Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Synthesis of Amphiphilic Hydantoin-based Universal Peptidomimetics as Antibiotic Agents

Alessio M. Caramiello,[a] Maria Cristina Bellucci,[b] Emerenziana Ottaviano,[c] Silvia Ancona, [c] Elisa Borghi,[c] and Alessandro Volonterio*[a]

Department of Chemistry, Materials, and Chemical Engineering "Giulio Natta", Politecnico di Milano, via Mancinelli 7, 20131 Milano, Italy; Department of Food, Environmental and Nutritional Sciences, Università degli Studi di Milano, via Celoria 2, 20133 Milano, Italy; Department of Health Science, Università degli Studi di Milano, via Di Rudinì 8, 20142 Milano, Italy;.

Email: alessandro.volonterio@polimi.it.

Table of content:

MATERIALS AND METHODS

Synthesis and characterization.

Commercially available reagent-grade solvents were employed without purification. TLC were run on silica gel 60 F254 Merck. Visualization of the developed chromatogram was achieved with UV light and ceric ammonium molybdate (CAM) or ninhydrin stains. Flash chromatography (FC) were performed with silica gel 60 (60-200 µm, Merck). ^{1}H-, and ^{13}C NMR spectra were run at 400 MHz. Chemical shifts are expressed in ppm (δ), using tetramethylsilane (TMS) as internal standard for ^{1}H and ^{13}C nuclei (δH and δC = 0.00). ESI mass spectra were performed by a Bruker Esquire 3000+ instrument equipped with a MS detector composed by an ESI ionization source and a Single Quadrupole mass selective detector or by an Agilent Technologies 1200 Series HPLC system equipped with a DAD and a 6120 MS detector composed by an ESI ionization source and a Single Quadrupole mass selective detector.

Antimicrobial susceptibility testing

Synthesized compounds were dissolved in sterile ddH_2O at the concentrations of 10,000 µg/mL and filtered with 0.22 µm pore size membrane. The final concentration tested ranged from 4-0.06µg/mL (two-fold dilution). Before testing, bacterial strains were thaw from glycerol stocks stored at −80 °C by seeding them on fresh Mueller-Hinton agar and culturing them for 24 h at 37 °C. A single colony was harvested in phosphate buffer saline (PBS) to obtain a 0.5 McFarland suspension (corresponding to about 10^8 CFU/mL). Serial dilutions were then performed in Mueller-Hinton broth until the desired concentration of 5×10^5 CFU/mL. Colony counts on inoculum suspensions were performed to ensure that the final inoculum concentrations closely approximated 5×10^5 CFU/mL. MIC were read manually after 24 h incubation at 37°C aerobically. The minimum inhibitory concentrations (MICs) were determined by a broth microdilution method according to the CLSI methodology in round-bottom 96-wells. Experiments were carried out in biological triplicate.

Molecular modeling:

Calculations were performed with Spartan 08 software. All the structures were first submitted to a Monte Carlo conformational search with MM (MMFF94 force field) minimization.

Synthesis of urea 6a,b. General procedure. To a solution of aspartic acid diester **5** (1 equiv) and TEA (1.2 equiv.) in DCM (0.1 M solution respect to **5**) isocyanate **4** (1 equiv.) in DCM (0.1 M solution) was added at rt. The solution was stirred for 30 minutes and then diluted with a 1M aqueous solution of HCl. The mixture was extracted with DCM, the collected organic layers dried over Na_2SO_4, filtered and the solvent evaporated under pressure. The crude was purified by flash chromatography.

4-(*tert*-butyl) 1-methyl ((2-(benzyloxy)-2-oxoethyl)carbamoyl)-L-aspartate, 6b. Yields: 98%. R_f = 0.30 (hexane/AcOEt = 50:50); $[\alpha]^{20}_D$= + 18.6 (c = 1.2, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33-7.31 (m, 5H), 6.1-5.5 (br s, 2H), 5.16 (s, 2H), 4.78 (t, *J* = 4.8 Hz, 1H), 4.13 (d, *J* = 18.4 Hz, 1H), 3.96 (d, *J* = 18.4 Hz, 1H), 3.71 (s, 3H), 2.89 (dd, *J* = 16.8 and 4.8 Hz, 1H), 2.74 (dd, *J* = 16.8 and 4.8 Hz, 1H), 1.40 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.8, 171.2, 170.5, 157.4, 135.4, 128.6, 128.3, 128.2, 81.4, 67.0, 52.5, 49.7, 42.2, 38.3, 28.0; ESI m/z 417.9 $[M+Na, (100)]^+$; Anal. calcd. for $C_{19}H_{26}N_2O_7$: C, 57.86; H, 6.64; N, 7.10; found: C, 57.86; H, 6.64; N, 7.11.

Synthesis of hydantoins 7a,b. General procedure. To a solution of urea **6** (1 equiv.) in CH_3CN (0.1M solution) a 1M aqueous solution of NaOH (10% in volume) was added. After 5 minutes the solution was quenched with a 1M aqueous solution of HCl until acidic pH was reached. The mixture was extracted with AcOEt, dried over Na_2SO_4, filtered and the solvent evaporated under pressure. The hydantoins **7** were used in the following steps without further purification.

***tert*-butyl (S)-2-(1-(2-ethoxy-2-oxoethyl)-2,5-dioxoimidazolidin-4-yl)acetate, 7a.** Yields: 98%. R_f = 0.31 (hexane/AcOEt = 50:50); $[\alpha]^{20}_D$= + 31.1 (c = 1.5, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.08 (br s, 1H), 4.39-4.36 (m, 1H), 4.19-4.16 (m, 4H), 2.89 (dd, *J* = 17.2 and 3.6 Hz, 1H), 2.56 (dd, *J* = 17.2 and 9.6 Hz, 1H), 1.41 (s, 9H), 1.24 (t, *J* = 7.2 Hz, 3H) ; ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.5, 169.2, 166.9, 156.5, 82.2, 61.9, 54.0, 39.4, 37.4, 27.9, 14.0; ESI m/z 323.1 $[M+Na, (100)]^+$; Anal. calcd. for $C_{13}H_{20}N_2O_6$: C, 51.99; H, 6.71; N, 9.33; found: C, 52.00; H, 6.71; N, 9.34.

benzyl (S)-2-(4-(2-(*tert*-butoxy)-2-oxoethyl)-2,5-dioxoimidazolidin-1-yl)acetate, 7b. Yields: 98%. R_f = 0.33 (hexane/AcOEt = 50:50); $[\alpha]^{20}_D$= + 21.5 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36-7.34 (m, 5H), 6.26 (br s, 1H), 5.19 (d, *J* = 12.0 Hz, 1H), 5.15 (d, *J* = 12.0 Hz, 1H), 4.36 (m, 1H), 4.29 (s, 2H), 2.92 (dd, *J* = 17.2 and 2.8 Hz, 1H), 2.50 (dd, *J* = 17.2 and 10.4 Hz, 1H), 1.45 (s, 9H) ; ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.3, 169.5, 166.8, 155.9, 134.9, 128.7, 128.4, 127.0, 82.4, 70.1, 67.7, 54.0, 39.4, 37.5, 28.0; ESI m/z 385.4 $[M+Na, (100)]^+$; Anal. calcd. for $C_{18}H_{22}N_2O_6$: C, 59.66; H, 6.12; N, 7.73; found: C, 59.67; H, 6.12; N, 7.72.

Synthesis of compounds 9a-c. General procedure. To a solution of hydanotin **7** (1 equiv) in DMF (0.1 M solution) K_2CO_3 (1.3 equiv.) followed by benzyl bromide **8** were added at rt. The mixture was stirred in a sealed tube at 80 °C overnight. The mixture was cooled to rt and diluted with a 1M aqueous solution of HCl. The mixture was extracted with AcOEt, the collected organic layers dried over Na_2SO_4, filtered and the solvent evaporated under pressure. The crude was purified by flash chromatography.

***tert*-butyl (S)-2-(3-(4-(tert-butyl)benzyl)-1-(2-ethoxy-2-oxoethyl)-2,5-dioxoimidazolidin-4-yl)acetate, 9a.** Yields: 84%. R_f = 0.45 (hexane/AcOEt = 70:30); $[\alpha]^{20}_D$= + 21.8 (c = 1.2, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.37 (d, *J* = 8.4 Hz, 2H), 7.22 (d, *J* = 8.4 Hz, 2H), 4.92 (d, *J* = 15.2 Hz, 1H), 4.31 (s, 2H), 4.26-4.19 (m, 4H), 2.79 (dd, *J*

= 16.8 Hz, 1H), 2.73 (dd, *J* = 16.8 and 4.8 Hz, 1H), 1.40 (s, 9H), 1.32 (s, 9H), 1.30 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.3, 168.1, 167.0, 156.0, 151.0, 132.5, 127.6, 125.9, 82.0, 61.8, 56.1, 44.8, 39.9, 35.4, 34.5, 31.3, 27.9, 14.1; ESI m/z 469.3 $[M+Na, (100)]^+$, 485.3 $[M+K, (46)]^+$; Anal. calcd. for $C_{24}H_{34}N_2O_6$: C, 64.55; H, 7.67; N, 6.27; found: C, 64.56; H, 7.68; N, 6.28.

***tert*-butyl (S)-2-(1-(2-ethoxy-2-oxoethyl)-3-(4-fluorobenzyl)-2,5-dioxoimidazolidin-4-yl)acetate, 9b.** Yields: 91%. R_f = 0.31 (hexane/AcOEt = 70:30); $[\alpha]^{20}_D$= + 29.3 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.35.7.26 (m, 2H), 7.06-7.01 (m, 2H), 4.86 (d, *J* = 15.6 Hz, 1H), 4.64 (s, 1H), 4.31 (d, *J* = 16.8 Hz, 1H), 4.26 (d, *J* = 16.8 Hz, 1H), 4.25-4.18 (m, 4H), 2.79-2.74 (m, 2H), 1.40 (s, 9H), 1.29 (t, *J* = 7.2 Hz, 3H); ESI m/z 409.2 $[M+H, (100)]^+$; Anal. calcd. for $C_{20}H_{25}FN_2O_6$: C, 58.82; H, 6.17; N, 6.86; found: C, 58.81; H, 6.19; N, 6.88.

benzyl (S)-2-(4-(2-(*tert*-butoxy)-2-oxoethyl)-3-(naphthalen-1-ylmethyl)-2,5-dioxoimidazolidin-1-yl)acetate, 9c. Yields: 78%. R_f = 0.37 (hexane/AcOEt = 70:30); $[\alpha]^{20}_D$= + 10.4 (c = 0.9, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99-7.97 (m, 1H), 7.80-7.78 (m, 2H), 7.44-7.42 (m, 2H), 7.36-7.24 (m, 6H), 5.32 (d, *J* = 15.6 Hz, 1H), 5.12 (s, 2H), 4.65 (d, *J* = 15.6 Hz, 1H), 3.89 (dd, *J* = 5.2 and 4.0 Hz, 1H), 2.69 (dd, *J* = 16.8 and 4.4 Hz, 1H), 2.57 (dd, *J* = 16.8 and 5.2 Hz, 1H), 1.20 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.6, 167.7, 166.9, 155.8, 135.0, 134.0, 131.3, 130.7, 129.2, 128.8, 128.7, 128.5, 128.3, 127.1, 126.7, 126.3, 125.2, 123.2, 82.0, 67.6, 56.5, 43.7, 40.0, 35.2, 27.8; ESI m/z 525.3 $[M+Na, (100)]^+$; Anal. calcd. for $C_{29}H_{30}N_2O_6$: C, 69.31; H, 6.02; N, 5.57; found: C, 69.30; H, 6.04; N, 5.57.

Synthesis of compounds 11a-c. General procedure. To a stirred solution of **9** (1 equiv.) in DCM (0.1M solution) neat TFA (30% in volume) was added. After 4 hours the solvents were evaporated and co-evaporated twice with cyclo-hexane. The crude was dissolved in DMF (0.1M solution) and cooled to 0°C and solid HBTU (1.2 equiv.) was added. After 10 minutes, TEA (1.5 equiv.) followed by a solution of **10** (1.2 equiv.) in minimum amount of DMF were added and the resulting solution stirred overnight at rt. The solution was diluted with a 1M aqueous solution of HCl and extracted with AcOEt. The collected organic phases were washed with brine (once), with a saturated aqueous solution of $NaHCO_3$ (twice) and brine (once). The organic phase was dried over Na_2SO_4, filtered and the solvent evaporated under pressure. The hydantoins **11** were used in the following steps without further purification.

ethyl (S)-2-(4-(2-((4-((*tert*-butoxycarbonyl)amino)butyl)amino)-2-oxoethyl)-3-(4-(tert-butyl)benzyl)-2,5-dioxoimidazolidin-1-yl)acetate, 11a. Yields: 74%. R_f = 0.21 (hexane/AcOEt = 50:50); $[\alpha]^{20}_D$= + 20.0 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34 (d, *J* = 8.0 Hz, 2H), 7.22 (d, *J* = 8.0 Hz, 2H), 6.22 (br s, 1H), 4.85 (d, *J* = 15.2 Hz, 1H), 4.74 (br s, 1H), 4.28-4.26 (m, 4H), 4.21 (q, *J* = 7.2 Hz, 2H), 3.20-3.18 (m, 2H), 3.11-3.09 (m, 2H), 2.71 (dd, *J* = 15.6 and 5.2 Hz, 1H), 2.62 (dd, *J* = 15.6 and 5.6 Hz, 1H), 1.46-1.44 (m, 4H), 1.43 (s, 9H), 1.30 (s, 9H), 1.29 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.4, 167.8, 167.1, 156.2, 155.8, 150.9, 132.8, 127.8,

125.7, 78.5, 61.9, 56.4, 44.8, 39.9, 39.4, 36.5, 34.5, 31.3, 28.4, 27.6, 14.1; ESI m/z 583.4 [M+Na, (100)]$^+$, 599.4 [M+K, (97)]$^+$; Anal. calcd. for $C_{29}H_{44}N_4O_7$: C, 62.12; H, 7.91; N, 9.99; found: C, 62.12; H, 7.92; N, 10.00.

ethyl (S)-2-(4-(2-((4-((*tert*-butoxycarbonyl)amino)butyl)amino)-2-oxoethyl)-3-(4-fluorobenzyl)-2,5-dioxoimidazolidin-1-yl)acetate, 11b. Yields: 80%. R_f = 0.18 (hexane/AcOEt = 50:50); $[\alpha]^{20}_D$= + 10.9 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27-7.25 (m, 2H), 6.95-6.93 (m, 2H), 6.46 (br s, 1H), 4.84 (br s, 1H), 4.73 (d, *J* = 15.2 Hz, 1H), 4.31 (d, *J* = 15.2 Hz, 1H), 4.28-4.26 (m, 3H), 4.19 (q, *J* = 7.2 Hz, 2H), 3.14-3.12 (m, 2H), 3.06-3.04 (m, 2H), 2.73 (dd, *J* = 16.0 Hz and 4.4 Hz, 1H), 2.59 (dd, *J* = 16.0 and 6.0 Hz, 1H), 1.43-1.42 (m, 4H), 1.39 (s, 9H), 1.25 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.4, 168.1, 167.4, 162.4 (d, *J* = 247.4 Hz), 156.3, 155.9, 131.9 (d, *J* = 3.0 Hz), 129.9 (d, *J* = 8.1 Hz), 115.6 (d, *J* = 21.2 Hz), 79.2, 62.0, 56.5, 44.5, 39.9, 39.3, 38.6, 36.1, 28.3, 14.0; ESI m/z 523.2 [M+H, (38)]$^+$, 545.3 [M+Na, (100)]$^+$; Anal. calcd. for $C_{25}H_{35}FN_4O_7$: C, 57.46; H, 6.75; N, 10.72; found: C, 57.44; H, 6.75; N, 10.73.

benzyl (S)-2-(4-(2-(*tert*-butoxy)-2-oxoethyl)-3-(naphthalen-1-ylmethyl)-2,5-dioxoimidazolidin-1-yl)acetate, 11c. Yields: 79%. R_f = 0.20 (hexane/AcOEt = 50:50); $[\alpha]^{20}_D$= + 22.1 (c = 0.8, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04-8.02 (m, 1H), 7.83-7.89 (m, 2H), 7.49-7.46 (m, 2H), 7.36-7.33 (m, 2H), 7.26 (br t, *J* = 5.6 Hz, 1H), 5.22 (d, *J* = 15.2 Hz, 1H), 4.78 (br s, 1H), 4.70 (d, *J* = 15.2 Hz, 1H), 4.19 (s, 2H), 3.67 (dd, *J* = 4.4 and 2.8 Hz, 1H), 3.24-3.17 (m, 2H), 3.03 (t, *J* = 6.8 Hz, 1H), 2.84 (dd, *J* = 17.6 and 2.8 Hz, 1H), 2.63 (dd, *J* = 17.6 and 4.8 Hz, 1H), 1.46-1.43 (m, 4H), 1.36 (s, 9H), 1.22 (s, 9H); ESI m/z 617.4 [M+H, (100)]$^+$; Anal. calcd. for $C_{34}H_{40}N_4O_7$: C, 66.22; H, 6.54; N, 9.08; found: C, 66.22; H, 6.55; N, 9.10.

Synthesis of compounds 12a,b. General procedure. To a stirred solution of **11** (1 equiv.) in MeOH (0.1M solution) a 1.0 M aqueous solution of NaOH (30% in volume) was added. After 2 hours the solution was acidified with a 1M aqueous solution of HCl and extracted with AcOEt. The collected organic phases were dried over Na_2SO_4, filtered and the solvent evaporated under pressure. The crude was dissolved in DMF (0.1M solution) and cooled to 0°C and solid HBTU (1.2 equiv.) was added. After 10 minutes, TEA (1.5 equiv.) followed by a solution of **10** (1.2 equiv.) in minimum amount of DMF were added and the resulting solution stirred overnight at rt. The solution was diluted with a 1M aqueous solution of HCl and extracted with AcOEt. The collected organic phases were washed with brine (once), with a saturated aqueous solution of $NaHCO_3$ (twice) and brine (once). The organic phase was dried over Na_2SO_4, filtered and the solvent evaporated under pressure. The hydantoins **12** were used in the following steps without further purification.

di-*tert*-butyl (((2,2'-(3-(4-(tert-butyl)benzyl)-2,5-dioxoimidazolidine-1,4-diyl)bis(acetyl))bis(azanediyl))bis(butane-4,1-diyl))(S)-dicarbamate, 12a. Yields: 71%. R_f = 0.28 (hexane/AcOEt = 20:80); $[\alpha]^{20}_D$= + 9.5 (c = 0.6, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (br t, *J* = 5.2 Hz, 1H), 7.33 (d, *J* = 8.4 Hz, 2H), 7.19 (d, *J* = 8.4 Hz, 2H), 6.96 (br s, 1H), 5.12 (br s, 1H), 4.95 (br s, 1H), 4.93 (d, *J* = 15.2

Hz, 1H), 4.24 (d, *J* = 16.8 Hz, 1H), 4.15 (d, *J* = 15.2 Hz, 1H), 4.13 (d, *J* = 16.8 Hz, 1H), 3.87 (dd, *J* = 4.4 and 2.4 Hz, 1H), 3.27-3.25 (m, 2H), 3.24-3.05 (m, 6H), 2.98-2.95 (m 1H), 2.88-2.85 (m, 1H), 1.50-1.47 (m, 8H), 2.42 (s, 9H), 2.41 (s, 9H), 1.28 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.4, 168.2, 167.0, 162.6, 156.6, 156.0, 151.2, 132.3, 128.0, 125.9, 79.3, 79.1, 55.7, 44.4, 41.8, 39.4, 39.1, 38.6, 36.5, 34.5, 33.8, 31.4, 31.3, 28.4, 27.0, 26.1; ESI m/z 725.4 [M+Na, (100)]$^+$; Anal. calcd. for $C_{36}H_{58}N_6O_8$: C, 61.52; H, 8.32; N, 11.96; found: C, 61.53; H, 8.30; N, 11.97.

di-tert-butyl (((2,2'-(3-(4-fluorobenzyl)-2,5-dioxoimidazolidine-1,4-diyl)bis(acetyl))bis(azanediyl))bis(butane-4,1-diyl))(S)-dicarbamate, 12b. Yields: 77%. R_f = 0.22 (hexane/AcOEt = 20:80); $[\alpha]^{20}_D$= + 11.9 (c = 0.8, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (br s, 1H), 7.22-7.20 (m, 2H), 6.96-6.92 (m, 3H), 5.08 (br s, 1H), 4.82 (br s, 1H), 4.71 (d, *J* = 15.2 Hz, 1H), 2.24 (d, *J* = 15.2 Hz, 1H), 4.18 (d, *J* = 16.8 Hz, 1H), 4.10 (d, *J* = 16.8 Hz, 1H), 3.84 (dd, *J* = 4.4 and 2.8 Hz, 1H), 3.20-3.17 (m 2H), 3.06-3.00 (m, 6H), 2.98 (m, 1H), 2.71 (dd, *J* = 16.4 and 4.8 Hz, 1H), 1.55-1.48 (m, 8H), 1.36 (s, 9H), 1.50 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.1, 167.9, 166.8, 162.4 (d, *J* = 248.5 Hz), 156.6, 156.2, 156.0, 131.5, 130.0 (d, *J* = 8.1 Hz), 115.8 (d, *J* = 21.2 Hz), 79.3, 79.0, 56.1, 44.4, 41.9, 39.5, 39.3, 33.9, 28.4, 27.1, 26.1; ESI m/z 687.3 [M+Na, (100)]$^+$; Anal. calcd. for $C_{32}H_{49}FN_6O_8$: C, 57.82; H, 7.43; N, 12.64; found: C, 57.84; H, 7.43; N, 12.64.

Synthesis of diamine 13c. General procedure. To a stirred solution of **11c** (1 equiv.) in a 1:1 mixture of AcOEt/MeOH (0.1M solution) a catalytic amount of Pd/C was added and the mixture vigorously stirred under hydrogen atmosphere. After 3 hours, the mixture was filtered on a Celite pad, washed with MeOH and the organic solvents evaporated under reduced pressure. The crude was dissolved in DMF (0.1M solution) and cooled to 0°C and solid HBTU (1.2 equiv.) was added. After 10 minutes, TEA (1.5 equiv.) followed by a solution of **10** (1.2 equiv.) in minimum amount of DMF were added and the resulting solution stirred overnight at rt. The solution was diluted with a 1M aqueous solution of HCl and extracted with AcOEt. The collected organic phases were washed with brine (once), with a saturated aqueous solution of $NaHCO_3$ (twice) and brine (once). The organic phase was dried over Na_2SO_4, filtered and the solvent evaporated under pressure. The crude was purified by flash chromatography. The resulting di-Boc derivative was dissolved in DCM (1.0 M solution) and treated with H3PO4 (85% solution in weight, 13 equiv.) and the solution stirred at rt for 4 hours. The solution was basified with a 1.0 M aqueous solution of NaOH and extracted with DCM. The collected organic phases were dried over Na_2SO_4, filtered and the solvent evaporated under pressure affording **13c** in high purity.

(S)-2,2'-(3-(naphthalen-1-ylmethyl)-2,5-dioxoimidazolidine-1,4-diyl)bis(N-(4-aminobutyl)acetamide), 13c. Yields: 64%. $[\alpha]^{20}_D$= + 1.6 (c = 1.2, MeOH); $[\alpha]^{20}_D$= + 11.6 (c = 1.0, $CHCl_3$); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.17-8.14 (m, 1H), 8.04 (br t, *J* = 5.6 Hz, 1H), 7.91-7.86 (m, 2H), 7.60-7.55 (m, 2H), 7.46-7.44 (m, 2H), 6.36 (br t, *J* = 5.2

Hz, 1H), 5.08 (d, *J* = 15.2 Hz, 1H), 5.04 (d, *J* = 15.2 Hz, 1H), 4.30 (d, *J* = 16.8 Hz, 1H), 4.24 (d, *J* = 16.8 Hz, 1H), 3.82 (dd, *J* = 4.8 and 2.4 Hz, 1H), 3.33-3.28 (m 2H), 2.96-2.93 (m, 1H), 2.86 (dd, *J* = 16.4 and 2.4 Hz, 1H), 2.68-66 (m, 4H), 2.64-2.62 (m, 1H), 2.43 (dd, *J* = 16.0 and 4.8 Hz, 1H), 1.59-1.56 (m, 2H), 1.45-1.34 (m, 10H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.0, 167.3, 166.5, 156.0, 133.9, 131.6, 131.5, 129.5, 128.7, 127.5, 127.2, 126.5, 125.1, 123.6, 57.9, 44.6, 42.1, 41.9, 41.5, 39.5, 39.3, 34.6, 31.0, 30.5, 26.6, 26.3; ESI m/z 497.4 $[M+H, (100)]^+$; Anal. calcd. for $C_{26}H_{36}N_6O_4$: C, 62.88; H, 7.31; N, 16.92; found: C, 62.90; H, 7.32; N, 16.91.

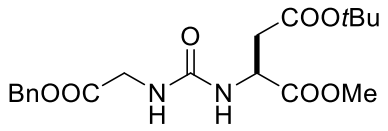
Synthesis of final peptidomimetics 3a-c. General procedure. To a stirred solution of **12** (1 equiv.) in DCM (0.1M solution) neat TFA (20% in volume) was added. After 4 hours the solvents were evaporated and co-evaporated twice with cyclo-hexane. The crude was dissolved in MeOH (0.1 M solution) and TEA (4.0 equiv.) followed by solid **14** (3.0 equiv.) were added and the resulting solution stirred 24 hours at rt. The solvent was evaporated under reduced pressure and the crude purified by flash chromatography. The resulting Boc protected guanidino derivative was dissolved in a 4.0 M solution of HCl in dioxane (1.0 M solution) or in a 1:1 mixture of TFA/DCM in the presence of a 3% in volume of triethyl silane. The solution was stirred for 4 hours, and the solvents evaporated under reduced pressure and co-evaporated with cyclo-hexane affording compounds **3a-c** in high purity.

(S)-2,2'-(3-(4-(tert-butyl)benzyl)-2,5-dioxoimidazolidine-1,4-diyl)bis(N-(4-guanidinobutyl)acetamide), 3a. Yields: 67%. $[\alpha]^{20}_D$= + 5.2 (c = 1.0, MeOH); ^{1}H NMR (400 MHz, CD_3OD) δ 7.41-7.39 (d, *J* = 7.6 Hz, 2H), 7.28 (d, *J* = 7.6 Hz, 2H), 4.79-4.75 (m, 1H), 4.37-4.35 (m, 1H), 4.22-4.14 (m, 2H), 3.33-3.22 (m, 8H), 2.90-2.88 (m, 2H), 1.64-1.58 (m, 8H), 1.32 (s, 9H); ^{13}C NMR (101 MHz, CD_3OD) δ 173.0, 169.1, 168.0, 157.2, 156.6, 150.7, 133.0, 127.6, 127.5, 125.4, 66.8, 56.6, 44.3, 41.1, 40.8, 38.5, 34.0, 33.9, 30.4, 26.1, 25.9, 25.7; ESI m/z 294.3 $[M+H, (100)]^{2+}$, 587.6 $[M+H, (48)]^+$; Anal. calcd. for $C_{28}H_{46}N_{10}O_4$: C, 57.32; H, 7.90; N, 23.87; found: C, 57.31; H, 7.89; N, 23.88.

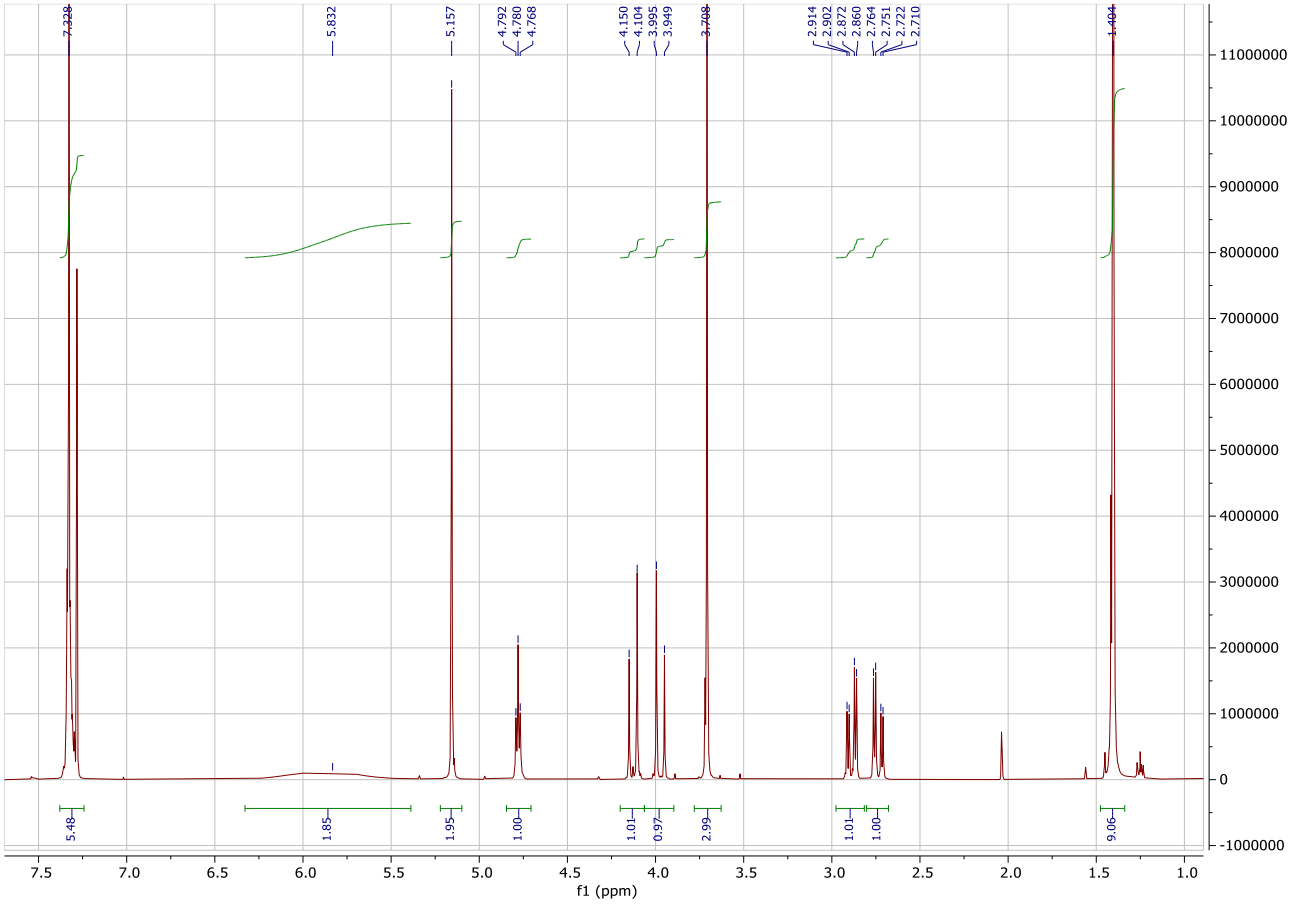
(S)-2,2'-(3-(4-fluorobenzyl)-2,5-dioxoimidazolidine-1,4-diyl)bis(N-(4-guanidinobutyl)acetamide), 3b. Yields: 60%. $[\alpha]^{20}_D$= + 3.4 (c = 0.8, MeOH); ^{1}H NMR (400 MHz, CD_3OD) δ 7.41-7.39 (m, 2H), 7.11-7.09 (m, 2H), 4.67 (d, *J* = 15.6 Hz, 1H), 4.51 (d, *J* = 15.6 Hz, 1H), 4.23-4.18 (m, 3H), 3.22-3.20 (m, 2H), 3.18-3.16 (m, 4H), 3.11-3.09 (m, 2H), 2.87-2.86 (m, 3H), 1.64-1.54 (m, 8H); ^{13}C NMR (101 MHz, CD_3OD) δ 172.9, 169.0, 168.0, 162.5 (d, *J* = 245.4 Hz), 159.3, 157.2, 156.7, 132.4, 129.8 (d, *J* = 8.1 Hz), 115.1 (d, *J* = 21.2 Hz), 57.0, 44.2, 41.0, 40.8, 40.7, 38.5, 38.4, 37.7, 34.0, 26.0, 25.96, 25.93, 25.7; ESI m/z 275.1 $[M+H, (81)]^{2+}$, 549.4 $[M+H, (100)]^+$; Anal. calcd. for $C_{24}H_{37}FN_{10}O_4$: C, 52.54; H, 6.80; N, 25.53; found: C, 52.54; H, 6.80; N, 25.52.

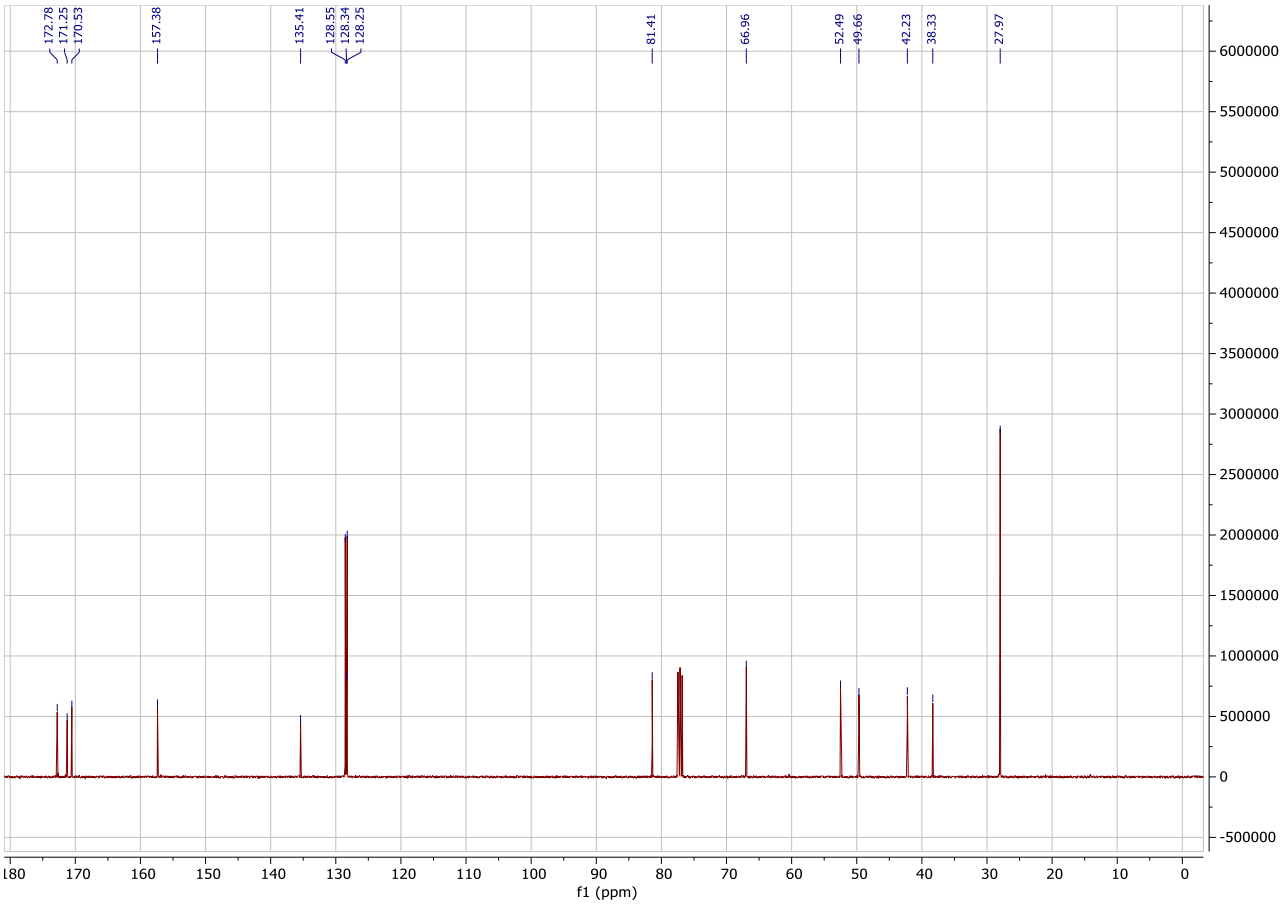
(S)-2,2'-(3-(naphthalen-1-ylmethyl)-2,5-dioxoimidazolidine-1,4-diyl)bis(N-(4-guanidinobutyl)acetamide), 3c. Yields: 71%. $[\alpha]^{20}_D$= + 1.1 (c = 0.6, MeOH); ^{1}H NMR (400 MHz, CD_3OD) δ 8.14-8.12 (m, 1H), 7.95 (br s, 1H), 7.89-7.84 (m, 2H), 7.53-7.45 (m, 4H), 5.08 (d, *J* = 15.6 Hz, 1H), 4.98 (d, *J* = 15.6 Hz, 1H), 4.23 (d, *J* = 16.8 Hz,

1H), 4.15 (d, *J* = 16.8 Hz, 1H), 4.09 (dd, *J* = 4.8 and 3.2 Hz, 1H), 3.28-3.26 (m, 2H), 3.18-3.16 (m, 2H), 3.10 (t, *J* = 6.8 Hz, 2H), 2.90-2.86 (m, 1H), 2.79-2.72 (m, 2H), 2.67 (dd, *J* = 16.8 and 4.8 Hz, 1H), 1.61-1.58 (m, 4H), 1.44-1.42 (m, 2H), 1.33-1.31 (m, 2H); ^{13}C NMR (101 MHz, CD_3OD) δ 173.0, 168.8, 168.0, 157.3, 157.2, 156.6, 134.4, 131.34, 131.31, 128.8, 128.5, 126.8, 126.3, 125.8, 125.1, 123.1, 57.3, 43.7, 41.0, 40.7, 40.6, 38.4, 38.3, 34.0, 25.9, 25.8, 25.6; ESI m/z 291.1 $[M+H, (100)]^{2+}$, 581.5 $[M+H, (100)]^{+}$; Anal. calcd. for $C_{28}H_{40}N_{10}O_4$: C, 57.91; H, 6.94; N, 24.12; found: C, 57.90; H, 6.95; N, 24.12.


BnOOC
N
H
O
N
H
COOtBu
COOMe

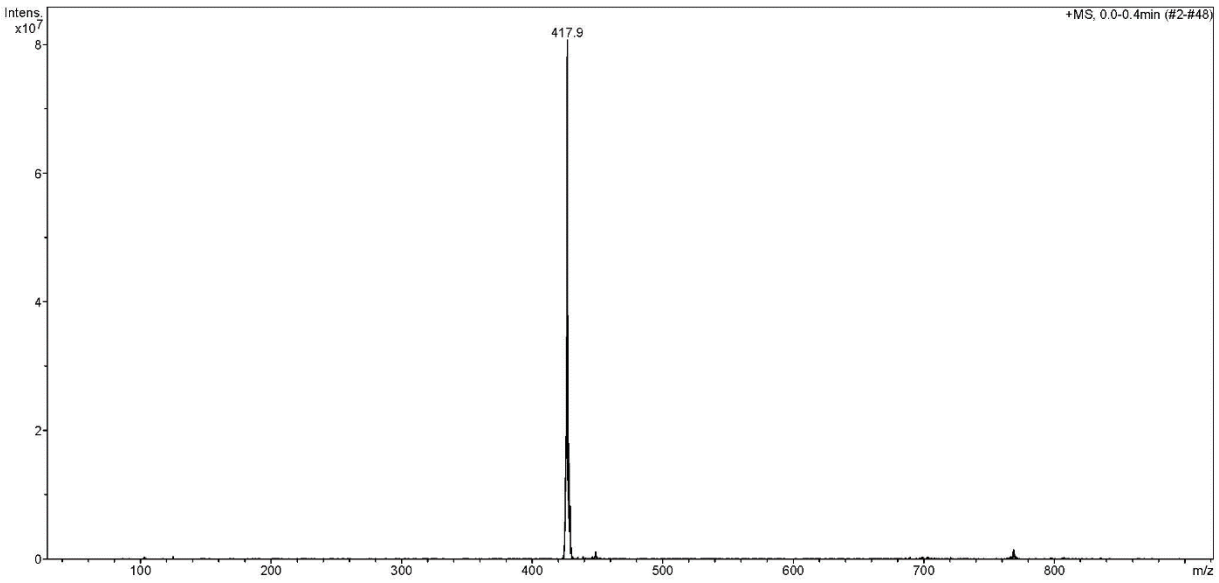
6b


7.328
5.832
5.157
4.792
4.780
4.768
4.150
4.104
3.995
3.949
3.708
2.914
2.902
2.872
2.860
2.764
2.751
2.722
2.710
1.404
11000000
10000000
9000000
8000000
7000000
6000000
5000000
4000000
3000000
2000000
1000000
0
-1000000
5.48
1.85
1.95
1.00
1.01
0.97
2.99
1.01
1.00
9.06
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)

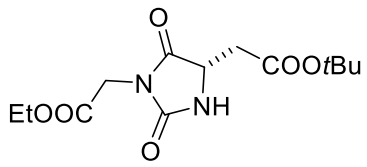


-L.G.S. - Laboratorio Grandi Strumenti - Display Report

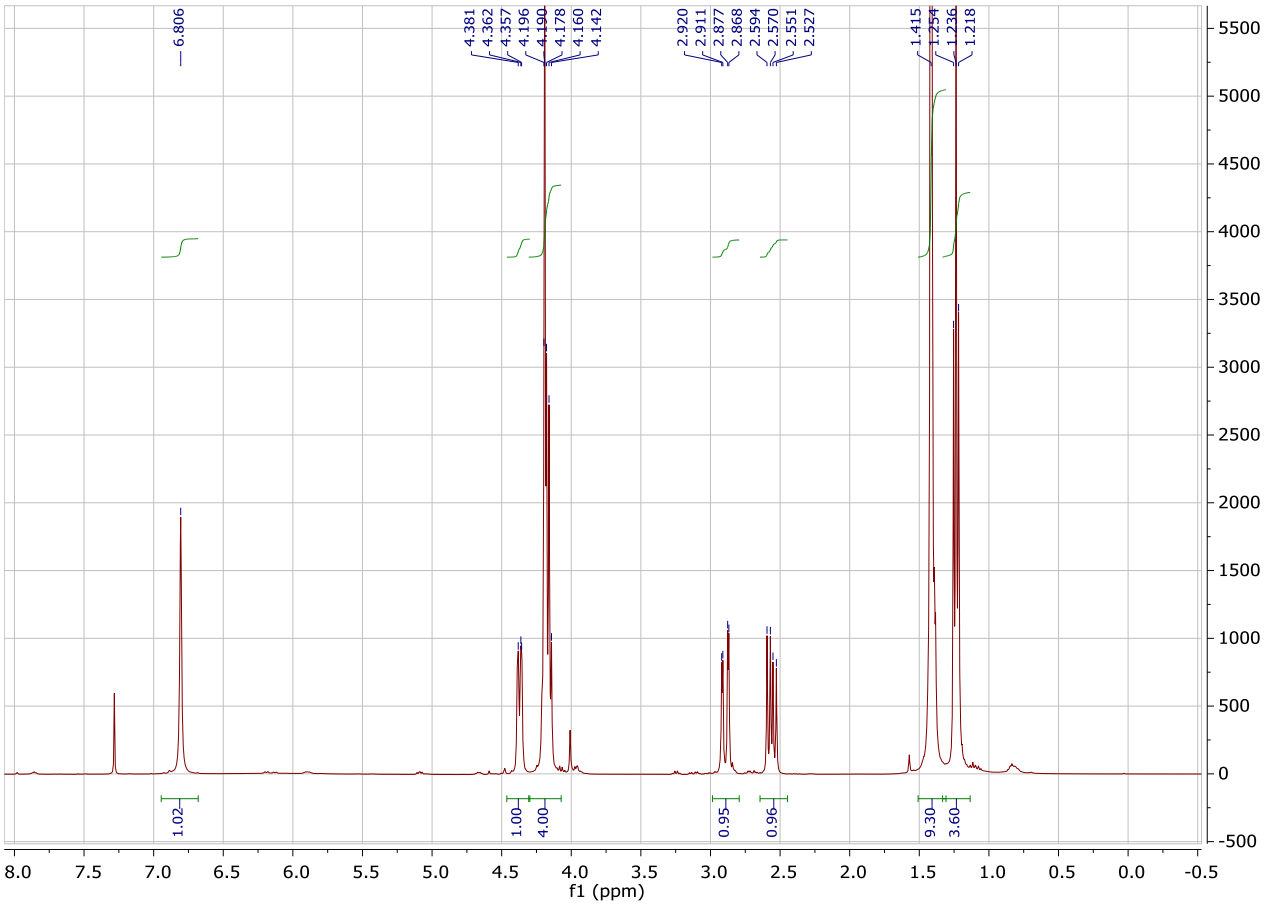
Analysis Name	av fm2684 f 10-12.d	Acquisition Date	06/16/15 11:57:39	Operator	Walter Panzeri
Sample Name		Method	Copy of _01tmix_posneg lm.MS	Instrument	esquire3000plus
Comment	1 mg/ml dil 1:100 MeOH + HCOOH 0.1%				
	Richiedente: Frigerio				

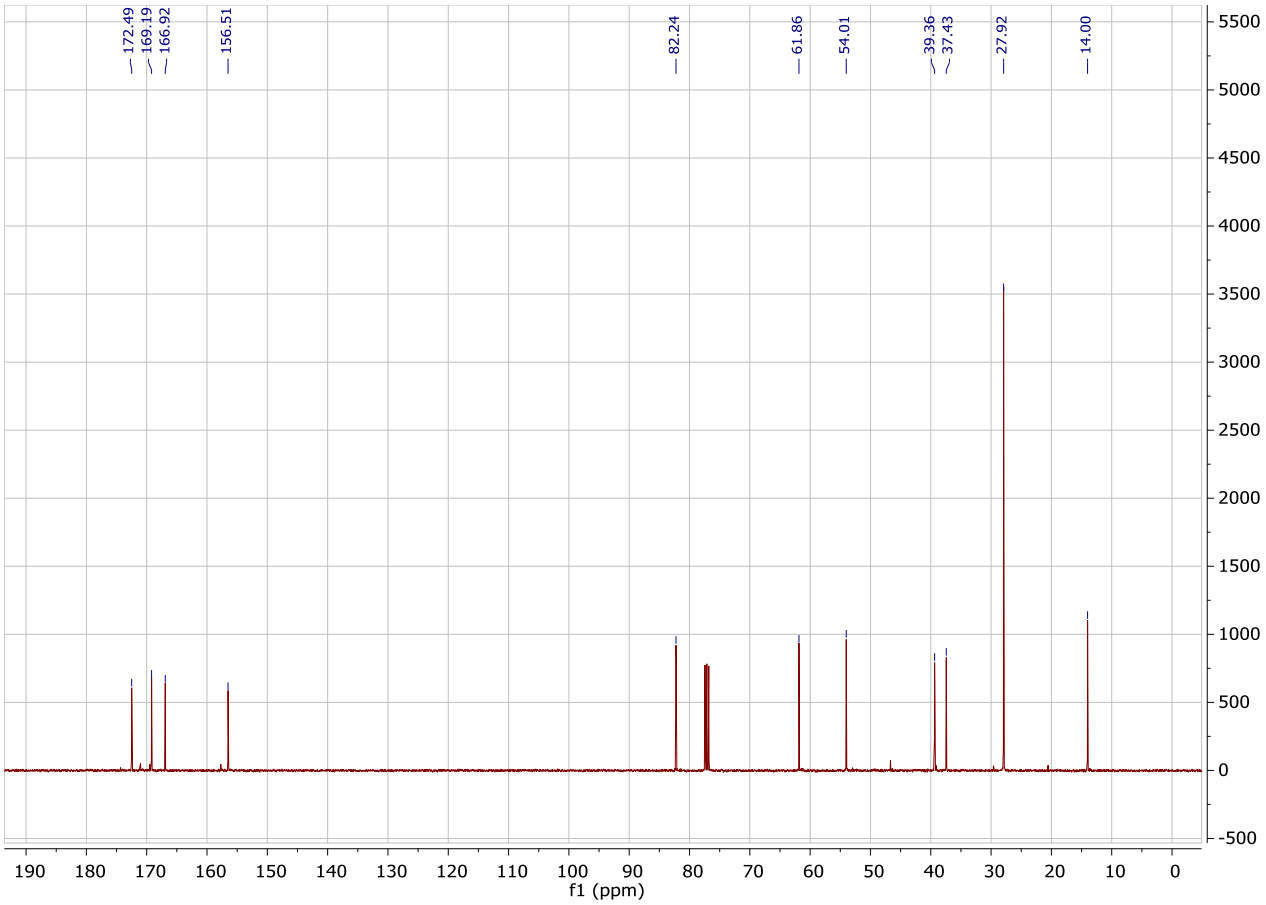


Bruker Daltonics DataAnalysis 3.1 printed: 06/16/15 12:01:20 Page 1 of 1


O
N
NH
O
EtOOC
COO*t*Bu

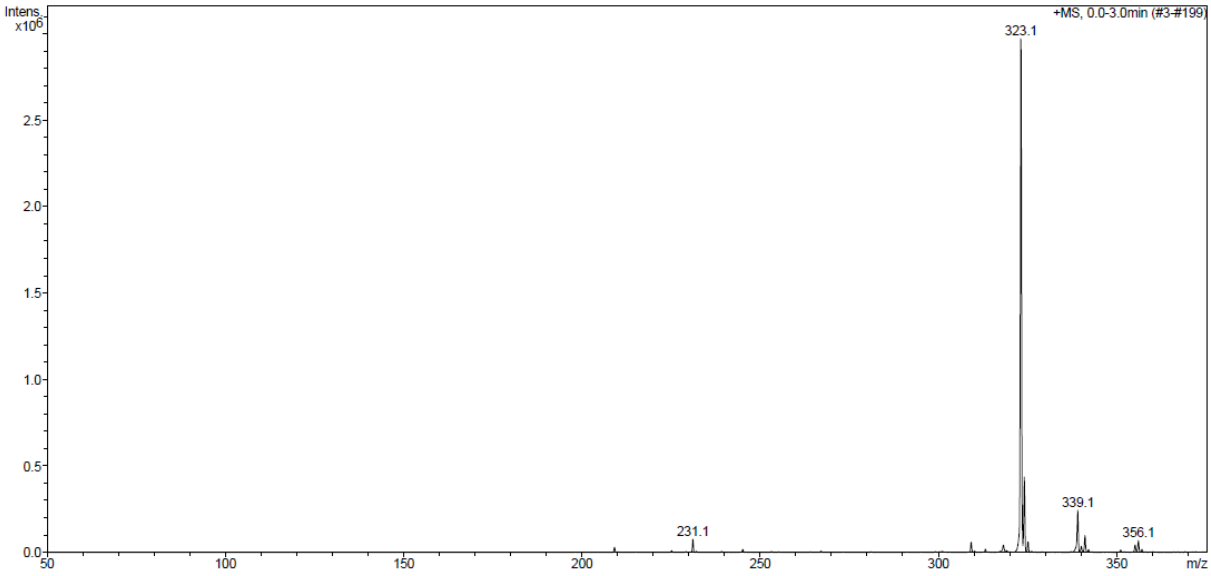
7a


6.806
4.381
4.362
4.357
4.196
4.190
4.178
4.160
4.142
2.920
2.911
2.877
2.868
2.594
2.570
2.551
2.527
1.415
1.254
1.236
1.218
1.02
1.00
4.00
0.95
0.96
9.30
3.60
f1 (ppm)

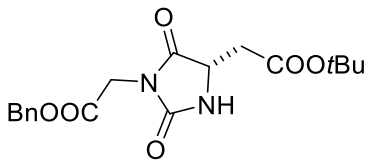


-L.G.S. - Laboratorio Grandi Strumenti - Display Report

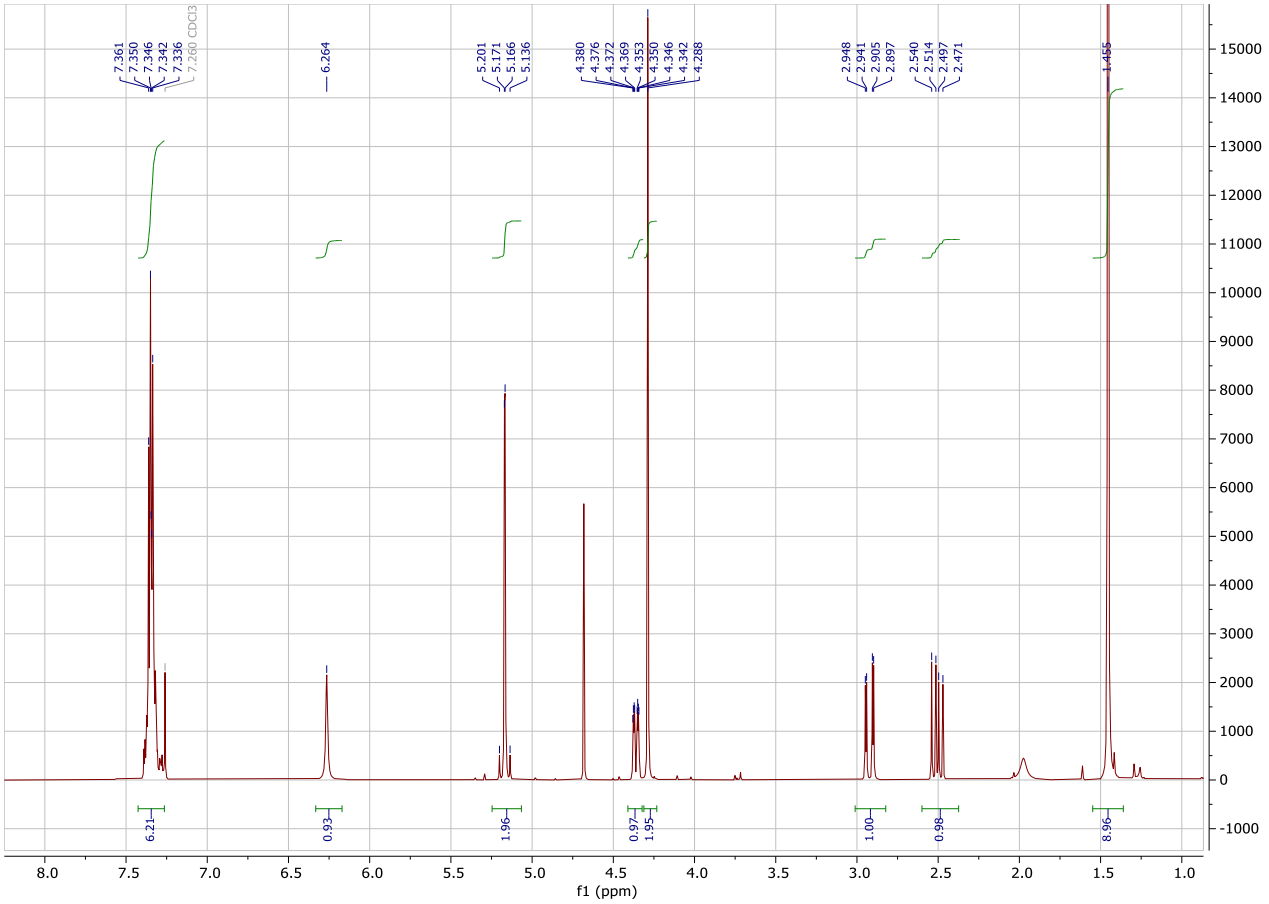
Analysis Name	av 2950.d	Acquisition Date	09/02/22 12:41:30	Operator	Walter Panzeri
Sample Name		Method	Copy of $opt0622.MS	Instrument	esquire3000plus
Comment	1 mg/mL dil 1:100 MeOH Richiedente: Volonterio				

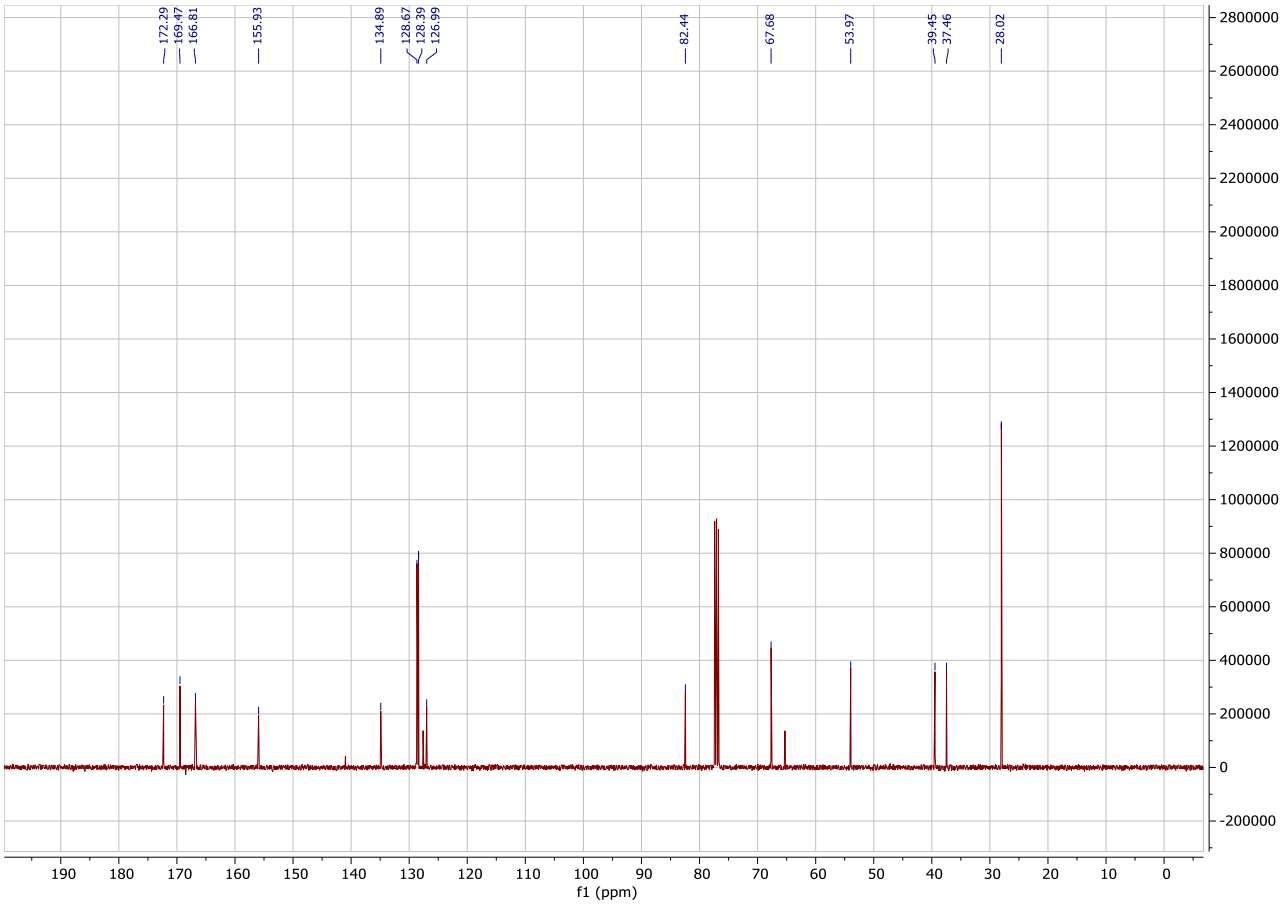


Bruker Daltonics DataAnalysis 3.1 printed: 09/02/22 12:51:33 Page 1 of 1


O
N
NH
O
COOtBu
BnOOC

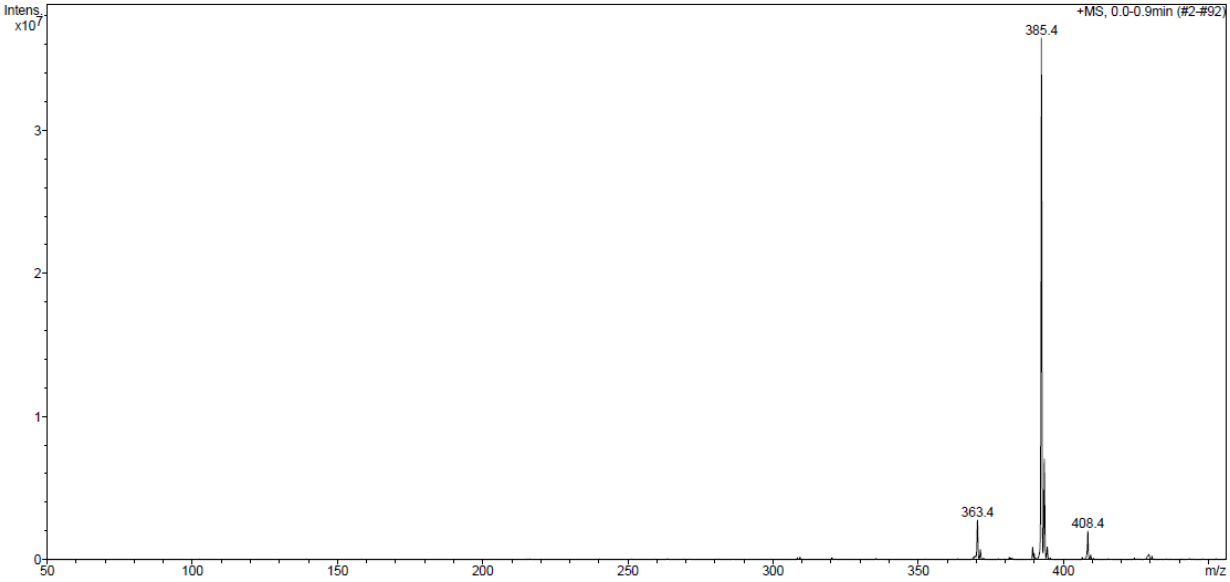
7b


7.361
7.350
7.346
7.342
7.336
7.260 CDCl3
6.264
5.201
5.171
5.166
5.136
4.380
4.376
4.372
4.369
4.353
4.350
4.346
4.342
4.288
2.948
2.941
2.905
2.897
2.540
2.514
2.497
2.471
1.456
6.21
0.93
1.96
0.97
1.95
1.00
0.98
8.96
f1 (ppm)

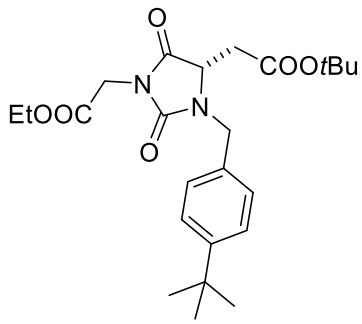


-L.G.S. - Laboratorio Grandi Strumenti - Display Report

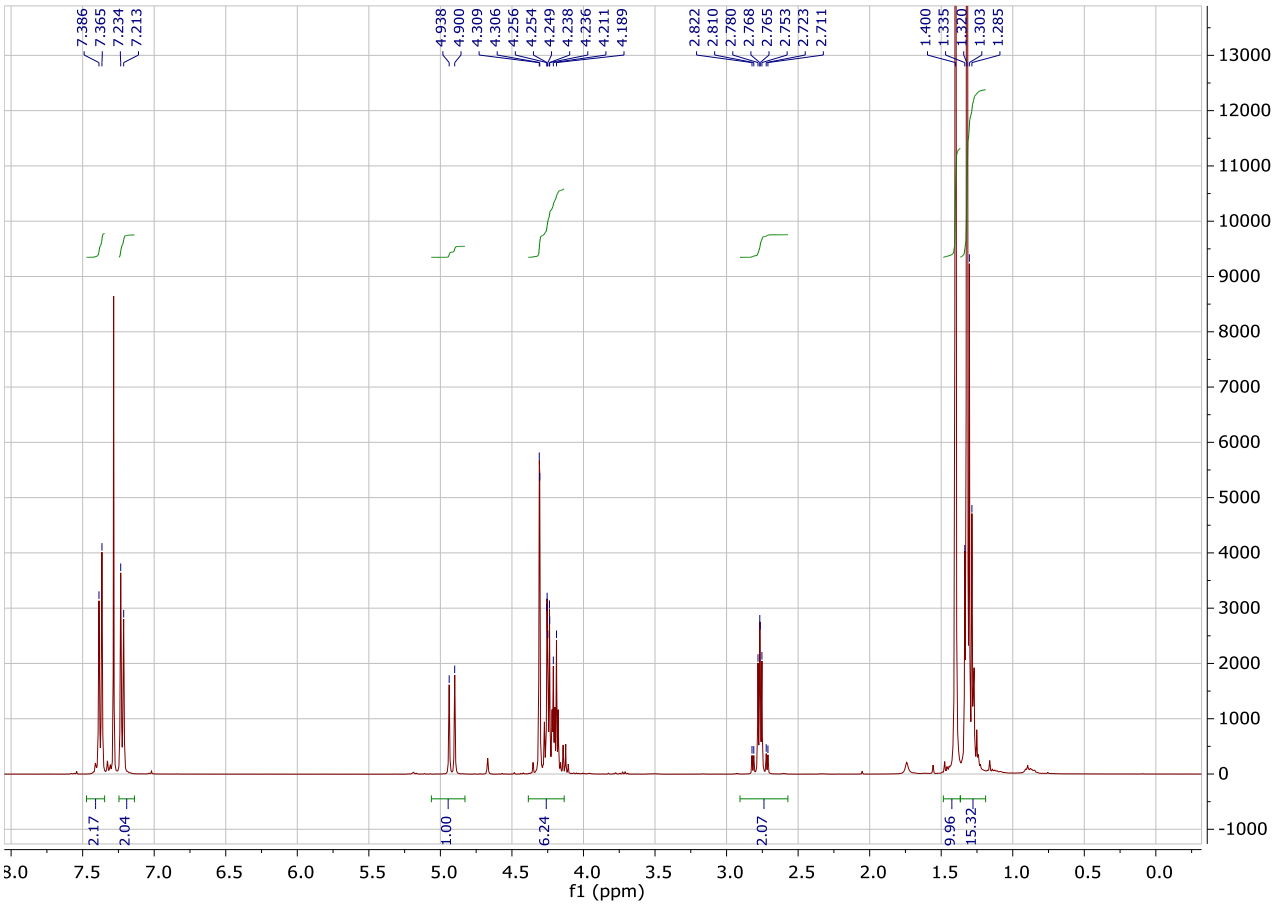
Analysis Name	av gc20_c.d	Acquisition Date	01/26/18 14:43:10	Operator	Walter Panzeri
Sample Name		Method	Copy of _01tmix_posneg lm.MS	Instrument	esquire3000plus
Comment	1 mg/ml H2O Richiedente: Cristina				

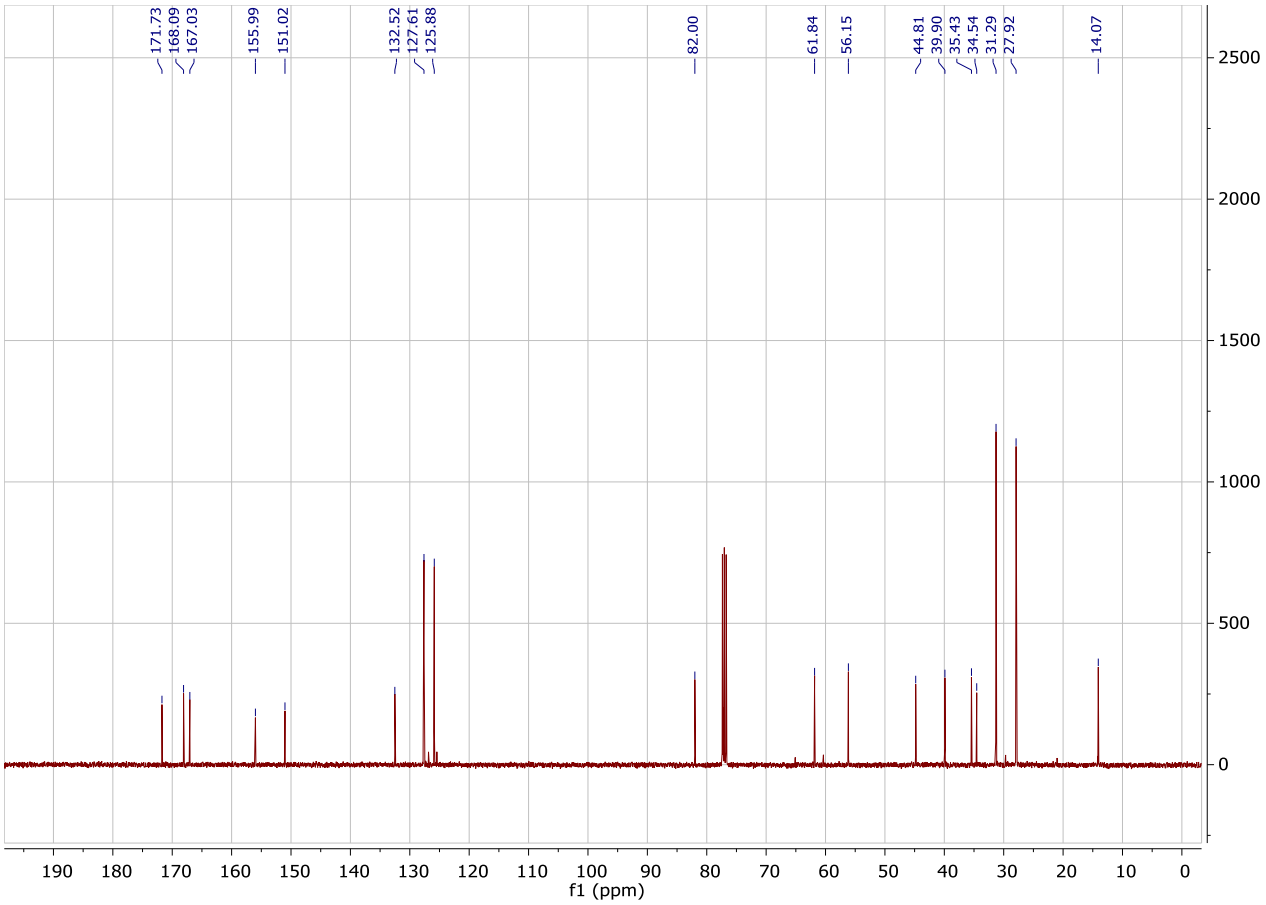


Bruker Daltonics DataAnalysis 3.1 printed: 01/26/18 14:44:33 Page 1 of 1


O
N
N
O
O
EtOOC
COO*t*Bu

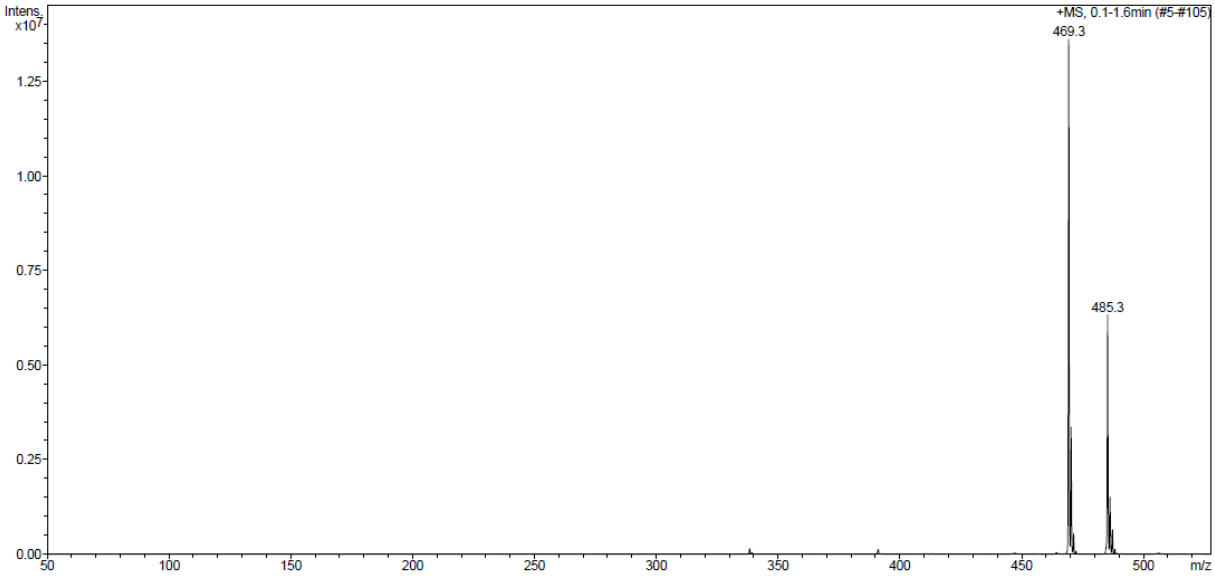
9a


7.386
7.365
7.234
7.213
4.938
4.900
4.309
4.306
4.256
4.254
4.249
4.238
4.236
4.211
4.189
2.822
2.810
2.780
2.768
2.765
2.753
2.723
2.711
1.400
1.335
1.320
1.303
1.285
2.17
2.04
1.00
6.24
2.07
9.96
15.32
f1 (ppm)

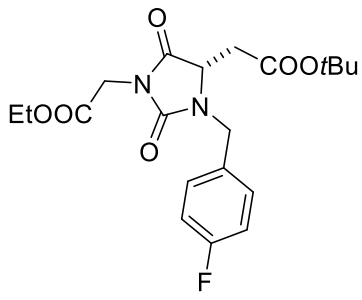


-L.G.S. - Laboratorio Grandi Strumenti - Display Report

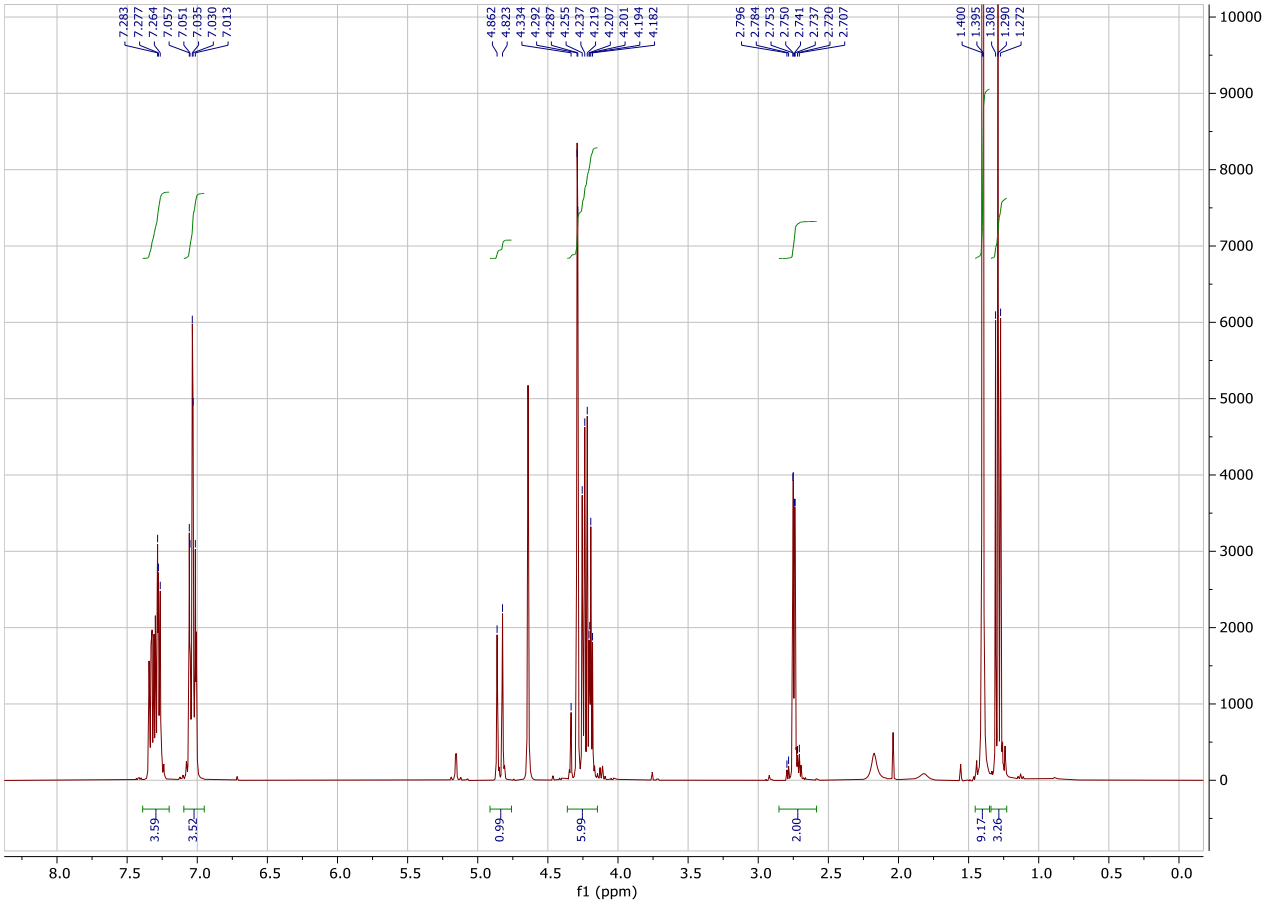
Analysis Name	av 2951.d	Acquisition Date	09/08/22 09:16:37	Operator	Walter Panzeri
Sample Name		Method	Copy of $opt0622.MS	Instrument	esquire3000plus
Comment	1 mg/mL dil 1:100 MeOH Richiedente: Volonterio				



Bruker Daltonics DataAnalysis 3.1 printed: 09/08/22 09:20:19 Page 1 of 1

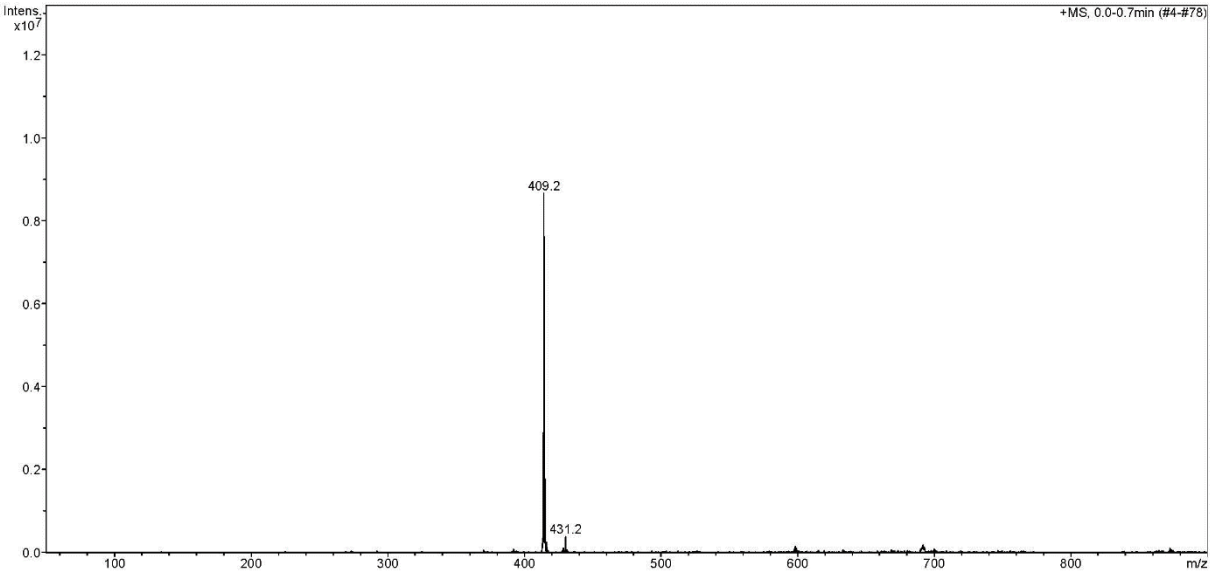

O
N
N
O
EtOOC
COO*t*Bu
F

9b

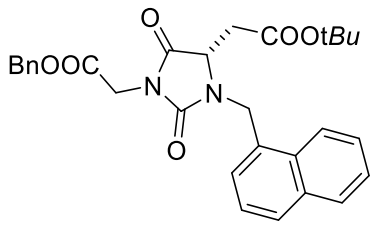

7.283
7.277
7.264
7.057
7.051
7.035
7.030
7.013
4.862
4.823
4.334
4.292
4.287
4.255
4.237
4.219
4.207
4.201
4.194
4.182
2.796
2.784
2.753
2.750
2.741
2.737
2.720
2.707
1.400
1.395
1.308
1.290
1.272
3.59
3.52
0.99
5.99
2.00
9.17
3.26
f1 (ppm)

-L.G.S. - Laboratorio Grandi Strumenti - Display Report

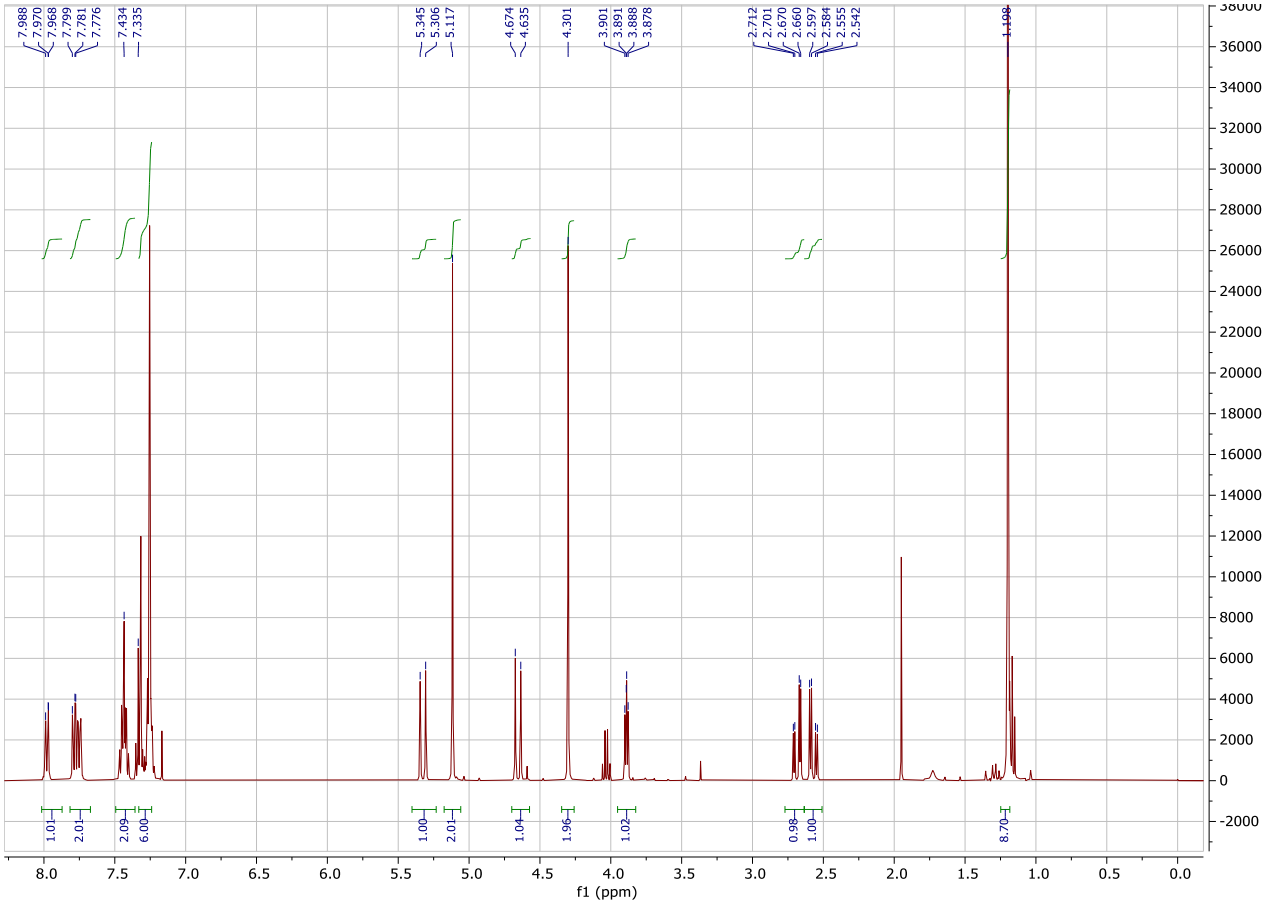
Analysis Name	av fm2686b.d	Acquisition Date	06/22/15 13:40:16	Operator	Walter Panzeri
Sample Name		Method	Copy of _01tmix_posneg lm.MS	Instrument	esquire3000plus
Comment	1 mg/ml dil 1:100 MeOH Richiedente: Frigerio				

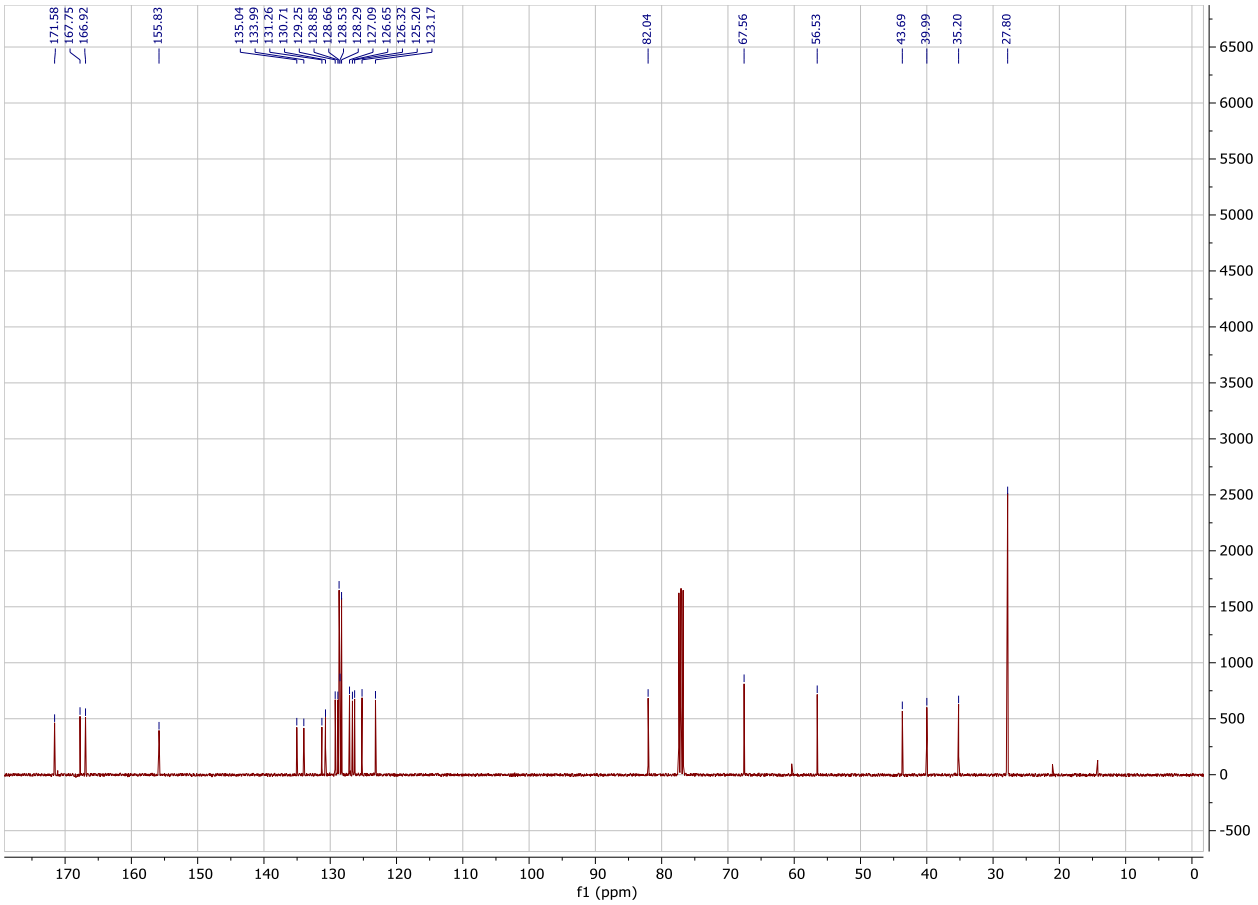


Bruker Daltonics DataAnalysis 3.1 printed: 06/22/15 13:41:30 Page 1 of 1


O
COOtBu
BnOOC
N
N
O

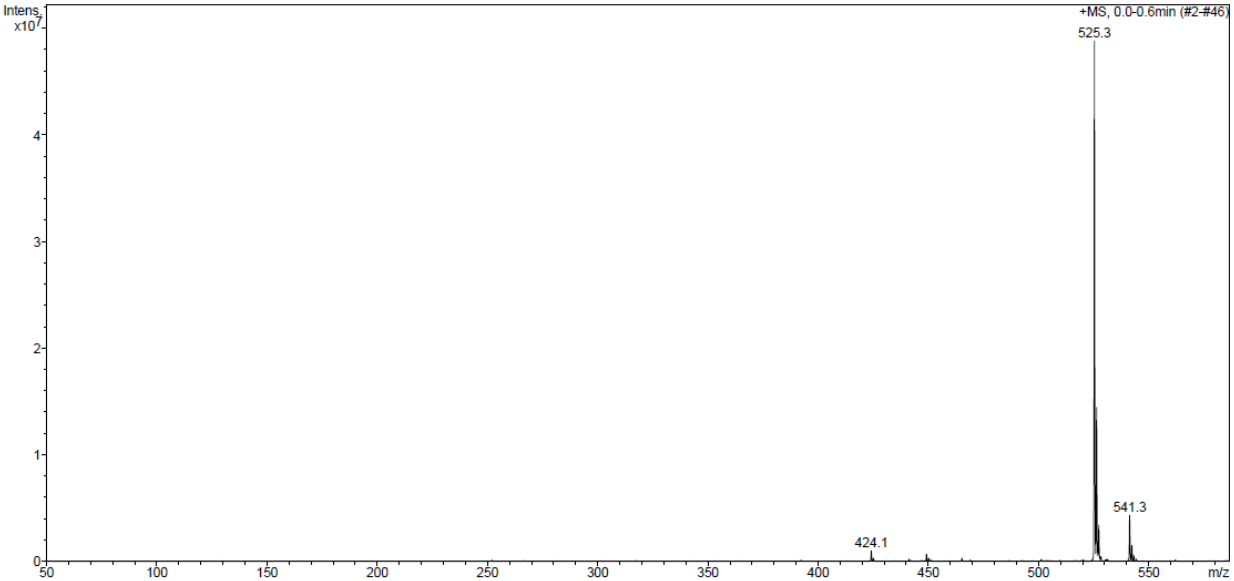
9c


7.988
7.970
7.968
7.799
7.781
7.776
7.434
7.335
5.345
5.306
5.117
4.674
4.635
4.301
3.901
3.891
3.888
3.878
2.712
2.701
2.670
2.660
2.597
2.584
2.555
2.542
1.108
1.01
2.01
2.09
6.00
1.00
2.01
1.04
1.96
1.02
0.98
1.00
8.70
f1 (ppm)

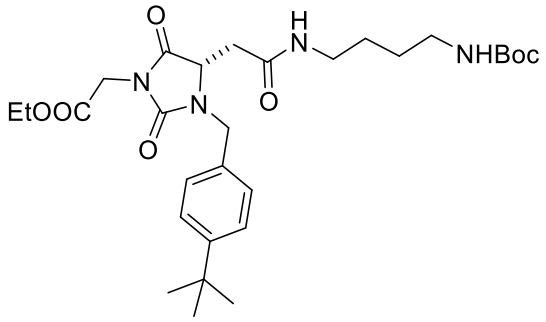


-L.G.S. - Laboratorio Grandi Strumenti - Display Report

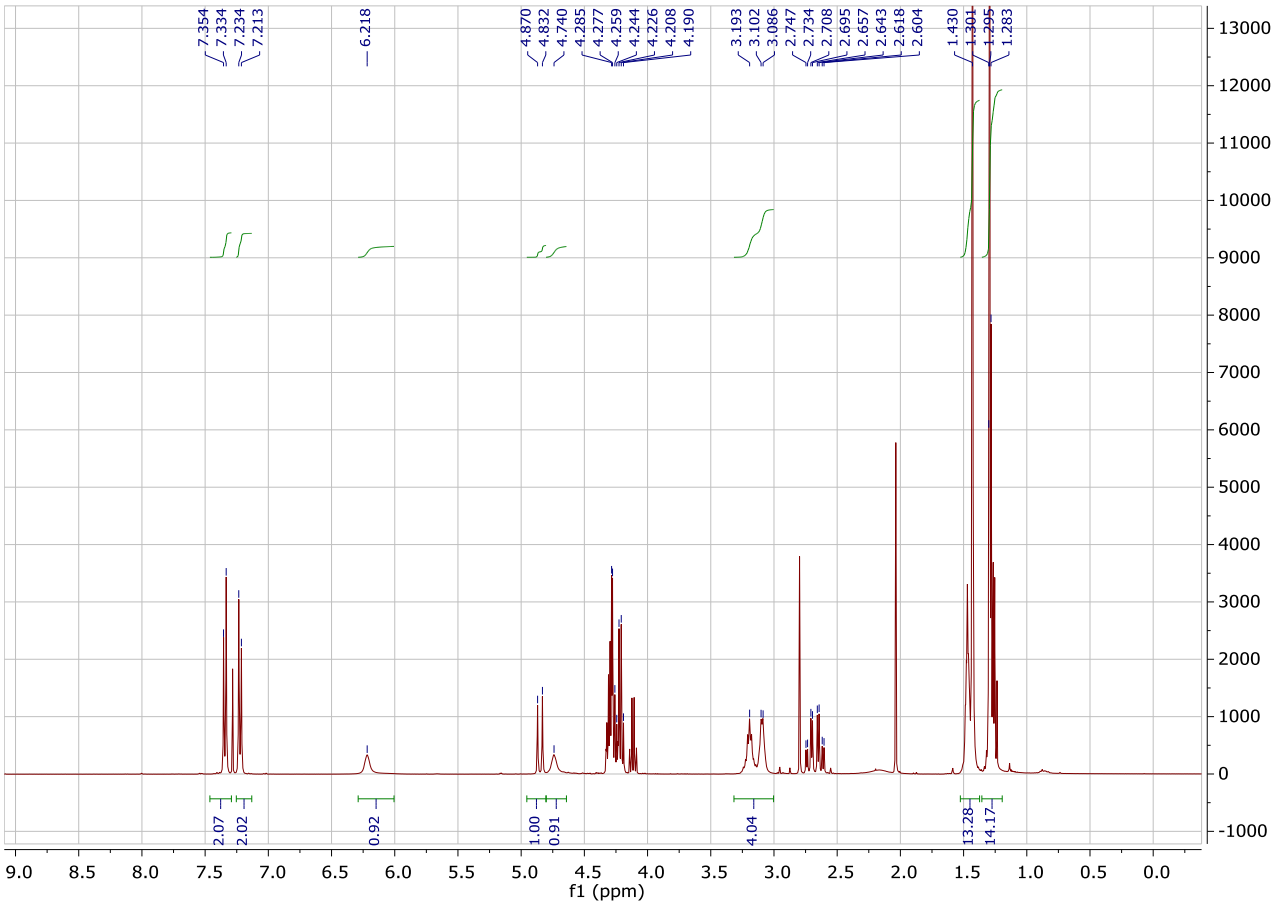
Analysis Name	av ac067.d	Acquisition Date	07/24/20 16:24:44	Operator	Administrator
Sample Name		Method	Copy of _01tmix_posneg lm.MS	Instrument	esquire3000plus
Comment	1mg/ml dil 1:100 MeOH Richiedente: Caramiello				

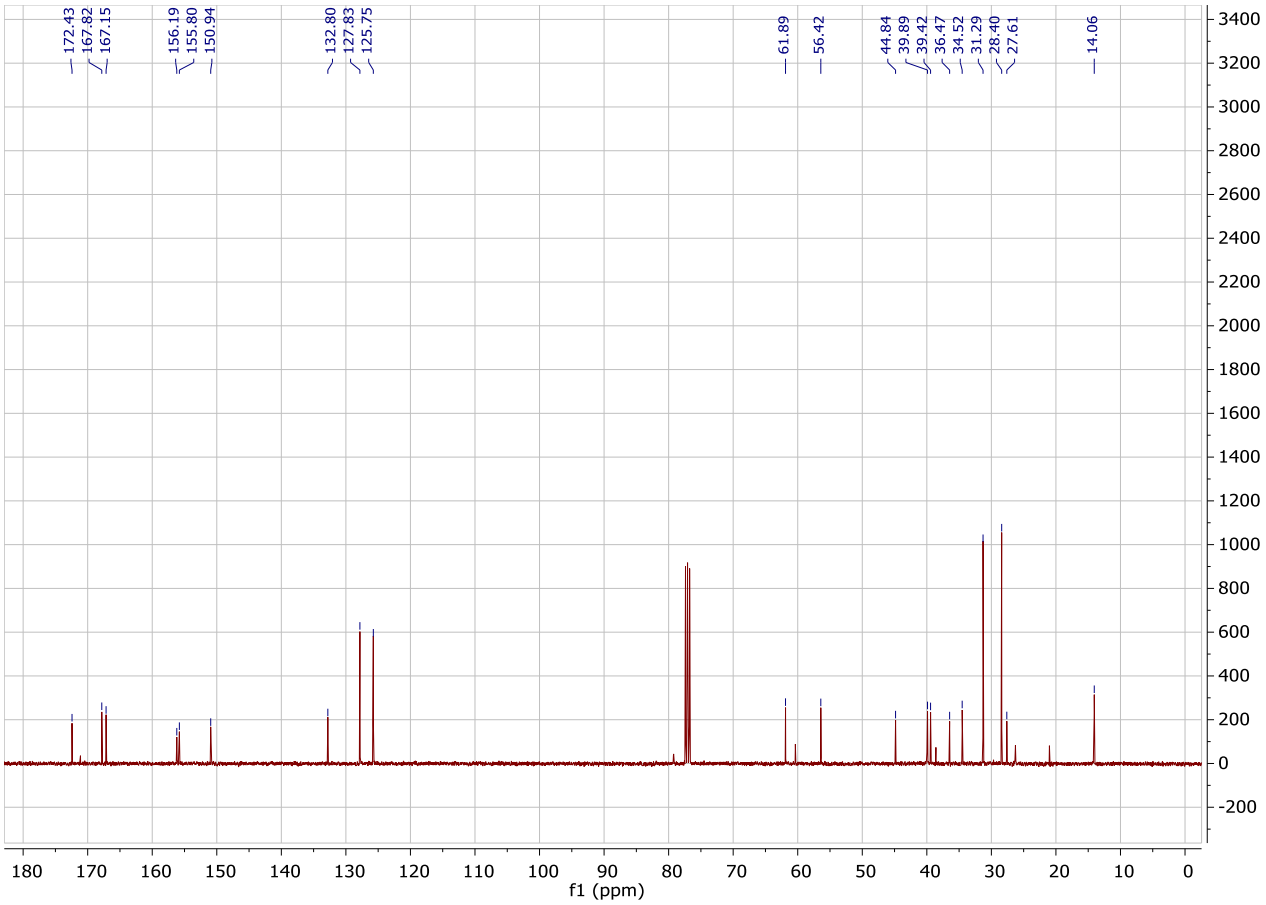


Bruker Daltonics DataAnalysis 3.1 printed: 07/24/20 16:25:33 Page 1 of 1


O
H
N
NHBoc
EtOOC
N
N
O
O
O

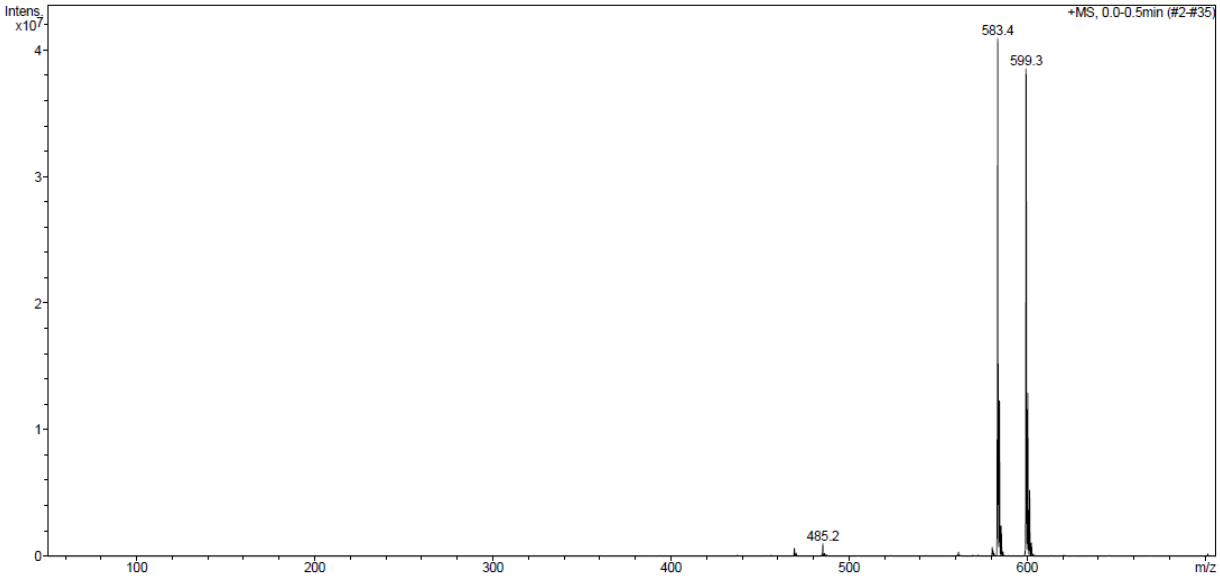
11a


7.354
7.334
7.234
7.213
6.218
4.870
4.832
4.740
4.285
4.277
4.259
4.244
4.226
4.208
4.190
3.193
3.102
3.086
2.747
2.734
2.708
2.695
2.657
2.643
2.618
2.604
1.430
1.301
1.295
1.283
2.07
2.02
0.92
1.00
0.91
4.04
13.28
14.17
f1 (ppm)

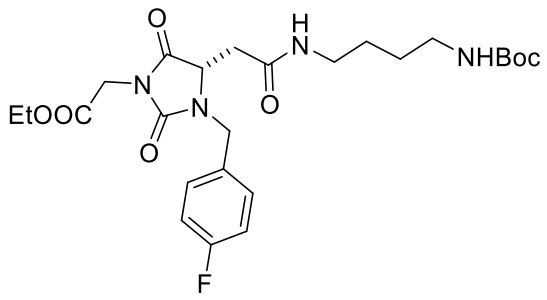


-L.G.S. - Laboratorio Grandi Strumenti - Display Report

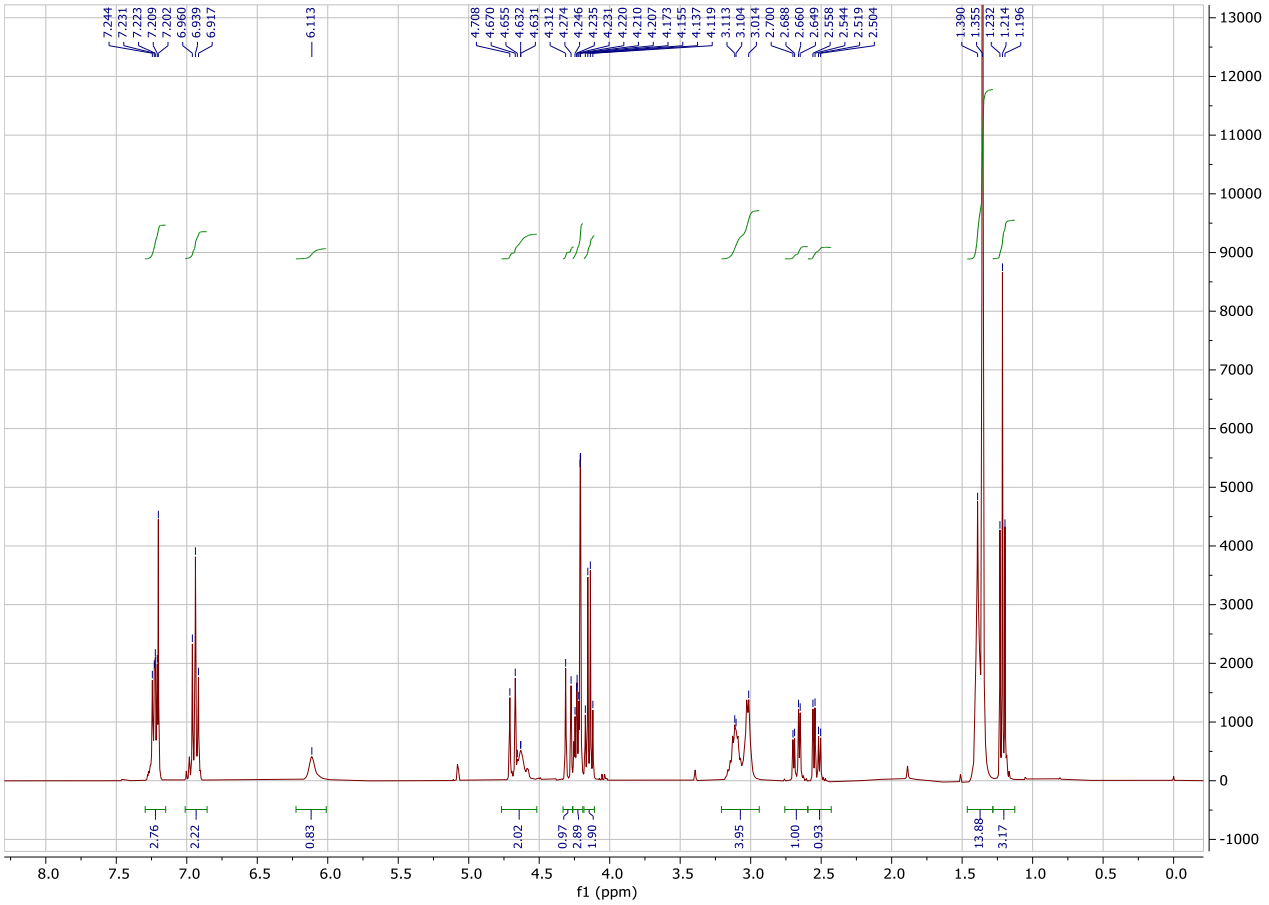
Analysis Name	av 2954.d	Acquisition Date	09/08/22 09:12:28	Operator	Walter Panzeri
Sample Name		Method	Copy of $opt0622.MS	Instrument	esquire3000plus
Comment	1 mg/mL dil 1:100 MeOH Richiedente: Volonterio				

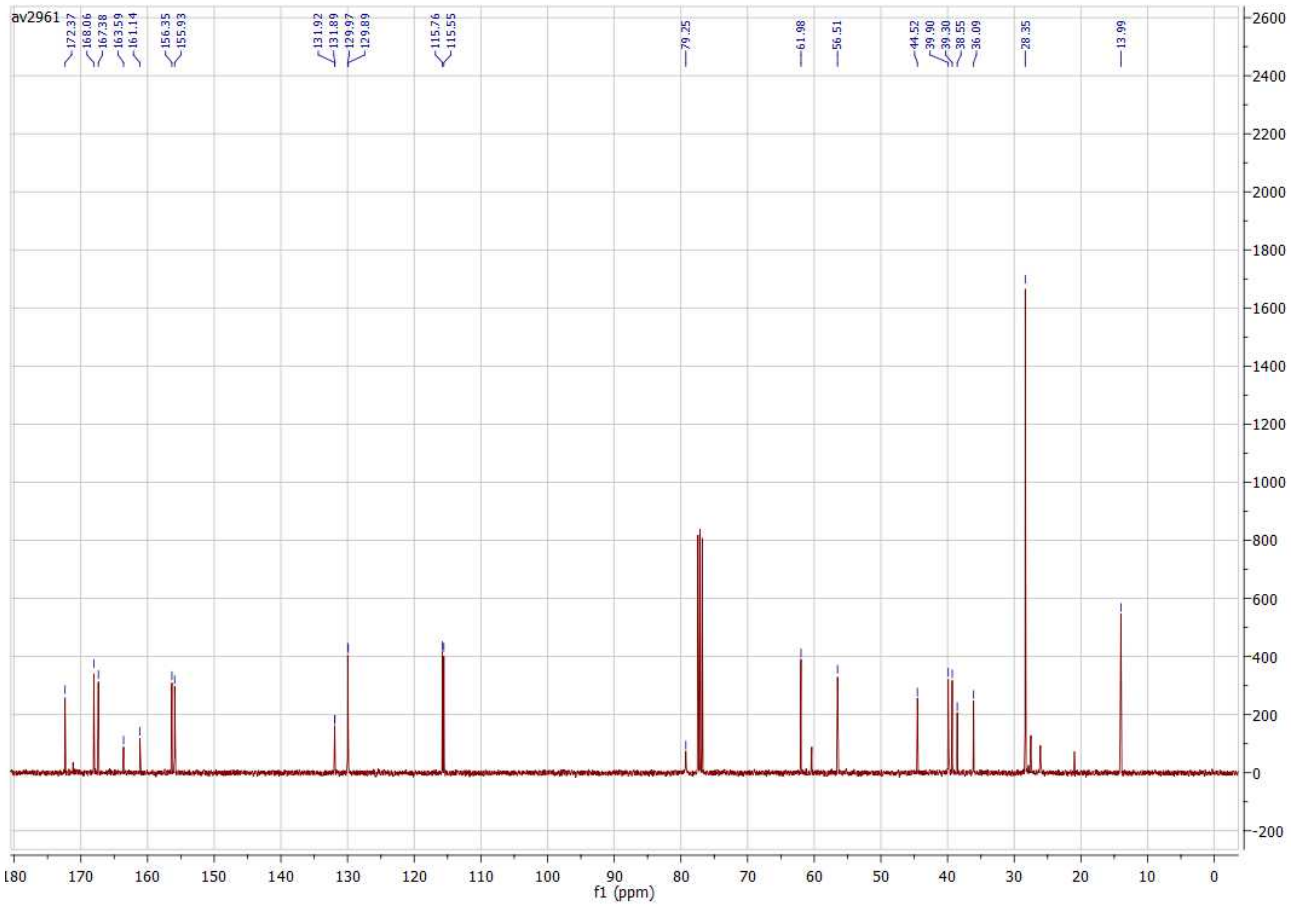


Bruker Daltonics DataAnalysis 3.1 printed: 09/08/22 09:14:11 Page 1 of 1


O
H
N
NHBoc
EtOOC
N
N
O
O
F

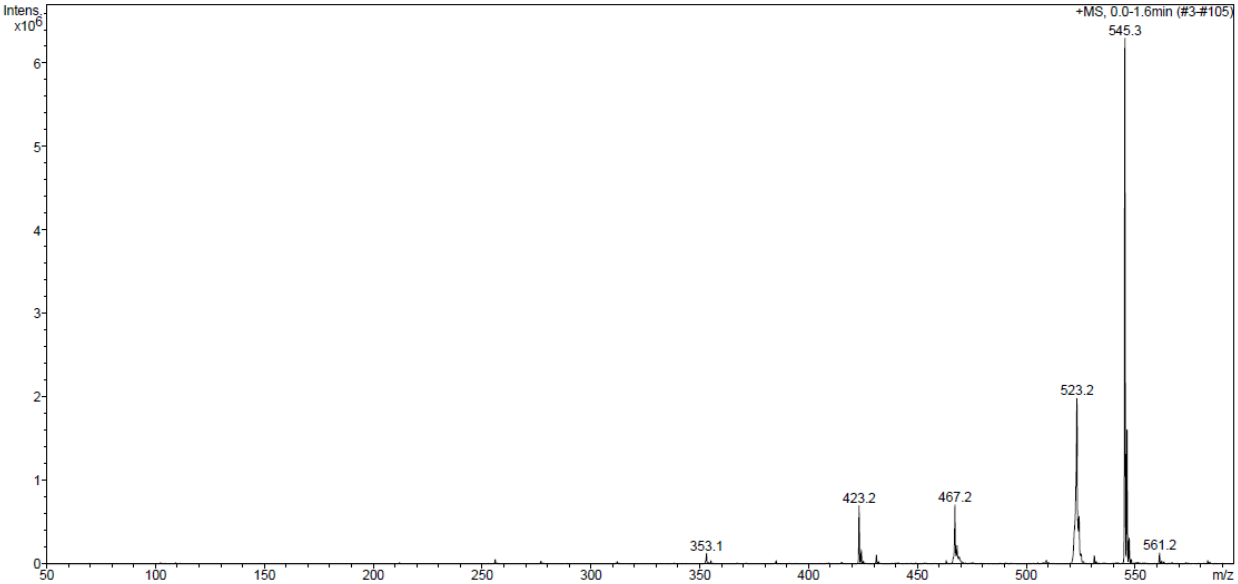
11b


7.244
7.231
7.223
7.209
7.202
6.960
6.939
6.917
6.113
4.708
4.670
4.655
4.632
4.631
4.312
4.274
4.246
4.235
4.231
4.210
4.207
4.173
4.155
4.137
4.119
3.113
3.104
3.014
2.700
2.688
2.660
2.649
2.558
2.544
2.519
2.504
1.390
1.355
1.232
1.214
1.196
2.76
2.22
0.83
2.02
0.97
2.89
1.90
3.95
1.00
0.93
13.88
3.17
f1 (ppm)

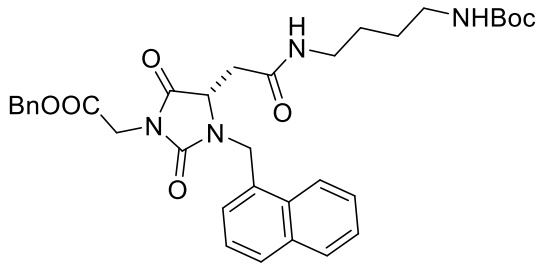


-L.G.S. - Laboratorio Grandi Strumenti - Display Report

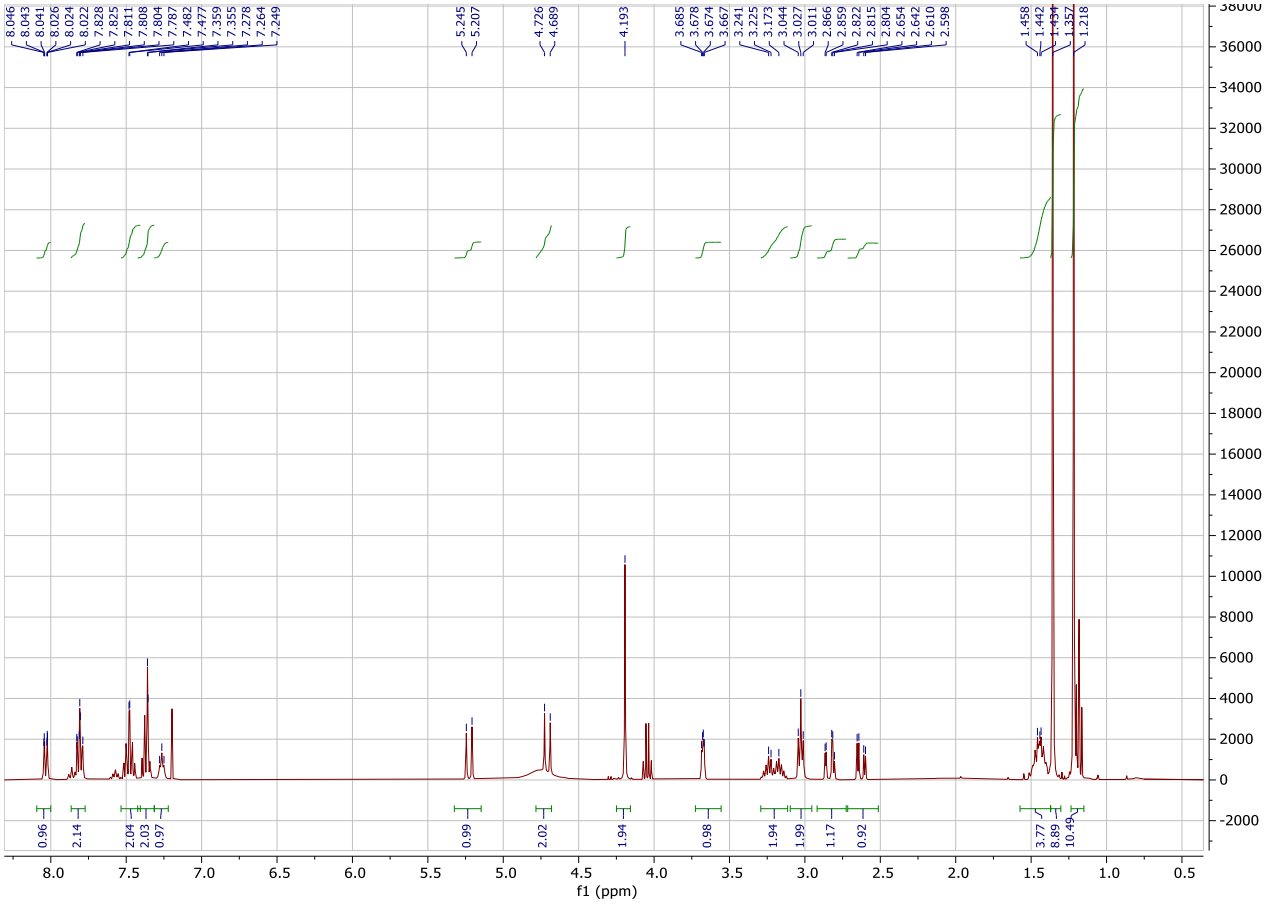
Analysis Name	av 2961.d	Acquisition Date	10/26/22 08:36:11	Operator	Walter Panzeri
Sample Name		Method	Copy of $opt0622.MS	Instrument	esquire3000plus
Comment	1 mg/mL Dil 1:100 MeOH Richiedente: Volonterio				



Bruker Daltonics DataAnalysis 3.1 printed: 10/26/22 08:38:07 Page 1 of 1

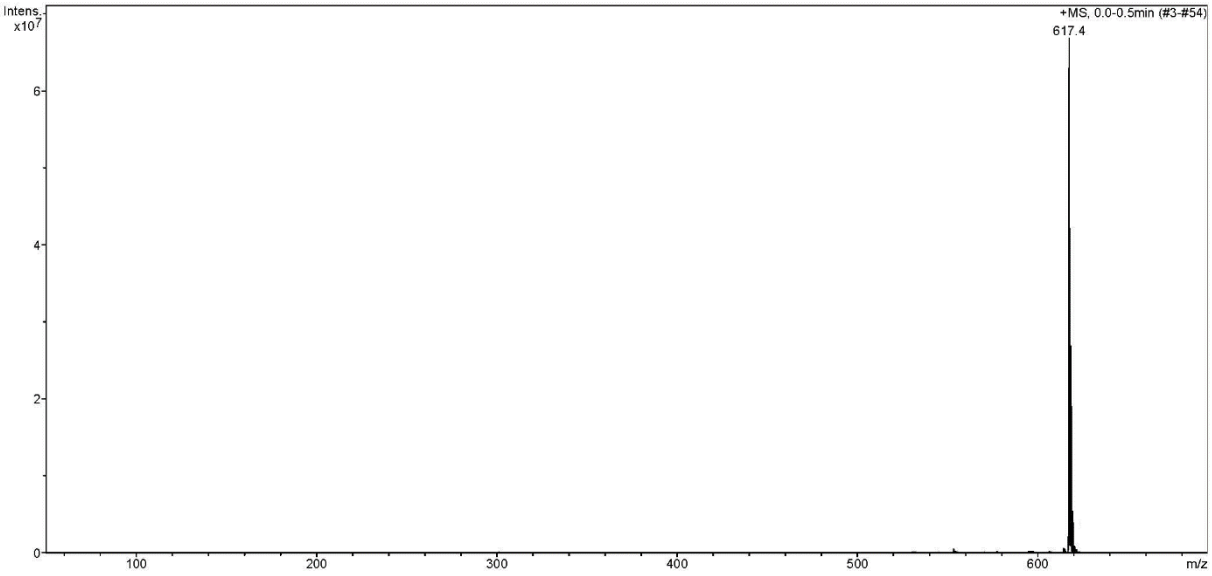

NHBoc
H
N
O
BnOOC
N
N
O
O
O

11c

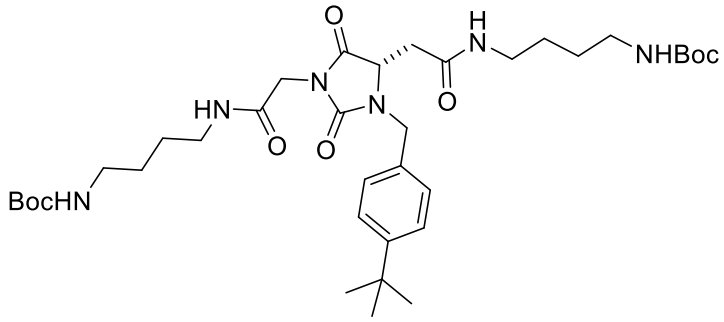

8.046
8.043
8.041
8.026
8.024
8.022
7.828
7.825
7.811
7.808
7.804
7.787
7.482
7.477
7.359
7.355
7.278
7.264
7.249
5.245
5.207
4.726
4.689
4.193
3.685
3.678
3.674
3.667
3.241
3.225
3.173
3.044
3.027
3.011
2.866
2.859
2.822
2.815
2.804
2.654
2.642
2.610
2.598
1.458
1.442
1.431
1.357
1.218
0.96
2.14
2.04
2.03
0.97
0.99
2.02
1.94
0.98
1.94
1.99
1.17
0.92
3.77
8.89
10.49
f1 (ppm)

-L.G.S. - Laboratorio Grandi Strumenti - Display Report

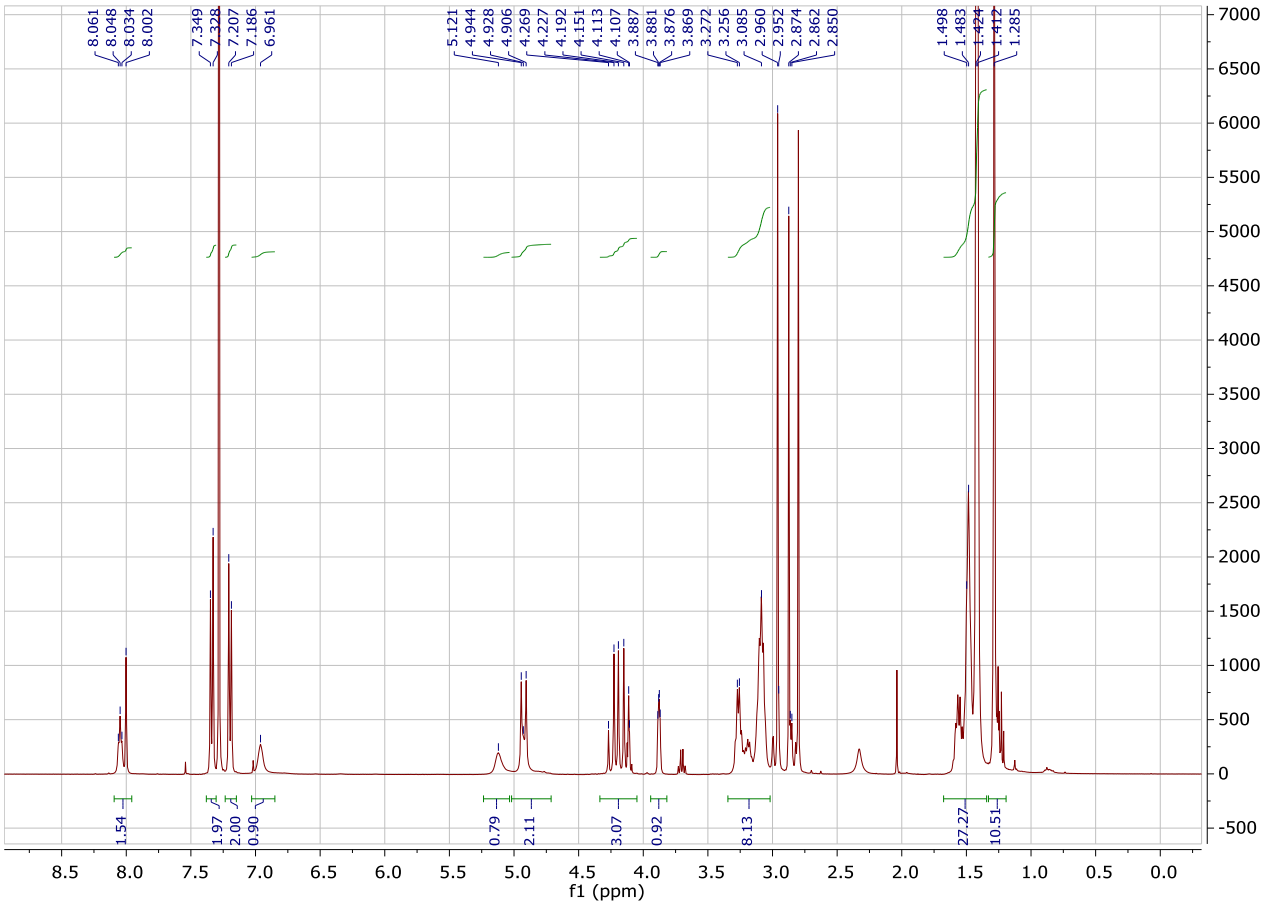
Analysis Name	av fm2856.d	Acquisition Date	07/13/17 13:23:26	Operator	Walter Panzeri
Sample Name		Method	Copy of _01tmix_posneg lm.MS	Instrument	esquire3000plus
Comment	1 mg/ml dil 1:100 MeOH Richiedente: Frigerio				

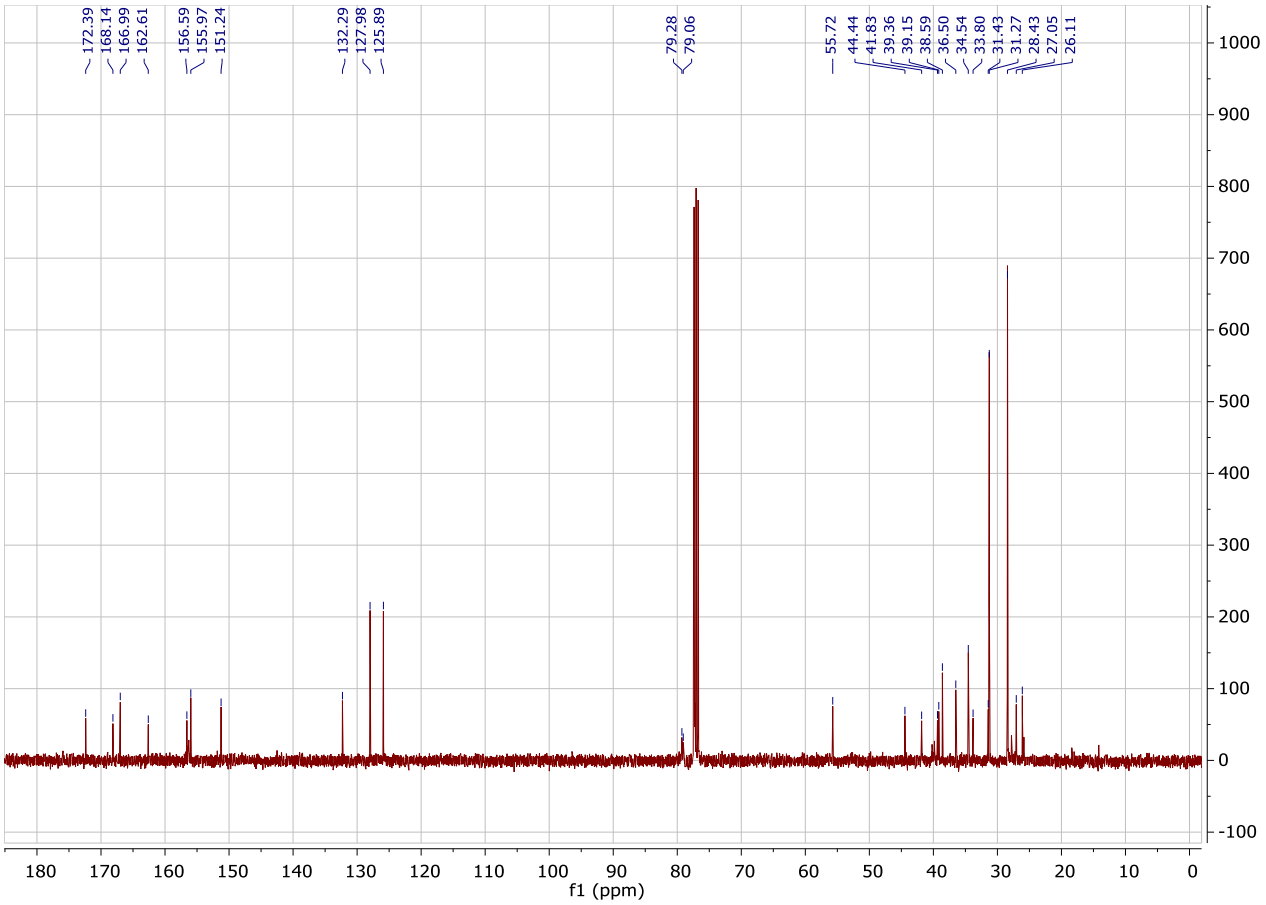


Bruker Daltonics DataAnalysis 3.1 printed: 07/13/17 13:24:17 Page 1 of 1


O
H
N
NHBoc
O
N
HN
N
O
O
BocHN

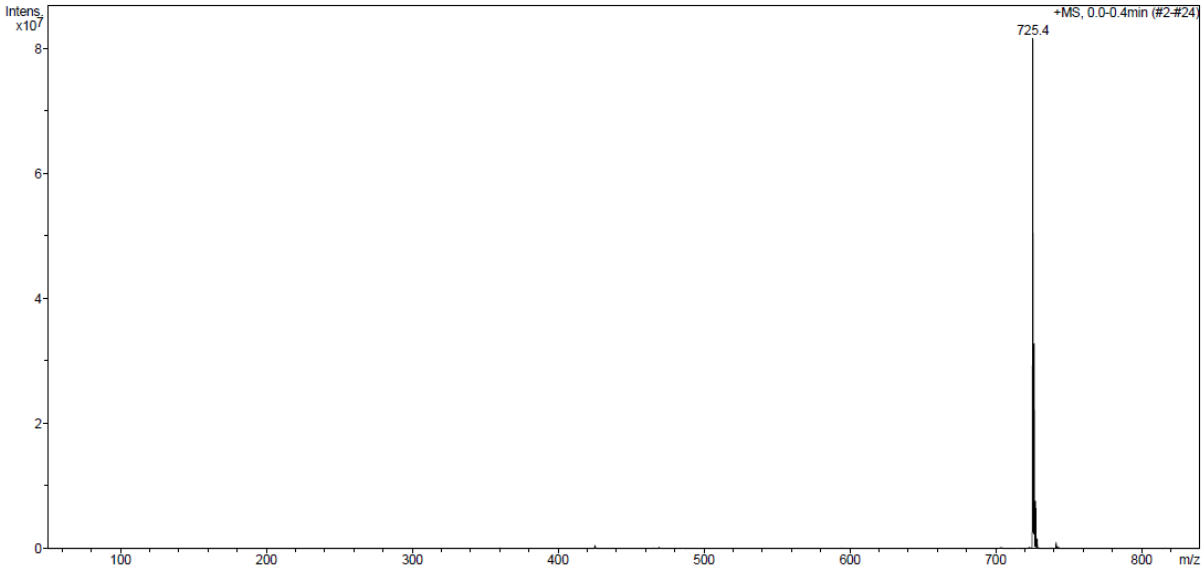
12a


8.061
8.048
8.034
8.002
7.349
7.328
7.207
7.186
6.961
5.121
4.944
4.928
4.906
4.269
4.227
4.192
4.151
4.113
4.107
3.887
3.881
3.876
3.869
3.272
3.256
3.085
2.960
2.952
2.874
2.862
2.850
1.498
1.483
1.424
1.412
1.285
1.54
1.97
2.00
0.90
0.79
2.11
3.07
0.92
8.13
27.27
10.51
f1 (ppm)

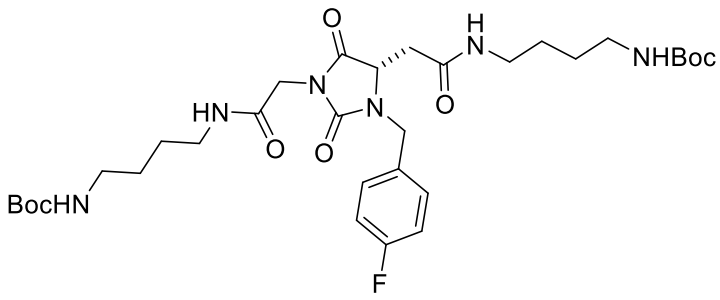


-L.G.S. - Laboratorio Grandi Strumenti - Display Report

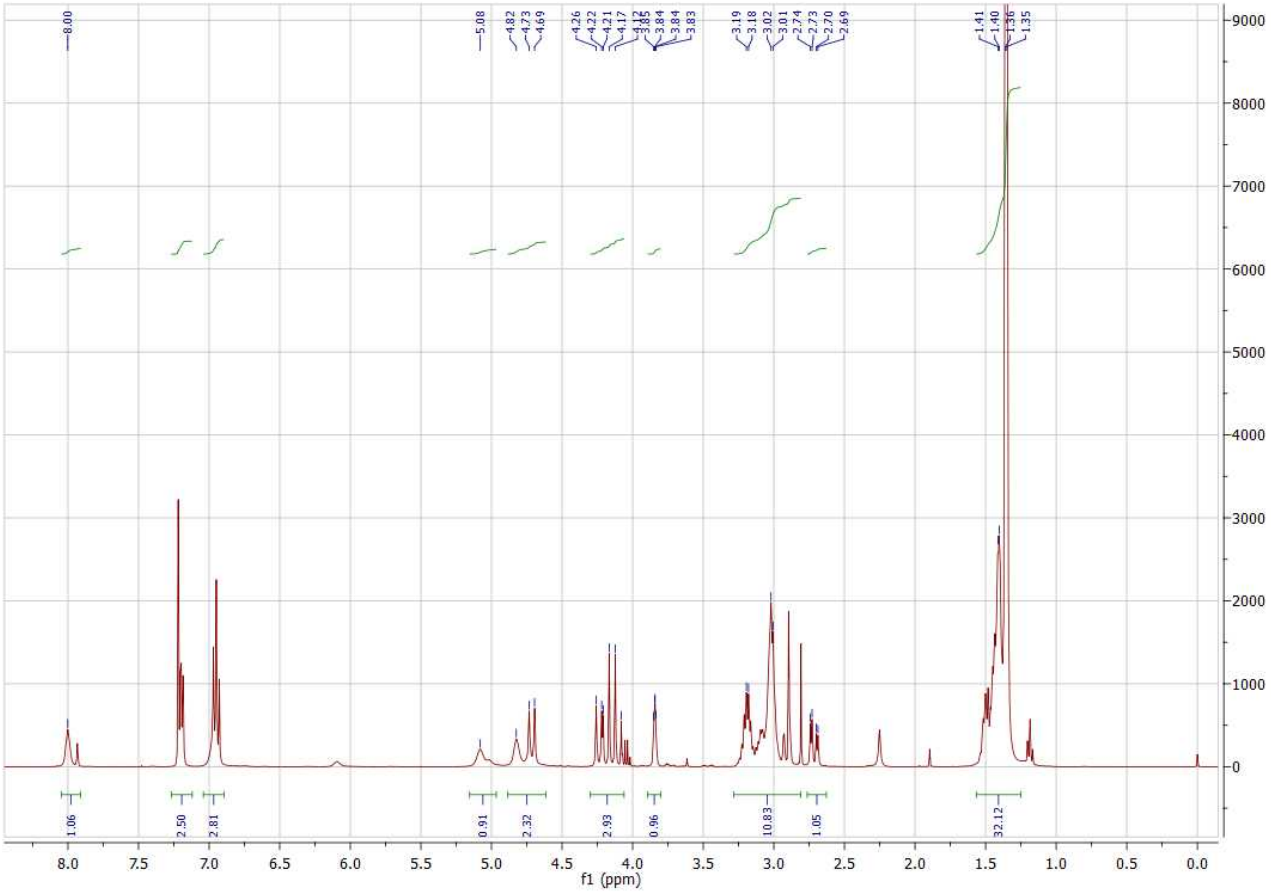
Analysis Name	av 2955.d	Acquisition Date	09/08/22 09:04:52	Operator	Walter Panzeri
Sample Name		Method	Copy of $opt0622.MS	Instrument	esquire3000plus
Comment	1 mg/mL dil 1:100 MeOH Richiedente: Volonterio				

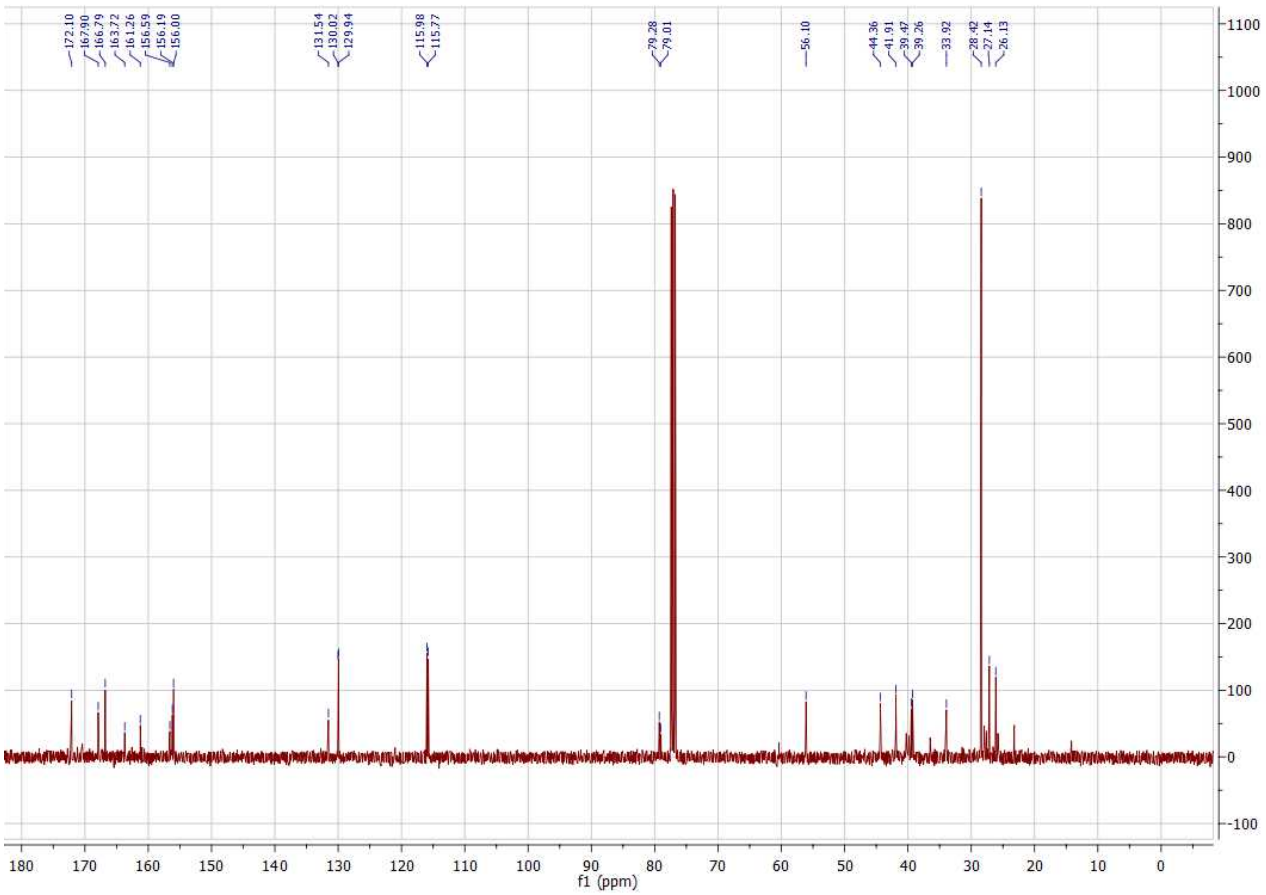


Bruker Daltonics DataAnalysis 3.1 printed: 09/08/22 09:06:33 Page 1 of 1


O
H
N
NHBoc
N
O
HN
N
O
O
BocHN
F

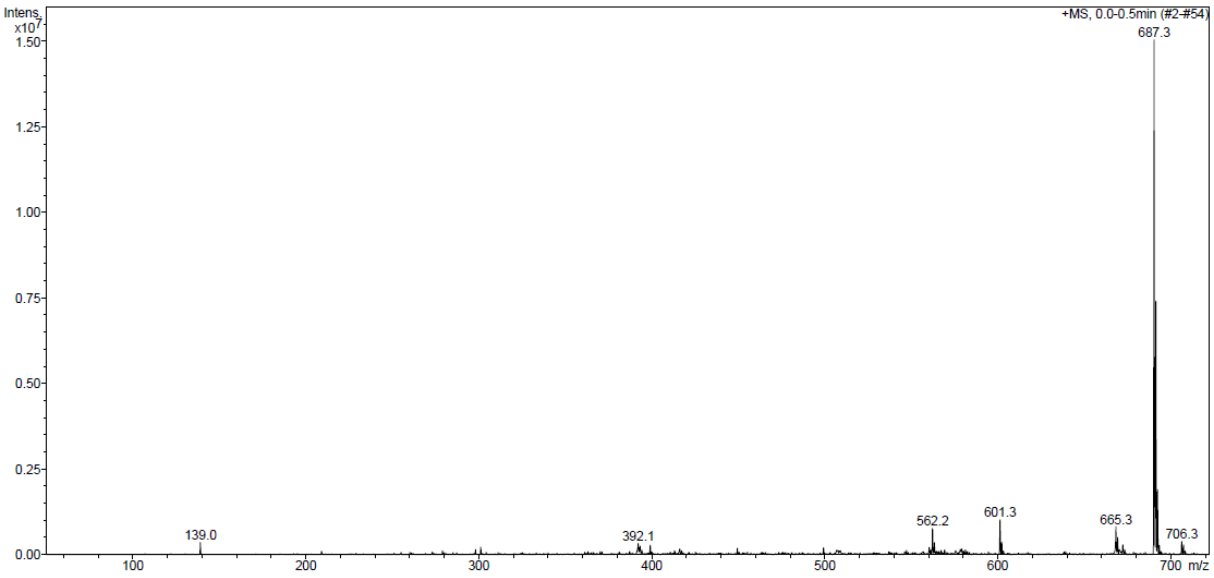
12b


8.00
5.08
4.82
4.73
4.69
4.26
4.22
4.21
4.17
3.85
3.84
3.84
3.83
3.19
3.18
3.02
3.01
2.74
2.73
2.70
2.69
1.41
1.40
1.36
1.35
1.06
2.50
2.81
0.91
2.32
2.93
0.96
10.83
1.05
32.12
f1 (ppm)

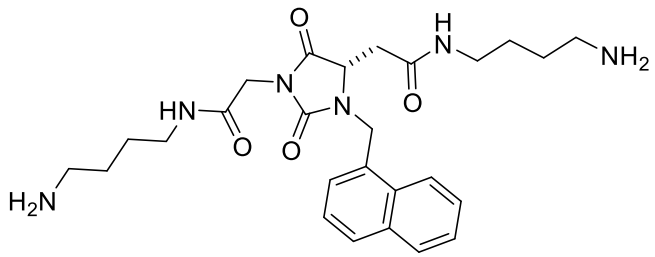


-L.G.S. - Laboratorio Grandi Strumenti - Display Report

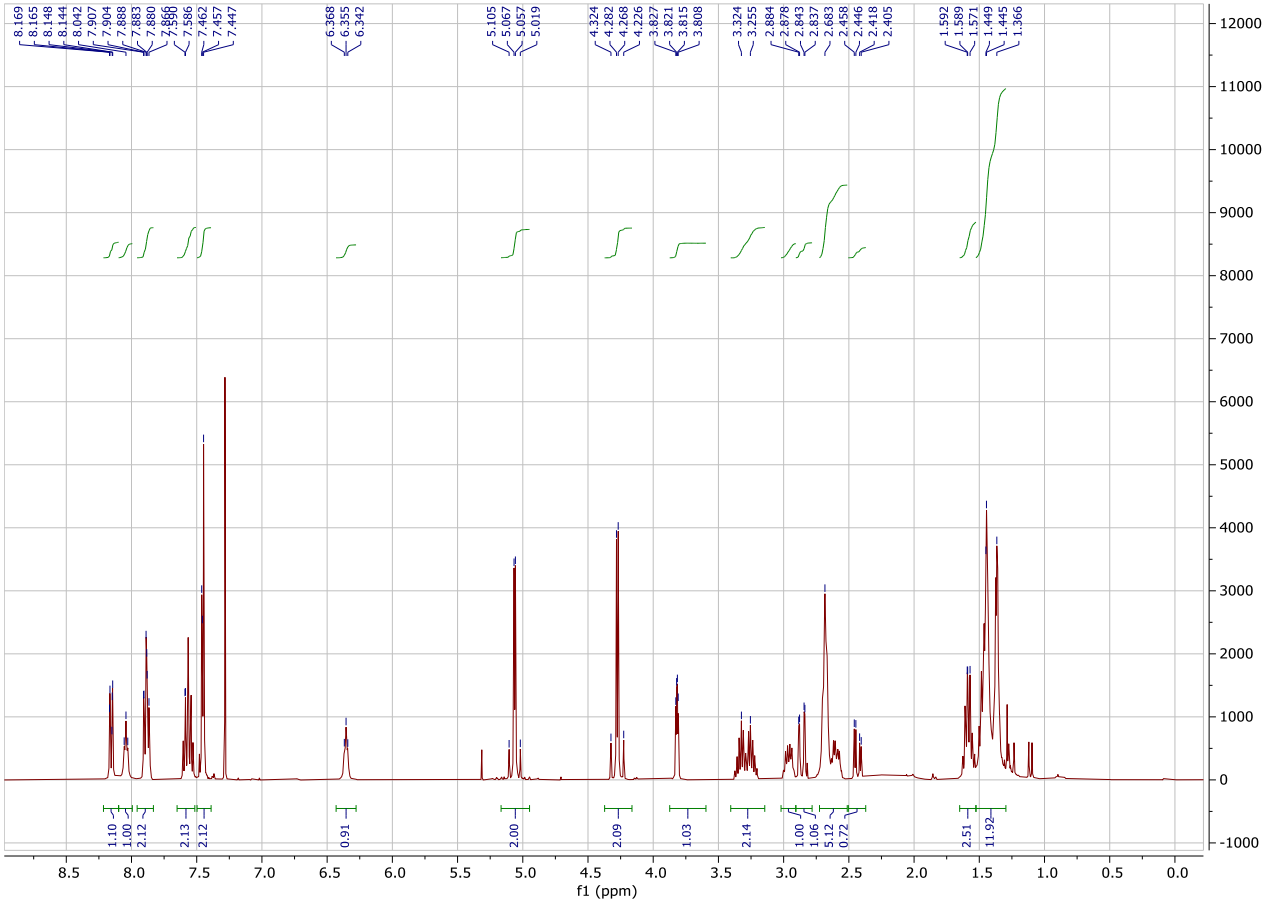
Analysis Name	av fm2662.d	Acquisition Date	06/08/15 13:47:42	Operator	Walter Panzeri
Sample Name		Method	Copy of _01tmix_posneg lm.MS	Instrument	esquire3000plus
Comment	1 mg/ml dil 1:100 MeOH Richiedente: Frigerio				

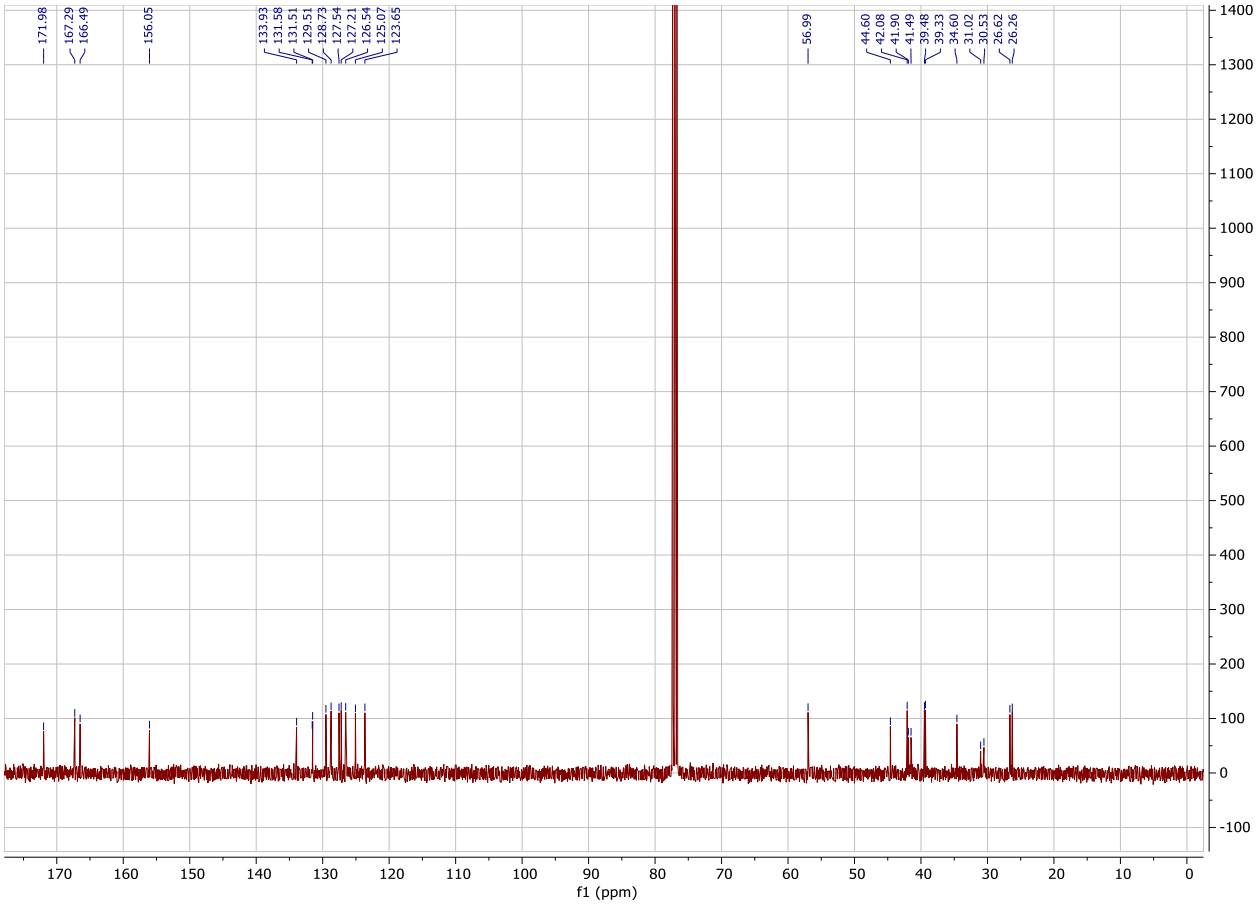


Bruker Daltonics DataAnalysis 3.1 printed: 06/08/15 14:03:38 Page 1 of 1



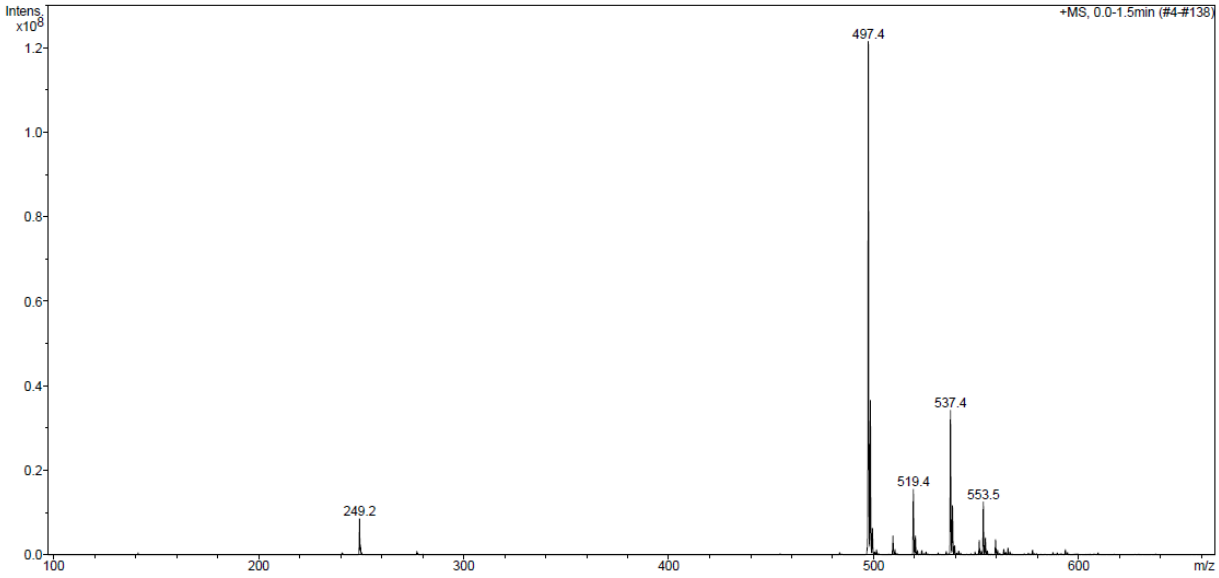
13c


8.169
8.165
8.148
8.144
8.042
7.907
7.904
7.888
7.883
7.880
7.586
7.462
7.457
7.447
6.368
6.355
6.342
5.105
5.067
5.057
5.019
4.324
4.282
4.268
4.226
3.827
3.821
3.815
3.808
3.324
3.255
2.884
2.878
2.843
2.837
2.683
2.458
2.446
2.418
2.405
1.592
1.589
1.571
1.449
1.445
1.366
1.10
1.00
2.12
2.13
2.12
0.91
2.00
2.09
1.03
2.14
1.00
1.06
5.12
0.72
2.51
11.92
f1 (ppm)

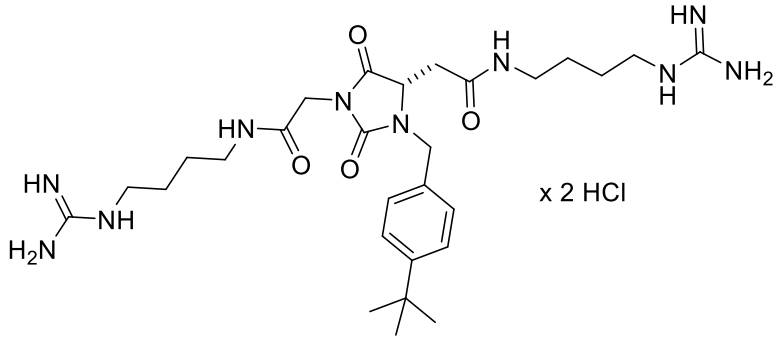


-L.G.S. - Laboratorio Grandi Strumenti - Display Report

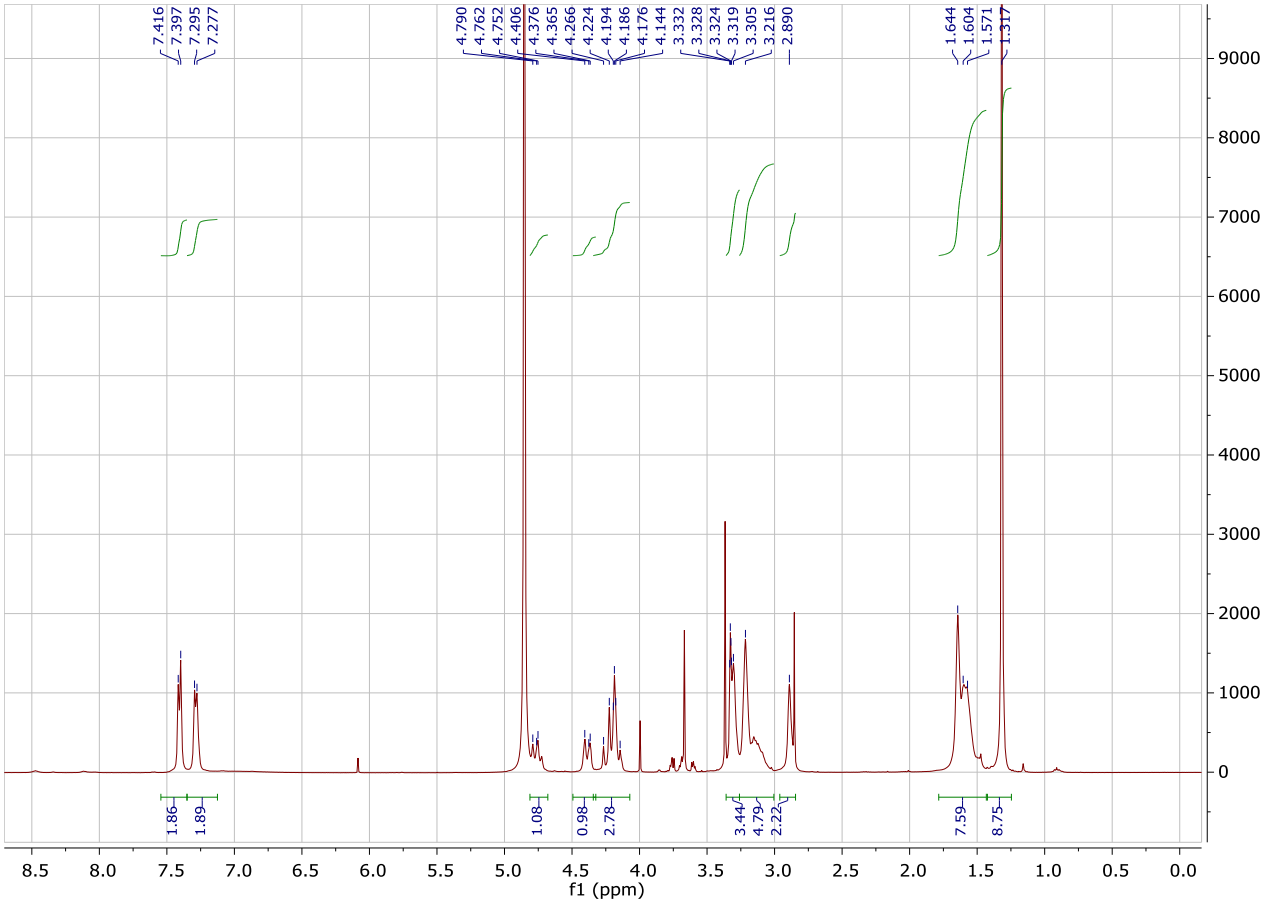
Analysis Name	av ac137.d	Acquisition Date	04/30/21 09:35:19	Operator	Walter Panzeri
Sample Name		Method	Copy of $wp_lm.MS	Instrument	esquire3000plus
Comment	1 mg/ml dil 1:100 MeOH Richiedente: Caramiello				

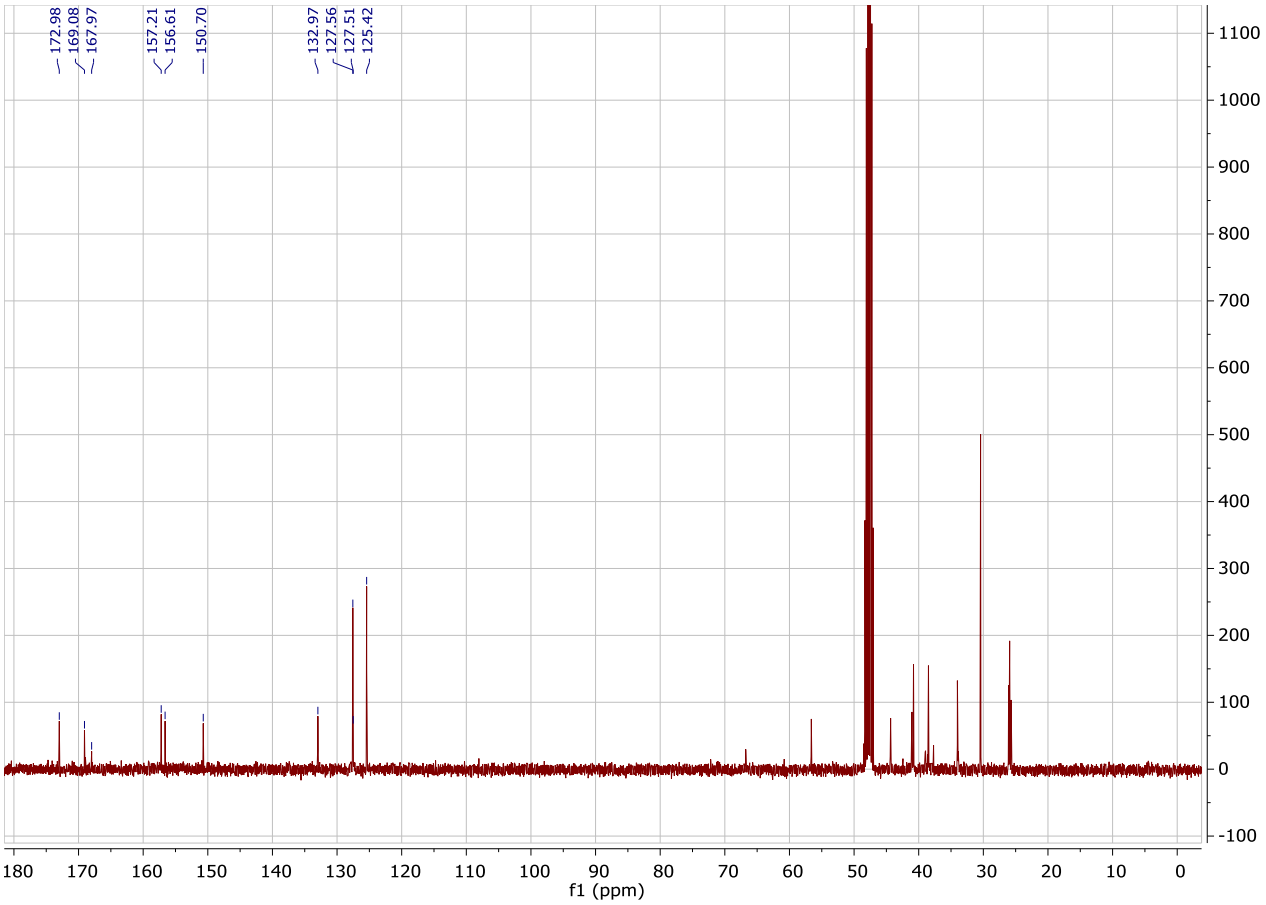


Bruker Daltonics DataAnalysis 3.1 printed: 04/30/21 09:50:42 Page 1 of 1


HN
O
H
N
HN
NH2
N
H
N
O
HN
O
O
HN
NH
H2N
x 2 HCl

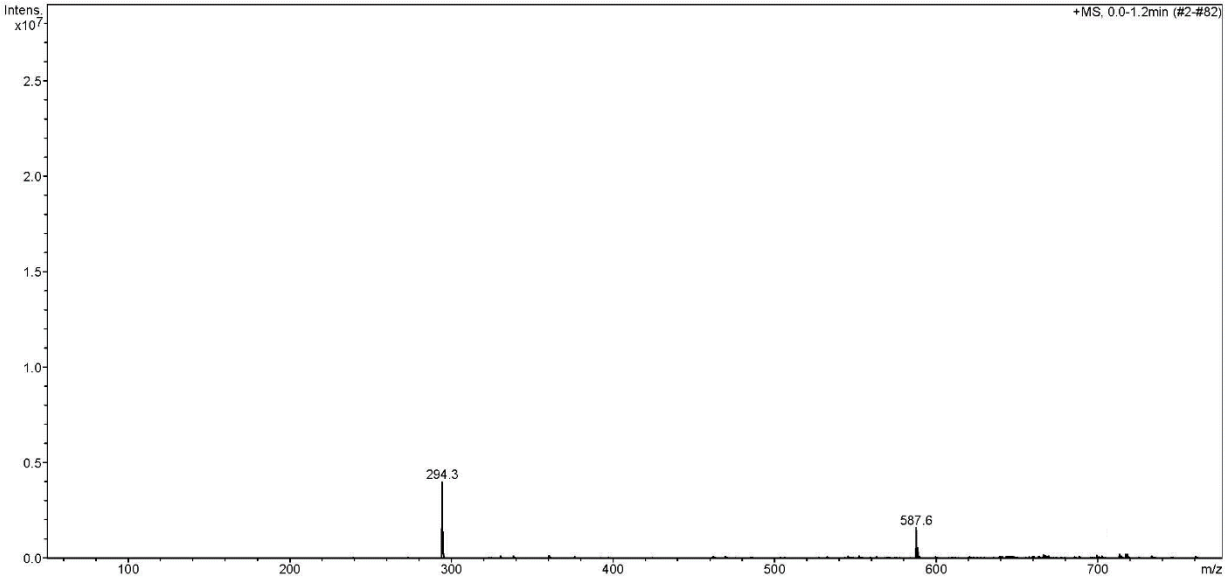
3a


7.416
7.397
7.295
7.277
4.790
4.762
4.752
4.406
4.376
4.365
4.266
4.224
4.194
4.186
4.176
4.144
3.332
3.328
3.324
3.319
3.305
3.216
2.890
1.644
1.604
1.571
1.317
1.86
1.89
1.08
0.98
2.78
3.44
4.79
2.22
7.59
8.75
f1 (ppm)

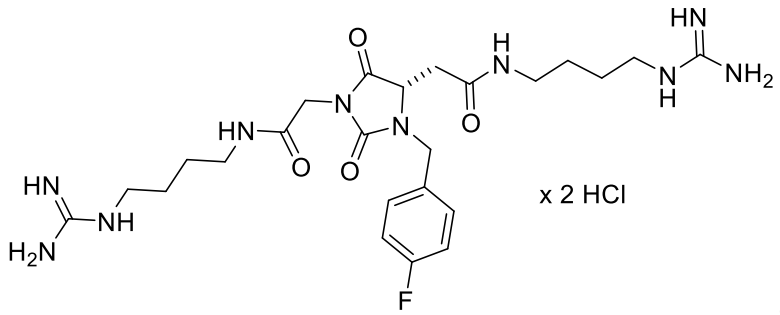


-L.G.S. - Laboratorio Grandi Strumenti - Display Report

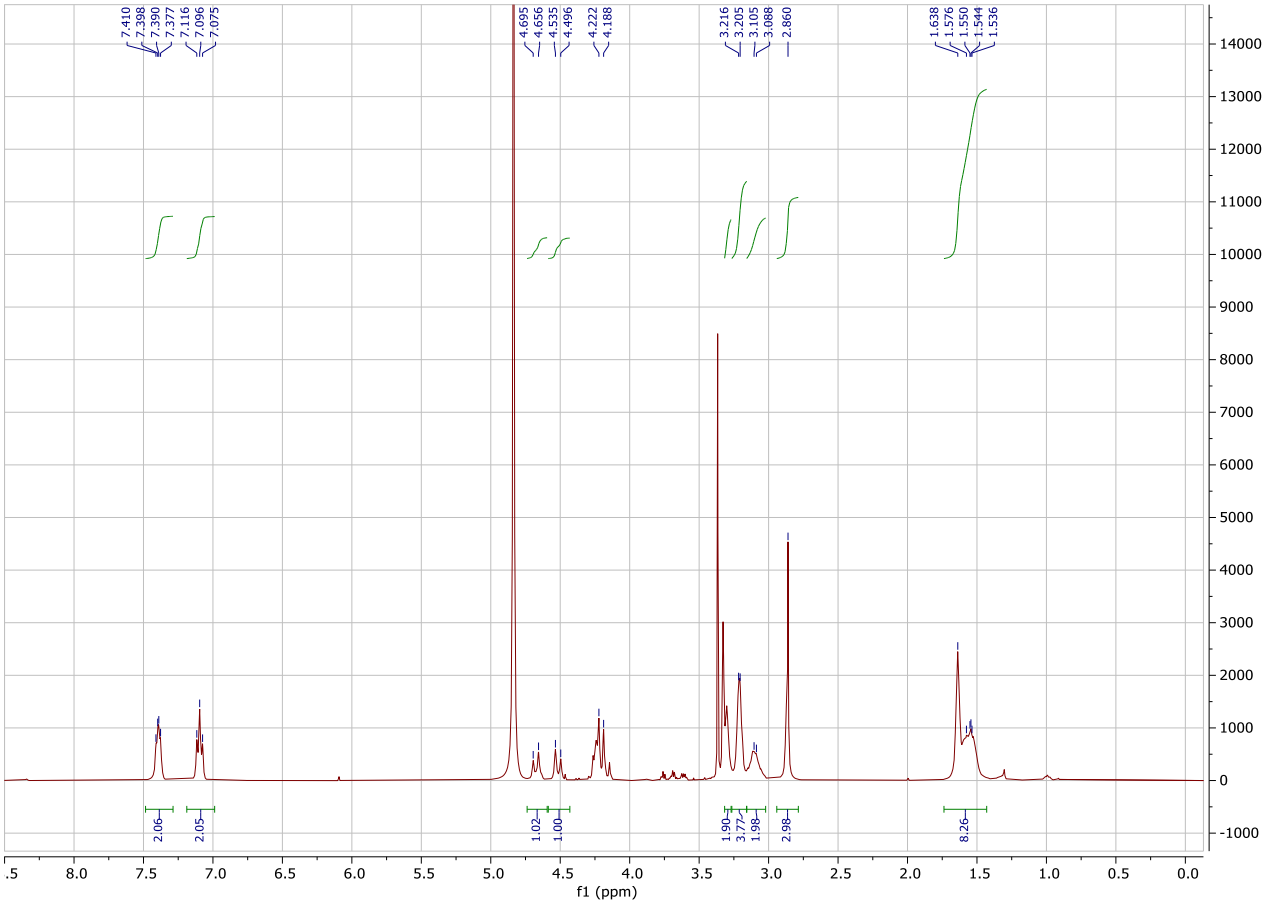
Analysis Name	av 2957.d	Acquisition Date	09/12/22 14:49:41	Operator	Walter Panzeri
Sample Name		Method	Copy of $opt0622.MS	Instrument	esquire3000plus
Comment	1 mg/mL dil 1:100 MeOH Richiedente: Volonterio				

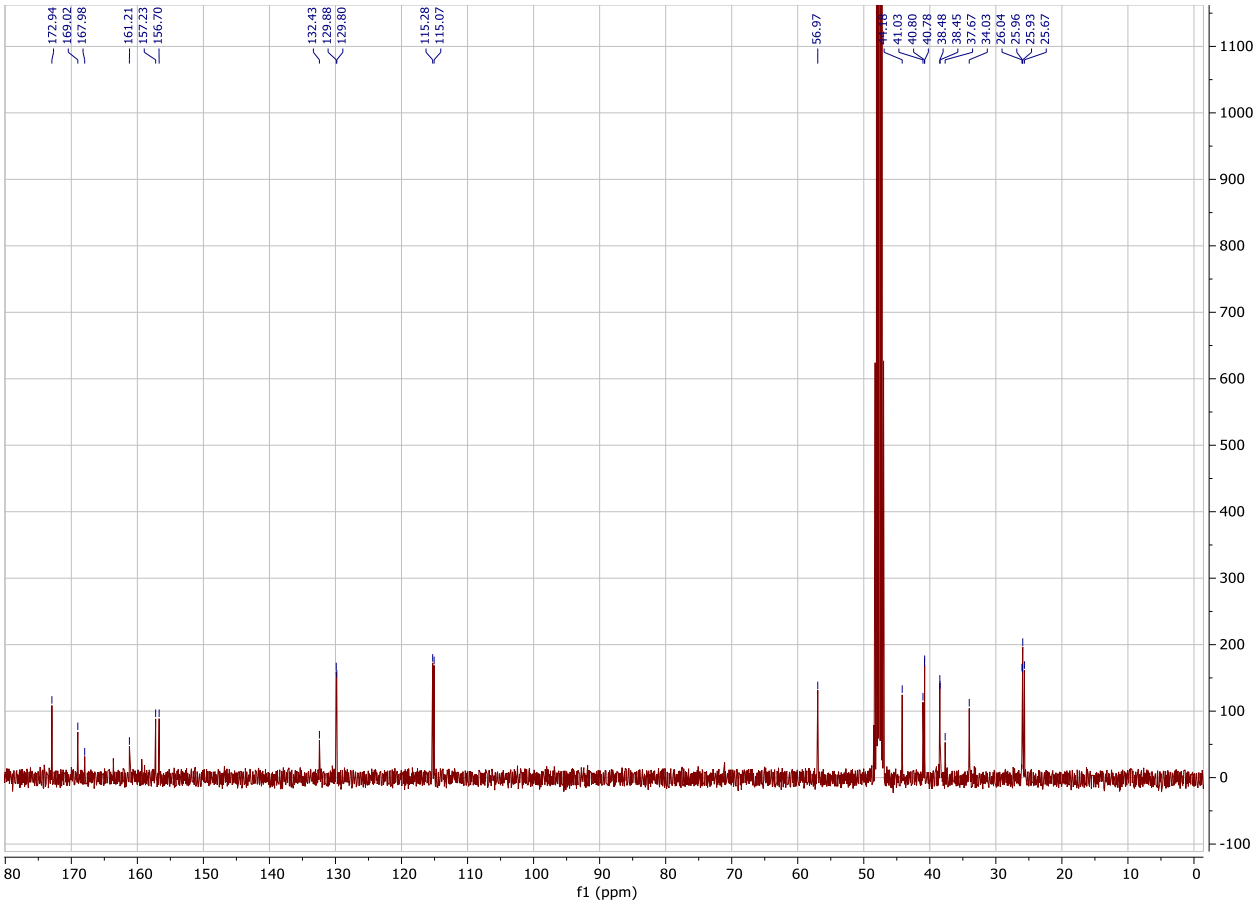


Bruker Daltonics DataAnalysis 3.1 printed: 09/12/22 14:52:28 Page 1 of 1


HN
O
H
N
NH2
N
H
N
O
HN
O
N
O
HN
NH
H2N
F
x 2 HCl

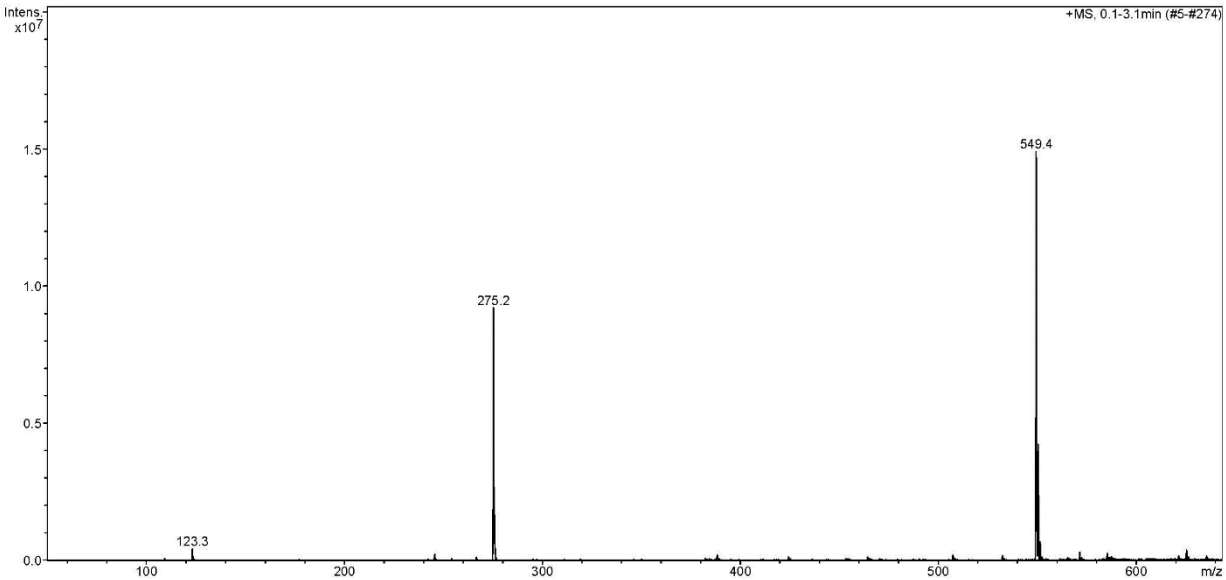
8b


7.410
7.398
7.390
7.377
7.116
7.096
7.075
4.695
4.656
4.535
4.496
4.222
4.188
3.216
3.205
3.105
3.088
2.860
1.638
1.576
1.550
1.544
1.536
2.06
2.05
1.02
1.00
1.90
3.77
1.98
2.98
8.26
f1 (ppm)

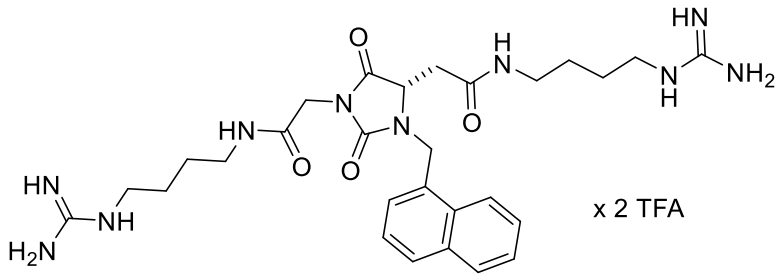


-L.G.S. - Laboratorio Grandi Strumenti - Display Report

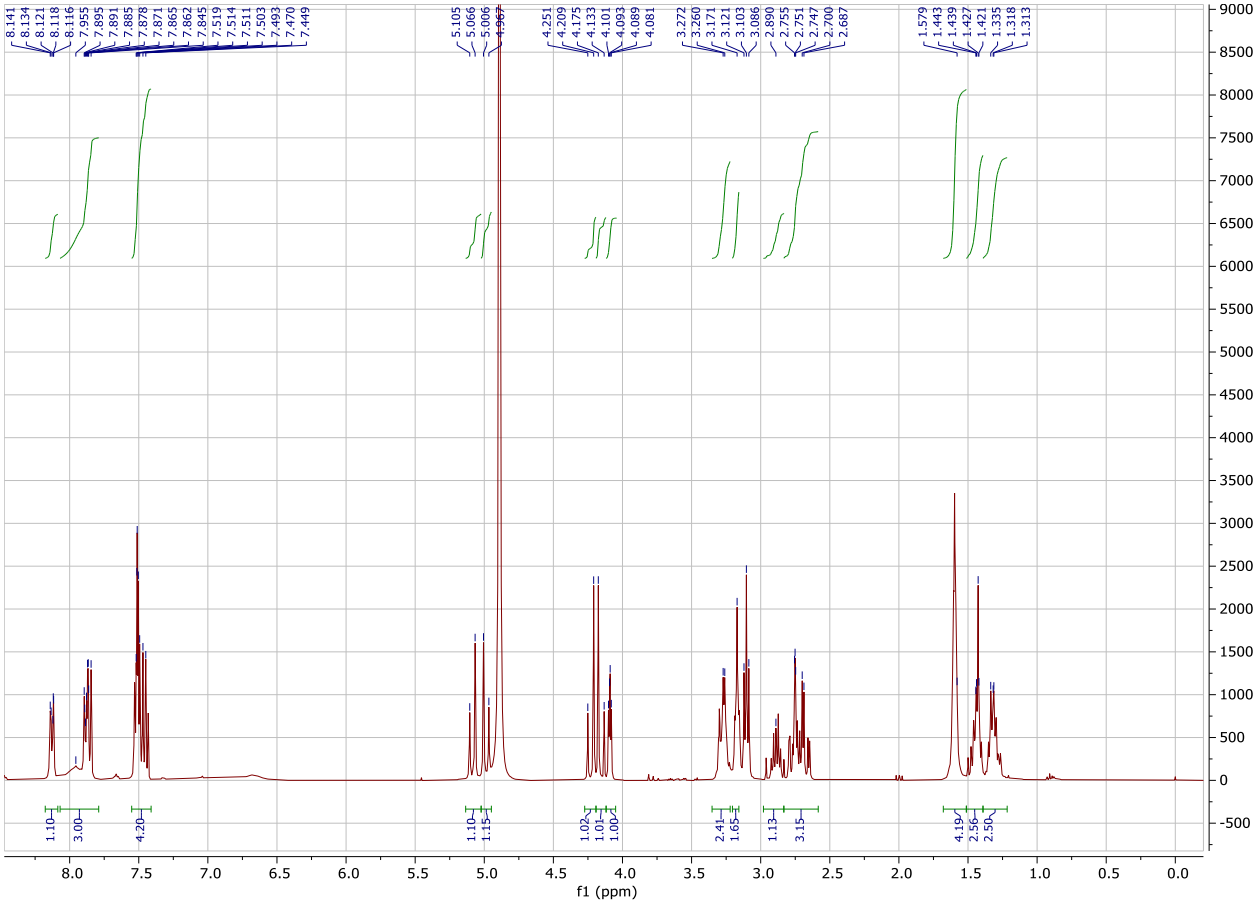
Analysis Name	av 2976.d	Acquisition Date	03/16/23 13:53:46	Operator	Administrator
Sample Name		Method	Copy of $opt0622.MS	Instrument	esquire3000plus
Comment	1 mg/ml dil 1:100 MeOH Richiedente: Volonterio				

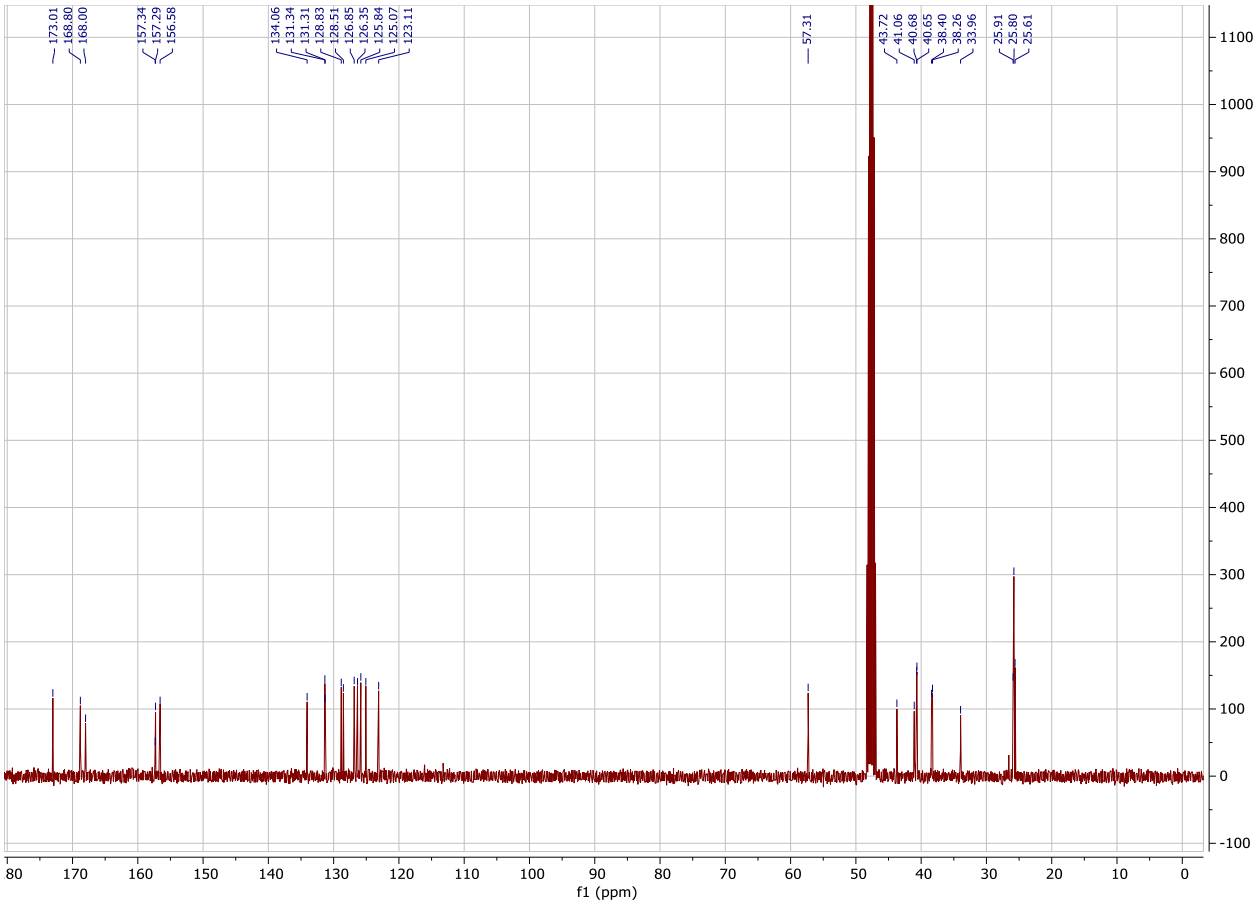


Bruker Daltonics DataAnalysis 3.1 printed: 03/16/23 13:57:16 Page 1 of 1


HN
NH2
H
N
N
H
O
O
N
N
HN
O
O
HN
NH
H2N
x 2 TFA

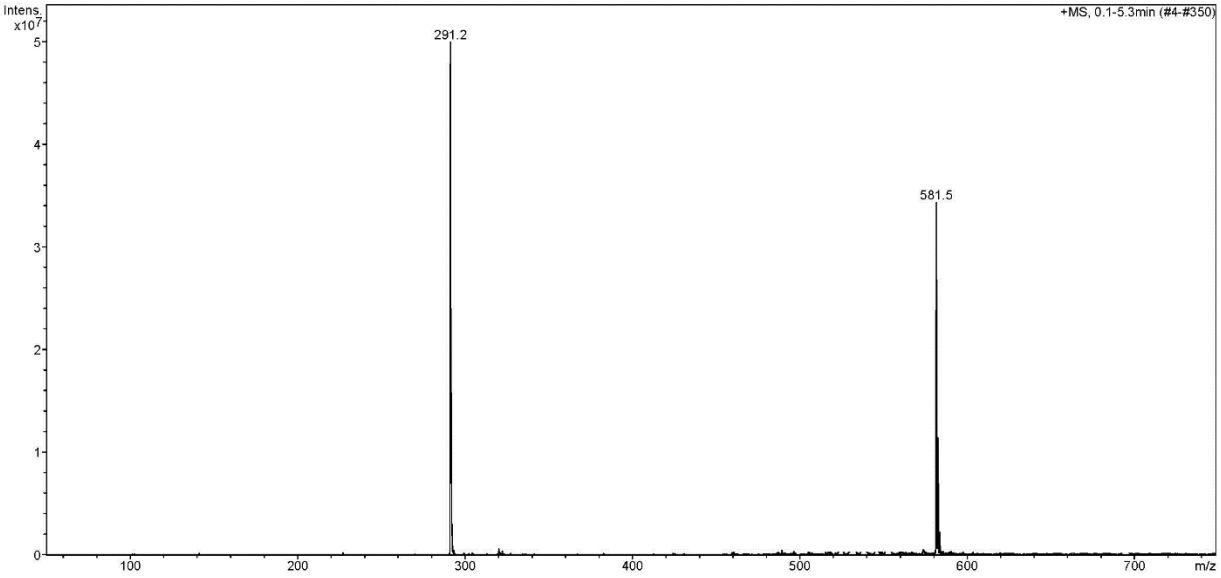
8c


8.141
8.134
8.121
8.118
8.116
7.955
7.895
7.891
7.885
7.878
7.871
7.865
7.862
7.845
7.519
7.514
7.511
7.503
7.493
7.470
7.449
5.105
5.066
5.006
4.967
4.251
4.209
4.175
4.133
4.101
4.093
4.089
4.081
3.272
3.260
3.171
3.121
3.103
3.086
2.890
2.755
2.751
2.747
2.700
2.687
1.579
1.443
1.439
1.427
1.421
1.335
1.318
1.313
1.10
3.00
4.20
1.10
1.15
1.02
1.01
1.00
2.41
1.65
1.13
3.15
4.19
2.56
2.50
f1 (ppm)



-L.G.S. - Laboratorio Grandi Strumenti - Display Report

Analysis Name	av ac139.d	Acquisition Date	05/07/21 10:29:57	Operator	Walter Panzeri
Sample Name		Method	Copy of _giov 1620 24713.MS	Instrument	esquire3000plus
Comment	1 mg/ml dil 1:100 MeOH Richiedente: Caramiello				



Bruker Daltonics DataAnalysis 3.1 printed: 05/07/21 10:36:01 Page 1 of 1

Table S1. Ideal atomic parameters used in the computational MM calculations.

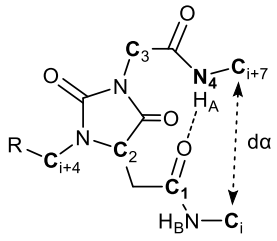
		**i – i+4**	**i – i+7**	**i+4 – i+7**	**dα**	**ω (C_1-C_2-C_3-N_4)**
	α-helix	6.2 Å	10.3 Å	5.8 Å	-	-
	β-turn	-	-	-	<7Å	-30°<X<+30°

Table S2. Summary of the results from QM/MM computational calculations

Mimic	% i – i +4[a]	% i +4 – i +7[a]	% i – i +7[a]	% α-helix[b]	% dα < 7Å	Angle β < |30°|	% β-turn[c]
13c	98	62	53	**27**	29	24	**18**
3c	96	42	50	**17**	32	31	**26**

[a] Values in the ± 10% range with respect to the ideal distance were considered; i − i + 4 = 5.6–6.8 Å; i − i +7 =9.3–11.3 Å; i +4 – I +7 = 5.2–6.4 Å.

[b] Percentage of conformers having the three interatomic distances in the correct range

[c] Percentage of conformers having dα and angle-β in the correct range

Table S3. Computational results for molecule **13c**

13c	Relative Energy [kcal/mol]	i – i+4 [Å]	i+4 – i+7 [Å]	i – i+7 [Å]	ω (C_1-C_2-C_3-N_4) [°]	d_α [Å]
M0001	0,00	5,64	5,93	8,77	159,80	8,77
M0002	3,94	5,43	7,20	8,60	13,79	8,60
M0003	4,28	6,59	6,36	8,58	128,18	8,58
M0004	5,38	6,20	6,71	7,85	-22,37	7,85
M0005	5,86	6,60	7,04	9,38	-82,64	9,38
M0006	6,21	6,29	6,26	7,55	108,42	7,55
M0007	6,48	6,92	6,23	9,71	125,04	9,71
M0008	6,83	6,93	7,47	6,81	-9,11	6,81
M0009	6,96	6,83	6,90	6,87	-31,45	6,87
M0010	6,99	6,50	5,98	8,87	143,58	8,87
M0011	7,28	6,58	6,07	8,88	-93,05	8,88
M0012	7,31	6,45	5,90	8,46	135,01	8,46
M0013	7,69	6,96	6,73	8,25	70,48	8,25
M0014	7,72	6,44	7,65	8,51	96,94	8,51
M0015	7,87	5,88	6,68	5,23	-9,98	5,23
M0016	7,90	7,11	6,29	7,96	-87,18	7,96
M0017	8,00	5,83	6,72	5,04	-0,02	5,04
M0018	8,09	6,96	7,91	7,44	-32,79	7,44

M0019	8,27	5,92	5,91	8,42	-166,43	8,42
M0020	8,29	6,57	6,20	7,67	112,72	7,67
M0021	8,35	6,59	6,14	9,04	-95,73	9,04
M0022	8,38	6,56	6,98	6,62	70,29	6,62
M0023	8,47	6,37	7,41	9,38	120,99	9,38
M0024	8,58	6,39	7,50	9,62	121,52	9,62
M0025	8,70	6,03	6,79	8,78	-46,17	8,78
M0026	8,71	6,39	7,80	8,83	68,18	8,83
M0027	8,84	7,01	7,83	6,01	-5,88	6,01
M0028	9,03	7,10	6,39	8,34	-93,39	8,34
M0029	9,03	6,85	7,30	6,95	-22,45	6,95
M0030	9,11	5,70	6,56	6,61	-7,56	6,61
M0031	9,12	6,53	7,75	8,95	100,60	8,95
M0032	9,16	6,19	6,65	6,46	-55,73	6,46
M0033	9,17	6,94	6,44	4,86	-44,26	4,86
M0034	9,20	5,72	7,32	9,11	-13,29	9,11
M0035	9,22	6,65	7,83	8,76	-44,25	8,76
M0036	9,31	6,68	6,80	9,54	140,82	9,54
M0037	9,42	6,58	7,62	9,35	-53,20	9,35
M0038	9,50	5,97	6,83	7,69	91,25	7,69
M0039	9,54	5,85	6,16	8,94	-168,80	8,94
M0040	9,65	5,47	7,84	10,45	151,93	10,45
M0041	9,66	4,50	6,68	6,67	1,70	6,67
M0042	9,67	6,23	6,50	6,34	-68,30	6,34
M0043	9,71	5,99	6,25	10,19	130,20	10,19
M0044	9,71	6,48	7,73	8,96	102,04	8,96
M0045	9,89	5,96	7,44	6,96	-22,60	6,96
TOTAL IN RANGE [%]		**98**	**62**	**53**	**24**	**29**

Table S4. Computational results for molecule **3c**

3c	Relative Energy [kcal/mol]	i – i+4 [Å]	i+4 – i+7 [Å]	i – i+7 [Å]	ω (C_1-C_2-C_3-N_4) [°]	d_α [Å]
M0032	-8,68	5,38	7,74	9,70	166,70	9,70
M0004	-8,45	5,44	7,75	9,69	172,84	9,69
M0267	-8,29	6,57	7,70	9,83	63,61	9,83
M0664	-8,15	5,19	7,57	9,24	169,88	9,24
M0603	-8,11	7,05	6,35	8,20	-89,09	8,20
M0656	-7,88	5,20	8,02	8,68	127,62	8,68
M0412	-7,67	6,65	6,26	8,90	-91,12	8,90
M0585	-7,38	5,23	7,74	9,27	160,16	9,27
M0529	-7,33	6,83	6,41	8,48	117,76	8,48
M0618	-7,30	6,84	6,44	8,39	113,48	8,39
M0687	-7,12	5,90	6,22	10,64	161,33	10,64

M0285	-7,04	7,06	6,37	7,51	-74,82	7,51
M0568	-6,88	6,09	7,56	8,68	164,46	8,68
M0199	-6,87	5,22	8,23	8,16	117,62	8,16
M0474	-6,47	5,24	7,92	8,52	126,02	8,52
M0650	-6,24	6,14	7,69	8,46	159,28	8,46
M0080	-6,13	5,31	8,15	8,79	108,88	8,79
M0016	-6,01	6,64	6,93	8,99	-84,27	8,99
M0531	-5,82	6,58	6,64	5,06	-22,70	5,06
M0382	-5,73	5,39	7,93	9,49	155,03	9,49
M0360	-5,70	5,43	6,66	6,77	-3,07	6,77
M0002	-5,68	7,03	6,23	7,98	-87,91	7,98
M0101	-5,55	6,79	8,01	8,14	-34,73	8,14
M0226	-5,54	5,20	7,95	8,82	145,58	8,82
M0570	-5,51	5,54	6,68	6,65	-2,45	6,65
M0079	-5,49	6,04	7,81	8,82	66,56	8,82
M0232	-5,49	5,30	7,70	9,30	-178,83	9,30
M0329	-5,47	5,10	7,86	9,30	168,32	9,30
M0513	-5,41	6,86	6,56	8,38	-73,19	8,38
M0281	-5,32	7,08	6,25	9,28	117,91	9,28
M0576	-5,32	5,24	8,18	8,34	120,74	8,34
M0424	-5,14	6,87	6,35	8,73	-83,15	8,73
M0337	-5,13	5,60	6,57	6,65	-6,59	6,65
M0408	-5,08	6,79	6,79	8,14	-49,24	8,14
M0261	-5,05	5,45	6,40	10,49	153,83	10,49
M0422	-5,01	7,00	6,28	8,24	-86,65	8,24
M0263	-4,98	5,53	6,29	10,32	146,98	10,32
M0471	-4,98	5,61	6,68	6,67	-3,42	6,67
M0340	-4,80	6,53	7,92	7,63	144,11	7,63
M0499	-4,76	5,67	6,12	10,91	-168,78	10,91
M0056	-4,75	6,66	7,21	7,48	-22,63	7,48
M0509	-4,75	6,93	6,20	8,41	-87,36	8,41
M0262	-4,74	5,50	6,11	10,86	-164,42	10,86
M0183	-4,71	5,58	6,78	6,48	1,84	6,48
M0441	-4,69	5,67	6,59	6,57	-5,81	6,57
M0083	-4,65	5,20	7,96	9,76	166,27	9,76
M0311	-4,56	6,11	7,20	10,13	-150,35	10,13
M0020	-4,51	7,03	6,16	8,31	-91,82	8,31
M0110	-4,48	6,73	5,80	9,07	147,22	9,07
M0521	-4,46	6,86	6,29	8,72	-87,89	8,72
M0486	-4,45	5,23	7,70	9,30	154,95	9,30
M0117	-4,43	5,68	6,58	6,56	-5,72	6,56
M0525	-4,42	5,46	7,91	8,96	-53,21	8,96
M0446	-4,39	6,16	6,91	8,59	-163,86	8,59
M0672	-4,39	6,40	6,56	7,83	-34,10	7,83
M0507	-4,23	5,71	7,49	9,41	1,55	9,41

M0667	-4,23	7,01	7,19	6,30	-33,57	6,30
M0163	-4,18	6,26	7,42	9,15	161,81	9,15
M0378	-4,18	5,21	8,03	8,98	140,97	8,98
M0283	-4,14	6,75	6,43	10,78	-130,27	10,78
M0674	-4,14	5,48	6,14	10,94	-158,04	10,94
M0683	-4,07	6,66	6,91	7,52	-32,35	7,52
M0302	-4,02	6,87	6,56	7,78	-56,61	7,78
M0034	-3,99	7,04	7,95	7,33	-27,93	7,33
M0438	-3,99	5,54	7,55	9,68	-129,56	9,68
M0165	-3,97	5,91	7,29	8,96	176,99	8,96
M0057	-3,79	5,74	7,79	10,36	-11,13	10,36
M0599	-3,79	5,45	7,41	8,91	23,54	8,91
M0381	-3,77	5,43	7,88	9,39	166,57	9,39
M0557	-3,77	6,53	6,64	9,33	-162,77	9,33
M0111	-3,74	6,66	8,02	8,27	-32,19	8,27
M0206	-3,74	5,20	7,60	9,70	162,53	9,70
M0395	-3,74	5,66	6,21	11,01	-166,31	11,01
M0416	-3,73	6,46	6,74	6,95	92,14	6,95
M0524	-3,64	5,91	7,67	9,75	89,68	9,75
M0298	-3,58	6,21	6,44	9,81	154,57	9,81
M0259	-3,57	5,76	6,60	6,54	-6,29	6,54
M0682	-3,55	6,35	6,35	8,99	-76,21	8,99
M0646	-3,53	6,66	7,28	9,40	-172,48	9,40
M0007	-3,50	6,03	7,11	4,95	17,67	4,95
M0406	-3,48	7,00	7,97	8,39	-37,16	8,39
M0419	-3,46	6,59	6,65	7,82	106,79	7,82
M0093	-3,45	6,39	7,57	9,62	-173,12	9,62
M0051	-3,43	5,89	6,73	5,04	3,25	5,04
M0257	-3,38	5,89	6,65	8,17	-18,51	8,17
M0277	-3,38	6,36	6,36	8,80	-73,36	8,80
M0604	-3,37	6,62	6,93	7,54	-28,92	7,54
M0370	-3,31	5,22	8,28	8,10	122,55	8,10
M0027	-3,28	6,83	6,63	7,55	-49,06	7,55
M0109	-3,27	5,51	7,26	9,81	-145,06	9,81
M0137	-3,26	6,05	7,60	8,49	155,50	8,49
M0498	-3,24	6,04	6,26	9,79	102,66	9,79
M0026	-3,21	6,97	6,71	6,44	-36,15	6,44
M0550	-3,21	6,52	7,96	7,56	138,47	7,56
M0349	-3,19	6,48	7,33	9,95	-172,16	9,95
M0391	-3,18	5,75	6,36	10,28	124,22	10,28
M0404	-3,15	6,20	6,31	8,46	-59,07	8,46
M0561	-3,13	6,66	7,37	9,39	179,50	9,39
M0031	-3,12	6,82	5,43	7,99	-48,95	7,99
M0323	-3,09	5,91	6,88	5,06	7,67	5,06
M0291	-3,08	5,88	7,06	9,69	-63,66	9,69

M0506	-3,07	6,26	6,35	9,10	-75,86	9,10
M0496	-3,05	5,70	6,68	8,32	-10,66	8,32
M0234	-3,04	5,28	8,03	9,47	145,54	9,47
M0493	-3,04	4,99	7,86	7,96	151,25	7,96
M0024	-3,02	6,85	6,33	8,82	-87,30	8,82
M0033	-3,01	6,68	7,27	9,52	-66,28	9,52
M0353	-3,01	5,94	7,55	8,73	153,48	8,73
M0077	-2,96	6,22	7,79	10,33	141,17	10,33
M0230	-2,96	5,40	7,89	9,35	153,61	9,35
M0238	-2,95	5,06	7,96	8,05	141,43	8,05
M0095	-2,90	6,67	6,07	9,69	165,61	9,69
M0011	-2,85	7,00	7,19	6,28	-31,22	6,28
M0162	-2,85	6,24	7,10	9,14	-167,52	9,14
M0671	-2,84	5,60	6,67	8,36	-8,41	8,36
M0085	-2,83	5,09	7,87	8,81	150,72	8,81
M0457	-2,82	6,58	7,16	9,27	-165,46	9,27
M0253	-2,80	4,99	7,91	7,94	148,76	7,94
M0325	-2,79	5,35	7,31	9,84	-148,50	9,84
M0655	-2,71	5,13	7,76	8,00	154,98	8,00
M0098	-2,70	6,73	7,58	9,13	-65,55	9,13
M0171	-2,69	6,46	7,66	8,99	152,94	8,99
M0351	-2,69	6,66	7,33	9,44	-179,40	9,44
M0158	-2,68	6,06	7,62	8,54	148,30	8,54
M0204	-2,67	5,30	7,80	7,85	142,17	7,85
M0624	-2,64	5,94	6,96	5,06	9,79	5,06
M0443	-2,63	6,93	5,85	8,55	161,31	8,55
M0195	-2,62	5,26	8,17	8,35	126,76	8,35
M0006	-2,59	6,46	6,11	9,07	-84,28	9,07
M0135	-2,59	6,13	7,89	10,31	138,60	10,31
M0115	-2,53	5,74	6,58	6,93	-15,72	6,93
M0112	-2,50	6,38	7,58	10,32	163,15	10,32
M0425	-2,48	6,00	6,69	5,24	-12,24	5,24
M0191	-2,45	5,10	8,04	8,39	111,28	8,39
M0623	-2,45	5,42	6,65	5,42	-8,61	5,42
M0304	-2,43	7,08	6,43	8,17	-92,97	8,17
M0087	-2,41	6,56	5,97	8,97	145,02	8,97
M0185	-2,41	6,39	7,82	9,42	136,91	9,42
M0491	-2,41	7,05	7,34	5,35	-15,96	5,35
M0235	-2,35	5,73	6,60	6,93	-14,89	6,93
M0690	-2,34	6,72	5,93	9,08	147,31	9,08
M0632	-2,32	5,67	7,17	9,69	-122,22	9,69
M0155	-2,27	6,68	7,27	9,29	-175,20	9,29
M0209	-2,26	5,30	7,97	9,39	125,78	9,39
M0152	-2,25	6,72	7,76	9,23	149,44	9,23
M0575	-2,25	5,11	8,07	8,32	110,24	8,32

M0217	-2,24	5,28	7,77	9,96	137,32	9,96
M0392	-2,23	5,47	7,21	8,80	13,63	8,80
M0681	-2,21	6,57	7,65	7,79	-5,68	7,79
M0397	-2,19	6,28	7,52	10,26	82,24	10,26
M0598	-2,18	5,79	6,20	9,92	109,16	9,92
M0409	-2,16	6,77	7,32	9,31	-66,35	9,31
M0480	-2,16	5,14	7,24	8,92	-159,90	8,92
M0293	-2,15	5,63	6,19	10,40	157,79	10,40
M0335	-2,11	5,73	6,63	6,92	-14,51	6,92
M0653	-2,10	5,11	7,63	8,52	165,47	8,52
M0626	-2,09	6,41	7,47	10,28	173,25	10,28
M0301	-2,08	6,92	6,08	9,16	136,58	9,16
M0693	-2,06	6,02	6,54	5,20	-9,77	5,20
M0361	-2,05	6,42	7,78	8,73	134,74	8,73
M0478	-2,04	5,27	7,66	9,96	145,89	9,96
M0078	-2,03	6,01	7,60	9,36	89,42	9,36
M0134	-2,02	6,99	5,85	8,67	163,83	8,67
M0410	-2,02	6,33	7,55	9,05	93,16	9,05
M0310	-1,98	6,60	7,36	9,54	125,18	9,54
M0686	-1,95	6,21	7,36	9,84	116,64	9,84
M0167	-1,92	5,29	8,21	5,46	34,21	5,46
M0354	-1,92	4,67	8,04	5,40	34,17	5,40
M0076	-1,91	6,17	7,40	7,57	72,41	7,57
M0366	-1,90	5,22	7,49	8,95	158,26	8,95
M0601	-1,89	6,06	6,78	9,09	-40,87	9,09
M0605	-1,89	5,41	7,53	8,96	27,90	8,96
M0066	-1,88	5,36	7,11	5,53	7,75	5,53
M0336	-1,88	5,73	6,82	6,56	-1,39	6,56
M0376	-1,88	5,41	7,98	9,27	131,89	9,27
M0654	-1,87	5,36	8,08	8,19	137,06	8,19
M0367	-1,86	5,12	8,09	8,25	107,88	8,25
M0156	-1,85	6,23	7,51	8,73	153,89	8,73
M0050	-1,84	6,32	8,01	6,71	-47,82	6,71
M0501	-1,84	6,26	7,38	8,28	-8,37	8,28
M0551	-1,84	6,36	7,65	7,66	172,86	7,66
M0642	-1,83	6,51	6,96	9,37	-159,73	9,37
M0573	-1,82	5,07	7,65	8,69	171,28	8,69
M0040	-1,81	6,26	6,67	5,08	-10,00	5,08
M0532	-1,81	5,33	8,00	9,03	112,80	9,03
M0021	-1,80	6,95	6,19	8,51	-90,12	8,51
M0198	-1,80	5,15	7,31	9,81	164,94	9,81
M0440	-1,77	5,88	6,95	6,21	4,05	6,21
M0466	-1,77	6,25	6,70	8,63	-157,22	8,63
M0633	-1,77	5,75	6,61	6,90	-16,13	6,90
M0008	-1,75	7,06	7,33	7,96	68,40	7,96

M0030	-1,75	6,65	5,91	8,93	143,03	8,93
M0035	-1,75	5,40	6,69	5,25	-10,37	5,25
M0037	-1,75	6,91	7,14	8,30	-62,16	8,30
M0342	-1,75	6,98	5,84	8,57	161,94	8,57
M0371	-1,67	5,36	7,91	9,58	139,61	9,58
M0403	-1,67	6,34	7,66	8,23	-4,01	8,23
M0485	-1,67	5,24	8,16	8,85	120,54	8,85
M0449	-1,66	6,56	6,52	4,33	-17,10	4,33
M0567	-1,66	6,07	7,45	8,98	162,36	8,98
M0295	-1,64	6,85	5,89	9,63	162,48	9,63
M0369	-1,61	5,07	7,82	7,74	152,77	7,74
M0384	-1,61	7,03	7,30	5,44	-20,92	5,44
M0214	-1,60	5,24	7,57	9,93	153,01	9,93
M0116	-1,58	5,74	6,85	6,58	-0,21	6,58
M0175	-1,58	4,81	7,95	5,27	24,74	5,27
M0393	-1,58	5,94	6,28	10,09	112,33	10,09
M0244	-1,56	5,67	8,17	5,96	-16,15	5,96
M0189	-1,52	5,32	8,07	8,23	139,66	8,23
M0019	-1,50	5,40	6,66	5,04	-3,34	5,04
M0379	-1,50	5,20	7,67	5,17	33,07	5,17
M0540	-1,50	5,70	7,33	9,89	-144,34	9,89
M0046	-1,44	5,59	8,24	9,45	101,22	9,45
M0213	-1,44	5,29	7,75	8,49	156,43	8,49
M0647	-1,44	4,65	7,89	5,20	25,49	5,20
M0305	-1,43	6,66	6,16	8,88	-94,50	8,88
M0649	-1,43	6,11	7,32	9,04	176,98	9,04
M0100	-1,42	6,27	7,81	10,21	151,00	10,21
M0223	-1,42	5,36	8,06	9,16	128,36	9,16
M0350	-1,41	6,06	6,20	6,58	-51,37	6,58
M0611	-1,41	7,02	6,17	8,24	-93,06	8,24
M0330	-1,40	5,44	7,43	9,87	-143,43	9,87
M0423	-1,40	6,72	8,00	8,65	85,03	8,65
M0224	-1,39	6,10	6,44	5,57	-18,78	5,57
M0161	-1,36	5,58	6,04	8,39	-139,98	8,39
M0266	-1,36	6,25	6,79	9,52	-61,27	9,52
M0610	-1,36	6,63	7,27	7,72	-25,96	7,72
M0170	-1,34	6,28	7,39	9,37	160,45	9,37
M0102	-1,31	6,74	7,74	9,19	101,87	9,19
M0459	-1,31	4,64	8,03	5,48	35,51	5,48
M0054	-1,30	5,19	7,91	7,71	8,63	7,71
M0662	-1,30	5,43	6,86	4,99	-3,08	4,99
M0463	-1,28	5,03	7,82	6,73	28,85	6,73
M0060	-1,27	5,80	7,93	10,15	165,36	10,15
M0482	-1,27	5,10	7,78	7,82	167,45	7,82
M0015	-1,25	5,73	6,75	5,19	1,69	5,19

M0038	-1,25	5,67	6,95	5,27	10,00	5,27
M0679	-1,24	5,80	6,37	9,91	-76,67	9,91
M0475	-1,21	5,09	7,62	8,69	173,24	8,69
M0659	-1,21	5,47	7,70	5,94	-29,93	5,94
M0181	-1,20	6,10	6,65	6,66	-14,70	6,66
M0421	-1,20	7,06	5,78	9,10	125,37	9,10
M0018	-1,19	6,86	7,09	7,02	-28,11	7,02
M0250	-1,19	5,18	7,83	4,77	15,93	4,77
M0303	-1,19	6,82	7,89	8,90	95,66	8,90
M0577	-1,15	5,26	7,87	8,71	141,12	8,71
M0465	-1,11	4,82	7,91	5,32	18,79	5,32
M0487	-1,11	5,32	7,58	9,05	148,46	9,05
M0511	-1,11	7,13	7,69	9,66	96,59	9,66
M0218	-1,10	5,41	7,72	6,19	10,18	6,19
M0526	-1,10	6,59	6,85	8,87	-75,76	8,87
M0619	-1,10	5,39	6,86	9,43	136,75	9,43
M0145	-1,08	6,63	6,69	4,89	-19,93	4,89
M0215	-1,05	5,30	7,73	6,11	42,51	6,11
M0345	-1,05	6,47	6,57	9,05	-157,24	9,05
M0396	-1,05	6,14	6,92	9,30	-46,09	9,30
M0276	-1,03	6,42	7,70	8,15	-1,58	8,15
M0554	-1,03	6,45	6,50	6,72	-71,69	6,72
M0142	-1,02	6,50	6,90	9,40	-146,87	9,40
M0246	-1,02	7,00	7,31	6,32	-30,58	6,32
M0411	-0,99	6,18	6,28	9,14	126,77	9,14
M0430	-0,99	5,58	6,56	5,15	-8,54	5,15
M0092	-0,98	5,42	7,46	9,81	-142,25	9,81
M0564	-0,98	4,64	7,76	5,08	17,15	5,08
M0168	-0,97	6,24	7,86	8,64	150,37	8,64
M0450	-0,97	6,05	6,76	5,11	-1,10	5,11
M0483	-0,97	5,38	8,10	9,06	124,57	9,06
M0104	-0,95	5,97	8,00	9,99	125,21	9,99
M0086	-0,93	5,00	5,77	9,00	160,07	9,00
M0595	-0,93	5,19	7,76	4,55	15,43	4,55
M0504	-0,92	6,39	7,71	8,15	1,89	8,15
M0691	-0,90	6,95	6,64	7,82	-62,34	7,82
M0364	-0,87	4,98	7,45	4,91	19,62	4,91
M0405	-0,87	5,28	7,50	9,30	22,05	9,30
M0502	-0,85	6,78	7,80	10,35	85,13	10,35
M0508	-0,84	7,00	6,55	9,17	95,80	9,17
M0284	-0,82	6,99	7,15	6,02	-11,67	6,02
M0287	-0,82	7,11	7,65	9,34	78,14	9,34
M0321	-0,81	5,49	6,68	5,26	-3,72	5,26
M0587	-0,80	5,22	7,38	9,35	171,06	9,35
M0347	-0,79	6,66	6,60	4,85	-22,84	4,85

M0075	-0,77	5,53	8,20	9,37	101,07	9,37
M0591	-0,77	5,50	6,56	5,18	-3,95	5,18
M0326	-0,75	5,40	6,93	5,62	-0,34	5,62
M0187	-0,74	5,13	7,28	9,14	177,78	9,14
M0139	-0,73	6,00	7,83	7,89	159,96	7,89
M0108	-0,72	5,31	6,86	6,81	0,03	6,81
M0630	-0,72	6,54	7,51	8,99	119,82	8,99
M0399	-0,71	6,79	7,84	10,29	83,88	10,29
M0229	-0,70	5,29	7,59	8,99	146,94	8,99
M0270	-0,69	5,98	6,20	9,13	-61,33	9,13
M0174	-0,67	6,34	6,84	5,12	-11,08	5,12
M0505	-0,65	5,43	7,21	8,56	11,98	8,56
M0029	-0,63	5,59	6,66	5,52	-8,58	5,52
M0562	-0,61	5,79	7,34	8,41	-168,67	8,41
M0188	-0,59	5,07	7,73	5,55	39,21	5,55
M0386	-0,59	5,27	7,86	9,59	160,88	9,59
M0451	-0,59	6,68	6,59	4,87	-24,13	4,87
M0545	-0,58	5,40	7,46	9,77	-141,84	9,77
M0455	-0,56	6,70	7,49	9,79	174,66	9,79
M0063	-0,55	5,47	6,98	5,55	4,01	5,55
M0553	-0,54	6,14	6,44	5,32	-53,02	5,32
M0600	-0,54	5,03	7,54	10,80	-41,45	10,80
M0447	-0,53	6,56	6,61	5,11	-23,58	5,11
M0153	-0,50	6,36	6,37	6,79	-53,63	6,79
M0398	-0,50	5,44	6,26	10,57	176,07	10,57
M0157	-0,49	5,46	7,45	9,43	-127,34	9,43
M0069	-0,48	6,11	7,34	8,76	-43,13	8,76
M0047	-0,47	5,61	6,90	5,41	3,68	5,41
M0548	-0,47	5,35	6,85	6,91	-2,46	6,91
M0675	-0,47	5,10	6,99	8,70	9,46	8,70
M0510	-0,46	7,01	5,20	7,23	-54,57	7,23
M0614	-0,46	6,54	5,87	8,85	145,01	8,85
M0426	-0,44	5,63	5,94	9,80	-145,42	9,80
M0676	-0,44	6,17	7,08	9,30	-40,85	9,30
M0645	-0,42	6,35	6,13	6,34	-52,77	6,34
M0280	-0,41	7,09	7,61	9,07	84,45	9,07
M0566	-0,41	5,90	7,73	8,55	164,23	8,55
M0275	-0,40	5,35	7,27	8,63	13,85	8,63
M0439	-0,40	5,27	6,80	6,93	-2,84	6,93
M0118	-0,39	5,77	7,02	6,98	-0,60	6,98
M0518	-0,39	5,69	7,03	8,84	-37,66	8,84
M0527	-0,39	6,45	6,01	8,69	138,79	8,69
M0258	-0,38	5,56	6,26	10,32	132,73	10,32
M0448	-0,38	6,92	6,12	9,29	138,01	9,29
M0523	-0,38	6,24	7,54	7,68	70,67	7,68

M0193	-0,37	5,30	7,95	5,81	6,80	5,81
M0055	-0,36	6,29	7,81	8,19	155,98	8,19
M0317	-0,35	5,60	6,27	7,26	-53,91	7,26
M0435	-0,35	5,22	7,86	8,89	116,35	8,89
M0517	-0,35	6,05	6,81	9,45	-68,12	9,45
M0249	-0,34	5,29	7,71	9,32	147,99	9,32
M0089	-0,33	5,70	6,56	5,19	-8,84	5,19
M0560	-0,33	6,61	5,70	9,94	-172,04	9,94
M0017	-0,32	7,02	8,02	8,19	-29,10	8,19
M0114	-0,32	6,79	7,94	8,07	-34,13	8,07
M0042	-0,30	5,83	8,30	9,09	95,34	9,09
M0464	-0,30	6,41	6,79	5,15	-13,47	5,15
M0473	-0,30	4,93	7,44	4,89	21,90	4,89
M0003	-0,29	6,50	7,80	8,35	70,06	8,35
M0149	-0,29	5,79	7,30	6,03	12,92	6,03
M0273	-0,29	5,92	6,38	9,21	-58,96	9,21
M0546	-0,29	5,19	7,37	9,40	-118,70	9,40
M0138	-0,28	6,43	7,52	8,42	170,33	8,42
M0394	-0,27	6,14	6,29	9,33	-58,01	9,33
M0631	-0,27	5,76	7,29	6,06	9,39	6,06
M0637	-0,27	5,02	8,09	8,43	149,05	8,43
M0059	-0,25	5,55	7,23	10,46	-150,96	10,46
M0479	-0,25	5,26	7,77	9,70	144,52	9,70
M0182	-0,24	6,42	6,59	5,31	-17,22	5,31
M0312	-0,24	5,73	7,68	6,76	33,01	6,76
M0103	-0,23	5,23	6,61	6,95	-10,93	6,95
M0282	-0,23	6,46	6,56	9,13	-77,91	9,13
M0685	-0,23	5,93	7,24	10,52	130,01	10,52
M0331	-0,22	5,88	7,87	9,87	-177,97	9,87
M0582	-0,22	5,30	7,57	5,71	11,65	5,71
M0608	-0,22	7,06	8,06	8,63	-56,72	8,63
M0617	-0,22	6,78	6,21	8,83	-85,17	8,83
M0309	-0,21	6,77	6,08	8,67	-93,06	8,67
M0641	-0,21	6,09	7,80	7,93	164,61	7,93
M0239	-0,20	5,46	6,85	5,28	1,90	5,28
M0012	-0,19	6,80	6,19	8,31	-76,27	8,31
M0689	-0,19	6,46	6,28	8,00	-59,76	8,00
M0219	-0,18	5,76	7,95	9,82	116,63	9,82
M0278	-0,18	5,38	7,56	9,33	20,67	9,33
M0428	-0,18	7,00	7,18	6,07	-26,99	6,07
M0180	-0,17	6,25	8,22	6,14	12,41	6,14
M0297	-0,17	6,29	7,50	9,22	96,97	9,22
M0427	-0,17	6,13	6,60	4,87	-10,95	4,87
M0669	-0,17	5,26	7,72	9,28	146,87	9,28
M0228	-0,16	5,19	7,66	5,11	33,58	5,11

M0240	-0,16	5,50	6,57	5,18	-3,35	5,18
M0023	-0,15	5,57	6,29	7,36	-54,23	7,36
M0194	-0,15	5,32	7,98	8,18	103,87	8,18
M0607	-0,15	6,99	7,10	8,30	-67,37	8,30
M0203	-0,14	5,18	7,64	8,81	153,11	8,81
M0320	-0,14	5,60	7,03	5,59	6,88	5,59
M0324	-0,14	5,78	6,48	5,35	-15,22	5,35
M0067	-0,10	6,69	7,91	8,84	139,21	8,84
M0402	-0,10	5,68	6,36	9,34	-54,46	9,34
M0227	-0,08	5,26	7,69	8,99	155,38	8,99
M0490	-0,07	4,97	7,87	7,82	146,33	7,82
M0515	-0,06	5,96	6,42	9,99	117,04	9,99
M0256	-0,05	5,98	7,31	8,36	2,22	8,36
M0271	-0,04	6,38	7,65	10,81	93,41	10,81
M0368	-0,04	5,09	7,56	8,02	139,65	8,02
M0143	-0,02	6,55	7,79	8,17	138,17	8,17
M0208	-0,02	5,27	7,64	6,01	28,80	6,01
M0264	-0,02	5,45	7,60	10,76	-40,08	10,76
M0492	-0,02	5,63	6,70	5,32	-8,76	5,32
M0001	0,00	7,07	7,73	8,65	-44,66	8,65
M0070	0,00	6,18	6,82	5,19	-5,39	5,19
M0010	0,01	7,01	7,14	5,94	-27,49	5,94
M0090	0,02	6,63	7,32	5,92	43,22	5,92
M0045	0,03	5,55	6,30	7,38	-53,48	7,38
M0099	0,03	5,65	6,53	6,74	-8,37	6,74
M0144	0,03	6,03	6,48	4,99	-39,57	4,99
M0458	0,03	6,50	6,85	9,73	-155,20	9,73
M0052	0,05	6,16	7,56	5,37	-22,99	5,37
M0452	0,06	5,94	7,64	8,68	161,37	8,68
M0172	0,08	6,10	7,80	8,24	166,44	8,24
M0200	0,08	5,23	7,61	9,42	169,36	9,42
M0470	0,08	6,26	8,15	6,13	8,35	6,13
M0105	0,09	6,77	7,75	9,24	102,98	9,24
M0164	0,09	6,00	7,70	8,64	164,07	8,64
M0049	0,10	5,70	6,15	6,68	-46,24	6,68
M0359	0,10	5,34	6,95	6,68	4,78	6,68
M0622	0,10	5,97	6,96	4,98	7,13	4,98
M0279	0,11	5,87	6,36	9,36	-64,91	9,36
M0565	0,11	5,73	6,19	8,36	-139,11	8,36
M0220	0,12	5,15	7,30	9,00	-156,30	9,00
M0432	0,12	6,81	5,69	9,80	-177,55	9,80
M0123	0,13	6,20	6,76	4,89	-14,23	4,89
M0272	0,14	5,40	5,57	9,26	-38,10	9,26
M0477	0,14	5,23	7,73	9,63	136,93	9,63
M0516	0,16	5,57	7,04	6,11	-9,80	6,11

M0173	0,17	6,53	6,33	9,57	-156,28	9,57
M0462	0,17	4,87	7,73	5,50	16,46	5,50
M0522	0,17	5,92	5,34	9,20	146,51	9,20
M0013	0,18	5,96	6,93	5,18	4,29	5,18
M0201	0,19	5,20	7,77	7,81	132,38	7,81
M0300	0,19	6,53	7,30	5,93	44,13	5,93
M0418	0,19	6,88	7,75	9,27	109,98	9,27
M0248	0,20	5,59	6,85	5,22	1,53	5,22
M0260	0,21	6,09	6,47	9,25	-50,01	9,25
M0692	0,21	6,79	6,39	7,62	103,18	7,62
M0237	0,22	6,91	6,47	7,06	-53,37	7,06
M0081	0,23	5,49	7,96	7,49	20,18	7,49
M0154	0,23	6,30	7,64	7,43	-26,37	7,43
M0621	0,23	7,04	7,18	6,07	-25,49	6,07
M0082	0,24	6,21	6,72	5,23	-12,98	5,23
M0292	0,24	6,20	6,93	8,85	74,59	8,85
M0343	0,24	5,92	6,89	4,87	7,47	4,87
M0043	0,27	5,54	6,61	5,39	-7,33	5,39
M0211	0,27	5,19	6,74	6,86	-5,14	6,86
M0222	0,27	5,07	8,03	7,70	143,66	7,70
M0255	0,27	6,21	7,98	7,18	-32,50	7,18
M0495	0,27	5,95	7,31	8,48	0,24	8,48
M0072	0,28	5,98	7,05	8,10	68,81	8,10
M0236	0,28	5,90	6,79	5,98	-3,68	5,98
M0420	0,29	6,82	8,10	8,75	-37,52	8,75
M0401	0,30	6,82	6,52	9,26	91,35	9,26
M0606	0,31	5,77	6,32	9,56	-66,80	9,56
M0064	0,32	6,51	7,75	7,75	-8,55	7,75
M0166	0,33	4,80	7,85	5,30	16,65	5,30
M0643	0,33	6,82	6,24	9,14	143,14	9,14
M0127	0,34	5,49	7,82	6,22	7,11	6,22
M0413	0,34	5,07	6,07	9,82	-179,30	9,82
M0299	0,35	5,71	6,17	9,32	-74,33	9,32
M0196	0,36	5,30	7,37	5,40	33,57	5,40
M0221	0,37	5,85	6,72	5,18	-10,44	5,18
M0680	0,37	5,61	5,57	9,39	-44,72	9,39
M0530	0,38	5,58	7,81	6,57	45,65	6,57
M0120	0,39	5,71	6,59	6,64	-12,31	6,64
M0571	0,39	5,04	7,28	8,98	174,83	8,98
M0184	0,40	6,26	6,39	6,41	-44,47	6,41
M0062	0,42	6,09	6,41	8,24	96,28	8,24
M0328	0,42	5,51	6,80	5,27	-4,21	5,27
M0612	0,42	6,14	7,59	7,66	-48,11	7,66
M0640	0,42	6,00	5,97	8,49	-160,92	8,49
M0061	0,43	6,11	6,15	8,82	154,09	8,82

M0265	0,43	5,57	6,07	10,58	-179,32	10,58
M0296	0,43	5,97	7,55	9,29	77,78	9,29
M0327	0,43	6,57	5,74	9,92	-177,34	9,92
M0586	0,43	5,31	7,54	8,91	165,67	8,91
M0615	0,44	6,35	7,55	9,32	99,93	9,32
M0130	0,45	6,15	6,41	4,98	-50,08	4,98
M0192	0,46	6,23	7,91	10,16	144,21	10,16
M0348	0,46	6,00	7,65	8,68	160,12	8,68
M0088	0,47	6,14	6,80	4,94	-3,40	4,94
M0389	0,47	6,19	8,00	7,09	-31,46	7,09
M0572	0,47	5,05	7,78	5,77	45,78	5,77
M0512	0,48	7,00	6,11	7,27	-84,18	7,27
M0374	0,49	6,98	6,31	9,79	-119,61	9,79
M0150	0,52	6,31	7,33	8,32	-5,31	8,32
M0028	0,53	6,77	6,61	7,61	-57,52	7,61
M0177	0,53	6,26	6,80	8,59	-150,27	8,59
M0233	0,53	5,29	5,85	9,25	-146,29	9,25
M0460	0,53	6,12	7,77	8,61	156,83	8,61
M0594	0,53	5,34	7,47	8,82	176,22	8,82
M0053	0,54	6,19	7,36	6,50	-11,17	6,50
M0058	0,54	5,53	6,83	5,26	1,79	5,26
M0372	0,54	5,30	8,15	8,78	118,16	8,78
M0574	0,54	5,33	8,08	8,23	140,95	8,23
M0025	0,55	6,50	7,49	7,82	-14,31	7,82
M0044	0,55	5,74	6,60	5,16	-8,47	5,16
M0362	0,55	6,01	6,59	6,72	-12,91	6,72
M0242	0,57	5,18	7,51	5,76	22,26	5,76
M0454	0,57	6,00	7,51	8,79	174,58	8,79
M0528	0,57	6,68	8,06	8,74	-40,76	8,74
M0563	0,57	5,03	8,28	5,62	44,71	5,62
M0014	0,58	5,86	6,75	6,52	-31,40	6,52
M0316	0,58	5,87	6,96	5,16	8,22	5,16
M0190	0,61	5,21	7,96	6,50	2,18	6,50
M0113	0,62	6,77	6,31	8,88	-90,35	8,88
M0121	0,62	6,07	6,69	6,42	-8,50	6,42
M0346	0,62	6,34	7,51	8,00	159,97	8,00
M0436	0,62	5,49	7,93	7,29	21,84	7,29
M0602	0,62	6,50	7,68	10,71	89,56	10,71
M0106	0,63	5,64	7,24	10,45	-151,40	10,45
M0131	0,63	5,68	7,26	9,73	131,85	9,73
M0251	0,63	5,55	6,36	6,52	-49,81	6,52
M0639	0,64	5,87	8,25	5,81	40,75	5,81
M0494	0,68	4,46	7,71	5,73	10,05	5,73
M0555	0,68	6,58	6,33	6,57	-58,94	6,57
M0660	0,68	6,99	6,33	9,81	-121,61	9,81

M0538	0,69	5,42	7,07	5,46	11,11	5,46
M0286	0,70	6,84	7,40	9,67	-76,49	9,67
M0363	0,70	5,92	6,71	8,77	123,42	8,77
M0597	0,70	5,96	7,33	8,44	2,86	8,44
M0243	0,71	5,26	6,89	4,80	0,56	4,80
M0657	0,71	5,28	7,28	4,35	24,25	4,35
M0084	0,72	5,28	7,61	7,14	67,12	7,14
M0269	0,72	5,40	6,57	8,10	10,83	8,10
M0179	0,73	6,35	8,18	6,88	36,20	6,88
M0241	0,73	5,29	8,03	8,32	109,56	8,32
M0380	0,73	5,29	7,63	8,85	139,73	8,85
M0588	0,73	5,29	5,82	9,26	-149,52	9,26
M0268	0,74	6,71	7,97	9,93	66,35	9,93
M0124	0,75	5,40	6,46	6,88	-11,24	6,88
M0205	0,75	5,06	8,11	6,40	22,49	6,40
M0444	0,75	6,26	6,85	4,79	0,27	4,79
M0556	0,75	6,11	7,58	8,29	164,16	8,29
M0609	0,75	6,83	7,56	10,64	92,92	10,64
M0039	0,76	6,17	6,76	5,16	-12,18	5,16
M0133	0,76	6,43	7,62	4,85	-21,51	4,85
M0169	0,76	5,82	7,59	8,74	163,78	8,74
M0539	0,76	5,51	6,80	5,37	0,49	5,37
M0073	0,77	6,35	7,48	8,02	86,54	8,02
M0307	0,77	6,75	7,59	9,50	119,27	9,50
M0314	0,77	5,54	6,52	9,00	-56,47	9,00
M0375	0,78	5,08	8,08	7,83	138,70	7,83
M0431	0,80	6,34	7,43	10,63	166,16	10,63
M0476	0,80	5,26	8,15	7,36	23,96	7,36
M0497	0,80	5,30	6,02	8,99	-48,88	8,99
M0648	0,80	6,40	7,28	9,19	176,72	9,19
M0159	0,81	6,06	7,30	8,27	-167,85	8,27
M0627	0,81	5,72	7,30	9,73	131,62	9,73
M0315	0,82	6,18	6,60	4,94	-13,01	4,94
M0207	0,83	5,12	7,65	8,54	174,94	8,54
M0365	0,83	5,01	7,39	9,18	175,89	9,18
M0417	0,84	6,66	7,07	9,22	-90,53	9,22
M0202	0,86	5,17	7,71	9,21	139,02	9,21
M0357	0,86	6,22	7,17	8,82	-165,59	8,82
M0652	0,86	6,36	7,90	8,39	133,09	8,39
M0290	0,87	6,12	7,41	7,98	-17,24	7,98
M0434	0,87	5,53	6,48	5,13	-10,89	5,13
M0151	0,88	6,45	7,76	8,07	122,32	8,07
M0590	0,88	5,67	6,84	5,14	-3,49	5,14
M0651	0,88	6,52	6,80	5,14	-14,83	5,14
M0048	0,89	5,36	7,11	5,51	15,19	5,51

M0245	0,89	5,46	6,63	5,72	-12,82	5,72
M0578	0,89	5,35	7,87	9,86	151,32	9,86
M0126	0,90	6,24	7,81	7,65	155,00	7,65
M0387	0,90	5,49	6,31	6,19	-49,46	6,19
M0503	0,91	5,24	7,28	8,85	10,69	8,85
M0684	0,91	6,58	6,28	9,22	-87,55	9,22
M0537	0,92	5,47	7,94	9,63	113,94	9,63
M0634	0,93	6,42	6,62	5,08	-13,94	5,08
M0665	0,93	5,28	7,69	8,81	136,93	8,81
M0128	0,94	6,46	7,82	8,12	5,88	8,12
M0429	0,95	5,47	6,89	5,27	3,82	5,27
M0461	0,95	6,17	7,40	8,98	170,09	8,98
M0129	0,96	6,12	7,84	5,92	11,51	5,92
M0677	0,96	6,73	8,11	10,07	70,55	10,07
M0022	0,97	7,09	6,91	8,06	-60,25	8,06
M0356	0,97	4,98	7,78	5,46	12,44	5,46
M0536	0,97	5,48	6,65	5,35	-5,02	5,35
M0625	0,97	5,48	6,37	4,72	-6,72	4,72
M0009	0,98	6,13	6,66	5,01	-9,37	5,01
M0041	1,00	5,87	7,18	7,13	-42,78	7,13
M0119	1,00	6,67	7,96	8,21	78,04	8,21
M0122	1,00	5,62	6,38	7,63	-36,66	7,63
M0160	1,00	4,96	7,56	5,31	-0,46	5,31
M0254	1,00	4,26	7,94	5,46	13,14	5,46
M0453	1,00	6,47	7,64	8,81	161,98	8,81
M0468	1,00	6,58	6,95	7,82	174,74	7,82
M0107	1,01	5,71	6,69	6,55	-6,91	6,55
M0140	1,01	6,32	6,30	5,45	-57,71	5,45
M0176	1,01	6,16	7,29	9,22	172,39	9,22
M0252	1,01	5,47	6,93	5,20	-1,07	5,20
M0533	1,01	6,20	6,85	5,23	-8,33	5,23
M0620	1,01	5,55	7,86	5,84	15,45	5,84
M0668	1,01	5,59	6,43	5,22	-15,09	5,22
M0074	1,02	6,10	6,14	8,50	123,85	8,50
M0308	1,03	6,83	5,74	8,15	-91,01	8,15
M0663	1,03	5,36	7,30	5,54	9,19	5,54
M0132	1,05	6,10	7,10	5,44	6,07	5,44
M0338	1,05	5,62	7,42	10,92	179,85	10,92
M0484	1,05	5,35	7,75	7,90	160,93	7,90
M0125	1,06	5,29	7,75	4,89	1,08	4,89
M0136	1,06	6,61	6,33	6,53	-59,31	6,53
M0339	1,06	5,25	7,66	4,83	-4,63	4,83
M0535	1,06	5,37	7,68	9,96	133,04	9,96
M0094	1,08	6,36	6,73	9,06	-132,53	9,06
M0352	1,08	6,67	6,65	6,50	-52,40	6,50

M0385	1,08	5,13	7,42	7,03	168,52	7,03
M0616	1,08	6,39	6,53	8,12	105,61	8,12
M0065	1,09	5,89	8,05	10,49	158,43	10,49
M0541	1,09	6,40	7,72	8,94	165,26	8,94
M0534	1,10	5,36	6,79	5,27	5,02	5,27
M0322	1,11	5,72	7,63	9,95	-149,10	9,95
M0666	1,11	5,68	6,86	5,33	-1,82	5,33
M0289	1,12	6,13	7,33	8,47	-35,81	8,47
M0456	1,12	6,49	7,82	8,01	118,47	8,01
M0481	1,12	5,54	7,45	5,77	15,52	5,77
M0569	1,12	6,28	6,13	6,53	-51,74	6,53
M0581	1,12	5,35	7,79	7,12	143,98	7,12
M0688	1,12	5,94	7,65	9,29	84,88	9,29
M0005	1,13	5,56	7,55	5,17	14,05	5,17
M0036	1,14	6,70	7,81	9,50	112,22	9,50
M0091	1,14	6,58	7,29	7,25	-33,22	7,25
M0210	1,14	5,36	8,12	8,70	109,35	8,70
M0231	1,14	5,35	7,72	7,74	151,82	7,74
M0445	1,15	6,14	7,72	8,49	147,68	8,49
M0358	1,16	6,29	6,71	5,21	-16,91	5,21
M0472	1,16	5,11	7,25	8,94	-179,16	8,94
M0068	1,17	6,42	5,91	9,92	-179,18	9,92
M0580	1,17	5,27	7,80	8,45	144,31	8,45
M0097	1,18	5,69	7,17	9,53	-118,53	9,53
M0148	1,18	6,21	7,52	8,76	166,10	8,76
M0247	1,18	5,04	7,82	9,23	160,83	9,23
M0294	1,18	6,27	7,76	8,87	-24,32	8,87
M0407	1,18	6,91	6,52	8,68	86,67	8,68
M0489	1,18	6,79	7,79	5,87	-28,39	5,87
M0596	1,18	5,55	6,82	5,23	-4,94	5,23
M0635	1,18	6,22	7,10	4,67	10,04	4,67
M0274	1,19	5,49	7,08	8,31	22,42	8,31
M0552	1,19	5,96	6,94	4,88	9,07	4,88
M0383	1,20	5,17	7,80	4,64	12,63	4,64
M0388	1,20	5,96	6,34	9,52	160,99	9,52
M0544	1,20	5,64	7,34	6,17	15,23	6,17
M0225	1,22	5,64	6,87	5,54	-3,10	5,54
M0318	1,22	5,40	7,65	9,98	132,32	9,98
M0373	1,22	5,22	7,74	9,24	127,13	9,24
M0071	1,23	5,39	6,58	5,21	-6,51	5,21
M0306	1,24	6,71	7,70	9,41	-61,97	9,41
M0216	1,25	5,37	7,79	8,69	107,61	8,69
M0288	1,25	5,60	7,69	8,69	-22,93	8,69
M0377	1,25	6,14	6,41	5,66	-19,78	5,66
M0141	1,26	5,52	7,64	9,02	-169,68	9,02

M0197	1,27	5,28	7,45	8,64	-166,44	8,64
M0658	1,27	5,31	7,75	8,47	149,68	8,47
M0178	1,29	6,22	7,27	8,73	-166,15	8,73
M0212	1,29	5,33	7,97	8,73	118,97	8,73
M0543	1,29	5,54	6,52	5,13	-8,57	5,13
M0096	1,30	6,67	6,33	8,50	114,53	8,50
M0147	1,30	6,39	7,84	7,91	144,39	7,91
M0313	1,30	5,41	7,86	7,15	56,84	7,15
M0589	1,30	6,88	7,91	7,50	-49,23	7,50
M0146	1,31	6,43	7,66	8,79	158,77	8,79
M0469	1,31	5,89	6,93	6,45	0,71	6,45
M0628	1,31	6,66	5,73	9,80	-179,46	9,80
M0678	1,31	5,31	6,59	8,24	8,82	8,24
M0186	1,32	5,13	8,04	6,26	13,40	6,26
M0333	1,32	5,41	6,36	9,40	143,46	9,40
M0558	1,32	6,36	7,84	7,97	156,55	7,97
M0319	1,33	5,68	6,82	5,32	-0,51	5,32
M0332	1,33	5,37	6,47	7,27	-16,31	7,27
M0334	1,34	5,83	7,13	6,31	10,47	6,31
M0341	1,34	6,36	5,75	8,89	-159,09	8,89
M0344	1,34	6,08	8,00	5,23	8,21	5,23
M0355	1,34	6,16	7,88	8,49	151,01	8,49
M0390	1,35	5,38	6,35	8,34	-51,16	8,34
M0400	1,35	5,43	5,54	9,35	-41,68	9,35
M0414	1,35	5,16	7,84	7,89	63,97	7,89
M0415	1,36	5,70	7,18	7,69	-48,27	7,69
M0433	1,36	5,24	7,22	5,46	20,85	5,46
M0437	1,36	5,51	7,97	7,55	21,19	7,55
M0442	1,36	5,43	6,61	6,82	-4,44	6,82
M0467	1,37	6,33	6,66	5,18	-19,15	5,18
M0488	1,37	6,96	6,45	6,51	-43,05	6,51
M0500	1,37	5,39	7,65	10,67	-33,18	10,67
M0514	1,37	5,88	7,91	9,00	-48,90	9,00
M0519	1,37	6,46	5,65	8,07	133,48	8,07
M0520	1,38	6,31	7,77	8,82	-24,60	8,82
M0542	1,38	5,44	6,89	5,26	0,33	5,26
M0547	1,39	5,38	6,39	9,37	141,89	9,37
M0549	1,39	6,11	7,12	5,33	7,71	5,33
M0559	1,39	6,26	7,79	6,04	-22,06	6,04
M0579	1,40	5,30	7,69	8,24	146,09	8,24
M0583	1,40	5,16	7,61	9,12	175,34	9,12
M0584	1,40	5,33	7,76	7,69	161,52	7,69
M0592	1,40	5,18	7,78	4,64	12,28	4,64
M0593	1,41	5,78	7,89	10,07	126,22	10,07
M0613	1,41	6,03	7,47	9,19	83,25	9,19

M0629	1,41	5,47	6,88	5,27	-0,37	5,27
M0636	1,42	6,37	7,04	8,40	139,26	8,40
M0638	1,42	6,25	7,19	8,91	-178,52	8,91
M0644	1,42	6,70	7,61	9,77	175,46	9,77
M0661	1,42	5,02	7,70	7,63	174,12	7,63
M0670	1,43	5,33	7,00	5,11	7,08	5,11
M0673	1,43	5,54	6,23	10,18	122,68	10,18
TOTAL IN RANGE [%]		**96**	**42**	**50**	**32**	**31**

Figure S1. VT ^{1}H NMR on **13c**

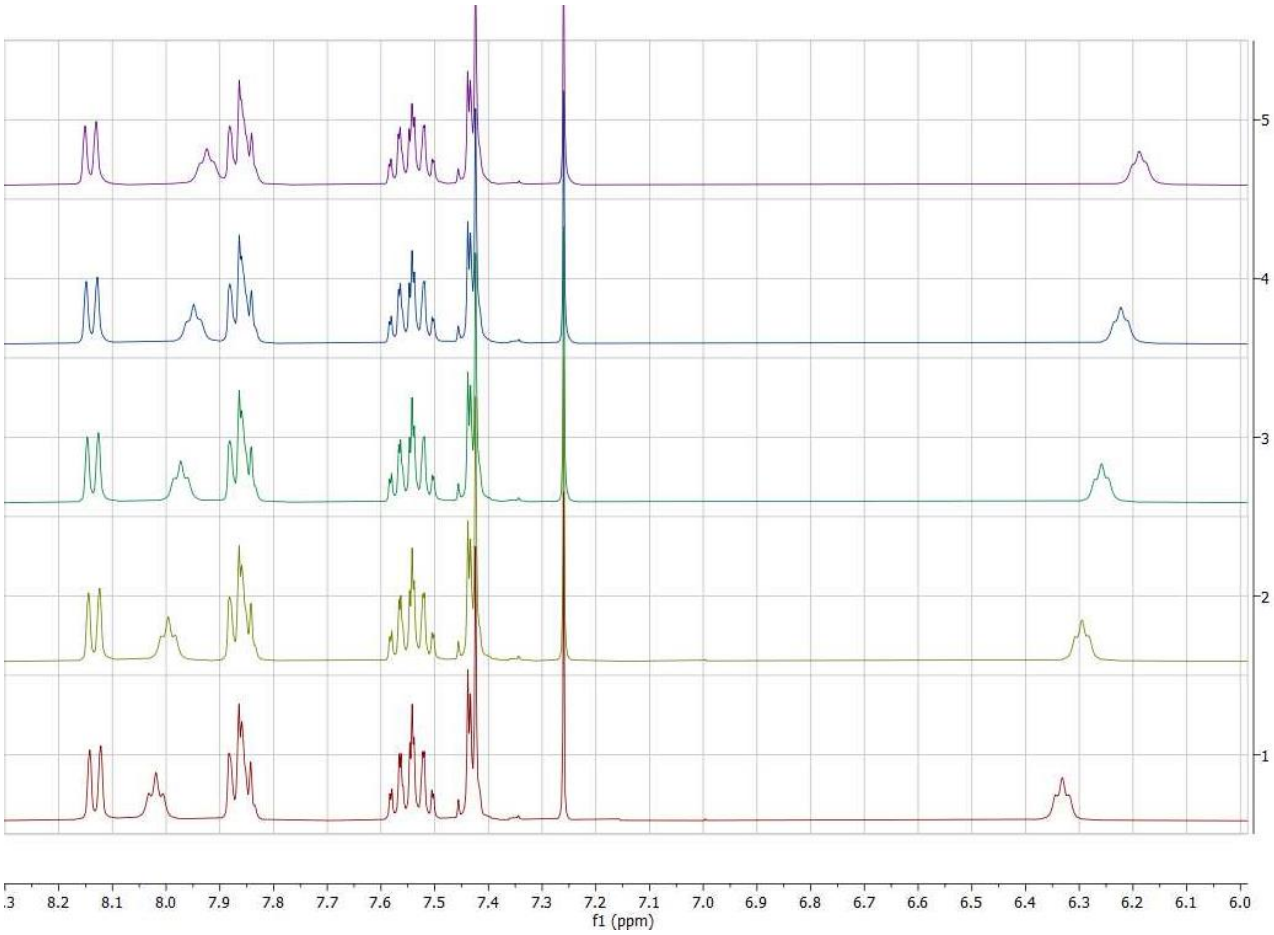


Figure S2. DMSO ^{1}H NMR titration on **13c**