SUPPLEMENTARY INFORMATION

Design, Synthesis, and Conformational Analysis of 3-*Cyclo*-Butylcarbamoyl Hydantoins as Novel Hydrogen Bond Driven Universal Peptidomimetics

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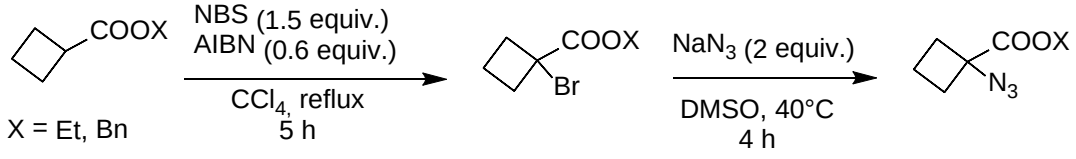
Experimental procedures

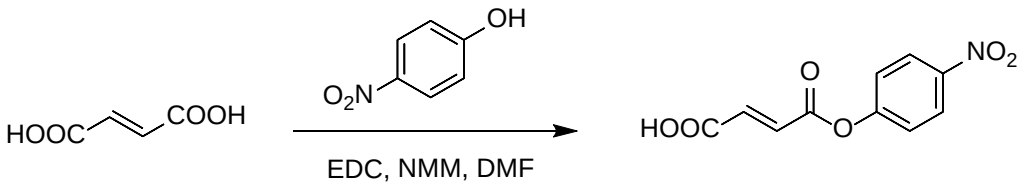
General Methods. *Synthesis and characterization:* commercially available reagent-grade solvents were employed without purification. TLC were run on silica gel 60 F254 Merck. Flash chromatography (FC) was performed with silica gel 60 (60-200 mm, Merck). ^{1}H NMR spectra were recorded on 400 MHz spectrometers. 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). ESIMS was performed with an Esquire 3000 plus ion-trap mass spectrometer equipped with an ESI source. Elemental analysis of the basic neomycin conjugates were obtained on FlashEA 1112 NC Analyzers. *Molecular modeling:* Calculations were performed with Spartan 08 software.[1] All the structures were first submitted to a Monte Carlo conformational search with MM (MMFF94 force field) minimization. The selected global minima were then submitted to HF/3-21G* full optimization followed by DFT/6-31G* single point calculations. *X-ray crystallography:* crystals of **1c**, **1i** and **1k** were obtained as colorless prisms from water/methanol 1:1 solutions at room temperature. Intensity data were collected at room temperature on a Bruker Apex II CCD diffractometer, using graphite-monochromatized Mo-Kα radiation (λ = 0.71073 Å). Intensity data were corrected for Lorentz-polarization effects and for absorption (*SADABS*)[2]. The structures were solved by direct methods (*SIR-97*)[3] and completed by iterative cycles of full-matrix least squares refinement on F_o^2 and ΔF synthesis using the *SHELXL-97*[4] program (*WinGX* suite)[5]. The positions of hydrogen atoms were introduced at calculated positions, in their described geometries and allowed to ride on the attached carbon atom with fixed isotropic thermal parameters (1.2Ueq of the parent carbon atom) or were detected in a difference Fourier and refined with isotropic thermal factors. All non-H-atoms were refined anisotropically. These data can be obtained free of charge *via* www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB21EZ, UK; fax: ++44 1223 336 033; or deposit@ccdc.cam.ac.uk). CCDC-1540951 (**1i**) and CCDC-1540950 (**1k**) numbers contain the supplementary crystallographic data for this paper.

1. Preparation of α-azido-*cyclo*-butyl carboxylic esters 2

α-Azido-*cyclo*-butyl carboxylic esters **2** were prepared by bromination of the corresponding esters followed by nucleophilic displacement of the bromine with sodium azides, according to the procedures reported in literature.[6]



2. Preparation of fumaric acid mono *p*-nitrophenyl ester 5



To a stirred solution of fumaric acid (1.0 equiv.) in DMF (0.1 M solution), solid *p*-nitrophenol (1.0 equiv.) followed by *N*-methylmorpholine (1.0 equiv.) and EDC (1.0 equiv.) were added at 0°C. The mixture was stirred at rt overnight. The mixture was poured in a 5% aqueous solution of $NaHCO_3$ and washed with AcOEt. The aqueous phase was acidified (pH = 2) with 1N aqueous HCl and extracted with Et_2O. The combined organic layers were dried on Na_2SO_4, filtered, and the organic solvent evaporated. The crude was crystalized from methanol affording compound **5** in 62 % yield as a white solid.

(E)-4-(4-nitrophenoxy)-4-oxobut-2-enoic acid 5 R_f = 0.17 (DCM/MeOH = 80:20); ^{1}H NMR (400 MHz, DMSO-d_6) δ 13.27 (br s, 1H), 8.29 (d, *J* = 8.8 Hz, 2H), 7.51 (d, *J* = 8.8 Hz, 2H), 6.92 (d, , *J* = 16.0 Hz, 1H), 6.87 (d, , *J* = 16.0 Hz, 1H); ^{13}C NMR (100.6 MHz, DMSO-d_6) δ 165.9, 163.1, 155.3, 145.8, 137.2, 131.7, 125.7, 123.5; ESI (*m/z)* 235.8 [M^--H, (100)], 137.9 [(*p*-NO_2-phenol)$^-$-H, (75)].

3. General procedure for the MC synthesis of intermediates 7.

To a stirred solution of azide **2** (1.0 equiv.) and isocyanate **3** (1.0 equiv.) in CH_3CN (0.1 M), solid Ph_3P (1.1 equiv.) was added and the resulting solution stirred overnight. 2,4,6 Trimethylpyridine (TMP, 1.1 equiv.) followed by acid **5** (1.1 equiv.) were added at rt. Once intermediate **6** is formed (3-4 h, TLC monitoring), the amine component (1.1 equiv.) is added and the mixture stirred at rt overnight. The solution was diluted with AcOEt and washed with a 1M aqueous HCl solution, with a saturated aqueous solution of $NaHCO_3$, and with brine. The combined organic layers were dried on Na_2SO_4, filtered, and the organic solvent evaporated. The crude was purified by flash chromatography affording compounds **7** in a 60-80 % range yields.

Ethyl 1-(3-ethyl-4-(2-((4-methoxybenzyl)amino)-2-oxoethyl)-2,5-dioxoimidazolidin-1-yl)cyclobutane-1-carboxylate 7a: Yield 73%. R_f = 0.21 (Hexane/AcOEt = 40:60); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.19 (d, *J* = 8.4 Hz, 2H), 6.85 (d, *J* = 8.4 Hz, 2H), 6.33 (br t, 1H), 4.39-4.28 (m, 3H), 4.23-4.18 (m, 2H), 3.78 (s, 3H), 3.64 (sextet, *J* = 7.2 Hz, 1H), 3.07 (sextet, *J* = 7.2 Hz, 1H), 2.82-2.70 (m, 5H), 2.54 (dd, *J* = 15.6 and 6.4 Hz, 1H), 3.31 (q, *J* = 2.4 Hz, 1H), 1.97-1.95 (m, 1H), 1.28 (t, *J* = 7.2 Hz, 3H), 1.13 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 172.8, 172.1, 168.0, 159.1, 155.4, 130.0, 129.2, 114.1, 61.8, 60.1, 55.8, 55.3, 43.3, 37.2, 36.1, 31.2, 30.9, 17.4, 14.1,

13.0; ESI (*m/z)* 454.1 [M^++Na, (100)]; Anal. calcd. for $C_{22}H_{29}N_3O_6$: C 61.24, H 6.77, N 9.74; found: C 61.25, H 6.73, N 9.76.

Benzyl 1-(4-(2-((2,2-diphenylethyl)amino)-2-oxoethyl)-3-ethyl-2,5-dioxoimidazolidin-1-yl)cyclobutane-1-carboxylate 7b: Yield 77%. R_f = 0.43 (Hexane/AcOEt = 40:60); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24-7.23 (m, 15H), 5.49 (br t, 1H), 5.13 (d, *J* = 12.0 Hz, 1H), 5.08 (d, *J* = 12.0 Hz, 1H), 4.23 (dd, *J* = 6.8 and 4.4 Hz, 1H), 4.14 (t, *J* = 8.0 Hz, 1H), 3.90-3.87 (m, 2H), 3.51 (sextet, *J* = 7.2 Hz, 1H), 2.88-2.85 (m, 3H), 2.79-2.74 (m, 2H), 2.40 (dd, *J* = 15.6 and 4.8 Hz, 1H), 2.31 (q, *J* = 10.8 Hz, 1H), 2.01-1.95 (m, 2H), 1.03 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 172.8, 171.8, 168.2, 155.3, 141.6, 141.5, 135.6, 128.8, 128.7, 128.6, 128.5, 128.2, 128.1, 128.0, 127.99, 127.94, 126.9, 67.4, 60.2, 55.5, 50.6, 44.0, 37.2, 35.9, 31.4, 31.0, 17.4, 13.0; ESI (*m/z)* 552,4 [M^--H, (100)]; Anal. calcd. for $C_{33}H_{35}N_3O_5$: C 71.59, H 6.37, N 7.59; found: C 71.61, H 6.38, N 7.61.

Benzyl 1-(3-benzyl-4-(2-((2,2-diphenylethyl)amino)-2-oxoethyl)-2,5-dioxoimidazolidin-1-yl)cyclobutane-1-carboxylate 7c: Yield 75%. R_f = 0.45 (Hexane/AcOEt = 40:60); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27-7.15 (m, 20H), 5.21 (br s, 1H), 5.18 (d, *J* = 12.0 Hz, 1H), 5.11 (d, *J* = 12.0 Hz, 1H), 4.56 (d, *J* = 15.2 Hz, 1H), 4.22 (d, *J* = 15.2 Hz, 1H), 4.13 (dd, *J* = 6.0 and 4.8 Hz, 1H), 4.04 (t, *J* = 8.0 Hz, 1H), 3.87-3.84 (m, 1H), 3.69-3.66 (m, 1H), 2.93-2.89 (m, 4H), 2.35-2.29 (m, 2H), 2.02-2.00 (m, 2H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 172.5, 171.9, 167.9, 156.0, 141.7, 141.6, 136.4, 135.5, 128.8, 128.73, 128.71, 128.6, 128.5, 128.2, 128.1, 128.06, 128.00, 127.96, 127.92, 127.7, 126.93, 126.91, 67.4, 60.3, 56.3, 50.5, 45.2, 43.9, 36.9, 31.4, 30.9, 17.4; ESI (*m/z)* 638.3 [M^++Na, (100)]; Anal. calcd. for $C_{38}H_{37}N_3O_5$: C 74.13, H 6.06, N 6.82; found: C 74.14, H 6.06, N 6.83.

Benzyl 1-(4-(2-((2-(1H-indol-3-yl)ethyl)amino)-2-oxoethyl)-3-benzyl-2,5-dioxoimidazolidin-1-yl)cyclobutane-1-carboxylate 7d: Yield 69%. R_f = 0.17 (Hexane/AcOEt = 40:60); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.25 (s, 1H), 7.52 (d, *J* = 7.6 Hz, 1H), 7.27-7.11 (m, 13H), 6.91 (s, 1H), 5.39 (br t, 1H), 5.18 (d, *J* = 12.4 Hz, 1H), 5.13 (d, *J* = 12.4 Hz, 1H), 4.59 (d, *J* = 15.6 Hz, 1H), 4.23 (d, *J* = 15.6 Hz, 1H), 4.15 (t, *J* = 5.6 Hz, 1H), 3.52-3.51 (m, 1H), 3.43-3.41 (m, 1H), 2.88-2.82 (m, 6H), 2.36-2.33 (m, 2H), 2.16 (dd, *J* = 15.6 and 6.4 Hz, 1H), 1.97-1.93 (m, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 172.5, 172.0, 167.9, 156.1, 136.5, 136.3, 135.5, 128.7, 128.6, 128.5, 128.2, 128.0, 127.9, 127.7, 127.4, 122.2, 122.15, 122.11, 119.5, 118.5, 112.6, 111.3, 67.5, 60.3, 56.4, 45.1, 39.9, 36.8, 31.4, 30.9, 25.0, 17.4 ESI (*m/z)* 601.3 [M^++Na, (100)]; Anal. calcd. for $C_{34}H_{34}N_4O_5$: C 70.57, H 5.92, N 9.68; found: C 70.58, H 5.90, N 9.68.

Benzyl 1-(3-benzyl-4-(2-(cyclohexylamino)-2-oxoethyl)-2,5-dioxoimidazolidin-1-yl)cyclobutane-1-carboxylate 7e: Yield 81%. R_f = 0.37 (Hexane/AcOEt = 40:60); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31-7.23 (m, 10H), 5.23 (br s, 1H), 5.21 (d, *J* = 12.4 Hz, 1H), 5.16 (d, *J* = 12.4 Hz, 1H), 4.70 (d, *J* = 15.6 Hz, 1H), 4.29 (d, *J* = 15.6 Hz, 1H), 4.18 (dd, *J* = 6.8 and 4.8 Hz, 1H), 3.66-3.64 (m, 1H), 2.92-2.88 (m, 2H), 2.80-2.77 (m, 2H), 2.47 (dd, *J* = 15.6 and 4.8 Hz, 1H), 2.33 (q, *J* = 9.6 Hz, 1H), 2.19 (dd, *J* = 15.6 and 6.8 Hz, 1H), 1.99-1.95 (m, 1H), 1.82-1.80 (m, 2H), 1.66-1.62 (m, 2H), 1.34-1.02 (m, 6H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 172.6, 171.9, 166.9, 156.0, 136.3,

135.6, 128.7, 128.6, 128.3, 128.1, 128.0, 127.7, 67.4, 60.3, 56.4, 48.6, 45.2, 37.3, 32.9, 31.4, 31.0, 25.5, 24.74, 24.70, 17.4 ESI (*m/z)* 540.3 [M^++Na, (100)]; Anal. calcd. for $C_{30}H_{35}N_3O_5$: C 69.61, H 6.82, N 8.12; found: C 69.59, H 6.83, N 8.12.

Benzyl 1-(4-(2-(hexylamino)-2-oxoethyl)-3-(naphthalen-1-ylmethyl)-2,5-dioxoimidazolidin-1-yl)cyclobutane-1-carboxylate 7f: Yield 77%. R_f = 0.43 (Hexane/AcOEt = 40:60); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04-8.02 (m, 1H), 7.78-7.74 (m, 2H), 7.36-7.34 (m, 2H), 7.33-7.18 (m, 7H), 5.18 (d, *J* = 12.4 Hz, 1H), 5.16 (d, *J* = 12.4 Hz, 1H), 5.05 (br s, 1H), 5.04 (d, *J* = 15.6 Hz, 1H), 4.85 (d, *J* = 15.6 Hz, 1H), 3.96 (t, *J* = 5.2 Hz, 1H), 2.86-2.75 (m, 5H), 2.50-2.45 (m, 1H), 2.31-2.28 (m, 3H), 1.94-1.90 (m, 1H), 1.15-1.13 (m, 8H), 0.79 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 172.6, 172.0, 167.5, 155.8, 135.6, 133.9, 131.5, 131.3, 129.0, 128.7, 128.6, 128.3, 127.9, 126.9, 126.2, 125.2, 123.5, 115.6, 67.5, 60.3, 56.9, 43.6, 39.7, 36.5, 31.4, 30.9, 29.1, 26.5, 22.5, 17.5, 14.0; ESI (*m/z)* 592.1 [M^++Na, (100)]; Anal. calcd. for $C_{34}H_{39}N_3O_5$: C 71.68, H 6.90, N 7.38; found: C 71.70, H 6.91, N 7.39.

Benzyl 1-(4-(2-((2,2-diphenylethyl)amino)-2-oxoethyl)-3-(2-ethoxy-2-oxoethyl)-2,5-dioxoimidazolidin-1-yl)cyclobutane-1-carboxylate 7g: Yield 63%. R_f = 0.32 (Hexane/AcOEt = 40:60); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18-7.15 (m, 15H), 5.44 (br t, *J* = 5.6 Hz, 1H), 5.11 (d, *J* = 12.0 Hz, 1H), 5.03 (d, *J* = 12.0 Hz, 1H), 4.39 (dd, *J* = 8.4 and 3.2 Hz, 1H), 4.17 (d, *J* = 18.0 Hz, 1H), 4.12-4.05 (m, 3H), 3.79-3.77 (m, 3H), 3.75 (d, *J* = 18.0 Hz, 1H), 2.81-2.78 (m, 1H), 2.71-2.67 (m, 2H), 2.47 (dd, *J* = 16.4 and 3.2 Hz, 1H), 2.26 (q, *J* = 10.4 Hz, 1H), 2.02 (dd, *J* = 16.4 and 8.4 Hz, 1H), 1.92-1.88 (m, 1H), 1.20 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 172.4, 171.7, 168.8, 168.6, 156.2, 141.6, 141.5, 135.5, 128.84, 128.83, 128.7, 128.6, 128.5, 128.2, 128.17, 128.11, 128.0, 127.9, 127.03, 127.00, 67.5, 61.5, 60.2, 56.8, 50.6, 44.0, 43.1, 37.3, 31.3, 30.9, 17.4, 14.2 ESI (*m/z)* 634.4 [M^++Na, (57)]; Anal. calcd. for $C_{35}H_{37}N_3O_7$: C 68.72, H 6.10, N 6.87; found: C 68.73, H 6.12, N 6.88.

4. General procedure for the synthesis of mimetics 1.

*Hydrolysis of the ethyl ester **7a***. To a solution of the ester (1 equiv.) in MeOH (0.1 M) a 1 M aqueous solution of NaOH was added and the mixture stirred at 40°C overnight. The mixture was acidified with a 1M aqueous solution of HCl and extracted with AcOEt. The combined organic layers were dried on Na_2SO_4, filtered, and the organic solvent evaporated. The crude was submitted to the next step without further purification.

*Hydrogenolysis of benzyl esters **7b-g***. To a solution of the ester **7b-g** in MeOH (0.1 M) a catalytic amount of Pd/C was added. The mixture was stirred under a H_2 atmosphere until completion of the reaction (TLC monitoring). The mixture was filtered over a Celite pad, the solvent evaporated and the crude submitted to the next step without further purification

Coupling. The acids obtained as describe above were dissolved in DMF (0.1 M solution) and the amine (1.05 equiv.), DIPEA (1.05 equiv.) followed by HBTU (1.05 equiv.) were added and the resulting solution stirred at

rt overnight. The organic solvent was evaporated, the crude dissolved in AcOEt and washed with a 1M aqueous HCl solution, with a saturated aqueous solution of $NaHCO_3$, and with brine. The combined organic layers were dried on Na_2SO_4, filtered, and the organic solvent evaporated. The crude was purified by flash chromatography affording compounds **1** in a 65-85 % range yields.

N-benzyl-1-(3-ethyl-4-(2-((4-methoxybenzyl)amino)-2-oxoethyl)-2,5-dioxoimidazolidin-1-yl)cyclobutane-1-carboxamide 1a: Yield 81%. R_f = 0.27 (Hexane/AcOEt = 20:80); ^{1}H NMR (400 MHz, $CDCl_3/CD_3OD$) δ 7.16-7.14 (m, 5H), 6.91 (d, *J* = 8.4 Hz, 2H), 6.69 (d, *J* = 8.4 Hz, 2H), 4.44 (d, *J* = 15.2 Hz, 1H), 4.33 (d, *J* = 15.2 Hz, 1H), 4.00 (dd, *J* = 4.8 and 3.2 Hz, 1H), 3.92 (d, *J* = 14.8 Hz, 1H), 3.86 (d, J = 14.8 Hz, 1H), 3.51 (sextet, *J* = 7.2 Hz, 1H), 3.24 (s, 3H), 3.00-2.92 (m, 4H), 2.68 (dd, *J* = 16.8 and 4.4 Hz, 1H), 2.66-2.61 (m, 1H), 2.53 (q, *J* = 12.0 Hz, 1H), 2.73 (sextet, *J* = 9.2 Hz, 1H), 1.87-1.84 (m, 1H), 1.05 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3/CD_3OD$) δ 172.7, 172.3, 167.7, 158.8, 155.3, 138.6, 129.9, 129.0, 128.2, 127.1, 126.6, 113.9, 61.0, 55.9, 55.2, 43.2, 42.6, 38.4, 35.4, 33.3, 32.0, 31.2, 17.1, 12.9 ESI (*m/z)* 515.2 [M^++Na, (100)]; Anal. calcd. for $C_{27}H_{32}N_4O_5$: C 65.84, H 6.55, N 11.37; found: C 65.84, H 6.57, N 11.38.

N-cyclohexyl-1-(3-ethyl-4-(2-((4-methoxybenzyl)amino)-2-oxoethyl)-2,5-dioxoimidazolidin-1-yl)cyclobutane-1-carboxamide 1b: Yield 74%. R_f = 0.23 (Hexane/AcOEt = 20:80); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (br d, *J* = 8.0 Hz, 1H), 7.12 (d, *J* = 6.8 Hz, 2H), 6.97 (br t, *J* = 5.6 Hz, 1H), 6.81 (d, *J* = 6.8 Hz, 2H), 4.34 (dd, *J* = 14.8 and 5.6 Hz, 1H), 4.27 (dd, *J* = 14.8 and 5.6 Hz, 1H), 4.05 (dd, *J* = 4.4 and 2.8 Hz, 1H), 3.77 (s, 3H), 3.76-3.75 (m, 1H), 3.61 (sextet, *J* = 7.6 Hz, 1H), 3.09 (sextet, *J* = 6.8 Hz, 1H), 3.04-3.01 (m, 1H), 2.65-2.63 (m, 1H), 2.51 (q, *J* = 9.2 Hz, 1H), 2.22 (q, *J* = 9.2 Hz, 1H), 1.88-1.60 (m, 8H), 1.26-1.23 (m, 8H), 1.12 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 171.9, 171.4, 167.8, 159.1, 155.3, 130.0, 128.8, 114.1, 61.0, 55.9, 55.3, 49.0, 43.0, 38.6, 35.5, 33.8, 32.6, 32.5, 32.1, 31.2, 25.6, 25.3, 25.2, 24.7, 17.2, 13.1 ESI (*m/z)* 507.2 [M^++Na, (100)], 485.2 [M^++H, (67)]; Anal. calcd. for $C_{26}H_{36}N_4O_5$: C 64.44, H 7.49, N 11.56; found: C 64.43, H 7.51, N 11.56.

N-butyl-1-(3-ethyl-4-(2-((4-methoxybenzyl)amino)-2-oxoethyl)-2,5-dioxoimidazolidin-1-yl)cyclobutane-1-carboxamide 1c: Yield 89%. R_f = 0.38 (Hexane/AcOEt = 20:80); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.64 (br t, *J* = 5.6 Hz, 1H), 7.14 (d, *J* = 8.8 Hz, 2H), 6.86 (d, *J* = 8.8 Hz, 2H), 6.23 (br t, *J* = 6.0 Hz, 1H), 4.36 (dd, *J* = 14.4 and 5.6 Hz, 1H), 4.28 (d, *J* = 14.6 and 5.6 Hz, 1H), 4.08 (dd, *J* = 4.8 and 3.2 Hz, 1H), 3.80 (s, 3H), 3.67 (sextet, *J* = 7.2 Hz, 1H), 3.27-3.23 (m, 2H), 3.09-3.04 (m, 2H), 2.94-2.90 (m, 2H), 2.75 (dd, *J* = 16.4 and 4.8 Hz, 1H), 2.75-2.66 (m, 1H), 2.56 (q, *J* = 12.4 Hz, 1H), 2.32 (sextet, *J* = 10.0 Hz, 1H), 1.92-1.88 (m, 1H), 1.54-1.50 (m, 2H), 1.31-1.27 (m, 2H), 1.16 (t, *J* = 7.2 Hz, 3H), 0.86 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 172.0, 171.6, 167.5, 159.3, 155.3, 129.5, 129.1, 114.3, 61.1, 55.7, 55.3, 43.2, 39.8, 35.6, 35.5, 33.9, 32.1, 31.5, 31.2, 20.0, 17.3, 13.7, 13.2; ESI (*m/z)* 481.3 [M^++Na, (100)]; Anal. calcd. for $C_{24}H_{34}N_4O_5$: C 62.86, H 7.47, N 12.22; found: C 62.87, H 7.49, N 12.24.

(1-(3-ethyl-4-(2-((4-methoxybenzyl)amino)-2-oxoethyl)-2,5-dioxoimidazolidin-1-yl)cyclobutane-1-carbonyl)glycine 1d: Yield 65%. R_f = 0.22 ($CHCl_3$/MeOH = 90:10); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.11 (br s, 1H), 7.12 (d, *J* = 8.0 Hz, 2H), 6.84 (d, *J* = 8.0 Hz, 2H), 6.82 (br s, 1H), 4.29-4.19 (m, 3H), 3.97-3.93 (m, 2H), 3.78 (s, 3H), 3.67-3.65 (m, 1H), 3.08, 3.06 (m, 1H), 3.00-2.68 (m, 5H), 2.65-2.62 (m, 1H), 2.20 (q, *J* = 9.6 Hz, 1H), 1.93-1.91 (m, 1H), 1.28 (s, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 173.7, 172.1, 171.8, 168.2, 159.2, 155.4, 129.6, 129.1, 114.2, 60.8, 55.9, 55.3, 43.3, 42.2, 35.7, 34.4, 31.6, 31.1, 29.6, 17.1, 13.1; ESI (*m/z)* 459.1 [M^--H, (100)]; Anal. calcd. for $C_{22}H_{28}N_4O_7$: C 57.38, H 6.13, N 12.17; found: C 57.37, H 6.15, N 12.15.

1-(4-(2-((2,2-diphenylethyl)amino)-2-oxoethyl)-3-ethyl-2,5-dioxoimidazolidin-1-yl)-N-hexylcyclobutane-1-carboxamide (1-(3-ethyl-4-(2-((4-methoxybenzyl)amino)-2-oxoethyl)-2,5-dioxoimidazolidin-1-yl)cyclobutane-1-carbonyl)glycinate 1e: Yield 76%. R_f = 0.41 (Hexane/AcOEt = 20:80); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (br t, *J* = 5.2 Hz, 1H), 7.25-7.21 (m, 10H), 5.63 (br s, *J* = 6.0 Hz, 1H), 4.13 (t, *J* = 8.0 Hz, 1H), 3.96 (dd, *J* = 4.4 and 2.8 Hz, 1H), 3.90-3.88 (m, 1H), 3.77-3.74 (m, 1H), 3.55 (sextet, *J* = 7.2 Hz, 1H), 3.25-3.22 (m, 2H), 2.96-2.85 (m, 2H), 2.70-2.67 (m, 1H), 2.58-2.52 (m, 1H), 2.31-2.28 (m, 1H), 1.85-1.83 (m, 2H), 1.52-1.50 (m, 2H), 1.21-1.20 (m, 8H), 1.05 (t, *J* = 7.2 Hz, 3H), 0.78 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 171.8, 171.5, 167.8, 155.2, 141.4, 141.3, 128.8, 127.87, 127.82, 127.0, 61.1, 55.5, 50.4, 44.0, 40.1, 35.4, 33.9, 32.2, 31.6, 31.4, 29.2, 29.1, 26.5, 22.5, 17.3, 13.9, 13.1; ESI (*m/z)* 569.3 [M^++Na, (100)]; Anal. calcd. for $C_{32}H_{42}N_4O_4$: C 70.30, H 7.74, N 10.25; found: C 70.28, H 7.74, N 10.26.

1-(3-benzyl-4-(2-((2,2-diphenylethyl)amino)-2-oxoethyl)-2,5-dioxoimidazolidin-1-yl)-N-(2-(3a,7a-dihydro-1H-indol-3-yl)ethyl)cyclobutane-1-carboxamide 1f: Yield 69%. R_f = 0.14 (Hexane/AcOEt = 20:80); ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.05 (br s, 1H), 7.81 (br s, 1H), 7.48 (d, *J* = 7.6 Hz, 1H), 7.23-7.08 (m, 17H), 6.90-6.86 (m, 2H), 5.52 (br s, 1H), 4.54 (d, *J* = 15.6 Hz, 1H), 4.03-3.97 (m, 1H), 3.95 (d, *J* = 15.6 Hz, 1H), 3.77 (s, 1H), 3.58-3.56 (m, 4H), 3.01 (t, *J* = 7.2 Hz, 2H), 2.90-2.61 (m, 5H), 2.32 (q, *J* = 9.2 Hz, 1H), 2.28-2.26 (m, 1H), 1.91-1.88 (m, 1H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 172.1, 171.5, 167.6, 155.8, 141.5, 141.4, 136.3, 136.0, 128.9, 128.8, 128.7, 128.6, 128.0, 127.99, 127.91, 127.8, 127.6, 126.9, 126.8, 122.2, 121.6, 119.2, 118.7, 113.3, 110.9, 61.2, 56.1, 50.3, 45.0, 43.8, 40.4, 38.7, 34.0, 32.2, 31.5, 25.0, 17.4; ESI (*m/z)* 690.3 [M^++Na, (100)]; Anal. calcd. for $C_{41}H_{43}N_5O_4$: C 73.52, H 6.47, N 10.46; found: C 73.53, H 6.46, N 10.45.

1-(4-(2-((2-(1H-indol-3-yl)ethyl)amino)-2-oxoethyl)-3-benzyl-2,5-dioxoimidazolidin-1-yl)-N-(6-aminohexyl)cyclobutane-1-carboxamide 1g: Yield 65%. ^{1}H NMR (400 MHz, CD_3OD) δ 7.95 (br s, 1H), 7.83 (br s, 1H), 7.48 (d, *J* = 8.0 Hz, 1H), 7.50-7.46 (m, 6H), 7.24-7.22 (m, 1H), 6.99 (s, 2H), 5.44 (br s, 1H), 4,56 (d, *J* = 15.6 Hz, 1H), 4.22 (d, *J* = 15.6 Hz, 1H), 4.04 (s, 1H), 3.36-3.33 (m, 2H), 3.19-3.17 (m, 1H), 3.03-3.01 (m, 1H), 2.83-2.80 (m, 6H), 2.70-2.66 (m, 4H), 2.55-2.52 (m, 1H), 1.92-1.87 (m, 1H), 1.57-1.54 (m, 2H), 1.48-1.45 (m, 2H), 1.28-1.25 (m, 6H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 173.3, 172.6, 168.6, 156.3, 136.2, 128.4, 127.6, 127.5, 121.9, 121.0, 118.3, 117.8, 111.8, 110.9, 61.1, 56.7, 44.4, 39.9, 39.5, 39.0, 37.5, 32.9, 31.7, 30.9, 28.4, 25.7,

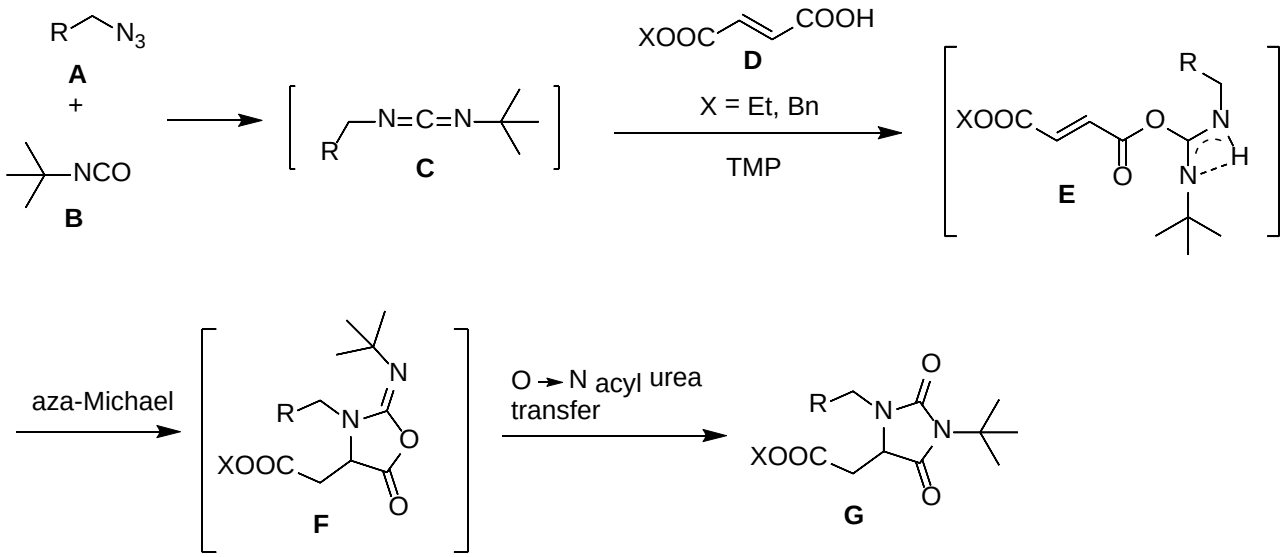
25.5, 24.7, 16.6; ESI (*m/z)* 587.3 [M^++H, (100)]; Anal. calcd. for $C_{33}H_{42}N_6O_4$: C 67.55, H 7.22, N 14.32; found: C 67.53, H 7.23, N 14.33.

1-(4-(2-((2-(1H-indol-3-yl)ethyl)amino)-2-oxoethyl)-3-benzyl-2,5-dioxoimidazolidin-1-yl)-N-(4-hydroxyphenethyl)cyclobutane-1-carboxamide 1h: Yield 64%. R_f = 0.22 (CH_2Cl_2/MeOH = 95:5); ^{1}H NMR (400 MHz, CD_3OD) δ 8.37 (br s, 1H), 7.47 (d, *J* = 12.0 Hz, 1H), 7.26-7.21 (m, 6H), 7.04 (t, *J* = 8.0 Hz, 1H), 6.95 (t, *J* = 3.2 Hz, 1H), 6.90 (d, *J* = 8.4 Hz, 2H), 6.59 (d, *J* = 8.4 Hz, 2H), 4.54 (d, *J* = 15.6 Hz, 1H), 4.18 (d, *J* = 15.6 Hz, 1H), 4.00 (dd, *J* = 4.8 and 3.2 Hz, 1H), 3.38-3.32 (m, 4H), 3.05-3.00 (m, 2H), 2.77-2.72 (m, 4H), 2.70-2.55 (m, 3H), 2.51 (m, 1H), 2.22 (q, *J* = 9.6 Hz, 1H), 1.89-1.87 (m, 1H); ^{13}C NMR (100.6 MHz, CD_3OD) δ 173.2, 172.5, 168.5, 156.3, 155.2, 136.8, 136.2, 130.1, 129.4, 129.3, 128.4, 127.6, 127.5, 127.4, 121.9, 120.9, 118.3, 117.8, 114.8, 111.8, 110.9, 61.1, 56.7, 44.4, 41.5, 39.9, 34.3, 33.0, 30.9, 30.2, 25.7, 16.6; ESI (*m/z)* 631.3 [M^++H, (100)]; Anal. calcd. for $C_{35}H_{37}N_5O_5$: C 69.18, H 6.14, N 11.52; found: C 69.21, H 6.16, N 11.54.

1-(3-benzyl-4-(2-(cyclohexylamino)-2-oxoethyl)-2,5-dioxoimidazolidin-1-yl)-N-(2,2-diphenylethyl)cyclobutane-1-carboxamide 1i: Yield 78%. R_f = 0.32 (Hexane/AcOEt = 20:80); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43 (br s, 1H), 7.24-7.20 (m, 15H), 5.10 (br d, *J* = 7.6 Hz, 1H), 4.54 (d, *J* = 15.2 Hz, 1H), 4.34 (t, *J* = 8.0 Hz, 1H), 4.27 (d, *J* = 15.2 Hz, 1H), 3.89-3.87 (m, 2H), 3.83-3.81 (m, 1H), 3.58-3.55 (m, 1H), 2.86-2.80 (m, 2H), 2.64 (dd, *J* = 16.4 and 3.6 Hz, 1H), 2.53-2.49 (m, 2H), 2.34 (dd, *J* = 16.4 and 4.8 Hz, 1H), 2.13 (q, *J* = 9.6 Hz, 1H), 1.82-1.80 (m, 3H), 1.66-1.55 (m, 3H), 1.29-1.25 (m, 2H), 1.14-1.04 (m, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 171.7, 171.3, 166.5, 155.8, 142.5, 142.4, 136.2, 128.9, 128.3, 128.2, 128.1, 127.9, 126.35, 126.31, 61.1, 56.4, 50.3, 48.8, 45.5, 44.4, 38.6, 34.7, 32.84, 32.81, 31.8, 31.3, 25.4, 24.74, 24.70, 17.2; ESI (*m/z)* 629.3 [M^++Na, (100)]; Anal. calcd. for $C_{37}H_{42}N_4O_4$: C 73.24, H 6.98, N 9.23; found: C 73.25, H 6.99, N 9.23.

1-(4-(2-(hexylamino)-2-oxoethyl)-3-(naphthalen-1-ylmethyl)-2,5-dioxoimidazolidin-1-yl)-N-(4-hydroxyphenethyl)cyclobutane-1-carboxamide 1j: Yield 81%. R_f = 0.41 (CH_2Cl_2/MeOH = 95:5); ^{1}H NMR (400 MHz, CD_3OD) δ 8.51 (t, *J* = 5.2 Hz, 1H), 8.19 (d, *J* = 9.6 Hz, 1H), 7.92-7.91 (m, 2H), 7.55-7.53 (m, 4H), 7.02 (d, *J* = 8.4 Hz, 2H), 6.70 (d, *J* = 8.4 Hz, 2H), 5.10 (d, *J* = 15.6 Hz, 1H), 4.93 (d, *J* = 15.6 Hz, 1H), 3.96 (dd, *J* = 4.8 and 2.8 Hz, 1H), 3.45-3.43 (m, 2H), 3.04 (q, *J* = 12.4 Hz, 1H), 2.95-2.65 (m, 8H), 2.55-2.53 (m, 1H), 2.30 (sextet, *J* = 10.4 Hz, 1H), 1.94-1.91 (m, 1H), 1.23-1.21 (m, 8H), 0.88 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (100.6 MHz, CD_3OD) δ 172.9, 168.6, 156.5, 155.8, 134.5, 131.9, 131.8, 130.5, 129.8, 129.3, 128.9, 127.5, 126.7, 126.2, 125.4, 123.7, 115.2, 61.5, 57.5, 43.9, 42.0, 39.4, 34.7, 33.6, 32.2, 31.6, 29.1, 26.8, 22.6, 17.0, 13.3; ESI (*m/z)* 621.2 [M^++Na, (100)]; Anal. calcd. for $C_{35}H_{42}N_4O_5$: C 70.21, H 7.07, N 9.36; found: C 70.22, H 7.07, N 9.37.

ethyl 2-(3-(1-((2-(1H-indol-3-yl)ethyl)carbamoyl)cyclobutyl)-5-(2-((2,2-diphenylethyl)amino)-2-oxoethyl)-2,4-dioxoimidazolidin-1-yl)acetate 1k: Yield 81%. R_f = 0.17 (Hexane/AcOEt = 20:80); ^{1}H NMR (400 MHz, DMSO-d_6) δ 10.77 (s, 1H), 8.36 (t, *J* = 5.2 Hz, 1H), 8.11 (t, *J* = 5.2 Hz, 1H), 7.50 (d, *J* = 8.0 Hz, 1H), 7.33 (d, *J* = 8.0 Hz, 1H), 7.19-7.16 (m, 8H), 7.06-7.02 (m, 2H), 6.90 (t, *J* = 7.2 Hz, 1H), 4.25 (t, *J* = 3.2 Hz, 1H), 4.18 (t, *J* = 8.0 Hz, 1H), 4.12 (q, *J* = 7.2 Hz, 2H), 3.98 (d, *J* = 18.0 Hz, 1H), 3.80-3.77 (m, 1H), 3.52 (d, *J* = 18.0 Hz, 1H), 3.42-3.40 (m, 2H), 2.90-2.86 (m, 3H), 2.80 (dd, *J* = 16.8 and 4.8 Hz, 1H), 2.72-2.69 (m, 2H), 2.47-2.45 (m, 4H), 2.15 (sextet, *J* = 9.6 Hz, 1H), 1.85-1.82 (m, 1H), 1.21 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (100.6 MHz, $CDCl_3$) δ 172.2, 171.7, 169.3, 168.9, 156.1, 142.9, 142.8, 136.7, 128.9, 128.2, 128.1, 126.8, 126.7, 123.0, 121.3, 118.7, 118.6, 112.0, 111.8, 61.4, 60.7, 57.0, 50.3, 43.6, 42.2, 33.9, 31.9, 31.2, 25.4, 17.3, 14.4; ESI (*m/z)* 686.4 [M^++Na, (100)]; Anal. calcd. for $C_{38}H_{41}N_5O_6$: C 68.76, H 6.23, N 10.55; found: C 68.77, H 6.22, N 10.53.



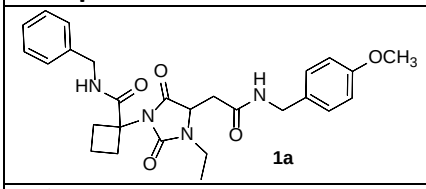
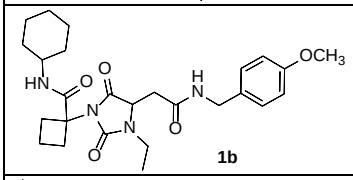
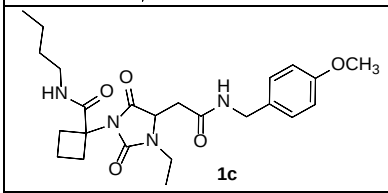
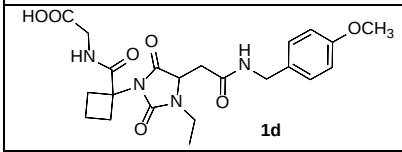
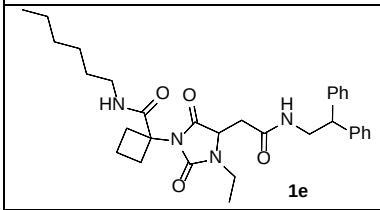
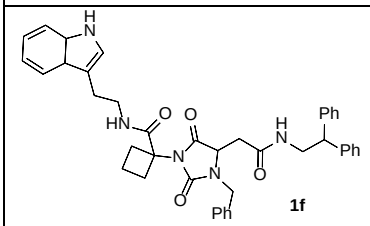
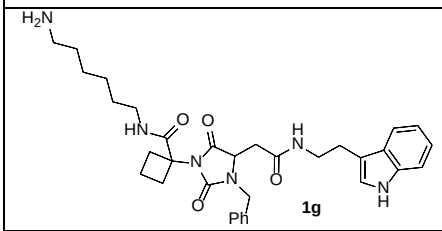
Scheme S1. Mechanism of the regioselective MC domino process.

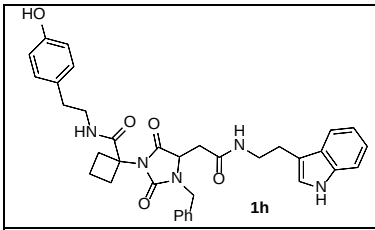
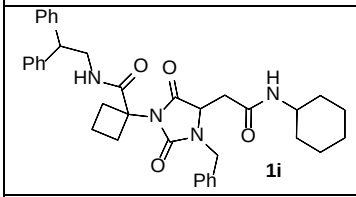
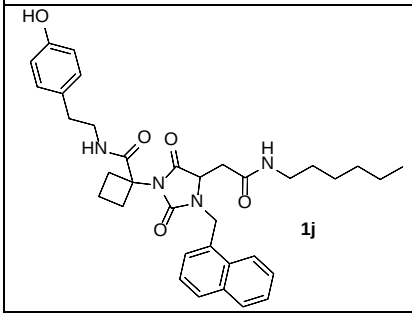
Primary azides **A** react in DCM or CH_3CN at rt with *tert*-butyl isocyanate **B** affording "weakly asymmetric"[7] carbodiimides **C** through Staudinger followed aza-Wittig reactions. Addition *in situ* of TMP and fumaric acid monoester **D** leads to the formation of *O*-acyl isourea **E** that undergoes intramolecular aza-Michael reaction producing intermediate **F** as the only regioisomer. Indeed, the latter step is regioselective because the nucleophilic attack of the less sterically hindered primary amine moiety is favored compared to the attack of sterically hindered tertiary *tert*-butyl amine. Intermediate **F** is not stable and undergoes spontaneously O → N acyl urea transfer producing final hydantoins **G**.

Table S1. Rule of five parameters for compounds **1a-k**

Lipinski's rule :

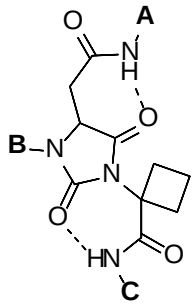
- A molecular mass less than 500 daltons. In most cases (especially when MW is greater than 500) the Polar Surface Area is a better discriminant. PSA should be no greater than 140 $Å^2$
- No more than 5 hydrogen bond donors (HBD)
- No more than 10 hydrogen bond acceptors (HBA)
- An octanol-water partition coefficient log P not greater than 5

Compound	MW	logP	HBD	HBA	PSA ($Å^2$)
 **1a**	492.57	0.94±0.78	2	9	108.05
 **1b**	484.59	1.16±0.76	2	9	108.05
 **1c**	458.55	0.69±0.76	2	9	108.05
 **1d**	460.48	-1.09±0.80[a]	3	11	145.35
 **1e**	546.7	3.82±0.77	2	8	98.82
 **1f**	669.81	3.64±0.98	3	9	110.85
 **1g**	586.72	1.59±0.76[a]	5	10	140.63

 **1h**	607.70	2.32±0.78[a]	4	10	134.84
 **1i**	606.75	4.61±0.78	2	8	98.82
 **1j**	598.73	4.11±0.76[a]	3	9	119.05

[a]logP has been calculated for the uncharged molecule

Table S2. Analysis of the inter-residue distances A-B, A-C and B-C as resulted from conformational analysis

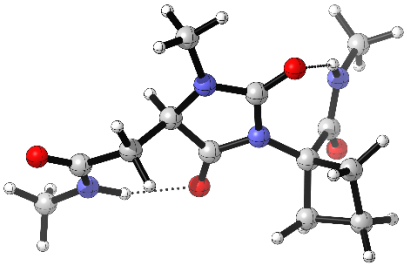


			A			1a			1b			1c			1d			1e			1f			1g			1h			1i			1j			1k		
	Distances		A-B	A-C	B-C	A-B	A-C	B-C	A-B	A-C	B-C	A-B	A-C	B-C	A-B	A-C	B-C	A-B	A-C	B-C	A-B	A-C	B-C	A-B	A-C	B-C	A-B	A-C	B-C	A-B	A-C	B-C	A-B	A-C	B-C	A-B	A-C	B-C
	residues	ideal value (Å)																																				
helix	*i* - *i*+1	5.2																																				
	i - *i*+2	7.1																																				
	i - *i*+3	5.6																																				
	i - *i*+4	6.5																																				
	i - *i*+5	9.8																																				
	i - *i*+6	10.8																																				
	i - *i*+7	10.7																																				
	i - *i*+8	12.9																																				
β turn	*i* - *i*+1	5.7																																				
	i - *i*+2	5.1																																				
	i - *i*+3	5.4																																				
	i+1 - *i*+2	5.2																																				
	i+1 - *i*+3	7.5																																				
	i+2 - *i*+3	5.6																																				
β sheet parallel	*i* - *i*+1	5.8																																				
	i - *i*+2	7.1																																				
	i - *i*+3	11.1																																				
	i - *i*+4	13.2																																				
	i-*i*'	5.5																																				
	i' - *i*+1	7.2																																				
	i' - *i*+2	9																																				
	i' - *i*+3	11.5																																				
	i' - *i*+4	14.4																																				
β sheet anti-parallel	*i* - *i*+1	5.8																																				
	i - *i*+2	6.5																																				
	i - *i*+3	11																																				
	i - *i*+4	12.8																																				
	i-*i*'	4.5																																				
	i' - *i*+1	7.6																																				
	i' - *i*+2	8.9																																				
	i' - *i*+3	12.7																																				
	i' - *i*+4	14.8																																				
γ turn classic	*i* - *i*+1	4.7																																				
	i - *i*+2	7.2																																				
	i+1 - *i*+2	5.1																																				
γ turn inverse	*i* - *i*+1	5.7																																				
	i - *i*+2	5.4																																				
	i+1 - *i*+2	6.2																																				

Results from DFT single point calculations

A conformer a

E = -1027.379880 Hartrees; ZPE = 895.51 kcal/mol

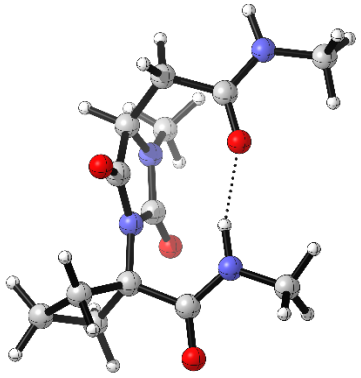


Atom	X	Y	Z
C1	0.5499308	-0.3801910	0.0594027
C2	-0.6047417	1.5519858	-0.4150285
C3	1.5382723	0.7910094	0.1317763
C4	2.7788909	0.6047504	-0.7744883
H4A	2.4928765	0.0703698	-1.6890133
H4B	3.1496512	1.5868626	-1.0755261
C5	3.9819597	-0.0940291	-0.1171069
C6	4.7418010	-2.0517923	1.1637194
H6A	5.6475514	-1.4457431	1.2115963
H6B	4.9576305	-2.9666722	0.5974101
C13	1.0916006	3.3063082	-0.0769119
H13A	0.2382182	3.9312870	-0.3431911
H13B	1.9354550	3.5553520	-0.7281623
C15	-1.9047539	-0.6325921	-0.5319456
C16	-2.7370231	-0.2457536	-1.7968509
H16A	-3.6085059	0.3938608	-1.6428078
H16B	-2.0950567	0.2099258	-2.5560377
C17	-2.9510947	-1.7591499	-2.0538810
H17A	-3.8844017	-2.1241912	-1.6167381
H17B	-2.8875365	-2.0974303	-3.0915697
C18	-1.7357249	-2.0504472	-1.1369280
H18A	-0.8067635	-2.1302316	-1.7049564
H18B	-1.8075826	-2.8698513	-0.4229018
C19	-2.7842885	-0.6610872	0.7517391
C20	-3.9926567	0.7474665	2.3723213
H20A	-4.1280686	-0.2289734	2.8390731
H20B	-4.9758649	1.1482333	2.0957896
N1	-0.6706151	0.1407489	-0.3019559
N2	0.6979808	1.9199577	-0.2497429
N3	3.7067957	-1.2609896	0.5211847
H3	2.7540398	-1.6190508	0.4908000
N4	-3.1470631	0.5688335	1.2053949
H4	-2.8719533	1.3804521	0.6594701
O1	-1.5672952	2.2825426	-0.6102198

O2	0.8162632	-1.5546640	0.2616725
O3	5.1000198	0.4065764	-0.1910192
O5	-3.1244119	-1.7150758	1.2758010
H31	1.8633708	0.9063814	1.1771067
H14	4.4348738	-2.3329057	2.1770066
H17	-3.5253378	1.4316936	3.0897910
H18	1.3780791	3.5068774	0.9639141

A conformer b

E = -1027.378397 Hartrees; ZPE = 896.09 kcal/mol

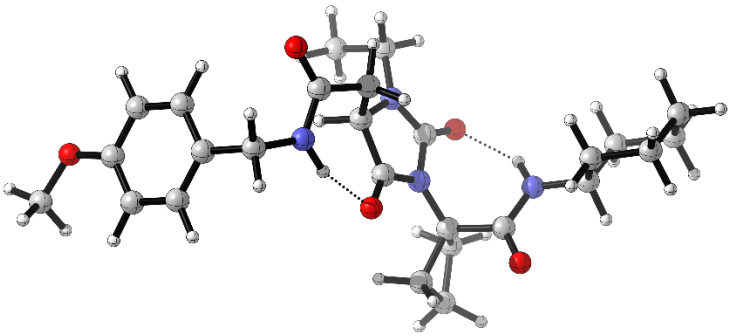


Atom	X	Y	Z
C1	-0.0334446	-1.0081716	-1.1385705
C2	-0.2752320	-1.0412398	1.1588380
C3	1.1686633	-1.7549322	-0.5355657
C4	2.5059439	-1.1867600	-1.0336453
H4A	3.3270962	-1.8690313	-0.7854993
H4B	2.4360577	-1.1443048	-2.1282763
C5	2.7902548	0.2228301	-0.5220554
C6	4.5716794	1.8349245	0.0624443
H6A	5.0116261	2.3758915	-0.7839413
H6B	5.3170640	1.7503504	0.8592618
C13	1.7500412	-2.2422747	1.9151135
H13A	1.2715483	-2.0404440	2.8750018
H13B	2.7525329	-1.7966304	1.9191691
C15	-2.1688653	0.0116954	-0.1343928
C16	-2.9899569	-0.2709289	-1.4419009
H16A	-3.6177071	0.6026197	-1.6333330
H16B	-2.4242195	-0.5254863	-2.3359051
C17	-3.7747692	-1.3782828	-0.7011854
H17A	-4.8552406	-1.4207957	-0.8684045
H17B	-3.3553352	-2.3740390	-0.8812823
C18	-3.2874979	-0.7669344	0.6335608
H18A	-2.9557519	-1.4321533	1.4305623
H18B	-3.9929625	-0.0369713	1.0350215
C19	-2.0594672	1.5068166	0.2194811
C20	-0.6720653	3.4890086	0.4711209

H20A	-0.9371428	3.7245292	1.5084835
H20B	-1.3172250	4.0853182	-0.1824242
N1	-0.8741703	-0.6948898	-0.0873742
N2	0.9202022	-1.6595603	0.8844063
N3	4.1045927	0.5147172	-0.3321096
H3	4.7921621	-0.1815003	-0.5830760
N4	-0.8320556	2.0725342	0.1946785
H4	-0.0005694	1.5306927	-0.0070647
O1	-0.7497216	-0.8237916	2.2561228
O2	-0.1687955	-0.7844137	-2.3254366
O3	1.8936666	1.0374760	-0.3097432
O5	-3.0839987	2.1463581	0.4532499
H31	1.1069542	-2.8006603	-0.8773130
H14	3.7111760	2.3946006	0.4300655
H17	0.3723778	3.7572907	0.2964680
H18	1.8466649	-3.3284208	1.7822793

1b conformer a

E = -1607.6303354 Hartrees; ZPE = 382.844 kcal/mol



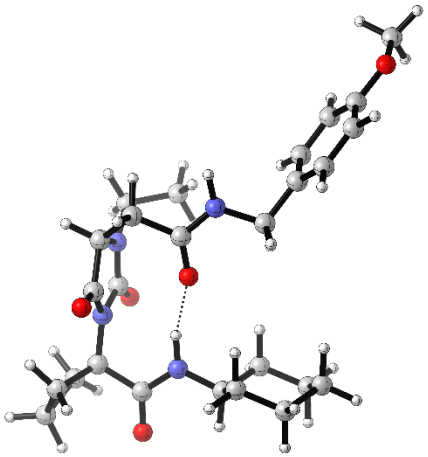
Atom	X	Y	Z
C1	0.0376434	0.3498330	-0.2225698
C2	1.3410046	0.2789144	1.6509323
C3	-0.5585304	-0.7048924	0.7115672
C4	-0.6189080	-2.0937423	0.0358586
C5	-1.9671541	-2.3555937	-0.6278143
C12	1.9450310	1.9753820	-0.1034512
C13	2.3188698	3.1337732	0.8819940
C14	2.1172293	4.1255016	-0.3113539
C15	1.2698045	3.0254406	-1.0298985
C16	3.2236110	1.4393937	-0.7572205
C31	0.2260967	-1.3836318	3.0876955
N1	1.1119222	0.8955962	0.4184006
N2	0.3806106	-0.6548870	1.8269412
N3	-2.3546448	-1.4393559	-1.5277352
N4	3.9998147	0.6936071	0.0499277
O1	2.2673404	0.5417464	2.3970236

O2	-0.3602338	0.6247996	-1.3345754
O3	-2.6311673	-3.3415218	-0.3326376
O4	3.5212128	1.7088654	-1.9108515
H3A	-1.5486063	-0.3916076	1.0193294
H4	3.7426931	0.5673268	1.0088421
H4A	0.1815598	-2.1946715	-0.6870175
H3	-1.7772451	-0.6423265	-1.7178657
H4B	-0.5078076	-2.8610133	0.7840928
H31B	1.1868177	-1.3557049	3.5793753
H15B	0.2207001	3.1299317	-0.8047529
H15A	1.4317642	2.8724403	-2.0802334
H13B	1.5483171	3.2590321	1.6285851
H13A	3.2869897	3.0735616	1.3491704
H14A	1.6194282	5.0553283	-0.0858272
H14B	3.0401206	4.3098836	-0.8400972
H11	-0.0162280	-2.4134423	2.8669503
C25	-0.8501236	-0.7574648	3.9879497
H2	-0.5857631	0.2645092	4.2297449
H5	-0.9322320	-1.3196655	4.9108638
H7	-1.8191743	-0.7634787	3.5032140
C6	-3.6542370	-1.5490204	-2.2026952
H6	-3.5588689	-1.0909945	-3.1776038
H9	-3.8675068	-2.5994385	-2.3335077
C7	-4.7714277	-0.8845292	-1.4190469
C8	-6.8004608	0.3281388	0.0636948
C9	-5.2615634	-1.4844956	-0.2582163
C10	-5.3137961	0.3195354	-1.8140947
C11	-6.3249592	0.9302052	-1.0820846
C26	-6.2601051	-0.8870855	0.4714192
H8	-4.8414201	-2.4180165	0.0568922
H10	-4.9555595	0.8003070	-2.7044412
H12	-6.7232108	1.8634285	-1.4203619
H13	-6.6492566	-1.3378579	1.3602348
O5	-7.7922702	0.8440470	0.8592524
C27	-8.4417580	2.0764041	0.5133571
H14	-7.7402241	2.9016204	0.4978059
H15	-9.1771748	2.2423807	1.2834239
H16	-8.9332712	2.0065504	-0.4492820
C17	5.2637483	0.1233752	-0.4323616
C18	7.4775908	-0.8535441	0.3077197
C19	6.3426086	-1.7296169	-1.7799201
C20	7.2318400	-2.0923187	-0.5752328
C21	5.0115791	-1.1150926	-1.3087721
C22	6.1441652	-0.2374562	0.7723736
H1	8.0346717	-0.1142585	-0.2607654
H17	6.8650982	-1.0141578	-2.4088408
H18	6.7393392	-2.8600707	0.0150482
H19	4.4567294	-1.8434771	-0.7242908

H20	5.6137669	-0.9543119	1.3938895
H21	5.7586267	0.8752635	-1.0339803
H22	8.0775176	-1.1208658	1.1708671
H23	6.1501993	-2.6108121	-2.3823664
H24	8.1783684	-2.4981003	-0.9165676
H25	4.4059073	-0.8206962	-2.1564981
H26	6.3251640	0.6507084	1.3685632

1b conformer b

E = -1607.6302484 Hartrees; ZPE = 382.858 kcal/mol



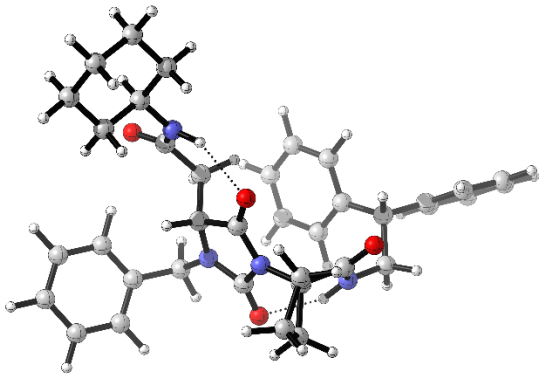
Atom	X	Y	Z
C1	-2.3687858	1.7398845	1.3367545
C2	-2.2637422	1.9387314	-0.9427497
C3	-1.2400629	2.7192786	1.0033512
C4	0.0730260	2.2920836	1.6548095
C5	0.5546606	0.9527943	1.1361887
C12	-4.1349417	0.5710413	-0.0170094
C13	-5.2053556	1.0759646	-1.0428150
C14	-6.3205402	0.7150623	-0.0132819
C15	-5.2314688	0.6752077	1.1042236
C16	-3.8267355	-0.8982384	-0.2819665
C31	-0.4204783	3.5323549	-1.3179794
N1	-2.9565240	1.4031042	0.1468309
N2	-1.2583007	2.7149609	-0.4436314
N3	1.8715625	0.7321665	1.2357195
N4	-2.5540386	-1.2772256	-0.1472636
O1	-2.5317754	1.7696039	-2.1091814
O2	-2.6765774	1.3791822	2.4454643
O3	-0.2180690	0.1151345	0.6812983
O4	-4.7421267	-1.6592226	-0.5812722
H3A	-1.5195533	3.6913842	1.3981716
H4	-1.8402238	-0.6331022	0.1268436
H4A	0.8339030	3.0486518	1.5152095

H3	2.4754519	1.4128598	1.6434738
H4B	-0.1150067	2.1895153	2.7196098
H31B	-0.0593908	4.3754644	-0.7424002
H15B	-5.1565403	1.6159431	1.6260816
H15A	-5.2597831	-0.1387450	1.8088085
H13B	-5.1182581	2.1424258	-1.1856410
H13A	-5.2154668	0.5659609	-1.9892389
H14A	-6.7139238	-0.2670499	-0.2069702
H14B	-7.1105997	1.4394039	0.1166348
H11	-1.0431308	3.9075447	-2.1183421
C25	0.7498653	2.7356547	-1.9162788
H2	1.4021886	2.3609036	-1.1378425
H5	1.3286650	3.3652681	-2.5830459
H7	0.3586032	1.8985775	-2.4793710
C6	2.4761965	-0.5535393	0.8401090
H6	2.3305842	-1.2853668	1.6251183
H9	1.9544360	-0.9025416	-0.0381340
C7	3.9508923	-0.3599113	0.5649982
C8	6.6659715	0.0286336	0.0501249
C9	4.9176983	-0.8830558	1.4142454
C10	4.3677002	0.3589645	-0.5408789
C11	5.7123455	0.5558239	-0.8031011
C26	6.2583082	-0.6932755	1.1625488
H8	4.6192599	-1.4463324	2.2770826
H10	3.6374328	0.7675265	-1.2124968
H12	5.9996406	1.1117827	-1.6702440
H13	7.0108751	-1.0939729	1.8080996
O5	8.0162619	0.1661558	-0.1190857
C27	8.5530845	0.8609532	-1.2572597
H14	8.2547403	0.3864860	-2.1837168
H15	9.6234890	0.8048076	-1.1497178
H16	8.2426769	1.8983783	-1.2670827
C17	-2.1218017	-2.6601160	-0.3548803
C18	-0.5445346	-4.1366282	-1.6916350
C19	-0.9765314	-4.6412279	0.7490927
C20	0.0651374	-4.6794786	-0.3852166
C21	-1.5169296	-3.2126271	0.9475068
C22	-1.0845614	-2.7085415	-1.4897636
H1	-1.3574312	-4.7873506	-2.0022254
H17	-1.7994413	-5.3050944	0.4984186
H18	0.9190091	-4.0668196	-0.1076425
H19	-0.7131954	-2.5496249	1.2525265
H20	-0.2699206	-2.0391444	-1.2294525
H21	-2.9999111	-3.2253640	-0.6278671
H22	0.1975241	-4.1436176	-2.4834463
H23	-0.5380268	-5.0027899	1.6736302
H24	0.4227443	-5.6936364	-0.5316302
H25	-2.2732681	-3.1964090	1.7243324

H26	-1.5392524	-2.3385573	-2.4017326

1i conformer a

E = -1955.2020964 Hartrees; ZPE = 1949.63 kcal/mol



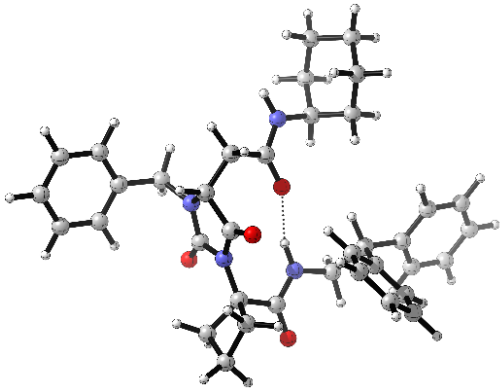
Atom	X	Y	Z
C1	0.8567978	0.0628018	-1.1769469
C2	-0.1167937	-1.9631504	-0.7672240
C3	1.5299196	-0.5378851	0.0488554
C4	1.4169626	0.4123538	1.2649284
C5	2.7350994	1.1350904	1.4757501
C6	4.3063142	2.7664294	0.5258713
C7	4.0759295	4.1621395	-0.0714108
C8	5.3838743	4.9763425	-0.0785215
C9	6.4898769	4.2317028	-0.8505850
C10	6.7185378	2.8306537	-0.2518334
C11	5.4086592	2.0200266	-0.2448013
C12	-0.9263009	-0.7060579	-2.8056425
C13	-0.9703244	-1.9892832	-3.7173130
C14	0.0206491	-1.2945941	-4.7042368
C15	-0.2753852	0.0658025	-3.9959840
C16	-2.2905761	-0.1809267	-2.3813683
C17	-4.2541951	-0.5644067	-0.9969493
C18	-4.1281644	0.5830953	0.0329766
C19	-3.2826454	0.2390726	1.2536752
C20	-2.7157291	1.2833372	1.9786390
C21	-1.9753760	1.0420498	3.1201143
C22	-1.7819927	-0.2577948	3.5621848
C23	-2.3333551	-1.3039095	2.8480102
C24	-3.0753401	-1.0573082	1.7016566
C25	-5.5357343	1.0363379	0.4157033
C26	-6.2235823	0.4895536	1.4886218
C27	-7.5213142	0.8834484	1.7677048
C28	-8.1487388	1.8308030	0.9789814
C29	-7.4693499	2.3837649	-0.0924511

C30	-6.1732957	1.9882905	-0.3700402
C31	1.0842369	-2.7647709	1.2476879
C32	2.5061099	-3.2827577	1.1351865
C33	2.7699434	-4.4281860	0.3986788
C34	4.0640333	-4.9005559	0.2741380
C35	5.1088125	-4.2255855	0.8818968
C36	4.8537184	-3.0774039	1.6100788
C37	3.5575659	-2.6060749	1.7400862
N1	-0.0416124	-0.8644653	-1.6411000
N2	0.7913234	-1.7754257	0.2077460
N3	3.0494679	2.0104932	0.5068445
N4	-2.9579722	-0.9786539	-1.5262974
O1	-0.8944014	-2.8972981	-0.8810288
O2	1.0768060	1.1732982	-1.6107915
O3	3.4531879	0.8895271	2.4381307
O4	-2.7481497	0.8685924	-2.8096610
H3A	2.5679913	-0.7455279	-0.1772340
H17A	-4.8675448	-0.2072104	-1.8116807
H18	-3.6454035	1.3987343	-0.4896032
H4	-2.5499097	-1.8457850	-1.2401089
H4A	0.6072323	1.1141497	1.1227762
H17B	-4.7422120	-1.4225414	-0.5590495
H3	2.4423446	2.1049401	-0.2853073
H8A	5.7097397	5.1399976	0.9448688
H4B	1.2200097	-0.1580158	2.1557920
H6	4.6009914	2.8535269	1.5620082
H8B	5.2067936	5.9494084	-0.5235950
H31B	0.9208304	-2.3165485	2.2175368
H31A	0.3698569	-3.5631150	1.1166005
H22	-1.2165248	-0.4473114	4.4531611
H15B	0.5521354	0.7044609	-3.7582638
H15A	-1.0477267	0.6309479	-4.4920988
H13B	-0.6654023	-2.9075179	-3.2515239
H33	1.9612177	-4.9529347	-0.0730443
H7A	3.7132539	4.0557944	-1.0906968
H26	-5.7399529	-0.2315008	2.1156276
H13A	-1.9557472	-2.1012421	-4.1465557
H9A	7.4111946	4.8039531	-0.8229042
H24	-3.4892895	-1.8883967	1.1687927
H20	-2.8727541	2.2925720	1.6500987
H9B	6.1957007	4.1332863	-1.8917310
H30	-5.6503891	2.4198622	-1.2024062
H23	-2.1960935	-2.3141641	3.1809371
H37	3.3854310	-1.7012243	2.2926069
H7B	3.3115054	4.6753262	0.5012186
H14A	-0.2285664	-1.3536797	-5.7525514
H10B	7.0829615	2.9316318	0.7667359
H11A	5.0723487	1.8595480	-1.2653708

H14B	1.0388495	-1.6226660	-4.5503578
H11B	5.5644669	1.0510763	0.2162642
H21	-1.5564742	1.8631807	3.6679318
H36	5.6579997	-2.5465883	2.0791149
H34	4.2555244	-5.7906065	-0.2917217
H35	6.1119875	-4.5912239	0.7878844
H10A	7.4775182	2.3013484	-0.8178127
H27	-8.0381425	0.4535960	2.6031215
H28	-9.1522356	2.1373236	1.1983360
H29	-7.9445888	3.1218723	-0.7080503

1i conformer b

E = -1955.2017278 Hartrees; ZPE = 1948.87 kcal/mol



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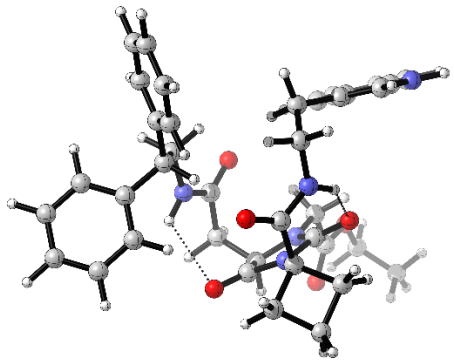
C3	-2.6304340	0.4545930	0.9691057
C4	-1.9089315	1.7328151	1.3776558
C5	-0.6507897	1.9451224	0.5585381
C6	0.9566779	3.5743129	-0.3439986
C7	2.1692033	3.5415725	0.6032705
C8	2.0923360	4.6568079	1.6598020
C9	1.9806509	6.0373423	0.9855103
C10	0.7482566	6.0927479	0.0631701
C11	0.7960422	4.9622765	-0.9856074
C12	-1.1992227	-2.8303420	-0.1296356
C13	-2.1107178	-3.9142276	-0.7948387
C14	-1.5897995	-4.9513805	0.2479094
C15	-1.0886955	-3.7654948	1.1307900
C16	0.1509620	-2.7896664	-0.8340659
C17	2.0851012	-1.4572766	-1.4900652
C18	2.9800427	-0.6941429	-0.4798234
C19	4.3393728	-0.3238054	-1.0636510
C20	4.9089677	-0.9928384	-2.1368543
C21	6.1535492	-0.6218893	-2.6247180

C22	6.8462400	0.4237329	-2.0476870
C23	6.2882755	1.0977360	-0.9726913
C24	5.0500544	0.7252768	-0.4889930
C25	3.1098623	-1.4987959	0.8120924
C26	2.1635546	-1.3367540	1.8150515
C27	2.2207886	-2.0954110	2.9714748
C28	3.2334517	-3.0219100	3.1450567
C29	4.1841770	-3.1854346	2.1525581
C30	4.1218029	-2.4304209	0.9946814
C31	-3.8642438	1.1665388	-1.1730268
C32	-5.3000256	0.8476206	-0.7950315
C33	-5.8456719	-0.3748389	-1.1718968
C34	-7.1424319	-0.6947059	-0.8222759
C35	-7.9097275	0.2014152	-0.0924608
C36	-7.3734971	1.4178544	0.2824365
C37	-6.0705254	1.7382356	-0.0688413
N1	-1.7950382	-1.5208619	0.0732419
N2	-2.9099016	0.3342752	-0.4465792
N3	-0.2811358	3.2162305	0.3756686
N4	0.7312982	-1.5893691	-0.9649722
O1	-2.6857580	-1.2954203	-2.0596069
O2	-1.1899142	-1.0281204	2.2577679
O3	0.0005492	0.9944353	0.1258360
O4	0.6576076	-3.8348296	-1.2234114
H3A	-3.5374358	0.3529984	1.5568924
H17A	2.4543794	-2.4545432	-1.6631869
H18	2.4592657	0.2260196	-0.2443625
H4	0.2955465	-0.7581532	-0.6223303
H4A	-2.5679522	2.5870750	1.3025296
H17B	2.0646086	-0.9159684	-2.4296010
H3	-0.8364664	3.9512811	0.7537998
H8A	2.9711846	4.6216877	2.2938855
H4B	-1.6134709	1.6198905	2.4164410
H6	1.0859570	2.8279137	-1.1133682
H8B	1.2293487	4.4924326	2.2977049
H31B	-3.6413778	2.2070628	-0.9771797
H31A	-3.7033215	0.9753178	-2.2239275
H22	7.8075900	0.7103296	-2.4255247
H15B	-1.8149411	-3.4868311	1.8770668
H15A	-0.1094131	-3.8369721	1.5724100
H13B	-3.1526161	-3.6769158	-0.6385262
H33	-5.2480642	-1.0591595	-1.7419110
H7A	2.2214169	2.5679082	1.0746816
H26	1.3658637	-0.6355832	1.6862352
H13A	-1.9150613	-4.1084442	-1.8340093
H9A	2.8745499	6.2195748	0.3959805
H24	4.6289093	1.2413718	0.3518217
H20	4.3926680	-1.8085695	-2.6001285

H9B	1.9187705	6.8185366	1.7353561
H30	4.8661098	-2.5598306	0.2355482
H23	6.8195531	1.9080583	-0.5130982
H37	-5.6617335	2.6886585	0.2185988
H7B	3.0685763	3.6691670	0.0085108
H14A	-0.7653535	-5.5137532	-0.1531857
H10B	0.7009519	7.0505838	-0.4431097
H11A	-0.0948587	4.9745007	-1.6040030
H14B	-2.3290089	-5.5985586	0.6955982
H11B	1.6490024	5.1277019	-1.6353867
H21	6.5759322	-1.1535586	-3.4546375
H36	-7.9626028	2.1159392	0.8435137
H34	-7.5576065	-1.6369136	-1.1201659
H35	-8.9167547	-0.0484377	0.1762767
H10A	-0.1527676	6.0146979	0.6666201
H27	1.4664191	-1.9635260	3.7216293
H28	3.2810234	-3.6104853	4.0400946
H29	4.9728494	-3.9013436	2.2771809

1k conformer a

E = -2197.9099629 Hartrees; ZPE = 1964.66 kcal/mol



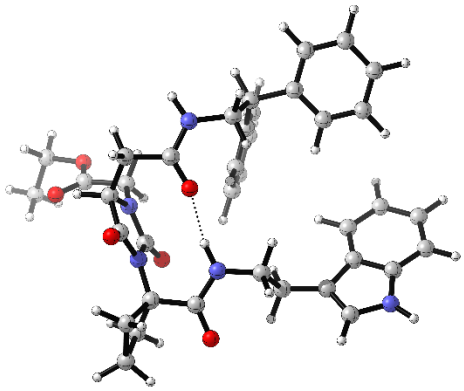
Atom	X	Y	Z
N5	0.3310913	1.1771492	-2.2637141
C28	0.9728772	0.0169606	-2.4487900
O6	2.1946294	-0.1167749	-2.3713435
C29	0.0755278	-1.1712833	-2.7706107
C30	0.7905304	-2.3634920	-3.4805431
C31	-0.4031532	-2.4575276	-4.4836032
C32	-0.8479522	-1.0298787	-4.0340730
N6	-0.6697531	-1.5682775	-1.5690880
C33	-0.2941006	-2.5208262	-0.6520211
C34	-1.3859774	-2.5637532	0.4096250
N7	-2.1838616	-1.4038862	0.0483288
C35	-1.7996551	-0.8622787	-1.1277041
C36	-0.7926489	-2.5282626	1.8239407

C37	-0.0625919	-1.2241276	2.0943284
O7	-0.6433793	-0.2504696	2.5658914
N8	1.2332155	-1.2267598	1.7502582
C38	1.0414603	2.4130571	-1.9251600
O8	-2.3061977	0.0797282	-1.7071382
O9	0.7062766	-3.2005089	-0.6480328
C39	-3.2781939	-0.8803042	0.8337997
H39	-0.6715764	1.1956695	-2.2802163
H40	1.0173698	-3.2174609	-2.8740184
H41	1.6876861	-1.9920600	-3.9499401
H42	-0.1498794	-2.5777492	-5.5256373
H43	-1.1201058	-3.2107648	-4.1898466
H44	-0.4529393	-0.2650453	-4.6876256
H45	-1.8895672	-0.8533044	-3.8435554
H46	-1.9689624	-3.4659604	0.2905858
H47	-1.5883353	-2.6221352	2.5484892
H48	-0.1296594	-3.3766865	1.9197702
H51	2.0861852	2.1675469	-1.8369882
H52	-2.9186375	-0.5686041	1.8039660
H53	-3.6763390	-0.0101821	0.3339849
C46	0.5292662	3.0188233	-0.6058222
H59	0.5774926	2.2545318	0.1582356
H60	1.2076386	3.8127447	-0.3079506
H61	-1.2309768	1.9647190	1.7760874
C47	-2.0416783	2.5753812	1.4332145
C48	-4.2520455	4.0834094	0.5359083
C49	-1.9459829	3.3311805	0.2647732
C50	-3.2245223	2.5920711	2.1367532
C51	-4.3205867	3.3426160	1.6913009
C52	-3.0551795	4.0728097	-0.1718555
H62	-3.3099533	2.0199535	3.0391256
H63	-5.2289838	3.3353319	2.2609413
H64	-5.0929772	4.6528535	0.1929687
C53	-0.8792733	3.5532110	-0.6948493
C54	-1.3789530	4.3864228	-1.6346009
H65	-0.9077097	4.7976474	-2.4982041
N9	-2.6962517	4.7086167	-1.3357742
H66	-3.2823835	5.2960812	-1.8826127
C1	-4.3622666	-1.9104272	0.9947388
O2	-4.3090941	-3.0646035	0.6443796
O3	-5.4121184	-1.3771717	1.6365287
C2	-6.5777808	-2.2145693	1.9241556
H3	-7.0982895	-1.6813826	2.7013076
H4	-6.2366369	-3.1708862	2.2892170
C3	-7.4349046	-2.3816653	0.6726256
H5	-6.8881040	-2.9348113	-0.0784448
H6	-7.7053610	-1.4115479	0.2763305
H7	-8.3399417	-2.9255913	0.9168591

H20	1.6512065	-2.0540440	1.3758063
H21	0.9280499	3.1275736	-2.7317957
C4	2.1096471	-0.0690678	1.9593900
H1	2.5733525	-0.1374590	2.9352763
H8	1.4977511	0.8190852	1.9341113
C5	3.1755499	-0.0261506	0.8461845
H9	2.6562276	-0.0390254	-0.0991864
C6	4.0501715	-1.2778551	0.8903200
C7	5.5711842	-3.6092776	0.9622998
C8	3.9461062	-2.2173927	-0.1250214
C9	4.9325757	-1.5125163	1.9378189
C10	5.6870938	-2.6687457	1.9748012
C11	4.7021326	-3.3797257	-0.0861629
H10	3.2809073	-2.0311520	-0.9444379
H11	5.0432635	-0.7816602	2.7143393
H12	6.3673493	-2.8360611	2.7866981
H13	4.6081463	-4.0983438	-0.8759913
H14	6.1573076	-4.5064950	0.9922738
C12	4.0248900	1.2388604	0.8672325
C13	5.6202414	3.5242655	0.7570096
C14	4.2821284	1.9755785	2.0126054
C15	4.5712079	1.6667513	-0.3400672
C16	5.3622028	2.7971171	-0.3949449
C17	5.0769923	3.1114109	1.9574025
H2	3.8669703	1.6795678	2.9550807
H15	4.3566256	1.1064668	-1.2298175
H16	5.7761048	3.1123015	-1.3325735
H17	5.2656596	3.6698712	2.8531812
H18	6.2339765	4.4021794	0.7154564

1k conformer b

E = -2197.9093950 Hartrees; ZPE = 1963.98 kcal/mol



Atom	X	Y	Z
C1	-2.7254913	0.8700671	0.3139374
C2	-3.1993197	1.1371568	-1.9112629

C3	-3.5035078	-0.3141248	-1.5462465
C4	-2.7427045	-1.2781004	-2.4528530
C5	-1.2497538	-1.1457770	-2.2339622
C6	0.9321185	-2.3020444	-2.2324109
C7	1.4296121	-3.2110925	-1.0852386
C8	2.9480315	-3.3204541	-1.2201450
C9	3.7797811	-2.3014923	-0.7780929
H9	3.3649050	-1.4521090	-0.2755495
C10	5.1480324	-2.3807825	-0.9618263
H10	5.7713064	-1.5844085	-0.6078659
C11	5.7040537	-3.4835967	-1.5885252
H11	6.7650022	-3.5458697	-1.7280955
C12	4.8835897	-4.5057223	-2.0286984
H12	5.3053052	-5.3658667	-2.5103332
C13	3.5133307	-4.4216250	-1.8458984
H13	2.8836617	-5.2205342	-2.1897234
C14	1.0163199	-2.7734575	0.3190696
C15	-2.5480847	3.1776696	-0.5708406
C16	-3.2889115	3.8838472	0.6143174
C17	-3.5755545	5.0964750	-0.3244235
H17A	-2.8260624	5.8581232	-0.2012533
H17B	-4.5712069	5.5119017	-0.2863203
C18	-3.2594308	4.1820894	-1.5495101
H18A	-2.6410796	4.5851820	-2.3342272
H18B	-4.1504009	3.7457300	-1.9687005
C19	-1.0624329	3.5013514	-0.5001331
C20	1.2415377	2.7694866	-0.7421409
C21	1.7132509	2.9407704	0.7210473
C22	3.2066376	3.1003042	0.7967075
C23	3.9242009	4.1990252	0.4761011
C24	5.4449658	2.6567816	1.0774937
C25	4.1659886	2.0873788	1.1935092
C26	4.0384777	0.7772379	1.6513781
H26	3.0702521	0.3304703	1.7655527
C27	5.1739759	0.0668678	1.9694628
H27	5.0897444	-0.9396685	2.3281602
C28	6.4433852	0.6460356	1.8372559
H28	7.3119391	0.0725585	2.0955201
C29	6.5929284	1.9392526	1.3942187
H29	7.5650407	2.3816617	1.3022852
C30	0.5226190	-1.5139415	0.6203484
H30	0.3819819	-0.7820341	-0.1446780
C31	0.1690957	-1.1821582	1.9236279
H31	-0.2536961	-0.2160498	2.1187804

C32	0.3200034	-2.1041442	2.9407472
H32	0.0493109	-1.8483804	3.9458309
C33	0.8199141	-3.3647439	2.6506105
H33	0.9423563	-4.0874420	3.4331329
C34	1.1583639	-3.6942017	1.3536866
H34	1.5503497	-4.6699159	1.1387076
C35	-3.2946219	-1.4809044	0.7288149
C36	-4.7585629	-1.8107675	0.8918320
C40	-6.2471623	-3.3106219	2.0778871
C38A	-6.9209672	-2.3701334	3.0729185
H38D	-7.0854562	-1.4037671	2.6165904
H38E	-6.2988091	-2.2499537	3.9502398
H38F	-7.8776232	-2.7798421	3.3752081
N1	-2.8299402	1.7644568	-0.7460811
N2	-3.1036459	-0.3585480	-0.1513843
N3	-0.5325277	-2.2689978	-2.3493033
N4	-0.2014490	2.5335107	-0.8288039
N5	5.2828038	3.9473026	0.6349686
O1	-2.3717360	1.1389136	1.4408370
O2	-3.3037652	1.6199282	-3.0101569
O3	-0.7437841	-0.0533366	-1.9796604
O4	-4.9020377	-2.8305039	1.7520342
O5	-0.7054196	4.6254422	-0.1573125
O6	-5.6793134	-1.2740712	0.3278511
H3	-4.5675914	-0.4783432	-1.6397633
H4	-0.5106378	1.6572163	-1.1974226
H7	1.0136591	-4.2010712	-1.2510374
H23	3.5823183	5.1542712	0.1475012
H41	-3.0722120	-2.2964047	-2.2967667
H42	-2.9624934	-0.9991368	-3.4787123
H50	6.0116404	4.6025474	0.4701266
H61	1.2708130	-1.2887297	-2.1009022
H62	1.3464724	-2.6765459	-3.1597534
H161	-4.1927194	3.3464530	0.8623598
H162	-2.6946998	4.0614669	1.4925007
H201	1.4996454	3.6613525	-1.2975066
H202	1.7370769	1.9227343	-1.1954874
H211	1.2102409	3.8066436	1.1269112
H212	1.4003380	2.0745713	1.2909543
H300	-0.9962562	-3.1279610	-2.5540830
H361	-2.7755222	-2.3637231	0.3789443
H362	-2.8859706	-1.2291196	1.6960515
H8	-6.0820067	-4.2890966	2.4956970
H14	-6.8194062	-3.3834270	1.1660331

Figure S1. VT-NMR experiments (d_6-DMSO) for compound **1b**.

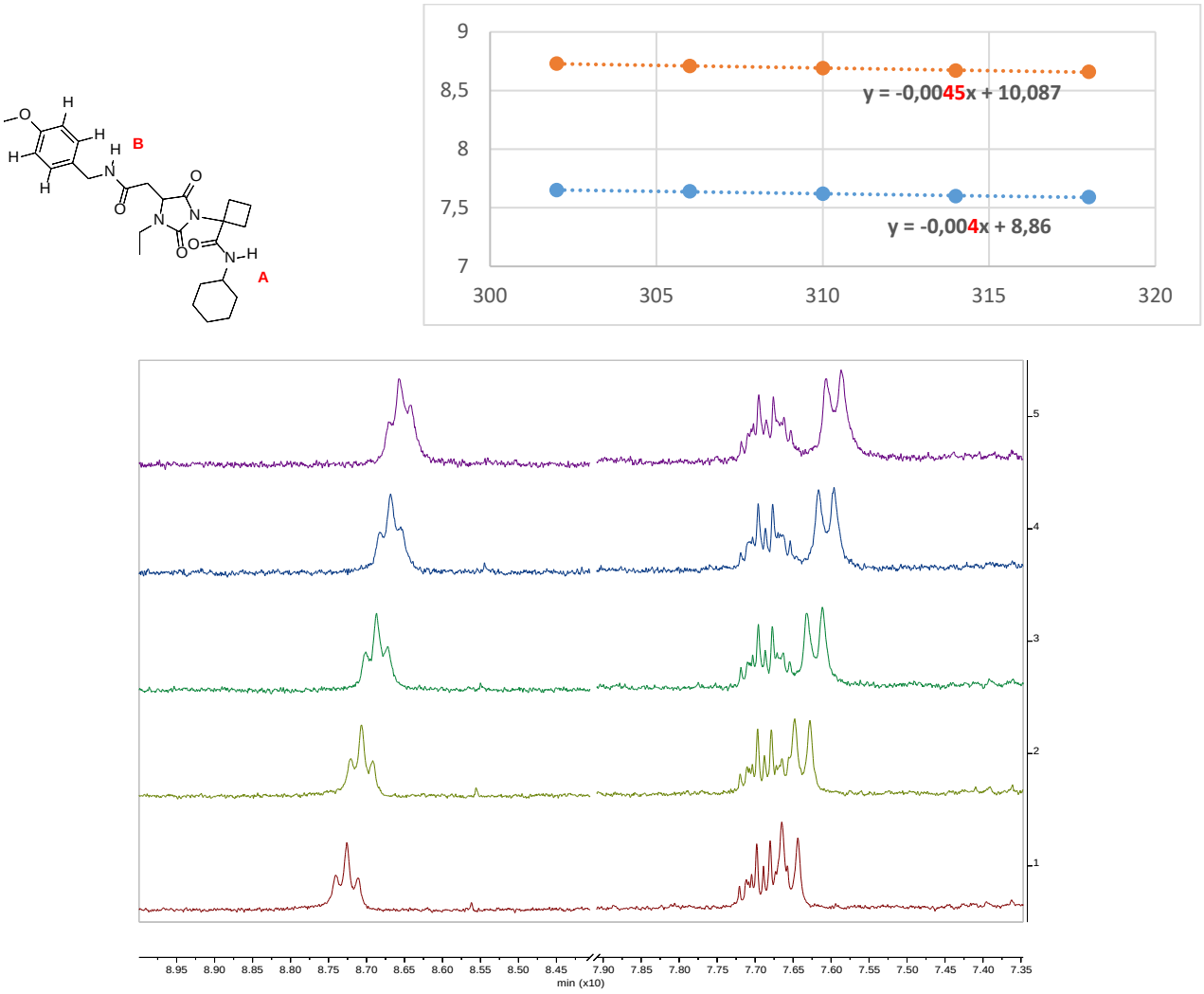
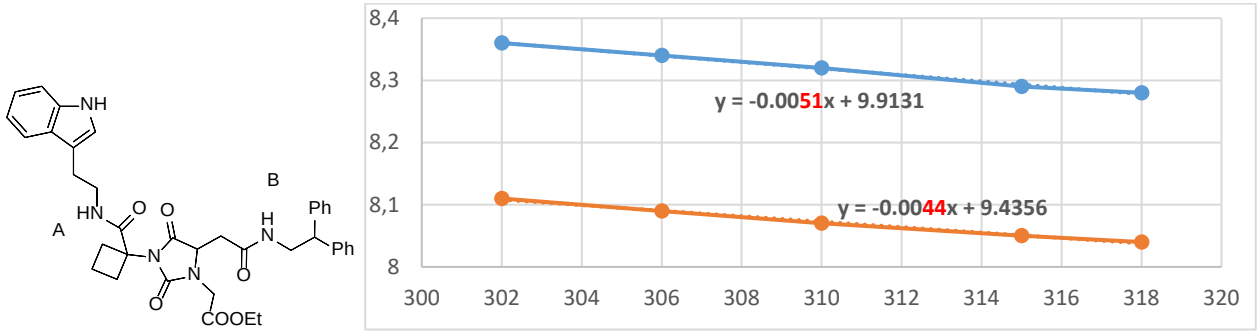


Figure S2. VT-NMR experiments (d_6-DMSO) for compound **1k**.



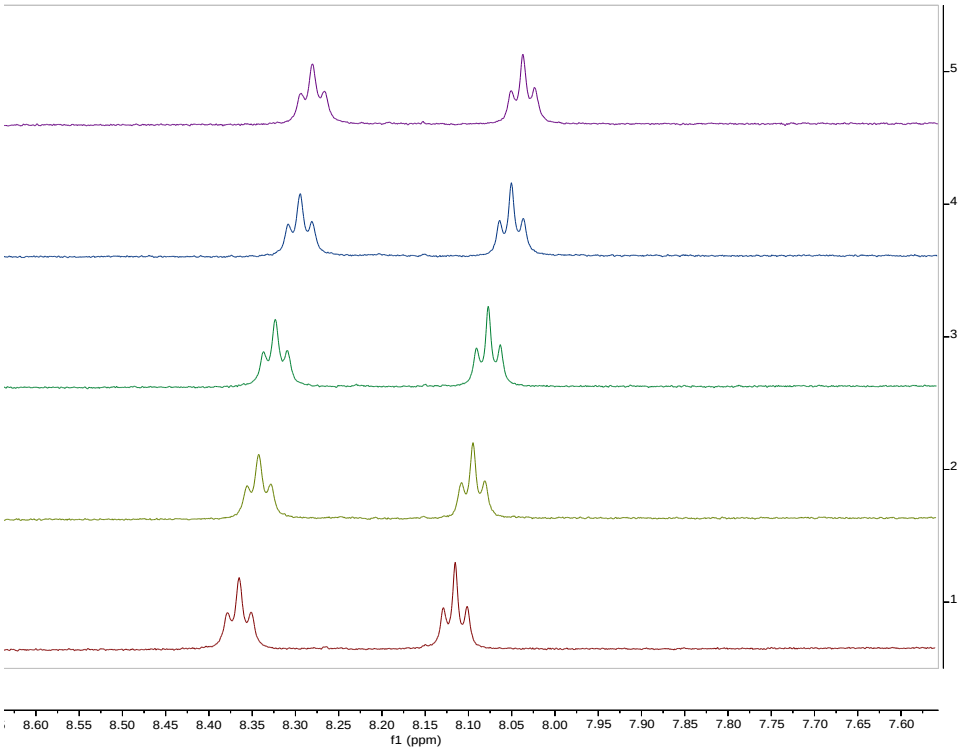


Figure S3. ORTEP[8] view of compound **1k**, showing the relative arbitrary atom-numbering scheme (ellipsoids are at the 40% probability and H atoms are as spheres of arbitrary radii).

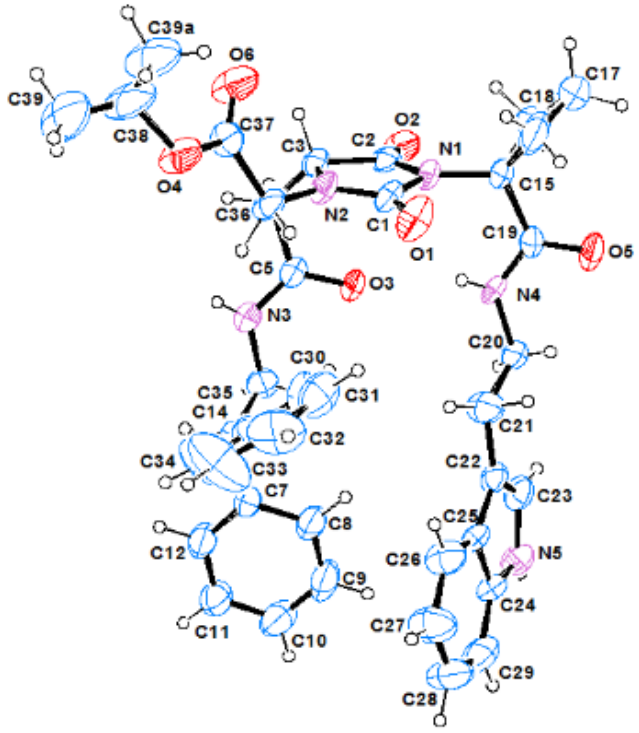


Figure S4. ORTEP[8] view of compound **1i**, showing the relative arbitrary atom-numbering scheme (ellipsoids are at the 40% probability and H atoms are as spheres of arbitrary radii).

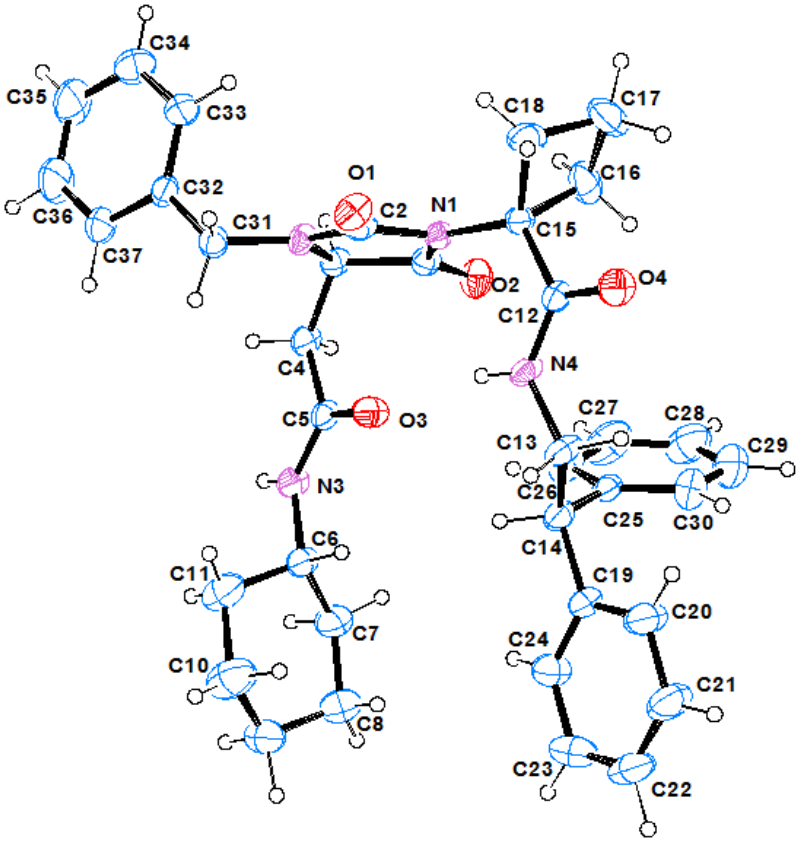


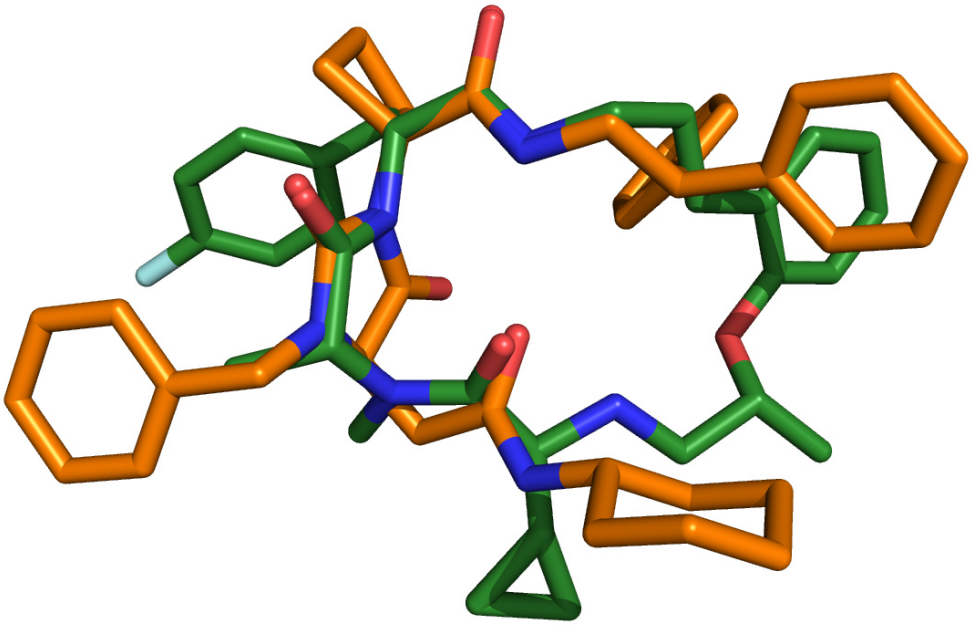
Table S3. Hydrogen bonds geometry (Å,°) of **1i** and **1k**.

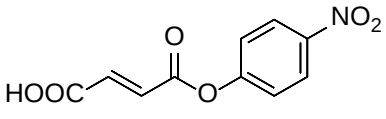
Compound	D-H…A	H…A distance (Å)	D-H…A angle (°)
1i	N4-H…O3	2.080(1)	165(1)
1i	C37-H…O1^{I}	2.607(1)	148(1)
1i	N3-H…O4^{II}	2.153(1)	179(1)
1k	N4-H…O3	2.296(1)	161(1)
1k	N3-H…O5^{III}	2.177(1)	168(1)
1k	N5-H…O2^{IV}	2.361(1)	151(1)

Equivalent positions:

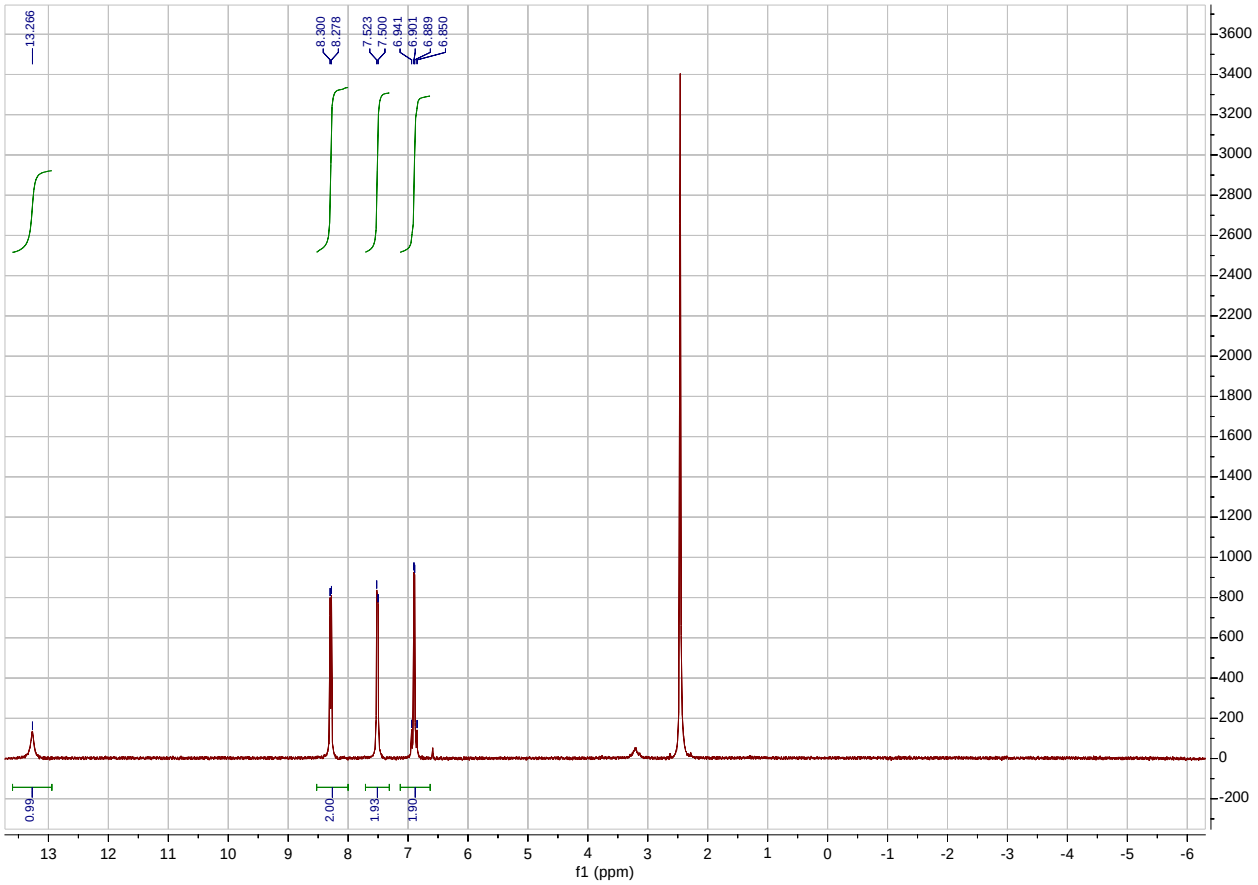
(I) at 1-x, y-1/2, z-1/2; (II) at x, y-1, z; (III) at x-1, y, z; (IV) at 2-x, 1-y, 1-z.

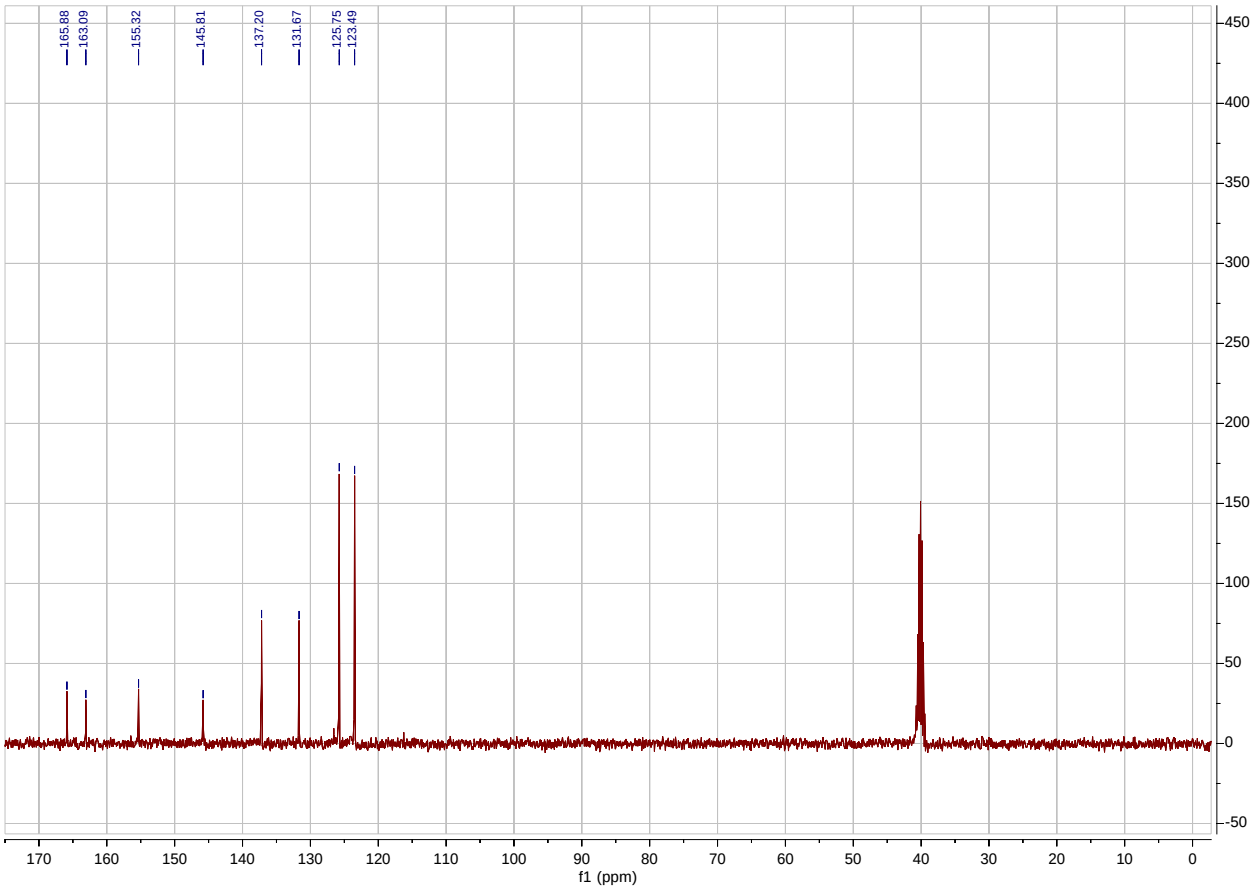
Figure S5. Superimposition of the crystal structure of compound **1i** (orange) with the crystal structure of macrocyclic β-turn mimetic, active toward ghrelin receptor agonist (green).[9] The two structures overlay each other very well, with a RMSD = 0.301 in the β-turn region.




HOOC
O
O
NO2

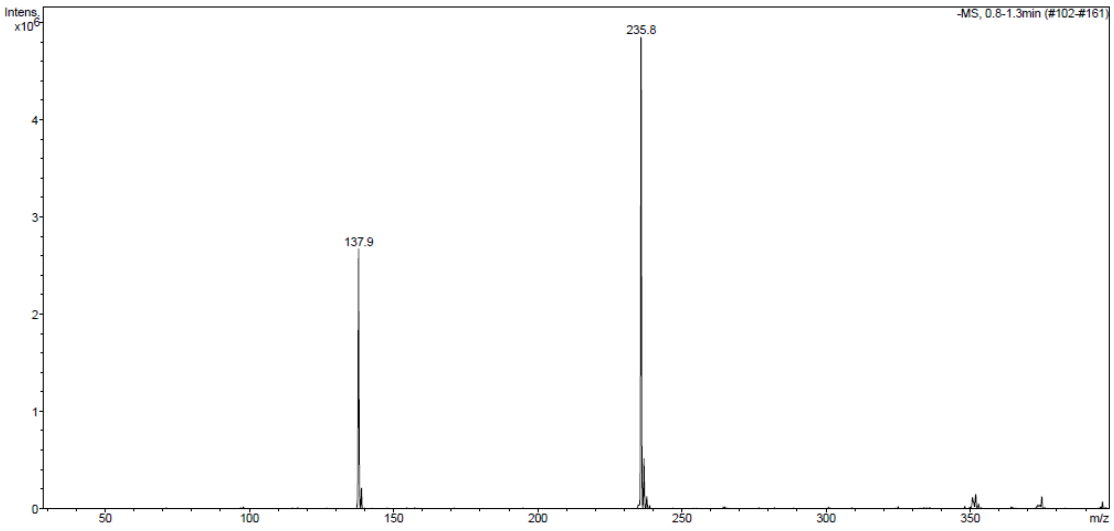
5


13.266
8.300
8.278
7.523
7.500
6.941
6.901
6.889
6.850
0.99
2.00
1.93
1.90
f1 (ppm)

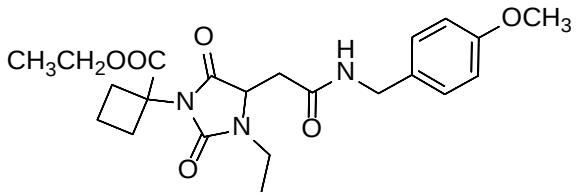


-L.G.S. - Laboratorio Grandi Strumenti - Display Report

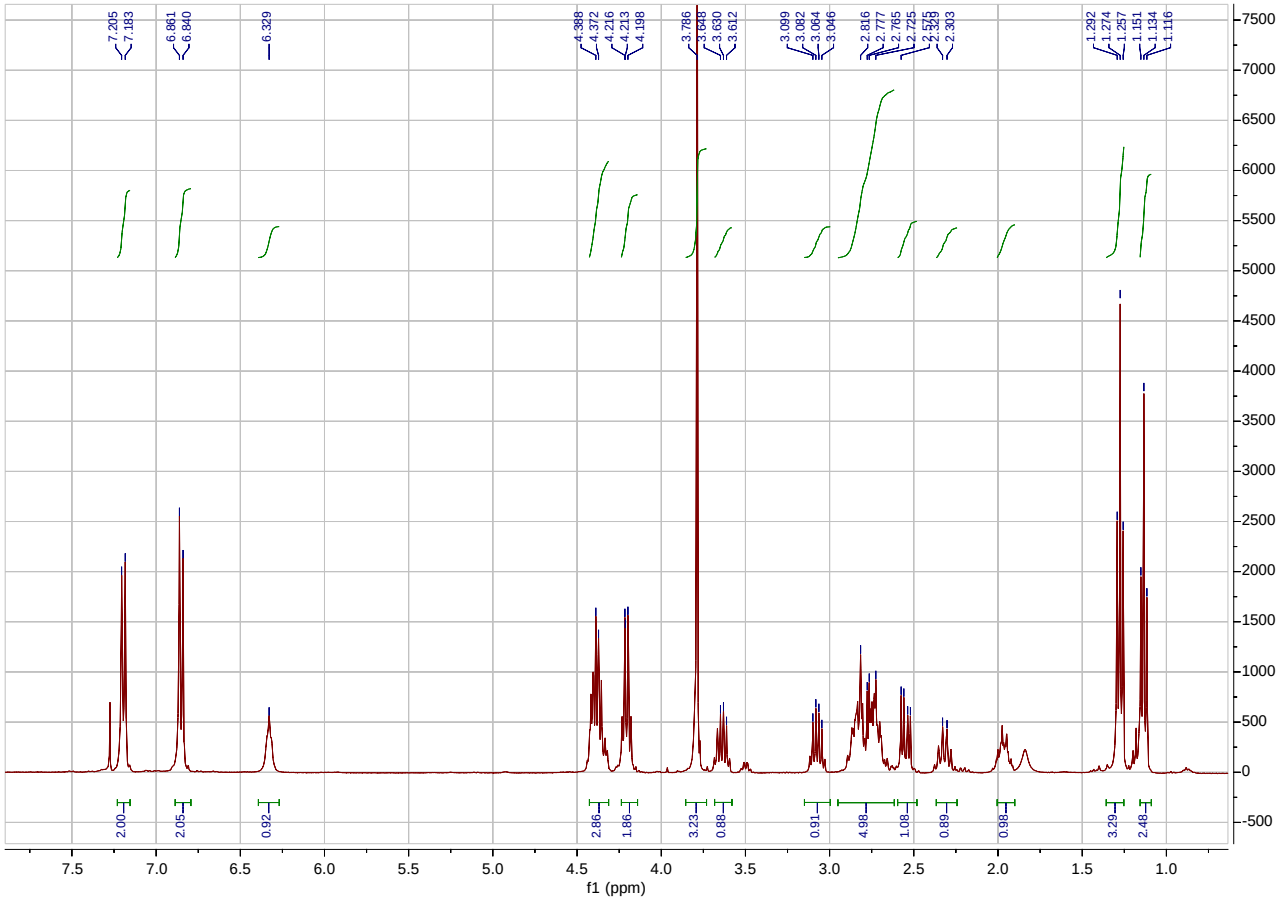
Analysis Name	av fm2669bisxx.d	Acquisition Date	03/18/15 13:57:32	Operator	Walter Panzeri
Sample Name		Method	Copy of _01tmix_posneg lm.MS	Instrument	esquire3000plus
Comment	1 mg/ml CH2Cl2 dil 1:100 MeOH Richiedente: Bertarelli				

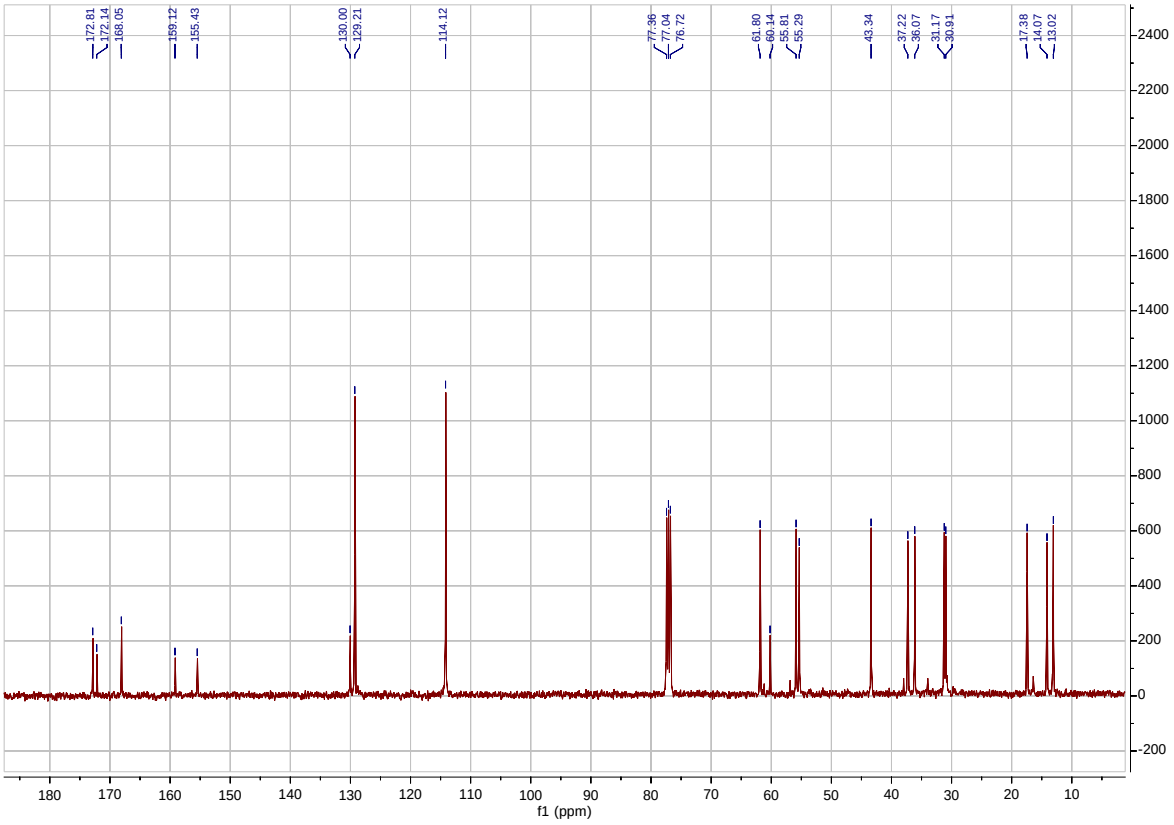


Bruker Daltonics DataAnalysis 3.1 printed: 03/18/15 15:02:24 Page 1 of 1


CH3CH2OOC
O
N
N
O
O
H
N
O
OCH3

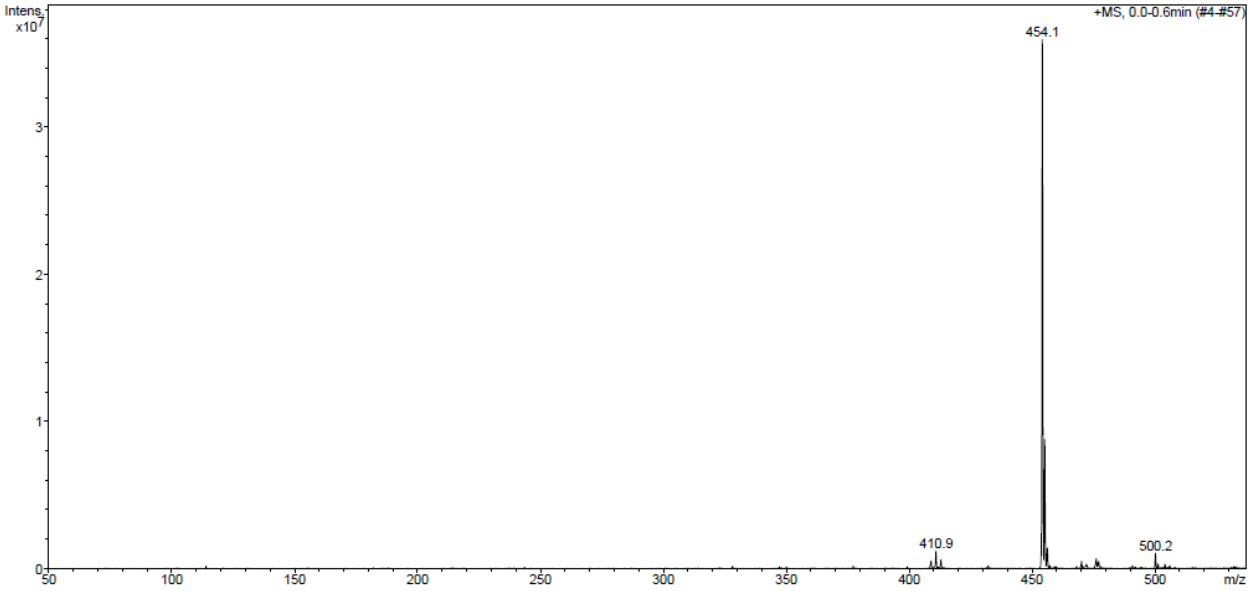
7a


7.205
7.183
6.861
6.840
6.329
4.388
4.372
4.216
4.213
4.198
3.786
3.648
3.630
3.612
3.099
3.082
3.064
3.046
2.816
2.777
2.765
2.725
2.575
2.529
2.303
1.292
1.274
1.257
1.151
1.134
1.116
2.00
2.05
0.92
2.86
1.86
3.23
0.88
0.91
4.98
1.08
0.89
0.98
3.29
2.48
f1 (ppm)

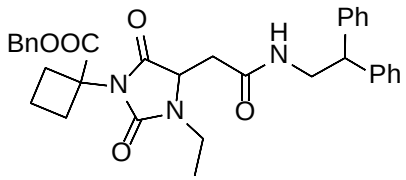


-L.G.S. - Laboratorio Grandi Strumenti - Display Report

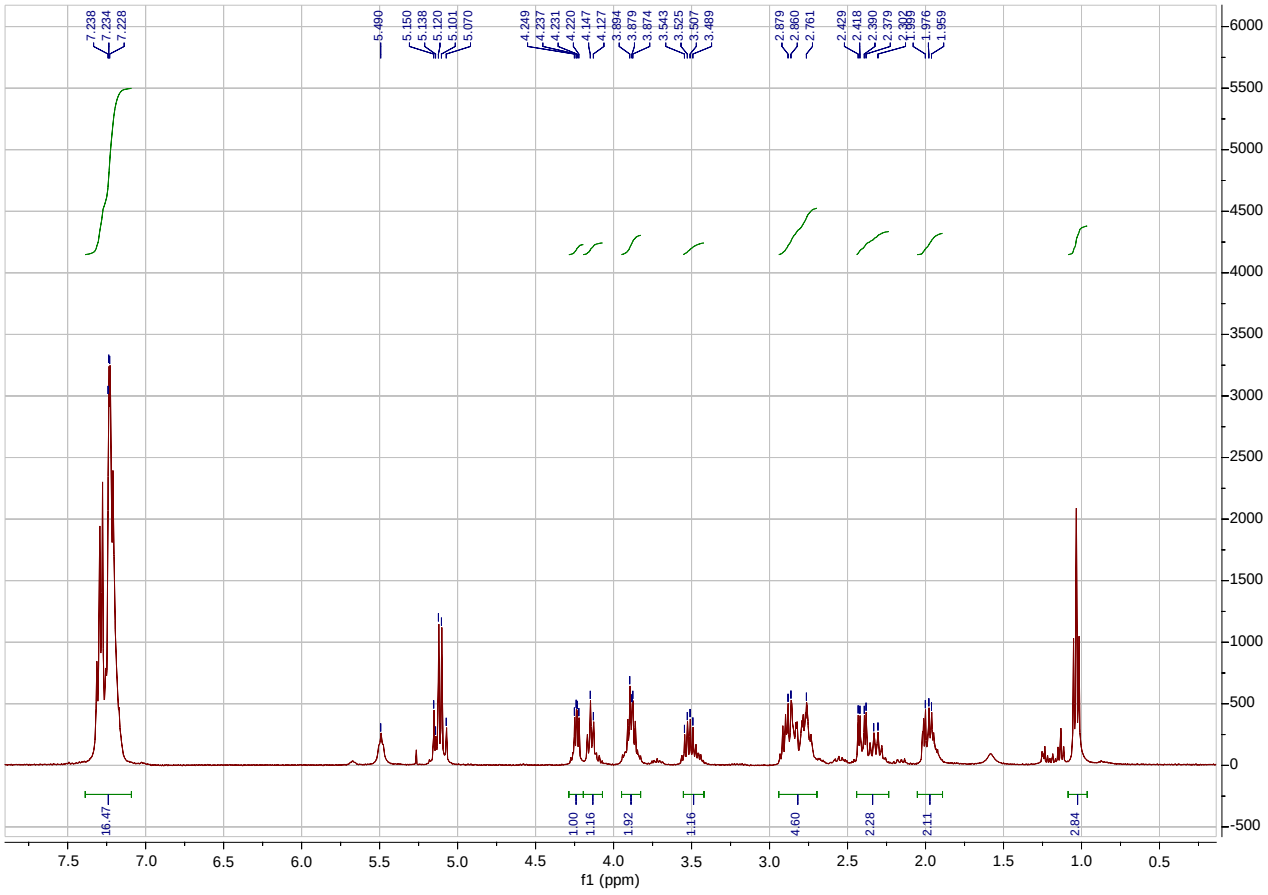
Analysis Name	av pc41.d	Acquisition Date	07/24/14 14:38:56	Operator	Walter Panzeri
Sample Name		Method	Copy of _01esquirew t 1500.MS	Instrument	esquire3000plus
Comment	1 mg/ml dil 1:100 MeOH Richiedente: Volonterio				



Bruker Daltonics DataAnalysis 3.1 printed: 07/24/14 14:40:04 Page 1 of 1


BnOOC
O
N
N
O
O
H
N
Ph
Ph

7b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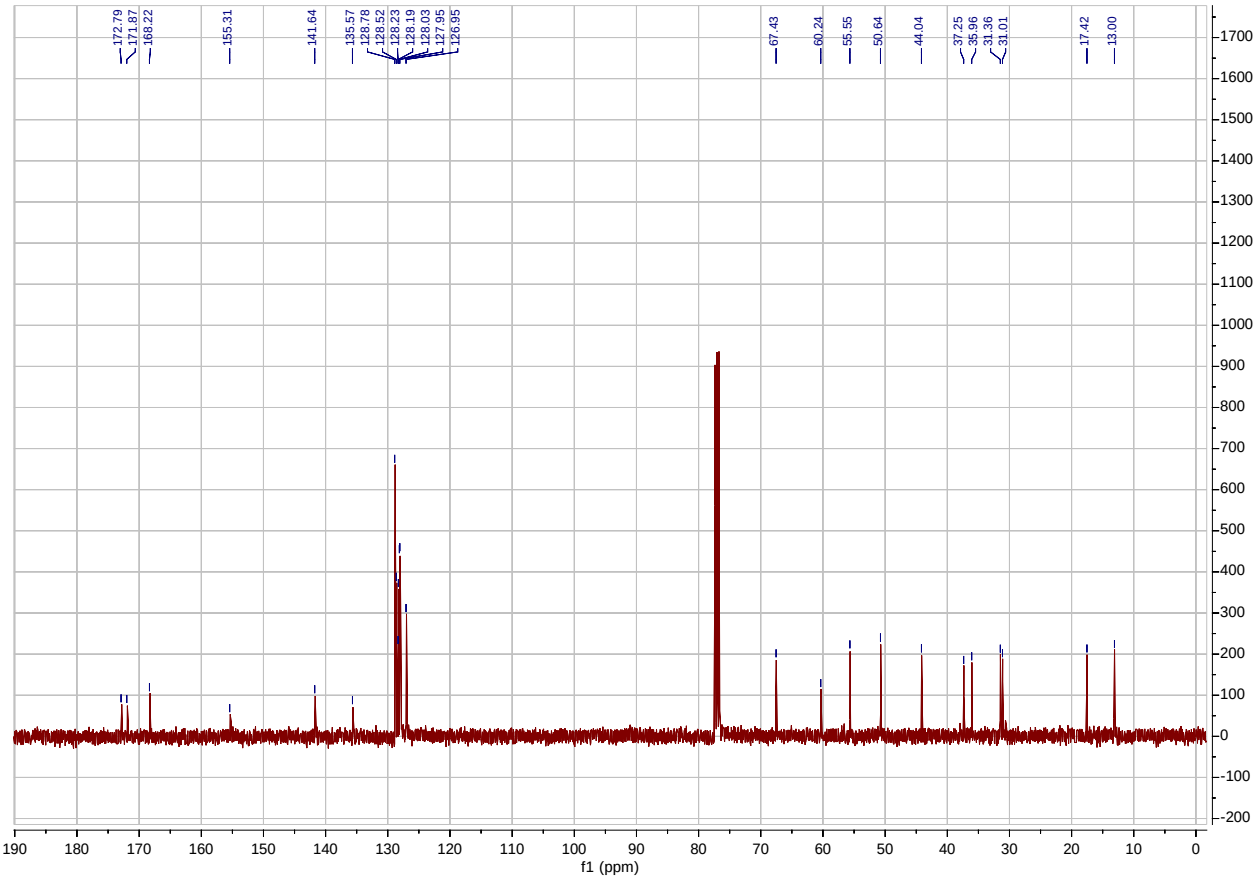
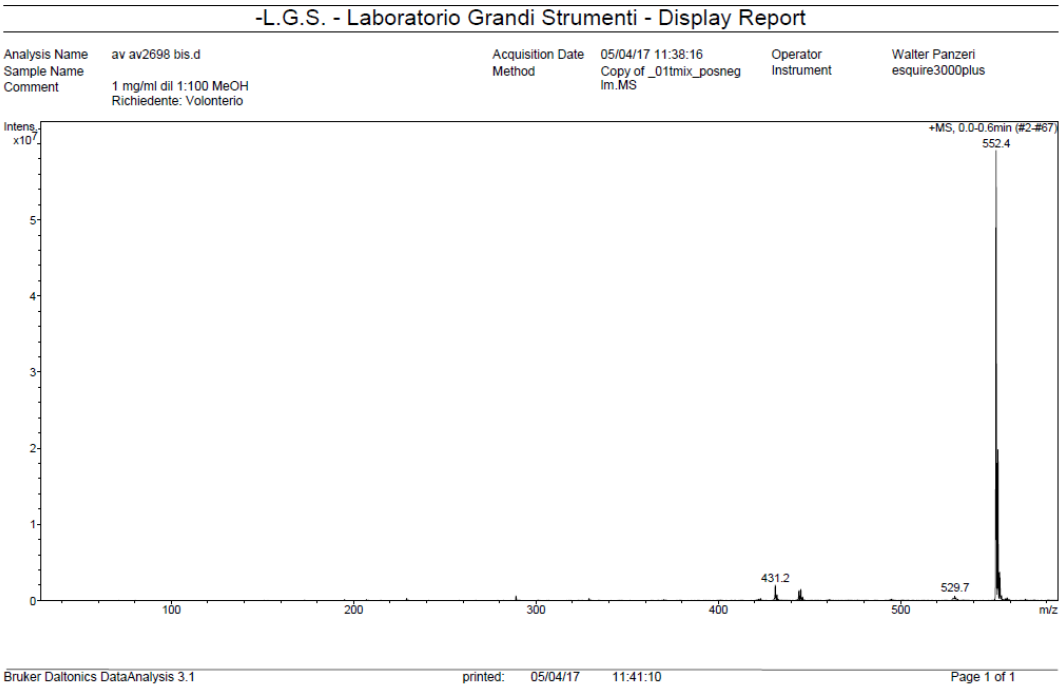
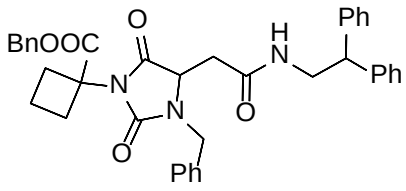
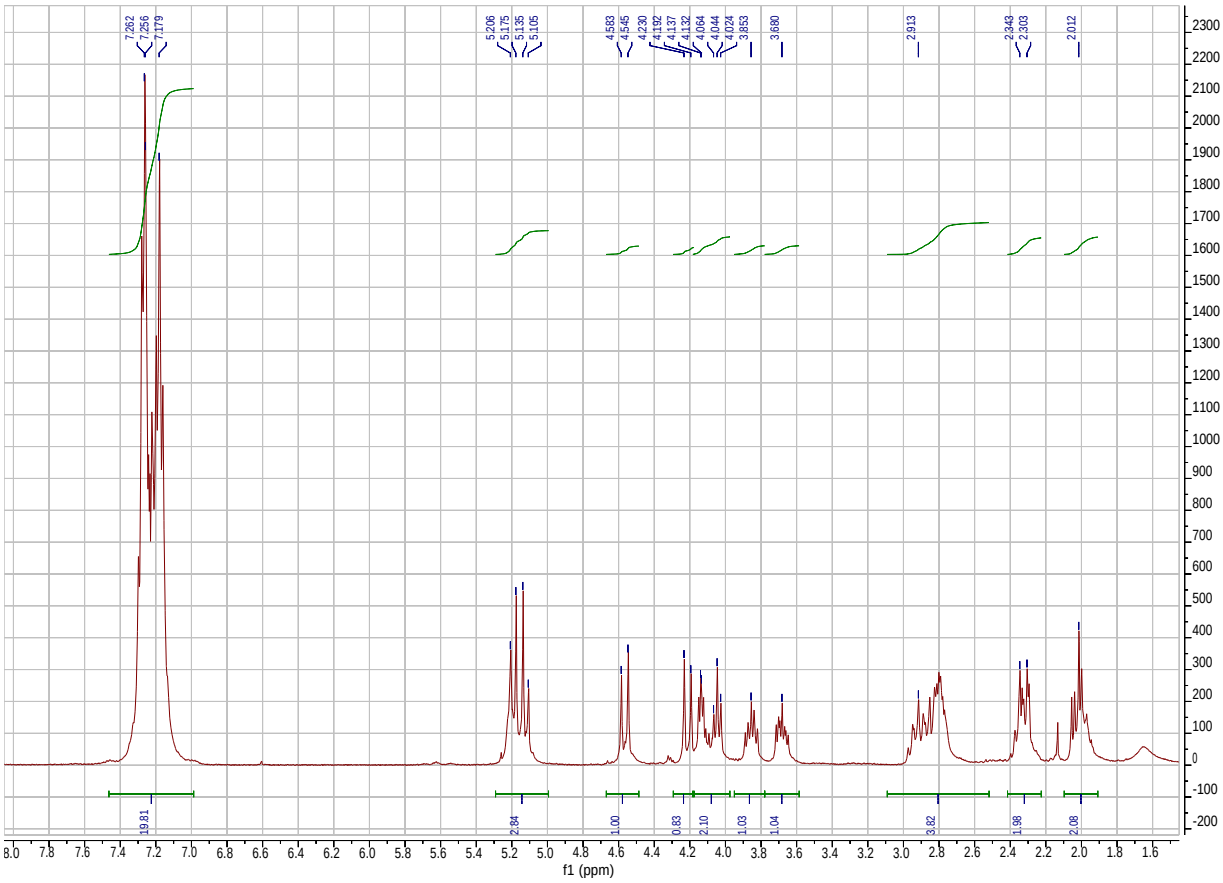
7.234
7.228
5.490
5.150
5.138
5.120
5.101
5.070
4.249
4.237
4.231
4.220
4.147
4.127
3.894
3.879
3.874
3.543
3.525
3.507
3.489
2.879
2.860
2.761
2.429
2.418
2.390
2.379
1.976
1.959
16.47
1.00
1.16
1.92
1.16
4.60
2.28
2.11
2.84
f1 (ppm)


172.79
171.87
168.22
155.31
141.64
135.57
128.78
128.52
128.23
128.19
128.03
127.95
126.95
67.43
60.24
55.55
50.64
44.04
37.25
35.96
31.36
31.01
17.42
13.00
f1 (ppm)


-L.G.S. - Laboratorio Grandi Strumenti - Display Report
Analysis Name av av2698 bis.d
Sample Name
Comment 1 mg/ml dil 1:100 MeOH
Richiedente: Volonterio
Acquisition Date 05/04/17 11:38:16
Method Copy of _01tmix_posneg lm.MS
Operator Walter Panzeri
Instrument esquire3000plus
+MS, 0.0-0.6min (#2-#67)
552.4
431.2
529.7
m/z
Bruker Daltonics DataAnalysis 3.1
printed: 05/04/17 11:41:10
Page 1 of 1


BnOOC
O
N
N
O
O
H
N
Ph
Ph
Ph

7c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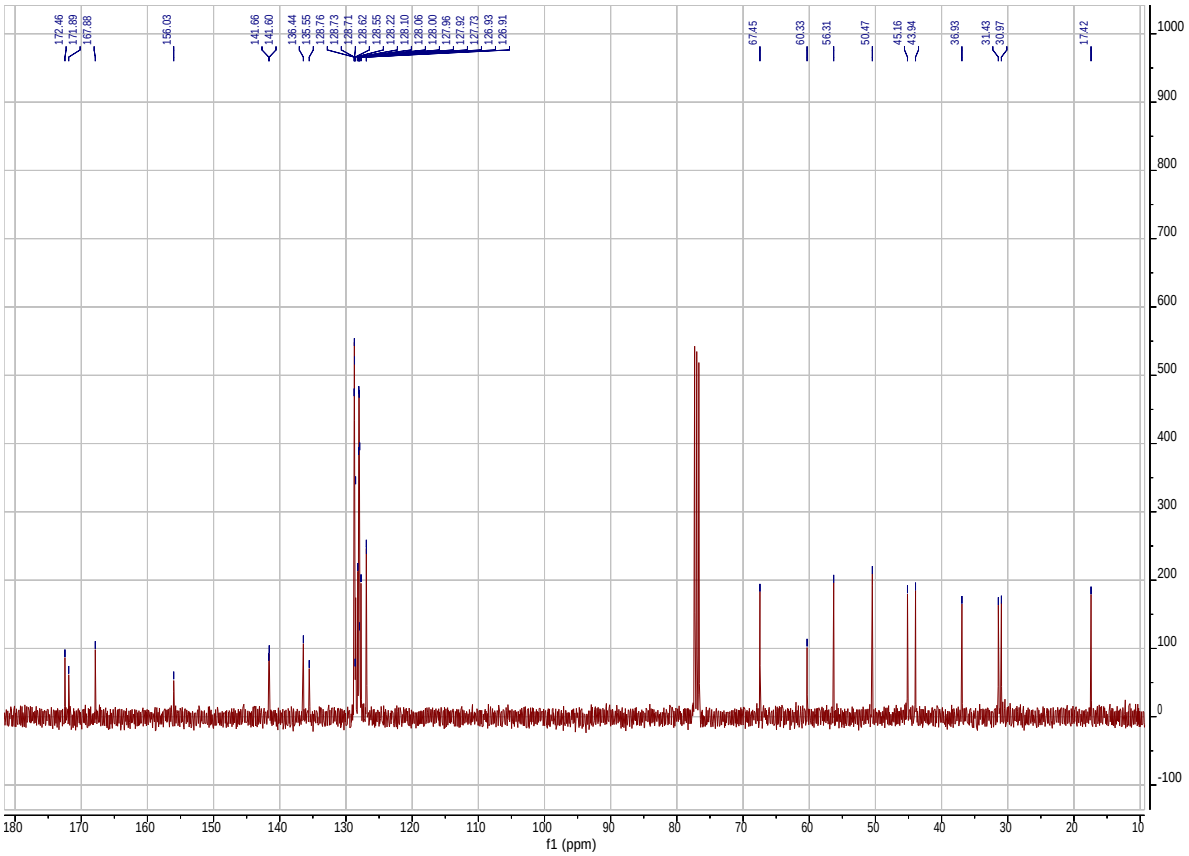
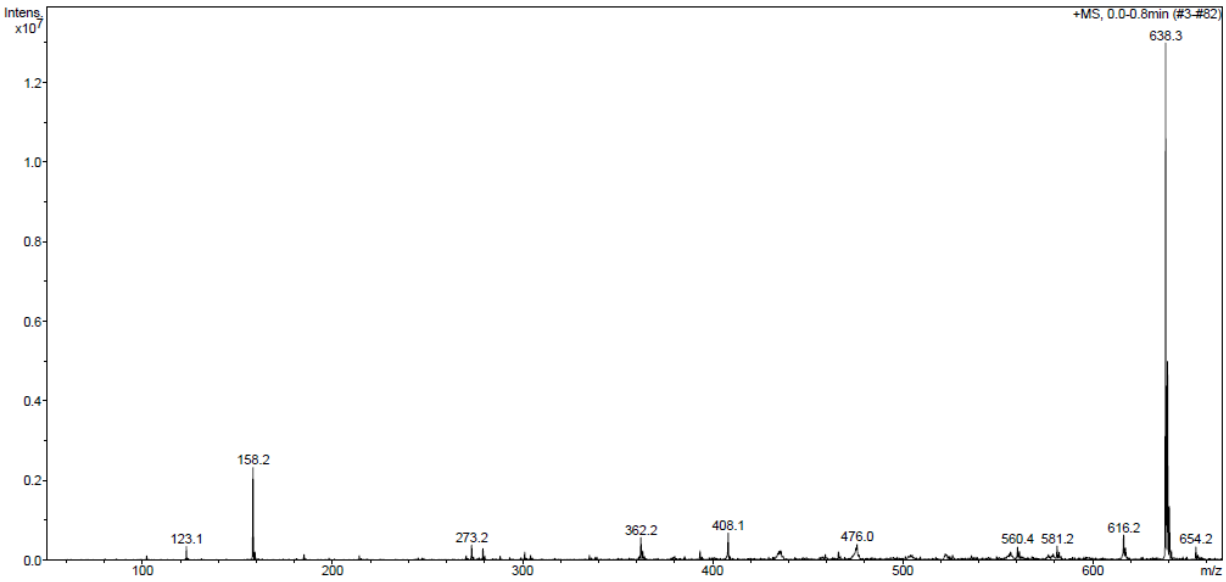
7.256
7.179
5.206
5.175
5.135
5.105
4.583
4.545
4.230
4.192
4.137
4.132
4.064
4.044
4.024
3.853
3.680
2.913
2.343
2.303
2.012
19.81
2.84
1.00
0.83
2.10
1.03
1.04
3.82
1.98
2.08
f1 (ppm)

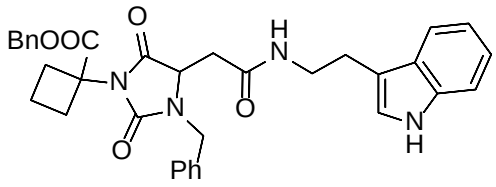


-L.G.S. - Laboratorio Grandi Strumenti - Display Report

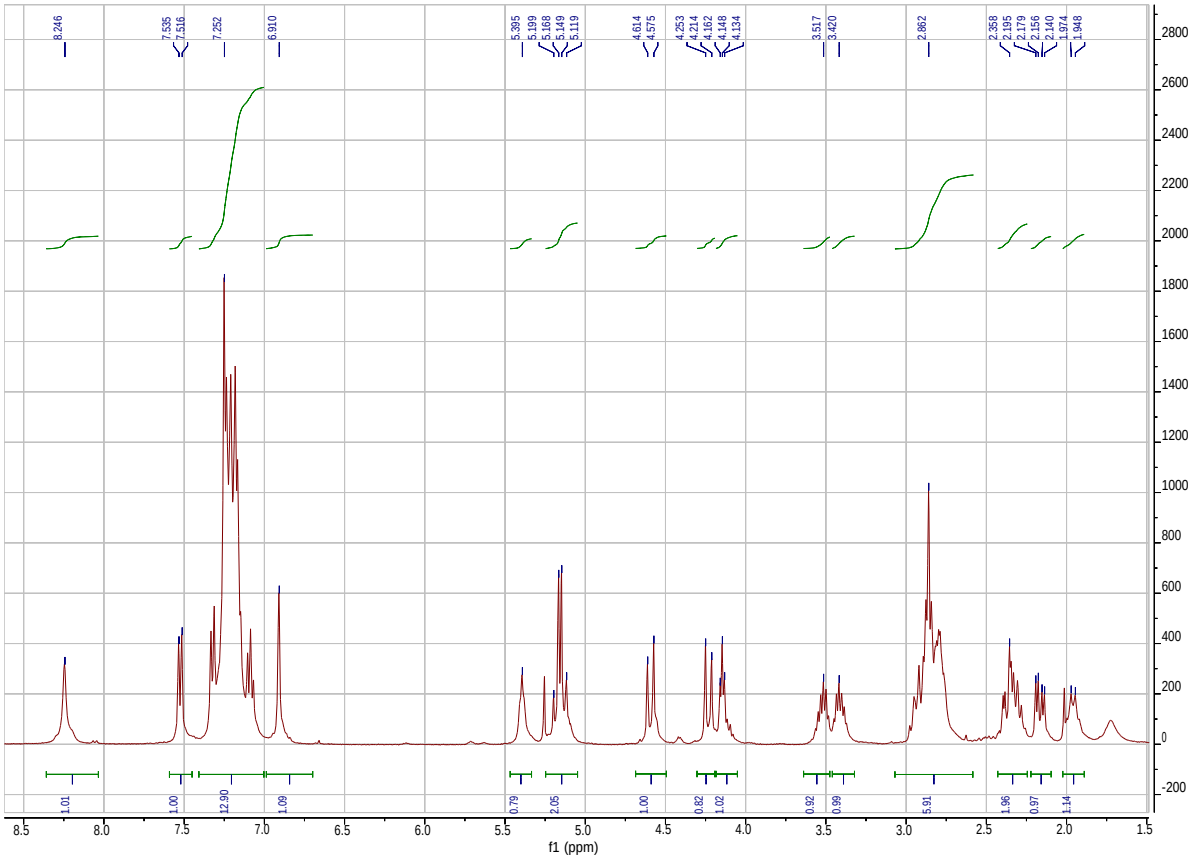
Analysis Name	av fm2659.d	Acquisition Date	05/04/15 16:37:22	Operator	Walter Panzeri
Sample Name		Method	Copy of _01tmix_posneg lm.MS	Instrument	esquire3000plus
Comment	1 mg/ml dil 1:100 MeOH Richiedente: Frigerio				



Bruker Daltonics DataAnalysis 3.1 printed: 05/04/15 16:38:31 Page 1 of 1


BnOOC
O
N
N
O
Ph
H
N
O
N
H

7d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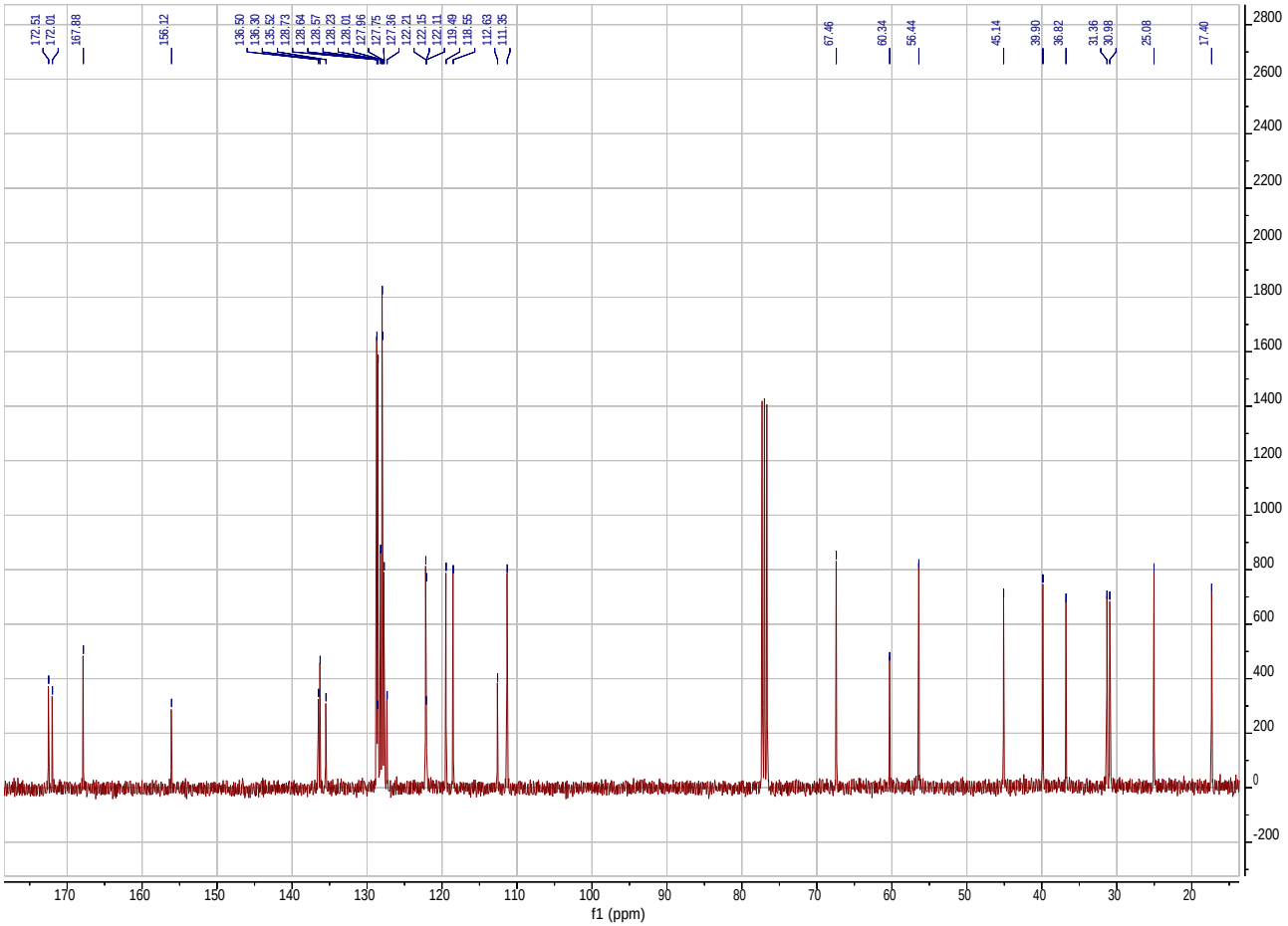
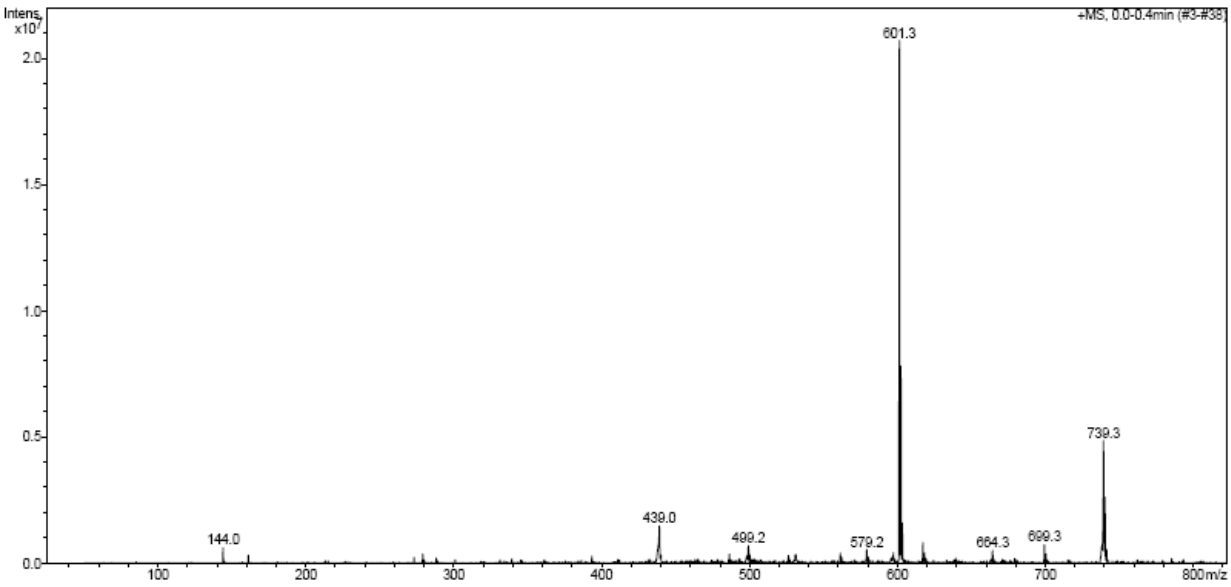
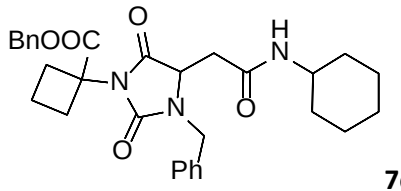
7.516
7.252
6.910
5.395
5.199
5.168
5.149
5.119
4.614
4.575
4.253
4.214
4.162
4.148
4.134
3.517
3.420
2.862
2.358
2.195
2.179
2.156
2.140
1.974
1.948
1.01
1.00
12.90
1.09
0.79
2.05
1.00
0.82
1.02
0.92
0.99
5.91
1.96
0.97
1.14
f1 (ppm)



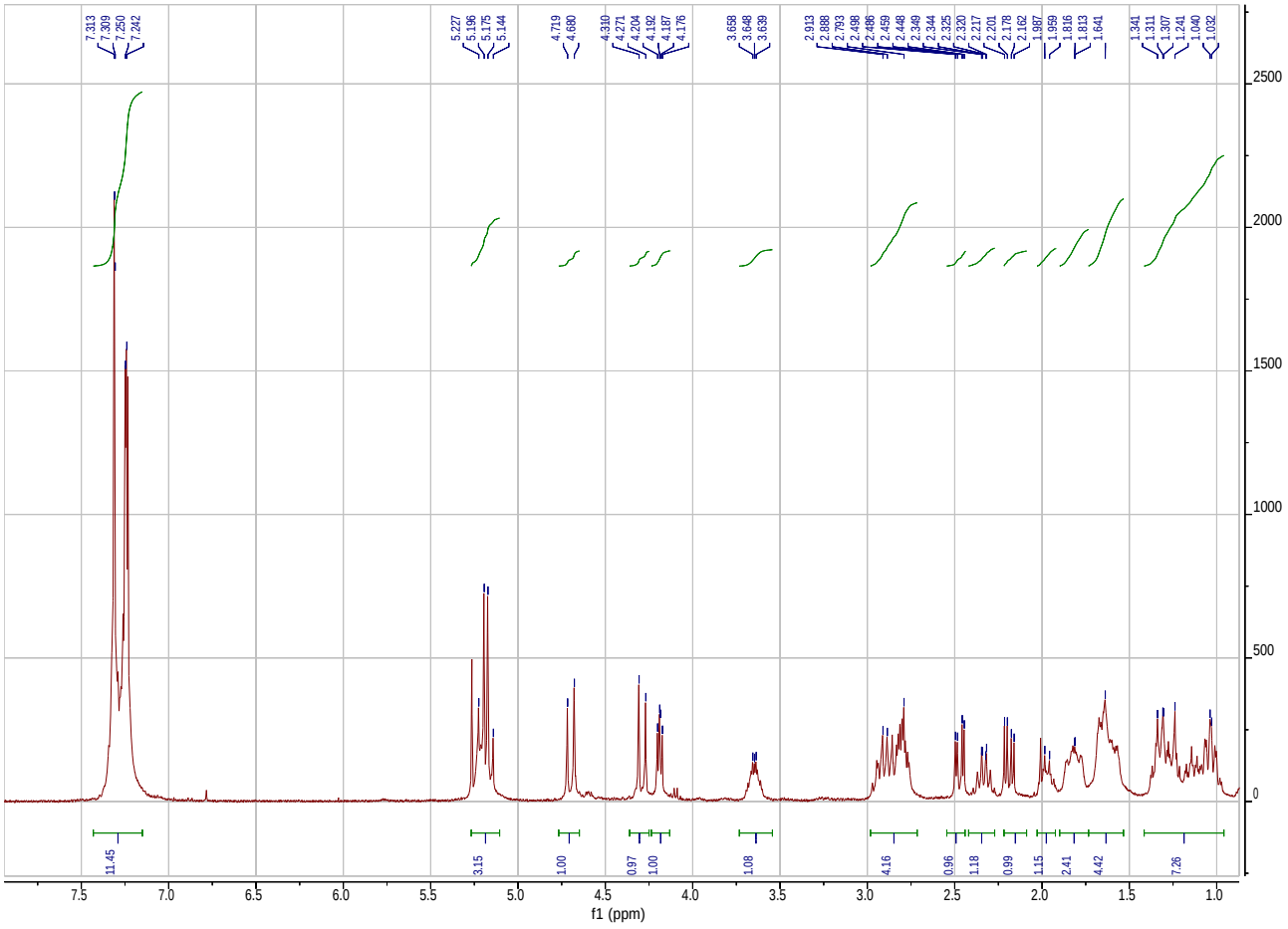
-L.G.S. - Laboratorio Grandi Strumenti - Display Report

Analysis Name	av fm2661.d	Acquisition Date	05/05/15 15:21:31	Operator	Walter Panzeri
Sample Name		Method	Copy of _01tmix_posneg lm.MS	Instrument	esquire3000plus
Comment	1 mg/ml dil 1:100 MeOH Richiedente: Frigerio				




BnOOC
O
N
N
O
H
N
O
O
Ph

7e


7.313
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7.250
7.242
5.227
5.196
5.175
5.144
4.719
4.680
4.310
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4.192
4.187
4.176
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3.639
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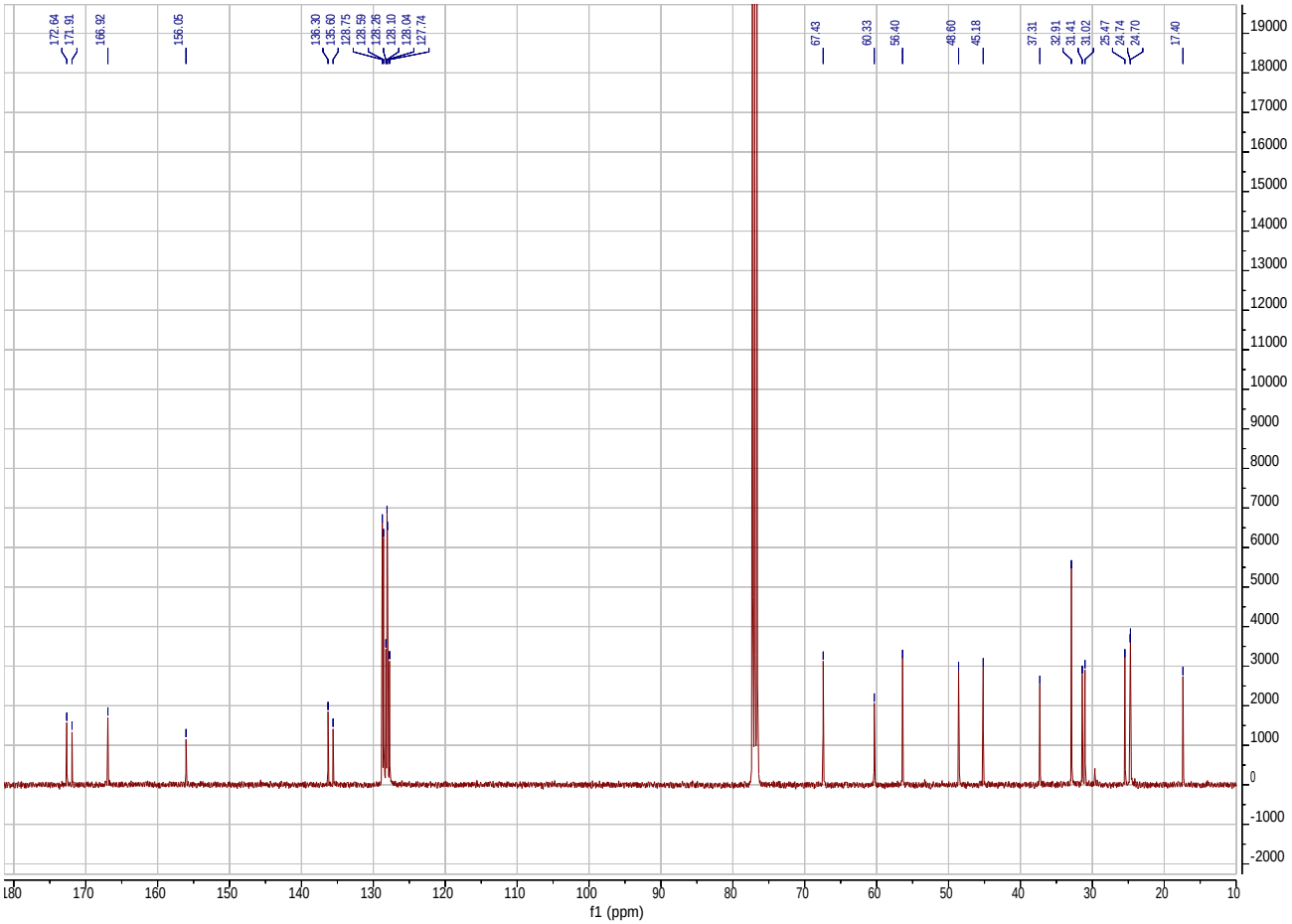
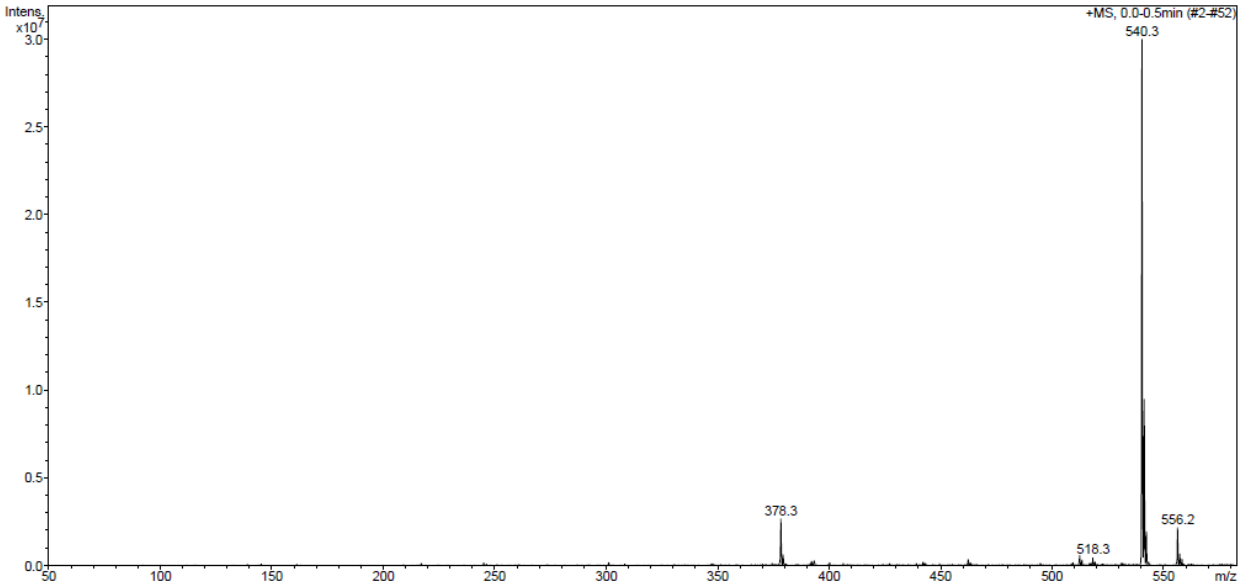
2.448
2.349
2.344
2.325
2.320
2.217
2.201
2.178
2.162
1.987
1.959
1.816
1.813
1.641
1.341
1.311
1.307
1.241
1.040
1.032
2500
2000
1500
1000
500
0
11.45
3.15
1.00
0.97
1.00
1.08
4.16
0.96
1.18
0.99
1.15
2.41
4.42
7.26
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
f1 (ppm)

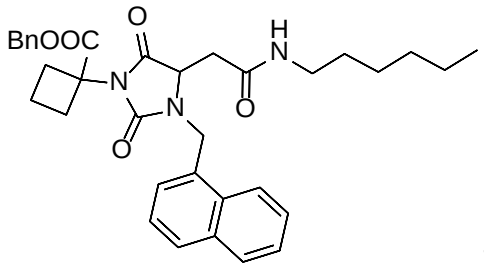


-L.G.S. - Laboratorio Grandi Strumenti - Display Report

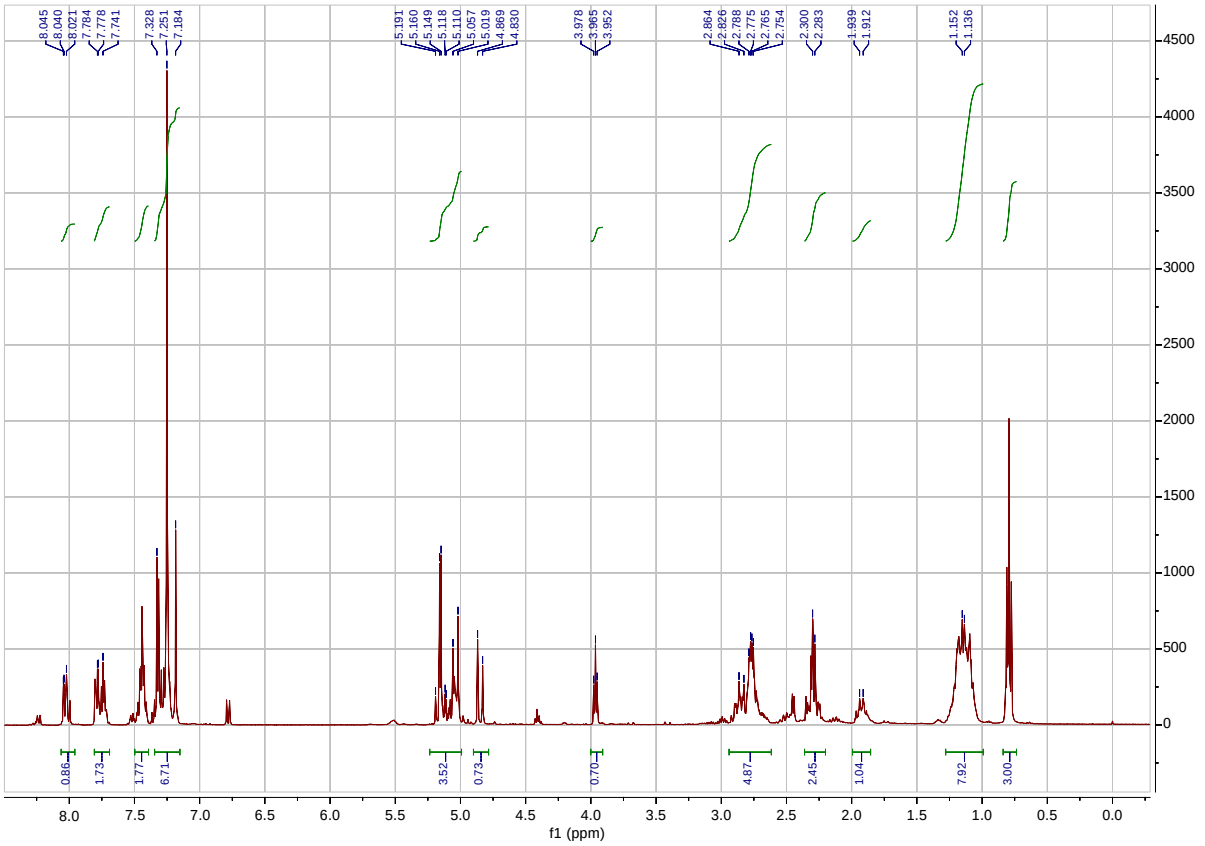
Analysis Name	av fm2676.d	Acquisition Date	06/08/15 14:06:00	Operator	Walter Panzeri
Sample Name		Method	Copy of _01tmix_posneg lm.MS	Instrument	esquire3000plus
Comment	1 mg/ml dil 1:100 MeOH Richiedente: Frigerio				

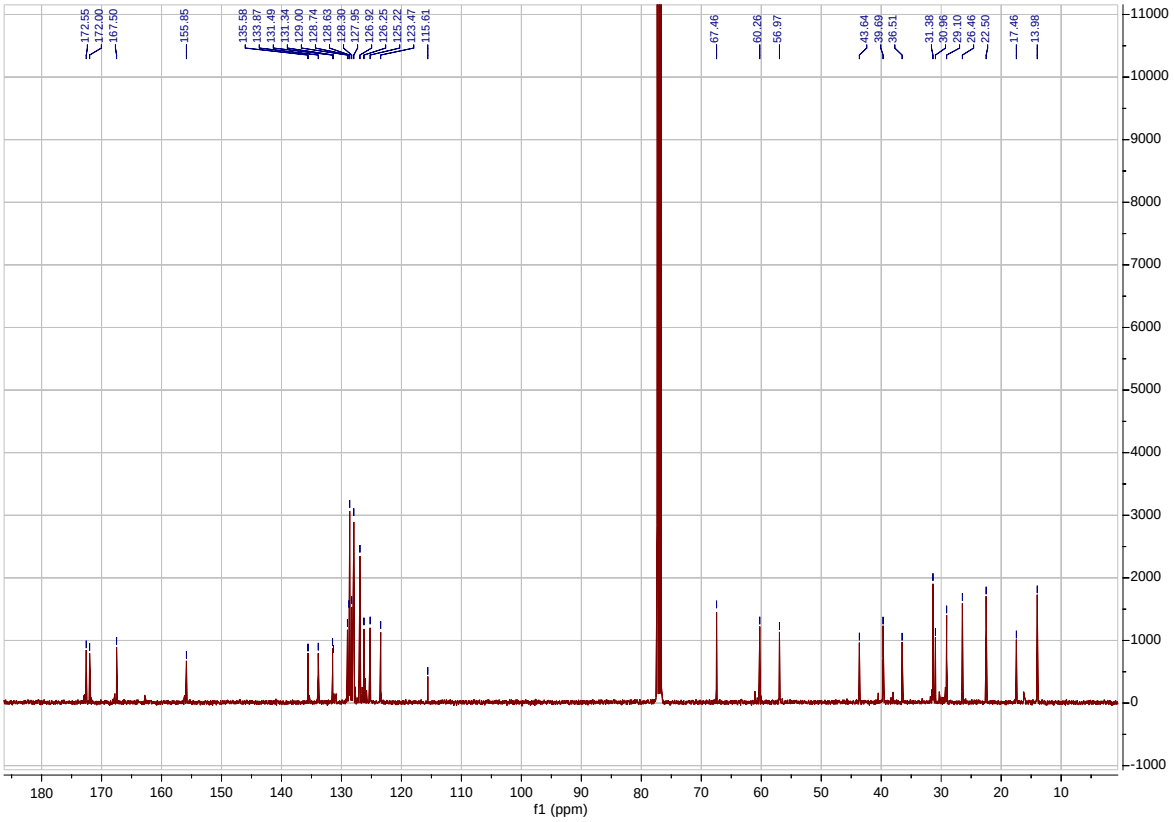


Bruker Daltonics DataAnalysis 3.1 printed: 06/08/15 14:07:36 Page 1 of 1


BnOOC
O
N
N
O
O
H
N

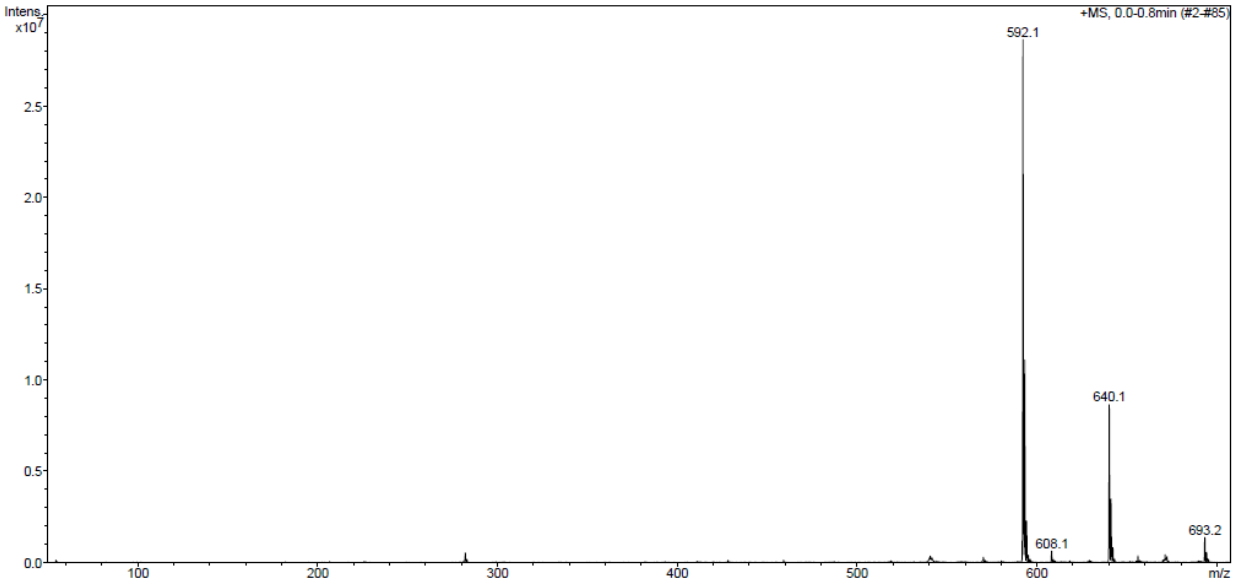
7f


8.045
8.040
8.021
7.784
7.778
7.741
7.328
7.251
7.184
5.191
5.160
5.149
5.118
5.110
5.057
5.019
4.869
4.830
3.978
3.965
3.952
2.864
2.826
2.788
2.775
2.765
2.754
2.300
2.283
1.939
1.912
1.152
1.136
0.86
1.73
1.77
6.71
3.52
0.73
0.70
4.87
2.45
1.04
7.92
3.00
f1 (ppm)

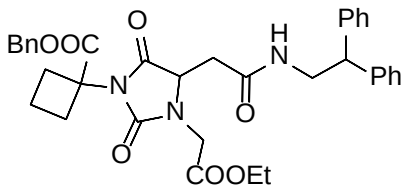


-L.G.S. - Laboratorio Grandi Strumenti - Display Report

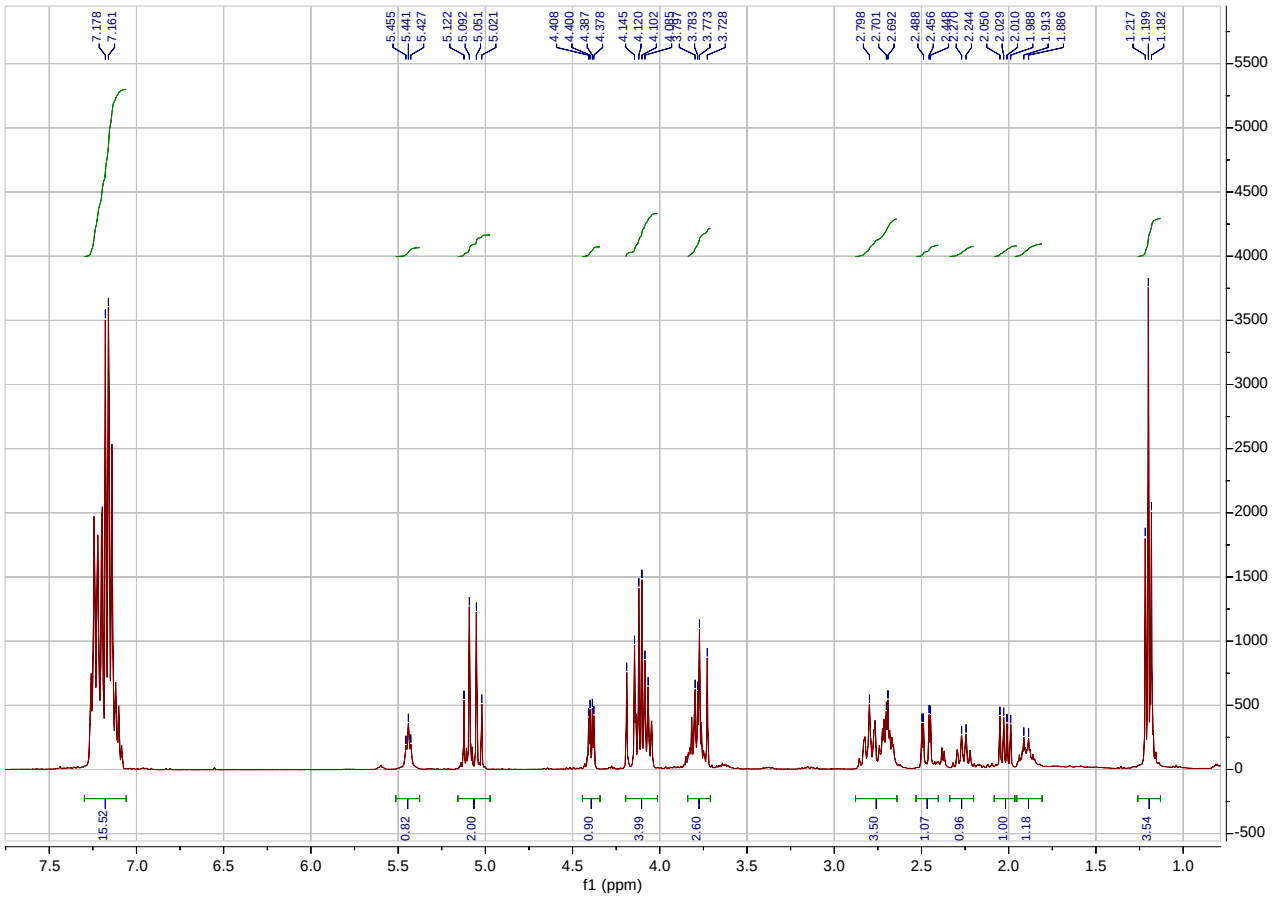
Analysis Name	av fm2722b.d	Acquisition Date	01/28/16 14:08:20	Operator	Walter Panzeri
Sample Name		Method	Copy of _01tmix_posneg lm.MS	Instrument	esquire3000plus
Comment	1 mg/ml dil 1:100 MeOH Richiedente: Frigerio				

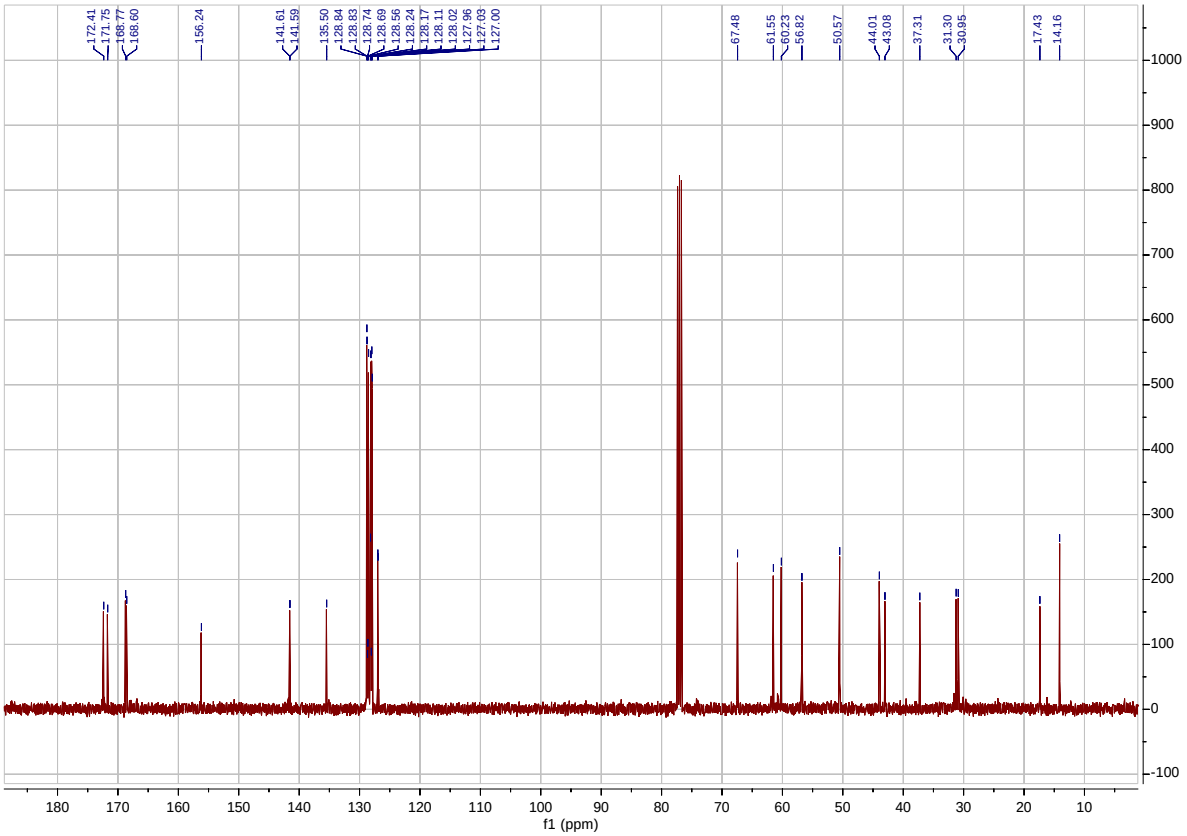


Bruker Daltonics DataAnalysis 3.1 printed: 01/28/16 14:12:13 Page 1 of 1


BnOOC
O
N
N
O
O
H
N
Ph
Ph
COOEt

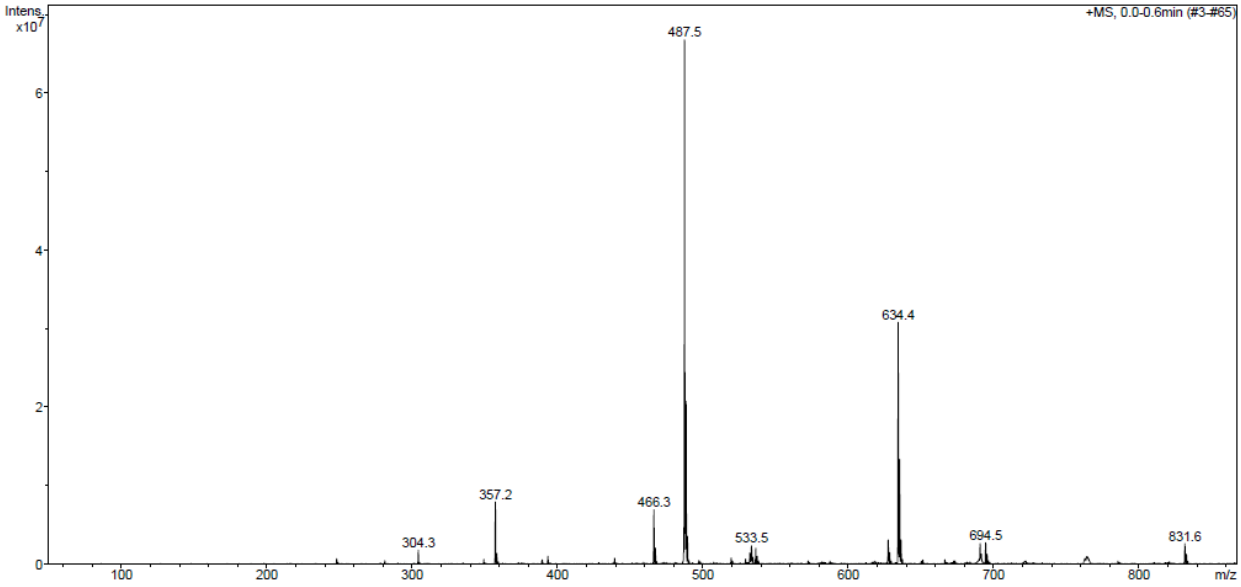
7g


7.178
7.161
5.455
5.441
5.427
5.122
5.092
5.051
5.021
4.408
4.400
4.387
4.378
4.145
4.120
4.102
3.783
3.773
3.728
2.798
2.701
2.692
2.488
2.456
2.448
2.244
2.050
2.029
2.010
1.988
1.913
1.886
1.217
1.199
1.182
15.52
0.82
2.00
0.90
3.99
2.60
3.50
1.07
0.96
1.00
1.18
3.54
f1 (ppm)



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

Analysis Name	av fm2746b.d	Acquisition Date	05/11/16 15:53:21	Operator	Walter Panzeri
Sample Name		Method	Copy of _01tmix_posneg lm.MS	Instrument	esquire3000plus
Comment	1 mg/ml dil 1:100 MeOH Richiedente: Frigerio				



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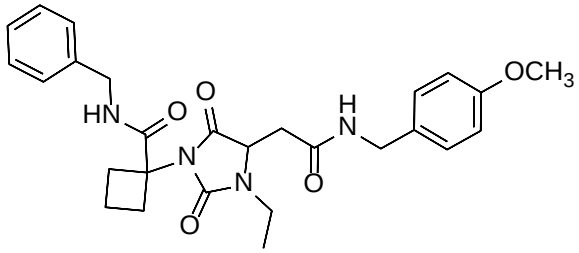
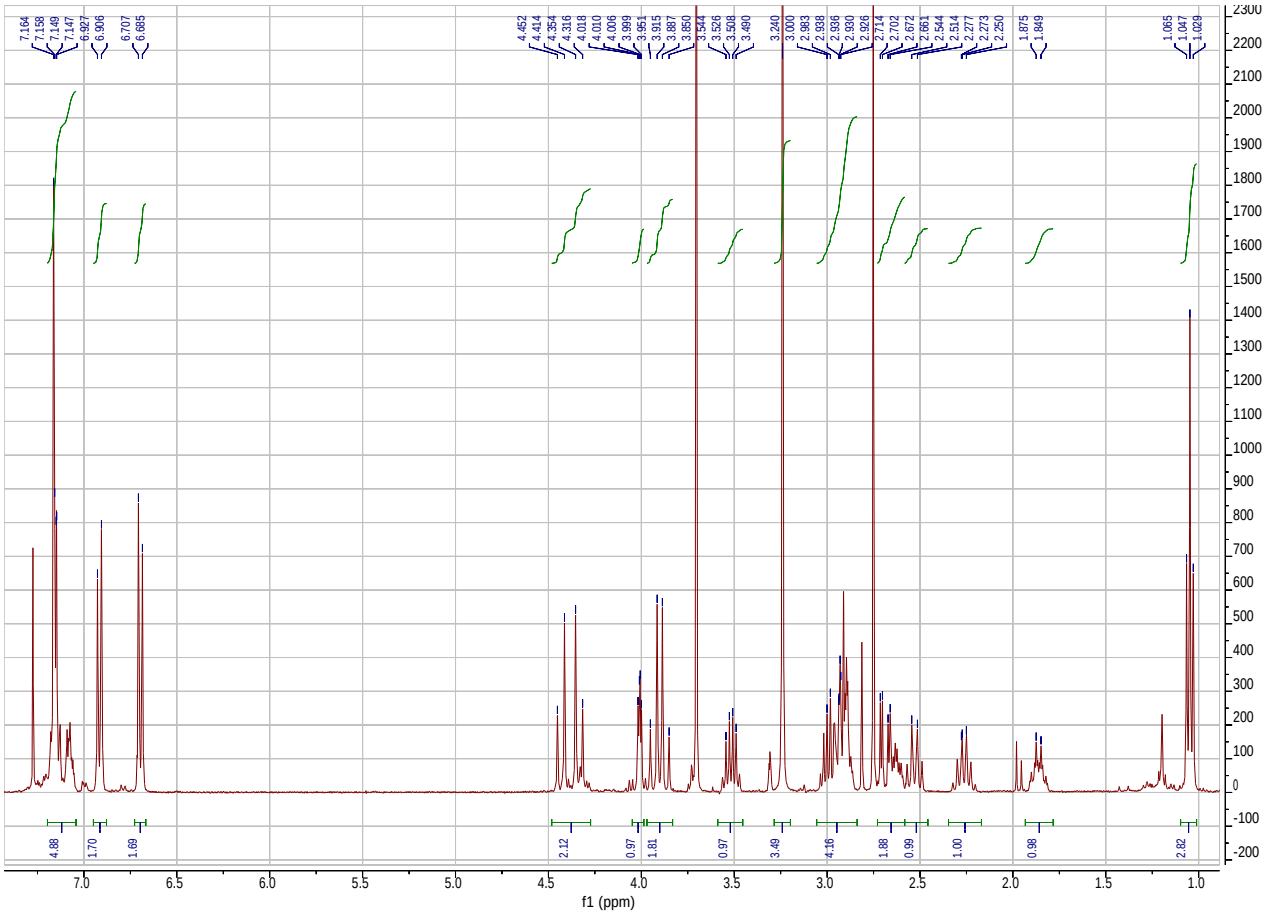
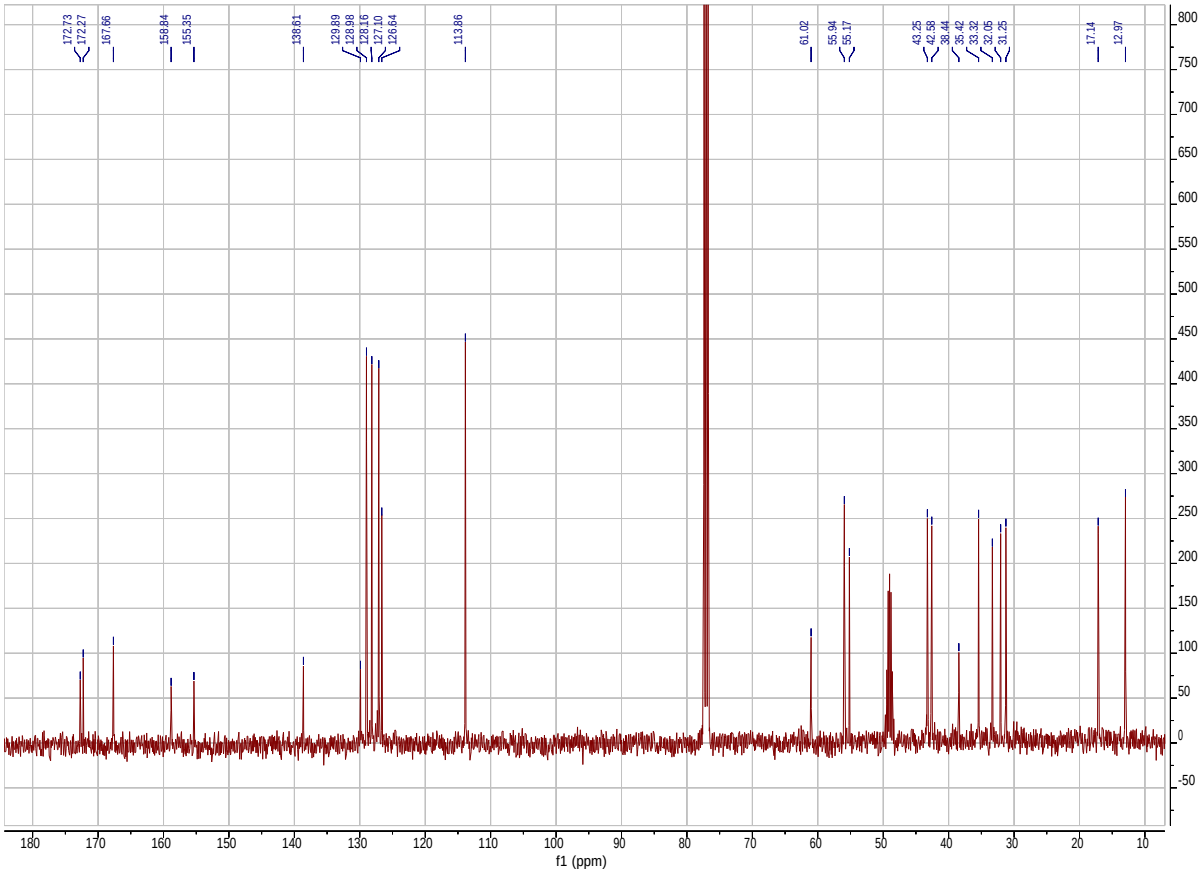

HN
O
O
N
N
O
O
H
N
O
OCH3

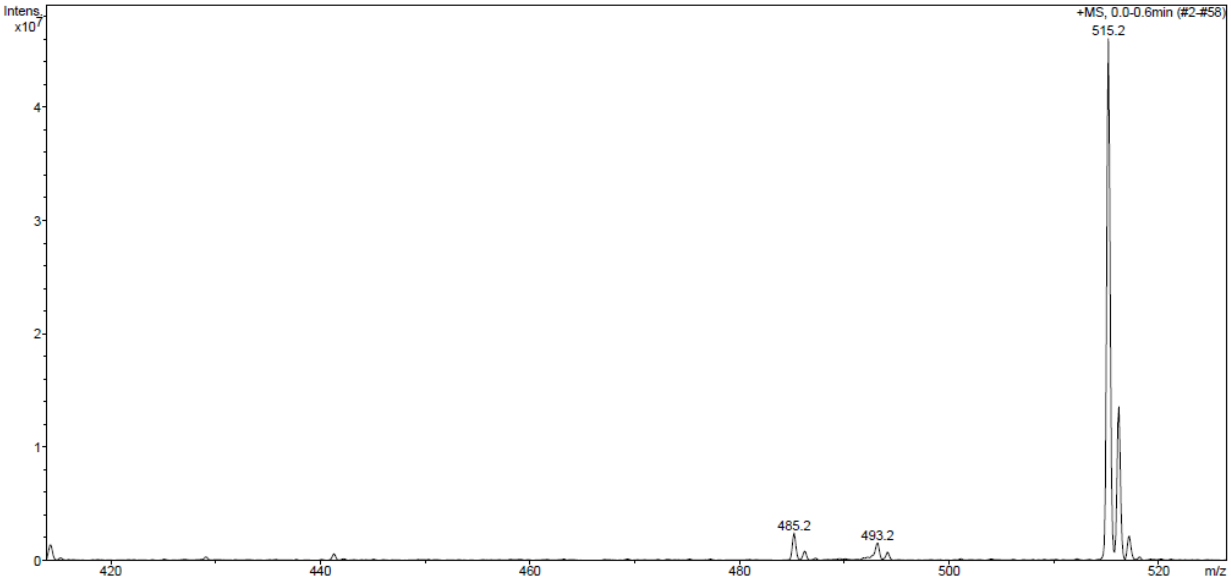
1a


7.164
7.158
7.149
7.147
6.927
6.906
6.707
6.685
4.452
4.414
4.354
4.316
4.018
4.010
4.006
3.999
3.951
3.915
3.887
3.850
3.544
3.526
3.508
3.490
3.240
3.000
2.983
2.938
2.936
2.930
2.926
2.714
2.702
2.672
2.861
2.544
2.514
2.277
2.273
2.250
1.875
1.849
1.065
1.047
1.029
4.88
1.70
1.69
2.12
0.97
1.81
0.97
3.49
4.16
1.88
0.99
1.00
0.98
2.82
f1 (ppm)



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

Analysis Name	av 2619.d	Acquisition Date	07/25/14 16:55:51	Operator	Administrator
Sample Name		Method	Copy of _01esquirew t.MS	Instrument	esquire3000plus
Comment	1 mg/ml dil1:100 MeOH Richiedente: Volonterio				



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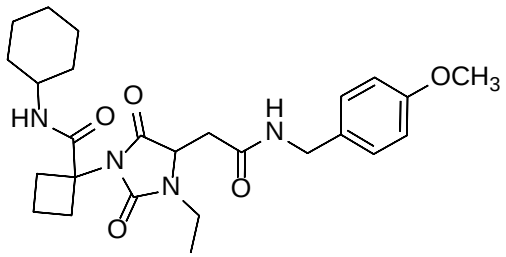
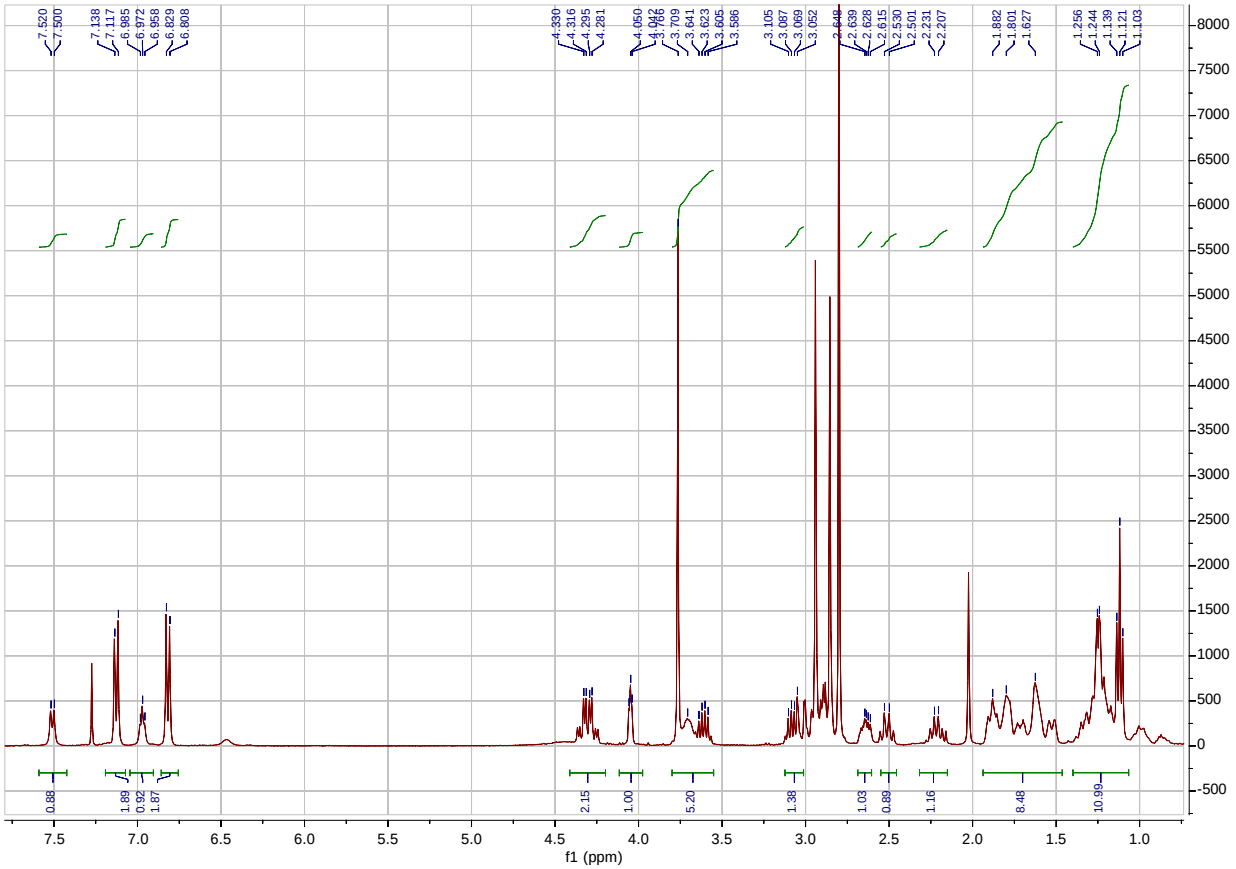
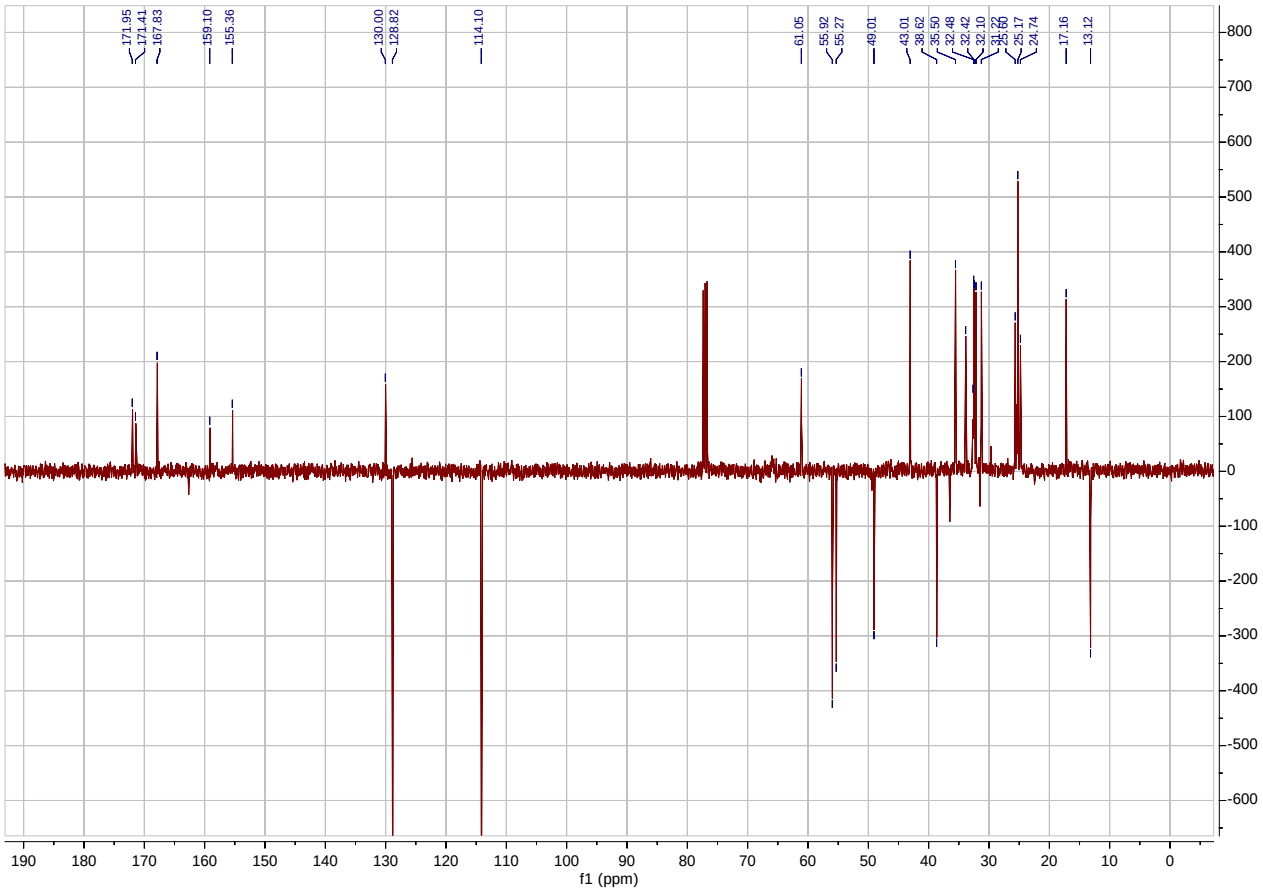
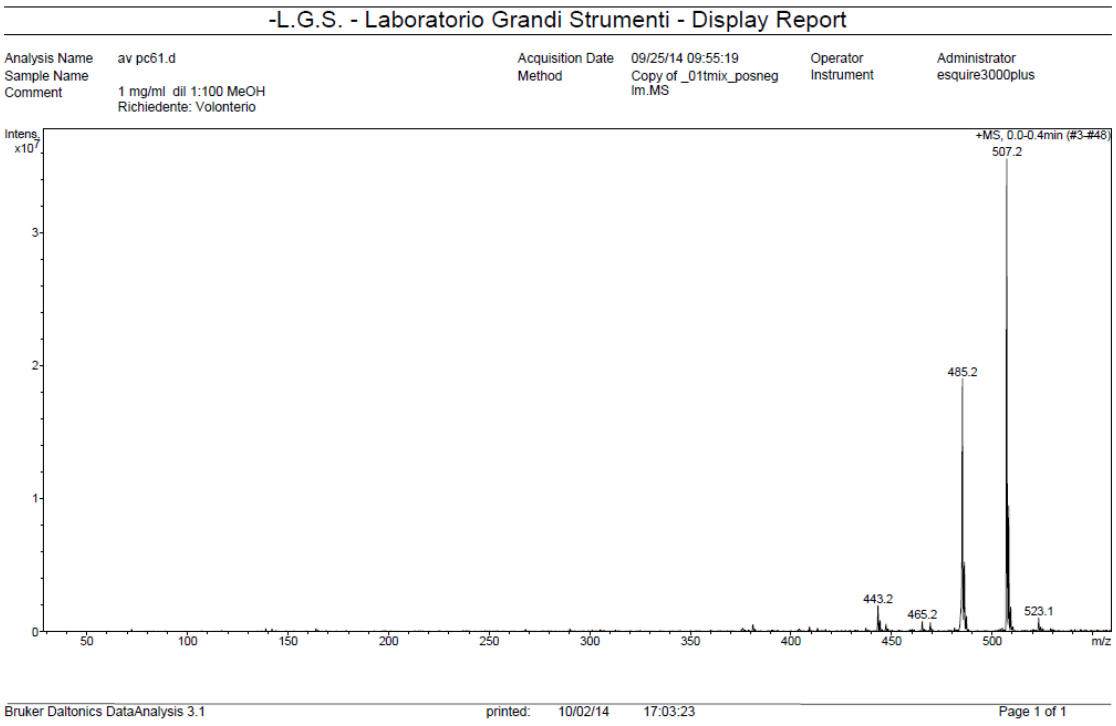
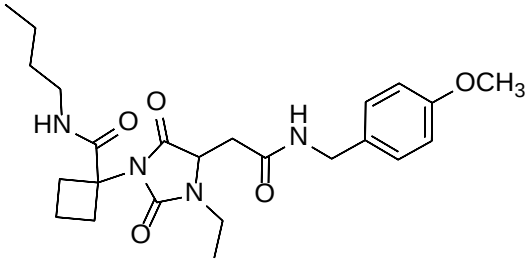

HN
O
O
N
N
O
O
H
N
OCH3

1b

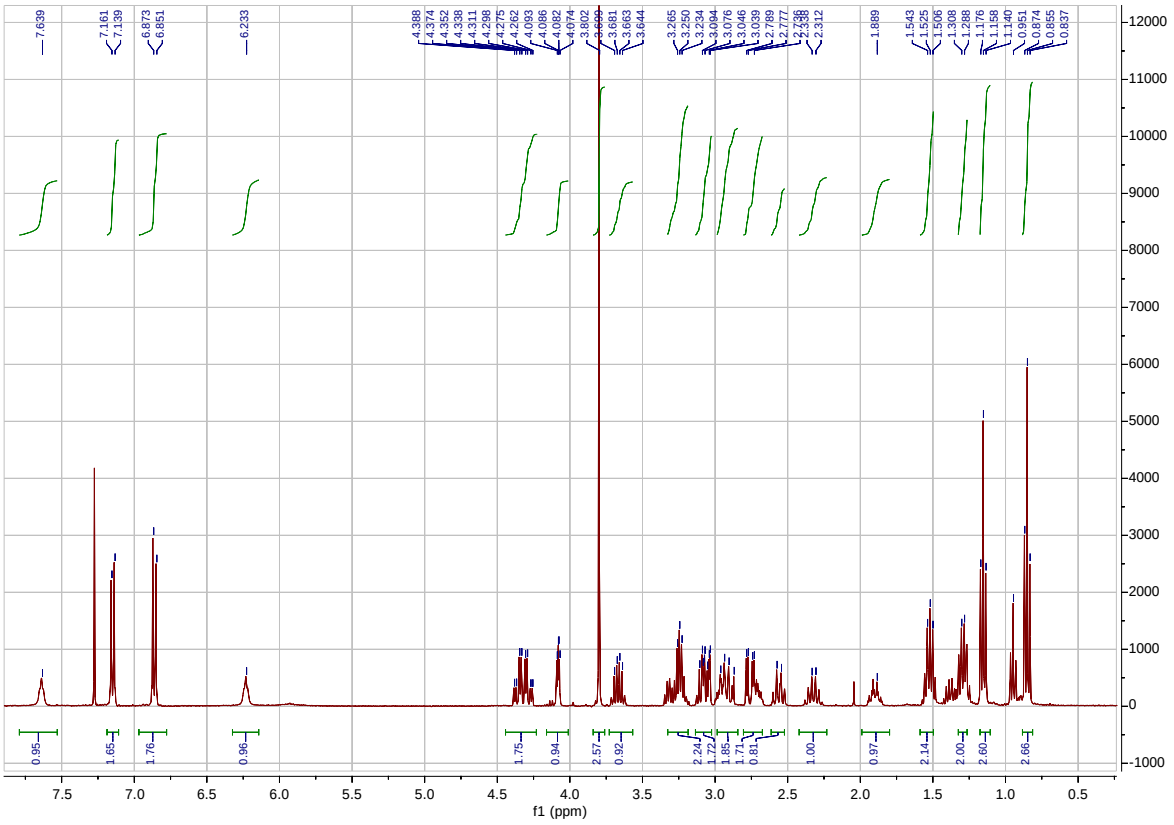

7.520
7.500
7.138
7.117
6.985
6.972
6.958
6.829
6.808
4.330
4.316
4.295
4.281
4.050
4.042
3.766
3.709
3.641
3.623
3.605
3.586
3.105
3.087
3.069
3.052
2.648
2.639
2.628
2.615
2.530
2.501
2.231
2.207
1.882
1.801
1.627
1.256
1.244
1.139
1.121
1.103
0.88
1.89
0.92
1.87
2.15
1.00
5.20
1.38
1.03
0.89
1.16
8.48
10.99
f1 (ppm)

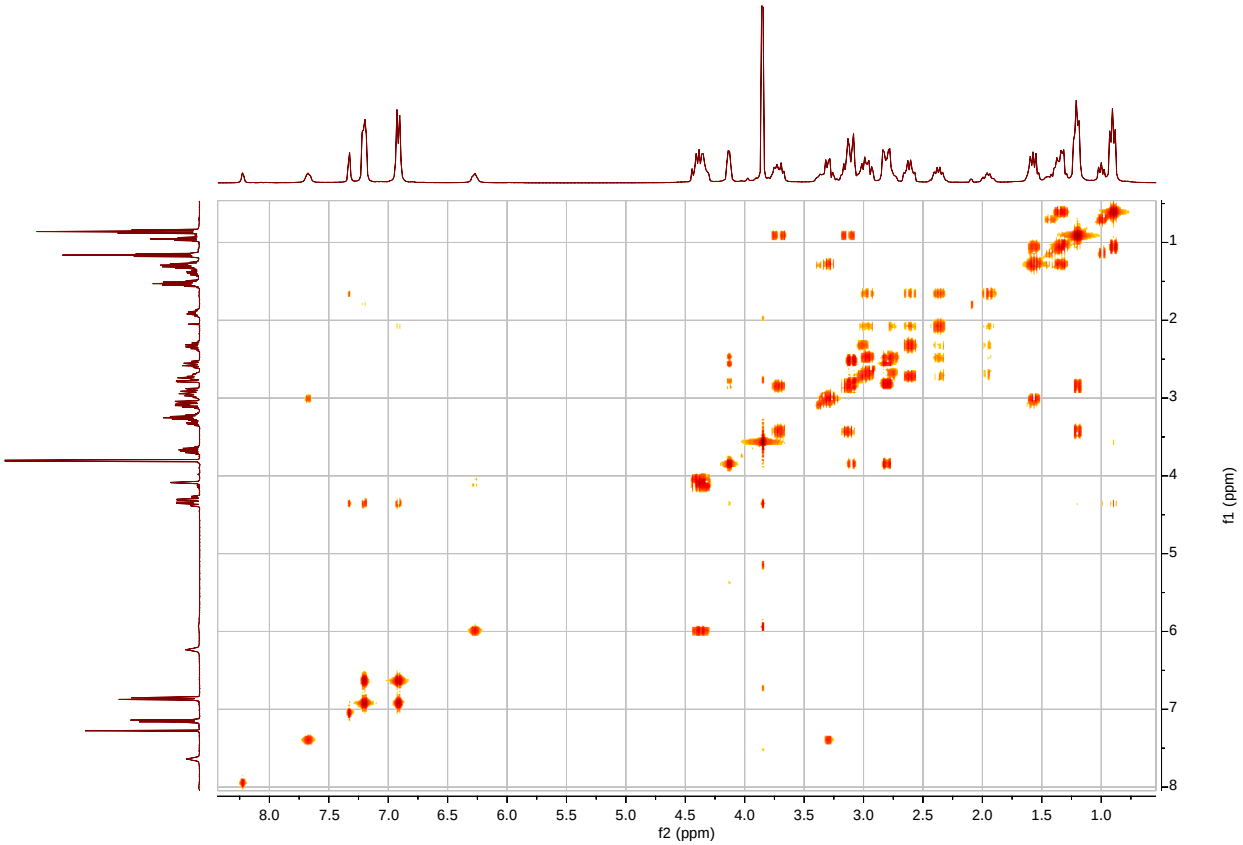

171.95
171.41
167.83
159.10
155.36
130.00
128.82
114.10
61.05
55.92
55.27
49.01
43.01
38.62
35.50
32.48
32.42
32.10
31.22
25.66
25.17
24.74
17.16
13.12
f1 (ppm)

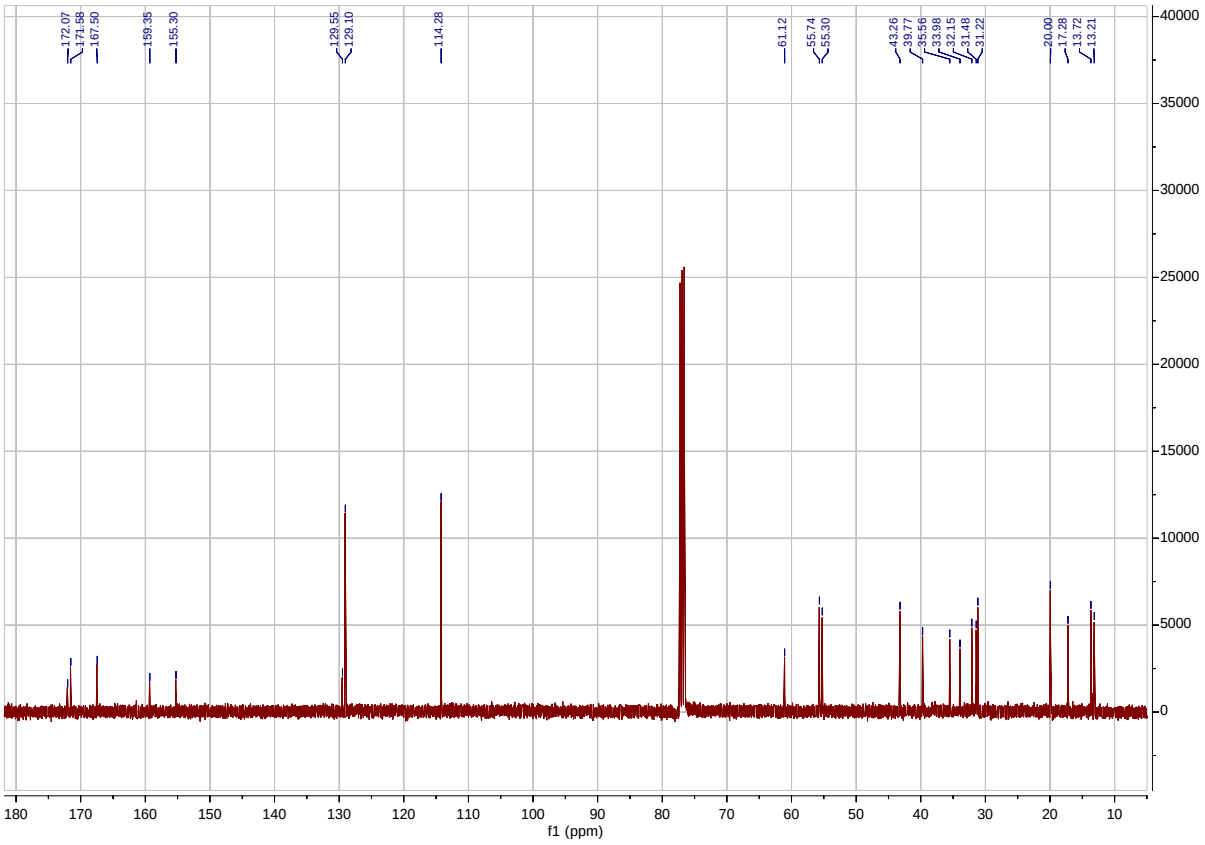

-L.G.S. - Laboratorio Grandi Strumenti - Display Report
Analysis Name av pc61.d
Sample Name
Comment 1 mg/ml dil 1:100 MeOH
Richiedente: Volonterio
Acquisition Date 09/25/14 09:55:19
Method Copy of _01tmix_posneg lm.MS
Operator
Instrument
Administrator
esquire3000plus
Intens. x10^7
+MS, 0.0-0.4min (#3-#48)
507.2
485.2
443.2
465.2
523.1
m/z
Bruker Daltonics DataAnalysis 3.1
printed: 10/02/14 17:03:23
Page 1 of 1



1c

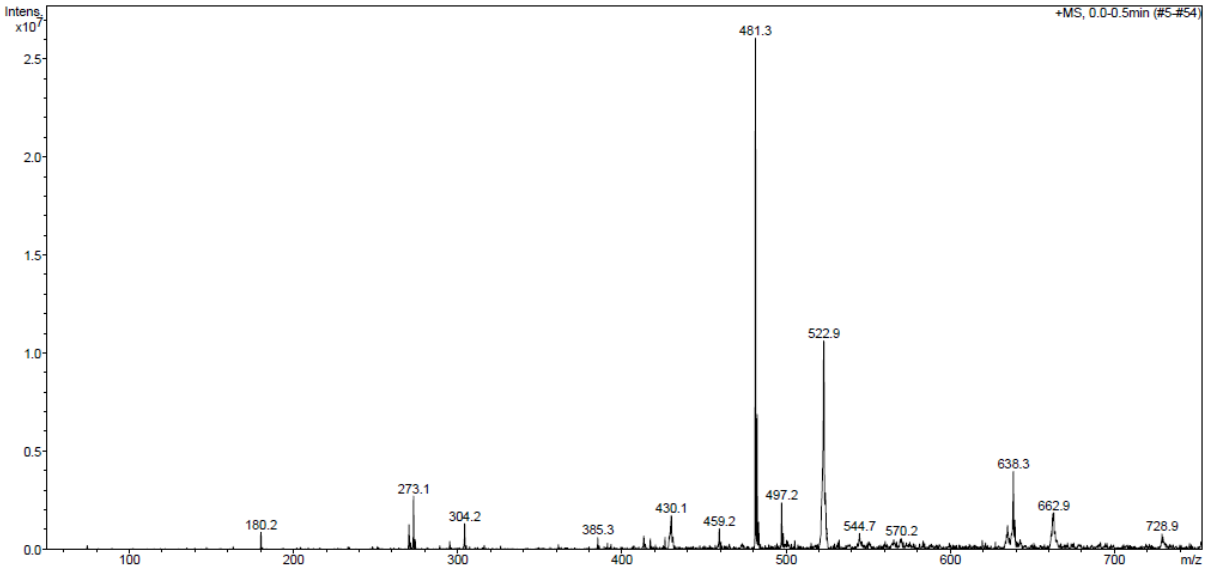



f2 (ppm)
f1 (ppm)


172.07
171.58
167.50
159.35
155.30
129.55
129.10
114.28
61.12
55.74
55.30
43.26
39.77
35.56
33.98
32.15
31.48
31.22
20.00
17.28
13.72
13.21
f1 (ppm)

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

Analysis Name	av pc69.d	Acquisition Date	04/28/15 13:55:25	Operator	Walter Panzeri
Sample Name		Method	Copy of _01tmix_posneg lm.MS	Instrument	esquire3000plus
Comment	1 mg/ml dil 1:100 MeOH Richiedente: Volonterio				



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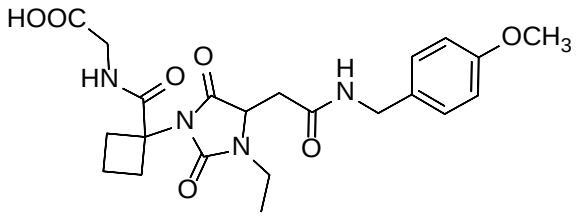
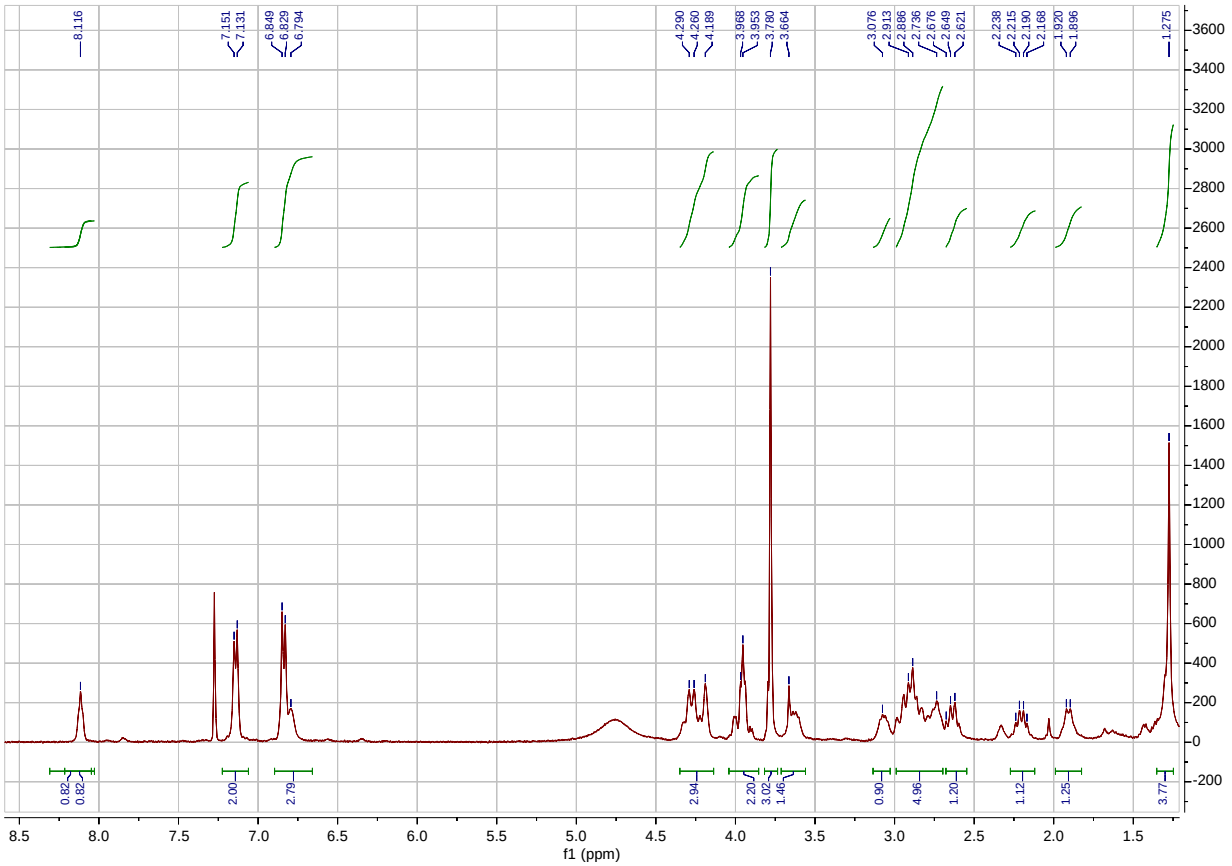
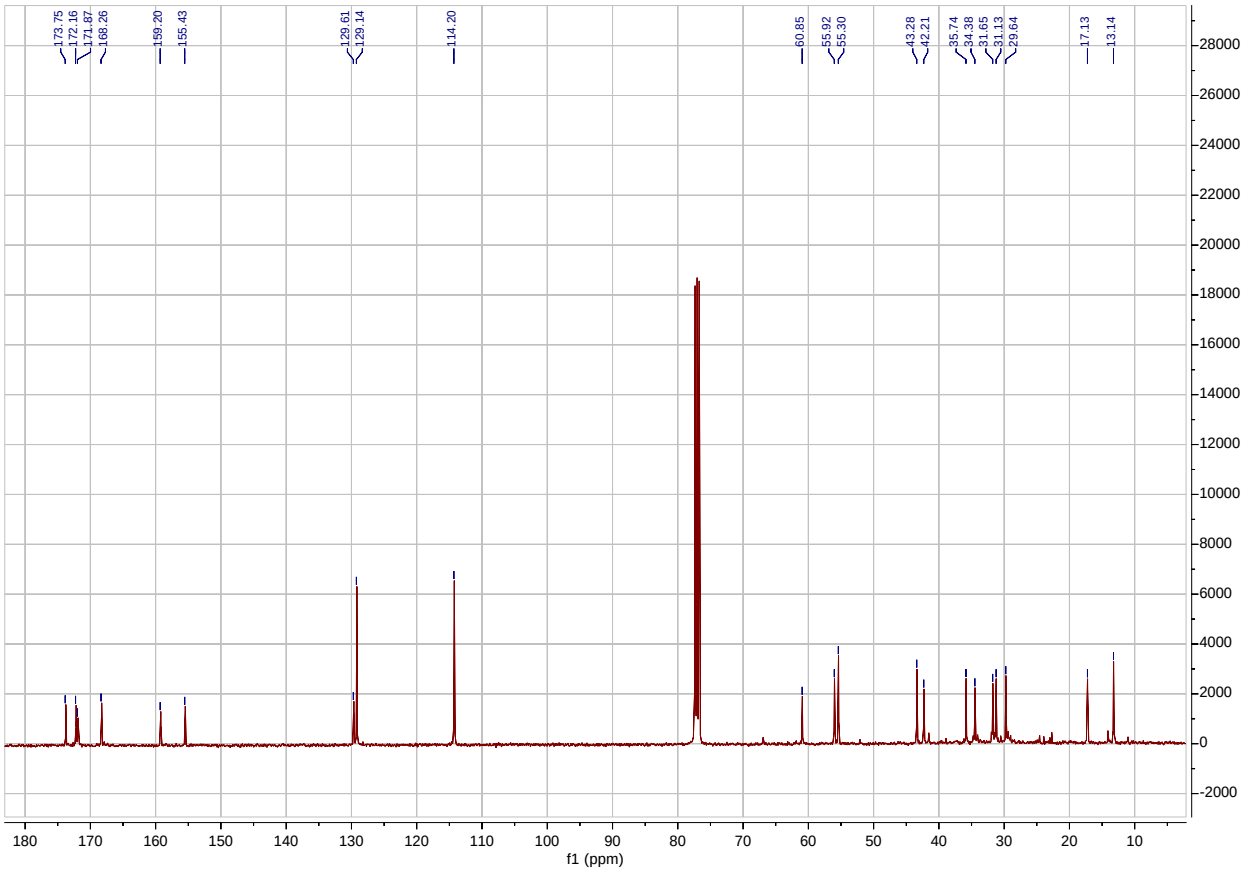

HOOC
HN
O
O
N
N
O
H
N
O
OCH3

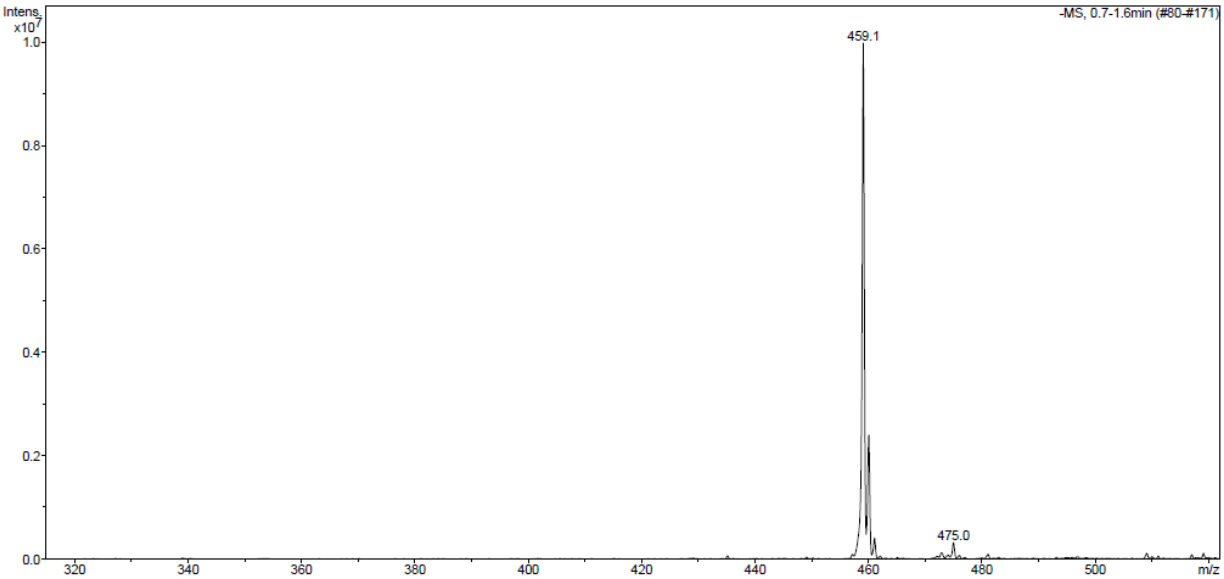
1d


8.116
7.151
7.131
6.849
6.829
6.794
4.290
4.260
4.189
3.968
3.953
3.780
3.664
3.076
2.913
2.886
2.736
2.676
2.649
2.621
2.238
2.215
2.190
2.168
1.920
1.896
1.275
0.82
0.82
2.00
2.79
2.94
2.20
3.02
1.46
0.90
4.96
1.20
1.12
1.25
3.77
f1 (ppm)



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

Analysis Name	av pc71.d	Acquisition Date	04/28/15 13:47:04	Operator	Walter Panzeri
Sample Name		Method	Copy of _01tmix_posneg lm.MS	Instrument	esquire3000plus
Comment	1 mg/ml dil 1:100 MeOH Richiedente: Volonterio				



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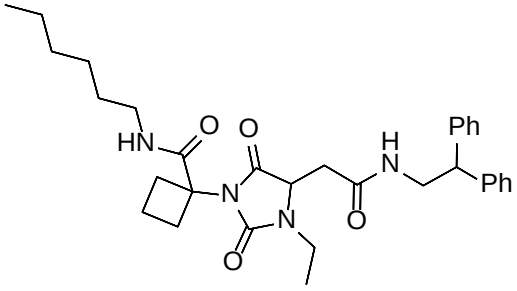
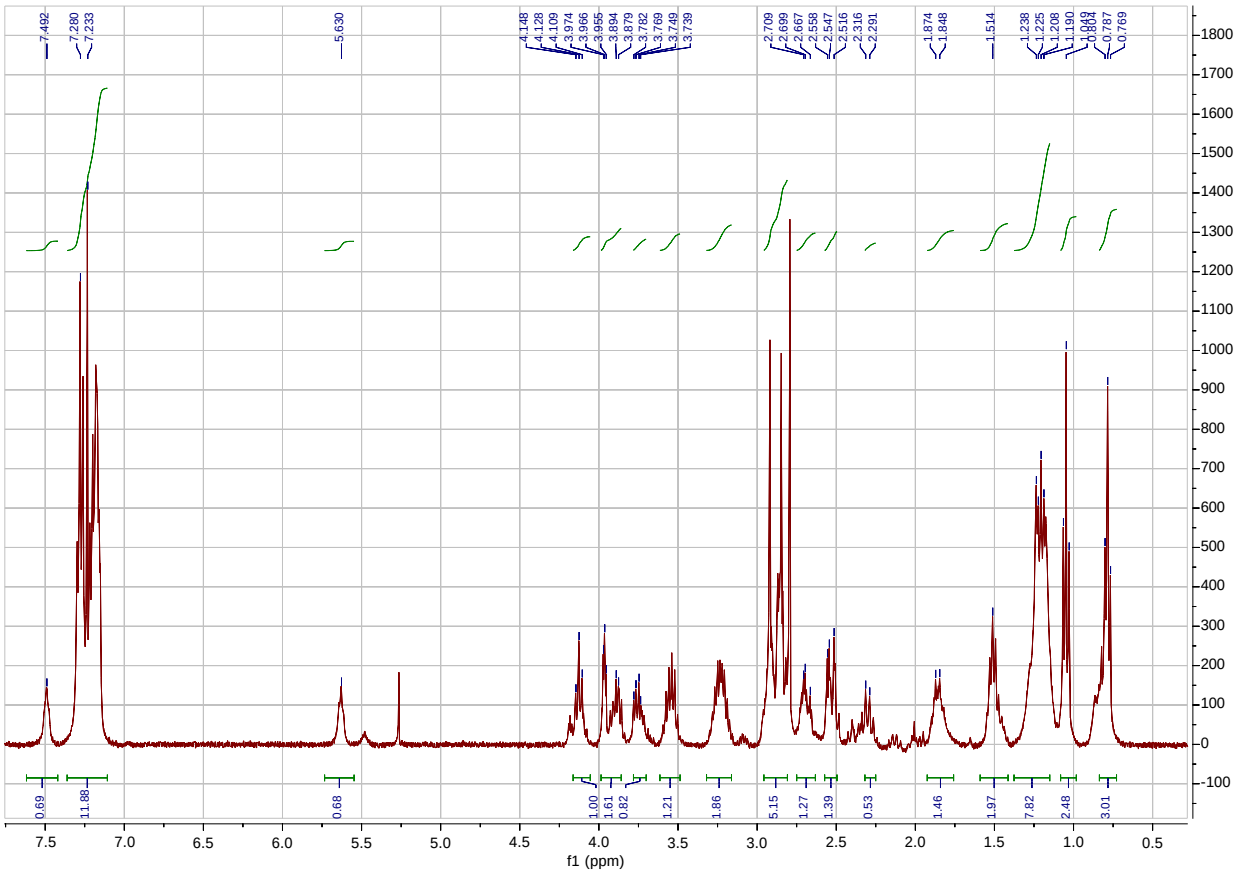
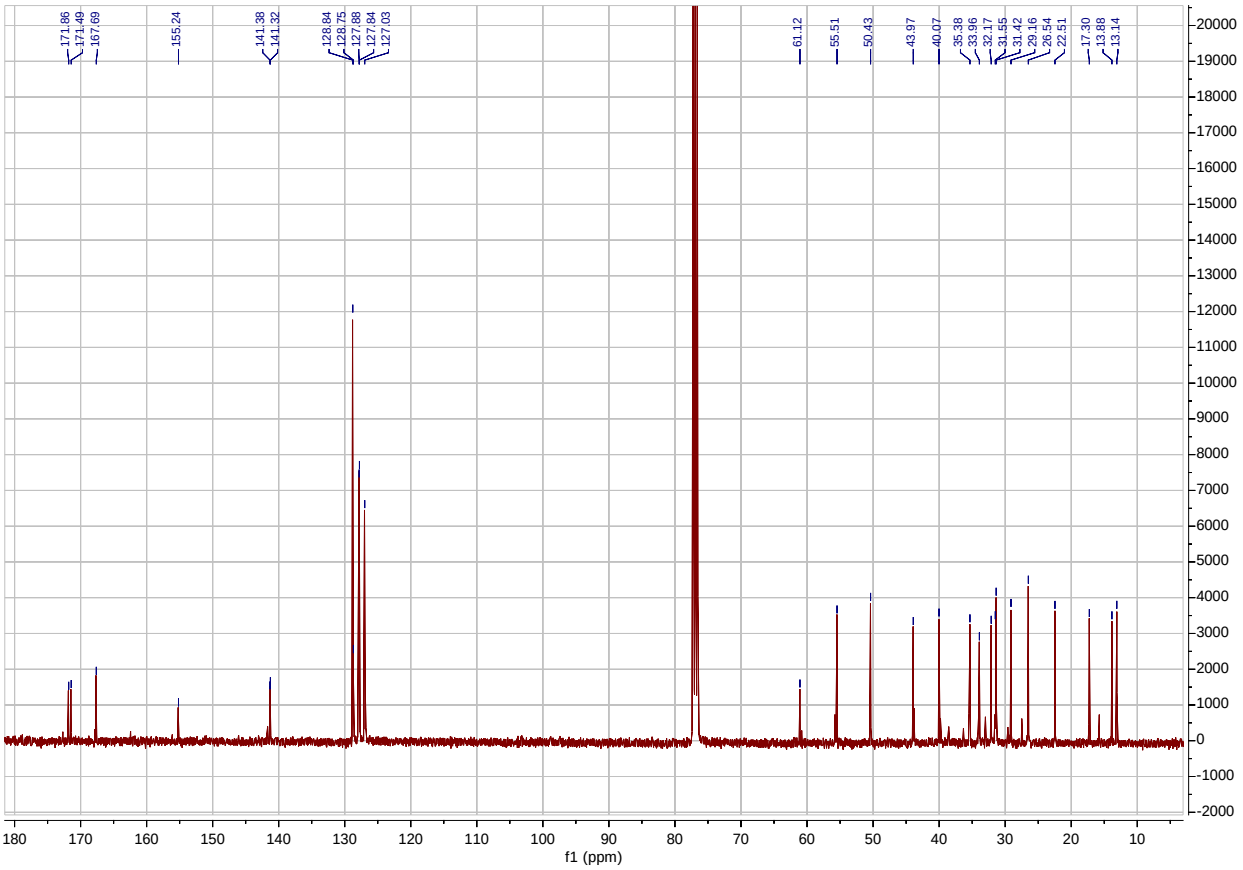

HN
O
O
N
N
O
O
H
N
Ph
Ph

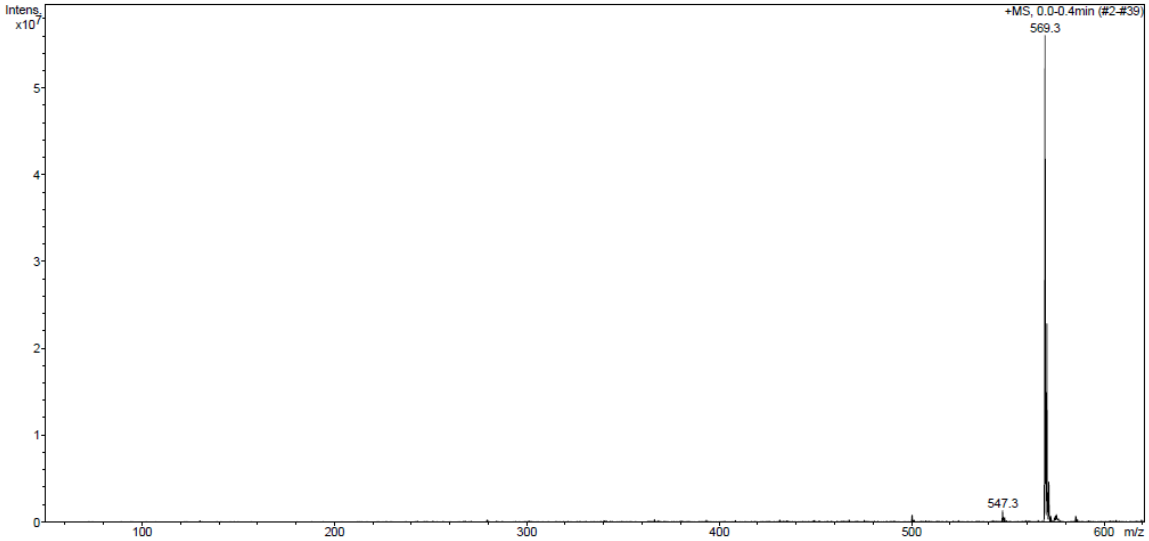
1e


7.492
7.280
7.233
5.630
4.148
4.128
4.109
3.974
3.966
3.955
3.894
3.879
3.782
3.769
3.749
3.739
2.709
2.699
2.667
2.558
2.547
2.516
2.316
2.291
1.874
1.848
1.514
1.238
1.225
1.208
1.190
0.804
0.787
0.769
0.69
11.88
0.68
1.00
1.61
0.82
1.21
1.86
5.15
1.27
1.39
0.53
1.46
1.97
7.82
2.48
3.01
f1 (ppm)



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

Analysis Name	av fm2653.d	Acquisition Date	04/16/15 15:34:04	Operator	Walter Panzeri
Sample Name		Method	Copy of _01tmix_posneg lm.MS	Instrument	esquire3000plus
Comment	1 mg/ml dil 1:100 MeOH Richiedente: Frigerio				



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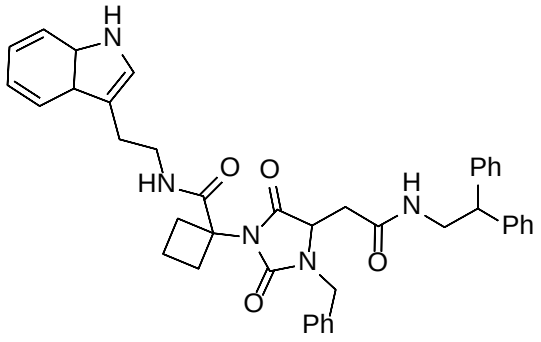
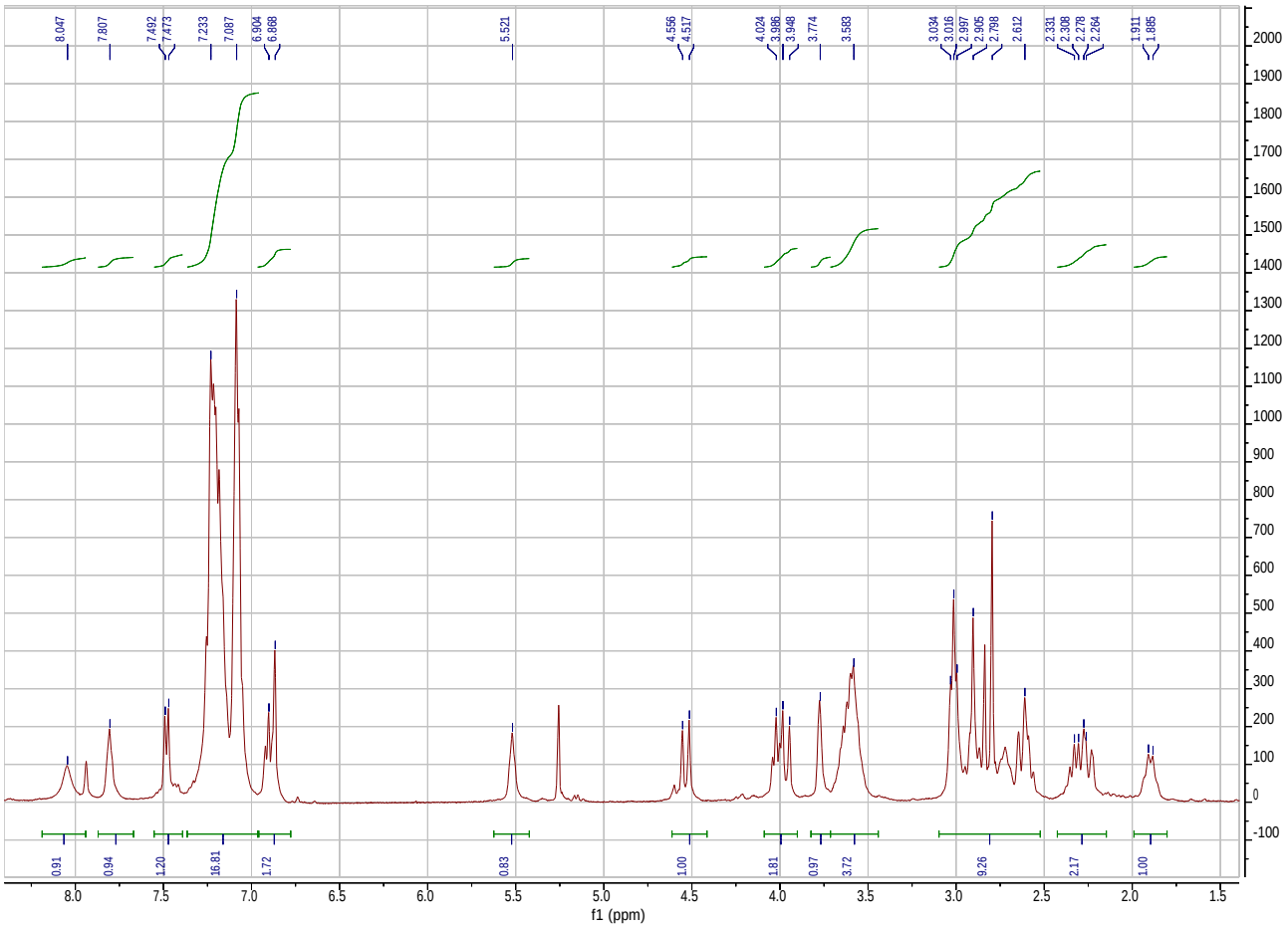
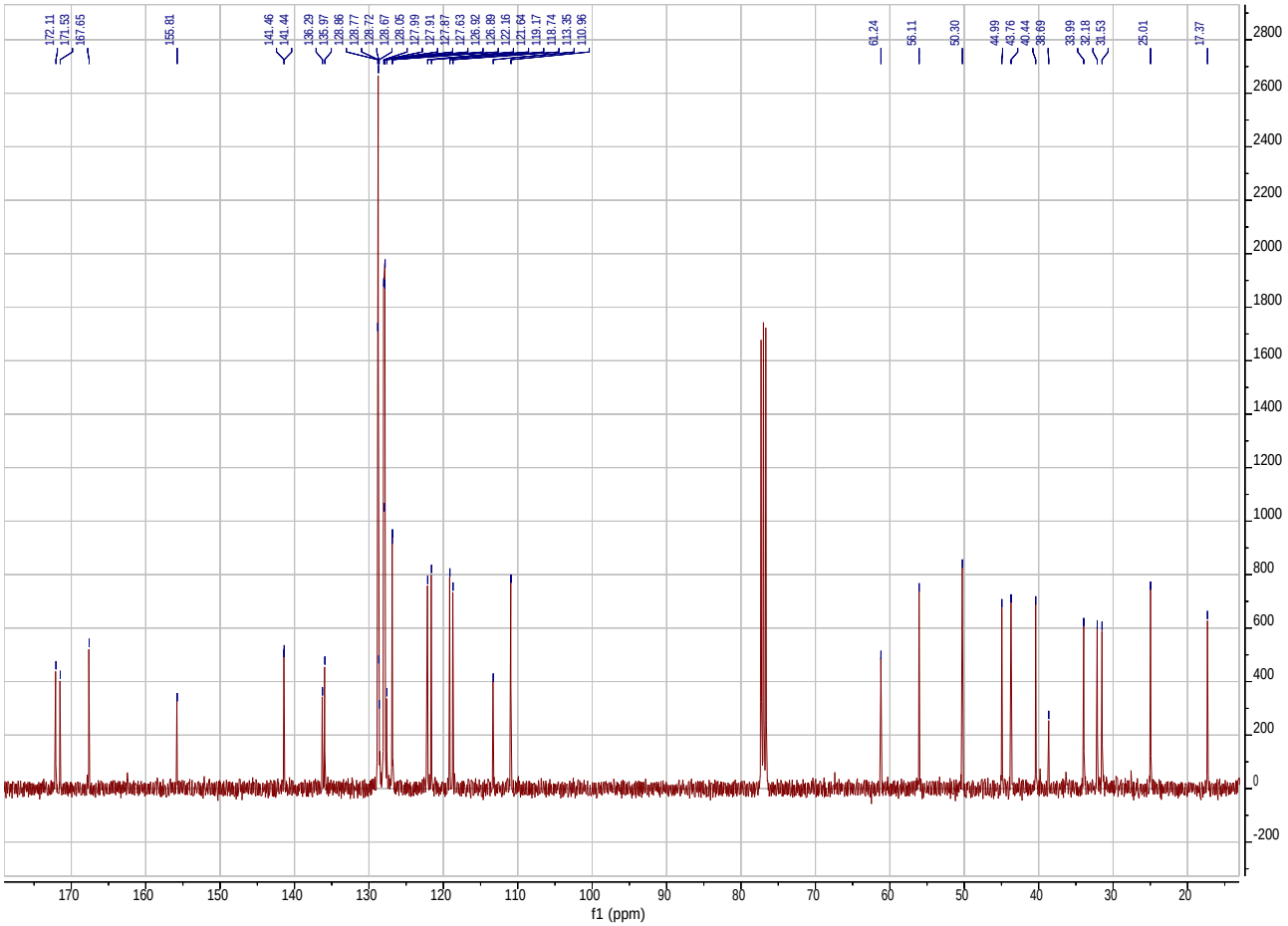
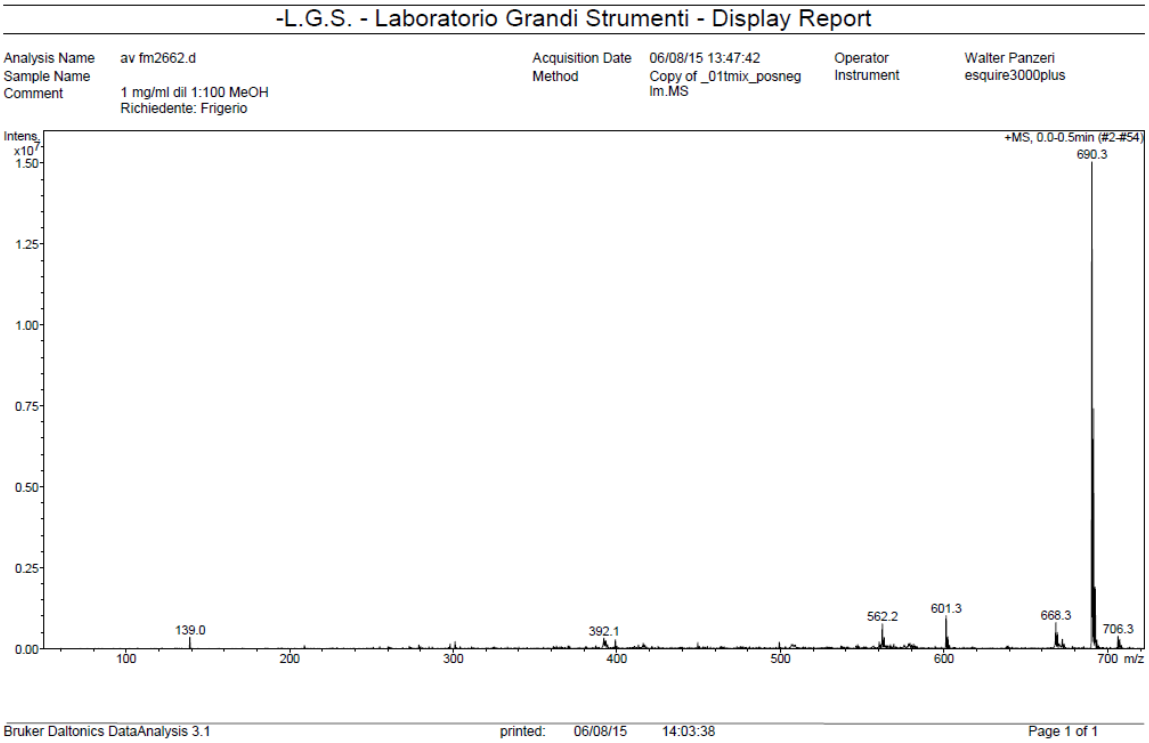
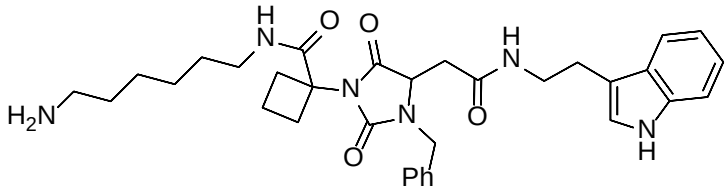


1f

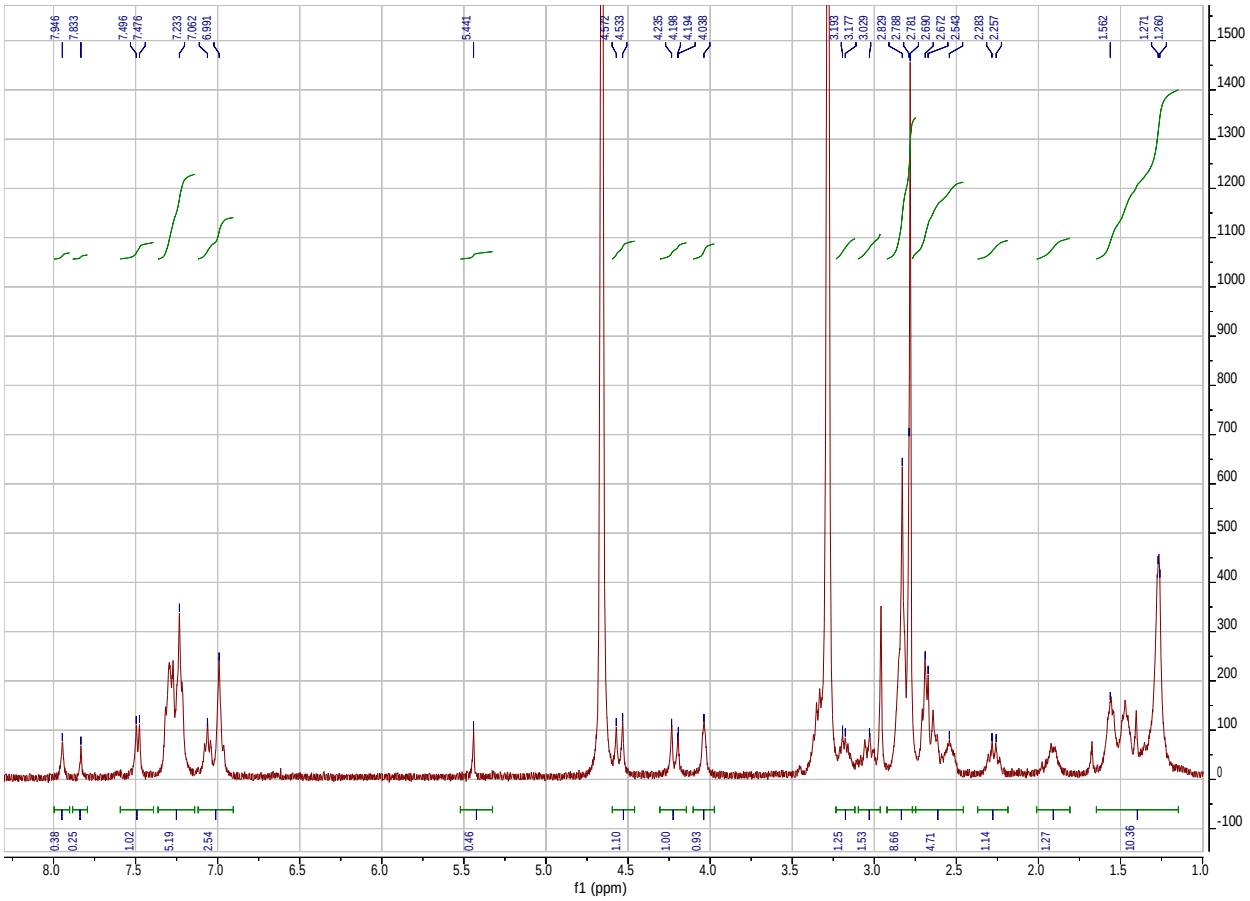

8.047
7.807
7.492
7.473
7.233
7.087
6.904
6.868
5.521
4.556
4.517
4.024
3.986
3.948
3.774
3.583
3.034
3.016
2.997
2.905
2.798
2.612
2.331
2.308
2.278
2.264
1.911
1.885
0.91
0.94
1.20
16.81
1.72
0.83
1.00
1.81
0.97
3.72
9.26
2.17
1.00
f1 (ppm)

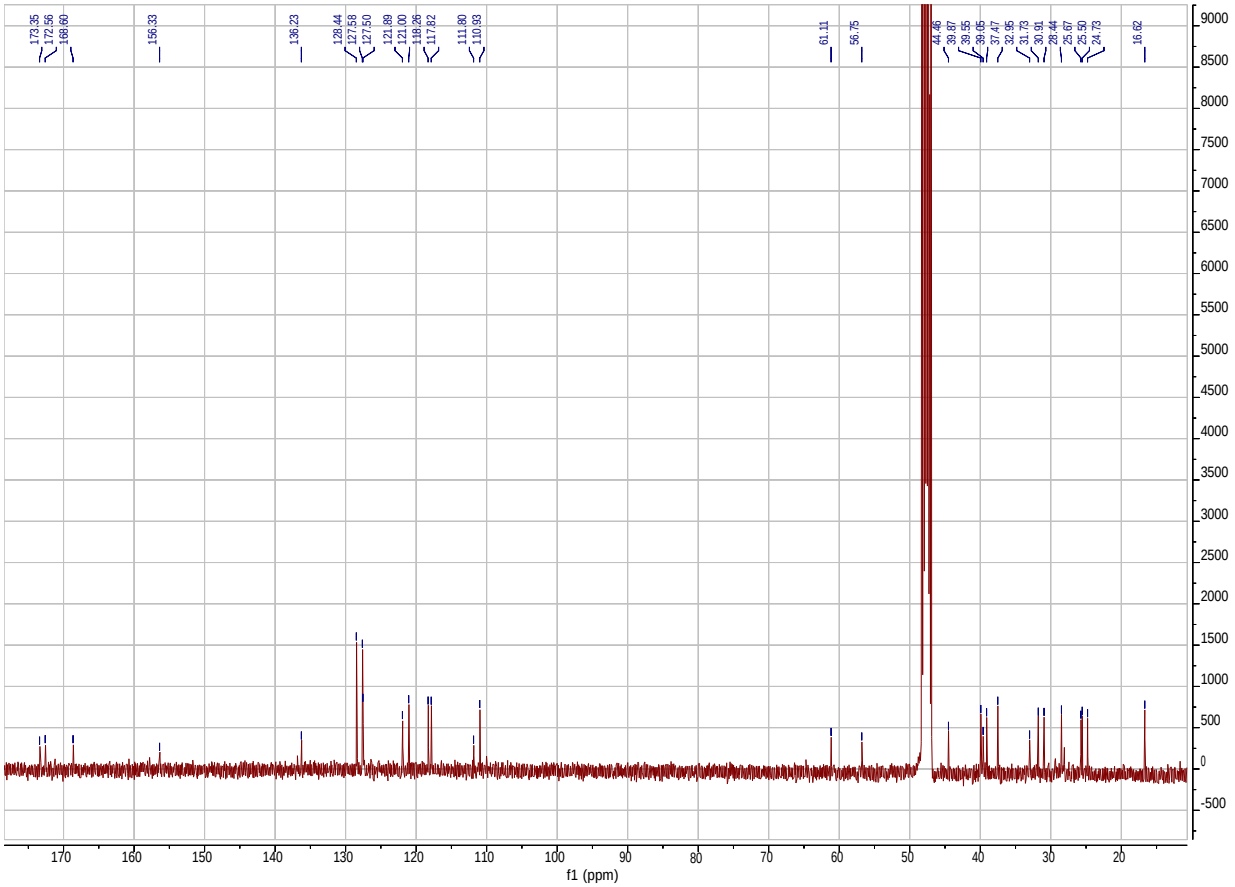

172.11
171.53
167.65
155.81
141.46
141.44
136.29
135.97
128.86
128.77
128.72
128.67
128.05
127.99
127.91
127.87
127.63
126.92
126.89
122.16
121.64
119.17
118.74
113.35
110.96
61.24
56.11
50.30
44.99
43.76
40.44
38.69
33.99
32.18
31.53
25.01
17.37
f1 (ppm)


-L.G.S. - Laboratorio Grandi Strumenti - Display Report
Analysis Name av fm2662.d
Sample Name
Comment 1 mg/ml dil 1:100 MeOH
Richiedente: Frigerio
Acquisition Date 06/08/15 13:47:42
Method Copy of _01tmix_posneg lm.MS
Operator Walter Panzeri
Instrument esquire3000plus
Intens. x10^7
+MS, 0.0-0.5min (#2-#54)
690.3
139.0
392.1
562.2
601.3
668.3
706.3
m/z
Bruker Daltonics DataAnalysis 3.1
printed: 06/08/15 14:03:38
Page 1 of 1



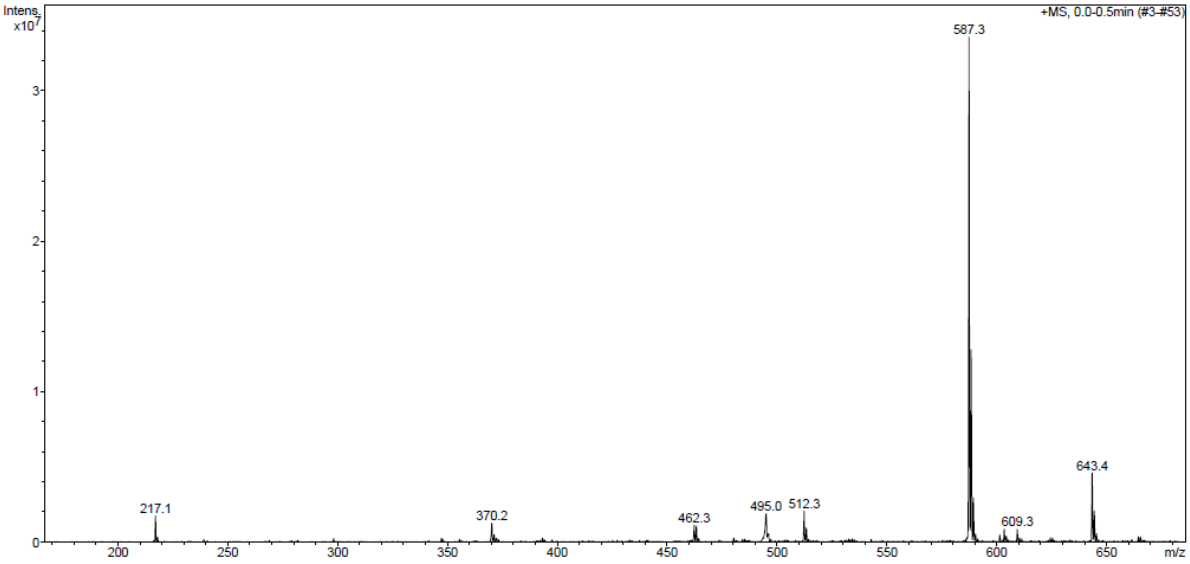
1g


7.946
7.833
7.496
7.476
7.233
7.062
6.991
5.441
4.572
4.533
4.235
4.198
4.194
4.038
3.193
3.177
3.029
2.829
2.788
2.781
2.690
2.672
2.543
2.283
2.257
1.562
1.271
1.260
0.38
0.25
1.02
5.19
2.54
0.46
1.10
1.00
0.93
1.25
1.53
8.66
4.71
1.14
1.27
10.36
f1 (ppm)



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

Analysis Name	av fm2665.d	Acquisition Date	06/08/15 14:00:07	Operator	Walter Panzeri
Sample Name		Method	Copy of _01tmix_posneg lm.MS	Instrument	esquire3000plus
Comment	1 mg/ml dil 1:100 MeOH Richiedente: Frigerio				



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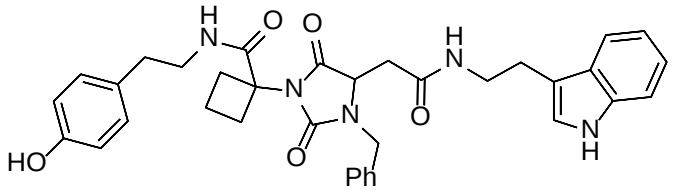
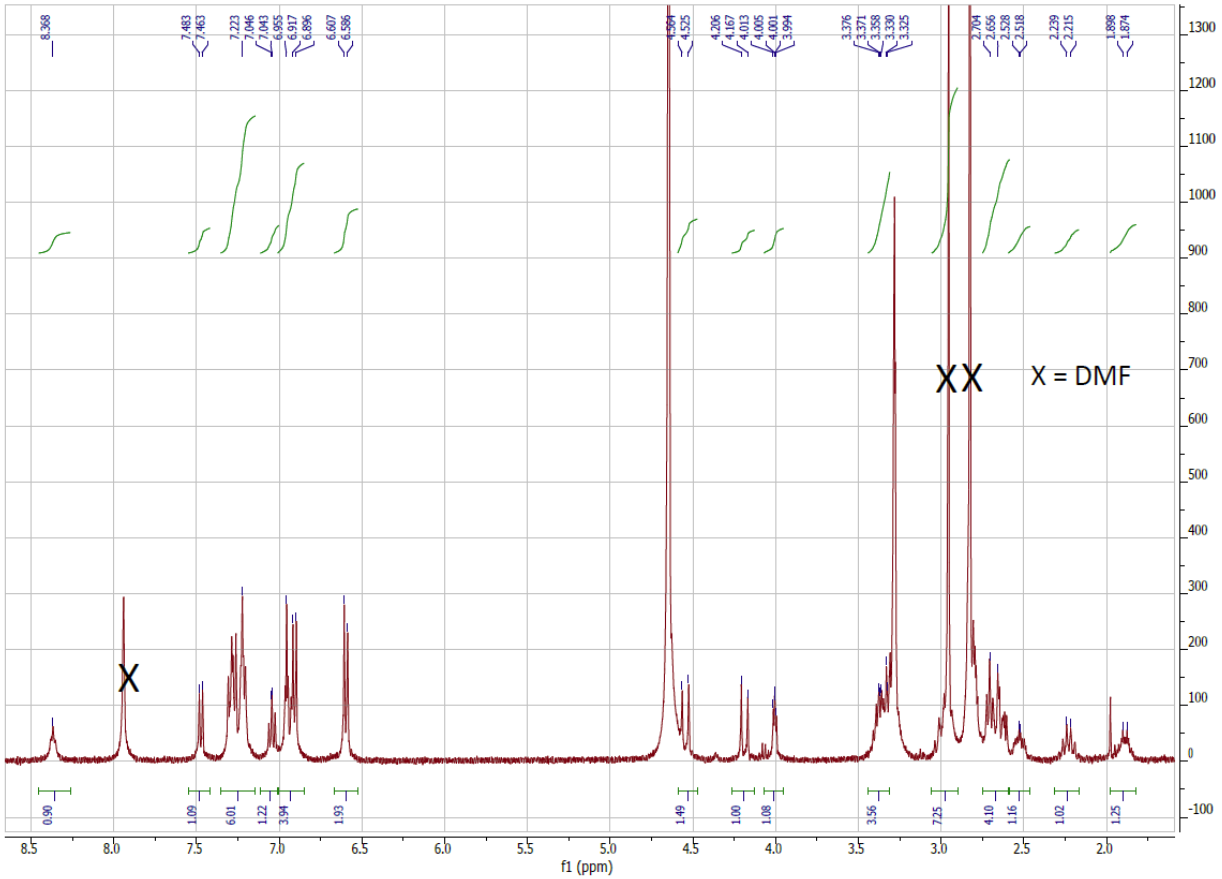
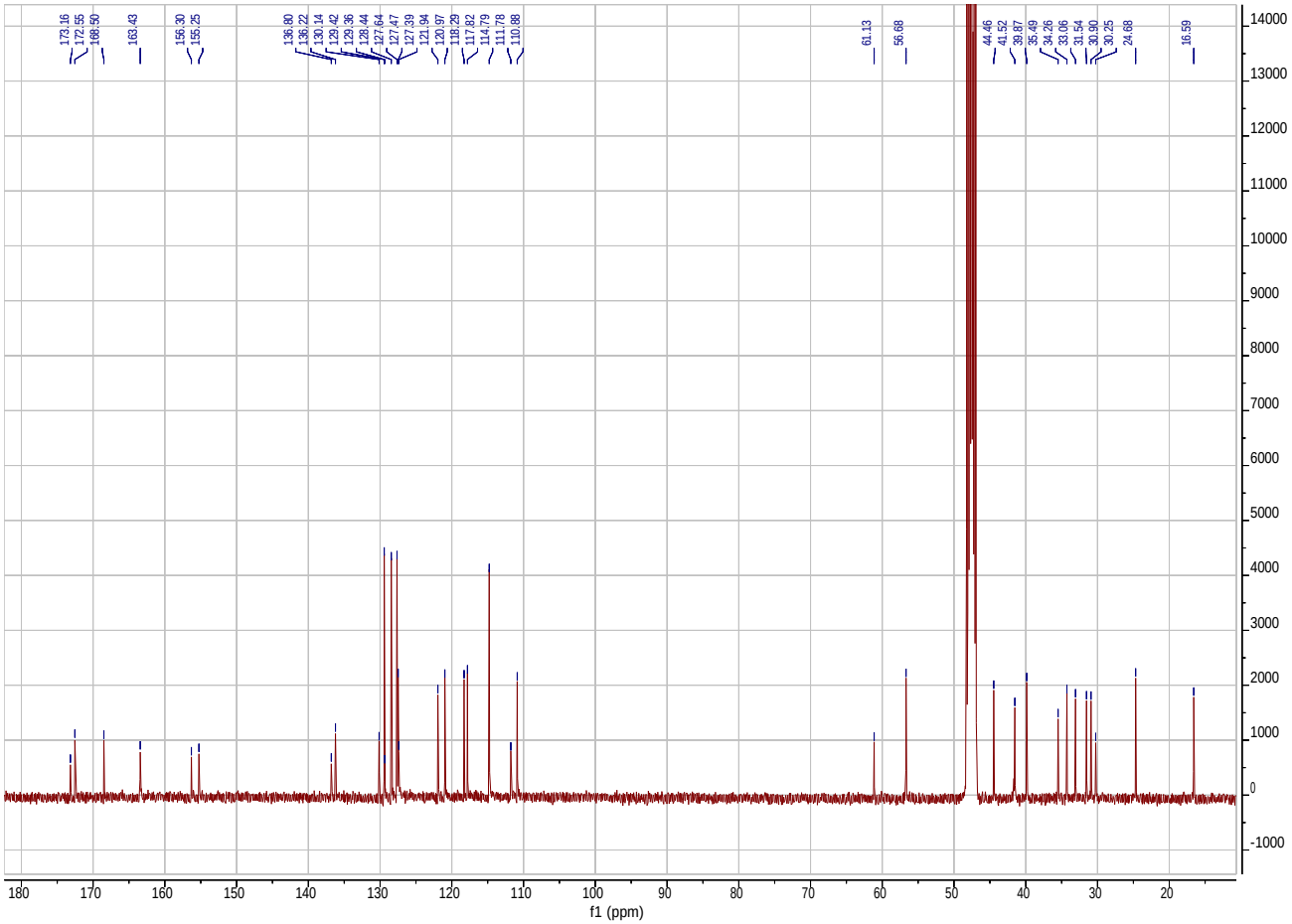


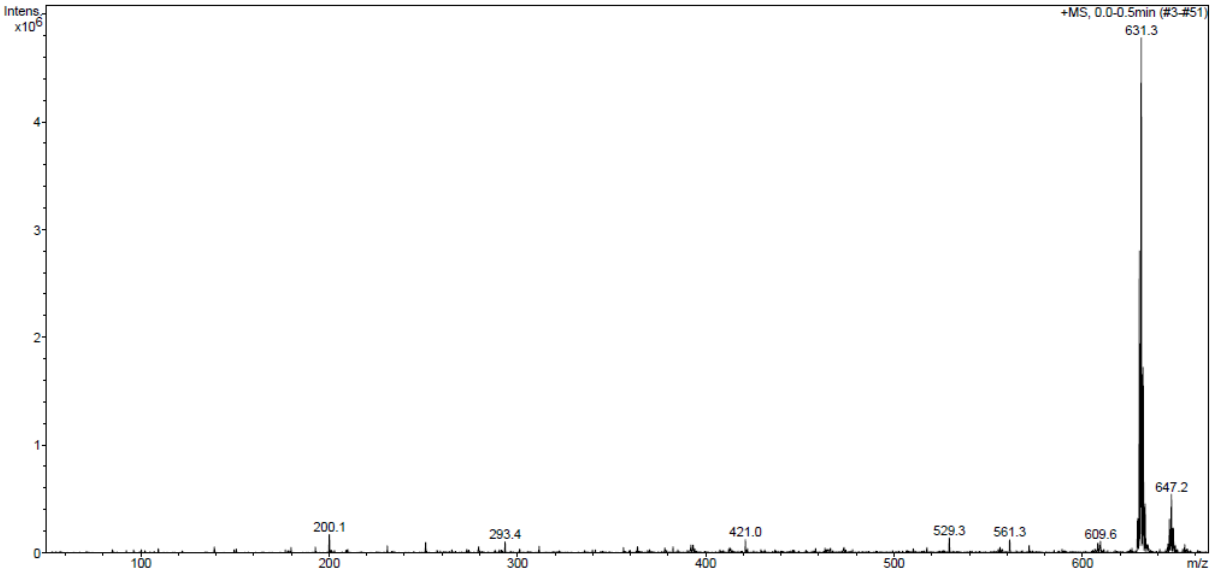
1h





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

Analysis Name	av fm2666.d	Acquisition Date	06/08/15 13:56:38	Operator	Walter Panzeri
Sample Name		Method	Copy of _01tmix_posneg lm.MS	Instrument	esquire3000plus
Comment	1 mg/ml dil 1:100 MeOH Richiedente: Frigerio				



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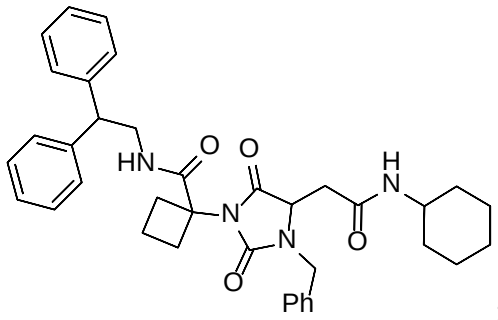
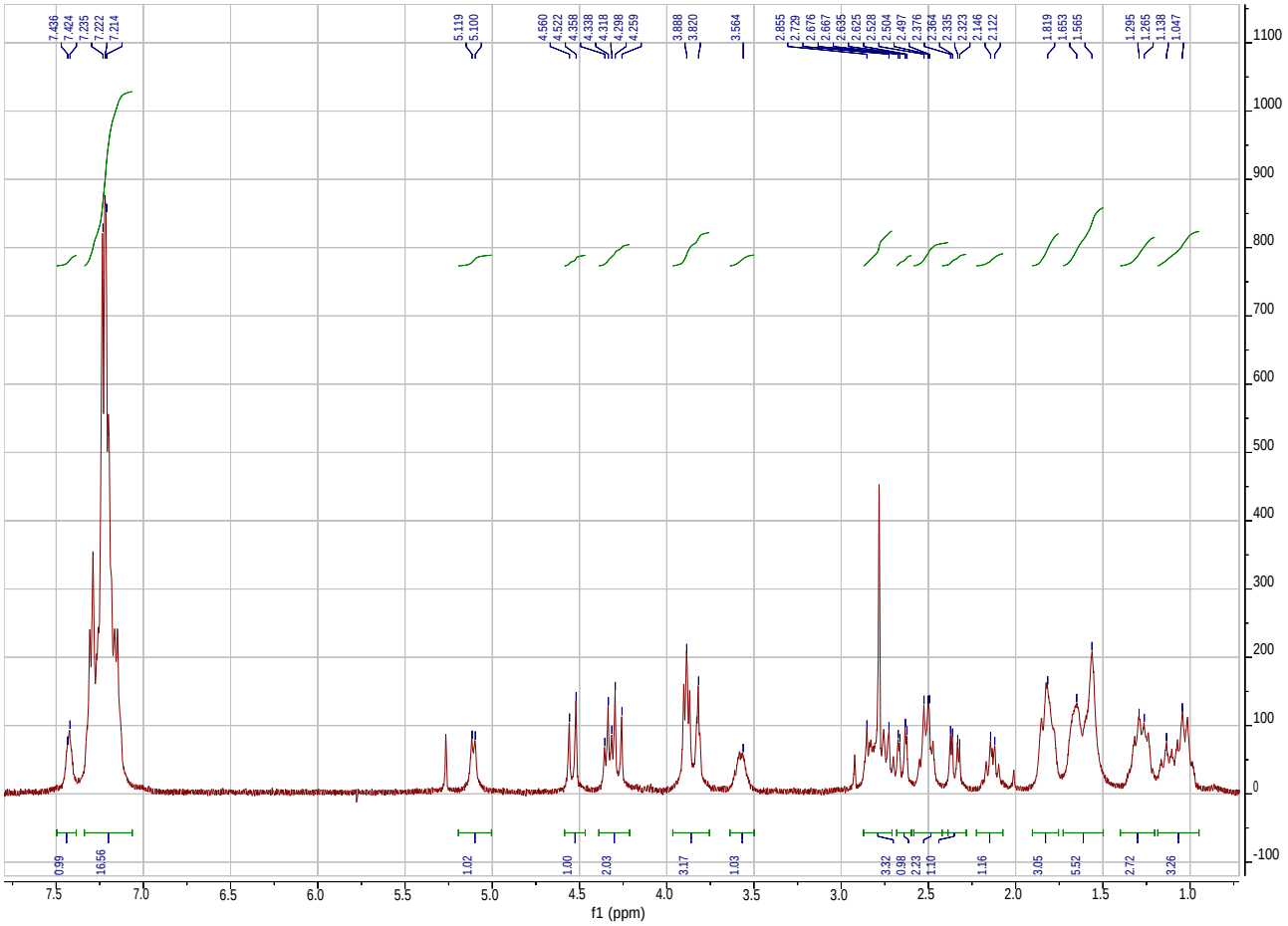
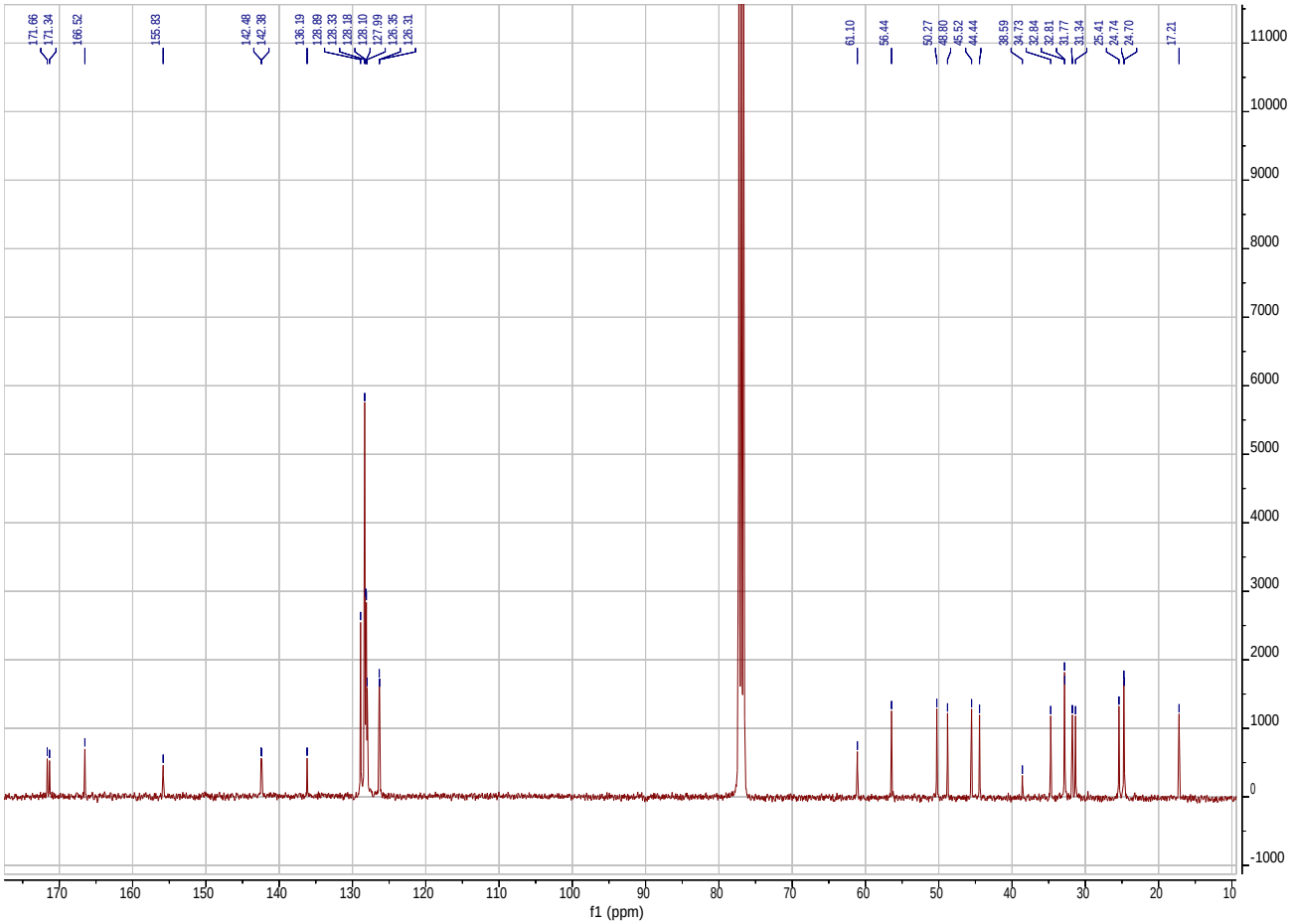

HN
O
O
N
N
O
O
H
N
Ph

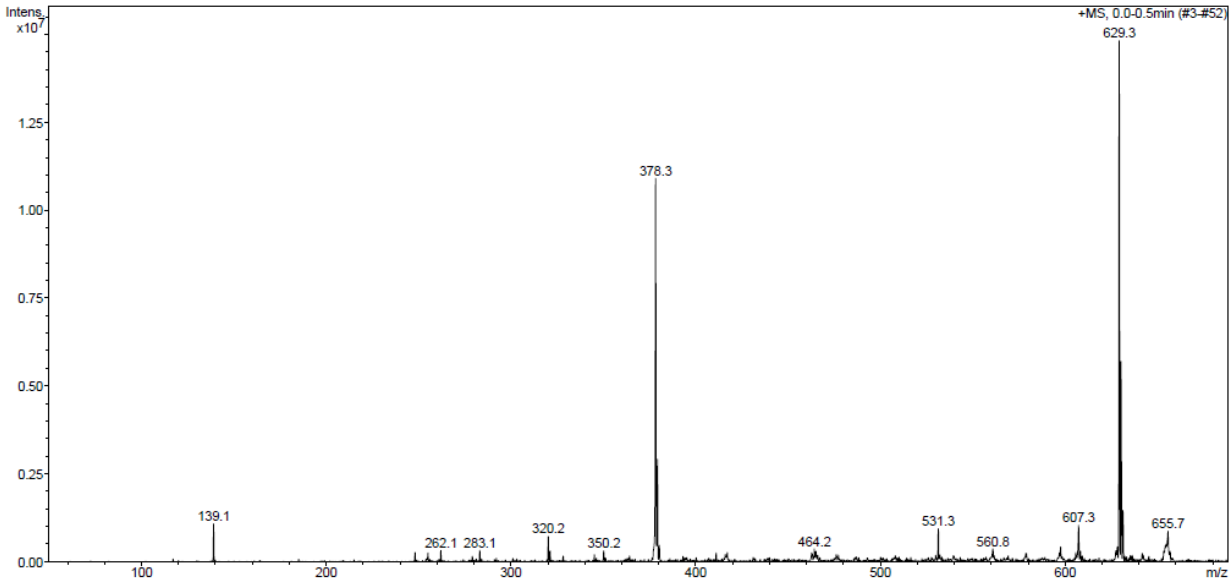
1i


7.436
7.424
7.235
7.222
7.214
5.119
5.100
4.560
4.522
4.358
4.338
4.318
4.298
4.259
3.888
3.820
3.564
2.855
2.729
2.676
2.667
2.635
2.625
2.528
2.504
2.497
2.376
2.364
2.335
2.323
2.146
2.122
1.819
1.653
1.565
1.295
1.265
1.138
1.047
0.99
16.56
1.02
1.00
2.03
3.17
1.03
3.32
0.98
2.23
1.10
1.16
3.05
5.52
2.72
3.26
f1 (ppm)



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

Analysis Name	av fm2678.d	Acquisition Date	06/08/15 13:53:03	Operator	Walter Panzeri
Sample Name		Method	Copy of _01tmix_posneg lm.MS	Instrument	esquire3000plus
Comment	1 mg/ml dil 1:100 MeOH Richiedente: Frigerio				



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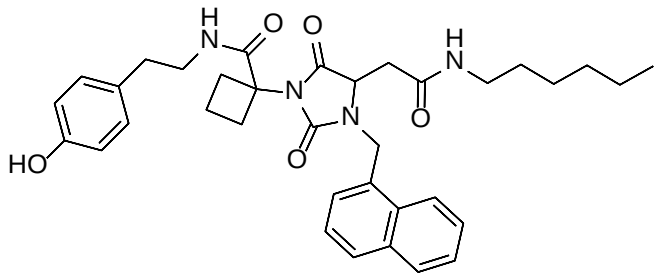
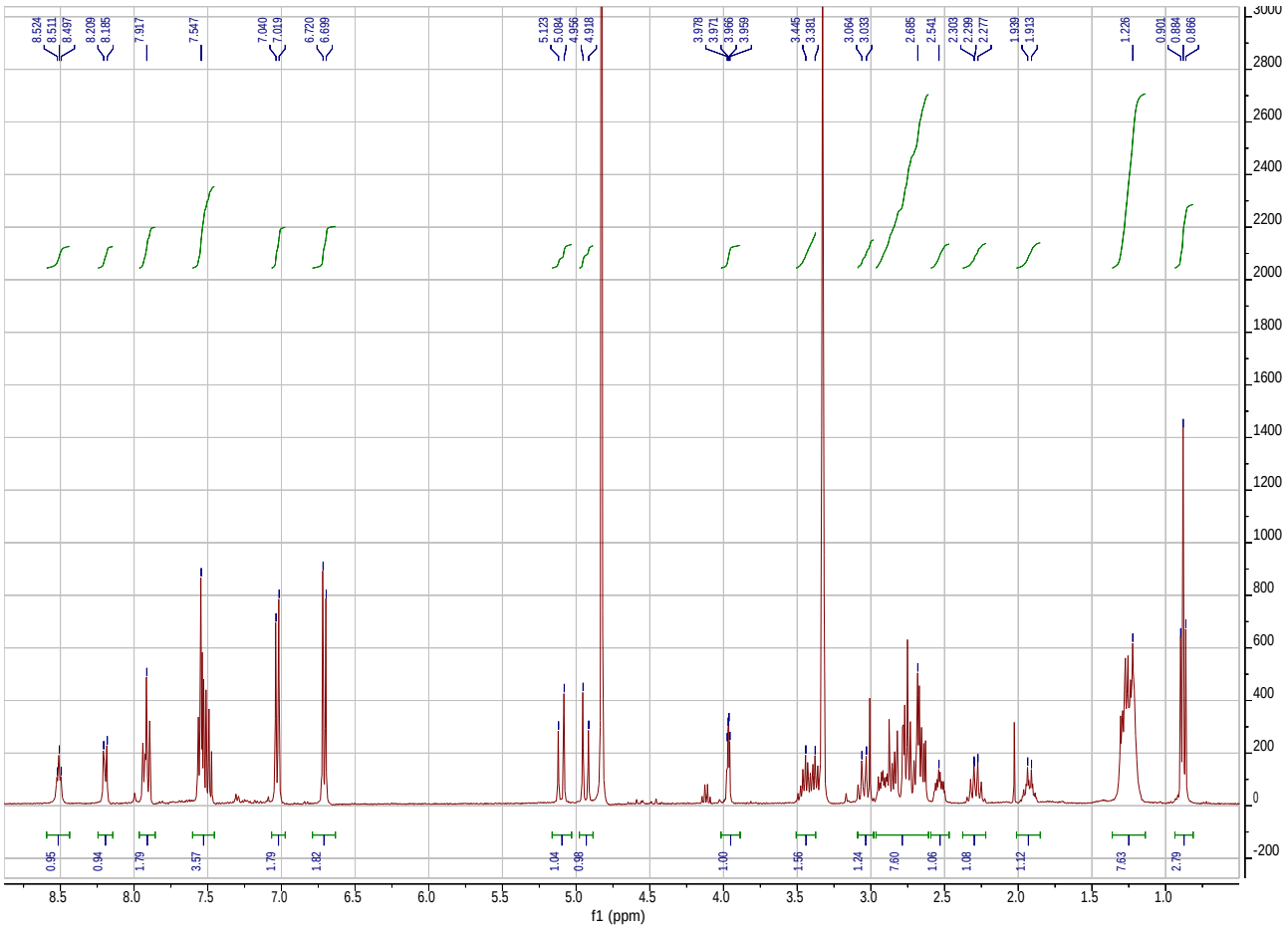
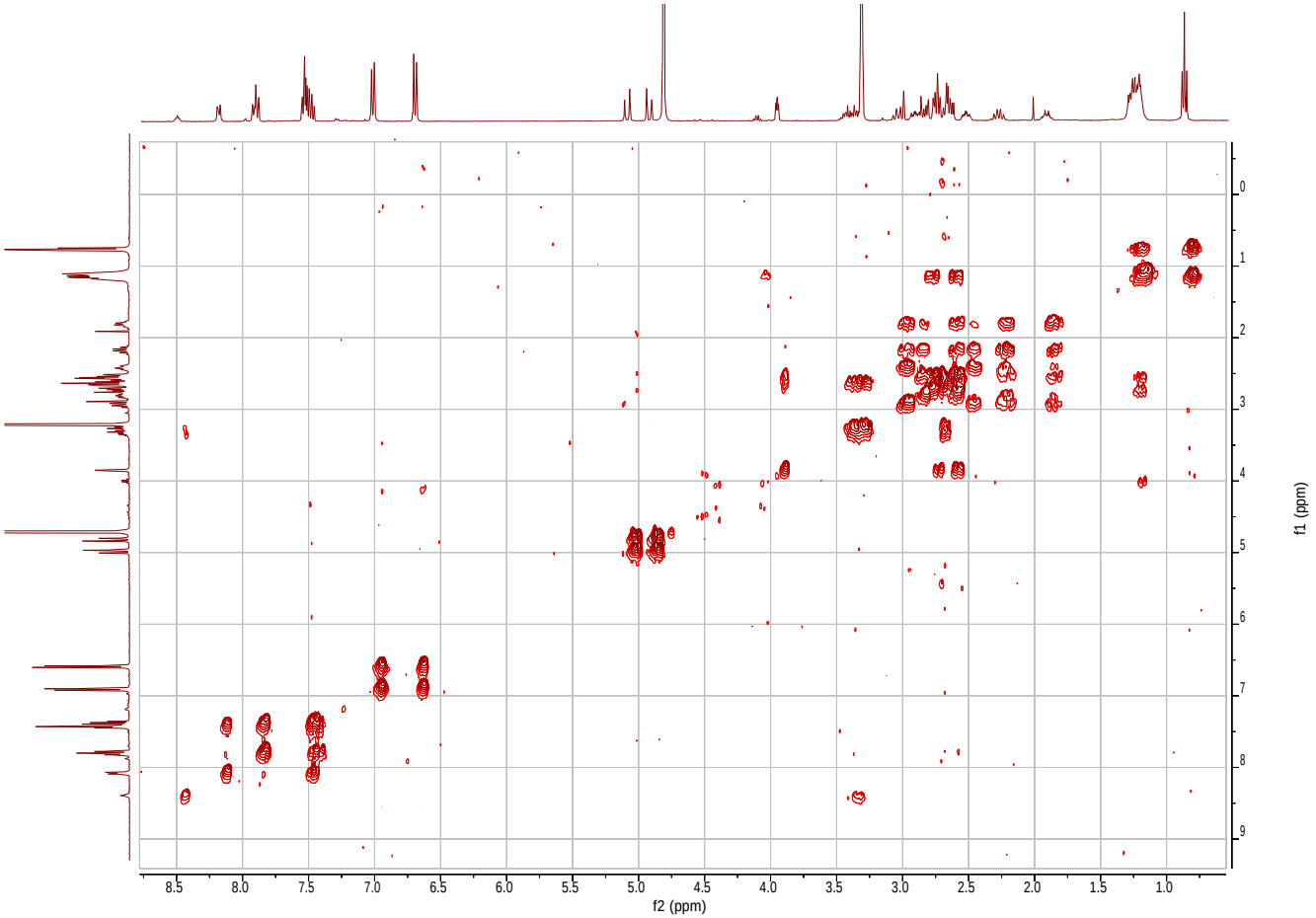
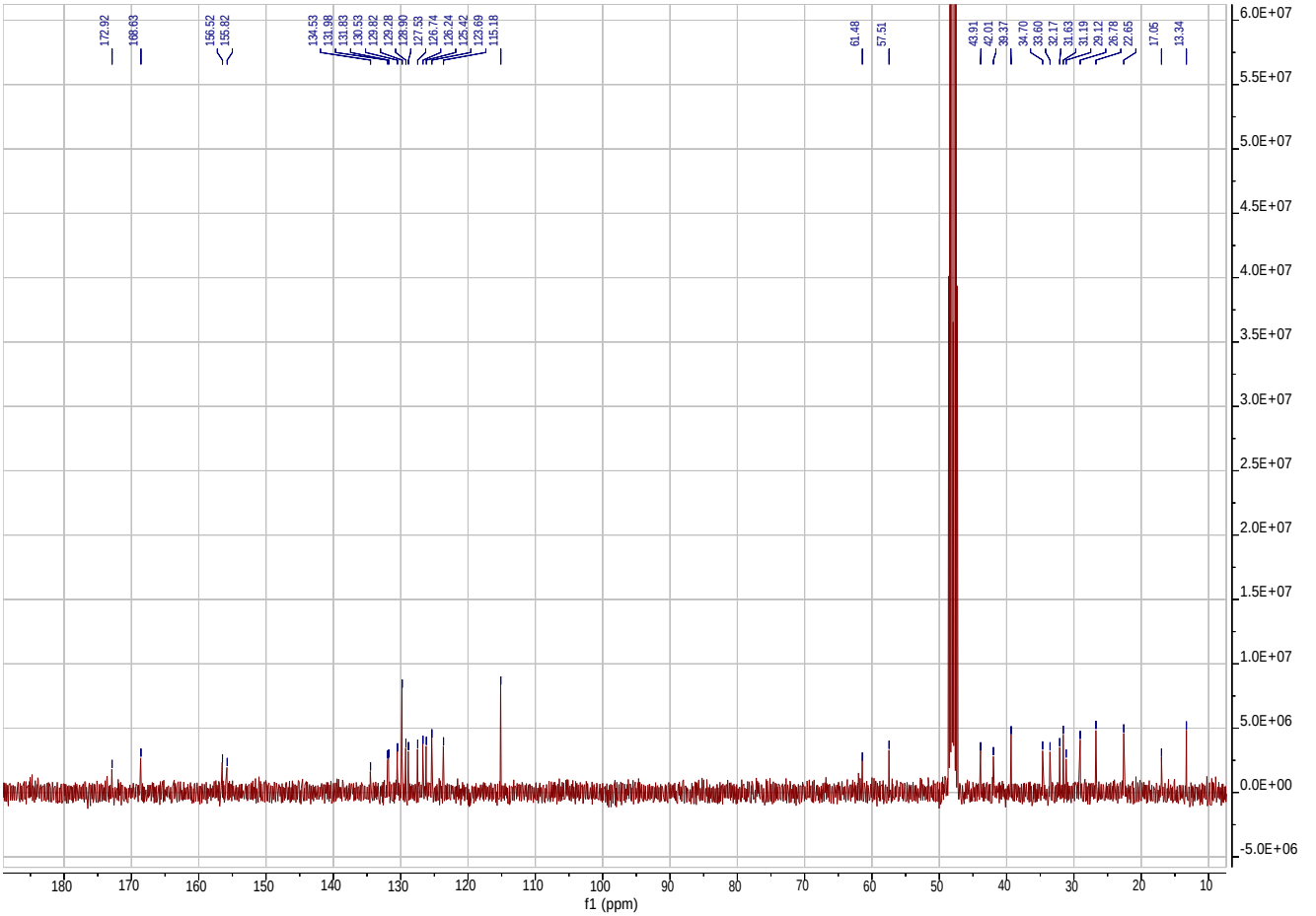


1j

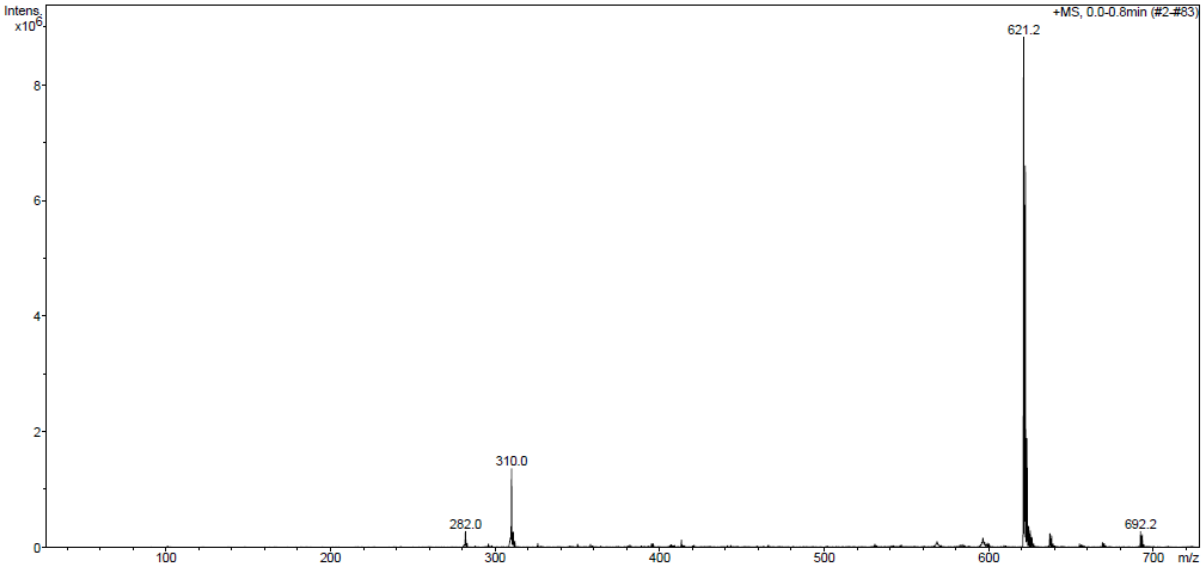

8.524
8.511
8.497
8.209
8.185
7.917
7.547
7.040
7.019
6.720
6.699
5.123
5.084
4.956
4.918
3.978
3.971
3.966
3.959
3.445
3.381
3.064
3.033
2.685
2.541
2.303
2.299
2.277
1.939
1.913
1.226
0.901
0.884
0.866
0.95
0.94
1.79
3.57
1.79
1.82
1.04
0.98
1.00
1.56
1.24
7.60
1.06
1.08
1.12
7.63
2.79
f1 (ppm)


f2 (ppm)
f1 (ppm)


172.92
166.63
156.52
155.82
134.53
131.98
131.83
130.53
129.82
129.28
126.90
127.53
126.74
126.24
125.42
123.69
115.18
61.48
57.51
43.91
42.01
39.37
34.70
33.60
32.17
31.63
31.19
29.12
26.78
22.65
17.05
13.34
f1 (ppm)

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

Analysis Name	av fm2724solido.d	Acquisition Date	02/04/16 14:05:25	Operator	Walter Panzeri
Sample Name		Method	Copy of _01tmix_posneg lm.MS	Instrument	esquire3000plus
Comment	1 mg/ml dil 1:100 MeOH Richiedente: Frigerio				



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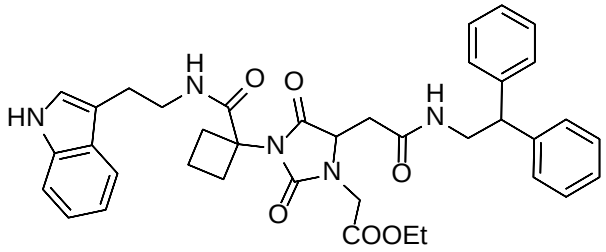
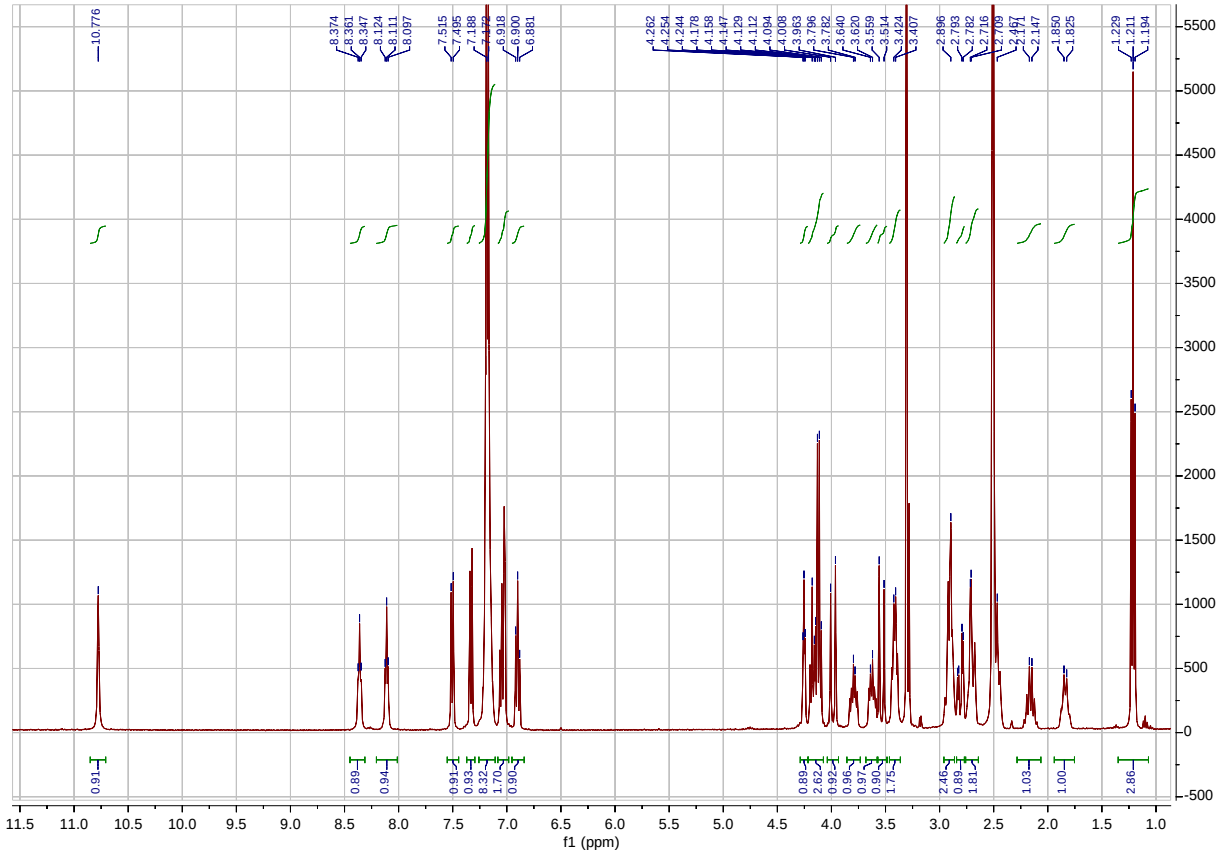
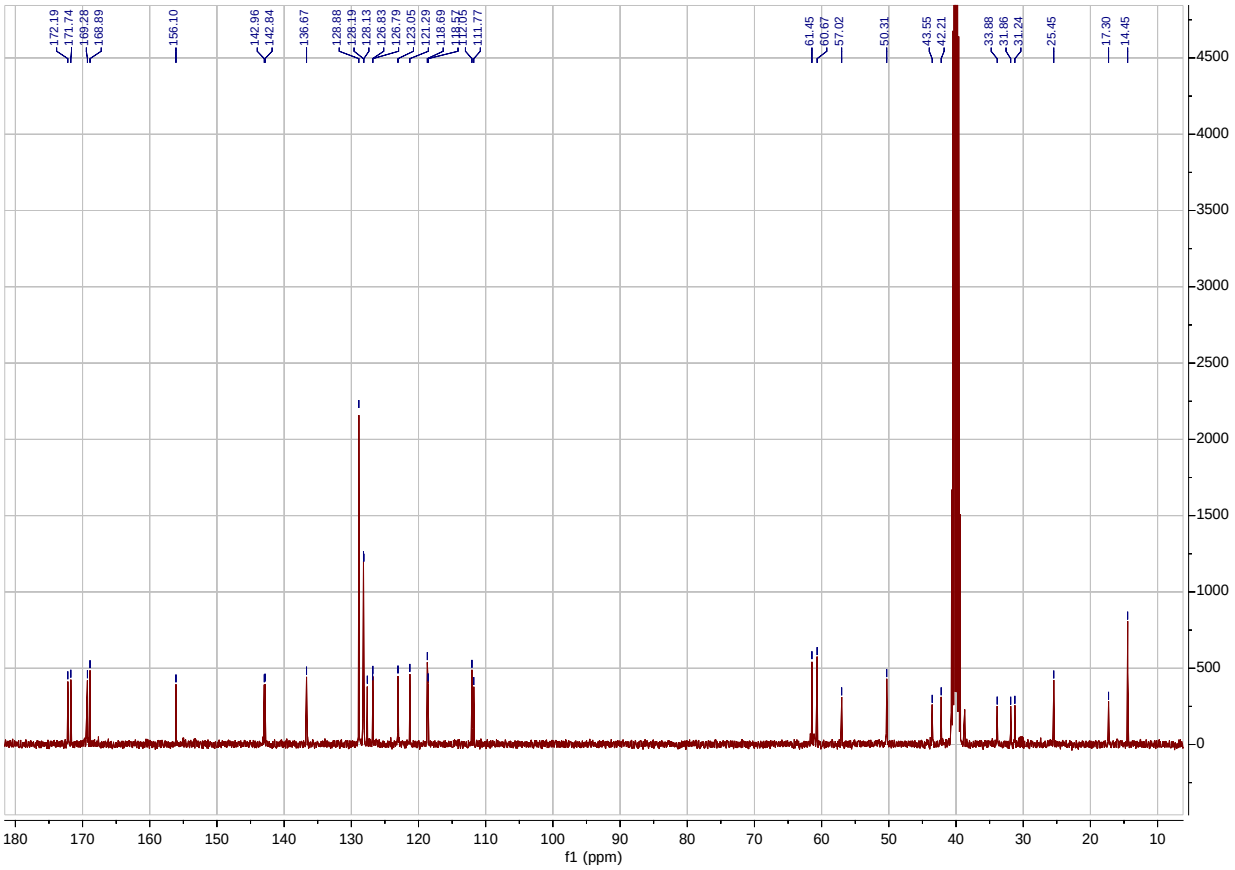

HN
H
N
O
O
N
N
O
H
N
O
COOEt

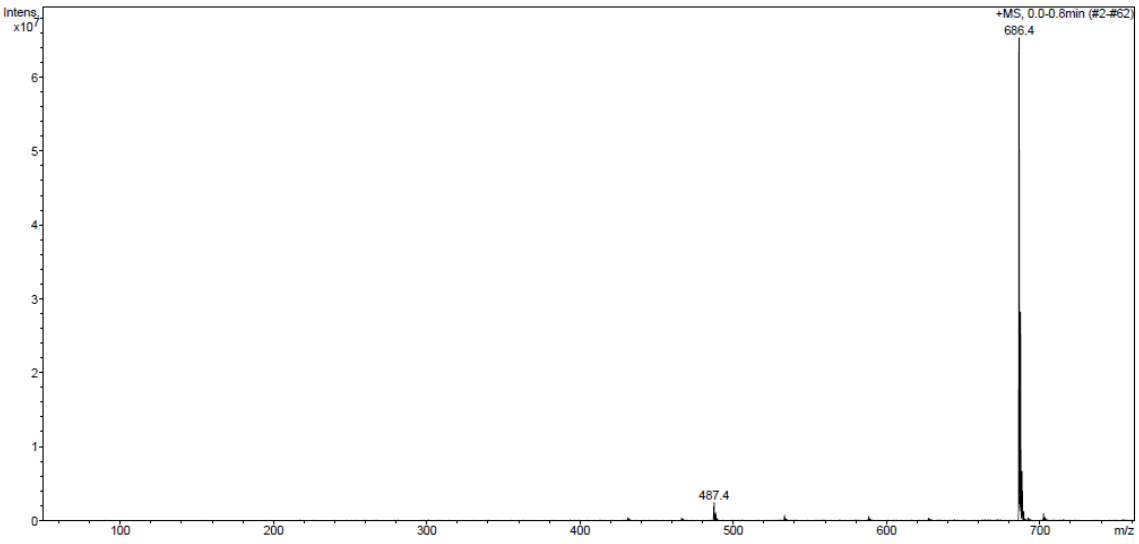
1k


10.776
8.374
8.361
8.347
8.124
8.111
8.097
7.515
7.495
7.188
7.172
6.918
6.900
6.881
4.262
4.254
4.244
4.178
4.158
4.147
4.129
4.112
4.094
4.008
3.963
3.796
3.782
3.640
3.620
3.559
3.514
3.424
3.407
2.896
2.793
2.782
2.746
2.709
2.491
2.147
1.850
1.825
1.229
1.211
1.194
0.91
0.89
0.94
0.91
0.93
8.32
1.70
0.90
0.89
2.62
0.92
0.96
0.97
0.90
1.75
2.46
0.89
1.81
1.03
1.00
2.86
f1 (ppm)



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

Analysis Name	av fm2748.d	Acquisition Date	05/18/16 16:17:40	Operator	Walter Panzeri
Sample Name		Method	Copy of _01tmix_posneg lm.MS	Instrument	esquire3000plus
Comment	1 mg/ml dil 1:100 MeOH Richiedente: Frigerio				



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