

Supporting Information

Synthesis of Novel Unnatural α -Amino Acid (UAAs) Containing 7-Hydroxy-2, 2-Dimethyl-Chroman using Isoxazole as Linker

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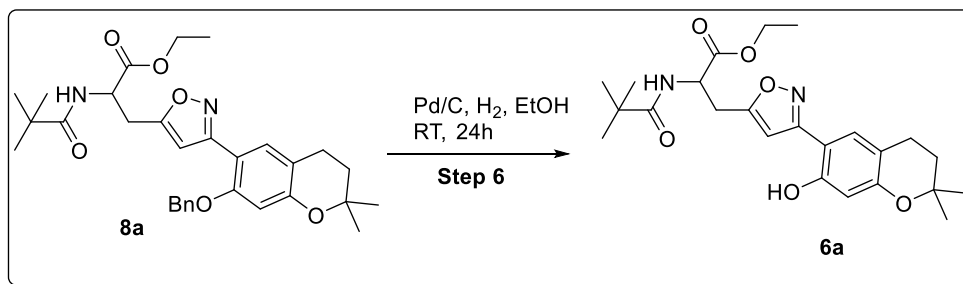
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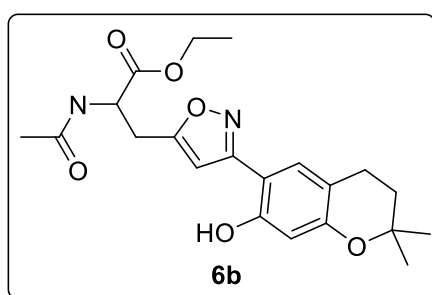
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General Information:

All the chemicals were commercially available and procured from companies like Aldrich, Spectrochem (India), S. D. Fine (India), combi-block, fluorochem, matrix and Avra (India) and have been carried forward without further purification. Solvents used in the present study are dried before prior use whenever required. Precoated TLC silica gel plates (Kieselgel 60 F254, Merck) were used for monitoring reactions. Purification was performed by column chromatography using silica gel (Particle size 60-120 mesh, Merck). Melting points were determined in open capillary tubes on cintex melting point apparatus and are uncorrected. IR (KBr) spectra were recorded on Perkin-Elmer FT/IR-4000 using ATR (ν_{max} in cm^{-1}) in the frequency range of 600-4000 cm^{-1} . ^1H NMR and ^{13}C NMR spectra were recorded in $\text{CDCl}_3/\text{DMSO}-d_6$ on a Bruker DRX-400 (400 MHz FT NMR). Chemical shifts are presented in δ ppm employing TMS as internal reference. Splitting patterns were reported as s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; br, broad.

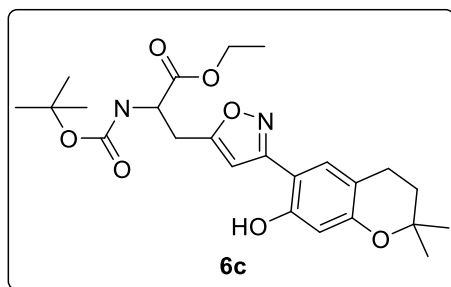


Experimental procedure for the preparation of ethyl 3-(3-(7-hydroxy-2,2-dimethylchroman-6-yl)isoxazol-5-yl)-2-pivalamidopropanoate (6a): To a stirred solution of compound **8a** (70 mg, 0.131mmol) in ethanol (10 ml), 10% Pd/C (30 mg) was added and stirred at room temperature for 24 h under hydrogen atmosphere (30 psi). The progress of the reaction was monitored by TLC analysis (20% ethyl acetate/pet ether). After completion of the reaction, the reaction mixture was filtered through celite bed and washed the celite bed with ethanol twice (2x10 ml). Combined organic layers were concentrated under reduced pressure to give the crude compound which was purified by Prep TLC to give compound **11** (50 mg, 86%); MR: 155-158⁰C; IR (KBr, cm⁻¹): 3380, 2973.4, 2932, 2867.3, 1743, 1644, 1520, 1450, 1376, 1288,1205, 1152, 1118, 1022, 955, 879, 867, 772, 621. ¹H NMR (500 MHz, CDCl₃): δ = 9.22 (s, 1H, -OH), 7.09 (s, 1H, Ar-H), 6.46 (s, 1H, Ar-H), 6.39-6.37 (d, *J* = 7 Hz, 1H, -NH), 6.34 (s, 1H, isoxazole-H), 4.89-4.86 (q, 1H, chiral-H), 4.30-4.22 (q, 2H, -OCH₂), 3.50-3.33 (m, 2H, -CH₂), 2.75-2.72 (t, *J* = 13.5 Hz, 2H, -CH₂), 1.82-1.79 (t, *J* = 13.5 Hz, 2H, Ar-CH₂), 1.34 (s, 6H, -(CH₃)₂), 1.32-1.30 (t, *J* = 13 Hz, 3H, -CH₃), 1.20 (s, 9H, -(CH₃)₃); ¹³C NMR (500 MHz, CDCl₃) = 178.50, 170.75, 167.53, 162.54, 157.18, 156.37, 128.67, 113.18, 106.14, 105.11, 100.48, 75.08, 62.38, 50.89, 38.90, 32.96, 29.100, 27.51, 27.00, 21.86, 14.24. MS (EI): *m/z* 445 (M+1, 100); HRMS: calcd for: C₂₄H₃₃N₂O₆ [M+H]: 445.2339; Found: 445.2340.

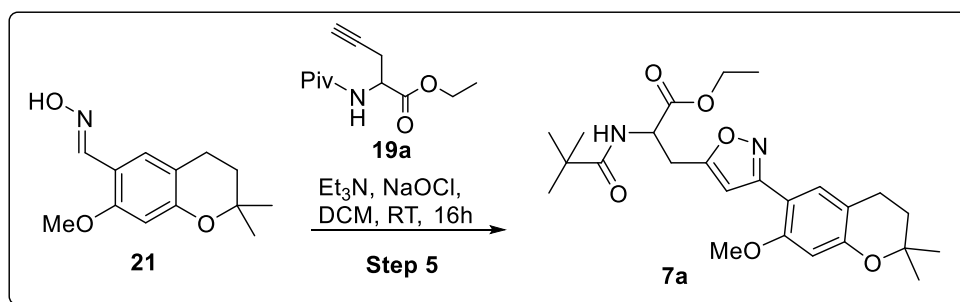


Ethyl 2-acetamido-3-(3-(7-hydroxy-2,2-dimethylchroman-6-yl)isoxazol-5-yl)propanoate (6b): MR: 76-79⁰C; IR (KBr, cm⁻¹): 3274.3, 3065, 2980.1, 2930, 2854.7, 1741.8, 1669.4, 1635.7, 1582.6, 1518, 1448.6, 1375.3, 1287.5, 1211.3, 1154.4, 1116.8, 1027.1, 961.5, 879.5, 755.1, 599.8; ¹H NMR (400 MHz, CDCl₃): δ = 9.20 (s, 1H, -OH), 7.12 (s, 1H, Ar-H), 6.46 (s, 1H, Ar-H), 6.37 (s, 1H, isoxazole-H), 6.26-6.25 (d, *J* = 7.2 Hz, 1H, -NH), 4.95-4.90 (q, 1H, chiral-H), 4.30-4.22 (q, 2H, -OCH₂), 3.48-3.33 (m, 2H, -CH₂), 2.76-2.72 (t, *J* = 13.6 Hz, 2H, -CH₂), 2.04 (s, 3H, -COCH₃), 1.82-1.79 (t, *J* =

13.6Hz, 2H, Ar-CH₂), 1.34 (s, 6H, -(CH₃)₂), 1.31-1.27 (t, *J* = 14 Hz, 3H, -CH₃); ¹³C NMR (100 MHz, CDCl₃) = 170.39, 169.94, 167.20, 162.43, 157.05, 156.20, 128.58, 113.03, 105.93, 104.95, 100.42, 74.93, 62.30, 50.80, 32.80, 29.67, 29.15, 26.83, 23.14, 21.68, 14.08; MS (ESI): *m/z* 403 (M+1, 100).



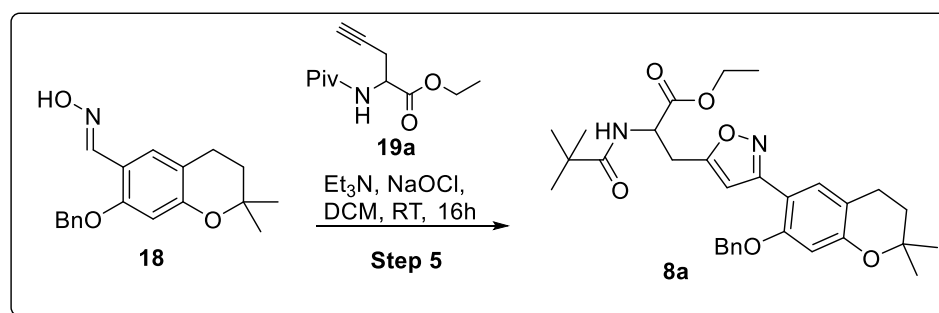
Ethyl 2-((tert-butoxycarbonyl)amino)-3-(3-(7-hydroxy-2,2-dimethylchroman-6-yl)isoxazol-5-yl)propanoate (6c): MR: 103-106⁰C; IR (KBr, cm⁻¹): 3356.2, 3247.3, 3148.9, 2977.2, 2931.9, 2852.8, 1737.9, 1709.9, 1638.6, 1585.5, 1514.1, 1450.5, 1369.5, 1289.4, 1222.9, 1187.2, 1160.2, 1017.4, 962.5, 878.6, 846.7, 792.7, 615.3; ¹H NMR (500 MHz, CDCl₃): δ= 9.23 (s, 1H, -OH), 7.12 (s, 1H, Ar-H), 6.46 (s, 1H, Ar-H), 6.39 (s, 1H, isoxazole-H), 5.25-5.24 (d, *J* = 7.5 Hz, 1H, -NH), 4.68-4.66 (m, 1H, chiral-H), 4.27-4.21 (q, 2H, -OCH₂), 3.41-3.32 (m, 2H, -CH₂), 2.75-2.73 (t, *J* = 13Hz, 2H, -CH₂), 1.82-1.80 (t, *J* = 13.5Hz, 2H, Ar-CH₂), 1.44 (s, 9H, -(CH₃)₃), 1.34 (s, 6H, -(CH₃)₂), 1.29-1.26 (t, *J* = 14.5 Hz, 3H, -CH₃); ¹³C NMR (150 MHz, CDCl₃) = 170.58, 167.38, 162.42, 156.98, 156.22, 155.07, 128.57, 112.97, 106.03, 104.93, 100.22, 80.41, 74.90, 62.09, 51.97, 32.81, 29.71, 28.24, 26.85, 21.69, 14.09; MS (ESI): *m/z* 461 (M+1, 100).



Experimental procedure for the preparation of ethyl 3-(3-(7-methoxy-2,2-dimethylchroman-6-yl)isoxazol-5-yl)-2-pivalamidopropanoate (7a): To a stirred solution of compound **21** (1 g, 4.255 mmol) and compound **19a** (1.148 g, 5.106 mmol) in dichloromethane (15 ml), was added triethylamine (0.888 ml, 6.382 mmol) at 0°C and stirred for 10 min then added 10% aqueous NaOCl solution (15 ml) and the reaction mixture was stirred at room temperature for 16 h. The progress of the reaction was monitored by TLC analysis (30% ethyl acetate/pet ether). After completion of the reaction, the reaction mixture was diluted with dichloromethane (250 ml) and washed with water and brine solution.

Organic layer was dried over anhydrous Na₂SO₄ and concentrated under reduced pressure to give the crude residue which was charged on silica gel column. The column was eluted with 40% ethyl acetate/pet ether to give the compound **7a** (1.5g, 77% yield) as off white solid.

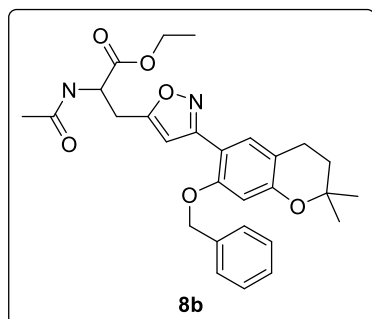
MR: 121-124⁰C; IR (KBr, cm⁻¹): 3433, 3408, 2976, 2931, 1814, 1741, 1659, 1623, 1601, 1469, 1439, 1363, 1274, 1262, 1199, 1158, 1119, 1065, 1025, 752; ¹H NMR (400 MHz, CDCl₃): δ = 7.60 (s, 1H, Ar-H), 6.51 (s, 1H, Ar-H), 6.41 (s, 1H, isoxazole-H), 6.38 (bs, 1H, -NH), 4.86-4.84 (q, 1H, chiral-CH), 4.30-4.19 (q, 2H, -OCH₂), 3.79 (s, 3H, -OCH₃), 3.46-3.32 (m, 2H, -CH₂), 2.75-2.72 (t, *J* = 13.2 Hz, 2H, -CH₂), 1.82-1.79 (t, *J* = 13.6 Hz, 2H, Ar-CH₂), 1.35 (s, 6H, -(CH₃)₂), 1.32-1.28 (t, *J* = 14.4 Hz, 3H, -CH₃), 1.21 (s, 9H, -(CH₃)₃); ¹³C NMR (400 MHz, CDCl₃) = 178.19, 170.71, 166.95, 129.88, 113.39, 104.50, 100.36, 75.06, 62.01, 55.44, 50.92, 38.72, 32.82, 29.00, 27.36, 26.83, 21.48, 14.10; MS (ESI): *m/z* 459 (M+1, 100).



Experimental procedure for the preparation of ethyl 3-(3-(7-(benzyloxy)-2,2-dimethylchroman-6-yl)isoxazol-5-yl)-2-pivalamidopropanoate (8a): To a stirred solution of compound **18** (150 mg, 0.482mmol) and compound **19a** (130.2 mg, 0.578mmol) in dichloromethane (10 ml), was added triethylamine (0.1 ml, 0.723 mmol) at 0^oC and stirred for 10 min then added 10% aqueous NaOCl solution (2 ml) and the reaction mixture was stirred at room temperature for 16 h. The progress of the reaction was monitored by TLC analysis (30% ethyl acetate/pet ether). After completion of the reaction, the reaction mixture was diluted with dichloromethane (25 ml) and washed with water and brine solution. Organic layer was dried over anhydrous Na₂SO₄ and concentrated under reduced pressure to give the crude residue which was charged on silica gel column. The column was eluted with 16% ethyl acetate/pet ether to give the compound **8a** (160mg, 62% yield) as off white solid.

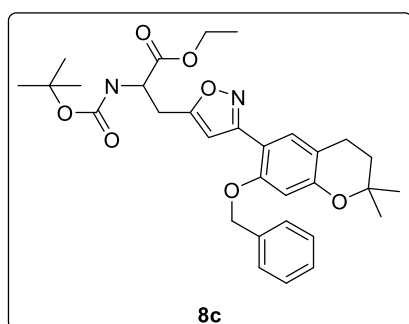
MR: 129-132⁰C; IR (KBr, cm⁻¹): 3364, 3176, 2968, 2925, 2864, 1748, 1666, 1606, 1515, 1463, 1383, 1291, 1191, 1120, 1018, 917, 732, 695, 604; ¹H NMR (400 MHz, CDCl₃): δ = 7.65 (s, 1H, Ar-H), 7.41-7.30 (m, 5H, Ar-H), 6.49 (s, 1H, Ar-H), 6.47 (s, 1H, isoxazole-H), 6.35 (d, *J* = 7.2 Hz, 1H, -NH), 5.06 (s, 2H, Bn-CH₂), 4.84-4.80 (q, 1H, chiral-H), 4.16-4.10 (q, 2H, -OCH₂), 3.38-3.27 (m, 2H, -CH₂), 2.76-2.73 (t, *J* = 13.2 Hz, 2H, -CH₂), 1.81-1.78 (t, *J* = 13.2Hz, 2H, Ar-CH₂), 1.34 (s, 6H, -(CH₃)₂), 1.25-1.21 (t, *J* = 15.2 Hz, 3H, -CH₃), 1.15 (s, 9H, -(CH₃)₃); ¹³C NMR (400 MHz, CDCl₃) = 178.14,

170.59, 167.0, 159.94, 156.47, 155.94, 136.55, 129.96, 128.64, 128.03, 127.31, 113.78, 109.86, 104.42, 101.53, 75.07, 70.44, 61.88, 50.83, 38.63, 32.76, 29.03, 27.30, 26.80, 21.50, 14.04. MS (ESI): m/z 535 ($M+1$, 100); HRMS: Calcd for: $C_{31}H_{39}N_2O_6$ [$M+H$]: 535.2808; Found: 535.2820.



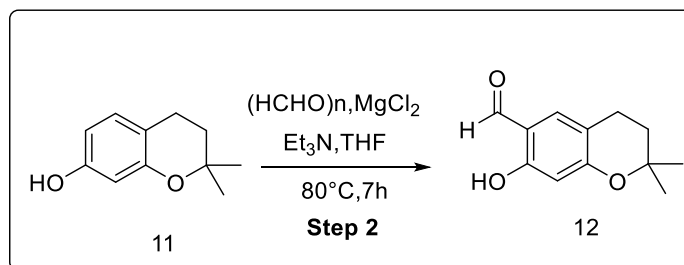
Ethyl 2-acetamido-3-(3-(7-(benzyloxy)-2,2-dimethylchroman-6-yl)isoxazol-5-yl)propanoate (8b):

MR: 111-114⁰C; IR (KBr, cm^{-1}): 3292.6, 3065, 2978.2, 2931.9, 1741.8, 1665.6, 1516.1, 1457.2, 1383.9, 1274, 1119.7, 753.2, 698.2; ¹H NMR (400 MHz, $CDCl_3$): δ = 7.64 (s, 1H, Ar-H), 7.41-7.34 (m, 5H, Ar-H), 6.49 (s, 1H, Ar-H), 6.48 (s, 1H, isoxazole-H), 6.15-6.13 (d, J = 7.6 Hz, 1H, -NH), 5.06-5.05 (s, 2H, Bn- CH_2), 4.87-4.85 (m, 1H, chiral-H), 4.17-4.12 (q, 2H, - OCH_2), 3.33-3.31 (m, 2H, - CH_2), 2.77-2.73 (t, J = 16 Hz, 2H, - CH_2), 1.90 (s, 3H, - $COCH_3$), 1.82-1.79 (t, J = 14 Hz, 2H, Ar- CH_2), 1.34 (s, 6H, - $(CH_3)_2$), 1.24-1.20 (t, J = 14.4 Hz, 3H, - CH_3); ¹³C NMR (100 MHz, $CDCl_3$) = 170.39, 169.75, 166.81, 160.01, 156.49, 155.94, 136.56, 129.98, 128.65, 128.12, 127.48, 113.78, 109.81, 104.39, 101.46, 75.09, 75.50, 62.00, 50.83, 32.74, 29.21, 26.81, 23.00, 21.50, 14.05; MS (ESI): m/z 493 ($M+1$, 100).



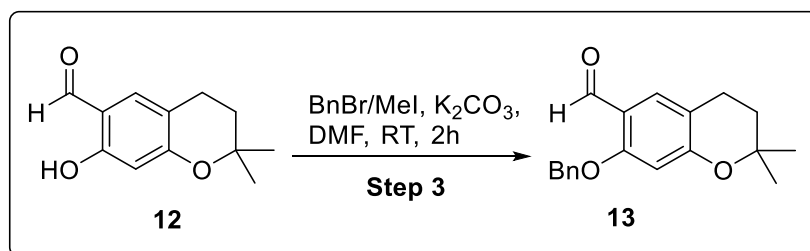
Ethyl 3-(3-(7-(benzyloxy)-2,2-dimethylchroman-6-yl)isoxazol-5-yl)-2-((tert-butoxycarbonyl)amino)propanoate (8c):MR: 149-152⁰C; IR (KBr, cm^{-1}): 3347.6, 2977.2, 2930, 2864.4, 1736.9, 1708, 1600.9, 1519.9, 1457.2, 1384.9, 1290.4, 1220.9, 1167.9, 1116.8, 1060.8, 1019.4, 926.8, 732.9, 696.3; ¹H NMR (400 MHz, $CDCl_3$): δ = 7.64 (s, 1H, Ar-H), 7.40-7.32 (m, 5H, Ar-H), 6.51 (s, 1H, Ar-H), 6.48 (s, 1H, isoxazole-H), 5.22-5.20 (d, J = 8 Hz, 1H, -NH), 5.07 (s, 2H, Bn- CH_2), 4.61-4.59 (m, 1H, chiral-H), 4.15-4.09 (q, 2H, - OCH_2), 3.28-3.27 (d, J = 4.4 Hz, 2H, - CH_2), 2.76-2.73 (t, J = 13.2 Hz, 2H, - CH_2),

1.82-1.79 (t, $J = 13.2$ Hz, 2H, Ar-CH₂), 1.42 (s, 9H, -(CH₃)₃), 1.34 (s, 6H, -(CH₃)₂), 1.22-1.18(t, $J = 14.4$ Hz, 3H, -CH₃); ¹³C NMR (100 MHz, CDCl₃): = 170.67, 166.97, 160.0, 156.44, 155.92, 155.06, 136.58, 130.17, 129.86, 128.78, 128.46, 128.15, 127.83, 127.16, 113.77, 109.98, 104.44, 104.17, 101.68, 101.43, 80.13, 75.06, 70.48. 70.13, 61.78, 52.2, 52.06, 32.76, 29.27, 28.27, 28.21, 26.86, 26.77, 21.72, 21.51, 14.12. 13.98; MS (ESI): m/z 551 (M+1, 100).



Experimental procedure for the preparation of (7-hydroxy-2, 2-dimethylchromane-6-carbaldehyde)

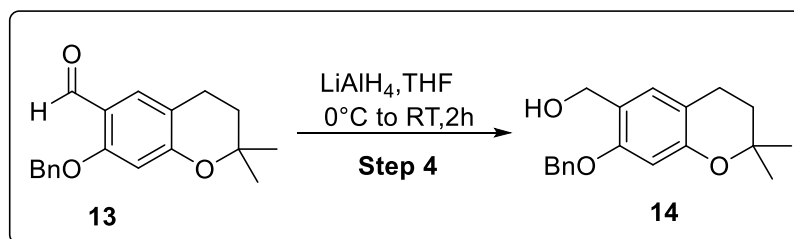
(12): To a stirred solution of compound **11** (1g, 5.617 mmol) in THF (30 ml), were added MgCl₂ (802 mg, 8.425 mmol) and triethylamine (2.892 ml, 20.782 mmol) at RT and stirred for 20 min. Then was added Para formaldehyde (3.145g, 37.92 mmol) and stirred for 1 h at RT followed by reflux for 7 h. The reaction was monitored by TLC analysis (10% ethyl acetate/pet ether). After completion of the reaction, THF was evaporated under reduced pressure and the reaction mixture was diluted with Ethyl acetate (100 ml) and passed through celite bed. Bed was washed with ethyl acetate (100 ml). Combined RM was washed with water (100 ml) and brine solution. Organic layer was dried over anhydrous Na₂SO₄ and concentrated under reduced pressure to give the crude residue which was charged on silica gel column. The column was eluted with 5% ethyl acetate/pet ether to give the compound **12** (810 mg, 70% yield). ¹H NMR (400 MHz, CDCl₃): δ 11.07 (s, 1H, -CHO), 9.66 (s, 1H, -OH), 7.21 (s, 1H, Ar-H), 6.31 (s, 1H, Ar-H), 2.77-2.73 (t, $J = 13.2$ Hz, 2H, -CH₂), 1.84-1.81 (t, $J = 13.2$ Hz, 2H, Ar-CH₂), 1.36 (s, 6H, -(CH₃)₂); MS (ESI): m/z 207 (M+1,100).



Experimental procedure for the preparation of 7-(benzyloxy)-2, 2-dimethylchromane-6-carbaldehyde (13):

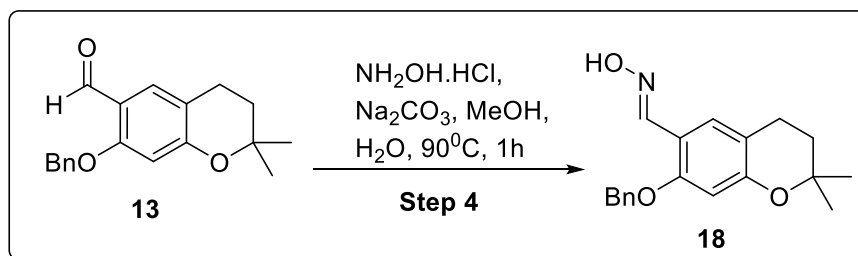
To a stirred solution of compound **12** (400 mg, 1.951 mmol) in DMF (5 ml), were added K₂CO₃ (538 mg, 3.902 mmol) and Benzyl bromide (0.243 ml, 2.048mmol), stirred for 2 h at RT. The reaction was monitored by TLC analysis (10% ethyl acetate/pet ether). After completion of

the reaction, the reaction mixture was diluted with Ethyl acetate (100 ml) and washed with water (100 ml) and brine solution. Organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to give the crude residue which was charged on silica gel column. The column was eluted with 8% ethyl acetate/pet ether to give the compound **13** (550 mg, 95% yield).: $^1\text{H NMR}$ (400 MHz, CDCl_3): δ 10.36 (s, 1H, -CHO), 7.62 (s, 1H, Ar-H), 7.44-7.34 (m, 5H, Ar-H), 6.42 (s, 1H, Ar-H), 5.10 (s, 2H, $-\text{OCH}_2$), 2.76-2.72 (t, $J = 13.6$ Hz, 2H, $-\text{CH}_2$), 1.83-1.79 (t, $J = 13.6$ Hz, 2H, Ar- CH_2), 1.35 (s, 6H, $-(\text{CH}_3)_2$); MS (ESI): m/z 297 ($\text{M}+1$, 100).



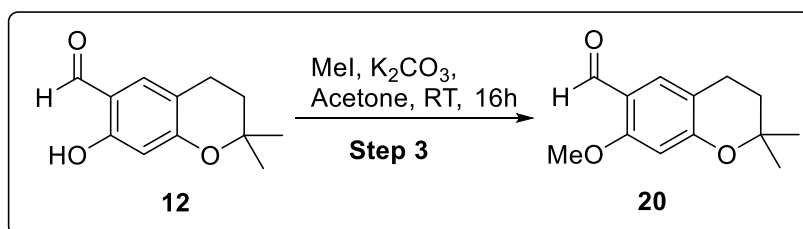
Experimental procedure for the preparation of (7-(benzyloxy)-2,2-dimethylchroman-6-yl)methanol (14): To a stirred solution of compound **13** (500mg, 1.689 mmol) in THF (10 ml) was added LAH (128.3 mg, 3.378 mmol (1M in THF)) at 0°C and stirred for 2 h at RT. The progress of the reaction was monitored by TLC analysis (10% ethyl acetate/pet ether). After completion of the reaction, the reaction mixture was diluted with ethyl acetate (100 ml) and washed with water and brine solution. Organic layer was dried over anhydrous Na_2SO_4 and concentrated under reduced pressure to give the crude residue which was charged on silica gel column. The column was eluted with 15% ethyl acetate/pet ether to give the compound **14** (420 mg, 83% yield) as off white solid.

$^1\text{H NMR}$ (400 MHz, CDCl_3): δ 7.40-7.33 (m, $J = 29.6$ Hz, 5H, Ar-H), 6.96 (s, 1H, Ar-H), 6.43 (s, 1H, Ar-H), 5.03 (s, 2H, $-\text{OCH}_2$), 4.63-4.62 (d, $J = 5.6$ Hz, 2H, $-\text{OCH}_2$), 2.71-2.68 (t, $J = 13.2$ Hz, 2H, $-\text{CH}_2$), 2.15 (bs, 1H, $-\text{OH}$), 1.79-1.76 (t, $J = 13.6$ Hz, 2H, Ar- CH_2), 1.32 (s, 6H, $-(\text{CH}_3)_2$); MS (APCI): m/z 280 ($[\text{M}-\text{OH}]^+$, 100).



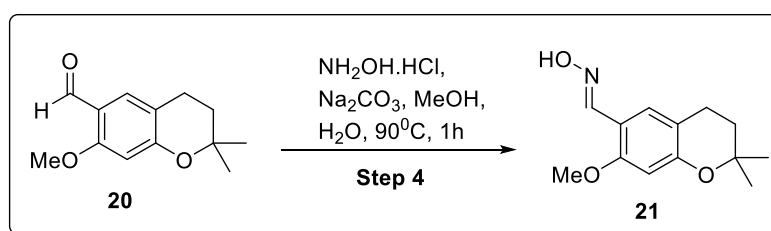
Experimental procedure for the preparation of (E)-7-(benzyloxy)-2,2-dimethylchroman-6-carbaldehyde oxime (18): To a stirred solution of compound **13** (400mg, 1.35 mmol) in Methanol: water (16:4 ml) were added $\text{NH}_2\text{OH}\cdot\text{HCl}$ (111.8 mg, 1.62 mmol), and Na_2CO_3 (171 mg, 1.62mmol) and heated at 90°C for 1 h. The progress of the reaction was monitored by TLC analysis (20% ethyl

acetate/pet ether). After completion of the reaction, the reaction mixture was concentrated under reduced pressure. Water was added to reaction mixture, white solid was precipitated. Filtered the precipitate and dried under vacuum to give the compound **18** (300 mg, 71% yield) as off white solid.; ¹H NMR (400 MHz, CDCl₃): δ = 8.48 (s, 1H, -N=CH), 7.48 (s, 1H, Ar-H), 7.40-7.32 (m, 5H, Ar-H), 7.03 (s, 1H, -OH), 6.41 (s, 1H, Ar-H), 5.01 (s, 2H, Bn-CH₂), 2.73-2.70 (t, *J* = 10.8 Hz, 2H, -CH₂), 1.80-1.77 (t, *J* = 13.2 Hz, 2H, Ar-CH₂), 1.33 (s, 6H, -(CH₃)₂). MS (ESI): *m/z* 312 (M+1, 100).



Experimental procedure for the preparation of 7-hydroxy-2, 2-dimethylchromane-6-carbaldehyde (20): To a stirred solution of compound **12** (2.5 g, 12.135 mmol) in Acetone (25 ml) were added K₂CO₃ (5.02 g, 36.20 mmol) and CH₃I (1.87 ml, 29.12 mmol) at 0°C and stirred at RT for 16 h. The progress of the reaction was monitored by TLC analysis (10% ethyl acetate/pet ether). After completion of the reaction, the reaction mixture was diluted with ethyl acetate (250 ml) and washed with water and brine solution. Organic layer was dried over anhydrous Na₂SO₄ and concentrated under reduced pressure to give the crude residue which was charged on silica gel column. The column was eluted with 5% ethyl acetate/pet ether to give the compound **20** (2.4 g, 90% yield).

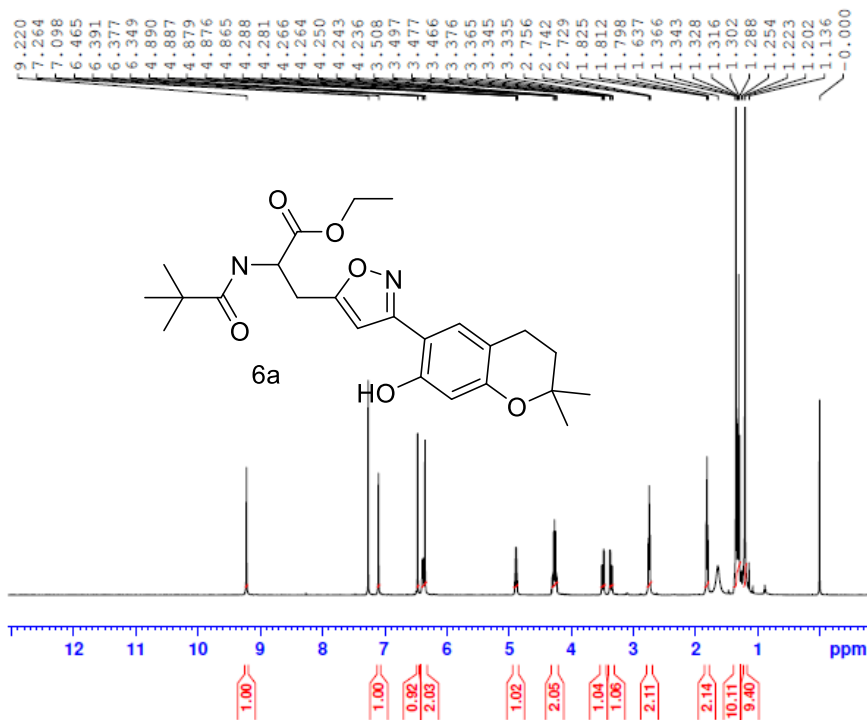
¹H NMR (400 MHz, CDCl₃): δ = 10.26 (s, 1H, -CHO), 7.59 (s, 1H, Ar-H), 6.34 (s, 1H, Ar-H), 3.84 (s, 3H, -OCH₃), 2.75-2.72 (t, *J* = 13.2 Hz, 2H, -CH₂), 1.83-1.79 (t, *J* = 14 Hz, 2H, Ar-CH₂), 1.35 (s, 6H, -(CH₃)₂); MS (ESI): *m/z* 221 (M+1, 100).



Experimental procedure for the preparation of (E)-7-methoxy-2, 2-dimethylchromane-6-carbaldehyde oxime (21): To a stirred solution of compound **20** (2.2g, 10 mmol) in Methanol and water (20:5 ml) were added NH₂OH.HCl (820.5 mg, 11.891 mmol) and Na₂CO₃ (1.26 g, 11.891mmol) and heated at 90°C for 1 h. The progress of the reaction was monitored by TLC analysis (20% ethyl acetate/pet ether). The reaction mixture was concentrated under reduced pressure. Water was added to reaction the mixture, white solid was precipitated. Filtered the precipitate and dried under vacuum to give the compound **21** (2g, 85% yield) as off white solid.; ¹H NMR (400 MHz, CDCl₃): δ = 8.38 (s,

1H, -N=CH), 7.80 (bs, 1H, -OH), 7.38 (s, 1H, Ar-H), 6.33 (s, 1H, Ar-H), 3.78 (s, 3H, -OCH₃), 2.72-2.69 (t, *J* = 13.2 Hz, 2H, -CH₂), 1.80-1.77 (t, *J* = 13.2 Hz, 2H, Ar-CH₂), 1.34 (s, 6H, -(CH₃)₂); MS (ESI): *m/z* 236 (*M*+1, 100).

GVK-RAG-1-51

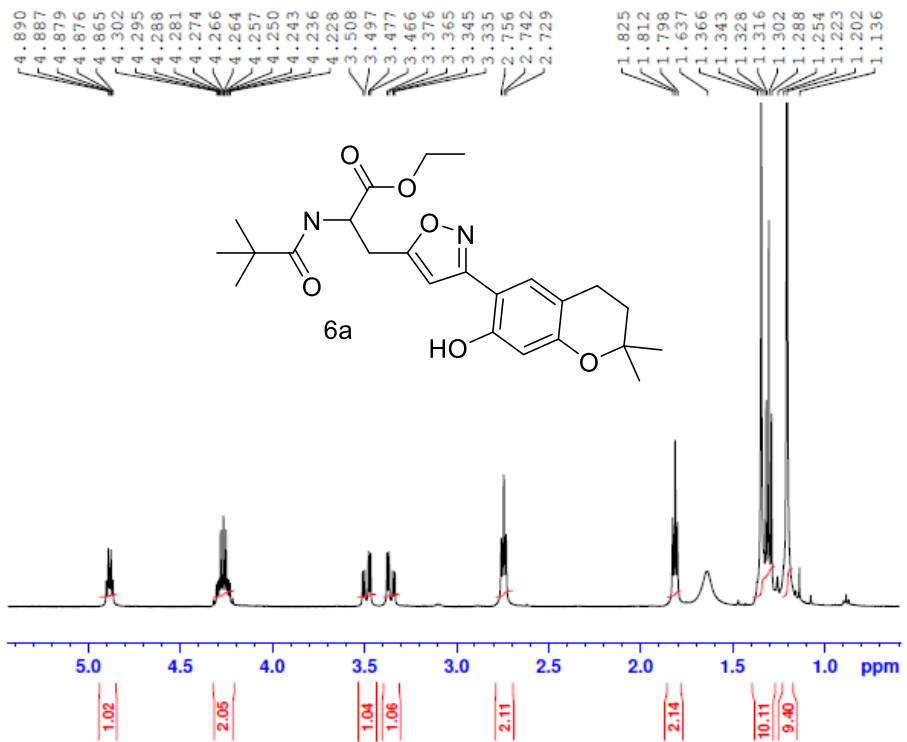


Current Data Parameters
 NAME 51805A6233
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180607
 Time 21.28 h
 INSTRUM spect
 PROBHD Z119470_0294 (zg30)
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 111.07
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TDO 1
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 10.00 usec
 PIW1 20.38699913 W

F2 - Processing parameters
 SI 65536
 SF 500.1300100 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

GVK-RAG-1-51

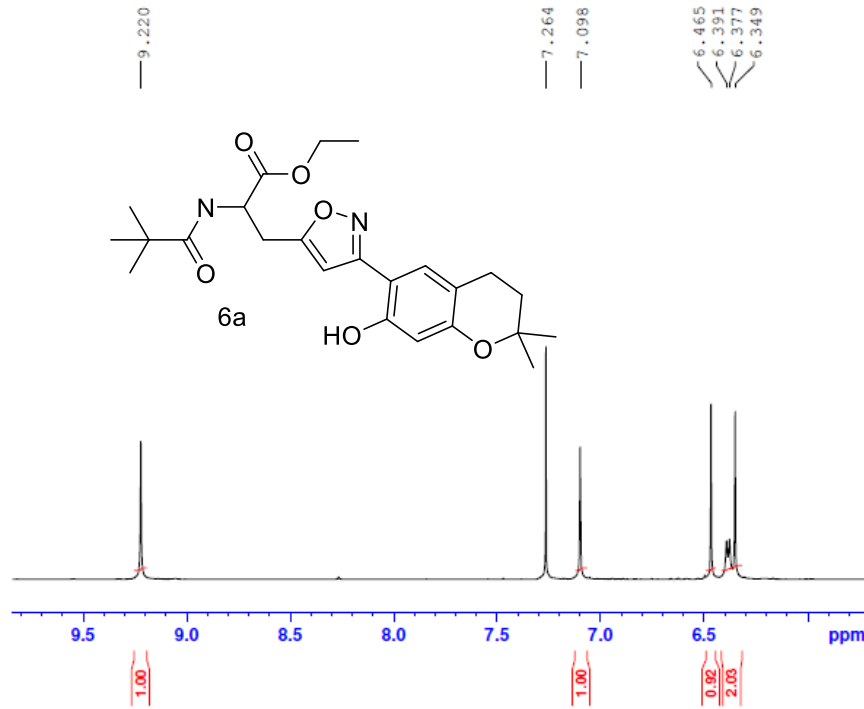


Current Data Parameters
 NAME 51805A6233
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20180607
 Time 21.28 h
 INSTRUM spect
 PROBHD Z119470_0294 (zg30)
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 10000.000 Hz
 FIDRES 0.152588 Hz
 AQ 3.2767999 sec
 RG 111.07
 DW 50.000 usec
 DE 6.50 usec
 TE 298.2 K
 D1 1.00000000 sec
 TDO 1
 SFO1 500.1330885 MHz
 NUC1 1H
 P1 10.00 usec
 PIW1 20.38699913 W

F2 - Processing parameters
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 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

GVK-RAG-1-51



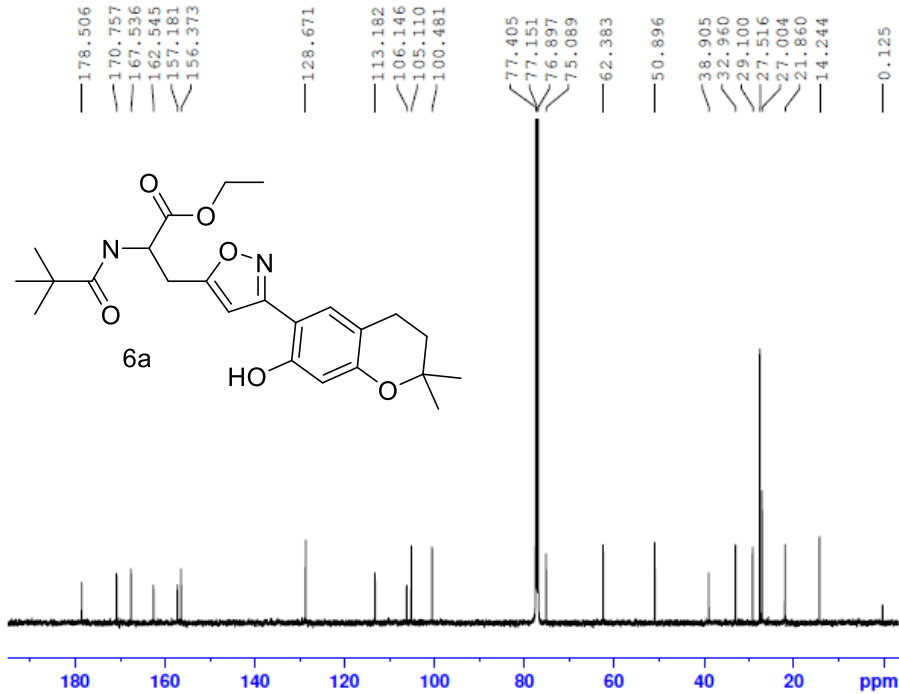
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Current Data Parameters
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EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
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INSTRUM  spect
PROBHD   Z119470_0294 (
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        8
DS        10000.000 Hz
SWH       0.152588 Hz
FIDRES    3.2767999 sec
AQ         111.07
RG         50.000 usec
DE         6.50 usec
TE         298.2 K
D1         1.00000000 sec
D11        1
SFO1      500.1330885 MHz
NUC1       1H
P1         10.00 usec
PIW1      20.38699913 W

F2 - Processing parameters
SI         65536
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WVW        EM
SSB         0
LB          0.30 Hz
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PC          1.00
    
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GVK-RAG-1-51



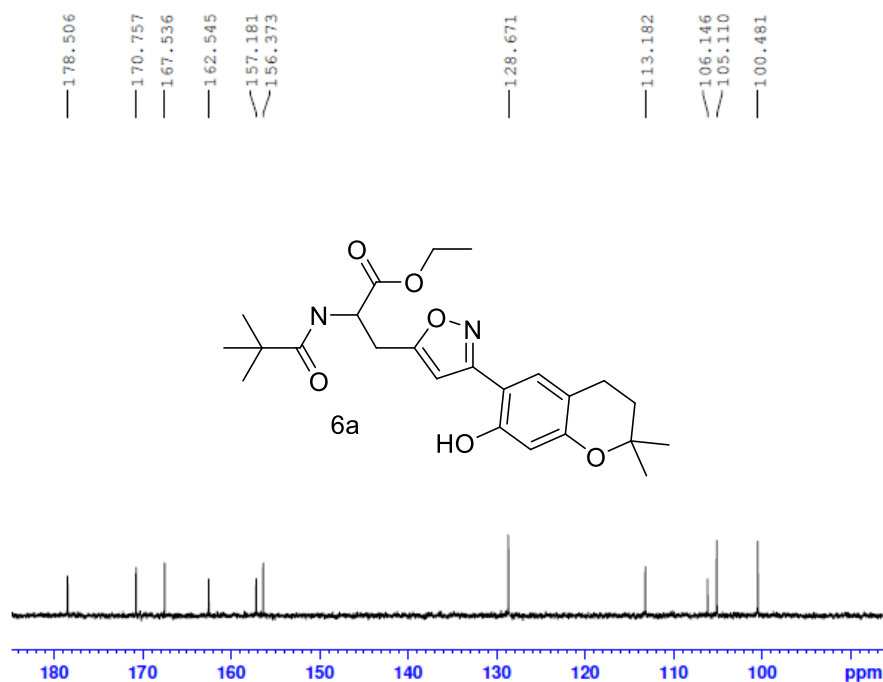
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Current Data Parameters
NAME      511806A6233
EXPNO    2
PROCNO   1

F2 - Acquisition Parameters
Date_    20180607
Time     22.48 h
INSTRUM  spect
PROBHD   Z119470_0294 (
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        1024
DS        4
SWH       29761.904 Hz
FIDRES    0.454131 Hz
AQ         1.1010048 sec
RG         197.72
DE         16.800 usec
TE         298.2 K
D1         3.00000000 sec
D11        0.03000000 sec
D12        1
SFO1      125.7703643 MHz
NUC1       13C
P1         10.00 usec
PIW1      79.88800049 W
SFO2      500.1320005 MHz
NUC2       1H
CPDPRG2  waltz16
PCPD2     90.00 usec
PIW2      20.38699913 W
PIW12     0.25169000 W
PIW13     0.16023000 W

F2 - Processing parameters
SI         32768
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WVW        EM
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GVK-RAG-1-51



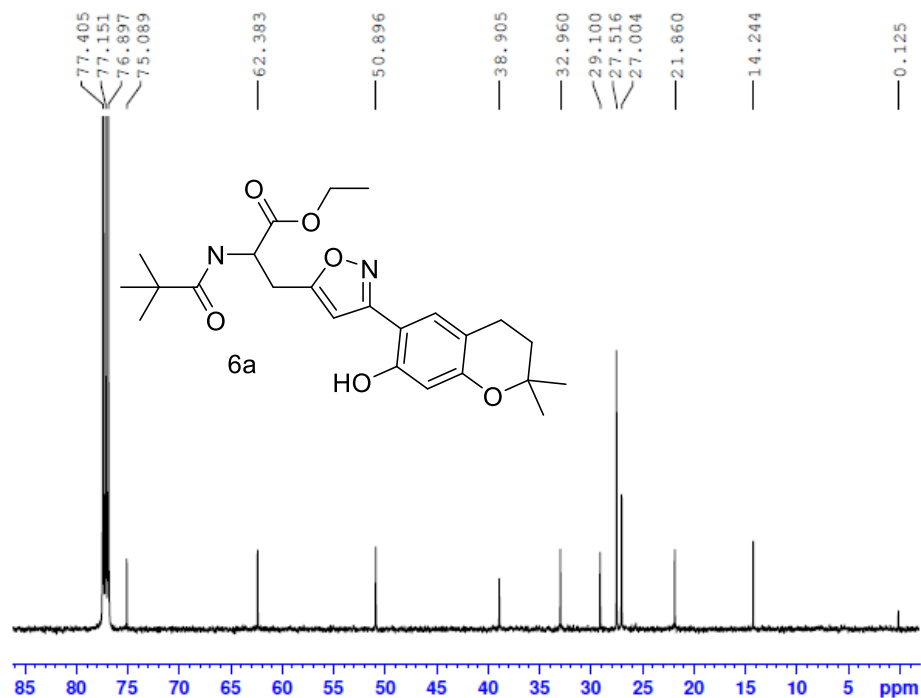
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Current Data Parameters
NAME      511806A6233
EXPNO    2
PROCNO   1

F2 - Acquisition Parameters
Date_    20180607
Time     22.48 h
INSTRUM  spect
PROBHD   Z119470_0294 (
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        1024
DS        4
SWH       29761.904 Hz
FIDRES    0.454131 Hz
AQ        1.1010048 sec
RG        197.72
DW        16.800 usec
DE        6.50 usec
TE        298.2 K
D1        3.0000000 sec
D11       0.0300000 sec
TDO       1
SF01      125.7703643 MHz
NUC1      13C
P1        10.00 usec
PIW1      79.8880049 W
SF02      500.1320005 MHz
NUC2      1H
CPDPRG2   waltz16
PCPD2     90.00 usec
PIW2      20.3869913 W
PIW12     0.25169000 W
PIW13     0.16023000 W

F2 - Processing parameters
SI         32768
SF         125.7577726 MHz
WVW        EM
SSB        0
LB         2.00 Hz
GB         0
PC         1.40
    
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GVK-RAG-1-51

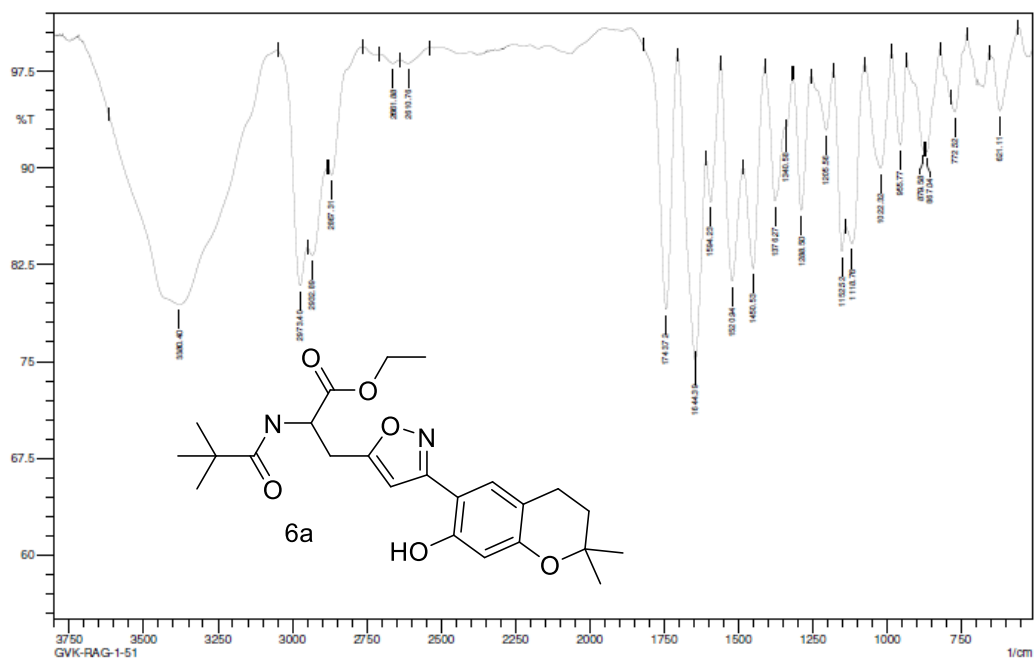


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Current Data Parameters
NAME      511806A6233
EXPNO    2
PROCNO   1

F2 - Acquisition Parameters
Date_    20180607
Time     22.48 h
INSTRUM  spect
PROBHD   Z119470_0294 (
PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        1024
DS        4
SWH       29761.904 Hz
FIDRES    0.454131 Hz
AQ        1.1010048 sec
RG        197.72
DW        16.800 usec
DE        6.50 usec
TE        298.2 K
D1        3.0000000 sec
D11       0.0300000 sec
TDO       1
SF01      125.7703643 MHz
NUC1      13C
P1        10.00 usec
PIW1      79.8880049 W
SF02      500.1320005 MHz
NUC2      1H
CPDPRG2   waltz16
PCPD2     90.00 usec
PIW2      20.3869913 W
PIW12     0.25169000 W
PIW13     0.16023000 W

F2 - Processing parameters
SI         32768
SF         125.7577726 MHz
WVW        EM
SSB        0
LB         2.00 Hz
GB         0
PC         1.40
    
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Comment: IN Kbr
GVK-RAG-1-51

No. of Scans:
Resolution:
Apodization:

Date: 6/8/2018 12:57:05 PM
User: Admin

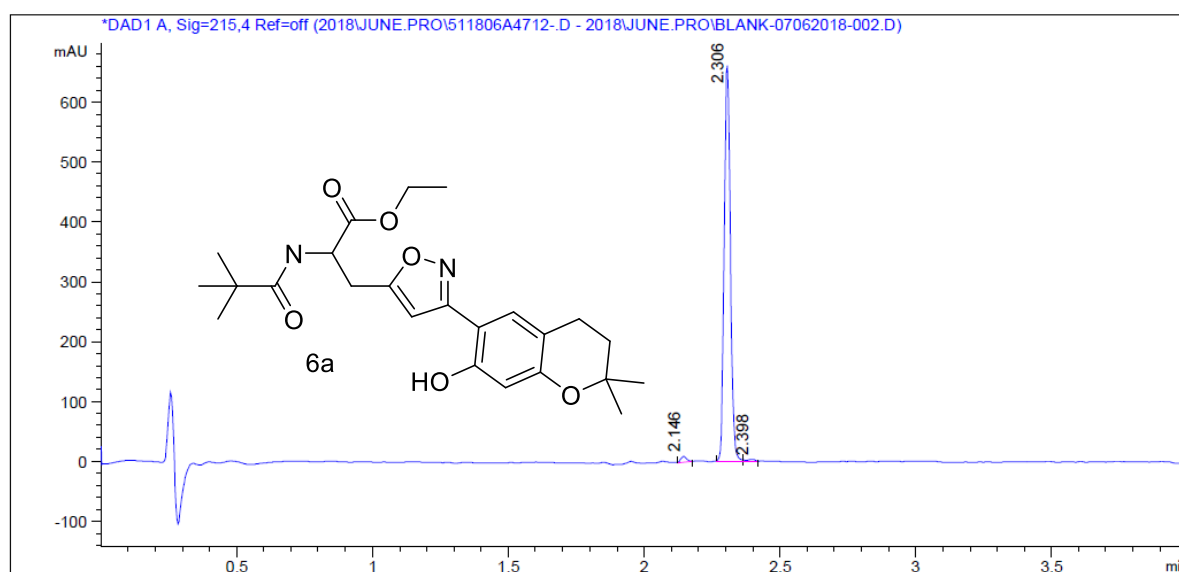
GVK BIOSCIENCES PVT. LTD.
 MEDICINAL CHEMISTRY LABORATORY - ANALYTICAL RESEARCH
 LCMS REPORT

```

=====
Date of Analysis : 6/7/2018           7:09:28 PM           Vial position : P1-B-05
Acq. Method      : RND-FA-4.01 MIN      Injection Vol  : 1.000µl
Sample Name      : GVK-RAG-1-51         Instrument ID  : ANL-MCL5-LCMS-001
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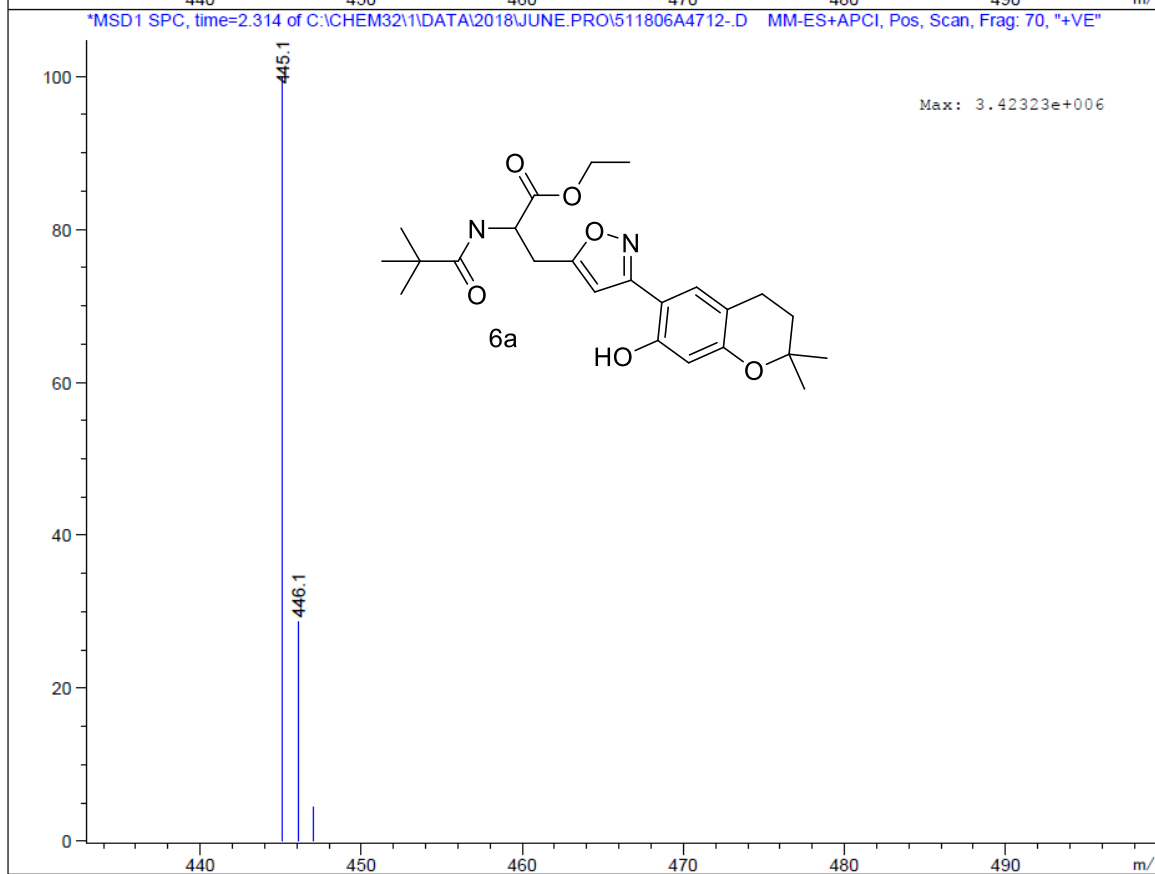
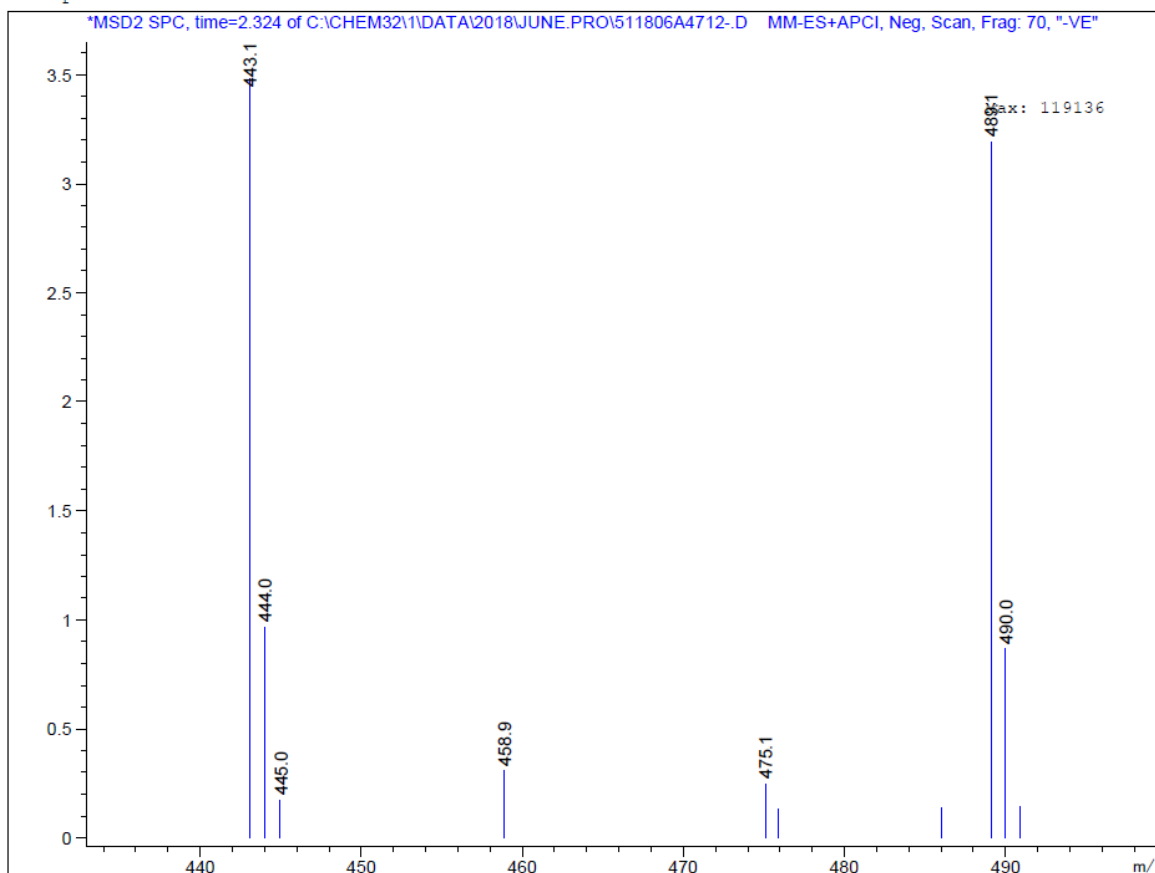
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RND-FA 4.01 MIN.M
Column          : ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7µm)
Mobile Phase    : B1: 0.1 % FA IN WATER A1: 0.1%FA IN ACN
Gradient        : Time (min) /%B1: 0/3, 0.3/3, 2.3/98,3.5/98,4/3,4.01/3
Column Flow     : 0.6 ml/min
Column Temp     : 50°C
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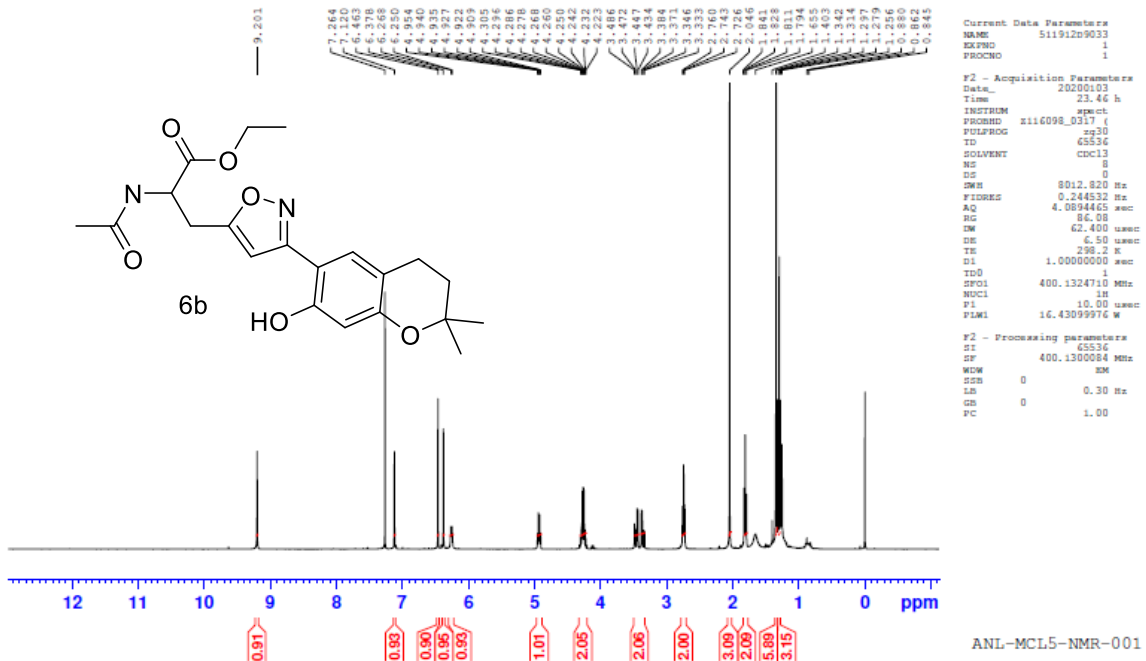
DAD1 A, Sig=215,4 Ref=off

Peak No	RT min	Height	Area	Area %
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2	2.31	666.513	1056.928	97.900
3	2.40	3.570	7.768	0.720

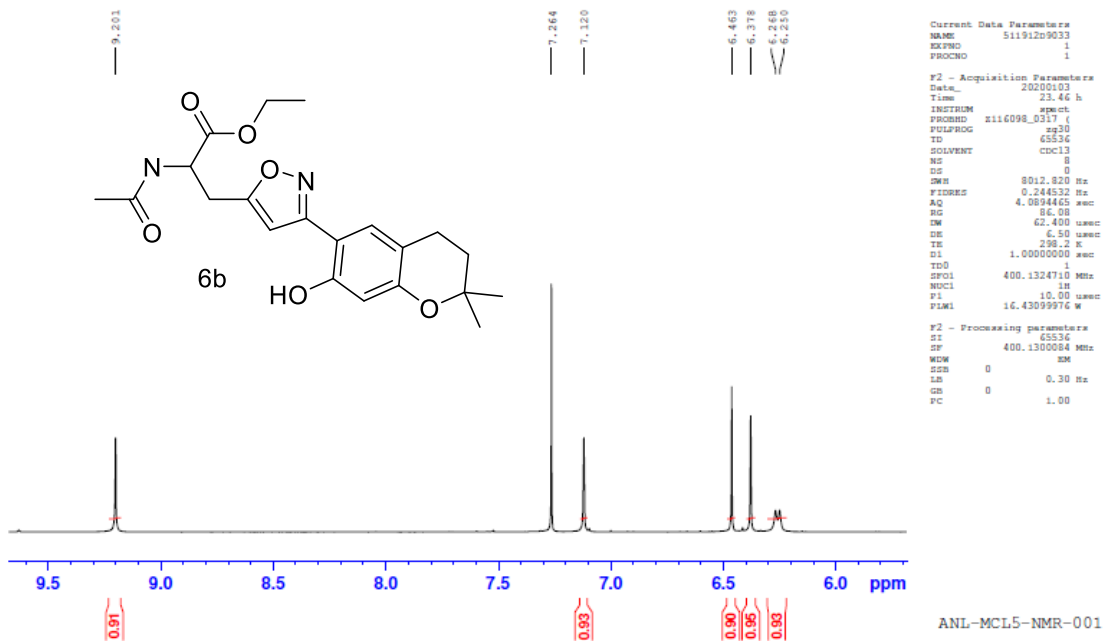
MS Spectrum



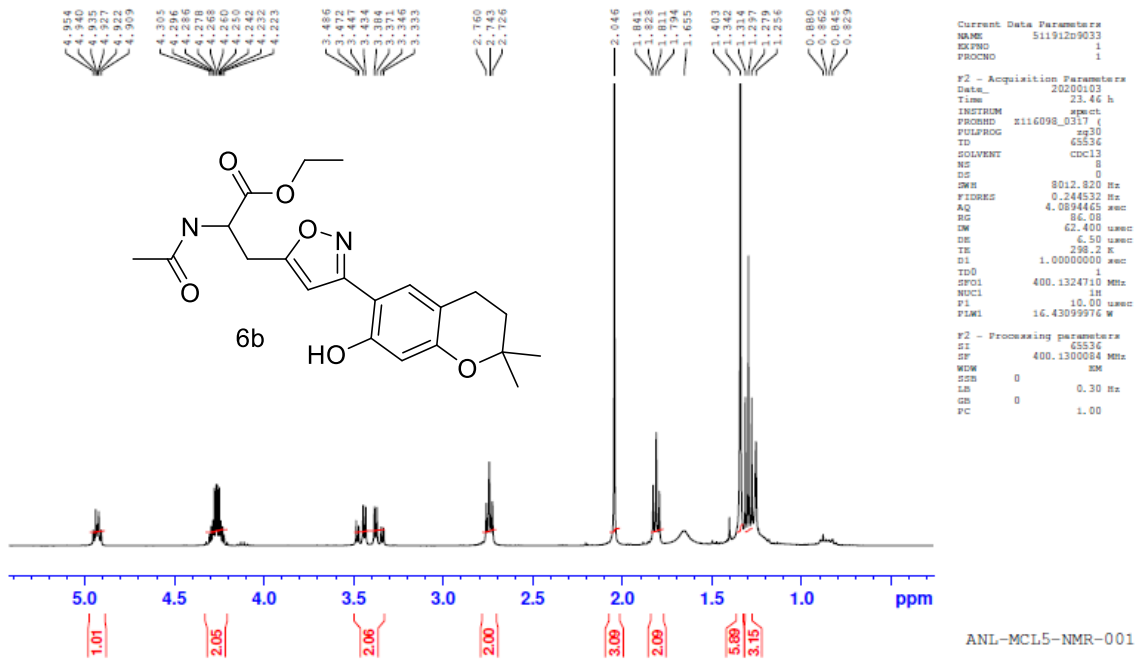
GVK-RAG-2-56



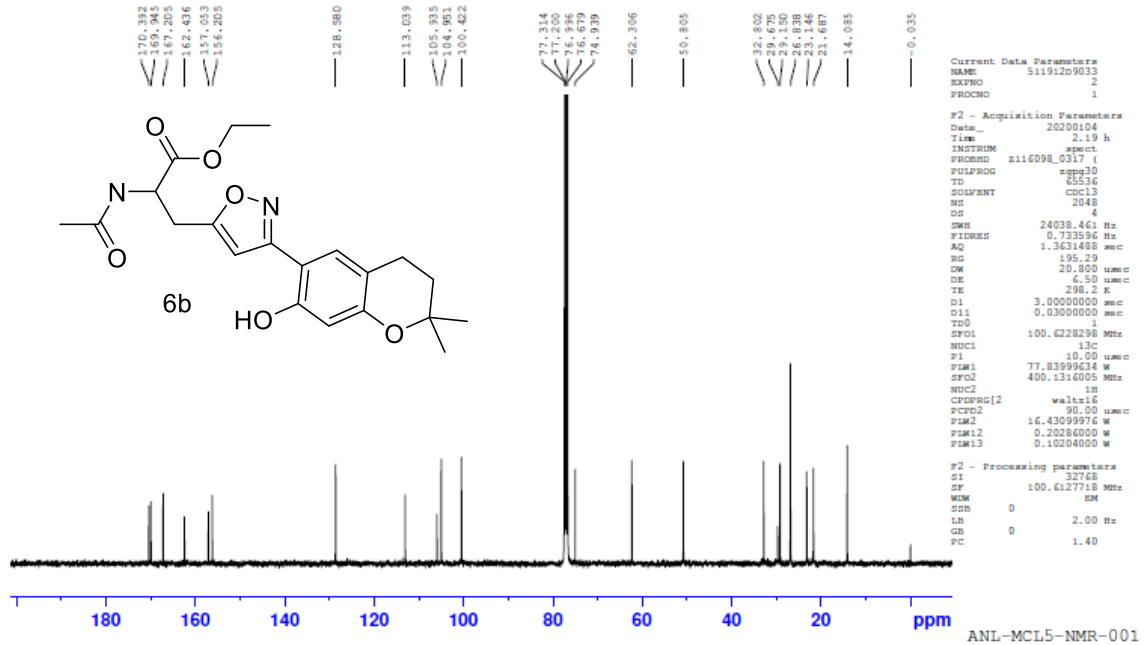
GVK-RAG-2-56



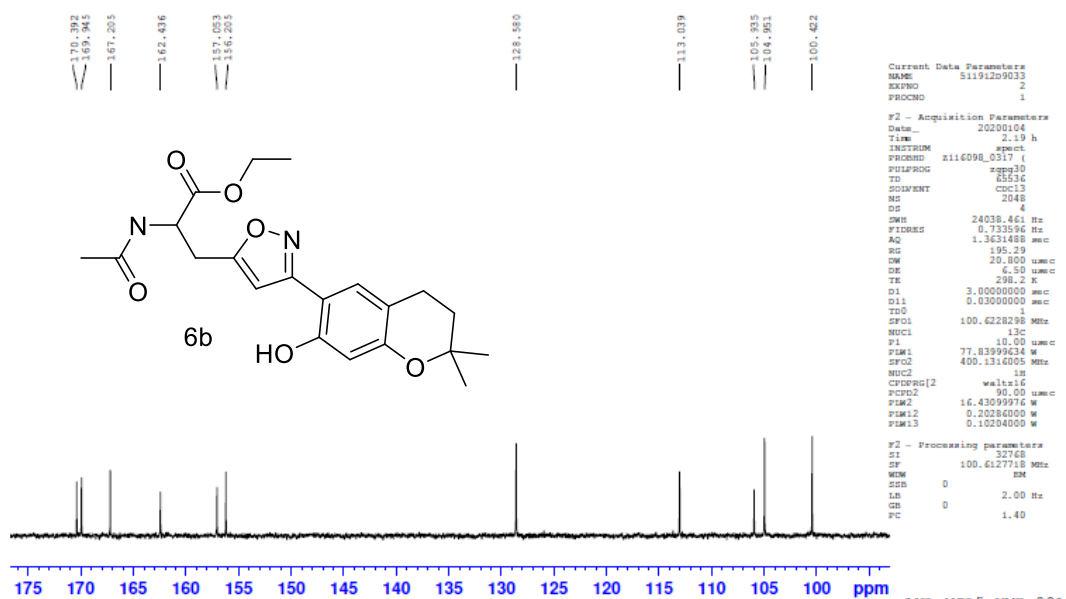
GVK-RAG-2-56



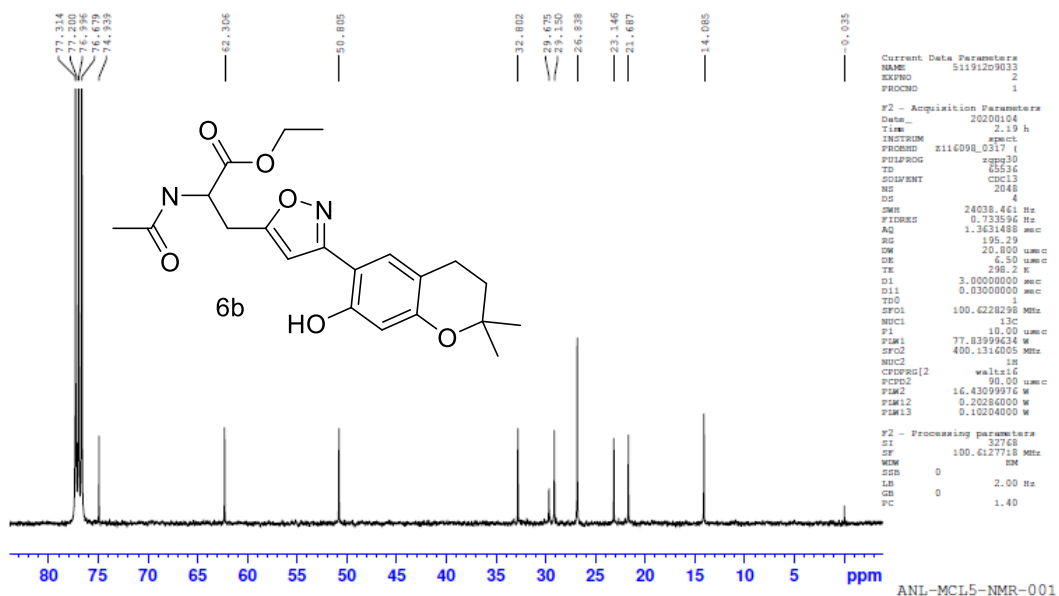
GVK-RAG-2-56



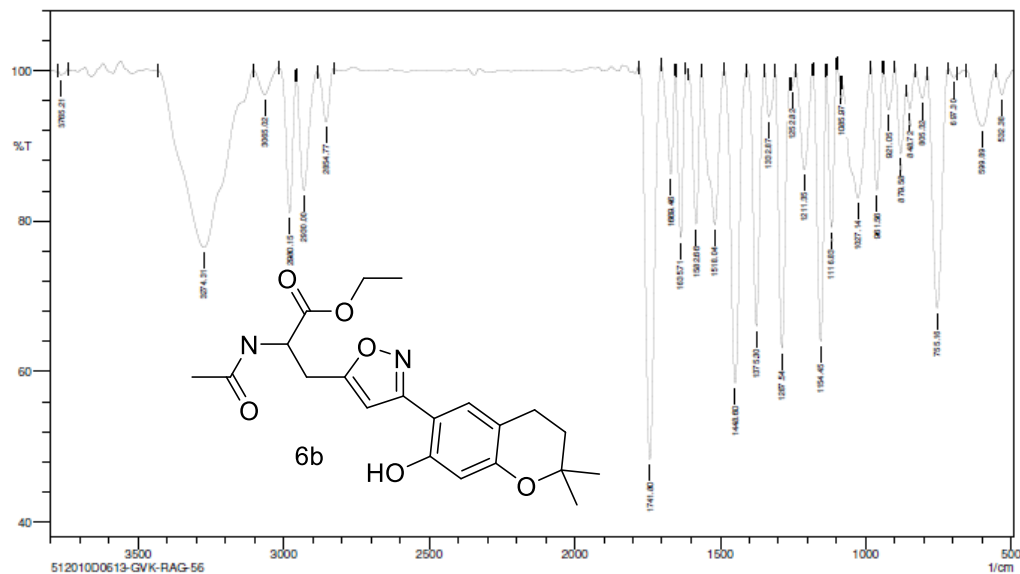
GVK-RAG-2-56



GVK-RAG-2-56



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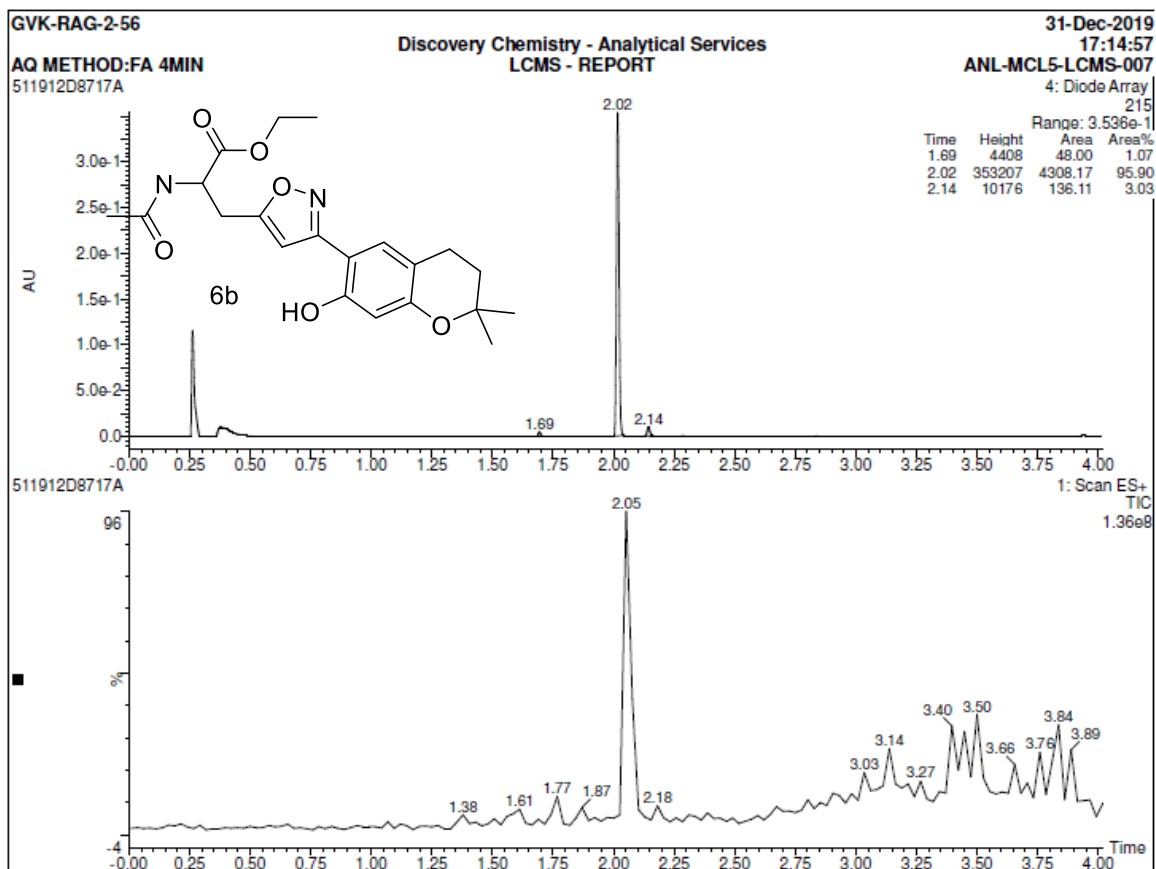


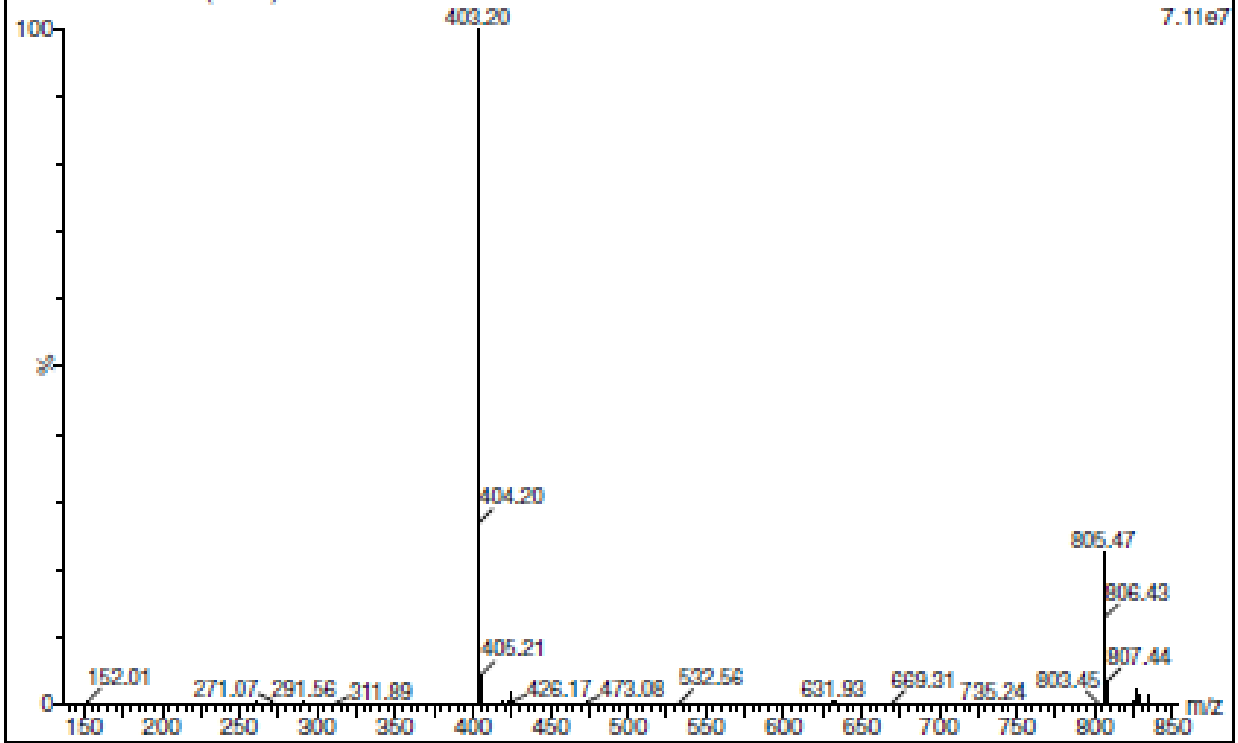
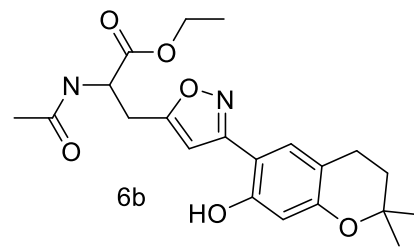
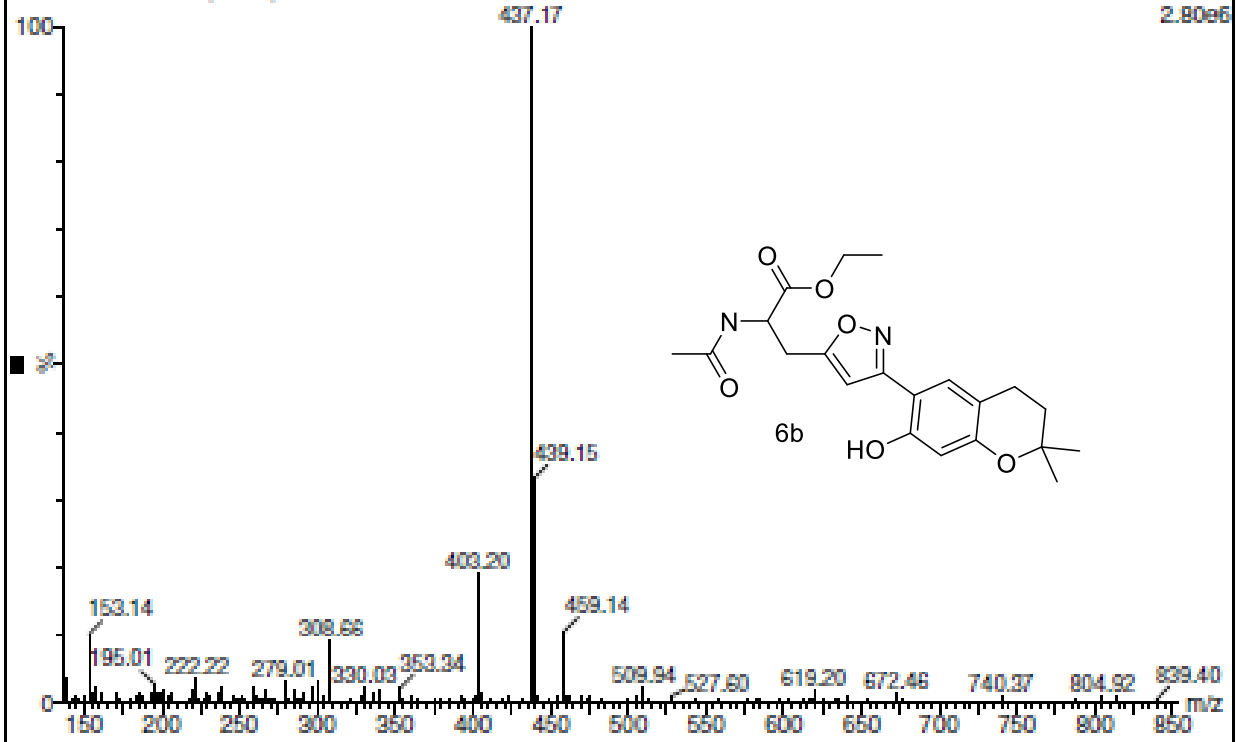
Sample Name:
512010D0613-GVK-RAG-56

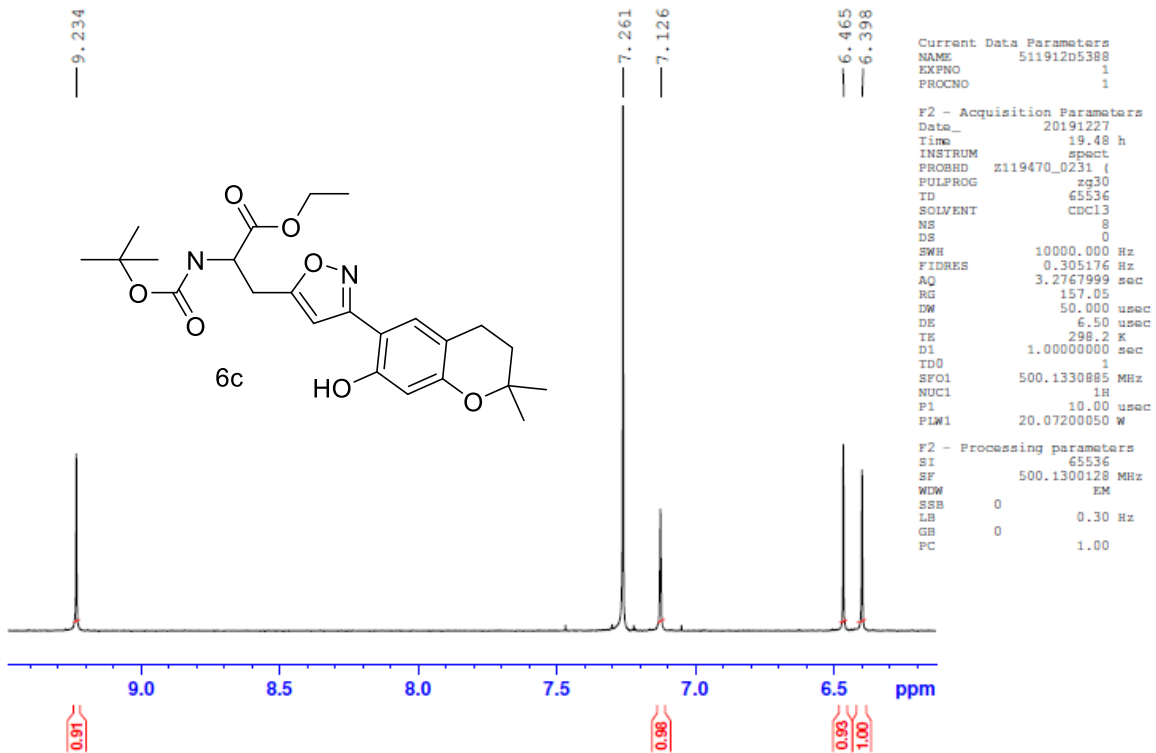
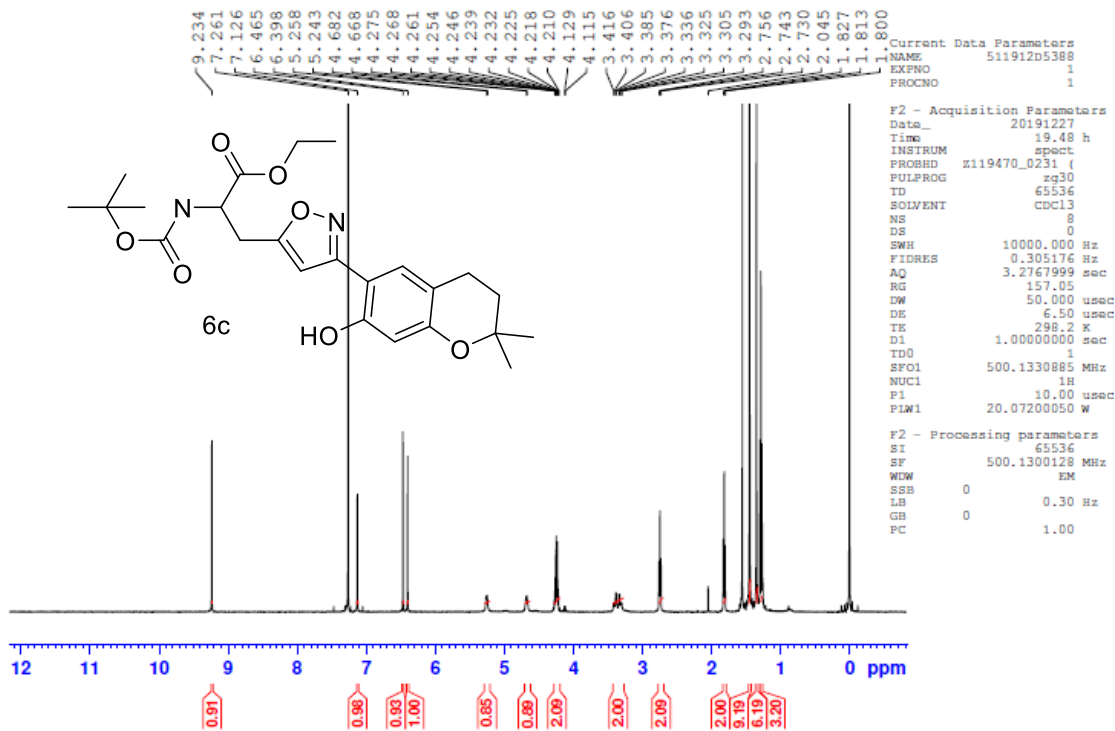
No. of Scans:

Date/Time: 10/31/2020 2:41:49 PM

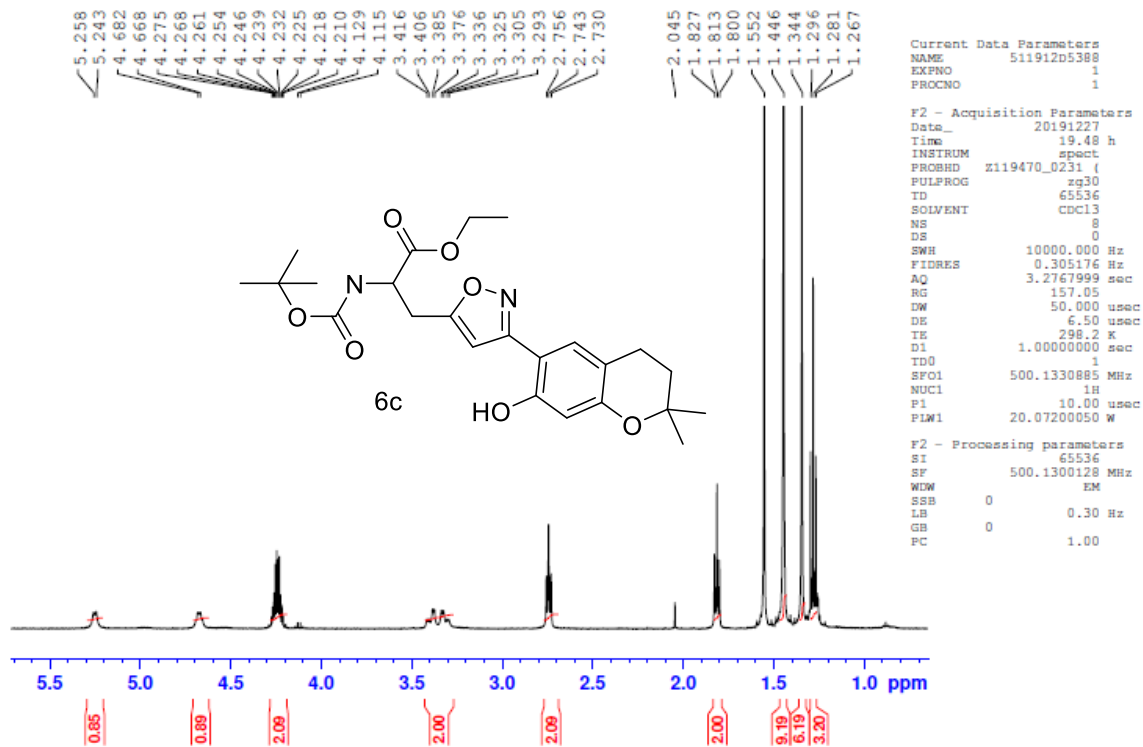
User: GVKBIO



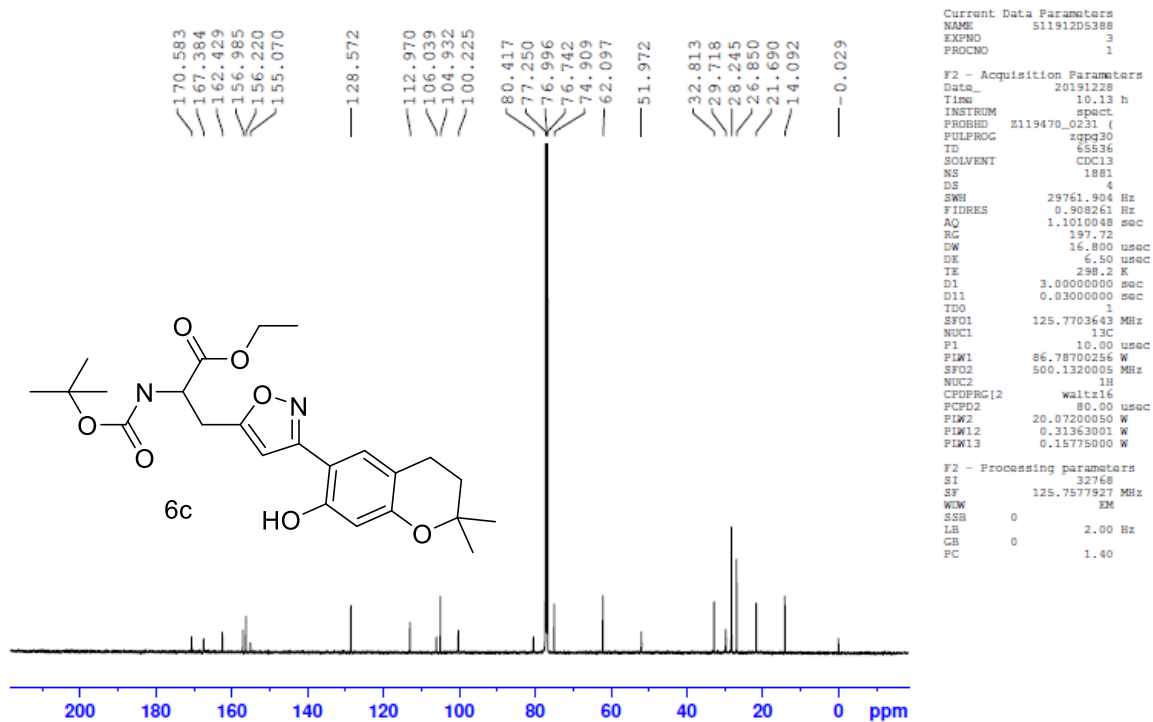




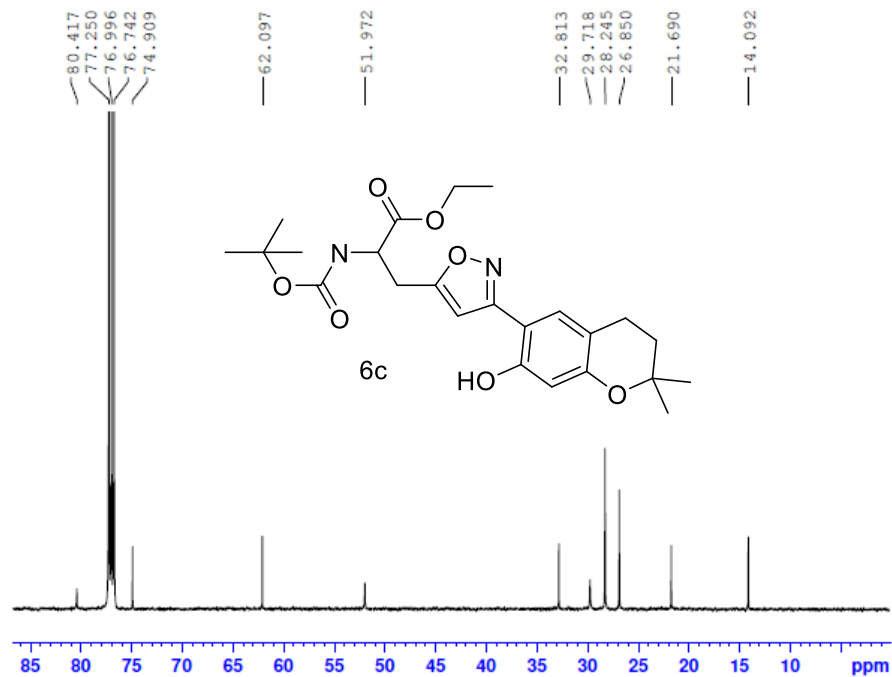
GVK-RAG-2-53



GVK-RAG-2-53



GVK-RAG-2-53



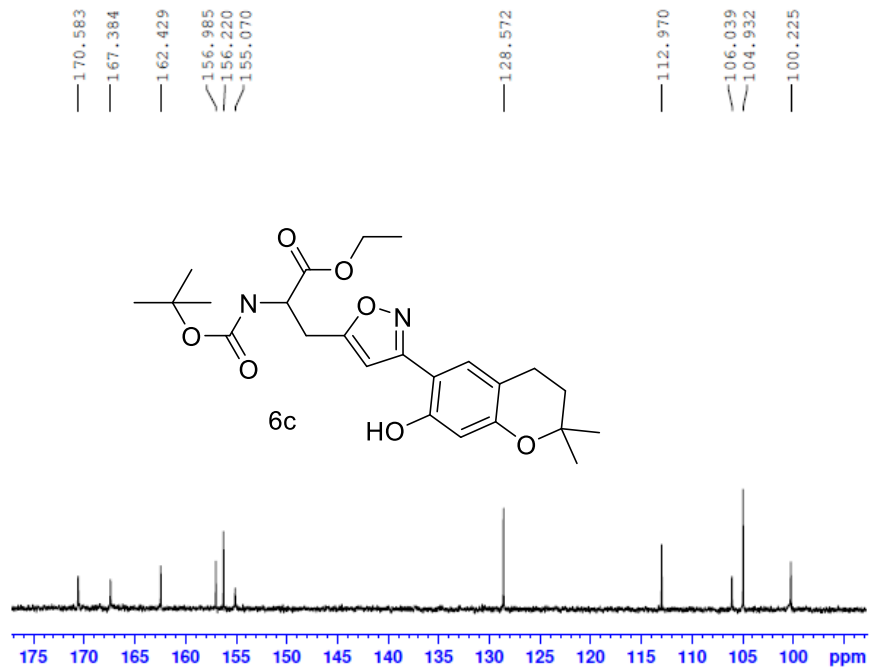
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EXPNO    3
PROCNO   1

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Time     10.13 h
INSTRUM spect
PROBHD   Z119470_0231 (
PULPROG zgpg30
TD       65536
SOLVENT  CDCl3
NS       1881
DS       4
SWH      29761.904 Hz
FIDRES   0.908261 Hz
AQ       1.1010048 sec
RG       197.72
DW       16.800 usec
DE       6.50 usec
TE       298.2 K
D1       3.0000000 sec
D11      0.0300000 sec
TD0      1
SF01     125.7703643 MHz
NUC1     13C
P1       10.00 usec
PLW1     86.78700256 W
SF02     500.1320005 MHz
NUC2     1H
CPDPRG2 waltz16
PCPD2    80.00 usec
PLW2     20.07200050 W
PLW12    0.31363001 W
PLW13    0.15775000 W

F2 - Processing parameters
SI       32768
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WVW      EM
SSB      0
LB       2.00 Hz
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PC       1.40
    
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GVK-RAG-2-53



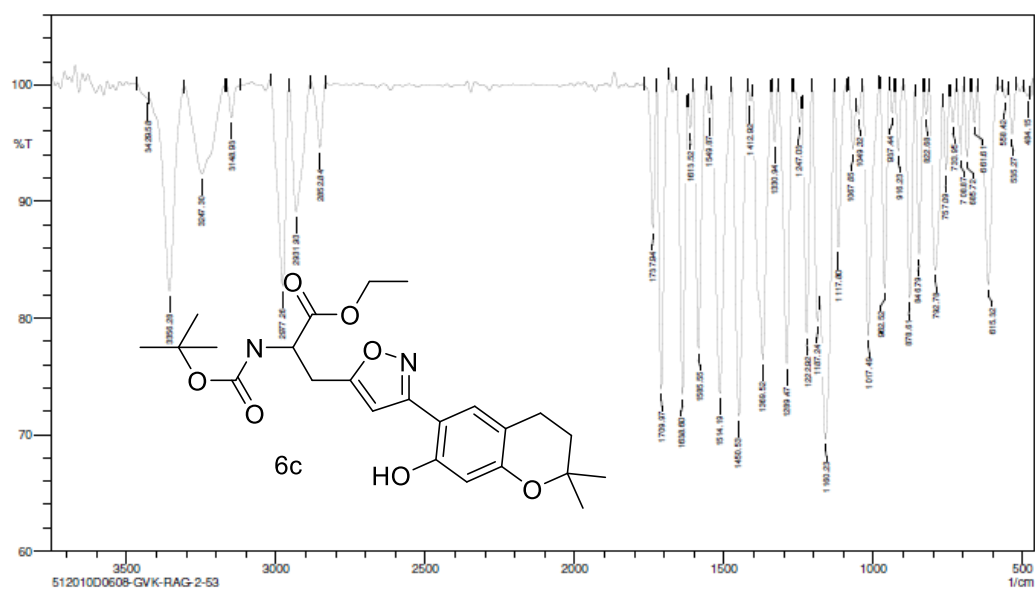
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Current Data Parameters
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EXPNO    3
PROCNO   1

F2 - Acquisition Parameters
Date_    20191228
Time     10.13 h
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PULPROG zgpg30
TD       65536
SOLVENT  CDCl3
NS       1881
DS       4
SWH      29761.904 Hz
FIDRES   0.908261 Hz
AQ       1.1010048 sec
RG       197.72
DW       16.800 usec
DE       6.50 usec
TE       298.2 K
D1       3.0000000 sec
D11      0.0300000 sec
TD0      1
SF01     125.7703643 MHz
NUC1     13C
P1       10.00 usec
PLW1     86.78700256 W
SF02     500.1320005 MHz
NUC2     1H
CPDPRG2 waltz16
PCPD2    80.00 usec
PLW2     20.07200050 W
PLW12    0.31363001 W
PLW13    0.15775000 W

F2 - Processing parameters
SI       32768
SF       125.7577927 MHz
WVW      EM
SSB      0
LB       2.00 Hz
GB       0
PC       1.40
    
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Sample Name:
512010D0608-GVK-RAG-2-53

No. of Scans:

Date/Time: 10/31/2020 12:29:26 PM

User: GVKBIO

GVK-RAG-2-53

Discovery Chemistry - Analytical Services
LCMS - REPORT

27-Dec-2019

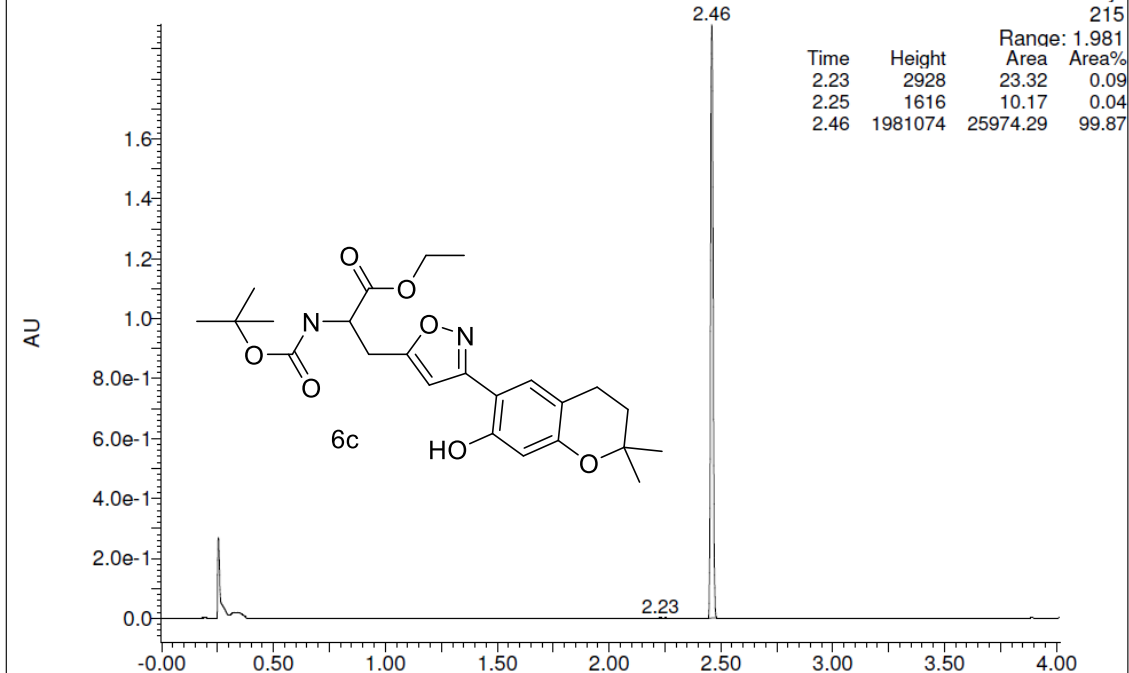
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ANL-MCL5-LCMS-007

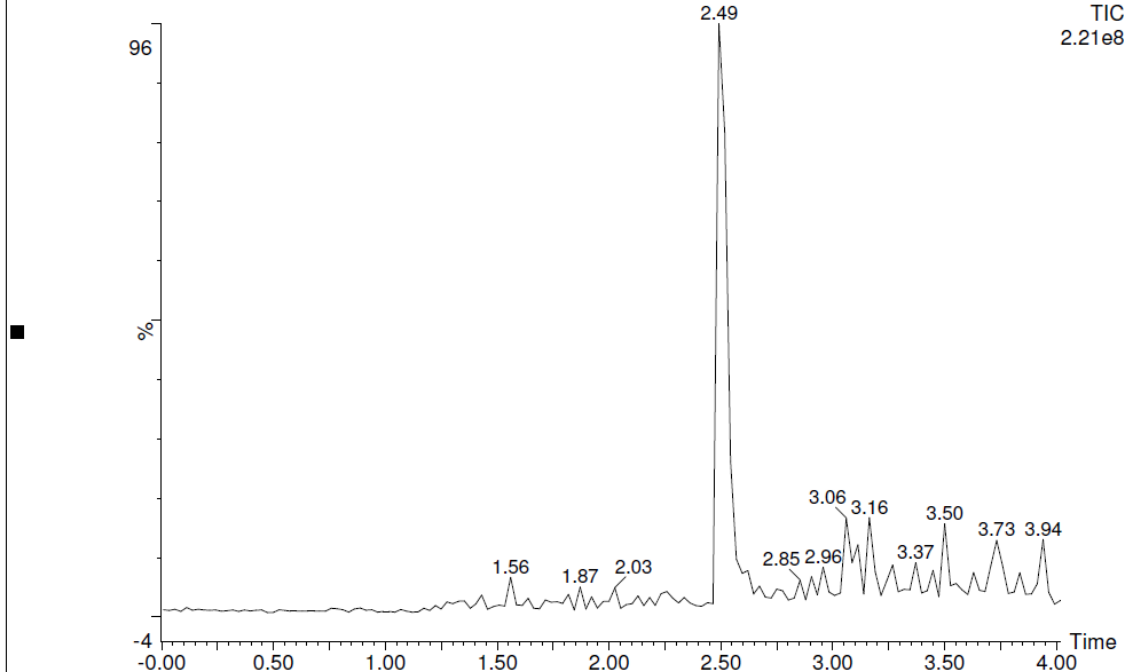
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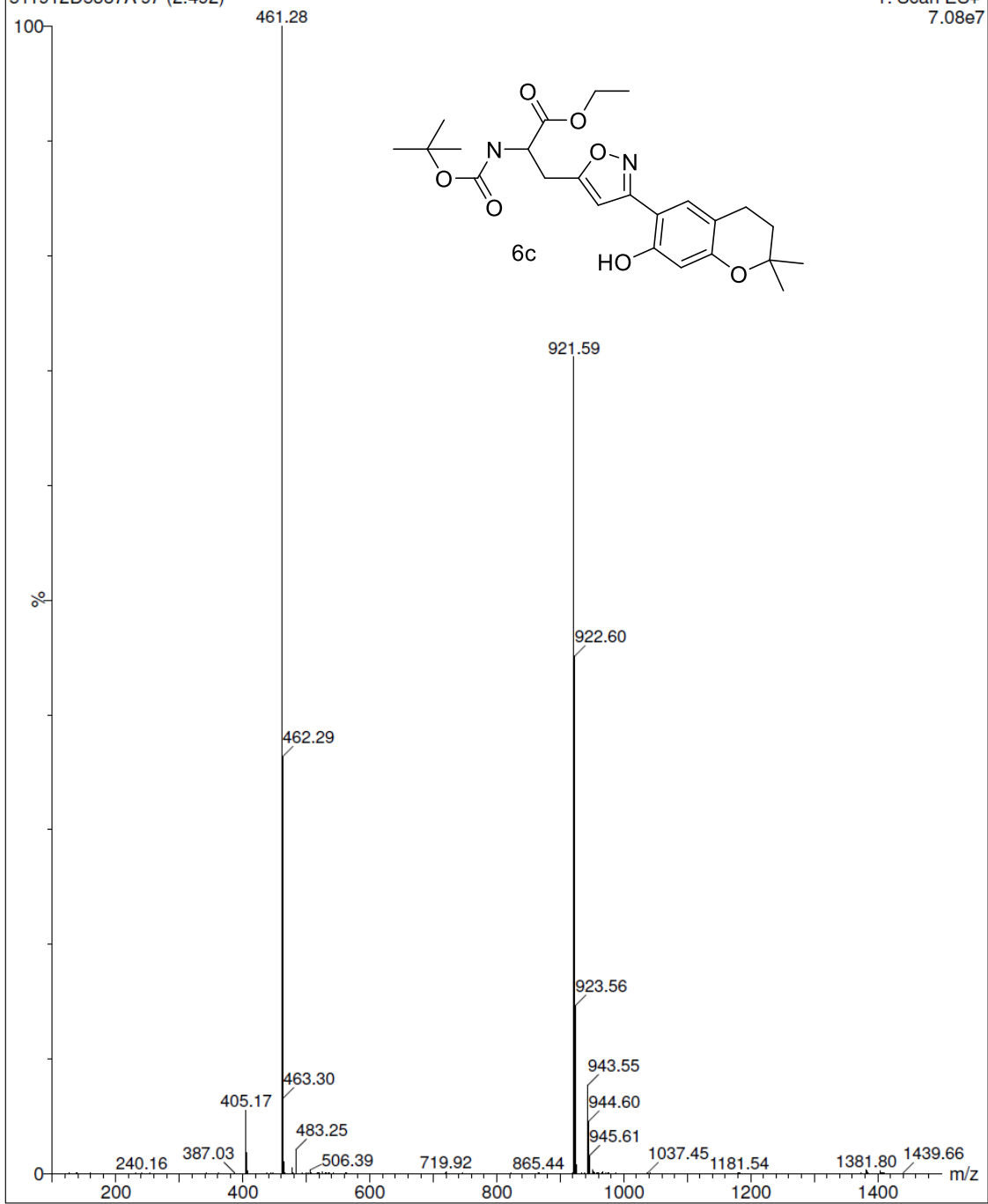
4: Diode Array



511912D5387A

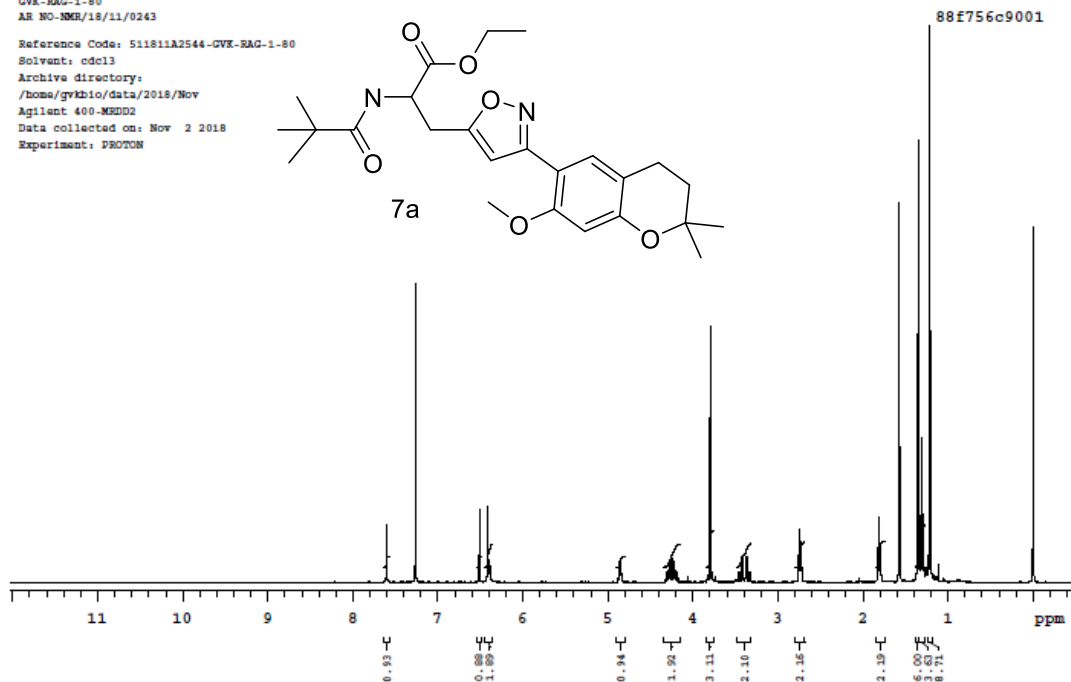
1: Scan ES+
TIC
2.21e8





GVX-RAG-1-80
AR NO-NMR/18/11/0243

Reference Code: 511811A2544-GVX-RAG-1-80
Solvent: cdcl3
Archive directory:
/home/gvxbio/data/2018/Nov
Agilent 400-MEDD2
Data collected on: Nov 2 2018
Experiment: PROTON

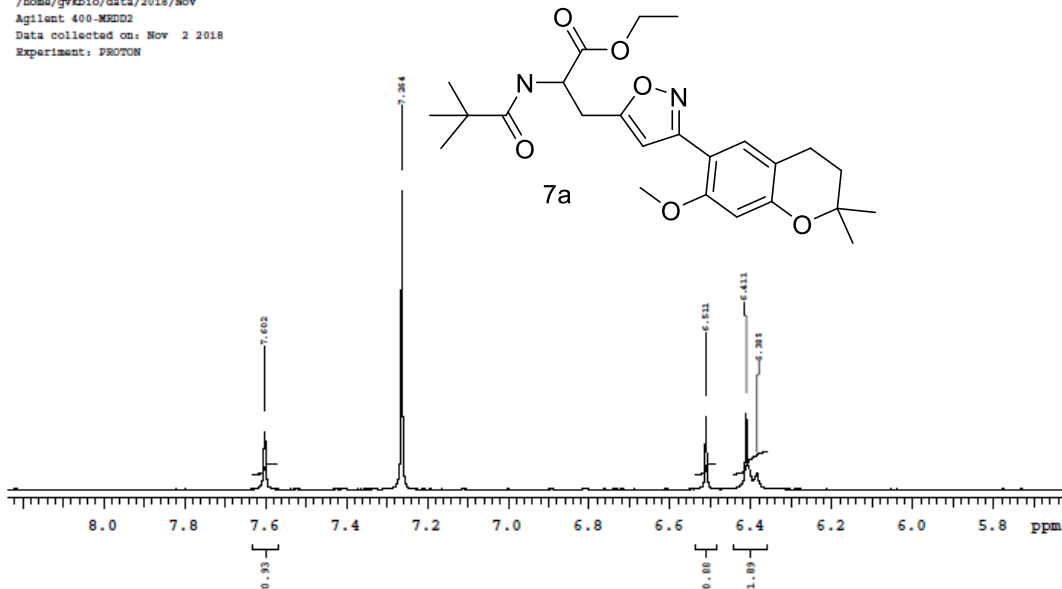


Plotname: 511811A2544-GVX-RAG-1-80_PROTON_01.REC_plot01

GVX-RAG-1-80
AR NO-NMR/18/11/0243

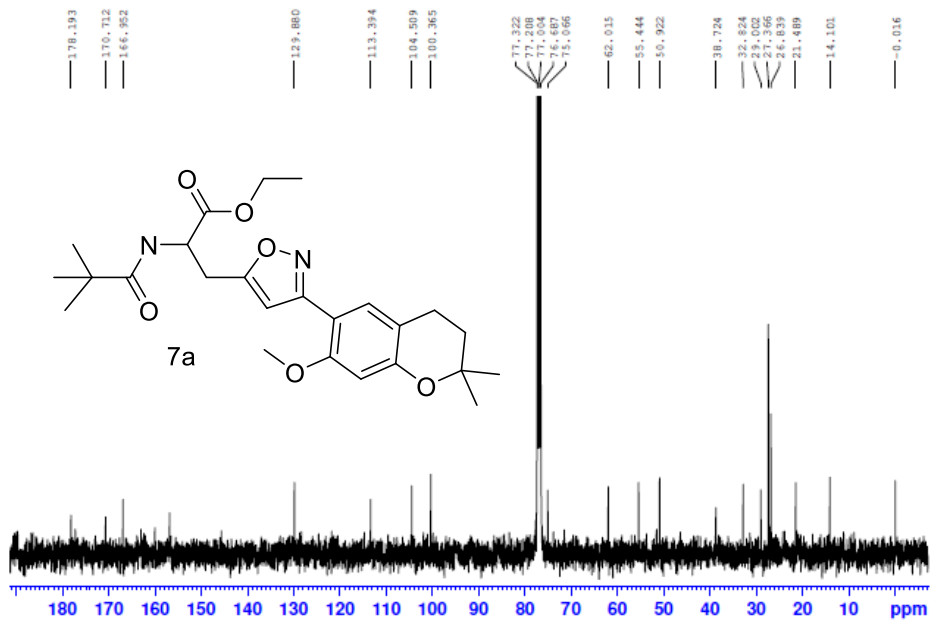
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Solvent: cdcl3
Archive directory:
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Agilent 400-MEDD2
Data collected on: Nov 2 2018
Experiment: PROTON

88f756c9001



Plotname: 511811A2544-GVX-RAG-1-80_PROTON_01.REC_plot02

GVK-RAG-1-80

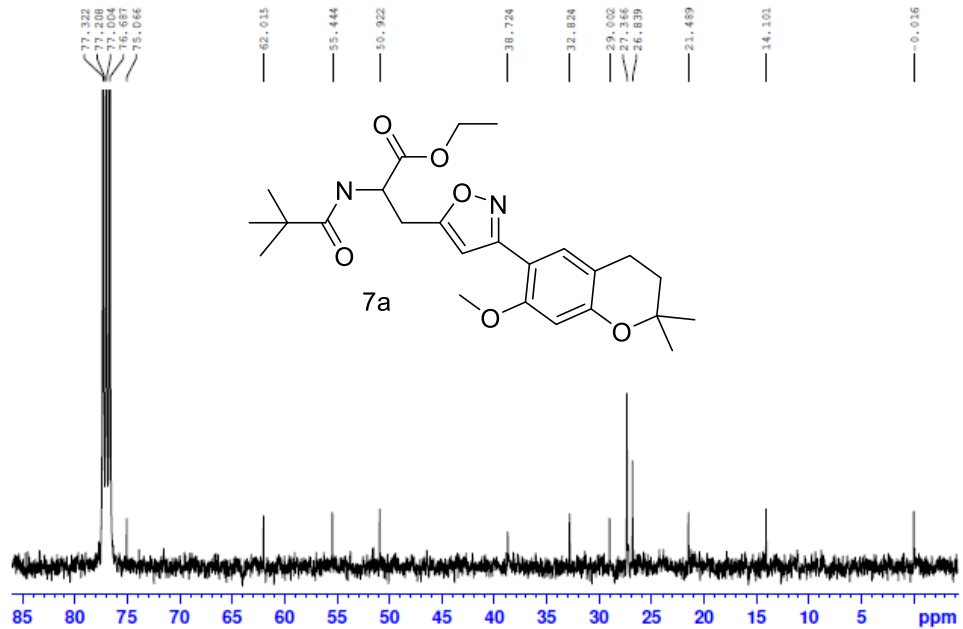


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EXPNO 2
PROCNO 1
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Time 6.10 h
INSTRUM spect
PROBHD 116098_017
PULPRG2 zgpg30
TD 65536
SOLVENT CDCl3
NS 4
DS 4
SWH 24028.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 159.29
SQ 20.100 usec
SE 6.50 usec
TE 300.2 K
SI 3.0000000 sec
S11 0.0300000 sec
TDD 1
SFO1 100.6228298 MHz
NUC1 13C
P1 10.00 usec
F1 70.6080071 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 30.00 usec
P2 16.8290047 W
F2 0.20776001 W
SFO3 0.1040000 W
F2 - Processing parameters
SI 32768
SF 100.6127485 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
    
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ANL-MCL5-NMR-001

GVK-RAG-1-80

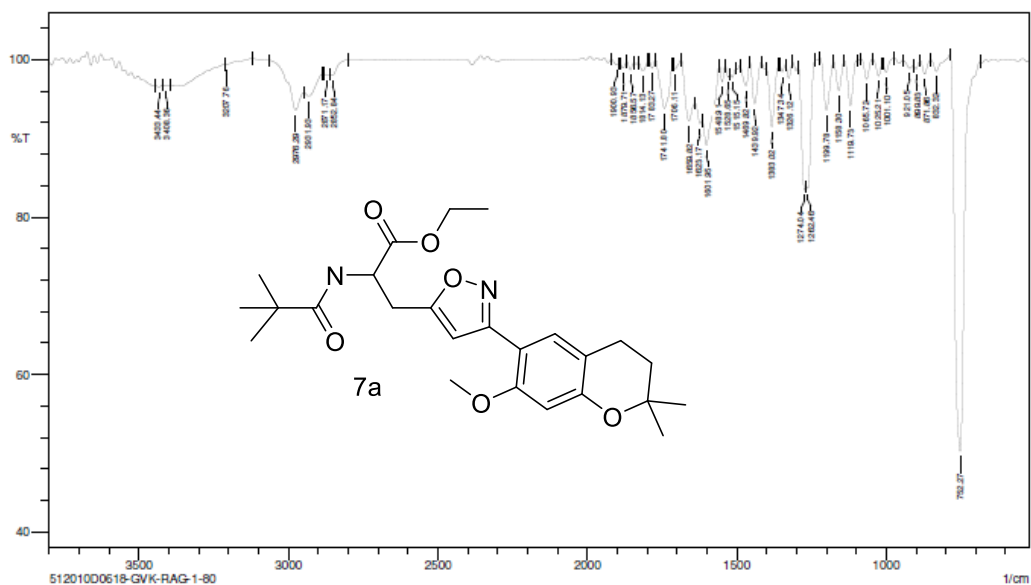


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Current Data Parameters
NAME 3121000020-DVS-RAG-1-80
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 2021101
Time 6.10 h
INSTRUM spect
PROBHD 116098_017
PULPRG2 zgpg30
TD 65536
SOLVENT CDCl3
NS 4
DS 4
SWH 24028.461 Hz
FIDRES 0.733596 Hz
AQ 1.3631488 sec
RG 159.29
SQ 20.100 usec
SE 6.50 usec
TE 300.2 K
SI 3.0000000 sec
S11 0.0300000 sec
TDD 1
SFO1 100.6228298 MHz
NUC1 13C
P1 10.00 usec
F1 70.6080071 W
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG2 waltz16
PCPD2 30.00 usec
P2 16.8290047 W
F2 0.20776001 W
SFO3 0.1040000 W
F2 - Processing parameters
SI 32768
SF 100.6127485 MHz
WDW EM
SSB 0
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GB 0
PC 1.40
    
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ANL-MCL5-NMR-001

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Discovery Chemistry- Analytical Services

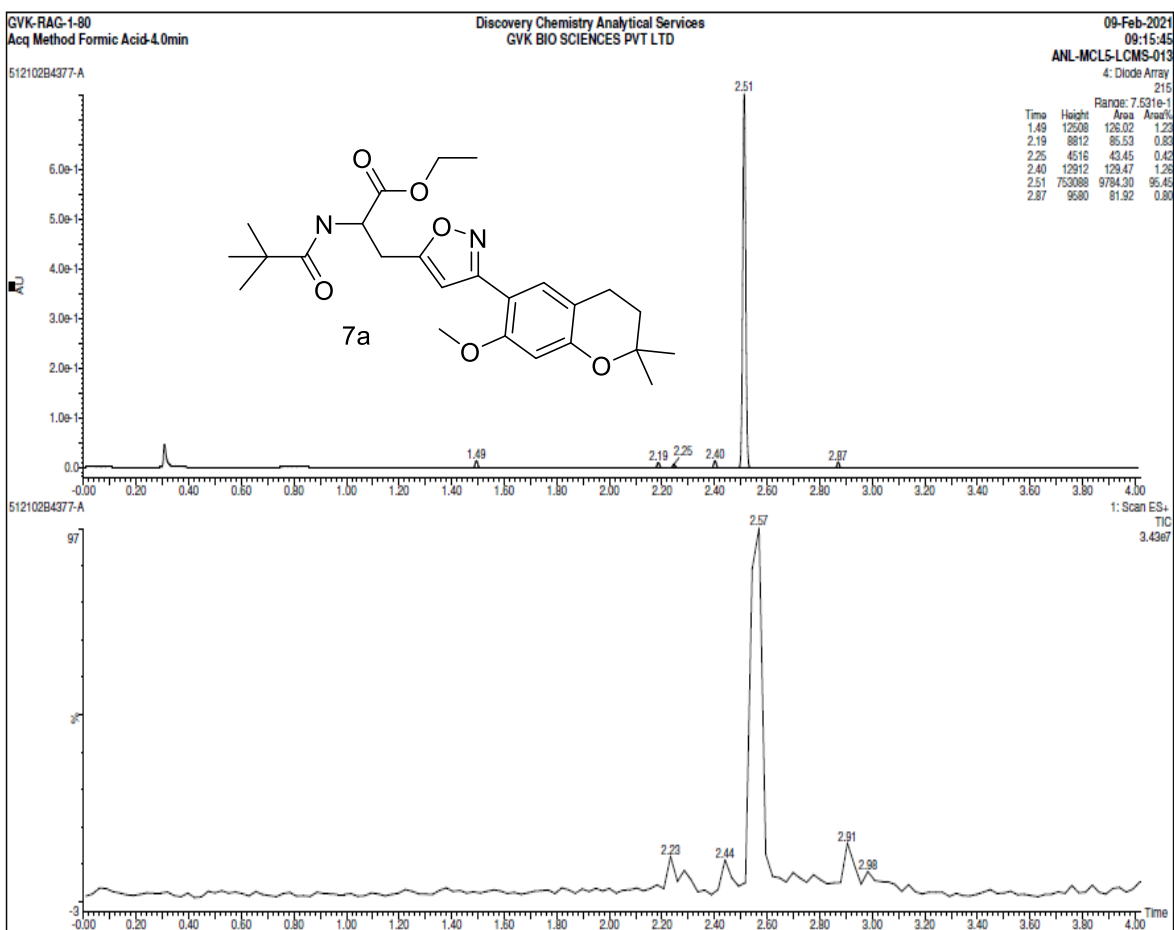


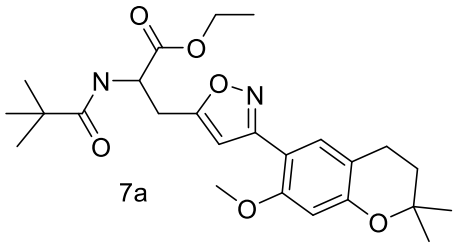
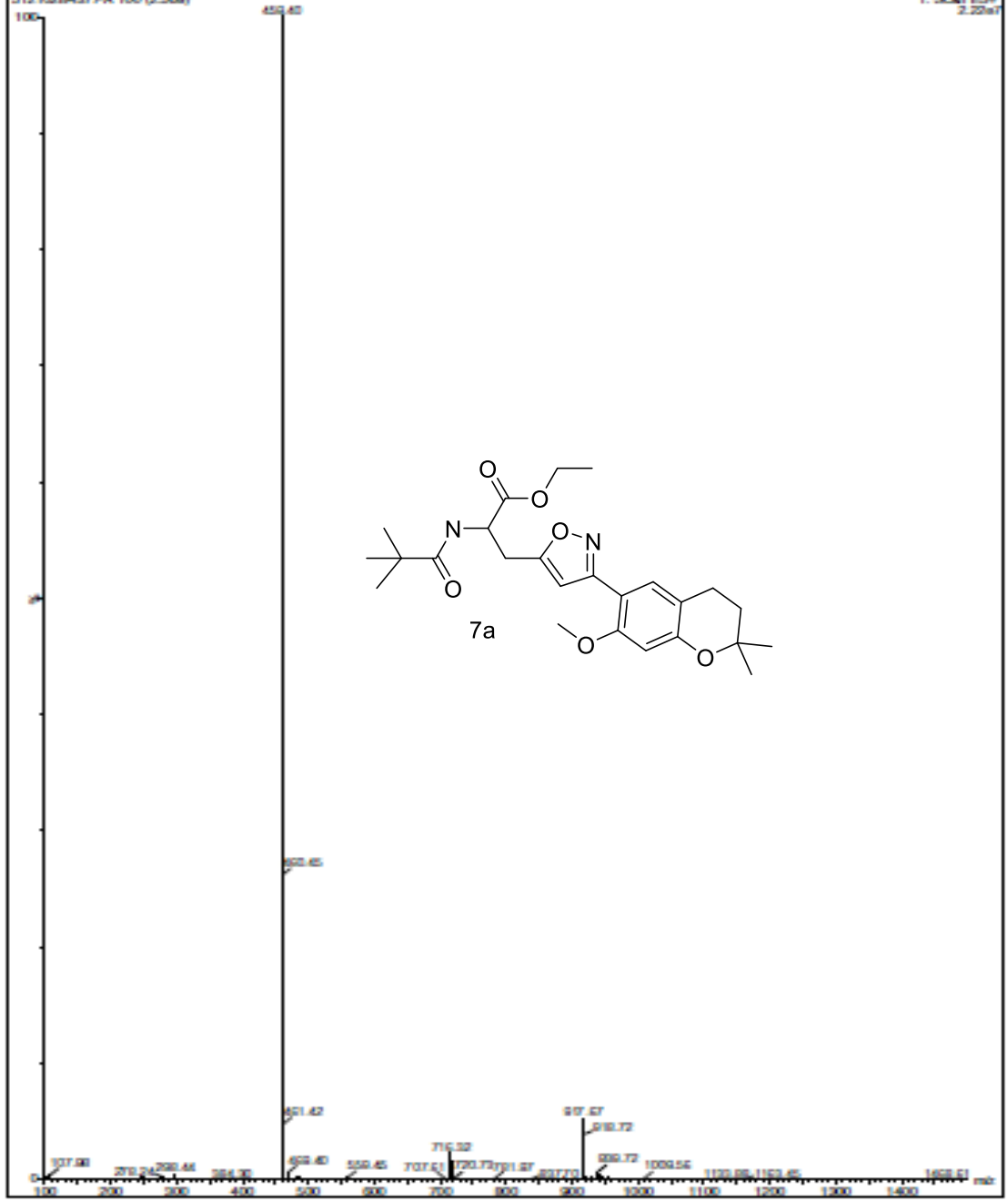
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512010D0618-GVK-RAG-1-80

No. of Scans:

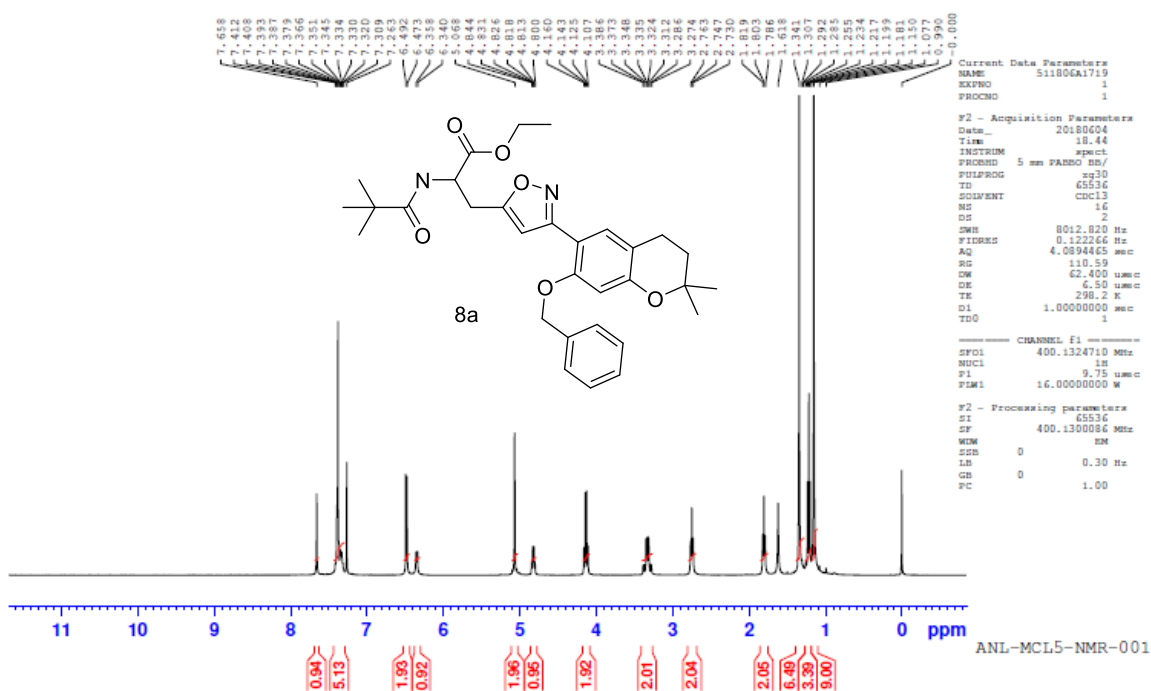
Date/Time: 10/31/2020 2:23:43 PM

User: GVKBIO

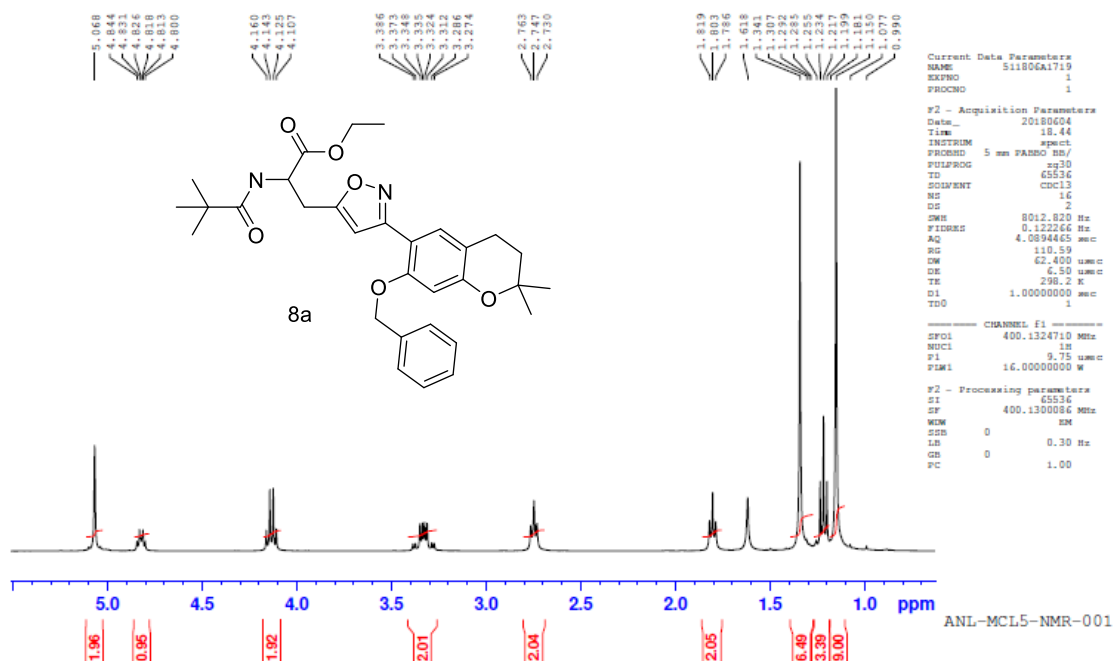




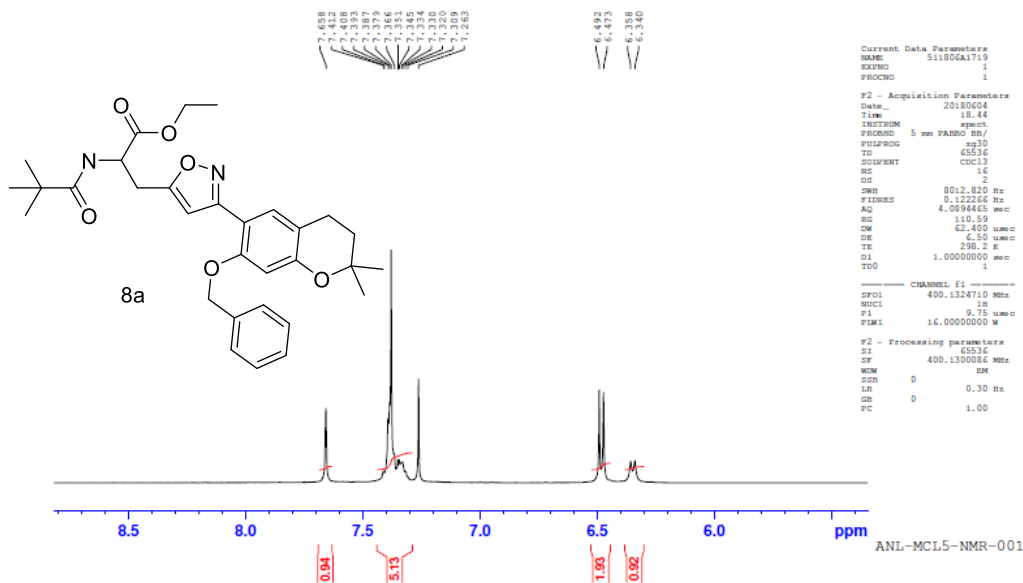
GVK-RAG-1-50



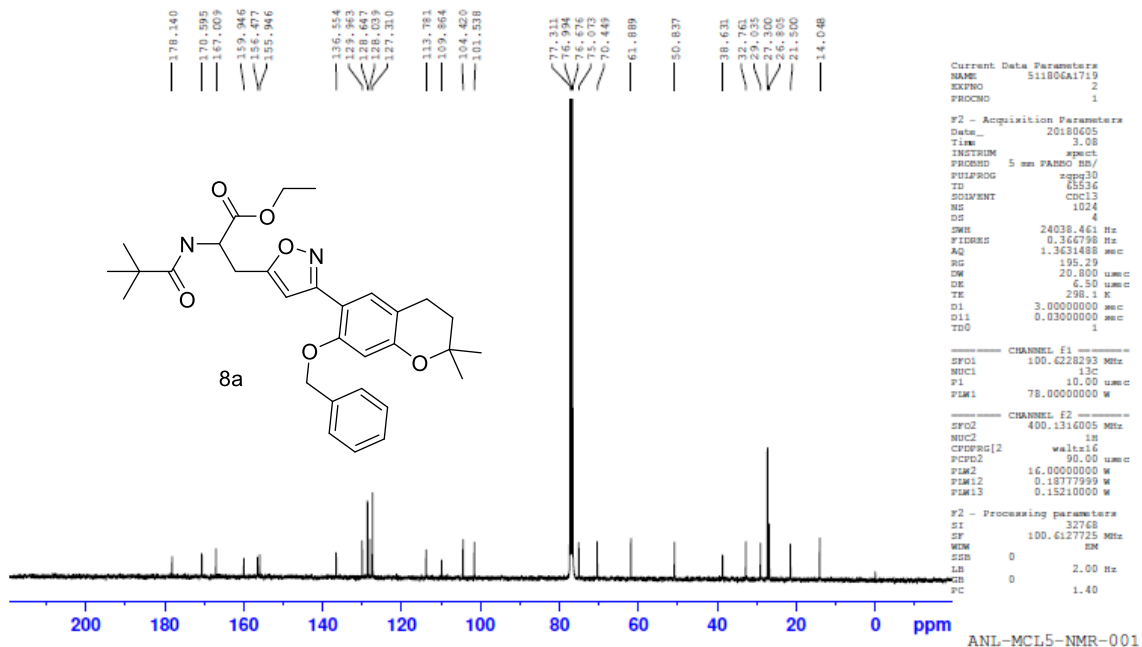
GVK-RAG-1-50



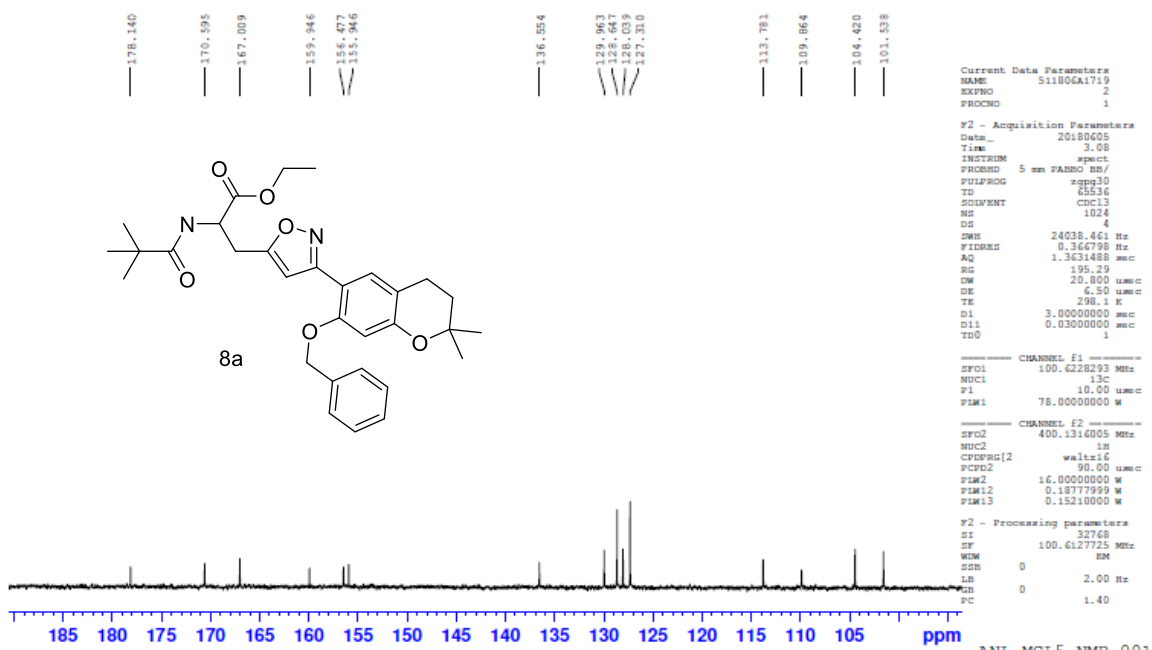
GVK-RAG-1-50



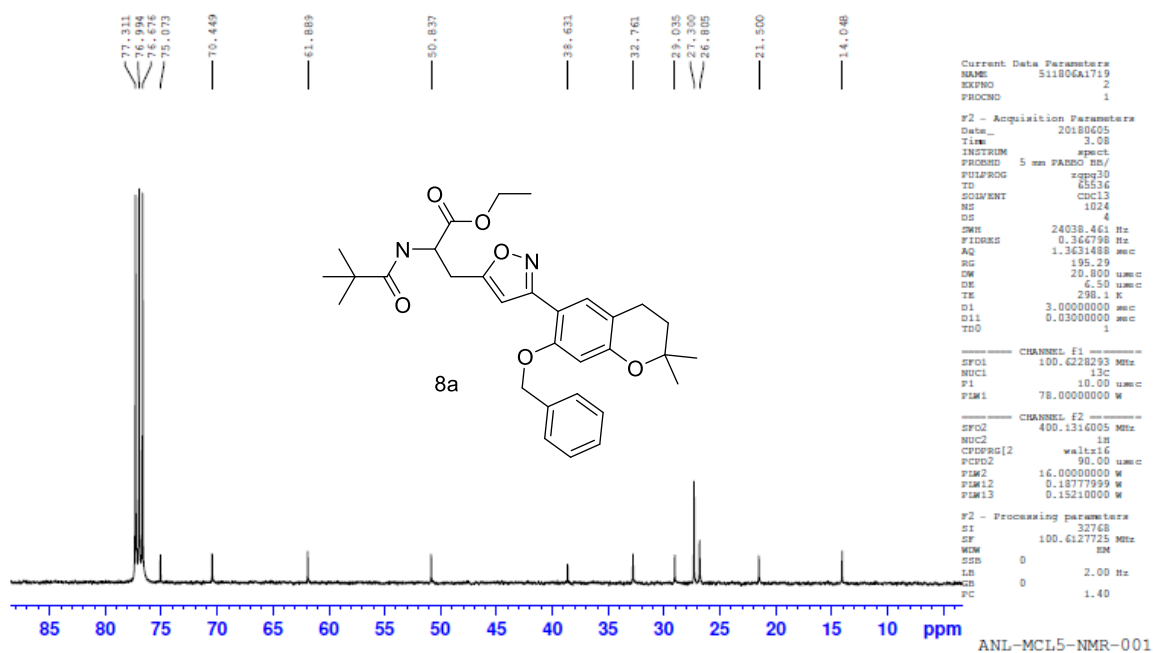
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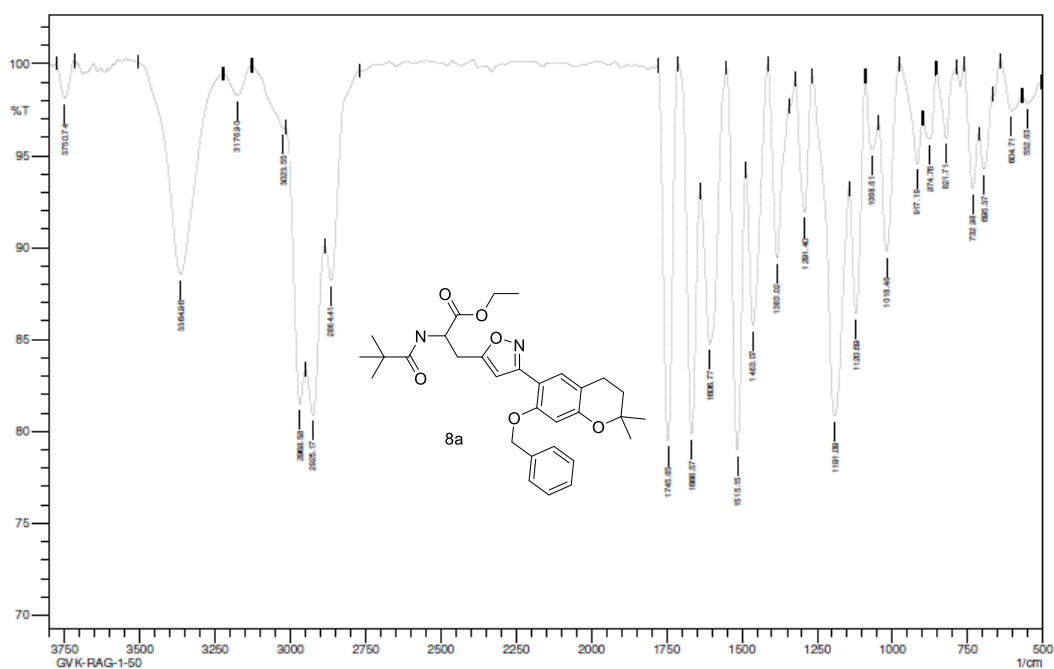


GVK-RAG-1-50



GVK-RAG-1-50

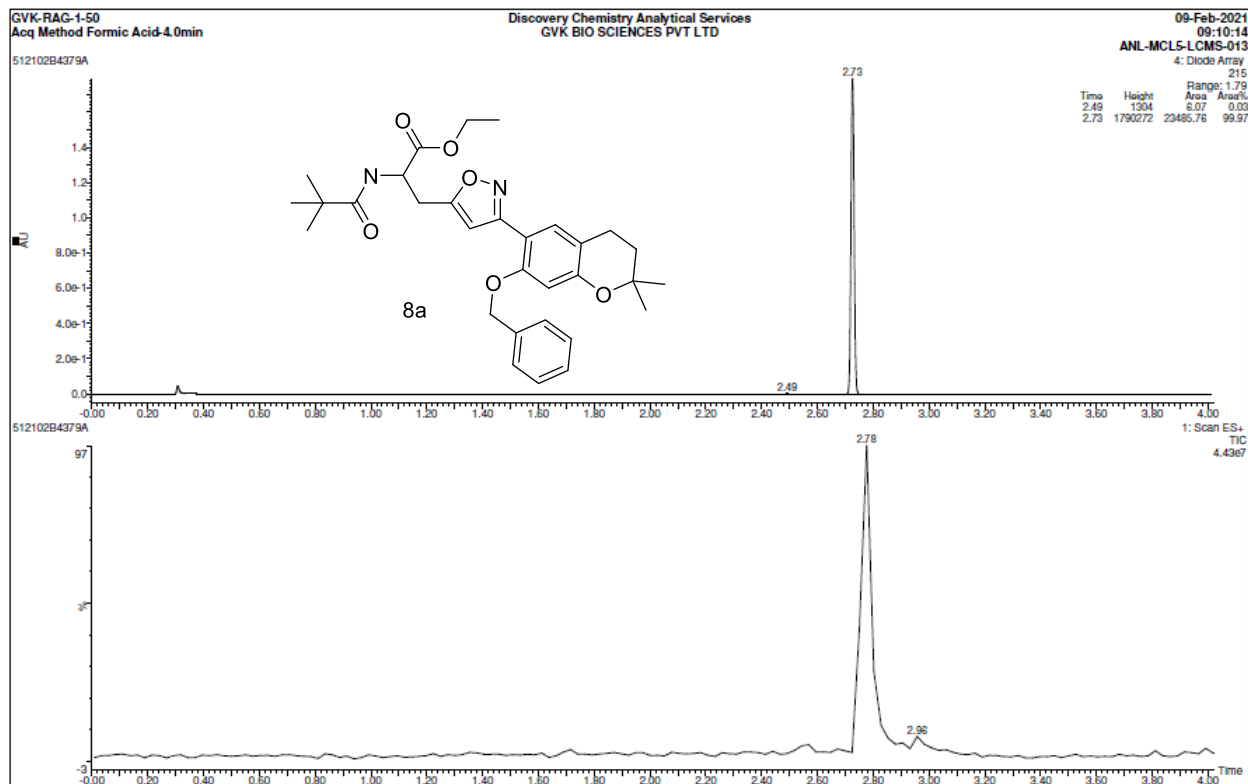




Comment: IN Kbr
GVK-RAG-1-50

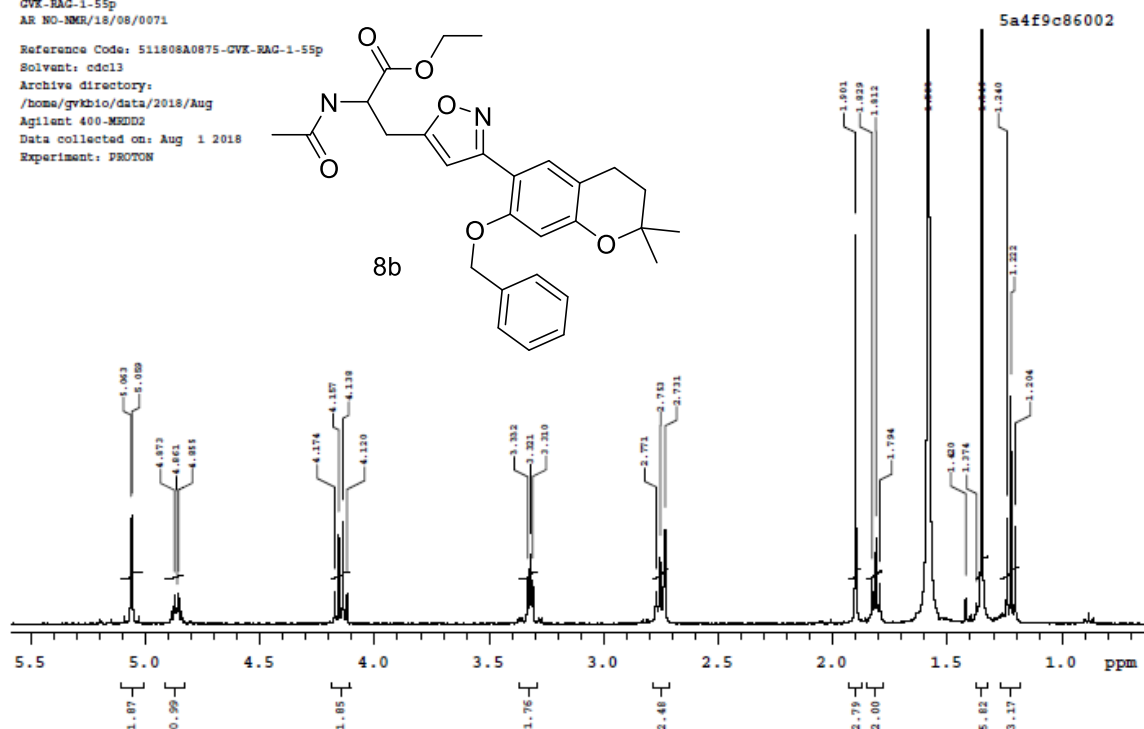
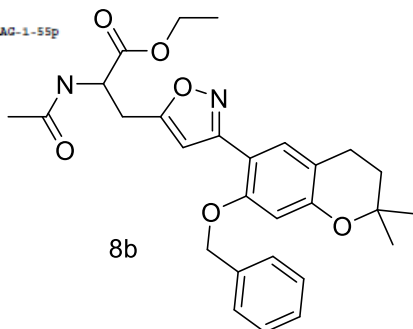
No. of Scans:
Resolution:
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Date: 6/4/2018 4:08:01 PM
User: Admin



GVK-RAG-1-55p
AR NO-NMR/18/08/0071

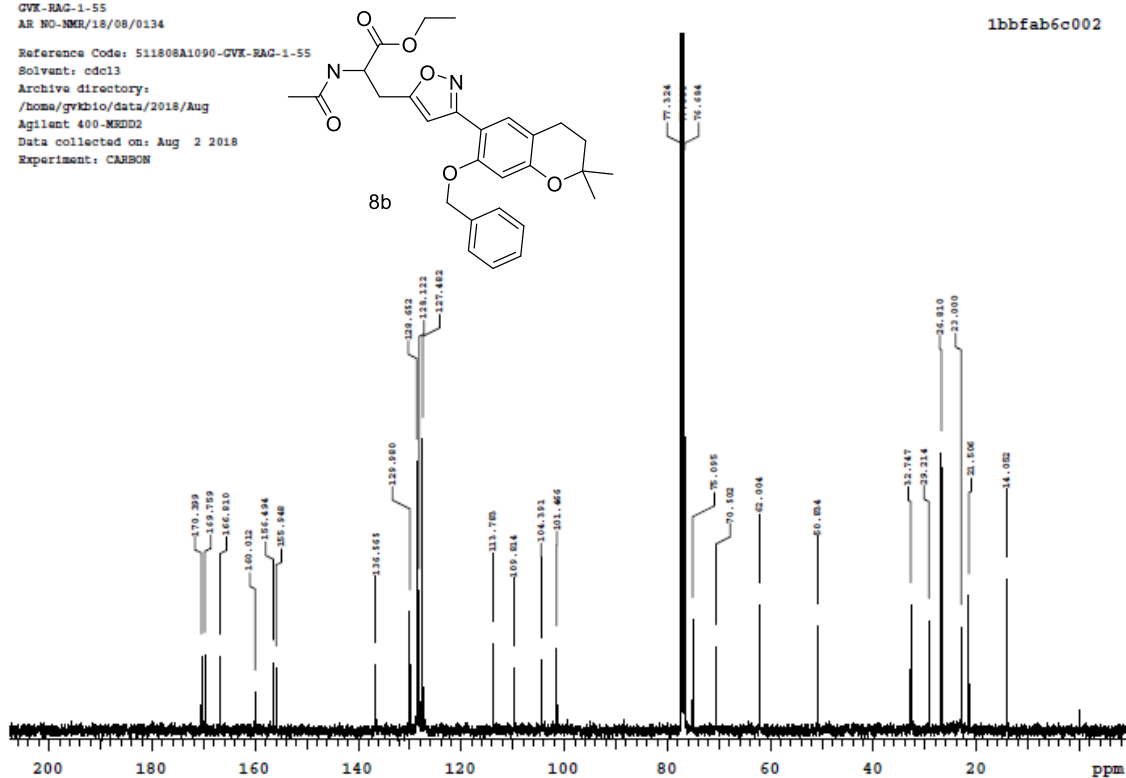
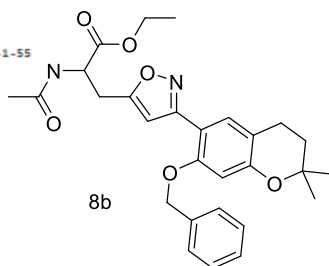
Reference Code: 511808A0875-GVK-RAG-1-55p
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2018/Aug
Agilent 400-MKDD2
Data collected on: Aug 1 2018
Experiment: PROTON



Plotname: 511808A0875-GVK-RAG-1-55p_PROTON_01.REC_plot03

GVK-RAG-1-55
AR NO-NMR/18/08/0134

Reference Code: 511808A1090-GVK-RAG-1-55
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2018/Aug
Agilent 400-MKDD2
Data collected on: Aug 2 2018
Experiment: CARBON

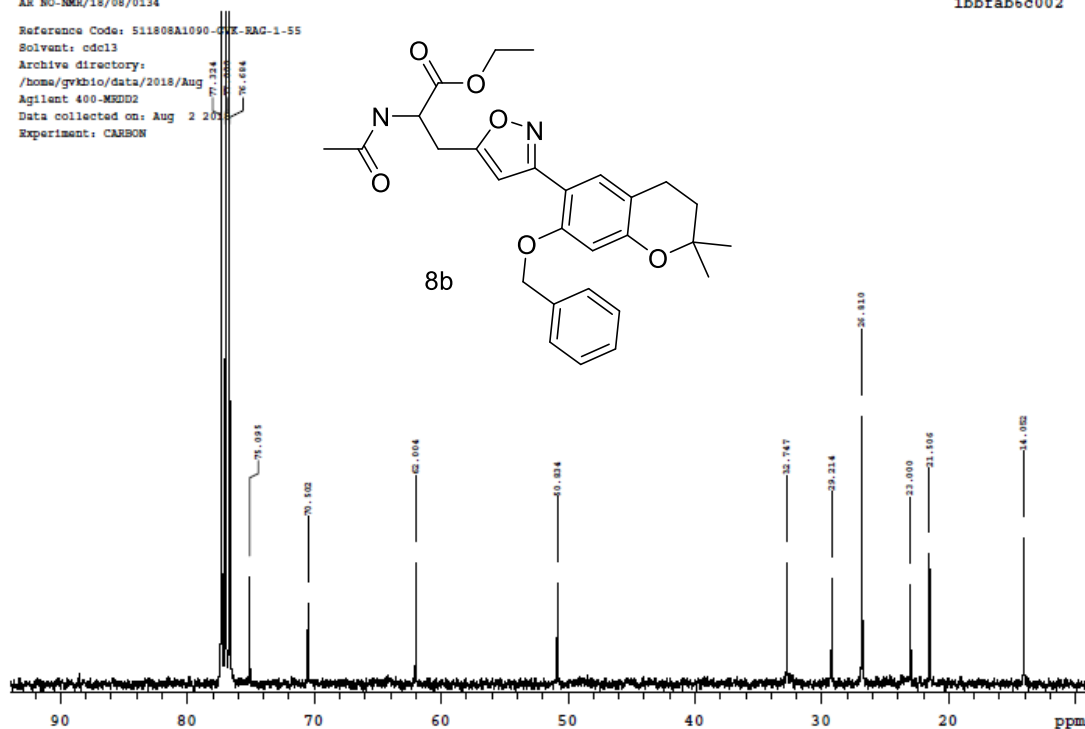


Plotname: 511808A1090-GVK-RAG-1-55_CARBON_01.REC_plot01

GVK-RAG-1-55
AR NO-NMR/18/08/0134

1bbfab6c002

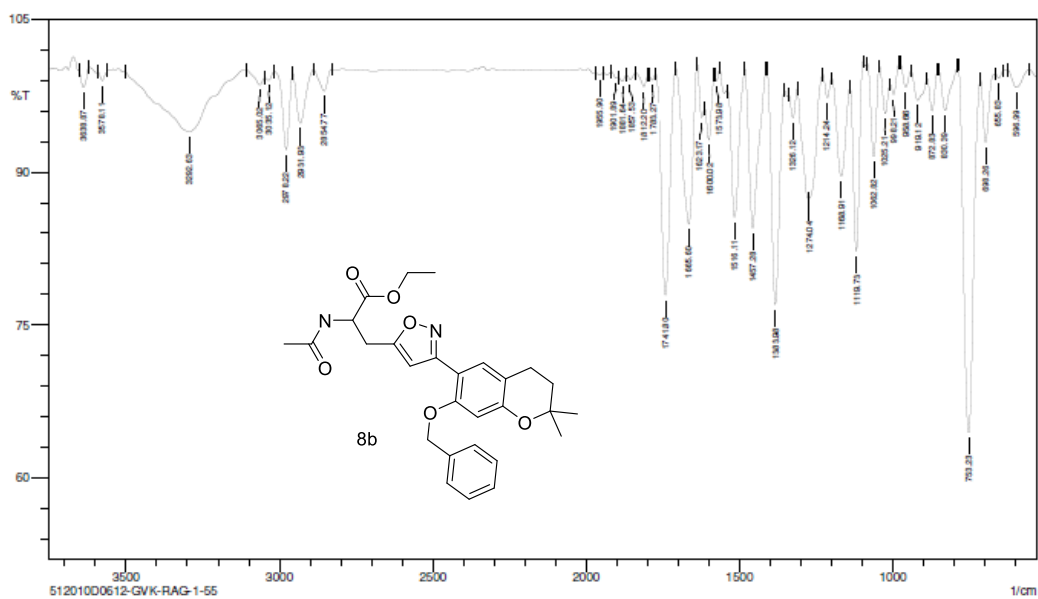
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Solvent: cdcl3
Archive directory:
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Agilent 400-MREDD2
Data collected on: Aug 2 2020
Experiment: CARBON



Plotname: 511808A1090-GVK-RAG-1-55_CARBON_01.REC_plot03

SHIMADZU

GVK BIOScience Private Limited
Discovery Chemistry- Analytical Services

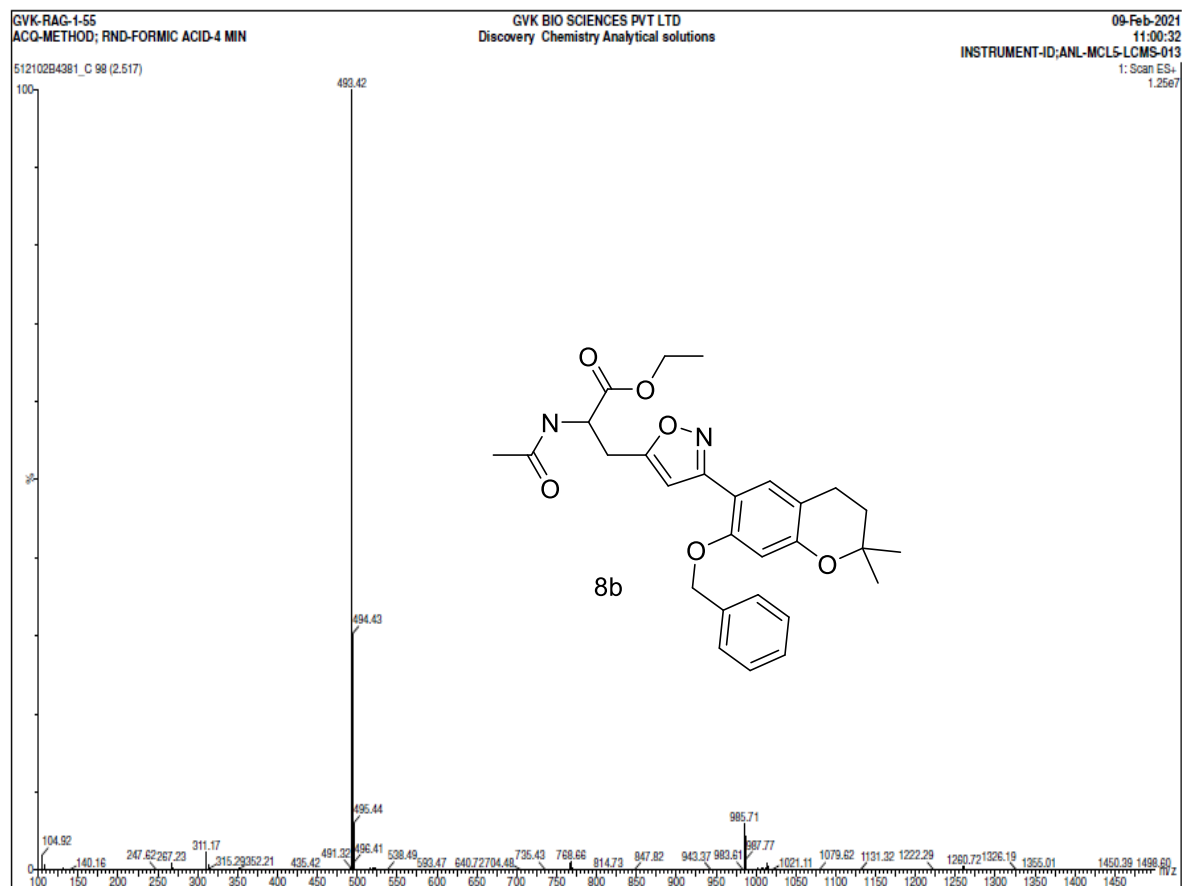
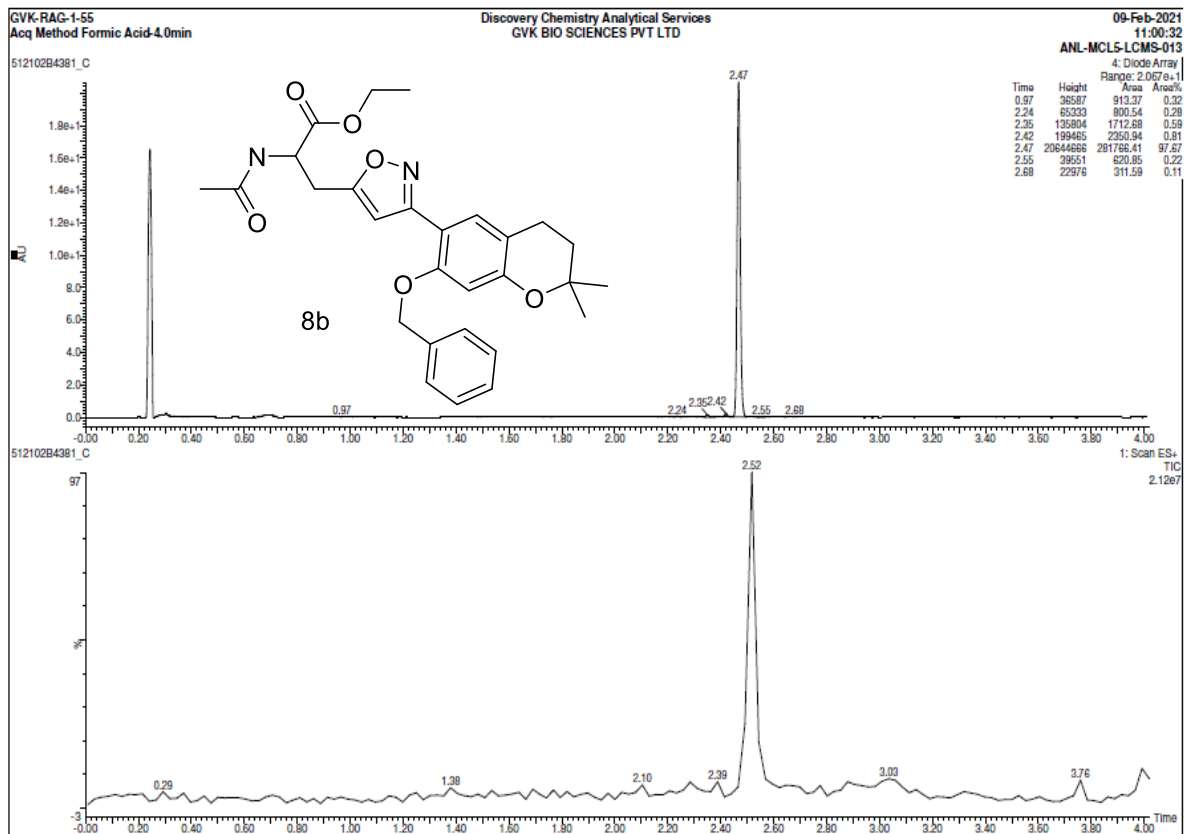


Sample Name:
512010D0612-GVK-RAG-1-55

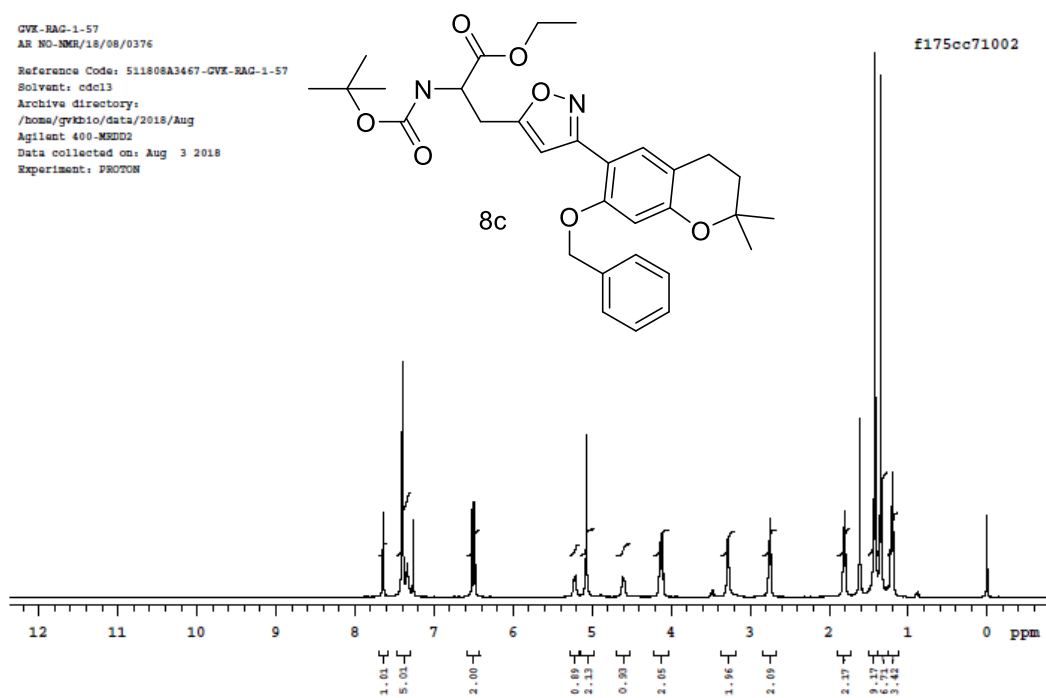
No. of Scans:

Date/Time: 10/31/2020 2:33:43 PM

User: GVKBIO



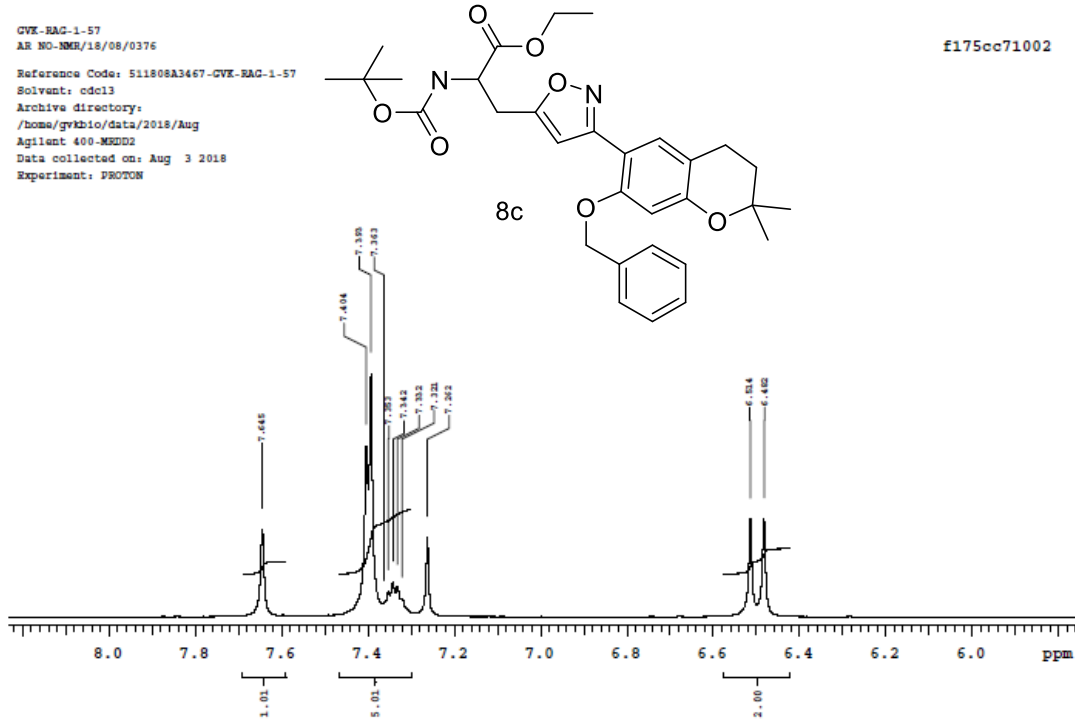
GVX-RAG-1-57
AR NO-MMR/18/08/0376
Reference Code: S11808A3467-GVX-RAG-1-57
Solvent: cdcl3
Archive directory:
/home/gvxbio/data/2018/Aug
Agilent 400-MRDD2
Data collected on: Aug 3 2018
Experiment: PROTON



Plotname: S11808A3467-GVX-RAG-1-57_PROTON_01.REC_plot01

GVK-RAG-1-57
AR NO-NMR/18/08/0376
Reference Code: 511808A3467-GVK-RAG-1-57
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2018/Aug
Agilent 400-MRDD2
Data collected on: Aug 3 2018
Experiment: PROTON

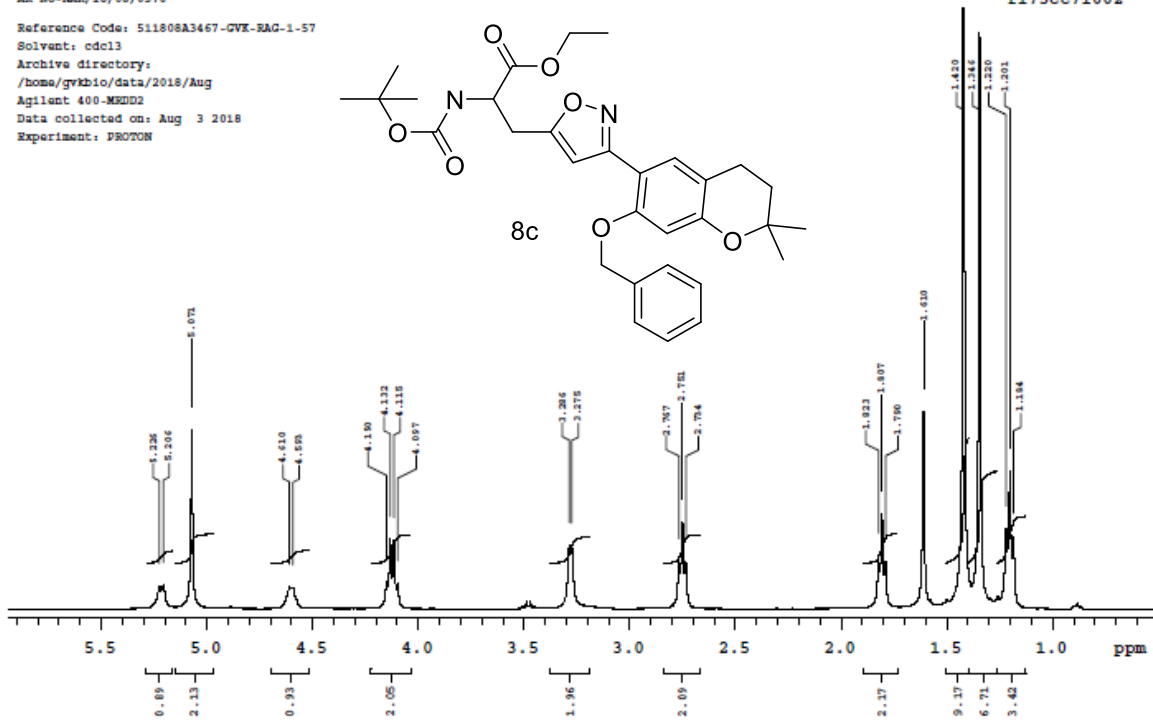
f175cc71002



Plotname: 511808A3467-GVK-RAG-1-57_PROTON_01.RRC_plot02

GVK-RAG-1-57
AR NO-NMR/18/08/0376
Reference Code: 511808A3467-GVK-RAG-1-57
Solvent: cdcl3
Archive directory:
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Agilent 400-MRDD2
Data collected on: Aug 3 2018
Experiment: PROTON

f175cc71002

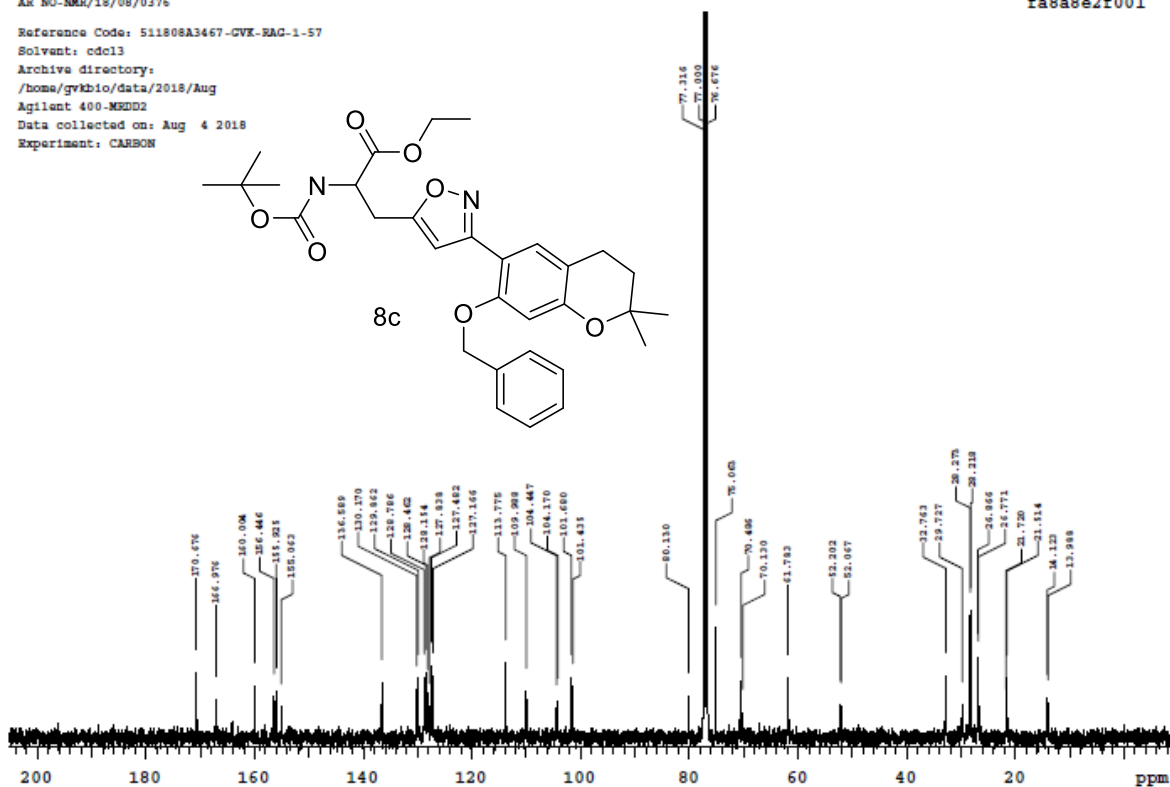
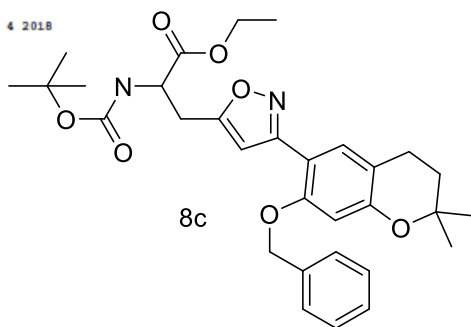


Plotname: 511808A3467-GVK-RAG-1-57_PROTON_01.RRC_plot03

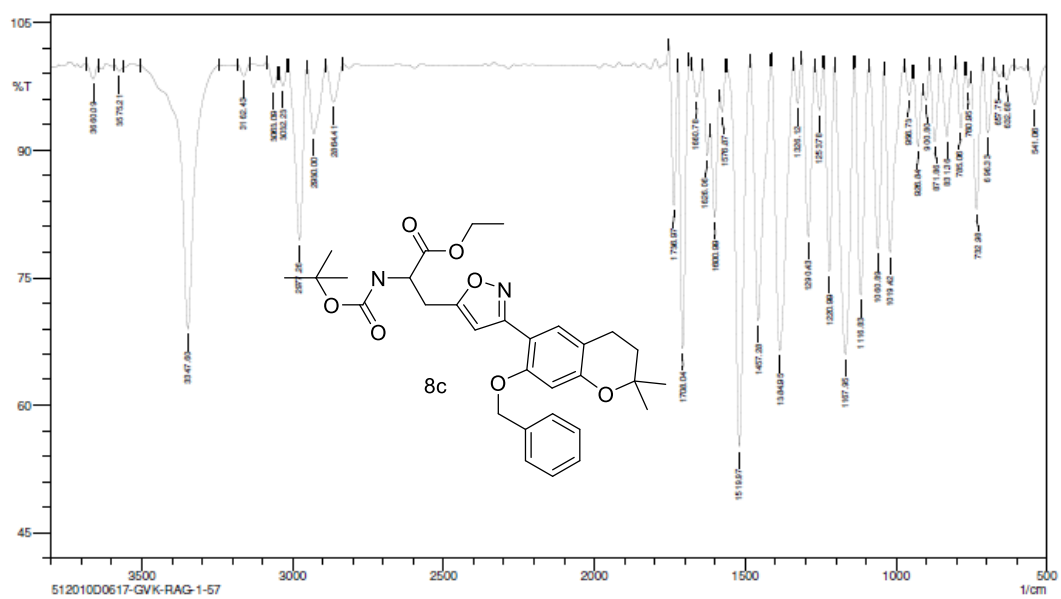
GVK-RAG-1-57
AR NO-NMR/18/08/0376

fa8a8e2f001

Reference Code: 511808A3467-GVK-RAG-1-57
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2018/Aug
Agilent 400-MEDD2
Data collected on: Aug 4 2018
Experiment: CARBON



Plotname: 511808A3467-GVK-RAG-1-57 CARBON_01.REC_plot01

GVK BIOScience Private Limited
Discovery Chemistry- Analytical ServicesSample Name:
512010D0617-GVK-RAG-1-57

No. of Scans:

Date/Time: 10/31/2020 12:52:12 PM

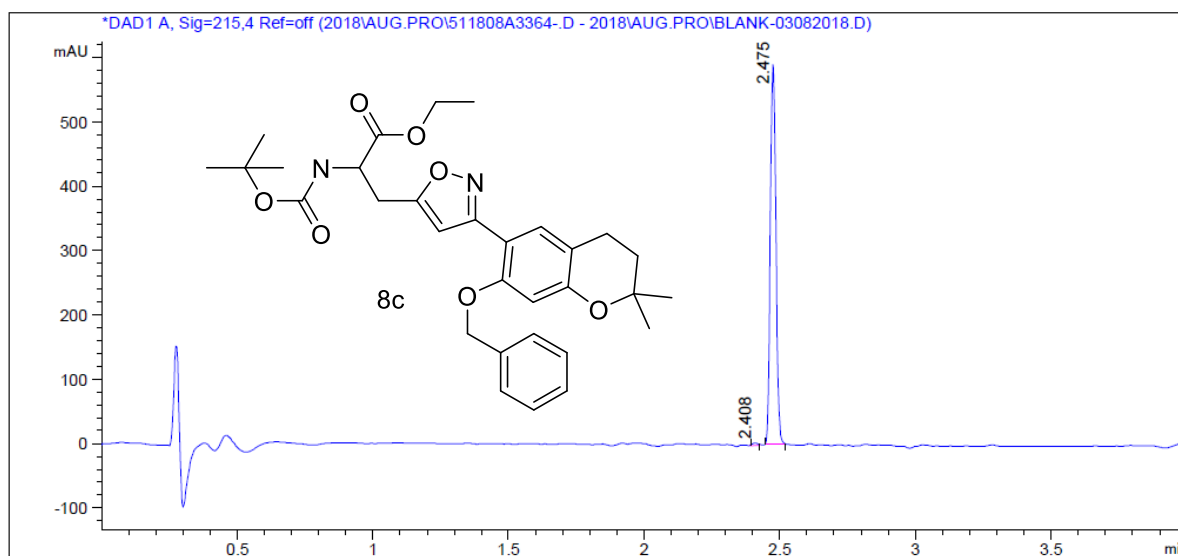
User: GVKBIO

GVK BIOSCIENCES PVT. LTD.
MEDICINAL CHEMISTRY LABORATORY - ANALYTICAL RESEARCH
LCMS REPORT

Sample Name : GVK-RAG-1-57 Vial position : P1-D-06
Date of Analysis : 8/3/2018 5:23:44 PM Injection Vol : 1.000µl
Acq. Method : RND-FA-4.01 Instrument ID : ANL-MCL5-LCMS-001

RND-FA-4.01 MIN :-

Column : ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7µm)
Mobile Phase : A1 - 0.1 % FA IN WATER ; B1: 0.1%FA IN ACN
Gradient : Time (min) / %B1:0/3,0.3/3,2.3/98,3.5/98,4.0/3,4.01/3
Flow Rate : 0.6 ml/min
Column Temp : 50°C



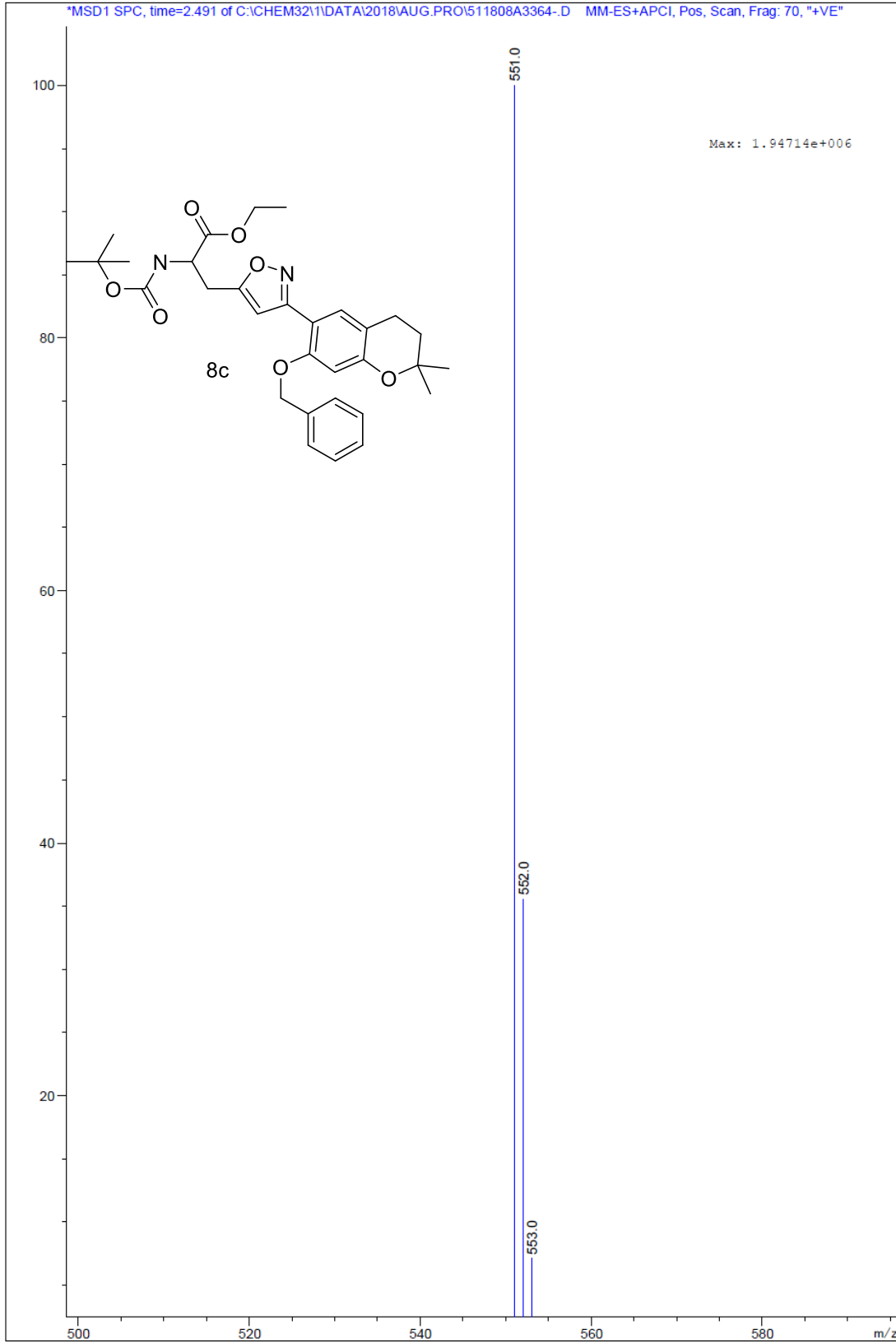
Pea No	RT min	Area	Area %
1	2.41	4.887	0.565
2	2.48	859.452	99.435

Analysed by :

Page 1 of 2

MS Spectrum

*MSD1 SPC, time=2.491 of C:\CHEM32\1\DATA\2018\AUG.PRO\511808A3364-D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"





GVK Biosciences Private Limited
Discovery Chemistry - Analytical Services
SFC Analytical Chromatogram

User Name: analyst

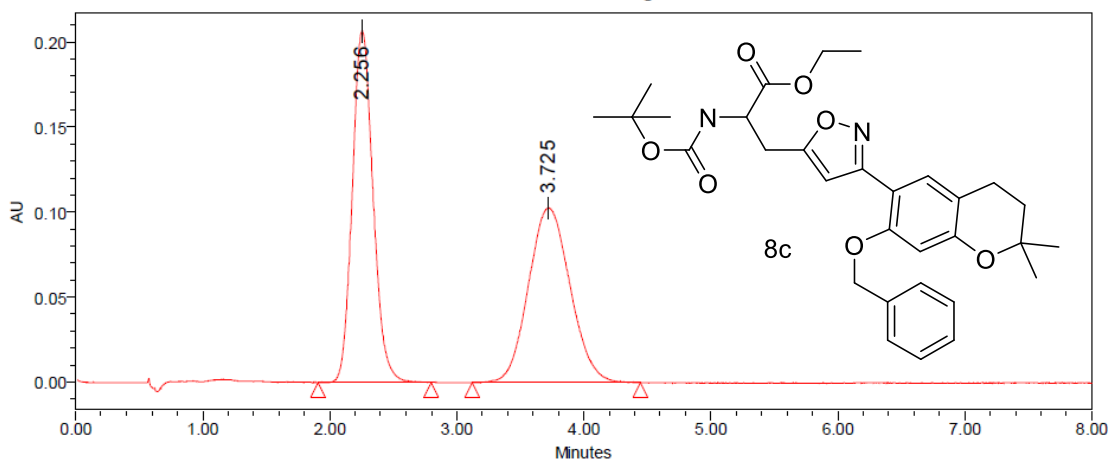
Project Name: 2021\APR-2021\MALLAPUR\ANL-MCL5-SFC-006-APR-2021

Sample Name:	GVK-RAG-1-57	Acquired By:	MLRAnalyst
Vial:	1:C,1	Sample Set Name:	19_APRIL_2021
Injection Volume:	10.00 ul	Acq. Method Set:	C2_SolvB2_3g_25
Date Acquired:	19-Apr-2021 07:42:40 PM IST	Proc. Chnl. Descr.:	PDA Spectrum PDA 215.0 nm (PDA Spectrum (200-400)nm)

SFC Method Conditions :

Column : CHIRALPAK AD-3 (4.6*150mm)3µm
Co-solvent : Methanol
Total flow : 3g/min
% of Co-Solvent : 25
ABPR : 1500psi
Temperature : 30°C

Auto-Scaled Chromatogram



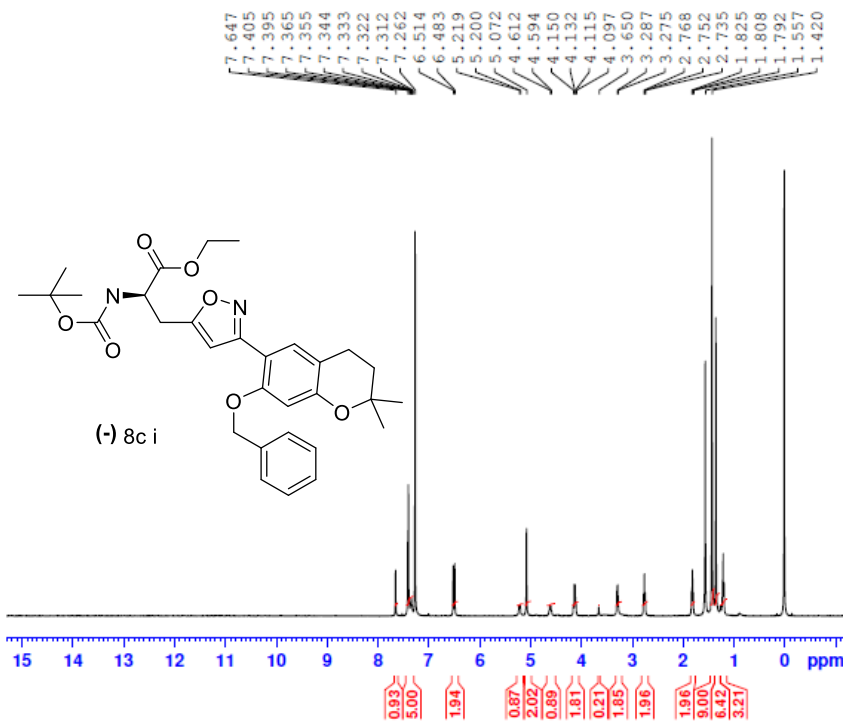
Peak Results

Name	RT	Area	% Area
1	2.26	2350432	50.01
2	3.73	2349802	49.99

Report Template: Chiral Report

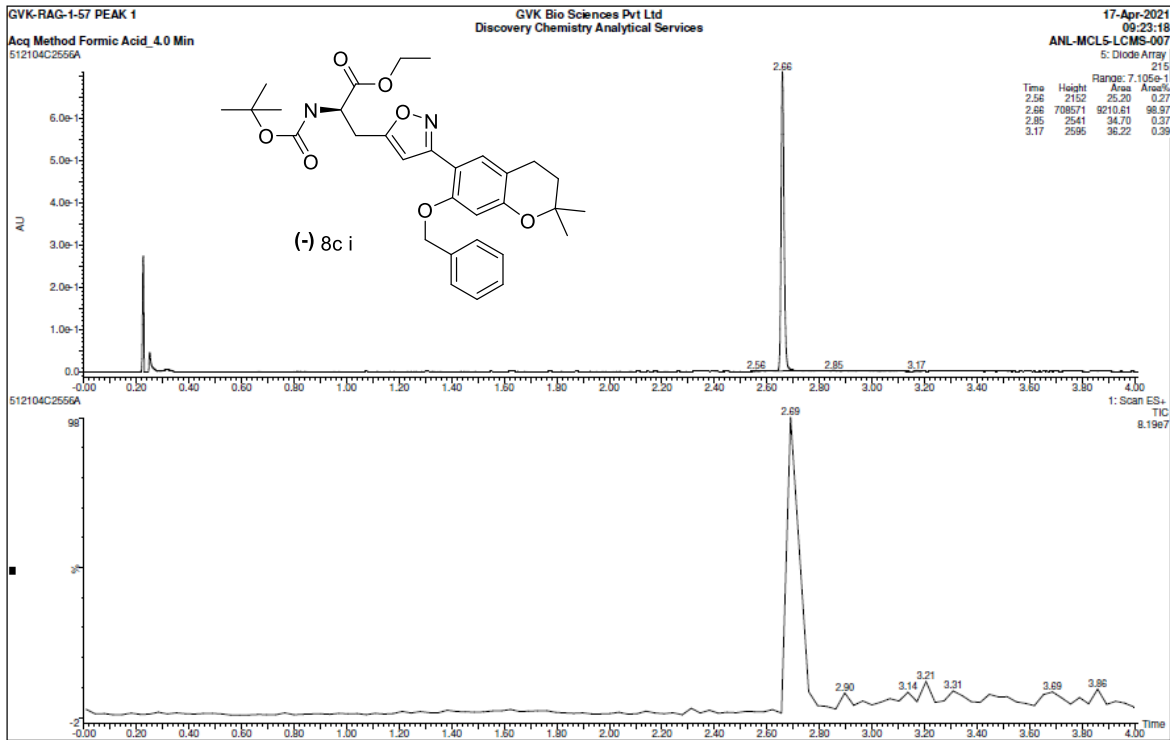
Print Date & Time: 19-Apr-2021 07:54:58 PM Asia/Kolkata

GVK-RAG-1-57 PEAK 1



Current Data Parameters
 NAME: 512104C2556A-GVK-RAG-1-57 PEAK 1
 METHOD: 1
 F2 - Acquisition Parameters
 Date_: 20210417
 Time: 3.39 h
 INJECTION: Average
 FOLDER: E163739_0135 (1)
 FILENAME: 1930
 TD: 65536
 SOLVENT: CDCl3
 NS: 8
 DS: 0
 SWH: 8196.722 Hz
 FIDRES: 0.250144 Hz
 AQ: 3.931900 sec
 RG: 101
 IN: 61.000 umsc
 DE: 13.493 umsc
 TE: 293.2
 CD: 1.00000000 sec
 TDD: 1
 SFO1: 400.3024719 MHz
 NUC1: 13C
 P1: 2.07 umsc
 F1: 8.00 umsc
 PCMR: 22.47400093 M
 F2 - Processing parameters
 SI: 65536
 SF: 400.3000092 MHz
 MSK: 0
 SSB: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.00

ANL-MCL5-NMR-003

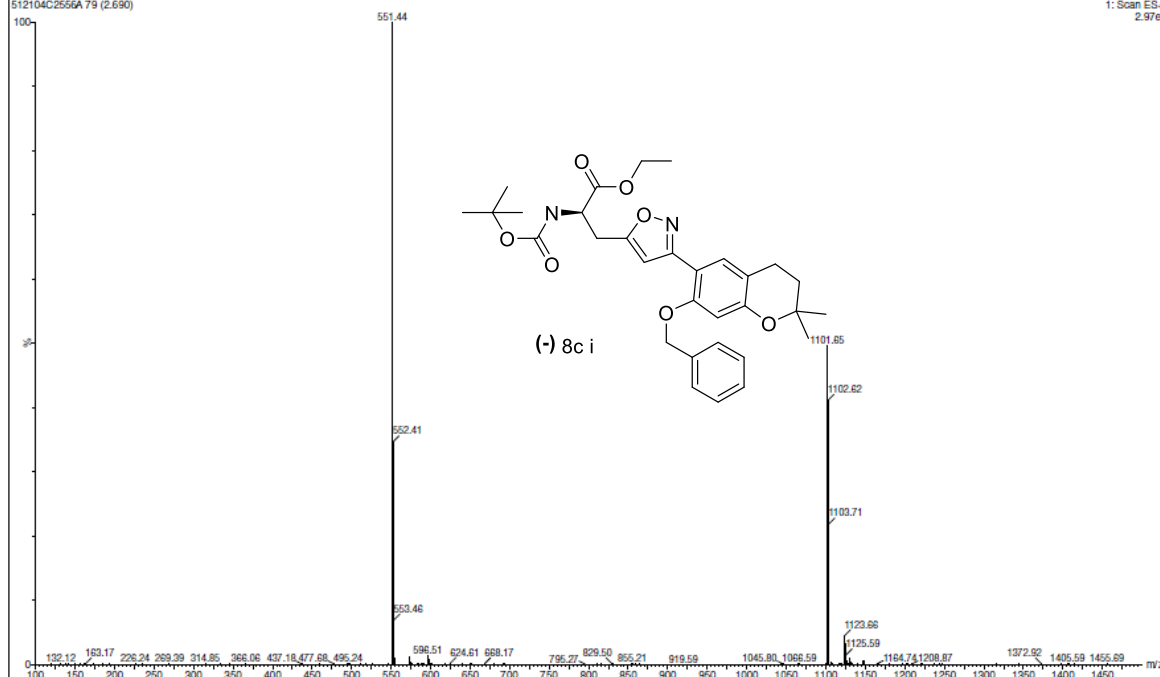


GVK-RAG-1-57 PEAK 1

Acq Method Formic Acid_4.0 Min
512104C2556A 79 (2.690)

GVK Bio Sciences Pvt Ltd
Discovery Chemistry - Analytical Services

17-Apr-2021
09:23:18
ANL-MCLS-LCMS-007
1: Scan ES-
2.9767





GVK Biosciences Private Limited
Discovery Chemistry - Analytical Services

SFC Analytical Chromatogram

User Name: analyst

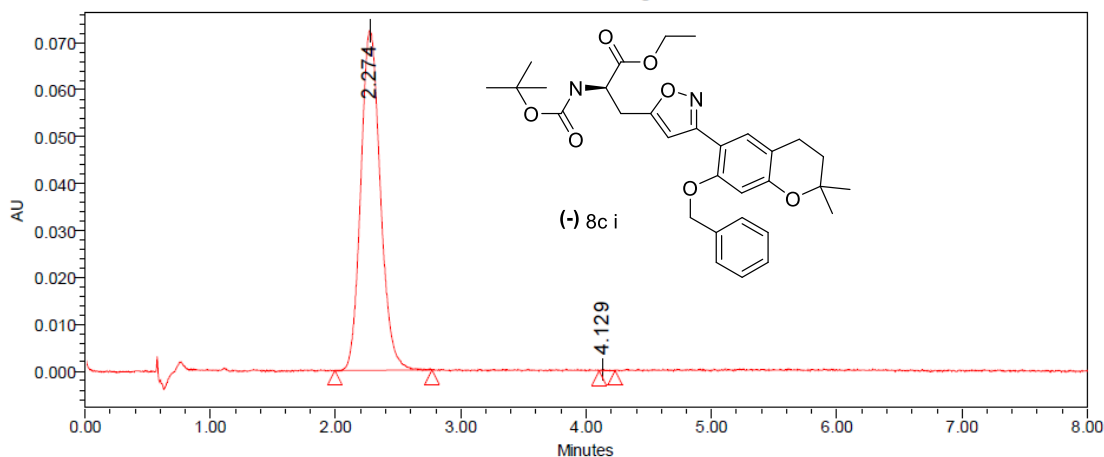
Project Name: 2021\APR-2021\MALLAPUR\ANL-MCL5-SFC-006-APR-2021

Sample Name:	GVK-RAG-1-57-PEAK-1	Acquired By:	MLRAnalyst
Vial:	1:C,2	Sample Set Name:	17_APRIL_2021
Injection Volume:	10.00 ul	Acq. Method Set:	C2_SolvB2_3g_25
Date Acquired:	17-Apr-2021 10:09:36 AM IST	Proc. Chnl. Descr.:	PDA Spectrum PDA 210.0 nm (PDA Spectrum (200-400)nm)

SFC Method Conditions :

Column : CHIRALPAK AD-3 (4.6*150mm)3µm
Co-solvent : Methanol
Total flow : 3g/min
% of Co-Solvent : 25
ABPR : 1500psi
Temperature : 30°C

Auto-Scaled Chromatogram



Peak Results

Name	RT	Area	% Area
1	2.27	787603	99.90
2	4.13	801	0.10

GVK-RAG-1-57 PEAK 1

[Data Information]

Creation Date 17-Apr-2021 17:36

[Measurement Information]

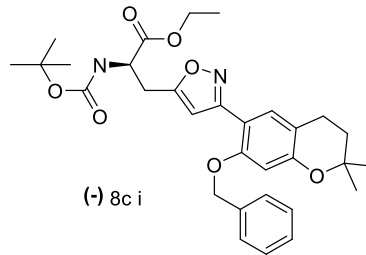
Instrument Name POLARIMETER
Model Name P-2000
Serial No. B160661232
Polarizer Dichrom
Faraday Cell Flint Glass

Accessory PTC-262
Accessory S/N C058861481
Temperature 25.00 C
Control Sensor Holder
Monitor Sensor Holder
Start Mode Start immediately

Light Source WI
Monitor wavelength 589 nm
D.I.T. 5 sec
No. of cycle 5
Cycle interval 5 sec
Temp. Monitor Holder
Temp. Corr. Factor None
Aperture(S) 8.0mm
Aperture(L) Auto
Mode Specific O.R.
Path Length 50 mm
Concentration 0.2 w/v%
Water content of sample 0 %
Factor 1

[Comment]

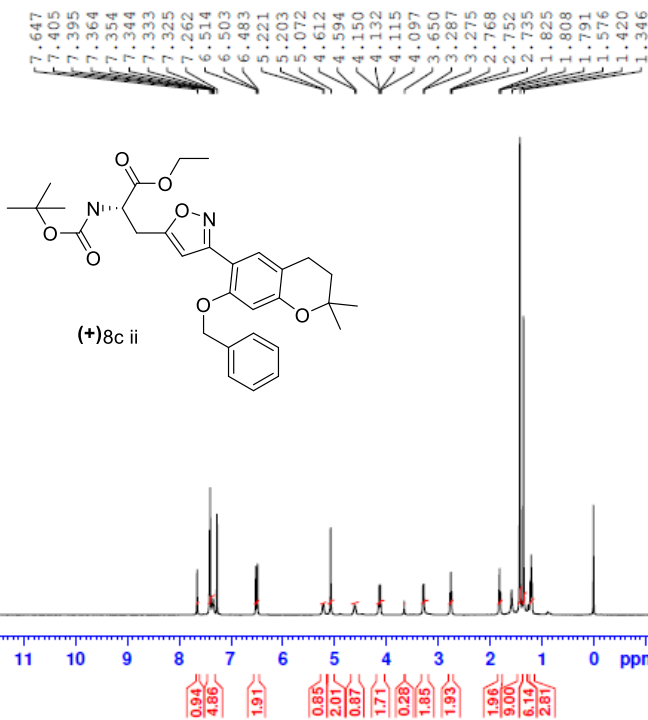
Sample name GVK-RAG-1-57 PEAK 1
Comment CONC= 0.2% in MeOH
User
Division
Company GVK BIO SCIENCES PVT LTD



	No.	Sample No.	Mode	Calc. Data	Meas. Data	Monitor(deg)	PMT Voltage[V]	
1	*	1	GVK-RAG-1-57 PEAK 1-1	Specific O.R.	-0.9000	-0.0009	-0.0015	253
2	*	2	GVK-RAG-1-57 PEAK 1-2	Specific O.R.	-1.5000	-0.0015	-0.0021	253
3	*	3	GVK-RAG-1-57 PEAK 1-3	Specific O.R.	-1.4000	-0.0014	-0.0020	253
4	*	4	GVK-RAG-1-57 PEAK 1-4	Specific O.R.	-1.1000	-0.0011	-0.0017	253
5	*	5	GVK-RAG-1-57 PEAK 1-5	Specific O.R.	-1.3000	-0.0013	-0.0019	253
6	*	6	Avg.		-1.2400			
7		7	S.D		0.2408			
8		8	C.V		19.4219			

	Temperature(C)	Blank	Measurement Date	Comment
1	24.99	-0.0006	17-Apr-2021 17:35	
2	24.99	-0.0006	17-Apr-2021 17:35	
3	24.99	-0.0006	17-Apr-2021 17:36	
4	25.00	-0.0006	17-Apr-2021 17:36	
5	25.00	-0.0006	17-Apr-2021 17:36	
6				
7				
8				

GVK-REAG-2-57 PEAK 2



Current Data Parameters
 NAME: 512104C2134-09-5-REAG-2-57 PEAK 2
 EXPNO: 1
 PROCNO: 1

F2 - Acquisition Parameters
 Date_: 20210417
 Time: 3.42 h
 INSTRUM: Avance
 PROCNO: 2163731_0135_1
 PULPROG: zg30
 TD: 65536
 SOLVENT: CDCl3
 NS: 8
 DS: 0
 SWH: 8196.722 Hz
 FIDRES: 0.250144 Hz
 AQ: 3.9974959 sec
 RG: 101
 CW: 61.000 usec
 DE: 13.89 usec
 TE: 292.7 K
 DQ: 1.0000000 sec
 TDO: 1
 SFO1: 400.3024719 MHz
 NUC1: 1H
 P0: 2.67 usec
 F1: 8.00 usec
 PL1: 22.47400093 W

F2 - Processing parameters
 SI: 65536
 SF: 400.3000091 MHz
 NH: 8M
 SSB: 0
 LB: 1.00 Hz
 GB: 0
 PC: 1.00

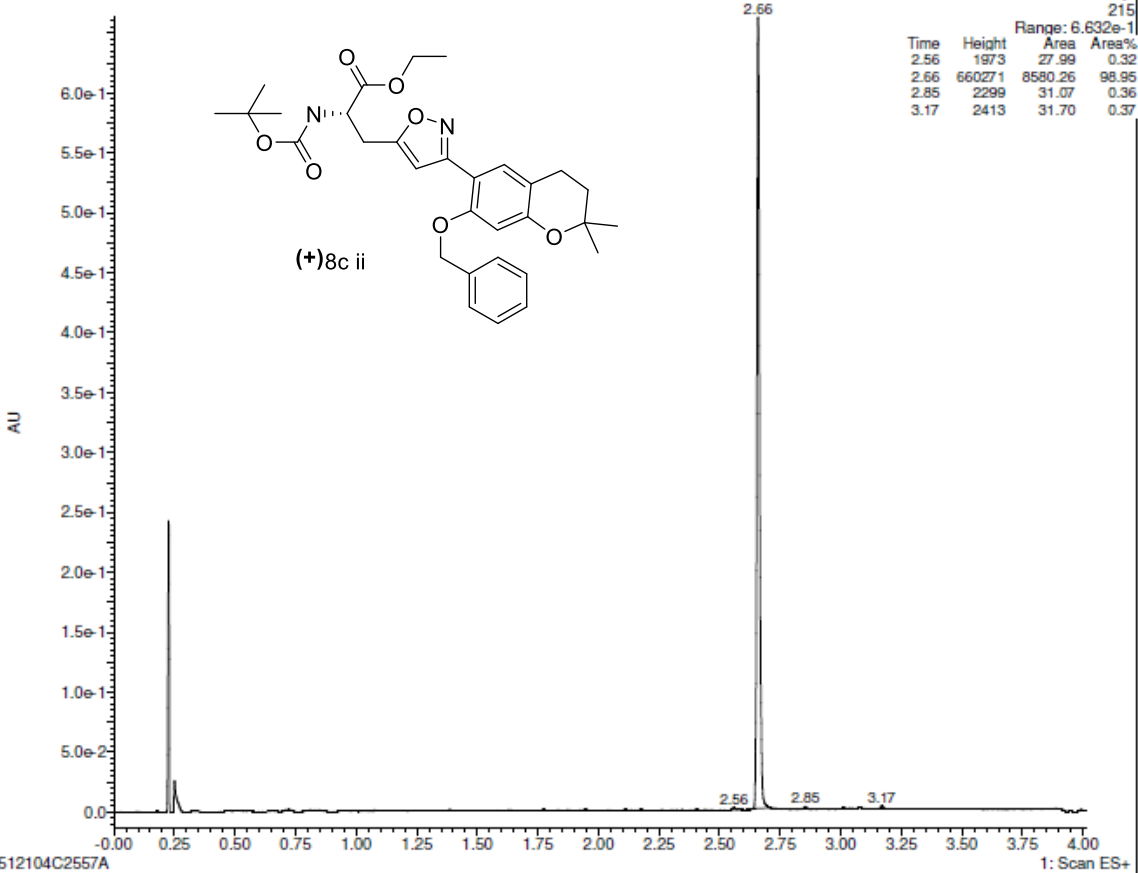
ANL-MCL5-NMR-003

Acq Method Formic Acid_4.0 Min

ANL-MCL5-LCMS-007

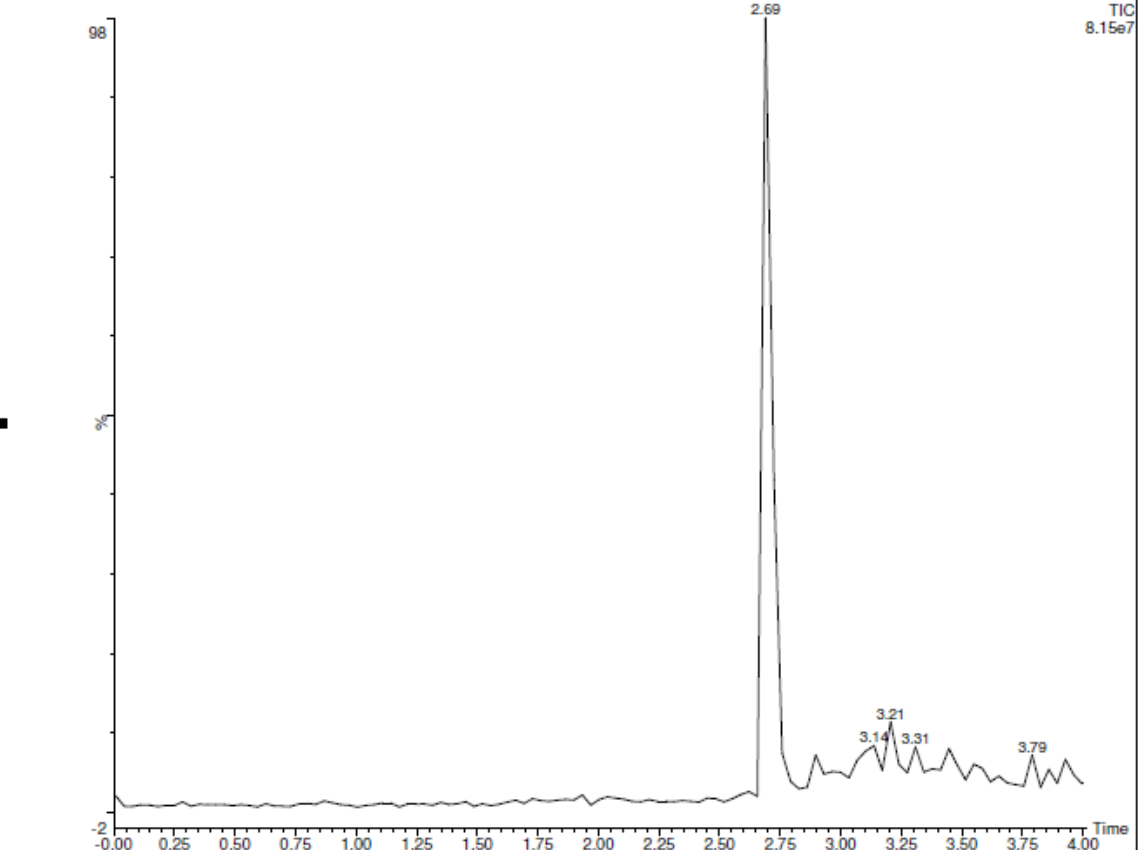
512104C2557A

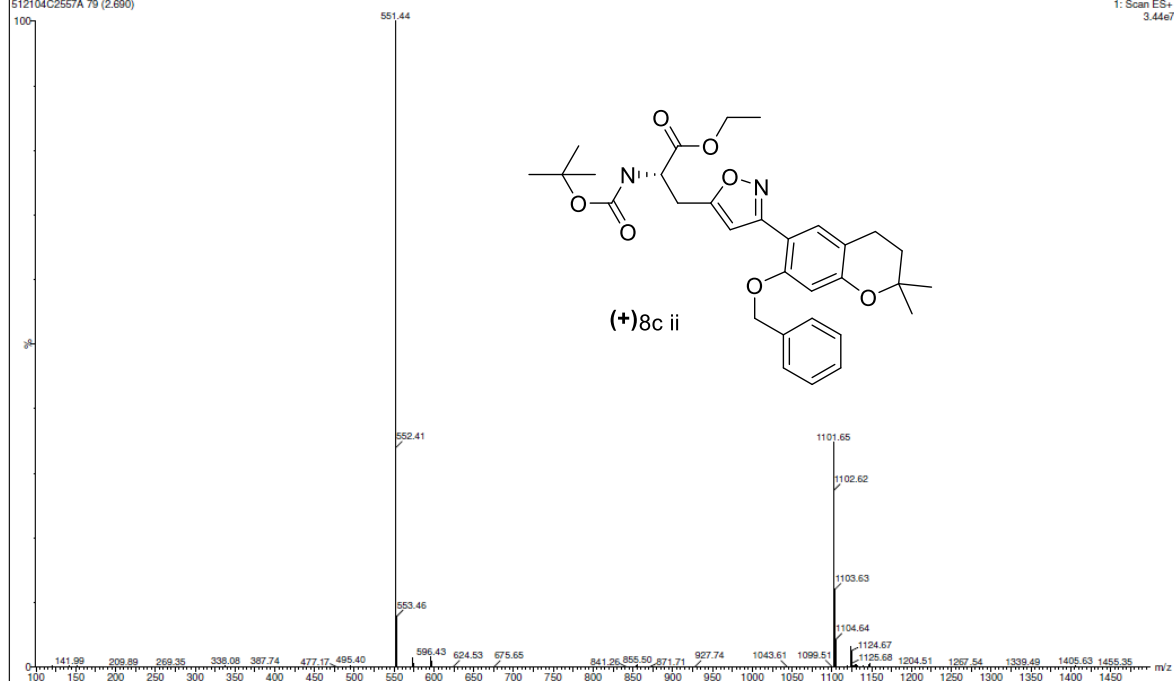
5: DiodeArray



512104C2557A

1: Scan ES+







GVK Biosciences Private Limited
Discovery Chemistry - Analytical Services

SFC Analytical Chromatogram

User Name: analyst

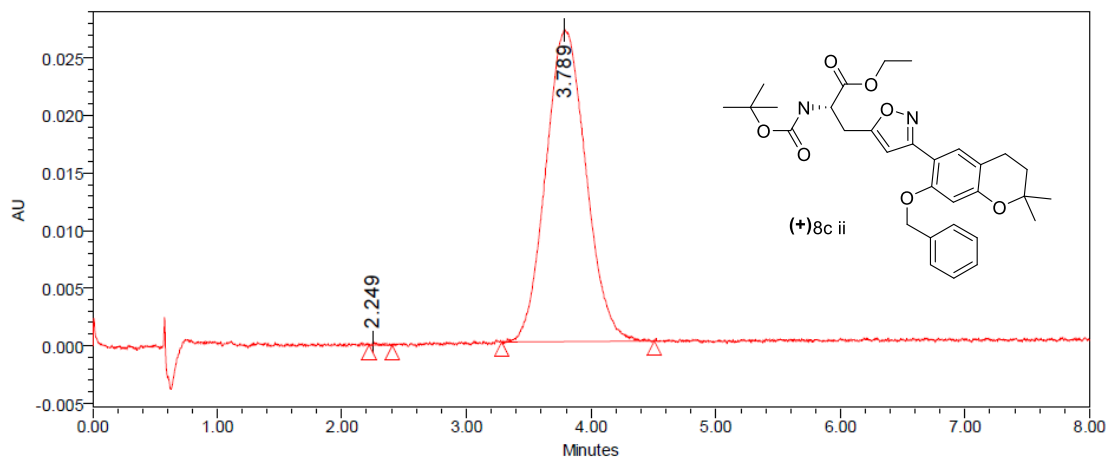
Project Name: 2021\APR-2021\MALLAPUR\ANL-MCL5-SFC-006-APR-2021

Sample Name:	GVK-RAG-1-57-PEAK-2	Acquired By:	MLRAnalyst
Vial:	1:C,1	Sample Set Name:	17_APRIL_2021
Injection Volume:	10.00 ul	Acq. Method Set:	C2_SolVB2_3g_25
Date Acquired:	17-Apr-2021 09:53:22 AM IST	Proc. Chnl. Descr.:	PDA Spectrum PDA 210.0 nm (PDA Spectrum (200-400)nm)

SFC Method Conditions :

Column : CHIRALPAK AD-3 (4.6*150mm)3µm
Co-solvent : Methanol
Total flow : 3g/min
% of Co-Solvent : 25
ABPR : 1500psi
Temperature : 30°C

Auto-Scaled Chromatogram



Peak Results

Name	RT	Area	% Area
1	2.25	876	0.14
2	3.79	607350	99.86

Report Template: Chiral Report

Print Date & Time: 17-Apr-2021 11:43:31 AM Asia/Kolkata

C5748-PEAK 2

[Data Information]

Creation Date 17-Apr-2021 17:49

[Measurement Information]

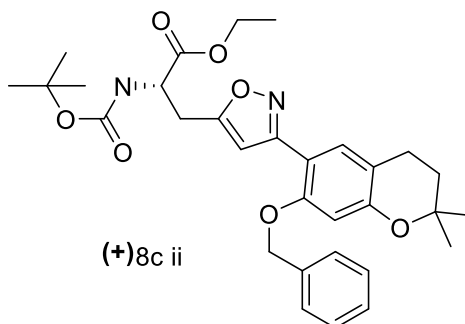
Instrument Name POLARIMETER
Model Name P-2000
Serial No. B160661232
Polarizer Dichrom
Faraday Cell Flint Glass

Accessory PTC-262
Accessory S/N C058861481
Temperature 25.00 C
Control Sensor Holder
Monitor Sensor Holder
Start Mode Start immediately

Light Source W1
Monitor wavelength 589 nm
D.I.T. 5 sec
No. of cycle 5
Cycle interval 5 sec
Temp. Monitor Holder
Temp. Corr. Factor None
Aperture(S) 8.0mm
Aperture(L) Auto
Mode Specific O.R.
Path Length 50 mm
Concentration 0.2 w/v%
Water content of sample 0 %
Factor 1

[Comment]

Sample name C5748-PEAK 2
Comment CONC= 0.2% in MeOH
User
Division
Company GVK BIO SCIENCES PVT LTD



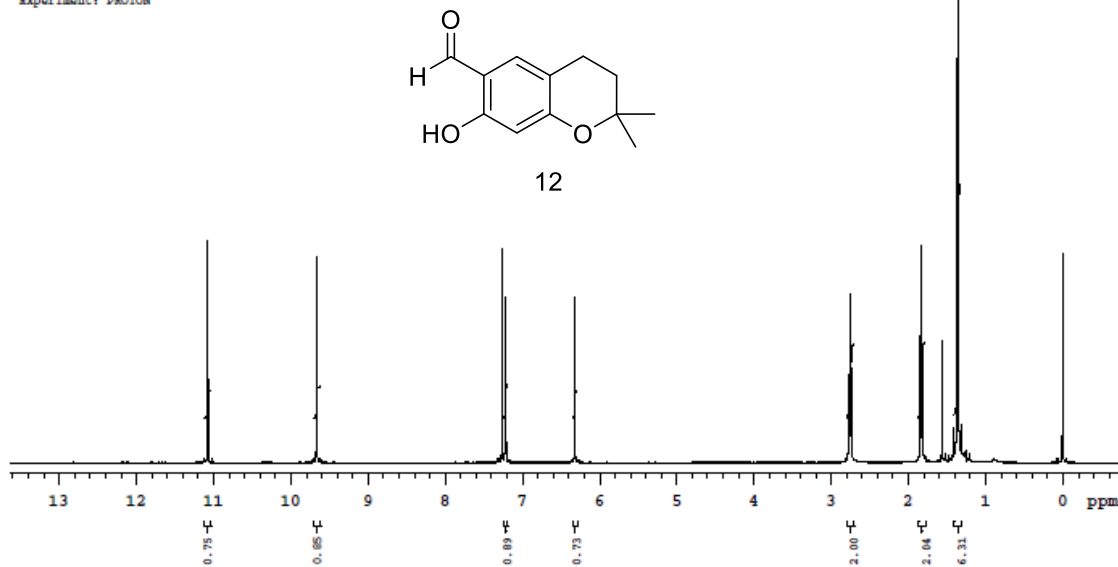
	No.	Sample No.	Mode	Calc. Data	Meas. Data	Monitor(deg)	PMT Voltage[V]	Temperature(C)
1	*	1 C5748-PEAK 2-1	Specific O.R.	+1.8000	+0.0018	+0.0012	263	25.00
2	*	2 C5748-PEAK 2-2	Specific O.R.	+1.7000	+0.0017	+0.0011	263	25.00
3	*	3 C5748-PEAK 2-3	Specific O.R.	+1.9000	+0.0019	+0.0013	263	24.99
4	*	4 C5748-PEAK 2-4	Specific O.R.	+1.5000	+0.0015	+0.0009	263	25.00
5	*	5 C5748-PEAK 2-5	Specific O.R.	+0.9000	+0.0009	+0.0003	263	25.00
6	*	6 Avg.		+1.5600				
7		7 S.D		0.3975				
8		8 C.V		25.4803				

	Blank	Measurement Date	Comment
1	-0.0006	17-Apr-2021 17:49	
2	-0.0006	17-Apr-2021 17:49	
3	-0.0006	17-Apr-2021 17:49	
4	-0.0006	17-Apr-2021 17:49	
5	-0.0006	17-Apr-2021 17:49	
6			
7			
8			

GVK-RAG-1-33
AR NO-NMR/18/03/0977

Reference Code: 511803A8655-GVK-RAG-1-33
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2018/Mar
Agilent 400-MXDD2
Data collected on: Mar 9 2018
Experiment: PROTON

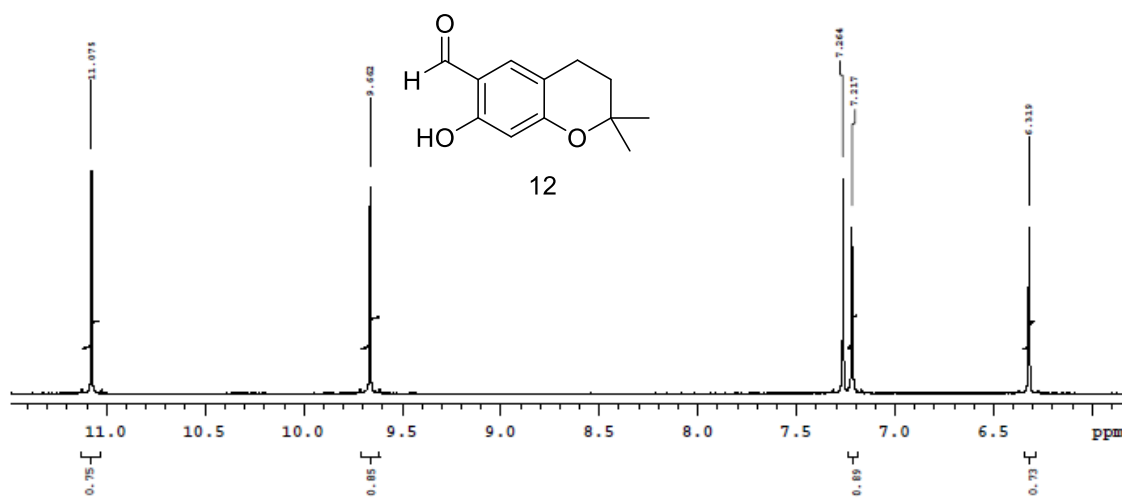
edb17206003



GVK-RAG-1-33
AR NO-NMR/18/03/0977

Reference Code: 511803A8655-GVK-RAG-1-33
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2018/Mar
Agilent 400-MXDD2
Data collected on: Mar 9 2018
Experiment: PROTON

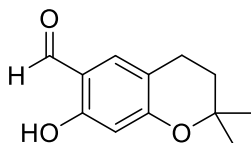
edb17206003



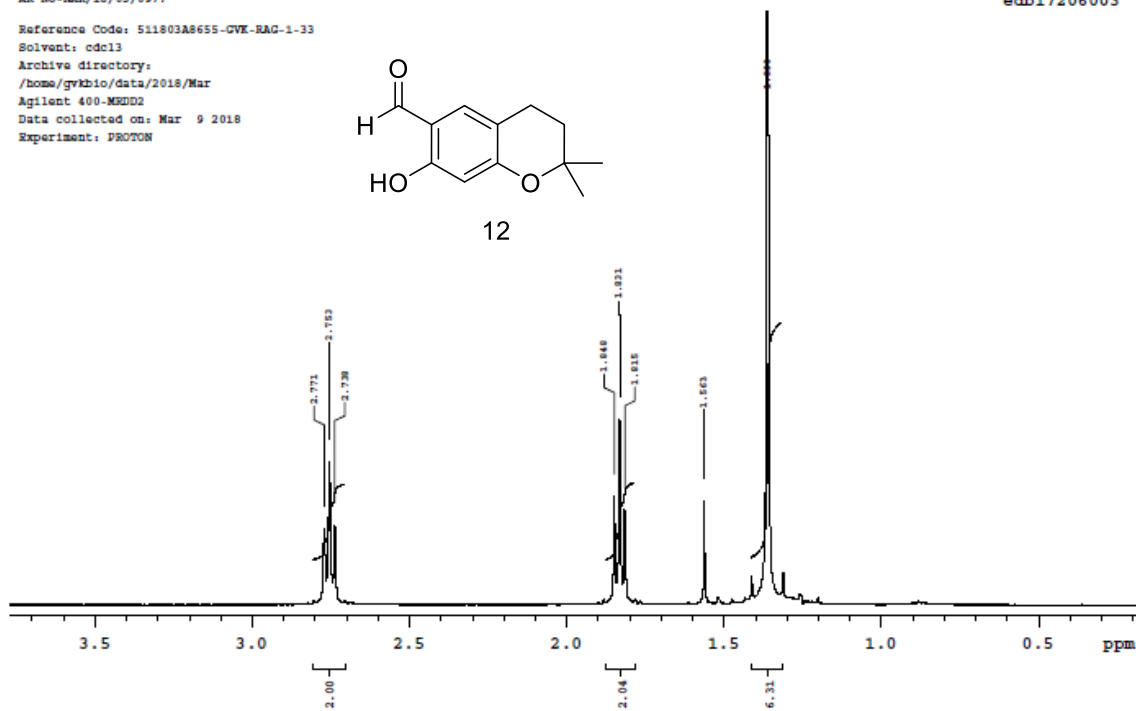
GVK-RAG-1-33
AR NO-NMR/18/03/0977

edb17206003

Reference Code: 511803A8655-GVK-RAG-1-33
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2018/Mar
Agilent 400-MEED2
Data collected on: Mar 9 2018
Experiment: PROTON



12



GVK Biosciences (Pvt.) Ltd.
Analytical Research and Development

Data File:	BG_511803A8654	Sample Name :	P-3323-8-FMC-GVK-G4920-40
Instrument Name :	N/A	Injection Volume(μl):	2.00
Comments:		Vial:	GE7
Sample Type:	Unknown	Run Time(min):	5.01
Acquisition Date:	03/09/18 05:45:29 PM		

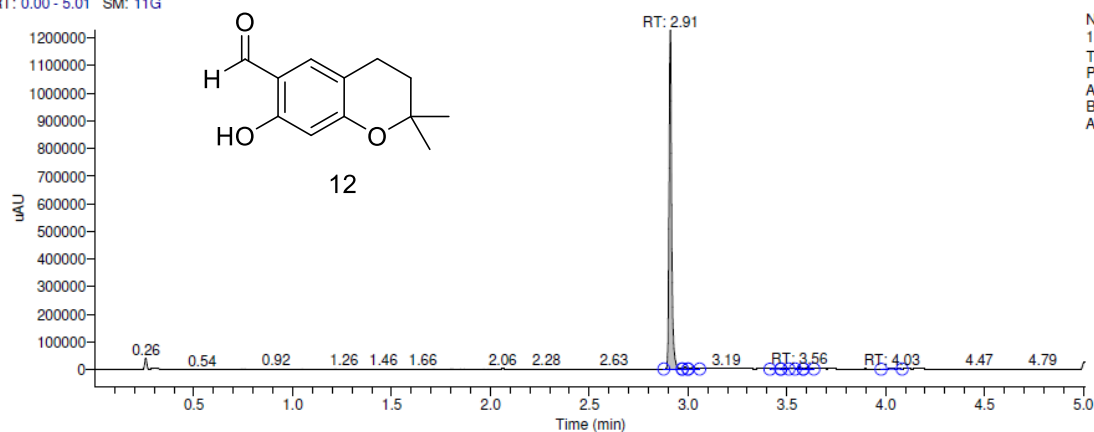
LC Method Details :

Method : GVK_5MIN; GVK_LCMS_40
 Mobile Phase A: 0.1% FA in Water
 Mobile Phase B: 0.1% FA in ACN
 Gradient % of B: 0/80,8/80
 Flow : 0.8ml/min
 Column : Acquity UPLC BEH C18, 2.1*50mm, 1.7um,
 Column temperature : 40c

Detector Type: PDA
 Wavelength Range 1 (nm): N/A

UV Chromatogram

RT: 0.00 - 5.01 SM: 11G

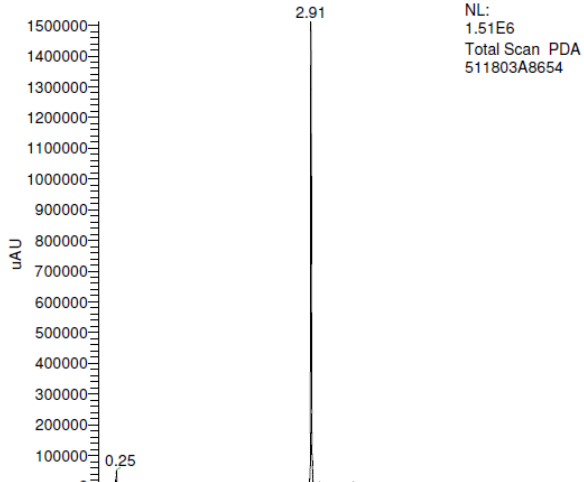


RT	Peak Height	Peak Area	Area %
2.91	1226029.98	1165595.71	95.37
2.99	7239.23	7425.10	0.61
3.03	8169.62	9797.23	0.80
3.43	3243.98	8213.00	0.67
3.49	4485.95	6531.16	0.53
3.56	6635.38	8743.25	0.72
3.60	6213.84	9172.04	0.75
4.03	2100.58	6669.41	0.55

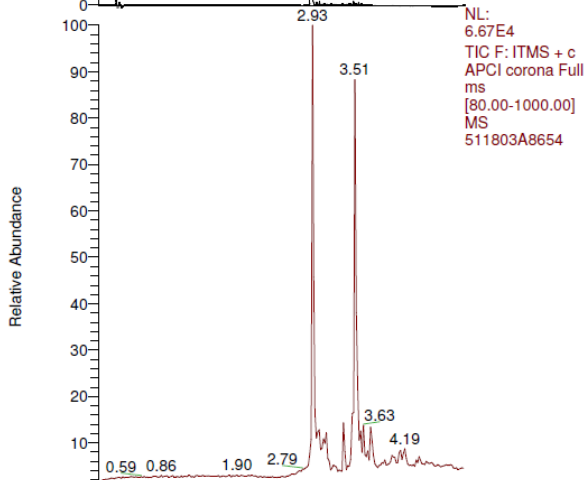
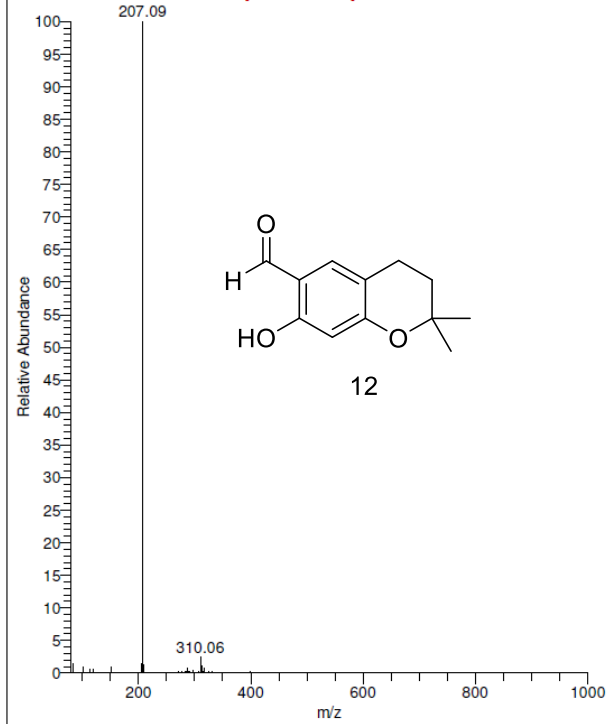
Operator: Thermo Scientific
 Instrument Name: N/A

Page 1 of 1
 Friday, March 09, 2018, 17:46:04

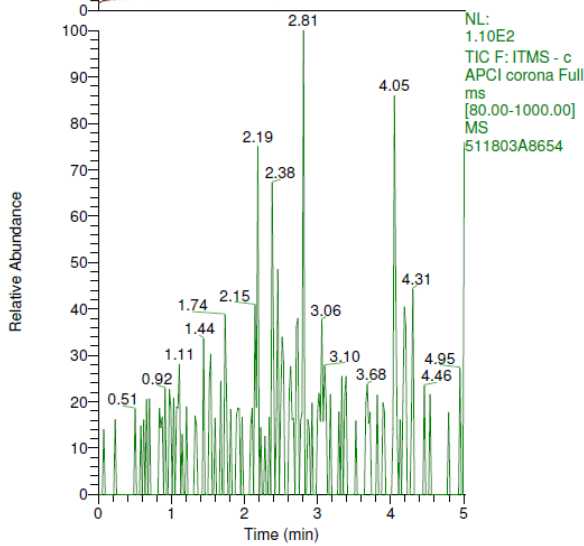
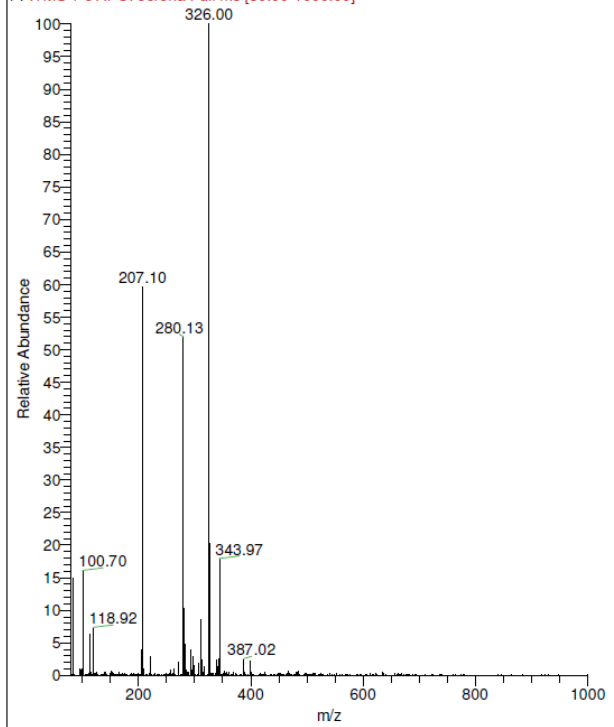
IT: 0.00 - 5.01



511803A8654 #303 RT: 2.95 AV: 1 NL: 2.30E4
F: ITMS + c APCI corona Full ms [80.00-1000.00]

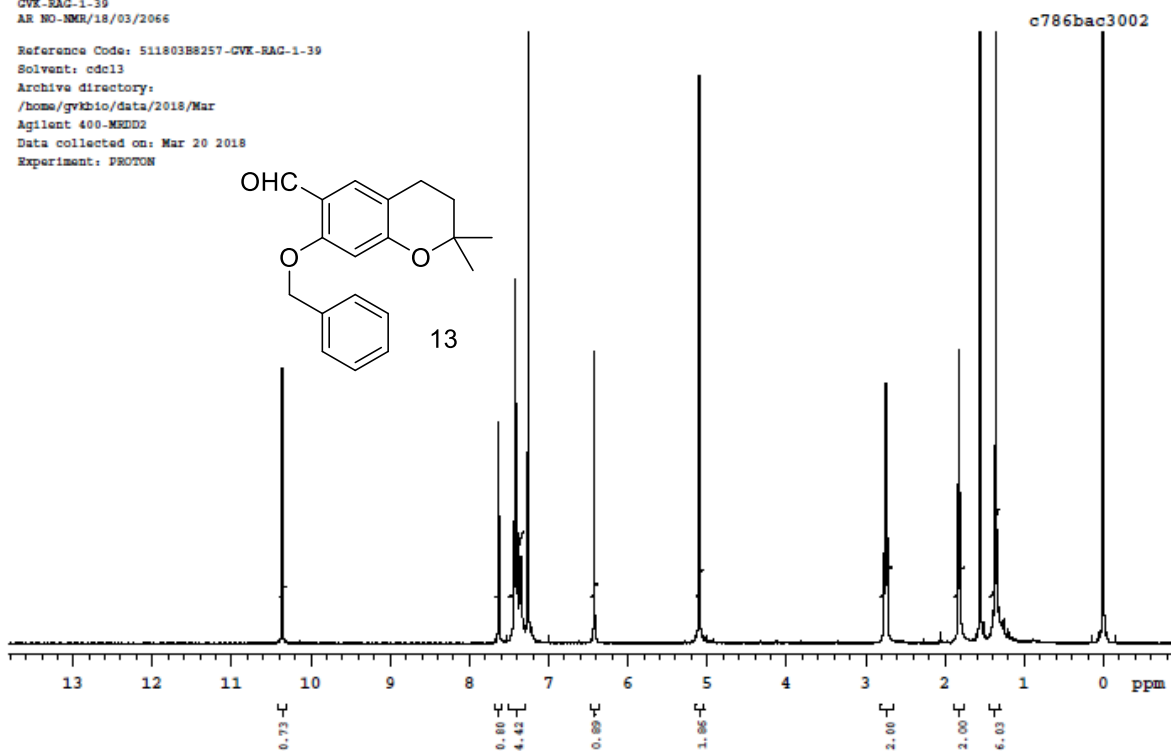
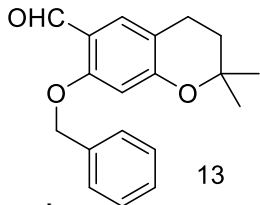


511803A8654 #311 RT: 3.03 AV: 1 NL: 1.94E3
F: ITMS + c APCI corona Full ms [80.00-1000.00]



GVK-RAG-1-39
AR NO-NMR/18/03/2066

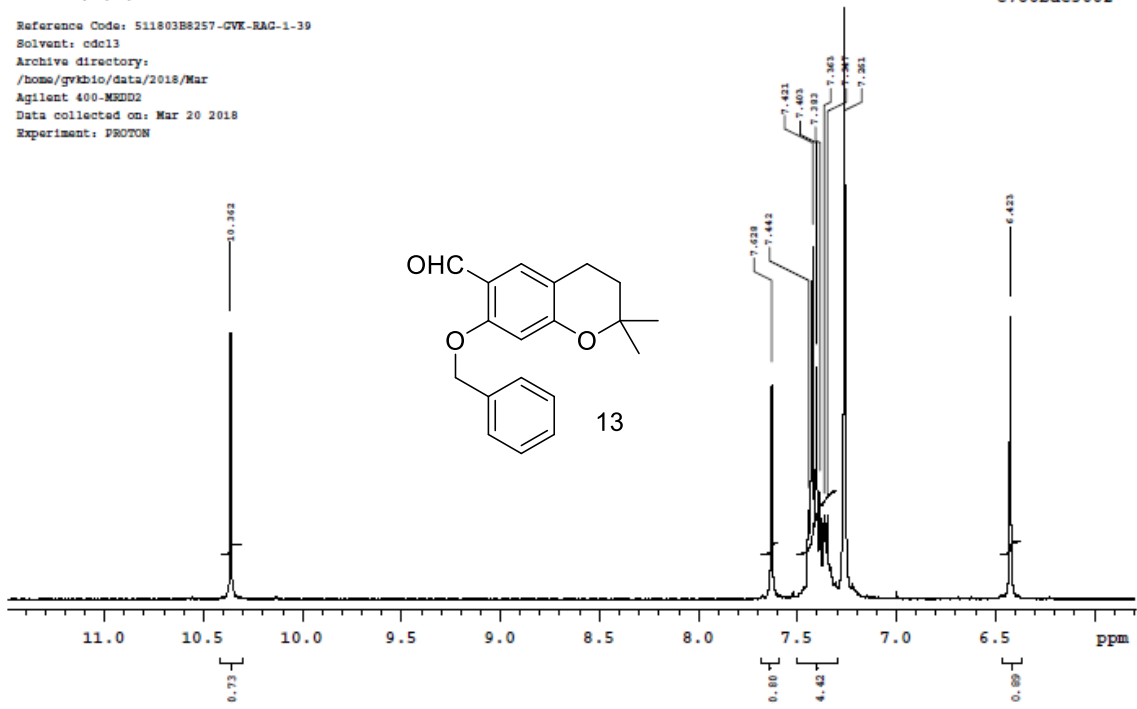
Reference Code: 511803B8257-GVK-RAG-1-39
Solvent: cdcl3
Archive directory:
/home/gvkhio/data/2018/Mar
Agilent 400-MRDD2
Data collected on: Mar 20 2018
Experiment: PROTON



GVK-RAG-1-39
AR NO-NMR/18/03/2066

c786bac3002

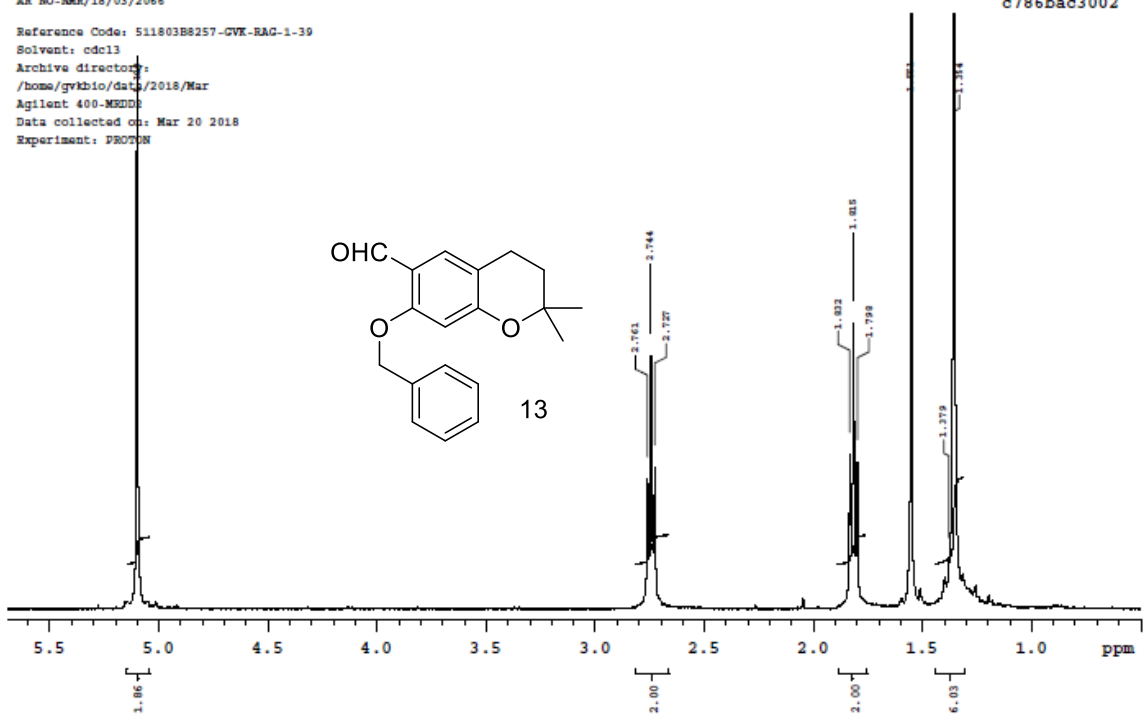
Reference Code: 511803B8257-GVK-RAG-1-39
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2018/Mar
Agilent 400-MXDD2
Data collected on: Mar 20 2018
Experiment: PROTON



GVK-RAG-1-39
AR NO-NMR/18/03/2066

c786bac3002

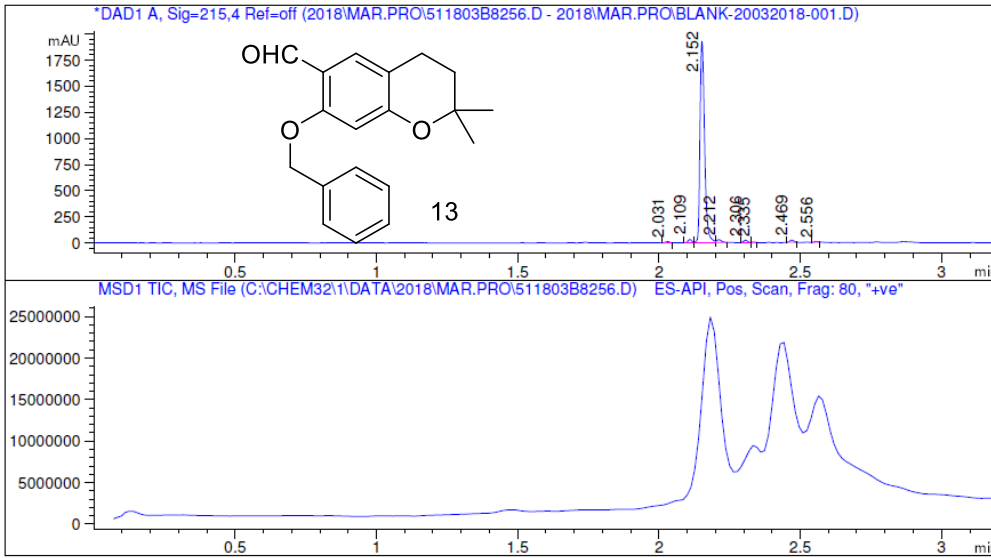
Reference Code: 511803B8257-GVK-RAG-1-39
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2018/Mar
Agilent 400-MXDD2
Data collected on: Mar 20 2018
Experiment: PROTON



LC/MS REPORT

 Date of Analysis : 3/20/2018 TIME : 3:06:14 PM Vial position: P1-A-03
 Sample Name : GVK-RAG-1-39 Injection Vol: 0.300 µL
 Acq. Method : C:\CHEM32\1\METHODS\RND-FA-3.2-MIN.M Instrument Name:ANL-MCL5-LCMS-002

Acq Method Conditions : RND-FA-3.2-MIN
 Column : Acquity UPLC BEH C18 (50mmx2.1 mm,1.7µm)
 Mobile phase:A: 0.1% of Formic Acid in Water,B: 0.1% of Formic acid in Acetonitrile
 Gradient : Time(min)/ %B 0/2,0.2/2,1.5/98,2.6/98,2.61/2,3.2/2
 Column temperature :45 C,Flow rate :0.8 ml/mn



DAD1 A, Sig=215,4 Ref=off

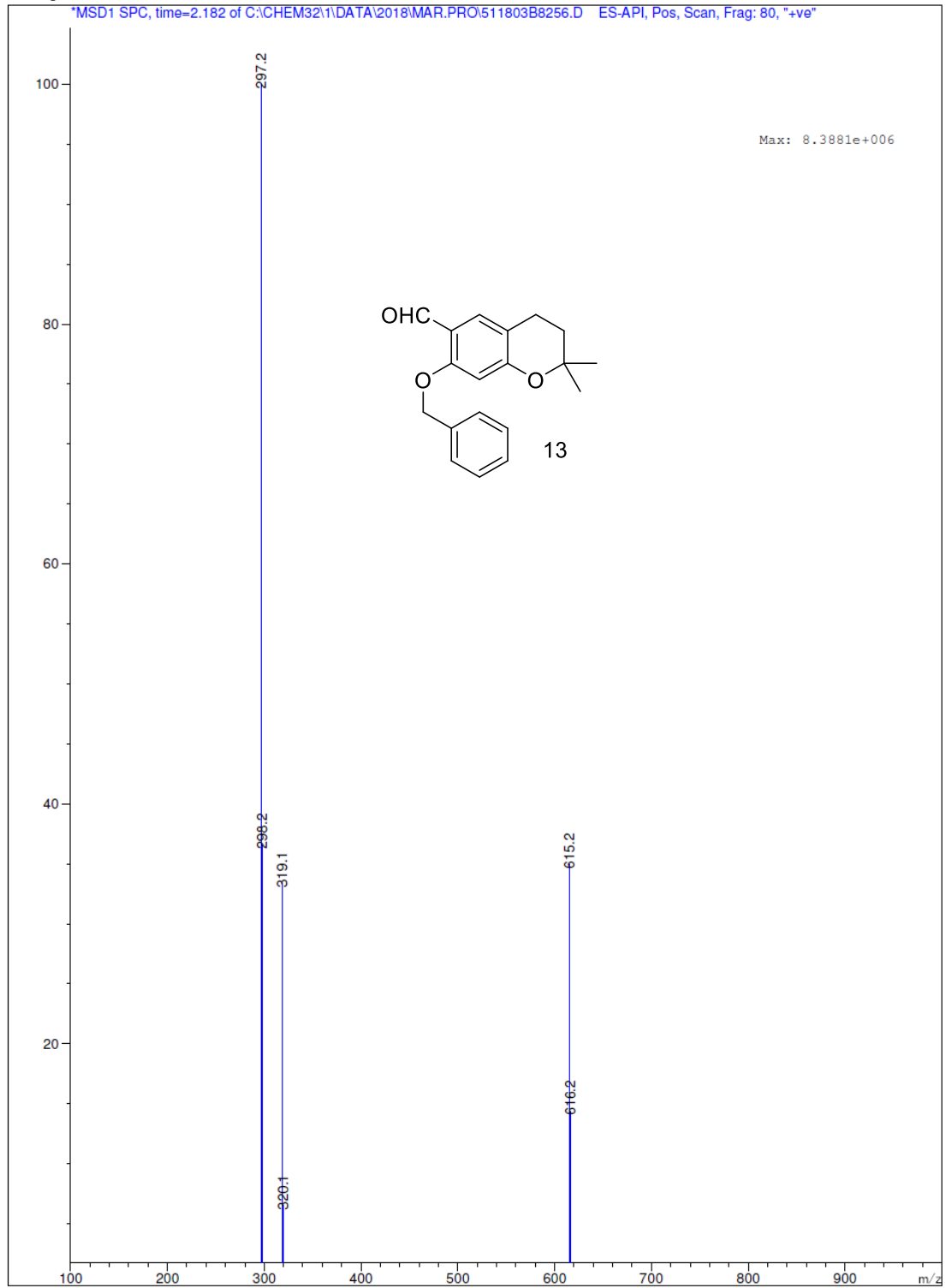
PEAK No	RT min	Height	Area	Area %
1	2.031	12.089	13.044	0.574
2	2.109	32.577	29.667	1.306
3	2.152	1.936e3	2144.274	94.360
4	2.212	27.662	32.752	1.441
5	2.306	20.950	19.598	0.862
6	2.335	3.254	2.783	0.122
7	2.469	20.614	21.121	0.929
8	2.556	8.668	9.187	0.404

MSD1 TIC, MS File

PEAK No	RT min	Height	Area	Area %

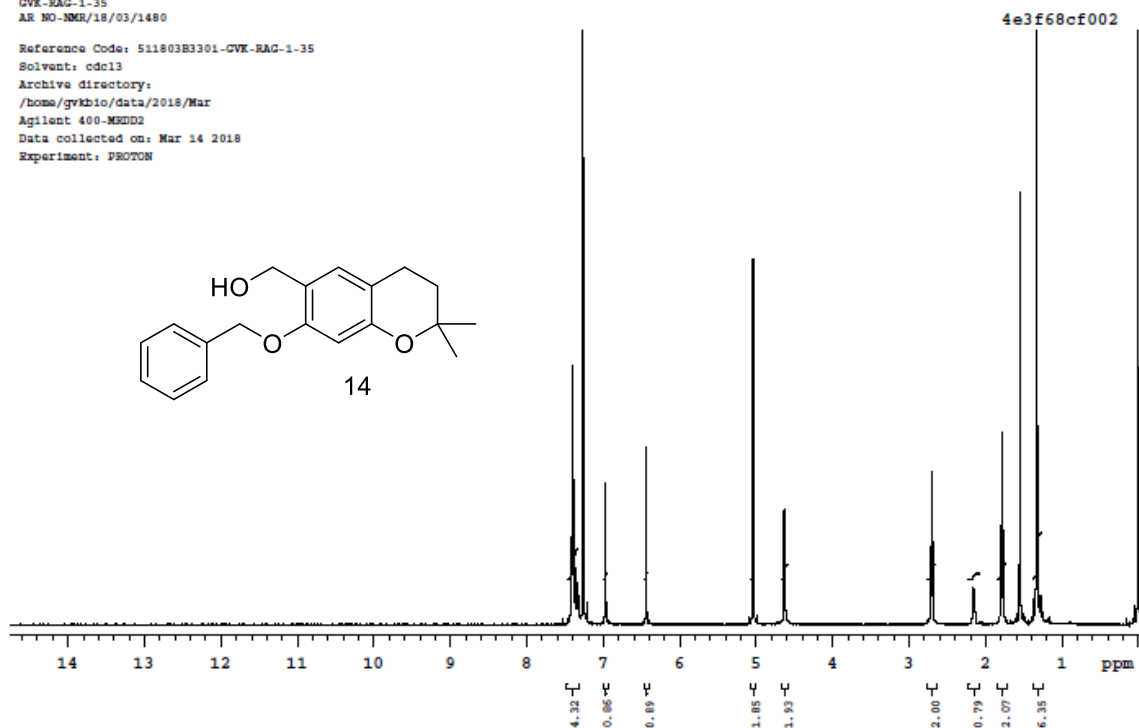
MS Spectrum

*MSD1 SPC, time=2.182 of C:\CHEM32\1\DATA\2018\MAR.PRO\511803B8256.D ES-API, Pos, Scan, Frag: 80, "+ve"



GVK-RAG-1-35
AR NO-NMR/18/03/1480

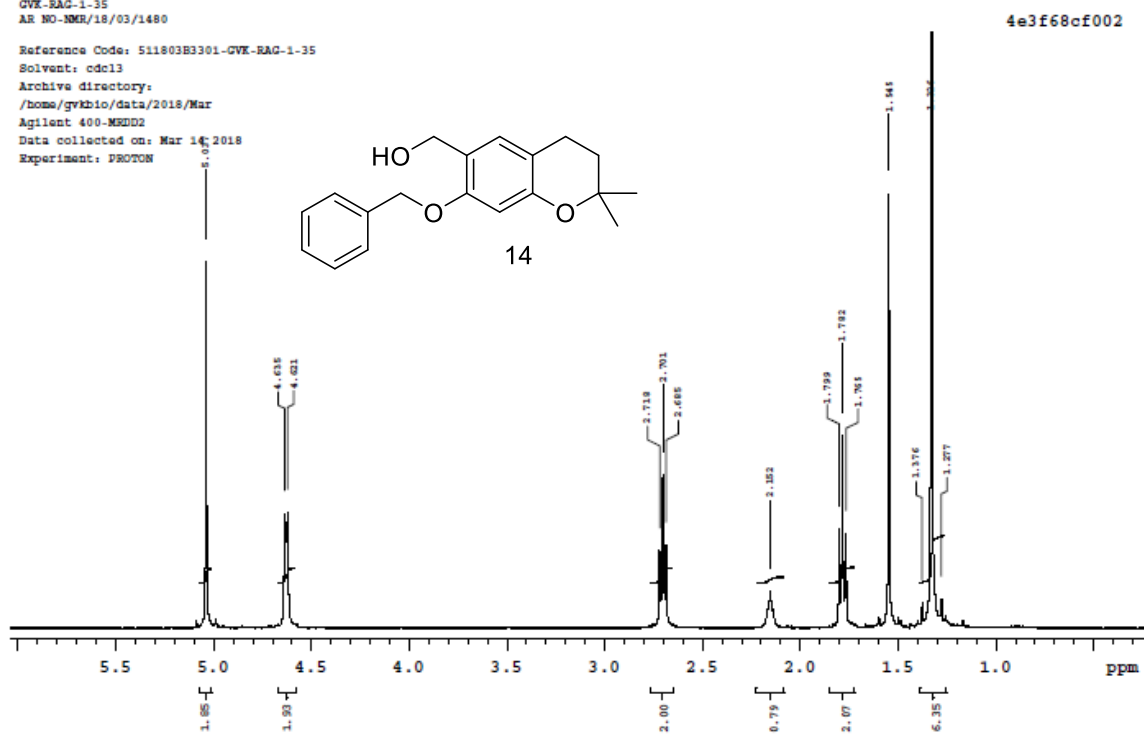
Reference Code: 511803B3301-GVK-RAG-1-35
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2018/Mar
Agilent 400-MKDD2
Data collected on: Mar 14 2018
Experiment: PROTON



Plotname: 511803B3301-GVK-RAG-1-35_PROTON_01.REC_plot01

GVK-RAG-1-35
AR NO-NMR/18/03/1480

Reference Code: 511803B3301-GVK-RAG-1-35
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2018/Mar
Agilent 400-MKDD2
Data collected on: Mar 14 2018
Experiment: PROTON

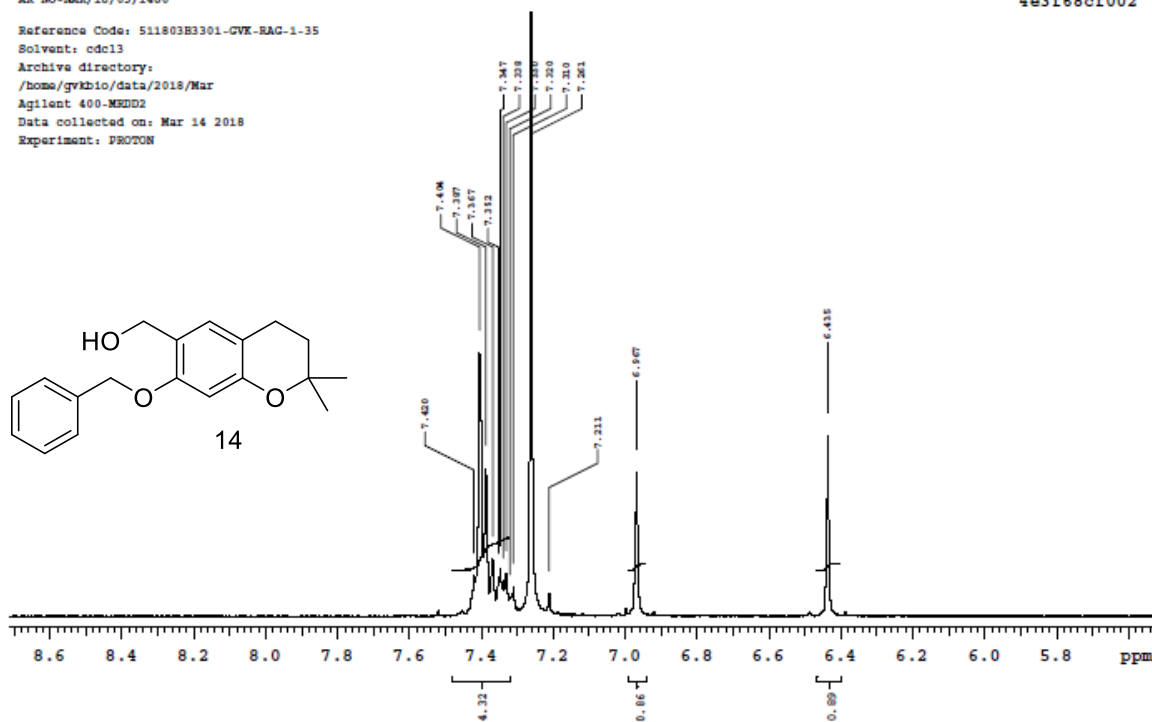


Plotname: 511803B3301-GVK-RAG-1-35_PROTON_01.REC_plot03

GVK-RAG-1-35
AR NO-NMR/18/03/1480

4e3f68cf002

Reference Code: 511803B3301-GVK-RAG-1-35
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2018/Mar
Agilent 400-MRDD2
Data collected on: Mar 14 2018
Experiment: PROTON

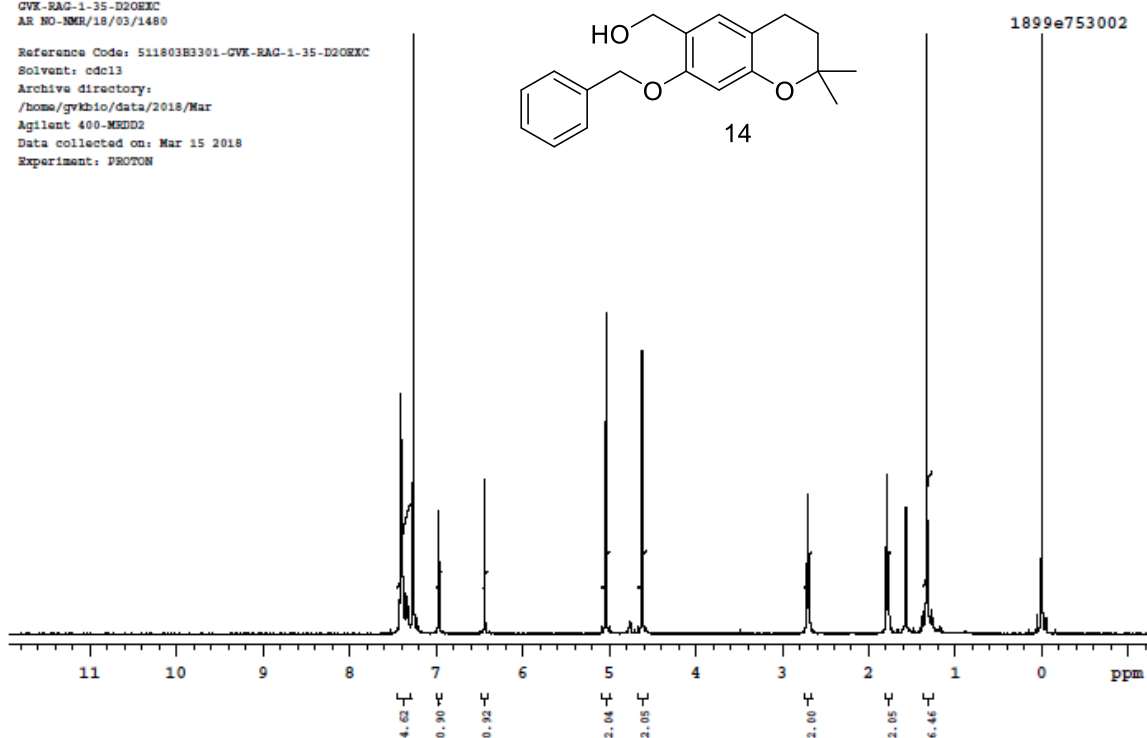


Plotname: 511803B3301-GVK-RAG-1-35_PROTON_01.REC plot02

GVK-RAG-1-35-D2OEXC
AR NO-NMR/18/03/1480

1899e753002

Reference Code: 511803B3301-GVK-RAG-1-35-D2OEXC
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2018/Mar
Agilent 400-MRDD2
Data collected on: Mar 15 2018
Experiment: PROTON



Plotname: 511803B3301-GVK-RAG-1-35-D2OEXC_PROTON_01.REC plot01

GVK Biosciences (Pvt.) Ltd.
Analytical Research and Development

Data File: BG_511803B3300 Sample ID: GVK-RAG-1-35
Sample Type: Unknown Vial: BA4
Instrument Name: N/A Injection Volume(μl): 2.00
Operator: Thermo Scientific Acquisition Date: 03/14/18 09:40:46 PM
Original Data Path: D:\GVKBIO\DATA\2018\DATA\MA R-2018\511803B3300 Run Time(min): 9.99

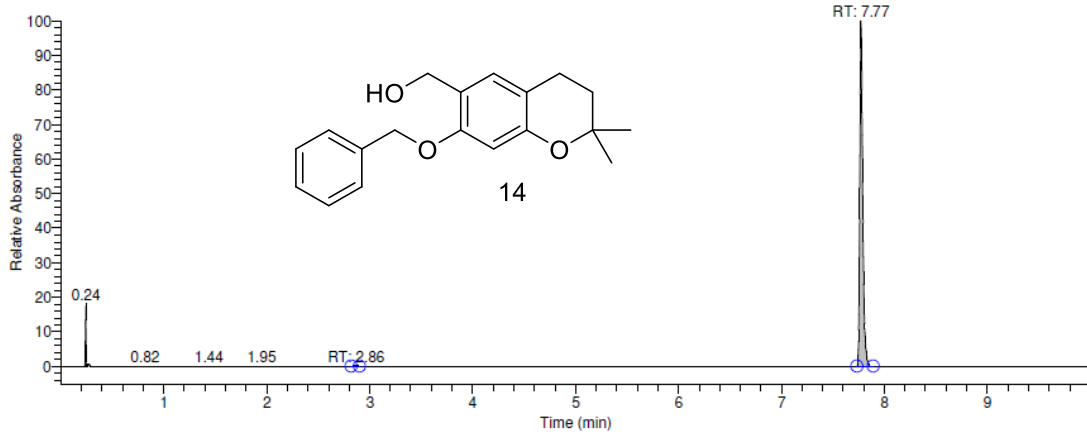
LC Method Details

Method : GVK_10MIN
Mobile Phase A: 0.1% FA in Water
Mobile Phase B: 0.1% FA in ACN
Gradient % of B: 0/2, 0.5/2, 9.5/98, 9.7/98, 10/2
Flow : 0.6ml/min
Column: BEH C18, 2.1*50mm, 1.7um,

Detector Type: PDA
Wavelength Range 1 (nm): 215.00000

UV Chromatogram

RT: 0.00 - 9.99 SM: 5G



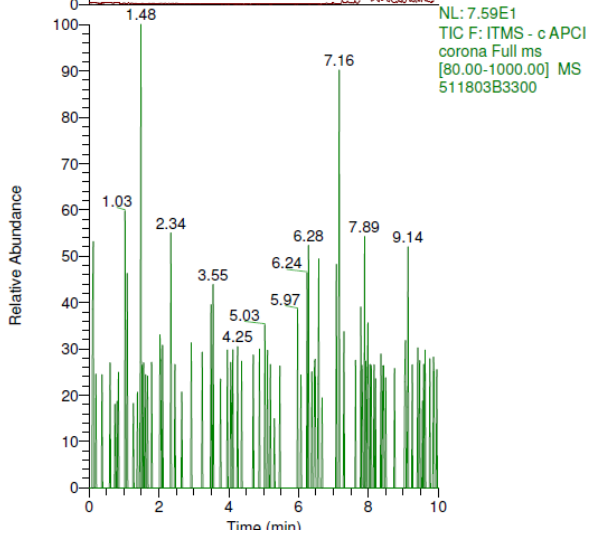
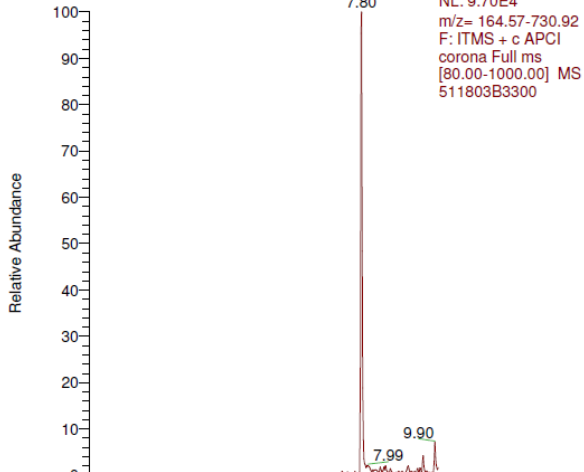
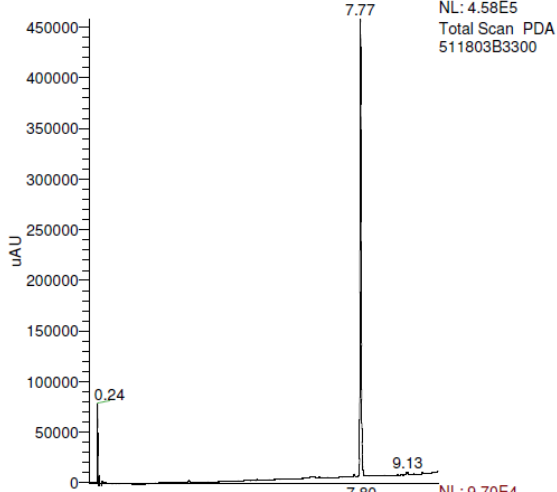
NL:
1.81E6
Spectrum
Maximum
nm=214.5
215.5 PDA
Avalon
BG_511803B:
00

RT	Peak Area	Area %
2.86	9658.10	0.25
7.77	3786128.60	99.75

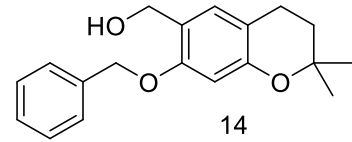
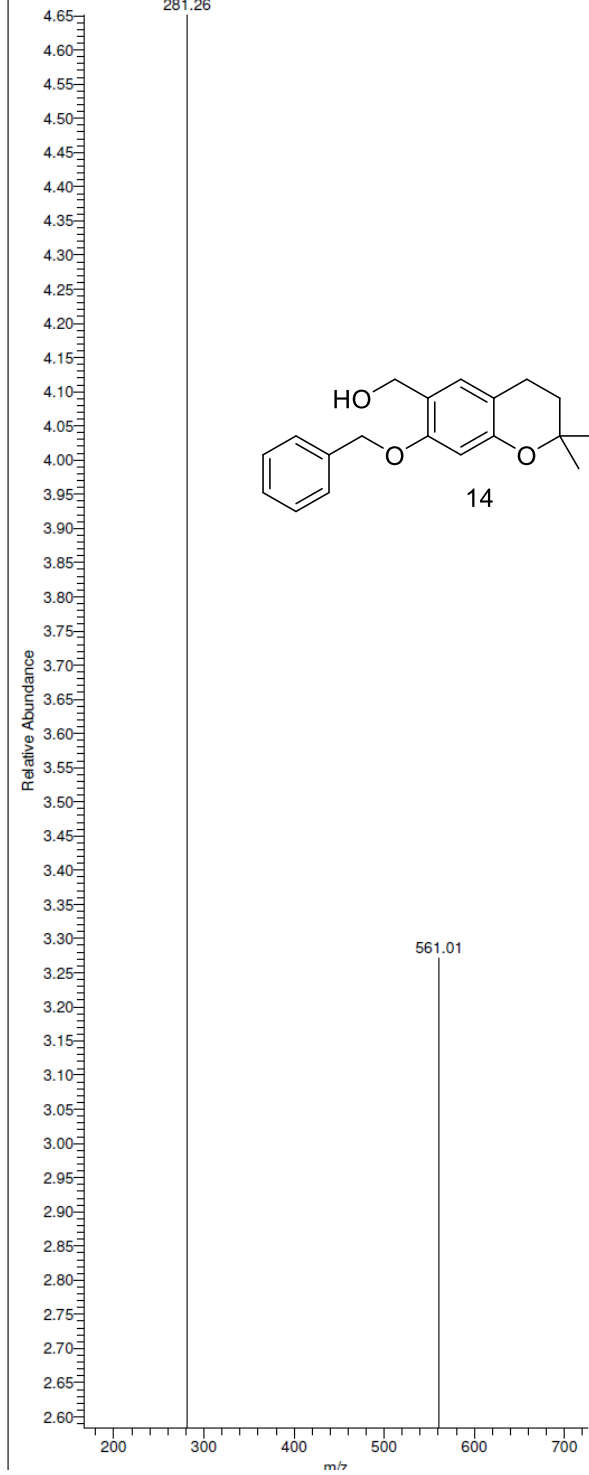
Operator: Thermo Scientific
Instrument Name: N/A

Page 1 of 1
Wednesday, March 14, 2018, 21:42:16

RT: 0.00 - 10.02

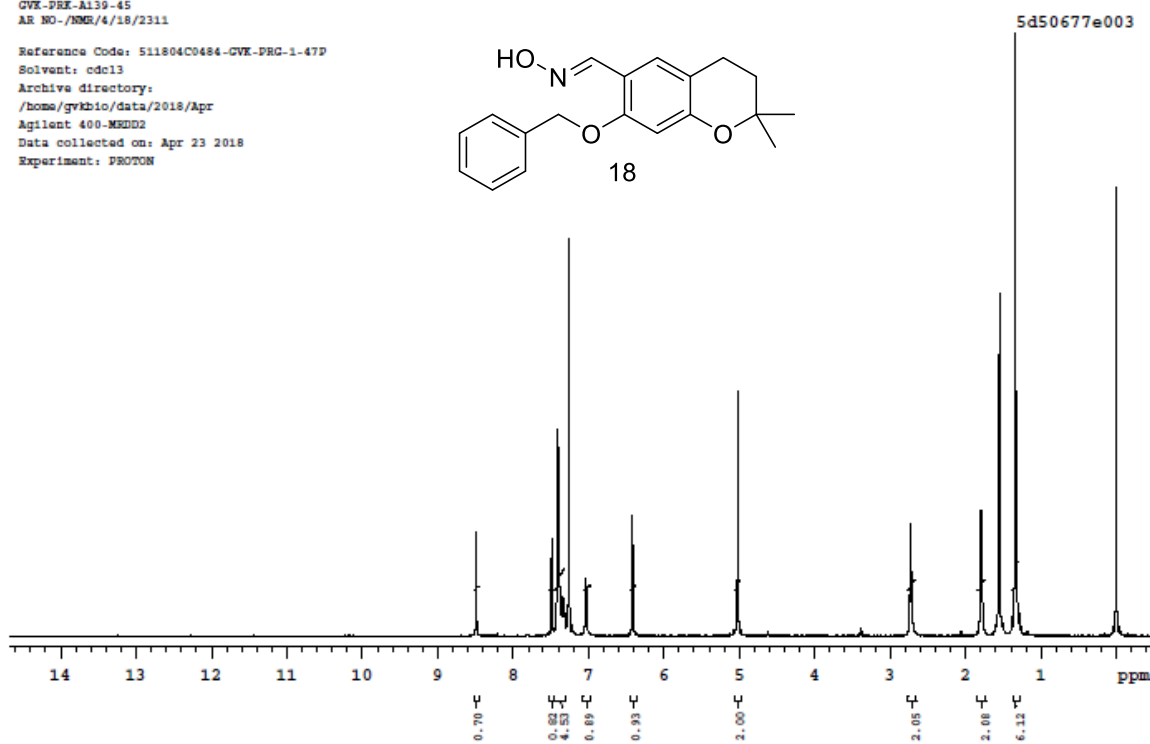
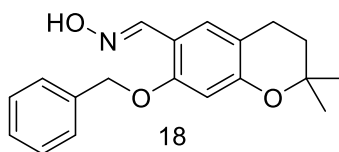


511803B3300 #801 RT: 7.80 AV: 1 NL: 8.31E4
F: ITMS + c APCI corona Full ms [80.00-1000.00]



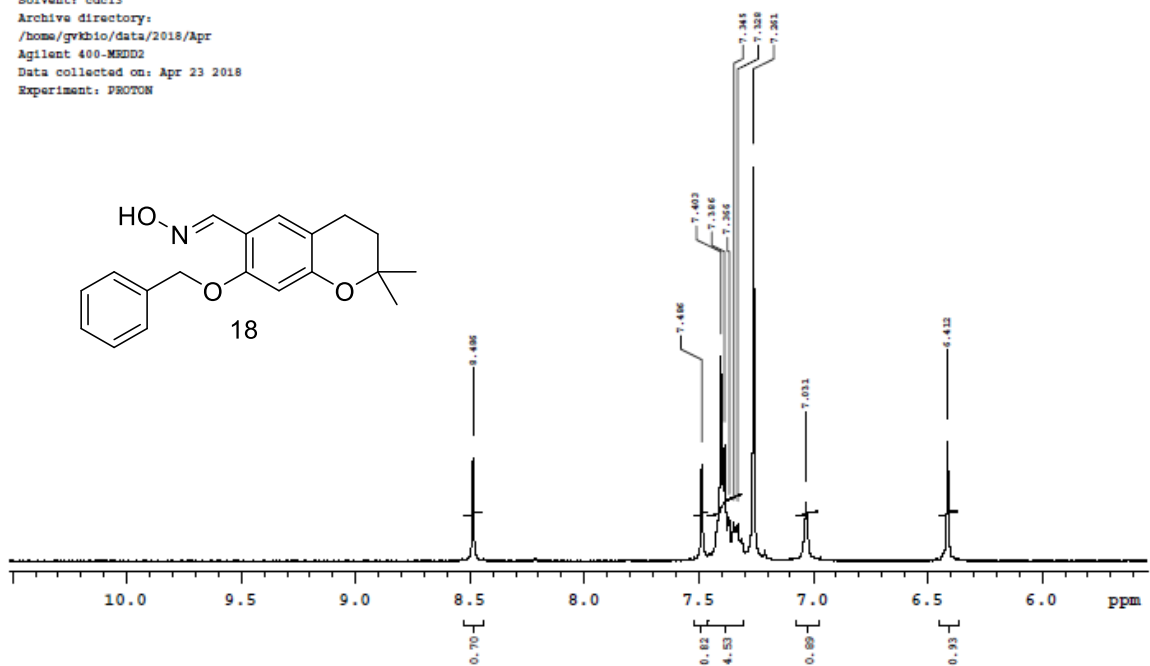
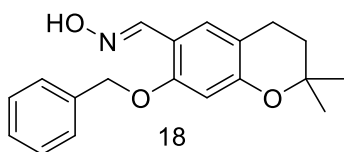
GVK-PRX-A139-45
AR NO-/NMR/4/18/2311

Reference Code: 511804C0484-GVK-PRG-1-47P
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2018/Apr
Agilent 400-MRDD2
Data collected on: Apr 23 2018
Experiment: PROTON



GVK-PRX-A139-45
AR NO-/NMR/4/18/2311

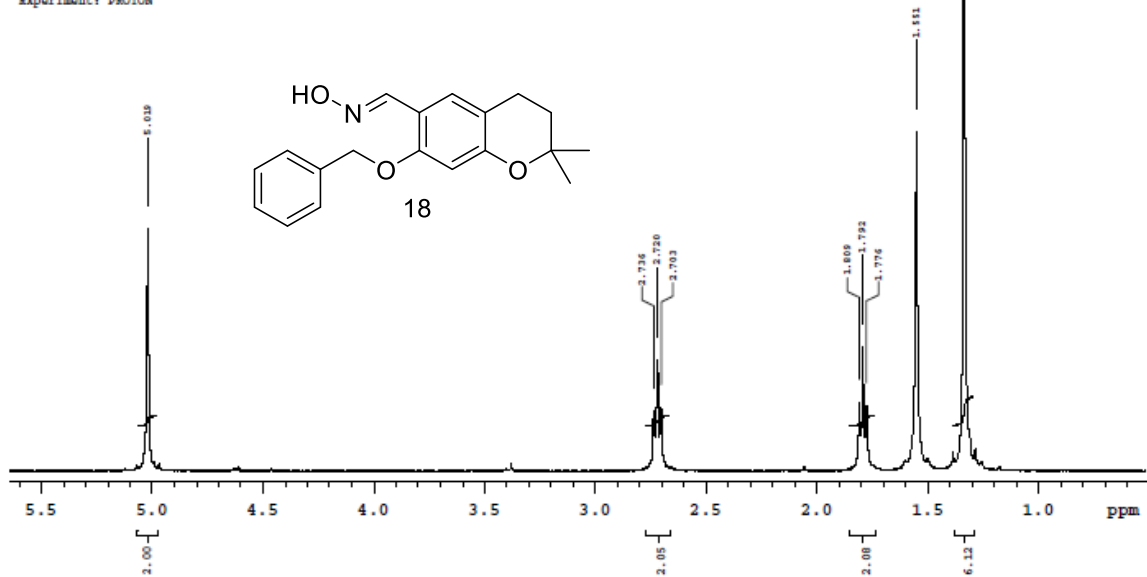
Reference Code: 511804C0484-GVK-PRG-1-47P
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2018/Apr
Agilent 400-MRDD2
Data collected on: Apr 23 2018
Experiment: PROTON



GVK-PRX-A139-45
AR NO-/NMR/4/18/2311

5d50677e003

Reference Code: 511804C0484-GVK-PRG-1-47D
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2018/Apr
Agilent 400-ME802
Data collected on: Apr 23 2018
Experiment: PROTON



GVK Biosciences (Pvt.) Ltd.
Analytical Research and Development

Data File:	BG_511804C0483-	Sample ID:	GVK-RAG-1-47p
Sample Name:		Vial:	BC6
Instrument Name:	N/A	Injection Volume(μl):	1.00
Operator:	Thermo Scientific	Run Time(min):	5.49
INSTRUMENT ID:	ANL-MCL5-LCMS-005	Acquisition Date:	04/23/18 09:19:06 AM

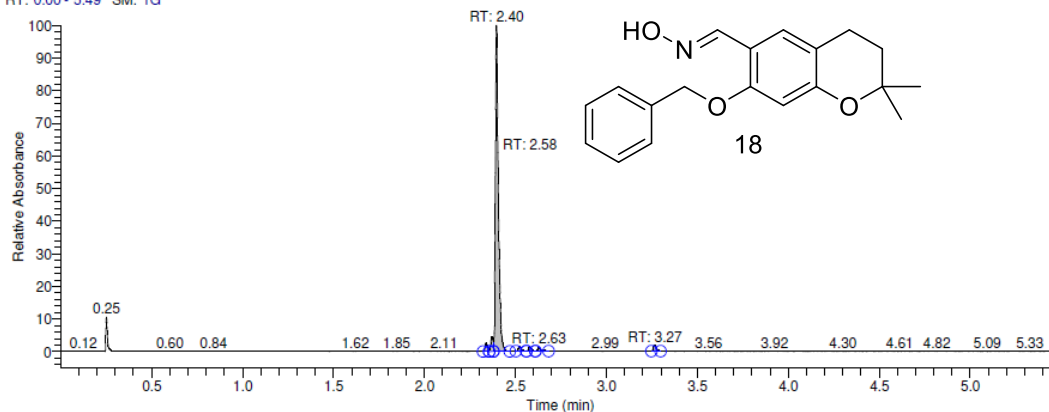
LC Method Details

Method : GVK_5.5MIN
 Mobile Phase A : 0.1% FA in Water
 Mobile Phase B : 0.1% FA in ACN
 Gradient % of B : 0/3, 0.3/3, 1.8/98, 4.5/98,4.51/3,5.5/3
 Flow Rate : 0.6ml/min
 Column : BEH C18, (2.1*50mm), 1.7um

Detector Type: PDA
 Wavelength Range 1 (nm): 215.00000

UV Chromatogram

RT: 0.00 - 5.49 SM: 1G



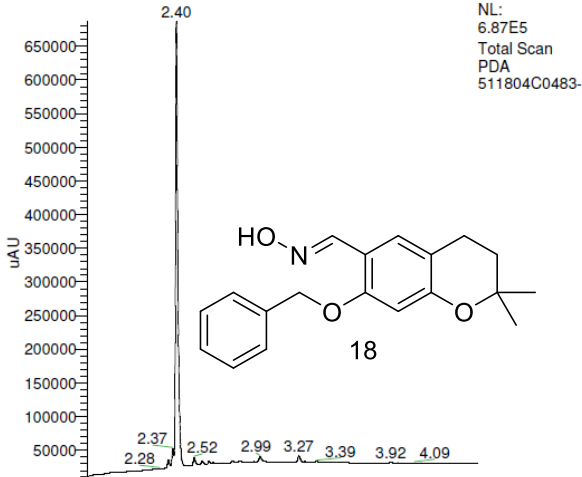
NL:
 1.77E6
 nm=214.5-
 215.5 PDA
 Avalon
 BG_511804
 C0483-

RT	Peak Area	Area %
2.34	48482.70	2.19
2.37	70026.70	3.16
2.40	1963930.18	88.67
2.52	32040.58	1.45
2.58	27014.08	1.22
2.63	29576.42	1.34
3.27	43907.36	1.98

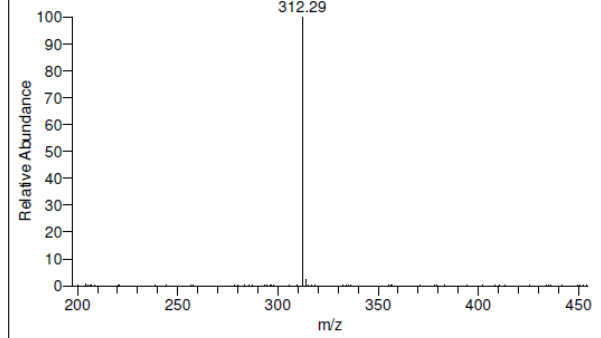
Operator: Thermo Scientific
 Instrument Name: N/A

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 Monday, April 23, 2018, 09:19:39

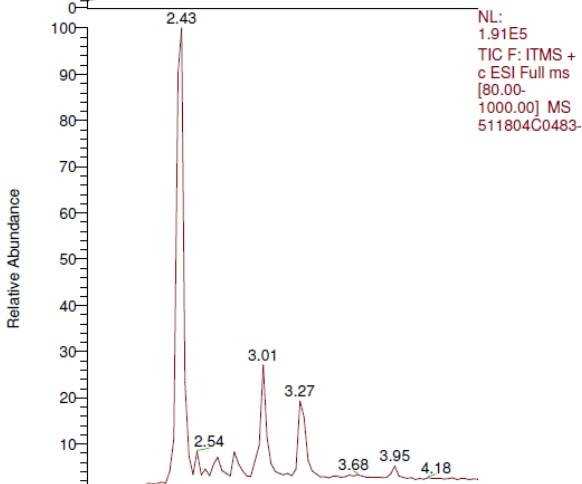
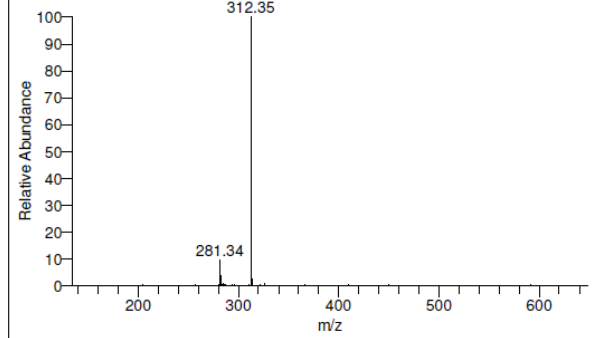
RT: 1.76 - 4.53



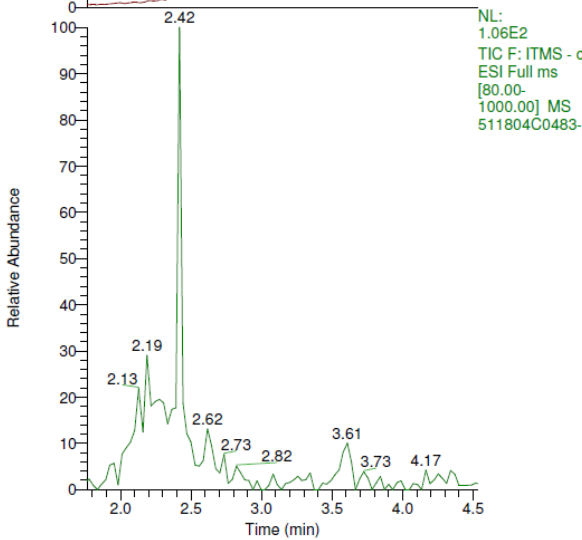
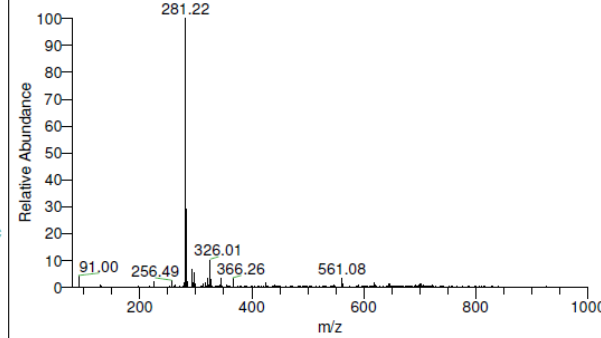
511804C0483- #167 RT: 2.43 AV: 1 NL: 1.66E5
F: ITMS + c ESI Full ms [80.00-1000.00]



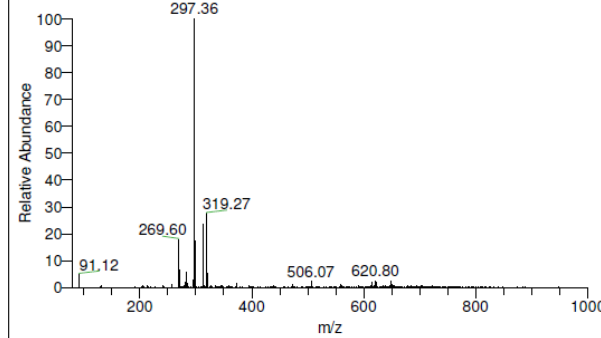
511804C0483- #163 RT: 2.38 AV: 1 NL: 1.33E4
F: ITMS + c ESI Full ms [80.00-1000.00]



511804C0483- #161 RT: 2.35 AV: 1 NL: 2.56E3
F: ITMS + c ESI Full ms [80.00-1000.00]

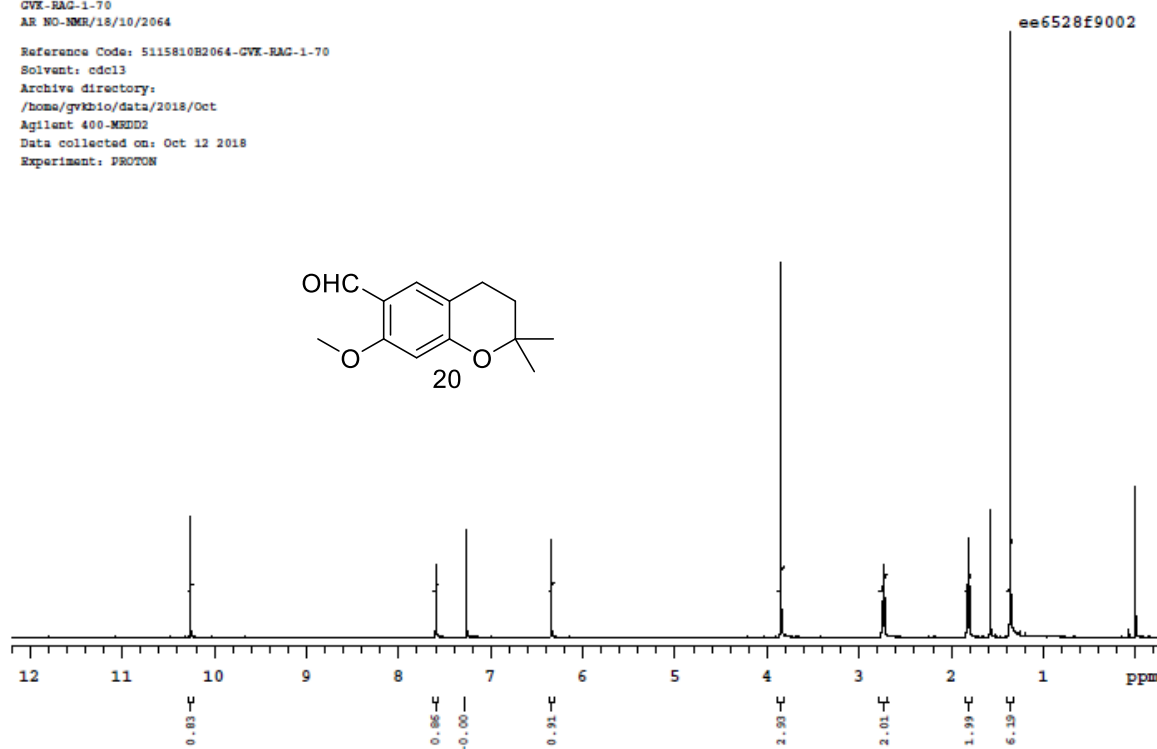


511804C0483- #175 RT: 2.54 AV: 1 NL: 4.45E3
F: ITMS + c ESI Full ms [80.00-1000.00]



GVK-RAG-1-70
AR NO-NMR/18/10/2064

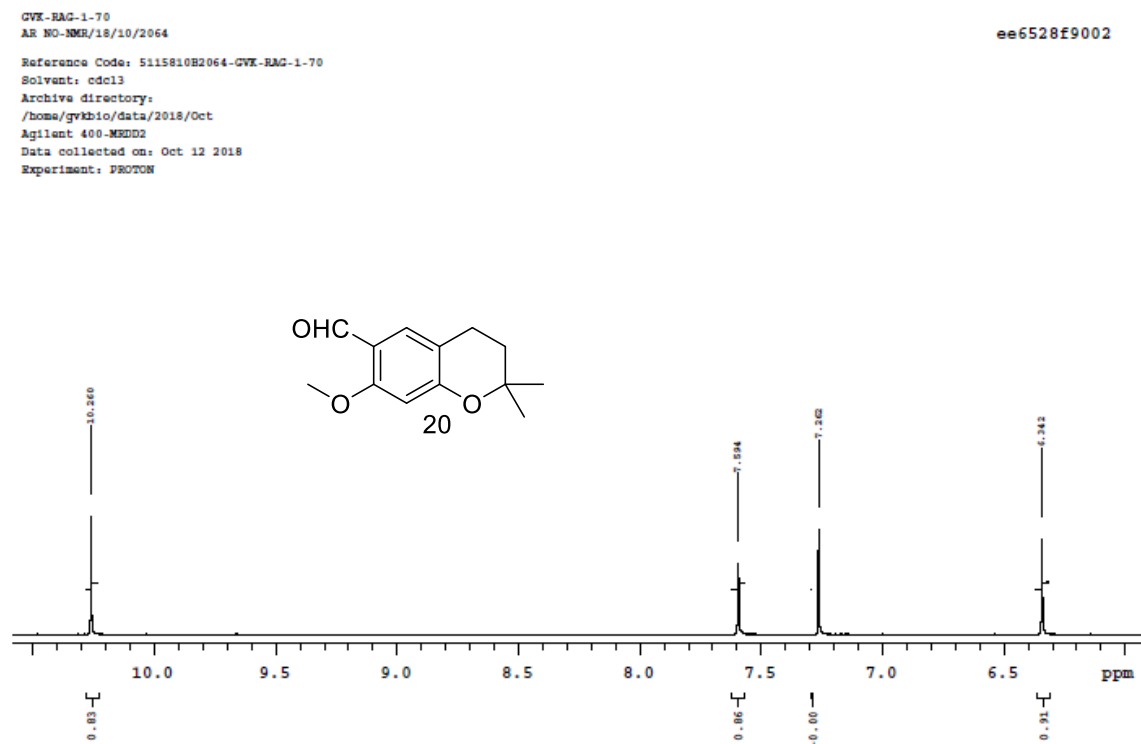
Reference Code: 511581082064-GVK-RAG-1-70
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2018/Oct
Agilent 400-MRSD2
Data collected on: Oct 12 2018
Experiment: PROTON



Plotname: 511581082064-GVK-RAG-1-70_PROTON_01.RRC_plot01

GVK-RAG-1-70
AR NO-NMR/18/10/2064

Reference Code: 511581082064-GVK-RAG-1-70
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2018/Oct
Agilent 400-MRSD2
Data collected on: Oct 12 2018
Experiment: PROTON



Plotname: 511581082064-GVK-RAG-1-70_PROTON_01.RRC_plot02

GVK-RAG-1-70
AR NO-NMR/18/10/2064

Reference Code: 5115810H2064-GVK-RAG-1-70

Solvent: cdcl3

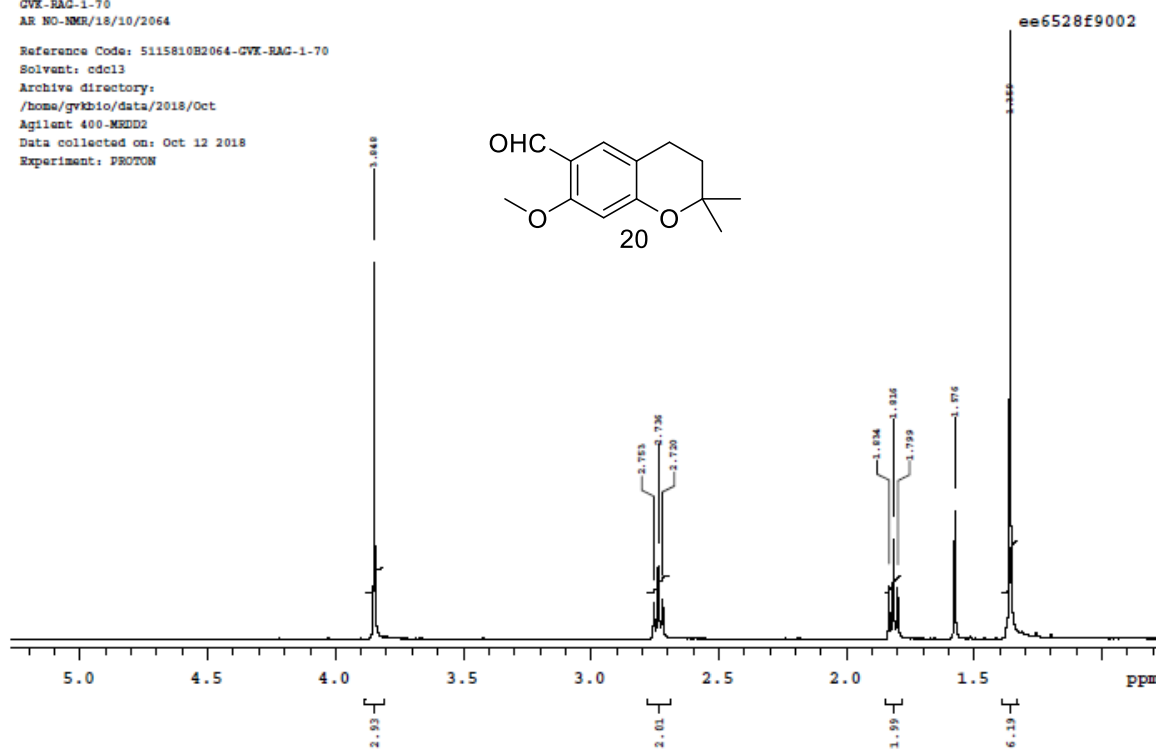
Archive directory:

/home/gvkbio/data/2018/Oct

Agilent 400-MRSD2

Data collected on: Oct 12 2018

Experiment: PROTON

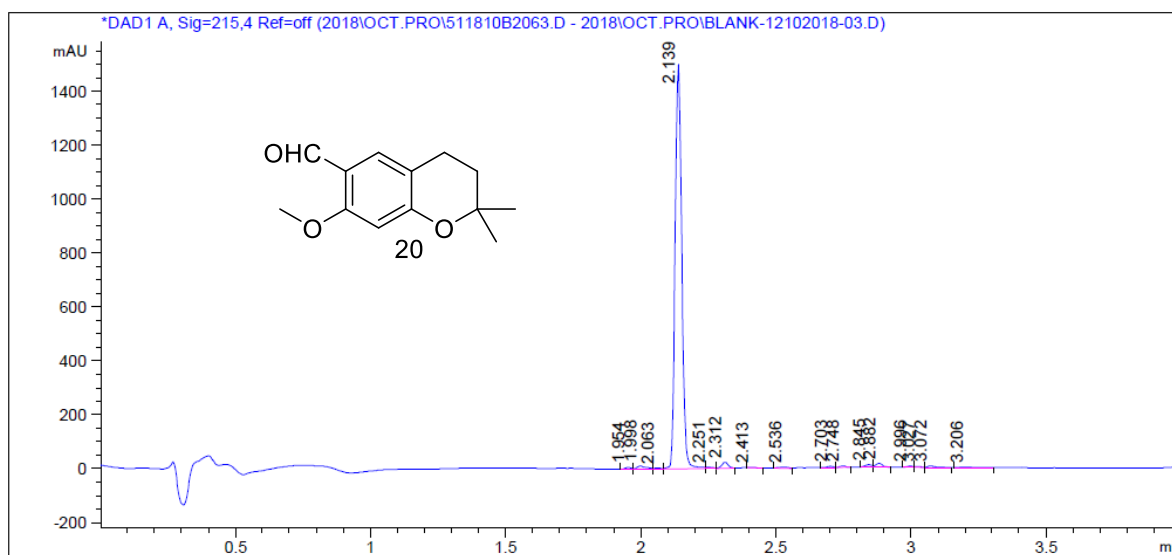


GVK BIOSCIENCES PVT. LTD.
 MEDICINAL CHEMISTRY LABORATORY - ANALYTICAL RESEARCH
 LCMS REPORT

Sample Name : GVK-RAG-1-70 Vial position : P1-C-01
 Date of Analysis : 10/12/2018 12:20:50 PM Injection Vol : 0.300µl
 Acq. Method : RND-FA-4.01 Instrument ID : ANL-MCL5-LCMS-001

RND-FA-4.01 MIN :-

Column : ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7µm)
 Mobile Phase : A1 - 0.1 % FA IN WATER ; B1: 0.1%FA IN ACN
 Gradient : Time (min) / %B1:0/3,0.3/3,2.3/98,3.5/98,4.0/3,4.01/3
 Flow Rate : 0.6 ml/min
 Column Temp : 50°C

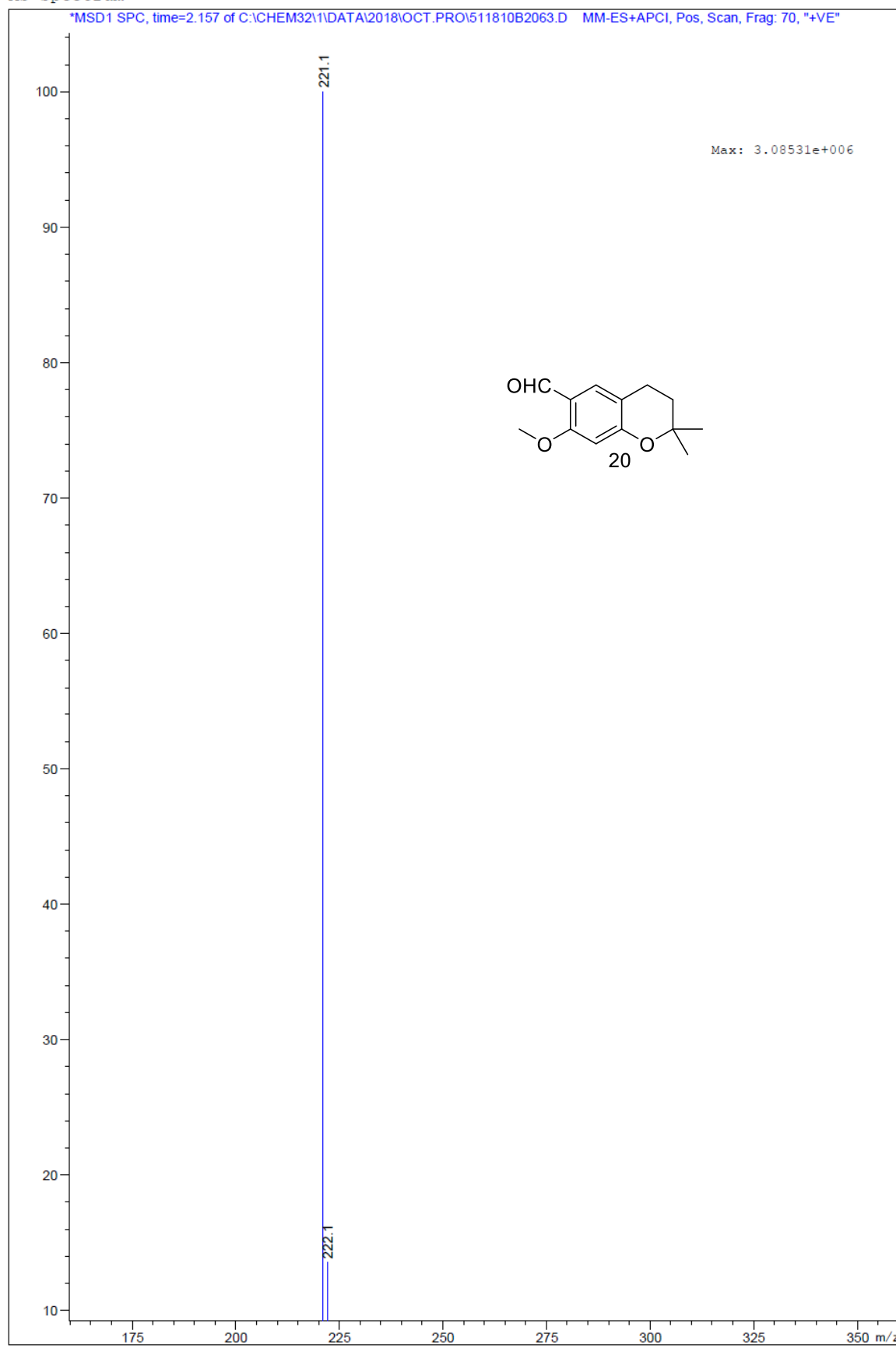


Peak No	RT min	Area	Area %
1	1.95	10.942	0.401
2	2.00	27.523	1.008
3	2.06	6.110	0.224
4	2.14	2542.948	93.140
5	2.25	9.294	0.340
6	2.31	38.671	1.416
7	2.41	2.306	0.084
8	2.54	8.980	0.329
9	2.70	5.802	0.213
10	2.75	6.768	0.248
11	2.84	16.009	0.586
12	2.88	22.676	0.831
13	3.00	5.883	0.215
14	3.03	4.806	0.176
15	3.07	12.971	0.475
16	3.21	8.567	0.314

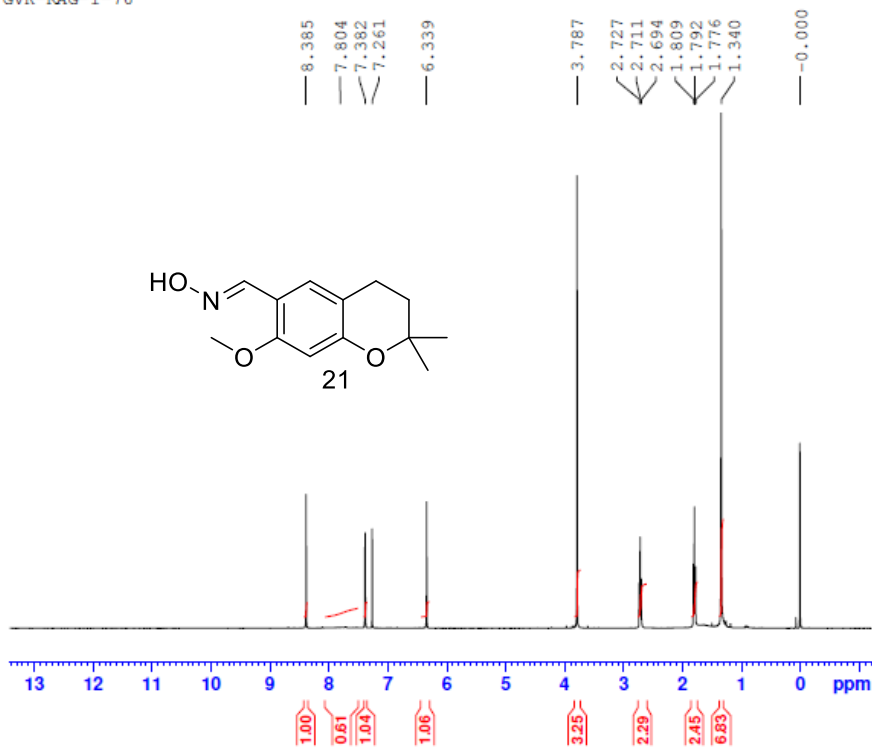
Analysed by :

Page 1 of 2

MS Spectrum



GVK-RAG-1-76



```

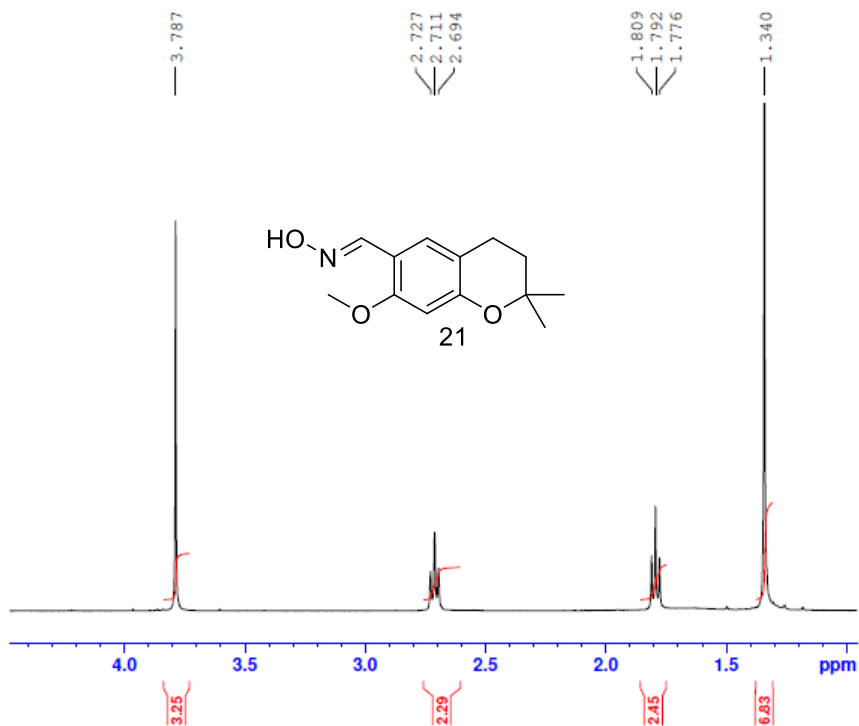
Current Data Parameters
NAME      5120100590-GVK-RAG-1-76
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20201020
Time     20.51 h
INSTRUM  Avance Neo nanobay
PROBHD   Z163739_0247 (
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        8
DS        0
SWH       8196.722 Hz
FIDRES   0.250144 Hz
AQ        3.9976959 sec
RG        101
DW        61.000 usec
DE        13.89 usec
TE        298.0 K
D1        1.00000000 sec
TDO       1
SFO1     400.2024712 MHz
NUC1      1H
PQ        2.67 usec
PI        8.00 usec
PLW1     23.09399986 W

F2 - Processing parameters
SI        65536
SF        400.2000094 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
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ANL-MCL5-NMR-004

GVK-RAG-1-76



```

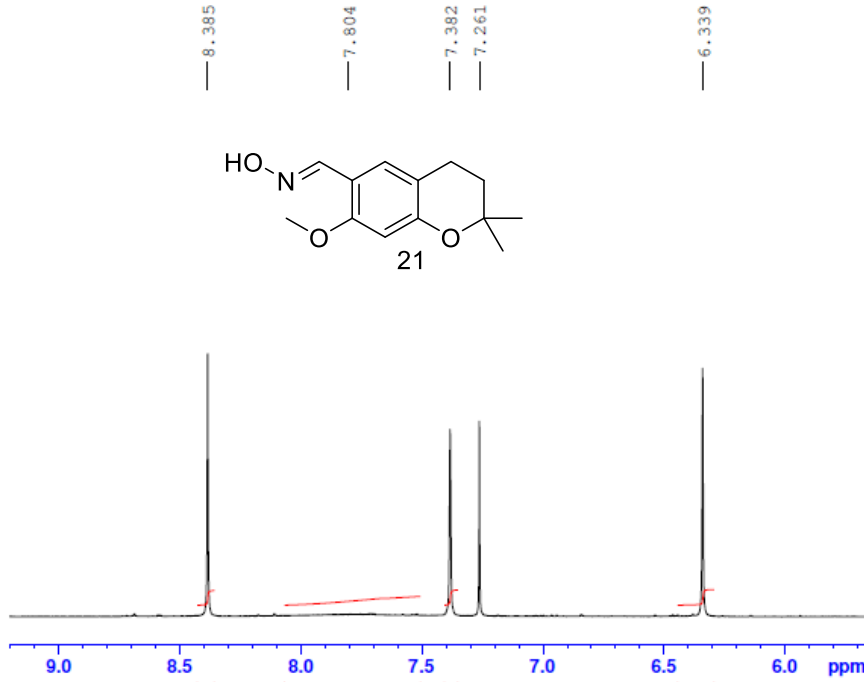
Current Data Parameters
NAME      5120100590-GVK-RAG-1-76
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20201020
Time     20.51 h
INSTRUM  Avance Neo nanobay
PROBHD   Z163739_0247 (
PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        8
DS        0
SWH       8196.722 Hz
FIDRES   0.250144 Hz
AQ        3.9976959 sec
RG        101
DW        61.000 usec
DE        13.89 usec
TE        298.0 K
D1        1.00000000 sec
TDO       1
SFO1     400.2024712 MHz
NUC1      1H
PQ        2.67 usec
PI        8.00 usec
PLW1     23.09399986 W

F2 - Processing parameters
SI        65536
SF        400.2000094 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
    
```

ANL-MCL5-NMR-004

GVK-RAG-1-76

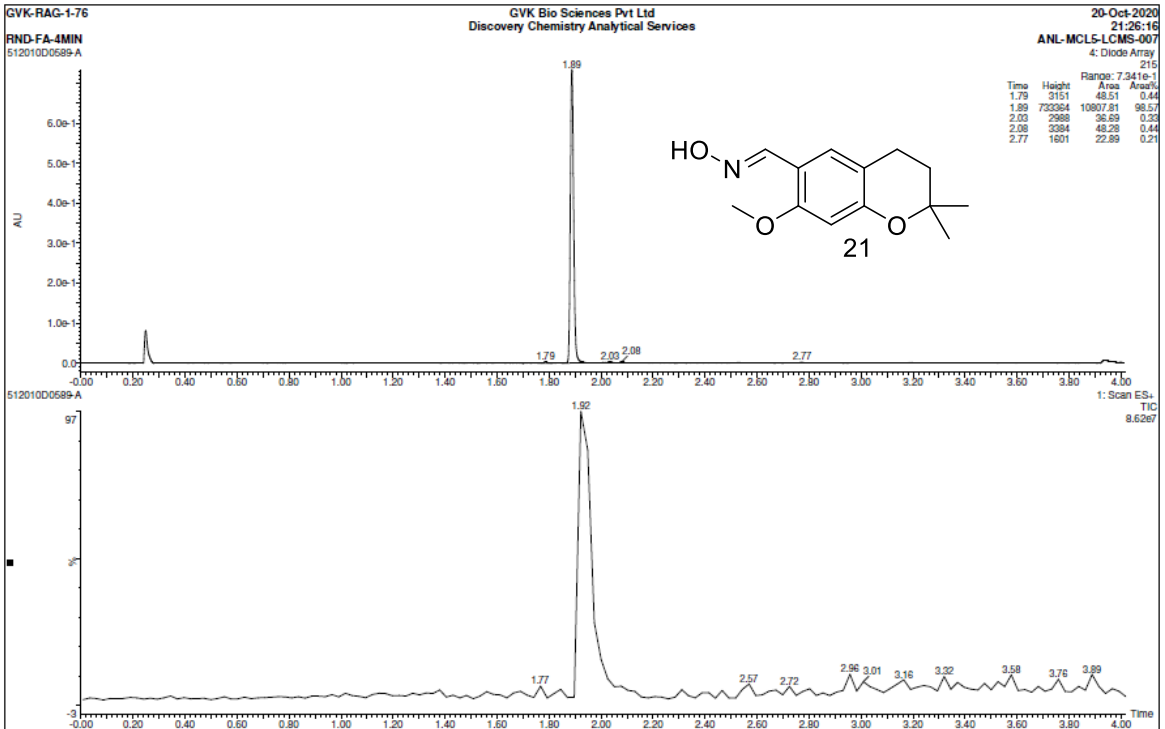


Current Data Parameters
 Name 512010D0590-GVK-RAG-1-76
 EXPNO 1
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20201020
 Time 20.51 h
 INSTRUM Avance Neo nanobay
 PROBRD z163739_0247 f1
 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 8
 DS 0
 SWH 8196.722 Hz
 FIDRES 0.250144 Hz
 AQ 3.9976959 sec
 RG 101
 DW 61.000 usec
 DE 13.89 usec
 TE 298.0 K
 D1 1.00000000 sec
 TDO 1
 SFO1 400.2024712 MHz
 NUC1 1H
 PD 2.67 usec
 P1 8.00 usec
 P1M1 23.09399986 W

F2 - Processing parameters
 SI 65536
 SF 400.2000094 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

ANL-MCL5-NMR-004



Acq Method Formic Acid_4.0 Min

21:26:16

512010D0589-A 75 (1.522)

ANL-MCLS-LCMS-007

1: Scan ES+

6.72e7

