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 F_{254}. Flash column chromatography (FC) was carried out using Brunschwig silica gel 60 Å (32-63 mesh). Commercially available products were used without further purification.

^{1}H- and ^{13}C-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 $CHCl_3$ (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 [SiO_2, hexane/EtOAc (1:1)] to furnish the desired product as a yellow solid (42.0 mg, 92 %); **^{1}H NMR** (360 MHz, $CDCl_3$) 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); **^{13}C NMR** (125 MHz, $CDCl_3$) 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 ($C_{26}H_{36}N_2O_5$ + Na^+ calcd 479.2516).

Ddz-Leu-Phe-O^{t}Bu (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 Et_3N (14 μL, 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 [SiO_2, hexane/EtOAc (2:1)] to provide the desired product as a yellow solid (45.1 mg, 81 %); **^{1}H NMR** (360 MHz, $CDCl_3$) 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); **^{13}C NMR** (125 MHz, $CDCl_3$) 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 ($C_{31}H_{44}N_2O_7$ + Na^+ calcd 579.3041).

Leu-Phe-O^{t}Bu (6): Ddz-L-Leu-L-Phe-OtBu (**5**) (27.8 mg, 0.050 mmol) was dissolved in deuterated MeCN (2.5 mL). The solution was then irradiated at 300 nm (Rayonnet®) in a quartz NMR tube for 8 hours. The mixture was concentrated to dryness and purified by flash column chromatography [SiO_2, CH_2Cl_2/$MeOH_{sat.NH_3}$ (95:5)] to provide the desired product as an orange solid (13.9 mg, 83 %). **^{1}H NMR** (360 MHz, $CDCl_3$) 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); **^{13}C NMR** (125 MHz, $CDCl_3$) 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 ($C_{19}H_{30}N_2O_3$ + Na^+ calcd 357.2149).

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

Ddz-Gly-Gly-O^{t}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 Et_3N (14 μL, 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 [SiO_2, Hexane/EtOAc (1:1)] to provide the desired product as a yellow solid (38.3 mg, 93 %). **^{1}H NMR** (360 MHz, $CDCl_3$) 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 ($C_{20}H_{30}N_2O_7$ + Na^+ calcd 433.1945).

Gly-Gly-O^{t}Bu (13): Ddz-Gly-Gly-O^{t}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 [SiO_2, CH_2Cl_2/$MeOH_{sat.NH_3}$ (95:5)] to provide the desired product as an orange solid (10.4 mg, 74 %). **^{1}H NMR** (360 MHz, $CDCl_3$) 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^{t}Bu (15): A mixture of Ddz-Phe-Dni (**14**) (28.9 mg, 0.018 mmol) and Gly-Gly-O^{t}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 [SiO_2, Hexane/EtOAc (1:3)] to provide the desired product as a yellow solid (25.1 mg, 90 %). **^{1}H NMR** (360 MHz, $CDCl_3$) 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 ($C_{29}H_{39}N_3O_8$ + Na^+ calcd 580.2629).

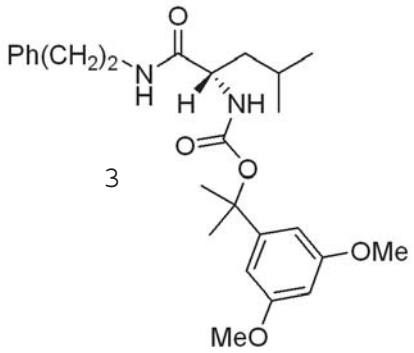
Phe-Gly-Gly-O^{t}Bu (16): Ddz-Phe-Gly-Gly-OtBu (**15**) (27.9 mg, 0.050 mmol) was dissolved in anhydrous MeCN (3 mL). The solution was then irradiated at 300 nm (Rayonnet®) in a quartz tube for 6 hours. The mixture was concentrated to dryness and purified by flash column chromatography [SiO_2, CH_2Cl_2/$MeOH_{sat.NH_3}$ (95:5)] to provide the desired product as a yellowish solid (13.5 mg, 80 %). **^{1}H NMR** (360 MHz, $CDCl_3$) 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^{t}Bu (17): A mixture of Ddz-Gly-Dni (**10**) (12.2 mg, 0.025 mmol), and Phe-Gly-Gly-O^{t}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 [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 (13.4 mg, 87 %). **^{1}H NMR** (360 MHz, $CDCl_3$) 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^{t}Bu (18): Ddz-Gly-Phe-Gly-Gly-O^{t}Bu (**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 %). **^{1}H NMR** (360 MHz, $CDCl_3$) δ = 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(^{t}Bu)-Gly-Phe-Gly-Gly-O^{t}Bu (20): A mixture of A mixture of Ddz-Tyr(^{t}Bu)-Dni (**19**) (1.3 mg, 2 μmol), and Gly-Phe-Gly-Gly-O^{t}Bu (**18**) (0.8 mg, 2 μmol) 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 %). **^{1}H NMR** (360 MHz, $CDCl_3$) δ = 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). **^{13}C NMR** (125 MHz, $CDCl_3$) δ = 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 $[M+Na]^+$.



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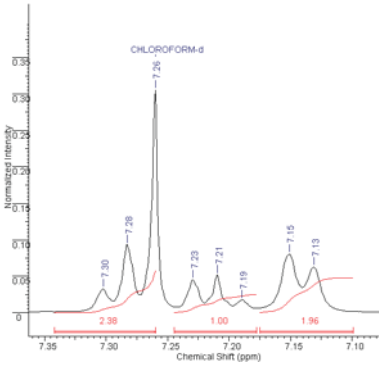

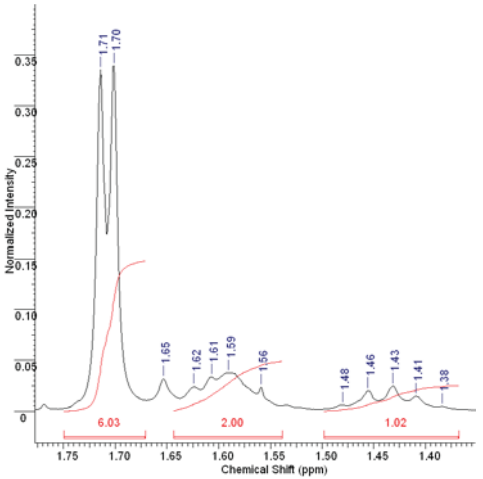

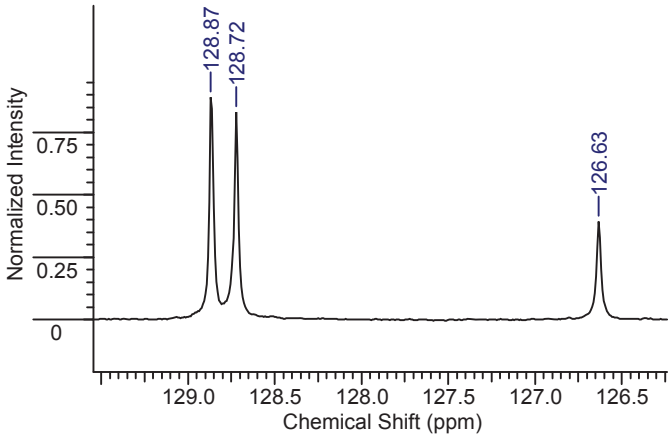

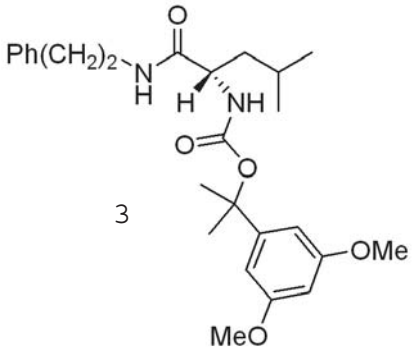

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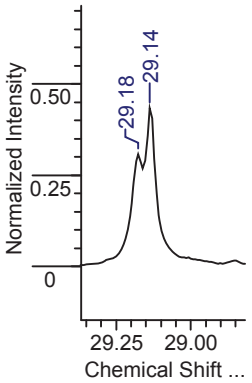

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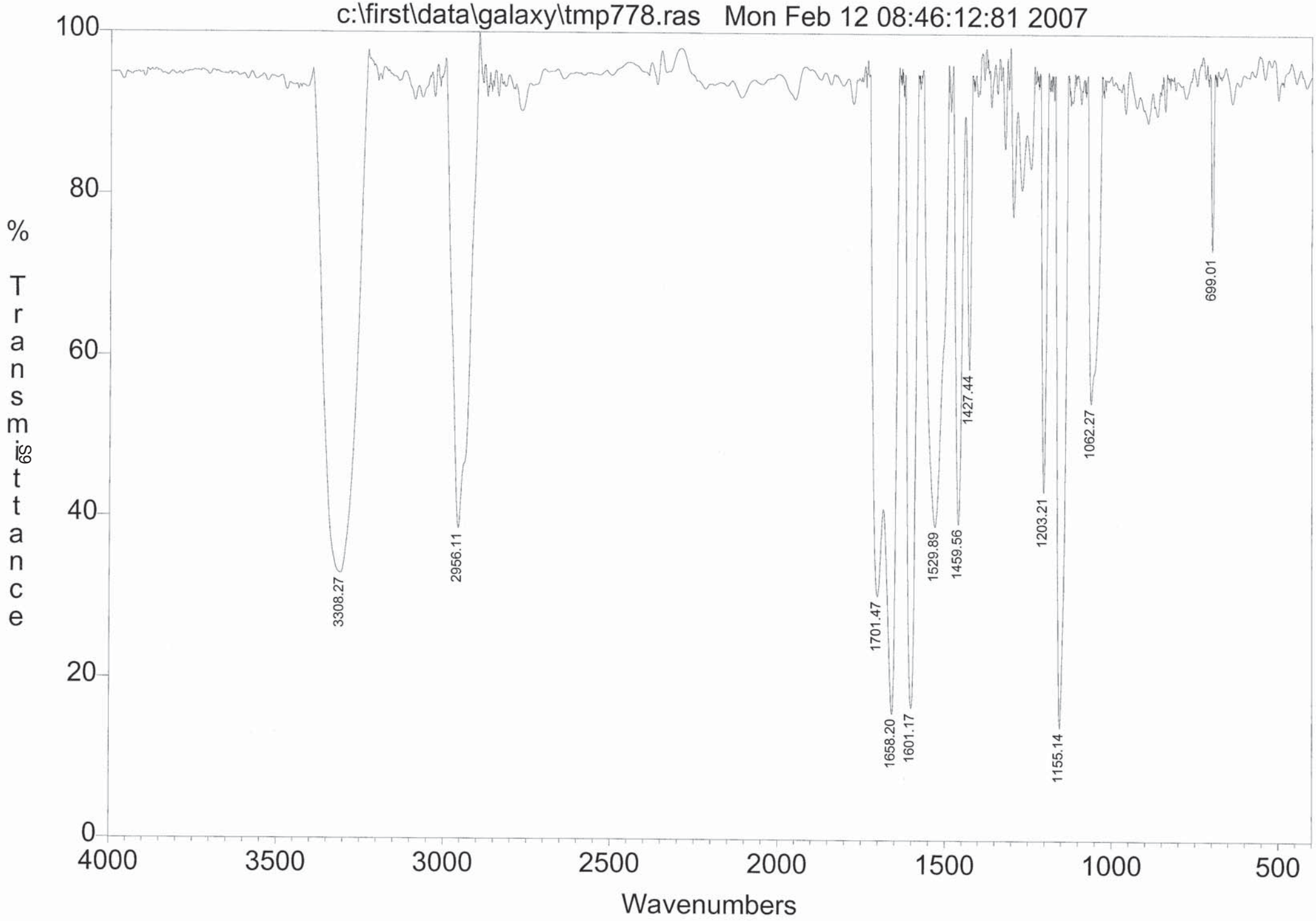

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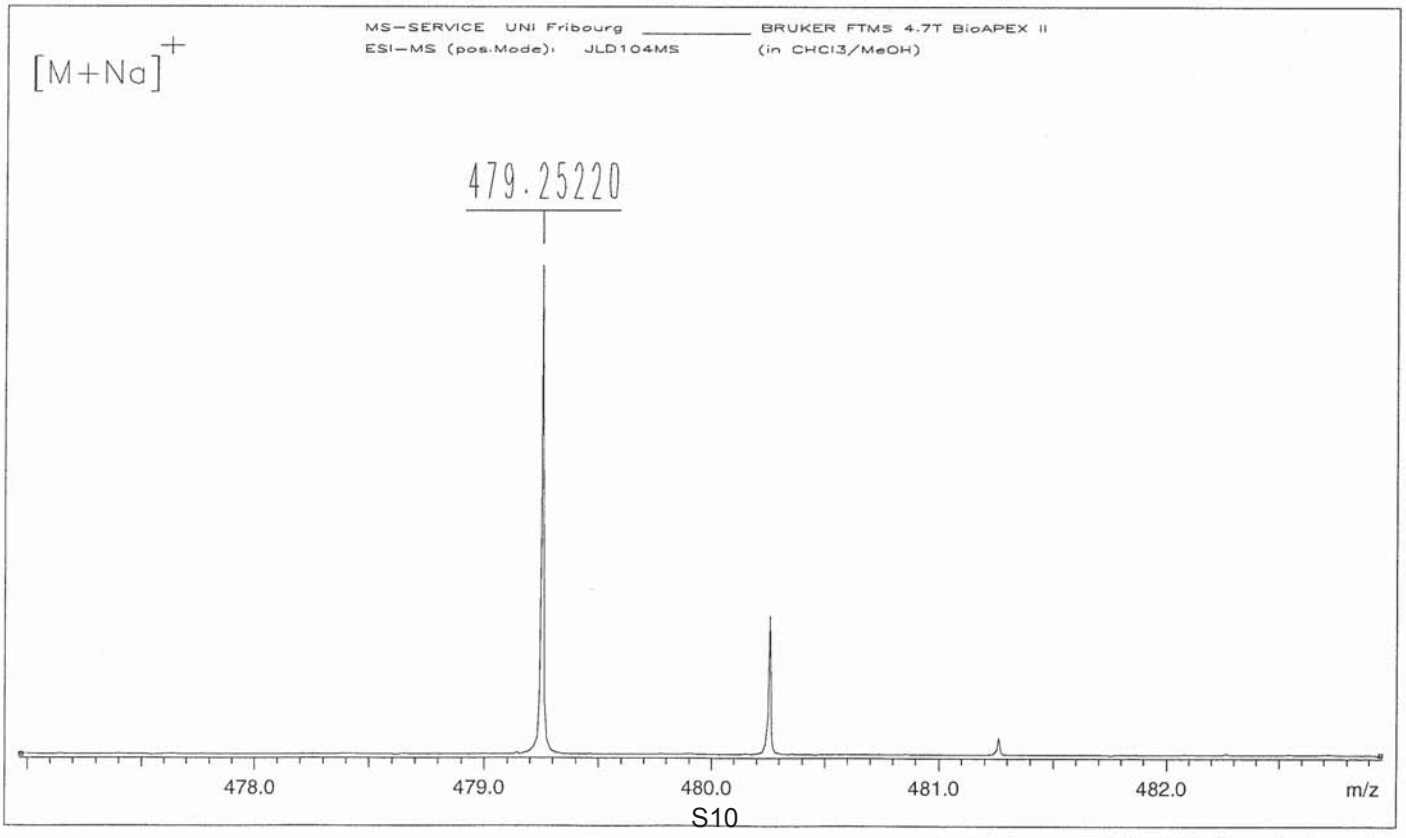

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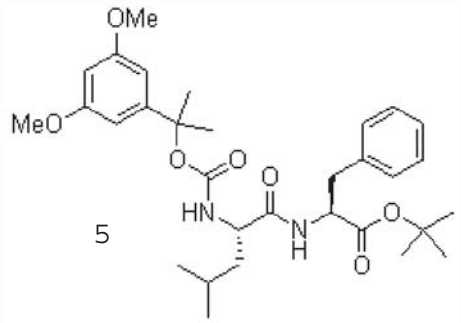

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19	1.65	592.8	0.0279
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31	3.74	1348.4	0.9501
32	4.01	1442.9	0.0120
33	4.03	1451.1	0.0255
34	4.04	1456.1	0.0280
35	4.07	1465.1	0.0132
36	4.65	1673.1	0.0144
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38	4.68	1685.8	0.0326
39	4.70	1692.2	0.0160

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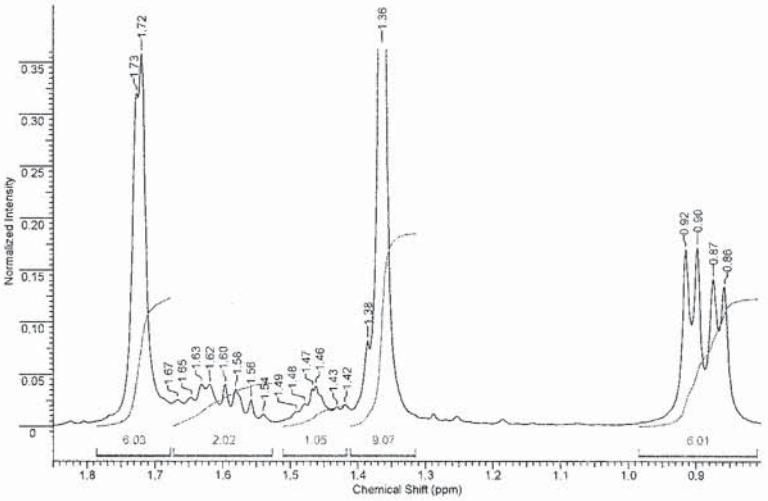

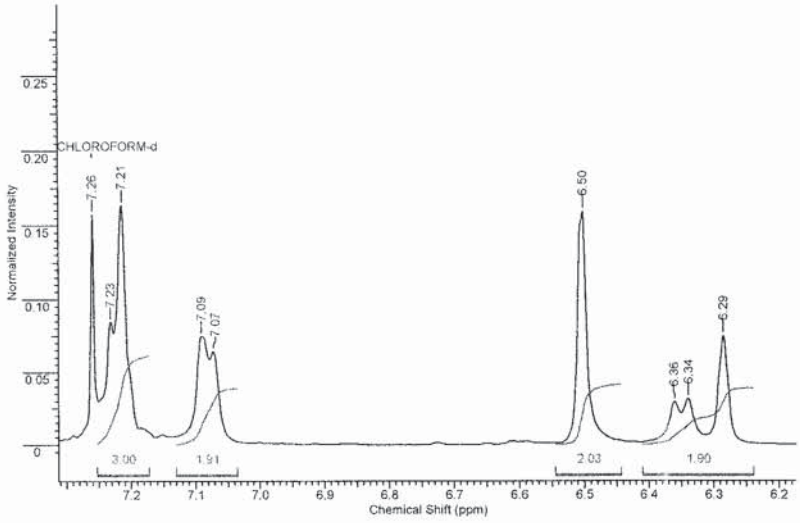

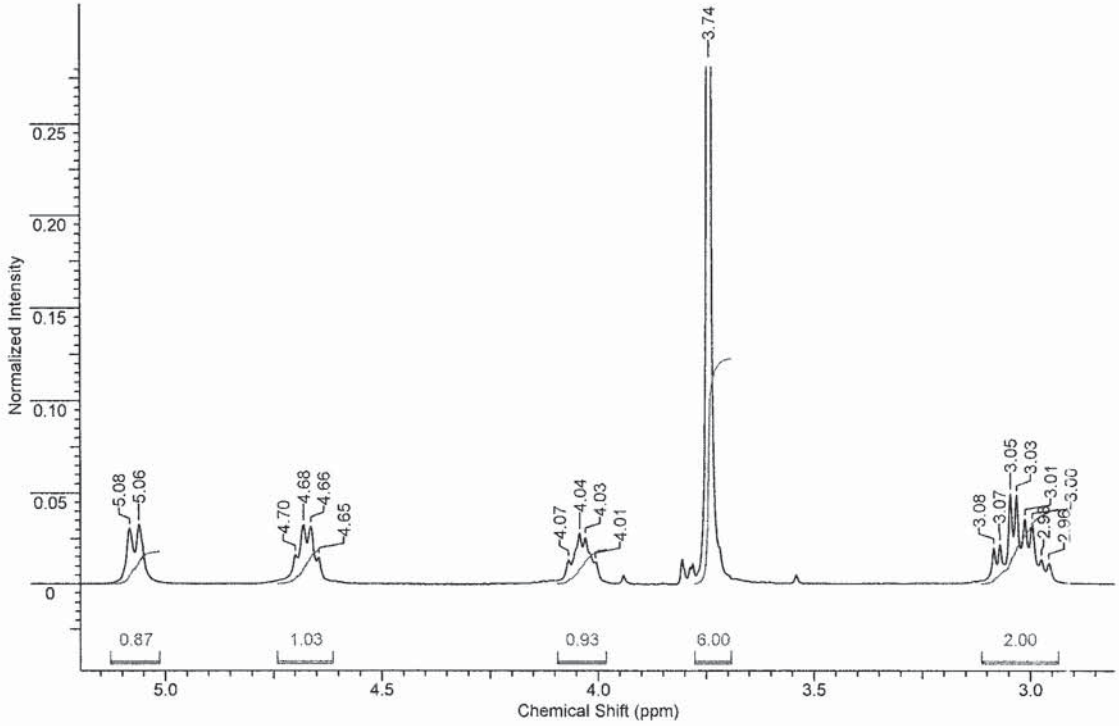

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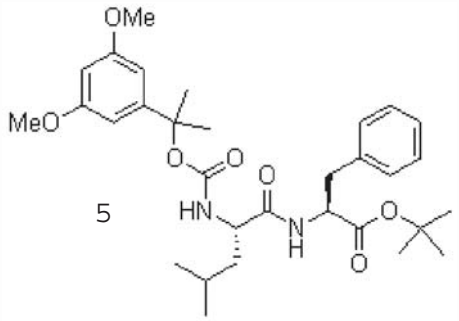
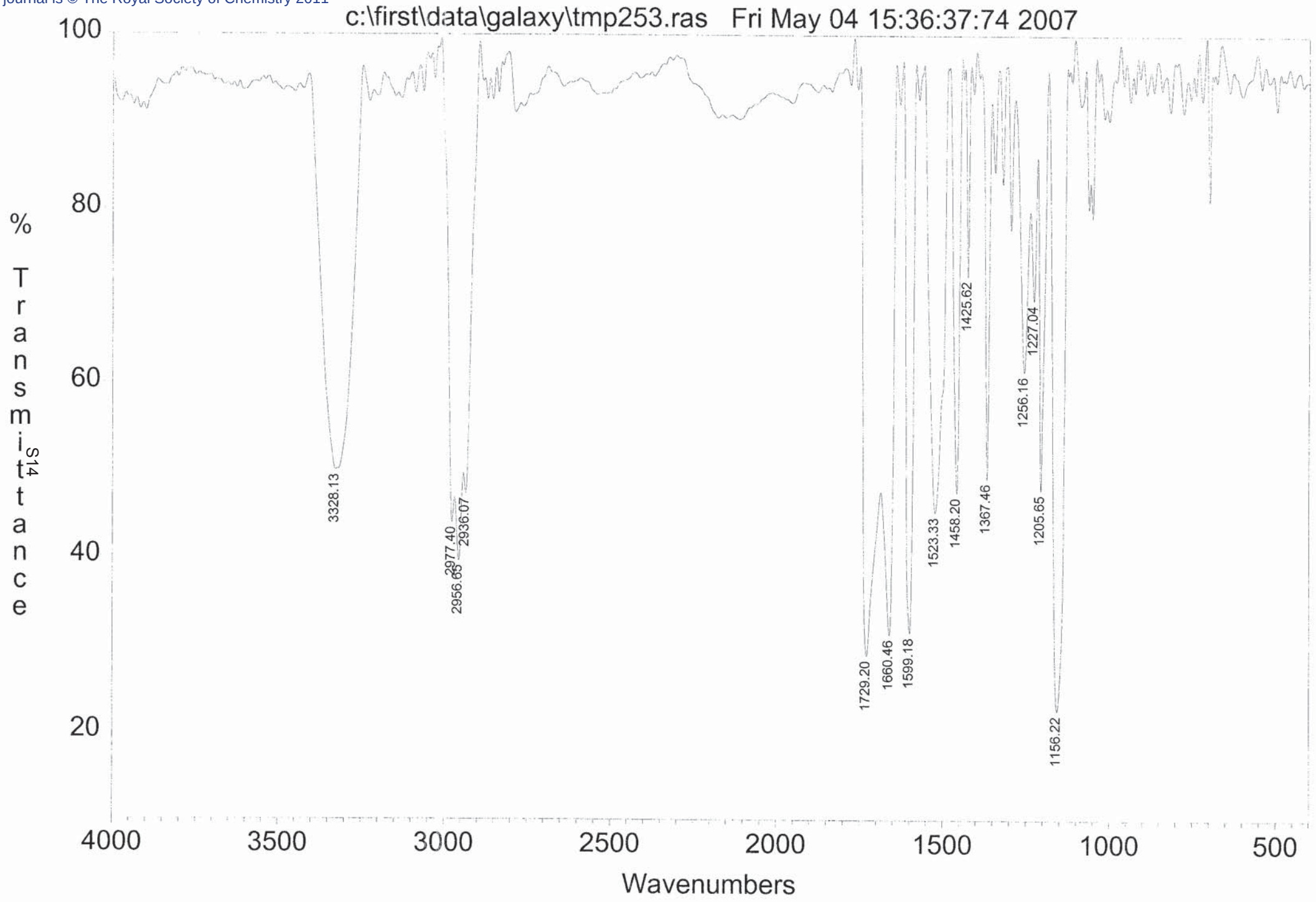
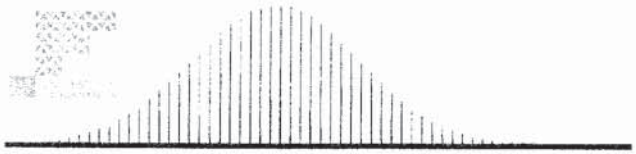
SW(cyclical) (Hz)	30120.48	*Solvent*	CHLOROFORM-d			*Spectrum Offset (Hz)*	12567.2520
Sweep Width (Hz)	30119.56	*Temperature (degree C)*	25.000				







BRUKER FTMS 4.7T BioAPEX II MS-Service UNI-Fribourg

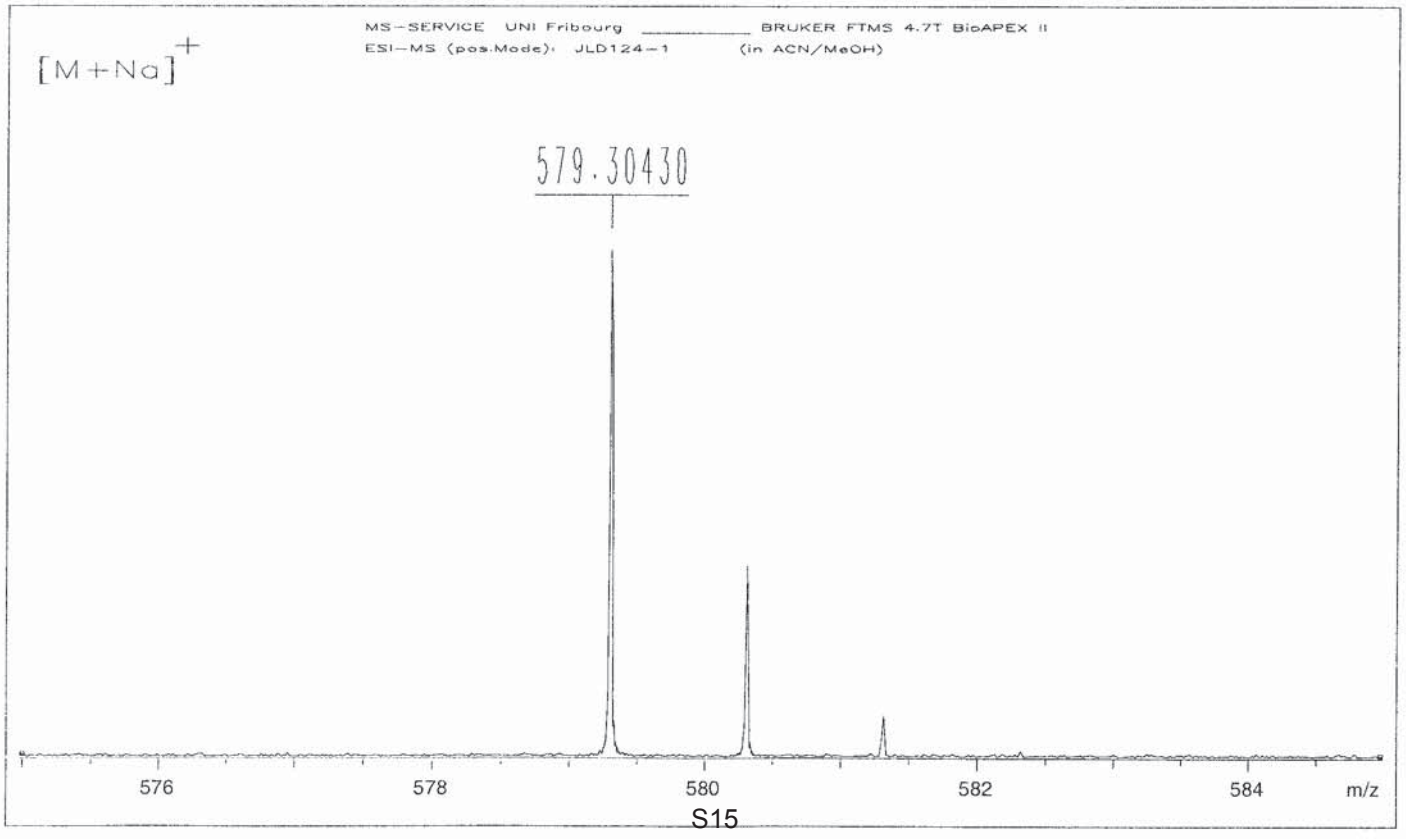
ESI-MS: JLD124-1

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

Ion mass = 579.3043030

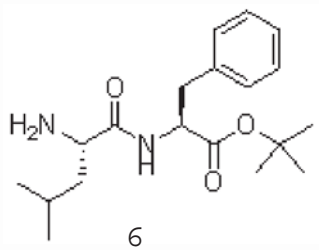
Charge = +1

#	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

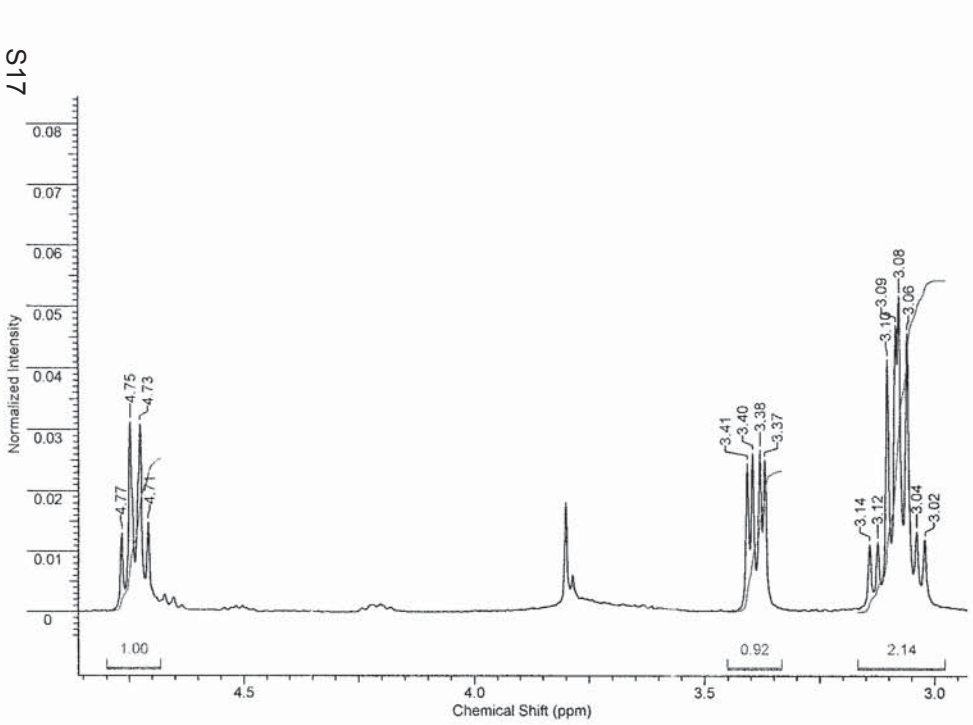
Acquisition Time (sec)	2.2021	*Comment*	PROTONNR CDCl3 u jld 16			*Date*	22 May 2007 12:39:28
File Name	\\HOME\DebieuxJ\My Documents\Chimie\Doctorat\NMR\jld125-2F1_001001r					*Frequency (MHz)*	360.13
Nucleus	1H	*Number of Transients*	16	*Origin*	dpx360	*Original Points Count*	16384
Owner	nmruser	*Points 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				

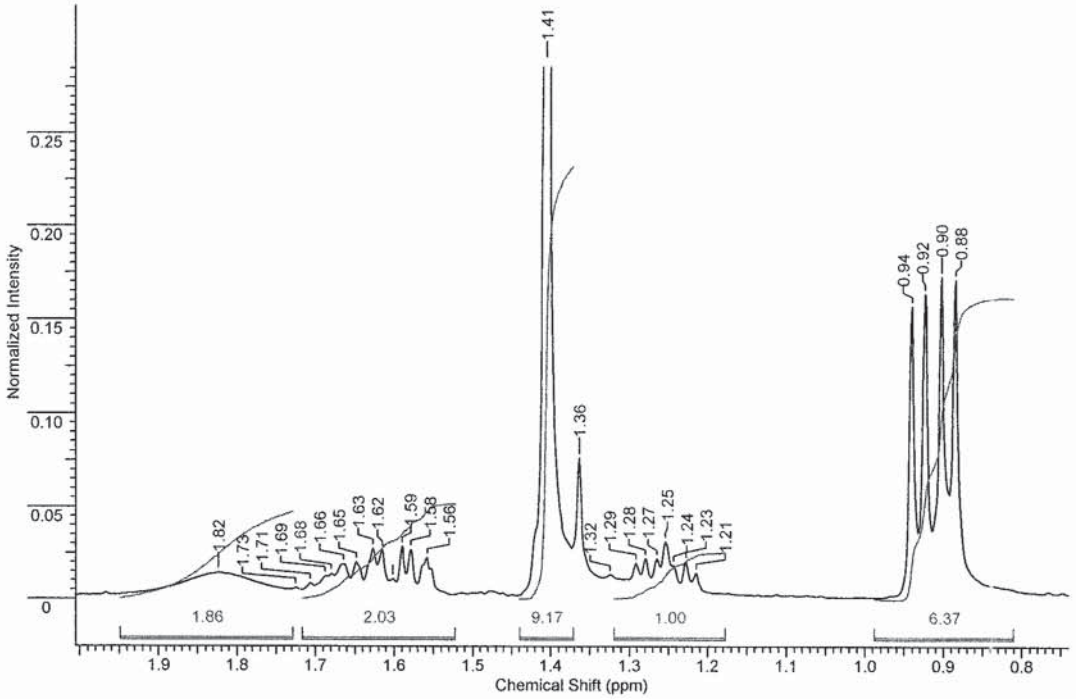


6

jld125

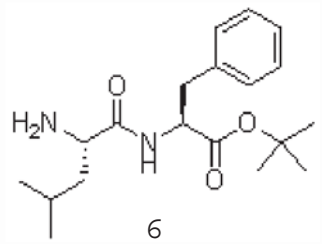
No.	(ppm)	(Hz)	Height
1	0.88	318.5	0.1711
2	0.90	324.8	0.1729
3	0.92	332.5	0.1635
4	0.94	338.4	0.1570
5	1.21	437.4	0.0141
6	1.23	442.0	0.0204
7	1.24	447.9	0.0182
8	1.25	451.5	0.0311
9	1.27	455.6	0.0218
10	1.28	460.6	0.0218
11	1.29	465.1	0.0194
12	1.32	477.0	0.0131
13	1.36	491.0	0.0762
14	1.41	506.0	1.0000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



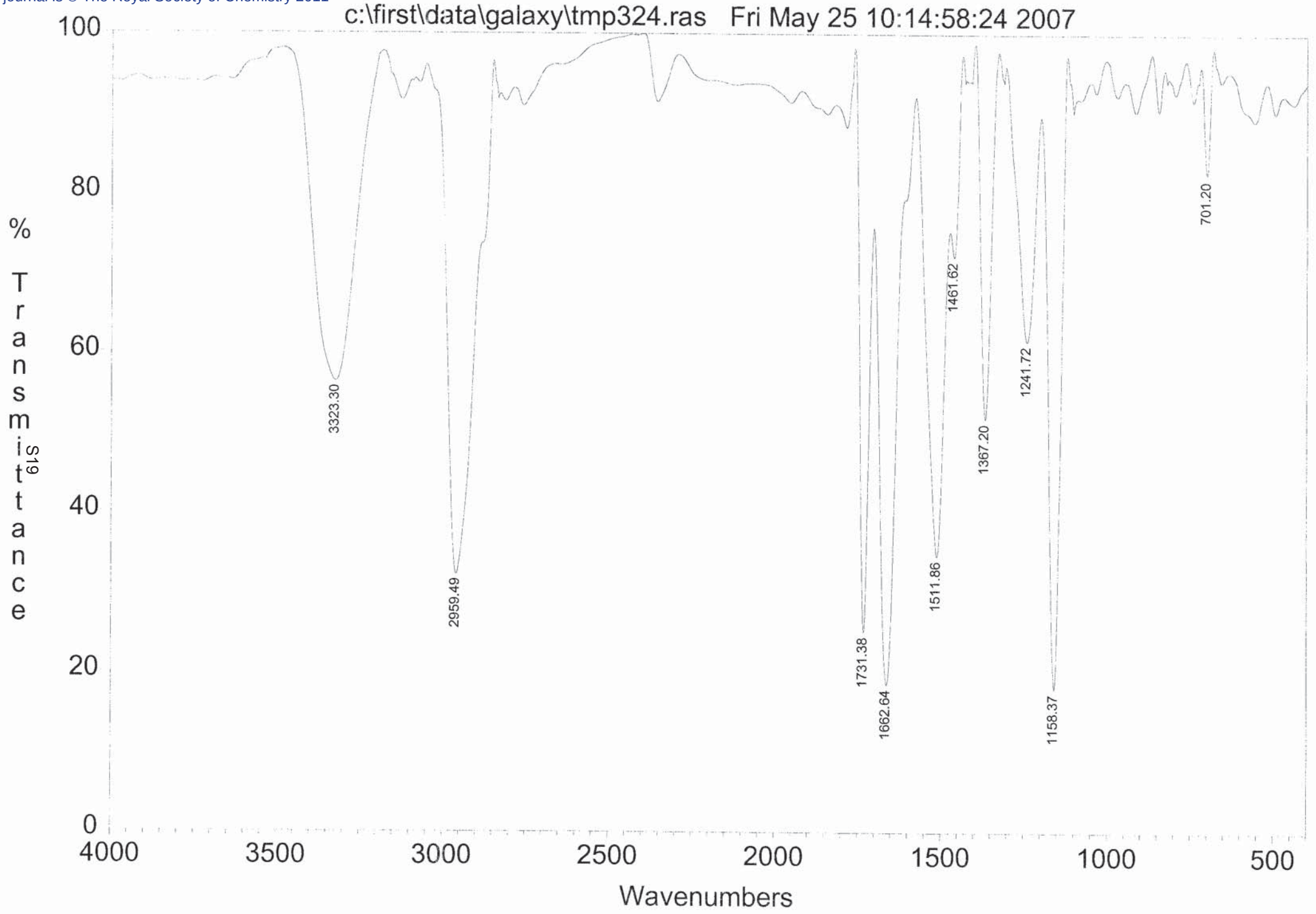


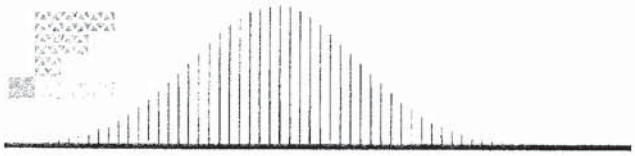
jld125, C13 CPD

Acquisition Time (sec)	1.0879	*Comment*	5 mm Multinuclear Z3149/0097			*Date*	25 May 2007 06:00:32
File Name	\\HOME\DebieuxJ\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				



6





BRUKER FTMS 4.7T BioAPEX II MS-Service UNI-Fribourg

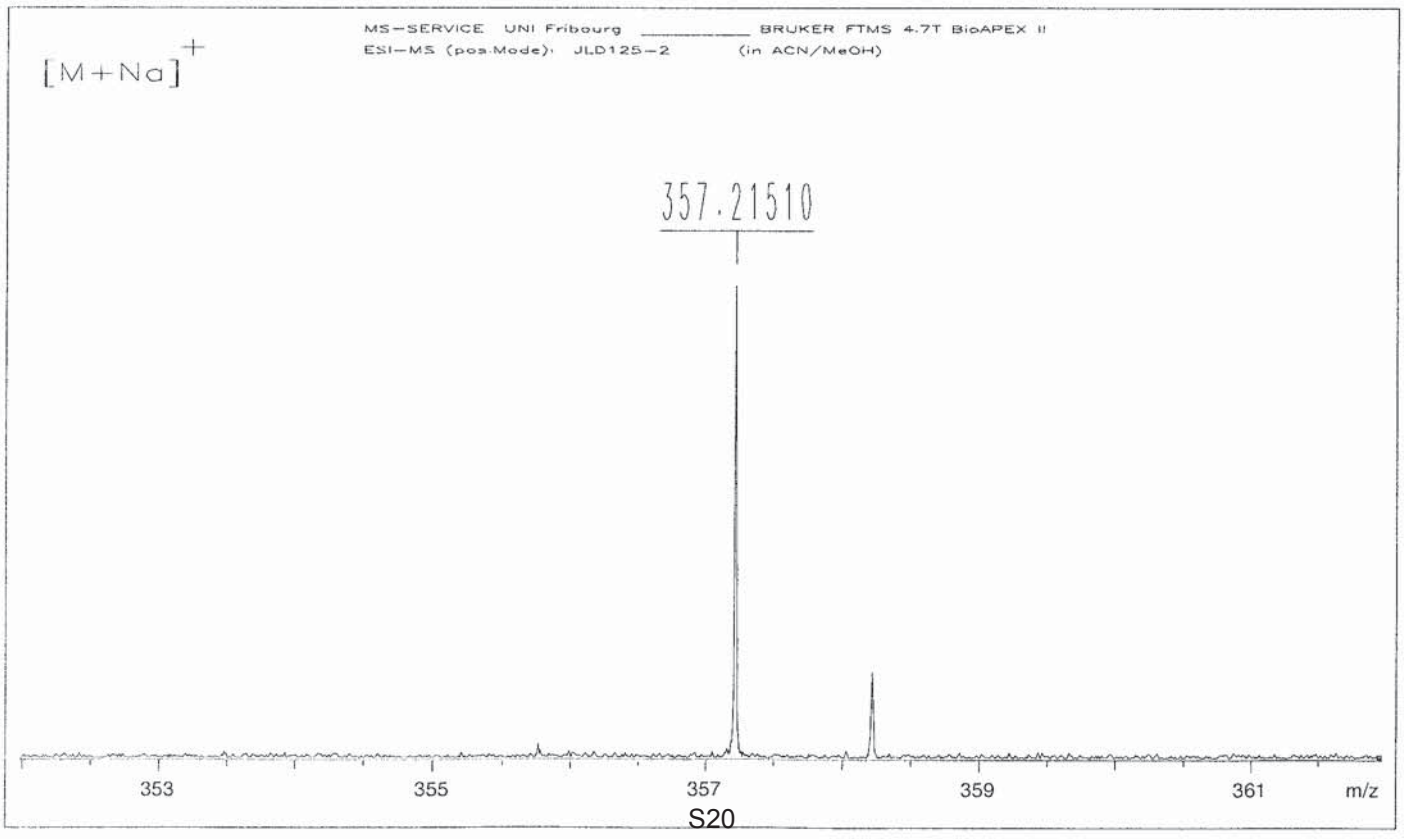
ESI-MS: JLD125-2

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

Ion mass = 357.2151030

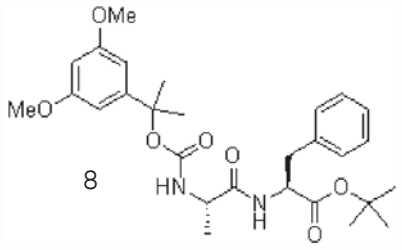
Charge = +1

#	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				



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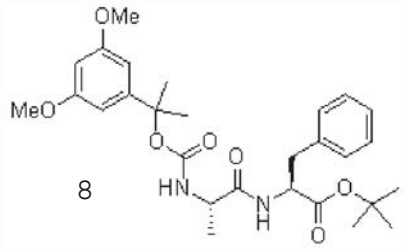
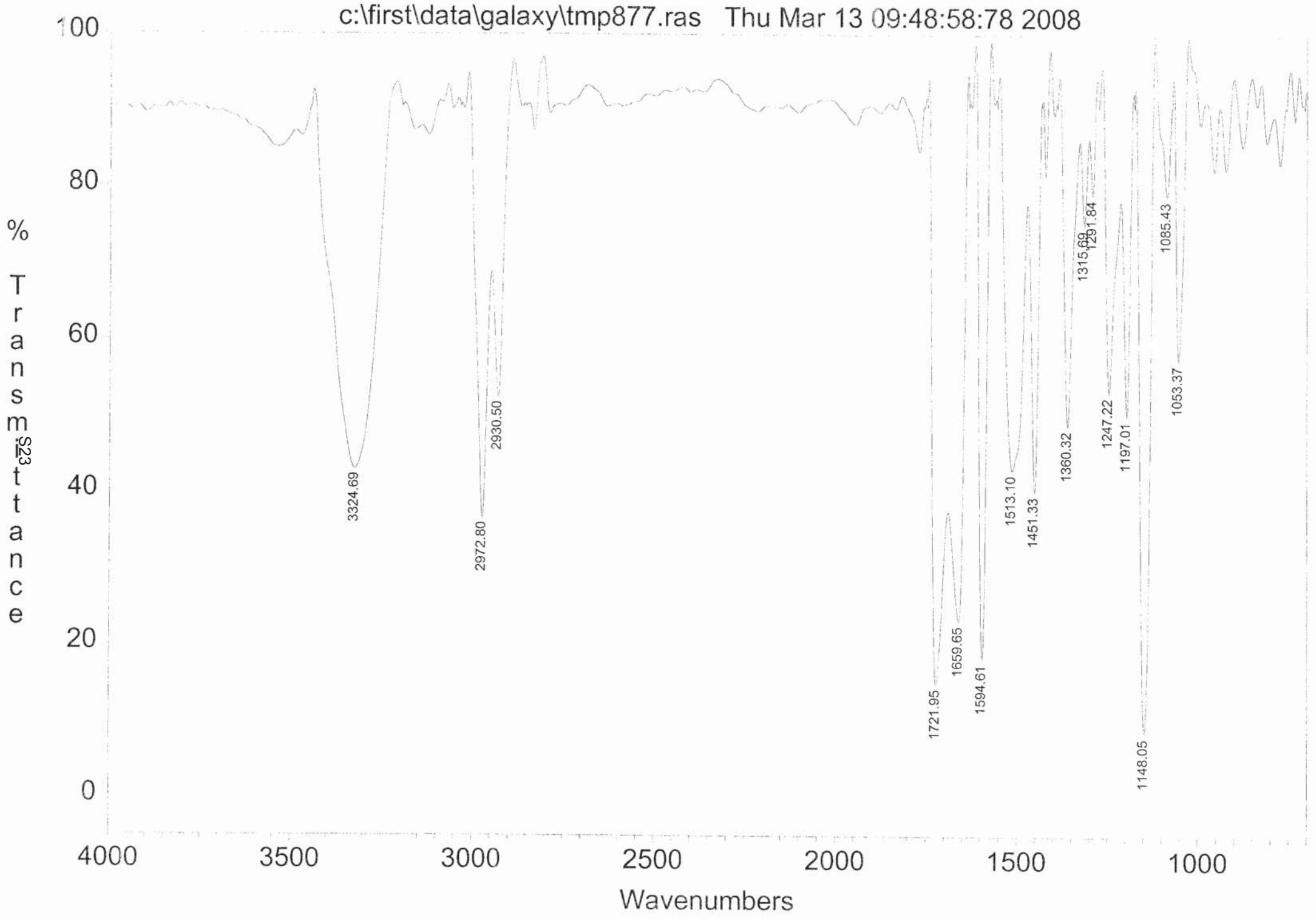
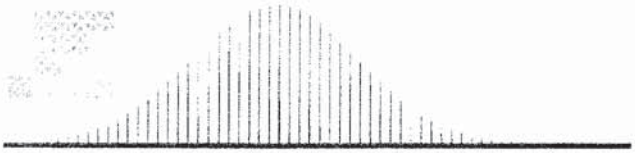
jld172, C13

Acquisition Time (sec)	1.0879	*Comment*	all_carbon	*Date*	14 Mar 2008 14:06:56		
File Name	\\HOME\DebieuxJ\My Documents\Chimie\Doctorat\NMR\debi3758.bbo_002001r					*Frequency (MHz)*	125.76
Nucleus	13C	*Number of Transients*	1974	*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)*	13923.0781
Sweep Width (Hz)	30119.56	*Temperature (degree C)*	25.000				



8





FTMS 4.7T BioAPEX II MS-Service UNI-Fribourg

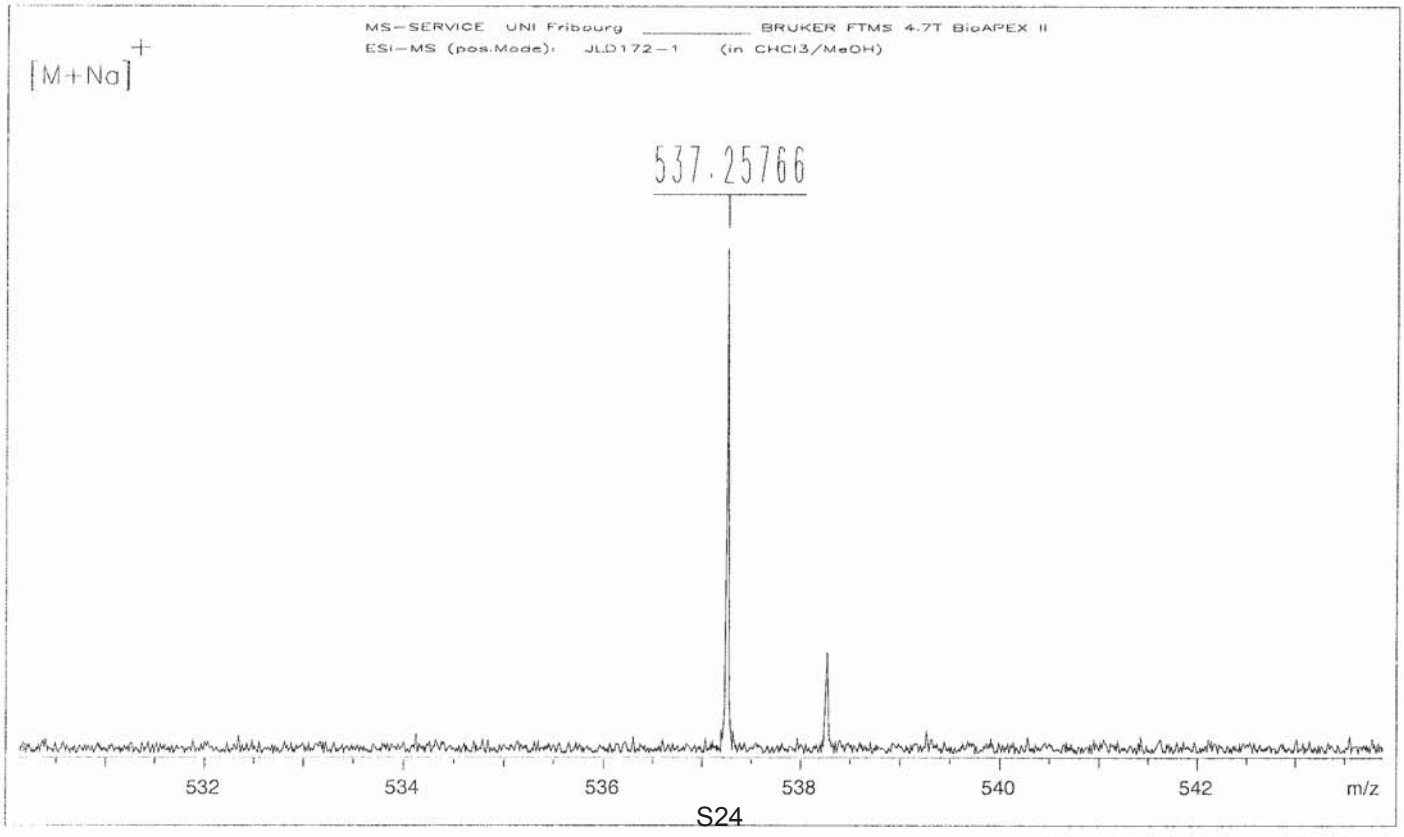
ESI-MS: JLD172-1

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

Ion mass = 537.2576570

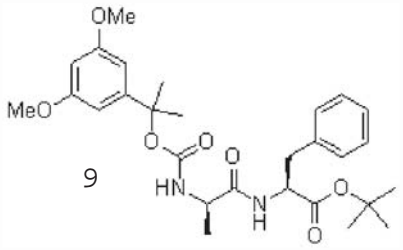
Charge = +1

#	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



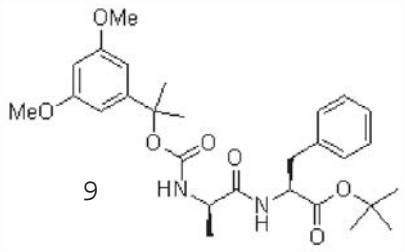
jld173

Acquisition Time (sec)	2.2021	*Comment*	PROTONNR CDCl3 u jld 43			*Date*	18 Mar 2008 12:41:36
File Name	\\HOME\DebieuxJ\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\DebieuxJ\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	*Points Count*	32768
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				



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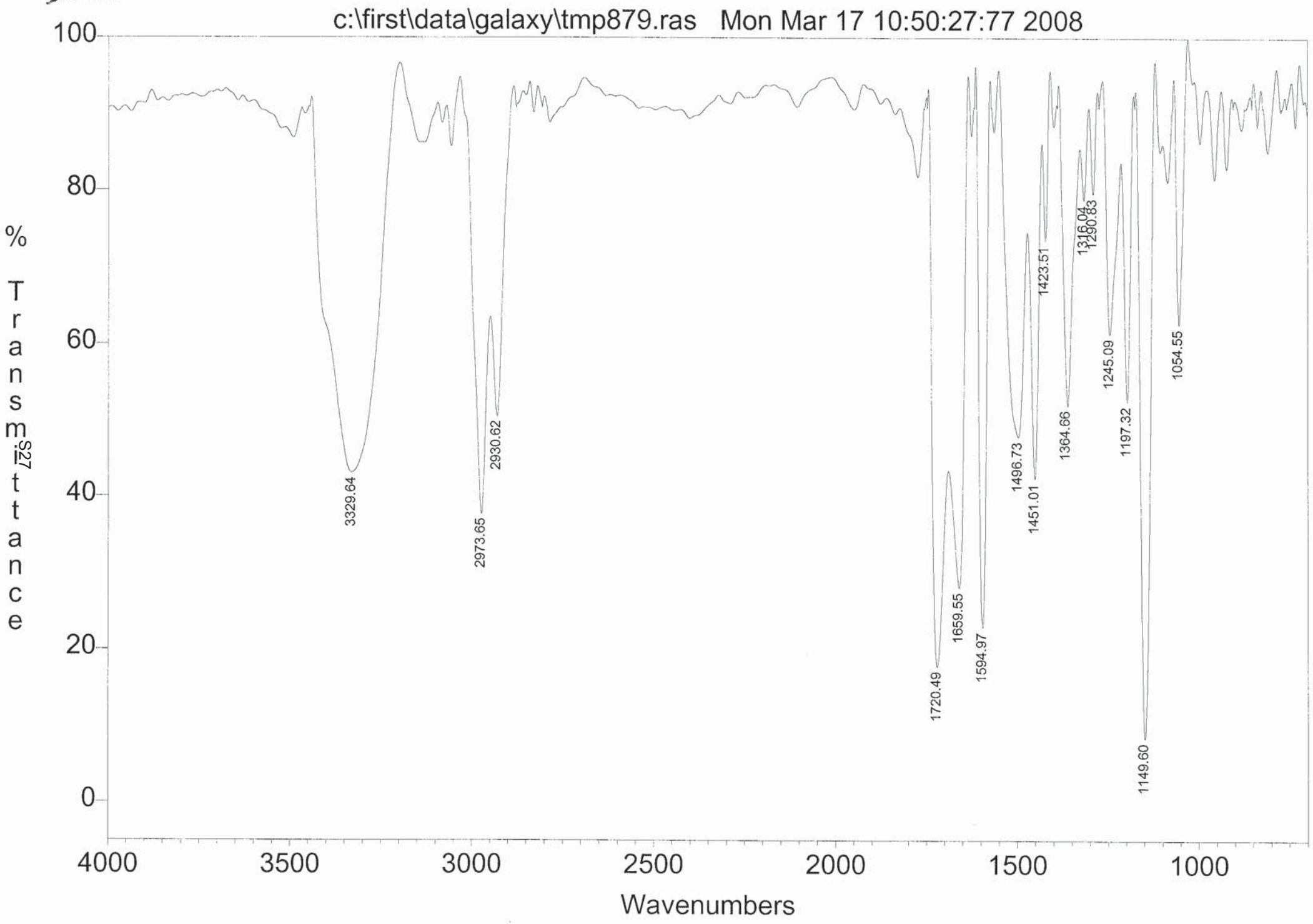
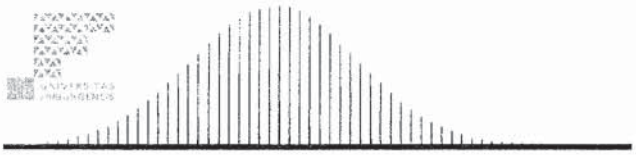




FTMS 4.7T BioAPEX II MS-Service UNI-Fribourg

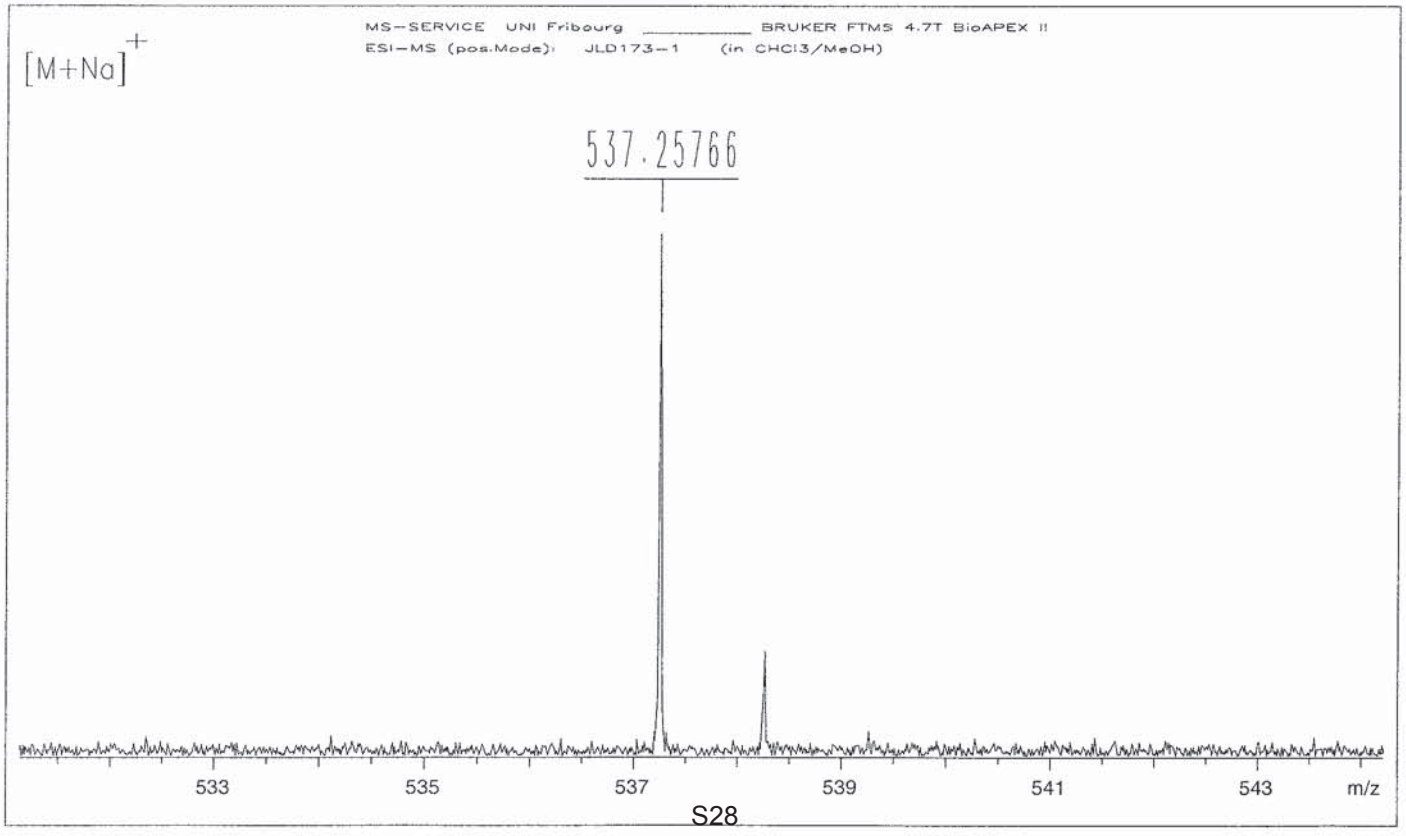
ESI-MS: JLD173-1

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

Ion mass = 537.2576570

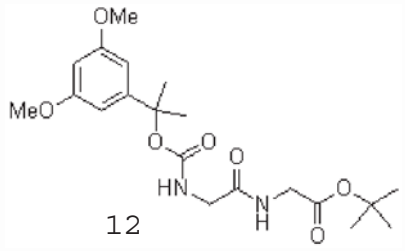
Charge = +1

#	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 CDCl3 u jld 60			***Date***	06 Dec 2007 13:07:12
File Name	\\HOME\DebieuxJ\My 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				



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FTMS 4.7T BioAPEX II MS-Service UNI-Fribourg

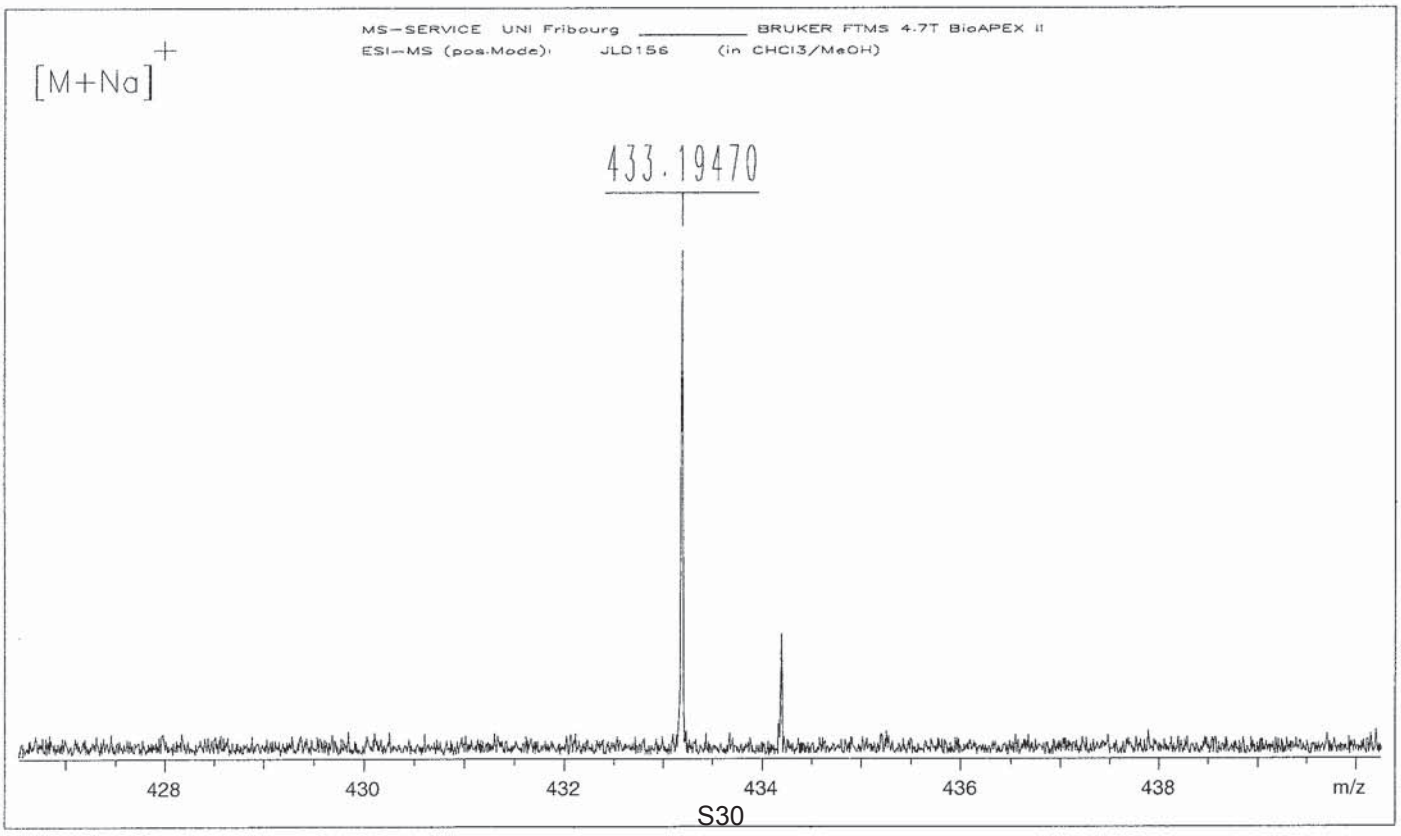
ESI-MS: JLD156

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

Ion mass = 433.1946960

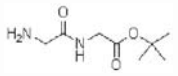
Charge = +1

#	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\DebieuxJ\My Documents\Chimie\Doctorat\NMR\jld157-3_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*	287.40
SW(cyclical) (Hz)	7440.48	*Solvent*	CHLOROFORM-d			*Spectrum Offset (Hz)*	2210.5947
Sweep Width (Hz)	7440.02	*Temperature (degree C)*	27.000				



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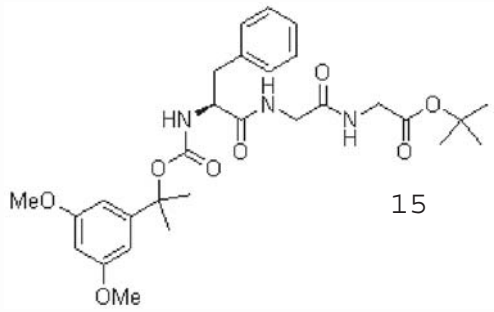
jld160

Acquisition Time (sec)	2.2021	*Comment*	PROTONNR CDCl3 u jld 60			*Date*	17 Dec 2007 14:13:20
File Name	\\HOME\DebieuxJ\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				



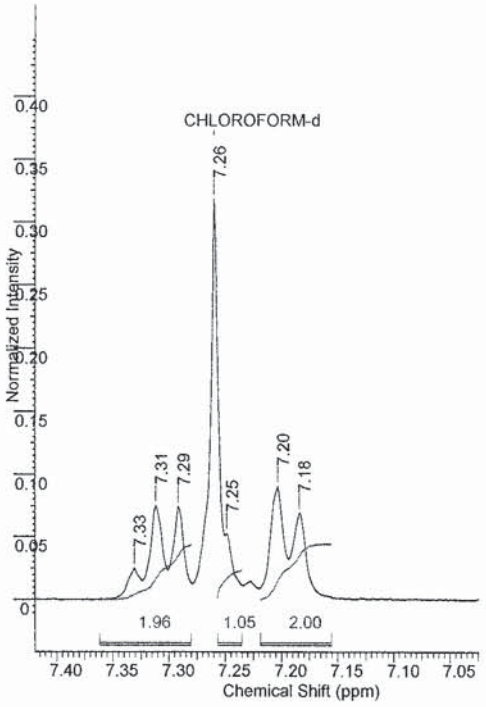
jld160

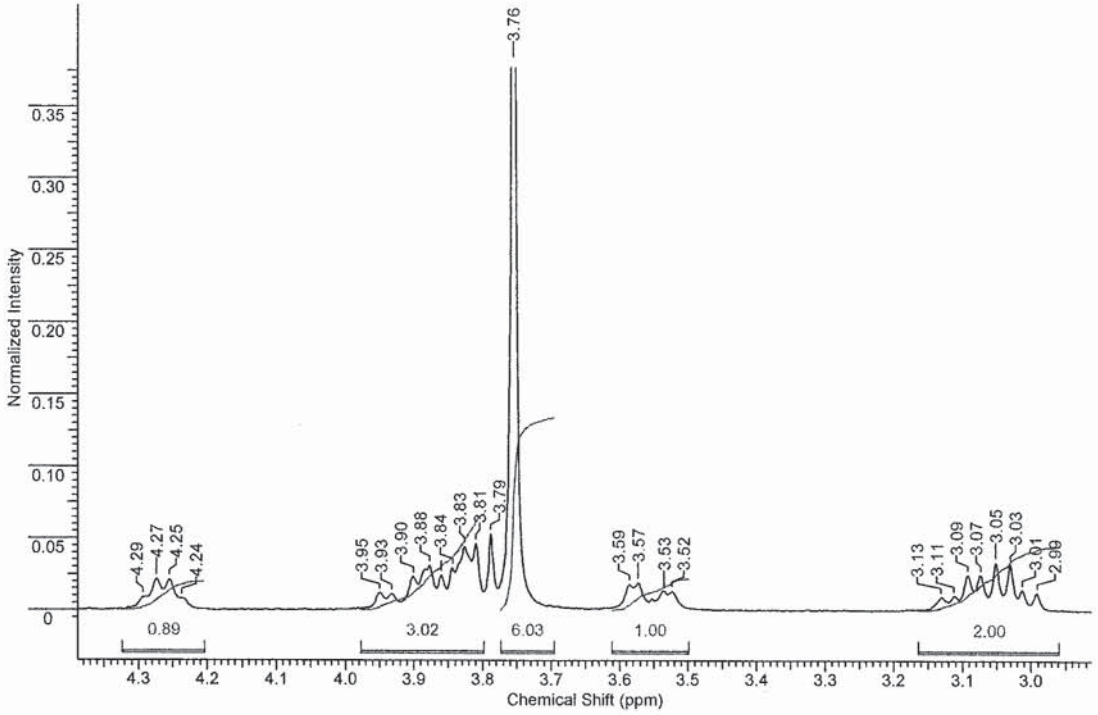
No.	(ppm)	(Hz)	Height
1	1.45	523.7	1.0000
2	1.65	595.9	0.2338
3	1.69	608.6	0.2415
4	2.99	1077.3	0.0127
5	3.01	1085.0	0.0150
6	3.03	1091.4	0.0322
7	3.05	1099.1	0.0336
8	3.07	1106.8	0.0251
9	3.09	1113.6	0.0251
10	3.11	1120.9	0.0106

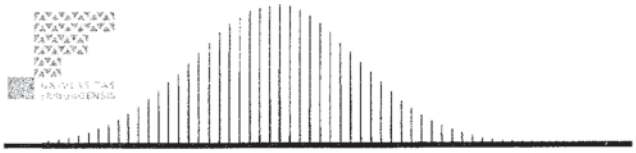
No.	(ppm)	(Hz)	Height
11	3.13	1127.7	0.0098
12	3.52	1269.0	0.0136
13	3.53	1273.0	0.0137
14	3.57	1286.7	0.0194
15	3.59	1291.2	0.0184
16	3.76	1352.5	0.6693
17	3.79	1364.3	0.0535
18	3.81	1372.0	0.0464
19	3.83	1377.9	0.0443
20	3.84	1384.3	0.0294

No.	(ppm)	(Hz)	Height
21	3.86	1390.2	0.0246
22	3.88	1396.1	0.0311
23	3.90	1404.7	0.0236
24	3.93	1416.1	0.0115
25	3.95	1422.5	0.0120
26	4.24	1526.0	0.0084
27	4.25	1532.4	0.0212
28	4.27	1539.2	0.0216
29	4.29	1546.4	0.0089
30	5.24	1888.4	0.0247

No.	(ppm)	(Hz)	Height
31	5.26	1894.7	0.0231
32	6.32	2276.7	0.0683
33	6.43	2314.8	0.1606
34	6.53	2352.1	0.0308
35	7.18	2587.3	0.0690
36	7.20	2594.1	0.0904
37	7.26	2614.5	0.3182
38	7.29	2625.9	0.0742
39	7.31	2633.2	0.0753
40	7.33	2640.0	0.0250







BRUKER FTMS 4.7T BioAPEX II MS-Service UNI-Fribourg

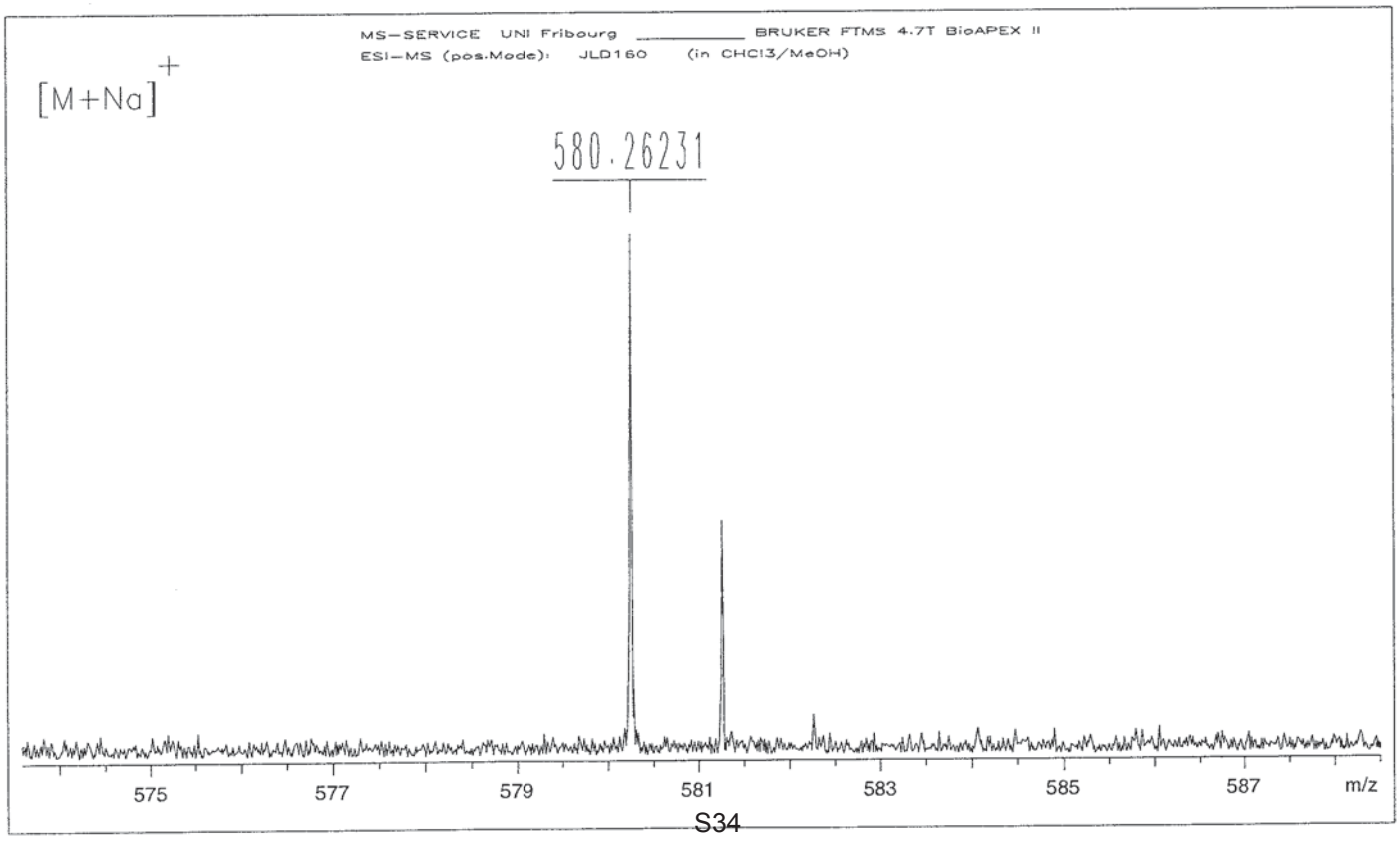
ESI-MS: JLD160

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

Ion mass = 580.2623080

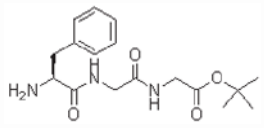
Charge = +1

#	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\DebieuxJ\My Documents\Chimie\Doctorat\NMR\jld163-2_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***	574.70
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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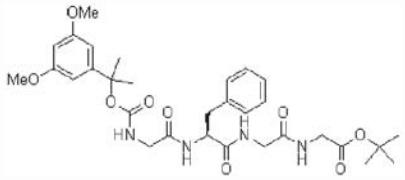
jld165

Acquisition Time (sec)	2.2021	***Comment***	PROTONNR CDCl3 u jld 47			***Date***	25 Jan 2008 13:49:52
File Name	\\HOME\DebieuxJ\My 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

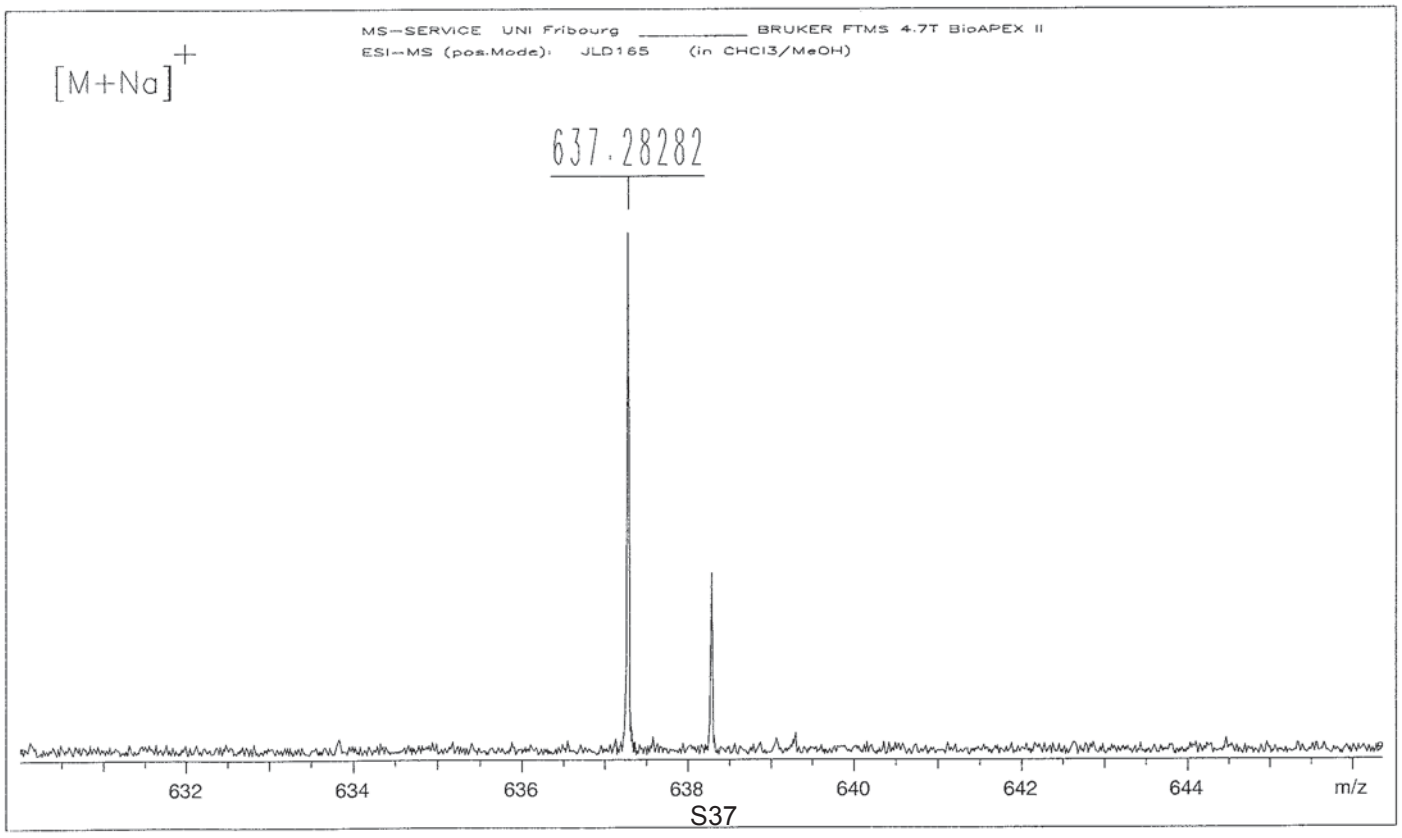
ESI-MS: JLD165

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

Ion mass = 637.2828190

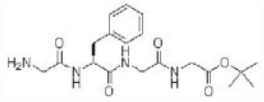
Charge = +1

#	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\DebieuxJ\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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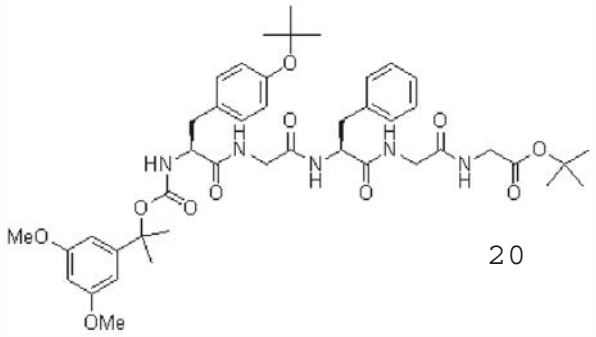
S38

jld167

Acquisition Time (sec)	2.2021	*Comment*	PROTONNR CDCl3 u jld 36			*Date*	10 Apr 2008 09:01:52
File Name	\\HOME\DebieuxJ\My 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				



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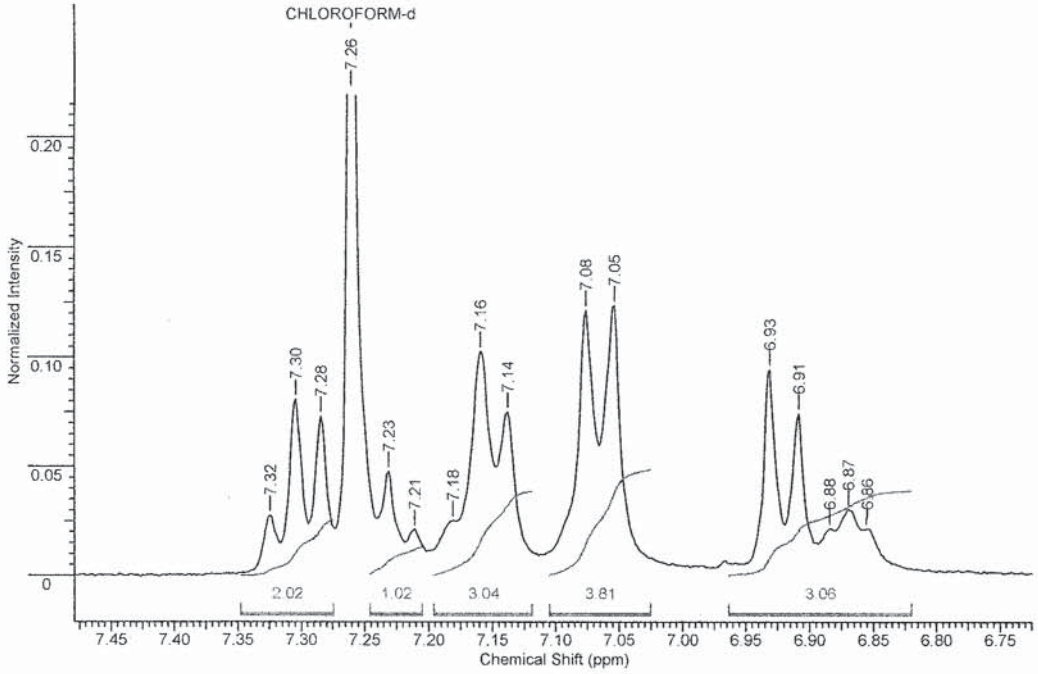
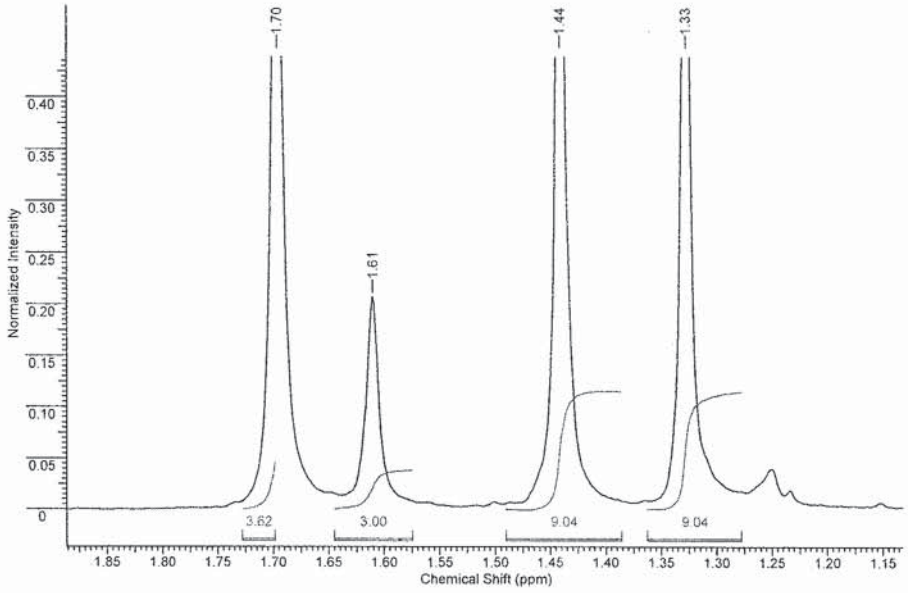
jld167

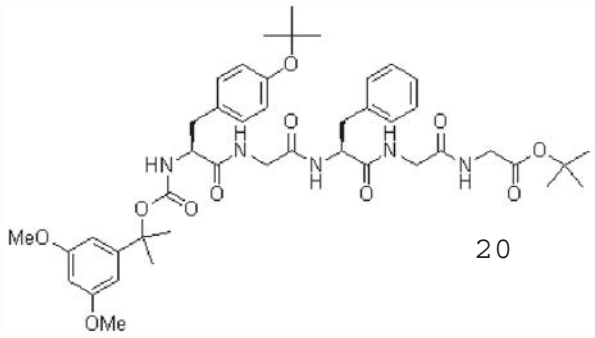
No.	(ppm)	(Hz)	Height
1	1.33	478.3	1.0000
2	1.44	519.2	0.8910
3	1.61	580.0	0.2071
4	1.70	610.9	0.7355
5	2.53	911.6	0.0144
6	2.56	921.1	0.0173
7	2.57	925.6	0.0185
8	2.60	934.7	0.0170
9	2.86	1028.3	0.0162
10	2.88	1036.9	0.0186
11	2.89	1041.9	0.0247
12	2.92	1051.0	0.0239
13	3.03	1092.3	0.0342
14	3.05	1096.8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





jld167, C13

Acquisition Time (sec)	1.0879	*Comment*	all_carbon	*Date*	23 Mar 2008 00:17:04		
File Name	\\HOME\DebieuxJ\My Documents\Chimie\Doctorat\NMR\debi3769.bbo_002001r					*Frequency (MHz)*	125.76
Nucleus	13C	*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)*	13922.1592	*Sweep Width (Hz)*	30119.56
Temperature (degree C)	20.000						



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Display Report

Analysis Info

Analysis Name	D:\Data\Debieux\EDAF3145_ESI.d	Acquisition Date	20.02.2008 15:07:03
Method	JLD148_MS.m	Operator	Administrator
Sample Name	JLD167-1	Instrument	HCT
Comment	(in CHCl3/MeOH/NaCl)		

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