

SUPPORTING INFORMATION

Photochemical Synthesis of *N*-Protected- α - Amino Acid Amides *via* *N*-Protected- α -Amino Acyl-5,7-Dinitroindolines

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Experimental Section

General: ^1H - and ^{13}C -NMR spectra were recorded with 500 MHz or 360 MHz spectrometers with residual solvent signals used as a reference. For ^{13}C NMR spectra, the hydrogen substitution pattern was determined by a DEPT sequence. IR spectra were recorded with a Fourier transform FTIR spectrometer, neat, in CHCl_3 (NaCl cell), or in KBr pellets; absorption bands are in cm^{-1} . UV spectra absorption bands are in nm. EI mass spectra were recorded with a quadrupole spectrometer, with electron impact ionization (70 eV), whereas ESI mass spectra were measured with a ion-cyclotron FT/MS mass 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. All the reactions subjected to microwave heating were performed in a Biotage InitiatorTM 2.0 microwave. Column chromatography was carried out on silica gel (32-63 mesh). Unless otherwise indicated, all commercial reagents were used without further purification.

Benzyl (S)-1-(5,7-dinitroindolin-1-yl)-1-oxopropan-2-ylcarbamate (3b): Purification by flash column chromatography [SiO_2 , hexane/EtOAc (1:2)]. Yellow solid (348 mg, 84 %); mp. 70-73°C; ^1H NMR (360 MHz, CDCl_3) δ = 8.59 (s, 1H), 8.28 (s, 1H), 7.32 (b, 5H), 5.53 (d, J = 7.8 Hz, 1H), 5.08 (dd, J = 21.0, 12.3 Hz, 2H), 4.76-4.68 (2H), 4.43 (q, J = 9.6 Hz, 1H), 3.49 (m, 1H), 3.31 (m, 1H), 1.48 (d, J = 6.8 Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ = 172.5, 156.1, 143.9, 140.0, 139.4, 138.8, 136.1, 128.7 (2xC), 128.4, 128.0 (2xC), 123.5, 120.0, 67.3, 50.4, 49.5, 29.0, 17.9. IR (neat): 3410, 3332, 1694, 1609, 1546, 1532, 1454, 1399, 1373, 1341, 1311, 1279, 1253, 1221, 1062. HR-MS 437.1064 ($\text{C}_{19}\text{H}_{18}\text{N}_4\text{O}_7 + \text{Na}^+$ calcd 437.1068).

N-Benzyloxycarbonyl-(S)-1'-[(5,7)-dinitroindolin-1-yl]-proline (3d): Purification by flash column chromatography [SiO_2 , hexane/EtOAc (3:1)]. Yellow solid (388 mg, 88 %); mp. 71 °C; ^1H NMR (500 MHz, $\text{DMSO}-d_6$) mixture of 2 rotamers δ = 8.48-8.47 (1H), 8.45-8.39 (1H), 7.38-7.17 (5H), 5.10-4.94

(2H), 4.83-4.80 (1H), 4.74-4.33 (1H), 4.32-4.23 (1H), 3.52-3.33 (3H), 3.22-2.78 (1H), 2.33-2.23 (1H), 2.00-1.85 (3H); ^{13}C NMR (125 MHz, $\text{DMSO}-d_6$) mixture of 2 rotamers δ = 171.9, 171.8, 154.0, 153.2, 143.03, 142.98, 139.8, 139.7, 139.4, 139.1, 138.24, 138.20, 136.8, 136.4, 128.4, 128.2, 127.8, 127.6, 127.4, 123.9, 123.8, 119.3, 66.4, 66.1, 58.7, 58.0, 50.2, 50.0, 47.0, 46.4, 29.8, 28.9, 28.3, 27.9, 24.0, 23.1. IR (neat): 2979, 2958, 1708, 1695, 1609, 1545, 1534, 1464, 1417, 1341, 1283, 1211, 1166, 739. HR-MS 463.1220 ($\text{C}_{21}\text{H}_{20}\text{N}_4\text{O}_7 + \text{Na}^+$ calcd 463.1224).

***tert*-Butyl (S)-1-(5,7-dinitroindolin-1-yl)-1-oxo-3-phenylpropan-2-ylcarbamate (3e):** Purification by flash column chromatography [SiO_2 , hexane/EtOAc (2:1)]. Yellow solid (369 mg, 81 %); mp. 86 °C; ^1H NMR (360 MHz, CDCl_3) δ = 8.58 (s, 1H), 8.21 (s, 1H), 7.32-7.26 (5H), 5.28 (d, J = 8.7 Hz, 1H), 4.80 (q, J = 7.7 Hz, 1H), 4.43 (td, J = 10.0, 5.6 Hz, 1H), 3.57 (m, 1H), 3.25 (m, 1H), 3.14-3.01 (2H), 2.99-2.90 (1H), 1.40 (s, 9H); ^{13}C NMR (125 MHz, CDCl_3) δ = 171.6, 155.5, 143.9, 139.7, 139.4, 138.9, 136.1, 129.6 (2xC), 128.9 (2xC), 127.4, 123.3, 119.9, 80.6, 54.8, 50.2, 39.3, 28.7, 28.4 (3xC). IR (neat): 3412, 3344, 2978, 2933, 1692, 1608, 1545, 1532, 1500, 1459, 1439, 1392, 1370, 1341, 1280, 1251, 1164. HR-MS 479.15041 ($\text{C}_{22}\text{H}_{24}\text{N}_4\text{O}_7 + \text{Na}^+$ calcd 479.1537).

Benzyl (S)-3-*tert*-butoxy-1-(5,7-dinitroindolin-1-yl)-1-oxopropan-2-ylcarbamate (3g): Purification by flash column chromatography [SiO_2 , hexane/EtOAc (1:1)]. Yellow solid (443 mg, 91 %); mp. 84 °C; ^1H NMR (360 MHz, CDCl_3) δ = 8.58 (s, 1H), 8.28 (s, 1H), 7.38-7.27 (5H), 5.59 (d, J = 7.8 Hz, 1H), 5.10 (dd, J = 14.8, 12.5 Hz, 2H), 4.82 (dd, J = 13.2, 7.3 Hz, 1H), 4.60 (m, 2H), 3.67 (m, 1H), 3.57 (t, J = 8.2 Hz, 1H), 3.33 (m, 2H), 1.17 (s, 9H); ^{13}C NMR (125 MHz, CDCl_3) δ = 170.7, 156.1, 144.0, 139.7, 139.6, 139.1, 136.1, 128.7 (2xC), 128.4, 128.1 (2xC), 123.4, 119.9, 74.2, 67.3, 62.7, 53.9, 50.6, 28.9, 27.4 (3xC). IR (neat): 3416, 3323, 2974, 1716, 1696, 1536, 1458, 1341, 1285, 1222, 1087. HR-MS 509.1630 ($\text{C}_{23}\text{H}_{26}\text{N}_4\text{O}_8 + \text{Na}^+$ calcd 509.1643).

***tert*-Butyl (S)-3-methyl-1-(5,7-dinitroindolin-1-yl)-1-oxobutan-2-ylcarbamate (3h):** Purification by flash column chromatography [SiO_2 , hexane/EtOAc (1:1)]. Yellow solid (343 mg, 84 %); mp. 107 °C; ^1H NMR (360 MHz, CDCl_3) δ = 8.56 (s, 1H), 8.27 (s, 1H), 5.17 (d, J = 9.1 Hz, 1H), 4.81 (td, J = 10.2,

3.7 Hz, 1H), 4.44 (dd, $J = 9.1, 5.9$ Hz, 1H), 4.34 (q, $J = 10$ Hz, 1H), 3.49 (m, 1H), 3.29 (m, 1H), 2.13 (m, 1H), 1.40 (s, 9H), 1.07 (d, $J = 6.8$ Hz, 3H), 1.02 (d, $J = 6.8$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3) $\delta = 172.3, 156.2, 143.9, 139.8, 139.7, 138.7, 123.3, 119.9, 80.4, 58.2, 50.6, 31.6, 28.9, 28.4$ (3xC), 19.5, 17.7. IR (neat): 3425, 2975, 2935, 1689, 1547, 1532, 1505, 1464, 1392, 1370, 1341, 1284, 1168, 1157. HR-MS 431.1544 ($\text{C}_{18}\text{H}_{24}\text{N}_4\text{O}_7 + \text{Na}^+$ calcd 431.1537).

***tert*-Butyl (S)-4-(methylthio)-1-(5,7-dinitroindolin-1-yl)-1-oxobutan-2-ylcarbamate (3i):**

Purification by flash column chromatography [SiO_2 , hexane/EtOAc (2:1)]. Yellow solid (352 mg, 80 %); mp. 87 °C; ^1H NMR (360 MHz, CDCl_3) $\delta = 8.57$ (s, 1H), 8.28 (s, 1H), 5.20 (d, $J = 8.7$ Hz, 1H), 4.83 (m, 2H), 4.43 (q, $J = 9.7$ Hz, 1H), 3.49 (m, 1H), 3.31 (m, 1H), 2.65 (b, 2H), 2.13 (s, 3H), 2.10 (m, 1H), 1.96 (m, 1H), 1.40 (s, 9H); ^{13}C NMR (125 MHz, CDCl_3) $\delta = 172.3, 155.9, 143.9, 139.9, 139.5, 139.0, 123.5, 119.9, 80.6, 51.8, 50.6, 32.0, 30.1, 29.0, 28.4$ (3xC), 15.7. IR (neat): 3339, 2977, 2922, 1692, 1609, 1545, 1533, 1463, 1439, 1392, 1370, 1341, 1280, 1251, 1163. HR-MS 463.1249 ($\text{C}_{18}\text{H}_{24}\text{N}_4\text{O}_7\text{S} + \text{Na}^+$ calcd 463.1258).

***tert*-Butyl (S)-3-(4-*tert*-butoxyphenyl)-1-(5,7-dinitroindolin-1-yl)-1-oxopropan-2-ylcarbamate (3m):**

Purification by flash column chromatography [SiO_2 , hexane/EtOAc (2:1)]. Yellow solid (433 mg, 82 %); mp. 120 °C; ^1H NMR (360 MHz, CDCl_3) $\delta = 8.56$ (s, 1H), 8.20 (s, 1H), 7.22 (d, $J = 8.1$ Hz, 2H), 6.92 (d, $J = 8.2$ Hz, 2H), 5.31 (d, $J = 8.2$ Hz, 1H), 4.77 (q, $J = 7.9$ Hz, 1H), 4.39 (m, 1H), 3.49 (q, $J = 9.2$ Hz, 1H), 3.24 (m, 1H), 3.08-2.90 (3H), 1.40 (s, 9H), 1.31 (s, 9H); ^{13}C NMR (125 MHz, CDCl_3) $\delta = 171.6, 155.5, 154.7, 143.9, 139.7, 139.3, 138.9, 130.9, 130.2$ (2xC), 124.6 (2xC), 123.3, 119.9, 80.5, 78.8, 54.9, 50.2, 38.8, 28.9 (3xC), 28.7, 28.4 (3xC). IR (neat): 3423, 3338, 2978, 1692, 1540, 1511, 1464, 1375, 1342, 1278, 1243, 1166. HR-MS 551.2112 ($\text{C}_{26}\text{H}_{32}\text{N}_4\text{O}_8 + \text{Na}^+$ calcd 551.2112).

***tert*-Butyl (S)-3-(1*H*-indol-3-yl)-1-(5,7-dinitroindolin-1-yl)-1-oxopropan-2-ylcarbamate (3n):**

Purification by flash column chromatography [SiO_2 , hexane/EtOAc (1:1)]. Yellow solid (396 mg, 80 %); mp. 115 °C; ^1H NMR (360 MHz, CDCl_3) $\delta = 8.53$ (s, 1H), 8.21 (b, 1H), 8.09 (s, 1H), 7.65 (d, $J = 7.7$ Hz, 1H), 7.35 (d, $J = 8.2$ Hz, 1H), 7.15 (m, 2H), 7.08 (t, $J = 7.5$ Hz, 1H), 5.33 (d, $J = 8.2$ Hz, 1H),

4.94 (q, $J = 7.6$ Hz, 1H), 4.32 (m, 1H), 3.46 (q, $J = 9.1$ Hz, 1H), 3.25 (d, $J = 7.2$ Hz, 2H), 3.04 (m, 1H), 2.62 (m, 1H), 1.42 (s, 9H); ^{13}C NMR (125 MHz, CDCl_3) $\delta = 172.2, 155.6, 143.8, 139.6, 139.4, 139.0, 136.2, 127.3, 124.0, 123.2, 122.6, 120.1, 119.7, 118.6, 111.5, 109.8, 80.5, 53.5, 50.2, 29.3, 28.5, 28.4$ (3xC). IR (neat): 3418, 3354, 2979, 1704, 1682, 1609, 1542, 1504, 1461, 1439, 1391, 1371, 1341, 1280, 1164, 742. HR-MS 518.1645 ($\text{C}_{24}\text{H}_{25}\text{N}_5\text{O}_7 + \text{Na}^+$ calcd 518.1646).

2-(3,5-dimethoxyphenyl)propan-2-yl 2-(5,7-dinitroindolin-1-yl)-2-oxoethylcarbamate (3o):

Purification by flash column chromatography [SiO_2 , hexane/EtOAc (1:2)]. Yellow solid (371 mg, 76 %); mp. 173 °C; ^1H NMR (360 MHz, CDCl_3) $\delta = 8.53$ (s, 1H), 8.26 (s, 1H), 6.49 (s, 2H), 6.30 (s, 1H), 5.54 (b, 1H), 4.27 (t, $J = 8.2$ Hz, 2H), 4.08 (d, $J = 5.0$ Hz, 2H), 3.75 (s, 6H), 3.32 (t, $J = 8.0$ Hz, 2H), 1.71 (s, 6H); ^{13}C NMR (125 MHz, CDCl_3) $\delta = 169.7, 160.8$ (2xC), 155.7, 151.4, 148.9, 146.5, 144.2, 127.6, 122.9, 118.2, 103.0 (2xC), 98.1, 81.8, 55.4 (2xC), 44.6, 38.4, 36.5, 29.2 (2xC). IR (neat): 3416, 1719, 1694, 1599, 1539, 1459, 1426, 1386, 1370, 1337, 1277, 1203, 1147, 1044, 731. UV (51 μM soln in MeCN) λ_{max} (ϵ) 222 (23860), 275 (7200), 343 (10830). HR-MS 511.1436 ($\text{C}_{22}\text{H}_{24}\text{N}_4\text{O}_9 + \text{Na}^+$ calcd 511.1435).

2-(3,5-dimethoxyphenyl)propan-2-yl (S)-1-(5,7-dinitroindolin-1-yl)-1-oxopropan-2-ylcarbamate (3p):

Purification by flash column chromatography [SiO_2 , hexane/EtOAc (1:1)]. Yellow solid (392 mg, 78 %); mp. 80-83 °C; ^1H NMR (360 MHz, CDCl_3) $\delta = 8.59$ (s, 1H), 8.26 (s, 1H), 6.46 (s, 2H), 6.29 (s, 1H), 5.38 (d, $J = 8.2$ Hz, 1H), 4.61 (m, 2H), 4.24 (q, $J = 9.5$ Hz, 1H), 3.73 (s, 6H), 3.41 (m, 1H), 3.24 (m, 1H), 1.72 (s, 3H), 1.66 (s, 3H), 1.44 (d, $J = 6.8$ Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3) $\delta = 172.7, 160.8$ (2xC), 154.9, 148.9, 143.8, 140.1, 139.3, 138.7, 123.4, 119.9, 102.7 (2xC), 98.7, 81.7, 55.4 (2xC), 50.3, 49.1, 29.6, 28.9, 28.8, 17.8. IR (neat): 3403, 3346, 2978, 2935, 1690, 1604, 1542, 1526, 1455, 1422, 1392, 1368, 1336, 1312, 1296, 1275, 1225, 1202, 1152, 1137, 1056. UV (52 μM soln in MeCN) λ_{max} (ϵ) 223 (24120), 275 (6810), 281 (6790), 346 (11490). HR-MS 525.1590 ($\text{C}_{23}\text{H}_{26}\text{N}_4\text{O}_9 + \text{Na}^+$ calcd 525.1592).

2-(3,5-dimethoxyphenyl)propan-2-yl (R)-1-(5,7-dinitroindolin-1-yl)-1-oxopropan-2-ylcarbamate

(3q): Purification by flash column chromatography [SiO_2 , hexane/EtOAc (1:1)]. Yellow solid (442 mg, 88 %); mp. 80-83 °C; ^1H NMR (360 MHz, CDCl_3) δ = 8.59 (s, 1H), 8.27 (s, 1H), 6.46 (s, 2H), 6.29 (s, 1H), 5.36 (d, J = 8.6 Hz, 1H), 4.61 (m, 2H), 4.25 (q, J = 9.5 Hz, 1H), 3.74 (s, 6H), 3.41 (m, 1H), 3.24 (m, 1H), 1.72 (s, 3H), 1.66 (s, 3H), 1.44 (d, J = 6.8 Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ = 172.7, 160.8 (2xC), 154.9, 148.9, 143.9, 140.1, 139.3, 138.7, 123.4, 119.9, 102.8 (2xC), 98.7, 81.7, 55.4 (2xC), 50.3, 49.1, 29.6, 28.9, 28.8, 17.8. IR (neat): 3401, 3343, 2976, 2933, 1711, 1691, 1602, 1593, 1540, 1525, 1454, 1421, 1389, 1367, 1335, 1310, 1294, 1273, 1200, 1151, 1137, 1054. UV (51 μM soln in MeCN) λ_{max} (ϵ) 223 (22900), 275 (6410), 281 (6380), 347 (10860). HR-MS 525.1592 ($\text{C}_{23}\text{H}_{26}\text{N}_4\text{O}_9 + \text{Na}^+$ calcd 525.1592).

2-(3,5-dimethoxyphenyl)propan-2-yl (S)-4-methyl-1-(5,7-dinitroindolin-1-yl)-1-oxopentan-2-ylcarbamate (3r):

Purification by flash column chromatography [SiO_2 , hexane/EtOAc (1:1)]. Yellow solid (479 mg, 88 %); mp. 80-84 °C; ^1H NMR (360 MHz, CDCl_3) δ = 8.58 (d, J = 1.8 Hz, 1H), 8.26 (s, 1H), 6.44 (m, 2H), 6.28 (m, 1H), 5.21 (d, J = 9.1 Hz, 1H), 4.69 (td, J = 10.0 Hz, J = 3.6 Hz, 1H), 4.57 (td, J = 9.1 Hz, J = 5.4 Hz, 1H), 4.23 (q, J = 9.8 Hz, 1H), 3.72 (s, 6H), 3.39 (m, 1H), 3.22 (m, 1H), 1.82 (m, 1H), 1.72 (s, 3H), 1.65 (s, 3H), 1.60 (m, 2H), 0.98 (t, J = 6.8 Hz, 6H); ^{13}C NMR (125 MHz, CDCl_3) δ = 172.9, 160.8 (2xC), 155.4, 148.9, 143.8, 140.0, 139.4, 138.8, 123.3, 119.9, 102.6 (2xC), 98.8, 81.7, 55.3 (2xC), 51.8, 50.2, 41.2, 29.6, 28.87, 28.85, 24.8, 23.3, 21.9. IR (neat): 2961, 1697, 1605, 1544, 1463, 1432, 1373, 1342, 1291, 1265, 1207, 1155, 736. UV (48 μM soln in MeCN) λ_{max} (ϵ) 223 (20440), 282 (6240), 348 (9880). HR-MS 567.2061 ($\text{C}_{26}\text{H}_{32}\text{N}_4\text{O}_9 + \text{Na}^+$ calcd 567.2061).

2-(3,5-dimethoxyphenyl)propan-2-yl (S)-1-(5,7-dinitroindolin-1-yl)-1-oxo-3-phenylpropan-2-ylcarbamate (3s):

Purification by flash column chromatography [SiO_2 , hexane/EtOAc (3:2)]. Yellow solid (399 mg, 69 %); mp. 82-85 °C; ^1H NMR (360 MHz, CDCl_3) δ = 8.58 (s, 1H), 8.20 (s, 1H), 7.30-7.26 (5H), 6.44 (s, 2H), 6.29 (s, 1H), 5.46 (d, J = 9.0 Hz, 1H), 4.77 (q, J = 7.7 Hz, 1H), 4.34 (m, 1H), 3.72 (s, 6H), 3.48 (q, J = 9.4 Hz, 1H), 3.22-3.02 (3H), 3.90 (m, 1H), 1.69 (s, 3H), 1.66 (s, 3H); ^{13}C NMR

(125 MHz, CDCl₃) δ = 171.4, 160.8 (2xC), 154.8, 148.8, 144.0, 139.7, 139.4, 138.9, 135.9, 129.6 (2xC), 128.9 (2xC), 127.4, 123.3, 119.9, 102.7 (2xC), 98.7, 81.8, 55.4 (2xC), 54.8, 50.2, 39.2, 29.4, 28.9, 28.7. IR (neat): 3405, 3343, 2975, 2935, 1715, 1686, 1599, 1539, 1496, 1456, 1426, 1385, 1369, 1336, 1290, 1200, 1149, 1046, 731. UV (50 μ M soln in MeCN) λ_{max} (ϵ) 276 (6630), 282 (6680) 346 (11010). HR-MS 601.1902 (C₂₉H₃₀N₄O₉ + Na⁺ calcd 601.1905).

2-(3,5-dimethoxyphenyl)propan-2-yl (S)-3-(1H-indol-3-yl)-1-(5,7-dinitroindolin-1-yl)-1-oxopropan-2-ylcarbamate (3t): Purification by flash column chromatography [SiO₂, hexane/EtOAc (1:1)]. Yellow solid (475 mg, 77 %); mp. 107 °C; ¹H NMR (360 MHz, CDCl₃) δ = 8.55 (s, 1H), 8.16 (s, 1H), 8.10 (s, 1H), 7.61 (d, J = 7.7 Hz, 1H), 7.33 (d, J = 7.7 Hz, 1H), 7.17 (t, J = 7.7 Hz, 1H), 7.14 (s, 1H), 7.06 (t, J = 7.5 Hz, 1H), 6.46 (s, 2H), 6.29 (s, 1H), 5.51 (d, J = 8.6 Hz, 1H), 4.91 (dd, J = 15.0, 8.2 Hz, 1H), 4.25 (m, 1H), 3.72 (s, 6H), 3.45 (dd, J = 17.9, 9.8 Hz, 1H), 3.24 (m, 2H), 3.00 (m, 1H), 2.62 (m, 1H), 1.71 (s, 3H), 1.68 (s, 3H); ¹³C NMR (125 MHz, CDCl₃) δ = 172.0, 160.8 (2xC), 154.9, 148.9, 143.8, 139.6, 139.4, 139.1, 136.2, 127.3, 123.9, 123.2, 122.5, 120.1, 119.7, 118.6, 111.5, 109.7, 102.9 (2xC), 98.7, 81.7, 55.4 (2xC), 53.5, 50.2, 29.4, 29.2, 29.0, 28.5. IR (neat): 3395, 2974, 2934, 1688, 1597, 1536, 1496, 1456, 1424, 1385, 1366, 1334, 1288, 1225, 1199, 1148, 1055, 733. UV (49 μ M soln in MeCN) λ_{max} (ϵ) 275 (25730), 346 (11410). HR-MS 640.2020 (C₃₁H₃₁N₅O₉ + Na⁺ calcd 640.2014).

N-2-(3',5'-dimethoxyphenyl)-prop-2-yloxycarbonyl-(S)-1'-[(5,7)-dinitroindolin-1-yl]-proline (3u): Purification by flash column chromatography [SiO₂, hexane/EtOAc (1:2)]. Yellow solid (428 mg, 81 %); mp. 86 °C; ¹H NMR (360 MHz, DMSO-*d*₆) mixture of 2 rotamers δ = 8.49-8.42 (2H), 6.43-6.34 (2H), 6.32-6.30 (1H), 4.92-4.73 (1H), 4.63-4.51 (1H), 4.43-4.26 (1H), 3.71-3.63 (6H), 3.59-3.50 (1H), 3.44-3.20 (3H), 2.38-2.18 (1H), 2.02-1.81 (3H), 1.66-1.54 (6H). ¹³C NMR (125 MHz, DMSO-*d*₆) mixture of 2 rotamers δ = 171.9, 171.7, 160.2, 160.1, 152.8, 151.8, 149.0, 148.8, 143.0, 142.8, 139.7, 139.6, 139.4, 139.1, 138.3, 138.1, 123.83, 123.79, 119.3, 102.8, 102.5, 98.1, 97.9, 80.7, 58.33, 58.26, 54.99, 54.97, 50.1, 46.6, 29.9, 28.91, 28.88, 28.8, 28.7, 28.20, 28.15, 27.7, 23.9, 23.0. IR (neat): 3089, 2972, 2937, 2876, 1704, 1675, 1598, 1535, 1458, 1388, 1334, 1279, 1266, 1196, 1149. UV (50 μ M soln

in MeCN) λ_{max} (ϵ) 223 (23440), 276 (6650), 282 (6710), 347 (11320). HR-MS 551.1755 ($\text{C}_{25}\text{H}_{28}\text{N}_4\text{O}_9$ + Na^+ calcd 551.1748).

2-(3,5-dimethoxyphenyl)propan-2-yl (S)-3-(4-*tert*-butoxyphenyl)-1-(5,7-dinitroindolin-1-yl)-1-oxopropan-2-ylcarbamate (3v): Purification by flash column chromatography [SiO_2 , hexane/EtOAc (3:2)]. Yellow solid (468 mg, 72 %); mp. 132-136 °C; ^1H NMR (360 MHz, CDCl_3) δ = 8.57 (s, 1H), 8.19 (s, 1H), 7.20 (d, J = 7.7 Hz, 2H), 6.91 (d, J = 8.2 Hz, 2H), 6.45 (s, 2H), 6.29 (s, 1H), 5.50 (d, J = 8.6 Hz, 1H), 4.70 (q, J = 7.7 Hz, 1H), 4.29 (m, 1H), 3.73 (s, 6H), 3.39 (q, J = 9.4 Hz, 1H), 3.16 (m, 1H), 3.03 (m, 2H), 2.89 (m, 1H), 1.70 (s, 3H), 1.66 (s, 3H), 1.31 (s, 9H); ^{13}C NMR (125 MHz, CDCl_3) δ = 171.4, 160.8 (2xC), 154.8, 154.7, 148.9, 143.9, 139.6, 139.3, 138.9, 130.7, 130.2 (2xC), 124.5 (2xC), 123.3, 119.8, 102.7 (2xC), 98.7, 81.7, 78.8, 55.4 (2xC), 55.0, 50.2, 38.7, 29.5, 28.9 (3xC), 28.8, 28.6. IR (neat): 3404, 3339, 2972, 2930, 1713, 1692, 1598, 1538, 1500, 1456, 1426, 1383, 1363, 1335, 1289, 1274, 1232, 1199, 1152, 1049, 731. UV (56 μM soln in MeCN) λ_{max} (ϵ) 223 (31560), 275 (7060), 346 (10963). HR-MS 673.2481 ($\text{C}_{33}\text{H}_{38}\text{N}_4\text{O}_{10}$ + Na^+ calcd 673.2480).

2-(3,5-dimethoxyphenyl)propan-2-yl (S)-3-*tert*-butoxy-1-(5,7-dinitroindolin-1-yl)-1-oxopropan-2-ylcarbamate (3w): Purification by flash column chromatography [SiO_2 , hexane/EtOAc (3:2)]. Yellow solid (459 mg, 80 %); mp. 75-79 °C; ^1H NMR (360 MHz, CDCl_3) δ = 8.58 (s, 1H), 8.27 (s, 1H), 6.48 (s, 2H), 6.31 (s, 1H), 5.48 (d, J = 8.2 Hz, 1H), 4.72 (m, 1H), 4.56 (m, 1H), 4.45 (m, 1H), 3.75 (s, 6H), 3.62 (m, 1H), 3.54 (t, J = 7.7 Hz, 1H), 3.28 (m, 2H), 1.74 (s, 3H), 1.68 (s, 3H), 1.17 (s, 9H); ^{13}C NMR (125 MHz, CDCl_3) δ = 170.9, 160.8 (2xC), 154.8, 148.9, 143.9, 139.7, 139.1, 123.3, 119.9, 102.8 (2xC), 98.8, 81.7, 74.1, 62.7, 55.4 (2xC), 53.4, 50.4, 29.5, 28.9, 28.8, 27.4 (3xC). IR (neat): 3419, 3351, 2973, 2935, 1718, 1692, 1600, 1541, 1498, 1460, 1426, 1367, 1338, 1293, 1279, 1200, 1152. UV (52 μM soln in MeCN) λ_{max} (ϵ) 223 (21680), 276 (6270), 282 (6240), 346 (9830). HR-MS 597.2164 ($\text{C}_{27}\text{H}_{34}\text{N}_4\text{O}_{10}$ + Na^+ calcd 597.2167).

2-(3,5-dimethoxyphenyl)propan-2-yl (2*S*,3*R*)-3-*tert*-butoxy-1-(5,7-dinitroindolin-1-yl)-1-oxobutan-2-ylcarbamate (3x): Purification by 2 successive flash column chromatographies [SiO_2 ,

hexane/EtOAc (3:2)] and then [SiO₂, CH₂Cl₂/EtOAc (95:5)] to remove the remaining starting product. Yellow solid (235 mg, 40 %, or 294 mg, 50 % after 9 h of reaction); mp. 132 °C; ¹H NMR (360 MHz, CDCl₃) δ = 8.56 (s, 1H), 8.26 (s, 1H), 6.46 (s, 2H), 6.30 (s, 1H), 5.57 (d, *J* = 8.6 Hz, 1H), 4.62-4.46 (3H), 3.95 (m, 1H), 3.74 (s, 6H), 3.34 (m, 1H), 3.21 (m, 1H), 1.75 (s, 3H), 1.66 (s, 3H), 1.24 (s, 9H), 1.21 (d, *J* = 6.4 Hz, 3H); ¹³C NMR (125 MHz, CDCl₃) δ = 170.2, 160.8 (2xC), 154.8, 148.9, 144.0, 140.0, 139.6, 139.1, 123.3, 119.8, 102.9 (2xC), 98.7, 81.6, 75.1, 69.4, 58.2, 55.4 (2xC), 51.2, 29.8, 28.9, 28.7, 28.6 (3xC), 18.9. IR (neat): 3422, 2973, 2933, 1714, 1680, 1597, 1539, 1492, 1456, 1426, 1385, 1369, 1340, 1281, 1195, 1147. UV (52 μM soln in MeCN) λ_{max} (ε) 223 (24350), 282 (7500), 344 (11440). HR-MS 611.2316 (C₂₈H₃₆N₄O₁₀ + Na⁺ calcd 611.2324).

2-(3,5-dimethoxyphenyl)propan-2-yl (S)-3-(tert-butoxycarbonyl)-1-(5,7-dinitroindolin-1-yl)-1-oxopropan-2-ylcarbamate (3y): Purification by flash column chromatography [SiO₂, hexane/EtOAc (2:1)]. Yellow solid (464 mg, 77 %); mp. 86-92 °C; ¹H NMR (360 MHz, CDCl₃) δ = 8.59 (s, 1H), 8.26 (s, 1H), 6.46 (s, 2H), 6.30 (s, 1H), 5.60 (d, *J* = 10.0 Hz, 1H), 4.89 (m, 1H), 4.49 (m, 2H), 3.71 (s, 6H), 3.26 (m, 2H), 2.84 (dd, *J* = 16.8, 8.2 Hz, 1H), 2.64 (dd, *J* = 16.6, 4.8 Hz, 1H), 1.75 (s, 3H), 1.67 (s, 3H), 1.43 (s, 9H); ¹³C NMR (125 MHz, CDCl₃) δ = 170.9, 169.8, 160.8 (2xC), 154.8, 148.7, 143.9, 140.1, 139.4, 139.3, 123.3, 119.9, 103.0 (2xC), 98.5, 82.1, 82.0, 55.3 (2xC), 50.7, 49.8, 37.7, 29.6, 28.9, 28.7, 28.1 (3xC). IR (neat): 3393, 3353, 2974, 2933, 1721, 1689, 1597, 1537, 1457, 1423, 1365, 1334, 1286, 1251, 1202, 1151, 1135. UV (50 μM soln in MeCN) λ_{max} (ε) 223 (21720), 276 (6770), 282 (6800), 348 (10470). HR-MS 625.2111 (C₂₈H₃₄N₄O₁₁ + Na⁺ calcd 625.2116).

2-(3,5-dimethoxyphenyl)propan-2-yl (S)-4-(tert-butoxycarbonyl)-1-(5,7-dinitroindolin-1-yl)-1-oxobutan-2-ylcarbamate (3z): Purification by flash column chromatography [SiO₂, hexane/EtOAc (2:1)]. Yellow solid (462 mg, 75 %); mp. 69-73 °C; ¹H NMR (360 MHz, CDCl₃) δ = 8.58 (s, 1H), 8.27 (s, 1H), 6.45 (s, 2H), 6.28 (s, 1H), 5.37 (d, *J* = 8.6 Hz, 1H), 4.65 (m, 2H), 4.39 (q, *J* = 9.8 Hz, 1H), 3.73 (s, 6H), 3.39 (m, 1H), 3.26 (m, 1H), 2.40 (m, 2H), 2.13 (m, 1H), 1.82 (m, 1H), 1.72 (s, 3H), 1.65 (s, 3H), 1.42 (s, 9H); ¹³C NMR (125 MHz, CDCl₃) δ = 172.1, 172.0, 160.8 (2xC), 155.3, 148.9, 143.9,

139.9, 139.5, 139.0, 123.4, 119.8, 102.7 (2xC), 98.8, 81.7, 81.1, 55.4 (2xC), 52.4, 50.5, 30.6, 29.6, 28.9, 28.8, 28.2 (3xC), 27.3. IR (neat): 3403, 3354, 2974, 2933, 1721, 1690, 1599, 1539, 1458, 1426, 1385, 1366, 1336, 1287, 1255, 1224, 1202, 1150, 1134. UV (52 μ M soln in MeCN) λ_{max} (ϵ) 223 (22550), 276 (6450), 282 (6460), 346 (10690). HR-MS 639.2284 ($\text{C}_{29}\text{H}_{36}\text{N}_4\text{O}_{11} + \text{Na}^+$ calcd 639.2278).

Benzyl (S)-1-(2-bromo-3,5-dinitrophenethylcarbamoyl)ethylcarbamate (9b): Purification by flash column chromatography [SiO_2 , hexane/EtOAc (1:2)]. Slightly yellow solid (559 mg, 94 %); ^1H NMR (500 MHz, CDCl_3) δ = 8.36 (d, J = 2.7 Hz, 1H), 8.23 (d, J = 2.4 Hz, 1H), 7.37-7.29 (5H), 6.52 (b, 1H), 5.23 (d, J = 6.8 Hz, 1H), 5.04 (m, 2H), 4.14 (q, J = 7.2 Hz, 1H), 3.58 (m, 2H), 3.20 (m, 2H), 1.34 (d, J = 7.2 Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ = 172.9, 156.3, 151.5, 146.6, 144.1, 136.0, 128.7 (2xC), 128.5, 128.2 (2xC), 127.6, 123.0, 118.3, 67.4, 50.7, 38.5, 36.6, 18.1. IR (neat): 3405, 3315, 3087, 1711, 1655, 1534, 1453, 1346, 1241, 1056, 1038. HR-MS 517.0319 ($\text{C}_{19}\text{H}_{19}\text{BrN}_4\text{O}_7 + \text{Na}^+$ calcd 517.0329).

(9H-Fluoren-9-yl)methyl (S)-1-(2-bromo-3,5-dinitrophenethylcarbamoyl)ethylcarbamate (9c): Purification by flash column chromatography [SiO_2 , hexane/EtOAc (1:2)]. Slightly yellow solid (644 mg, 92 %); ^1H NMR (360 MHz, $\text{DMSO}-d_6$) δ = 8.76 (d, J = 2.8 Hz, 1H), 8.30 (d, J = 2.3 Hz, 1H), 8.00 (t, J = 5.5 Hz, 1H), 7.89 (d, J = 7.3 Hz, 2H), 7.72 (t, J = 6.6 Hz, 2H), 7.47 (d, J = 7.7 Hz, 1H), 7.41 (t, J = 7.3 Hz, 2H), 7.33 (t, J = 7.5 Hz, 2H), 4.23-4.17 (3H), 3.88 (q, J = 7.3 Hz, 1H), 3.44 (m, 2H), 3.10 (t, J = 6.2 Hz, 2H), 1.12 (d, J = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) δ = 172.7, 155.6, 151.1, 146.3, 143.9, 143.8 (2xC), 140.7 (2xC), 127.7, 127.6 (2xC), 127.1 (2xC), 125.30, 125.28, 121.9, 120.1 (2xC), 117.7, 65.5, 50.1, 46.6, 37.1, 35.8, 18.1. HR-MS 605.0649 ($\text{C}_{26}\text{H}_{23}\text{BrN}_4\text{O}_7 + \text{Na}^+$ calcd 605.0642).

(S)-Benzyl 2-(2-bromo-3,5-dinitrophenethylcarbamoyl)pyrrolidine-1-carboxylate (9d): Purification by flash column chromatography [SiO_2 , hexane/EtOAc (3:1)]. Slightly yellow solid (588 mg, 94 %); ^1H NMR (360 MHz, $\text{DMSO}-d_6$) mixture of 2 rotamers δ = 8.75-8.74 (1H), 8.31-8.28 (1H), 8.07-8.00 (1H), 7.38-7.25 (5H), 5.07-5.02 (1H), 4.96-4.93 (1H), 4.12-4.01 (1H), 3.50-3.29 (4H), 3.12-2.98 (2H), 2.13-1.98 (1H), 1.77-1.64 (3H); ^{13}C NMR (125 MHz, $\text{DMSO}-d_6$) mixture of 2 rotamers δ =

172.2, 172.0, 153.9, 153.8, 151.2, 151.1, 146.4, 146.2, 143.9, 143.7, 136.93, 136.90, 128.4, 128.2, 127.83, 127.79, 127.5, 127.3, 127.0, 121.9, 121.8, 117.71, 117.67, 65.8, 65.7, 60.1, 59.7, 47.0, 46.4, 37.3, 37.1, 35.8, 35.6, 31.1, 30.0, 23.8, 23.0. IR (neat): 3319, 1693, 1679, 1547, 1534, 1448, 1415, 1350, 1120, 736. HR-MS 543.0488 ($C_{21}H_{21}BrN_4O_7 + Na^+$ calcd 543.0486).

***tert*-Butyl (S)-1-(2-bromo-3,5-dinitrophenethylcarbamoyl)-2-phenylethylcarbamate (9e):**

Purification by flash column chromatography [SiO_2 , hexane/EtOAc (1:1)]. Slightly yellow solid (580 mg, 90 %); 1H NMR (360 MHz, $CDCl_3$) δ = 8.38 (d, J = 2.3 Hz, 1H), 8.21 (d, J = 2.3 Hz, 1H), 7.30-7.17 (5H), 6.16 (t, J = 5.0 Hz, 1H), 4.94 (d, J = 5.4 Hz, 1H), 4.27 (q, J = 7.3 Hz, 1H), 3.51 (q, J = 6.8 Hz, 2H) 3.16-3.03 (4H), 1.37 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 171.9, 155.7, 151.5, 146.7, 144.1, 136.7, 129.4 (2xC), 128.9 (2xC), 127.3, 127.2, 122.9, 118.3, 80.7, 56.1, 38.4, 38.3, 36.6, 28.4 (3xC). IR (neat): 3336, 3089, 3066, 2978, 2934, 1690, 1650, 1546, 1531, 1440, 1388, 1364, 1346, 1252, 1230, 1173. HR-MS 559.0782 ($C_{22}H_{25}BrN_4O_7 + Na^+$ calcd 559.0799).

***tert*-Butyl (S)-1-(2-bromo-3,5-dinitrophenethylcarbamoyl)-2-hydroxyethylcarbamate (9f):**

Purification by flash column chromatography [SiO_2 , CH_2Cl_2 (to remove 5,7-dinitroindoline) and then EtOAc]. Slightly yellow solid (447 mg, 78 %); 1H NMR (360 MHz, $CDCl_3$) δ = 8.40 (d, J = 2.7 Hz, 1H), 8.29 (d, J = 2.3 Hz, 1H), 7.00 (b, 1H), 5.55 (d, J = 6.8 Hz, 1H), 4.12-4.02 (2H), 3.62 (m, 3H), 3.23 (m, 3H), 1.41 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 172.0, 156.5, 151.5, 146.6, 144.1, 127.6, 123.0, 118.3, 81.0, 62.7, 55.0, 38.4, 36.7, 28.4 (3xC). HR-MS 499.0435 ($C_{16}H_{21}BrN_4O_8 + Na^+$ calcd 499.0435).

Benzyl (S)-1-(2-bromo-3,5-dinitrophenethylcarbamoyl)-2-*tert*-butoxyethylcarbamate (9g):

Purification by flash column chromatography [SiO_2 , hexane/EtOAc (1:1)]. Slightly yellow solid (647 mg, 95 %); mp. 110-113°C; 1H NMR (360 MHz, $CDCl_3$) δ = 8.39 (d, J = 2.3 Hz, 1H), 8.28 (d, J = 2.8 Hz, 1H), 7.39-7.31 (5H), 6.71 (b, 1H), 5.61 (b, 1H), 5.09 (s, 2H), 4.18 (m, 1H), 3.84 (m, 1H), 3.61 (q, J = 6.4 Hz, 2H), 3.38 (q, J = 7.8 Hz, 1H), 3.21 (m, 2H), 1.15 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 171.1, 156.3, 151.8, 147.0, 144.3, 136.4, 128.7 (2xC), 128.5, 128.3 (2xC), 127.3, 122.8, 118.2, 77.4,

67.4, 61.7, 55.3, 38.6, 36.9, 27.6 (3xC). IR (neat): 3411, 3319, 3083, 2976, 2937, 1718, 1666, 1541, 1349, 1230, 1195, 1089, 1061. HR-MS 589.0899 ($C_{23}H_{27}BrN_4O_8 + Na^+$ calcd 589.0904).

***tert*-Butyl (S)-1-(2-bromo-3,5-dinitrophenethylcarbamoyl)-2-methylpropylcarbamate (9h):**

Purification by flash column chromatography [SiO_2 , hexane/EtOAc (1:1)]. Slightly yellow solid (552 mg, 94 %); mp. 166.167 °C; 1H NMR (360 MHz, $CDCl_3$) δ = 8.40 (d, J = 2.3 Hz, 1H), 8.30 (d, J = 2.2 Hz, 1H), 6.48 (t, J = 5.7 Hz, 1H), 4.97 (d, J = 8.1 Hz, 1H), 3.85 (m, 1H), 3.61 (m, 2H), 3.23 (t, J = 7.0 Hz, 2H), 2.12 (m, 1H), 1.41 (s, 9H), 0.92 (d, J = 6.8 Hz, 3H), 0.88 (d, J = 6.8 Hz, 3H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 172.4, 156.2, 151.6, 146.7, 144.2, 127.5, 123.0, 118.3, 80.4, 60.3, 38.5, 36.9, 30.5, 28.4 (3xC), 19.5, 17.9. IR (neat): 3337, 3317, 2973, 1686, 1649, 1546, 1531, 1365, 1346, 1301, 1246, 1227, 1175, 736. HR-MS 511.0803 ($C_{18}H_{25}BrN_4O_7 + Na^+$ calcd 511.0799).

***tert*-Butyl (S)-1-(2-bromo-3,5-dinitrophenethylcarbamoyl)-3-(methylthio)propylcarbamate (9i):**

Purification by flash column chromatography [SiO_2 , hexane/EtOAc (1:1)]. Slightly yellow solid (607 mg, 97 %); mp. 94 °C; 1H NMR (360 MHz, $CDCl_3$) δ = 8.41 (d, J = 2.7 Hz, 1H), 8.29 (d, J = 2.7 Hz, 1H), 6.62 (b, 1H), 5.11 (d, J = 7.7 Hz, 1H), 4.21 (q, J = 7.7 Hz, 1H), 3.61 (q, J = 6.8 Hz, 2H), 3.23 (t, J = 6.8 Hz, 2H), 2.52 (m, 2H), 2.09 (s, 3H), 2.05 (m, 1H), 1.90 (m, 1H), 1.41 (s, 9H); ^{13}C NMR (125 MHz, $CDCl_3$) δ = 172.3, 155.9, 151.6, 146.7, 144.1, 127.5, 123.0, 118.3, 80.7, 53.7, 38.6, 36.8, 31.1, 30.5, 28.4 (3xC), 15.5. IR (neat): 3326, 3090, 2980, 1686, 1649, 1546, 1532, 1441, 1365, 1346, 1238, 1173. HR-MS 543.0514 ($C_{18}H_{25}BrN_4O_7S + Na^+$ calcd 543.0520).

(9H-Fluoren-9-yl)methyl

(S)-1-(2-bromo-3,5-dinitrophenethylcarbamoyl)-3-

(methylthio)propylcarbamate (9j): Slightly yellow solid (633 mg, 82 %); 1H NMR (360 MHz, $DMSO-d_6$) δ = 8.76 (d, J = 2.3 Hz, 1H), 8.31 (d, J = 2.7 Hz, 1H), 8.06 (t, J = 5.5 Hz, 1H), 7.99 (d, J = 7.7 Hz, 2H), 7.72 (t, J = 6.4 Hz, 2H), 7.52 (d, J = 7.8 Hz, 1H), 7.42 (t, J = 7.5 Hz, 2H), 7.32 (t, J = 7.3 Hz, 2H), 4.29-4.15 (3H), 3.92 (m, 1H), 3.46 (m, 2H), 3.10 (t, J = 6.2 Hz, 2H), 2.43-2.28 (2H), 1.99 (s, 3H), 1.80-1.63 (2H); ^{13}C NMR (125 MHz, $DMSO-d_6$) δ = 171.7, 155.9, 151.2, 146.3, 143.9, 143.7

(2xC), 140.7 (2xC), 127.67, 127.63 (2xC), 127.0 (2xC), 125.3 (2xC), 121.9, 120.1 (2xC), 117.7, 65.5, 53.8, 46.7, 37.1, 35.7, 31.3, 29.8, 14.5. HR-MS 665.0685 ($C_{28}H_{27}BrN_4O_7S + Na^+$ calcd 665.0676).

***tert*-Butyl (R)-1-(2-bromo-3,5-dinitrophenethylcarbamoyl)-2-(benzylthio)ethylcarbamate (9k):** Purification by washing the residue with a mixture of solvents ($CHCl_3$ /hexane (1:2)). Slightly yellow solid (644 mg, 92 %); mp. 156-158 °C; 1H NMR (360 MHz, $DMSO-d_6$) δ = 8.75 (s, 1H), 8.34 (s, 1H), 8.13 (t, J = 5.5 Hz, 1H), 7.31-7.22 (5H), 6.92 (d, J = 8.2 Hz, 1H), 4.04 (m, 1H), 3.68 (t, J = 14.1 Hz, 2H), 3.45 (m, 2H), 3.10 (t, J = 6.2 Hz, 2H), 2.63 (dd, J = 13.6, 5.4 Hz, 1H), 2.45 (dd, J = 13.2, 9.1 Hz, 1H), 1.36 (s, 9H); ^{13}C NMR (125 MHz, $DMSO-d_6$) δ = 170.4, 154.9, 151.0, 146.3, 143.7, 138.1, 128.5 (2xC), 128.1 (2xC), 127.3, 126.6, 121.6, 117.5, 78.1, 53.8, 37.3, 35.5, 35.2, 33.4, 27.9 (3xC). IR (neat): 3326, 1685, 1650, 1536, 1451, 1356, 1232, 1178, 706, 657. HR-MS 605.0668 ($C_{23}H_{27}BrN_4O_7S + Na^+$ calcd 605.0676).

***tert*-Butyl (R)-1-(2-bromo-3,5-dinitrophenethylcarbamoyl)-2-((acetamidomethyl)sulfanyl)ethylcarbamate (9l):** Purification by flash column chromatography (SiO_2 , EtOAc). Yellow solid (657 mg, 97 %); mp. 70-72 °C; 1H NMR (360 MHz, $DMSO-d_6$) δ = 8.75 (d, J = 2.2 Hz, 1H), 8.45 (t, J = 5.8 Hz, 1H), 8.35 (d, J = 2.2 Hz, 1H), 7.97 (t, J = 5.5 Hz, 1H), 6.86 (d, J = 8.5 Hz, 1H), 4.18 (m, 2H), 4.00 (m, 1H), 3.45 (m, 2H), 3.10 (t, J = 6.3 Hz, 2H), 2.79 (dd, J = 13.6, 5.1 Hz, 1H), 2.61 (dd, J = 13.6, 9.5 Hz, 1H), 1.83 (s, 3H), 1.35 (s, 9H); ^{13}C NMR (125 MHz, $DMSO-d_6$) δ = 170.7, 169.5, 155.2, 151.2, 146.3, 143.7, 127.6, 121.8, 117.7, 78.1, 54.3, 40.3, 37.3, 35.7, 32.6, 28.1 (3xC), 22.6. IR (neat): 3300, 3082, 2980, 1707, 1662, 1542, 1349, 1256, 1168, 735. HR-MS 586.0572 ($C_{19}H_{26}BrN_5O_8S + Na^+$ calcd 586.0578).

***tert*-Butyl (S)-1-(2-bromo-3,5-dinitrophenethylcarbamoyl)-2-(4-*tert*-butoxyphenyl)ethylcarbamate (9m):** Purification by flash column chromatography [SiO_2 , hexane/EtOAc (3:2)]. Slightly yellow solid (622 mg, 85 %); 1H NMR (360 MHz, $CDCl_3$) δ = 8.39 (d, J = 2.3 Hz, 1H), 8.21 (d, J = 2.3 Hz, 1H), 7.06 (d, J = 8.2 Hz, 2H), 6.88 (d, J = 8.2 Hz, 2H), 6.15 (t, J = 5.7 Hz, 1H), 4.97 (d, J = 6.8 Hz, 1H), 4.23 (q, J = 7.3 Hz, 1H), 3.49 (q, J = 6.5 Hz, 2H), 3.10 (t, J = 7.1

Hz, 2H), 2.97 (d, $J = 7.3$ Hz, 2H), 1.37 (s, 9H), 1.30 (s, 9H); ^{13}C NMR (125 MHz, CDCl_3) $\delta = 172.0$, 155.7, 154.5, 151.5, 146.6, 144.0, 131.4, 129.8 (2xC), 127.3, 124.5 (2xC), 122.9, 118.4, 80.6, 78.7, 56.2, 38.4, 37.7, 36.6, 28.9 (3xC), 28.4 (3xC). IR (neat): 3419, 3309, 2979, 2937, 1668, 1539, 1355, 1245, 1169. HR-MS 631.1376 ($\text{C}_{26}\text{H}_{33}\text{BrN}_4\text{O}_8 + \text{Na}^+$ calcd 631.1374).

***tert*-Butyl (S)-1-(2-bromo-3,5-dinitrophenethylcarbamoyl)-2-(1*H*-indol-3-yl)ethylcarbamate (9n):** Purification by flash column chromatography [SiO_2 , hexane/EtOAc (1:1)]. Slightly yellow solid (657 mg, 95 %); mp. 116 °C; ^1H NMR (500 MHz, CDCl_3) $\delta = 8.31$ (d, $J = 2.6$ Hz, 1H), 8.30 (b, 1H), 8.02 (d, $J = 2.6$ Hz, 1H), 7.60 (d, $J = 8.0$ Hz, 1H), 7.32 (d, $J = 8.1$ Hz, 1H), 7.16 (t, $J = 7.6$ Hz, 1H), 7.09 (t, $J = 7.6$ Hz, 1H), 7.03 (d, $J = 2.3$ Hz, 1H), 6.03 (b, 1H), 5.11 (b, 1H), 4.38 (m, 1H), 3.42 (q, $J = 6.5$ Hz, 2H), 3.28 (dd, $J = 14.6, 5.7$ Hz, 1H), 3.13 (dd, $J = 14.5, 7.7$ Hz, 1H), 2.91 (m, 2H), 1.39 (s, 9H); ^{13}C NMR (125 MHz, CDCl_3) $\delta = 172.4$, 155.7, 151.4, 146.6, 144.0, 136.3, 127.4, 127.1, 123.2, 122.8, 122.6, 120.0, 119.1, 118.2, 111.4, 110.8, 80.6, 55.4, 38.3, 36.4, 28.4 (3xC), 28.3. IR (neat): 3416, 3319, 2980, 1699, 1665, 1541, 1455, 1348, 1249, 1166, 740. HR-MS 598.0914 ($\text{C}_{24}\text{H}_{26}\text{BrN}_5\text{O}_7 + \text{Na}^+$ calcd 598.0908).

2-(3,5-dimethoxyphenyl)propan-2-yl (2-bromo-3,5-dinitrophenethylcarbamoyl)methylcarbamate (9o): Purification by flash column chromatography [SiO_2 , CH_2Cl_2 (to remove 5,7-dinitroindoline) and then hexane/EtOAc (1:2)]. Slightly yellow solid (526 mg, 77 %); ^1H NMR (360 MHz, CDCl_3) $\delta = 8.35$ (s, 1H), 8.13 (s, 1H), 6.57 (b, 1H), 6.44 (s, 2H), 6.23 (s, 1H), 5.44 (b, 1H), 3.80-3.69 (8H), 3.47 (m, 2H), 3.06 (m, 2H), 1.69 (s, 6H); ^{13}C NMR (125 MHz, CDCl_3) $\delta = 169.7$, 160.8 (2xC), 155.7, 151.4, 148.9, 146.5, 144.2, 127.6, 122.9, 118.2, 103.0 (2xC), 98.1, 81.8, 55.4 (2xC), 44.6, 38.4, 36.5, 29.2 (2xC). IR (neat): 3412, 3330, 1715, 1670, 1599, 1540, 1457, 1425, 1345, 1262, 1201, 1153, 1046, 734. HR-MS 591.0708 ($\text{C}_{22}\text{H}_{25}\text{BrN}_4\text{O}_9 + \text{Na}^+$ calcd 591.0697).

2-(3,5-dimethoxyphenyl)propan-2-yl (S)-1-(2-bromo-3,5-dinitrophenethylcarbamoyl)ethylcarbamate(9p): Purification by flash column chromatography

[SiO₂, CH₂Cl₂ (to remove 5,7-dinitroindoline) and then hexane/EtOAc (1:1)]. Slightly yellow solid (658 mg, 94 %); ¹H NMR (360 MHz, CDCl₃) δ = 8.37 (d, *J* = 1.8 Hz, 1H), 8.14 (s, 1H), 6.61 (b, 1H), 6.44 (s, 2H), 6.25 (s, 1H), 5.21 (d, *J* = 6.9 Hz, 1H), 4.05 (m, 1H), 3.73 (s, 6H), 3.45 (m, 2H), 3.04 (m, 2H), 1.73 (s, 3H), 1.64 (s, 3H), 1.28 (d, *J* = 6.8 Hz, 3H); ¹³C NMR (125 MHz, CDCl₃) δ = 172.9, 160.8 (2xC), 155.2, 151.4, 149.0, 146.5, 144.3, 127.6, 122.9, 118.2, 103.0 (2xC), 98.2, 81.7, 55.4 (2xC), 50.2, 38.4, 36.6, 29.8, 28.6, 18.0. IR (neat): 3402, 3319, 2968, 2927, 1701, 1649, 1587, 1530, 1444, 1417, 1336, 1236, 1186, 1135, 1041, 721. HR-MS 605.0863 (C₂₃H₂₇BrN₄O₉ + Na⁺ calcd 605.0854).

2-(3,5-dimethoxyphenyl)propan-2-yl **(*R*)-1-(2-bromo-3,5-dinitrophenethylcarbamoyl)ethylcarbamate (9q):** Purification by flash column chromatography [SiO₂, CH₂Cl₂ (to remove 5,7-dinitroindoline) and then hexane/EtOAc (1:1)]. Slightly yellow solid (637 mg, 91 %); ¹H NMR (360 MHz, CDCl₃) δ = 8.36 (s, 1H), 8.13 (s, 1H), 6.63 (b, 1H), 6.44 (s, 2H), 6.24 (s, 1H), 5.23 (d, *J* = 6.4 Hz, 1H), 4.05 (m, 1H), 3.72 (s, 6H), 3.45 (m, 2H), 3.04 (m, 2H), 1.73 (s, 3H), 1.64 (s, 3H), 1.27 (d, *J* = 7.3 Hz, 3H); ¹³C NMR (125 MHz, CDCl₃) δ = 172.9, 160.8 (2xC), 155.2, 151.4, 149.0, 146.5, 144.3, 127.6, 122.9, 118.2, 102.9 (2xC), 98.2, 81.7, 55.4 (2xC), 50.2, 38.4, 36.5, 29.8, 28.6, 18.1. IR (neat): 3413, 3321, 2977, 2934, 1707, 1666, 1604, 1594, 1538, 1453, 1423, 1343, 1317, 1202, 1153, 1138, 1061, 1046, 733. HR-MS 605.0853 (C₂₃H₂₇BrN₄O₉ + Na⁺ calcd 605.0854).

2-(3,5-dimethoxyphenyl)propan-2-yl **(*S*)-1-(2-bromo-3,5-dinitrophenethylcarbamoyl)-3-methylbutylcarbamate (9r):** Purification by flash column chromatography [SiO₂, hexane/EtOAc (1:1)]. Slightly yellow solid (691 mg, 92 %); ¹H NMR (360 MHz, CDCl₃) δ = 8.38 (m, 1H), 8.16 (m, 1H), 6.45 (m, 3H), 6.27 (m, 1H), 5.00 (d, *J* = 8.2 Hz, 1H), 3.94 (m, 1H), 3.74 (s, 6H), 3.47 (m, 2H), 3.11 (m, 1H), 2.99 (m, 1H), 1.75-1.56 (8H), 1.44 (m, 1H), 0.91 (d, *J* = 5.9 Hz, 3H), 0.86 (d, *J* = 5.4 Hz, 3H); ¹³C NMR (125 MHz, CDCl₃) δ = 173.0, 160.8 (2xC), 155.5, 151.4, 148.9, 146.6, 144.3, 127.6, 122.9, 118.3, 102.9 (2xC), 98.4, 81.8, 55.4 (2xC), 53.3, 40.4, 38.5, 36.7, 29.8, 28.6, 24.9, 23.0, 21.9. IR (neat): 3310, 2959, 1704, 1664, 1601, 1543, 1460, 1427, 1347, 1205, 1162, 1143, 737. HR-MS 647.1330 (C₂₆H₃₃BrN₄O₉ + Na⁺ calcd 647.1323).

2-(3,5-dimethoxyphenyl)propan-2-yl (S)-1-(2-bromo-3,5-dinitrophenethylcarbamoyl)-2-phenylethylcarbamate (9s): Purification by flash column chromatography [SiO_2 , CH_2Cl_2 (to remove 5,7-dinitroindoline) and then hexane/EtOAc (1:1)]. Yellow solid (720 mg, 91 %); mp. 68-71 °C; ^1H NMR (360 MHz, CDCl_3) δ = 8.36 (s, 1H), 8.11 (s, 1H), 7.29-7.13 (5H), 6.43 (s, 2H), 6.26 (s, 1H), 6.22 (b, 1H), 5.21 (d, J = 7.3 Hz, 1H), 4.21 (m, 1H), 3.72 (s, 6H), 3.41 (m, 2H), 2.98 (m, 4H), 1.70 (s, 3H), 1.64 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ = 171.7, 160.8 (2xC), 155.1, 151.4, 148.9, 146.6, 144.1, 136.5, 129.3 (2xC), 128.8 (2xC), 127.4, 127.2, 122.9, 118.2, 103.0 (2xC), 98.3, 81.8, 56.0, 55.4 (2xC), 38.4, 38.0, 36.6, 29.6, 28.6. IR (neat): 3411, 3320, 3080, 2976, 2935, 1708, 1658, 1599, 1540, 1453, 1424, 1342, 1293, 1257, 1197, 1149, 1055, 1036, 732. HR-MS 681.1171 ($\text{C}_{29}\text{H}_{31}\text{BrN}_4\text{O}_9 + \text{Na}^+$ calcd 681.1167).

2-(3,5-dimethoxyphenyl)propan-2-yl (S)-1-(2-bromo-3,5-dinitrophenethylcarbamoyl)-2-(1H-indol-3-yl)ethylcarbamate (9t): Purification by flash column chromatography [SiO_2 , CH_2Cl_2 (to remove 5,7-dinitroindoline) and then hexane/EtOAc (1:1)]. Orange solid (729 mg, 87 %); ^1H NMR (360 MHz, CDCl_3) δ = 8.28 (s, 2H), 7.96 (d, J = 2.3 Hz, 1H), 7.56 (d, J = 7.7 Hz, 1H), 7.30 (d, J = 7.8 Hz, 1H), 7.15 (t, J = 7.5 Hz, 1H), 7.08 (t, J = 7.3 Hz, 1H), 6.94 (s, 1H), 6.45 (s, 2H), 6.29 (s, 1H), 6.10 (b, 1H), 5.34 (d, J = 6.8 Hz, 1H), 4.30 (m, 1H), 3.73 (s, 6H), 3.36 (m, 2H), 3.17 (m, 2H), 2.84 (m, 2H), 1.70 (s, 3H), 1.66 (s, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ = 172.2, 160.8 (2xC), 155.2, 151.3, 149.0, 146.4, 144.0, 136.3, 127.4, 127.2, 123.2, 122.8, 122.5, 119.9, 118.9, 118.2, 111.4, 110.6, 103.0 (2xC), 98.3, 81.6, 55.4 (2xC), 55.3, 38.3, 36.3, 29.4, 28.9, 28.0. IR (neat): 3407, 3330, 2975, 2932, 1704, 1660, 1595, 1535, 1453, 1423, 1341, 1257, 1196, 1147, 1051, 734. HR-MS 720.1279 ($\text{C}_{31}\text{H}_{32}\text{BrN}_5\text{O}_9 + \text{Na}^+$ calcd 720.1276).

(S)-2-(3,5-dimethoxyphenyl)propan-2-yl 2-(2-bromo-3,5-dinitrophenethylcarbamoyl)pyrrolidine-1-carboxylate (9u): Purification by flash column chromatography [SiO_2 , hexane/EtOAc (1:2)]. Slightly yellow solid (563 mg, 77 %); mp. 72-74 °C: ^1H NMR (360 MHz, $\text{DMSO}-d_6$) mixture of 2 rotamers δ = 8.78-8.72 (1H), 8.35-8.29 (1H), 8.17-7.89 (1H),

6.45-6.33 (3H), 4.12-3.92 (1H), 3.72 (s, 6H), 3.58-3.38 (3H), 3.28-3.04 (3H), 2.15-1.94 (1H), 1.79-1.49 (9H); ^{13}C NMR (125 MHz, $\text{DMSO-}d_6$) mixture of 2 rotamers δ = 172.6, 172.1, 160.2, 160.1, 152.8, 152.3, 151.3, 151.1, 149.3, 149.1, 146.3, 143.9, 143.8, 127.6, 127.3, 121.9, 121.8, 117.71, 117.66, 102.8, 102.6, 98.0, 97.9, 80.4, 80.1, 59.8, 59.6, 55.1, 55.0, 46.7, 46.6, 37.4, 37.1, 35.8, 31.1, 30.0, 29.8, 28.8, 28.4, 27.8, 23.9, 23.0. IR (neat): 3411, 3319, 3078, 2974, 2936, 2875, 1695, 1596, 1536, 1453, 1396, 1341, 1196, 1148, 1108, 1050. HR-MS 631.1004 ($\text{C}_{25}\text{H}_{29}\text{BrN}_4\text{O}_9 + \text{Na}^+$ calcd 631.1010).

2-(3,5-dimethoxyphenyl)propan-2-yl (S)-1-(2-bromo-3,5-dinitrophenethylcarbamoyl)-2-(4-tert-butoxyphenyl)ethylcarbamate (9v): Purification by flash column chromatography [SiO_2 , CH_2Cl_2 (to remove 5,7-dinitroindoline) and then hexane/EtOAc (1:2)]. Slightly yellow solid (702 mg, 80 %); mp. 76 °C; ^1H NMR (360 MHz, CDCl_3) δ = 8.37 (s, 1H), 8.10 (s, 1H), 7.04 (d, J = 8.1 Hz, 2H), 6.88 (d, J = 8.2 Hz, 2H), 6.43 (s, 2H), 6.27 (s, 1H), 6.08 (b, 1H), 5.20 (d, J = 6.8 Hz, 1H), 4.15 (m, 1H), 3.74 (s, 6H), 3.40 (m, 2H), 2.96 (m, 4H), 1.70 (s, 3H), 1.63 (s, 3H), 1.31 (s, 9H); ^{13}C NMR (125 MHz, CDCl_3) δ = 171.8, 160.8 (2xC), 155.1, 154.5, 151.4, 148.9, 146.6, 144.0, 131.3, 129.8 (2xC), 127.3, 124.5 (2xC), 122.9, 118.4, 103.0 (2xC), 98.3, 81.7, 78.7, 56.2, 55.4 (2xC), 38.4, 37.3, 36.5, 29.7, 28.9 (3xC), 28.5. IR (neat): 3413, 3319, 2974, 2932, 1703, 1660, 1597, 1537, 1503, 1455, 1423, 1342, 1292, 1253, 1232, 1198, 1153, 1054, 731. HR-MS 753.1741 ($\text{C}_{33}\text{H}_{39}\text{BrN}_4\text{O}_{10} + \text{Na}^+$ calcd 753.1742).

2-(3,5-dimethoxyphenyl)propan-2-yl (S)-1-(2-bromo-3,5-dinitrophenethylcarbamoyl)-2-tert-butoxyethylcarbamate (9w): Purification by flash column chromatography [SiO_2 , CH_2Cl_2 (to remove 5,7-dinitroindoline) and then hexane/EtOAc (1:1)]. Slightly yellow solid (653 mg, 83 %); mp. 65 °C; ^1H NMR (360 MHz, CDCl_3) δ = 8.37 (s, 1H), 8.20 (s, 1H), 6.65 (b, 1H), 6.46 (s, 2H), 6.31 (s, 1H), 5.57 (d, J = 5.0 Hz, 1H), 4.06 (m, 1H), 3.81-3.75 (7H), 3.54 (m, 2H), 3.37 (m, 1H), 3.15 (m, 2H), 1.76 (s, 3H), 1.66 (s, 3H), 1.15 (s, 9H); ^{13}C NMR (125 MHz, CDCl_3) δ = 171.1, 160.8 (2xC), 155.1, 151.4, 149.0, 146.6, 144.2, 127.6, 122.9, 118.3, 103.0 (2xC), 98.3, 81.6, 74.1, 61.4, 55.4 (2xC), 54.7, 38.5, 36.8, 29.9, 28.3, 27.5 (3xC). IR (neat): 3416, 3334, 2972, 2933, 1714, 1667, 1597, 1538, 1457, 1423, 1343, 1195, 1150, 1053. HR-MS 677.1429 ($\text{C}_{27}\text{H}_{35}\text{BrN}_4\text{O}_{10} + \text{Na}^+$ calcd 677.1429).

2-(3,5-dimethoxyphenyl)propan-2-yl (1*S*,2*R*)-1-(2-bromo-3,5-dinitro-phenethylcarbamoyl)-2-*tert*-butoxypropylcarbamate (9x): Purification by flash column chromatography [SiO_2 , CH_2Cl_2 (to remove 5,7-dinitroindoline) and then gradient hexane/EtOAc (2:1) to hexane/EtOAc (1:1)]. Slightly yellow solid (530 mg, 66 %); mp. 79 °C; ^1H NMR (360 MHz, CDCl_3) δ = 8.39 (s, 1H), 8.26 (s, 1H), 6.99 (b, 1H), 6.50 (s, 2H), 6.33 (s, 1H), 5.76 (d, J = 4.5 Hz, 1H), 4.11 (m, 1H), 3.98 (m, 1H), 3.78 (s, 6H), 3.68 (m, 1H), 3.55 (m, 1H), 3.19 (m, 2H), 1.74 (s, 3H), 1.71 (s, 3H), 1.16 (s, 9H), 1.03 (d, J = 5.4 Hz, 3H); ^{13}C NMR (125 MHz, CDCl_3) δ = 170.7, 161.0 (2xC), 155.0, 151.7, 149.2, 146.9, 144.3, 127.4, 122.9, 118.3, 103.3 (2xC), 98.7, 81.5, 75.4, 66.8, 59.1, 55.5 (2xC), 38.5, 37.0, 29.4, 29.0, 28.5 (3xC), 18.2. IR (neat): 3404, 3348, 2974, 2934, 1714, 1671, 1598, 1540, 1479, 1459, 1424, 1343, 1196, 1150, 1055, 733. HR-MS 691.1581 ($\text{C}_{28}\text{H}_{37}\text{BrN}_4\text{O}_{10}$ + Na^+ calcd 691.1585).

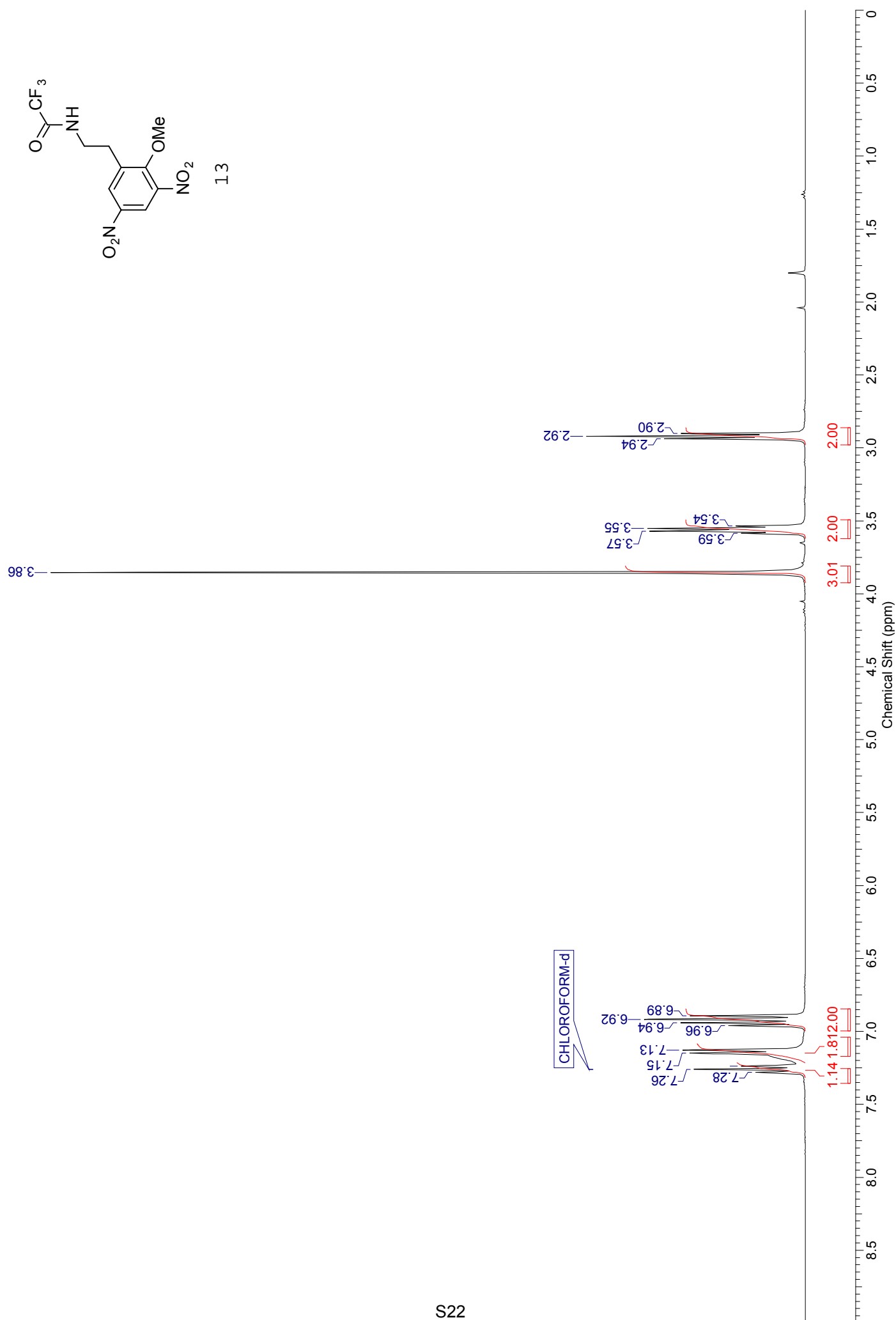
2-(3,5-dimethoxyphenyl)propan-2-yl (S)-1-(2-bromo-3,5-dinitrophenethylcarbamoyl)-2-(*tert*-butoxycarbonyl)ethylcarbamate (9y): Purification by flash column chromatography [SiO_2 , gradient hexane/EtOAc (2:1) to hexane/EtOAc (1:1)]. Slightly yellow solid (697 mg, 85 %); ^1H NMR (360 MHz, CDCl_3) δ = 8.38 (s, 1H), 8.28 (s, 1H), 6.63 (b, 1H), 6.48 (s, 2H), 6.32 (s, 1H), 6.02 (d, J = 7.8 Hz, 1H), 4.29 (m, 1H), 3.76 (s, 6H), 3.51 (m, 2H), 3.10 (m, 2H), 2.83 (dd, J = 17.7, 3.2 Hz, 1H), 2.51 (dd, J = 16.8, 5.0 Hz, 1H), 1.78 (s, 3H), 1.66 (s, 3H), 1.42 (s, 9H); ^{13}C NMR (125 MHz, CDCl_3) δ = 171.5, 171.4, 160.9 (2xC), 155.5, 151.4, 148.9, 146.6, 144.2, 127.7, 122.9, 118.3, 103.1 (2xC), 98.2, 82.0, 81.8, 55.4 (2xC), 50.8, 38.3, 36.8, 36.3, 30.1, 28.0, 27.9 (3xC). IR (neat): 3402, 3327, 2975, 2930, 1720, 1656, 1594, 1534, 1452, 1419, 1340, 1291, 1248, 1228, 1196, 1149, 1132, 1043. HR-MS 705.1374 ($\text{C}_{28}\text{H}_{35}\text{BrN}_4\text{O}_{11}$ + Na^+ calcd 705.1378).

2-(3,5-dimethoxyphenyl)propan-2-yl (S)-1-(2-bromo-3,5-dinitrophenethylcarbamoyl)-3-(*tert*-butoxycarbonyl)propylcarbamate (9z): Purification by flash column chromatography [SiO_2 , CH_2Cl_2 (to remove 5,7-dinitroindoline) and then gradient hexane/EtOAc (2:1) to hexane/EtOAc (1:1)]. Slightly yellow solid (711 mg, 85 %); ^1H NMR (360 MHz, CDCl_3) δ = 8.37 (s, 1H), 8.18 (s, 1H), 6.53 (b, 1H), 6.46 (s, 2H), 6.29 (s, 1H), 5.56 (d, J = 6.4 Hz, 1H), 3.96 (m, 1H), 3.76 (s, 6H), 3.51 (m, 2H), 3.10 (m,

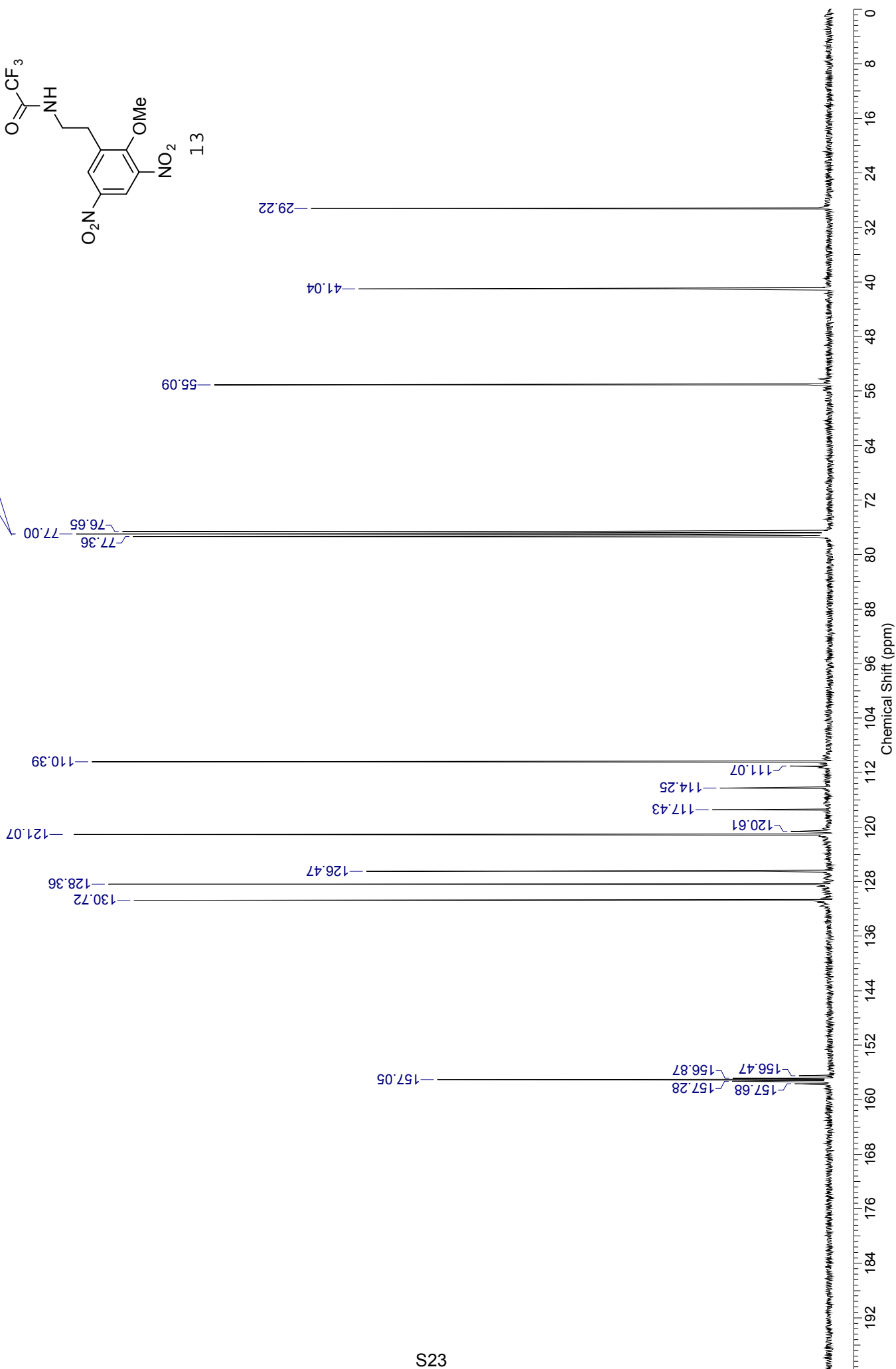
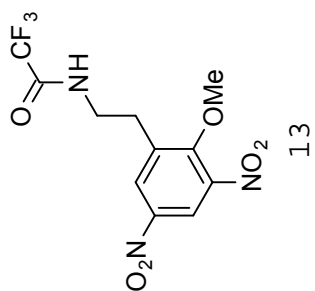
2H), 2.39 (m, 1H), 2.27 (m, 1H), 2.02 (m, 1H), 1.88 (m, 1H), 1.76 (s, 3H), 1.63 (s, 3H), 1.43 (s, 9H); ^{13}C NMR (125 MHz, CDCl_3) δ = 173.1, 172.1, 160.9 (2xC), 155.5, 151.4, 149.0, 146.6, 144.2, 127.7, 122.9, 118.3, 103.0 (2xC), 98.5, 81.7, 81.4, 55.4 (2xC), 54.5, 38.5, 36.7, 32.0, 30.1, 28.3, 28.2 (3xC), 27.0. IR (neat): 3400, 3324, 2977, 2934, 1721, 1667, 1595, 1542, 1454, 1423, 1363, 1343, 1296, 1251, 1203, 1154, 1046, 733. HR-MS 719.1536 ($\text{C}_{29}\text{H}_{37}\text{BrN}_4\text{O}_{11} + \text{Na}^+$ calcd 719.1534).

Benzyl (S)-1-(phenethylcarbamoyl)-2-*tert*-butoxyethylcarbamate (22 g): Purification by flash column chromatography [SiO_2 , hexane/EtOAc (3:2)]. Yellow solid (30.7 mg, 77 %); mp. 113-114 °C; ^1H NMR (360 MHz, CDCl_3) δ = 7.42-7.24 (10H), 6.66 (b, 1H), 5.74 (b, 1H), 5.17 (s, 2H), 4.22 (m, 1H), 3.87 (m, 1H), 3.61 (m, 2H), 3.39 (t, J = 7.7 Hz, 1H), 2.86 (t, J = 6.1 Hz, 2H), 1.17 (s, 9H); ^{13}C NMR (125 MHz, CDCl_3) δ = 170.3, 156.2, 138.9, 136.3, 128.9, 128.8 (2xC), 128.7 (2xC), 128.4 (2xC), 128.3 (2xC), 126.7, 74.2, 67.2, 61.8, 54.8, 40.7, 35.8, 27.5 (3xC). IR (neat): 3296, 3024, 2967, 2924, 2852, 1685, 1642, 1534, 1454, 1354, 1285, 1272, 1231, 1188, 1089, 1049, 740, 696. HR-MS 421.2096 ($\text{C}_{23}\text{H}_{30}\text{N}_2\text{O}_4 + \text{Na}^+$ calcd 421.2098).

2-(3,5-dimethoxyphenyl)propan-2-yl (S)-1-(phenethylcarbamoyl)-3-methylbutylcarbamate (22 r): Purification by flash column chromatography [SiO_2 , hexane/EtOAc (1:1)]. Yellow solid (42 mg, 92 %); ^1H 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 ($\text{C}_{26}\text{H}_{36}\text{N}_2\text{O}_5 + \text{Na}^+$ calcd 479.2516).

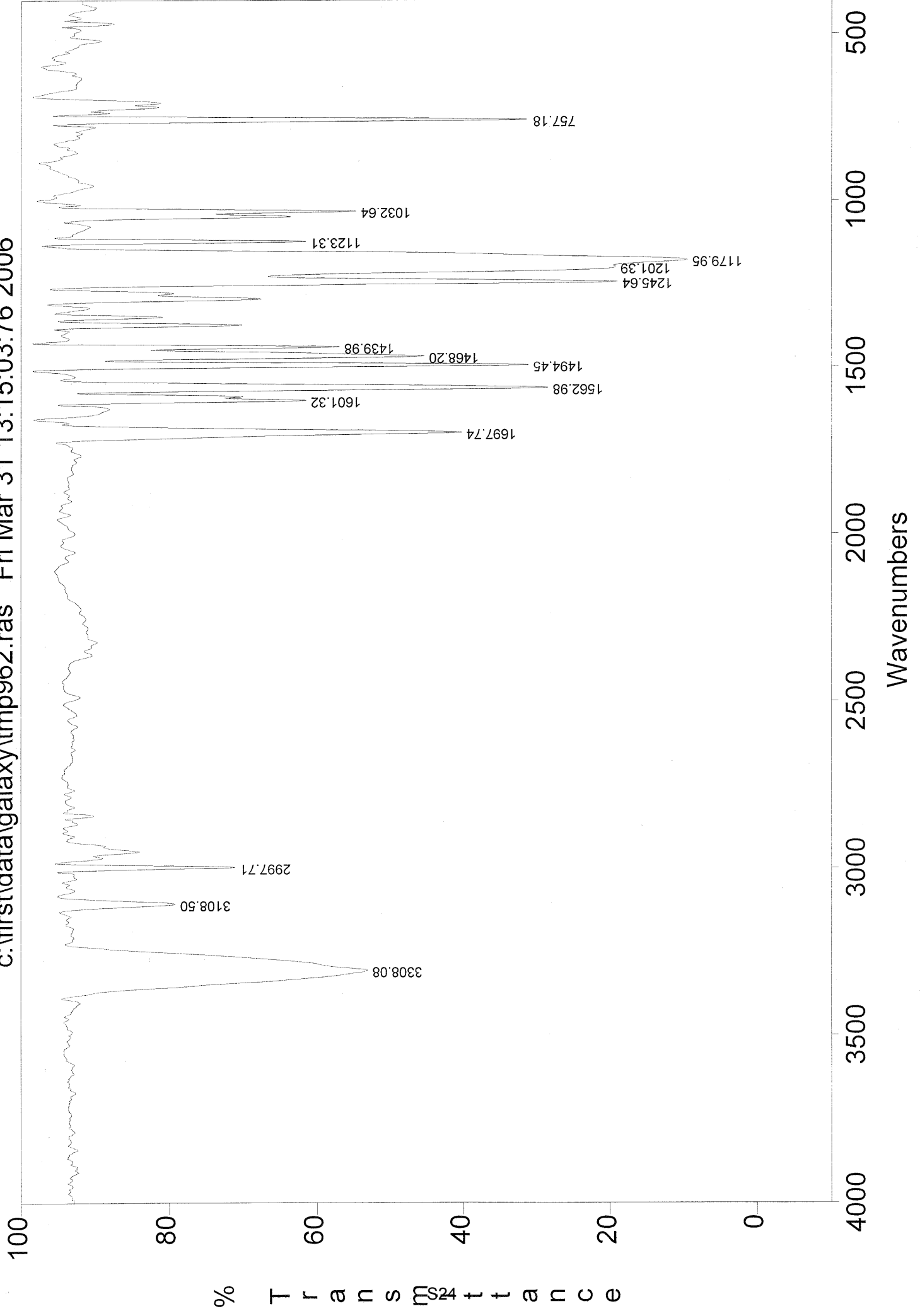


CHLOROFORM-d



2052

c:\first\data\galaxy\tmp962.ras Fri Mar 31 13:15:03:76 2006





FTMS 4.7T BioAPEX II MS-Service UNI-Fribourg

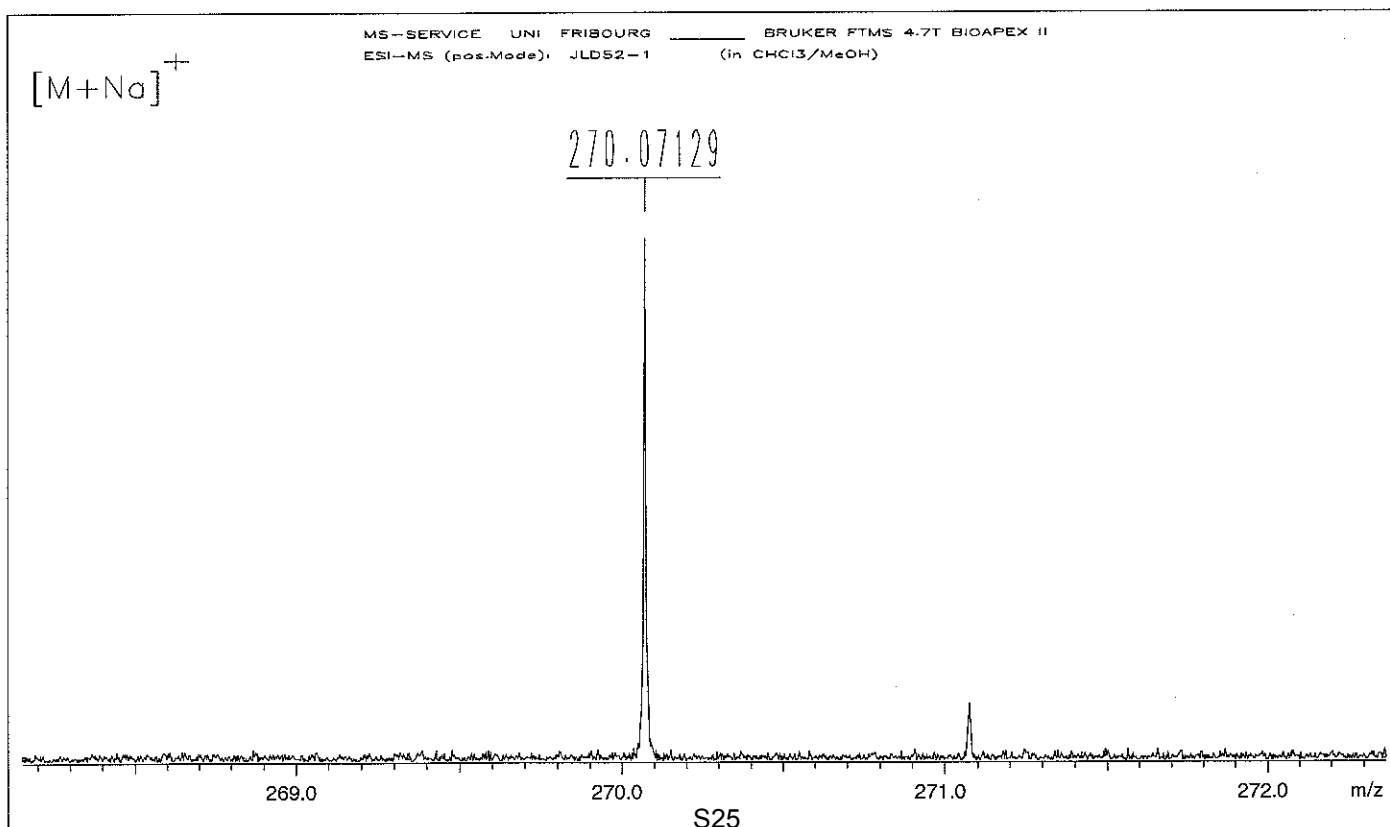
ESI-MS: JLD52-1

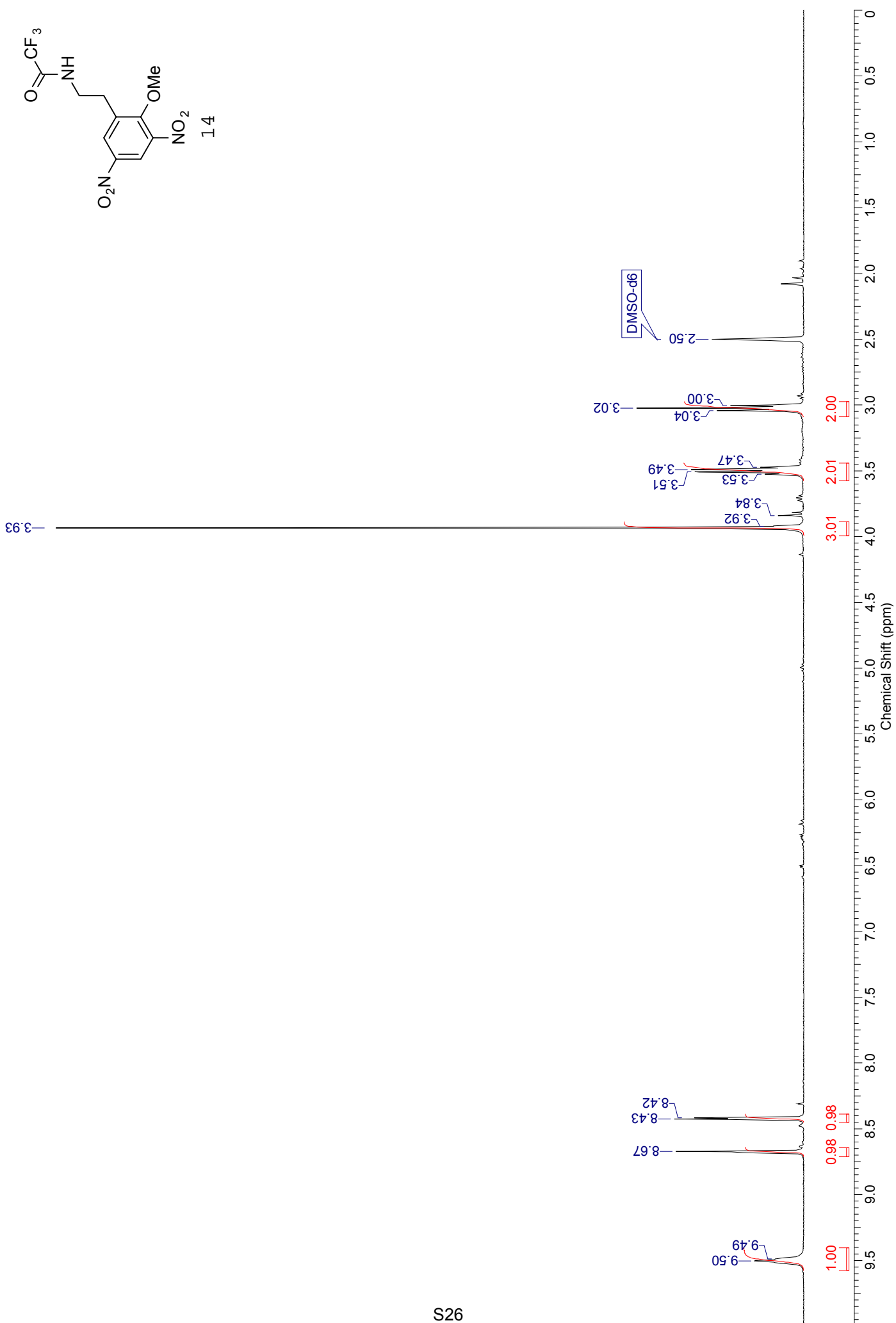
XMASS Mass Analysis for /Data/UNI_FR/DEBI1290_ESI/5/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

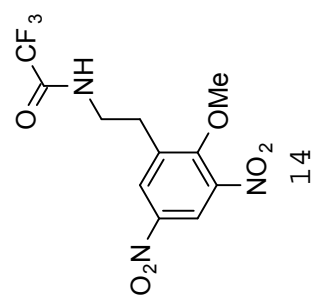
Ion mass = 270.0712950

Charge = +1

#	C	H	F	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 270.0712950									
1	11	12	3	1	2	1	270.0712343	4.5	6.068e-05
2	11	9	3	4	1	0	270.0722970	8.0	1.002e-03
3	16	10	2	1	1	0	270.0724968	11.5	1.202e-03
4	14	11	2	1	1	1	270.0700915	8.5	1.204e-03
5	13	11	3	1	2	0	270.0736396	7.5	2.345e-03
6	11	10	2	3	3	0	270.0684740	7.5	2.821e-03
7	10	12	4	1	3	0	270.0747825	3.5	3.487e-03
8	10	14	1	1	5	1	270.0748219	3.5	3.527e-03
9	14	9	1	3	2	0	270.0673312	11.5	3.964e-03
10	10	11	1	4	4	0	270.0758845	7.0	4.589e-03







DMSO-d6

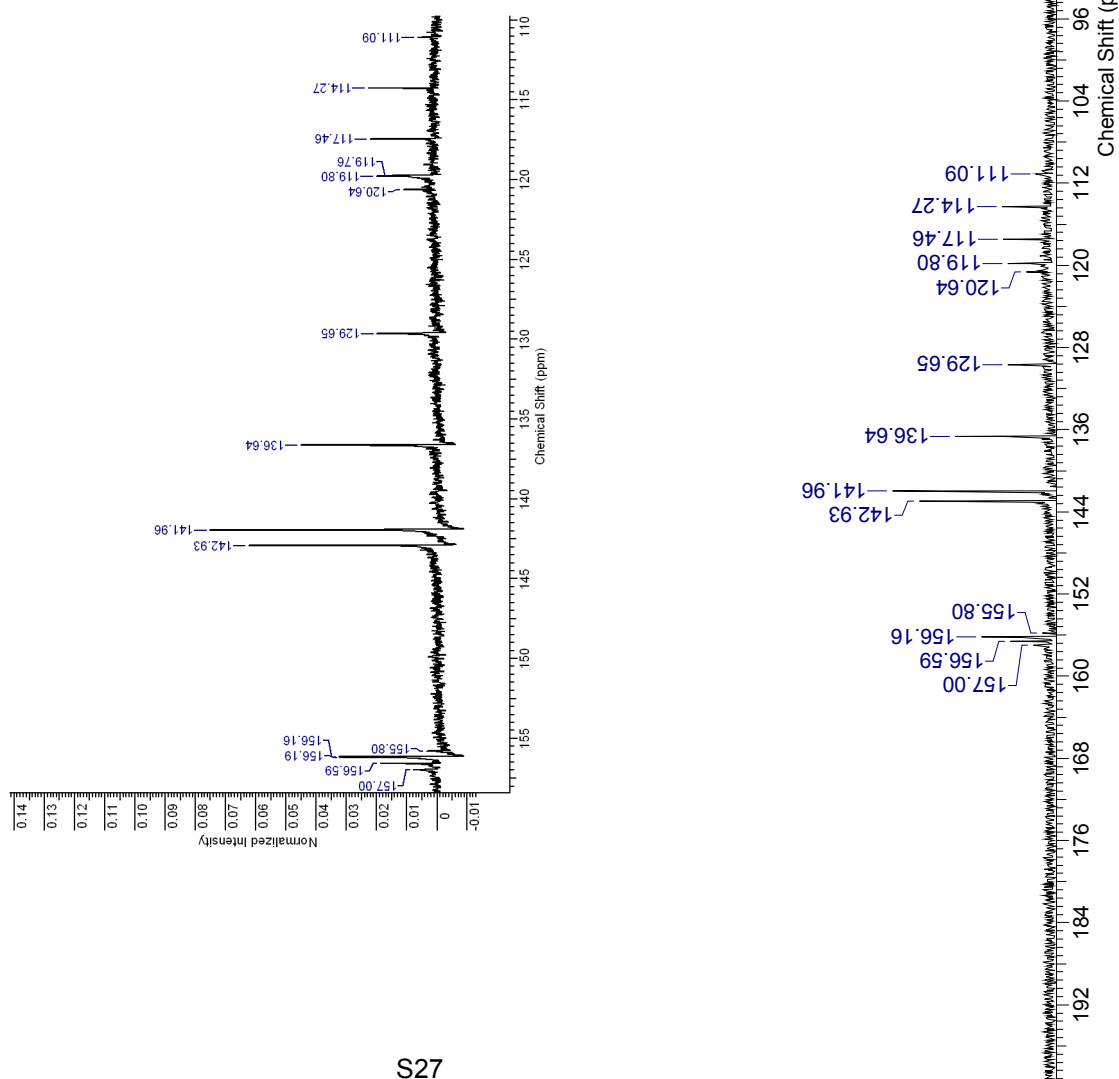
39.75
39.52
39.29

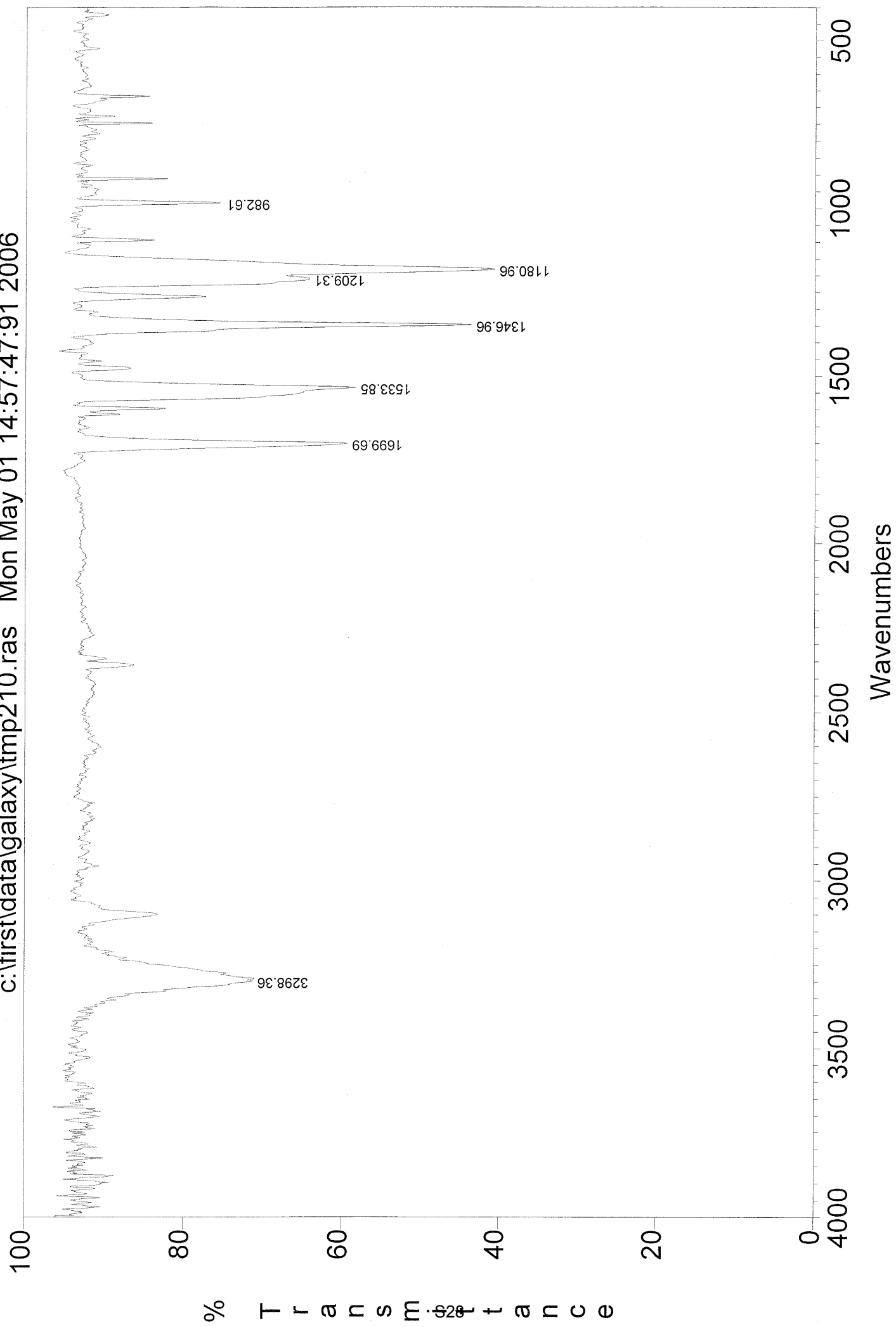
39.99
39.06

40.22
38.83

28.80

63.56
62.68





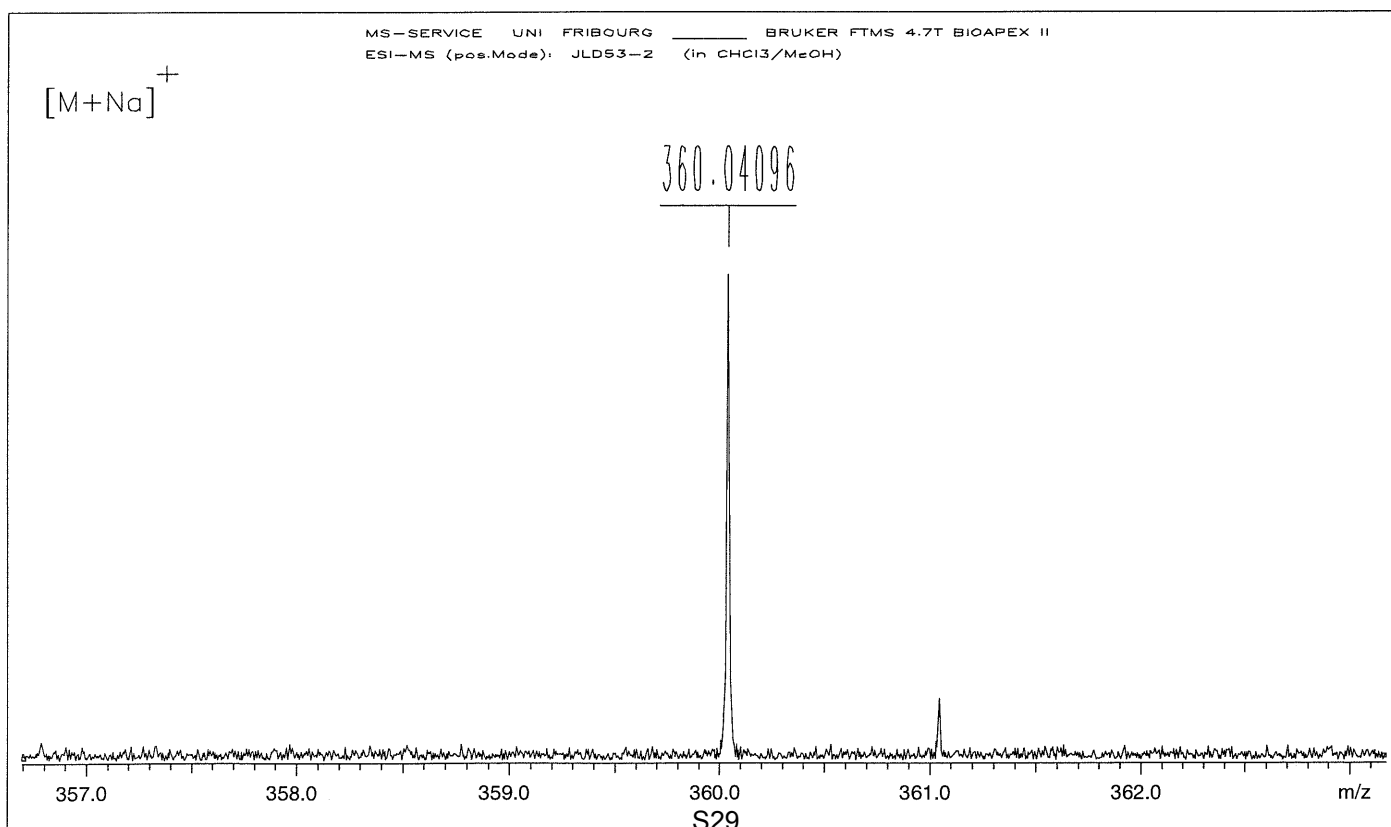
ESI-MS: JLD53-2

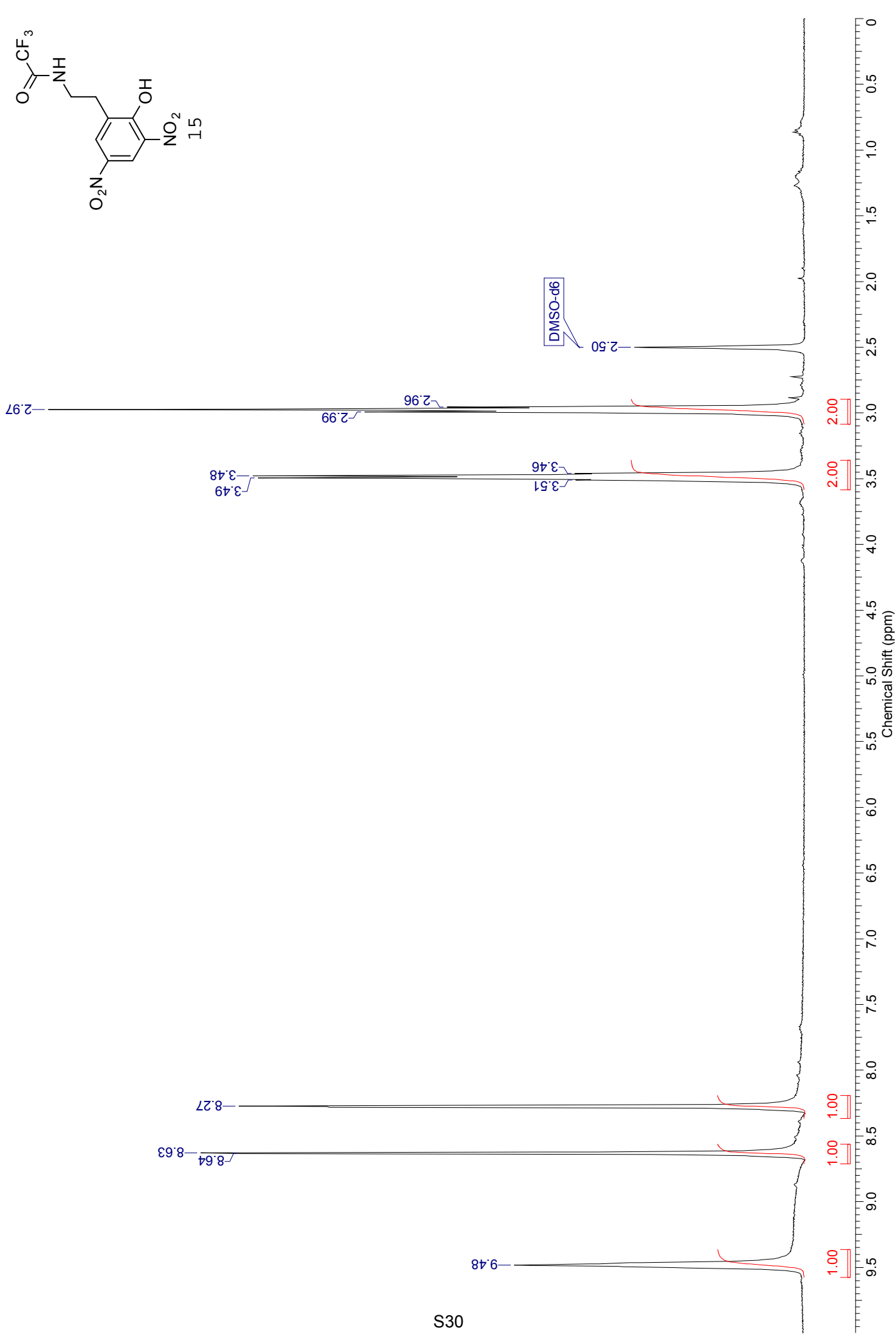
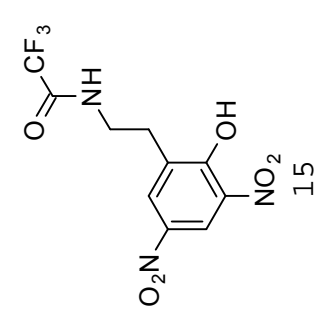
XMASS Mass Analysis for /Data/UNI_FR/DEBI1304_ESI/3/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

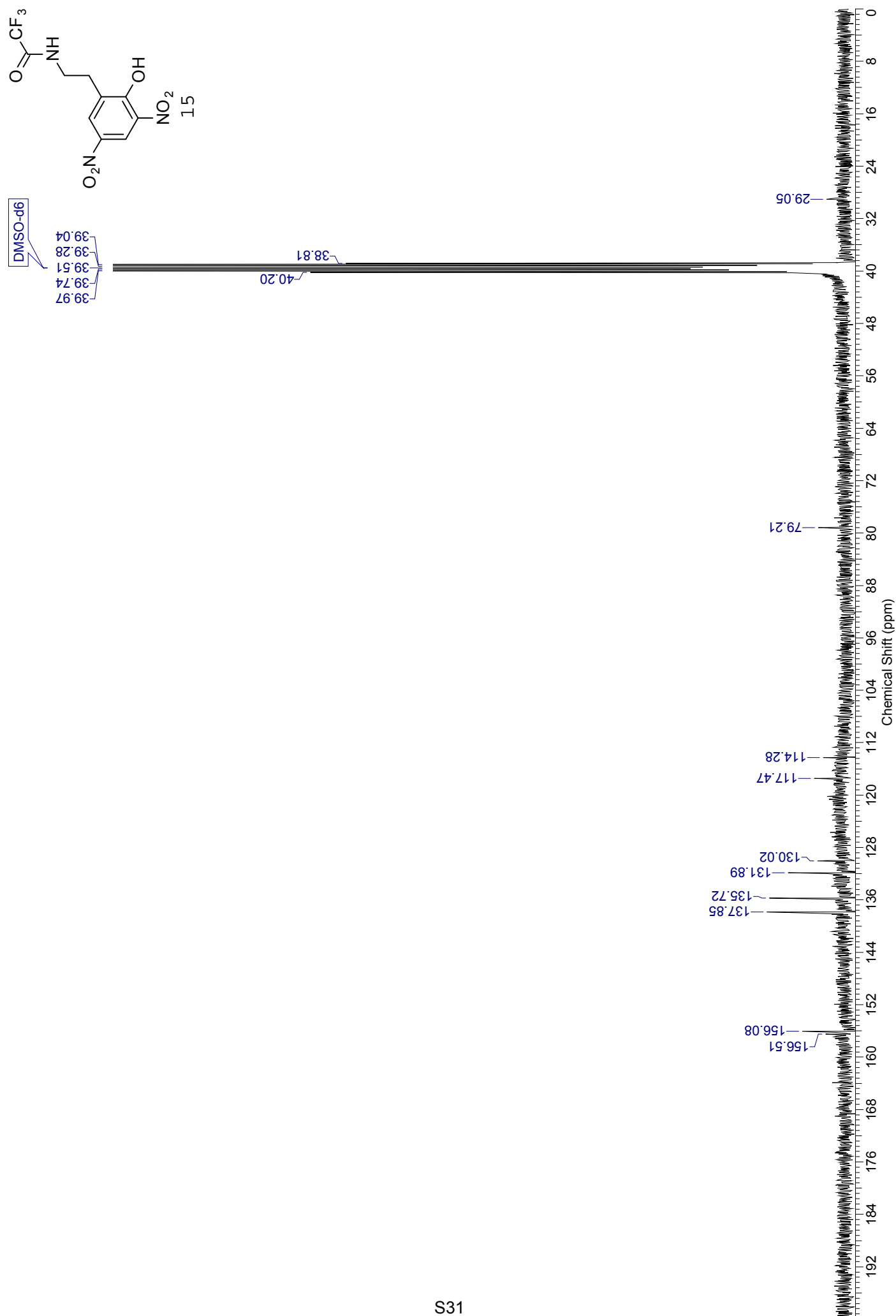
Ion mass = 360.0409590

Charge = +1

#	C	H	F	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 360.0409590									
1	11	10	3	3	6	1	360.0413908	6.5	4.318e-04
2	19	7	1	3	4	0	360.0415103	17.5	5.513e-04
3	14	9	2	3	5	1	360.0402479	10.5	7.111e-04
4	14	7	5	3	3	0	360.0402085	10.5	7.505e-04
5	13	10	2	2	8	0	360.0399731	9.0	9.859e-04
6	8	9	3	5	8	0	360.0397733	5.5	1.186e-03
7	8	11	4	3	7	1	360.0425336	2.5	1.575e-03
8	16	8	2	3	5	0	360.0426532	13.5	1.694e-03
9	17	8	1	3	4	1	360.0391051	14.5	1.854e-03
10	17	6	4	3	2	0	360.0390657	14.5	1.893e-03

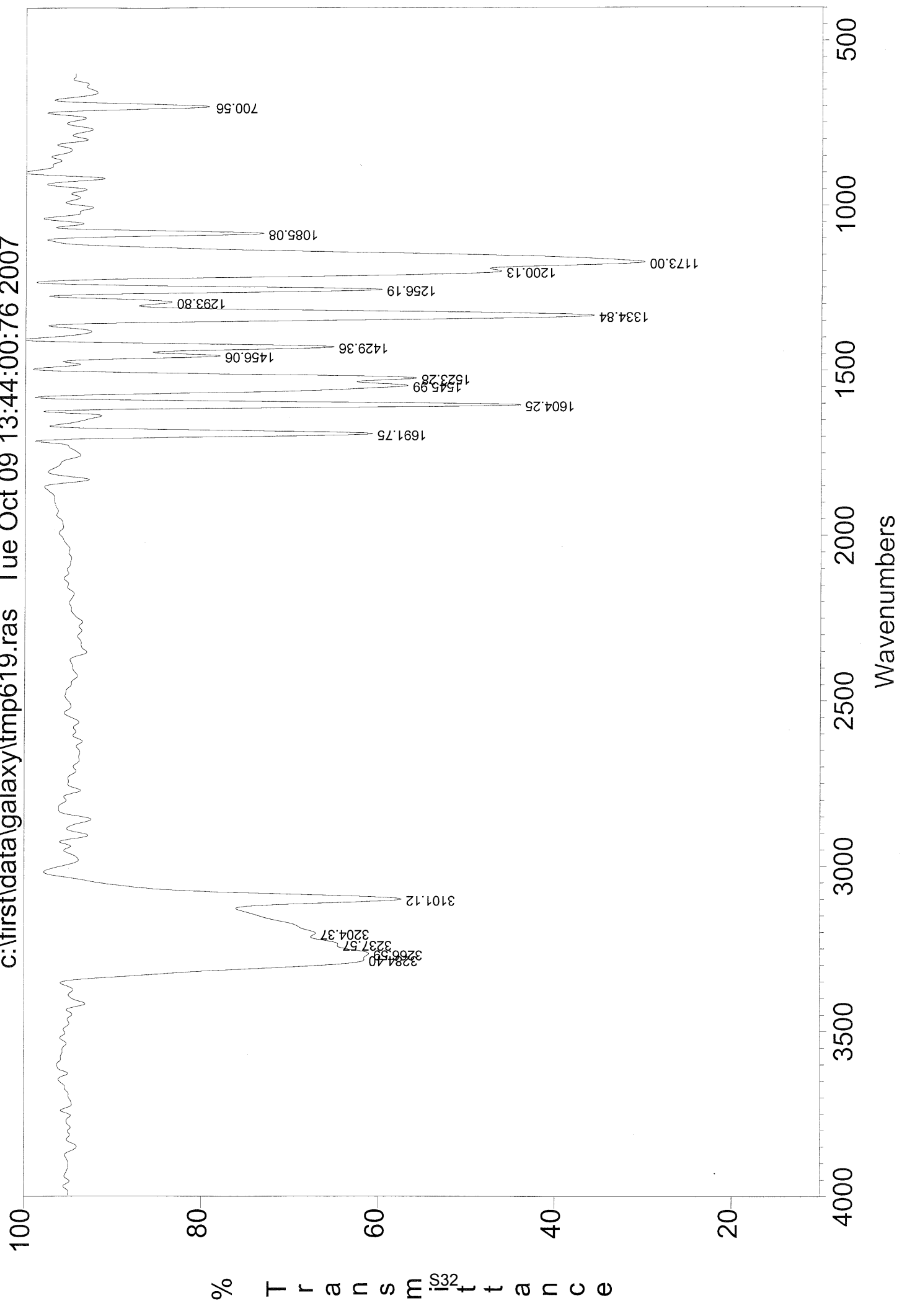






9655

c:\first\data\galaxy\tmp619.ras Tue Oct 09 13:44:00:76 2007



ESI-MS: JLD55-3

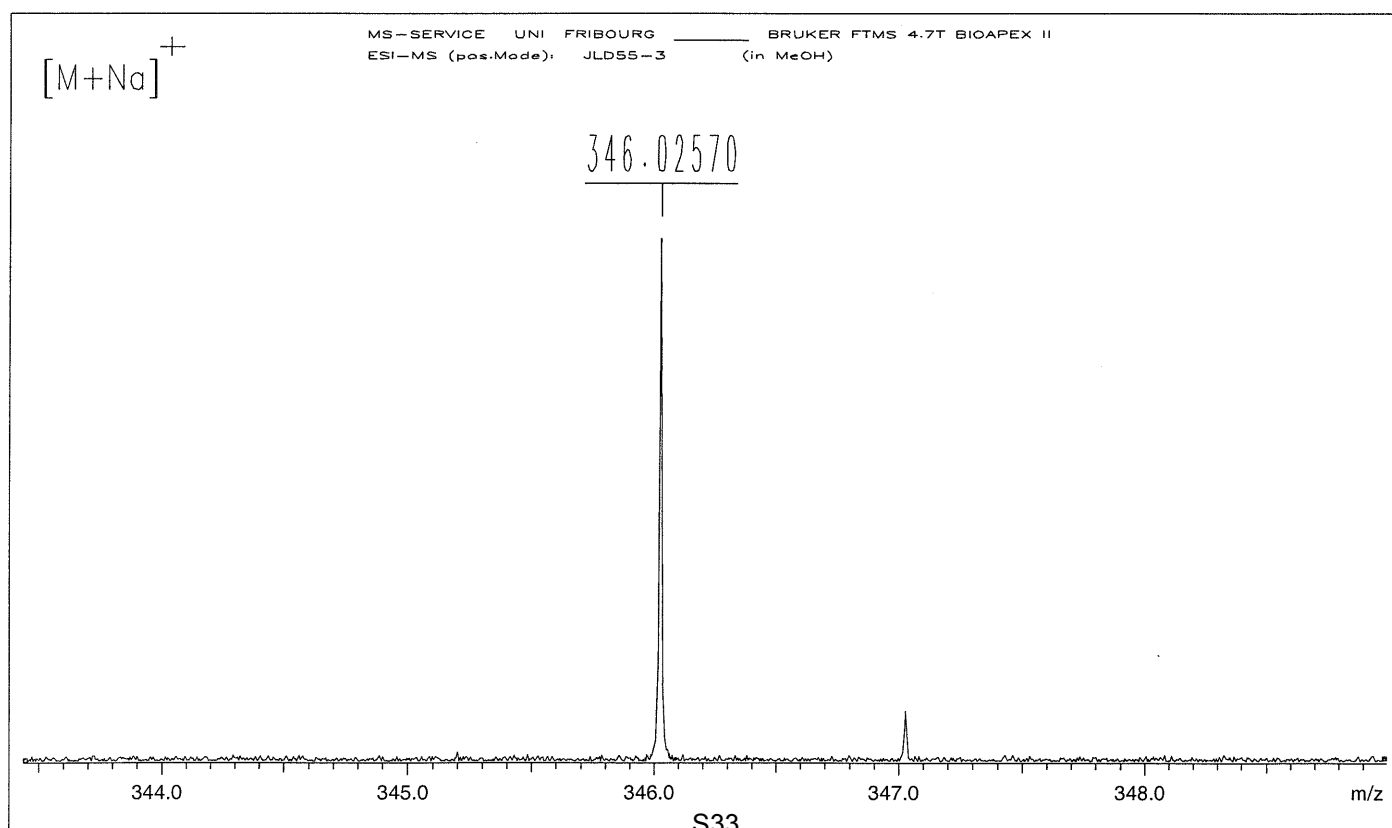
XMASS Mass Analysis for /Data/UNI_FR/DEBI1437_ESI/2/pdata/1/massanal.res:

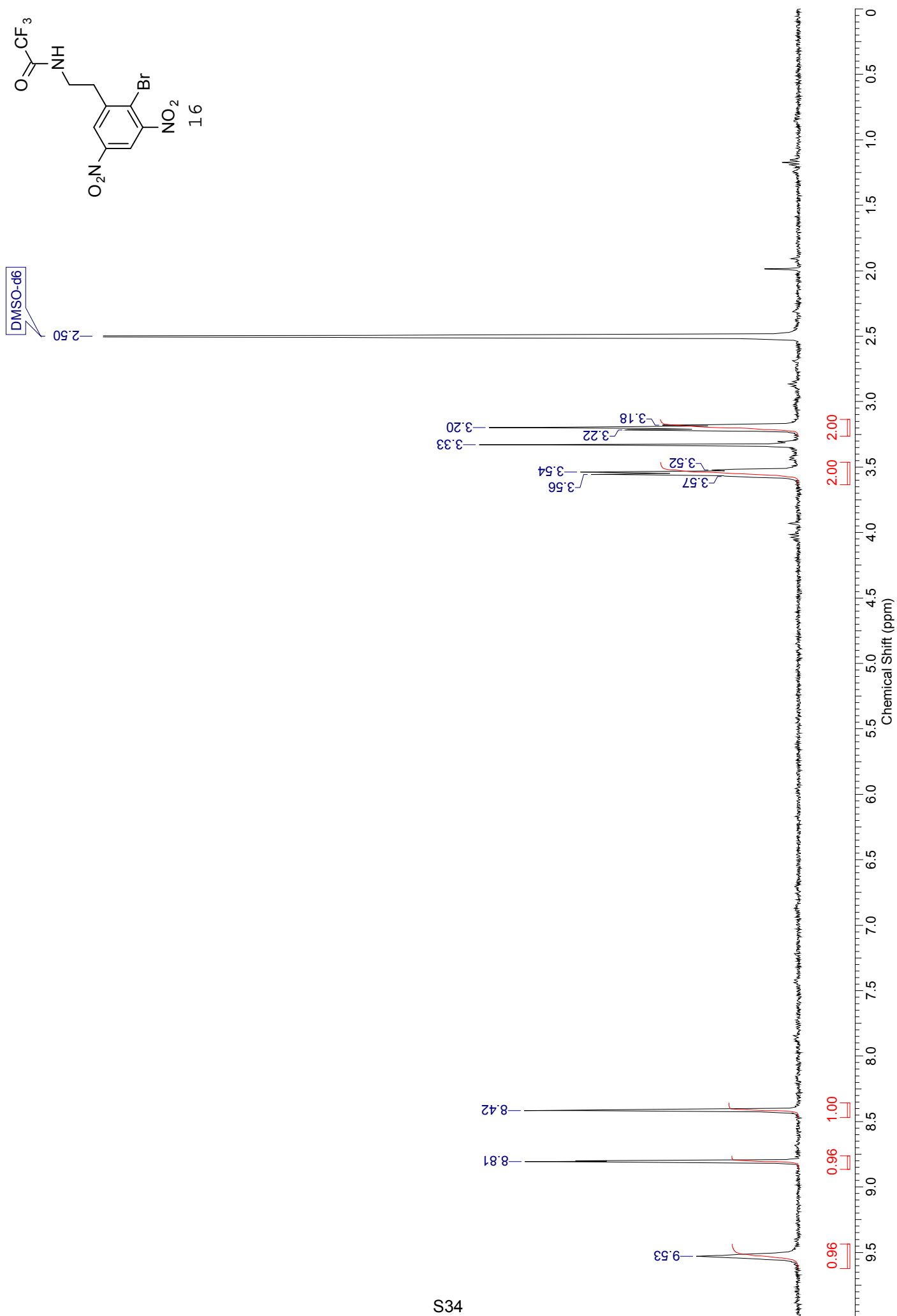
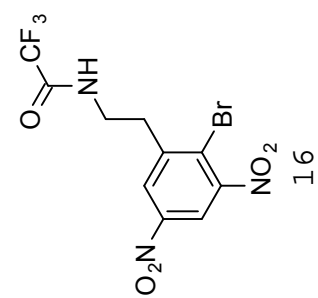
XMASS Mass Analysis Constraints

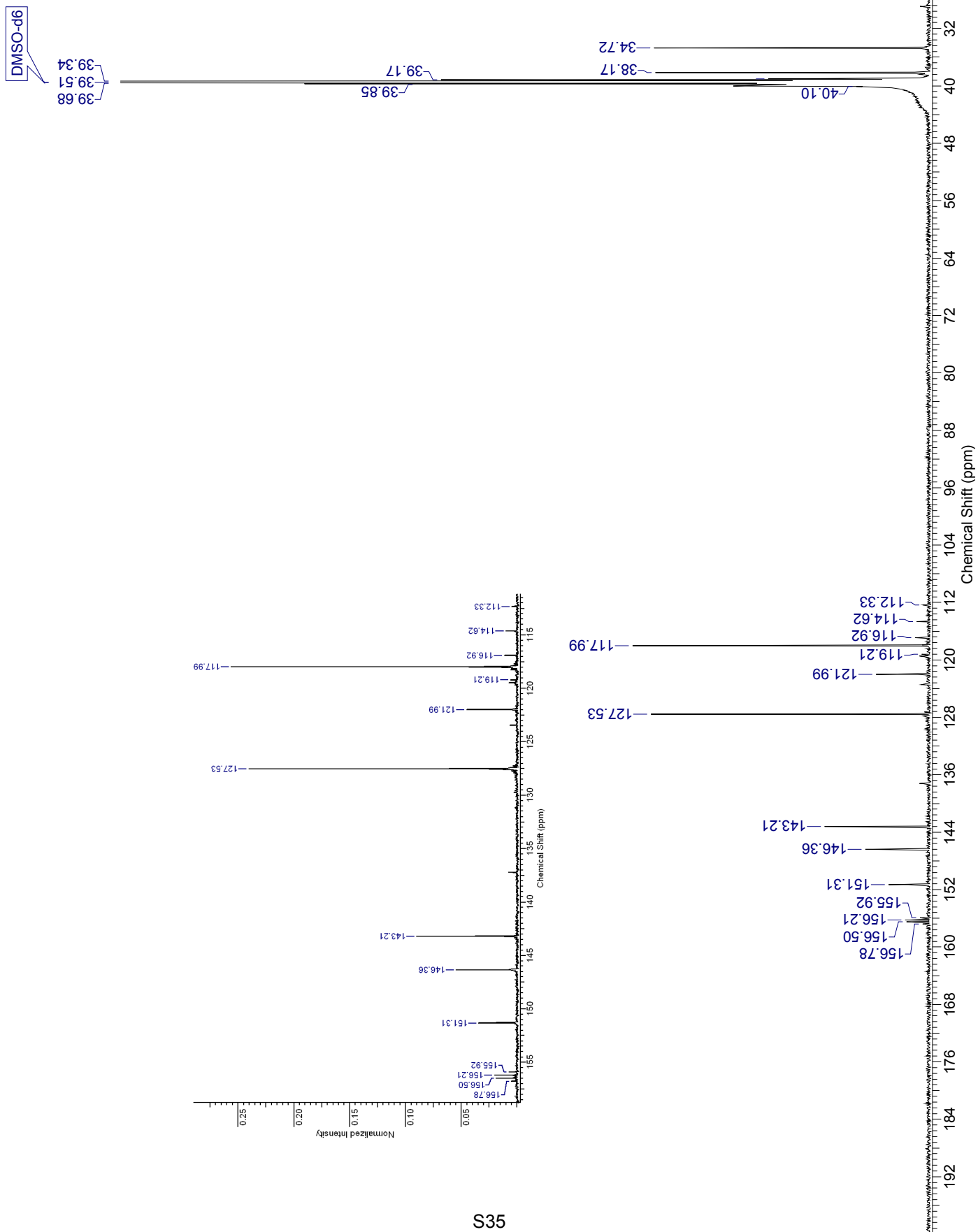
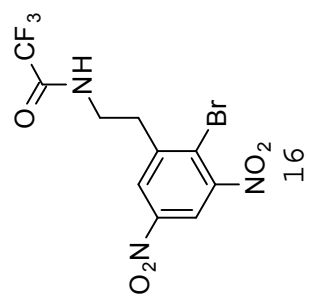
Ion mass = 346.0256960

Charge = +1

#	C	H	F	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 346.0256960									
1	10	8	3	3	6	1	346.0257407	6.5	4.470e-05
2	9	9	3	2	9	0	346.0254659	5.0	2.301e-04
3	6	10	4	2	10	0	346.0266088	1.0	9.128e-04
4	13	7	2	3	5	1	346.0245978	10.5	1.098e-03
5	7	9	4	3	7	1	346.0268835	2.5	1.188e-03
6	15	6	2	3	5	0	346.0270031	13.5	1.307e-03
7	12	8	2	2	8	0	346.0243231	9.0	1.373e-03
8	7	7	3	5	8	0	346.0241232	5.5	1.573e-03
9	16	5	2	4	2	1	346.0272779	15.0	1.582e-03
10	12	7	3	3	6	0	346.0281460	9.5	2.450e-03

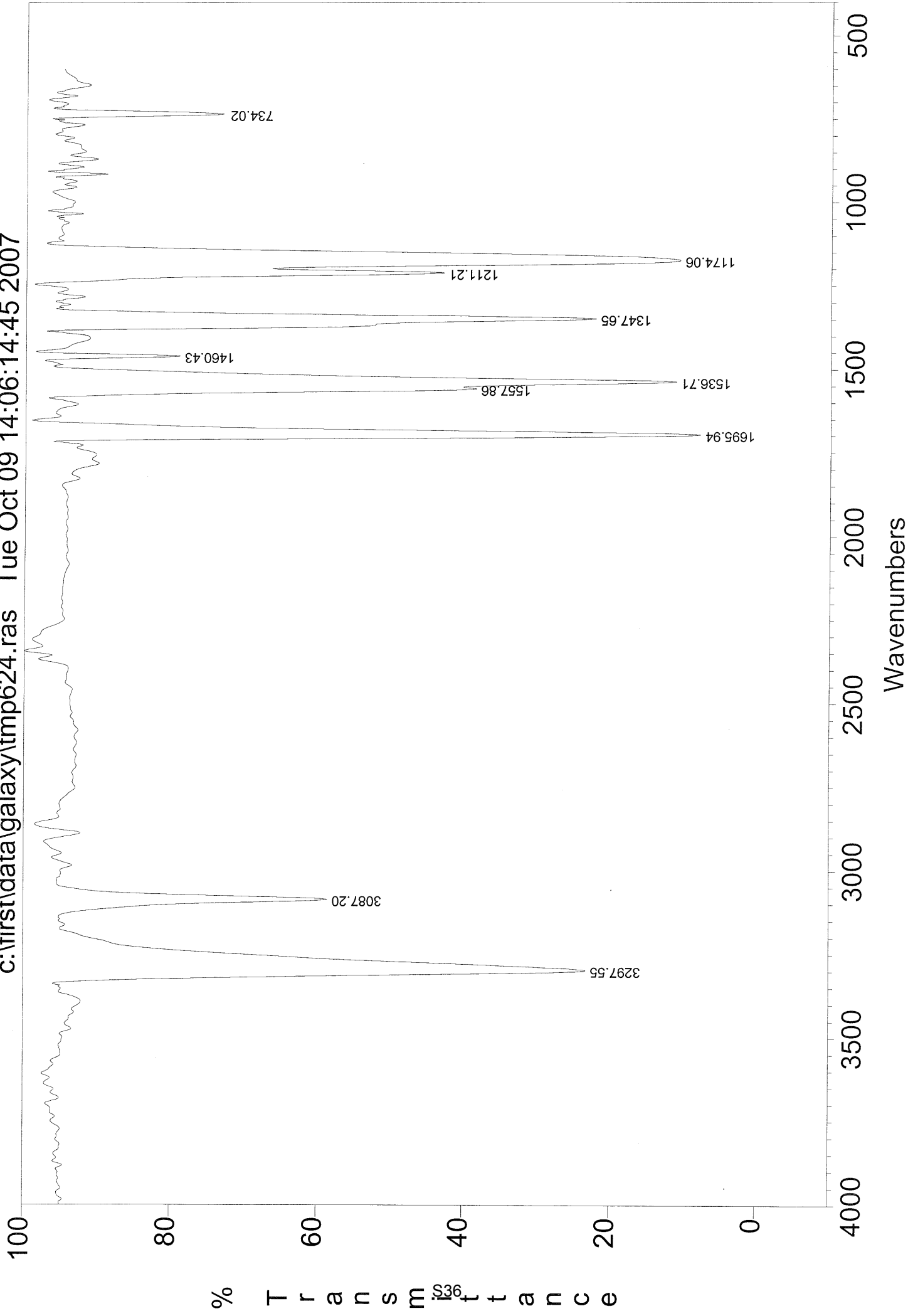






36056

c:\first\data\galaxy\tmp624.ras Tue Oct 09 14:06:14:45 2007



ESI-MS: JLD56-1

XMASS Mass Analysis for /Data/UNI_FR/DEBI1338_ESI/5/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

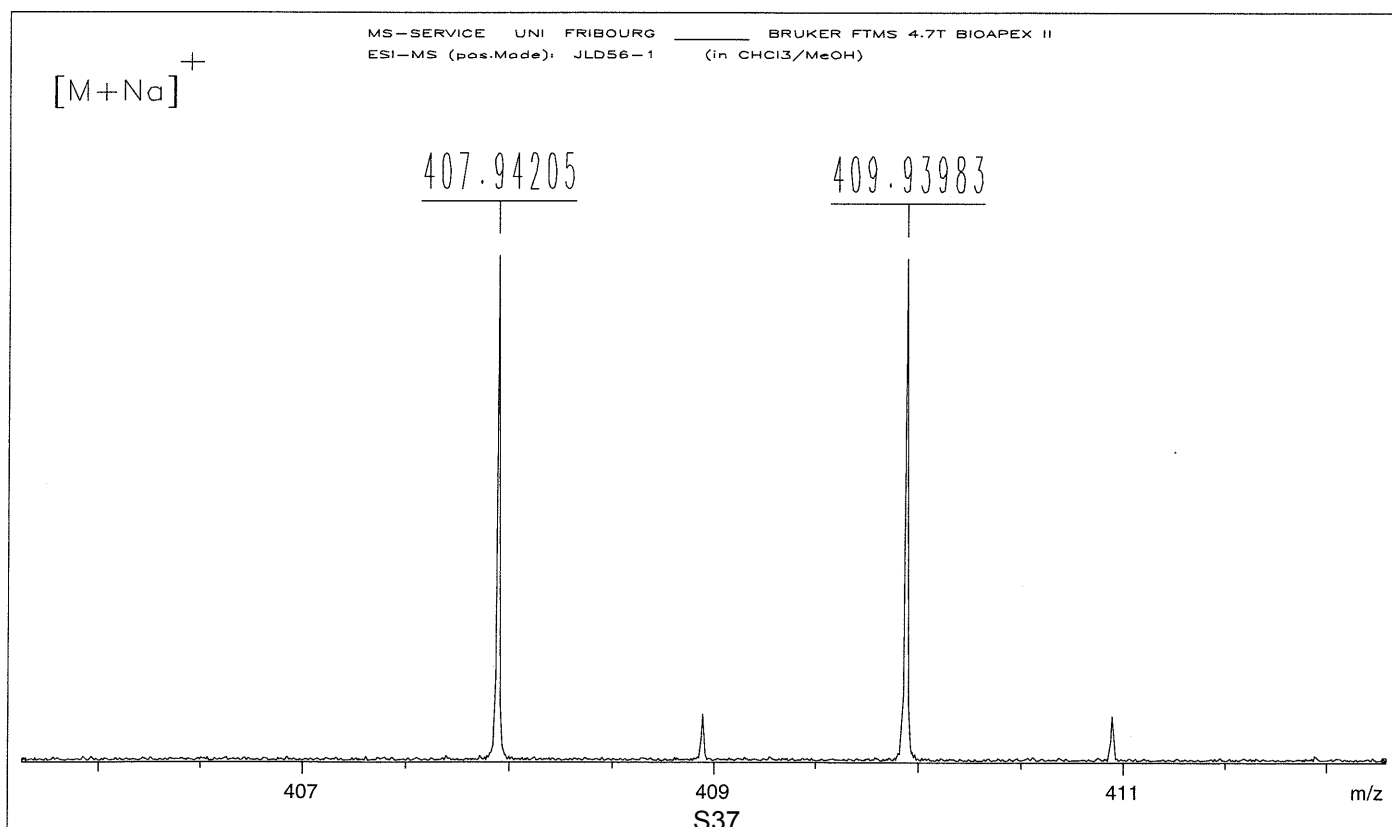
Ion mass [1] = 407.9420520

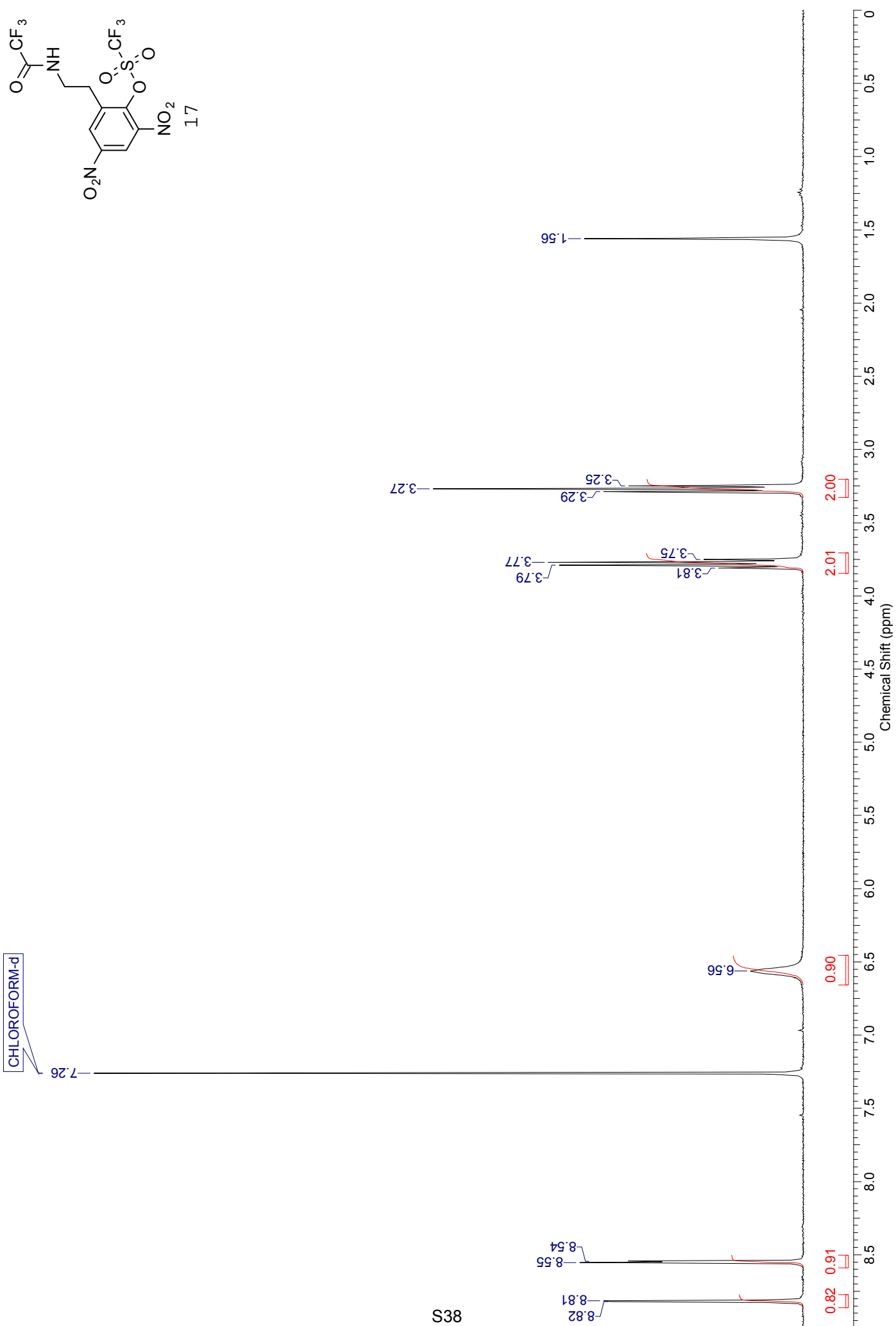
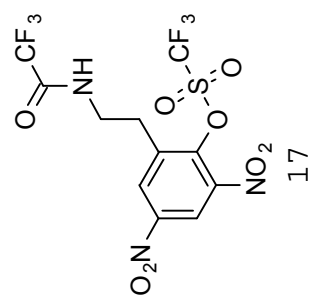
Ion mass [2] = 409.9398320

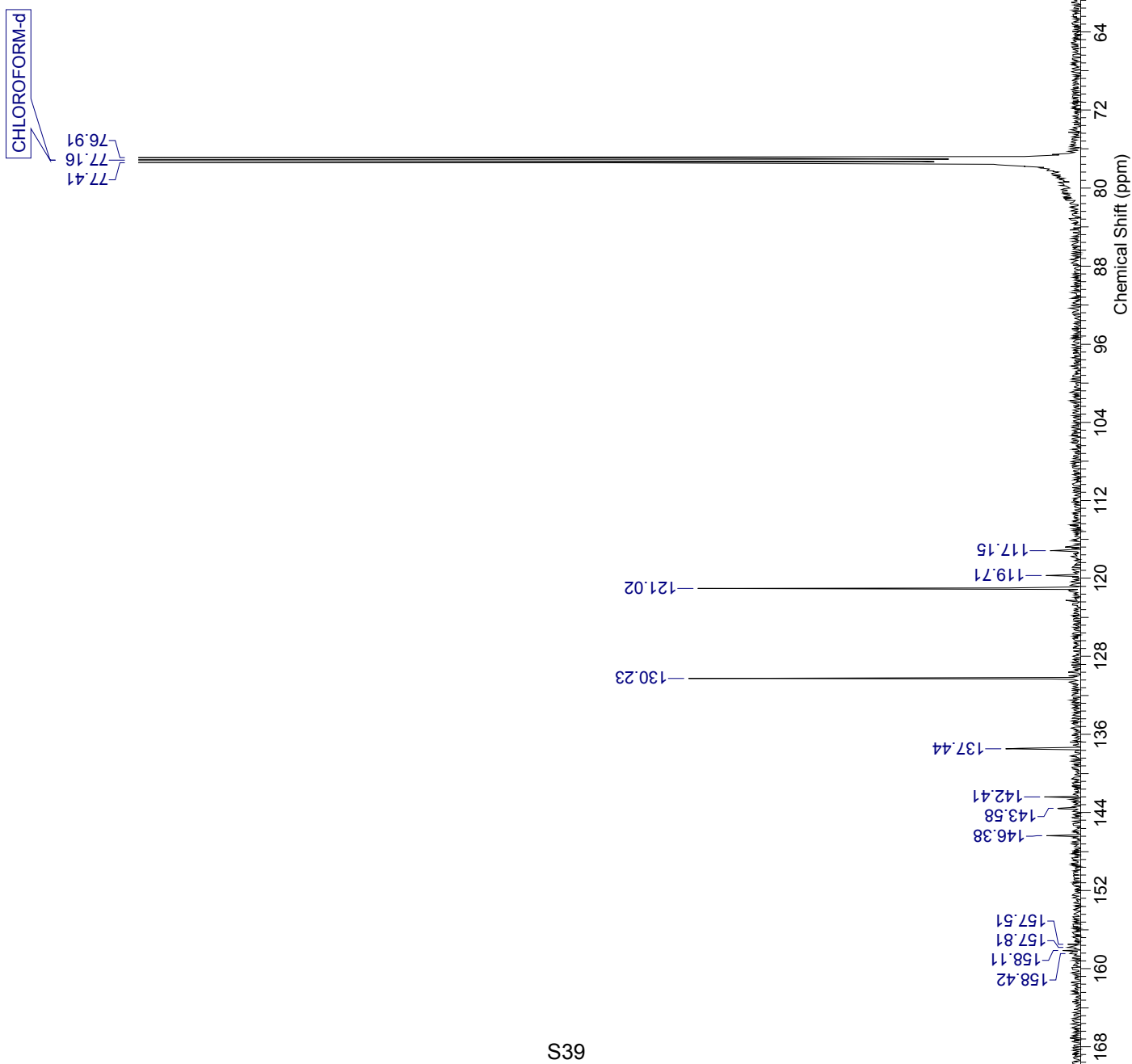
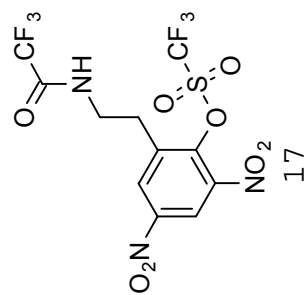
Charge = +1

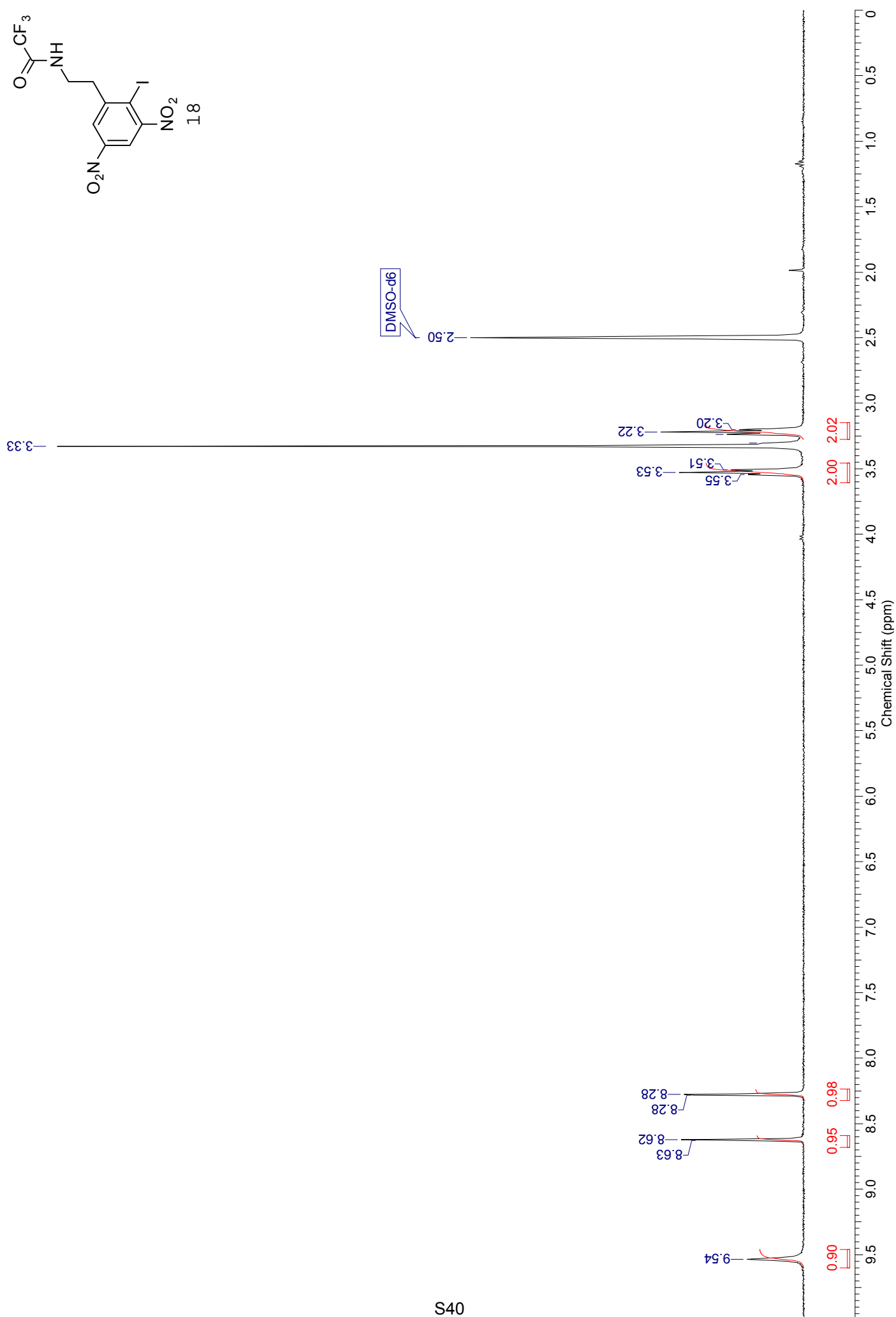
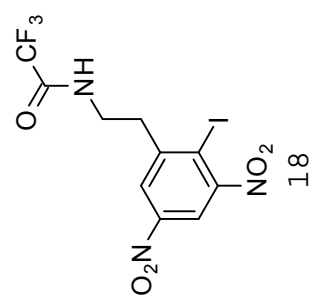
#	C	H	79Br	81Br	F	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 407.9420520											
1	10	7	1	0	3	3	5	1	407.9413386	6.5	7.134e-04
2	10	8	0	1	2	3	6	1	407.9436285	6.5	1.576e-03
3	12	6	1	0	3	3	5	0	407.9437439	9.5	1.692e-03
4	11	6	0	1	4	3	3	1	407.9400410	7.5	2.011e-03
5	10	7	0	1	4	2	6	0	407.9397662	6.0	2.286e-03

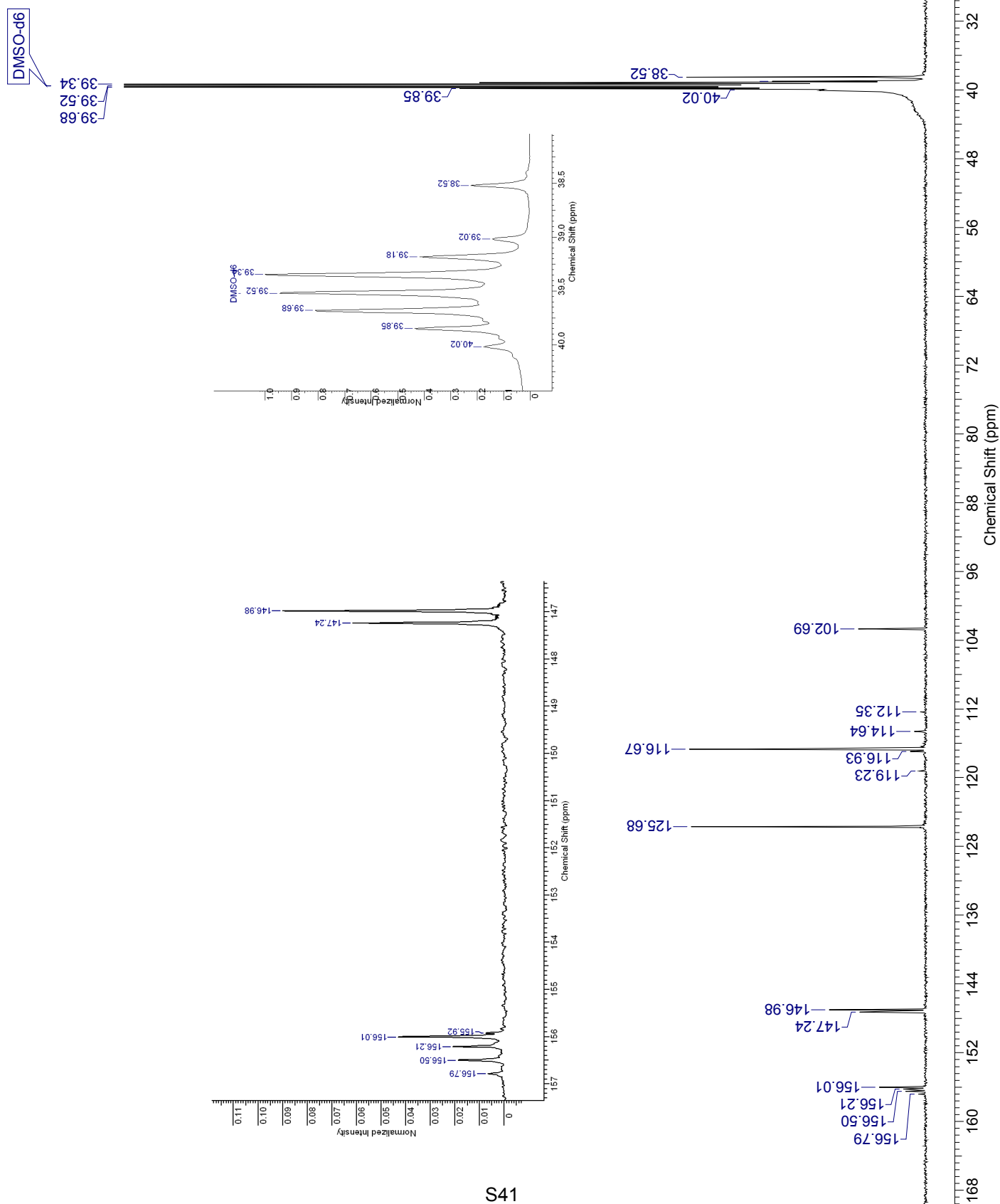
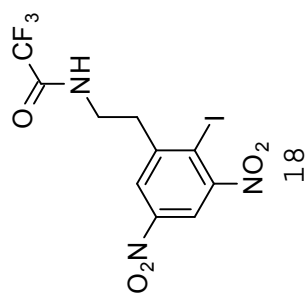
*** Mass Analysis for mass 409.9398320											
1	10	7	0	1	3	3	5	1	409.9392920	6.5	5.400e-04
2	12	6	0	1	3	3	5	0	409.9416973	9.5	1.865e-03
3	10	6	1	0	4	3	4	1	409.9370022	6.5	2.830e-03
4	9	7	0	1	4	3	6	0	409.9428402	5.5	3.008e-03
5	10	6	0	1	4	4	3	1	409.9431150	7.0	3.283e-03











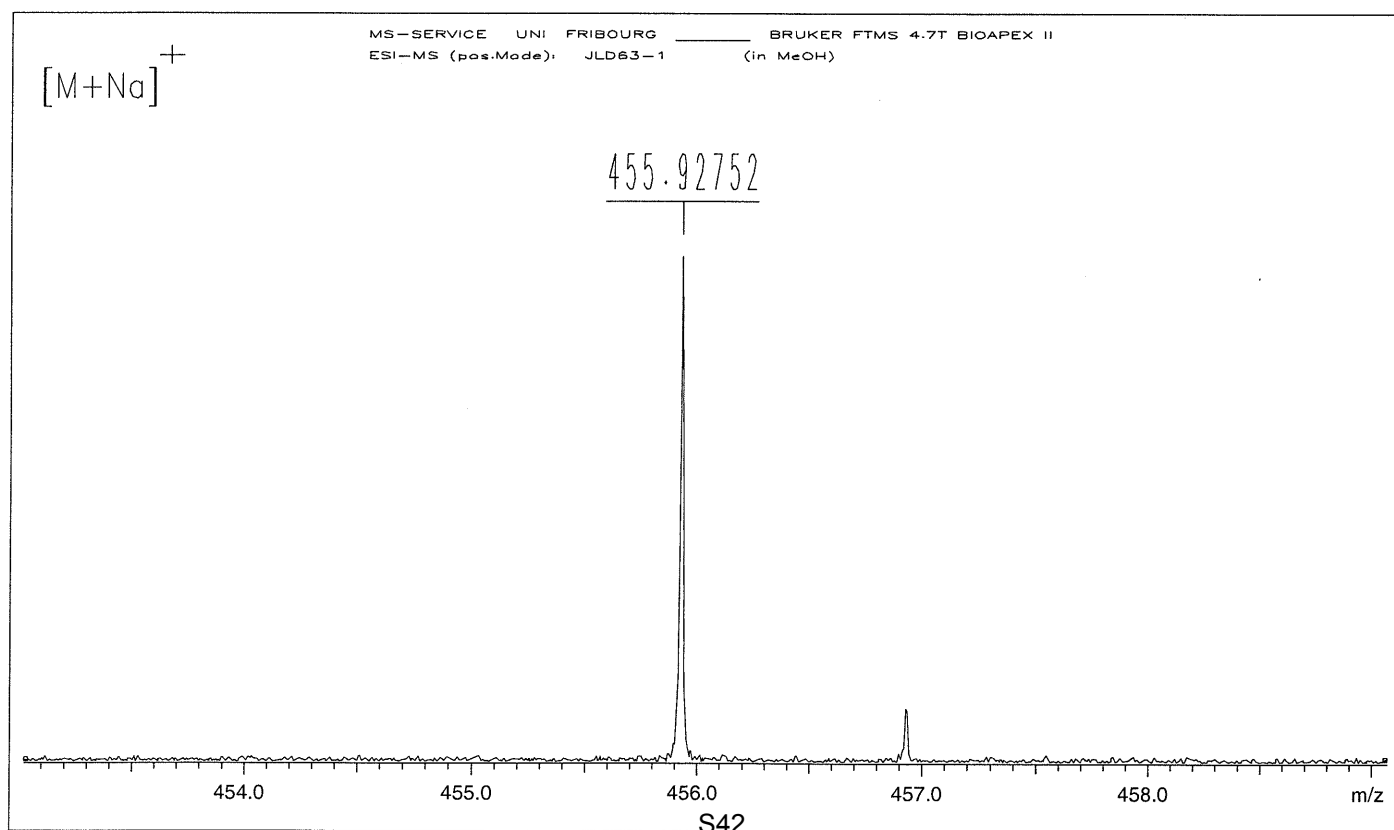
ESI-MS: JLD1452 63-1

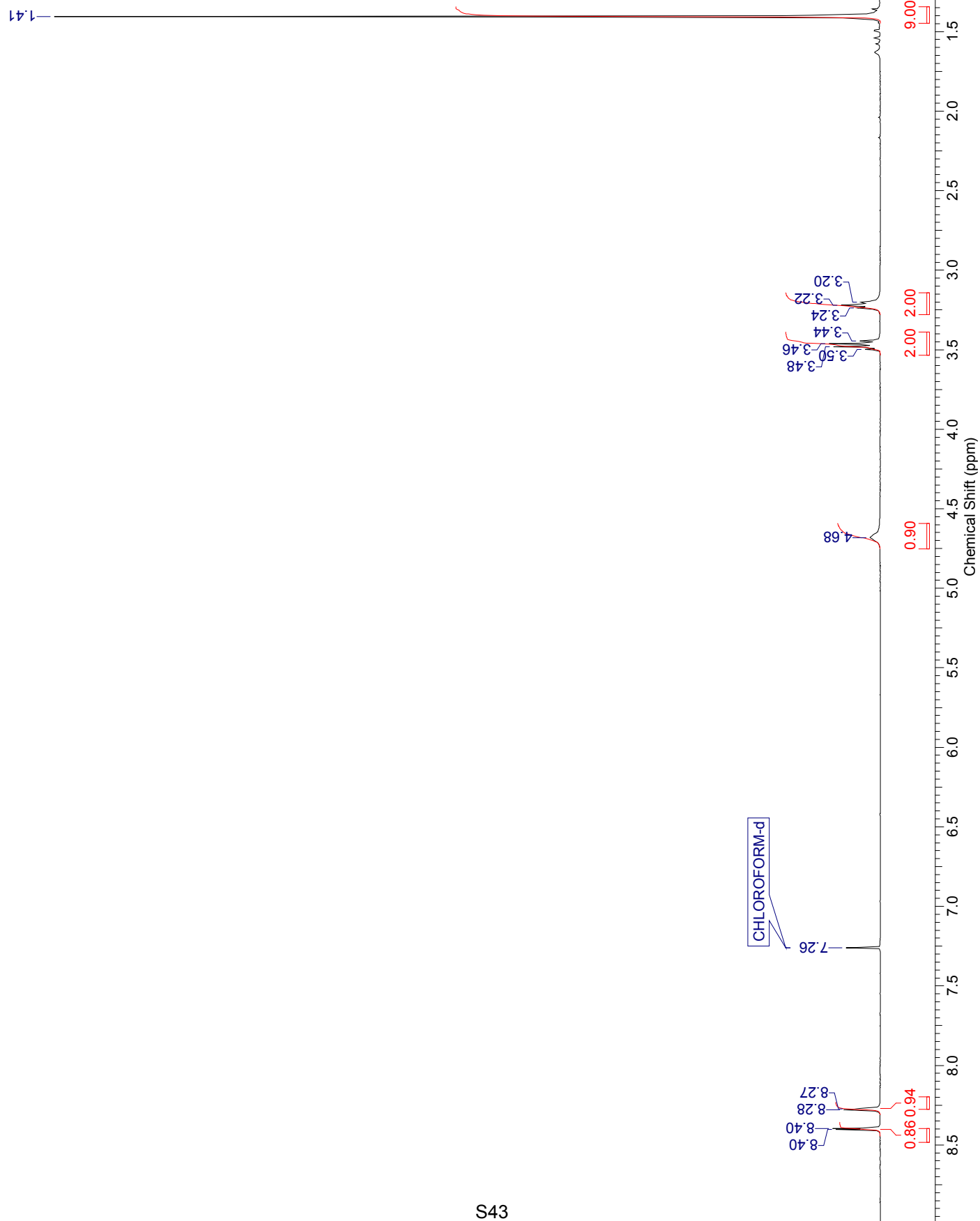
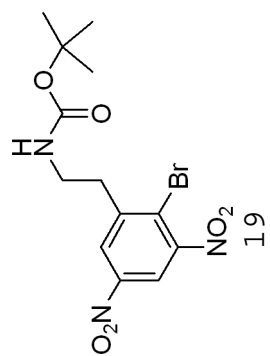
XMASS Mass Analysis for /Data/UNI_FR/DEBI1452_ESI/5/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

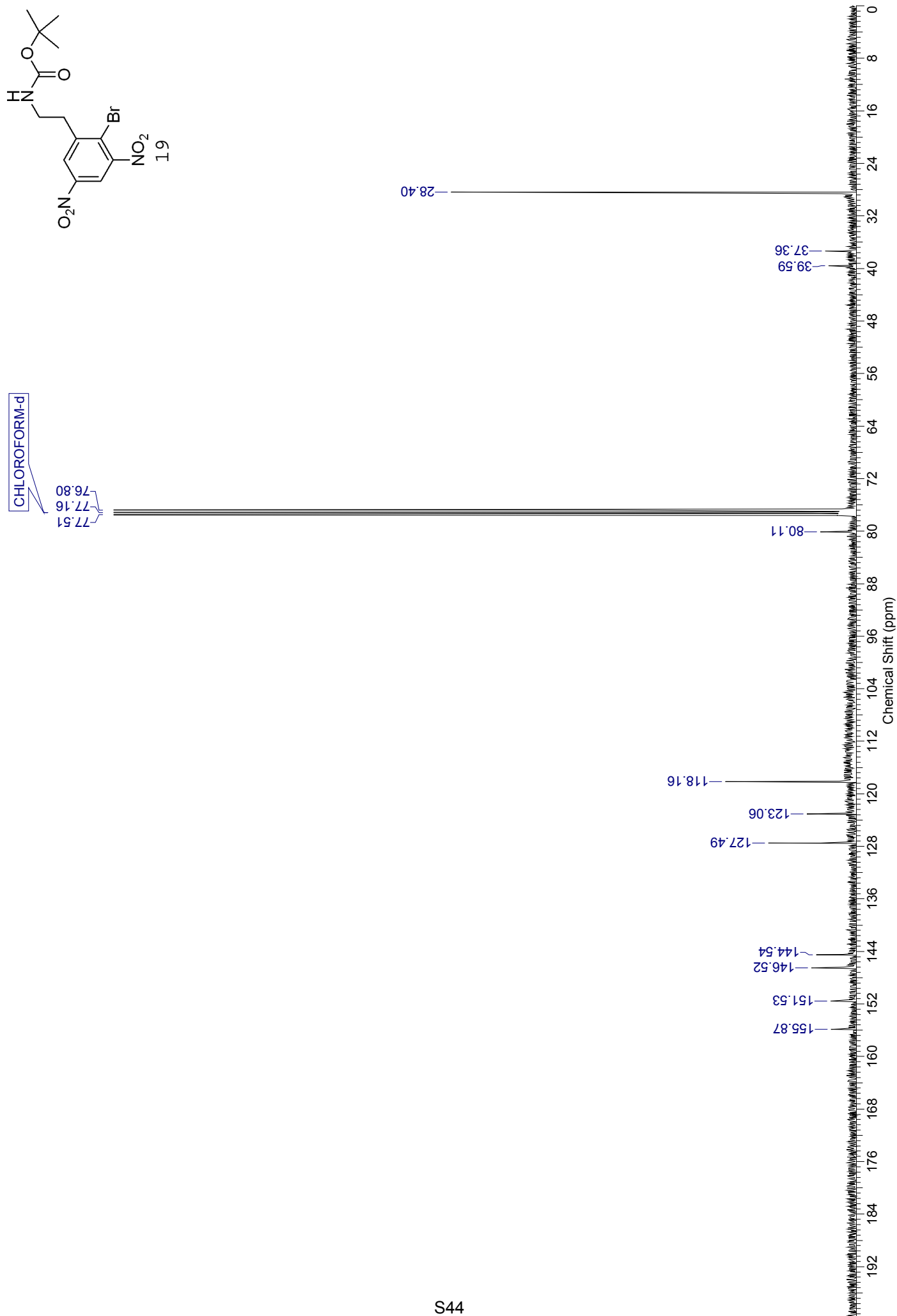
Ion mass = 455.9275210

Charge = +1

#	C	H	F	I	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 455.9275210										
1	10	7	3	1	3	5	1	455.9274690	6.5	5.196e-05
2	9	8	3	1	2	8	0	455.9271943	5.0	3.267e-04
3	6	9	4	1	2	9	0	455.9283371	1.0	8.161e-04
4	7	8	4	1	3	6	1	455.9286119	2.5	1.091e-03
5	13	6	2	1	3	4	1	455.9263262	10.5	1.195e-03
6	15	5	2	1	3	4	0	455.9287315	13.5	1.210e-03
7	12	7	2	1	2	7	0	455.9260514	9.0	1.470e-03
8	7	6	3	1	5	7	0	455.9258516	5.5	1.669e-03
9	12	6	3	1	3	5	0	455.9298743	9.5	2.353e-03
10	6	15	3	2	3	1	0	455.9251091	-1.5	2.412e-03

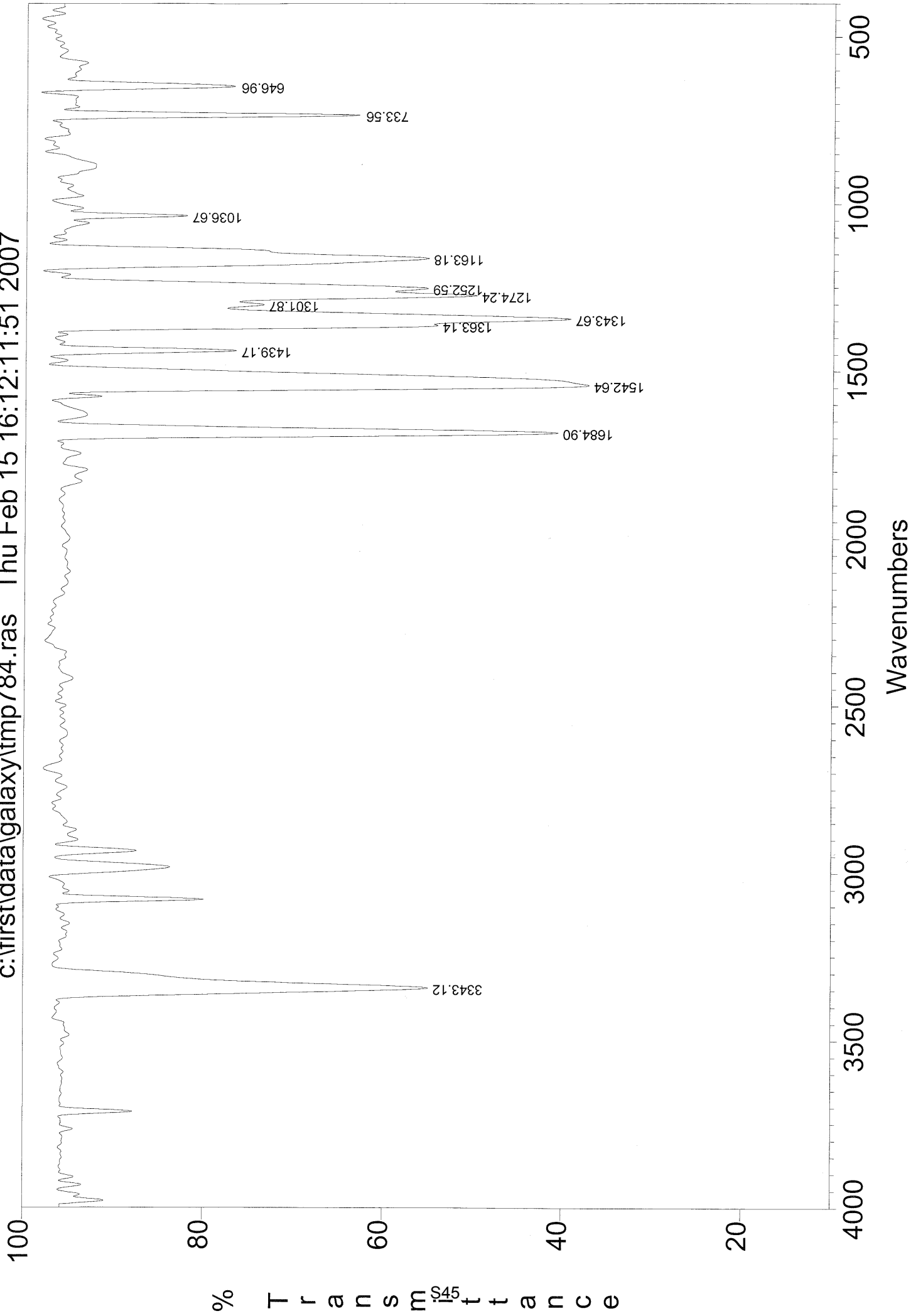






900 68

c:\first\data\galaxy\tmp784.ras Thu Feb 15 16:12:11:51 2007



% Transmittance

ESI-MS: JLD83-1

XMASS Mass Analysis for /Data/UNI_FR/DEBI1807_ESI/5/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

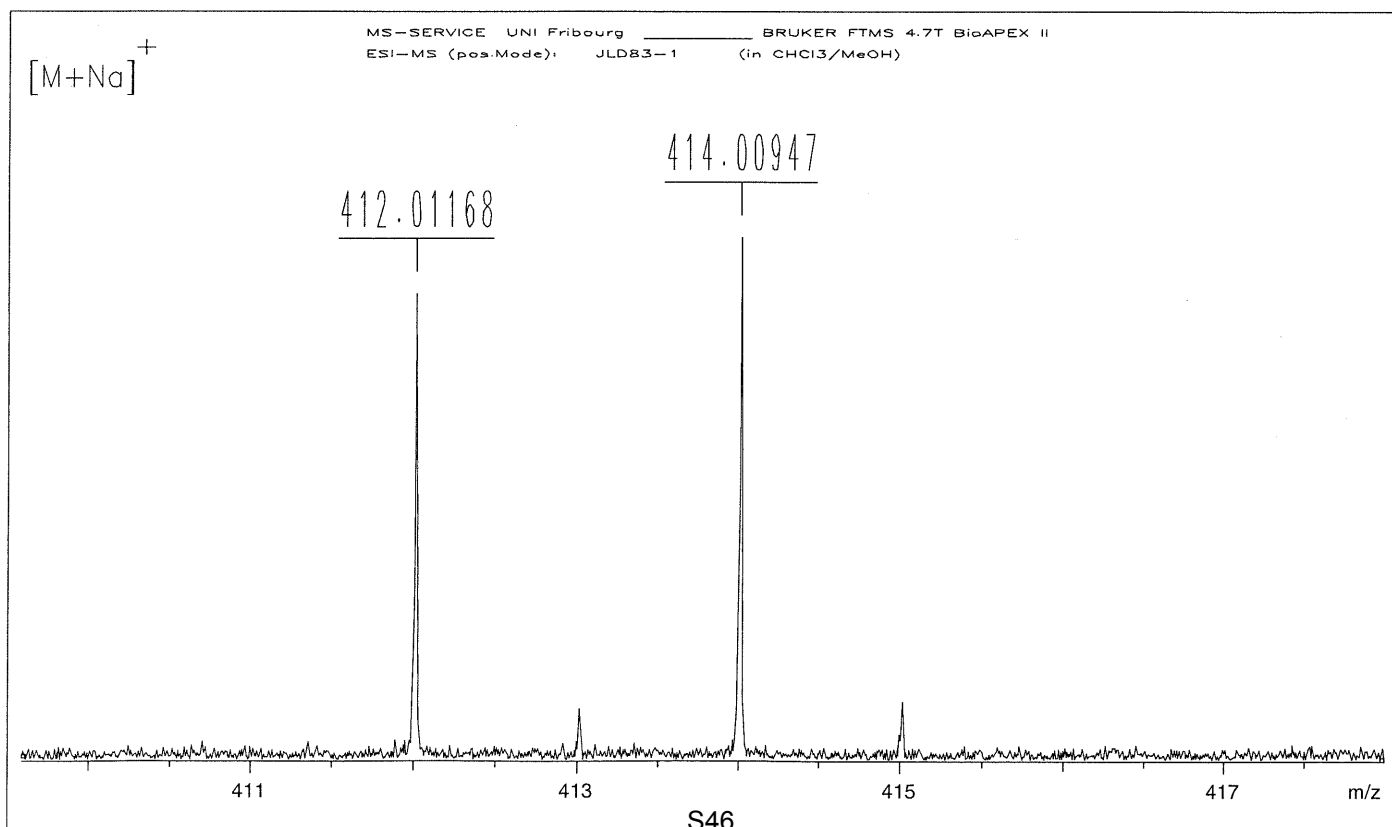
Ion mass [1] = 414.0094680

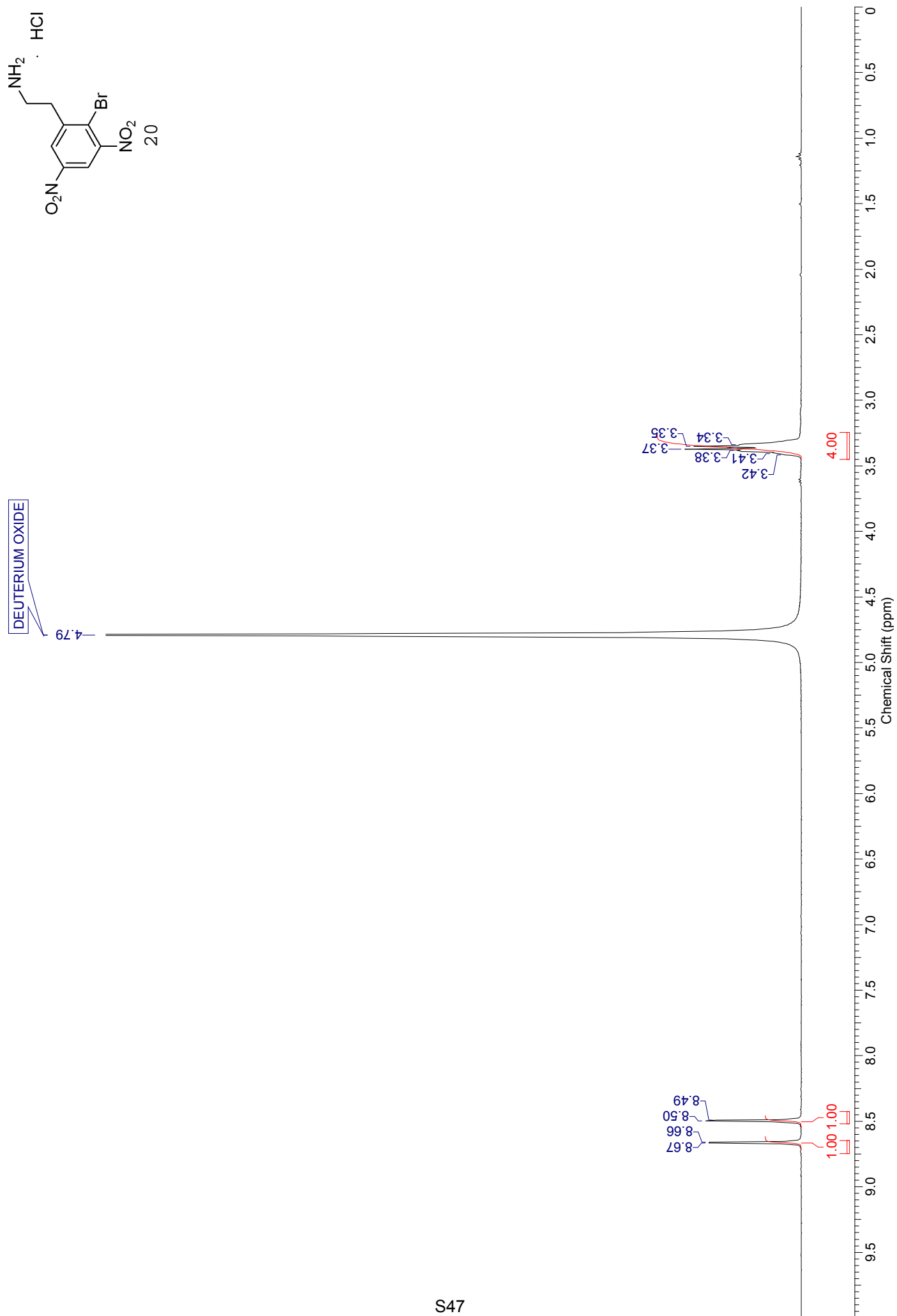
Ion mass [2] = 412.0116840

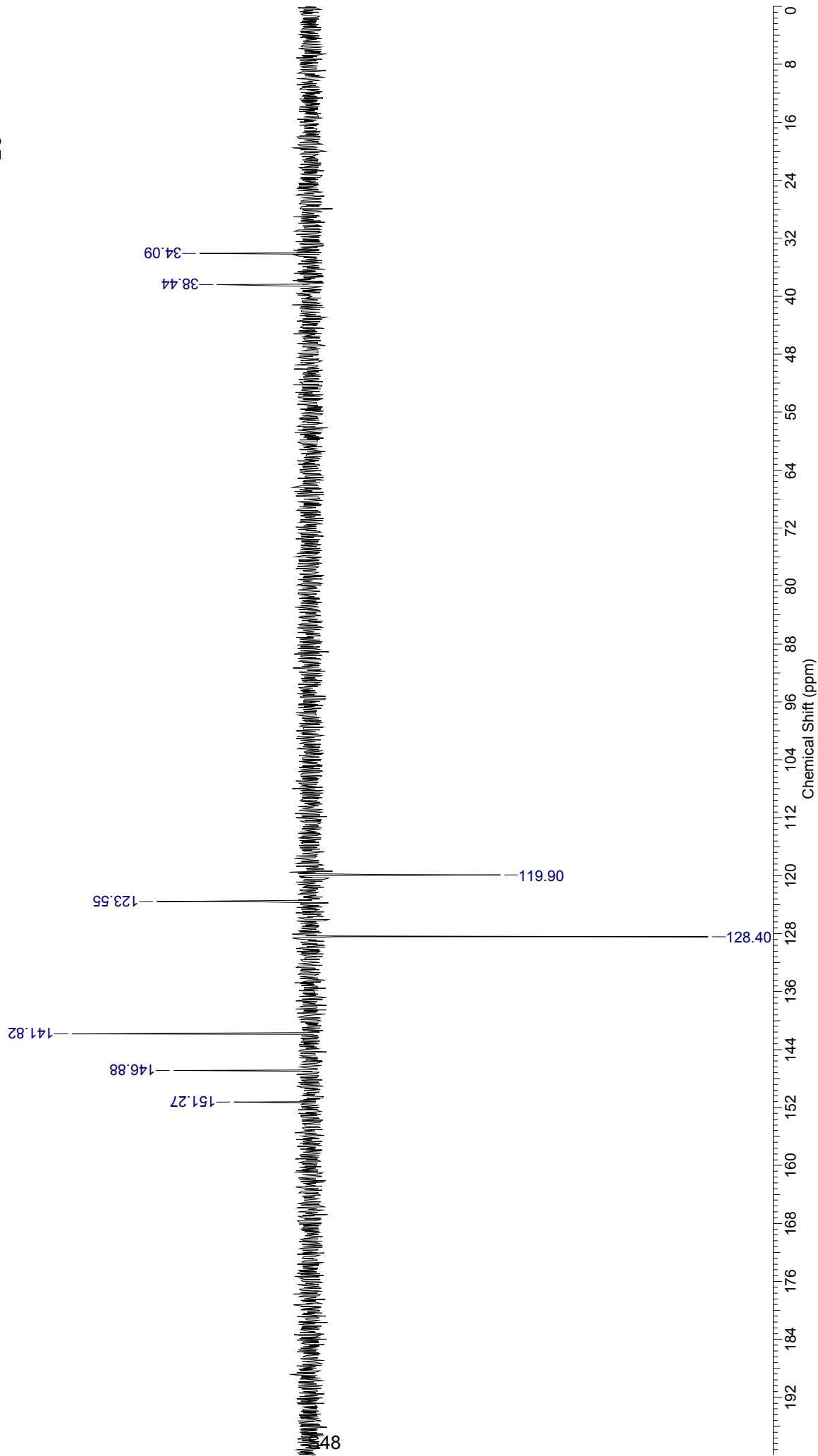
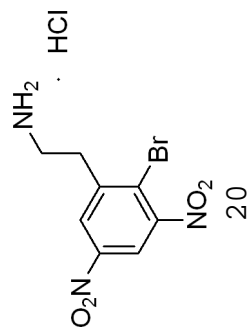
Charge = +1

#	C	H	79Br	81Br	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 414.0094680										
1	13	16	0	1	3	6	1	414.0094224	6.5	4.565e-05
2	14	24	1	1	1	3	0	414.0096987	2.5	2.307e-04
3	18	13	1	0	3	4	0	414.0083949	13.5	1.073e-03
4	12	25	1	1	1	3	1	414.0072934	-0.5	2.175e-03
5	15	15	0	1	3	6	0	414.0118276	9.5	2.360e-03

*** Mass Analysis for mass 412.0116840										
1	13	16	1	0	3	6	1	412.0114690	6.5	2.150e-04
2	19	13	0	1	3	3	0	412.0114337	14.5	2.503e-04
3	15	15	1	0	3	6	0	412.0138742	9.5	2.190e-03
4	16	14	1	0	4	3	1	412.0141490	11.0	2.465e-03
5	23	5	0	0	2	5	1	412.0090674	22.0	2.617e-03

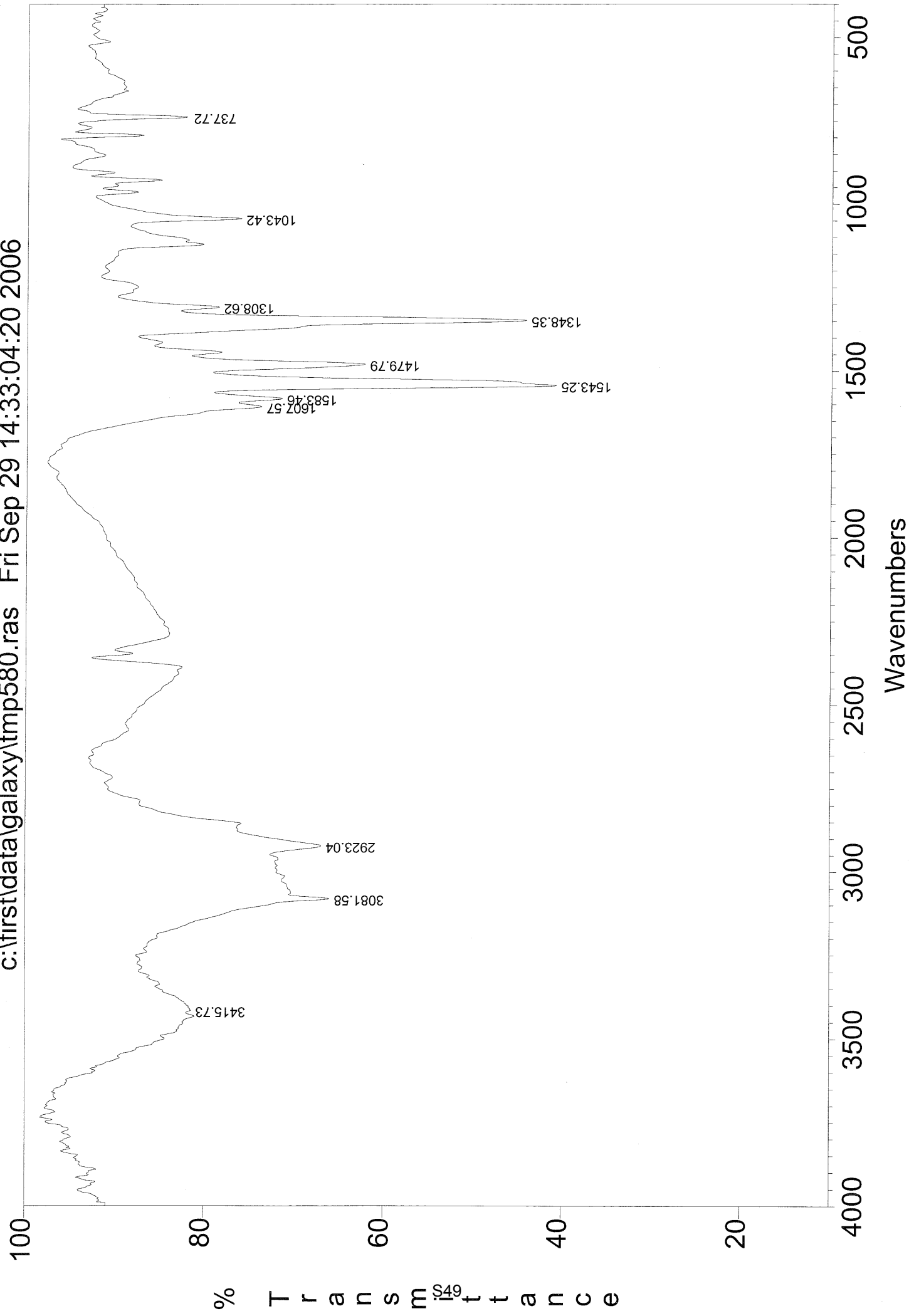






100%

c:\first\data\galaxy\tmp580.ras Fri Sep 29 14:33:04:20 2006



ESI-MS: JLD87-2

XMASS Mass Analysis for /Data/UNI_FR/DEBI1827_ESI/3/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

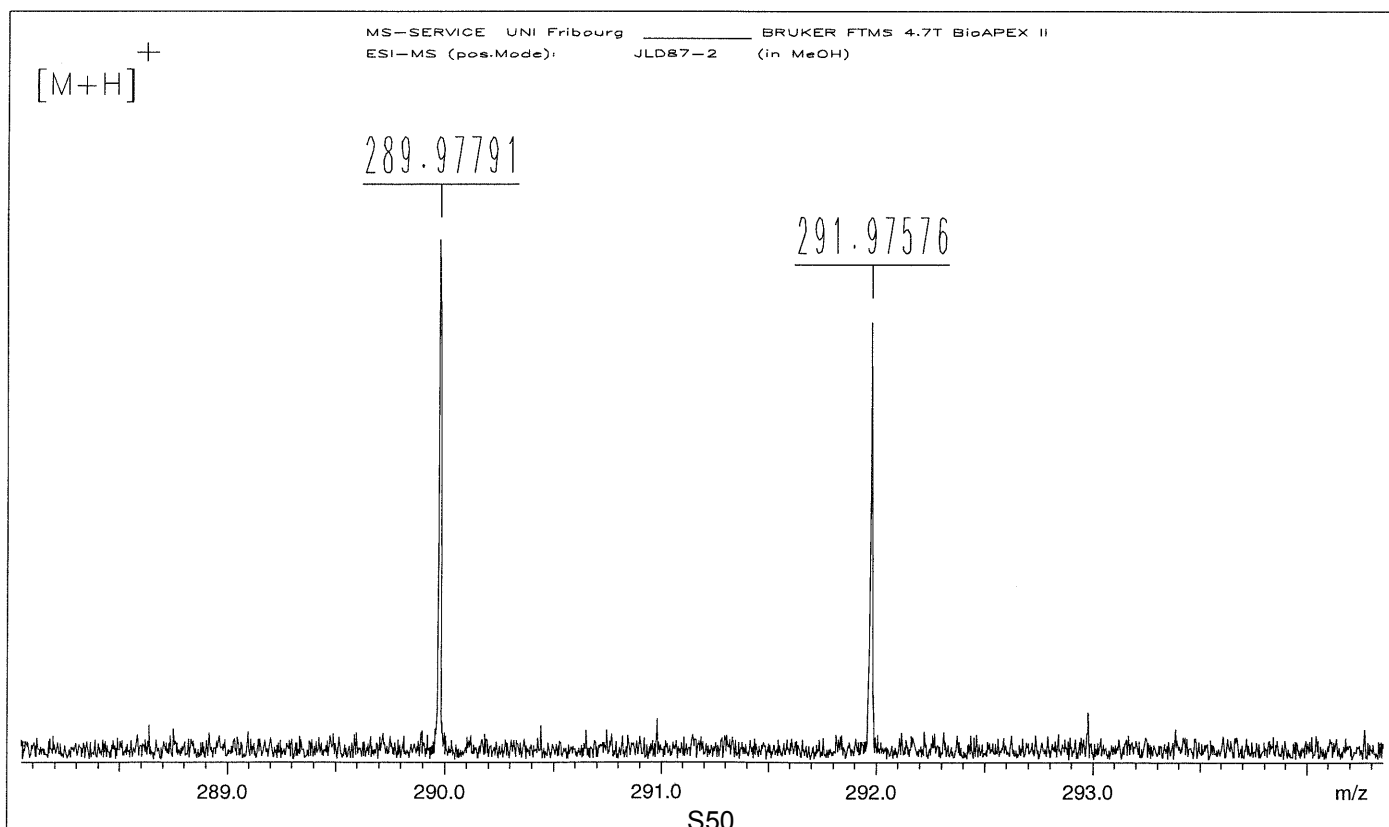
Ion mass [1] = 289.9779100

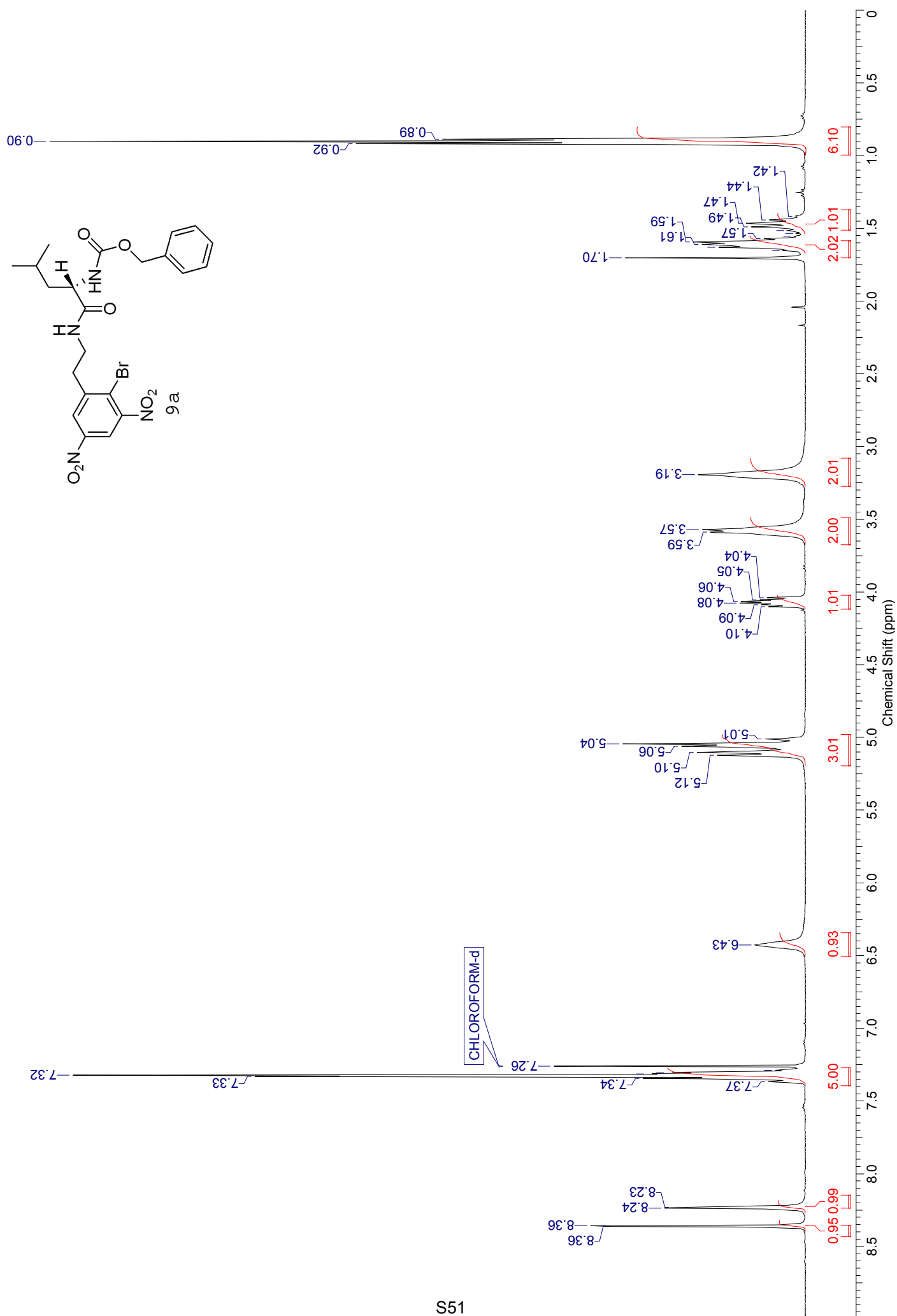
Ion mass [2] = 291.9757640

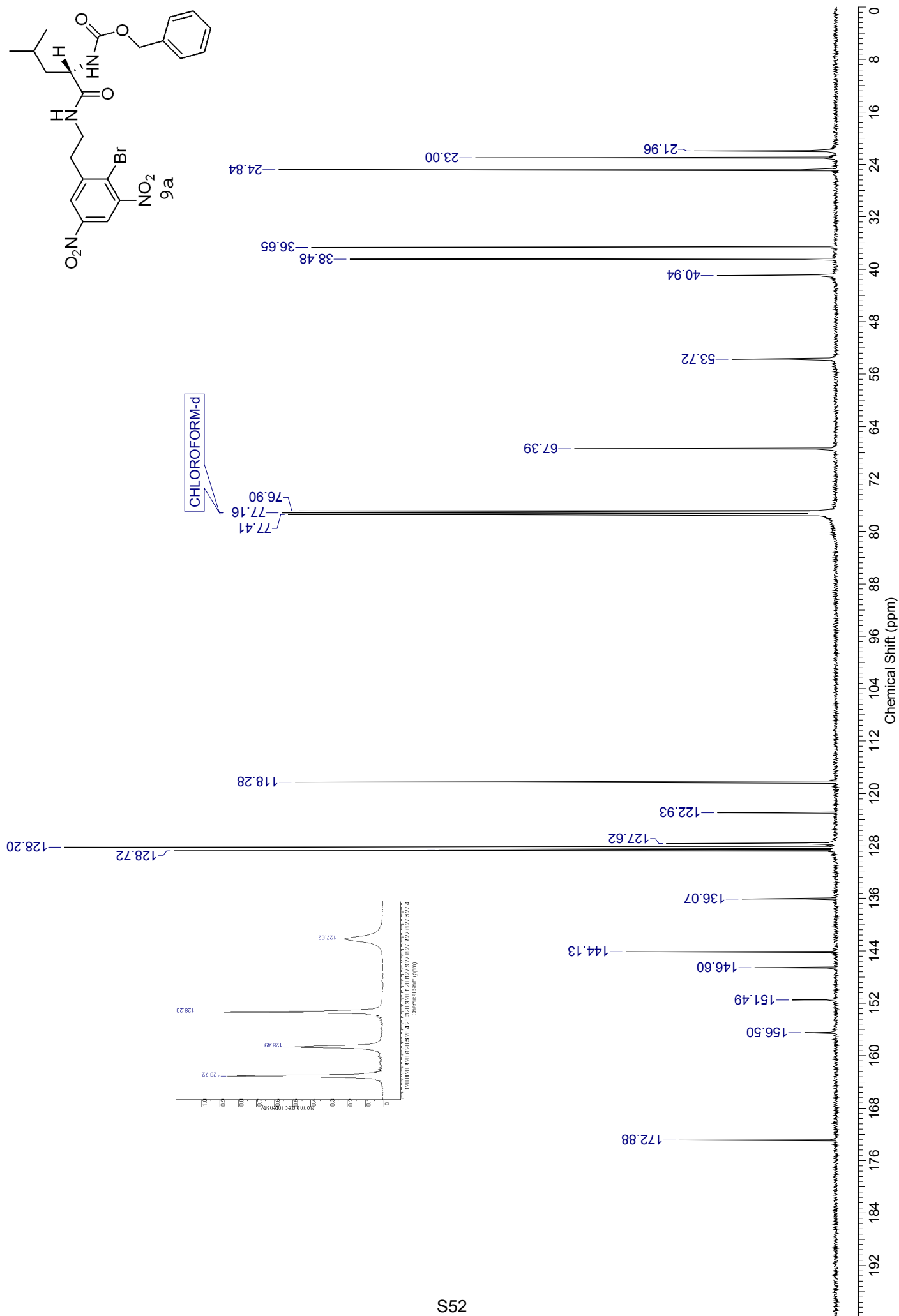
Charge = +1

#	C	H	79Br	81Br	N	O	mass	DBE	error
*** Mass Analysis for mass 289.9779100									
1	8	9	1	0	3	4	289.9770948	5.5	8.152e-04
2	11	7	1	0	4	1	289.9797749	10.0	1.865e-03
3	13	9	1	0	1	2	289.9811176	9.5	3.208e-03
4	12	7	0	1	3	1	289.9746543	10.5	3.256e-03
5	8	9	0	1	4	3	289.9832076	6.0	5.298e-03

*** Mass Analysis for mass 291.9757640									
1	8	9	0	1	3	4	291.9750482	5.5	7.158e-04
2	11	7	0	1	4	1	291.9777283	10.0	1.964e-03
3	7	18	1	1	1	1	291.9729192	-1.5	2.845e-03
4	13	9	0	1	1	2	291.9790710	9.5	3.307e-03
5	11	7	1	0	3	2	291.9716155	9.5	4.148e-03

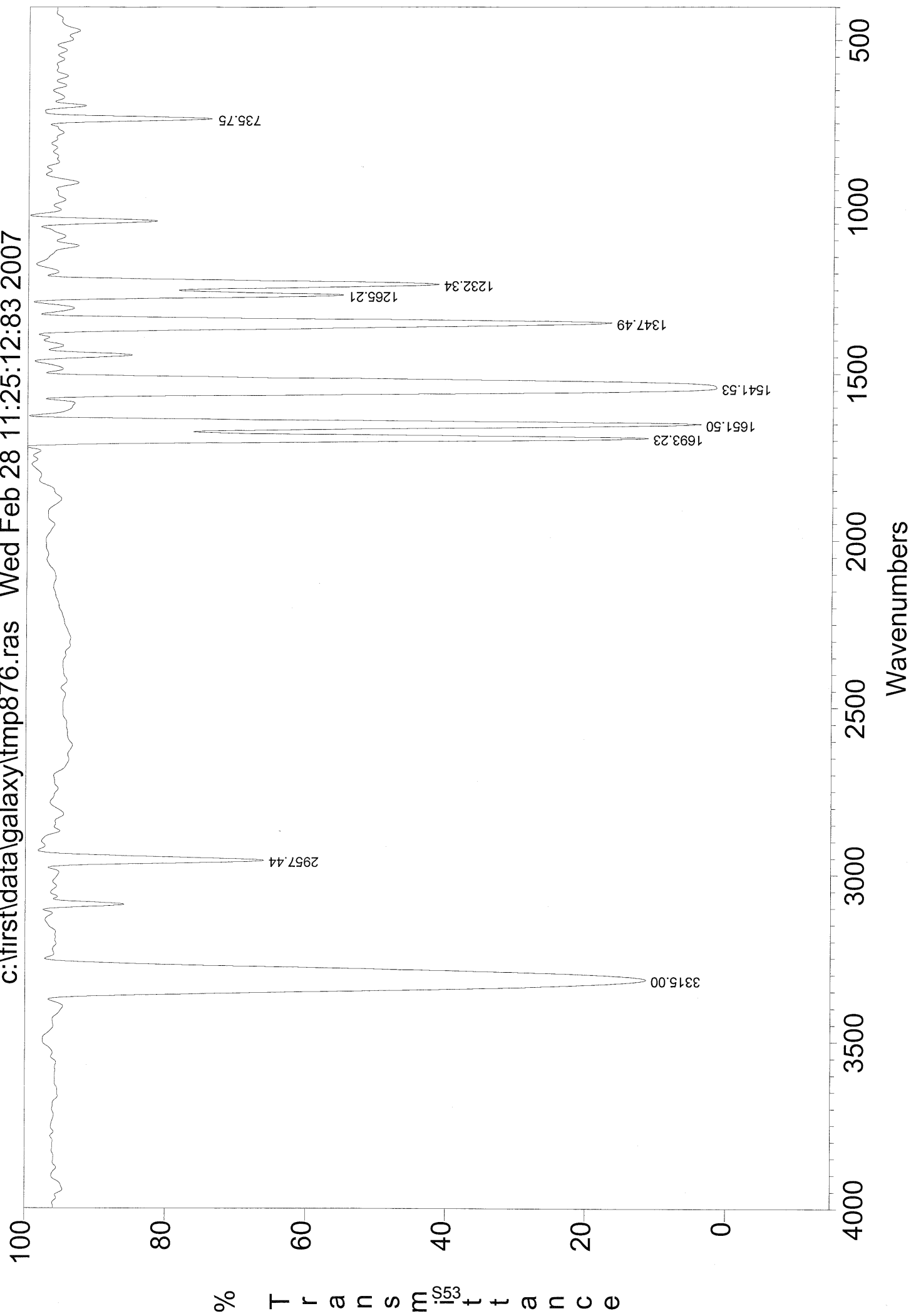






507105

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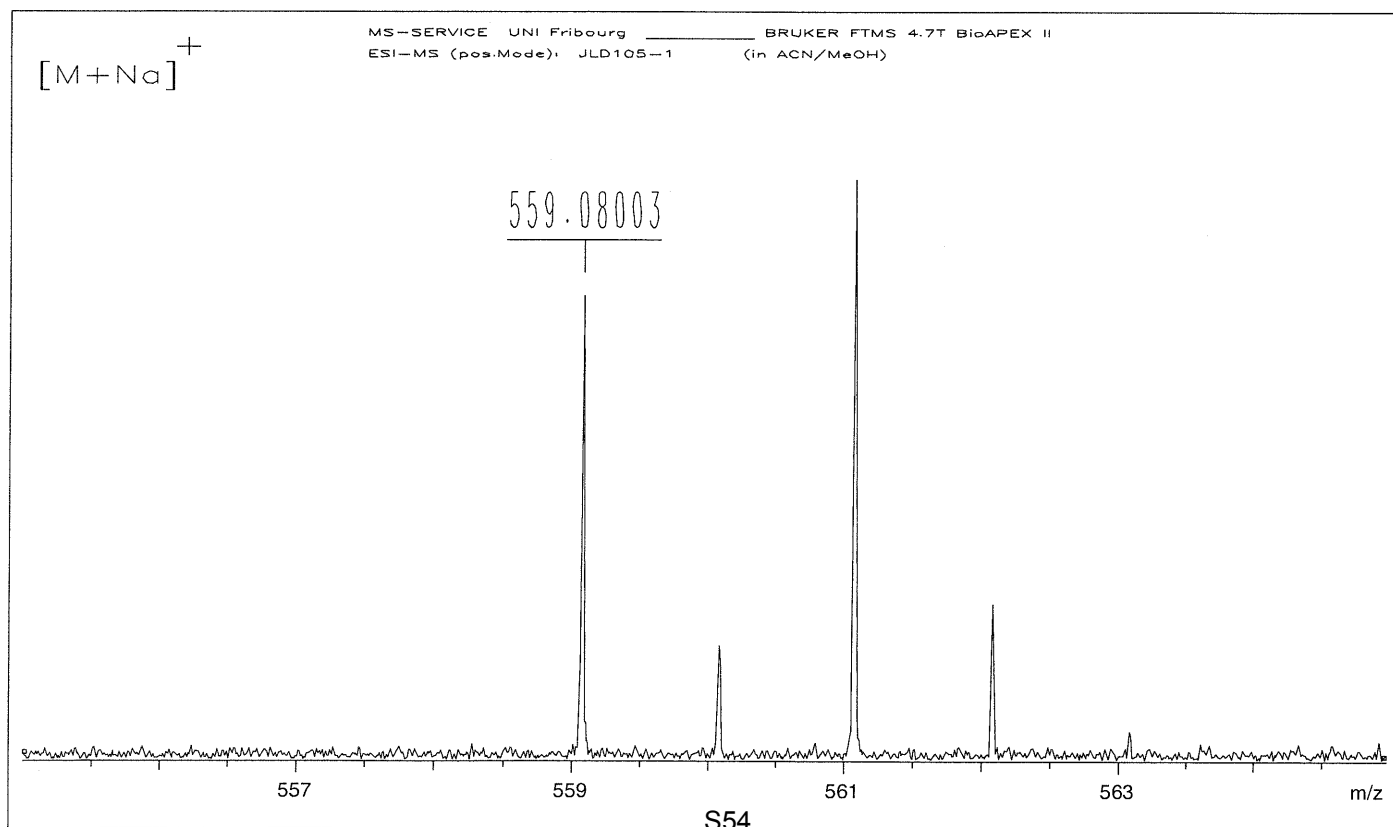
ESI-MS: JLD105-1

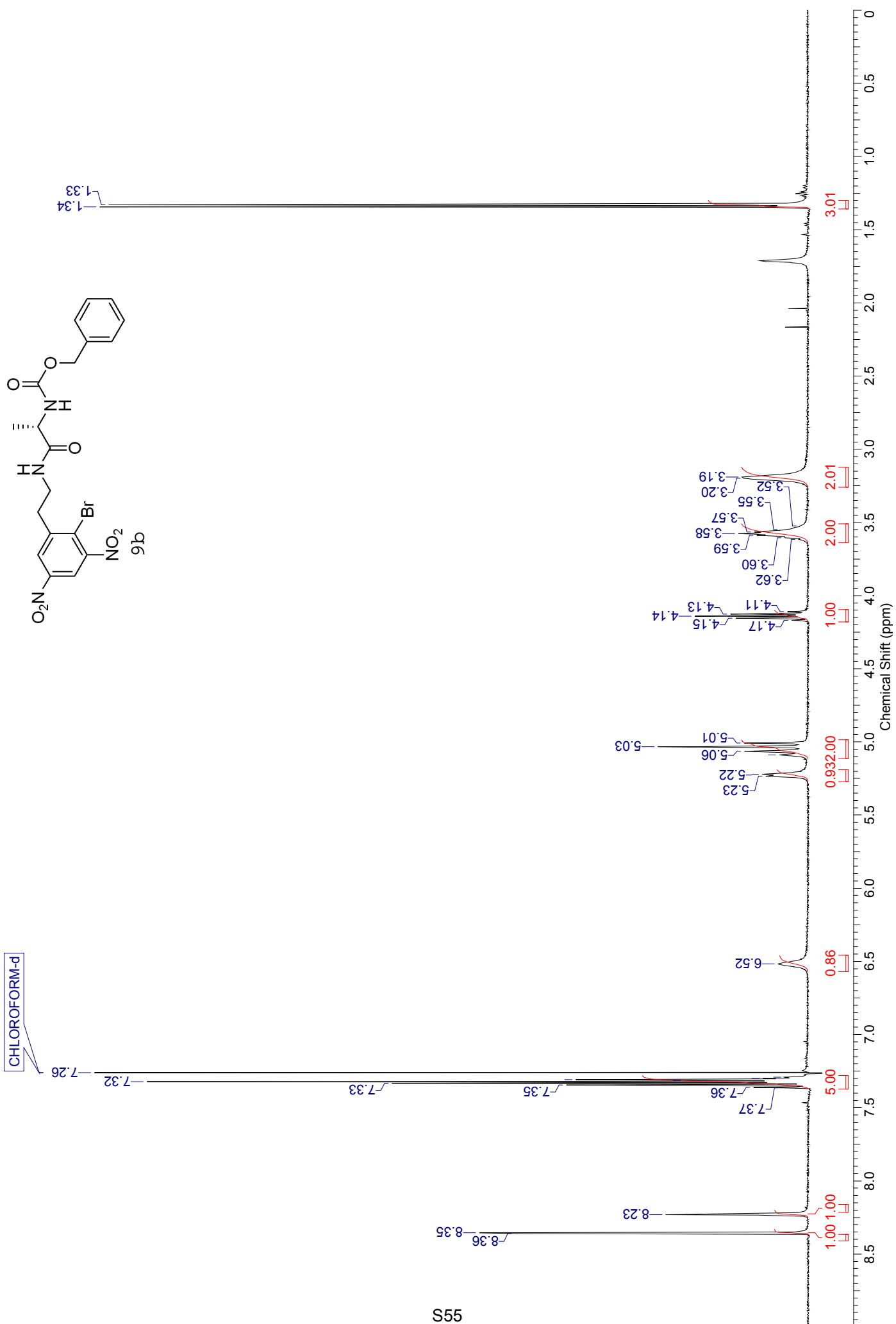
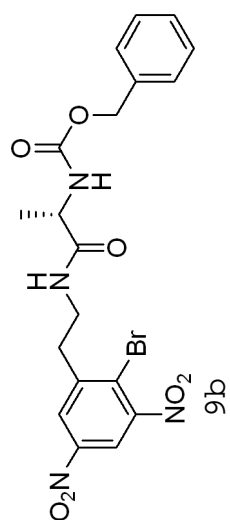
XMASS Mass Analysis for /Data/UNI_FR/DEBI2631_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

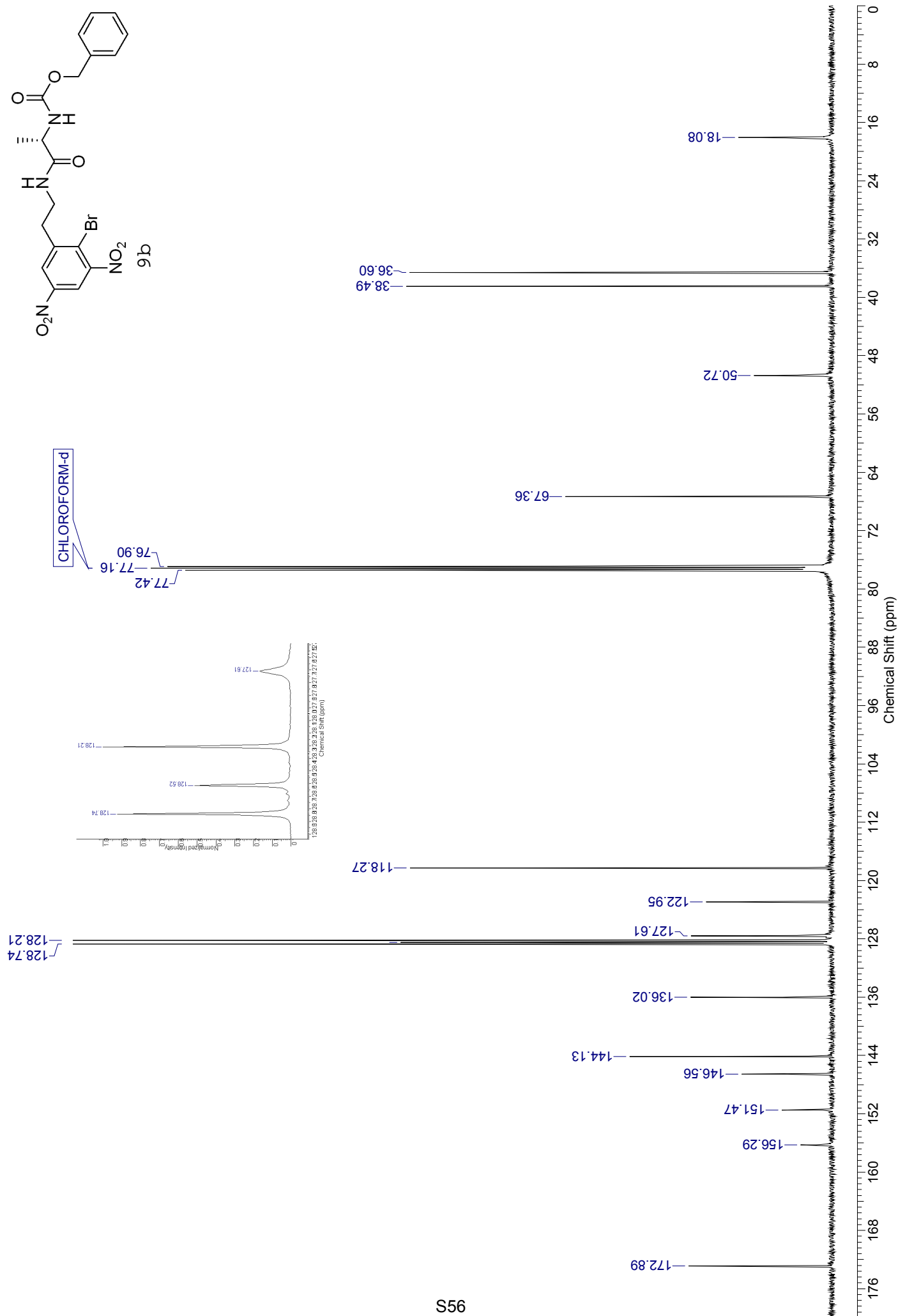
Ion mass = 559.0800340

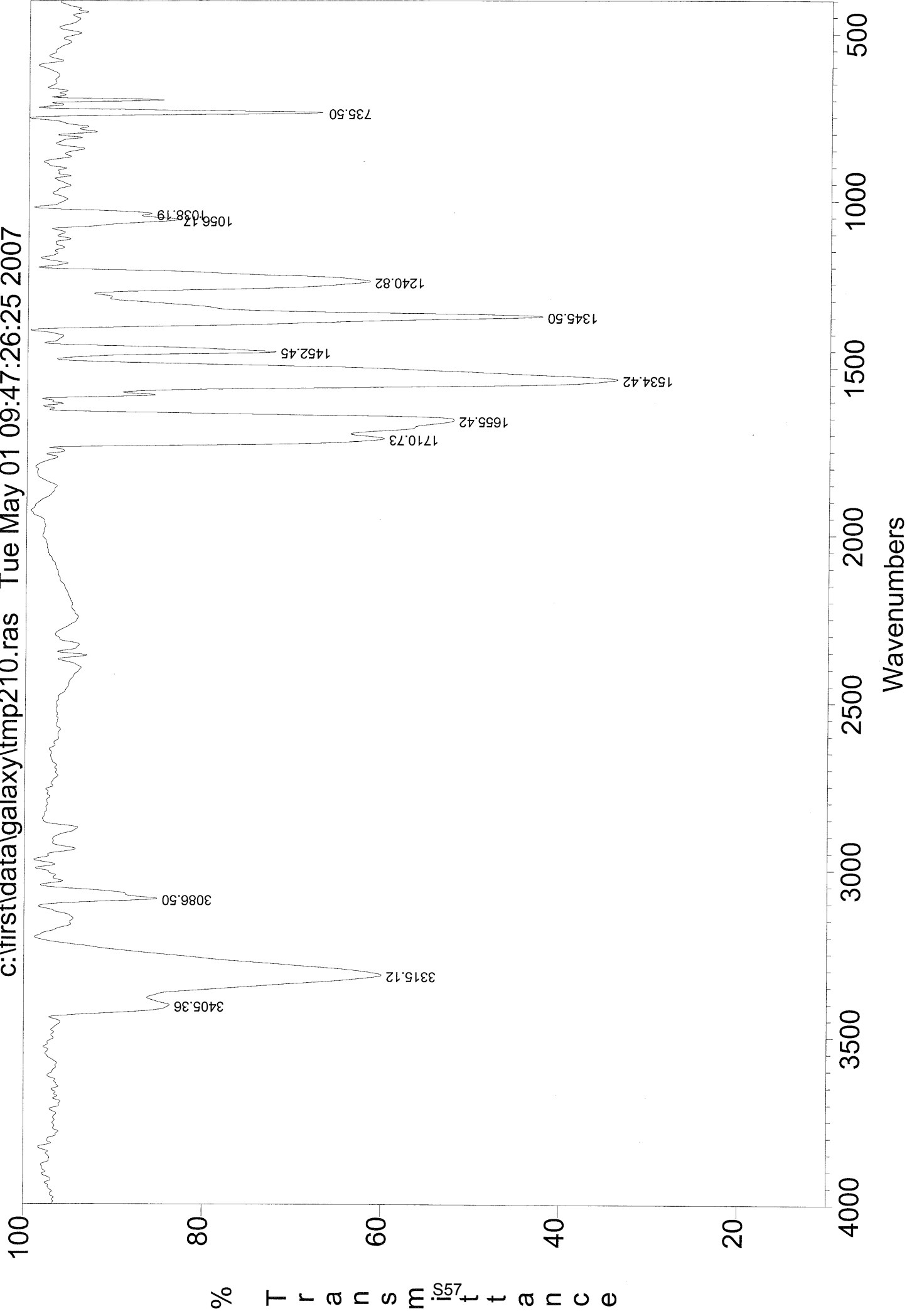
Charge = +1

#	C	H	79Br	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 559.0800340									
1	22	25	1	4	7	1	559.0798829	11.5	1.511e-04
2	24	24	1	4	7	0	559.0822882	14.5	2.254e-03
3	25	23	1	5	4	1	559.0825629	16.0	2.529e-03
4	18	33	2	4	6	0	559.0761364	3.5	3.898e-03
5	14	35	2	5	8	0	559.0846897	-1.0	4.656e-03
6	27	22	1	5	4	0	559.0849682	19.0	4.934e-03
7	17	36	2	3	6	1	559.0863072	0.0	6.273e-03
8	28	22	1	3	5	0	559.0737349	19.0	6.299e-03
9	16	34	2	4	6	1	559.0737311	0.5	6.303e-03
10	19	35	2	3	6	0	559.0887125	3.0	8.678e-03









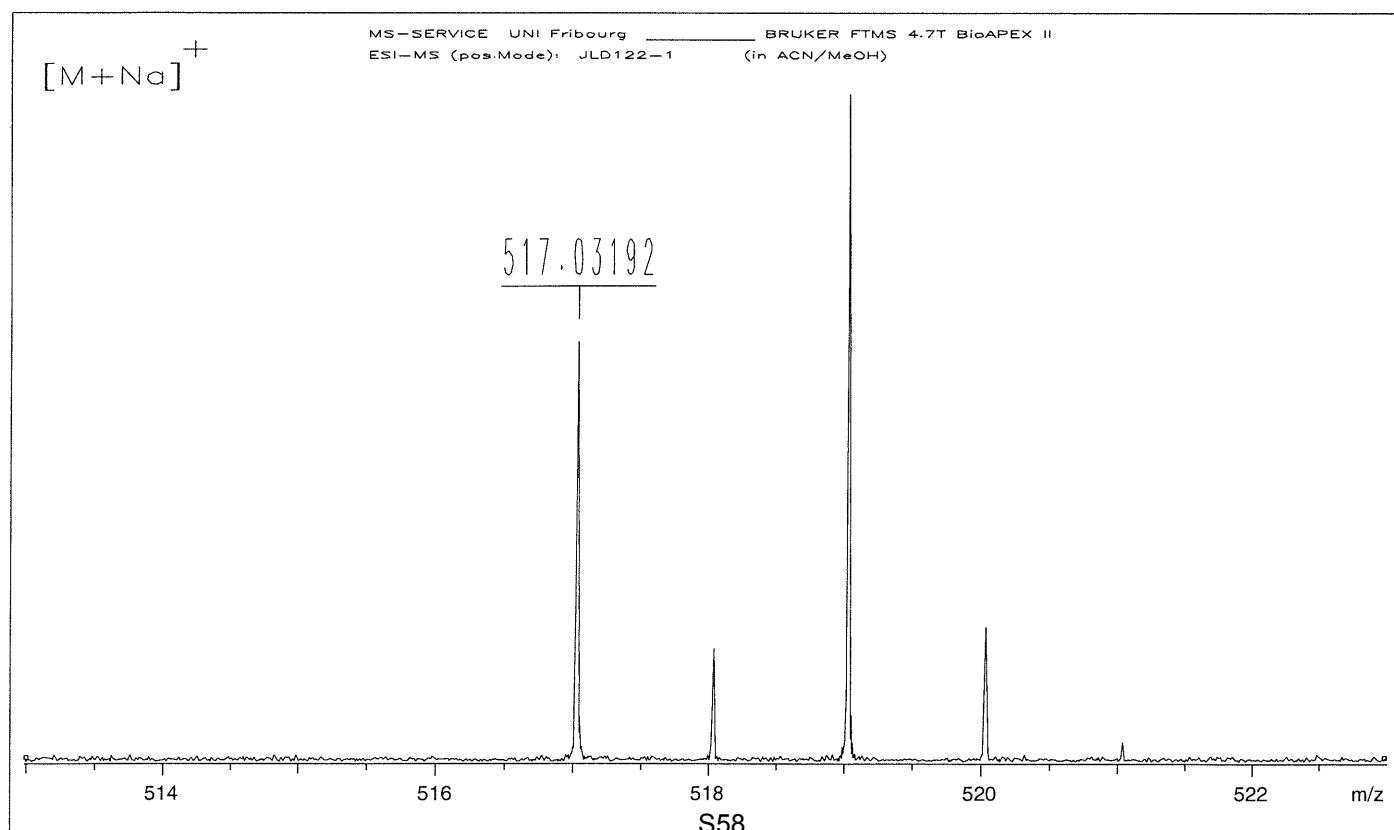
ESI-MS: JLD122-1

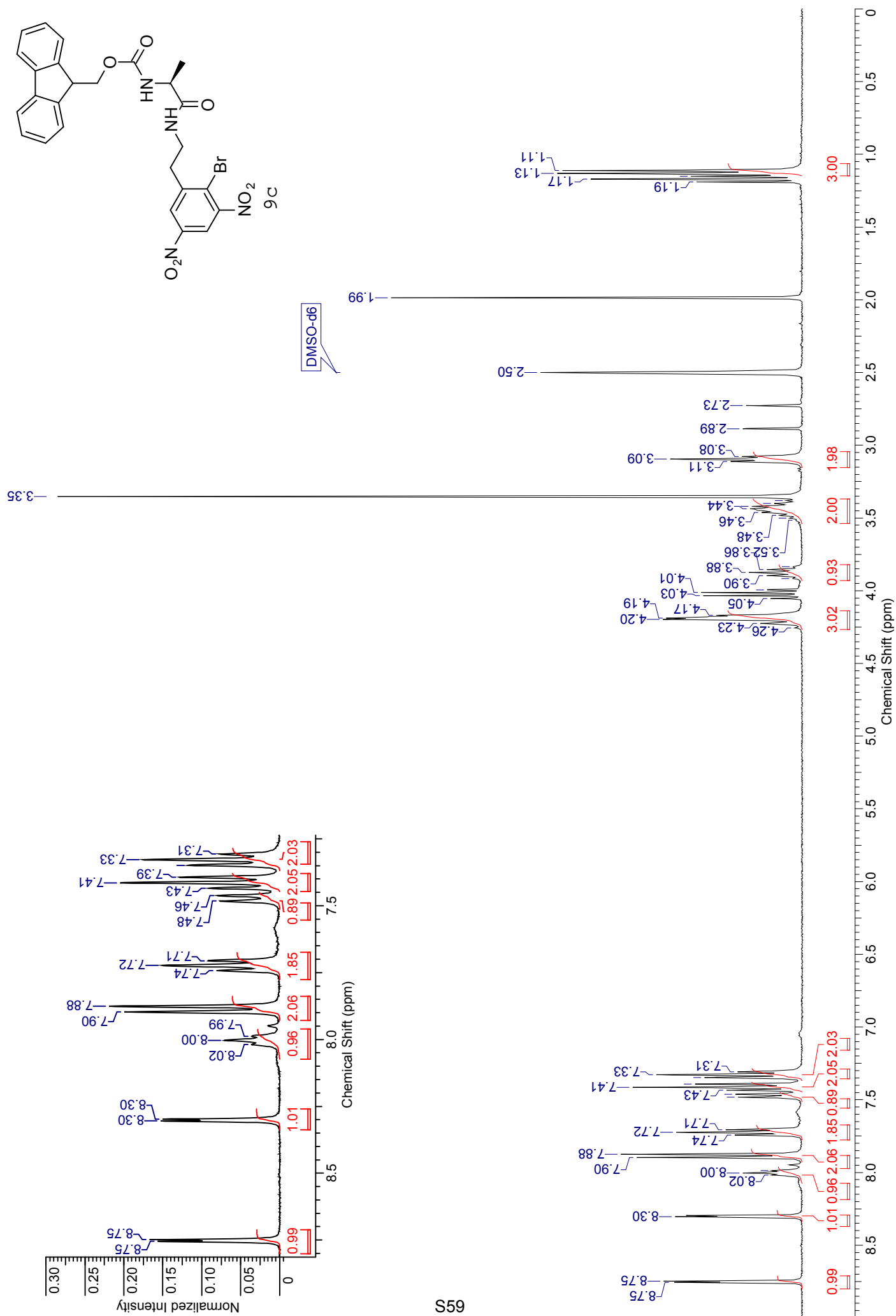
XMASS Mass Analysis for /Data/UNI_FR/DEBI2620_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

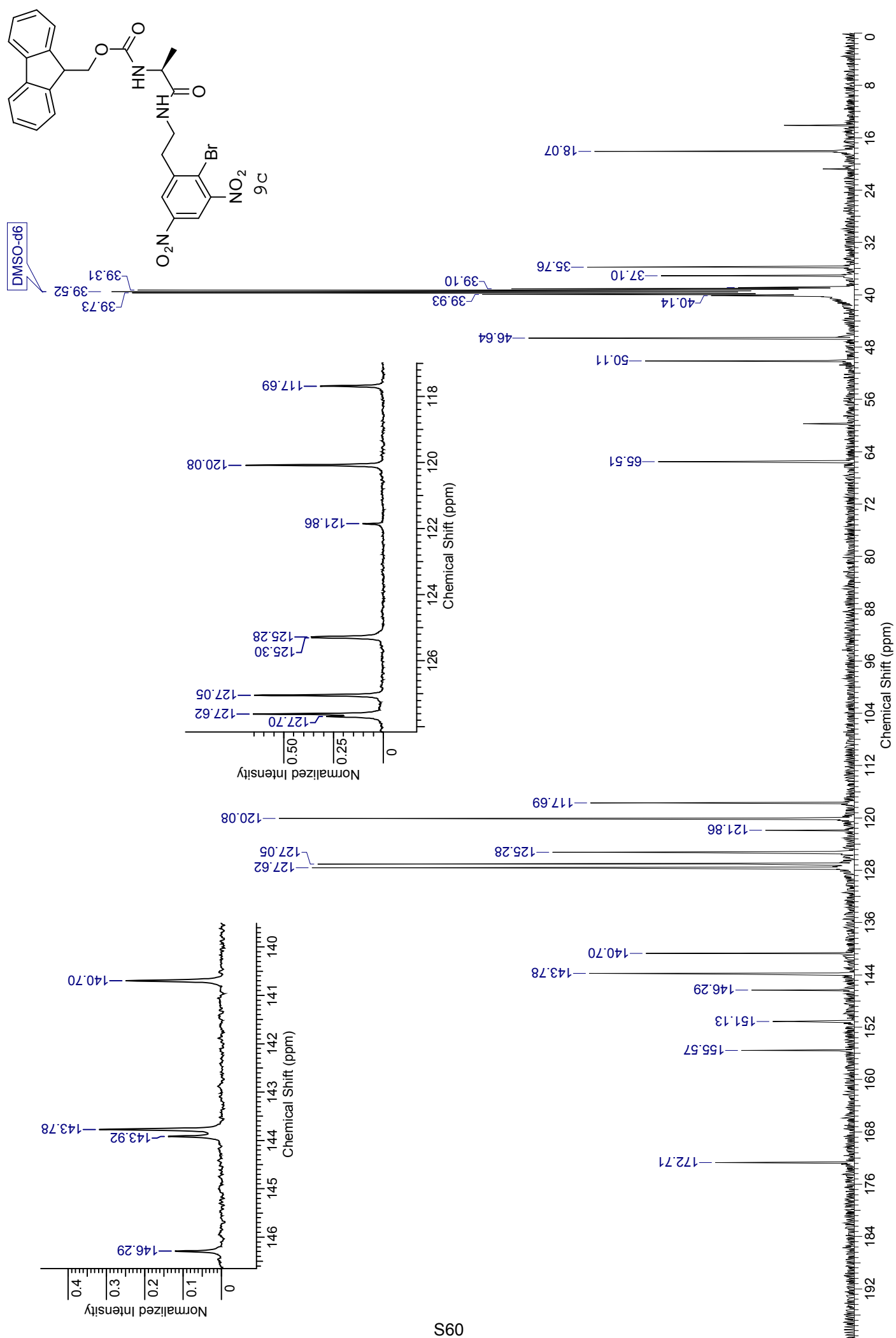
Ion mass = 517.0319240

Charge = +1

#	C	H	79Br	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 517.0319240									
1	19	19	1	4	7	1	517.0329327	11.5	1.009e-03
2	15	27	2	4	6	0	517.0291862	3.5	2.738e-03
3	21	18	1	4	7	0	517.0353380	14.5	3.414e-03
4	22	17	1	5	4	1	517.0356128	16.0	3.689e-03
5	25	16	1	3	5	0	517.0267847	19.0	5.139e-03
6	13	28	2	4	6	1	517.0267809	0.5	5.143e-03
7	11	29	2	5	8	0	517.0377396	-1.0	5.816e-03
8	24	16	1	5	4	0	517.0380180	19.0	6.094e-03
9	14	30	2	3	6	1	517.0393570	0.0	7.433e-03
10	23	17	1	3	5	1	517.0243794	16.0	7.545e-03







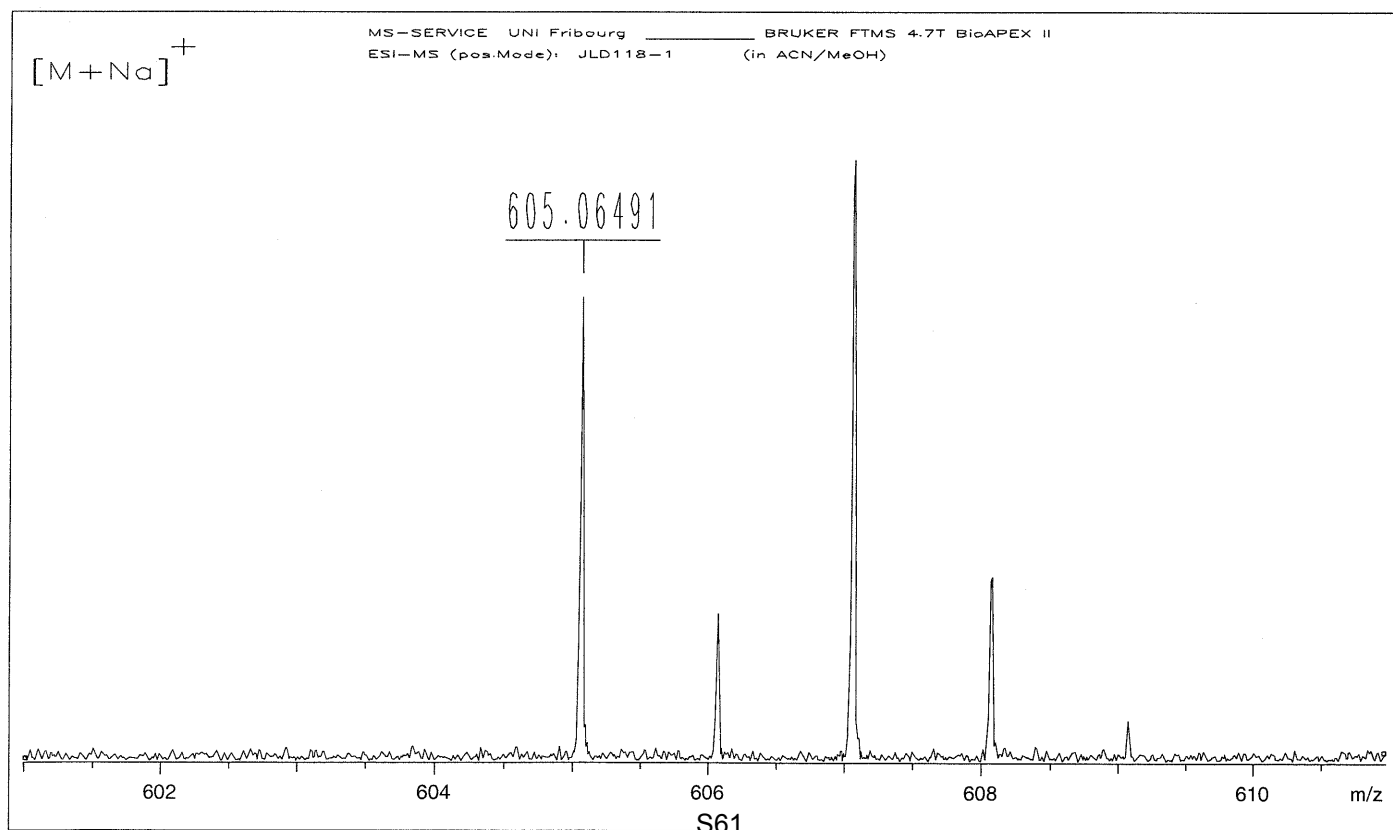
ESI-MS: JLD118-1

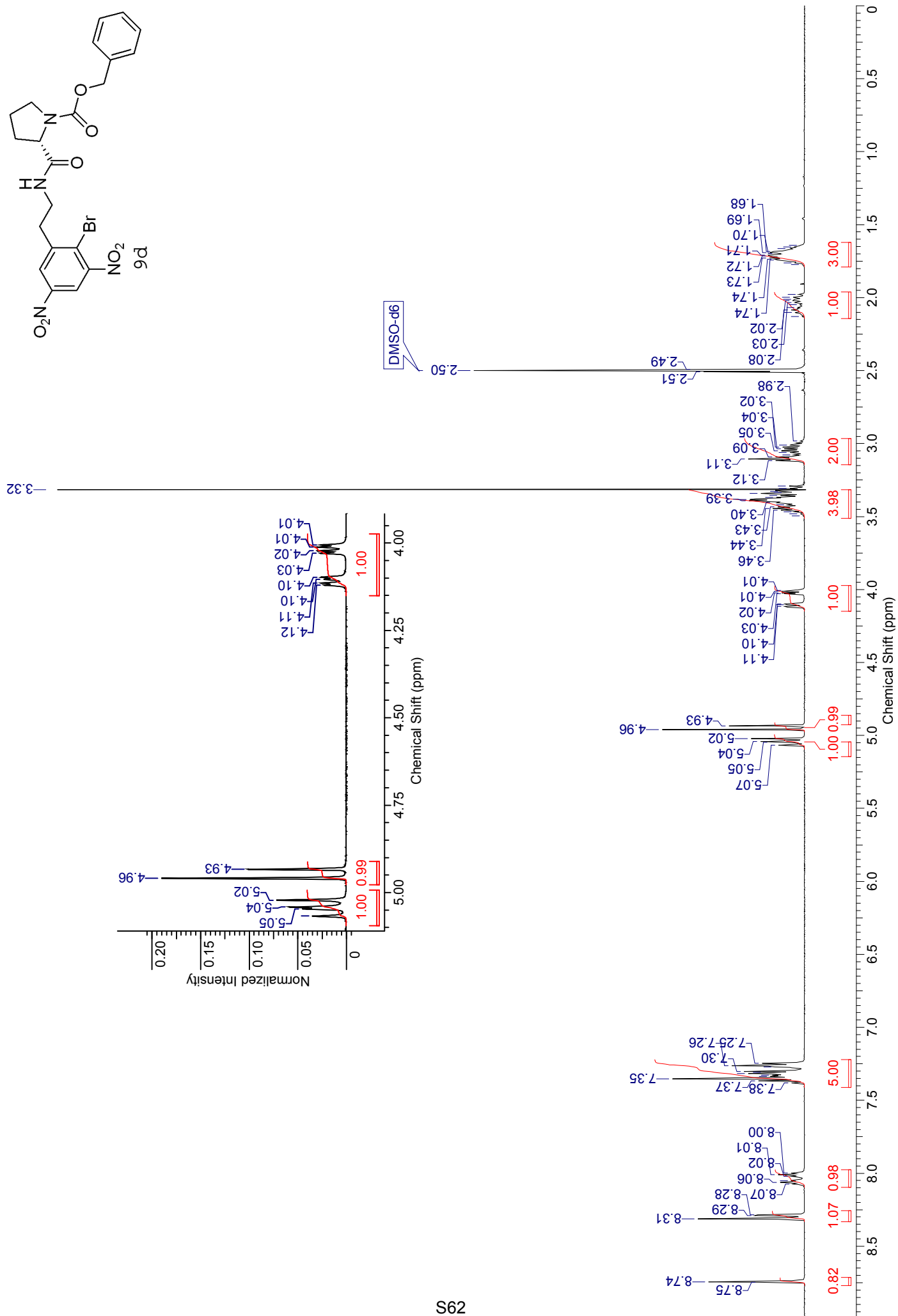
XMASS Mass Analysis for /Data/UNI_FR/DEBI2622_ESI/20/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

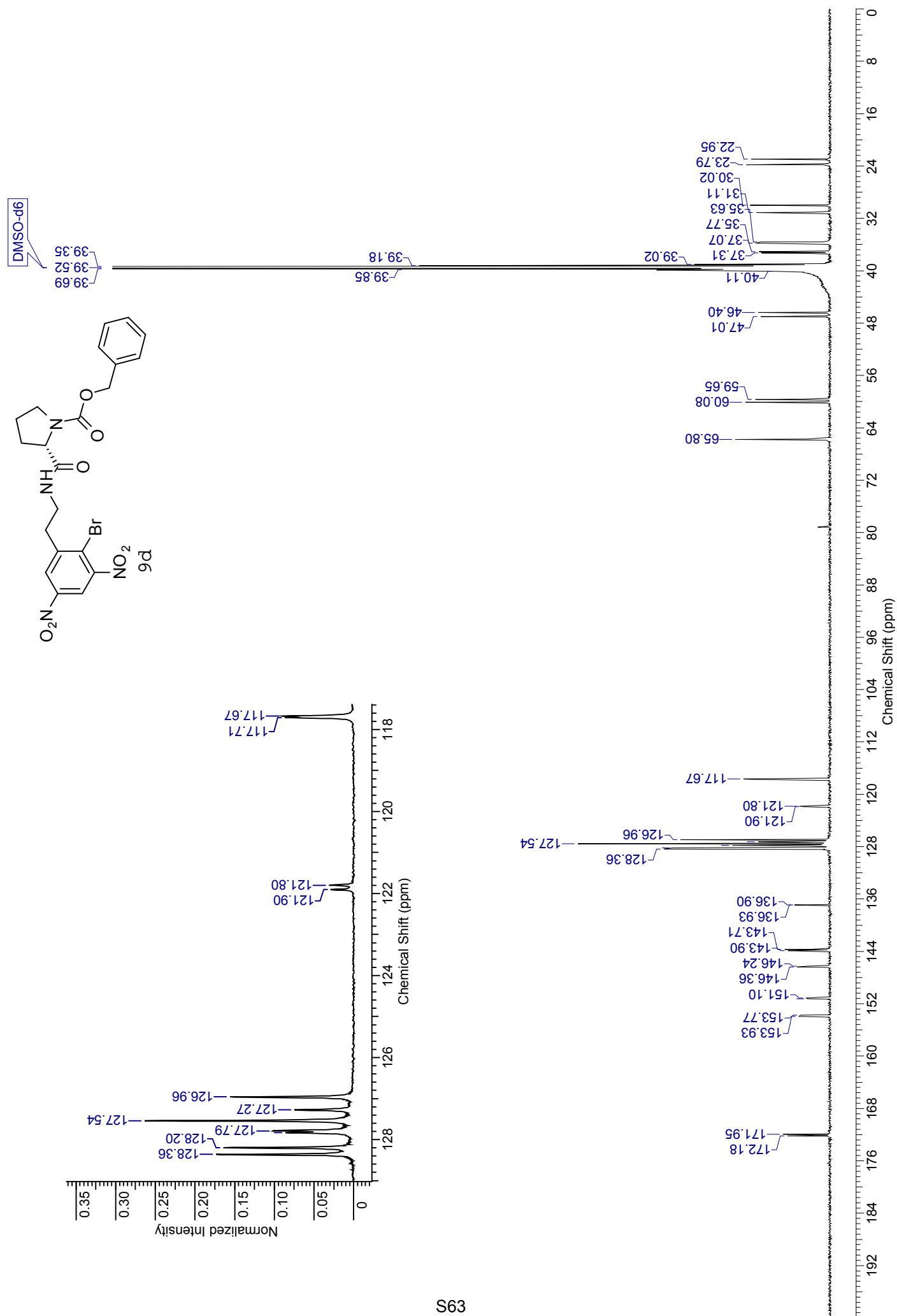
Ion mass = 605.0649130

Charge = +1

#	C	H	79Br	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 605.0649130									
1	26	23	1	4	7	1	605.0642328	16.5	6.802e-04
2	16	34	2	5	8	1	605.0666344	1.0	1.721e-03
3	28	22	1	4	7	0	605.0666381	19.5	1.725e-03
4	29	21	1	5	4	1	605.0669129	21.0	2.000e-03
5	18	33	2	5	8	0	605.0690397	4.0	4.127e-03
6	31	20	1	5	4	0	605.0693182	24.0	4.405e-03
7	22	31	2	4	6	0	605.0604864	8.5	4.427e-03
8	21	34	2	3	6	1	605.0706571	5.0	5.744e-03
9	32	20	1	3	5	0	605.0580848	24.0	6.828e-03
10	20	32	2	4	6	1	605.0580811	5.5	6.832e-03

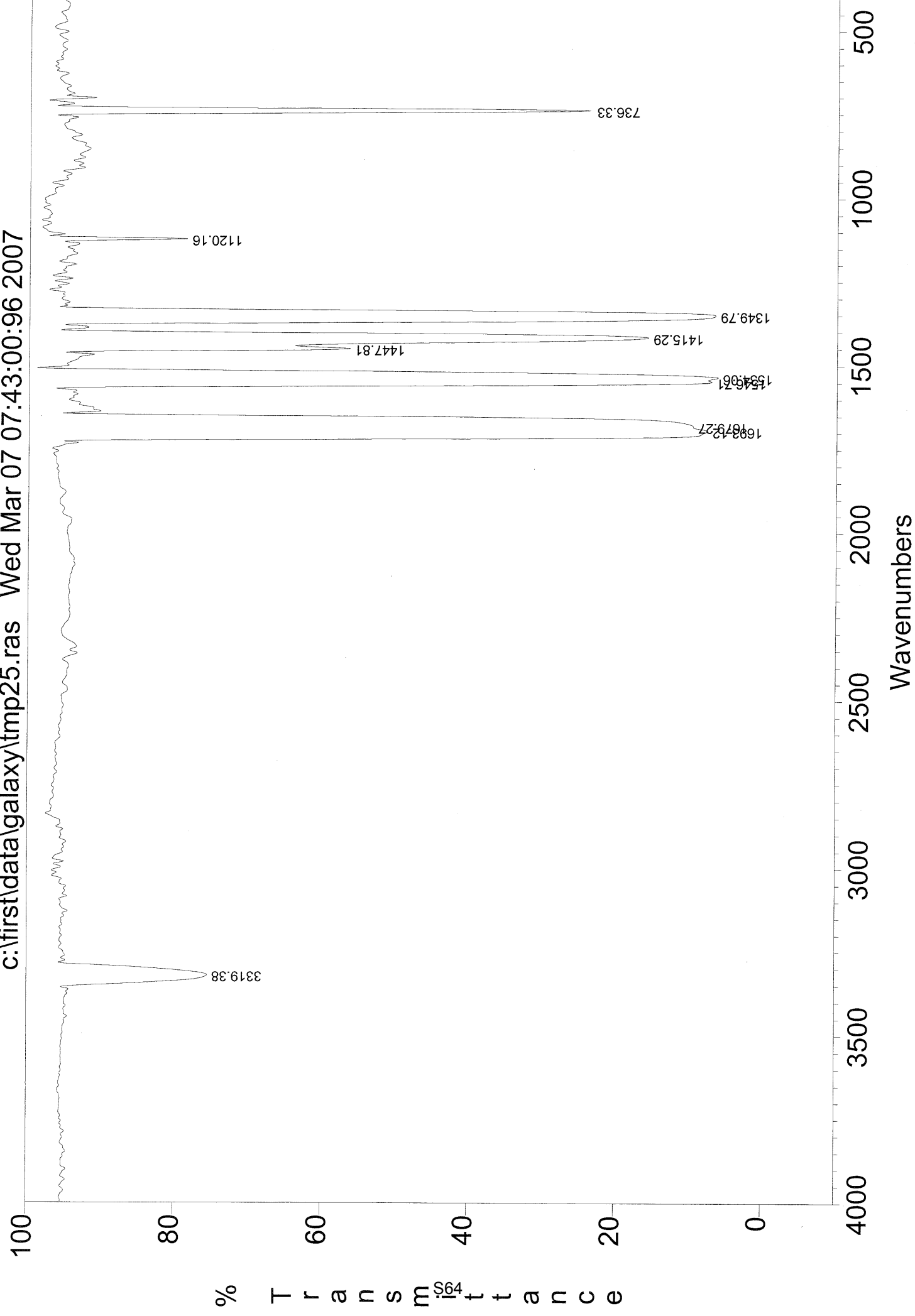






560107

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FTMS 4.7T BioAPEX II MS-Service UNI-Fribourg

ESI-MS: JLD107-1

XMASS Mass Analysis for /Data/UNI_FR/DEBI2628_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

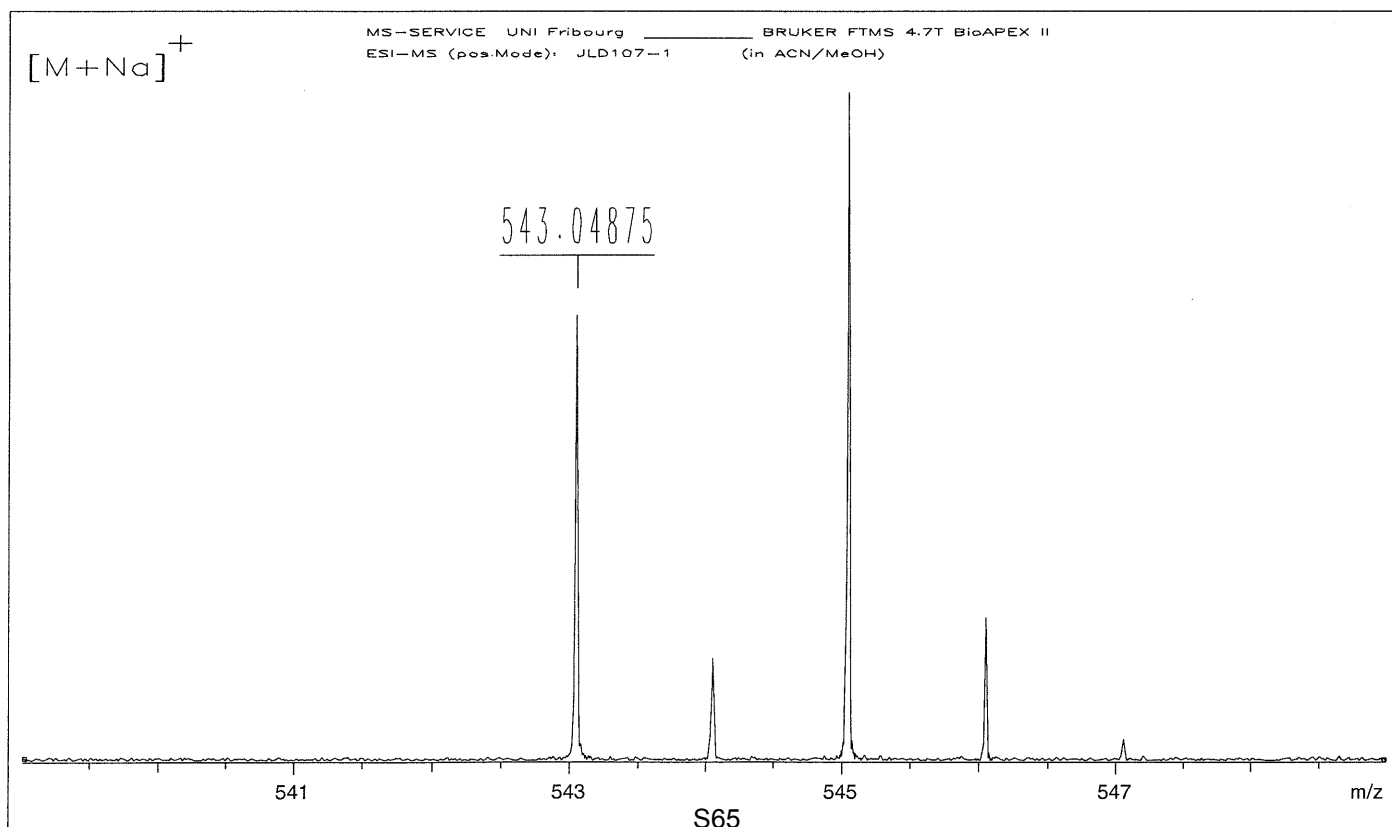
Ion mass = 543.0487460

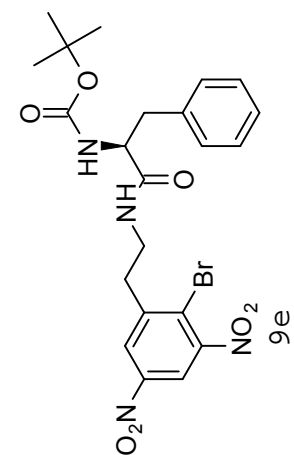
Charge = +1

#	C	H	79Br	N	O	Na	mass	DBE	error
---	---	---	------	---	---	----	------	-----	-------

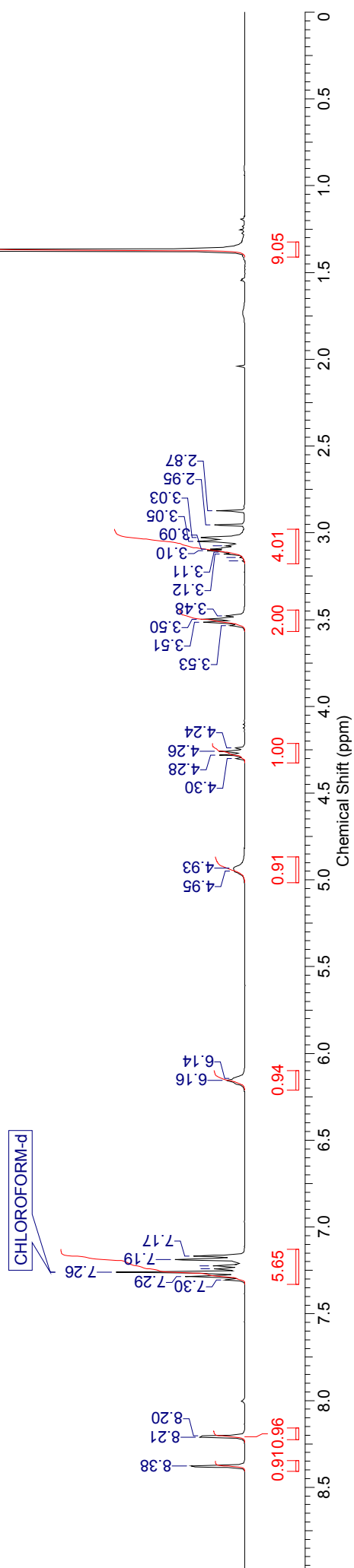
*** Mass Analysis for mass 543.0487460

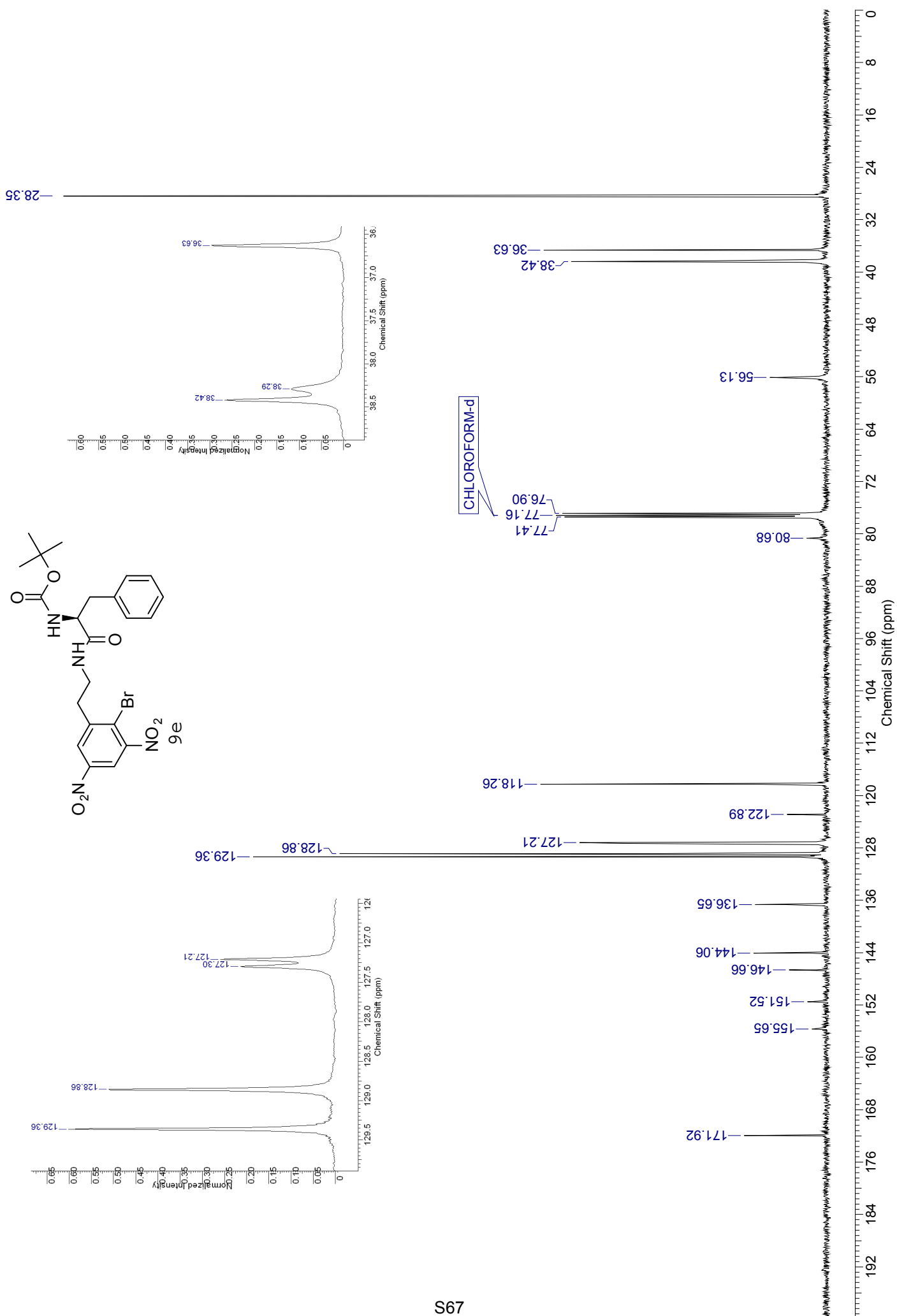
1	21	21	1	4	7	1	543.0485827	12.5	1.633e-04
2	23	20	1	4	7	0	543.0509880	15.5	2.242e-03
3	24	19	1	5	4	1	543.0512628	17.0	2.517e-03
4	17	29	2	4	6	0	543.0448363	4.5	3.910e-03
5	13	31	2	5	8	0	543.0533896	0.0	4.644e-03
6	26	18	1	5	4	0	543.0536681	20.0	4.922e-03
7	16	32	2	3	6	1	543.0550071	1.0	6.261e-03
8	27	18	1	3	5	0	543.0424347	20.0	6.311e-03
9	15	30	2	4	6	1	543.0424310	1.5	6.315e-03
10	18	31	2	3	6	0	543.0574124	4.0	8.666e-03





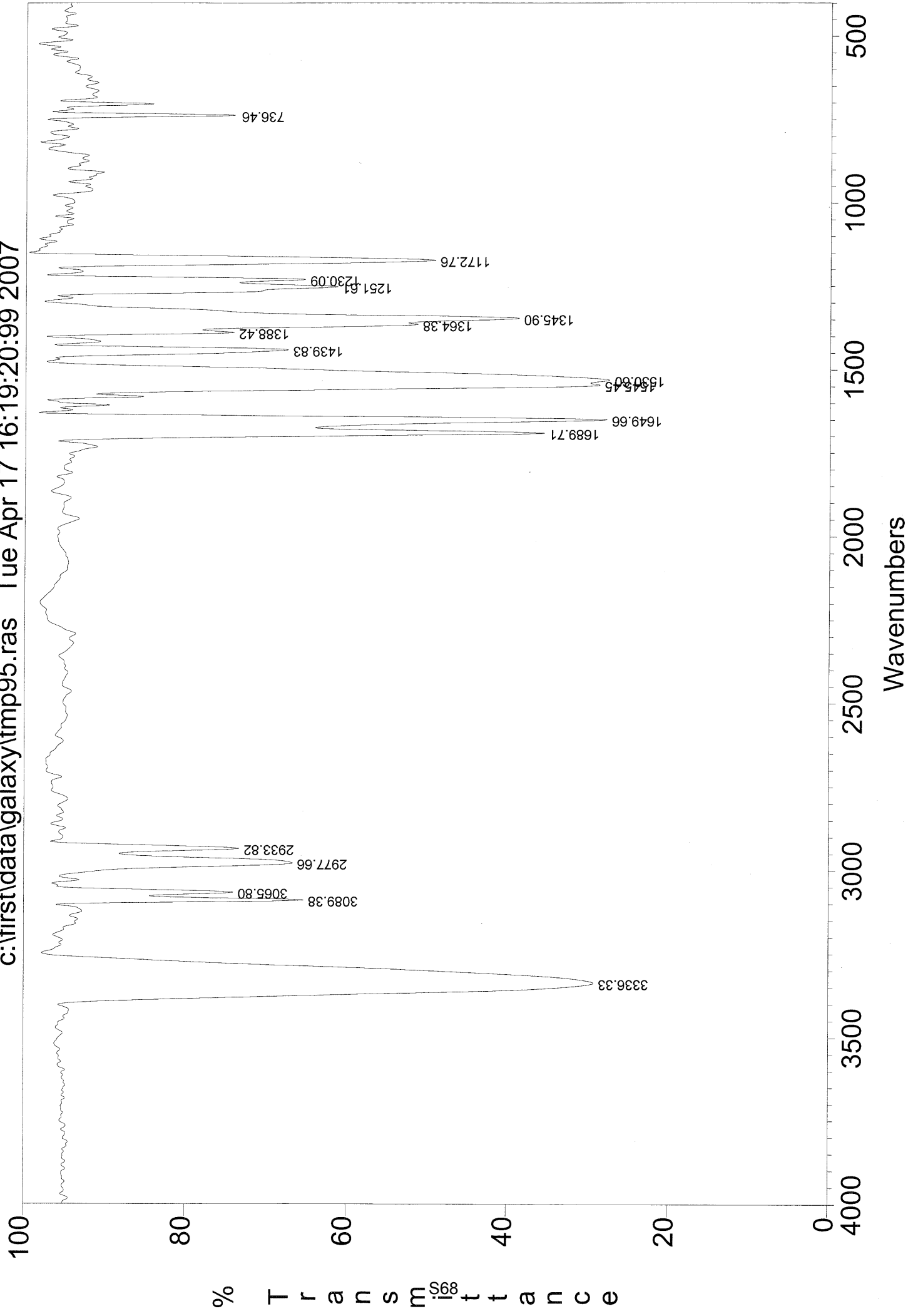
1.37





96884

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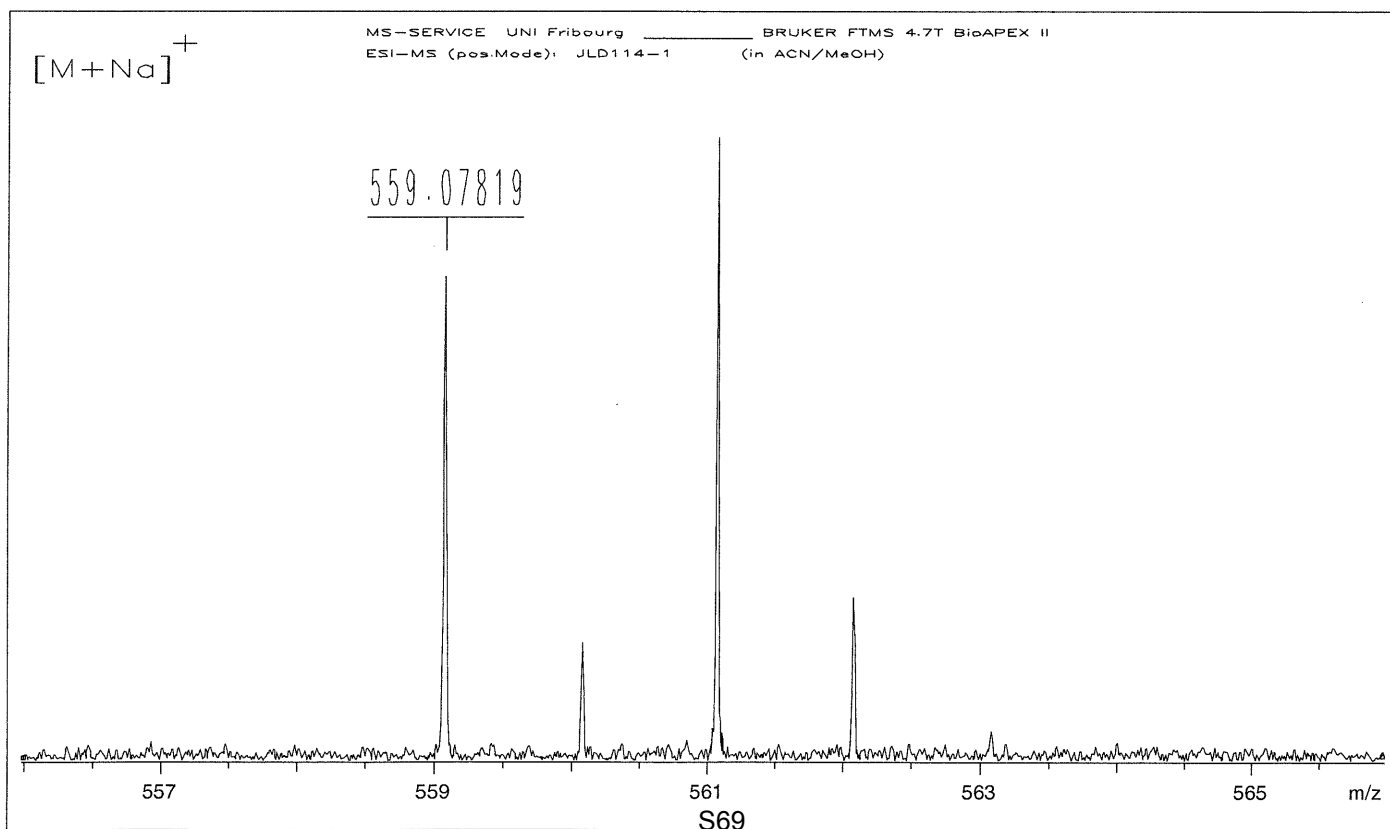
ESI-MS: JLD114-1

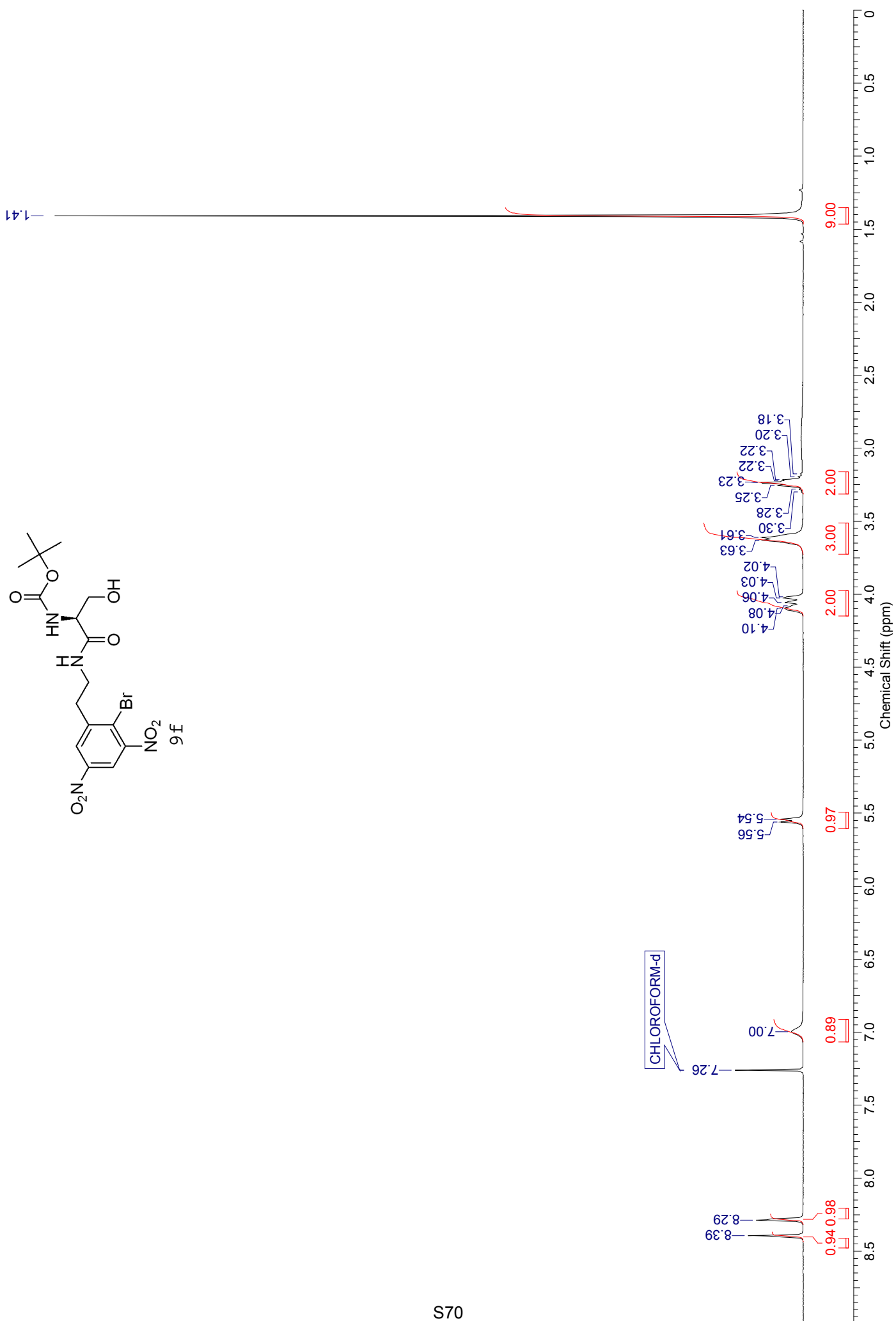
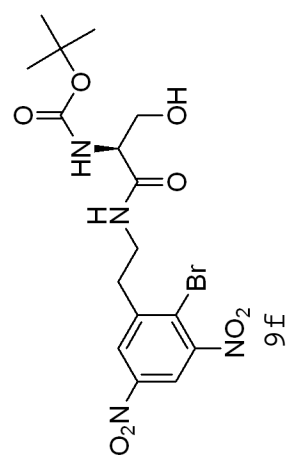
XMASS Mass Analysis for /Data/UNI_FR/DEBI2625_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

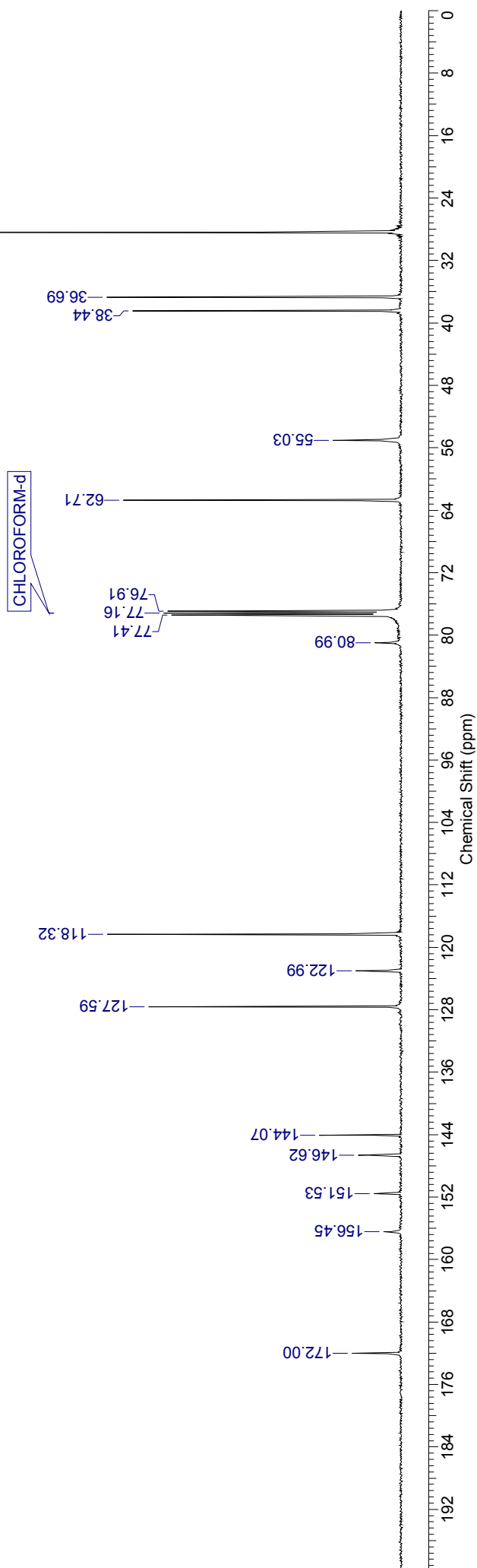
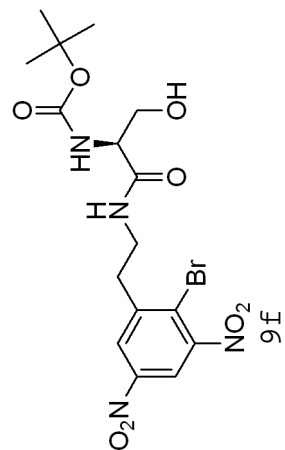
Ion mass = 559.0781910

Charge = +1

#	C	H	79Br	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 559.0781910									
1	22	25	1	4	7	1	559.0798829	11.5	1.692e-03
2	18	33	2	4	6	0	559.0761364	3.5	2.055e-03
3	24	24	1	4	7	0	559.0822882	14.5	4.097e-03
4	25	23	1	5	4	1	559.0825629	16.0	4.372e-03
5	28	22	1	3	5	0	559.0737349	19.0	4.456e-03
6	16	34	2	4	6	1	559.0737311	0.5	4.460e-03
7	14	35	2	5	8	0	559.0846897	-1.0	6.499e-03
8	27	22	1	5	4	0	559.0849682	19.0	6.777e-03
9	26	23	1	3	5	1	559.0713296	16.0	6.861e-03
10	17	36	2	3	6	1	559.0863072	0.0	8.116e-03







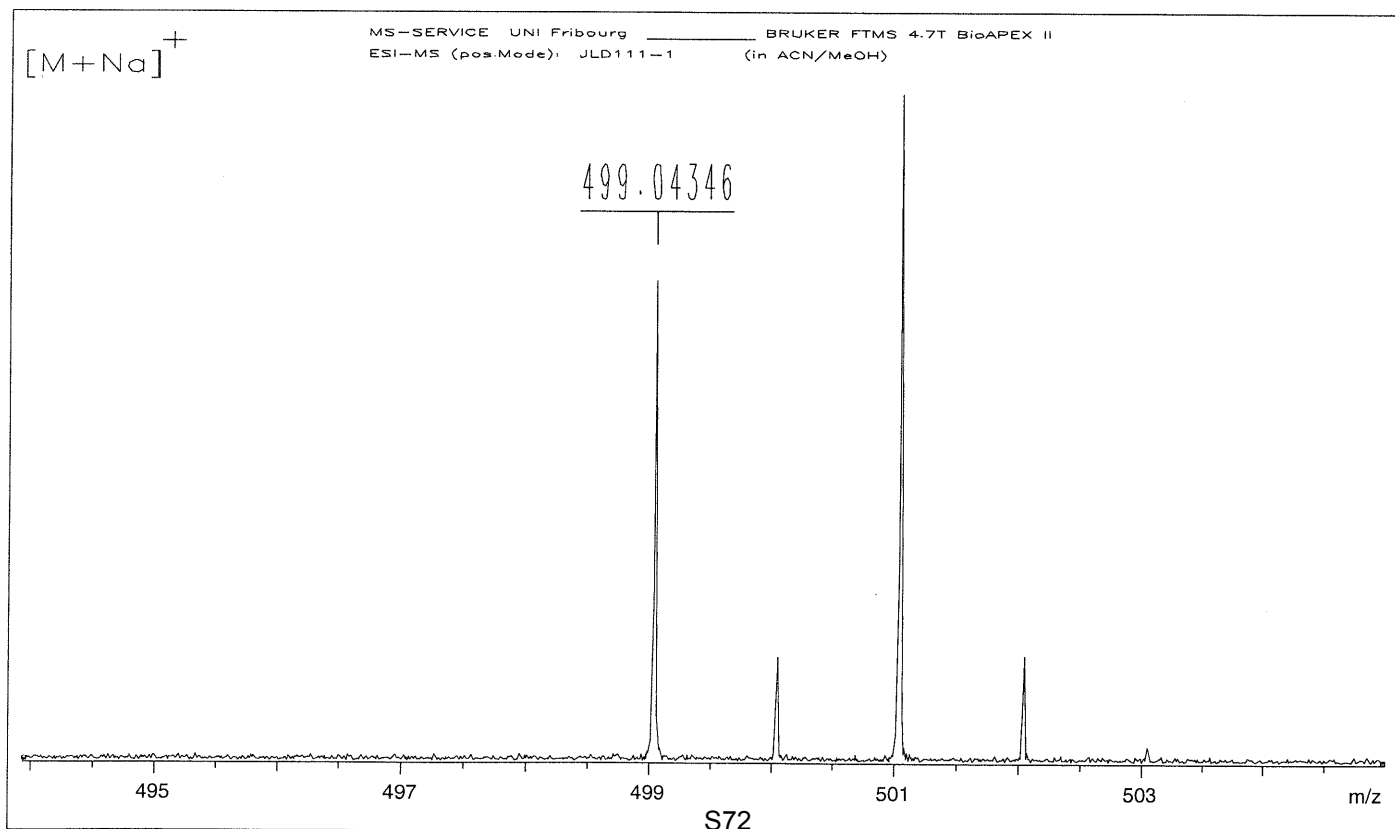
ESI-MS: JLD111-1

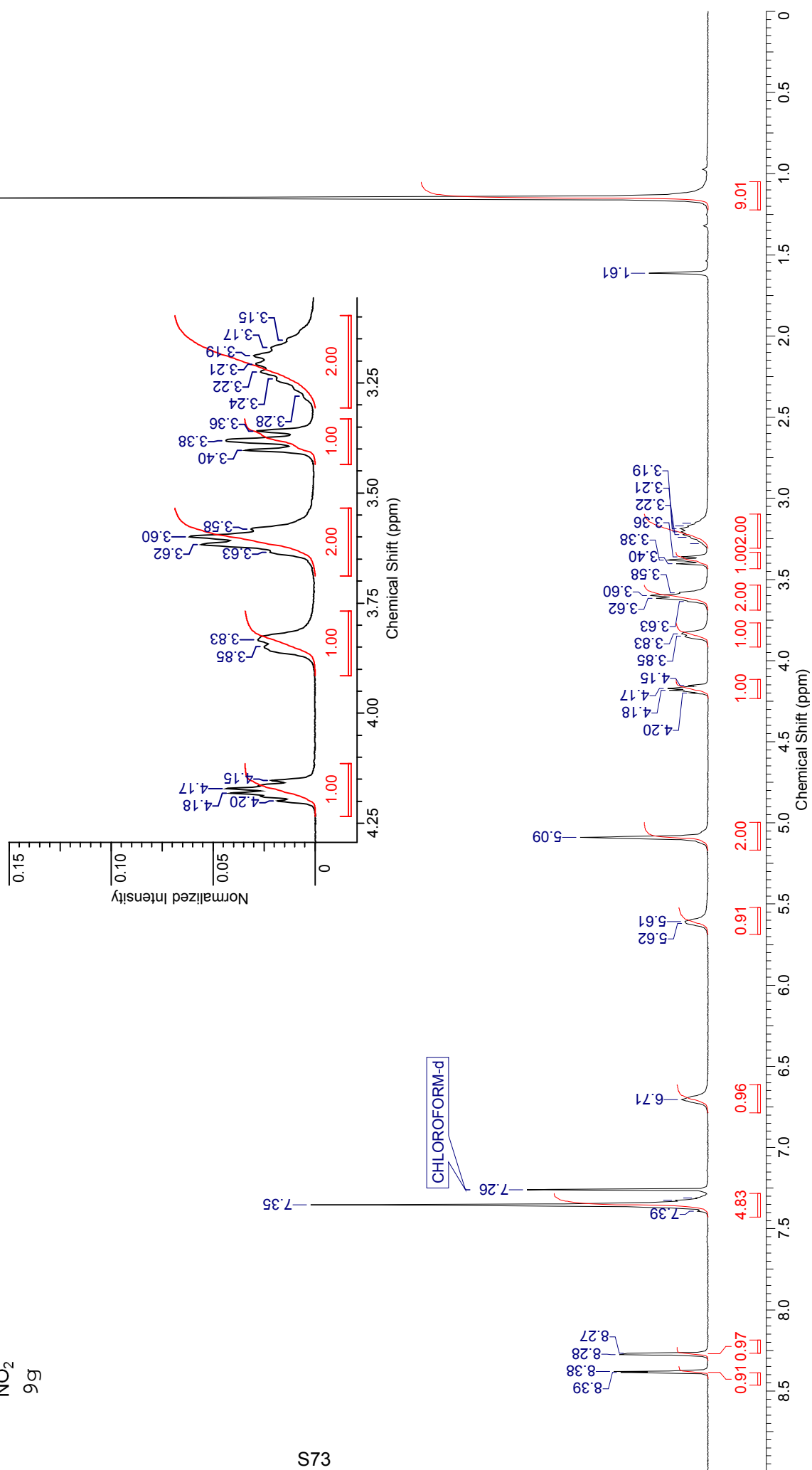
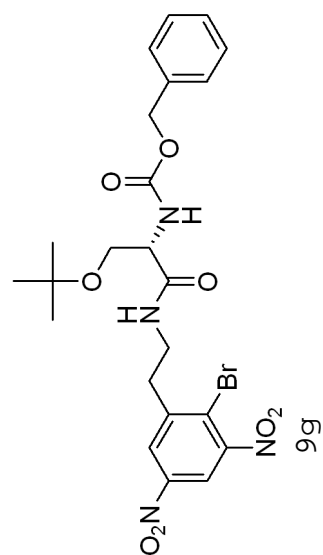
XMASS Mass Analysis for /Data/UNI_FR/DEBI2626_ESI/10/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

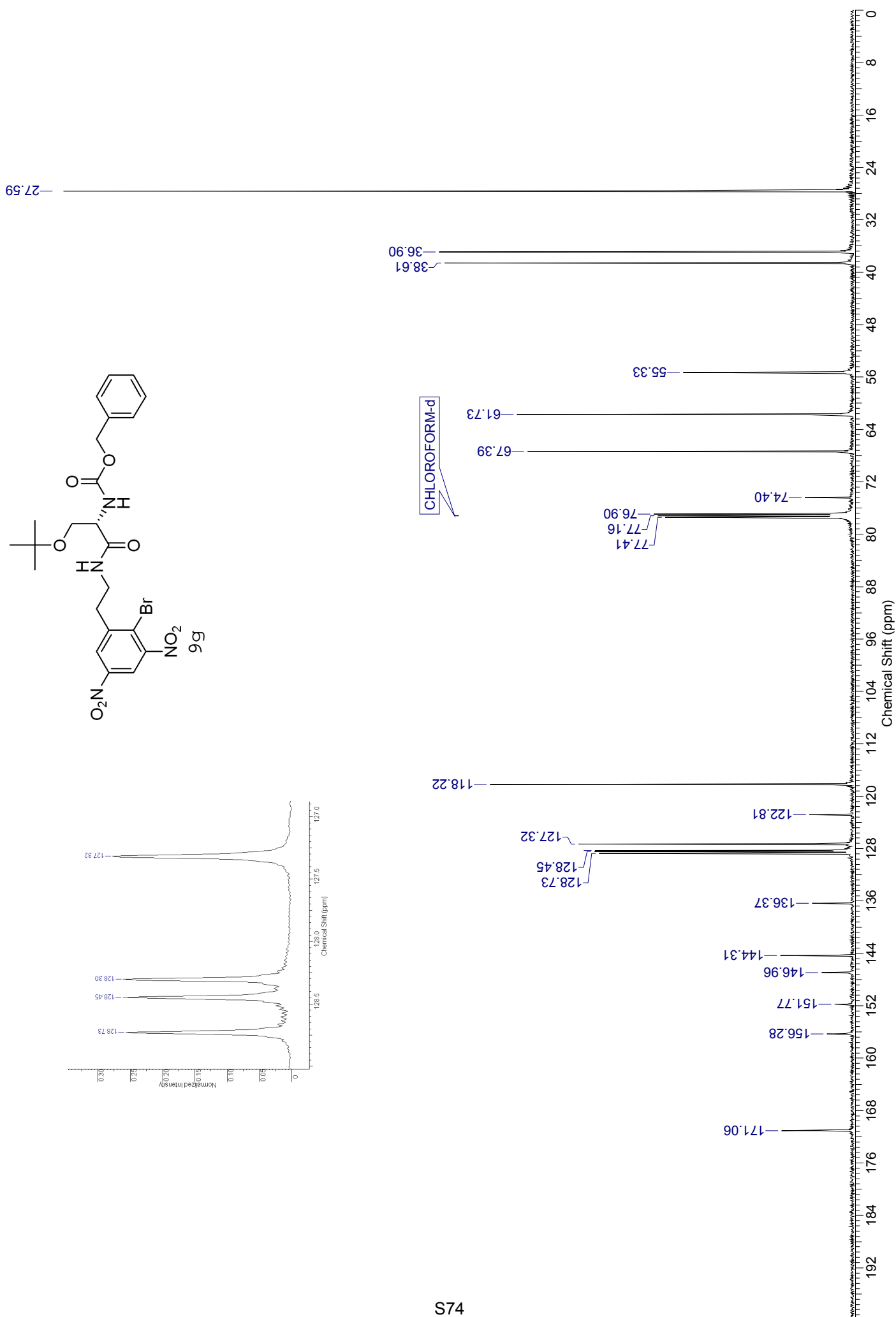
Ion mass = 499.0434590

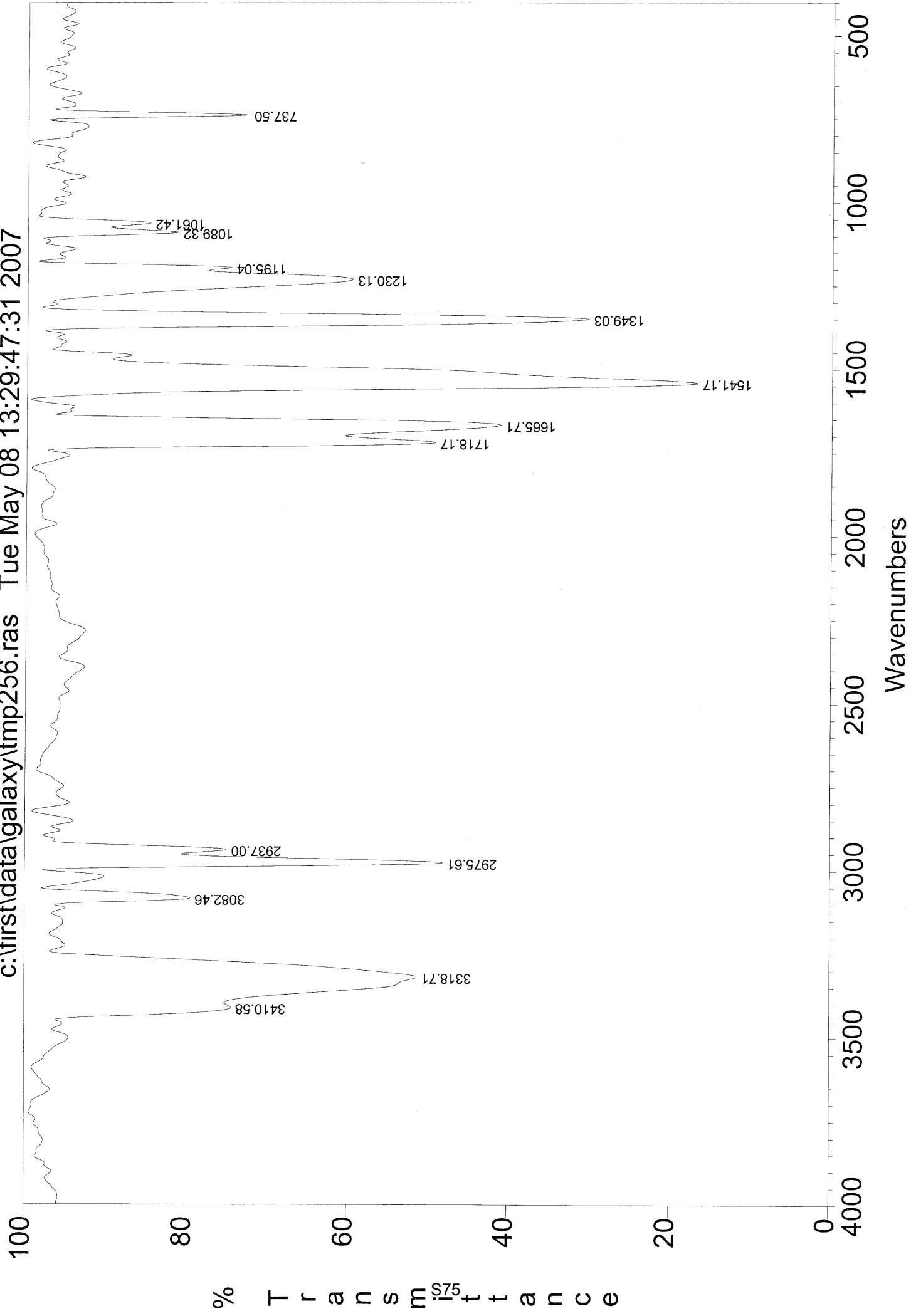
Charge = +1

#	C	H	79Br	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 499.0434590									
1	16	21	1	4	8	1	499.0434974	7.5	3.836e-05
2	15	27	2	5	4	0	499.0424310	4.0	1.028e-03
3	18	20	1	4	8	0	499.0459027	10.5	2.444e-03
4	19	19	1	5	5	1	499.0461774	12.0	2.718e-03
5	13	28	2	5	4	1	499.0400257	1.0	3.433e-03
6	12	29	2	4	7	0	499.0397509	-0.5	3.708e-03
7	21	18	1	5	5	0	499.0485827	15.0	5.124e-03
8	22	18	1	3	6	0	499.0373493	15.0	6.110e-03
9	20	19	1	3	6	1	499.0349440	12.0	8.515e-03
10	13	31	2	3	7	0	499.0523270	-1.0	8.868e-03











FTMS 4.7T BioAPEX II MS-Service UNI-Fribourg

ESI-MS: JLD126-1

XMASS Mass Analysis for /Data/UNI_FR/DEBI2616_ESI/20/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

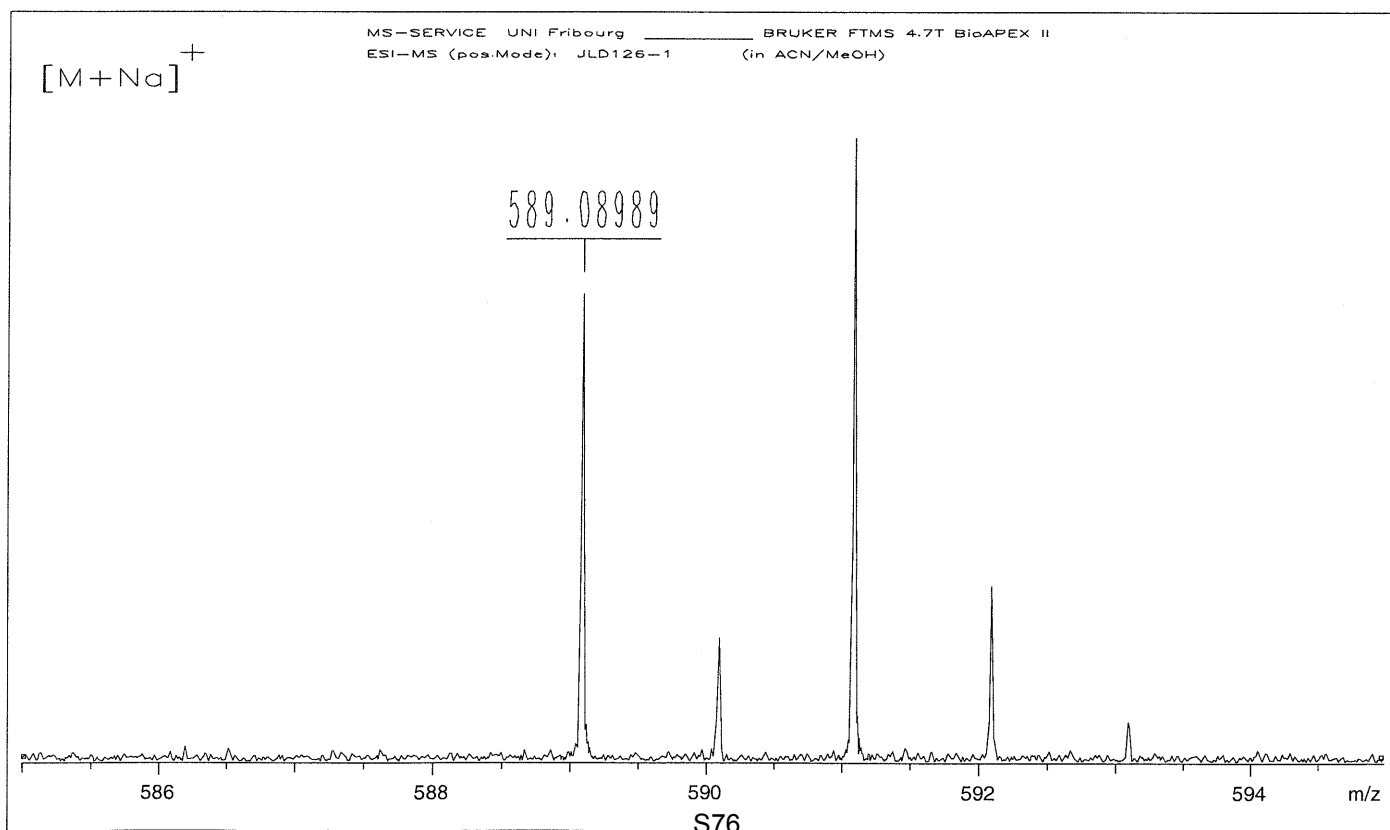
Ion mass = 589.0898910

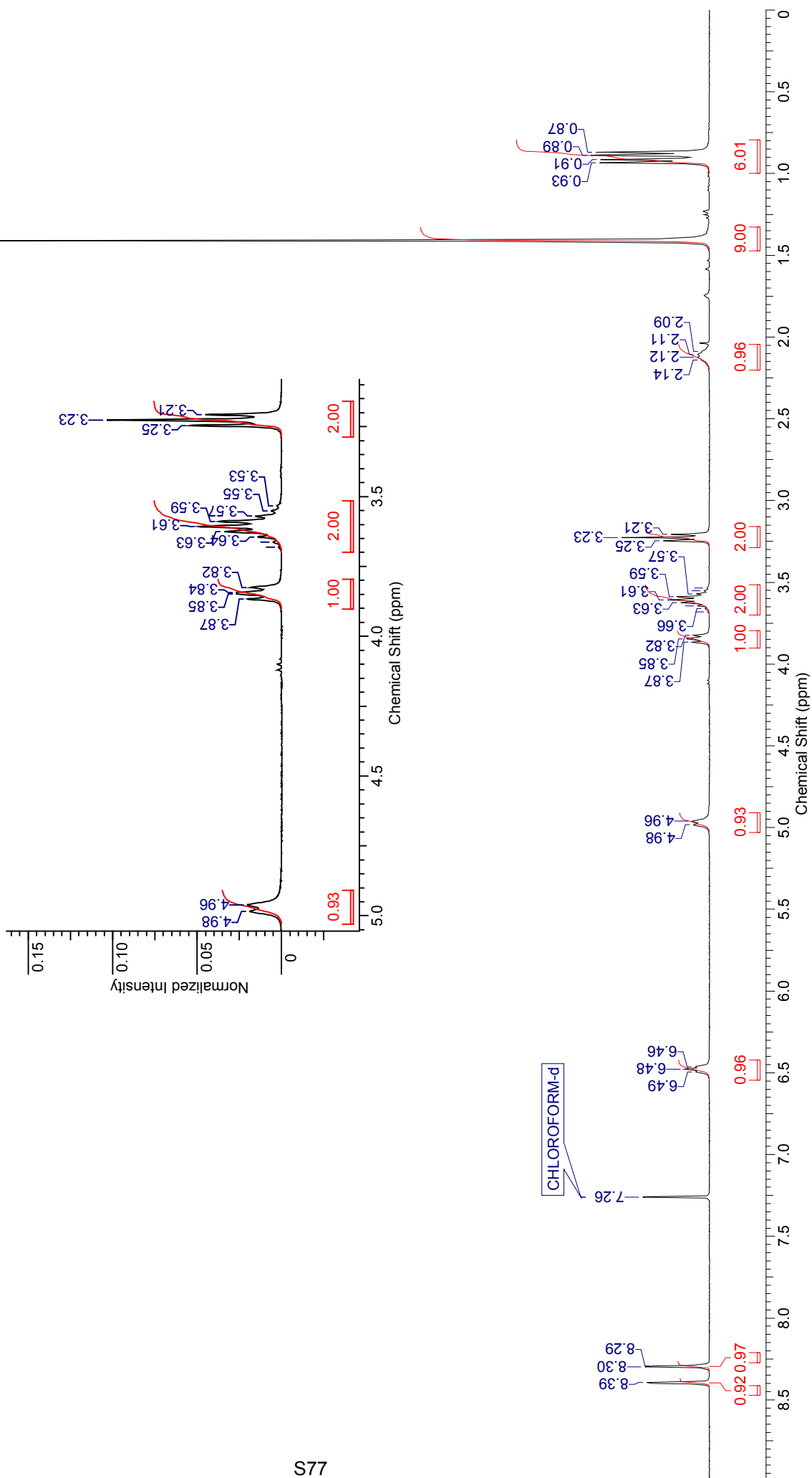
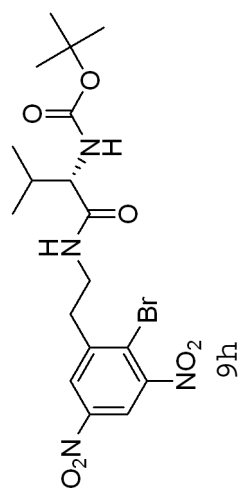
Charge = +1

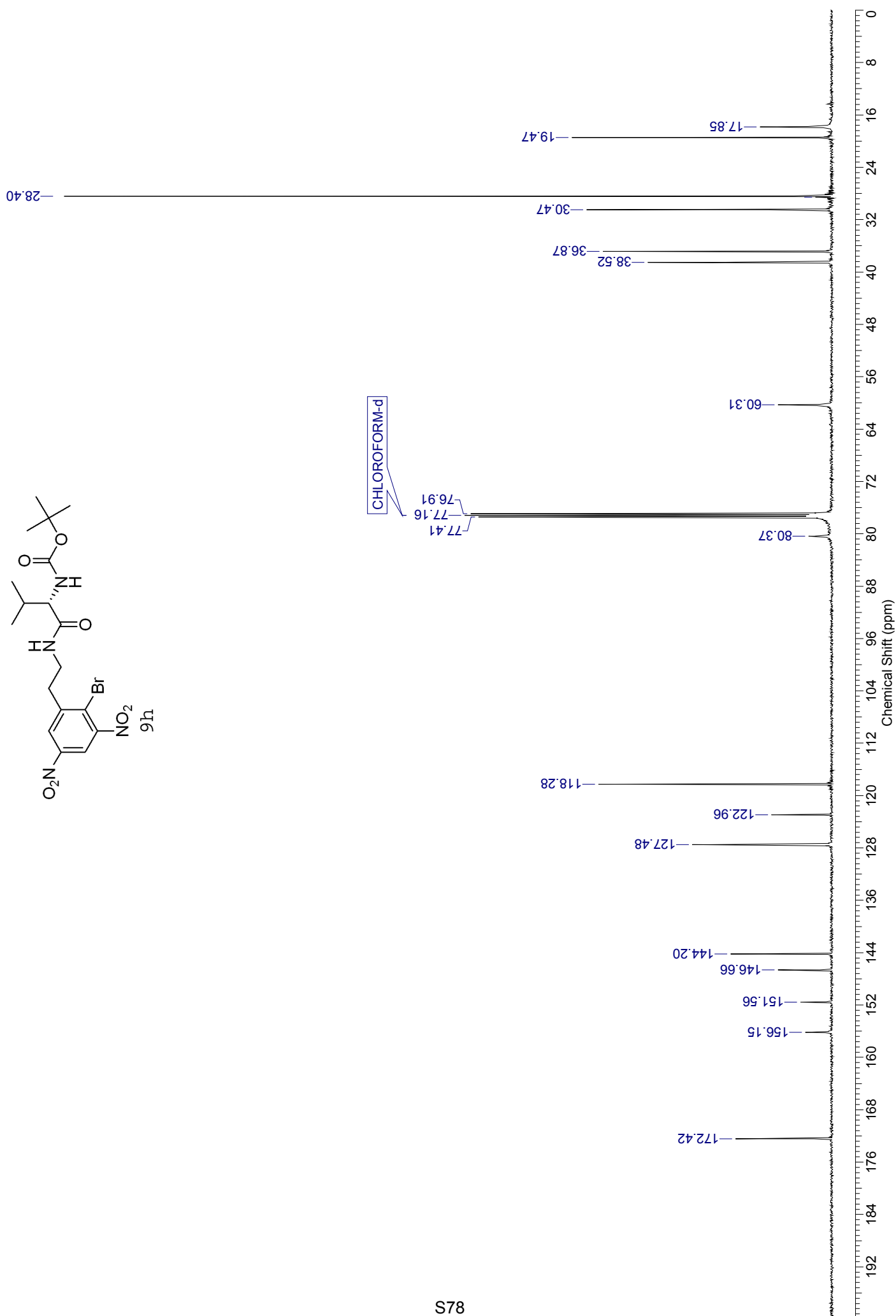
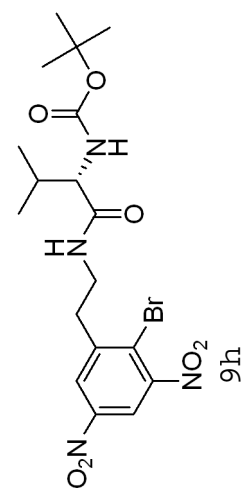
#	C	H	79Br	N	O	Na	mass	DBE	error
---	---	---	------	---	---	----	------	-----	-------

*** Mass Analysis for mass 589.0898910

1	23	27	1	4	8	1	589.0904476	11.5	5.566e-04
2	25	26	1	4	8	0	589.0928529	14.5	2.962e-03
3	26	25	1	5	5	1	589.0931276	16.0	3.237e-03
4	29	24	1	3	6	0	589.0842995	19.0	5.591e-03
5	28	24	1	5	5	0	589.0955329	19.0	5.642e-03
6	27	25	1	3	6	1	589.0818942	16.0	7.997e-03
7	24	24	1	5	8	0	589.0802768	15.0	9.614e-03
8	22	25	1	5	8	1	589.0778715	12.0	1.202e-02
9	24	29	1	3	8	1	589.1030236	11.0	1.313e-02
10	26	28	1	3	8	0	589.1054289	14.0	1.554e-02

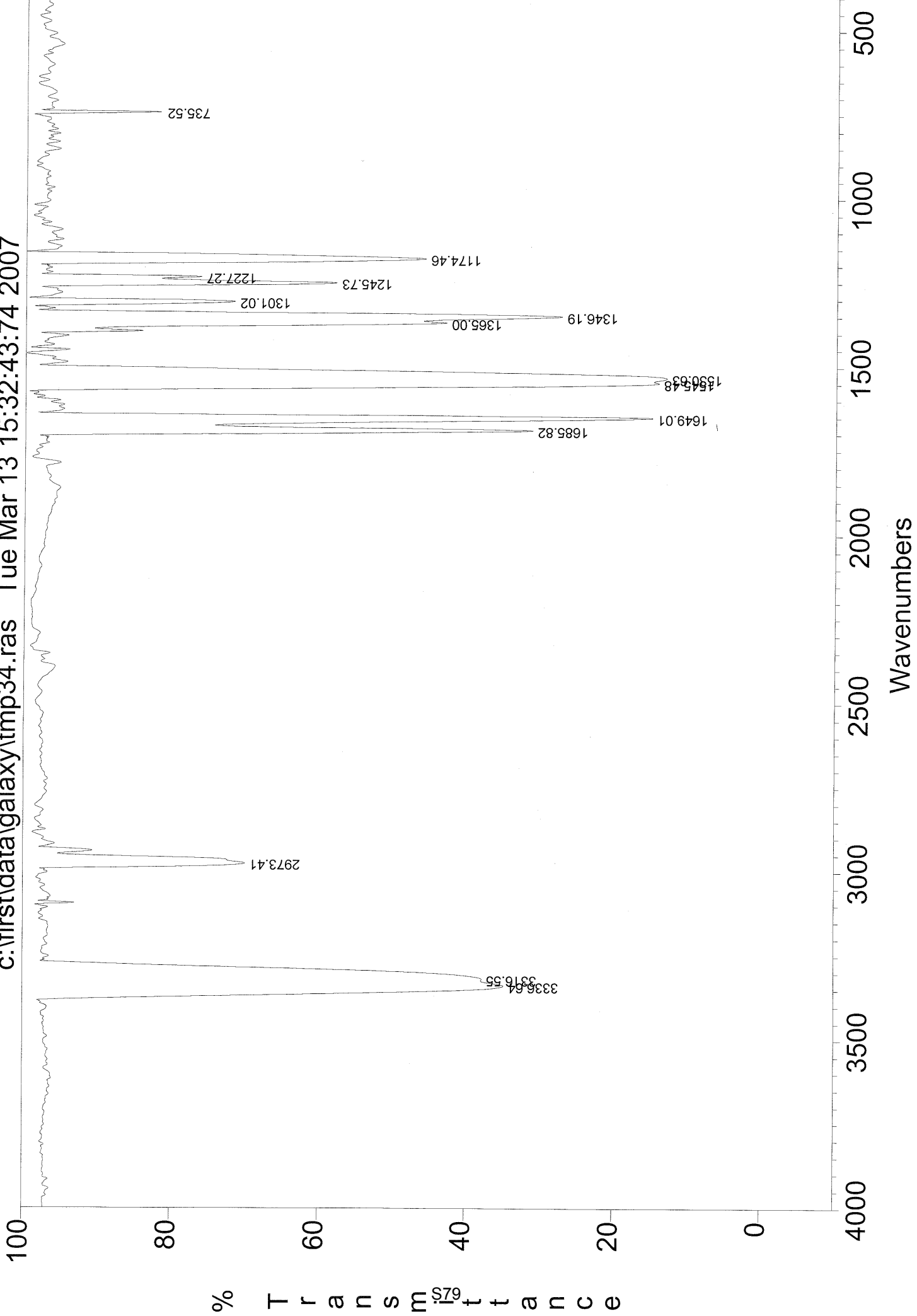






710109

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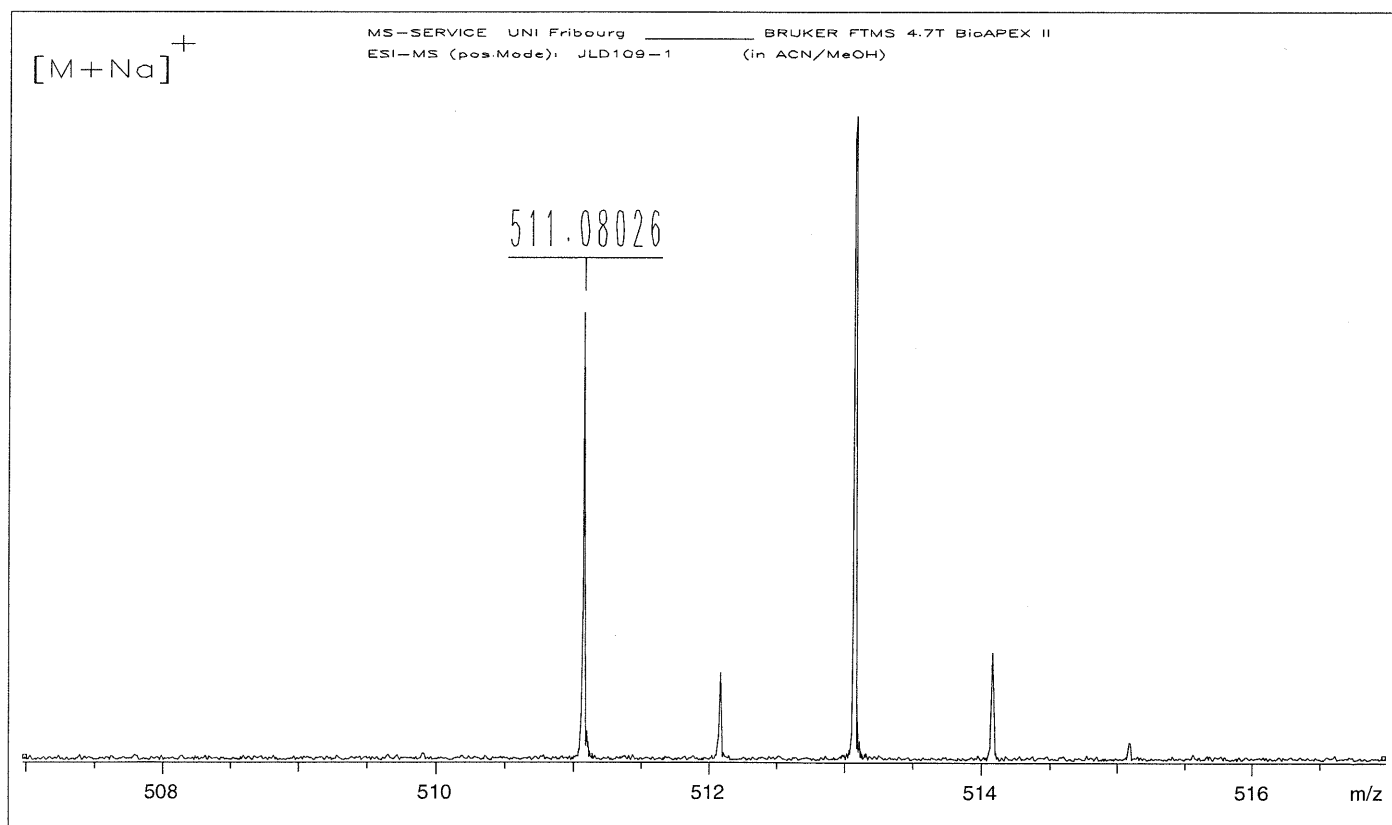
ESI-MS: JLD109-1

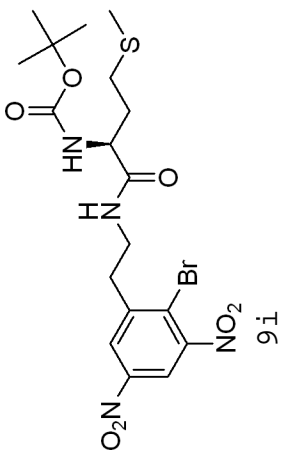
XMASS Mass Analysis for /Data/UNI_FR/DEBI2629_ESI/10/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 511.0802650

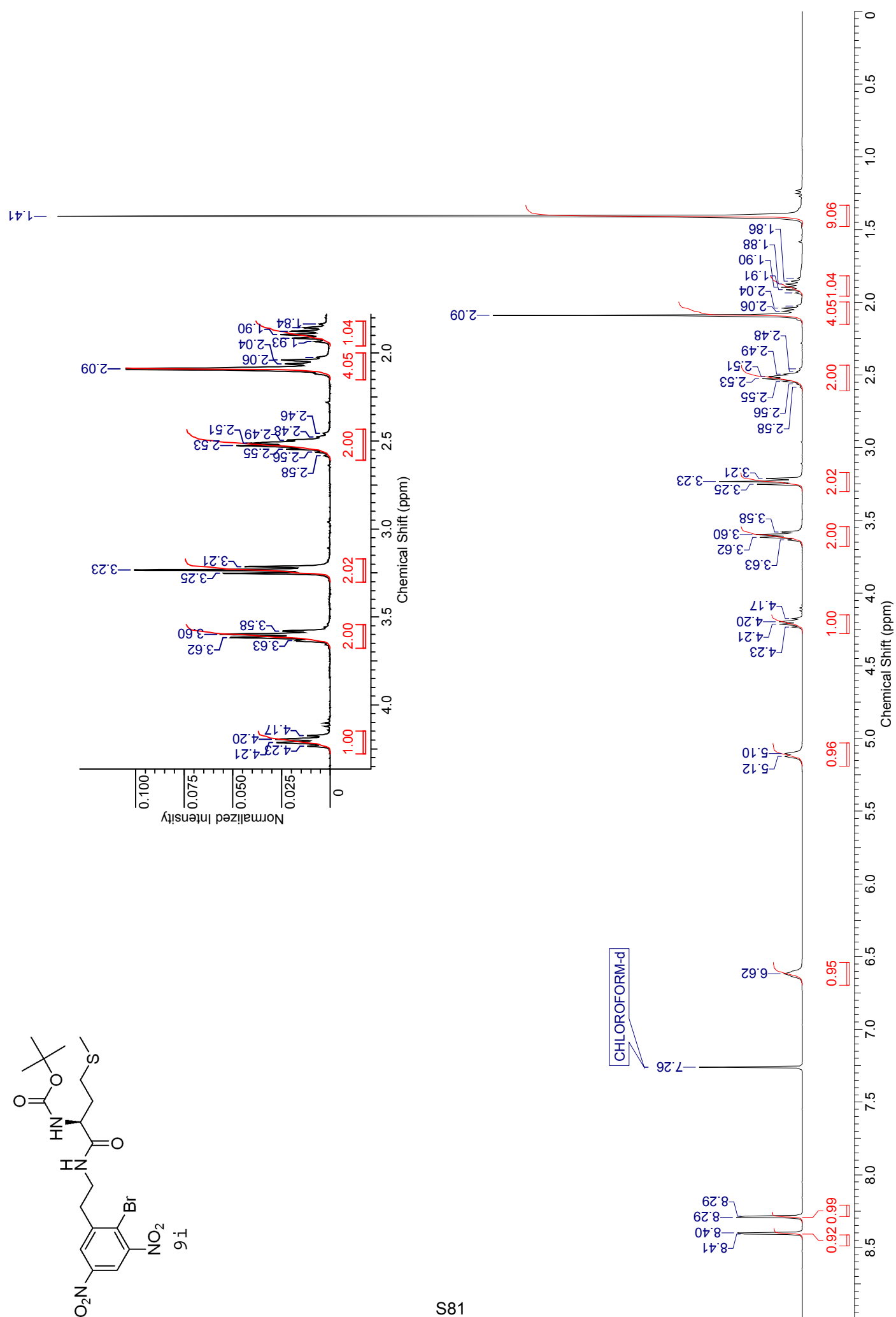
Charge = +1

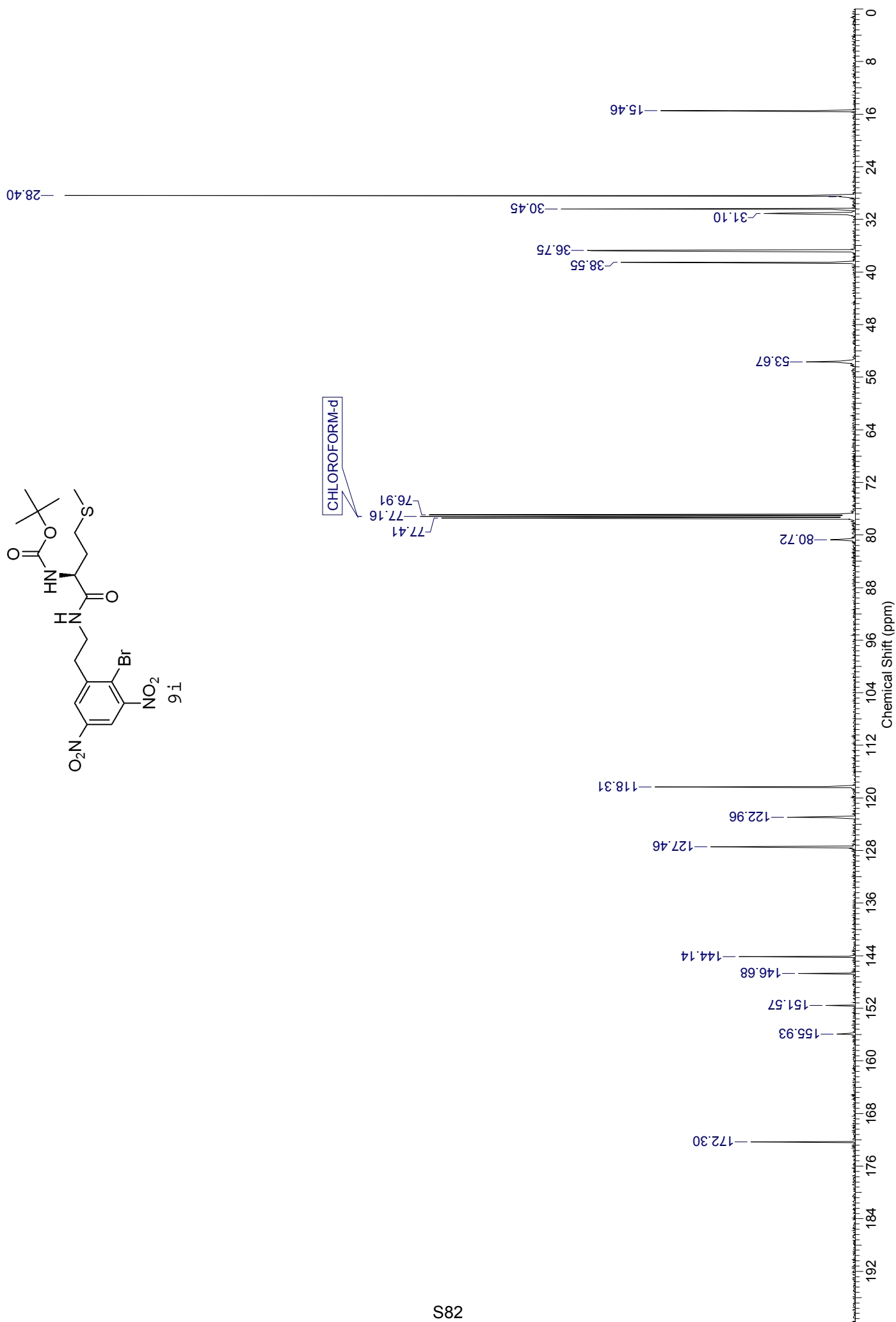
#	C	H	79Br	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 511.0802650									
1	18	25	1	4	7	1	511.0798829	7.5	3.821e-04
2	20	24	1	4	7	0	511.0822882	10.5	2.023e-03
3	21	23	1	5	4	1	511.0825629	12.0	2.298e-03
4	14	33	2	4	6	0	511.0761364	-0.5	4.129e-03
5	23	22	1	5	4	0	511.0849682	15.0	4.703e-03
6	24	22	1	3	5	0	511.0737349	15.0	6.530e-03
7	15	35	2	3	6	0	511.0887125	-1.0	8.447e-03
8	22	23	1	3	5	1	511.0713296	12.0	8.935e-03
9	19	22	1	5	7	0	511.0697121	11.0	1.055e-02
10	19	27	1	3	7	1	511.0924589	7.0	1.219e-02





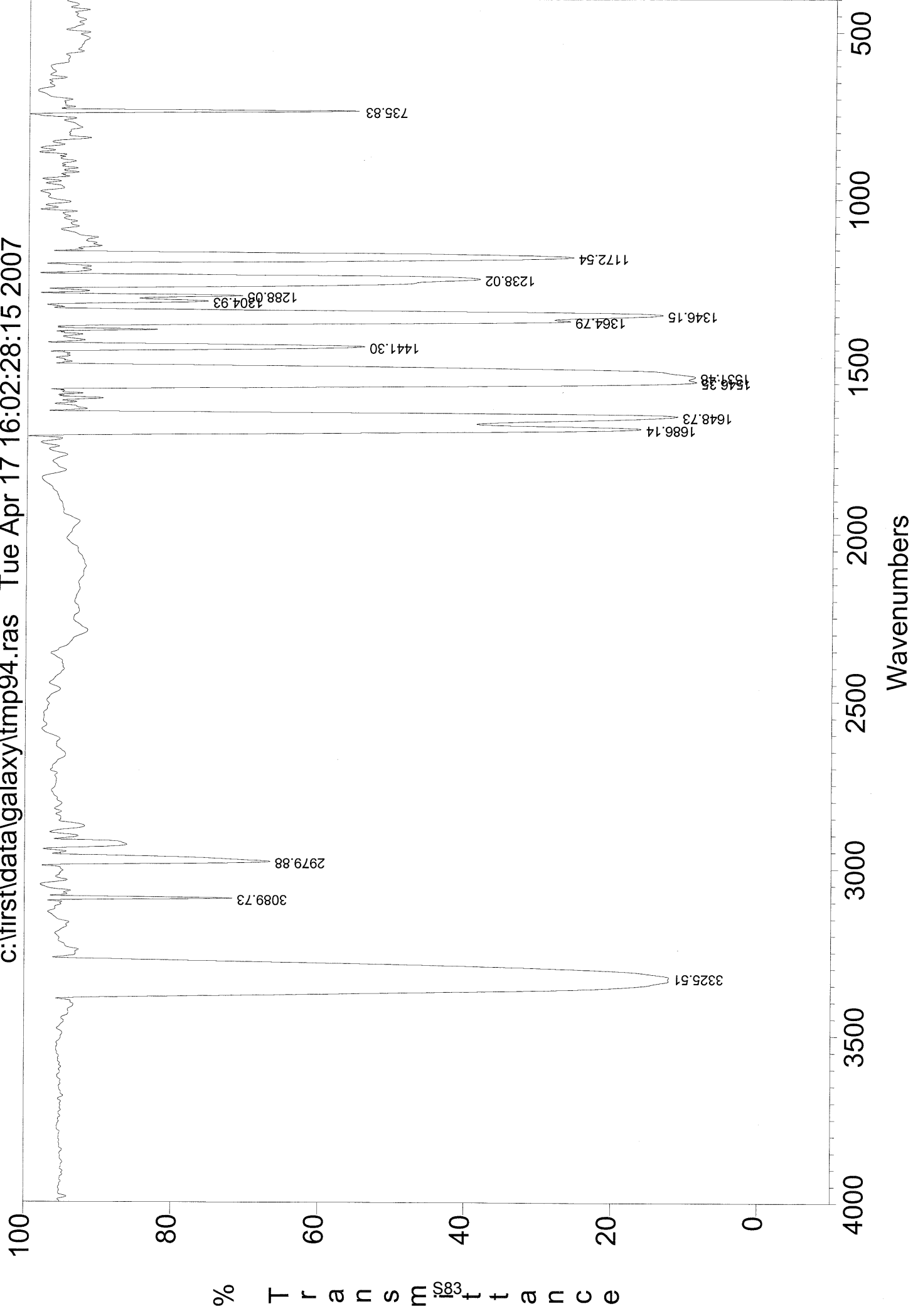
S81





960 120

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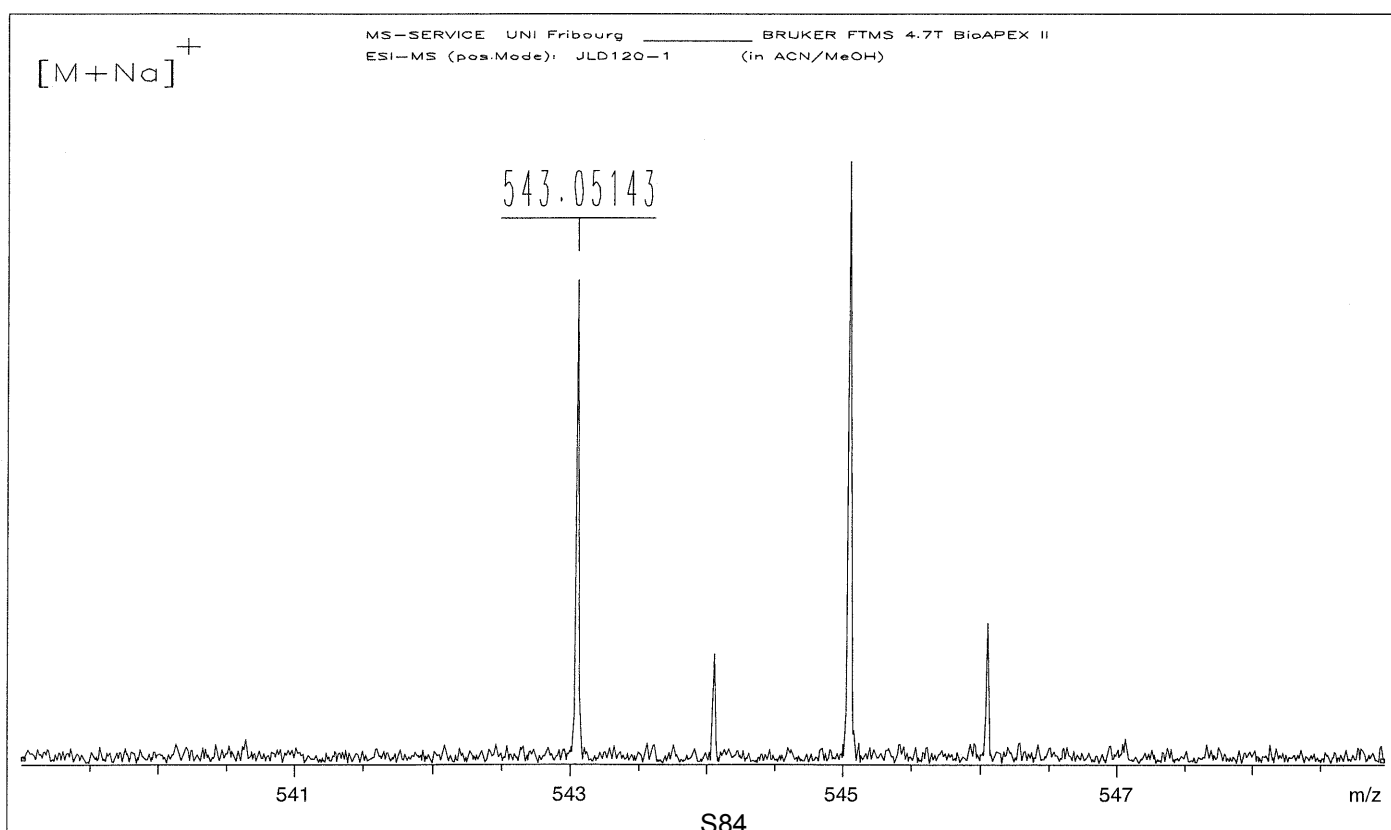
ESI-MS: JLD120-1

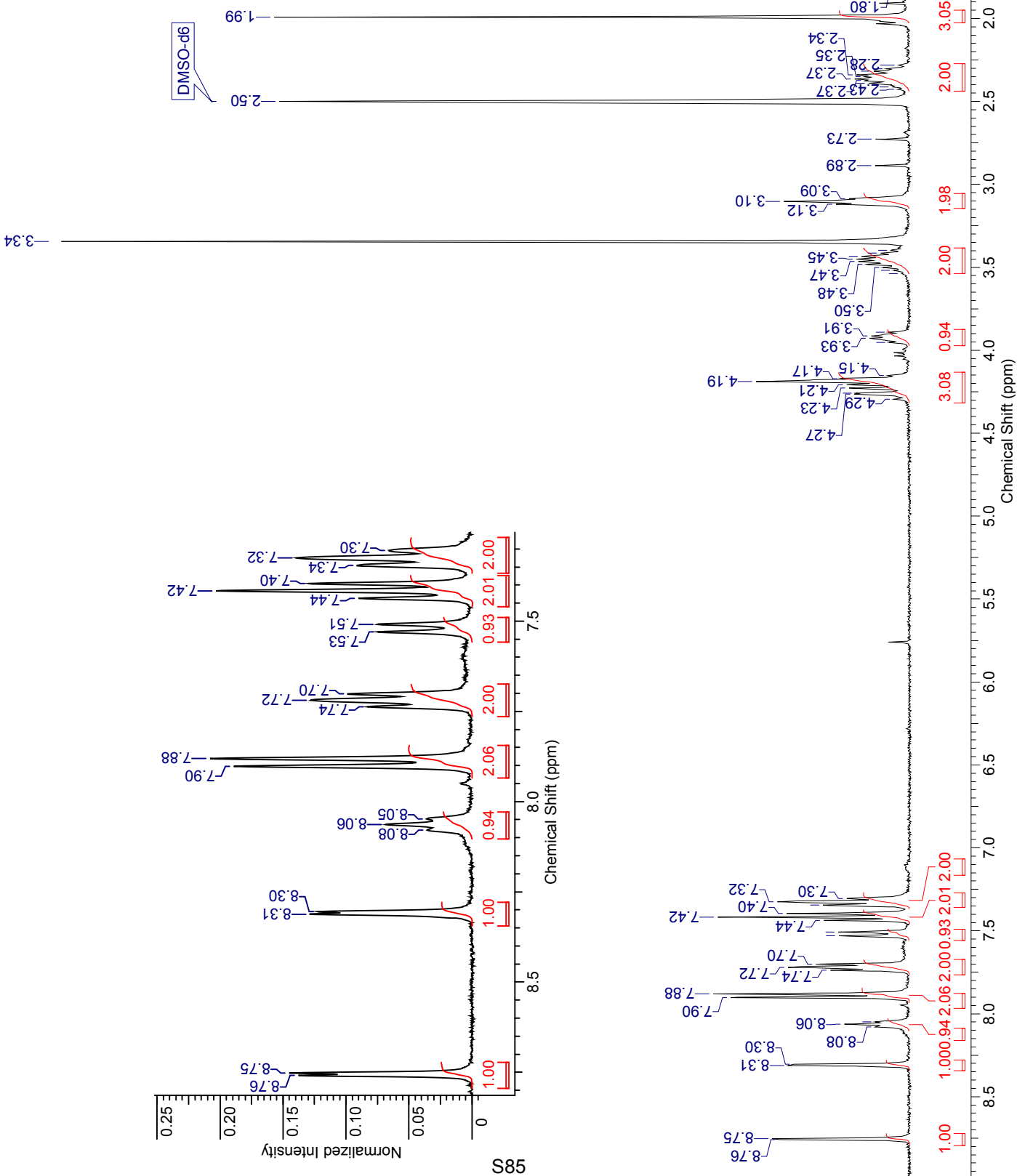
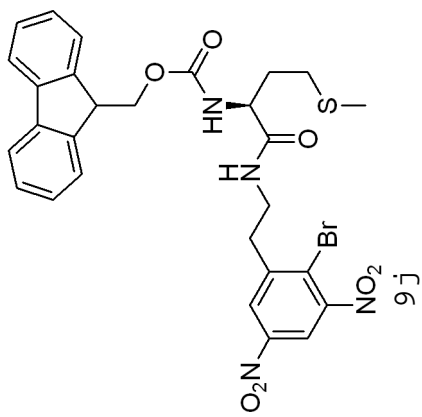
XMASS Mass Analysis for /Data/UNI_FR/DEBI2613_ESI/20/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

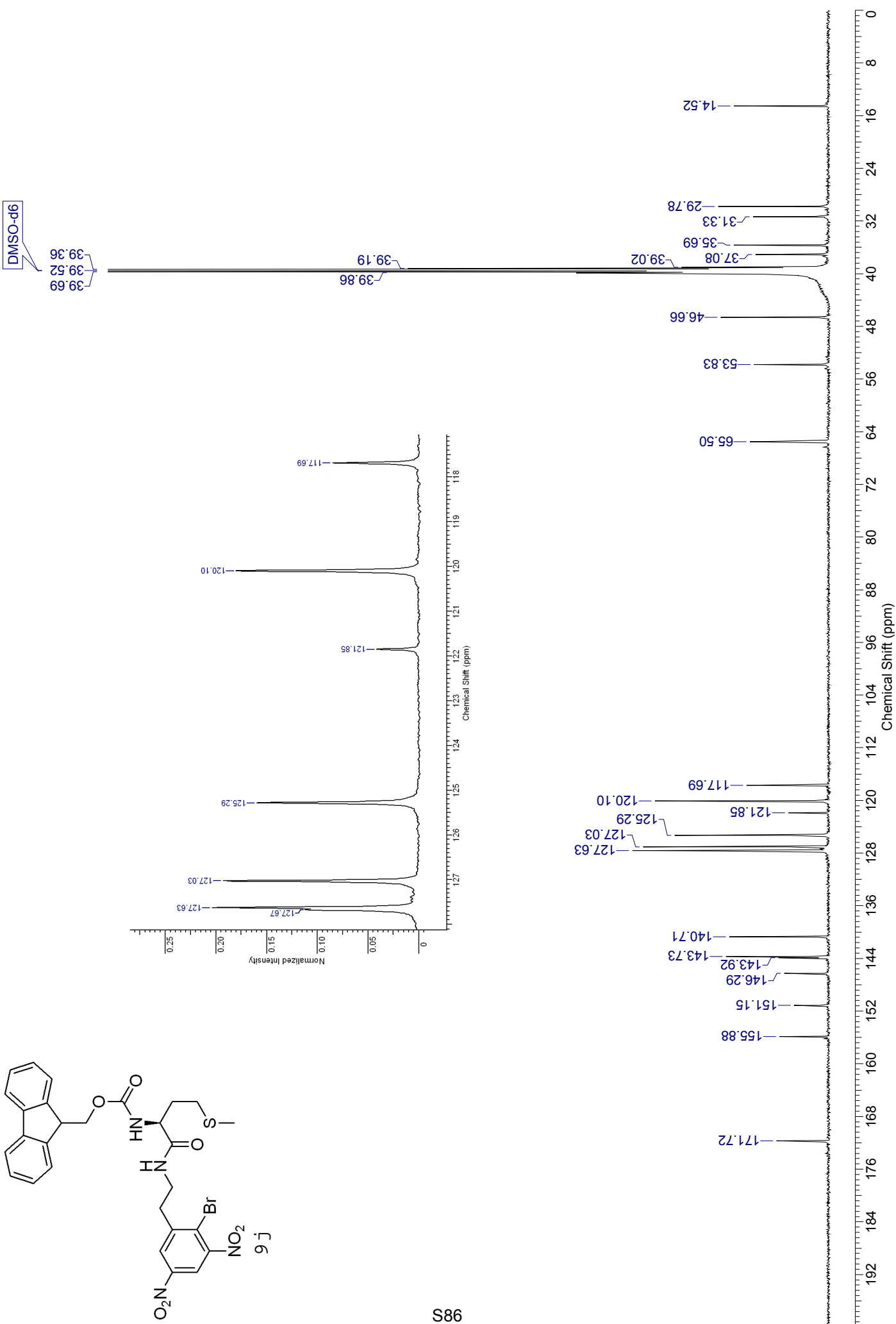
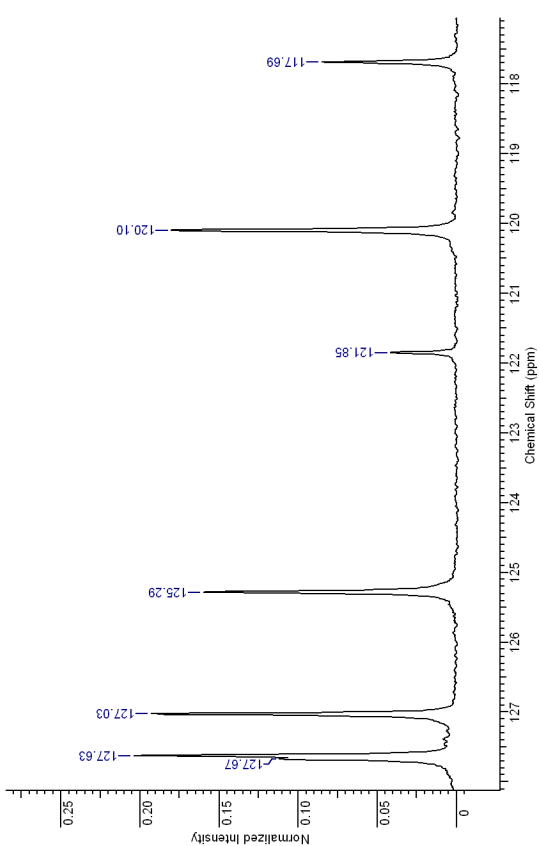
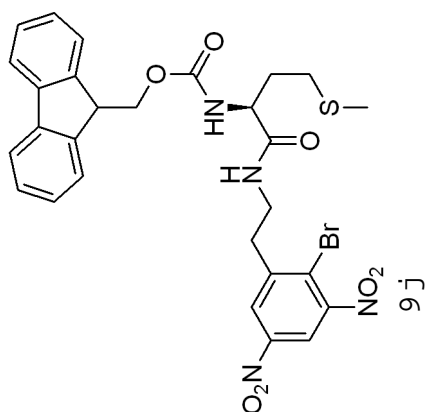
Ion mass = 543.0514270

Charge = +1

#	C	H	79Br	N	O	S	Na	mass	DBE	error
*** Mass Analysis for mass 543.0514270										
1	18	25	1	4	7	1	1	543.0519536	7.5	5.266e-04
2	20	24	1	4	7	1	0	543.0543589	10.5	2.932e-03
3	21	23	1	5	4	1	1	543.0546336	12.0	3.207e-03
4	14	33	2	4	6	1	0	543.0482071	-0.5	3.220e-03
5	23	22	1	5	4	1	0	543.0570389	15.0	5.612e-03
6	24	22	1	3	5	1	0	543.0458055	15.0	5.621e-03
7	22	23	1	3	5	1	1	543.0434002	12.0	8.027e-03
8	15	35	2	3	6	1	0	543.0607832	-1.0	9.356e-03
9	19	22	1	5	7	1	0	543.0417828	11.0	9.644e-03
10	18	31	2	3	4	1	0	543.0396538	4.0	1.177e-02







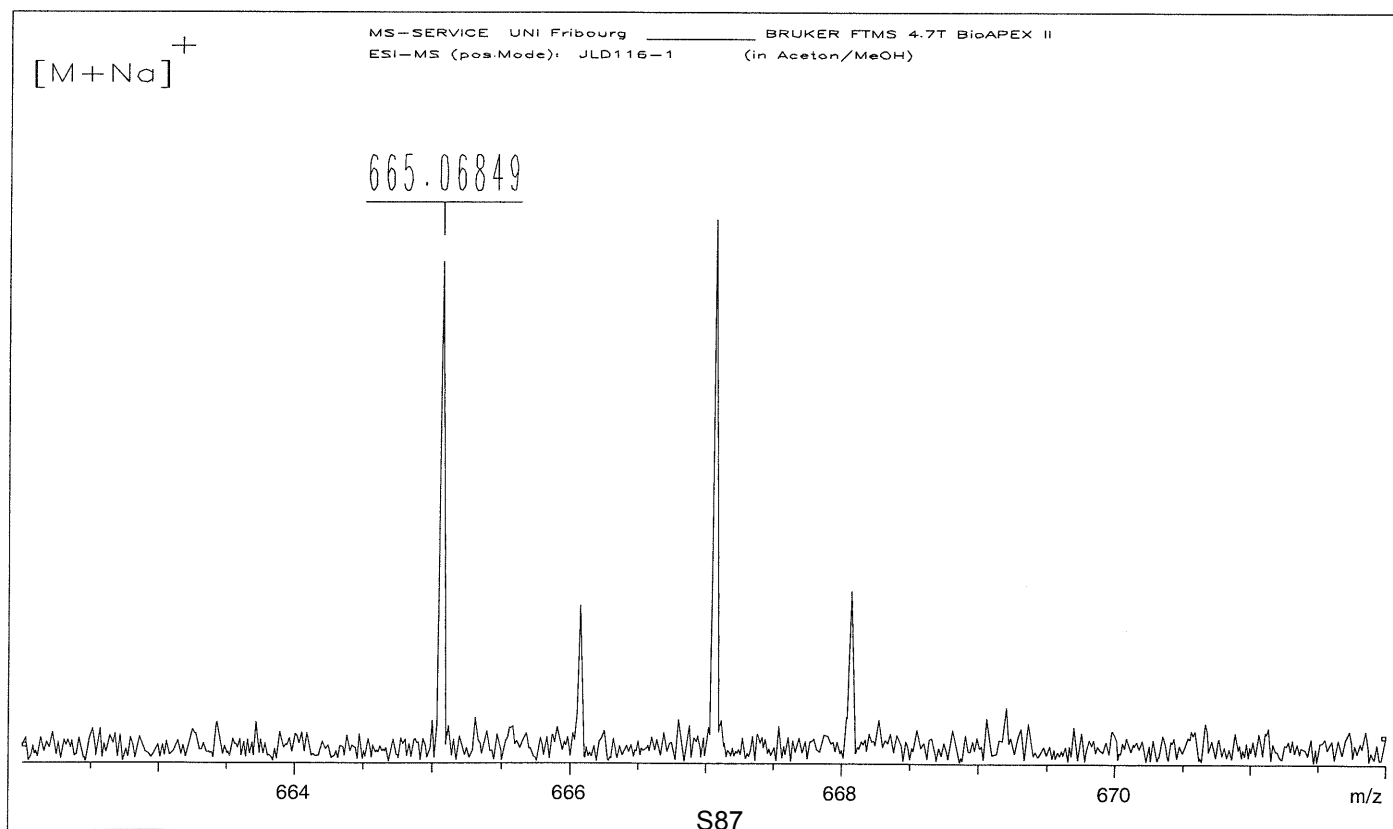
ESI-MS: JLD116-1

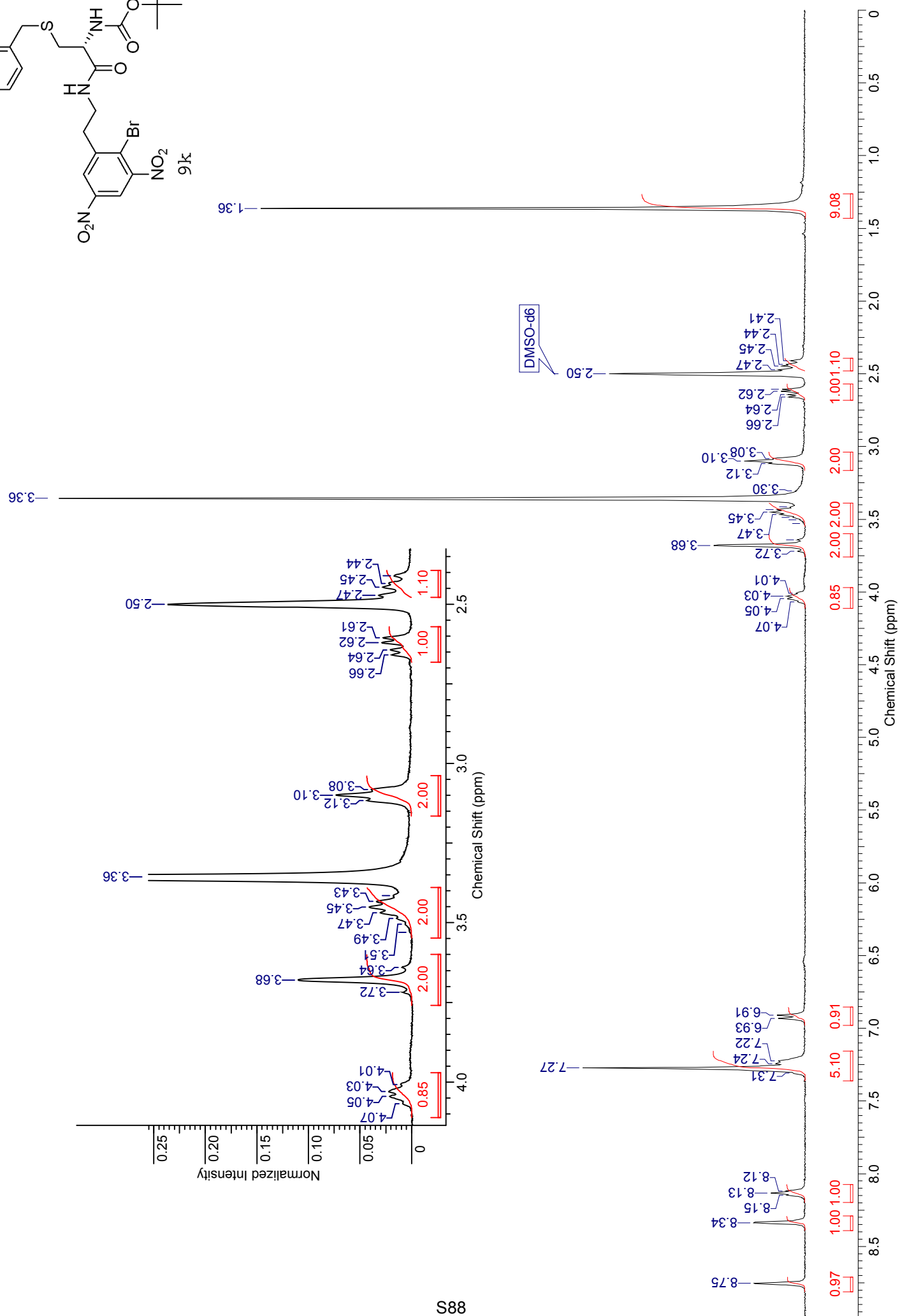
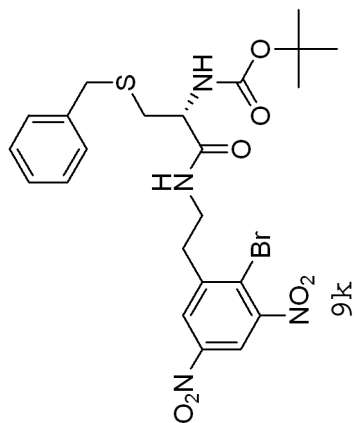
XMASS Mass Analysis for /Data/UNI_FR/DEBI2623_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

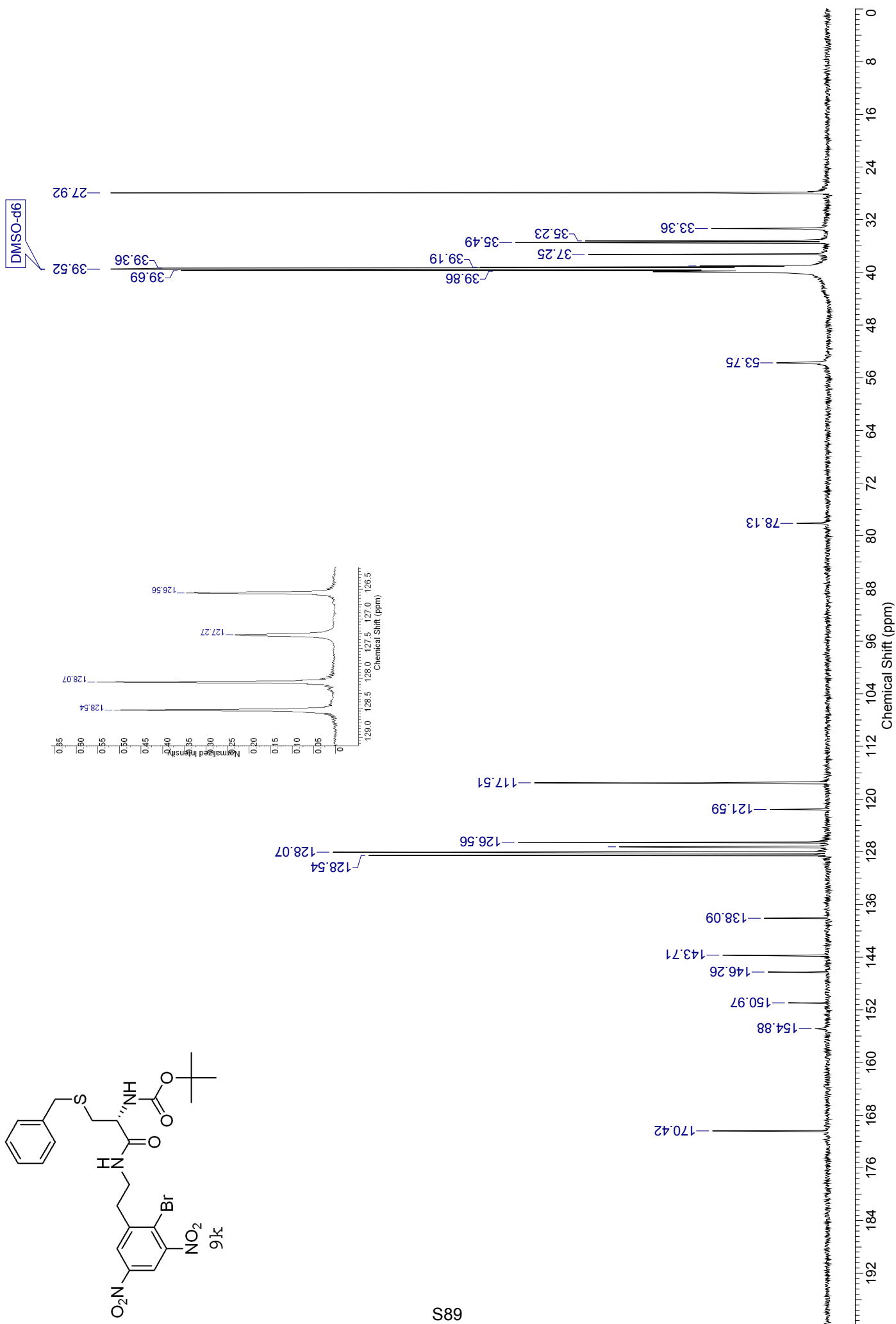
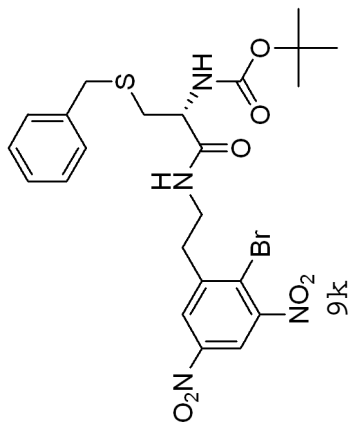
Ion mass = 665.0684900

Charge = +1

#	C	H	79Br	N	O	S	Na	mass	DBE	error
*** Mass Analysis for mass 665.0684900										
1	28	27	1	4	7	1	1	665.0676036	16.5	8.864e-04
2	21	39	2	4	6	2	0	665.0672280	3.5	1.262e-03
3	18	38	2	5	8	1	1	665.0700052	1.0	1.515e-03
4	30	26	1	4	7	1	0	665.0700089	19.5	1.519e-03
5	31	25	1	5	4	1	1	665.0702837	21.0	1.794e-03
6	25	31	1	4	7	2	1	665.0709744	11.5	2.484e-03
7	31	28	1	3	5	2	0	665.0648264	19.0	3.664e-03
8	19	40	2	4	6	2	1	665.0648227	0.5	3.667e-03
9	20	37	2	5	8	1	0	665.0724105	4.0	3.921e-03
10	33	24	1	5	4	1	0	665.0726890	24.0	4.199e-03

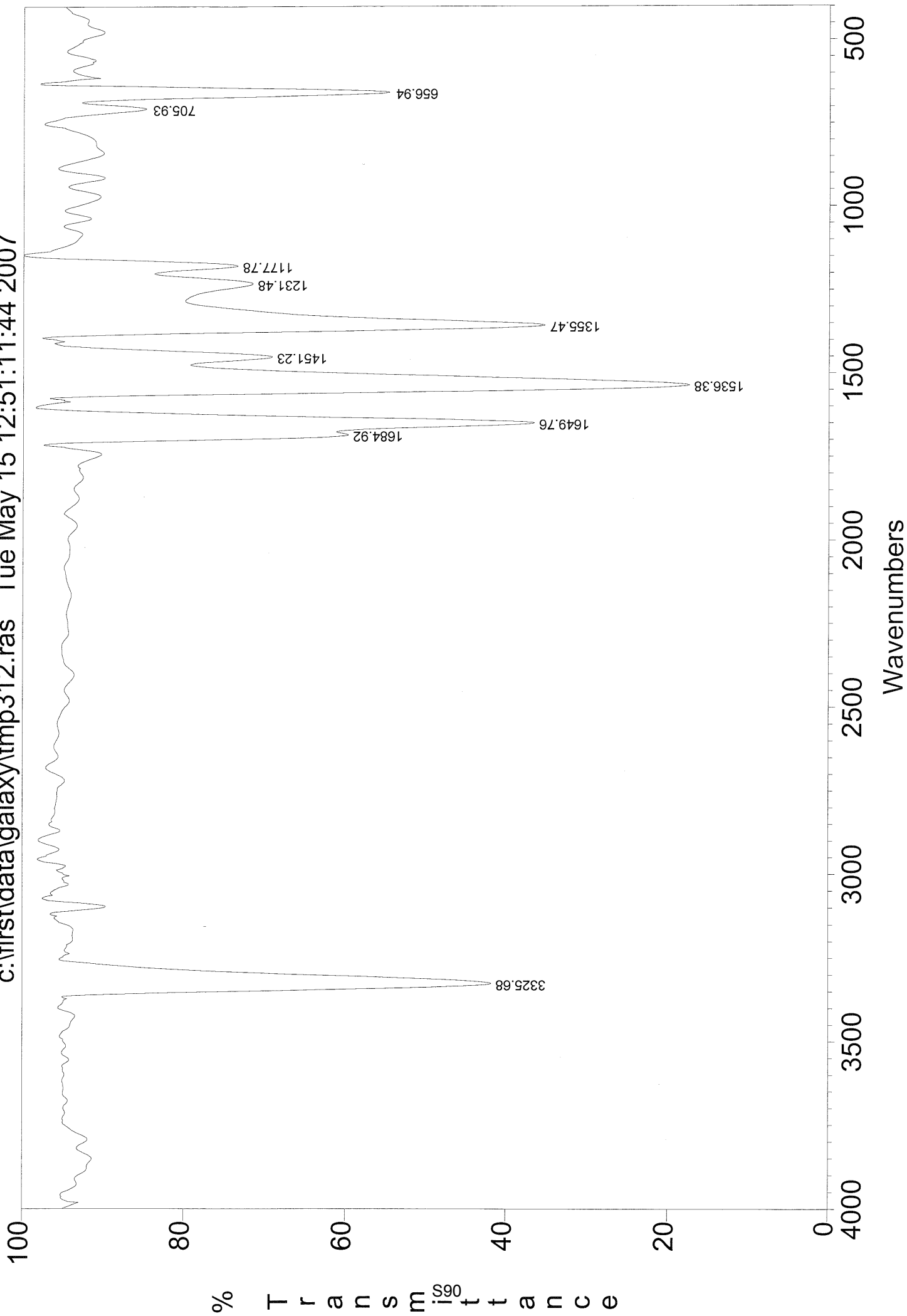






960128

c:\first\data\galaxy\tmp312.ras Tue May 15 12:51:11:44 2007



ESI-MS: JLD128-1

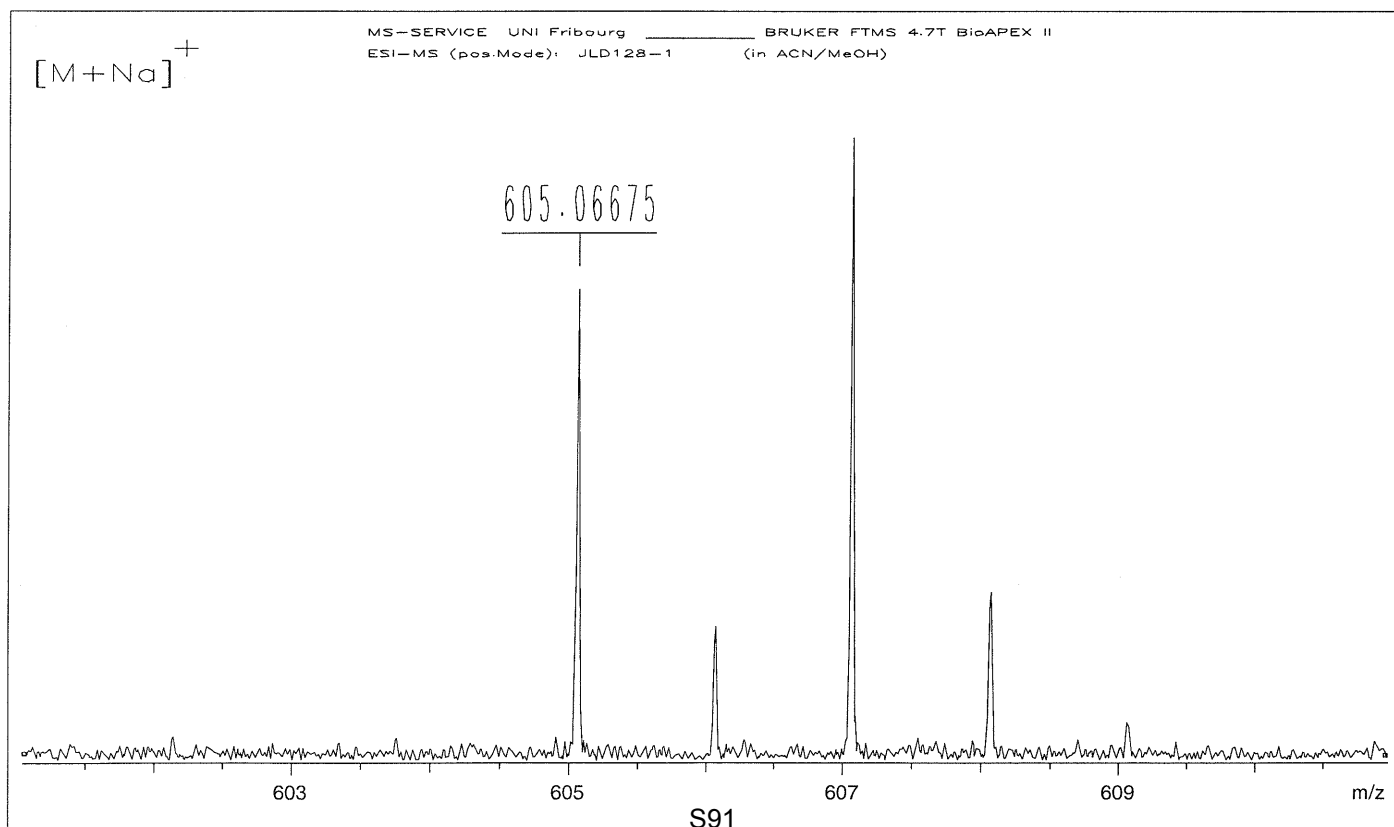
XMASS Mass Analysis for /Data/UNI_FR/DEBI2615_ESI/20/pdata/1/massanal.res:

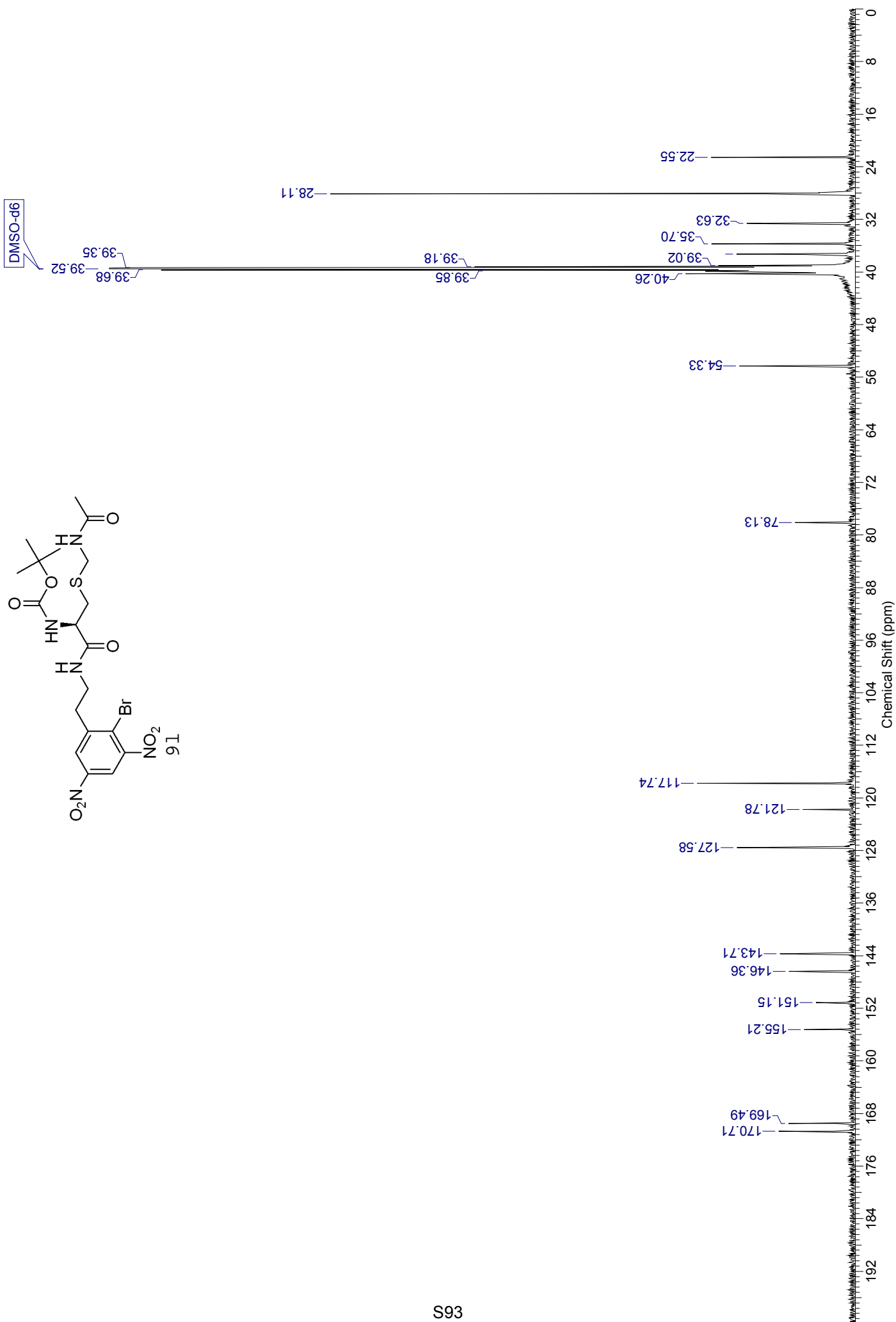
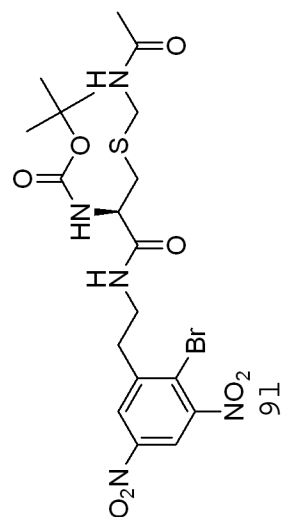
XMASS Mass Analysis Constraints

Ion mass = 605.0667460

Charge = +1

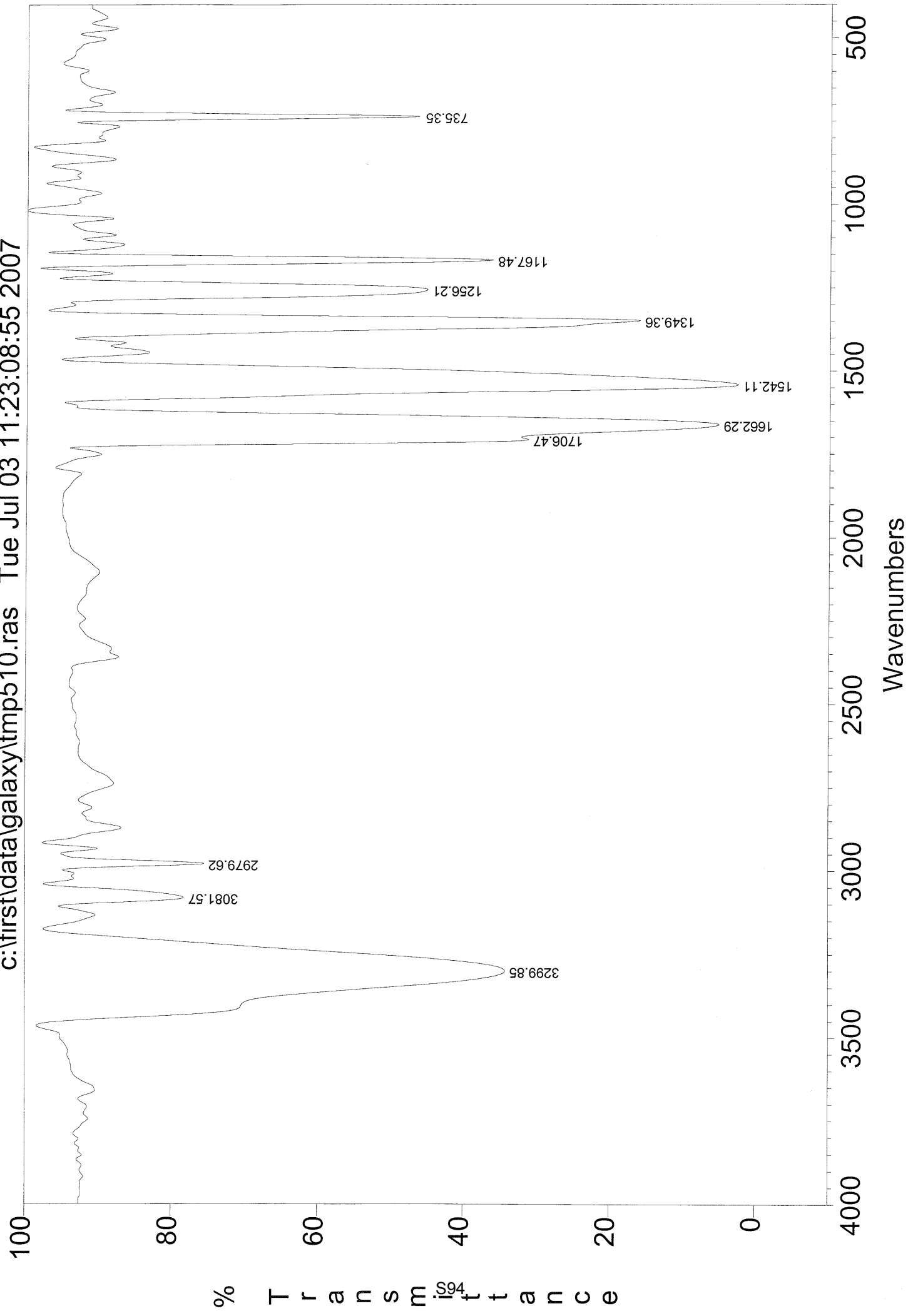
#	C	H	79Br	N	O	S	Na	mass	DBE	error
*** Mass Analysis for mass 605.0667460										
1	23	27	1	4	7	1	1	605.0676036	11.5	8.576e-04
2	26	28	1	3	5	2	0	605.0648264	14.0	1.920e-03
3	25	26	1	4	7	1	0	605.0700089	14.5	3.263e-03
4	26	25	1	5	4	1	1	605.0702837	16.0	3.538e-03
5	20	31	1	4	7	2	1	605.0709744	6.5	4.228e-03
6	24	29	1	3	5	2	1	605.0624211	11.0	4.325e-03
7	29	24	1	3	5	1	0	605.0614556	19.0	5.290e-03
8	21	28	1	5	7	2	0	605.0608037	10.0	5.942e-03
9	28	24	1	5	4	1	0	605.0726890	19.0	5.943e-03
10	22	30	1	4	7	2	0	605.0733797	9.5	6.634e-03





710A37

c:\first\data\galaxy\tmp510.ras Tue Jul 03 11:23:08:55 2007



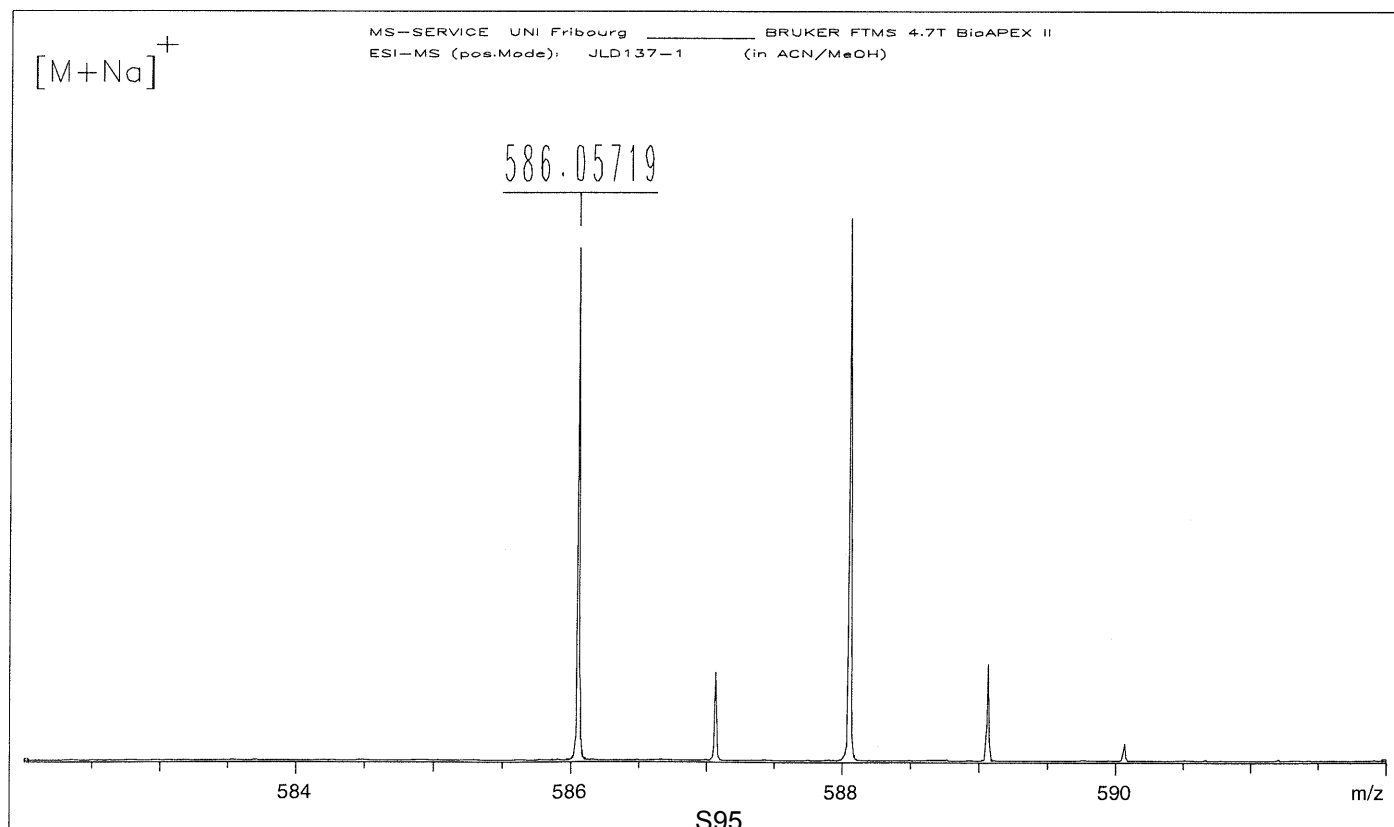
ESI-MS: JLD137-1

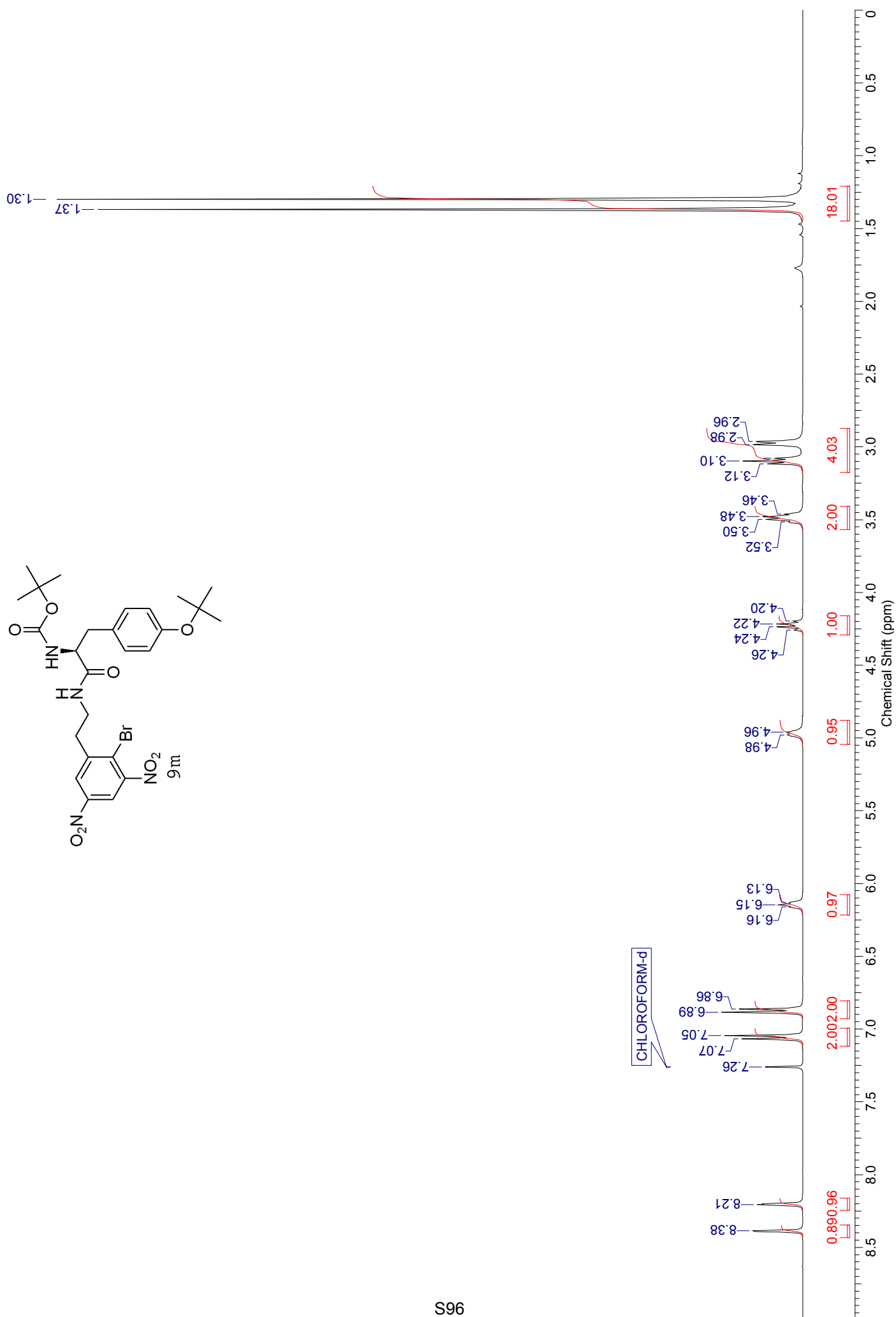
XMASS Mass Analysis for /Data/UNI_FR/DEBI2714_ESI/10/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

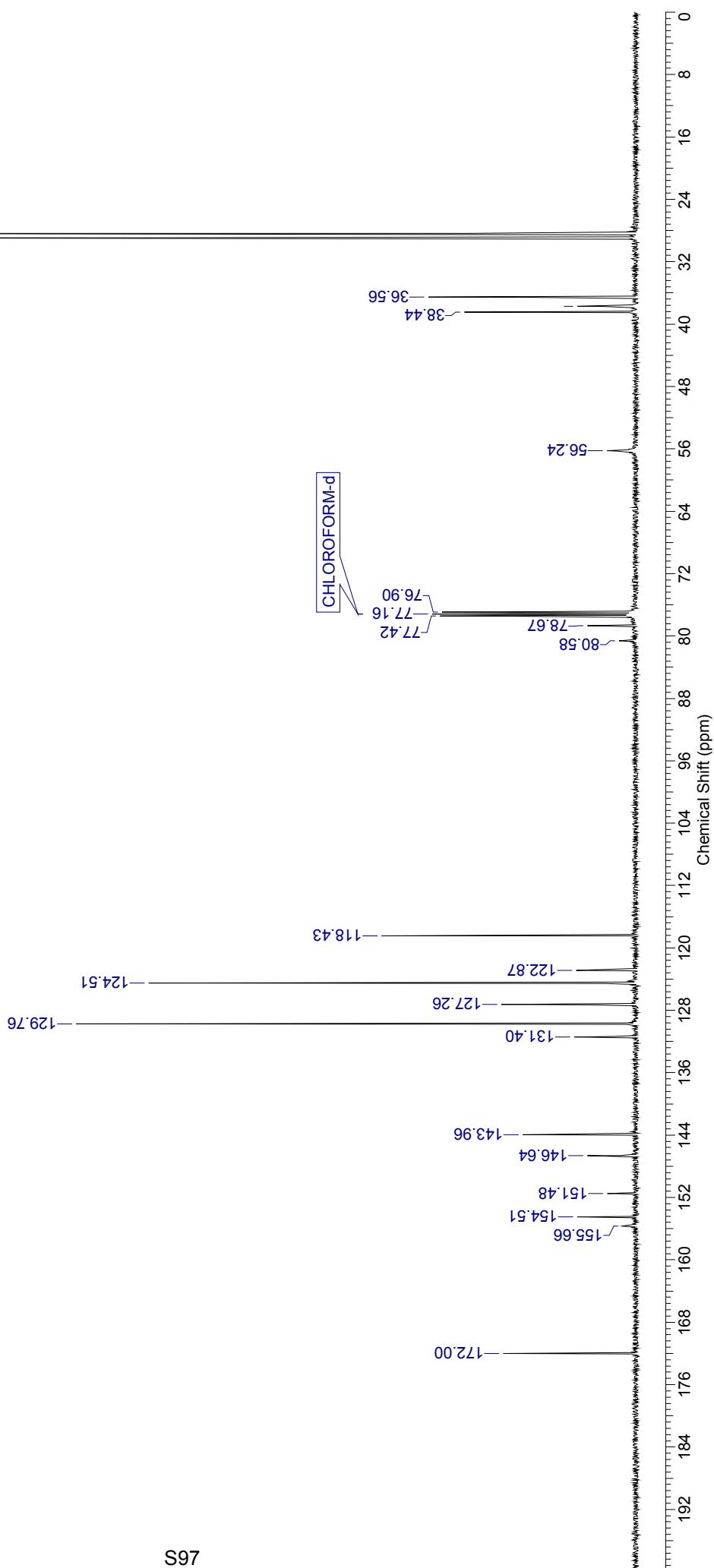
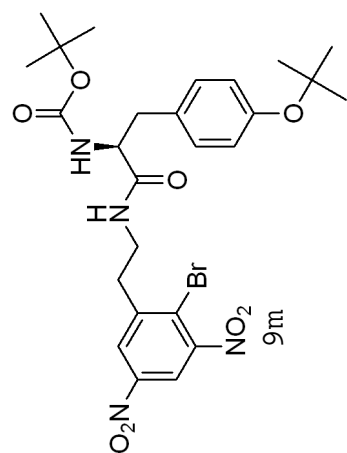
Ion mass = 586.0571940

Charge = +1

#	C	H	79Br	N	O	S	Na	mass	DBE	error
*** Mass Analysis for mass 586.0571940										
1	19	26	1	5	8	1	1	586.0577672	8.5	5.732e-04
2	20	34	2	3	5	1	0	586.0580435	4.5	8.495e-04
3	14	31	1	5	8	2	2	586.0587327	0.5	1.539e-03
4	18	35	2	3	5	1	1	586.0556382	1.5	1.556e-03
5	17	27	1	5	8	1	2	586.0553619	5.5	1.832e-03
6	22	27	1	3	6	1	2	586.0593847	9.5	2.191e-03
7	22	27	1	4	6	2	0	586.0549900	11.0	2.204e-03
8	21	25	1	5	8	1	0	586.0601725	11.5	2.979e-03
9	15	34	2	5	7	1	0	586.0540208	0.5	3.173e-03
10	16	30	1	5	8	2	1	586.0611380	3.5	3.944e-03

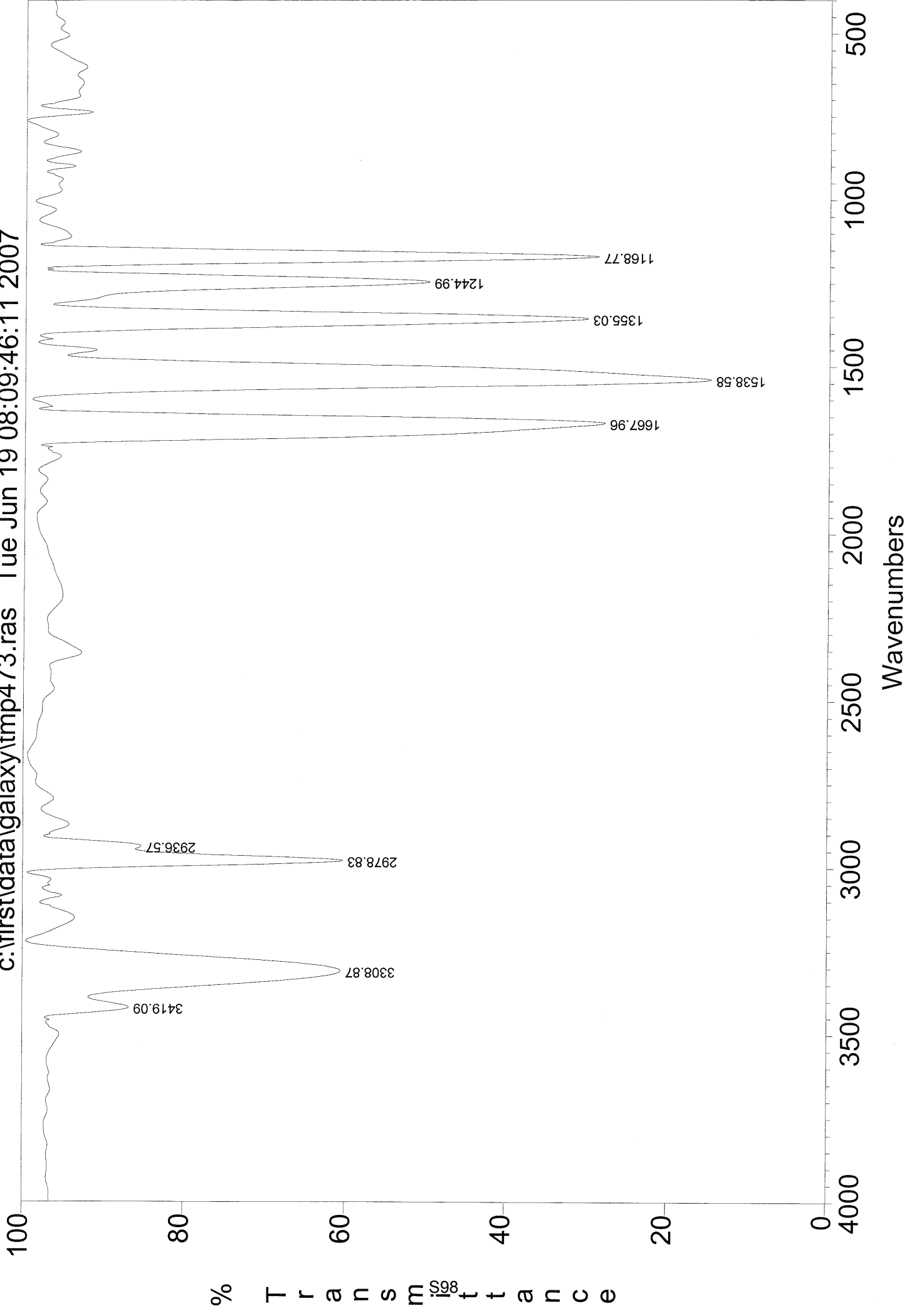






7/01/32

c:\first\data\galaxy\tmp473.ras Tue Jun 19 08:09:46:11 2007





FTMS 4.7T BioAPEX II MS-Service UNI-Fribourg

ESI-MS: JLD132-1

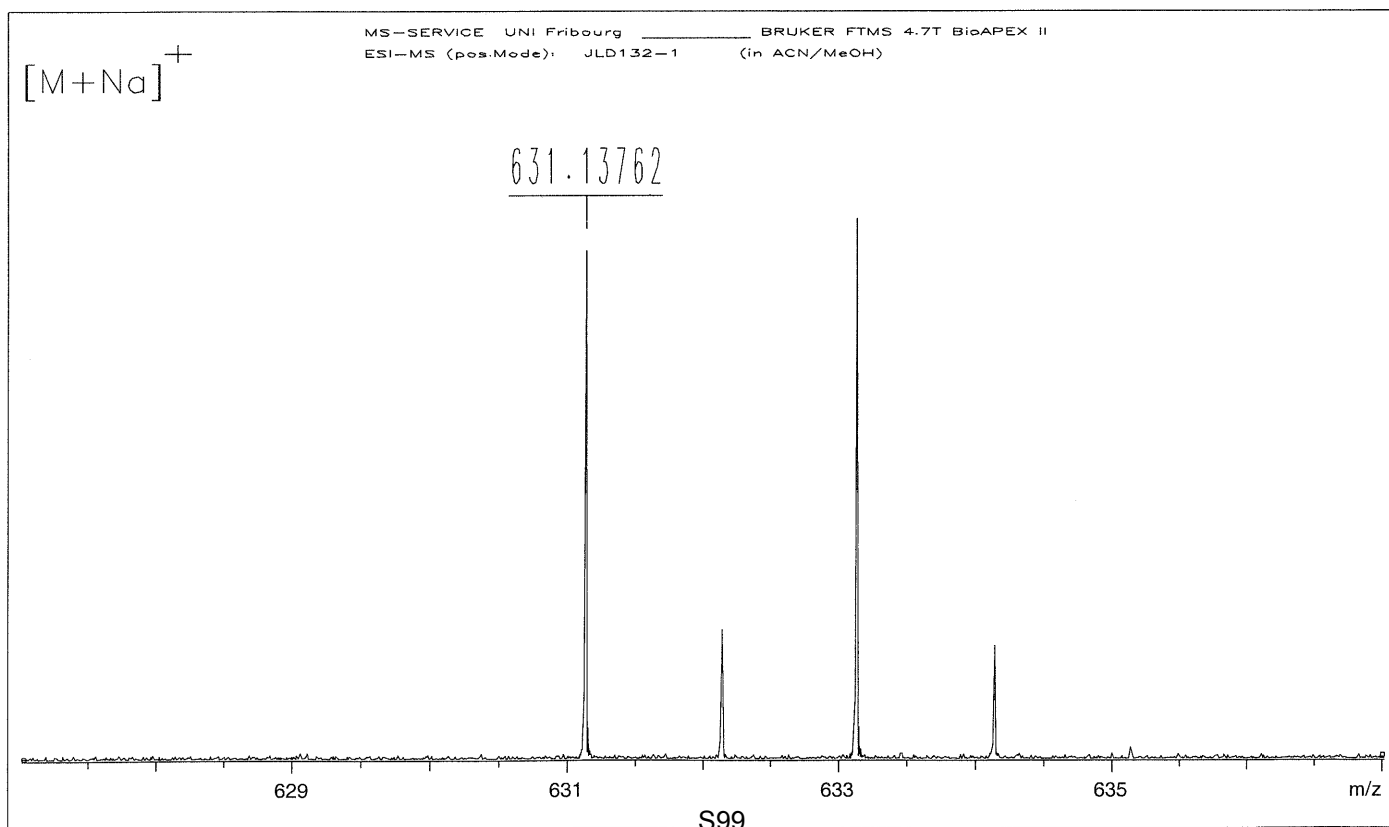
XMASS Mass Analysis for /Data/UNI_FR/DEBI2676_ESI/10/pdata/1/massanal.res:

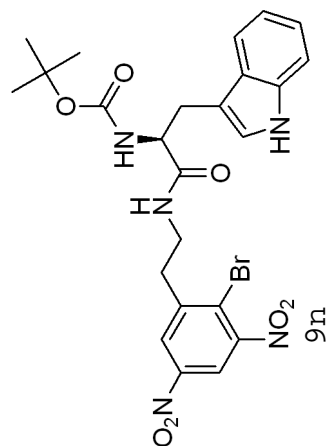
XMASS Mass Analysis Constraints

Ion mass = 631.1376210

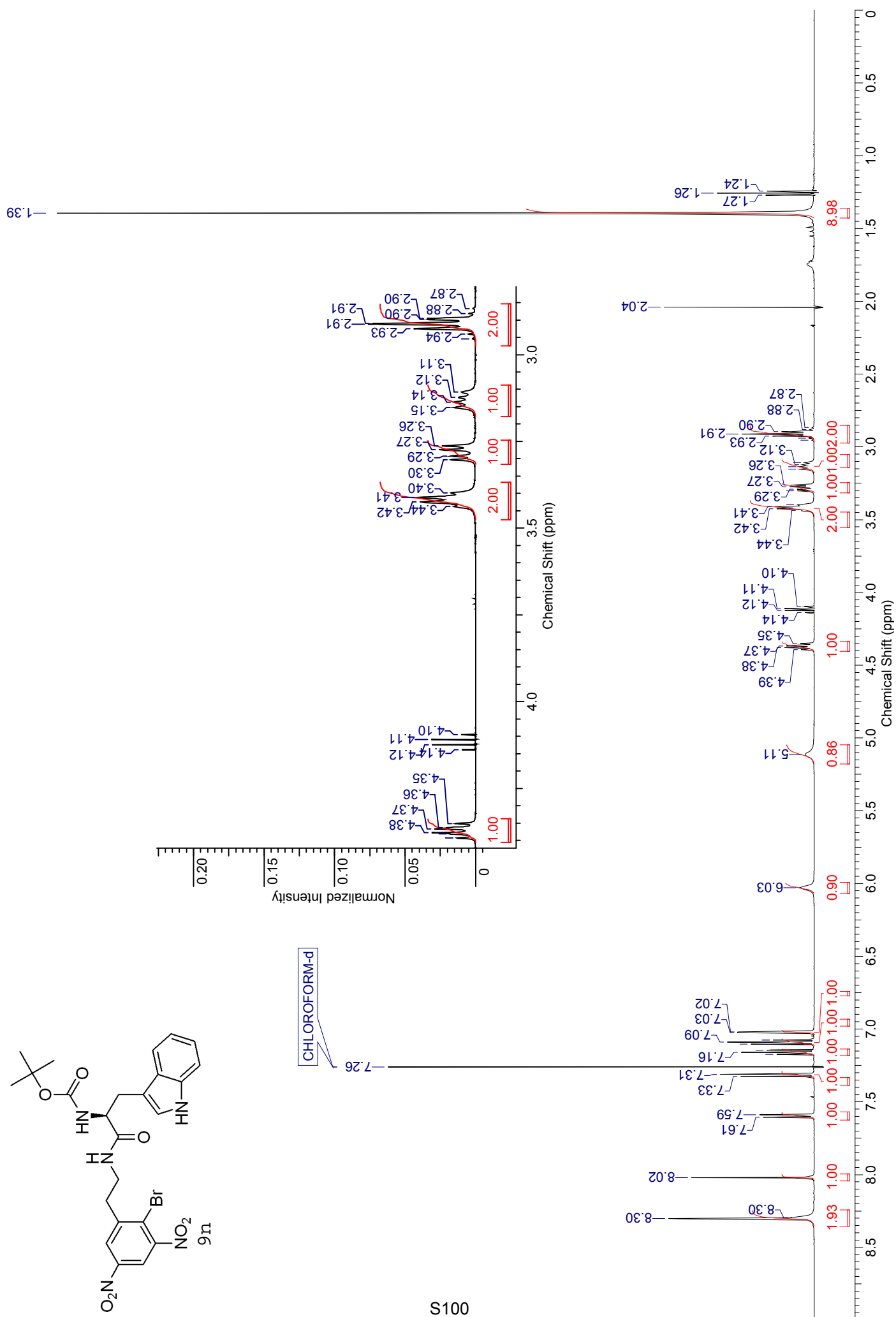
Charge = +1

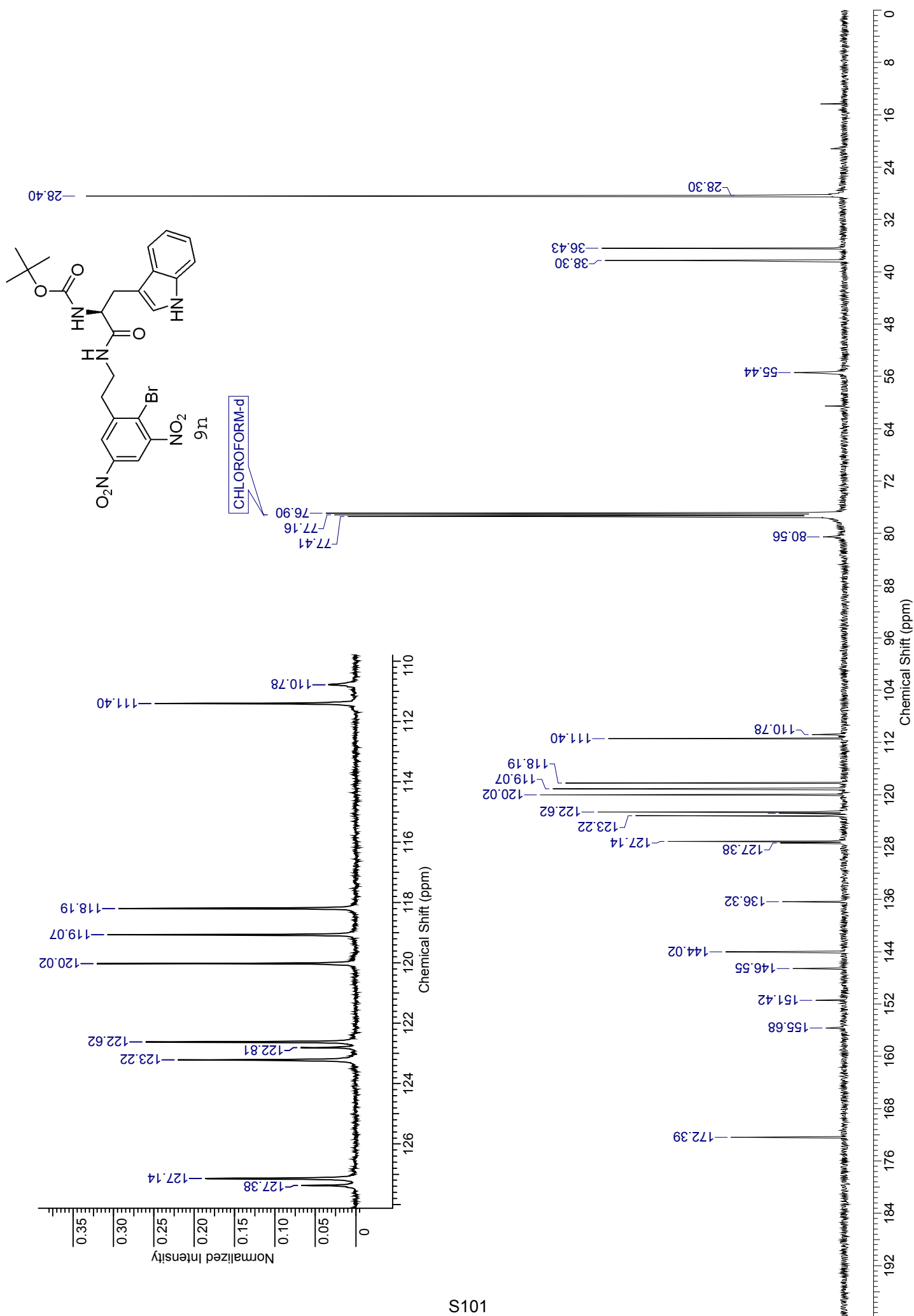
#	C	H	79Br	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 631.1376210									
1	26	33	1	4	8	1	631.1373977	11.5	2.233e-04
2	25	39	2	5	4	0	631.1363314	8.0	1.290e-03
3	28	32	1	4	8	0	631.1398030	14.5	2.182e-03
4	29	31	1	5	5	1	631.1400778	16.0	2.457e-03
5	23	40	2	5	4	1	631.1339261	5.0	3.695e-03
6	22	41	2	4	7	0	631.1336513	3.5	3.970e-03
7	19	42	2	6	6	1	631.1424794	0.5	4.858e-03
8	31	30	1	5	5	0	631.1424831	19.0	4.862e-03
9	20	42	2	4	7	1	631.1312460	0.5	6.375e-03
10	21	41	2	6	6	0	631.1448847	3.5	7.264e-03





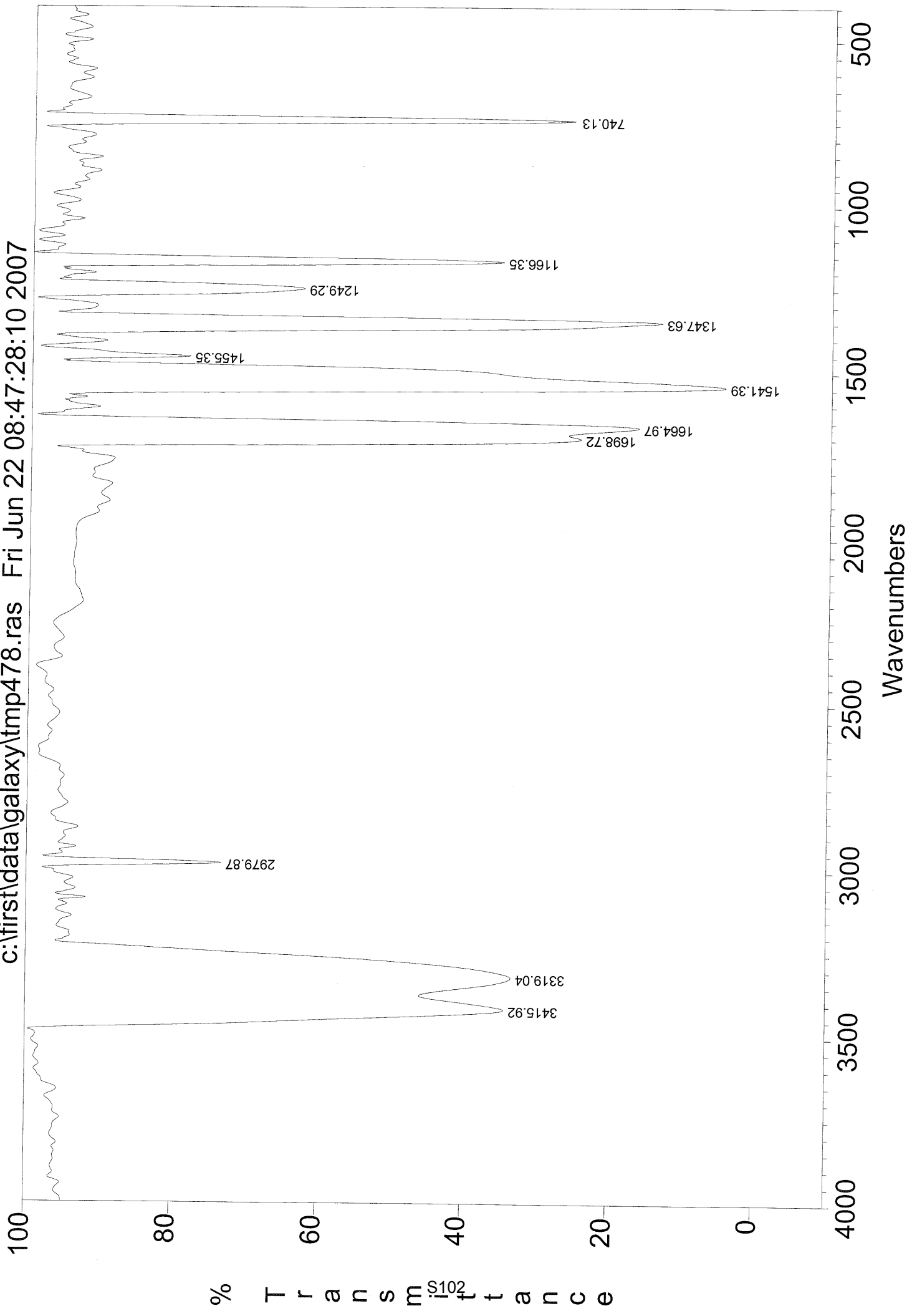
S100





960135

c:\first\data\galaxy\tmp478.ras Fri Jun 22 08:47:28:10 2007



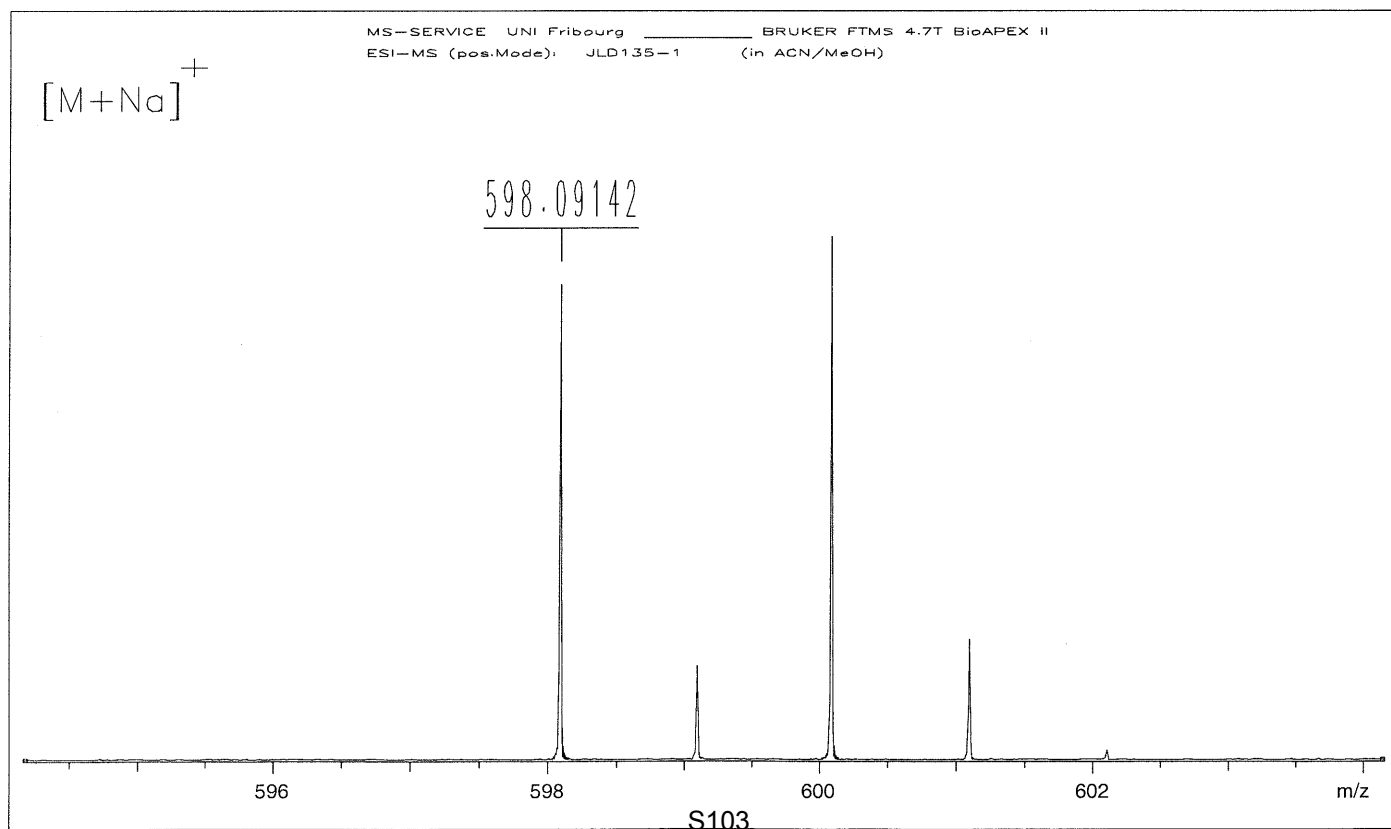
ESI-MS: JLD135-1

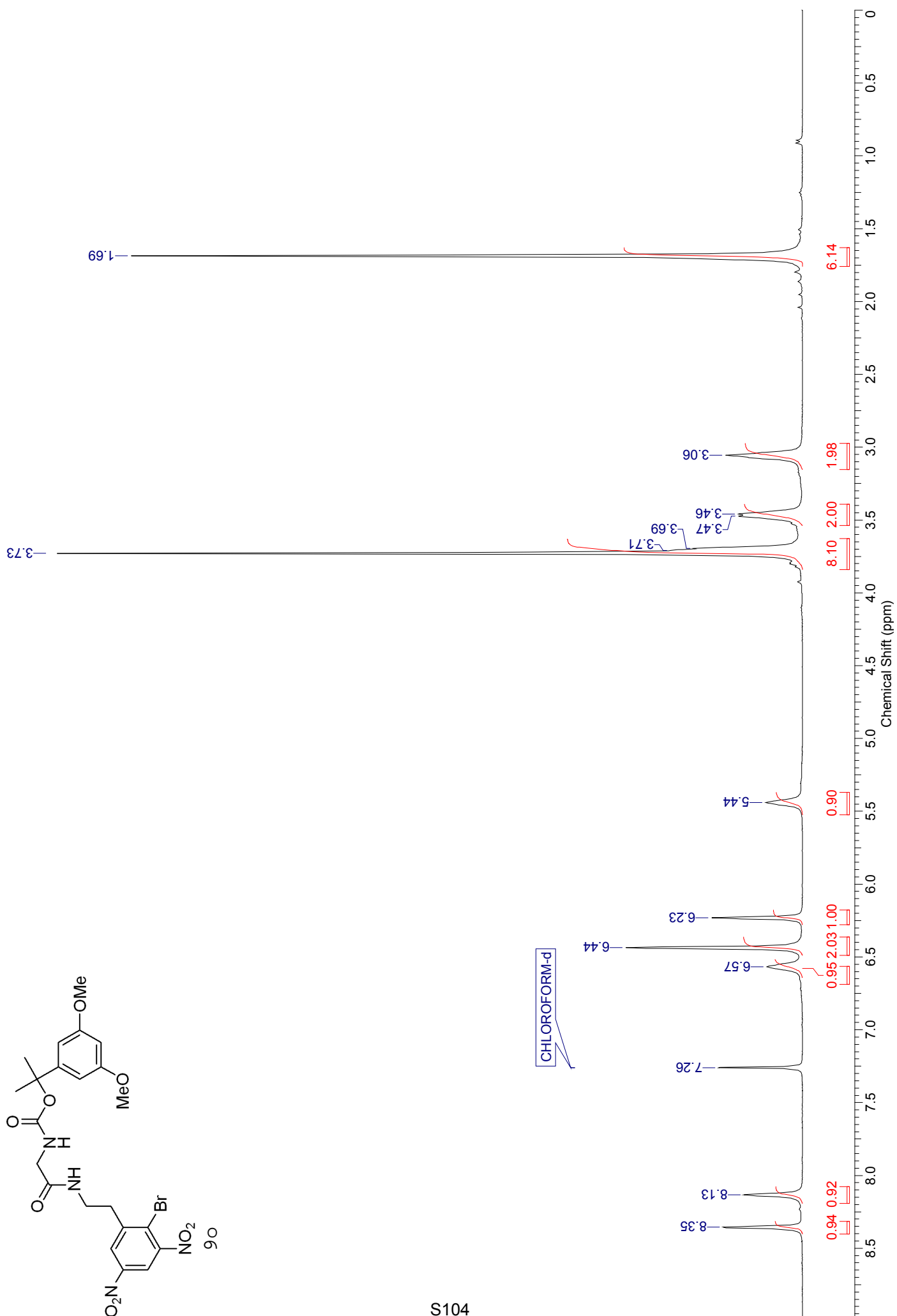
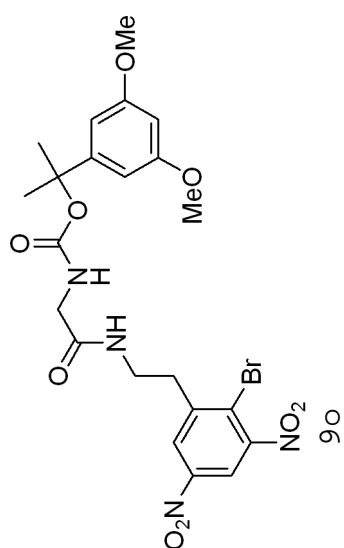
XMASS Mass Analysis for /Data/UNI_FR/DEBI2678_ESI/5/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

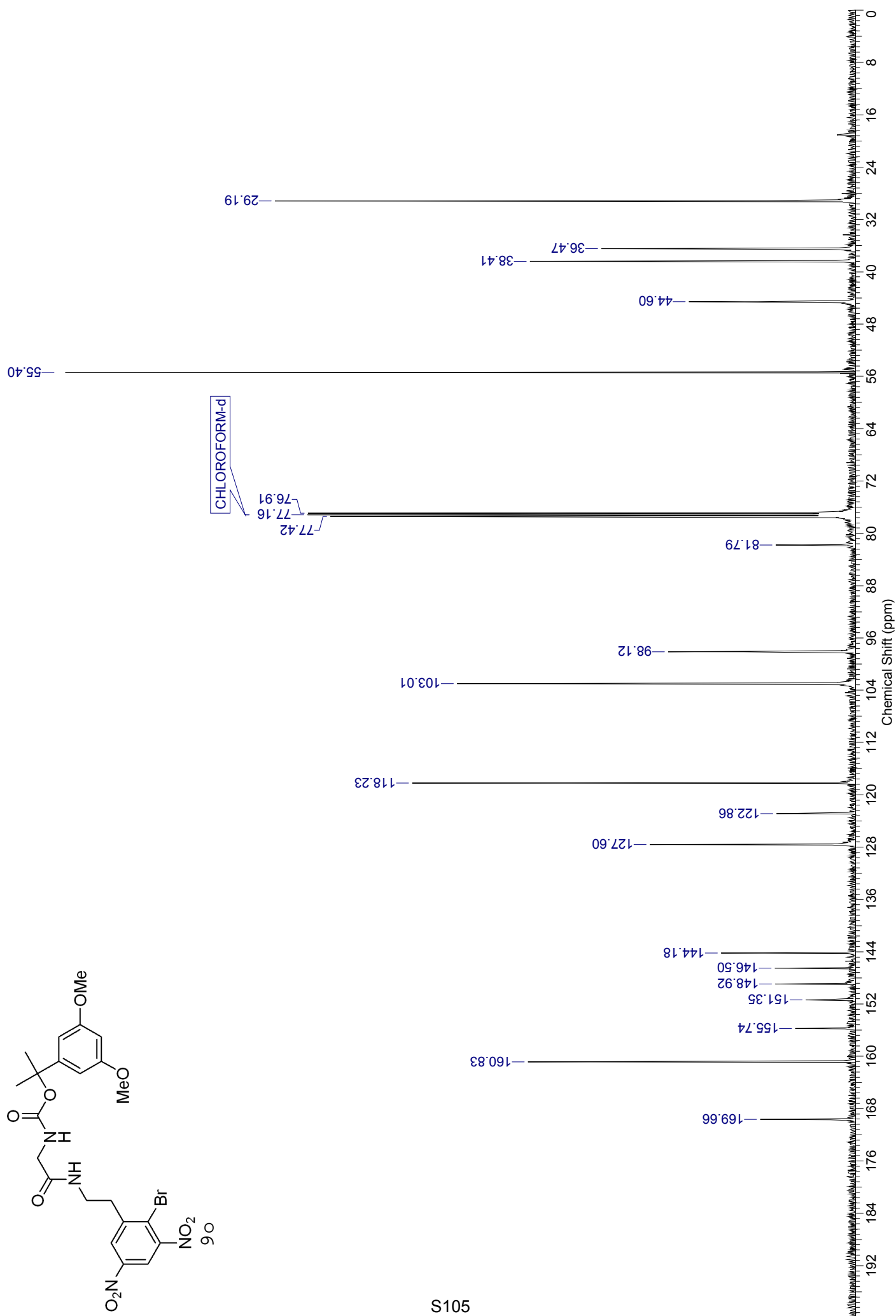
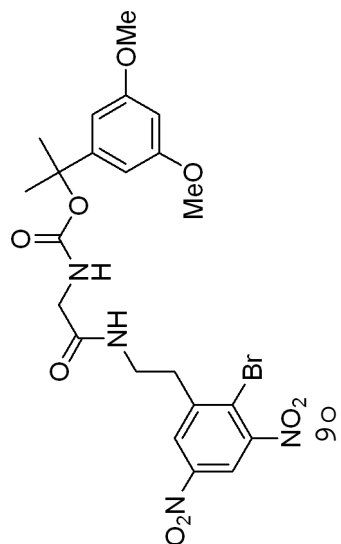
Ion mass = 598.0914220

Charge = +1

#	C	H	79Br	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 598.0914220									
1	24	26	1	5	7	1	598.0907819	13.5	6.401e-04
2	14	37	2	6	8	1	598.0931835	-2.0	1.761e-03
3	26	25	1	5	7	0	598.0931872	16.5	1.765e-03
4	27	24	1	6	4	1	598.0934620	18.0	2.040e-03
5	16	36	2	6	8	0	598.0955888	1.0	4.167e-03
6	20	34	2	5	6	0	598.0870355	5.5	4.387e-03
7	29	23	1	6	4	0	598.0958673	21.0	4.445e-03
8	19	37	2	4	6	1	598.0972062	2.0	5.784e-03
9	30	23	1	4	5	0	598.0846339	21.0	6.788e-03
10	18	35	2	5	6	1	598.0846302	2.5	6.792e-03

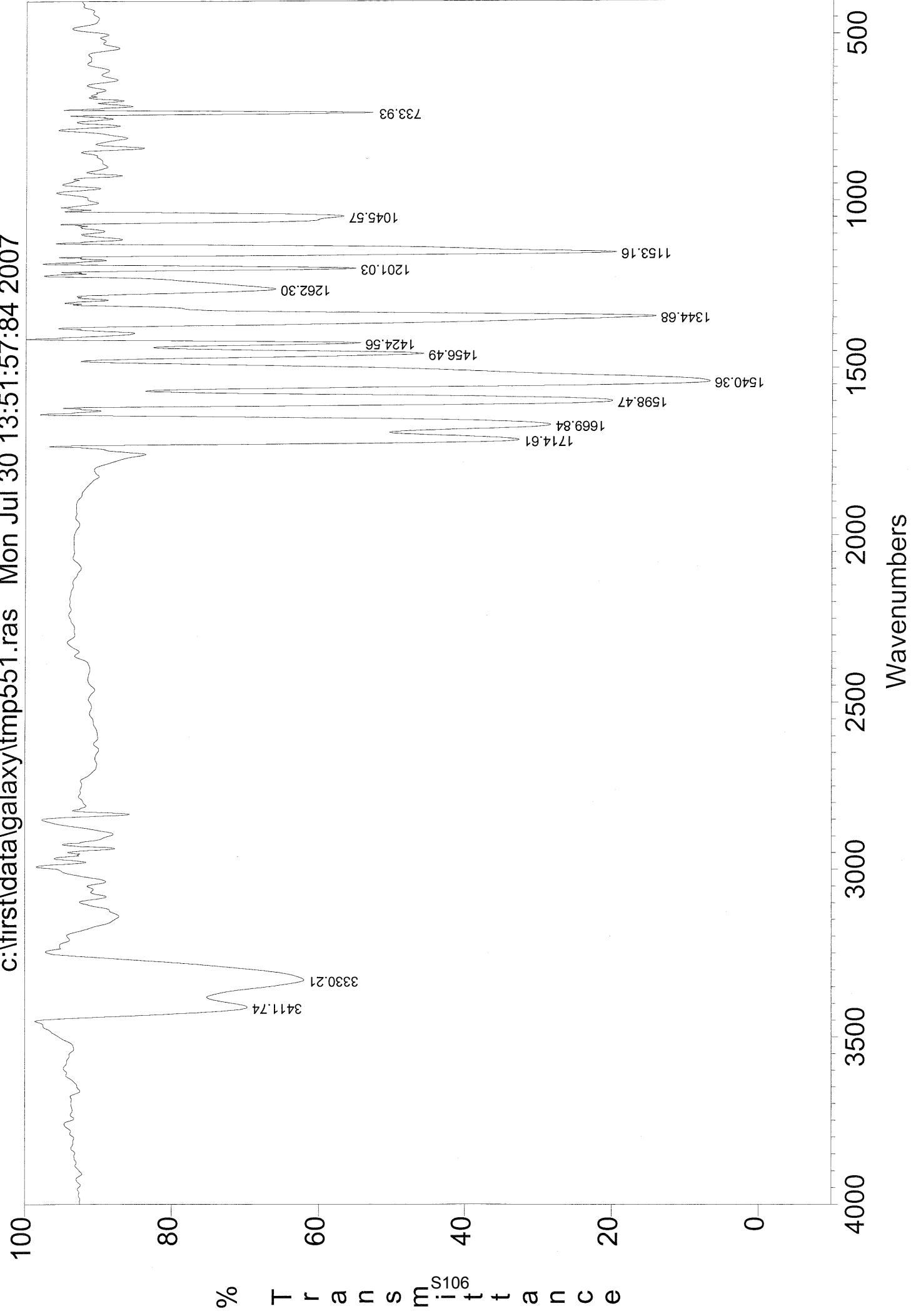






920144

c:\first\data\galaxy\tmp551.ras Mon Jul 30 13:51:57:84 2007



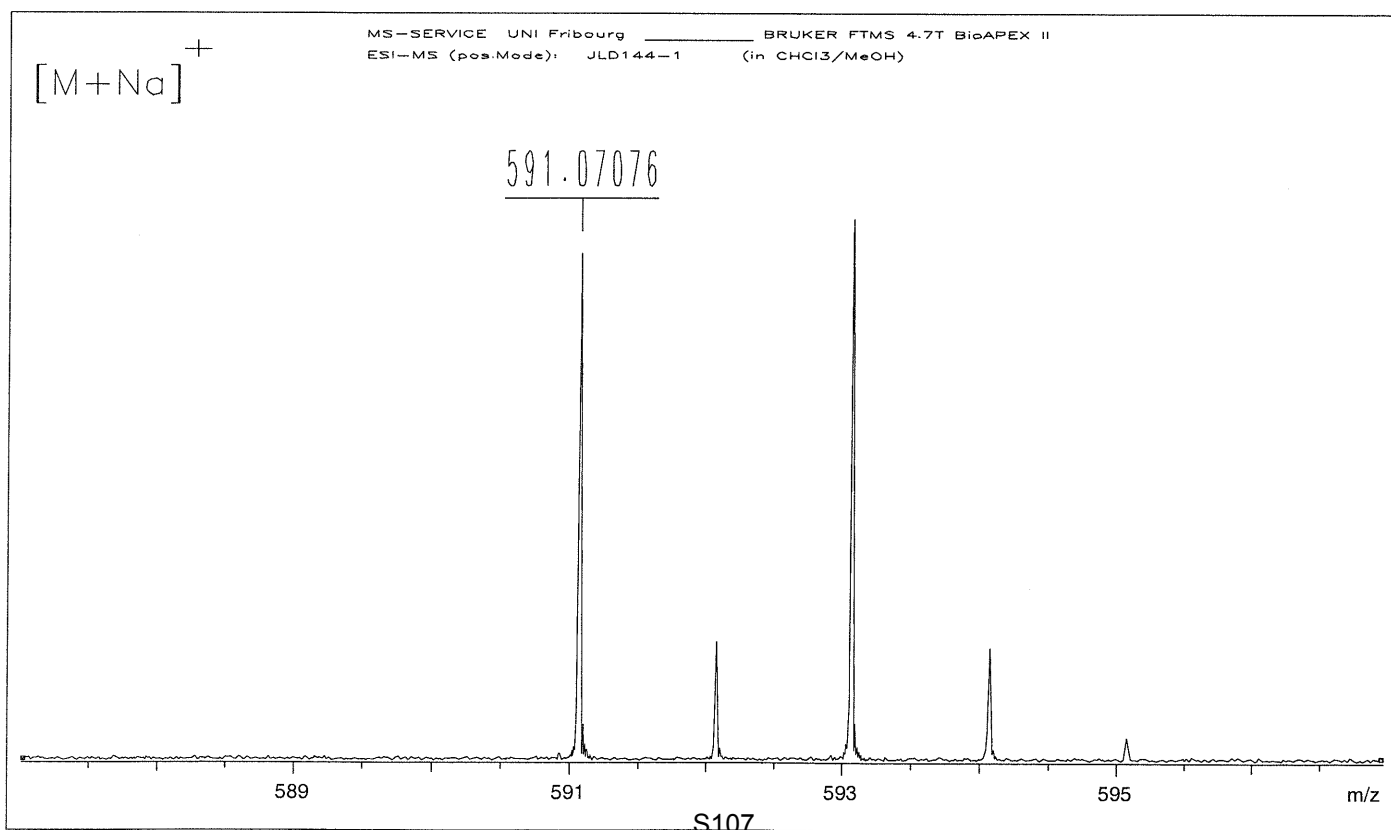
ESI-MS: JLD144-1

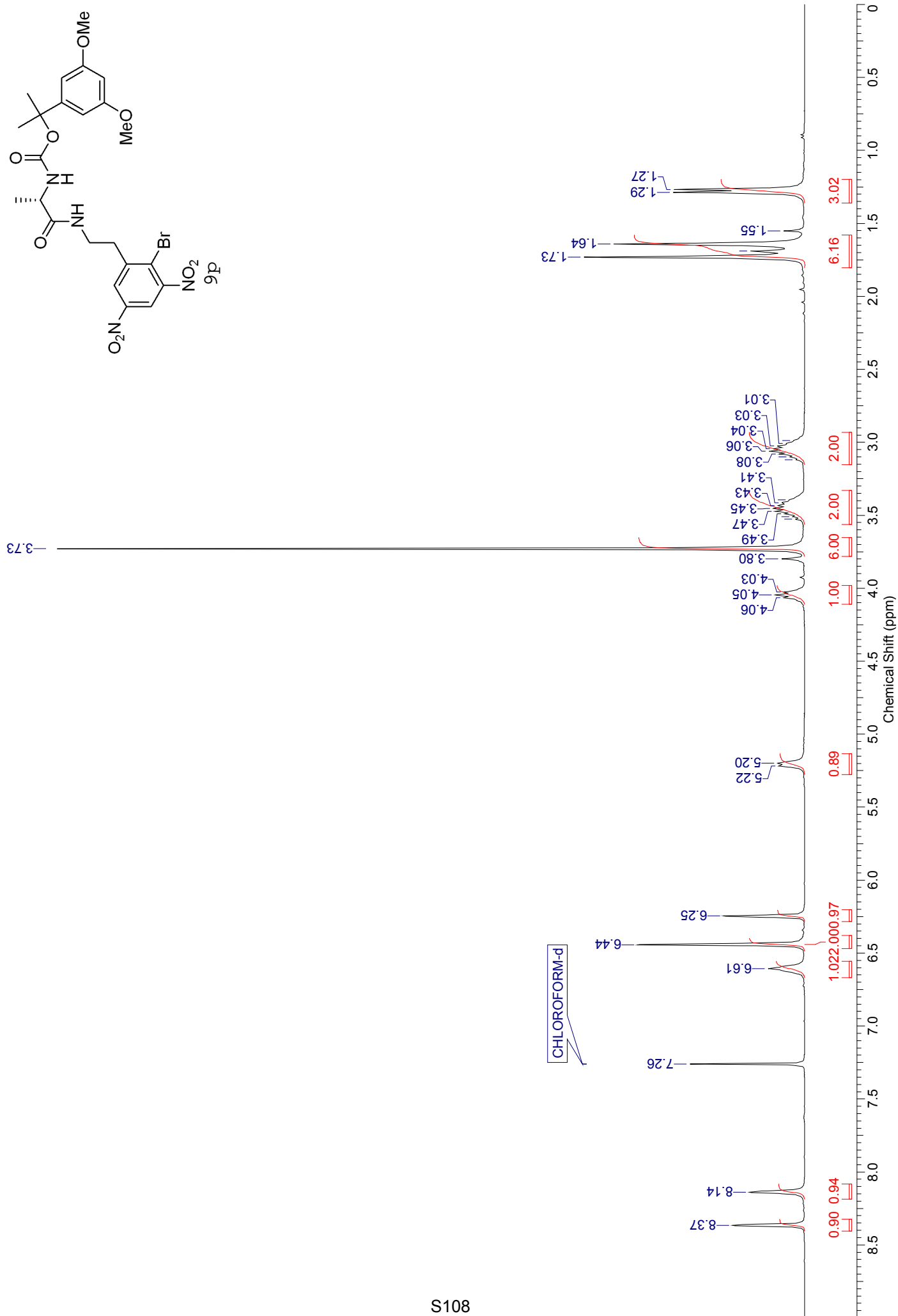
XMASS Mass Analysis for /Data/UNI_FR/DEBI2790_ESI/10/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

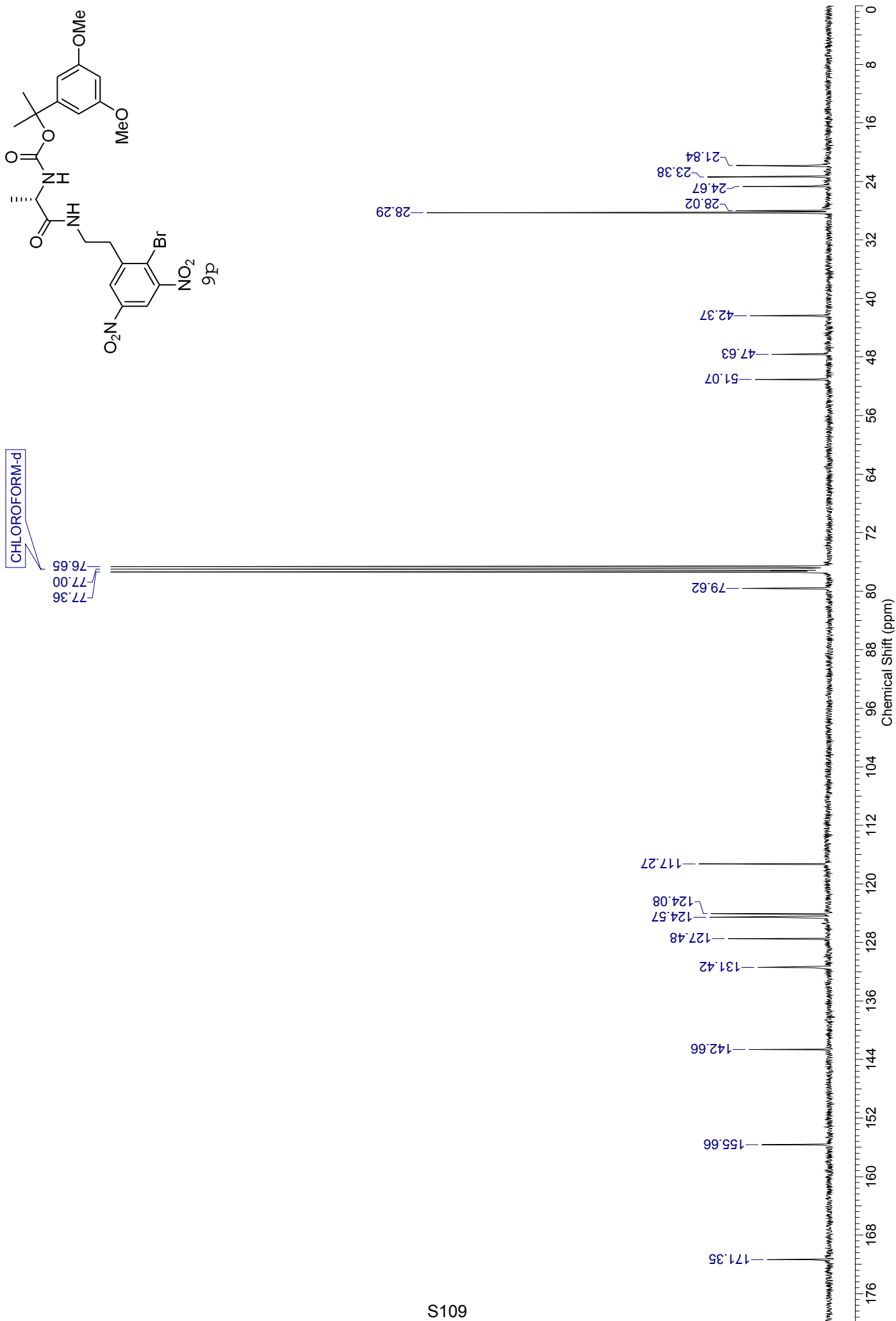
Ion mass = 591.0707590

Charge = +1

#	C	H	79Br	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 591.0707590									
1	22	25	1	4	9	1	591.0697121	11.5	1.047e-03
2	24	24	1	4	9	0	591.0721174	14.5	1.358e-03
3	14	35	2	5	10	0	591.0745190	-1.0	3.760e-03
4	18	33	2	4	8	0	591.0659657	3.5	4.793e-03
5	17	36	2	3	8	1	591.0761364	0.0	5.377e-03
6	28	22	1	3	7	0	591.0635641	19.0	7.195e-03
7	16	34	2	4	8	1	591.0635604	0.5	7.199e-03
8	15	35	2	3	11	0	591.0632856	-1.0	7.473e-03
9	18	27	1	5	11	1	591.0782654	7.0	7.506e-03
10	19	35	2	3	8	0	591.0785417	3.0	7.783e-03

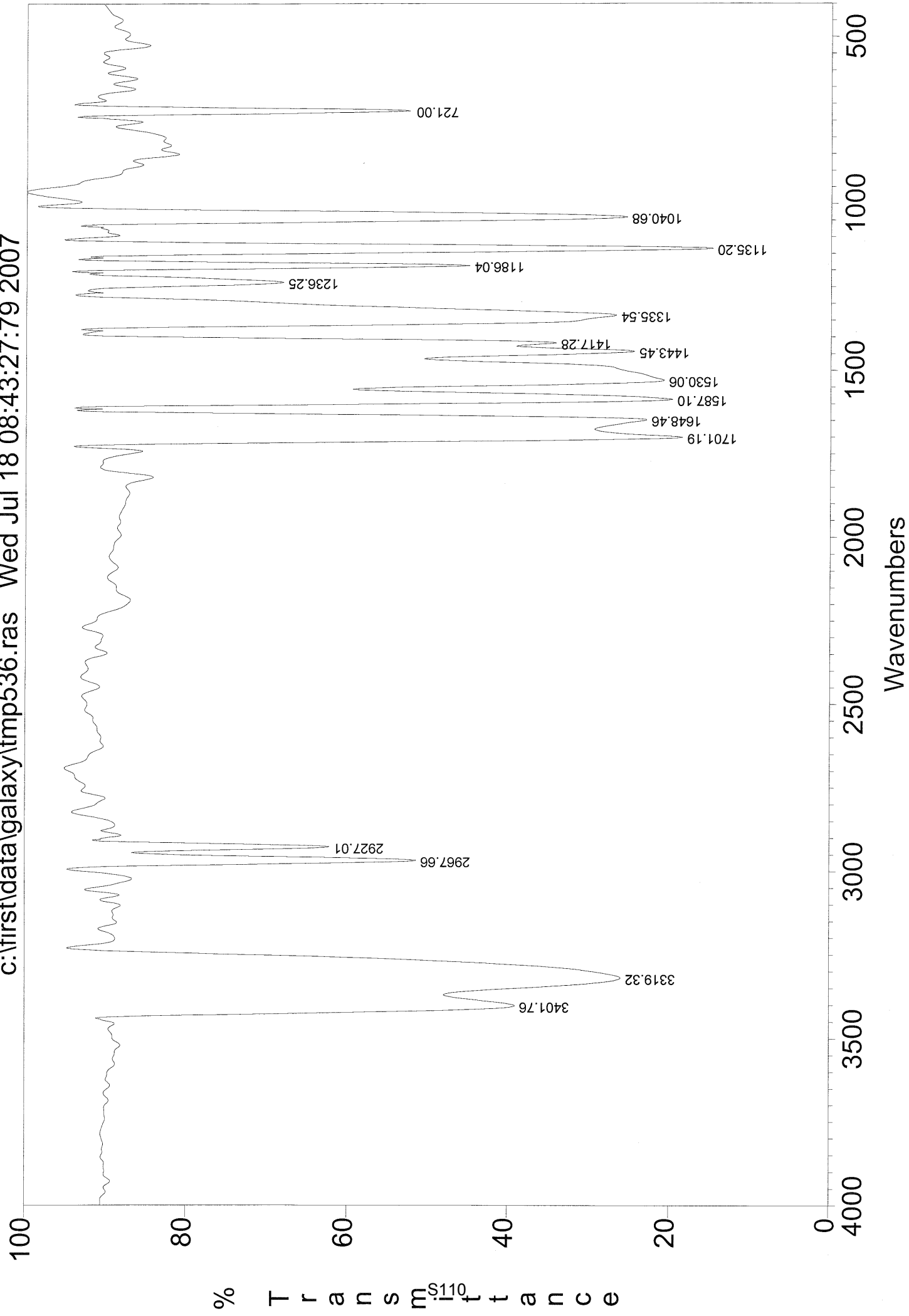






76D142

c:\first\data\galaxy\tmp536.ras Wed Jul 18 08:43:27:79 2007



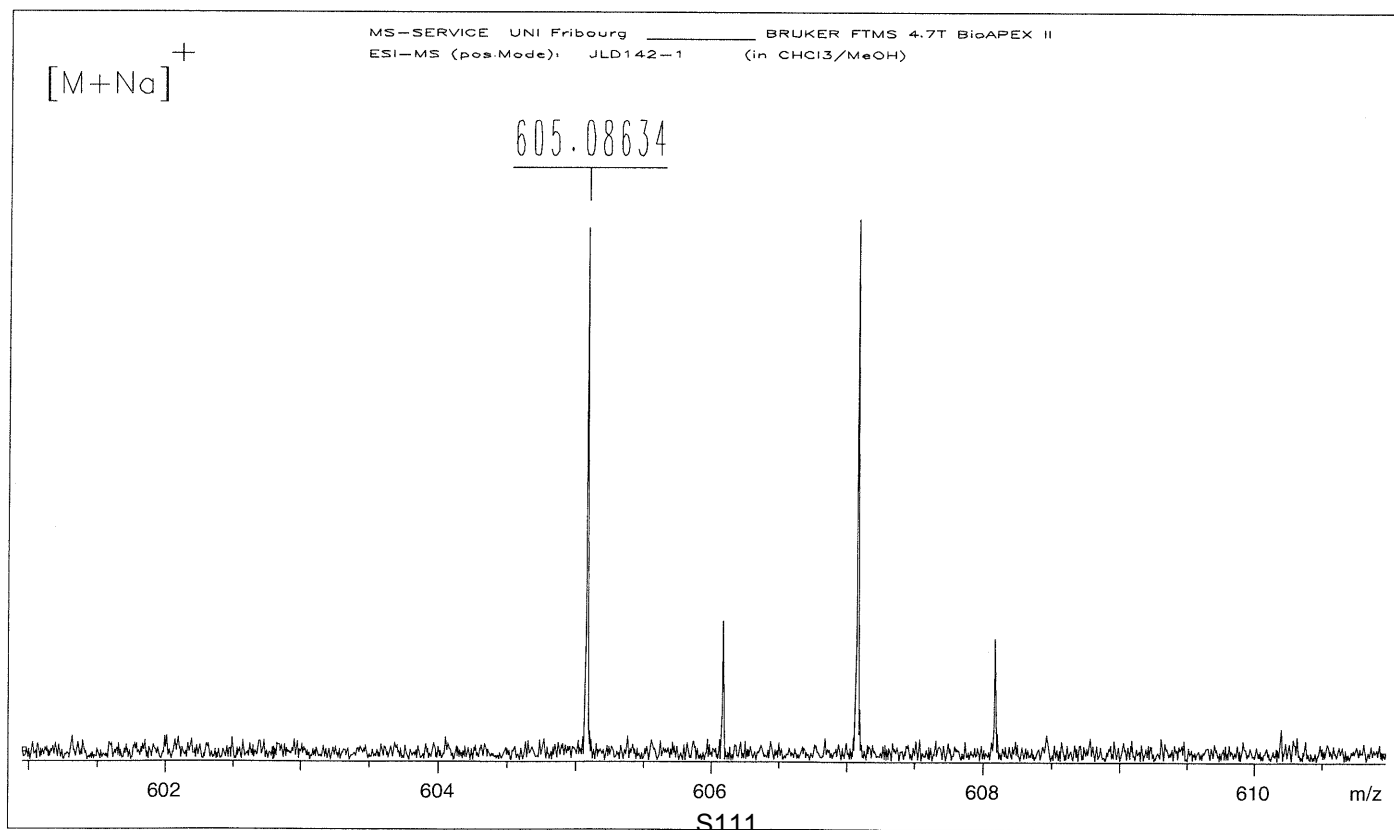
ESI-MS: JLD142-1

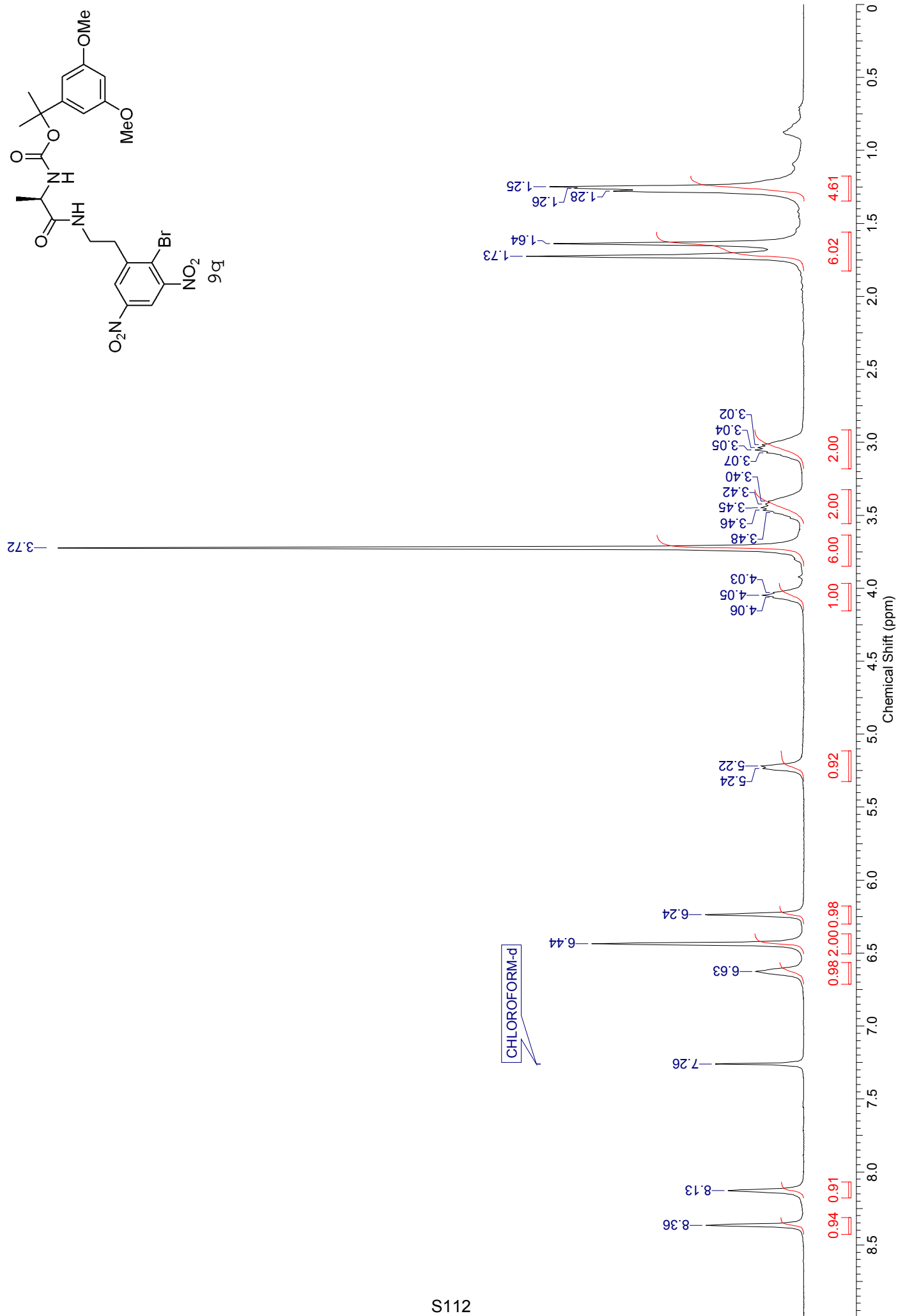
XMASS Mass Analysis for /Data/UNI_FR/DEBI2758_ESI/5/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

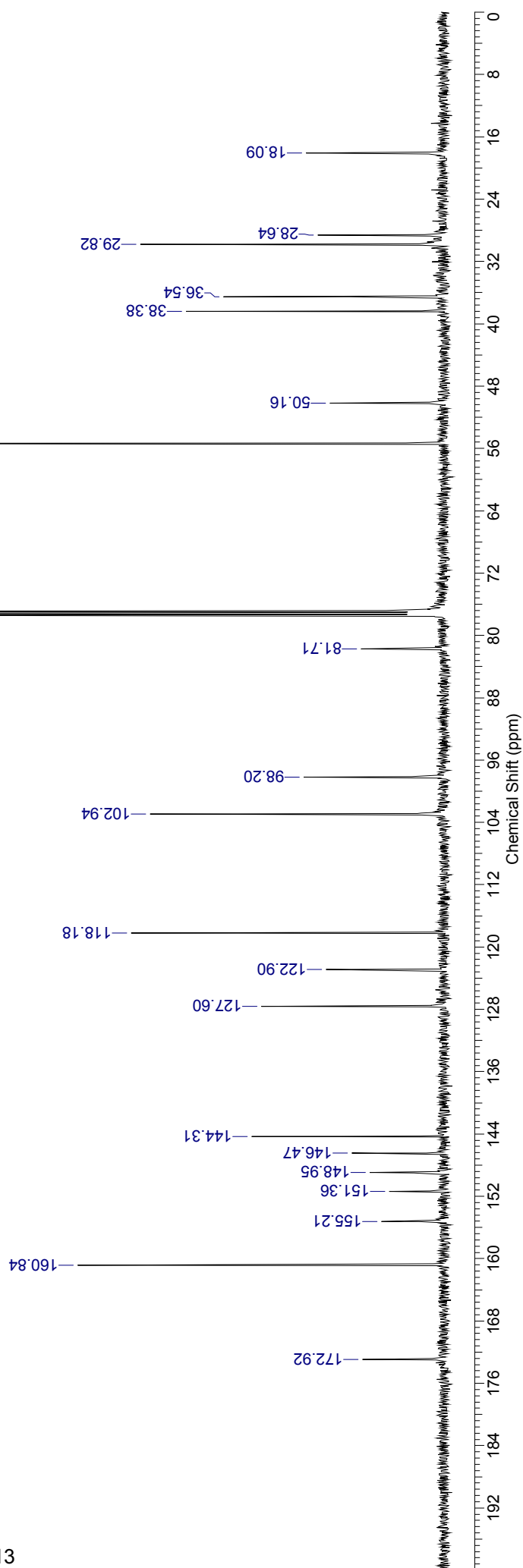
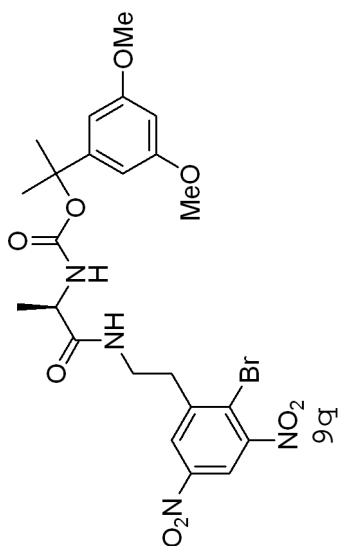
Ion mass = 605.0863380

Charge = +1

#	C	H	79Br	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 605.0863380									
1	23	27	1	4	9	1	605.0853622	11.5	9.758e-04
2	25	26	1	4	9	0	605.0877675	14.5	1.429e-03
3	26	25	1	5	6	1	605.0880423	16.0	1.704e-03
4	15	37	2	5	10	0	605.0901691	-1.0	3.831e-03
5	28	24	1	5	6	0	605.0904475	19.0	4.110e-03
6	19	35	2	4	8	0	605.0816157	3.5	4.722e-03
7	18	38	2	3	8	1	605.0917865	0.0	5.449e-03
8	29	24	1	3	7	0	605.0792142	19.0	7.124e-03
9	17	36	2	4	8	1	605.0792104	0.5	7.128e-03
10	16	37	2	3	11	0	605.0789357	-1.0	7.402e-03

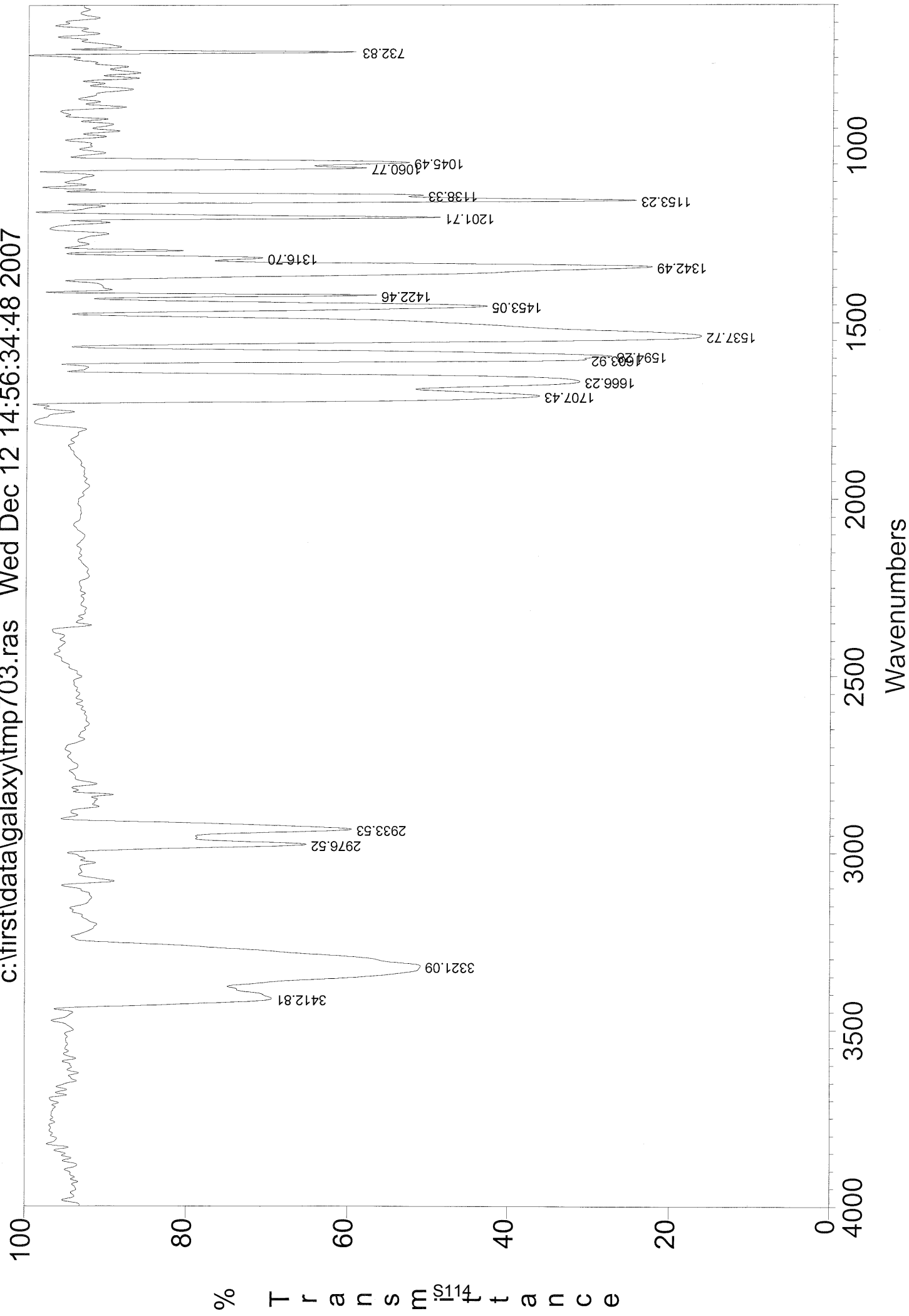






90158

c:\first\data\galaxy\tmp703.ras Wed Dec 12 14:56:34:48 2007





FTMS 4.7T BioAPEX II MS-Service UNI-Fribourg

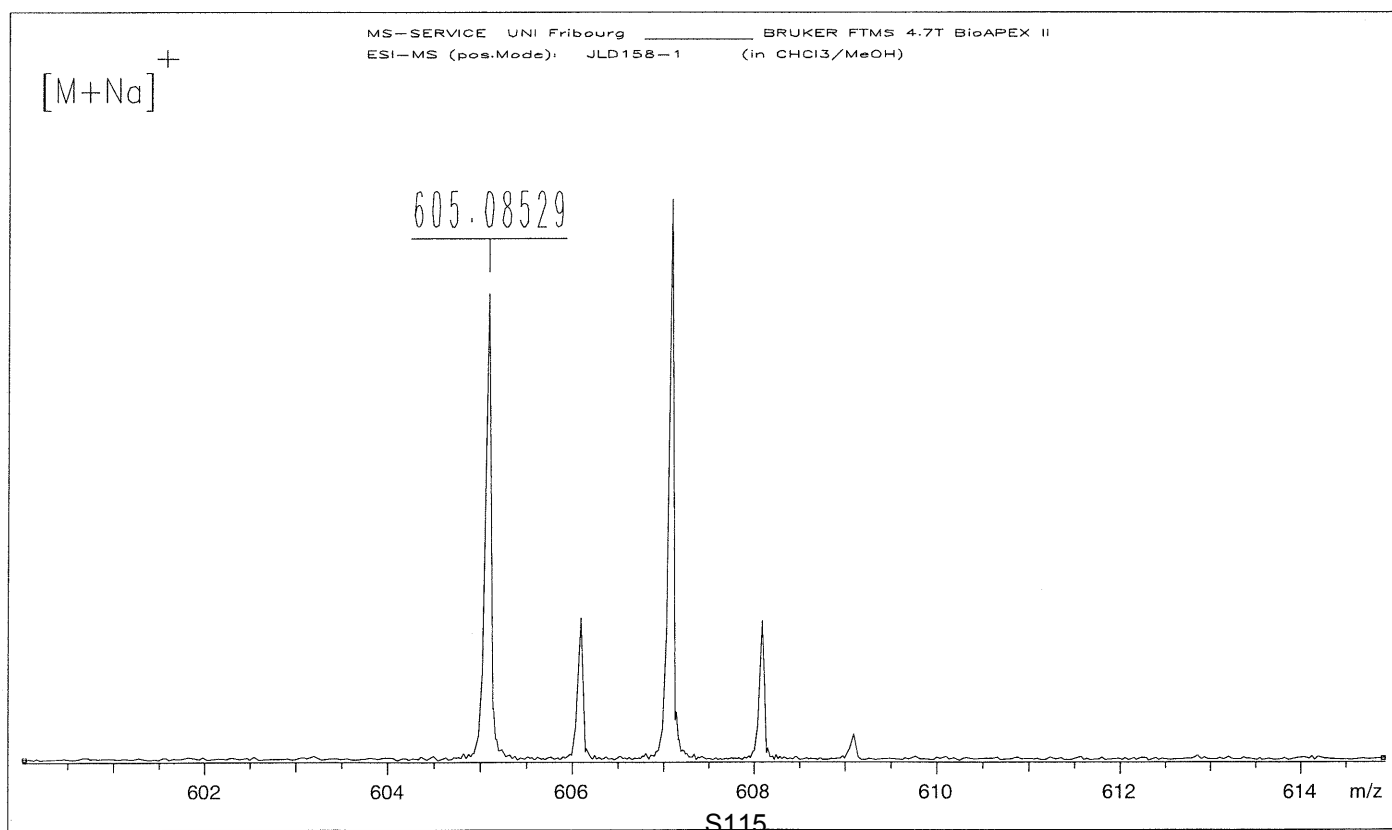
ESI-MS: JLDK158-1

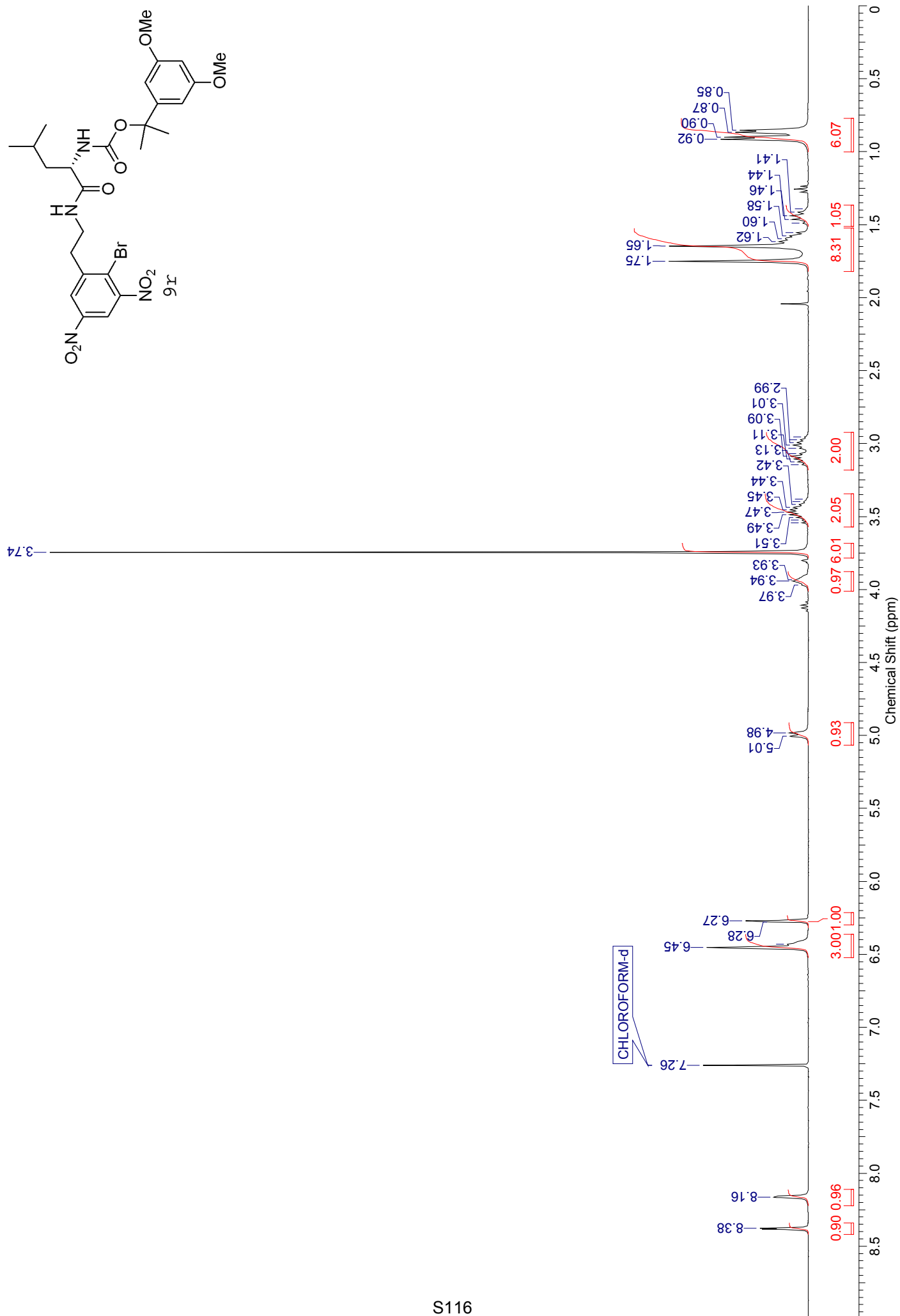
XMASS Mass Analysis for /Data/UNI_FR/DEBI3064_ESI/10/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

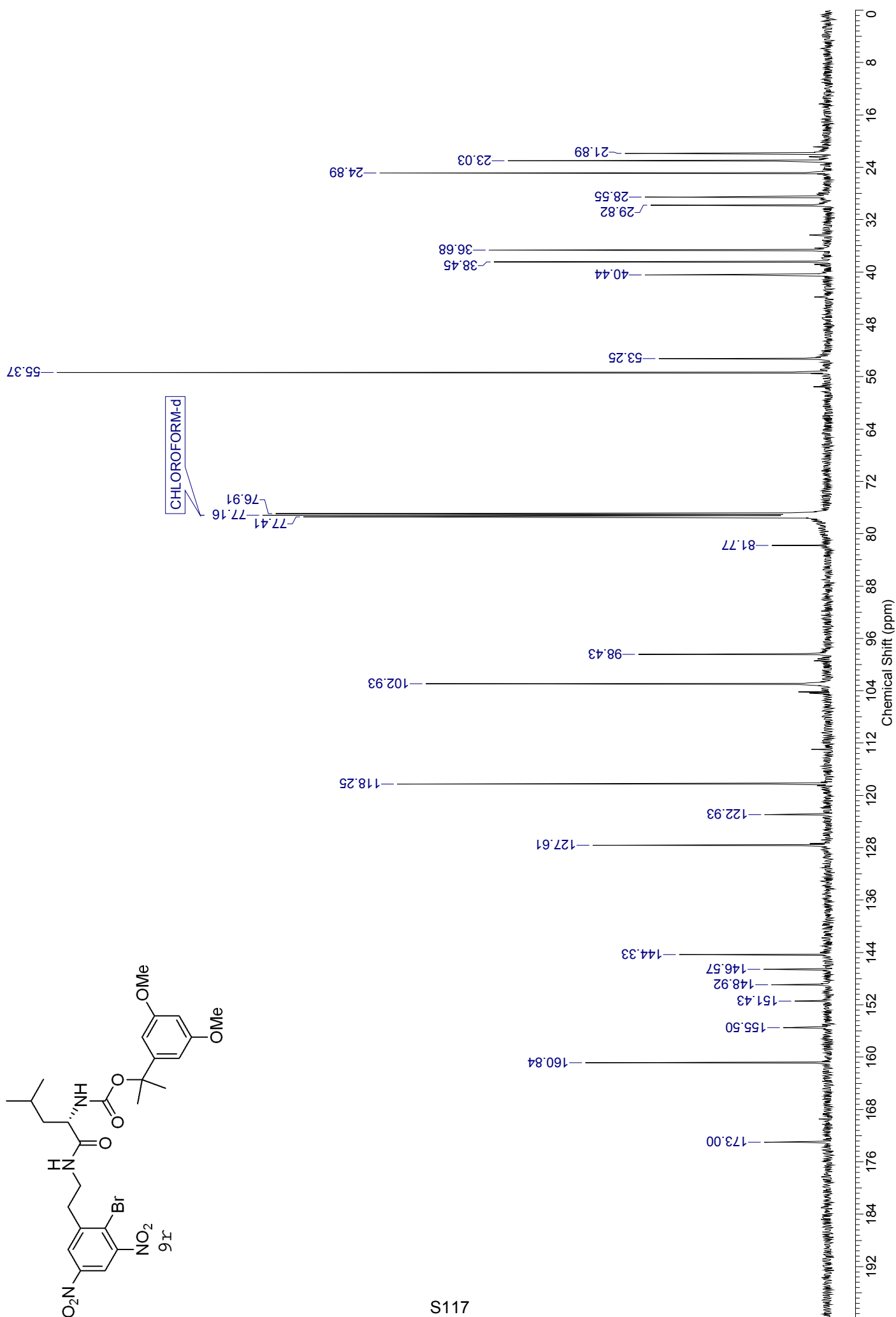
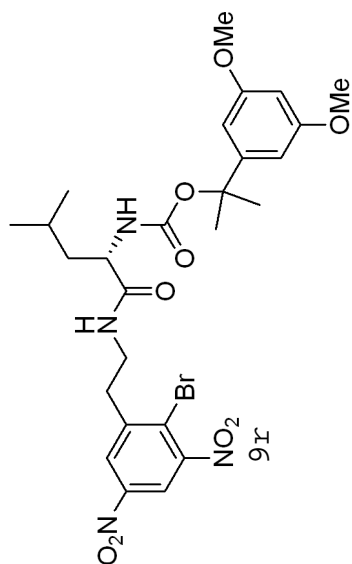
Ion mass = 605.0852950

Charge = +1

#	C	H	79Br	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 605.0852950									
1	23	27	1	4	9	1	605.0853622	11.5	6.718e-05
2	22	28	1	3	12	0	605.0850874	10.0	2.076e-04
3	21	22	1	10	7	0	605.0850821	15.5	2.129e-04
4	24	35	2	2	6	0	605.0856385	7.5	3.435e-04
5	22	33	2	5	5	0	605.0842958	8.0	9.992e-04
6	23	24	1	7	8	0	605.0864248	15.0	1.130e-03
7	21	25	1	7	8	1	605.0840195	12.0	1.275e-03
8	24	23	1	8	5	1	605.0866996	16.5	1.405e-03
9	25	29	1	1	10	1	605.0867048	11.0	1.410e-03
10	20	26	1	6	11	0	605.0837447	10.5	1.550e-03

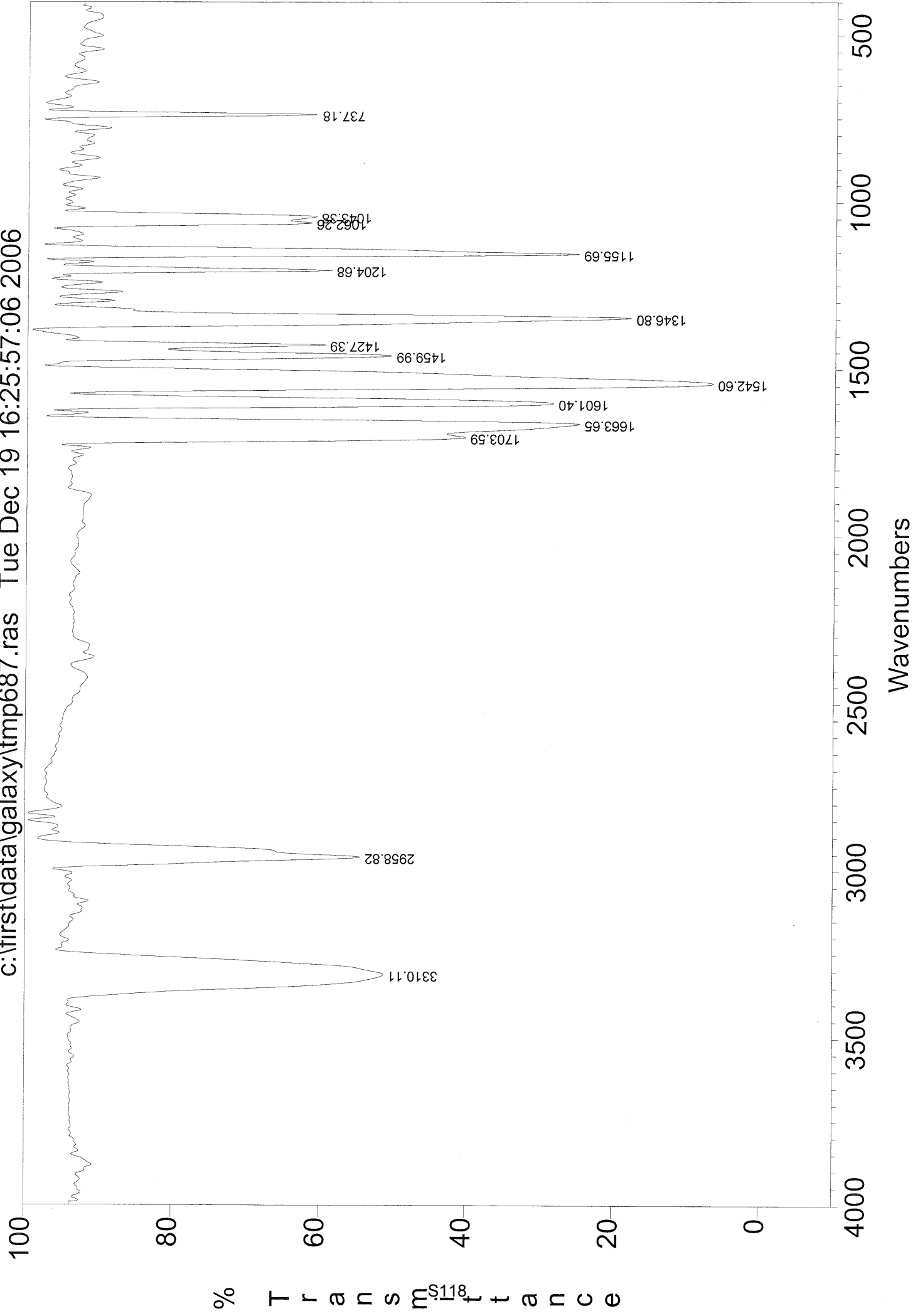






2692

c:\first\data\galaxy\tmp687.ras Tue Dec 19 16:25:57:06 2006



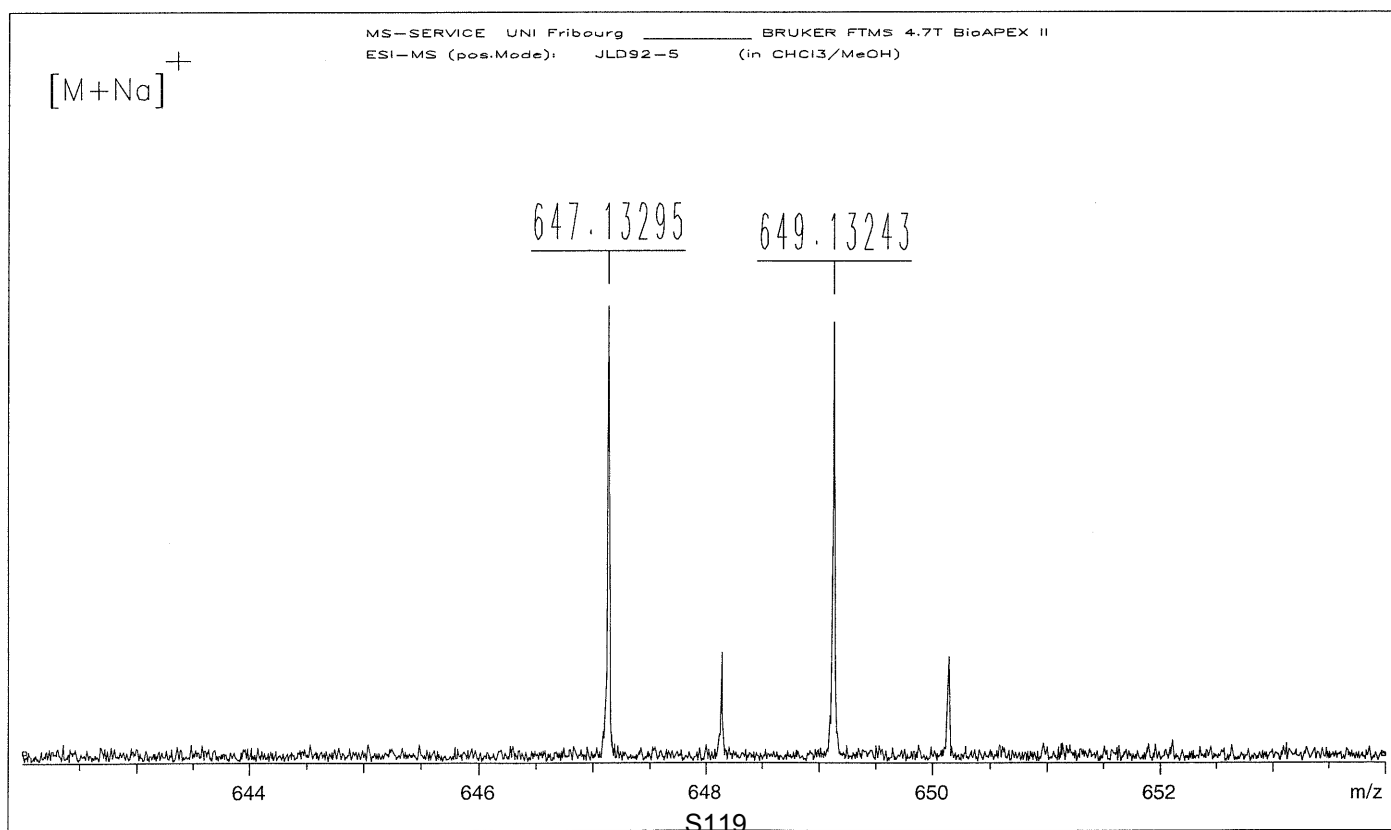
ESI-MS: JLD92-5

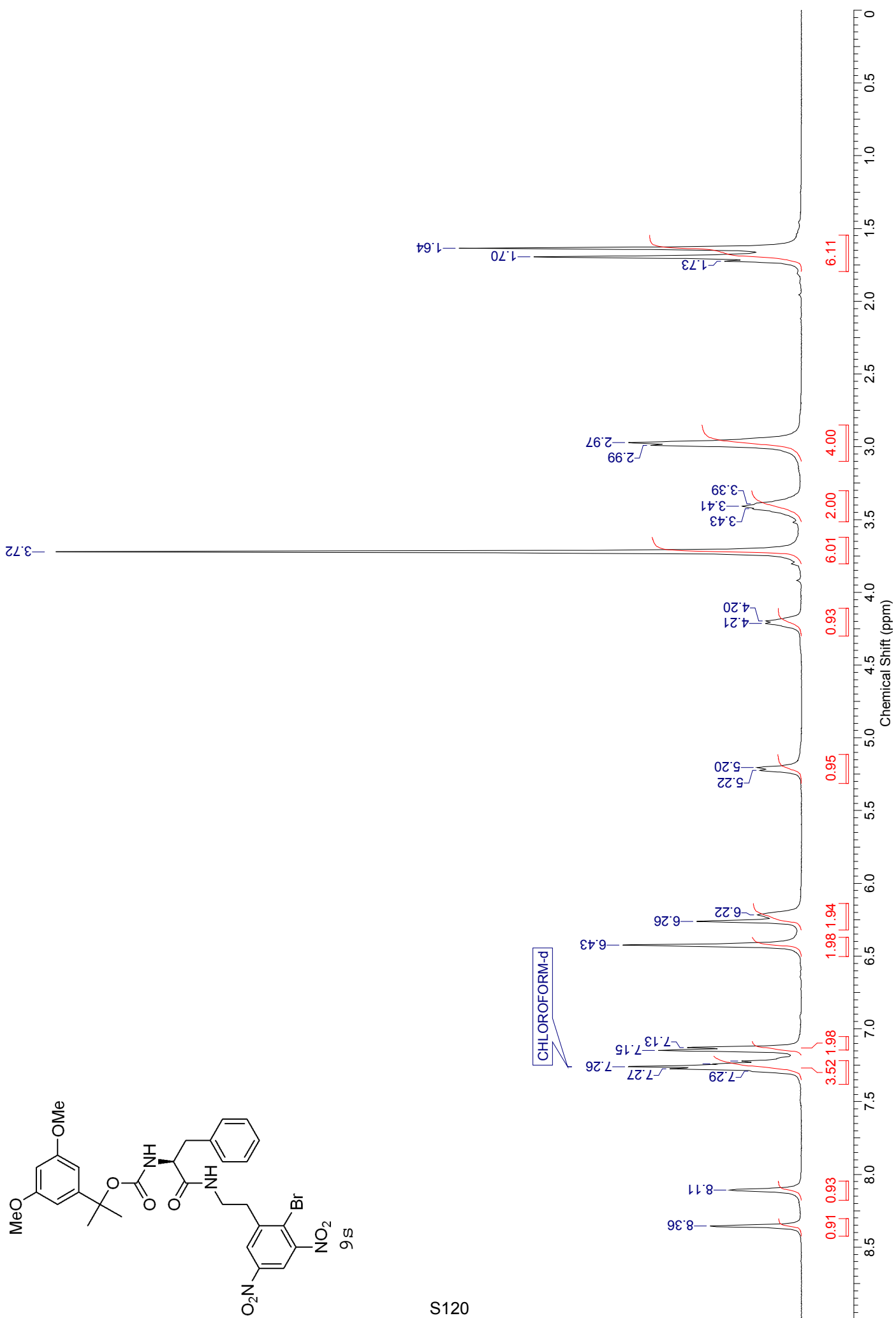
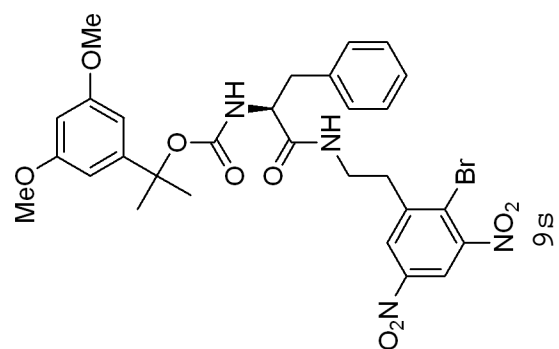
XMASS Mass Analysis for /Data/UNI_FR/DEBI2173_ESI/10/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

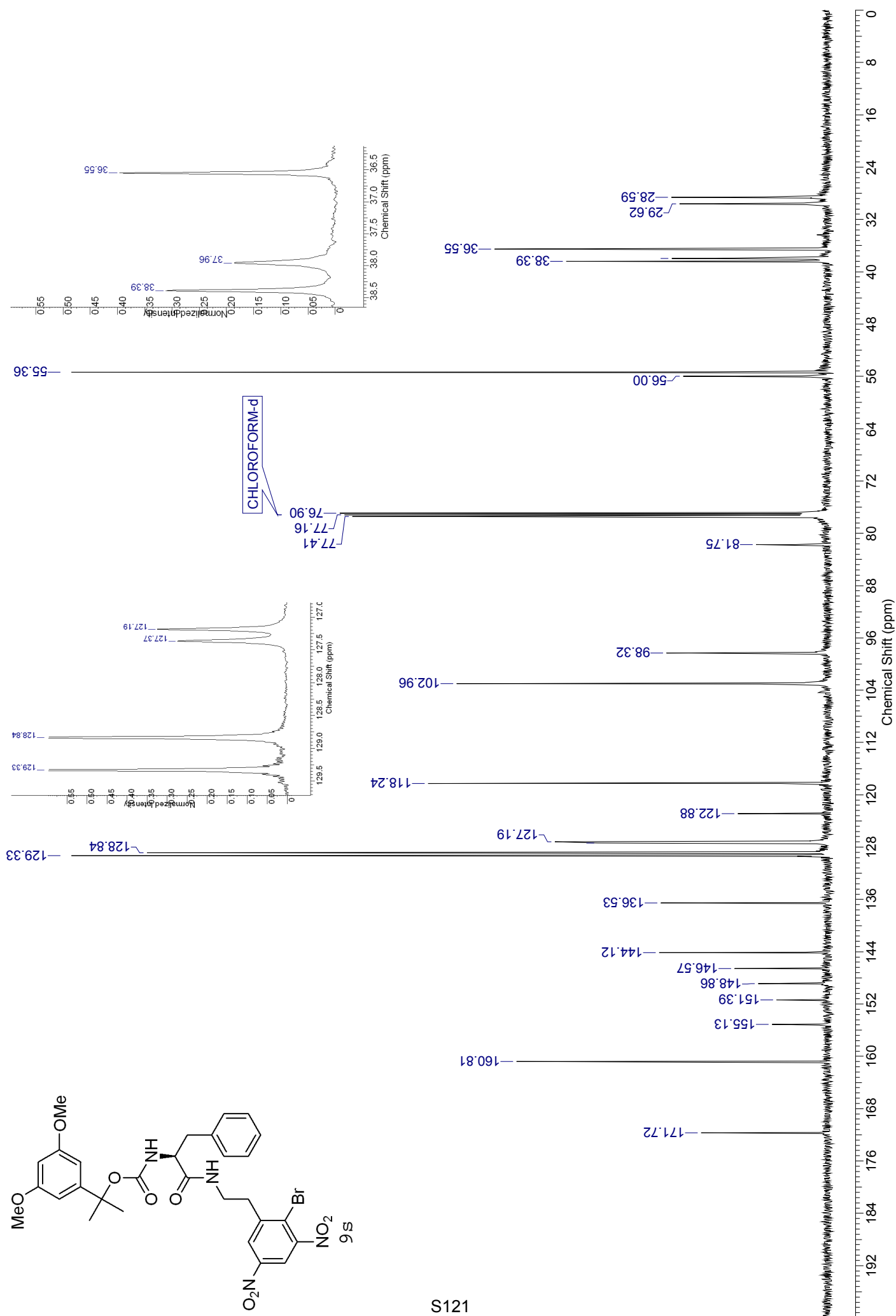
Ion mass = 647.1329490

Charge = +1

#	C	H	79Br	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 647.1329490									
1	26	33	1	4	9	1	647.1323124	11.5	6.366e-04
2	25	34	1	3	12	0	647.1320376	10.0	9.114e-04
3	25	39	2	5	5	0	647.1312460	8.0	1.703e-03
4	28	32	1	4	9	0	647.1347177	14.5	1.769e-03
5	29	31	1	5	6	1	647.1349924	16.0	2.043e-03
6	23	35	1	3	12	1	647.1296323	7.0	3.317e-03
7	23	40	2	5	5	1	647.1288407	5.0	4.108e-03
8	18	43	2	5	10	0	647.1371192	-1.0	4.170e-03
9	22	41	2	4	8	0	647.1285659	3.5	4.383e-03
10	31	30	1	5	6	0	647.1373977	19.0	4.449e-03

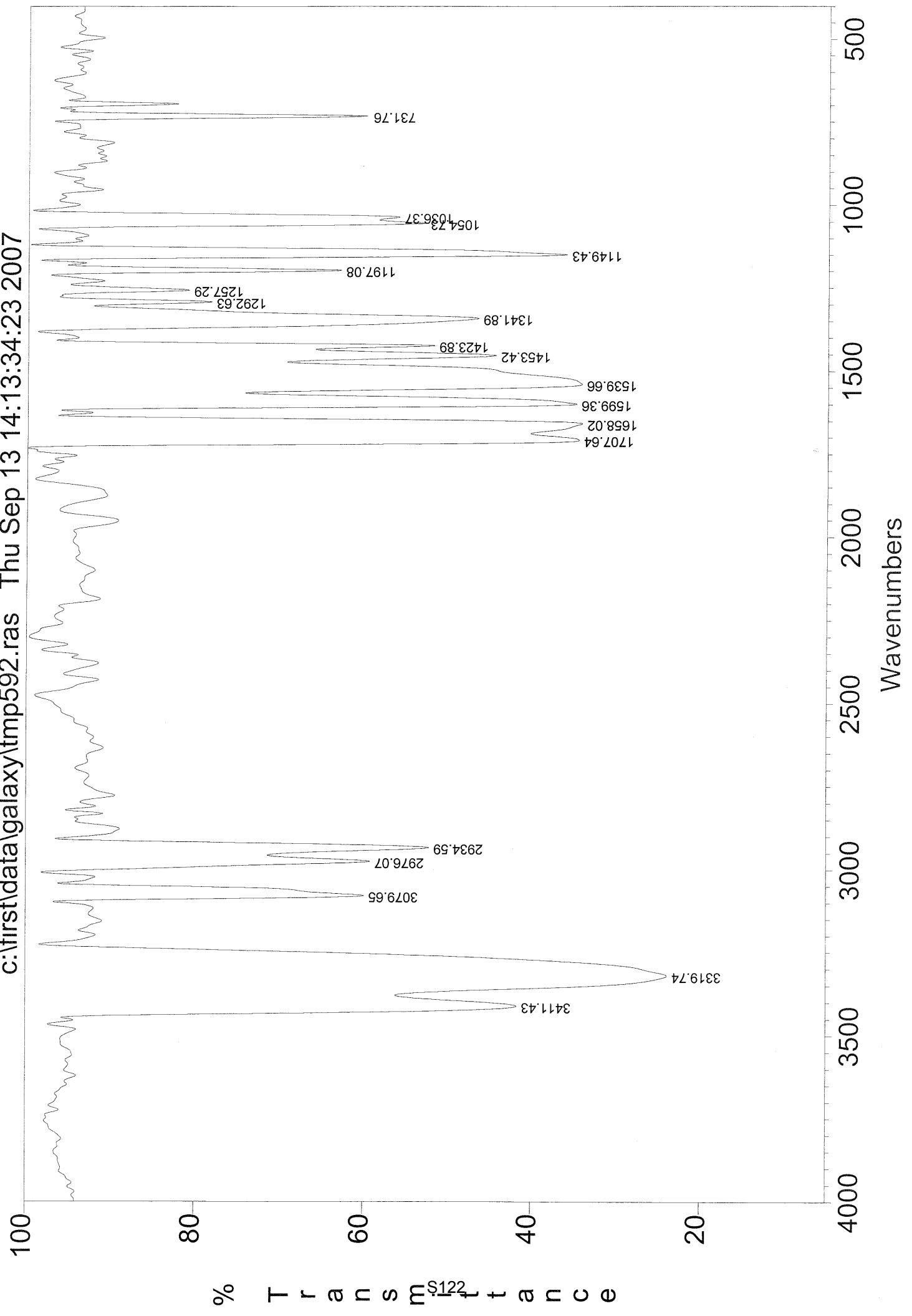






90149

c:\first\data\galaxy\tmp592.ras Thu Sep 13 14:13:34:23 2007



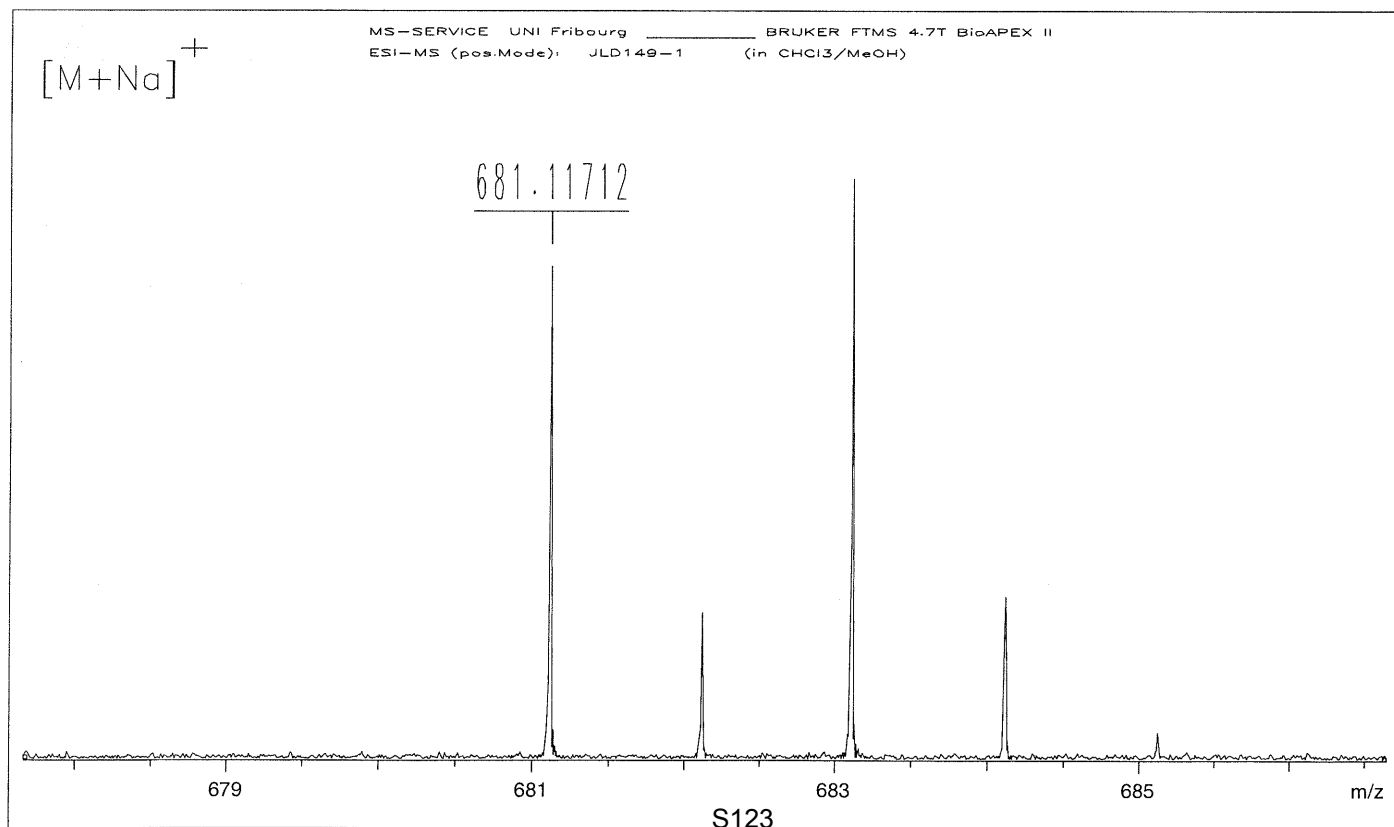
ESI-MS: JLD149-1

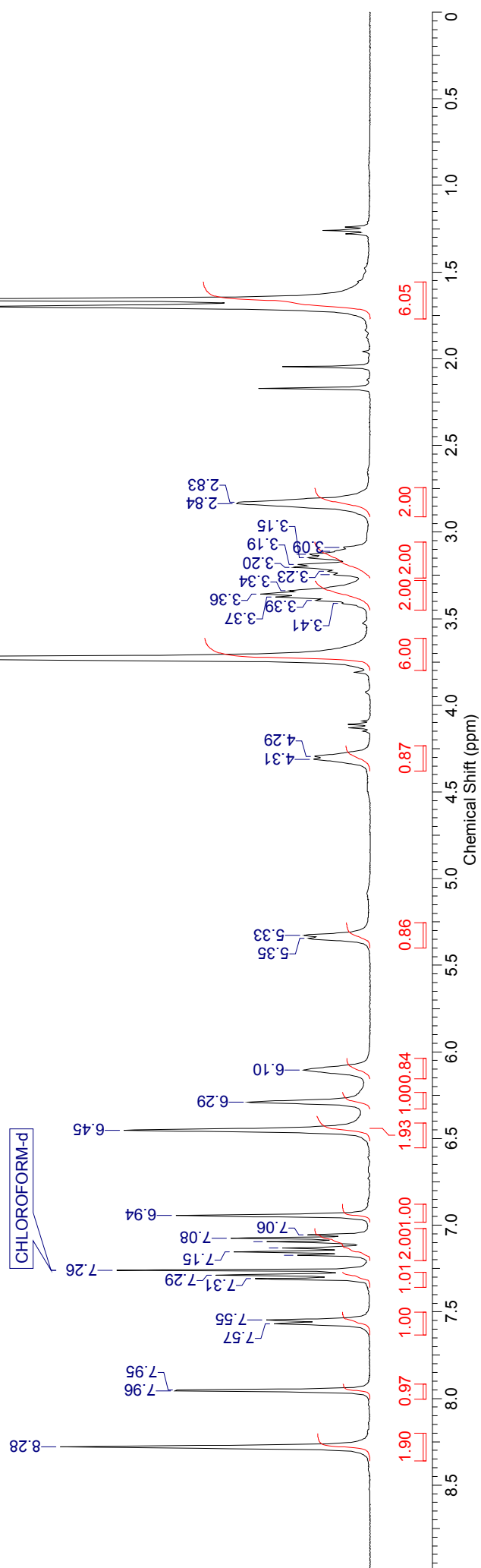
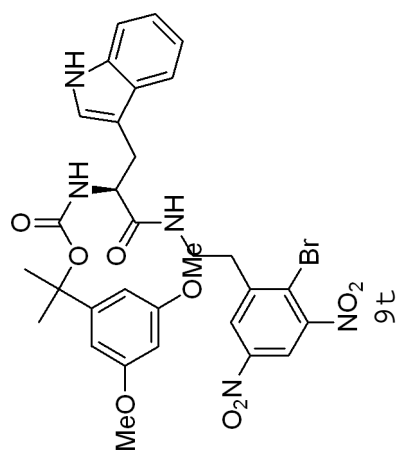
XMASS Mass Analysis for /Data/UNI_FR/DEBI2851_ESI/2/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

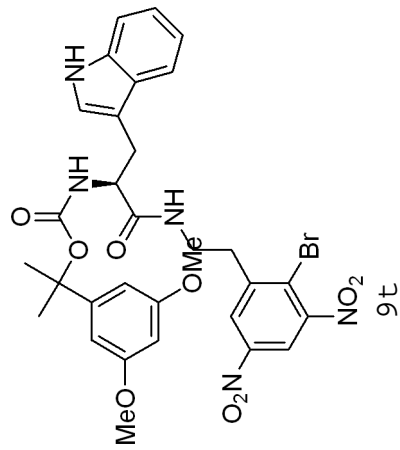
Ion mass = 681.1171240

Charge = +1

#	C	H	79Br	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 681.1171240									
1	29	31	1	4	9	1	681.1166623	15.5	4.617e-04
2	19	42	2	5	10	1	681.1190639	0.0	1.940e-03
3	31	30	1	4	9	0	681.1190676	18.5	1.944e-03
4	32	29	1	5	6	1	681.1193424	20.0	2.218e-03
5	25	39	2	4	8	0	681.1129159	7.5	4.208e-03
6	21	41	2	5	10	0	681.1214692	3.0	4.345e-03
7	34	28	1	5	6	0	681.1217477	23.0	4.624e-03
8	24	42	2	3	8	1	681.1230866	4.0	5.963e-03
9	35	28	1	3	7	0	681.1105143	23.0	6.610e-03
10	23	40	2	4	8	1	681.1105106	4.5	6.613e-03

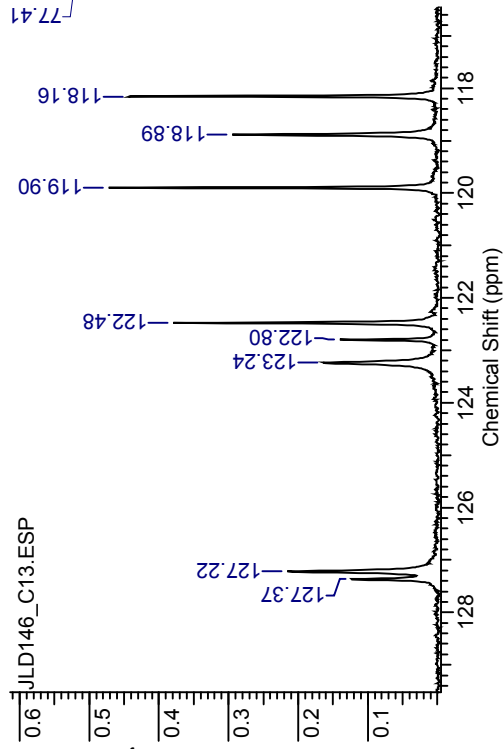






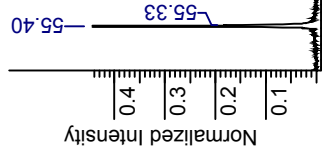
JULD146_C13.ESP

Normalized Intensity

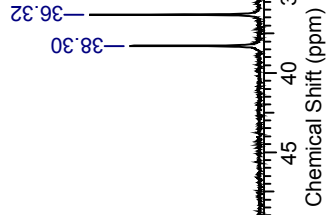


CHLOROFORM-d

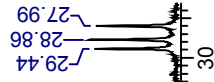
55.40



Normalized Intensity



Chemical Shift (ppm)



160.79

119.90

118.16

103.13

148.96

146.42

144.04

172.20

136.25

127.37

127.22

123.24

122.48

111.40

110.55

98.29

81.62

29.44

28.86

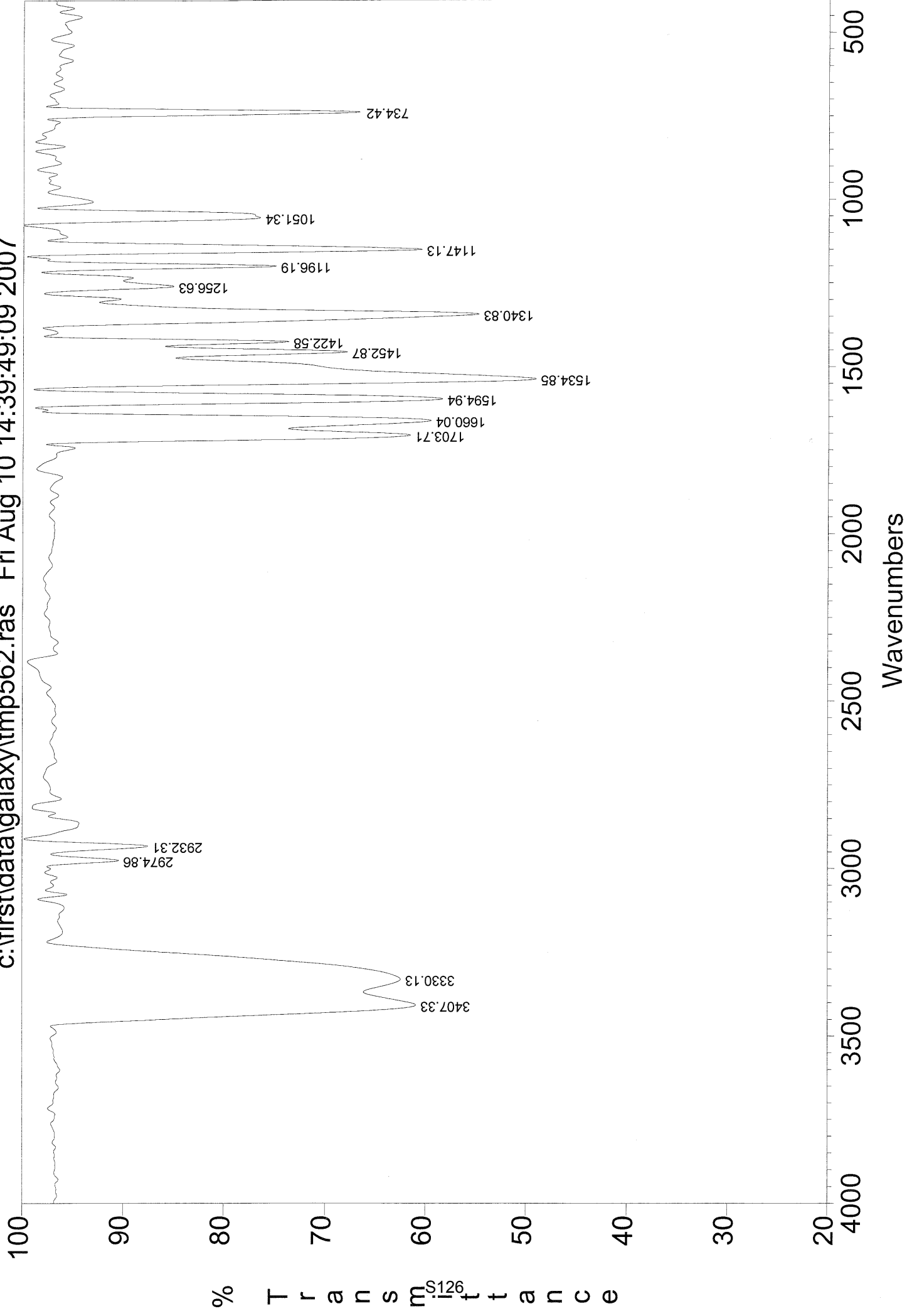
27.99

38.30

36.32

00146

c:\first\data\galaxy\tmp562.ras Fri Aug 10 14:39:49:09 2007



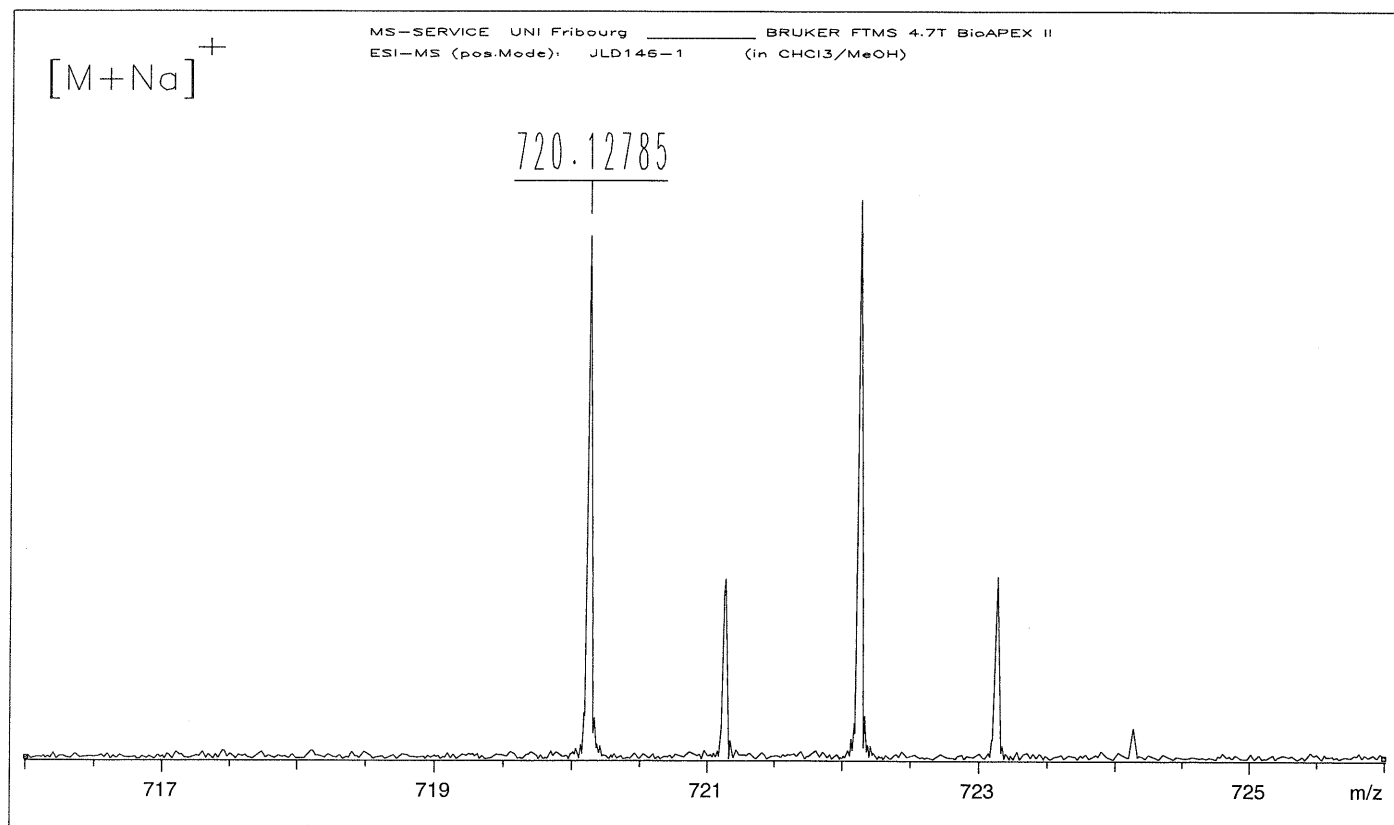
ESI-MS: JLD146-1

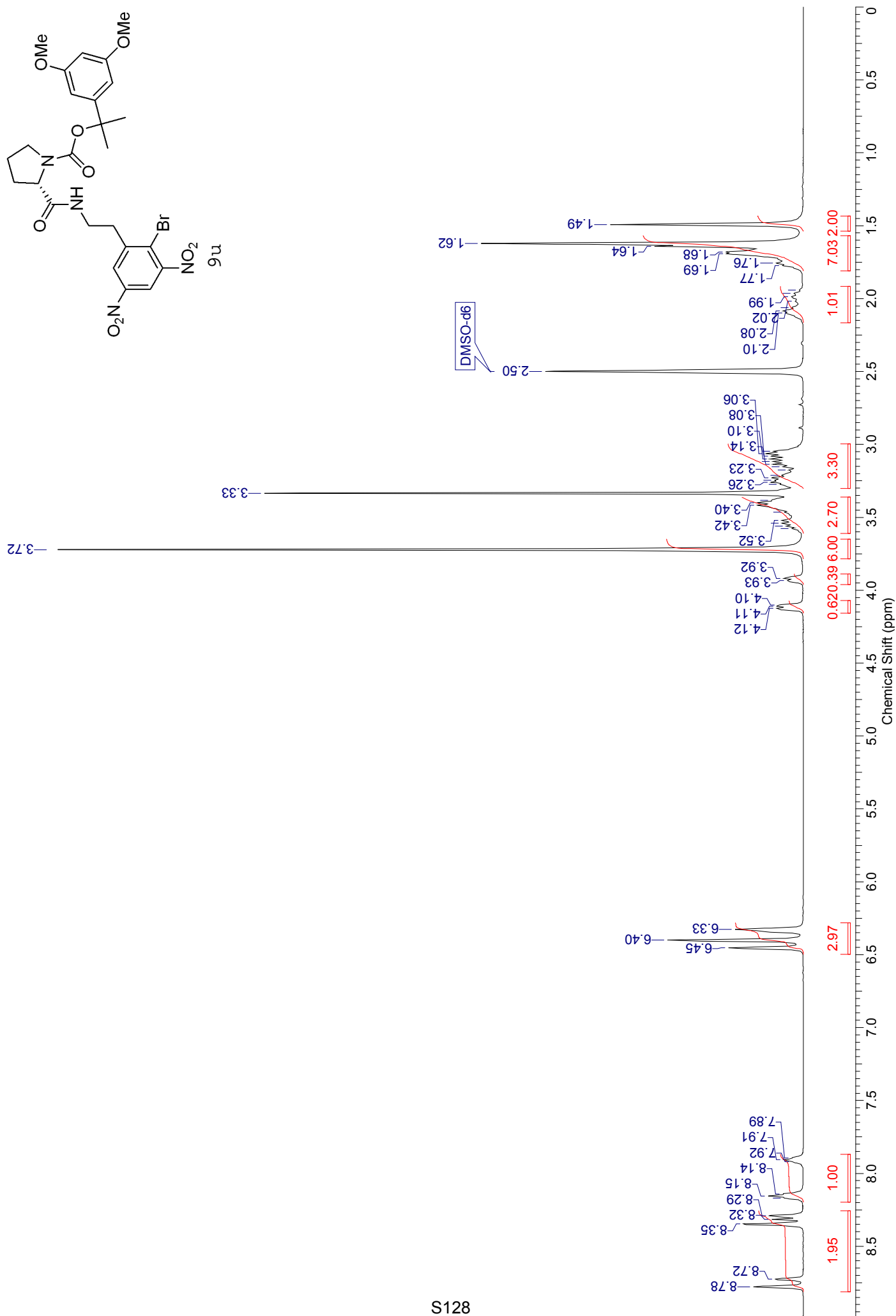
XMASS Mass Analysis for /Data/UNI_FR/DEBI2787_ESI/10/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

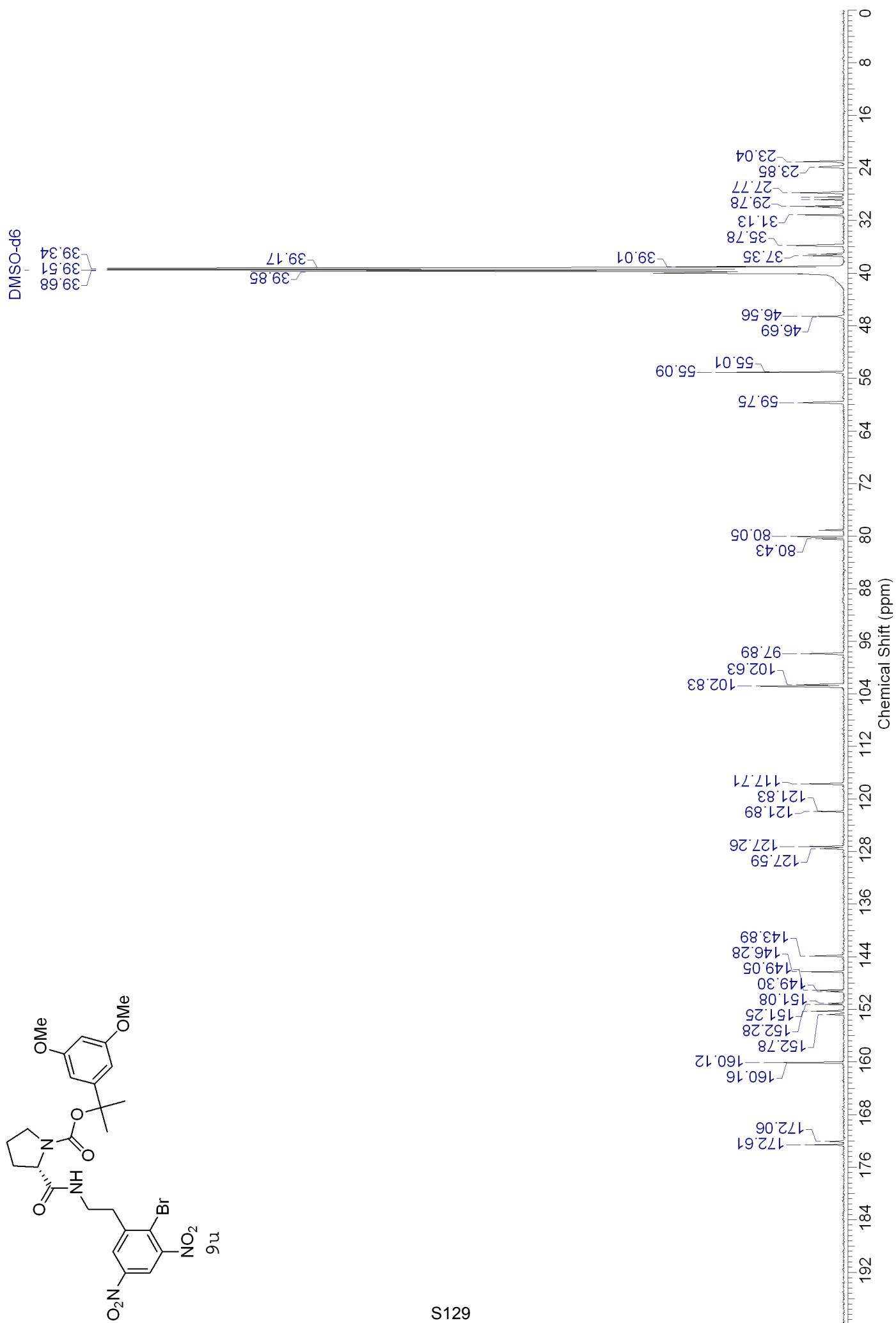
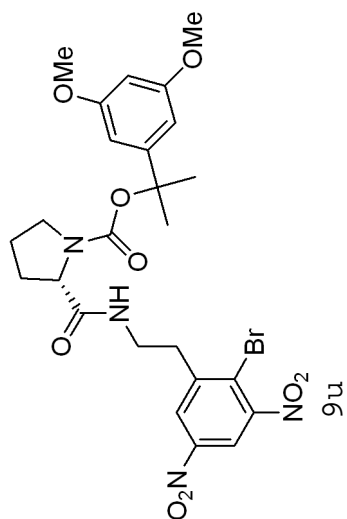
Ion mass = 720.1278470

Charge = +1

#	C	H	79Br	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 720.1278470									
1	31	32	1	5	9	1	720.1275613	17.5	2.857e-04
2	33	31	1	5	9	0	720.1299666	20.5	2.120e-03
3	23	45	2	3	11	1	720.1313056	1.5	3.459e-03
4	36	32	1	3	7	1	720.1315841	21.5	3.737e-03
5	27	40	2	5	8	0	720.1238149	9.5	4.032e-03
6	25	44	2	3	11	0	720.1337109	4.5	5.864e-03
7	26	43	2	4	8	1	720.1339857	6.0	6.139e-03
8	38	31	1	3	7	0	720.1339894	24.5	6.142e-03
9	37	29	1	4	7	0	720.1214133	25.0	6.434e-03
10	25	41	2	5	8	1	720.1214096	6.5	6.437e-03

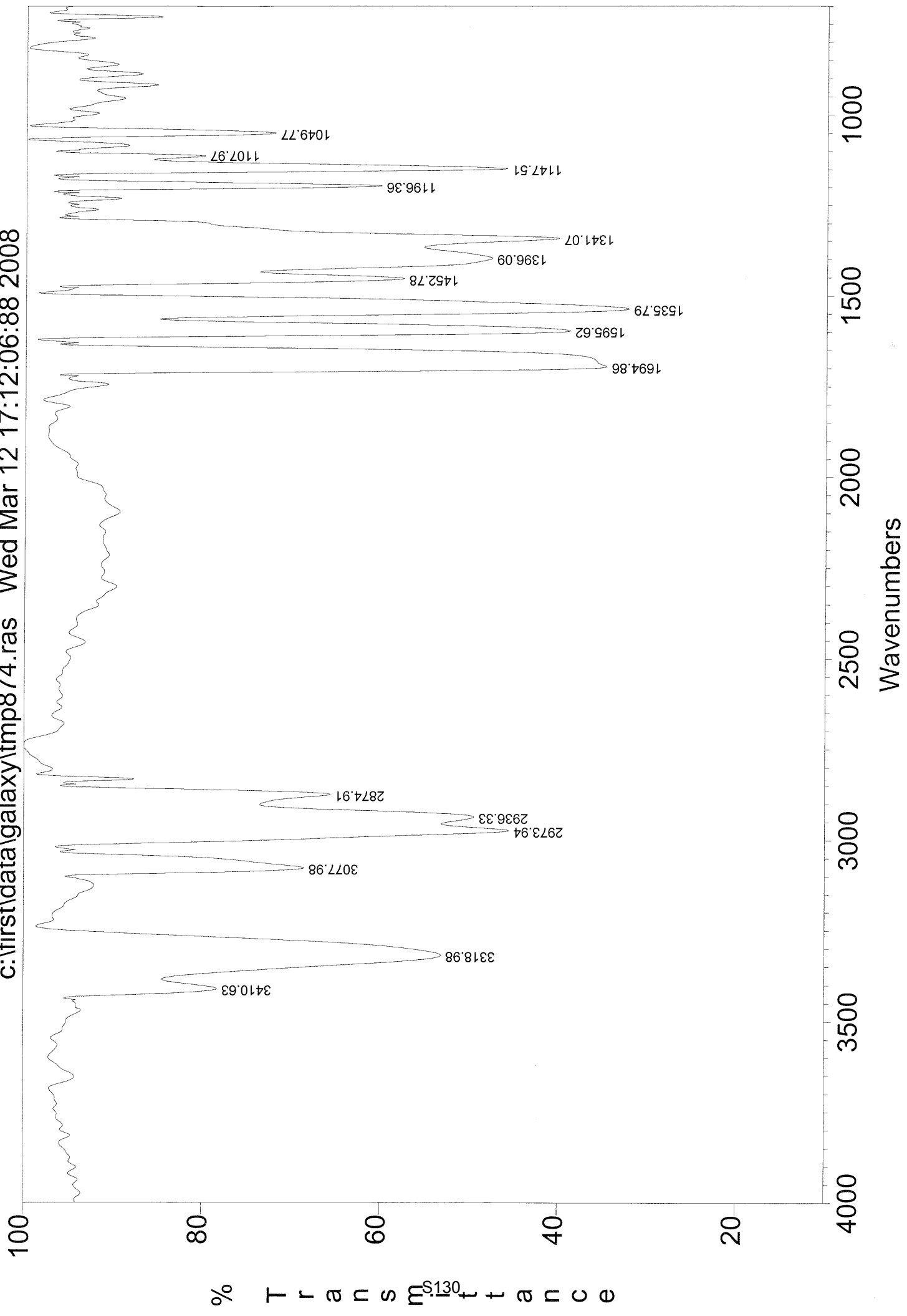






100120

c:\first\data\galaxy\tmp874.ras Wed Mar 12 17:12:06:88 2008



ESI-MS: JLD170-1

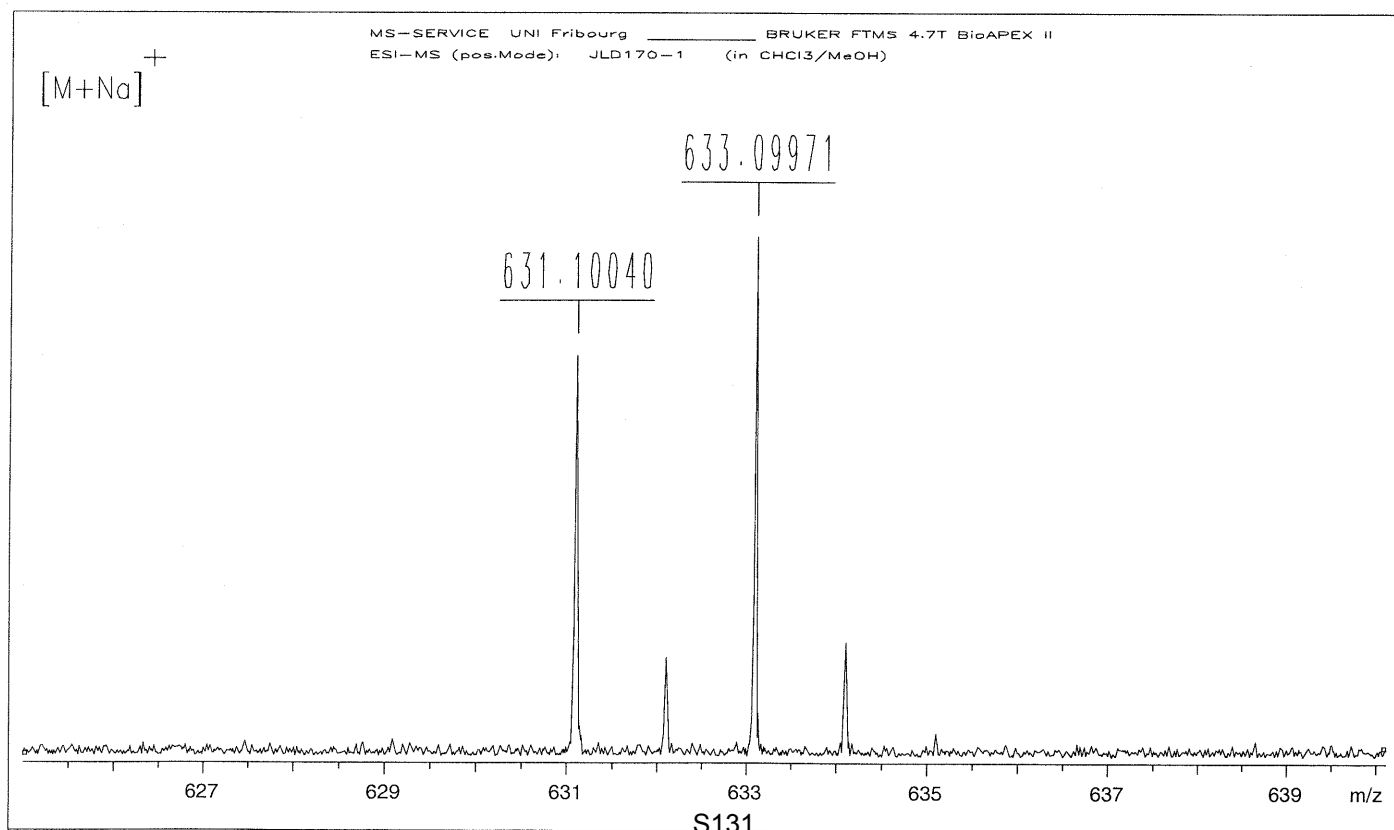
XMASS Mass Analysis for /Data/UNI_FR/DEBI3229_ESI/5/pdata/1/massanal.res:

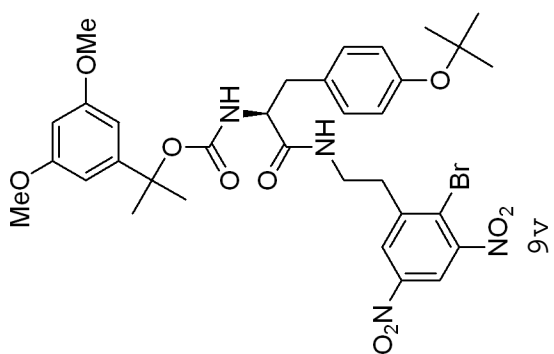
XMASS Mass Analysis Constraints

Ion mass = 631.1004050

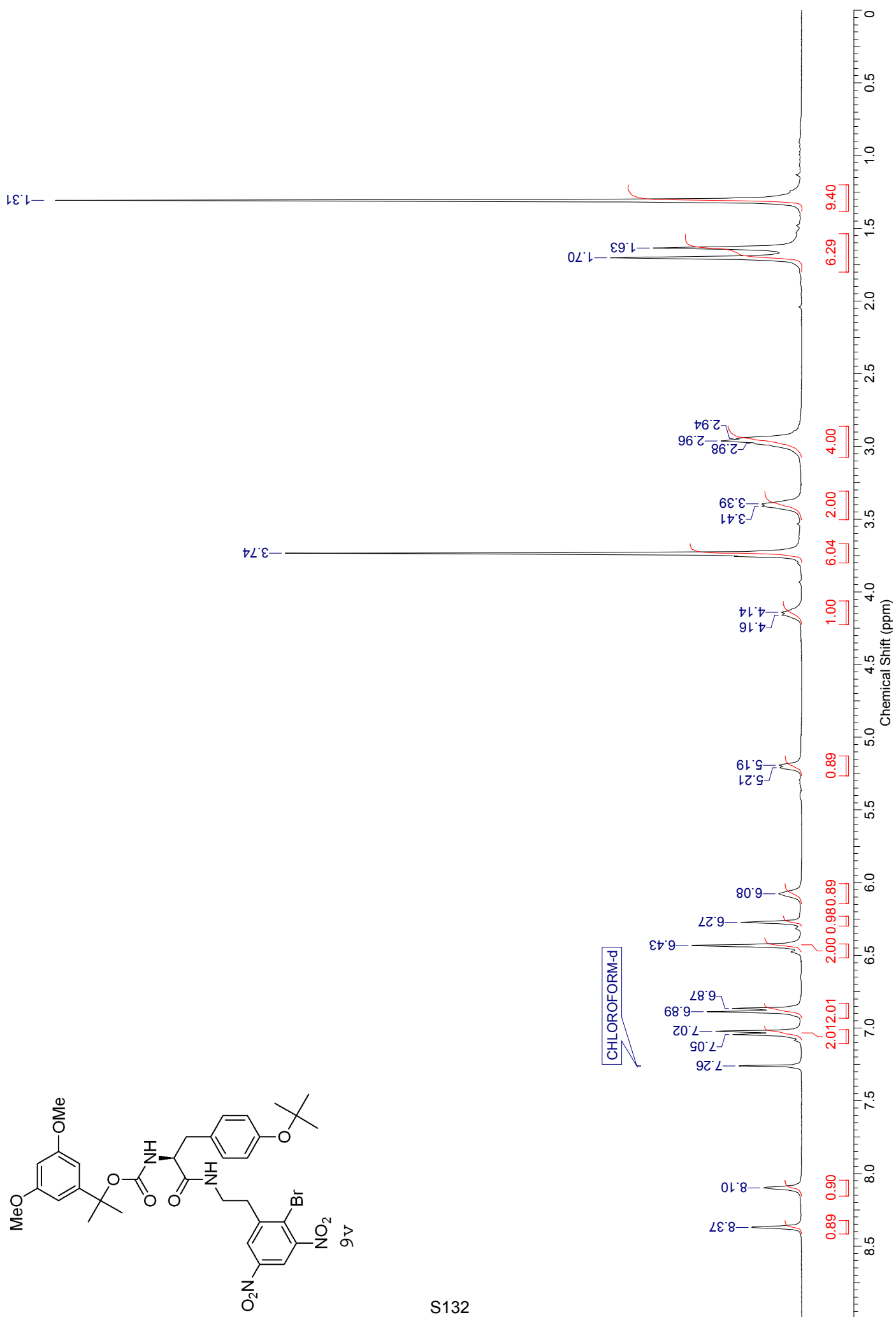
Charge = +1

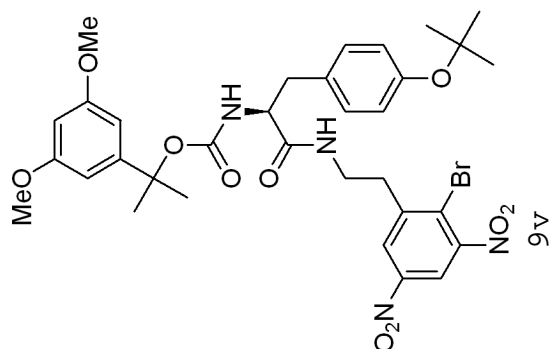
#	C	H	79Br	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 631.1004050									
1	25	29	1	4	9	1	631.1010122	12.5	6.072e-04
2	26	37	2	2	6	0	631.1012886	8.5	8.836e-04
3	22	28	1	6	11	0	631.0993948	11.5	1.010e-03
4	24	38	2	2	6	1	631.0988833	5.5	1.522e-03
5	23	39	2	1	9	0	631.0986085	4.0	1.797e-03
6	27	31	1	1	10	1	631.1023549	12.0	1.950e-03
7	27	28	1	4	9	0	631.1034175	15.5	3.013e-03
8	21	37	2	4	8	0	631.0972658	4.5	3.139e-03
9	28	27	1	5	6	1	631.1036923	17.0	3.287e-03
10	20	29	1	6	11	1	631.0969895	8.5	3.416e-03



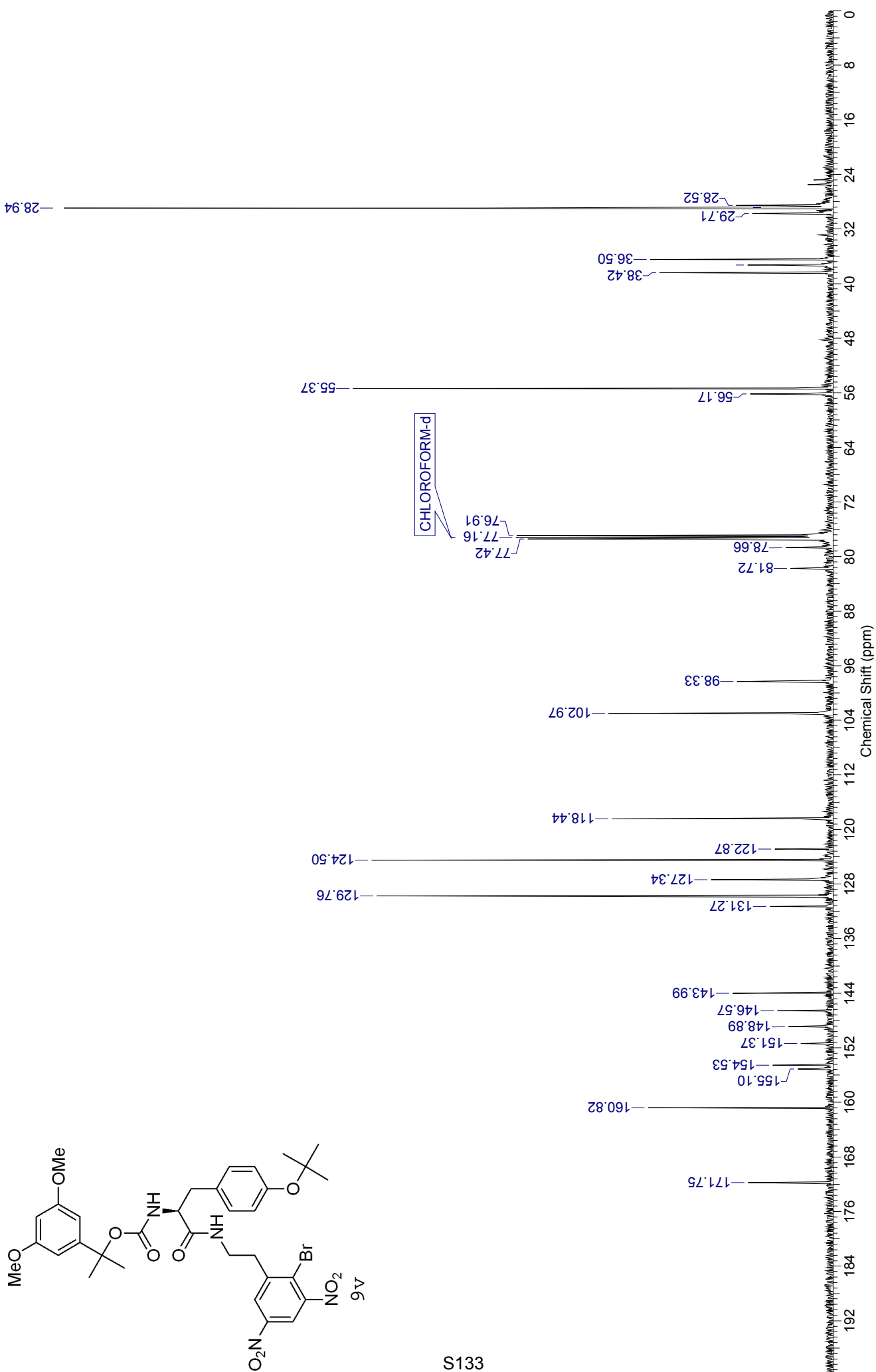


S132



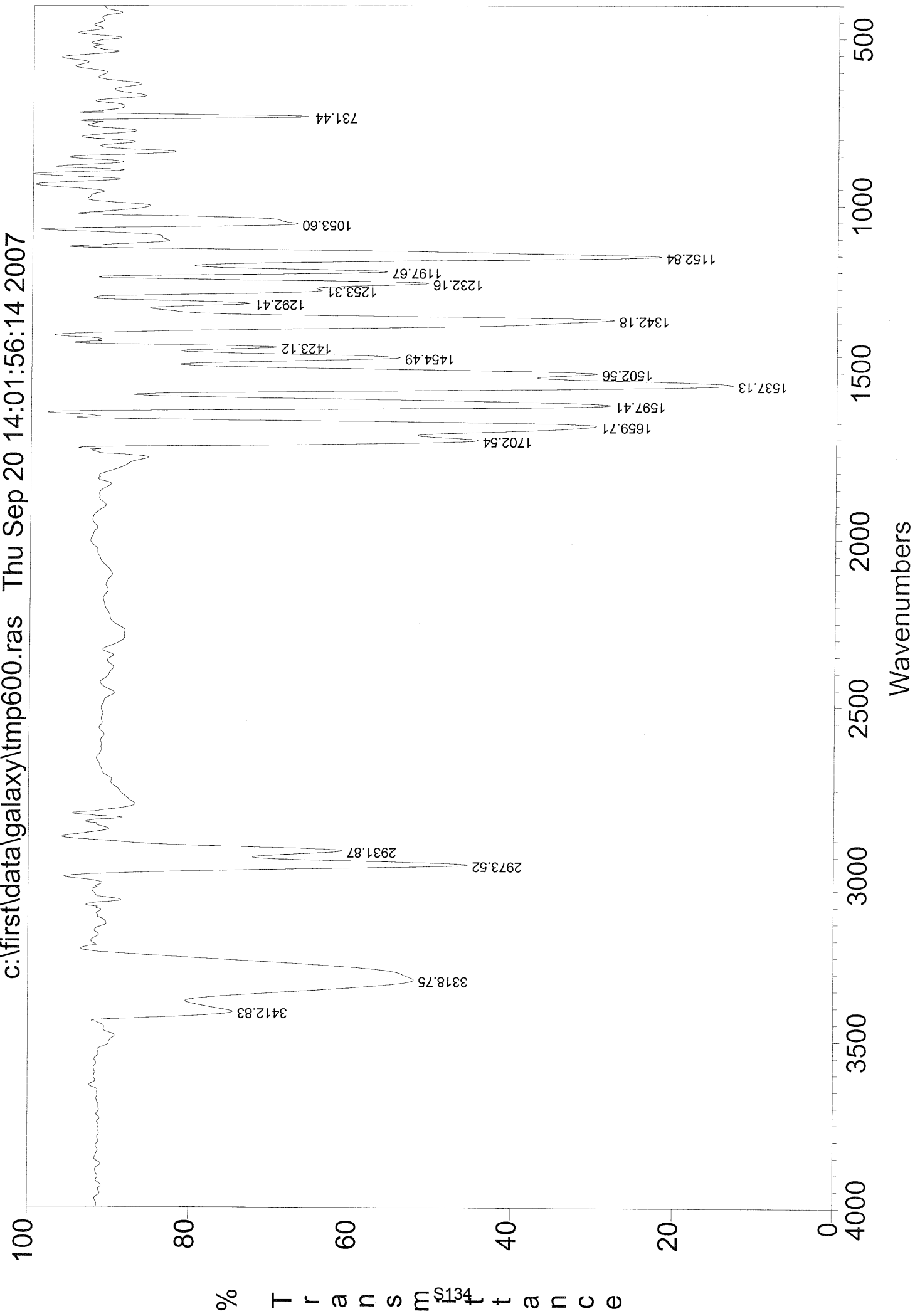


S133



960151

c:\first\data\galaxy\tmp600.ras Thu Sep 20 14:01:56:14 2007





FTMS 4.7T BioAPEX II MS-Service UNI-Fribourg

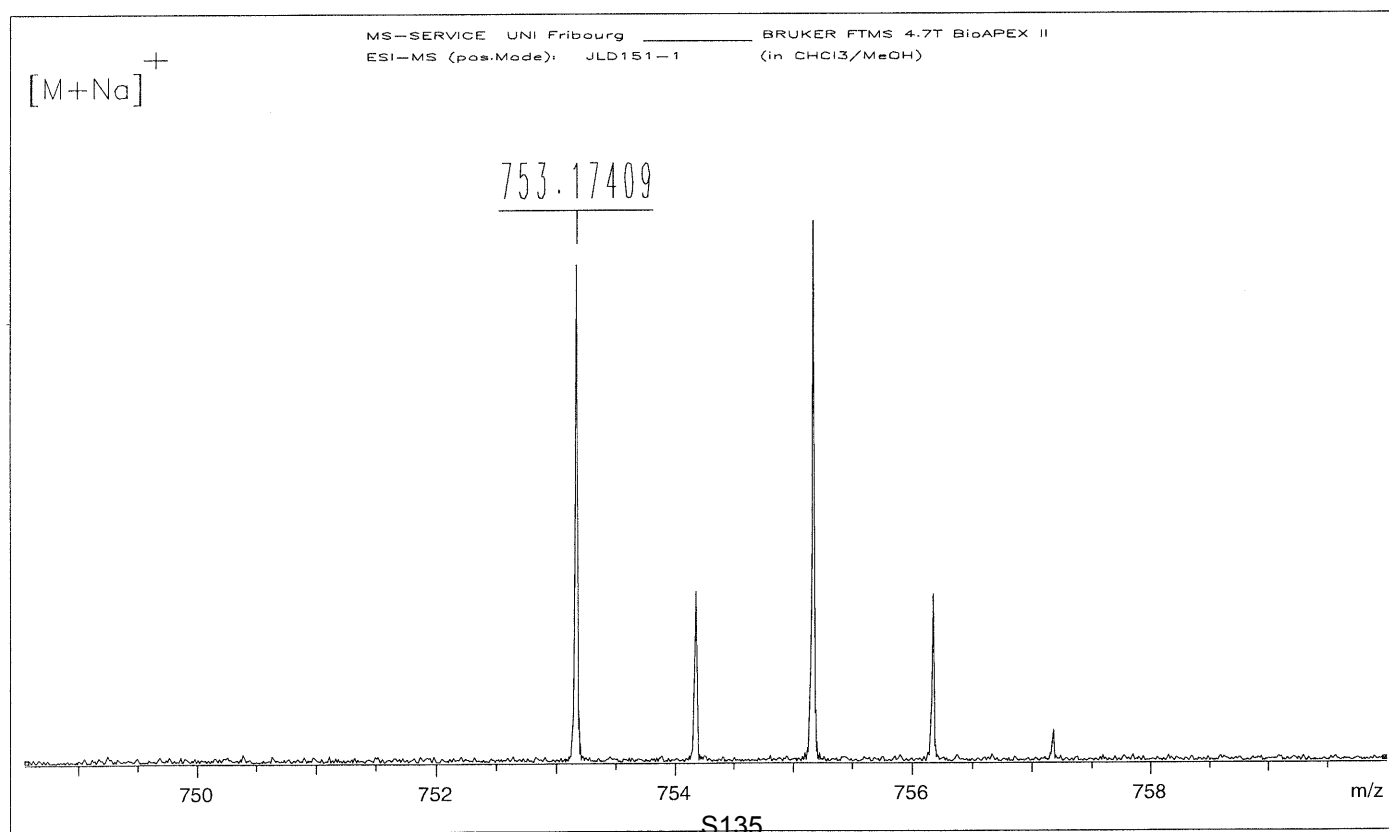
ESI-MS: JLD151-1

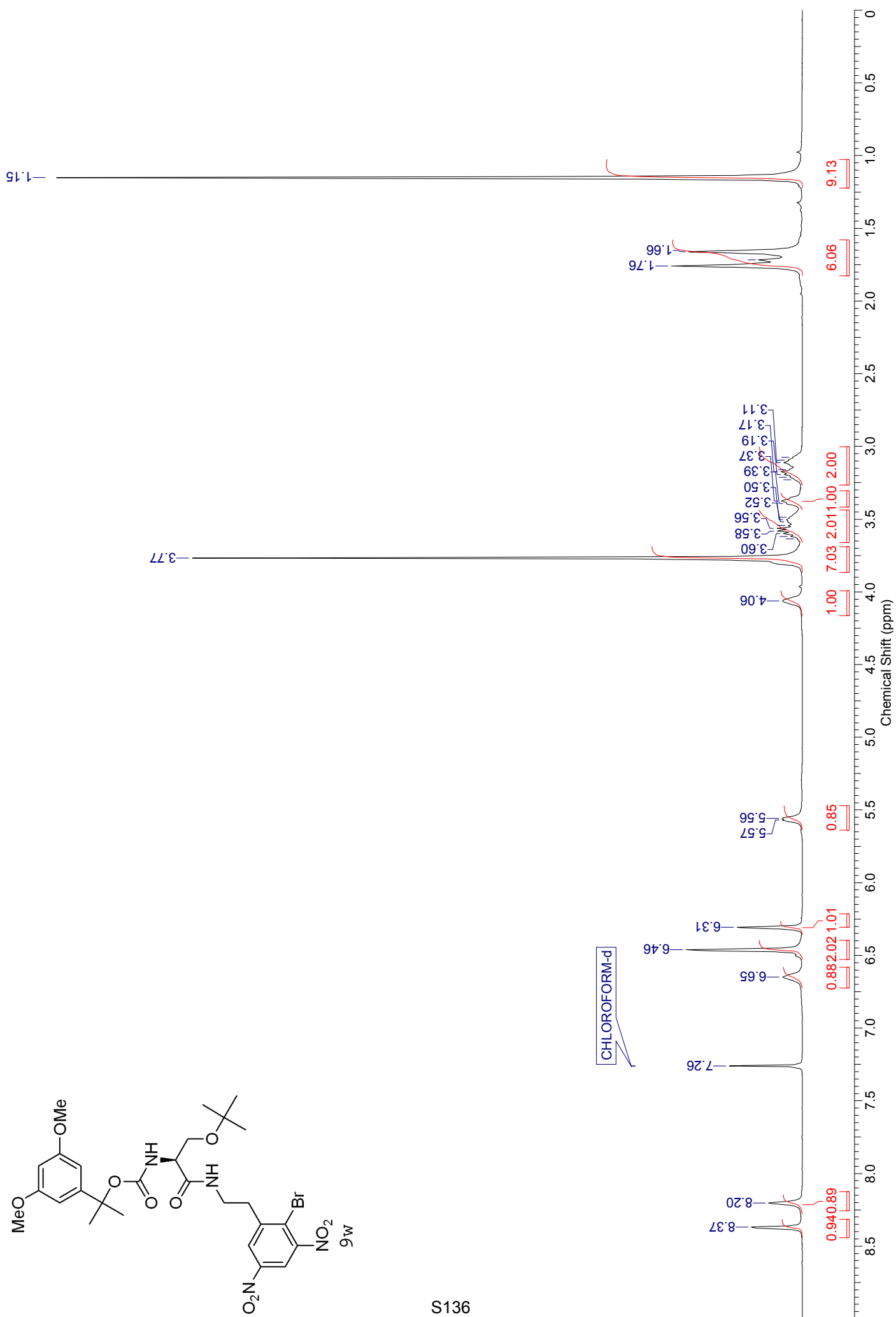
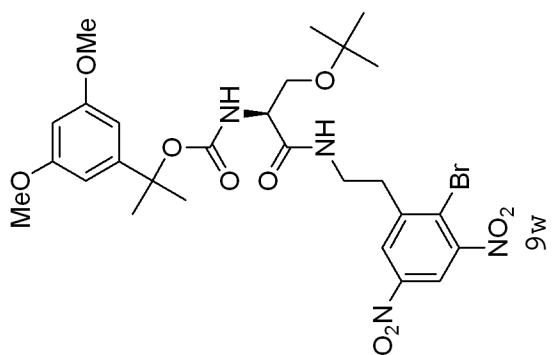
XMASS Mass Analysis for /Data/UNI_FR/DEBI2864_ESI/10/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

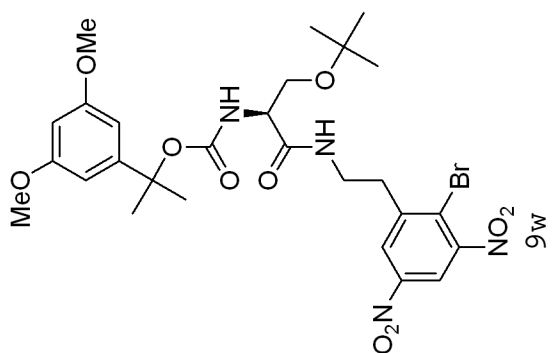
Ion mass = 753.1740930

Charge = +1

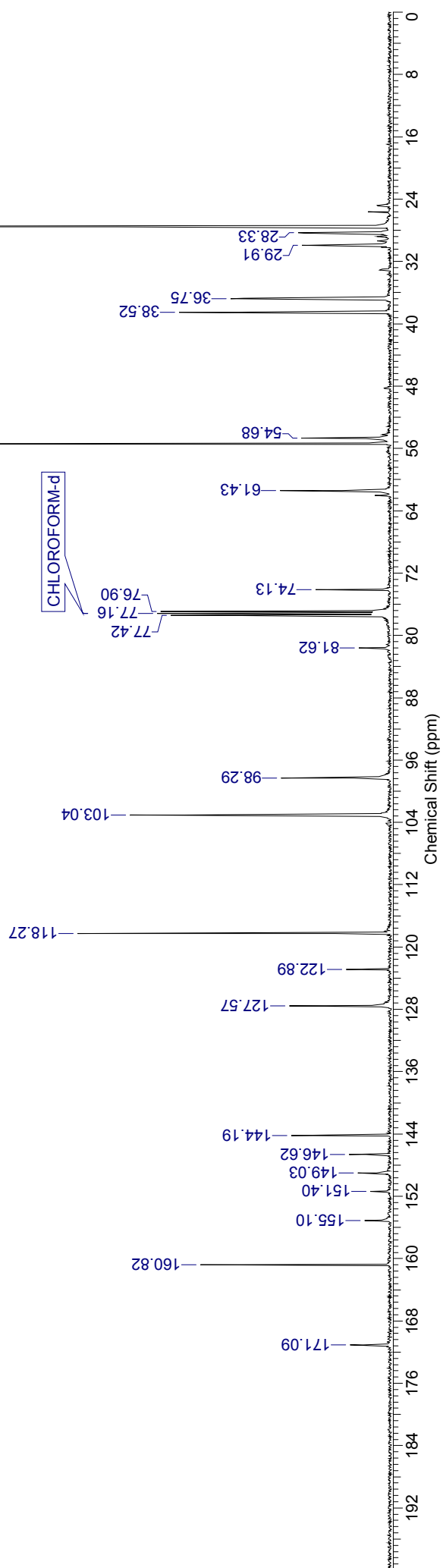
#	C	H	79Br	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 753.1740930									
1	33	39	1	4	10	1	753.1741772	15.5	8.418e-05
2	35	46	2	3	4	1	753.1747283	13.0	6.353e-04
3	32	45	2	5	6	0	753.1731108	12.0	9.822e-04
4	23	50	2	5	11	1	753.1765788	0.0	2.486e-03
5	35	38	1	4	10	0	753.1765825	18.5	2.489e-03
6	36	37	1	5	7	1	753.1768573	20.0	2.764e-03
7	37	45	2	3	4	0	753.1771336	16.0	3.041e-03
8	30	46	2	5	6	1	753.1707055	9.0	3.387e-03
9	29	47	2	4	9	0	753.1704307	7.5	3.662e-03
10	25	49	2	5	11	0	753.1789841	3.0	4.891e-03





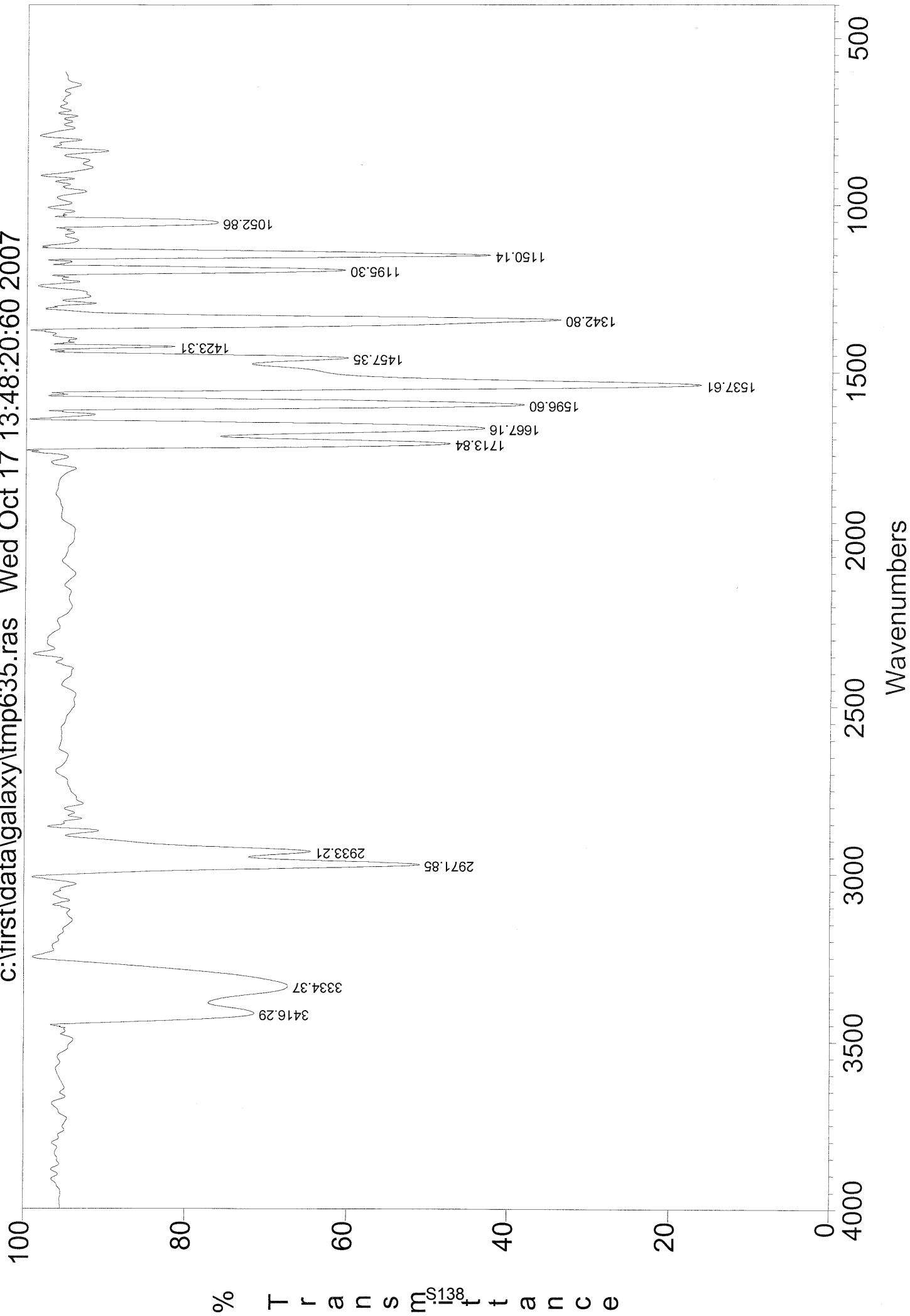


S137



157076

c:\first\data\galaxy\tmp635.ras Wed Oct 17 13:48:20:60 2007



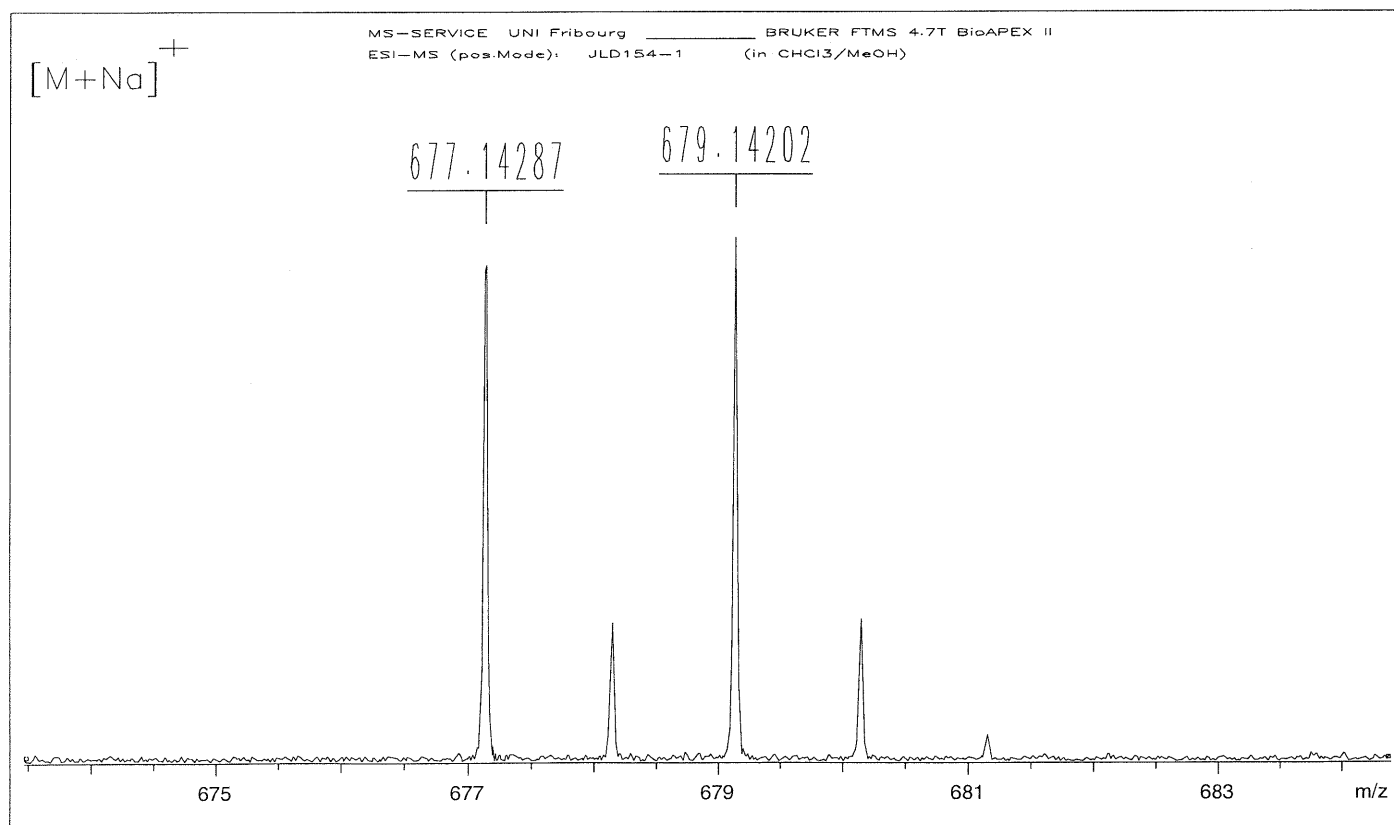
ESI-MS: JLD154-1

XMASS Mass Analysis for /Data/UNI_FR/DEBI2945_ESI/5/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

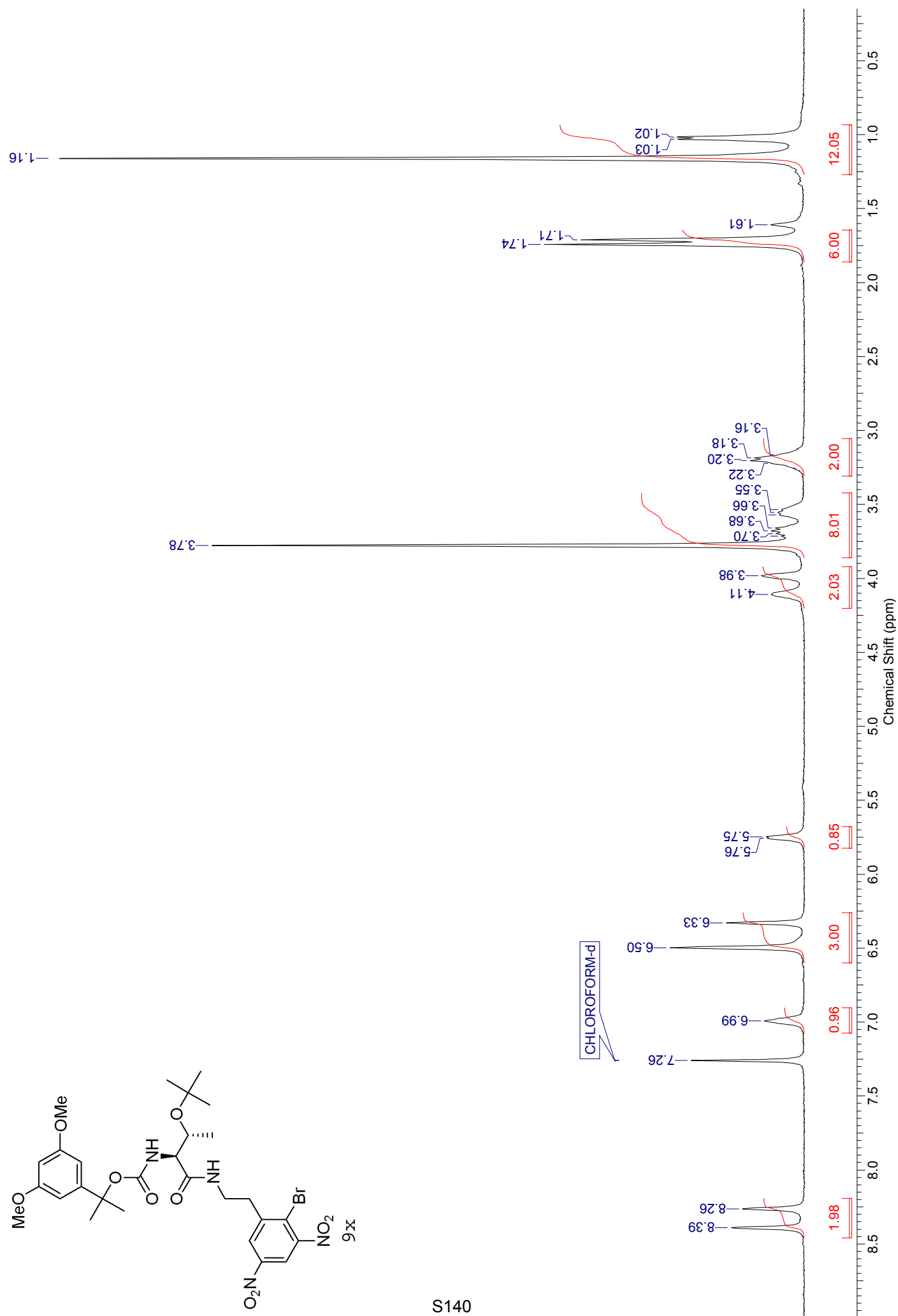
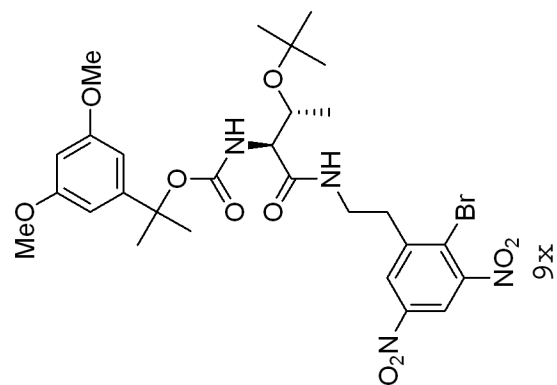
Ion mass = 677.1428670

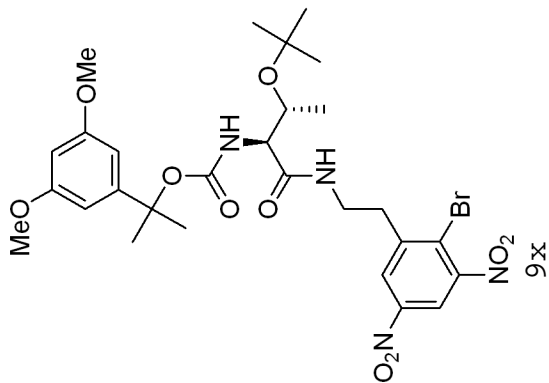
Charge = +1

#	C	H	79Br	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 677.1428670									
1	27	35	1	4	10	1	677.1428771	11.5	1.006e-05
2	25	30	1	10	8	0	677.1425970	15.5	2.700e-04
3	28	43	2	2	7	0	677.1431534	7.5	2.864e-04
4	26	41	2	5	6	0	677.1418107	8.0	1.056e-03
5	27	32	1	7	9	0	677.1439397	15.0	1.073e-03
6	25	33	1	7	9	1	677.1415344	12.0	1.333e-03
7	28	31	1	8	6	1	677.1442145	16.5	1.347e-03
8	29	37	1	1	11	1	677.1442197	11.0	1.353e-03
9	24	34	1	6	12	0	677.1412596	10.5	1.607e-03
10	38	32	1	1	6	0	677.1407518	23.0	2.115e-03

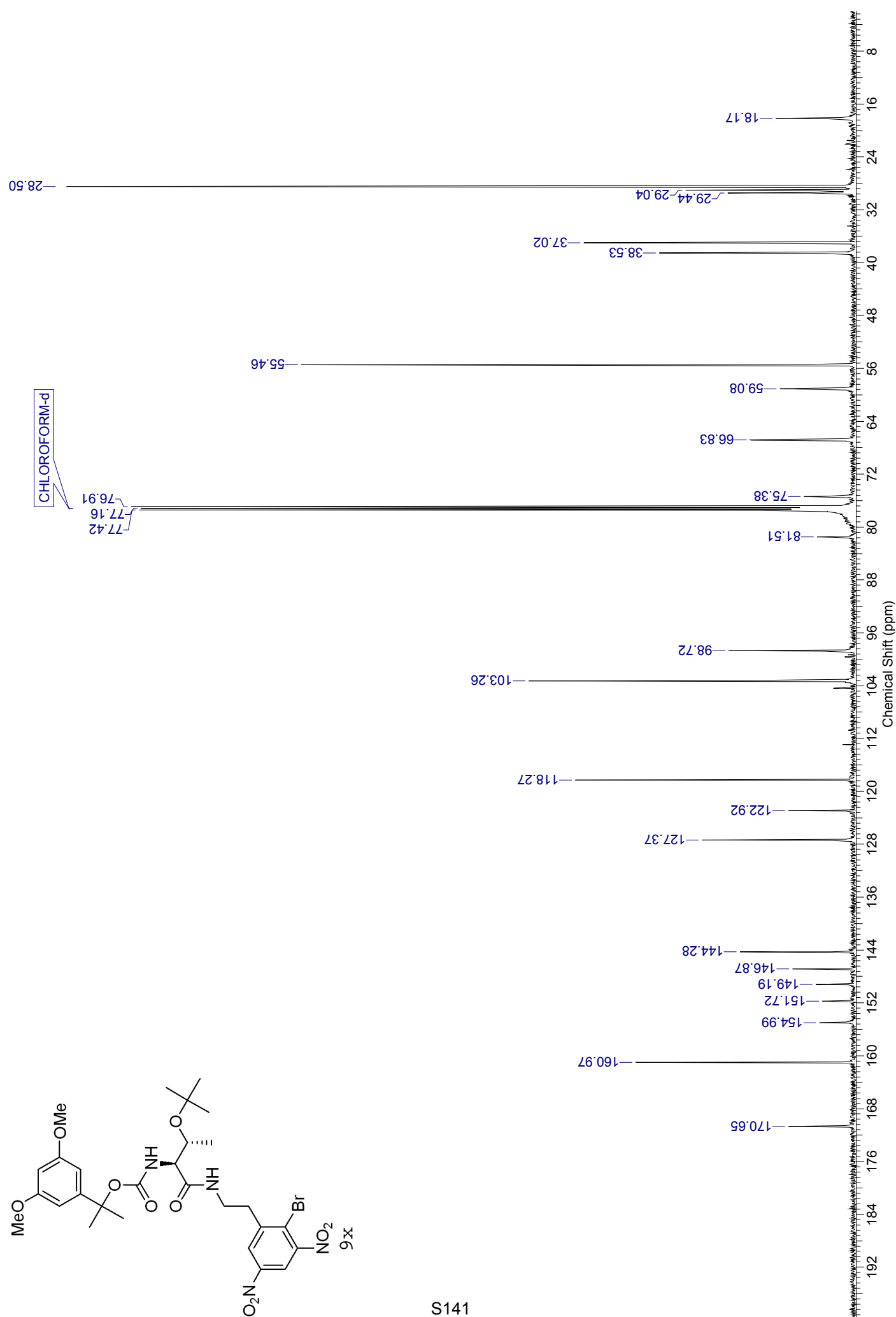


S139



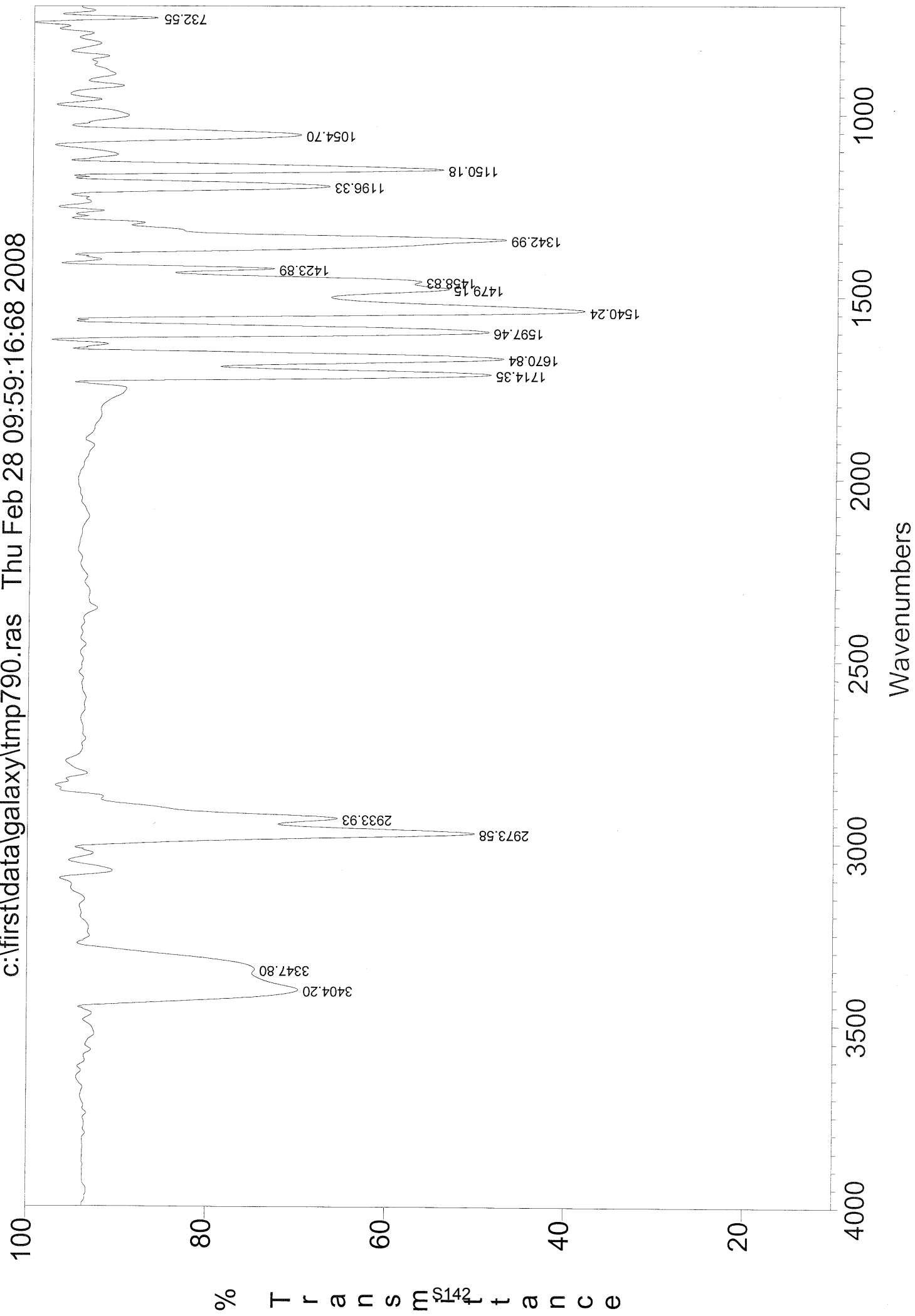


141S



960166

c:\first\data\galaxy\tmp790.ras Thu Feb 28 09:59:16:68 2008





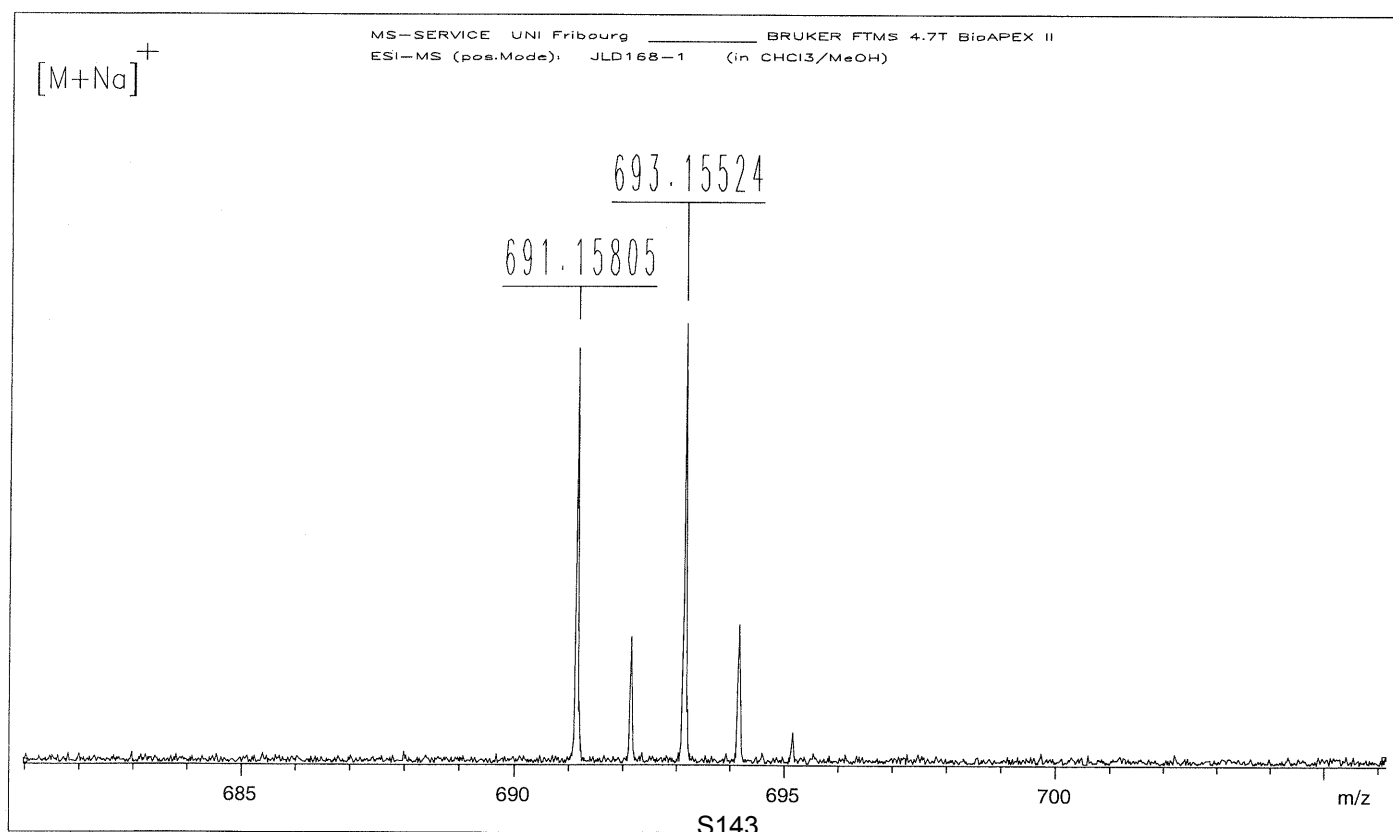
ESI-MS: JLD168-1

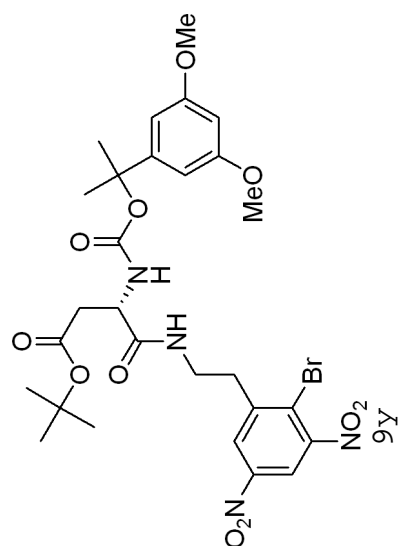
XMASS Mass Analysis for /Data/UNI_FR/DEBI3217_ESI/5/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 691.1580450

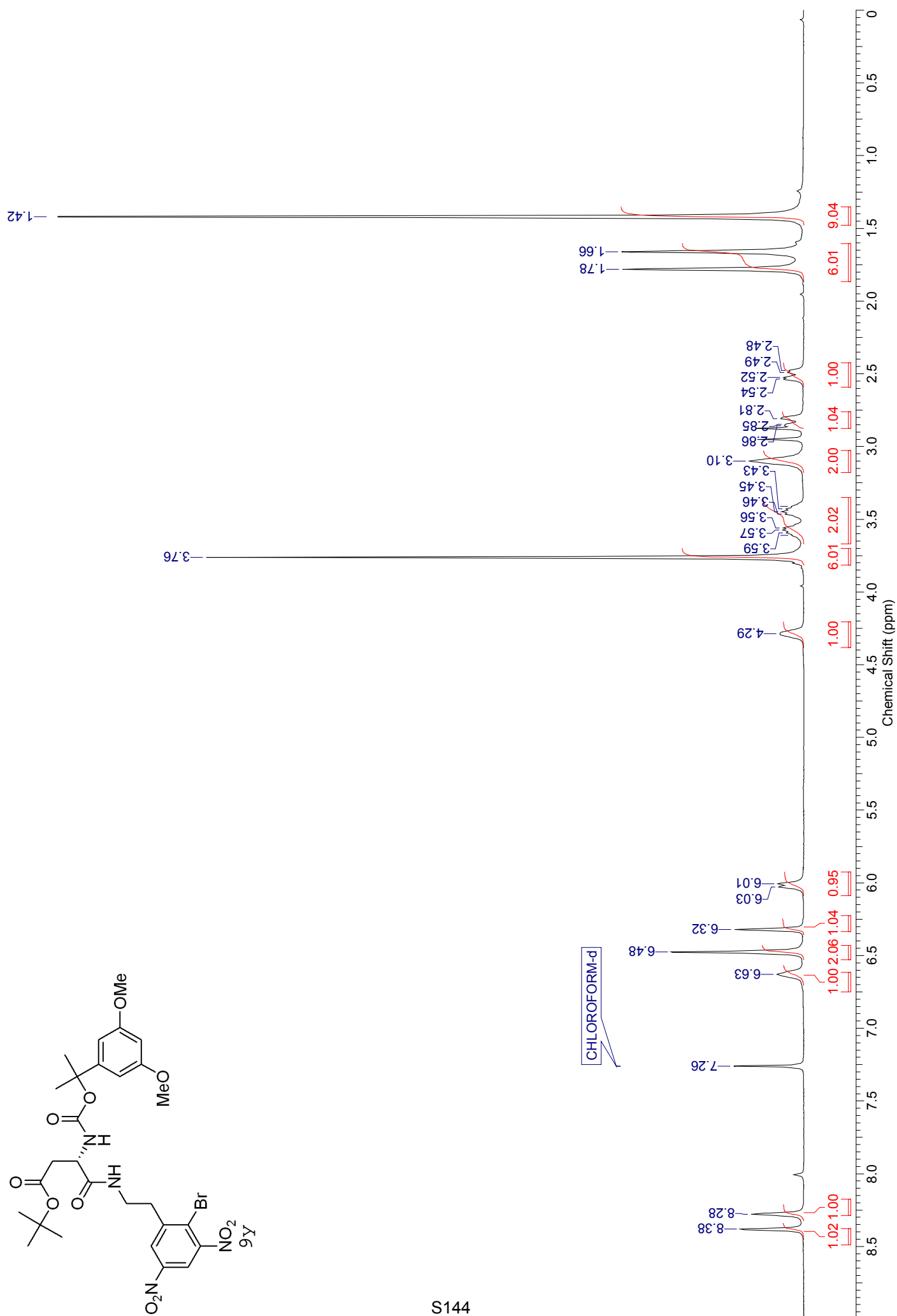
Charge = +1

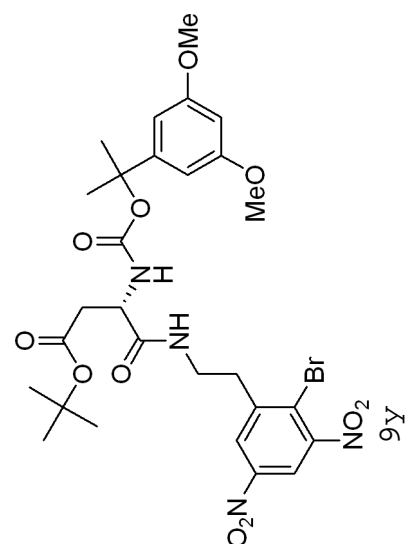
#	C	H	79Br	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 691.1580450									
1	28	37	1	4	10	1	691.1585271	11.5	4.821e-04
2	27	43	2	5	6	0	691.1574608	8.0	5.842e-04
3	29	45	2	2	7	0	691.1588034	7.5	7.584e-04
4	39	34	1	1	6	0	691.1564018	23.0	1.643e-03
5	27	46	2	2	7	1	691.1563981	4.5	1.647e-03
6	30	39	1	1	11	1	691.1598698	11.0	1.825e-03
7	26	47	2	1	10	0	691.1561234	3.0	1.922e-03
8	30	36	1	4	10	0	691.1609324	14.5	2.887e-03
9	25	44	2	5	6	1	691.1550555	5.0	2.990e-03
10	31	35	1	5	7	1	691.1612072	16.0	3.162e-03



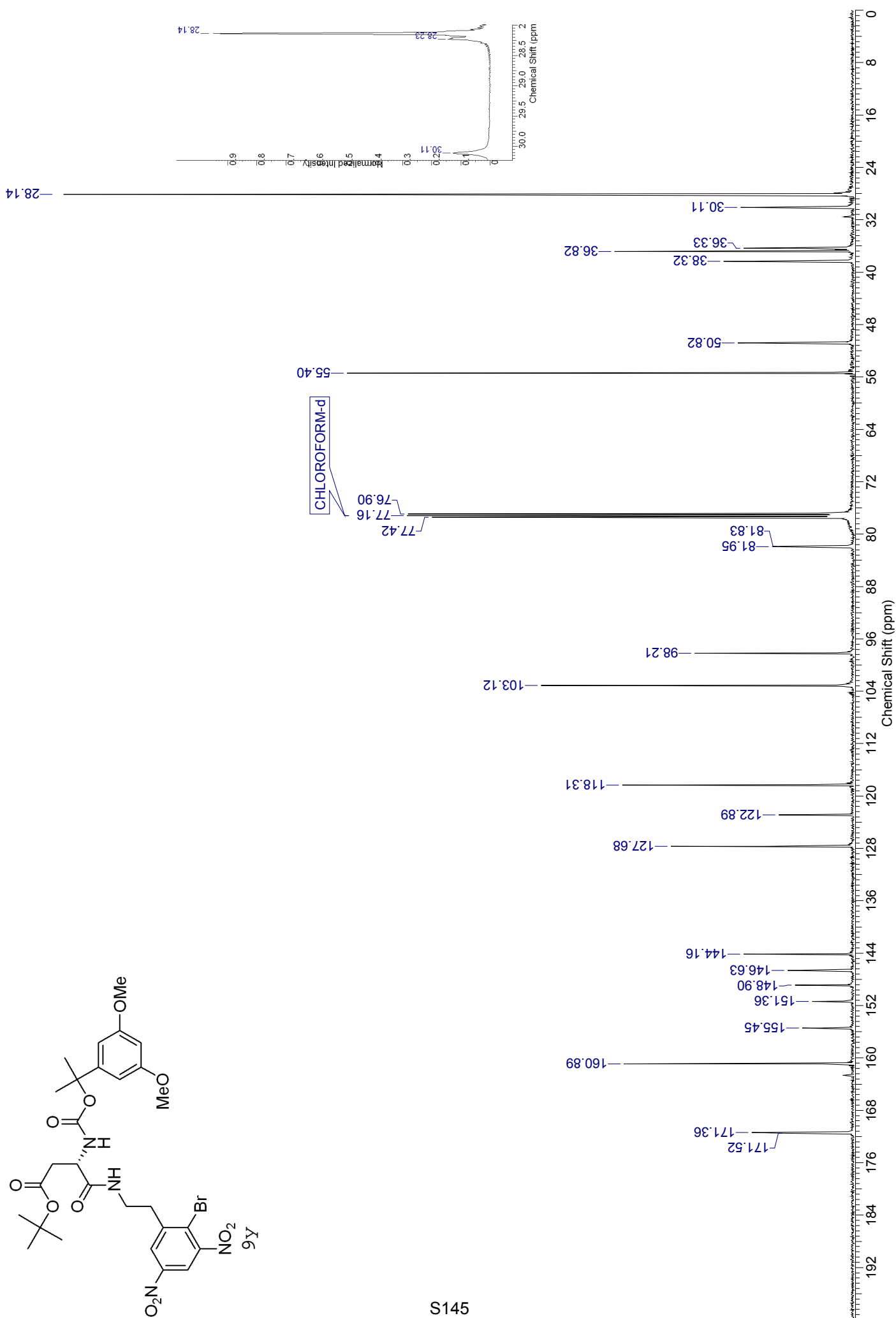


S144



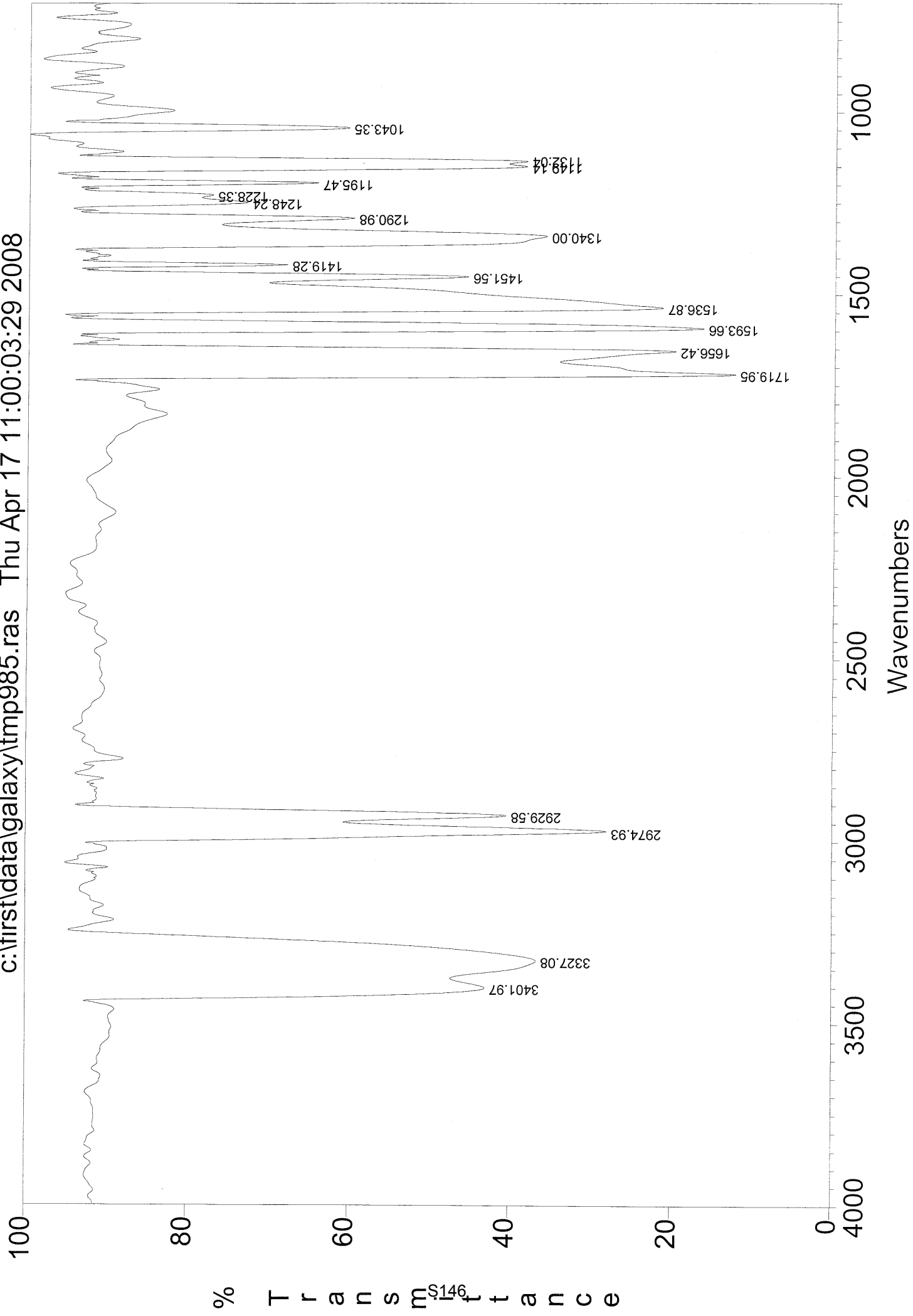


S145



96174

c:\first\data\galaxy\tmp985.ras Thu Apr 17 11:00:03:29 2008



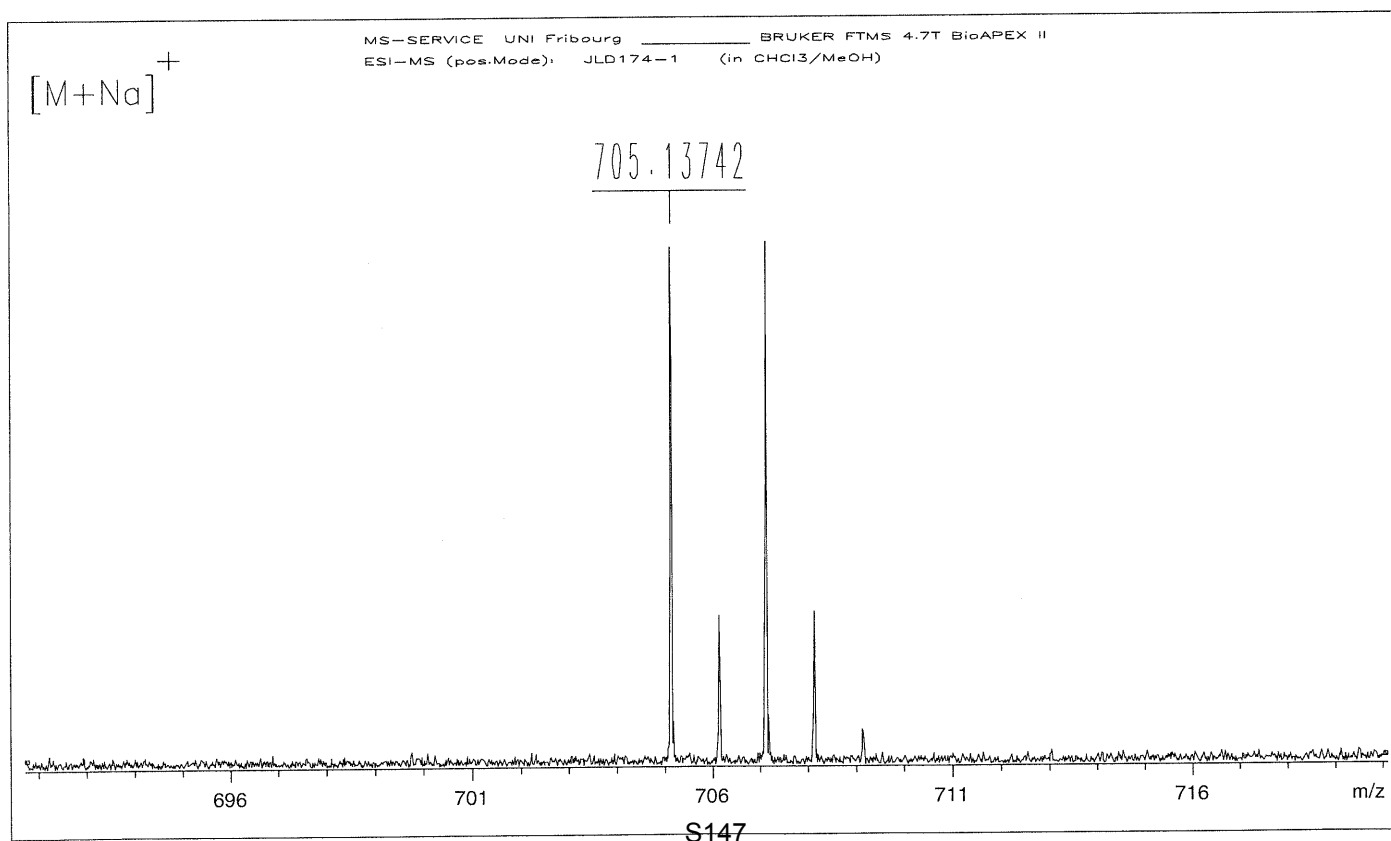
ESI-MS: JLD174-1

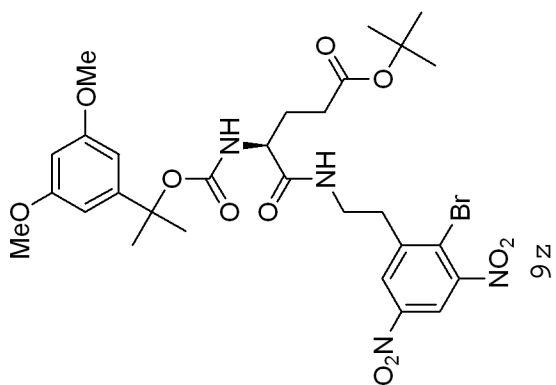
XMASS Mass Analysis for /Data/UNI_FR/DEBI3336_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 705.1374160

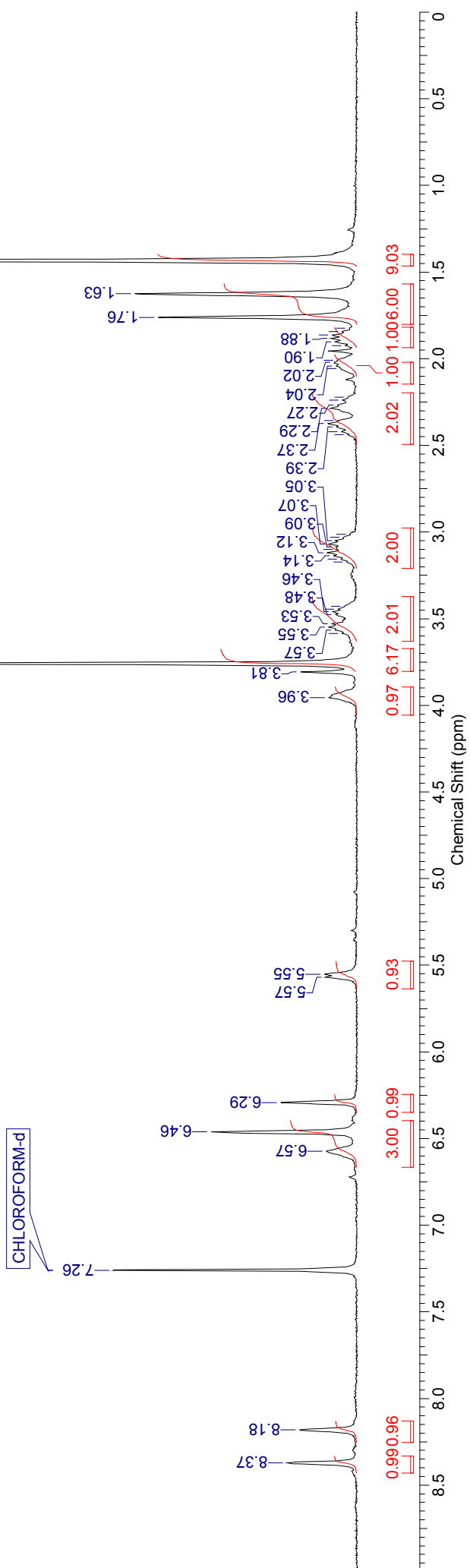
Charge = +1

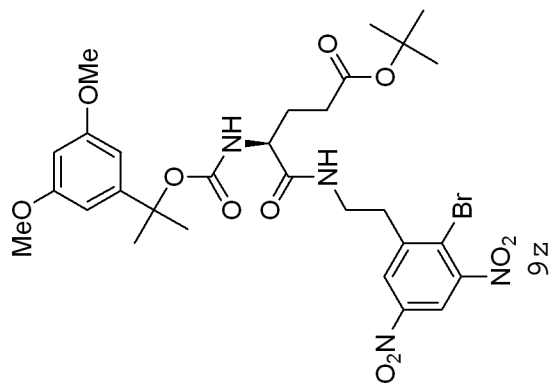
#	C	H	79Br	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 705.1374160									
1	28	35	1	4	11	1	705.1377917	12.5	3.757e-04
2	27	41	2	5	7	0	705.1367253	9.0	6.907e-04
3	30	42	2	3	5	1	705.1383428	10.0	9.268e-04
4	30	34	1	4	11	0	705.1401970	15.5	2.781e-03
5	31	33	1	5	8	1	705.1404718	17.0	3.056e-03
6	37	30	1	4	6	0	705.1343237	24.5	3.092e-03
7	25	42	2	5	7	1	705.1343200	6.0	3.096e-03
8	32	41	2	3	5	0	705.1407481	13.0	3.332e-03
9	24	43	2	4	10	0	705.1340452	4.5	3.371e-03
10	20	45	2	5	12	0	705.1425986	0.0	5.183e-03



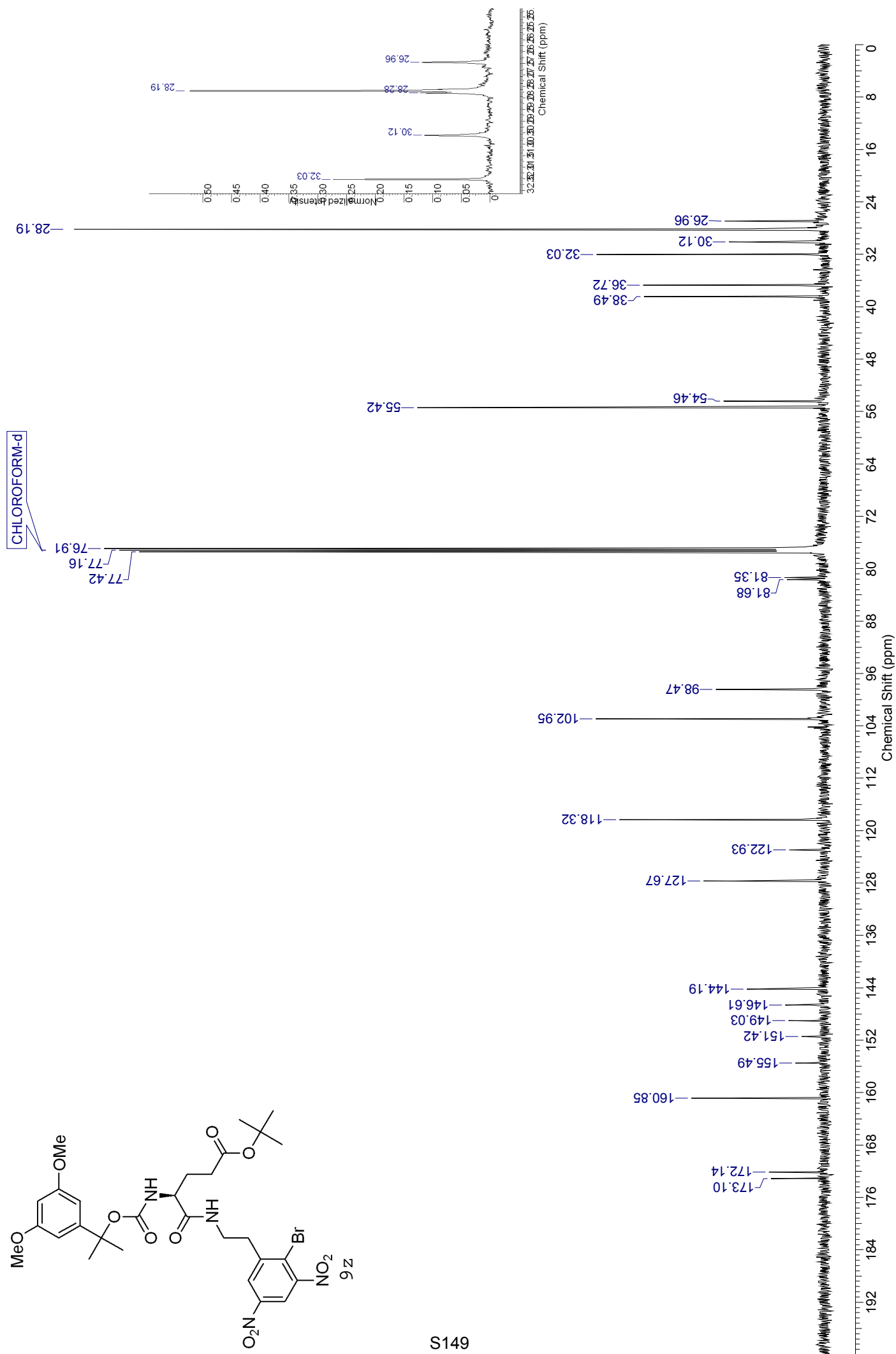


S148



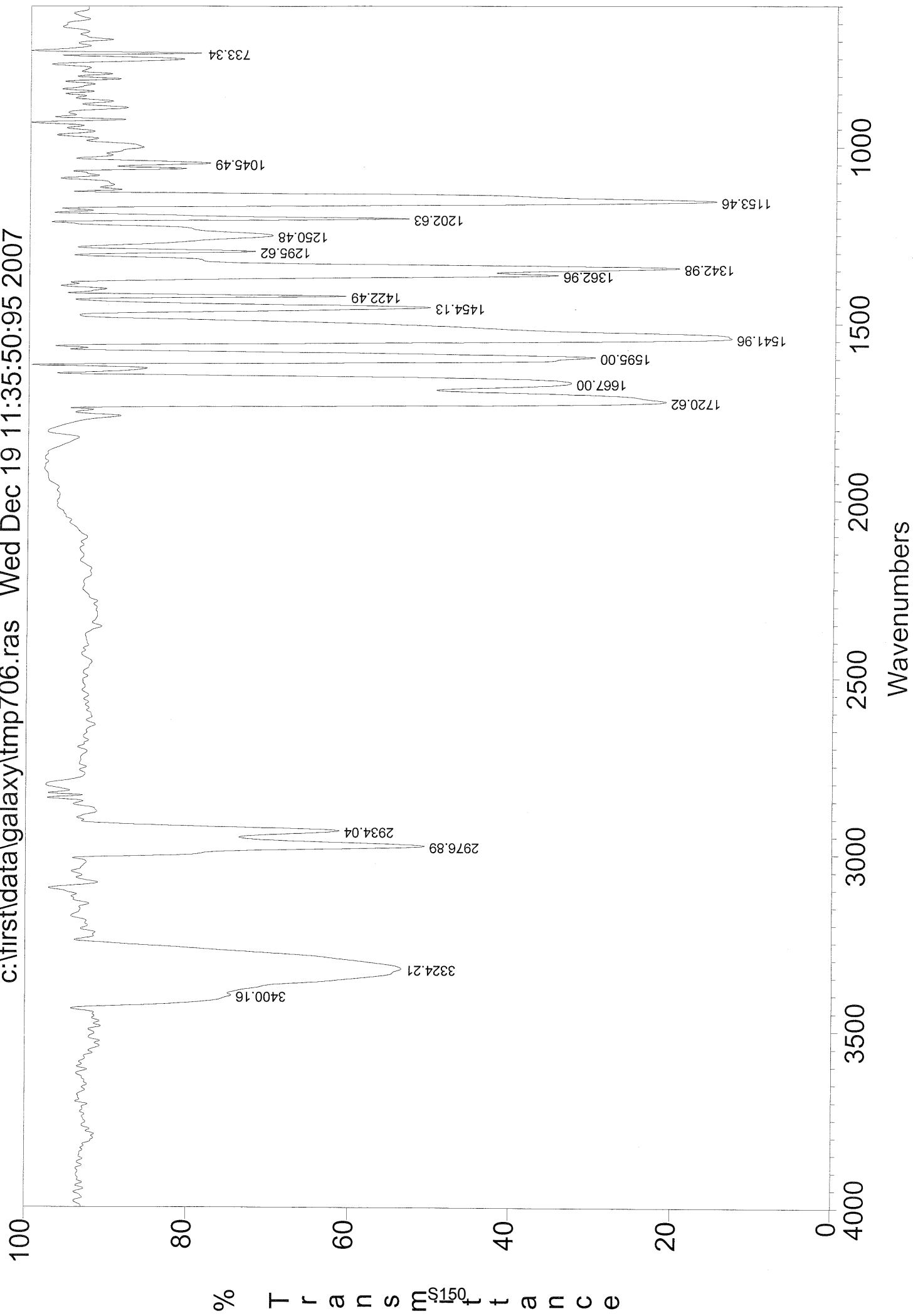


6149



56016A

c:\first\data\galaxy\tmp706.ras Wed Dec 19 11:35:50:95 2007



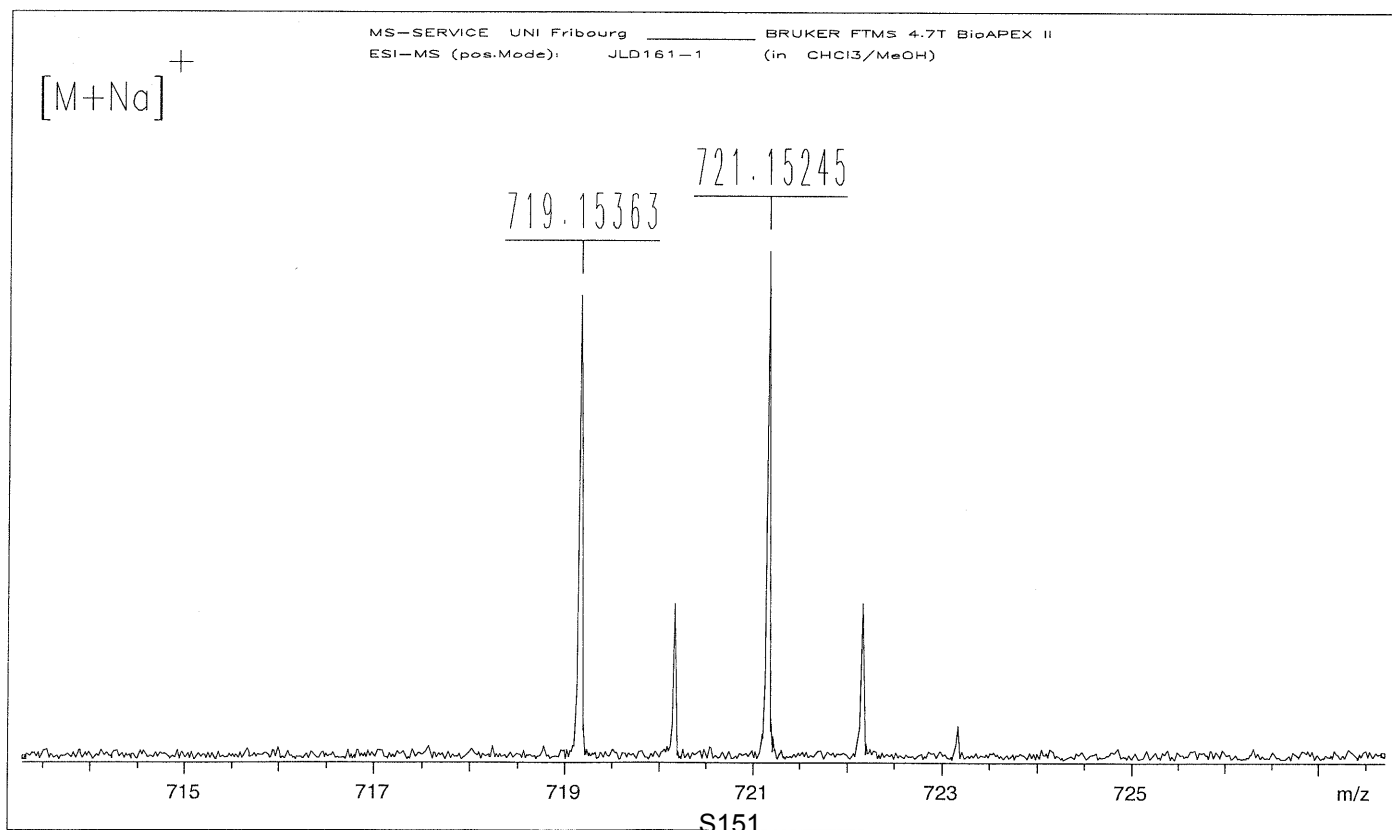
ESI-MS: JLD161-1

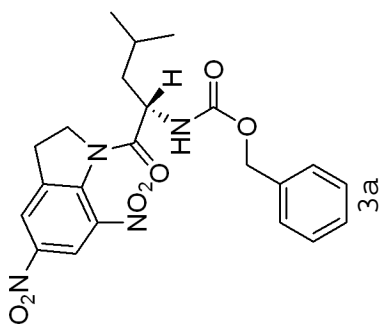
XMASS Mass Analysis for /Data/UNI_FR/DEBI3093_ESI/5/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 719.1536250

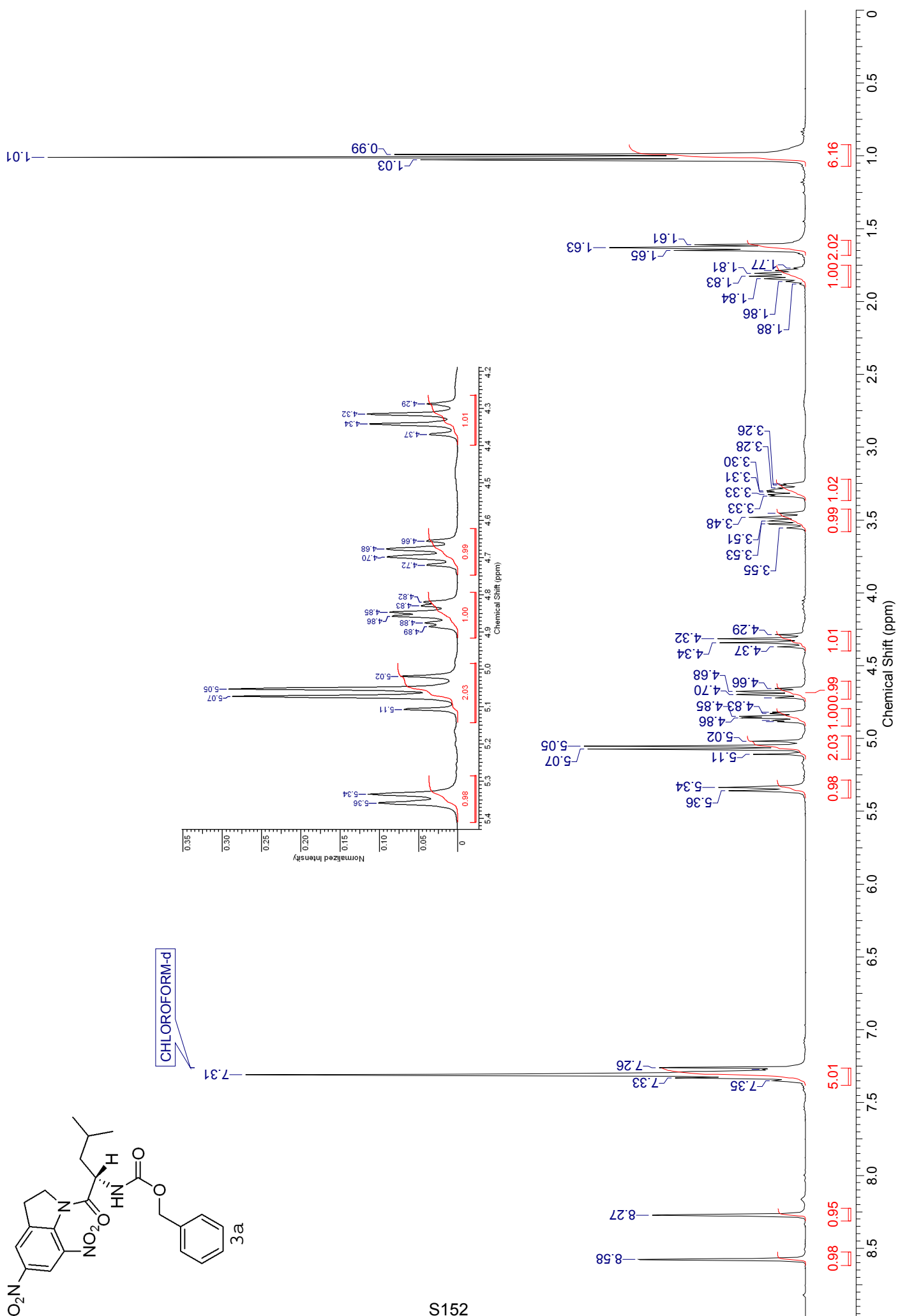
Charge = +1

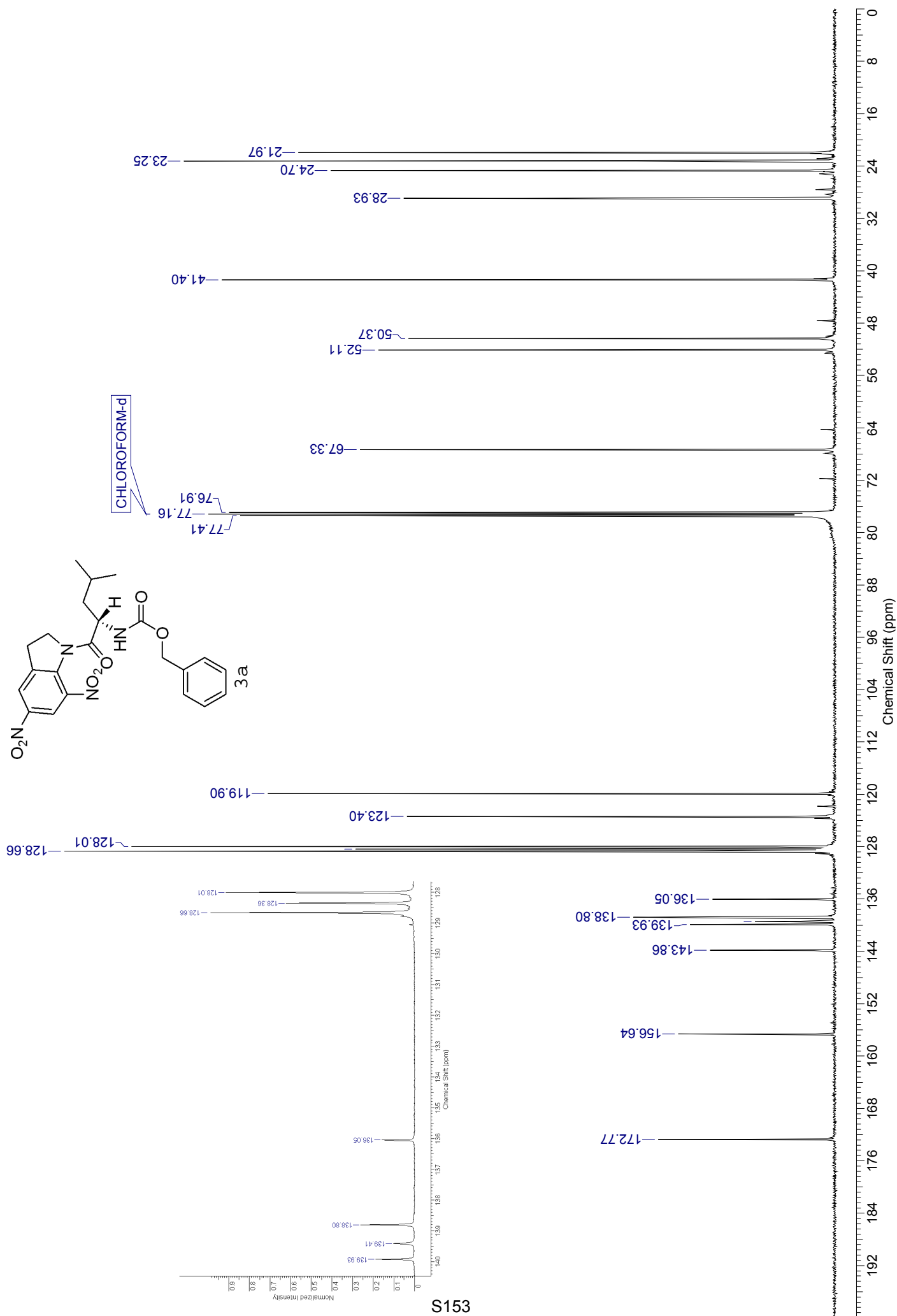
#	C	H	79Br	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 719.1536250									
1	29	37	1	4	11	1	719.1534417	12.5	1.833e-04
2	31	44	2	3	5	1	719.1539928	10.0	3.678e-04
3	28	38	1	3	14	0	719.1531670	11.0	4.580e-04
4	28	43	2	5	7	0	719.1523754	9.0	1.250e-03
5	31	36	1	4	11	0	719.1558470	15.5	2.222e-03
6	32	35	1	5	8	1	719.1561218	17.0	2.497e-03
7	33	43	2	3	5	0	719.1563981	13.0	2.773e-03
8	26	39	1	3	14	1	719.1507617	8.0	2.863e-03
9	38	32	1	4	6	0	719.1499738	24.5	3.651e-03
10	26	44	2	5	7	1	719.1499701	6.0	3.655e-03





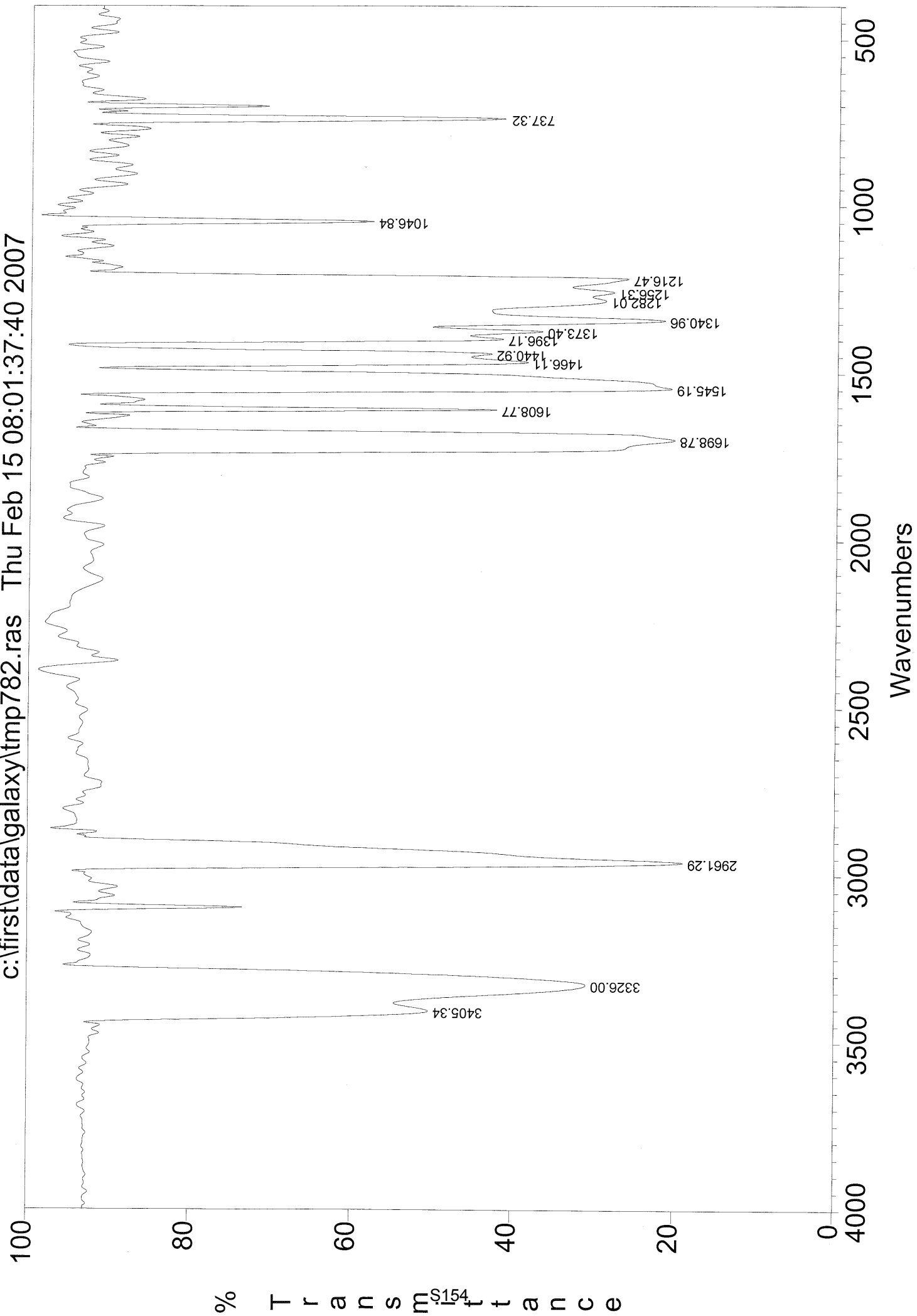
CHLOROFORM-d





50107

c:\first\data\galaxy\tmp782.ras Thu Feb 15 08:01:37:40 2007



ESI-MS: JLD102-MS

XMASS Mass Analysis for /Data/UNI_FR/DEBI2362_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

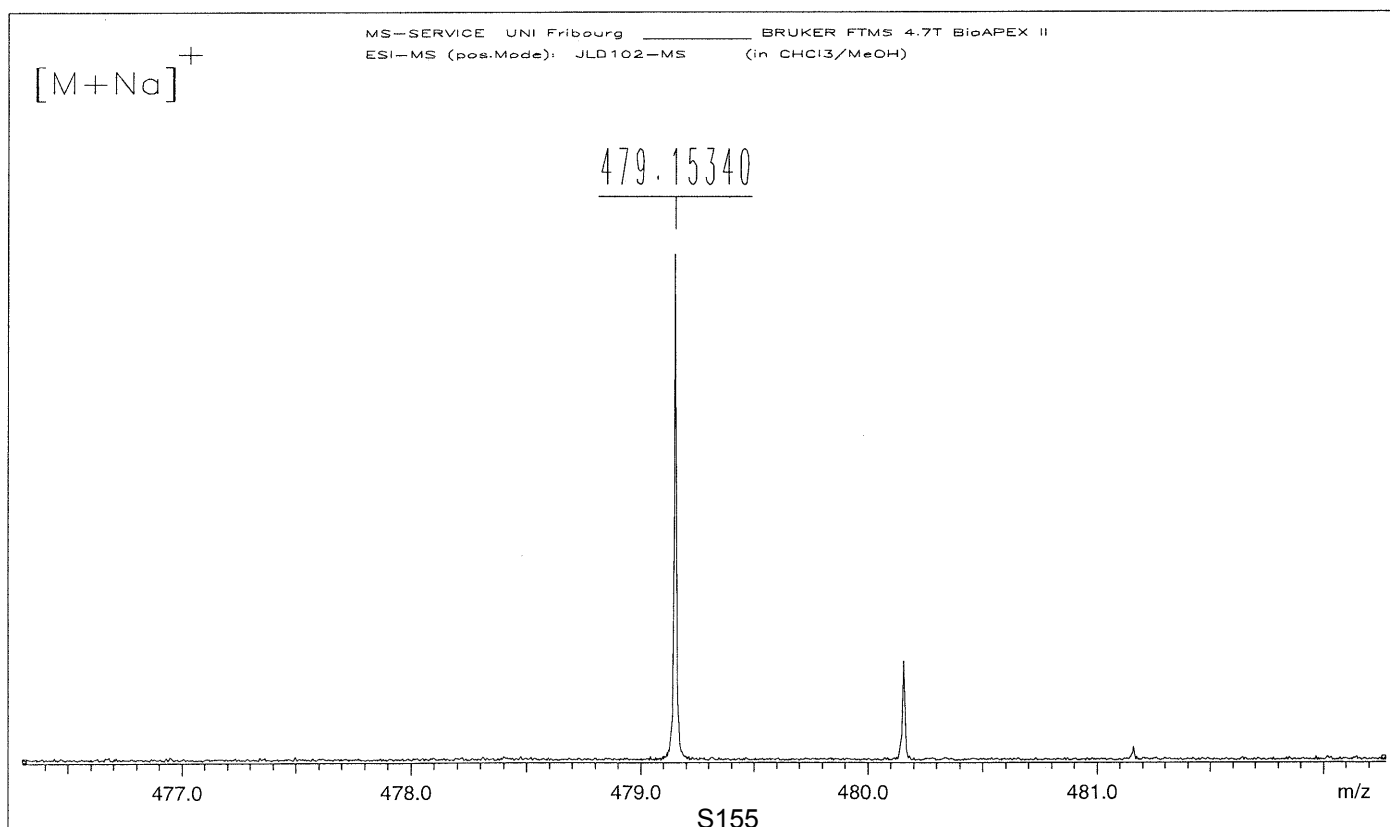
Ion mass = 479.1533970

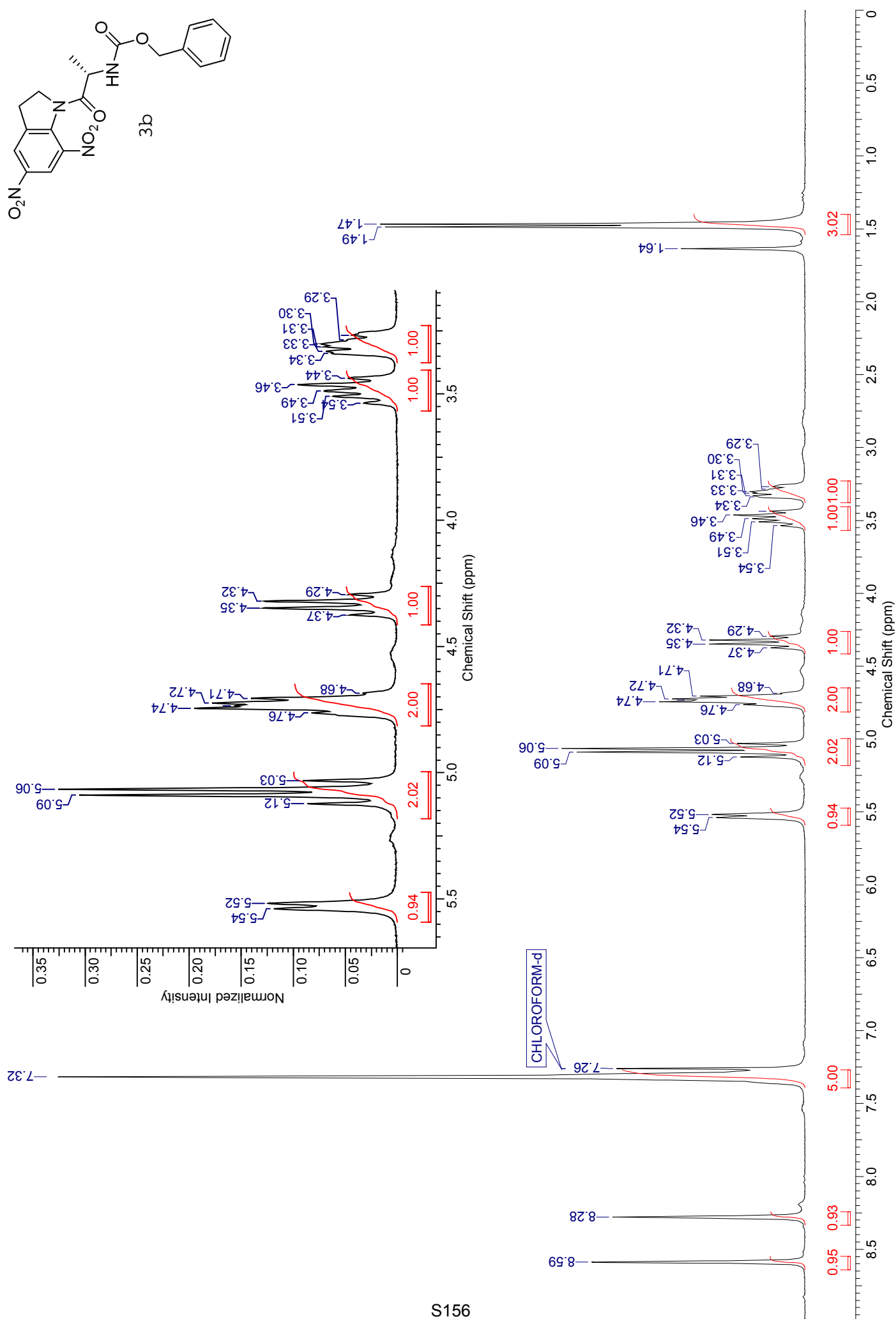
Charge = +1

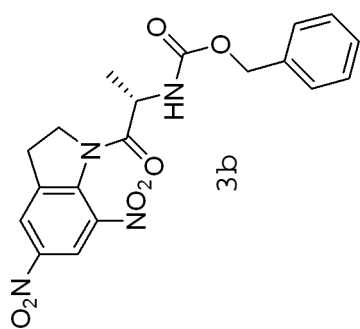
#	C	H	N	O	Na	mass	DBE	error
---	---	---	---	---	----	------	-----	-------

*** Mass Analysis for mass 479.1533970

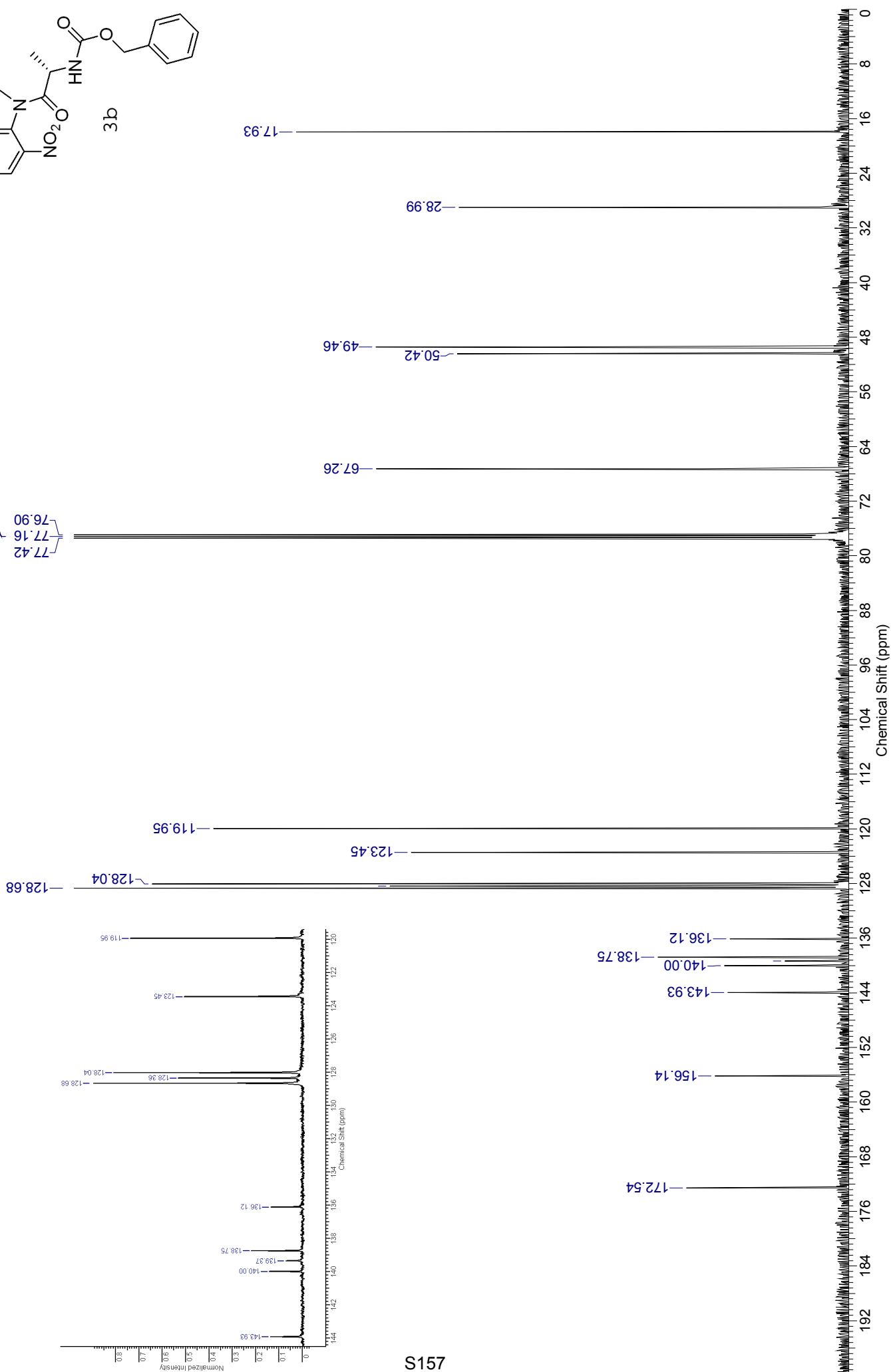
1	22	24	4	7	1	479.1537202	12.5	3.232e-04
2	20	22	7	6	1	479.1523776	13.0	1.019e-03
3	19	23	6	9	0	479.1521028	11.5	1.294e-03
4	22	21	7	6	0	479.1547829	16.0	1.386e-03
5	23	20	8	3	1	479.1550576	17.5	1.661e-03
6	24	23	4	7	0	479.1561255	15.5	2.729e-03
7	25	22	5	4	1	479.1564003	17.0	3.003e-03
8	17	24	6	9	1	479.1496975	8.5	3.700e-03
9	25	19	8	3	0	479.1574629	20.5	4.066e-03
10	16	24	8	8	1	479.1609309	8.5	7.534e-03





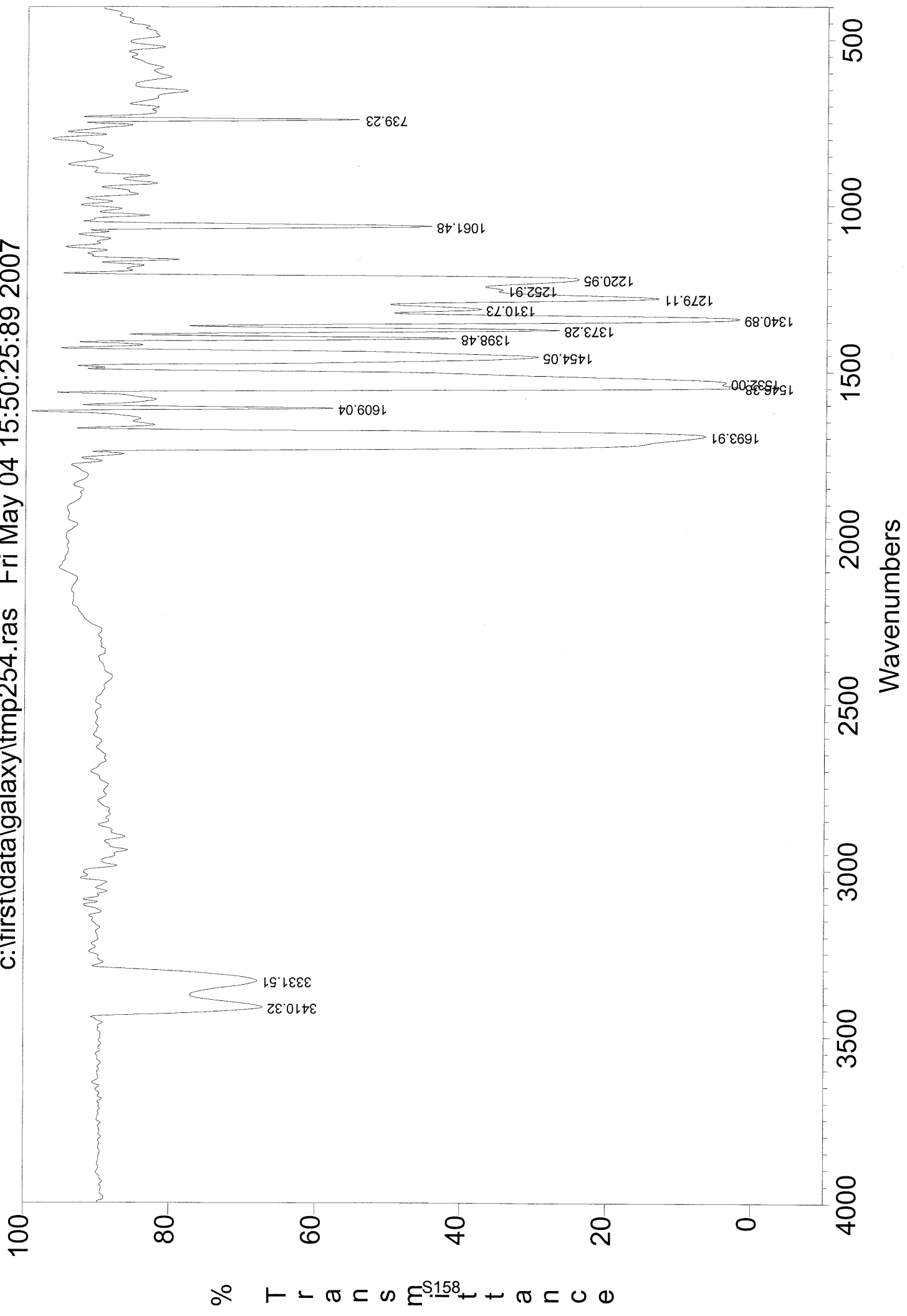


CHLOROFORM-d



920 123

c:\first\data\galaxy\tmp254.ras Fri May 04 15:50:25:89 2007



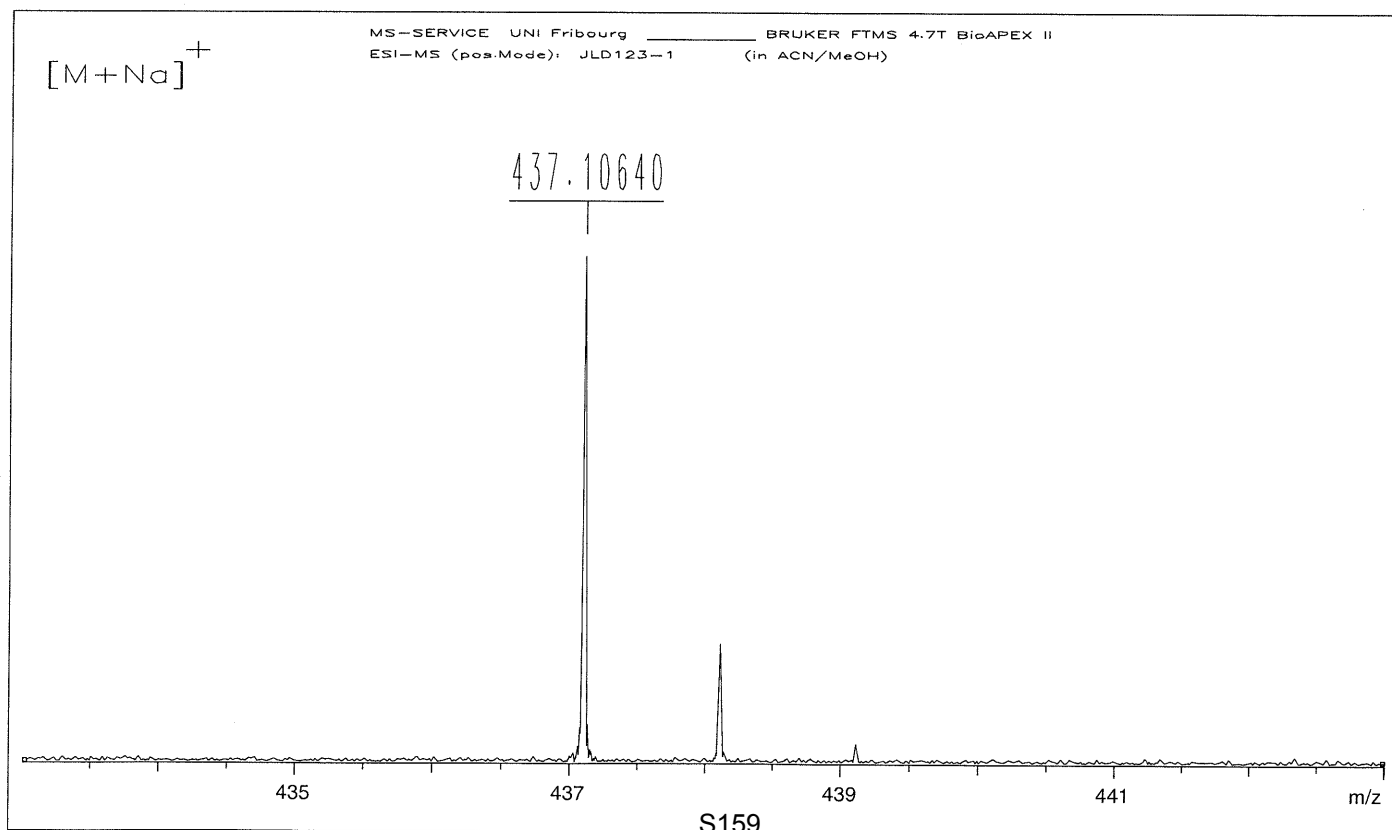
ESI-MS: JLD123-1

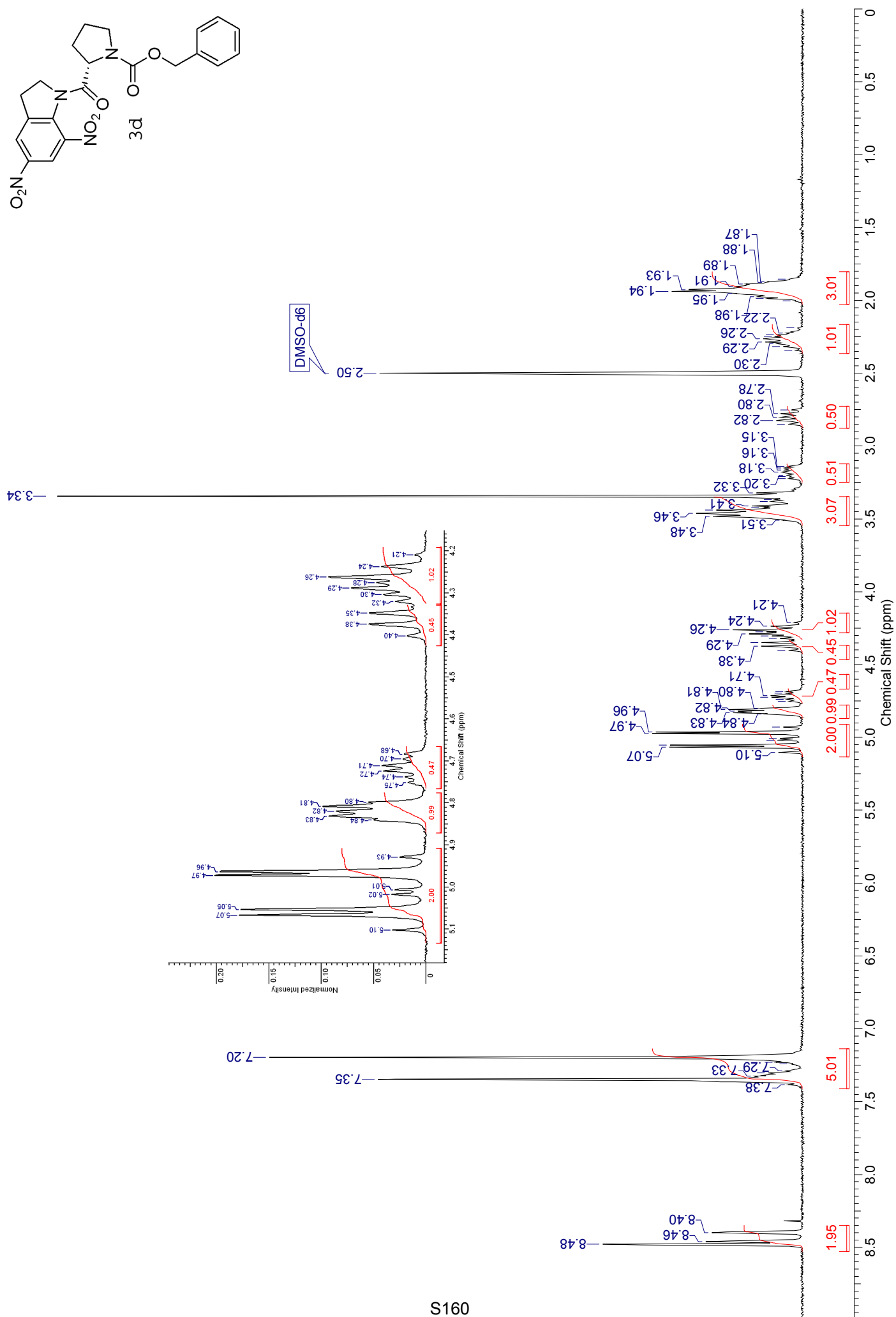
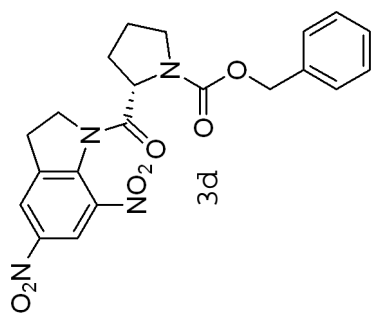
XMASS Mass Analysis for /Data/UNI_FR/DEBI2619_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

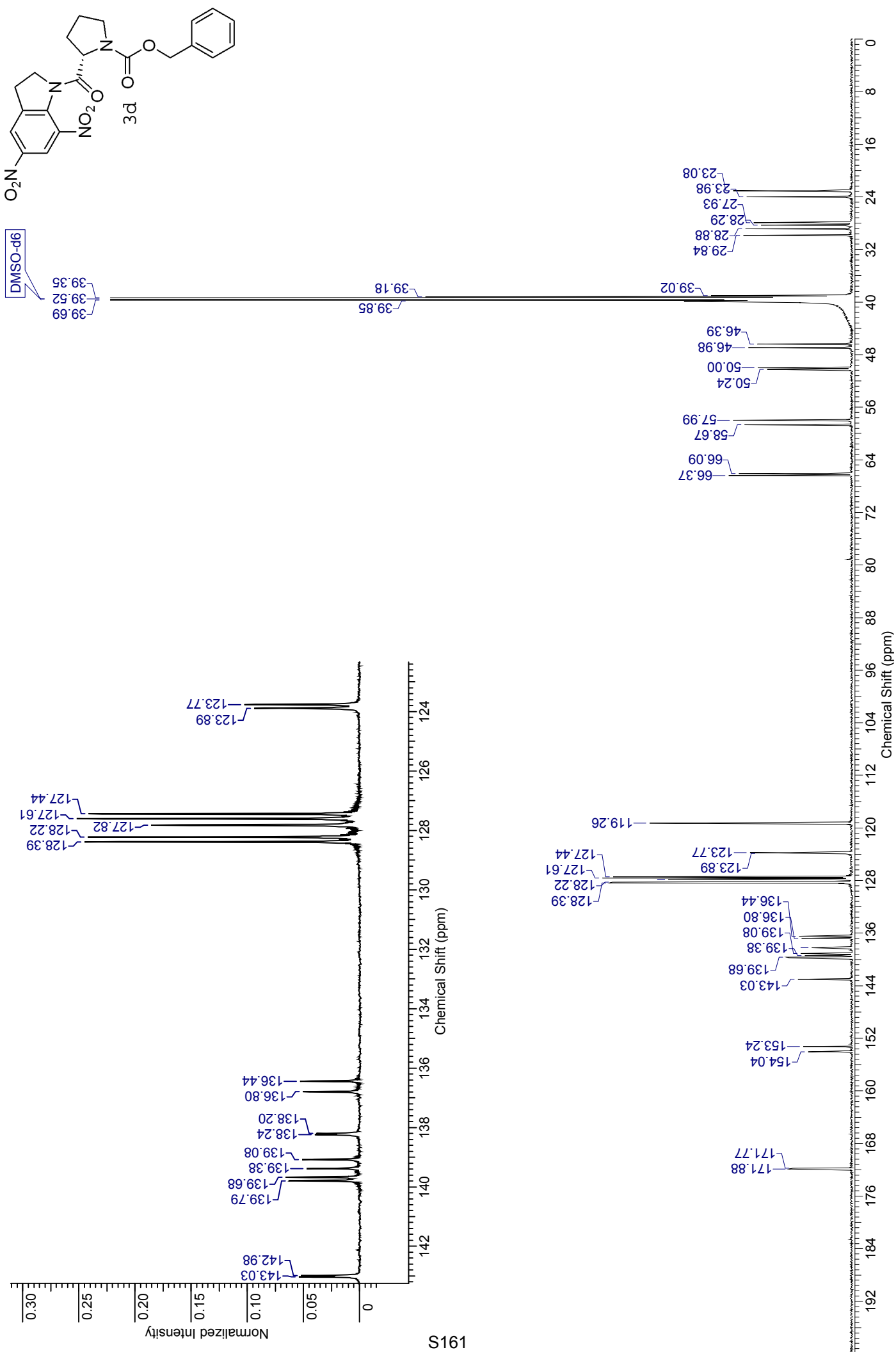
Ion mass = 437.1063960

Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 437.1063960								
1	19	18	4	7	1	437.1067700	12.5	3.740e-04
2	21	17	4	7	0	437.1091753	15.5	2.779e-03
3	22	16	5	4	1	437.1094501	17.0	3.054e-03
4	24	15	5	4	0	437.1118554	20.0	5.459e-03
5	25	15	3	5	0	437.1006220	20.0	5.774e-03
6	23	16	3	5	1	437.0982167	17.0	8.179e-03
7	20	15	5	7	0	437.0965993	16.0	9.797e-03
8	18	16	5	7	1	437.0941940	13.0	1.220e-02
9	20	20	3	7	1	437.1193461	12.0	1.295e-02
10	22	19	3	7	0	437.1217514	15.0	1.536e-02

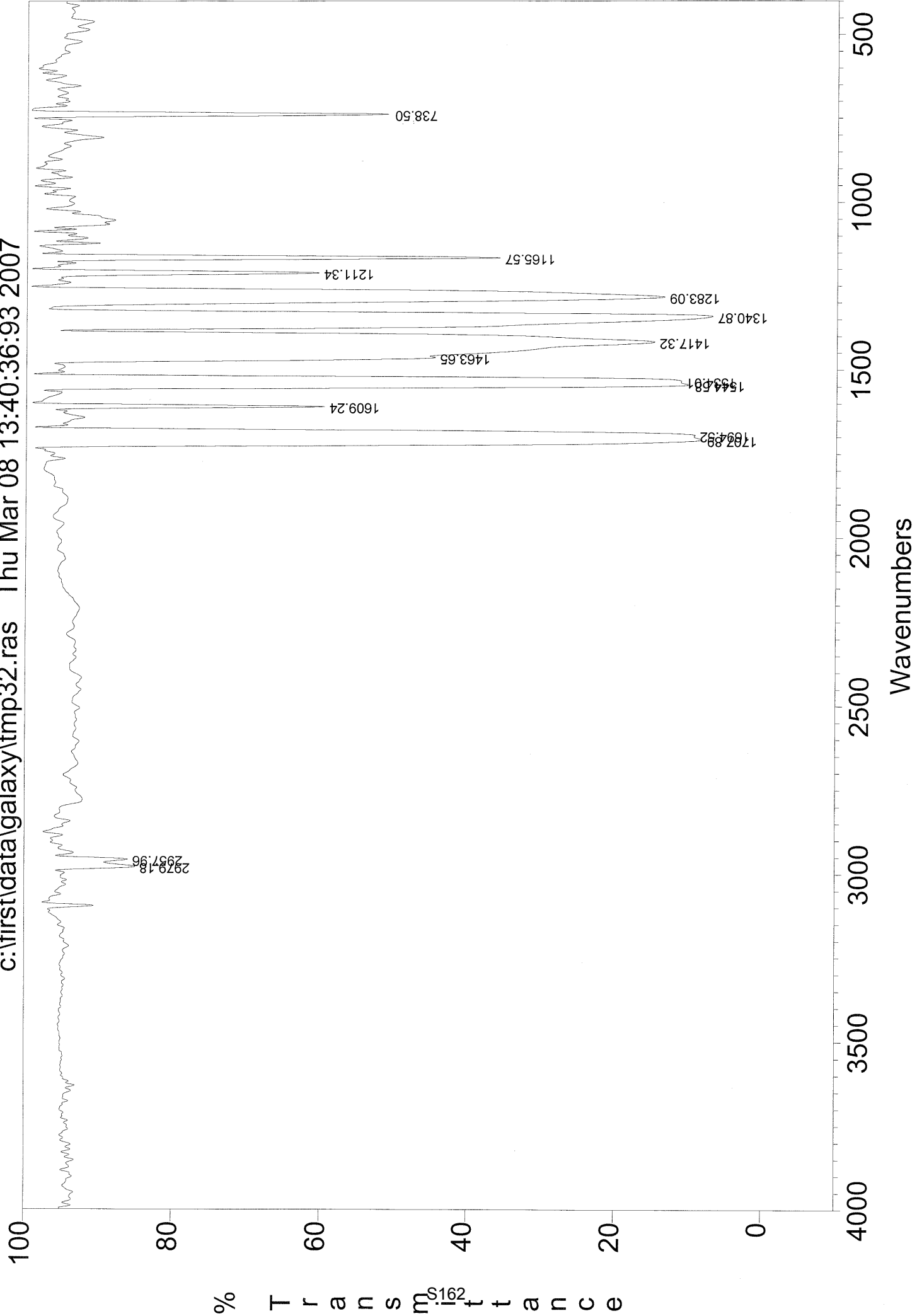






7CD108

c:\first\data\galaxy\tmp32.ras Thu Mar 08 13:40:36:93 2007



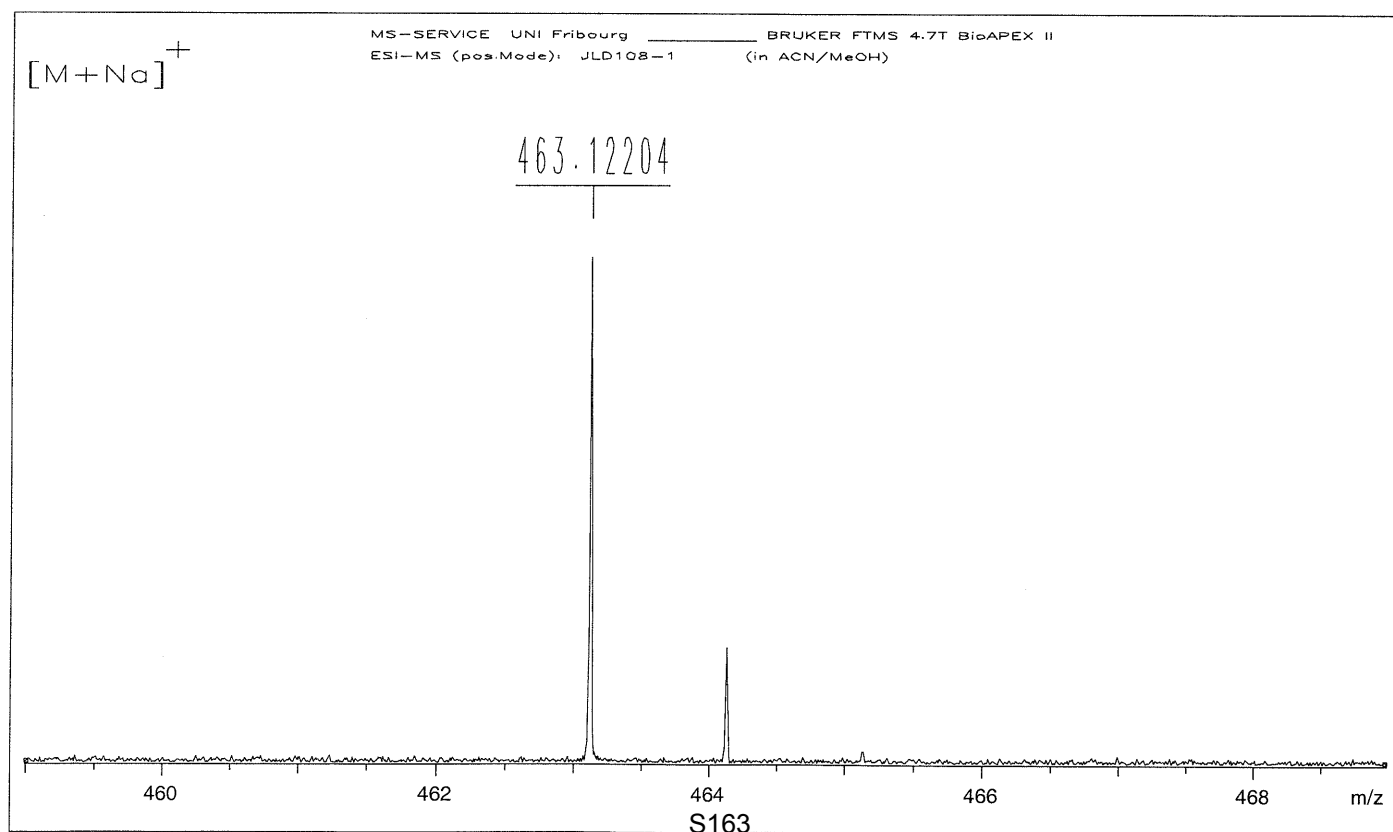
ESI-MS: JLD108-1

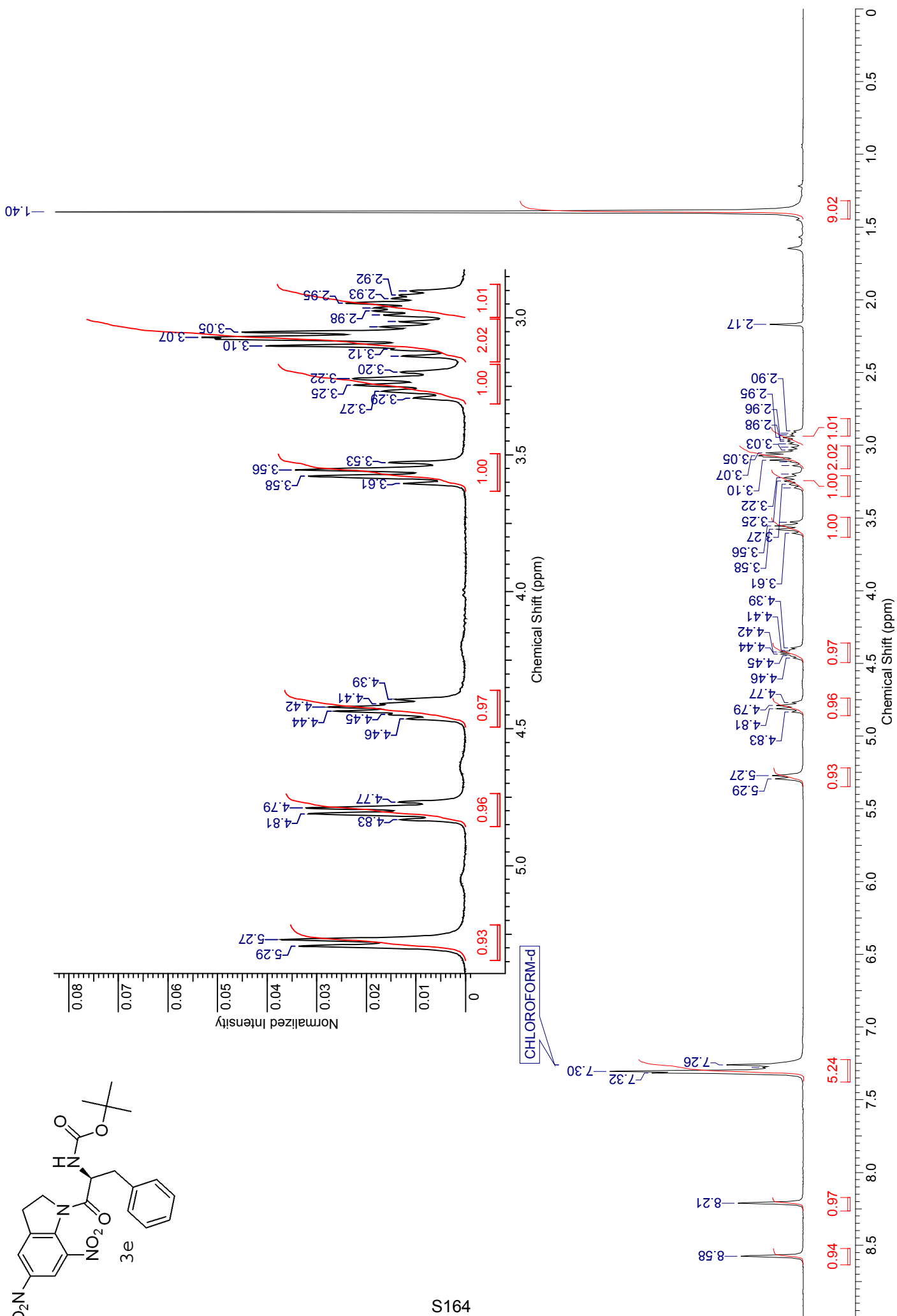
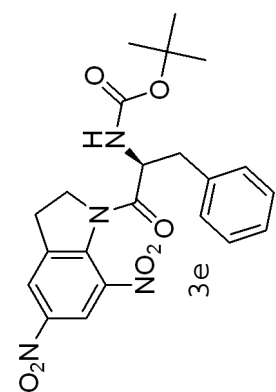
XMASS Mass Analysis for /Data/UNI_FR/DEBI2630_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

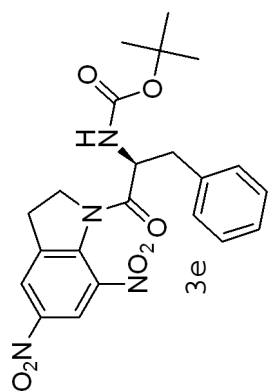
Ion mass = 463.1220380

Charge = +1

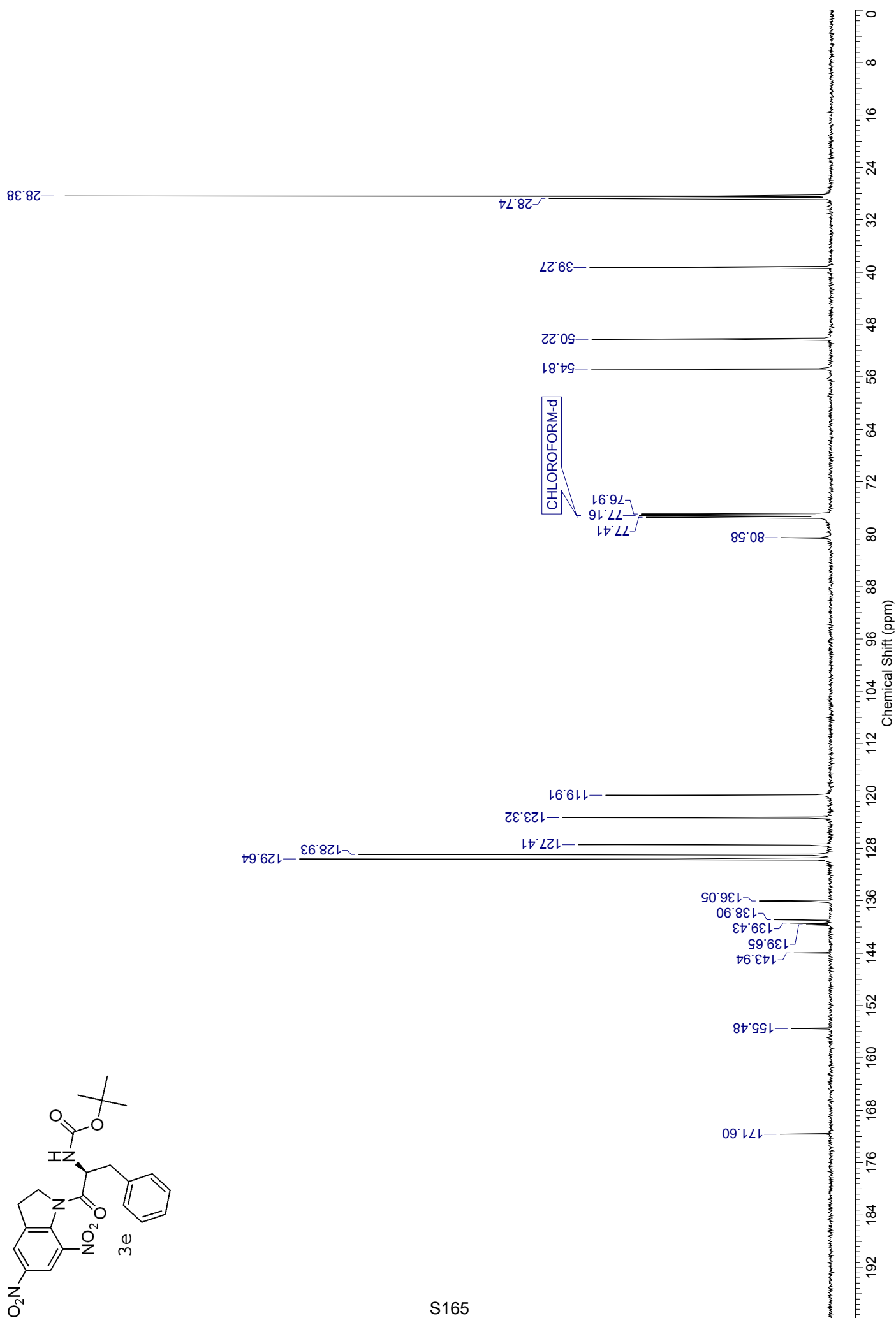
#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 463.1220380								
1	21	20	4	7	1	463.1224201	13.5	3.821e-04
2	23	19	4	7	0	463.1248254	16.5	2.787e-03
3	24	18	5	4	1	463.1251002	18.0	3.062e-03
4	25	18	3	5	1	463.1138668	18.0	8.171e-03
5	17	22	5	9	1	463.1309734	9.0	8.935e-03
6	22	17	5	7	0	463.1122493	17.0	9.789e-03
7	19	21	5	9	0	463.1333787	12.0	1.134e-02
8	20	18	5	7	1	463.1098440	14.0	1.219e-02
9	22	22	3	7	1	463.1349962	13.0	1.296e-02
10	24	21	3	7	0	463.1374015	16.0	1.536e-02





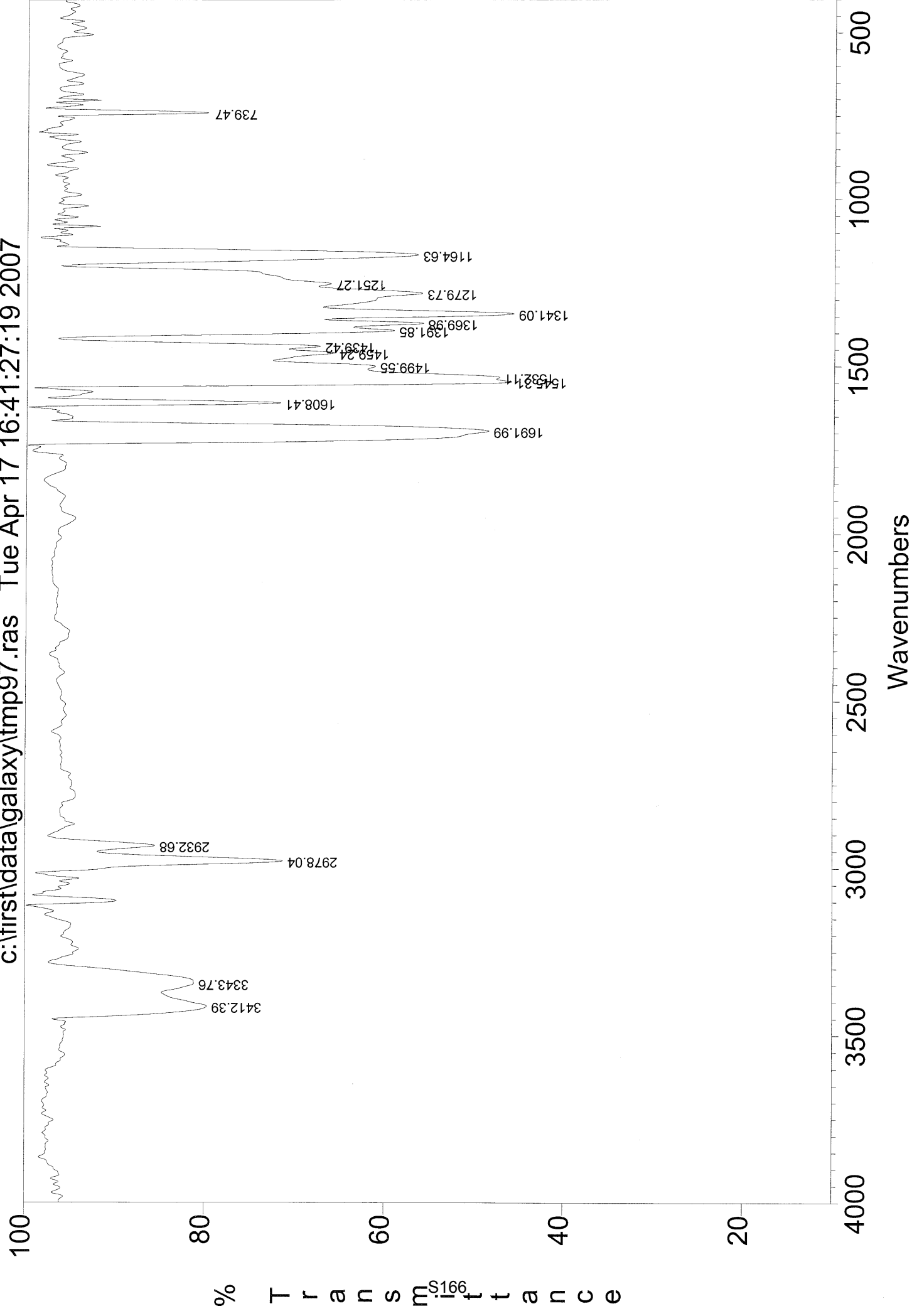


S165



5115

c:\firstdata\galaxy\tmp97.ras Tue Apr 17 16:41:27:19 2007



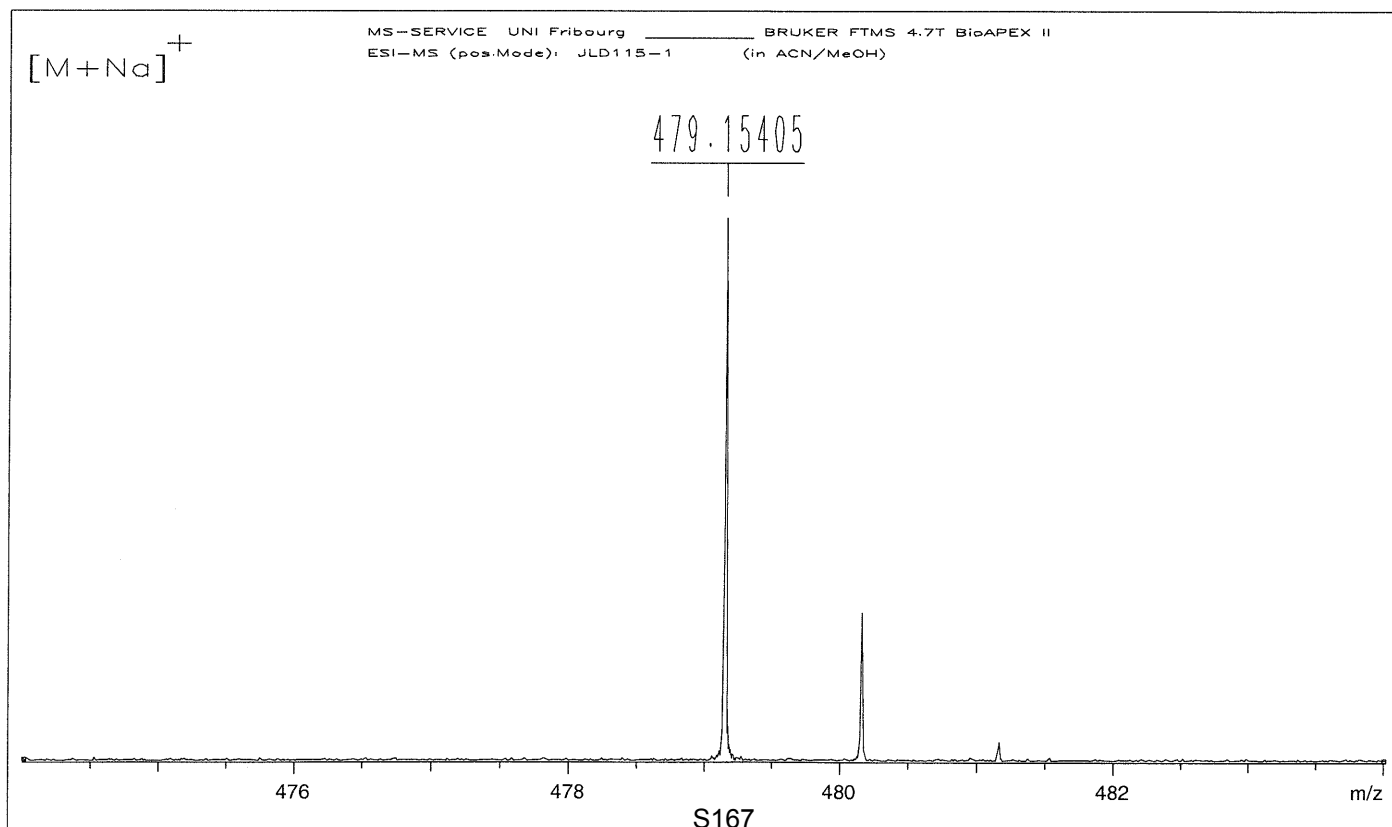
ESI-MS: JLD115-1

XMASS Mass Analysis for /Data/UNI_FR/DEBI2624_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 479.1540480

Charge = +1

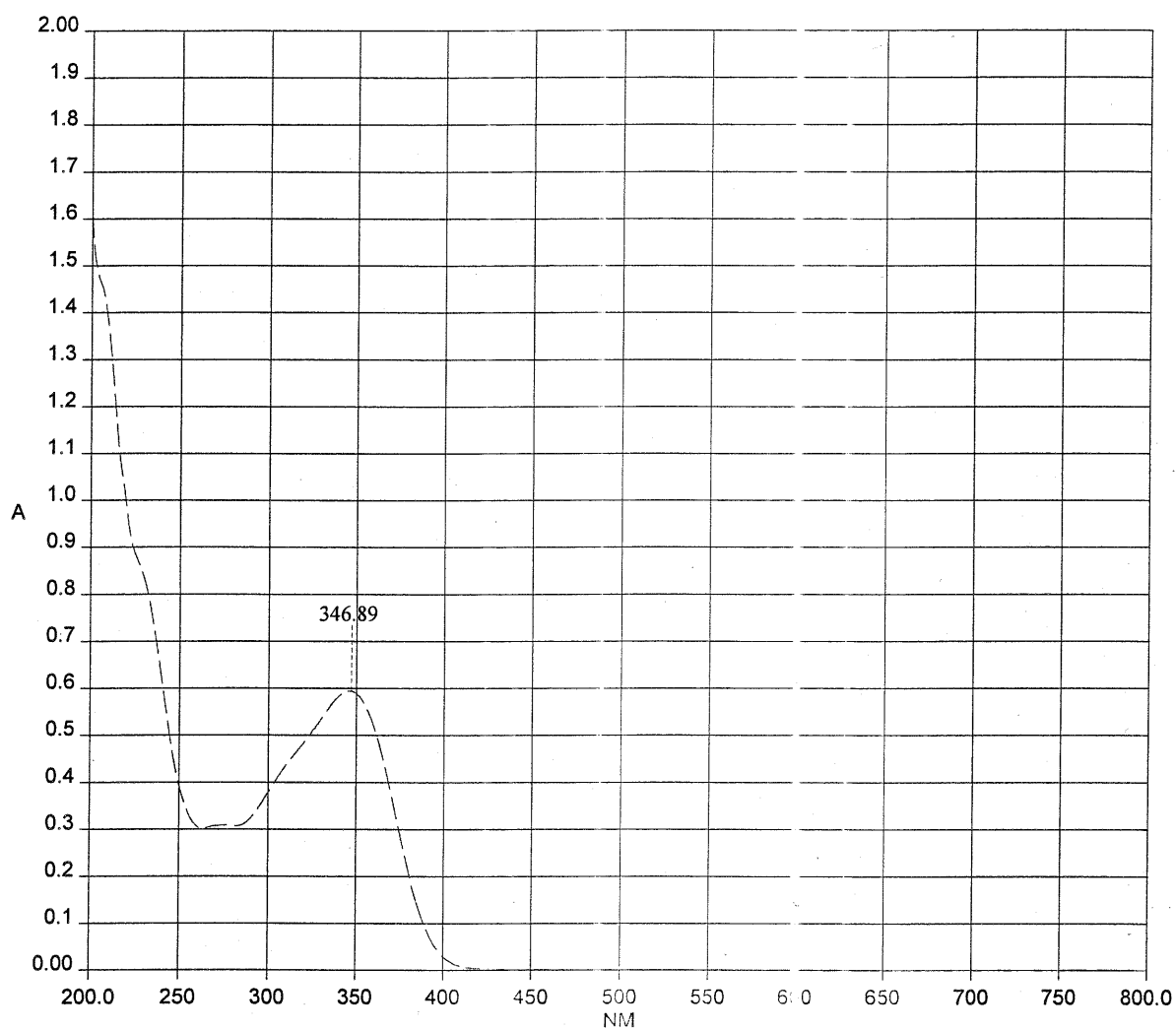
#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 479.1540480								
1	22	24	4	7	1	479.1537202	12.5	3.278e-04
2	24	23	4	7	0	479.1561255	15.5	2.078e-03
3	25	22	5	4	1	479.1564003	17.0	2.352e-03
4	27	21	5	4	0	479.1588056	20.0	4.758e-03
5	28	21	3	5	0	479.1475722	20.0	6.476e-03
6	26	22	3	5	1	479.1451669	17.0	8.881e-03
7	23	21	5	7	0	479.1435495	16.0	1.050e-02
8	23	26	3	7	1	479.1662963	12.0	1.225e-02
9	21	22	5	7	1	479.1411442	13.0	1.290e-02
10	25	25	3	7	0	479.1687016	15.0	1.465e-02



3e

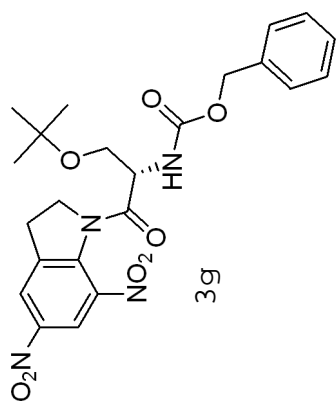
Date: 15.04.2009

Time: 14:50:46

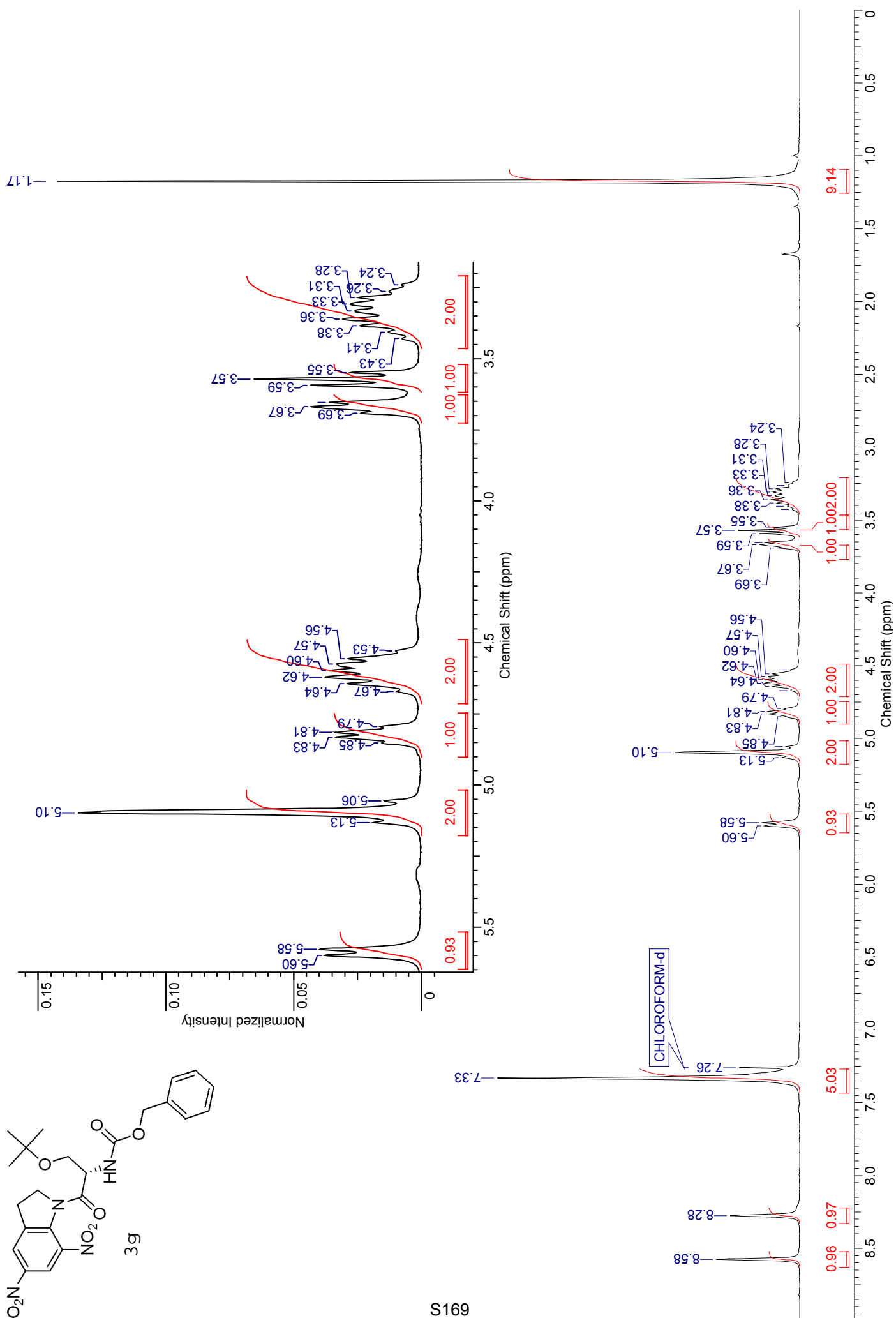


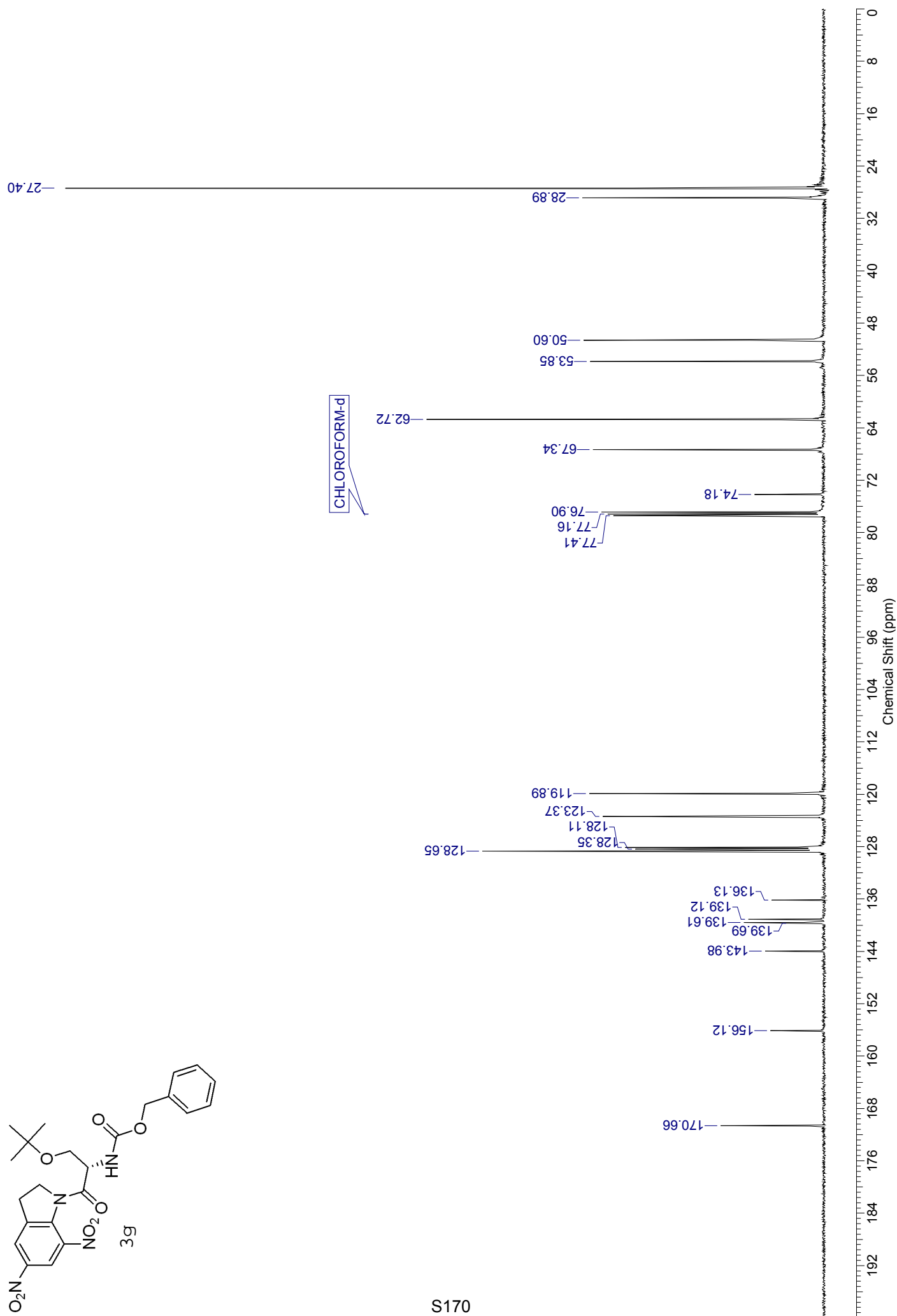
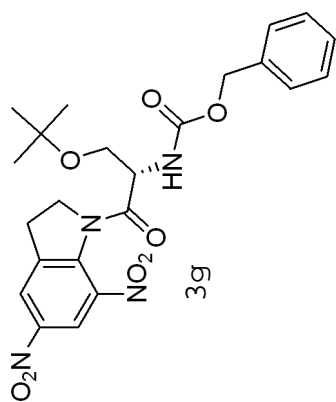
—— JLD115.SP - 15.04.2009 - 4.995*10⁻⁵ M

UV (50 μ l soln in MeCN) λ_{max} (E) 347 (11900).



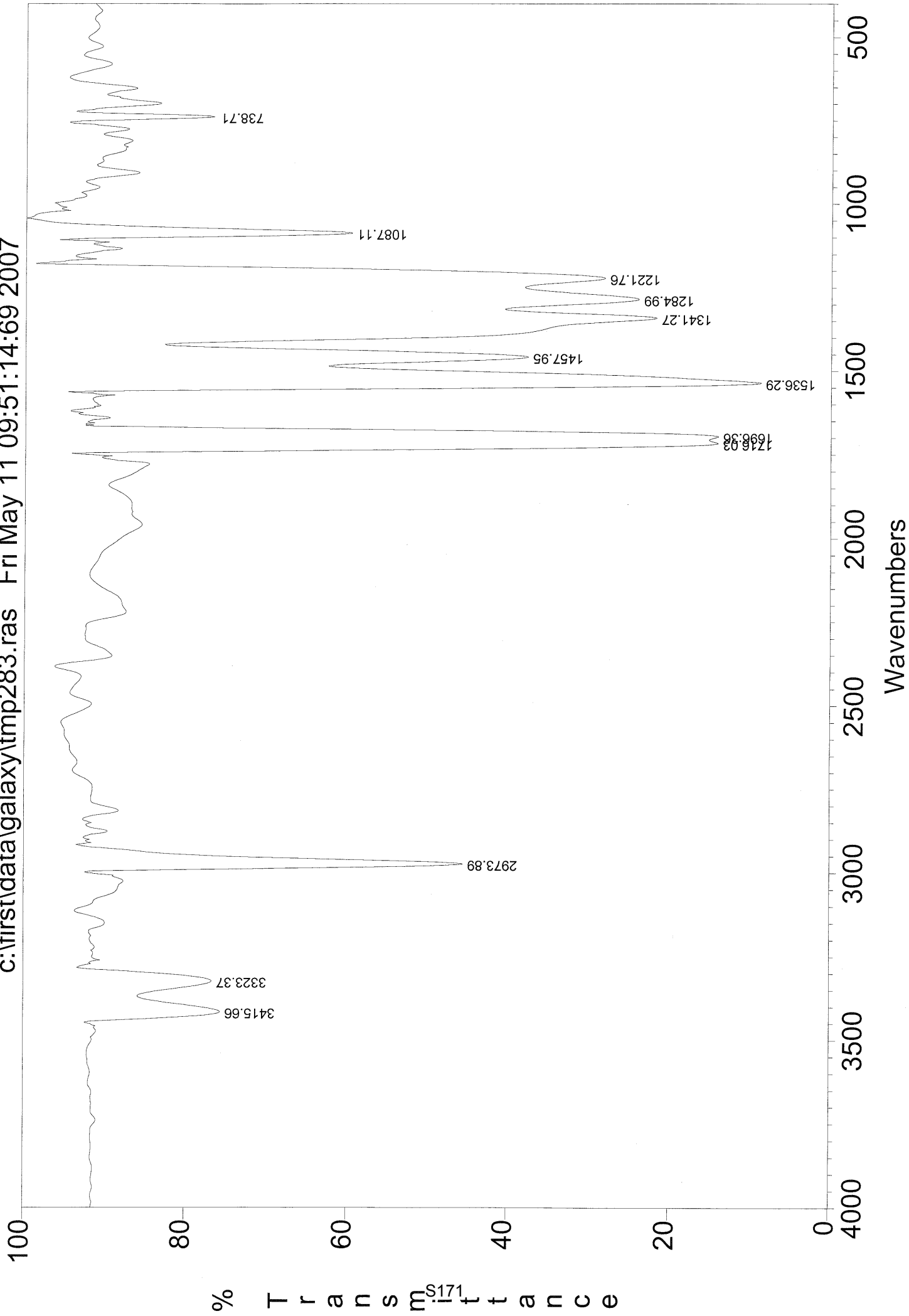
S169





000112

c:\first\data\galaxy\tmp283.ras Fri May 11 09:51:14:69 2007



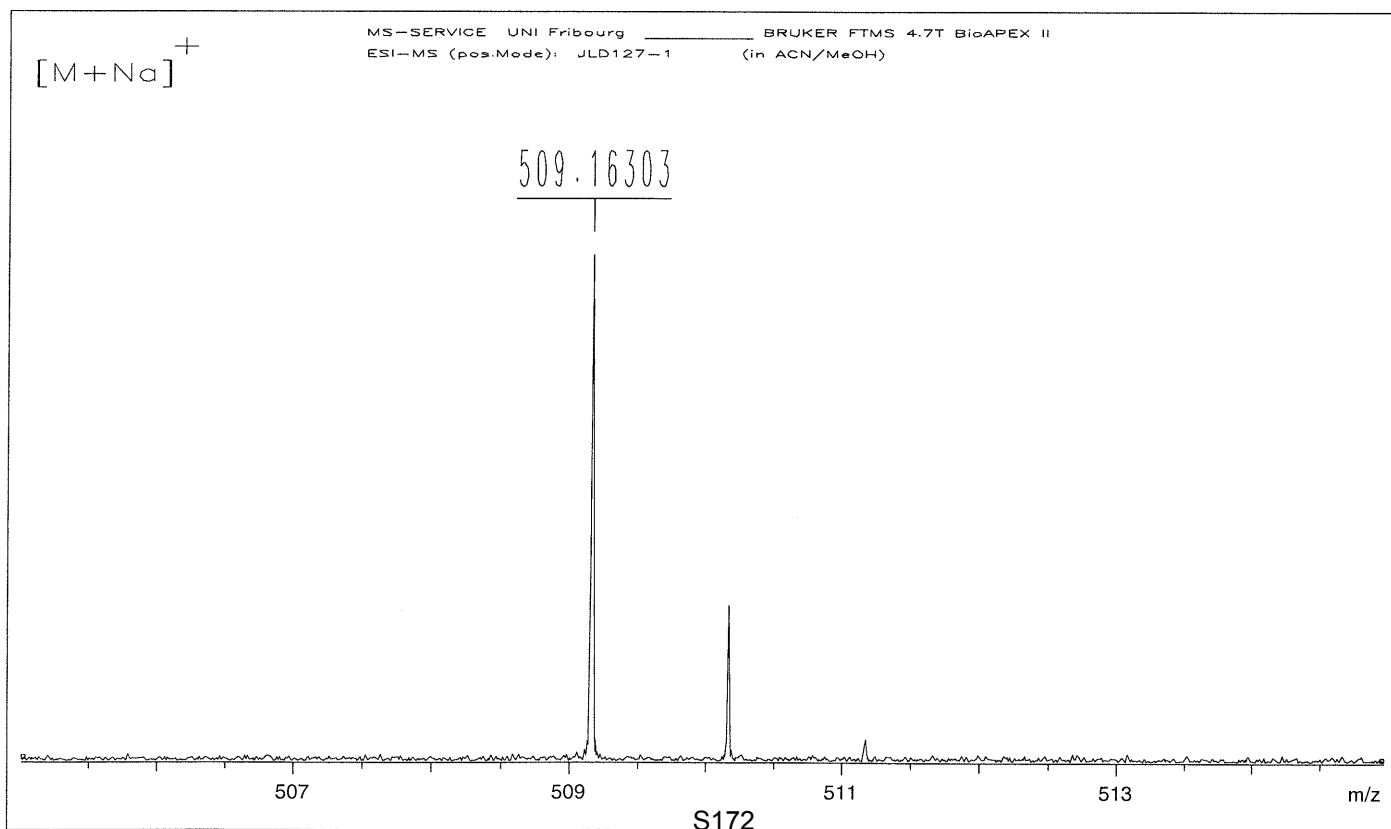
ESI-MS: JLD127-1

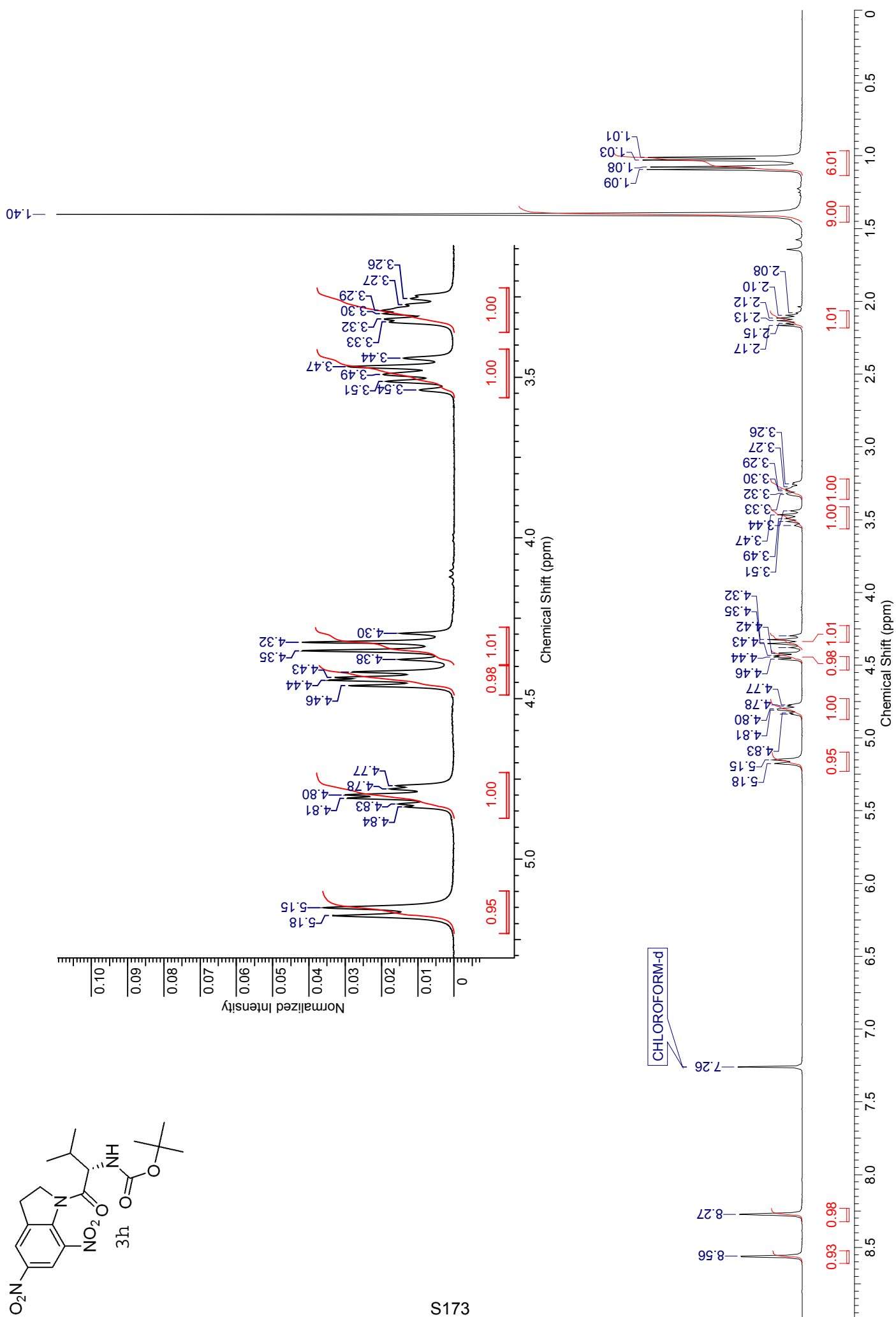
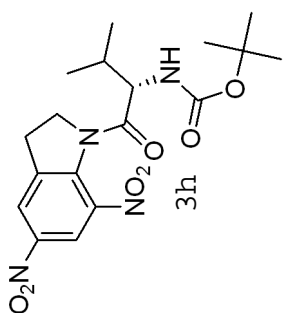
XMASS Mass Analysis for /Data/UNI_FR/DEBI2618_ESI/10/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

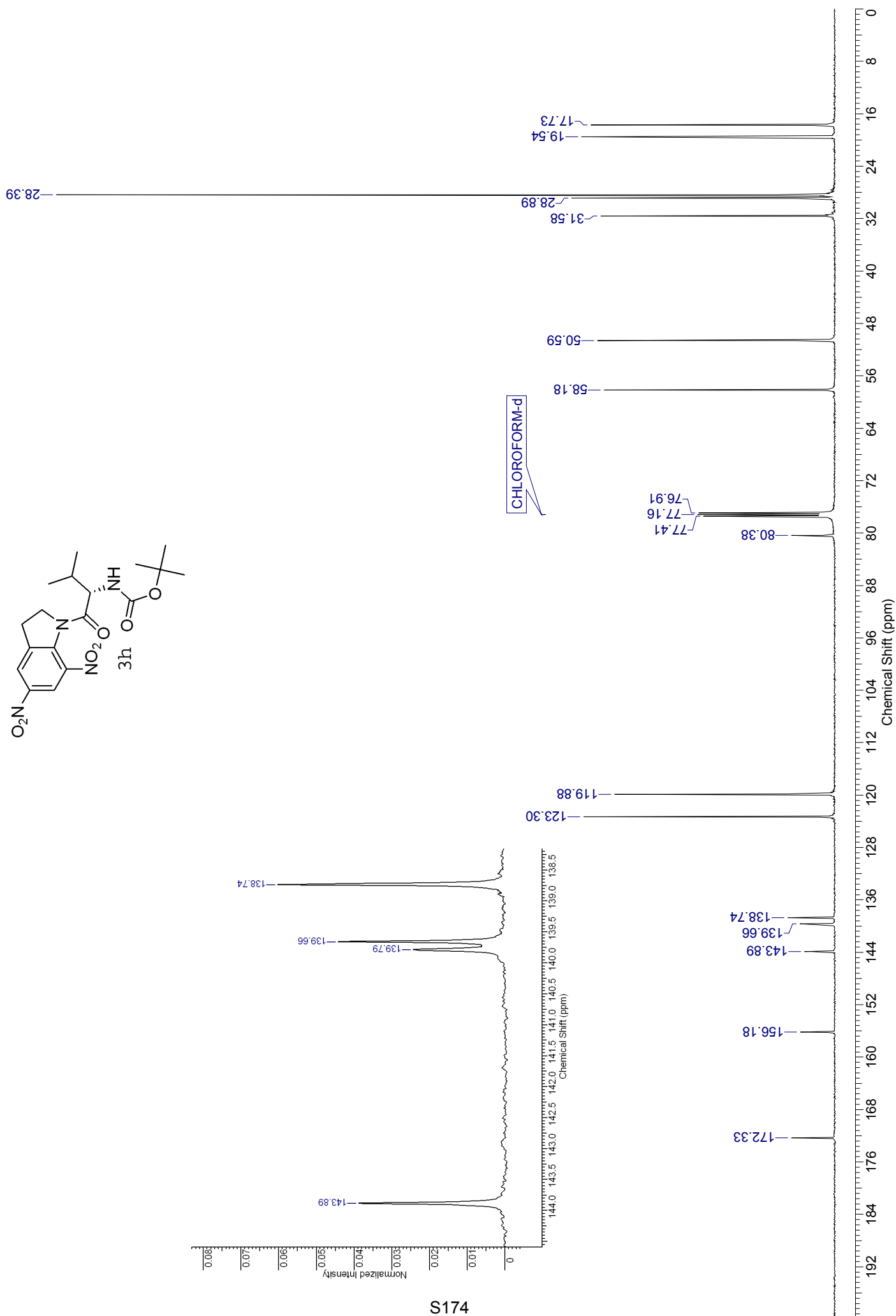
Ion mass = 509.1630290

Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 509.1630290								
1	23	26	4	8	1	509.1642849	12.5	1.256e-03
2	25	25	4	8	0	509.1666902	15.5	3.661e-03
3	26	24	5	5	1	509.1669650	17.0	3.936e-03
4	29	23	3	6	0	509.1581369	20.0	4.892e-03
5	28	23	5	5	0	509.1693703	20.0	6.341e-03
6	27	24	3	6	1	509.1557316	17.0	7.297e-03
7	24	23	5	8	0	509.1541142	16.0	8.915e-03
8	22	24	5	8	1	509.1517089	13.0	1.132e-02
9	24	28	3	8	1	509.1768610	12.0	1.383e-02
10	26	27	3	8	0	509.1792663	15.0	1.624e-02

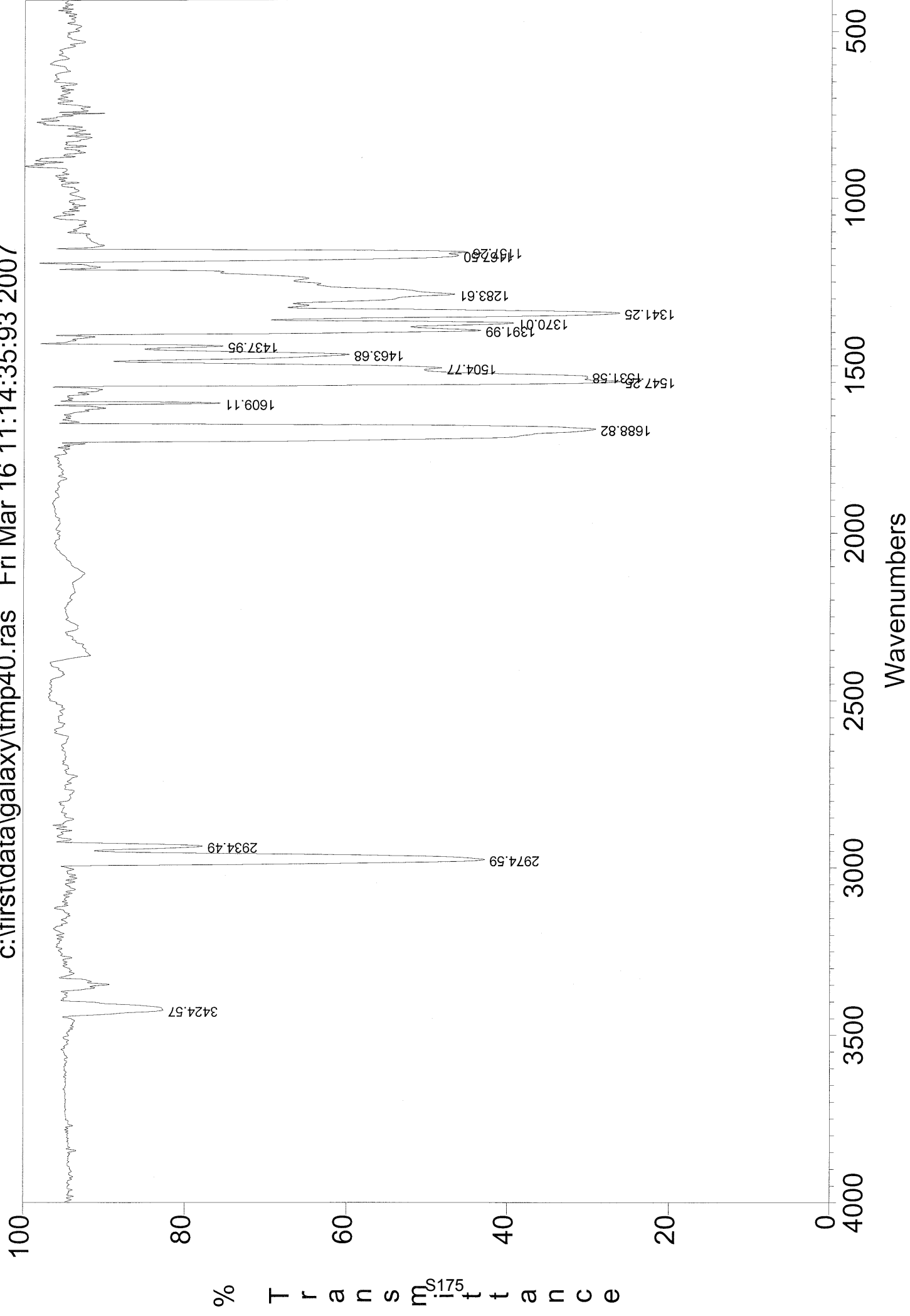






01110

c:\first\data\galaxy\tmp40.ras Fri Mar 16 11:14:35:93 2007



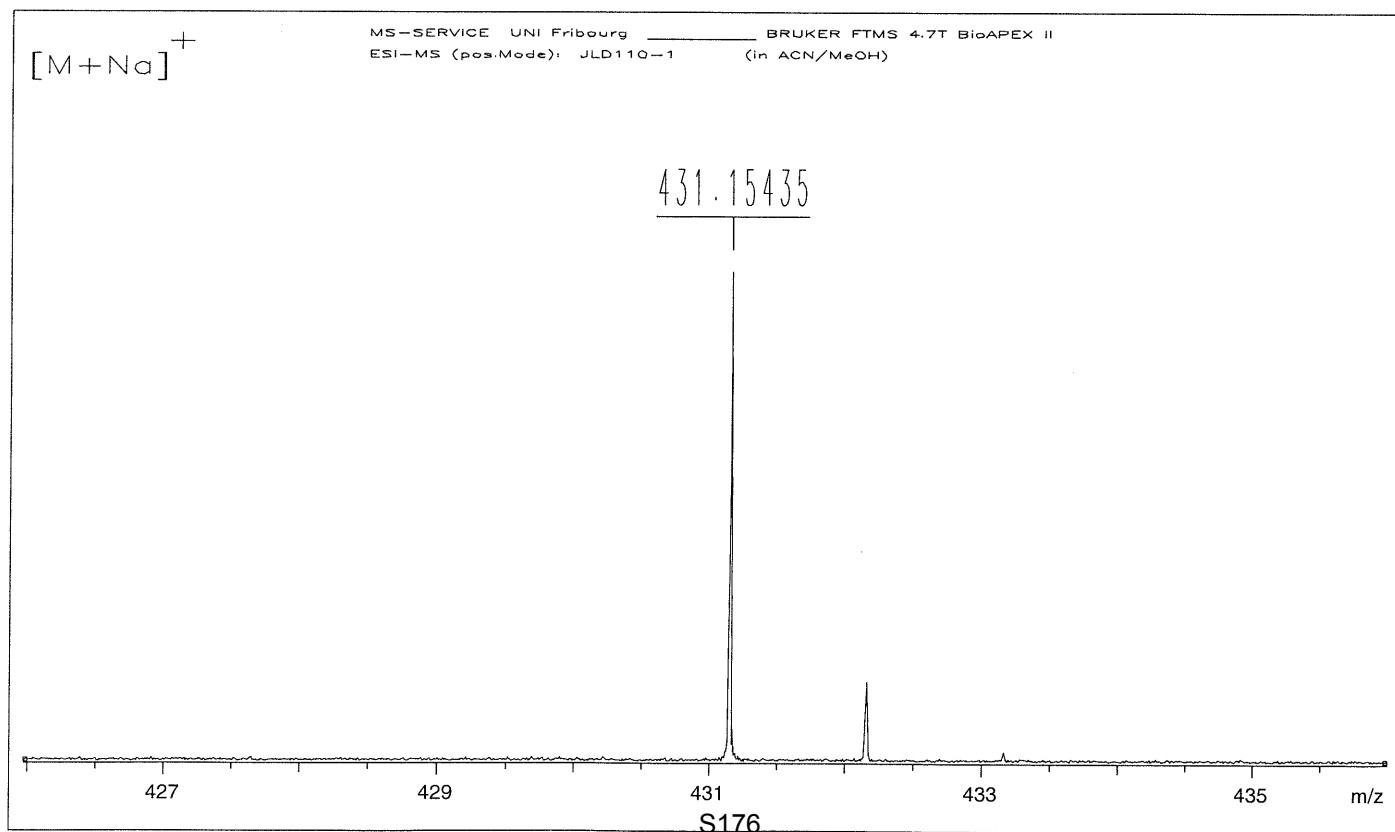
ESI-MS: JLD110-1

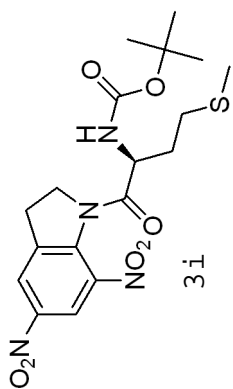
XMASS Mass Analysis for /Data/UNI_FR/DEBI2627_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 431.1543510

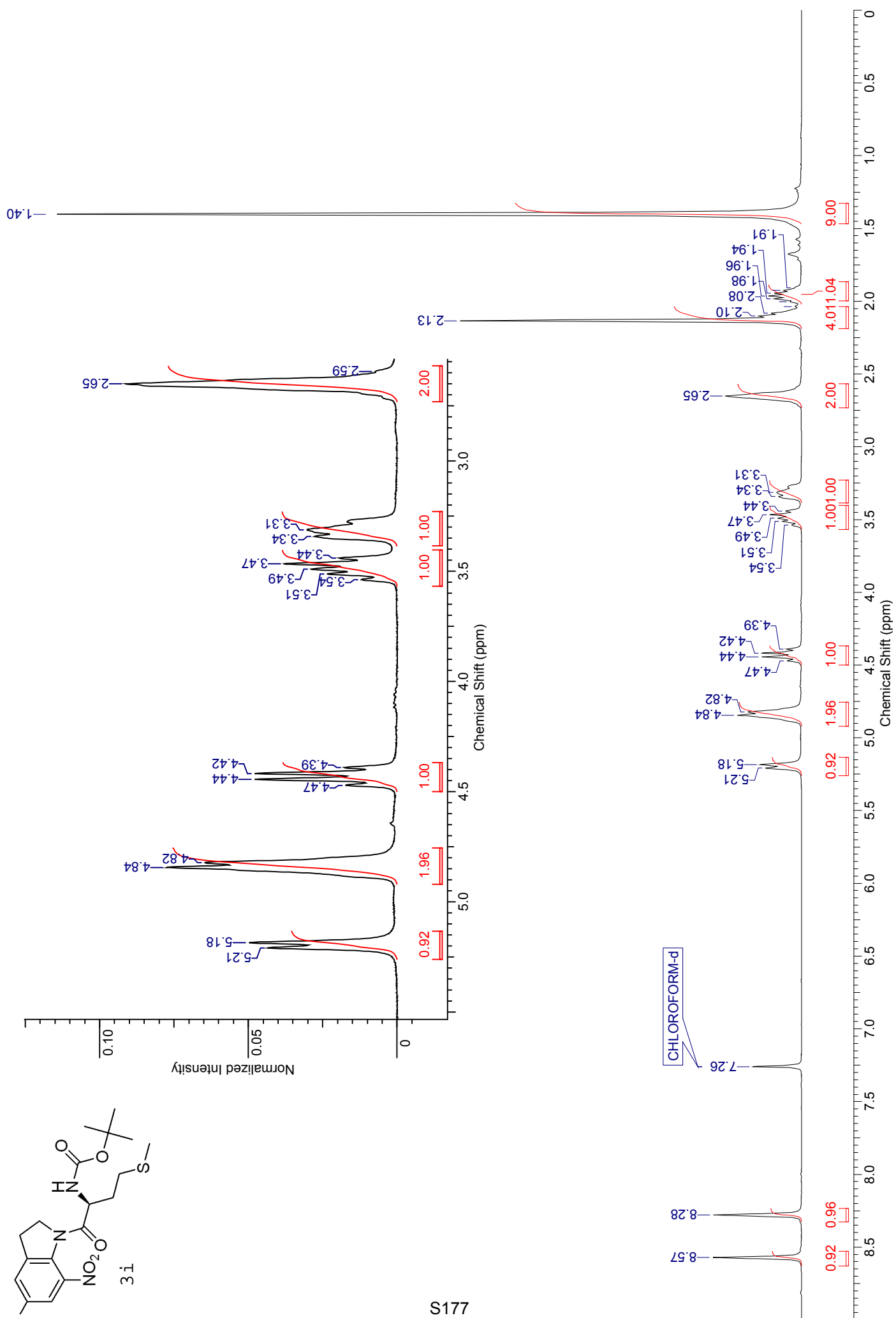
Charge = +1

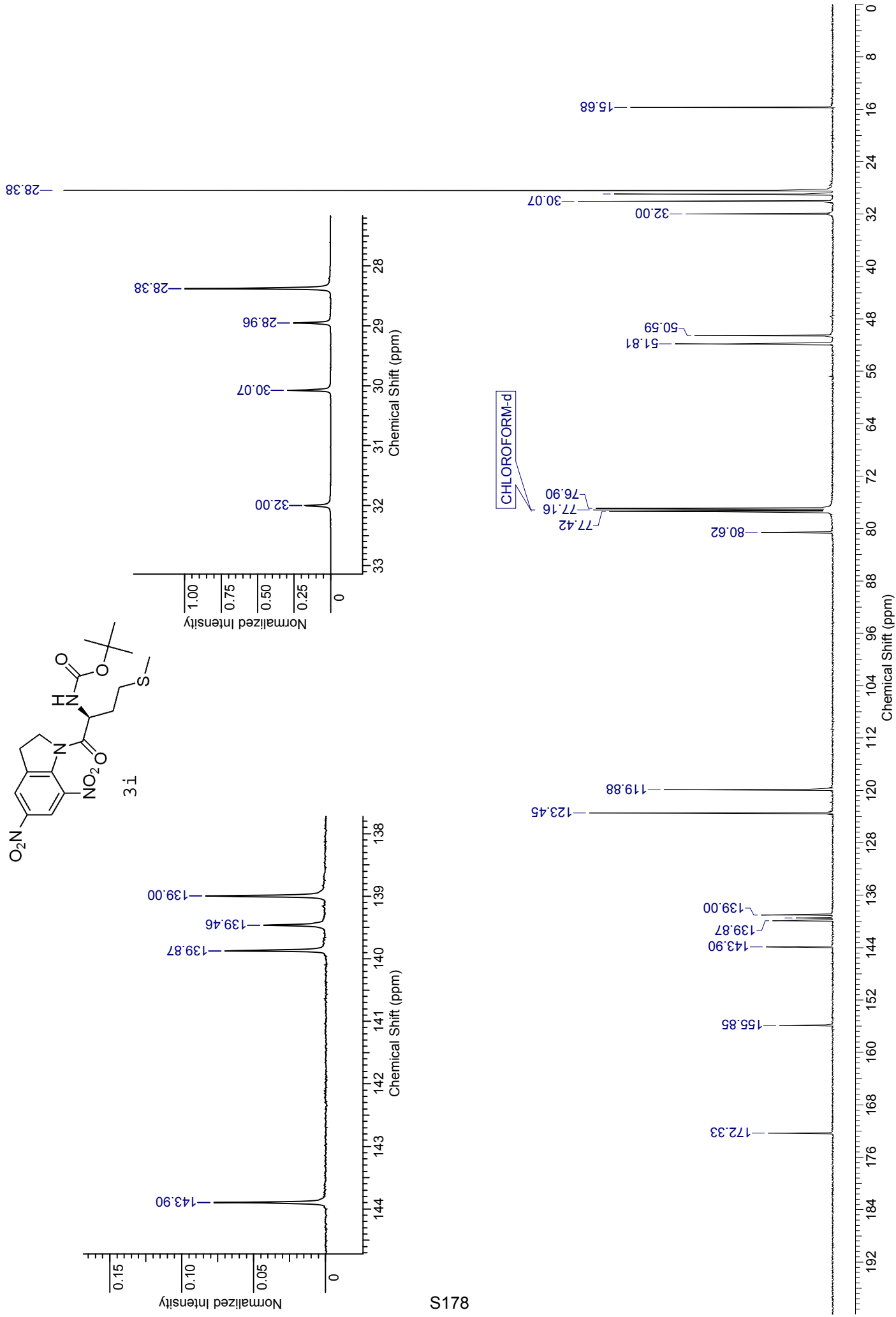
#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 431.1543510								
1	18	24	4	7	1	431.1537202	8.5	6.308e-04
2	20	23	4	7	0	431.1561255	11.5	1.775e-03
3	21	22	5	4	1	431.1564003	13.0	2.049e-03
4	23	21	5	4	0	431.1588056	16.0	4.455e-03
5	24	21	3	5	0	431.1475722	16.0	6.779e-03
6	22	22	3	5	1	431.1451669	13.0	9.184e-03
7	19	21	5	7	0	431.1435495	12.0	1.080e-02
8	19	26	3	7	1	431.1662963	8.0	1.195e-02
9	17	22	5	7	1	431.1411442	9.0	1.321e-02
10	21	25	3	7	0	431.1687016	11.0	1.435e-02





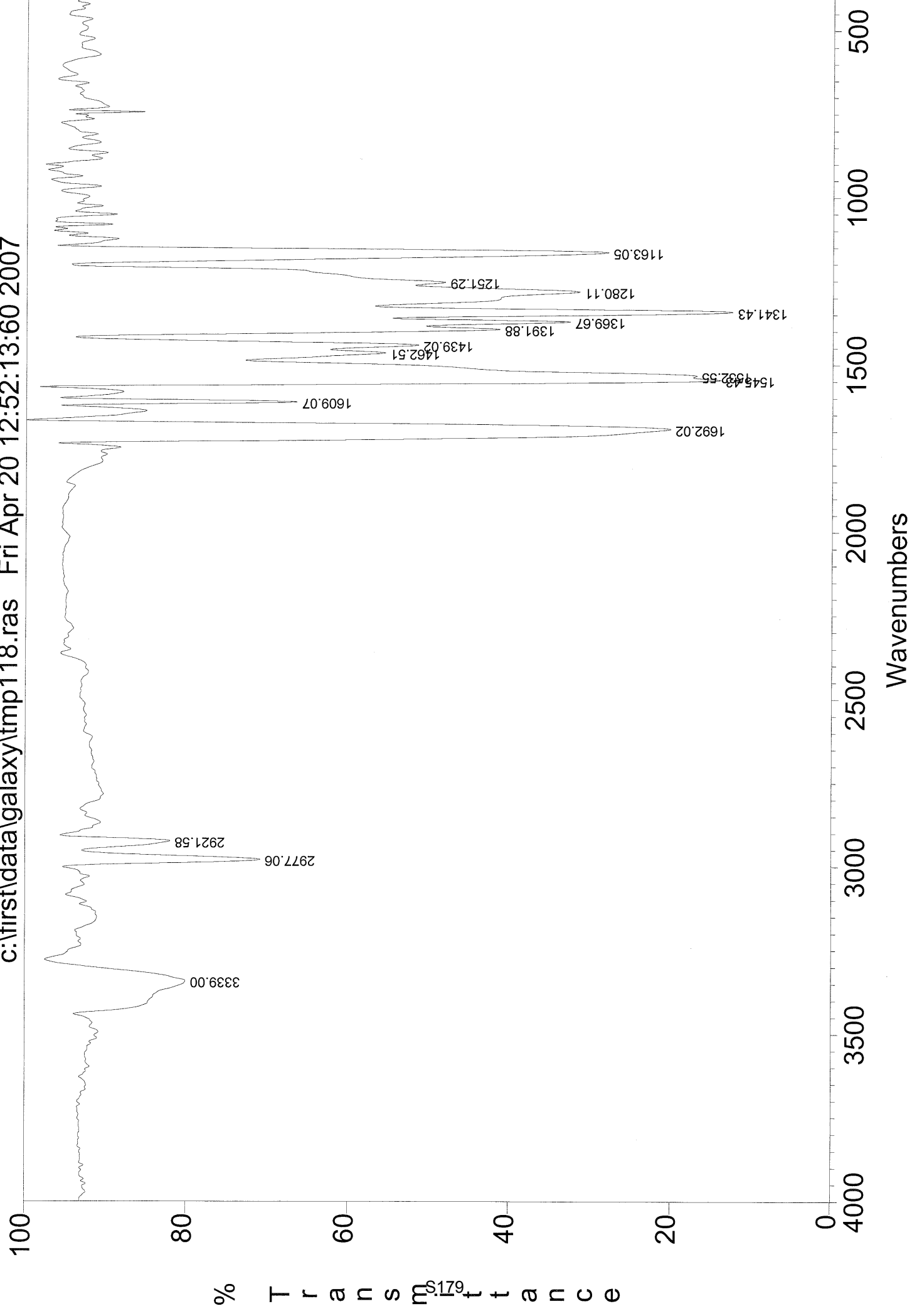
S177





179

c:\first\data\galaxy\tmp118.ras Fri Apr 20 12:52:13:60 2007



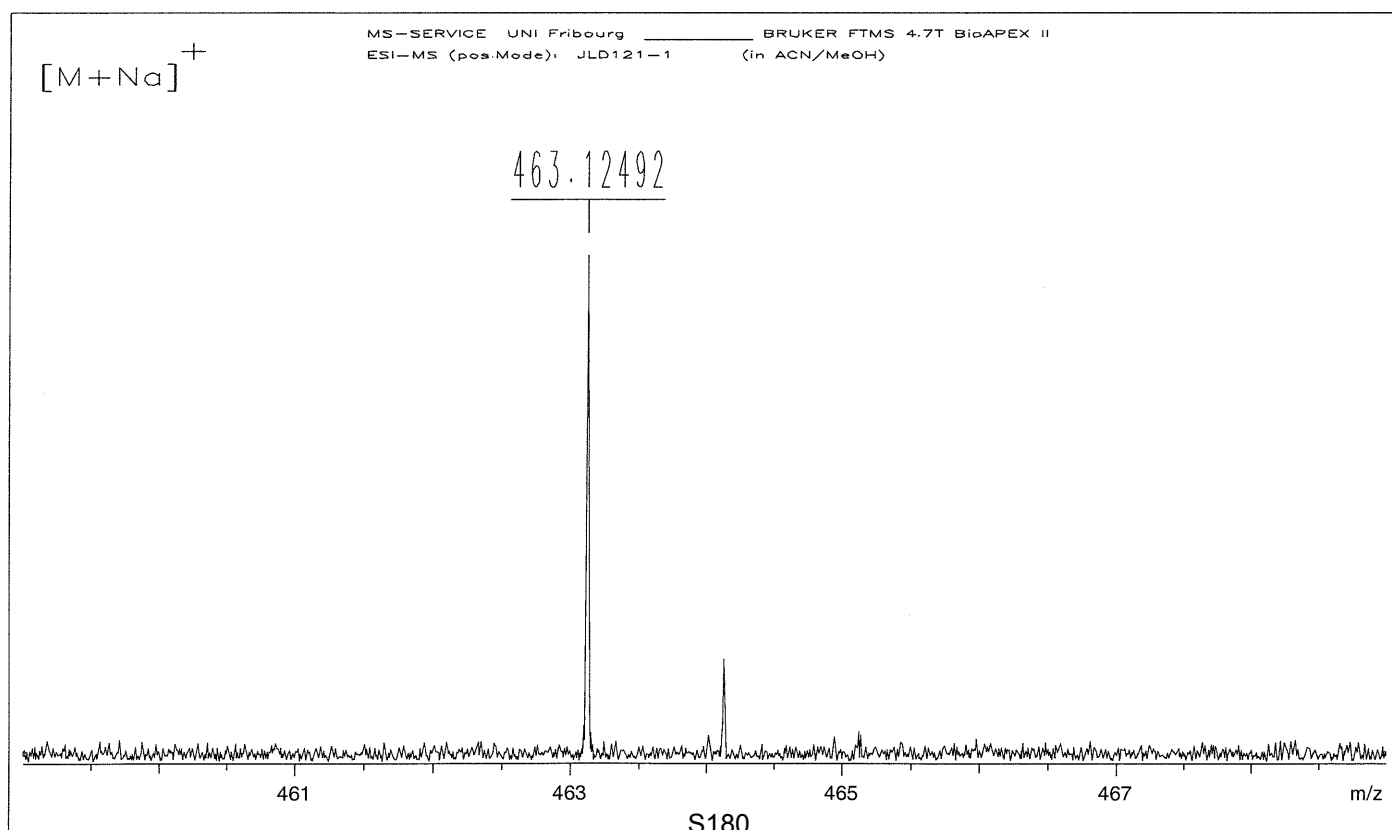
ESI-MS: JLD121-1

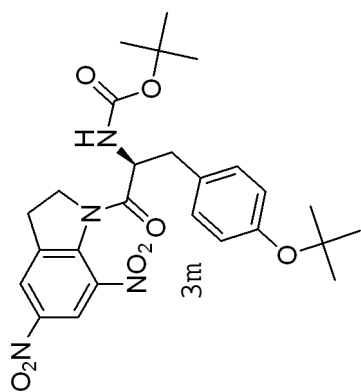
XMASS Mass Analysis for /Data/UNI_FR/DEBI2621_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 463.1249170

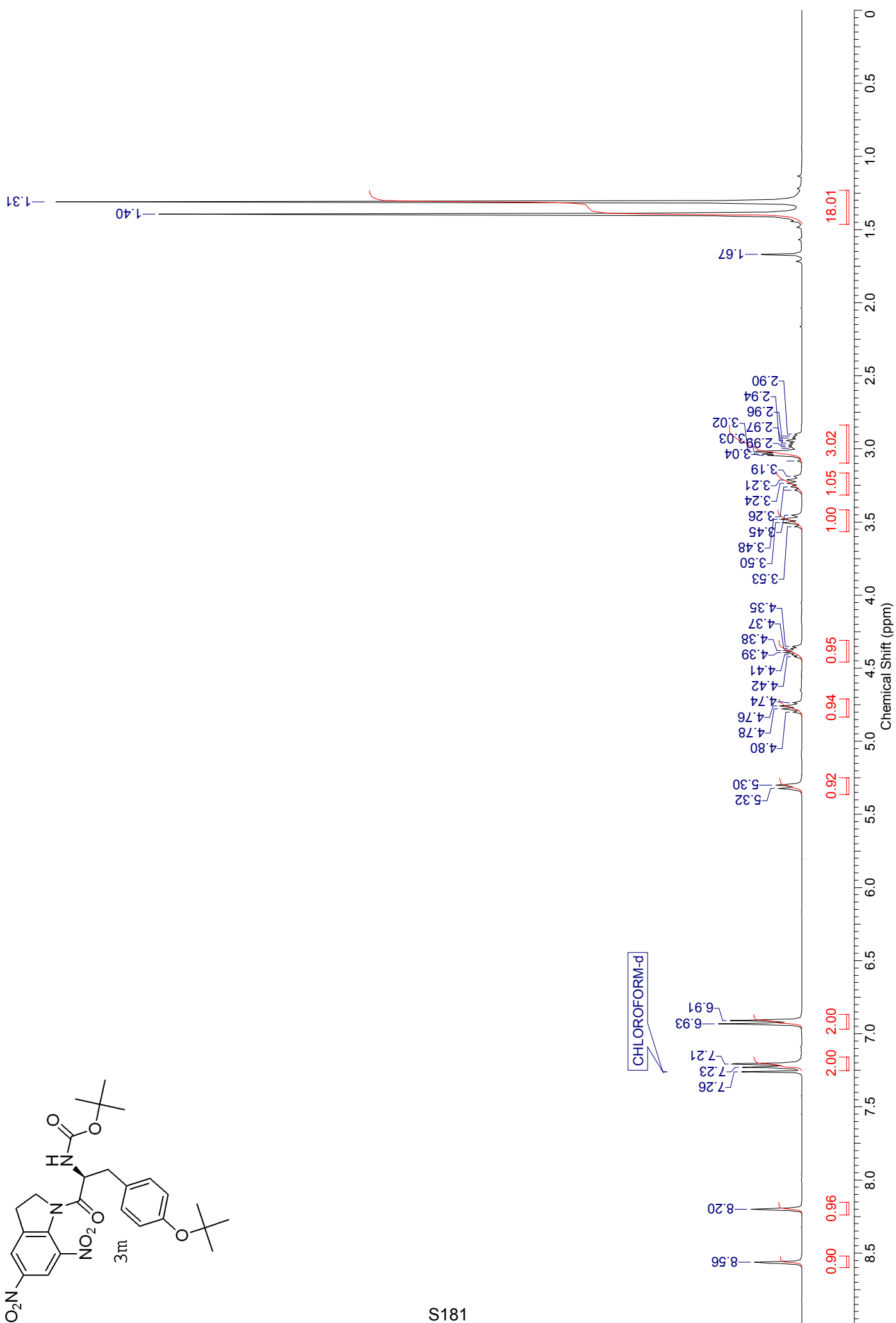
Charge = +1

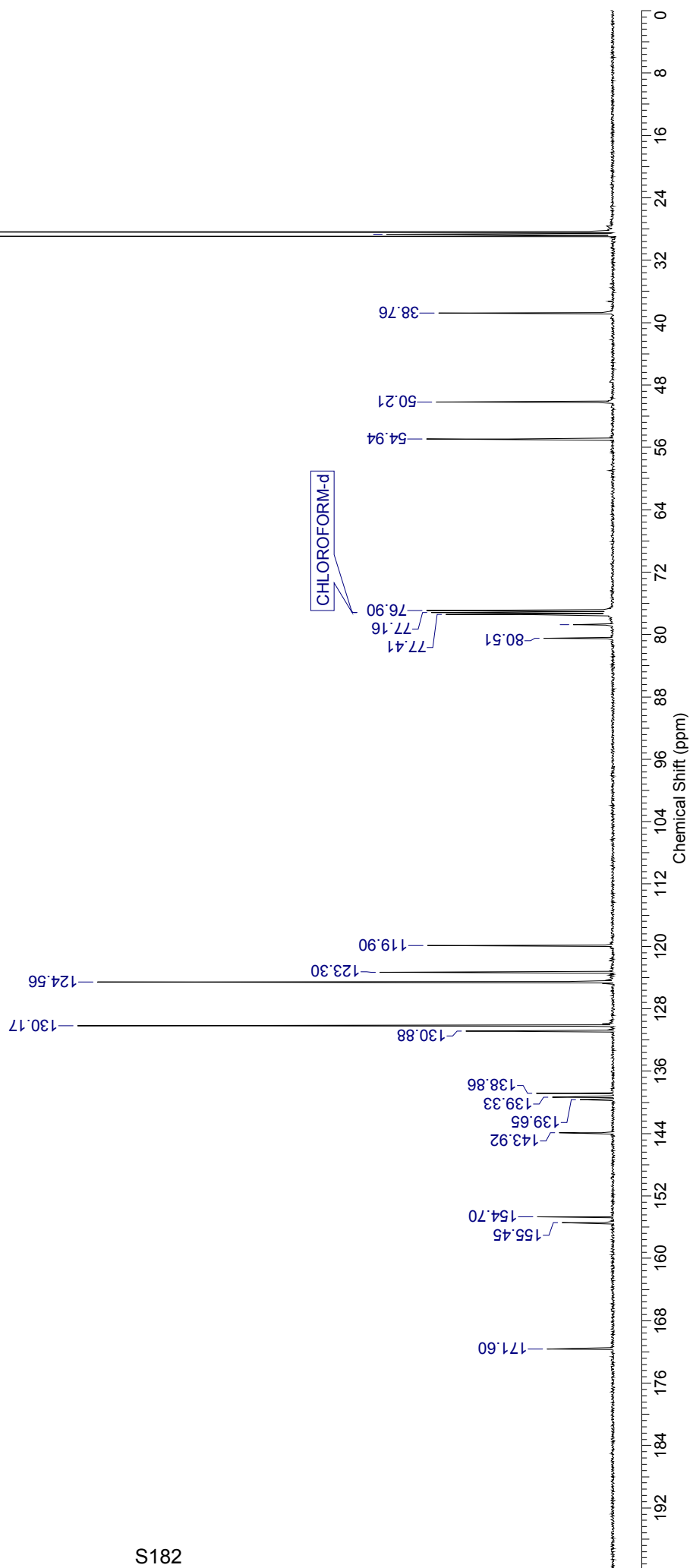
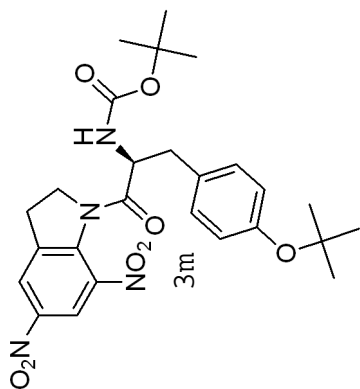
#	C	H	N	O	S	Na	mass	DBE	error
*** Mass Analysis for mass 463.1249170									
1	18	24	4	7	1	1	463.1257909	8.5	8.739e-04
2	21	25	3	5	2	0	463.1230137	11.0	1.903e-03
3	20	23	4	7	1	0	463.1281962	11.5	3.279e-03
4	24	21	3	5	1	0	463.1196429	16.0	5.274e-03
5	16	25	5	7	2	0	463.1189910	7.0	5.926e-03
6	22	22	3	5	1	1	463.1172376	13.0	7.679e-03
7	19	21	5	7	1	0	463.1156202	12.0	9.297e-03
8	17	22	5	7	1	1	463.1132149	9.0	1.170e-02
9	20	23	4	5	2	0	463.1104377	11.5	1.448e-02
10	21	25	3	7	1	0	463.1407723	11.0	1.586e-02





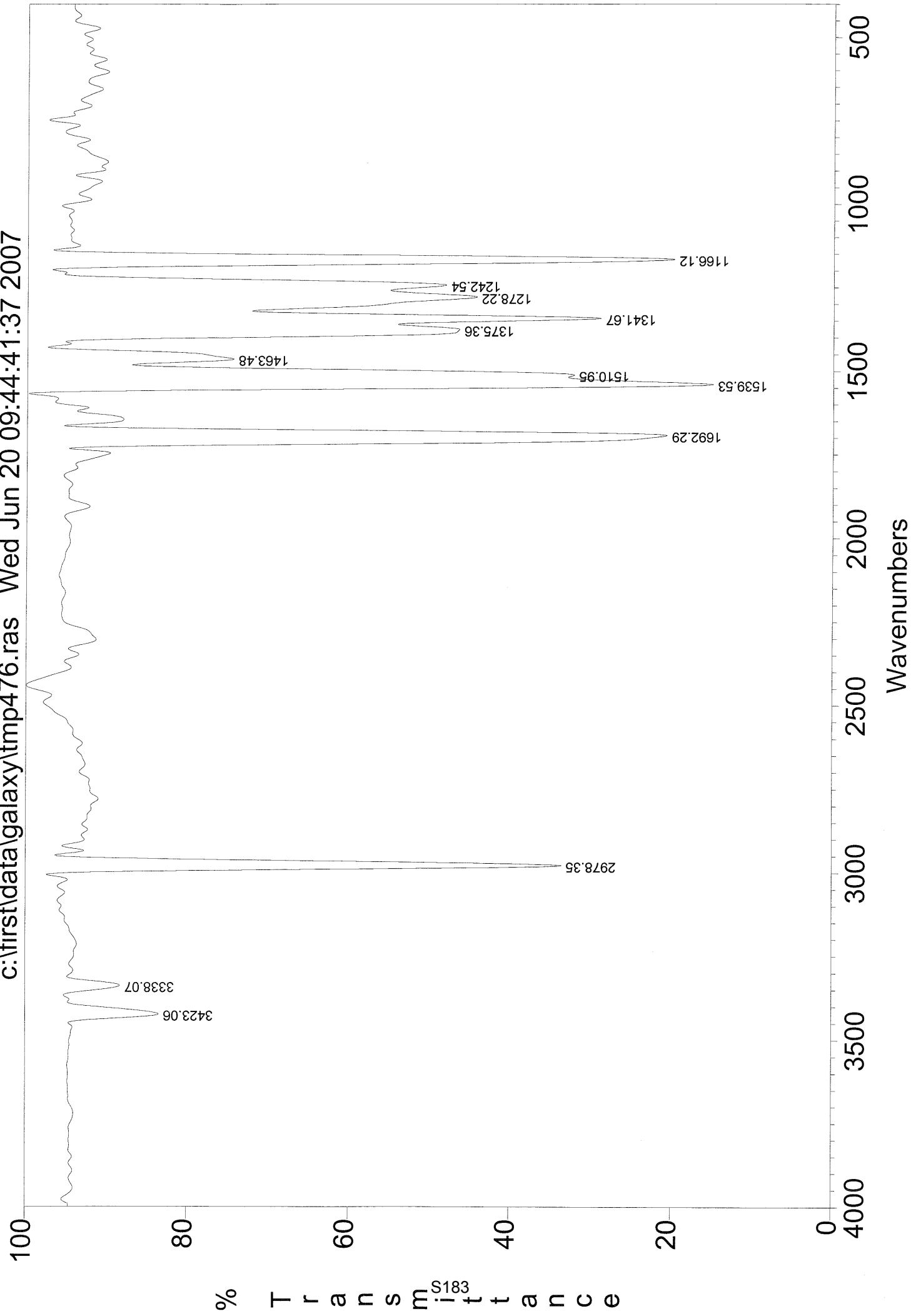
S181





010.134

c:\first\data\galaxy\tmp476.ras Wed Jun 20 09:44:41:37 2007



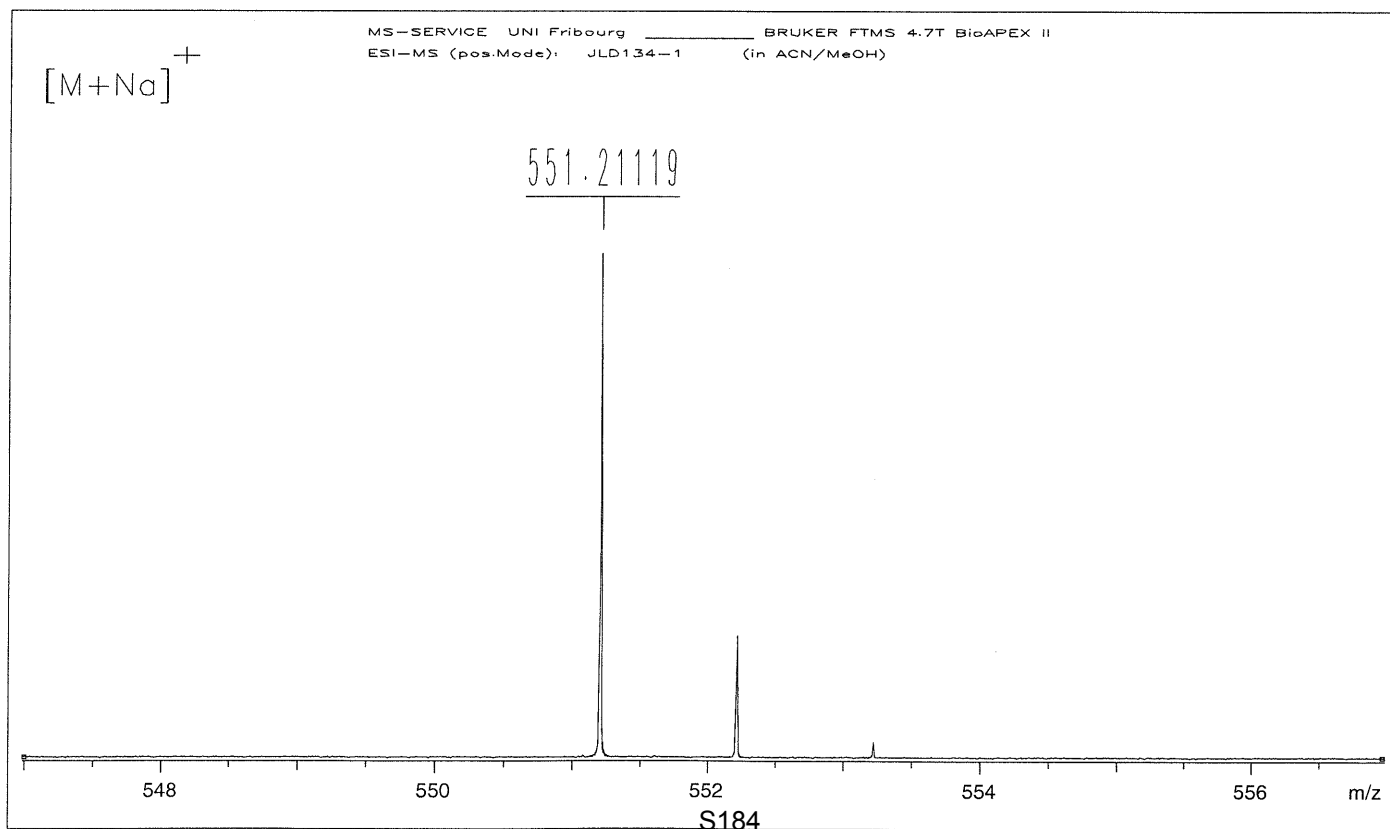
ESI-MS: JLD134-1

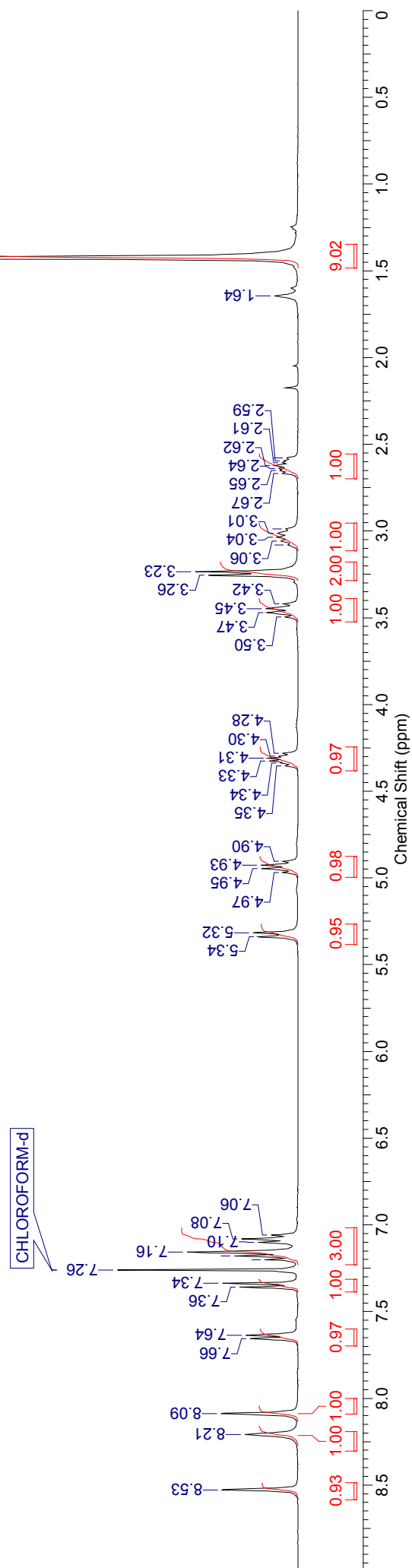
XMASS Mass Analysis for /Data/UNI_FR/DEBI2677_ESI/10/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 551.2111940

Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 551.2111940								
1	26	32	4	8	1	551.2112351	12.5	4.111e-05
2	28	31	4	8	0	551.2136404	15.5	2.446e-03
3	29	30	5	5	1	551.2139152	17.0	2.721e-03
4	31	29	5	5	0	551.2163205	20.0	5.126e-03
5	30	27	6	5	0	551.2037444	20.5	7.450e-03
6	28	28	6	5	1	551.2013391	17.5	9.855e-03
7	27	29	5	8	0	551.2010644	16.0	1.013e-02
8	25	32	6	7	1	551.2224685	12.5	1.127e-02
9	25	30	5	8	1	551.1986591	13.0	1.253e-02
10	27	31	6	7	0	551.2248738	15.5	1.368e-02

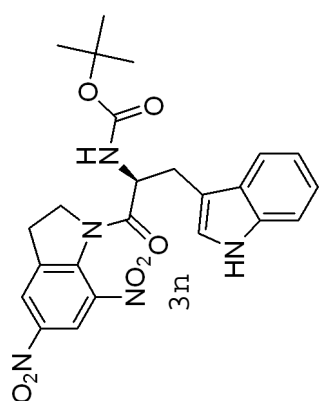


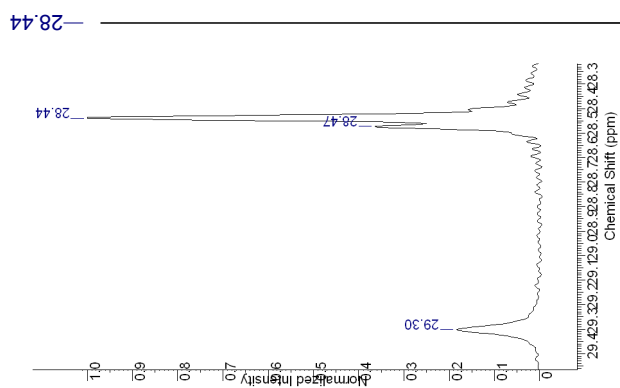


CHLOROFORM-d

Chemical Shift (ppm)

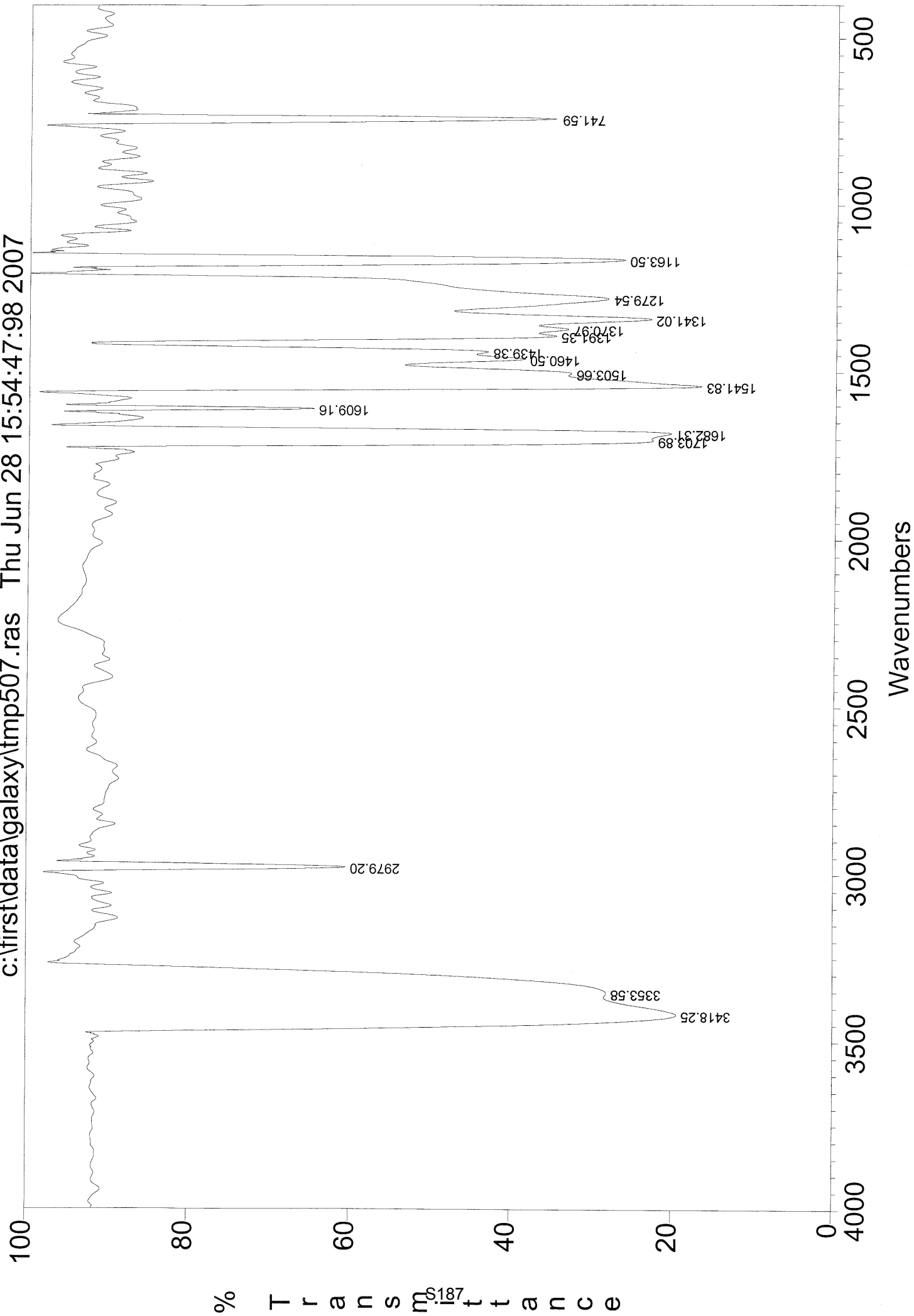
Normalized Intensity





710136

c:\first\data\galaxy\tmp507.ras Thu Jun 28 15:54:47:98 2007



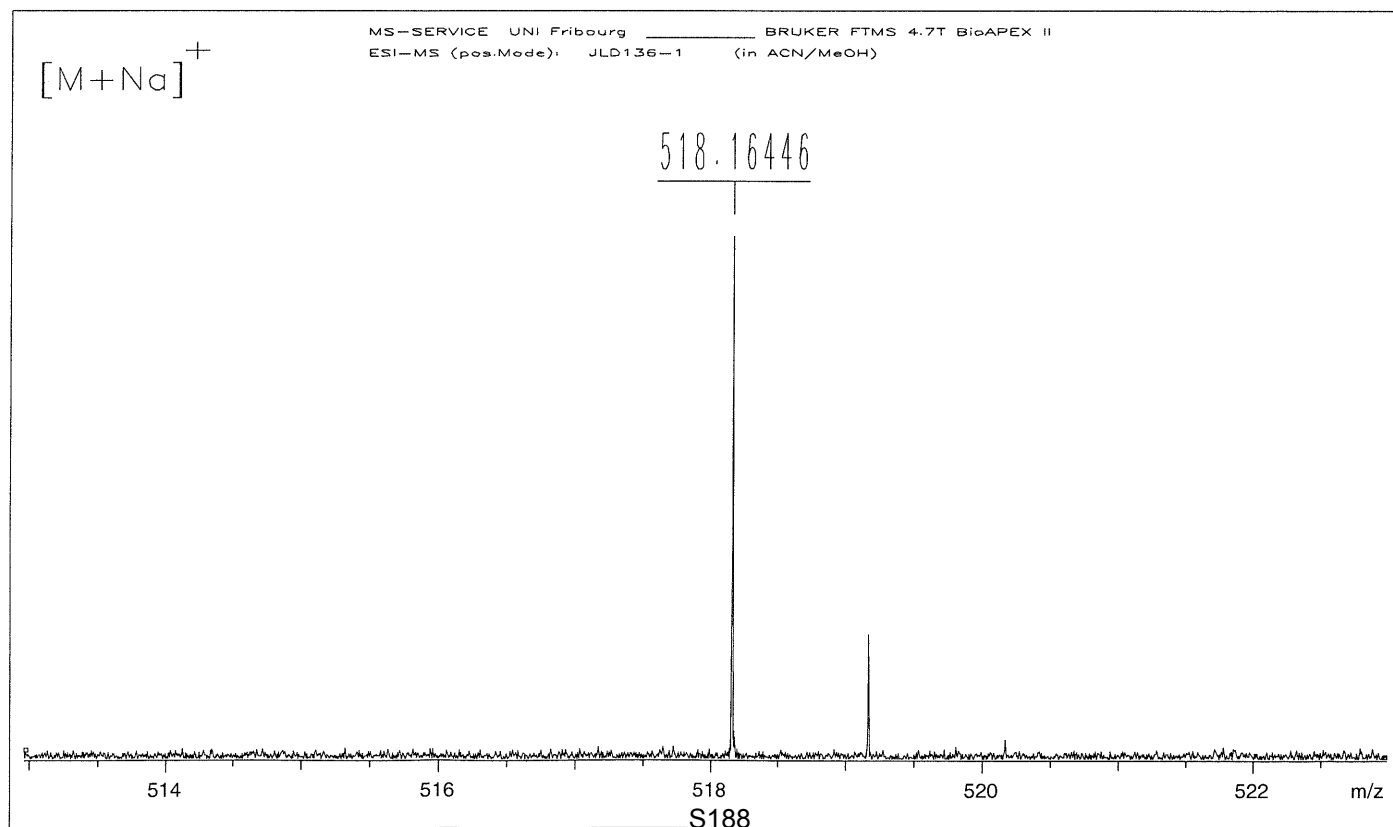
ESI-MS: JLD136-1

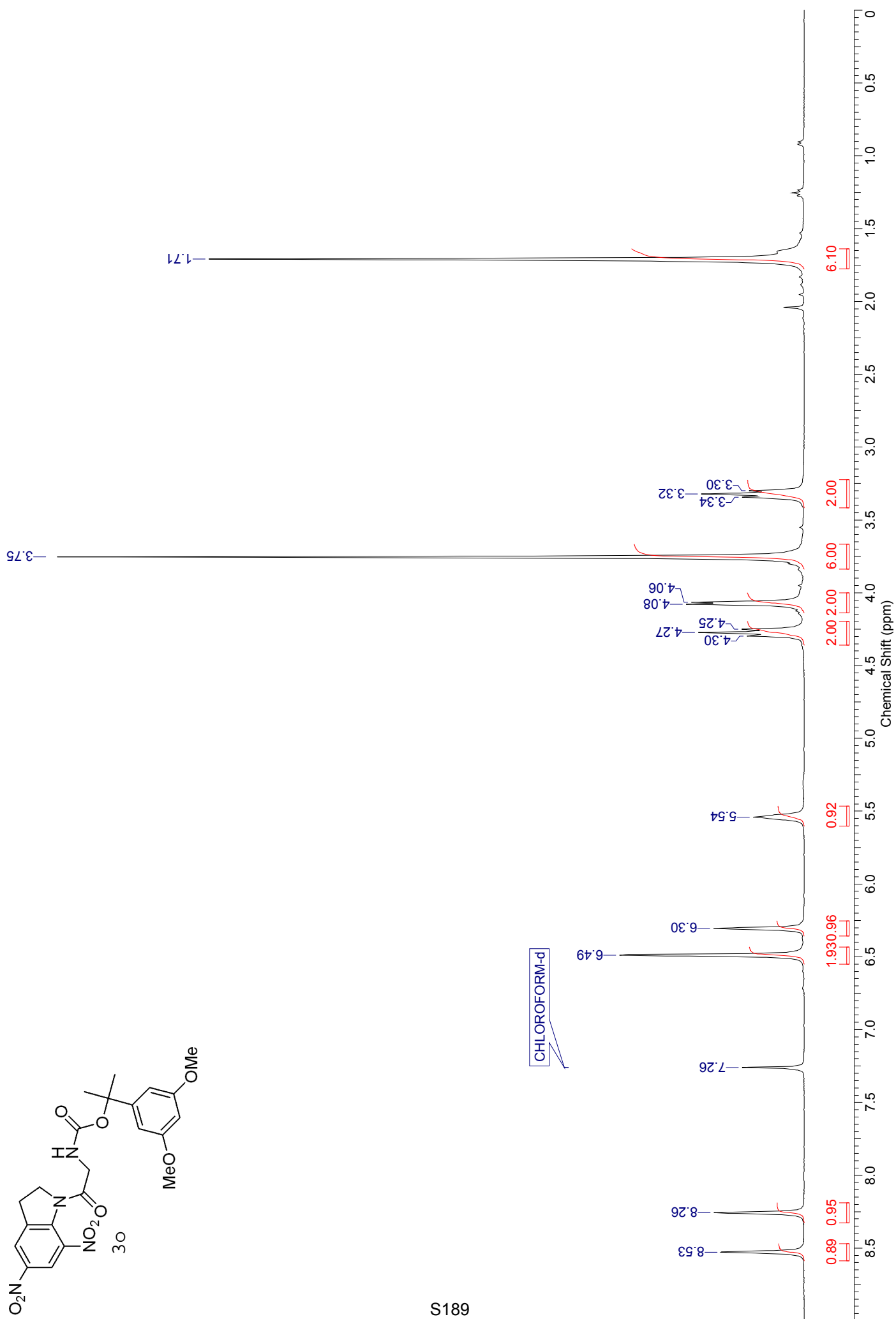
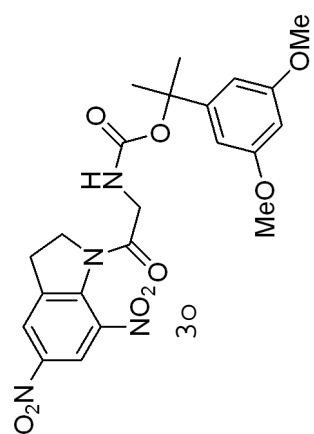
XMASS Mass Analysis for /Data/UNI_FR/DEBI2687_ESI/10/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

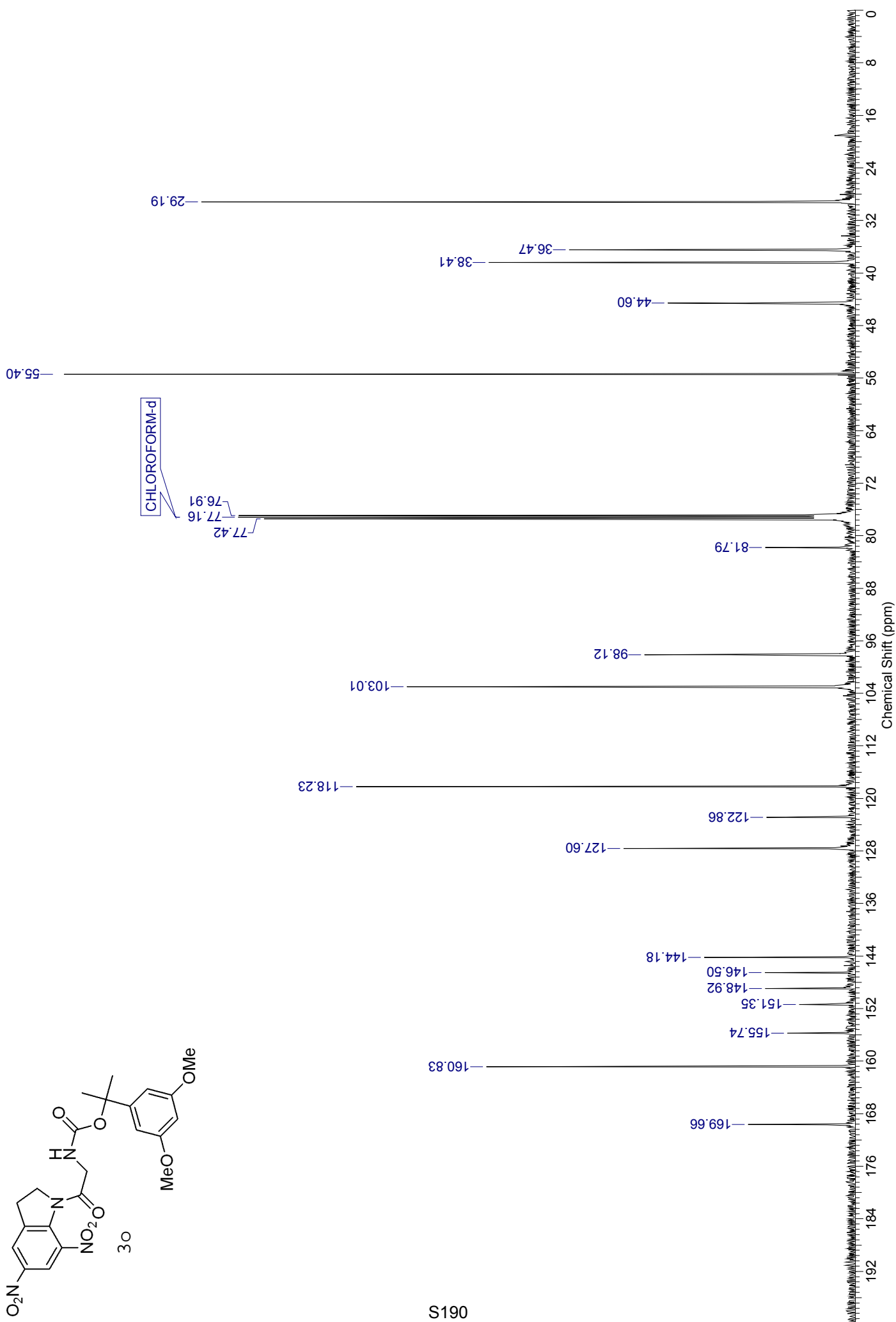
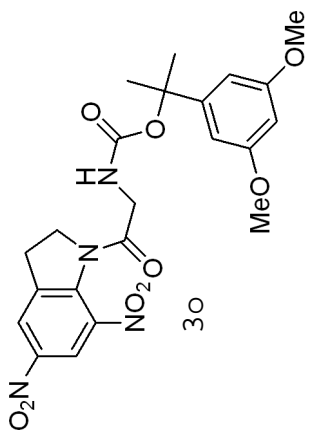
Ion mass = 518.1644650

Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 518.1644650								
1	24	25	5	7	1	518.1646193	14.5	1.543e-04
2	22	23	8	6	1	518.1632766	15.0	1.188e-03
3	24	22	8	6	0	518.1656819	18.0	1.217e-03
4	21	24	7	9	0	518.1630018	13.5	1.463e-03
5	25	21	9	3	1	518.1659567	19.5	1.492e-03
6	19	22	10	8	0	518.1616592	14.0	2.806e-03
7	19	25	7	9	1	518.1605965	10.5	3.868e-03
8	17	23	10	8	1	518.1592539	11.0	5.211e-03
9	18	25	9	8	1	518.1718299	10.5	7.365e-03
10	20	24	9	8	0	518.1742352	13.5	9.770e-03

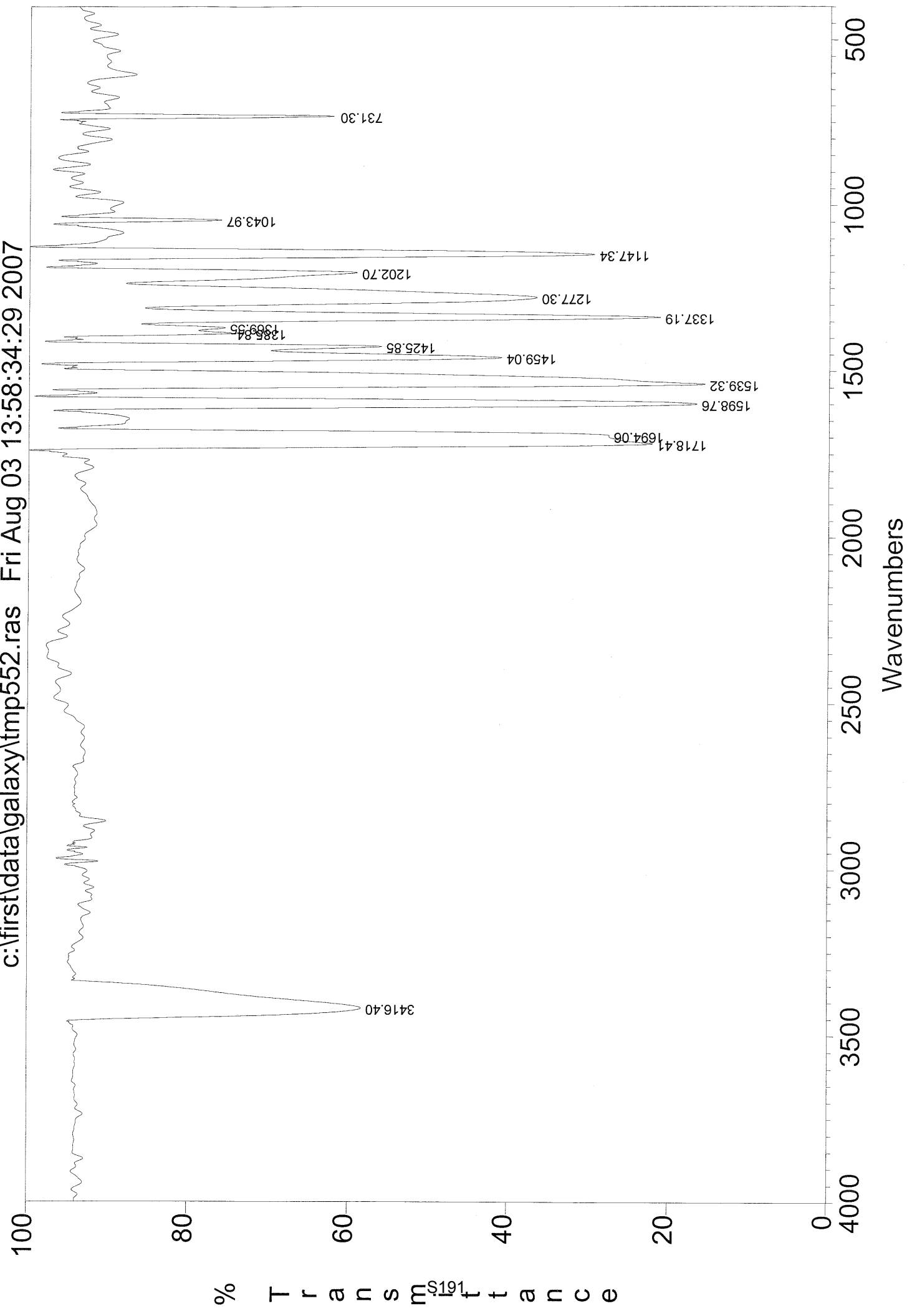






960 145

c:\first\data\galaxy\tmp552.ras Fri Aug 03 13:58:34:29 2007



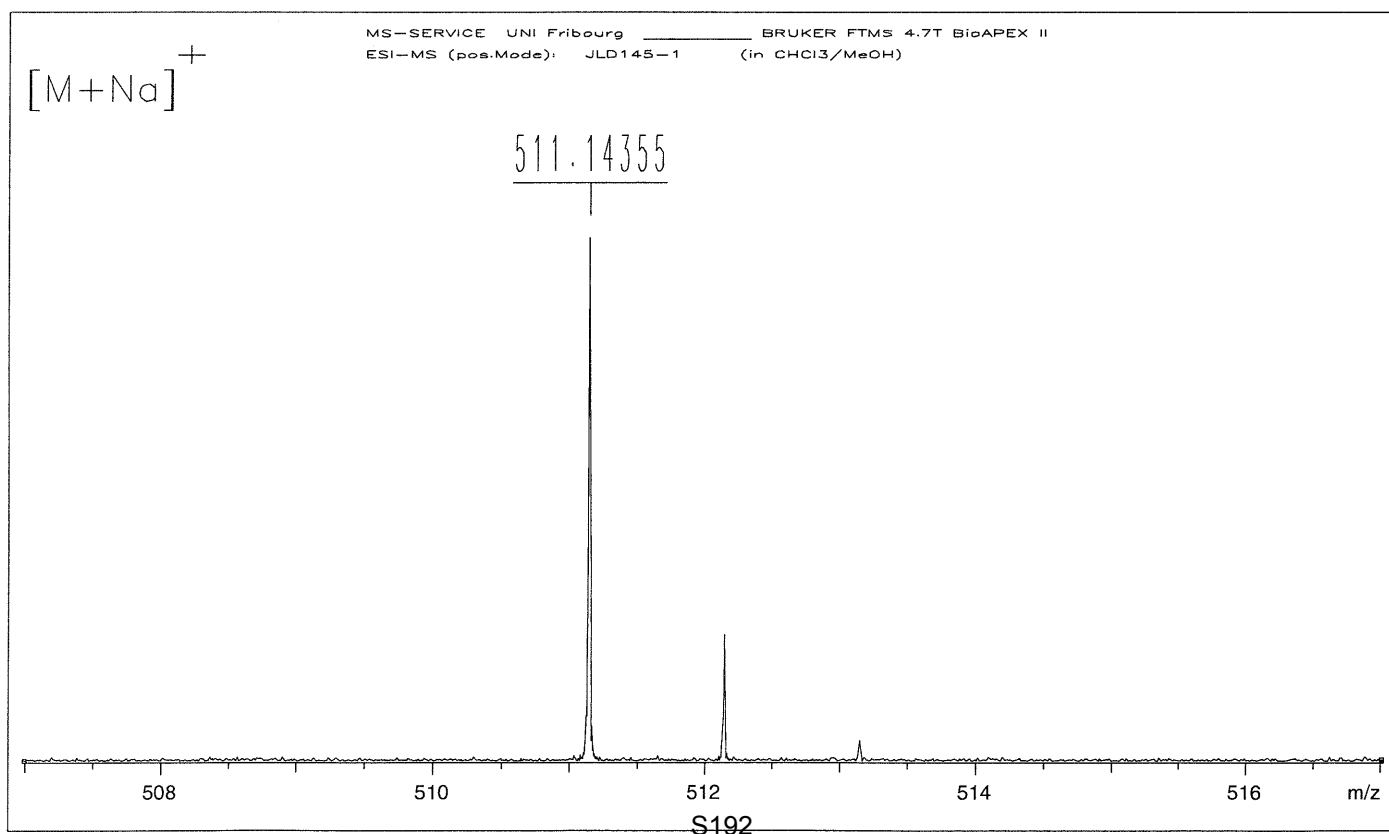
ESI-MS: JLD145-1

XMASS Mass Analysis for /Data/UNI_FR/DEBI2788_ESI/10/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 511.1435470

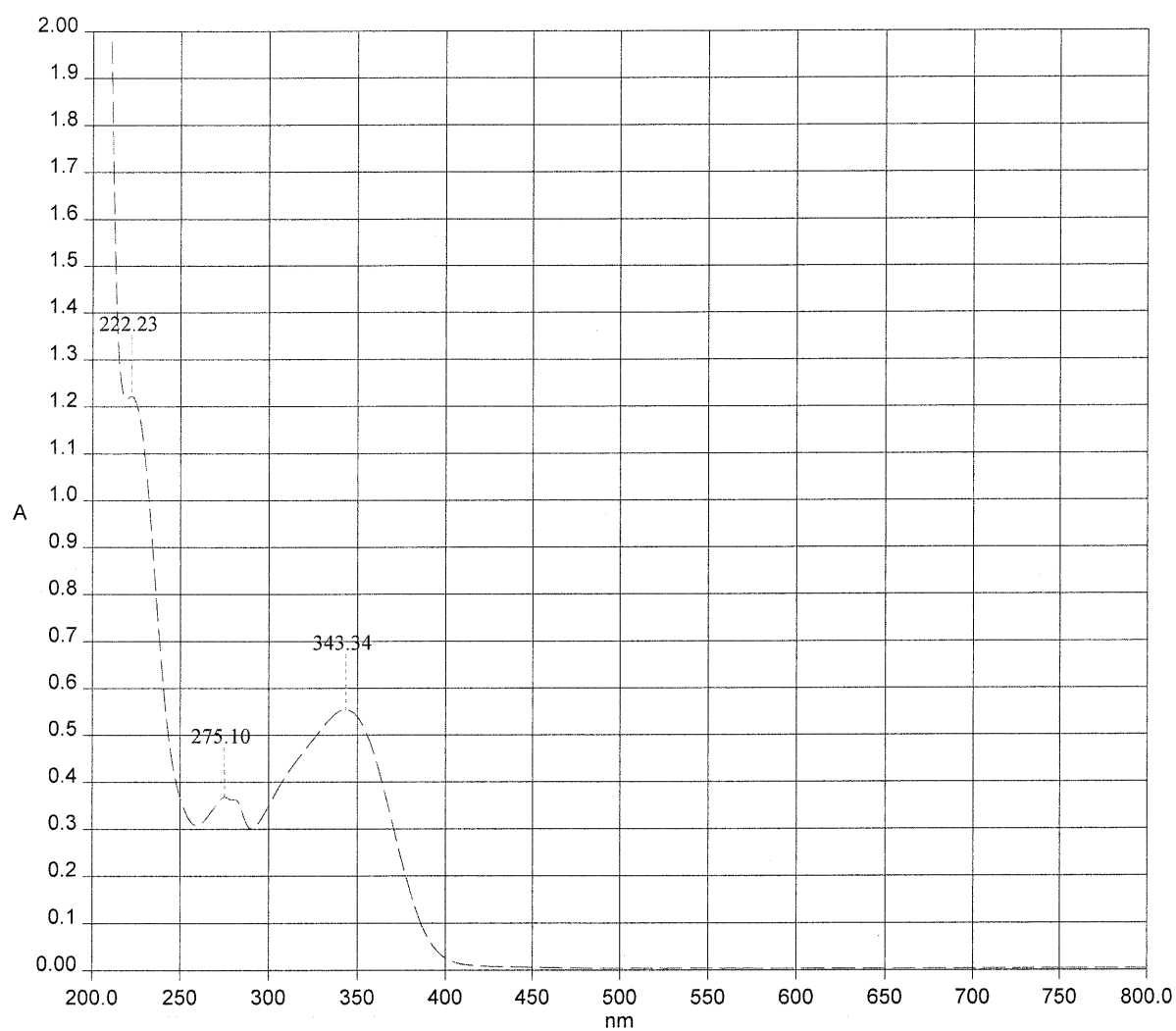
Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 511.1435470								
1	22	24	4	9	1	511.1435495	12.5	2.480e-06
2	20	19	10	7	0	511.1432694	16.5	2.776e-04
3	36	19	2	2	0	511.1441043	28.5	5.573e-04
4	34	17	5	1	0	511.1427616	29.0	7.854e-04
5	22	21	7	8	0	511.1446121	16.0	1.065e-03
6	23	20	8	5	1	511.1448869	17.5	1.340e-03
7	20	22	7	8	1	511.1422068	13.0	1.340e-03
8	24	26	1	10	1	511.1448922	12.0	1.345e-03
9	34	20	2	2	1	511.1416990	25.5	1.848e-03
10	33	21	1	5	0	511.1414242	24.0	2.123e-03

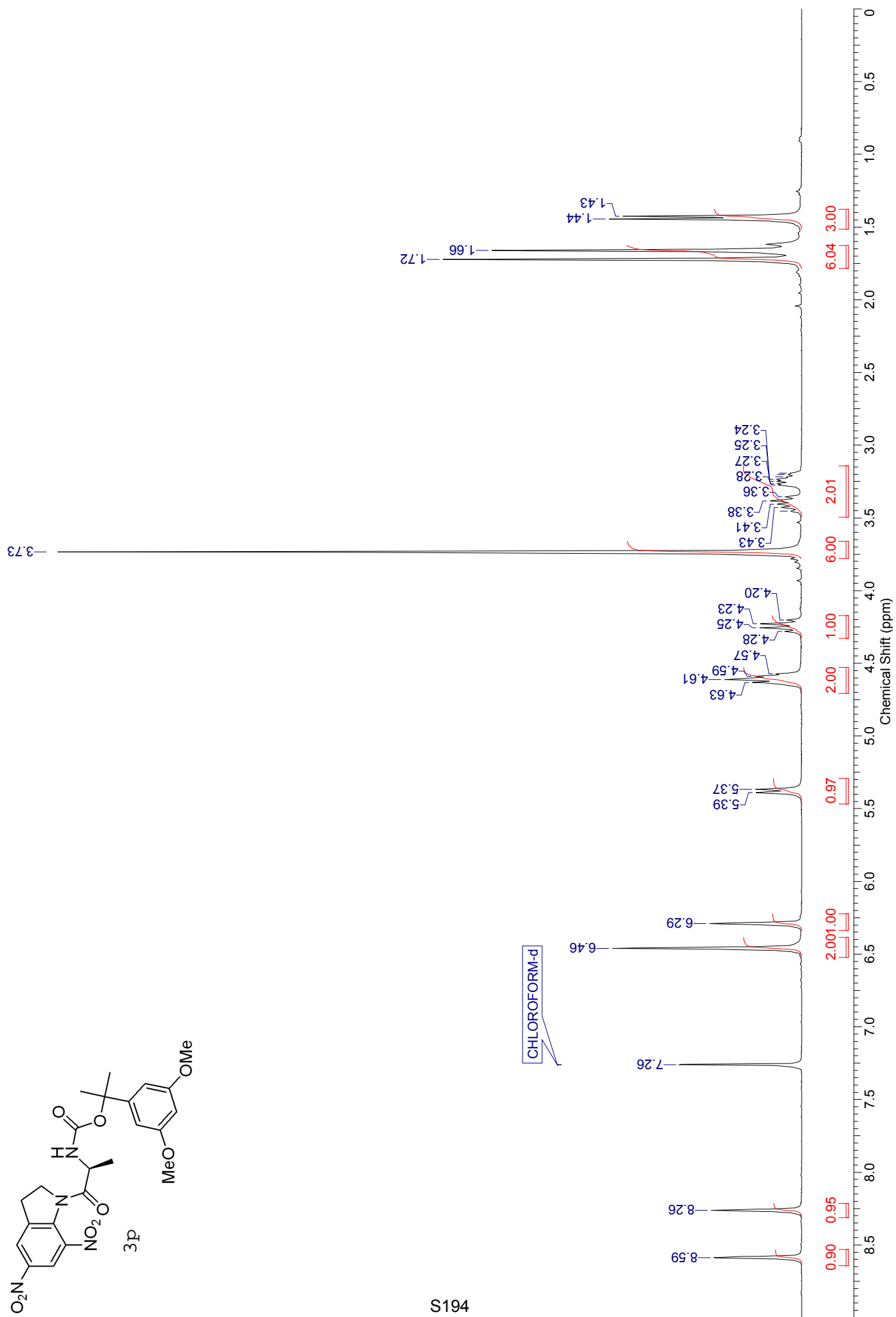
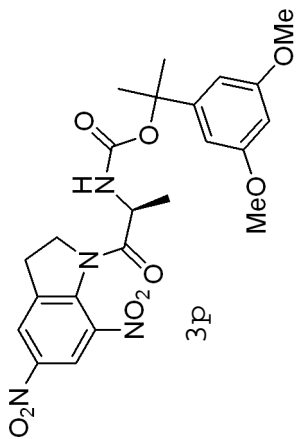


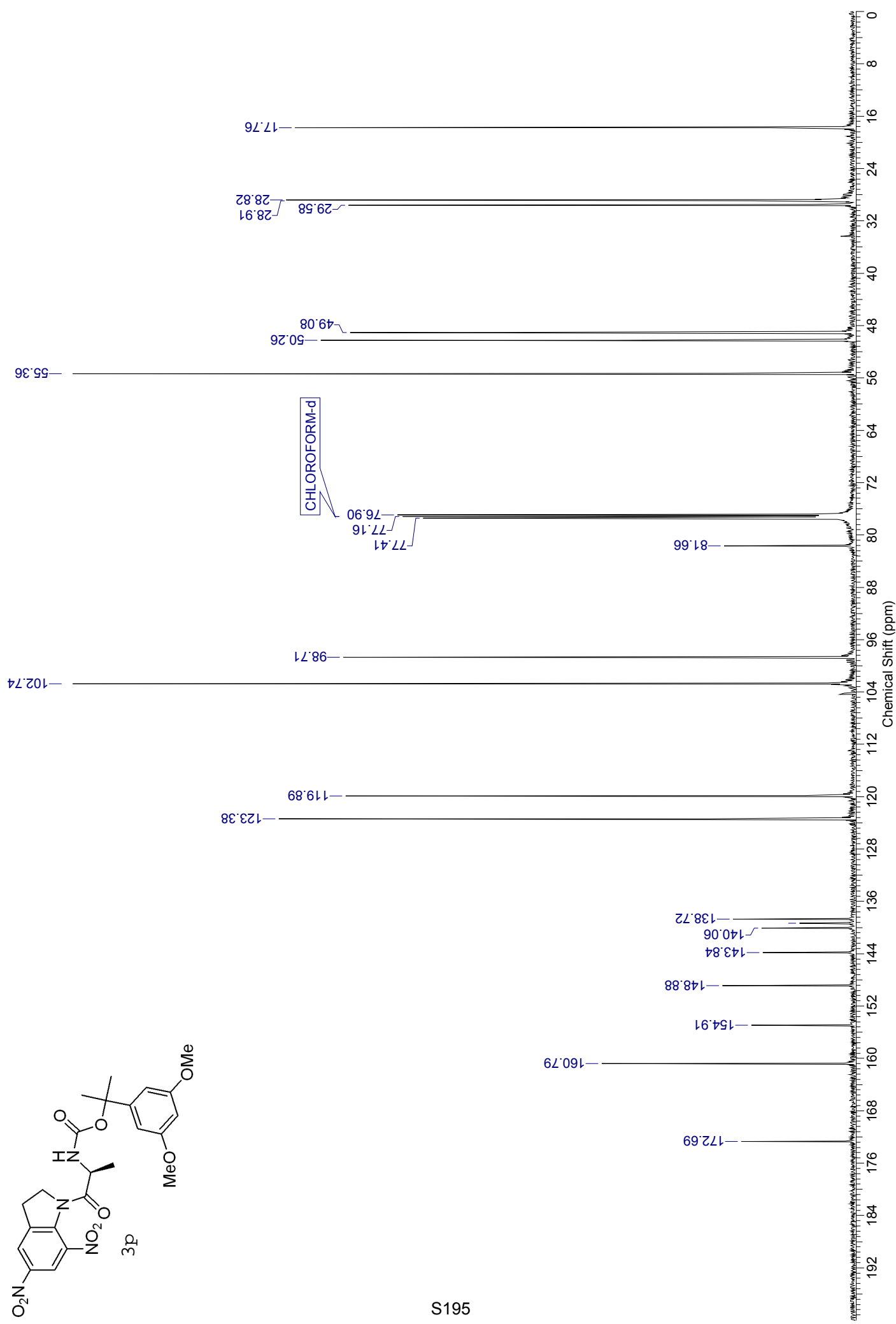
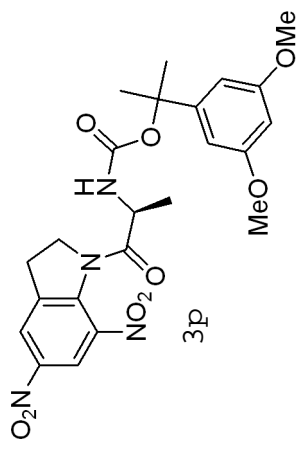
Date: 23.04.2008

Time: 09:41:35



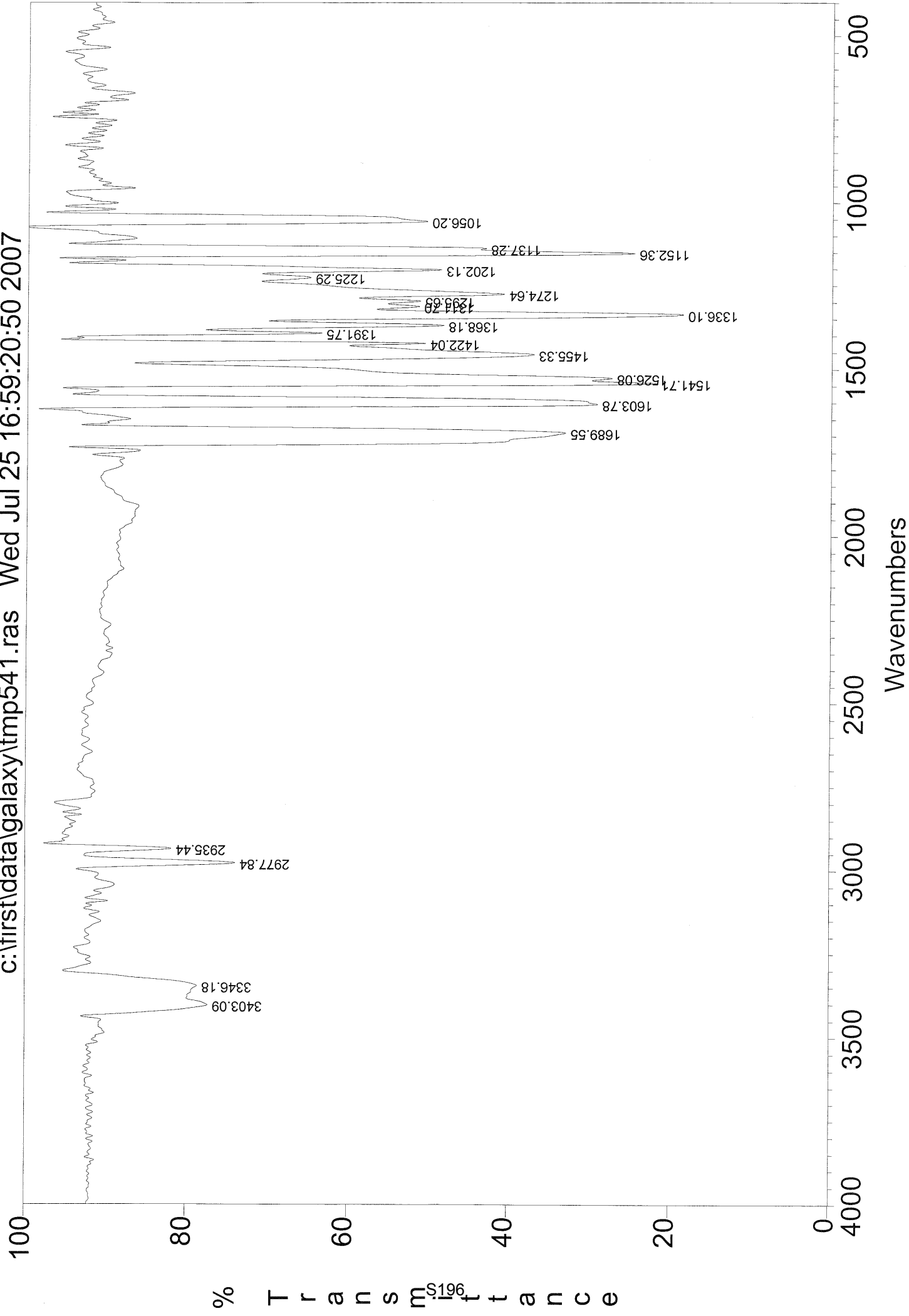
—— JLD145.SP - 23.04.2008 - $5.12 \cdot 10^{-5}$ M in MeCN





9615

c:\first\data\galaxy\tmp541.ras Wed Jul 25 16:59:20:50 2007



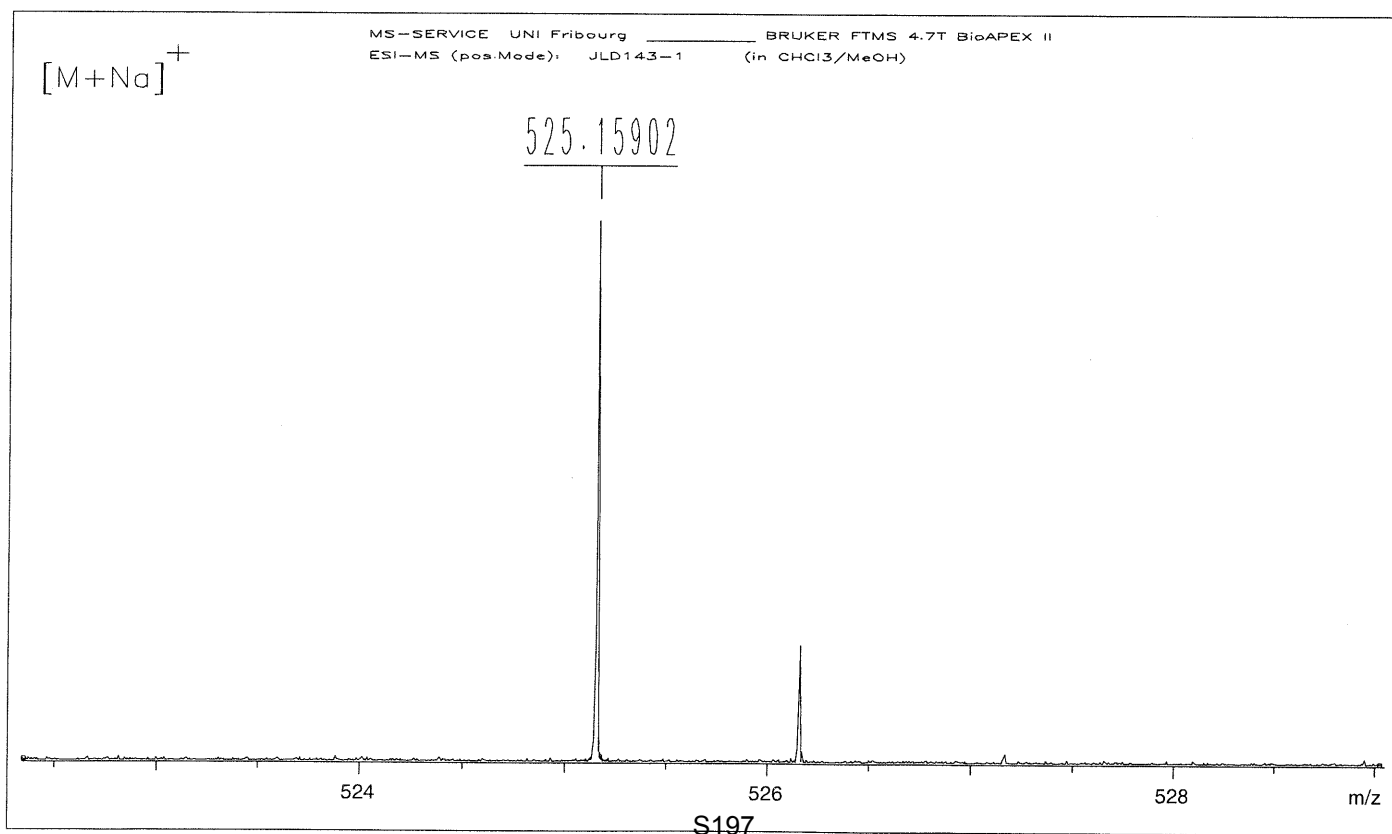
ESI-MS: JLD143-1

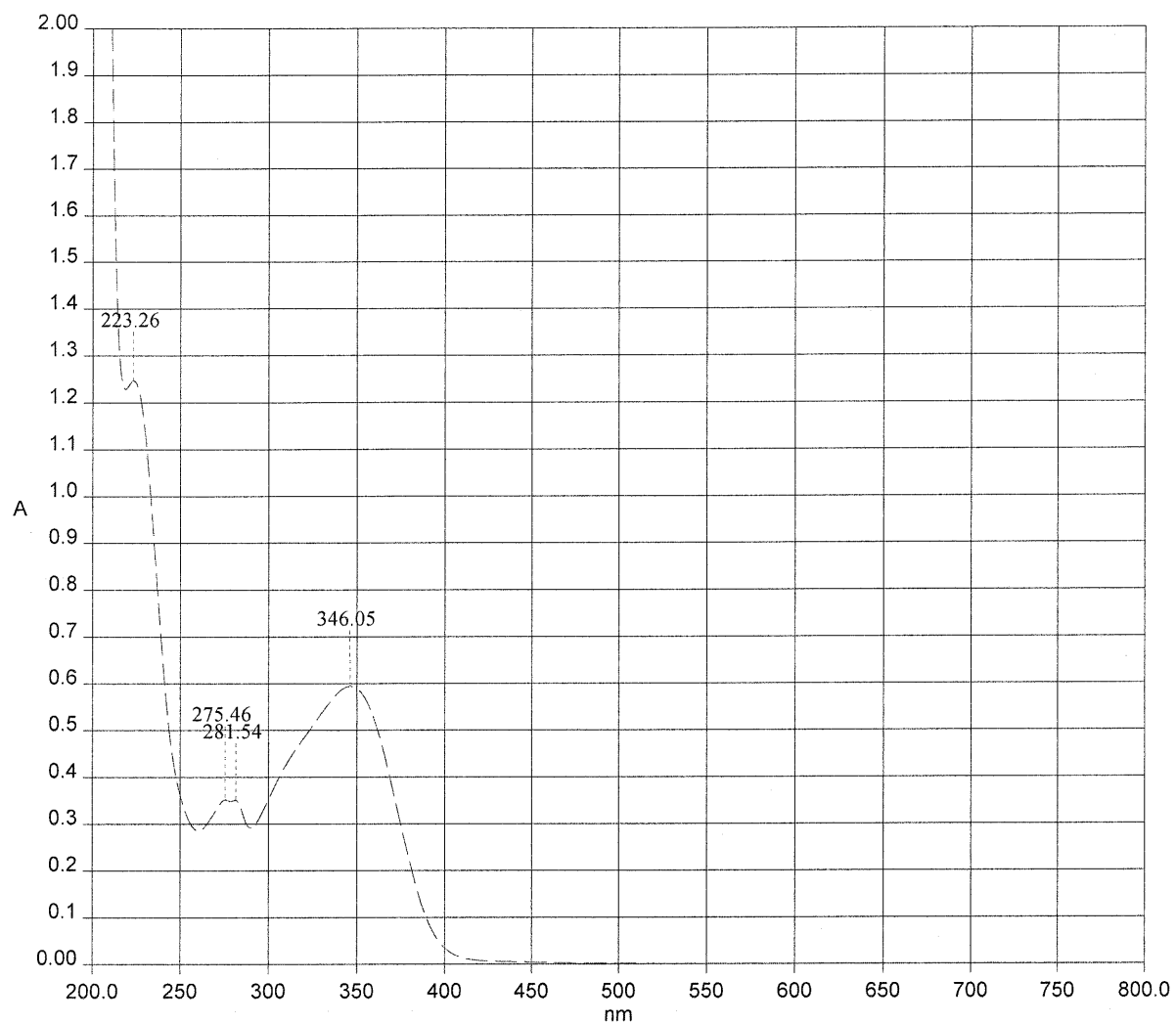
XMASS Mass Analysis for /Data/UNI_FR/DEBI2763_ESI/5/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 525.1590180

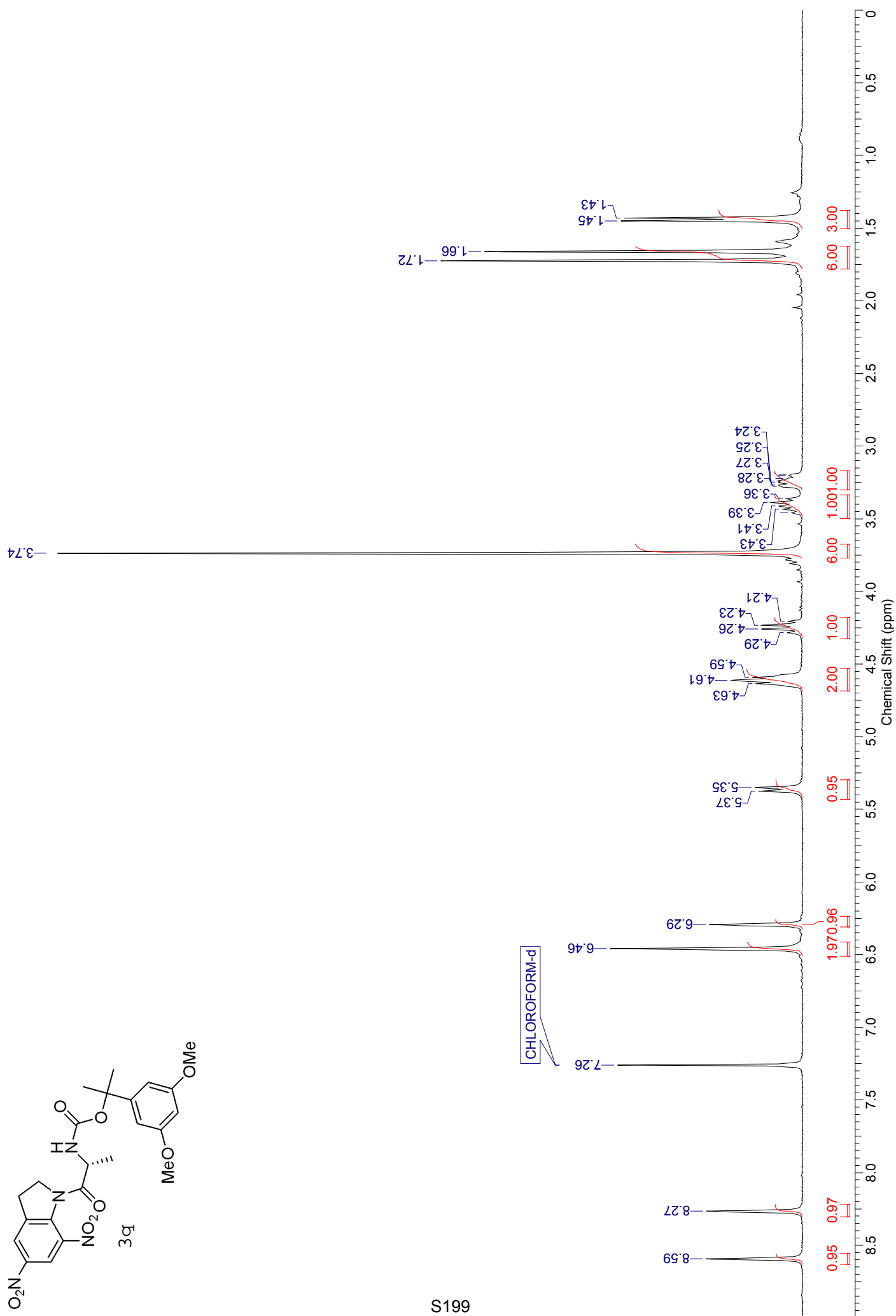
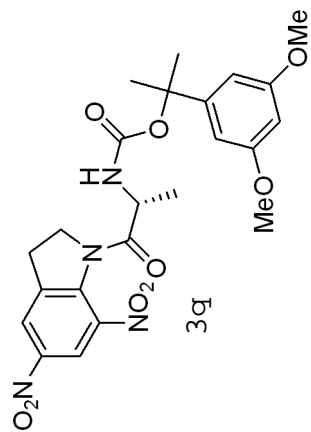
Charge = +1

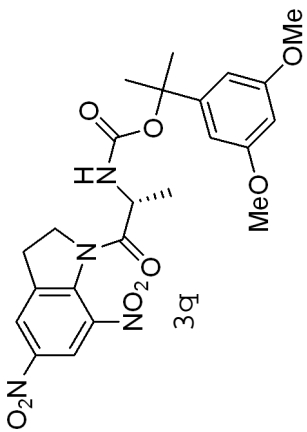
#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 525.1590180								
1	23	26	4	9	1	525.1591995	12.5	1.815e-04
2	25	25	4	9	0	525.1616048	15.5	2.587e-03
3	26	24	5	6	1	525.1618796	17.0	2.862e-03
4	28	23	5	6	0	525.1642849	20.0	5.267e-03
5	29	23	3	7	0	525.1530515	20.0	5.966e-03
6	27	24	3	7	1	525.1506462	17.0	8.372e-03
7	19	28	5	11	1	525.1677529	8.0	8.735e-03
8	24	23	5	9	0	525.1490288	16.0	9.989e-03
9	21	27	5	11	0	525.1701582	11.0	1.114e-02
10	22	24	5	9	1	525.1466235	13.0	1.239e-02



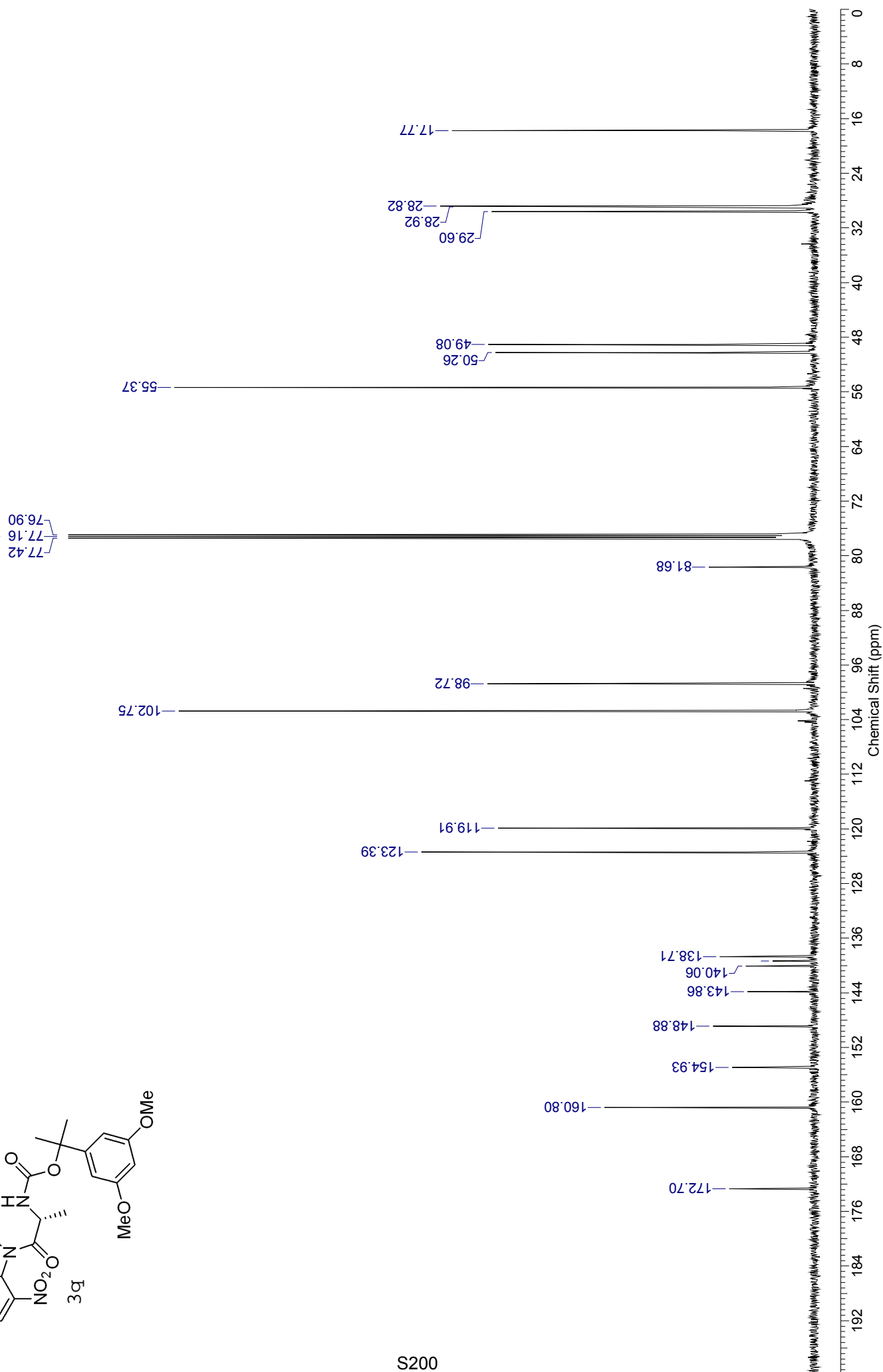


—— JLD143.SP - 23.04.2008 - $5.17 \cdot 10^{-5}$ M in MeCN



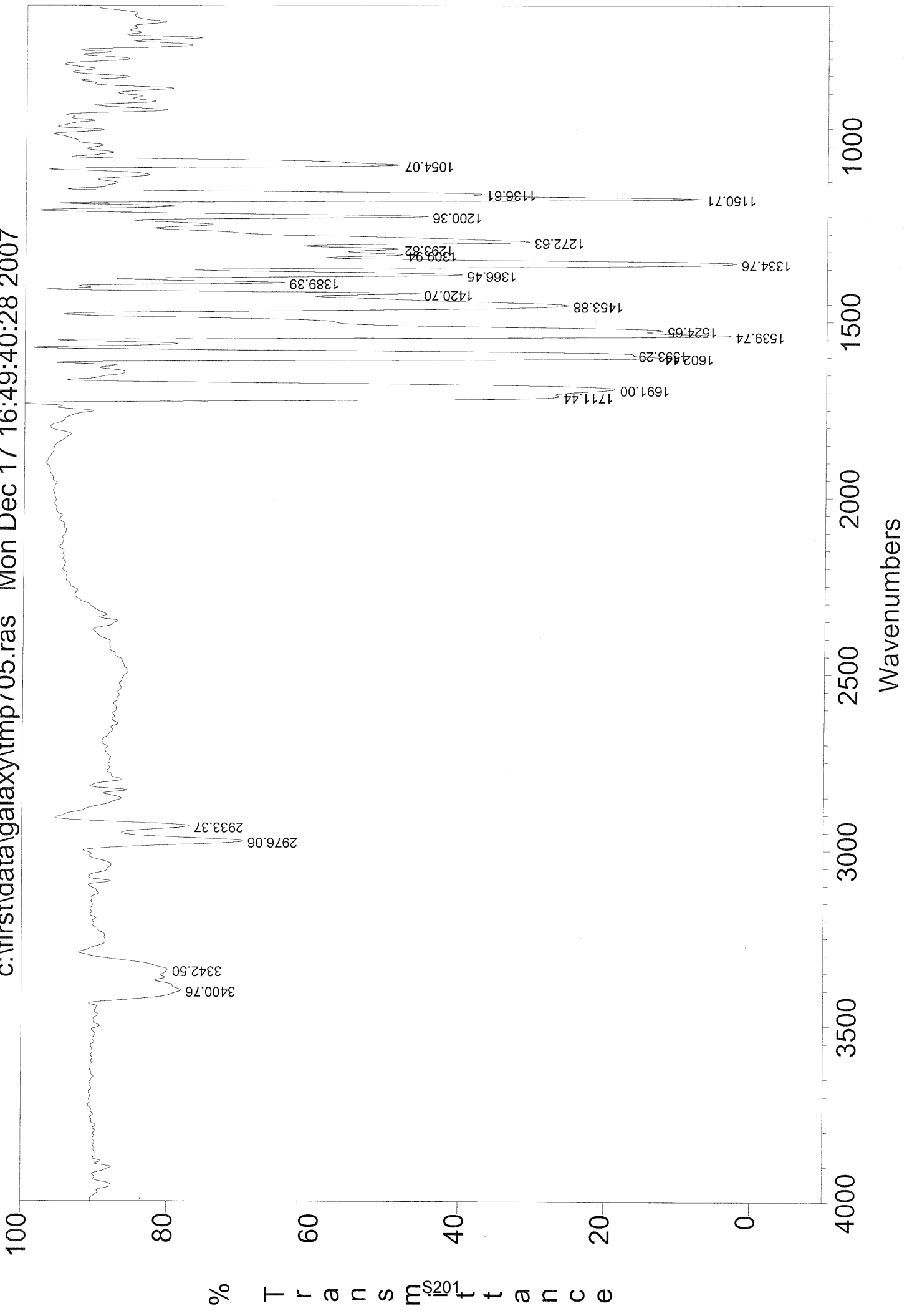


CHLOROFORM-d



500159

c:\first\data\galaxy\tmp705.ras Mon Dec 17 16:49:40:28 2007





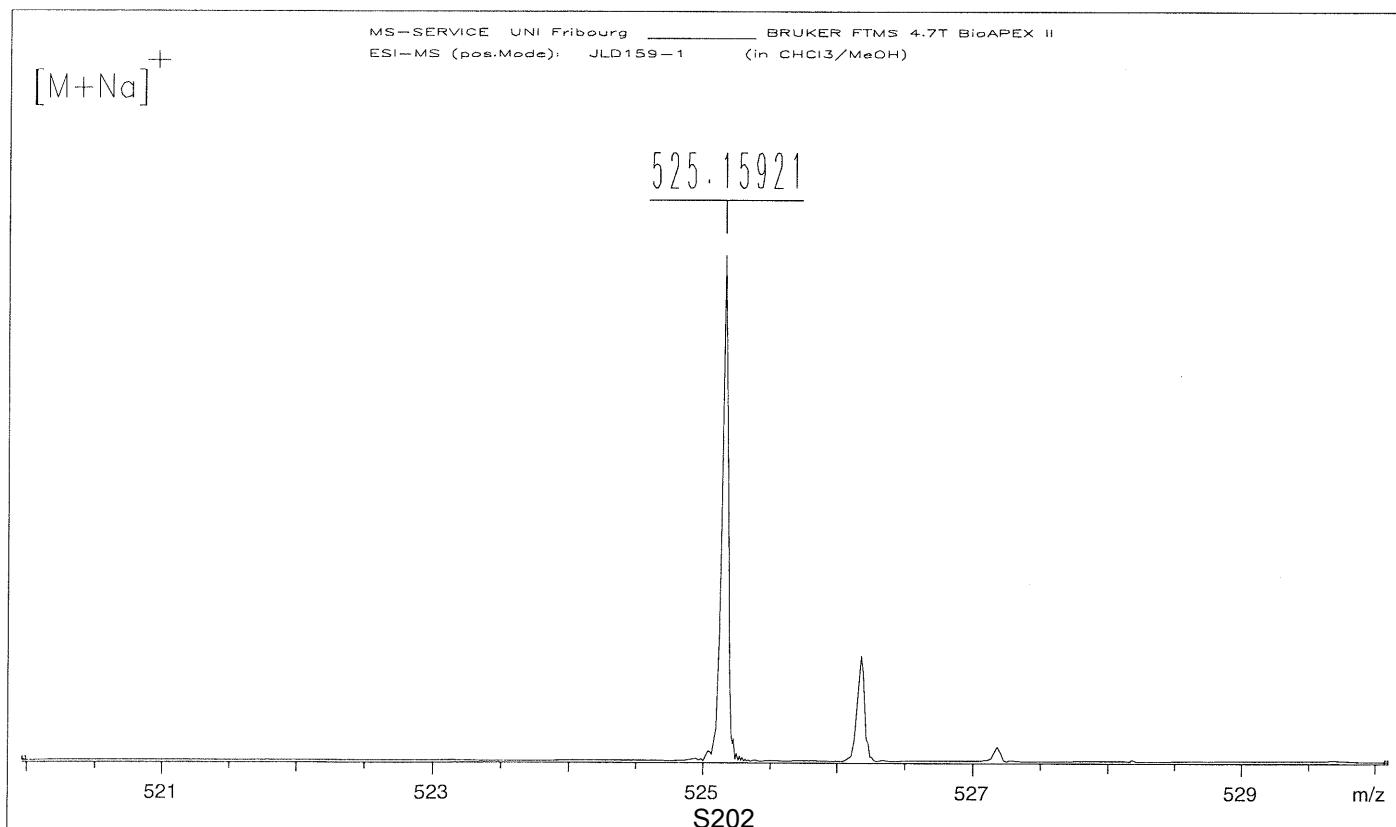
ESI-MS: JLD159-1

XMASS Mass Analysis for /Data/UNI_FR/DEBI3056_ESI/10/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 525.1592090

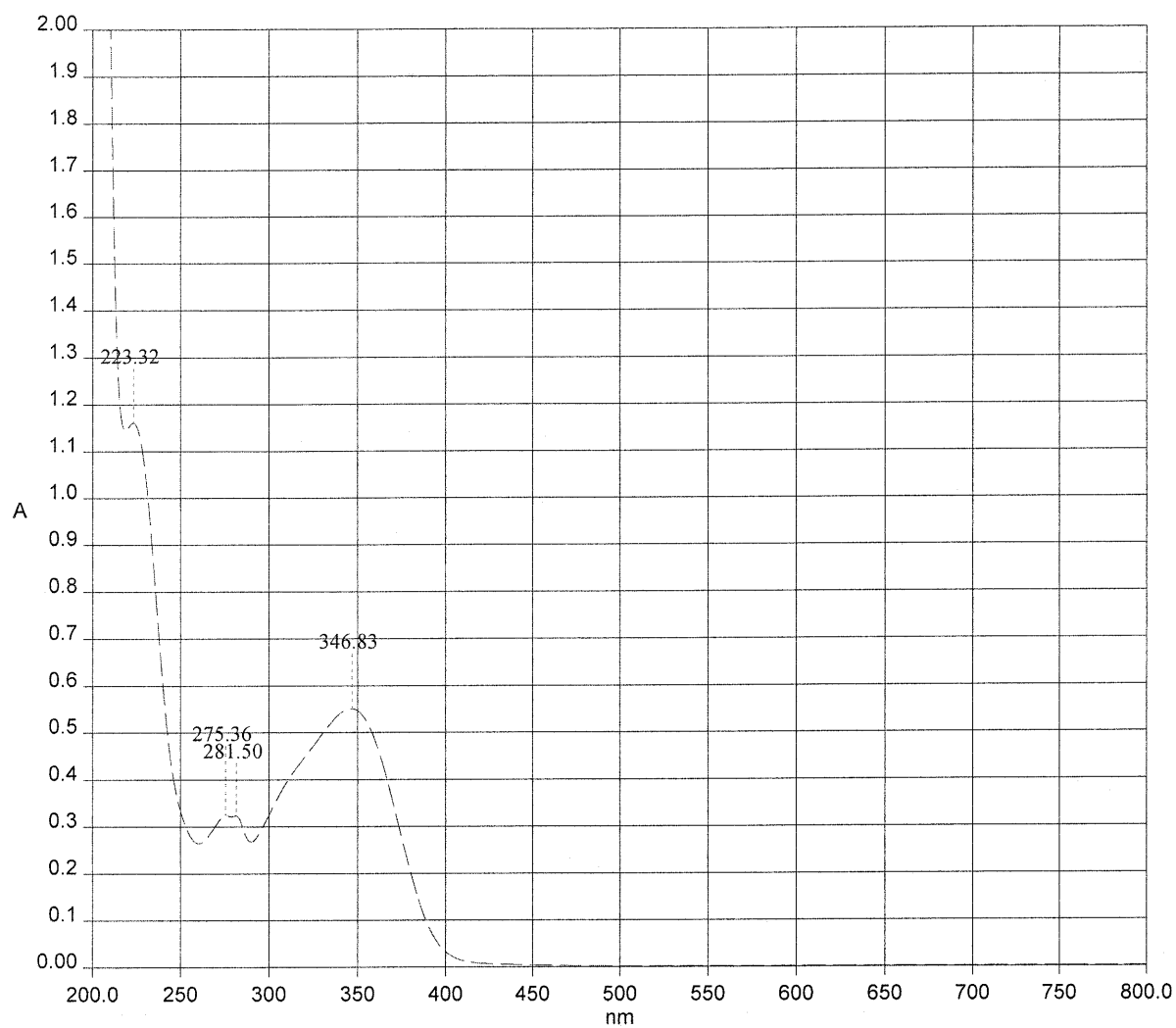
Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 525.1592090								
1	23	26	4	9	1	525.1591995	12.5	9.456e-06
2	21	21	10	7	0	525.1589195	16.5	2.895e-04
3	23	23	7	8	0	525.1602622	16.0	1.053e-03
4	24	22	8	5	1	525.1605369	17.5	1.328e-03
5	25	28	1	10	1	525.1605422	12.0	1.333e-03
6	21	24	7	8	1	525.1578569	13.0	1.352e-03
7	25	25	4	9	0	525.1616048	15.5	2.396e-03
8	19	22	10	7	1	525.1565142	13.5	2.695e-03
9	18	23	9	10	0	525.1562394	12.0	2.970e-03
10	16	24	9	10	1	525.1538341	9.0	5.375e-03

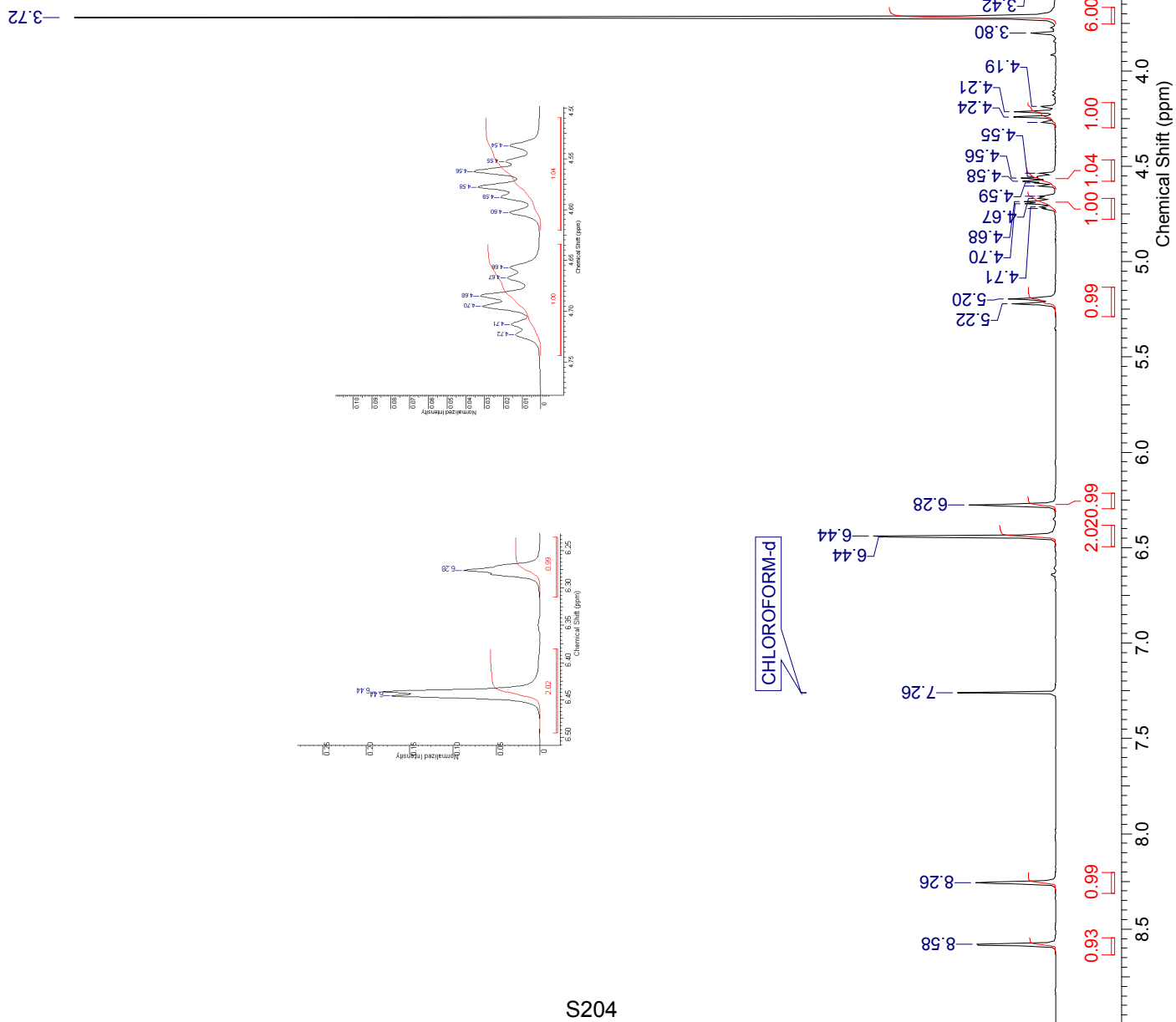
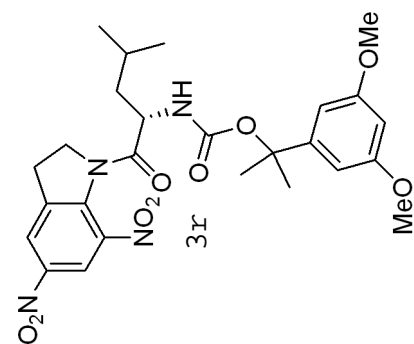


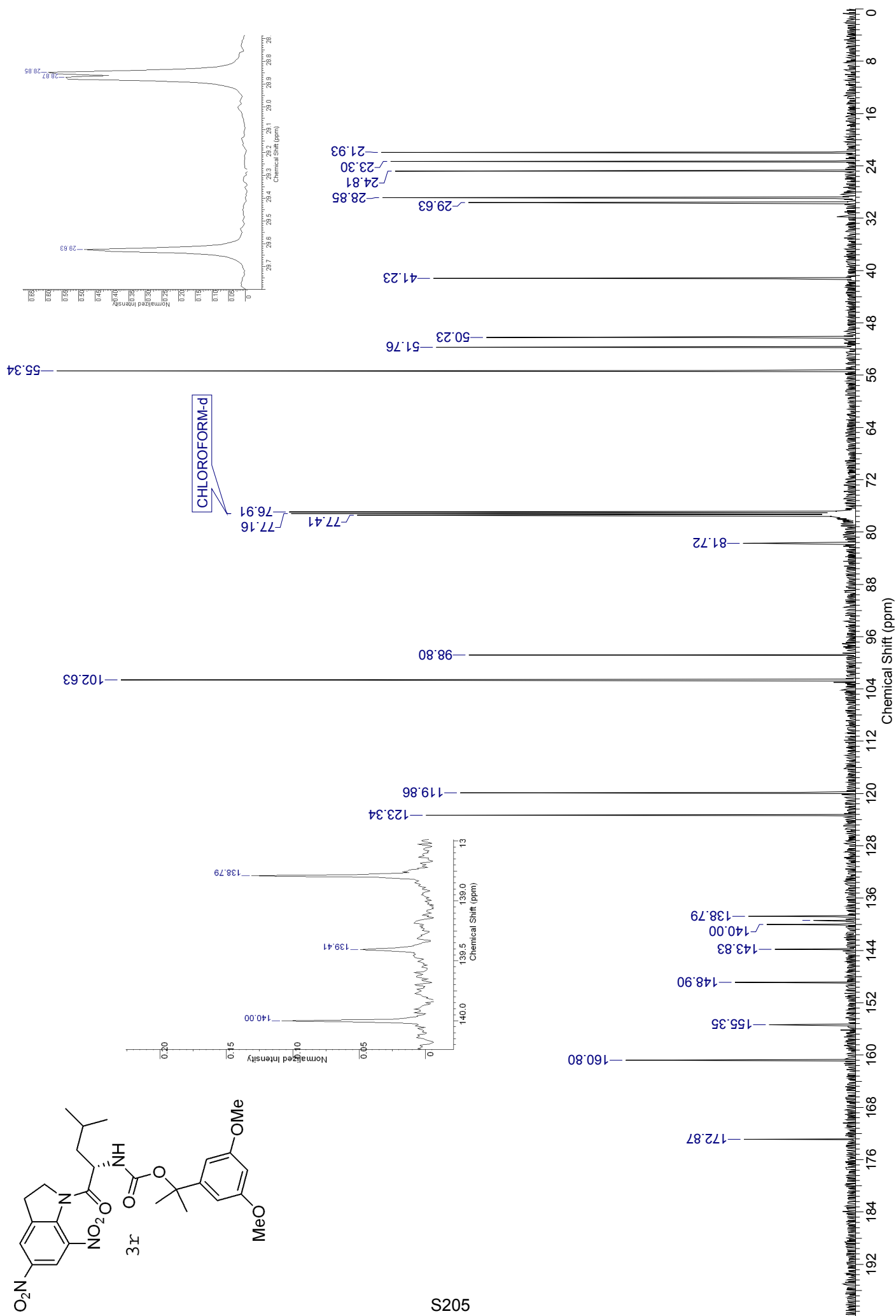
Date: 23.04.2008

Time: 09:59:47



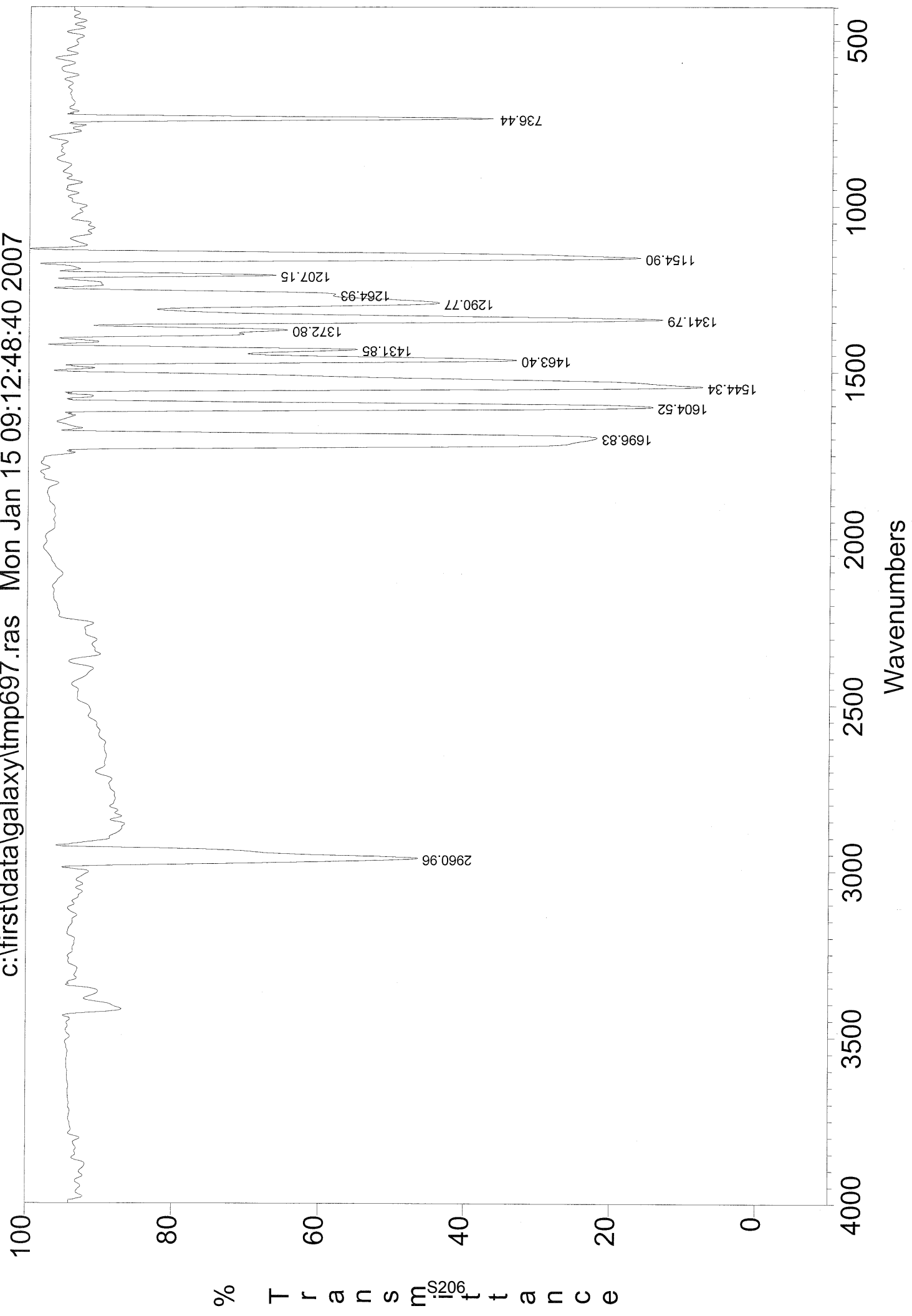
----- JLD159.SP - 23.04.2008 - $5.07 \cdot 10^{-5}$ M in MeCN





DL0100

c:\first\data\galaxy\tmp697.ras Mon Jan 15 09:12:48:40 2007



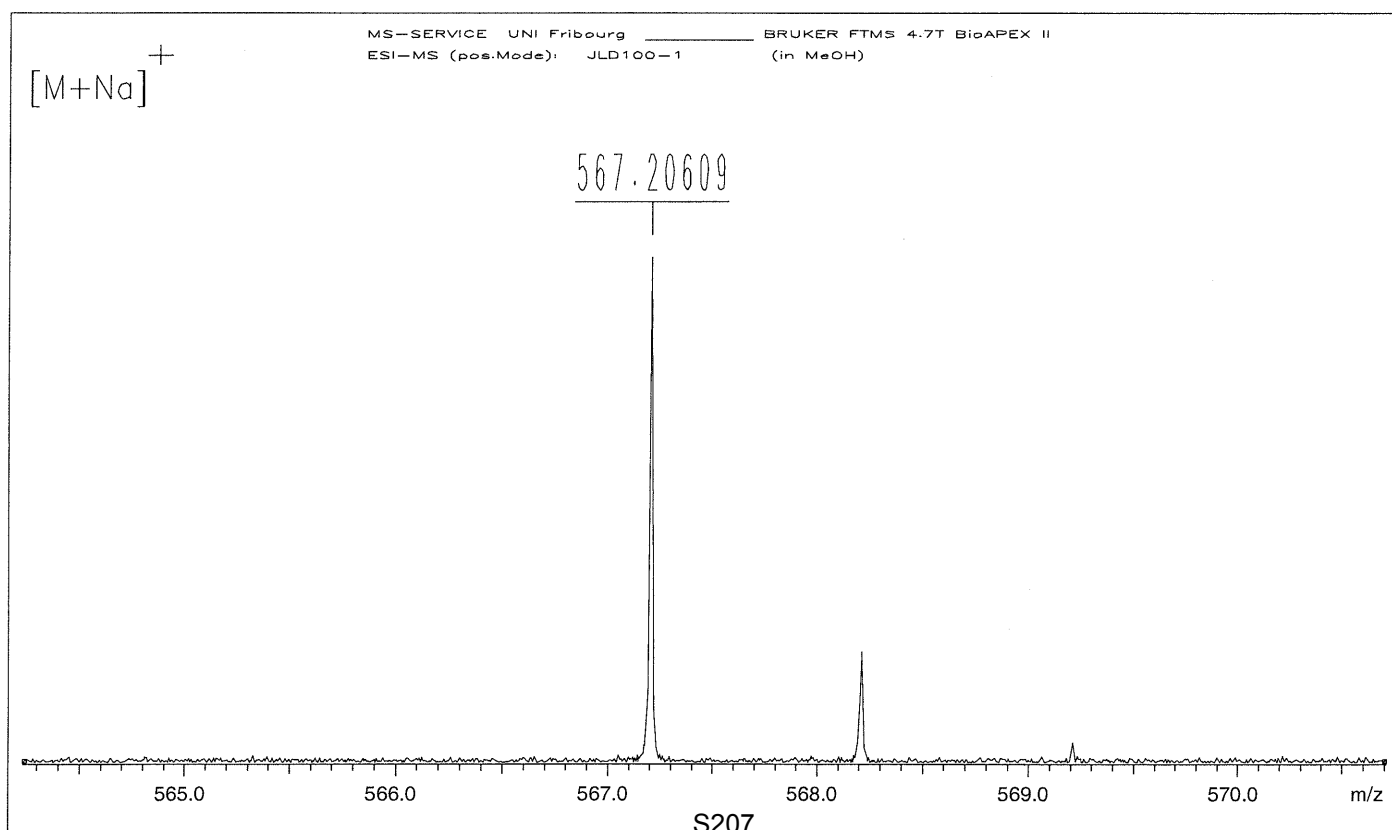
ESI-MS: JLD100-1

XMASS Mass Analysis for /Data/UNI_FR/DEBI2216_ESI/10/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 567.2060950

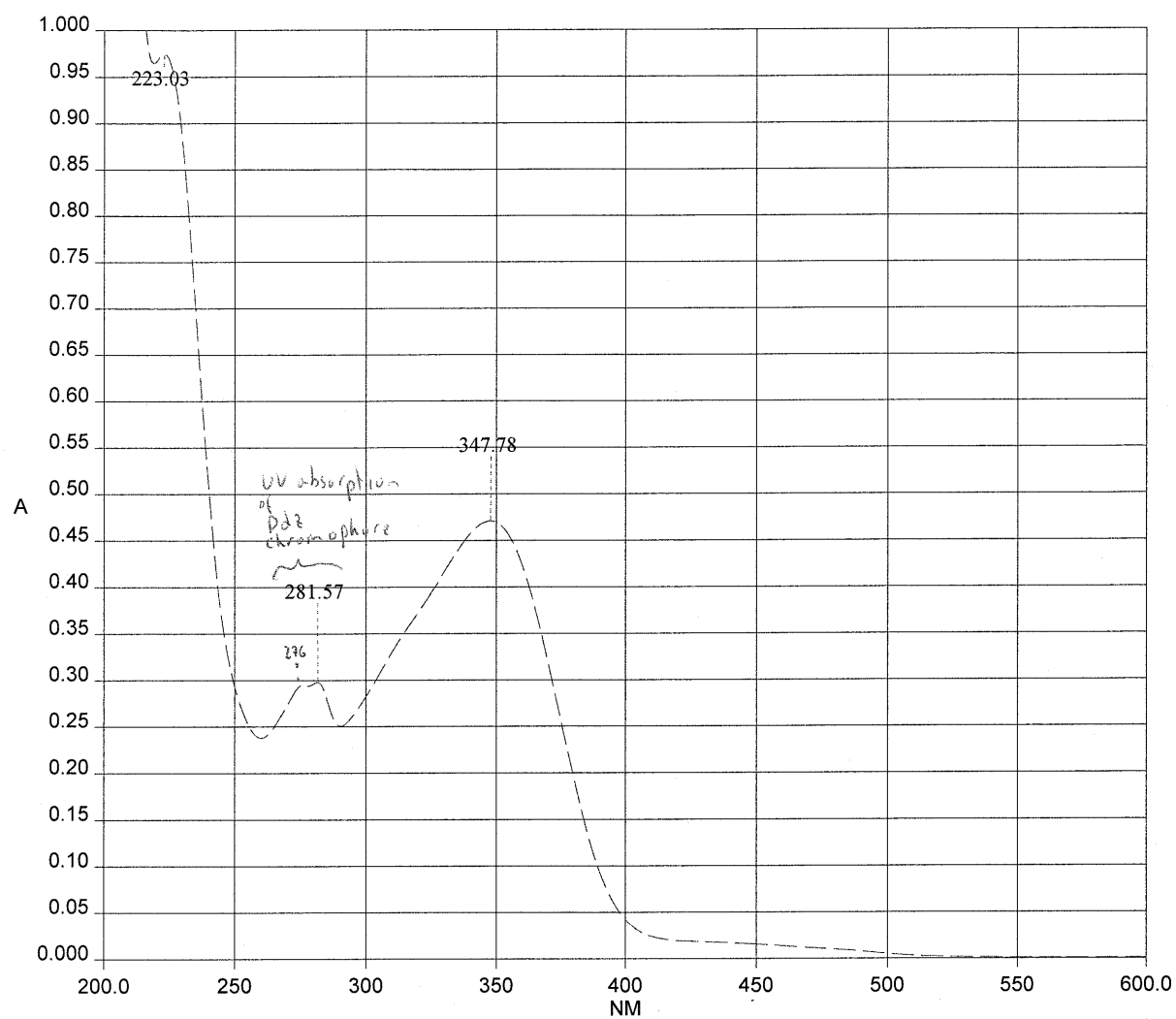
Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 567.2060950								
1	26	32	4	9	1	567.2061497	12.5	5.474e-05
2	24	27	10	7	0	567.2058697	16.5	2.253e-04
3	40	27	2	2	0	567.2067045	28.5	6.095e-04
4	38	25	5	1	0	567.2053619	29.0	7.331e-04
5	26	29	7	8	0	567.2072124	16.0	1.117e-03
6	24	30	7	8	1	567.2048071	13.0	1.288e-03
7	27	28	8	5	1	567.2074871	17.5	1.392e-03
8	28	34	1	10	1	567.2074924	12.0	1.397e-03
9	38	28	2	2	1	567.2042992	25.5	1.796e-03
10	37	29	1	5	0	567.2040245	24.0	2.071e-03

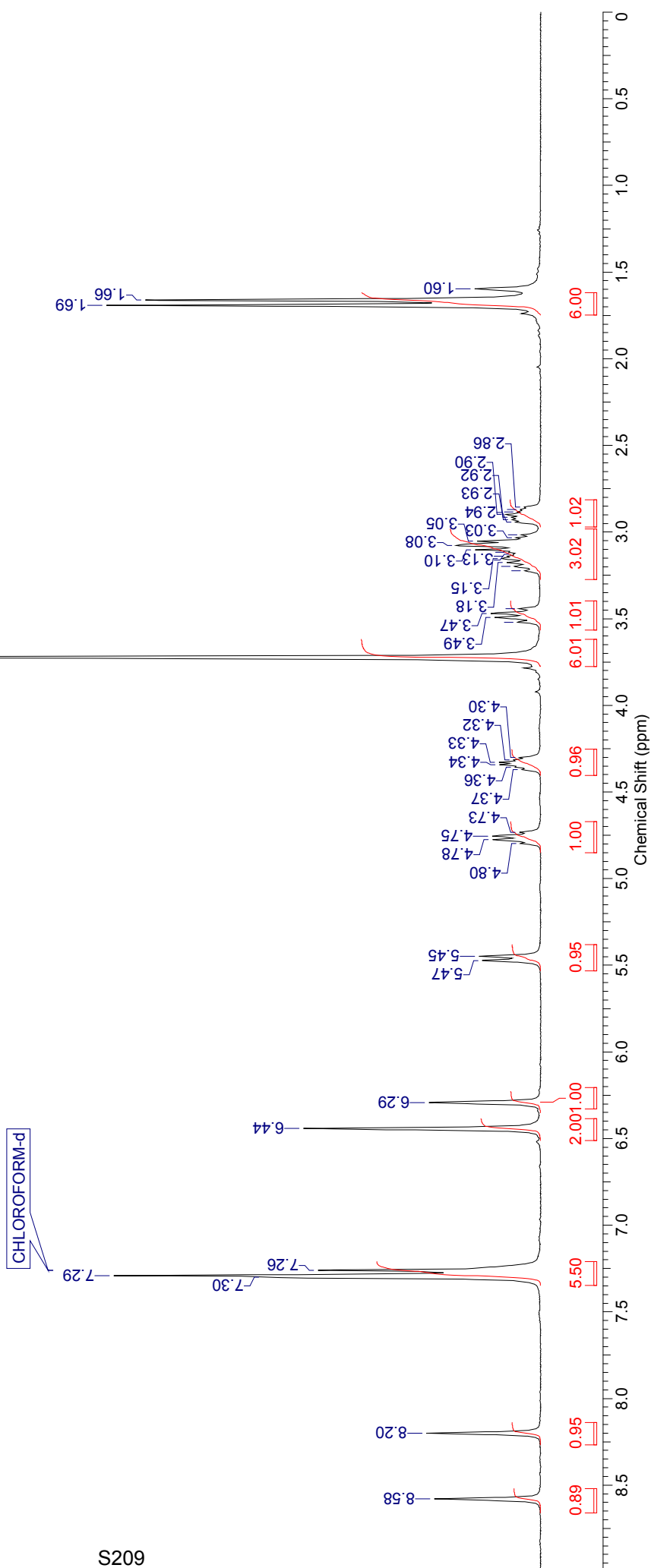
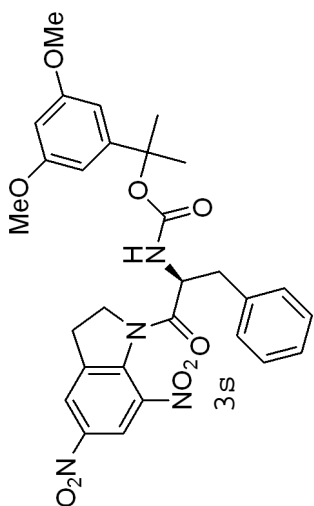


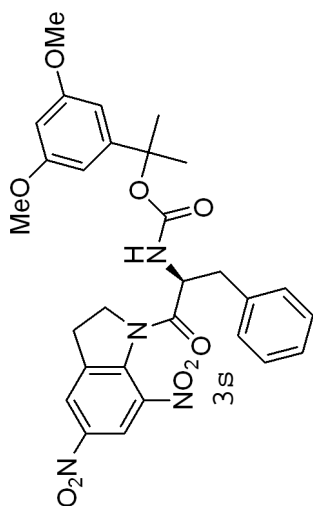
Date: 15.01.2007

Time: 13:13:23

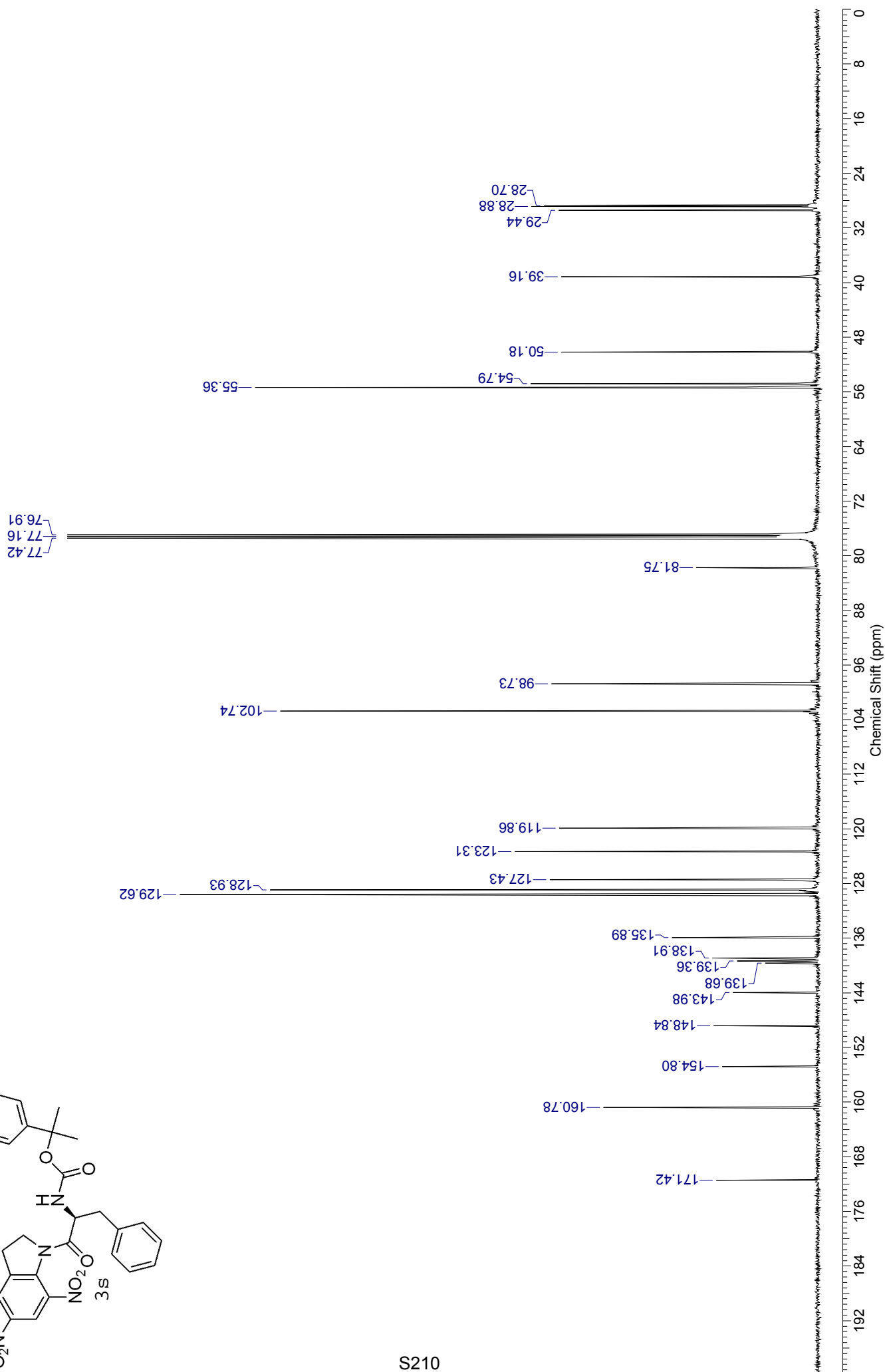


----- JLD100A.SP - 15.01.2007 - 4.77×10^{-5} M



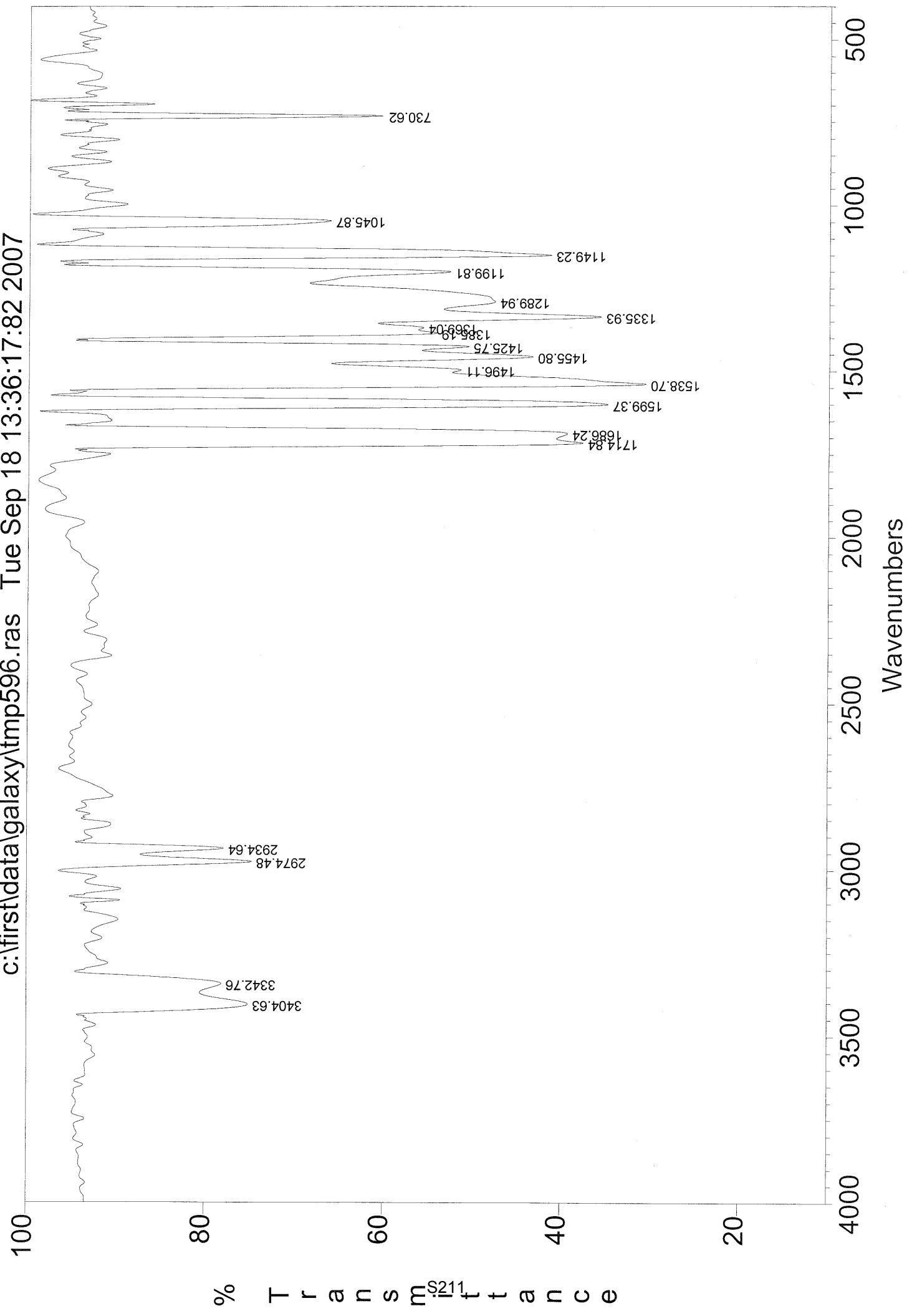


CHLOROFORM-d



50450

c:\first\data\galaxy\tmp596.ras Tue Sep 18 13:36:17:82 2007



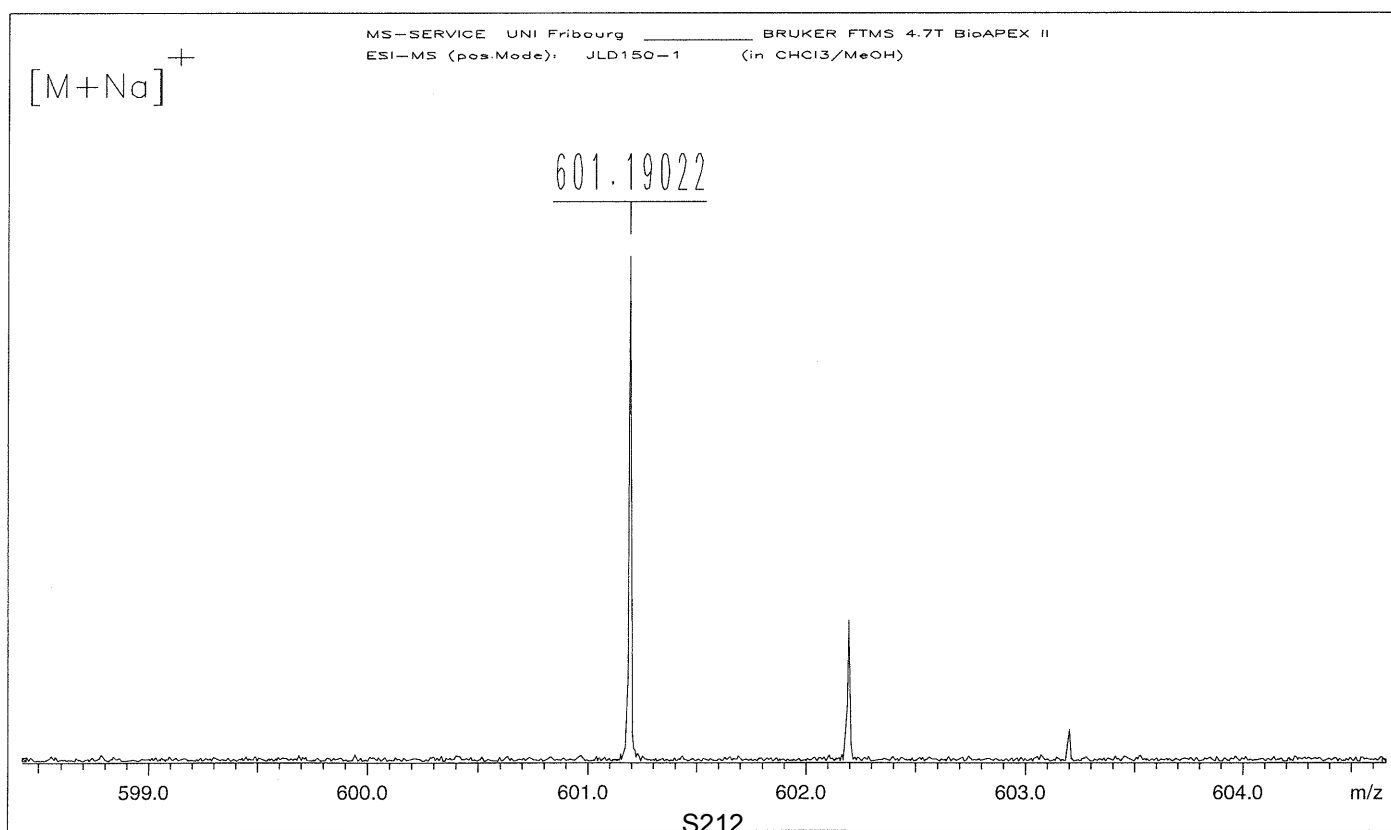
ESI-MS: JLD150-1

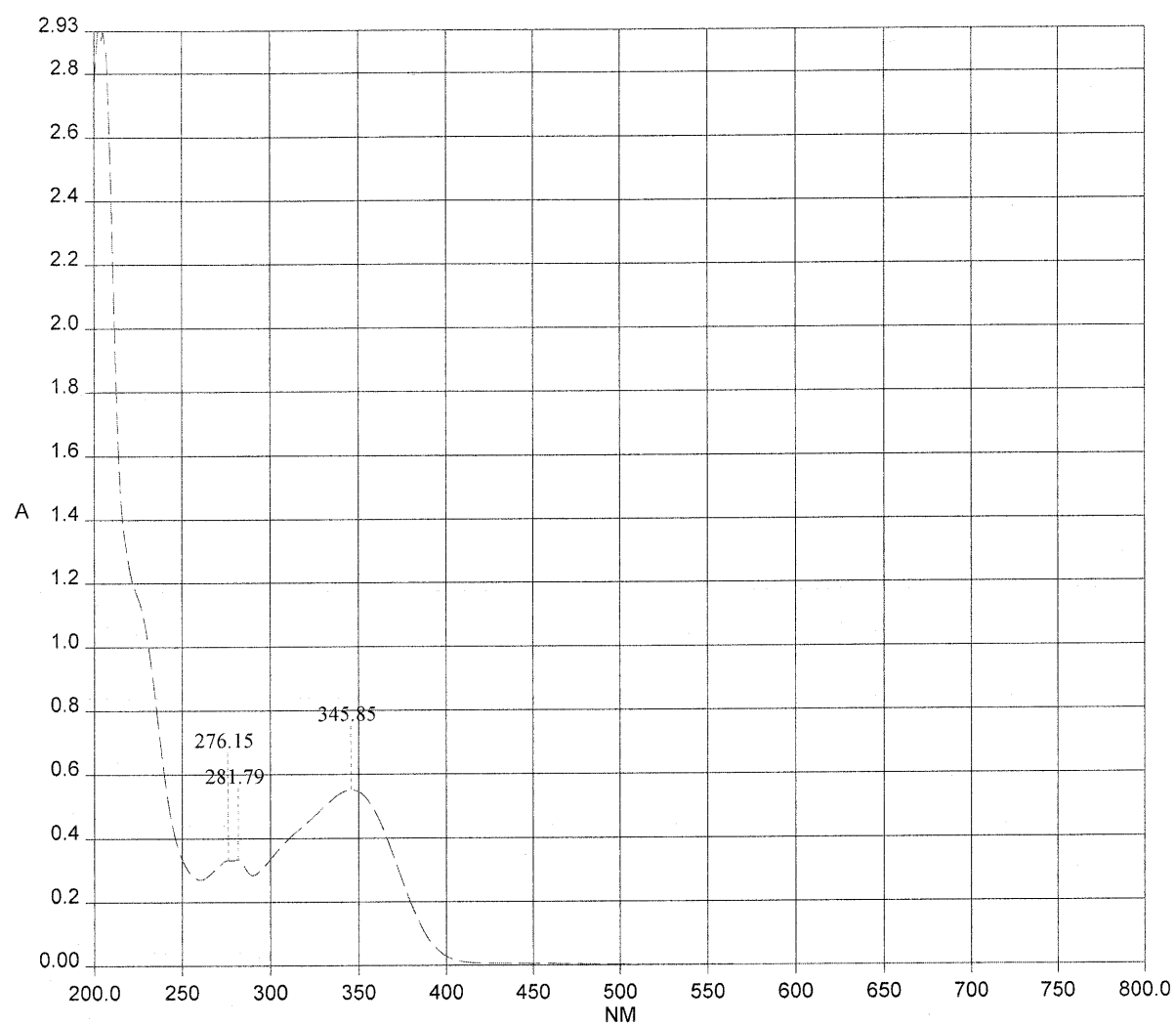
XMASS Mass Analysis for /Data/UNI_FR/DEBI2856_ESI/2/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 601.1902160

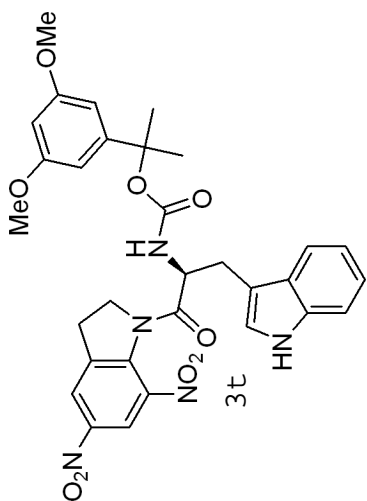
Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 601.1902160								
1	29	30	4	9	1	601.1904997	16.5	2.837e-04
2	27	28	7	8	1	601.1891570	17.0	1.059e-03
3	29	27	7	8	0	601.1915623	20.0	1.346e-03
4	30	26	8	5	1	601.1918371	21.5	1.621e-03
5	31	29	4	9	0	601.1929050	19.5	2.689e-03
6	32	28	5	6	1	601.1931797	21.0	2.964e-03
7	32	25	8	5	0	601.1942424	24.5	4.026e-03
8	34	27	5	6	0	601.1955850	24.0	5.369e-03
9	35	26	6	3	1	601.1958598	25.5	5.644e-03
10	35	27	3	7	0	601.1843517	24.0	5.864e-03

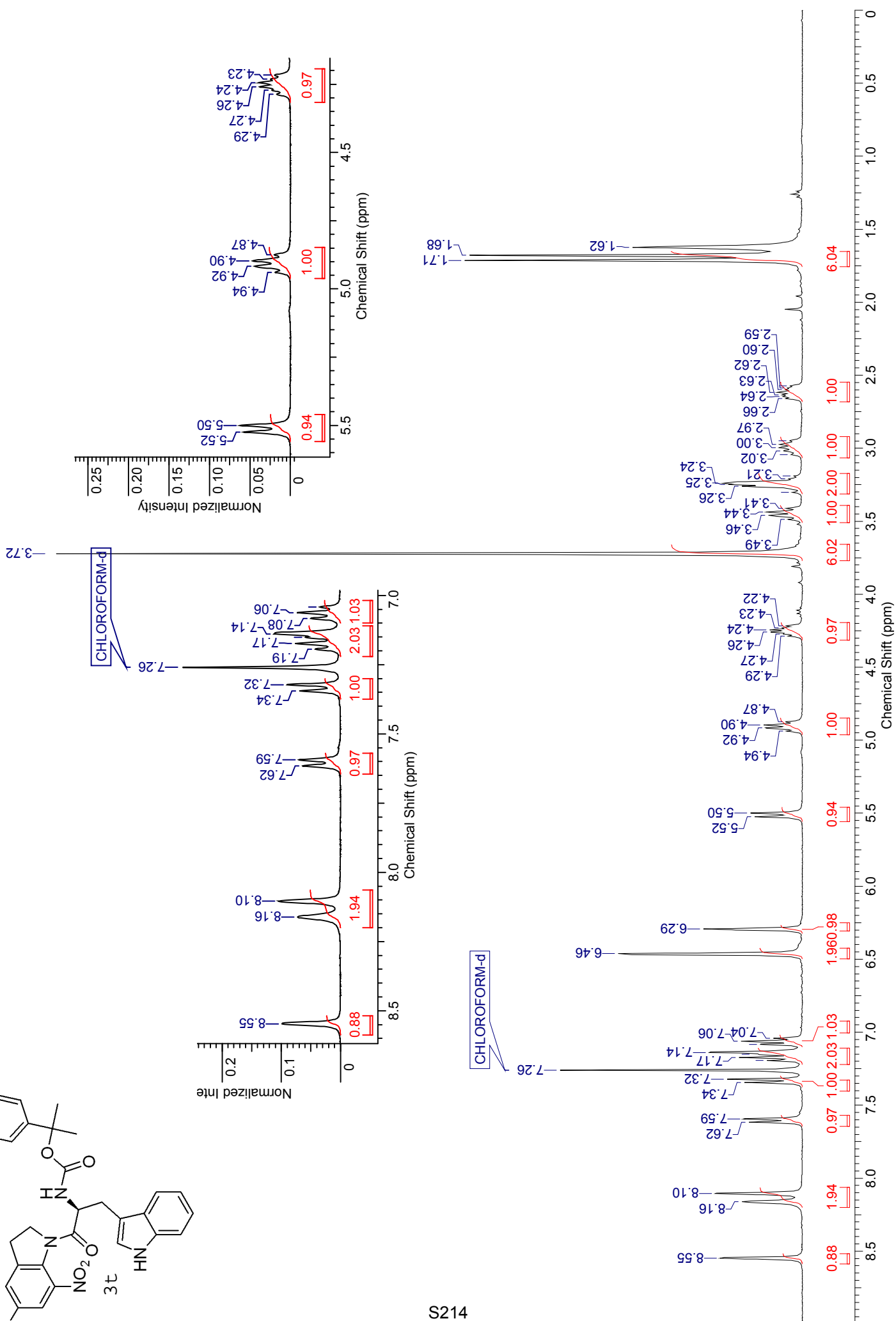


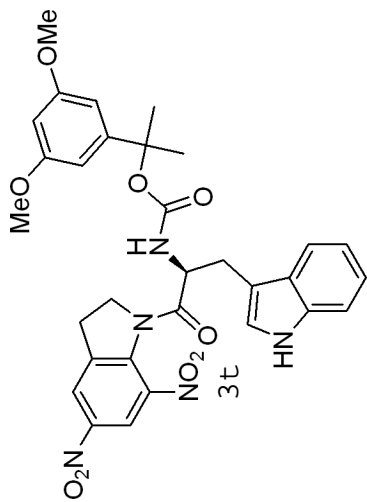


—— JLD150.SP - 21.04.2008 - $5.01 \cdot 10^{-5}$ M in MeCN



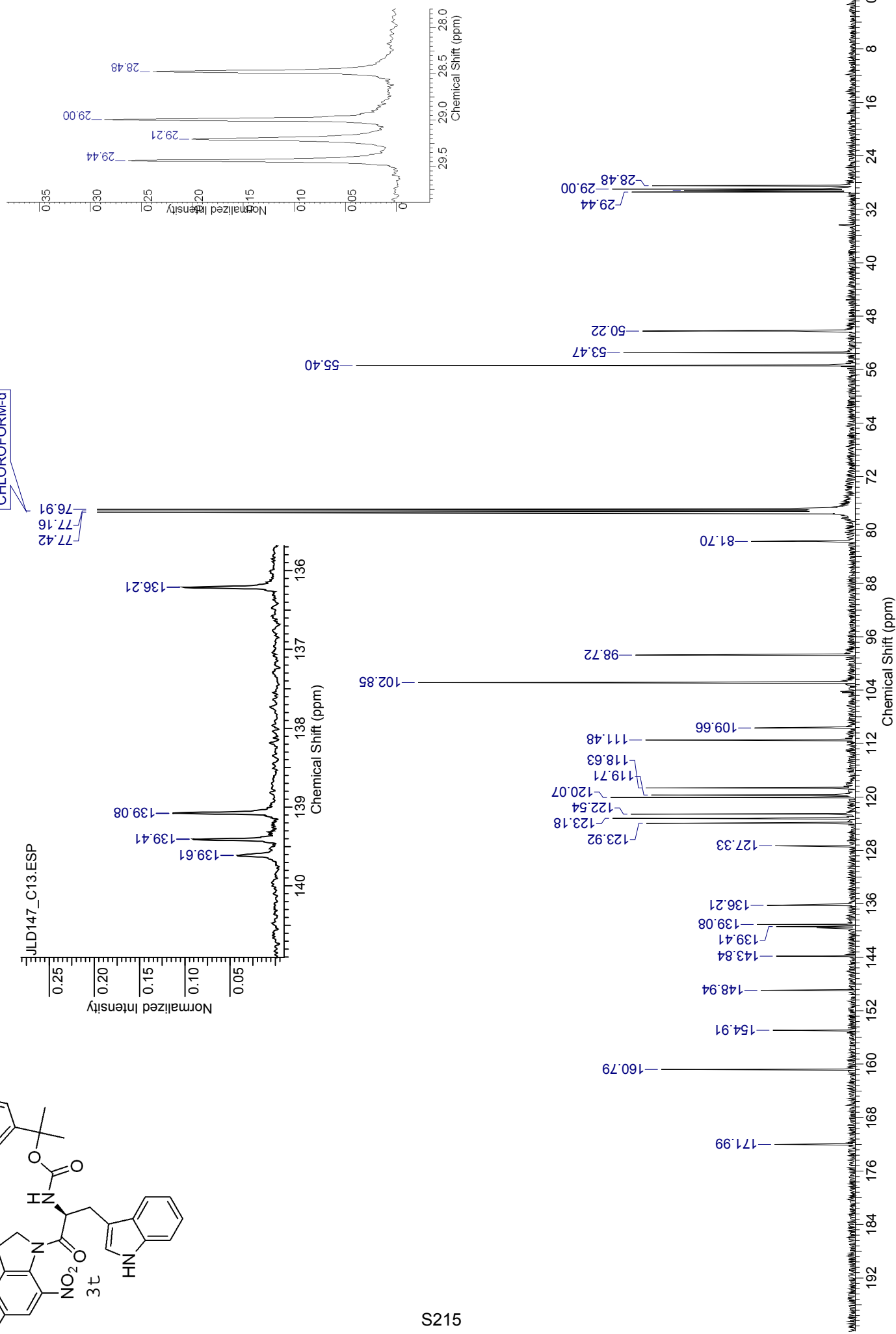
S214





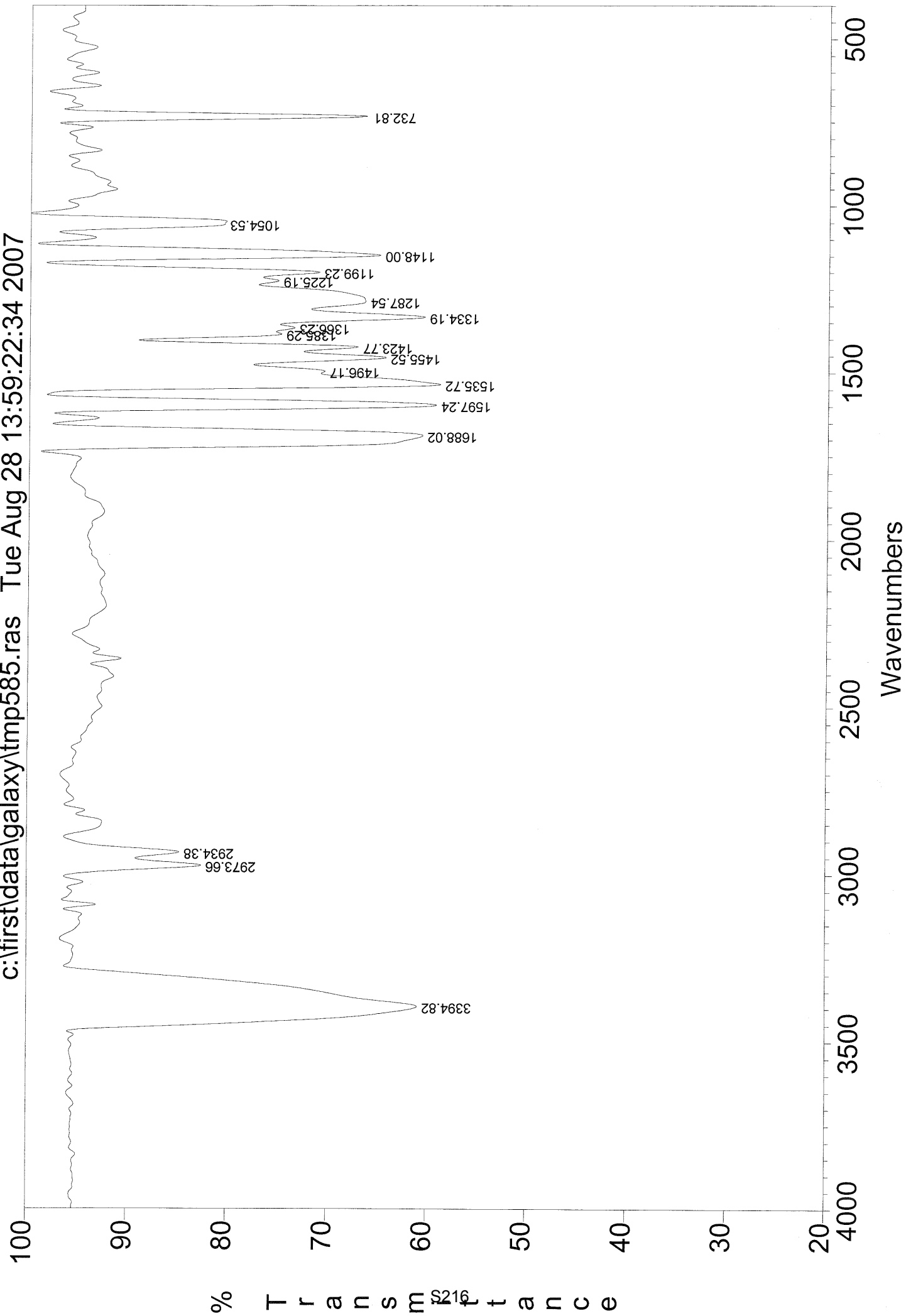
S215

CHLOROFORM-d



90147

c:\first\data\galaxy\tmp585.ras Tue Aug 28 13:59:22:34 2007



ESI-MS: JLD147-1

XMASS Mass Analysis for /Data/UNI_FR/DEBI2816_ESI/10/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

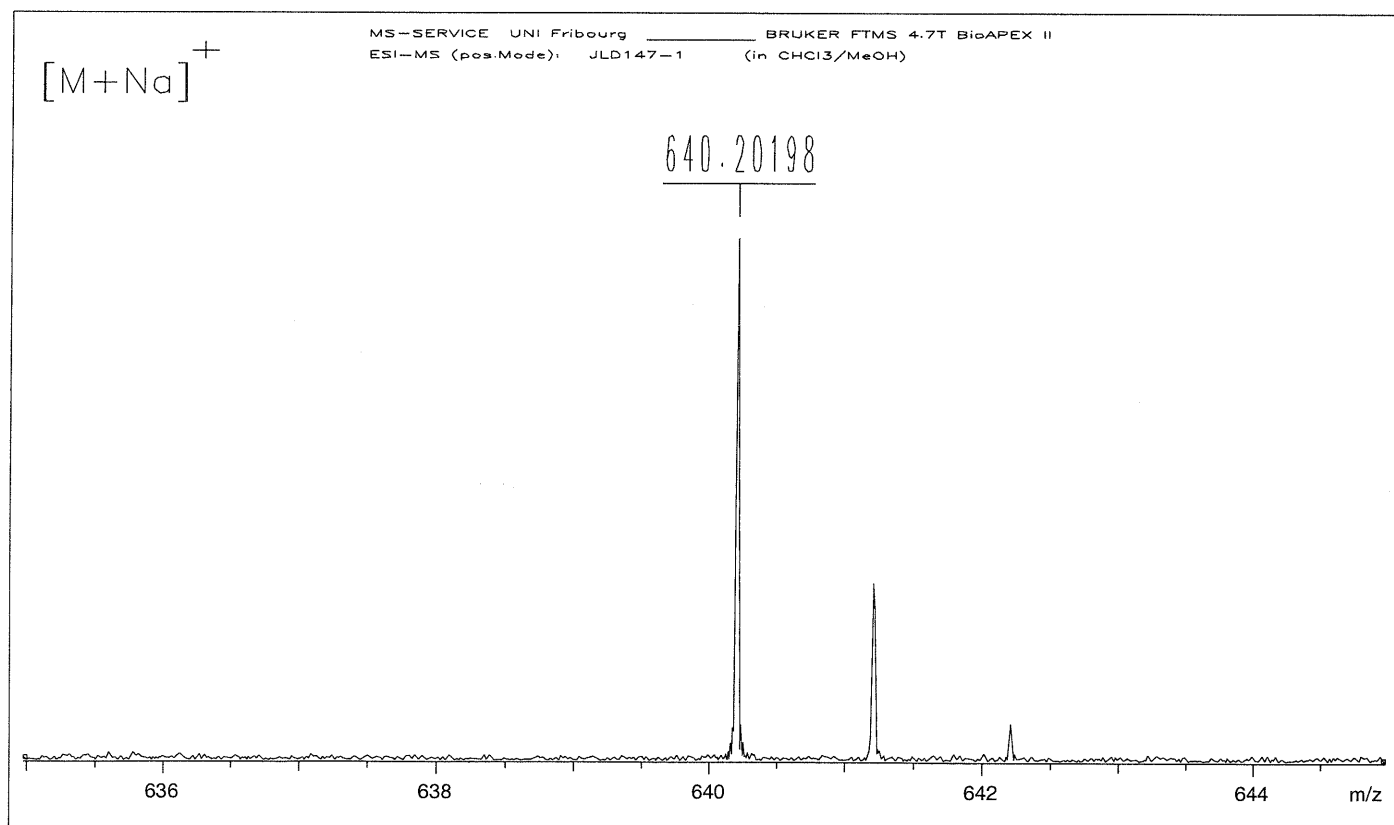
Ion mass = 640.2019820

Charge = +1

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

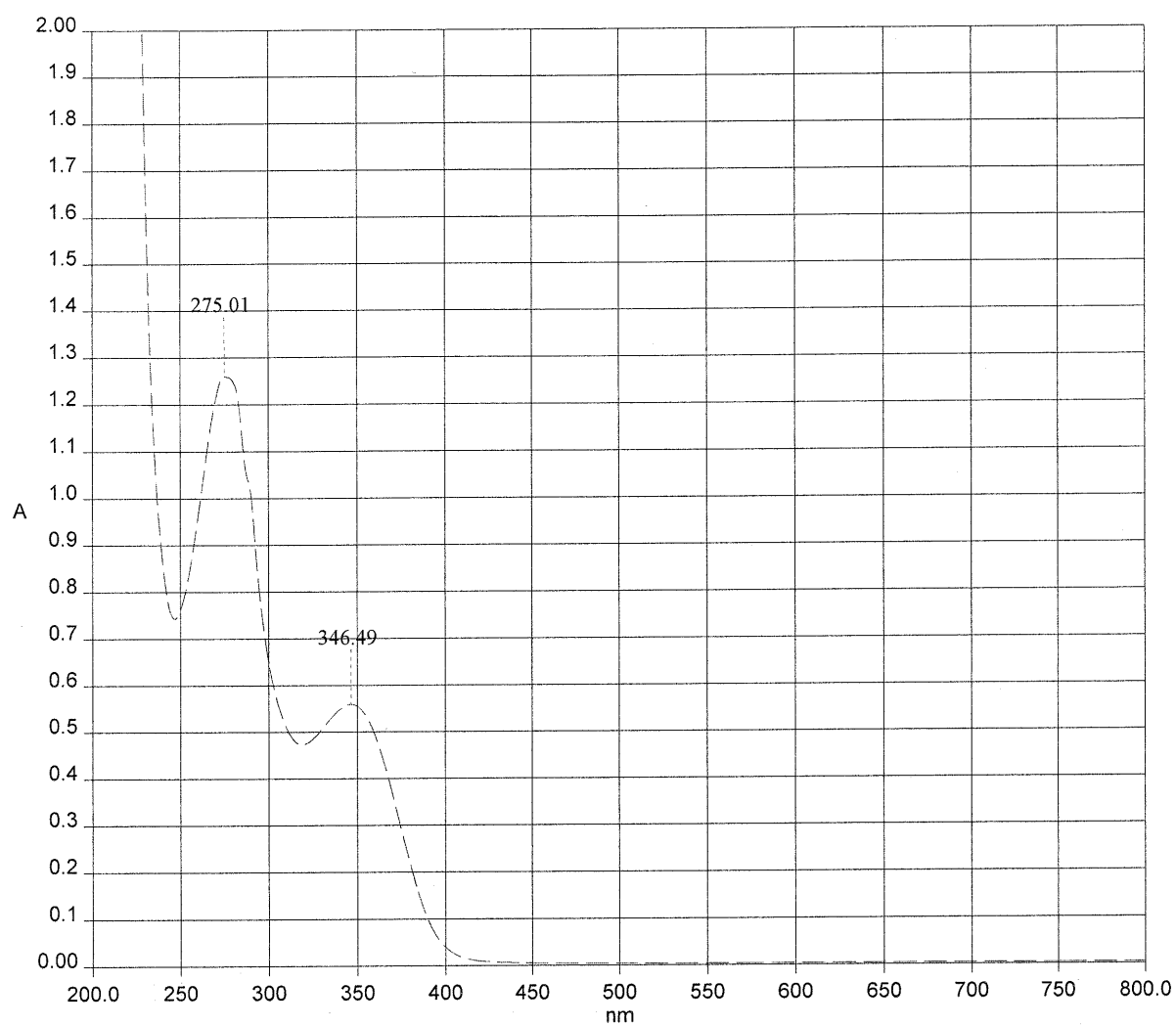
*** Mass Analysis for mass 640.2019820

1	31	31	5	9	1	640.2013987	18.5	5.833e-04
2	33	33	2	10	1	640.2027414	18.0	7.594e-04
3	33	30	5	9	0	640.2038040	21.5	1.822e-03
4	34	29	6	6	1	640.2040788	23.0	2.097e-03
5	35	32	2	10	0	640.2051467	21.0	3.165e-03
6	36	31	3	7	1	640.2054215	22.5	3.439e-03
7	40	26	5	4	0	640.1979308	30.5	4.051e-03
8	36	28	6	6	0	640.2064841	26.0	4.502e-03
9	37	27	7	3	1	640.2067589	27.5	4.777e-03
10	40	29	2	5	1	640.1968681	27.0	5.114e-03

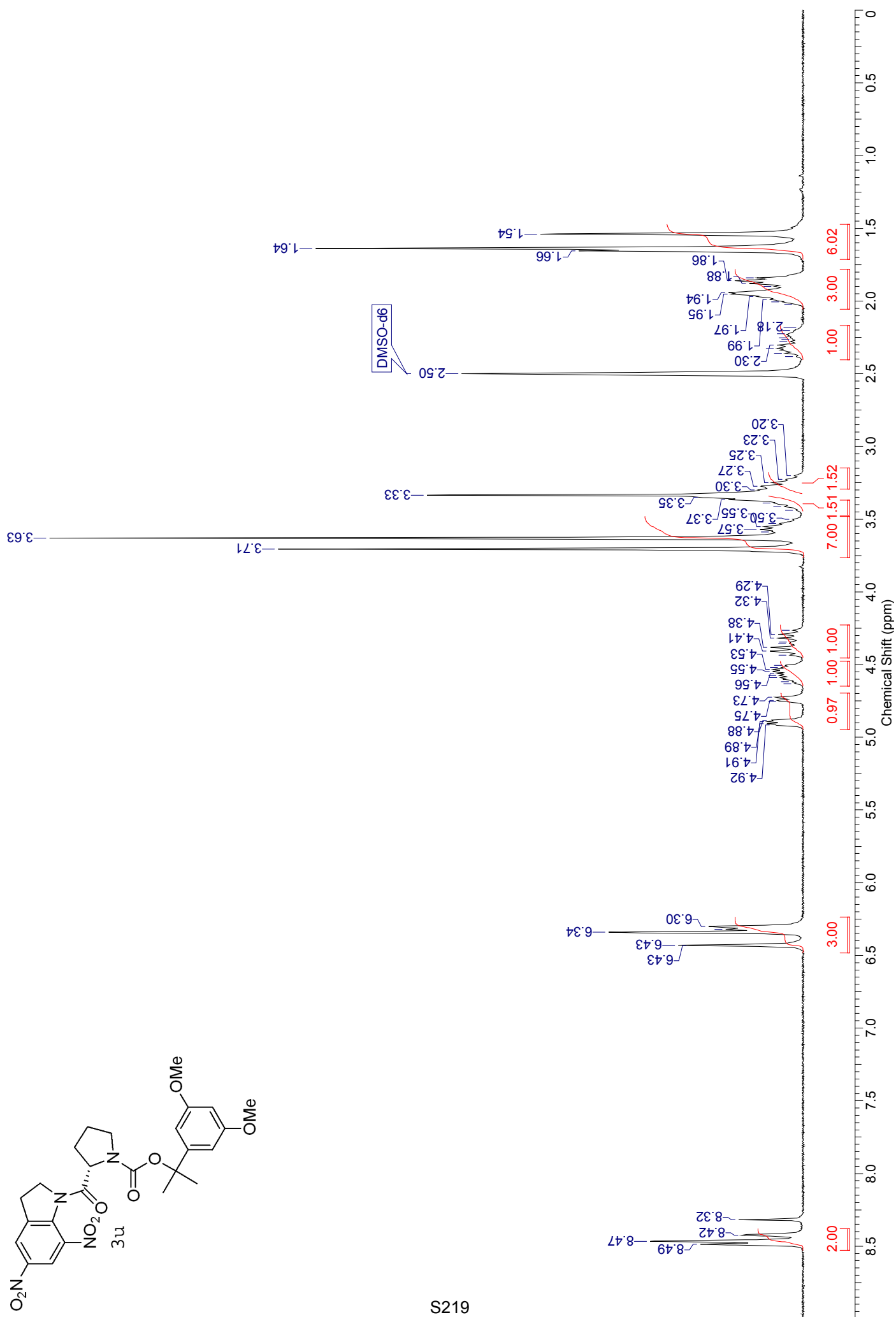
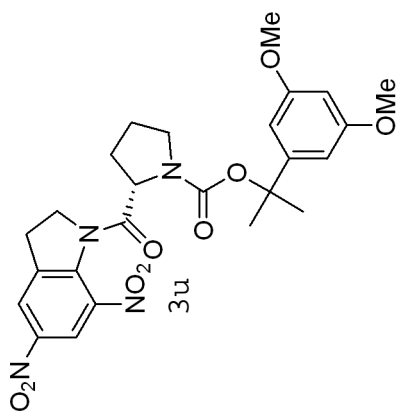


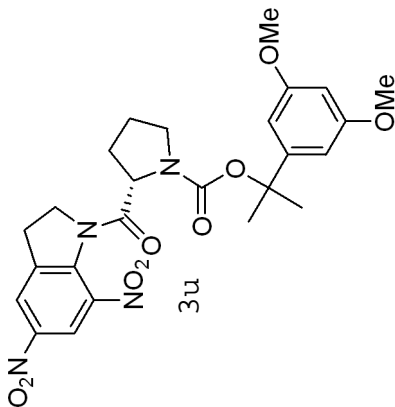
Date: 23.04.2008

Time: 10:42:18



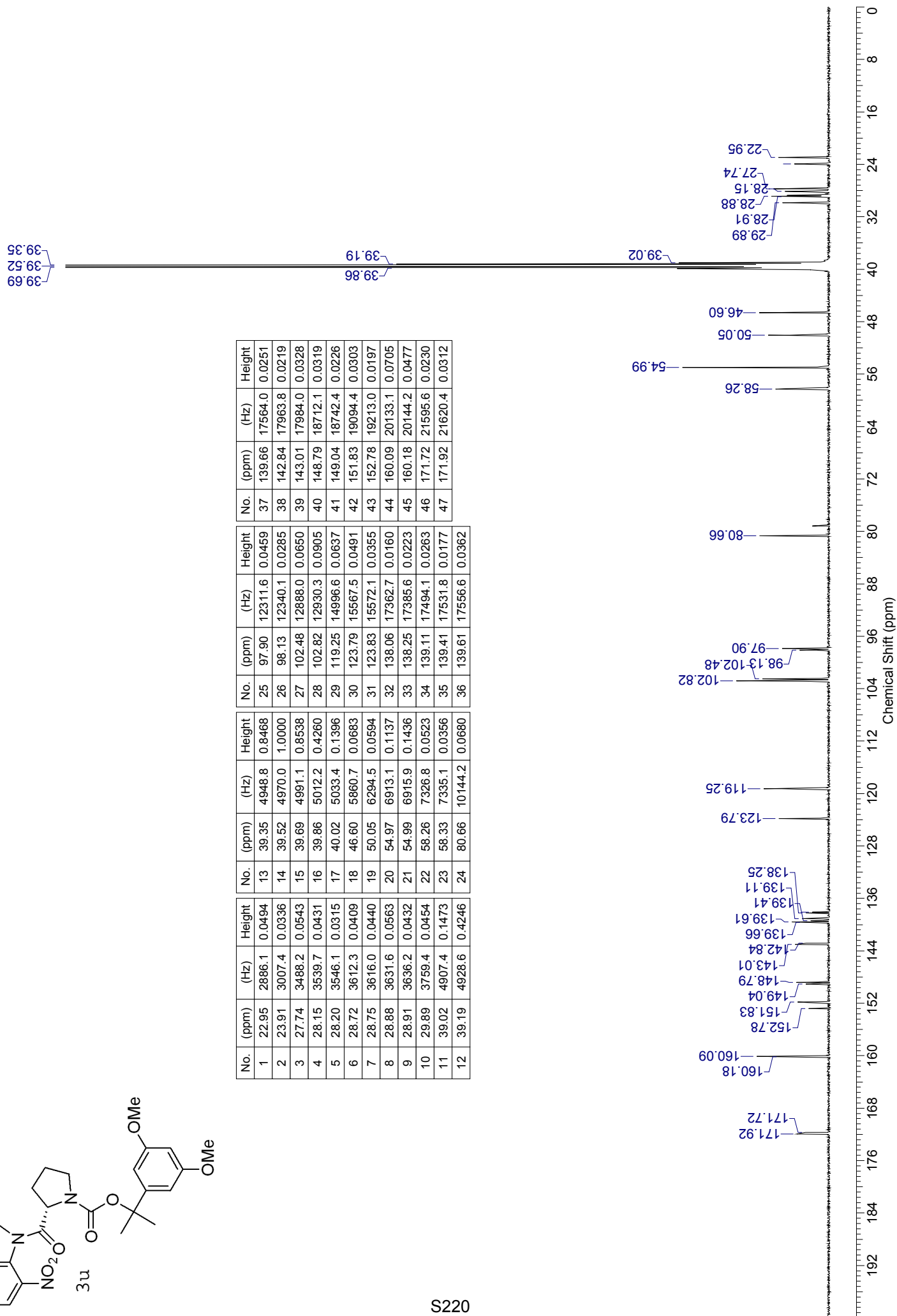
----- JLD147.SP - 23.04.2008 - in MeCN





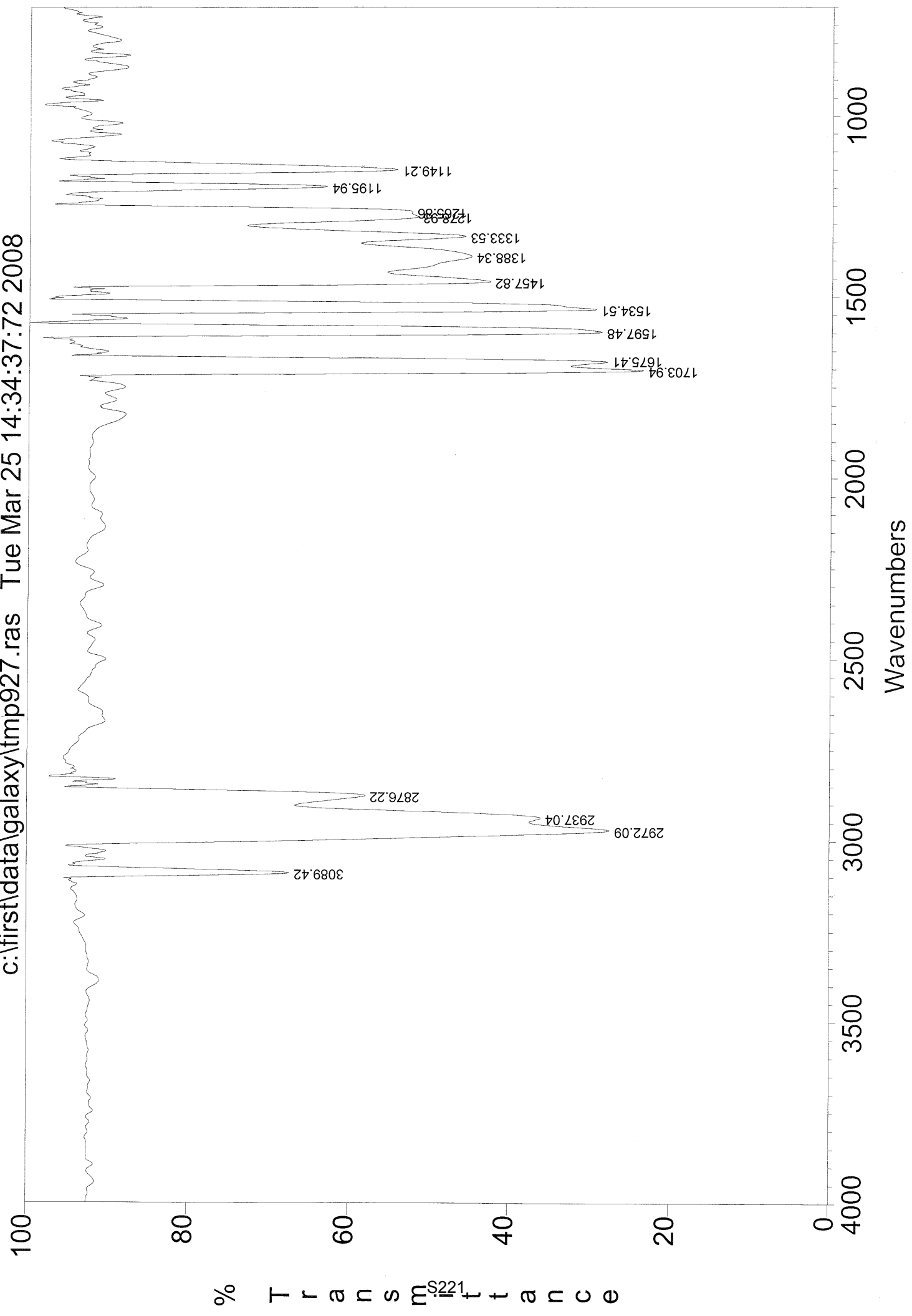
3u

No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	22.95	2886.1	0.0494	13	39.35	4948.8	0.8468	25	97.90	12311.6	0.0459
2	23.91	3007.4	0.0336	14	39.52	4970.0	1.0000	26	98.13	12340.1	0.0285
3	27.74	3488.2	0.0543	15	39.69	4991.1	0.8538	27	102.48	12888.0	0.0650
4	28.15	3539.7	0.0431	16	39.86	5012.2	0.4260	28	102.82	12930.3	0.0905
5	28.20	3546.1	0.0315	17	40.02	5033.4	0.1396	29	119.25	14996.6	0.0637
6	28.72	3612.3	0.0409	18	46.60	5860.7	0.0683	30	123.79	15567.5	0.0491
7	28.75	3616.0	0.0440	19	50.05	6294.5	0.0594	31	123.83	15572.1	0.0355
8	28.88	3631.6	0.0563	20	54.97	6913.1	0.1137	32	138.06	17362.7	0.0160
9	28.91	3636.2	0.0432	21	54.99	6915.9	0.1436	33	138.25	17385.6	0.0223
10	29.89	3759.4	0.0454	22	58.26	7326.8	0.0523	34	139.11	17494.1	0.0263
11	39.02	4907.4	0.1473	23	58.33	7335.1	0.0356	35	139.41	17531.8	0.0177
12	39.19	4928.6	0.4246	24	80.66	10144.2	0.0680	36	139.61	17556.6	0.0362



DATA

c:\first\data\galaxy\tmp927.ras Tue Mar 25 14:34:37:72 2008



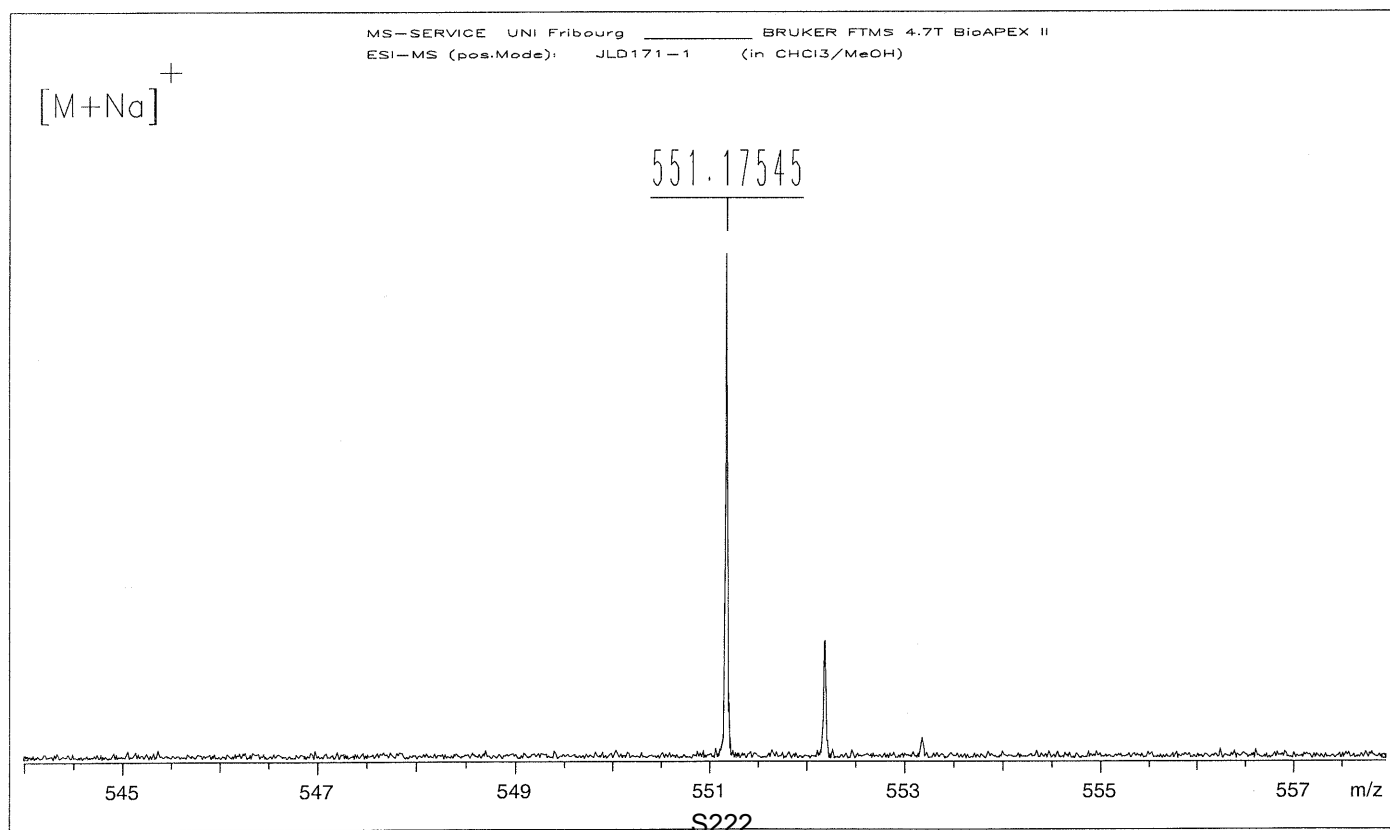
ESI-MS: JLD171-1

XMASS Mass Analysis for /Data/UNI_FR/DEBI3334_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 551.1754520

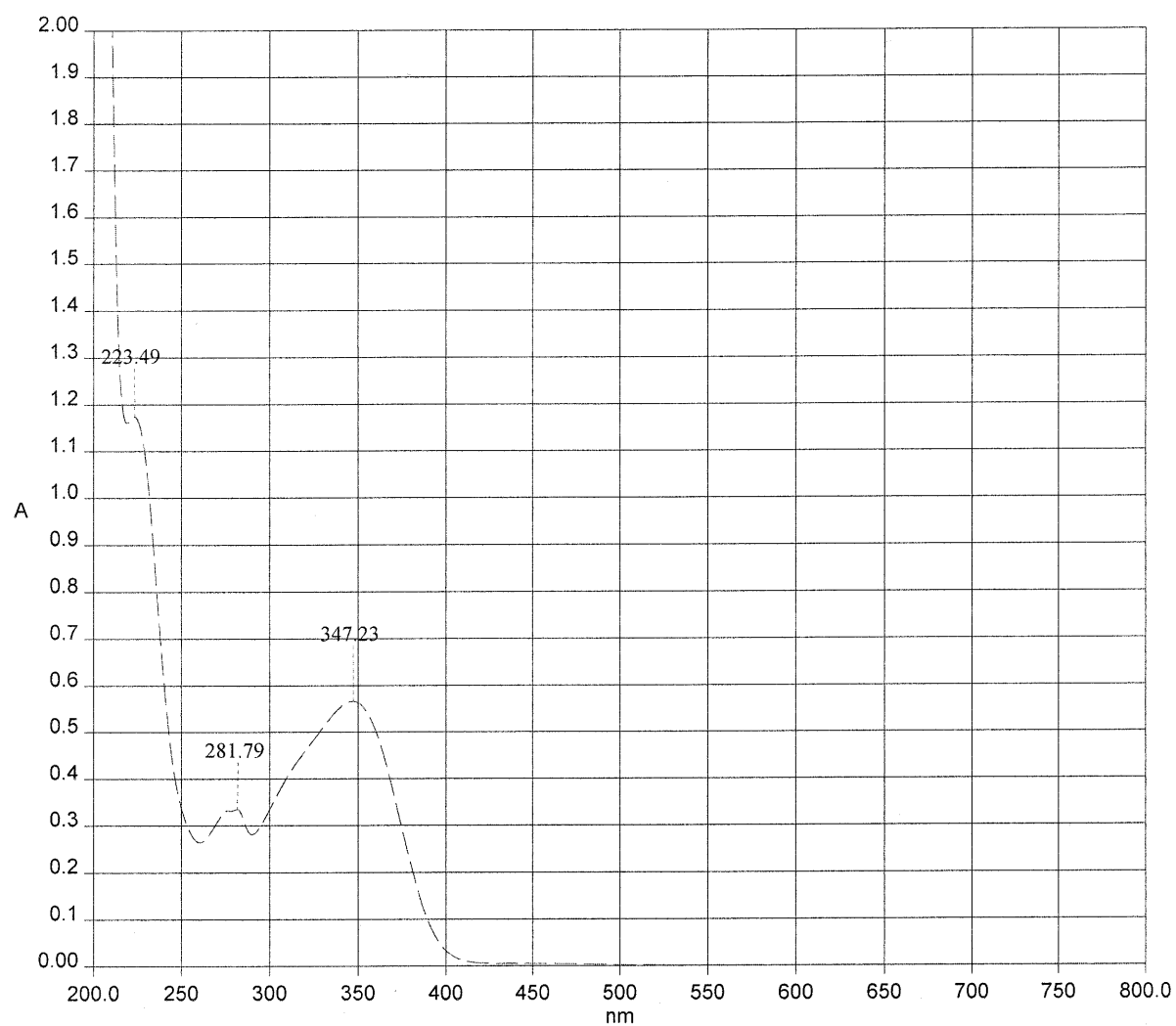
Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 551.1754520								
1	25	28	4	9	1	551.1748496	13.5	6.024e-04
2	24	29	3	12	0	551.1745748	12.0	8.772e-04
3	27	27	4	9	0	551.1772549	16.5	1.803e-03
4	28	26	5	6	1	551.1775297	18.0	2.078e-03
5	22	27	6	11	0	551.1732322	12.5	2.220e-03
6	22	30	3	12	1	551.1721695	9.0	3.282e-03
7	30	28	2	7	1	551.1788724	17.5	3.420e-03
8	30	25	5	6	0	551.1799350	21.0	4.483e-03
9	20	28	6	11	1	551.1708269	9.5	4.625e-03
10	21	30	5	11	1	551.1834029	9.0	7.951e-03

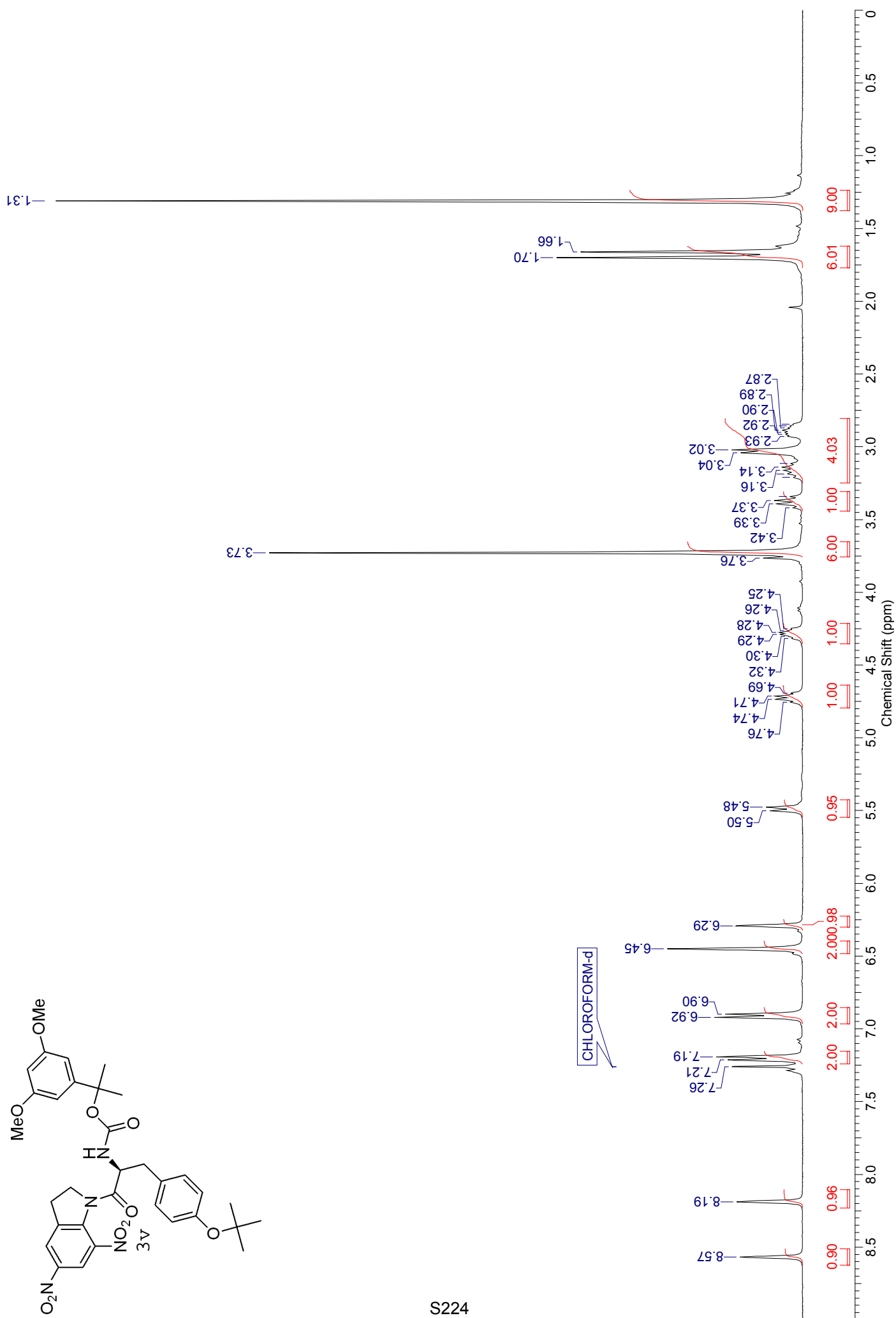
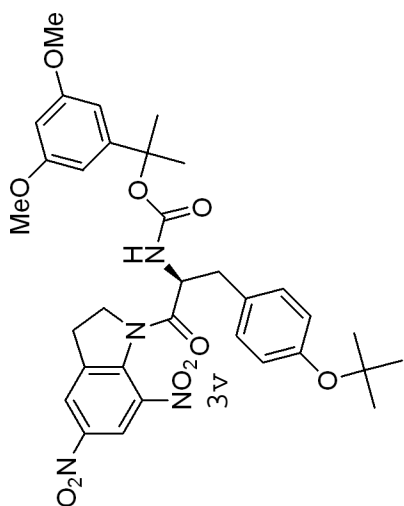


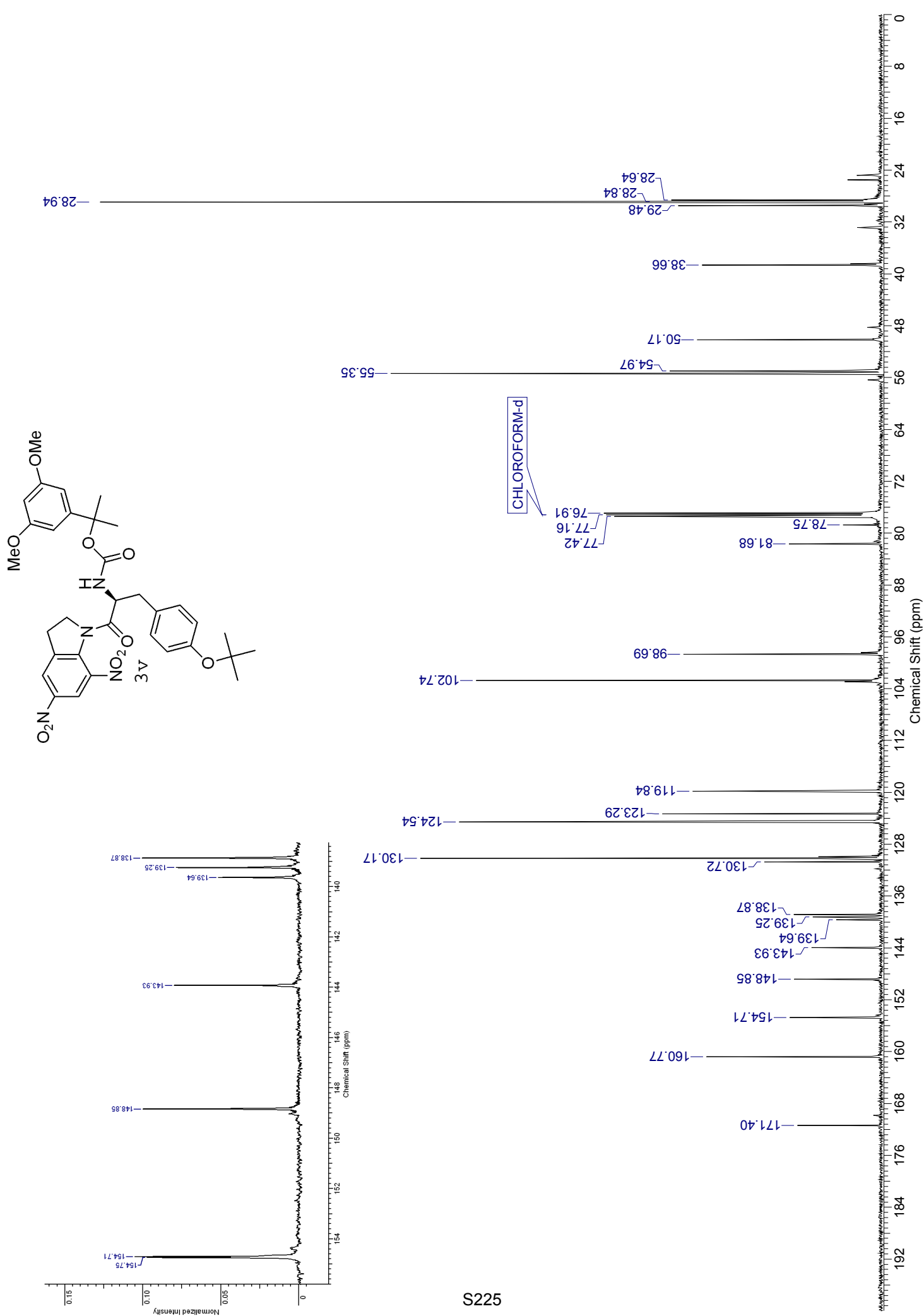
Date: 21.04.2008

Time: 16:46:43



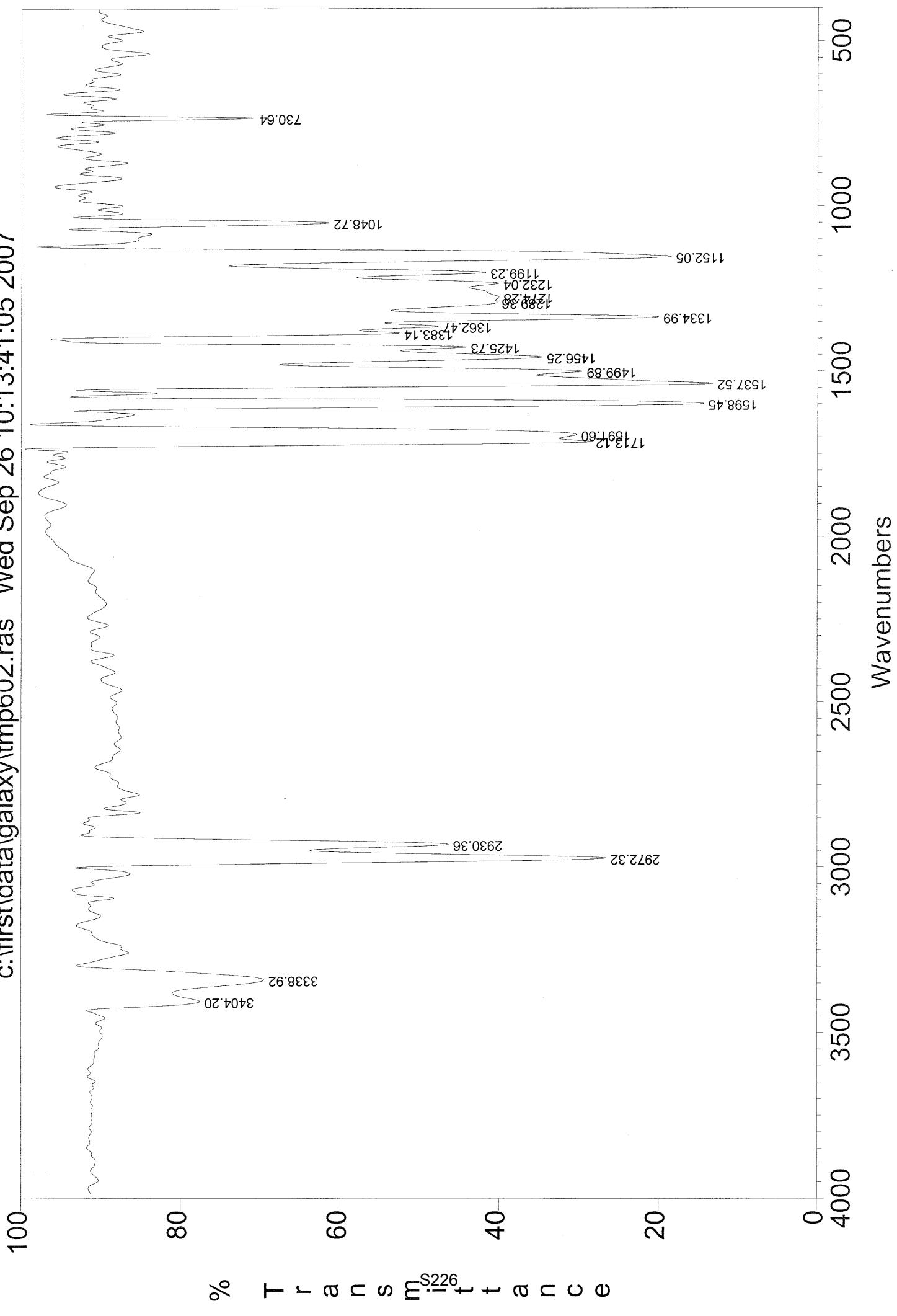
----- JLD171.SP - 21.04.2008 - 5.01×10^{-5} M in MeCN





900152

c:\first\data\galaxy\tmp602.ras Wed Sep 26 10:13:41:05 2007



ESI-MS: JLD152-1

XMASS Mass Analysis for /Data/UNI_FR/DEBI2865_ESI/10/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

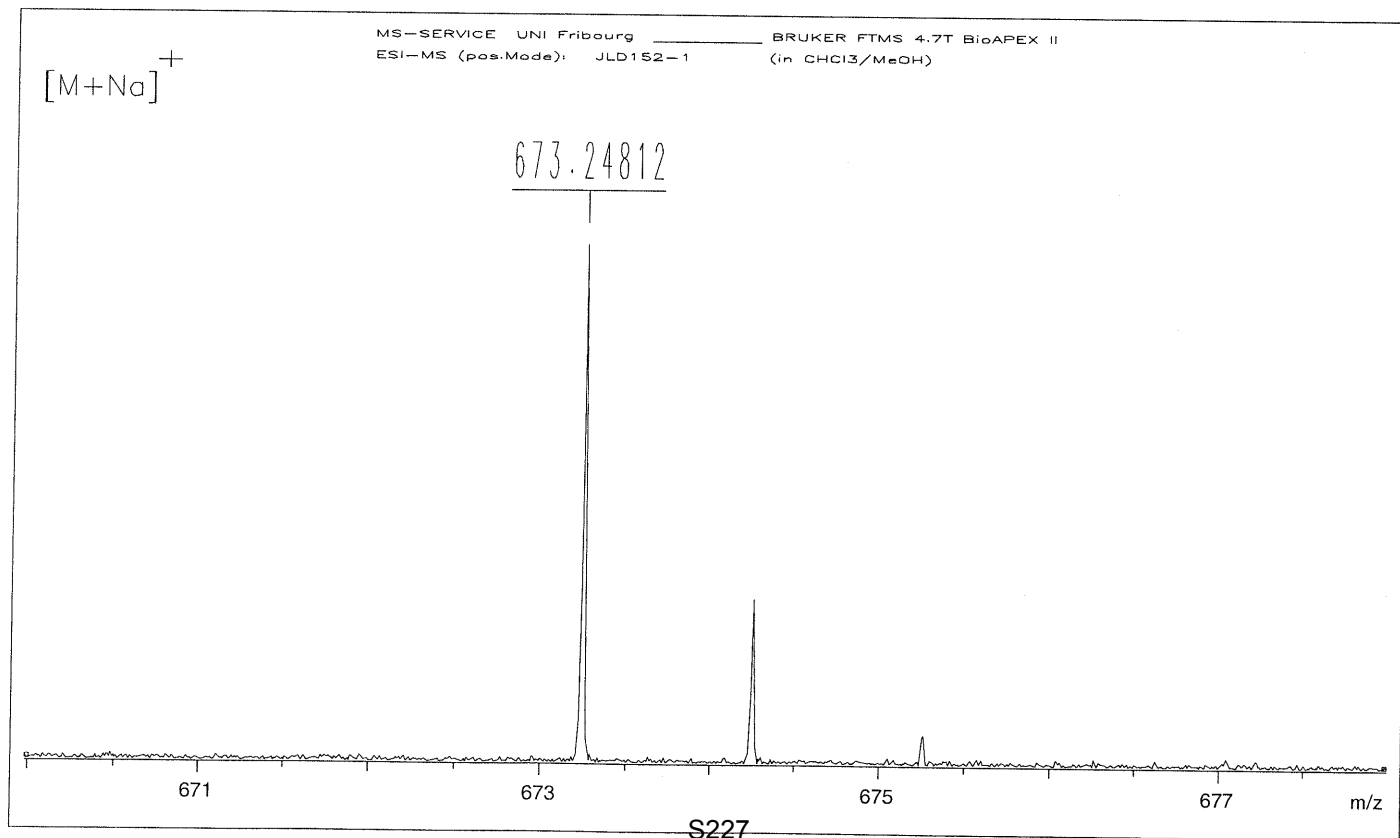
Ion mass = 673.2481210

Charge = +1

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

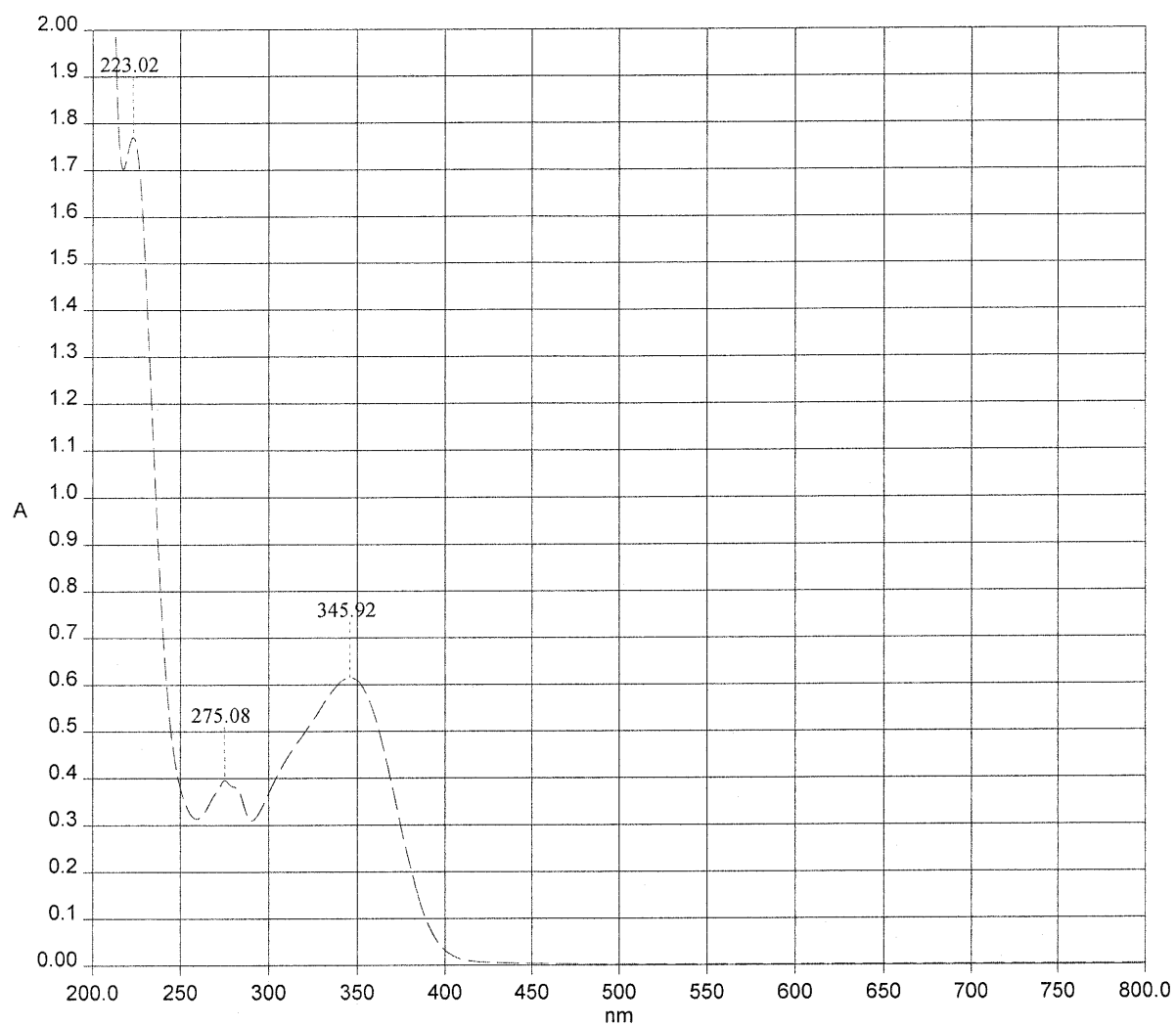
*** Mass Analysis for mass 673.2481210

1	33	38	4	10	1	673.2480146	16.5	1.064e-04
2	33	35	7	9	0	673.2490772	20.0	9.562e-04
3	35	40	1	11	1	673.2493572	16.0	1.236e-03
4	31	36	7	9	1	673.2466719	17.0	1.449e-03
5	30	37	6	12	0	673.2463971	15.5	1.724e-03
6	35	37	4	10	0	673.2504198	19.5	2.299e-03
7	36	36	5	7	1	673.2506946	21.0	2.574e-03
8	37	39	1	11	0	673.2517625	19.0	3.642e-03
9	38	38	2	8	1	673.2520373	20.5	3.916e-03
10	28	38	6	12	1	673.2439918	12.5	4.129e-03

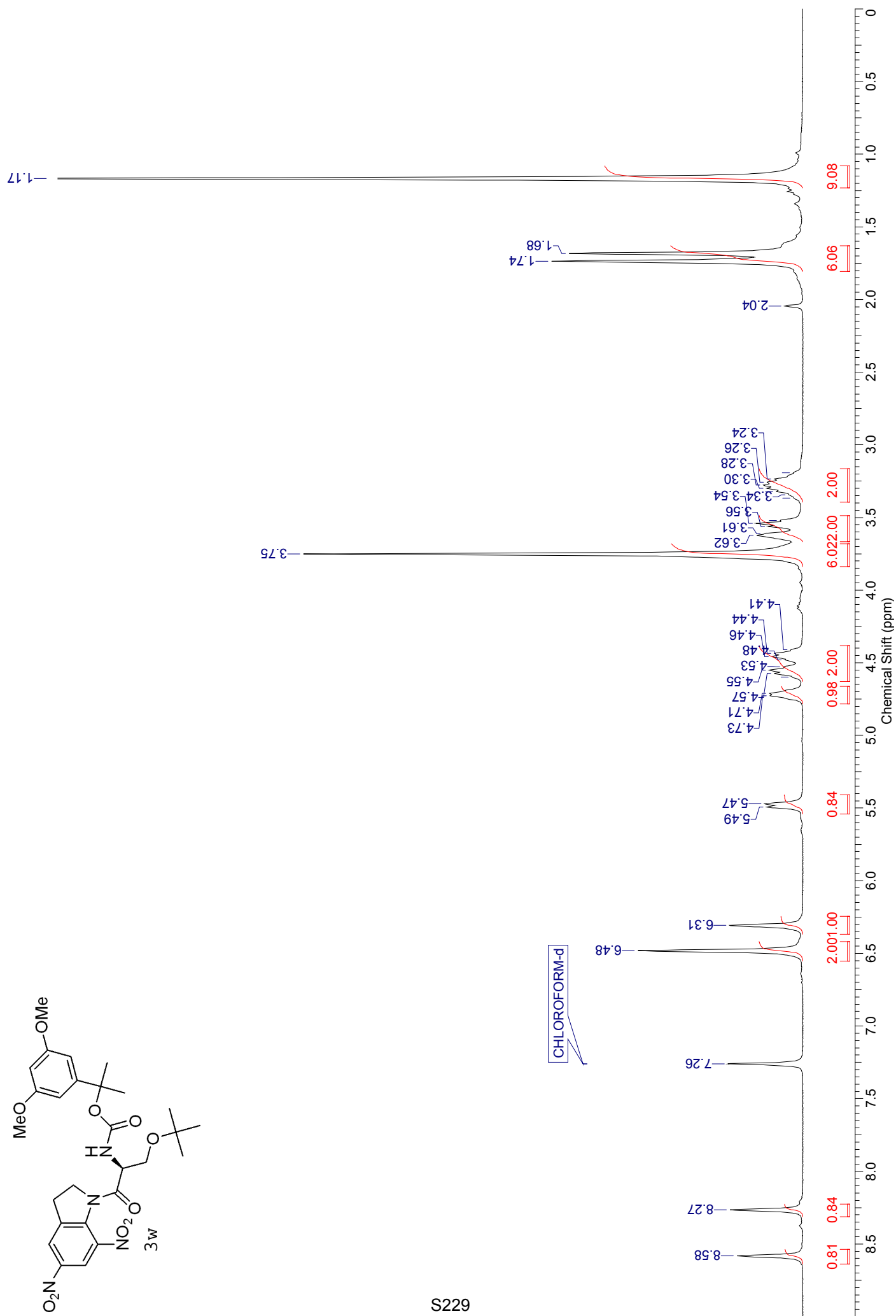
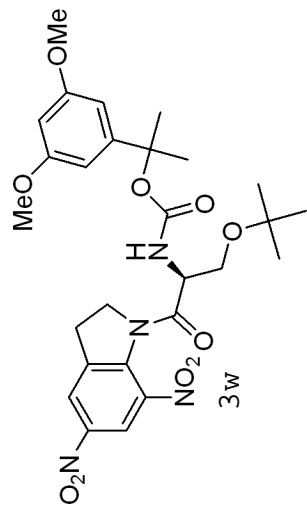


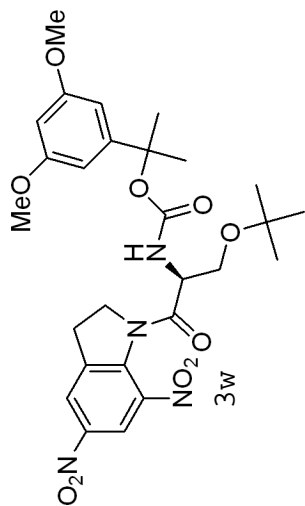
Date: 23.04.2008

Time: 11:02:33

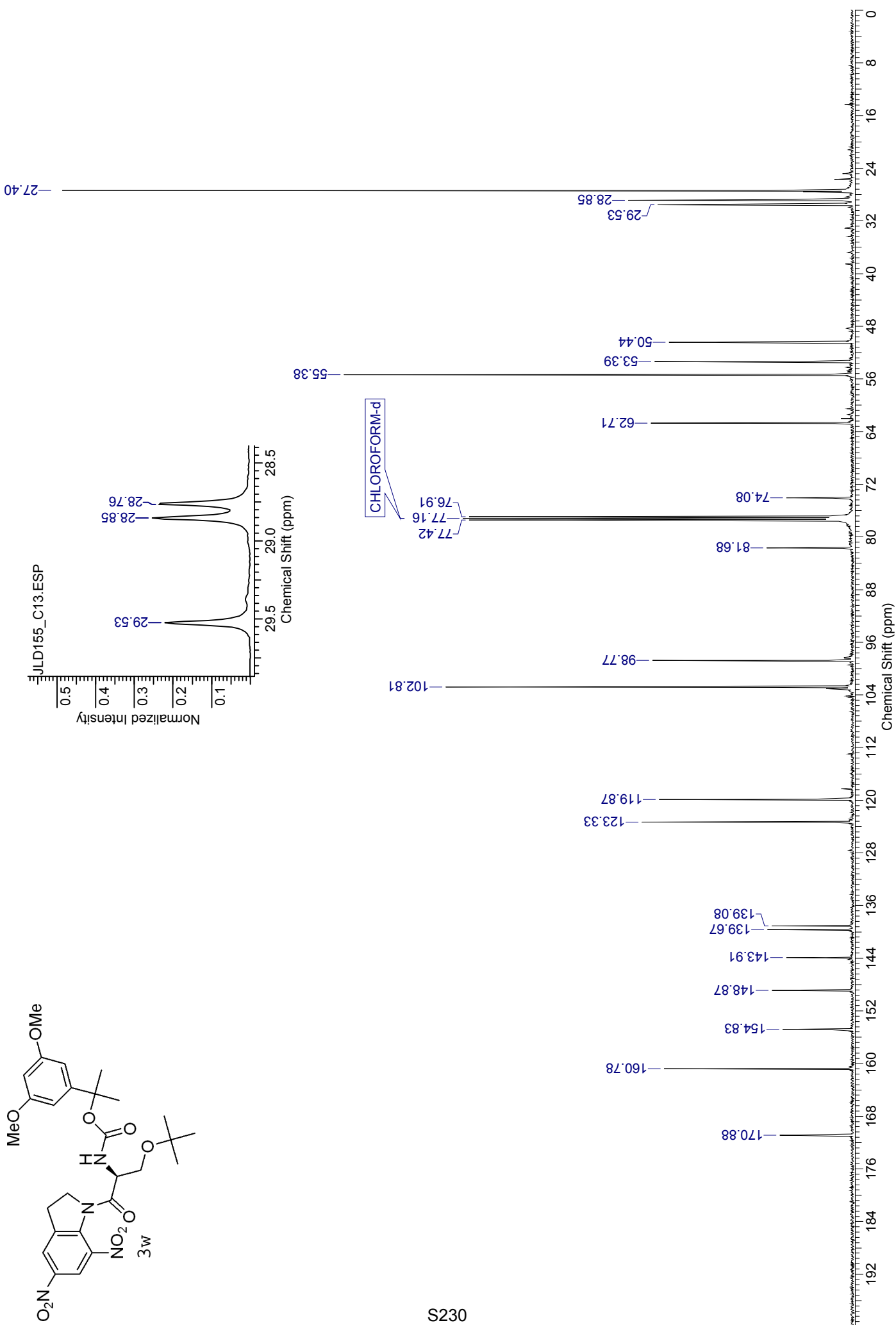


----- JLD152.SP - 23.04.2008 - $5.61 \cdot 10^{-5}$ M in MeCN



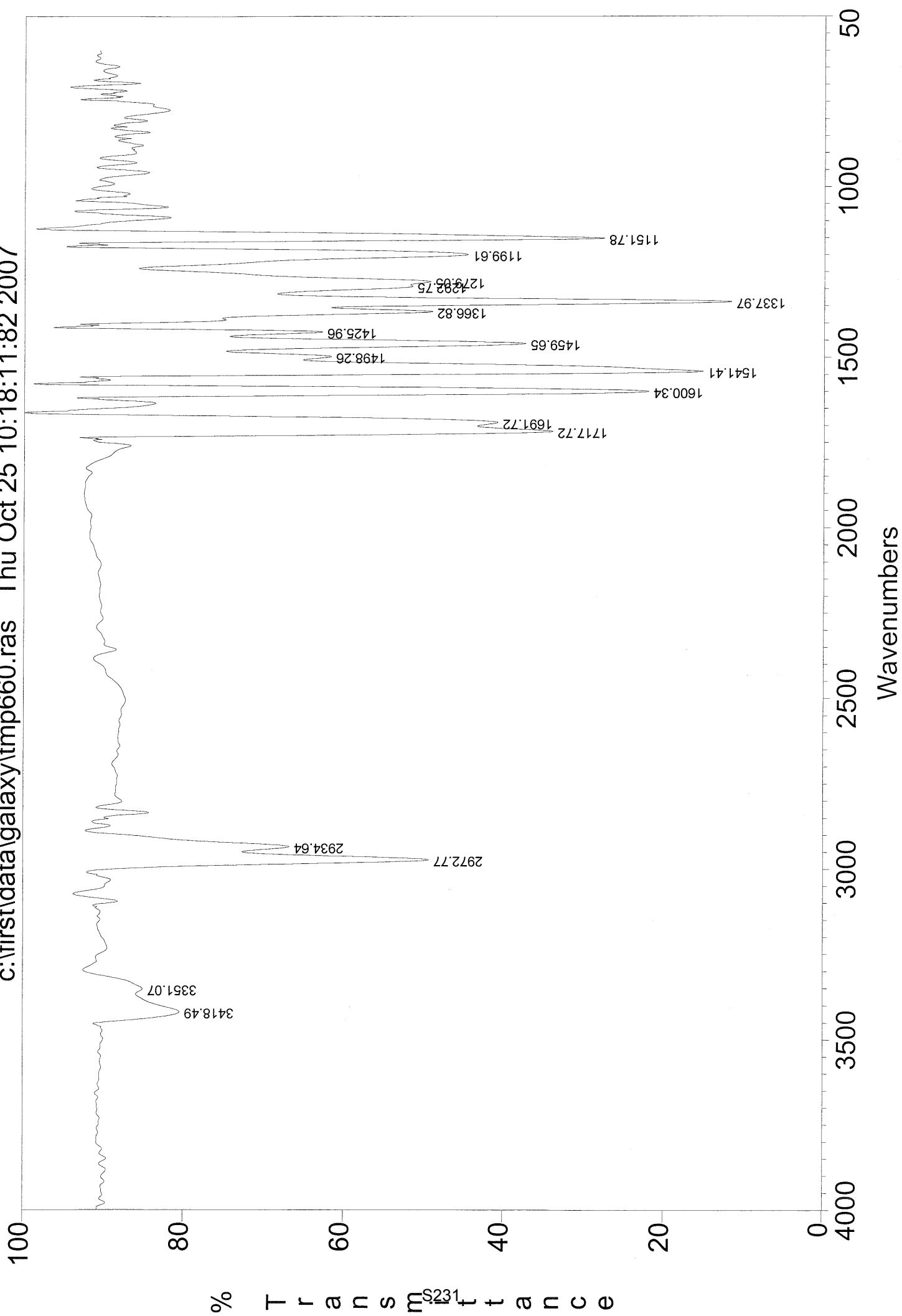


S230



96D 155

c:\first\data\galaxy\tmp660.ras Thu Oct 25 10:18:11:82 2007



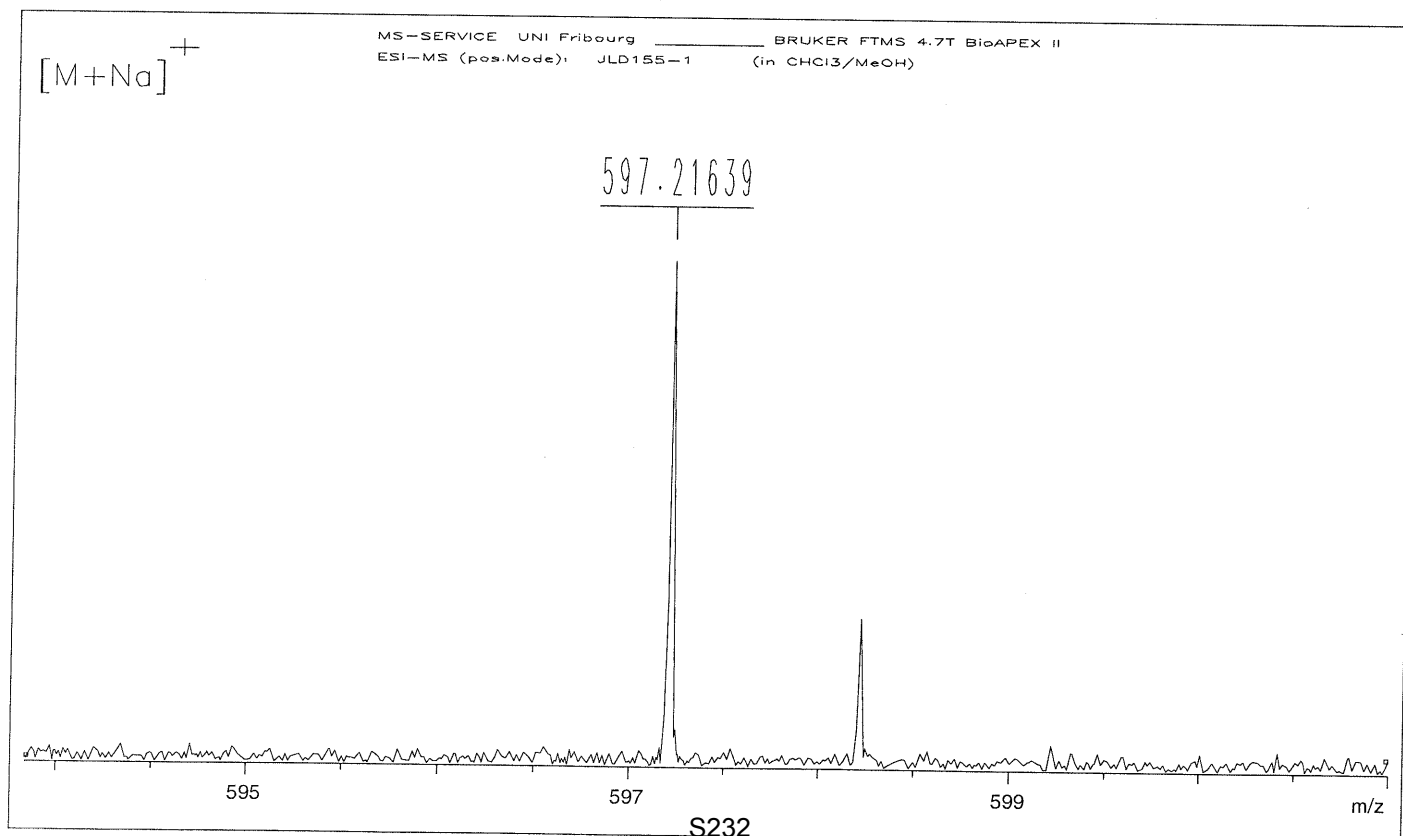
ESI-MS: JLD155-1

XMASS Mass Analysis for /Data/UNI_FR/DEBI2948_ESI/5/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 597.2163930

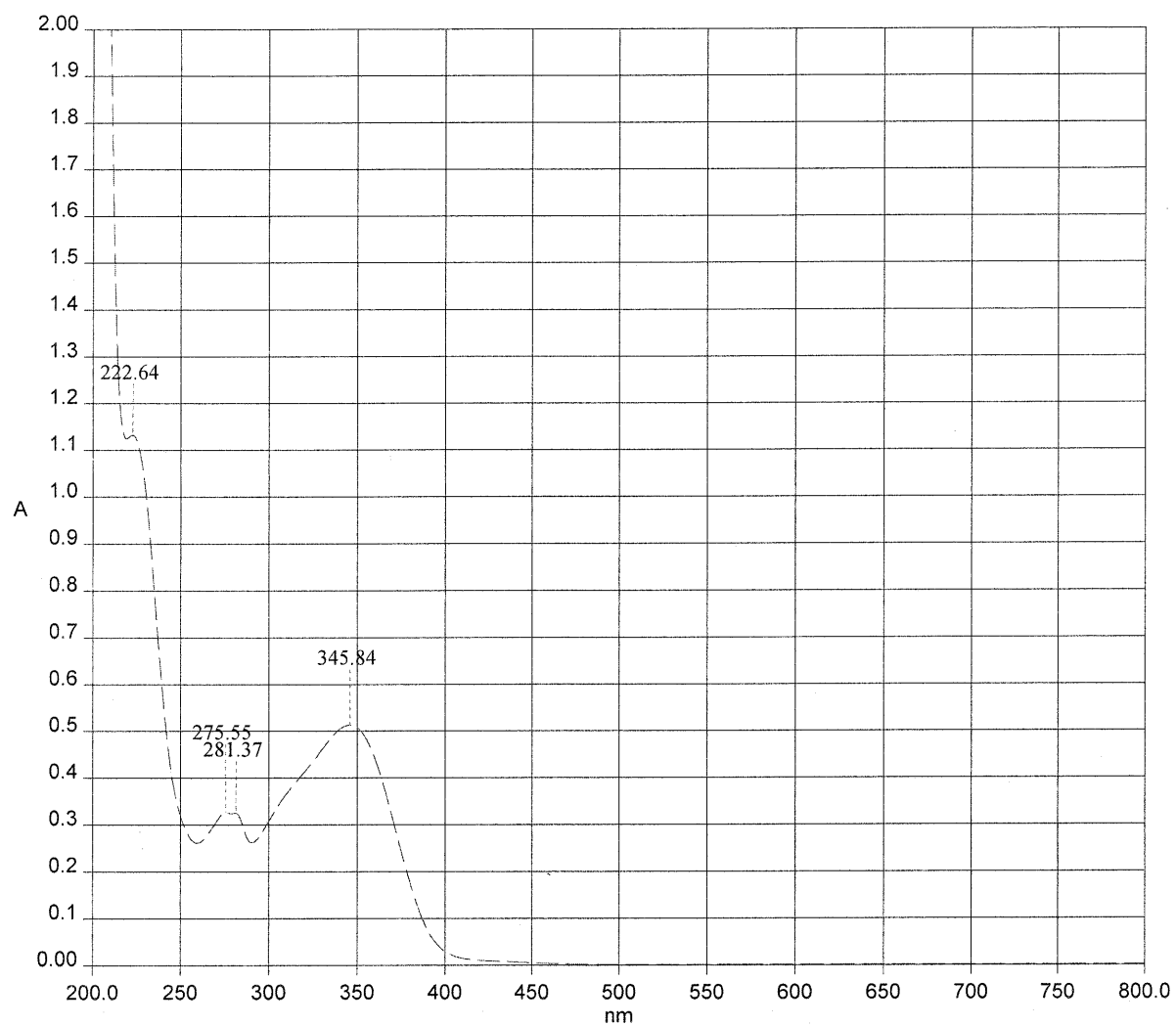
Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 597.2163930								
1	27	34	4	10	1	597.2167144	12.5	3.214e-04
2	24	33	6	12	0	597.2150970	11.5	1.296e-03
3	29	36	1	11	1	597.2180571	12.0	1.664e-03
4	38	31	1	6	0	597.2145892	24.0	1.804e-03
5	29	33	4	10	0	597.2191197	15.5	2.727e-03
6	30	32	5	7	1	597.2193945	17.0	3.001e-03
7	36	29	4	5	0	597.2132465	24.5	3.147e-03
8	22	34	6	12	1	597.2126917	8.5	3.701e-03
9	31	35	1	11	0	597.2204624	15.0	4.069e-03
10	36	32	1	6	1	597.2121839	21.0	4.209e-03

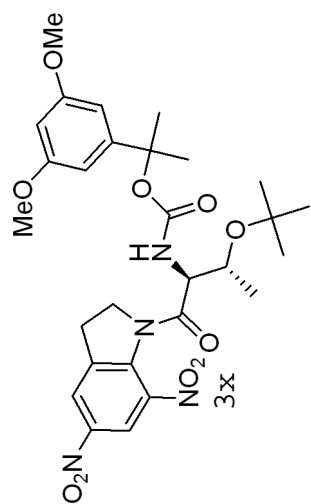


Date: 23.04.2008

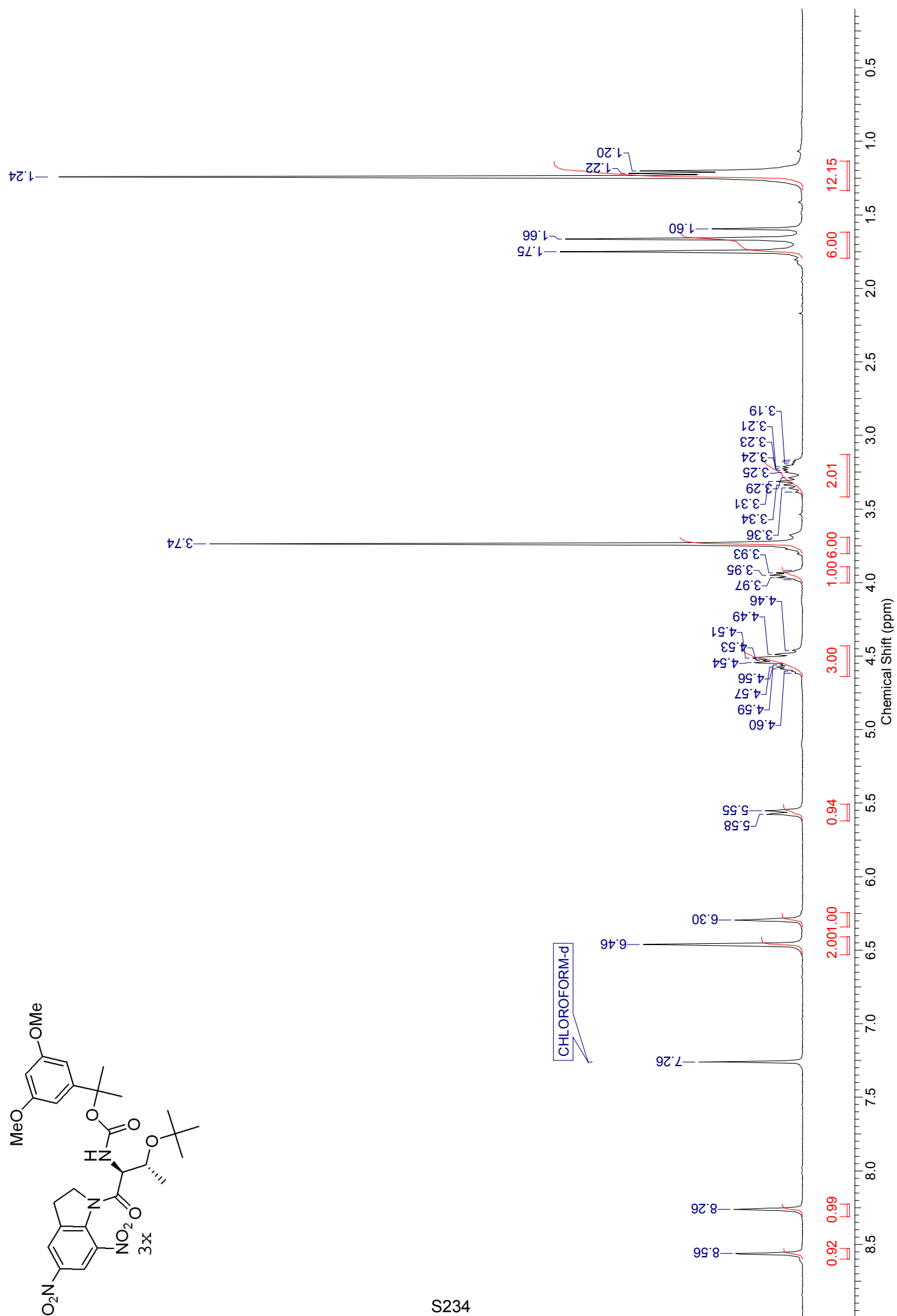
Time: 11:29:07

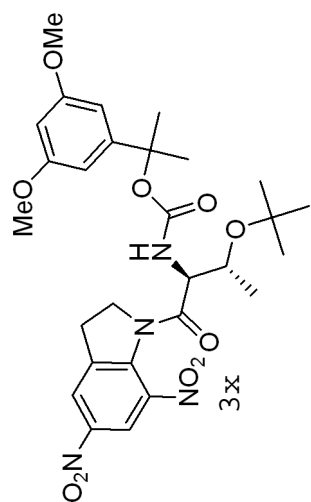


----- JLD155.SP - 23.04.2008 - $5.22 \cdot 10^{-5}$ M in MeCN



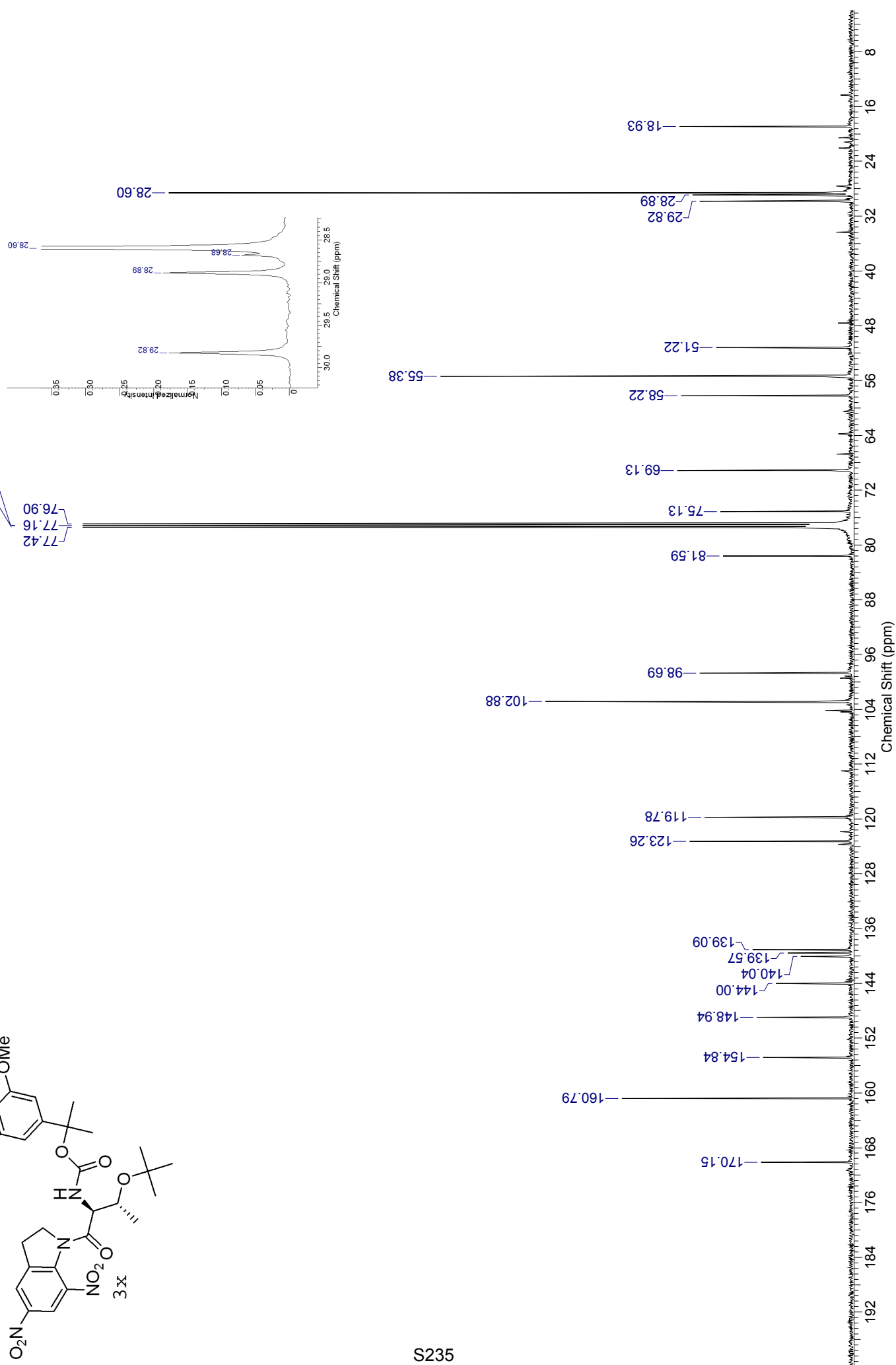
S234





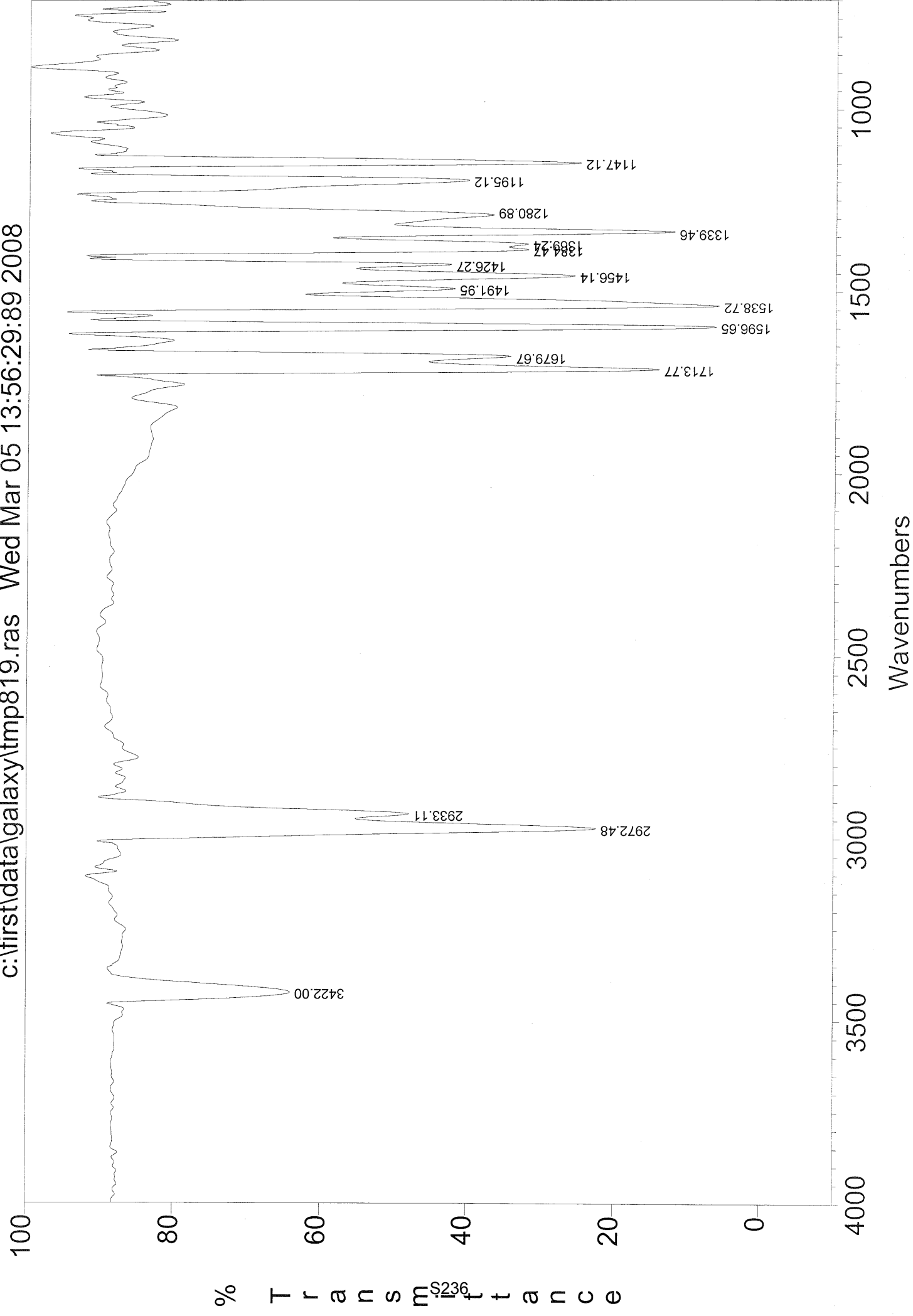
S235

CHLOROFORM-d



169

c:\first\data\galaxy\tmp819.ras Wed Mar 05 13:56:29:89 2008



ESI-MS: JLD169-2

XMASS Mass Analysis for /Data/UNI_FR/DEBI3216_ESI/5/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

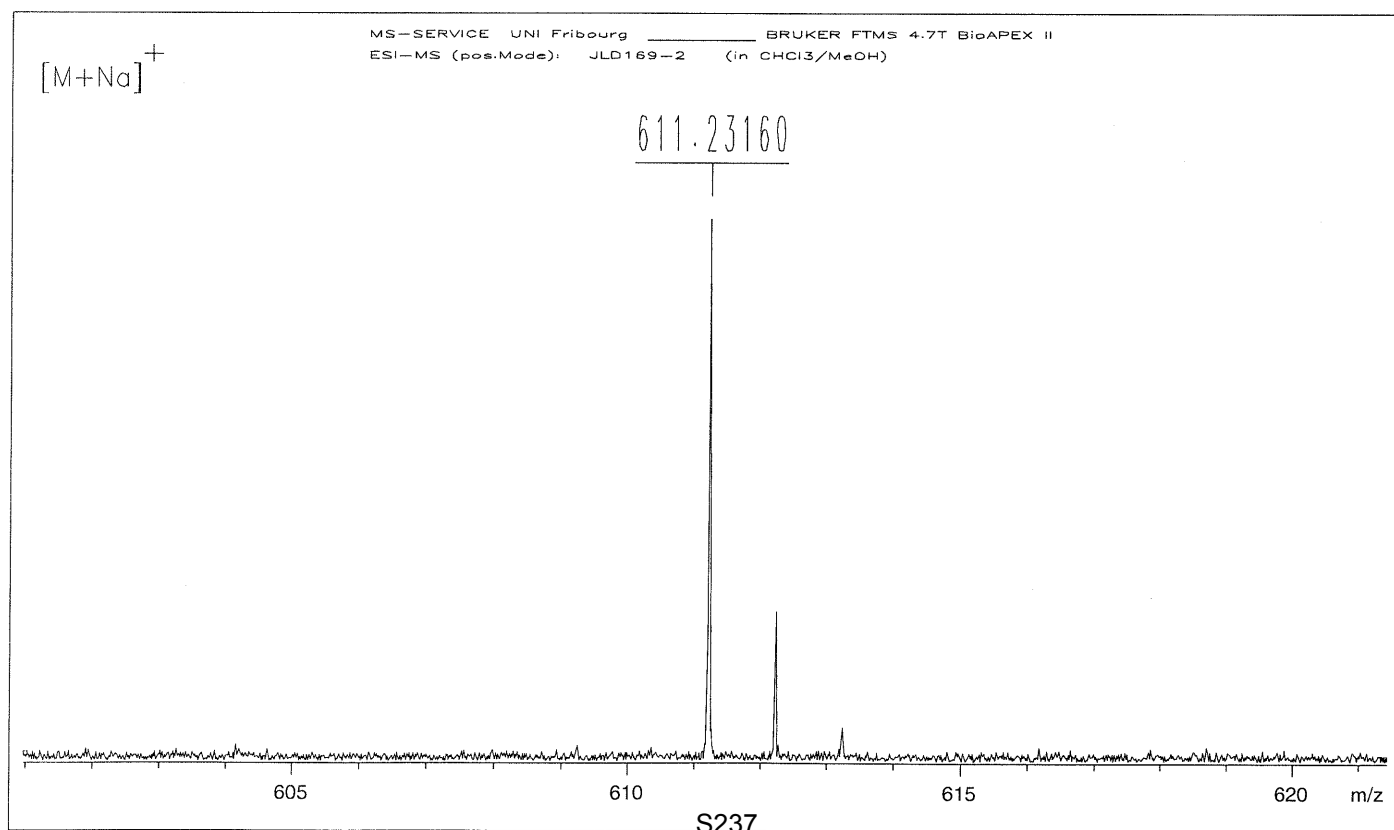
Ion mass = 611.2315980

Charge = +1

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

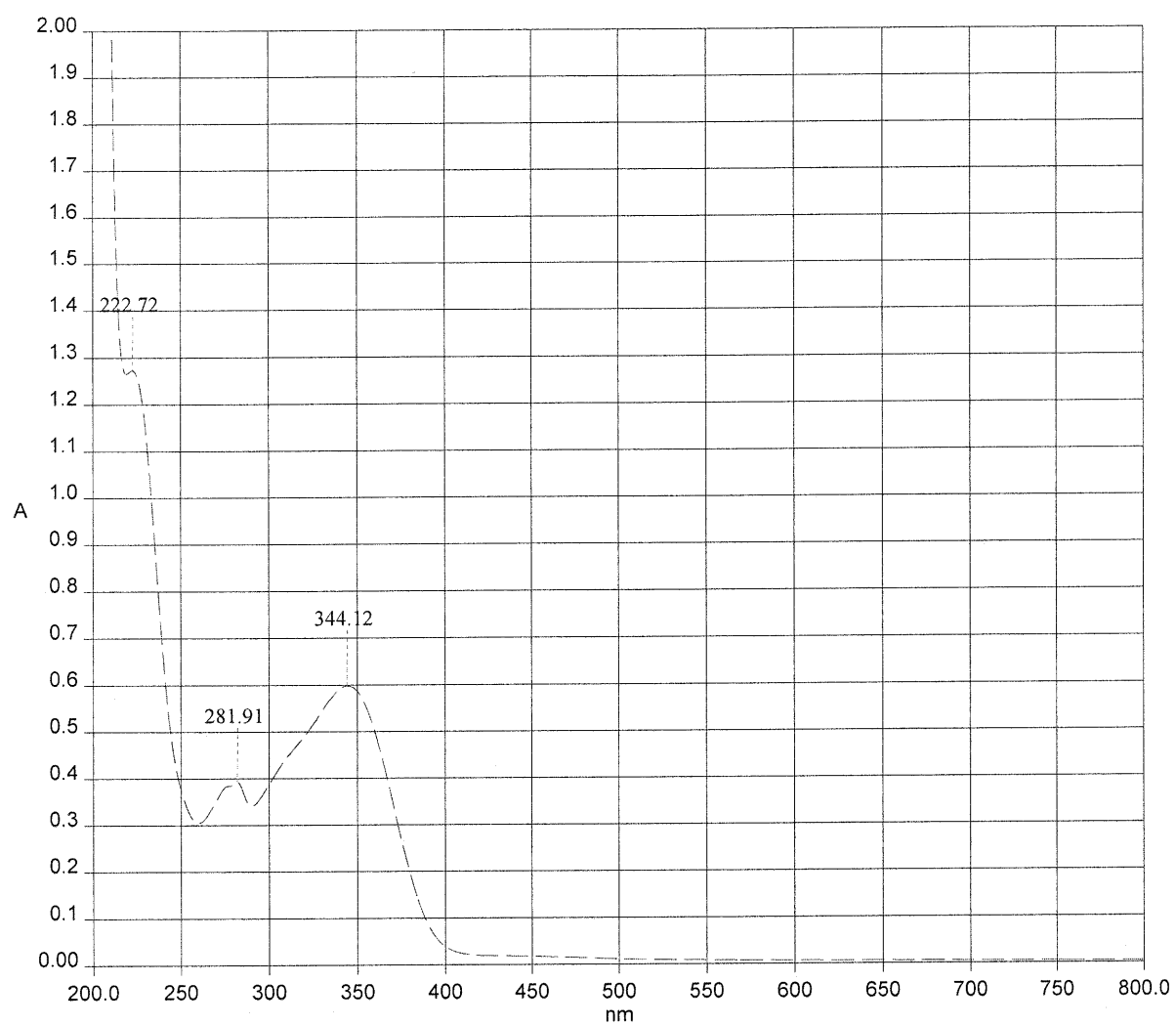
*** Mass Analysis for mass 611.2315980

1	28	36	4	10	1	611.2323645	12.5	7.665e-04
2	39	33	1	6	0	611.2302392	24.0	1.359e-03
3	30	38	1	11	1	611.2337072	12.0	2.109e-03
4	30	35	4	10	0	611.2347698	15.5	3.172e-03
5	31	34	5	7	1	611.2350446	17.0	3.447e-03
6	37	34	1	6	1	611.2278339	21.0	3.764e-03
7	32	37	1	11	0	611.2361125	15.0	4.514e-03
8	33	36	2	8	1	611.2363872	16.5	4.789e-03
9	34	33	3	8	0	611.2262165	20.0	5.382e-03
10	33	33	5	7	0	611.2374499	20.0	5.852e-03

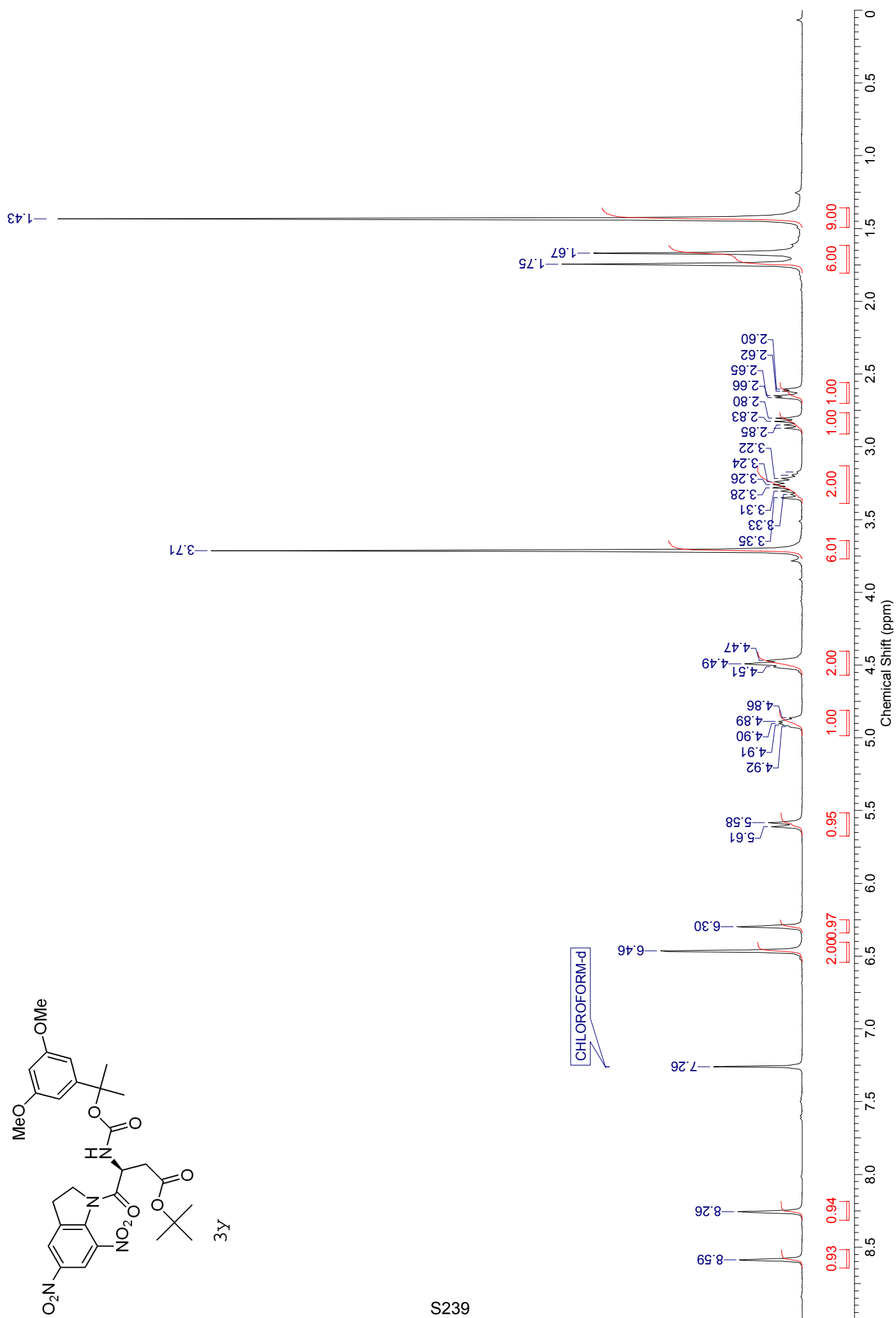
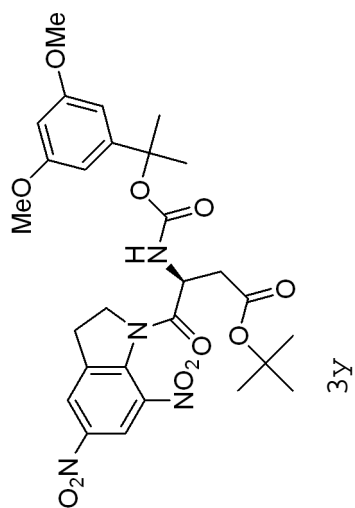


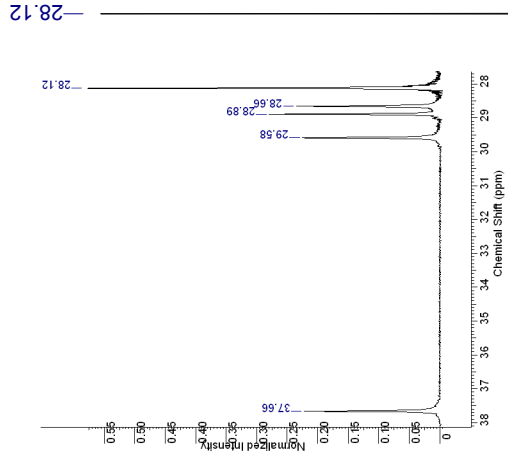
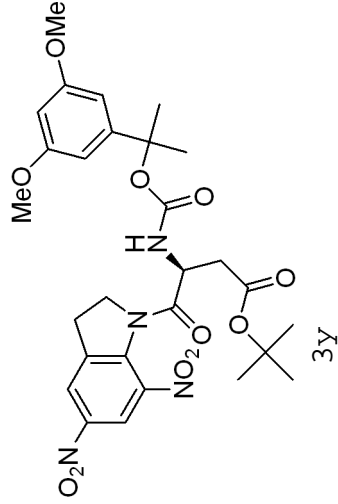
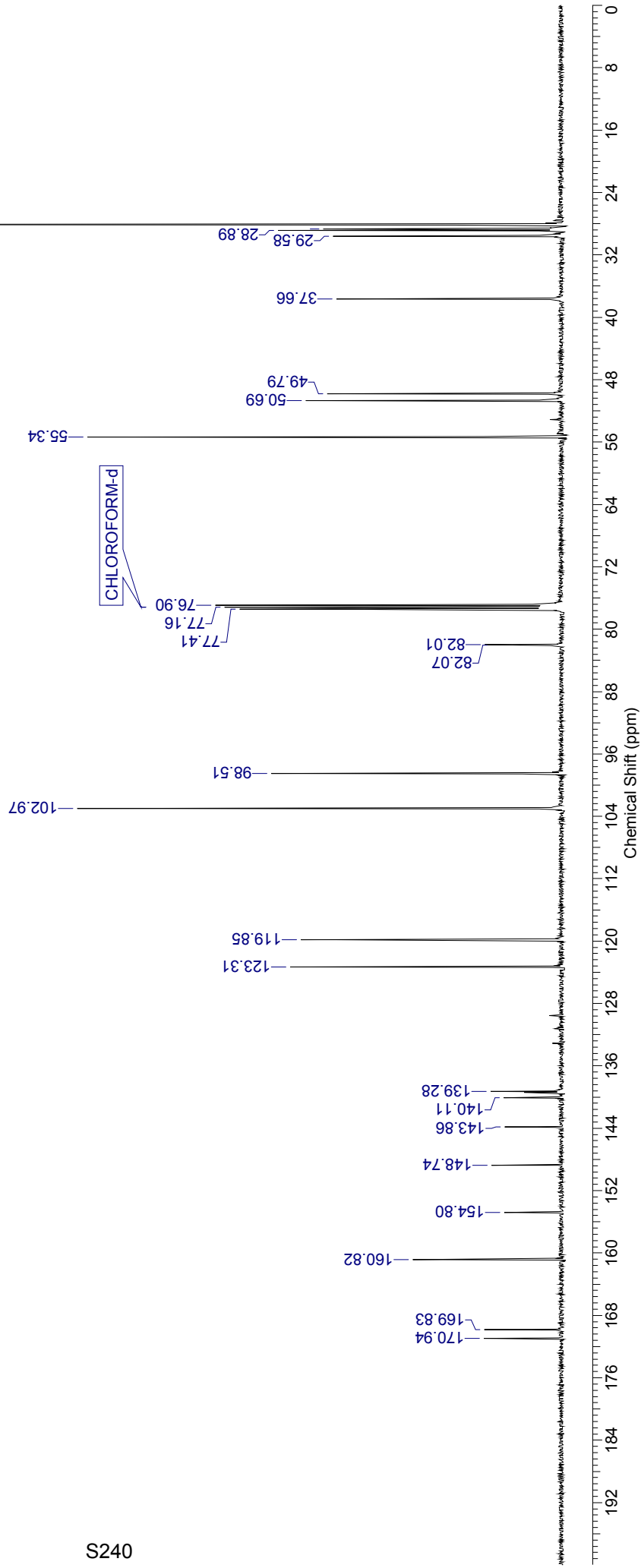
Date: 21.04.2008

Time: 17:13:23



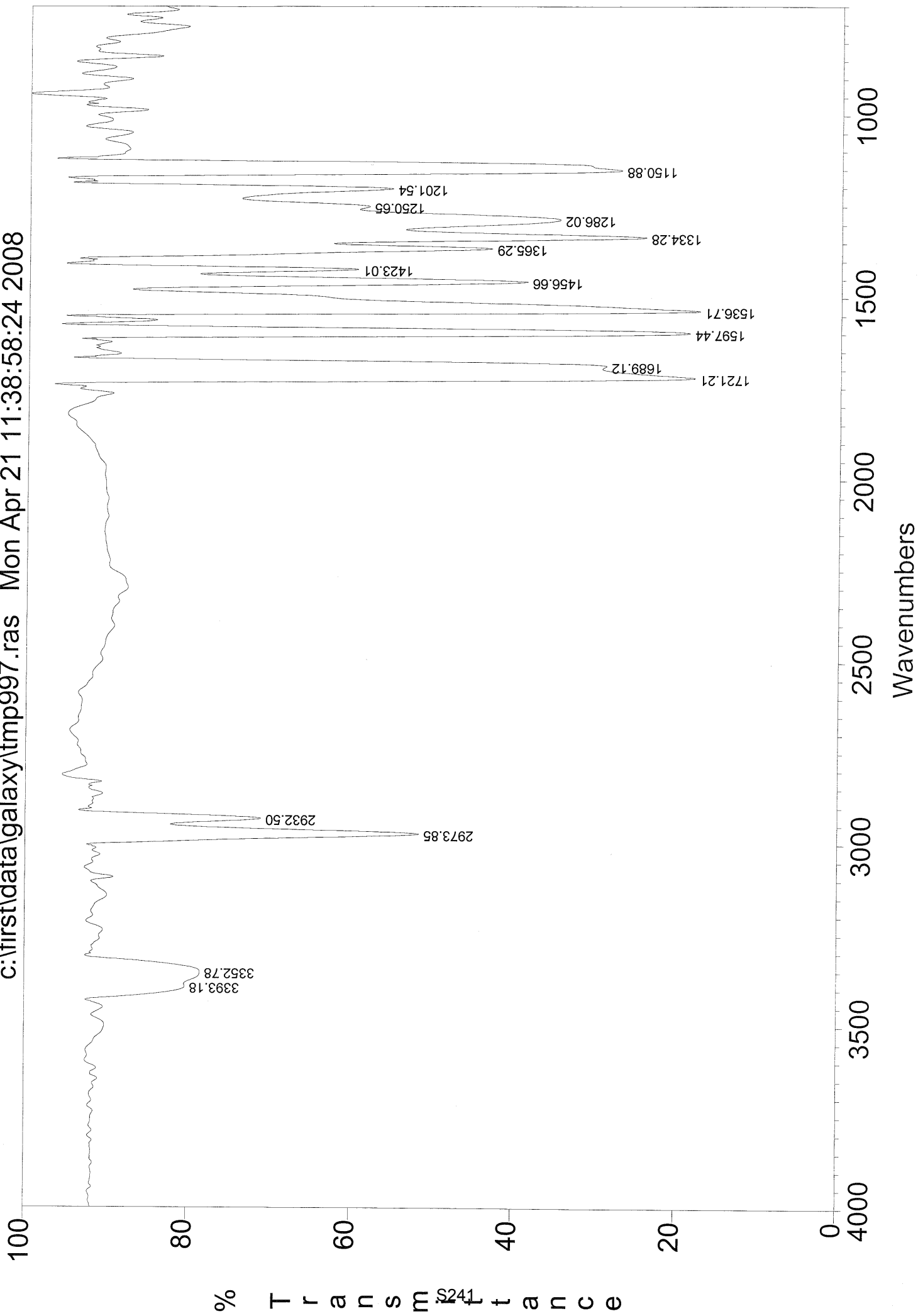
----- JLD169.SP - 21.04.2008 - 5.23×10^{-5} M in MeCN





5-47-07

c:\first\data\galaxy\tmp997.ras Mon Apr 21 11:38:58:24 2008





FTMS 4.7T BioAPEX II MS-Service UNI-Fribourg

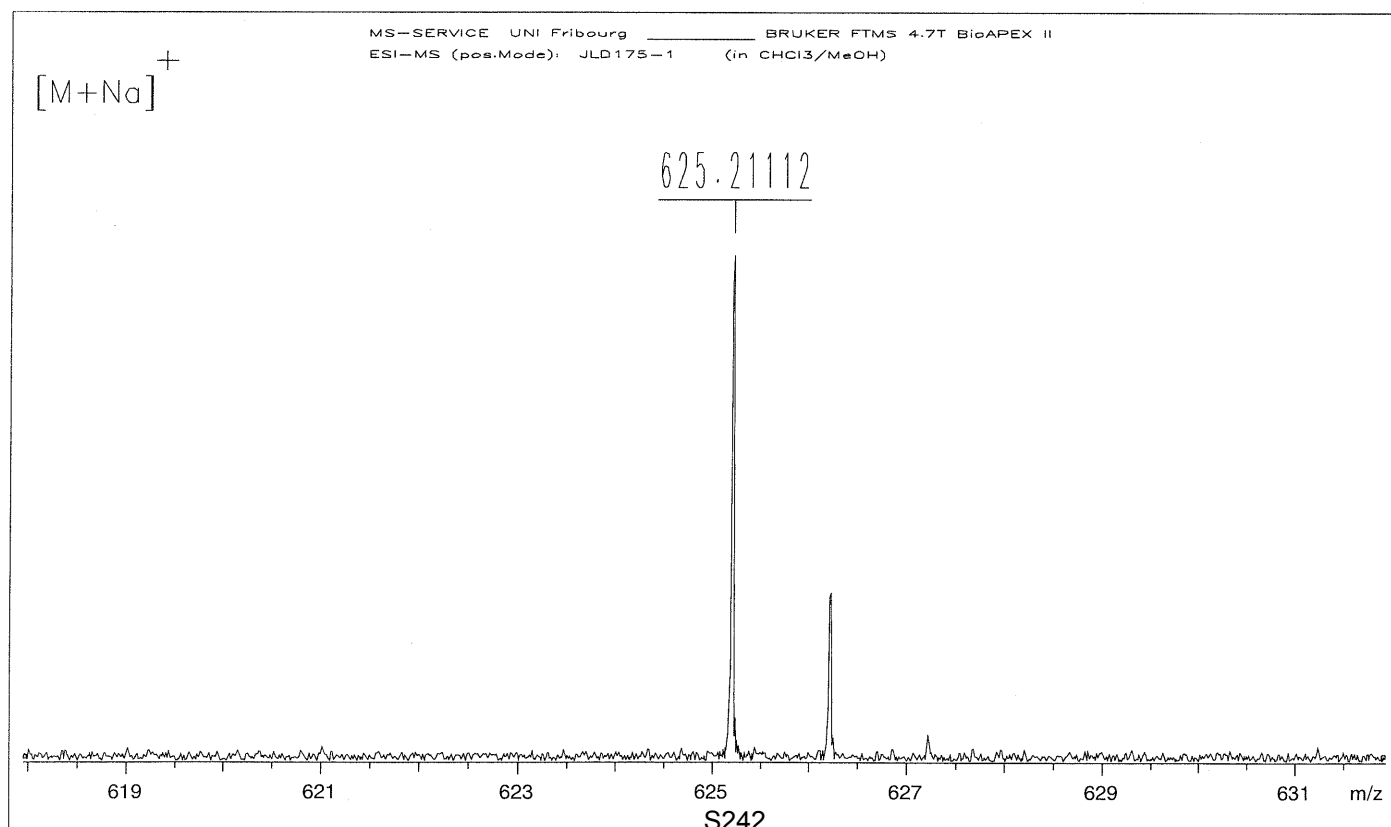
ESI-MS: JLD175-1

XMASS Mass Analysis for /Data/UNI_FR/DEBI3331_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 625.2111240

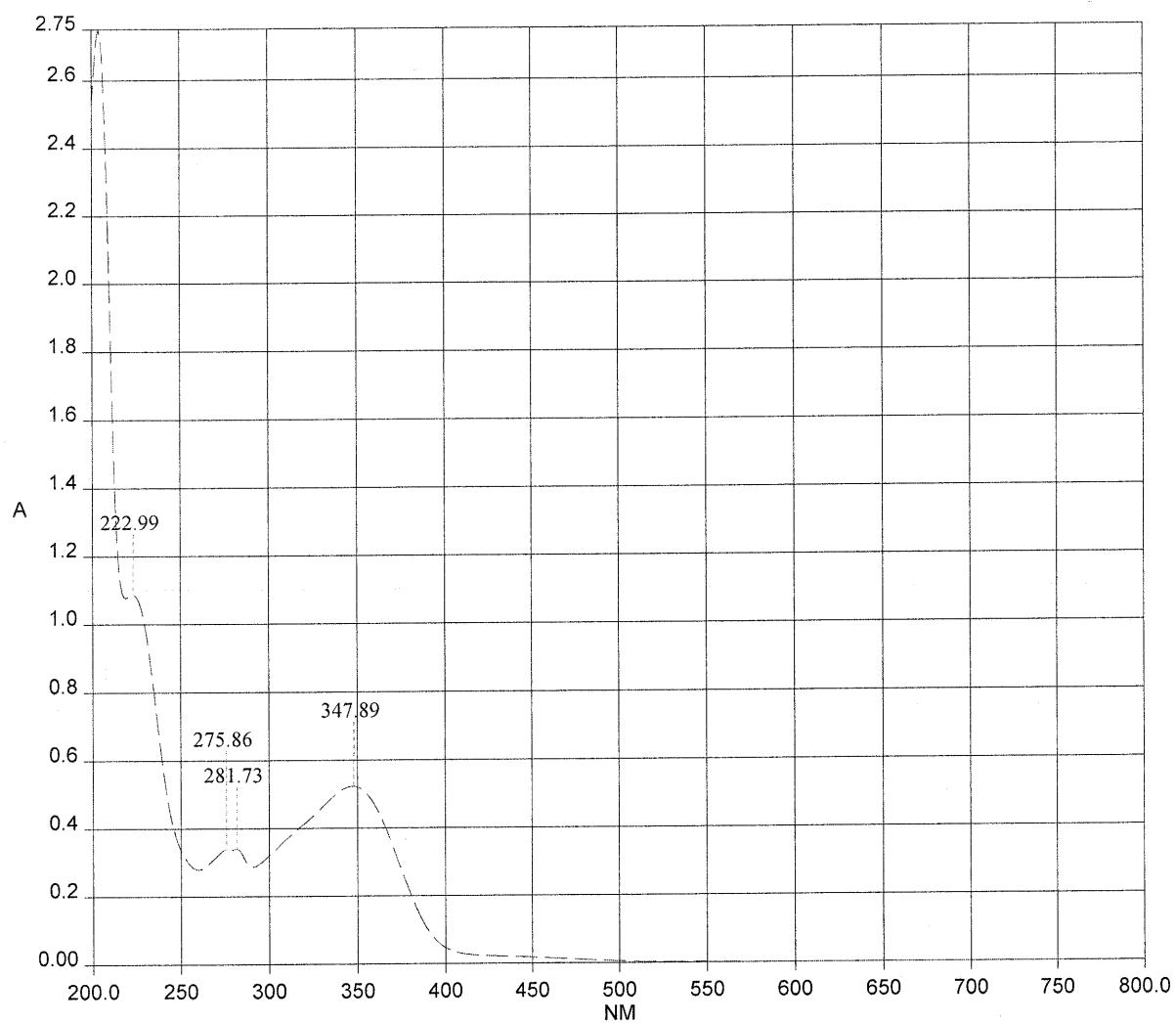
Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 625.2111240								
1	28	34	4	11	1	625.2116290	13.5	5.050e-04
2	30	33	4	11	0	625.2140343	16.5	2.910e-03
3	37	29	4	6	0	625.2081611	25.5	2.963e-03
4	31	32	5	8	1	625.2143091	18.0	3.185e-03
5	33	34	2	9	1	625.2156518	17.5	4.528e-03
6	35	30	4	6	1	625.2057558	22.5	5.368e-03
7	33	31	5	8	0	625.2167144	21.0	5.590e-03
8	34	31	3	9	0	625.2054810	21.0	5.643e-03
9	34	30	6	5	1	625.2169892	22.5	5.865e-03
10	35	33	2	9	0	625.2180571	20.5	6.933e-03

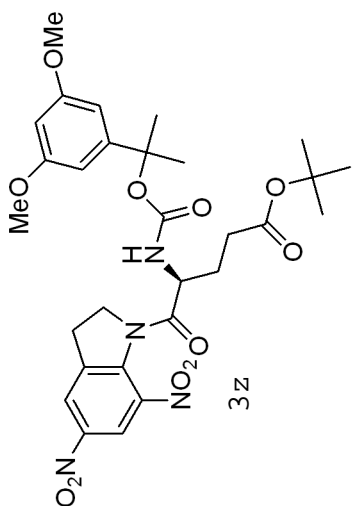


Date: 21.04.2008

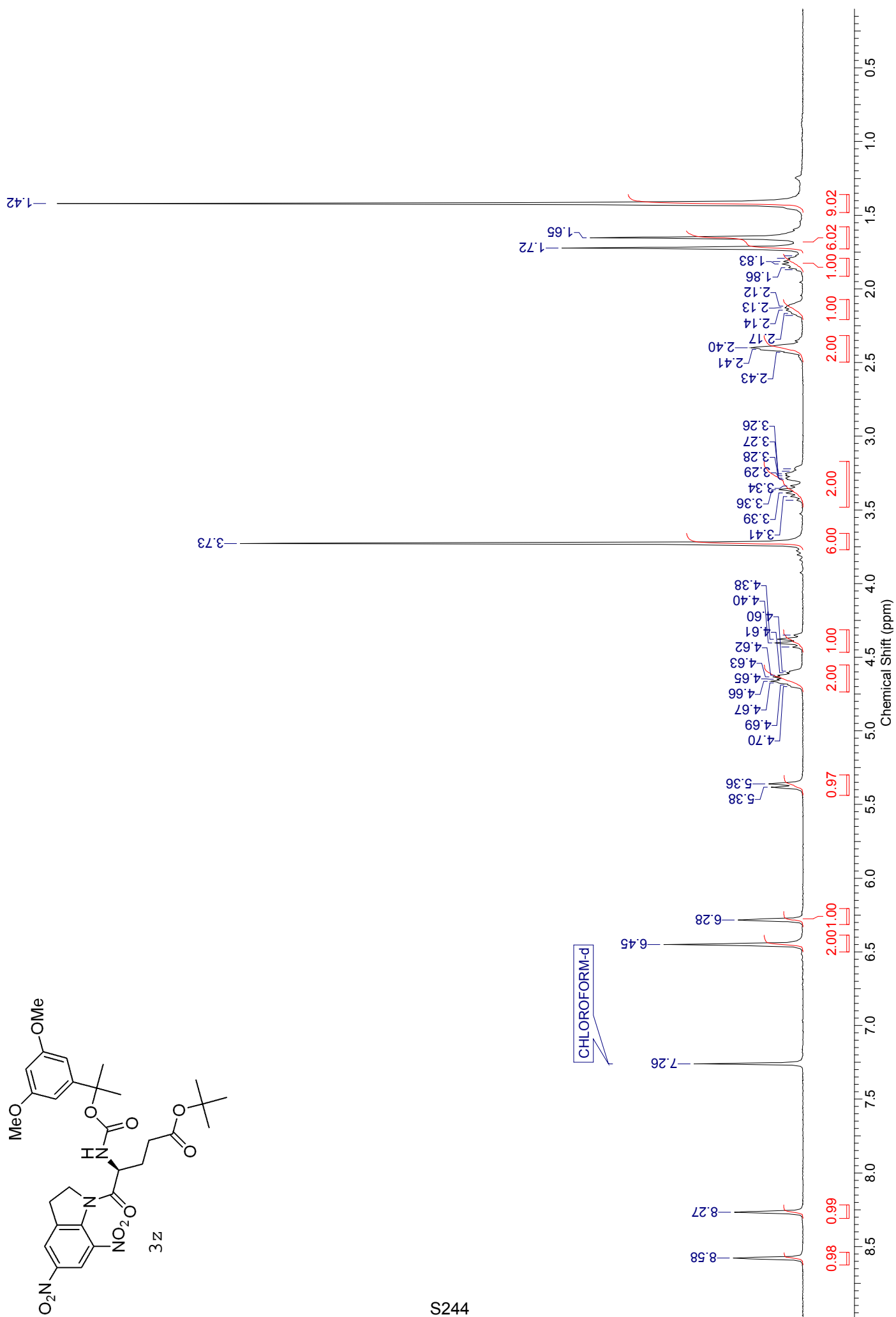
Time: 17:18:01

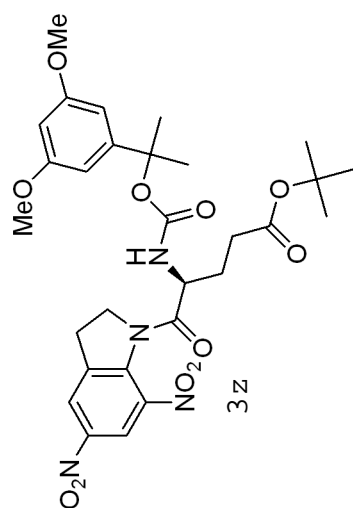


----- JLD175.SP - 21.04.2008 - 5.00×10^{-5} M in MeCN

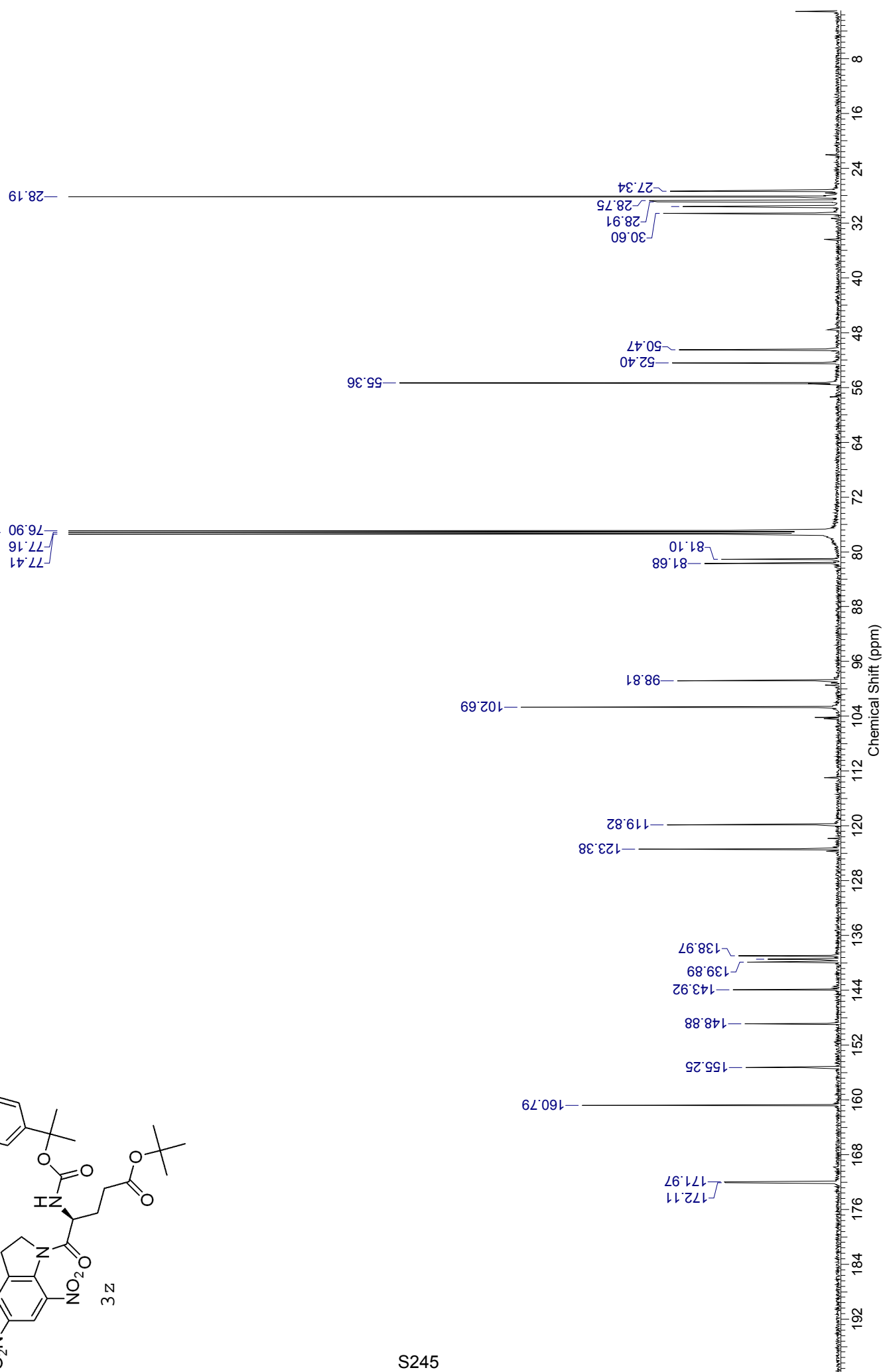


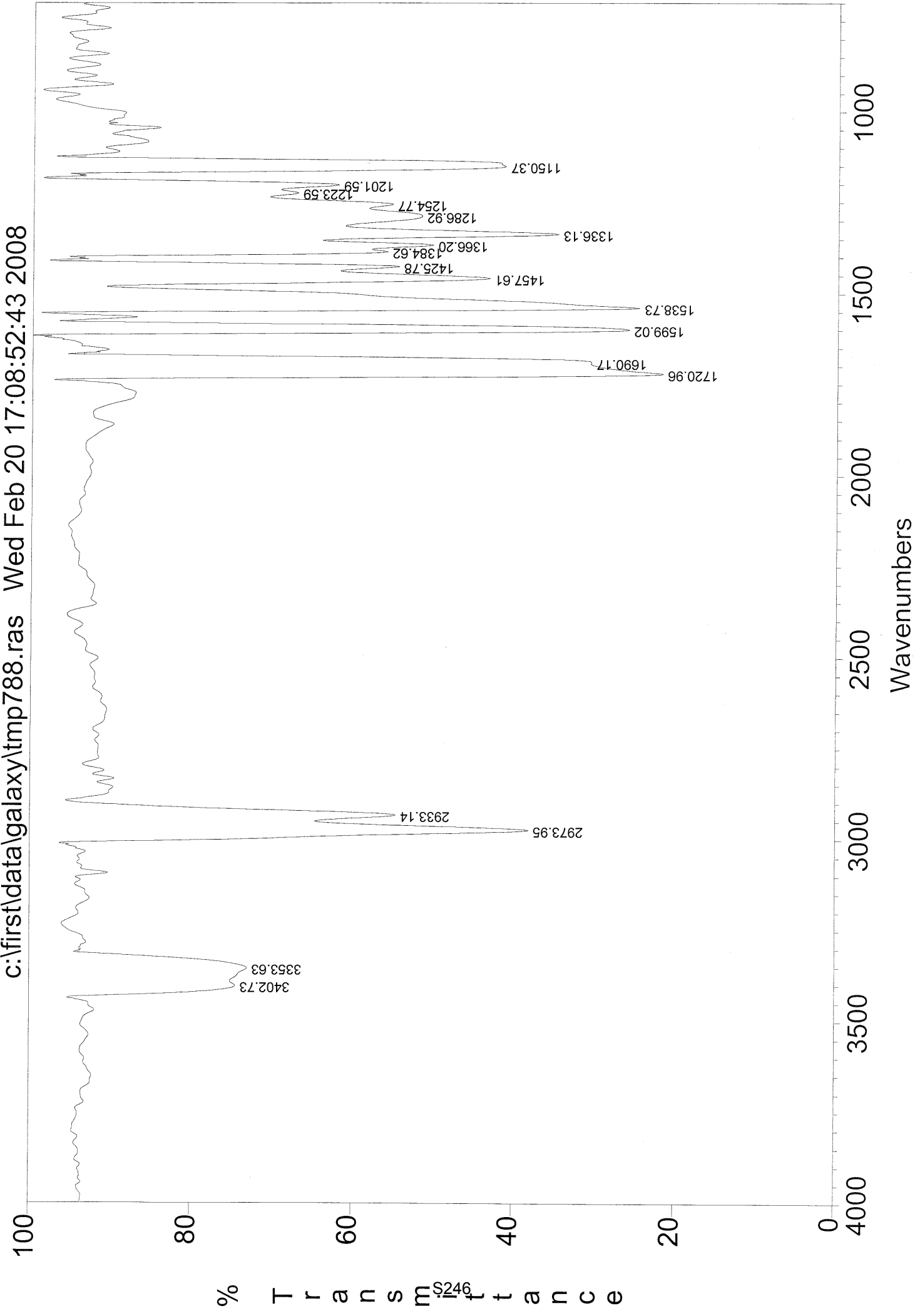
S244





CHLOROFORM-d





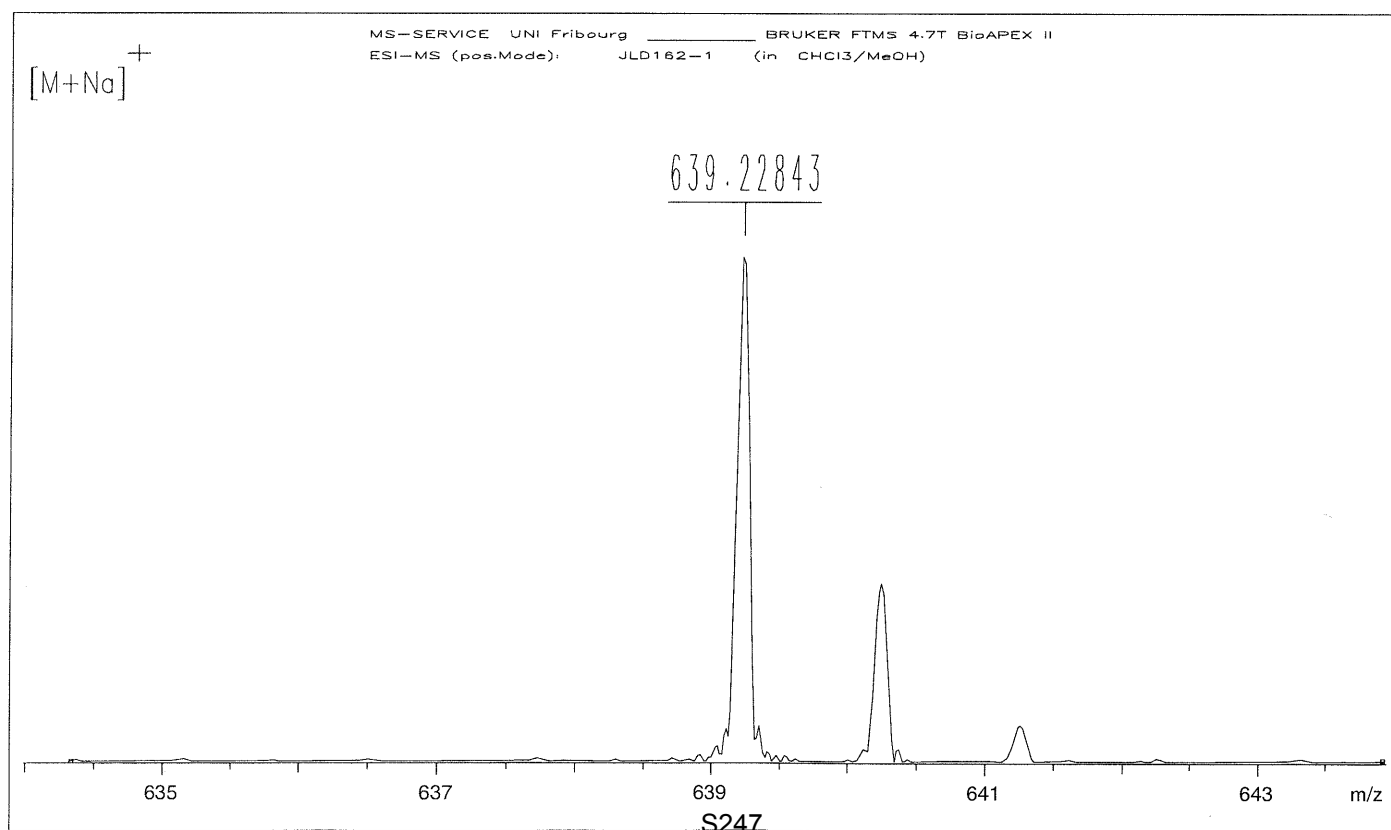
ESI-MS: JLD162-1

XMASS Mass Analysis for /Data/UNI_FR/DEBI3159_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 639.2284320

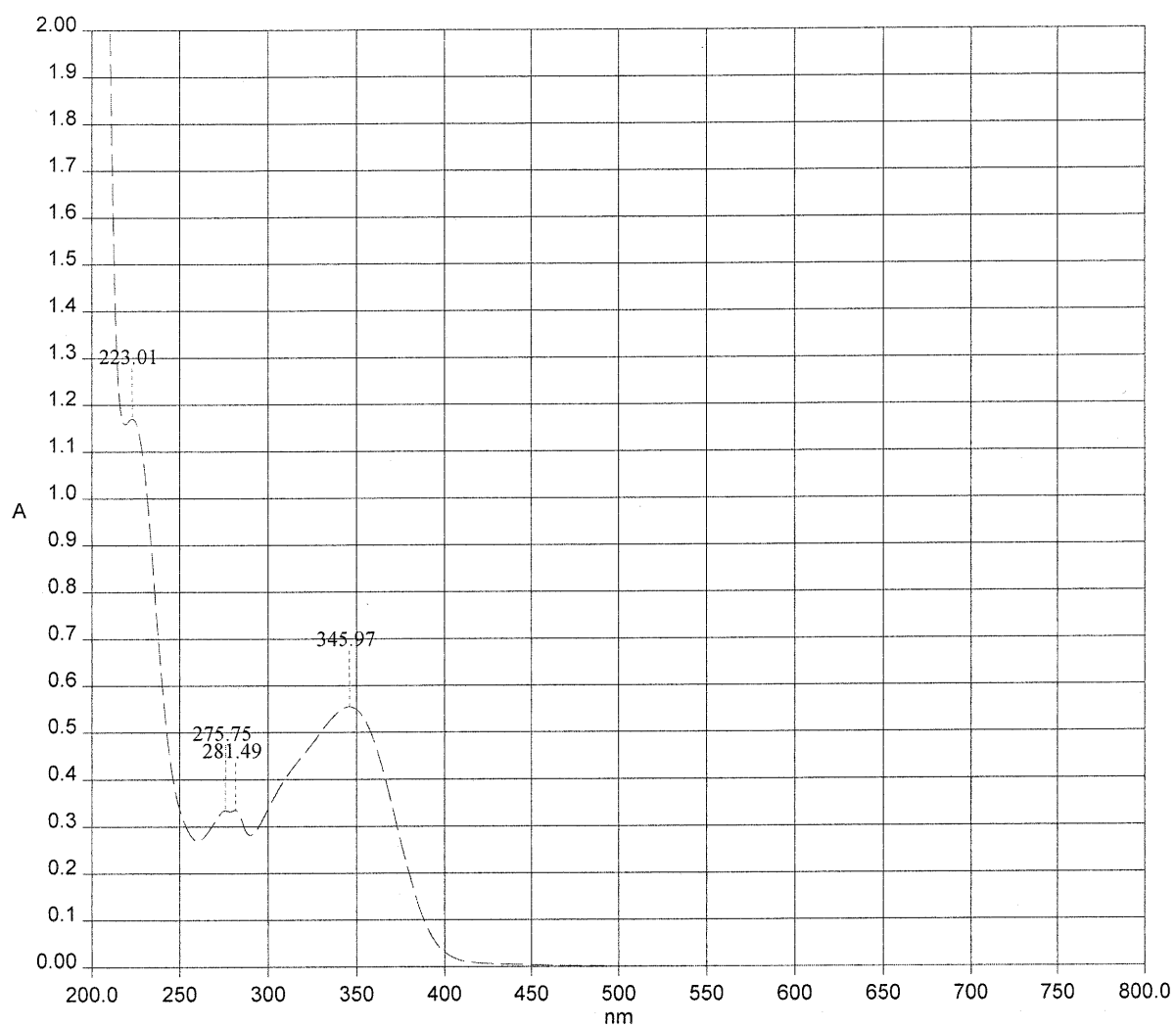
Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 639.2284320								
1	29	36	4	11	1	639.2272791	13.5	1.153e-03
2	31	35	4	11	0	639.2296844	16.5	1.252e-03
3	32	34	5	8	1	639.2299592	18.0	1.527e-03
4	26	35	6	13	0	639.2256617	12.5	2.770e-03
5	34	36	2	9	1	639.2313019	17.5	2.870e-03
6	34	33	5	8	0	639.2323645	21.0	3.932e-03
7	24	36	6	13	1	639.2232564	9.5	5.176e-03
8	36	35	2	9	0	639.2337072	20.5	5.275e-03
9	35	33	3	9	0	639.2211311	21.0	7.301e-03
10	25	38	5	13	1	639.2358324	9.0	7.400e-03



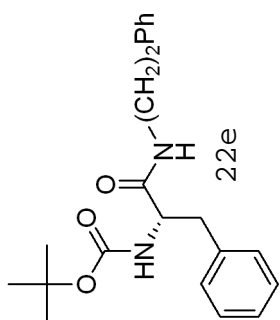
Date: 23.04.2008

Time: 08:58:27

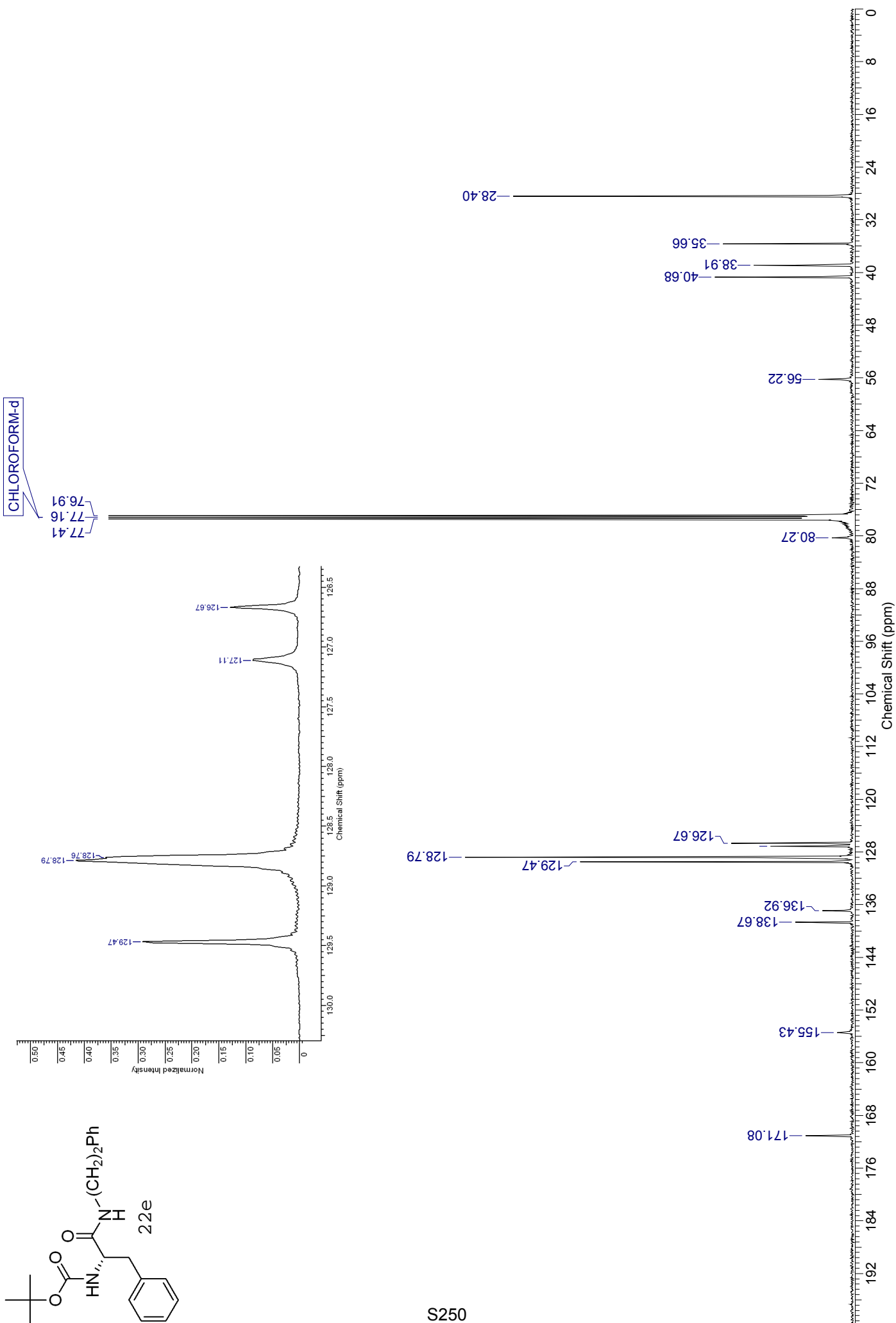


----- JLD162.SP - 23.04.2008 - $5.19 \cdot 10^{-5}$ M in MeCN



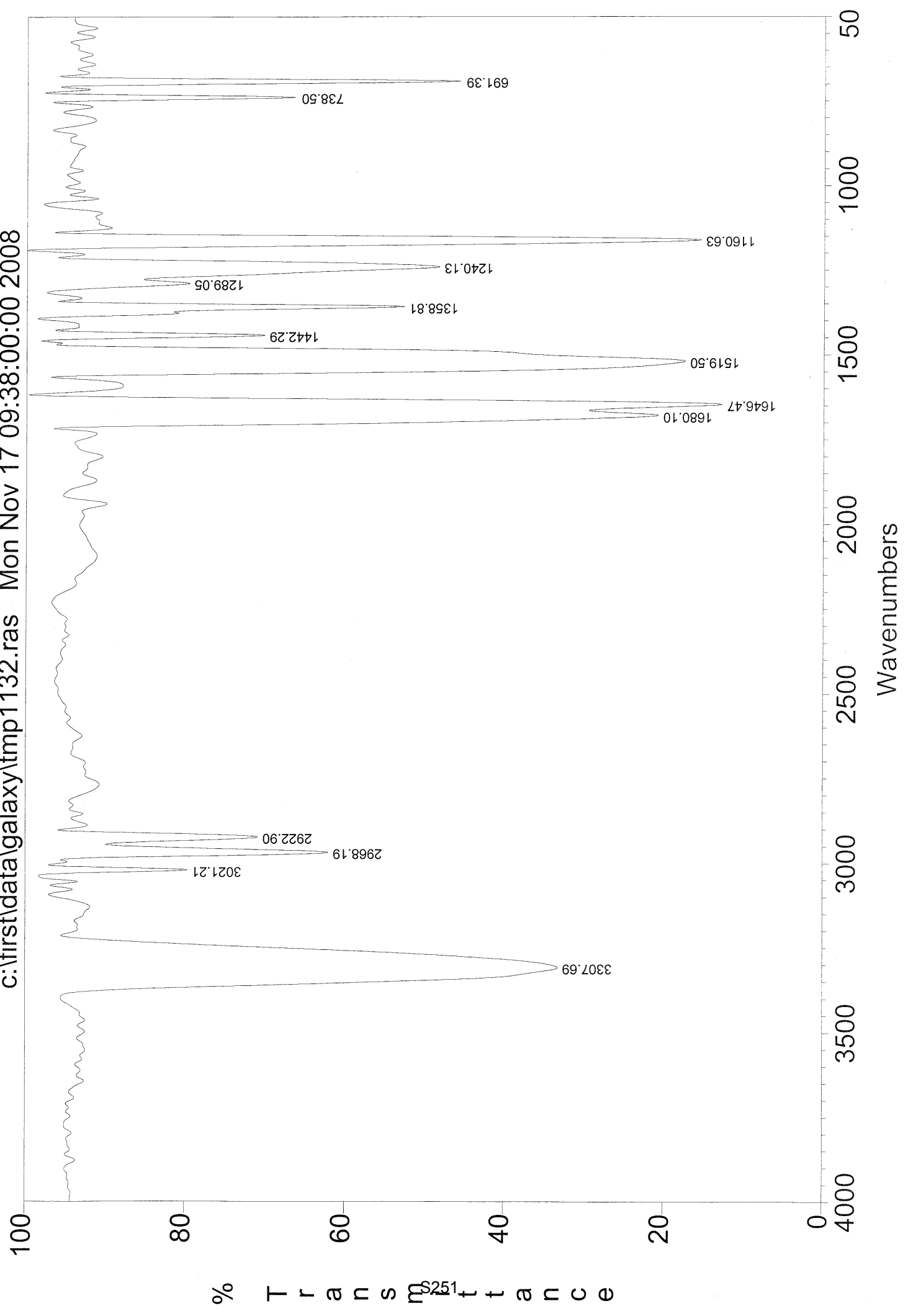


S250



510 209

c:\first\data\galaxy\tmp1132.ras Mon Nov 17 09:38:00:00 2008





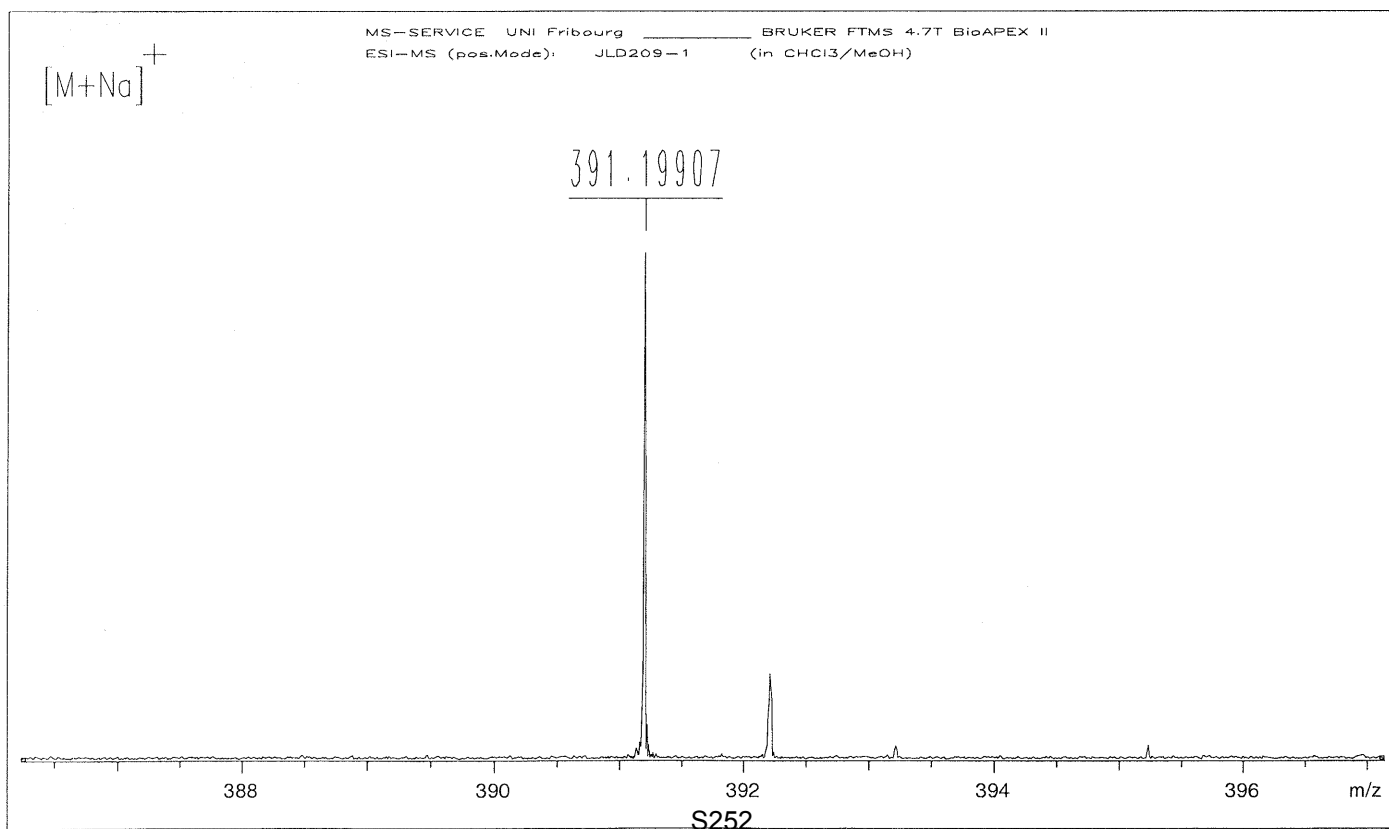
ESI-MS: JLD209-1

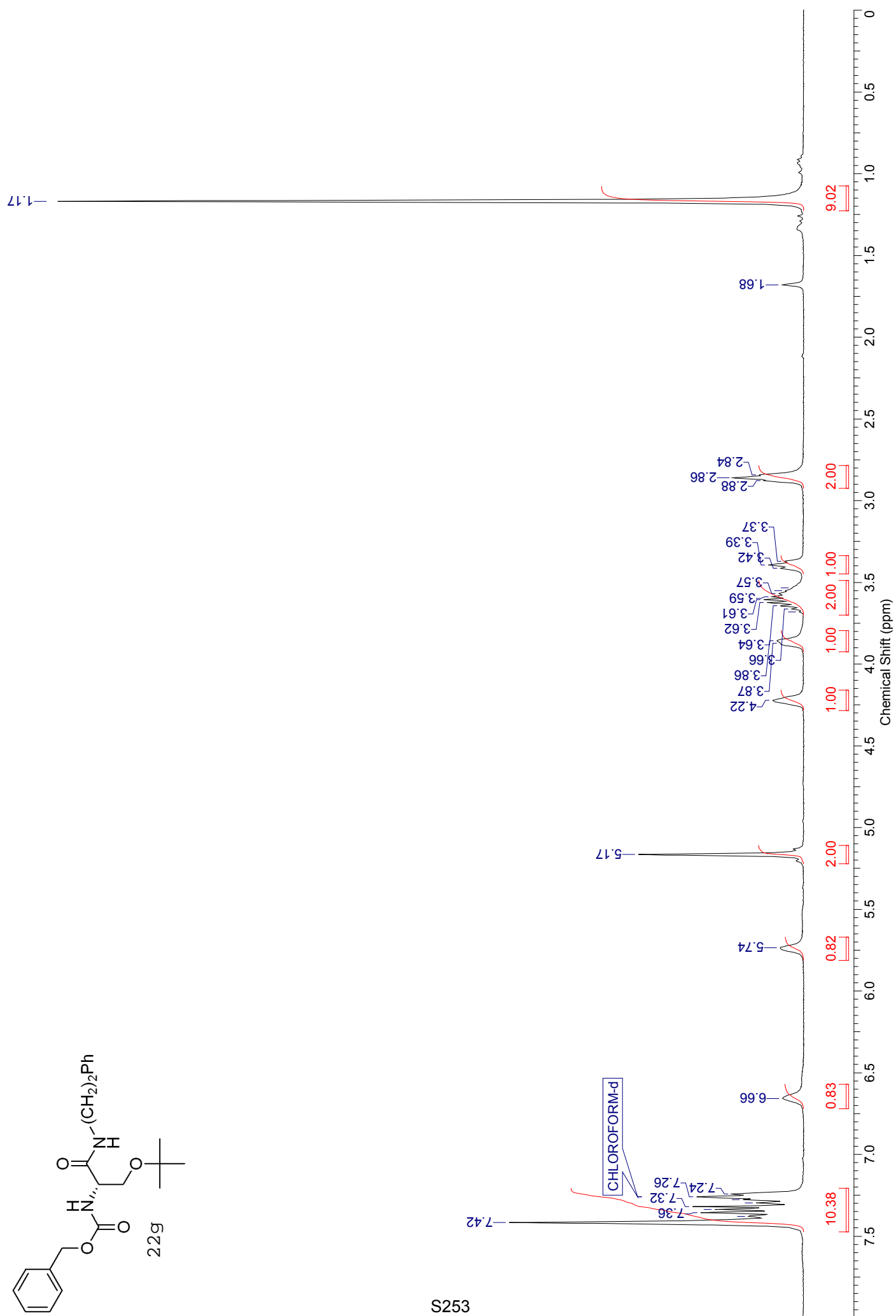
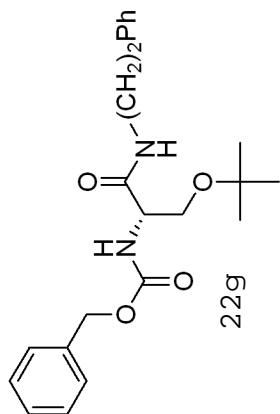
XMASS Mass Analysis for /Data/UNI_FR/DEBI3857_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

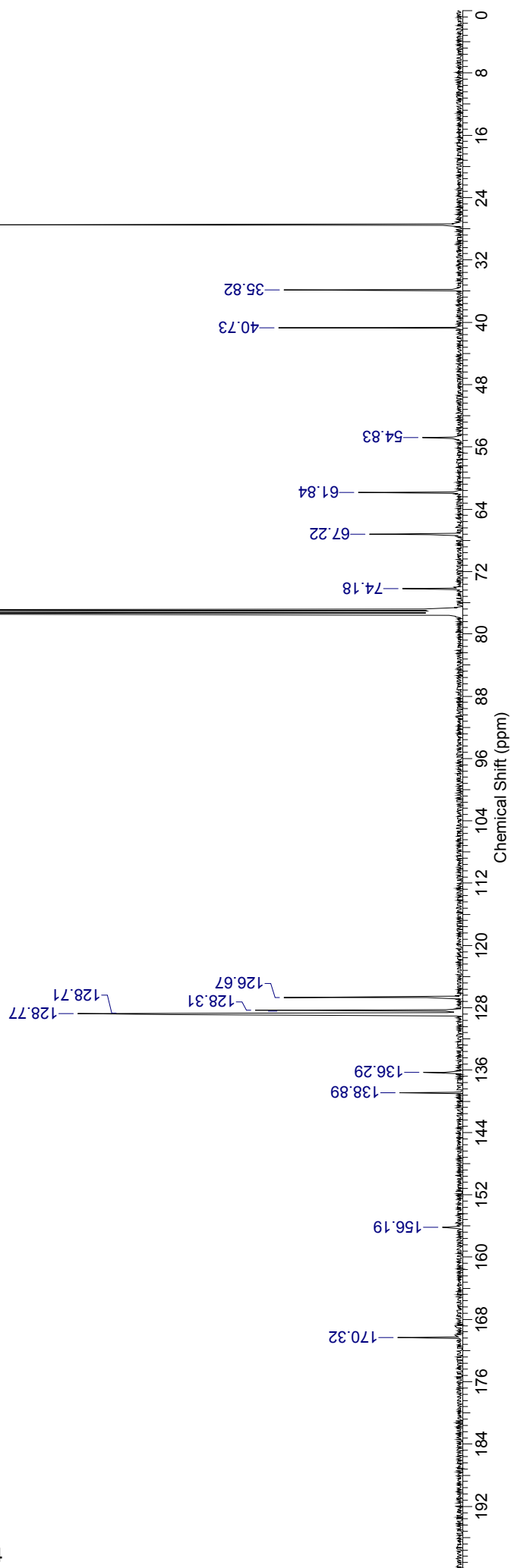
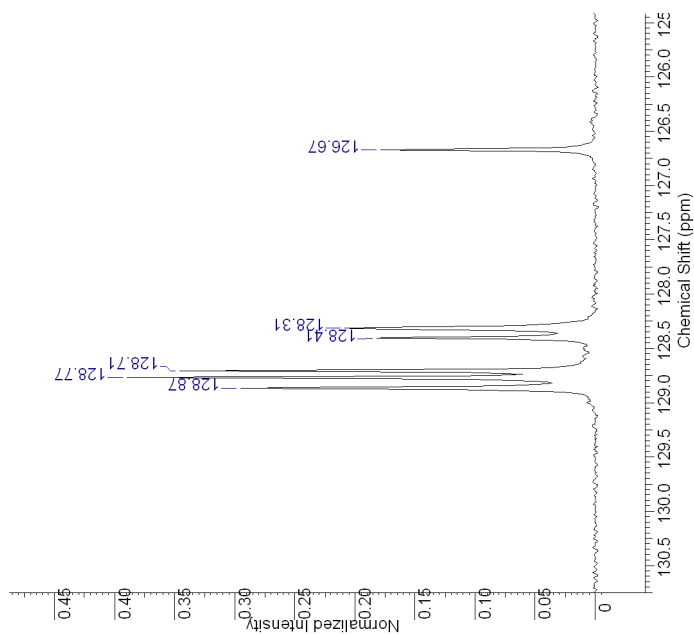
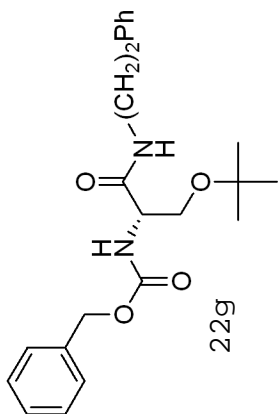
Ion mass = 391.1990710

Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 391.1990710								
1	22	28	2	3	1	391.1992139	9.5	1.429e-04
2	24	27	2	3	0	391.2016192	12.5	2.548e-03
3	18	30	3	5	1	391.2077672	5.0	8.696e-03
4	23	25	3	3	0	391.1890431	13.0	1.003e-02
5	20	29	3	5	0	391.2101725	8.0	1.110e-02
6	21	26	3	3	1	391.1866378	10.0	1.243e-02
7	23	30	1	3	1	391.2117899	9.0	1.272e-02
8	25	29	1	3	0	391.2141952	12.0	1.512e-02
9	24	25	1	4	0	391.1778097	13.0	2.126e-02
10	19	32	2	5	1	391.2203432	4.5	2.127e-02

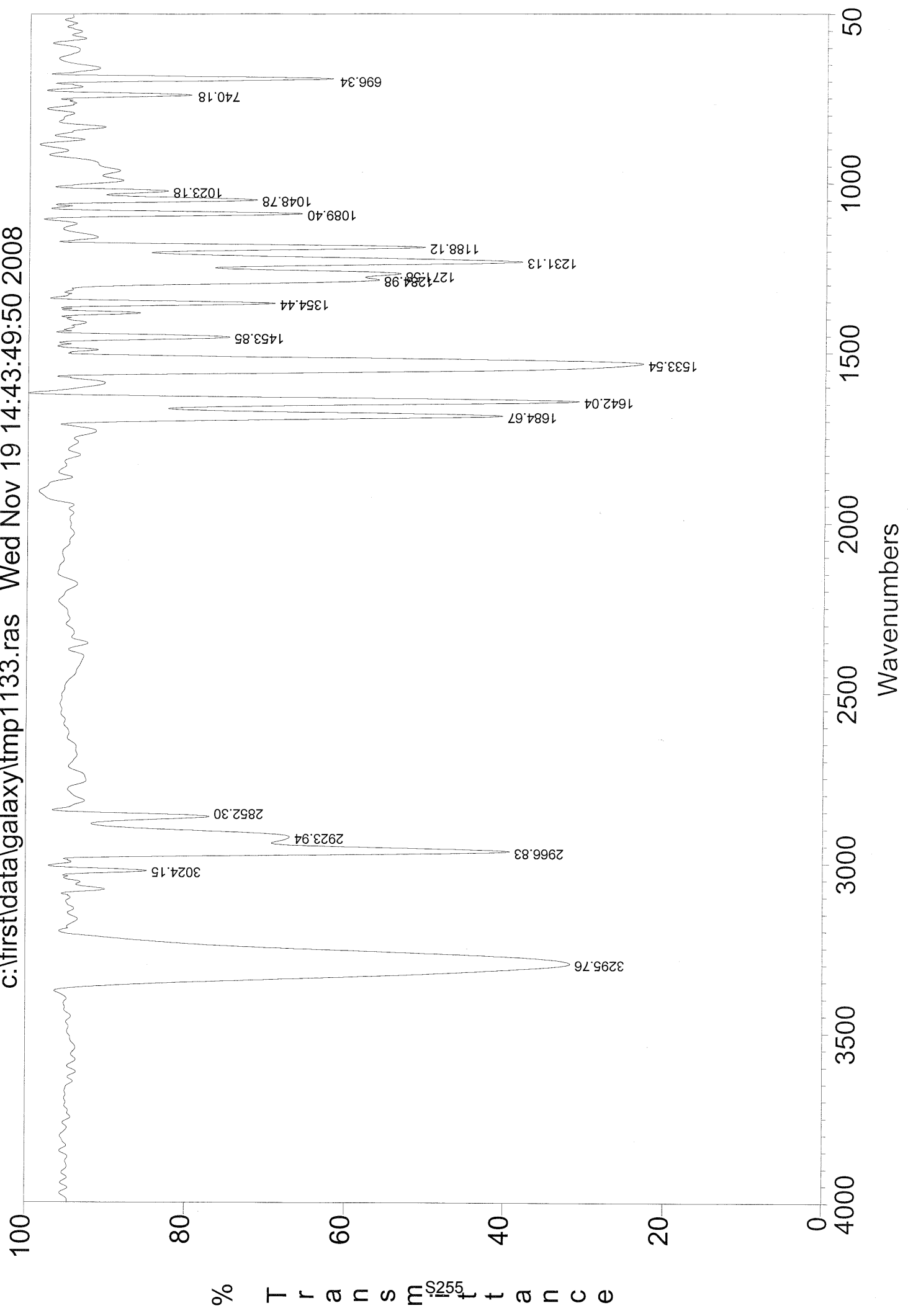






9/10/2008

c:\first\data\galaxy\tmp1133.ras Wed Nov 19 14:43:49:50 2008





FTMS 4.7T BioAPEX II MS-Service UNI-Fribourg

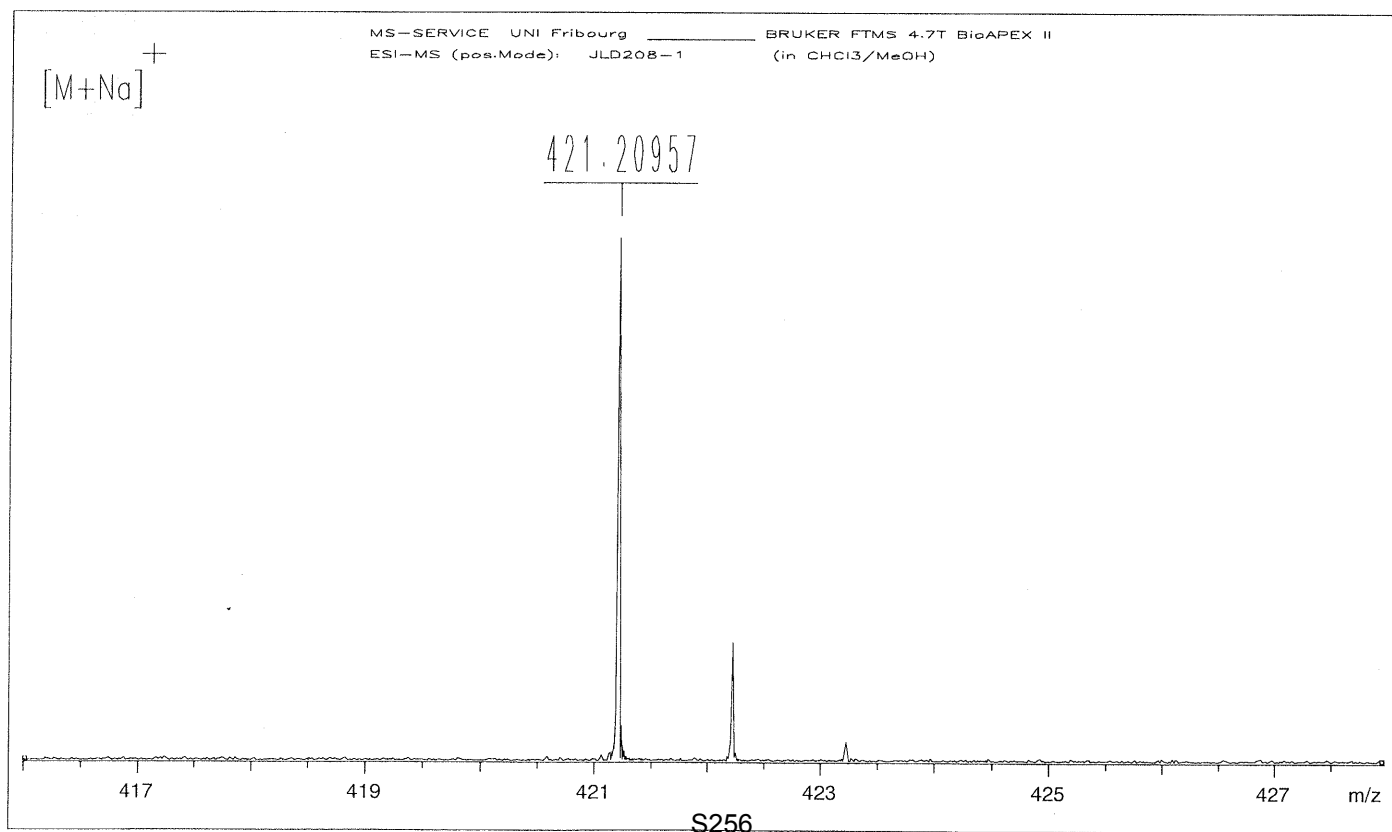
ESI-MS: JLD208-1

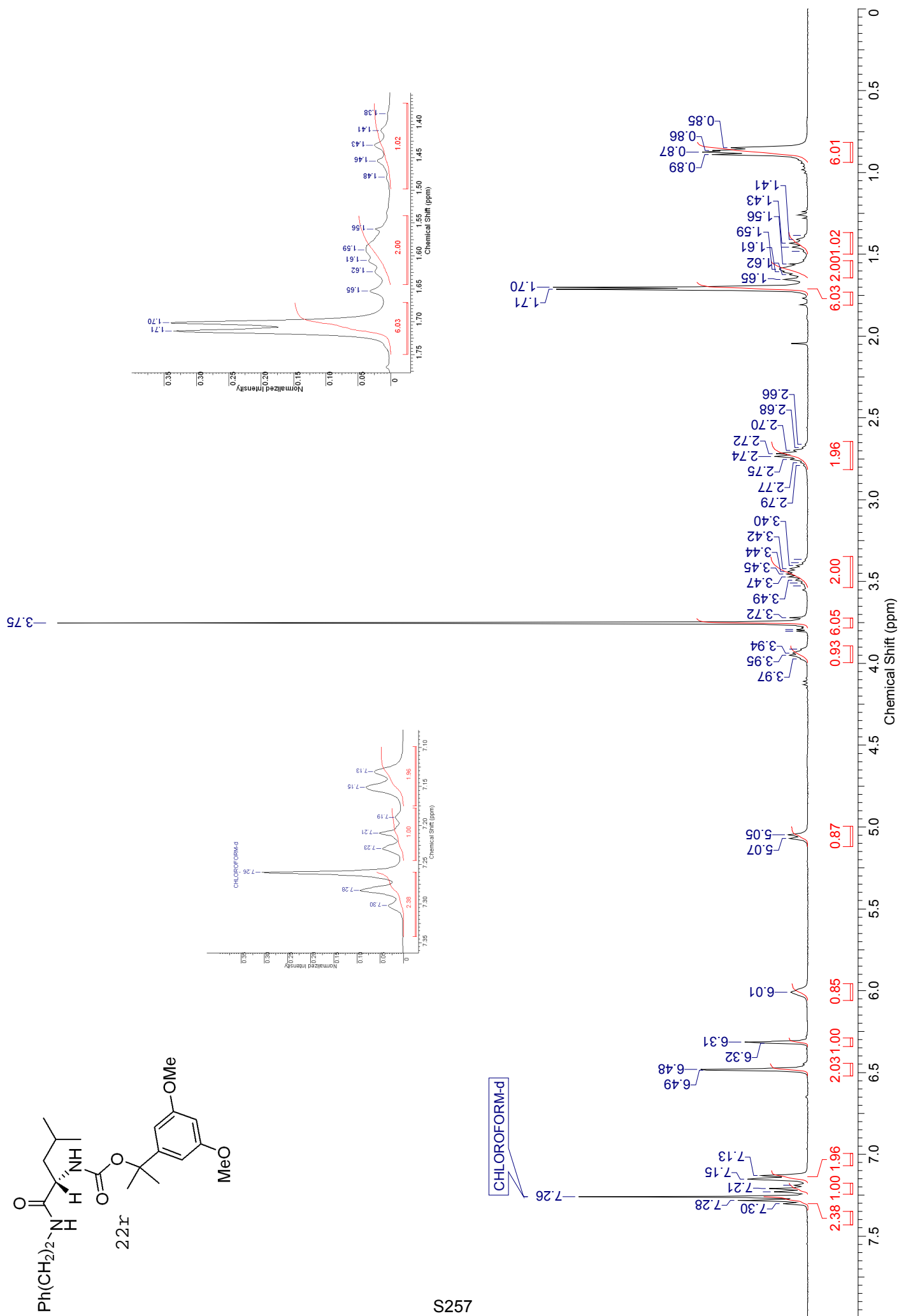
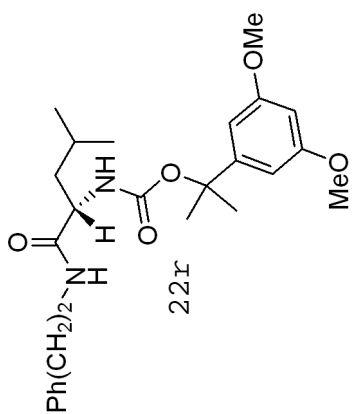
XMASS Mass Analysis for /Data/UNI_FR/DEBI3858_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

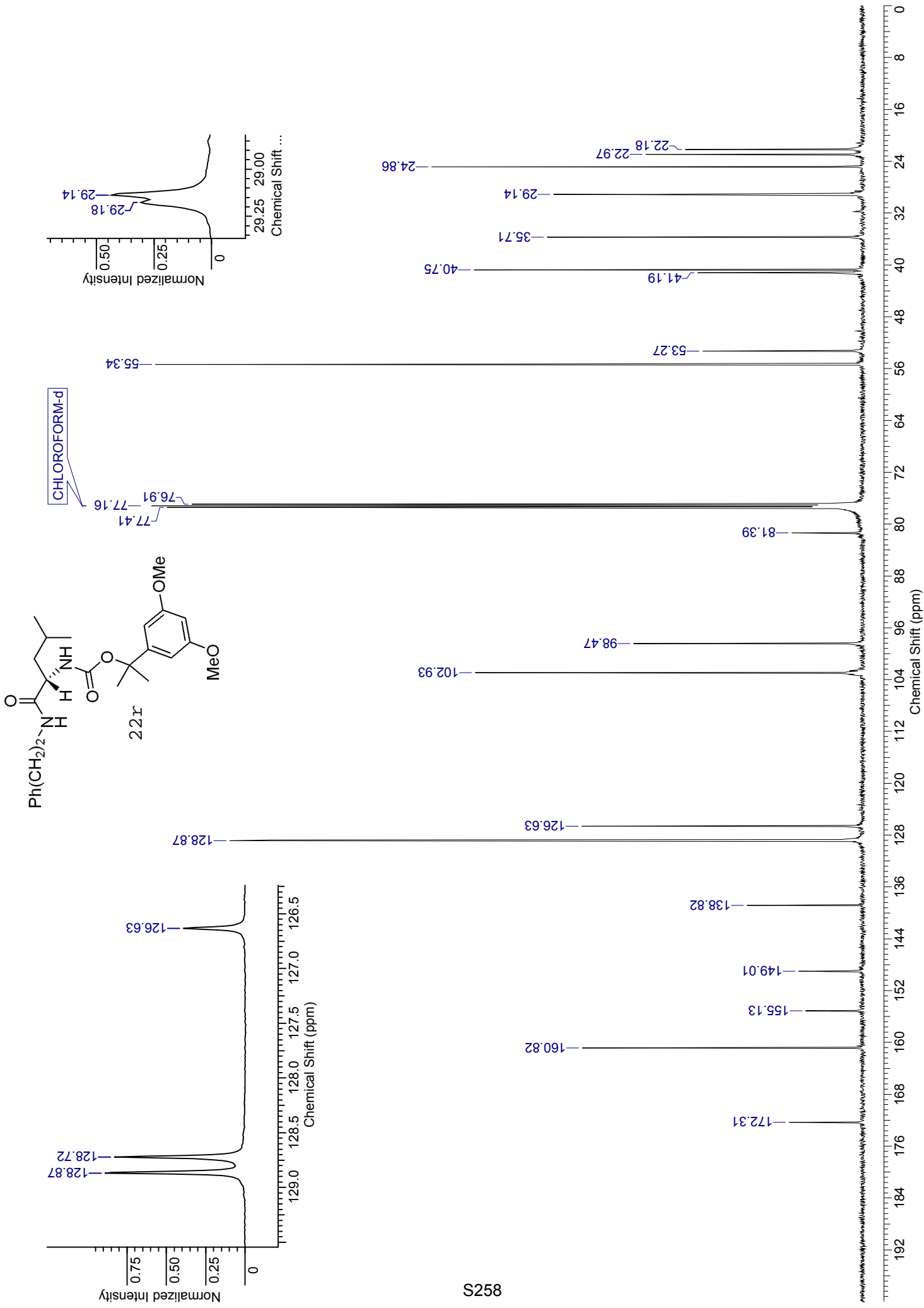
Ion mass = 421.2095670

Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 421.2095670								
1	23	30	2	4	1	421.2097786	9.5	2.116e-04
2	25	29	2	4	0	421.2121838	12.5	2.617e-03
3	24	27	3	4	0	421.1996078	13.0	9.959e-03
4	22	28	3	4	1	421.1972025	10.0	1.236e-02
5	24	32	1	4	1	421.2223546	9.0	1.279e-02
6	25	27	1	5	0	421.1883744	13.0	2.119e-02
7	23	28	1	5	1	421.1859691	10.0	2.360e-02
8	23	32	3	3	1	421.2335880	9.0	2.402e-02
9	25	31	3	3	0	421.2359933	12.0	2.643e-02
10	25	24	3	2	1	421.1760731	15.0	3.349e-02

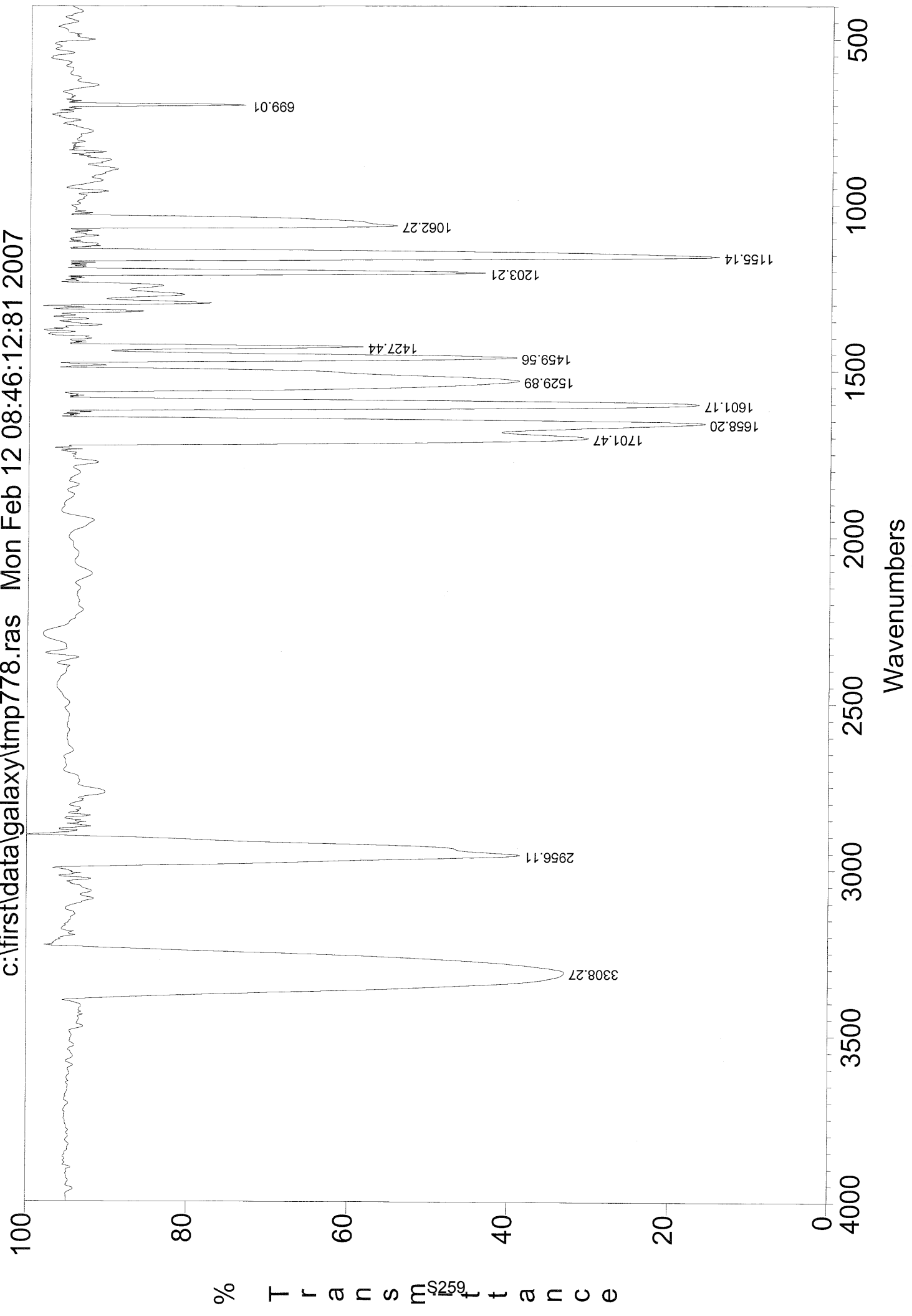






00009

c:\first\data\galaxy\tmp778.ras Mon Feb 12 08:46:12:81 2007



ESI-MS: JLD104-MS

XMASS Mass Analysis for /Data/UNI_FR/DEBI2339_ESI/1/pdata/1/massanal.res:
XMASS Mass Analysis Constraints

Ion mass = 479.2521950

Charge = +1

#	C	H	N	O	Na	mass	DBE	error
*** Mass Analysis for mass 479.2521950								
1	26	36	2	5	1	479.2516434	9.5	5.516e-04
2	25	37	1	8	0	479.2513686	8.0	8.264e-04
3	28	35	2	5	0	479.2540487	12.5	1.854e-03
4	29	34	3	2	1	479.2543234	14.0	2.128e-03
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
9	20	37	3	10	0	479.2473458	4.0	4.849e-03
10	19	40	2	10	1	479.2575166	0.5	5.322e-03

