SUPORTING INFORMATION SECTION

The Total Synthesis of Calcium Atorvastatin

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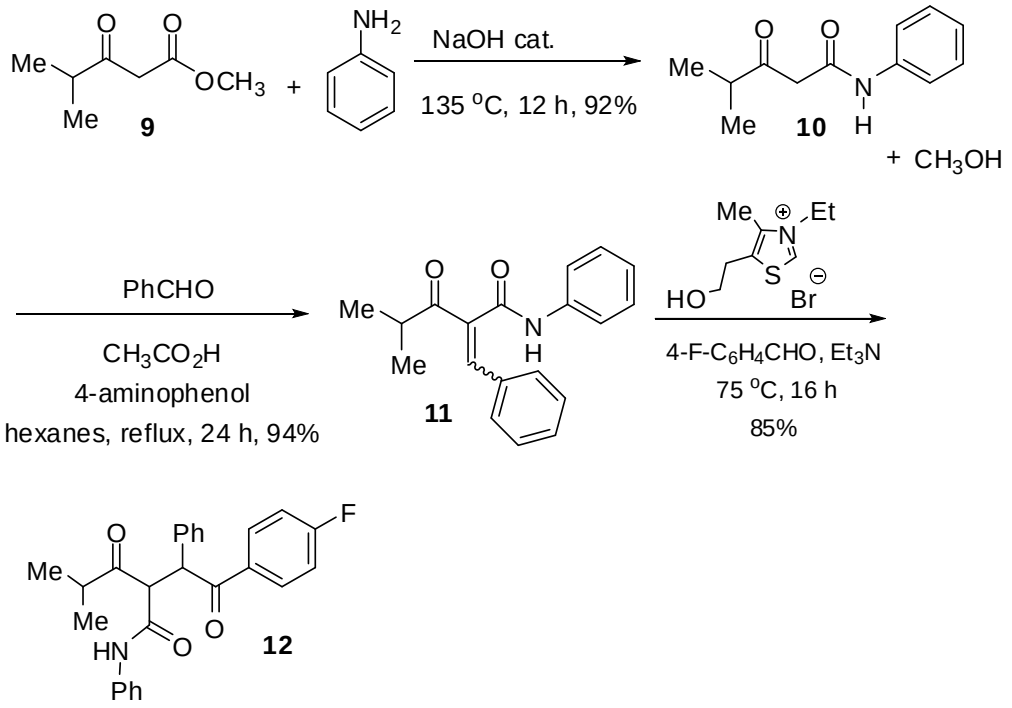
1. General Experimental

The air-sensitive and/or water-sensitive reactions were performed under nitrogen atmosphere with dry solvents under anhydrous conditions. Standard syringe techniques were applied for the transfer of dry solvents and air-sensitive reagents. The reactions were monitored by TLC performed on Merck silica gel (60 F_{254}) using UV light as the visualizing agent and 5% vanillin in 10% H_2SO_4 and heat as developing agents. Merck silica gel (particle size 0.040-0.063 mm) was used for flash chromatography. Dry THF and Et_2O were distilled from sodium/benzophenone under nitrogen prior to use. Some reagents and solvents were commercially available and were used without further purification. All of the yields were calculated as gross yields. ^1H (250 and 500 MHz) and ^{13}C (62.5 and 125 MHz) NMR spectra were recorded on Bruker DPX250 and INOVA 500 MHz spectrometers in $CDCl_3$, acetone-d_6, C_6D_6, MeOD or DMSO-d_6 using tetramethylsilane (TMS) as internal standards.

2. Preparation of aldehyde 3

4-Methyl-3-oxo-*N*-phenylpentanamide (**10**) was prepared from the inexpensive and commercially available 4-methyl-3-oxo-methylpentanoate (**9**) and aniline (Scheme 1).[1,4,13] Many reaction conditions were evaluated, and improvements were made to the original Pfizer route.[1] Among the several reaction conditions tested, the best result was obtained using NaOH (2 mol%) as the catalyst in the absence of solvent followed by the removal of methanol at 135 °C (92% yield). *N*-phenylpentanamide (**10**) was obtained as a viscous yellow oil in a pure form.



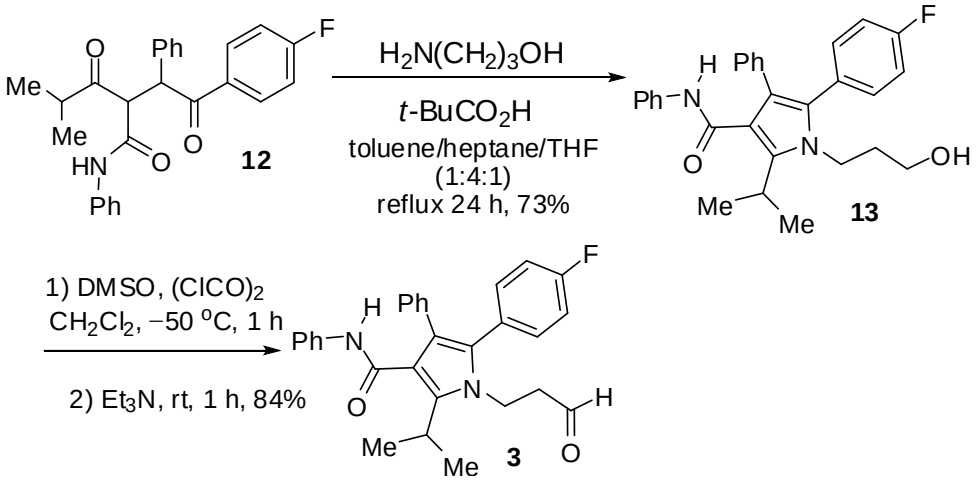
Scheme 1. Preparation of 1,4-diketone (**12**).

In the next step, to obtain 2-benzylidene-4-methyl-3-oxo-*N*-phenylpentanamide (**11**), 4-methyl-3-oxo-*N*-phenylpentanamide (**10**) was subjected to a reaction with benzaldehyde in the presence of acid catalysts in hexanes as the solvent (Scheme 1).[13] Among the several reaction conditions evaluated, we obtained the best results using 4-aminophenol (20 mol%) and acetic acid (20 mol%) as catalysts in refluxing hexanes for 24 h. Under these conditions, *Z*+*E*-2-benzylidene-4-methyl-3-oxo-*N*-phenylpentanamide (**11**) was obtained in 94% isolated yield. 2-Benzylidene-4-methyl-3-oxo-*N*-phenylpentanamide (**11**) is a white solid and was purified by washing with hot hexanes (60 °C) to remove the remaining benzaldehyde, followed by washing with distilled water to remove catalyst residues.

The synthesis of 2-[2-(4-fluorophenyl)-2-oxo-1-phenylethyl]-4-methyl-3-oxo-*N*-phenylpentanamide (**12**) was performed via the Stetter reaction, according to the work of Sagyan and coworkers (Scheme 1).[14c] *N*-phenylpentanamide (**11**) was subjected to a reaction with 4-fluorobenzaldehyde in the presence of triethylamine as the base and 3-ethyl-5-(2-hydroxyethyl)-4-methyl-3-thiazolium bromide as the catalyst (20 mol%) in anhydrous ethanol, according to the reported procedure.[4b,13] Using this protocol, 1,4-diketone (**12**) was obtained in only 39% yield after recrystallization. Considering this result, we decided to test the reaction in the absence of

solvent at 75 °C for 16 h. To our delight, these conditions afforded 2-[2-(4-fluorophenyl)-2-oxo-1-phenylethyl]-4-methyl-3-oxo-*N*-phenylpentanamide (**12**) in 85% isolated yield (Scheme 1).

Then, pyrrolic aldehyde (**3**) was prepared by a Pall-Knorr reaction.[1b,15] This process is composed of the reaction between 2-[2-(4-fluorophenyl)-2-oxo-1-phenylethyl]-4-methyl-3-oxo-*N*-phenylpentanamide (**12**) (previously prepared) with 3-aminopropan-1-ol and the subsequent oxidation of the resulting pyrrolic alcohol (**13**) (Scheme 2). For this purpose, 1,4-diketone (**12**) was treated with 1.5 equiv of 3-aminopropan-1-ol under pivalic acid catalysis in a mixture of toluene-heptane-tetrahydrofuran (1:4:1) under reflux with azeotropic removal of water for 24 h. Thus, 5-(4-fluorophenyl)-1-(3-hydroxypropyl)-2-isopropyl-*N*,4-diphenyl-1*H*-pyrrole-3-carboxamide (**13**) was obtained as a pale yellow solid in 73% isolated yield after purification by passing through a plug of silica gel. In the next step, pyrrolic alcohol (**13**) was subjected to oxidation under Swern conditions[16] to give the corresponding pyrrolic aldehyde (**3**) in 84% yield, which was used in the next step without further purification.[1b]

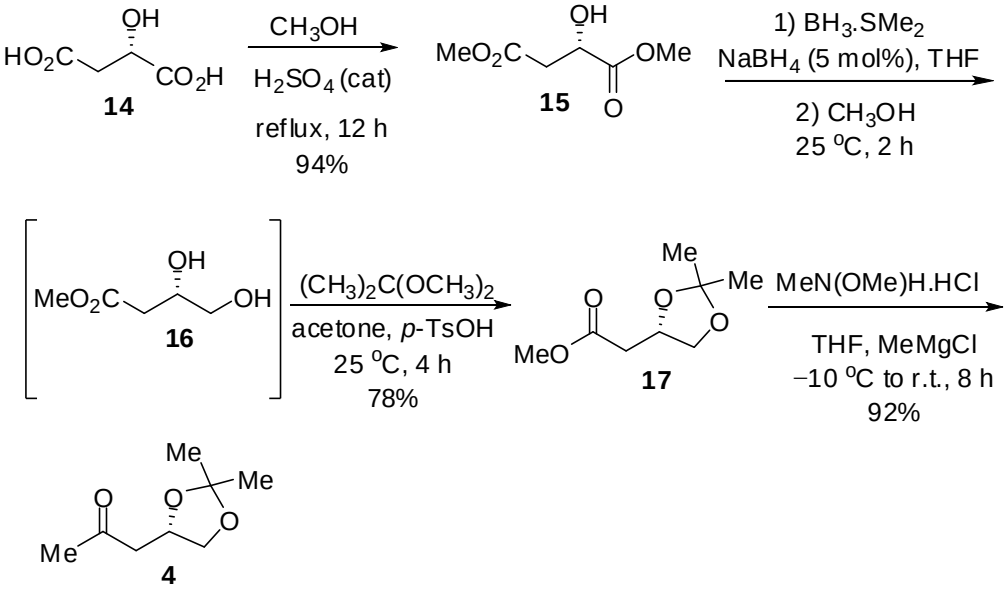


Scheme 2. Preparation of pyrrolic aldehyde (**3**)

3. Preparation of methylketone 4

The preparation of (*S*)-1-(2,2-dimethyl-1,3-dioxolan-4-yl)propan-2-one (**4**) was easily performed in four steps from inexpensive *L*-(*S*)-malic acid (**14**), according to the procedure described in the literature[17] (Scheme 3). In the first step, *L*-(S)-malic acid (**14**) was converted to its corresponding methyl ester (**15**) by a Fischer esterification reaction with methanol in the presence of catalytic amounts of sulfuric acid. Importantly, the product (*S*)-dimethylmalate (**15**) does not require

purification and can be used directly in the next step. In the next step, (*S*)-dimethyl malate (**15**) was converted to acetonide methyl ester (**17**) via Moriwake's regioselective reduction reaction[18] employing $BH_3.SMe_2$ and $NaBH_4$ (78% isolated yield). In this reaction, the intermediate 1,2-diol ester (**16**) was not isolated and was submitted directly to the ketalization reaction with 2,2-dimethoxy propane in the presence of catalytic amounts of *p*-TsOH (Scheme 3).



Scheme 3. Synthesis of methyl ketone (**4**) from *L*-(*S*)-malic acid (**14**)

The acetonide methyl ester (**17**) was easily purified by distillation under reduced pressure. Then, acetonide methyl ester (**17**) was submitted to a reaction with CH_3MgCl in THF in the presence of *N*-methyl-*N*-methoxy amine hydrochloride to produce the corresponding methyl ketone (**4**) via Weinreb's amide (Scheme 3).[19] The product (*S*)-1-(2,2-dimethyl-1,3-dioxolan-4-yl)propan-2-one (**4**) can be easily purified by vacuum distillation and was obtained in 62% overall yield from the 4-step sequence.

4. Experimental

4-methyl-3-oxo-*N*-phenylpentanamide (**10**). To a mixture of 4-methyl-3-oxo methyl pentanoate (**9**) (100.0 g, 700 mmol) and NaOH (0.5 g) was added aniline (68.4 g, 730.5 mmol) at 135 °C, with simultaneous removal of methanol over 2 h. The reaction mixture was maintained for another 12 h at 135 °C and was monitored by thin layer chromatography. The reaction was cooled to room temperature and was slowly added to a 0 °C 5% aqueous HCl solution (until pH = 6) followed by water (300 mL). The reaction mixture was extracted with ethyl acetate (3 x 300 mL), and the organic phase was washed with water (3 x 300 mL). The organic phase was dried with anhydrous magnesium sulfate and then concentrated under *vacuum* to provide 4-methyl-3-oxo-*N*-phenylpentanamide (**10**) as a viscous yellow oil in 92% yield (130.5 g) in pure form (bp 262-263 °C). ^{1}H NMR (250 MHz, DMSO-d_6) δ 1.03 (d, J = 7.0 Hz, 6H), 2.77-2.83 (m, 1H), 3.61 (s, 2H); 7.04 (t, J = 8.1 Hz, 1H), 7.30 (t, J = 8.1 Hz, 2H), 7.58 (d, J = 8.1 Hz, 2H); 10.07 (s, 1H). ^{13}C NMR (62.5 MHz, DMSO-d_6) δ 17.5, 40.3, 49.4, 118.9, 123.3, 128.6, 138.8, 165.1, 208.2. IR (KBr, cm^{-1}): 3298, 3044, 1729, 1658.

2-benzylidene-4-methyl-3-oxo-*N*-phenylpentanamide (**11**)**.** A mixture of 4-methyl-3-oxo-*N*-phenylpentanamide (**10**) (100.0 g, 480 mmol), 4-aminophenol (10.4 g, 96.0 mmol), benzaldehyde (53.0 g, 504.0 mmol) and acetic acid (5.7 g, 96.0 mmol) in hexanes (1 L) was refluxed for 24 h with azeotropic removal of water. The remaining solid was filtered, washed with hexanes (1 L) followed by distilled water (1.5 L) and dried under high *vacuum* (12 h) to give 2-benzylidene-4-methyl-3-oxo-*N*-phenylpentanamide (**11**) in 94% yield (131.0 g) as a white solid, mp 191-192 °C. ^{1}H NMR (250 MHz, DMSO-d_6) δ 1.12 (d, J = 7.1 Hz, 6H), 3.30-3.47 (m, 1H), 7.08 (t, J = 8.0 Hz, 1H), 7.30-7.41 (m, 5H), 7.66-7.70 (m, 5H), 9.61 (s, 1H). ^{13}C NMR (62.5 MHz, DMSO-d_6) δ 18.3, 36.0, 121.1, 124.2, 128.3, 129.5, 130.3, 132.7, 135.1, 136.0, 137.3, 140.2, 165.3, 202.8. IR (KBr, cm^{-1}): 3312, 3049, 1728, 1663.

2-[2-(4-fluorophenyl)-2-oxo-1-phenylethyl]-4-methyl-3-oxo-*N*-phenylpentanamide (**12**) **(diketone of Atorvastatin)**. A mixture of 2-benzylidene-4-methyl-3-oxo-*N*-phenylpentanamide (**11**) (130.0 g, 443.1 mmol), 3-ethyl-5-(2-hydroxyethyl)-4-methyl-3-thiazolium bromide (22.3 g, 88.6 mmol), triethylamine (135.8 mL, 974.8 mmol) and 4-fluorobenzaldehyde (60.5 g, 487.4 mmol) was heated at 75 °C under argon atmosphere with vigorous stirring for 16 h. The reaction

was monitored by thin layer chromatography (TLC) until consumption of *N*-phenylpentanamide (**11**) was achieved. Isopropyl alcohol (650 mL) was added, and the reaction mixture was maintained at 25 °C for 4 h under stirring. The remaining solid was *vacuum* filtered and washed with 700 mL of water followed by 500 mL of isopropyl alcohol. The product 2-[2-(4-fluorophenyl)-2-oxo-1-phenylethyl]-4-methyl-3-oxo-*N*-phenylpentanamide (**12**) was dried under high *vacuum* for 4 h, affording a white crystalline solid (mp 205-209 °C, Lit.[4b] 206-209 °C) in 85% yield (167.2 g). ^{1}H NMR (250 MHz, DMSO-d_6) δ 0.92 (d, J = 6.5 Hz, 3H), 1.15 (d, J = 7.5 Hz, 3H), 2.83-2.94 (m, 1H), 4.87 (d, J = 11.0 Hz, 1H), 5.42 (d, J = 11.0 Hz, 1H), 6.97-7.40 (m, 12H), 8.13 (d, J = 8.2 Hz, 2H), 10.18 (s, 1H). ^{13}C NMR (62.5 MHz, DMSO-d_6) δ 18.1, 18.6, 40.9, 54.1, 64.1, 115.6 (d, $J_{C\text{-}F}$ = 22.0 Hz), 120.6, 124.7, 128.0, 128.6, 129.4, 131.5, 131.6 (d, $J_{C\text{-}F}$ = 9.4 Hz) , 132.2 (d, $J_{C\text{-}F}$ = 2.5 Hz), 135.2, 136.7, 165.5, 165.6 (d, $J_{C\text{-}F}$ = 255.3 Hz), 196.4, 209.6. IR (KBr, cm^{-1}): 3296, 1720, 1684, 1598.

5-(4-fluorophenyl)-1-(3-hydroxypropyl)-2-isopropyl-*N*,4-diphenyl-1*H*-pyrrole-3-carboxamide (13). To a solution of 2-[2-(4-fluorophenyl)-2-oxo-1-phenylethyl]-4-methyl-3-oxo-*N*-phenylpentanamide (**12**) (140.0 g, 335.3 mmol) and 3-aminopropan-1-ol (37.8 g, 502.9 mmol) in toluene-heptane-tetrahydrofuran (1:4:1) (1 L) was added pivalic acid (6.8 g, 67.0 mmol) under nitrogen atmosphere. The reaction mixture was refluxed for 24 h with azeotropic removal of water, monitored by thin layer chromatography (TLC), cooled to room temperature and extracted with ethyl acetate (3 x 700 mL). The organic phase was washed with brine (500 mL). The solvent was removed under *vacuum*, and pyrrolic alcohol (**13**) was obtained as a pale yellow solid in 73% yield (113.8 g, 251.4 mmol) after purification by passing through a plug of silica. Alternatively, pyrrolic alcohol (**13**) can be purified by recrystallization from hexane-isopropyl alcohol. Mp 175-178 ºC. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.53 (d, J = 7.0 Hz, 6H), 1.71-1.82 (m, 2H), 3.46-3.61 (m, 3H), 3.99 (t, J = 7.7 Hz, 2H), 6.87 (s, 1H), 6.95-7.21 (m, 14H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 21.7 (2C), 26.1, 34.3, 41.7, 59.8, 115.4 (d, $J_{C\text{-}F}$ = 21.3 Hz), 119.6, 121.8, 123.5, 126.5, 128.2 (d, $J_{C\text{-}F}$ = 2.5 Hz), 128.3, 128.6, 128.8, 130.4, 133.1 (d, $J_{C\text{-}F}$ = 8.8 Hz), 133.2, 134.6, 138.3, 141.4, 162.2 (d, $J_{C\text{-}F}$ = 247.6 Hz), 164.8. IR (KBr, cm^{-1}): 3335, 3367, 1669.

5-(4-fluorophenyl)-2-isopropyl-1-(3-oxopropyl)-*N*,4-diphenyl-1H-pyrrole-3-carboxamide (3). To a solution of oxalyl chloride (33.3 g, 262.8 mmol) in CH_2Cl_2 (800 mL) under an atmosphere of dry argon at −50 °C was added DMSO (34.2 g, 438 mmol) over 30 min. After 20 min at −50 °C, pyrrolic alcohol (**13**) (100.0 g, 219.0 mmol) dissolved in CH_2Cl_2 (200 mL) was slowly added over 30 min. The reaction mixture was maintained at −50 °C for 1 h, and Et_3N was added (88.4 g, 876 mmol, 4.0 eq.). The reaction was continued for 1 h at room temperature and was extracted with ethyl acetate (3 x 500 mL). Pyrrolic aldehyde (**3**) was purified by passing through a plug of silica and eluted with hexane/acetate (9:1 mixture) to obtain a pale yellow solid in 84% yield (84.2 g, 186.1 mmol). Mp 160-163 °C. Lit.[1b] mp 164-165 °C. ^{1}H NMR (500 MHz, $CDCl_3$) δ 1.51 (d, J = 7.0 Hz, 6H), 2.67 (t, J = 7.5 Hz, 2H), 3.61 (quint, J = 7.0 Hz, 1H), 4.25 (t, J = 7.5 Hz, 2H), 6.85 (s, 1H), 6.95-7.21 (m, 14H), 9.58 (s 1H). ^{13}C NMR (125 MHz, $CDCl_3$) δ 21.6 (2C), 25.9, 37.6, 45.2, 115.7 (d, $J_{C\text{-}F}$ = 21.4 Hz), 119.5, 122.1, 123.5, 126.7, 127.6, 127.7 (d, $J_{C\text{-}F}$ = 3.8 Hz), 128.5, 128.6, 130.5, 133.0 (d, $J_{C\text{-}F}$ = 8.7 Hz), 133.4, 134.7, 138.5, 141.5, 162.3 (d, $J_{C\text{-}F}$ = 248.8 Hz), 164.4, 198.5. IR (KBr, cm^{-1}): 3402, 2965, 1722, 1674, 1596, 1510.

(*S*)-dimethylmalate (15). To a mixture of *L*-(*S*)-malic acid (**14**) (100.0 g, 745.7 mmol) in anhydrous methanol (600 mL) was added sulfuric acid (3.65 g, 2 mL), and the resulting mixture was refluxed for 12 h. Methanol was distilled off to obtain a final volume of approximately 100 mL. To the mixture was added a saturated aqueous $NaHCO_3$ solution until reaching pH = 8.0 (100 mL). The reaction was extracted with ethyl acetate (3 x 500 mL), and the organic phase was collected and dried with anhydrous Na_2SO_4. The solvent was removed in a rotary evaporator (40 °C/100 mmHg), and the remaining solvent was removed under high *vacuum* (1 mmHg) for 5 h. (*S*)-Dimethyl malate (**15**) was obtained in 94% yield (113.9 g) as a pale yellow oil and was used in the next step without purification. ^{1}H NMR (250 MHz, $CDCl_3$) δ 2.67 (dd, J = 15.1 Hz, 7.4 Hz, 1H), 2.71 (s, 1H), 2.78 (dd, J = 15.1 Hz, 7.4 Hz, 1H), 3.69 (s, 3H), 3.70 (s, 3H), 4.50 (t, J = 7.3 Hz, 1H). ^{13}C NMR (62.5 MHz, $CDCl_3$) δ 38.2, 51.6, 51.8, 68.9, 172.1, 172.3. IR (thin film, cm^{-1}): 3368, 2964, 1740.

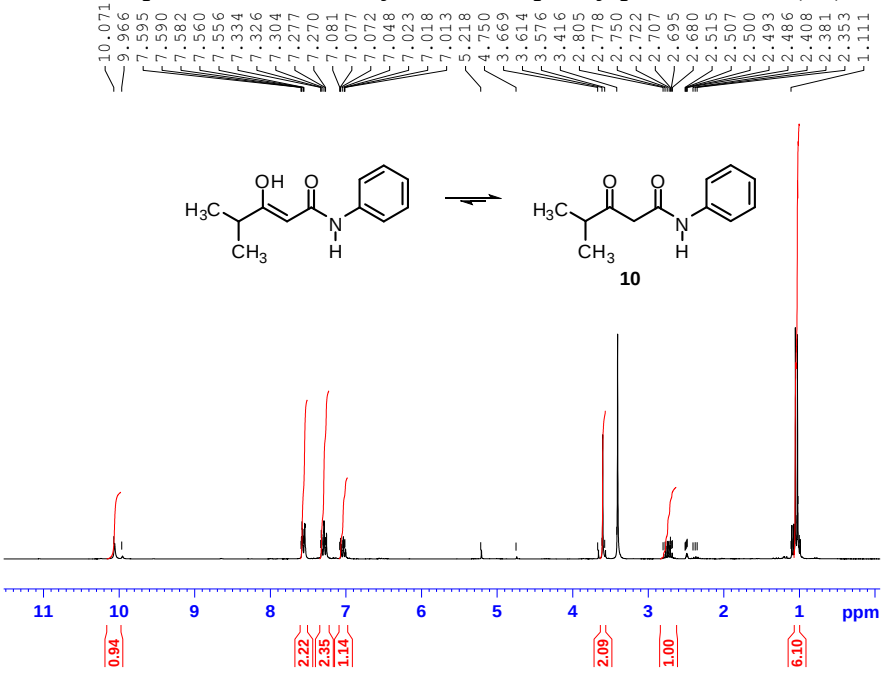
(*S*)-methyl 2-(2,2-dimethyl-1,3-dioxolan-4-yl)acetate (17). To a solution of (*S*)-dimethyl malate (**15**) (110.0 g, 678.7 mmol) in anhydrous THF (1.0 L) at 20 °C under argon atmosphere was added $BH_3.SMe_2$ (10 M) (60.5 mL, 605.0 mmol) over 40 min. The solution was stirred for

30 min at 20 °C until the hydrogen evolution ceased. The reaction temperature was reduced to 10 °C, and the solution was maintained for 10 min at this temperature. Then, $NaBH_4$ was added in portions (0.23 g in 5 portions) (1.15 g, 28.6 mmol) over 50 min. The reaction mixture was maintained under intense agitation for 1 h at 20 °C. The reaction was monitored by thin layer chromatography until total consumption of (*S*)-dimethyl malate (**15**) was achieved. Next, anhydrous methanol (500 mL) was slowly added to the reaction at 0 °C, and the mixture was stirred for 30 min at 20 °C. The solvent was removed completely on a rotary evaporator and then under high *vacuum* for 4 h. The viscous oil residue containing **16** was dissolved in a mixture of acetone (600 mL) and 2,2-dimethoxypropane (200 mL). To this mixture was added *p*-TsOH (4.95 g), and the reaction was stirred for 4 h at 20 °C. The mixture was extracted with ethyl acetate (3 x 500 mL), and the residue was subjected to distillation under reduced pressure (bp 74-75 °C/6 mbar). The product (**17**) was obtained as a colorless liquid in 78% yield (92.2 g, 529.3 mmol). ^{1}H NMR (250 MHz, $CDCl_3$) δ 1.35 (s, 3H), 1.41 (s, 3H), 2.52 (dd, J = 15.0 Hz, 7.5 Hz, 1H); 2.72 (dd, J = 15.0 Hz, 7.5 Hz, 1H), 3.65 (dd, J = 10.0 Hz, 7.5 Hz, 1H), 3.70 (s, 3H); 4.15 (dd, J = 8.7 Hz, 7.5 Hz, 1H), 4.47 (quint, J = 7.5 Hz, 1H). ^{13}C NMR (62.5 MHz, $CDCl_3$) δ 25.4, 26.8, 38.7, 51.7, 69.1, 72.0, 109.2, 171.0. IR (thin film, cm^{-1}): 2966, 1738, 1230.

(*S*)-1-(2,2-dimethyl-1,3-dioxolan-4-yl)propan-2-one (4). To a slurry of (*S*)-methyl 2-(2,2-dimethyl-1,3-dioxolan-4-yl)acetate (**17**) (90.0 g, 516.7 mmol) and $CH_3(OCH_3)NH.HCl$ (57.6 g, 593.8 mmol) in anhydrous THF (1.0 L) at −10 °C was slowly added a solution of CH_3MgCl (3.0 M in THF) (689.0 mL, 2.06 mol) over 1 h. After 1 h at –5 °C, the reaction mixture was warmed to 25 °C over 1 h, aged for 8 h then quenched into 1 M HCl (pH = 7.0). The layers were separated, and the THF solution was concentrated to 100 mL. The crude mixture was extracted with ethyl acetate (3 x 400 mL) and washed with brine (300 mL), and the residue was subjected to distillation under reduced pressure (bp 68-69 °C/7 mmHg). The product (*S*)-1-(2,2-dimethyl-1,3-dioxolan-4-yl)propan-2-one (**4**) was obtained as a light yellow liquid in 92% yield (75.2 g, 475.3 mmol). ^{1}H NMR (250 MHz, $CDCl_3$) δ 1.34 (s, 3H), 1.40 (s, 3H), 2.19 (s, 3H), 2.60 (dd, J = 17.5 Hz, 7.0 Hz, 1H), 2.89 (dd, J = 17.5 Hz, 6.0 Hz, 1H), 3.53 (dd, J = 7.5 Hz, 6.7 Hz, 1H); 4 17 (dd, J = 7.5 Hz, 6.7 Hz, 1H), 4.45 (quint, J = 6.7 Hz, 1H). ^{13}C NMR (62.5 MHz, $CDCl_3$) δ 25.3, 26.8, 30.5, 47.7, 69.3, 71.6, 108.7, 206.2. IR (thin film, cm^{-1}): 2960, 1732, 1235.

5. Appendix – Copies of ^{1}H and ^{13}C NMR data

^{1}H NMR spectrum of 4-methyl-3-oxo-*N*-phenylpentanamide (**10**) in DMSO-d_6 at 250 MHz

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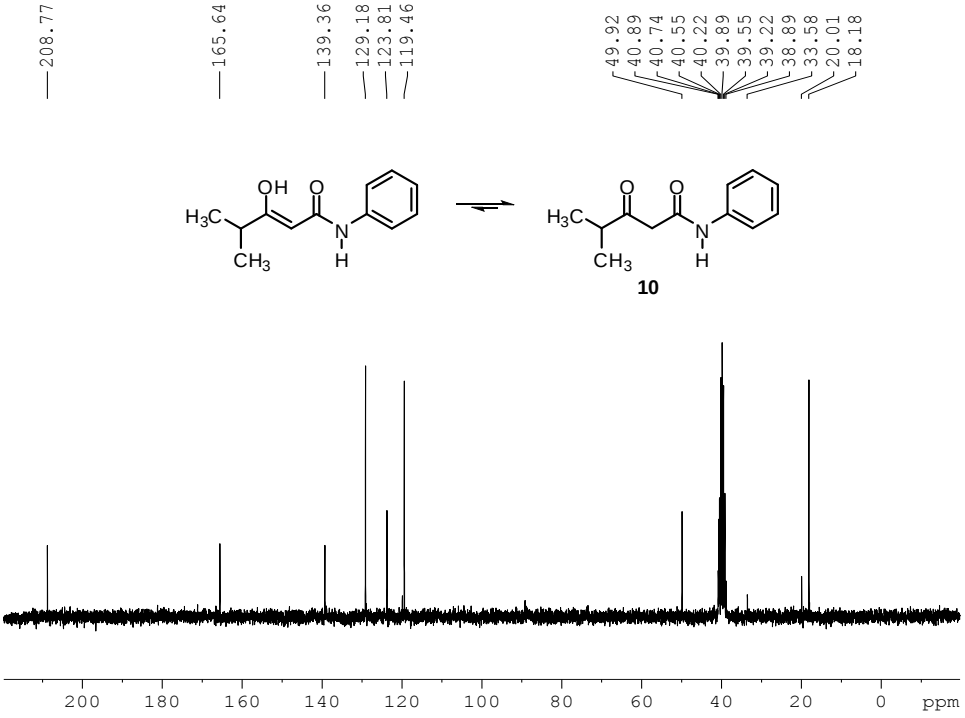
^{13}C NMR spectrum of 4-methyl-3-oxo-*N*-phenylpentanamide (**10**) in DMSO-d_6 at 62.5 MHz

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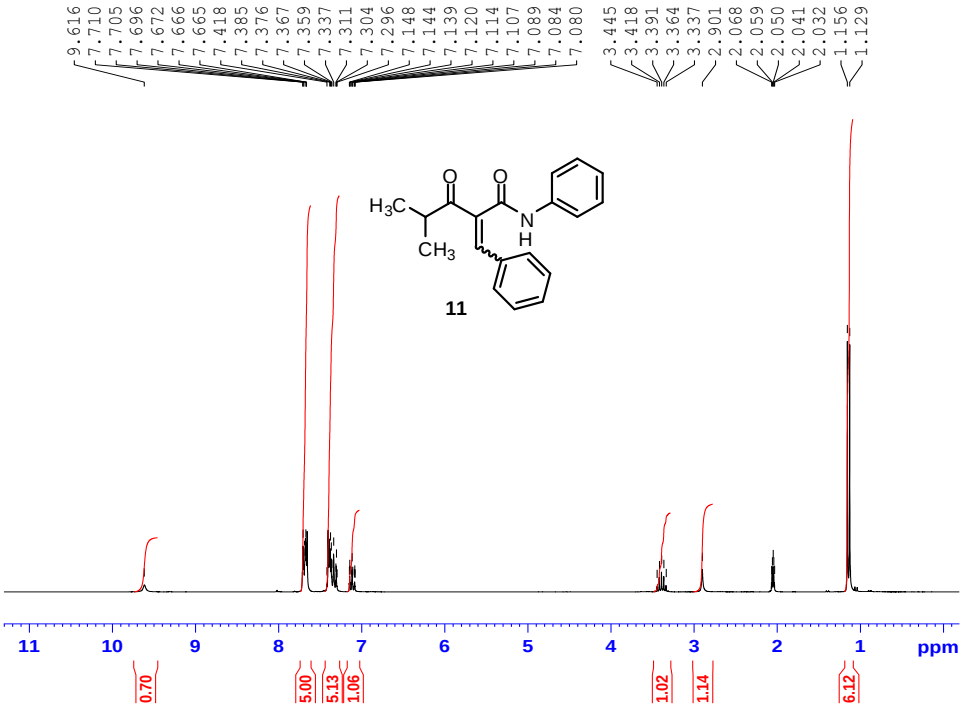
[1]H NMR spectrum of (*Z*)-2-benzylidene-4-methyl-3-oxo-*N*-phenylpentanamide (**11**) in acetone-d_6 at 250 MHz

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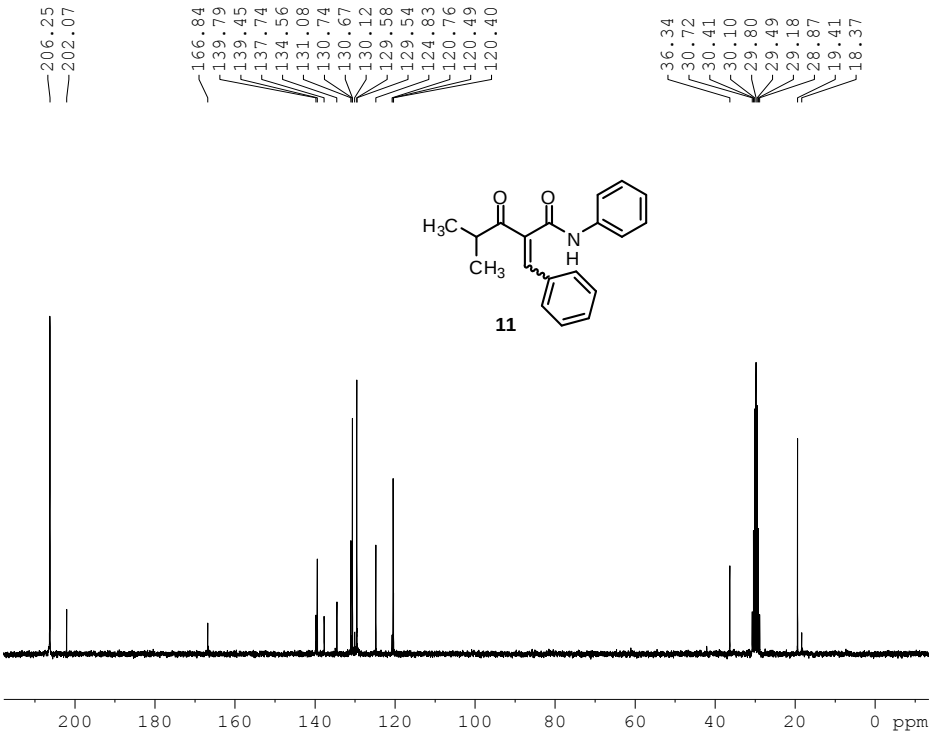
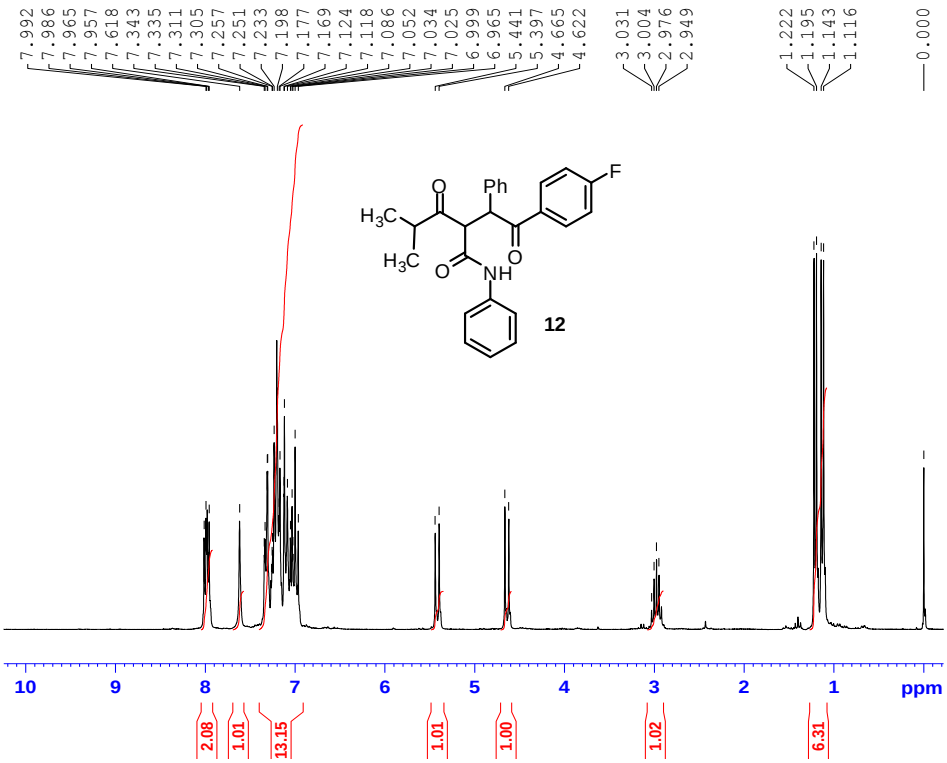
[13]C NMR spectrum of (*Z*)-2-benzylidene-4-methyl-3-oxo-*N*-phenylpentanamide (**11**) in acetone-d_6 at 62.5 MHz



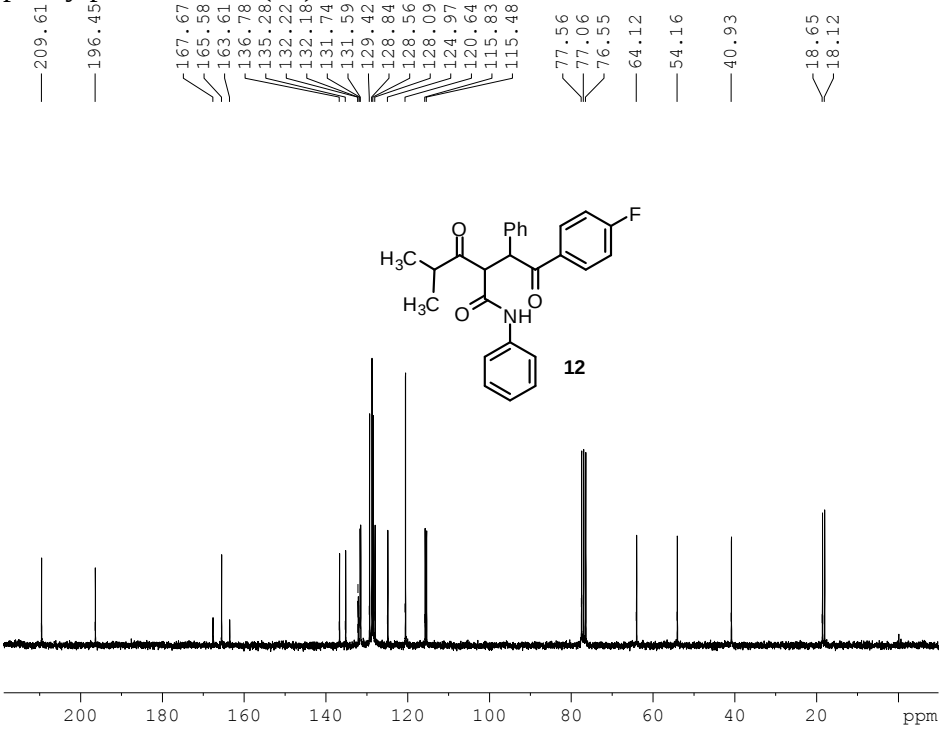

```
Current Data Parameters
NAME            nov12asvC
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20091112
Time               18.48
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                 16384
SOLVENT          Acetone
NS                   226
DS                     0
SWH            15060.241 Hz
FIDRES          0.919204 Hz
AQ              0.5439488 sec
RG                 456.1
DW                33.200 usec
DE                 6.00 usec
TE                300.0 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                    1
SFO1          62.9015280 MHz
NUC1                  13C
P1                10.00 usec
PLW1          -1.00000000 W
SFO2         250.1310005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              100.00 usec
PLW2          -1.00000000 W
PLW12         -1.00000000 W
PLW13         -1.00000000 W

F2 - Processing parameters
SI                 32768
SF            62.8951897 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

^{1}H NMR spectrum of 2-[2-(4-fluorophenyl)-2-oxo-1-phenylethyl]-4-methyl-3-oxo-*N*-phenylpentanamide (**12**) in $CDCl_3$ at 250 MHz



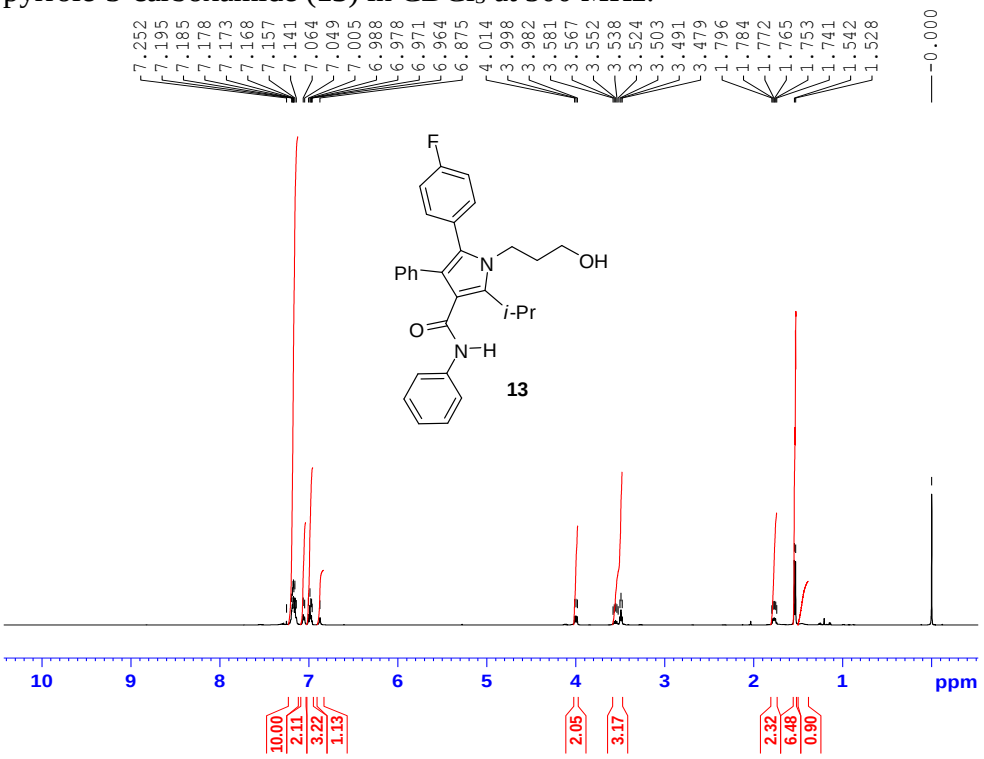

```
Current Data Parameters
NAME          jul08asvH1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20100708
Time_              18.34
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    0
SWH            5175.983 Hz
FIDRES         0.157958 Hz
AQ            3.1653888 sec
RG                  256
DW               96.600 usec
DE                6.00 usec
TE               298.3 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 13.00 usec
PL1                -6.00 dB
SFO1         250.1315447 MHz

F2 - Processing parameters
SI                 32768
SF           250.1300024 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{13}C NMR spectrum of 2-[2-(4-fluorophenyl)-2-oxo-1-phenylethyl]-4-methyl-3-oxo-*N*-phenylpentanamide (**12**) in $CDCl_3$ at 62.5 MHz



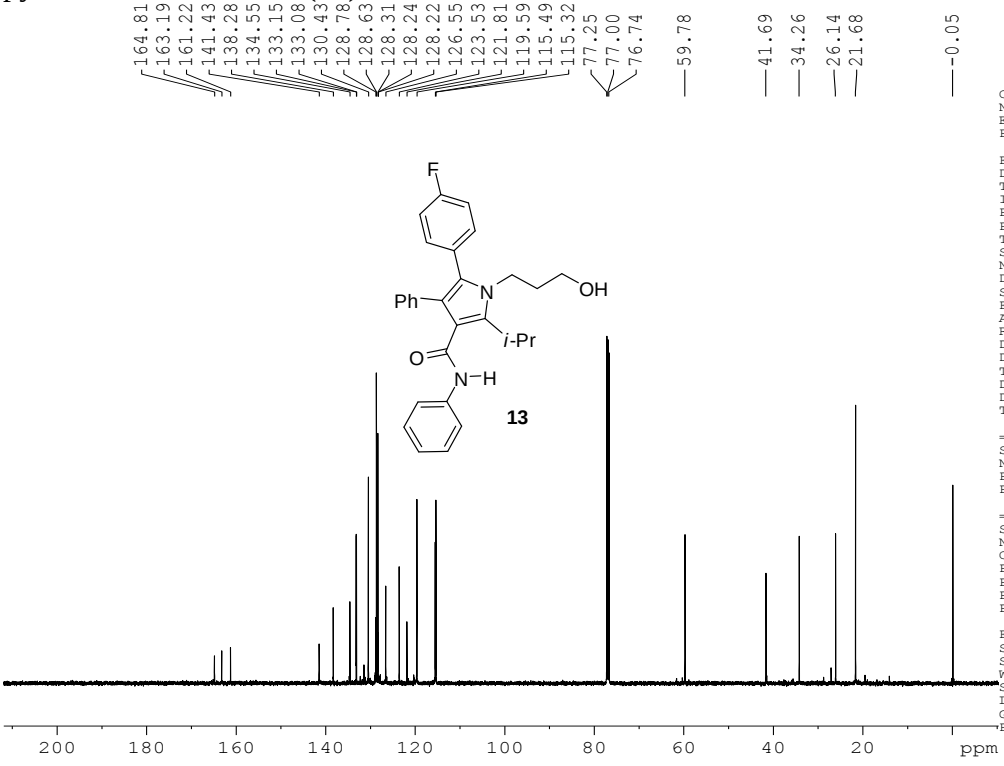

```
Current Data Parameters
NAME          jul12asvC1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20100712
Time_              8.59
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG          zgpg30
TD                16384
SOLVENT           CDCl3
NS                  782
DS                    0
SWH           15060.241 Hz
FIDRES         0.919204 Hz
AQ            0.5439488 sec
RG                456.1
DW               33.200 usec
DE                6.00 usec
TE               298.3 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    1
SFO1         62.9015280 MHz
NUC1                  13C
P1                10.00 usec
PLW1         -1.00000000 W
SFO2         250.1310005 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             100.00 usec
PLW2         -1.00000000 W
PLW12        -1.00000000 W
PLW13        -1.00000000 W

F2 - Processing parameters
SI                 32768
SF           62.8952425 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

[1]H NMR spectrum of [5-(4-fluorophenyl)-1-(3-hydroxypropyl]-2-isopropyl-*N*,4-diphenyl-1*H*-pyrrole-3-carboxamide (**13**) in $CDCl_3$ at 500 MHz.



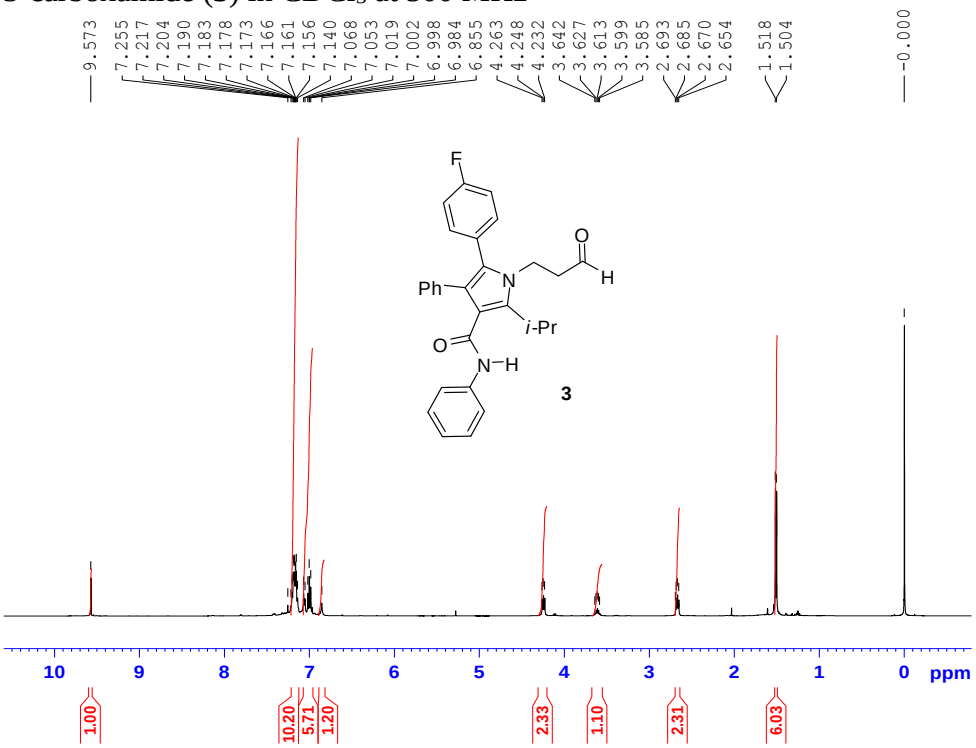

```
Current Data Parameters
NAME          jun241cdH2
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140624
Time_              15.11
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            1.6384000 sec
RG                   57
DW               50.000 usec
DE                6.50 usec
TE               298.2 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         499.8730869 MHz
NUC1                 1H
P1                11.75 usec
PLW1         25.00000000 W

F2 - Processing parameters
SI                 65536
SF           499.8700208 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

[13]C NMR spectrum of [5-(4-fluorophenyl) -1-(3-hydroxypropyl]-2-isopropyl-*N*,4-diphenyl-1H-pyrrole-3-carboxamide (**13**) in $CDCl_3$ at 125 MHz



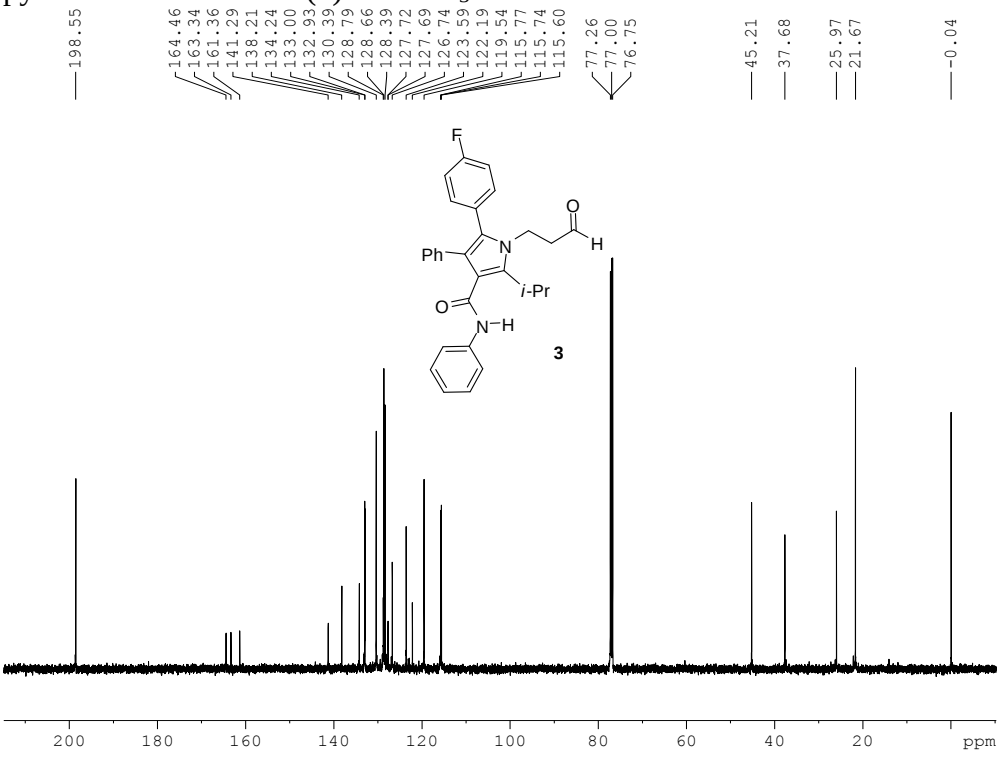

```
Current Data Parameters
NAME          jun241cdH2
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140624
Time_              15.37
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT           CDCl3
NS                  640
DS                    4
SWH           29761.904 Hz
FIDRES        0.908261 Hz
AQ            0.5505024 sec
RG                 2050
DW               16.800 usec
DE                6.50 usec
TE               298.2 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         125.7049801 MHz
NUC1                 13C
P1                10.00 usec
PLW1         91.00000000 W

======== CHANNEL f2 ========
SFO2         499.8719995 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2             80.00 usec
PLW2         26.85300064 W
PLW12         0.57928002 W
PLW13         0.37074000 W

F2 - Processing parameters
SI                 32768
SF           125.6924211 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

^{1}H NMR spectrum of 5-(4-fluorophenyl)-2-isopropyl-1-(3-oxopropyl)-*N*,4-diphenyl-1H-pyrrole-3-carboxamide (**3**) in $CDCl_3$ at 500 MHz



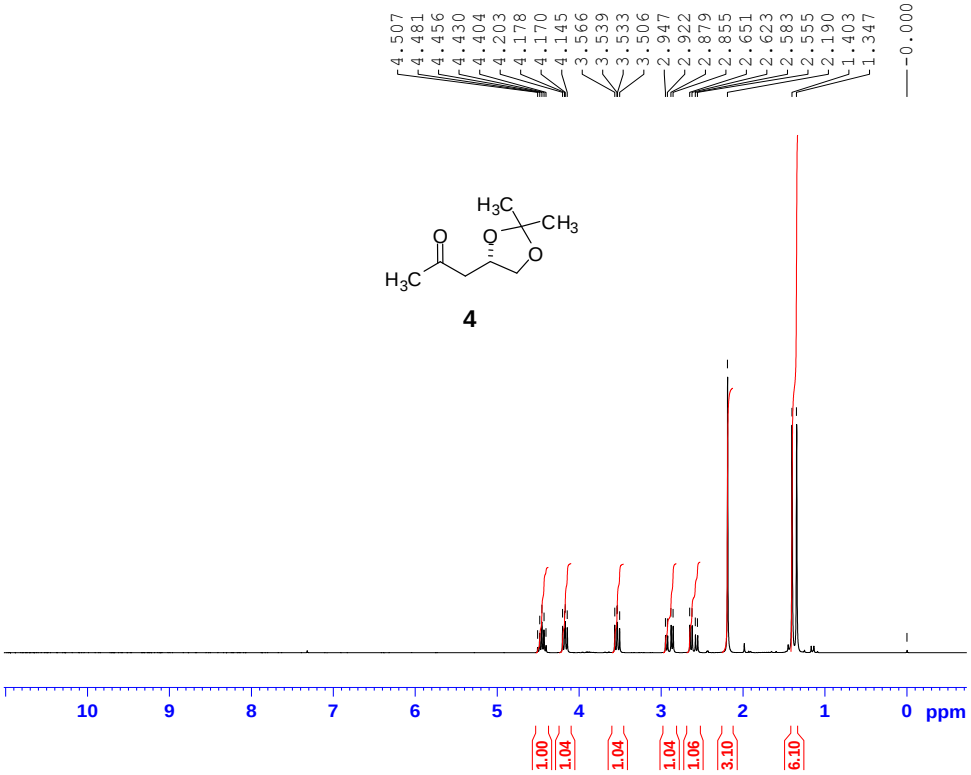

```
Current Data Parameters
NAME          jun241cdH1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140624
Time              13.37
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                  16
DS                   2
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            1.6384000 sec
RG                  57
DW               50.000 usec
DE                6.50 usec
TE               298.2 K
D1            1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1         499.8730869 MHz
NUC1               1H
P1               11.75 usec
PLW1         25.00000000 W

F2 - Processing parameters
SI                65536
SF           499.8700196 MHz
WDW                EM
SSB       0
LB               0.30 Hz
GB        0
PC               1.00
```

^{13}C NMR spectrum of 5-(4-fluorophenyl)-2-isopropyl-1-(3-oxopropyl)-*N*,4-diphenyl-1H-pyrrole-3-carboxamide (**3**) in $CDCl_3$ at 125 MHz.



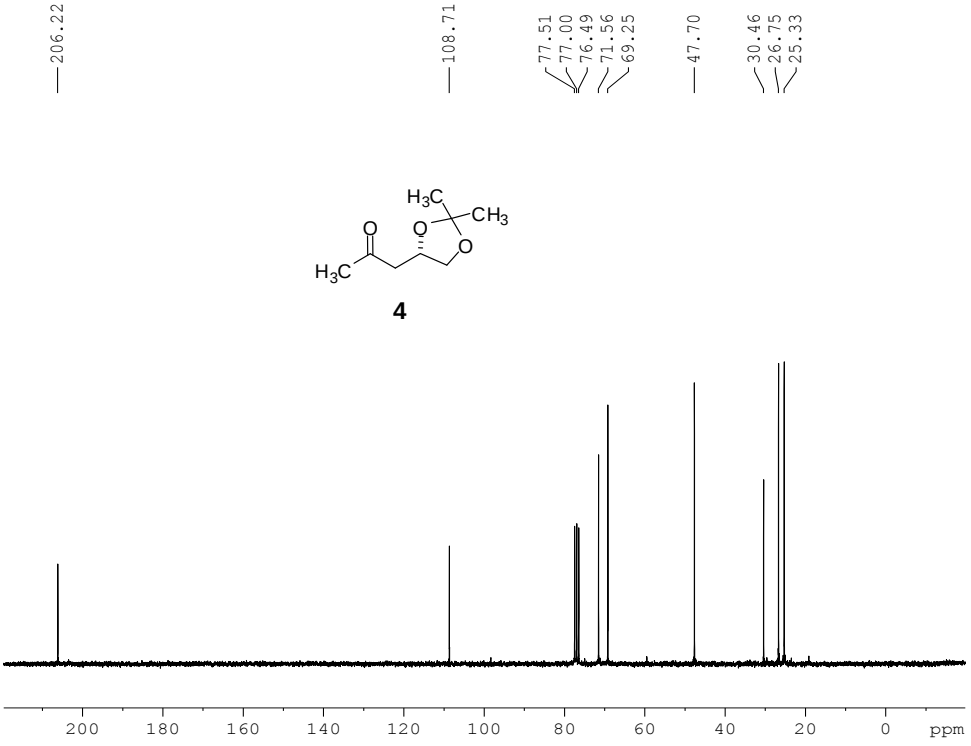

```
Current Data Parameters
NAME          jun241cdH1
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20140624
Time              13.45
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD               32768
SOLVENT          CDCl3
NS                 256
DS                   4
SWH           29761.904 Hz
FIDRES        0.908261 Hz
AQ            0.5505024 sec
RG                2050
DW               16.800 usec
DE                6.50 usec
TE               298.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1         125.7049801 MHz
NUC1               13C
P1               10.00 usec
PLW1         91.00000000 W

======== CHANNEL f2 ========
SFO2         499.8719995 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2            80.00 usec
PLW2         26.85300064 W
PLW12         0.57928002 W
PLW13         0.37074000 W

F2 - Processing parameters
SI                32768
SF           125.6924203 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```

^{1}H NMR spectrum of (*S*)-1-(2,2-dimethyl-1,3-dioxolan-4-yl)propan-2-one (**4**) in $CDCl_3$ at 250 MHz



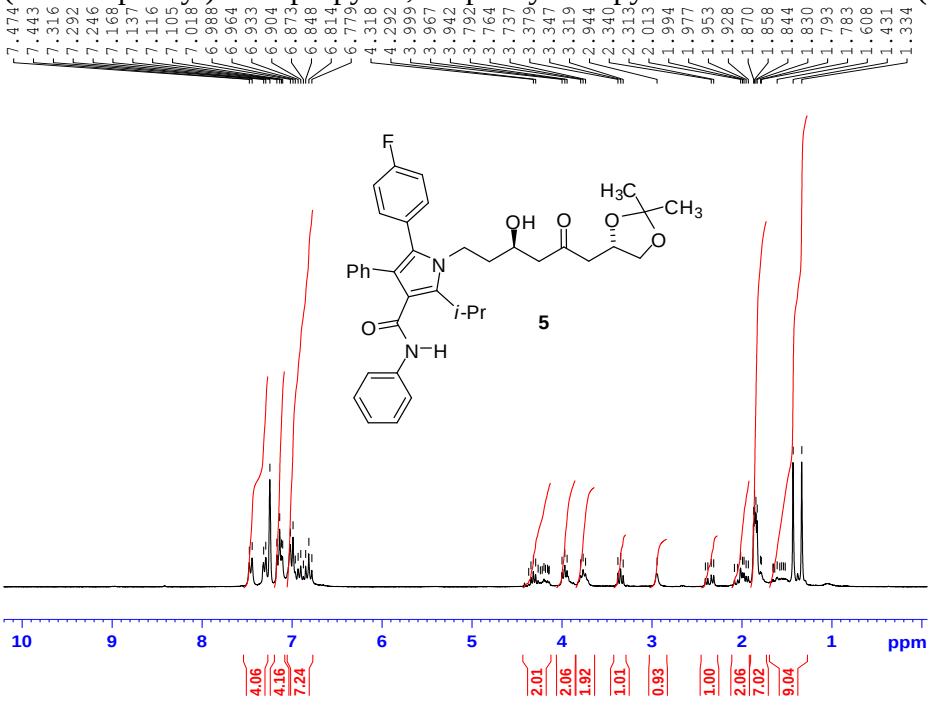

```
Current Data Parameters
NAME          set22asvH1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20100922
Time               12.40
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG             zg30
TD                 32768
SOLVENT            CDCl3
NS                    16
DS                     0
SWH             5175.983 Hz
FIDRES          0.157958 Hz
AQ             3.1653888 sec
RG                 161.3
DW                96.600 usec
DE                 6.00 usec
TE                298.2 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 13.00 usec
PL1                -6.00 dB
SFO1         250.1315447 MHz

F2 - Processing parameters
SI                 32768
SF           250.1299849 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

^{13}C NMR spectrum of (*S*)-1-(2,2-dimethyl-1,3-dioxolan-4-yl)propan-2-one (**4**) in $CDCl_3$ at 62.5 MHz



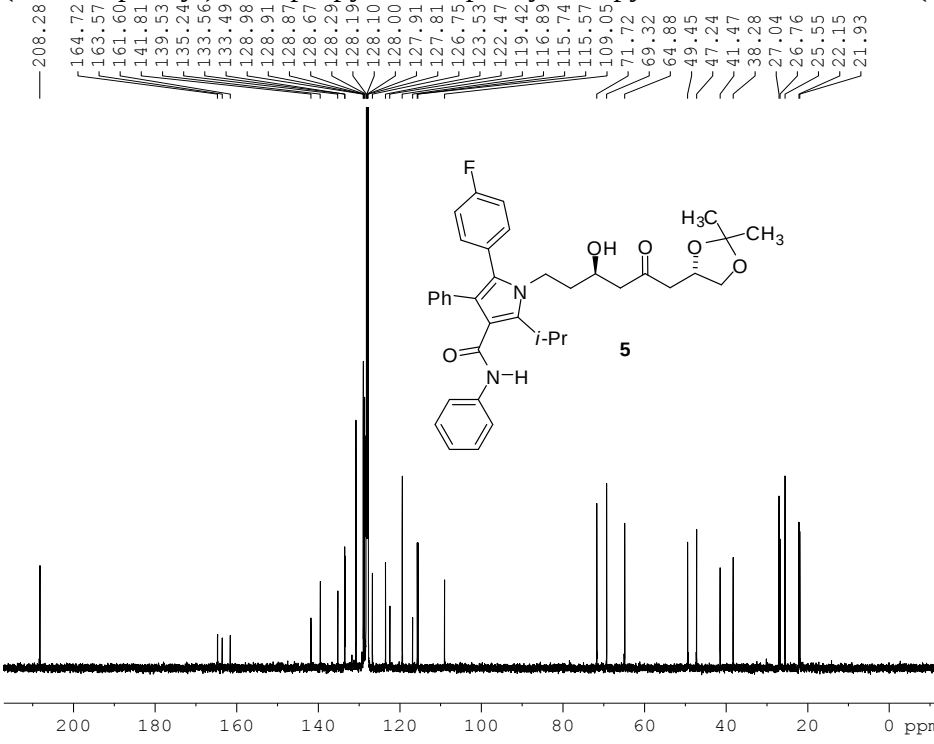

```
Current Data Parameters
NAME          set22asvC1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20100922
Time               13.03
INSTRUM            spect
PROBHD   5 mm QNP 1H/13
PULPROG           zgpg30
TD                 16384
SOLVENT            CDCl3
NS                   474
DS                     0
SWH            15060.241 Hz
FIDRES          0.919204 Hz
AQ             0.5439488 sec
RG                 645.1
DW                33.200 usec
DE                 6.00 usec
TE                298.2 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    1
SFO1          62.9015280 MHz
NUC1                  13C
P1                10.00 usec
PLW1         -1.00000000 W
SFO2         250.1310005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             100.00 usec
PLW2         -1.00000000 W
PLW12        -1.00000000 W
PLW13        -1.00000000 W

F2 - Processing parameters
SI                 32768
SF            62.8952422 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

^{1}H NMR spectrum of 1-[(*R*)-6-((*S*)-2,2-dimethyl-1,3-dioxolan-4-yl)-3-hydroxy-5-oxohexyl]-5-(4-fluorophenyl)-2-isopropyl-*N*,4-diphenyl-1*H*-pyrrole-3-carboxamide (**5**) in C_6D_6 at 250 MHz



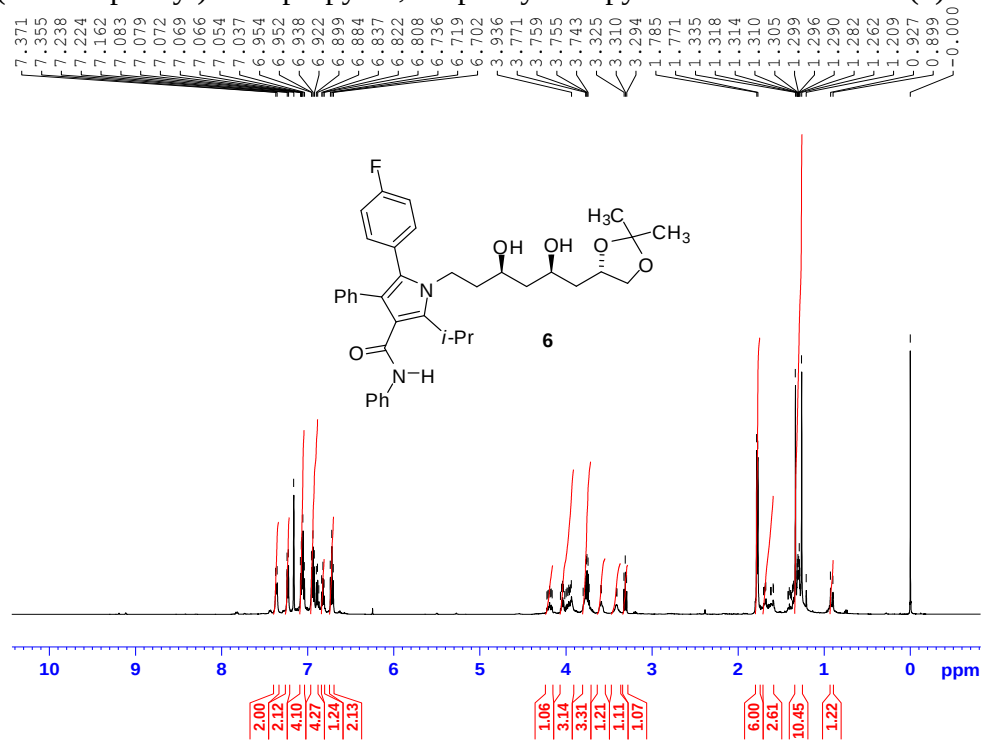

```
Current Data Parameters
NAME                  ago24asvH
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_               20110824
Time                   12.48
INSTRUM                spect
PROBHD    5 mm QNP 1H/13
PULPROG                zg30
TD                    32768
SOLVENT                C6D6
NS                       16
DS                        0
SWH                5175.983 Hz
FIDRES            0.157958 Hz
AQ                3.1653888 sec
RG                      256
DW                   96.600 usec
DE                    6.00 usec
TE                   298.2 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                     1H
P1                    13.00 usec
PL1                   -6.00 dB
SFO1           250.1315447 MHz

F2 - Processing parameters
SI                    32768
SF             250.1300000 MHz
WDW                      no
SSB          0
LB           0 Hz
GB           0
PC                     1.00
```

^{13}C NMR spectrum of 1-[(*R*)-6-((*S*)-2,2-dimethyl-1,3-dioxolan-4-yl)-3-hydroxy-5-oxohexyl]-5-(4-fluorophenyl)-2-isopropyl-*N*,4-diphenyl-1H-pyrrole-3-carboxamide (**5**) in C_6D_6 at 125 MHz



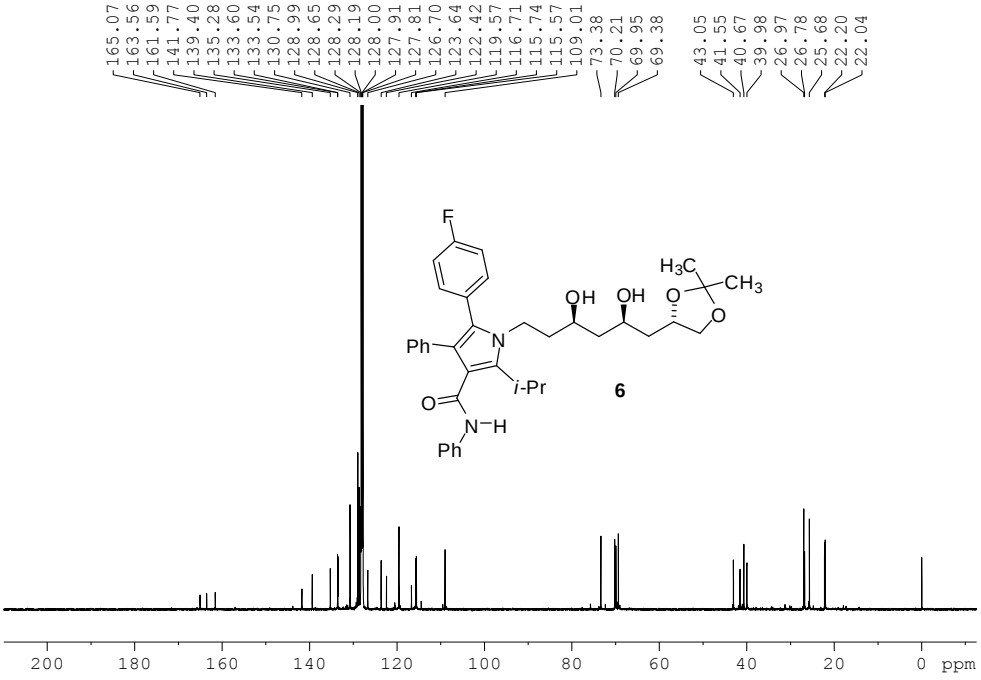

```
Current Data Parameters
NAME                  jun241cdH3
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_               20140624
Time                   15.59
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                    32768
SOLVENT               CDC13
NS                      512
DS                        4
SWH               29761.904 Hz
FIDRES            0.908261 Hz
AQ                0.5505024 sec
RG                     2050
DW                   16.800 usec
DE                    6.50 usec
TE                   298.1 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           125.7049801 MHz
NUC1                    13C
P1                    10.00 usec
PLW1           91.00000000 W

======== CHANNEL f2 ========
SFO2           499.8719995 MHz
NUC2                     1H
CPDPRG[2             waltz16
PCPD2                 80.00 usec
PLW2           26.85300064 W
PLW12           0.57928002 W
PLW13           0.37074000 W

F2 - Processing parameters
SI                    32768
SF             125.6923843 MHz
WDW                      EM
SSB          0
LB                    1.00 Hz
GB           0
PC                     1.40
```

^{1}H NMR spectrum of 1-[(3*R*,5*R*)-6-((*S*)-2,2-dimethyl-1,3-dioxolan-4-yl)-3,5-dihydroxyhexyl]-5-(4-fluorophenyl)-2-isopropyl-*N*,4-diphenyl-1*H*-pyrrole-3-carboxamide (**6**) in C_6D_6 at 500 MHz



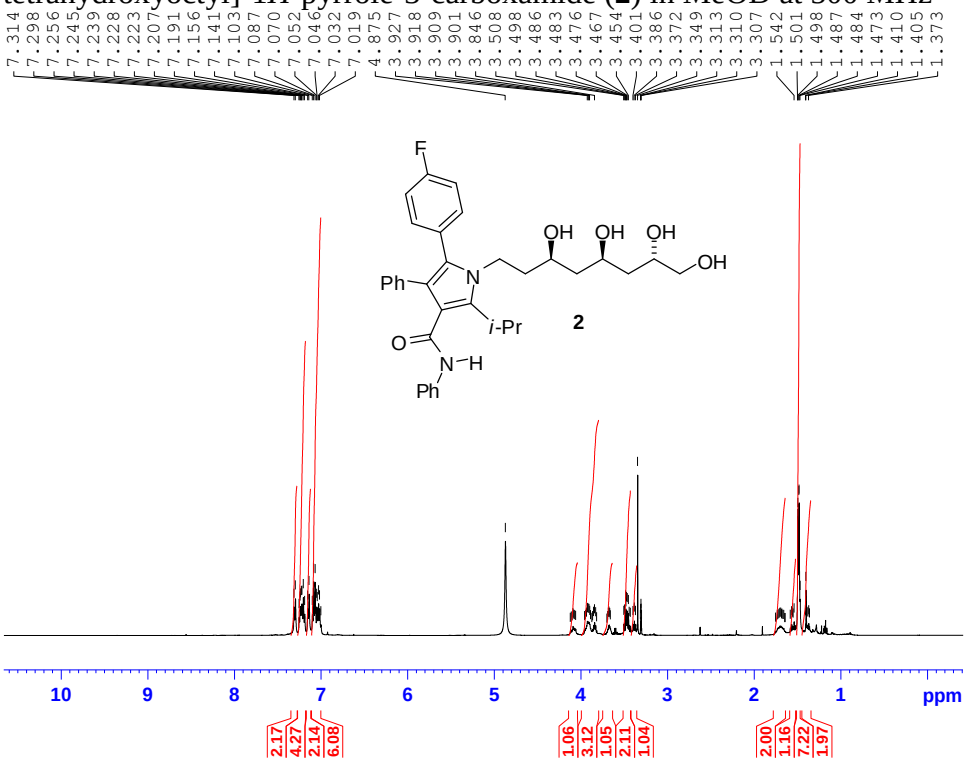

```
Current Data Parameters
NAME                 abr061cdH1
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_               20150406
Time                    9.36
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    32768
SOLVENT                C6D6
NS                       16
DS                        2
SWH               10000.000 Hz
FIDRES                0.305176 Hz
AQ                1.6384000 sec
RG                       32
DW                   50.000 usec
DE                    6.50 usec
TE                   298.1 K
D1                1.00000000 sec
TD0                           1

======== CHANNEL f1 ========
SFO1             499.8730869 MHz
NUC1                       1H
P1                     11.75 usec
PLW1            25.00000000 W

F2 - Processing parameters
SI                        65536
SF               499.8700000 MHz
WDW                        EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

^{13}C NMR spectrum of 1-[(3*R*,5*R*)-6-((S)-2,2-dimethyl-1,3-dioxolan-4-yl)-3,5-dihydroxyhexyl]-5-(4-fluorophenyl)-2-isopropyl-*N*,4-diphenyl-1*H*-pyrrole-3-carboxamide (**6**) in C_6D_6 at 125 MHz



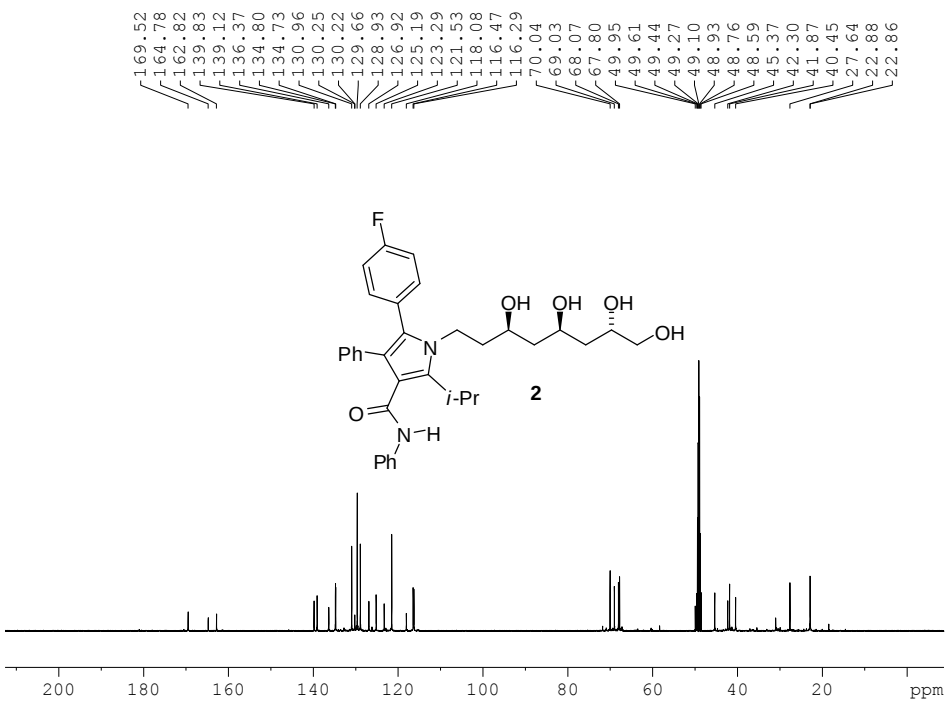

```
Current Data Parameters
NAME                 abr061cdH1
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_               20150406
Time                    9.38
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg30
TD                    32768
SOLVENT                C6D6
NS                     2048
DS                        4
SWH               29761.904 Hz
FIDRES                0.908261 Hz
AQ                0.5505024 sec
RG                     2050
DW                   16.800 usec
DE                    6.50 usec
TE                   298.2 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                           1

======== CHANNEL f1 ========
SFO1             125.7049801 MHz
NUC1                      13C
P1                     10.00 usec
PLW1            91.00000000 W

======== CHANNEL f2 ========
SFO2             499.8719995 MHz
NUC2                       1H
CPDPRG[2             waltz16
PCPD2                  80.00 usec
PLW2            26.85300064 W
PLW12            0.57928002 W
PLW13            0.37074000 W

F2 - Processing parameters
SI                        32768
SF               125.6923743 MHz
WDW                        EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

[1]H-NMR spectrum of 5-(4-fluorophenyl)-2-isopropyl-*N*,4-diphenyl-1-[(3*R*,5*R*,7*S*)-3,5,7,8-tetrahydroxyoctyl]-1*H*-pyrrole-3-carboxamide (**2**) in MeOD at 500 MHz



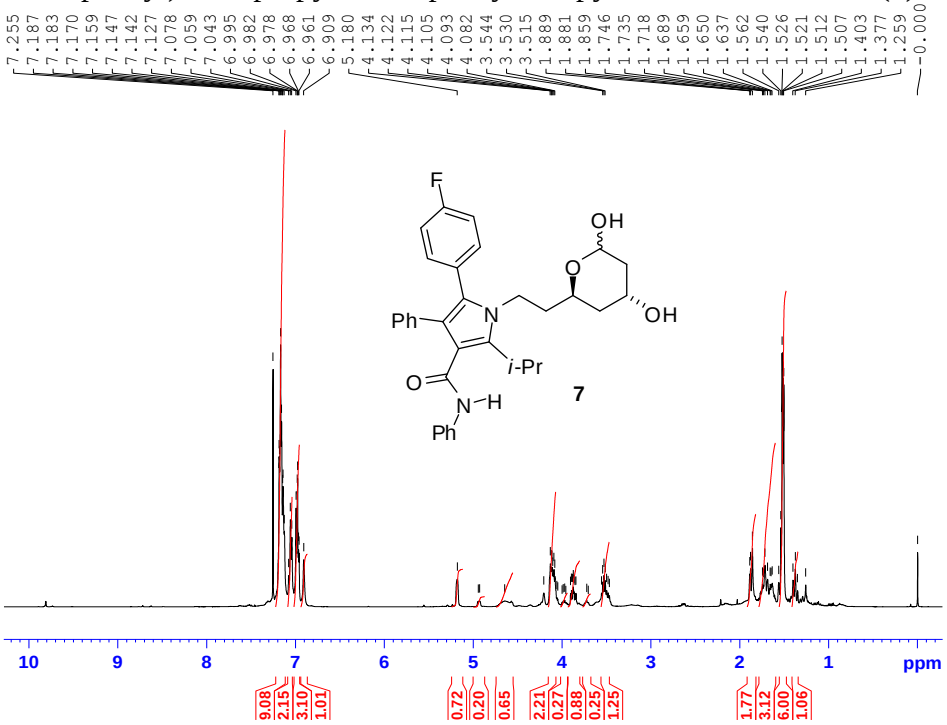

```
Current Data Parameters
NAME          ago301cdH3
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150830
Time              17.17
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                32768
SOLVENT            MeOD
NS                    8
DS                    0
SWH           10302.198 Hz
FIDRES        0.314398 Hz
AQ            1.5903403 sec
RG                   32
DW               48.533 usec
DE                6.50 usec
TE               298.1 K
D1           1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         499.8730869 MHz
NUC1                 1H
P1                11.75 usec
PLW1         25.00000000 W

F2 - Processing parameters
SI                65536
SF           499.8700149 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

[13]C NMR spectrum of 5-(4-fluorophenyl)-2-isopropyl-*N*,4-diphenyl-1-[(3*R*,5*R*,7*S*)-3,5,7,8-tetrahydroxyoctyl)-1*H*-pyrrole-3-carboxamide (**2**) in MeOD at 125 MHz




```
Current Data Parameters
NAME          ago301cdH3
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150830
Time              18.45
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                32768
SOLVENT            MeOD
NS                 2048
DS                    0
SWH           32894.738 Hz
FIDRES        1.003868 Hz
AQ            0.4980736 sec
RG                 2050
DW               15.200 usec
DE                6.50 usec
TE               298.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         125.7062372 MHz
NUC1                 13C
P1               10.00 usec
PLW1         91.00000000 W

======== CHANNEL f2 ========
SFO2         499.8719995 MHz
NUC2                 1H
CPDPRG[2          waltz16
PCPD2            80.00 usec
PLW2         26.85300064 W
PLW12         0.57928002 W
PLW13         0.37074000 W

F2 - Processing parameters
SI                32768
SF           125.6922379 MHz
WDW                  EM
SSB       0
LB               1.00 Hz
GB        0
PC                1.40
```

^{1}H NMR spectrum of 1-[2-((2*R*,4*R*)-4,6-dihydroxytetrahydro-2*H*-pyran-2-yl)ethyl]-5-(4-fluorophenyl)-2-isopropyl-*N*,4-diphenyl-1*H*-pyrrole-3-carboxamide (**7**) in $CDCl_3$ at 500 MHz

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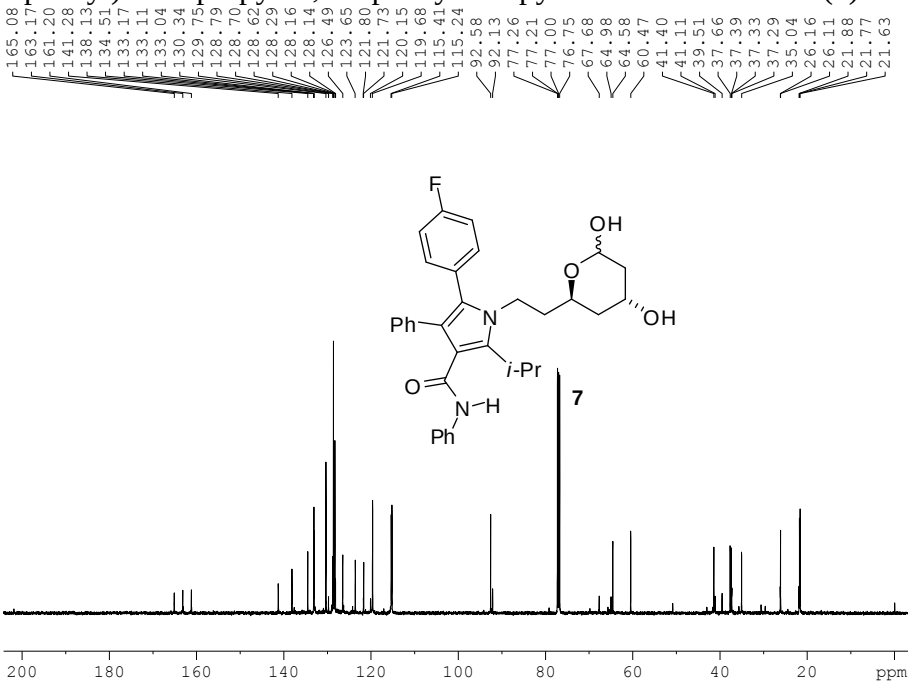
Current Data Parameters
NAME          set111cdH1
EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150911
Time              14.21
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32768
SOLVENT          CDCl3
NS                  16
DS                   0
SWH          10302.198 Hz
FIDRES        0.314398 Hz
AQ            1.5903403 sec
RG                25.4
DW              48.533 usec
DE                6.50 usec
TE              298.2 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        499.8730869 MHz
NUC1                  1H
P1                11.75 usec
PLW1        25.00000000 W

F2 - Processing parameters
SI                 65536
SF          499.8700194 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

^{13}C NMR spectrum of 1-[2-((2*R*,4*R*)-4,6-dihydroxytetrahydro-2*H*-pyran-2-yl)ethyl]-5-(4-fluorophenyl)-2-isopropyl-*N*,4-diphenyl-1*H*-pyrrole-3-carboxamide (**7**) in $CDCl_3$ at 125 MHz

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Current Data Parameters
NAME          set111cdH1
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20150911
Time              14.37
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               32768
SOLVENT          CDCl3
NS                1024
DS                   0
SWH          32894.738 Hz
FIDRES        1.003868 Hz
AQ            0.4980736 sec
RG                2050
DW              15.200 usec
DE                6.50 usec
TE              298.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        125.7062372 MHz
NUC1                  13C
P1               10.00 usec
PLW1        91.00000000 W

======== CHANNEL f2 ========
SFO2        499.8719995 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         26.85300064 W
PLW12         0.57928002 W
PLW13         0.37074000 W

F2 - Processing parameters
SI                 32768
SF          125.6924244 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```
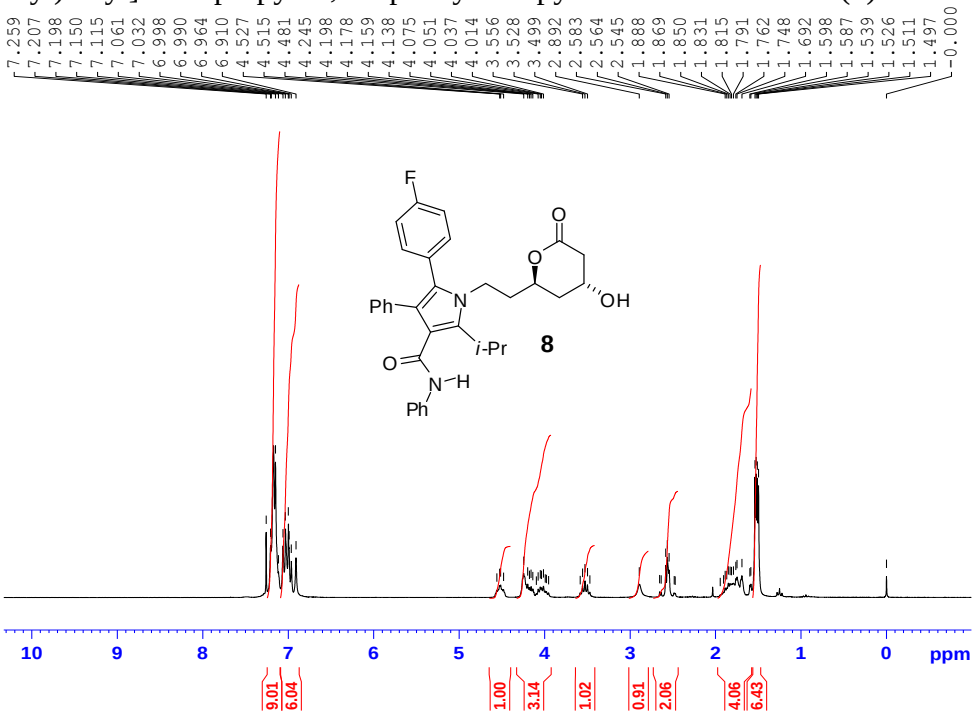

^{1}H NMR spectrum of 5-(4-fluorophenyl)-1-[2-((2*R*,4*R*)-4-hydroxy-6-oxo-tetrahydro-2*H*-pyran-2-yl)ethyl]-2-isopropyl-*N*,4-diphenyl-1*H*-pyrrole-3-carboxamide (**8**) in $CDCl_3$ at 250 MHz

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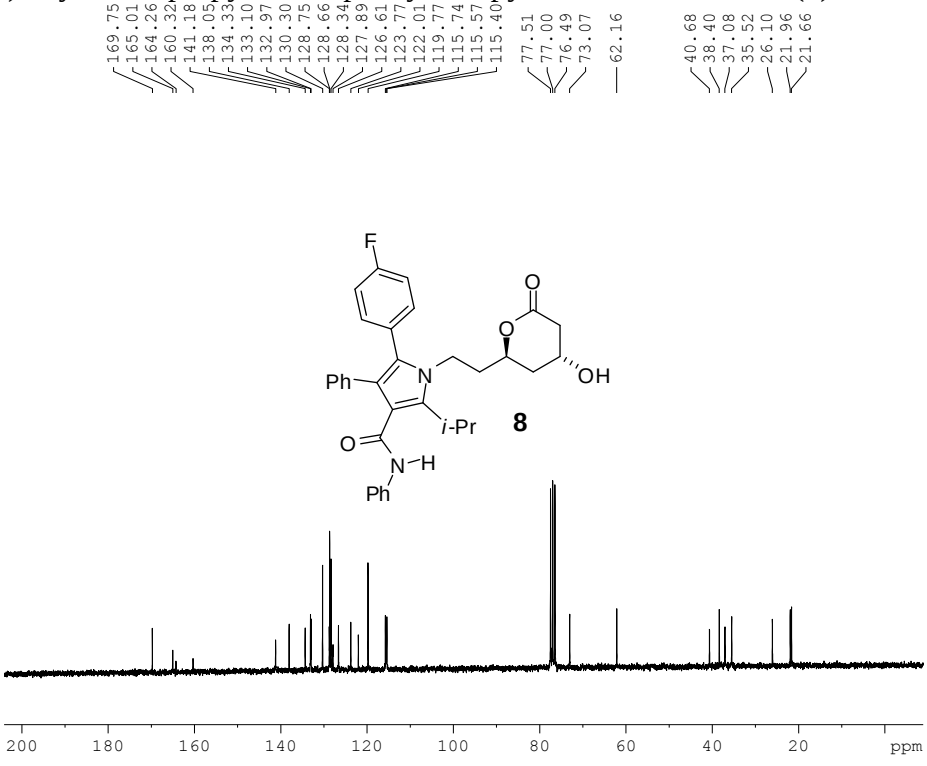
Current Data Parameters
NAME                  nov24asvH
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20101124
Time                      12.16
INSTRUM                   spect
PROBHD    5 mm QNP 1H/13
PULPROG                   zg30
TD                       32768
SOLVENT                  CDCl3
NS                          16
DS                           0
SWH                5175.983 Hz
FIDRES             0.157958 Hz
AQ                 3.1653888 sec
RG                       322.5
DW                     96.600 usec
DE                       6.00 usec
TE                      298.2 K
D1                 1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                       13.00 usec
PL1                      -6.00 dB
SFO1           250.1315447 MHz

F2 - Processing parameters
SI                       32768
SF                250.1300001 MHz
WDW                         EM
SSB          0
LB                       0.30 Hz
GB           0
PC                       1.00
```

^{13}C NMR spectrum of 5-(4-fluorophenyl)-1-[2-((2*R*,4*R*)-4-hydroxy-6-oxo-tetrahydro-2*H*-pyran-2-yl)ethyl]-2-isopropyl-*N*,4-diphenyl-1*H*-pyrrole-3-carboxamide (**8**) in $CDCl_3$ at 62.5 MHz

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Current Data Parameters
NAME                  nov25asvC
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_                  20101125
Time                       8.10
INSTRUM                   spect
PROBHD    5 mm QNP 1H/13
PULPROG                 zgpg30
TD                       16384
SOLVENT                  CDCl3
NS                        1024
DS                           0
SWH               15060.241 Hz
FIDRES             0.919204 Hz
AQ                 0.5439488 sec
RG                       724.1
DW                     33.200 usec
DE                       6.00 usec
TE                      298.2 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                          1
SFO1           62.9015280 MHz
NUC1                       13C
P1                      10.00 usec
PLW1          -1.00000000 W
SFO2           250.1310005 MHz
NUC2                       1H
CPDPRG[2                waltz16
PCPD2                  100.00 usec
PLW2          -1.00000000 W
PLW12         -1.00000000 W
PLW13         -1.00000000 W

F2 - Processing parameters
SI                       32768
SF                62.8952416 MHz
WDW                         EM
SSB          0
LB                       1.00 Hz
GB           0
PC                       1.40
```
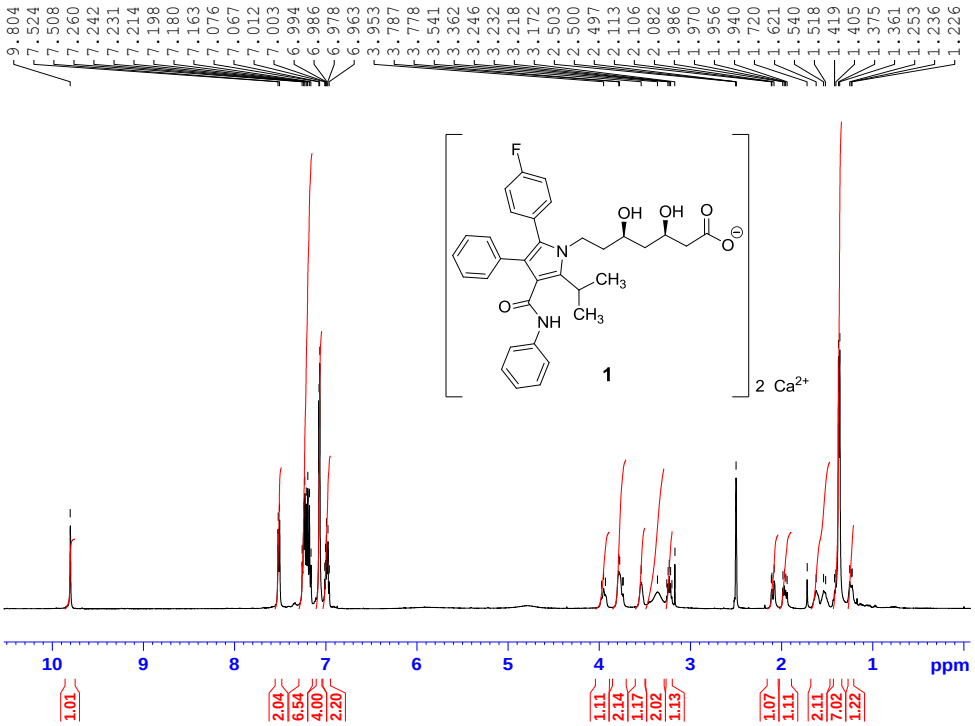

^{1}H NMR spectrum of Calcium Atorvastatin (**1**) in DMSO-d_6 at 500 MHz

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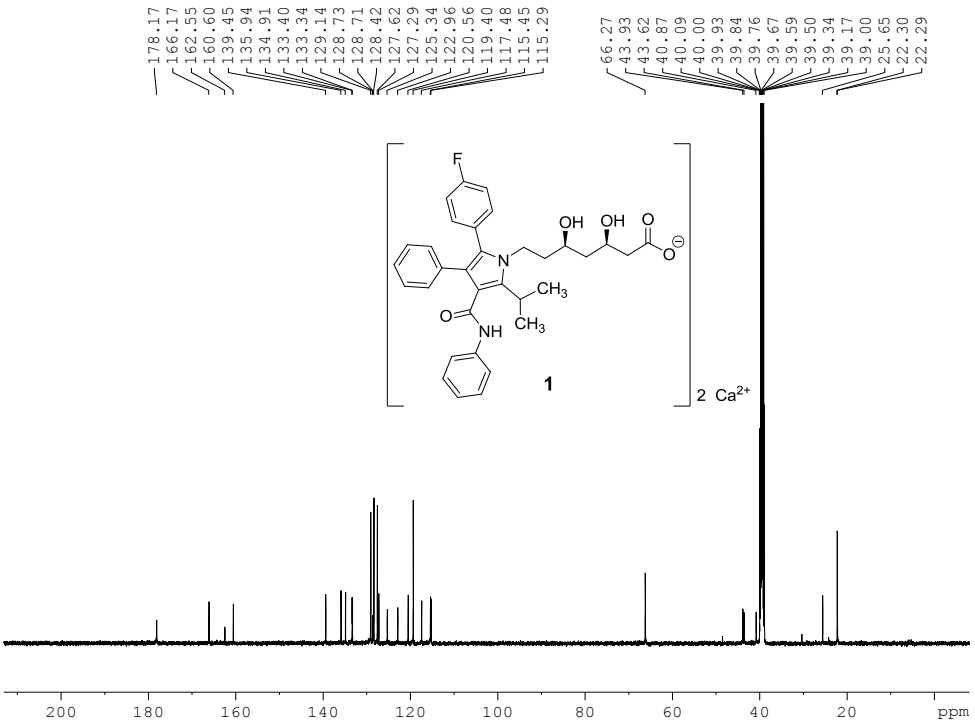
Current Data Parameters
NAME                 ago301cdH2
EXPNO                         1
PROCNO                        1

F2 - Acquisition Parameters
Date_               20150830
Time_                  15.45
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    32768
SOLVENT                DMSO
NS                        4
DS                        0
SWH                10302.198 Hz
FIDRES             0.314398 Hz
AQ                 1.5903403 sec
RG                      80.6
DW                    48.533 usec
DE                     6.50 usec
TE                    298.1 K
D1                 1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1              499.8730869 MHz
NUC1                      1H
P1                     11.75 usec
PLW1              25.00000000 W

F2 - Processing parameters
SI                        65536
SF                499.8700093 MHz
WDW                       EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

^{13}C NMR spectrum of Calcium Atorvastatin (**1**) in DMSO-d_6 at 125 MHz

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Current Data Parameters
NAME                 ago301cdH2
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_               20150830
Time_                  17.14
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg30
TD                    32768
SOLVENT                DMSO
NS                     2048
DS                        0
SWH                32894.738 Hz
FIDRES             1.003868 Hz
AQ                 0.4980736 sec
RG                     2050
DW                   15.200 usec
DE                     6.50 usec
TE                    298.2 K
D1                 2.00000000 sec
D11                0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1              125.7062372 MHz
NUC1                      13C
P1                     10.00 usec
PLW1              91.00000000 W

======== CHANNEL f2 ========
SFO2              499.8719995 MHz
NUC2                      1H
CPDPRG[2             waltz16
PCPD2                  80.00 usec
PLW2              26.85300064 W
PLW12              0.57928002 W
PLW13              0.37074000 W

F2 - Processing parameters
SI                        32768
SF                125.6924729 MHz
WDW                       EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

Amorphous Calcium Atorvastatin (1) XR Diffractogram

Measurement Condition

X-ray tube

target = Cu

voltage = 40.0 (kV)

current = 20.0 (mA)

Slits

divergence slit = 1.00000 (deg)

scatter slit = 1.00000 (deg)

receiving slit = 0.30000 (mm)

Scanning

drive axis = Theta-2Theta

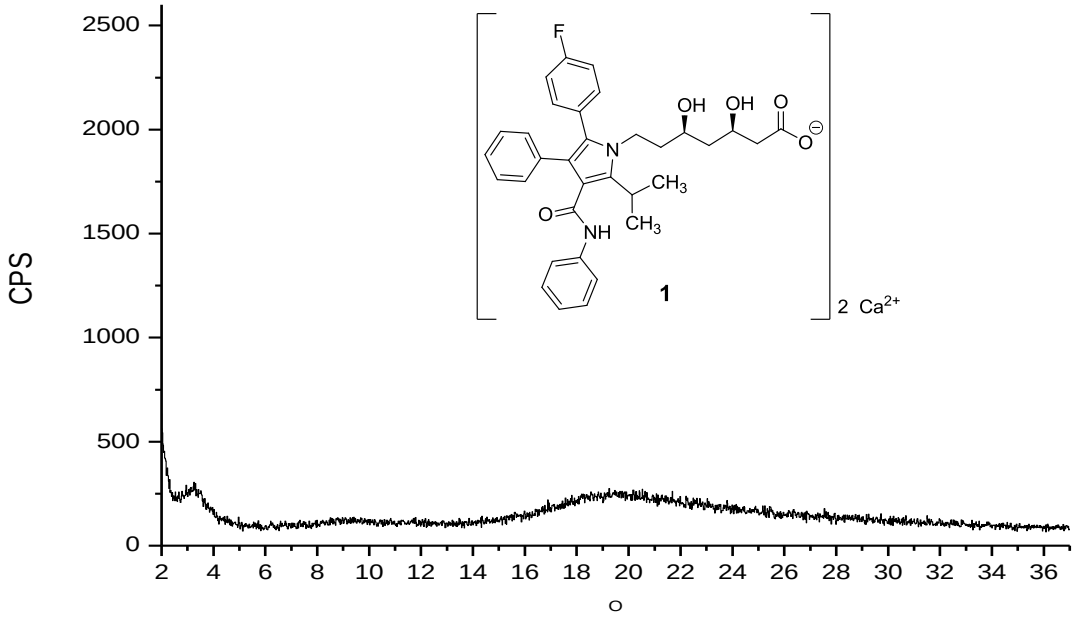
scan range = 2.000 - 37.000

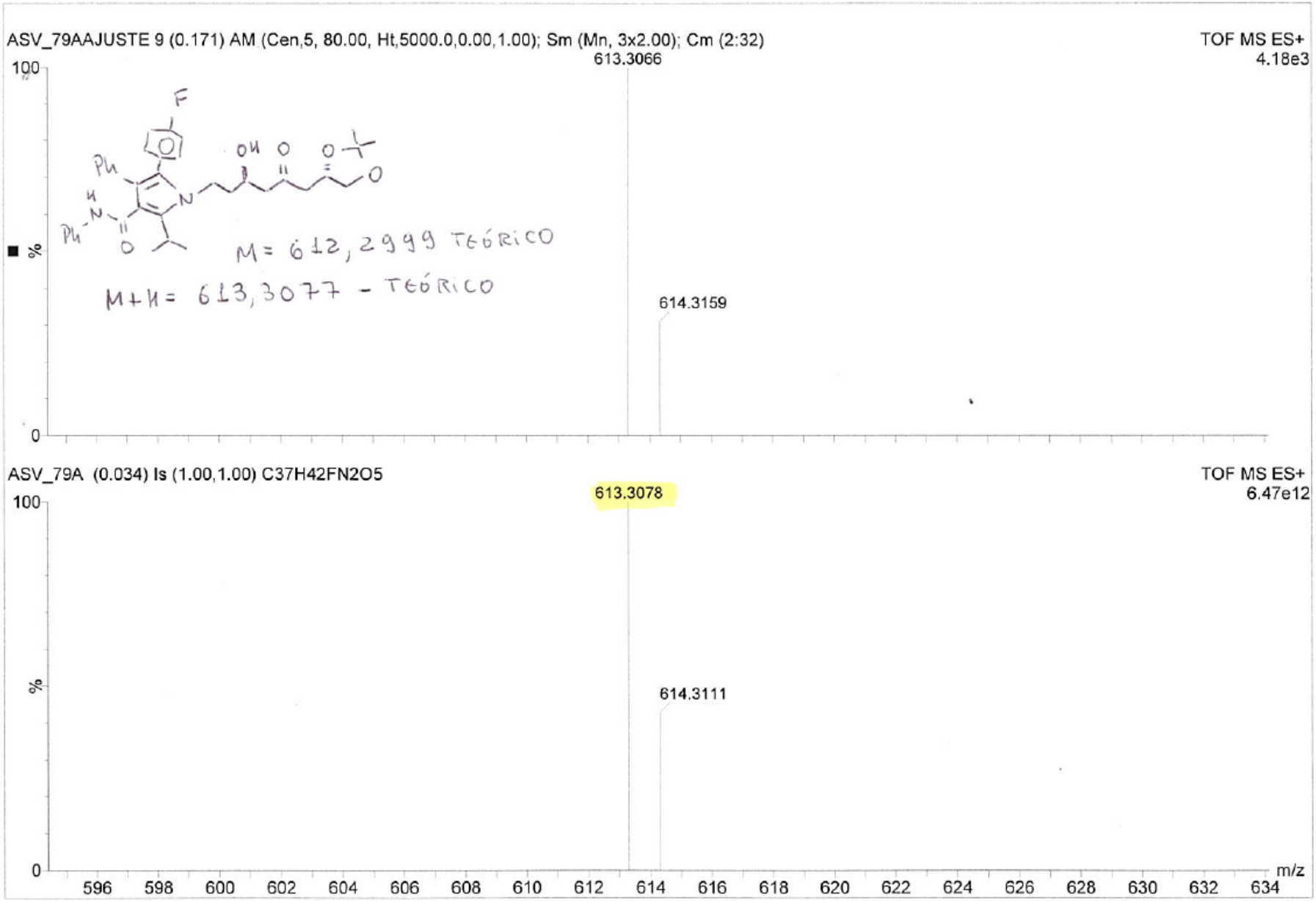
scan mode = Continuous Scan

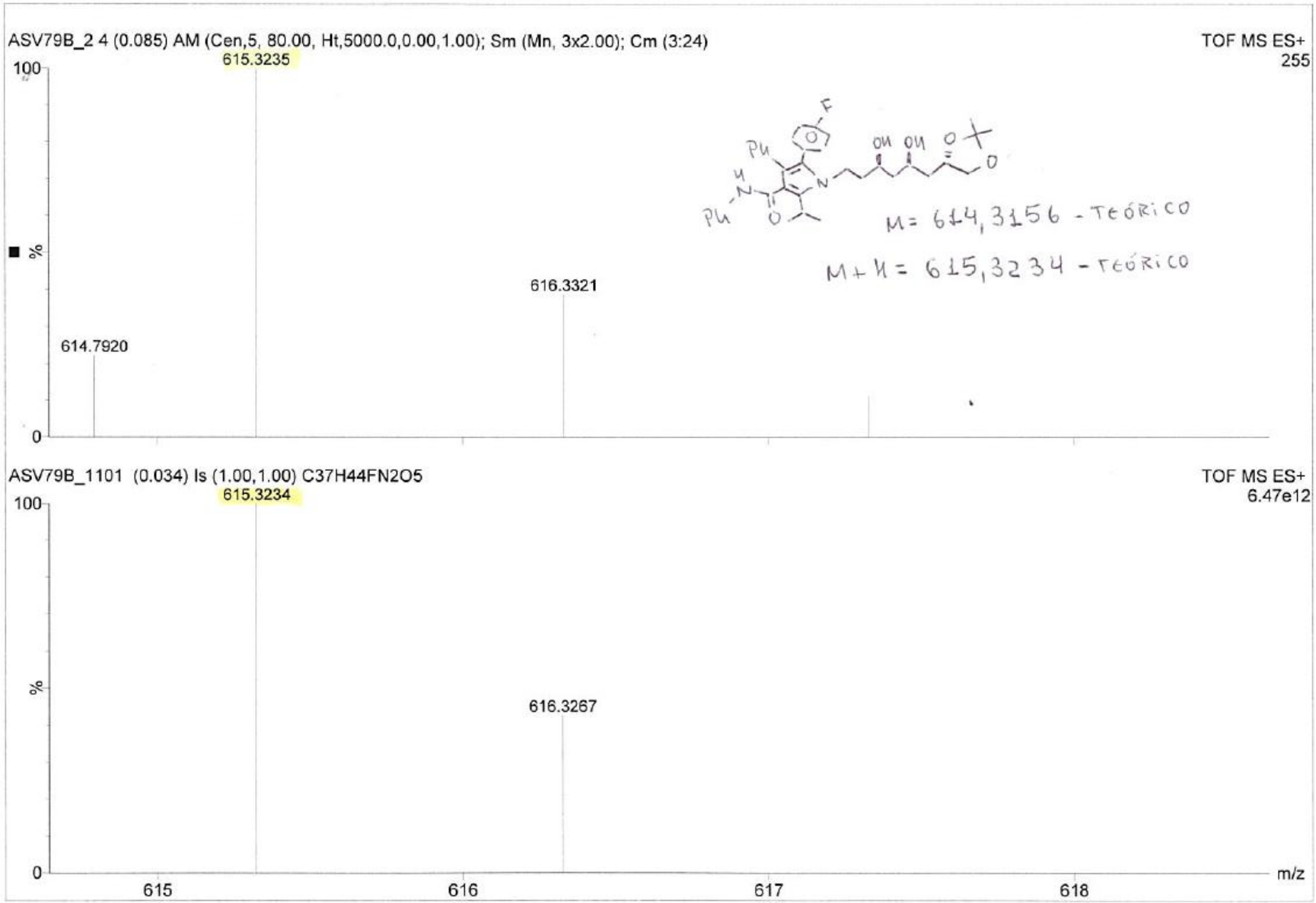
scan speed = 2.0000 (deg/min)

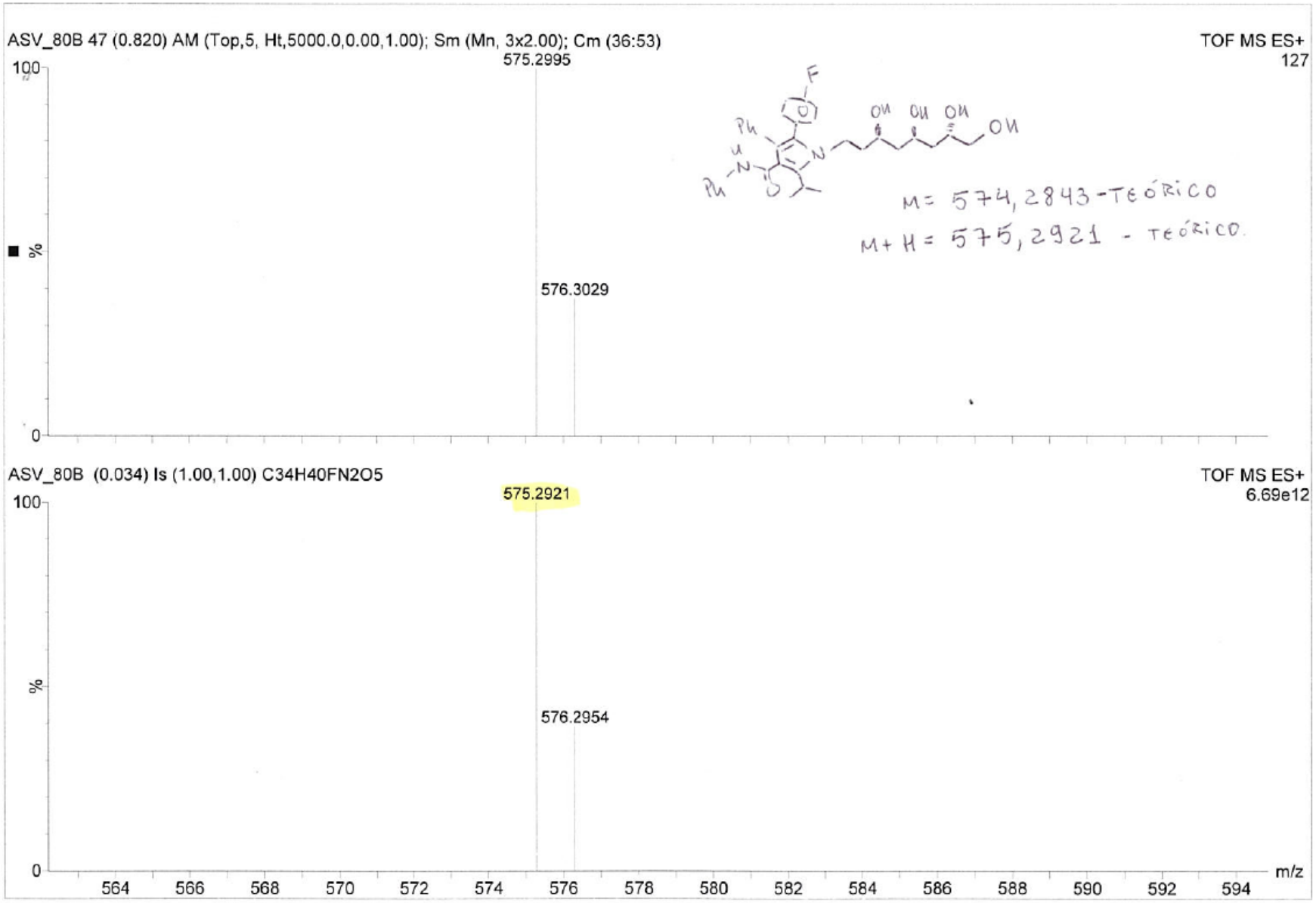
sampling pitch = 0.0200 (deg)

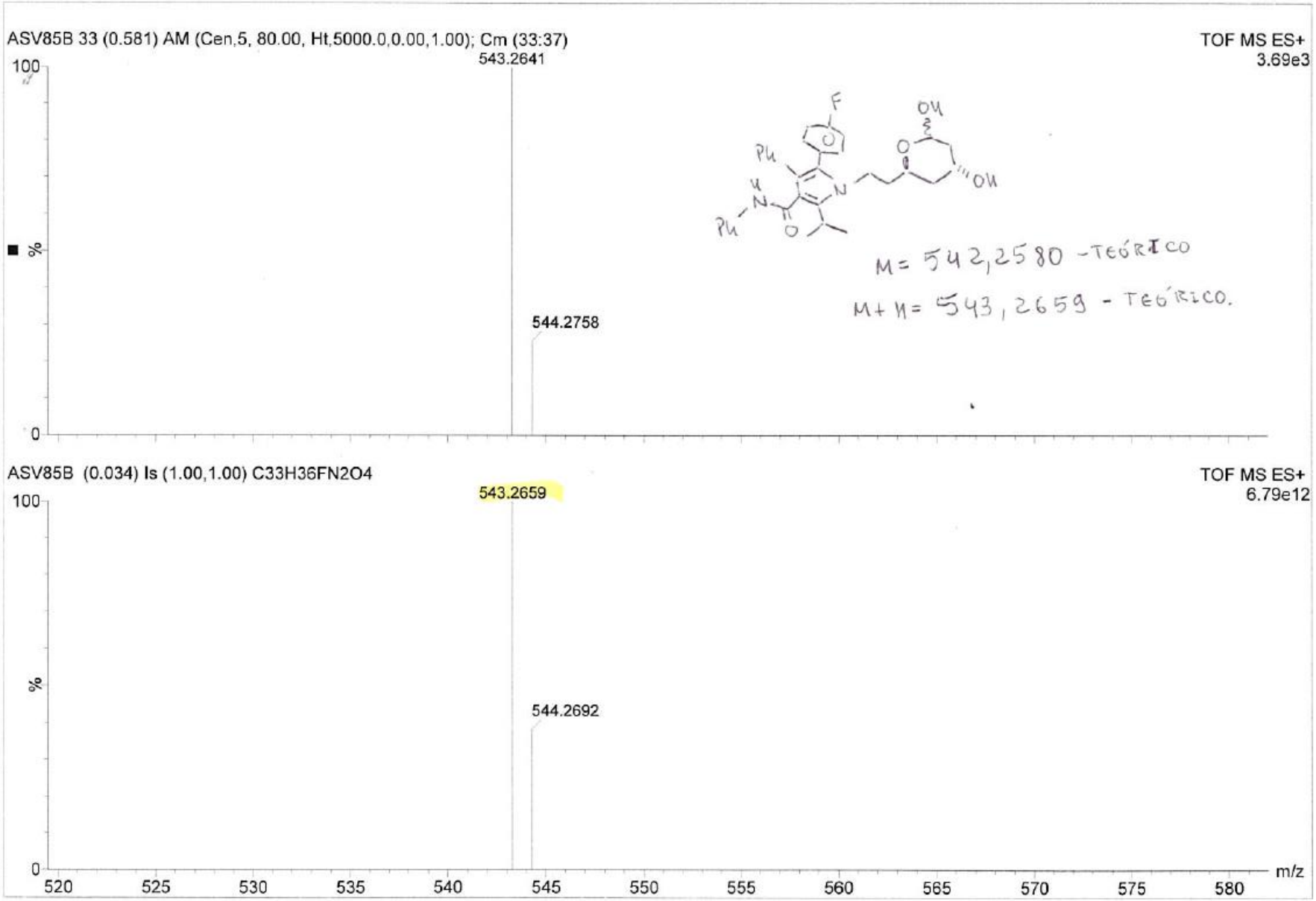
preset time = 0.60 (sec)




ASV_79AAJUSTE 9 (0.171) AM (Cen,5, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 3x2.00); Cm (2:32)
613.3066
TOF MS ES+
4.18e3
100
%
0
M = 612,2999 TEÓRICO
M+H = 613,3077 - TEÓRICO
614.3159
ASV_79A (0.034) Is (1.00,1.00) C37H42FN2O5
613.3078
TOF MS ES+
6.47e12
100
%
0
614.3111
596 598 600 602 604 606 608 610 612 614 616 618 620 622 624 626 628 630 632 634
m/z


ASV79B_2 4 (0.085) AM (Cen,5, 80.00, Ht,5000.0,0.00,1.00); Sm (Mn, 3x2.00); Cm (3:24)
TOF MS ES+
255
615.3235
100
%
616.3321
614.7920
0
M = 614,3156 - TEÓRICO
M+H = 615,3234 - TEÓRICO
ASV79B_1101 (0.034) Is (1.00,1.00) C37H44FN2O5
TOF MS ES+
6.47e12
615.3234
100
%
616.3267
0
615
616
617
618
m/z


ASV_80B 47 (0.820) AM (Top,5, Ht,5000.0,0.00,1.00); Sm (Mn, 3x2.00); Cm (36:53)
TOF MS ES+
127
575.2995
100
%
576.3029
0
M = 574,2843 - TEÓRICO
M+H = 575,2921 - TEÓRICO
ASV_80B (0.034) Is (1.00,1.00) C34H40FN2O5
TOF MS ES+
6.69e12
575.2921
100
%
576.2954
0
564
566
568
570
572
574
576
578
580
582
584
586
588
590
592
594
m/z


ASV85B 33 (0.581) AM (Cen,5, 80.00, Ht,5000.0,0.00,1.00); Cm (33:37)
TOF MS ES+
3.69e3
543.2641
544.2758
100
%
0
M = 542,2580 - TEÓRICO
M+H = 543,2659 - TEÓRICO.
ASV85B (0.034) Is (1.00,1.00) C33H36FN2O4
TOF MS ES+
6.79e12
543.2659
544.2692
100
%
0
m/z
520
525
530
535
540
545
550
555
560
565
570
575
580

Data File D:\ACIDOS\DADOS\ADRIANO-ATORVASTATINA\AMOSTRA 1.D
Sample Name: atorvastatina

ATV Ca^{2+}

```
==========================================================================
Acq. Operator    : ricardo
Acq. Instrument  : Instrument 1                    Location : Vial 2
Injection Date   : 9/28/2011 11:04:01 AM
                                                   Inj Volume : 20.0 µl
Method           : C:\CHEM32\1\METHODS\ATORVASTATINA-ADRIANO.M
Last changed     : 9/28/2011 10:25:07 AM by ricardo
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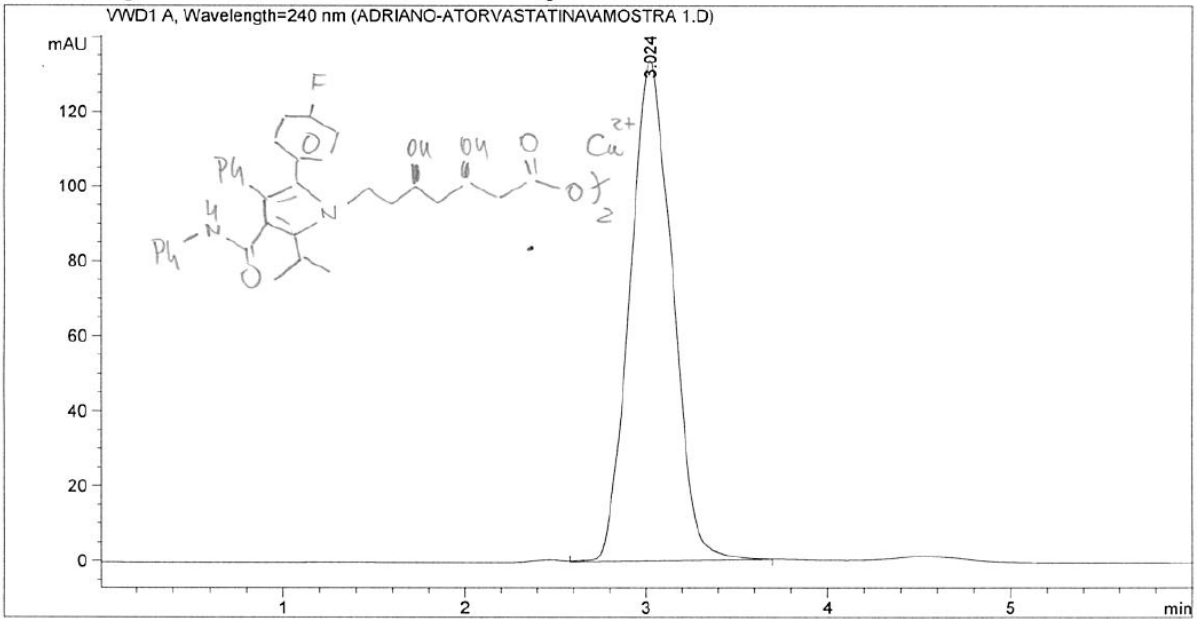


```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: VWD1 A, Wavelength=240 nm

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1   3.024 VB    0.2259 2177.05591  133.77722 100.0000

Totals :                   2177.05591  133.77722

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                        *** End of Report ***
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