A Convenient Synthesis of 4-Alkyl-5-Amino Isoxazoles

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Experimental procedures

4-methyl-3-phenylisoxazol-5-amine (1b), Standard Procedure

To a solution of propiononitrile (0.42 g, 7.7 mmol) in 15 mL of THF at -78 °C was added tert-butyllithium (4.5 mL of a 1.7 M solution in heptane, 7.7 mmol). The mixture was stirred for 20 min. (Z)-benzaldehyde (α)-chloro-oxime (.30 g, 1.9 mmol) was then added slowly in 2 mL of THF. The mixture was stirred for 30 min and then quenched with aq. NH₄Cl. The biphasic mixture was extracted twice with EtOAc and the combined organic extracts were washed with brine and dried over MgSO₄. Filtration and concentration under reduced pressure, followed by flash chromatography on silica gel (10% to 50% EtOAc/hexanes), afforded 4-methyl-3-phenylisoxazol-5-amine (0.30 g, 1.7 mmol, 89% yield) as a white crystalline solid. ¹H NMR (400 MHz, CDCl₃) δ ppm 7.64-7.62 (m, 2H), 7.48-7.43 (m, 3H), 4.23 (s, 2H), 1.95 (s, 3H); ¹³C NMR (400 MHz, CDCl₃) δ ppm 165.57, 163.59, 130.27, 129.25, 128.64, 127.93, 87.27, 7.27; Melting point range 88-92 °C; ES HRMS m/e calcd for (M + H) C₁₀H₁₀N₂O 175.0866, found 175.0871.

3-phenylisoxazol-5-amine (1a)

The standard procedure was followed using acetonitrile (0.26 g, 6.4 mmol), tert-butyl lithium (2.8 mL of a 1.7 M solution in heptane, 6.4 mmol), and (Z)-benzaldehyde (α)-chloro-oxime (0.25 g, 1.6 mmol), affording 3-phenylisoxazol-5-amine (0.13 g, 51% yield) as a white crystalline solid. ¹H NMR (400 MHz, CDCl₃) δ ppm 7.74-7.72 (m, 2H), 7.43-7.40 (m, 3H), 5.46 (s, 1H), 4.49 (s, 2H); ¹³C NMR (100 MHz, CDCl₃) δ ppm 168.73, 163.84, 129.72, 128.69, 126.57, 78.26; Melting point range 99-103 °C; ES HRMS m/e calcd for (M + H) C₉H₈N₂O 161.0709, found 161.0715.

4-isopropyl-3-phenylisoxazol-5-amine (1c)

The standard procedure was followed using isovaleronitrile (0.64 g, 7.7 mmol), tert-butyl lithium (4.5 mL of a 1.7 M solution in heptane, 7.7 mmol), and (Z)-benzaldehyde (α)-chloro-oxime (0.30 g, 1.9 mmol), affording 4-isopropyl-3-phenylisoxazol-5-amine (0.25 g, 64% yield) as a clear oil. ^1H NMR (400 MHz, CDCl_3) δ ppm 7.51-7.43 (m, 5H), 4.27 (s, 1H), 2.84-2.77 (m, 1H), 1.20 (d, $J = 7.1$ Hz, 6H); ^{13}C NMR (100 MHz, CDCl_3) δ ppm 164.66, 164.06, 130.43, 129.13, 128.62, 128.50, 98.07, 22.48, 21.85; ES HRMS m/e calcd for ($M + H$) $\text{C}_{12}\text{H}_{14}\text{N}_2\text{O}$ 203.1179, found 203.1187.

4-cyclopropyl-3-phenylisoxazol-5-amine (1d)

The standard procedure was followed using 2-cyclopropylacetonitrile (0.63 g, 7.7 mmol), tert-butyl lithium (4.5 mL of a 1.7 M solution in heptane, 7.7 mmol), and (Z)-benzaldehyde (α)-chloro-oxime (0.30 g, 1.9 mmol), affording 4-cyclopropyl-3-phenylisoxazol-5-amine (0.38 g, 78% yield) as a white crystalline solid with the odor of butterscotch. ^1H NMR (400 MHz, CDCl_3) δ ppm 7.85-7.82 (m, 2H), 7.47-7.40 (m, 3H), 4.45 (s, 2H), 1.56-1.53 (m, 1H), 0.84-0.79 (m, 2H), 0.38-0.35 (m, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ ppm 167.02, 163.47, 129.91, 129.20, 128.30, 127.95, 92.36, 6.11, 2.90; Melting point range 108-112 $^\circ\text{C}$; ES HRMS m/e calcd for ($M + H$) $\text{C}_{12}\text{H}_{12}\text{N}_2\text{O}$ 201.1022, found 201.1036.

3,4-diphenylisoxazol-5-amine (1e)

The standard procedure was followed using 2-phenylacetonitrile (0.90 g, 7.7 mmol), tert-butyl lithium (4.5 mL of a 1.7 M solution in heptane, 7.7 mmol), and (Z)-benzaldehyde (α)-chloro-oxime (0.30 g, 1.9 mmol), affording 3,4-diphenylisoxazol-5-amine (0.39 g, 86% yield) as a white crystalline solid. ^1H NMR (400 MHz, CDCl_3) δ ppm 7.47-7.18 (m, 10H), 4.58 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ ppm 165.52, 161.96, 130.64, 129.41, 129.33, 129.17, 129.02, 128.39, 128.34, 126.98, 94.35; Melting

point range 148-152 °C; ES HRMS m/e calcd for (M + H) C₁₅H₁₂N₂O 237.1022, found 237.1026.

4-benzyl-3-phenylisoxazol-5-amine (1f)

The standard procedure was followed using 3-phenylpropionitrile (1.0 g, 7.7 mmol), tert-butyl lithium (4.5 mL of a 1.7 M solution in heptane, 7.7 mmol), and (Z)-benzaldehyde (α)-chloro-oxime (0.30 g, 1.9 mmol), affording 4-benzyl-3-phenylisoxazol-5-amine (0.44 g, 91% yield) as a white crystalline solid. ¹H NMR (400 MHz, CDCl₃) δ ppm 7.58-7.22 (m, 10H), 4.09 (s, 2H), 3.77 (s, 2H); ¹³C NMR (100 MHz, CDCl₃) δ ppm 166.2, 164.00, 138.44, 129.86, 129.35, 128.85, 128.65, 128.14, 126.67, 89.90, 28.03; Melting point range 70-74 °C; ES HRMS m/e calcd for (M + H) C₁₆H₁₄N₂O 251.1179, found 251.1188.

3-(4-methoxyphenyl)-4-methylisoxazol-5-amine (2a)

The standard procedure was followed using propionitrile (0.24 g, 4.3 mmol), tert-butyl lithium (2.5 mL of a 1.7 M solution in heptane) and (Z)-4-methoxybenzaldehyde (α)-chloro-oxime (0.20 g, 1.1 mmol), affording 3-(4-methoxyphenyl)-4-methylisoxazol-5-amine (.17 g, 77% yield) as a white crystalline solid. ¹H NMR (400 MHz, CDCl₃) δ ppm 7.58 (d, J = 8.8 Hz, 2H), 6.98 (d, J = 8.6 Hz, 2H), 4.20 (s, 2H), 3.85 (s, 3H), 1.94 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ ppm 165.44, 163.20, 160.39, 129.21, 122.74, 114.08, 87.11, 55.34, 7.39; Melting point range 131-135 °C; ES HRMS m/e calcd for (M + H) C₁₁H₁₂N₂O₂ 205.0972, found 205.0989.

3-(4-chlorophenyl)-4-methylisoxazol-5-amine (2b)

The standard procedure was followed using propionitrile (0.232 g, 4.21 mmol), tert-butyl lithium (2.48 mL of a 1.7 M solution in heptane) and (Z)-4-chlorobenzaldehyde (α)-chloro-oxime (0.200 g, 1.05 mmol), affording 4-methyl-3-(pyridin-2-yl)isoxazol-5-amine (0.160 g, 73% yield) as a white crystalline solid. ¹H NMR (400 MHz, CDCl₃) δ ppm

7.56 (d, $J = 8.0$ Hz, 2H), 7.41 (d, $J = 8.0$ Hz, 2H), 4.28 (s, 2H), 1.95 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ ppm 165.39, 159.16, 135.41, 131.00, 128.77, 126.66, 126.04, 124.43, 87.11, 7.48; Melting point range 113–117 °C; ES HRMS m/e calcd for ($M + H$) $\text{C}_{10}\text{H}_9\text{ClN}_2\text{O}$ 209.0476, found 209.0484.

3-(3-chlorophenyl)-4-methylisoxazol-5-amine (2c)

The standard procedure was followed using propionitrile (0.262 g, 4.21 mmol), tert-butyl lithium (2.48 mL of a 1.7 M solution in heptane) and (*Z*)-3-chlorobenzaldehyde (α -chloro-oxime) (0.200 g, 1.05 mmol), affording 4-methyl-3-(pyridin-2-yl)isoxazol-5-amine (0.178 g, 81% yield) as a white crystalline solid. ^1H NMR (400 MHz, CDCl_3) δ ppm 7.63 (s, 1H), 7.52 (dt, $J = 8$ Hz, $J = 4$ Hz, 1H), 7.39 (m, 2H), 4.30 (s, 2H), 1.93 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ ppm 165.80, 162.38, 134.61, 132.04, 129.94, 129.36, 127.98, 126.05, 87.16, 7.23; Melting point range 70–74 °C; ES HRMS m/e calcd for ($M + H$) $\text{C}_{10}\text{H}_9\text{ClN}_2\text{O}$ 209.0476, found 209.0484.

3-(2-chlorophenyl)-4-methylisoxazol-5-amine (2d)

The standard procedure was followed using propionitrile (0.232 g, 4.21 mmol), tert-butyl lithium (2.48 mL of a 1.7 M solution in heptane) and (*Z*)-2-chlorobenzaldehyde (α -chloro-oxime), affording 4-methyl-3-(pyridin-2-yl)isoxazol-5-amine (0.151 g, 69% yield) as a white crystalline solid. ^1H NMR (400 MHz, CDCl_3) δ ppm 7.48 (d, $J = 8.0$ Hz, 1H), 7.37 (m, 3H), 4.30 (s, 2H), 1.74 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ ppm 165.08, 163.27, 133.62, 131.50, 130.61, 129.78, 129.39, 126.77, 89.33, 6.62; Melting point range 98–102 °C; ES HRMS m/e calcd for ($M + H$) $\text{C}_{10}\text{H}_9\text{ClN}_2\text{O}$ 209.0476, found 209.0453.

3-cyclohexyl-4-methylisoxazol-5-amine (2e)

The standard procedure was followed using propionitrile (0.55 g, 10.0 mmol), tert-butyl lithium (5.9 mL of a 1.7 M solution in heptane) and (*Z*)-cyclohexanecarboxaldehyde (α -chloro-oxime) (0.40 g, 2.5 mmol), affording 3-cyclohexyl-4-methylisoxazol-5-amine (0.24 g, 53% yield) as a dark amorphous solid. ^1H

NMR (400 MHz, CDCl_3) δ ppm 4.06 (s, 2H), 2.59-2.38 (m, 1H), 1.98-1.80 (m, 4H), 1.78 (s, 3H), 1.63-1.44 (m, 2H), 1.43-1.20 (m, 4H); ^{13}C NMR (100 MHz, CDCl_3) δ ppm 168.52, 164.52, 86.80, 36.27, 30.85, 26.39, 26.04, 6.33; ES HRMS m/e calcd for ($M + H$) $\text{C}_{10}\text{H}_{16}\text{N}_2\text{O}$ 181.1335, found 181.1345.

4-methyl-3-propylisoxazol-5-amine (2f)

The standard procedure was followed using propionitrile (0.53 g, 9.8 mmol), tert-butyl lithium (5.7 mL of a 1.7 M solution in heptane) and (*Z*)-butanal (α -chloro-oxime) (0.29 g, 2.4 mmol), affording 4-methyl-3-propylisoxazol-5-amine (0.25 g, 74% yield) as a white amorphous solid. ^1H NMR (400 MHz, CDCl_3) δ ppm 4.04 (s, 2H), 2.47 (t, $J = 7.3$ Hz, 2H), 1.71-1.60 (m, 2H), 0.98 (t, $J = 7.3$ Hz, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ ppm 164.77, 164.55, 87.33, 27.48, 20.87, 13.95, 6.05; ES HRMS m/e calcd for ($M + H$) $\text{C}_7\text{H}_{12}\text{N}_2\text{O}$ 141.1022, found 141.1028.

4-methyl-3-(thiophen-3-yl)isoxazol-5-amine (2g)

The standard procedure was followed using propionitrile (0.27 g, 5.0 mmol), tert-butyl lithium (2.9 mL of a 1.7 M solution in heptane) and (*Z*)-thiophene-3-carbaldehyde (α -chloro-oxime) (0.200 g, 1.2 mmol), affording 4-methyl-3-(pyridin-2-yl)isoxazol-5-amine (0.22 g, 33% yield) as a white crystalline solid. ^1H NMR (400 MHz, CDCl_3) δ ppm 7.63 (m, 1H), 7.46 (d, $J = 4$ Hz, 1H), 7.30 (m, 1H), 4.30 (s, 2H), 1.98 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ ppm 165.77, 162.56, 135.37, 129.19, 128.93, 128.76, 87.10, 7.26; Melting point range 81-85 $^\circ\text{C}$; ES HRMS m/e calcd for ($M + H$) $\text{C}_8\text{H}_8\text{N}_2\text{OS}$ 181.0430, found 181.0435. Additionally, 1.3 mg of 3-(2-chlorothiophen-3-yl)-4-methylisoxazol-5-amine was isolated. ^1H NMR (400 MHz, CDCl_3) δ ppm 7.17 (d, $J = 8.0$ Hz, 1H), 7.03 (d, $J = 8.0$ Hz, 1H), 4.28 (s, 2H), 1.84 (s, 3H); ^{13}C NMR (100 MHz, CDCl_3) δ ppm 165.51, 158.68, 129.32, 128.11, 127.84, 123.47, 88.63, 6.95.

4-methyl-3-(pyridin-2-yl)isoxazol-5-amine (2h)

The standard procedure was followed using propionitrile (0.28 g, 5.1 mmol), tert-butyl lithium (3.0 mL of a 1.7 M solution in heptane) and (Z)-picolinaldehyde (α)-chloro-oxime (0.20 g, 1.3 mmol), affording 4-methyl-3-(pyridin-2-yl)isoxazol-5-amine (0.11 g, 49% yield) as a white crystalline solid. ^1H NMR (400 MHz, CDCl_3) δ ppm 8.69 (d, J = 4.9 Hz, 1H), 7.89 (d, J = 8.0 Hz, 1H), 7.76 (dt, J = 1.8 Hz, 7.8 Hz, 1H), 7.31 (dd, J = 1.1 Hz, 4.8 Hz, 1H), 4.26 (s, 2H); ^{13}C NMR (100 MHz, CDCl_3) δ ppm 166.06, 162.21, 150.62, 149.34, 136.56, 123.70, 122.70, 88.61, 7.32; Melting point range 139-143 $^\circ\text{C}$; ES HRMS m/e calcd for ($\text{M} + \text{H}$) $\text{C}_9\text{H}_9\text{N}_3\text{O}$ 176.0818, found 176.0934.

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Acquisition Time (sec)	5.1120	Comment	bourbeau	Date	24 Mar 2005 00:56:01
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Frequency (MHz)	400.16	Nucleus	1H	Number of Transients	32
Origin	Bruker BioSpin GmbH			Original Points Count	32768
Owner	chemist	Points Count	32768	SW(cyclical) (Hz)	6410.26
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	2390.9109
Sweep Width (Hz)	6410.06

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[4.36 .. 4.58]	1.924	1.11743e+10	1.924
2	[5.89 .. 5.52]	0.965	5.60271e+9	0.965
3	[7.32 .. 7.48]	3.000	1.74238e+10	3.000
4	[7.65 .. 7.79]	1.959	1.13760e+10	1.959

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Acquisition Time (sec)	1.1535	Comment	bourbeau	Date	15 May 2006 23:57:46
File Name	\\scone\nmr-archive\camp\bourbeau\2006\77020-26-20_10.dx			Frequency (MHz)	100.62
Nucleus	¹³ C	Number of Transients	512	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	smallmolecules	Points Count	32768
SW(cyclical) (Hz)	28409.09	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	12070.4248	Sweep Width (Hz)	28408.22	Temperature (degree C)	23.800

No.	(ppm)	(Hz)	Height
1	78.26	7874.7	0.1997
2	126.57	12735.8	0.3597
3	128.69	12949.1	0.3227
4	129.67	13047.9	0.0674
5	129.72	13053.1	0.2022
6	163.84	16486.4	0.0500
7	168.73	16977.9	0.0639

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Acquisition Time (sec)	5.1120	Comment	bourbeau	Date	29 Mar 2005 00:26:40
File Name	\\scone\nmr-archive\camp\bourbeau\2005\65441-25-1_10.dx				
Frequency (MHz)	400.16	Nucleus	1H	Number of Transients	32
Origin	Bruker BioSpin GmbH			Original Points Count	32768
Owner	chemist	Points Count	32768	SW(cyclical) (Hz)	6410.26
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	2392.9358
Sweep Width (Hz)	6410.06	Temperature (degree C)	25.000

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[1.90 .. 1.98]	3.000	3.90012e+9	3.000
2	[4.18 .. 4.29]	1.755	2.28195e+9	1.755
3	[7.40 .. 7.50]	3.012	3.91608e+9	3.012
4	[7.60 .. 7.69]	1.924	2.50072e+9	1.924

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Acquisition Time (sec)	1.1600	Comment	bourbeau	Date	05 Jan 2006 05:58:25
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Nucleus	¹³ C	Number of Transients	4096	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	chemist	Points Count	32768
SW(cyclical) (Hz)	28248.59	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	12075.7510	Sweep Width (Hz)	28247.73

No.	(ppm)	(Hz)	Height
1	7.27	732.1	0.1186
2	87.27	8782.2	0.0586
3	127.93	12873.6	0.3161
4	128.64	12945.2	0.3244
5	129.25	13007.2	0.1330
6	130.27	13109.8	0.0471
7	163.59	16462.4	0.0518
8	165.57	16661.6	0.0624

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Acquisition Time (sec)	5.1120	Comment	bourbeau	Date	04 Apr 2005 23:48:55
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Frequency (MHz)	400.16	Nucleus	1H	Number of Transients	32
Origin	Bruker BioSpin GmbH			Original Points Count	32768
Owner	chemist	Points Count	32768	SW(cyclical) (Hz)	6410.26
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	2393.1921
Sweep Width (Hz)	6410.06	Temperature (degree C)	25.000

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[1.14 .. 1.24]	6.407	1.21756e+10	6.407
2	[2.73 .. 2.88]	1.005	1.90990e+9	1.005
3	[4.20 .. 4.38]	1.964	3.73262e+9	1.964
4	[7.39 .. 7.47]	3.000	5.70027e+9	3.000
5	[7.47 .. 7.53]	2.026	3.84950e+9	2.026

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Acquisition Time (sec)	1.1535	Comment	bourbeau	Date	12 May 2006 21:39:04
File Name	\\scone\nmr-archive\jcamp\bourbeau\2006\77020-26-1 10.dx			Frequency (MHz)	100.62
Nucleus	¹³ C	Number of Transients	512	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	smallmolecules	Points Count	32768
SW(cyclical) (Hz)	28409.09	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	12076.2061	Sweep Width (Hz)	28408.22	Temperature (degree C)	23.700

No.	(ppm)	(Hz)	*(ppm)	*(Hz)	Height	*Height	*FWHH	*Area	*LF	*Function
1	21.85	2198.3	21.85	2198.31	0.1946	0.1946	0.87	0.22	0.50	Gauss+Lorentz
2	22.48	2261.6	22.48	2261.60	0.1221	0.1221	0.87	0.14	0.50	Gauss+Lorentz
3	98.07	9868.4	98.07	9868.45	0.0369	0.0369	0.87	0.04	0.50	Gauss+Lorentz
4	127.44	12824.0	127.44	12823.97	0.0212	0.0212	0.87	0.02	0.50	Gauss+Lorentz
5	128.50	12930.6	128.50	12930.61	0.1711	0.1711	0.87	0.20	0.50	Gauss+Lorentz
6	128.62	12942.7	128.62	12942.75	0.2059	0.2059	0.87	0.24	0.50	Gauss+Lorentz
7	129.13	12993.9	129.13	12993.90	0.1005	0.1005	0.87	0.11	0.50	Gauss+Lorentz
8	130.43	13124.8	130.43	13124.82	0.0341	0.0341	0.87	0.04	0.50	Gauss+Lorentz
9	164.06	16508.6	164.06	16508.63	0.0312	0.0312	0.87	0.04	0.50	Gauss+Lorentz
10	164.66	16569.3	164.66	16569.31	0.0437	0.0437	0.87	0.05	0.50	Gauss+Lorentz

- noise

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Acquisition Time (sec)	5.1120	Comment	bourbeau	Date	06 Apr 2005 18:31:13
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Frequency (MHz)	400.16	Nucleus	1H	Number of Transients	32
Origin	Bruker BioSpin GmbH			Original Points Count	32768
Owner	chemist	Points Count	32768	SW(cyclical) (Hz)	6410.26
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	2393.0642
Sweep Width (Hz)	6410.06	Temperature (degree C)	25.000

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[0.33 .. 0.42]	2.025	9.15134e+9	2.025
2	[0.77 .. 0.87]	2.060	9.30946e+9	2.060
3	[1.50 .. 1.59]	1.086	4.90727e+9	1.086
4	[4.35 .. 4.54]	1.957	8.84538e+9	1.957
5	[7.38 .. 7.48]	3.003	1.35701e+10	3.003
6	[7.79 .. 7.89]	1.923	8.68808e+9	1.923

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Acquisition Time (sec)	1.1535	Comment	bourbeau	Date	12 May 2006 23:11:54
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Nucleus	¹³ C	Number of Transients	512	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	smallmolecules	Points Count	32768
SW(cyclical) (Hz)	28409.09	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	12070.4248	Sweep Width (Hz)	28408.22	Temperature (degree C)	23.800

No.	(ppm)	(Hz)	*(ppm)	*(Hz)	Height	*Height	*FWHH	*Area	*LF	*Function
1	2.90	292.1	2.90	292.11	0.1961	0.1961	0.87	0.22	0.50	Gauss+Lorentz
2	6.11	614.6	6.11	614.63	0.3824	0.3824	0.87	0.44	0.50	Gauss+Lorentz
3	92.36	9293.9	92.36	9293.93	0.0621	0.0621	0.87	0.07	0.50	Gauss+Lorentz
4	127.95	12875.4	127.95	12875.41	0.3425	0.3425	0.87	0.39	0.50	Gauss+Lorentz
5	128.30	12910.1	128.30	12910.09	0.4130	0.4130	0.87	0.47	0.50	Gauss+Lorentz
6	129.20	13000.3	129.20	13000.26	0.1911	0.1911	0.87	0.22	0.50	Gauss+Lorentz
7	129.91	13072.2	129.91	13072.22	0.0686	0.0686	0.87	0.08	0.50	Gauss+Lorentz
8	163.47	16449.1	163.47	16449.09	0.0546	0.0546	0.87	0.06	0.50	Gauss+Lorentz
9	167.02	16806.3	167.02	16806.29	0.0751	0.0751	0.87	0.09	0.50	Gauss+Lorentz

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Acquisition Time (sec)	5.1120	Comment	bourbeau	Date	12 Apr 2005 01:05:19
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Origin	Bruker BioSpin GmbH			Original Points Count	32768
Owner	chemist	Points Count	32768	SW(cyclical) (Hz)	6410.26
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	2393.4924
Sweep Width (Hz)	6410.06	Temperature (degree C)	23.400

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[4.49 .. 4.67]	2.000	3.53432e+9	2.000
2	[7.10 .. 7.22]	2.005	3.54272e+9	2.005
3	[7.28 .. 7.41]	5.918	1.04586e+10	5.918
4	[7.41 .. 7.50]	1.998	3.53057e+9	1.998

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Acquisition Time (sec)	1.1535	Comment	bourbeau	Date	12 May 2006 23:38:49
File Name	\\scone\nmr-archive\camp\bourbeau\2006\77020-26-4_10.dx			Frequency (MHz)	100.62
Nucleus	¹³ C	Number of Transients	512	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	smallmolecules	Points Count	32768
SW(cyclical) (Hz)	28409.09	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	12071.2920	Sweep Width (Hz)	28408.22	Temperature (degree C)	23.800

No.	(ppm)	(Hz)	* (ppm)	* (Hz)	Height	*Height	*FWHH	*Area	*LF	*Function
1	94.35	9494.2	94.35	9494.20	0.0422	0.0422	0.87	0.05	0.50	Gauss+Lorentz
2	126.98	12777.4	126.98	12777.44	0.1526	0.1526	0.87	0.17	0.50	Gauss+Lorentz
3	128.34	12914.4	128.34	12914.42	0.3476	0.3476	0.87	0.40	0.50	Gauss+Lorentz
4	128.39	12919.6	128.39	12919.63	0.2731	0.2731	0.87	0.31	0.50	Gauss+Lorentz
5	129.02	12982.9	129.02	12982.92	0.3553	0.3553	0.87	0.41	0.50	Gauss+Lorentz
6	129.17	12997.7	129.17	12997.66	0.3481	0.3481	0.87	0.40	0.50	Gauss+Lorentz
7	129.33	13014.1	129.33	13014.13	0.1769	0.1769	0.87	0.20	0.50	Gauss+Lorentz
8	129.41	13021.9	129.41	13021.93	0.0545	0.0545	0.87	0.06	0.50	Gauss+Lorentz
9	130.64	13145.9	130.64	13145.91	0.0529	0.0529	0.87	0.06	0.50	Gauss+Lorentz
10	161.96	16297.4	161.96	16297.37	0.0389	0.0389	0.87	0.04	0.50	Gauss+Lorentz
11	165.52	16655.4	165.52	16655.43	0.0615	0.0615	0.87	0.07	0.50	Gauss+Lorentz

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Acquisition Time (sec)	5.1120	Comment	bourbeau	Date	14 Apr 2005 23:39:11
File Name	\\scone\nmr-archive\camp\bourbeau\2005\65519-25-1_10.dx				
Frequency (MHz)	400.16	Nucleus	1H	Number of Transients	32
Origin	Bruker BioSpin GmbH			Original Points Count	32768
Owner	chemist	Points Count	32768	SW(cyclical) (Hz)	6410.26
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	2400.9949
Sweep Width (Hz)	6410.06	Temperature (degree C)	23.300

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[3.71 .. 3.81]	2.000	9.67681e+9	2.000
2	[4.02 .. 4.14]	1.907	9.22567e+9	1.907
3	[7.19 .. 7.28]	3.168	1.53299e+10	3.168
4	[7.30 .. 7.39]	2.101	1.01660e+10	2.101
5	[7.39 .. 7.48]	2.895	1.40052e+10	2.895
6	[7.52 .. 7.63]	1.918	9.27785e+9	1.918

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Acquisition Time (sec)	1.1535	Comment	bourbeau	Date	13 May 2006 00:05:36
File Name	\\scone\mr-archive\camp\bourbeau\2006\77020-26-5_10.dx			Frequency (MHz)	100.62
Nucleus	¹³ C	Number of Transients	512	Origin	Brüker BioSpin GmbH
Original Points Count	32768	Owner	smallmolecules	Points Count	32768
SW(cyclical) (Hz)	28408.09	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	12071.2920	Sweep Width (Hz)	28408.22	Temperature (degree C)	23.900

No.	(ppm)	(Hz)	Height
1	28.03	2820.2	0.0959
2	89.90	9046.0	0.0363
3	126.67	12746.2	0.1091
4	128.14	12893.6	0.2660
5	128.65	12945.6	0.2091
6	128.85	12965.6	0.2314
7	129.35	13015.9	0.0943
8	129.86	13067.0	0.0359
9	138.44	13930.5	0.0378
10	164.00	16502.0	0.0260
11	166.32	16736.1	0.0451

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Acquisition Time (sec)	5.1120	Comment	bourbeau	Date	10 Jun 2005 04:22:29
File Name	\\scone\mr-archiv\jcamp\bourbeau\2005\65751-3-1_10.dx			Frequency (MHz)	400.16
Nucleus	¹ H	Number of Transients	32	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	chemist	Points Count	32768
SW(cyclical) (Hz)	6410.26	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2392.8201	Sweep Width (Hz)	6410.06	Temperature (degree C)	23.300

No.	(ppm)	(Hz)	Height
1	1.94	777.2	0.7725
2	3.85	1541.6	0.7801
3	4.20	1681.2	0.0952
4	6.97	2787.3	0.1845
5	6.99	2795.9	0.1910
6	7.57	3027.5	0.1956
7	7.59	3036.3	0.1774

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[1.88 .. 1.99]	2.895	5.07119e+9	2.895
2	[3.83 .. 3.91]	3.057	5.35385e+9	3.057
3	[4.13 .. 4.28]	1.898	3.32524e+9	1.898
4	[6.92 .. 7.05]	1.999	3.50059e+9	1.999
5	[7.52 .. 7.70]	1.929	3.37803e+9	1.929

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Acquisition Time (sec)	1.1535	Comment	bourbeau	Date	16 May 2006 09:19:24
File Name	\\scone\nmr-archive\camp\bourbeau\2006\77020-26-9_10.dx			Frequency (MHz)	100.65
Nucleus	¹³ C	Number of Transients	4096	Origin	Brüker BioSpin GmbH
Original Points Count	32768	Owner	smallmolecules	Points Count	32768
SW(cyclical) (Hz)	28409.09	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	12080.0889	Sweep Width (Hz)	28408.22	Temperature (degree C)	23.500

No.	(ppm)	(Hz)	Height
1	7.39	743.9	0.2102
2	55.34	5569.5	0.2767
3	87.11	8767.8	0.0820
4	114.08	11482.3	0.5600
5	122.74	12353.6	0.0827
6	129.21	13004.7	0.4640
7	160.39	16143.2	0.1054
8	163.20	16425.8	0.0641
9	165.44	16651.2	0.1104

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Acquisition Time (sec)	5.1120	Comment	Jrider	Date	17 Jun 2005 16:28:29	Frequency (MHz)	400.16
File Name	\iscor\nmr-archive\JCAMP\JRIDER\2005065769-02-01_10.DX						
Nucleus	¹ H	Number of Transients	32	Origin	Bruker BioSpin GmbH		
Original Points Count	32768	Owner	chemist	Points Count	32768	SW(cyclical) (Hz)	6410.26
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	2393.3879	Sweep Width (Hz)	6410.06
Temperature (degree C)	25.000

No	Color	Structure	Visible
1			True

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[1.90 .. 1.96]	3.000	6.17774e+9	3.000
2	[4.12 .. 4.39]	1.870	3.85083e+9	1.870
3	[7.40 .. 7.46]	1.958	4.03166e+9	1.958
4	[7.53 .. 7.60]	1.937	3.98938e+9	1.937

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Acquisition Time (sec)	1.1600	Comment	Jrider	Date	19 Jan 2006 11:55:38	Frequency (MHz)	100.63
File Name	Vaconehnm-archiv\JCAMP\JRIDER2006\65769-1-1 10.DX						
Nucleus	13C	Number of Transients	4096	Origin	Bruker Biospin GmbH		
Original Points Count	32768	Owner	chemist	Points Count	32768	SW(cyclical) (Hz)	28248.59
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	12075.9717	Sweep Width (Hz)	28247.73

No.	Color	Structure	Visible
1			True

No.	(ppm)	(Hz)	Height
1	7.26	730.6	0.1231
2	87.10	8765.2	0.0497
3	128.76	12957.4	0.0610
4	128.93	12974.7	0.3140
5	129.19	13000.8	0.3146
6	135.37	13622.1	0.0542
7	162.56	16359.2	0.0406
8	165.77	16681.6	0.0604

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Acquisition Time (sec)	5.1120	Comment	jider	Date	10 Jun 2005 04:48:17
File Name	\seconelm-archival\CAMPURIDER2005065883-20-01 10.DX				
Nucleus	¹ H	Number of Transients	32	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	chemist	Points Count	32768
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	2393.8884
Temperature (degree C)	23.200			Sweep Width (Hz)	6410.06

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[1.90..1.97]	3.010	4.63503e+9	3.010
2	[4.17..4.45]	1.891	2.91105e+9	1.891
3	[7.35..7.44]	2.000	3.07986e+9	2.000
4	[7.49..7.54]	0.953	1.46716e+9	0.953
5	[7.59..7.65]	0.928	1.42828e+9	0.928

No	Color	Structure	Visible
1			True

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Acquisition Time (sec)	1.1600	Comment	Index	Date	19 Jan 2006 08:57:20	Frequency (MHz)	100.63
File Name	Isconetnmt-archivelJCAMPJRIDER2006165683-20-1 10.DX						
Nucleus	13C	Number of Transients	4096	Origin	Bruker BioSpin GmbH		
Original Points Count	32768	Owner	chemist	Points Count	32768	SW(cyclical) (Hz)	28248.59
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	12076.2139	Sweep Width (Hz)	28247.73

Vertical Scale Factor = 1

No.	(ppm)	(Hz)	Height
1	7.23	727.4	0.0521
2	87.16	8771.4	0.0252
3	126.05	12684.4	0.0712
4	127.98	12879.2	0.0615
5	129.36	13018.0	0.0680
6	129.94	13076.7	0.0701
7	132.04	13287.0	0.0297
8	134.61	13545.6	0.0239
9	162.38	16340.5	0.0209
10	165.80	16685.3	0.0270

No.	Color	Structure	Visible
1			True

5/22/2006 1:55 PM

Acquisition Time (sec)	5.120	Comment	Jrdr	Date	10 Jun 2005 04:13:51	Frequency (MHz)	400.16
File Name	\scone\nmr-archive\JCAMPURIDER\2005\65683-19-01_10.DX						
Nucleus	¹ H	Number of Transients	32	Origin	Bruker BioSpin GmbH		
Original Points Count	32768	Owner	chemist	Points Count	32768	SW(cyclical) (Hz)	6410.26
Solvent	CHLOROFORM-d						Sweep Width (Hz) 6410.06
Temperature (degree C)	23.300

No	Color	Structure	Visible
1			True

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[1.71 .. 1.77]	3.105	3.47010e+9	3.105
2	[4.19 .. 4.41]	1.911	2.13481e+9	1.911
3	[7.29 .. 7.44]	3.001	3.35289e+9	3.001
4	[7.45 .. 7.51]	0.964	1.07768e+9	0.964

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Acquisition Time (sec)	1.1600	Comment	Index	Date	19 Jan 2006 05:59:24	Frequency (MHz)	100.63
File Name	\Isconelmr-archiv\JCAMP\JRIDER\2006\65683-19-1_10.DX						
Nucleus	13C	Number of Transients	4096	Origin	Bruker BioSpin GmbH	SW(cyclical) (Hz)	28248.59
Original Points Count	32768	Owner	chemist	Points Count	32768	Sweep Width (Hz)	28247.73
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	12075.7998

No.	Color	Structure	Visible
1			True

No.	(ppm)	(Hz)	Height
1	6.62	665.8	0.1019
2	89.33	8989.1	0.0440
3	126.77	12757.3	0.1414
4	129.39	13021.1	0.0447
5	129.78	13059.9	0.1216
6	130.61	13143.5	0.1348
7	131.50	13233.1	0.1434
8	133.62	13446.9	0.0423
9	163.27	16430.6	0.0368
10	165.08	16612.5	0.0484

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Acquisition Time (sec)	5.1120	Comment	bourbeau	Date	27 Jun 2005 17:56:03
File Name	\\scone\hmr-archive\camp\bourbeau\2005\65785-6-1_10.dx			Frequency (MHz)	400.13
Nucleus	1H	Number of Transients	32	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	chemist	Points Count	32768
SW(cyclical) (Hz)	6410.26	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2392.1042	Sweep Width (Hz)	6410.06	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	4.06	1624.0	0.0413

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[1.14 .. 1.43]	4.537	1.06909e+10	4.537
2	[1.44 .. 1.63]	2.929	6.90203e+9	2.929
3	[1.64 .. 1.76]	2.460	5.79544e+9	2.460
4	[1.76 .. 1.80]	2.971	7.00082e+9	2.971
5	[1.80 .. 1.98]	3.971	9.35720e+9	3.971
6	[2.38 .. 2.58]	1.614	3.80275e+9	1.614
7	[3.97 .. 4.13]	2.001	4.71444e+9	2.001

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Acquisition Time (sec)	1.1535	Comment	bourbeau	Date	16 May 2006 06:41:12
File Name	\\scone\nmr-archive\camp\bourbeau\2006\77020-26-8_10.dx			Frequency (MHz)	100.85
Nucleus	¹³ C	Number of Transients	4096	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	smallmolecules	Points Count	32768
SW(cyclical) (Hz)	28409.09	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	12080.9248	Sweep Width (Hz)	28408.22	Temperature (degree C)	23.500

No.	(ppm)	(Hz)	Height
1	6.33	637.3	0.2059
2	26.04	2620.9	0.2924
3	26.39	2656.5	0.5542
4	30.85	3104.7	0.4586
5	36.27	3650.9	0.1974
6	86.80	8736.6	0.0597
7	164.52	16559.3	0.0833
8	168.52	16961.6	0.0852

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Acquisition Time (sec)	5.1120	Comment	bourbeau	Date	17 Jun 2005 16:47:10
File Name	\\scone\nmr-archive\jcamp\bourbeau\2005\65751-17-1_10.dx				
Frequency (MHz)	400.16	Nucleus	1H	Number of Transients	32
Origin	Bruker BioSpin GmbH			Original Points Count	32768
Owner	chemist	Points Count	32768	SW(cyclical) (Hz)	6410.26
Solvent	CHLOROFORM-d			Spectrum Offset (Hz)	2394.5125
Sweep Width (Hz)	6410.06	Temperature (degree C)	25.000

No.	(ppm)	(Hz)	Height
1	0.97	386.7	0.2017
2	0.98	394.1	0.4137
3	1.00	401.4	0.2082
4	1.60	642.2	0.0296
5	1.71	685.2	0.0186
6	2.45	981.4	0.1774
7	2.47	989.4	0.2568
8	2.49	996.7	0.1502
9	4.04	1615.6	0.0117

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[0.93 .. 1.05]	3.000	6.44961e+9	3.000
2	[1.59 .. 1.73]	2.464	5.29800e+9	2.464
3	[2.40 .. 2.57]	2.135	4.58915e+9	2.135
4	[3.80 .. 4.26]	1.487	3.19580e+9	1.487

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Acquisition Time (sec)	1.1535	Comment	bourbeau	Date	16 May 2006 00:43:20
File Name	\\scone\nmr-archive\camp\bourbeau\2006\77020-6-1_10.dx			Frequency (MHz)	100.62
Nucleus	¹³ C	Number of Transients	512	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	smallmolecules	Points Count	32768
SW(cyclical) (Hz)	28409.09	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	12076.6807	Sweep Width (Hz)	28408.22	Temperature (degree C)	23.800

No.	(ppm)	(Hz)	Height
1	6.05	608.7	0.1617
2	13.95	1403.8	0.2857
3	20.87	2099.9	0.2270
4	27.48	2764.9	0.2275
5	87.38	8793.0	0.0584
6	164.55	16557.7	0.0569
7	164.77	16580.2	0.0639

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Acquisition Time (sec)	5.1120	Comment	jld	Date	28 Jun 2005 00:01:37	Frequency (MHz)	400.16
File Name	\\aconetnmt-archivel\JCAMP\JRIDER2005\65769-17-001_10.DX						
Nucleus	¹ H	Number of Transients	16	Origin	Bruker BioSpin GmbH	SW(cyclical) (Hz)	6410.26
Original Points Count	32768	Owner	chemist	Points Count	32768	Sweep Width (Hz)	6410.06
Solvent	CHLOROFORM-d						
Temperature (degree C)	25.000

No	Color	Structure	Visible
1			True

No.	(ppm)	Value	Absolute Value	Non-Negative Value
1	[1.95 .. 1.99]	3.040	8.52206e+9	3.040
2	[4.15 .. 4.56]	1.677	4.70066e+9	1.677
3	[7.36 .. 7.43]	1.000	2.80380e+9	1.000
4	[7.44 .. 7.50]	0.975	2.73249e+9	0.975
5	[7.59 .. 7.67]	0.962	2.69798e+9	0.962

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Acquisition Time (sec)	1.1600	Comment	jider	Date	20 Jan 2006 05:59:05
File Name	\\lsone\mr-archive\JCAMP\JRIDR\2006\65769-17-2_10.DX				
Nucleus	¹³ C	Number of Transients	4096	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	chemist	Points Count	32768
Solvent	CHLOROFORM-d			SW(cyclical) (Hz)	28248.59
				Sweep Width (Hz)	28247.72
				Spectrum Offset (Hz)	12076.0039

No.	ppm	Height	Color	Structure	Visible
1	6.95	0.0368			True

No.	ppm	Height
1	6.95	0.0368
2	88.63	0.0191
3	123.47	0.0478
4	127.84	0.0167
5	128.11	0.0414
6	129.32	0.0112
7	158.68	0.0118
8	165.51	0.0185

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Acquisition Time (sec)	5.1120	Comment	bourbeau	Date	10 Jun 2005 03:56:36
File Name	\\scone\nmr-archive\camp\bourbeau\2005\65751-2-1_10.dx			Frequency (MHz)	400.16
Nucleus	¹ H	Number of Transients	32	Origin	Brüker BioSpin GmbH
Original Points Count	32768	Owner	chemist	Points Count	32768
SW(cyclical) (Hz)	6410.26	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	2393.3804	Sweep Width (Hz)	6410.06	Temperature (degree C)	23.300

¹H NMR (400 MHz, CHLOROFORM-d) δ ppm 8.69 (d, $J=4.89$ Hz, 1 H) 7.89 (d, $J=8.02$ Hz, 1 H) 7.76 (td, $J=7.73, 1.76$ Hz, 1 H) 7.31 (ddd, $J=7.53, 4.89, 1.08$ Hz, 1 H) 4.26 (s, 2 H) 2.13 (s, 3 H)
VerticalScaleFactor = 1

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	Value	Absolute Value	Non-Negative Value	No.	Multiplet1	S
1	2.13	854.3	0.5976	11	7.74	3096.4	0.0261	1	[2.13 .. 2.15]	3.168	2.55715e+9	3.168	1	M00	
2	4.26	1702.7	0.0457	12	7.74	3098.1	0.0274	2	[4.21 .. 4.30]	1.773	1.43152e+9	1.773	2	M01	
3	7.29	2918.0	0.0326	13	7.76	3104.0	0.0544	3	[7.28 .. 7.33]	1.077	8.69367e+8	1.077	3	M02	
4	7.29	2919.1	0.0328	14	7.76	3105.8	0.0561	4	[7.74 .. 7.78]	1.009	8.14163e+8	1.009	4	M02	
5	7.30	2922.8	0.0347	15	7.78	3111.8	0.0332	5	[7.88 .. 7.91]	0.991	7.99977e+8	0.991	5	M02	
6	7.31	2924.0	0.0369	16	7.78	3113.6	0.0335	6	[8.68 .. 8.71]	0.982	7.92453e+8	0.982	6	M03	
7	7.31	2925.6	0.0391	17	7.88	3154.9	0.0717						7	M03	
8	7.31	2926.6	0.0363	18	7.90	3162.9	0.0543						8	M03	
9	7.32	2930.5	0.0361	19	8.68	3475.1	0.0465						9	M04	
10	7.33	2931.4	0.0351	20	8.70	3480.0	0.0473						10	M05	

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Acquisition Time (sec)	1.1535	Comment	bourbeau	Date	16 May 2006 01:10:25
File Name	\\scone\nmr-archive\camp\bourbeau\2006\77020-7-1_10.dx			Frequency (MHz)	100.62
Nucleus	¹³ C	Number of Transients	512	Origin	Bruker BioSpin GmbH
Original Points Count	32768	Owner	smallmolecules	Points Count	32768
SW(cyclical) (Hz)	28409.09	Solvent	CHLOROFORM-d		
Spectrum Offset (Hz)	12075.8252	Sweep Width (Hz)	28408.22	Temperature (degree C)	23.800

No.	(ppm)	(Hz)	Height
1	7.32	736.2	0.1385
2	88.61	8916.1	0.0401
3	122.70	12346.8	0.1404
4	123.70	12447.3	0.1930
5	136.56	13741.7	0.1441
6	149.34	15027.4	0.1449
7	150.62	15155.8	0.0413
8	162.21	16322.7	0.0326
9	166.06	16710.2	0.0544