Electronic Supplementary Information (ESI)

C−H cycloamination of *N*-aryl-2-aminopyridines and *N*-arylamidines catalyzed by in situ generated hypervalent iodine(III) reagent

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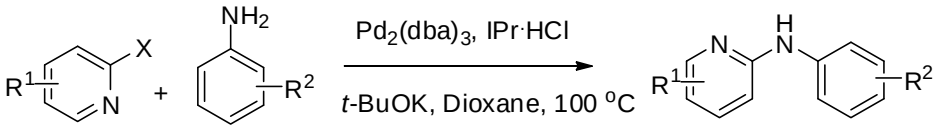
1. General Information

Reactions were monitored by using thin-layer chromatography (TLC) on commercial silica gel plates (GF 254). Visualization of the developed plates was performed under UV lights (GF 254 nm). Flash column chromatography was performed on silica gel (200-300 mesh). ^{1}H and ^{13}C NMR spectra were recorded on a Bruker AV400 or 500 MHz spectrometer. Chemical shifts (δ) were reported in ppm referenced to an internal TMS 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 D_6-DMSO (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 and Characterization of Substrates

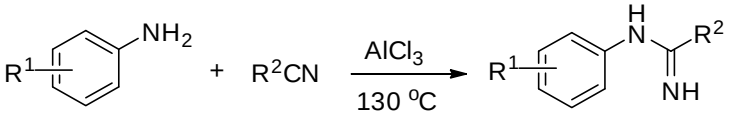
2.1 Synthesis of Substrates

Substrates **1b-1w** were prepared according to the following general procedure. [1]



Under an atmosphere of argon, 1,4-dioxane (10 mL), *t*-BuOK (504 mg, 4.5 mmol), 2-halopyridine (3.0 mmol), and aniline (3.6 mmol) were added in turn to a Schlenk tube charging with $Pd_2(dba)_3$ (60 mg, 0.06 mmol), IPr·HCl (1,3-bis(2,6-diisopropyl phenyl) imidazolium chloride) (54 mg, 0.12 mmol), and a magnetic stirring bar. The Schlenk tube was placed in a 100 °C oil bath and stirred for 2-48 h. The mixture was then allowed to cool to room temperature, then diluted with water, and extracted with ethyl acetate. The extracts were combined, washed with brine, and then dried over anhydrous Na_2SO_4. The solvent was removed under vacuum and the residue was purified by flash chromatography.

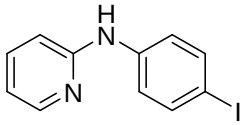
Substrates **3a-3d** were prepared according to the following general procedure. [2]



A mixture of $AlCl_3$ (11.0 mmol, 1.1 equiv), aniline (11.0 mmol, 1.1 equiv) and carbonitrile (10.0 mmol) was stirred at 130 °C under an inert atmosphere in a sealed tube for about an hour. The hot mixture was poured into a solution of concentrated NaOH solution (40 mL) in mixed water and ice (100 mL) and stirred for about 15 minutes. Then the mixture was extracted with EtOAc (25 mL × 3). The combined organic layers were washed with brine (30 mL × 3), dried over anhydrous Na_2SO_4, and evaporated under vacuum. The residue was purified either by column chromatography on silica gel or by recrystallization.

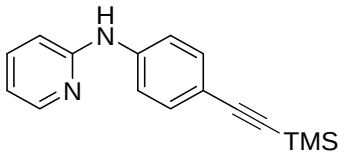
2.2 Characterization of Some New Substrates

***N*-(4-iodophenyl)-2-aminopyridine (1h)**



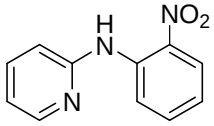
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.21 (d, *J* = 6.4 Hz, 1H), 7.61-7.58 (m, 2H), 7.53-7.49 (m, 1H), 7.16 (d, *J* = 8.4 Hz, 2H), 6.82 (d, *J* = 8.4 Hz, 1H), 6.78-6.75 (m, 1H), 6.66 (br s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 155.4, 148.2, 140.4, 138.0, 137.7, 121.7, 115.4, 108.8, 84.7.

***N*-(4-(2-(trimethylsilyl)ethynyl)phenyl)-2-aminopyridine (1i)**



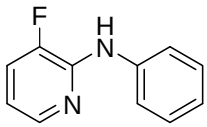
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.23 (d, *J* = 8.0 Hz, 1H), 7.55-7.50 (m, 1H), 7.42 (d, *J* = 8.8 Hz, 2H), 7.30 (d, *J* = 8.8 Hz, 2H), 6.87 (d, *J* = 8.0 Hz, 1H), 6.78 (t, *J* = 5.6 Hz, 1H), 6.61(br s, 1H), 0.25 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 155.1, 148.4, 140.9, 137.7, 133.1, 118.6, 116.4, 115.7, 109.2, 105.3, 92.9.

***N*-(2-nitrophenyl)-2-aminopyridine (1n)**



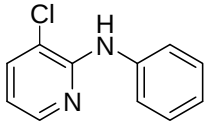
^{1}H NMR (400 MHz, $CDCl_3$): δ 10.15 (br s, 1H), 8.75 (d, *J* = 7.6 Hz, 1H), 8.35 (t, *J* = 4.4 Hz, 1H), 8.23 (d, *J* = 6.8 Hz, 1H), 7.84 (t, *J* = 5.6 Hz, 1H), 7.64 (t, *J* = 5.6 Hz, 1H), 7.55 (d, *J* = 5.6 Hz, 1H), 7.21 (d, *J* = 5.6 Hz, 1H), 6.94 (t, *J* = 4.4 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 153.5, 147.9, 138.9, 138.0, 135.6, 129.0, 126.2, 122.5, 119.6, 117.8, 113.8.

3-fluoro-*N*-phenyl-2-aminopyridine (1r)



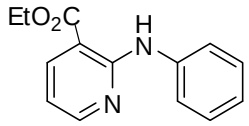
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.01 (d, *J* = 7.6 Hz, 1H), 7.66 (d, *J* = 7.6 Hz, 2H), 7.33 (t, *J* = 5.6 Hz, 2H), 7.30-7.25 (m, 1H), 7.04 (t, *J* = 7.2 Hz, 1H), 6.72 (d, *J* = 3.6 Hz, 1H), 6.61 (br s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 148.0, 145.9, 145.4, 145.3, 142.6, 142.5, 139.6, 128.9, 122.3, 120.9, 120.8, 119.1, 114.4.

3-chloro-*N*-phenyl-2-aminopyridine (1s)



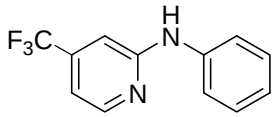
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.13 (d, *J* = 4.0 Hz, 1H), 7.63 (d, *J* = 7.6 Hz, 2H), 7.57 (d, *J* = 7.6 Hz, 1H), 7.34 (d, *J* = 8.4 Hz, 2H), 7.05 (t, *J* = 7.2 Hz, 1H), 6.97 (br s, 1H), 6.70 (d, *J* = 7.6 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 151.4, 145.8, 139.8, 136.6, 128.9, 122.8, 120.0, 116.1, 115.2.

ethyl 2-(phenylamino)pyridine-3-carboxylate (1t)



^{1}H NMR (400 MHz, $CDCl_3$): δ 10.20 (br s, 1H), 8.38-8.36 (m, 1H), 8.26-8.23 (m, 1H), 7.70 (t, *J* = 7.6 Hz, 2H), 7.36-7.32 (m, 2H), 7.05 (t, *J* = 7.6 Hz, 1H), 6.73-6.70 (m, 1H), 4.40 (t, *J* = 7.2 Hz, 2H), 1.42 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 167.5, 156.2, 140.1, 139.7, 133.0, 128.8, 122.7, 120.8, 113.2, 107.2, 61.2, 14.2.

4-(trifluoromethyl)-*N*-phenyl-2-aminopyridine (1u)

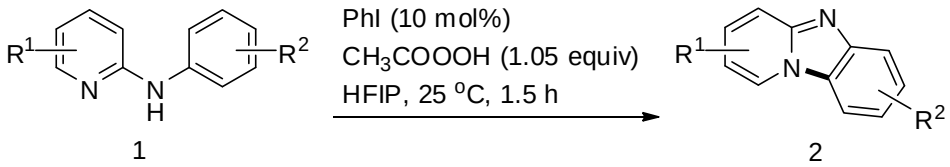


^{1}H NMR (400 MHz, MeOD): δ 8.28 (d, *J* = 5.2 Hz, 1H), 7.58-7.56 (m, 2H), 7.30 (t, *J* = 5.2 Hz, 2H), 7.02-6.99 (m, 2H), 6.90 (t, *J* = 4.8 Hz, 1H), 6.76 (br s, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 156.9, 156.8, 149.6, 140.4, 140.1, 139.9, 139.6, 139.4, 139.3, 129.5, 126.1, 124.0, 123.8, 121.8, 121.3, 121.1, 110.0, 103.7, 103.6.

3. General Procedure and Product Characterization

3.1 General Procedure

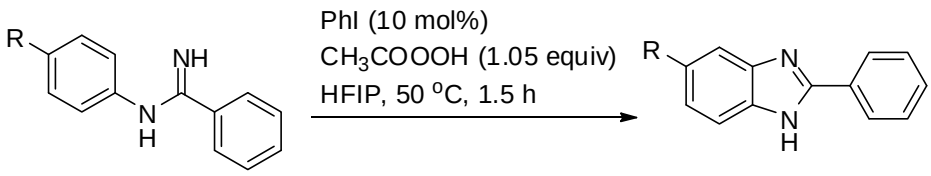
Substrates **2a-2w** were afforded according to the following procedure



1 2

A tube was charged with **1** (0.2 mmol), PhI (0.02 mmol), peracetic acid (41-45 wt %, 34 μL), and 1,1,1,3,3,3-hexafluoro-2-propanol (2 mL). The reaction mixture was stirred at room temperature for 1.5 h. The reaction mixture was quenched with saturated solution of sodium thiosulphate and extracted with ethyl acetate. The organic layer was washed with brine, and dried over anhydrous Na_2SO_4. The organic extracts were filtered and concentrated under reduced pressure. Purification by column chromatography on silica gel afforded the pure product.

Substrates **4a-4d** were afforded according to the following procedure



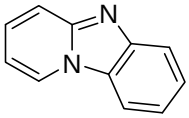
3 **4**

A tube was charged with **3** (0.2 mmol), PhI (0.02 mmol), peracetic acid (41-45 wt %, 34 μL), and 1,1,1,3,3,3-Hexafluoro-2-propanol (2 mL). The reaction mixture was

stirred at 50 ^{o}C for 1.5 h. The reaction mixture was quenched with saturated solution of sodium thiosulphate and extracted with ethyl acetate. The organic layer was washed with brine, dried over anhydrous Na_2SO_4. The organic extracts were filtered and concentrated under reduced pressure. Purification by column chromatography on silica gel afforded the pure product.

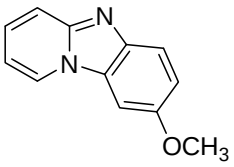
3.2 Product Characterization

Pyrido[1,2-*a*]benzimidazole (2a)



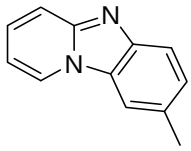
Yield: 91%. mp 181-182 ^{o}C, white solid. ^{1}H NMR (400 MHz, D_6-DMSO): δ 9.08 (d, *J* = 6.8 Hz, 1H), 8.30 (d, *J* = 8.4 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 1H), 7.66 (d, *J* = 9.2 Hz, 1H), 7.57-7.48 (m, 2H), 7.39-7.35 (m, 1H), 7.00-6.98 (m, 1H); ^{13}C NMR (125 MHz, D_6-DMSO): δ 148.0, 144.3, 130.4, 128.9, 127.3, 125.6, 120.8, 119.2, 117.2, 112.3, 110.5; HRMS (ESI): Exact mass calcd for $C_{11}H_9N_2$ $[M+H]^+$, 169.0760; Found :169.0765.

8-methoxypyrido[1,2-*a*]benzimidazole (2b)



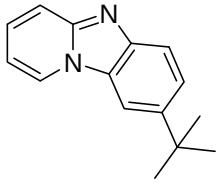
Yield: 85%. mp 155-156 ^{o}C, dark solid. ^{1}H NMR (400 MHz, D_6-DMSO): δ 8.99 (d, *J* = 6.8 Hz, 1H), 7.90 (d, *J* = 2.4 Hz, 1H), 7.70 (d, *J* = 8.8 Hz, 1H), 7.59 (d, *J* = 9.2 Hz, 1H), 7.46-7.42 (m, 1H), 7.14-7.12 (m, 1H), 6.95-6.92 (m, 1H), 3.88 (s, 3H); ^{13}C NMR (100 MHz, D_6-DMSO): δ 154.6, 147.1, 138.4, 128.7, 128.4, 126.3, 119.4, 116.9, 115.4, 109.6, 94.6, 55.7; HRMS (ESI): Exact mass calcd for $C_{12}H_{11}N_2O$ $[M+H]^+$, 199.0866; Found: 199.0870.

8-methylpyrido[1,2-*a*]benzimidazole (2c)



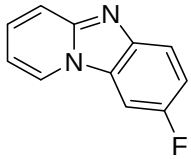
Yield: 93%. mp 83-85 °C, off-white solid. ^{1}H NMR (400 MHz, D_6-DMSO): δ 8.98 (d, *J* = 6.8 Hz, 1H), 8.10 (s, 1H), 7.68 (d, *J* = 8.4 Hz, 1H), 7.61 (d, *J* = 9.2 Hz, 1H), 7.52-7.47 (m, 1H), 7.34-7.32 (m, 1H), 6.97-6.93 (m, 1H), 2.53 (s, 3H); ^{13}C NMR (125 MHz, D_6-DMSO): δ 147.5, 142.1, 130.0, 129.5, 128.7, 127.0, 126.7, 118.6, 117.0, 111.3, 110.1, 21.4; HRMS (ESI): Exact mass calcd for $C_{12}H_{11}N_2$ $[M+H]^+$, 183.0917; Found: 183.0923.

8-(*tert*-butyl)pyrido[1,2-*a*]benzimidazole (2d)



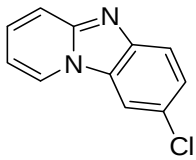
Yield: 94%. mp 90-92 °C, pale yellow solid. ^{1}H NMR (400 MHz, D_6-DMSO): δ 9.12 (d, *J* = 6.8 Hz, 1H), 8.29 (d, *J* = 1.6 Hz, 1H), 7.71 (d, *J* = 8.8 Hz, 1H), 7.63- 7.57(m, 2H), 7.52-7.48 (m, 1H), 6.97-6.93 (m, 1H), 1.41 (s, 9H); ^{13}C NMR (125 MHz, D_6-DMSO): δ 147.8, 143.8, 142.0, 129.4, 128.4, 126.9, 123.4, 118.3, 116.9, 109.8, 107.9, 34.8, 31.6; HRMS (ESI): Exact mass calcd for $C_{15}H_{17}N_2$ $[M+H]^+$, 225.1386; Found: 225.1391.

8-fluoropyrido[1,2-*a*]benzimidazole (2e)



Yield: 94%. mp 182-183 °C, white solid. ^{1}H NMR (400 MHz, D_6-DMSO): δ 9.00 (d, *J* = 6.8 Hz, 1H), 8.26-8.23 (m, 1H), 7.83-7.80 (m, 1H), 7.65 (d, *J* = 9.2 Hz, 1H), 7.56-7.51 (m, 1H), 7.40-7.35 (m, 1H), 7.01-6.98 (m, 1H); ^{13}C NMR (125 MHz, D_6-DMSO): δ 158.1, 156.2, 148.5, 140.5, 130.0, 128.4, 128.2, 127.0, 120.1, 120.0, 117.2, 113.9, 113.7, 110.4, 98.7, 98.5; HRMS (ESI): Exact mass calcd for $C_{11}H_8FN_2$ $[M+H]^+$, 187.0666; Found: 187.0665.

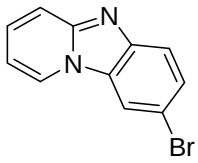
8-chloropyrido[1,2-*a*]benzimidazole (2f)



Yield: 99%. mp 110-112 °C, white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.36 (d, *J* = 6.8 Hz, 1H), 7.89 (s, 1H), 7.85 (d, *J* = 8.8 Hz, 1H), 7.68 (d, *J* = 9.2 Hz, 1H), 7.50 (d, *J* =

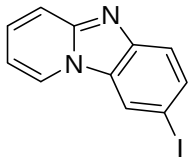
2.0 Hz, 1H), 7.48-7.42 (m, 1H), 6.87 (t, J = 6.4 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 149.0, 143.0, 129.6, 129.0, 126.6, 126.4, 125.0, 120.8, 118.2, 110.8, 110.5; HRMS (ESI): Exact mass calcd for $C_{11}H_8ClN_2$ $[M+H]^+$, 203.0371; Found: 203.0369.

8-bromopyrido[1,2-*a*]benzimidazole (2g)



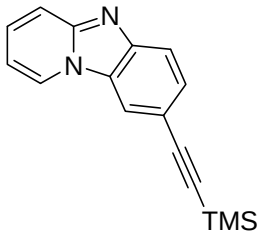
Yield: 91%. mp 151-153 °C, off-white solid. ^{1}H NMR (400 MHz, D_6-DMSO): δ 9.05 (d, J = 6.8 Hz, 1H), 8.62 (d, J = 2.0 Hz, 1H), 7.73 (d, J = 8.8 Hz, 1H), 7.65 (d, J = 9.2 Hz, 1H), 7.61-7.54 (m, 2H), 7.02-6.99 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 149.0, 143.6, 129.6, 129.0, 125.1, 121.3, 118.4, 113.9, 113.6, 110.8; HRMS (ESI): Exact mass calcd for $C_{11}H_8BrN_2$ $[M+H]^+$, 246.9865; Found: 246.9873.

8-iodopyrido[1,2-*a*]benzimidazole (2h)



Follow the general procedure, yield: 39%. mp 181-182 °C, off-white solid. The yield of **2h** was improved significantly to 91% by slowly addition of a solution of peracetic acid (34 μL) in HFIP (1.0 mL) during 5 minutes to a HFIP (1.0 mL) solution of *N*-(4-iodophenyl)-2-aminopyridine. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.38 (d, J = 6.8 Hz, 1H), 8.25(s, 1H), 7.80-7.77 (m, 1H), 7.71-7.68 (m, 1H), 7.48-7.43 (m, 1H), 6.88 (t, J = 6.8 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 148.5, 143.8, 134.4, 130.1, 129.9, 125.0, 121.6, 119.5, 118.1, 110.9, 83.3; HRMS (ESI): Exact mass calcd for $C_{11}H_8IN_2$ $[M+H]^+$, 294.9727; Found: 294.9725.

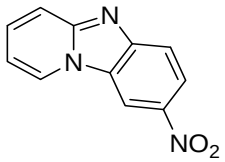
8-(trimethylsilyl)ethynylpyrido[1,2-*a*]benzimidazole (2i)



Yield: 78%. mp 209-210 °C, pale yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.41 (d, J = 6.8 Hz, 1H), 8.05 (s, 1H), 7.83 (d, J = 8.4 Hz, 1H), 7.69 (d, J = 9.2 Hz, 1H), 7.64-7.61 (m, 1H), 7.48-7.44 (m, 1H), 6.89 (t, J = 6.8 Hz, 1H), 0.29 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 149.5, 144.6, 130.0, 129.8, 128.3, 125.2, 119.7, 118.2, 115.5,

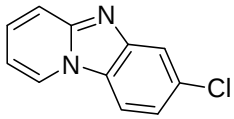
114.3, 110.9, 105.7, 93.6; HRMS (ESI): Exact mass calcd for $C_{16}H_{16}N_2Si[M+H]^+$,265.1156; Found: 265.1154.

8-nitropyrido[1,2-*a*]benzimidazole (2j)



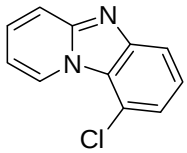
Yield: 97%. mp 275-276 °C, dark solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.92(s, 1H), 8.60 (d, *J* = 6.8 Hz, 1H), 8.47-8.44 (m, 1H), 7.96 (d, *J* = 9.2 Hz, 1H), 7.80 (d, *J* = 9.2 Hz, 1H), 7.64 (t, *J* = 7.2 Hz, 1H), 7.06 (t, *J* = 6.4 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 152.2, 148.9, 141.7, 132.0, 128.0, 125.8, 121.4, 119.8, 118.7, 112.1, 108.0; HRMS (ESI): Exact mass calcd for $C_{11}H_7N_3O_2[M+H]^+$, 214.0611; Found: 214.0614.

7-chloropyrido[1,2-*a*]benzimidazole (2k)



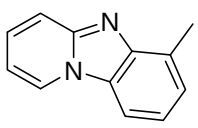
Yield: 44%. mp 209-210 °C, off-white solid. ^{1}H NMR (400 MHz, D_6-DMSO): δ 9.09 (d, *J* = 6.8 Hz, 1H), 8.34 (d, *J* = 8.8 Hz, 1H), 7.84 (s, 1H), 7.67 (d, *J* = 8.8 Hz, 1H), 7.60 (t, *J* = 6.8 Hz, 1H), 7.39-7.37 (m, 1H), 7.04 (t, *J* = 6.8 Hz, 1H); ^{13}C NMR (125 MHz, D_6-DMSO): δ 148.9, 144.8, 130.9, 129.8, 127.5, 127.3, 120.6, 118.1, 116.9, 113.5, 110.9; HRMS (ESI): Exact mass calcd for $C_{11}H_8ClN_2[M+H]^+$, 203.0371; Found: 203.0370.

9-chloropyrido[1,2-*a*]benzimidazole (2k')



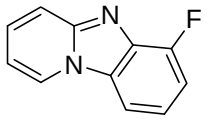
Yield: 44%. mp 225-226 °C, off-white solid. ^{1}H NMR (400 MHz, D_6-DMSO): δ 9.36 (d, *J* = 6.8 Hz, 1H), 7.79-7.77 (m, 1H), 7.71 (d, *J* = 9.2 Hz, 1H), 7.63-7.59 (m, 1H), 7.48 (t, *J* = 8.0 Hz, 1H), 7.41-7.39 (m, 1H), 7.06-7.02 (m, 1H); ^{13}C NMR (125 MHz, D_6-DMSO): δ 148.6, 145.9, 130.7, 127.9, 125.9, 124.3, 121.8, 118.2, 117.5, 117.2, 110.1; HRMS (ESI): Exact mass calcd for $C_{11}H_8ClN_2[M+H]^+$, 203.0375; Found: 203.0374.

6-methylpyrido[1,2-*a*]benzimidazole (2l)



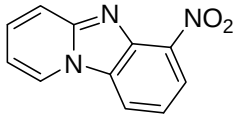
Yield: 79%. mp 139-140 °C, white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.42 (d, *J* = 6.8 Hz, 1H), 7.76-7.72 (m, 2H), 7.43-7.39 (m, 1H), 7.35-7.28 (m, 2H), 6.86-6.82 (m, 1H), 2.80 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.0, 144.0, 130.0, 128.8, 128.3, 125.6, 125.2, 121.0, 118.2, 110.1, 107.7, 17.0; HRMS (ESI): Exact mass calcd for $C_{12}H_{11}N_2$ $[M+H]^+$, 183.0917; Found: 183.0918.

6-fluoropyrido[1,2-*a*]benzimidazole (2m)



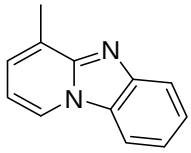
Yield: 71%. mp 207-208 °C, off-white solid. ^{1}H NMR (400 MHz, D_6-DMSO): δ 9.10 (d, *J* = 6.8 Hz, 1H), 8.17-8.15 (m, 1H), 7.72 (d, *J* = 9.2 Hz, 1H), 7.64-7.60 (m, 1H), 7.35-7.31 (m, 2H), 7.08-7.04 (m, 1H); ^{13}C NMR (100 MHz, D_6-DMSO): δ 154.0, 151.5, 147.9, 132.9, 132.7, 131.4, 131.3, 130.7, 126.9, 120.6, 120.5, 117.0, 110.8, 110.0, 109.9, 108.2, 108.1; HRMS (ESI): Exact mass calcd for $C_{11}H_8FN_2$ $[M+H]^+$, 187.0666; Found: 187.0665.

6-nitropyrido[1,2-*a*]benzimidazole (2n)



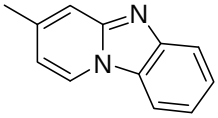
Yield: 88%. mp 300-301 °C, dark solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.55 (d, *J* = 6.8 Hz, 1H), 8.46 (d, *J* = 8.0 Hz, 1H), 8.23 (d, *J* = 8.0 Hz, 1H), 7.94 (d, *J* = 9.6 Hz, 1H), 7.65-7.60 (m, 1H), 7.45 (t, *J* = 8.0 Hz, 1H), 7.05 (t, *J* = 6.8 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 151.1, 138.6, 138.5, 132.0, 131.8, 125.2, 123.0, 119.4, 119.0, 116.7, 112.3; HRMS (ESI): Exact mass calcd for $C_{11}H_7N_3O_2$ $[M+H]^+$, 214.0611; Found: 214.0608.

4-methylpyrido[1,2-*a*]benzimidazole (2o)



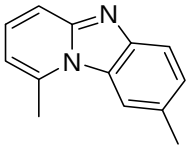
Yield: 85%. mp 135-136 °C, white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.33 (d, *J* = 6.8 Hz, 1H), 7.98 (d, *J* = 8.0 Hz, 1H), 7.87 (d, *J* = 8.4 Hz, 1H), 7.54-7.50 (m, 1H), 7.38-7.34 (m, 1H), 7.22 (d, *J* = 6.4 Hz, 1H), 6.78 (t, *J* = 6.8 Hz, 1H), 2.71 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 149.0, 144.1, 129.1, 127.7, 127.6, 125.4, 122.8 120.9, 119.9, 110.4, 110.3, 17.5; HRMS (ESI): Exact mass calcd for $C_{12}H_{11}N_2$ $[M+H]^+$, 183.0917; Found: 183.0920.

3-methylpyrido[1,2-*a*]benzimidazole (2p)



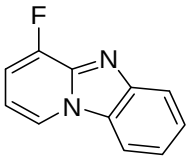
Yield: 97%. mp 163-164 °C, white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.32 (d, *J* = 6.8 Hz, 1H), 7.89 (d, *J* = 8.4 Hz, 1H), 7.84 (d, *J* = 8.4 Hz, 1H), 7.49 (t, *J* = 7.6 Hz, 1H), 7.43 (s, 1H), 7.33 (t, *J* = 7.6 Hz, 1H), 6.68 (d, *J* = 6.4 Hz, 1H), 2.47 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 149.1, 144.8, 140.7, 128.7, 125.4, 124.2, 120.5, 119.6, 116.0, 113.1, 110.1, 21.9; HRMS (ESI): Exact mass calcd for $C_{12}H_{11}N_2$ $[M+H]^+$, 183.0917; Found: 183.0919.

1,8-dimethylpyrido[1,2-*a*]benzimidazole (2q)



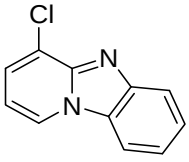
Yield: 94%. mp 118-120 °C, white solid. ^{1}H NMR (400 MHz, D_6-DMSO): δ 8.09 (s, 1H), 7.70 (d, *J* = 8.4 Hz, 1H), 7.49 (d, *J* = 9.2 Hz, 1H), 7.44-7.40 (m, 1H), 7.33 (d, *J* = 8.4 Hz, 1H), 6.74 (d, *J* = 6.4 Hz, 1H), 3.03 (s, 3H), 2.54 (s, 3H); ^{13}C NMR (100 MHz, D_6-DMSO): δ 148.6, 142.7, 139.4, 129.5, 129.4, 129.1, 126.3, 118.2, 114.8, 114.3, 110.2, 21.3, 20.6; Exact mass calcd for $C_{13}H_{13}N_2$ $[M+H]^+$, 197.1073; Found: 197.1076.

4-fluoropyrido[1,2-*a*]benzimidazole (2r)



Yield: 94%. mp 225-226 °C, off-white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.29 (d, *J* = 6.8 Hz, 1H), 8.01 (d, *J* = 8.0 Hz, 1H), 7.90 (d, *J* = 8.4 Hz, 1H), 7.57 (t, *J* = 7.6 Hz, 1H), 7.43 (t, *J* = 8.0 Hz, 1H), 7.14 (t, *J* = 7.6 Hz, 1H), 6.81-6.77 (m, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 152.5, 150.5, 144.2, 141.4, 141.2, 129.1, 126.1, 121.9, 121.4, 120.6, 111.1, 111.0, 110.7, 109.0; HRMS (ESI): Exact mass calcd for $C_{11}H_7FN_2$ $[M+H]^+$, 187.0666; Found: 187.0666.

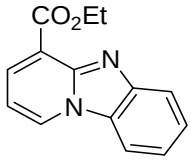
4-chloropyrido[1,2-*a*]benzimidazole (2s)



Yield: 84%. mp 147-148 °C, off-white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.42 (d, *J* = 6.8 Hz, 1H), 8.05 (d, *J* = 8.4 Hz, 1H), 7.89 (d, *J* = 8.4 Hz, 1H), 7.57-7.52 (m, 2H), 7.43 (d, *J* = 7.6 Hz, 1H), 6.82 (t, *J* = 6.8 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 145.8,

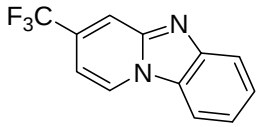
144.1, 129.5, 127.8, 126.2, 123.8, 123.5, 122.0, 120.7, 110.7, 109.8; HRMS (ESI): Exact mass calcd for $C_{11}H_7ClN_2$ $[M+H]^+$, 203.0371; Found: 203.0372.

ethyl benzo[4,5]imidazo[1,2-*a*]pyridine-4-carboxylate (2t)



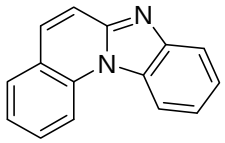
Yield: 67%. mp 98-100 °C, green solid. ^{1}H NMR (400 MHz, D_6-DMSO): δ 9.34 (d, *J* = 6.4 Hz, 1H), 8.35 (d, *J* = 8.0 Hz, 1H), 8.17 (d, *J* = 6.4 Hz, 1H), 7.90 (d, *J* = 8.4 Hz, 1H), 7.56 (t, *J* = 7.6 Hz, 1H), 7.43 (t, *J* = 7.6 Hz, 1H), 7.10 (t, *J* = 7.2 Hz, 1H), 4.42 (t, *J* = 6.8 Hz, 2H), 1.37 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100 MHz, D_6-DMSO): δ 163.8, 144.5, 144.0, 133.6, 131.0, 128.2, 125.7, 121.1, 119.2, 119.0, 111.8, 108.9, 60.8, 14.0; HRMS (ESI): Exact mass calcd for $C_{14}H_{12}N_2O_2$ $[M+H]^+$, 241.0972; Found: 241.0974.

3-(trifluoromethyl)pyrido[1,2-*a*]benzimidazole (2u)



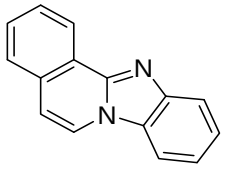
Yield: 93%. mp 226-227 °C, white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.57 (d, *J* = 7.2 Hz, 1H), 8.01 (t, *J* = 7.2 Hz, 2H), 7.95 (d, *J* = 8.0 Hz, 1H), 7.62-7.58 (m, 1H), 7.47 (t, *J* = 7.6 Hz, 1H), 7.01 (t, *J* = 7.2 Hz, 1H), ^{13}C NMR (125 MHz, $CDCl_3$): δ 146.3, 145.1, 131.0, 130.7, 128.5, 126.5, 126.2, 124.1, 122.6, 121.9, 120.7, 116.3, 110.7, 105.9; HRMS (ESI): Exact mass calcd for $C_{12}H_7F_3N_2$ $[M+H]^+$, 237.0634; Found: 237.0636.

Benzimidazo[1,2-*a*]quinoline (2v)



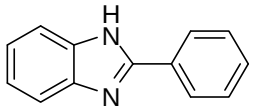
Yield: 93%. mp 97-99 °C, yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.58 (d, *J* = 8.4 Hz, 1H), 8.39 (d, *J* = 8.4 Hz, 1H), 8.02 (d, *J* = 8.0 Hz, 1H), 7.84 (d, *J* = 8.0 Hz, 1H), 7.78-7.74 (m, 1H), 7.70 (d, *J* = 9.6 Hz, 1H), 7.62 (d, *J* = 9.2 Hz, 1H), 7.57-7.47 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 148.3, 145.0, 135.9, 131.0, 129.6, 129.5, 124.4, 124.1, 123.6, 122.7, 120.7, 118.0, 115.3, 113.9; HRMS (ESI): Exact mass calcd for $C_{15}H_{11}N_2$ $[M+H]^+$, 219.0917; Found: 219.0923.

Benzimidazo[2,1-*a*]isoquinoline (2w)



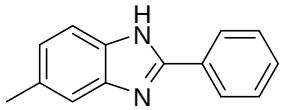
Yield: 77%. mp 129-130 °C, yellow solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ 8.83 (d, *J* = 8.0 Hz, 1H), 8.17 (d, *J* = 8.0 Hz, 1H), 8.03 (d, *J* = 8.0 Hz, 1H), 7.85 (d, *J* = 8.0 Hz, 1H), 7.77-7.75 (m, 1H), 7.70-7.67 (m, 2H), 7.54-7.50 (m, 1H), 7.44-7.40 (m, 1H), 7.08 (d, *J* = 7.2 Hz, 1H); ^{13}C NMR (125 MHz, $CDCl_3$): δ 147.3, 143.8, 131.6, 130.0, 128.2, 127.1, 125.0, 124.7, 123.6, 121.9, 121.4, 119.9, 111.4, 111.1, 109.8; HRMS (ESI): Exact mass calcd for $C_{15}H_{11}N_2$ $[M+H]^+$, 219.0917; Found: 219.0914.

2-phenyl-1*H*-benzo[*d*]imidazole (4a)



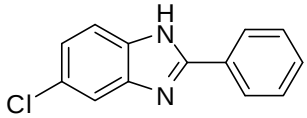
Yield: 95%. mp 302-303 °C, off-white solid. ^{1}H NMR (400 MHz, D_6-DMSO): δ 12.89 (br s, 1H), 8.98 (d, *J* = 6.4 Hz, 1H), 8.20 (d, *J* = 6.4 Hz, 1H), 7.86 (d, *J* = 8.8 Hz, 1H), 7.68 (t, *J* = 8.0 Hz, 1H), 7.55-7.50 (m, 3H), 7.20 (t, *J* = 6.8 Hz, 1H); ^{13}C NMR (125 MHz, D_6-DMSO): δ 162.9, 151.1, 130.6, 130.5, 130.1, 129.1, 129.0, 126.8, 115.9, 114.4; HRMS (ESI): Exact mass calcd for $C_{13}H_{11}N_2$ $[M+1]^+$ 195.0917, found: 195.0918.

5-methyl-2-phenyl-1*H*-benzo[*d*]imidazole (4b)



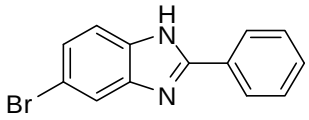
Yield: 91%. mp 247-249 °C, off-white solid. ^{1}H NMR (400 MHz, D_6-DMSO): δ 12.74 (br s, 1H), 8.14 (d, *J* = 7.6 Hz, 2H), 7.55-7.45 (m, 4H), 7.40-7.31 (m, 1H), 7.03 (t, *J* = 8.0 Hz, 1H), 2.43 (s, 3H); ^{13}C NMR (125 MHz, D_6-DMSO): δ 151.1, 150.7, 144.2, 141.9, 135.2, 133.0, 131.8, 130.5, 130.3, 129.6, 128.9, 126.2, 123.9, 123.2, 118.6, 118.4, 111.0, 110.8, 21.3, 21.2; HRMS (ESI): Exact mass calcd for $C_{14}H_{13}N_2$ $[M+1]^+$ 209.1073, found: 209.1074.

5-chloro-2-phenyl-1*H*-benzo[*d*]imidazole (4c)



Yield: 90%. mp 213-215 °C, off-white solid. ^{1}H NMR (400 MHz, D_6-DMSO): δ 13.09 (br s, 1H), 8.16 (d, *J* = 6.8 Hz, 2H), 7.72-7.66 (m, 1H), 7.58-7.49 (m, 4H), 7.22 (t, *J* = 9.2 Hz, 1H); ^{13}C NMR (125 MHz, D_6-DMSO): δ 152.8, 152.4, 144.7, 142.6, 135.7, 133.8, 130.2, 129.7, 129.0, 126.8, 126.6, 126.1, 122.6, 122.1, 120.1, 118.2, 112.6, 111.0; HRMS (ESI): Exact mass calcd for $C_{13}H_{10}ClN_2$ $[M+1]^+$ 229.0527, found: 229.0527.

5-bromo-2-phenyl-1*H*-benzo[*d*]imidazole (4d)



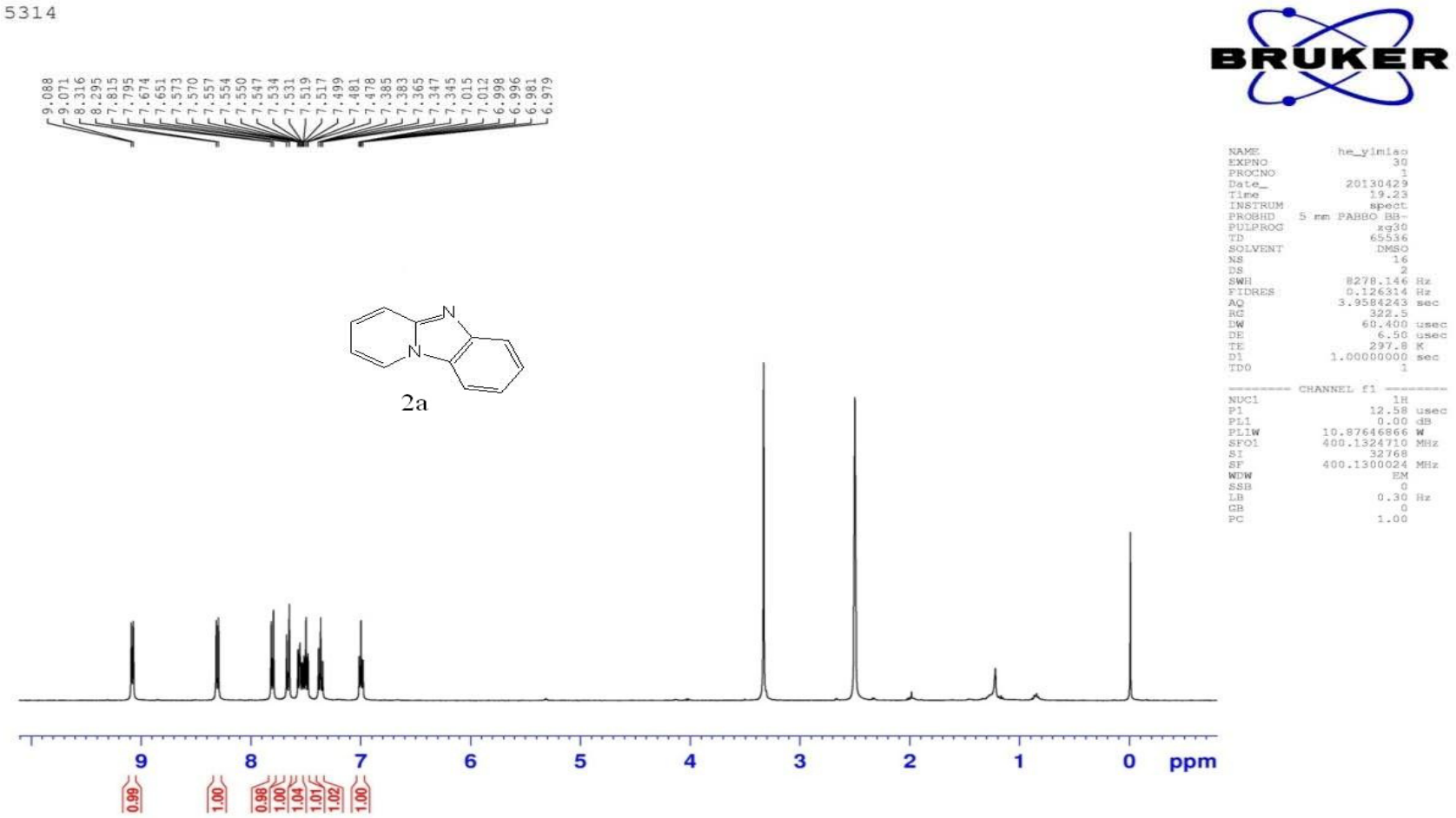
Yield: 91%. mp 201-202 ^{o}C, off-white solid. ^{1}H NMR (400 MHz, D_6-DMSO): δ 13.07 (br s, 1H), 8.15 (t, J = 6.8 Hz, 2H), 7.84-7.66 (m, 1H), 7.61-7.47 (m, 4H), 7.32 (t, J = 8.8 Hz, 1H); ^{13}C NMR (125 MHz, D_6-DMSO): δ 152.6, 152.3, 145.3, 142.9, 136.3, 134.1, 130.2, 129.6, 129.0, 126.6, 125.2, 124.7, 121.2, 120.5, 114.7, 113.9, 113.1; HRMS (ESI): Exact mass calcd for $C_{13}H_{10}BrN_2$ $[M+1]^+$ 273.0022, found: 273.0022.

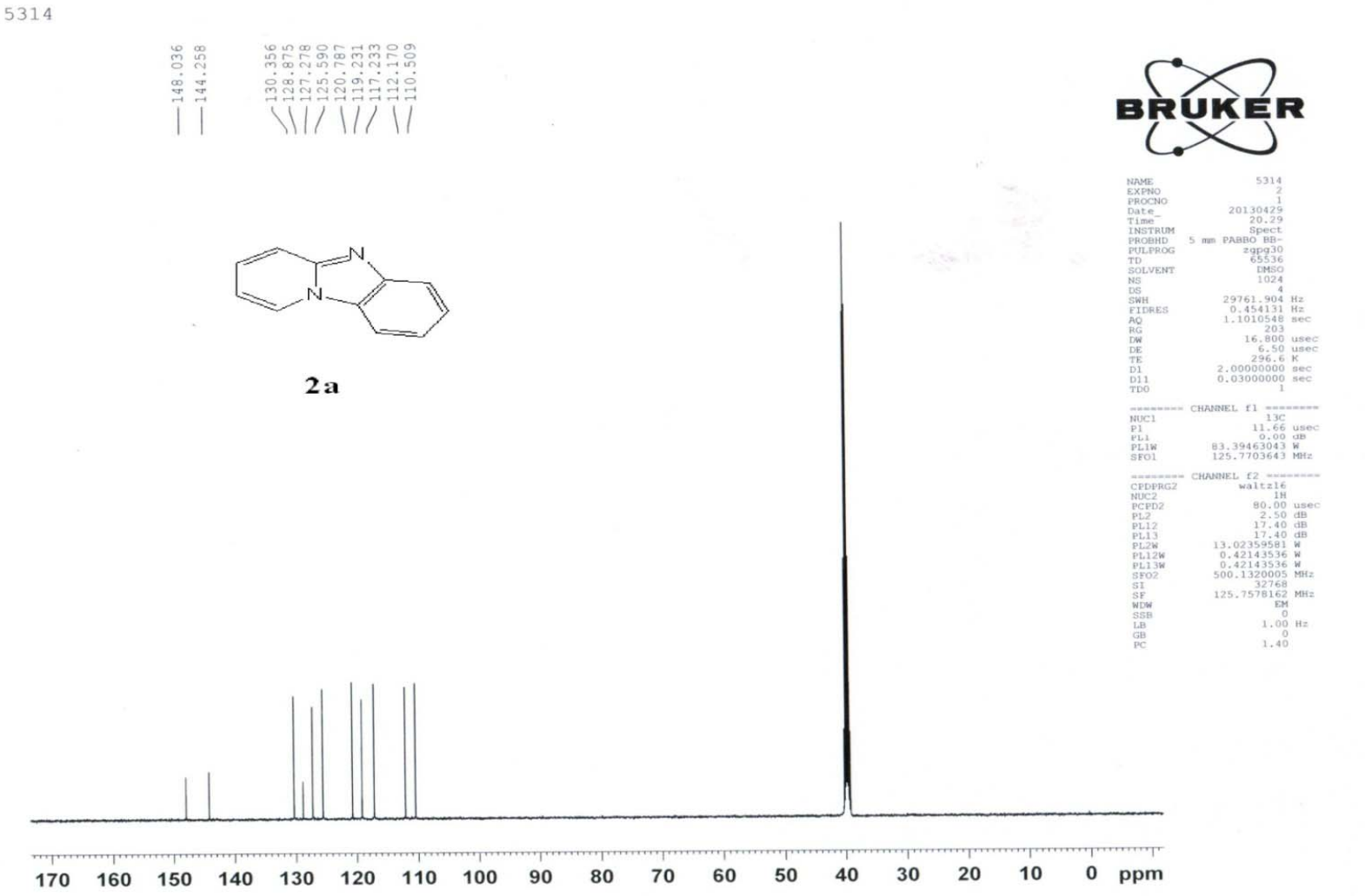
4. References

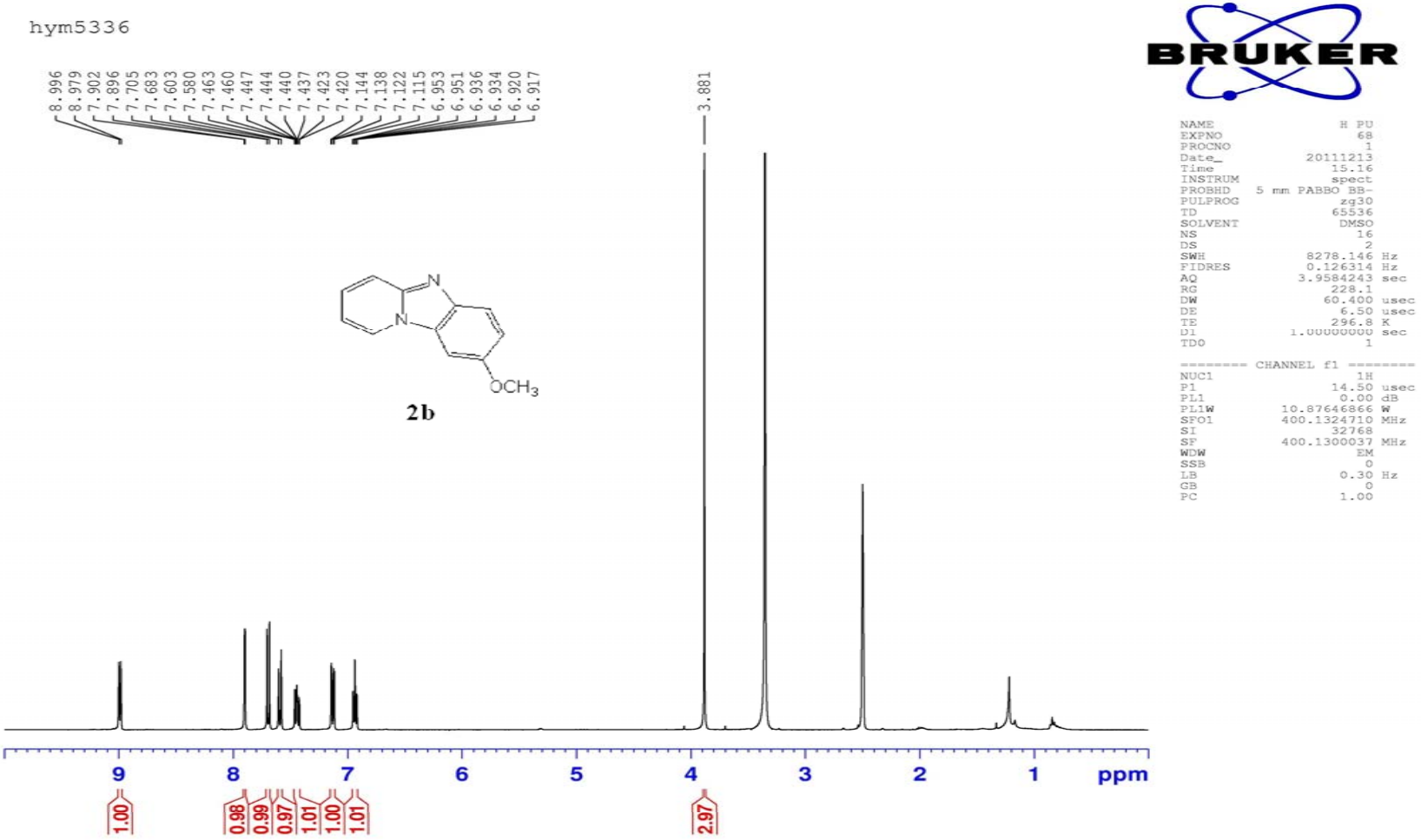
(1) (a) G. A. Grasa, M. S. Viciu, J. Huang and S. P. Nolan, *J. Org. Chem.*, 2001, **66**, 7729; (b) H. Wang, Y. Wang, C. Peng, J. Zhang and Q. Zhu, *J. Am. Chem. Soc.*, 2010, **132**, 13217.

(2) J. Huang, Y. He, Y. Wang and Q. Zhu, *Chem. Eur. J.*, 2012, **18**, 13964.

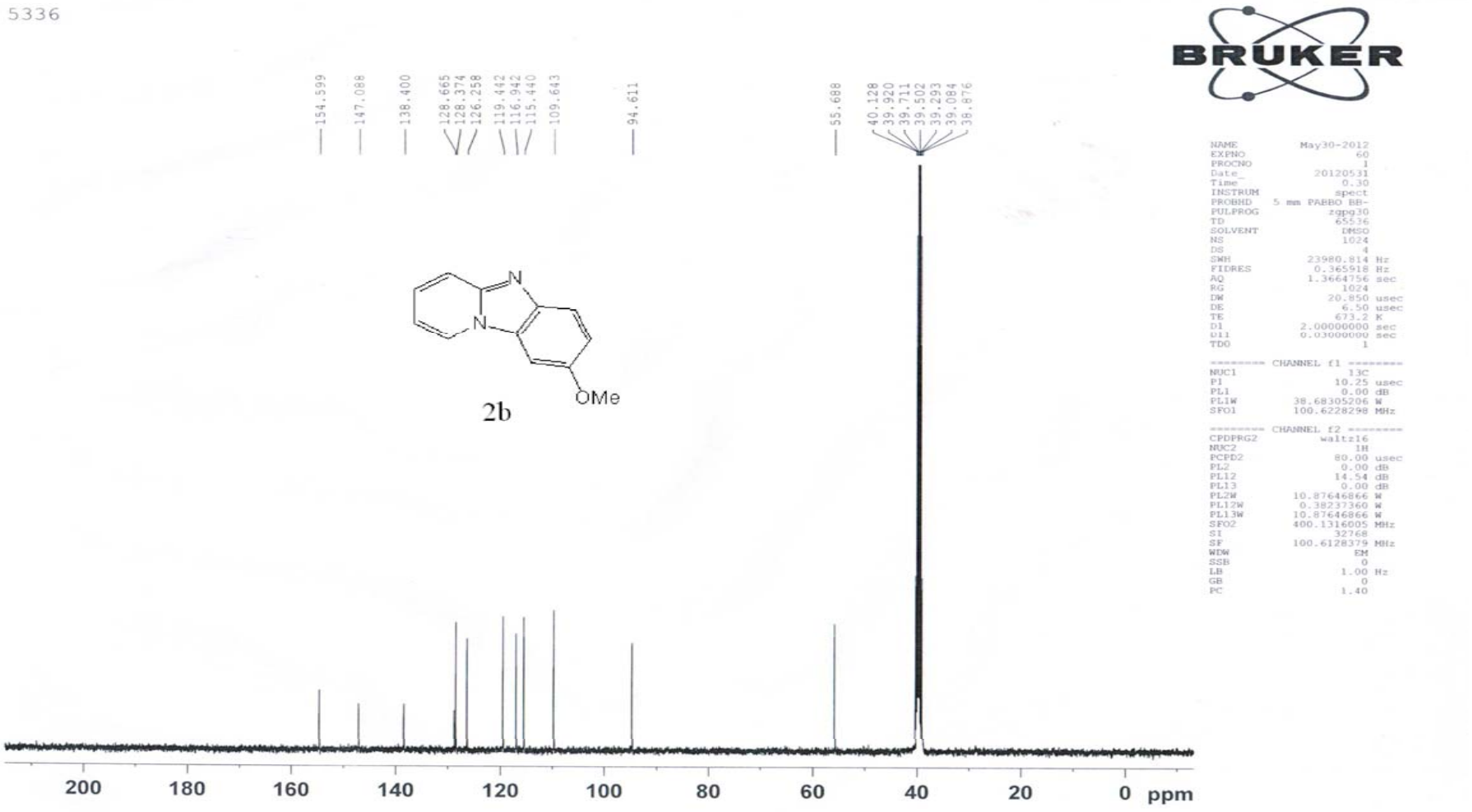
5. Copies of ^{1}H NMR and ^{13}C NMR Spectra

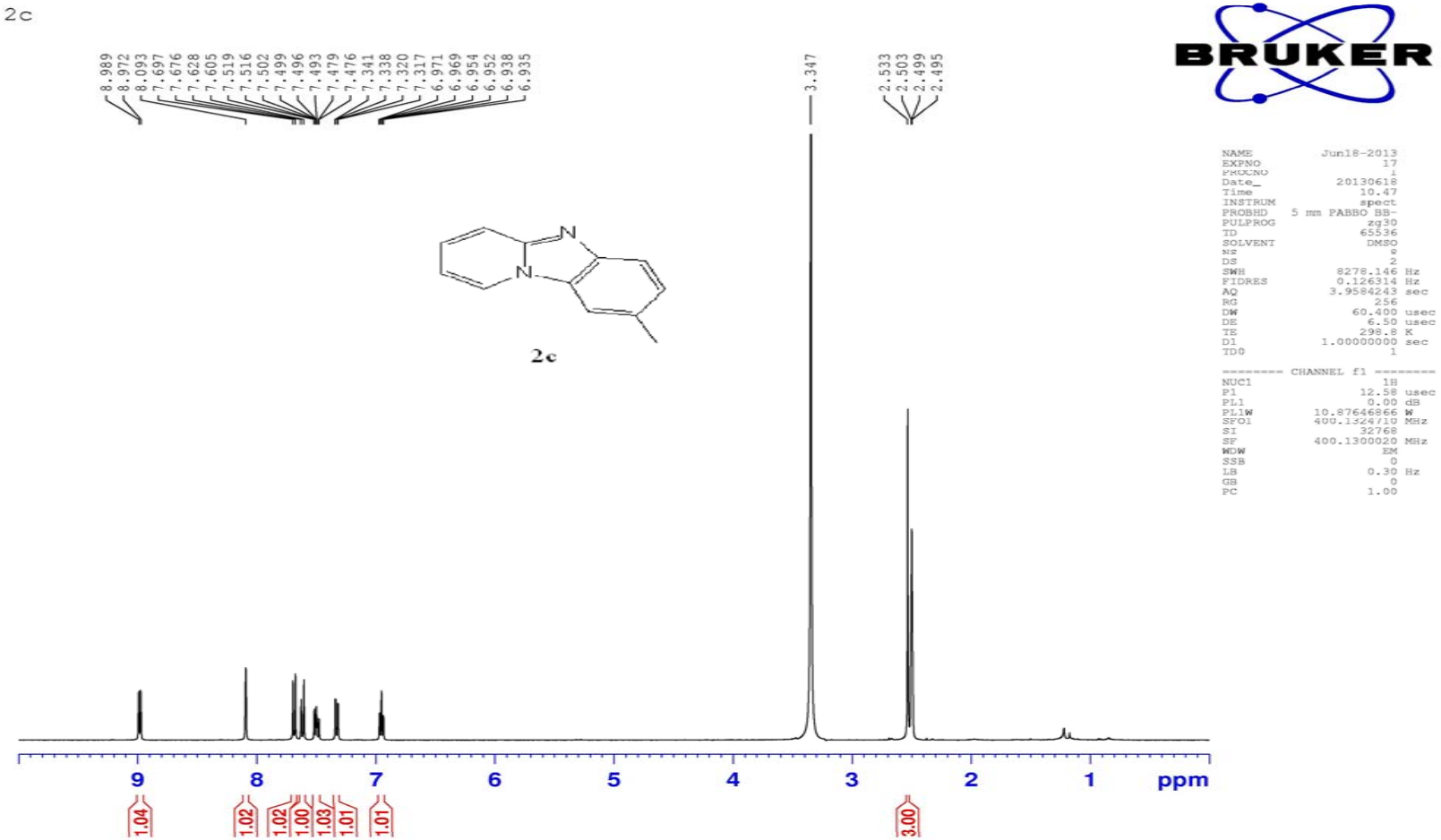

5314
9.088
9.071
8.316
8.295
7.815
7.795
7.674
7.651
7.573
7.570
7.557
7.554
7.550
7.547
7.534
7.531
7.519
7.517
7.499
7.481
7.478
7.385
7.383
7.365
7.347
7.345
7.015
7.012
6.998
6.996
6.981
6.979
BRUKER
NAME he_yimiao
EXPNO 30
PROCNO 1
Date_ 20130429
Time 19.23
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 322.5
DW 60.400 usec
DE 6.50 usec
TE 297.8 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 12.58 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
N
N
2a
9
8
7
6
5
4
3
2
1
0
ppm
0.99
1.00
0.98
1.00
1.04
1.01
1.02
1.00

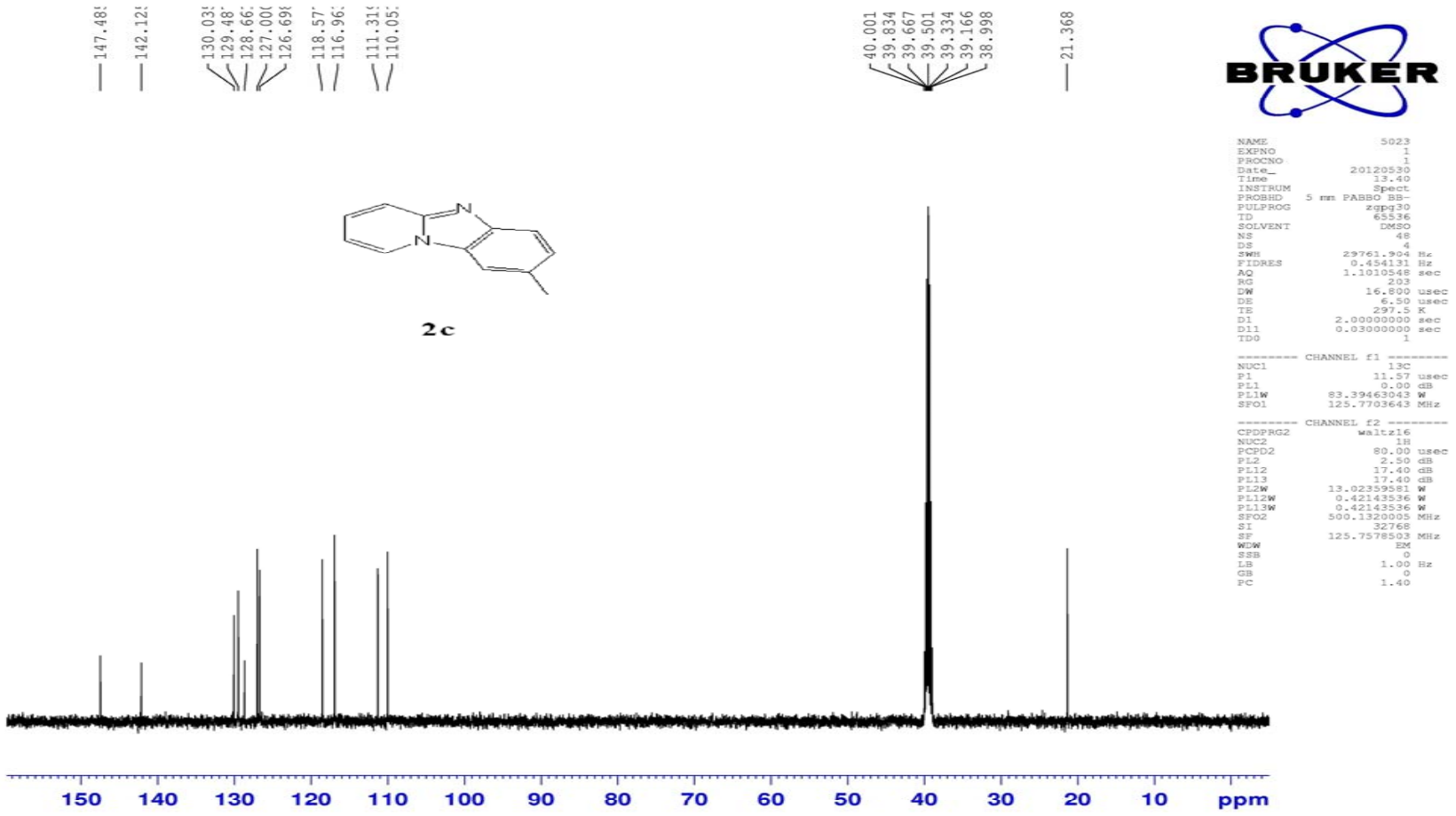

5314
148.036
144.258
130.356
128.875
127.278
125.590
120.787
119.231
117.233
112.170
110.509
N
N
2a
BRUKER
NAME 5314
EXPNO 2
PROCNO 1
Date_ 20130429
Time_ 20.29
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 296.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 11.66 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 125.7578162 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

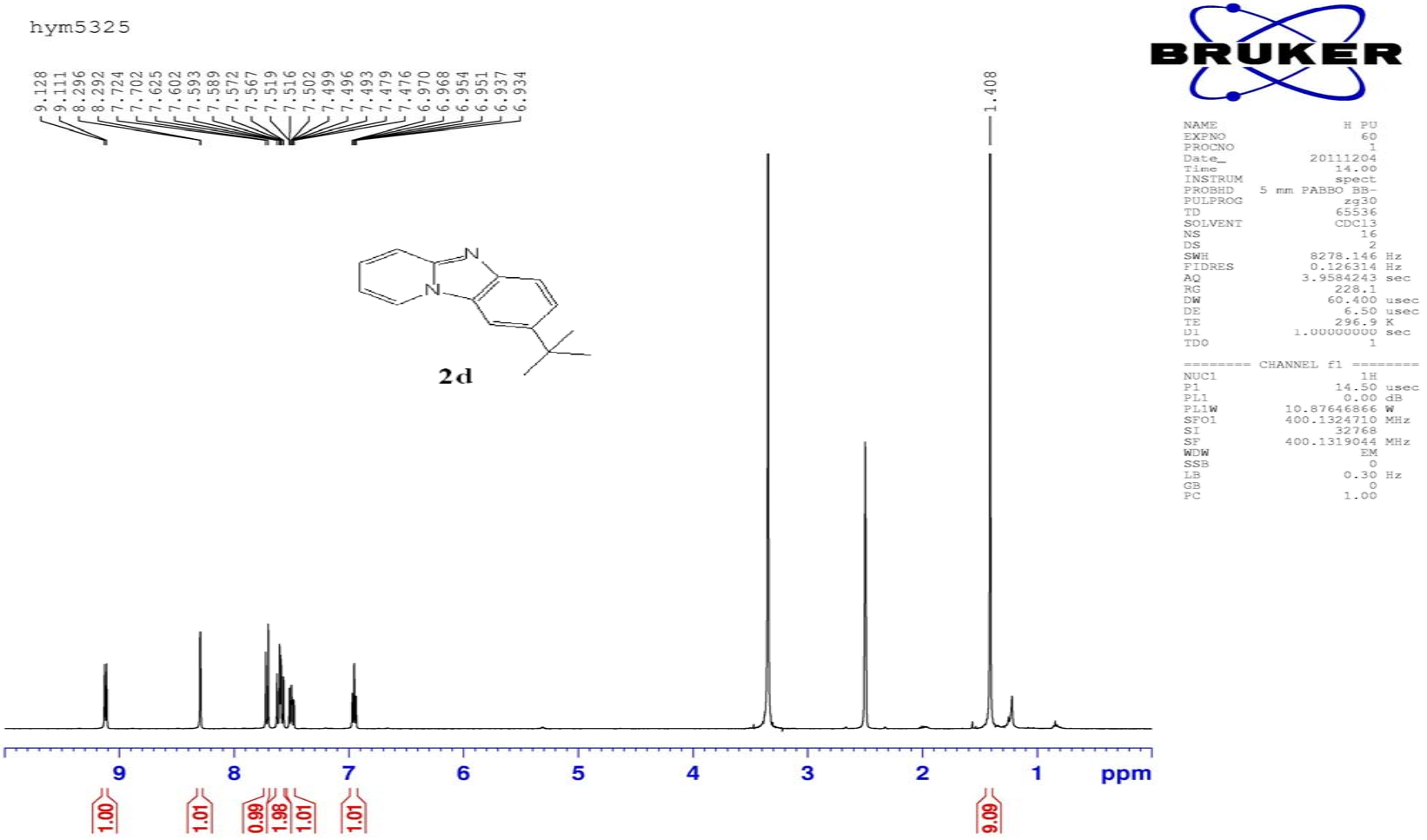


NAME	H PU
EXPNO	68
PROCNO	1
Date_	20111213
Time	15.16
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	228.1
DW	60.400 usec
DE	6.50 usec
TE	296.8 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.00 dB
PL1W	10.87646866 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300037 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00


5336
154.599
147.088
138.400
128.665
128.374
126.258
119.442
116.942
115.440
109.643
94.611
55.688
40.128
39.920
39.711
39.502
39.293
39.084
38.876
N
N
OMe
2b
BRUKER
NAME May30-2012
EXPNO 60
PROCNO 1
Date_ 20120531
Time 0.30
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
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 673.2 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 100.6128379 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0 ppm

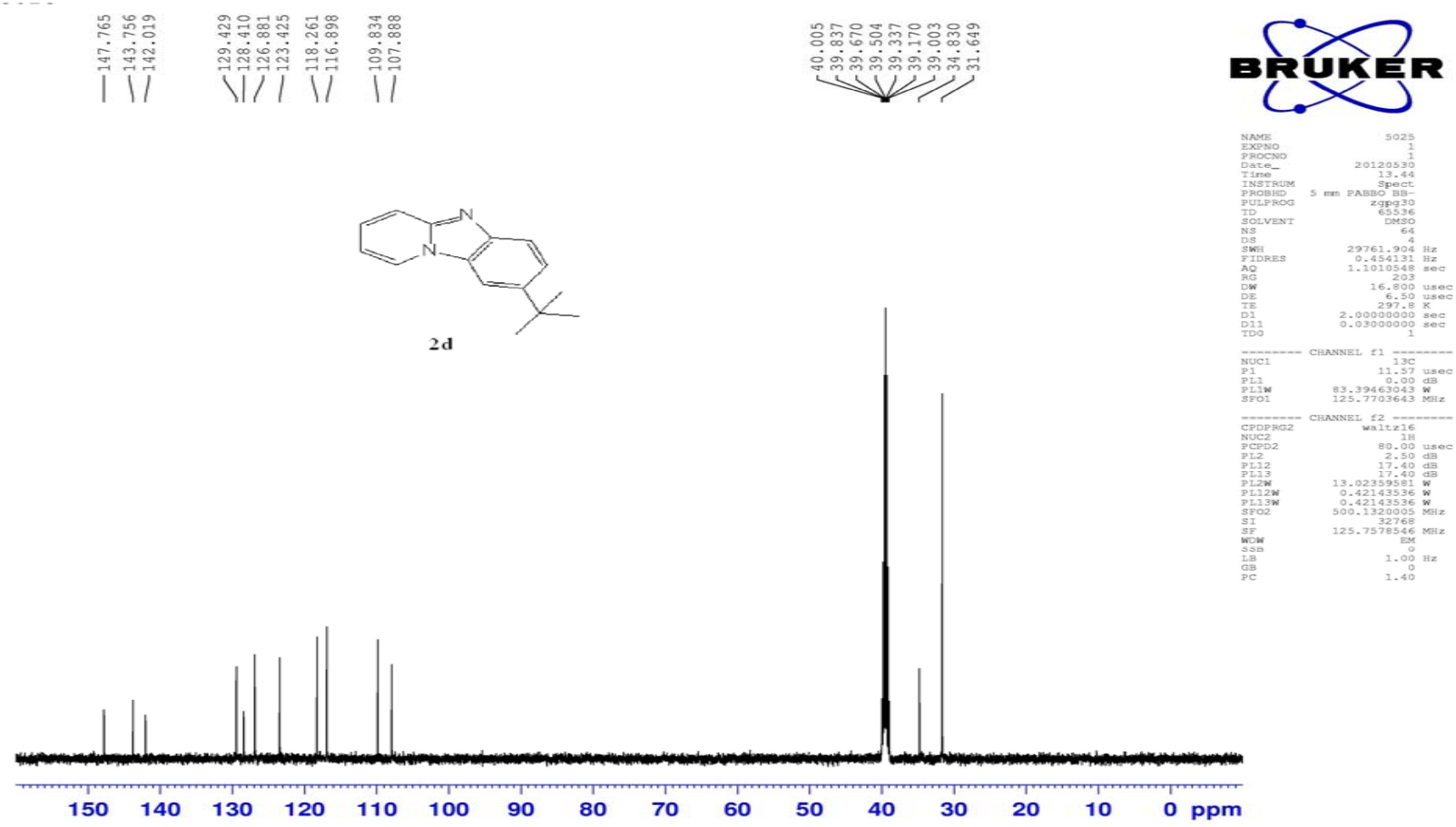

2c
8.989
8.972
8.093
7.697
7.676
7.628
7.605
7.519
7.516
7.502
7.499
7.496
7.493
7.479
7.476
7.341
7.338
7.320
7.317
6.971
6.969
6.954
6.952
6.938
6.935
3.347
2.533
2.503
2.499
2.495
2c
NAME Jun18-2013
EXPNO 17
PROCNO 1
Date_ 20130618
Time 10.47
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
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 298.8 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 12.58 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
9
8
7
6
5
4
3
2
1
ppm
1.04
1.02
1.02
1.00
1.03
1.01
1.01
3.00

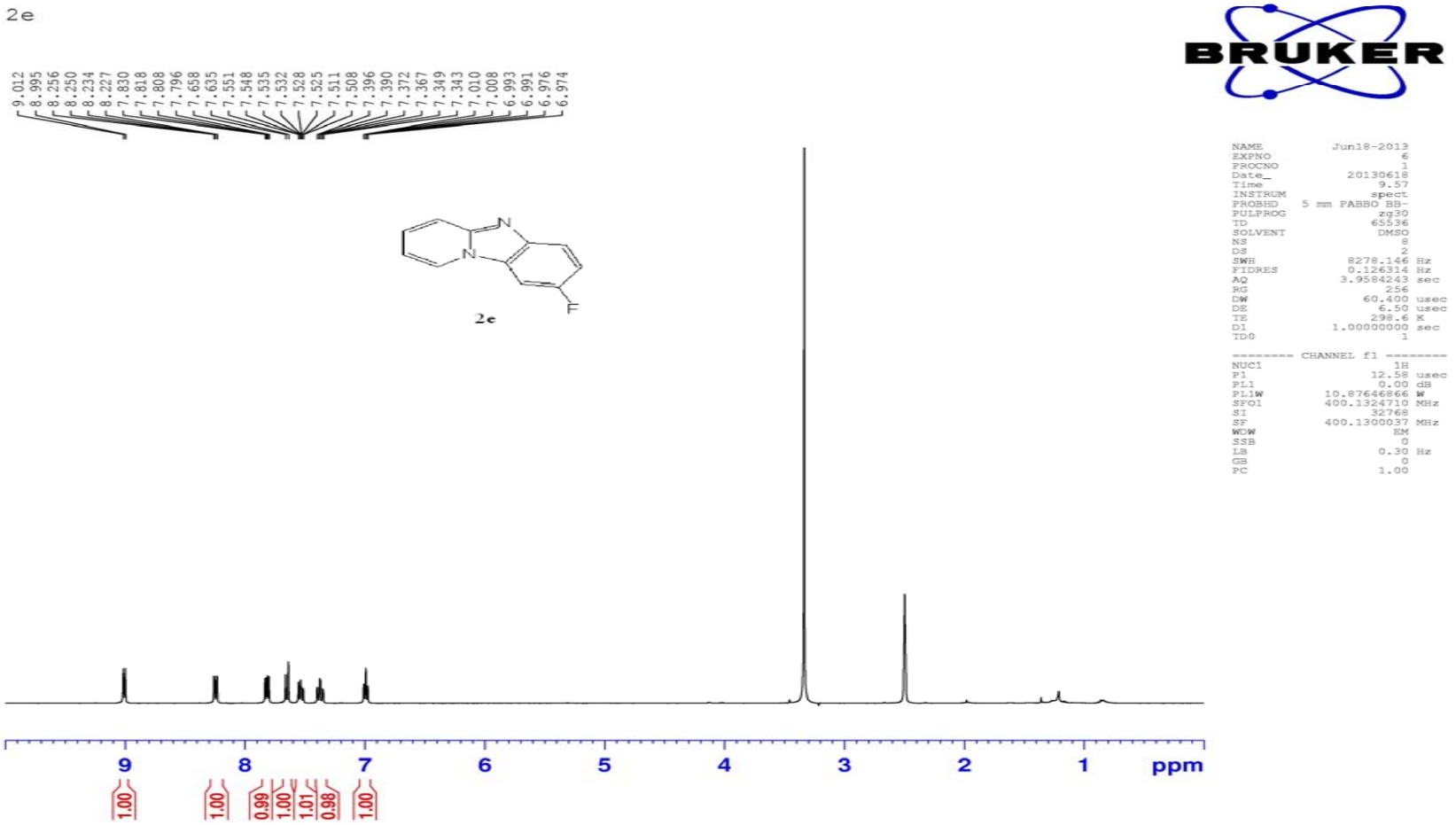

147.48
142.12
130.03
129.48
128.66
127.00
126.69
118.57
116.96
111.31
110.05
40.001
39.834
39.667
39.501
39.334
39.166
38.998
21.368
BRUKER
NAME 5023
EXPNO 1
PROCNO 1
Date_ 20120530
Time 13.40
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 48
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 297.5 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 125.7578503 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
2c
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm

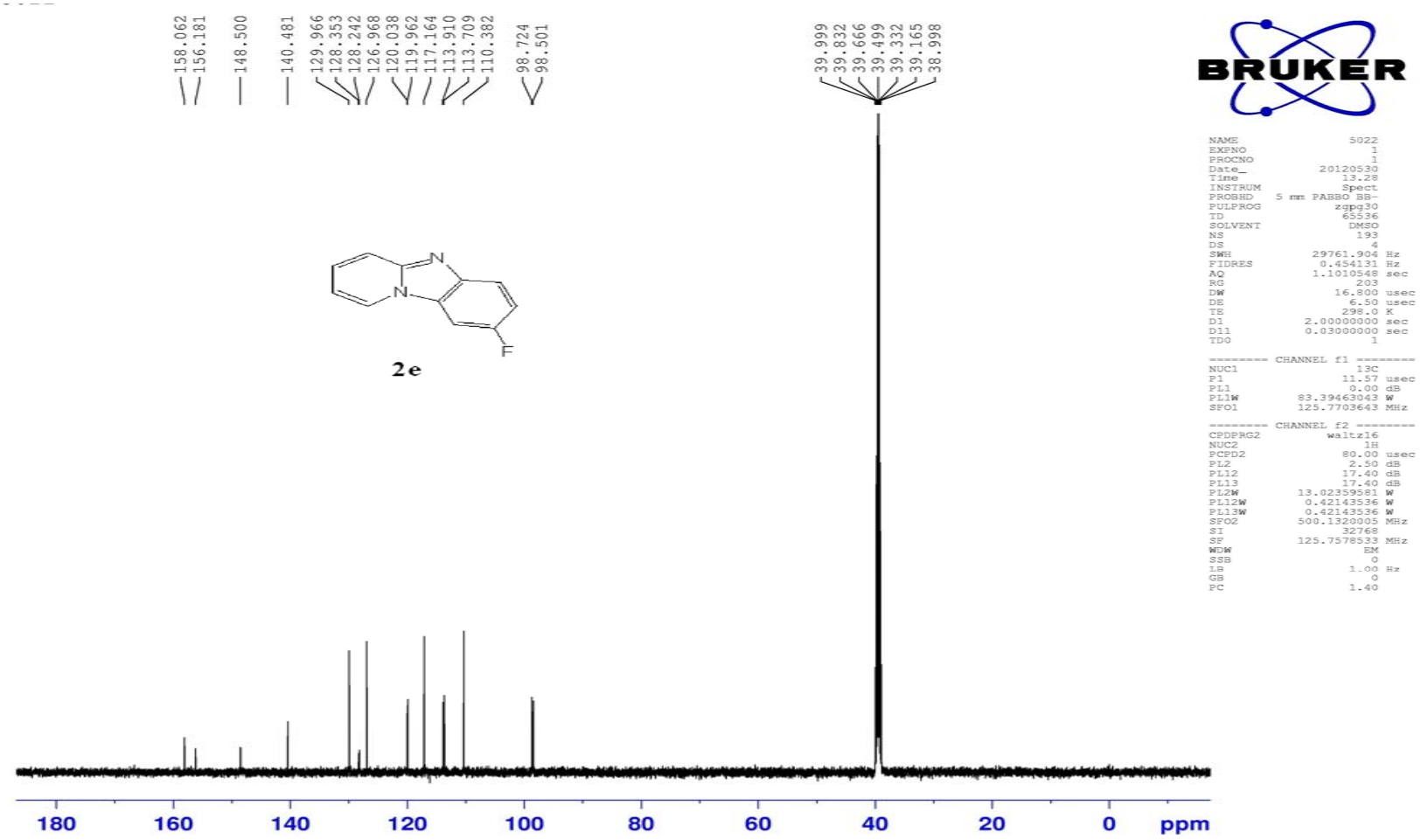


BRUKER

NAME	H PU
EXPNO	60
PROCNO	1
Date_	20111204
Time	14.00
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	228.1
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	400.1319044 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

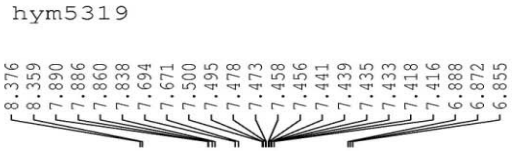

147.765
143.756
142.019
129.429
128.410
126.881
123.425
118.261
116.898
109.834
107.888
40.005
39.837
39.670
39.504
39.337
39.170
39.003
34.830
31.649
N
N
2d
BRUKER
NAME 5025
EXPNO 1
PROCNO 1
Date_ 20120530
Time 13.44
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 64
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 297.8 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 125.7578546 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

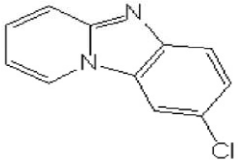

2e
9.012
8.995
8.256
8.250
8.234
8.227
7.830
7.818
7.808
7.796
7.658
7.635
7.551
7.548
7.535
7.532
7.528
7.525
7.511
7.508
7.396
7.390
7.372
7.367
7.349
7.343
7.010
7.008
6.993
6.991
6.976
6.974
N
N
F
2e
BRUKER
NAME Jun18-2013
EXPNO 6
PROCNO 1
Date_ 20130618
Time 9.57
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
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 298.6 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 12.58 usec
PL1 0.00 dB
PL1W 10.87646866 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300037 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
1.00
1.00
0.99
1.00
1.01
0.98
1.00



BRUKER

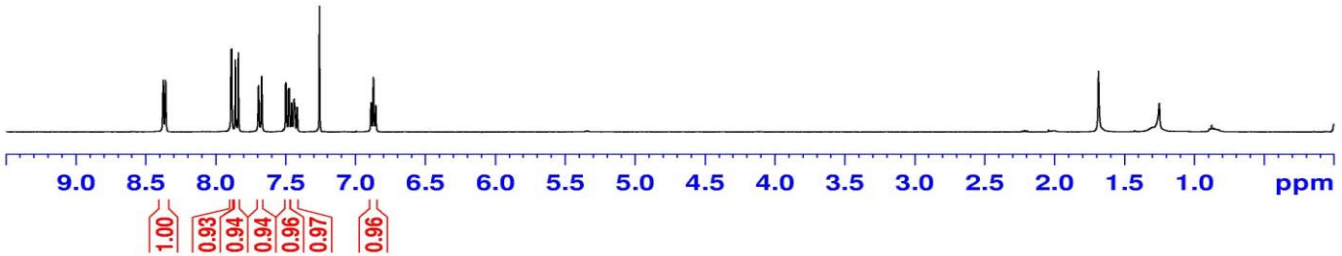
NAME	5022
EXPNO	1
PROCNO	1
Date_	20120530
Time	13.28
INSTRUM	Spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	193
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	11.57 usec
PL1	0.00 dB
PL1W	83.39463043 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.50 dB
PL12	17.40 dB
PL13	17.40 dB
PL2W	13.02359581 W
PL12W	0.42143536 W
PL13W	0.42143536 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7578533 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

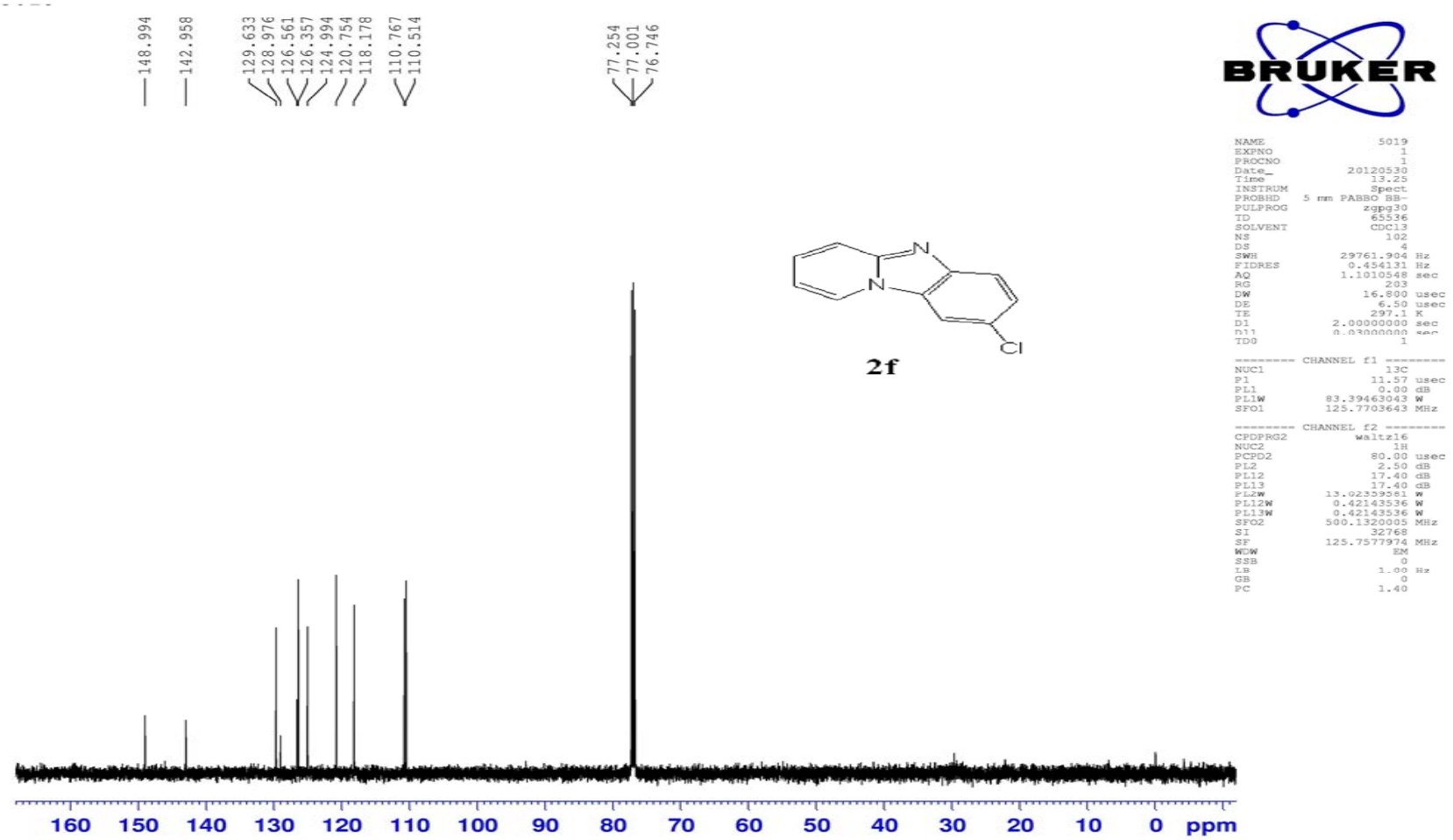




2f

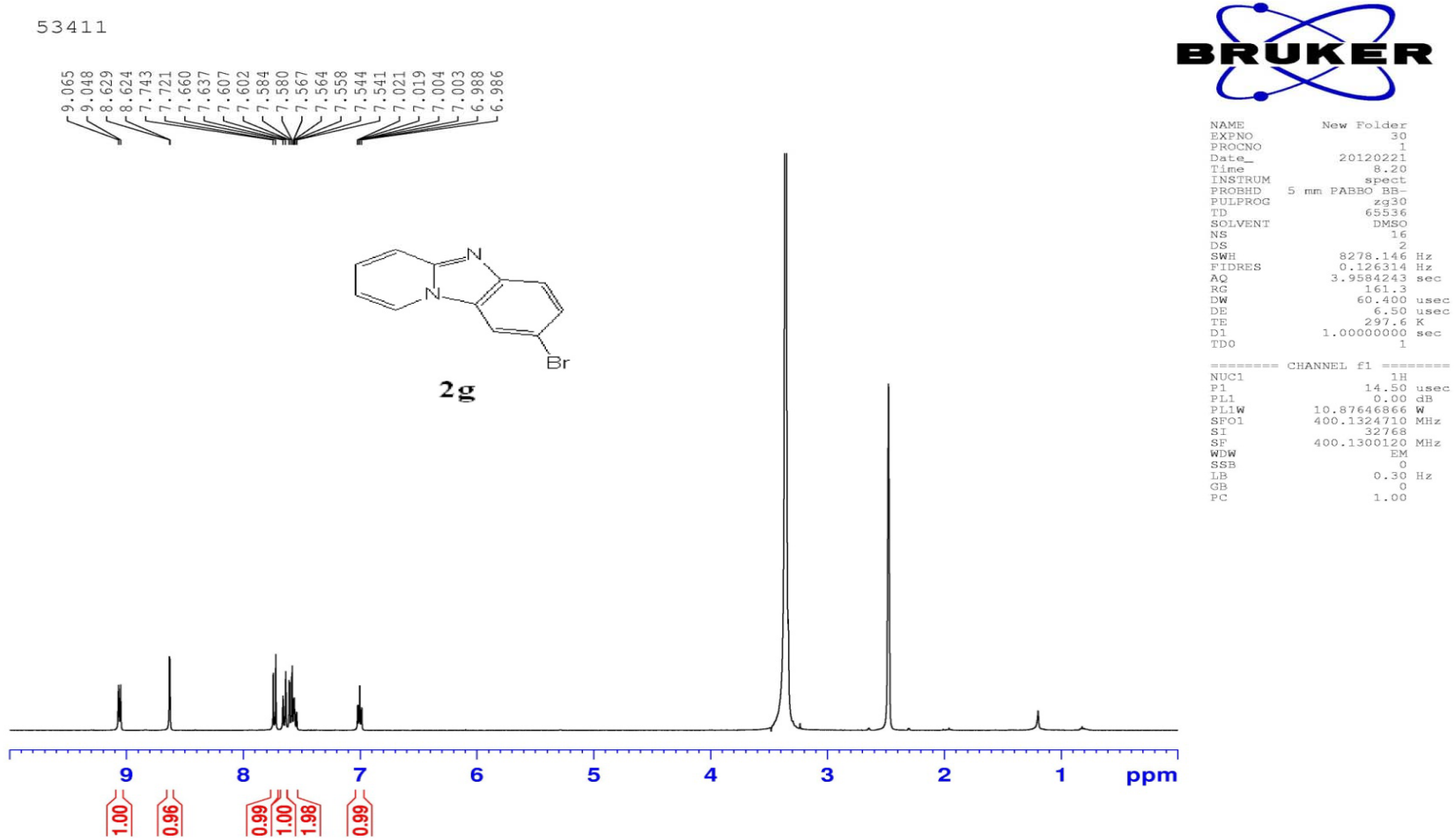
NAME	H PU
EXPNO	54
PROCNO	1
Date_	20111204
Time	9.11
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	322.5
DW	60.400 usec
DE	6.50 usec
TE	297.1 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.00 dB
PL1W	10.87646866 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300102 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

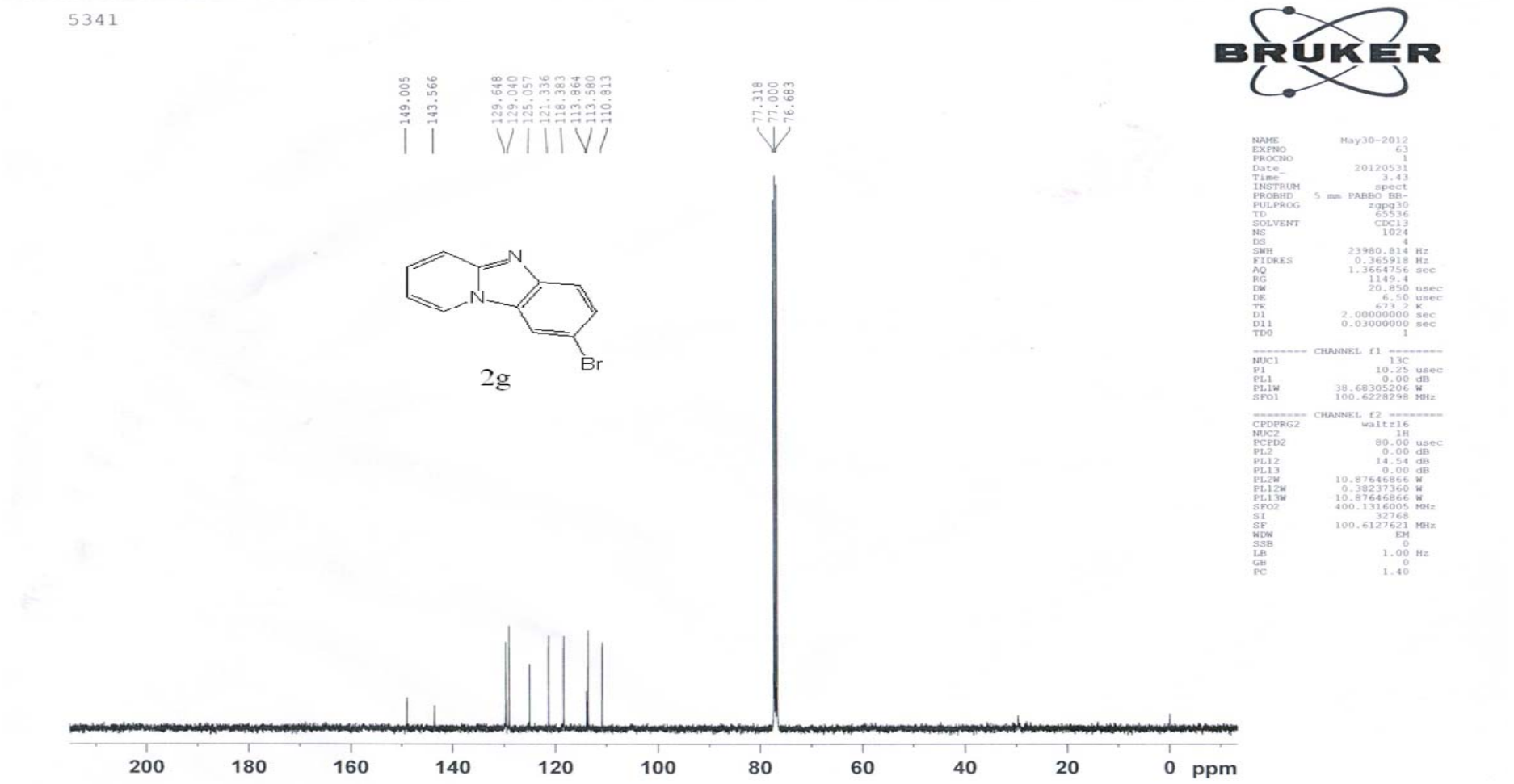


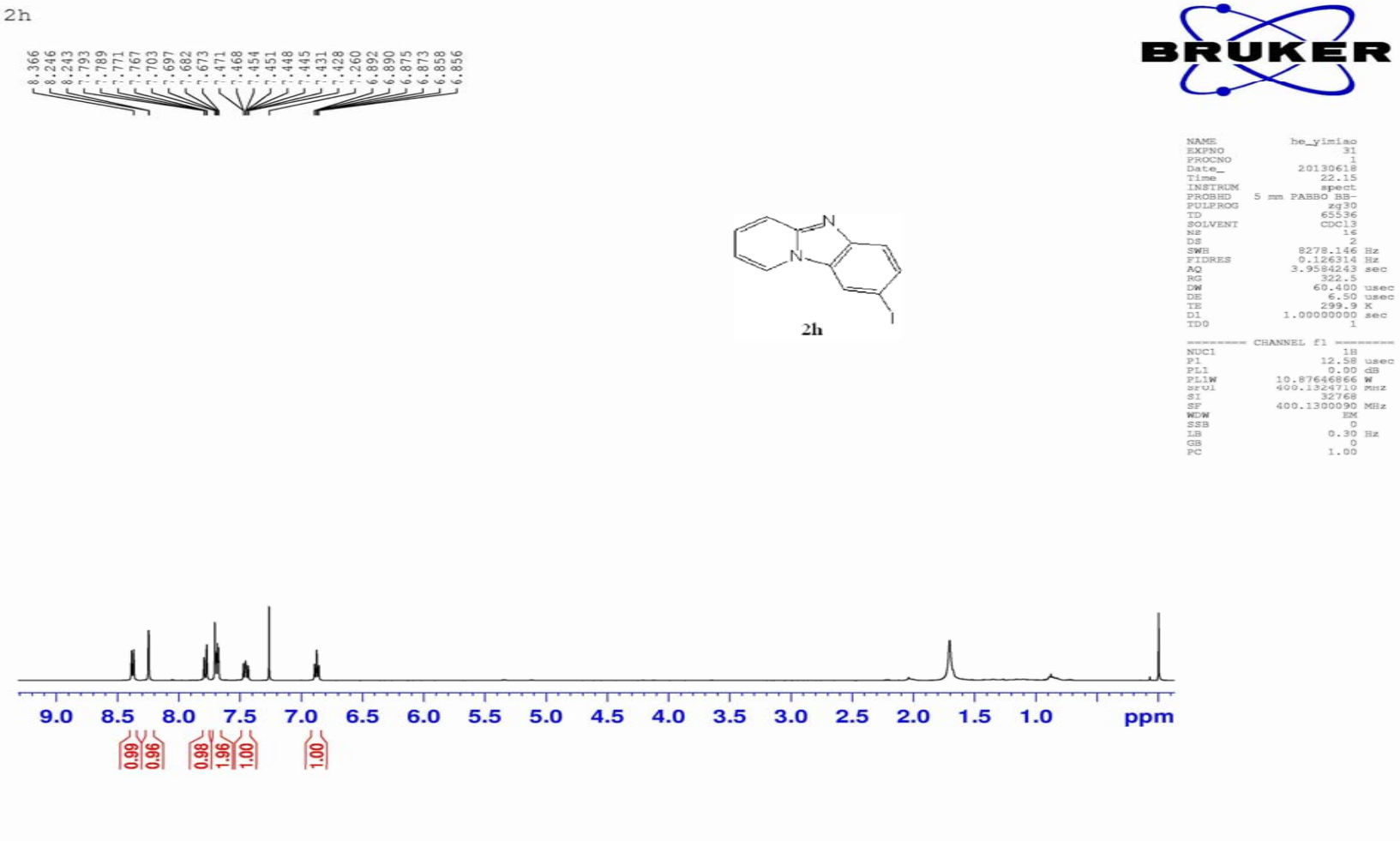


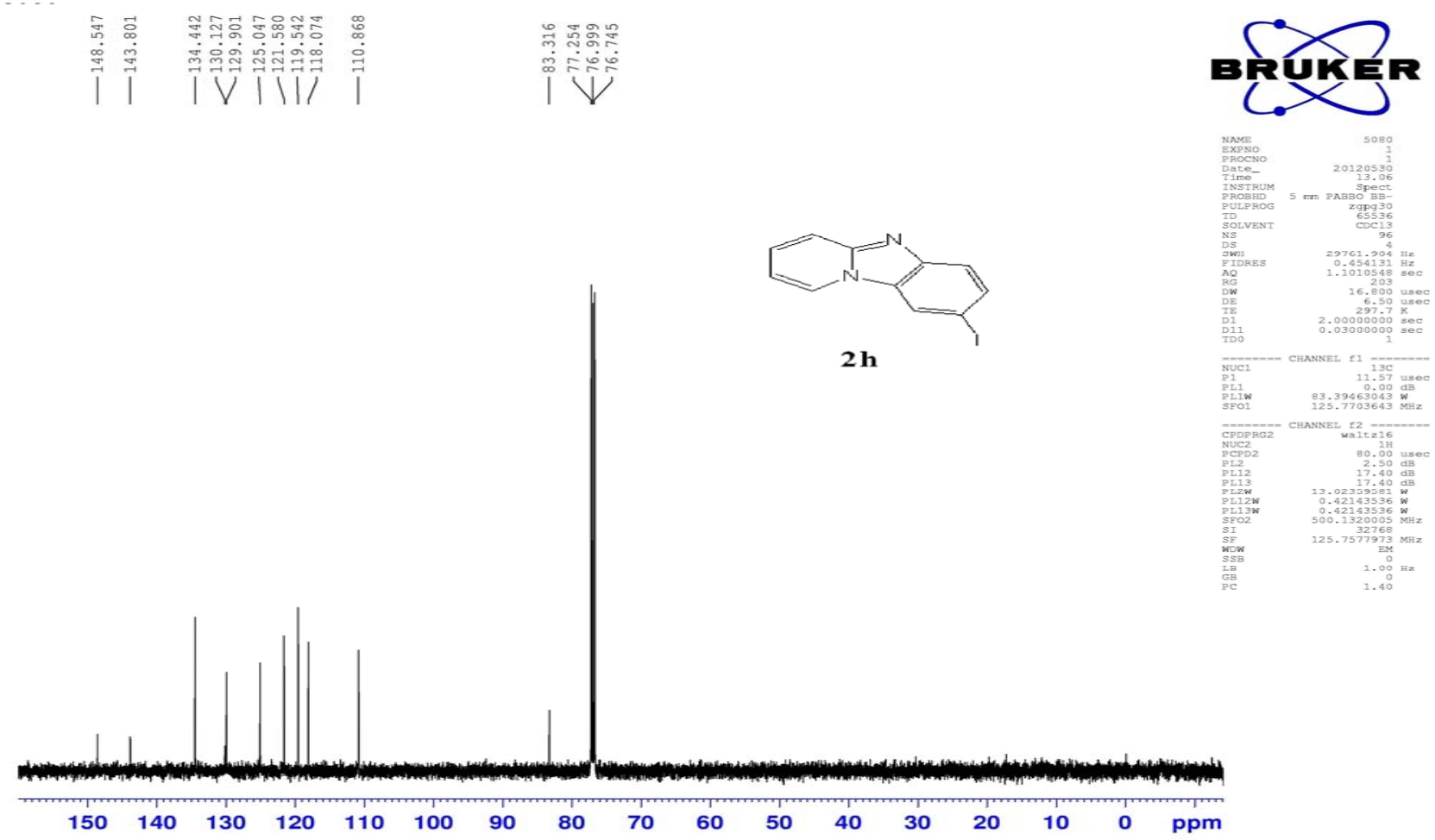
BRUKER

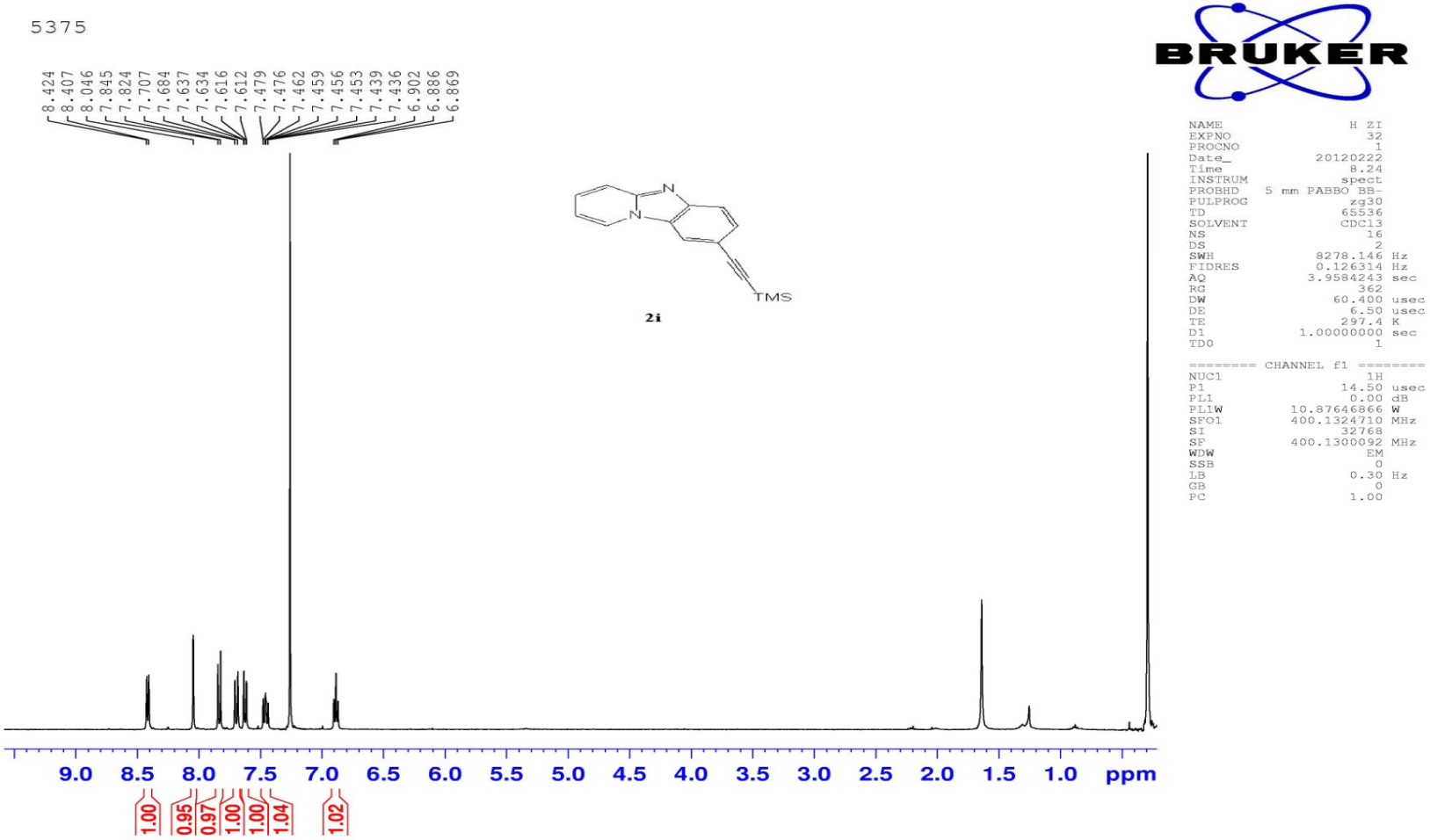
NAME	5019	
EXPNO	1	
PROCNO	1	
Date_	20120530	
Time	13.25	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zgpg30	
TD	65536	
SOLVENT	CDCl3	
NS	102	
DS	4	
SWH	29761.904	Hz
FIDRES	0.454131	Hz
AQ	1.1010548	sec
RG	203	
DW	16.800	usec
DE	6.50	usec
TE	297.1	K
D1	2.00000000	sec
D11	0.03000000	sec
TD0	1	
======== 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	13.02392581	W
PL12W	0.42143536	W
PL13W	0.42143536	W
SFO2	500.1320005	MHz
SI	32768	
SF	125.7577974	MHz
WDW	EM	
SSB	0	
LB	1.00	Hz
GB	0	
PC	1.40	


53411
9.065
9.048
8.629
8.624
7.743
7.721
7.660
7.637
7.607
7.602
7.584
7.580
7.567
7.564
7.558
7.544
7.541
7.021
7.019
7.004
7.003
6.988
6.986
N
N
Br
2g
NAME New Folder
EXPNO 30
PROCNO 1
Date_ 20120221
Time 8.20
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 297.6 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 400.1300120 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
ppm
1.00
0.96
0.99
1.00
1.98
0.99


5341
149.005
143.566
129.648
129.040
125.057
121.336
118.383
113.864
113.580
110.813
77.318
77.000
76.683
N
N
Br
2g
BRUKER
NAME May30-2012
EXPNO 63
PROCNO 1
Date_ 20120531
Time 3.43
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 673.2 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 100.6127621 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0 ppm

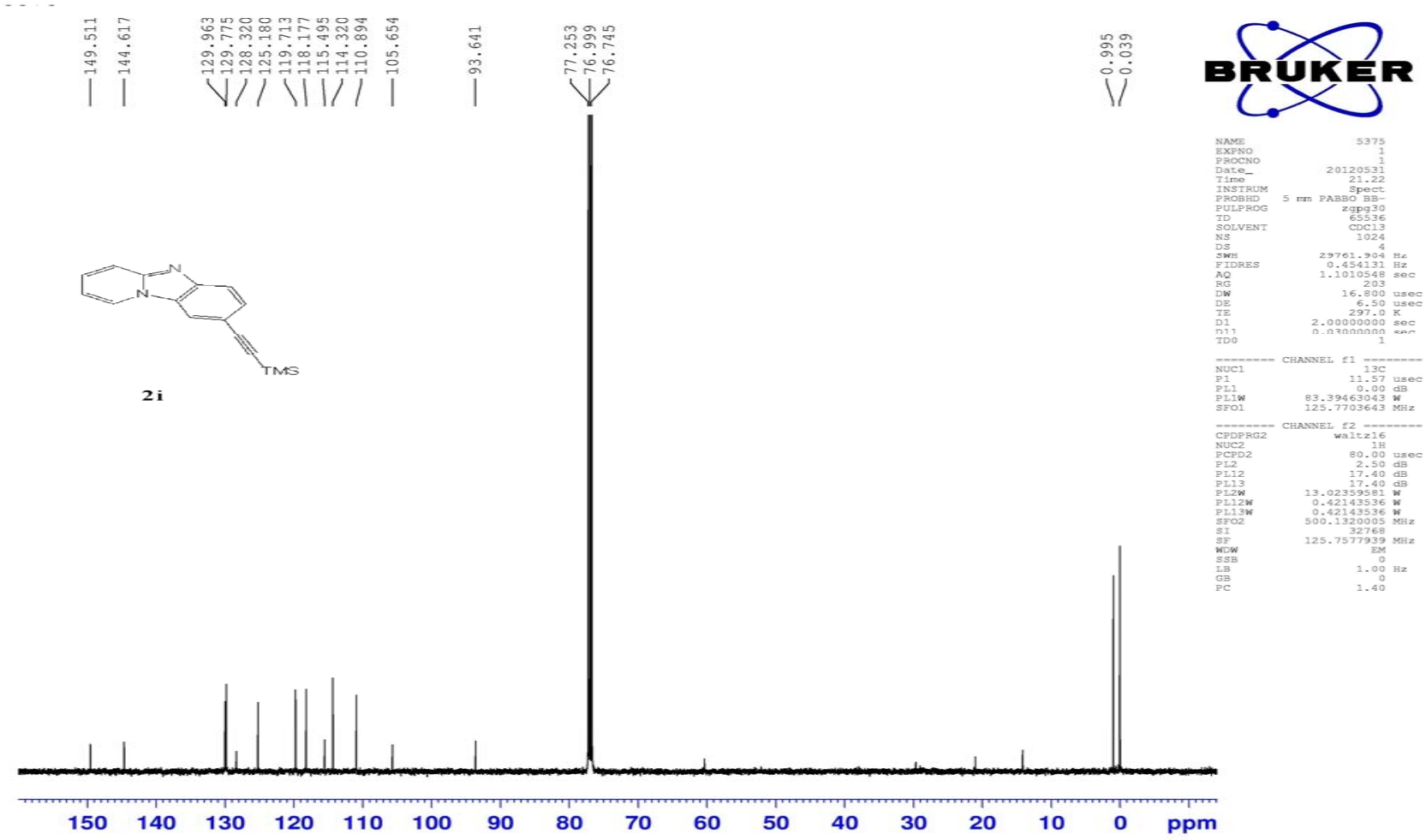

2h
8.366
8.246
8.243
7.793
7.789
7.771
7.767
7.703
7.697
7.682
7.673
7.471
7.468
7.454
7.451
7.448
7.445
7.431
7.428
7.260
6.892
6.890
6.875
6.873
6.858
6.856
BRUKER
N
N
I
2h
NAME be_yimiao
EXPNO 31
PROCNO 1
Date_ 20130618
Time 22.15
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 322.5
DW 60.400 usec
DE 6.50 usec
TE 299.9 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
NUC1 1H
P1 12.58 usec
PL1 0.00 dB
PL1W 10.87646866 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300090 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
0.99
0.96
0.98
1.96
1.00
1.00


148.547
143.801
134.442
130.127
129.901
125.047
121.580
119.542
118.074
110.868
83.316
77.254
76.999
76.745
BRUKER
NAME 5080
EXPNO 1
PROCNO 1
Date_ 20120530
Time 13.06
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 96
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 297.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 11.57 usec
PL1 0.00 dB
PL1W 83.39463043 W
SFO1 125.7703643 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577973 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
N
N
I
2h
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



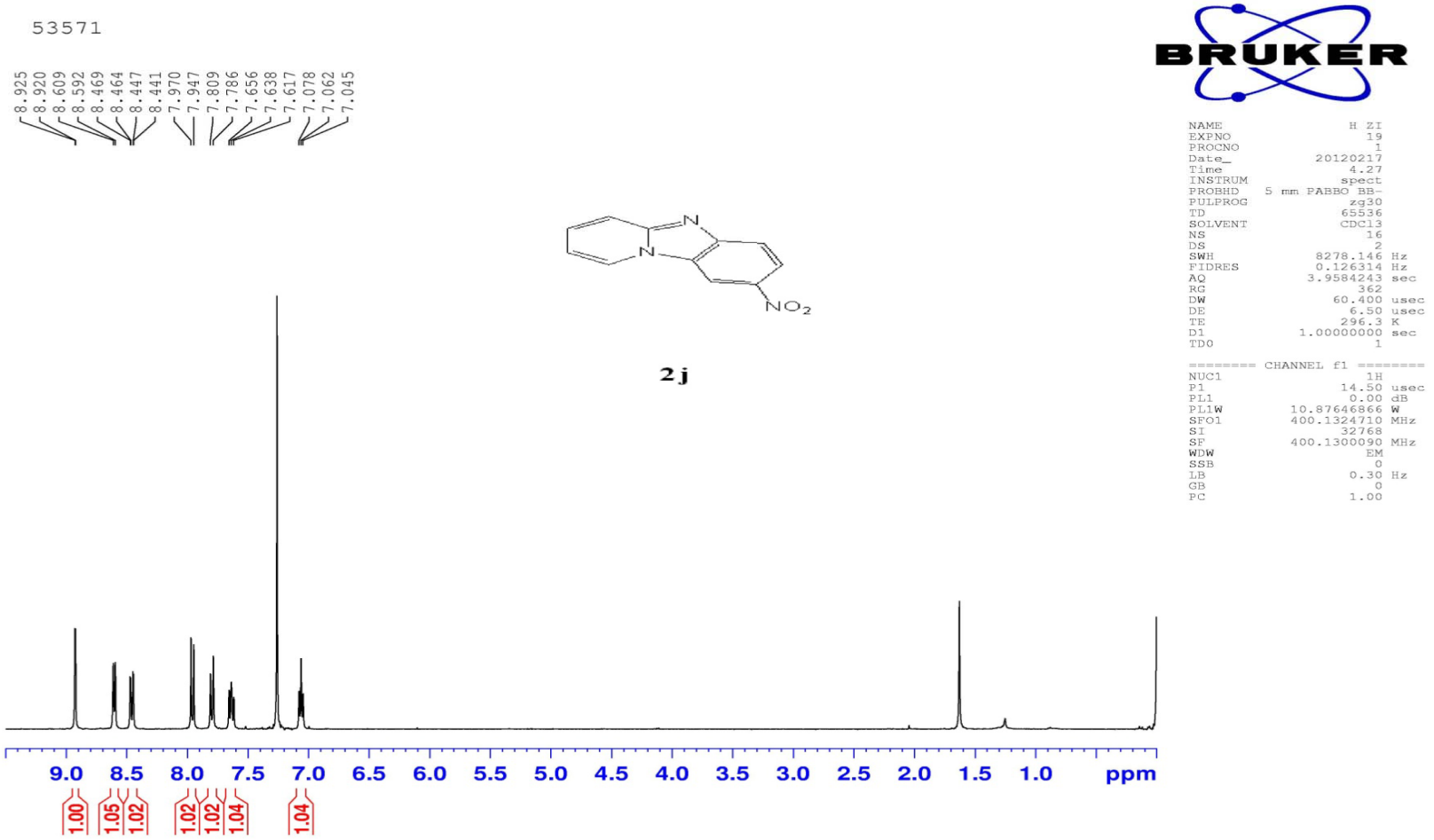
BRUKER

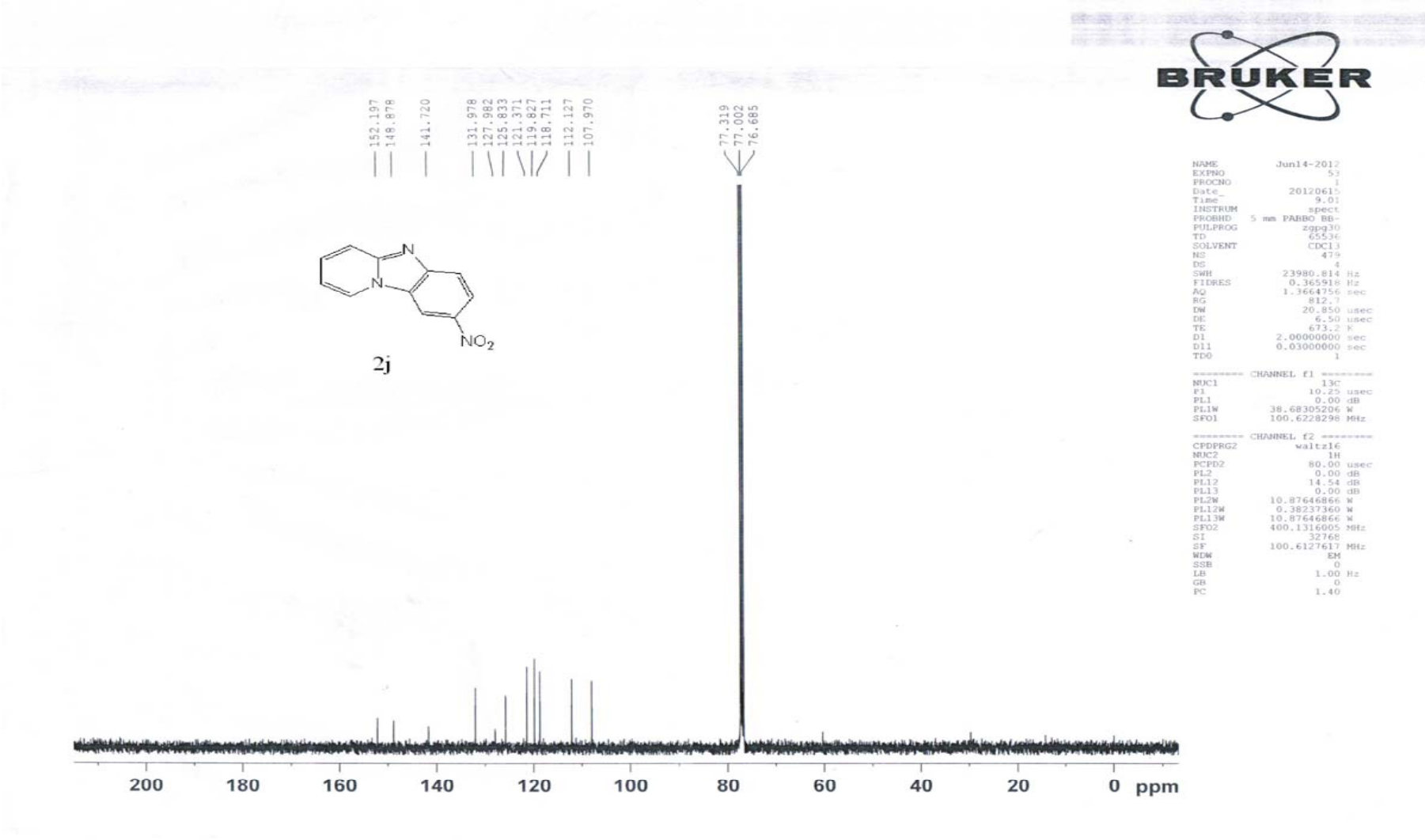
NAME	H ZI
EXPNO	32
PROCNO	1
Date_	20120222
Time	8.24
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	362
DW	60.400 usec
DE	6.50 usec
TE	297.4 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.00 dB
PL1W	10.87646866 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300092 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

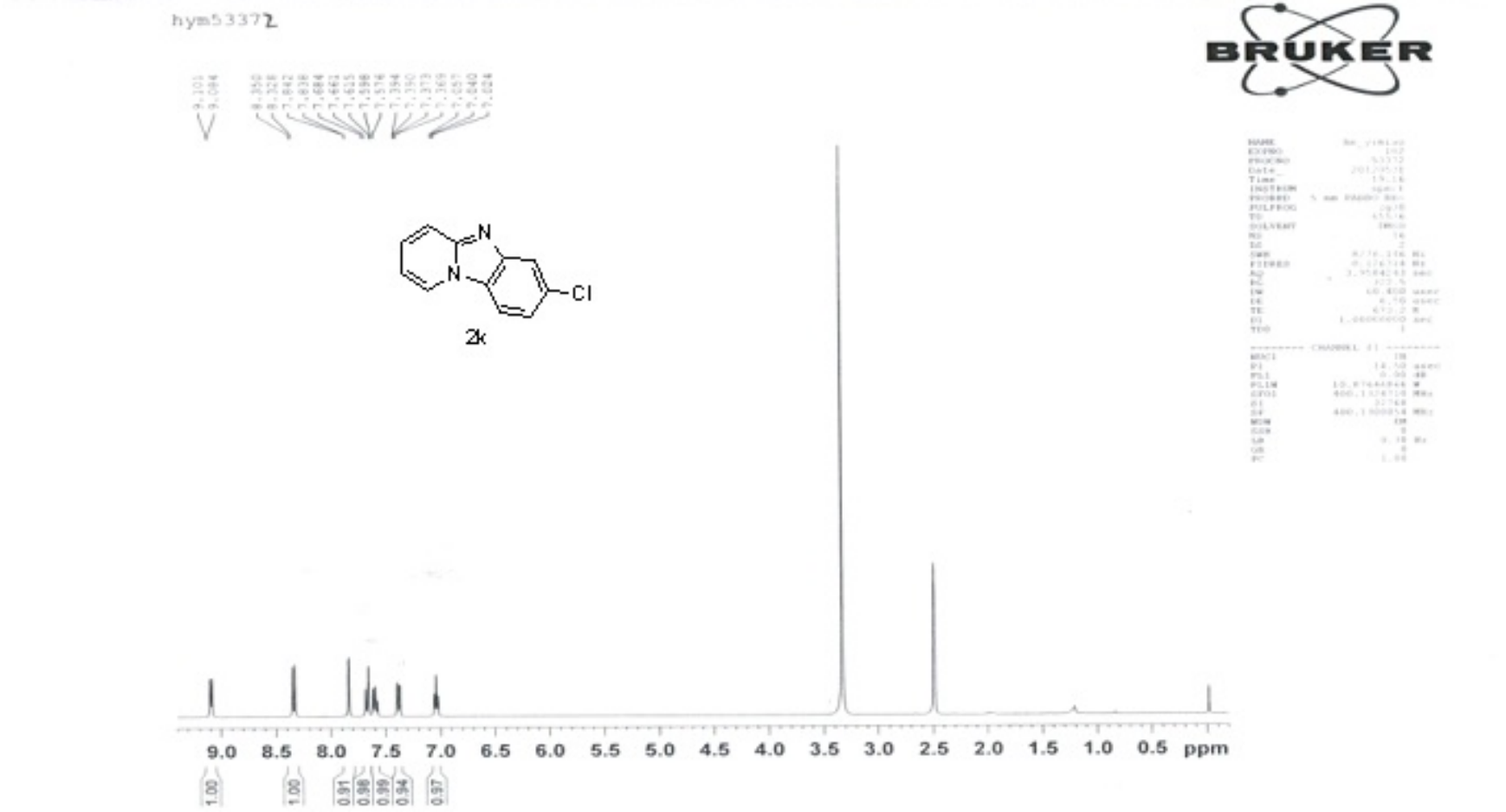


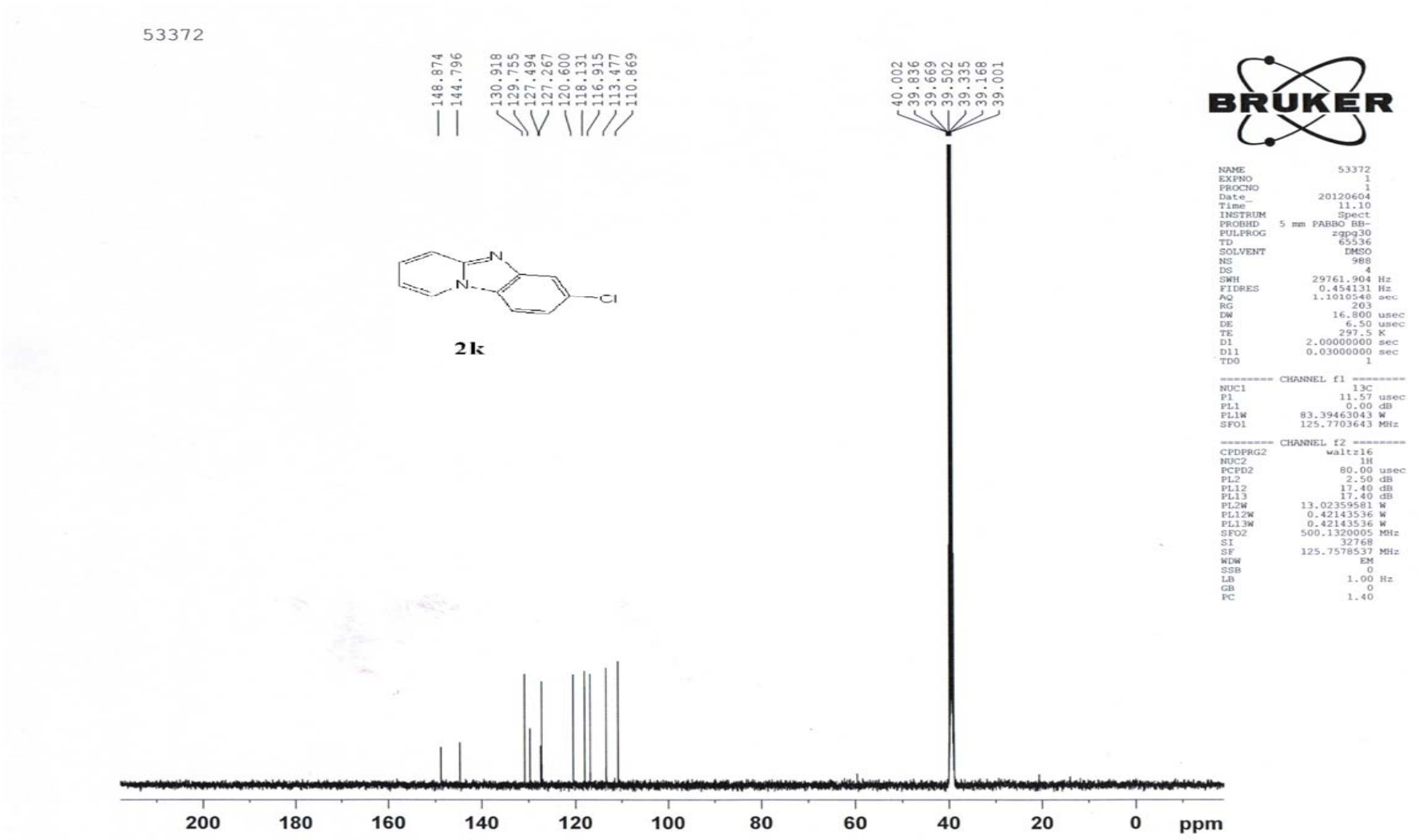
BRUKER

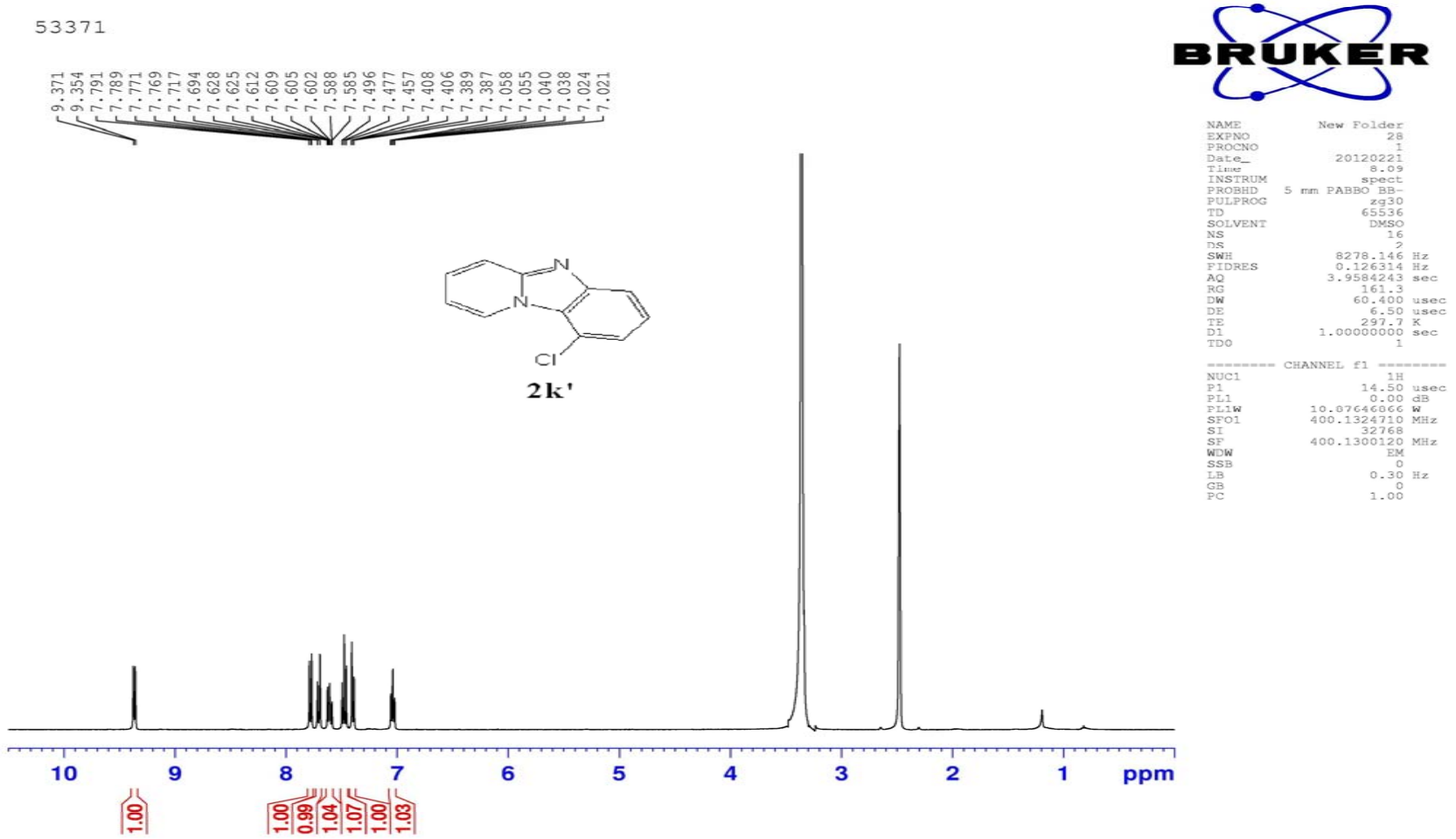
NAME	5375
EXPNO	1
PROCNO	1
Date_	20120531
Time	21.22
INSTRUM	Spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	297.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	11.57 usec
PL1	0.00 dB
PL1W	83.39463043 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.50 dB
PL12	17.40 dB
PL13	17.40 dB
PL2W	13.02359581 W
PL12W	0.42143536 W
PL13W	0.42143536 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7577939 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40


53571
8.925
8.920
8.609
8.592
8.469
8.464
8.447
8.441
7.970
7.947
7.809
7.786
7.656
7.638
7.617
7.078
7.062
7.045
N
N
NO2
2j
BRUKER
NAME H ZI
EXPNO 19
PROCNO 1
Date_ 20120217
Time 4.27
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 362
DW 60.400 usec
DE 6.50 usec
TE 296.3 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
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.00
1.05
1.02
1.02
1.02
1.04
1.04


152.197
148.878
141.720
131.978
127.982
125.833
121.371
119.827
118.711
112.127
107.970
77.319
77.002
76.685
N
N
NO2
2j
BRUKER
NAME Jun14-2012
EXPNO 53
PROCNO 1
Date_ 20120615
Time 9.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 479
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 673.2 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 100.6127617 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0 ppm

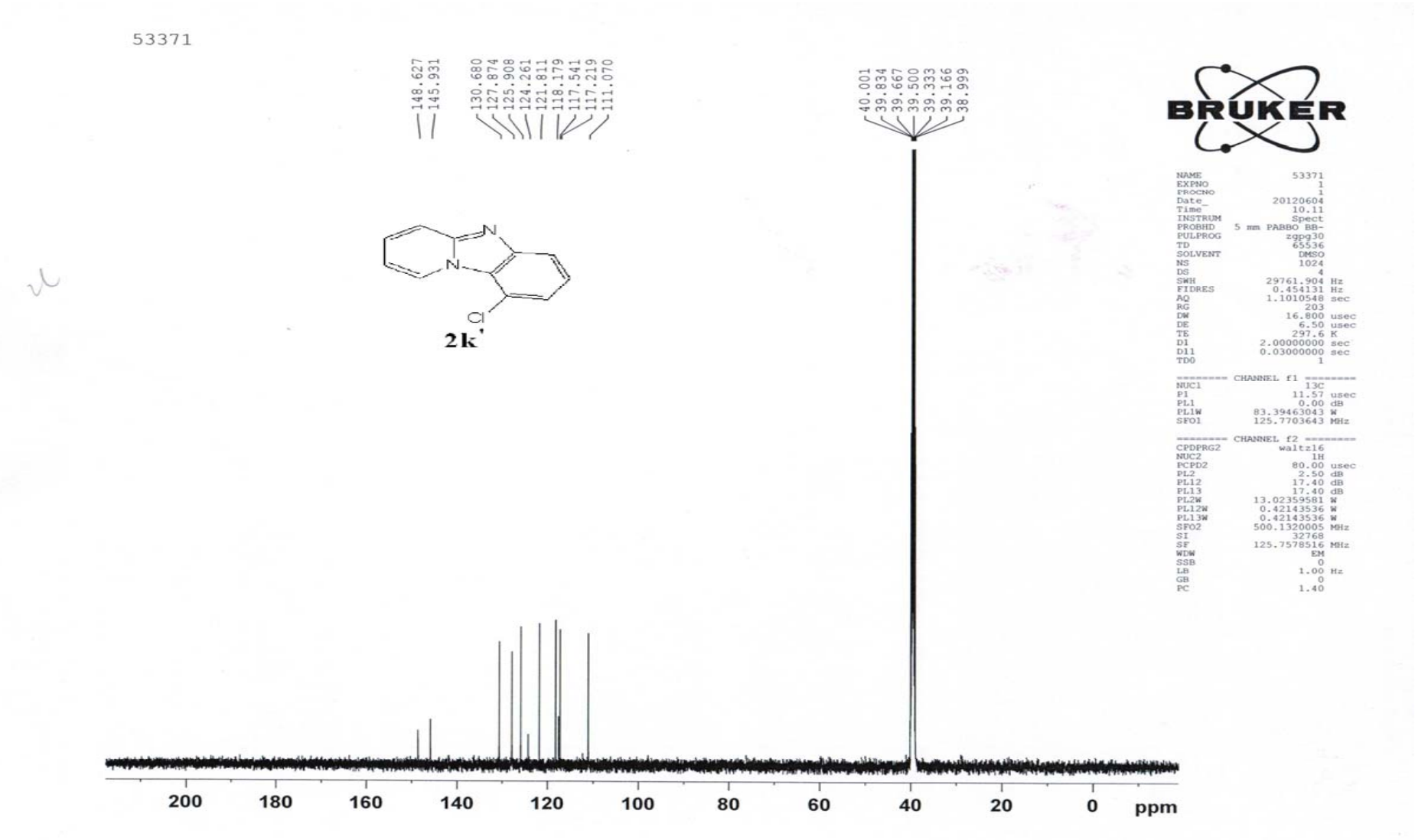

hym53372
BRUKER
N
N
Cl
2k
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm
1.00
1.00
0.91
0.98
0.99
0.94
0.97

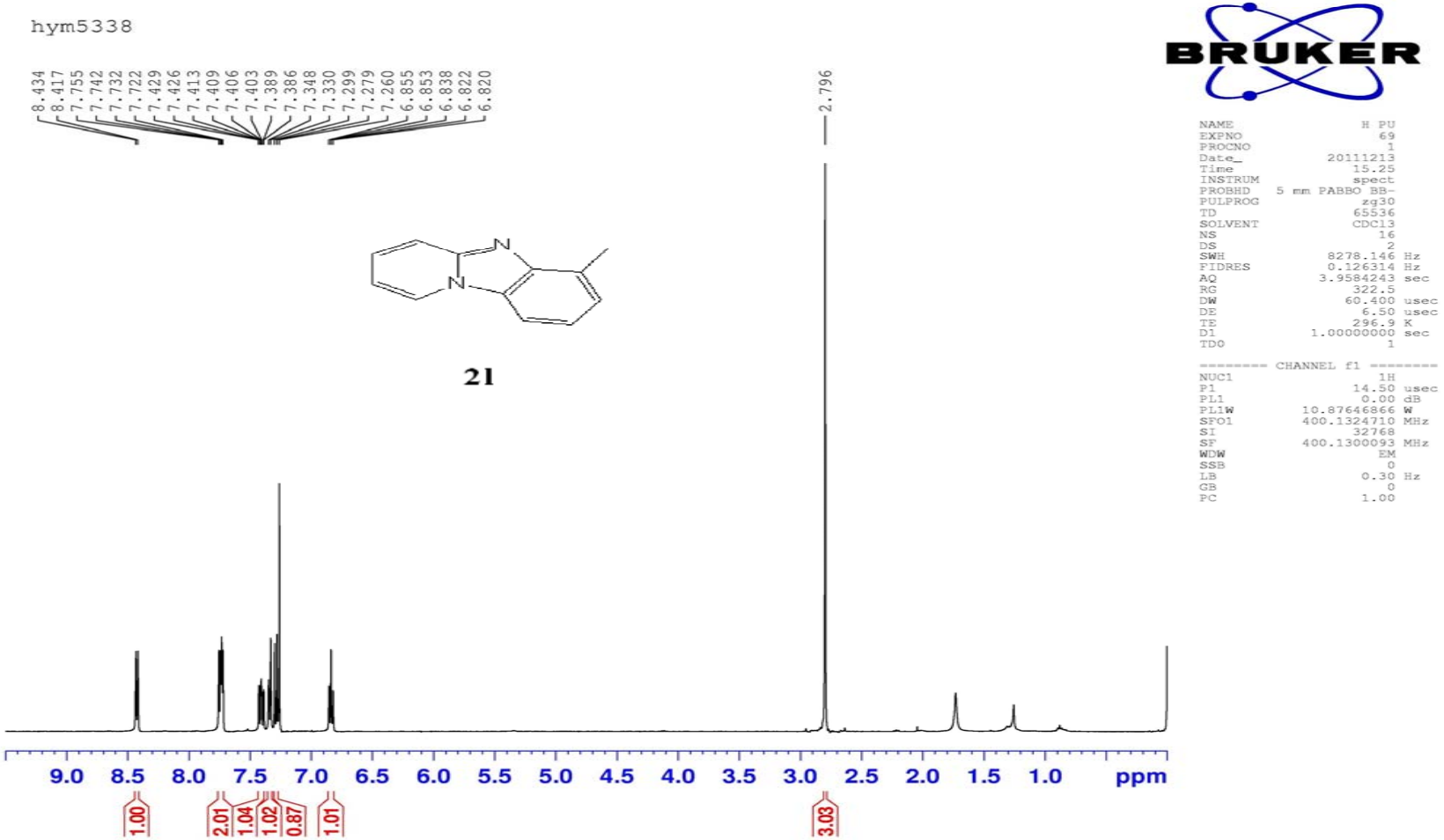

53372
148.874
144.796
130.918
129.755
127.494
127.267
120.600
118.131
116.915
113.477
110.869
40.002
39.836
39.669
39.502
39.335
39.168
39.001
N
N
Cl
2k
BRUKER
NAME 53372
EXPNO 1
PROCNO 1
Date_ 20120604
Time 11.10
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 988
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010540 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 297.5 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 125.7578537 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0
ppm

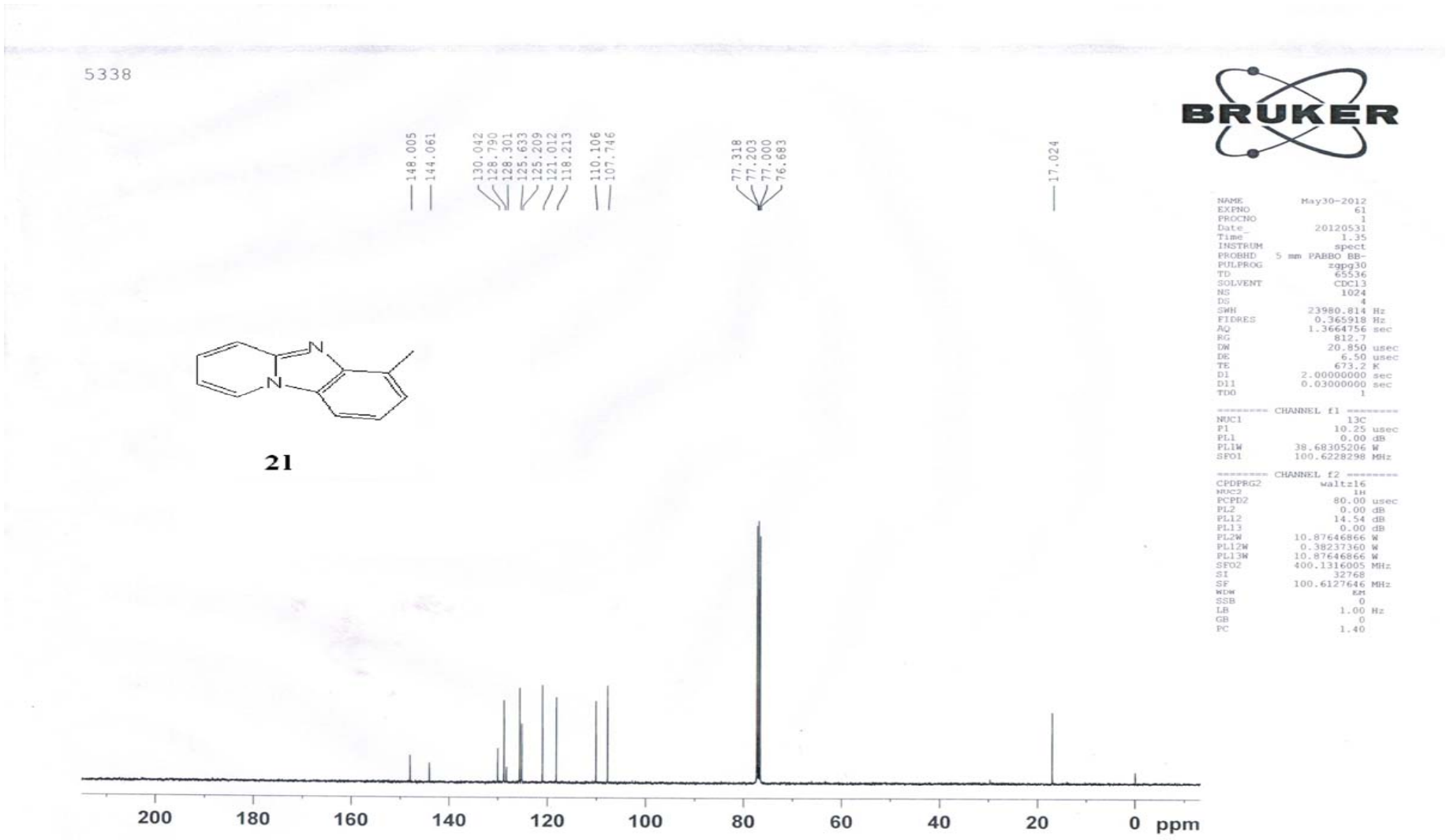


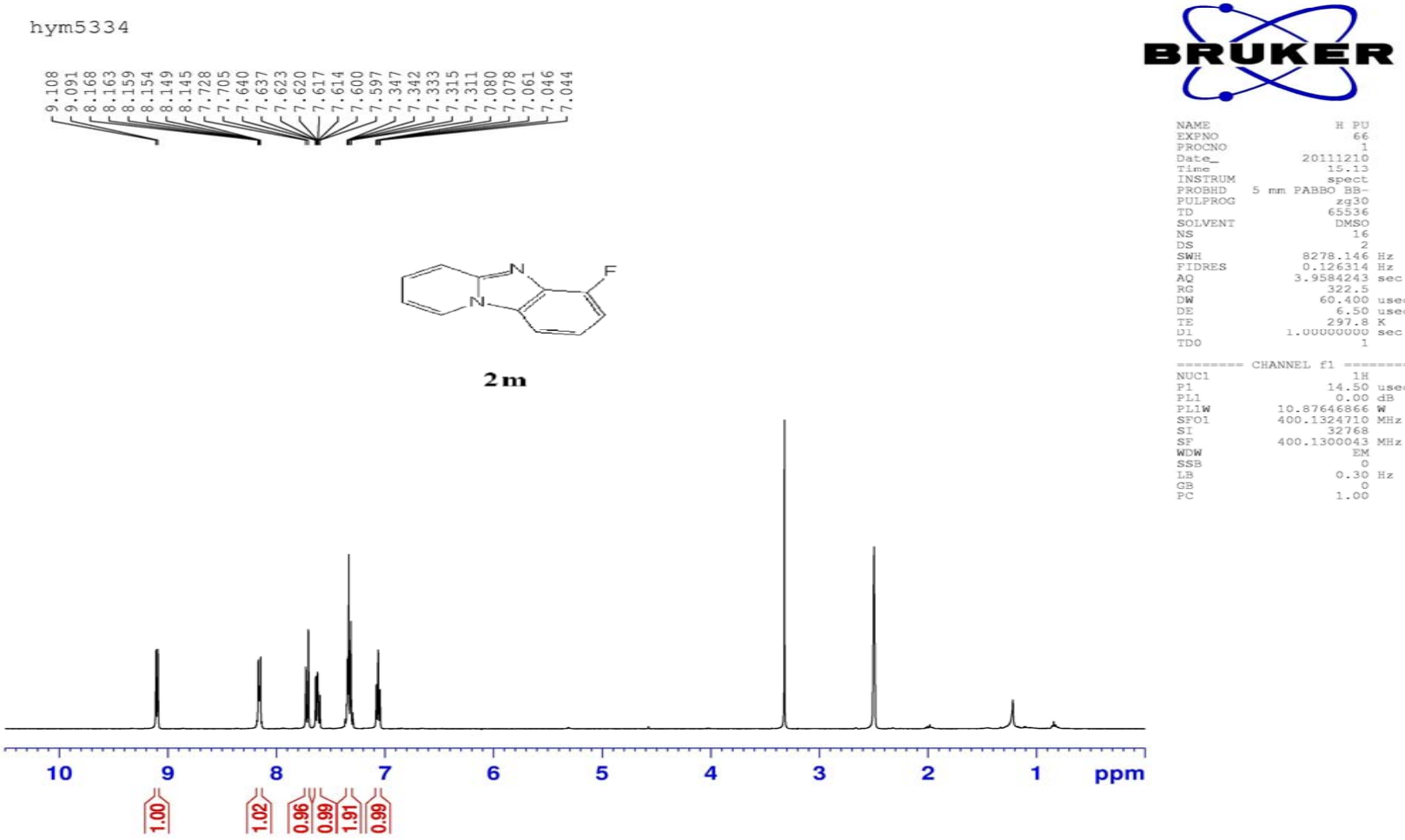
BRUKER

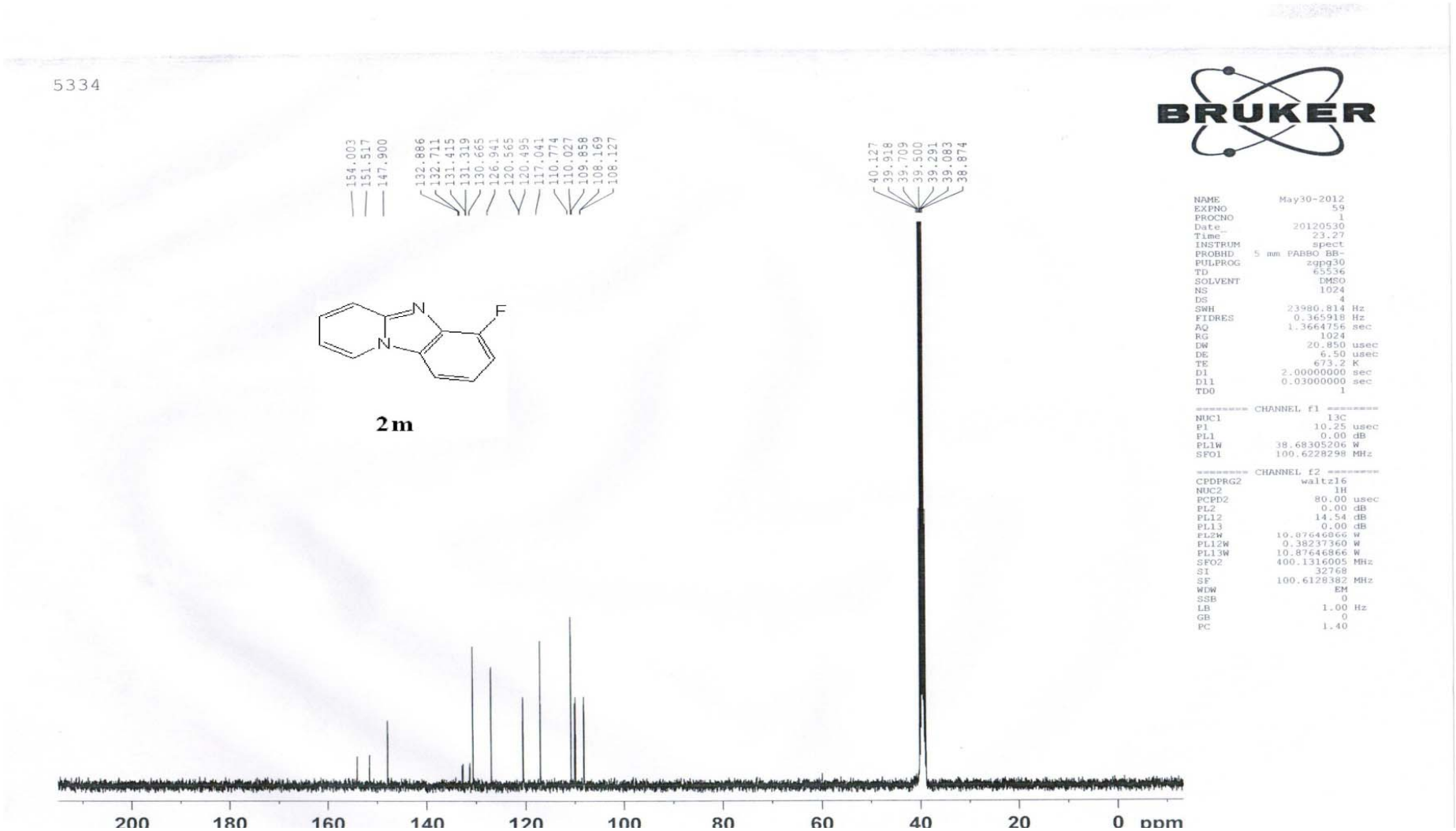
NAME	New Folder	
EXPNO	28	
PROCNO	1	
Date_	20120221	
Time	8.09	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	DMSO	
NS	16	
DS	2	
SWH	8278.146	Hz
FIDRES	0.126314	Hz
AQ	3.9584243	sec
RG	161.3	
DW	60.400	usec
DE	6.50	usec
TE	297.7	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	14.50	usec
PL1	0.00	dB
PL1W	10.07646866	W
SFO1	400.1324710	MHz
SI	32768	
SF	400.1300120	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	

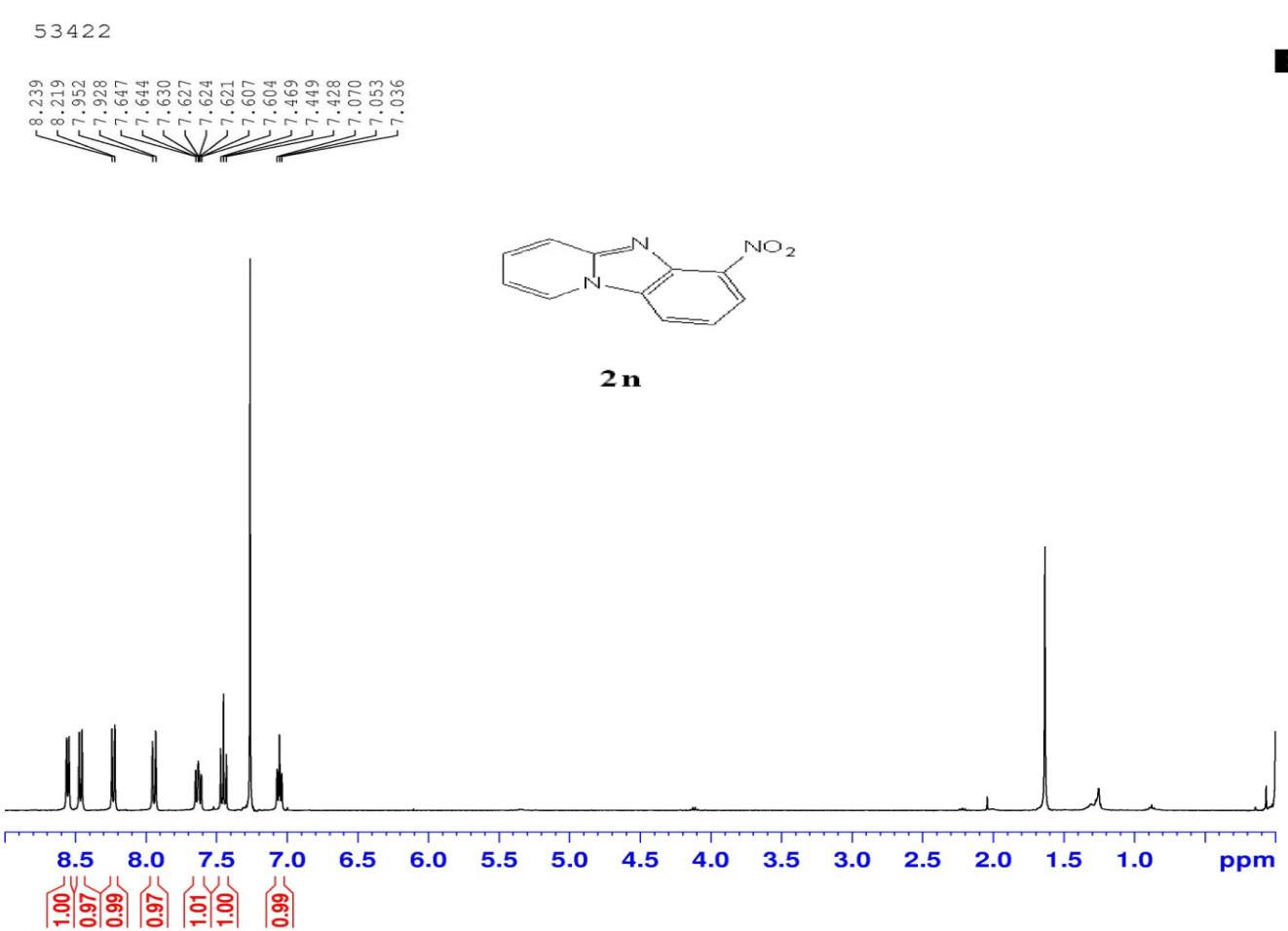

53371
148.627
145.931
130.680
127.874
125.908
124.261
121.811
118.179
117.541
117.219
111.070
40.001
39.834
39.667
39.500
39.333
39.166
38.999
BRUKER
NAME 53371
EXPNO 1
PROCNO 1
Date_ 20120604
Time 10.11
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 297.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 11.57 usec
PL1 0.00 dB
PL1W 83.39463043 W
SFO1 125.7703643 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7578516 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
N
N
Cl
2k'
200
180
160
140
120
100
80
60
40
20
0
ppm


hym5338
8.434
8.417
7.755
7.742
7.732
7.722
7.429
7.426
7.413
7.409
7.406
7.403
7.389
7.386
7.348
7.330
7.299
7.279
7.260
6.855
6.853
6.838
6.822
6.820
2.796
21
BRUKER
NAME H PU
EXPNO 69
PROCNO 1
Date_ 20111213
Time 15.25
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 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 400.1300093 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
2.01
1.04
1.02
0.87
1.01
3.03


5338
148.005
144.061
130.042
128.790
128.301
125.633
125.209
121.012
118.213
110.106
107.746
77.318
77.203
77.000
76.683
17.024
BRUKER
NAME May30-2012
EXPNO 61
PROCNO 1
Date_ 20120531
Time_ 1.35
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 812.7
DW 20.850 usec
DE 6.50 usec
TE 673.2 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 100.6127646 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
N
N
21
200
180
160
140
120
100
80
60
40
20
0
ppm

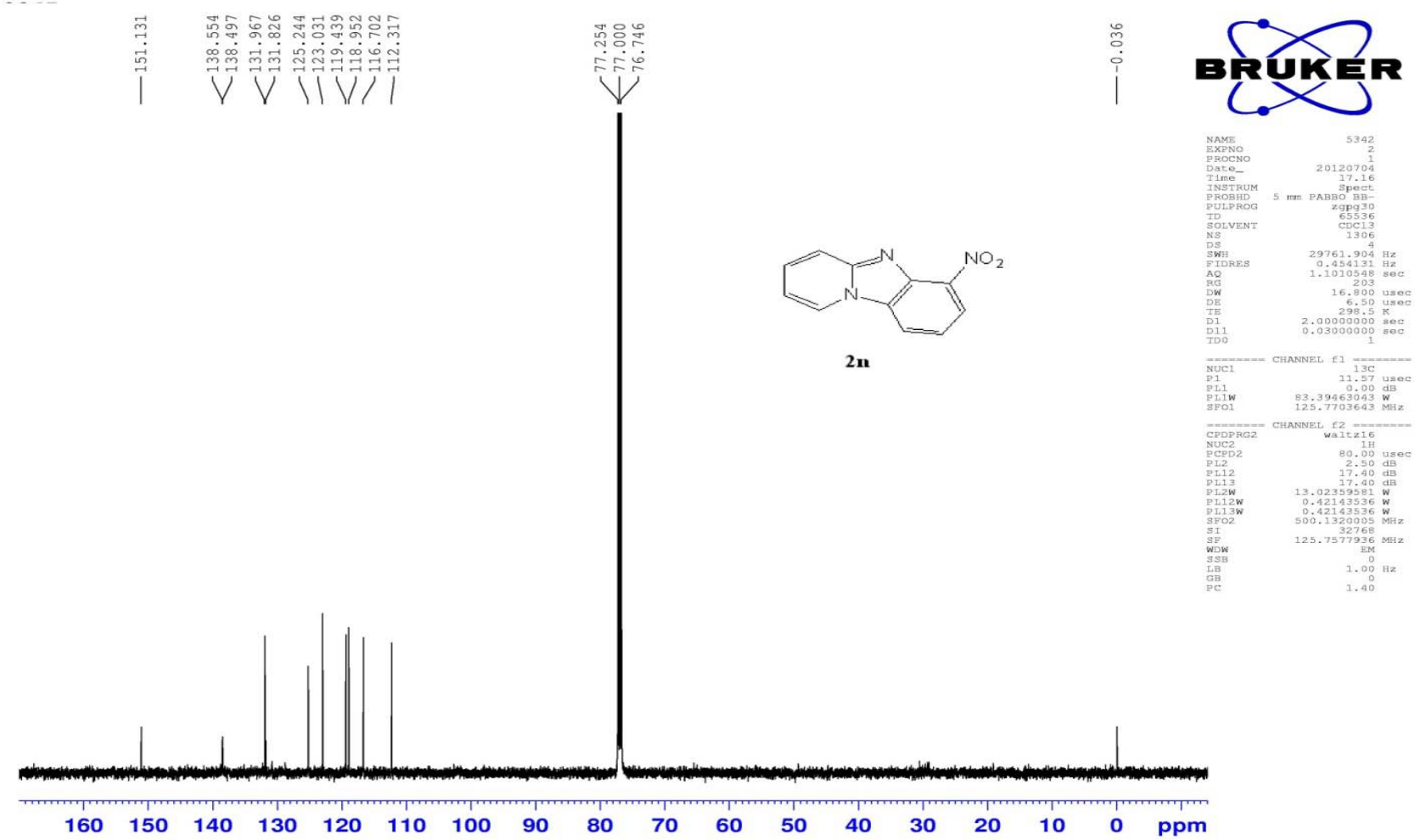

hym5334
9.108
9.091
8.168
8.163
8.159
8.154
8.149
8.145
7.728
7.705
7.640
7.637
7.623
7.620
7.617
7.614
7.600
7.597
7.347
7.342
7.333
7.315
7.311
7.080
7.078
7.061
7.046
7.044
N
N
F
2m
BRUKER
NAME H PU
EXPNO 66
PROCNO 1
Date_ 20111210
Time 15.13
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 322.5
DW 60.400 usec
DE 6.50 usec
TE 297.8 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 400.1300043 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
1.02
0.96
0.99
1.91
0.99

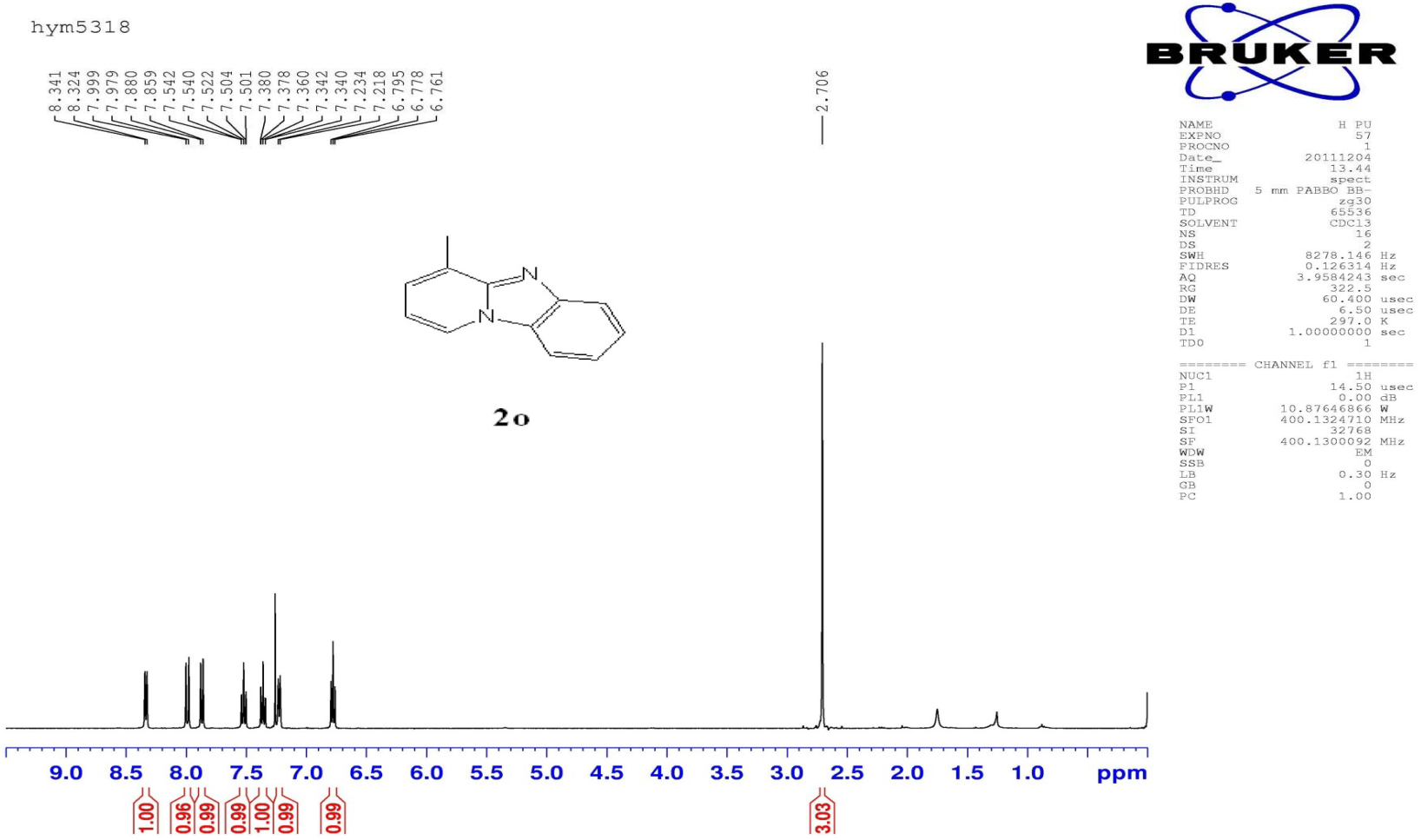

5334
154.003
151.517
147.900
132.886
132.711
131.415
131.319
130.665
126.941
120.565
120.495
117.041
110.774
110.027
109.858
108.169
108.127
40.127
39.918
39.709
39.500
39.291
39.083
38.874
N
N
F
2m
BRUKER
NAME May30-2012
EXPNO 59
PROCNO 1
Date_ 20120530
Time 23.27
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
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 673.2 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 100.6128382 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0 ppm



BRUKER

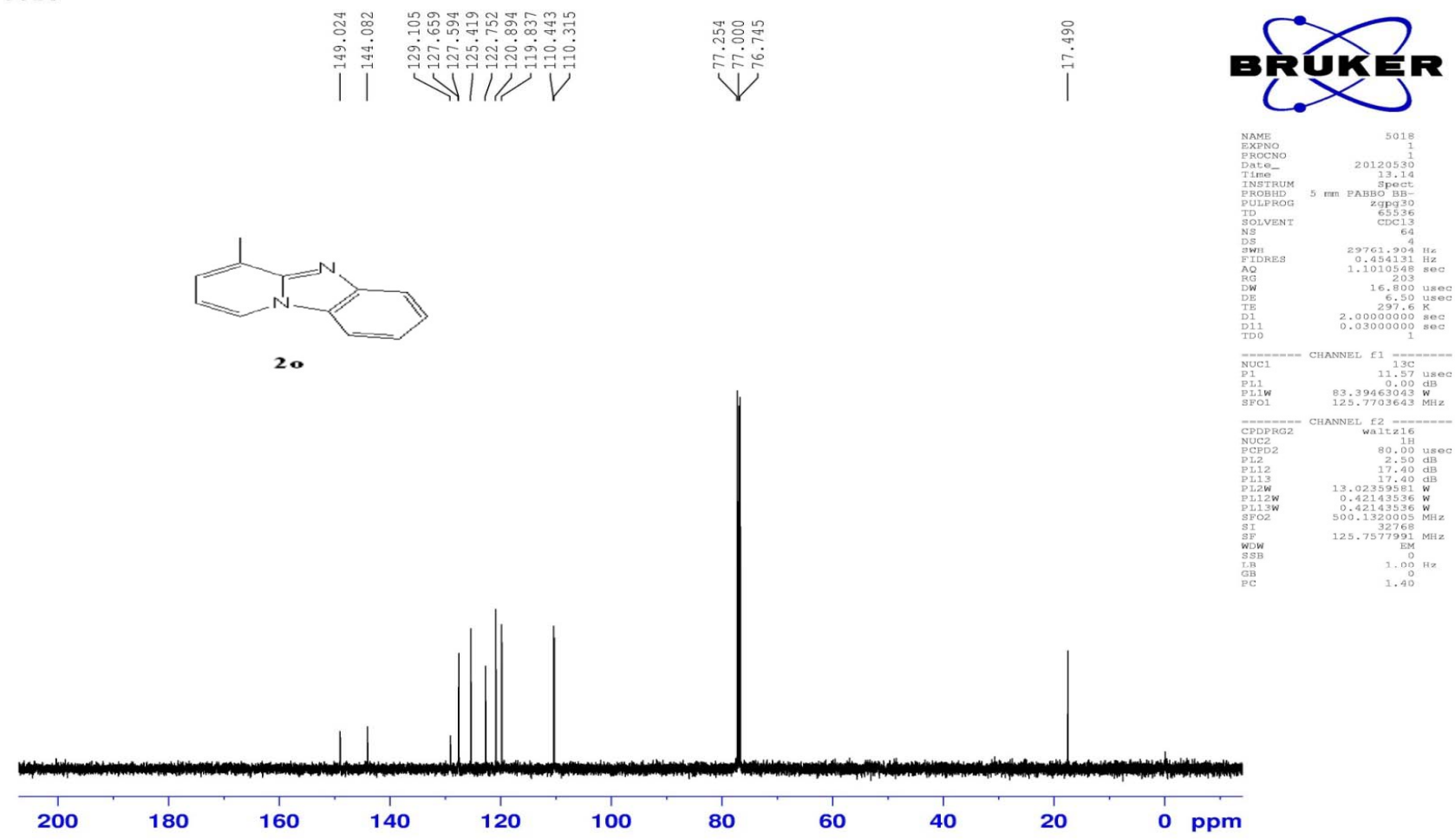
NAME	H ZI
EXPNO	29
PROCNO	1
Date_	20120222
Time	8.04
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	CDCl3
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	456.1
DW	60.400 usec
DE	6.50 usec
TE	297.6 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	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


151.131
138.554
138.497
131.967
131.826
125.244
123.031
119.439
118.952
116.702
112.317
77.254
77.000
76.746
-0.036
N
N
NO2
2n
BRUKER
NAME 5342
EXPNO 2
PROCNO 1
Date_ 20120704
Time 17.16
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1306
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 298.5 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 125.7577936 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

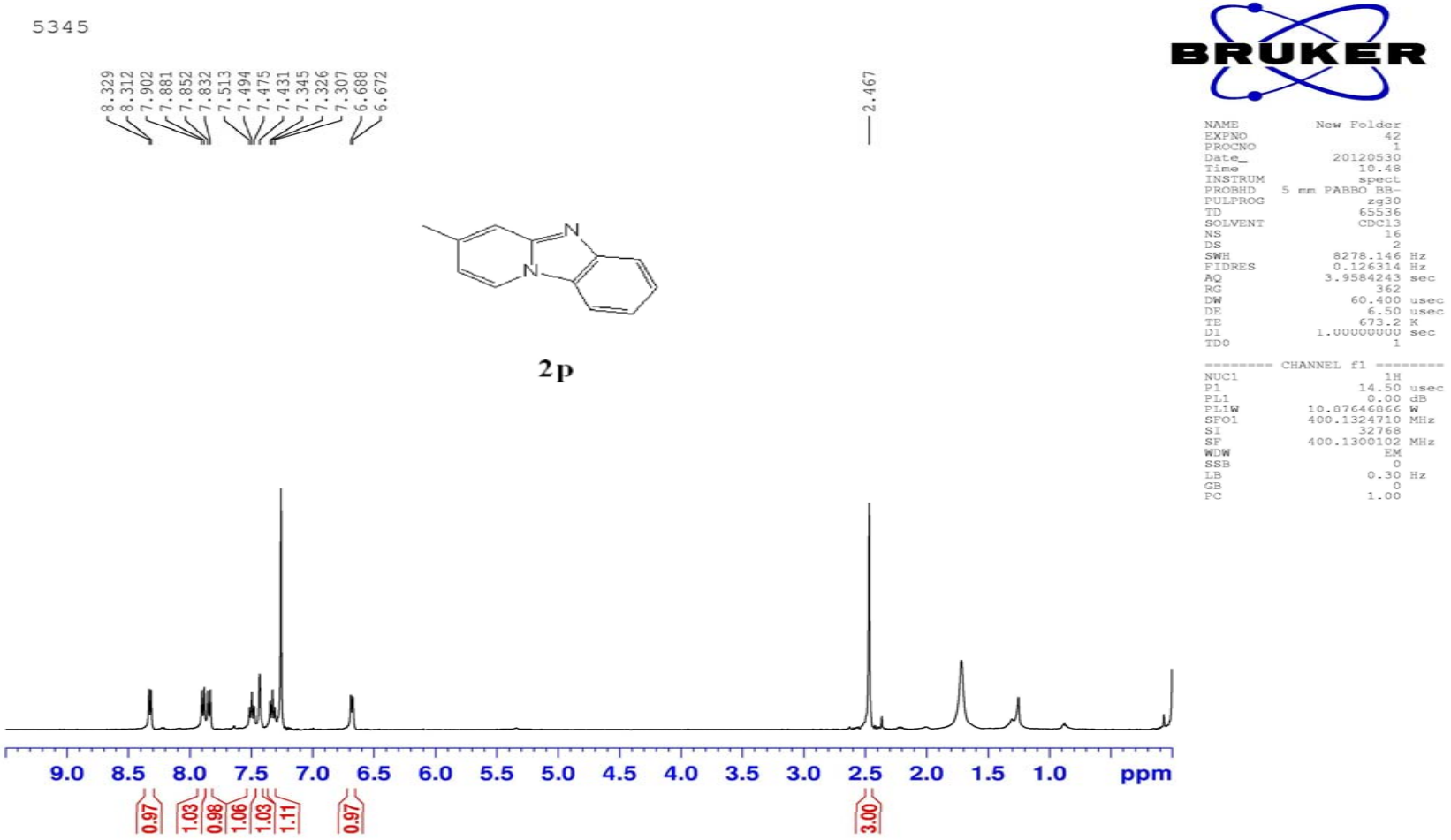


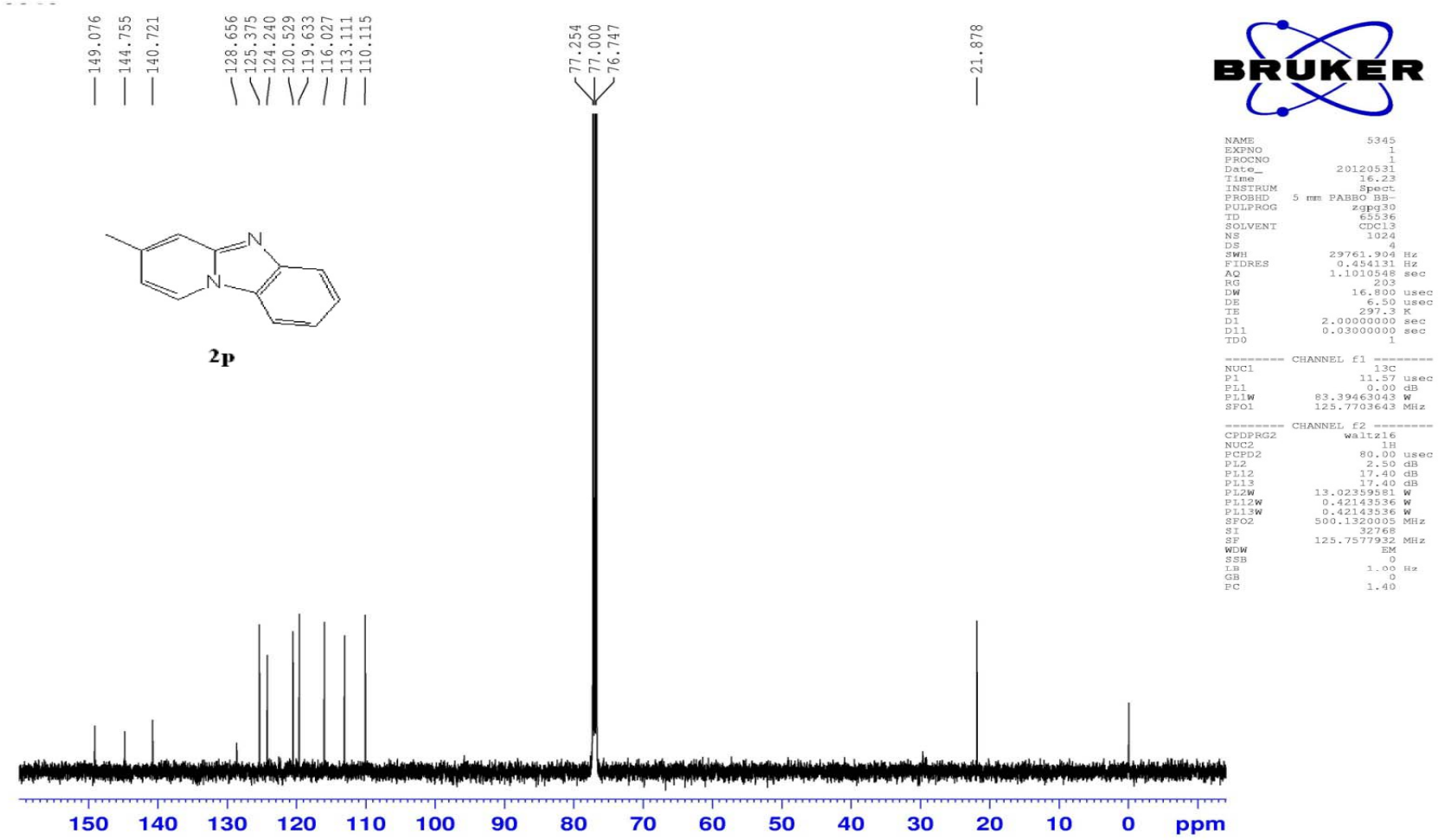
BRUKER

NAME	H PU
EXPNO	57
PROCNO	1
Date_	20111204
Time	13.44
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	322.5
DW	60.400 usec
DE	6.50 usec
TE	297.0 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


149.024
144.082
129.105
127.659
127.594
125.419
122.752
120.894
119.837
110.443
110.315
77.254
77.000
76.745
17.490
BRUKER
NAME 5018
EXPNO 1
PROCNO 1
Date_ 20120530
Time 13.14
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 297.6 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 11.57 usec
PL1 0.00 dB
PL1W 83.39463043 W
SFO1 125.7703643 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577791 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
N
N
200
180
160
140
120
100
80
60
40
20
0 ppm

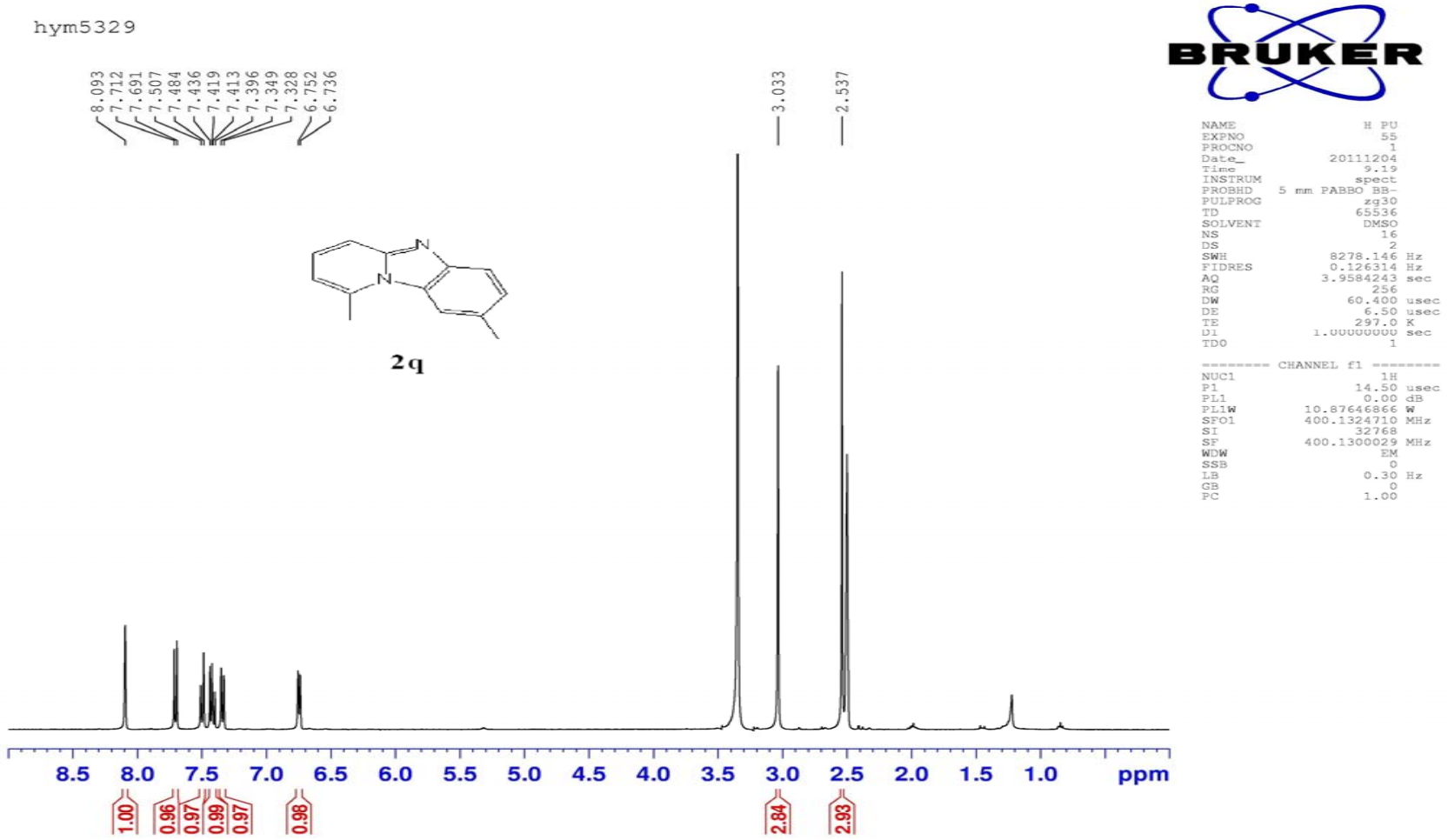
2o


5345
8.329
8.312
7.902
7.881
7.852
7.832
7.513
7.494
7.475
7.431
7.345
7.326
7.307
6.688
6.672
2.467
N
N
2p
BRUKER
NAME New Folder
EXPNO 42
PROCNO 1
Date_ 20120530
Time 10.48
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 362
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 10.07646066 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300102 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
0.97
1.03
0.98
1.06
1.03
1.11
0.97
3.00



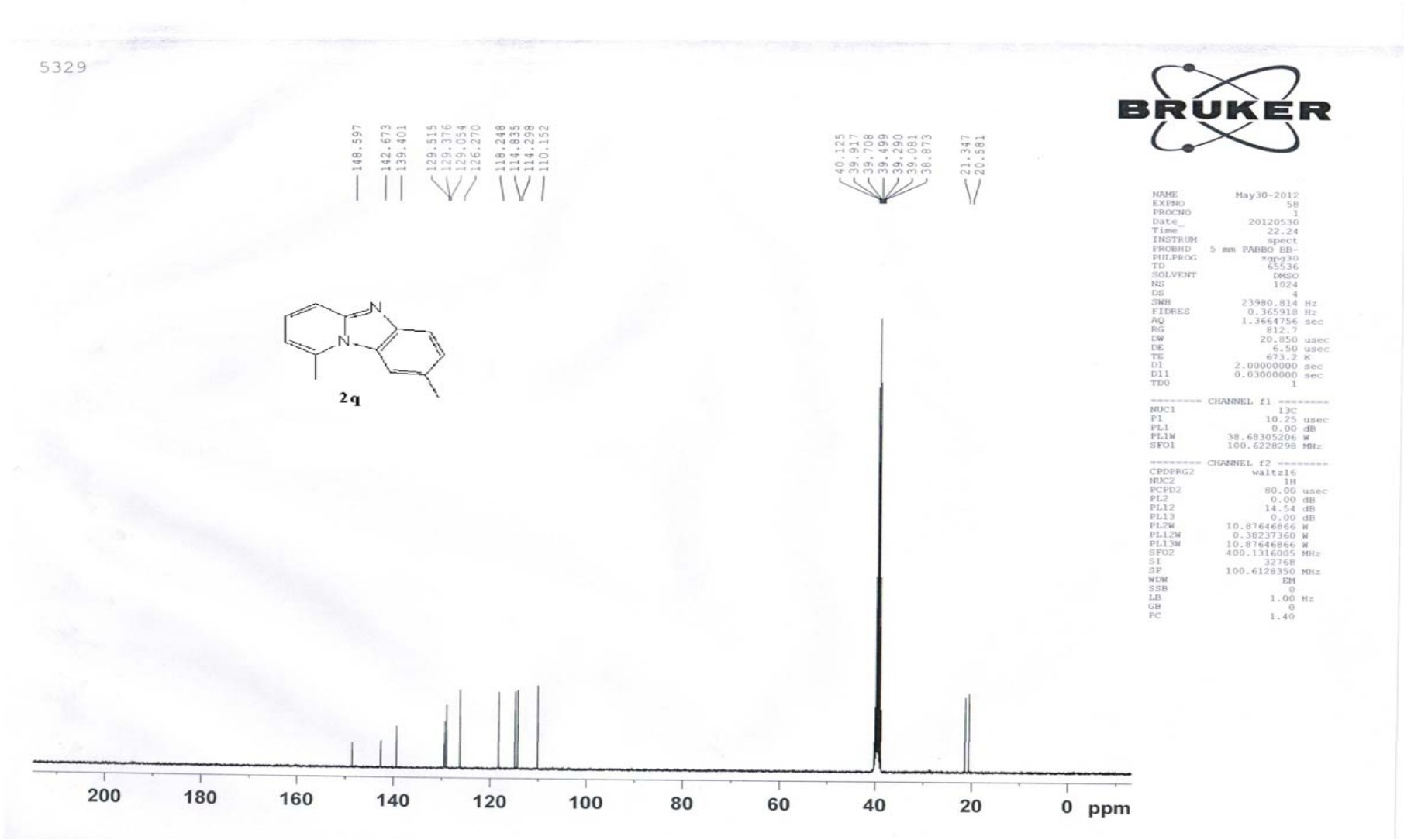
BRUKER

NAME	5345
EXPNO	1
PROCNO	1
Date_	20120531
Time	16.23
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	297.3 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	125.7577932 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

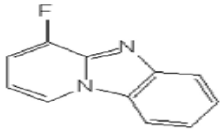


BRUKER

NAME	H PU
EXPNO	55
PROCNO	1
Date_	20111204
Time	9.19
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	256
DW	60.400 usec
DE	6.50 usec
TE	297.0 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	400.1300029 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

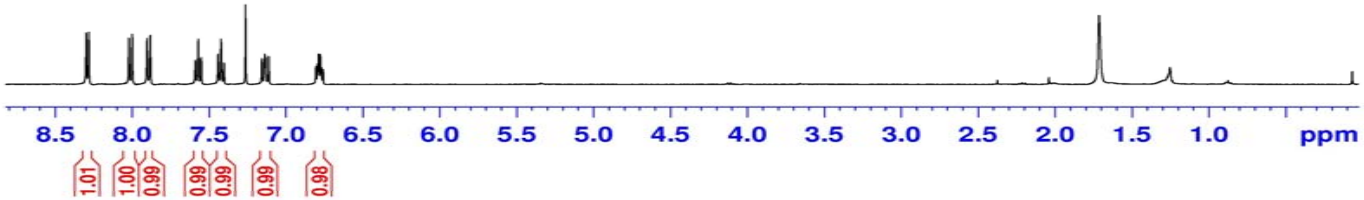

5329
148.597
142.673
139.401
129.515
129.376
129.054
126.270
118.248
114.835
114.298
110.152
40.125
39.917
39.708
39.499
39.290
39.081
38.873
21.347
20.581
2q
200
180
160
140
120
100
80
60
40
20
0 ppm
NAME May30-2012
EXPNO 58
PROCNO 1
Date_ 20120530
Time 22.24
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
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 673.2 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 100.6128350 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

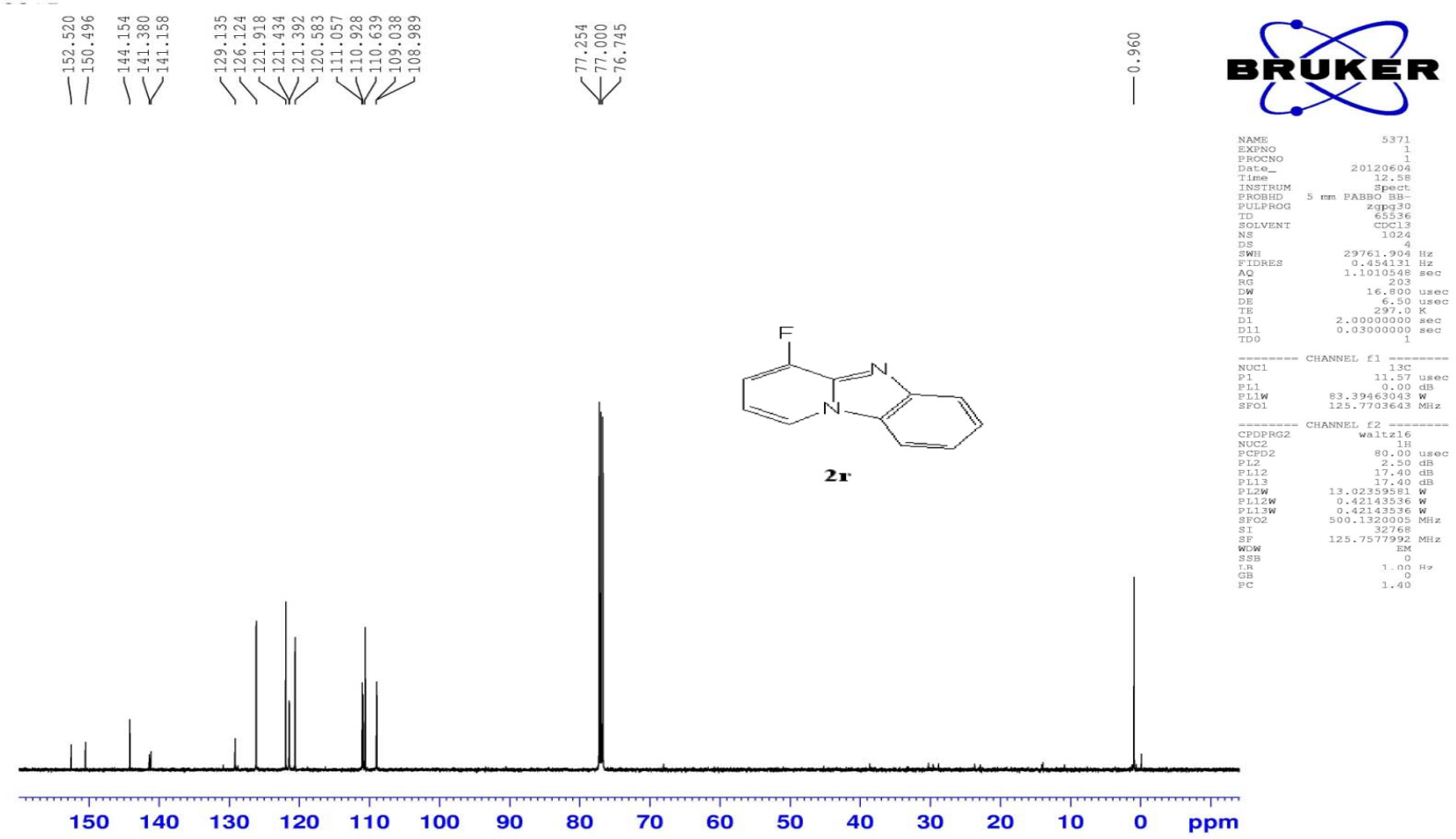
2r



2r

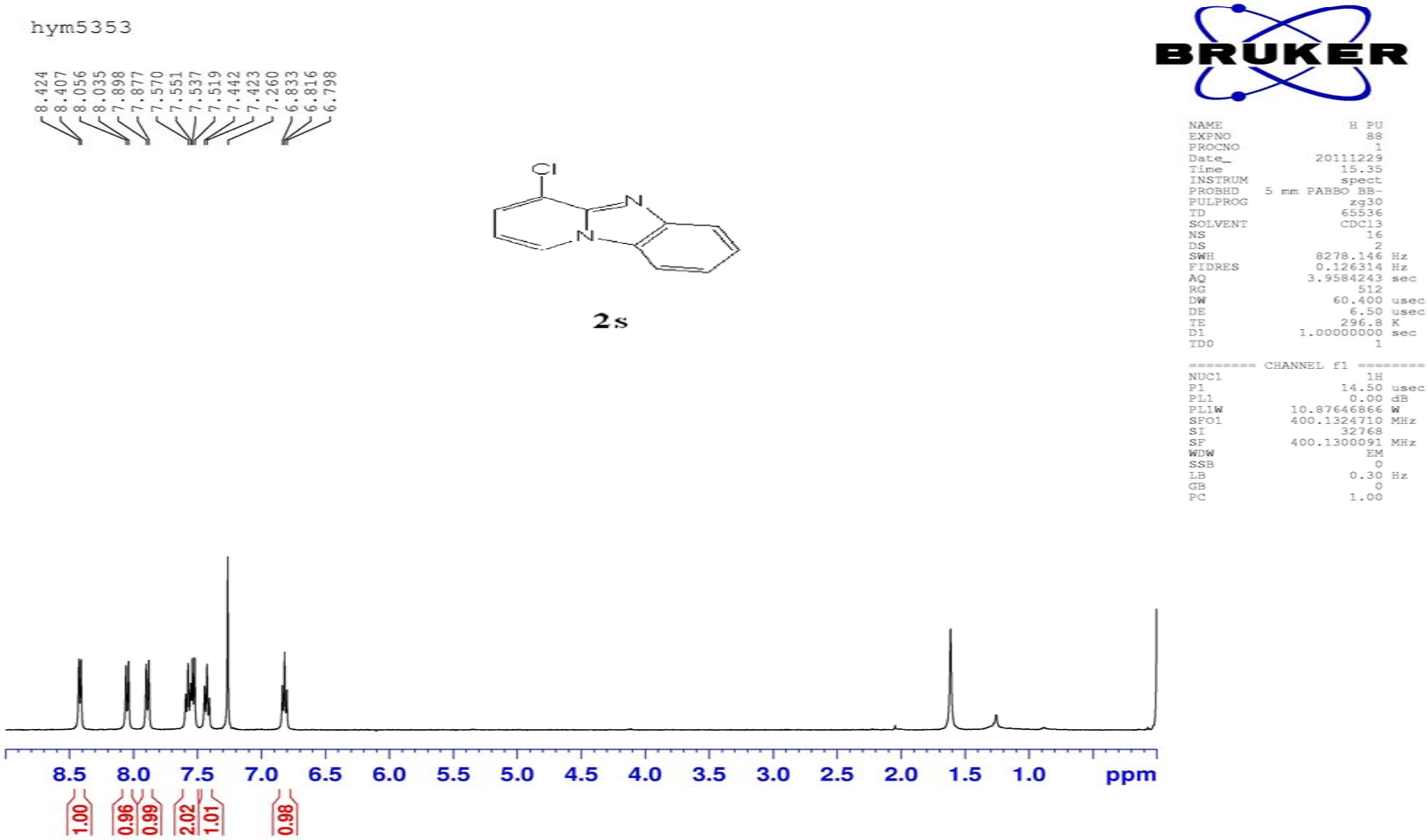
```
NAME                Jun18-2013
EXPNO                        9
PROCNO                       1
Date_             20130618
Time                     10.08
INSTRUM                  spect
PROBHD     5 mm PABBO BB-
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                           8
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                     298.6 K
D1                  1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       1H
P1                      12.58 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
```

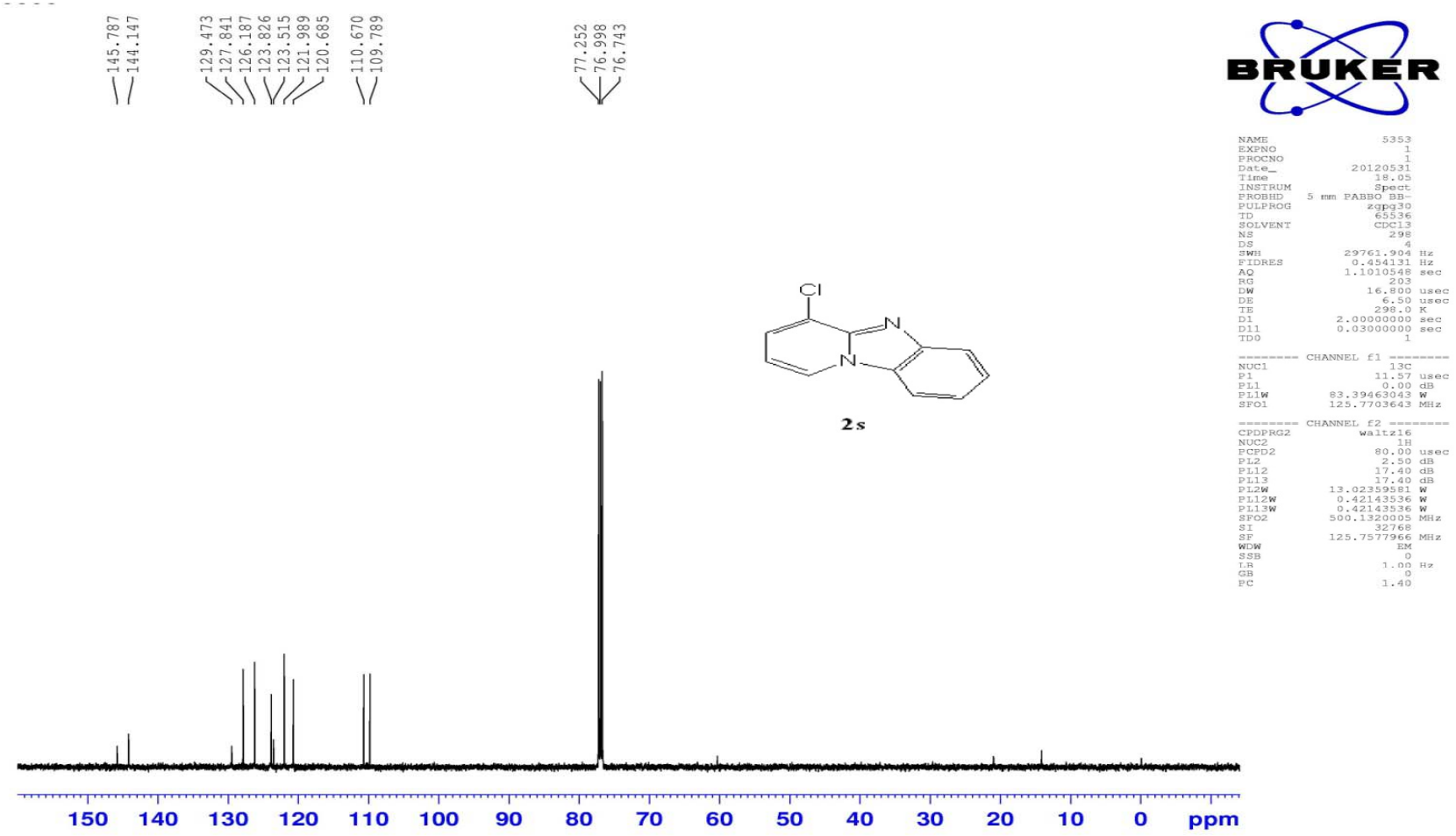




BRUKER

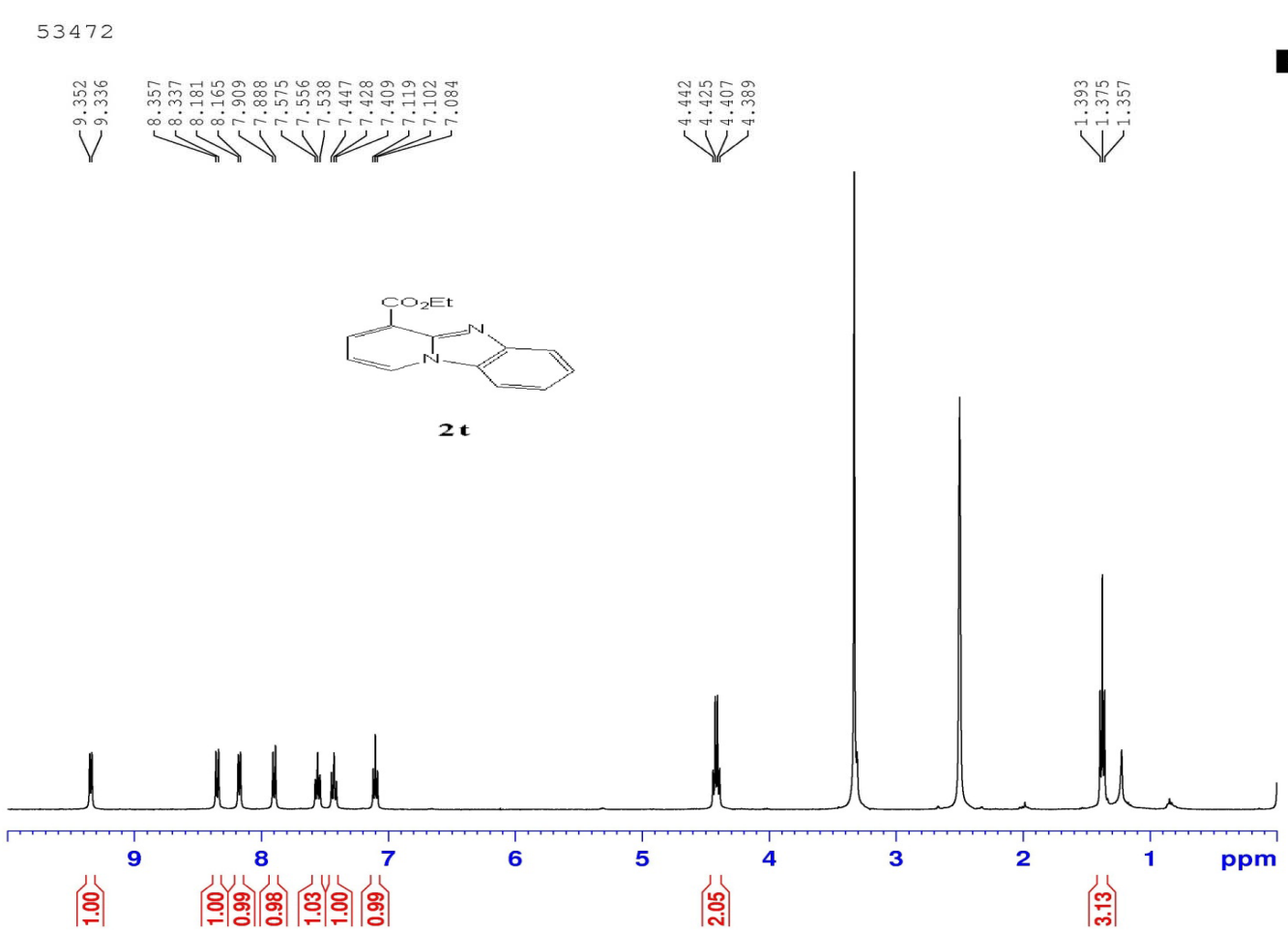
NAME	5371
EXPNO	1
PROCNO	1
Date_	20120604
Time	12.58
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	1024
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	297.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	11.57 usec
PL1	0.00 dB
PL1W	83.39463043 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.50 dB
PL12	17.40 dB
PL13	17.40 dB
PL2W	13.02359581 W
PL12W	0.42143536 W
PL13W	0.42143536 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7577992 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40


hym5353
8.424
8.407
8.056
8.035
7.898
7.877
7.570
7.551
7.537
7.519
7.442
7.423
7.260
6.833
6.816
6.798
Cl
N
N
2s
BRUKER
NAME H PU
EXPNO 88
PROCNO 1
Date_ 20111229
Time 15.35
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 512
DW 60.400 usec
DE 6.50 usec
TE 296.8 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 14.50 usec
PL1 0.00 dB
PL1W 10.87646866 W
SFO1 400.1324710 MHz
SI 32768
SF 400.1300091 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.00
0.96
0.99
2.02
1.01
0.98

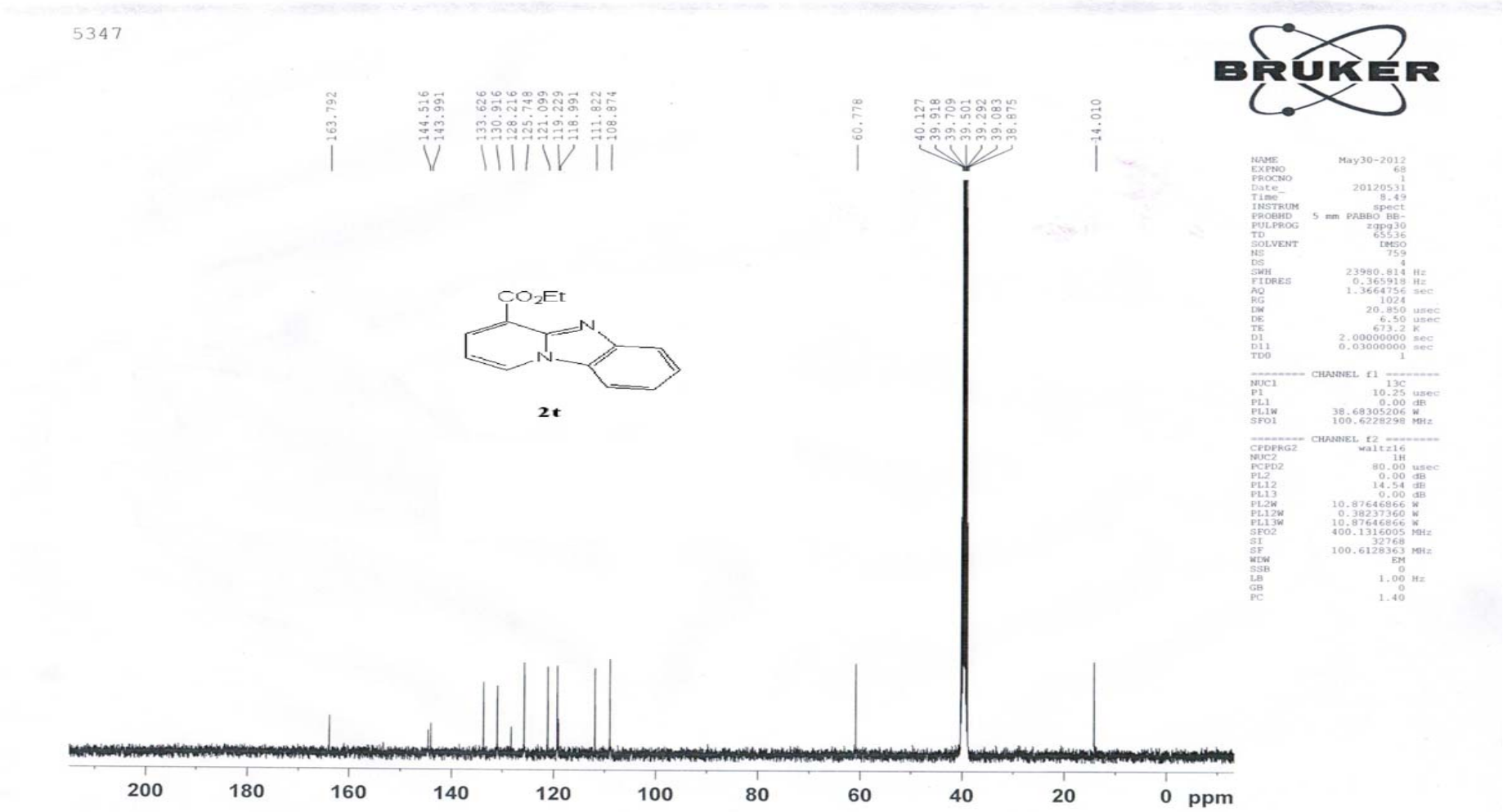


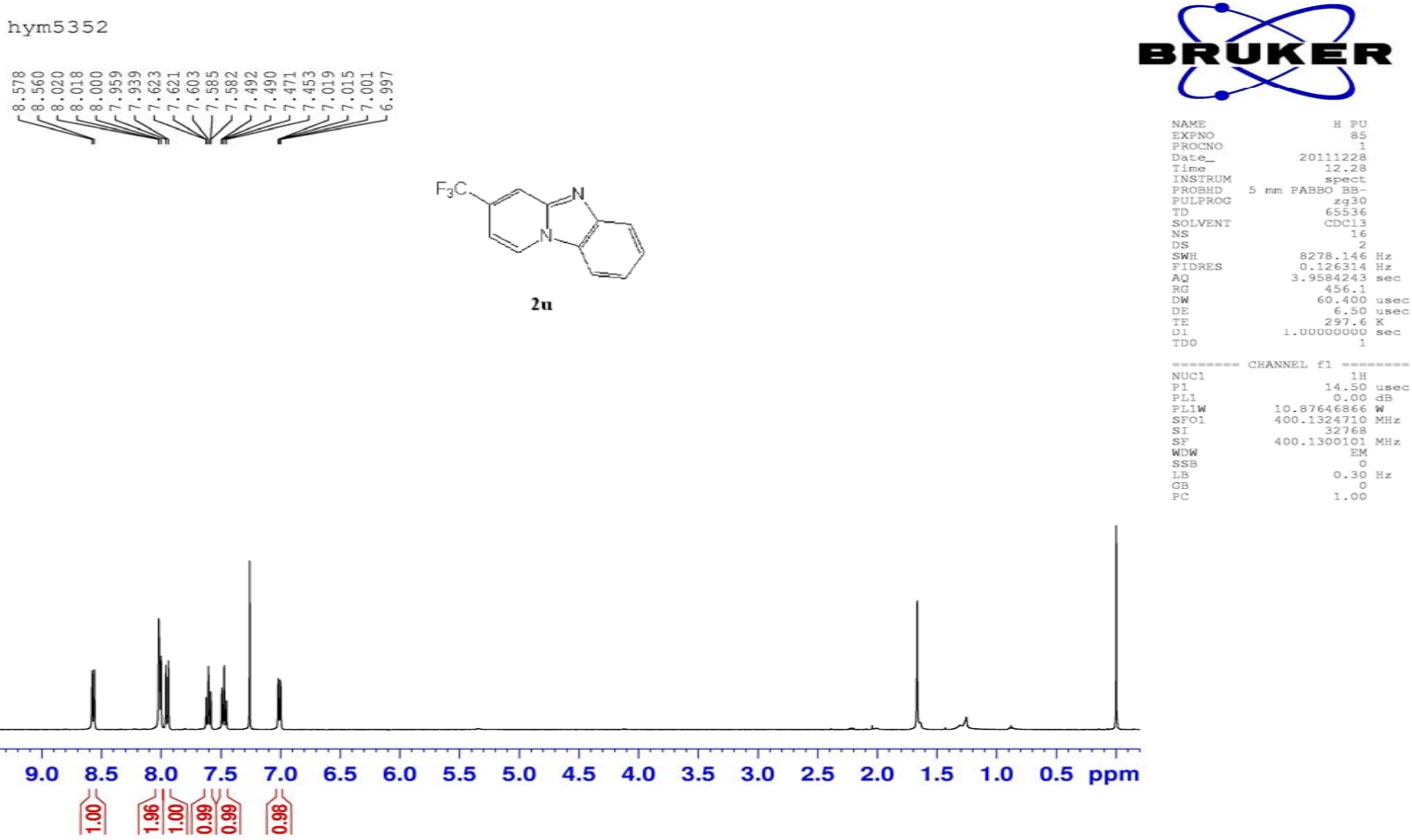
BRUKER

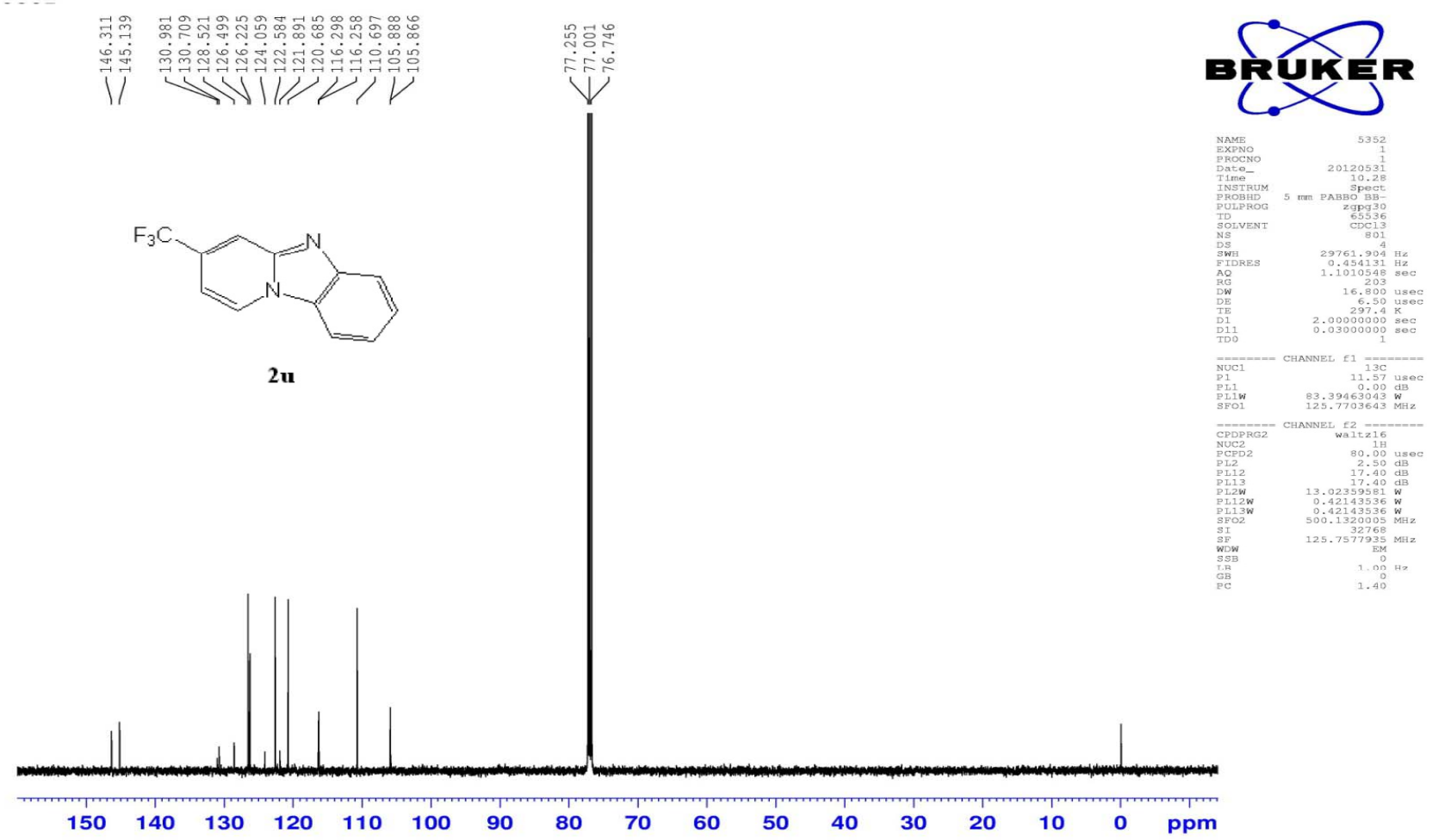
NAME	5353
EXPNO	1
PROCNO	1
Date_	20120531
Time	18.05
INSTRUM	Spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	298
DS	4
SWH	29761.904 Hz
FIDRES	0.454131 Hz
AQ	1.1010548 sec
RG	203
DW	16.800 usec
DE	6.50 usec
TE	298.0 K
D1	2.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	11.57 usec
PL1	0.00 dB
PL1W	83.39463043 W
SFO1	125.7703643 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.50 dB
PL12	17.40 dB
PL13	17.40 dB
PL2W	13.02359581 W
PL12W	0.42143536 W
PL13W	0.42143536 W
SFO2	500.1320005 MHz
SI	32768
SF	125.7577966 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

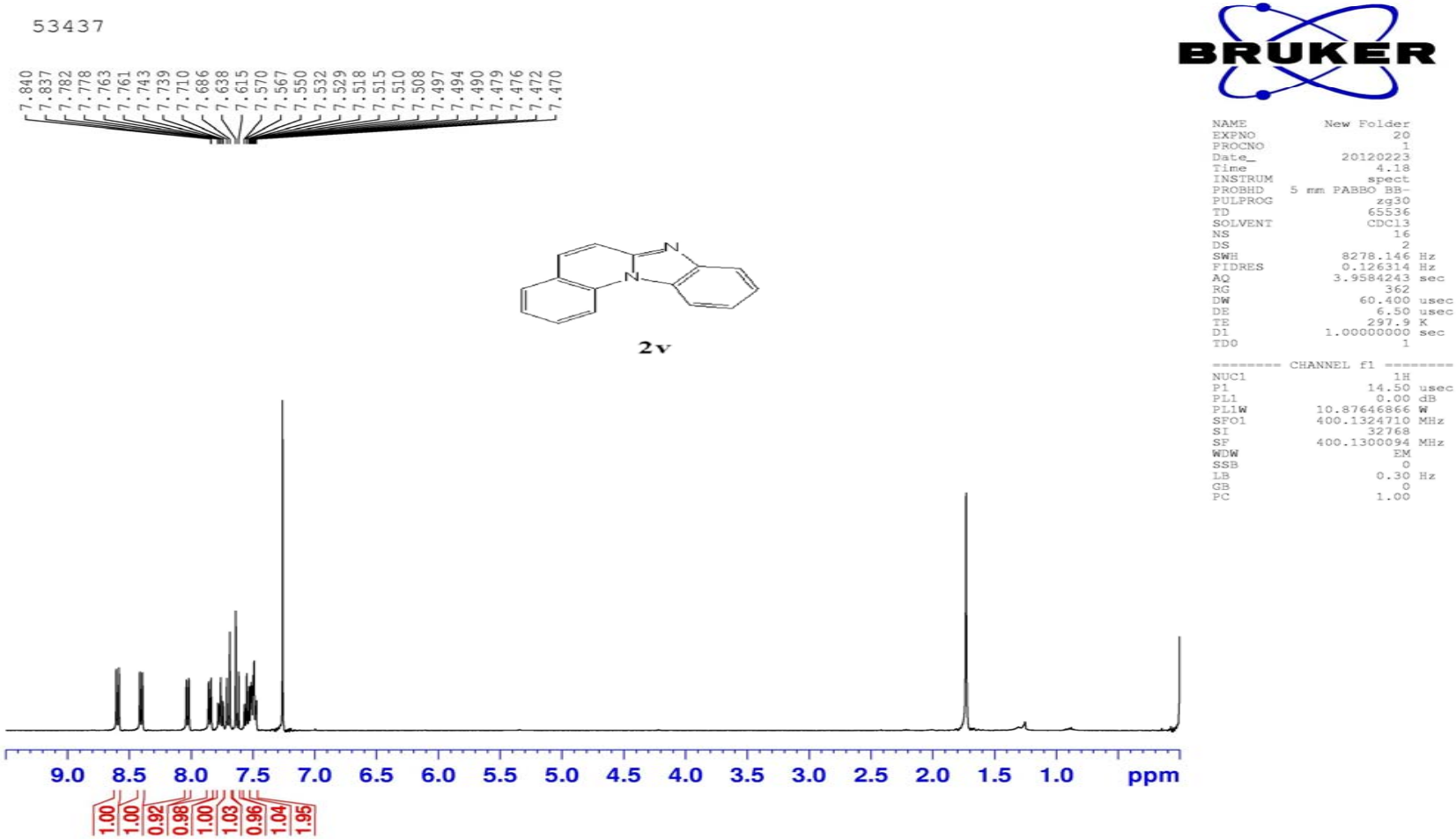


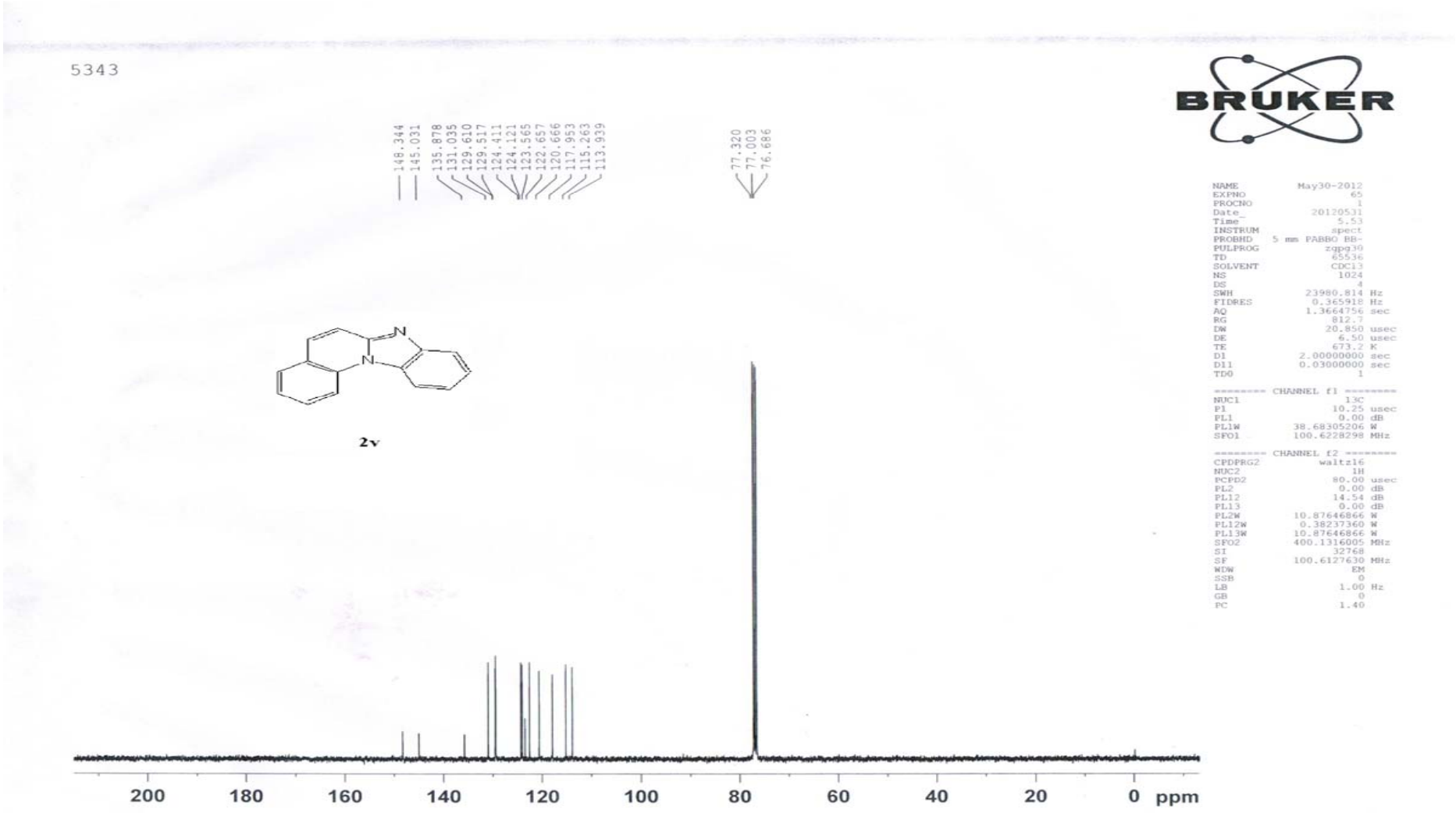
NAME	H ZI
EXPNO	60
PROCNO	1
Date_	20120217
Time	10.29
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	362
DW	60.400 usec
DE	6.50 usec
TE	296.9 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.00 dB
PL1W	10.87646866 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300028 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00

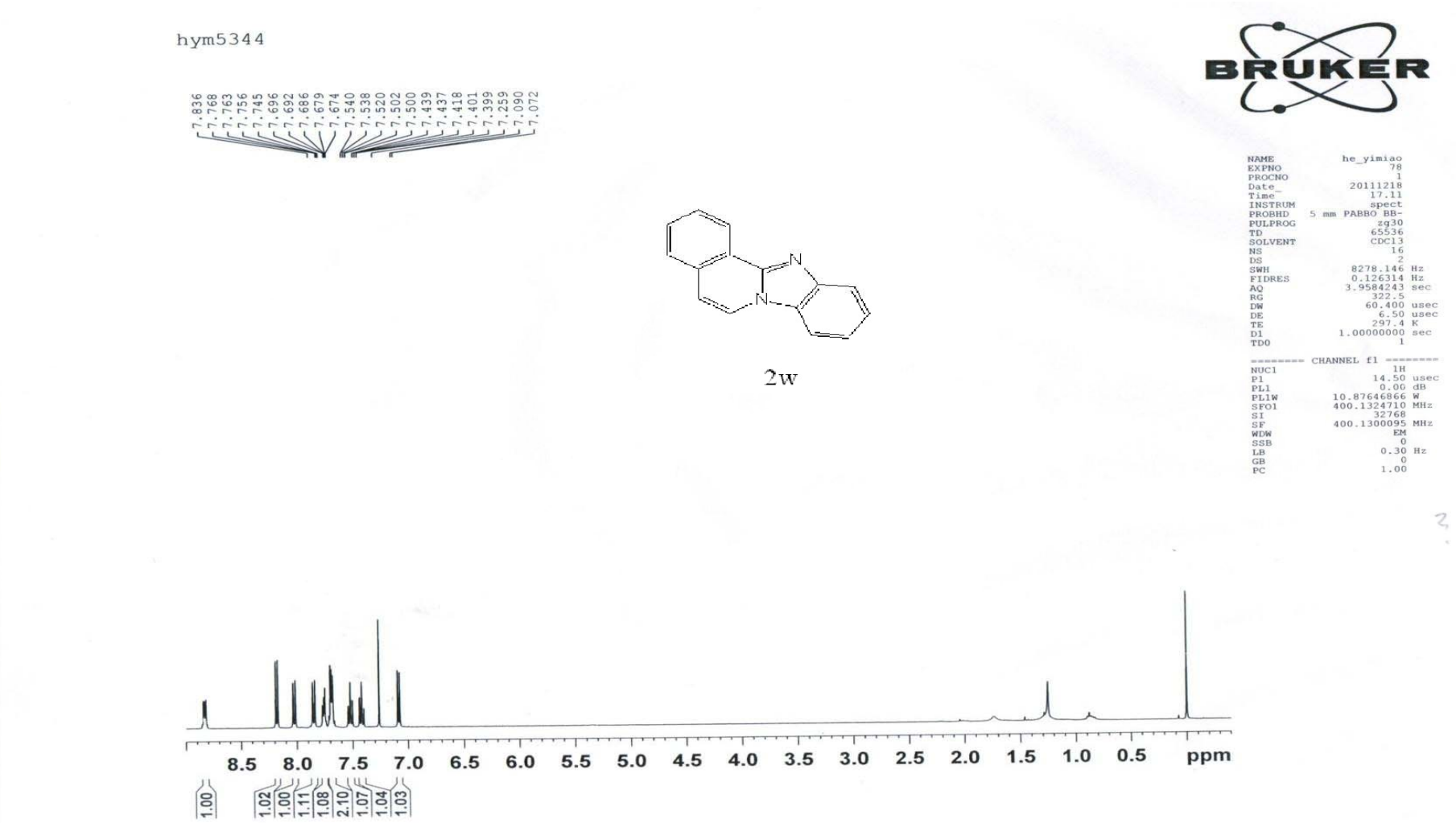

5347
163.792
144.516
143.991
133.626
130.916
128.216
125.748
121.099
119.229
118.991
111.822
108.874
60.778
40.127
39.918
39.709
39.501
39.292
39.083
38.875
14.010
CO2Et
N
N
2t
BRUKER
NAME May30-2012
EXPNO 68
PROCNO 1
Date_ 20120531
Time 8.49
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 759
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 673.2 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 100.6128363 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
0 ppm


hym5352
8.578
8.560
8.020
8.018
8.000
7.959
7.939
7.623
7.621
7.603
7.585
7.582
7.492
7.490
7.471
7.453
7.019
7.015
7.001
6.997
F3C
N
N
2u
NAME H PU
EXPNO 85
PROCNO 1
Date_ 20111228
Time 12.28
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 456.1
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 400.1300101 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.00
1.96
1.00
0.99
0.99
0.98

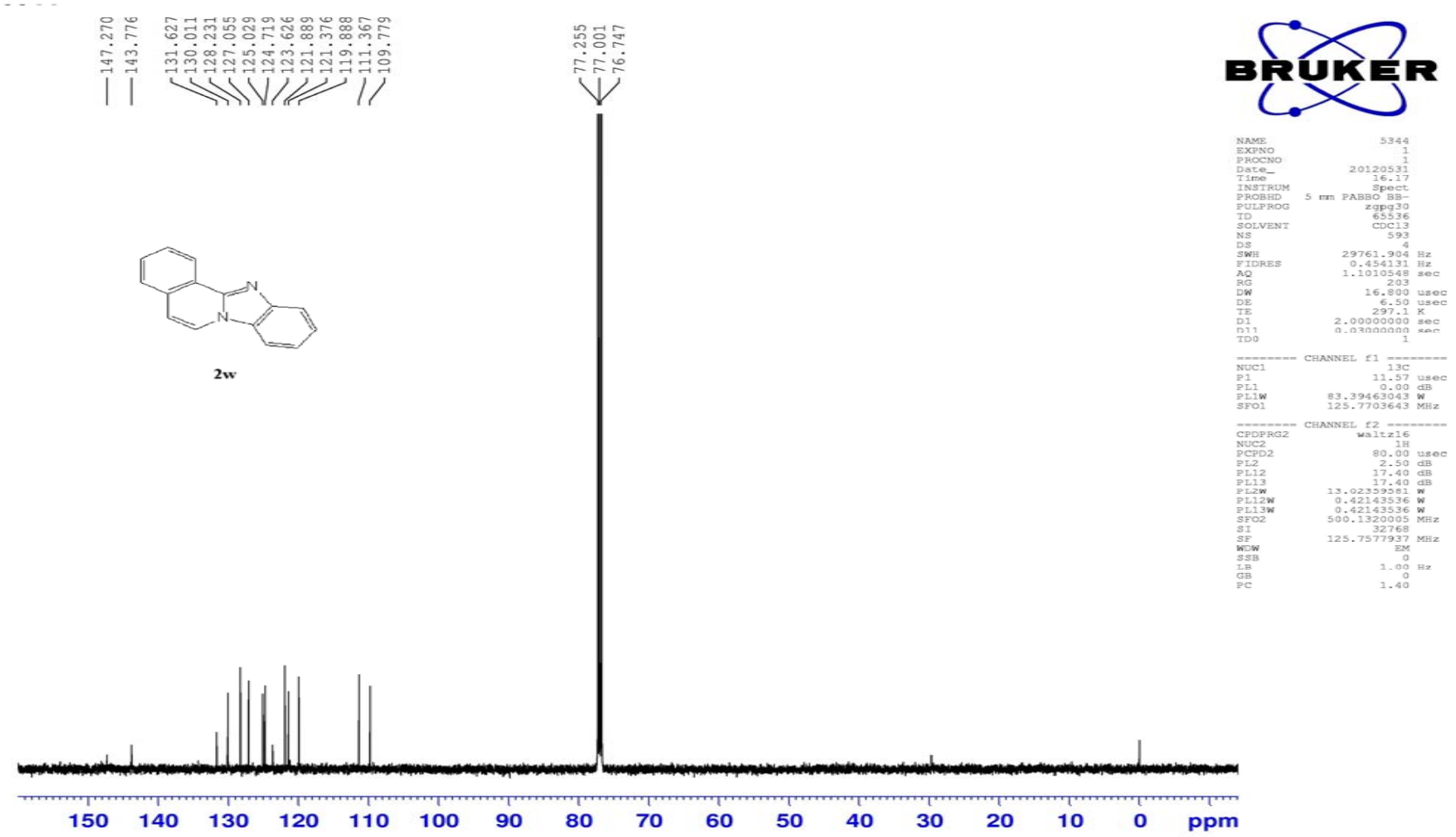

146.311
145.139
130.981
130.709
128.521
126.499
126.225
124.059
122.584
121.891
120.685
116.298
116.258
110.697
105.888
105.866
77.255
77.001
76.746
F3C
N
N
2u
BRUKER
NAME 5352
EXPNO 1
PROCNO 1
Date_ 20120531
Time 10.28
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 801
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 125.7577935 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

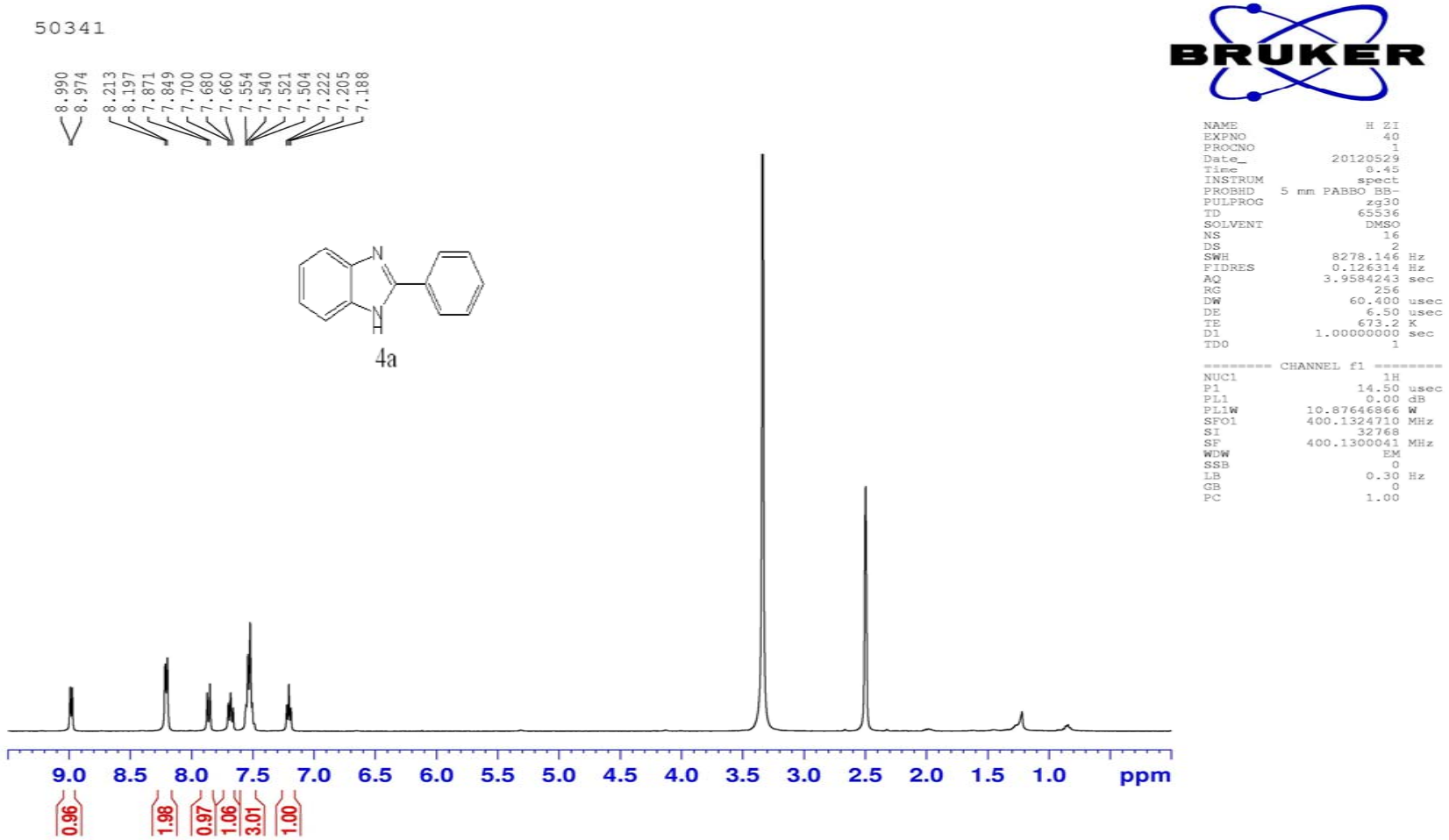

53437
7.840
7.837
7.782
7.778
7.763
7.761
7.743
7.739
7.710
7.686
7.638
7.615
7.570
7.567
7.550
7.532
7.529
7.518
7.515
7.510
7.508
7.497
7.494
7.490
7.479
7.476
7.472
7.470
BRUKER
NAME New Folder
EXPNO 20
PROCNO 1
Date_ 20120223
Time 4.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8278.146 Hz
FIDRES 0.126314 Hz
AQ 3.9584243 sec
RG 362
DW 60.400 usec
DE 6.50 usec
TE 297.9 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 400.1300094 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
N
N
2v
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
ppm
1.00
1.00
0.92
0.98
1.00
1.03
0.96
1.04
1.95


5343
148.344
145.031
135.878
131.035
129.610
129.517
124.411
124.121
123.565
122.657
120.666
117.953
115.263
113.939
77.320
77.003
76.686
BRUKER
NAME May30-2012
EXPNO 65
PROCNO 1
Date_ 20120531
Time_ 5.53
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 812.7
DW 20.850 usec
DE 6.50 usec
TE 673.2 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 100.6127630 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
N
N
2v
200
180
160
140
120
100
80
60
40
20
0 ppm


hym5344
7.836
7.768
7.763
7.756
7.745
7.696
7.692
7.686
7.679
7.674
7.540
7.538
7.520
7.502
7.500
7.439
7.437
7.418
7.401
7.399
7.259
7.090
7.072
N
N
NAME he_yimiao
EXPNO 78
PROCNO 1
Date_ 20111218
Time 17.11
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 297.4 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 400.1300095 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.00
1.02
1.00
1.11
1.08
2.10
1.07
1.04
1.03

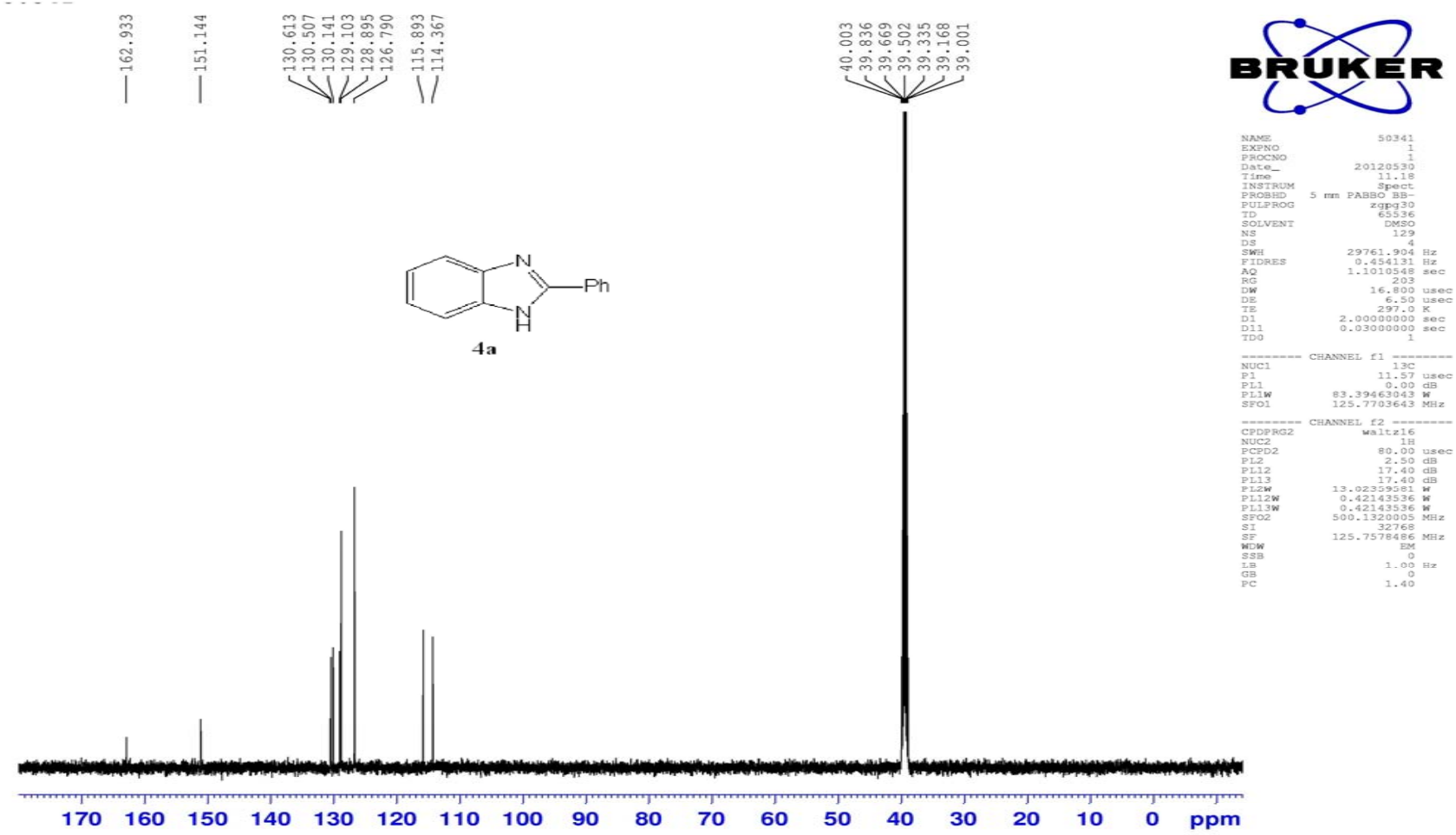
2w

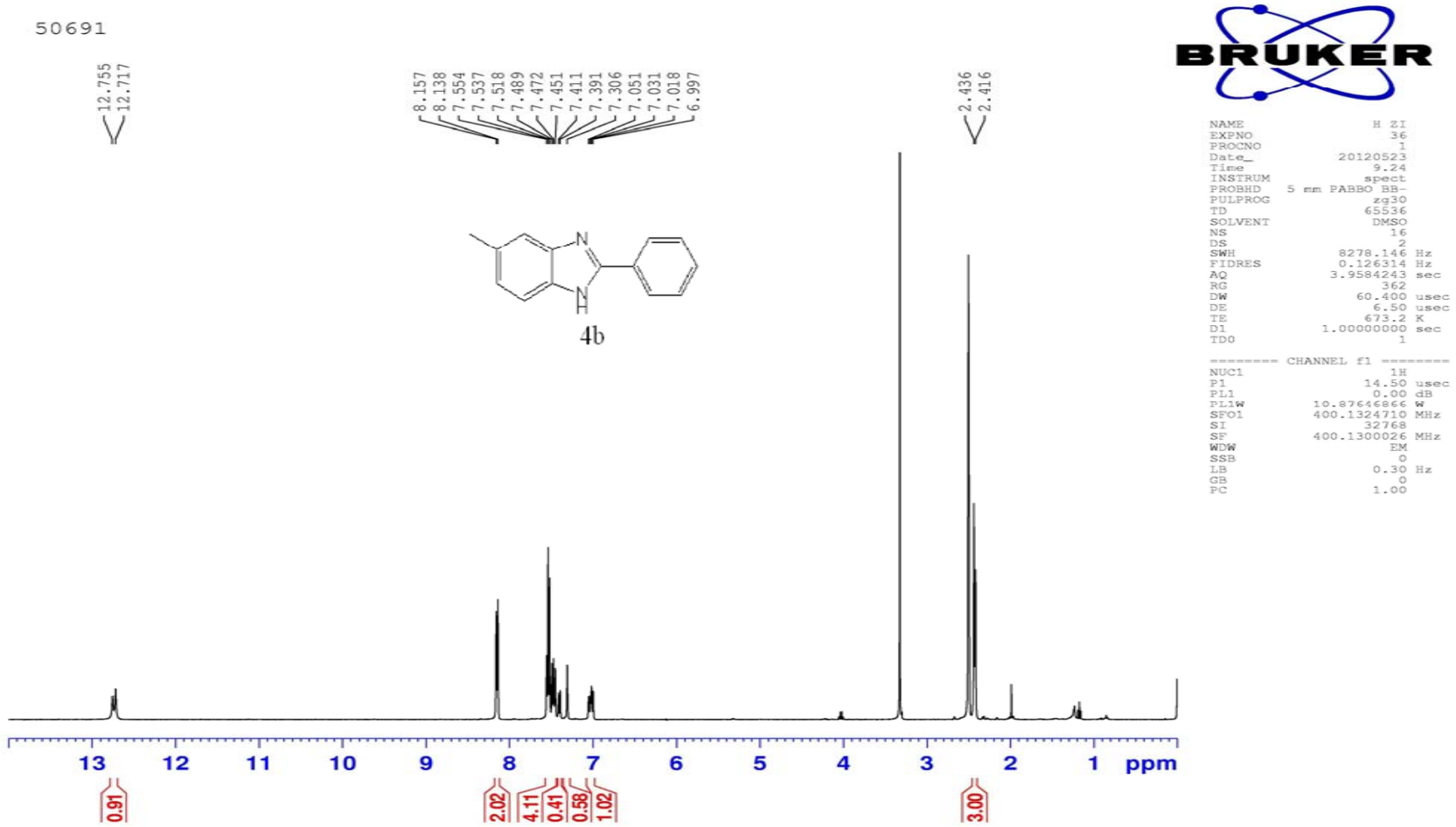

147.270
143.776
131.627
130.011
128.231
127.055
125.029
124.719
123.626
121.889
121.376
119.888
111.367
109.779
77.255
77.001
76.747
BRUKER
NAME 5344
EXPNO 1
PROCNO 1
Date_ 20120531
Time 16.17
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 592
DS 4
SWH 29761.904 Hz
FIDRES 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 13.02359551 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7577937 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
2w
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



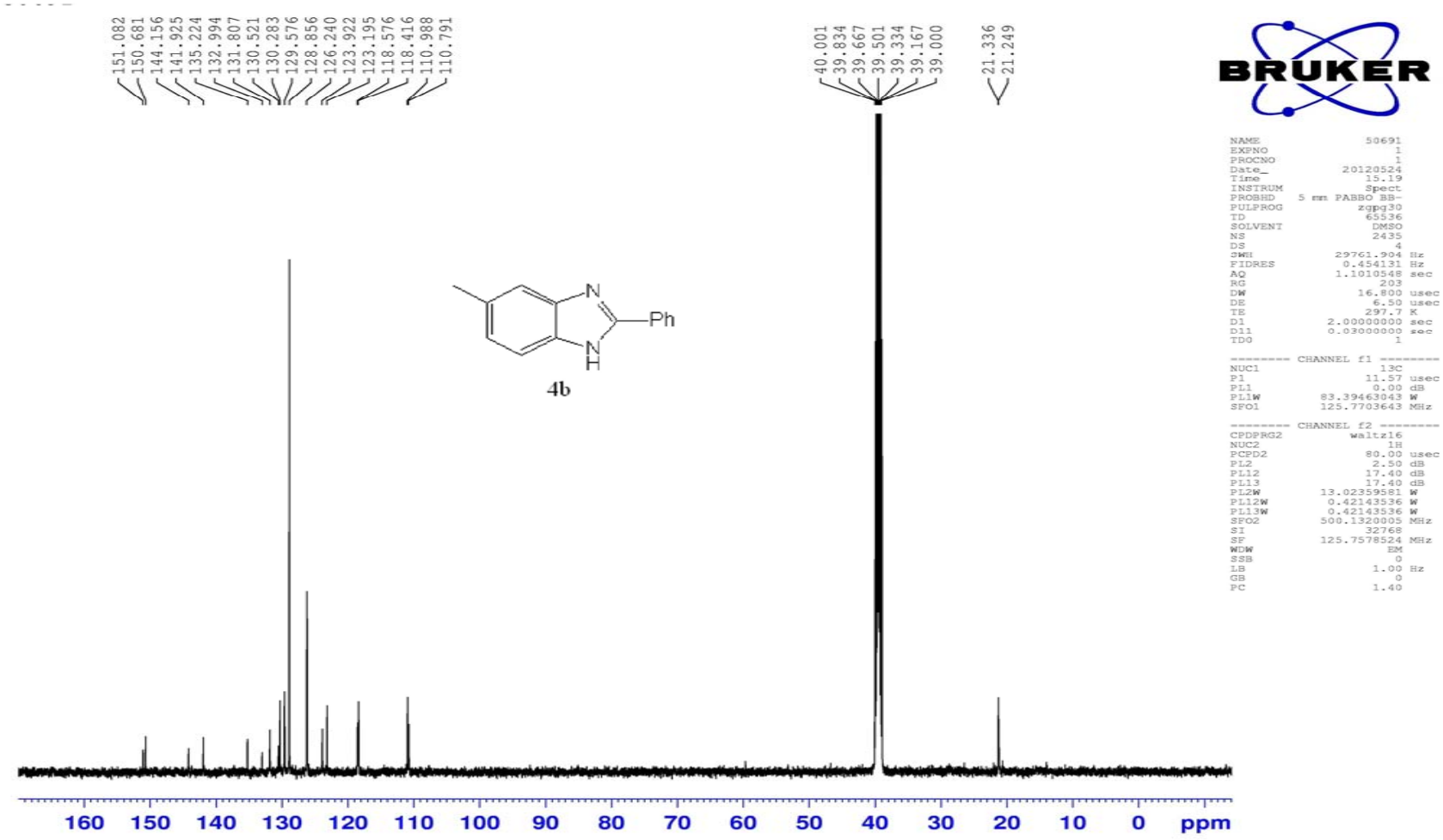
BRUKER

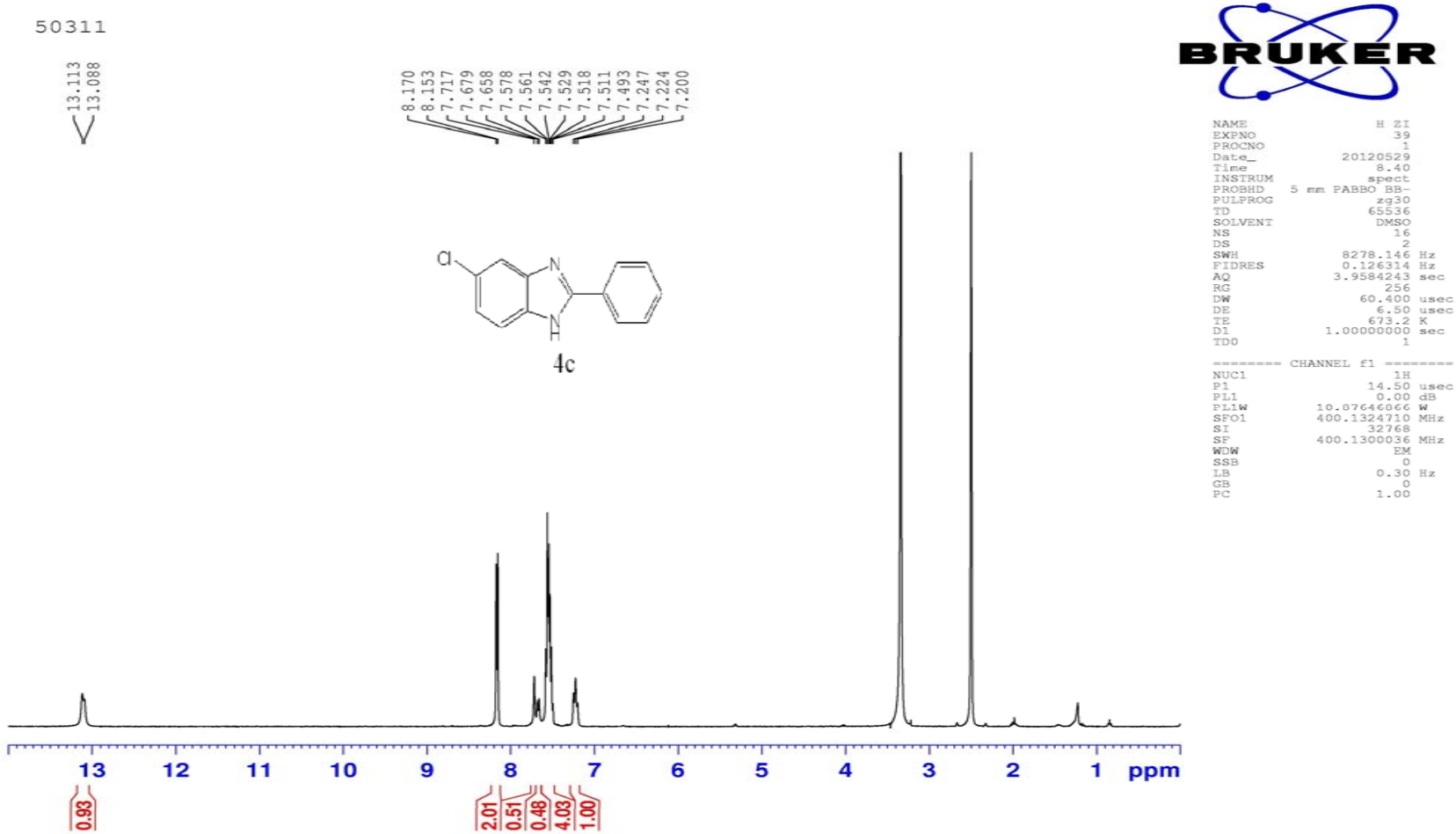
NAME	H ZI
EXPNO	40
PROCNO	1
Date_	20120529
Time	0.45
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	65536
SOLVENT	DMSO
NS	16
DS	2
SWH	8278.146 Hz
FIDRES	0.126314 Hz
AQ	3.9584243 sec
RG	256
DW	60.400 usec
DE	6.50 usec
TE	673.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	14.50 usec
PL1	0.00 dB
PL1W	10.87646866 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300041 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00


162.933
151.144
130.613
130.507
130.141
129.103
128.895
126.790
115.893
114.367
40.003
39.836
39.669
39.502
39.335
39.168
39.001
N
Ph
N
H
4a
BRUKER
NAME 50341
EXPNO 1
PROCNO 1
Date_ 20120530
Time 11.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 655536
SOLVENT DMSO
NS 129
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 297.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 11.57 usec
PL1 0.00 dB
PL1W 83.39463043 W
SFO1 125.7703643 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7578486 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



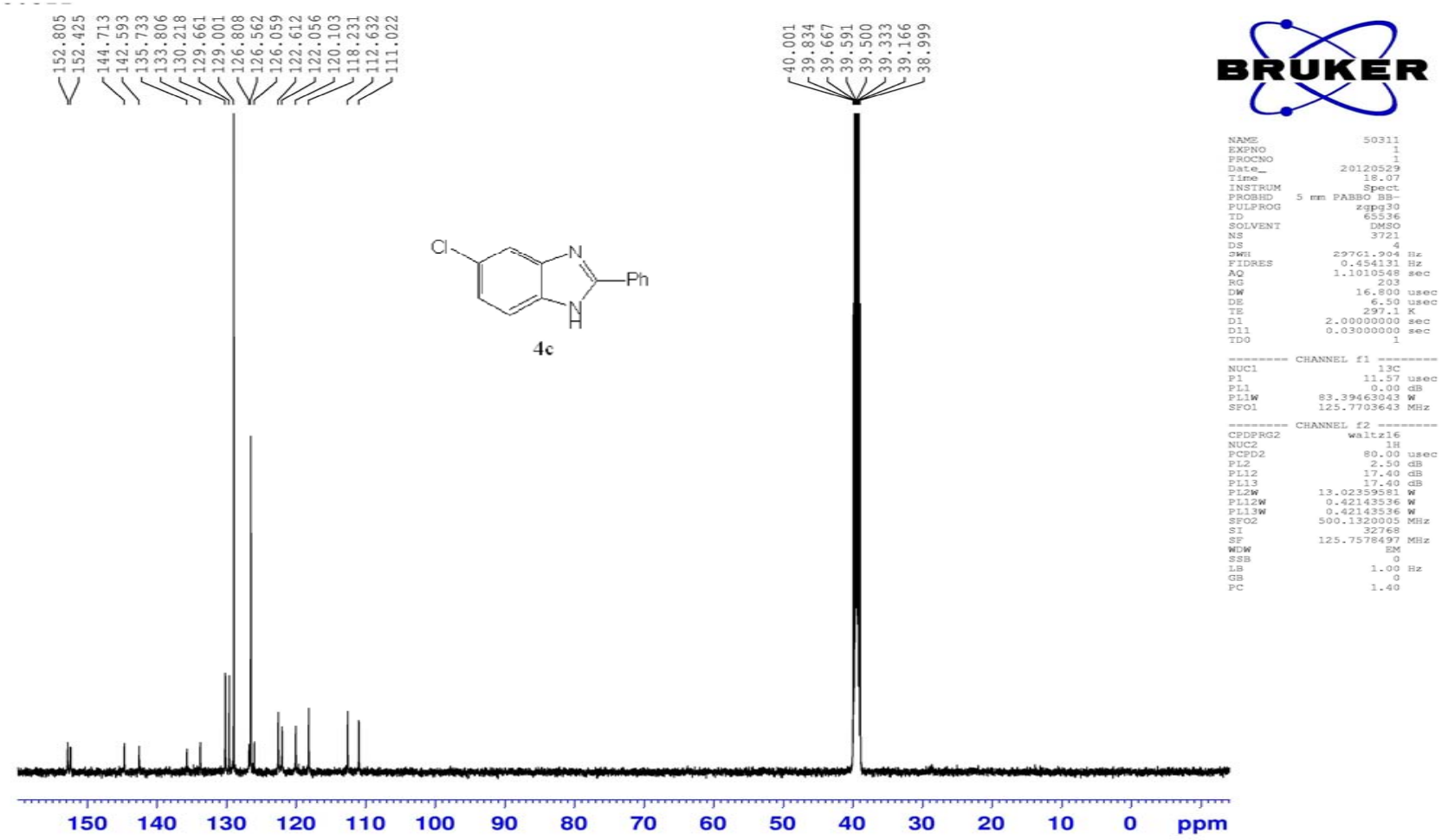
NAME	H ZI	
EXPNO	36	
PROCNO	1	
Date_	20120523	
Time	9.24	
INSTRUM	spect	
PROBHD	5 mm PABBO BB-	
PULPROG	zg30	
TD	65536	
SOLVENT	DMSO	
NS	16	
DS	2	
SWH	8278.146	Hz
FIDRES	0.126314	Hz
AQ	3.9584243	sec
RG	362	
DW	60.400	usec
DE	6.50	usec
TE	673.2	K
D1	1.00000000	sec
TD0	1	
======== CHANNEL f1 ========		
NUC1	1H	
P1	14.50	usec
PL1	0.00	dB
PL1W	10.87646866	W
SFO1	400.1324710	MHz
SI	32768	
SF	400.1300026	MHz
WDW	EM	
SSB	0	
LB	0.30	Hz
GB	0	
PC	1.00	


151.082
150.681
144.156
141.925
135.224
132.994
131.807
130.521
130.283
129.576
128.856
126.240
123.922
123.195
118.576
118.416
110.988
110.791
40.001
39.834
39.667
39.501
39.334
39.167
39.000
21.336
21.249
N
Ph
N
H
4b
BRUKER
NAME 50691
EXPNO 1
PROCNO 1
Date_ 20120524
Time 15.19
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2435
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 297.7 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 11.57 usec
PL1 0.00 dB
PL1W 83.39463043 W
SFO1 125.7703643 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7578524 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm



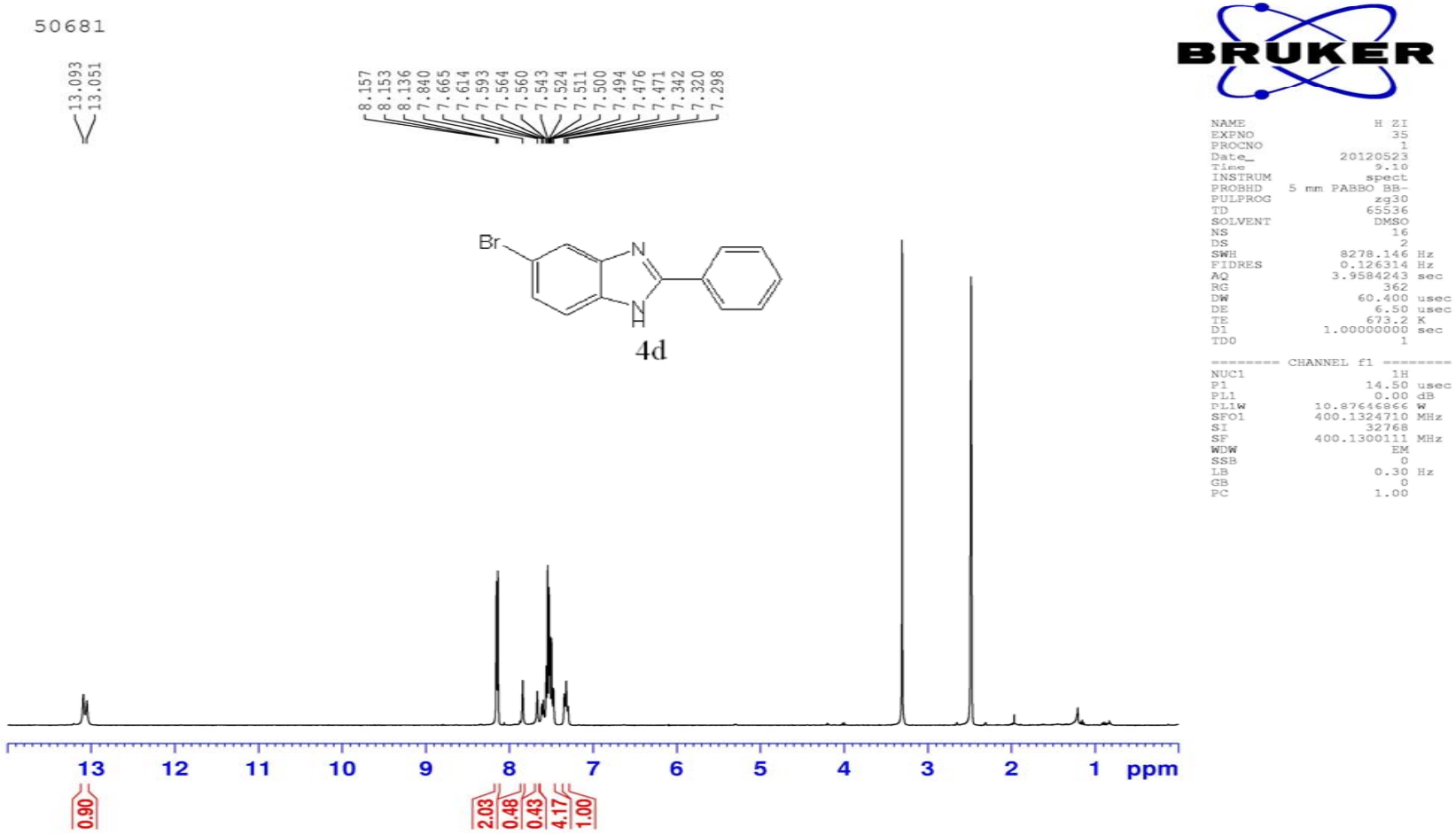
BRUKER

NAME	H ZI
EXPNO	39
PROCNO	1
Date_	20120529
Time	8.40
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	256
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	10.07646066 W
SFO1	400.1324710 MHz
SI	32768
SF	400.1300036 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00



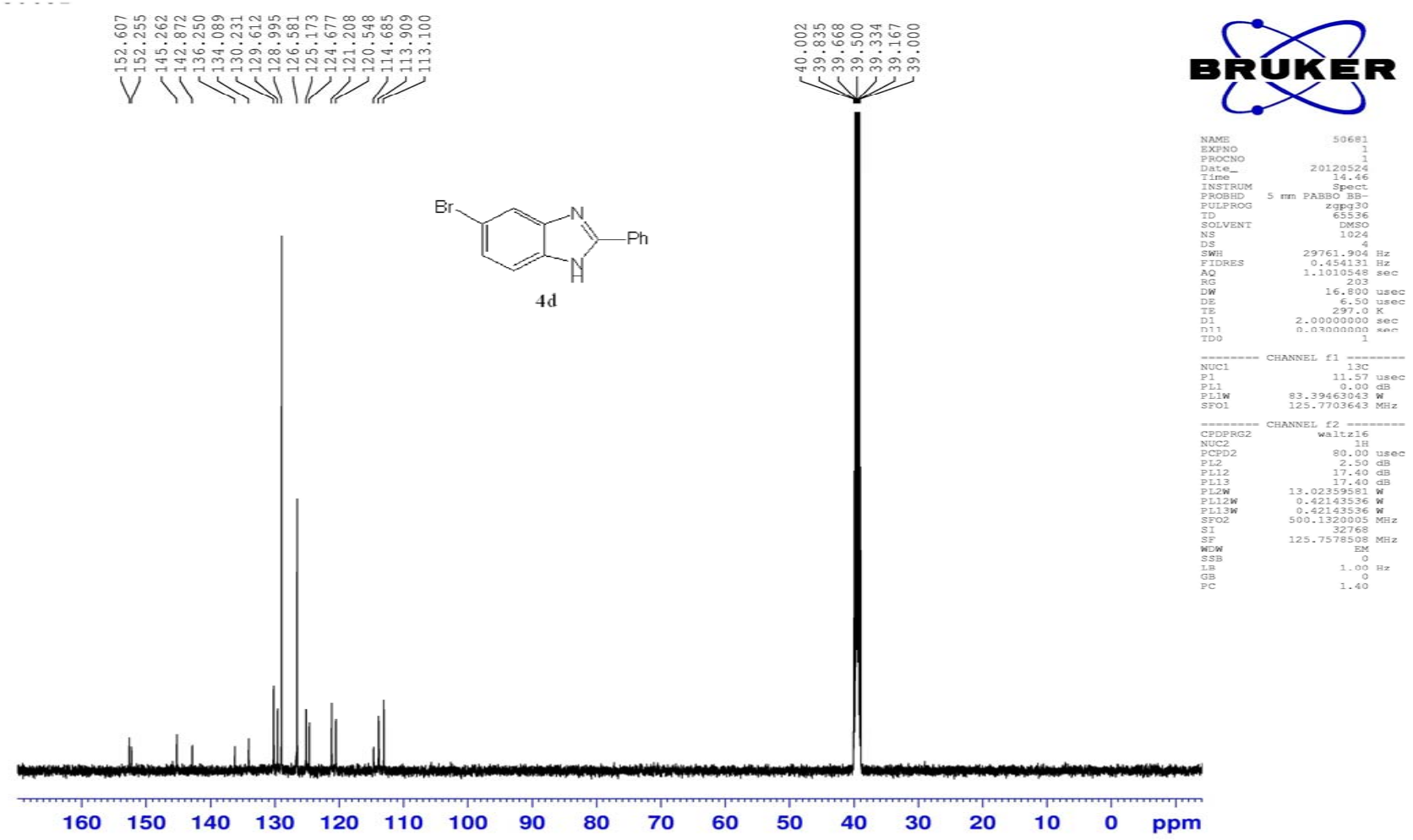
BRUKER

NAME	50311
EXPNO	1
PROCNO	1
Date_	20120529
Time	18.07
INSTRUM	Spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	DMSO
NS	3721
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	125.7578497 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40



BRUKER

NAME	H ZI
EXPNO	35
PROCNO	1
Date_	20120523
Time	9.10
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	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	400.1300111 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	1.00


152.607
152.255
145.262
142.872
136.250
134.089
130.231
129.612
128.995
126.581
125.173
124.677
121.208
120.548
114.685
113.909
113.100
40.002
39.835
39.668
39.500
39.334
39.167
39.000
Br
N
Ph
N
H
4d
BRUKER
NAME 50681
EXPNO 1
PROCNO 1
Date_ 20120524
Time 14.46
INSTRUM Spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010548 sec
RG 203
DW 16.800 usec
DE 6.50 usec
TE 297.0 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 11.57 usec
PL1 0.00 dB
PL1W 83.39463043 W
SFO1 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 2.50 dB
PL12 17.40 dB
PL13 17.40 dB
PL2W 13.02359581 W
PL12W 0.42143536 W
PL13W 0.42143536 W
SFO2 500.1320005 MHz
SI 32768
SF 125.7578508 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm