Unexpected Intermolecular Pd-Catalyzed Cross-Coupling Reaction Employing Heteroaromatic Carboxylic Acids as Coupling Partners.

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Supporting Information

I. General

All reactions were carried out using the Biotage Initiator 60 microwave apparatus and the corresponding vials. Anhydrous dimethylformamide was purchased from Aldrich and degassed by bubbling with Argon once for 30 minutes before being used. 4-methyl-1,3-oxazole-5-carboxylic acid and 2-bromo-5-methylthiophene were purchased from Maybridge, 3-methyl-2-furan carboxylic acid was obtained from Alfa Aesar, 1,3-thiazole-5-carboxylic acid was obtained from Combi-Blocks and 3-methyl-2-benzofuran carboxylic acid was purchased from Avocado. 3-methyl-2-thiophene carboxylic acid, 1-methyl-2-pyrrole carboxylic acid, 4-methyl-1,3-thiazole-5-carboxylic acid, 2-furan carboxylic acid, 4-methyl-2-thiophene carboxylic acid, 3-methylthiophene, phenyl bromide, 4-nitro bromobenzene, 3-bromopyridine and 4-bromoanisole were bought from Aldrich co. Every chemicals were used as received from the specified supplier. Cesium carbonate, tetra-*n*-butylammonium chloride hydrate and tetra-*n*-butylammonium bromide were obtained from Aldrich co. and used as received. Potassium acetate was obtained from American Chemicals Ltd and used as received. Palladium (0) [bis(tri-*tert*-butylphosphine)] was purchased from Strem Chemicals, stored under inert gas and used as is.

Unless otherwise noted, the compounds were purified using a CombiFlash Companion (Isco) with corresponding 12g normal phase columns. When necessary, the products were purified using Preparative TLC (Layer thickness: 1.00 μ m, Fluorescent indicator, 20 x 20 cm, purchased from Aldrich co.). HPLC analyses were performed on a Waters 2695 system (YMC CombiScreen ODS-AQ column (50 x 4.6 mm ID, S-5 μ m)) using a water/acetonitrile gradient (both containing 0.06% TFA). When specified, compounds were purified with a Waters Semi-Preparative HPLC system (SunFire Prep C18 ODB 5 μ m, 19 x 50 mm column), using a water/acetonitrile gradient (both containing 0.06% TFA). ^1H and ^{13}C NMR data were collected using a 400 MHz Bruker apparatus. HRMS data was obtained using a ZAB-1F VG-micromass apparatus in electronic impact (EI) mode.

II. Experimental procedures

A) General procedure for cross-coupling reaction between heteroaromatic carboxylic acid and phenyl bromide.

Unless otherwise noted each reaction was performed using the following procedure. In a microwave vial (2 to 5 ml), opened to air, were added phenyl bromide (42 μ l, 0.40 mmol, 1 eq), heterocyclic carboxylic acid (0.80 mmol, 2 eq), tetra-*n*-butylammonium chloride hydrate (0.40 mmol, 1 eq), cesium carbonate (0.60 mmol, 1.5 eq) and palladium (0) [bis(tri-*tert*-butylphosphine)] (0.020 mmol, 0.05 eq). Anhydrous DMF (4 ml) was then added after what the mixture was stirred for 30 seconds and submitted to the microwave conditions (170 $^{\circ}$ C, 8 min, high absorption level).

The reaction mixture was then diluted with ethyl acetate (50 ml), the organic layer was washed with brine (3x), saturated NaHCO₃ solution (2x), water (1x) and back with brine (1x). The organic layer was finally dried over MgSO₄, filtered and solvent evaporation over silica afforded a solid residue that was purified using the CombiFlash Companion.

4-Methyl-5-phenyloxazole (Table 1, entry 1). Starting from 4-methyl-1,3-oxazole-5-carboxylic acid, the compound was prepared (except that $t^0=190^{\circ}\text{C}$, no additive was used and water (72 μL , 4.00 mmol, 10 eq) was added) and purified according to the general procedure ($R_f=0.32$ in 20:80 EtOAc/hexanes) to yield the title compound as a white solid (34 mg, 0.214 mmol, 54%).

HPLC (220 nm): 100% (3.82 min)

¹H NMR (400 MHz, DMSO-*d*₆) δ ppm 8.34 (s, 1H), 7.62 (d, $J=7.4$ Hz, 2H), 7.50 (t, $J=7.4$ Hz, 2H), 7.38 (t, $J=7.4$ Hz, 1H), 2.37 (s, 3H).

¹³C NMR (101 MHz, DMSO-*d*₆) δ ppm 150.5, 144.7, 131.2, 129.3, 128.6, 128.1, 125.3, 13.2.

HRMS (EI) calcd for C₁₀H₉NO (M^+) 159.0684 found 159.0689 (+3.1 ppm).

2-phenyl-1-methylpyrrole (3b: Table 2, entry 2). Starting from 1-methyl-2-pyrrole carboxylic acid, the compound was prepared and purified according to the general procedure ($R_f=0.38$ in 5:95 EtOAc/hexanes) to yield the title compound as a white solid (55 mg, 0.350 mmol, 88%).

HPLC (220 nm): 100% (4.75 min)

¹H NMR (400 MHz, DMSO-*d*₆) δ ppm 7.48-7.35 (m, 4H), 7.33-7.24 (m, 1H), 6.83 (s, 1H), 6.15 (m, 1H), 6.06 (s, 1H), 3.64 (s, 3H).

¹³C NMR (101 MHz, DMSO-*d*₆) δ ppm 133.4, 133.0, 128.5, 127.9, 126.5, 124.3, 108.4, 107.4, 34.9.

HRMS (EI) calcd for $C_{11}H_{11}N$ (M^+) 157.0891 found 157.0895 (+2.5 ppm).

2,3-diphenyl-1-methylpyrrole (5) The compound was purified using a Semi-Preparative HPLC from the 2-phenyl-1-methylpyrrole experiment to yield the title compound as a clear oil (<5 mg, isolated only for structure confirmation).

HPLC (220 nm): 100% (6.26 min)

1H NMR (400 MHz, $DMSO-d_6$) δ ppm 7.46-7.33 (m, 3H), 7.30-7.24 (m, 2H), 7.18-7.10 (m, 2H), 7.09-6.99 (m, 3H), 6.89 (s, 1H), 6.32 (s, 1H), 3.45 (s, 3H).

COSY, HMBC, HMQC and ROESY experiments were performed in order to support the proposed structure.

3-Methyl-2-phenylfuran (6b: Table 2, entry 3). Starting from 3-methyl-2-furan carboxylic acid, the compound was prepared and purified according to the general procedure (R_f =0.57 in 5:95 EtOAc/hexanes) to yield the title compound as a yellow oil (54 mg, 0.343 mmol, 86%).

HPLC (220 nm): 99.6% (5.45 min)

1H NMR (400 MHz, $DMSO-d_6$) δ ppm 7.64 (d, J =1.5 Hz, 1H), 7.60 (d, J =7.5 Hz, 2H), 7.45 (t, J =7.5 Hz, 2H), 7.29 (t, J =7.5 Hz, 1H), 6.47 (d, J =1.5 Hz, 1 H), 2.24 (s, 3 H).

^{13}C NMR (101 MHz, $DMSO-d_6$) δ ppm 147.6, 141.5, 131.2, 128.8, 126.8, 124.8, 116.3, 115.5, 11.6.

HRMS (EI) calcd for $C_{11}H_{10}O$ (M^+) 157.0732 found 158.0734 (+1.3 ppm).

2-phenylfuran (7b: Table 2, entry 4). Starting from 2-furan carboxylic acid, the compound was prepared and purified according to the general procedure (R_f =0.71 in 5:95 EtOAc/hexanes) to yield the title compound as an orange oil (23 mg, 0.262 mmol, 41%).

HPLC (220 nm): 94.8% (4.85 min)

¹H NMR (400 MHz, DMSO-*d*₆) δ ppm 7.75 (s, 1H), 7.70 (d, *J*=7.7 Hz, 2H), 7.42 (t, *J*=7.7 Hz, 2H), 7.29 (t, *J*=7.7 Hz, 1H), 6.95 (s, 1H), 6.60 (s, 1H).

¹³C NMR (101 MHz, DMSO-*d*₆) δ ppm 153.0, 142.9, 130.3, 128.9, 127.4, 126.7, 123.4, 112.1, 105.8.

HRMS (EI) calcd for C₁₀H₈O (M⁺) 144.0575 found 144.0577 (+1.4 ppm).

2,3-diphenylfuran. The compound was purified using a Semi-Preparative HPLC from the 2-phenylfuran experiment to yield the title compound as a clear oil (<5 mg, isolated only for structure confirmation).

HPLC (220 nm): 99.6% (6.48 min)

¹H NMR (400 MHz, DMSO-*d*₆) δ ppm 7.83 (s, 1H), 7.51-7.19 (m, 10H), 6.75 (s, 1H).

COSY, HMBC, HMQC and ROESY experiments were performed in order to support the proposed structure.

2,5-diphenylfuran. The compound was purified using a Semi-Preparative HPLC from the 2-phenylfuran experiment to yield the title compound as a clear oil (<5 mg, isolated only for structure confirmation).

HPLC (220 nm): 100% (6.77 min)

¹H NMR (400 MHz, DMSO-*d*₆) δ ppm 7.82 (d, *J*=7.6 Hz, 4H), 7.46 (t, *J*=7.6 Hz, 4H), 7.31 (t, *J*=7.6 Hz, 2H), 7.09 (s, 2H).

COSY, HMBC, HMQC and ROESY experiments were performed in order to support the proposed structure.

4-methyl-5-phenyl-1,3-thiazole (8b: Table 2, entry 5). Starting from 4-methyl-1,3-thiazole-5-carboxylic acid, the compound was prepared according to the general procedure and purified using a preparative TLC ($R_f=0.34$ in 20:80 EtOAc/hexanes) to yield the title compound as a white solid (52 mg, 0.296 mmol, 74%).

HPLC (220 nm): 100% (3.21 min)

^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ ppm 9.01 (s, 1H), 7.54-7.44 (m, 4H), 7.43-7.29 (m, 1H), 2.46 (s, 3H).

^{13}C NMR (101 MHz, $\text{DMSO}-d_6$) δ ppm 151.7, 147.9, 131.5, 131.2, 129.0, 128.0, 16.0.

HRMS (EI) calcd for $\text{C}_{10}\text{H}_9\text{NS}$ (M^+) 175.0456 found 175.0452 (-2.3 ppm).

5-phenyl-1,3-thiazole (9b: Table 2, entry 6). Starting from 1,3-thiazole-5-carboxylic acid, the compound was prepared according to the general procedure (except that $t^0=200^\circ\text{C}$) and purified using a preparative TLC ($R_f=0.51$ in 30:70 EtOAc/hexanes) to yield the title compound as a white solid (15 mg, 0.094 mmol, 23%).

HPLC (220 nm): 100% (3.30 min)

^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ ppm 9.09 (s, 1H), 8.32 (s, 1H), 7.69 (d, $J=7.4$ Hz, 2H), 7.46 (t, $J=7.4$ Hz, 2H), 7.37 (t, $J=7.4$ Hz, 1H).

^{13}C NMR (101 MHz, $\text{DMSO}-d_6$) δ ppm 153.6, 139.4, 138.6, 130.8, 129.3, 128.4, 126.6.

HRMS (EI) calcd for $\text{C}_9\text{H}_7\text{NS}$ (M^+) 161.0299 found 161.0302 (+1.9 ppm).

2-phenyl-3-methylthiophene (10b: Table 2, entry 7). Starting from 3-methyl-2-thiophene carboxylic acid, the compound was prepared according to the general procedure and purified using

a preparative TLC ($R_f=0.59$ in 5:95 EtOAc/hexanes) to yield the title compound as a clear oil (44 mg, 0.251 mmol, 63%).

HPLC (220 nm): 96.3% (5.84 min)

^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ ppm 7.46-7.43 (m, 5H), 7.41-7.29 (m, 1H), 7.00 (d, $J=5.1$ Hz, 1H), 2.28 (s, 3H).

^{13}C NMR (101 MHz, $\text{DMSO}-d_6$) δ ppm 136.8, 134.1, 133.0, 131.5, 128.8, 128.5, 127.3, 124.2, 14.7.

HRMS (EI) calcd for $\text{C}_{11}\text{H}_{10}\text{S}$ (M^+) 174.0503 found 174.0500 (-1.7 ppm).

2-phenyl-3-methylbenzofuran (11b: Table 2, entry 8). Starting from 3-methyl-2-benzofuran carboxylic acid, the compound was prepared and purified according to the general procedure ($R_f=0.65$ in 5:95 EtOAc/hexanes) to yield the title compound as a white solid (72 mg, 0.346 mmol, 86%).

HPLC (220 nm): 99.1% (6.65 min)

^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ ppm 7.82 (d, $J=8.2$ Hz, 2H), 7.67 (d, $J=7.5$ Hz, 1H), 7.61-7.50 (m, 3H), 7.43 (t, $J=7.5$ Hz, 1H), 7.37-7.25 (m, 2H), 2.47 (s, 3H).

^{13}C NMR (101 MHz, $\text{DMSO}-d_6$) δ ppm 153.1, 149.9, 130.5, 128.9, 128.2, 126.3, 124.7, 122.7, 119.7, 111.3, 110.9, 9.1.

HRMS (EI) calcd for $\text{C}_{15}\text{H}_{12}\text{O}$ (M^+) 208.0888 found 208.0891 (+1.4 ppm).

B) Regioselectivity experiments (scheme 3)

4-methyl-2-phenylthiophene (13b). Starting from 4-methyl-2-thiophene carboxylic acid, the compound was prepared according to the general procedure and purified using a preparative TLC

(R_f =0.71 in 5:95 EtOAc/hexanes) to yield the title compound as a pale yellow oil (13 mg, 0.074 mmol, 19%).

HPLC (220 nm): 78.3% (5.93 min) [biphenyl: 5.49 min (12.8%), unknown: 5.68 min (9.0%), no trace of **10b** (see data for entry 7)].

^1H NMR (400 MHz, DMSO- d_6) δ ppm 7.61 (d, J =7.5 Hz, 2H), 7.40 (t, J =7.5 Hz, 2H), 7.34 (s, 1H), 7.29 (t, J =7.5 Hz, 1H), 7.11 (s, 1H), 2.24 (s, 3H).

2-phenyl-3-methylthiophene (10b): see Table 2, entry 7

C-H activation using 3-methylthiophene (10b/13b mixture). Starting from 3-methylthiophene, the compound was prepared according to the general procedure (except that we used tetra-*n*-butylammonium bromide as the additive and potassium acetate as the base: very little conversion was observed with other reagents). It was purified using a preparative TLC (R_f =0.71 in 5:95 EtOAc/hexanes) to yield the mixture of **A/B** as a clear oil (27 mg, 0.156 mmol, 39%).

HPLC (220 nm): 73.2% (5.79 min) [**10b**, 2-phenyl-3-methylthiophene] and 21.9% (5.93 min) [**13b**, 4-methyl-2-phenylthiophene].

2-(4-methoxyphenyl)-1-methylpyrrole (Table 3, entry 1). Starting from 1-methyl-2-pyrrole carboxylic acid and 4-bromoanisole, the compound was prepared and purified according to the general procedure (R_f =0.37 in 10:90 EtOAc/hexanes) to yield the title compound as a clear oil (58 mg, 0.308 mmol, 77%).

HPLC (220 nm): 99.4% (4.64 min)

¹H NMR (400 MHz, DMSO-*d*₆) δ ppm 7.34 (d, *J*=8.7 Hz, 2H), 6.97 (d, *J*=8.7 Hz, 2H), 6.78 (s, 1H), 6.04 (m, 2H), 3.78 (s, 3H), 3.59 (s, 3H).

¹³C NMR (101 MHz, DMSO-*d*₆) δ ppm 158.1, 133.3, 129.4, 125.5, 123.4, 113.9, 107.6, 107.1, 55.1, 34.7.

HRMS (EI) calcd for C₁₂H₁₃NO (M⁺) 187.0997 found 187.1001 (+2.1 ppm).

2-(4-nitrophenyl)-1-methylpyrrole (Table 3, entry 2). Starting from 1-methyl-2-pyrrole carboxylic acid and 4-bromo nitrobenzene, the compound was prepared and purified according to the general procedure (R_f=0.30 in 10:90 EtOAc/hexanes) to yield the title compound as a yellow solid (54 mg, 0.267 mmol, 66%).

HPLC (220 nm): 100% (6.58 min)

¹H NMR (400 MHz, DMSO-*d*₆) δ ppm 8.24 (d, *J*=8.5 Hz, 2H), 7.74 (d, *J*=8.5 Hz, 2H), 7.01 (m, 1H), 6.48 (m, 1H), 6.15 (m, 1H), 3.32 (s, 3H).

¹³C NMR (101 MHz, DMSO-*d*₆) δ ppm 145.1, 139.4, 131.3, 127.7, 127.4, 123.9, 111.6, 108.3, 35.6.

2-(2-(5-methylthiophene))-1-methylpyrrole (Table 3, entry 3). Starting from 1-methyl-2-pyrrole carboxylic acid and 2-bromo-5-methylthiophene, the compound was prepared and purified according to the general procedure (R_f=0.61 in 10:90 EtOAc/hexanes) to yield the title compound as a pale yellow oil (57 mg, 0.324 mmol, 78%).

HPLC (220 nm): 100% (7.03 min)

¹H NMR (400 MHz, DMSO-*d*₆) δ ppm 6.90 (m, 1H), 6.82 (m, 1H), 6.78 (m, 1H), 6.14 (m, 1H), 6.01 (m, 1H), 3.66 (s, 3H), 2.43 (s, 3H).

¹³C NMR (101 MHz, DMSO-*d*₆) δ ppm 137.9, 132.3, 126.5, 126.0, 124.3, 108.9, 107.4, 34.9, 14.8.

2-(3-pyridyl)-1-methylpyrrole (Table 3, entry 4). Starting from 1-methyl-2-pyrrole carboxylic acid and 3-bromopyridine, the compound was prepared and purified according to the general procedure (R_f=0.43 in 70:30 EtOAc/hexanes) to yield the title compound as a clear oil (54 mg, 0.338 mmol, 85%).

HPLC (220 nm): Too polar: solvent front

¹H NMR (400 MHz, DMSO-*d*₆) δ ppm 8.67 (s, 1H), 8.49 (m, 1H), 7.87 (m, 1H), 7.43 (m, 1H), 6.91 (s, 1H), 6.28 (s, 1H), 6.10 (m, 1H), 3.67 (s, 3H).

¹³C NMR (101 MHz, DMSO-*d*₆) δ ppm 148.4, 147.3, 134.9, 130.0, 128.9, 125.4, 123.5, 109.5, 107.7, 34.9.

HRMS (EI) calcd for C₁₀H₁₀N₂ (M⁺) 158.0844 found 158.0847 (+1.9 ppm).

2-phenyl-1-methylpyrrole (Table 3, entry 5): Thermal conditions. Starting from 1-methyl-2-pyrrole carboxylic acid and bromobenzene, the compound was prepared (except that an oil bath was used, t⁰=140⁰C for 1 hr) and purified according to the general procedure R_f=0.38 in 5:95 EtOAc/hexanes) to yield the title compound as a white solid (57%). *Note:* the yield is an average of 3 experiments. Yields of 43%, 55% and 72% were obtained, unoptimized conditions.

HPLC (220 nm): always obtained purities 95+%.

For complete characterization, see entry 2 of Table 2.

Acquisition Time (sec)	5.1120	Comment	1Dproton DMSO D ₆ mcbrochu 31	Date	02 Feb 2006 19:31:12
File Name	\\LAVFS01\nmrdata\Data\mcbrochu\nmr\MCB-4082-0040PA1_020001r			Frequency (MHz)	400.13
Nucleus	1H			Original Points Count	32768
Owner	chemistry			Receiver Gain	574.70
SW(cyclical) (Hz)	6410.26			Sweep Width (Hz)	6410.06
				Spectrum Offset (Hz)	2468.7878
				Solvent	DMSO-d6
				Pulse Sequence	zg60
				Number of Transients	16
				Points Count	32768
				Origin	spect

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[2.33 .. 2.40]	2.985	6.13649e+9	2.985
2	[7.34 .. 7.41]	0.952	1.95751e+9	0.952
3	[7.46 .. 7.54]	1.979	4.06857e+9	1.979
4	[7.58 .. 7.67]	1.945	3.99745e+9	1.945
5	[8.31 .. 8.36]	0.752	1.54585e+9	0.752

No.	Annotation	(ppm)
1	DMSO-d6	2.50

No.	(ppm)	(Hz)	Height
1	2.37	946.9	1.0000
2	2.50	998.8	0.2841
3	2.50	1000.3	0.3785
4	2.50	1002.1	0.2944
5	3.33	1331.9	0.2975
6	7.36	2944.3	0.0423
7	7.38	2951.7	0.1116
8	7.40	2959.1	0.0750
9	7.48	2993.7	0.1270
10	7.50	3001.8	0.2354
11	7.52	3009.2	0.1309
12	7.62	3047.4	0.2312
13	7.63	3054.6	0.1739
14	8.34	3337.7	0.2353

59

Acquisition Time (sec)	1.3566	Comment	1Dcarbon DMSO D: mcbrochu 69	Date	18 Feb 2006 08:57:36
File Name	\\LAVFS01\nmrdata\Data\mcbrochu\mcb-4082-0041PA1_010001r	Number of Transients	3720	Frequency (MHz)	100.61
Nucleus	13C	Points Count	32768	Original Points Count	32768
Owner	chemistry	Solvent	DMSO-d6	Receiver Gain	14596.50
SW(cyclical) (Hz)	24154.59	Pulse Sequence	zgpg60	Sweep Width (Hz)	24153.85

VerticalScaleFactor = 1

No.	Annotation	(ppm)
1	DMSO-d6	39.51

No.	(ppm)	(Hz)	Height
9	125.34	12610.8	0.2927
10	128.12	12890.2	0.1582
11	128.58	12936.6	0.0286
12	129.27	13005.9	0.3013
13	131.19	13199.0	0.0181
14	144.67	14556.1	0.0122
15	150.53	15145.1	0.1483

No.	(ppm)	(Hz)	Height
1	13.16	1324.5	0.0824
2	39.09	3933.2	0.1378
3	39.30	3954.6	0.4249
4	39.51	3975.2	0.8376
5	39.72	3996.6	1.0000
6	39.93	4017.2	0.8442
7	40.14	4038.6	0.4361
8	40.35	4059.2	0.1576

S10

Sample Name: MCB-4082-0041PA1
Sample Set Name: zMCB2006_Exp
System Name: MCSN_LC3_2695_2487
Run Time: 11.5 Minutes
Channel Name: 2487Channel 1

Result_Id: 13171
Date Acquired: Thursday, February 02, 2006 2:40:34 PM
Acq. Method Set: All_ODSAQ5to100_MB_Exp
Project Name: MCSN_LC3_1Q_2006
Channel Description: 220nm

Peak Results

	RT	Height	Area	% Area
1	3.820	676723	3218774	100.00

RÉSULTAT HAUTE RÉOLUTION**Date :** 8/3/2006**Produit :** 4082-0041pa1

2006B059

Formule : C₁₀H₉N₁O₁**Référence :** 1) m₁/e = 161.99042) m₂/e = 154.9920m₁/m₂ (calculé) = 1.045153**Inconnu :** m_i/e (théorique) = 159.0684m_i/m₂ = 1.026304 ±0.000003m_i/e (expérimental) = 159.0689 ±0.0005 +3.1 ppm**Responsable :**

Spectre de masse

c:\masspec\bordeleau\mcb40820041pa1.mas ionisation électronique:70eV

Échantillon : MCB-4082-0041PA1

7/3/2006

2006059

Acquisition Time (sec)	5.1120	Comment	1Dproton DMSO D: mcbrochu 41	Date	30 Jan 2006 20:58:40
File Name	\\LAVFS01\inmdata\Archive\2006\mcbrochu\NMR\MCB-4082-0036PA1_010001r	Origin	spect	Frequency (MHz)	400.13
Nucleus	¹ H	Number of Transients	16	Original Points Count	32768
Owner	chemistry	Points Count	32768	Receiver Gain	574.70
SW(cyclical) (Hz)	6410.26	Solvent	DMSO-d6	Spectrum Offset (Hz)	2468.7878
				Sweep Width (Hz)	6410.06

VerticalScaleFactor = 1

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[3.61 .. 3.69]	3.000	5.03899e+9	3.000
2	[6.01 .. 6.10]	0.922	1.54805e+9	0.922
3	[6.11 .. 6.17]	0.917	1.54074e+9	0.917
4	[6.80 .. 6.86]	0.896	1.50532e+9	0.896
5	[7.24 .. 7.33]	0.965	1.62145e+9	0.965
6	[7.35 .. 7.48]	3.949	6.63378e+9	3.949

No.	Annotation	(ppm)
1	DMSO-d6	2.50

No.	(ppm)	Height
9	6.15	2461.8
10	6.16	2463.6
11	6.83	2734.5
12	7.29	2916.7
13	7.41	2963.6
14	7.42	2970.3
15	7.44	2978.1

No.	(ppm)	Height
1	2.50	1000.3
2	3.33	1331.9
3	3.64	1456.9
4	6.05	2419.8
5	6.06	2423.1
6	6.06	2425.8
7	6.14	2458.5
8	6.15	2460.3

Acquisition Time (sec)	1.3566	Comment	1Carbon DMSO D: mcbrochu 66	Date	18 Feb 2006 03:31:12
File Name	\\LAVFS01\mmdata\Archive\2006\mcbrochu\NMR\MCB-4082-0036PA1_020001r	Origin	spec	Frequency (MHz)	100.61
Nucleus	¹³ C	Number of Transients	3720	Original Points Count	32768
Owner	chemistry	Points Count	32768	Receiver Gain	16384.00
SW(cyclical) (Hz)	24154.59	Solvent	DMSO-d6	Spectrum Offset (Hz)	9975.1582
				Sweep Width (Hz)	24153.85

VerticalScaleFactor = 1

No.	Annotation	(ppm)
1	DMSO-d6	39.51

No.	(ppm)	(Hz)	Height
1	34.89	3510.8	0.0670
2	38.89	3912.6	0.1340
3	39.09	3933.2	0.4170
4	39.30	3954.6	0.8425
5	39.51	3975.2	1.0000
6	39.72	3996.6	0.8516
7	39.93	4017.2	0.4471
8	40.14	4038.6	0.1626
9	107.36	10801.9	0.1377

Sample Name: MCB-4082-0036PA1
Sample Set Name: zMCB2006_Exp
System Name: MCSN_LC3_2695_2487
Run Time: 11.5 Minutes
Channel Name: 2487Channel 1

Result_Id: 13112
Date Acquired: Tuesday, January 31, 2006 11:10:10 AM
Acq. Method Set: All_ODSAQ5to100_MB_Exp
Project Name: MCSN_LC3_1Q_2006
Channel Description: 220nm

Peak Results

	RT	Height	Area	% Area
1	4.754	410137	2100815	100.00

RÉSULTAT HAUTE RÉOLUTION**Date :** 8/3/2006**Produit :** 4082-0036pa1

2006 B057

Formule : C₁₁H₁₁N₁**Référence :** 1) m₁/e = 161.99042) m₂/e = 154.9920m₁/m₂ (calculé) = 1.045153**Inconnu :** m_i/e (théorique) = 157.0891m_i/m₂ = 1.013533 ±0.000003m_i/e (expérimental) = 157.0895 ±0.0005 + 2.5 ppm**Responsable :**

815

Spectre de masse

Université de Sherbrooke

c:\masspec\bordeleau\mcb40820036pal.mas

Échantillon : MCB-4082-0036PA1

7/3/2006

20060057

ionisation électronique:70eV

Commentaires

François Bilodeau

DMSO

3872-103/10

16 Janvier 2006

[Signature]

Commentaires

François Bilodeau
DMSO
3872-103/11 cosy
16 Janvier 2006

M. Duchey

Commentaires

François Bilodeau
DMSO
3872-103/13 hmqc
18 janvier 2006

[Signature]

Commentaires

François Bilodeau
DMSO
3872-103/13 hmbc
16 Janvier 2006

[Signature]

Commentaires

François Bilodeau
DMSO
3872-103/14 roesy
16 Janvier 2006

M. Ruby

S24

Sample Name: xx-MCB-4082-0002@f9NMR
Sample Set Name: zMCB2006_Exp
System Name: MCSN_LC3_2695_2487
Run Time: 11.5 Minutes
Channel Name: 2487Channel 1

Result_Id: 18635
Date Acquired: Wednesday, January 11, 2006 9:47:14
Acq. Method Set: All_ODSAQ5to100_MB_Exp
Project Name: MCSN_2006\MCSN_LC3_1Q_2006
Channel Description: 220nm

Peak Results

	RT	Height	Area	% Area
1	6.260	378566	1725157	100.00

Acquisition Time (sec)	5.1120	Comment	1Dproton DMSO D: mcbrochu 39	Date	31 Jan 2006 20:30:56
File Name	\\LAVFS01\nmrdata\Archive\2006\mcbrochu\NMR\MCB-4082-0037PA1_010001r				
Nucleus	1H	Number of Transients	16	Origin	spect
Owner	chemistry	Points Count	32768	Pulse Sequence	zg60
SW(cyclical) (Hz)	6410.26	Solvent	DMSO-d6	Spectrum Offset (Hz)	2468.7878
				Receiver Gain	574.70
				Sweep Width (Hz)	6410.06

VerticalScaleFactor = 1

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[2.18 .. 2.30]	3.000	6.69122e+9	3.000
2	[6.41 .. 6.53]	0.873	1.94808e+9	0.873
3	[7.22 .. 7.37]	0.958	2.13761e+9	0.958
4	[7.39 .. 7.50]	1.975	4.40535e+9	1.975
5	[7.55 .. 7.62]	1.909	4.25718e+9	1.909
6	[7.62 .. 7.68]	0.861	1.91981e+9	0.861

No.	Annotation	(ppm)
1	DMSO-d6	2.50

No.	(ppm)	Height	(Hz)
9	7.43	2972.4	0.1312
10	7.45	2980.4	0.2421
11	7.47	2988.1	0.1400
12	7.59	3035.4	0.2295
13	7.60	3042.9	0.1848
14	7.64	3056.7	0.1644
15	7.64	3058.1	0.1669

Acquisition Time (sec)	1.3566	Comment	1Dcarbon DMSO D: mcbrochu 65			Date	18 Feb 2006 01:42:24
File Name	\\LAVFS01\mrdata\Archive\2006\mcbrochu\NMR\MCB-4082-0037PA1_020001r						
Nucleus	13C	Number of Transients	3720	Origin	spect	Original Points Count	32768
Owner	chemistry	Points Count	32768	Pulse Sequence	zgpg60	Receiver Gain	13004.00
SW(cyclical) (Hz)	24154.59	Solvent	DMSO-d6	Spectrum Offset (Hz)	9974.4219	Sweep Width (Hz)	24153.85

VerticalScaleFactor = 1

No.	Annotation	(ppm)
1	DMSO-d6	39.51

No.	(ppm)	(Hz)	Height
1	11.55	1162.3	0.1857
2	38.88	3911.8	0.1357
3	39.09	3933.2	0.4199
4	39.30	3953.8	0.8430
5	39.51	3975.2	1.0000
6	39.72	3995.9	0.8623
7	39.93	4017.2	0.4460
8	40.13	4037.9	0.1659
9	115.50	11620.8	0.3607
10	116.33	11704.1	0.0543
11	124.80	12556.3	0.6117
12	126.83	12761.2	0.3790
13	128.78	12957.3	0.6640
14	131.16	13196.1	0.0691
15	141.49	14235.5	0.3435
16	147.63	14853.9	0.0410

Sample Name: MCB-4082-0037PA1
Sample Set Name: zMCB2006_Exp
System Name: MCSN_LC3_2695_2487
Run Time: 11.5 Minutes
Channel Name: 2487Channel 1

Result_Id: 13130
Date Acquired: Tuesday, January 31, 2006 3:19:46 PM
Acq. Method Set: All_ODSAQ5to100_MB_Exp
Project Name: MCSN_LC3_1Q_2006
Channel Description: 220nm

Peak Results

	RT	Height	Area	% Area
1	5.451	2178778	12147656	99.56
2	7.151	11397	53477	0.44

RÉSULTAT HAUTE RÉOLUTION

Date : 29/3/2006

Produit : 40820111pa1

2006C053

Formule : C₁₁H₁₀O₁

Référence : 1) m₁/e = 161.9904

2) m₂/e = 154.9920

m₁/m₂ (calculé) = 1.045153

Inconnu : m_i/e (théorique) = 158.0732

m_i/m₂ = 1.019881 ±0.000003

m_i/e (expérimental) = 158.0734 ±0.0005 +1.3 ppm

Responsable :

Spectre de masse

ionisation électronique: 70eV

c:\masspec\bordeleau\mcb40820111pal.mas

Échantillon : MCB-4082-0111PA1

29/3/2006

2006C053

S30

Acquisition Time (sec)	5.1120	Comment	1Dproton DMSO-D: mcbrochu 36	Date	09 Feb 2006 20:33:04
File Name	\\LAVFS01\mrdata\Archive\2006\mcbrochu\NMR\MCB-4082-0048PA1_010001r			Frequency (MHz)	400.13
Nucleus	¹ H	Number of Transients	16	Original Points Count	32768
Owner	chemistry	Points Count	32768	Receiver Gain	574.70
SW(cyclical) (Hz)	6410.26	Solvent	DMSO-d6	Spectrum Offset (Hz)	2469.1790
				Sweep Width (Hz)	6410.06

VerticalScaleFactor = 1

DMSO-d6

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[6.55 .. 6.63]	0.926	6.03961e+9	0.926
2	[6.91 .. 6.99]	1.000	6.52536e+9	1.000
3	[7.25 .. 7.33]	1.007	6.56857e+9	1.007
4	[7.36 .. 7.50]	2.417	1.57732e+10	2.417
5	[7.63 .. 7.73]	2.246	1.46546e+10	2.246
6	[7.73 .. 7.79]	0.891	5.81307e+9	0.891

No.	Annotation	(ppm)
1	DMSO-d6	2.50

No.	(ppm)	Height	(Hz)	Height
1	2.50	0.9937	1000.3	0.4593
2	3.33	0.8059	1332.1	0.3157
3	6.59	0.3600	2635.9	0.5463
4	6.59	0.4950	2637.7	1.0000
5	6.60	0.5481	2639.1	0.5127
6	6.60	0.5056	2641.0	0.9786
7	6.95	0.6449	2779.1	0.8368
8	6.95	0.6520	2782.5	0.7396
9	7.27	0.1803	2908.5	

Acquisition Time (sec)	1.3566	Comment	1Dcarbon DMSO D: mcbrochu 67	Date	18 Feb 2006 05:20:00
File Name	\\LAVFS01\nmrdata\Archive\2006\mcbrochu\NMR\MCB-4082-0048PA1_020001r			Frequency (MHz)	100.61
Nucleus	¹³ C	Number of Transients	3720	Original Points Count	32768
Owner	chemistry	Points Count	32768	Pulse Sequence	zgpg60
SW(cyclical) (Hz)	24154.59	Solvent	DMSO-d6	Receiver Gain	14596.50
				Sweep Width (Hz)	24153.85

VerticalScaleFactor = 1

No.	Annotation	(ppm)
1	DMSO-d6	39.51

No.	(ppm)	(Hz)	Height
1	38.88	3911.8	0.1407
2	39.09	3933.2	0.4209
3	39.30	3953.8	0.8572
4	39.51	3975.2	1.0000
5	39.72	3995.9	0.8738
6	39.93	4017.2	0.4439
7	40.13	4037.9	0.1684
8	105.83	10647.8	0.2217
9	112.05	11273.6	0.2659
10	123.38	12413.2	0.4686
11	126.70	12747.2	0.0505
12	127.44	12821.6	0.3182
13	128.89	12967.6	0.5025
14	130.32	13112.1	0.0482
15	142.91	14378.5	0.2458
16	152.98	15391.3	0.0357

Sample Name: MCB-4082-0048PA1
Sample Set Name: zMCB2006_Exp
System Name: MCSN_LC3_2695_2487
Run Time: 11.5 Minutes
Channel Name: 2487Channel 1

Result_Id: 13178
Date Acquired: Thursday, February 09, 2006 3:45:05 PM
Acq. Method Set: All_ODSAQ5to100_MB_Exp
Project Name: MCSN_LC3_1Q_2006
Channel Description: 220nm

Peak Results

	RT	Height	Area	% Area
1	4.854	1954662	10682574	94.80
2	5.534	82761	399732	3.55
3	6.489	41886	186552	1.66

RÉSULTAT HAUTE RÉOLUTION**Date :** 8/3/2006**Produit :** 4082-0048pa1

2006C002

Formule : C₁₀H₈O₁**Référence :** 1) m₁/e = 149.99042) m₂/e = 142.9920m₁/m₂ (calculé) = 1.048943**Inconnu :** m_i/e (théorique) = 144.0575m_i/m₂ = 1.007453 ±0.000003m_i/e (expérimental) = 144.0577 ±0.0004 +1.4 ppm**Responsable :**

S35

Spectre de masse

Université de Sherbrooke

c:\masspec\bordeleau\mcb40820048pa1.mas ionisation électronique: 70eV

Échantillon : MCB-4082-0048PA1

7/3/2006

2006C002

Acquisition Time (sec)	5.1120	Comment	1Dproton DMSO D: mcbrochu 43	Date	15 Feb 2006 19:03:28		
File Name	\\LAVFS01\mrdata\Archive\2006\mcbrochu\NMR\MCB-4082-0055PB2_010001r				Frequency (MHz)	400.13	
Nucleus	¹ H	Number of Transients	16	Origin	spect	Original Points Count	32768
Owner	chemistry	Points Count	32768	Pulse Sequence	zg60	Receiver Gain	574.70
SW(cyclical) (Hz)	6410.26	Solvent	DMSO-d6	Spectrum Offset (Hz)	2469.1790	Sweep Width (Hz)	6410.06

VerticalScaleFactor = 1

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[6.69 .. 6.79]	1.000	3.38926e+9	1.000
2	[7.19 .. 7.51]	10.427	3.53393e+10	10.427
3	[7.80 .. 7.91]	0.940	3.18566e+9	0.940

No.	Annotation	(ppm)
1	DMSO-d6	2.50

No.	(ppm)	(Hz)	Height
1	2.50	1000.3	0.6855
2	3.33	1332.1	0.6680
3	6.75	2699.1	0.2439
4	6.75	2700.7	0.2999
5	7.33	2934.9	0.2723
6	7.35	2942.3	0.3648
7	7.39	2955.0	1.0000
8	7.39	2958.1	0.4361
9	7.44	2976.3	0.3470
10	7.83	3134.0	0.2810

Commentaires

François Biloiseau MC-4082-055PB2

dms0

3872-131

17 Février 2006

[Signature]

Commentaires

François Bilodeau MC-4082-055PB2

dmsd

3872-131/10 cosy

17 Février 2006

[Signature]

Commentaires

François Bilodeau MC-4082-055PB2

dmsd

3872-131/13 hmbc

17 Février 2006

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Commentaires

François Bilodeau MC-4082-055PB2

dmsd

3872-131/11 hmqc

17 Février 2006

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Commentaires

François Bilodeau MC-4082-055PB2

dmso

3872-131/14 roesy

17 Février 2006

[Signature]

Sample Name: MCB-4082-0055PB2

Sample Set Name: zMCB2006_Exp

System Name: MCSN_LC3_2695_2487

Run Time: 11.5 Minutes

Channel Name: 2487Channel 1

Result_Id: 18632

Date Acquired: Wednesday, February 15, 2006 3:00:15

Acq. Method Set: All_ODSAQ5to100_MB_Exp

Project Name: MCSN_2006\MCSN_LC3_1Q_2006

Channel Description: 220nm

Peak Results

	RT	Height	Area	% Area
1	6.481	2701166	14822826	99.59
2	6.635	12230	60472	0.41

S42

Acquisition Time (sec)	5.1120	Comment	1Dproton DMSO D: mcbrochu 113	Date	15 Feb 2006 22:15:28
File Name	\\LAVFS01\mrdata\Archive\2006\mcbrochu\NMR\MCB-4082-0055PC1_010001r	Number of Transients	16	Frequency (MHz)	400.13
Nucleus	¹ H	Points Count	32768	Original Points Count	32768
Owner	chemistry	Solvent	DMSO-d6	Receiver Gain	1024.00
SW(cyclical) (Hz)	6410.26			Sweep Width (Hz)	6410.06

VerticalScaleFactor = 1

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[7.00 .. 7.12]	1.000	2.07358e+9	1.000
2	[7.22 .. 7.37]	1.026	2.12745e+9	1.026
3	[7.39 .. 7.53]	2.017	4.18283e+9	2.017
4	[7.72 .. 7.89]	1.987	4.11975e+9	1.987

No.	Annotation	(ppm)
1	DMSO-d6	2.50

No.	(ppm)	(Hz)	Height
1	2.50	1000.3	1.0000
2	2.50	1001.7	0.9543
3	3.33	1332.1	0.8452
4	7.09	2837.4	0.3788
5	7.31	2926.8	0.1395
6	7.44	2975.6	0.1606
7	7.46	2983.4	0.2944
8	7.48	2991.0	0.1452
9	7.81	3125.8	0.2859
10	7.83	3134.0	0.2534

S43

Commentaires

François Bilodeau MC-4082-055PC1

dmsd

3872-132

17 Février 2006

M. Bilodeau

Commentaires

François Bilodeau MC-4082-055PC1

dmsd

3872-132/11 cosy

17 Février 2006

Handwritten signature

S45

Commentaires

François Bilodeau MC-4082-055PC1

dmso

3872-132/12 hmqc

17 Février 2006.

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546

Commentaires

François Bilodeau MC-4082-055PC1

dmso

3872-132/13 HMBC

17 Février 2006

M. Bilodeau

Commentaires

François Bilodeau MC-4082-055PC1

dmso

3872-132/14 roesy

17 Février 2006

M. Bilodeau

S48

Sample Name: MCB-4082-0055PC1
Sample Set Name: zMCB2006_Exp
System Name: MCSN_LC3_2695_2487
Run Time: 11.5 Minutes
Channel Name: 2487Channel 1

Result_Id: 18634
Date Acquired: Wednesday, February 15, 2006 5:19:47
Acq. Method Set: All_ODSAQ5to100_MB_Exp
Project Name: MCSN_2006\MCSN_LC3_1Q_2006
Channel Description: 220nm

Peak Results

	RT	Height	Area	% Area
1	6.772	637536	2953269	100.00

Acquisition Time (sec)	5.1120	Comment	1Dproton DMSO D: mcbrochu 95	Date	07 Feb 2006 20:48:00		
File Name	\\LAVFS01\nmrdata\Archive\2006\mcbrochu\NMR\MCB-4082-0046PA1_010001r				Frequency (MHz)	400.13	
Nucleus	1H	Number of Transients	16	Origin	spect	Original Points Count	32768
Owner	chemistry	Points Count	32768	Pulse Sequence	zg60	Receiver Gain	574.70
SW(cyclical) (Hz)	6410.26	Solvent	DMSO-d6	Spectrum Offset (Hz)	2468.7878	Sweep Width (Hz)	6410.06

VerticalScaleFactor = 1

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[2.43 .. 2.48]	3.000	4.11646e+9	3.000
2	[7.29 .. 7.43]	0.967	1.32649e+9	0.967
3	[7.44 .. 7.54]	3.970	5.44703e+9	3.970
4	[8.92 .. 9.06]	0.771	1.05753e+9	0.771

No.	Annotation	(ppm)
1	DMSO-d6	2.50

No.	(ppm)	Height
1	2.46	984.5
2	2.50	1000.3
3	3.33	1331.3
4	7.40	2960.5
5	7.41	2966.8
6	7.48	2992.2
7	7.49	2996.1
8	7.49	2998.4
9	9.01	3603.9

SSD

Acquisition Time (sec)	1.3566	Comment	1Dcarbon DMSO D: mcbrochu 70	Date	18 Feb 2006 10:44:16
File Name	\\LAVFS01\inmdata\Archive\2006\mcbrochu\NMR\WCB-4082-0046PA1_0200001r			Frequency (MHz)	100.61
Nucleus	13C	Number of Transients	3720	Origin	spect
Owner	chemistry	Points Count	32768	Pulse Sequence	zgpg60
SW(cyclical) (Hz)	24154.59	Solvent	DMSO-d6	Receiver Gain	11585.20
				Spectrum Offset (Hz)	9974.4219
				Sweep Width (Hz)	24153.85

VerticalScaleFactor = 1

DMSO-d6

No.	Annotation	(ppm)
1	DMSO-d6	39.51

No.	(ppm)	(Hz)	Height
1	15.97	1606.8	0.1352
2	38.89	3912.6	0.1369
3	39.09	3933.2	0.4204
4	39.30	3954.6	0.8311
5	39.51	3975.2	1.0000
6	39.72	3996.6	0.8409
7	39.93	4017.2	0.4417

No.	(ppm)	(Hz)	Height
8	40.13	4037.9	0.1608
9	127.98	12876.2	0.2311
10	128.95	12974.2	0.6021
11	131.20	13200.5	0.0263
12	131.48	13228.5	0.0354
13	147.93	14884.1	0.0296
14	151.68	15260.8	0.2187

Sample Name: MCB-4082-0046PA1
Sample Set Name: zMCB2006_Exp
System Name: MCSN_LC3_2695_2487
Run Time: 11.5 Minutes
Channel Name: 2487Channel 1

Result_Id: 13176
Date Acquired: Tuesday, February 07, 2006 3:22:43 PM
Acq. Method Set: All_ODSAQ5to100_MB_Exp
Project Name: MCSN_LC3_1Q_2006
Channel Description: 220nm

Peak Results

	RT	Height	Area	% Area
1	3.210	2671346	14001944	100.00

RÉSULTAT HAUTE RÉOLUTION**Date :** 8/3/2006**Produit :** 4082-0046pa1 2006C00/**Formule :** C₁₀H₉N₁S₁**Référence :** 1) m₁/e = 180.98882) m₂/e = 168.9888m₁/m₂ (calculé) = 1.071011**Inconnu :** m_i/e (théorique) = 175.0456m_i/m₂ = 1.035839 ±0.000003m_i/e (expérimental) = 175.0452 ±0.0005 -2.3 ppm**Responsable :**

Spectre de masse

c:\masspec\bordeleau\mcb40820046pa1.mas ionisation électronique:70eV

Échantillon : MCB-4082-0046PA1 2006 C001

7/3/2006

Acquisition Time (sec)	5.1120	Comment	1Dproton DMSO D: mcbrochu 9	Date	27 Feb 2006 22:17:36
File Name	\\LAVFS01\1nmrdata\Data\mcbrochu\1nmr\MCB-4082-0072PA1_010001r				
Nucleus	1H	Number of Transients	16	Origin	spect
Owner	chemistry	Points Count	32768	Pulse Sequence	zg60
SW(cyclical) (Hz)	6410.26	Solvent	DMSO-d6	Spectrum Offset (Hz)	2468.7878
				Sweep Width (Hz)	6410.06

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[7.29 .. 7.41]	1.018	1.21510e+9	1.018
2	[7.41 .. 7.52]	2.106	2.51429e+9	2.106
3	[7.65 .. 7.74]	2.053	2.45073e+9	2.053
4	[8.27 .. 8.36]	1.000	1.19399e+9	1.000
5	[9.03 .. 9.13]	0.872	1.04170e+9	0.872

No.	Annotation	(ppm)
1	DMSO-d6	2.50

No.	(ppm)	(Hz)	Height
1	2.50	1000.3	1.0000
2	3.33	1331.3	0.9449
3	7.37	2950.3	0.0872
4	7.39	2957.6	0.0689
5	7.44	2975.9	0.1142
6	7.46	2983.8	0.1846
7	7.48	2991.0	0.0831
8	7.68	3074.7	0.1839
9	7.70	3082.2	0.1570
10	8.32	3330.4	0.2208
11	9.09	3637.9	0.1898

Acquisition Time (sec)	1.3566	Comment	1Dcarbon DMSO D: mcbrochu 23	Date	03 Mar 2006 04:07:28
File Name	11LAVFS01\nmrdata\mcbrochu\mmr\MCB-4082-0072PA1		020001r	Frequency (MHz)	100.61
Nucleus	¹³ C	Number of Transients	10240	Original Points Count	32768
Owner	chemistry	Points Count	32768	Receiver Gain	13004.00
SW(cyclical) (Hz)	24154.59	Solvent	DMSO-d6	Sweep Width (Hz)	24153.85

No.	Annotation	(ppm)
1	DMSO-d6	39.51

No.	(ppm)	(Hz)	Height
1	38.89	3912.6	0.1331
2	39.09	3933.2	0.4222
3	39.30	3954.6	0.8336
4	39.51	3975.2	1.0000
5	39.72	3995.9	0.8423
6	39.93	4017.2	0.4452
7	40.13	4037.9	0.1597

Sample Name: MCB-4082-0072PA1
Sample Set Name: zMCB2006_Exp
System Name: MCSN_LC3_2695_2487
Run Time: 11.5 Minutes
Channel Name: 2487Channel 1

Result_Id: 13203
Date Acquired: Thursday, March 02, 2006 11:25:55 AM
Acq. Method Set: All_ODSAQ5to100_MB_Exp
Project Name: MCSN_LC3_1Q_2006
Channel Description: 220nm

Peak Results

	RT	Height	Area	% Area
1	3.295	891341	5072453	100.00

RÉSULTAT HAUTE RÉOLUTION

Date : 8/3/2006

Produit : 4082-0072pa1

2006C004

Formule : C9H7N1S1

Référence : 1) $m1/e = 161.9904$

2) $m2/e = 154.9920$

$m1/m2$ (calculé) = 1.045153

Inconnu : mi/e (théorique) = 161.0299

$mi/m2 = 1.038958 \pm 0.000003$

mi/e (expérimental) = 161.0302 ± 0.0005 +69 ppm

Responsable :

Spectre de masse

c:\masspec\bordeleau\mcb40820072pal.mas ionisation électronique:70eV

Échantillon : MCB-4082-0072PA1 20060004

7/3/2006

559

Acquisition Time (sec)	5.1120	Comment	1Dproton DMSO D: mcbrochu 6	Date	06 Feb 2006 16:49:04
File Name	\\LAVFS01\mrdata\Archive\2006\mcbrochu\NMR\MCB-4082-0044PA1_010001r	Number of Transients	16	Frequency (MHz)	400.13
Nucleus	¹ H	Points Count	32768	Original Points Count	32768
Owner	chemistry	Solvent	DMSO-d6	Receiver Gain	574.70
SW(cyclical) (Hz)	6410.26			Sweep Width (Hz)	6410.06

VerticalScaleFactor = 1

No.	(ppm)	(Hz)	Height
1	2.28	913.5	1.0000
2	2.50	1000.3	0.3660
3	3.33	1332.5	0.2180
4	6.99	2798.3	0.1511
5	7.01	2803.4	0.1614
6	7.35	2940.7	0.0697
7	7.36	2943.7	0.0664
8	7.36	2946.8	0.0666
9	7.45	2980.6	0.3245
10	7.45	2982.8	0.4288
11	7.46	2985.9	0.6795

No.	Annotation	(ppm)
1	DMSO-d6	2.50

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[2.22 .. 2.34]	3.131	6.54332e+9	3.131
2	[6.93 .. 7.05]	0.947	1.97934e+9	0.947
3	[7.29 .. 7.41]	1.079	2.25482e+9	1.079
4	[7.41 .. 7.53]	5.000	1.04512e+10	5.000
5	[7.61 .. 7.72]	0.213	4.45056e+8	0.213

Acquisition Time (sec)	1.3566	Comment	1Dcarbon DMSO D: mcbrochu 68	Date	18 Feb 2006 07:08:48
File Name	\\LAVFS01\mrdata\Archive\2006\mcbrochu\NMR\MCB-4082-0044PA1_020001r			Frequency (MHz)	100.61
Nucleus	13C	Number of Transients	3720	Origin	spect
Owner	chemistry	Points Count	32768	Pulse Sequence	zgpg80
SW(cyclical) (Hz)	24154.59	Solvent	DMSO-d6	Receiver Gain	14596.50
				Spectrum Offset (Hz)	9974.4219
				Sweep Width (Hz)	24153.85

VerticalScaleFactor = 1

No.	Annotation	(ppm)
1	DMSO-d6	39.51

No.	(ppm)	(Hz)	Height
1	147.2	1481.5	0.0924
2	38.88	3911.8	0.1405
3	39.09	3933.2	0.4291
4	39.30	3953.8	0.8428
5	39.51	3975.2	1.0000
6	39.72	3995.9	0.8530
7	39.93	4017.2	0.4400
8	40.13	4037.9	0.1594
9	124.17	12492.9	0.1615

Sample Name: MCB-4082-0044PA1
Sample Set Name: zMCB2006_Exp
System Name: MCSN_LC3_2695_2487
Run Time: 11.5 Minutes
Channel Name: 2487Channel 1

Result_Id: 13174
Date Acquired: Monday, February 06, 2006 12:37:00 PM
Acq. Method Set: All_ODSAQ5to100_MB_Exp
Project Name: MCSN_LC3_1Q_2006
Channel Description: 220nm

Peak Results

	RT	Height	Area	% Area
1	5.546	37134	177424	3.08
2	5.838	1123030	5543463	96.33
3	6.077	6441	33809	0.59

RÉSULTAT HAUTE RÉOLUTION**Date :** 8/3/2006**Produit :** 4082-0044pa1 2006B060**Formule :** C₁₁H₁₀S₁**Référence :** 1) m₁/e = 180.98882) m₂/e = 168.9888m₁/m₂ (calculé) = 1.071011**Inconnu :** m_i/e (théorique) = 174.0503m_i/m₂ = 1.029950 ±0.000003m_i/e (expérimental) = 174.0500 ±0.0005 -1.7ppm**Responsable :**

563

Spectre de masse

c:\masspec\bordeleau\mcb40820044pa1.mas ionisation électronique:70eV

Échantillon : MCB-4082-0044PA1

7/3/2006

2006B060

S64

Acquisition Time (sec)	5.1120	Comment	1Dproton DMSO D: mcbrochu 5	Date	16 Feb 2006 14:21:52
File Name	\\LAVFS01\mmrdata\Archive\2006\mcbrochu\NMR\MCB-4082-0054PA1_010001r	Number of Transients	16	Frequency (MHz)	400.13
Nucleus	¹ H	Points Count	32768	Original Points Count	32768
Owner	chemistry	Solvent	DMSO-d6	Receiver Gain	574.70
SW(cyclical) (Hz)	6410.26			Sweep Width (Hz)	6410.06

VerticalScaleFactor = 1

No.	Value	Absolute Value	Non-Negative Value
1	[2.44 .. 2.48]	3.000	3.000
2	[7.25 .. 7.37]	2.066	2.066
3	[7.39 .. 7.46]	0.990	0.990
4	[7.50 .. 7.61]	3.006	3.006
5	[7.64 .. 7.70]	1.054	1.054
6	[7.75 .. 7.89]	2.033	2.033

No.	Annotation	(ppm)
1	DMSO-d6	2.50

No.	(ppm)	Height	(Hz)
1	2.47	987.8	1.0000
2	2.50	1000.3	0.3650
3	2.50	1001.7	0.3419
4	3.34	1334.6	0.3453
5	7.29	2916.1	0.1332
6	7.31	2923.5	0.1100
7	7.32	2929.4	0.0973
8	7.34	2937.2	0.1266
9	7.43	2971.3	0.1180
10	7.44	2978.7	0.0858

S65

Acquisition Time (sec)	1.3566	Comment	1Dcarbon DMSO D: mcbrochu 71	Date	18 Feb 2006 12:33:04
File Name	\\LAVFS01\mrdata\Archive\2006\mcbrochu\NMR\MCB-4082-0054PA1_020001r	Origin	spect	Frequency (MHz)	100.61
Nucleus	13C	Number of Transients	32768	Original Points Count	32768
Owner	chemistry	Points Count	32768	Pulse Sequence	zgpg60
SW(cyclical) (Hz)	24154.59	Solvent	DMSO-d6	Receiver Gain	14596.50
				Spectrum Offset (Hz)	9973.6846
				Sweep Width (Hz)	24153.85

VerticalScaleFactor = 1

No.	Annotation	(ppm)
1	DMSO-d6	39.51

No.	(ppm)	(Hz)	Height
1	9.13	918.3	0.1356
2	38.88	3911.8	0.1504
3	39.09	3933.2	0.4318
4	39.30	3953.8	0.8726
5	39.51	3975.2	1.0000
6	39.72	3995.9	0.8745
7	39.92	4016.5	0.4345
8	40.13	4037.9	0.1589
9	110.86	11153.5	0.2021
10	111.34	11202.1	0.0373
11	119.69	12042.5	0.2061
12	122.68	12343.2	0.2156
13	124.74	12550.4	0.2074
14	126.31	12708.8	0.4098
15	128.22	12900.5	0.2159
16	128.94	12973.5	0.3936
17	130.54	13134.2	0.0474
18	130.61	13140.8	0.0473
19	149.88	15080.2	0.0263
20	153.07	15400.9	0.0340

566

Sample Name: MCB-4082-0054PA1
Sample Set Name: zMCB2006_Exp
System Name: MCSN_LC3_2695_2487
Run Time: 11.5 Minutes
Channel Name: 2487Channel 1

Result_Id: 13180
Date Acquired: Thursday, February 16, 2006 9:11:34 AM
Acq. Method Set: All_ODSAQ5to100_MB_Exp
Project Name: MCSN_LC3_1Q_2006
Channel Description: 220nm

Peak Results

	RT	Height	Area	% Area
1	5.523	24277	118469	0.93
2	6.649	1979348	12670359	99.07

567

RÉSULTAT HAUTE RÉOLUTION**Date :** 8/3/2006**Produit :** 4082-0054_{pa1}

2006003

Formule : C₁₅H₁₂O₁**Référence :** 1) m₁/e = 218.98562) m₂/e = 204.9888m₁/m₂ (calculé) = 1.068281**Inconnu :** m_i/e (théorique) = 208.0888m_i/m₂ = 1.015124 ±0.000003m_i/e (expérimental) = 208.0891 ±0.0006 +1.4 ppm**Responsable :**

Spectre de masse

c:\masspec\bordeleau\mcb40820054pa1.mas ionisation électronique:70eV

Échantillon : MCB-4082-0054PA1

7/3/2006

20060003

Acquisition Time (sec)	5.1120	Comment	1Dproton DMSO D: mcbrochu 7	Date	27 Feb 2006 22:06:56
File Name	\\LAVFS01\mmdata\Archive\2006\mcbrochu\NMR\MCB-4082-0068PA1_010001r	Number of Transients	16	Frequency (MHz)	400.13
Nucleus	¹ H	Points Count	32768	Original Points Count	32768
Owner	chemistry	Solvent	DMSO-d6	Receiver Gain	574.70
SW(cyclical) (Hz)	6410.26			Sweep Width (Hz)	6410.06

VerticalScaleFactor = 1

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[2.20 .. 2.26]	3.000	6.24578e+9	3.000
2	[7.08 .. 7.13]	0.769	1.60191e+9	0.769
3	[7.23 .. 7.32]	1.043	2.17223e+9	1.043
4	[7.32 .. 7.35]	1.026	2.13590e+9	1.026
5	[7.35 .. 7.43]	2.514	5.23420e+9	2.514
6	[7.43 .. 7.50]	0.893	1.85906e+9	0.893
7	[7.58 .. 7.64]	1.876	3.90606e+9	1.876
8	[7.64 .. 7.70]	0.818	1.70379e+9	0.818

No.	Annotation	(ppm)
1	DMSO-d6	2.50

No.	(ppm)	Height	(Hz)
9	7.40	2959.7	0.2977
10	7.42	2967.5	0.1645
11	7.47	2988.5	0.1335
12	7.60	3041.5	0.2956
13	7.62	3048.9	0.2347
14	7.65	3061.6	0.1258
15	7.67	3068.9	0.0990

No.	(ppm)	Height	(Hz)
1	2.24	894.7	1.0000
2	2.50	1000.3	0.4974
3	3.33	1332.3	0.4257
4	7.11	2846.6	0.2004
5	7.29	2915.3	0.1412
6	7.30	2922.5	0.1049
7	7.34	2936.2	0.2932
8	7.38	2951.9	0.1769

Sample Name: MCB-4082-0068PA1
Sample Set Name: zMCB2006_Exp
System Name: MCSN_LC3_2695_2487
Run Time: 11.5 Minutes
Channel Name: 2487Channel 1

Result_Id: 17308
Date Acquired: Friday, February 24, 2006 10:02:00 AM
Acq. Method Set: All_ODSAQ5to100_MB_Exp
Project Name: MCSN_LC3_1Q_2006
Channel Description: 220nm

Peak Results

	RT	Height	Area	% Area
1	5.489	205418	974909	12.76
2	5.681	130769	684903	8.96
3	5.928	1230849	5983497	78.28

Sample Name: MCB-4082-0070PA1

Sample Set Name: zMCB2006_Exp

System Name: MCSN_LC3_2695_2487

Run Time: 11.5 Minutes

Channel Name: 2487Channel 1

Result_Id: 18637

Date Acquired: Friday, February 24, 2006 2:59:24 PM EST

Acq. Method Set: All_ODSAQ5to100_MB_Exp

Project Name: MCSN_2006\MCSN_LC3_1Q_2006

Channel Description: 220nm

Peak Results

	RT	Height	Area	% Area
1	5.499	86683	439730	4.83
2	5.792	1366087	6671692	73.24
3	5.930	415004	1997503	21.93

10b (5.79 min)

and

13b (5.93 min)

Acquisition Time (sec)	2.5559	Comment	1Dproton DMSO D: mcbrochu 86	Date	10 Mar 2006 19:05:36
Date Stamp	10 Mar 2006 19:05:36	File Name	\\LAVFS01\Nmrdata\Archive\2006\mcbrochu\NMR\MCB-4082-0088PA1_010001r	Origin	spect
Frequency (MHz)	400.13	Nucleus	¹ H	Number of Transients	16
Original Points Count	16384	Owner	chemistry	Points Count	32768
Receiver Gain	406.40	SW(cyclical) (Hz)	6410.26	Pulse Sequence	zg60
Sweep Width (Hz)	6410.06	Solvent	DMSO-d6	Spectrum Offset (Hz)	2468.5920

No.	(ppm)	(Hz)	Height
1	2.50	1000.3	0.2109
2	3.33	1332.5	0.1629
3	3.59	1436.6	0.9763
4	3.78	1511.5	1.0000
5	6.02	2408.6	0.1629
6	6.04	2417.2	0.1470
7	6.05	2419.0	0.1534
8	6.78	2711.9	0.1613
9	6.96	2785.8	0.2430
10	6.98	2794.4	0.2662
11	7.33	2932.7	0.2735
12	7.35	2941.5	0.2364

CFS

Acquisition Time (sec)	0.6783	Comment	1Dcarbon DMSO D: mcbrochu 89	Date	11 Mar 2006 17:46:40
Date Stamp	11 Mar 2006 17:46:40	File Name	\\LAVFS01\Nmrdata\Archive\2006\mcbrochu\NMR\MCB-4082-0088PA1_020001r		
Frequency (MHz)	100.61	Nucleus	¹³ C	Number of Transients	10240
Original Points Count	16384	Owner	chemistry	Points Count	32768
Receiver Gain	16384.00	SW(cyclical) (Hz)	24154.59	Pulse Sequence	zgpg60
Sweep Width (Hz)	24153.85			Spectrum Offset (Hz)	9974.4219

No.	(ppm)	(Hz)	Height
1	34.67	3488.7	0.1806
2	38.88	3911.8	0.1417
3	39.09	3933.2	0.4309
4	39.30	3953.8	0.8481
5	39.51	3975.2	1.0000
6	39.72	3995.9	0.8496
7	39.93	4017.2	0.4337
8	40.13	4037.9	0.1554
9	55.10	5543.8	0.2496
10	107.12	10777.5	0.3262
11	107.61	10826.9	0.3181
12	113.92	11461.6	0.5882

hfs

Sample Name: MCB-4082-0088PA1
Sample Set Name: zMCB2006_Exp
System Name: MCSN_LC3_2695_2487
Run Time: 11.5 Minutes
Channel Name: 2487Channel 1

Result_Id: 14732
Date Acquired: Friday, March 10, 2006 1:16:18 PM
Acq. Method Set: All_ODSAQ5to100_MB_Exp
Project Name: MCSN_LC3_1Q_2006
Channel Description: 220nm

Peak Results

	RT	Height	Area	% Area
1	4.641	2562180	16204442	99.39
2	4.880	7313	44119	0.27
3	5.428	11144	55262	0.34

RÉSULTAT HAUTE RÉOLUTION

Date : 29/3/2006

Produit : 40820088pa1 2006C049

Formule : C₁₂H₁₃N₁O₁

Référence : 1) m₁/e = 192.9888

2) m₂/e = 180.9888

m₁/m₂ (calculé) = 1.066302

Inconnu : m_i/e (théorique) = 187.0997

m_i/m₂ = 1.033766 ±0.000003

m_i/e (expérimental) = 187.1001 ±0.0005 +2.1 ppm

Responsable :

A. B. G.

576

577

Spectre de masse

Université de Sherbrooke

2006C049

ionisation électronique: 70eV

c:\masspec\bordeleau\mcb40820088pal.mas

Échantillon : MCB-4082-0088PA1

29/3/2006

Acquisition Time (sec)	2.5559	Comment	1Dproton DMSO D: kthesen 44	Date	15 Jun 2006 20:24:32
Date Stamp	15 Jun 2006 20:24:32	File Name	\\LAVFS01\Nmrdata\Data\kthesen\kt-4083-0186PB1_010001r	Origin	spect
Frequency (MHz)	400.13	Nucleus	¹ H	Points Count	32768
Original Points Count	16384	Owner	chemistry	Pulse Sequence	zg60
Receiver Gain	1625.50	SW(cyclical) (Hz)	6410.26	Solvent	DMSO-d6
Sweep Width (Hz)	6410.06			Spectrum Offset (Hz)	2467.2227

KT-4083-0186PB1_010001 VerticalScaleFactor = 1

No.	(ppm)	(Hz)	Height
1	2.50	999.0	1.0000
2	3.32	1328.4	0.2908
3	3.76	1503.3	0.2960
4	6.14	2457.1	0.0264
5	6.15	2460.5	0.0380
6	6.16	2463.4	0.0287
7	6.47	2590.0	0.0303
8	6.48	2591.7	0.0339
9	6.49	2593.7	0.0324
10	6.49	2595.3	0.0301
11	7.00	2801.8	0.0440
12	7.01	2803.8	0.0295

875

Acquisition Time (sec) 0.6783	Comment 1Dcarbon DMSO D: kthesen 22	Date 14 Jul 2006 03:16:16
Date Stamp 14 Jul 2006 03:16:16	File Name \\LAVFS01\Nmrdata\Data\kthesen\nmr\KT-4083-0186PB1_053001r	
Frequency (MHz) 100.61	Nucleus ¹³ C	Origin spect
Original Points Count 16384	Owner chemistry	Pulse Sequence zgpg60
Receiver Gain 14596.50	SW(cyclical) (Hz) 24154.59	Spectrum Offset (Hz) 9975.1582
Sweep Width (Hz) 24153.85	Solvent DMSO-d6	

KT-4083-0186PB1_053001r VerticalScaleFactor = 1

No.	(ppm)	Annotation	Layer No.	Created By	Created At	Modified By	Modified At
1	39.51	DMSO-d6	1	fbilodea	Fri 07/14/2006 9:32:25 AM		

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	35.60	3581.6	0.0993	10	111.57	11225.7	0.1538
2	38.89	3912.6	0.1387	11	123.90	12466.3	0.2832
3	39.09	3933.2	0.4233	12	127.44	12822.4	0.1484
4	39.30	3954.6	0.8401	13	127.66	12843.7	0.2896
5	39.51	3975.2	1.0000	14	131.33	13213.0	0.0234
6	39.72	3996.6	0.8454	15	139.41	14026.1	0.0356
7	39.93	4017.2	0.4390	16	145.05	14593.7	0.0232
8	40.13	4037.9	0.1558				
9	108.32	10898.4	0.1551				

SampleName KT-4083-0186PB1

System Name MCSN_LC2_2695_2487

Sample Set Name 1Punit03_Exp

Channel Description 254nm

Date Acquired Friday, June 16, 2006 11:36:43 AM

Acq Method Set

Peak Results

	RT	% Area	Area	Height
1	6.576	100.00	4329189	944542

Handwritten signature

June 16, 2006

Acquisition Time (sec)	2.5559	Comment	1Dproton DMSO D: kthesen 76	Date	09 Jun 2006 20:28:48
Date Stamp	09 Jun 2006 20:28:48	File Name	\\LA\F501\Nmrdata\Data\kthesen\hnm\KT-4083-0159PA1_020001r	Origin	spect
Frequency (MHz)	400.13	Nucleus	¹ H	Pulse Sequence	zg60
Original Points Count	16384	Owner	chemistry	Spectrum Offset (Hz)	2468.3965
Receiver Gain	574.70	SW(cyclical) (Hz)	6410.26	Solvent	DMSO-d6
Sweep Width (Hz)	6410.06

No.	(ppm)	(Hz)	No.	(ppm)	(Hz)	Height
1	2.43	972.5	13	6.82	2727.1	0.1753
2	2.50	998.8	14	6.90	2759.2	0.1647
3	2.50	1000.3	15	6.90	2762.3	0.1821

No.	(ppm)	(Hz)	Height
4	3.66	1463.0	1.0000
5	6.00	2401.0	0.1601
6	6.01	2403.7	0.1522
7	6.13	2453.2	0.1483
8	6.14	2454.8	0.1546
9	6.14	2456.8	0.1439
10	6.78	2711.3	0.1606
11	6.78	2712.4	0.1598
12	6.81	2725.2	0.1843

581

Acquisition Time (sec)	0.6783	Comment	1Dcarbon DMSO D: kthesen 88	Date	27 May 2006 08:19:12
Date Stamp	27 May 2006 08:19:12	File Name	\\LAVFS01\Nmrdata\kthesen\mrKT-4083-0159PA1_011001r	Origin	spec
Frequency (MHz)	100.61	Nucleus	13C	Number of Transients	10240
Original Points Count	16384	Owner	chemistry	Points Count	32768
Receiver Gain	13004.00	SW(cyclical) (Hz)	24154.59	Solvent	DMSO-d6
Sweep Width (Hz)	24153.85			Pulse Sequence	zgpg60
				Spectrum Offset (Hz)	9975.8955

No.	(ppm)	Height	(Hz)	Height
1	14.78	0.2508	12681.6	0.3719
2	34.92	0.2287	12725.8	0.0488
3	38.89	0.1379	13306.7	0.0529
4	39.09	0.4234	13869.8	0.0771
5	39.30	0.8399		
6	39.51	1.0000		
7	39.72	0.8478		
8	39.93	0.4452		
9	40.14	0.1621		
10	107.35	0.4236		
11	108.87	0.3794		
12	124.27	0.6626		

782

SampleName KT-4083-0159PA1

System Name MCSN_LC2_2695_2487

Channel Description 254nm

Sample Set Name 1Punit03_Exp

Date Acquired Friday, May 26, 2006 12:47:20 PM

Acq Method Set

Peak Results

	RT	% Area	Area	Height
1	7.025	100.00	3841670	863268

Kyl
May 26, 2006

Acquisition Time (sec)	2.5559	Comment	1Dproton DMSO D: mcbrochu 18	Date	13 Mar 2006 16:10:40
Date Stamp	13 Mar 2006 16:10:40	File Name	\\LAVFS01\Nmrdata\Archive\2006\mcbrochu\NMR\MCB-4082-0089PA1_010001r	Origin	spect
Frequency (MHz)	400.13	Nucleus	¹ H	Number of Transients	16
Original Points Count	16384	Owner	chemistry	Points Count	32768
Receiver Gain	574.70	SW(cyclical) (Hz)	6410.26	Pulse Sequence	zg60
Sweep Width (Hz)	6410.06	Solvent	DMSO-d6	Spectrum Offset (Hz)	2468.5920

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	2.50	1000.3	0.4562	13	7.41	2966.8	0.0757
2	3.33	1333.1	0.2955	14	7.43	2971.6	0.0859
3	3.67	1469.4	1.0000	15	7.43	2974.6	0.0863
4	6.09	2438.2	0.1054	16	7.45	2979.3	0.0772
5	6.10	2441.3	0.1469	17	7.86	3144.2	0.0980
6	6.11	2444.2	0.0977	18	7.88	3152.2	0.0878
7	6.28	2512.1	0.1242	19	8.48	3392.6	0.1075
8	6.28	2513.7	0.1323	20	8.48	3393.8	0.1081
9	6.29	2515.4	0.1178	21	8.49	3397.3	0.1022
10	6.29	2517.2	0.0981	22	8.67	3469.3	0.1559
11	6.91	2764.9	0.1237	23	8.67	3470.9	0.1431
12	6.91	2766.8	0.1577				

Acquisition Time (sec)	0.6783	Comment	1Dcarbon DMSO D: mcbrochu 49	Date	03 Apr 2006 08:21:20
Date Stamp	03 Apr 2006 08:21:20	File Name	\\LAVFS01\Nmrdata\Archive\2006\mcbrochu\NMR\MCB-4082-0089PA1_0200001r	Origin	spect
Frequency (MHz)	100.61	Nucleus	¹³ C	Points Count	32768
Original Points Count	16384	Owner	chemistry	Solvent	DMSO-d6
Receiver Gain	11585.20	SW(cyclical) (Hz)	24154.59	Pulse Sequence	zgpg60
Sweep Width (Hz)	24153.85			Spectrum Offset (Hz)	9975.8955

No.	(ppm)	(Hz)	Height
1	34.93	3514.5	0.0834
2	38.89	3912.6	0.1382
3	39.09	3933.2	0.4212
4	39.30	3954.6	0.8407
5	39.51	3975.2	1.0000
6	39.72	3996.6	0.8469
7	39.93	4017.2	0.4426
8	40.14	4038.6	0.1581
9	107.70	10835.8	0.1493
10	109.49	11015.6	0.1370
11	123.50	12425.8	0.1145
12	125.35	12611.5	0.1403

No.	(ppm)	(Hz)	Height
13	128.89	12968.3	0.0225
14	129.97	13076.7	0.0169
15	134.85	13567.6	0.1185
16	147.34	14824.4	0.1425
17	148.39	14929.8	0.1199

RÉSULTAT HAUTE RÉOLUTION

Date : 29/3/2006

Produit : 40820089_{pa1} 2006C050

Formule : C₁₀H₁₀N₂

Référence : 1) m₁/e = 161.9904

2) m₂/e = 154.9920

m₁/m₂ (calculé) = 1.045153

Inconnu : m_i/e (théorique) = 158.0844

m_i/m₂ = 1.019954 ±0.000003

m_i/e (expérimental) = 158.0847 ±0.0005 + 1.9 ppm

Responsable :

Spectre de masse

Université de Sherbrooke

2006 C050

c:\masspec\bordeleau\mcb40820089pal.mas

Échantillon : MCB-4082-0089PA1

29/3/2006

ionisation électronique: 70eV