Supplementary data

Assignment of Absolute Configuration of natural products with alcohols by ^{13}C-NMR, using derivatization with Methyl-1-(chloromethyl)-5-oxopyrrolidine-2-carboxylate and Quantum-Mechanical GIAO Calculations.

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General methods

^{1}H and ^{13}C NMR were recorder on Bruker Avance 300 MHz or Bruker Avance III 400 MHz instruments using $CDCl_3$ (99.9% D) as the solvent, with chemical shifts (δ) referenced to internal standards residual $CHCl_3$ and $CDCl_3$, (7.26 ppm ^{1}H, 77.0 ppm ^{13}C) Mass spectra were recorded on MStation JMS-700 high-resolution mass spectrometer. THF was distilled from potassium and benzophenone, and dichloromethane was distilled from calcium hydride. All reagents and solvents were purchased from Sigma Aldrich México and were used without further purification. Glassware for anhydrous reactions was dried in an oven at 100 ºC overnight and cooled under molecular sieves as a moisture trap.

Computational Method

B3LYP/6-311+(2d,p) model has been used for 1H and 13C NMR modeling. First, systematic conformational search has been performed using MMFF94 force field to ensure that all conformations have been tested and the global minimum conformation has been selected. Then the geometries of lowest energy conformers were optimized at B3LYP/6-311+(2d,p) level and GIAO Magnetic shielding tensor were calculated at the same level. The same calculations were repeated for TMS standard. The difference between the corresponding isotropic shielding tensors gave chemical shifts.

Experimental Procedures

General procedure for preparation of Derivatization Chiral agent

Methyl-1-(Chloromethyl)-2-pyrrolidon-5-carboxylate 1-*(S)* and 1-(R).

A mixture of methyl pyroglutamate (500 mg, 3.49 mmol), paraformaldehyde (170 mg, 5.6mmol) and chlorotrimethylsilane (2.3 mL, 17.9 mmol) was stirred at room temperature for 3 h. Excess of chlorotrimethylsilane was removed under vacuum and paraformaldehyde was removed by distillation in Kugelrohr at 100 ºC. ^{1}H NMR (300 MHz, $CDCl_3$), 5.72 ppm (d, *J*=10.2 Hz, 1H), 4.9 ppm (d, *J*=10.2 Hz, 1H), 4.45 ppm (dd, J= 8, 4 Hz, 1H), 3.79 ppm (s, 3H), 2.3 ppm (m, 4H).

General procedure for preparation 1-(alkoxy-methyl)-methyl-2-pyrrolidine-5-carboxylate derivatives with 1-(S) or 1-(R) and NaH.

Sodium hydride (2.5 equiv., 60% in mineral oil) was added to a solution of alcohol (1 equiv.) in dried THF at 0ºC, under nitrogen atmosphere. The mixture was stirred by 10 minutes, then s **1-(S)** or **1-(R)** (3 equiv.) in THF was added. The mixture was stirred by refluxed for 6-12 h. A saturated solution of NH_4Cl was added and THF was removed and extracted with ethyl acetate. Organic extracts were dried over anhydrous sodium sulfate, filtered, and concentrated. The mixture was purified by flash chromatography.

General procedure for preparation 1-(alkoxy-methyl)-methyl-2-pyrrolidine-5-carboxylate derivatives with 1-(S) or 1-(R) with Silver triflate.

Silver trifluoromethanesulfonate (AgOtf) (1.2 equiv.) was added in absence of light to a mixture of alcohol (1 equiv), **1-(S**) or **1-(R)** (3 equiv) and Hydrotalcite (HT) (50 mg per mmol of alcohol) in dried DCM. The mixture was stirred for 3-12h. The mixture was filtered over Celite and washed with brine. Organic extracts were dried over calcium chloride, and concentrated. The mixture was purified by flash chromatography.

Methyl-(S)-1-((((1R,2S,5R)-2-isopropyl-5-methylcyclohexyl)oxy)methyl)-5-oxopyrrolidine-2-carboxylate 2a.

A mixture of (-)-Menthol **2-(R)** (78 mg, 0.5 mmol), NaH (24 mg, 0.6 mmol), **1-(S)** (114 mg, 0.6 mmol) in dried THF was refluxed for 12 h, as a general procedure. the crude reaction mixture was purified by column chromatography with n-hexane/Ethyl acetate 80:20 to yield 83 mg of **2a** (52%). ^{1}H NMR (400 MHz, $CDCl_3$), δ 5.29 (d, J = 11.2 Hz, 1H), 4.40 (dd, J = 9.2, 3.0 Hz, 1H), 4.32 (d, J = 11.2, 1H), 3.76 (s, 3H), 3.15 (td, J =10.4, 4.2 Hz, 1H), 2.55 – 2.26 (m, 3H), 2.22-2.17(m,1H), 2.14-2.06(m, 2H), 1.65 – 1.57 (m, 2H), 1.42-1.31 (m, 1H), 1.20-1.12 (m, 1H), 0.92-0.71 (m,3H), 0.92 (d, J = 6.5 Hz, 3H),

0.88 (d, J = 7.0 Hz, 3H), 0.69 (d, J = 7.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.85, 172.4, **76.4, 68.6**, 57.7, 52.6, **48.1**, **40.1**, 34.5, 31.4, 29.7, 25.6, 23.0, 22.3, 21.2, 15.8. ESI-MS m/z (rel. intensity, %): M^+ 311(0.5), 268 (1), 252(13), 224(2), 222(1), 182(1), 172(8), 156(100), 128(75), 84(62), 68(19), 41(15), 29(4), 27(3), 15(2). ESI-HRMS m/z: $C_{17}H_{30}N_1O_4$ [M+1] calculated 312.21748 observed. 312.21717. $[\alpha]_D^{20}$= -105.2(c 0.25, $CHCl_3$)

Methyl-(S)-1-((((1S,2R,5S)-2-isopropyl-5-methylcyclohexyl)oxy)methyl)-5-oxopyrrolidine-2-carboxylate 2b.

A mixture of (+)-Menthol **2-(S)** (78 mg, 0.5 mmol), NaH (24 mg, 0.6 mmol), **1-(S)** (114 mg, 0.6 mmol) in dried THF was refluxed for 12 h, as a general procedure. The crude material was purified by column chromatography with n-hexane/Ethyl acetate 80:20 to yield 104 mg of **2b** (65%). ^{1}H NMR (400 MHz, $CDCl_3$), δ 5.20 (d, J = 9.9 Hz, 1H), 4.38 (dd, J = 8.9, 3.7 Hz, 1H), 4.32 (d, J = 10.0 Hz, 1H), 3.69 (s, 3H), 3.14 (td, J = 10.6, 4.4 Hz, 1H), 2.53 – 2.20 (m, 3H), 2.12 – 1.94 (m, 2H), 1.92-1.87 (m, 1H), 163-1.55(m, 2H), 1.38 – 1.28 (m, 1H), 1.2-1.1 (m-1H), 0.99-0.80(m-3H), 0.83 (d, J = 1.72 Hz, 3H), 0.81 (d, J = 1.15 Hz, 3H), 0.71 (d, J = 7.0 Hz, 3H). ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.4, 172.4, **79.4**, **71.8**, 57.6, 52.5, **48.6**, **41.9**, 34.4, 31.5, 29.9, 25.7, 23.2, 22.9, 22.4, 21.2, 16.2, $DART^+$ m/z (rel intensity, %): [2M+2] 624 (14), [2M+1] 623 (32), 467 (28), 329 (14), [M+2] 313 (13), [M+1] 312 (100), 299 (14), 174(17), 156 (98), 128 (23). ESI-HRMS m/z: $C_{17}H_{30}N_1O_4$ [M+1] calculated 312.21748, observed 312.21750. $[\alpha]_D^{20}$= +11.29 (c 1, $CHCl_3$).

Methyl-(S)-1-((((3S,4aR,6aR,6bS,8aS,11R,12S,12aS,14aR,14bR)-8a-(methoxycarbonyl)-4,4,6a,6b,11,12,14b-heptamehyll-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,10,11,12,12a,14,14a,14b-icosahydropicen-3-yl)oxy)methyl)-5-oxopyrrolidyne-2-carboxylate, 3a.

A mixture of **Ursolic acid Methyl ester 3** (42 mg, 0.089 mmol), NaH (8mg, 0.2 mmol), **1-(S)** (37 mg, 0.19 mmol) in dried THF was refluxed for 16 h, as a general procedure. the crude reaction mixture was purified by column chromatography with n-hexane/Ethyl acetate 90:10 to yield 16 mg of **3a** (28%). ^{1}H NMR (300 MHz, $CDCl_3$), δ. 5.22 (t, J = 3.9 Hz, 1H), 5.18 (d, J = 10.3 Hz, 1H), 4.47 (d, J = 10.2 Hz, 1H), 4.11 (dd, J = 8.6, 3.24 Hz, 1H), 3.75 (s, 3H), 3.59 (s, 3H), 3.00 (dd, J = 9.9, 5.2 Hz, 1H), 2.58-2.10 (m, 7H), 1.97 (dd, J = 12.3, 4.47 Hz, 1H), 1.88 (dd, J = 8.64, 3.57 Hz, 1H), 1.79-1.29 (m, 18H), 1.05 (s, 3H), 0.94 (s, 6H), 0.89 (s, 3H), 0.84 (d, J = 6.4 Hz, 3H), 0.73 (d, J = 5.7 Hz, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 178.2, 175.5, 172.4, 138.3, 125.6, **87.2**, **72.9**, 57.9, 55.4, 53.0, 52.6, 51.6, 48.2, 47.6, 42.1, 39.6, 39.1, **39.0**, 39.0, 38.7, 36.9, 36.8, 33.0, 30.8, 29.9, 28.1, 28.1, **24.8**, 24.3, 23.7, 23.4, 23.1, 21.3, 18.3, 17.2, 17.0, 16.5, 15.6. $DART^+$ m/z (rel intensidad, %): [M+2] 627 (31), [M+1] 626 (75) 608 (45), 454 (35), 453 (100), 329 (12), 299 (13), 156 (56), 144 (16), 117 (29), ESI-HRMS m/z: $C_{38}H_{60}N_1O_6$ [M+1] calculated 626.44206 observed. 626.44055 $[\alpha]_D^{20}$= +17.95 (c 0.49, $CHCl_3$).

Methyl-(R)-1-((((3S,4aR,6aR,6bS,8aS,11R,12S,12aS,14aR,14bR)-8a-(methoxycarbonyl)-4,4,6a,6b,11,12,14b-heptamehyll-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,10,11,12,12a,14,14a,14b-icosahydropicen-3-yl)oxy)methyl)-5-oxopyrrolidyne-2-carboxylate, 3b.

A mixture of **Ursolic acid methyl ester 3** (42 mg, 0.089 mmol), NaH (8mg, 0.2 mmol), **1-(R)** (37 mg, 0.19 mmol) in dried THF was refluxed for 16 h, as a general procedure. the crude product was purified by column chromatography with n-hexane/Ethyl acetate 90:10 to yield 14 mg of **3b** (16%). ^{1}H NMR (300 MHz, $CDCl_3$), δ. 5.30 – 5.18 (m, 2H), 4.44 (dd, J = 9.0, 2.9 Hz, 1H), 4.37 (d, J = 11.1 Hz, 1H), 3.77 (s, 3H), 3.59 (s, 3H), 2.91 (dd, J = 11.6, 4.3 Hz, 1H), 2.57 – 2.02 (m, 7H), 1.97 (dd, J = 12.9, 4.8 Hz, 1H), 1.89 (dd, J = 8.8, 3.3 Hz, 1H), 1.78 – 1.22 (m, 18H), 1.06 (s, 3H), 0.94 (s, 3H), 0.91 (s, 3H), 0.88 (s, 3H), 0.84 (d, J = 6.4 Hz, 3H), 0.73 (d, J = 6.2 Hz, 6 H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 178.2, 176.1, 172.5, 138.2, 125.7, **84.2**, **69.1**, 57.8, 55.6, 53.0, 52.6, 51.6, 48.2, 47.5, 42.1, 39.6, 39.2, 39.0, **38.4**, 38.4, 37.0, 36.8, 33.1, 30.8, 29.8, 28.2, 28.1, 24.3, 23.7, 23.4, 23.1, **22.3**, 21.3, 18.4, 17.1, 17.1, 16.4, 15.6. ESI-MS (rel. Int. %): M+ 625(1), 610 (1), 566 (3), 565(3), 482 (5), 409 (6), 393 (5), 364

(9), 317 (3), 262 (68), 261(10), 203 (66), 156 (100), 128 (69), 69 (33), 57 (45), 41 (29), 27 (25). ESI-HRMS m/z: $C_{38}H_{60}N_1O_6$ [M+1] calculated 626.44206 observed. 626.44211, $[\alpha]_D^{20}$= +55.7142 (c 0.14, $CHCl_3$).

Estradiol 3-methyl ether, 4.

KOH (160 mg, 2.8 mmol) was added to a solution of Estrone (1g, 3.69 mmol) in dried Acetone (100 mL). Methyl iodide (0.3 mL, 4.8 mmol) was added at 0°C, in 16 mL of Acetone, the mixture was stirred at room temperature by 2.5 h; then Methyl iodide (0.04 mL, 0.64 mmol) in 5 mL of Acetone was added. The reaction mixture was stirred at room temperature for 4 h. Acetone was removed under vacuum and extracts was dissolved in ethyl acetate. Organic extracts were washed with brine and dried over anhydrous sodium sulfate, filtered and concentrated. Crude material was purified by crystallization in methanol to yield 992mg (94%) of Estrone methyl ether **4i**. NMR-^{1}H (400 MHz, $CDCl_3$), δ 7.23 (dd, J = 8.6, 1.2 Hz, 1H), 6.75 (dd, J = 8.6, 2.8 Hz, 1H), 6.68 (d, J = 2.8 Hz, 1H), 3.81 (s, 3H), 3.00 – 2.87 (m, 2H), 2.58 – 1.93 (m, 7H), 1.75 – 1.38 (m, 6H), 0.94 (s, 3H). $NaBH_4$ (125 mg, 3.12 mmol) was added to a solution of **4i** (148 mg, 0.5 mmol) in 15 mL of methanol at 0°C. The mixture was stirred by 4 h. Acetic acid (0.2 mL) was added, methanol was removed under vacuum, the mixture was dissolved in ethyl acetate and washed by brine, dried over anhydrous sodium sulfate, filtered, concentrated and crystalized in methanol providing 103 mg with a yield of 69% of **4**. -^{1}H NMR (300 MHz, $CDCl_3$), δ. 7.22 (d, J = 8.4 Hz, 1H), 6.72 (dd, J = 8.4, 2.7 Hz, 1H), 6.64 (d, J = 2.7 Hz, 1H), 3.79 (s, 3H), 3.74 (t, J = 8.4 Hz, 1H),2.90-2.84 (m, 2H), 2.45 – 1.09 (m, 14H), 0.79 (s, 3H).

Methyl-(S)-1-((((8R,9S,13S,14S,17S)-3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)oxy)methyl)-5-oxopyrrolidin-2-carboxilate, 4a.

A mixture of **4** (40 mg, 0.13 mmol), NaH (7 mg, 0.16 mmol), **1-(S)** (52 mg, 0.27 mmol) in dried THF was refluxed for 16 h, as a general procedure. the crude product was purified by column chromatography with n-hexane/Ethyl acetate 80:20 to yield 36 mg of **4a** (57%). ^{1}H NMR (300 MHz, $CDCl_3$), δ. 7.20 (d, J = 8.6 Hz, 1H), 6.70 (dd, J = 8.6, 2.7 Hz, 1H), 6.62 (d, J = 2.6 Hz, 1H), 5.11 (d, J = 10.5 Hz, 1H), 4.57 (d, J = 10.4 Hz, 1H), 4.38 (dd, J = 8.9, 3.2 Hz, 1H), 3.7705 (s, 3H), .3.7703 (s, 3H), 3.49 (t, J = 8.2 Hz, 1H), 2.86-2.81 (m, 2H), 2.63 – 1.13 (m, 17H), 0.76 (s, 3H). ^{13}C-NMR-(75 MHz, $CDCl_3$) δ 175.6, 172.1, 157.4, 138.1, 132.7, 126.5, 113.9, 111.6, **88.0**, **72.2**, 57.8, 55.3, 52.6, 49.8, 44.0, **43.5**, 38.7, 37.5, 30.0, 29.9, **28.4**, 27.3, 26.4, 23.2, 23.1, 11.8. ESI-MS m/z (rel intensity %): 441(28), 413 (1), 382 (3), 352 (0.5), 314 (0.5), 285 (25), 267 (23), 227 (9), 201 (20), 173 (42), 157 (91), 128 (100), 91 (21), 57 (30), 41 (33), 28 (18), 18 (4). ESI-HRMS m/z: $C_{26}H_{36}N_1O_5$ [M+1] calculated 442.25935, observed. 442.25883, $[\alpha]_D^{20}$= +1.81° (c 0.55, $CHCl_3$).

Methyl-(R)-1-((((8R,9S,13S,14S,17S)-3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)oxy)methyl)-5-oxopyrrolidin-2-carboxilate, 4b.

A mixture of **4** (68 mg, 0.238 mmol), NaH (12 mg, 0.28 mmol), **1-(R)** (67 mg, 0.35 mmol) in dried THF was refluxed for 16 h, as a general procedure. the crude product was purified by column chromatography with n-hexane/Ethyl acetate 80:20 to yield 56 mg of **4b** (53%). ^{1}H NMR (300 MHz, $CDCl_3$), δ 7.18 (d, J = 8.5 Hz, 1H), 6.70 (dd, J = 8.6, 2.7 Hz, 1H), 6.62 (d, J = 2.6 Hz, 1H), 5.11 (d, J = 10.6 Hz, 1H), 4.53 (d, J = 10.6 Hz, 1H), 4.37 (dd, J = 8.9, 3.2 Hz, 1H), 3.78 (s, 3H), 3.77 (s, 3H), 3.42 (t, J = 8.2 Hz, 1H), 2.92 – 2.76 (m, 2H), 2.66 – 1.07 (m, 17H), 0.77 (s, 3H). NMR-^{13}C (75 MHz, $CDCl_3$) δ 175.8, 172.5, 157.6, 138.1, 132.7, 126.4, 113.9, 111.6, **86.4**, **70.9**, 57.6, 55.3, 52.6, 50.1, 44.0, **43.1**, 38.7, 37.4, 30.0, 29.9, **27.5**, 27.3, 26.4, 23.2, 23.1, 11.8. ESI-MS m/z (rel intensity %): 441(93), 413 (2), 382 (7), 352 (1), 316 (1), 285(58), 267 (33), 241 (10.3), 201 (16), 173 (45), 156 (100), 128 (87), 84 (20), 59 (20), 43(34), 41 (15), 29 (4), 15 (3). ESI-HRMS m/z: $C_{26}H_{36}N_1O_5$ [M+1] calculated 442.25935, observed. 442.25806, $[\alpha]_D^{20}$= +45.2° (c 0.46, $CHCl_3$).

(5R,6S,8aS)-5,6-dihidroxi-5,8a-dimethyl-3-(propan-2-iliden)octahydronaphtalen-2(1H)-ona, Cuauhtemone, **5.**

A 2.5 N aqueous solution of LiOH (2mL, 5 mmol) was added to a solution of 3-O-[2,3-epoxi-2-metilbutiroil] Cuauhtemone (100 mg, 0.29 mmol) in THF (10 mL). The mixture was stirred at room temperature for 1.5 h. THF was removed by distillation; then the mixture was acidulated with HCl 1N and dissolved in Ethyl acetate, the mixture was washed with brine and dried over anhydrous sodium sulfate, filtered, and concentrated to give 67 mg (91%) of **5**. ^{1}H-NMR (300 MHz, $CDCl_3$), δ 3.68 (d, J = 2.9 Hz, 1H), 2.96 (dd, J = 14.7, 3.5 Hz, 1H), 2.24 (d, J = 4.7 Hz, 2H), 2.11 – 2.05 (m, 3H), 2.03 (s, 3H), 1.85 (s, 1H), 1.81-170 (m, 4H), 1.23 (s, 6H), 0.95 (s, 3H).

Methyl-(2S)-1-((((1R,2S,4aS)-1-hydroxy-1,4a-dimethyl-6-oxo-7-(propan-2-iliden)decahydronaphtalen-2-yl)oxy)methyl)-5-oxopirrolydine-2-carboxylate, 5a.

A mixture of **5** (40 mg, 0.15 mmol), NaH (7 mg, 1.8 mmol), **1-(S)** (35mg, 0.18 mmol) in dried THF was refluxed by 12 h, as a general procedure. the crude product was purified by column chromatography with n-hexane/Ethyl acetate to yield 34mg of **5a** (53%). ^{1}H NMR (300 MHz, $CDCl_3$), δ 4.95 (d, J = 10.7 Hz, 1H), 4.79 (d, J = 10.7 Hz, 1H), 4.34 (dd, J = 8.87, 3.72 Hz, 1H), 3.79 (s, 3H), 3.53 (dd, J = 3.7, 1.8 Hz, 1H), 2.98 (dd, J = 15.3, 4.2 Hz, 1H), 2.70 – 2.25 (m, 6H), 2.18 (d, J = 2.9 Hz, 3H), 2.17 – 2.07 (m, 3H), 2.01 (s, 3H), 1.92-1.85 (m, 3H), 1.83 (s, 1H), 1.17 (s, 6H), 0.93 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) 202.9, 176.1, 172.5, 144.4, 131.5, **81.9**, 72.4, **71.9**, 60.2, 59.5, 52.8, 47.2, 36.3, 33.3, 29.8, 29.6, 25.6, 23.4, 23.3, 23.0, 22.8, 20.9, 18.9. ESI-MS m/z (rel intensity %): 406 (20), 388 (10), 329(18), 299 (24), 156 (100), 144 (24), 128 (12). ESI-HRMS m/z: $C_{22}H_{33}N_1O_6$ [M+1] calculated 407.23079, observed 407.23011 $[\alpha]_D^{20}$= +26.3 (c 0.285, $CHCl_3$).

Methyl-(2R)-1-((((1R,2S,4aS)-1-hydroxy-1,4a-dimethyl-6-oxo-7-(propan-2-iliden)decahydronaphtalen-2-yl)oxy)methyl)-5-oxopirrolydine-2-carboxylate, 5b.

A mixture of **5** 40 mg, 0.15 mmol), NaH (7 mg, 1.8 mmol), **1-(R)** (35mg, 0.18 mmol) in dried THF was refluxed for 12 h, as a general procedure. the crude product was purified by column chromatography with n-hexane/Ethyl acetate to yield 28 mg of **5b** (45%). ^{1}H NMR (300 MHz, $CDCl_3$), δ 5.02 (d, J = 11.4 Hz, 3H), 4.72 (d, J = 11.4 Hz, 3H), 4.45 (dd, J = 8.9, 3.2 Hz, 5H), 4.14 (q, J = 6.9 Hz, 4H), 3.75 (s, 3H), 3.70 (s, 3H), 2.28-2.03 (m, 4H), 1.35 (d, J = 6.9 Hz, 9H). NMR-^{13}C (75 MHz, $CDCl_3$) δ 202.9, 176.2, 172.3, 144.3, 134.5, **79.1**, 72.5, **69.5**, 60.2, 58.1, 52.8, 47.5, 36.4, 33.4, 29.7, 25.8, 23.5, 23.0, 21.6, 22.8, 20.8, 18.9.

Methyl-(S)-1-(((S)-1-(naphtalen-2-yl)etoxy)methyl)-5-oxopyrrolidin-2-carboxylate, 6a.

A mixture of (S)-1-(naphtalen-2-yl)-ethan-1-ol **6** (69 mg, 0.40 mmol), **1-(S)** (86 mg, 0.45 mmol), HT (30 mg) and AgOTf (103 mg, 0.4 mmol) in dried DCM was stirred at room temperature for 6 h, as a general procedure. The crude product was purified by column chromatography with n-hexane/Ethyl acetate 80/20 to yield 61 mg of **8a** (46 %). ^{1}H NMR (300 MHz, $CDCl_3$), δ 7.84-7.76 (m, 4H), 7.51 – 7.41 (m, 3H), 5.06 (d, J = 10.6 Hz, 1H), 4.66 (q, J = 6.5 Hz, 1H), 4.41 (d, J = 10.84 Hz, 1H) , 4.38 (dd, J = 8.99, 3.45 Hz, 1H), 3.54 (s, 3H), 258-2.27 (m, 3H), 2.09-2.01 (m,1H), 1.50 (d, J = 6.5 Hz, 2H).NMR ^{13}C (75 MHz, $CDCl_3$) δ 175.8, 172.3, 140.3, 133.3, 133.2, 128.4, 128.0, 127.7, 126.2, 125.9, 125.5, 124.2, 75.8, 70.0, 57.9, 52.4, 29.7, 23.6, 22.9. DART^{+} m/z (rel intensity, %): [2M+2] 656 (12), [2M+1] 655 (28), 552 (12), 484 (15), 483 (40), 330 (20), 329 (100), 328 (16), 174 (14), 156 (32). ESI-HRMS m/z: $C_{19}H_{22}N_1O_4$ [M+1] calculated 328.15488, observed 328.15588. $[\alpha]_D^{20}$=-5.45° (c 0.22, $CHCl_3$),

Methyl-(R)-1-(((S)-1-(naphtalen-2-yl) ethoxy) methyl)-5-oxopyrrolidin-2-carboxylate, 6b.

A mixture of (S)-1-(naphtalen-2-yl)-ethan-1-ol **8** (35 mg, 0.420 mmol), **1-*(R)*** (46 mg, 0.24 mmol), HT (20 mg) and AgOTf (50 mg, 0.2 mmol) in dried DCM was stirred at room temperature for 6 h, as a

general procedure. the crude product was purified by column chromatography with n-hexane/Ethyl acetate 80/20 to yield 13 mg of **7b** (20 %). ^{1}H NMR (300 MHz, $CDCl_3$), δ 7.94 – 7.68 (m, 4H), 7.59 – 7.38 (m, 3H), 5.16 (d, J = 11.1 Hz, 1H), 4.70 (q, J = 6.6 Hz, 1H), 4.62 (d, J = 11.2 Hz, 1H) , 4.03 (dd, J = 9.5, 2.7 Hz, 1H), 3.74 (s, 3H), 2.49 – 2.16 (m, 3H), 1.94 – 1.58 (m, 1H), 1.49 (d, J = 6.5 Hz, 4H). NMR ^{13}C (75 MHz, $CDCl_3$) δ 175.8, 172.7, 141.3, 133.3, 133.1, 128.4, 128.0, 127.7, 126.4, 126.1, 124.8, 124.0, 77.9, 71.5, 57.9, 52.6, 29.5, 24.1, 22.3. DART^{+} m/z (rel intensity): [2M+2] 656 (13), [2M+1] 655 (30), 483 (30),[M+3] 330 (17), [M+2] 329 (100), 310 (24), 174 (25), 156 (94), 128 (32). ESI-HRMS m/z: $C_{19}H_{22}N_1O_4$ [M+1] calculated 328.15488, observed 328.15532$[\alpha]_D^{20}$= -20° (c 0.12, $CHCl_3$).

Methyl-(S)-1-(((S)-1-(2-bromophenyl) ethoxy) methyl)-5-oxopyrrolidine-2-carboxylate, 7a.

A mixture of (S)-(-)-2-Bromide- α-methyl benzyl alcohol **7** (50 mg, 0.25 mmol), 1-(S) (60 mg, 0.33 mmol), HT (20 mg) and AgOTf (77 mg, 0.33 mmol) in dried DCM was stirred at room temperature for 8 h, as a general procedure. The crude product was purified by column chromatography with n-hexane/Ethyl acetate 90/10 to yield 31 mg of **7a** (34 %). ^{1}H NMR (300 MHz, $CDCl_3$), δ 7.51 (d, J = 7.9 Hz, 1H), 7.46 (dd, J = 7.9, 1.5 Hz, 1H), 7.31 (t, J = 7.6 Hz, 1H), 7.12 (td, J = 7.6, 1.62 Hz, 1H), 5.00 (d, J = 10.4 Hz, 1H), 4.89 (q, J = 6.4 Hz, 1H), 4.44 (d, J = 10.4 Hz, 1H), 4.36 (dd, J = 9.0, 3.4 Hz, 1H), 3.66 (s, 3H), 2.57 – 2.7 (m, 3H), 2.15 – 2.03 (m, 1H), 1.4 (d, J = 6.39 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 175.5, 172.4, 142.3, 132.9, 129.0, 127.9, 127.1, 122.5, 74.5, 70.5, 58.1, 52.5, 29.7, 23.0, 22.5. DART^{+} m/z (rel intensity, %):[2M+1] 713 (18), 514 9), 513 (43), [M] 356 (13), 329 (67), 299 (3), 174 (18), 156 (100), 128 (32). ESI-HRMS m/z: $C_{15}H_{19}Br_1N_1O_4$ [M+1] calculated 356.04975, observed 356.05105. $[\alpha]_D^{20}$= -44.7° (c 0.275, $CHCl_3$).

Methyl-(R)-1-(((S)-1-(2-bromophenyl)ethoxy)methyl)-5-oxopyrrolidine-2-carboxylate, 7b.

A mixture of (S)-(-)-2-Bromide- α-methyl benzyl alcohol **7** (50 mg, 0.25 mmol), **1-*(R)*** (60 mg, 0.33 mmol), HT (20 mg) and AgOTf (77 mg, 0.33 mmol) in dried DCM was stirred at room temperature for 8 h, as a general procedure. The crude product was purified by column chromatography with n-hexane/Ethyl acetate 90/10 to yield 64 mg of **7b** (71 %). ^{1}H NMR (300 MHz, $CDCl_3$), δ 7.50-7.45 (m, 2H), 7.32 (td, J = 7.5, 1.3 Hz, 1H), 7.10 (td, J = 7.79, 1.84 Hz, 1H), 5.11 (d, J = 10.8 Hz, 1H), 4.92 (q, J = 6.4 Hz, 1H), 4.49 (d, J = 10.8 Hz, 1H), 4.21 – 4.13 (m, 1H), 3.73 (s, 3H), 2.48- 2.37 (m, 1H), 2.24 – 2.11 (m, 1H), 2.03 – 1.88 (m, 2H), 1.38 (d, J = 6.4 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 175.5, 172.5, 142.9, 132.8, 128.8, 127.8, 127.3, 122.0, 75.3, 71.0, 58.1, 52.5, 29.5, 22.7, 22.3. DART^{+} ^{m}/z (rel intensity): [2M+1] 713 (9), 511 (34), [M] 356 (15), 329 (66), 299 (19), 174 (16), 156 (100), 128 (35). ESI-HRMS m/z: $C_{15}H_{19}Br_1N_1O_4$ [M+1] calculated 356.04975, observed 356.04896. $[\alpha]_D^{20}$= -10.9635 (c 0.602, $CHCl_3$)

Methyl-(S)-1-((((S)-1-methoxy-1-oxopropan-2-yl)oxy)methyl)-5-oxopyrrolydin-2-carboxylate, 8a.

A mixture of Methyl (S)-Lactate **6** (56 mg, 0.54 mmol), **1-(S)** (124 mg, 0.65 mmol), HT (25 mg) and AgOTf (166 mg, 0.65 mmol) in dried DCM was stirred at room temperature by 6 h, as a general procedure. the crude product was purified by column chromatography with n-hexane/Ethyl acetate 50/50 to yield 44 mg of **6a** (31%). ^{1}H NMR (300 MHz, $CDCl_3$), δ 5.10 (d, J = 10.8 Hz, 1H), 4.58 (d, J = 10.8 Hz, 1H), 4.42 (dd, J = 8.7, 3.3 Hz, 2H), 4.11 (q, J = 6.9 Hz, 1H), 3.75 (s, 3H), 3.73 (s, 3H), 2.60-2.29 (m. 4H), 1.38 (d, J = 6.9 Hz, 3H). NMR-^{13}C (75 MHz, $CDCl_3$) δ 176.1, 173.2, 172.4, 72.1, 71.0, 57.9, 52.6, 52.2, 29.6, 23.1, 18.5. DART^{+} m/z (rel intensity %): 440 (18), [M+2] 426(14), [M+K]299(33), 285(100), 271(76), 228 (10), 156 (68), 144 (66), 130(56), 102(55). ESI-HRMS m/z: $C_{11}H_{18}N_1O_6$ [M+1] calculated 260.11341 observed. 260.11224. $[\alpha]_D^{20}$=-29.54° (c 0.44, $CHCl_3$).

Methyl-(R)-1-((((S)-1-methoxy-1-oxopropan-2-yl) oxy)methyl)-5-oxopyrrolydin-2-carboxylate, 8b.

A mixture of methyl (S)-Lactate **6** (57 mg, 0.54 mmol), **1-(R)** (124 mg, 0.65 mmol), HT (25 mg) and AgOTf (166 mg, 0.65 mmol) in dried DCM was stirred at room temperature for 6 h, as a general procedure. The crude product was purified by column chromatography with n-hexane/Ethyl acetate 50/50 to yield 24 mg of **6a** (17 %). ^{1}H NMR (300 MHz, $CDCl_3$), δ: 5.02 (d, J = 11.4 Hz, 3H), 4.72 (d, J = 11.4 Hz, 3H), 4.45 (dd, J = 8.9, 3.2 Hz, 5H), 4.14 (q, J = 6.9 Hz, 4H), 3.75 (s, 3H), 3.70 (s, 3H), 2.28-2.03 (m, 4H), 1.35 (d, J = 6.9 Hz, 9H). ^{13}C NMR- (75 MHz, $CDCl_3$) δ 176.3, 173.7, 172.6, 73.5, 71.8, 58.3, 52.6, 52.1, 29.6, 23.0, 18.6. DART^{+} m/z (rel intensity %): [2M+1] 518 (4), 415 (14), [M+2] 261 (12), [M+1] 260 (100), 156 (41). ESI-HRMS m/z: $C_{11}H_{18}N_1O_5$ [M+1] calculated 260.11341 observed. 260.113003. $[\alpha]_D^{20}$= -9.92° (c 0.252, $CHCl_3$)

One derivatization product

Hispanolone reduction to *β*-alcohol, 9.
(1R,2R,3R,8aS)-1-(2-(furan-3-yl)ethyl)-2,5,5,8a-tetramethyldecahydronaphthalene-1,3-diol. *β*-alcohol of hispanolone.

$NaBH_4$ (300 mg, 0.94 mmol) was added to solution of Hispanolone (300 mg, 0.94 mmol) in dried methanol (10 mL), at 0 °C, the mixture was stirred for 16 h. sulfuric acid was added, then mixture was concentrated and dissolved in Ethyl acetate, extracted with water. Organic extracts were dried over anhydrous sodium sulfate, filtered, and concentrated. The crude product was purified by column chromatography with n-hexane/Ethyl acetate 90/10 to yield 60 mg of α-alcohol (20 %) m.p. 129 °C, 134 mg of BO_3 derivative (35%) m.p. 205°C, and 45 mg (15%) *β*-alcohol, m.p, 105°C ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.33 (t, *J* = 1.6 Hz, 1H), 7.23 – 7.17 (m, 1H), 6.26 (dd, *J* = 1.8, 0.9 Hz, 1H), 3.49 (td, *J* = 10.7, 5.2 Hz, 1H), 2.59 – 2.36 (m, 3H), 1.95 – 1.24 (m, 23H), 1.10 (d, *J* = 6.6 Hz, 2H), 0.96 (s, 2H), 0.87 (d, *J* = 10.7 Hz, 5H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 143.0, 138.6, 125.4, 110.9, 78.7, 73.2, 44.4, 44.0, 43.1, 41.7, 35.4, 33.7, 33.3, 32.3, 31.7, 22.1, 21.7, 18.6, 16.5, 11.5.

Methyl (2S)-1-((((2R,3R,4R,4aS)-4-(2-(furan-3-yl)ethyl)-4-hydroxy-3,4a,8,8-tetramethyldecahydronaphthalen-2-yl)oxy)methyl)-5-oxopyrrolidine-2-carboxylate, 9.1

A mixture of ***β*-alcohol of hispanolone** (32 mg, 0.1 mmol), NaH (6 mg, 0.4 mmol), **1-(S)** (57 mg, 0.3 mmol) in dried THF was stirred 3 h in Microwave at 100°C, as a general procedure. the crude product was purified by column chromatography with n-hexane/Ethyl acetate to yield 20 mg of **9** (40%). ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.35 (t, *J* = 1.7 Hz, 1H), 7.22 (dd, *J* = 1.6, 0.9 Hz, 1H), 6.28 – 6.26 (m, 2H), 5.28 (d, *J* = 10.0 Hz, 1H), 4.48 (dd, *J* = 8.6, 3.5 Hz, 1H), 4.43 (d, *J* = 9.9 Hz, 1H), 3.78 (s, 3H), 3.29 (td, *J* = 10.7, 5.1 Hz, 1H), 2.65 – 2.28 (m, 3H), 2.21 – 2.04 (m, 1H), 1.95 – 1.79 (m, 2H), 1.80 – 1.65 (m, 2H), 1.57 (s, 9H), 1.54 – 1.13 (m, 7H), 1.06 (d, *J* = 6.5 Hz, 3H), 0.95 (s, 3H), 0.87 (d, *J* = 10.2 Hz, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 175.1, 172.2, 142.9, 138.5, 125.2, 110.8, 80.9, 78.4, 77.2, 72.0, 57.7, 52.5, 43.5, 42.8, 42.8, 41.5, 35.2, 33.5, 33.2, 32.0, 29.7, 28.5, 22.9, 21.9, 21.5, 18.5, 16.3, 11.3.

Mixture of Methyl (2S)-1-((((2R,3R,3aR,4aS,4bS,8R,10aR)-2-hydroxy-3,7,7,10a-tetramethyltetradecahydro-3,4b-methanonaphtho[2',1':3,4]cyclohepta[1,2-b]oxiren-8-yl)oxy)methyl)-5-oxopyrrolidine-2-carboxylate--methyl (2S)-1-((((2R,3R,3aR,4aS,4bS,8R,10aR)-8-hydroxy-3,7,7,10a-tetramethyltetradecahydro-3,4b-methanonaphtho[2',1':3,4]cyclohepta[1,2-b]oxiren-2-yl)oxy)methyl)-5-oxopyrrolidine-2-carboxylate, 10.1 and **methyl (2S)-1-((((2R,3R,3aR,4aS,4bS,8R,10aR)-8-hydroxy-3,7,7,10a-tetramethyltetradecahydro-3,4b-methanonaphtho[2',1':3,4]cyclohepta[1,2-b]oxiren-2-yl)oxy)methyl)-5-oxopyrrolidine-2-carboxylate, 10.2.**

A mixture of ***epoxide beyerene of Viguiera insignis*** (40 mg, 0.12 mmol), NaH (11 mg, 0.8 mmol), **1-(S)** (77 mg, 0.4 mmol) in dried THF was stirred 3 h in Microwave at 110°C, as a general procedure. the crude product was purified by column chromatography with n-hexane/Ethyl acetate 70/30 to yield 34 mg (30%) of **a mixture of 10.1 and 10.2**. ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.22 (t, *J* = 10.7 Hz, 1H), 4.41 (ddt, *J* = 11.2, 6.2, 3.6 Hz, 4H), 3.78 (d, *J* = 1.0 Hz, 3H), 3.50 – 3.42 (m, 1H), 3.37 (d, *J* = 2.9 Hz, 1H), 3.22 (dd, *J* = 11.5, 4.5 Hz, 1H), 3.00 (dd, *J* = 10.9, 2.8 Hz, 1H), 2.91 (dd, *J* = 11.6, 4.2 Hz, 1H), 2.60 – 2.24 (m, 4H), 1.98 – 1.83 (m, 1H), 1.62 (d, *J* = 19.1 Hz, 2H), 1.26 (s, 1H), 1.11 (s, 2H), 1.03 (s, 2H), 0.91 (d, *J* = 2.1 Hz, 7H), 0.80 (d, *J* = 8.3 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 175.9, 175.8, 172.3, 172.2, 83.7, 78.8, 77.2, 77.2, 72.1, 69.3, 69.1, 59.6, 59.2, 57.7, 57.6, 55.7, 55.5, 55.4, 55.1, 52.6, 52.5, 52.0, 51.6, 44.6, 44.3, 44.0, 43.9, 39.0, 38.8, 38.7, 38.3, 37.4, 37.1, 36.9, 36.8, 32.7, 29.7, 29.3, 28.8, 28.2, 28.2, 27.2, 23.9, 22.9, 22.1, 19.5, 18.1, 17.7, 16.2, 15.9, 15.6.

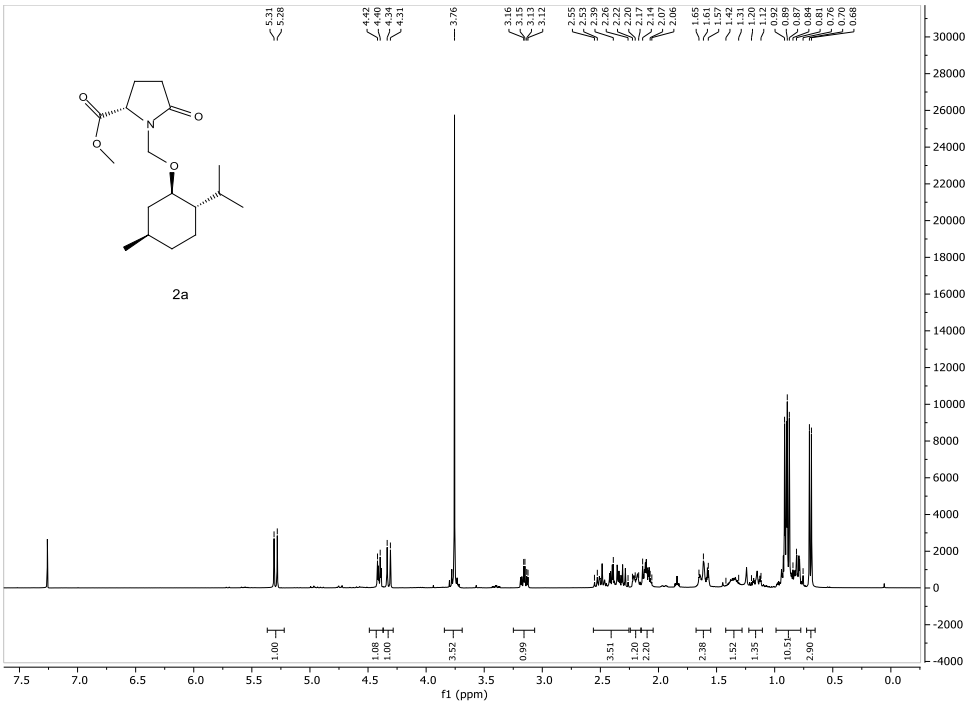
Isoborneol/Borneol

A mixture of dry methanol (10 mL) and (-)-camphor (100 mg, 0.65 mmol) was stirred into round-bottom flask, then sodium borohydride (59 mg, 1.58 mmol) was added into the solution, and stirred for 1 h. The mixture was poured into ice water (15 mL) and filtrated under vacuum, to yield 63 mg (66.8%) of (+)-Isoborneol/(-)-borneol.

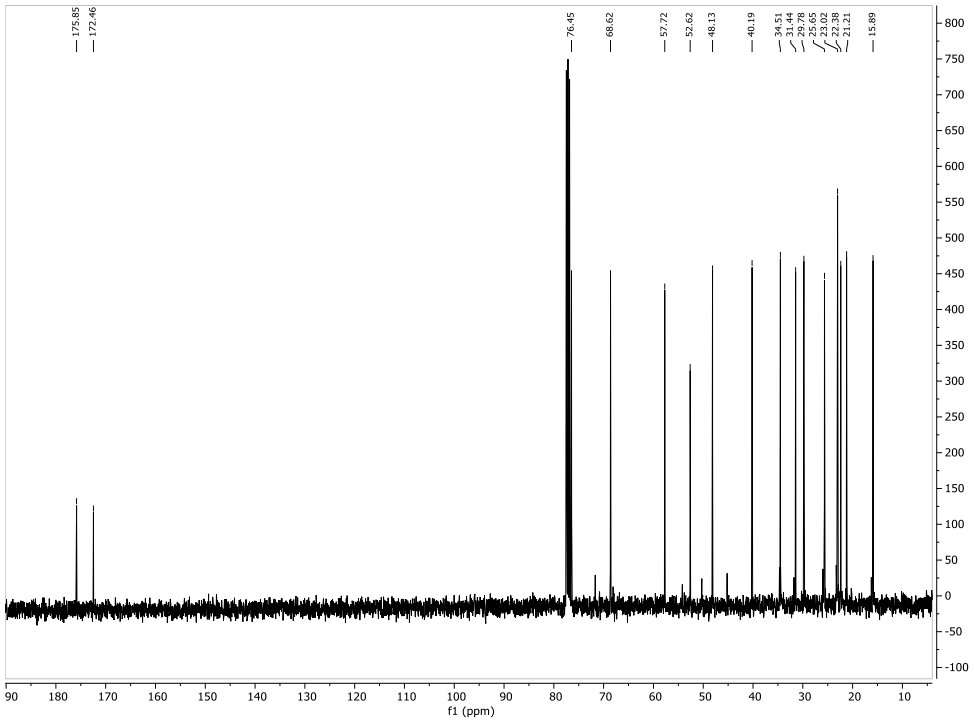
Mixture of methyl **5-oxo-1-((((1S,2R,4S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl)oxy)methyl)pyrrolidine-2-carboxylate** and **methyl 5-oxo-1-((((1S,2S,4S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl)oxy)methyl)pyrrolidine-2-carboxylate. 11.1 and 12.1**

A mixture of 80/20 (+)-isoborneo/(-)-borneol (50 mg, 0.25 mmol), **1-(S)** (60 mg, 0.33 mmol), HT (20 mg) and AgOTf (77 mg, 0.33 mmol) in dried DCM was stirred at room temperature for 8 h, as a general procedure. The crude product was purified by column chromatography with n-hexane/Ethyl acetate 90/10 to yield 31 mg of **11.1** and **12.1** ^{1}H NMR (300 MHz, $CDCl_3$) δ 5.05 (d, *J* = 10.5 Hz, 0.2H), 4.99 (d, *J* = 10.5 Hz, 1H), 4.46 (d, *J* = 10.5 Hz, 1H), 4.44 (d, *J* = 10.5 Hz, 0.2H), 4.30 (dd, *J* = 8.7, 3.3 Hz, 1H), 3.73 (s, 1H), 3.72 (s, 3H), 3.35 – 3.24 (m, 1H), 2.60 – 1.98 (m, 5H), 1.77 – 1.35 (m, 5H), 0.95 (td, *J* = 7.3, 6.4, 2.9 Hz, 1H), 0.89 (s, 3H), 0.83 (s, 3H), 0.79 (s, 1H), 0.77 (s,), 0.75 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 175.6, 175.5, 172.4, 86.5, 82.4, 72.2, 70.8, 57.8, 57.5, 52.4, 49.2, 48.9, 47.8, 46.6, 45.1, 44.9, 39.1, 35.9, 34.3, 29.9, 29.8, 29.7, 28.2, 27.1, 26.5, 23.1, 23.0, 20.2, 20.2, 19.8, 18.9.

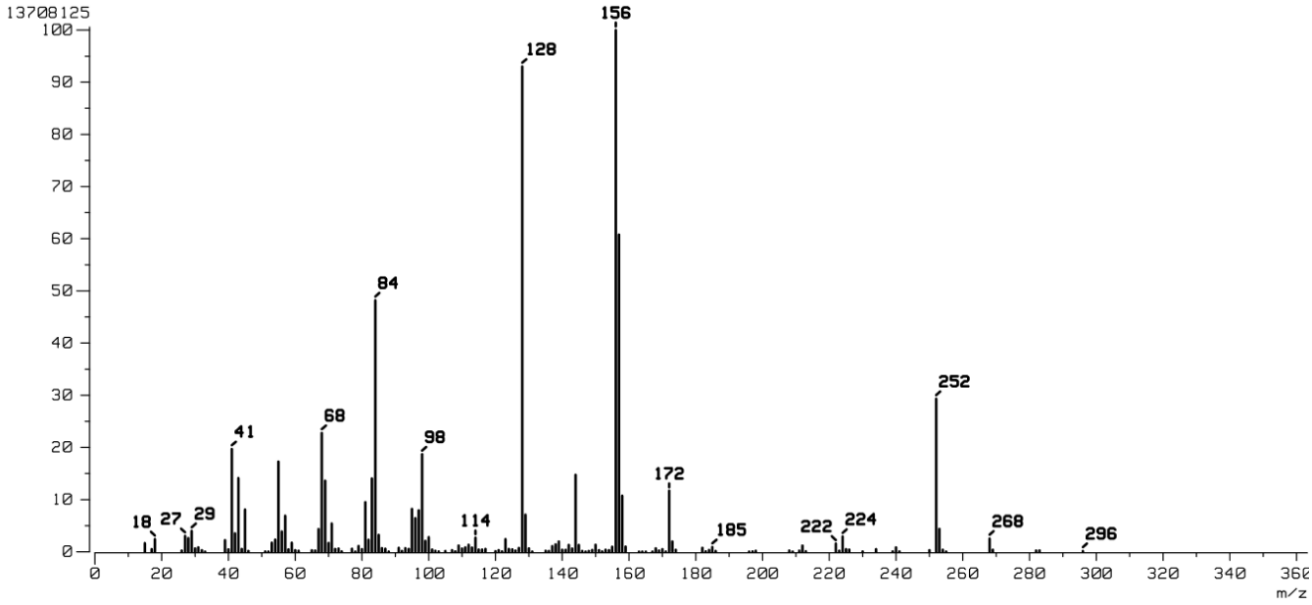
3. NMR spectra



S 1.NMR-^{1}H (400.1 MHz, $CDCl_3$) of 2a



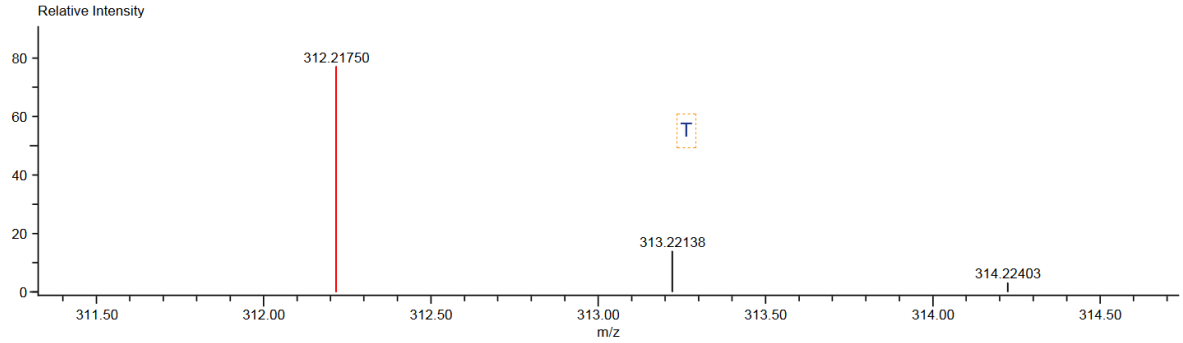
S 2. NMR-^{13}C (100.6 MHz, $CDCl_3$) of 2a



S 3. ESI-MS of 2a

Charge number:1 Tolerance:3.00(mmu) Unsaturation Number:0.0 .. 30.0 (Fraction:Both)

Element:^{12}C:0 .. 40, ^{1}H:0 .. 60, ^{14}N:0 .. 4, ^{16}O:4 .. 4



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
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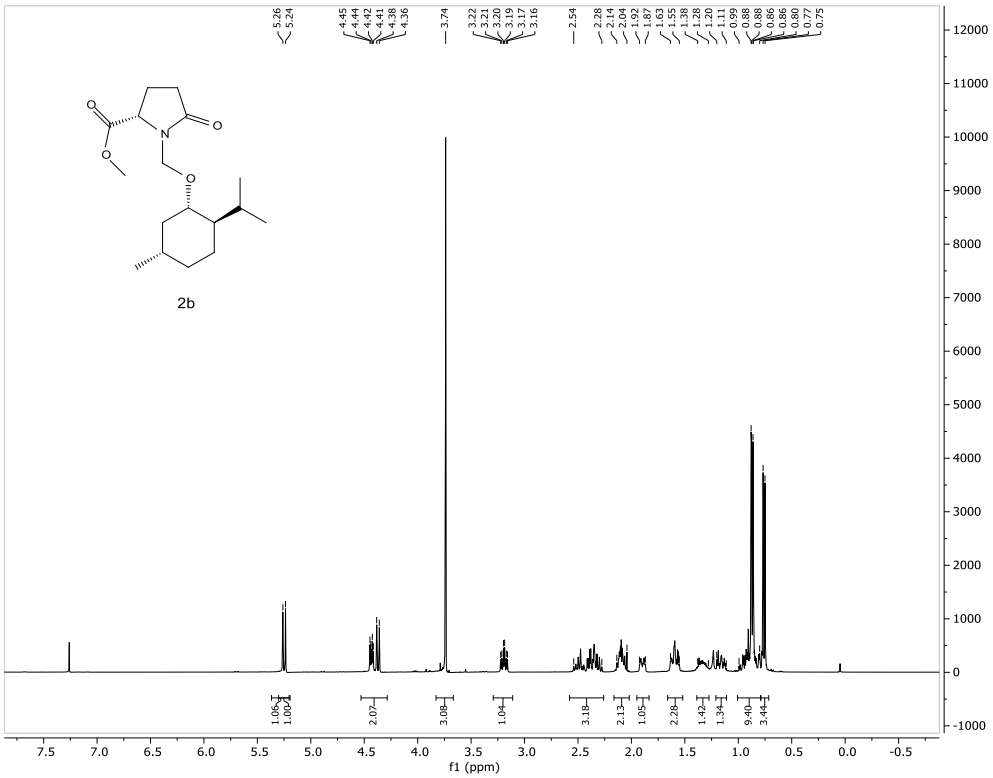
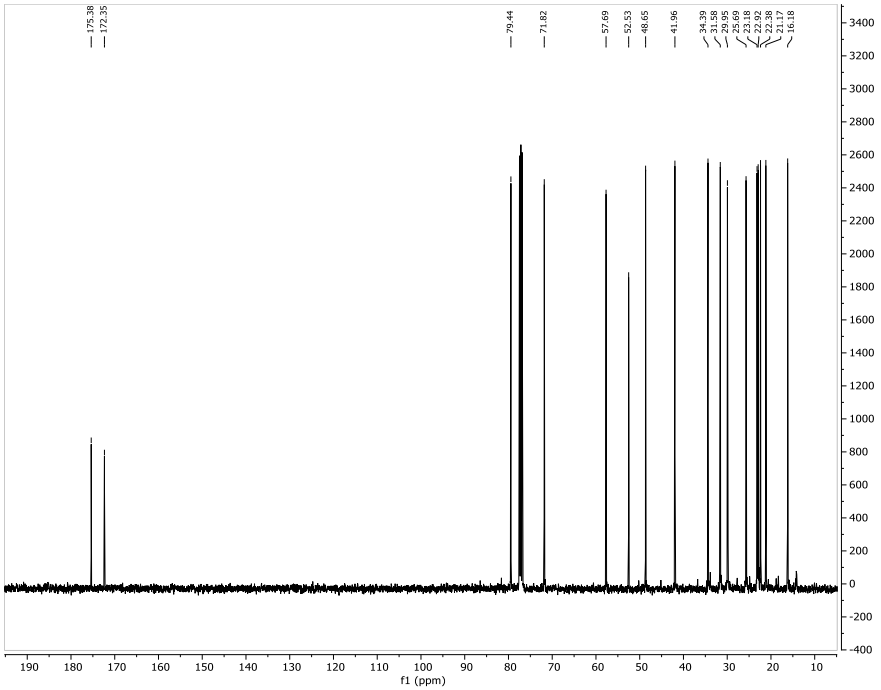
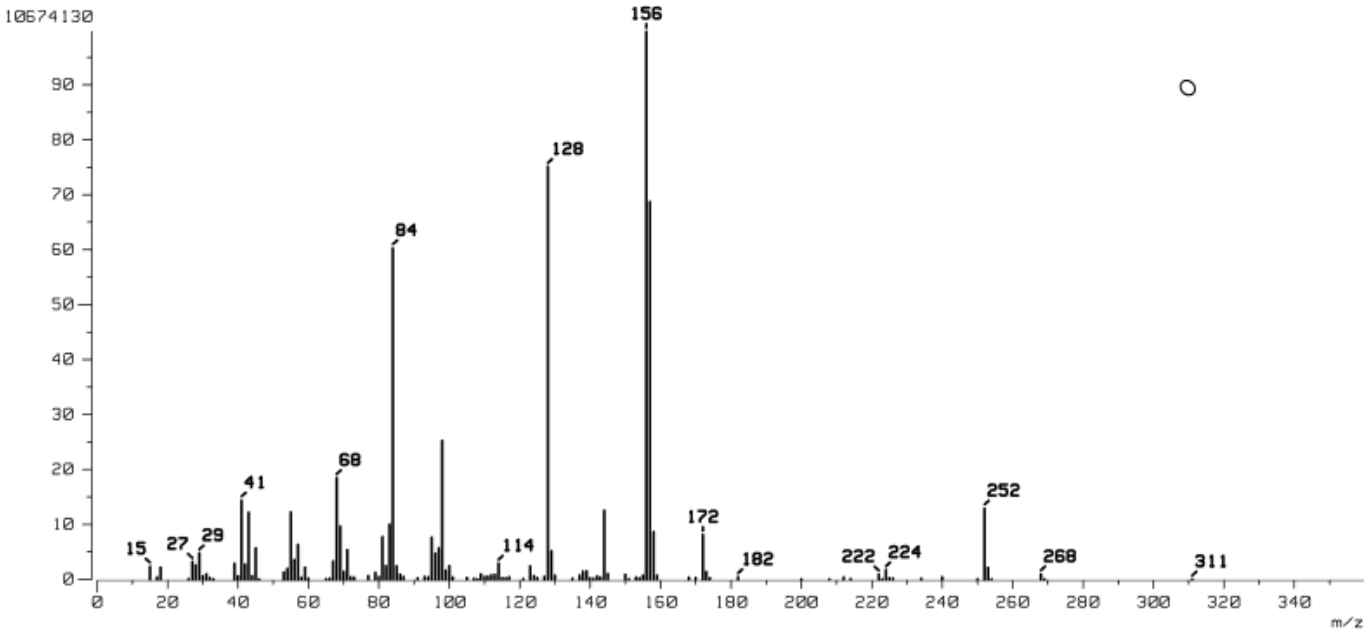
S 4. ESI-HRMS of 2a



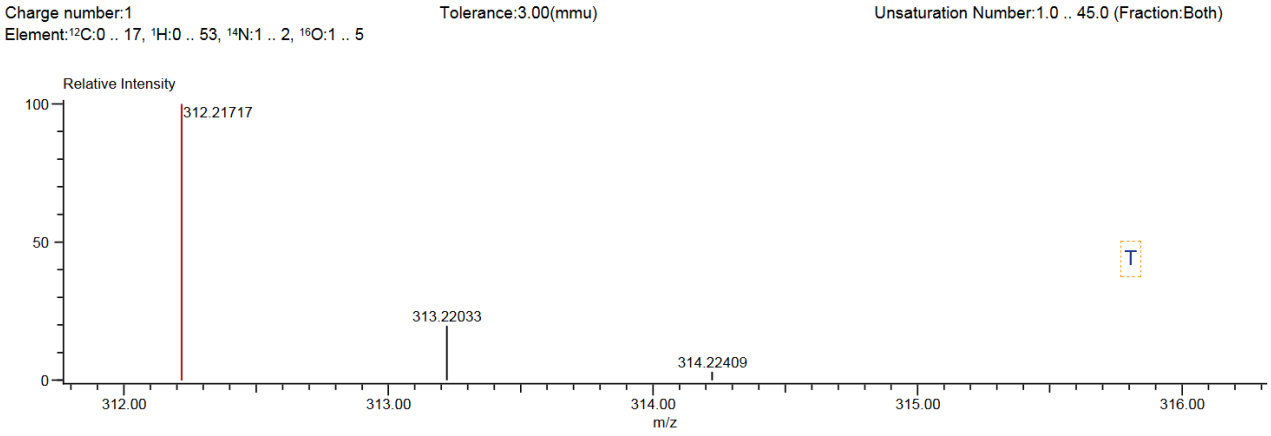
S 5. NMR-^{1}H (400.1 MHz, $CDCl_3$) of 2b



S 6. NMR-^{13}C (100.6 MHz, $CDCl_3$) of 2b.



S. 7. DART⁺ of 2b



Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
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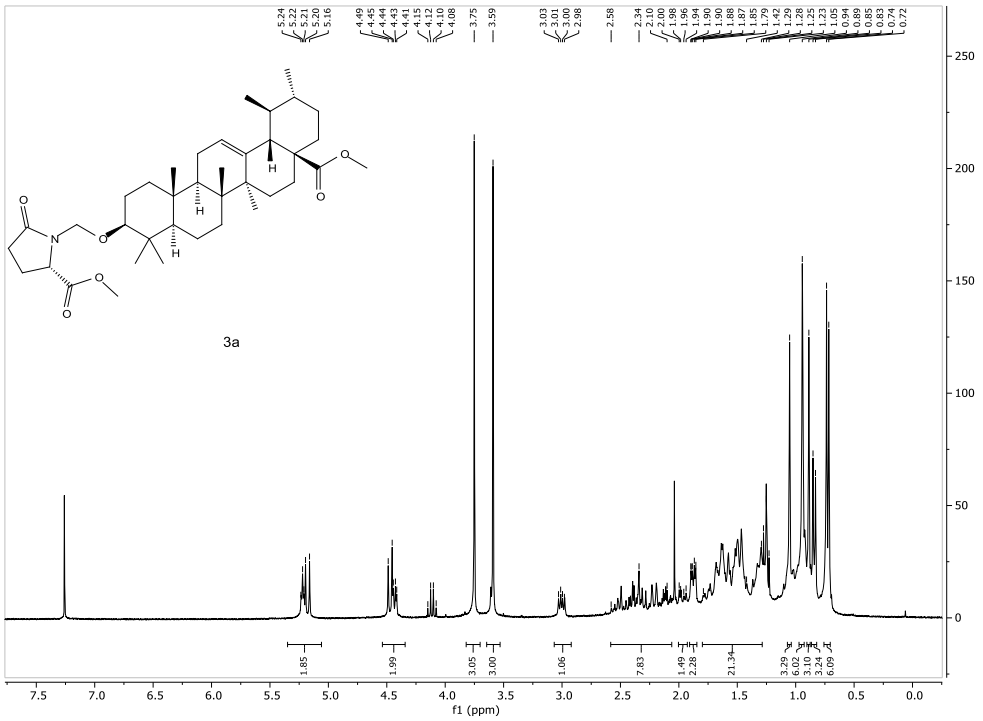
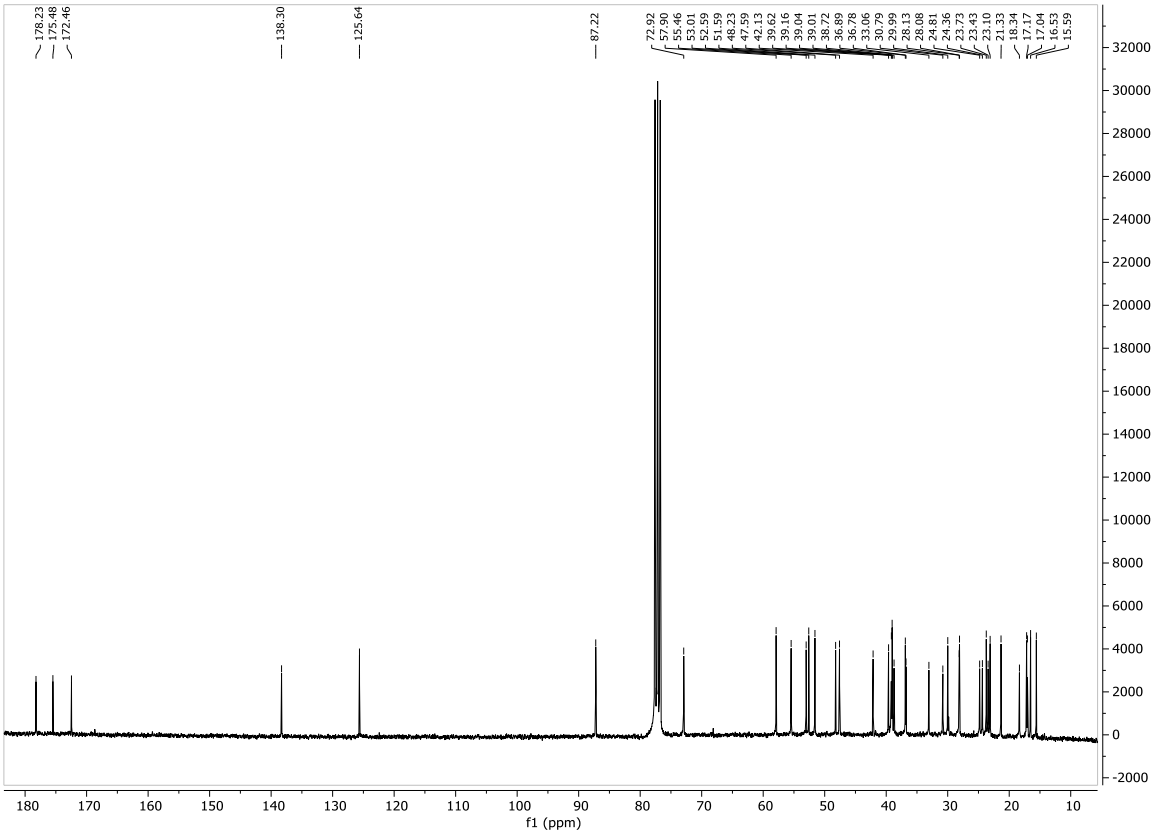
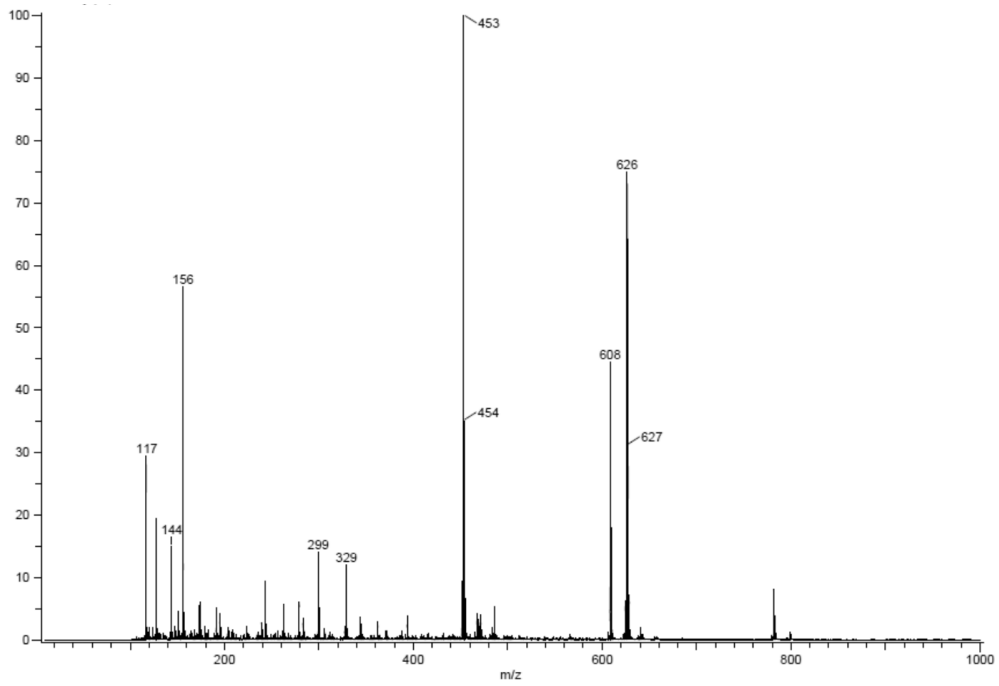
S 8. ES-HRMS⁺ of 2b



S 9. NMR-^{1}H (300 MHz, $CDCl_3$) of 3a.



S 10. NMR-^{13}C (75 MHz, $CDCl_3$) of 3a.

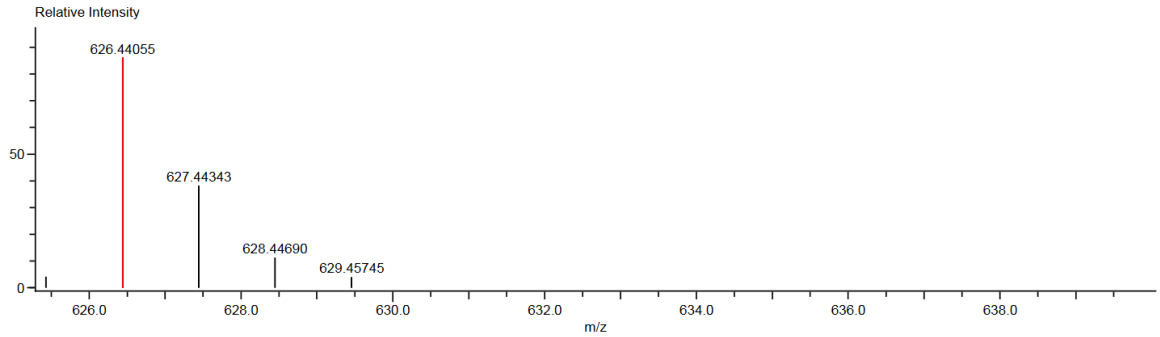


S 11. DART+ of 3a

Charge number:1
Element:^{12}C:0 .. 40, ^{1}H:0 .. 80, ^{14}N:0 .. 1, ^{16}O:0 .. 6

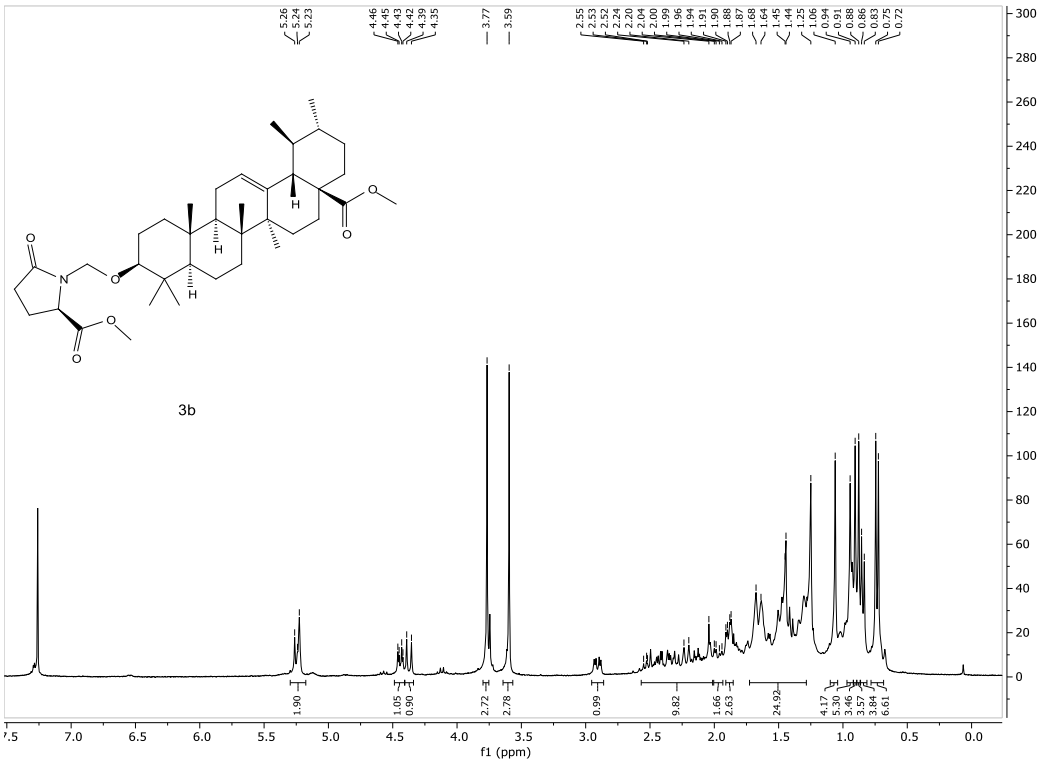
Tolerance:3.00(ppm), 5.00 .. 15.00(mmu)

Unsaturation Number:0.0 .. 60.0 (Fraction:Both)

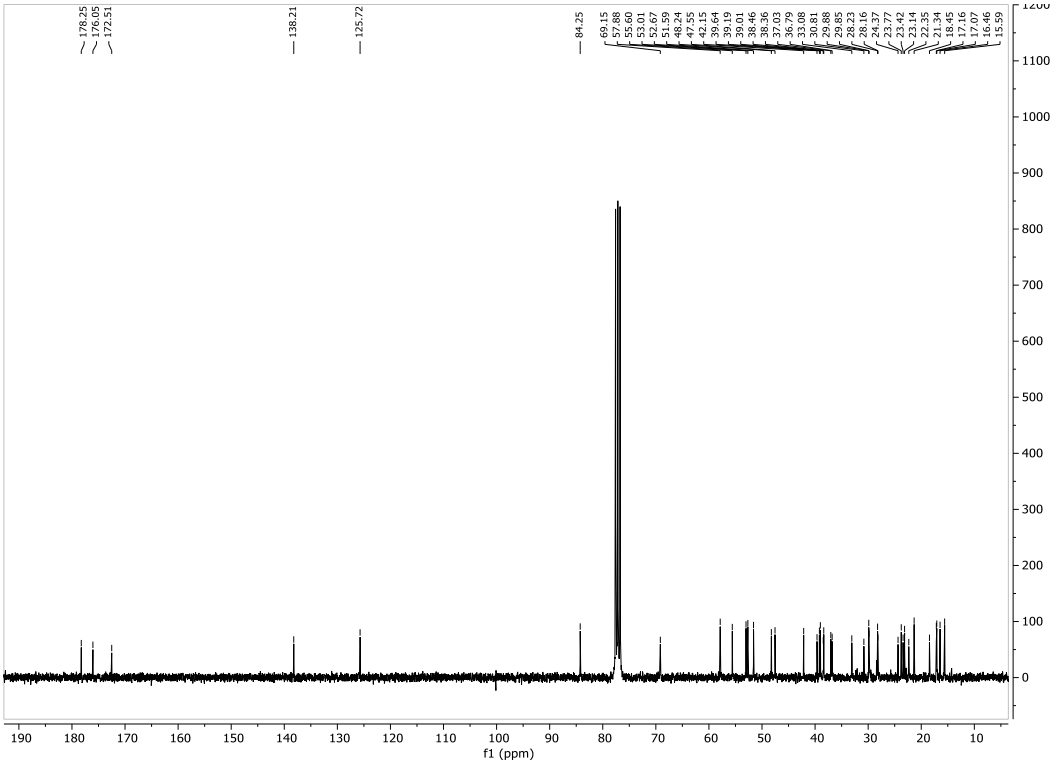


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
626.44055	2092054.95	626.44206	-1.51	-2.41	$^{12}C_{38}{}^{1}H_{60}{}^{14}N_{1}{}^{16}O_{6}$	9.5

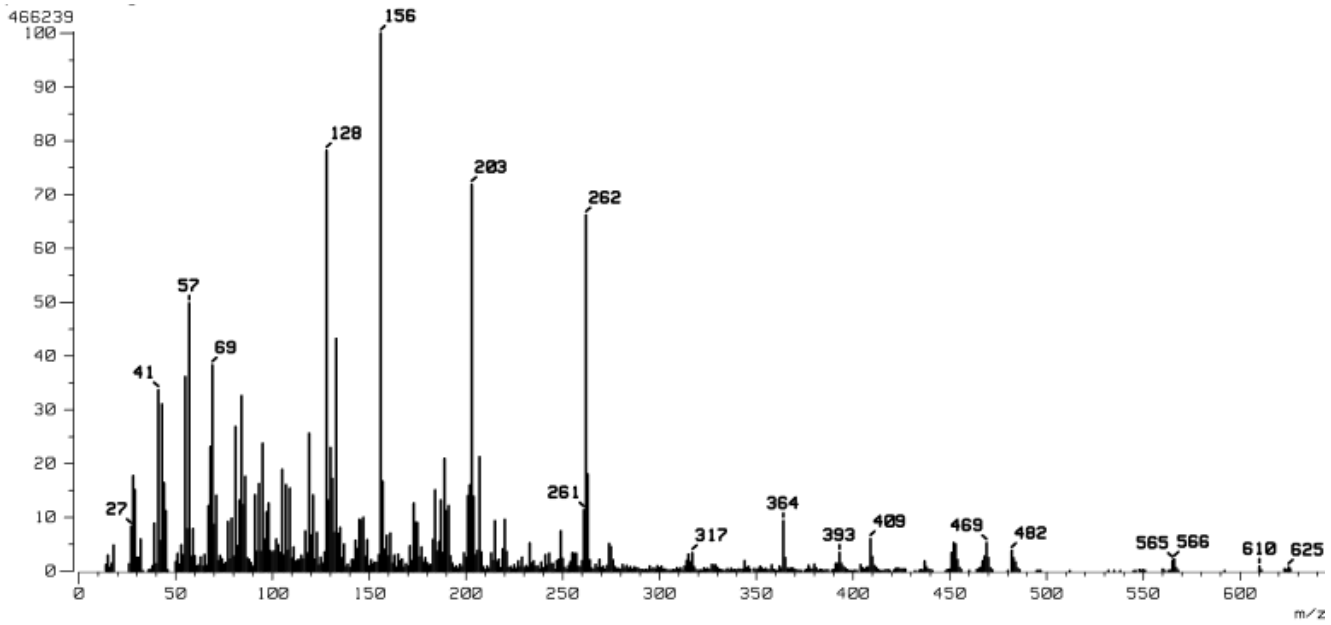
S 12. ESI-HRMS of 3 a



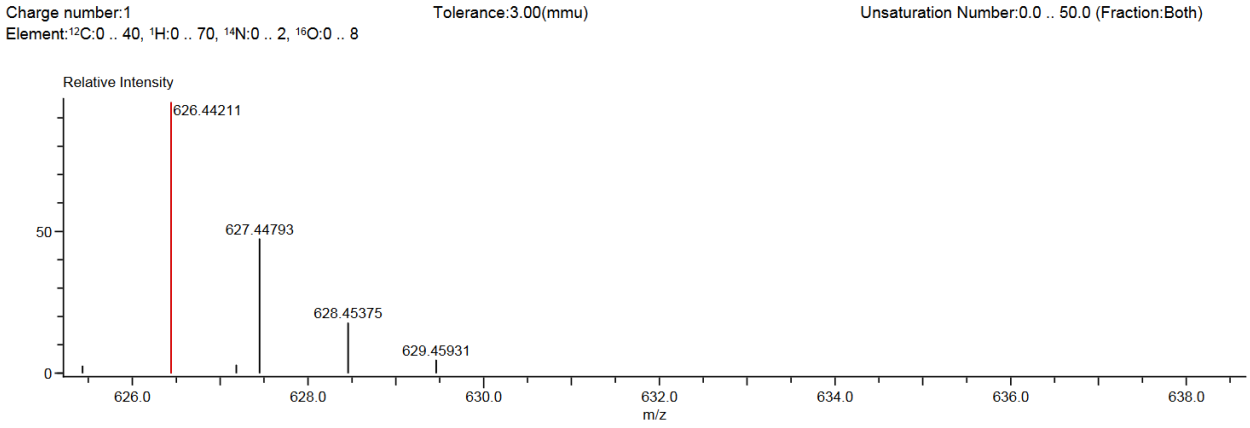
S 13. NMR-^{1}H (300 MHz, $CDCl_3$) of 3b.



S 14. NMR-^{13}C (75 MHz, $CDCl_3$) of 3a

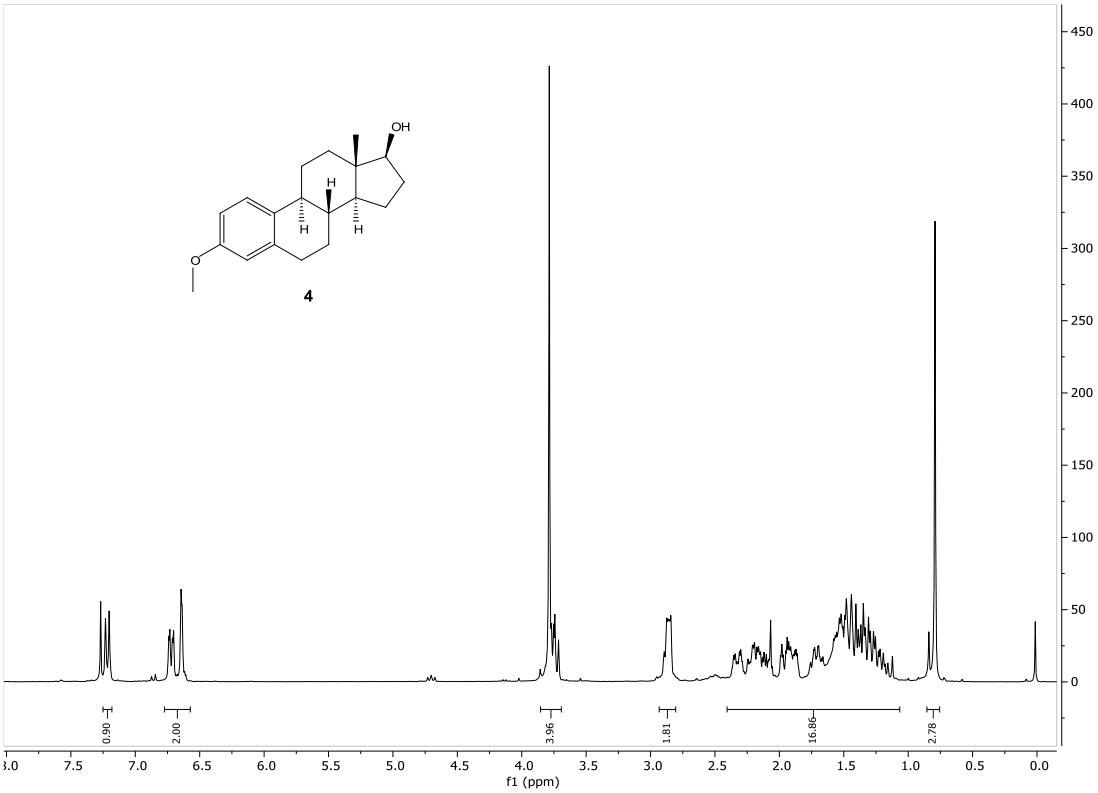


S 15. ESI-MS of 3b

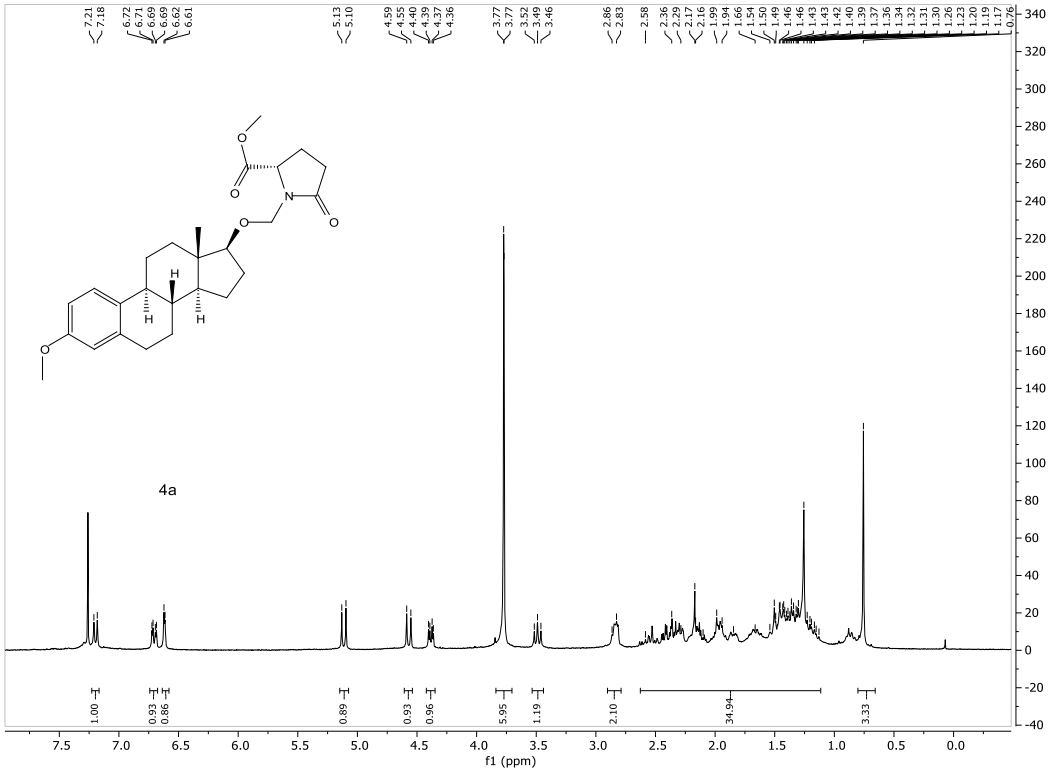


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
626.44211	13539.87	626.44206	0.05	0.08	$^{12}C_{38}{}^{1}H_{60}{}^{14}N_{1}{}^{16}O_{6}$	9.5

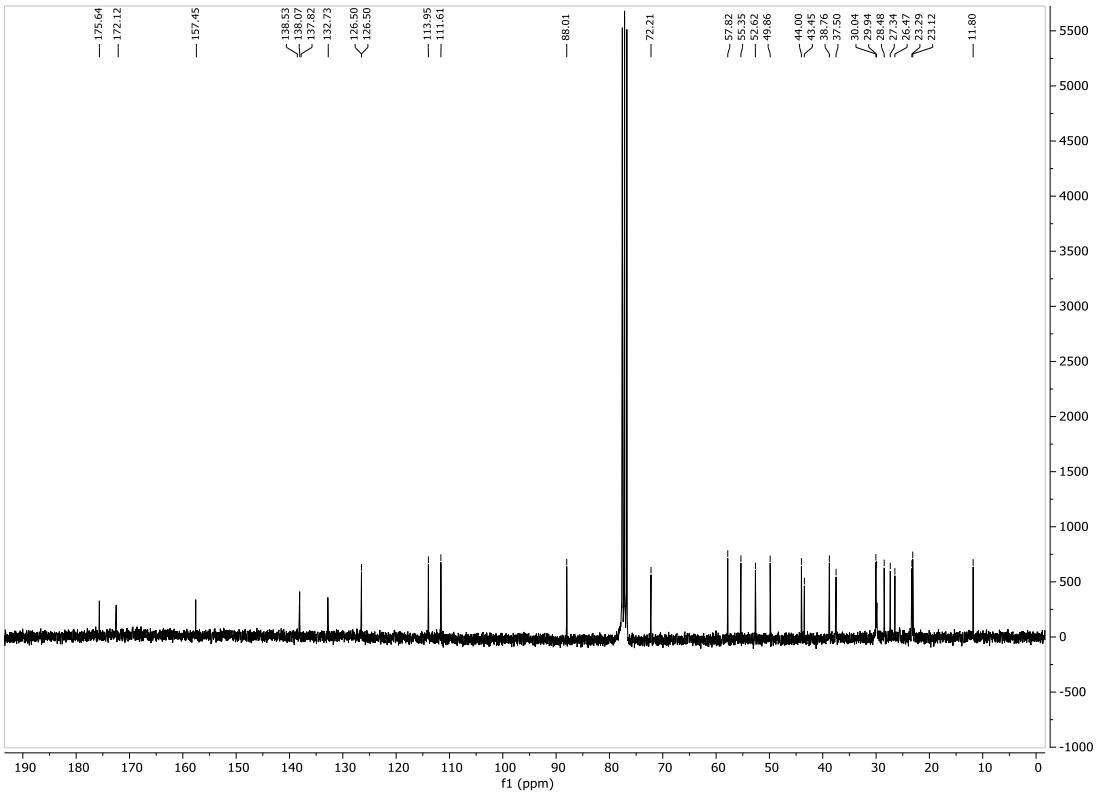
S 16. ESI-HRMS of 3b



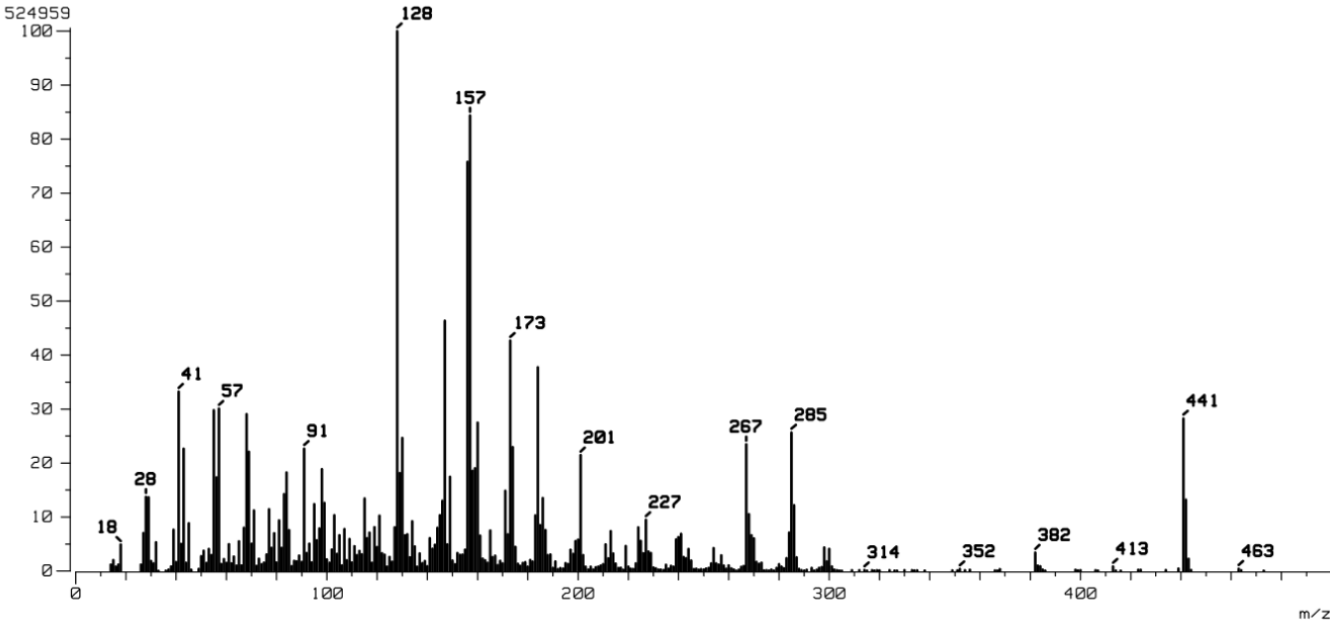
S 17. NMR-^{1}H (300 MHz, $CDCl_3$) of 4



S 18. NMR-^{1}H (300 MHz, $CDCl_3$) of 4a

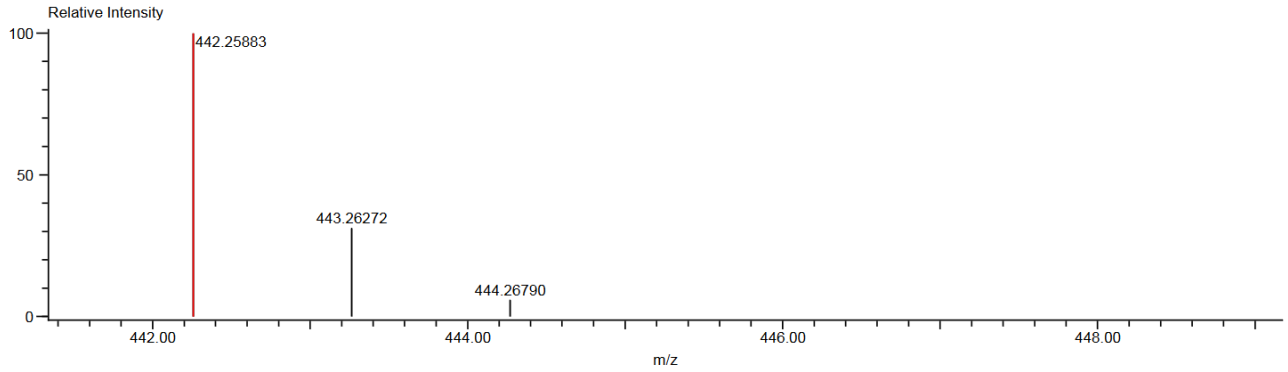


S 19. NMR-^{13}C (75 MHz, $CDCl_3$) of 4a.



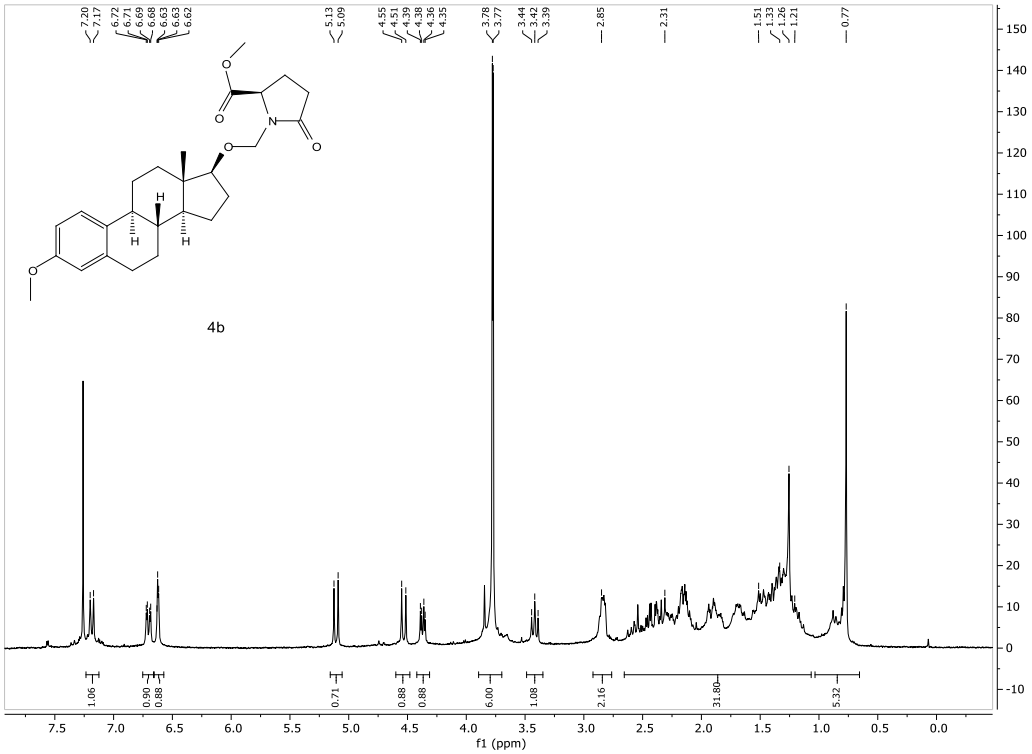
S 20. ESI-MS of 4a

Charge number:1 Tolerance:3.00(mmu) Unsaturation Number:0.0 .. 50.0 (Fraction:Both)
Element:^{12}C:0 .. 40, ^{1}H:0 .. 70, ^{14}N:0 .. 2, ^{16}O:0 .. 5

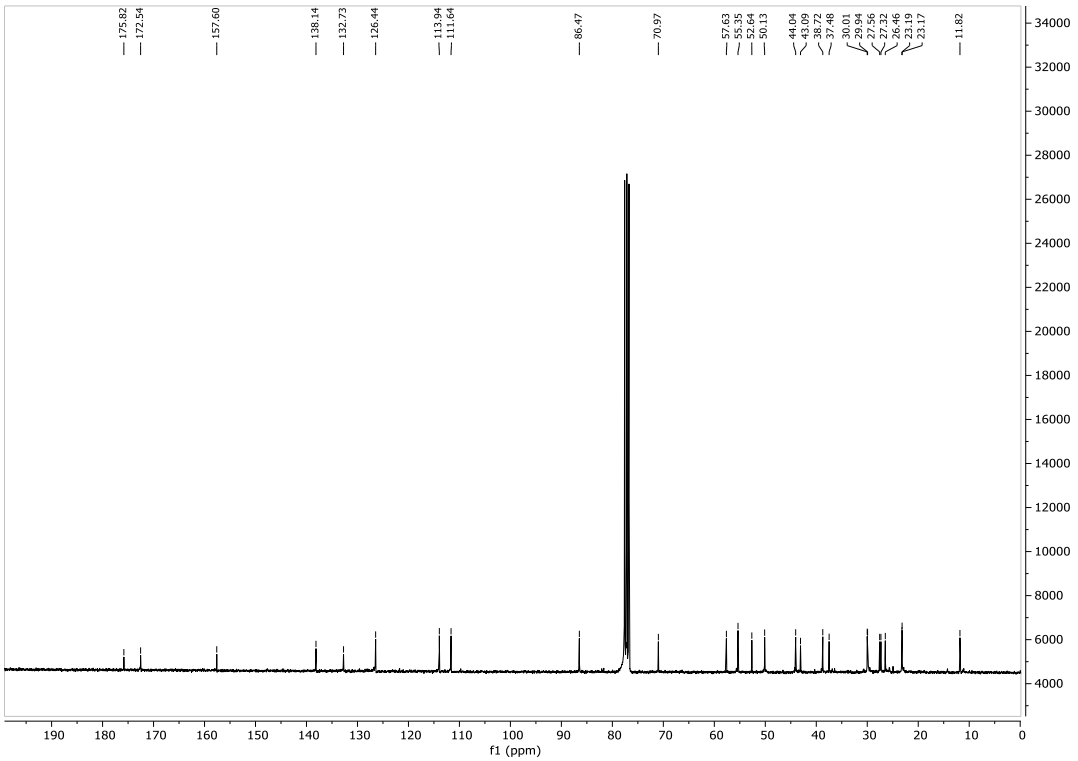


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
442.25883	338260.88	442.25935	-0.52	-1.17	$^{12}C_{26}{}^{1}H_{36}{}^{14}N_{1}{}^{16}O_{5}$	9.5

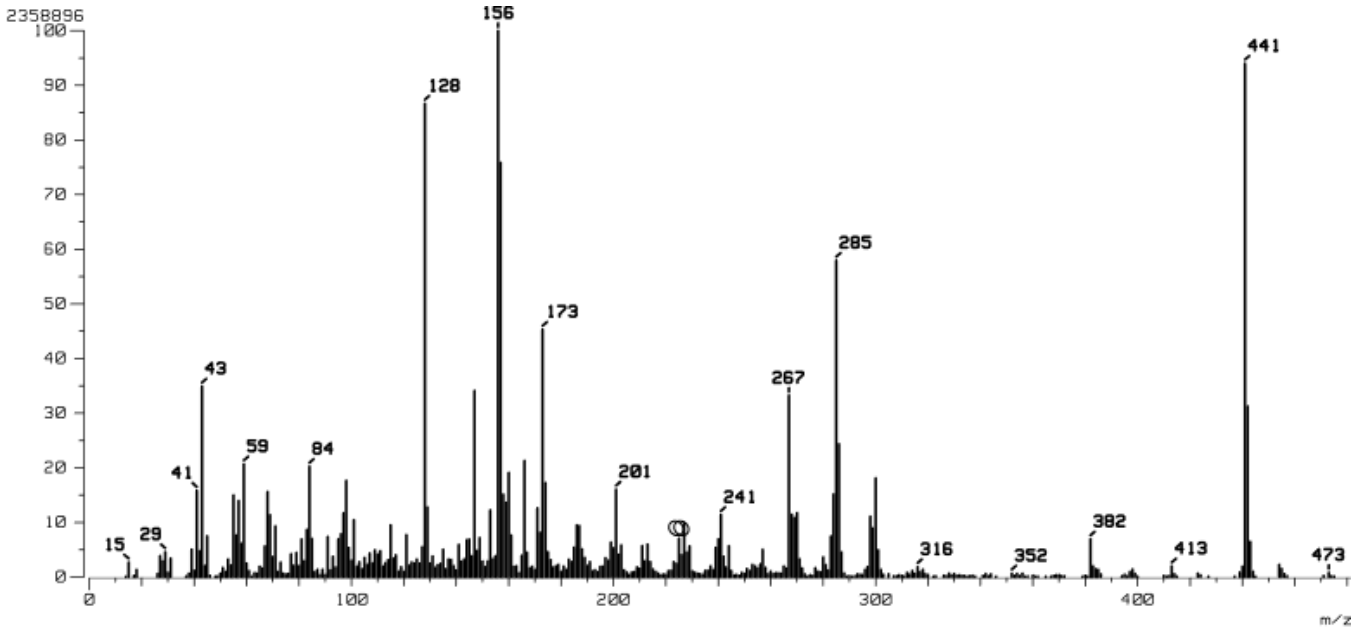
S 21. ESI-HRMS of 4a.



S 22. NMR-^{1}H (300 MHz, $CDCl_3$) of 4b.

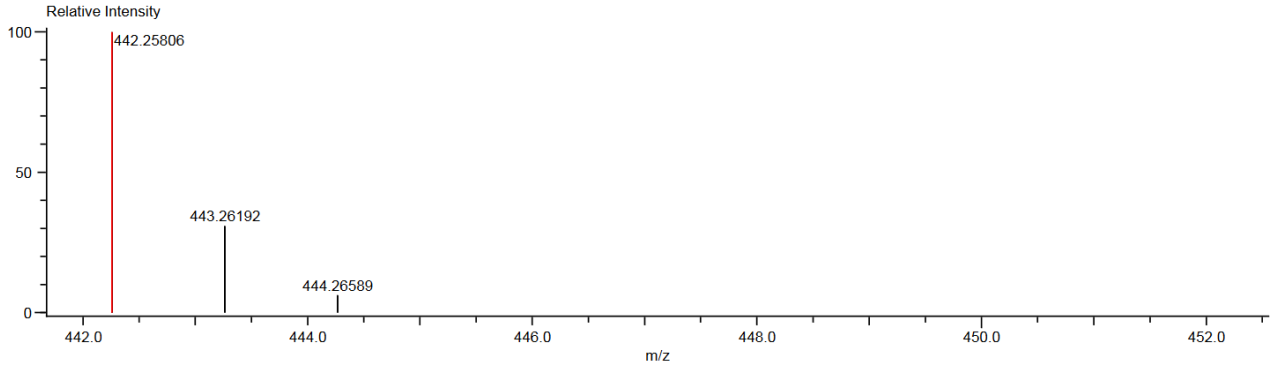


S 23. NMR-^{13}C (75 MHz, $CDCl_3$) of 4b.



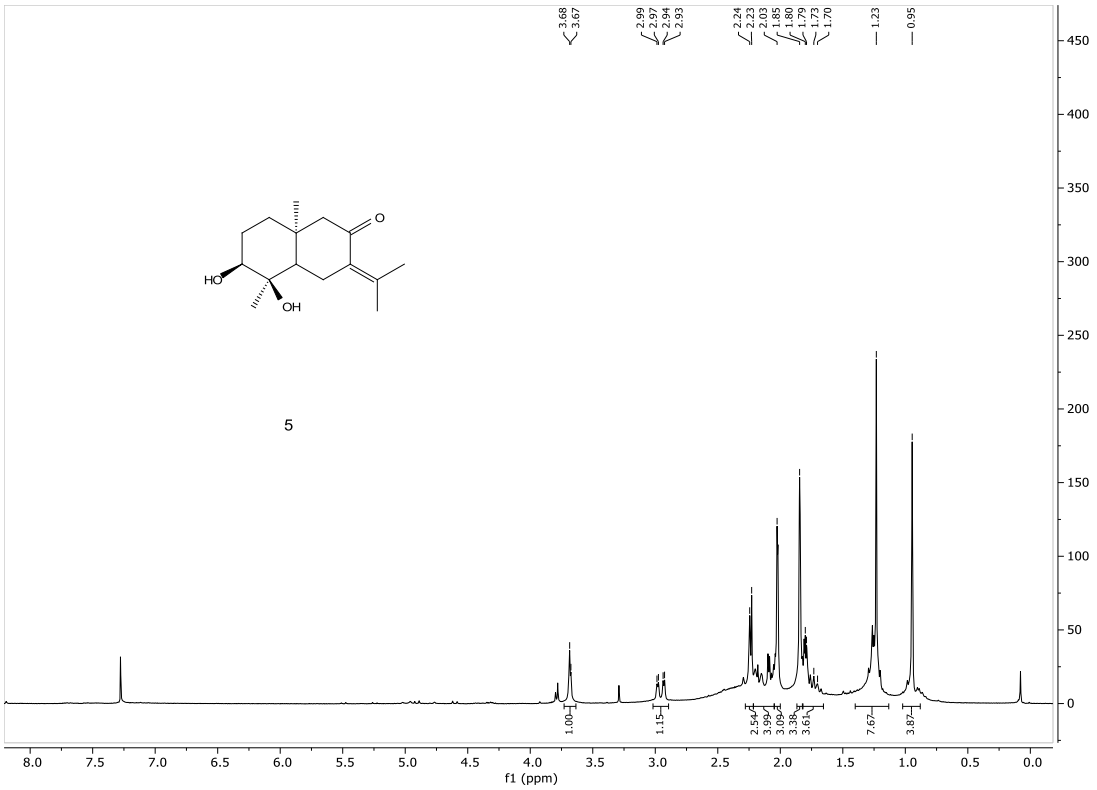
S 24. ESI-MS of 4b.

Charge number:1 Tolerance:3.00(ppm), 5.00 .. 15.00(mmu) Unsaturation Number:0.0 .. 50.0 (Fraction:Both)
Element:^{12}C:1 .. 26, ^{1}H:1 .. 40, ^{14}N:1 .. 2, ^{16}O:1 .. 6

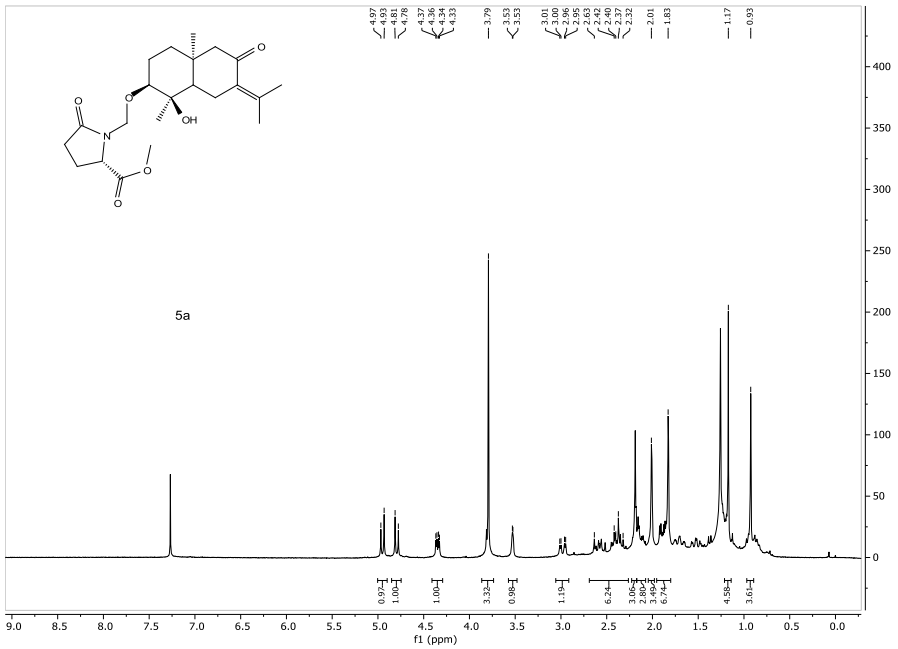


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
442.25806	249075.92	442.25935	-1.29	-2.91	$^{12}C_{26}{}^{1}H_{36}{}^{14}N_{1}{}^{16}O_{5}$	9.5

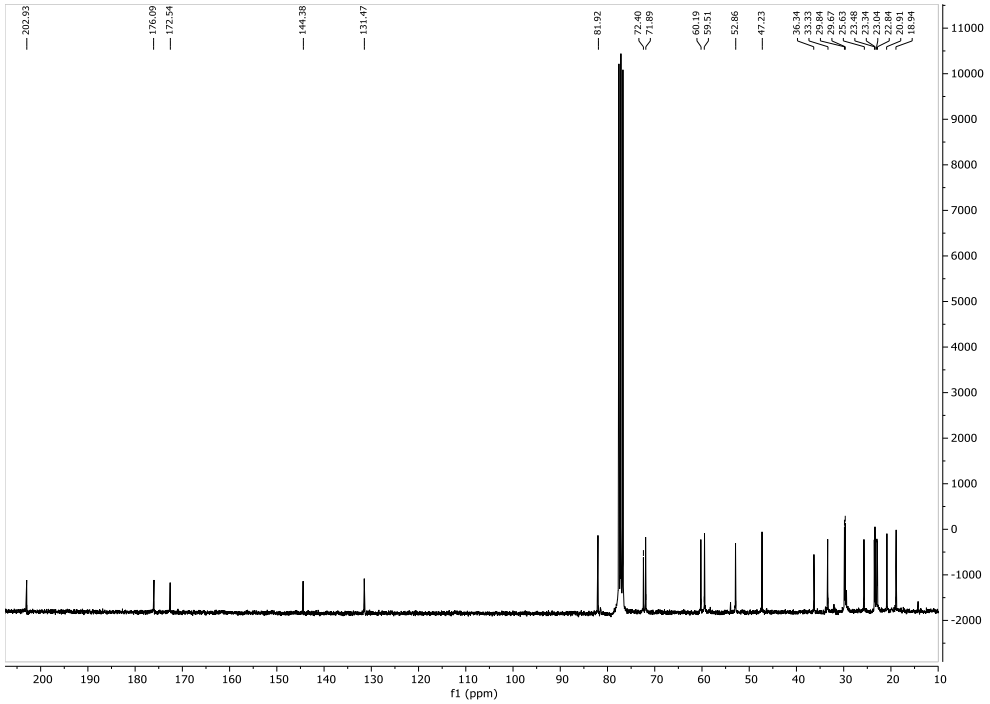
S 25. ESI-HRMS of 4b.



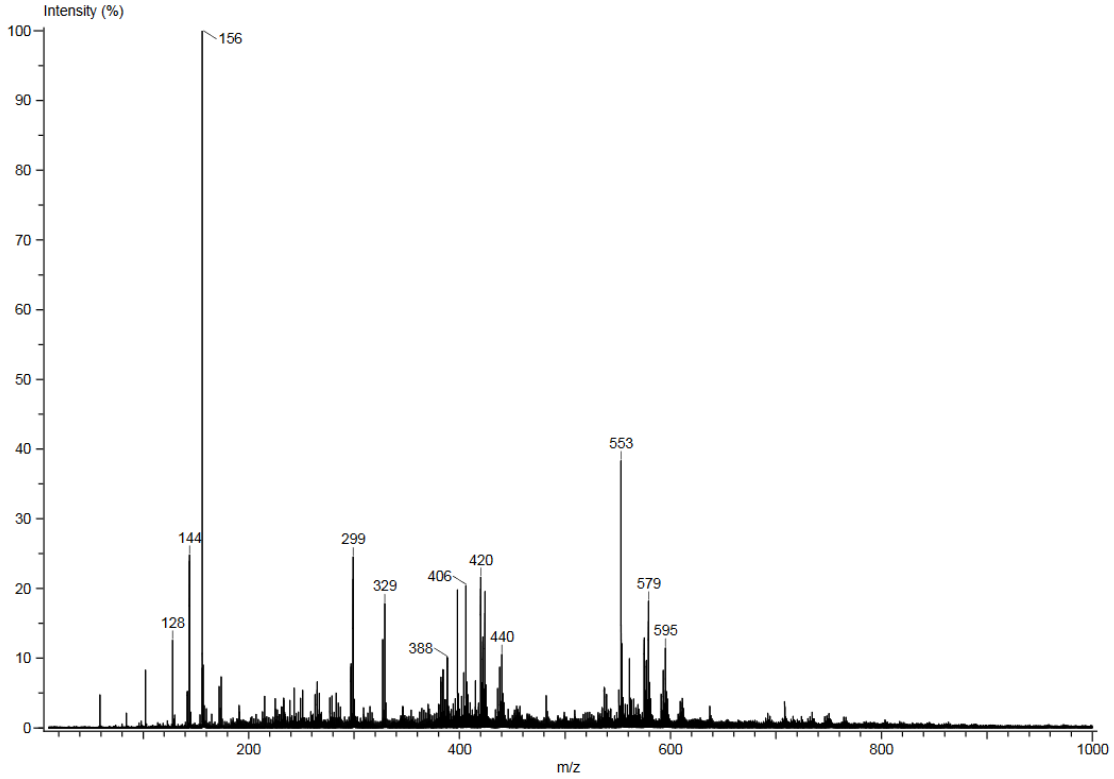
S 26. NMR-^{1}H (300 MHz, $CDCl_3$) of 5.



S 27. NMR-^{1}H (300 MHz, $CDCl_3$) of 5a.



S 28. NMR-^{13}C (75 MHz, $CDCl_3$) of 5a

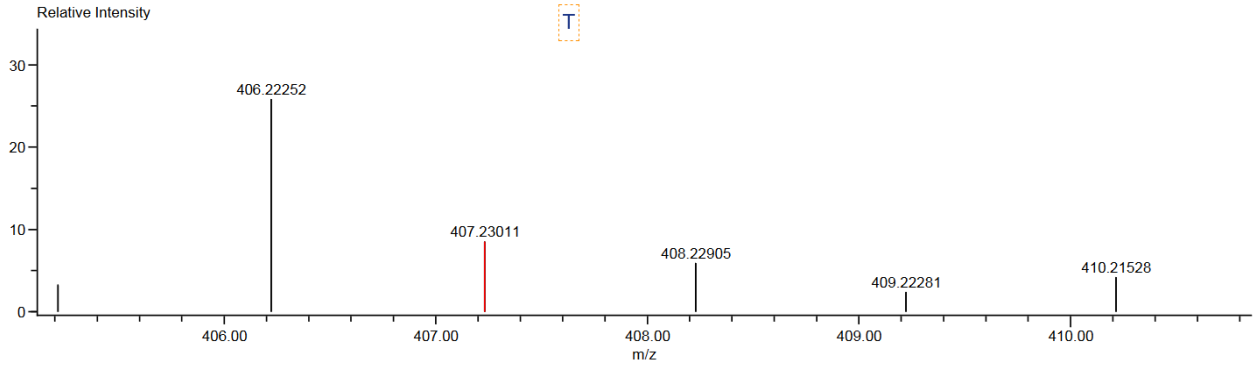


S 29. ESI-MS of 5a

Charge number:1
Element:^{12}C:0 .. 40, ^{1}H:0 .. 40, ^{14}N:0 .. 1, ^{16}O:0 .. 6

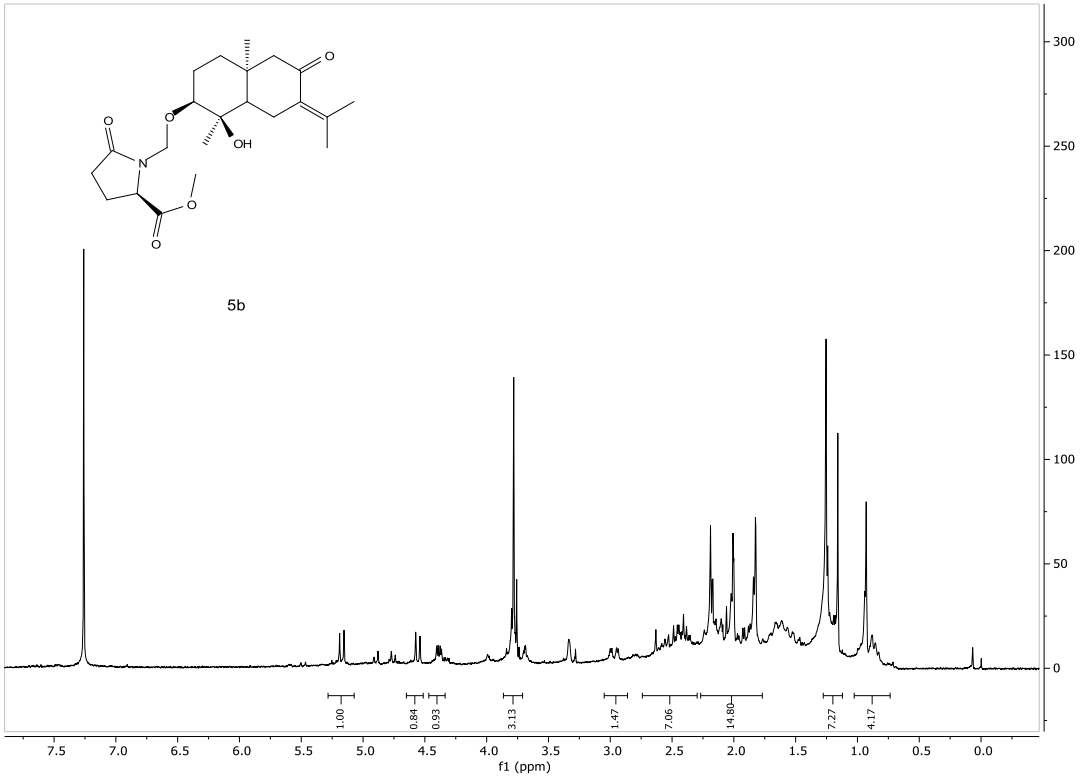
Tolerance:3.00(ppm), 5.00 .. 15.00(mmu)

Unsaturation Number:0.0 .. 50.0 (Fraction:Both)

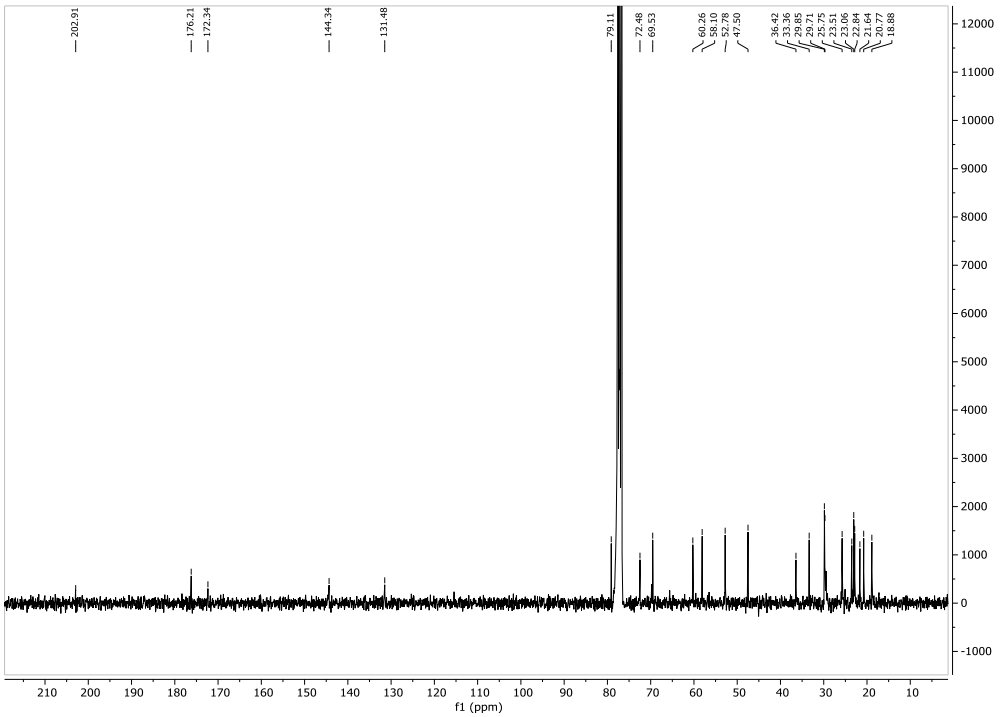


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
407.23011	3243.74	407.23079	-0.68	-1.66	$^{12}C_{22}{}^{1}H_{33}{}^{14}N_{1}{}^{16}O_{6}$	7.0

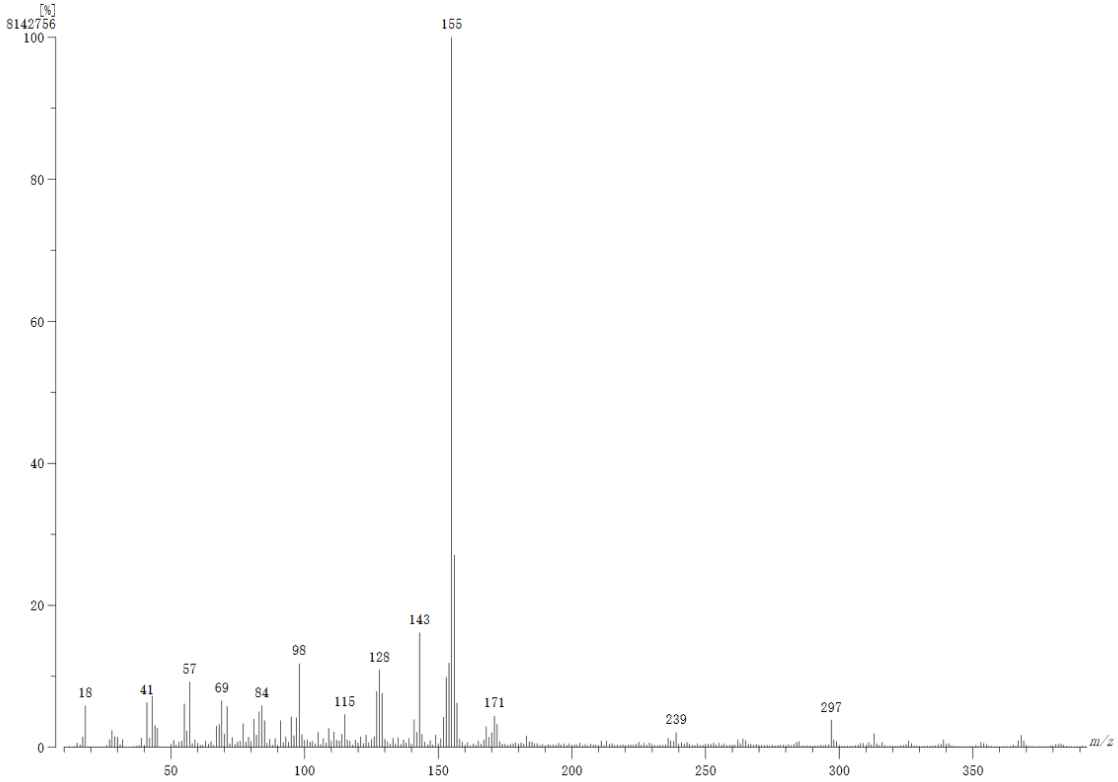
S 30. ESI-HRMS of 5a



S 31. NMR-^{1}H (300 MHz, $CDCl_3$) of 5b.

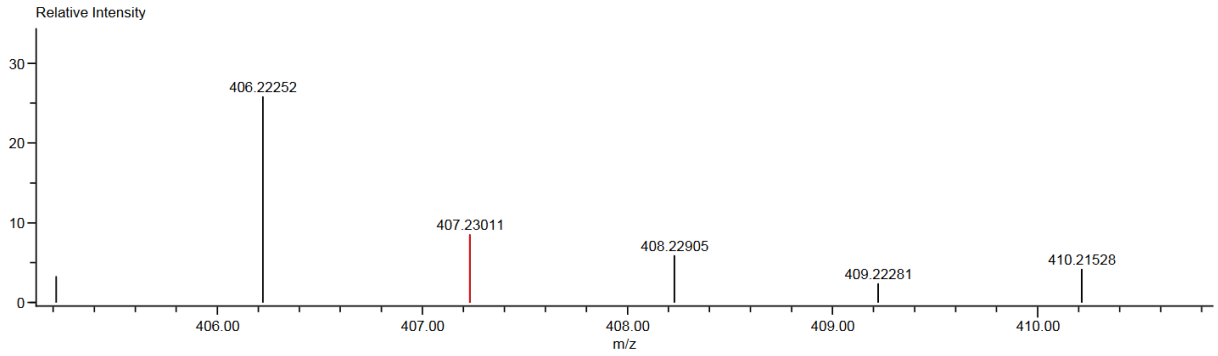


S 32. NMR-^{13}C (75 MHz, $CDCl_3$) of 5b.



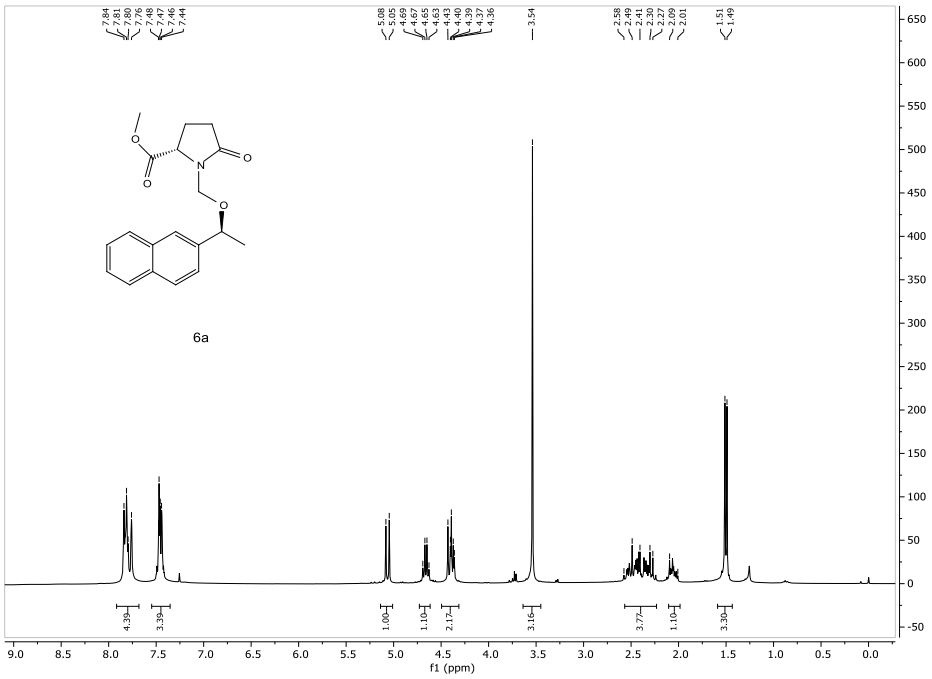
S 33. ESI-MS of 5b

Charge number:1
Tolerance:3.00(ppm), 5.00 .. 15.00(mmu)
Unsaturation Number:0.0 .. 50.0 (Fraction:Both)
Element:^{12}C:0 .. 40, ^{1}H:0 .. 40, ^{14}N:0 .. 1, ^{16}O:0 .. 6

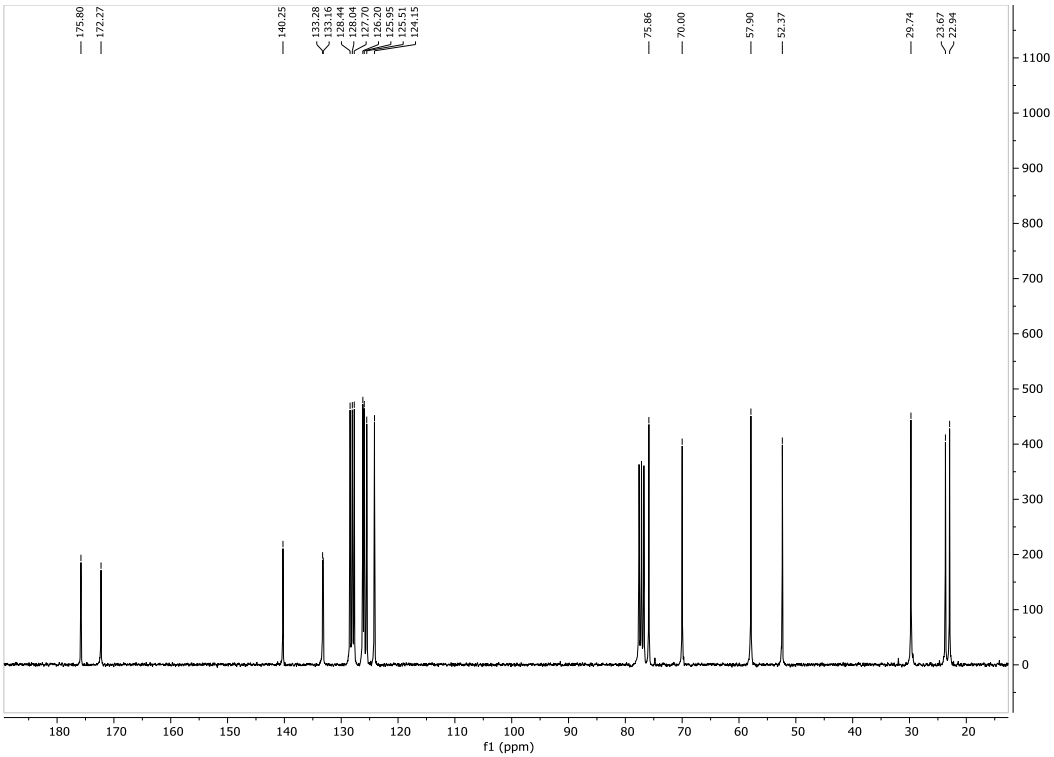


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
407.23011	3243.74	407.23079	-0.68	-1.66	$^{12}C_{22}{}^{1}H_{33}{}^{14}N_{1}{}^{16}O_{6}$	7.0

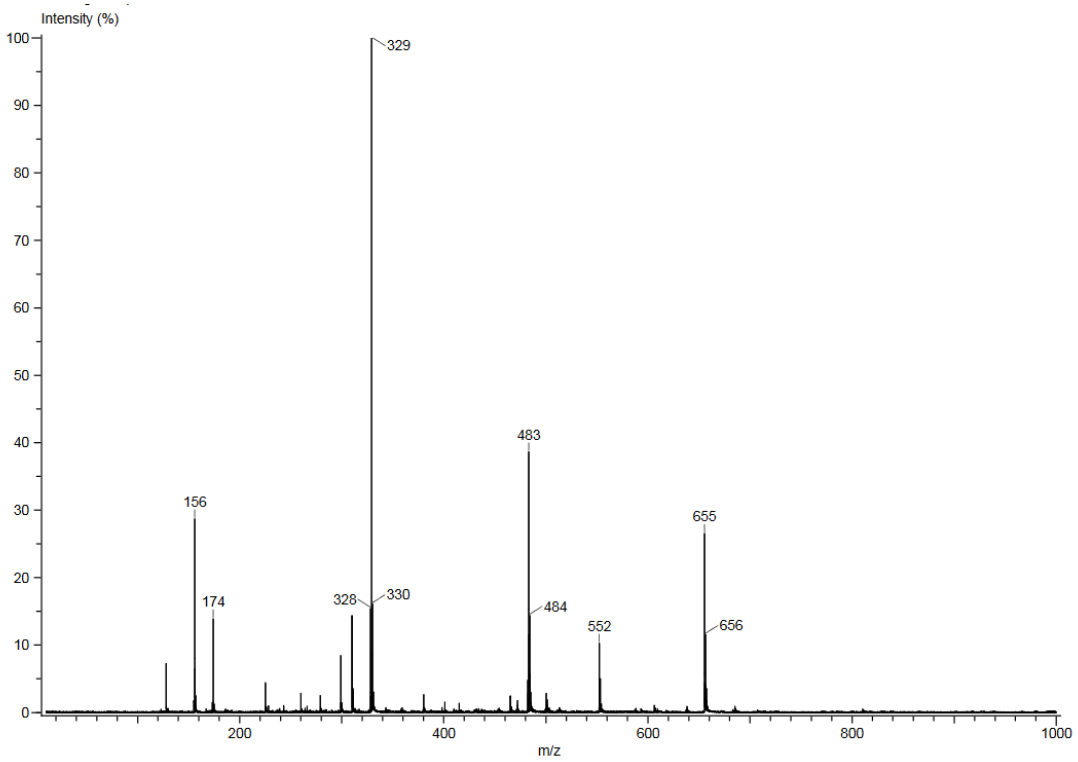
S 34. ESI-HRMS of 5b.



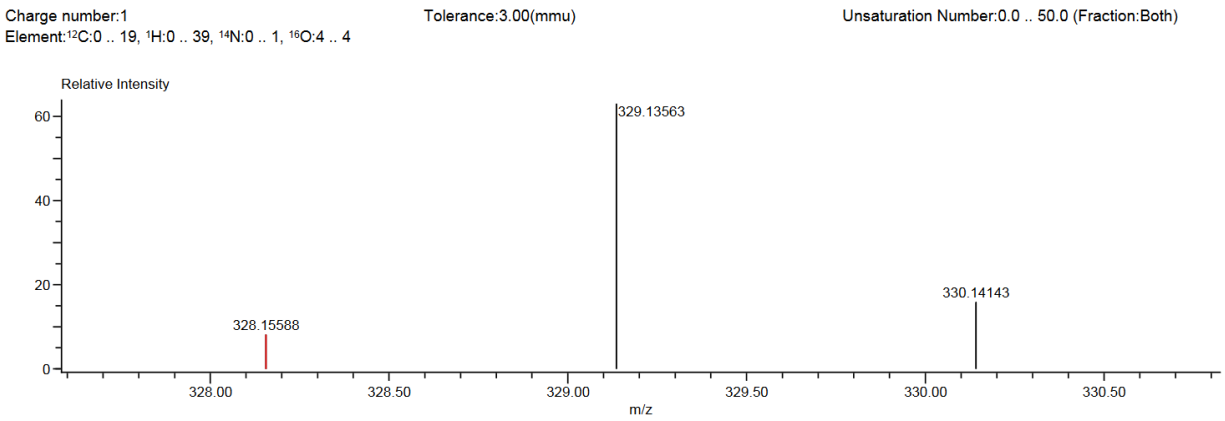
S 35. NMR-^{1}H (300 MHz, $CDCl_3$) of 6a.



S 36. NMR-^{13}C (75 MHz, $CDCl_3$) of 6a.

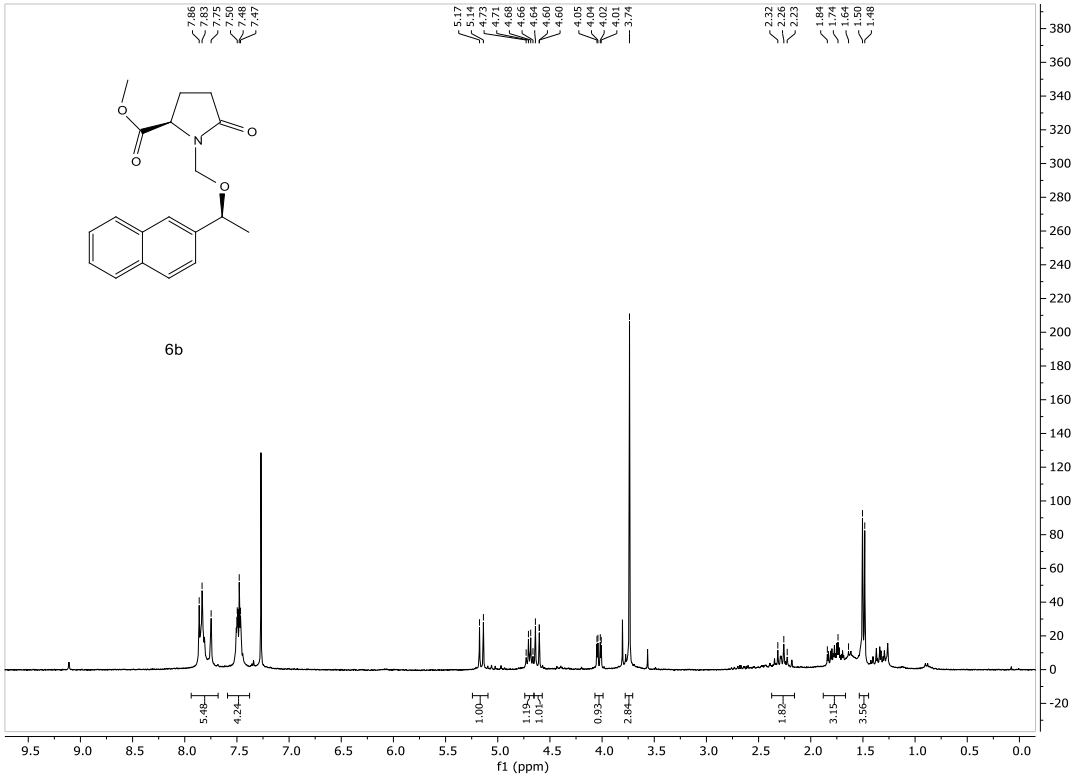


S 37. DART+ of 6a.

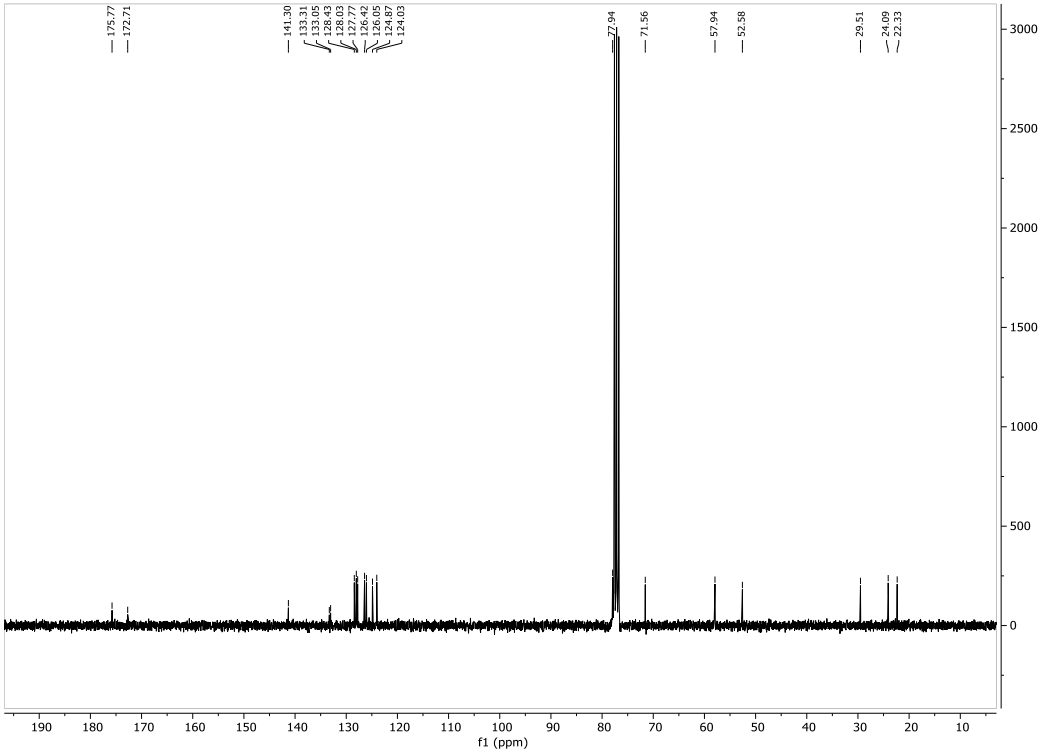


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
328.15588	4225.64	328.15488	1.00	3.03	$^{12}C_{19}{}^{1}H_{22}{}^{14}N_{1}{}^{16}O_{4}$	9.5

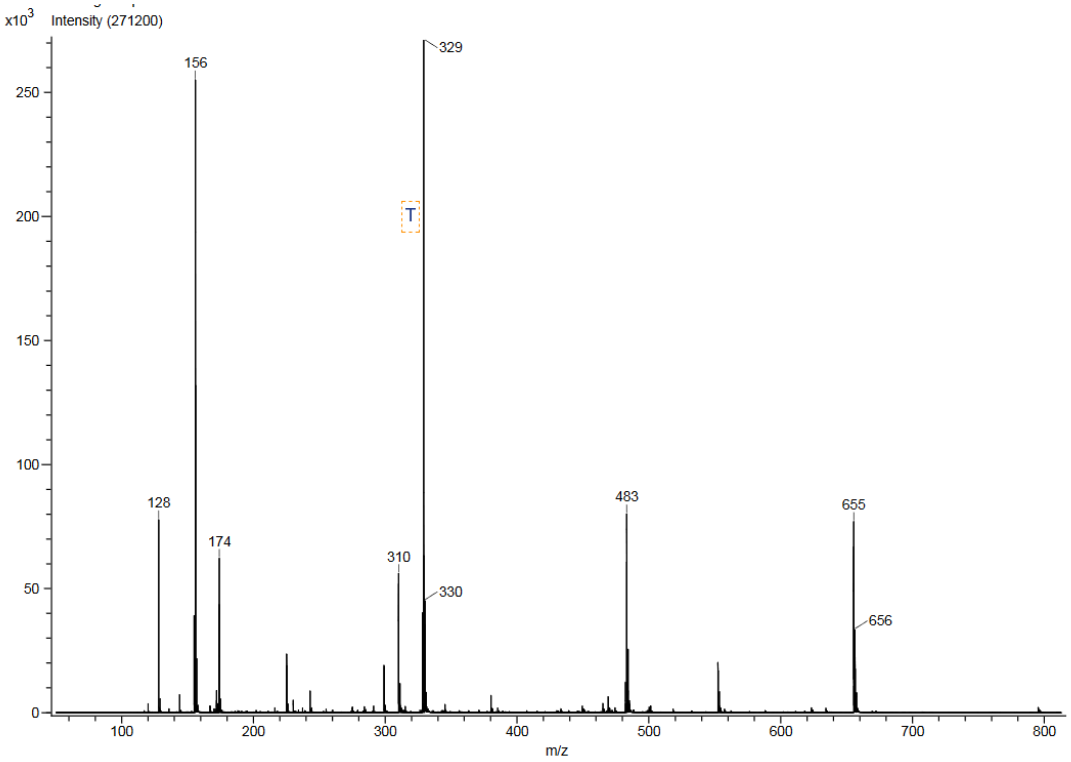
S 38. ESI-HRMS of 6a.



S 39. NMR-^{1}H (300 MHz, $CDCl_3$) of 6b.

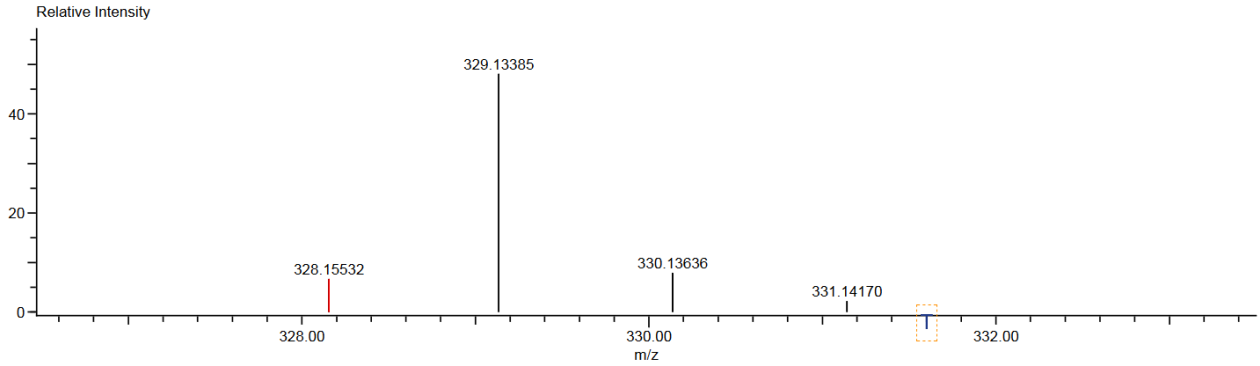


S 40. NMR-^{13}C (75 MHz, $CDCl_3$) of 6b.



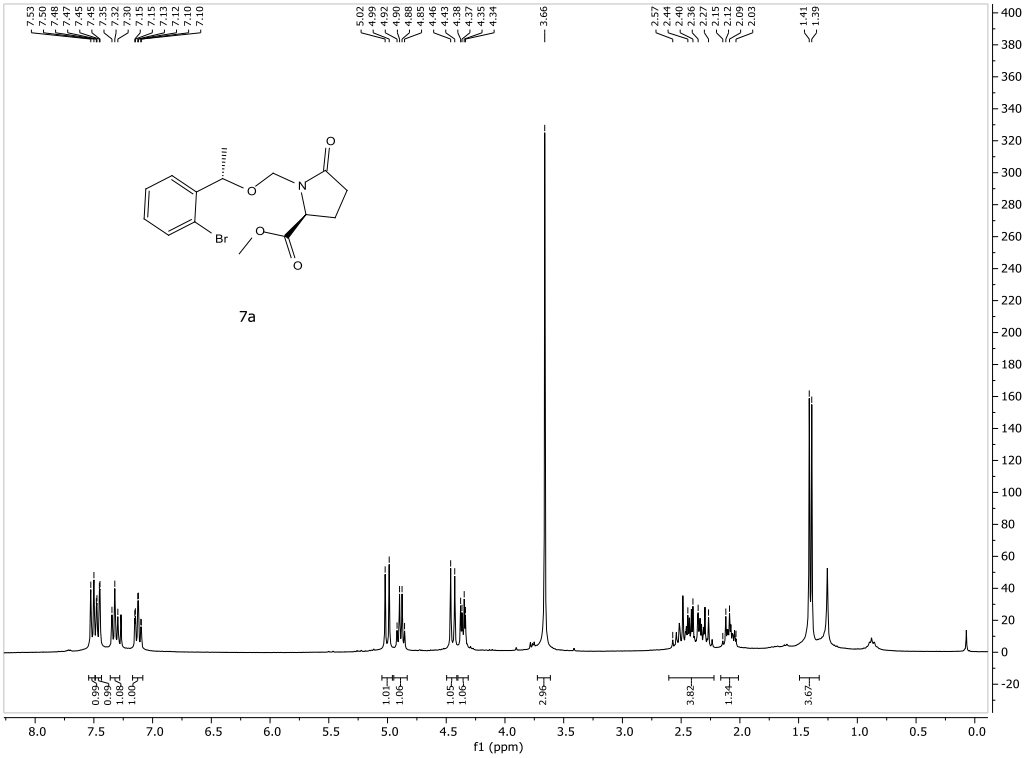
S 41. DART+ of 6b.

Charge number:1 Tolerance:3.00(mmu) Unsaturation Number:0.0 .. 50.0 (Fraction:Both)
Element:^{12}C:0 .. 19, ^{1}H:0 .. 39, ^{14}N:0 .. 1, ^{16}O:4 .. 4

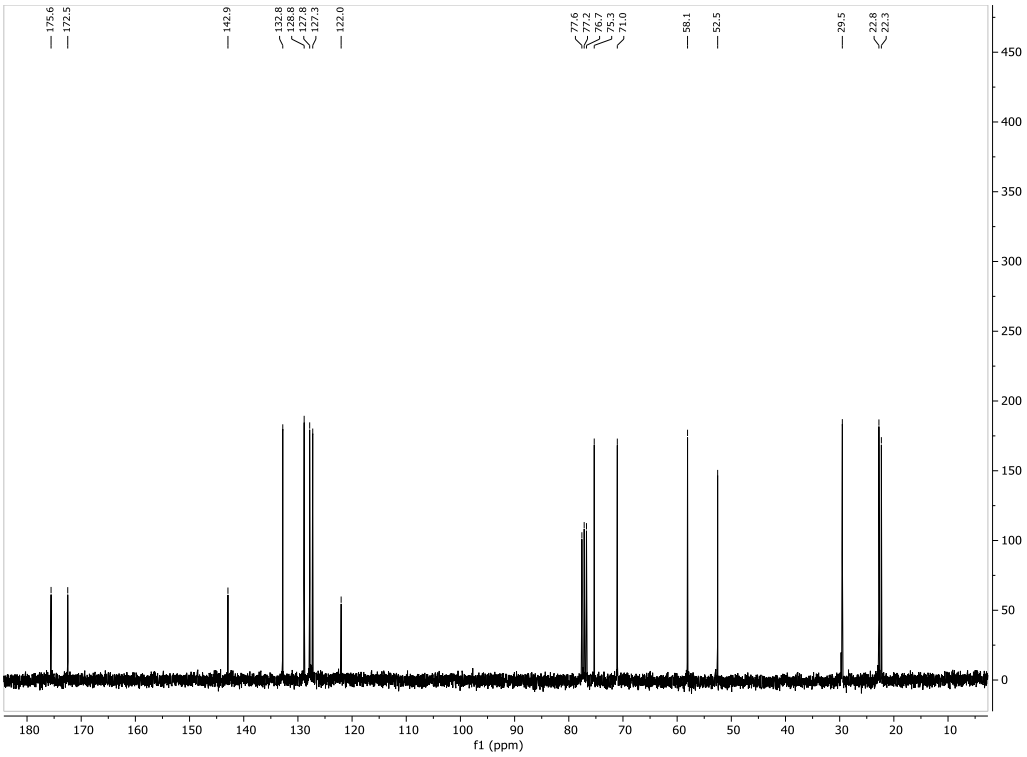


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
328.15532	22765.79	328.15488	0.44	1.35	$^{12}C_{19}{}^{1}H_{22}{}^{14}N_{1}{}^{16}O_{4}$	9.5

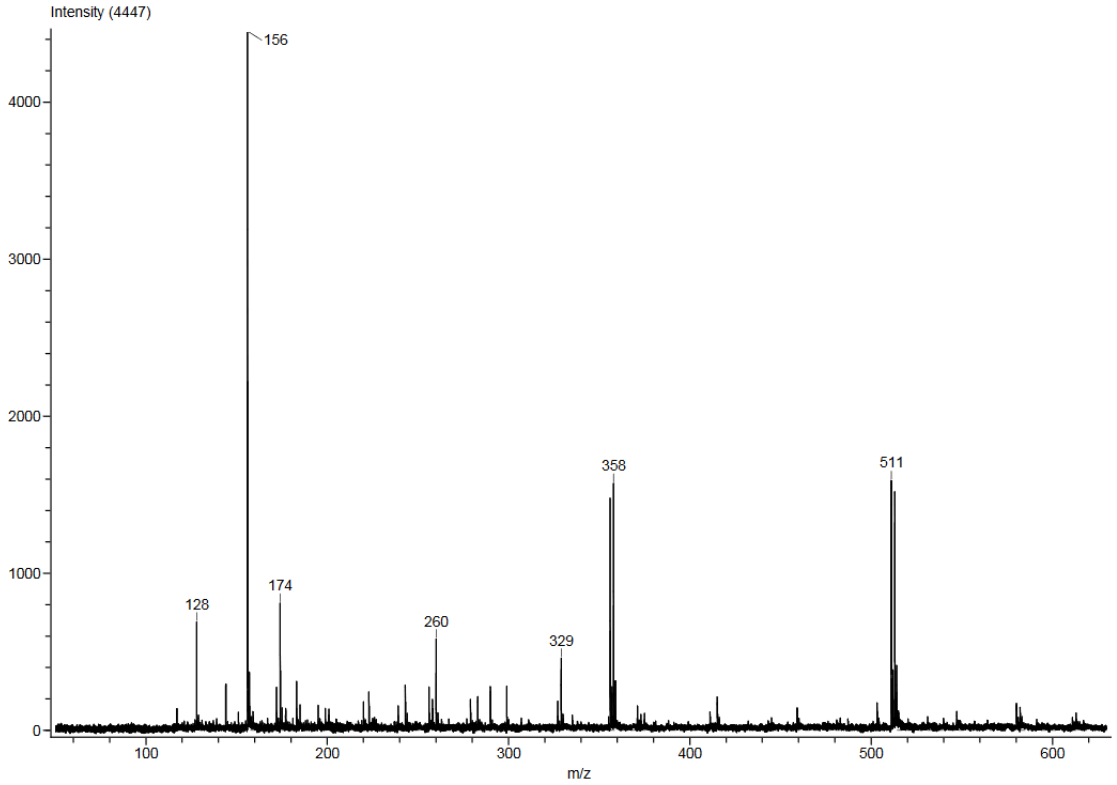
S 42. ESI-HRMS of 6b.



S 43. NMR-^{1}H (300 MHz, $CDCl_3$) of 7a.

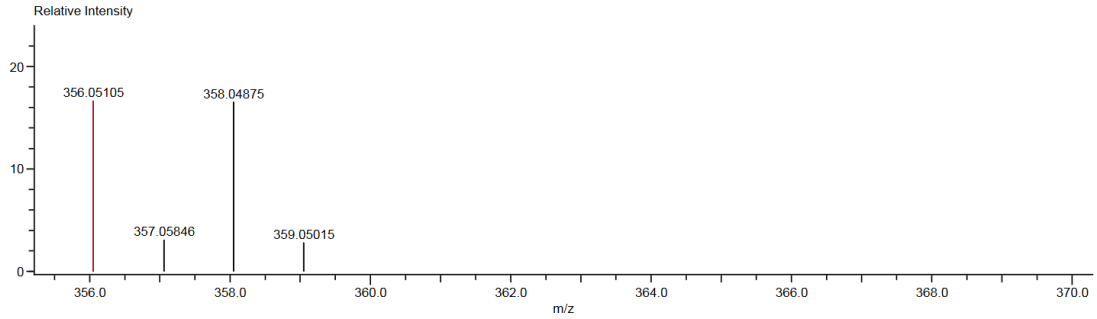


S 44. NMR-^{13}C (75 MHz, $CDCl_3$) of 7a.



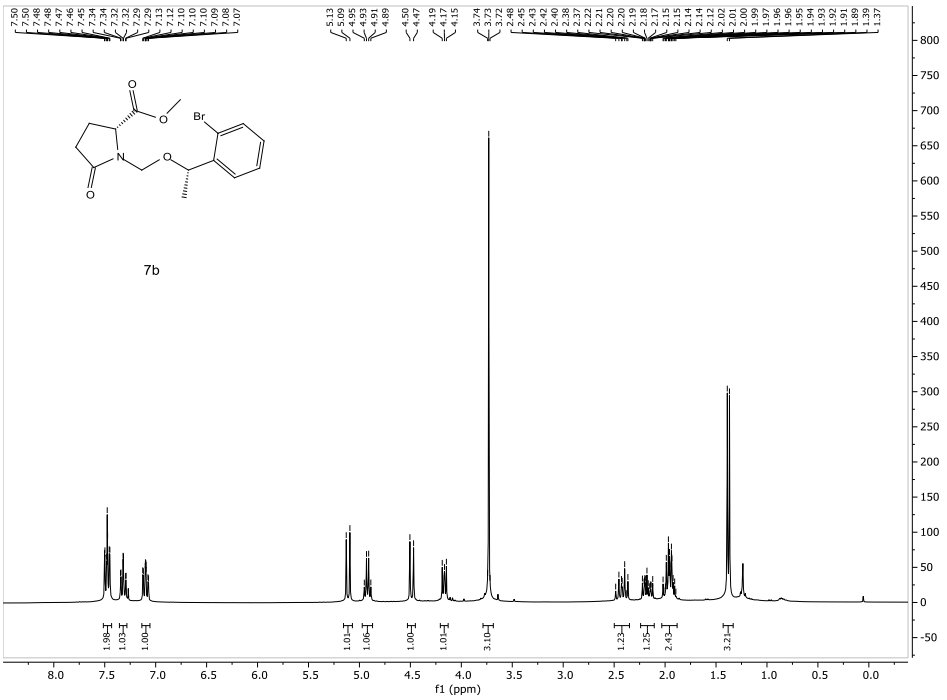
S 45. DART+ of 7a

Charge number:1 Tolerance:3.00(mmu) Unsaturation Number:0.0 .. 100.0 (Fraction:Both)
Element:^{12}C:1 .. 15, ^{1}H:0 .. 30, ^{79}Br:0 .. 1, ^{81}Br:0 .. 1, ^{14}N:1 .. 1, ^{16}O:0 .. 4

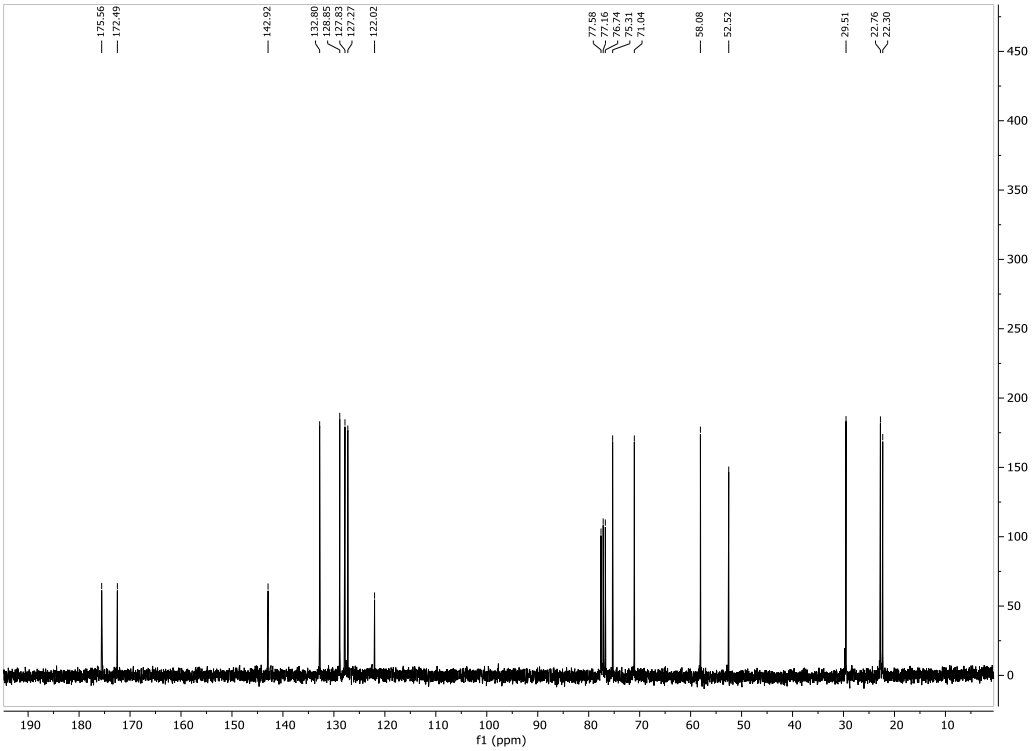


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
356.05105	3358.29	356.04975	1.31	3.67	$^{12}C_{15}{}^{1}H_{19}{}^{79}Br_{1}{}^{14}N_{1}{}^{16}O_{4}$	6.5

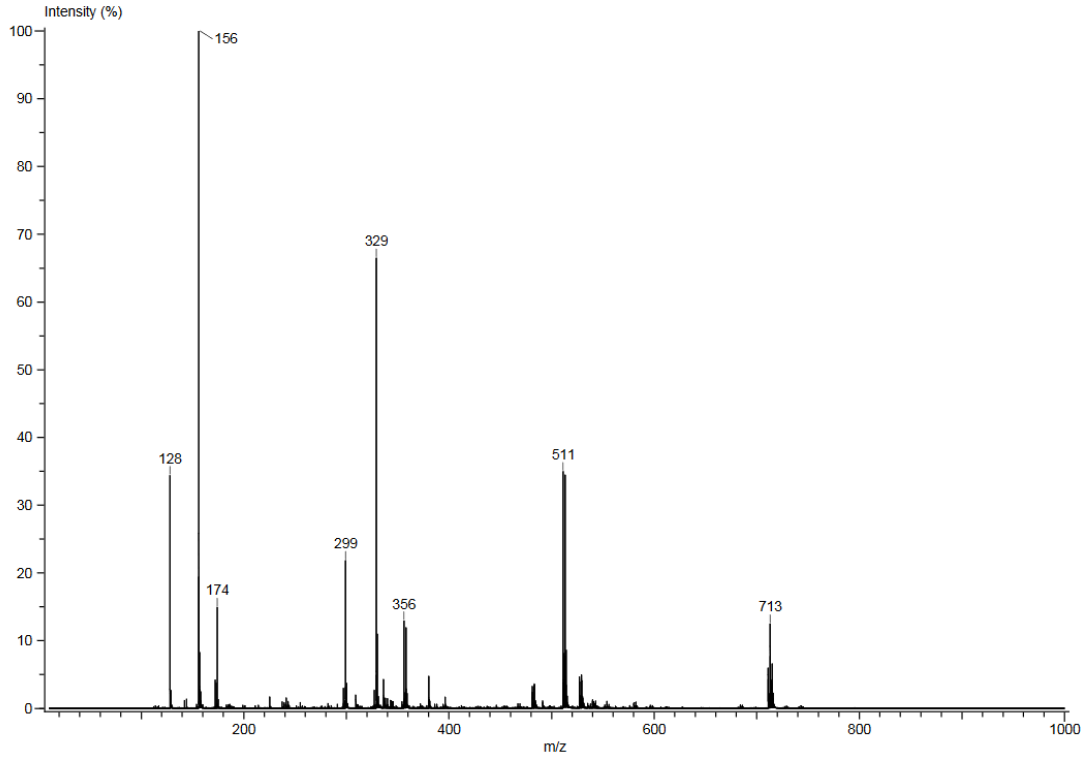
S 46. ESI-HRMS of 7a



S 47. NMR-^{1}H (300 MHz, $CDCl_3$) of 7b.

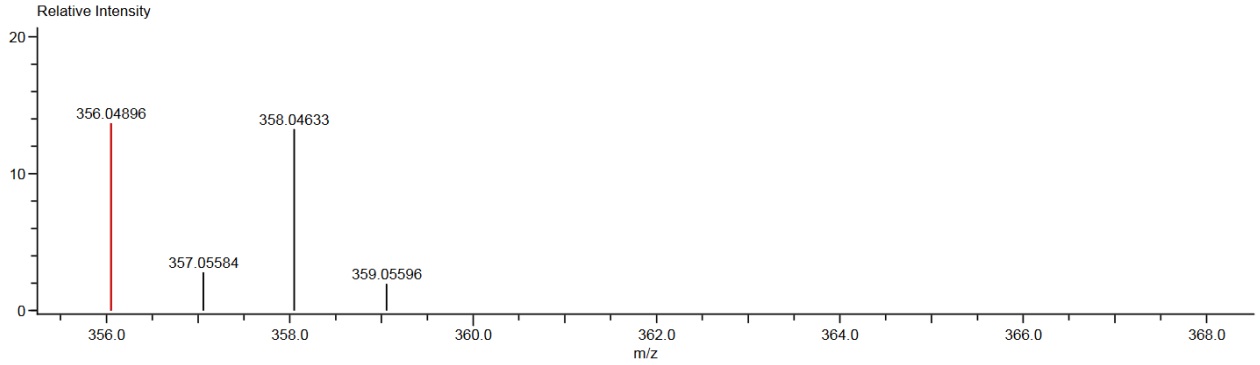


S 48. NMR-^{13}C (75 MHz, $CDCl_3$) of 7b.



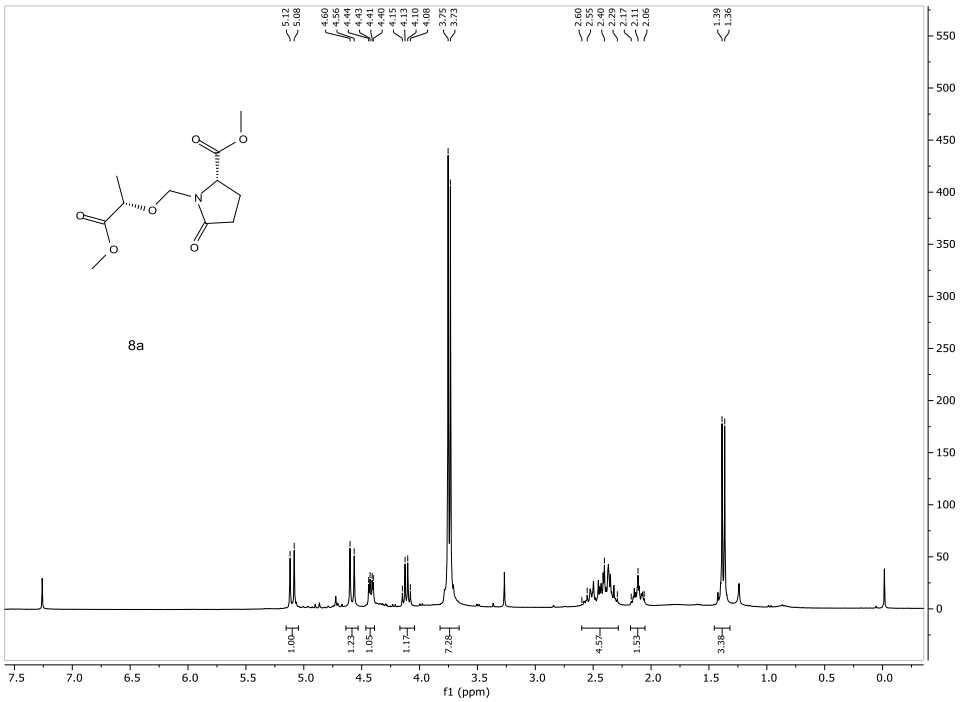
S 49. DART+ of 7b.

Charge number:1 Tolerance:5.00(mmu) Unsaturation Number:0.0 .. 100.0 (Fraction:Both)
Element:^{12}C:1 .. 15, ^{1}H:0 .. 20, ^{79}Br:0 .. 1, ^{81}Br:0 .. 1, ^{14}N:0 .. 1, ^{16}O:0 .. 4

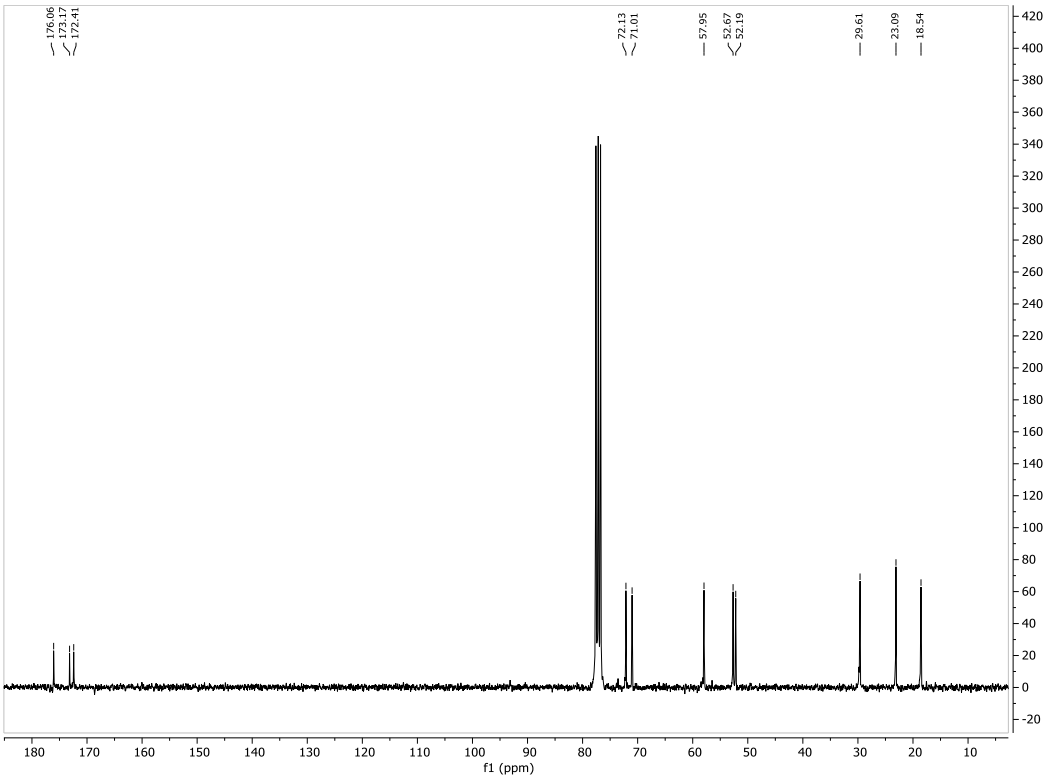


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
356.04896	6729.57	356.04975	-0.78	-2.20	$^{12}C_{15}{}^{1}H_{19}{}^{79}Br_{1}{}^{14}N_{1}{}^{16}O_{4}$	6.5

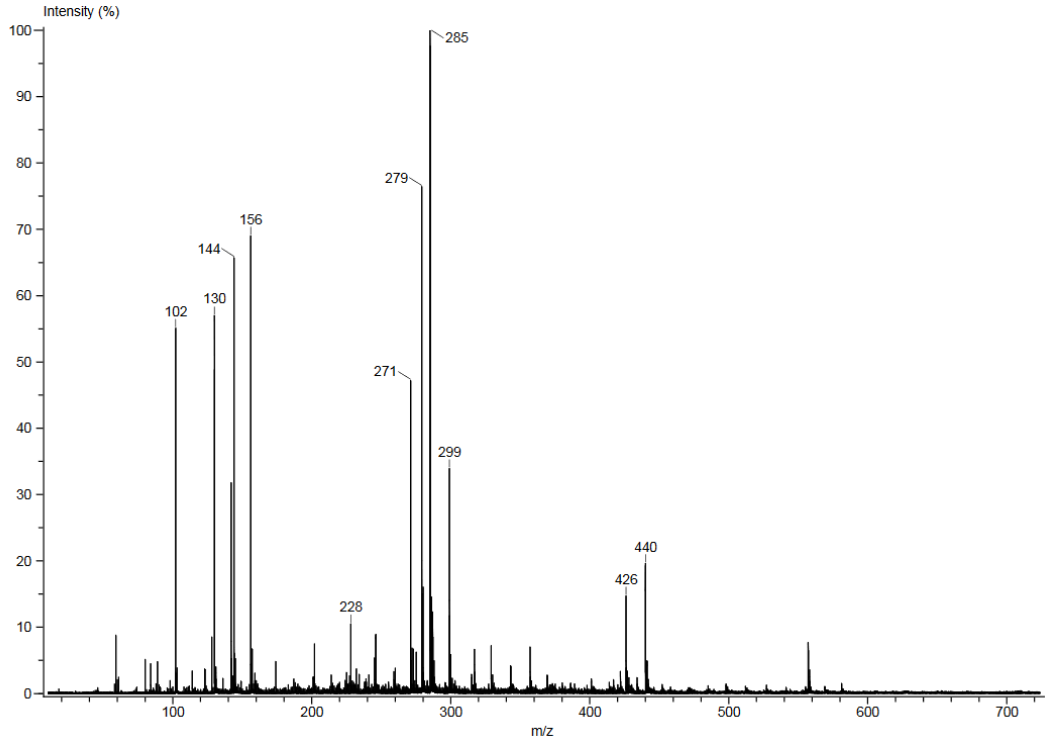
S 50. ESI-HRMS of 7b.



S 51. NMR-^{1}H (300 MHz, $CDCl_3$) of 8a



S 52. NMR-^{13}C (75 MHz, $CDCl_3$) of 8a.

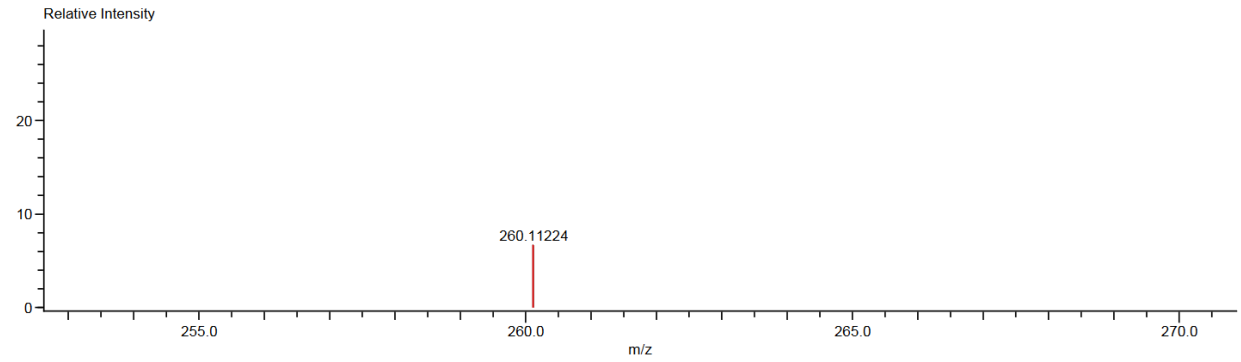


S 53. ESI-MS of 8a.

Charge number:1
Element:^{12}C:0 .. 11, ^{1}H:0 .. 40, ^{14}N:0 .. 1, ^{16}O:0 .. 6

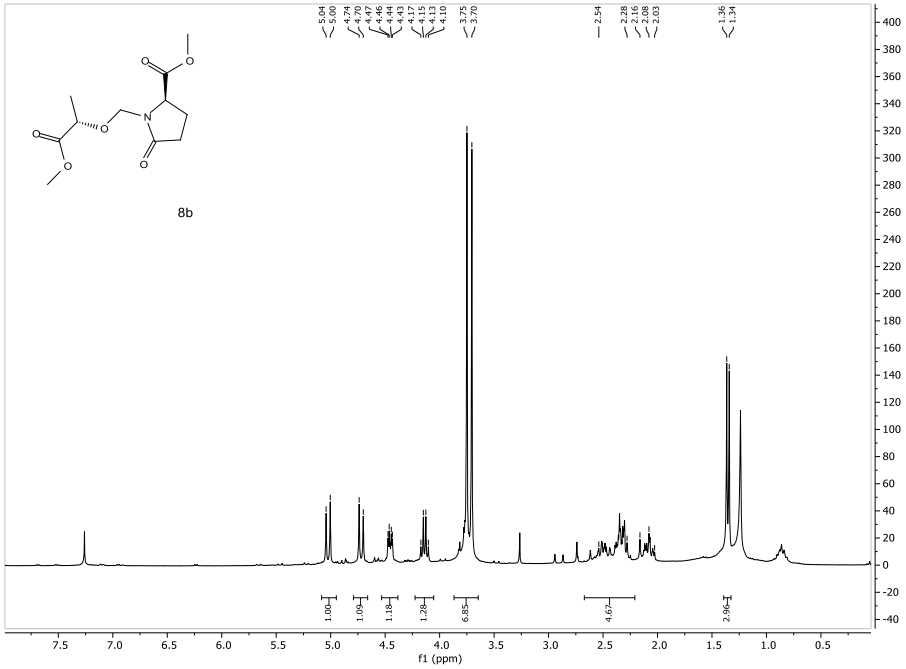
Tolerance:3.00(ppm), 5.00 .. 15.00(mmu)

Unsaturation Number:0.0 .. 50.0 (Fraction:Both)

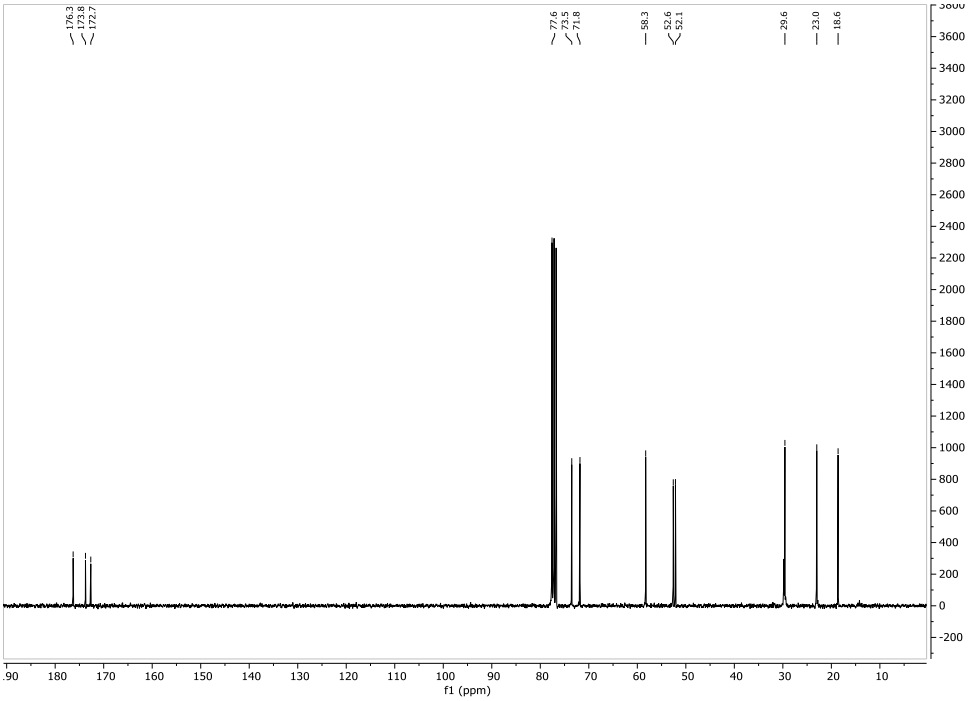


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
260.11224	5096.69	260.11341	-1.17	-4.52	$^{12}C_{11}{}^{1}H_{18}{}^{14}N_{1}{}^{16}O_{6}$	3.5

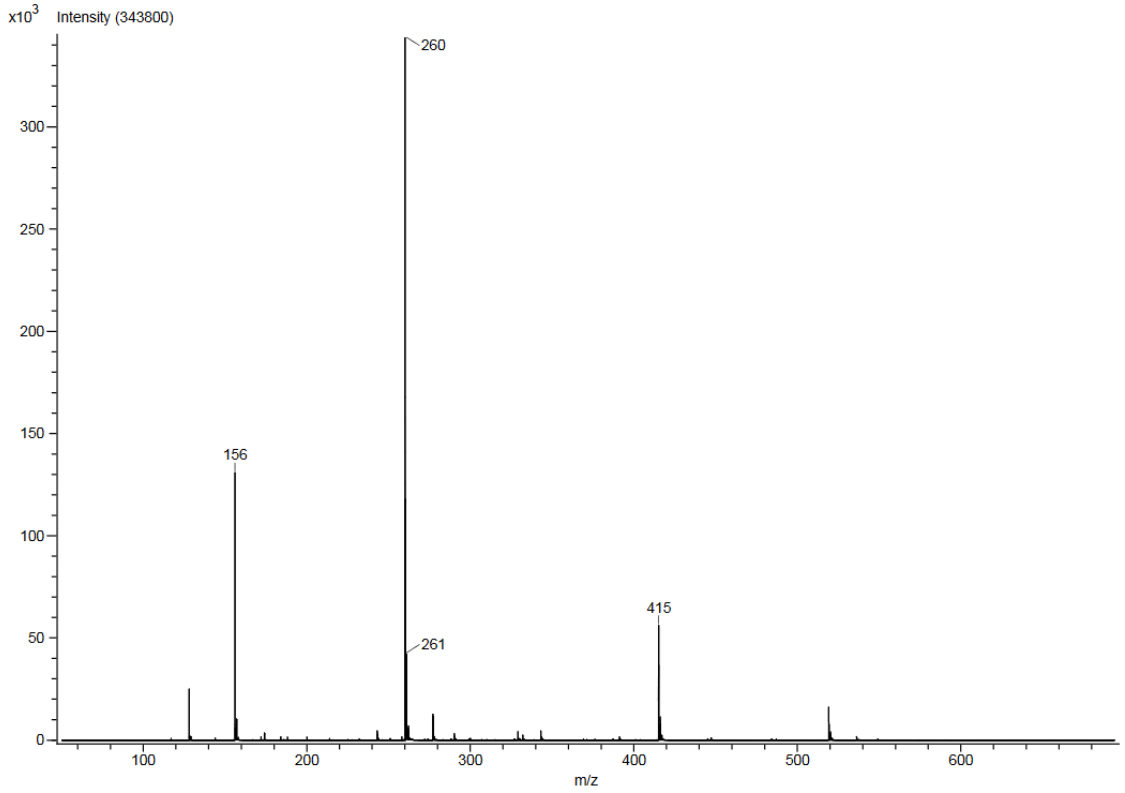
S 54. ESI-HRMS of 8a



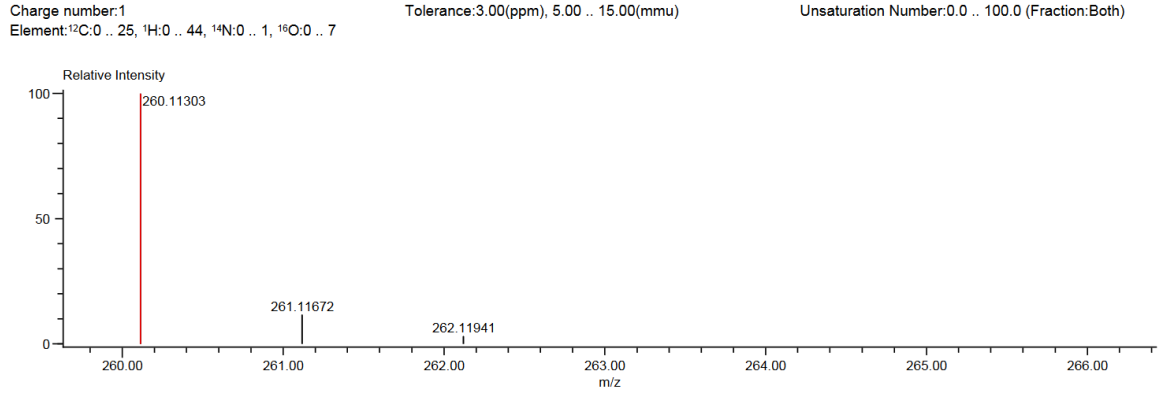
S 55. NMR-^{1}H (300 MHz, $CDCl_3$) of 8b.



S 56. NMR-^{13}C (75 MHz, $CDCl_3$) of 8b.

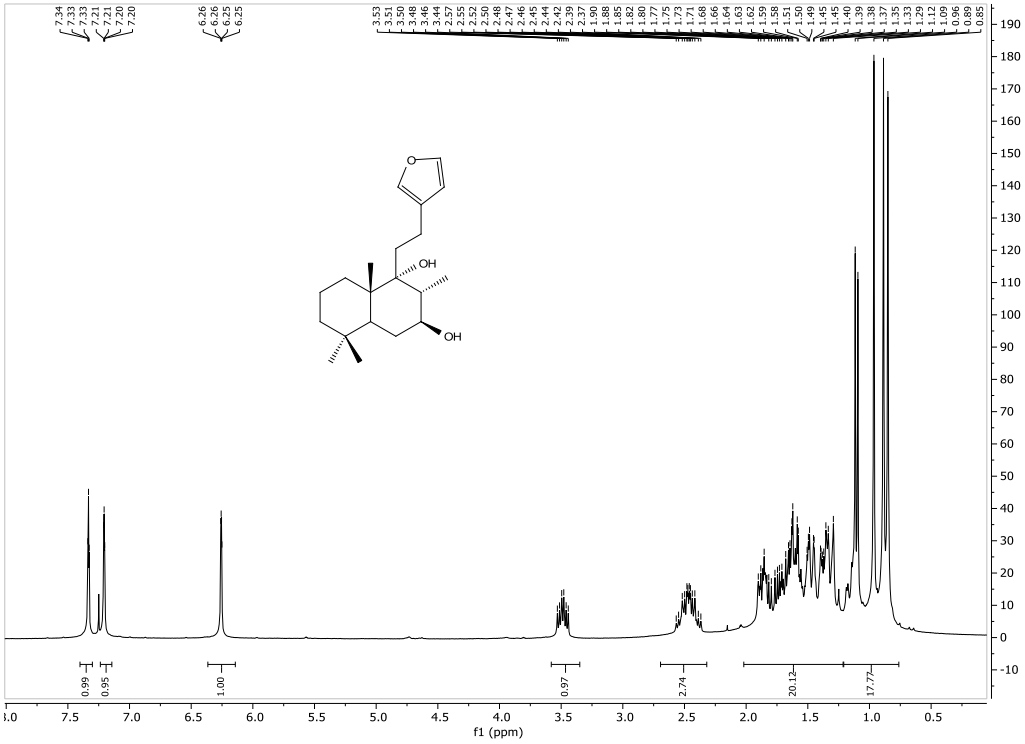


S 57. DART+ of 8b.

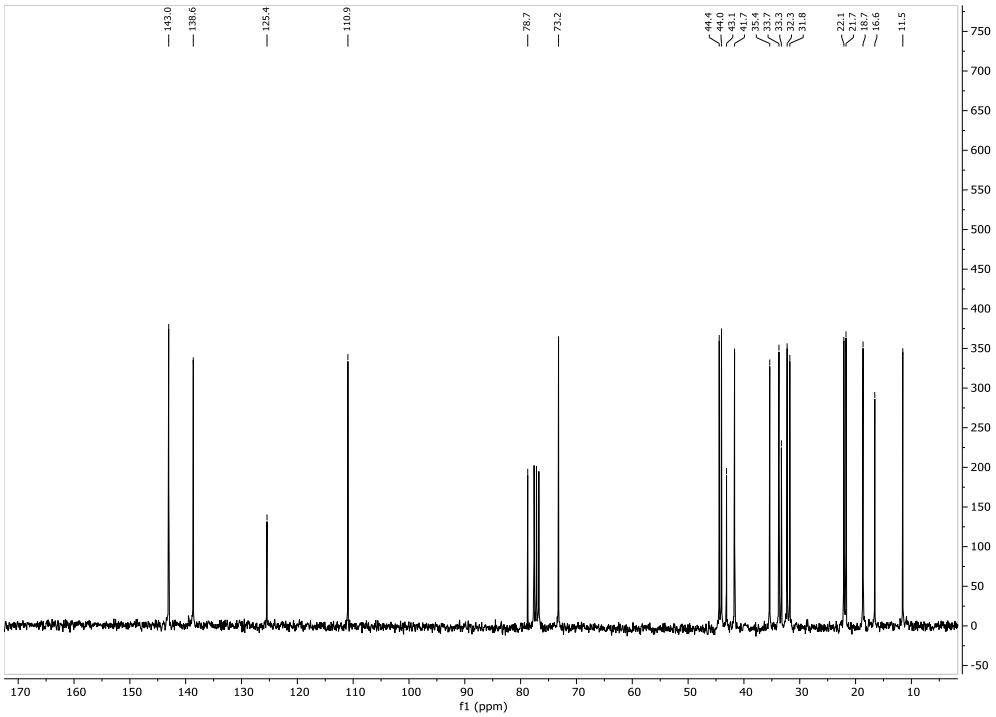


Mass	Intensity	Calc. Mass	Mass Difference (mmu)	Mass Difference (ppm)	Possible Formula	Unsaturation Number
260.11303	416648.92	260.11341	-0.38	-1.46	$^{12}C_{11}{}^{1}H_{18}{}^{14}N_{1}{}^{16}O_{6}$	3.5

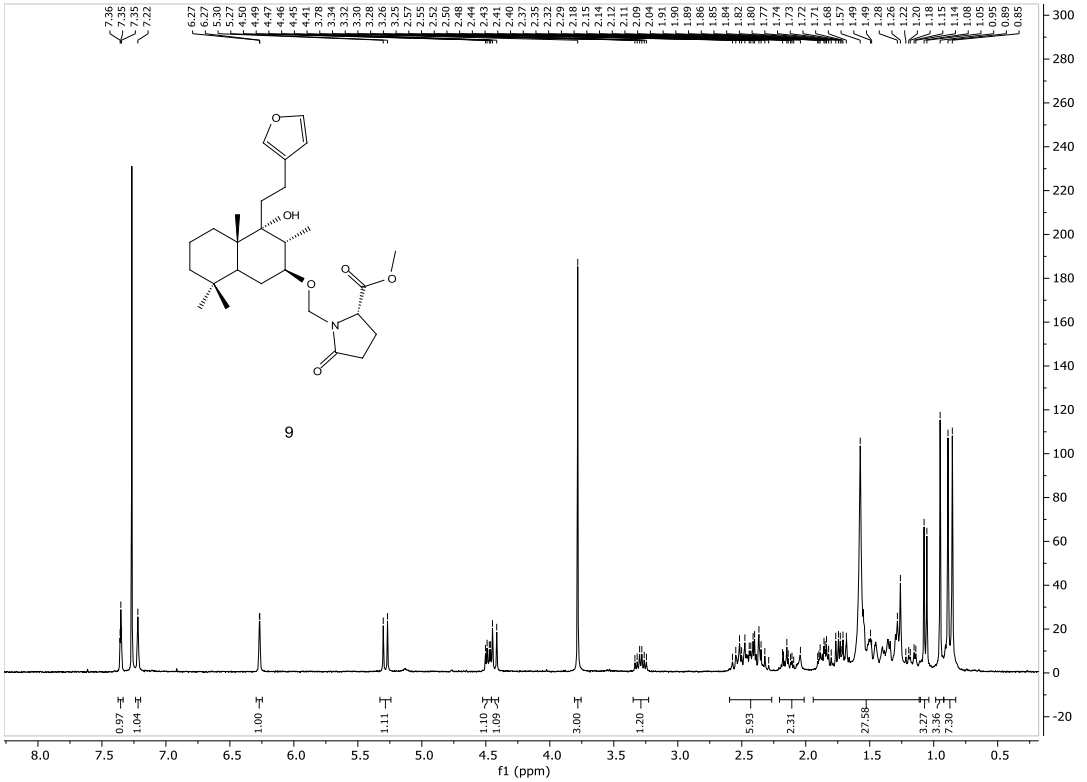
S 58. ESI-HRMS of 8b.



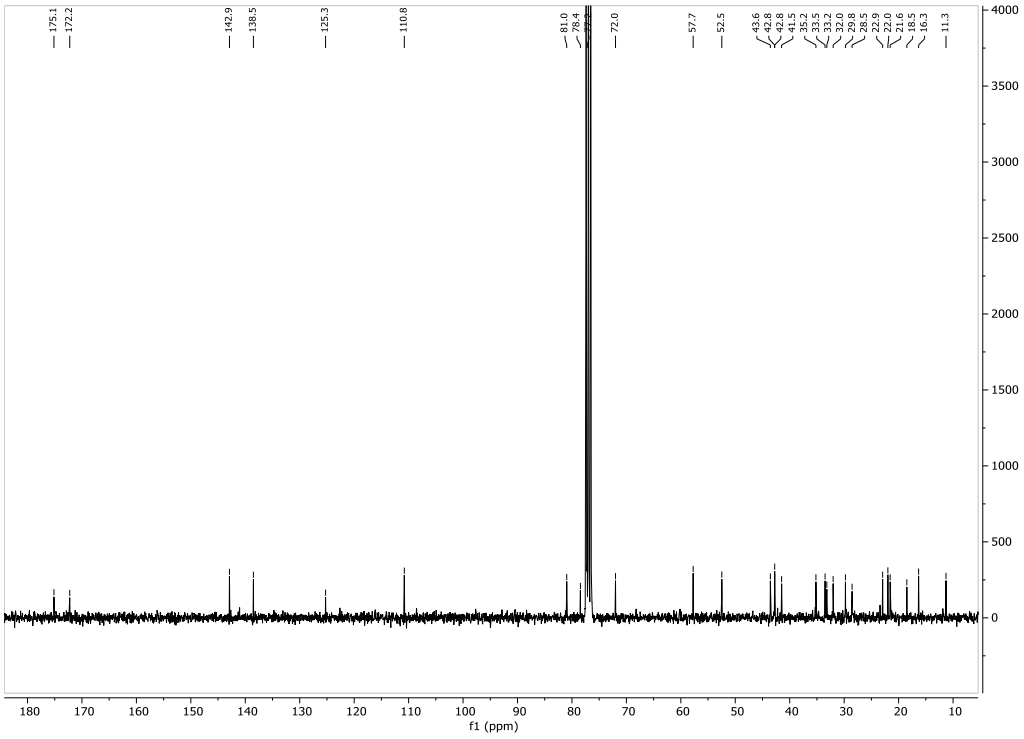
S 59. NMR-^{1}H (300 MHz, $CDCl_3$) of hispanolone β alcohol.



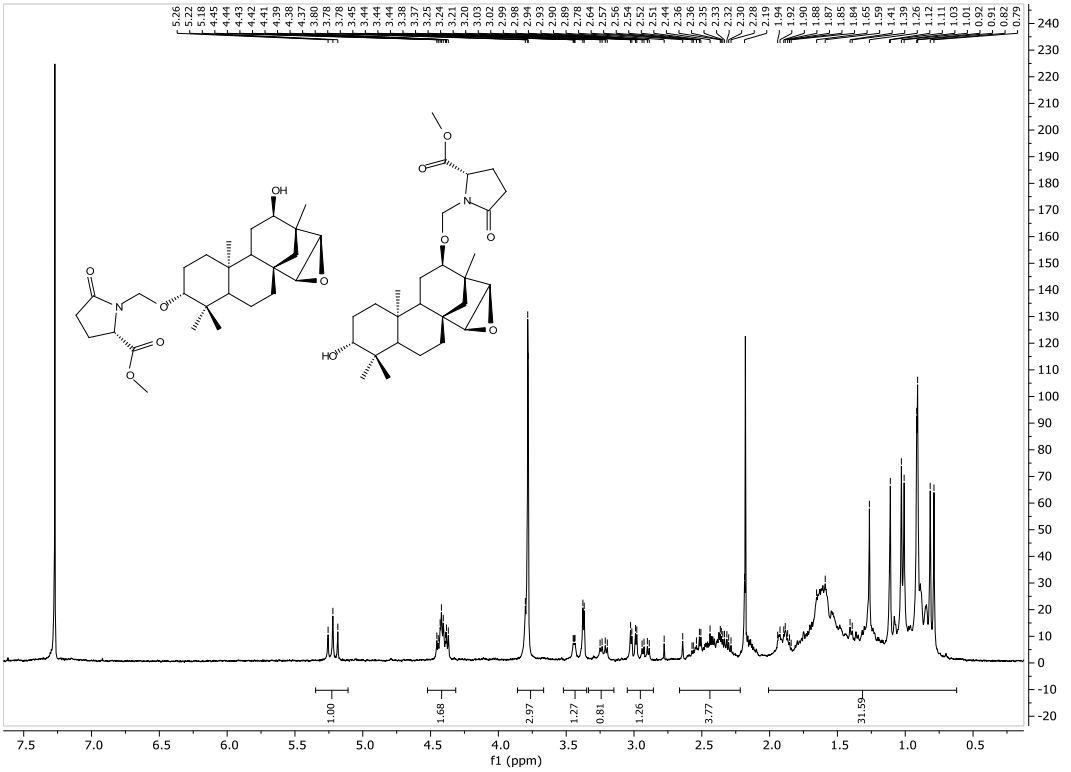
S 60. NMR-^{13}C (75 MHz, $CDCl_3$) of hispanolone β alcohol.



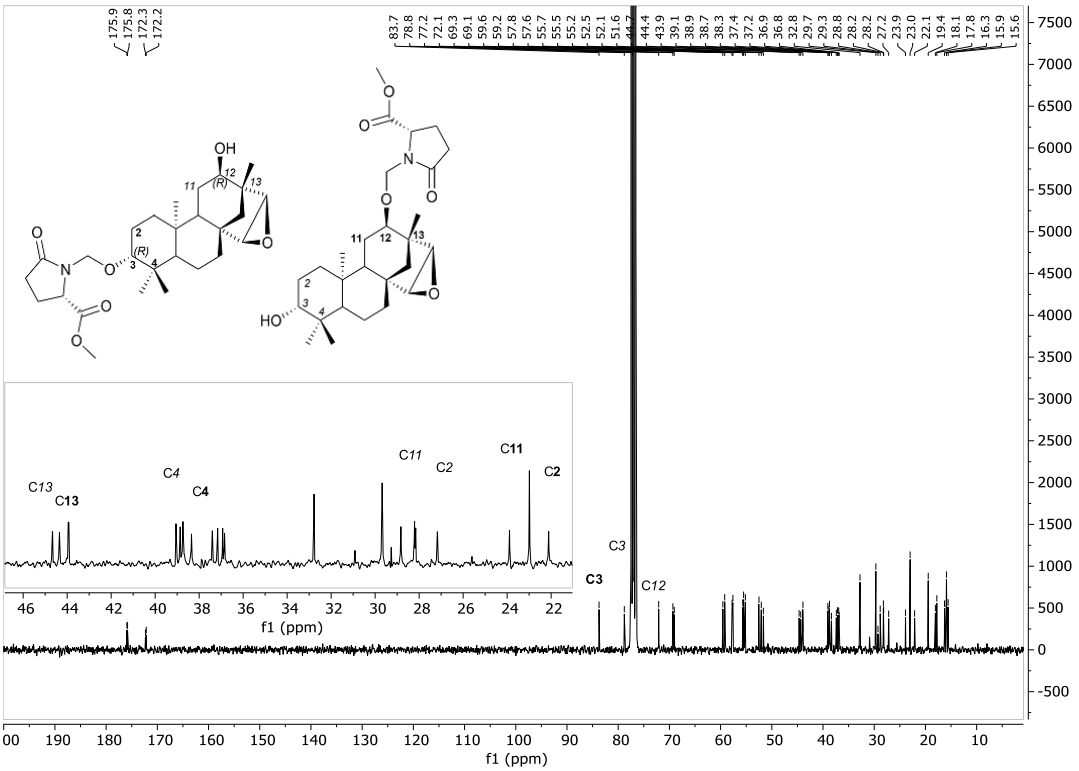
S 61. NMR-^{1}H (300 MHz, $CDCl_3$) of 9



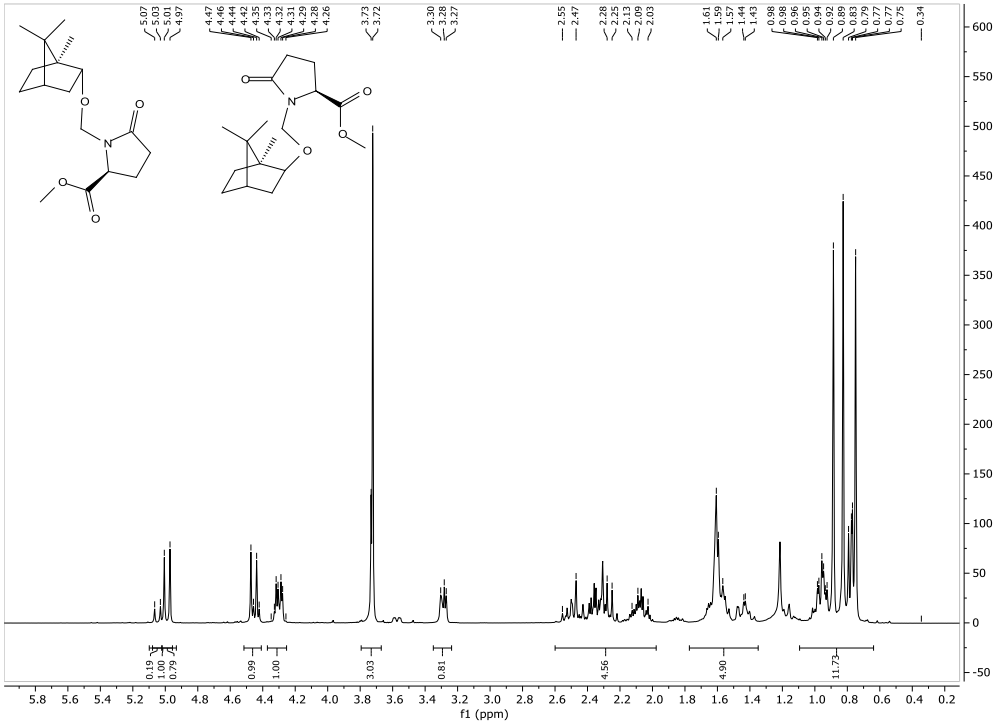
S 62. NMR-^{13}C (75MHz, $CDCl_3$) of 9.



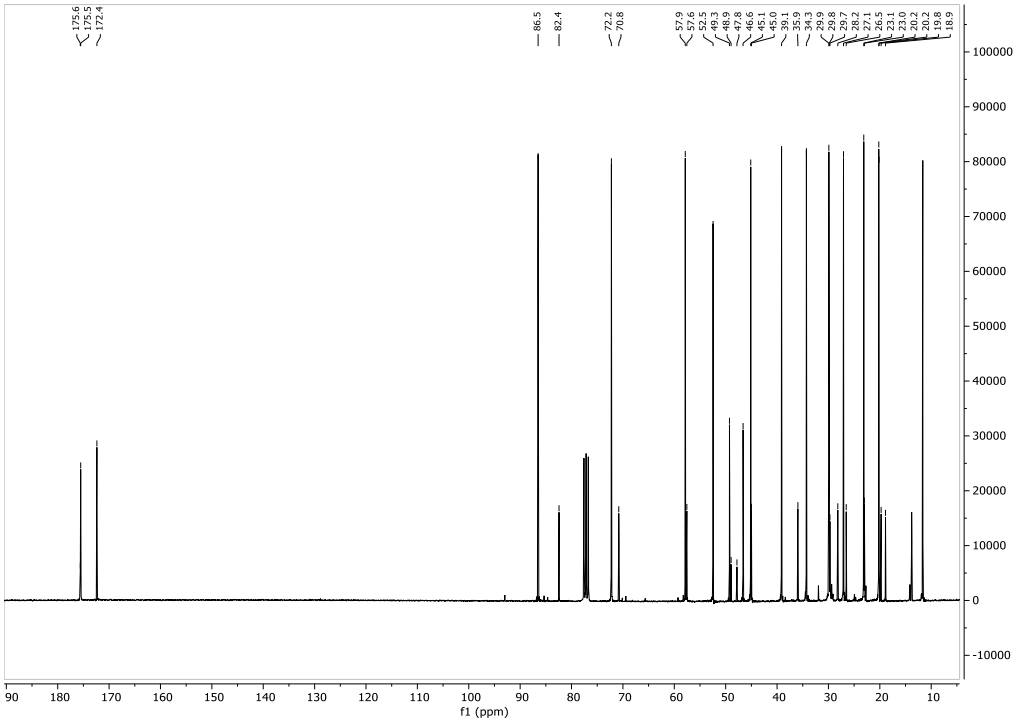
*S 63. NMR-^{1}H (300 MHz, $CDCl_3$) mixture of **10.1** and **10.2***



*S 64. NMR-^{13}C (75MHz, $CDCl_3$) mixture of **10.1** and **10.2**.*



S 65. NMR-^{1}H (300 MHz, $CDCl_3$) mixture of borneol and isoborneol with 1-(S).



*S 66. NMR-^{13}C (75 MHz, $CDCl_3$) of mixture of borneol and isoborneol **11.1** and **12.1**.*

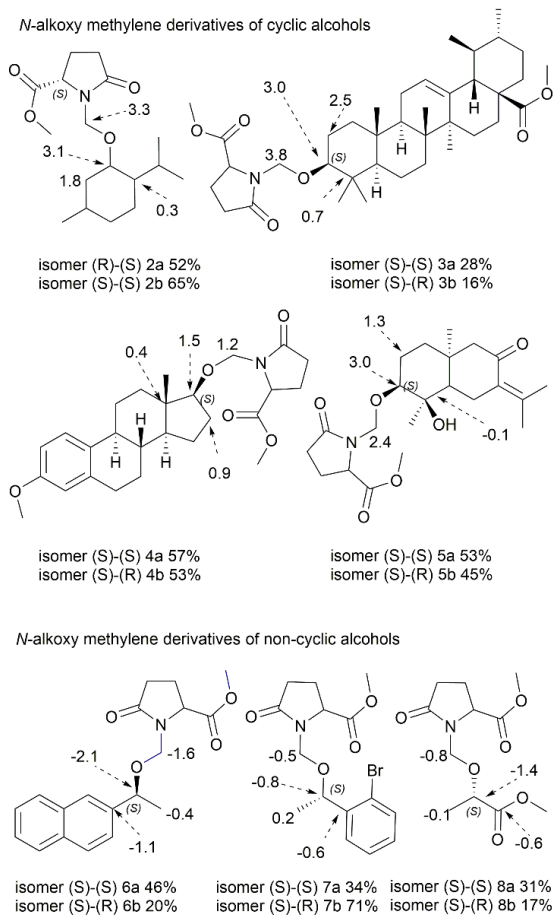


Figure 1. ^{13}C NMR $\Delta\delta_{S-R}$ between diastereomeric *N*-alkoxy methylene derivatives

Table 1. ^{13}C NMR $\Delta\delta_{S-R}$ between diastereomeric *N*-alkoxy methylene derivatives and GIAO/B3LYP (gas phase)/6-31+G(d) $\Delta\delta_{S-R}$ calculated, considering only the lowest-energy conformers.

Derivatives	Experimental $\Delta\delta_{S-R}$				Calculated $\Delta\delta_{S-R}$			
	C^1	C^2	C^3	*N*-alkoxy methylene	C^1	C^2	C^3	*N*-alkoxy methylene
2a- 2b	3.1	0.3	1.8	3.3	3.3	0.2	0.5	1.5
3a-3b	3.0	0.7	2.5	3.8	-0.3	-0.2	-0.2	-0.1
4a-4b	1.5	0.4	0.9	1.2	0.5	0.1	0.04	0.8
5a-5b	3.0	-0.1	1.3	2.4	7.1	2.6	-0.3	2.3
6a-6b	-2.7	-1.5	-0.4	-1.5	-1.3	-0.9	-1.1	-2.8
7a-7b	-0.8	-0.6	0.2	-0.5	3	-0.6	5	0.9
8a-8b	-1.4	-0.6	-0.1	-0.8	-3.8	-0.7	-5	-0.6

Table 2. Dihedral angles of some *N*-alkoxy methylene derivatives calculated by GIAO model.

Alcohol	**1** configuration	dihedral angle
2-(R)	(S)	175.7°
2-(S)	(S)	164.9°
3-(S)	(S)	175.2°
	(R)	-104.5°
4-(S)	(S)	173.2°
	(R)	175.3°
5-(S)	(S)	136.7°
	(R)	-173.9°
6-(S)	(S)	-175.2°
	(R)	180.0°
7-(S)	(S)	162.6°
	(R)	162.6°
8-(S)	(S)	180.0°
	(R)	180.0°

Gaussian 16 revision.

(+)-Menthol. **2-(R)**

O	-0.04964100	-0.08799000	-0.25892700
C	-1.44611000	-0.04225300	-0.58591200
C	4.34991800	-0.18153500	-0.11743400
C	4.28955000	0.90470800	-1.19739300
C	3.02725400	-0.97616900	-0.27886500
H	5.21177200	-0.84039100	-0.21283400
H	4.37825700	0.27209100	0.87175100
H	4.83270400	0.62765900	-2.10513400
H	4.67151100	1.87173100	-0.87307500
H	3.17535600	-1.89222400	-0.85914900
N	2.15939300	-0.05561200	-1.00597500
C	2.81789400	1.01727800	-1.56574400
O	2.30639200	1.86334000	-2.26881000
C	2.42431300	-1.44073400	1.04793200
O	2.12844400	-2.58841400	1.27242000
O	2.28666000	-0.43911600	1.92502000
C	1.65211700	-0.78018700	3.17057600
H	2.22520100	-1.54631500	3.69188300
H	1.62675300	0.14156500	3.74555100
H	0.64295200	-1.14555400	2.98456900
C	0.80391200	-0.37594200	-1.35185900
H	0.53573400	0.23603500	-2.21816000
H	0.74884900	-1.43939900	-1.61482800
C	-2.02039300	-1.45290000	-0.76441300
C	-2.16459000	0.72618200	0.53446300
H	-1.55717800	0.51130200	-1.52991700
C	-3.53352000	-1.45377600	-1.02242600
H	-1.80213700	-2.02734600	0.14360800
C	-3.67984700	0.72948300	0.26164300
H	-1.99690100	0.14492100	1.45182600
C	-4.24934600	-0.68177600	0.09158500
H	-3.71479600	-0.91916000	-1.96517200
H	-3.88893800	1.30662800	-0.64565500
H	-5.32198400	-0.62885900	-0.12107700
H	-4.14617600	-1.23654400	1.03295700
C	-4.07483700	-2.87628600	-1.17809500
H	-3.57758500	-3.40506500	-1.99560100
H	-3.91795300	-3.45640900	-0.26364400
H	-5.14765100	-2.87036200	-1.38809200
C	-1.56313700	2.13275400	0.79218700
H	-0.48448300	1.98163700	0.87964700
C	-1.79033500	3.13503700	-0.34774200
H	-1.25958600	4.06704600	-0.13854100
H	-1.41774100	2.76447300	-1.30485700
H	-2.84821600	3.38379300	-0.46816300
C	-2.04920900	2.71727400	2.12553400
H	-3.11697000	2.95253800	2.10690500
H	-1.87504300	2.02349900	2.95302700

H	-1.51841800	3.64516400	2.35364900
H	-1.51042800	-1.96273600	-1.58755600
H	-4.19929100	1.24004900	1.07606000

(-)-Menthol. **2 (S)**

C	-0.13101800	1.46084800	-0.15260000
C	0.66356500	0.32165300	0.50586000
C	-1.62490400	1.37764500	0.18013500
H	-0.00215200	1.42098900	-1.23706800
H	0.46734600	0.38292100	1.58588000
C	-2.22877100	0.02385600	-0.21795300
H	-1.76958800	1.53002700	1.25824500
H	-2.16751200	2.18570900	-0.32116200
C	-1.41568300	-1.11625800	0.41136600
H	-2.14205700	-0.06849400	-1.30687800
H	-1.80565600	-2.08657900	0.07836800
H	-1.54247600	-1.09727200	1.50115100
C	2.20141500	0.48786200	0.36844800
H	2.42265200	1.43205800	0.88383200
C	2.97041500	-0.61264000	1.11140500
H	2.88326300	-1.57670800	0.60362700
H	4.03457600	-0.36874700	1.16179300
H	2.61041500	-0.73698600	2.13705500
C	2.72929300	0.63311700	-1.06614900
H	2.25507000	1.46262800	-1.59390500
H	3.80478200	0.83137200	-1.04600600
H	2.55647500	-0.27271800	-1.64687500
C	-3.70983300	-0.07357200	0.15234300
H	-4.28930200	0.72256400	-0.32265700
H	-4.13840700	-1.02951200	-0.16153700
H	-3.85143900	0.01390600	1.23431200
C	0.08463600	-1.04244700	0.09750600
H	0.59559000	-1.82973200	0.66471900
O	0.33025400	-1.25125800	-1.30413400
H	-0.07108100	-2.08879400	-1.56088500
H	0.27277700	2.42305300	0.17890000

Methyl-(S)-1-((((1R,2S,5R)-2-isopropyl-5-methylcyclohexyl)oxy)methyl)-5-oxopyrrolidine-2-carboxylate 2a.

C	-4.34991800	-0.18153500	0.11743400
C	-4.28955000	0.90470800	1.19739300
C	-3.02725400	-0.97616900	0.27886500
H	-5.21177200	-0.84039100	0.21283400
H	-4.37825700	0.27209100	-0.87175100
H	-4.83270400	0.62765900	2.10513400
H	-4.67151100	1.87173100	0.87307500
H	-3.17535600	-1.89222400	0.85914900

N	-2.15939300	-0.05561200	1.00597500
C	-2.81789400	1.01727800	1.56574400
O	-2.30639200	1.86334000	2.26881000
C	-2.42431300	-1.44073400	-1.04793200
O	-2.12844400	-2.58841400	-1.27242000
O	-2.28666000	-0.43911600	-1.92502000
C	-1.65211700	-0.78018700	-3.17057600
H	-2.22520100	-1.54631500	-3.69188300
H	-1.62675300	0.14156500	-3.74555100
H	-0.64295200	-1.14555400	-2.98456900
C	-0.80391200	-0.37594200	1.35185900
H	-0.53573400	0.23603500	2.21816000
H	-0.74884900	-1.43939900	1.61482800
O	0.04964100	-0.08799000	0.25892700
C	1.44611000	-0.04225300	0.58591200
C	2.02039300	-1.45290000	0.76441300
C	2.16459000	0.72618200	-0.53446300
H	1.55717800	0.51130200	1.52991700
C	3.53352000	-1.45377600	1.02242600
H	1.80213700	-2.02734600	-0.14360800
C	3.67984700	0.72948300	-0.26164300
H	1.99690100	0.14492100	-1.45182600
C	4.24934600	-0.68177600	-0.09158500
H	3.71479600	-0.91916000	1.96517200
H	3.88893800	1.30662800	0.64565500
H	5.32198400	-0.62885900	0.12107700
H	4.14617600	-1.23654400	-1.03295700
C	4.07483700	-2.87628600	1.17809500
H	3.57758500	-3.40506500	1.99560100
H	3.91795300	-3.45640900	0.26364400
H	5.14765100	-2.87036200	1.38809200
C	1.56313700	2.13275400	-0.79218700
H	0.48448300	1.98163700	-0.87964700
C	1.79033500	3.13503700	0.34774200
H	1.25958600	4.06704600	0.13854100
H	1.41774100	2.76447300	1.30485700
H	2.84821600	3.38379300	0.46816300
C	2.04920900	2.71727400	-2.12553400
H	3.11697000	2.95253800	-2.10690500
H	1.87504300	2.02349900	-2.95302700
H	1.51841800	3.64516400	-2.35364900
H	1.51042800	-1.96273600	1.58755600
H	4.19929100	1.24004900	-1.07606000

Methyl-(S)-1-((((1S,2R,5S)-2-isopropyl-5-methylcyclohexyl)oxy)methyl)-5-oxopyrrolidine-2-carboxylate 2b.

.C	-4.34991800	-0.18153500	0.11743400
C	-4.28955000	0.90470800	1.19739300
C	-3.02725400	-0.97616900	0.27886500
H	-5.21177200	-0.84039100	0.21283400
H	-4.37825700	0.27209100	-0.87175100

H	-4.83270400	0.62765900	2.10513400
H	-4.67151100	1.87173100	0.87307500
H	-3.17535600	-1.89222400	0.85914900
N	-2.15939300	-0.05561200	1.00597500
C	-2.81789400	1.01727800	1.56574400
O	-2.30639200	1.86334000	2.26881000
C	-2.42431300	-1.44073400	-1.04793200
O	-2.12844400	-2.58841400	-1.27242000
O	-2.28666000	-0.43911600	-1.92502000
C	-1.65211700	-0.78018700	-3.17057600
H	-2.22520100	-1.54631500	-3.69188300
H	-1.62675300	0.14156500	-3.74555100
H	-0.64295200	-1.14555400	-2.98456900
C	-0.80391200	-0.37594200	1.35185900
H	-0.53573400	0.23603500	2.21816000
H	-0.74884900	-1.43939900	1.61482800
O	0.04964100	-0.08799000	0.25892700
C	1.44611000	-0.04225300	0.58591200
C	2.02039300	-1.45290000	0.76441300
C	2.16459000	0.72618200	-0.53446300
H	1.55717800	0.51130200	1.52991700
C	3.53352000	-1.45377600	1.02242600
H	1.80213700	-2.02734600	-0.14360800
C	3.67984700	0.72948300	-0.26164300
H	1.99690100	0.14492100	-1.45182600
C	4.24934600	-0.68177600	-0.09158500
H	3.71479600	-0.91916000	1.96517200
H	3.88893800	1.30662800	0.64565500
H	5.32198400	-0.62885900	0.12107700
H	4.14617600	-1.23654400	-1.03295700
C	4.07483700	-2.87628600	1.17809500
H	3.57758500	-3.40506500	1.99560100
H	3.91795300	-3.45640900	0.26364400
H	5.14765100	-2.87036200	1.38809200
C	1.56313700	2.13275400	-0.79218700
H	0.48448300	1.98163700	-0.87964700
C	1.79033500	3.13503700	0.34774200
H	1.25958600	4.06704600	0.13854100
H	1.41774100	2.76447300	1.30485700
H	2.84821600	3.38379300	0.46816300
C	2.04920900	2.71727400	-2.12553400
H	3.11697000	2.95253800	-2.10690500
H	1.87504300	2.02349900	-2.95302700
H	1.51841800	3.64516400	-2.35364900
H	1.51042800	-1.96273600	1.58755600
H	4.19929100	1.24004900	-1.07606000

Ursolic acid Methyl ester. 3

C	3.62216600	0.80294500	-1.78826600
C	5.15132400	0.82203100	-1.85537900
C	5.77623100	1.08204000	-0.48976200
C	5.35411400	0.05930600	0.59310300
C	3.78646300	0.01390600	0.59827500
C	3.17280400	-0.88283100	1.68126900
C	1.70572300	-0.50921500	1.91770100
C	0.80818700	-0.58709000	0.65787600
C	1.53625800	0.11780400	-0.53700800
C	3.06400900	-0.22470500	-0.76931600
C	0.68828100	0.03046800	-1.81360800
C	-0.77957300	0.20472400	-1.57555600
C	-1.38261800	0.28177200	-0.38919300
C	-0.58411400	0.17404600	0.91706100
C	-1.46025100	-0.58469300	1.96675300
C	-2.56443900	-1.44634800	1.35442700
C	-3.62088800	-0.59926500	0.59155300
C	-2.90481000	0.44426900	-0.36330200
C	-3.43858800	1.90148800	-0.15197400
C	-4.98343500	1.86092100	-0.21646900
C	-5.55566700	1.06231000	0.97830200
C	-4.54433600	0.09792500	1.60678800
C	5.84849500	0.60855800	1.95042500
C	6.03604300	-1.30494500	0.37359300
C	3.29446200	-1.64109600	-1.35127600
C	0.54234600	-2.07789700	0.35181900
C	-0.35508600	1.60292400	1.47980100
C	-4.45662900	-1.60650200	-0.20585600
C	-2.83561200	2.86164300	-1.18113900
C	-5.65447800	3.23665800	-0.29259700
C	-4.50404900	-3.07005700	-2.05916400
H	1.29202400	-1.14507900	2.70599800
H	3.50288000	1.04047300	0.87414500
H	3.27051800	-1.93859700	1.41818100
H	3.70635900	-0.76103700	2.62549500
H	1.56375700	1.17806100	-0.27046200
H	1.70446100	0.50760100	2.31287200
H	3.22314500	0.60211500	-2.78568700
H	5.47050100	1.60994600	-2.54815000
H	3.27149700	1.80418500	-1.51049500
H	5.54591300	-0.11320300	-2.25988400
H	5.43324300	2.06854800	-0.14178700
H	2.49799800	-1.92272700	-2.03981800
H	4.22255500	-1.68835400	-1.91874000
H	3.35484800	-2.41599700	-0.59007800
H	5.87957000	-1.71171100	-0.62328900
H	7.11203100	-1.20699300	0.51911700
H	5.66656700	-2.03714800	1.09471000
H	6.91212000	0.84041600	1.88938300
H	5.31726300	1.52421000	2.22695400

H	5.71369400	-0.11538800	2.75536600
H	1.01638500	0.78872300	-2.53193500
H	0.83579700	-0.92645200	-2.32778100
H	-1.39179900	0.25151900	-2.47316300
H	-0.08766100	-2.21614000	-0.52647700
H	1.46921700	-2.61843600	0.17991900
H	0.05108000	-2.56656800	1.19385500
H	-1.29677200	2.14817800	1.50793300
H	0.02114200	1.57437300	2.50373800
H	0.33724700	2.19095800	0.87719600
H	-0.83144800	-1.20593700	2.60587600
H	-1.91560800	0.14394000	2.64112800
H	-3.21908300	0.20466600	-1.38021200
H	-2.12840400	-2.17462900	0.67123900
H	-3.07409700	-2.01194000	2.14035900
H	-3.16271200	2.26554600	0.84326500
H	-5.23831200	1.32612500	-1.14177700
H	-1.74650700	2.83361500	-1.16221200
H	-3.15304100	2.59961800	-2.19601500
H	-3.14517600	3.89014300	-0.99101500
H	-5.42003600	3.76878300	-1.21575000
H	-6.74129100	3.12645100	-0.24414300
H	-5.35225600	3.86839000	0.54903800
H	-5.06996900	-0.66187200	2.18695000
H	-3.91561200	0.64656200	2.31047700
O	-5.55107600	-2.00803800	0.11039400
O	-3.80996800	-2.06610800	-1.30042600
H	-5.45252700	-2.68159800	-2.42962700
H	-3.84310600	-3.31884900	-2.88590100
H	-4.69680700	-3.94855700	-1.44355500
H	-6.44412800	0.51434300	0.65852000
H	-5.88788800	1.76282700	1.75163400
O	7.20803500	1.09500200	-0.56747600
H	7.47249000	1.75348600	-1.21860700

Methyl-(S)-1-((((3S,4aR,6aR,6bS,8aS,11R,12S,12aS,14aR,14bR)-8a-(methoxycarbonyl)-4,4,6a,6b,11,12,14b-heptamehyll-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,10,11,12,12a,14,14a,14b-icosahydropicen-3-yl)oxy)methyl)-5-oxopyrrolidyne-2-carboxylate, 3a.

C	1.29758300	-0.71371600	-1.55958900
C	2.80825800	-0.95421800	-1.51286600
C	3.45616500	-0.26477600	-0.31550800
C	2.84931800	-0.68254900	1.04860500
C	1.29621100	-0.49096000	0.94666500
C	0.52863800	-0.77345700	2.24475000
C	-0.85844400	-0.12445900	2.19823900
C	-1.74066000	-0.57115400	1.00637700
C	-0.89059200	-0.52266800	-0.30889500
C	0.56166000	-1.15059300	-0.26677300
C	-1.72459500	-0.99138600	-1.50927100
C	-3.14708400	-0.52631700	-1.47365400
C	-3.74457300	0.10798800	-0.46531800

C	-2.99095900	0.42412200	0.83367300
C	-3.99308100	0.29243200	2.02657100
C	-5.20991800	-0.58253300	1.72684500
C	-6.10720500	0.01404300	0.60827200
C	-5.22086100	0.48024800	-0.62120500
C	-5.51798500	1.96021700	-1.03640500
C	-7.04736800	2.11358300	-1.20886200
C	-7.77086500	1.93135900	0.14646900
C	-6.93983600	1.17226700	1.18582200
C	3.40710800	0.29085600	2.11032300
C	3.29635500	-2.10252400	1.44489700
C	0.56064100	-2.69826600	-0.22223800
C	-2.24587400	-2.00206900	1.29487000
C	-2.53636600	1.90803500	0.79768700
C	-7.06699300	-1.10626200	0.19590800
C	-4.74797400	2.33898500	-2.30441200
C	-7.48498000	3.42995600	-1.85985800
C	-7.27820900	-3.18867200	-0.88792400
C	7.66637900	1.38461500	0.99470800
C	7.70842200	0.04210000	0.28085100
C	9.16232100	-0.34281100	-0.10383200
C	8.99713400	-1.18771200	-1.37003800
C	7.66130600	-0.74835300	-1.95605500
C	7.77106000	3.72257600	0.76806000
C	5.62632200	0.34001000	-1.12793900
O	4.86665500	-0.51468200	-0.28704200
H	-1.38143400	-0.31941200	3.13902100
H	1.18427200	0.58932900	0.77052400
H	0.45234500	-1.84750500	2.42880400
H	1.06277300	-0.36185100	3.10277400
H	-0.69022500	0.53833000	-0.48202900
H	-0.69556900	0.95346100	2.15672600
H	0.88187500	-1.23368500	-2.42612500
H	3.25893500	-0.58235800	-2.43693700
H	1.11732400	0.35535200	-1.72589400
H	3.04242000	-2.02037900	-1.47570800
H	3.29803400	0.82102000	-0.41417000
H	-0.26357100	-3.11219600	-0.80252500
H	1.47386200	-3.10593100	-0.65260800
H	0.48256100	-3.10142400	0.78527700
H	3.07708800	-2.85242400	0.68798400
H	4.37340900	-2.11469700	1.61307100
H	2.81130900	-2.41212700	2.37281600
H	4.49536000	0.32374800	2.05317100
H	3.02729600	1.30561600	1.95863700
H	3.14516500	-0.01697200	3.12328900
H	-1.26700200	-0.64214400	-2.44036400
H	-1.72899200	-2.08455700	-1.59131600
H	-3.73226700	-0.75840400	-2.36030400
H	-2.88638800	-2.38379000	0.50037200
H	-1.41991700	-2.69774400	1.41490600
H	-2.81470400	-2.03372500	2.22466600

H	-3.37537900	2.54955800	0.53430200
H	-2.18109600	2.24180000	1.77401800
H	-1.75036500	2.09372100	0.06576400
H	-3.48106300	-0.09169700	2.90983800
H	-4.33761300	1.28926400	2.31111200
H	-5.55527300	-0.09813200	-1.48398900
H	-4.88507600	-1.57882500	1.43034500
H	-5.81428400	-0.70092200	2.63146200
H	-5.20781200	2.64557600	-0.24060800
H	-7.36262500	1.30164400	-1.87835000
H	-3.67864000	2.16608900	-2.18814100
H	-5.08503000	1.74427700	-3.15985700
H	-4.88996400	3.39108000	-2.55428000
H	-7.14475800	3.52260300	-2.89222100
H	-8.57601000	3.50003400	-1.86623000
H	-7.10557300	4.29041200	-1.29935900
H	-7.59602600	0.77840900	1.96324500
H	-6.25608400	1.86709700	1.67736800
O	-8.23445900	-1.17222900	0.49342700
O	-6.44878700	-2.07685000	-0.51579000
H	-8.10837300	-2.85480700	-1.51016300
H	-6.63107000	-3.86395000	-1.44202100
H	-7.67806100	-3.68013700	-0.00115100
H	-8.71990600	1.41731300	-0.01432500
H	-8.01779200	2.91592100	0.55692200
H	5.37616700	0.20617500	-2.18281400
H	5.46169300	1.38481600	-0.83712100
H	7.28407500	-0.67914300	0.98300400
H	8.92030700	-2.25585800	-1.14757500
H	9.79503000	-1.06072900	-2.10010000
H	9.66178400	-0.85957400	0.71359800
H	9.72617300	0.56342100	-0.33017800
O	7.22453200	-1.01286700	-3.05293800
N	7.01109200	0.00245700	-0.99565200
O	7.61624200	1.49425400	2.19262400
O	7.74502200	2.42460400	0.14498100
H	7.81933200	4.43688800	-0.04931600
H	6.87130800	3.87492600	1.36303300
H	8.64401000	3.81453800	1.41350000

Methyl-(R)-1-((((3S,4aR,6aR,6bS,8aS,11R,12S,12aS,14aR,14bR)-8a-(methoxycarbonyl)-4,4,6a,6b,11,12,14b-heptamehyll-1,2,3,4,4a,5,6,6a,6b,7,8,8a,9,10,11,12,12a,14,14a,14b-icosahydropicen-3-yl)oxy)methyl)-5-oxopyrrolidyne-2-carboxylate, 3b.

C	1.74657700	-0.85742100	0.37155000
C	3.26237400	-0.70277200	0.21820000
C	3.62936400	-0.16636200	-1.16009000
C	2.95125600	1.18173800	-1.51614400
C	1.41128800	1.00800200	-1.27833800
C	0.56042900	2.22529700	-1.66369600
C	-0.90558600	1.81759800	-1.84426800

C	-1.54741200	1.15011900	-0.60277800
C	-0.57195500	0.05861200	-0.04528300
C	0.95414600	0.44767500	0.10809300
C	-1.16132700	-0.60556200	1.20673200
C	-2.63885900	-0.83326100	1.13041300
C	-3.45522600	-0.40116100	0.16969800
C	-2.92803500	0.43217700	-1.00636300
C	-4.02212500	1.47877500	-1.39577200
C	-5.01735500	1.78770900	-0.27783200
C	-5.87120200	0.55060300	0.11294600
C	-4.94617400	-0.72552600	0.28984800
C	-5.45555300	-1.94544200	-0.54871500
C	-6.95702900	-2.14901300	-0.23839600
C	-7.78770000	-0.94752100	-0.74793200
C	-6.95983600	0.32545700	-0.95134600
C	3.20291200	1.43670600	-3.01872400
C	3.59017100	2.34790000	-0.73709300
C	1.22715300	1.41451300	1.28634600
C	-1.81645200	2.25109100	0.44676900
C	-2.74733600	-0.49874200	-2.23539200
C	-6.55941300	0.91305200	1.43231700
C	-4.62476100	-3.19749900	-0.25484100
C	-7.54662700	-3.45626500	-0.77832900
C	-6.26500500	1.31125800	3.73666800
C	7.05064100	0.48705600	1.03943400
C	7.61394100	-0.69743000	0.25212700
C	8.36057000	-1.66904300	1.20606000
C	7.29625500	-2.70623700	1.58392600
C	6.30749600	-2.66940900	0.42506100
C	7.26873600	2.79433400	1.44947200
C	5.82593500	-1.15343000	-1.48660000
O	5.05085200	0.01087800	-1.31973700
H	-1.49164100	2.69340300	-2.13814800
H	1.13122400	0.21815300	-1.99105200
H	0.65593900	3.02079600	-0.92103000
H	0.90779100	2.65366900	-2.60556900
H	-0.54645900	-0.72139100	-0.81114300
H	-0.93484500	1.13167800	-2.69213200
H	1.53277700	-1.23493700	1.37439500
H	3.72770200	-1.68053600	0.35786600
H	1.40062800	-1.62902200	-0.32696900
H	3.68248500	-0.05123900	0.98642000
H	3.30129900	-0.89922500	-1.91267400
H	0.56152200	1.21551800	2.12589300
H	2.24124700	1.29643500	1.66445700
H	1.10965800	2.46357900	1.02171600
H	3.60793200	2.18488500	0.33822200
H	4.62100800	2.48412600	-1.06594900
H	3.05241900	3.27876200	-0.92881000
H	4.26901800	1.35496800	-3.23160900
H	2.67481000	0.70765300	-3.64024200
H	2.88154200	2.43368700	-3.32312500

H	-0.66890300	-1.56670100	1.38481900
H	-0.95731200	-0.01461800	2.10729900
H	-3.06465900	-1.39156800	1.96082800
H	-2.28005600	1.85727300	1.35076200
H	-0.89820300	2.75290900	0.73953800
H	-2.47512700	3.02093000	0.04332500
H	-3.65164000	-1.08253900	-2.39757100
H	-2.57574400	0.07299700	-3.14891100
H	-1.92727400	-1.20644100	-2.11530100
H	-3.55576900	2.40635800	-1.73059100
H	-4.57198800	1.10960100	-2.26454200
H	-5.06744900	-1.05791300	1.32213700
H	-4.48524800	2.14613300	0.60213000
H	-5.69150100	2.59076400	-0.59151200
H	-5.36831900	-1.73124200	-1.61915400
H	-7.04093600	-2.18466700	0.85639300
H	-3.56258300	-3.01830700	-0.41735200
H	-4.74807500	-3.51430600	0.78608100
H	-4.92353400	-4.02966300	-0.89335700
H	-7.11103500	-4.33956300	-0.30921300
H	-8.62419100	-3.48486900	-0.59553400
H	-7.39626600	-3.53785200	-1.85963000
H	-7.62004800	1.19383000	-0.96659300
H	-6.47354200	0.28616400	-1.92797200
O	-7.72347800	1.20520200	1.55759400
O	-5.69744700	0.92561000	2.47530200
H	-7.06053500	0.62391500	4.02402400
H	-5.44631200	1.27015400	4.45074100
H	-6.67468100	2.31956400	3.67871200
H	-8.60478200	-0.74937000	-0.05229100
H	-8.25194100	-1.21157800	-1.70378400
H	5.21907000	-2.01780400	-1.76362800
H	6.54359100	-0.93198200	-2.28241000
H	6.75663300	-2.42671400	2.49100000
H	7.68378400	-3.71537900	1.71626200
H	8.79128400	-1.15377400	2.06356500
H	9.17456500	-2.14033500	0.65296600
O	5.44387900	-3.48267900	0.17193400
N	6.56587800	-1.53165900	-0.30460400
H	8.26265000	-0.31308500	-0.53652700
O	6.19697600	0.40097200	1.88453400
O	7.68234600	1.62687900	0.71407200
H	7.92885600	3.59336900	1.12288000
H	6.23186300	3.03421500	1.21762000
H	7.36747900	2.62236800	2.52056100

Estradiol 3-methyl ether, 4.

C	-0.14675200	2.15146900	-0.42127300
C	-0.78097400	0.83489700	0.02957000
C	0.01491200	-0.34818900	-0.57585900
C	1.26692000	2.28116300	0.14413600

C	-0.59212300	-1.70956300	-0.17486800
C	-2.24959600	0.68636600	-0.36060800
C	-2.87938800	-0.63522200	0.14348700
C	-2.10159800	-1.80737100	-0.46674100
C	2.36109700	-1.32846100	-0.39087000
C	3.73656800	-1.23992500	-0.19530600
C	4.30004100	-0.00175200	0.10036500
C	3.47270100	1.11425100	0.19202000
C	2.09854300	1.02157500	-0.00187400
C	1.51331800	-0.22469200	-0.29952000
C	-2.91097900	-0.75597500	1.68026200
C	-4.31342400	-0.44775000	-0.38585300
C	-3.27495900	1.76727000	0.02927400
C	-4.64492100	1.04040800	-0.09449500
O	5.63288500	0.21913000	0.31204500
C	6.51734800	-0.88628300	0.21973200
H	-0.12042600	2.18331900	-1.51734600
H	-0.74860400	3.00441100	-0.09675100
H	-0.69755700	0.78717900	1.12329000
H	-0.11423300	-0.26150100	-1.66633000
H	1.20021400	2.52876000	1.21096300
H	1.79172000	3.11862200	-0.32430400
H	-0.09065600	-2.51488000	-0.71568400
H	-0.39728700	-1.89274900	0.88618200
H	-2.26890400	0.62617000	-1.45968400
H	-2.48800000	-2.76233400	-0.09912600
H	-2.25437000	-1.80535300	-1.55297900
H	1.95151700	-2.30242600	-0.62538900
H	4.34267500	-2.13117900	-0.27791300
H	3.92819500	2.07171400	0.42023200
H	-3.41579500	0.08729100	2.15378600
H	-3.45395000	-1.65815000	1.96394500
H	-1.90920000	-0.81803900	2.10444400
H	-4.29539000	-0.61422400	-1.47097900
H	-3.11049200	2.11450000	1.05244500
H	-3.21391200	2.64497600	-0.61583300
H	-5.26622600	1.46914600	-0.88401400
H	-5.21722800	1.10142300	0.83310800
H	7.51167900	-0.49120400	0.41804000
H	6.27836100	-1.65338000	0.96307300
H	6.49797000	-1.33183200	-0.77989100
O	-5.21830700	-1.37932200	0.20634000
H	-6.07714000	-1.29201900	-0.21983500

Methyl-(S)-1-((((8R,9S,13S,14S,17S)-3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)oxy)methyl)-5-oxopyrrolidin-2-carboxilate, 4a.

C	3.27401500	2.37112300	-0.61927900
C	2.38583000	1.21112400	-0.15439600
C	3.00075600	-0.12990200	-0.63939700
C	4.64461000	2.29138800	0.05959700

H	2.38642900	1.21742500	0.94675100
H	3.38816600	2.32619600	-1.71239500
H	2.80719900	3.33686200	-0.39048500
H	4.53898600	2.61176300	1.10740100
H	5.34274300	3.00291900	-0.39937500
H	2.95840200	-0.09150900	-1.74281000
C	2.13538300	-1.34131200	-0.21635500
C	0.93968400	1.29480600	-0.64983900
C	0.05453800	0.13239600	-0.12956000
C	0.65323000	-1.19479300	-0.62150000
H	2.52261900	-2.25683400	-0.67708300
H	0.07595800	-2.04694100	-0.24125400
H	2.22403200	-1.48825000	0.86776100
H	0.57960100	-1.23251500	-1.71854500
H	0.98212600	1.17382200	-1.74654300
C	5.12523600	-1.48929700	-0.22531500
C	6.48059100	-1.62742400	0.07947300
C	7.23215300	-0.48515800	0.36775900
C	6.60684900	0.76460900	0.34101800
C	5.25159900	0.89837900	0.03839200
C	4.47745600	-0.24871600	-0.25077000
H	4.56715100	-2.39194000	-0.45294200
H	6.92777100	-2.61502800	0.08547600
H	7.20835900	1.64233000	0.56395700
C	-0.09967200	0.11407300	1.40732900
H	-0.48199900	1.06136200	1.80073800
H	-0.80980700	-0.66751000	1.69244500
H	0.84768500	-0.09143300	1.91252300
C	-1.29132200	0.52996600	-0.77347300
H	-1.24670500	0.28840400	-1.84883300
C	0.09547000	2.55869500	-0.38663100
H	0.24709600	2.92720100	0.63481700
H	0.35821400	3.37998400	-1.06071900
C	-1.37299900	2.07715500	-0.59166200
H	-1.84188200	2.56071600	-1.45502000
H	-1.99580800	2.30263600	0.28096800
O	-2.37155400	-0.19389200	-0.19573500
C	-3.58483900	-0.08735900	-0.92244200
H	-3.91435300	0.96151200	-0.96891900
H	-3.47725600	-0.48018800	-1.94125300
N	-4.58044100	-0.88203300	-0.26802900
C	-5.81042200	-1.87110600	1.47837500
H	-6.66624400	-1.68080600	2.13015600
H	-5.09050500	-2.47612200	2.03802000
C	-6.16468400	-2.55599400	0.15105100
H	-7.16325900	-2.27655400	-0.20714700
H	-6.11808400	-3.64690100	0.18305400
C	-5.13611900	-2.01064900	-0.84036900
O	-4.86234500	-2.45341000	-1.94072900
C	-6.09691500	0.62243500	1.05929300
O	-6.38433800	1.22599900	2.06961300
O	-6.63683700	0.87132500	-0.15044300

C	-7.60772300	1.93371300	-0.18268500
H	-7.15640800	2.87275900	0.14741300
H	-7.92892200	2.00356900	-1.22191300
H	-8.45313300	1.69769100	0.46875600
C	-5.10998100	-0.55007500	1.04174700
H	-4.30531500	-0.28130000	1.73112700
O	8.56422400	-0.48135500	0.67935700
C	9.24358300	-1.72464000	0.71218000
H	10.27775500	-1.49530700	0.97676900
H	8.81845700	-2.39952600	1.46745300
H	9.22297100	-2.22421500	-0.26589500

Methyl-(R)-1-((((8R,9S,13S,14S,17S)-3-methoxy-13-methyl-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl)oxy)methyl)-5-oxopyrrolidin-2-carboxilate, 4b.

C	2.86869700	-0.67833300	0.18726500
C	1.66191000	-0.45307300	-0.76646000
C	1.91884500	0.97281200	-1.34386500
C	3.27506300	1.36738700	-0.72290900
C	4.34774700	0.48329600	-1.39428800
C	4.06604600	-0.91837300	-0.77603600
C	3.18297300	0.77266700	0.71349800
C	2.08615300	1.40587400	1.58463700
C	4.49264400	0.88291700	1.51234300
C	2.66731900	-1.78480900	1.20816200
C	-3.21808900	1.09585100	-0.23455600
C	-2.50213700	0.05115000	0.62267600
C	-3.50656300	-0.74999400	1.50013500
C	-3.75203800	-2.03886100	0.70802500
C	-2.52319900	-2.18345800	-0.18069500
C	-4.19573600	3.24540300	-0.18273200
C	-0.68945200	-0.73082300	-0.95394900
H	4.24869000	0.48972000	-2.48158600
H	5.35739600	0.82760200	-1.16621100
H	3.82391300	-1.67079500	-1.52965900
H	4.92836000	-1.29522300	-0.22416100
H	1.11975800	1.64568200	-1.02939000
H	1.94930800	0.98799400	-2.43525100
H	1.67400700	-1.21547000	-1.55460200
H	3.48464300	2.43776800	-0.77281600
H	2.03807400	0.90803800	2.55683200
H	2.32206100	2.45786100	1.77212700
H	1.09430100	1.34906100	1.14525300
H	4.71310800	1.93348600	1.72233800
H	4.39664700	0.37663100	2.47630400
H	5.36008200	0.46228400	1.00663500
H	2.47460700	-2.74076900	0.71303500
H	3.55917300	-1.90867500	1.82791800
H	1.81737800	-1.58133000	1.86008200
O	0.41687300	-0.57823300	-0.07539100
H	-0.82315900	0.17081400	-1.56311200
H	-0.54786100	-1.59537000	-1.60875900

H	-1.77155000	0.57142300	1.24335000
H	-3.03084600	-0.97331300	2.45558600
H	-4.41104200	-0.17971300	1.70557500
H	-3.86957900	-2.92452400	1.33044900
H	-4.62808300	-1.97078900	0.05779500
N	-1.86741200	-0.97260600	-0.17903200
O	-2.18186700	-3.16977000	-0.79738100
O	-3.53435600	0.96059700	-1.38825200
O	-3.47294500	2.19875100	0.49443700
H	-4.30940900	4.04023300	0.54945900
H	-3.63207300	3.59499700	-1.04686300
H	-5.16875000	2.88204800	-0.51191000

(5R,6S,8aS)-5,6-dihidroxi-5,8a-dimethyl-3-(propan-2-iliden)octahydronaphtalen-2(1H)-ona, Cuauhtemona, **5.**

C	-1.90200500	-1.80085600	-0.57291100
C	-3.16274700	-1.04120100	-0.15125200
C	-3.02793000	0.46019300	-0.40252100
C	-1.79675000	1.08386100	0.29812400
C	-0.52354700	0.25004200	-0.04487600
C	0.74785700	0.82057200	0.60182900
C	2.02529400	0.15611300	0.10618700
C	1.94409800	-1.32412300	-0.09066000
C	0.61092900	-1.88503800	-0.56877000
C	-0.62913200	-1.29327500	0.13581900
C	3.16787500	0.83137800	-0.14748000
C	4.42821800	0.20815400	-0.69101600
C	3.31431700	2.31634300	0.06979200
C	-0.61365700	-1.78480700	1.59853500
C	-2.07752000	1.28438500	1.78737600
H	-0.41084000	0.39565700	-1.12616700
H	-1.77577600	-1.68580200	-1.65289500
H	-2.02886100	-2.87106100	-0.38268000
H	-4.02985800	-1.41802800	-0.70372200
H	-3.38647400	-1.20702500	0.90648800
H	-3.91806800	0.99028100	-0.04661400
H	0.65216200	-2.97074400	-0.46128700
H	0.54752700	-1.66382600	-1.64191000
H	0.69147000	0.70761100	1.69034700
H	0.76426400	1.88903100	0.40465600
H	-0.54384300	-2.87545600	1.61202800
H	0.24221600	-1.40333800	2.15789800
H	-1.51289000	-1.51266900	2.14918500
H	4.89652900	0.89250900	-1.40522200
H	5.14906600	0.05168900	0.11858000
H	4.26906100	-0.75706900	-1.16176400
H	3.40349800	2.83484800	-0.89140500
H	2.50098900	2.77165700	0.62826900
H	4.24555000	2.51296600	0.61064800
O	2.88604500	-2.07577300	0.09314500
H	-2.94722400	1.93419400	1.89877900
H	-2.26966200	0.35287300	2.31519500

H	-1.23446200	1.78066100	2.26746900
O	-1.62039300	2.41390000	-0.21198500
H	-1.80831200	2.36980500	-1.16037500
O	-2.86592700	0.72641700	-1.81275900
H	-3.72565900	0.67444400	-2.24176600

Methyl-(2S)-1-((((1R,2S,4aS)-1-hydroxy-1,4a-dimethyl-6-oxo-7-(propan-2-iliden)decahydronaphtalen-2-yl)oxy)methyl)-5-oxopirrolydine-2-carboxylate, 5a.

C	1.31688200	-2.13183600	-1.68856600
C	0.13778200	-2.74337500	-0.92698500
C	-0.54192400	-1.70028300	-0.03372700
C	0.44425300	-1.06662900	0.98754800
C	1.69063900	-0.52765100	0.23282700
C	2.70482000	0.15419400	1.16585100
C	3.82145800	0.87083800	0.41821300
C	4.34475800	0.16276500	-0.79062300
C	3.34329700	-0.64849800	-1.60135200
C	2.37960000	-1.51132100	-0.75754400
C	4.32286700	2.06724500	0.79592200
C	5.38660400	2.82610800	0.04413000
C	-3.71586400	0.24555900	1.28281300
C	3.85717600	2.80600000	2.02532200
C	3.21437300	-2.62921000	-0.09724400
C	0.72367100	-2.07439000	2.11361600
C	-3.15899400	1.12389900	0.16544700
C	-3.99226300	2.39221500	-0.13561400
C	-3.81183400	2.60525200	-1.64319400
C	-3.42742900	1.23814400	-2.19054800
C	-5.60321900	-0.88848600	2.13381600
C	-2.43514800	-0.82568500	-1.26772500
H	1.26786200	0.26423600	-0.39525400
H	0.92940900	-1.35400400	-2.35203100
H	1.78324100	-2.88778900	-2.32780700
H	-0.59836500	-3.13900200	-1.63325000
H	0.45954100	-3.59273500	-0.31870600
H	-1.35589900	-2.17074100	0.53475900
H	3.90794400	-1.25766200	-2.30987900
H	2.75541200	0.07249700	-2.18342300
H	3.15057400	-0.58896900	1.83683700
H	2.15606700	0.84728100	1.79643200
H	3.76627900	-3.17114000	-0.86943700
H	3.95159400	-2.23889500	0.60656900
H	2.60641900	-3.35808800	0.43635500
H	5.16153900	3.89683600	0.07213300
H	6.35862400	2.69278700	0.53095000
H	5.50401100	2.50548000	-0.98641500
H	3.30573400	3.70912700	1.74063500
H	3.22977300	2.21961800	2.69110000
H	4.72792300	3.14605000	2.59515400
O	5.50796000	0.22531900	-1.15045700
O	-1.09833500	-0.65512200	-0.83771500
H	-0.20808700	-2.28045500	2.64759800

H	1.12092400	-3.02493700	1.76257400
H	1.42607200	-1.65337300	2.83204500
O	-0.14191900	0.09585900	1.58594900
H	-1.01131000	-0.12474600	1.95603400
H	-2.48832400	-1.08530400	-2.32680400
H	-2.91919900	-1.61156300	-0.67504300
H	-2.98774800	3.28711200	-1.87120000
H	-4.69903100	2.98369600	-2.14887900
H	-3.65343700	3.23444200	0.46607300
H	-5.04014800	2.20528900	0.09604900
N	-3.14673700	0.41766600	-1.11456400
O	-3.35440200	0.91326000	-3.35580400
O	-3.04987100	-0.16426600	2.20926500
O	-5.01117300	-0.04131400	1.12759700
H	-5.09461900	-1.85123400	2.16263800
H	-5.53446300	-0.41447100	3.11198100
H	-6.64042600	-1.00944700	1.83439500
H	-2.13783400	1.36740600	0.46479600

Methyl-(2R)-1-((((1R,2S,4aS)-1-hydroxy-1,4a-dimethyl-6-oxo-7-(propan-2-iliden)decahydronaphtalen-2-yl)oxy)methyl)-5-oxopirrolydine-2-carboxylate, 5b.

C	0.42469500	-2.43175100	-1.09643900
C	-0.35215600	-3.01409400	0.08748100
C	-0.65727100	-1.94530600	1.13762300
C	0.61094200	-1.22550600	1.65869900
C	1.46368600	-0.72649600	0.45203900
C	2.73833100	0.00940100	0.89331300
C	3.46936500	0.69068600	-0.25590100
C	3.50913300	-0.08075300	-1.53845800
C	2.29645100	-0.94014800	-1.86656000
C	1.74839600	-1.76006100	-0.67793400
C	4.05907400	1.90200000	-0.15364800
C	4.74465100	2.61900100	-1.28902300
C	4.09646500	2.69743000	1.12698400
C	2.79602600	-2.83848000	-0.33049300
C	1.34435000	-2.11083500	2.66664600
C	-2.47391700	1.93269100	0.10727500
C	-3.75548000	1.15337200	0.42558000
C	-4.94283900	1.68899700	-0.41524500
C	-4.96638800	0.78651000	-1.65619300
C	-4.27982600	-0.49485700	-1.20939800
C	-0.70590200	3.20168200	1.02911000
C	-2.90314500	-1.21959800	0.70154200
H	0.81813100	0.02446300	-0.02013400
H	-0.20975800	-1.69311300	-1.59312300
H	0.62545400	-3.21680300	-1.83158400
H	-1.28847600	-3.45479600	-0.26525700
H	0.20256900	-3.82844000	0.56195200
H	-1.16588300	-2.38752500	2.00331400
H	2.56535800	-1.58419000	-2.70595400
H	1.51269500	-0.25619000	-2.21618700
H	3.42283500	-0.69697600	1.37607000

H	2.45634200	0.72989000	1.65672000
H	3.02645200	-3.41854700	-1.22758400
H	3.73606300	-2.41107200	0.02279500
H	2.44975500	-3.54068800	0.42648900
H	4.54360800	3.69254700	-1.21992500
H	5.82985400	2.49273600	-1.21306500
H	4.45420500	2.25702800	-2.27045800
H	3.50636600	3.61507200	1.02441300
H	3.74466700	2.15881100	2.00276600
H	5.12486900	3.01889700	1.32199800
O	4.44791900	-0.03206400	-2.31414600
O	-1.51400200	-0.92832500	0.57981500
H	0.67076300	-2.33789000	3.49478700
H	1.69344900	-3.04676500	2.23641600
H	2.20420400	-1.58329100	3.07883500
O	0.19408300	-0.08532800	2.42734200
H	-0.54903500	0.31310000	1.95186300
H	-3.14522900	-2.18585300	0.25428800
H	-3.17567300	-1.21996500	1.76521000
H	-4.38657700	1.20718000	-2.47977600
H	-5.96700800	0.56415000	-2.02455800
H	-4.82990900	2.74518300	-0.65306600
H	-5.85922300	1.56701700	0.16437700
N	-3.66588900	-0.23704400	0.00318000
O	-4.27046700	-1.56414500	-1.77886800
O	-1.88083400	2.38508600	1.22811900
O	-2.06706300	2.14523200	-1.00543600
H	-0.35481300	3.44943100	2.02669700
H	0.05220900	2.64563200	0.48046700
H	-0.96840500	4.10141200	0.47376300
H	-3.94356700	1.21188900	1.49858900

(S)-1-(naphtalen-2-yl)-ethan-1-ol **6**

C	-1.36761700	0.22189400	-0.21366100
C	-0.45679000	-0.79678200	-0.08693800
C	0.93483700	-0.53485000	-0.01212800
C	1.39458000	0.81481000	-0.07127100
C	0.43450700	1.84817500	-0.21034500
C	-0.90207900	1.55969900	-0.28151300
H	1.54094500	-2.60032200	0.16198900
H	-0.80374600	-1.82152500	-0.05237900
C	1.88934200	-1.57429500	0.11898900
C	2.78542000	1.07193000	0.00382300
H	0.77450100	2.87647700	-0.26733200
H	-1.61809700	2.36651300	-0.39956000
C	3.68370400	0.04287100	0.13254400
C	3.23045100	-1.29353600	0.19045800
H	3.13134400	2.09890600	-0.04218500
H	4.74543900	0.25181200	0.18948100
H	3.94887100	-2.09855400	0.29108600
C	-2.85913900	-0.03325400	-0.26108400

H	-3.28111700	0.59401700	-1.05893200
C	-3.54357100	0.32846000	1.06049100
H	-3.37736300	1.37730100	1.31390900
H	-4.62442000	0.16991900	0.99041800
H	-3.14875900	-0.28976200	1.86908900
O	-3.07645400	-1.40768200	-0.58781700
H	-4.01784200	-1.59405500	-0.50923000

Methyl-(S)-1-(((S)-1-(naphtalen-2-yl)etoxy)methyl)-5-oxopyrrolidin-2-carboxylate, 6a.

C	-4.23030600	-1.80468300	-0.26021800
C	-3.20933800	-2.94370700	-0.34284900
H	-5.13888300	-1.99067800	-0.83161100
H	-4.50889900	-1.61684000	0.77623500
H	-3.29854800	-3.52428100	-1.26558600
H	-3.25790000	-3.64508900	0.48890900
N	-2.07262900	-0.91224700	-0.61245900
C	-1.85582900	-2.24793800	-0.36706500
O	-0.76675200	-2.76516400	-0.22448000
C	-1.00098400	0.01090900	-0.92598700
H	-0.08326700	-0.57638000	-0.97414300
H	-1.20269400	0.46558900	-1.89904800
O	-0.90535100	1.08969400	-0.02041200
C	-0.00265400	0.93560900	1.10731800
C	5.70116900	-1.40615200	0.05065300
C	4.41287400	-1.40261300	0.52093000
C	3.57467900	-0.27708800	0.33120800
C	4.09157900	0.85648500	-0.36258400
C	5.42551700	0.82245200	-0.83459700
C	6.21290300	-0.28237400	-0.63300300
H	1.86420900	-1.11825000	1.32816400
H	6.33217300	-2.27402800	0.20178100
H	4.01699500	-2.26611600	1.04397000
C	2.23865700	-0.24498300	0.80862900
C	3.24206000	1.97635900	-0.55244500
H	5.81660600	1.68640200	-1.36099700
H	7.23260900	-0.29722100	-0.99954000
C	1.95951200	1.97138000	-0.08002700
C	1.43393300	0.85050900	0.61768500
H	3.62819000	2.84289000	-1.07847800
H	1.31822200	2.83070400	-0.24001000
H	-0.11876900	1.90010800	1.60905700
C	-0.44346600	-0.15243500	2.07803100
H	0.15900800	-0.10035300	2.98791600
H	-1.48861300	0.00489700	2.34549800
H	-0.33907500	-1.15289600	1.65750200
C	-3.47952000	-0.56264200	-0.78912200
H	-3.68859500	-0.36719100	-1.84650400
C	-3.83140100	0.70132800	0.00231900
O	-4.02081900	0.73775300	1.19026800
O	-3.90869100	1.76539400	-0.81112400
C	-4.13374700	3.02591600	-0.15408900

H	-4.24244900	3.75613500	-0.95149700
H	-5.03405100	2.98047400	0.45702900
H	-3.27877700	3.26844700	0.47583500

Methyl-(R)-1-(((S)-1-(naphtalen-2-yl) ethoxy) methyl)-5-oxopyrrolidin-2-carboxylate, 6b.

C	2.29904400	-2.46379100	-0.42974500
C	1.76112300	-2.11941100	-1.82049900
C	2.87867900	-1.12480100	0.09750100
H	1.48402100	-2.79259000	0.21788800
H	3.05914000	-3.24245000	-0.42654300
H	0.83460700	-2.62919500	-2.08171700
H	2.48517900	-2.33133000	-2.61242200
H	3.94327700	-1.04444700	-0.15075900
N	2.10793400	-0.11652200	-0.63328800
C	1.54995900	-0.61323600	-1.79187600
C	2.81063100	-1.08611700	1.62873900
O	1.02088900	0.05676200	-2.65688300
O	3.79556600	-1.41461500	2.24919400
C	1.51932300	-0.69753000	2.29903300
H	0.64868900	-1.11132700	1.78752400
H	1.54488100	-1.01810200	3.33878400
H	1.41555400	0.38823200	2.24584000
C	2.39192100	1.30731600	-0.51263600
H	3.42734600	1.41173700	-0.18063700
H	2.28355300	1.73365200	-1.50859500
O	1.63366300	2.00931100	0.44424300
C	0.36251100	2.62193200	0.07667300
C	-4.09859400	-1.59554600	-1.11200200
C	-3.05502000	-0.75555800	-1.40284300
C	-2.46355100	0.04358500	-0.39206300
C	-2.97281900	-0.04142800	0.93838700
C	-4.05375300	-0.91722700	1.20502200
C	-4.60363000	-1.67656800	0.20479400
H	-1.00656200	0.95778500	-1.68044500
H	-4.54254900	-2.20135600	-1.89317600
H	-2.66405700	-0.69078000	-2.41223000
C	-1.38490100	0.92060900	-0.66719700
C	-2.37410900	0.76169700	1.93998500
H	-4.44092800	-0.97800100	2.21637800
H	-5.43011400	-2.34338800	0.42071700
C	-1.32867700	1.59260400	1.63851900
C	-0.80858600	1.68161300	0.32126500
H	-2.76023700	0.71334700	2.95242700
H	-0.88497900	2.20245400	2.41838000
H	0.28972600	3.41388800	0.82583500
C	0.37716100	3.28740200	-1.29420900
H	1.23068000	3.96416200	-1.37350100
H	0.42021100	2.57161900	-2.11444200
H	-0.53419100	3.87681100	-1.40980800

(S)-(-)-2-Bromide- α-methyl benzyl alcohol **7**

C	2.11258500	-0.58793600	0.03965800
C	2.17044100	-1.96906000	-0.08817400
C	0.99657500	-2.70968100	-0.16149700
C	-0.23049100	-2.06150300	-0.10436500
C	-0.26819900	-0.67892200	0.02274600
C	0.89211100	0.09171500	0.09481300
H	3.02162300	-0.00681500	0.11430400
H	3.13228900	-2.46600300	-0.12526800
H	1.02826100	-3.78816300	-0.25788600
H	-1.15317100	-2.62357200	-0.15390400
Br	-2.01572100	0.13902200	0.10356700
C	0.72576100	2.26807200	-1.17270800
H	0.69428500	3.35678800	-1.06587400
H	1.57161600	2.00309300	-1.81001600
H	-0.19668000	1.95526000	-1.66379400
C	0.87101900	1.60362700	0.19915400
H	0.02299800	1.89194900	0.82806200
O	2.08665900	2.01236600	0.83689800
H	2.11692300	2.97490200	0.83659100

Methyl-(S)-1-(((S)-1-(2-bromophenyl) ethoxy) methyl)-5-oxopyrrolidine-2-carboxylate, 7a.

C	-1.28333000	1.78124300	0.69241900
C	-2.02305700	2.89435400	0.31733700
C	-3.24837000	2.73136800	-0.31943500
C	-3.72767800	1.45311700	-0.57303700
C	-2.97532500	0.35004300	-0.18773100
C	-1.74048500	0.48213700	0.44632000
H	-0.32504800	1.90593200	1.17960100
H	-1.64243100	3.88729700	0.52426900
H	-3.83413400	3.59186800	-0.61925100
H	-4.67890000	1.30991300	-1.06739200
Br	-3.72339100	-1.38815200	-0.56309400
C	-1.29353200	-1.09649700	2.34823000
H	-0.75832100	-1.99280000	2.66834100
H	-1.06094300	-0.28076200	3.03595800
H	-2.36178100	-1.30922300	2.41129700
C	-0.92126200	-0.70377900	0.91338100
H	-1.10960800	-1.55247200	0.24809400
O	0.45845600	-0.33903200	0.78774600
C	1.37727800	-1.39082700	1.04255800
H	1.53437400	-1.49245300	2.12286200
H	1.02361400	-2.33766900	0.62511000
C	3.44184400	0.05298000	0.76412700
C	4.43637400	-1.20368900	-1.07592200
C	4.79942200	-0.26242400	0.08020500
H	3.53624900	0.13829900	1.84751600
H	4.28946400	-0.66914200	-2.01636100
H	5.16678200	-1.99276000	-1.25011400
H	5.31509300	0.64182400	-0.24001100

H	5.43875100	-0.77272100	0.80214400
N	2.62763300	-1.09787800	0.40852400
O	2.60440300	1.38190600	-1.02397400
O	2.70747600	2.34539100	1.01117600
C	2.05073000	2.59350200	-1.57148000
H	1.97122900	2.41825000	-2.64097300
H	1.06705300	2.77959400	-1.14287400
H	2.70667300	3.43821600	-1.36394700
O	2.54492200	-2.76207400	-1.18214800
C	2.86063900	1.38973300	0.29220500
C	3.10093600	-1.81297500	-0.67218400

Methyl-(R)-1-(((S)-1-(2-bromophenyl)ethoxy)methyl)-5-oxopyrrolidine-2-carboxylate, 7b.

C	-2.93793700	2.25923000	-0.25430700
C	-4.03170300	2.28854700	-1.11059300
C	-4.63773000	1.10002500	-1.49544900
C	-4.14297500	-0.11028300	-1.02492400
C	-3.04552100	-0.12038200	-0.17460500
C	-2.41738400	1.05989100	0.23709100
H	-2.47748600	3.19334000	0.03844900
H	-4.40783300	3.23748100	-1.47265800
H	-5.49422400	1.10676000	-2.15865400
H	-4.60621500	-1.04320000	-1.31614200
Br	-2.41570100	-1.83877400	0.41566700
C	-0.96626800	2.32757400	1.93503000
H	-0.15319800	2.19101400	2.64977300
H	-0.69560600	3.15290000	1.27465200
H	-1.85687300	2.60655500	2.50165600
C	-1.20867700	1.03808300	1.15396700
H	-1.35006300	0.22154600	1.87097300
O	-0.08260300	0.70254900	0.32063000
C	1.03747200	0.18227600	1.01944200
H	1.55206300	0.98354400	1.56490300
H	0.74199400	-0.60610200	1.71708800
C	3.12246700	-2.02938600	-1.14273000
C	3.09629000	-0.73572100	-1.96511900
H	2.79377800	-2.90603500	-1.69865400
H	4.11092500	-2.24348400	-0.73125400
H	2.38588200	-0.81248100	-2.78811700
H	4.06466800	-0.47134300	-2.38819300
N	1.92803500	-0.41410900	0.06730800
O	1.72842200	-2.58878100	0.79431300
C	2.17683700	-1.77402100	0.02125800
C	2.56872500	0.35248600	-0.98148600
H	1.85886800	1.02474500	-1.46293300
C	3.69155500	1.22854300	-0.46285200
O	3.88138900	2.37609000	-0.67138200
O	4.63182200	0.42300600	0.35066900
C	5.64913100	0.97425100	0.95705400
H	5.58867100	2.07101200	0.75511800

Methyl (S)-Lactate **6**

C	0.28507000	-0.30195100	-0.03960100
O	1.21812700	0.61873200	-0.30351100
O	0.51679900	-1.39309500	0.42758700
C	2.57692500	0.24742400	0.00714800
H	2.86563700	-0.63433300	-0.56341300
H	3.18194900	1.10450000	-0.27519600
H	2.67634200	0.03825200	1.07146000
C	-1.11836900	0.16577100	-0.39911400
H	-1.10247000	0.43196800	-1.46359300
C	-1.54027100	1.39053900	0.41404800
H	-1.51498000	1.16662100	1.48239500
H	-0.88832800	2.24083800	0.20975000
H	-2.56315200	1.65571000	0.14497900
O	-2.02889800	-0.89709700	-0.20584900
H	-1.52335000	-1.64256600	0.15291900

Methyl-(S)-1-((((S)-1-methoxy-1-oxopropan-2-yl)oxy)methyl)-5-oxopyrrolydin-2-carboxylate, 8a.

C	-2.22892000	1.78415700	-0.73760700
C	-1.15686800	2.80430000	-0.33549400
H	-3.22630600	2.21300600	-0.82850700
H	-1.96666900	1.32199600	-1.68677300
H	-1.56174400	3.62801400	0.26010900
H	-0.62190700	3.24025700	-1.17756800
N	-0.83371600	0.86192700	0.92775000
C	-0.20038300	2.01870900	0.54864700
O	0.91700800	2.34345600	0.89869200
C	-0.26055700	-0.04952200	1.88789300
H	0.40963100	0.53192800	2.52573100
H	-1.06813400	-0.48701400	2.47328800
O	0.42868800	-1.14939900	1.32162900
C	-2.18102300	0.71114800	0.37202500
H	-2.92613400	0.90006600	1.15223100
C	-2.42532100	-0.73491500	-0.06609100
O	-2.91453600	-1.55757900	0.66767200
O	-2.01827000	-0.98043200	-1.31310900
C	-2.05836300	-2.36041200	-1.71641100
H	-3.08114500	-2.73491600	-1.68713800
H	-1.66573800	-2.37764900	-2.72906500
H	-1.43410000	-2.95457800	-1.05091500
C	1.97364100	-0.33909600	-0.39374800
O	3.22019400	0.15323400	-0.51850400
O	1.15331300	-0.33378900	-1.27284600
C	3.51807600	0.76591900	-1.78385800
H	2.90316100	1.65532400	-1.91872400
H	4.57020800	1.03483600	-1.73903300
H	3.33088000	0.06953900	-2.60059700
C	1.79352500	-0.93859400	1.00322400

H	2.24365800	-0.23693200	1.71285500
C	2.49931600	-2.29002600	1.08784300
H	2.04366200	-2.99422600	0.38949000
H	3.55741000	-2.18593900	0.84683700
H	2.39936700	-2.69114100	2.09671600

Methyl-(R)-1-((((S)-1-methoxy-1-oxopropan-2-yl) oxy)methyl)-5-oxopyrrolydin-2-carboxylate, 8b.

C	-2.06420500	1.22466900	1.50582100
C	-1.03589000	2.36060700	1.55053500
H	-1.71399600	0.38104400	2.09644300
H	-3.05152400	1.51287500	1.86593700
H	-0.44300200	2.38793700	2.46322200
H	-1.49188900	3.34714000	1.42238600
N	-0.78277700	1.21302600	-0.47209800
C	-0.13732200	2.09957400	0.35096000
O	0.94805800	2.59985800	0.12721500
C	-0.23370800	0.78683800	-1.73402300
H	-1.04772800	0.66990500	-2.44741600
H	0.45191700	1.56505700	-2.06502100
O	0.39234800	-0.48764800	-1.70584500
C	1.87957900	-0.76482000	0.21928700
O	3.16939200	-0.98555800	0.54842100
O	0.98332000	-0.75302900	1.02002900
C	3.42131900	-1.17715800	1.95082800
H	3.13906900	-0.28580800	2.51031900
H	2.85494300	-2.02897400	2.32643900
H	4.48964100	-1.35890400	2.03399100
C	1.75021900	-0.60049800	-1.30019900
H	2.05871400	-1.56580300	-1.71495700
C	2.69235400	0.47266200	-1.85139900
H	2.51816000	1.44079100	-1.38254300
H	3.72210400	0.17675900	-1.65615000
H	2.55591900	0.55843800	-2.93116700
C	-2.10464100	0.81175100	0.02171900
H	-2.87834900	1.36275000	-0.52580000
C	-2.39626100	-0.65895700	-0.28490400
O	-2.83813800	-1.01616900	-1.34866100
O	-2.12145300	-1.48364900	0.72934200
C	-2.27627400	-2.88374000	0.43933600
H	-1.61354300	-3.16618200	-0.37751800
H	-2.00376900	-3.40176400	1.35469200
H	-3.30645600	-3.10245100	0.16005400

Isoborneol/Borneol

C	0.04221500	1.64269500	-1.13920600
C	0.45574300	1.41143900	0.32974000
C	-0.19546900	-0.66354100	-0.34371400

C	-0.42468900	0.22847300	-1.59322500
H	-0.75190300	2.38752700	-1.21702500
H	0.87854100	2.00443400	-1.73980400
H	-1.46952100	0.20945900	-1.89757700
H	0.16386600	-0.14037600	-2.43516100
C	1.09124900	-0.01185500	0.28820500
C	-0.84243300	1.17414500	1.13011200
H	-0.68033500	1.23291400	2.20821200
H	-1.61671800	1.90013900	0.87417700
C	-1.27296800	-0.25756000	0.69277600
H	1.09499700	2.19526100	0.74144700
C	1.48862800	-0.55870100	1.67022000
H	1.81445100	-1.59948400	1.59351600
H	2.33170700	0.01309600	2.06833200
H	0.69300800	-0.51903500	2.41268100
C	-0.16883100	-2.15399300	-0.64018900
H	-1.12729000	-2.47767600	-1.05277300
H	0.60704700	-2.40213500	-1.36898400
H	0.01671400	-2.74233700	0.26307100
C	2.34266500	-0.11051200	-0.59755600
H	3.14560400	0.50405500	-0.18021000
H	2.70963400	-1.13980300	-0.63129500
H	2.18183200	0.21353500	-1.62414400
H	-1.24110400	-0.95044800	1.53919100
O	-2.57684900	-0.33241200	0.10729900
H	-3.23239900	-0.23336700	0.80497500

Mixture of methyl **5-oxo-1-((((1S,2R,4S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl)oxy)methyl)pyrrolidine-2-carboxylate** and **methyl 5-oxo-1-((((1S,2S,4S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-yl)oxy)methyl)pyrrolidine-2-carboxylate.**

C	2.38416400	-0.54658000	0.71491000
C	1.36925200	-1.01809300	-0.36452700
C	2.01295100	-0.54082800	-1.70177800
C	3.36262200	0.05395600	-1.25039900
C	4.24133600	-1.12736600	-0.78446500
C	3.57313900	-1.53750600	0.56169400
C	2.99460900	0.76203400	0.08664200
C	2.00758200	1.92805700	-0.07422000
C	4.21174500	1.31912100	0.84408800
C	1.81784800	-0.47321000	2.12223400
C	-2.42527000	1.56816600	-0.55359300
C	-3.07654300	0.20034600	-0.76513100
C	-4.39041200	0.02056600	0.04306000
C	-4.37281700	-1.43897000	0.51023000
C	-2.92703300	-1.88782500	0.36979300
C	-1.64529400	3.13272400	1.02594000
C	-0.93935200	-1.17395500	-0.87219200
H	4.24229100	-1.93791400	-1.51600800
H	5.28069300	-0.82803000	-0.64248100
H	3.22927600	-2.57400000	0.56403900

H	4.26313600	-1.43507500	1.40052900
H	1.37689600	0.21217500	-2.16891200
H	2.14317600	-1.35297200	-2.42027400
H	1.28537000	-2.11062700	-0.32723500
H	3.83356300	0.69075400	-2.00180900
H	1.76295600	2.35025200	0.90443100
H	2.46619100	2.72675600	-0.66501200
H	1.07271500	1.64528500	-0.54990300
H	4.65389900	2.14540400	0.28009300
H	3.90866900	1.71954900	1.81503200
H	4.99855300	0.58823000	1.02260300
H	1.45026300	-1.45129200	2.44482400
H	2.58506500	-0.15733500	2.83399100
H	0.97961900	0.22153500	2.18240500
O	0.05817300	-0.49351300	-0.13063600
H	-0.92150800	-0.85164300	-1.92136900
H	-0.77434500	-2.25418400	-0.81441100
H	-3.25501000	0.13666800	-1.84292300
H	-4.38109700	0.69132600	0.90003300
H	-5.25605500	0.26754500	-0.56979500
H	-4.71176100	-1.57739700	1.53609700
H	-4.97820100	-2.09321700	-0.12285000
N	-2.24258000	-0.91430900	-0.32860000
O	-2.45341200	-2.93805800	0.74793600
O	-2.14069600	2.31093200	-1.46082500
O	-2.24431300	1.85434200	0.74140600
H	-1.55719100	3.17613000	2.10819300
H	-0.66603800	3.20207500	0.55640200
H	-2.28223700	3.93671900	0.65775200