861, 1571, 1463, 1329, 1125, 979 cm^{-1}; EI-MS: m/z = 738(M^{+}-192, 9%), 737(27%), 736(21%), 546(53%), 193(100%).

Spectral data for 3-Benzylbenzofuran (10):

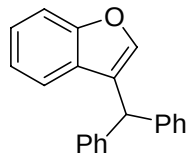


^{1}H NMR (600 MHz, $CDCl_3$): δ 7.46 (d, *J* = 12 Hz, 1H), 7.41 (d, *J* = 12 Hz, 1H), 7.37 (s, 1H), 7.30–7.15 (m, 7H), 4.02 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 155.9, 142.6, 139.5, 129.2, 129.0 (2C), 128.9 (2C), 126.7, 124.6, 122.7, 120.2,

Electronic Supplementary Material (ESI) for Chemical Communications
This journal is © The Royal Society of Chemistry 2011

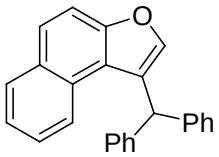
120.0, 111.8, 30.3; IR (neat): ν = 3030, 2918, 1599, 1452, 1184, 1092, 854, 747 cm^{-1}; EI-MS: m/z = 209(M^++1, 16%), 208(100%), 207 (87%), 178 (26%), 131 (37%), 91(49%).

Spectral data for 3-Benzhydrylbenzofuran (7a):



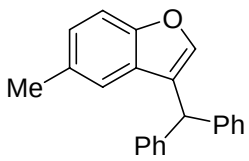
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.37 (dd, *J* = 8.3, 0.7 Hz, 1H), 7.22-7.12 (m, 11H), 7.04–6.97 (m, 2H), 6.92 (d, *J* = 1.0 Hz, 1H), 5.43 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 158.8, 144.0, 142.2, 128.8 (4C), 128.5 (4C), 128.3, 127.6, 126.7 (2C), 124.3, 124.0, 122.4, 120.7, 111.5, 47.4; IR (neat): ν = 3028, 2906, 1589, 1436, 1173, 1094, 845, 743 cm^{-1}; EI-MS: m/z = 285(M^++1, 25%), 284(100%), 283 (26%), 207 (63%), 178 (31%).

Spectral data for 1-benzhydrylnaphtho[2,1-*b*]furan (7b):



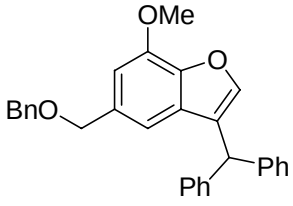
^{1}H NMR (600 MHz, $CDCl_3$): δ 7.93–7.91 (m, 2H), 7.75–7.67 (m, 2H), 7.39 (t, *J* = 7.8, 1H), 7.33–7.24 (m, 11H), 6.99 (s, 1H), 6.02 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 154.2, 144.8 (2C), 143.1, 131.1, 129.4 (4C), 129.2, 128.9 (4C), 128.6, 127.1 (2C), 126.4, 126.3, 126.2, 124.4, 124.2, 121.4, 113.1, 49.3; IR (neat): ν = 3034, 2913, 1594, 1446, 1178, 1087, 873, 756 cm^{-1}; EI-MS: m/z = 335(M^++1, 34%), 334(100%), 333 (14%), 257 (26%).

Spectral data for 3-benzhydryl-5-methylbenzofuran (7c):



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.27–7.15 (m, 11H), 6.98 (d, *J* = 8.4 Hz, 1H), 6.89 (s, 1H), 6.84 (s, 1H), 5.42 (s, 1H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 154.6, 144.6 (2C), 142.7, 132.2, 129.1 (4C), 128.8 (4C), 128.0, 127.0 (2C), 125.9, 124.0, 120.7, 111.3, 47.9, 21.7; IR (neat): ν = 2923, 1594, 1450, 1172, 1083, 836, 794, 698 cm^{-1}; EI-MS: m/z = 299(M^++1, 24%), 298 (100%), 297 (19%), 221 (44%), 178 (16%).

Spectral data for 3-benzhydryl-5-(benzyloxymethyl)-7-methoxybenzofuran (7d):

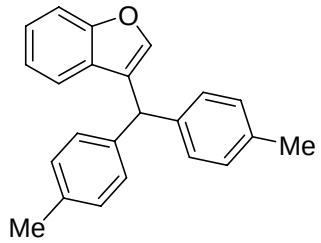


^{1}H NMR (600 MHz, $CDCl_3$): δ 7.38–7.25 (m, 15H), 7.03 (s, 1H), 6.85 (s, 1H), 6.71 (s, 1H), 5.52 (s, 1H), 4.49 (s, 2H), 4.46 (s, 2H), 4.01 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 145.7, 145.1, 144.8, 142.5 (2C),

Electronic Supplementary Material (ESI) for Chemical Communications
This journal is © The Royal Society of Chemistry 2011

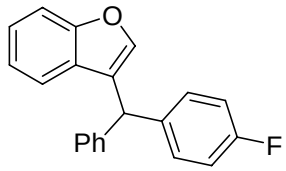
138.5, 133.8, 129.4, 129.1 (4C), 128.8 (4C), 128.7 (2C), 128.2 (2C), 127.9, 127.0 (2C), 124.7, 121.5, 114.4, 112.8, 110.9, 106.9, 72.6, 72.0, 56.4, 47.9; IR (neat): ν = 3471, 2928, 2865, 1603, 1479, 1332, 1073, 838, 741 cm^{-1}; EI-MS: m/z = 329(M^++1, 29%), 328(100%), 327 (9%), 91 (14%).

Spectral data for 3-(di-p-tolylmethyl)benzofuran (7e):



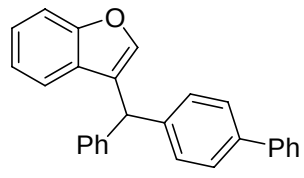
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.36 (dd, *J* = 8.3, 0.7 Hz, 1H), 7.17–7.13 (m, 2H), 7.05–6.97 (m, 9H), 6.93 (s, 1H), 5.35 (s, 1H), 2.23 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.8, 143.9, 139.5, 136.1(2C), 129.2 (2C), 129.1 (2C), 128.8(2C), 128.6 (2C), 127.7, 126.9, 124.3, 124.2, 122.3, 120.8, 111.4, 46.9, 21.1 (2C); IR (neat): ν = 3021, 2920, 1511, 1451, 1098, 856, 746 cm^{-1}; EI-MS: m/z = 313(M^++1, 31%), 312(100%), 297 (45%), 221 (46%), 178 (16%).

Spectral data for 3-((4-fluorophenyl)(phenyl)methyl)benzofuran (7f):



^{1}H NMR (600 MHz, $CDCl_3$): δ 7.47 (d, *J* = 8.4 Hz, 1H), 7.32–7.29 (m, 2H), 7.26–7.18 (m, 6H), 7.09 (d, *J* = 4.2 Hz, 2H), 6.98 (t, *J* = 9.0 Hz, 3H), 5.50 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 161.6 (d, J_{CF} = 244.5 Hz), 143.9, 142.0, 137.9 (d, J_{CF} = 3.0 Hz), 130.3 (d, J_{CF} = 7.5 Hz, 2C), 128.7 (2C), 128.6 (2C), 127.4, 126.9, 124.4, 123.9, 122.4, 120.6, 115.3 (d, J_{CF} = 21.0 Hz), 111.5, 46.9; IR (neat): ν = 2923, 2857, 1893, 1602, 1505, 1452, 1227, 1099, 809, 745 cm^{-1}; EI-MS: m/z = 303(M^++1, 21%), 302(100%), 301 (23%), 225 (36%), 207 (25%).

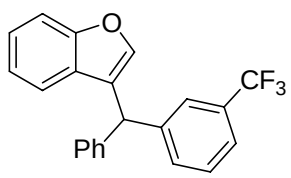
Spectral data for 3-(biphenyl-4-yl(phenyl)methyl)benzofuran (7g):



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.51–7.44 (m, 4H), 7.39 (d, *J* = 8.3 Hz, 1H), 7.33 (dt, *J* = 7.3, 1.3 Hz, 1H), 7.26–7.15 (m, 10H), 7.08–7.02 (m, 2H), 6.98 (d, *J* = 8.0, 1.3 Hz, 1H), 5.48 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 155.8, 144.0, 142.2, 141.3, 140.7, 139.5, 129.2 (2C), 129.0 (2C), 128.8 (2C), 128.7, 128.6 (2C), 127.0, 126.9 (2C), 126.8 (2C), 126.7, 124.3, 123.9, 122.4, 120.7, 111.5, 47.3 IR (neat): ν = 3027, 2906, 1585, 1443, 1176, 1085, 851, 767 cm^{-1}; EI-MS: m/z = 361(M^++1, 33%), 360(100%), 359 (20%), 283 (23%), 207 (11%).

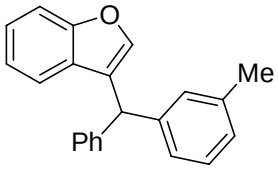
Supplementary Material (ESI) for Chemical Communications
This journal is (c) The Royal Society of Chemistry 2011

Spectral data for 3-(phenyl(3-(trifluoromethyl)phenyl)methyl)benzofuran (7h):



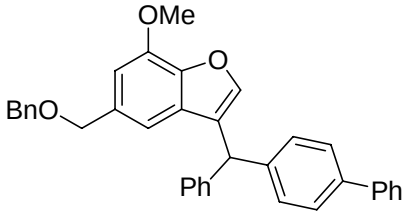
^{1}H NMR (600 MHz, $CDCl_3$): δ 7.46–7.35 (m, 6H), 7.22–7.15 (m, 5H), 7.05–7.00 (m, 2H), 6.93 (s, 1H), 5.51 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$): δ 156.2, 144.4, 143.6, 141.6, 132.5, 130.9, 129.4, 129.1 (2C), 129.1 (2C), 128.8, 127.6, 127.5, 125.9, 124.9, 124.1, 123.7, 122.9, 120.8, 111.9, 47.8; IR (neat): ν = 3042, 2908, 1587, 1462, 1179, 1089, 862, 753 cm^{-1}; EI-MS: m/z = 353(M^++1, 26%), 352(100%), 351 (23%), 275 (38%), 207 (38%), 178 (15%).

Spectral data for 3-(phenyl(m-tolyl)methyl)benzofuran (7i):



^{1}H NMR (300 MHz, $CDCl_3$): δ 7.48 (d, *J* = 5.4 Hz, 1H), 7.31–7.03 (m, 13H), 5.49 (s, 1H), 2.31 (s, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 156.1, 144.3 (2C), 142.7, 142.5, 138.4, 129.9, 129.1 (2C), 128.8 (2C), 128.7 (2C), 127.8, 127.0, 126.2, 124.6, 122.7, 121.0, 111.8, 48.0, 21.8; IR (neat): ν = 3029, 2920, 1600, 1452, 1182, 1098, 856, 744 cm^{-1}; EI-MS: m/z = 299(M^++1, 30%), 298 (100%), 297 (18%), 283 (14%), 221 (21%), 207 (24%), 178 (16%).

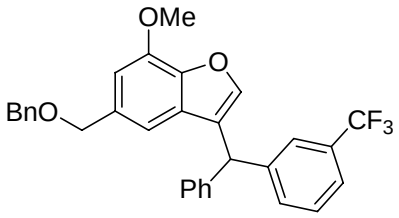
Spectral data for 5-(benzyloxymethyl)-3-(biphenyl-4-yl(phenyl)methyl)-7-methoxybenzofuran (7j):



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.51–7.45 (m, 4H), 7.35–7.32 (m, 2H), 7.26–7.17 (m, 13H), 6.99 (d, *J* = 1.0 Hz, 1H), 6.76 (s, 1H), 6.65 (d, *J* = 1.0 Hz, 1H), 5.46 (s, 1H), 4.41(s, 2H), 4.37 (s, 2H), 3.93 (s, 3H);^{13}C NMR (100 MHz, $CDCl_3$): δ 145.4, 144.7, 144.4, 142.1, 41.3, 140.7, 139.5, 138.2, 133.5, 129.2 (2C), 129.1, 128.8 (2C), 128.7 (2C), 128.6 (2C), 128.4 (2C), 127.9, 127.6 (3C), 127.2 (2C), 127.0, 126.8, 124.3, 112.4, 106.6, 72.3, 71.7, 56.1, 47.2; IR (neat): ν = 3386, 2969, 1600, 1459, 1372, 1143, 950, 734cm^{-1}; EI-MS: m/z = 405(M^++1, 28%), 404(100%), 396 (6%).

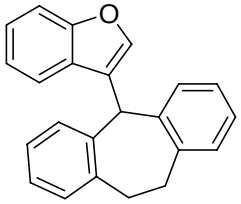
Supplementary Material (ESI) for Chemical Communications
This journal is (c) The Royal Society of Chemistry 2011

Spectral data for 5-(benzyloxymethyl)-7-methoxy-3-(phenyl(3-(trifluoromethyl)phenyl) methyl)benzofuran (7k):



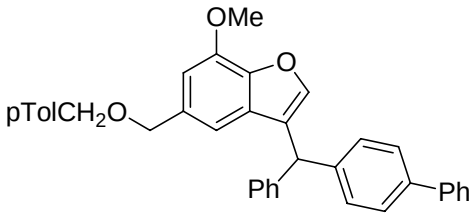
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.50 (s, 1H), 7.43–7.38 (m, 1H), 7.34–7.18 (m, 12H), 6.98 (d, *J* = 1.3 Hz, 1H), 6.83 (d, *J* = 1.0 Hz, 1H), 6.65 (d, *J* = 1.3 Hz, 1H), 5.55 (s, 1H), 4.47(s, 2H), 4.43 (s, 2H), 3.99 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.5, 144.8, 144.4, 143.2, 141.2, 138.1, 133.8, 132.1, 130.9 (d, *J* = 30.0 Hz), 129.0, 128.8 (2C), 128.7 (2C), 128.4 (2C), 128.3, 127.8 (2C), 127.6, 127.1, 125.5 (q, *J* = 3.7 Hz), 125.1 (d, *J* = 277.3 Hz), 123.8, 123.7, 112.0, 106.8, 72.2, 71.7, 56.1, 47.4; IR (neat): ν = 3468, 2922, 2855, 1600, 1488, 1328, 1076, 843, 739 cm^{-1}; EI-MS: m/z = 397(M^++1, 42%), 396(100%), 395 (12%), 91.3 (18%).

Spectral data for 3-(10,11-dihydro-5H-dibenzo[a,d]cyclohepten-5-yl)benzofuran (7l):



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.46–7.40 (m, 3H), 7.26–7.13 (m, 7H), 6.99 (t, *J* = 8 Hz, 1H), 6.82-6.80 (m, 2H), 5.26 (s, 1H), 3.35-3.26 (m, 2H), 2.79-2.71 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 156.3, 143.7 (2C), 140.5 (2C), 139.4, 131.1 (2C), 131.0 (2C), 127.8 (2C), 127.2, 126.5 (2C), 125.3, 124.3, 122.6, 121.2, 111.7, 51.4, 32.5 (2C); IR (neat): ν = 2925, 1489, 1449, 1170, 1093, 853, 746 cm^{-1}; EI-MS: m/z = 311(M^++1, 12%), 310(45%), 193 (23%), 192 (100%), 191 (99%).

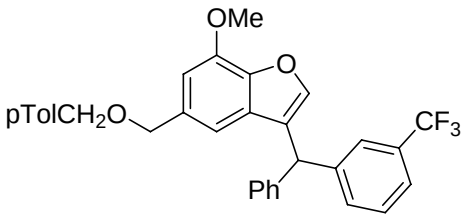
Spectral data for 3-(biphenyl-4-yl(phenyl)methyl)-7-methoxy-5-((4-methylbenzyloxy) methyl)benzofuran (7m):



^{1}H NMR (400 MHz, $CDCl_3$): δ 7.51–7.45 (m, 4H), 7.36–7.32 (m, 2H), 7.27–7.16 (m, 8H), 7.07 (d, *J* = 8.3 Hz, 1H), 7.01 (d, *J* = 8.0 Hz, 2H), 6.99 (d, *J* = 1.3 Hz, 1H), 6.76 (d, *J* = 1.3 Hz, 1H), 6.65 (s, 1H), 5.46 (s, 1H), 4.38 (s, 2H), 4.33 (s, 2H), 3.93 (s, 3H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.4, 144.7, 144.4, 142.2, 141.3, 140.7, 139.5, 137.3, 135.1, 133.7, 129.2 (2C), 129.0 (2C), 128.8 (2C), 128.7 (2C), 128.6 (2C), 128.0 (2C), 127.2 (3C), 127.0 (2C), 126.8, 124.3, 112.4, 106.6, 72.1, 71.5, 56.1, 47.2, 21.1; IR (neat): ν = 3436, 2920, 2853, 1601, 1486, 1379, 1145, 910, 806 cm^{-1}; EI-MS: m/z = 405(M^++1, 35%), 404(100%), 105 (7%).

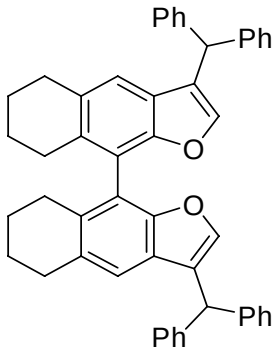
Supplementary Material (ESI) for Chemical Communications
This journal is (c) The Royal Society of Chemistry 2011

Spectral data for 7-methoxy-5-((4-methylbenzyloxy)methyl)-3-(phenyl(3-(trifluoromethyl) phenyl)methyl)benzofuran (7n):



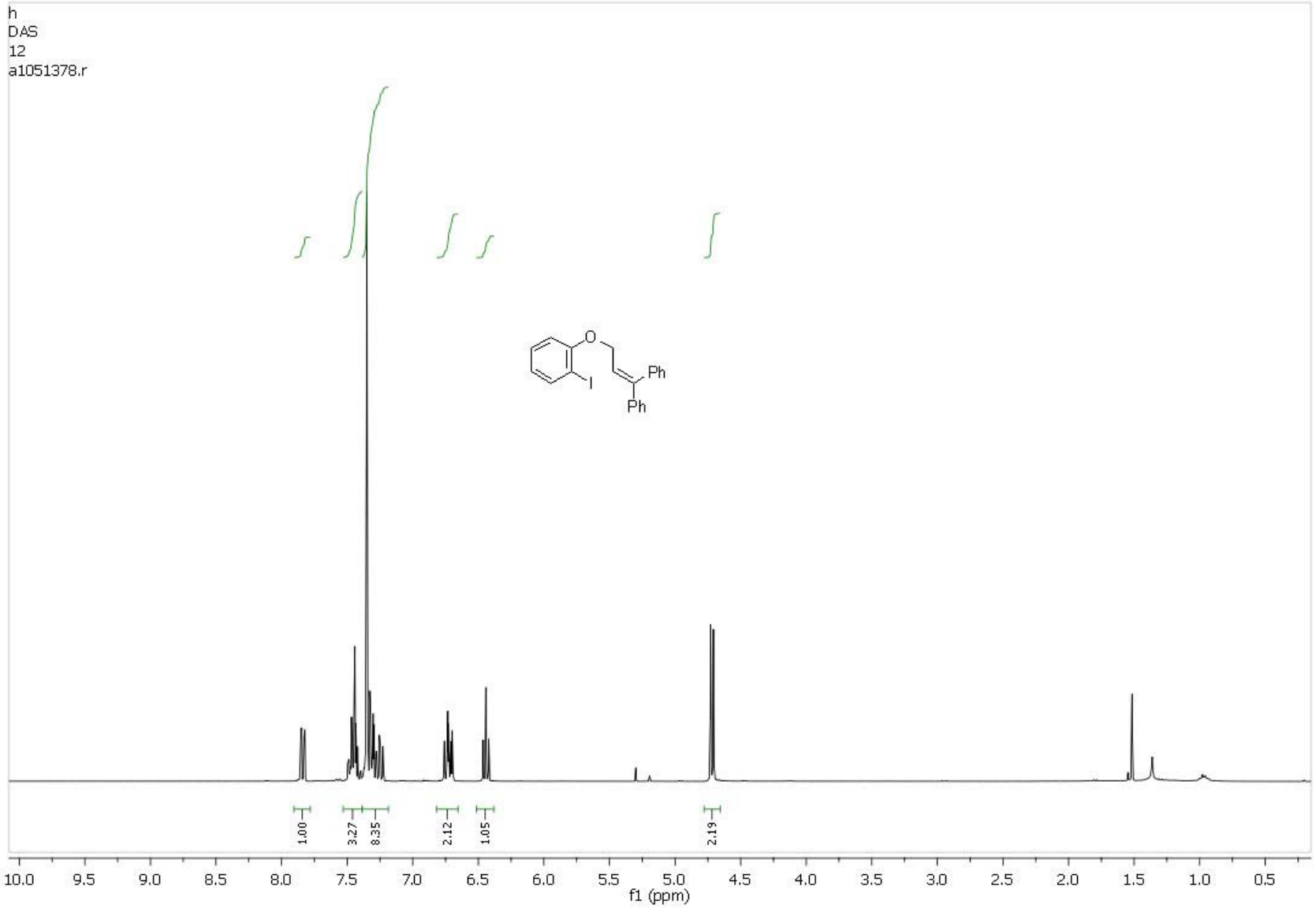
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.44 (s, 1H), 7.35–7.31 (m, 1H), 7.28–7.03 (m, 11H), 6.92 (d, *J* = 1.3 Hz, 1H), 6.76 (d, *J* = 1.0 Hz, 1H), 6.58 (d, *J* = 1.3 Hz, 1H), 5.48 (s, 1H), 4.38 (s, 2H), 4.33 (s, 2H), 3.93 (s, 3H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 145.4, 144.7, 144.4, 143.2, 141.2, 137.3, 135.1, 133.9, 132.1, 130.9 (d, *J* = 32.2 Hz), 129.0 (2C), 128.9, 128.8 (2C), 128.7 (2C), 128.6, 127.9 (2C), 127.1, 125.5 (q, *J* = 3.8 Hz), 125.1 (d, *J* = 276.7 Hz), 123.7, 123.6, 112.0, 106.8, 72.0, 71.5, 56.1, 47.4, 21.1; IR (neat): ν = 3431, 2909, 2863, 1605, 1476, 1383, 1162, 908, 796 cm^{-1}; EI-MS: m/z = 397(M^++1, 40%), 396 (100%), 395 (14%), 105 (14%).

Spectral data for 3,3'-dibenzhydryl-5,5',6,6',7,7',8,8'-octahydro-9,9'-binaphtho[2,3-b]furan (7o):

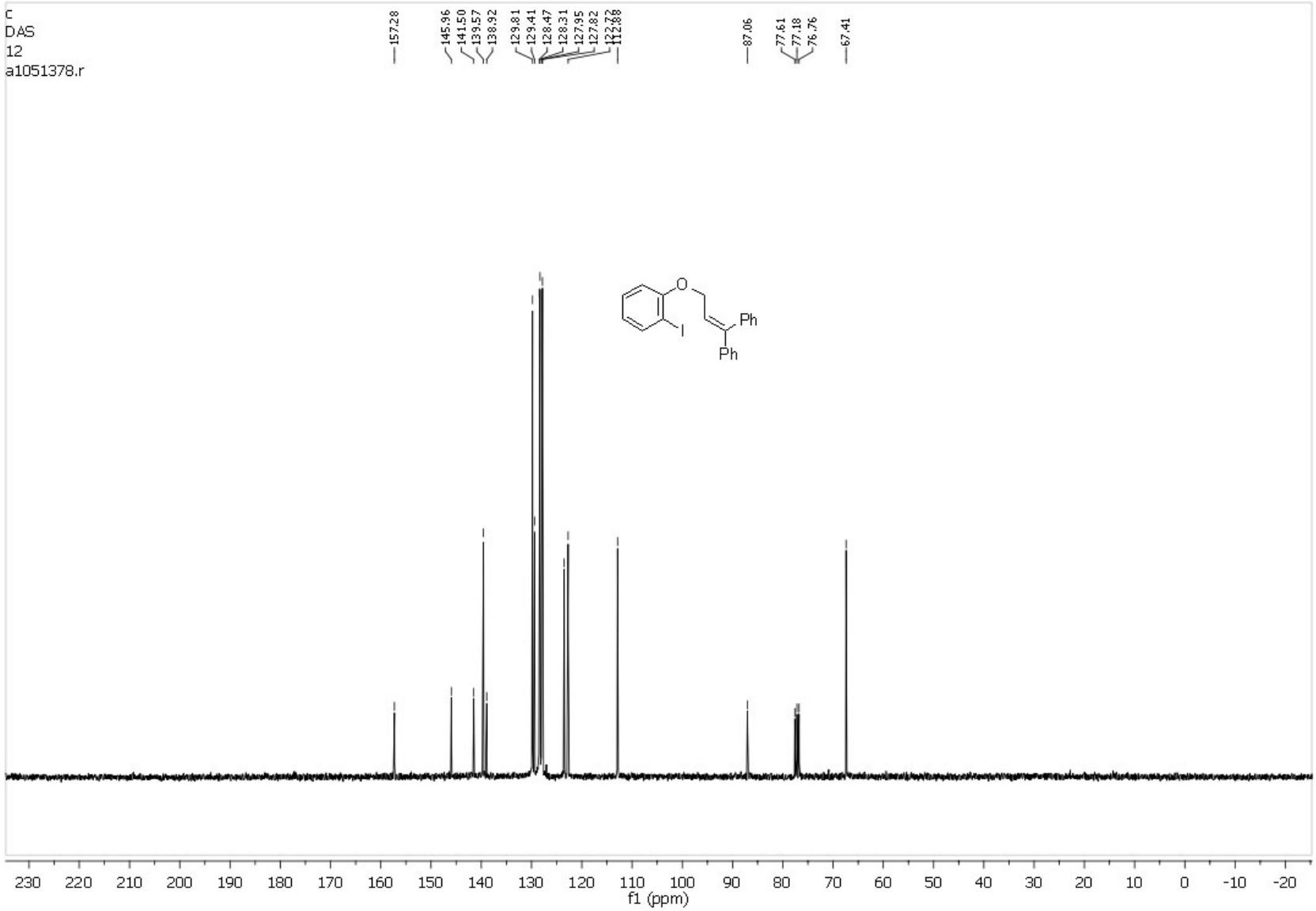


^{1}H NMR (400 MHz, $CDCl_3$): δ 7.25–7.14 (m, 20 H), 6.84 (s, 2 H), 6.74 (s, 2H), 5.42 (s, 2H), 2.75–2.72 (s, 4H), 2.42–2.40 (m, 4H), 1.69–1.53 (m, 8H) ^{13}C NMR (100 MHz, $CDCl_3$): δ 153.0 (2C), 144.1 (2C), 142.9 (2C), 142.8 (2C), 133.0 (2C), 132.3 (2C), 129.1 (8C), 128.8 (4C), 128.8 (4C), 126.9 (4C), 125.6 (2C), 123.7 (2C), 120.3 (2C), 118.6 (2C), 48.1 (2C), 30.6 (2C), 27.5 (2C), 23.5 (2C), 23.4 (2C); IR (neat): ν = 2926, 1580, 1445, 1241, 1099, 908, 698 cm^{-1}; EI-MS: m/z = 675(M^++1, 53%), 674 (100%).

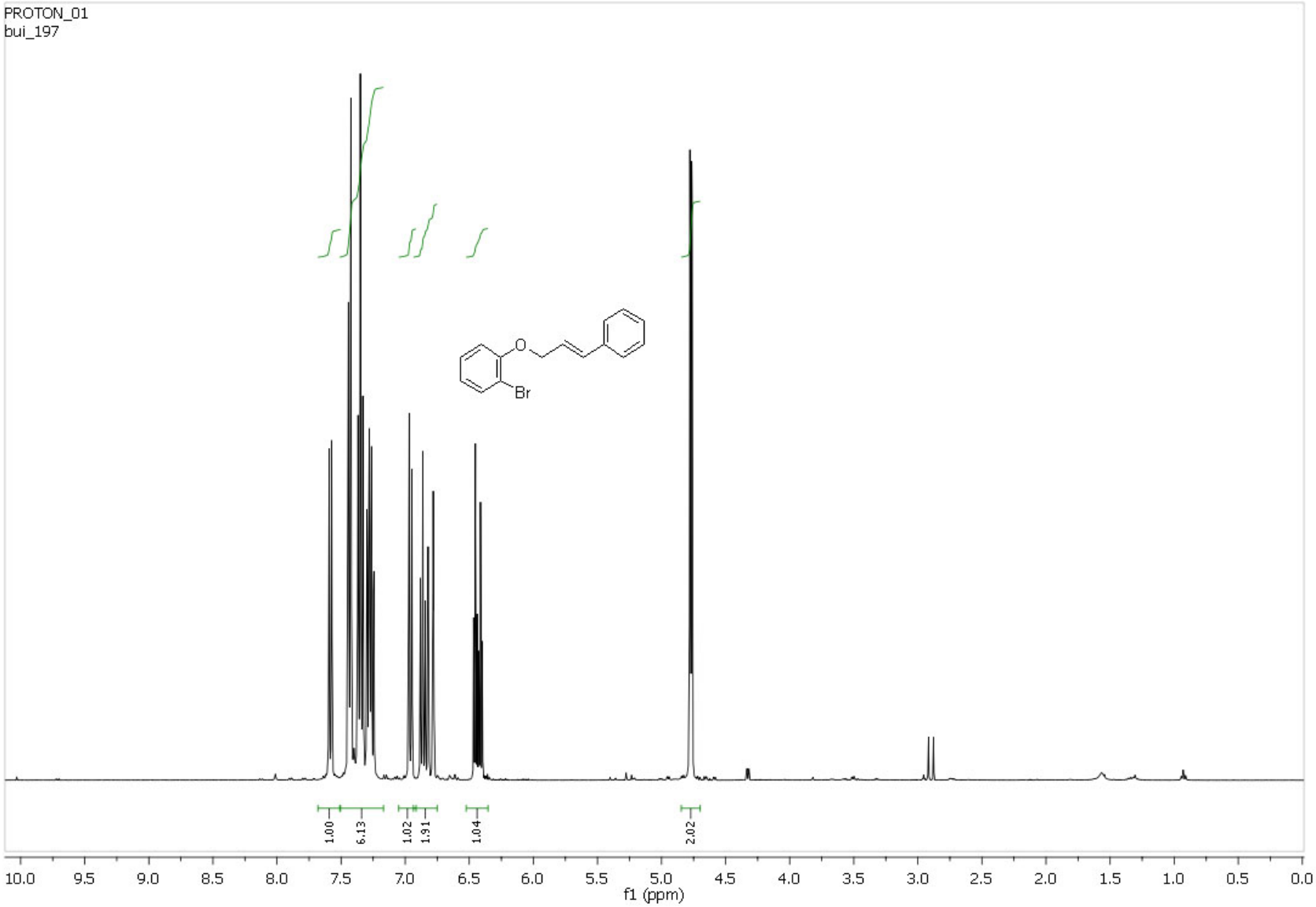
This journal is © The Royal Society of Chemistry 2011



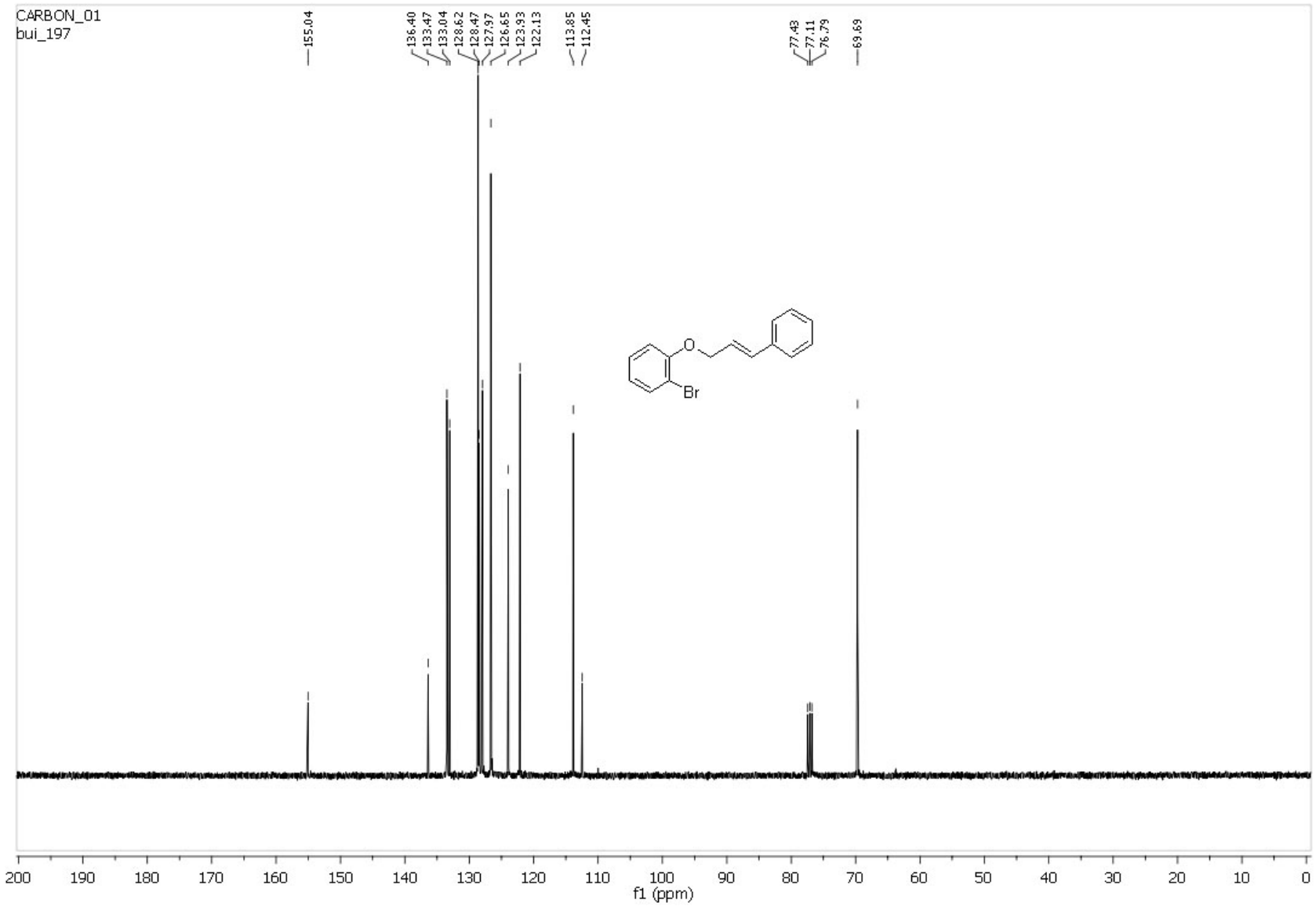
This journal is © The Royal Society of Chemistry 2011



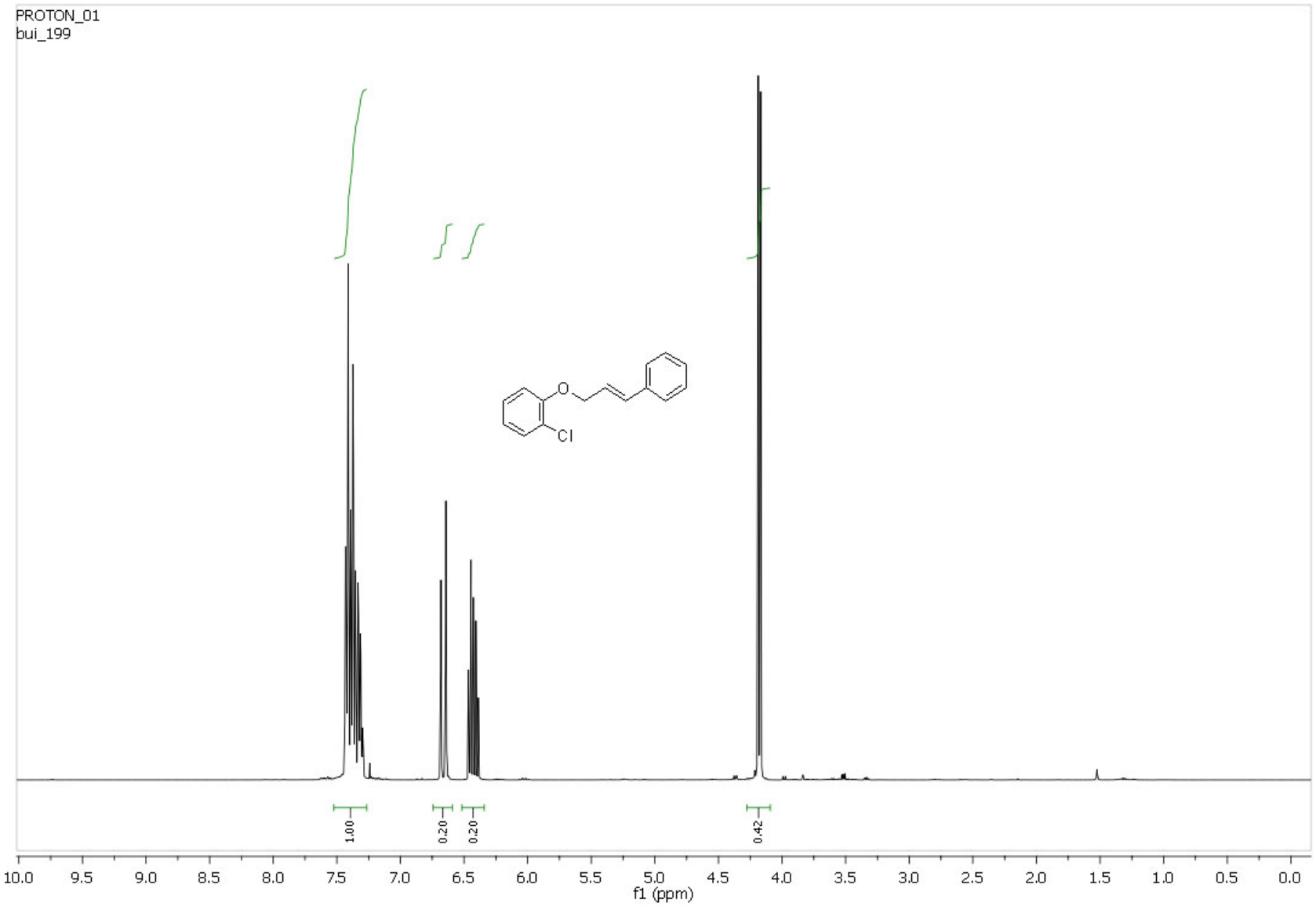
This journal is © The Royal Society of Chemistry 2011



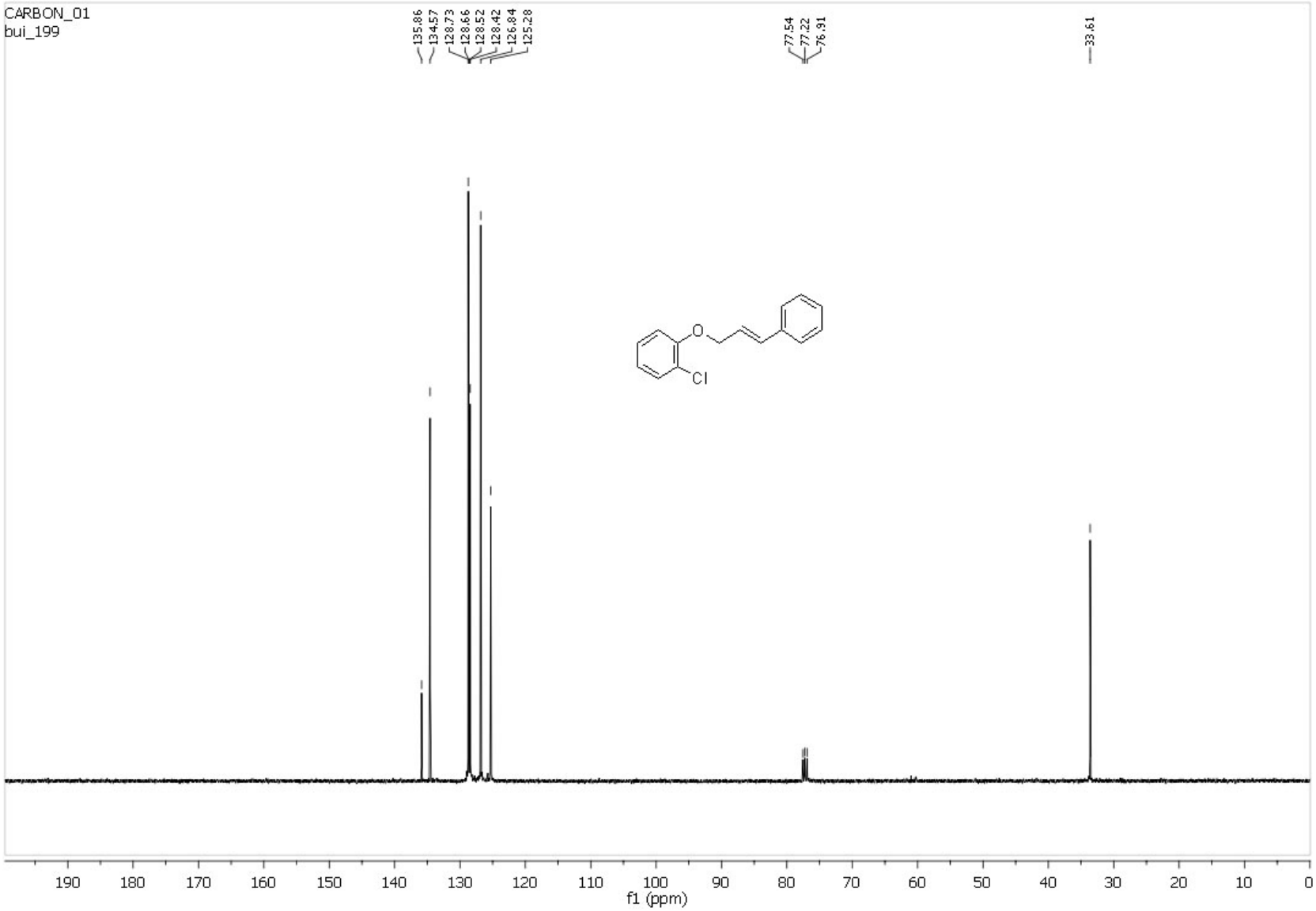
This journal is © The Royal Society of Chemistry 2011



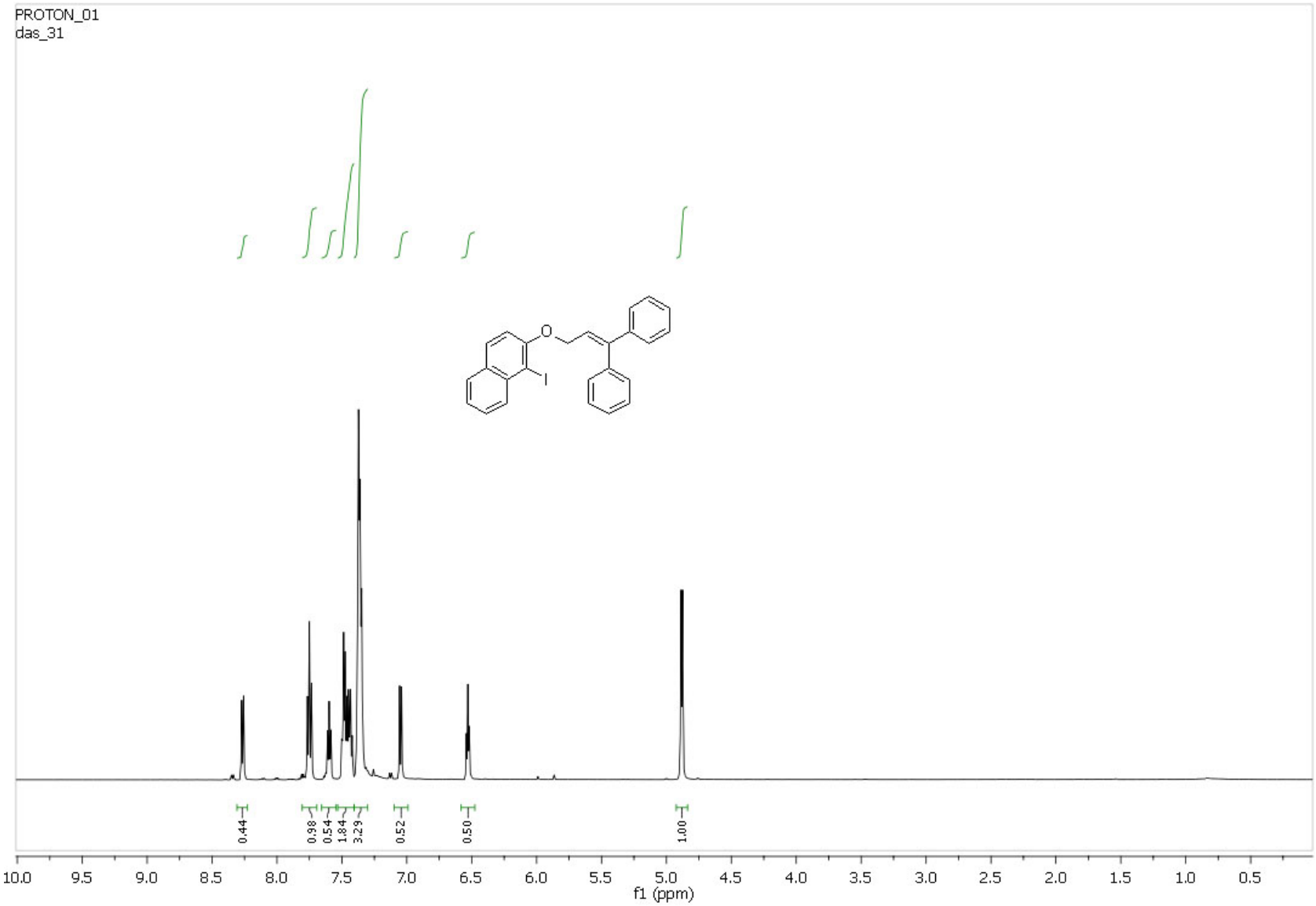
This journal is © The Royal Society of Chemistry 2011



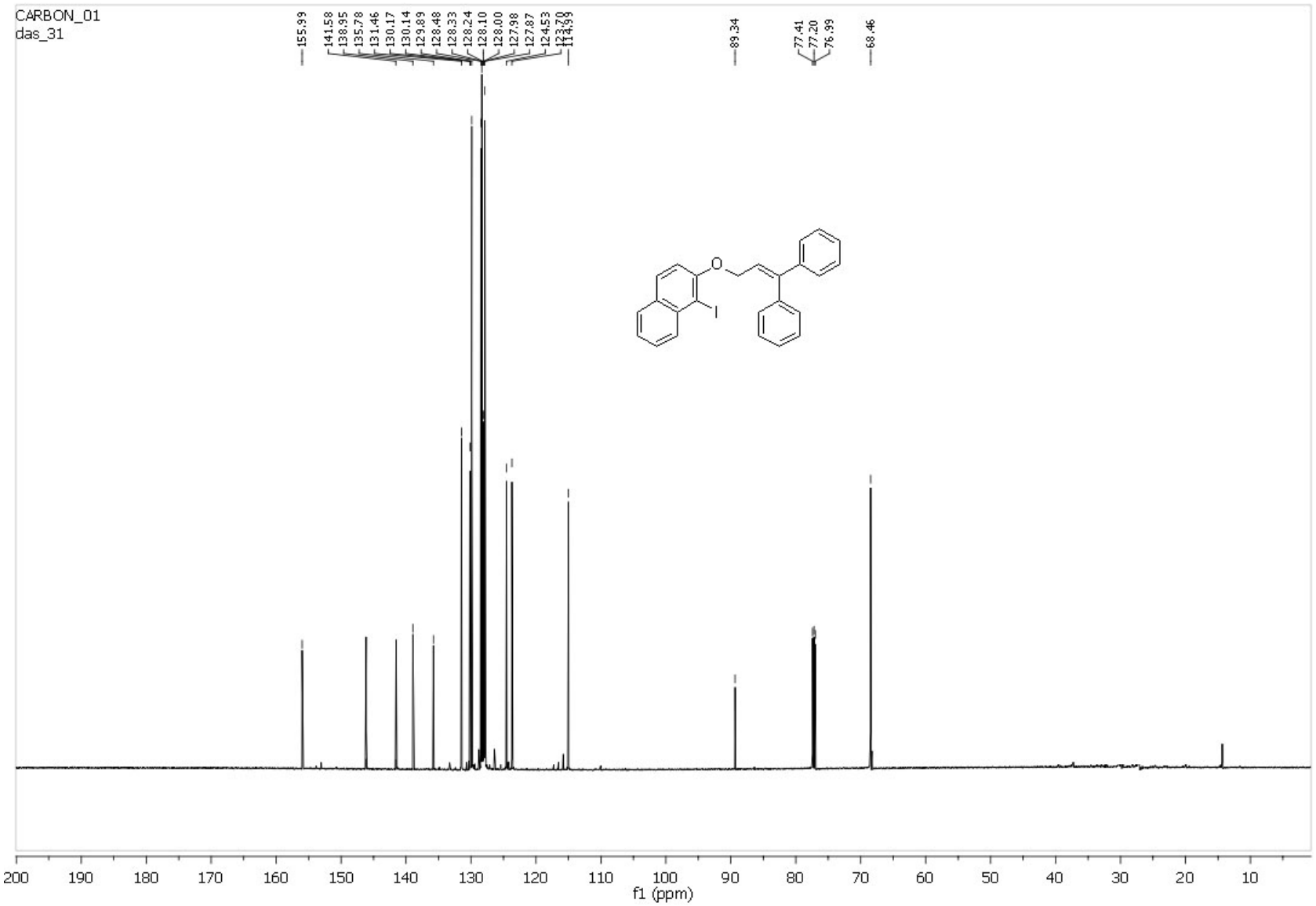
This journal is © The Royal Society of Chemistry 2011



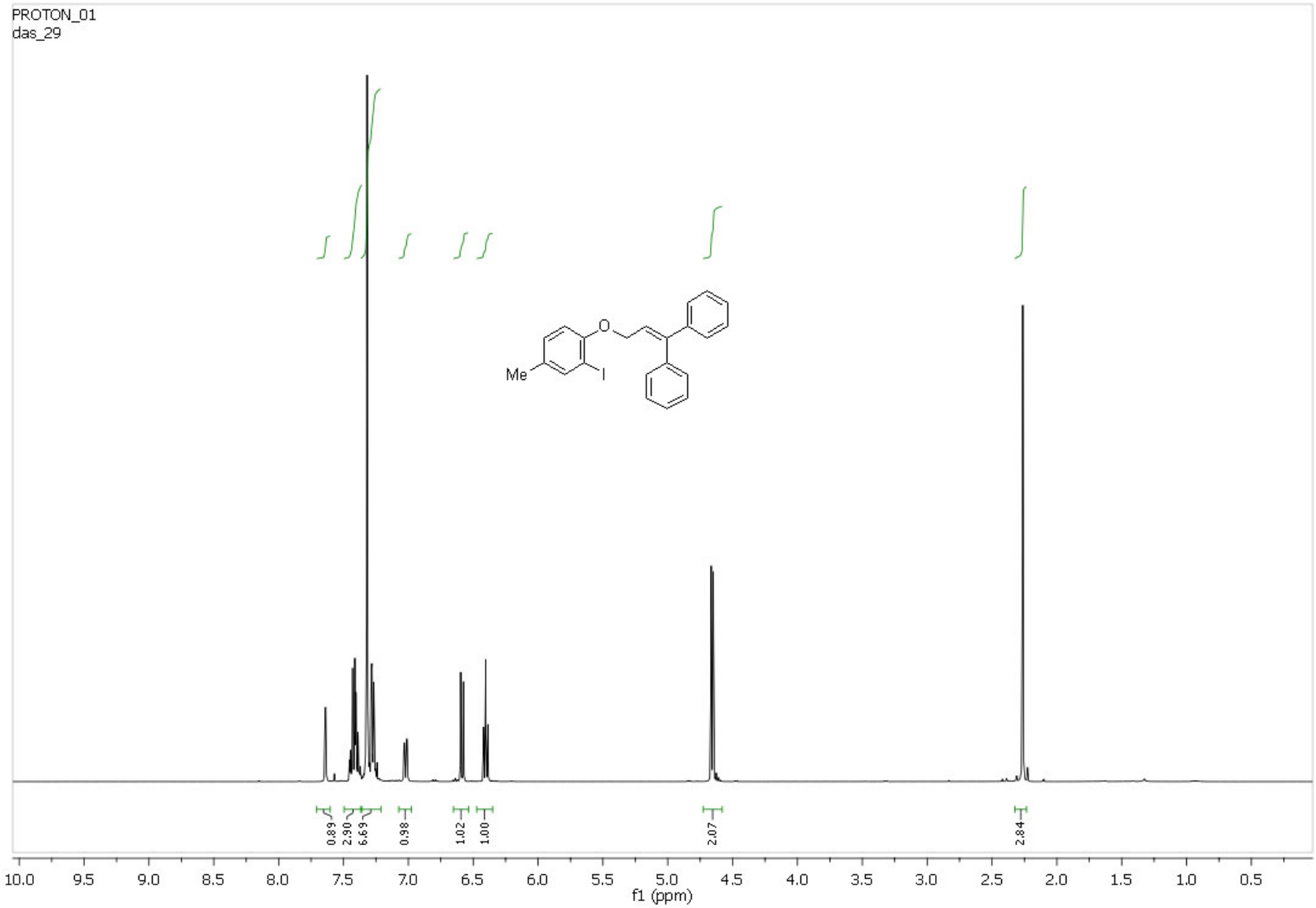
This journal is © The Royal Society of Chemistry 2011



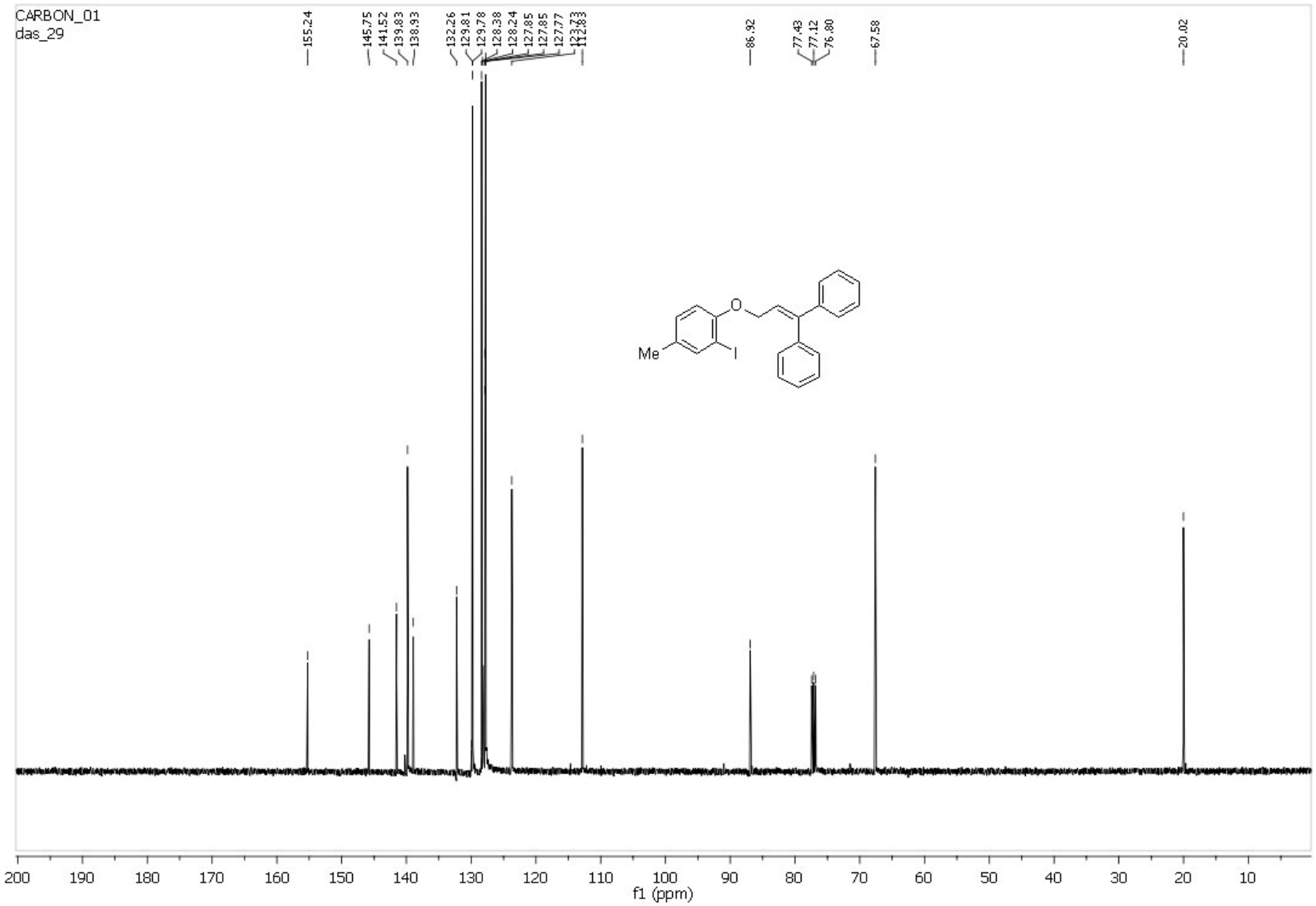
This journal is © The Royal Society of Chemistry 2011



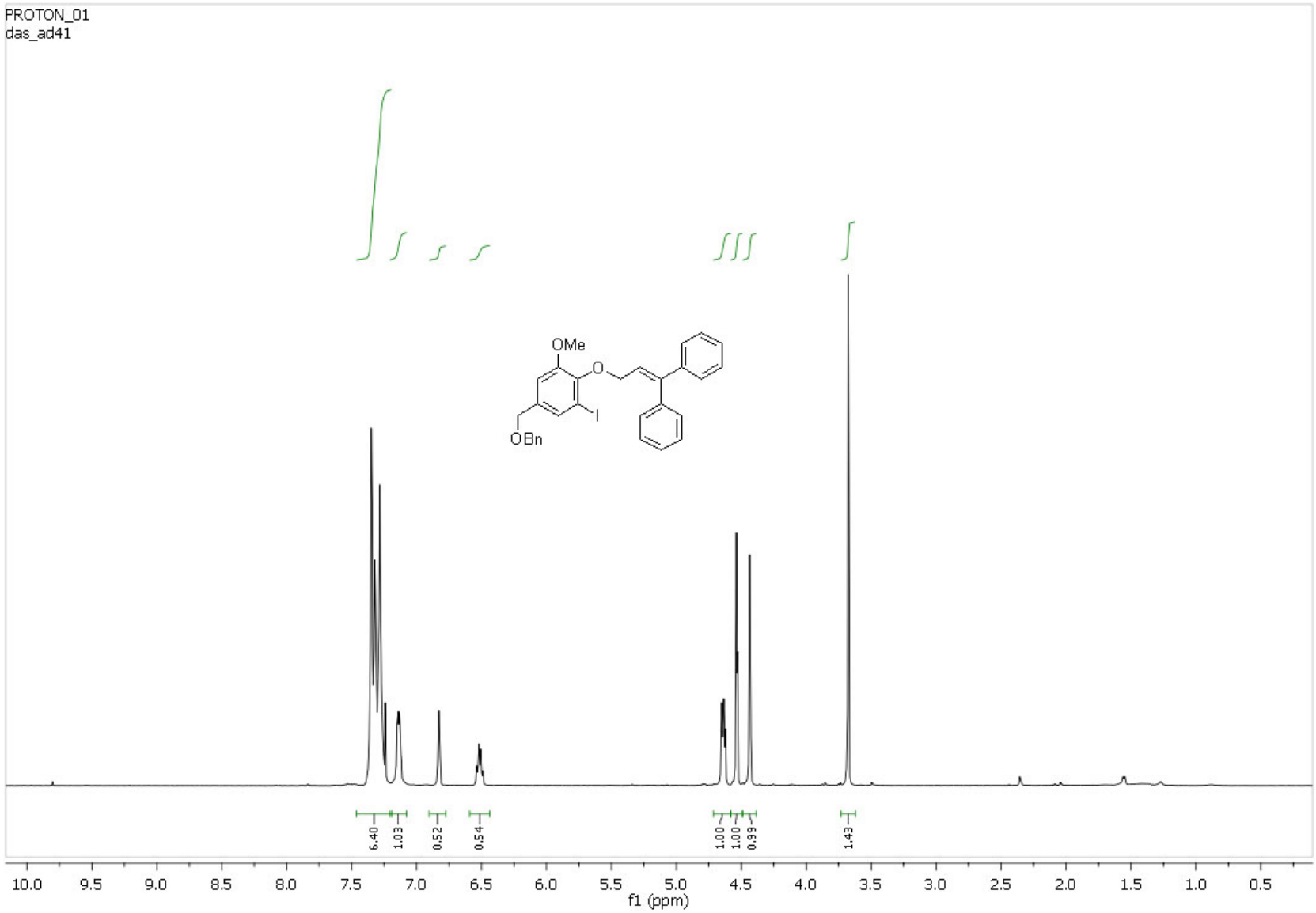
This journal is © The Royal Society of Chemistry 2011



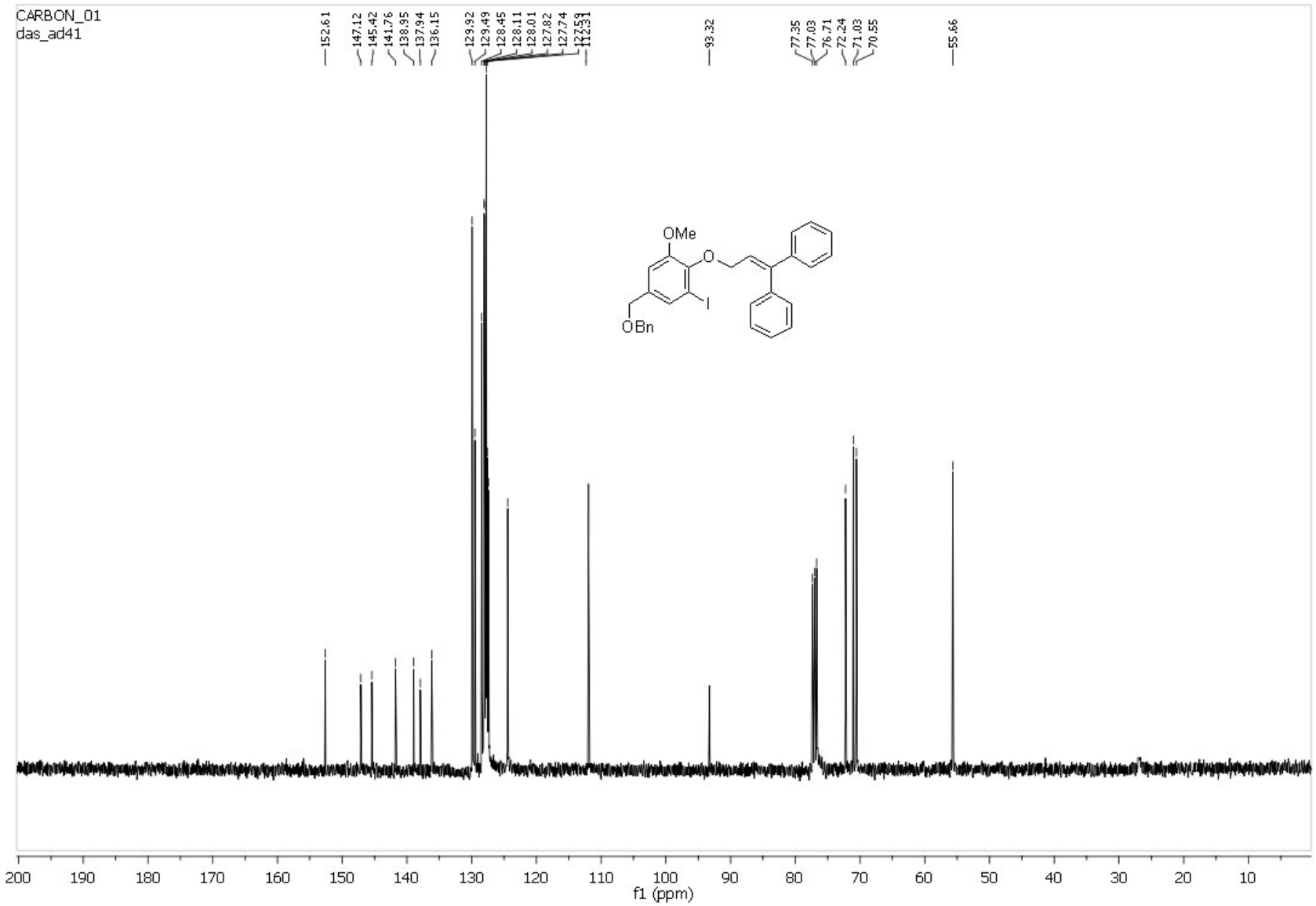
This journal is © The Royal Society of Chemistry 2011



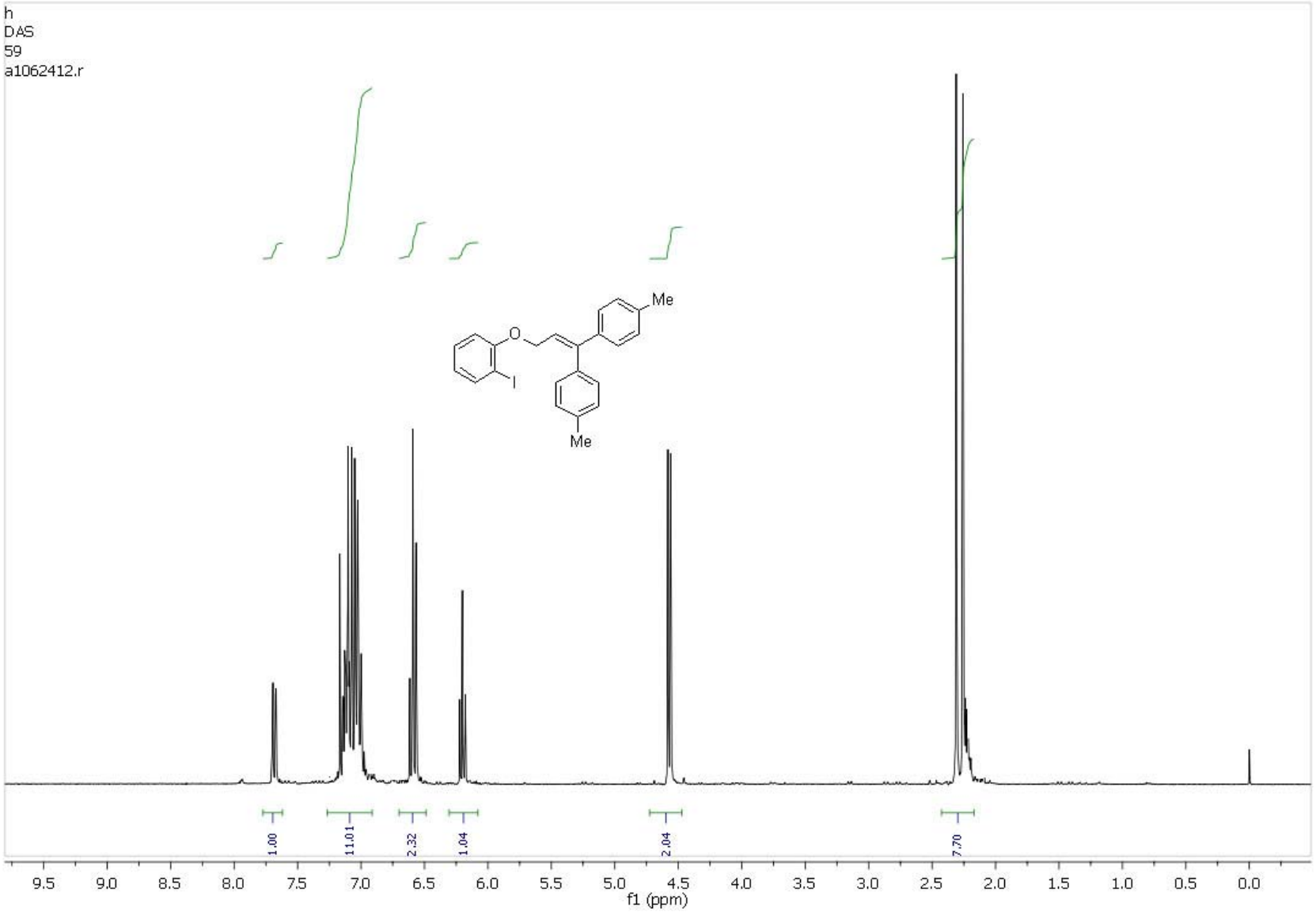
This journal is © The Royal Society of Chemistry 2011



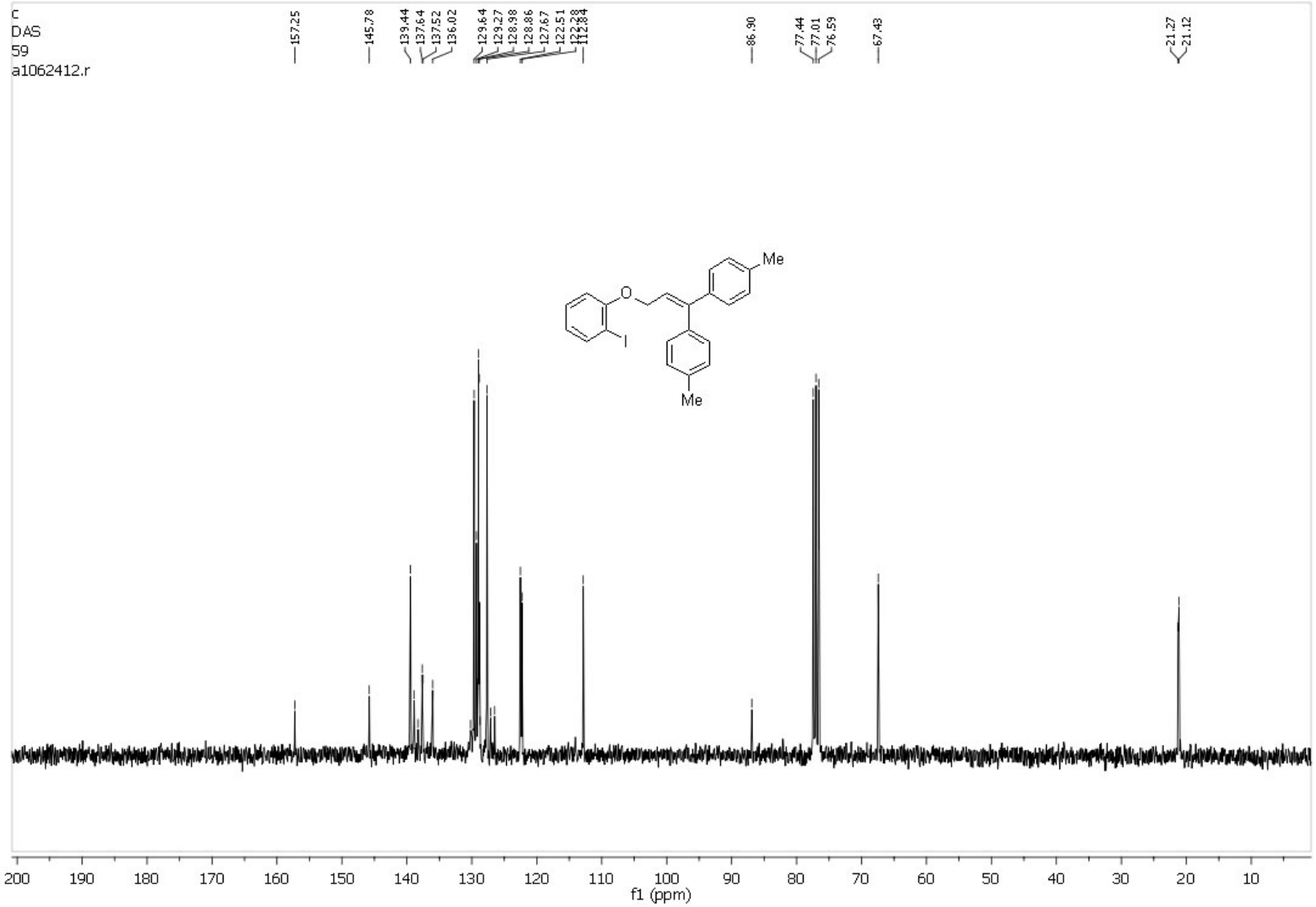
This journal is © The Royal Society of Chemistry 2011



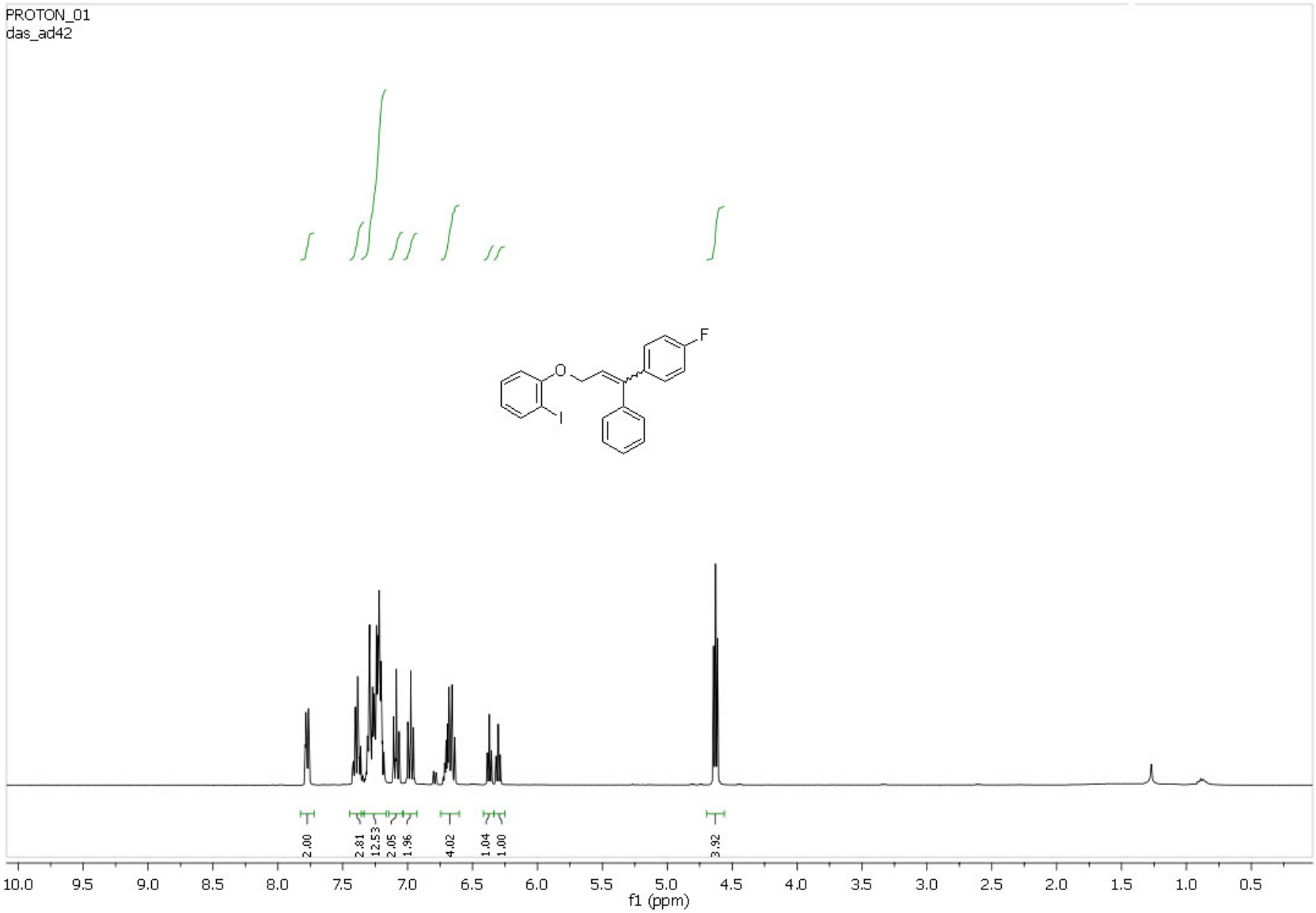
This journal is © The Royal Society of Chemistry 2011



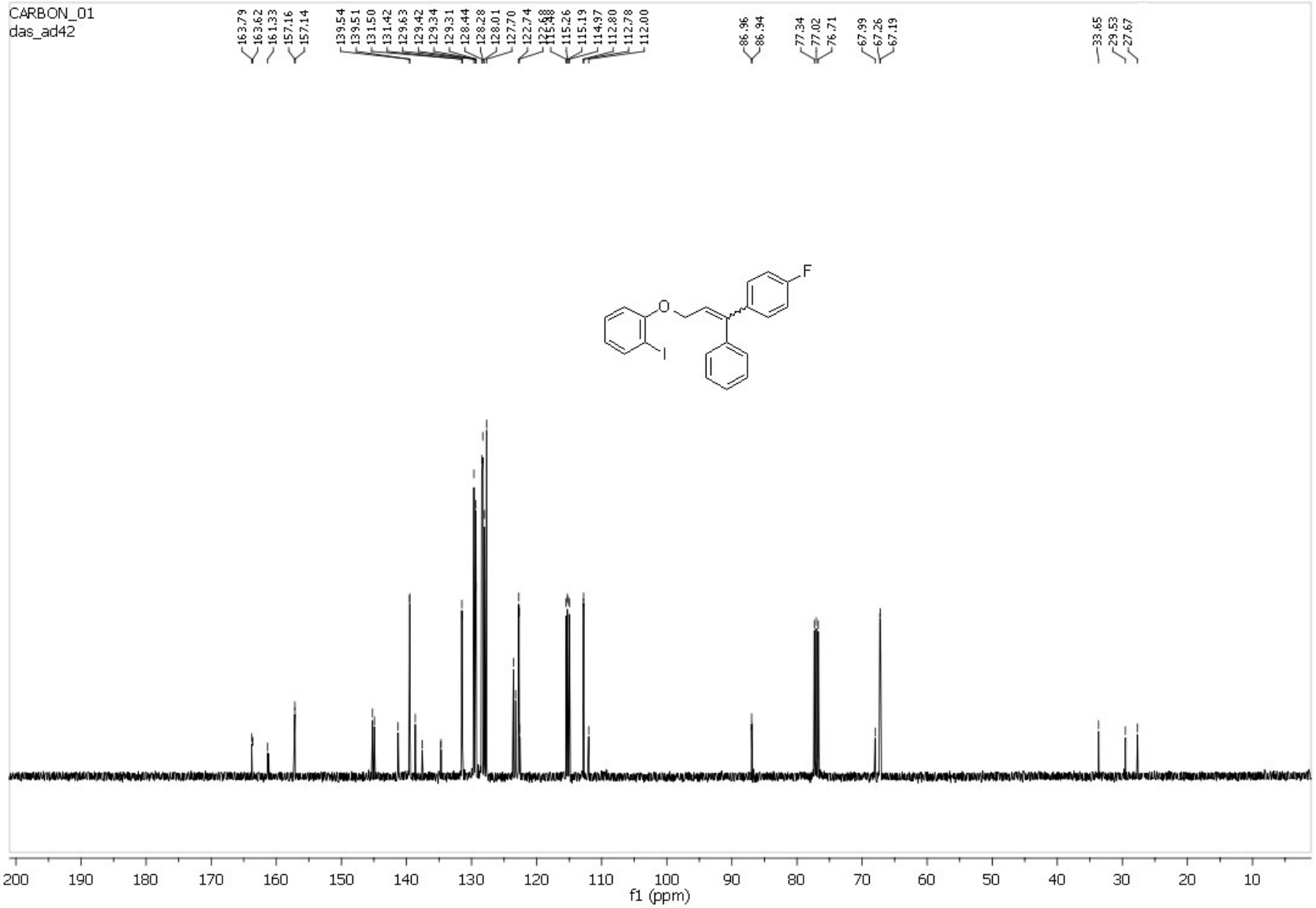
This journal is © The Royal Society of Chemistry 2011



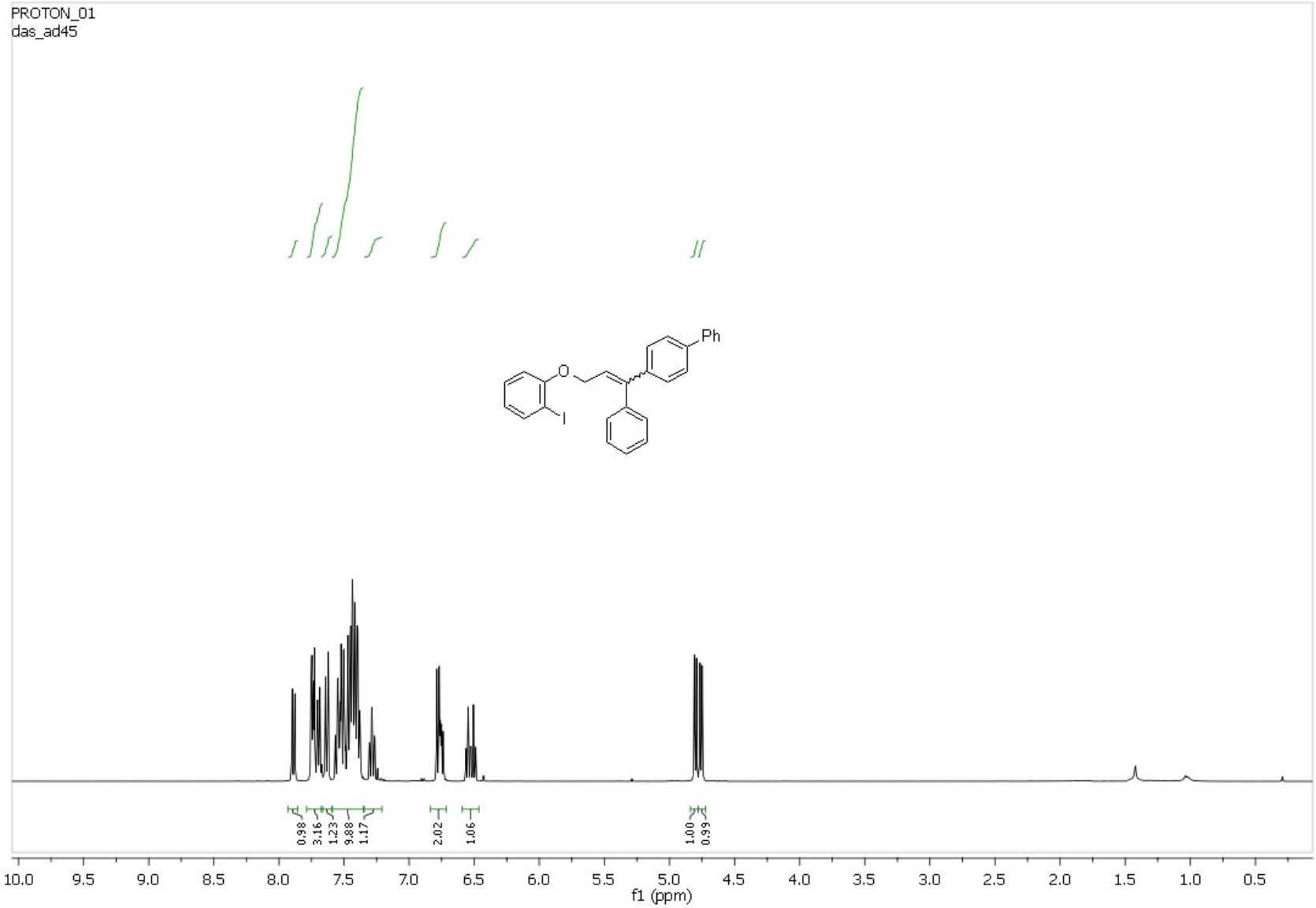
This journal is © The Royal Society of Chemistry 2011



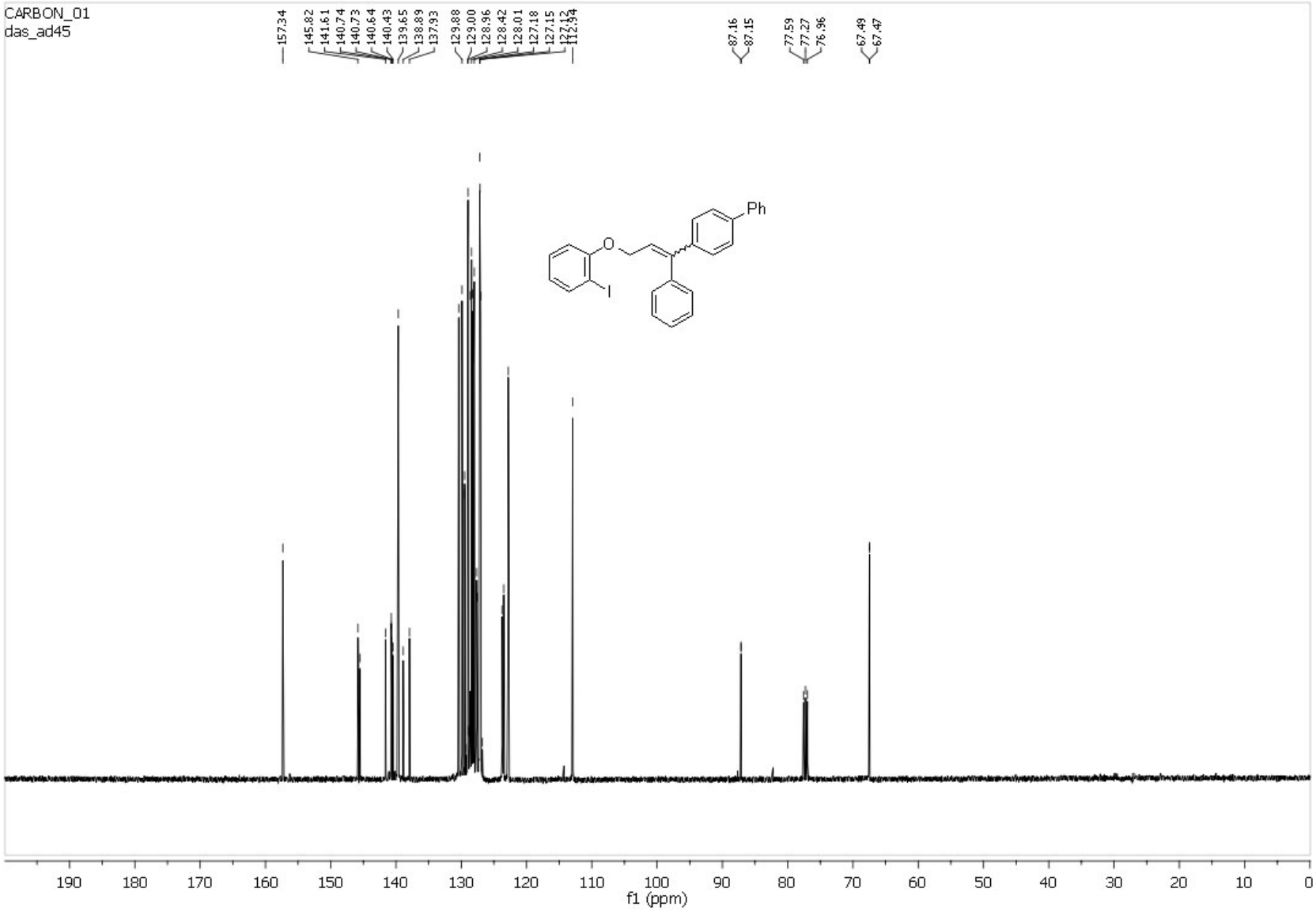
This journal is © The Royal Society of Chemistry 2011



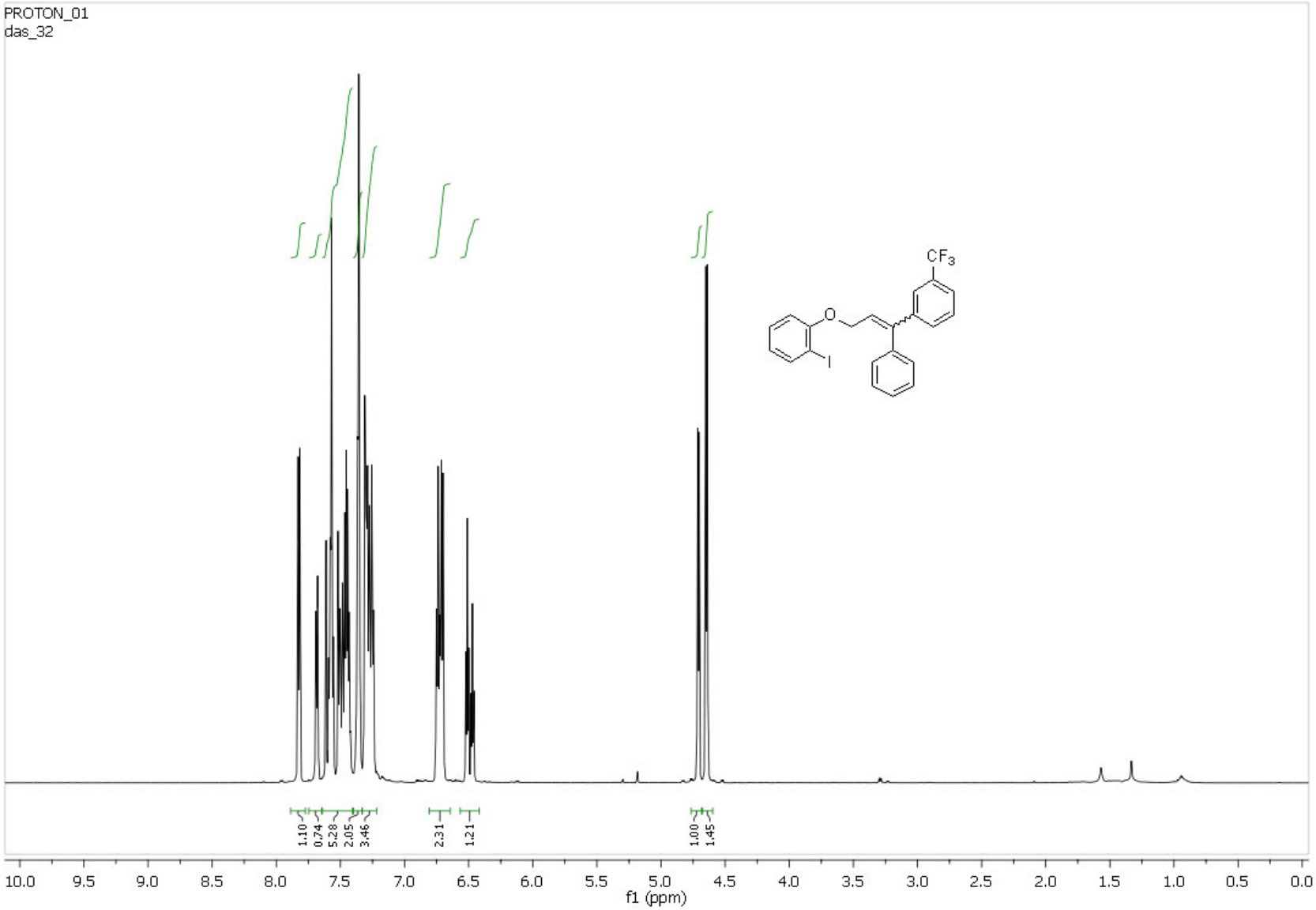
This journal is © The Royal Society of Chemistry 2011



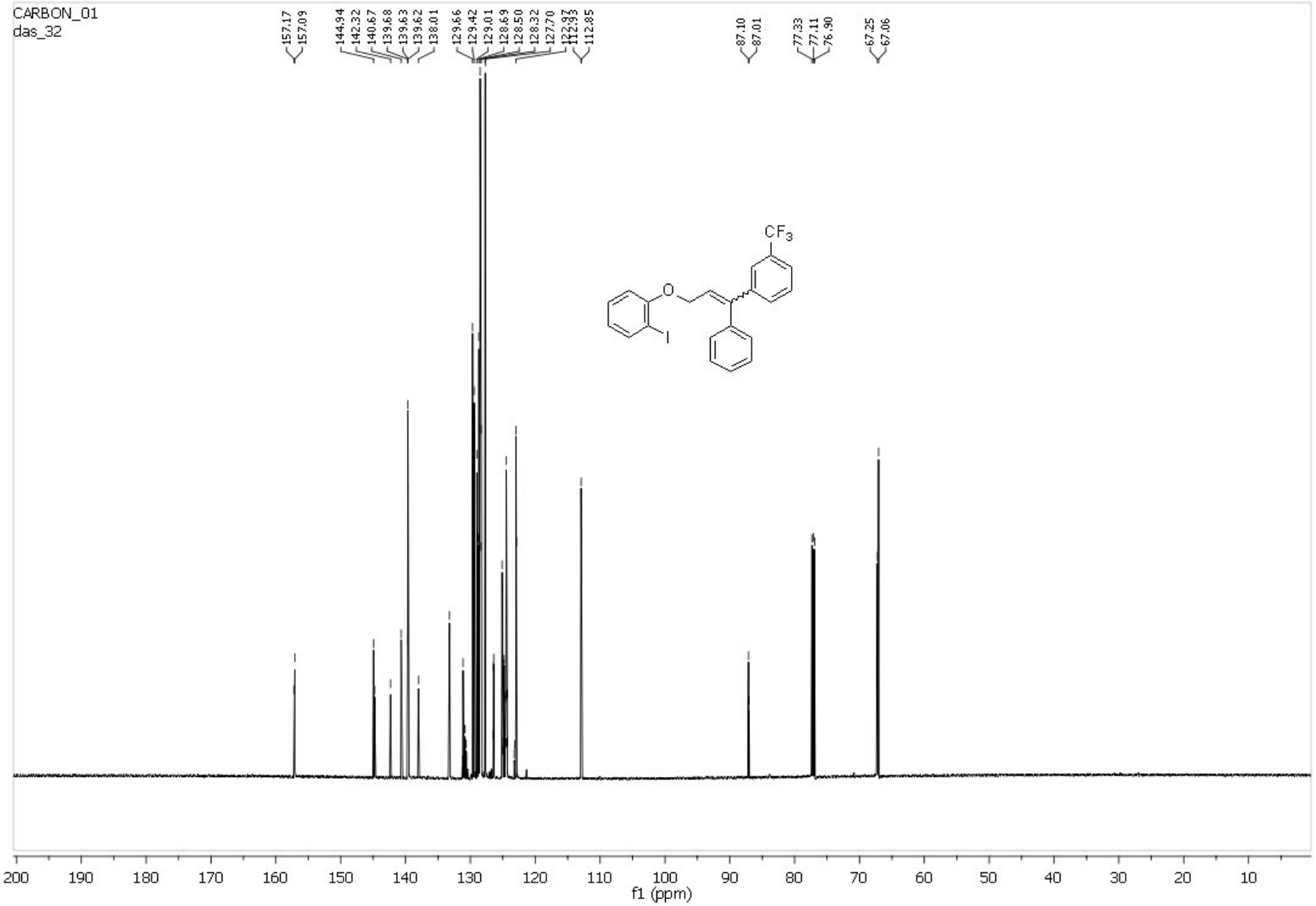
This journal is © The Royal Society of Chemistry 2011



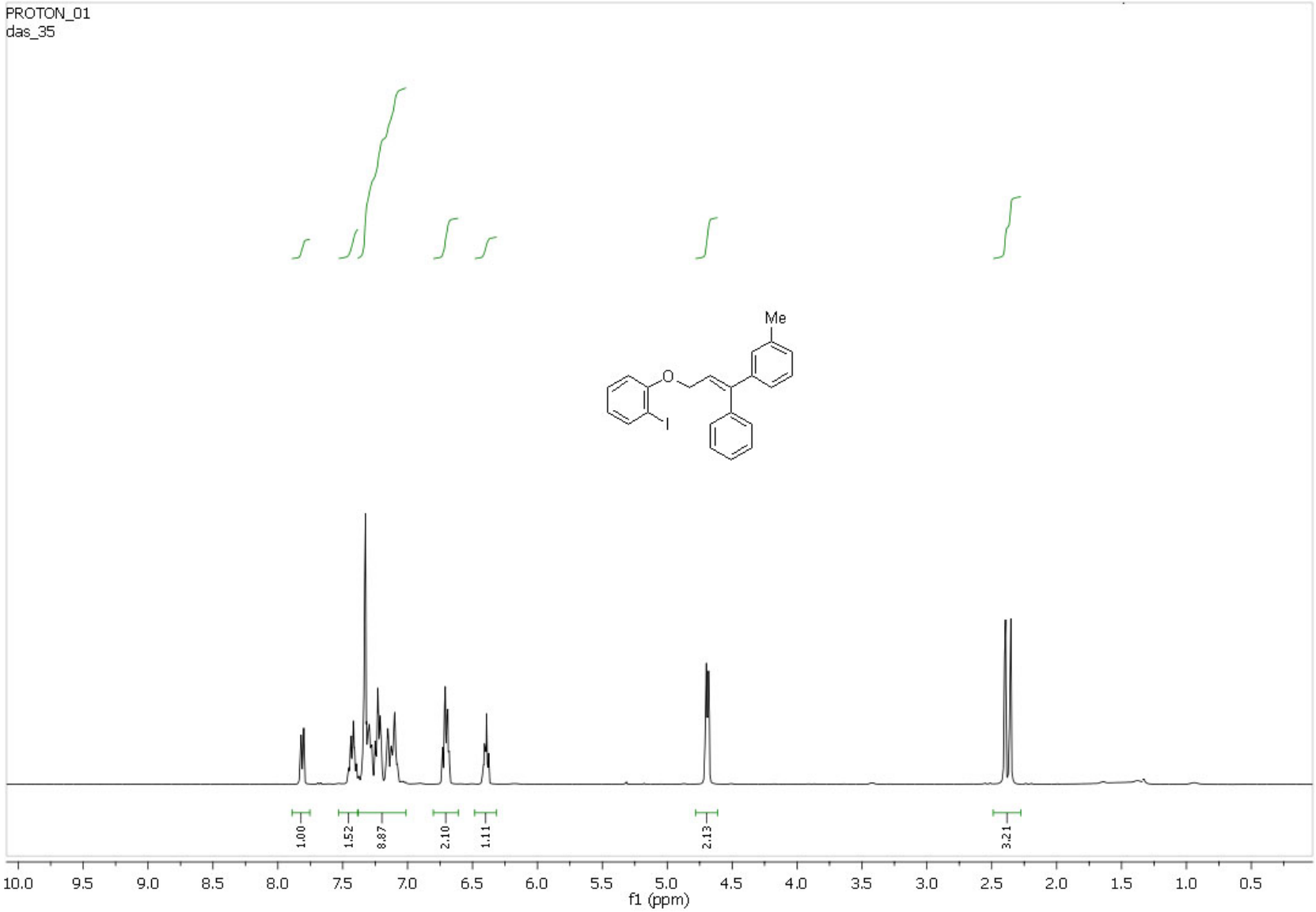
This journal is © The Royal Society of Chemistry 2011



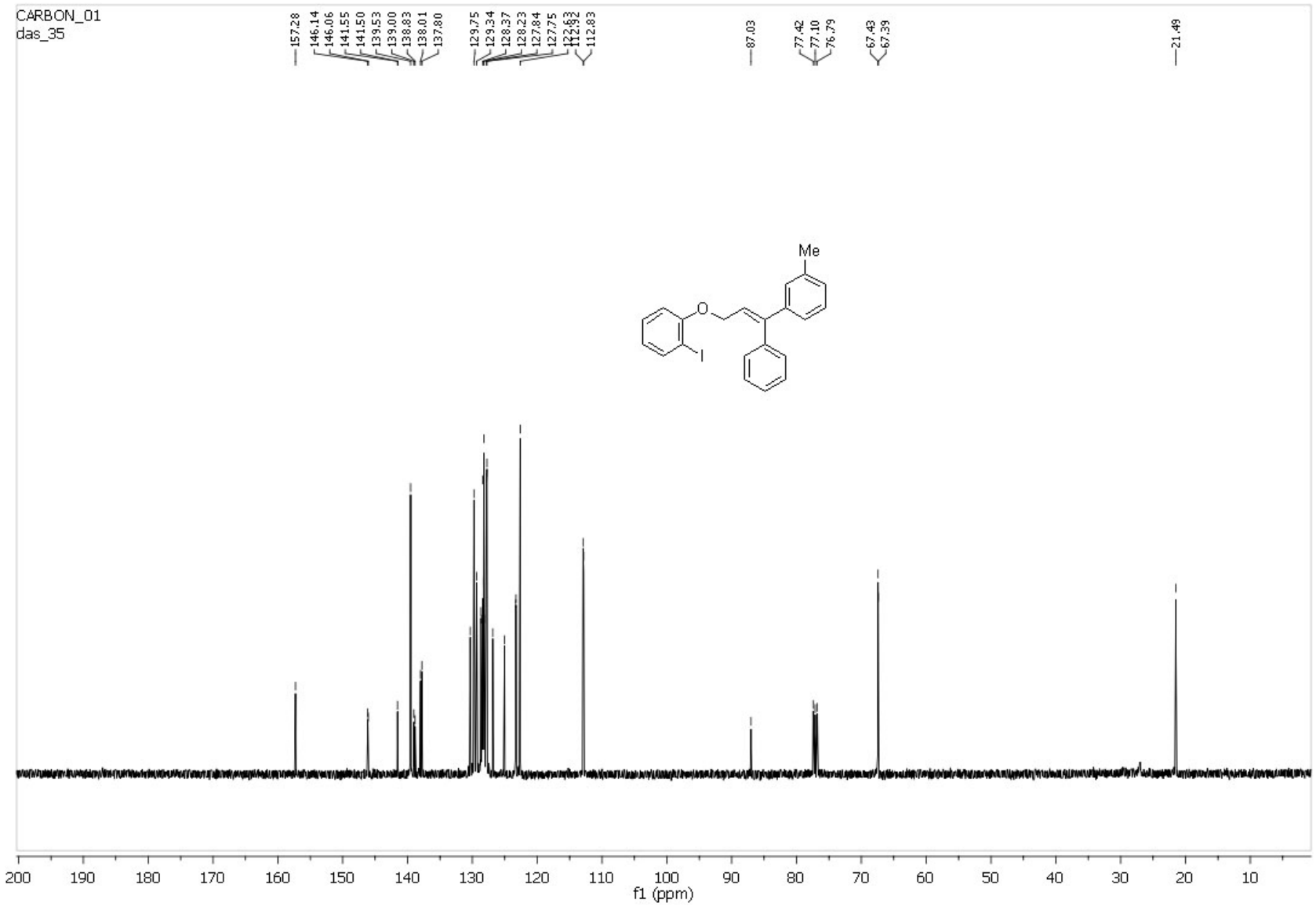
This journal is © The Royal Society of Chemistry 2011



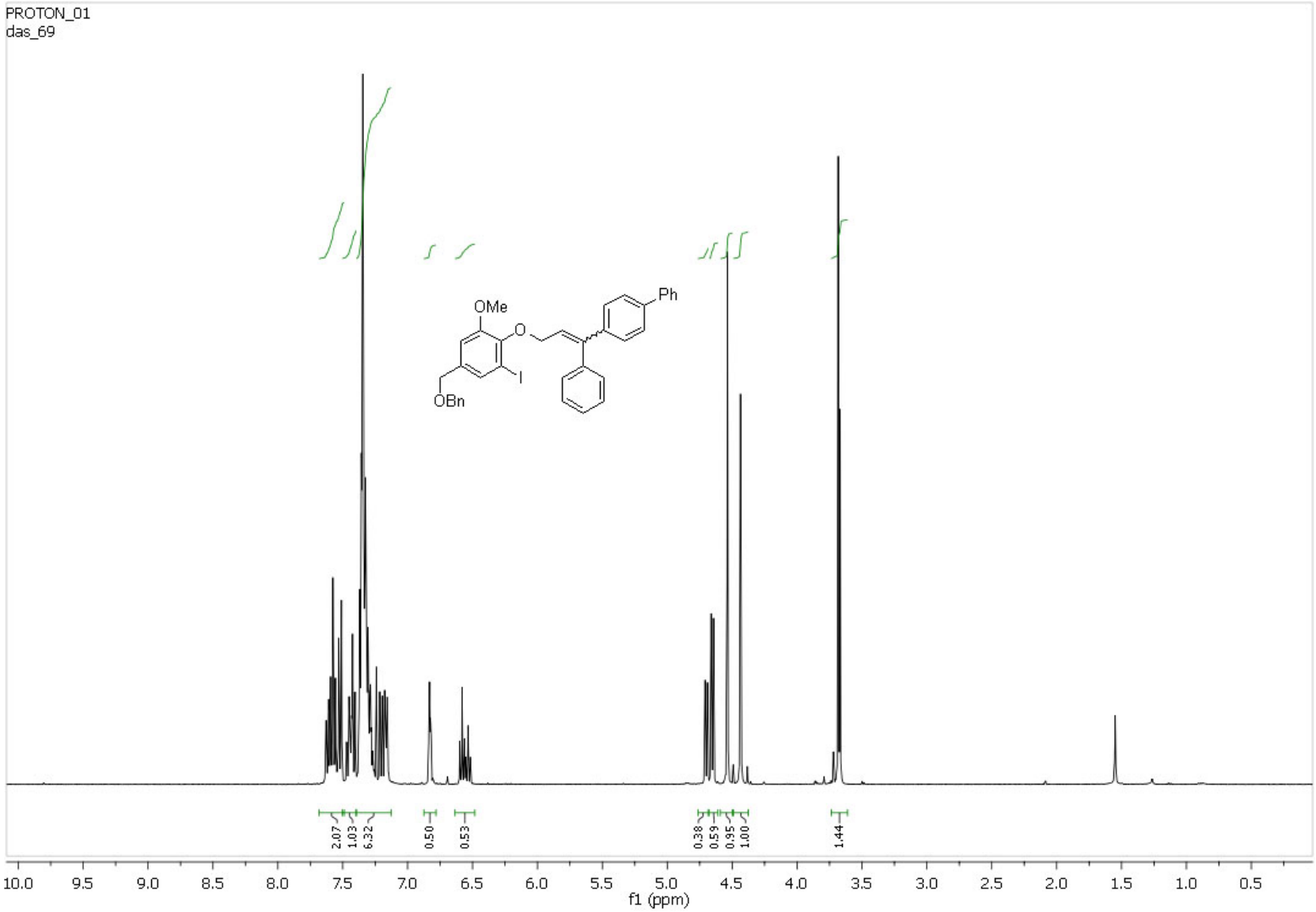
This journal is © The Royal Society of Chemistry 2011



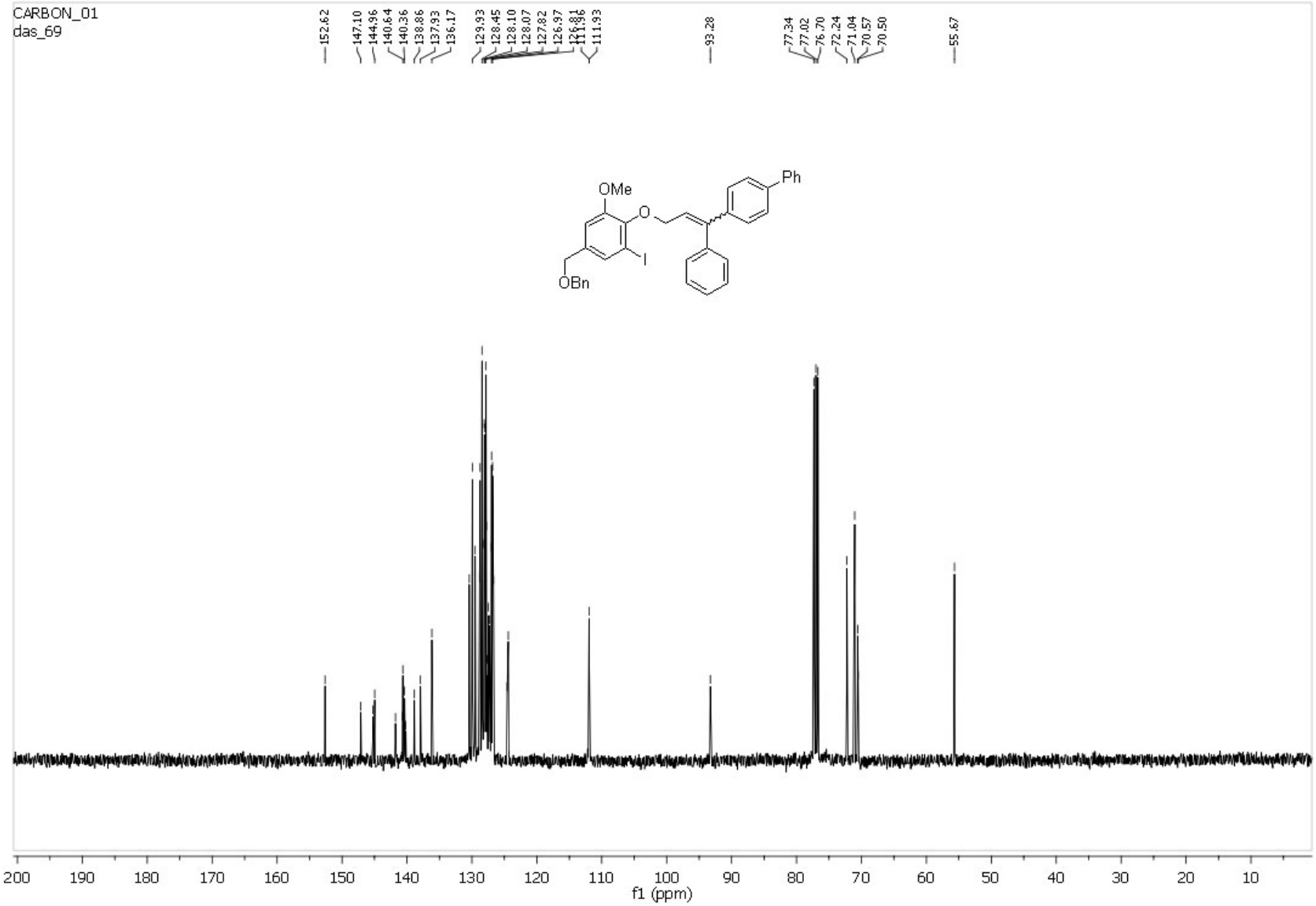
This journal is © The Royal Society of Chemistry 2011



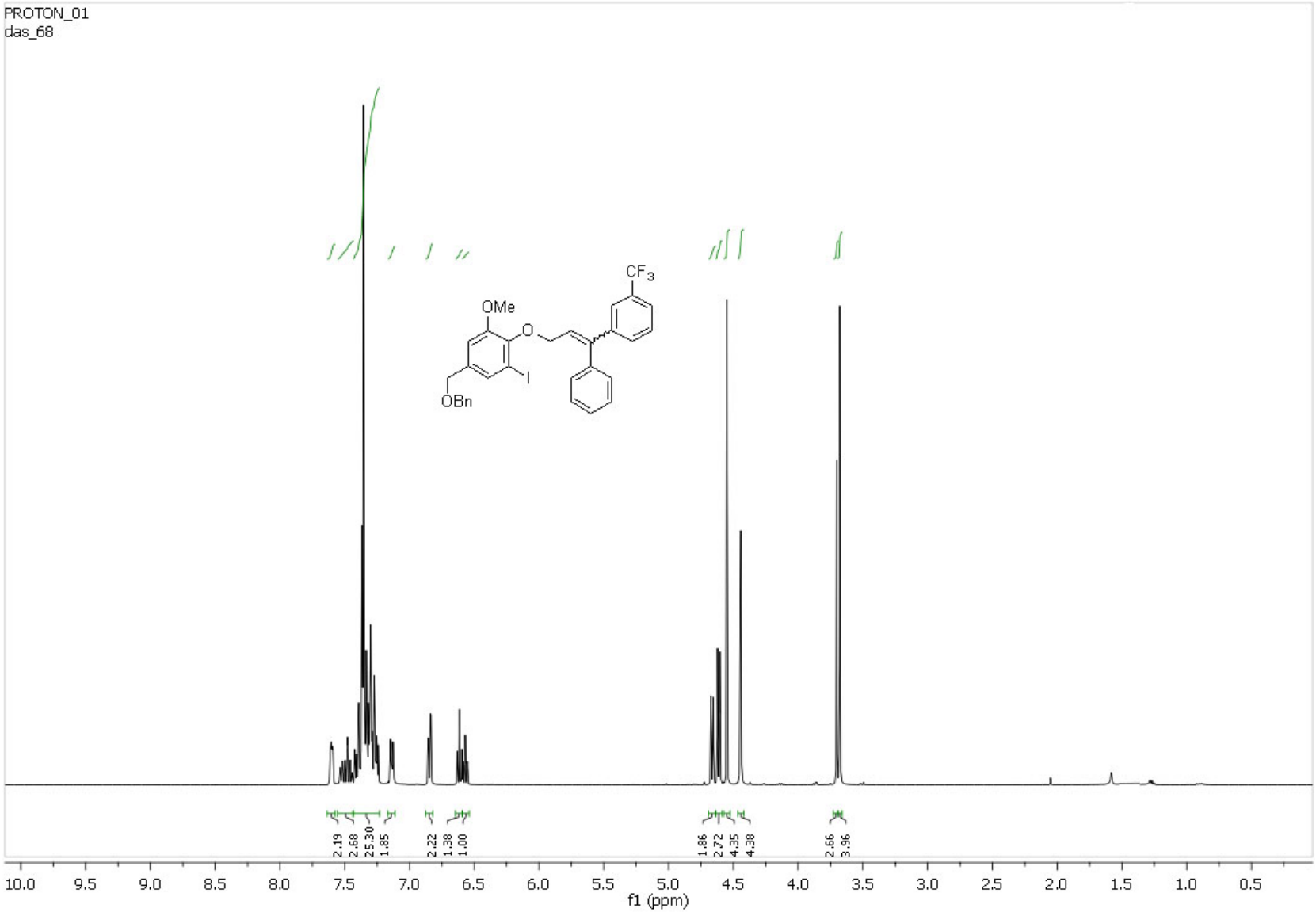
This journal is © The Royal Society of Chemistry 2011



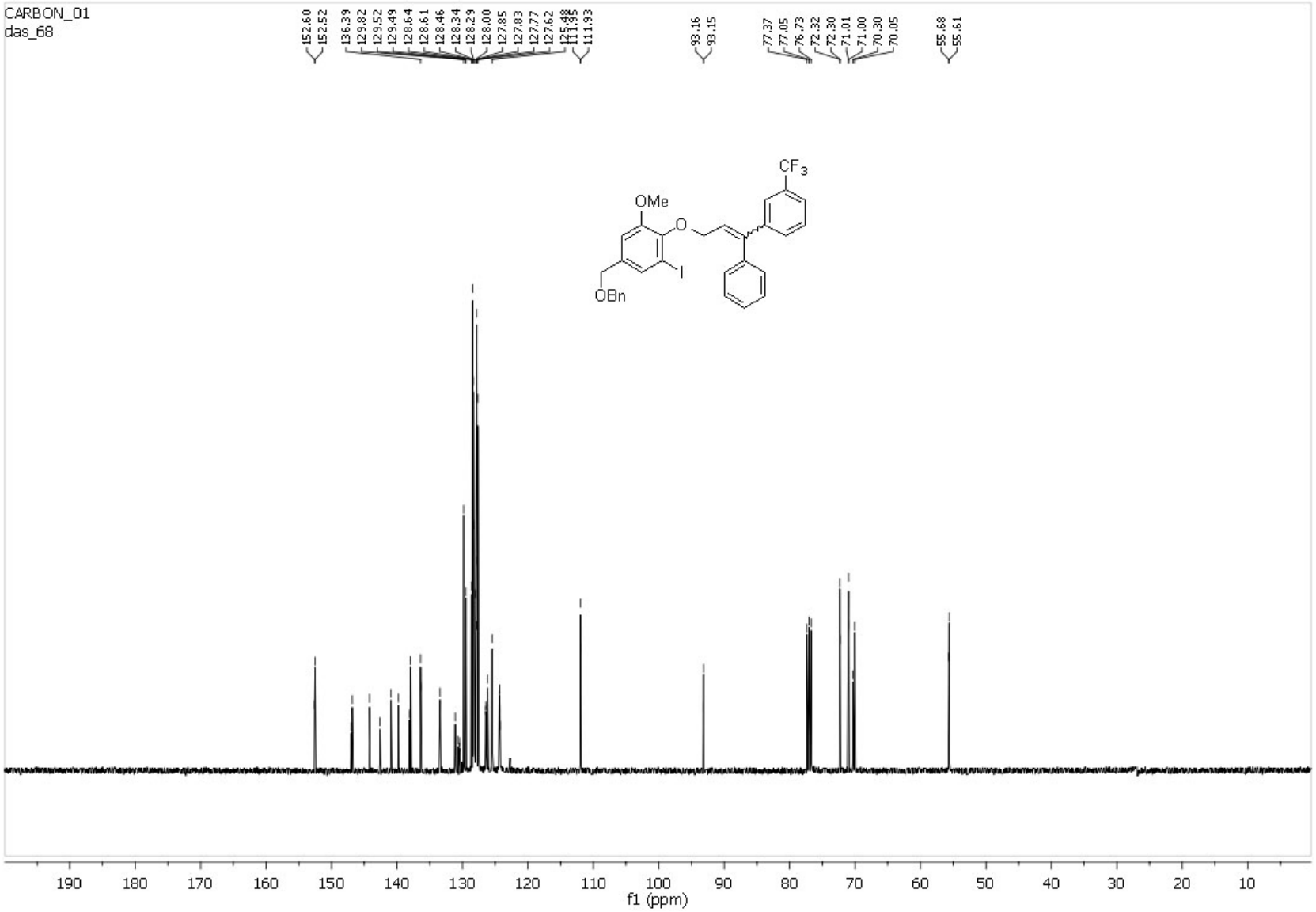
This journal is © The Royal Society of Chemistry 2011



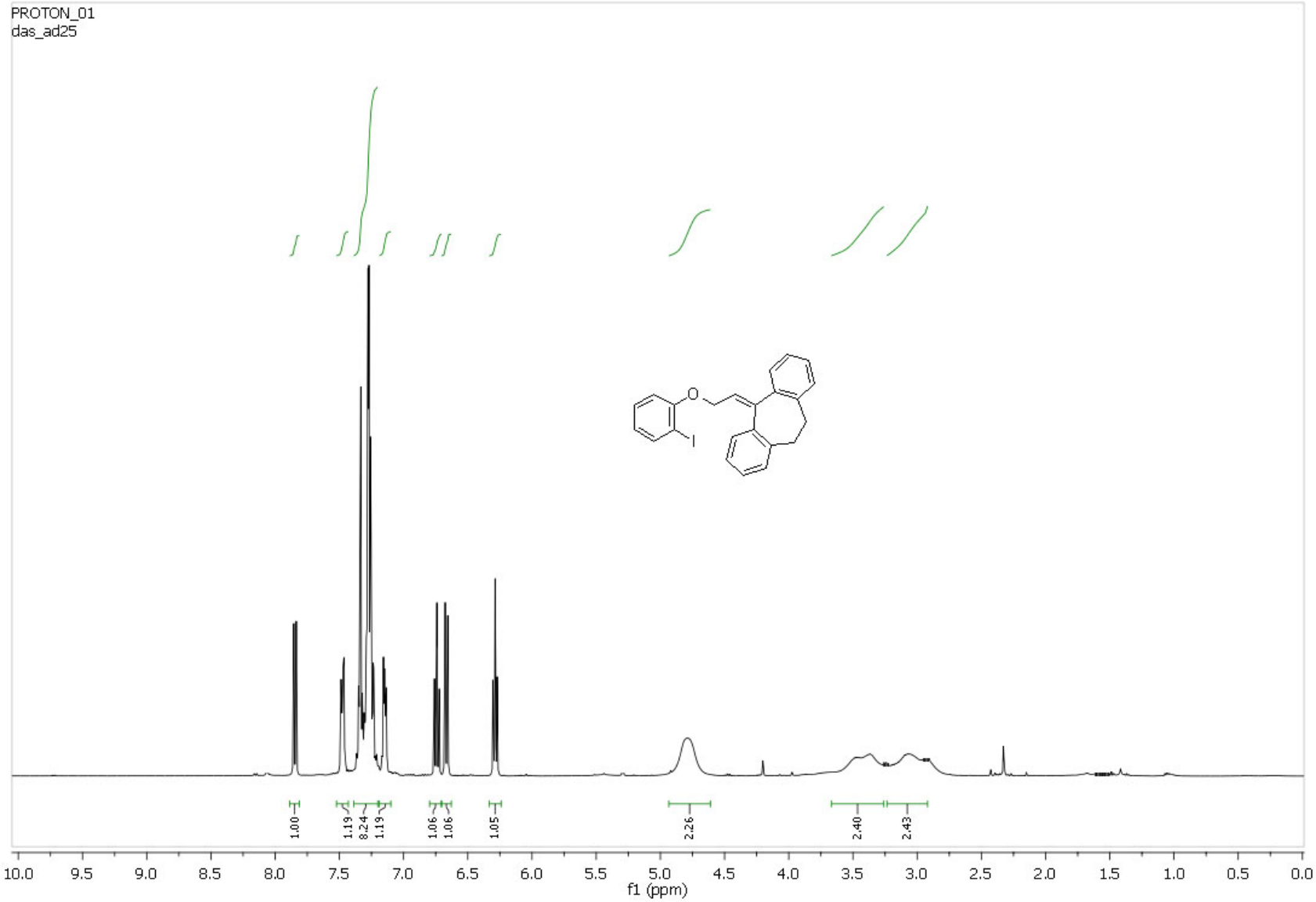
This journal is © The Royal Society of Chemistry 2011



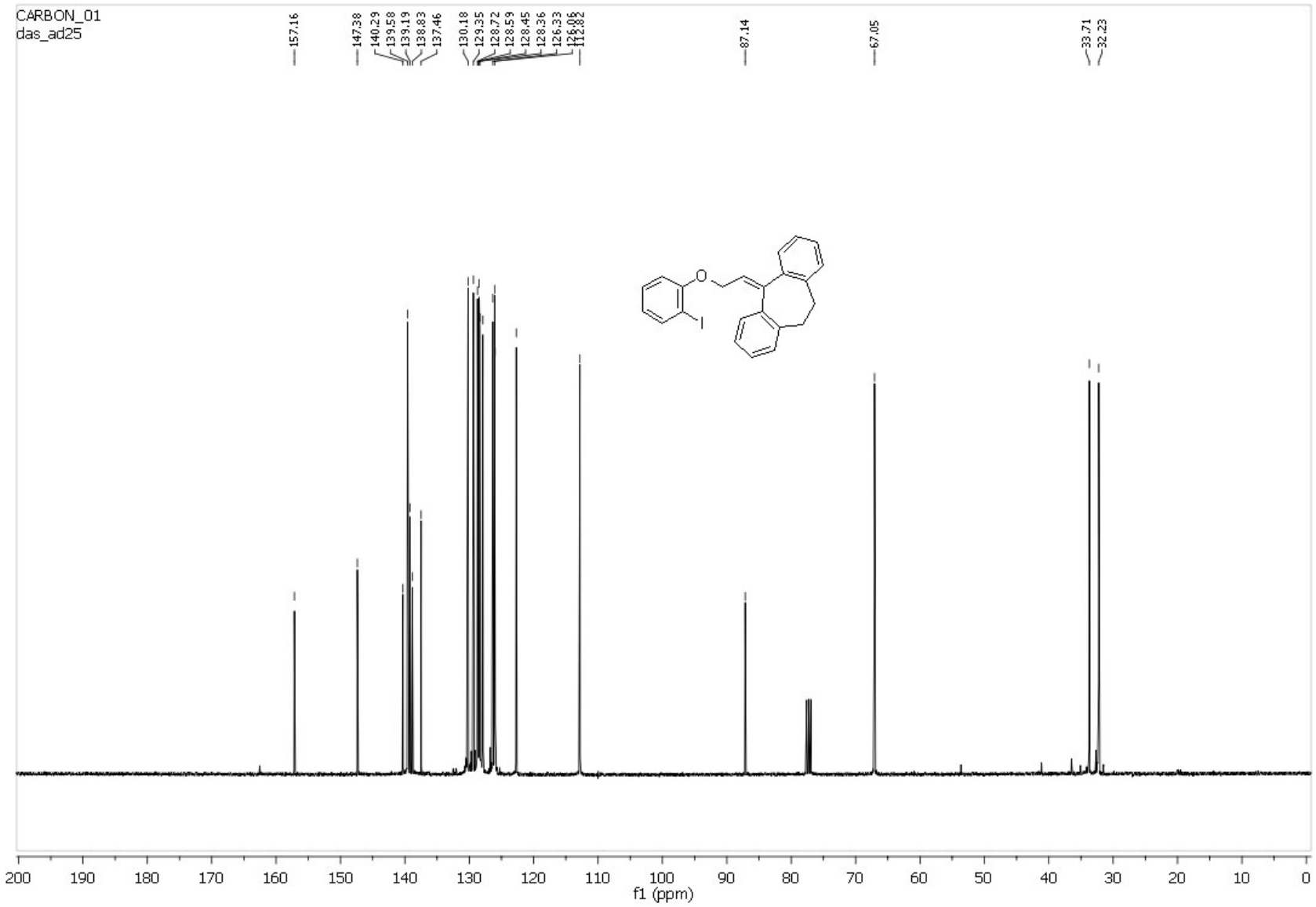
This journal is © The Royal Society of Chemistry 2011



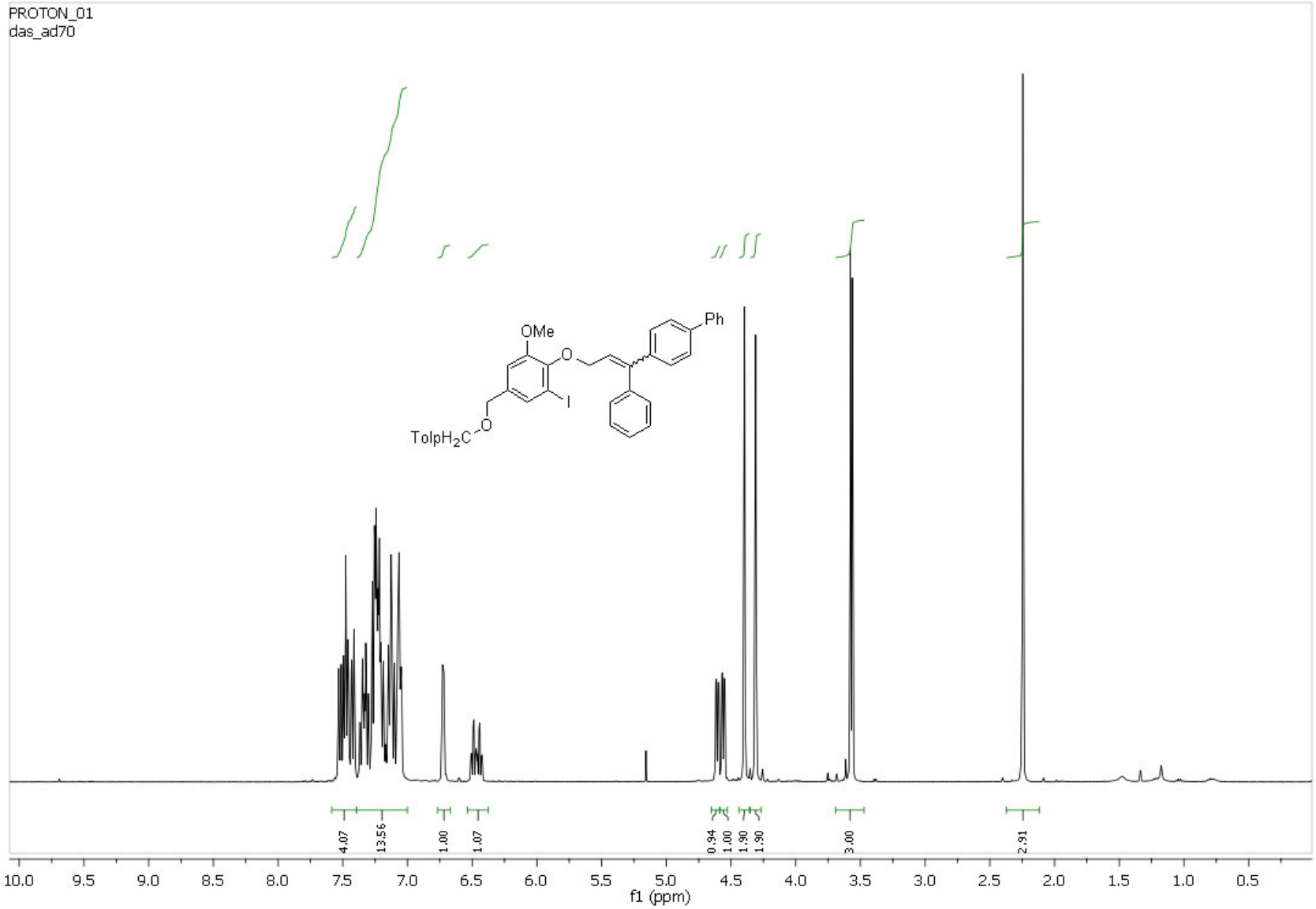
This journal is © The Royal Society of Chemistry 2011



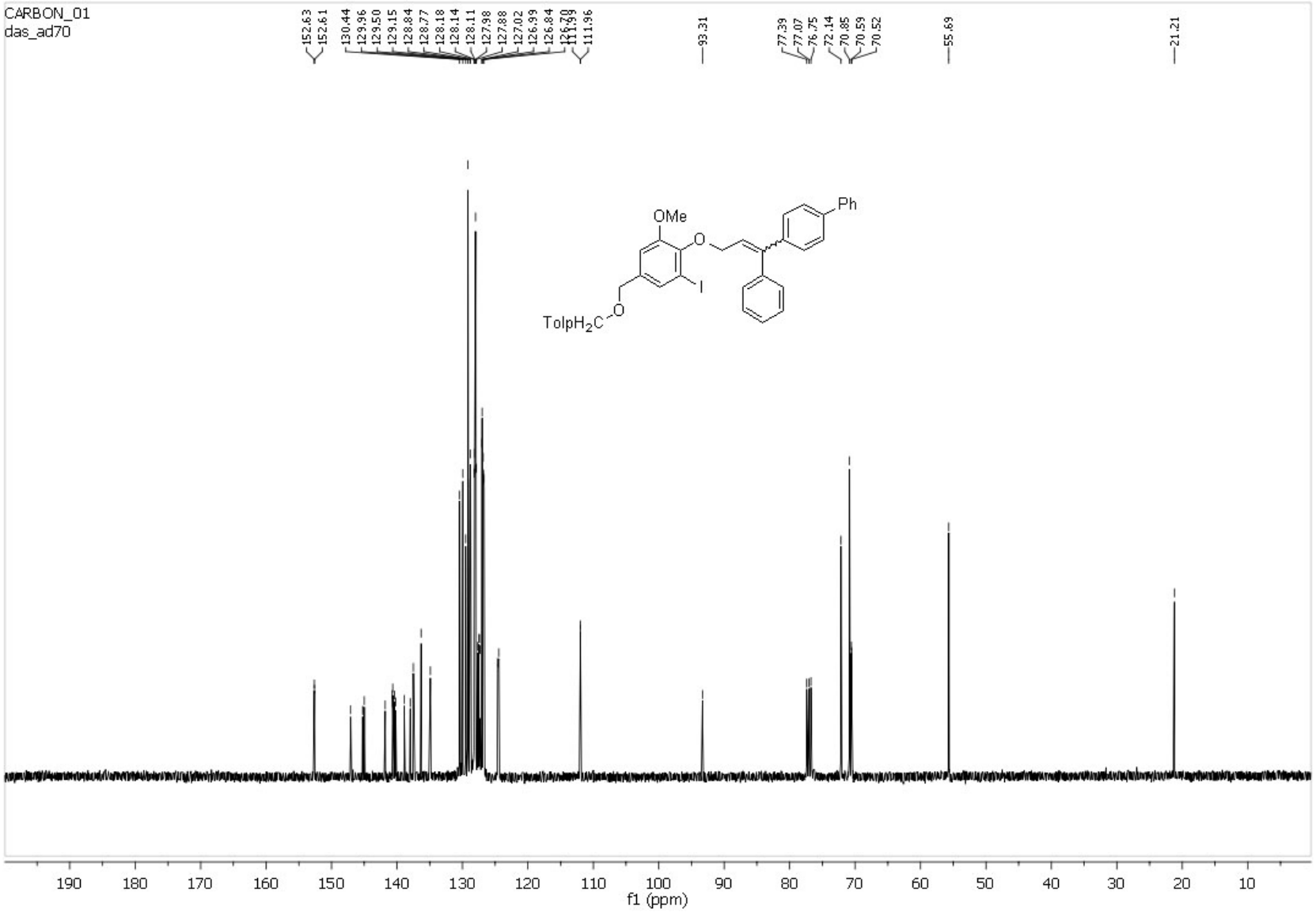
This journal is © The Royal Society of Chemistry 2011



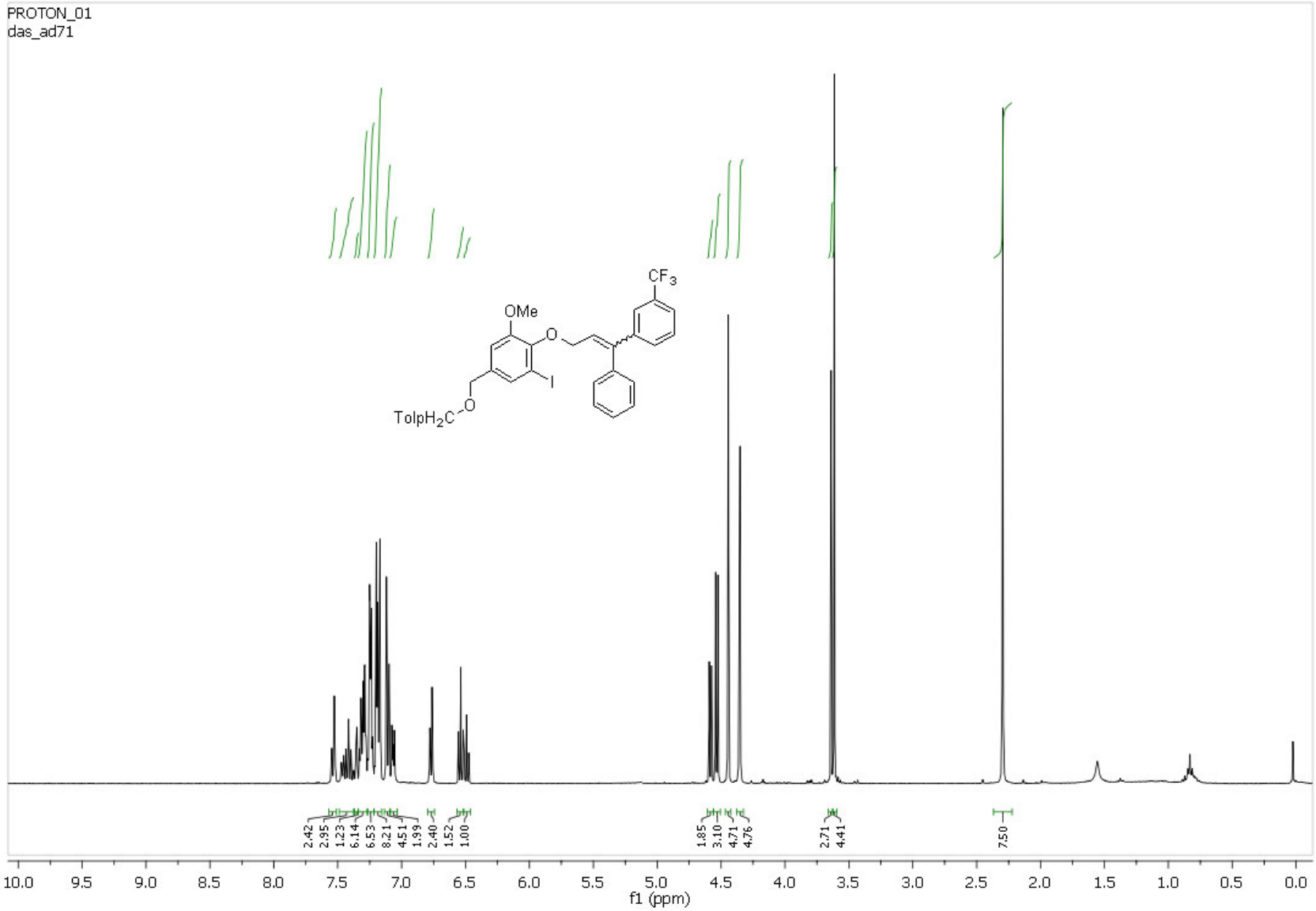
This journal is © The Royal Society of Chemistry 2011



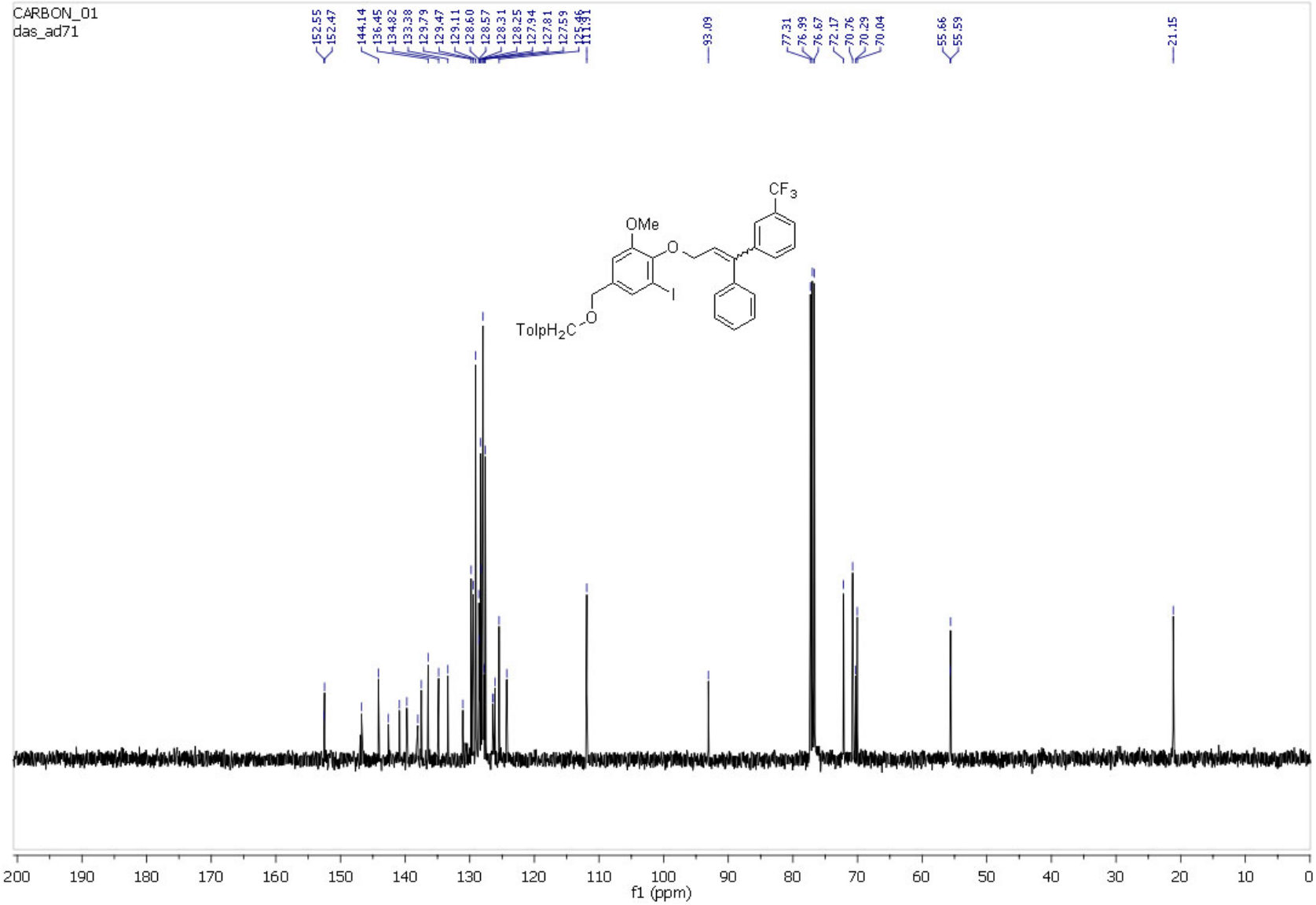
This journal is © The Royal Society of Chemistry 2011



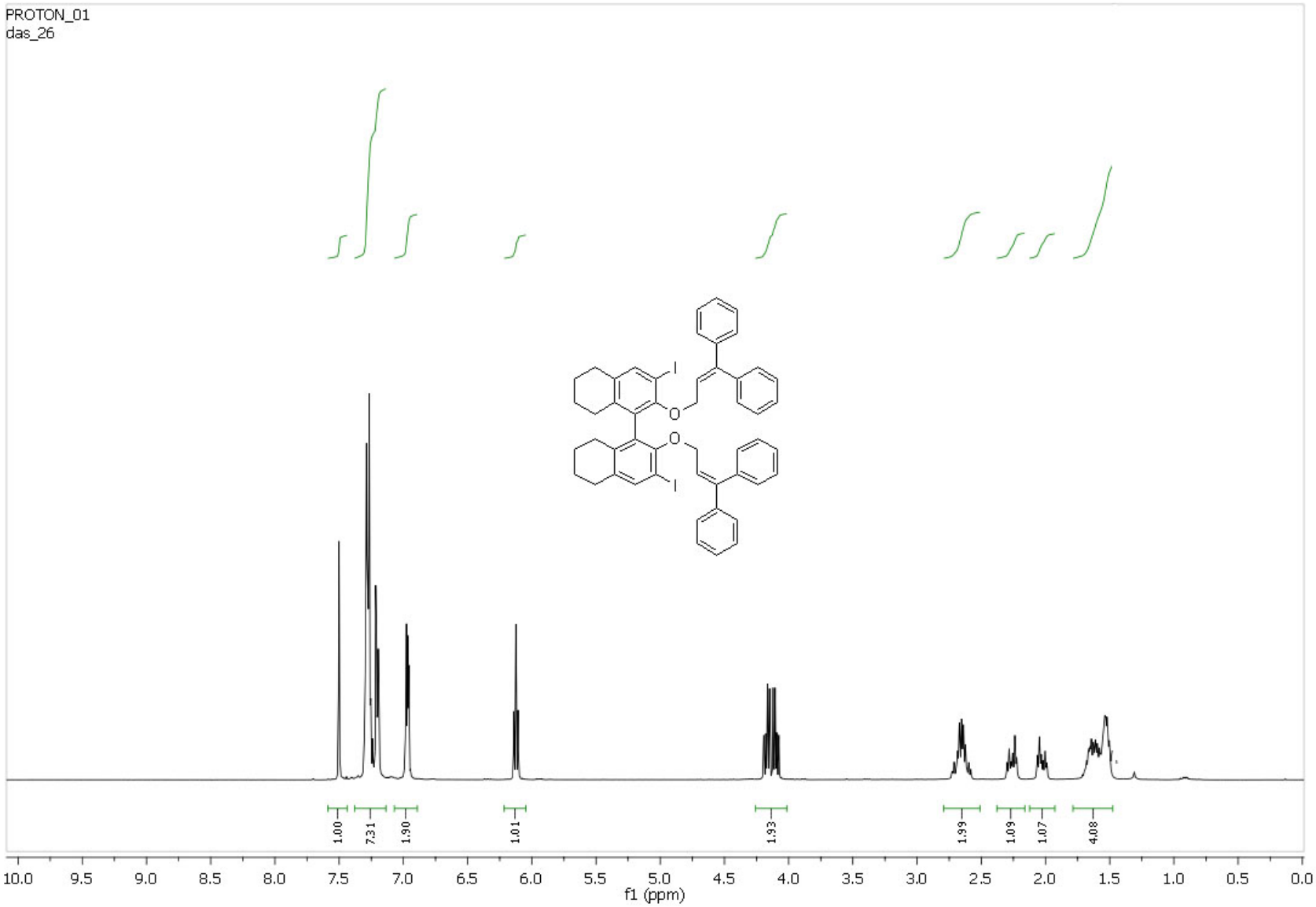
This journal is © The Royal Society of Chemistry 2011



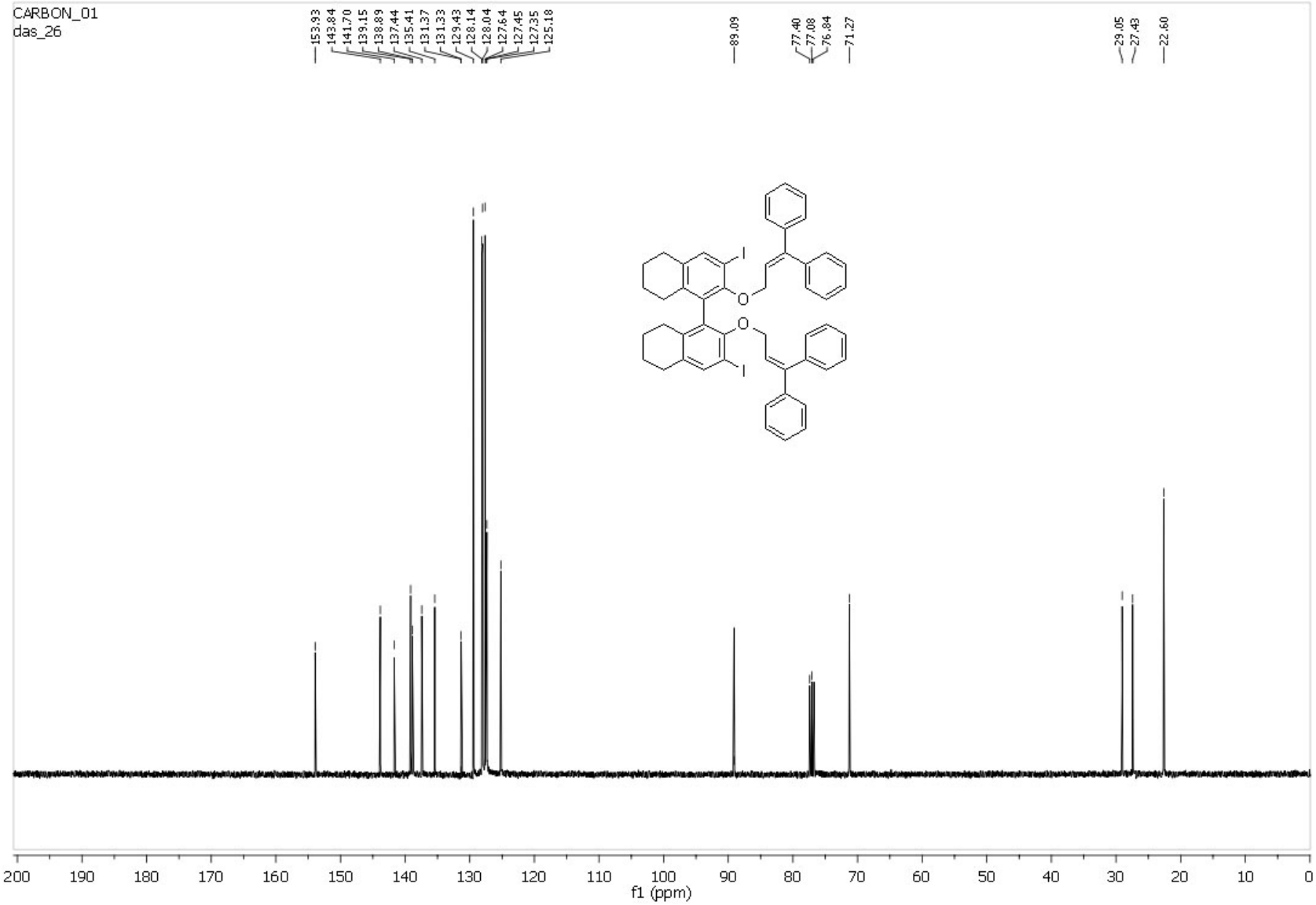
This journal is © The Royal Society of Chemistry 2011



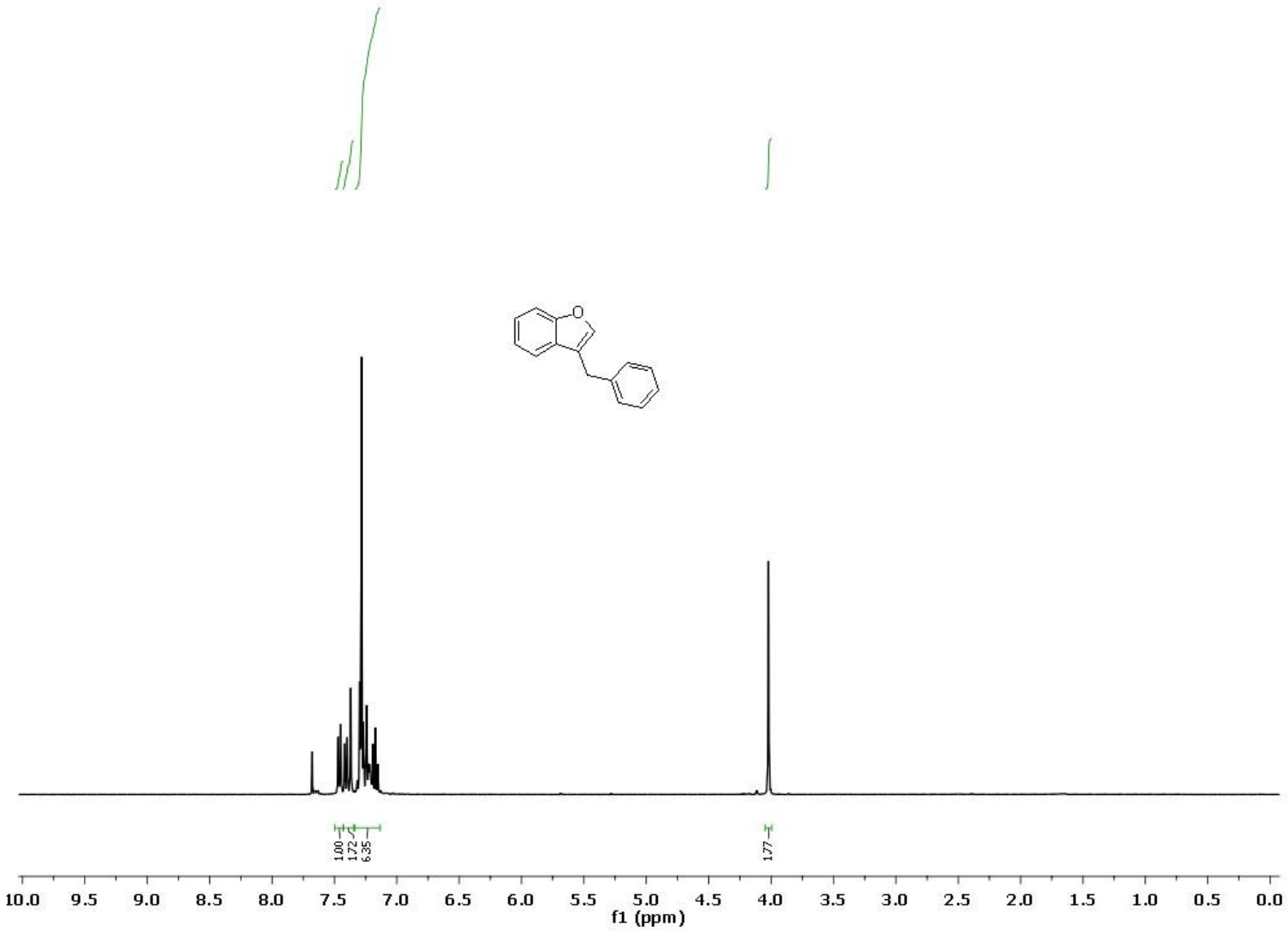
This journal is © The Royal Society of Chemistry 2011



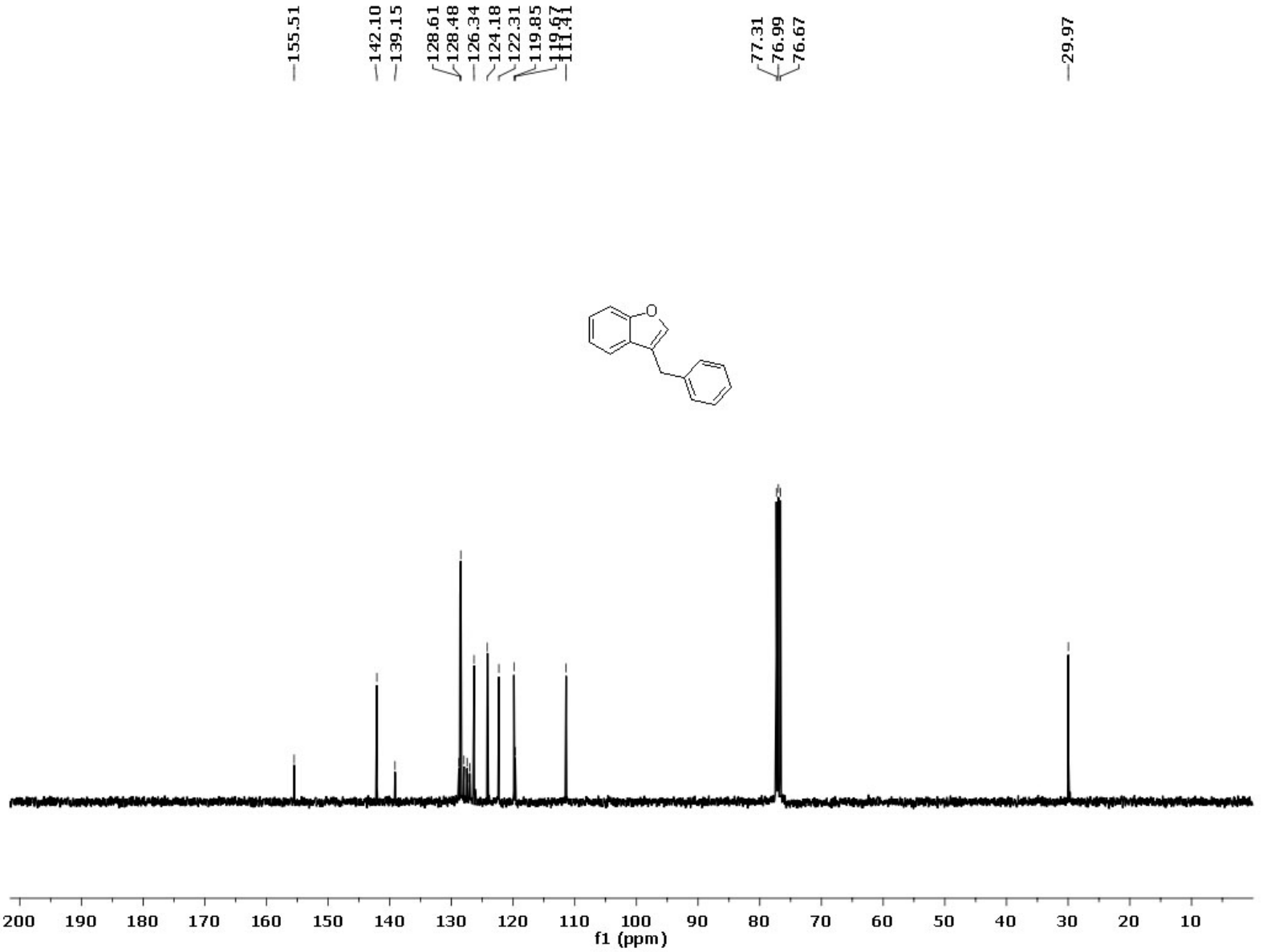
This journal is © The Royal Society of Chemistry 2011



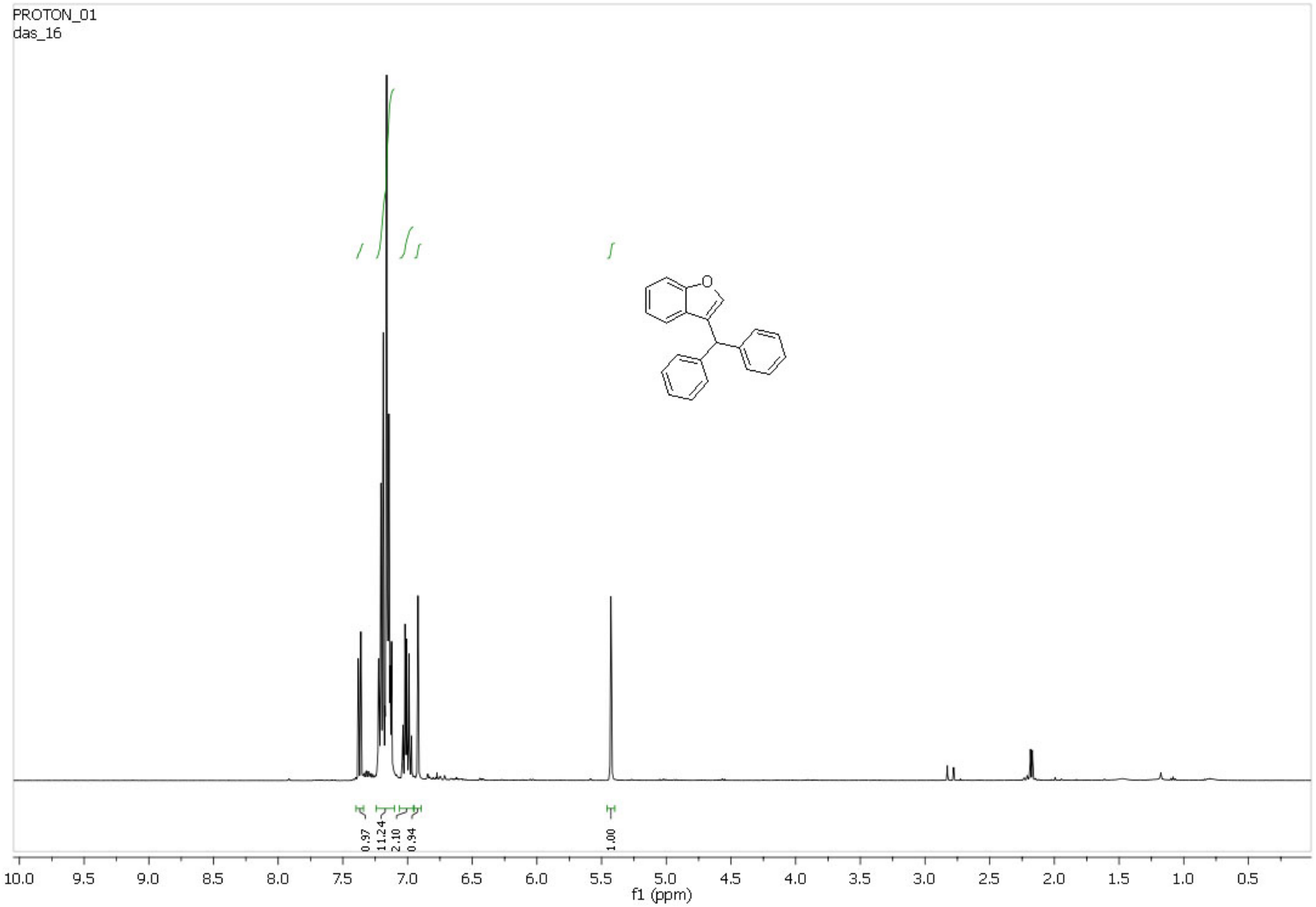
This journal is © The Royal Society of Chemistry 2011



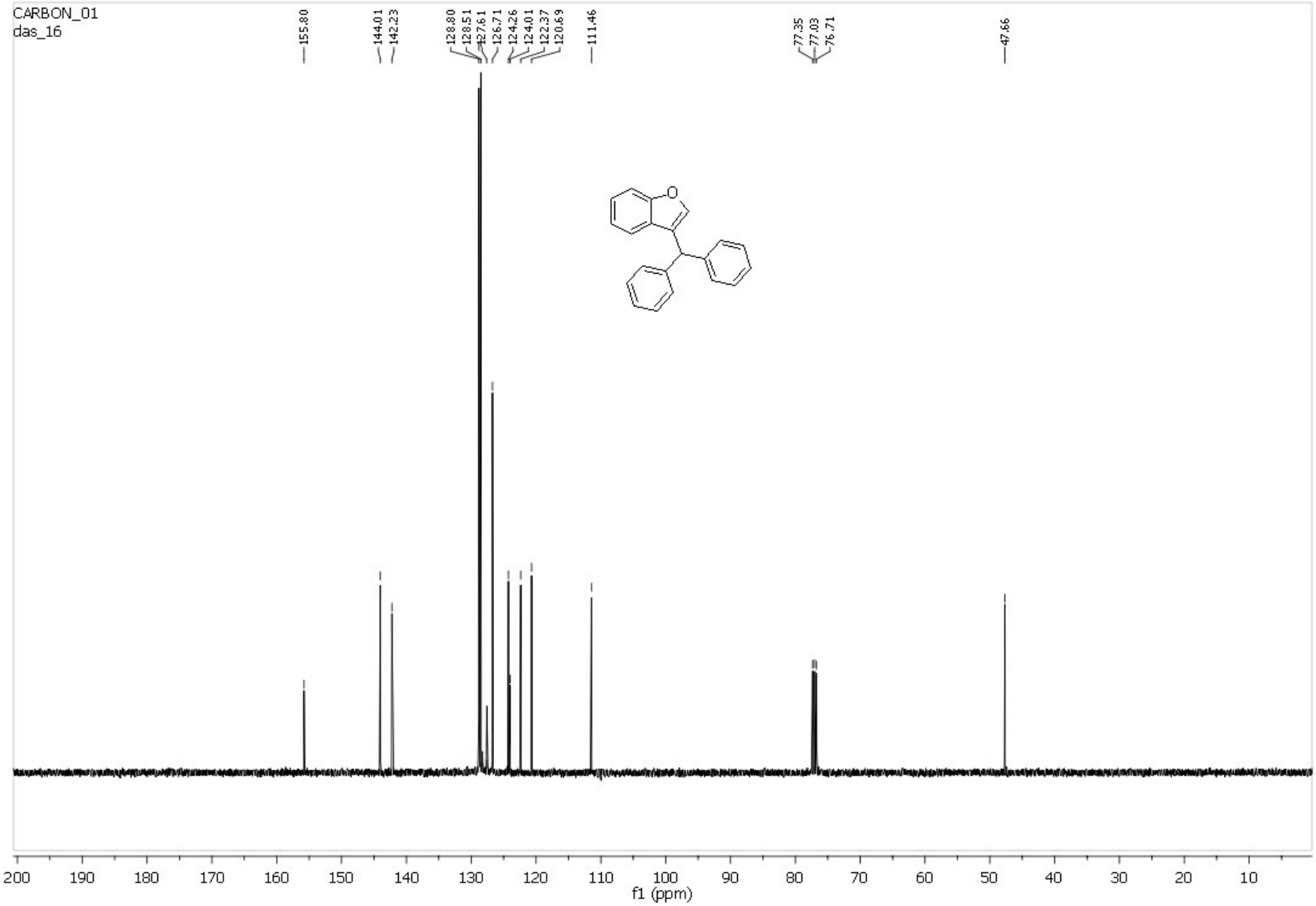
This journal is © The Royal Society of Chemistry 2011



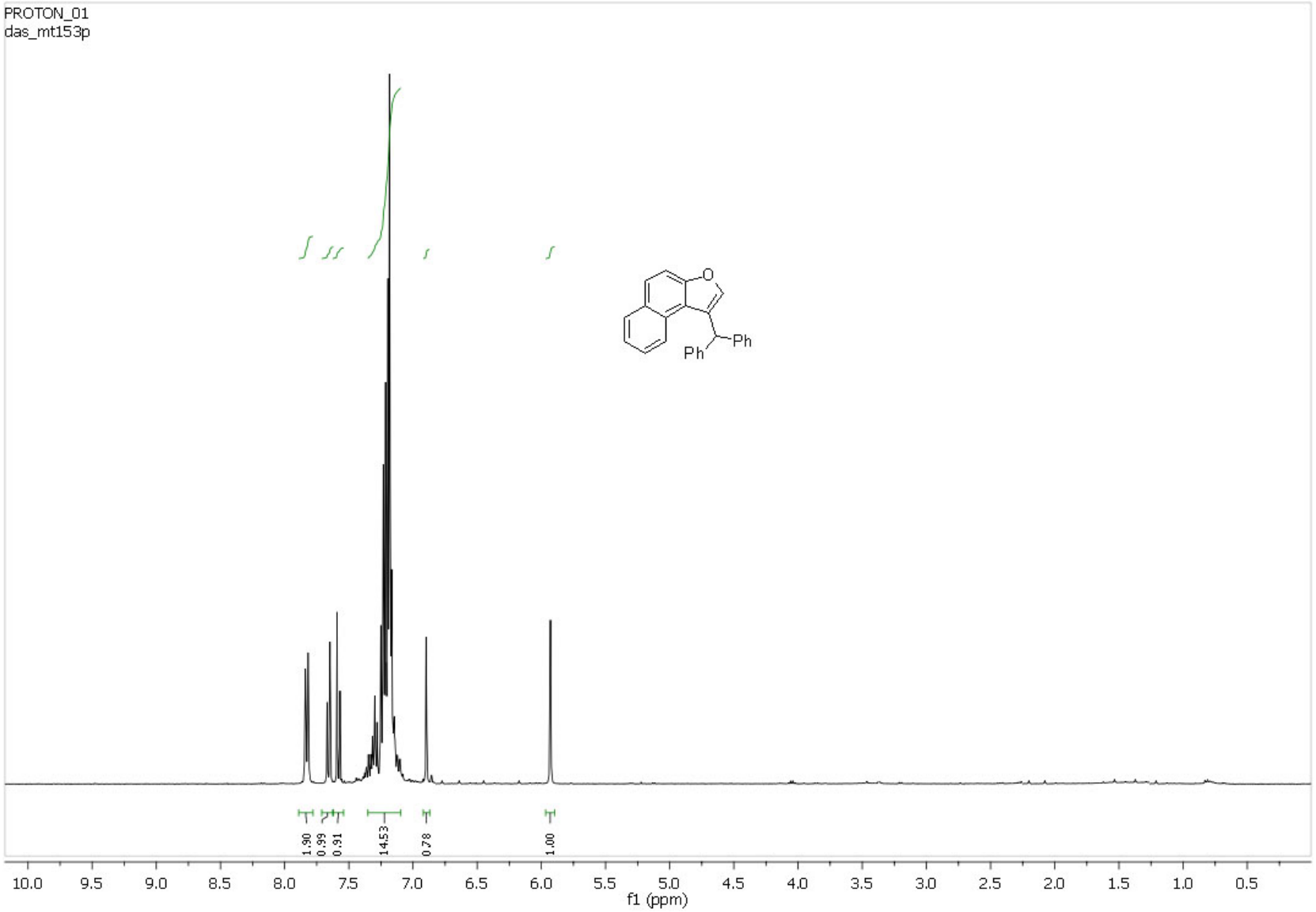
This journal is © The Royal Society of Chemistry 2011



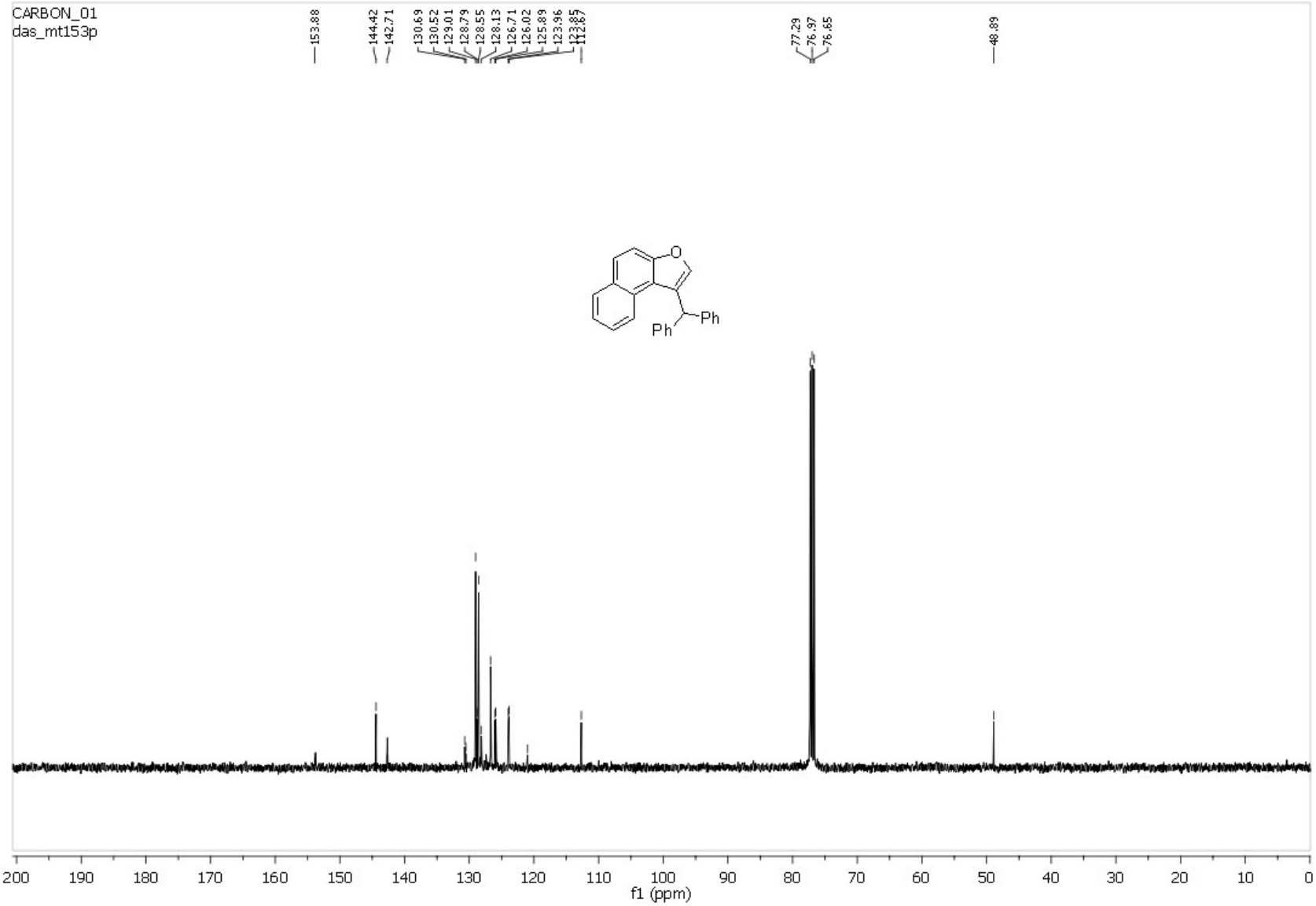
This journal is © The Royal Society of Chemistry 2011



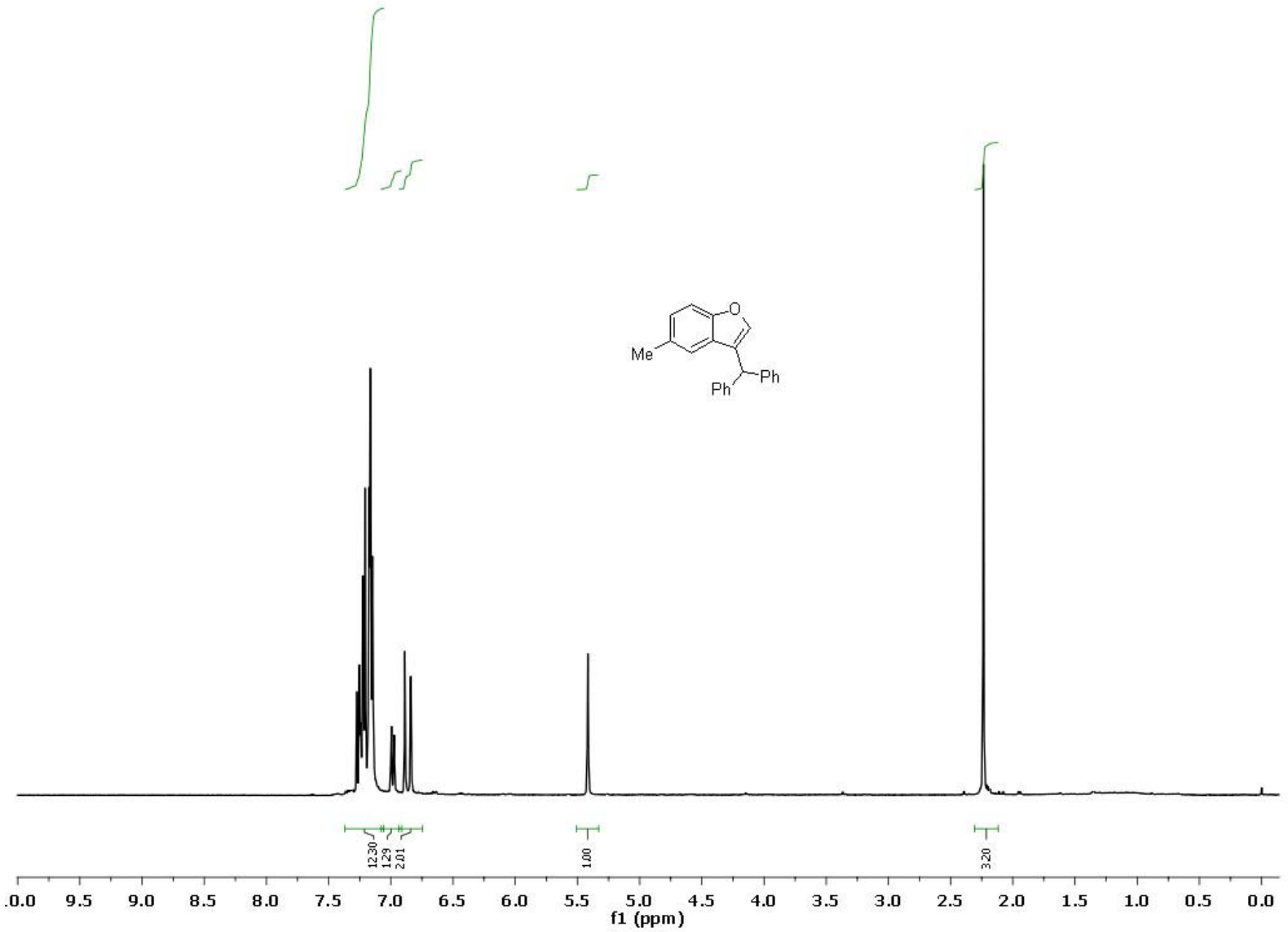
This journal is © The Royal Society of Chemistry 2011



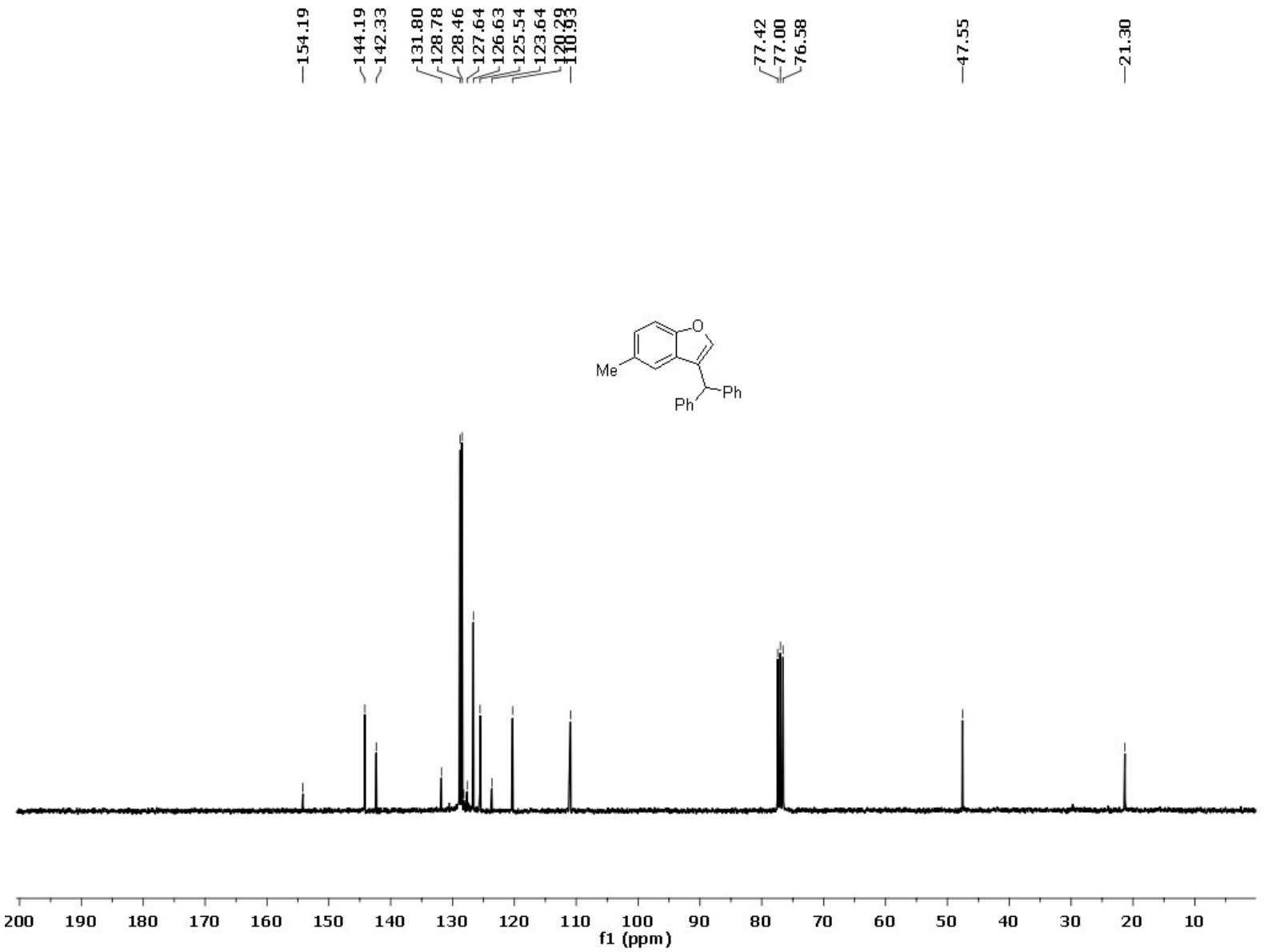
Electronic Supplementary Material (ESI) for Chemical Communications
This journal is © The Royal Society of Chemistry 2011



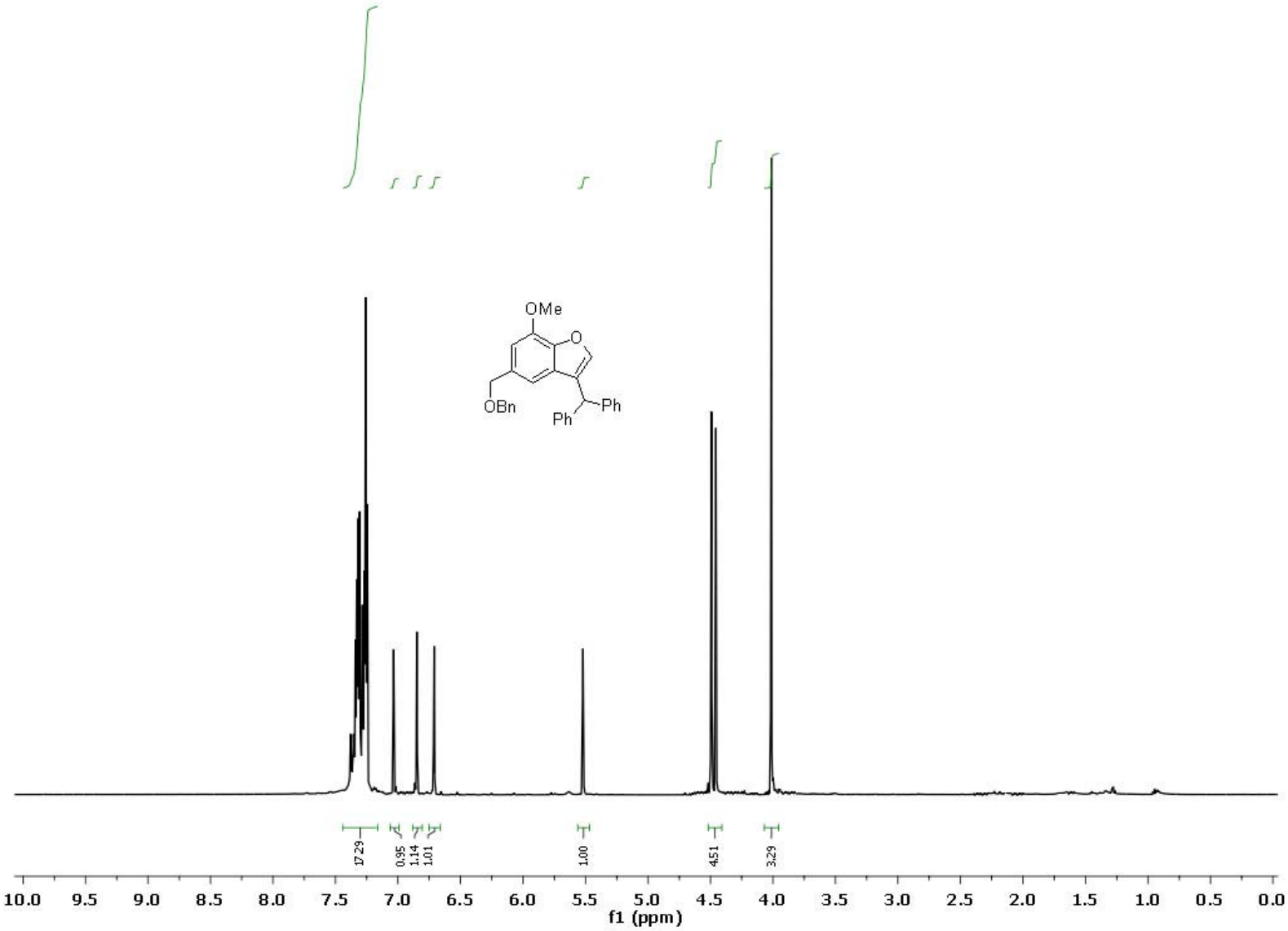
This journal is © The Royal Society of Chemistry 2011



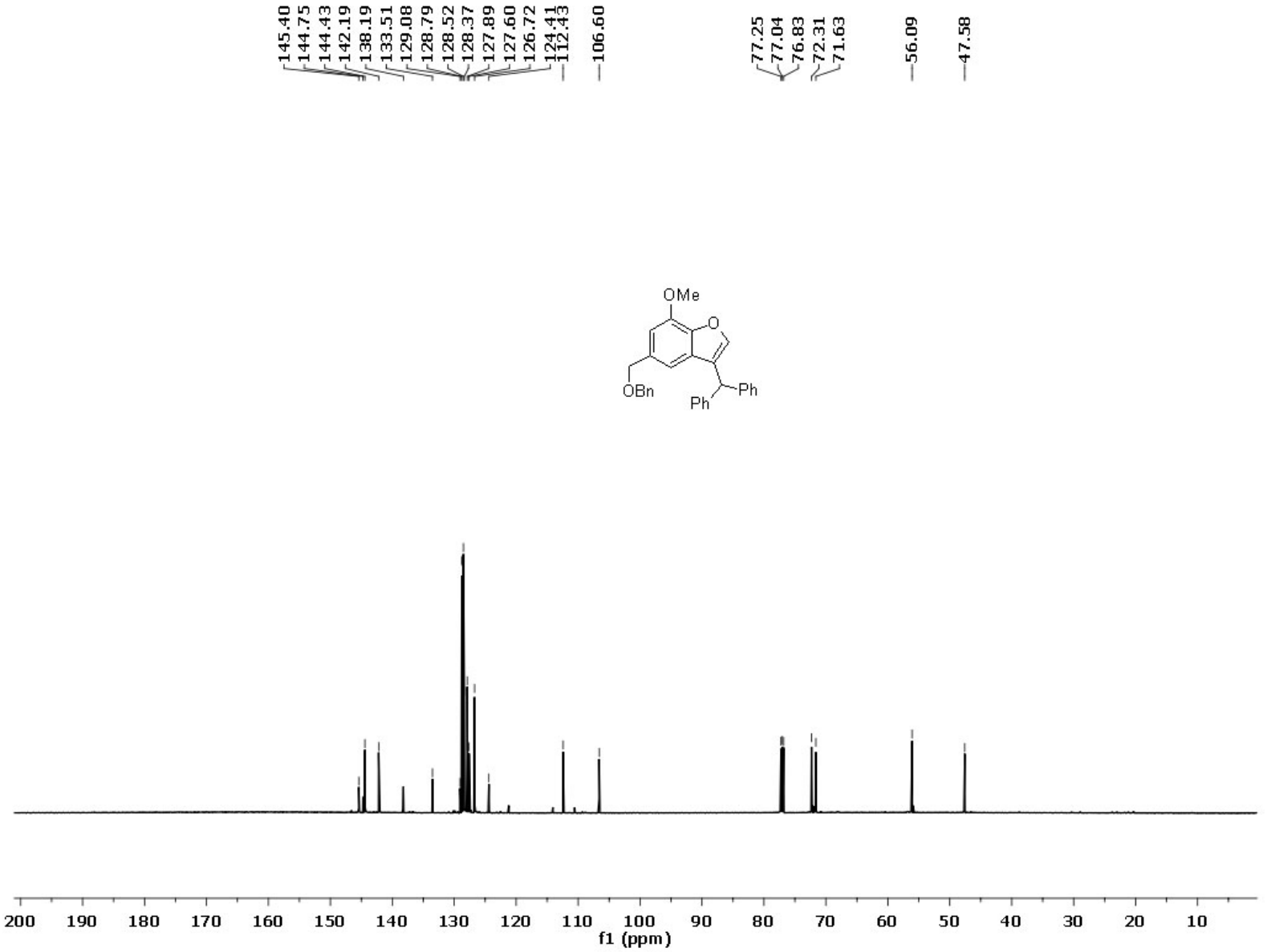
This journal is © The Royal Society of Chemistry 2011



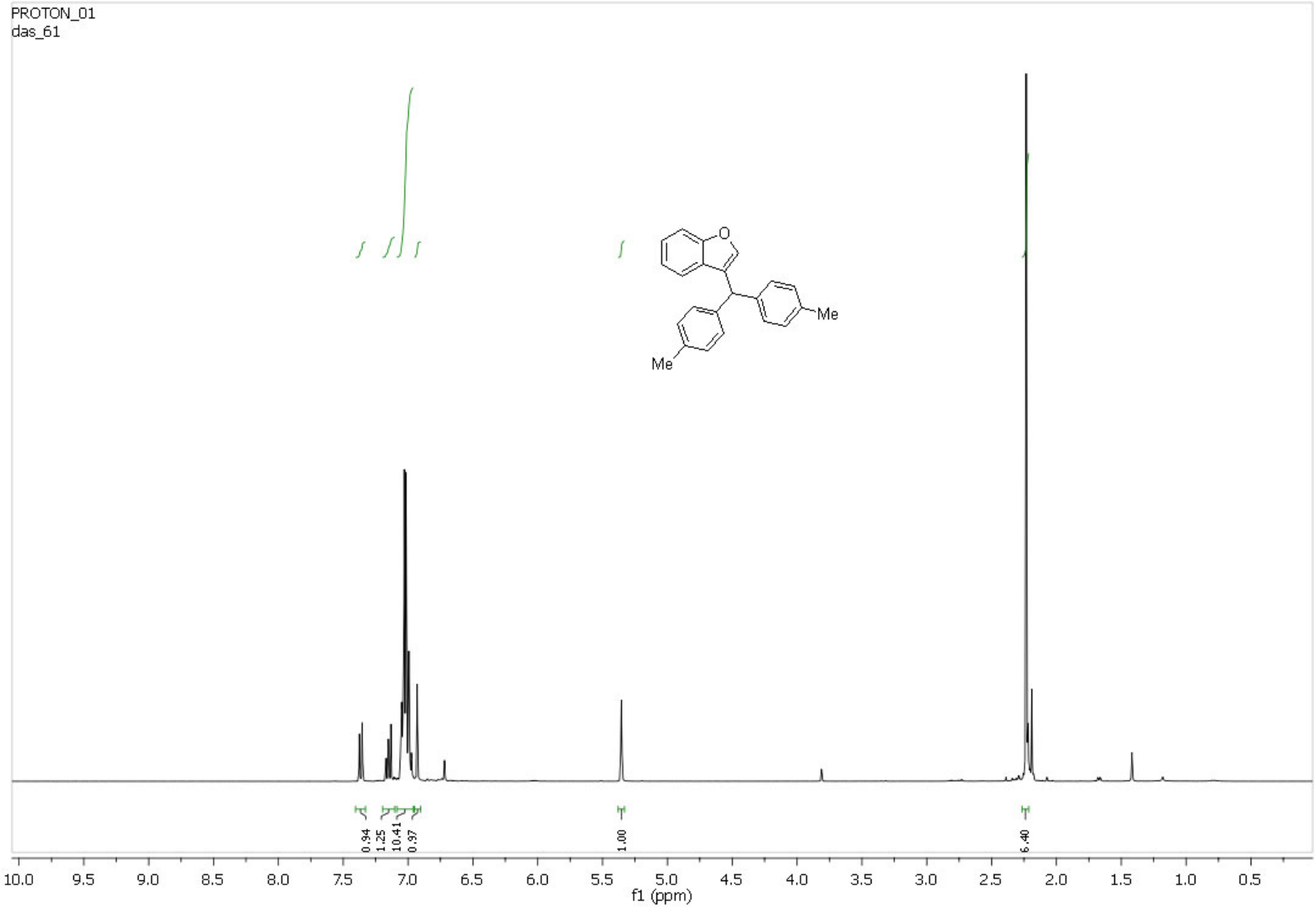
This journal is © The Royal Society of Chemistry 2011



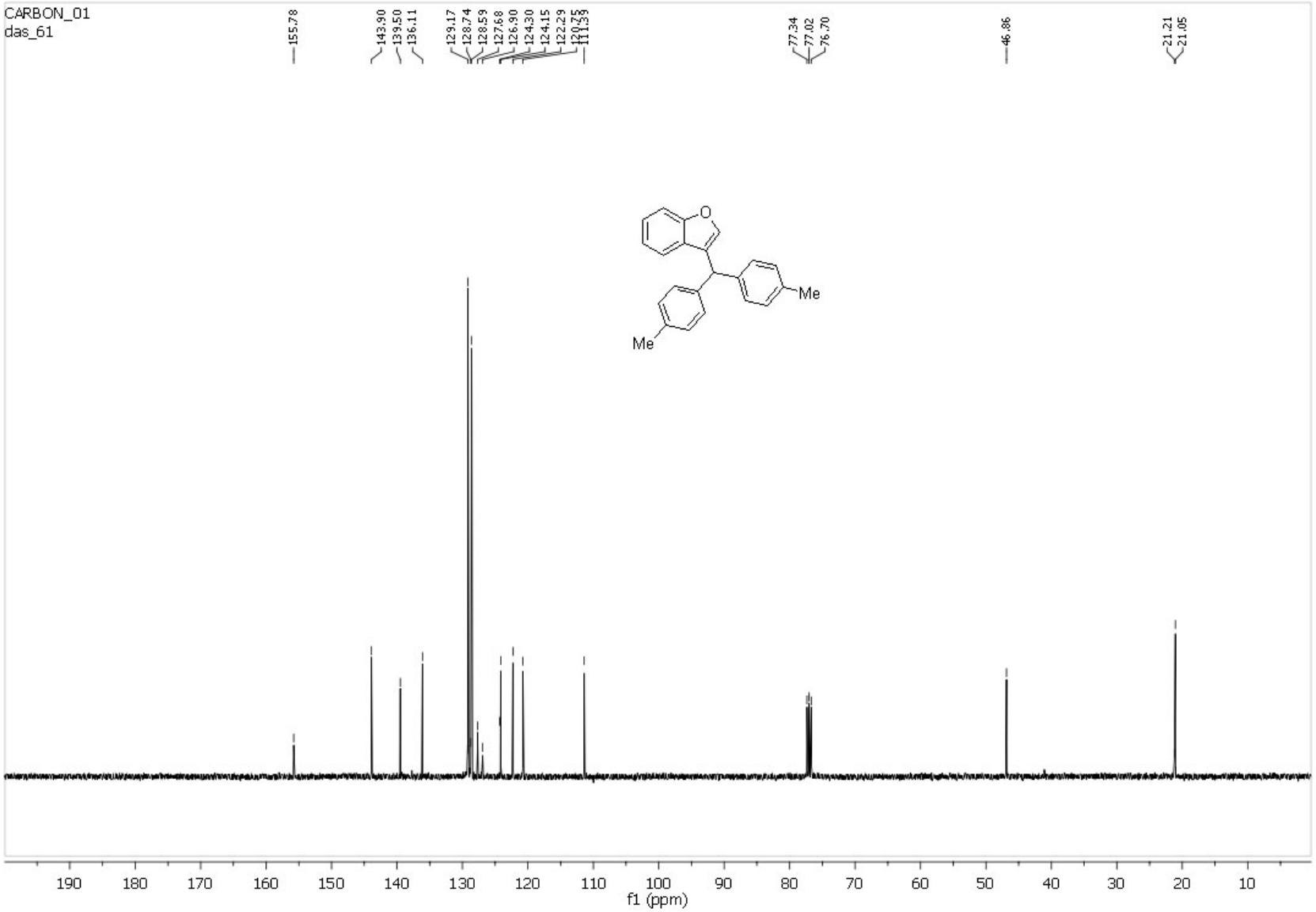
This journal is © The Royal Society of Chemistry 2011



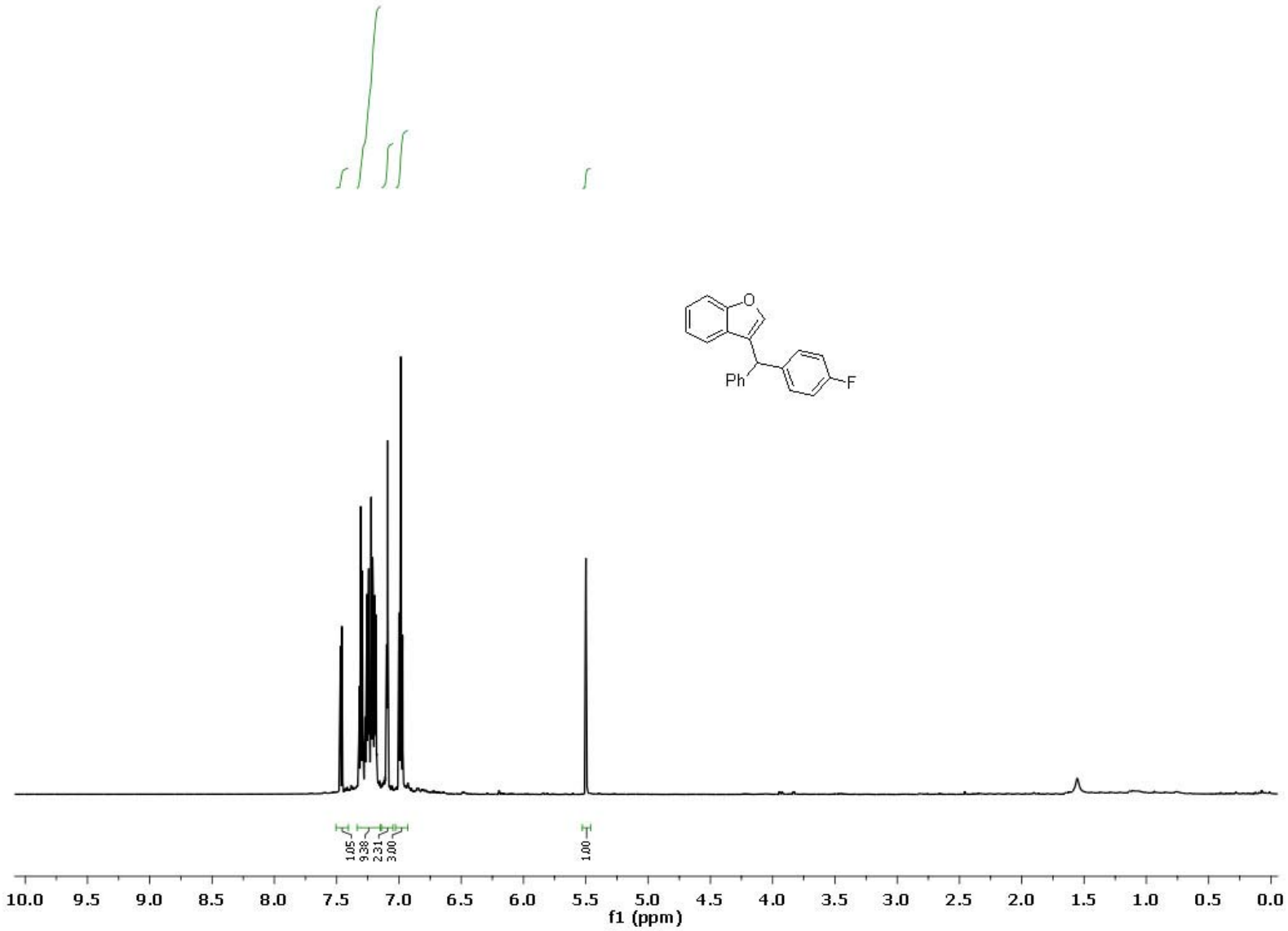
This journal is © The Royal Society of Chemistry 2011



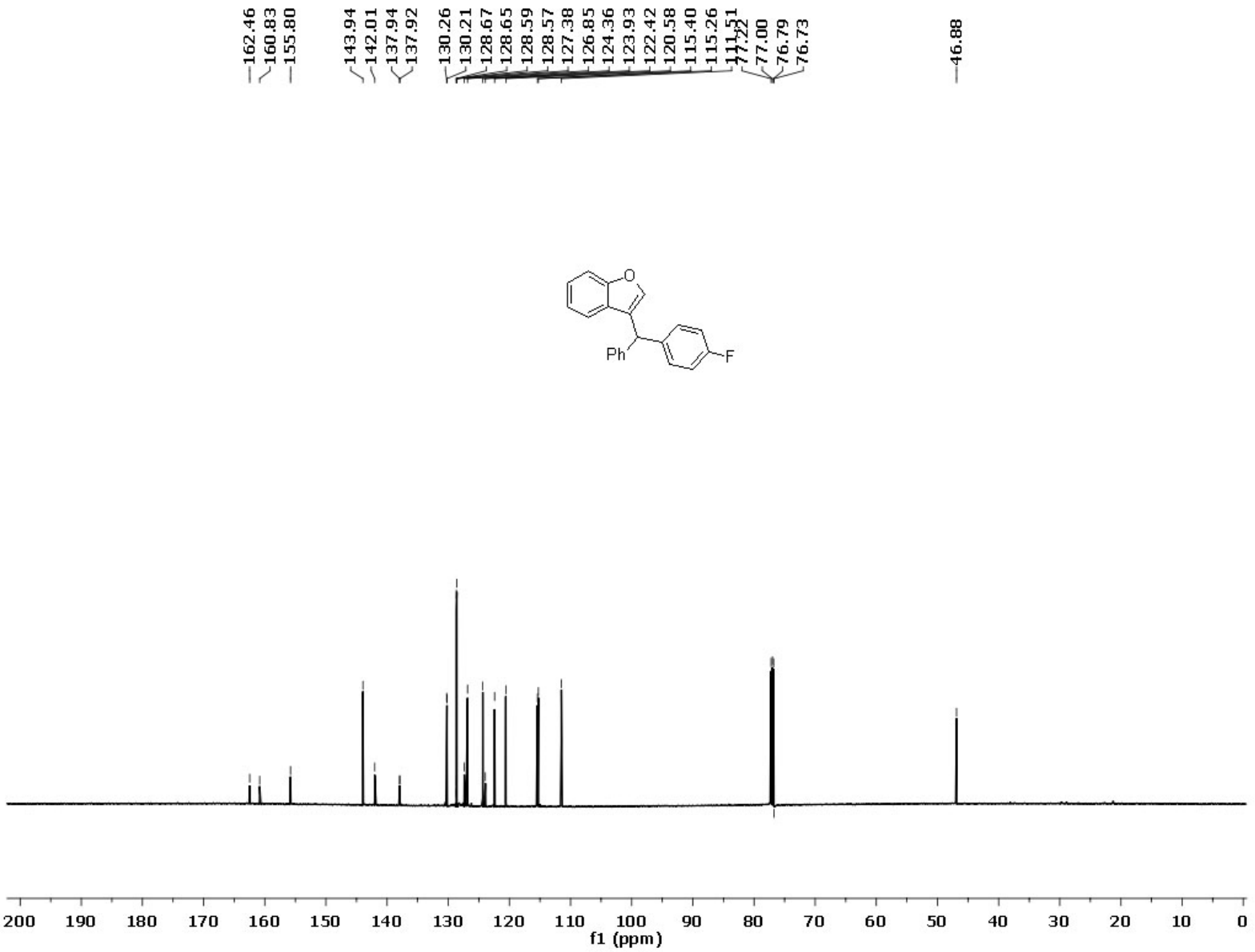
This journal is © The Royal Society of Chemistry 2011



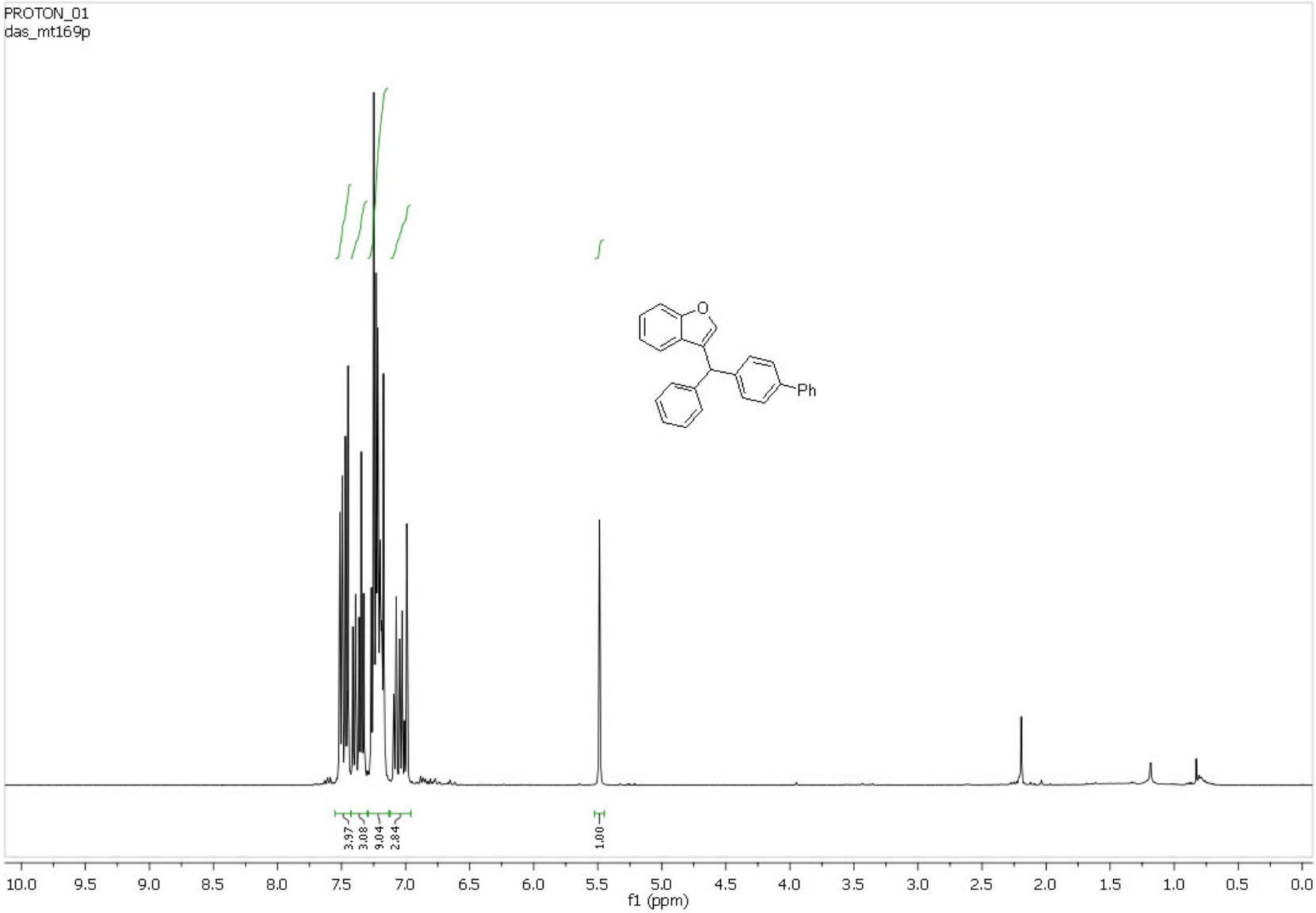
Electronic Supplementary Material (ESI) for Chemical Communications
This journal is © The Royal Society of Chemistry 2011



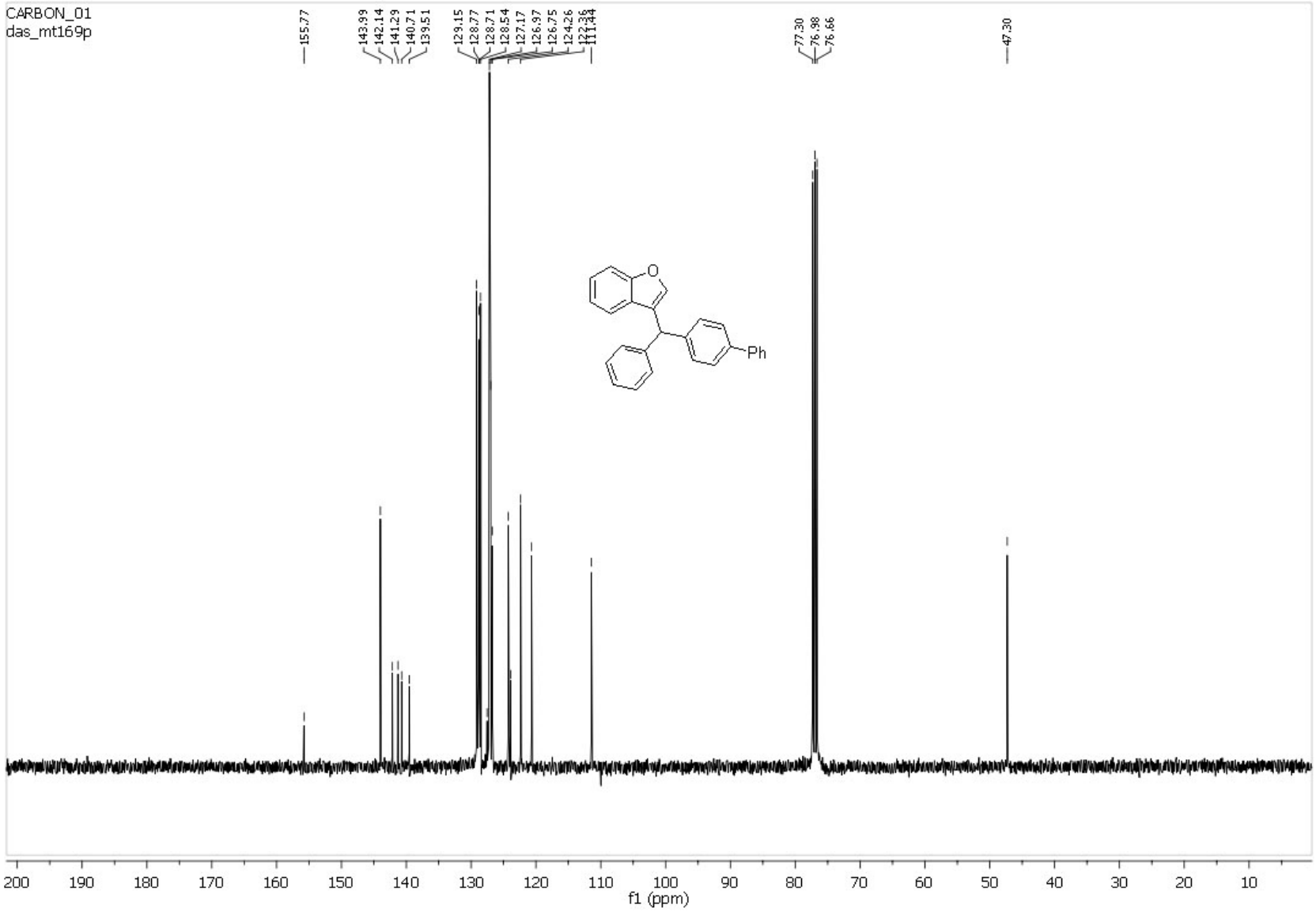
This journal is © The Royal Society of Chemistry 2011



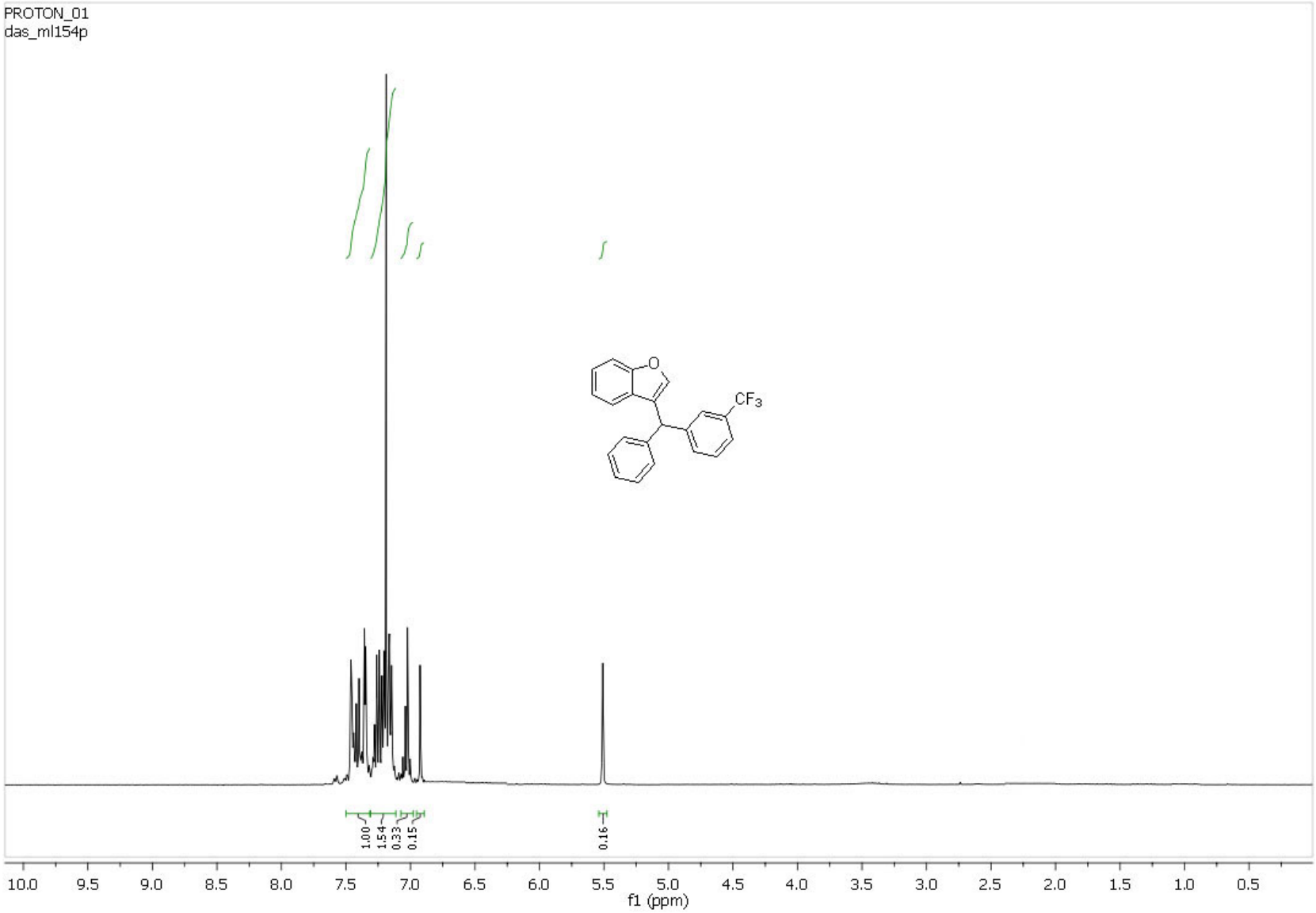
This journal is © The Royal Society of Chemistry 2011



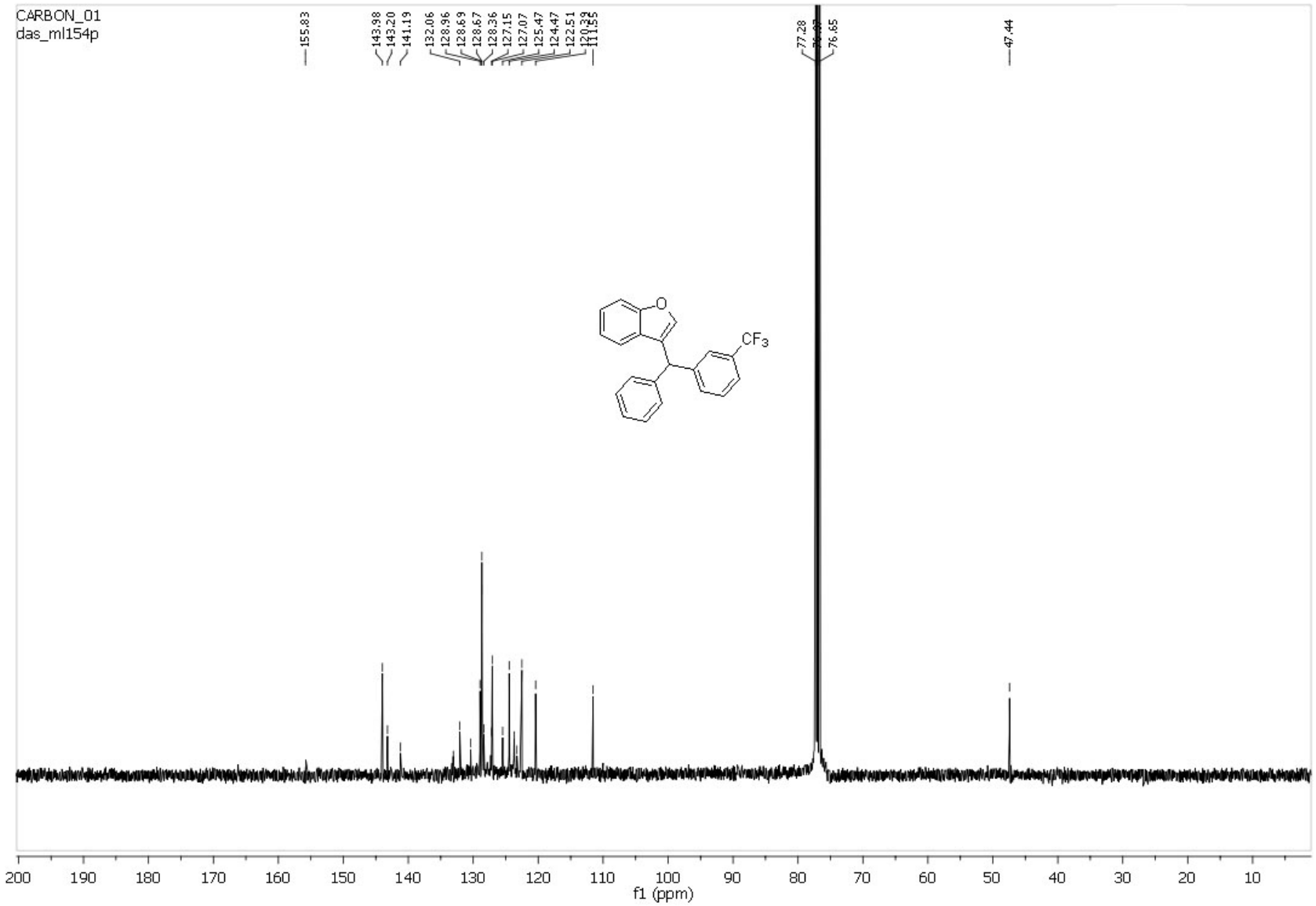
This journal is © The Royal Society of Chemistry 2011



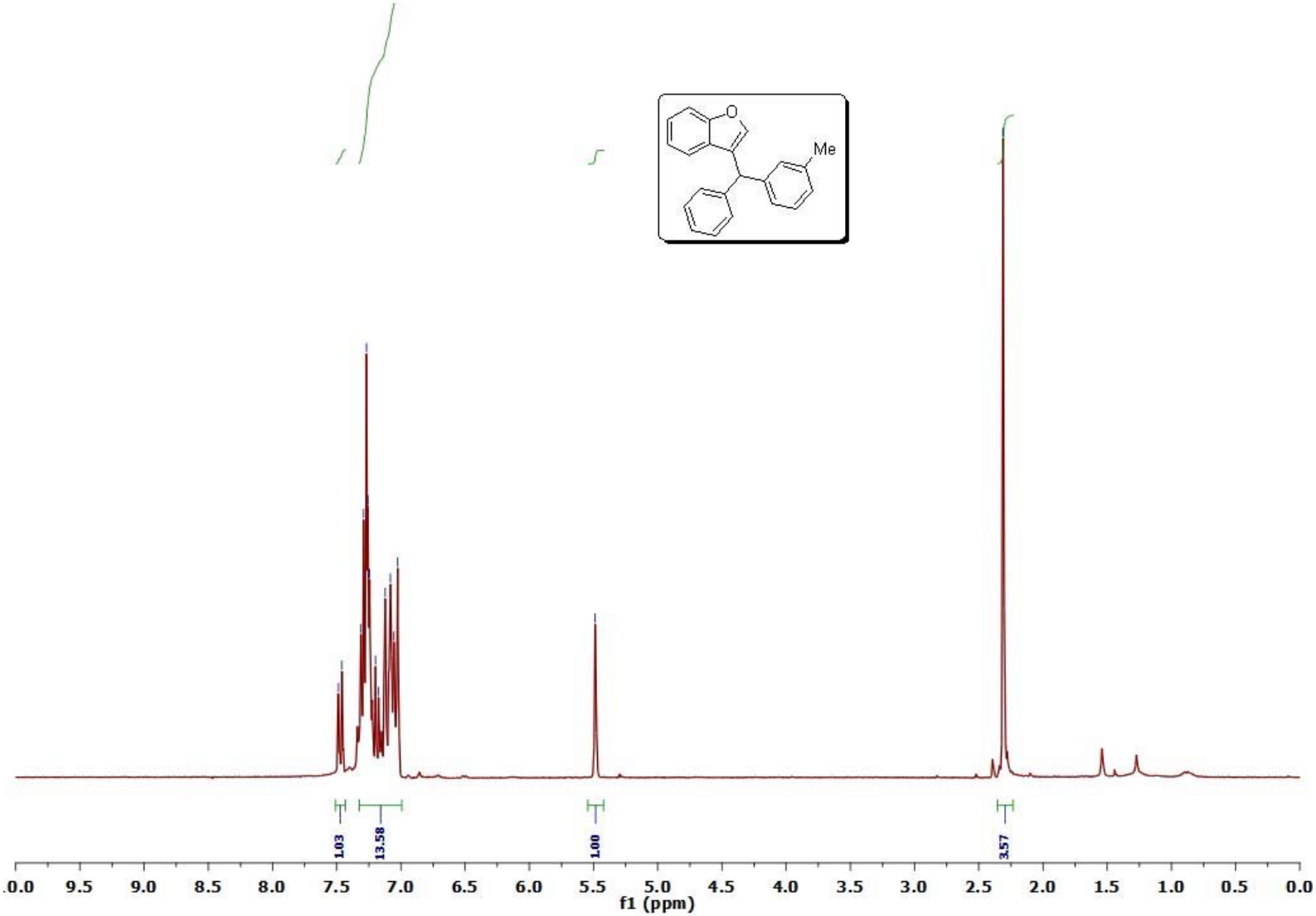
This journal is © The Royal Society of Chemistry 2011



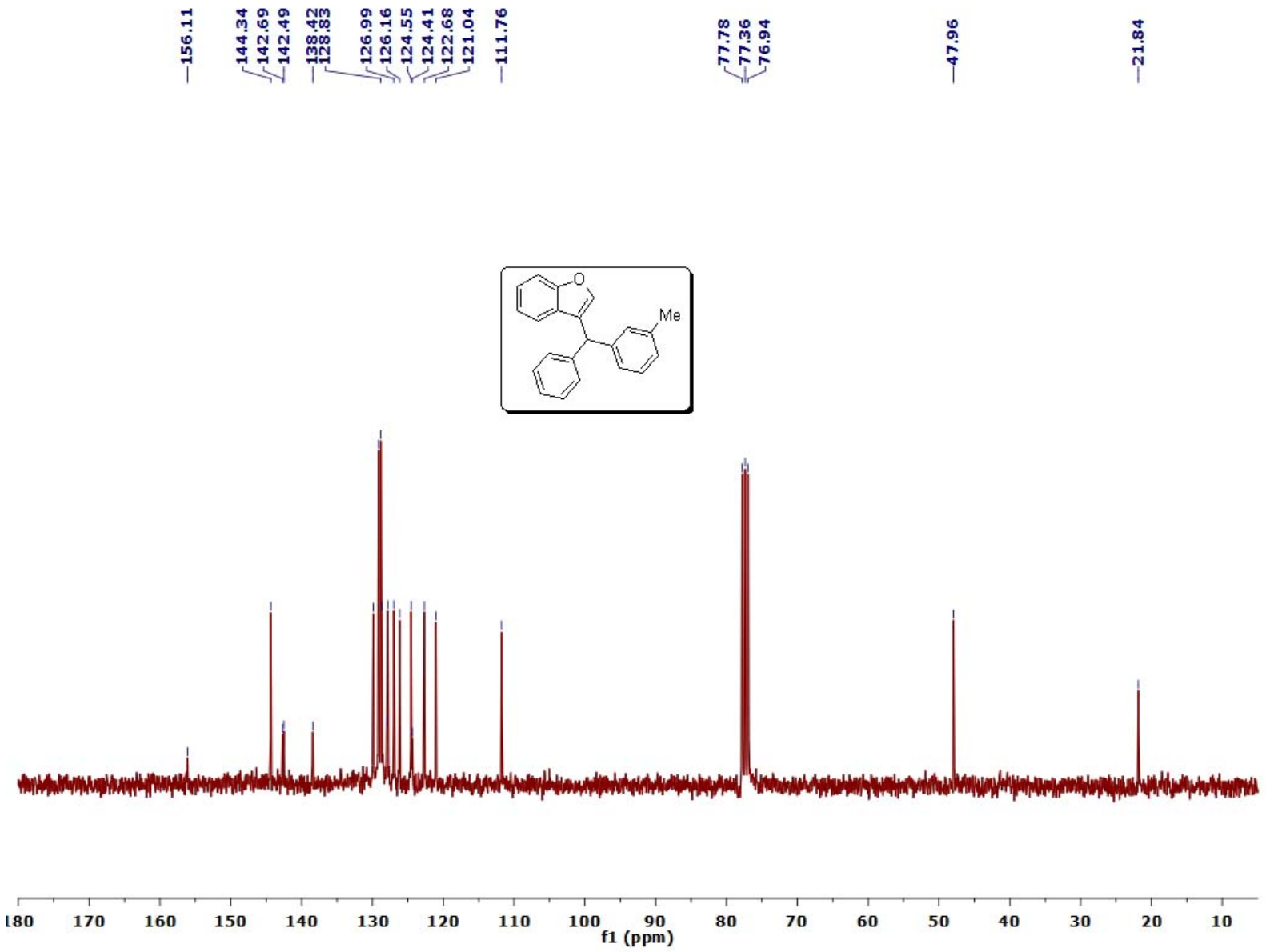
This journal is © The Royal Society of Chemistry 2011



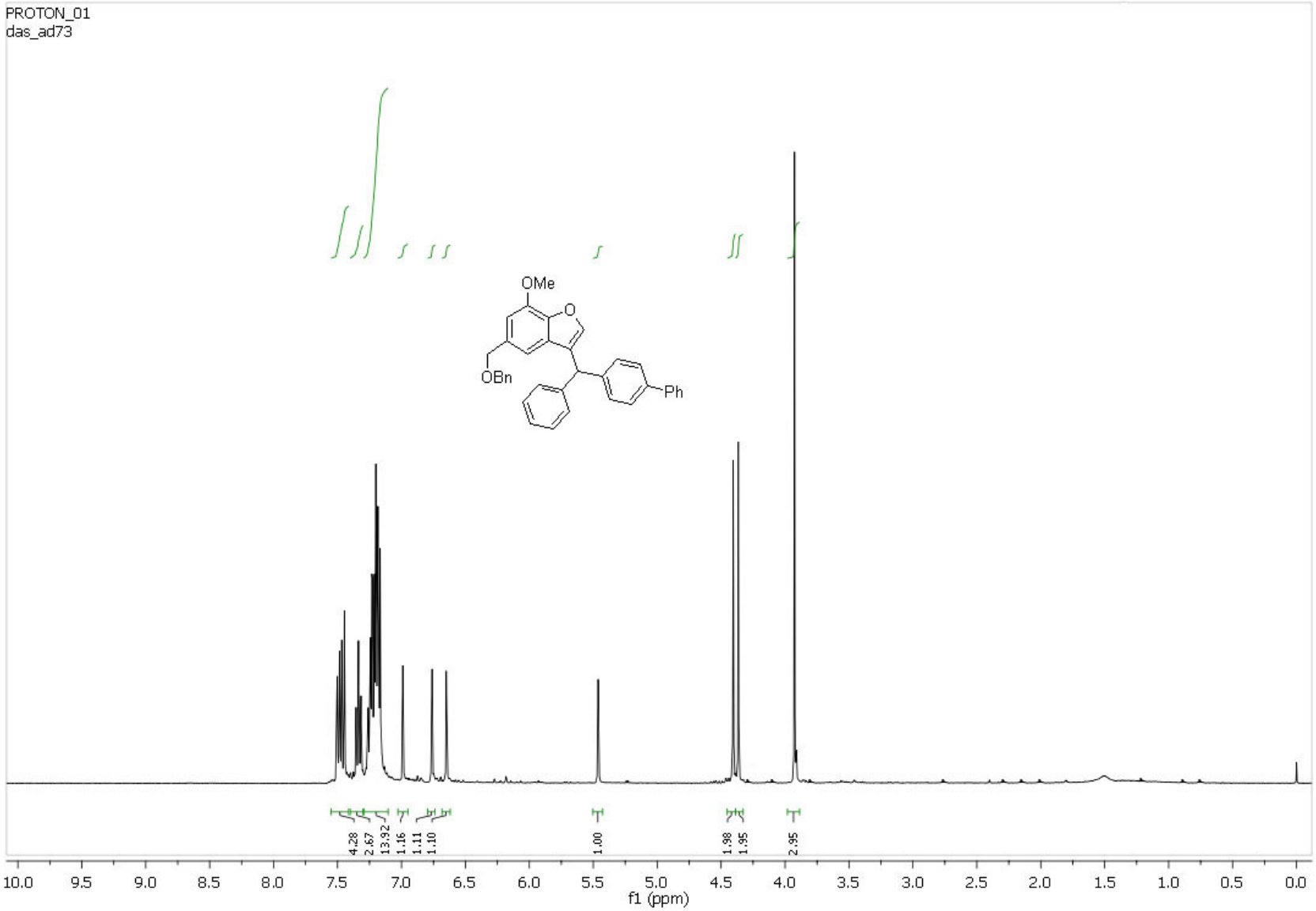
This journal is © The Royal Society of Chemistry 2011



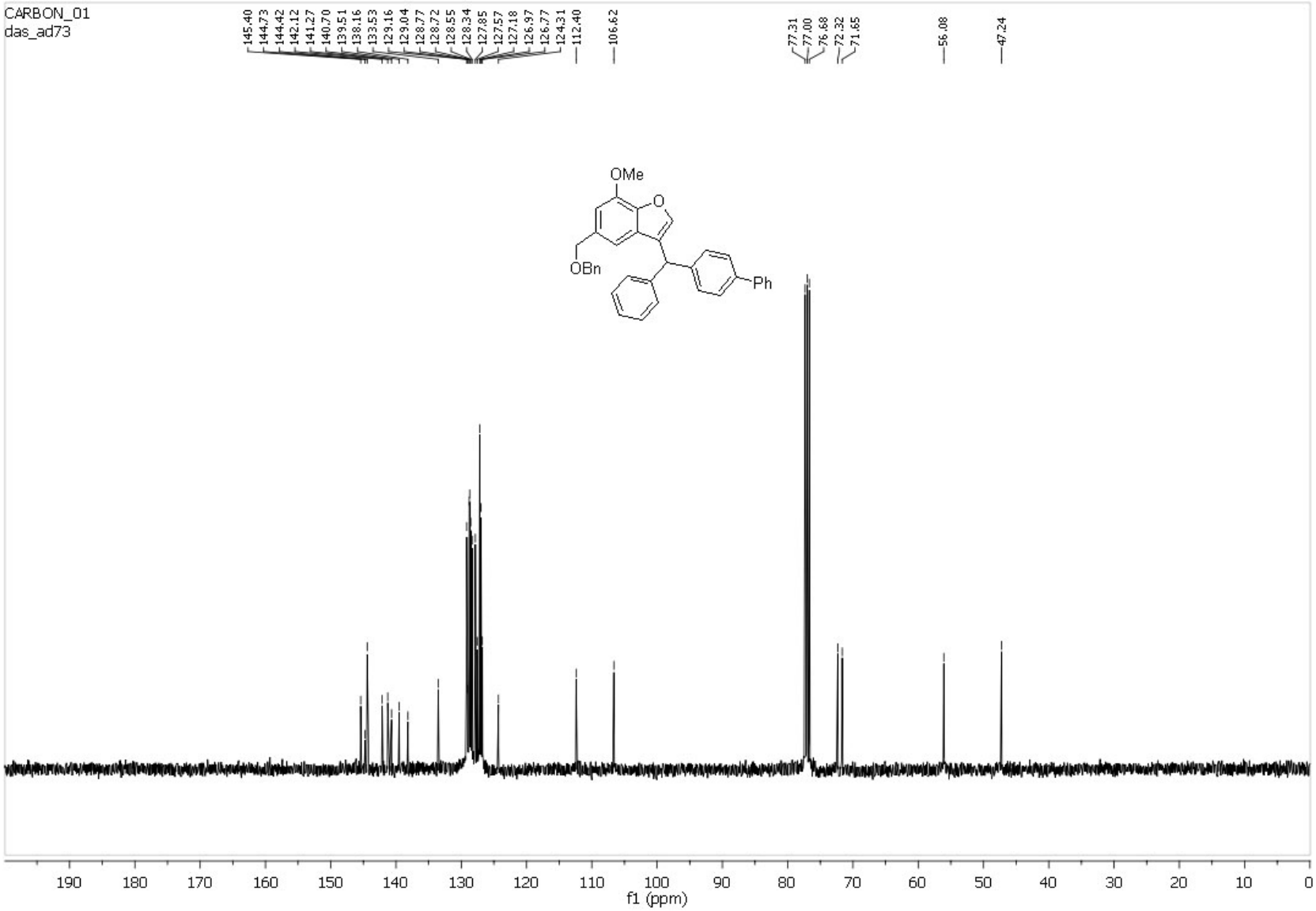
This journal is © The Royal Society of Chemistry 2011



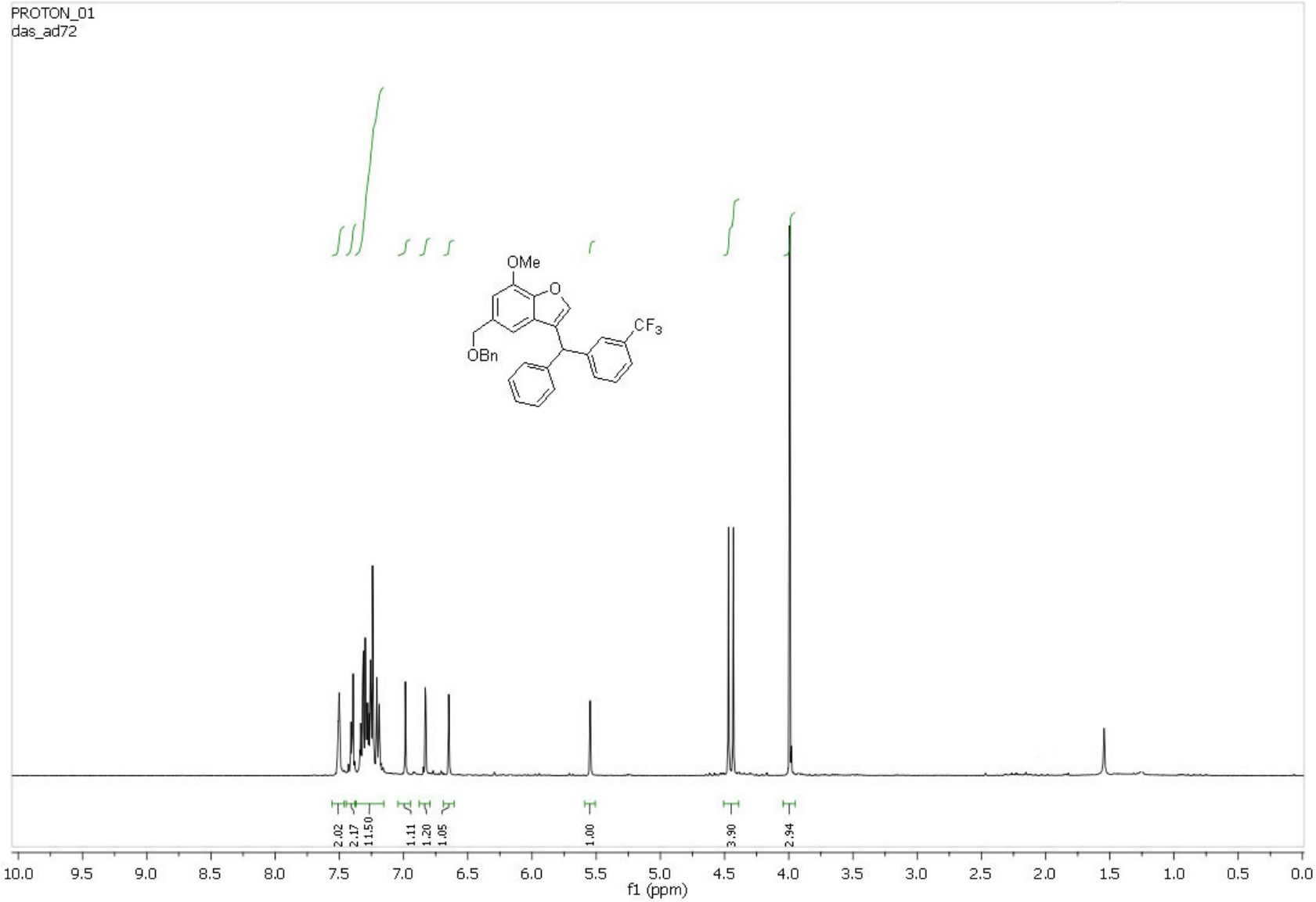
Electronic Supplementary Material (ESI) for Chemical Communications
This journal is © The Royal Society of Chemistry 2011



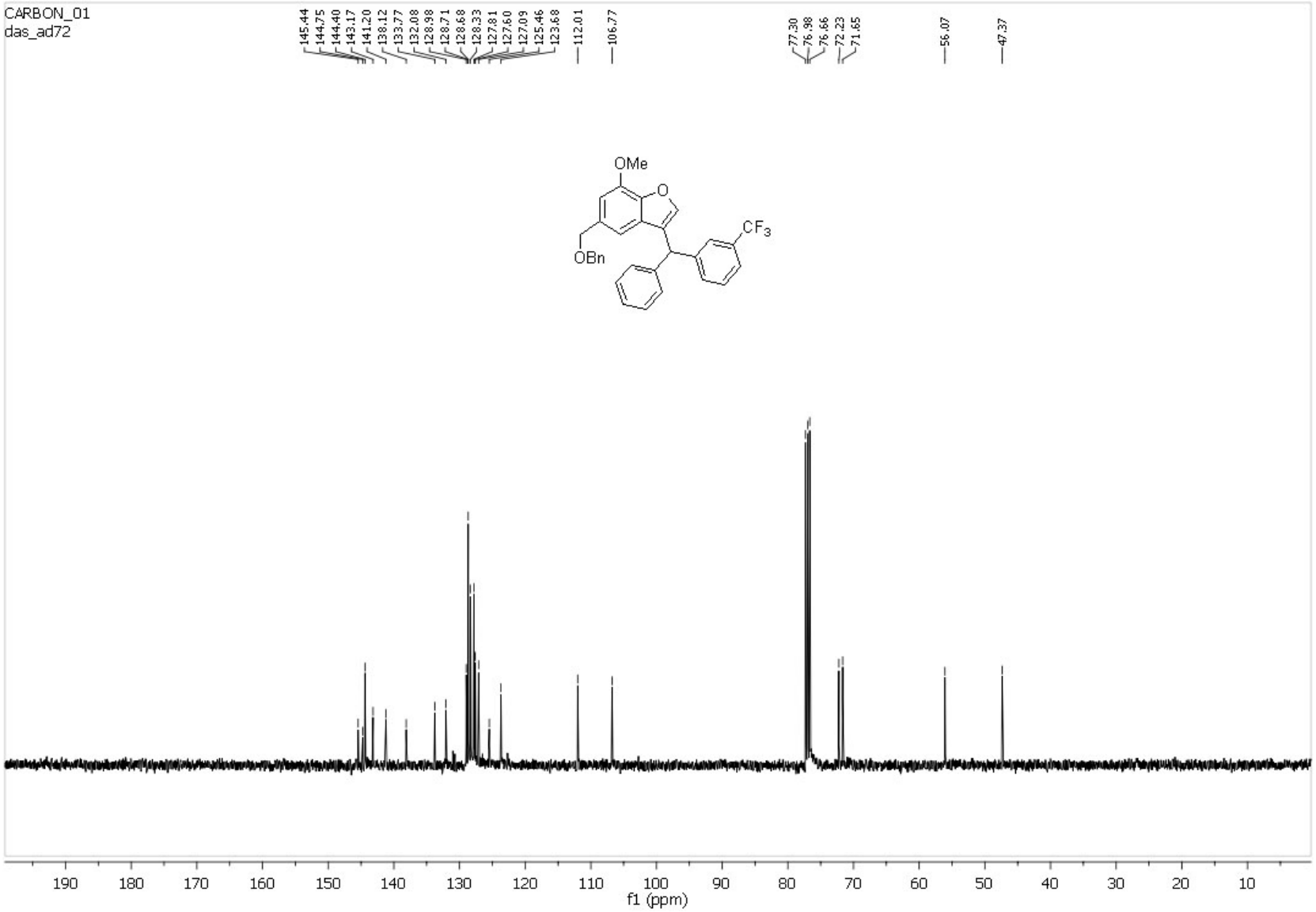
This journal is © The Royal Society of Chemistry 2011



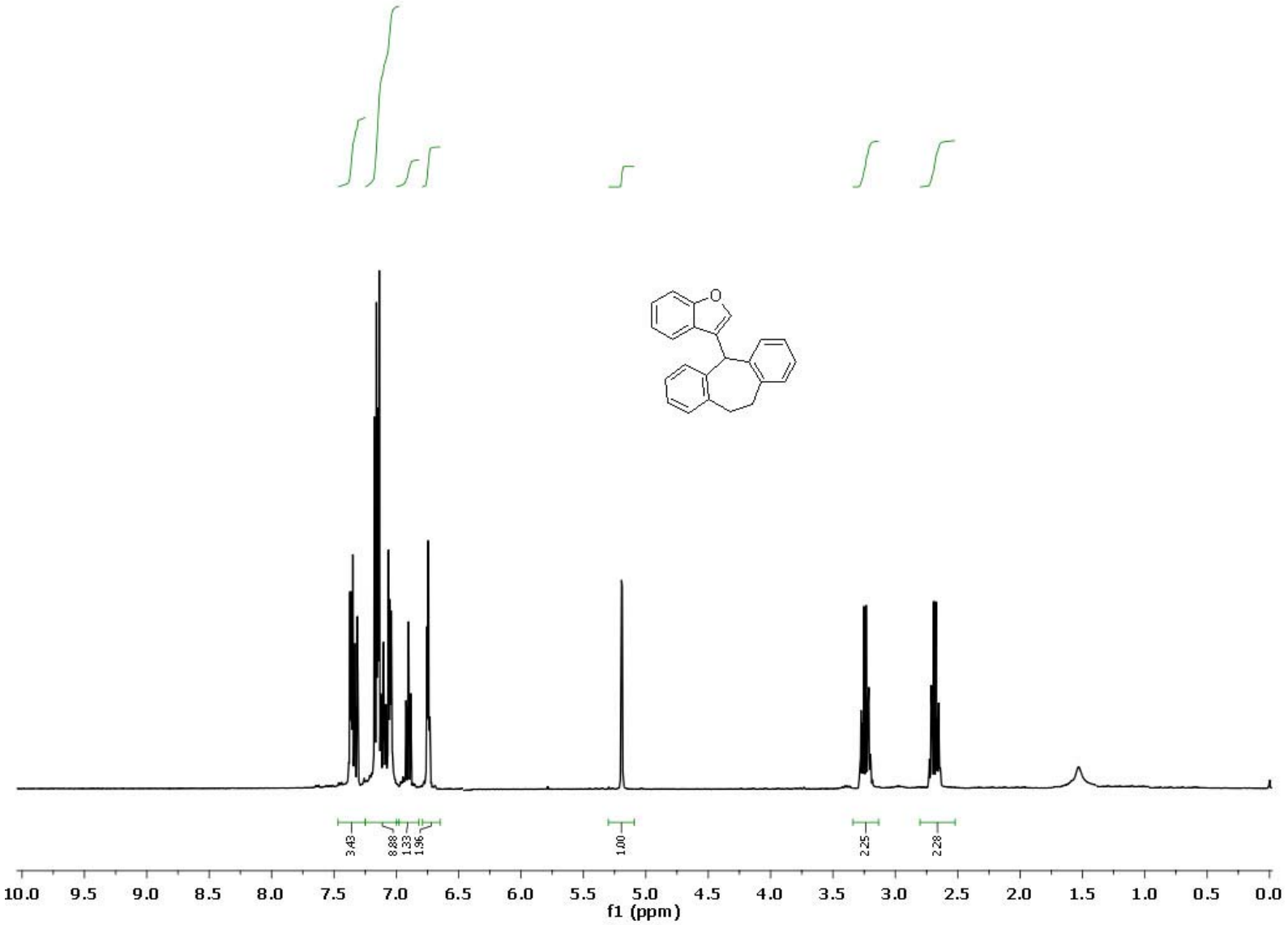
This journal is © The Royal Society of Chemistry 2011



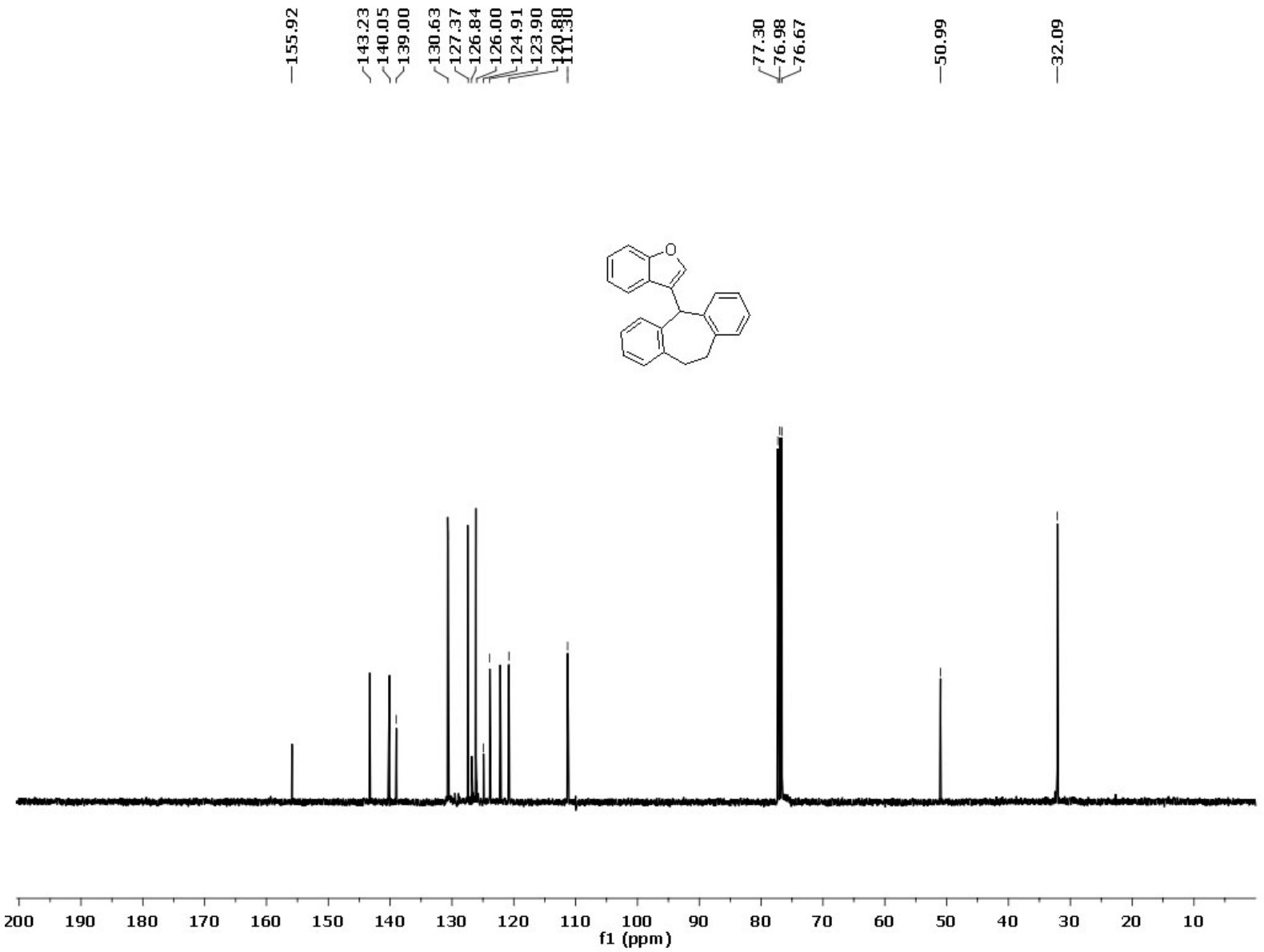
This journal is © The Royal Society of Chemistry 2011



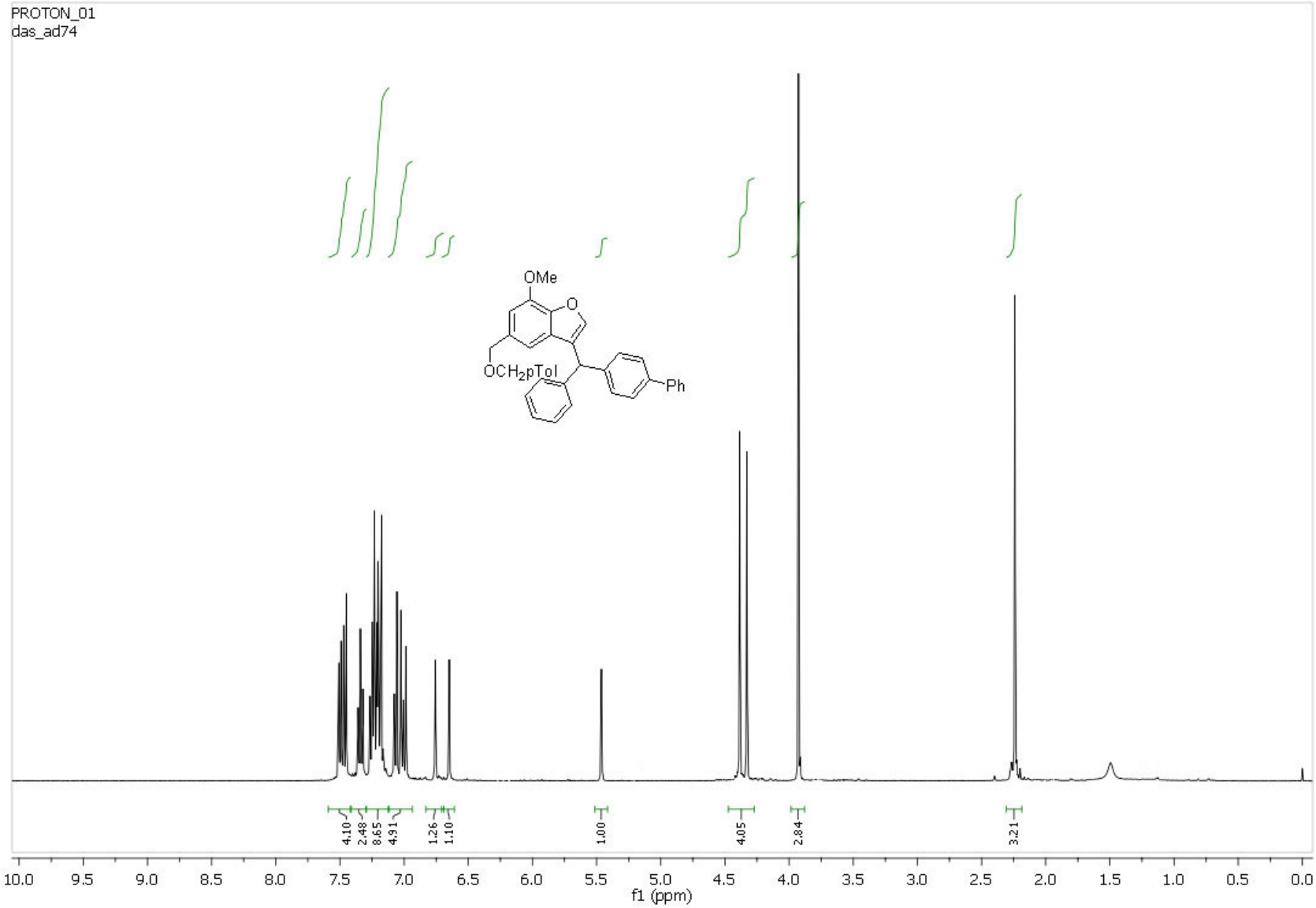
This journal is © The Royal Society of Chemistry 2011



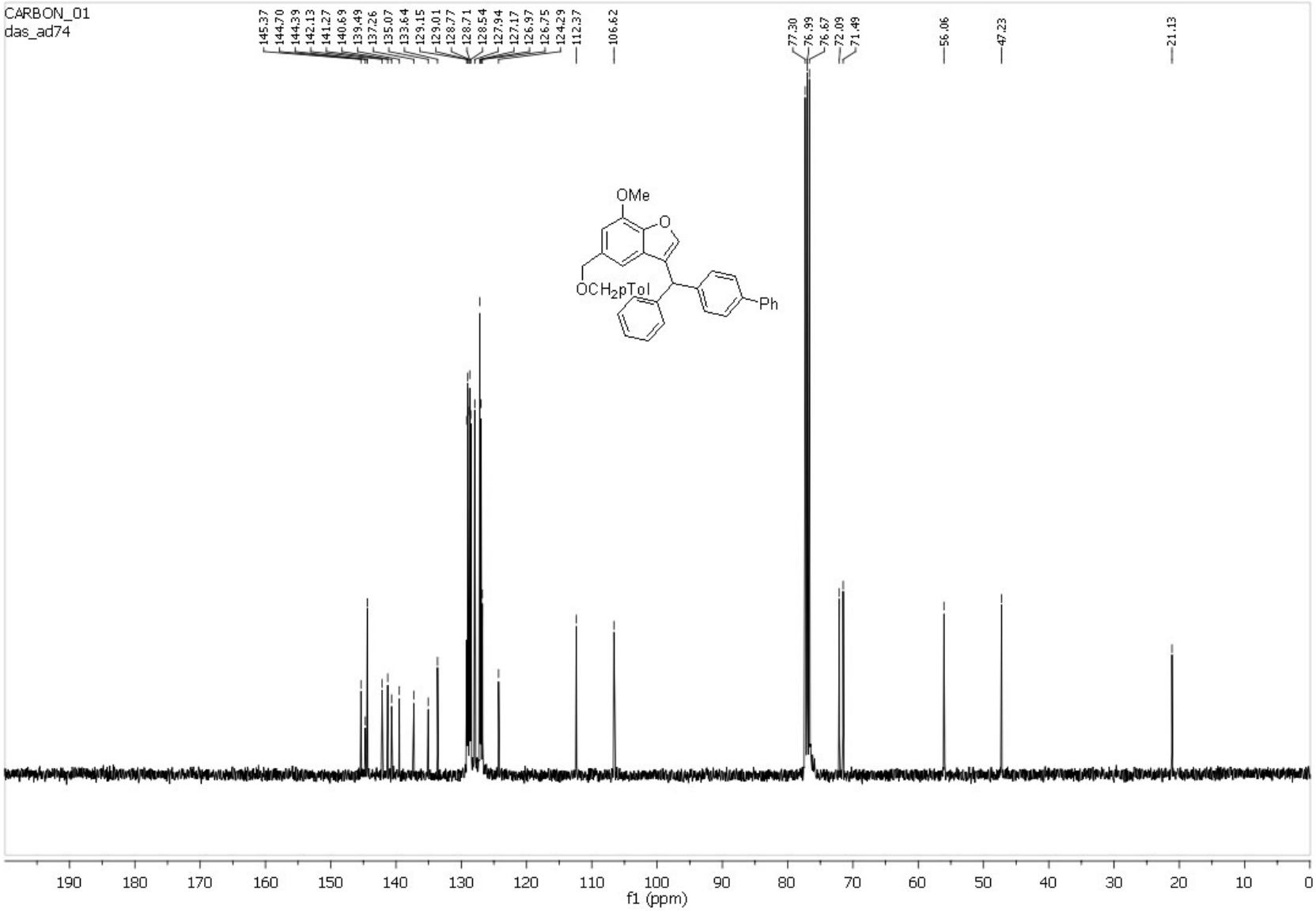
This journal is © The Royal Society of Chemistry 2011



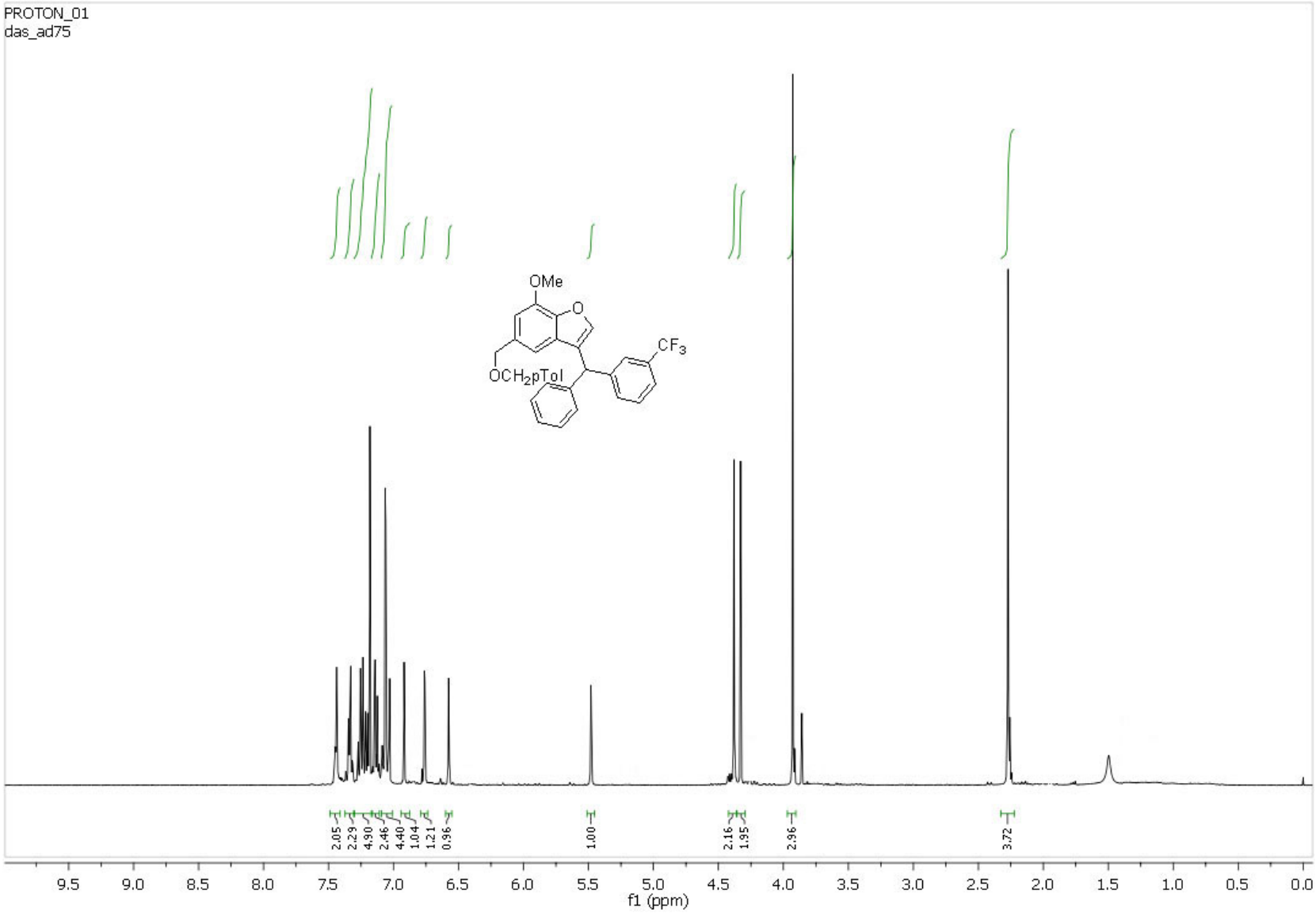
This journal is © The Royal Society of Chemistry 2011



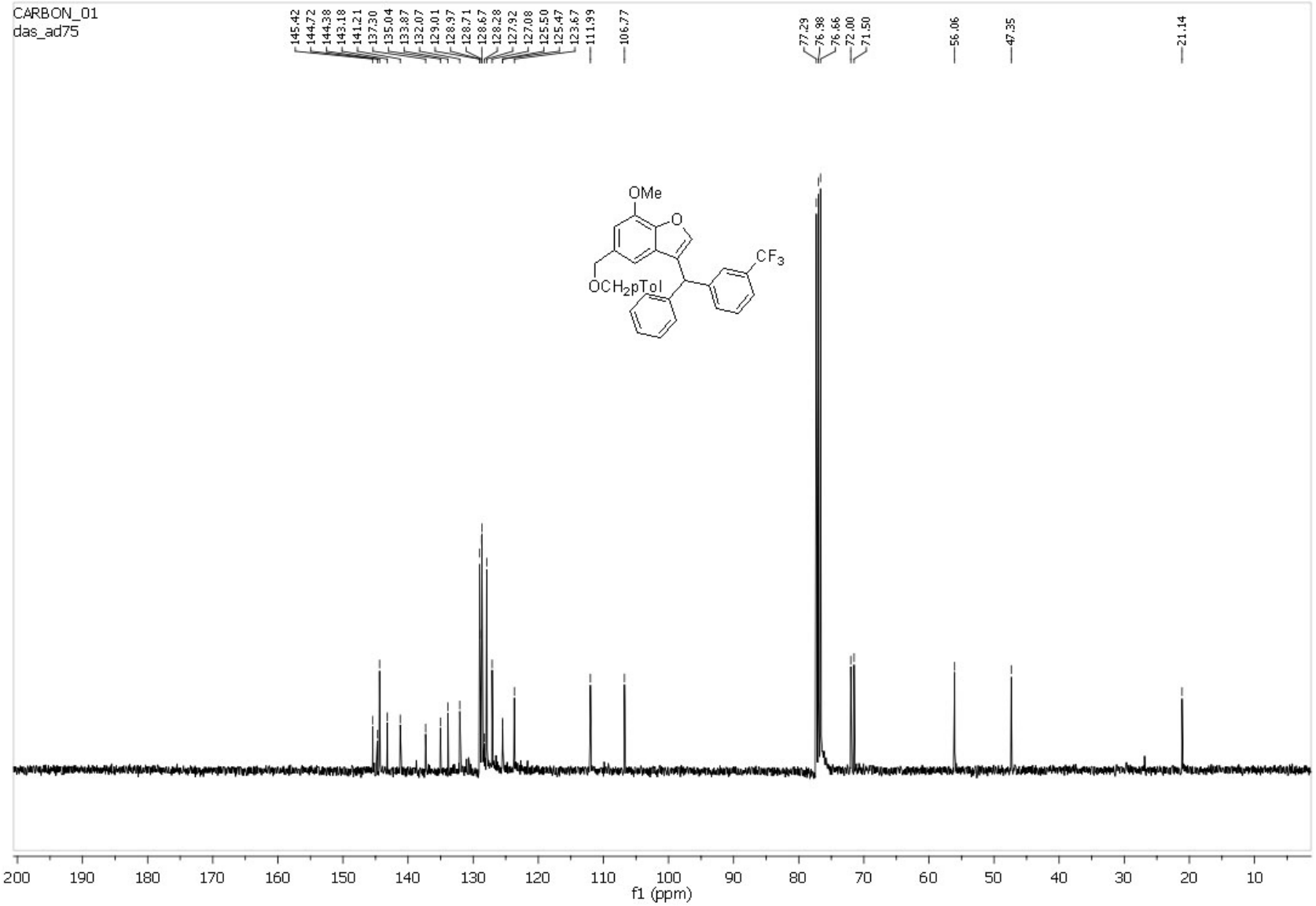
This journal is © The Royal Society of Chemistry 2011



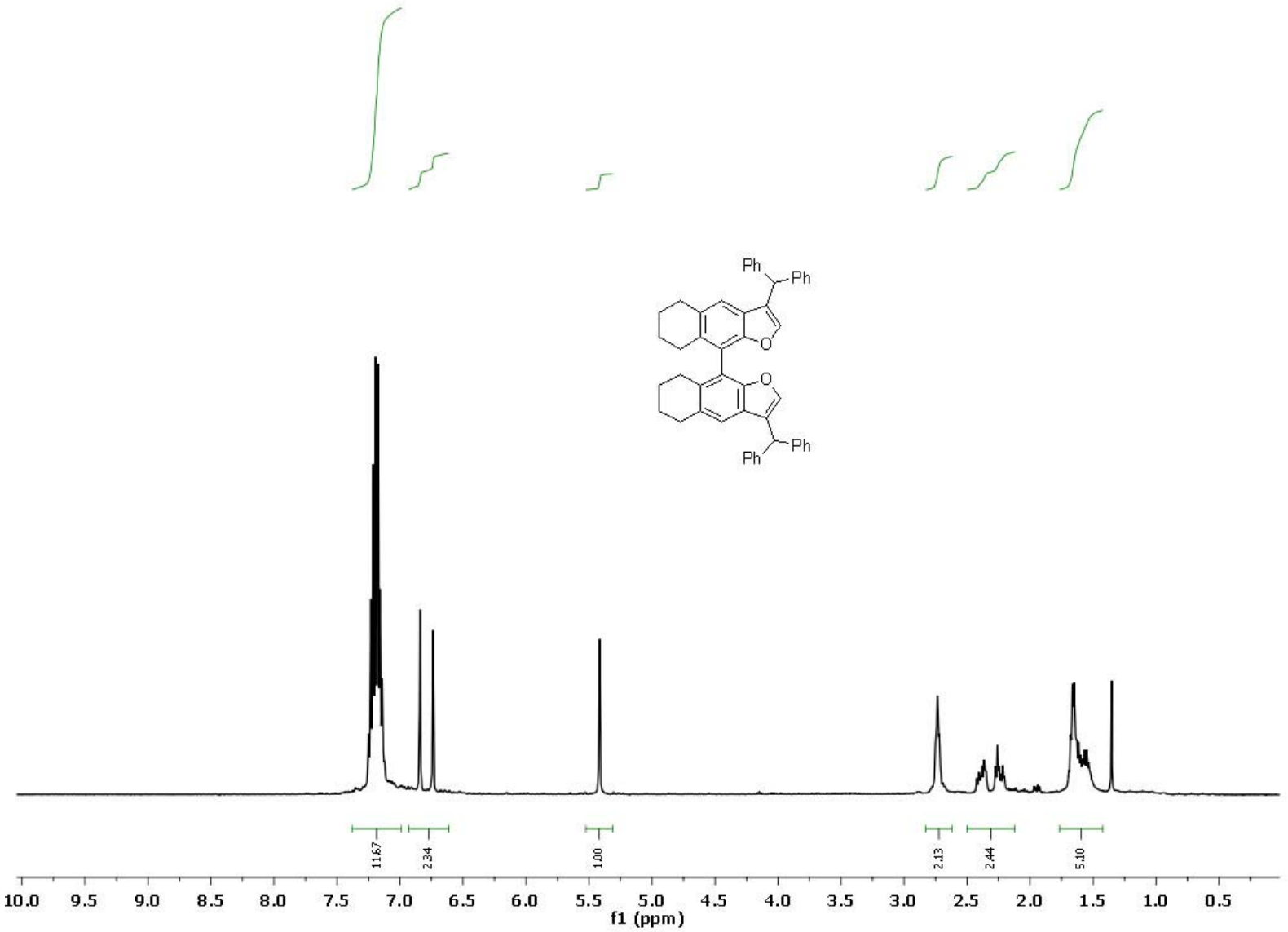
This journal is © The Royal Society of Chemistry 2011



This journal is © The Royal Society of Chemistry 2011



This journal is © The Royal Society of Chemistry 2011



This journal is © The Royal Society of Chemistry 2011