

SUPPORTING INFORMATION

The all-Photochemical Synthesis an OGP (10-14) Precursor

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General methods: All reactions were carried out under an atmosphere of nitrogen or argon using flame dried glassware. Solvents were dried by filtration, under an argon atmosphere, though a purification system similar to the one proposed by Grubbs *and co-workers*.¹ Thin layer chromatography (TLC) analyses were done using aluminium sheets coated with silica gel 60 F₂₅₄. Flash column chromatography (FC) was carried out using Brunschwig silica gel 60 Å (32-63 mesh). Commercially available products were used without further purification.

¹H- and ¹³C-NMR spectra were recorded with a Fourier transform Bruker-DRX-500 (500 MHz) or Bruker-DPX-360 (360 MHz) spectrometer with solvent residual signals used as a reference. Chemical shifts are given in ppm, coupling constants “*J*” are expressed in Hertz (multiplicity: s = singulet, d = doublet, dd = double doublet, t = triplet, dt = double tiplet, q = quadruplet, quint = quintuplet, sext = sextuplet, sept = septuplet, m = multiplet). IR spectra were recorded with a Fourier transform Mattson 5000 FTIR spectrometer, neat, in CHCl₃ (NaCl cell) or in KBr; absorption bands are in cm⁻¹. UV spectra were recorded with a Perkin Elmer Lambda 40 spectrometer; absorption bands are in nm. EI mass spectra were recorded with an HP 5988A Quadrupol spectrometer, with electron impact (70 eV) and ESI mass spectra with a Bruker FT/MS 4.7 T BioApex II spectrometer. Photochemical irradiations were carried out in a LUMOS 43 photoreactor (Atlas Photonics Inc.), in a quartz vessel, with 1 diode at 365, 375, 385, 405 or 430 nm, or in a Srinivasan-Griffin (Rayonet-RPR-100) photoreactor, in a quartz vessel, with 16 lamps at 254, 300, 350 or 420 nm.

¹ Pangborn, A. B.; Giardello, M. A.; Grubbs, R. H.; Rosen, R. K.; Timmers, F. J. *Organometallics* **1996**, *15*, 1518–1520.

Experimental procedures for the synthesis of the substrates 3, 5 and 6

2-(3,5-dimethoxyphenyl)propan-2-yl (S)-1-(phenethylcarbamoyl)-3-methylbutyl-carbamate (3): A mixture of *N*-protected- α -amino acyl-5,7-dinitroindolines (**1**) (0.10 mmol) and phenethylamine (0.10 mmol, 1 equiv.) in anhydrous MeCN (2 mL) was irradiated at 385 nm in a quartz tube for 16 hours, under an argon atmosphere, with vigorous stirring. The mixture was filtered, concentrated to dryness and purified by flash column chromatography [SiO₂, hexane/EtOAc (1:1)] to furnish the desired product as a yellow solid (42.0 mg, 92 %); ¹H NMR (360 MHz, CDCl₃) δ = 7.28 (m, 2H), 7.21 (m, 1H), 7.14 (d, *J* = 7.3 Hz, 2H), 6.49 (m, 2H), 6.32 (m, 1H), 6.01 (m, 1H), 5.06 (d, *J* = 8.7 Hz, 1H), 3.95 (m, 1H), 3.75 (s, 6H), 3.45 (m, 2H), 2.73 (m, 2H), 1.71 (s, 3H), 1.70 (s, 3H), 1.62-1.56 (2H), 1.43 (m, 1H), 0.87 (m, 6H); ¹³C NMR (125 MHz, CDCl₃) δ = 172.3, 160.8 (2xC), 155.1, 149.0, 138.8, 128.9 (2xC), 128.7 (2xC), 126.6, 102.9 (2xC), 98.5, 81.4, 55.3 (2xC), 53.3, 41.2, 40.8, 35.7, 29.2, 29.1, 24.9, 23.0, 22.2. IR (neat): 3308, 2956, 1702, 1658, 1601, 1530, 1460, 1427, 1203, 1155, 1062, 699. HR-MS 479.2522 (C₂₆H₃₆N₂O₅ + Na⁺ calcd 479.2516).

Ddz-Leu-Phe-O^tBu (5): A mixture of *N*-Ddz- α -amino acyl-5,7-dinitroindoline (**1**) (0.10 mmol), amino acids *tert*-butyl ester hydrochloride (**4**) (0.10 mmol, 1 equiv.) and Et₃N (14 μ L, 0.1 mmol) in anhydrous MeCN (2 mL) was irradiated at 375 nm in a quartz tube for 17 hours, under an argon, with stirring. The mixture was concentrated to dryness and purified by flash column chromatography [SiO₂, hexane/EtOAc (2:1)] to provide the desired product as a yellow solid (45.1 mg, 81 %); ¹H NMR (360 MHz, CDCl₃) δ = 7.23-7.21 (3H), 7.09-7.07 (2H), 6.50 (br s, 2H), 6.35 (d, *J* = 7.7 Hz, 1H), 6.29 (br s, 1H), 5.07 (d, *J* = 8.2 Hz, 1H), 4.67 (q, *J* = 6.4 Hz, 1H), 4.07-4.01 (1H), 3.74 (s, 6H), 3.02 (m, 2H), 1.73 (br s, 6H), 1.67-1.54 (2H), 1.49-1.42 (1H), 1.36 (s, 9H), 0.91 (d, *J* = 6.3 Hz, 3H), 0.87 (d, *J* = 5.9 Hz, 3H); ¹³C NMR (125 MHz, CDCl₃) δ = 171.9, 170.3, 160.8 (2xC), 154.9, 149.0, 136.1, 129.7 (2xC), 128.4 (2xC), 127.0, 103.0 (2xC), 98.5, 82.4, 81.3, 55.3 (2xC), 53.7, 53.3, 41.5, 38.1, 29.3, 28.9, 28.0 (3xC), 24.8, 23.0, 22.1. IR (neat): 3328, 2977, 2957, 2936, 1729, 1661, 1599, 1523, 1458, 1426, 1368, 1256, 1227, 1206, 1156. HR-MS 579.3043 (C₃₁H₄₄N₂O₇ + Na⁺ calcd 579.3041).

Leu-Phe-O^tBu (6): Ddz-L-Leu-L-Phe-O^tBu (**5**) (27.8 mg, 0.050 mmol) was dissolved in deuterated MeCN (2.5 mL). The solution was then irradiated at 300 nm (Rayonet[®]) in a quartz NMR tube for 8 hours. The mixture was concentrated to dryness and purified by flash column chromatography [SiO₂, CH₂Cl₂/MeOH_{sat.}NH₃ (95:5)] to provide the desired product as an orange solid (13.9 mg, 83 %). ¹H NMR (360 MHz, CDCl₃) δ = 7.79 (d, *J* = 8.2 Hz, 1H), 7.29-7.15 (5H), 4.73 (q, *J* = 6.8 Hz, 1H), 3.39 (dd, *J* = 9.8, 3.9 Hz, 1H), 3.09 (m, 2H), 1.82 (br s, 2H), 1.71-1.56 (2H), 1.41 (s, 9H), 1.25 (m, 1H), 0.93 (d, *J* = 5.9 Hz, 3H), 0.89 (d, *J* = 6.3 Hz, 3H); ¹³C NMR (125 MHz, CDCl₃) δ = 175.0, 171.0, 136.6, 129.7 (2xC), 128.4 (2xC), 127.0, 82.3, 53.6, 53.2, 44.1, 38.4, 28.1 (3xC), 25.0, 23.5, 21.5. IR (neat): 3323, 2960, 1731, 1663, 1512, 1462, 1367, 1242, 1158, 701. HR-MS 357.2151 (C₁₉H₃₀N₂O₃ + Na⁺ calcd 357.2149).

The all-photochemical synthesis of the OGP (10-14) precursor 20.

Ddz-Gly-Gly-O'Bu (12): A mixture of Ddz-Gly-Dni (**10**) (48.9 mg, 0.1 mmol), glycine *tert*-butyl ester hydrochloride (**11**) (16.9 mg, 0.1 mmol) and Et₃N (14 μ L, 0.1 mmol) in anhydrous MeCN (2 mL) was irradiated at 385 nm in a quartz tube for 16 hours, under argon, with stirring. The mixture was filtered, concentrated to dryness and purified by flash column chromatography [SiO₂, Hexane/EtOAc (1:1)] to provide the desired product as a yellow solid (38.3 mg, 93 %). ¹H NMR (360 MHz, CDCl₃) δ = 6.51 (s, 2H), 6.41 (br s, 1H), 6.34 (s, 1H), 5.35 (br s, 1H), 3.91 (d, *J* = 4.6 Hz, 2H), 3.82 (d, *J* = 5.4 Hz, 2H), 3.78 (s, 6H), 1.74 (s, 6H), 1.46 (s, 9H). **HR-MS** 433.1947 (C₂₀H₃₀N₂O₇ + Na⁺ calcd 433.1945).

Gly-Gly-O'Bu (13): Ddz-Gly-Gly-O'Bu (**12**) (30.8 mg, 0.075 mmol) was dissolved in anhydrous MeCN (3 mL). The solution was then irradiated at 300 nm (Rayonnet) in a quartz tube for 5 hours. The mixture was concentrated to dryness and purified by flash column chromatography [SiO₂, CH₂Cl₂/MeOH_{sat.NH₃} (95:5)] to provide the desired product as an orange solid (10.4 mg, 74 %). ¹H NMR (360 MHz, CDCl₃) δ = 7.73 (br s, 1H), 3.98 (d, *J* = 5.0 Hz, 2H), 3.46 (s, 2H), 2.12 (br s, 2H), 1.47 (s, 9H).

Ddz-Phe-Gly-Gly-O'Bu (15): A mixture of Ddz-Phe-Dni (**14**) (28.9 mg, 0.018 mmol) and Gly-Gly-O'Bu (**13**) (9.4 mg, 0.050 mmol) in anhydrous MeCN (1 mL) was irradiated at 385 nm in a quartz tube for 5 hours, under argon, with stirring. The mixture was filtered and concentrated to dryness and purified by flash column chromatography [SiO₂, Hexane/EtOAc (1:3)] to provide the desired product as a yellow solid (25.1 mg, 90 %). ¹H NMR (360 MHz, CDCl₃) δ = 7.33-7.18 (5H), 6.53 (br s, 1H), 6.43 (s, 3H), 6.32 (s, 1H), 5.25 (d, *J* = 6.3 Hz, 1H), 4.26 (q, *J* = 6.8 Hz, 1H), 3.95-3.81 (3H), 3.76 (s, 6H), 3.55 (m, 1H), 3.06 (m, 2H), 1.69 (s, 3H), 1.65 (s, 3H), 1.45 (s, 9H). **HR-MS** 580.2623 (C₂₉H₃₉N₃O₈ + Na⁺ calcd 580.2629).

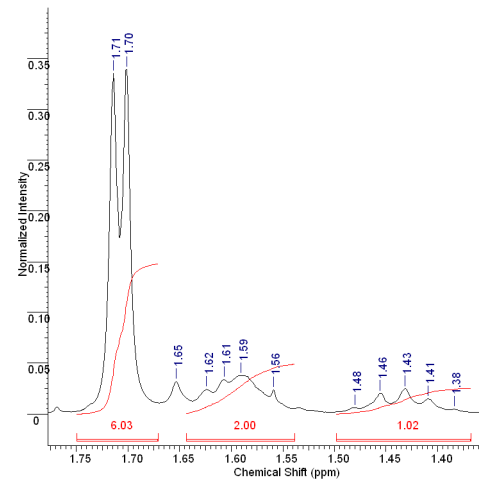
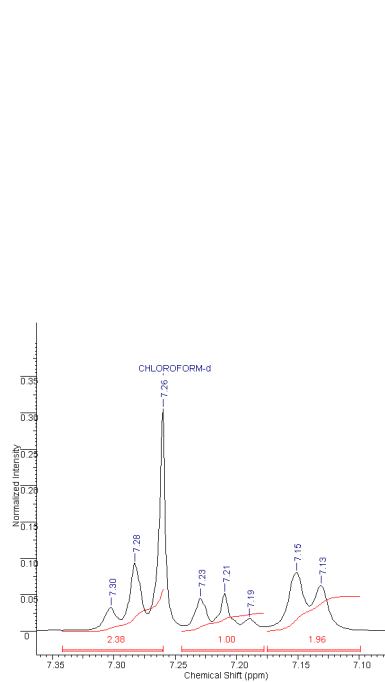
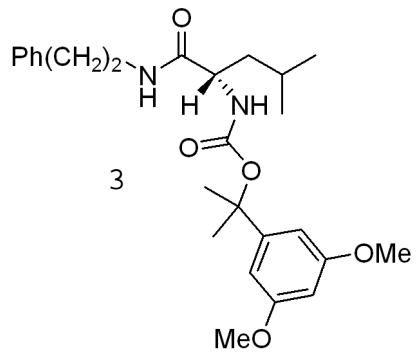
Phe-Gly-Gly-O'Bu (16): Ddz-Phe-Gly-Gly-OtBu (**15**) (27.9 mg, 0.050 mmol) was dissolved in anhydrous MeCN (3 mL). The solution was then irradiated at 300 nm (Rayonnet[®]) in a quartz tube for 6 hours. The mixture was concentrated to dryness and purified by flash column chromatography [SiO₂, CH₂Cl₂/MeOH_{sat.NH₃} (95:5)] to provide the desired product as a yellowish solid (13.5 mg, 80 %). ¹H NMR (360 MHz, CDCl₃) δ = 7.94 (br s, 1H), 7.34-7.21 (5H), 6.57 (br s, 1H), 3.99 (d, *J* = 5.9 Hz, 2H), 3.92 (d, *J* = 5.0 Hz, 2H), 3.68 (dd, *J* = 9.1, 3.6 Hz, 1H), 3.28 (dd, *J* = 13.9, 3.6 Hz, 1H), 2.74 (dd, *J* = 13.6, 9.5 Hz, 1H), 1.58 (br s, 2H), 1.46 (s, 9H).

Ddz-Gly-Phe-Gly-Gly-O'Bu (17): A mixture of Ddz-Gly-Dni (**10**) (12.2 mg, 0.025 mmol), and Phe-Gly-Gly-O'Bu (**16**) (8.4 mg, 0.025 mmol) in anhydrous MeCN (1 mL) was irradiated at 385 nm in a quartz tube for 5 hours, under argon, with stirring. The mixture was filtered and concentrated to dryness and purified by microscale flash column chromatography in a Pasteur pipette [SiO₂, EtOAc then CH₂Cl₂ and CH₂Cl₂/MeOH_{sat.NH₃} (95:5)] to provide the desired product as a yellow solid (13.4 mg, 87 %). ¹H NMR (360 MHz, CDCl₃) δ = 7.28-7.07 (6H), 6.85-6.80 (2H), 6.48 (s, 2H), 6.32 (s, 1H), 5.65 (d, *J* = 4.1 Hz, 1H), 4.63 (dd, *J* = 7.1, 13.9 Hz, 1H), 3.85-3.70 (12H), 3.07 (dd, *J* = 7.1, 13.9 Hz,

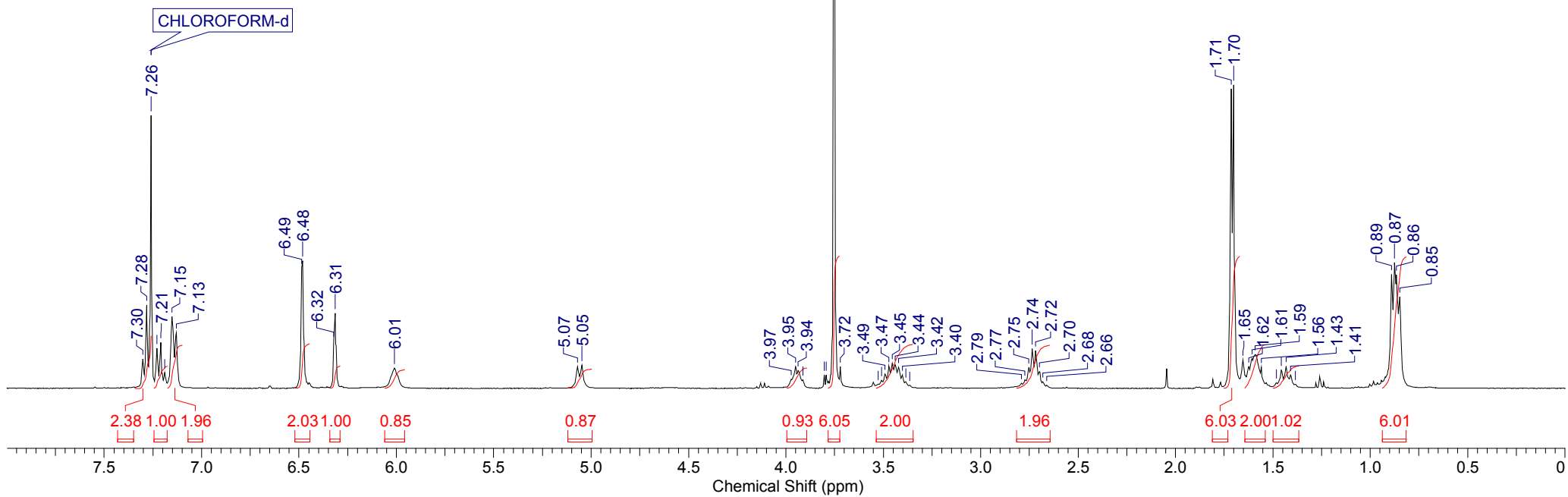
1H), 2.92 (dd, $J = 7.3, 13.2$ Hz, 1H), 1.70 (s, 6H), 1.46 (s, 9H). **HR-MS** 637.2828 ($C_{31}H_{42}N_4O_9 + Na^+$ calcd 637.2844).

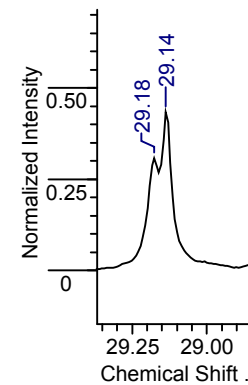
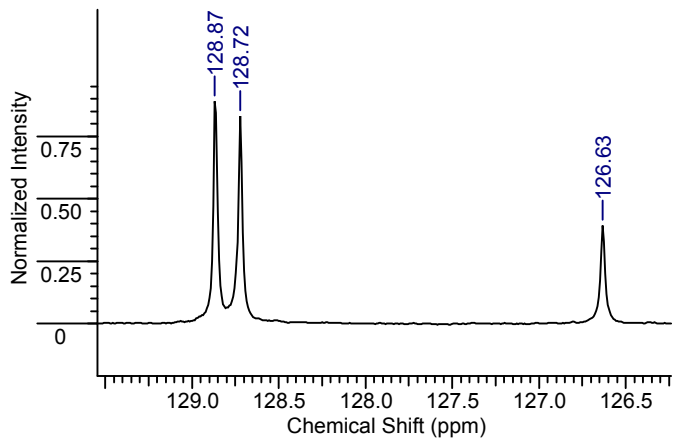
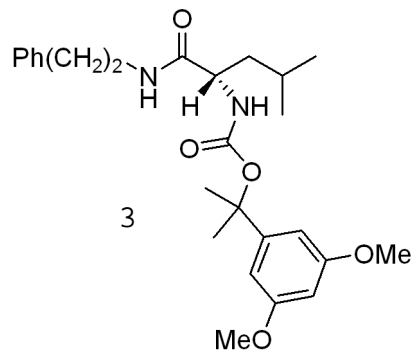
Gly-Phe-Gly-Gly-O^tBu (18): Ddz-Gly-Phe-Gly-Gly-O^tBu (**17**) (16.6 mg, 0.027 mmol) was dissolved in anhydrous MeCN (2 mL). The solution was then irradiated at 300 nm (Rayonnet[®]) in a quartz tube for 3 hours. The mixture was concentrated to dryness and purified by microscale flash column chromatography in a Pasteur pipette [SiO_2 , EtOAc then CH_2Cl_2 and $CH_2Cl_2/MeOH_{sat.NH_3}$ (95:5)] to provide the desired product as a yellowish solid (4.8 mg, 45 %). **¹H NMR** (360 MHz, $CDCl_3$) $\delta = 7.85$ (d, $J = 6.8$ Hz, 1H), 7.32-7.17 (5H), 6.92 (t, $J = 5.5$ Hz, 1H), 6.67 (t, $J = 4.5$ Hz, 1H), 4.59 (q, $J = 7.3$ Hz, 1H), 4.02-3.80 (6H), 3.20 (dd, $J = 6.8, 14.1$ Hz, 1H), 3.07 (dd, $J = 8.0, 14.4$ Hz, 1H), 1.73 (br s, 2H), 1.45 (s, 9H).

Ddz-Tyr(^tBu)-Gly-Phe-Gly-Gly-O^tBu (20): A mixture of A mixture of Ddz-Tyr(^tBu)-Dni (**19**) (1.3 mg, 2 μ mol), and Gly-Phe-Gly-Gly-O^tBu (**18**) (0.8 mg, 2 μ mol) in anhydrous MeCN (0.5 mL) was irradiated at 385 nm in a quartz tube for 2.5 hours, under argon, with stirring. The mixture was filtered and concentrated to dryness and purified by microscale flash column chromatography in a Pasteur pipette [SiO_2 , EtOAc then CH_2Cl_2 and $CH_2Cl_2/MeOH_{sat.NH_3}$ (95:5)] to provide the desired product as a yellow solid (1.2 mg, 75 %). **¹H NMR** (360 MHz, $CDCl_3$) $\delta = 7.34$ -7.22 (3H), 7.16 (d, $J = 6.8$, 3H), 7.07 (d, $J = 8.5$, 3H), 6.98 (d, $J = 5.9$, 1H), 6.92 (d, $J = 8.2$, 2H), 6.82 (br s, 1H), 6.43 (s, 2H), 6.23 (s, 1H), 5.33 (d, $J = 5.0$ Hz, 1H), 4.24 (m, 1H), 4.16-4.00 (4H), 3.70-3.59 (8H), 3.30 (dd, $J = 15.2, 4.3$ Hz, 1H), 3.06 (dd, $J = 13.2, 5.5$ Hz, 2H), 2.89 (dd, $J = 14.1, 8.7$ Hz, 1H), 2.53 (dd, $J = 13.4, 10.2$ Hz, 1H), 1.70 (s, 3H), 1.61 (s, 3H), 1.44 (s, 9H), 1.33 (s, 9H). **¹³C NMR** (125 MHz, $CDCl_3$) $\delta = 173.2, 171.4, 170.6, 170.3, 169.6, 160.9$ (2xC), 155.5, 154.8, 148.5, 136.8, 130.6, 129.7 (2xC), 129.2 (2xC), 128.9 (2xC), 127.2, 124.6 (2xC), 103.1 (2xC), 98.2, 82.5, 81.9, 76.6, 56.8, 56.5, 55.4 (2xC), 44.0, 42.7, 41.6, 36.9, 36.8, 30.4, 29.0 (3xC), 28.22 (3xC), 28.15. **ESI-MS:** 856.4 [M+Na]⁺.

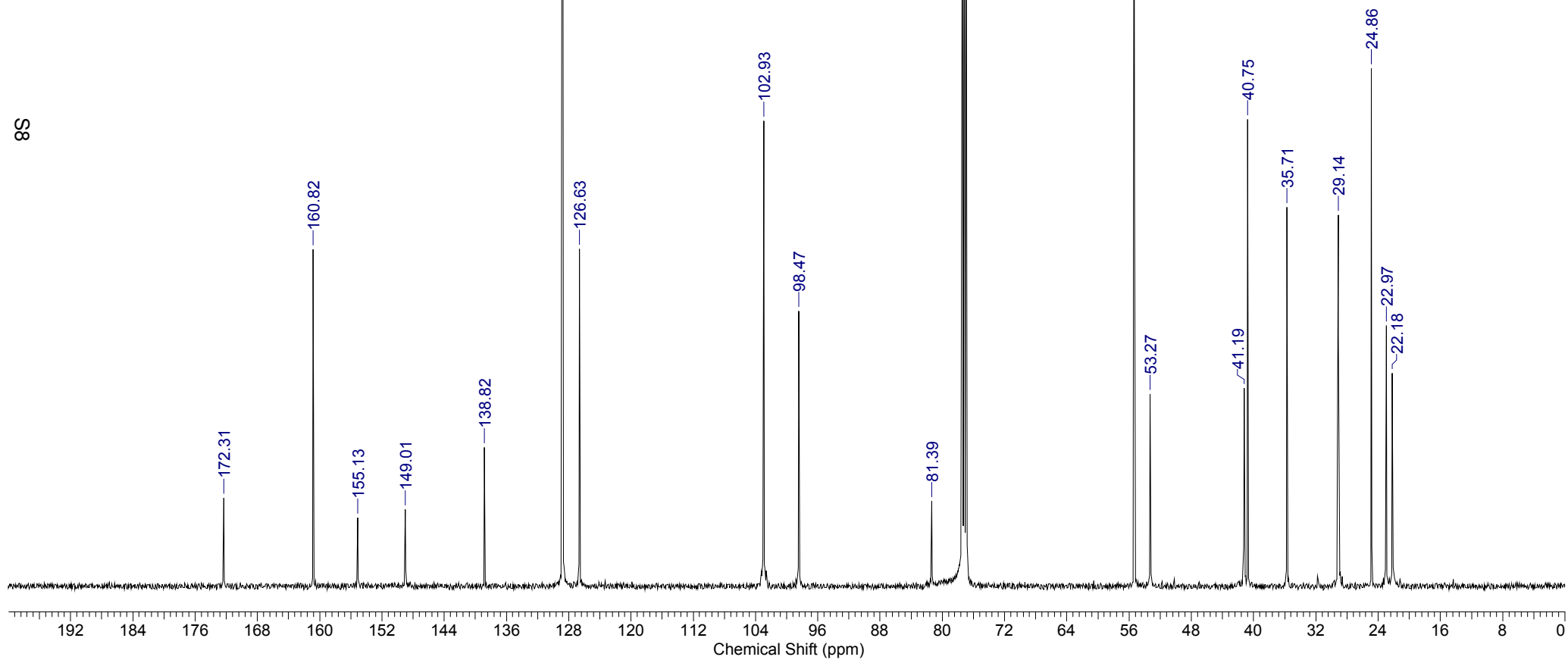


S7

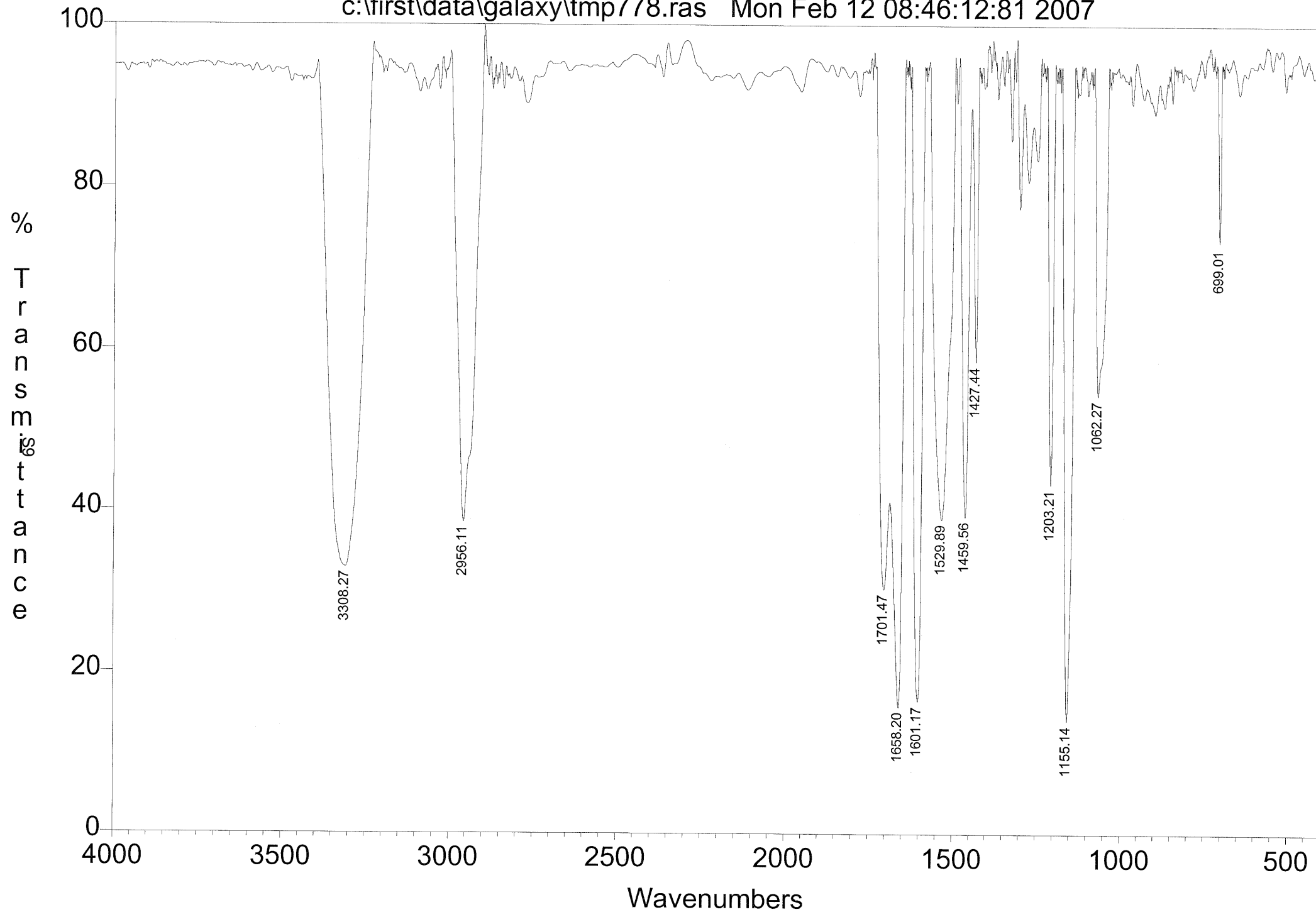




8S



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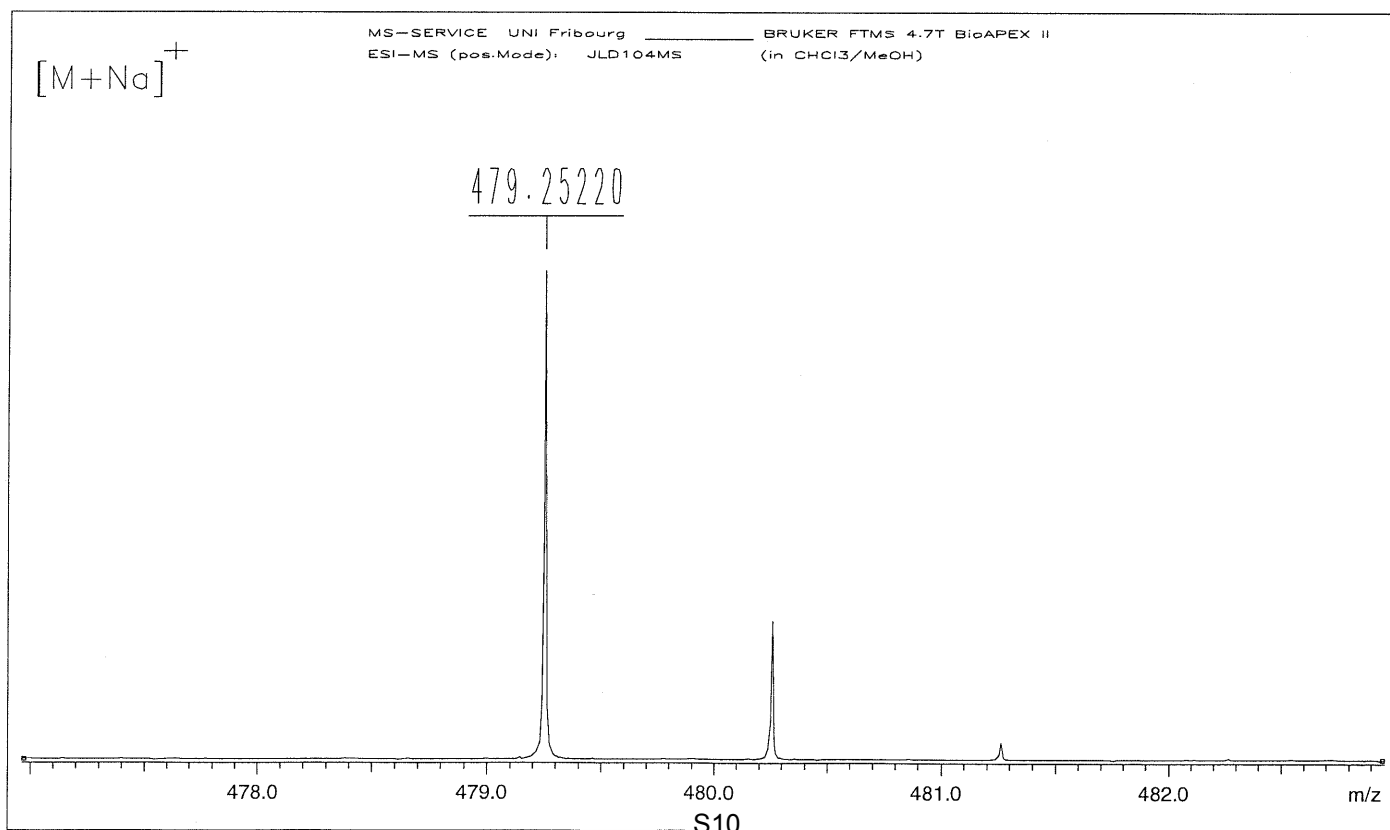
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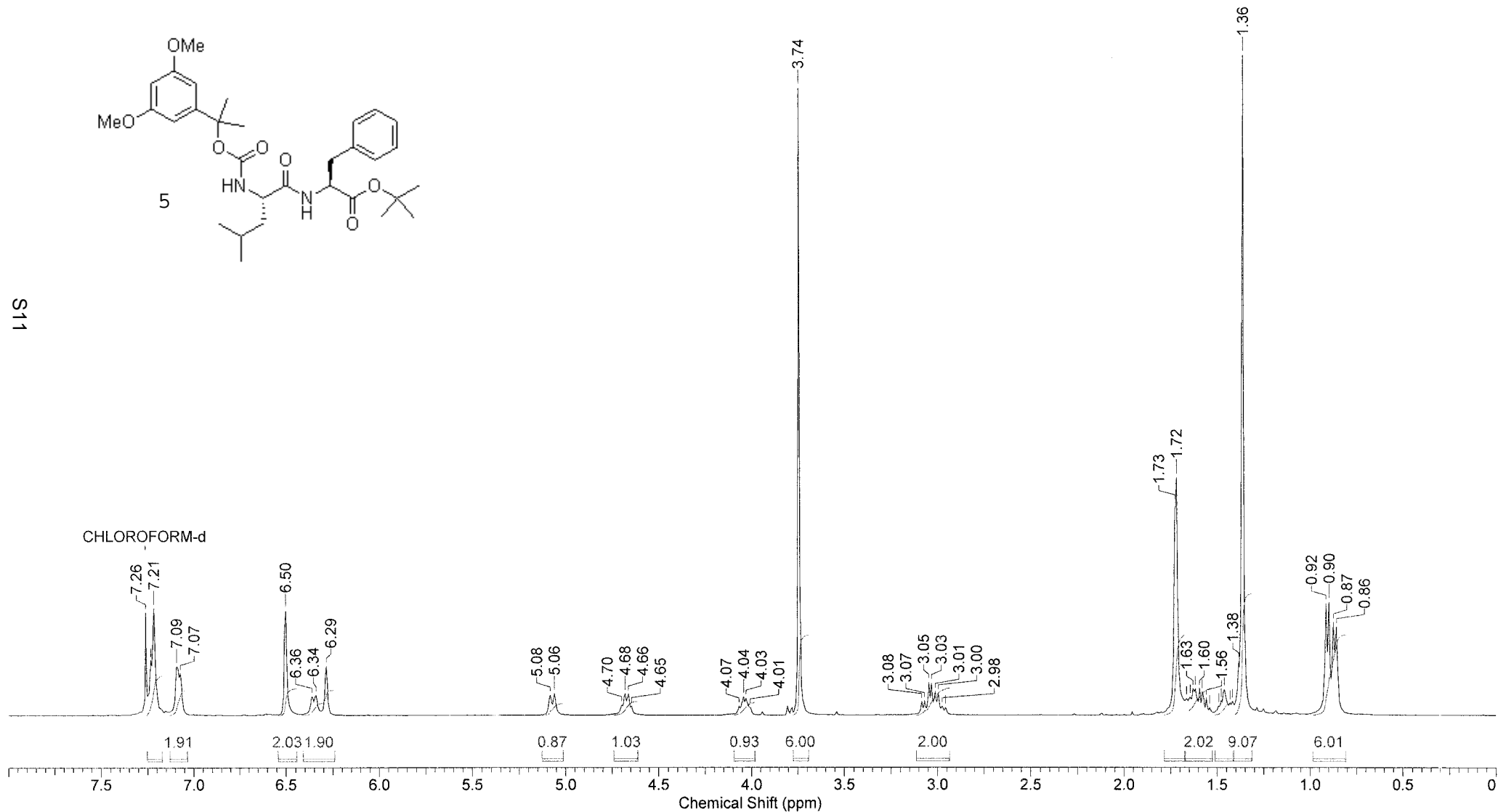
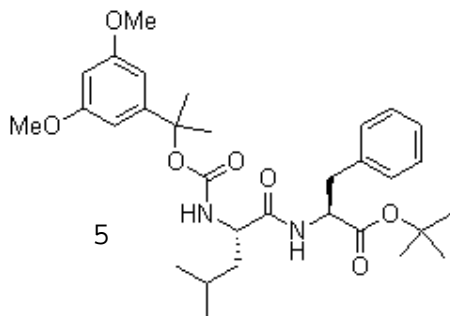
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5	23	35	4	7	0	479.2500259	8.5	2.169e-03
6	23	38	1	8	1	479.2489633	5.0	3.232e-03
7	31	33	3	2	0	479.2567287	17.0	4.534e-03
8	21	36	4	7	1	479.2476206	5.5	4.574e-03
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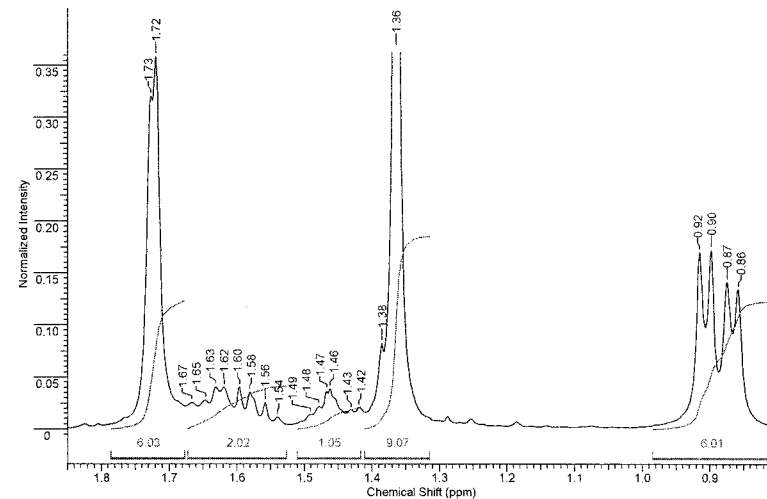
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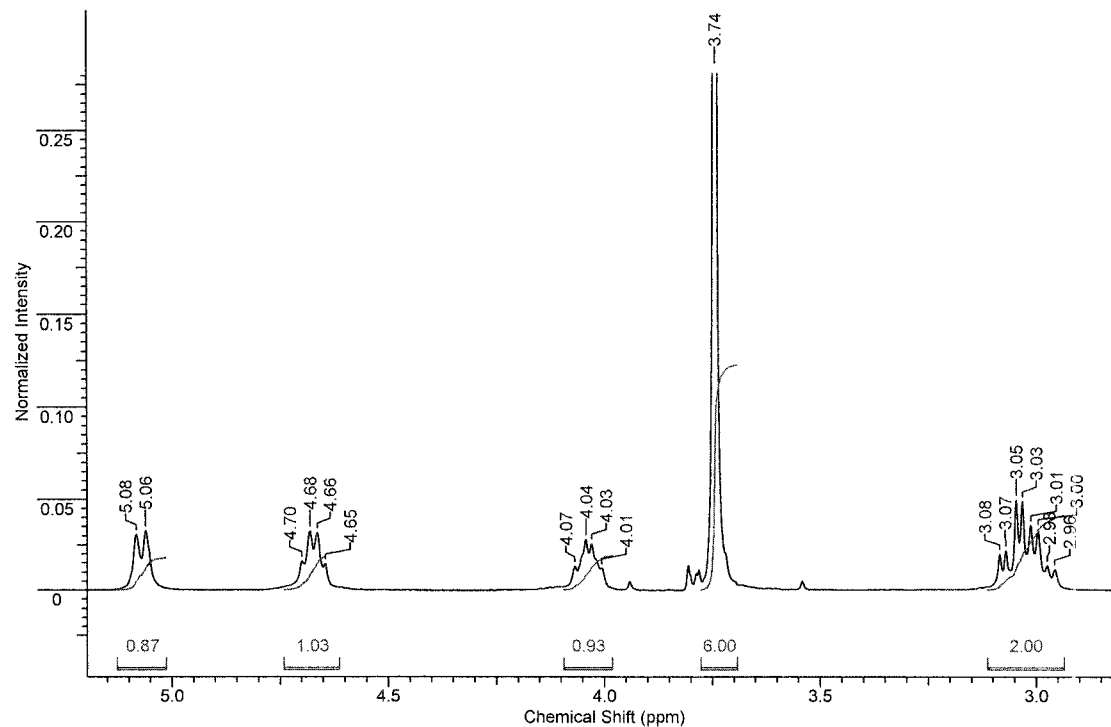
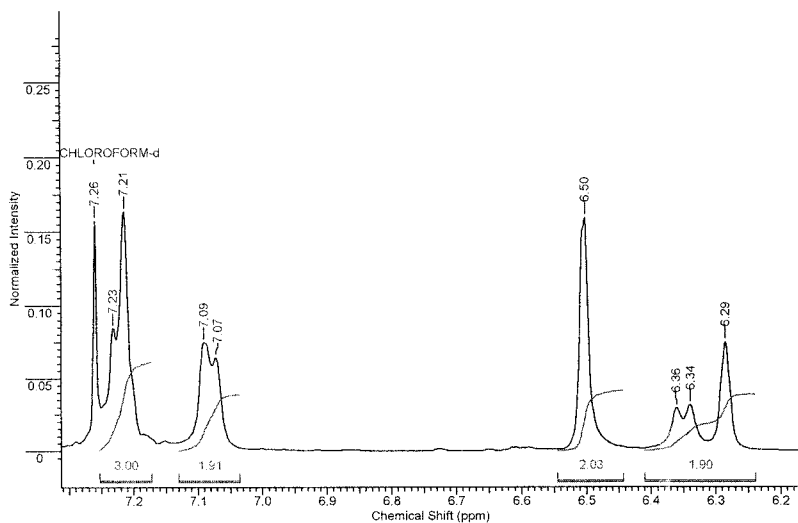


jld124

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3	0.90	323.5	0.1727	16	1.60	574.6	0.0404	29	3.07	1105.5	0.0216	42	6.29	2263.5	0.0750
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9	1.46	526.5	0.0392	22	1.73	621.8	0.3205	35	4.07	1465.1	0.0132	48	7.21	2598.2	0.1638
10	1.47	528.3	0.0368	23	2.96	1065.1	0.0114	36	4.65	1673.1	0.0144	49	7.23	2604.6	0.0844
11	1.48	532.4	0.0217	24	2.98	1071.4	0.0135	37	4.66	1679.5	0.0316	50	7.26	2614.5	0.1572
12	1.49	536.9	0.0139	25	3.00	1078.7	0.0337	38	4.68	1685.8	0.0326				
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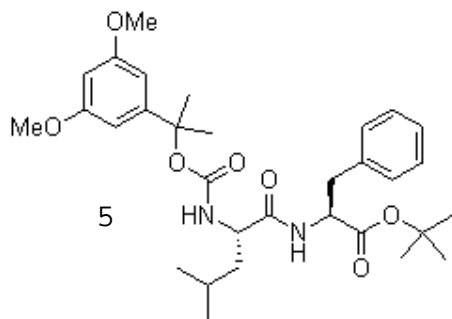


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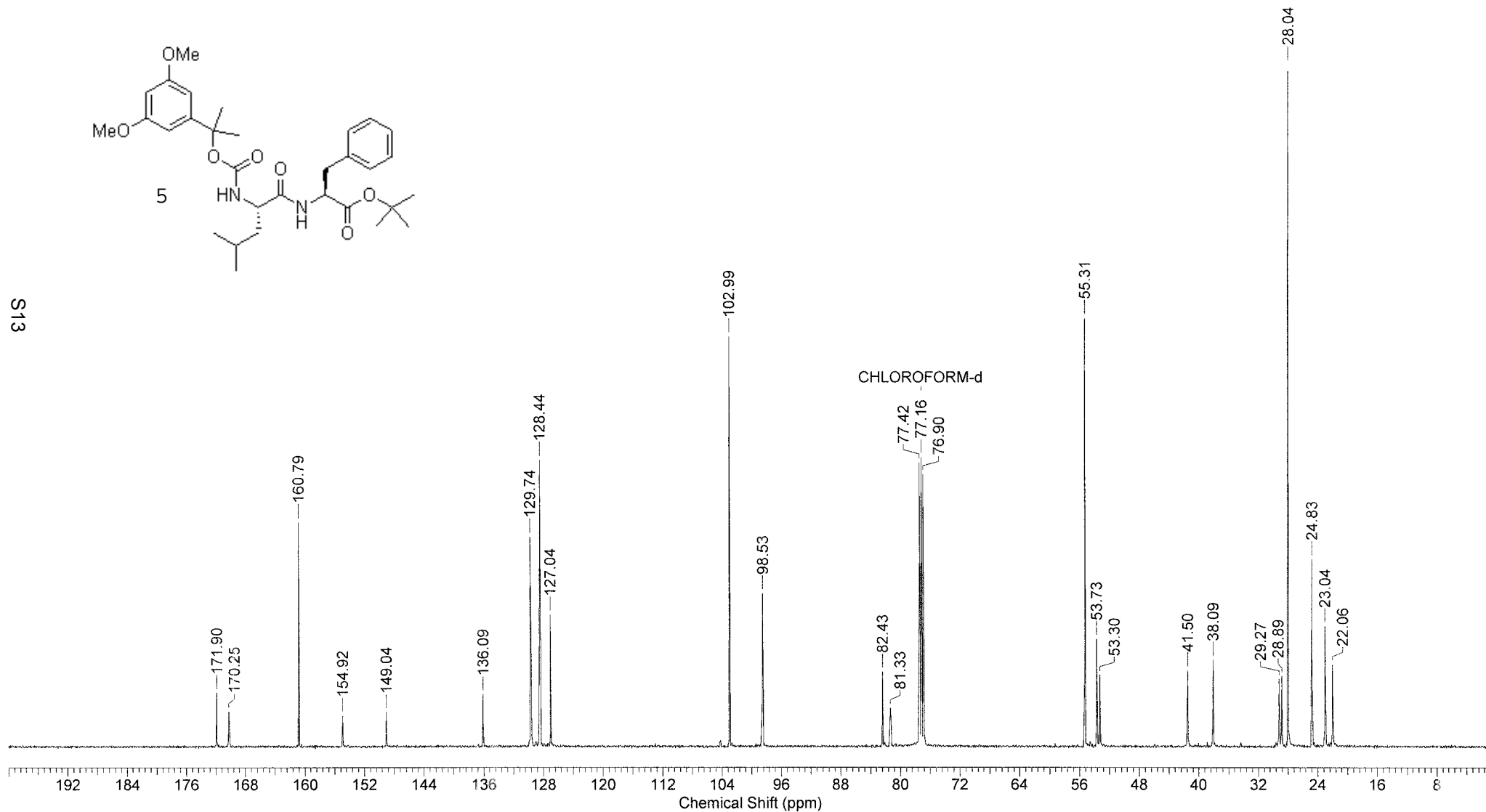


jld124, C13 CPD

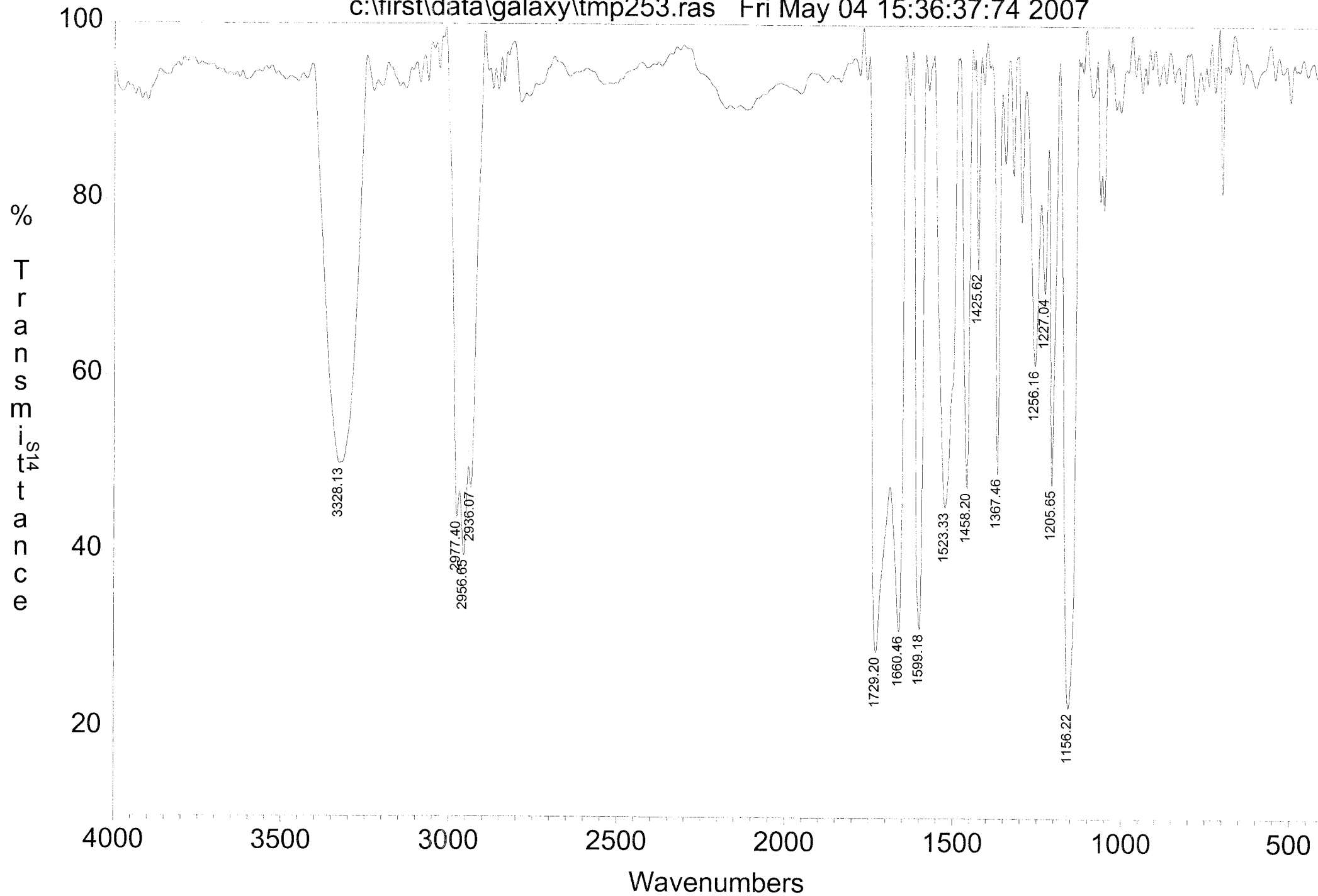
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File Name	\HOME\Debieux\My Documents\Chimie\Doctorat\NMR\debi3282.bbo_002001r			Frequency (MHz)	125.76
Nucleus	13C	Number of Transients	7322	Origin	drx500
Owner	nmruser	Points Count	32768	Pulse Sequence	zgdc
SW(cyclical) (Hz)	30120.48	Solvent	CHLOROFORM-d	Receiver Gain	16384.00
Sweep Width (Hz)	30119.56	Temperature (degree C)	25.000	Spectrum Offset (Hz)	12567.2520

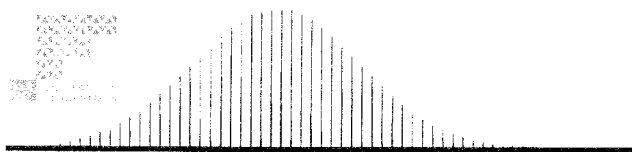


S15



c:\first\data\galaxy\tmp253.ras Fri May 04 15:36:37:74 2007





FTMS 4.7T BioAPEX II MS-Service UNI-Fribourg

ESI-MS: JLD124-1

XMASS Mass Analysis for /Data/UNI_FR/DEBI2617_ESI/20/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

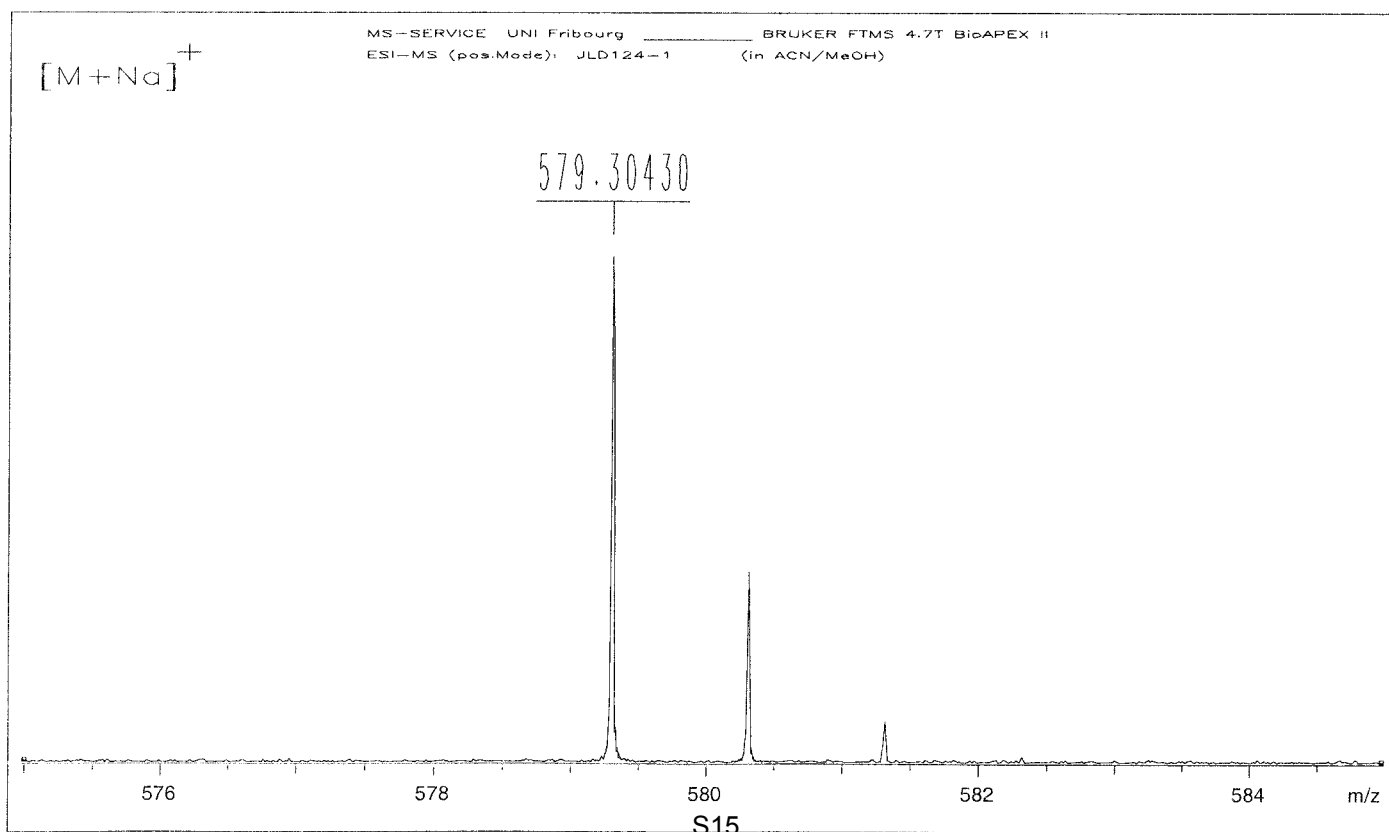
Ion mass = 579.3043030

Charge = +1

#	C	H	N	O	Na	mass	DBE	error
---	---	---	---	---	----	------	-----	-------

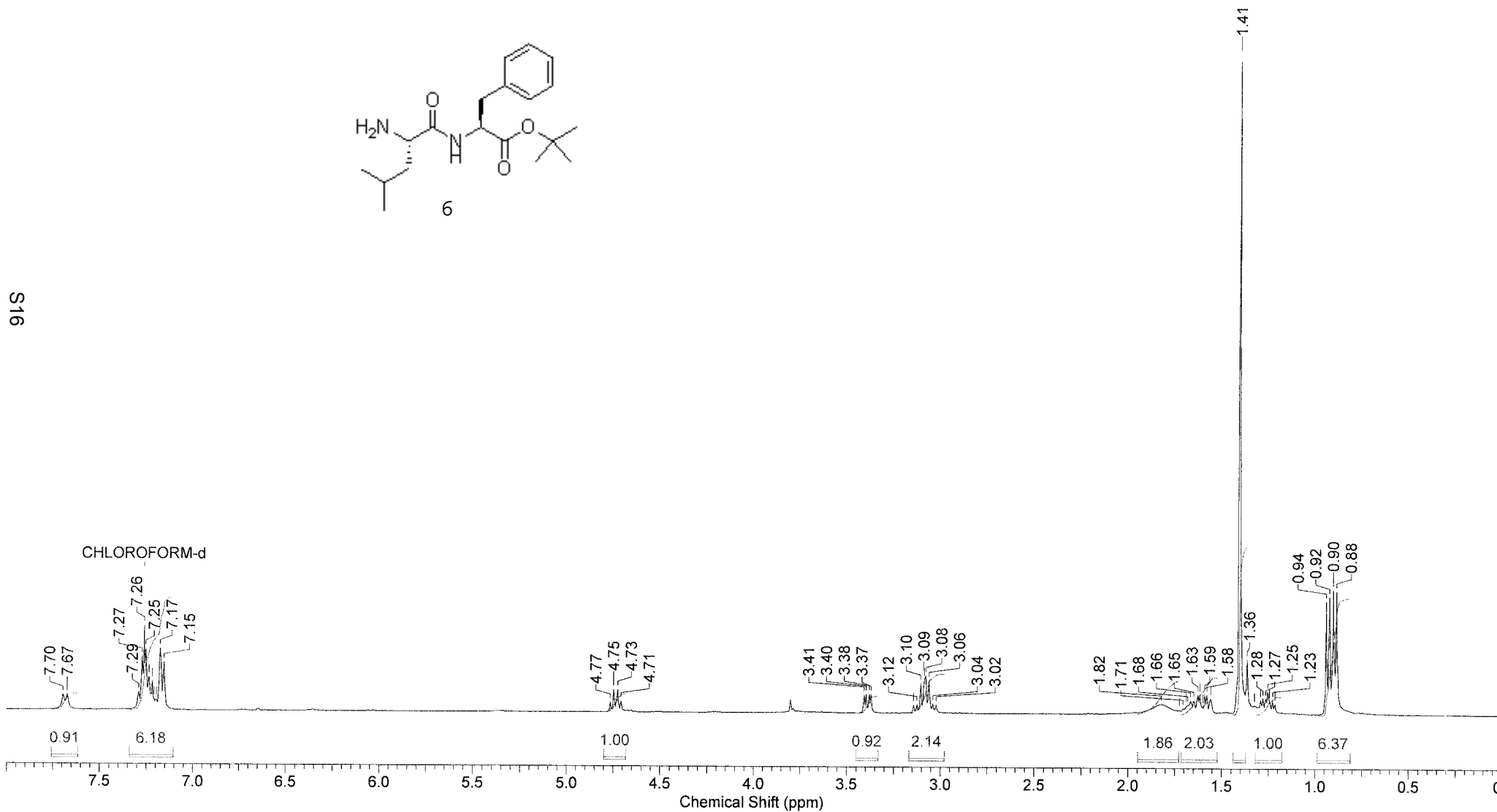
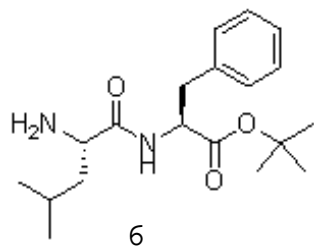
*** Mass Analysis for mass 579.3043030

1	31	44	2	7	1	579.3040729	10.5	2.301e-04
2	29	39	8	5	0	579.3037928	14.5	5.102e-04
3	31	41	5	6	0	579.3051355	14.0	8.325e-04
4	29	42	5	6	1	579.3027302	11.0	1.573e-03
5	33	43	2	7	0	579.3064782	13.5	2.175e-03
6	34	42	3	4	1	579.3067529	15.0	2.450e-03
7	27	40	8	5	1	579.3013875	11.5	2.915e-03
8	26	41	7	8	0	579.3011127	10.0	3.190e-03
9	36	41	3	4	0	579.3091582	18.0	4.855e-03
10	24	42	7	8	1	579.2987075	7.0	5.596e-03



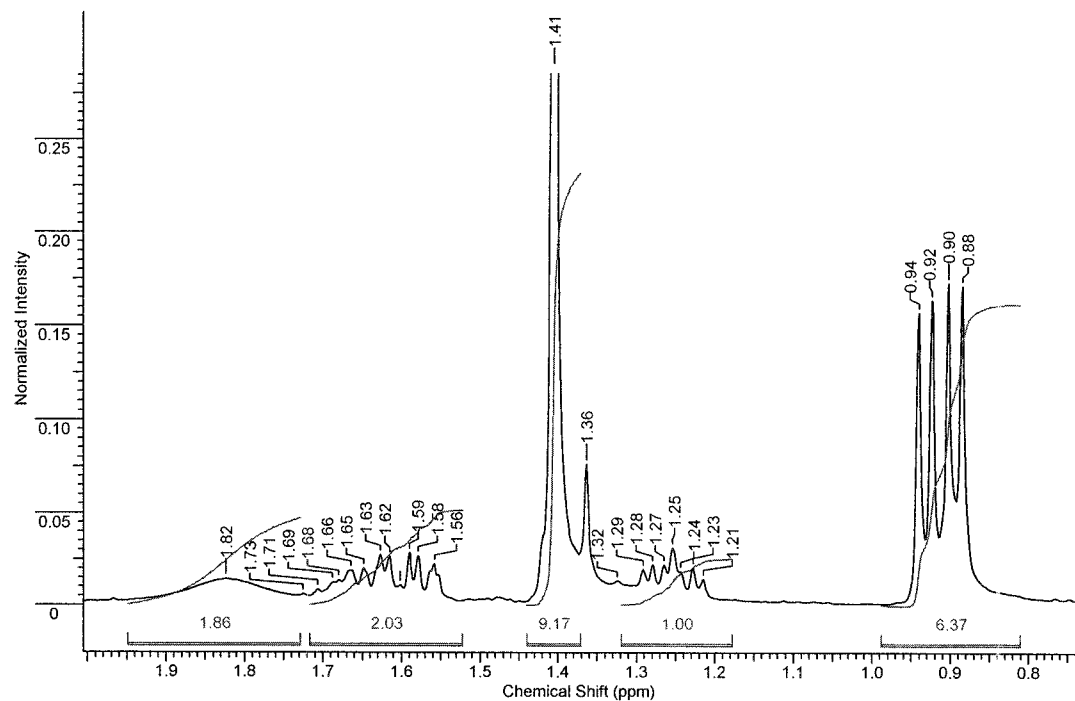
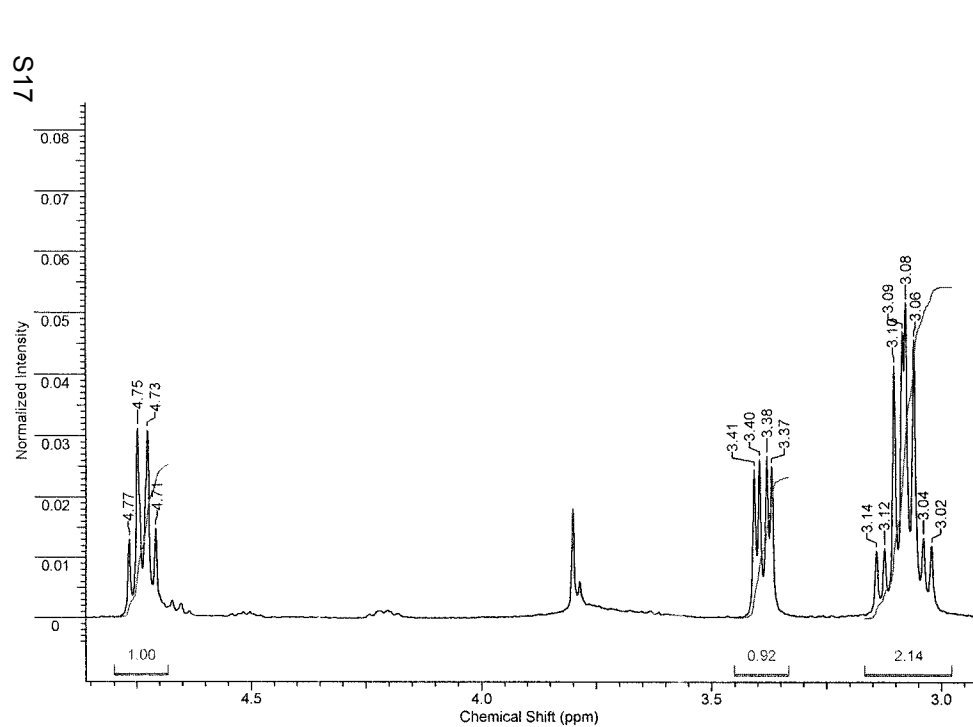
jld125

Acquisition Time (sec)	2.2021	Comment	PROTONNR CDCl3 u jld 16		Date	22 May 2007 12:39:28	
File Name	\\HOME\Debieux\My Documents\Chimie\Doctorat\NMR\jld125-2F1_001001r			Frequency (MHz)	360.13		
Nucleus	1H	Number of Transients	16	Origin	dpx360	Original Points Count	16384
Owner	nmruser	Points Count	16384	Pulse Sequence	zg30	Receiver Gain	143.70
SW(cyclical) (Hz)	7440.48	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	2210.5950	
Sweep Width (Hz)	7440.02	Temperature (degree C)	27.000				



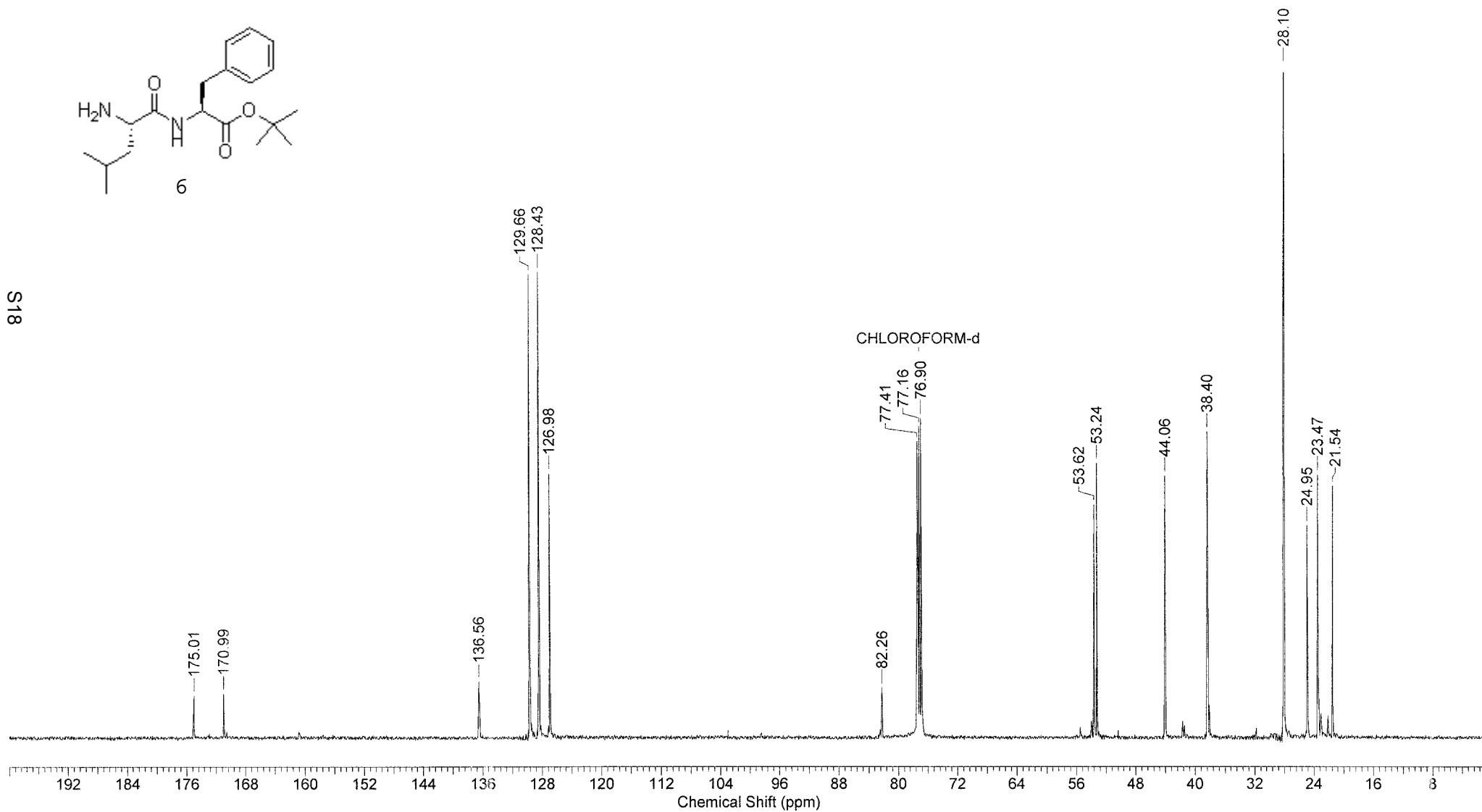
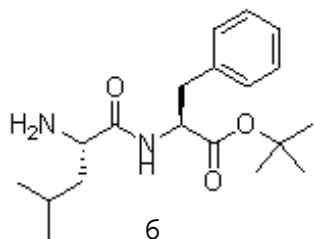
jld125

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	0.88	318.5	0.1711	15	1.56	561.0	0.0221	29	3.04	1095.0	0.0133	43	4.77	1716.3	0.0131
2	0.90	324.8	0.1729	16	1.58	568.7	0.0267	30	3.06	1102.3	0.0457	44	7.15	2576.4	0.0667
3	0.92	332.5	0.1635	17	1.59	572.8	0.0286	31	3.08	1108.6	0.0517	45	7.17	2583.7	0.0863
4	0.94	338.4	0.1570	18	1.60	576.9	0.0108	32	3.09	1111.4	0.0470	46	7.20	2591.4	0.0153
5	1.21	437.4	0.0141	19	1.62	581.9	0.0265	33	3.10	1117.7	0.0415	47	7.21	2595.5	0.0151
6	1.23	442.0	0.0204	20	1.63	585.9	0.0272	34	3.12	1125.0	0.0116	48	7.22	2598.6	0.0407
7	1.24	447.9	0.0182	21	1.65	593.7	0.0198	35	3.14	1131.4	0.0112	49	7.23	2605.5	0.0464
8	1.25	451.5	0.0311	22	1.66	599.6	0.0188	36	3.37	1213.6	0.0250	50	7.25	2611.4	0.0857
9	1.27	455.6	0.0218	23	1.68	605.0	0.0136	37	3.38	1217.2	0.0268	51	7.26	2614.5	0.1180
10	1.28	460.6	0.0218	24	1.69	607.7	0.0122	38	3.40	1223.1	0.0261	52	7.27	2618.6	0.0748
11	1.29	465.1	0.0194	25	1.71	614.6	0.0085	39	3.41	1227.2	0.0245	53	7.29	2625.4	0.0244
12	1.32	477.0	0.0131	26	1.73	621.4	0.0059	40	4.71	1695.8	0.0148	54	7.67	2763.0	0.0208
13	1.36	491.0	0.0762	27	1.82	656.8	0.0141	41	4.73	1702.2	0.0309	55	7.70	2771.2	0.0206
14	1.41	506.0	1.0000	28	3.02	1088.2	0.0119	42	4.75	1709.9	0.0313				

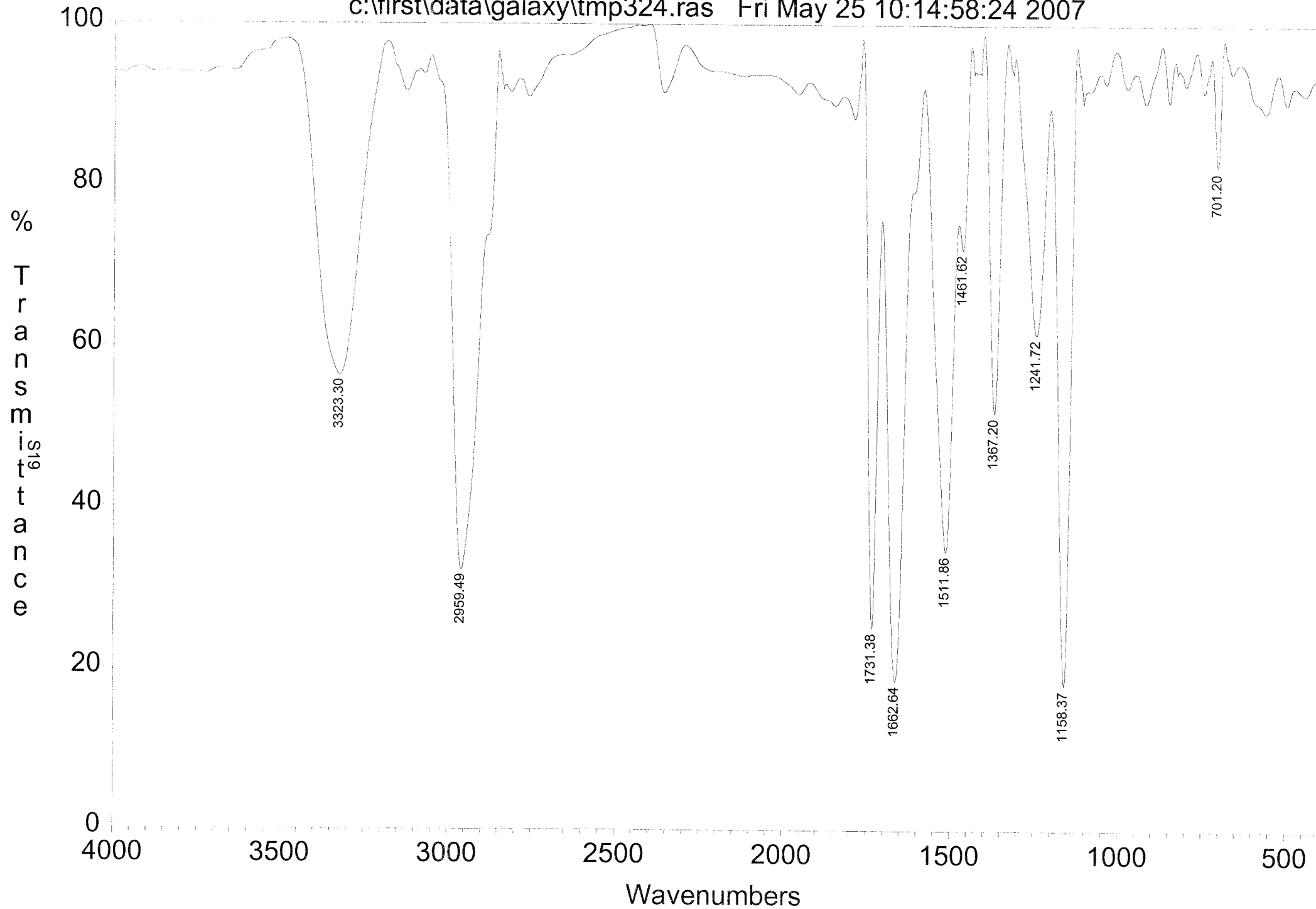


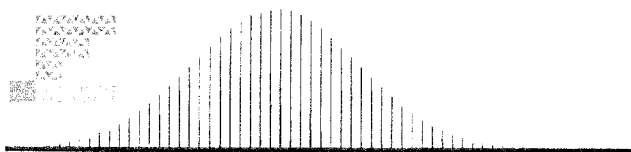
jld125, C13 CPD

Acquisition Time (sec)	1.0879	Comment	5 mm Multinuclear Z3149/0097		Date	25 May 2007 06:00:32	
File Name	\\HOME\Debieux\My Documents\Chimie\Doctorat\NMR\debi3316.bbo_002001r			Frequency (MHz)	125.76		
Nucleus	13C	Number of Transients	15646	Origin	drx500	Original Points Count	32768
Owner	nmruser	Points Count	32768	Pulse Sequence	zgdc	Receiver Gain	16384.00
SW(cyclical) (Hz)	30120.48	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	12568.1719	
Sweep Width (Hz)	30119.56	Temperature (degree C)	25.000				



c:\first\data\galaxy\tmp324.ras Fri May 25 10:14:58:24 2007





FTMS 4.7T BioAPEX II MS-Service UNI-Fribourg

ESI-MS: JLD125-2

XMASS Mass Analysis for /Data/UNI_FR/DEBI2614_ESI/10/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

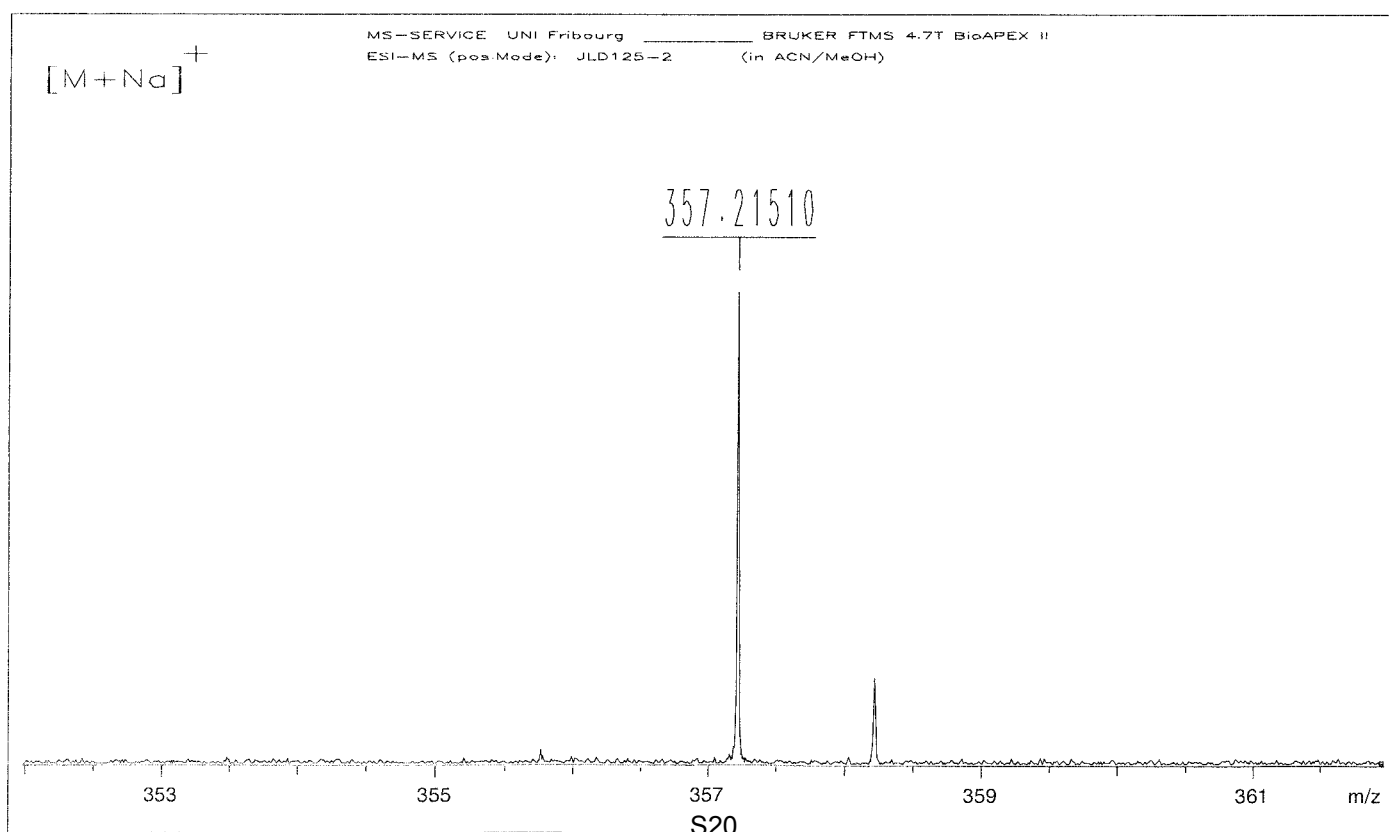
Ion mass = 357.2151030

Charge = +1

#	C	H	N	O	Na	mass	DBE	error
---	---	---	---	---	----	------	-----	-------

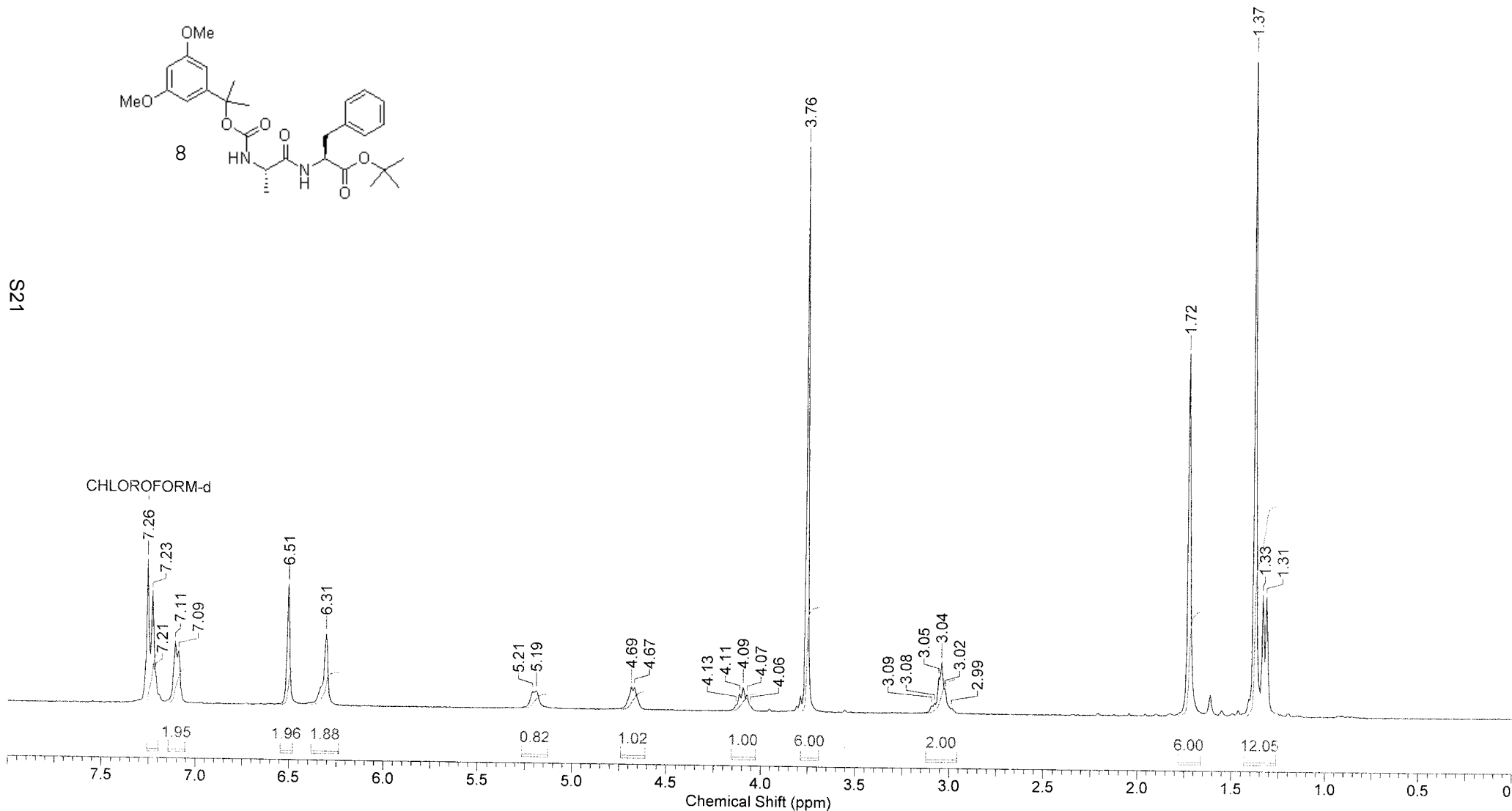
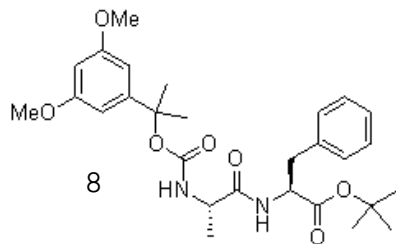
*** Mass Analysis for mass 357.2151030

1	19	30	2	3	1	357.2148639	5.5	2.391e-04
2	18	31	1	6	0	357.2145892	4.0	5.138e-04
3	17	25	8	1	0	357.2145839	9.5	5.191e-04
4	19	27	5	2	0	357.2159266	9.0	8.236e-04
5	17	28	5	2	1	357.2135213	6.0	1.582e-03
6	16	29	4	5	0	357.2132465	4.5	1.857e-03
7	21	29	2	3	0	357.2172692	8.5	2.166e-03
8	16	32	1	6	1	357.2121839	1.0	2.919e-03
9	15	26	8	1	1	357.2121786	6.5	2.924e-03
10	8	30	8	6	1	357.2180518	-2.5	2.949e-03



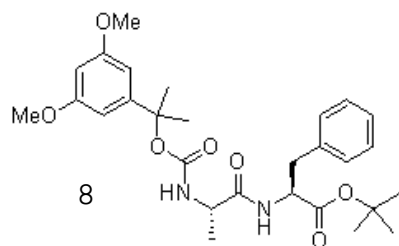
jld172

Acquisition Time (sec)	2.2021	Comment	PROTONNR CDCl3 u jld 12		Date	12 Mar 2008 14:17:36	
File Name	\\HOME\DebieuxJ\My Documents\Chimie\Doctorat\NMR\jld172-1_001001r			Frequency (MHz)	360.13		
Nucleus	1H	Number of Transients	16	Origin	dpx360	Original Points Count	16384
Owner	nmruser	Points Count	16384	Pulse Sequence	zg30	Receiver Gain	812.70
SW(cyclical) (Hz)	7440.48	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	2210.5950	
Sweep Width (Hz)	7440.02	Temperature (degree C)	27.000				

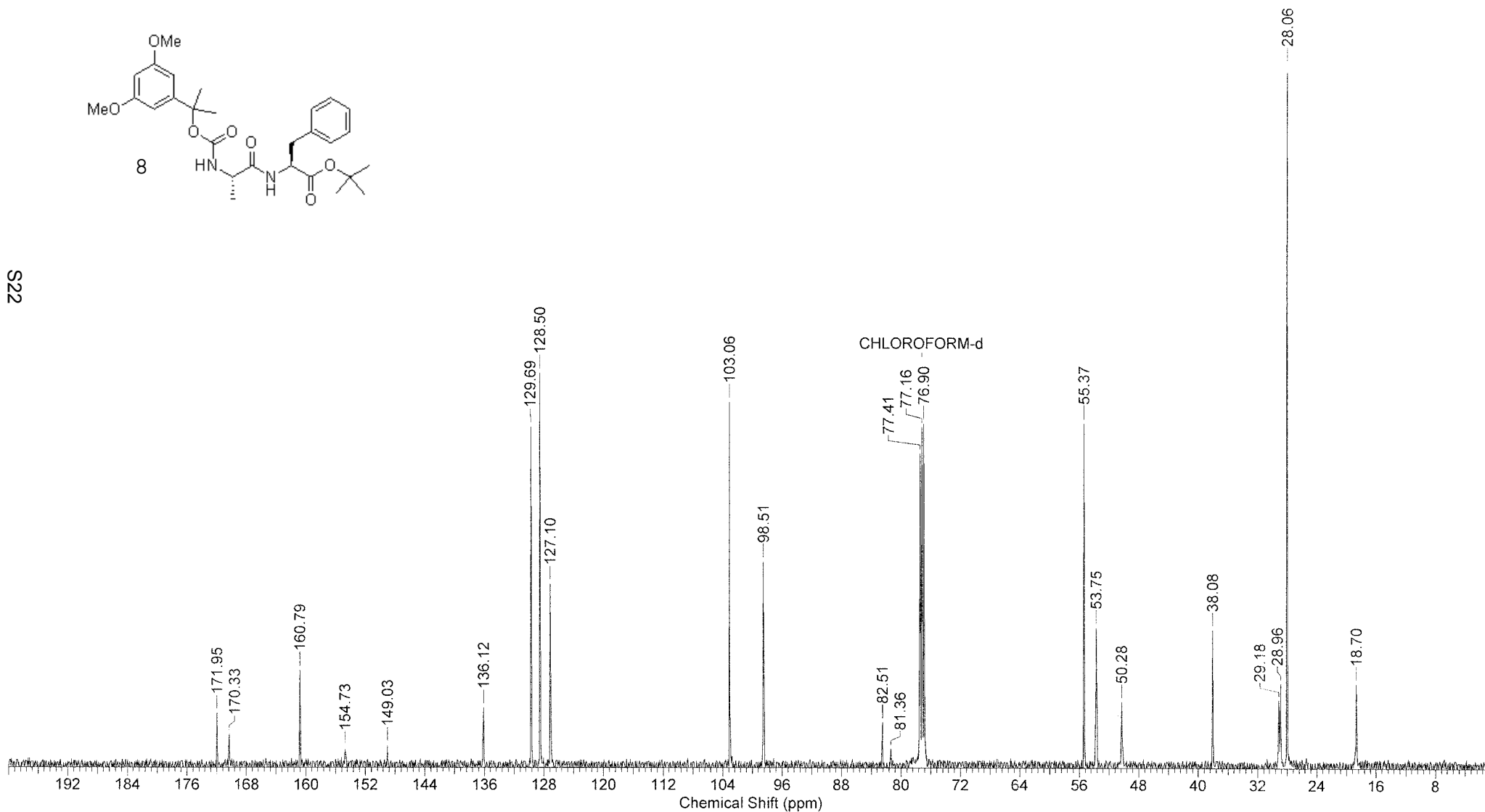


jld172, C13

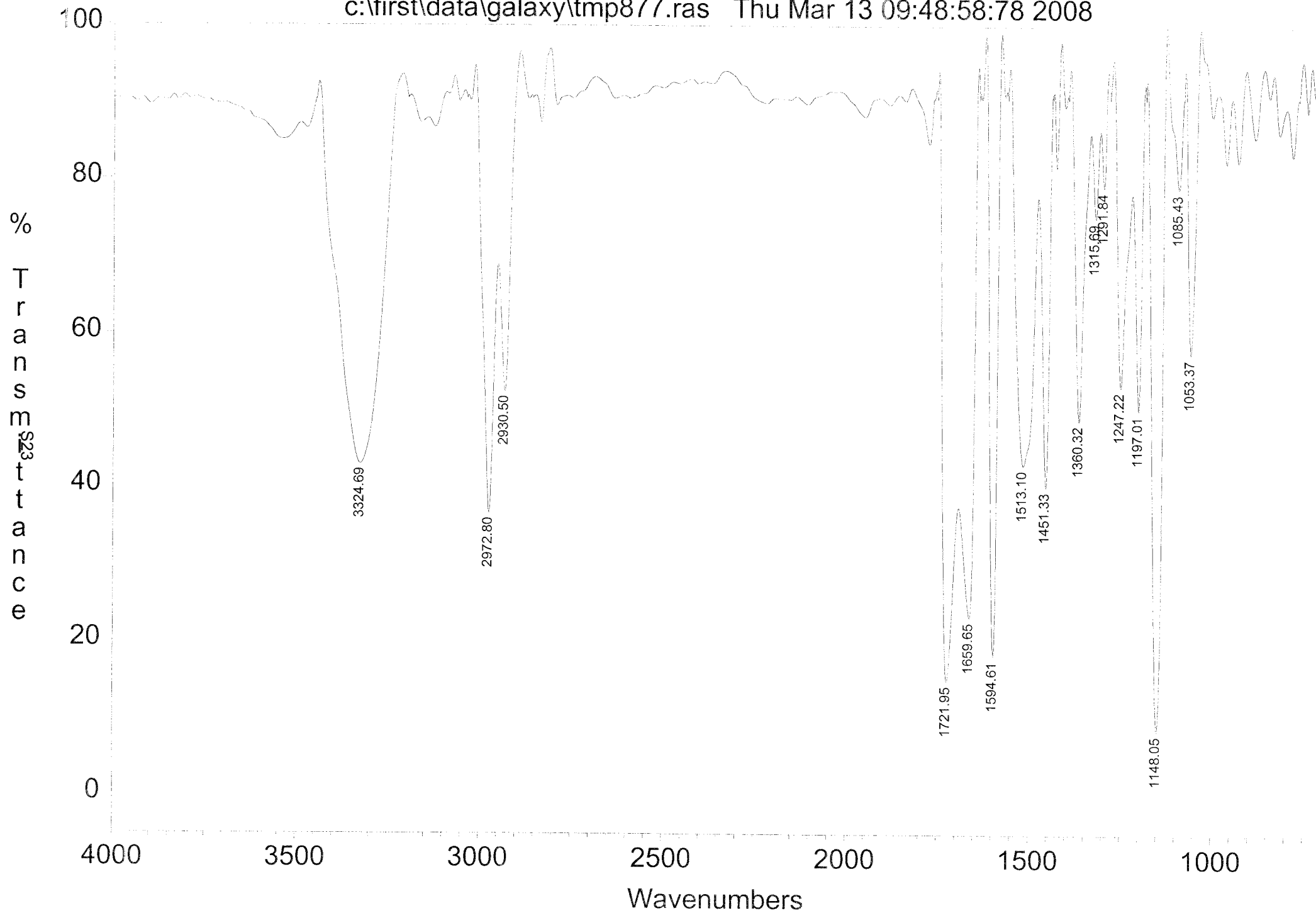
Acquisition Time (sec)	1.0879	Comment	all_carbon	Date	14 Mar 2008 14:06:56
File Name	\\HOME\Debieux\My Documents\Chimie\Doctorat\NMR\debi3758.bbo_002001r			Frequency (MHz)	125.76
Nucleus	13C	Number of Transients	1974	Origin	drx500
Owner	nmruser	Points Count	32768	Pulse Sequence	zgdc
SW(cyclical) (Hz)	30120.48	Solvent	CHLOROFORM-d	Receiver Gain	16384.00
Sweep Width (Hz)	30119.56	Temperature (degree C)	25.000	Spectrum Offset (Hz)	13923.0781

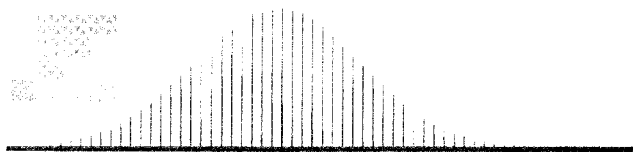


S22



c:\first\data\galaxy\tmp877.ras Thu Mar 13 09:48:58:78 2008





FTMS 4.7T BioAPEX II MS-Service UNI-Fribourg

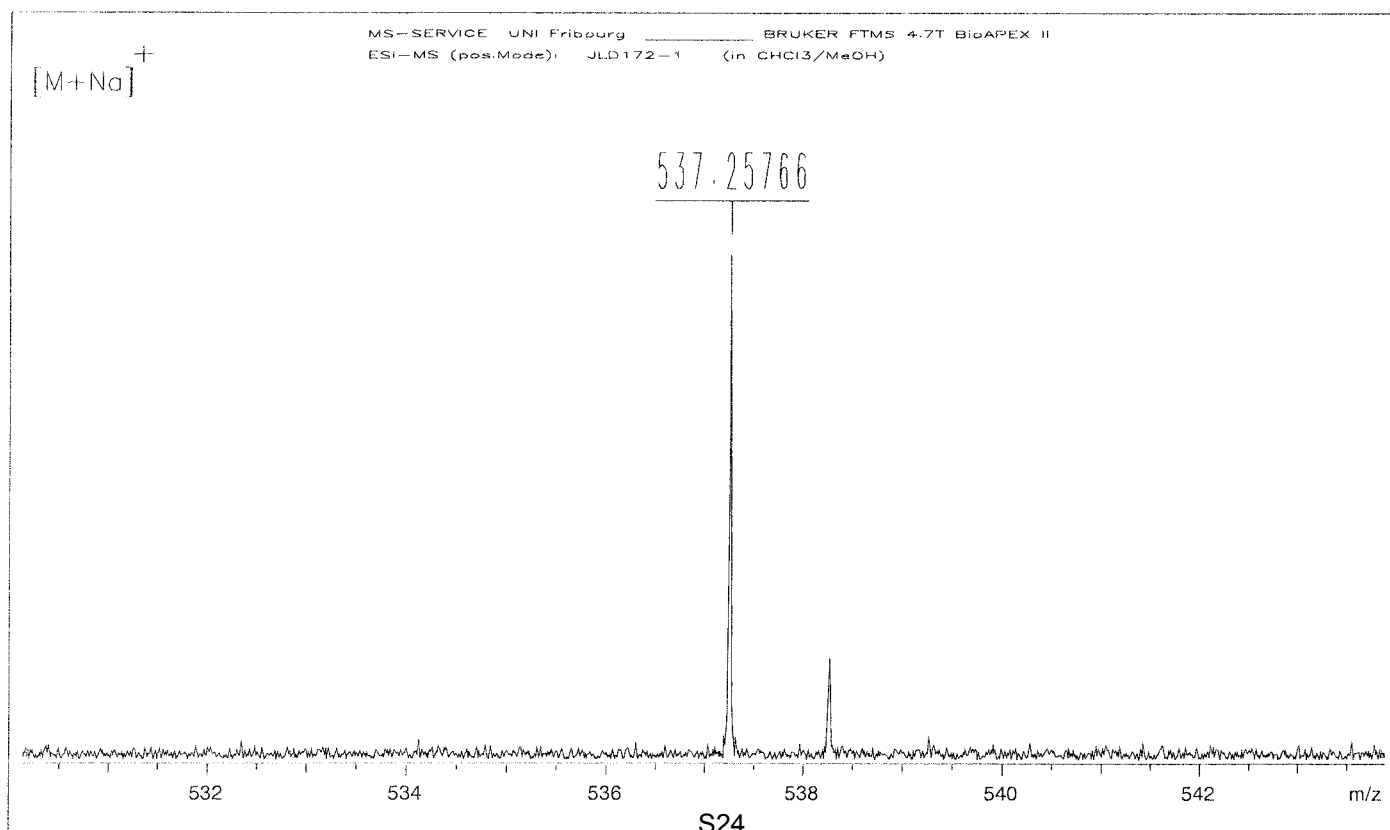
ESI-MS: JLD172-1

XMASS Mass Analysis for /Data/UNI_FR/DEBI3230_ESI/5/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 537.2576570

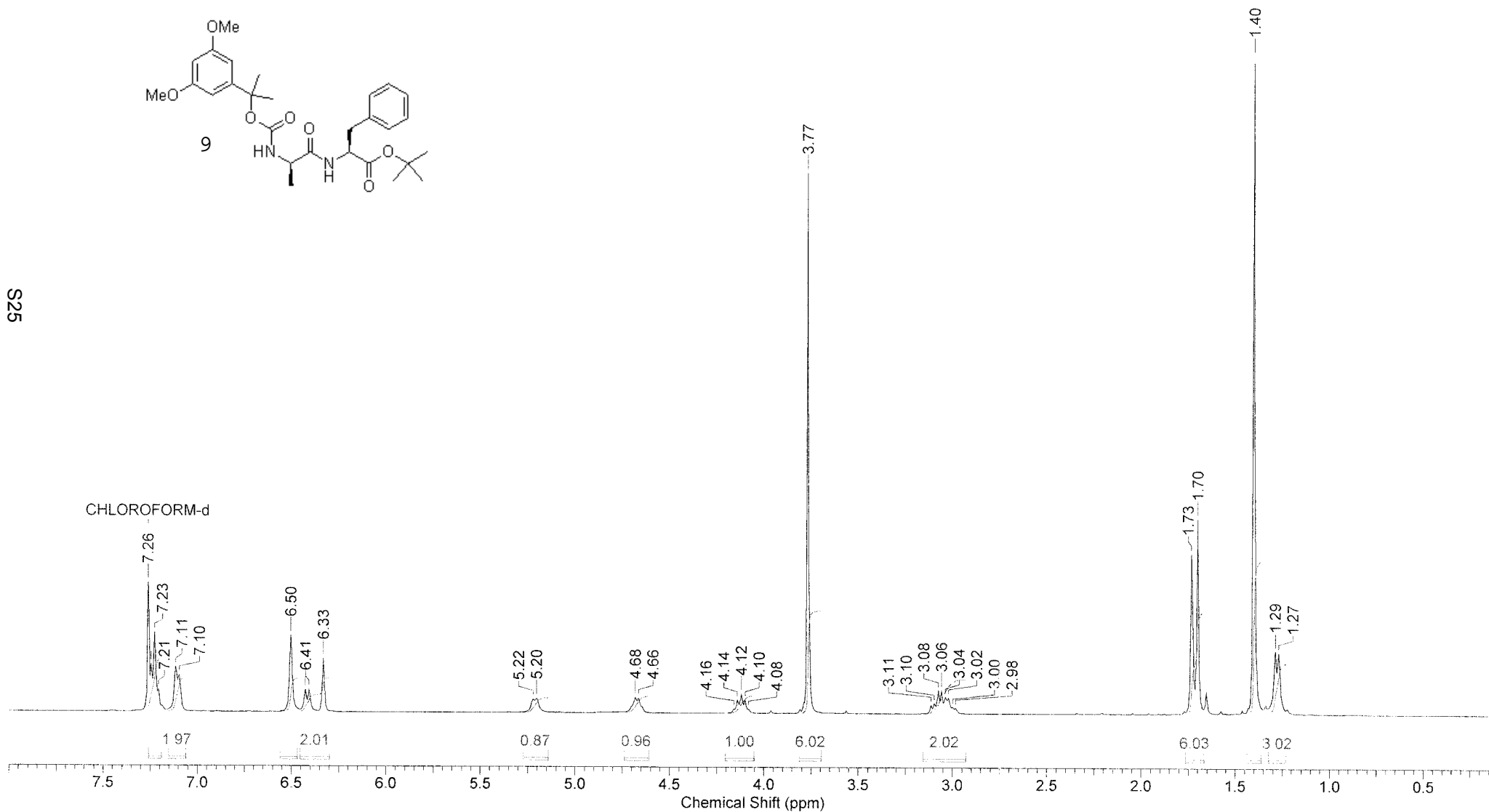
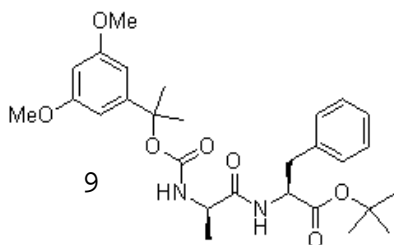
Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 537.2576570								
1	28	38	2	7	1	537.2571227	10.5	5.343e-04
2	27	39	1	10	0	537.2568479	9.0	8.091e-04
3	30	37	2	7	0	537.2595280	13.5	1.871e-03
4	25	37	4	9	0	537.2555052	9.5	2.152e-03
5	25	40	1	10	1	537.2544426	6.0	3.214e-03
6	23	38	4	9	1	537.2530999	6.5	4.557e-03
7	24	40	3	9	1	537.2656760	6.0	8.019e-03
8	26	39	3	9	0	537.2680813	9.0	1.042e-02
9	27	38	4	6	1	537.2683561	10.5	1.070e-02
10	29	35	3	7	0	537.2469519	14.0	1.071e-02



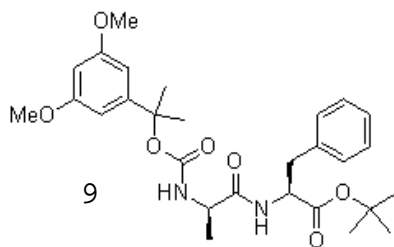
jld173

Acquisition Time (sec)	2.2021	Comment	PROTONNR CDCl3 u jld 43		Date	18 Mar 2008 12:41:36	
File Name	\HOME\Debieux\My Documents\Chimie\Doctorat\NMR\jld173-1_001001r			Frequency (MHz)	360.13		
Nucleus	1H	Number of Transients	16	Origin	dpx360	Original Points Count	16384
Owner	nmruser	Points Count	16384	Pulse Sequence	zg30	Receiver Gain	128.00
SW(cyclical) (Hz)	7440.48	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	2210.5950	
Sweep Width (Hz)	7440.02	Temperature (degree C)	27.000				

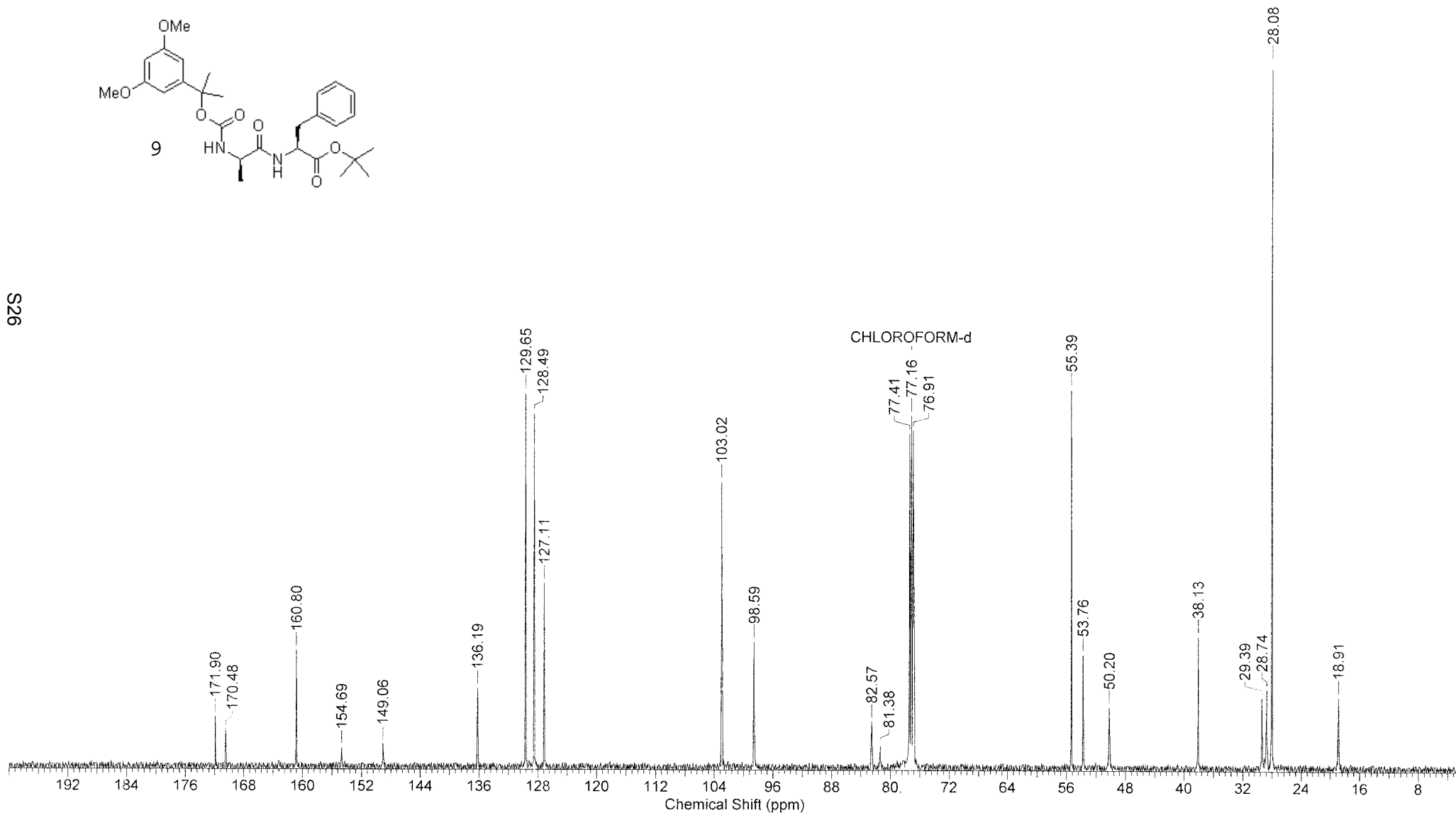


jld173, C13

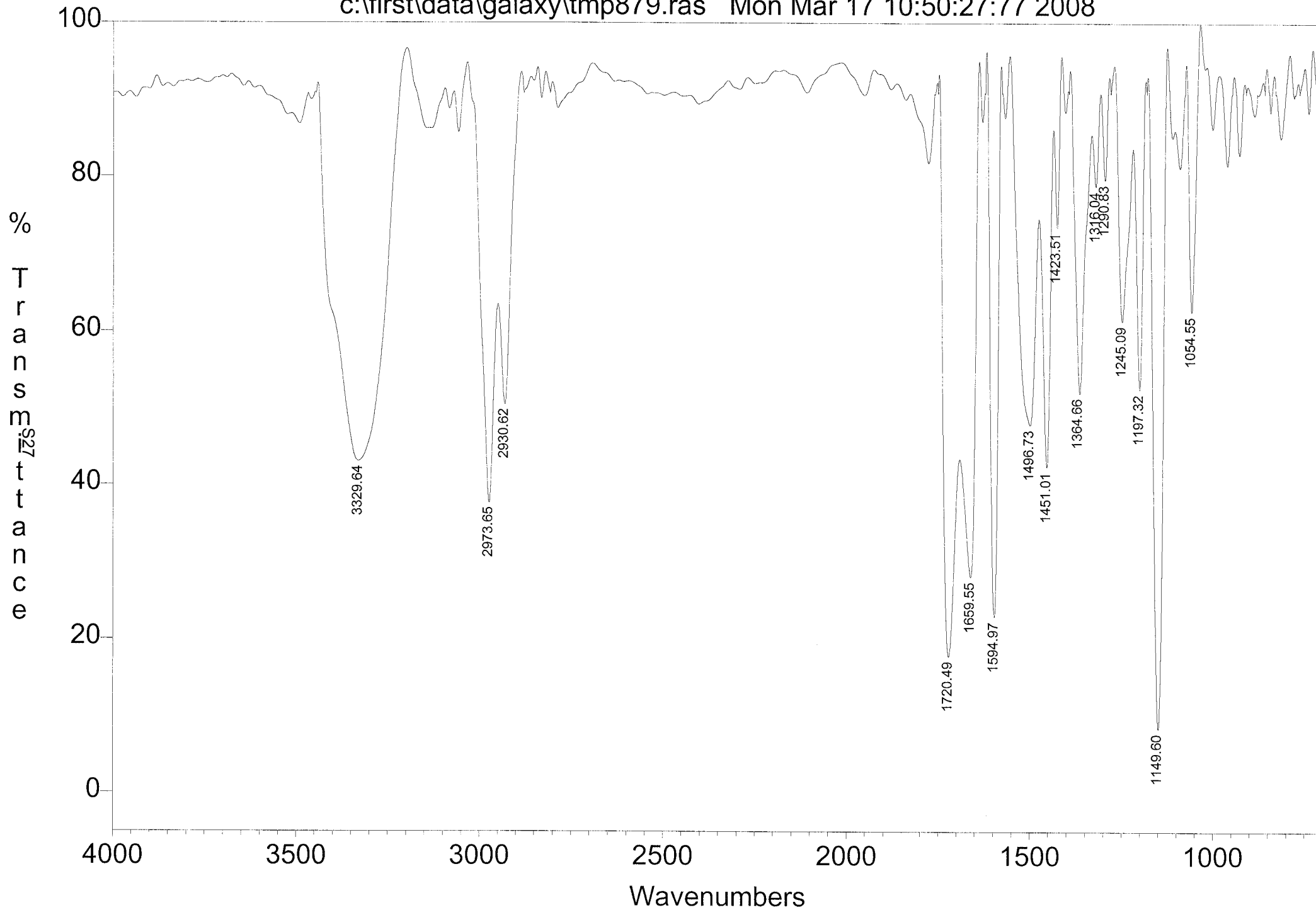
Acquisition Time (sec)	1.0421	Comment	all_carbon	Date	19 Mar 2008 14:34:40		
File Name	\HOME\Debieux\My Documents\Chimie\Doctorat\NMR\debi3765.bbo_002001r			Frequency (MHz)	125.76	Nucleus	13C
Number of Transients	1316	Origin	drx500	Original Points Count	32768	Owner	nmruser
Pulse Sequence	zgdc	Receiver Gain	8192.00	SW(cyclical) (Hz)	31446.54	Solvent	CHLOROFORM-d
Spectrum Offset (Hz)	13109.8271	Sweep Width (Hz)	31445.58	Temperature (degree C)	25.000	Points Count	32768

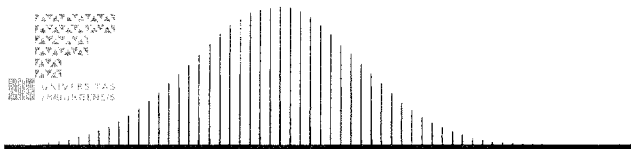


S26



c:\first\data\galaxy\tmp879.ras Mon Mar 17 10:50:27:77 2008





FTMS 4.7T BioAPEX II MS-Service UNI-Fribourg

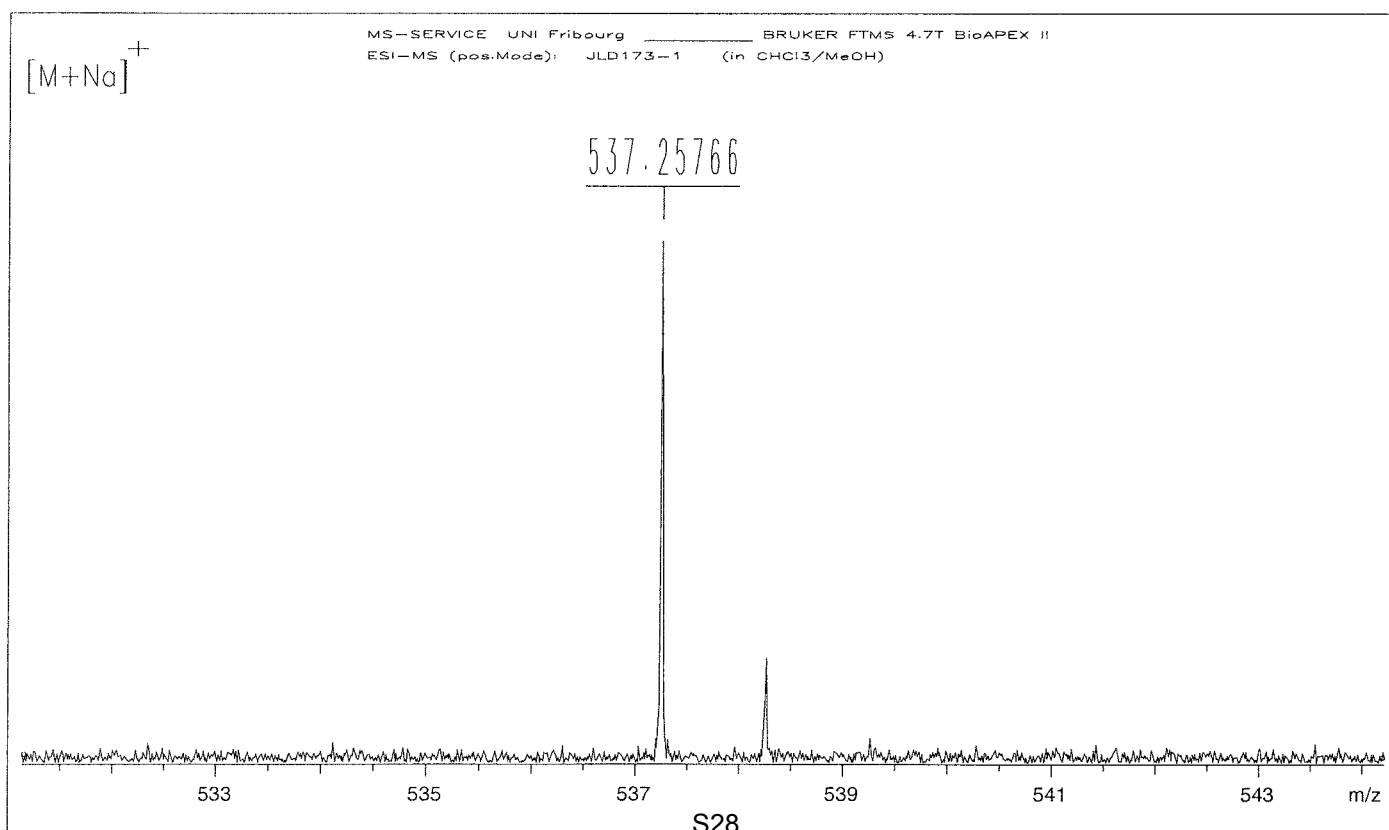
ESI-MS: JLD173-1

XMASS Mass Analysis for /Data/UNI_FR/DEBI3234_ESI/5/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 537.2576570

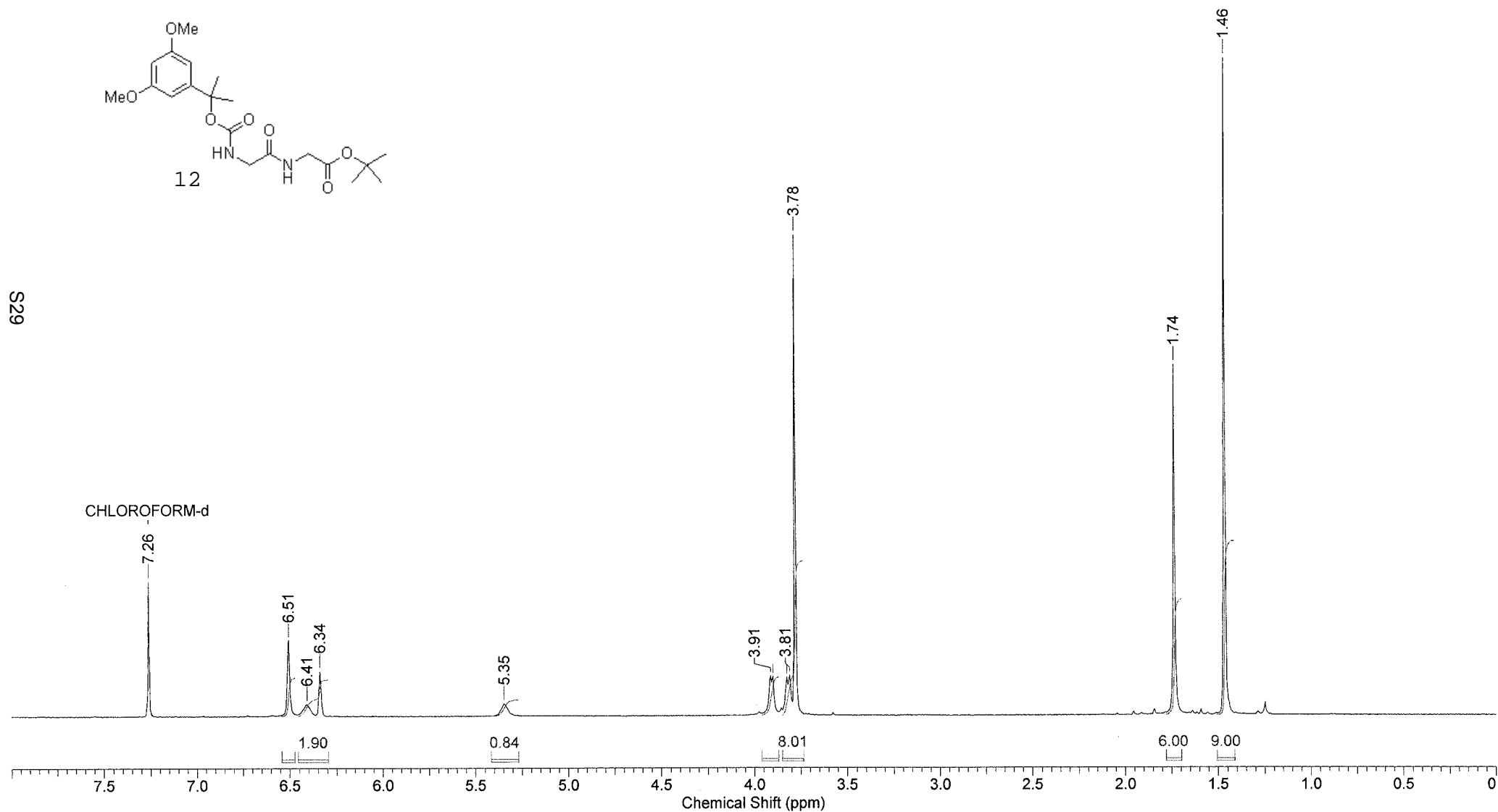
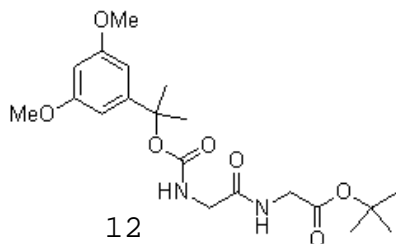
Charge = +1

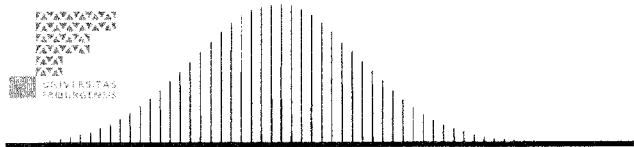
#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 537.2576570								
1	28	38	2	7	1	537.2571227	10.5	5.343e-04
2	27	39	1	10	0	537.2568479	9.0	8.091e-04
3	30	37	2	7	0	537.2595280	13.5	1.871e-03
4	25	37	4	9	0	537.2555052	9.5	2.152e-03
5	25	40	1	10	1	537.2544426	6.0	3.214e-03
6	23	38	4	9	1	537.2530999	6.5	4.557e-03
7	24	40	3	9	1	537.2656760	6.0	8.019e-03
8	26	39	3	9	0	537.2680813	9.0	1.042e-02
9	30	34	4	4	1	537.2472267	15.5	1.043e-02
10	27	38	4	6	1	537.2683561	10.5	1.070e-02



jld156

Acquisition Time (sec)	2.2021	Comment	PROTONNR CDCI3 u jld 60	Date	06 Dec 2007 13:07:12		
File Name	\\HOME\Debieux\JMy Documents\Chimie\Doctorat\NMR\jld156-1_001001r			Frequency (MHz)	360.13		
Nucleus	1H	Number of Transients	16	Origin	dpx360	Original Points Count	16384
Owner	nmruser	Points Count	16384	Pulse Sequence	zg30	Receiver Gain	228.10
SW(cyclical) (Hz)	7440.48	Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	2210.5950		
Sweep Width (Hz)	7440.02	Temperature (degree C)	27.000				





FTMS 4.7T BioAPEX II MS-Service UNI-Fribourg

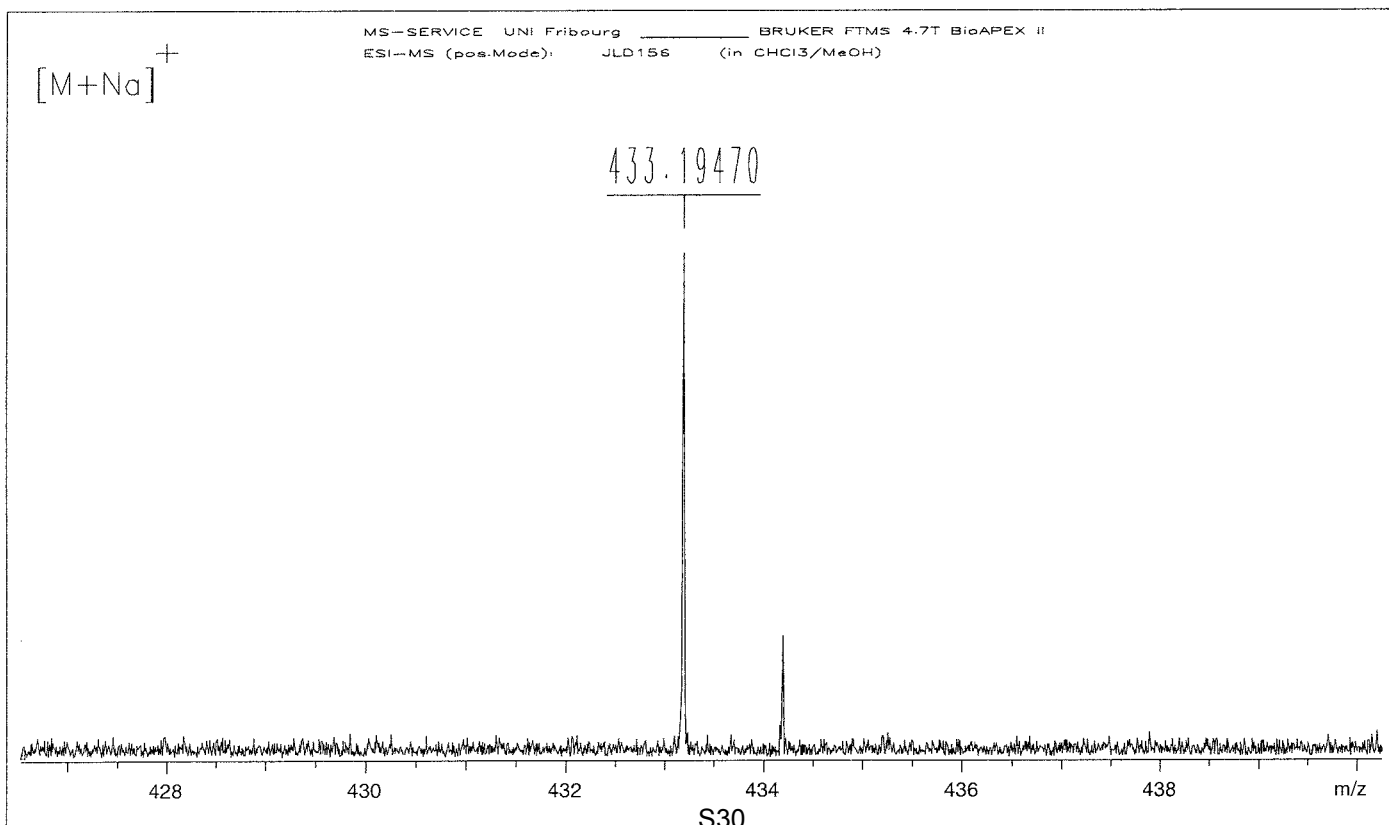
ESI-MS: JLD156

XMASS Mass Analysis for /Data/UNI_FR/DEBI3335_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 433.1946960

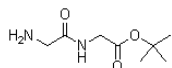
Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 433.1946960								
1	20	30	2	7	1	433.1945224	6.5	1.736e-04
2	20	27	5	6	0	433.1955850	10.0	8.890e-04
3	18	28	5	6	1	433.1931797	7.0	1.516e-03
4	17	29	4	9	0	433.1929050	5.5	1.791e-03
5	22	29	2	7	0	433.1969277	9.5	2.232e-03
6	15	30	4	9	1	433.1904997	2.5	4.196e-03
7	14	30	6	8	1	433.2017331	2.5	7.037e-03
8	16	32	3	9	1	433.2030757	2.0	8.380e-03
9	16	29	6	8	0	433.2041384	5.5	9.442e-03
10	21	27	3	7	0	433.1843517	10.0	1.034e-02

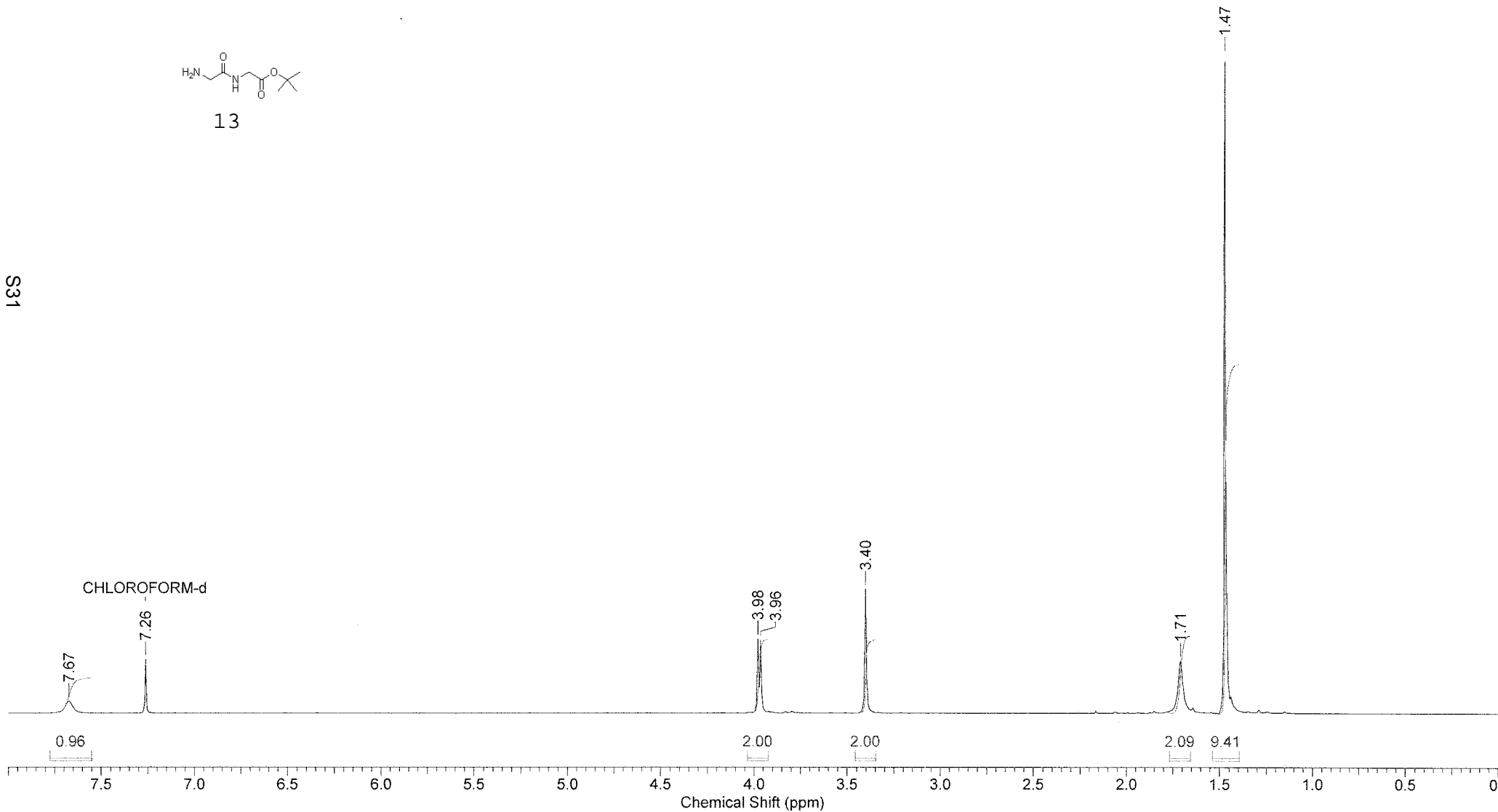


jld157

Acquisition Time (sec)	2.2021	Comment	PROTONNR CDCl3 u jld 47	Date	28 Mar 2008 13:07:12
File Name	\\HOME\Debieux\My Documents\Chimie\Doctorat\NMR\jld157-3_001001r			Frequency (MHz)	360.13
Nucleus	1H	Number of Transients	16	Origin	dpx360
Owner	nmruser	Points Count	16384	Pulse Sequence	zg30
SW(cyclical) (Hz)	7440.48	Solvent	CHLOROFORM-d	Receiver Gain	287.40
Sweep Width (Hz)	7440.02	Temperature (degree C)	27.000	Spectrum Offset (Hz)	2210.5947



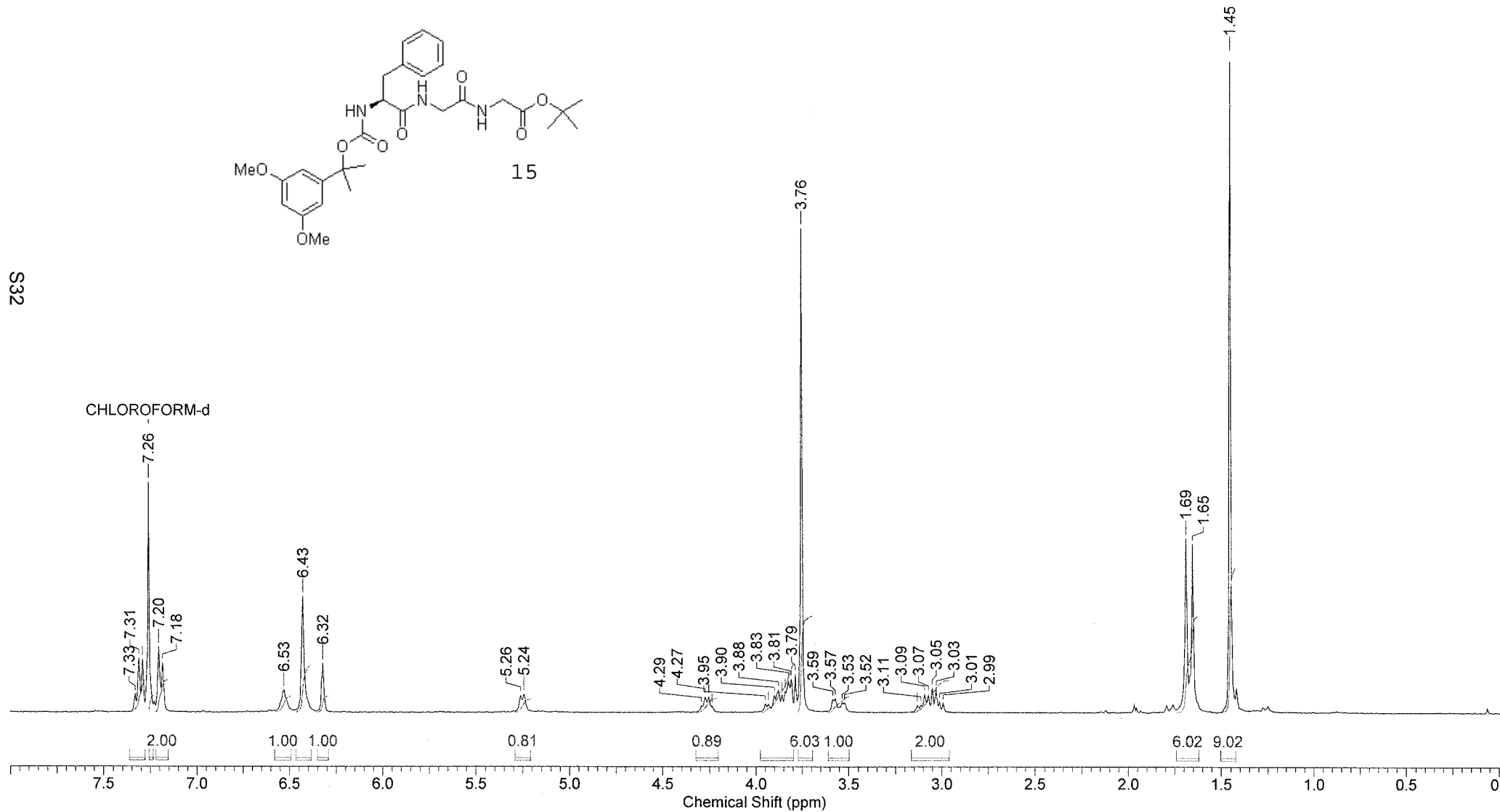
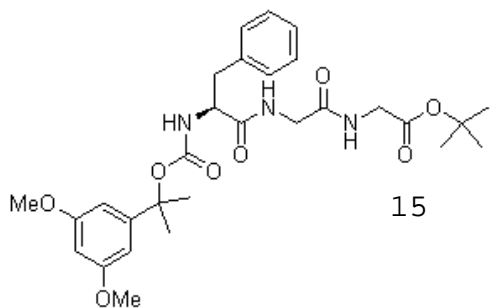
13



S31

jld160

Acquisition Time (sec)	2.2021	Comment	PROTONNR CDCl3 u jld 60		Date	17 Dec 2007 14:13:20	
File Name	\HOME\Debieux\My Documents\Chimie\Doctorat\NMR\jld160-1_001001r			Frequency (MHz)	360.13		
Nucleus	1H	Number of Transients	32	Origin	dpx360	Original Points Count	16384
Owner	nmruser	Points Count	16384	Pulse Sequence	zg30	Receiver Gain	1149.40
SW(cyclical) (Hz)	7440.48	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	2210.5950	
Sweep Width (Hz)	7440.02	Temperature (degree C)	27.000				

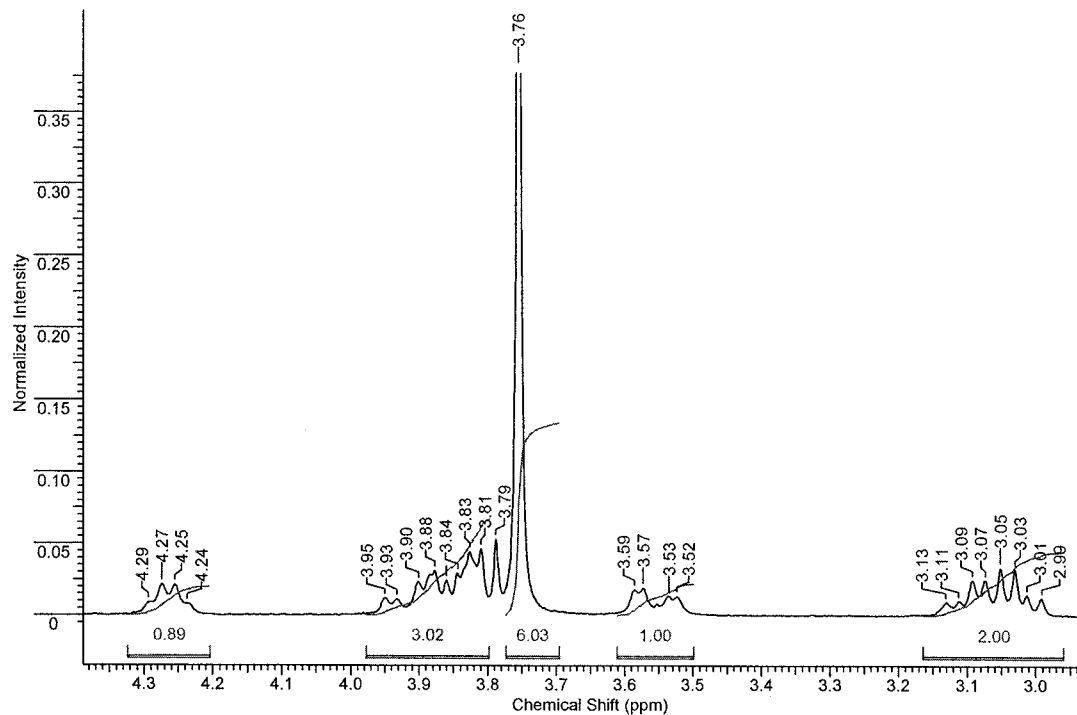
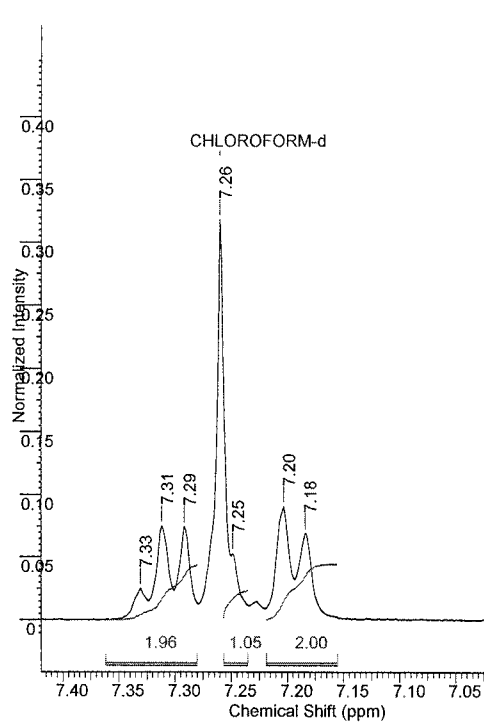


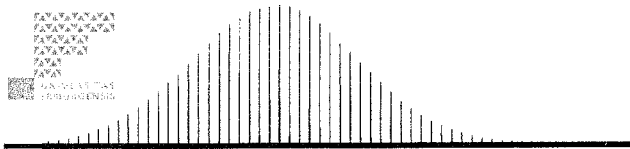
S32

jld160

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	1.45	523.7	1.0000	11	3.13	1127.7	0.0098	21	3.86	1390.2	0.0246	31	5.26	1894.7	0.0231
2	1.65	595.9	0.2338	12	3.52	1269.0	0.0136	22	3.88	1396.1	0.0311	32	6.32	2276.7	0.0683
3	1.69	608.6	0.2415	13	3.53	1273.0	0.0137	23	3.90	1404.7	0.0236	33	6.43	2314.8	0.1606
4	2.99	1077.3	0.0127	14	3.57	1286.7	0.0194	24	3.93	1416.1	0.0115	34	6.53	2352.1	0.0308
5	3.01	1085.0	0.0150	15	3.59	1291.2	0.0184	25	3.95	1422.5	0.0120	35	7.18	2587.3	0.0690
6	3.03	1091.4	0.0322	16	3.76	1352.5	0.6693	26	4.24	1526.0	0.0084	36	7.20	2594.1	0.0904
7	3.05	1099.1	0.0336	17	3.79	1364.3	0.0535	27	4.25	1532.4	0.0212	37	7.26	2614.5	0.3182
8	3.07	1106.8	0.0251	18	3.81	1372.0	0.0464	28	4.27	1539.2	0.0216	38	7.29	2625.9	0.0742
9	3.09	1113.6	0.0251	19	3.83	1377.9	0.0443	29	4.29	1546.4	0.0089	39	7.31	2633.2	0.0753
10	3.11	1120.9	0.0106	20	3.84	1384.3	0.0294	30	5.24	1888.4	0.0247	40	7.33	2640.0	0.0250

S33





FTMS 4.7T BioAPEX II MS-Service UNI-Fribourg

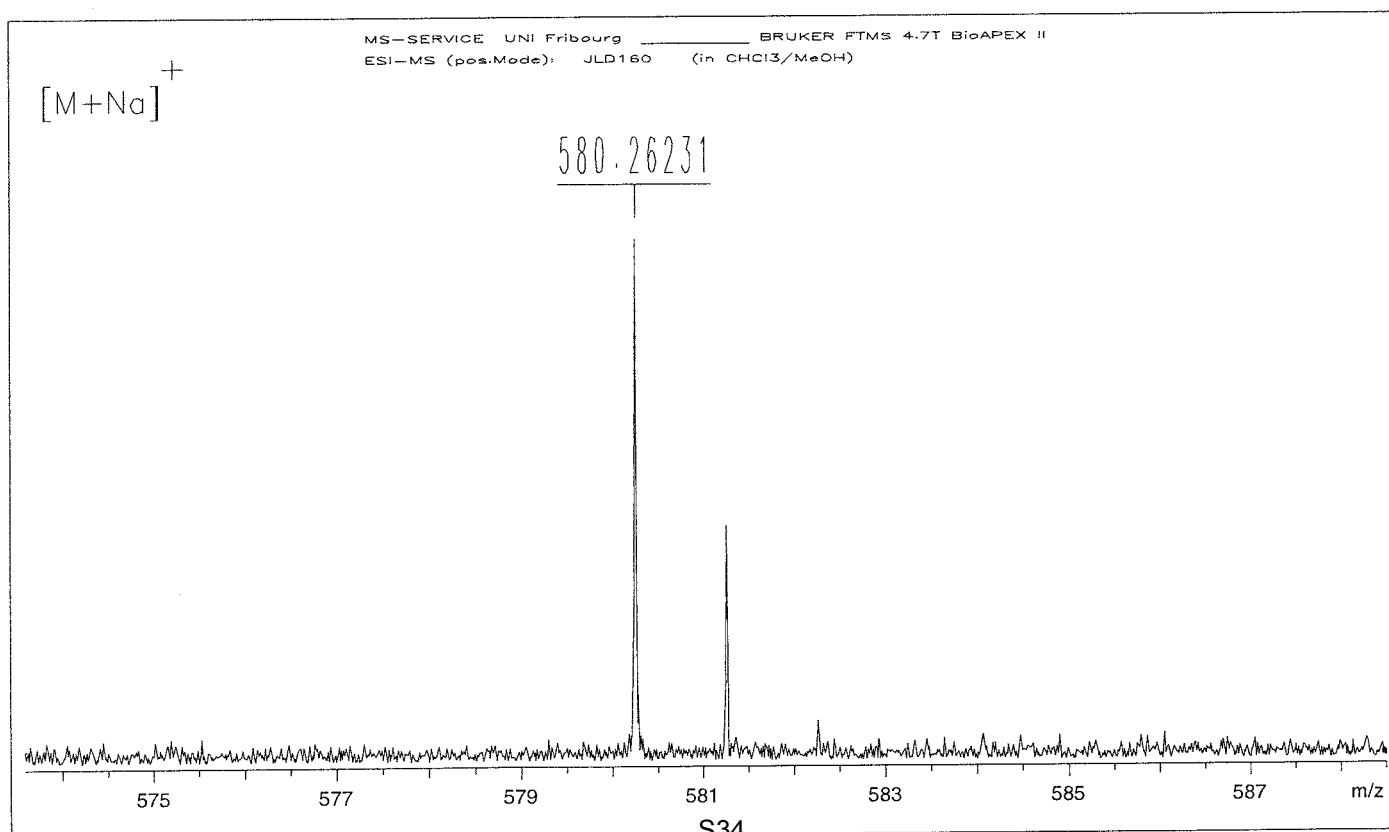
ESI-MS: JLD160

XMASS Mass Analysis for /Data/UNI_FR/DEBI3332_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 580.2623080

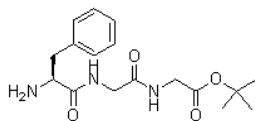
Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 580.2623080								
1	29	39	3	8	1	580.2629363	11.5	6.283e-04
2	27	37	6	7	1	580.2615937	12.0	7.143e-04
3	26	38	5	10	0	580.2613189	10.5	9.891e-04
4	29	36	6	7	0	580.2639990	15.0	1.691e-03
5	24	39	5	10	1	580.2589136	7.5	3.394e-03
6	25	41	4	10	1	580.2714896	7.0	9.182e-03
7	30	36	4	8	0	580.2527656	15.0	9.542e-03
8	27	40	4	10	0	580.2738949	10.0	1.159e-02
9	28	39	5	7	1	580.2741697	11.5	1.186e-02
10	28	37	4	8	1	580.2503603	12.0	1.195e-02

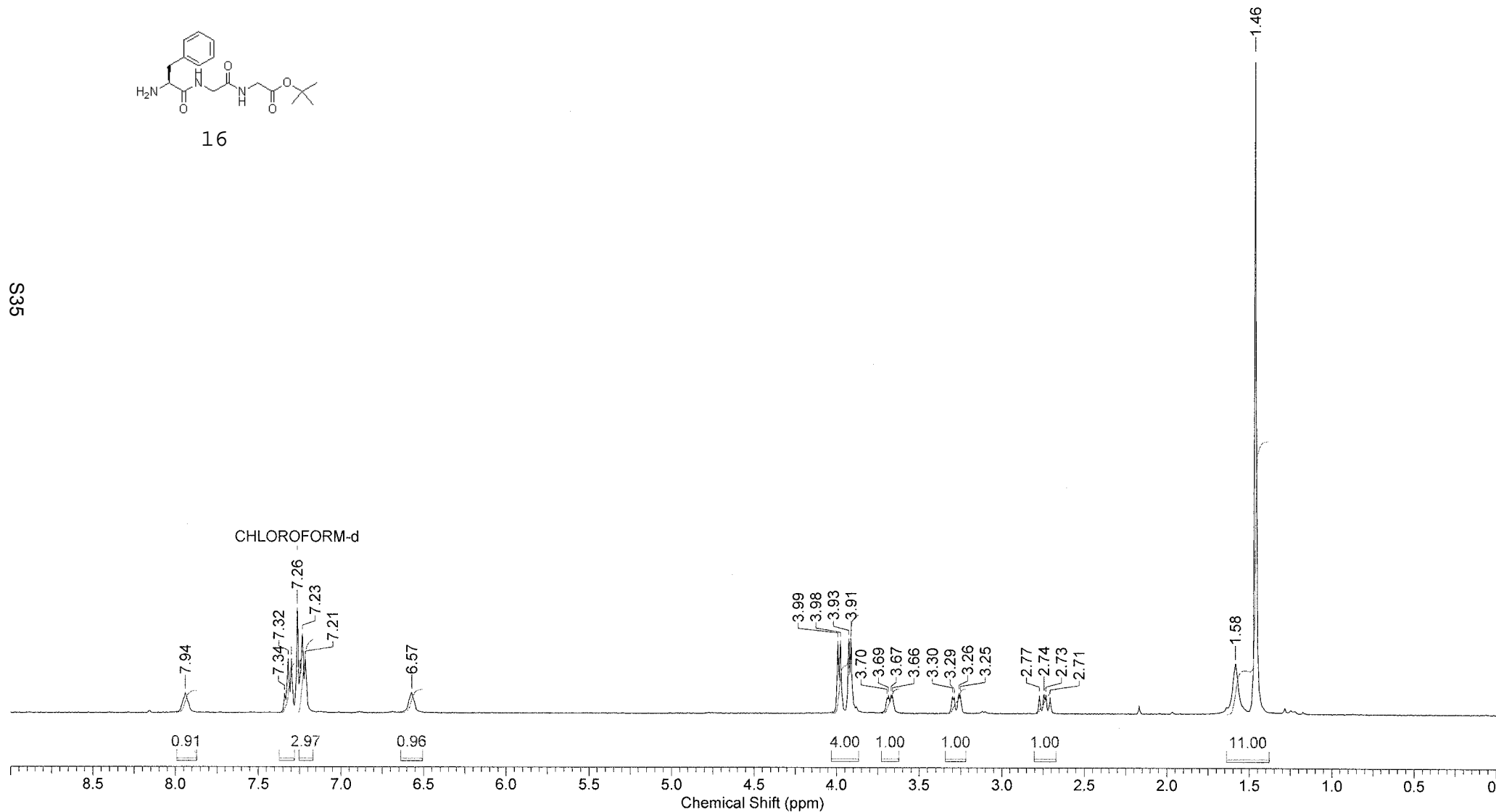


jld163

Acquisition Time (sec)	2.2021	Comment	PROTONNR CDCl3 u jld 60	Date	24 Jan 2008 08:51:12
File Name	\\HOME\Debieux\J\My Documents\Chimie\Doctorat\NMR\jld163-2_001001r			Frequency (MHz)	360.13
Nucleus	1H	Number of Transients	16	Origin	dpx360
Owner	nmruser	Points Count	16384	Pulse Sequence	zg30
SW(cyclical) (Hz)	7440.48	Solvent	CHLOROFORM-d	Receiver Gain	574.70
Sweep Width (Hz)	7440.02	Temperature (degree C)	27.000	Spectrum Offset (Hz)	2210.5950



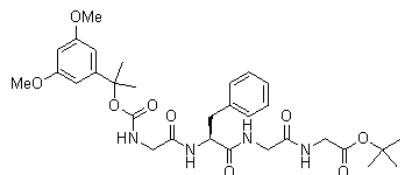
16



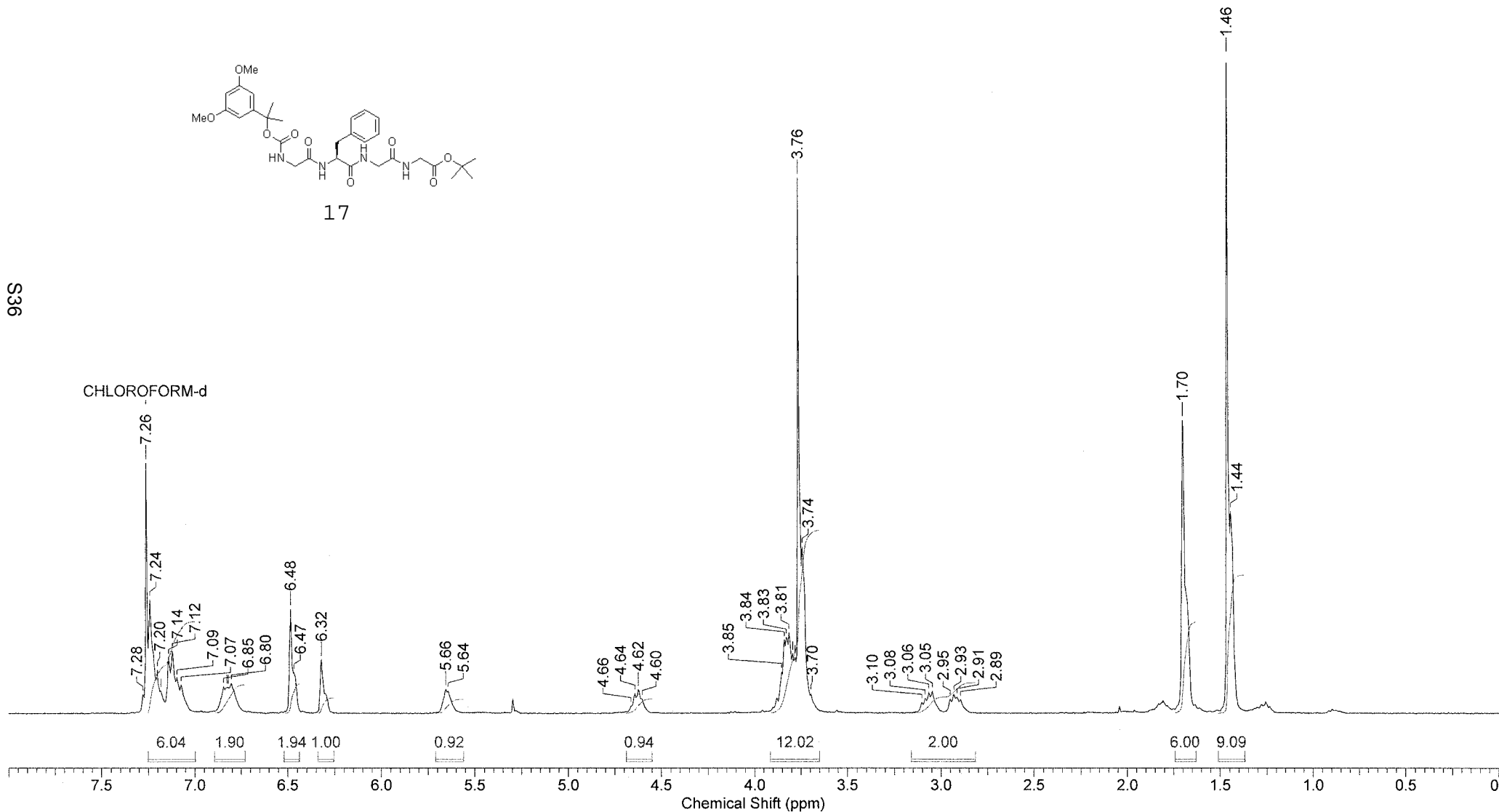
S89

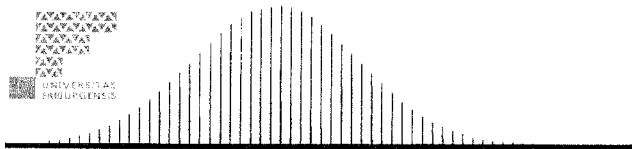
jld165

Acquisition Time (sec)	2.2021	Comment	PROTONNR CDCI3 u jld 47		Date	25 Jan 2008 13:49:52	
File Name	\\HOME\Debieux\JMy Documents\Chimie\Doctorat\NMR\jld165-1_001001r			Frequency (MHz)	360.13		
Nucleus	1H	Number of Transients	16	Origin	dpx360	Original Points Count	16384
Owner	nmruser	Points Count	16384	Pulse Sequence	zg30	Receiver Gain	645.10
SW(cyclical) (Hz)	7440.48	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	2210.1406	
Sweep Width (Hz)	7440.02	Temperature (degree C)	27.000				



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FTMS 4.7T BioAPEX II MS-Service UNI-Fribourg

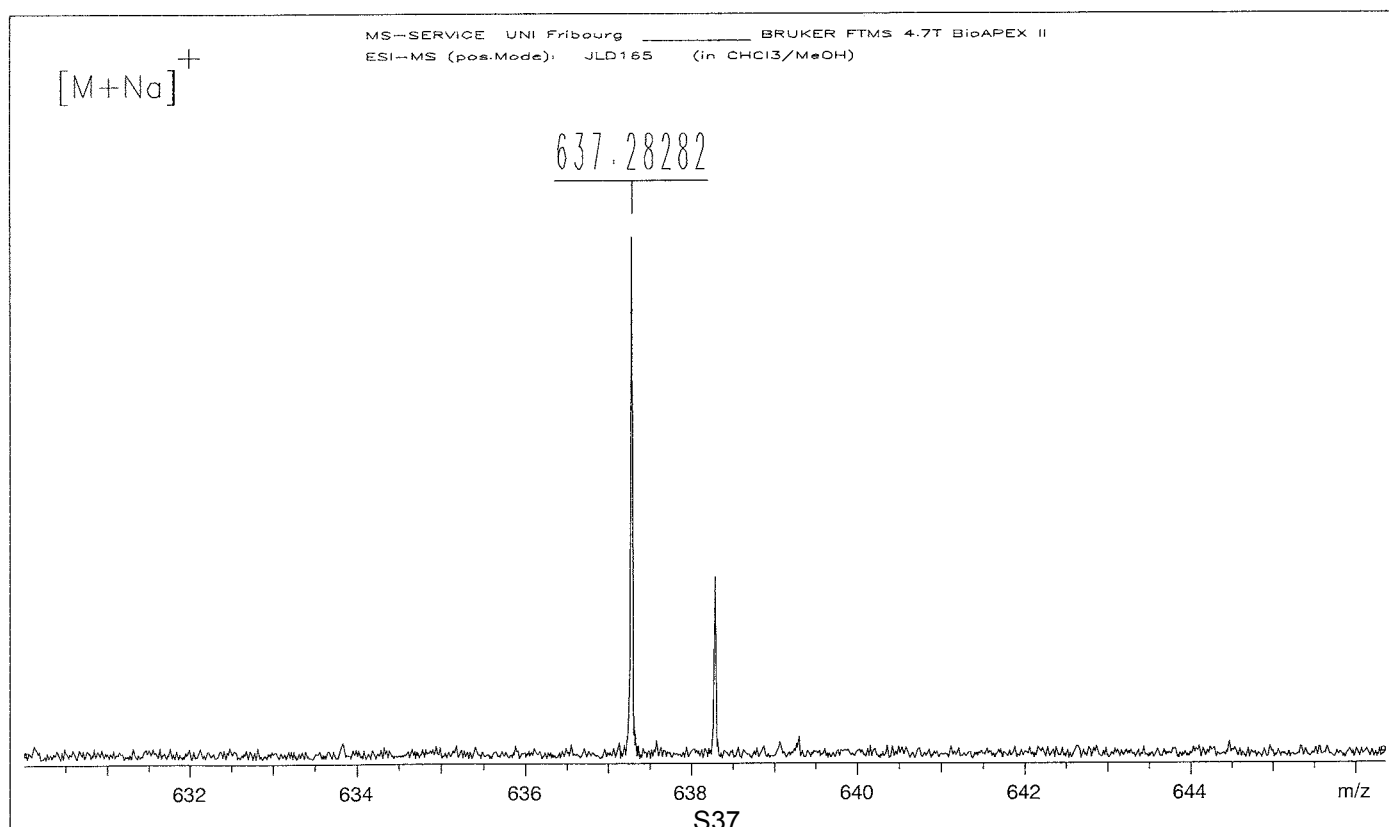
ESI-MS: JLD165

XMASS Mass Analysis for /Data/UNI_FR/DEBI3333_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 637.2828190

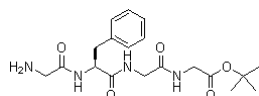
Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 637.2828190								
1	31	42	4	9	1	637.2844001	12.5	1.581e-03
2	33	41	4	9	0	637.2868054	15.5	3.986e-03
3	34	40	5	6	1	637.2870801	17.0	4.261e-03
4	37	39	3	7	0	637.2782520	20.0	4.567e-03
5	36	42	2	7	1	637.2884228	16.5	5.604e-03
6	35	37	6	6	0	637.2769094	20.5	5.910e-03
7	36	39	5	6	0	637.2894854	20.0	6.666e-03
8	35	40	3	7	1	637.2758467	17.0	6.972e-03
9	34	41	2	10	0	637.2755720	15.5	7.247e-03
10	38	41	2	7	0	637.2908281	19.5	8.009e-03

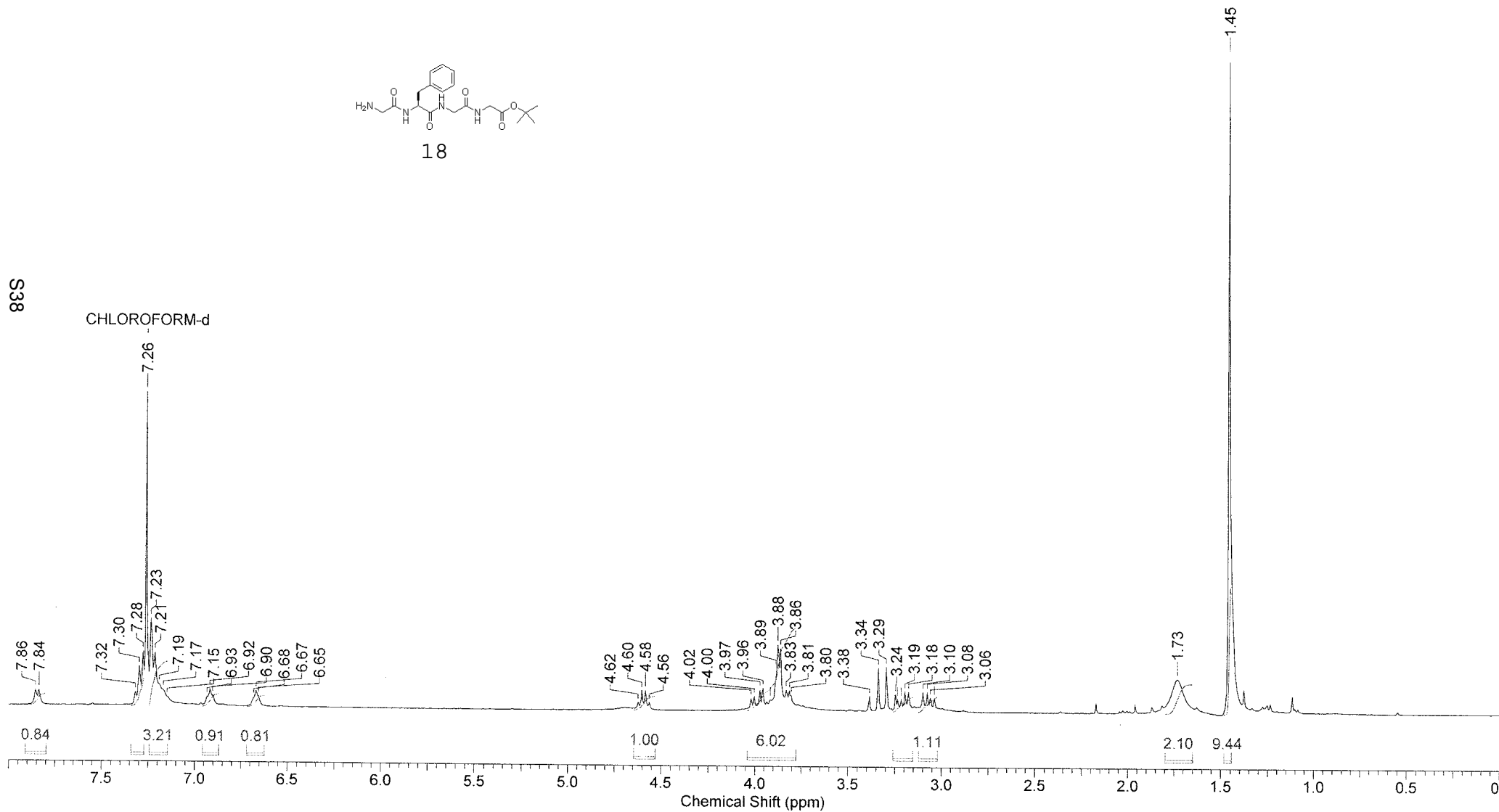


jld166

Acquisition Time (sec)	2.2021	Comment	PROTONNR CDCl3 u jld 36		Date	07 Apr 2008 16:06:24	
File Name	\HOME\Debieux\My Documents\Chimie\Doctorat\NMR\jld166-3_001001r			Frequency (MHz)	360.13		
Nucleus	1H	Number of Transients	64	Origin	dpx360	Original Points Count	16384
Owner	nmruser	Points Count	16384	Pulse Sequence	zg30	Receiver Gain	456.10
SW(cyclical) (Hz)	7440.48	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	2210.5950	
Sweep Width (Hz)	7440.02	Temperature (degree C)	27.000				

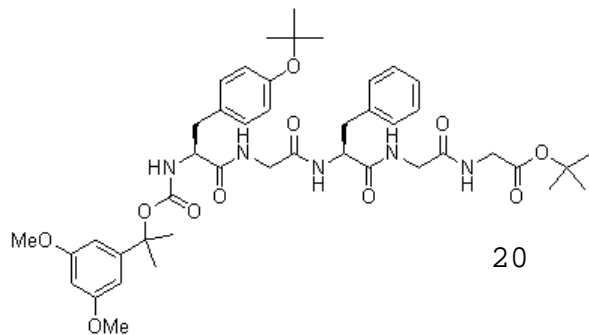


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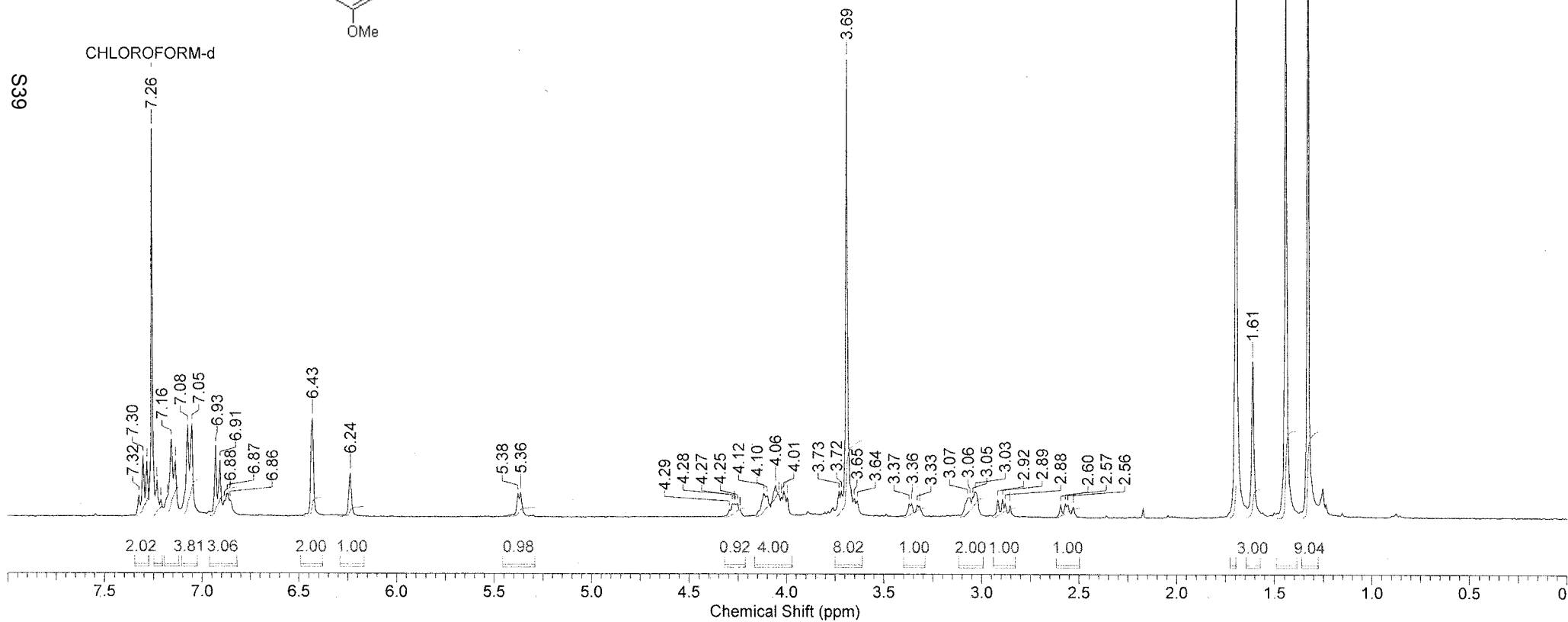


jld167

Acquisition Time (sec)	2.2021	Comment	PROTONNR CDCl3 u jld 36		Date	10 Apr 2008 09:01:52	
File Name	\HOME\Debieux\JMy Documents\Chimie\Doctorat\NMR\jld167-2b_001001r			Frequency (MHz)	360.13		
Nucleus	1H	Number of Transients	16	Origin	dpx360	Original Points Count	16384
Owner	nmruser	Points Count	16384	Pulse Sequence	zg30	Receiver Gain	456.10
SW(cyclical) (Hz)	7440.48	Solvent	CHLOROFORM-d		Spectrum Offset (Hz)	2210.5947	
Sweep Width (Hz)	7440.02	Temperature (degree C)	27.000				



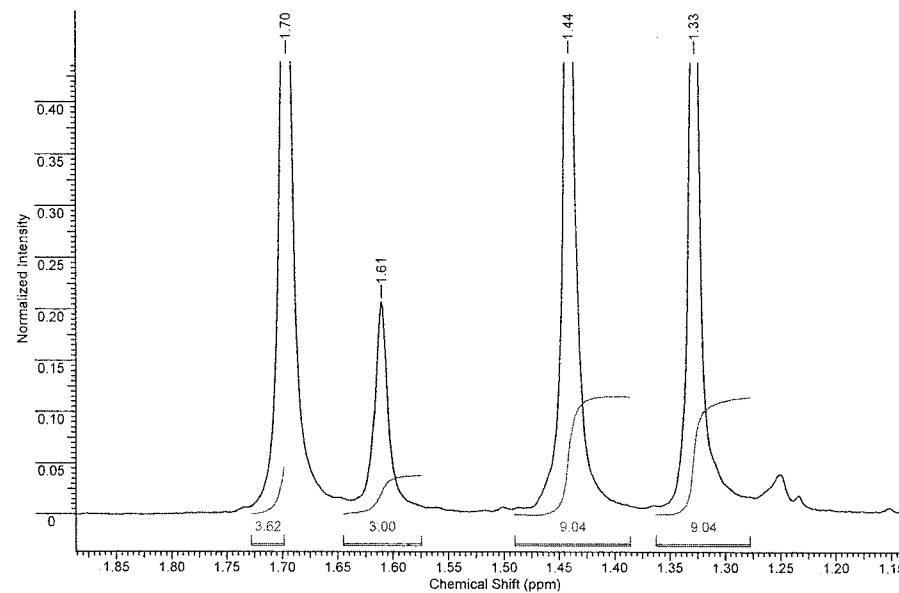
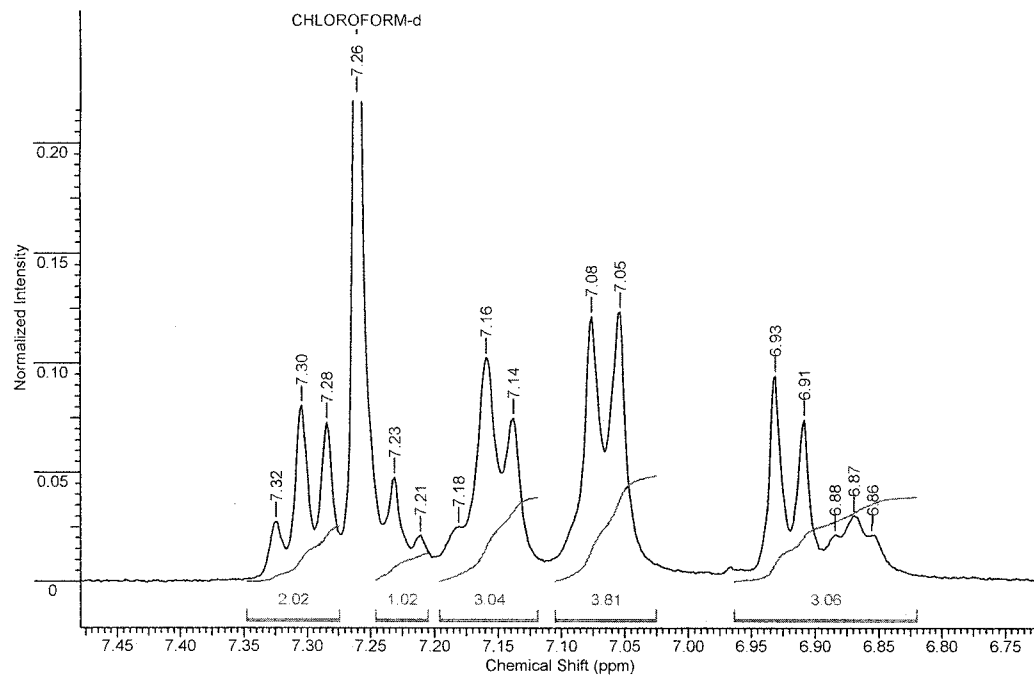
20



jld167

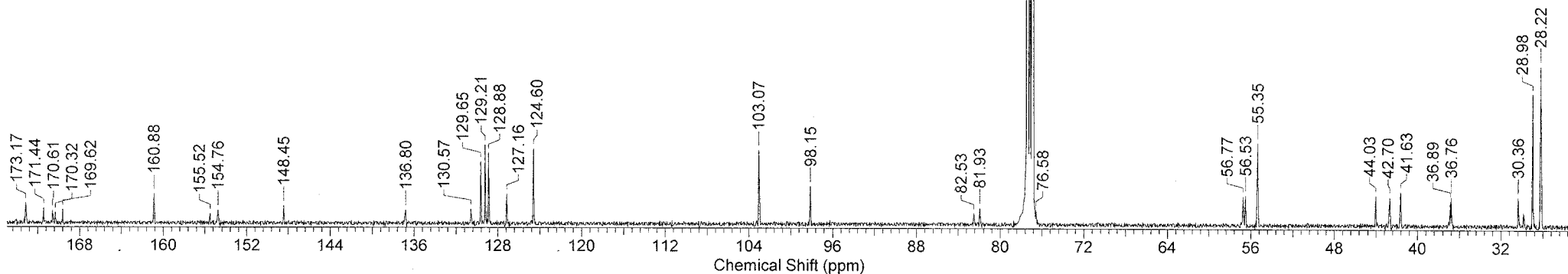
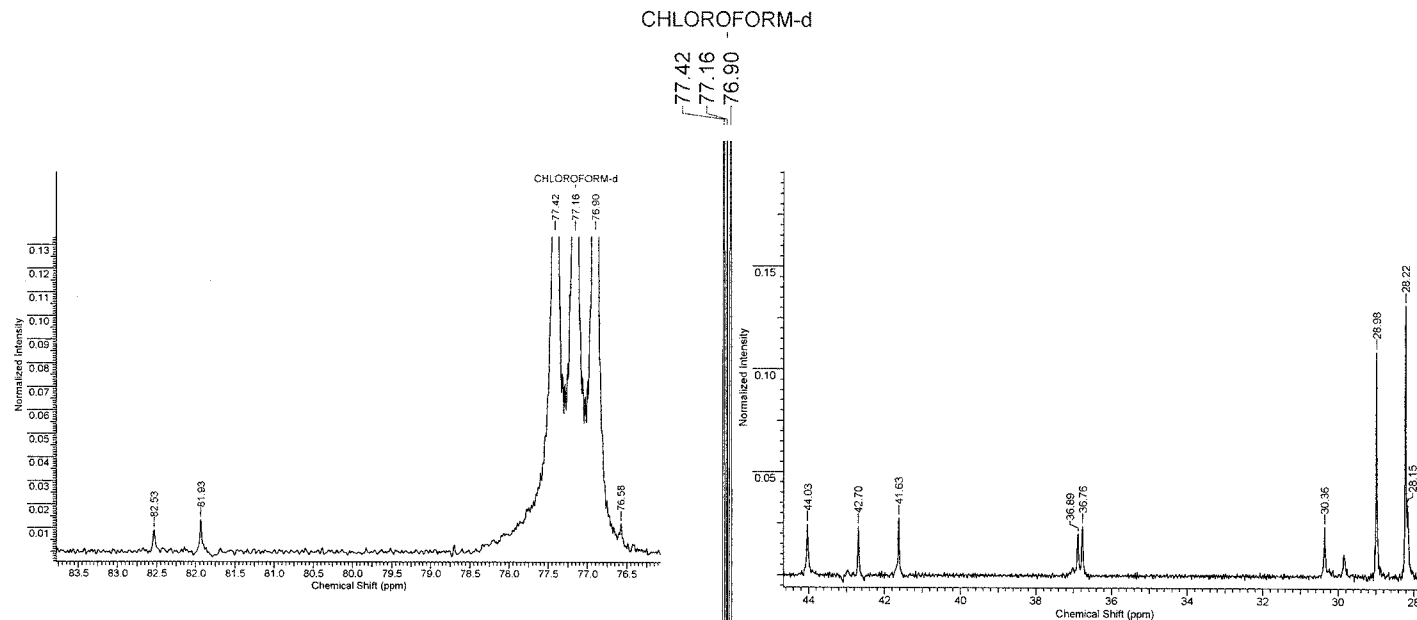
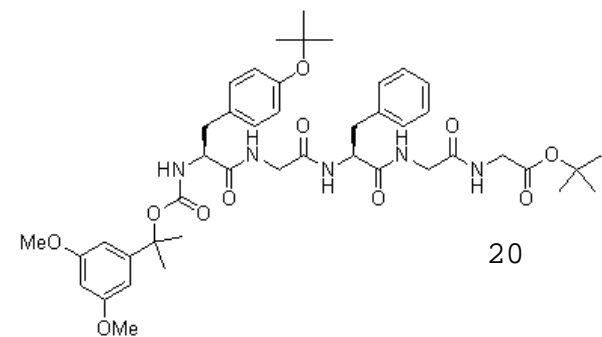
No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	1.33	478.3	1.0000	16	3.07	1106.8	0.0261	31	4.10	1476.0	0.0282	46	6.91	2487.8	0.0743
2	1.44	519.2	0.8910	17	3.32	1194.0	0.0158	32	4.12	1482.4	0.0320	47	6.93	2496.0	0.0943
3	1.61	580.0	0.2071	18	3.33	1198.6	0.0171	33	4.24	1526.4	0.0099	48	7.05	2540.1	0.1235
4	1.70	610.9	0.7355	19	3.36	1209.5	0.0191	34	4.25	1531.4	0.0183	49	7.08	2548.2	0.1215
5	2.53	911.6	0.0144	20	3.37	1214.0	0.0183	35	4.27	1536.0	0.0177	50	7.14	2570.5	0.0750
6	2.56	921.1	0.0173	21	3.64	1309.8	0.0217	36	4.27	1537.8	0.0173	51	7.16	2578.2	0.1029
7	2.57	925.6	0.0185	22	3.65	1315.3	0.0248	37	4.28	1541.0	0.0180	52	7.18	2585.9	0.0253
8	2.60	934.7	0.0170	23	3.69	1329.4	0.6038	38	4.29	1546.4	0.0094	53	7.21	2596.8	0.0213
9	2.86	1028.3	0.0162	24	3.72	1339.3	0.0349	39	5.36	1932.0	0.0314	54	7.23	2604.1	0.0479
10	2.88	1036.9	0.0186	25	3.73	1343.9	0.0337	40	5.38	1937.0	0.0303	55	7.26	2614.5	0.5112
11	2.89	1041.9	0.0247	26	4.00	1438.8	0.0262	41	6.24	2246.2	0.0582	56	7.28	2623.2	0.0730
12	2.92	1051.0	0.0239	27	4.01	1445.6	0.0342	42	6.43	2316.2	0.1305	57	7.30	2630.4	0.0809
13	3.03	1092.3	0.0342	28	4.03	1450.2	0.0267	43	6.86	2468.8	0.0216	58	7.32	2637.7	0.0277
14	3.05	1096.8	0.0279	29	4.04	1454.7	0.0301	44	6.87	2473.8	0.0304				
15	3.06	1102.3	0.0267	30	4.06	1461.1	0.0423	45	6.88	2479.2	0.0216				

S40



jld167, C13

Acquisition Time (sec)	1.0879	Comment	all_carbon	Date	23 Mar 2008 00:17:04
File Name	\HOME\Debieux\My Documents\Chimie\Doctorat\NMR\debi3769.bbo_002001r			Frequency (MHz)	125.76
Nucleus	13C	Origin	drx500	Original Points Count	32768
Points Count	32768	Pulse Sequence	zgdc	Receiver Gain	16384.00
Solvent	CHLOROFORM-d	Spectrum Offset (Hz)	13922.1592	SW(cyclical) (Hz)	30120.48
Temperature (degree C)	20.000	Sweep Width (Hz)	30119.56		



Display Report

Analysis Info

Analysis Name D:\Data\Debieux\EDAF3145_ESI.d
Method JLD148_MS.m
Sample Name JLD167-1
Comment (in CHCl₃/MeOH/NaCl)

Acquisition Date 20.02.2008 15:07:03

Operator Administrator
Instrument HCT

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	off
Mass Range Mode	Std/Enhanced	Scan Begin	100 m/z	Scan End	1200 m/z
Capillary Exit	133.0 Volt	Skim 1	40.0 Volt	Trap Drive	67.8
Accumulation Time	56 µs	Averages	5 Spectra	Auto MS/MS	off

