Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting information

T3P® Mediated Domino C(sp2)-H Sulfenylation/Annulation of Enaminones and Methylsulfinyls for the synthesis of Chromone Thioethers Derivatives

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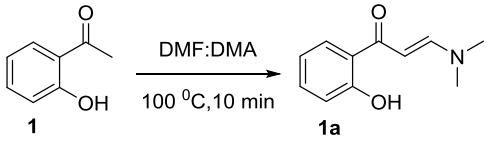
General Methods

Dry solvents were purchased from chemical suppliers and used without further purification. Analytical thin-layer chromatography (TLC) was performed on commercially available Merck TLC Silica gel 60 F_{254}. Silica gel column chromatography was performed on silica gel (spherical 100-200 µm). IR spectra were recorded on Perkin-Elmer FT/IR-4000 using ATR.^{1}H-NMR spectra were recorded on Varian-400 (400 MHz) spectrometer. Chemical shifts of ^{1}H-NMR spectra were reported relative to tetra methyl silane (^{13}C NMR spectra were recorded on Varian-400 (100 MHz) spectrometer. Chemical shifts of ^{13}C NMR spectra were reported to relative to $CDCl_3$ (77.16) and DMSO-d_6 (39.5). Splitting patterns were reported as s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet; br, broad. Melting points (m.p.) were measured by Büchi 510 melting point apparatus and uncorrected.

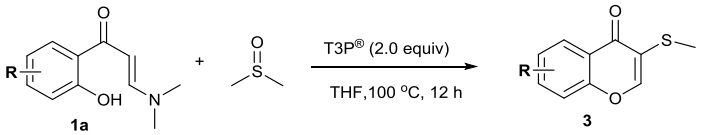
General procedure for the synthesis of Enaminone:



1 1a

A mixture of 2-hydroxy acetophenone **1** (200 mg, 1.47 mmol) and DMF-DMA (0.96 ml, 1.47 mmol) were introduced into a 2–5 mL initiator reaction vial. The mixture was irradiated for 10 minutes at 100 ˚C under MW. The reaction mixture was cooled to room temperature then wash with diethyl ether and filtered to get yellow solid.

General procedure for the synthesis 3-(methylthio)-4H-chromen-4-one (3a):



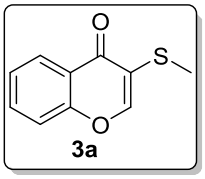
Enaminone **1a** (100 mg, 0.523mmol) was added to a dried sealed tube containing DMSO (0.297 mL, 4.18 mmol) in THF (1 mL) followed by the addition of T3P® (343 mg, 1.04 mmol) at 10 °C. After 15 min, the reaction mixture was heated to 100 ° C for 12 h. The reaction progress was monitored by TLC. Then the reaction mixture was cooled to room temperature, diluted with ethyl acetate, washed with water and brine, dried with anhydrous Na_2SO_4, and concentrated under vacuum. The residue was purified by flash chromatography (silica gel, hexane/EtOAc) to give desired product **3a** (91%) as a colourless solid. The same procedure was used to prepare compounds **3b**–**3n**

General procedure for the synthesis 3-(phenylthio)-4H-chromen-4-one (4a):

Enaminone **1a** (100 mg, 0.523 mmol) was added to a dried sealed tube containing DMAC (0.3 mL), followed by the addition of T3P® (343 mg, 1.04 mmol.) and methyl phenyl sulfoxide (145 mg, 1.04 mmol) at 0 ° C. After 15 min, the reaction mixture was heated to 90 ° C for 10 h. The reaction progress was monitored by TLC. Then the reaction mixture was cooled to room temperature, diluted with ethyl acetate, washed with water and brine,

dried with anhydrous Na_2SO_4, and concentrated under vacuum. The crude residue was purified by flash chromatography (silica gel, hexane /EtOAc) to give desired product **4a** (81 %) as a colourless solid. The same procedure was used to prepare compounds **4b**–**4p**

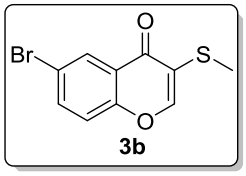
3-(methylthio)-4H-chromen-4-one:



3a

Off white solid; Yield (91%); m.p. 104-108 ^oC; IR (KBr, cm^{-1}): 3066, 1625, 1559, 1463, 1359, 1106, 1078, 891, 755; ^{1}H-NMR (400 MHz, $CDCl_3$): 8.27-8.25 (d, J= 7.6 Hz, 1H), 8.06 (s, 1H), 7.68 (s, 1H), 7.45-7.43 (m, 2H), 2.41 (s, 3H); ^{13}C NMR (400 MHz,$CDCl_3$): 175.58, 156.23, 153.86, 133.74, 126.06, 125.42, 123.12, 121.80, 118.03, 16.24; MS (EI): *m/z* 193 (M+1, 100); HRMS: (ESI): Calcd for $C_{10}H_8O_2S$[M+H]:193.0323, Found: 193.0329.

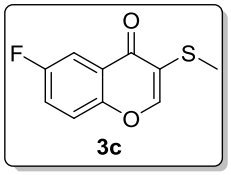
6-bromo-3-(methylthio)-4H-chromen-4-one*:*



3b

Yellow solid; Yield (82%); m.p. 124-127 ^oC; IR (KBr, cm^{-1}): 1627, 1463, 1432, 1311, 1120, 1080, 815, 754; ^{1}H-NMR (500 MHz, $CDCl_3$): 8.37 (d, J= 2.4 Hz, 1H), 8.0 (s, 1H), 7.76-7.74 (m, 1H), 7.37 (d, J= 8.8 Hz, 1H), 2.40 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): 174.32, 155.00, 153.67, 136.75, 128.63, 124.31, 122.28, 120.04, 118.80, 16.11; MS (EI): *m/z* 270 (M+1, 100); HRMS: (ESI): Calcd for $C_{10}H_7BrO_2S$[M+H]:270.9430, Found: 270.9428

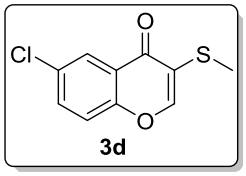
6-fluoro-3-(methylthio)-4H-chromen-4-one:



3c

Colourless liquid; Yield (80%); IR (KBr, cm^{-1}): 3079, 1628, 1558, 1479, 1370, 1102, 884, 814; ^{1}H-NMR (400 MHz, $CDCl_3$): 8.06 (s, 1H), 7.90-7.85 (m, 1H), 7.49-7.37 (m, 2H), 2.40 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 174.89, 160.55, 158.59, 153.91, 152.49, 124.23, 124.17, 122.18, 121.98, 121.36, 120.27, 120.20, 110.89, 110.70, 16.15; MS (EI): *m/z* 211 (M+1, 100); HRMS: (ESI): Calcd for $C_{10}H_7O_2FS$[M+H]:211.099, Found: 211.0231.

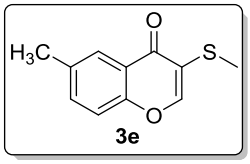
6-chloro-3-(methylthio)-4H-chromen-4-one:



3d

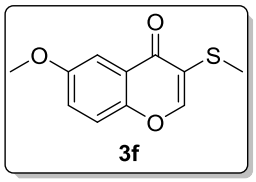
White Solid; Yield (74%); m.p.133-137 ^{o}C. IR (KBr, cm^{-1}): 3086, 1628, 1549, 1465, 1359, 1117, 1080, 814, 643; ^{1}H-NMR (400 MHz, $CDCl_3$): 8.21 (d, J= 2.8 Hz, 1H), 8.03 (s, 1H), 7.63-7.60 (m, 1H), 7.43 (d, 1H), 2.40 (s, 3H); ^{13}C NMR (400 MHz,$CDCl_3$): 174.47, 154.56, 153.70, 134.00, 131.36, 125.41, 123.95, 122.17, 119.82, 16.11; MS (EI): *m/z* 227 (M+1, 100); HRMS: (ESI): Calcd for $C_{10}H_7ClO_2S$[M+H]:226.9927, Found: 226.9934.

6-methyl-3-(methylthio)-4H-chromen-4-one:



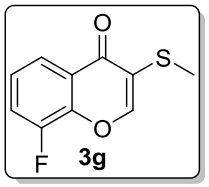
Off white Solid; Yield (83%); m.p. 97-101 °C; IR (KBr, cm^{-1}): 2918, 1639, 1482, 1367, 867, 824, 779, 720; ^{1}H-NMR (400 MHz, $CDCl_3$): 8.05-8.03 (m, 2H), 7.49-7.47 (m, 1H), 7.36 (d, J=8.8Hz, 1H), 2.46 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): 175.65, 154.52, 153.96, 135.46, 135.01, 125.28, 122.81, 121.43, 117.78, 20.90, 16.34; MS (EI): *m/z* 207 (M+1, 100); HRMS: (ESI): Calcd for $C_{11}H_{10}O_2S$[M+H]:207.0480, Found: 207.0488.

6-methoxy-3-(methylthio)-4H-chromen-4-one:



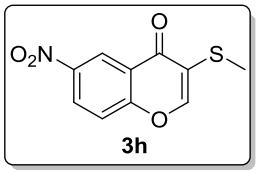
White Solid; Yield (79%); m.p. 87-91° C; IR (KBr,cm^{-1}): 3075, 1622, 1484, 1377, 1195, 1107, 1076, 1020, 814; ^{1}H-NMR (500 MHz, $CDCl_3$): 8.06 (s, 1H), 7.60 (d, J=3Hz, 1H), 7.40-7.25 (m, 2H), 3.90 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): 175.47, 157.07, 153.89, 151.12, 123.93, 123.75, 120.80, 119.47, 104.87, 55.90, 16.34; MS (EI): *m/z* 223 (M+1, 100); HRMS: (ESI): Calcd for $C_{11}H_{10}O_3S$[M+H]:222.9985, Found: 222.9987.

8-fluoro-3-(methylthio)-4H-chromen-4-one:



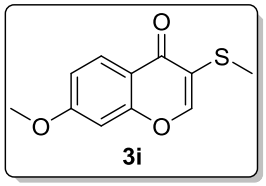
Off white Solid; Yield (81%); m.p. 237-241 °C; IR (KBr, cm^{-1}): 3079, 1630, 1557, 1484, 1340, 1256, 1099, 885; ^{1}H-NMR (500 MHz, $CDCl_3$): 8.05 (s, 1H), 8.02-8.0 (m, 1H),7.46-7.43 (m, 1H), 7.38-7.35 (m, 1H), 2.41 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): 174.61, 174.61, 174.59, 152.76, 152.00, 149.99, 145.12, 145.03, 125.07, 125.02, 124.82, 122.81, 121.09, 121.06, 119.52, 119.39, 15.98; MS (EI): *m/z* 211 (M+1, 100); HRMS: (ESI): Calcd for $C_{10}H_7FO_2S$[M+H]:211.0229, Found: 211.0222.

3-*(methylthio)-6-nitro-4H-chromen-4-one:*



Yellow Solid; Yield (72%); m.p. 150-152 °C; IR (KBr, cm^{-1}): 3095, 1642, 1517, 1448, 1337, 1220, 1080, 1058, 885, 734; ^{1}H-NMR (400 MHz, $CDCl_3$): 9.12 (d, J= 2.8Hz, 1H), 8.52-8.49 (dd, J= 9.2Hz, 1H), 8.02 (s, 1H), 7.64 (d, 1H), 2.43 (s, 3H);^{13}C NMR (400 MHz, $CDCl_3$): 174.14, 158.93, 152.74, 144.87, 128.02, 123.74, 122.92, 122.84, 119.92, 15.67; MS (EI): *m/z* 238 (M+1,100); HRMS: (ESI): Calcd for $C_{10}H_7NO_4S$[M-H]:236.0018, Found: 236.0021.

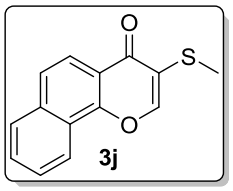
7-methoxy-3-(methylthio)-4H-chromen-4-one:



Off white solid; Yield (76%); m.p. 153-157 °C; IR (KBr, cm^{-1}): 3073, 1622, 1615, 1606, 1435, 1233, 1090, 935, 828; ^{1}H-NMR (500 MHz, $CDCl_3$): 8.16 (d, J= 9.2Hz, 1H), 7.97 (s, 1H), 7.00-6.97 (m, 1H),

6.82 (d, J=2.4Hz, 1H), 3.90 (s, 3H), 2.39 (s, 3H);^{13}C NMR (400 MHz, $CDCl_3$): 174.93, 164.10, 158.04, 153.30, 127.46, 121.71, 117.05, 114.83, 100.07, 55.81, 16.27; MS (EI): *m/z* 223 (M+1,100); HRMS: (ESI): Calcd for $C_{11}H_{10}O_3S$[M+H]:223.0428, Found: 223.0429.

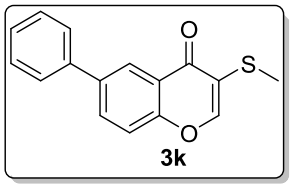
3-(methylthio)-4H-benzo[h]chromen-4-one:



3j

Light yellow Solid; Yield (87%); m.p. 134-138 °C; IR (KBr, cm^{-1}): 3063, 1559, 1387, 1207, 1105, 884, 759, 576; ^{1}H-NMR (400 MHz, $CDCl_3$): 8.49 (d, J=8, 1H), 8.20-8.18 (m, 2H), 7.95-7.93 (m, 1H), 7.80 (d, J=10 Hz, 1H) 7.74-7.67 (m, 2H), 2.46 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): 175.35, 153.75, 152.05, 135.74, 129.43, 128.09, 127.22, 125.58, 123.85, 123.83, 122.18, 120.86, 119.18, 15.84; MS (EI): *m/z* 243 (M+1,100); HRMS: (ESI): Calcd for $C_{14}H_{10}O_2S$[M+H]:243.0480, Found: 243.0479.

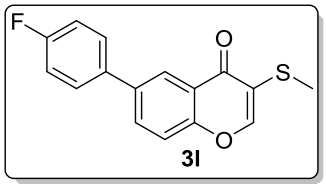
3-(methylthio)-6-phenyl-4H-chromen-4-one:



3k

Off white solid; Yield (84 %); m.p. 146-150 °C; IR (KBr,cm^{-1}): 2918, 1643, 1559, 1460, 1316, 1072, 762, 700; ^{1}H-NMR (500 MHz, $CDCl_3$): 8.4 (d, J= 2.4 Hz, 1H), 8.08 (s, 1H), 7.93-7.90 (m, 1H), 7.67-7.65 (m, 2H), 7.54-7.39 (m, 4H), 2.42 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): 175.63, 155.62, 153.80, 139.13, 138.64, 132.65, 128.96, 127.90, 127.15, 123.83, 123.24, 121.88, 118.56, 16.27; MS (EI): *m/z* 268 (M+1,100); HRMS: (ESI): Calcd for $C_{16}H_{12}O_2S$[M+H]:269.0636, Found: 269.0637

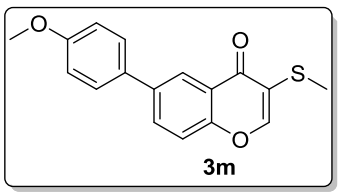
6-(4-fluorophenyl)-3-(methylthio)-4H-chromen-4-one:



3l

Light Yellow solid; Yield (86%); m.p. 120-125 °C; IR (KBr, cm^{-1}): 2919, 1633, 1472, 1324, 1220, 1079, 863, 814; ^{1}H-NMR (500 MHz, $CDCl_3$): 8.41 (d, J= 2.4Hz, 1H), 8.07 (s, 1H), 7.87-7.85 (m, 1H),7.63-7.59 (m, 2H), 7.54 (d, J= 8.8 Hz, 1H), 7.18-7.14 (m, 2H), 2.42(s, 3H);^{13}C NMR (400 MHz, $CDCl_3$): 175.56, 163.98, 161.52, 155.55, 153.77, 137.64, 135.29, 135.26, 132.46, 128.83, 128.75, 123.68, 123.22, 121.94, 118.66, 116.01, 115.79, 16.23; MS (EI): *m/z* 287 (M+1,100); HRMS: (ESI): Calcd for $C_{16}H_{11}FO_2S$[M+H]:287.0542, Found: 287.0546.

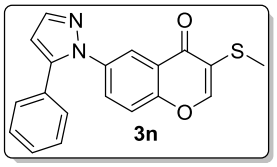
6-(4-methoxyphenyl)-3-(methylthio)-4H-chromen-4-one:



3m

Off white solid; Yield (84%); m.p. 114-117 °C; IR (KBr, cm^{-1}): 3445, 3423, 2922, 1635, 1558, 1465, 1246, 811, 532; ^{1}H-NMR (500 MHz, $CDCl_3$): 8.41 (d, J= 2.4Hz, 1H), 8.0 (s, 1H), 7.89-7.86 (m, 1H), 7.60-7.58 (m, 2H), 7.51 (d, J= 8.8 Hz , 1H), 7.01 (m, 2H), 3.86 (s, 3H), 2.42 (s, 3H);^{13}C NMR (400 MHz, $CDCl_3$): 175.64, 159.53, 155.19, 153.74, 138.20, 132.23, 131.52, 128.16, 123.16, 122.95, 121.67, 118.44, 114.34, 55.30, 16.23; MS (EI): *m/z* 299 (M+1, 100); HRMS: (ESI): Calcd for $C_{17}H_{14}O_3S$[M+H]:299.0742, Found: 299.0744.

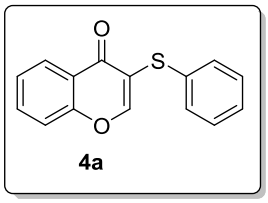
3-(methylthio)-6-(5-phenyl-1H-pyrazol-1-yl)-4H-chromen-4-one:



3n

Off white solid; Yield (87%); m.p. 167-171 ^{o}C; IR (KBr, cm^{-1}): 1624, 1497, 1456, 1118, 1090, 967, 934, 908; ^{1}H-NMR (500 MHz, $CDCl_3$): 8.77 (d, J= 2.4Hz, 1H), 8.49 (s, 1H), 8.35-8.32 (m, 2H), 7.97-7.95 (m, 2H), 7.89-7.87 (m, 1H), 7.45-7.38 (m, 3H), 7.11 (s, 1H), 2.39 (s, 3H); ^{13}C NMR (400 MHz, $CDCl_3$): 175.21, 154.20, 153.87, 153.50, 137.63, 132.66, 128.69, 128.29, 128.21, 125.85, 125.42, 123.49, 121.81, 119.71, 113.54, 105.87, 16.21; MS (EI): *m/z* 335 (M+1, 100); HRMS: (ESI): Calcd for $C_{19}H_{14}N_2O_2S$[M+H]:335.0854, Found: 335.0862

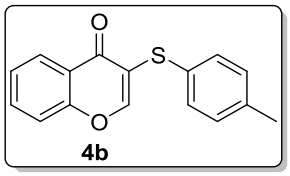
3-(phenylthio)-4H-chromen-4-one



4a

Color less liquid; Yield (81%); IR (KBr, cm^{-1}): 3061, 1652, 1467, 1350, 1313, 1109, 753, 692; ^{1}H-NMR (400 MHz, $CDCl_3$): 8.27 (dd, J=8.4Hz, 1H), 8.16 (s, 1H), 7.72 (m, 1H), 7.49-7.38 (m, 4H), 7.30-7.20 (m, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 175.16, 157.47, 156.43, 134.10, 129.91, 129.29, 127.21, 126.53, 125.84, 123.76, 120.00, 118.25; MS (EI): *m/z* 255 (M+1,100); HRMS: (ESI): Calcd for $C_{15}H_{10}O_2S$[M+H]:255.0480, Found: 255.0483.

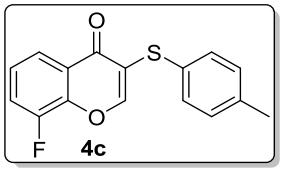
3-(p-tolylthio)-4H-chromen-4-one*:*



4b

Yellow solid; Yield (73%); m.p. 102-107 ^{o}C; IR (KBr, cm^{-1}): 3418, 2921, 1643, 1547, 1455, 1346, 1098, 750; ^{1}H-NMR (400 MHz, $CDCl_3$):8.25-8.23 (m, 1H), 8.04 (s, 1H), 7.70-7.65 (m, 1H), 7.46-7.40 (m, 2H), 7.36-7.33 (m, 2H), 7.12-7.10 (m, 2H), 2.31 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 175.04, 156.25, 156.21, 137.55, 133.83, 130.95, 130.00, 129.77, 126.34, 125.55, 123.51, 121.06, 118.06, 21.04; MS (EI): *m/z* 269 (M+1,100); HRMS: (ESI): Calcd for $C_{16}H_{12}O_2S$[M+H]:269.0636, Found: 269.0642.

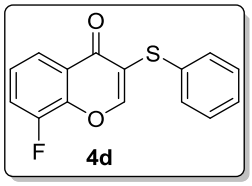
8-fluoro-3-(p-tolylthio)-4H-chromen-4-one:



4c

Yellow solid; Yield (70%); m.p. 139-143 ^{o}C; IR (KBr, cm^{-1}): 3055, 1653, 1544, 1484, 1306, 1255, 1101, 751; ^{1}H-NMR (400 MHz, $CDCl_3$): 7.99-7.97 (m, 2H), 7.44-7.42 (m, 1H), 7.38-7.33 (m, 3H), 7.14-7.12 (m, 2H), 2.32 (s, 3H);^{13}C NMR (125 MHz, $CDCl_3$): 174.05, 174.03, 154.80, 152.00, 149.98, 145.11, 145.02, 138.09, 131.65, 130.16, 128.83, 125.18, 125.14, 122.44, 121.31, 121.27, 119.60, 119.47, 21.08; MS (EI): *m/z* 287 (M+1,100); HRMS: (ESI): Calcd for $C_{16}H_{11}FO_2S$[M+H]:287.0542, Found: 287.0545.

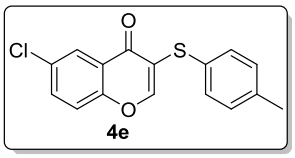
8-fluoro-3-(phenylthio)-4H-chromen-4-one:



4d

White solid; Yield (79%); m.p.114-118 ° C; IR (KBr, cm^{-1}): 3057, 1655, 1559, 1474, 1350, 1257, 1106, 750; ^{1}H-NMR (400 MHz, $CDCl_3$): 8.10 (s, 1H), 8.01 (d, J= 8.0 Hz, 1H), 7.49-7.43 (m, 3H), 7.41-.7.24 (m, 4H); ^{13}C NMR (125 MHz, $CDCl_3$): 174.17, 174.14, 156.11, 152.39, 149.86, 145.27, 145.16, 133.20, 130.63, 129.42, 127.66, 125.78, 125.74, 125.50, 125.43, 122.12, 121.95, 121.50, 121.46, 121.35, 119.90, 119.73, 118.24, MS (EI): *m/z* 273 (M+1,100); HRMS: (ESI): Calcd for $C_{15}H_9FO_2S$[M+H]:273.0386, Found: 237.0390.

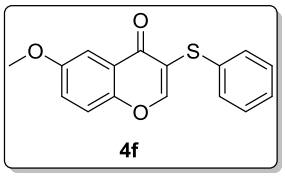
6-chloro-3-(p-tolylthio)-4H-chromen-4-one:



4e

Yellow solid; Yield (71%); m.p.123-127 ° C; IR (KBr, cm^{-1}): 3066, 1651, 1461, 1298, 1085, 910, 817, 654; ^{1}H-NMR (400 MHz, $CDCl_3$): 8.19 (d, J= 2.4 Hz, 1H), 7.97, (s, 1H), 7.62-7.59 (m, 1H), 7.41-7.39 (d, J= 7.2 Hz, 1H), 7.36-7.34 (m, 2H) ,7.13-7.11 (d, J= 8.0 Hz, 2H), 2.32 (s, 3H).), ^{13}C NMR (125 MHz, $CDCl_3$): 173.94, 155.78, 154.58, 137.95, 134.07, 131.52, 131.40, 130.13, 129.14, 125.67, 124.33, 121.70, 119.83, 21.08; MS (EI): *m/z* 303 (M+1,100); HRMS: (ESI): Calcd for $C_{16}H_{11}ClO_2S$[M+H]:303.0247, Found: 303.0255.

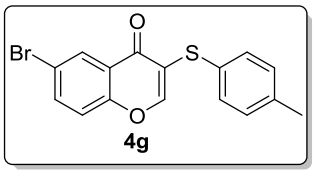
6-methoxy-3-(phenylthio)-4H-chromen-4-one:



4f

Light yellow solid; Yield (74%); m.p.94-98 ° C; IR (KBr, cm^{-1}): 3064, 1640, 1479, 1431, 1363, 1311, 1016, 729; ^{1}H-NMR (400 MHz, $CDCl_3$): 8.17 (s, 1H), 7.60 (d, J= 3.2Hz, 1H), 7.43-7.37 (m, 3H), 7.30-.7.21 (m, 4H), 3.95 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 174.96, 157.30, 151.17, 134.24, 133.75, 130.20, 129.86, 129.62, 129.20, 129.11, 126.96, 124.33, 124.08, 119.55, 118.82, 105.32, 55.92; MS (EI): *m/z* 285 (M+1,100); HRMS: (ESI): Calcd for $C_{16}H_{12}O_3S$[M+H]:285.0585, Found: 285.0587.

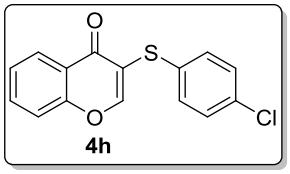
6-bromo-3-(p-tolylthio)-4H-chromen-4-one:



4g

Yellow solid; Yield (75%); m.p.234-238 ° C; IR (KBr, cm^{-1}): 3061, 1647, 1458, 1296, 1115, 1084, 906, 816; ^{1}H-NMR (400 MHz, $CDCl_3$): 8.36.(d, J= 2 Hz, 1H), 7.97, (s, 1H), 7.76-7.73 (m, 1H), 7.36-7.33 (m, 3H), 7.13 (d, J= 8 Hz, 2H), 2.32 (s, 3H).); ^{13}C NMR (125 MHz, $CDCl_3$): 173.80, 155.76, 155.02, 137.98, 136.83, 131.42, 130.14, 129.11, 128.89, 124.69, 121.83, 120.05, 118.97, 21.09; MS (EI): *m/z* 347 (M+1,100); HRMS: (ESI): Calcd for $C_{16}H_{11}BrO_2S$[M+H]:346.9741, Found: 346.9746.

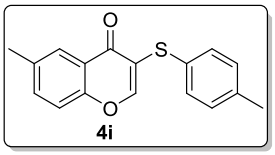
3-((4-chlorophenyl)thio)-4H-chromen-4-one:



4h

White solid; Yield (72%); m.p.154-158 ^{o}C; IR (KBr, cm^{-1}): 3418, 3047, 1640, 1547, 1462, 1379, 1099, 750; ^{1}H-NMR (400 MHz, $CDCl_3$): 8.24-8.22 (m, 2H), 7.73-7.69 (m, 1H), 7.49-7.42 (m, 2H), 7.33-.7.31 (m, 2H), 7.26-7.24 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): 175.07, 158.02, 156.48, 134.29, 133.22, 132.92, 131.00, 129.39, 126.57, 126.02, 123.84, 119.35, 118.33; MS (EI): *m/z* 289 (M+1,100); HRMS: (ESI): Calcd for $C_{15}H_9ClO_2S$[M+H]:289.0090, Found: 289.0079.

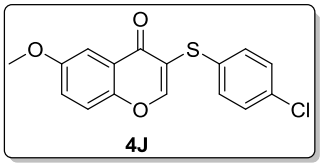
***6-methyl-3-(p-tolylthio)-4H-chromen-4-one**:*



4i

Yellow solid; Yield (76%); m.p.122-126 ^{o}C; IR (KBr, cm^{-1}): 3061, 1645, 1484, 1304, 1115, 814, 786, 511; ^{1}H-NMR (400 MHz, $CDCl_3$): 8.04-8.02 (m, 2H), 7.48-7.46 (m, 1H), 7.35-7.32 (m, 3H), 7.10-7.09 (m, 2H), 2.45 (s, 3H), 2.31 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 175.31, 156.56, 154.70, 137.53, 135.80, 135.26, 130.85, 130.21, 130.12, 125.76, 123.36, 120.70, 117.97, 21.20, 21.08; MS (EI): *m/z* 283 (M+1,100); HRMS: (ESI): Calcd for $C_{17}H_{14}O_2S$[M+H]:283.0793, Found: 283.0801.

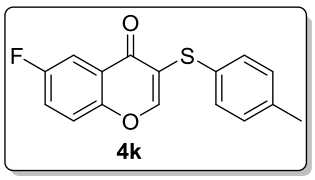
3-((4-chlorophenyl)thio)-6-methoxy-4H-chromen-4-one:



4J

Off white solid; Yield (70%); m.p. 161-165 ^{o}C; IR (KBr, cm^{-1}): 3072, 1649, 1562, 1478, 1432, 1303, 1084, 818; ^{1}H-NMR (400 MHz, $CDCl_3$): 8.23 (s, 1H), 7.58-7.57 (d, J= 3.2Hz, 1H), 7.43 (d, J=8.8Hz, 1H), 7.32-7.22 (m, 5H), 3.88 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 175.01, 157.91, 157.56, 151.35, 133.16, 133.12, 130.86, 129.36, 124.55, 124.40, 119.76, 118.33, 105.46, 56.17; MS (EI): *m/z* 319 (M+1,100); HRMS: (ESI): Calcd for $C_{16}H_{11}ClO_3S$[M+H]:319.0196, Found: 319.0200.

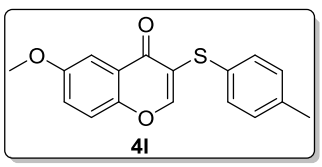
6-fluoro-3-(p-tolylthio)-4H-chromen-4-one:



4k

Yellow solid; Yield (73%); m.p. 151-155 ^{o}C; IR (KBr, cm^{-1}): 3073, 1650, 1557, 1478, 1346, 1302, 1103, 816; ^{1}H-NMR (400 MHz, $CDCl_3$): 8.01 (s, 1H), 7.87-7.84 (m, 1H), 7.48-7.40 (m, 2H), 7.39-7.34 (m, 2H), 7.13-7.11 (m, 2H), 2.32 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 174.51, 161.03, 158.56, 156.21, 152.65, 152.67, 138.00, 131.38, 130.25, 129.46, 124.81, 124.74, 122.44, 122.18, 120.95, 120.46, 120.38, 111.39, 111.16, 21.23; MS (EI): *m/z* 287 (M+1,100); HRMS: (ESI): Calcd for $C_{16}H_{11}FO_2S$[M+H]:287.0542, Found: 287.0553.

6-methoxy-3-(p-tolylthio)-4H-chromen-4-one:

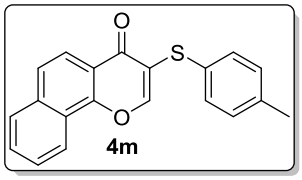


4l

Pale Yellow solid; Yield (77%); m.p. 121-126 ^{o}C; IR (KBr, cm^{-1}): 3425, 2920, 1639, 1434, 1303, 1270, 1083, 810; ^{1}H-NMR (400 MHz, $CDCl_3$): 8.06 (s, 1H), 7.59 (d, J= 2.0Hz, 1H), 7.40 (m, 1H), 7.38-7.09 (m, 5H), 3.88 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 174.54, 157.37, 156.44, 151.34, 137.61, 130.95,

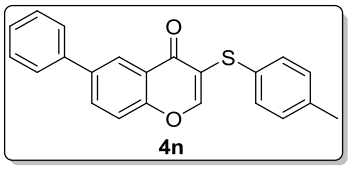
130.25, 130.15, 124.40, 124.19, 119.69, 105.42, 56.10, 21.23;.MS (EI): *m/z* 299 (M+1,100); HRMS: (ESI): Calcd for $C_{17}H_{14}O_3S$[M+H]:299.0749, Found: 299.0742.

3-(p-tolylthio)-4H-benzo[h]chromen-4-one:



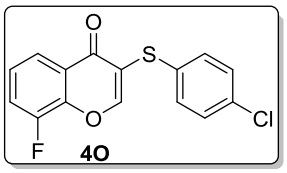
Yellow solid; Yield (80%); m.p. 131-134 °C; IR (KBr, cm^{-1}): 3425, 2920, 1639, 1434, 1303, 1270, 1083, 810; ^{1}H-NMR (400 MHz, $CDCl_3$): 8.45 (d, J= 8 Hz, 1H), 8.18-8.16 (d, J= 8.8Hz, 1H),8.10 (s, 1H), 7.94 (d, J= 7.6 Hz, 1H), 7.79-7.70 (m, 3H), 7.69-7.40 (m, 2H), 7.16 (d, J= 8 Hz, 2H), 2.33 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 174.94, 154.38, 153.87, 138.09, 135.91, 131.80, 130.32, 129.61, 129.22, 128.25, 127.41, 125.83, 123.93, 123.57, 122.28, 121.17, 119.73, 21.26; MS (EI): *m/z* 319 (M+1,100); HRMS: (ESI): Calcd for $C_{20}H_{14}O_2S$[M+H]:319.0798, Found: 319.0793.

6-phenyl-3-(p-tolylthio)-4H-chromen-4-one:



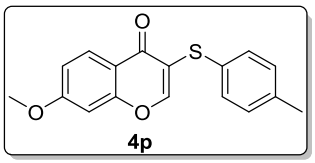
Off white solid; Yield (76%); m.p. 154-159 °C; IR (KBr, cm^{-1}): 3438, 3063, 2920, 1645, 1551, 1464, 1083, 697; ^{1}H-NMR (400 MHz, $CDCl_3$): 8.45 (d, J=2.4 Hz, 1H), 8.06 (s, 1H), 7.93-7.90 (m, 1H), 7.65-7.63 (m, 2H), 7.54-7.35 (m, 6H), 7.13 (d, J= 8.0 Hz, 2H), 2.33 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 175.28, 156.32, 155.80, 139.23, 138.93, 137.76, 132.89, 131.15, 130.21, 129.90, 129.14, 128.10, 127.31, 124.29, 123.80, 121.28, 118.76, 21.24; MS (EI): *m/z* 345 (M+1,100); HRMS: (ESI): Calcd for $C_{22}H_{16}O_2S$[M+H]:345.0798, Found: 345.0793.

3-((4-chlorophenyl)thio)-8-fluoro-4H-chromen-4-one:



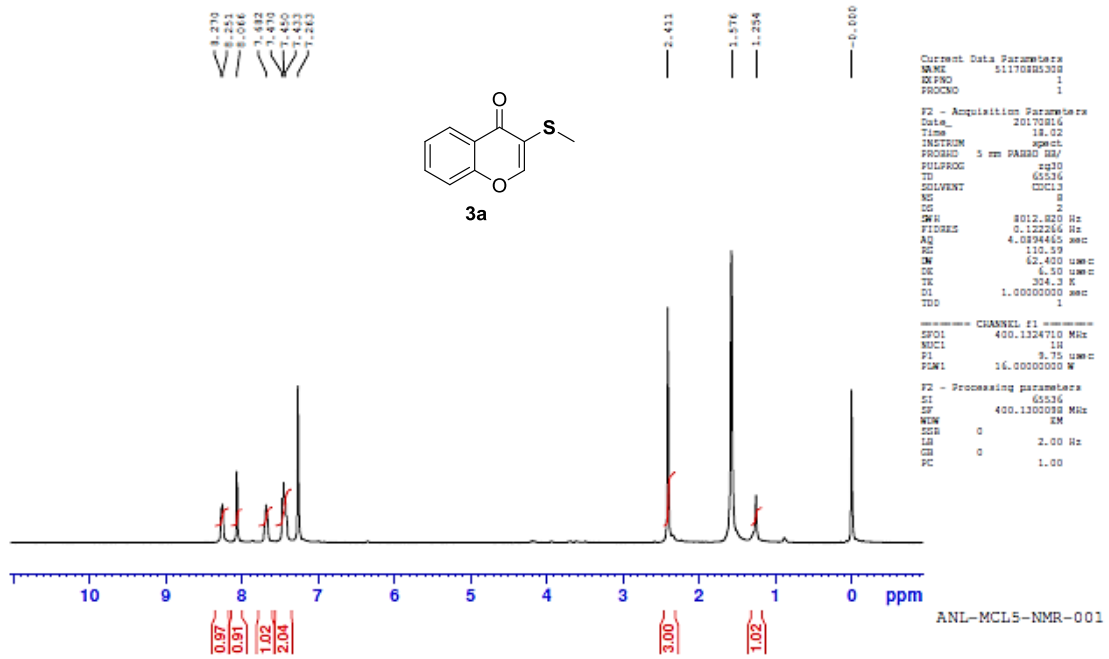
Off white solid; Yield (72%); m.p.177-181 °C; IR (KBr, cm^{-1}): 3063, 1645, 1556, 1479, 1259, 1112, 807, 759; ^{1}H-NMR (400 MHz, $CDCl_3$): 8.20 (s, 1H), 8.00-7.97 (m, 1H), 7.50-7.45 (m, 1H), 7.40-7.34 (m, 3H), 7.27-7.25 (m, 2H); ^{13}C NMR (125 MHz, $CDCl_3$): 173.95, 156.68, 152.03, 150.01, 145.18, 145.09, 133.57, 131.94, 131.50, 129.38, 125.57, 125.52, 125.40, 121.39, 121.36, 120.44, 119.95, 119.82; MS (EI): *m/z* 307 (M+1,100); HRMS: (ESI): Calcd for $C_{16}H_8ClFO_2S$[M+H]:306.9996, Found: 307.0003

7-methoxy-3-(p-tolylthio)-4H-chromen-4-one:

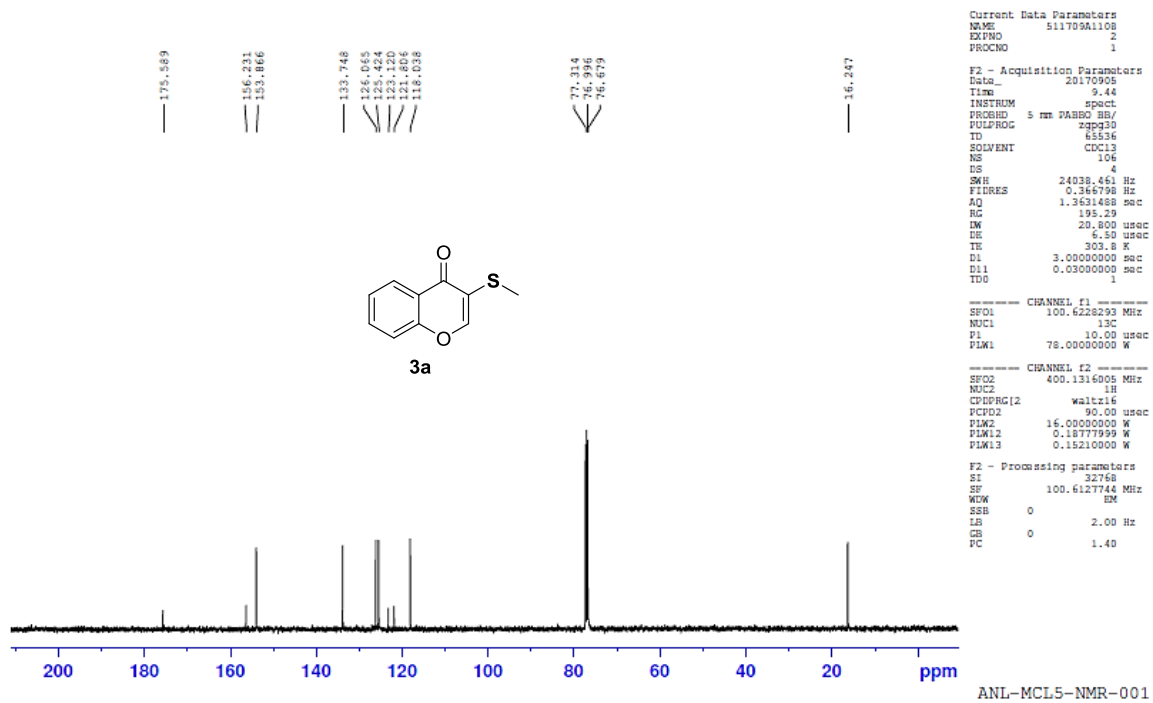


Pale yellow solid; Yield (74%); m.p.121-125 °C; IR (KBr, cm^{-1}): 3425, 2920, 1639, 1434, 1303, 1270, 1083, 810; ^{1}H-NMR (400 MHz, $CDCl_3$): 8.14 (d, J= 7.2 Hz, 1H), 7.96 (s, 1H), 7.34-7.32 (m, 2H), 7.11-7.09 (m, 2H), 6.96-6.82 (m, 1H), 6.81 (s, 1H), 3.89 (s, 3H), 2.30 (s, 3H); ^{13}C NMR (125 MHz, $CDCl_3$): 174.55, 164.33, 158.22, 156.00, 137.58, 130.97, 130.14, 127.93, 121.02, 117.61, 115.03, 100.36, 56.01, 21.22; MS (EI): *m/z* 299 (M+1,100); HRMS: (ESI): Calcd for $C_{17}H_{14}O_3S$[M+H]:299.0742, Found: 299.0753.

GVK-CBK-3-Phd-44



GVK-CBK-1-41



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

Vial position : P1-D-05
Date of Analysis : 9/13/2017 1:03:42 PM Injection Vol : 0.300uL
Acq. Method : RND-FA-3.5mns Instrument ID : ANL-MCL5-LCMS-(
Sample Name : GVK-CBK-3-Phd-44

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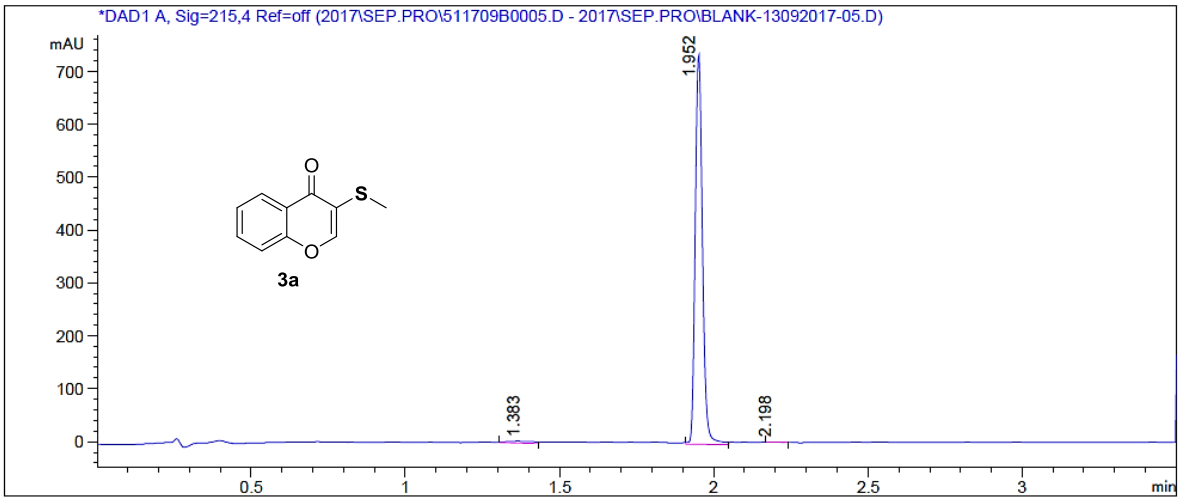
Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: B1: 0.1 % FA IN WATER A1: 0.1%FA IN ACN
Gradient: Time (min) /%A1: 0/2, 0.4/2, 2.8/98,3.4/98,3.41/2,3.5/2
Column Flow Rate: 0.6 ml/min
Column Temperature: 60°C ->



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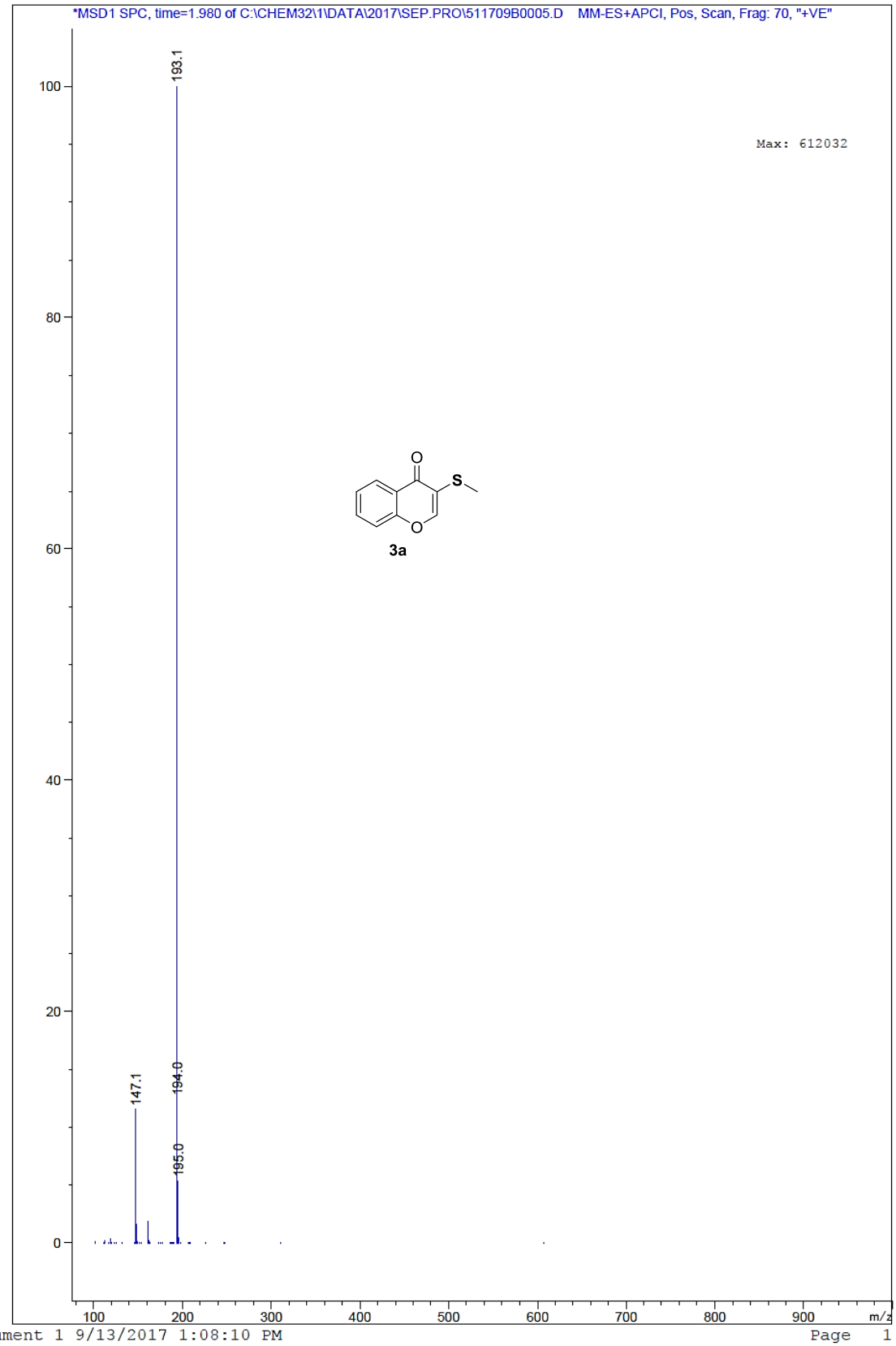
MS Spectrum

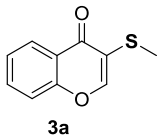


trument 1 9/13/2017 1:08:10 PM Page 1 of 1

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None



3a

Monoisotopic Mass, Even Electron Ions

5 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)

Elements Used:

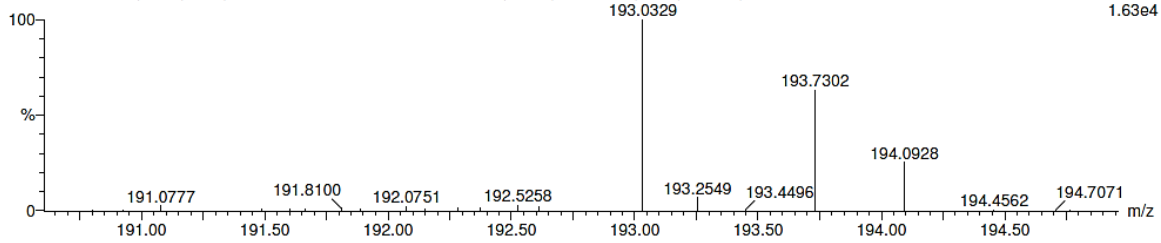
C: 0-10 H: 0-9 O: 0-2 S: 0-1

GVK-CBK-1-44

GVK Bio sciences (pvt)Ltd
Analytical Research and Development

Date of analysis:04-Oct-201715:10:46
Instru ment ID:ANL-MCL3-LCMS-001
1: TOF MS ES+
1.63e4

511709B4714 12 (0.384) AM (Cen,4, 20.00, Ar,5.0,195.13,1.00,LS 5); Sm (Mn, 5x2.00); Sb (1,40.00)



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
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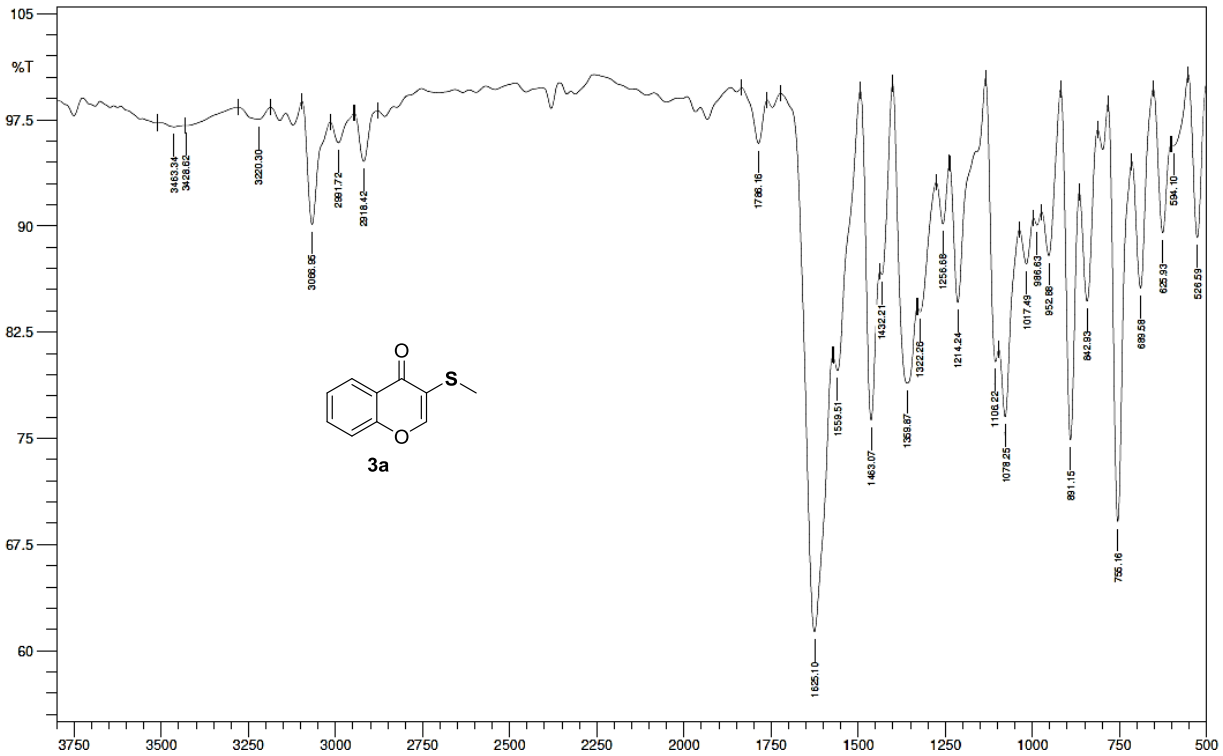
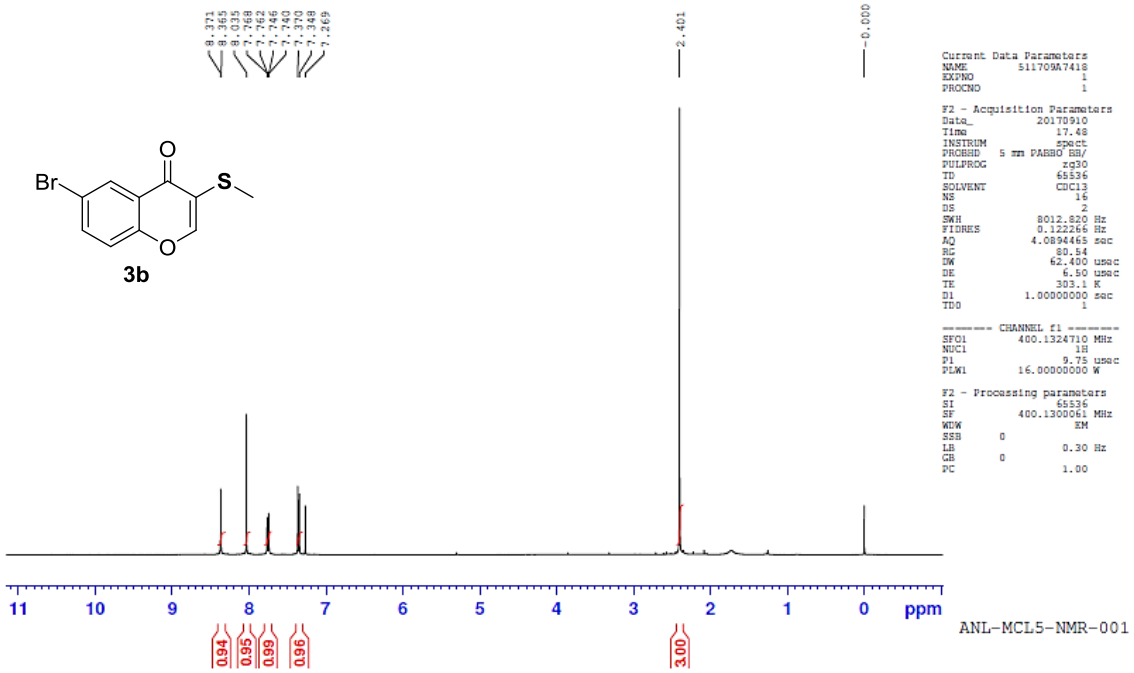


3a


8.371
8.365
8.035
7.768
7.762
7.746
7.740
7.370
7.348
7.269
2.401
0.000
Br
O
S
O
3b
Current Data Parameters
NAME 511709A7418
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Data_ 20170910
Time 17.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
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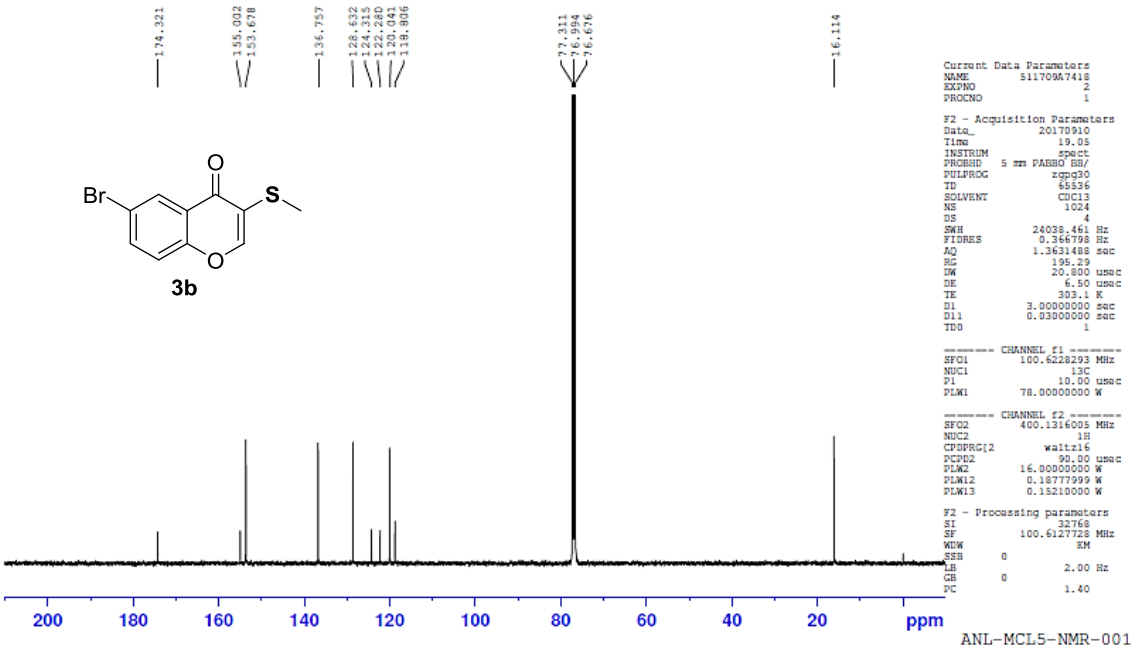
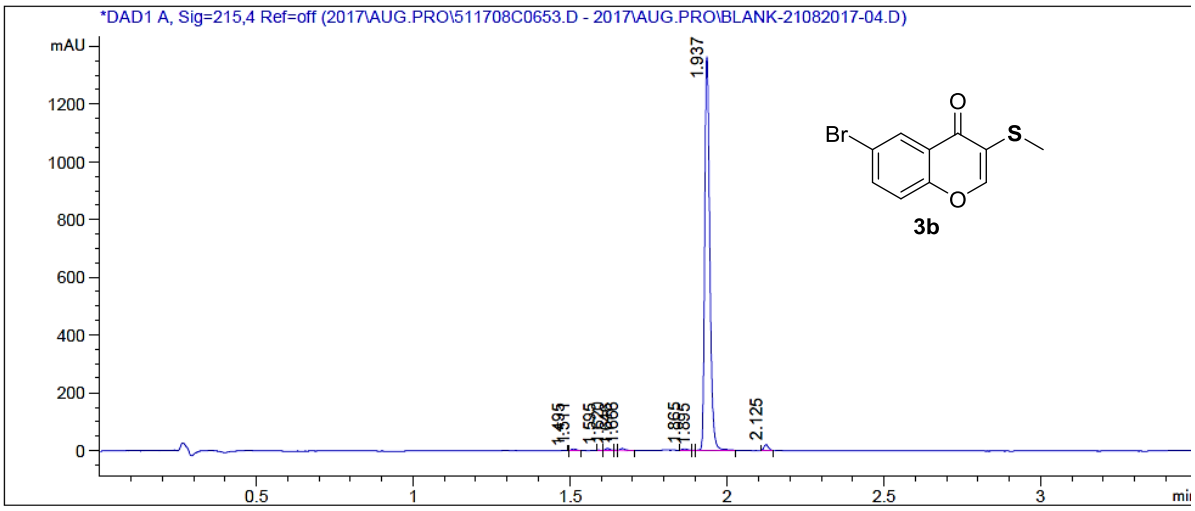
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 80.54
DW 62.400 usec
DE 6.50 usec
TE 303.1 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 9.75 usec
PLW1 16.00000000 W
F2 - Processing parameters
SI 65536
SF 400.1300061 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.94 0.95 0.99 0.96 3.00
ANL-MCL5-NMR-001


174.321
155.002
153.678
136.757
128.632
124.715
122.280
120.041
118.806
77.311
77.094
76.676
16.114
Br
O
S
O
3b
Current Data Parameters
NAME 511709A7418
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Data_ 20170910
Time 19.05
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 195.29
DW 20.800 usec
DE 6.50 usec
TE 303.1 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 78.00000000 W
CHANNEL f2
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.18777999 W
PLW13 0.15210000 W
F2 - Processing parameters
SI 32768
SF 100.6127728 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 ppm
ANL-MCL5-NMR-001

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

Vial position : P1-D-04
Date of Analysis : 8/21/2017 9:39:31 PM Injection Vol : 0.300uL
Acq. Method : RND-FA-3.5mns Instrument ID : ANL-MCL5-LCMS-
Sample Name : GVK-PHD-VK-KLU-MB-142

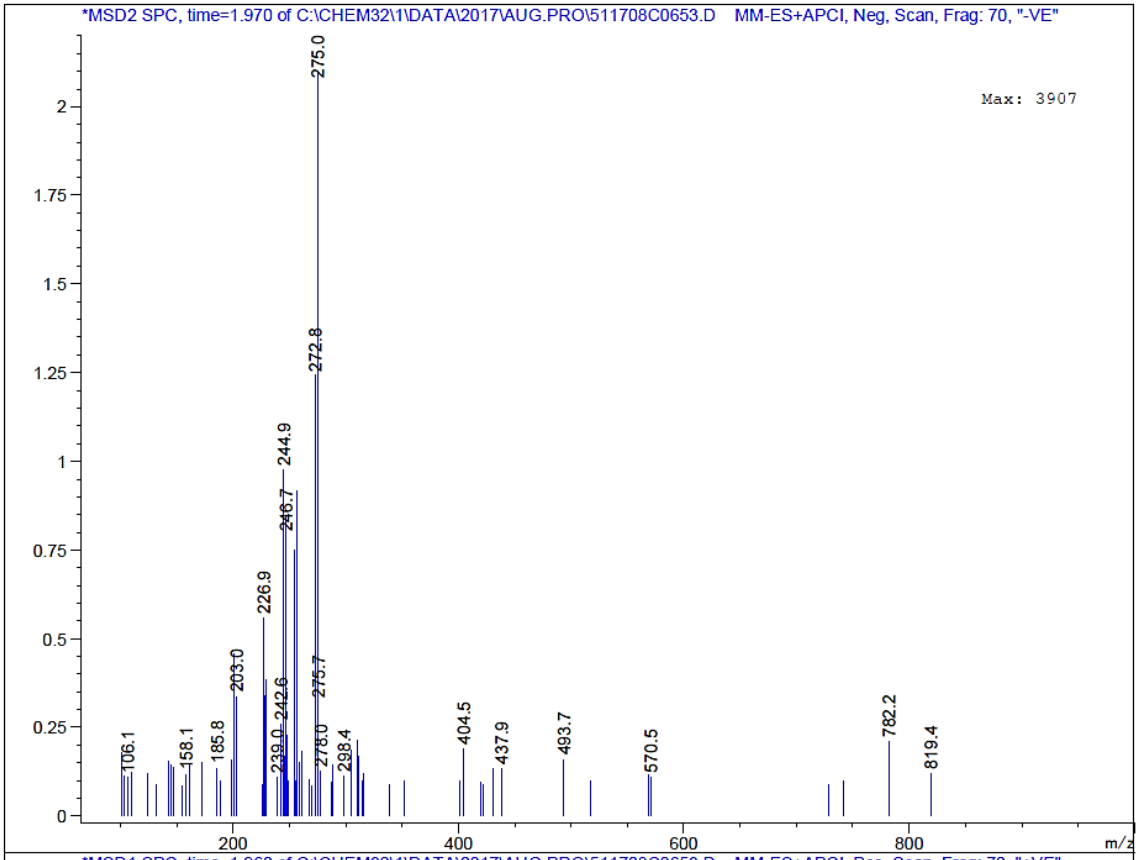
RND-FA-3.5 MIN.M
Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: B1: 0.1 % FA IN WATER A1: 0.1%FA IN ACN
Gradient: Time (min) /%A1: 0/2, 0.2/2, 2.3/98,3.4/98,3.41/2,3.5/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 50°C ->

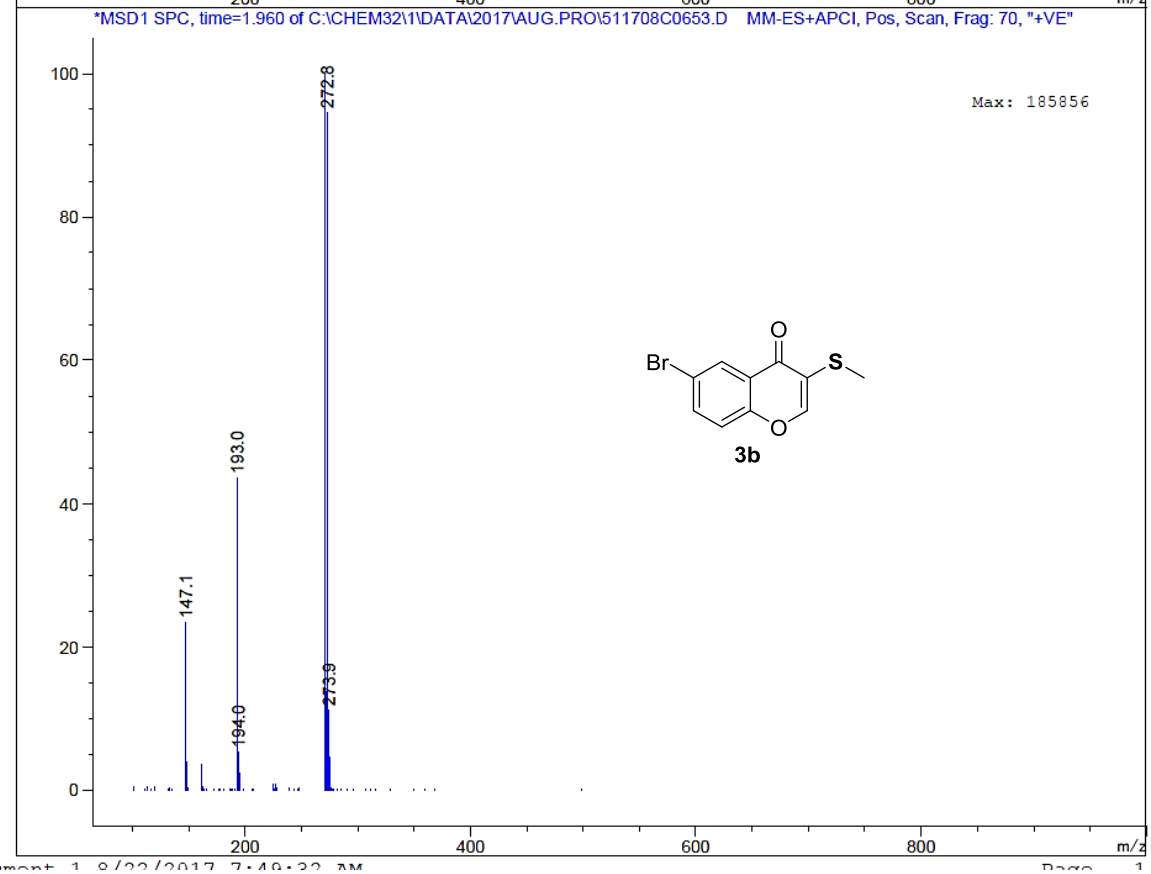


DAD1 A, Sig=215,4 Ref=off

Peak No	RT min	Height	Area	Area %
1	1.50	1.420	0.123	0.008
2	1.51	7.019	7.643	0.479
3	1.59	3.610	3.635	0.228
4	1.62	8.665	10.102	0.633
5	1.65	2.328	1.256	0.079
6	1.67	7.400	9.655	0.605
7	1.87	6.384	7.932	0.497
8	1.89	1.354	0.761	0.048
9	1.94	1368.751	1530.293	95.922
10	2.12	22.041	23.947	1.501

MS Spectrum



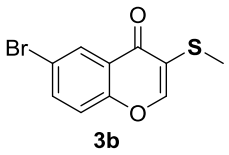


3b

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None



3b

Monoisotopic Mass, Odd and Even Electron Ions

11 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)

Elements Used:

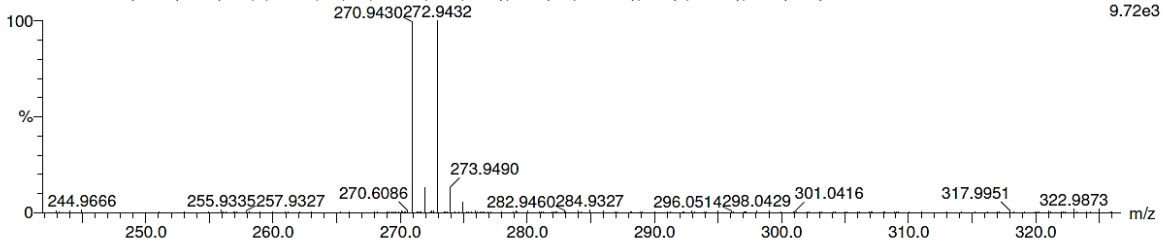
C: 0-10 H: 0-8 O: 0-2 S: 0-1 Br: 0-1

GVK-CBK-1-Phd-142(v)

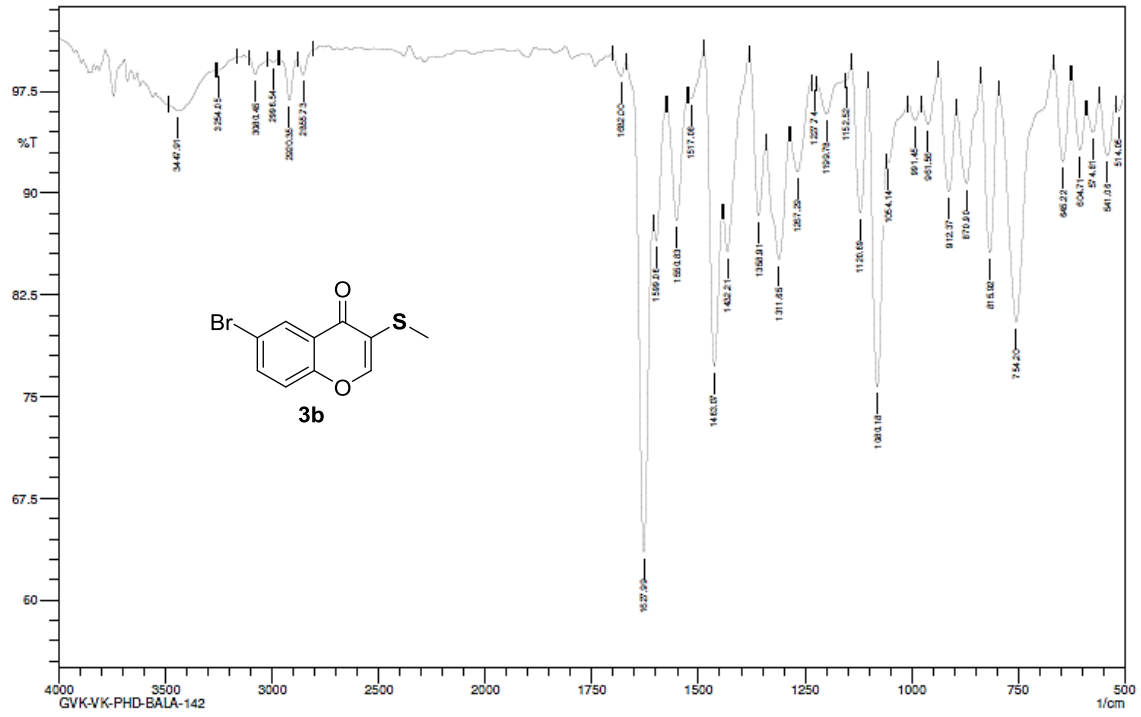
GVK Bio sciences (pvt)Ltd
Analytical Research and Development

Date of analysis:19-Feb-201811:48:40
Instru ment ID:ANL-MCL3-LCMS-001
1: TOF MS ES+
9.72e3

511802B3844- 7 (0.283) AM (Cen,2, 50.00, Ar,5.0,195.09,1.00,LS 5); Sm (Mn, 5x2.00); Sb (1,40.00); Cm (5:21)



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
270.9430	270.9428	0.2	0.7	6.5	12.2	C10 H8 O2 S Br



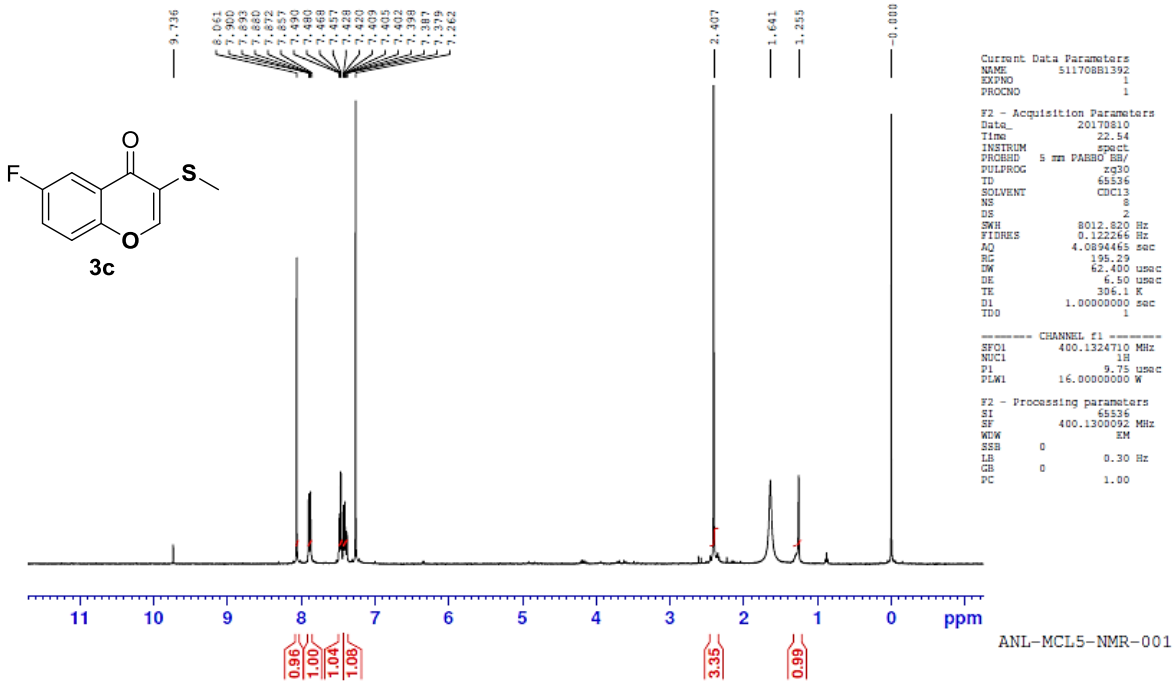
3b

Comment: IN Kbr
GVK-VK-PHD-BALA-142

No. of Scans:
Resolution:
Apodization:

Date:9/18/2017 6:15:10 PM
User: Admin

GVK-CBK-1-40

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Current Data Parameters
NAME          511708B1392
EXPNO                   1
PROCNO                  1

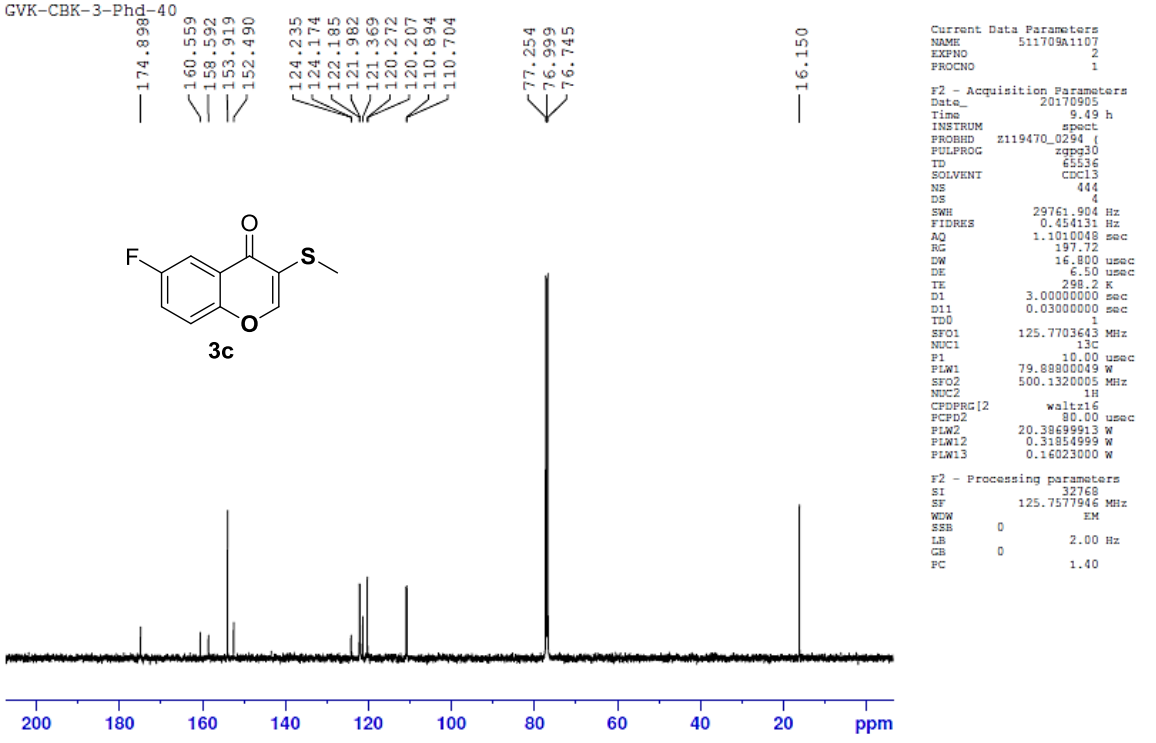
F2 - Acquisition Parameters
Date_           20170810
Time              22.54
INSTRUM           spect
PROBHD    5 mm PABBO BB/
PULPROG           zg30
TD               65536
SOLVENT          CDCl3
NS                   8
DS                   2
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.089465 sec
RG               195.29
DW              62.400 usec
DE               6.50 usec
TE              306.1 K
D1          1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1               1H
P1                9.75 usec
PLW1        16.00000000 W

F2 - Processing parameters
SI               65536
SF          400.1300092 MHz
WDW                EM
SSB       0
LB              0.30 Hz
GB        0
PC              1.00
```

ANL-MCL5-NMR-001

GVK-CBK-3-Phd-40




```
Current Data Parameters
NAME          511709A1107
EXPNO                   2
PROCNO                  1

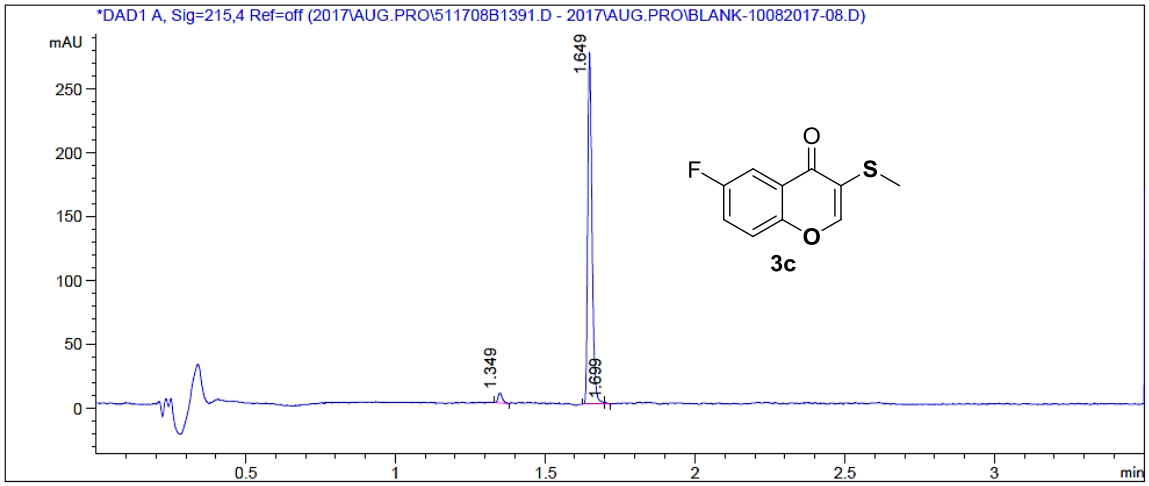
F2 - Acquisition Parameters
Date_           20170905
Time              9.49 h
INSTRUM           spect
PROBHD    Z119470_0294 (
PULPROG          zgpg30
TD               65536
SOLVENT          CDCl3
NS                 444
DS                   4
SWH          29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010048 sec
RG               197.72
DW              16.800 usec
DE               6.50 usec
TE              298.2 K
D1          3.00000000 sec
D11         0.03000000 sec
TD0                  1
SFO1        125.7703643 MHz
NUC1               13C
P1               10.00 usec
PLW1        79.88800049 W
SFO2        500.1320005 MHz
NUC2               1H
CPDPRG[2         waltz16
PCPD2            80.00 usec
PLW2        20.38699913 W
PLW12        0.31854999 W
PLW13        0.16023000 W

F2 - Processing parameters
SI               32768
SF          125.7577946 MHz
WDW                EM
SSB       0
LB              2.00 Hz
GB        0
PC              1.40
```

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

Vial position : P1-A-09
Date of Analysis : 8/10/2017 8:24:01 PM Injection Vol : 0.300uL
Acq. Method : RND-FA-3.5mns Instrument ID : ANL-MCL5-LCMS-001
Sample Name : GVK-CBK-3-Phd-40

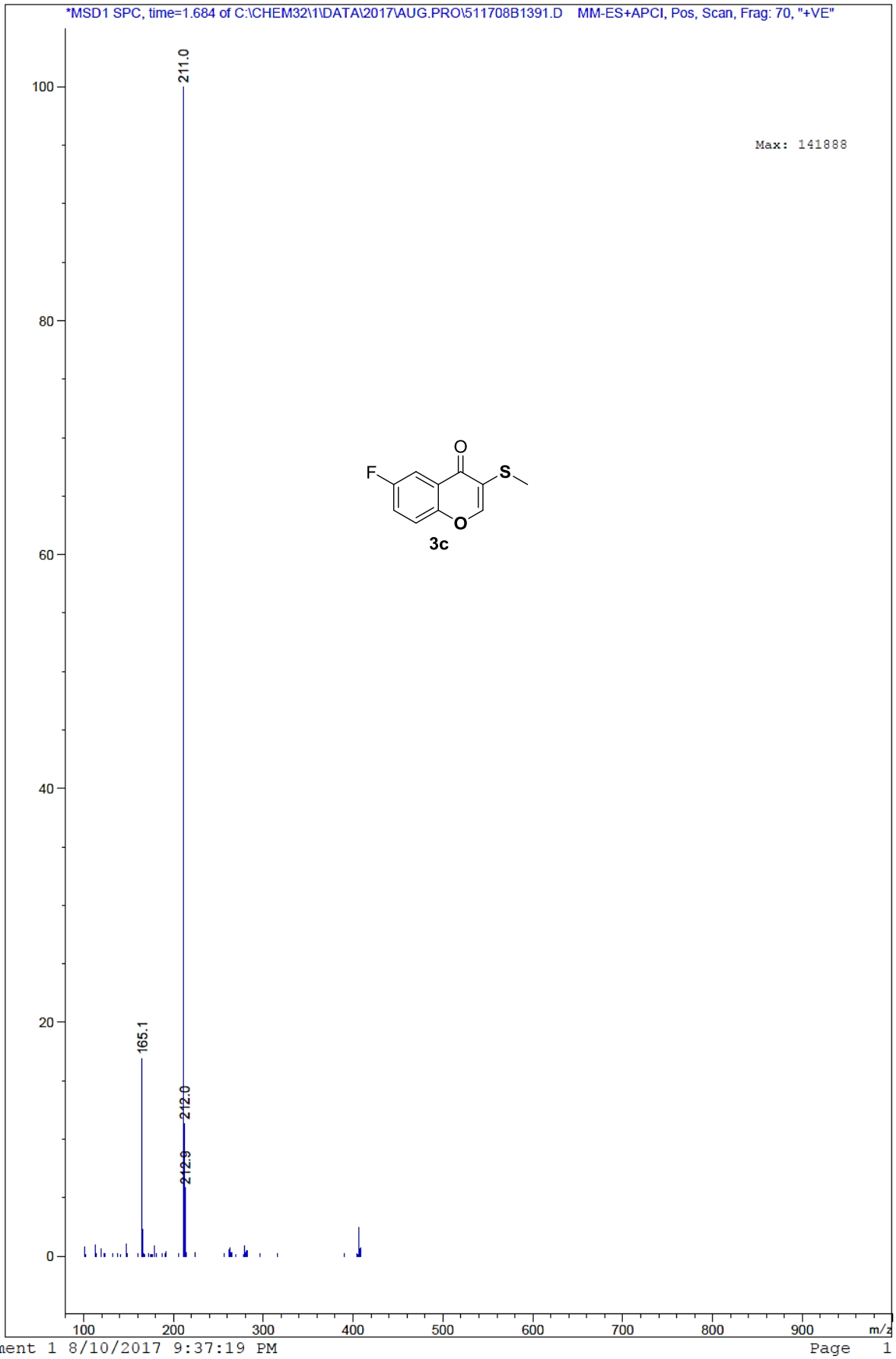
RND-FA-3.5 MIN.M
Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: B1: 0.1 % FA IN WATER A1: 0.1%FA IN ACN
Gradient: Time (min) /%A1: 0/2, 0.2/2, 2.3/98,3.4/98,3.41/2,3.5/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 50°C ->



DAD1 A, Sig=215,4 Ref=off

Peak No	RT min	Height	Area	Area %
1	1.35	7.978	8.050	2.858
2	1.65	276.320	272.950	96.896
3	1.70	0.974	0.694	0.246

MS Spectrum

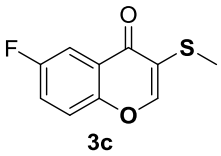


trument 1 8/10/2017 9:37:19 PM Page 1 of 1

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None



3c

Monoisotopic Mass, Odd and Even Electron Ions

10 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)

Elements Used:

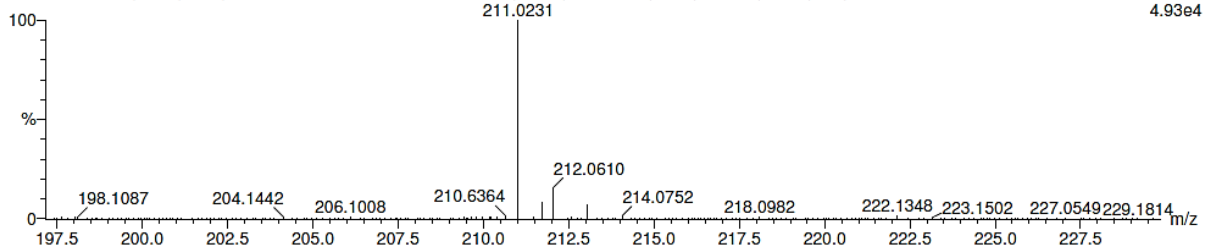
C: 0-10 H: 0-8 O: 0-2 F: 0-1 S: 0-1

GVK-CBK-1-Phd-40

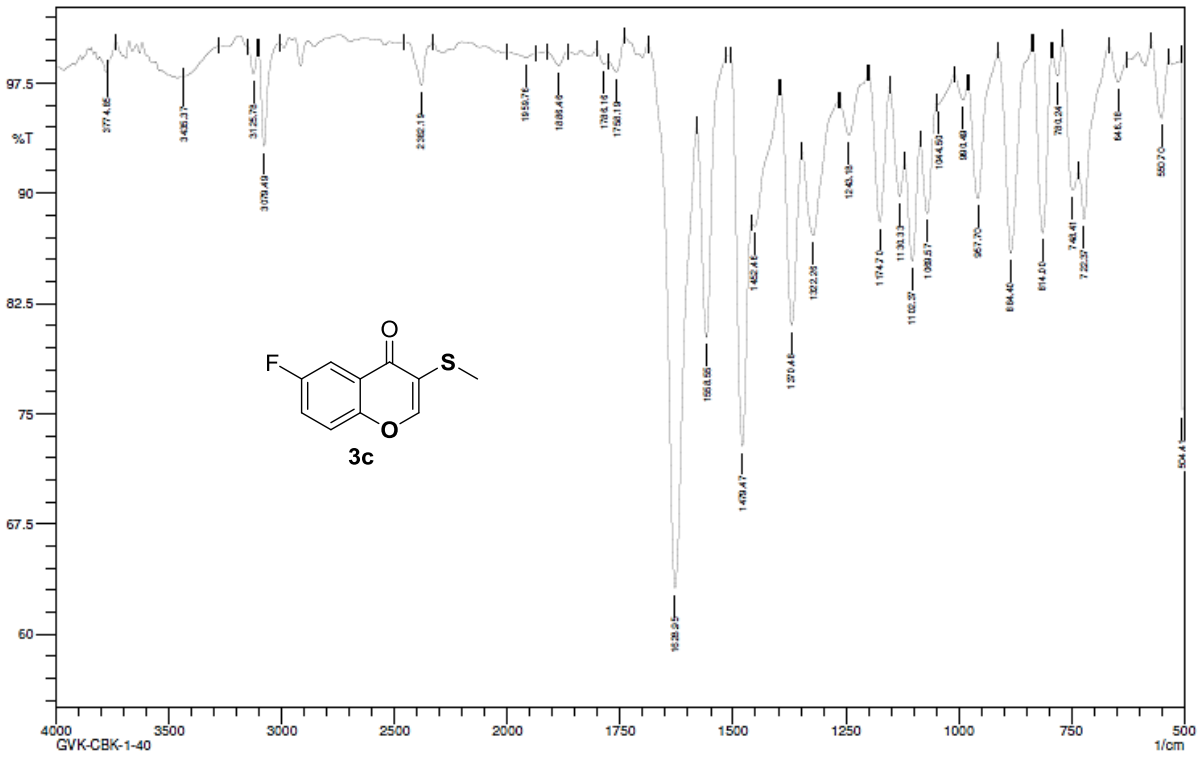
GVK Bio sciences (pvt)Ltd
Analytical Research and Development

Date of analysis:16-Feb-201815:31:50
Instru ment ID:ANL-MCL3-LCMS-001
1: TOF MS ES+
4.93e4

511802B3835 7 (0.282) AM (Cen,2, 50.00, Ar,5.0,195.11,1.00,LS 5); Sm (Mn, 5x2.00); Sb (1,40.00); Cm (5:15)



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
211.0231	211.0229	0.2	0.9	6.5	1080.4	C10 H8 O2 F S

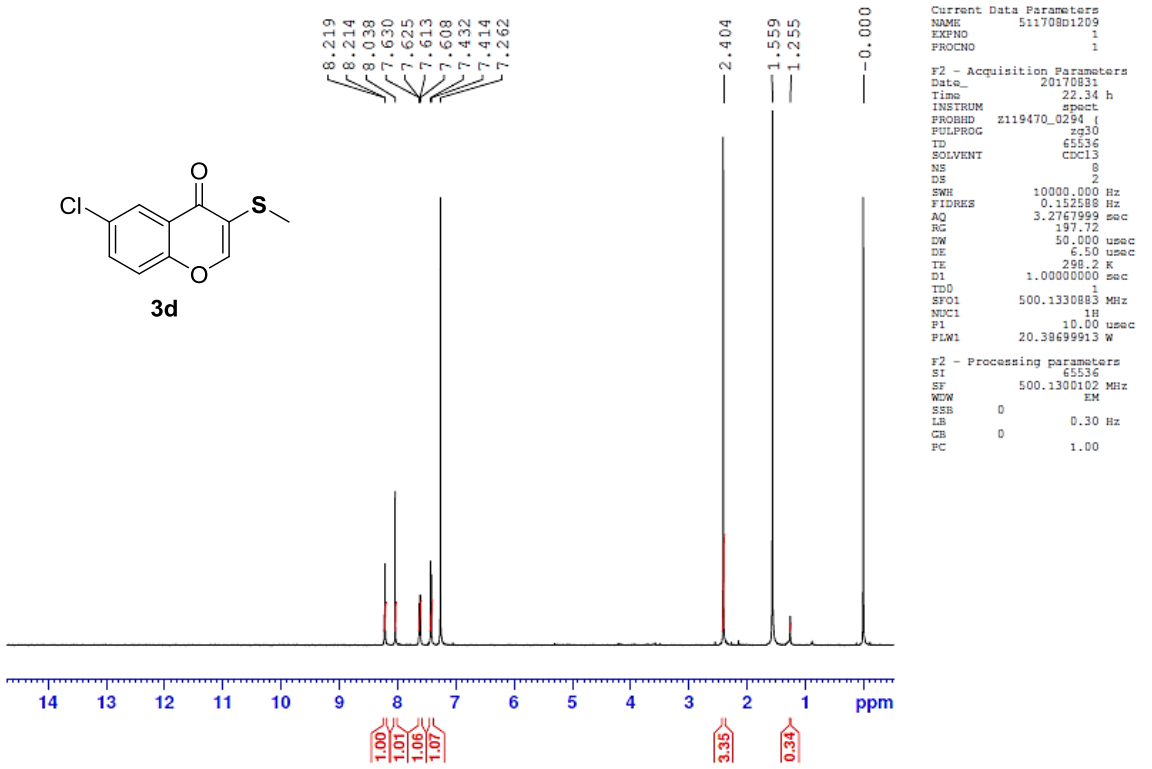


Comment: IN Kbr
GVK-CBK-1-40

No. of Scans:
Resolution:
Apodization:

Date: 9/13/2017 12:18:51 PM
User: Admin

GVK-CBK-3-Phd-47

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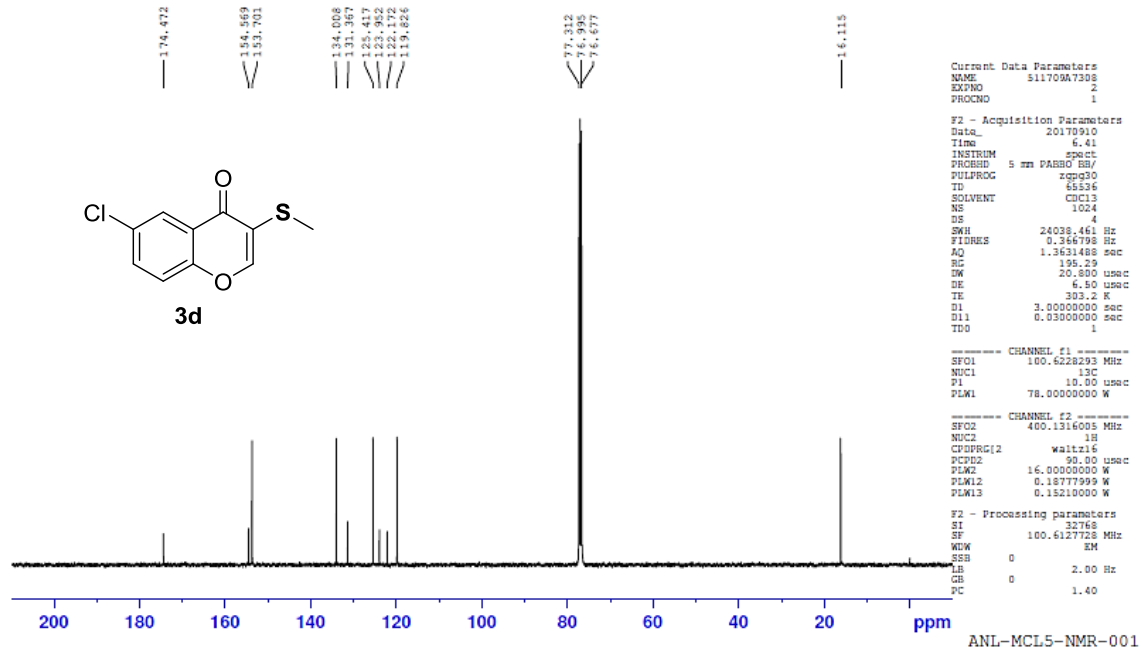
Current Data Parameters
NAME          511708d1209
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20170831
Time              22.34 h
INSTRUM             spect
PROBHD    Z119470_0294 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     2
SWH           10000.000 Hz
FIDRES            0.152588 Hz
AQ             3.2767999 sec
RG                 197.72
DW                50.000 usec
DE                 6.50 usec
TE                298.2 K
D1             1.00000000 sec
TD0                    1
SFO1          500.1330883 MHz
NUC1                  1H
P1                 10.00 usec
PLW1          20.38699913 W

F2 - Processing parameters
SI                 65536
SF            500.1300102 MHz
WDW                   EM
SSB          0
LB                 0.30 Hz
GB           0
PC                 1.00
```

GVK-CBK-3-Phd-47




```
Current Data Parameters
NAME          511709A7308
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20170910
Time                6.41
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     4
SWH           24038.461 Hz
FIDRES            0.366798 Hz
AQ             1.3631488 sec
RG                 195.29
DW                20.800 usec
DE                 6.50 usec
TE                303.2 K
D1             3.00000000 sec
D11            0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          100.6228293 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          78.00000000 W

======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              90.00 usec
PLW2          16.00000000 W
PLW12          0.18777999 W
PLW13          0.15210000 W

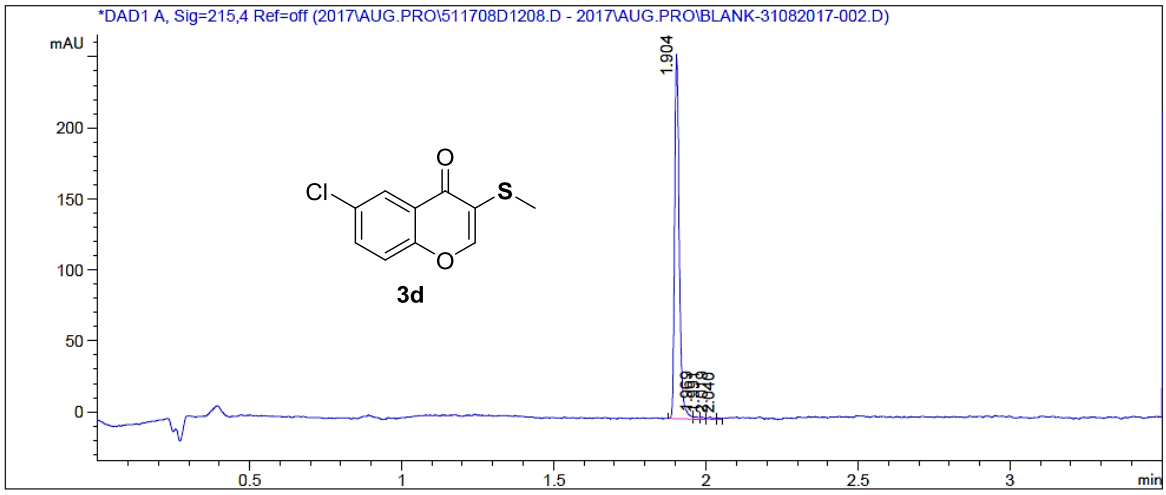
F2 - Processing parameters
SI                 32768
SF            100.6127728 MHz
WDW                   EM
SSB          0
LB                 2.00 Hz
GB           0
PC                 1.40
```

ANL-MCL5-NMR-001

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

Vial position : P1-C-04
Date of Analysis : 8/31/2017 8:52:06 PM Injection Vol : 0.300uL
Acq. Method : RND-FA-3.5mns Instrument ID : ANL-MCL5-LCMS-0(
Sample Name : GVK-CBK-1-47

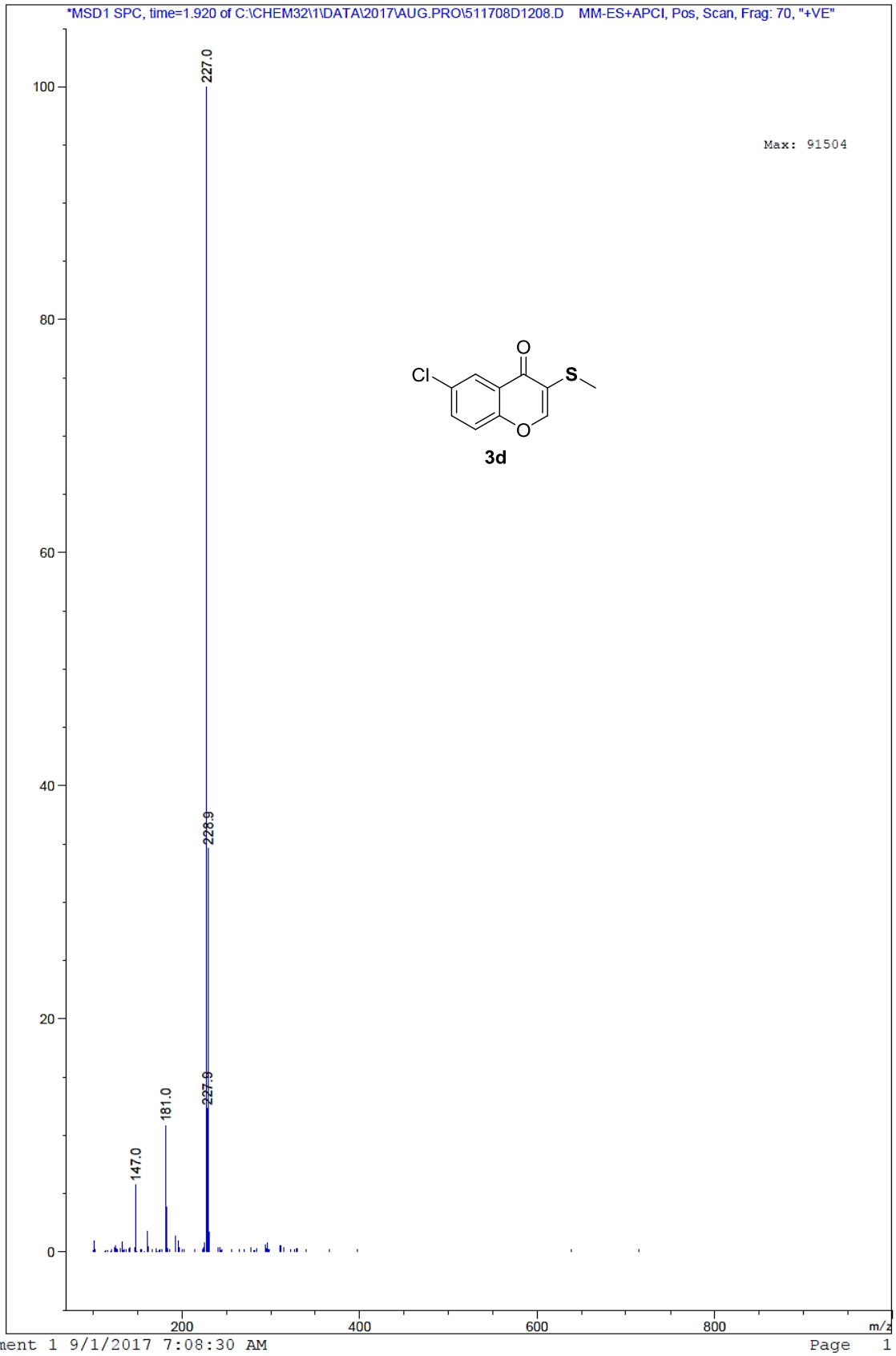
RND-FA-3.5 MIN.M
Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: B1: 0.1 % FA IN WATER A1: 0.1%FA IN ACN
Gradient: Time (min) /%A1: 0/2, 0.2/2, 2.3/98,3.4/98,3.41/2,3.5/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 50°C ->



DAD1 A, Sig=215,4 Ref=off

Peak No	RT min	Height	Area	Area %
1	1.90	257.532	279.700	97.958
2	1.97	1.661	1.947	0.682
3	1.99	1.460	1.290	0.452
4	2.02	1.447	1.800	0.630
5	2.04	0.987	0.796	0.279

MS Spectrum



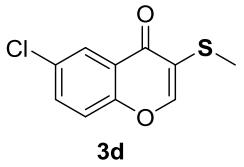
3d

rument 1 9/1/2017 7:08:30 AM Page 1 of 1

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None



3d

Monoisotopic Mass, Even Electron Ions

11 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)

Elements Used:

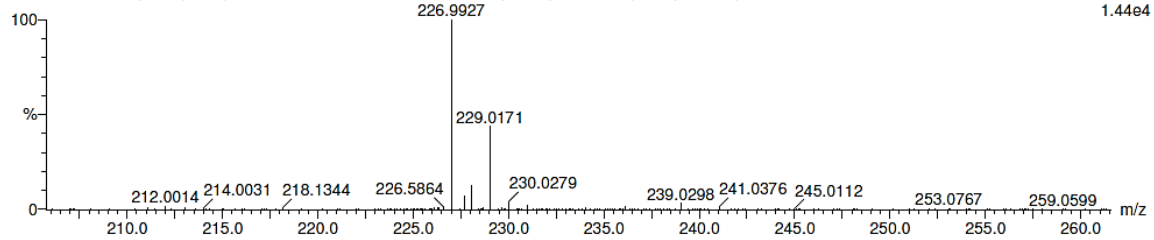
C: 0-10 H: 0-8 O: 0-2 S: 0-1 Cl: 0-1

GVK-CBK-1-47

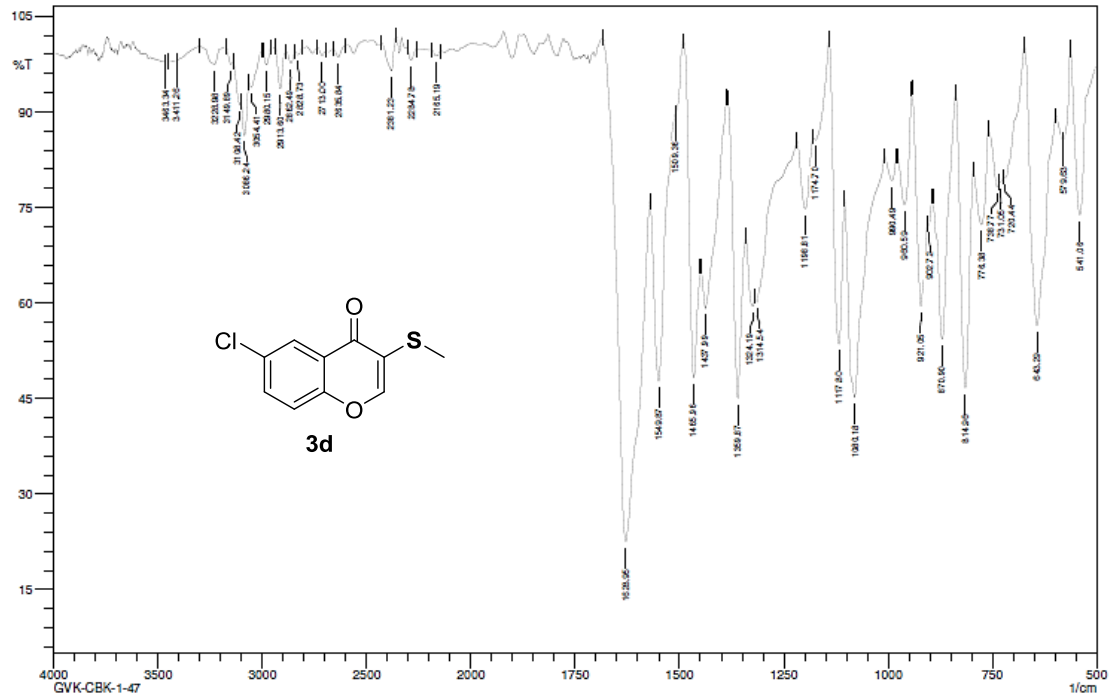
GVK Bio sciences (pvt)Ltd
Analytical Research and Development

Date of analysis:04-Oct-201715:05:51
Instru ment ID:ANL-MCL3-LCMS-001
2: TOF MS ES+
1.44e4

511709B4416 13 (0.335) AM (Cen,4, 20.00, Ar,5.0,195.11,1.00,LS 5); Sm (Mn, 5x2.00); Sb (1,40.00)



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
226.9927	226.9934	-0.7	-3.1	6.5	382.7	C10 H8 O2 S Cl



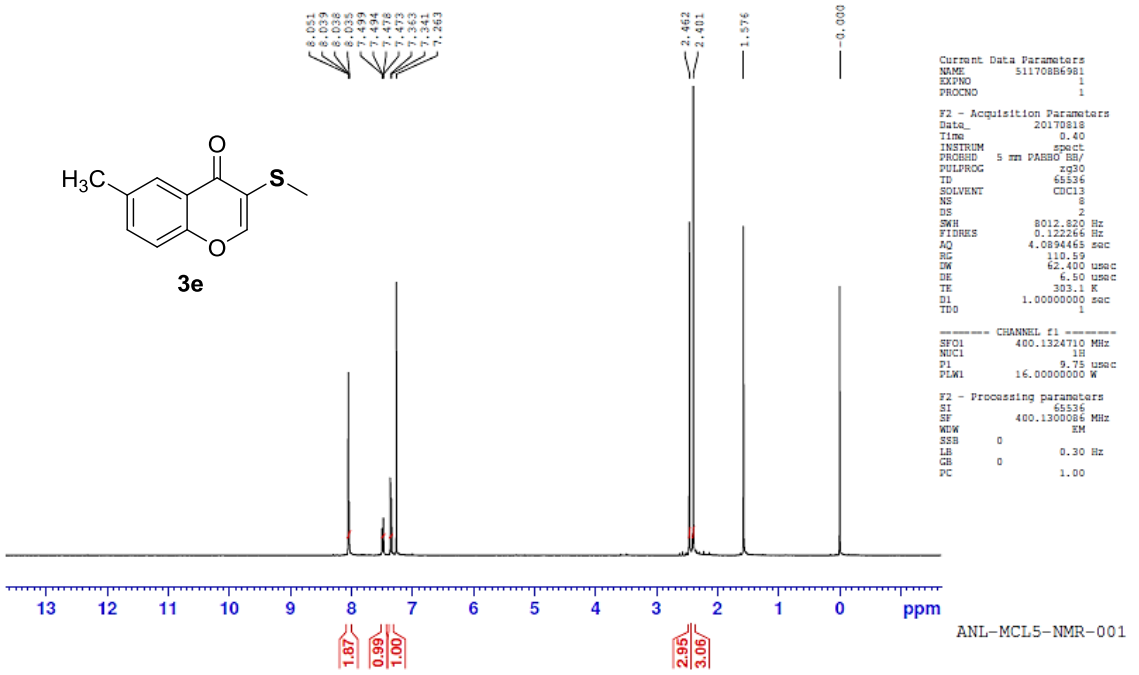
3d

Comment: IN Kbr
GVK-CBK-1-47

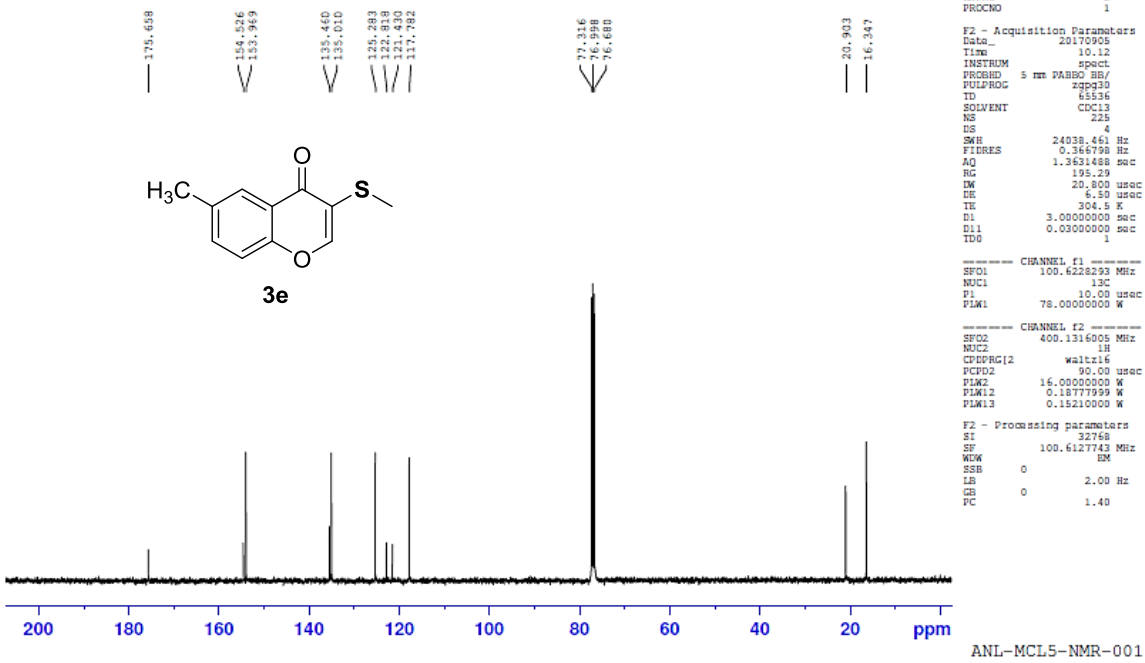
No. of Scans:
Resolution:
Apodization:

Date:9/13/2017 12:13:23 PM
User: Admin

GVK-CBK-1-42



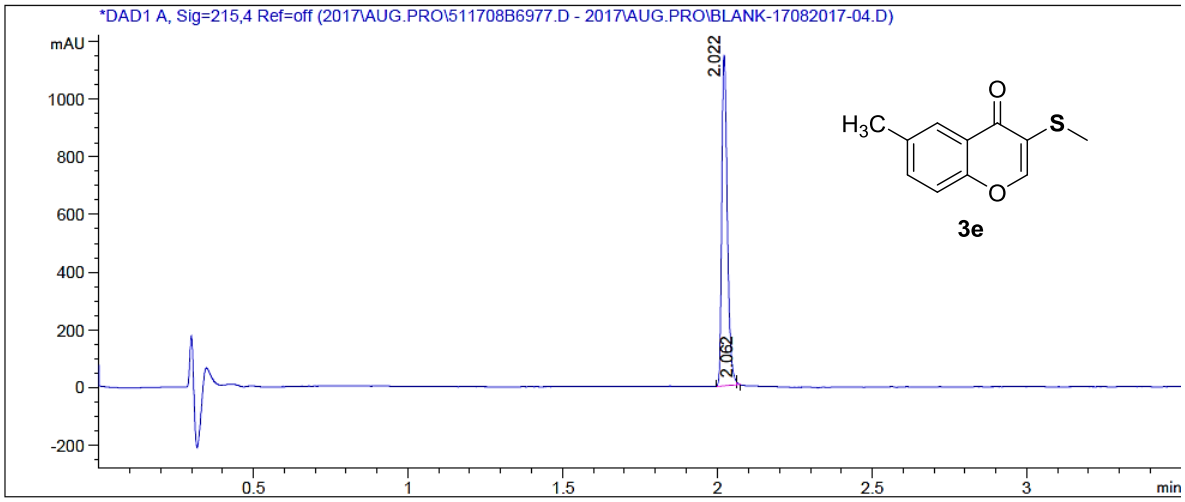
GVK-CBK-1-42



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

Vial position : P1-A-01
Date of Analysis : 8/17/2017 6:42:56 PM Injection Vol : 0.300uL
Acq. Method : RND-FA-3.5mns Instrument ID : ANL-MCL5-LCMS-
Sample Name : GVK-CBK-1-42

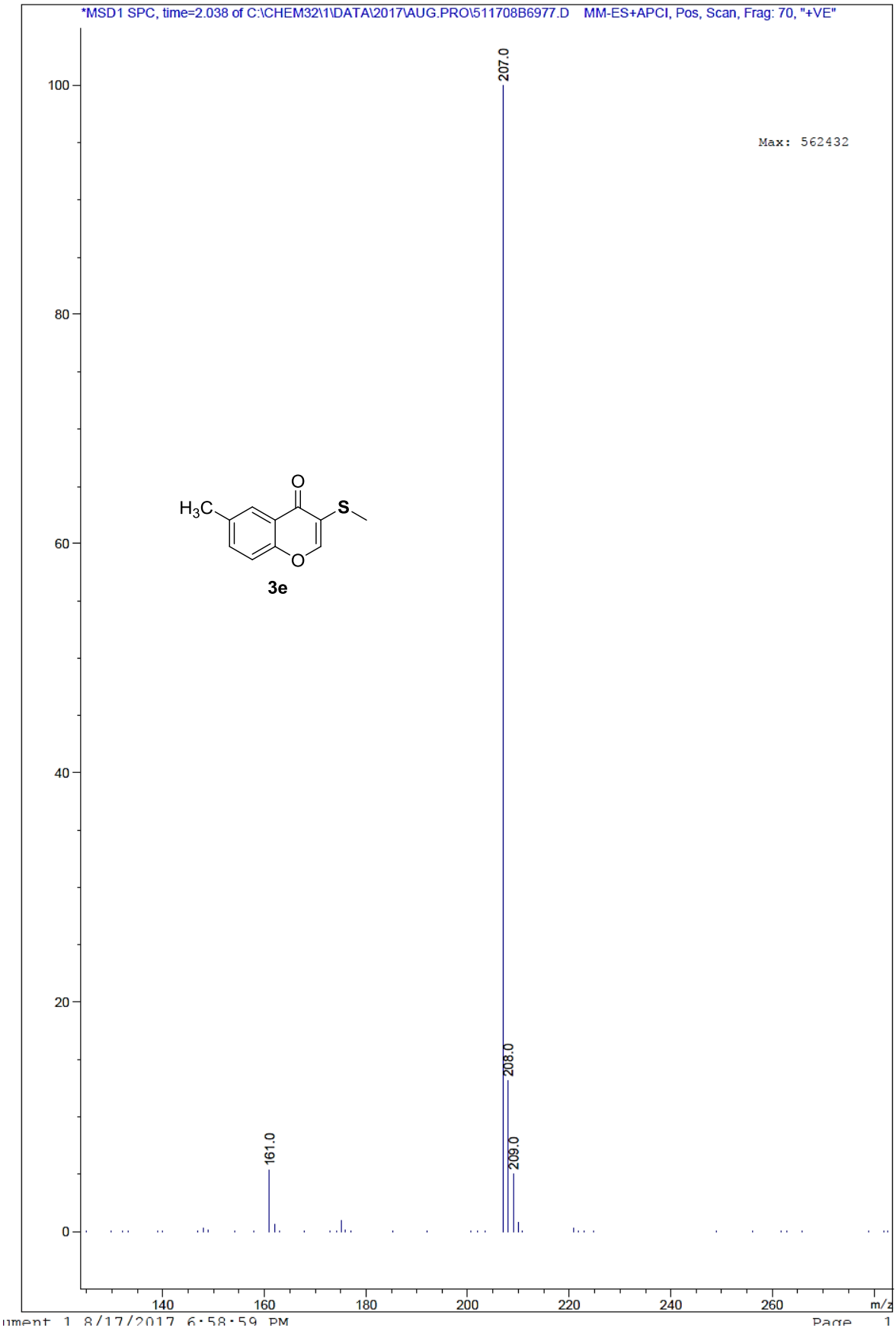
RND-FA-3.5 MIN.M
Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: B1: 0.1 % FA IN WATER A1: 0.1%FA IN ACN
Gradient: Time (min) /%A1: 0/2, 0.2/2, 2.3/98,3.4/98,3.41/2,3.5/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 50°C ->



DAD1 A, Sig=215,4 Ref=off

Pea No	RT min	Height	Area	Area %
1	2.02	1150.126	1425.981	99.838
2	2.06	10.408	2.309	0.162

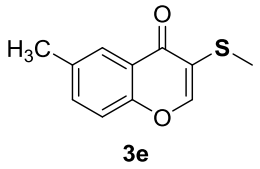
MS Spectrum


*MSD1 SPC, time=2.038 of C:\CHEM32\1\DATA\2017\AUG.PRO\511708B6977.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 562432
207.0
208.0
209.0
161.0
100
80
60
40
20
0
140
160
180
200
220
240
260
m/z
O
H3C
S
O
3e

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None



3e

Monoisotopic Mass, Even Electron Ions

5 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)

Elements Used:

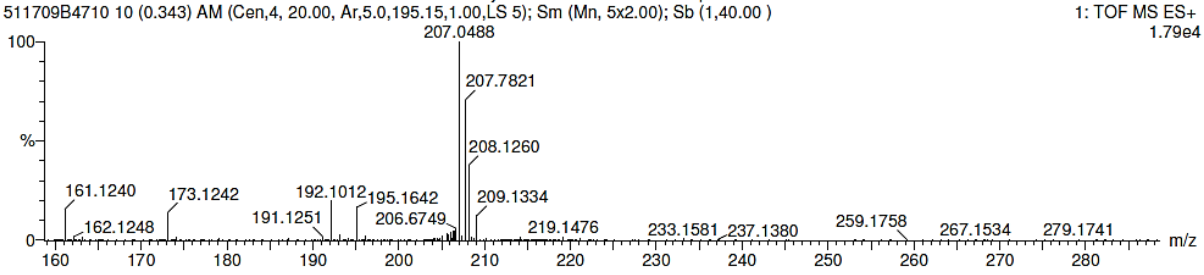
C: 0-11 H: 0-11 O: 0-2 S: 0-1

GVK-CBK-1-42

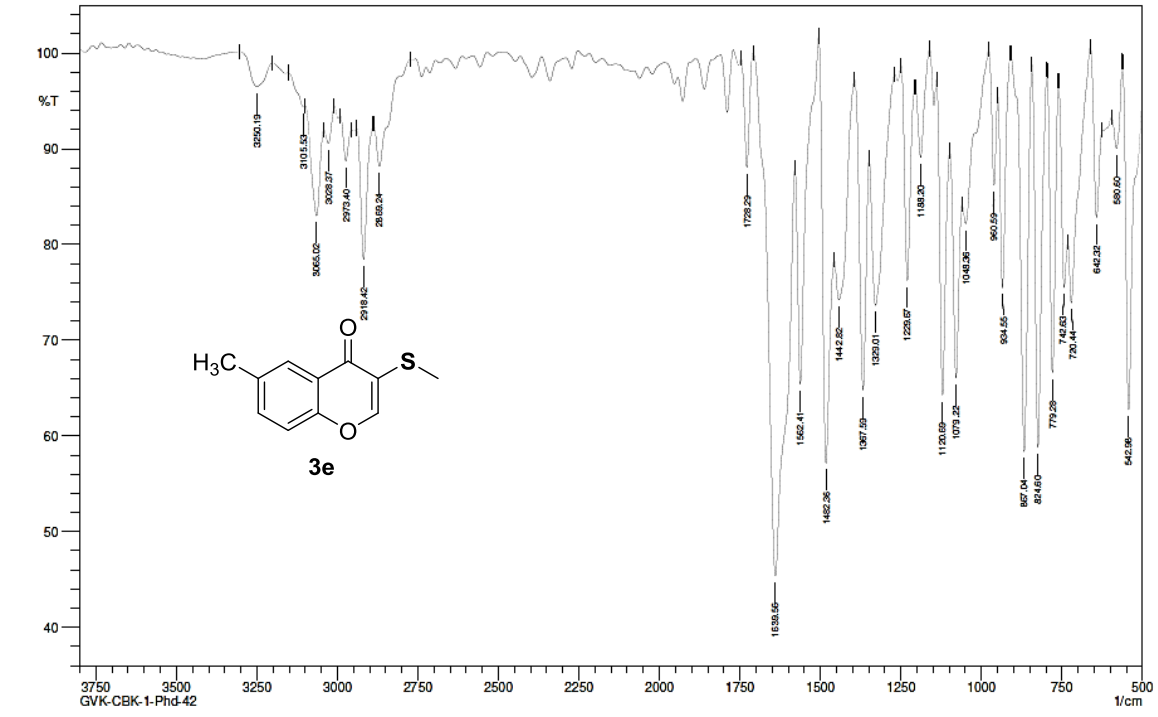
GVK Bio sciences (pvt)Ltd
Analytical Research and Development

Date of analysis:04-Oct-201715:33:33
Instru ment ID:ANL-MCL3-LCMS-001
1: TOF MS ES+
1.79e4

511709B4710 10 (0.343) AM (Cen,4, 20.00, Ar,5.0,195.15,1.00,LS 5); Sm (Mn, 5x2.00); Sb (1,40.00)



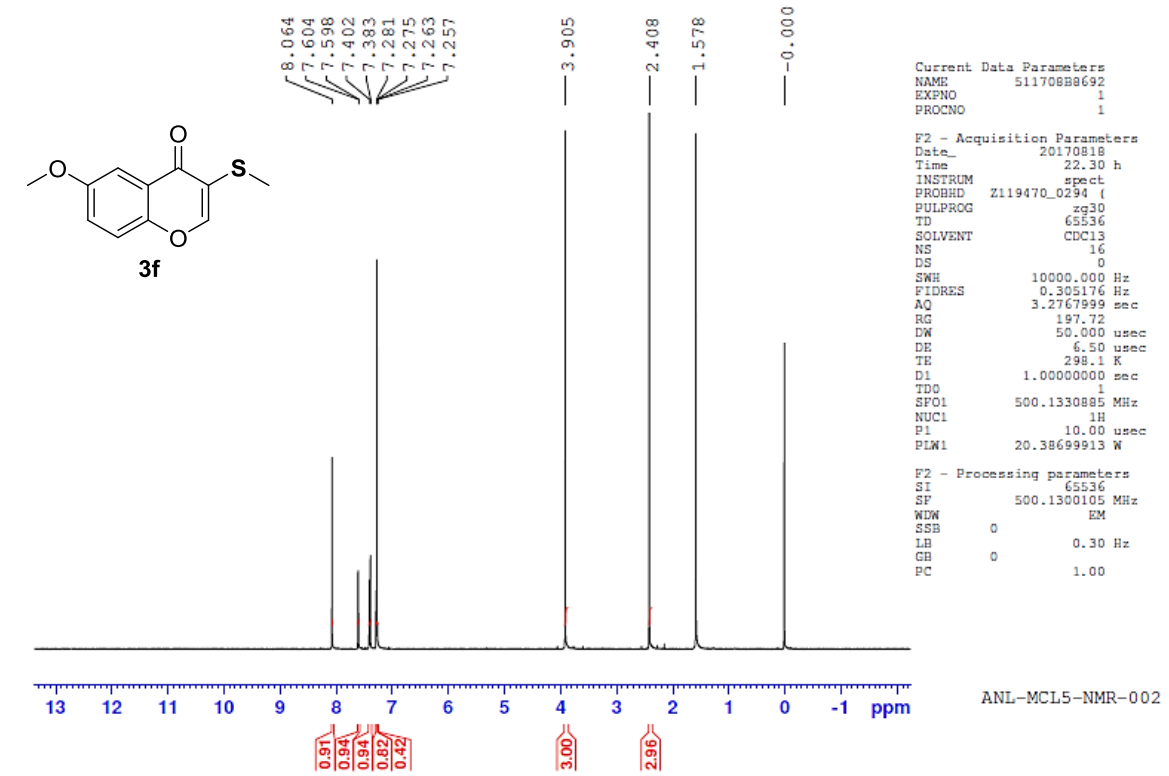
Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
207.0488	207.0480	0.8	3.9	6.5	5044.3	C11 H11 O2 S



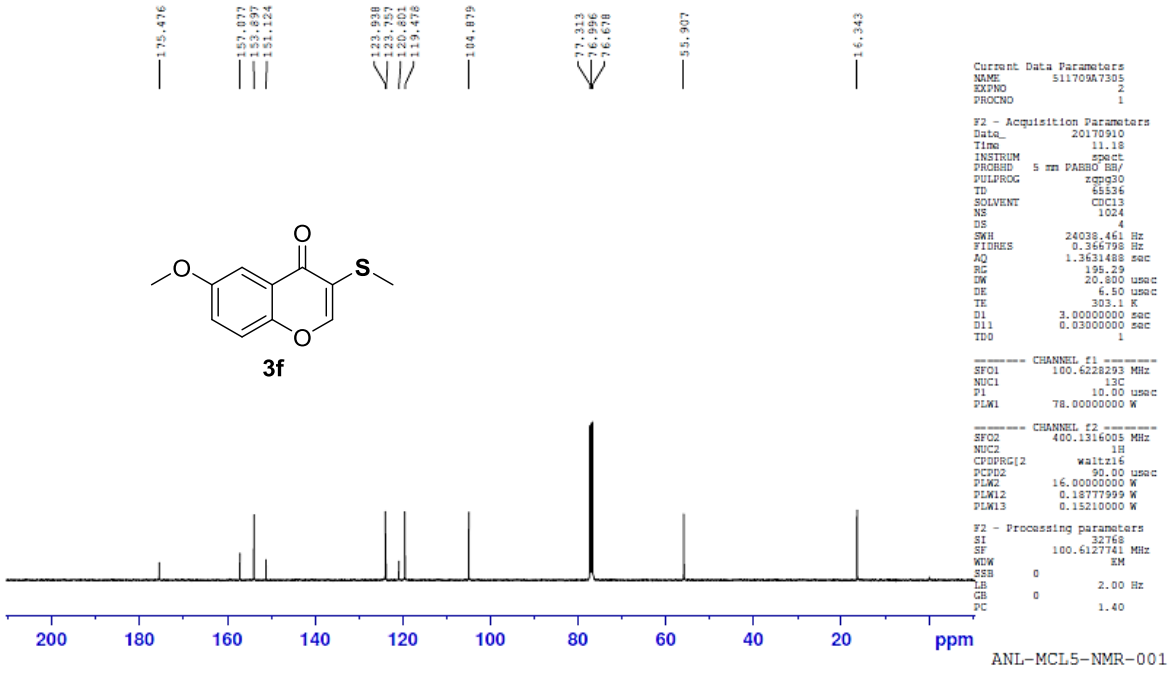
Comment: IN Kbr

No. of Scans:

Date:11/30/2018 4:14:59 PM



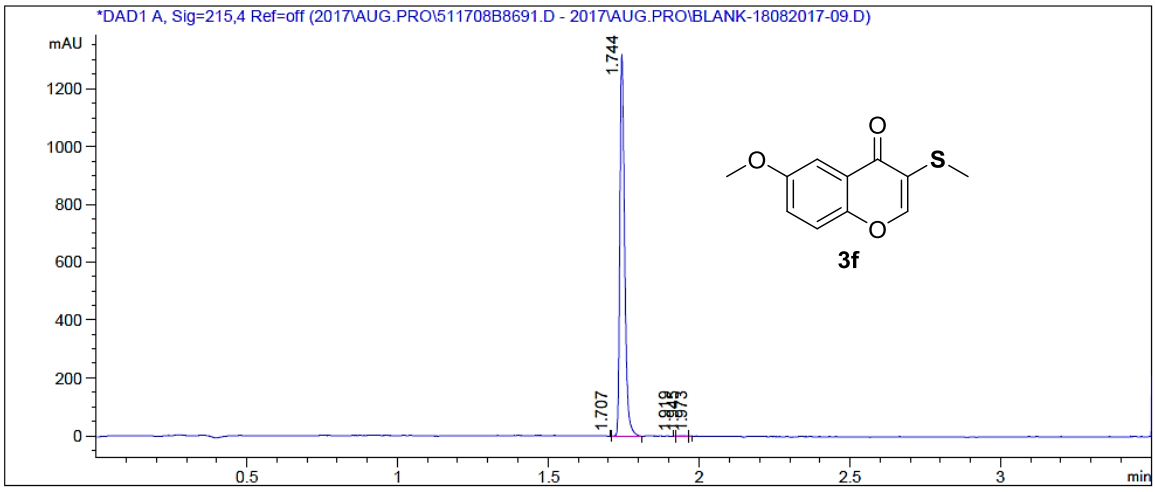
GVK-CBK-3-Phd-46



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

Vial position : P2-A-01
Date of Analysis : 8/18/2017 11:07:04 PM Injection Vol : 0.300uL
Acq. Method : RND-FA-3.5mns Instrument ID : ANL-MCL5-LCMS-0(
Sample Name : E119851-46

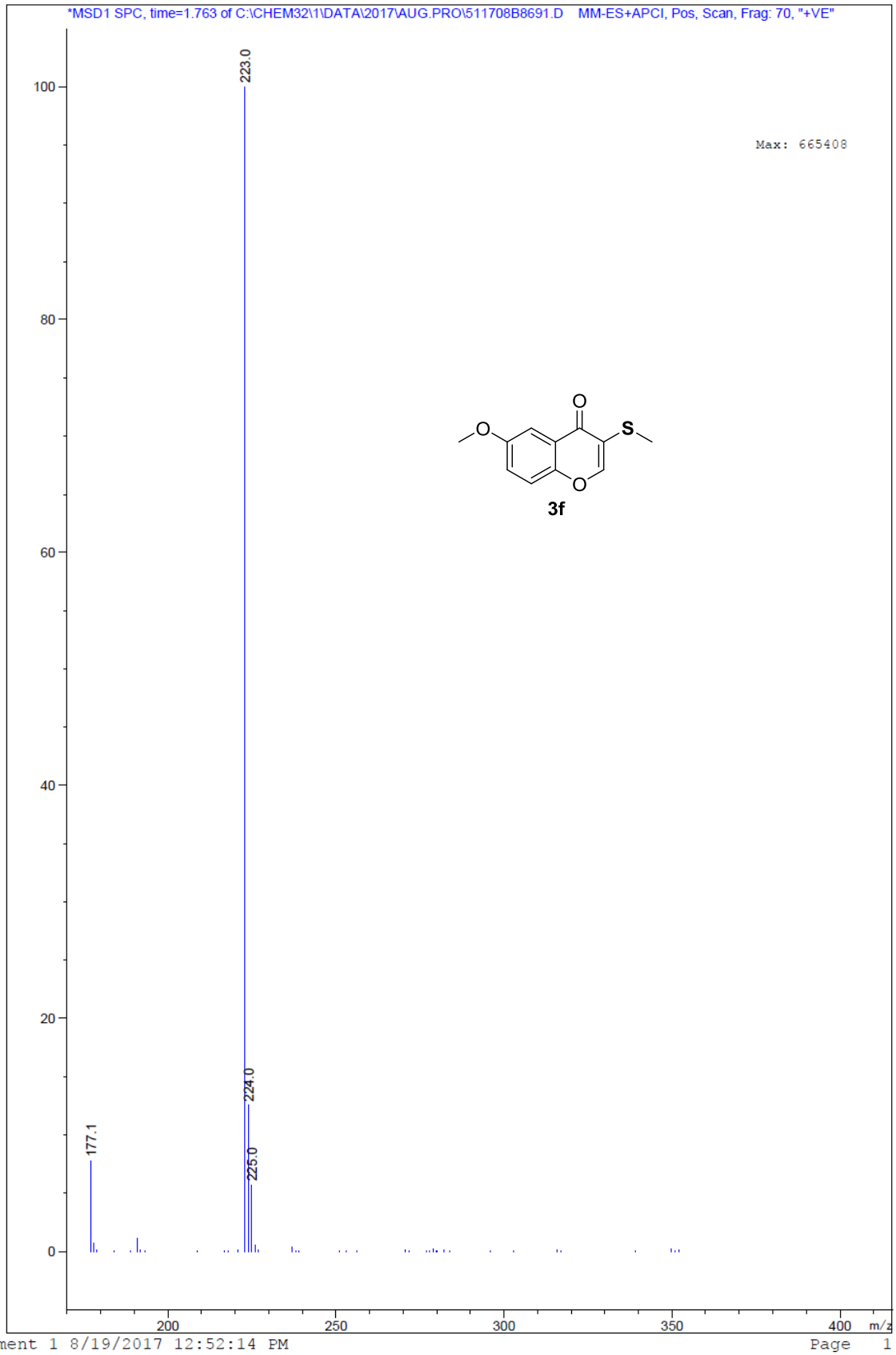
RND-FA-3.5 MIN.M
Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: B1: 0.1 % FA IN WATER A1: 0.1%FA IN ACN
Gradient: Time (min) /%A1: 0/2, 0.2/2, 2.3/98,3.4/98,3.41/2,3.5/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 50°C ->



DAD1 A, Sig=215,4 Ref=off

Peak No	RT min	Height	Area	Area %
1	1.71	1.086	0.320	0.022
2	1.74	1326.049	1454.485	99.793
3	1.92	0.530	0.210	0.014
4	1.95	1.509	2.320	0.159
5	1.97	0.487	0.168	0.012

MS Spectrum

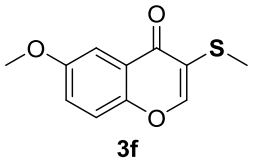


ument 1 8/19/2017 12:52:14 PM Page 1 of 1

Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None



3f

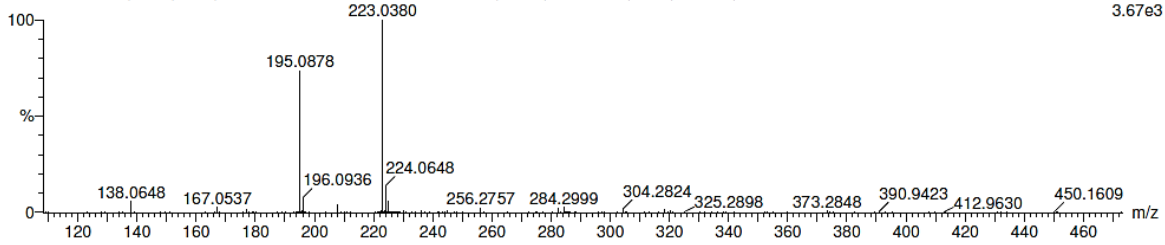
Monoisotopic Mass, Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-11 H: 0-11 O: 0-3 S: 0-1

GVKCBK-1-46

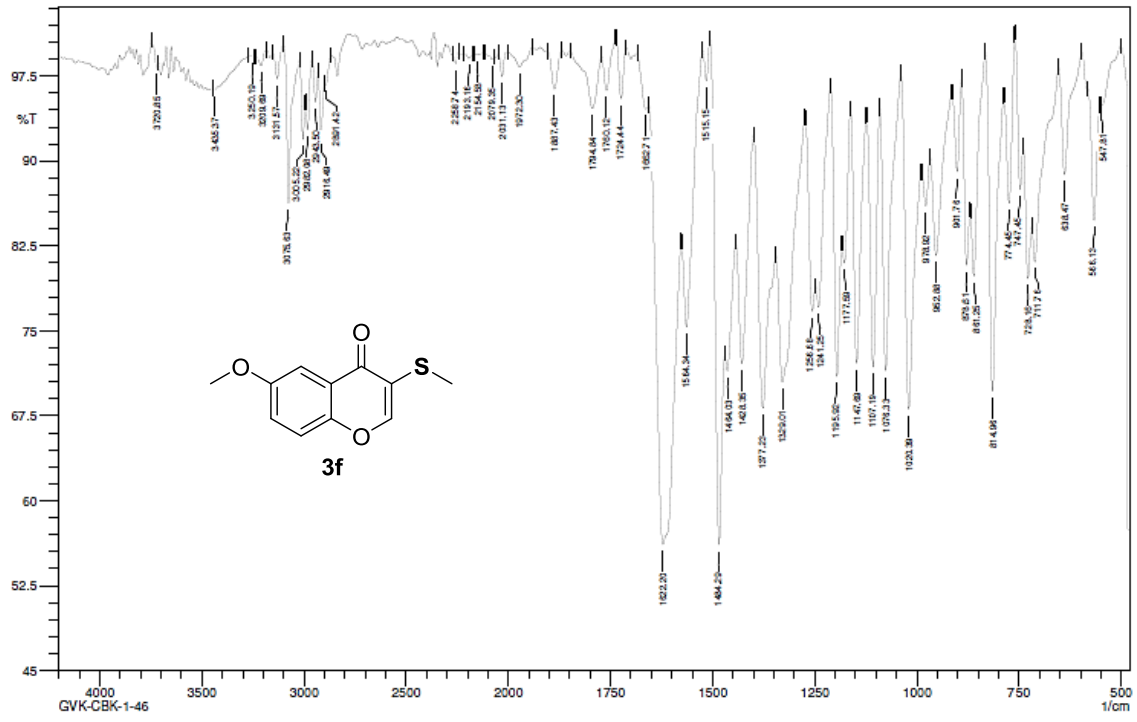
GVK Bio sciences (pvt)Ltd
Analytical Research and Development

Date of analysis:07-Mar-201812:42:04
Instru ment ID:ANL-MCL3-LCMS-001
1: TOF MS ES+
3.67e3

511803A4221 7 (0.282) AM (Cen,2, 50.00, Ar,5.0,195.10,1.00,LS 5); Sm (Mn, 5x2.00); Sb (1,40.00)



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
223.0380	223.0429	-4.9	-22.0	6.5	15.4	C11 H11 O3 S



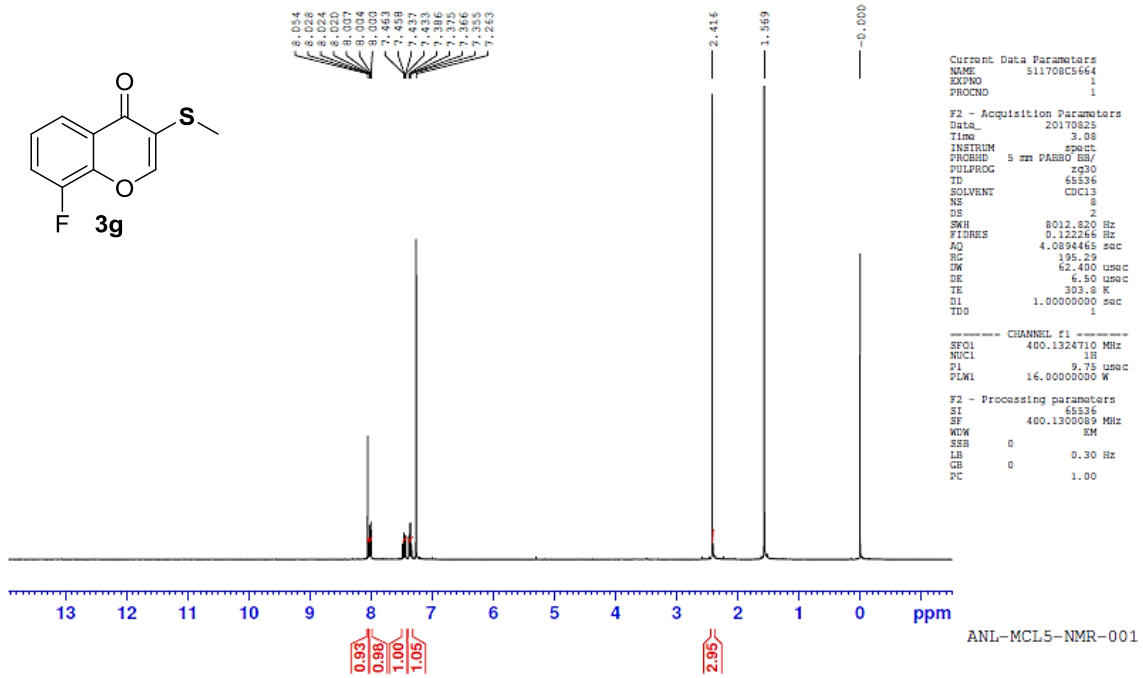
3f

Comment: IN Kbr
GVK-CBK-1-46

No. of Scans:
Resolution:
Apodization:

Date:9/13/2017 12:16:18 PM
User: Admin

GVK-CBK-3-Phd-49-I

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Current Data Parameters
NAME          511708C5664
EXPNO                   1
PROCNO                  1

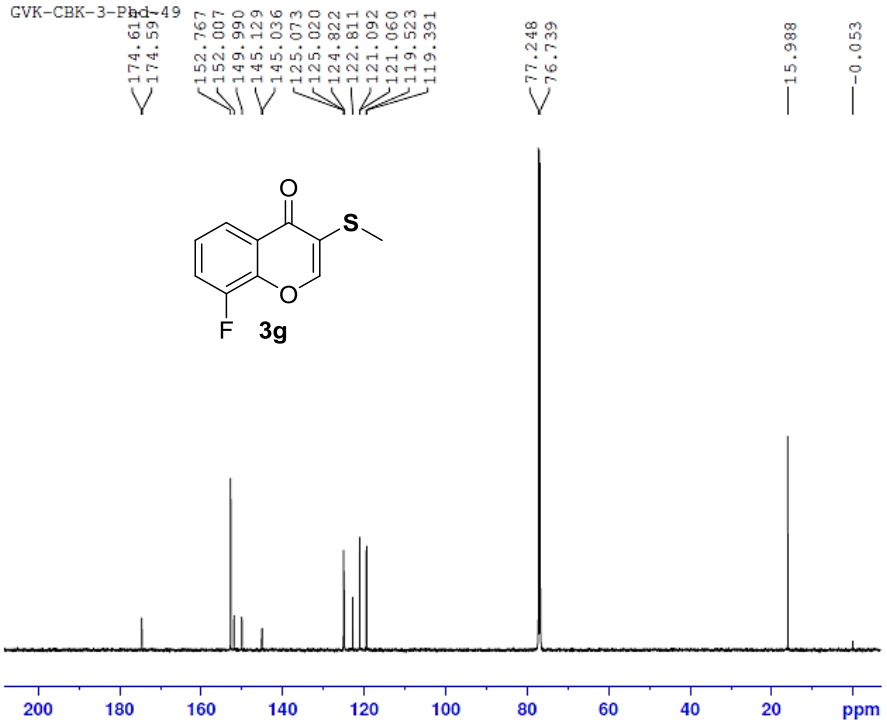
F2 - Acquisition Parameters
Date_              20170825
Time                   3.08
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       8
DS                       2
SWH               8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894465 sec
RG                   195.29
DW                 62.400 usec
DE                  6.50 usec
TE                  303.8 K
D1                1.00000000 sec
TD0                      1

====== CHANNEL f1 ======
SFO1            400.1324710 MHz
NUC1                    1H
P1                   9.75 usec
PLW1            16.00000000 W

F2 - Processing parameters
SI                   65536
SF              400.1300089 MHz
WDW                     EM
SSB                  0
LB                   0.30 Hz
GB                   0
PC                   1.00
```

ANL-MCL5-NMR-001

GVK-CBK-3-Phd-49

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Current Data Parameters
NAME          511709A7310
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_              20170911
Time                   1.16 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                3.00000000 sec
D11               0.03000000 sec
TD0                      1
SFO1            125.7703643 MHz
NUC1                    13C
P1                  10.00 usec
PLW1            79.88800049 W
SFO2            500.1320005 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2               80.00 usec
PLW2            20.38699913 W
PLW12            0.31854999 W
PLW13            0.16023000 W

F2 - Processing parameters
SI                   32768
SF              125.7577945 MHz
WDW                     EM
SSB                  0
LB                   2.00 Hz
GB                   0
PC                   1.40
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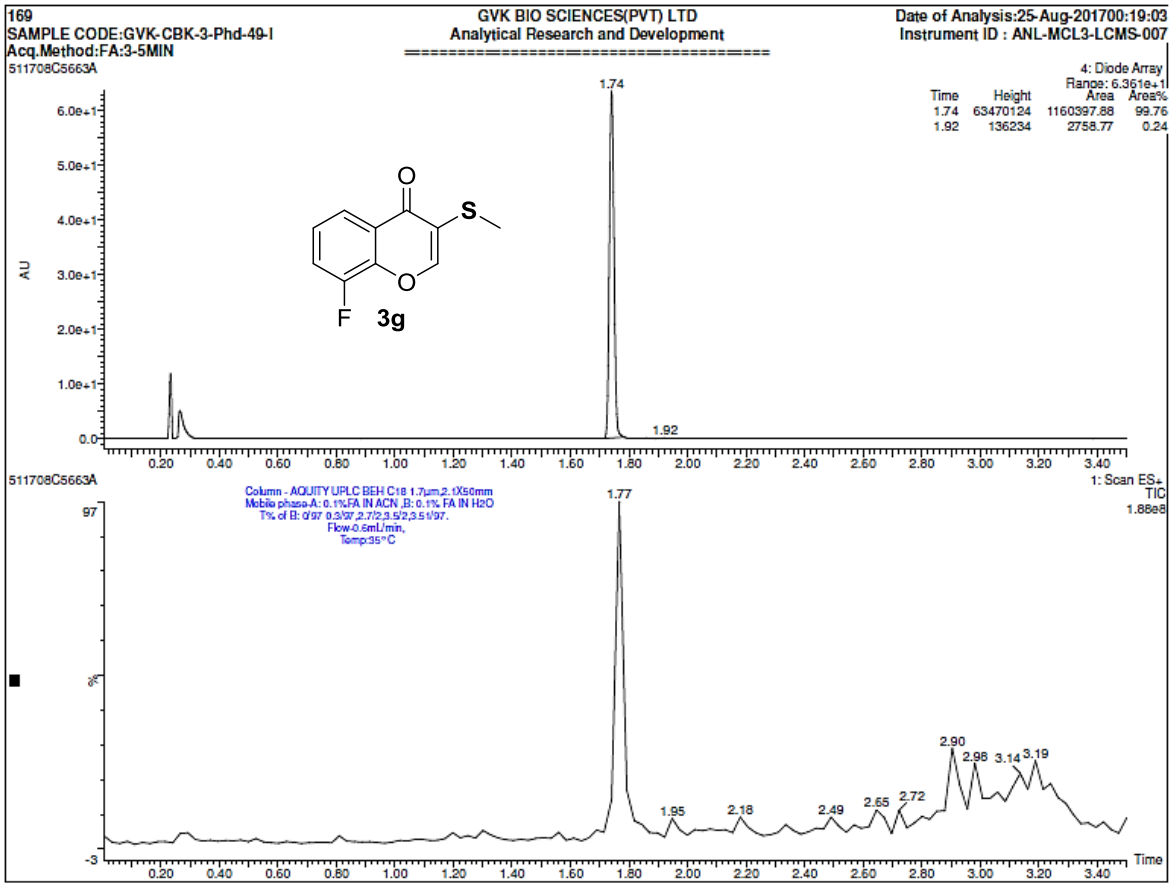
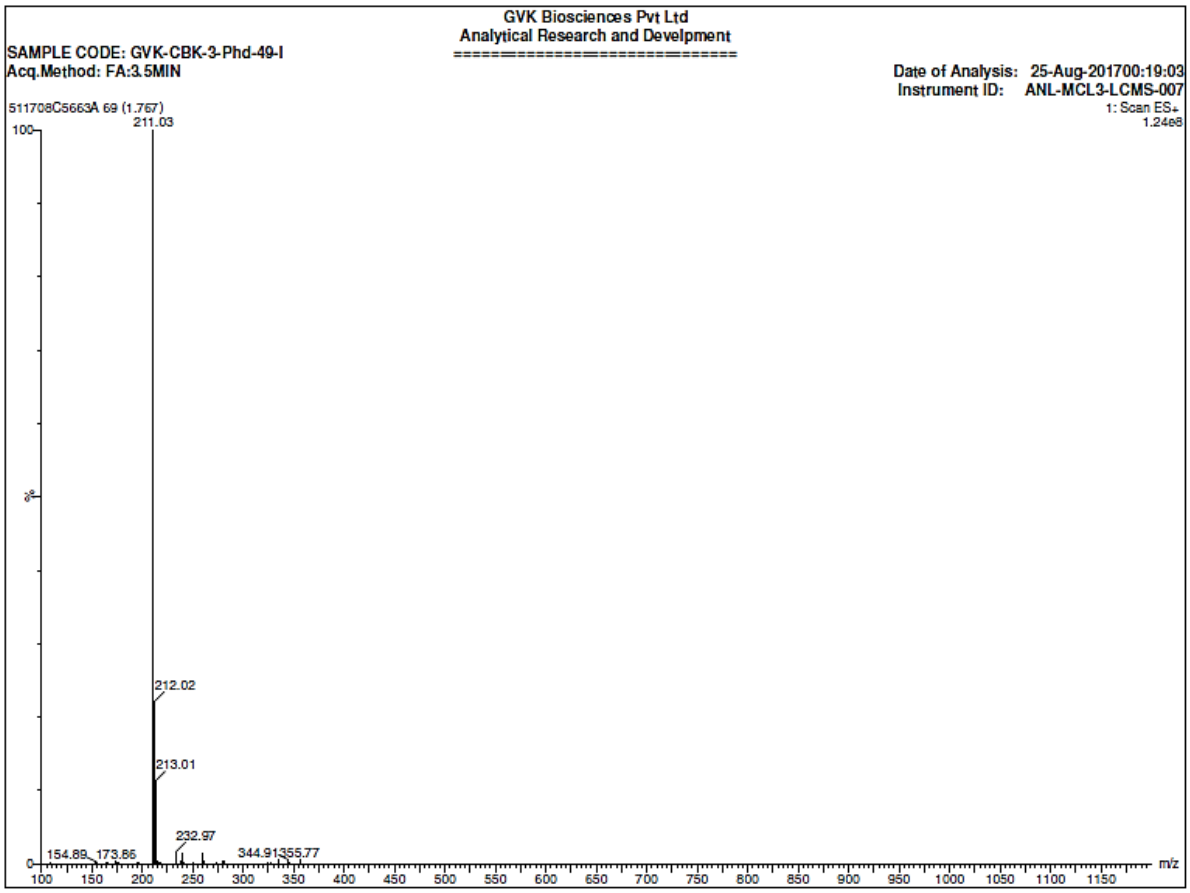
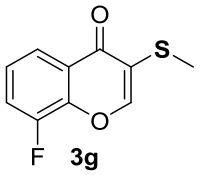

169
SAMPLE CODE:GVK-CBK-3-Phd-49-I
Acq.Method:FA:3-5MIN
GVK BIO SCIENCES(PVT) LTD
Analytical Research and Development
Date of Analysis:25-Aug-201700:19:03
Instrument ID : ANL-MCL3-LCMS-007
511708C5663A
4: Diode Array
Range: 6.361e+1
Time Height Area Area%
1.74 63470124 1160397.88 99.76
1.92 136234 2758.77 0.24
AU
1.74
1.92
O
S
O
F
3g
511708C5663A
1: Scan ES+
TIC
1.88e8
Column - AQUITY UPLC BEH C18 1.7µm,2.1X50mm
Mobile phase-A: 0.1%FA IN ACN ,B: 0.1% FA IN H2O
T% of B: 0/97 0.3/97,2.7/2,3.5/2,3.51/97.
Flow-0.6mL/min,
Temp:35°C
1.77
1.95
2.18
2.49
2.65
2.72
2.90
2.98
3.14
3.19
%
Time


GVK Biosciences Pvt Ltd
Analytical Research and Develpment
SAMPLE CODE: GVK-CBK-3-Phd-49-I
Acq.Method: FA:3.5MIN
Date of Analysis: 25-Aug-201700:19:03
Instrument ID: ANL-MCL3-LCMS-007
511708C5663A 69 (1.767)
1: Scan ES+
1.24e8
211.03
212.02
213.01
232.97
154.89
173.86
344.91
355.77
%
m/z

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None



3g

Monoisotopic Mass, Odd and Even Electron Ions

10 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)

Elements Used:

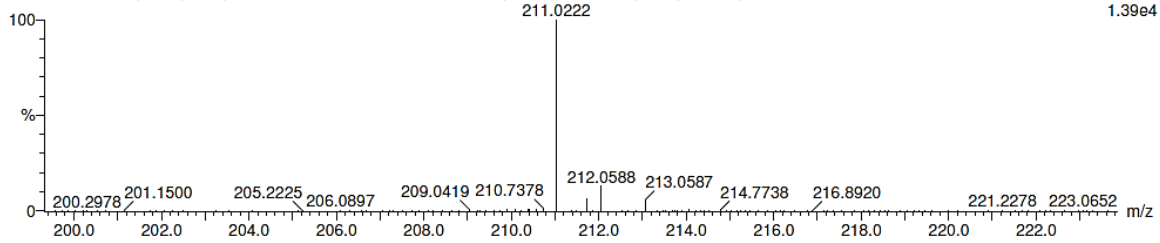
C: 0-10 H: 0-8 O: 0-2 F: 0-1 S: 0-1

GVK-CBK-1-49

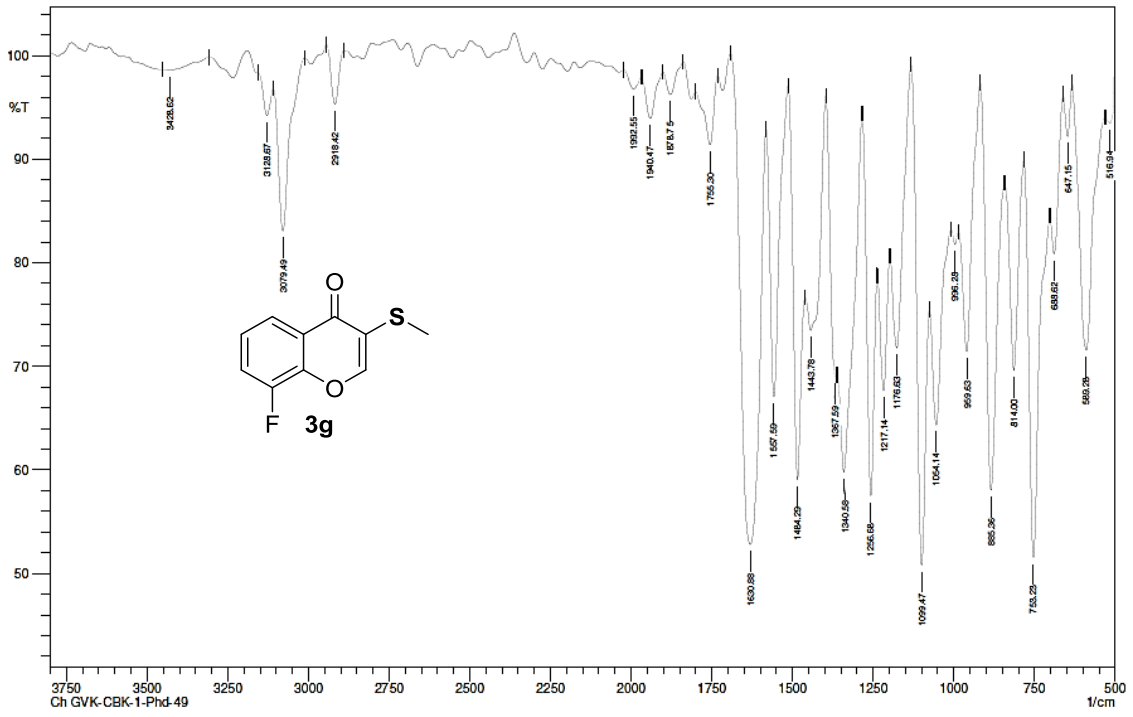
GVK Bio sciences (pvt)Ltd
Analytical Research and Development

Date of analysis:04-Oct-201715:08:26
Instru ment ID:ANL-MCL3-LCMS-001
1: TOF MS ES+
1.39e4

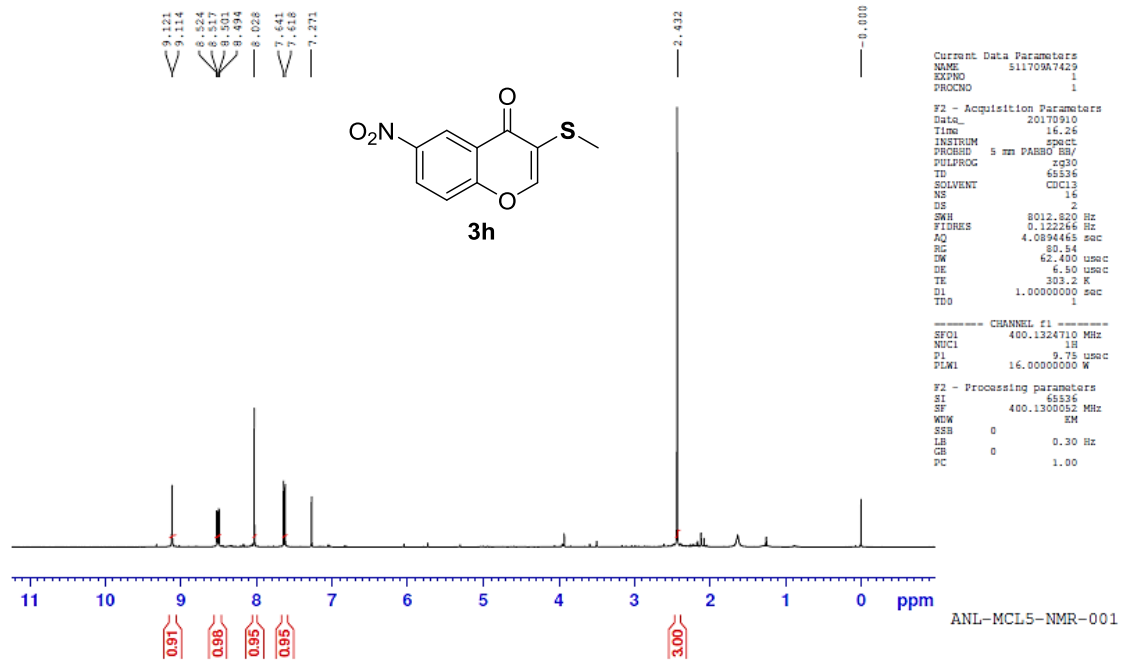
511709B4717 10 (0.346) AM (Cen,4, 20.00, Ar,5.0,195.11,1.00,LS 5); Sm (Mn, 5x2.00); Sb (1,40.00)

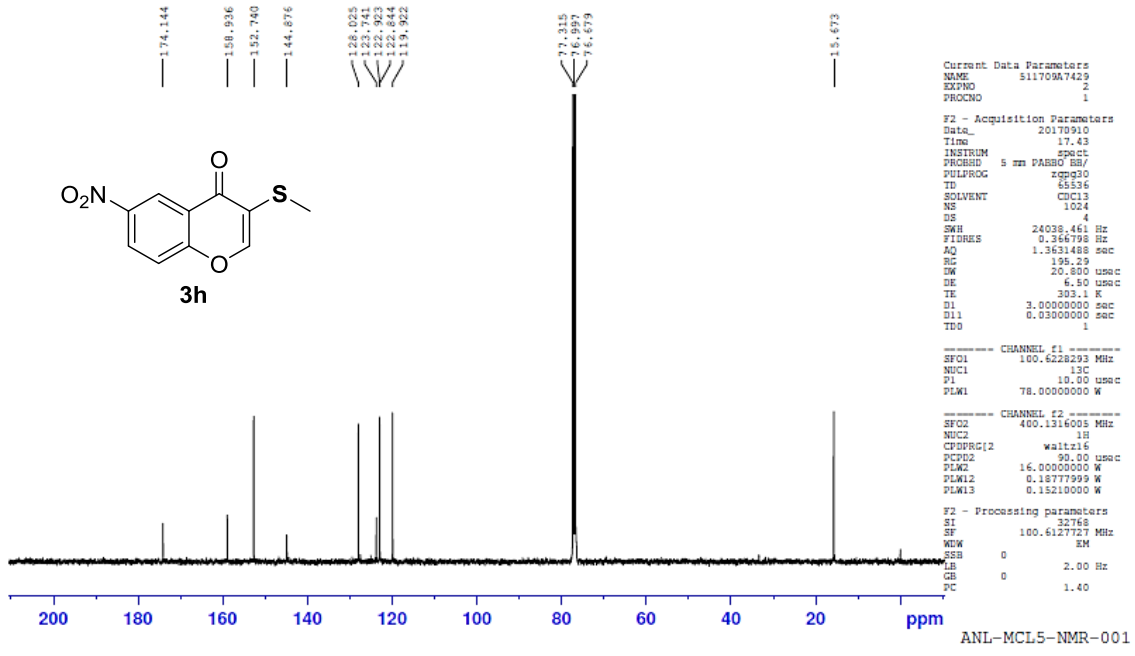


Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
211.0222	211.0229	-0.7	-3.3	6.5	190.7	C10 H8 O2 F S



3g

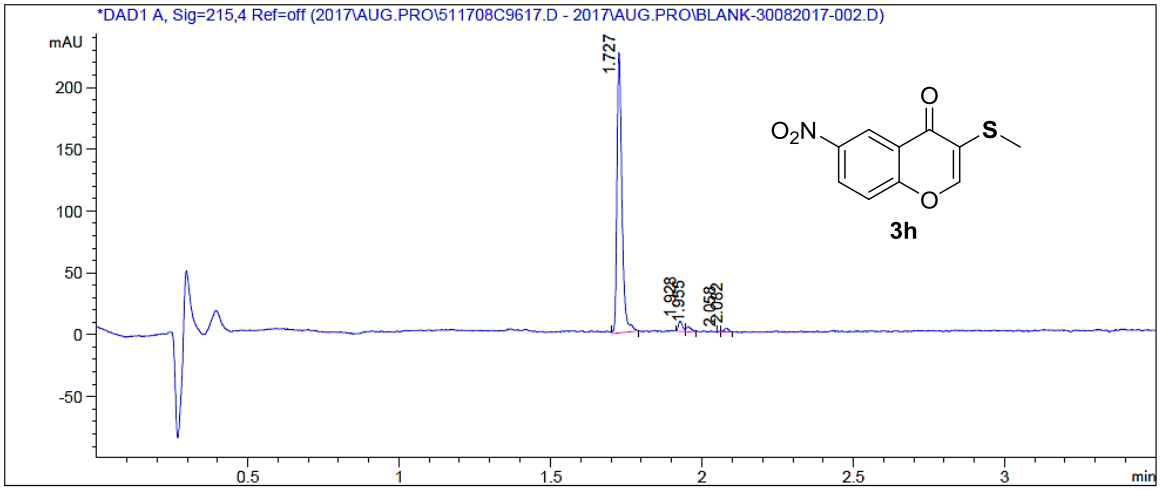

9.121
9.114
8.524
8.517
8.501
8.494
8.028
7.641
7.618
7.271
2.432
0.000
O2N
S
O
O
3h
Current Data Parameters
NAME 511709A7429
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Data_ 20170910
Time 16.26
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 80.64
DW 62.400 usec
DE 6.50 usec
TE 303.2 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 9.75 usec
PLW1 16.00000000 W
F2 - Processing parameters
SI 65536
SF 400.1300052 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.91 0.98 0.95 0.95 3.00
ANL-MCL5-NMR-001


174.144
158.936
152.740
144.876
128.025
123.741
122.923
122.644
119.922
77.315
76.997
76.679
15.673
O2N
S
O
O
3h
Current Data Parameters
NAME 511709A7429
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Data_ 20170910
Time 17.43
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 195.29
DW 20.800 usec
DE 6.50 usec
TE 303.1 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 78.00000000 W
CHANNEL f2
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.18777999 W
PLW13 0.15210000 W
F2 - Processing parameters
SI 32768
SF 100.6127727 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 ppm
ANL-MCL5-NMR-001

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

Vial position : P1-E-03
Date of Analysis : 8/30/2017 9:43:50 PM Injection Vol : 0.300uL
Acq. Method : RND-FA-3.5mns Instrument ID : ANL-MCL5-LCMS-00
Sample Name : GVK-VK-PHD-32

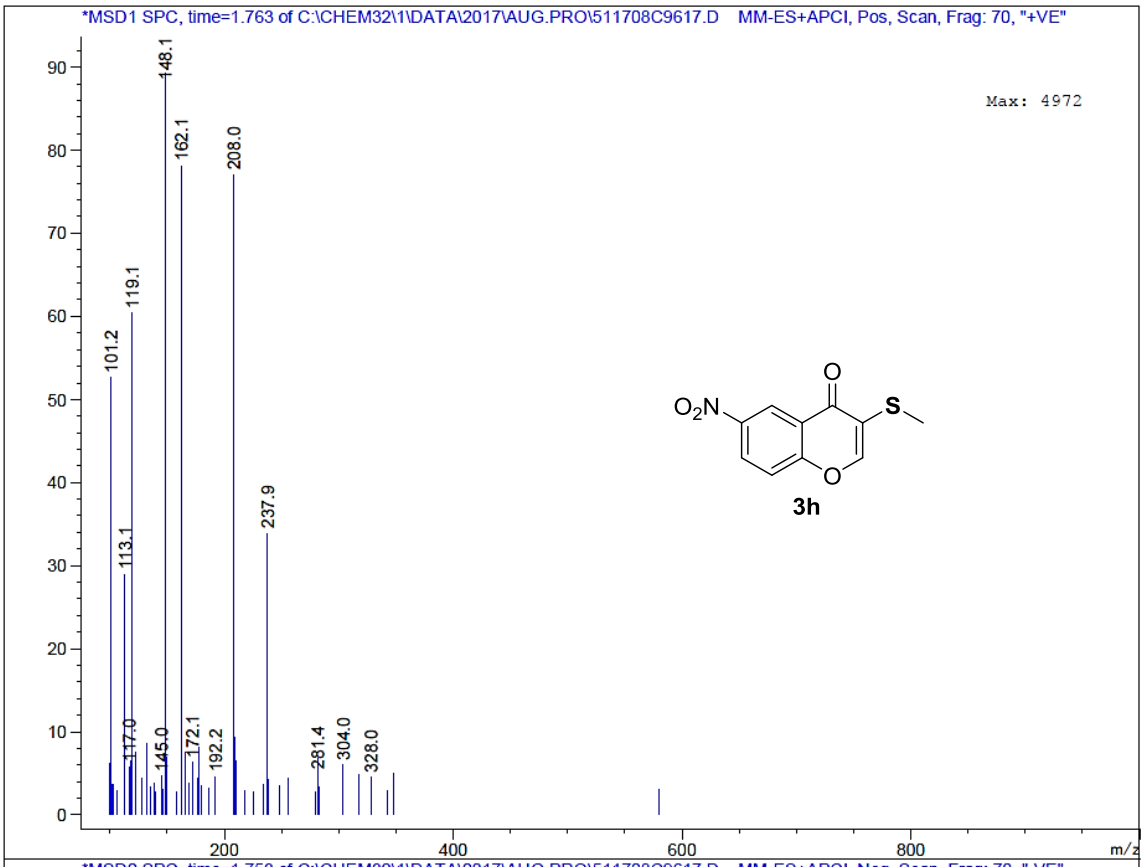
RND-FA-3.5 MIN.M
Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: B1: 0.1 % FA IN WATER A1: 0.1%FA IN ACN
Gradient: Time (min) /%A1: 0/2, 0.2/2, 2.3/98,3.4/98,3.41/2,3.5/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 50°C ->



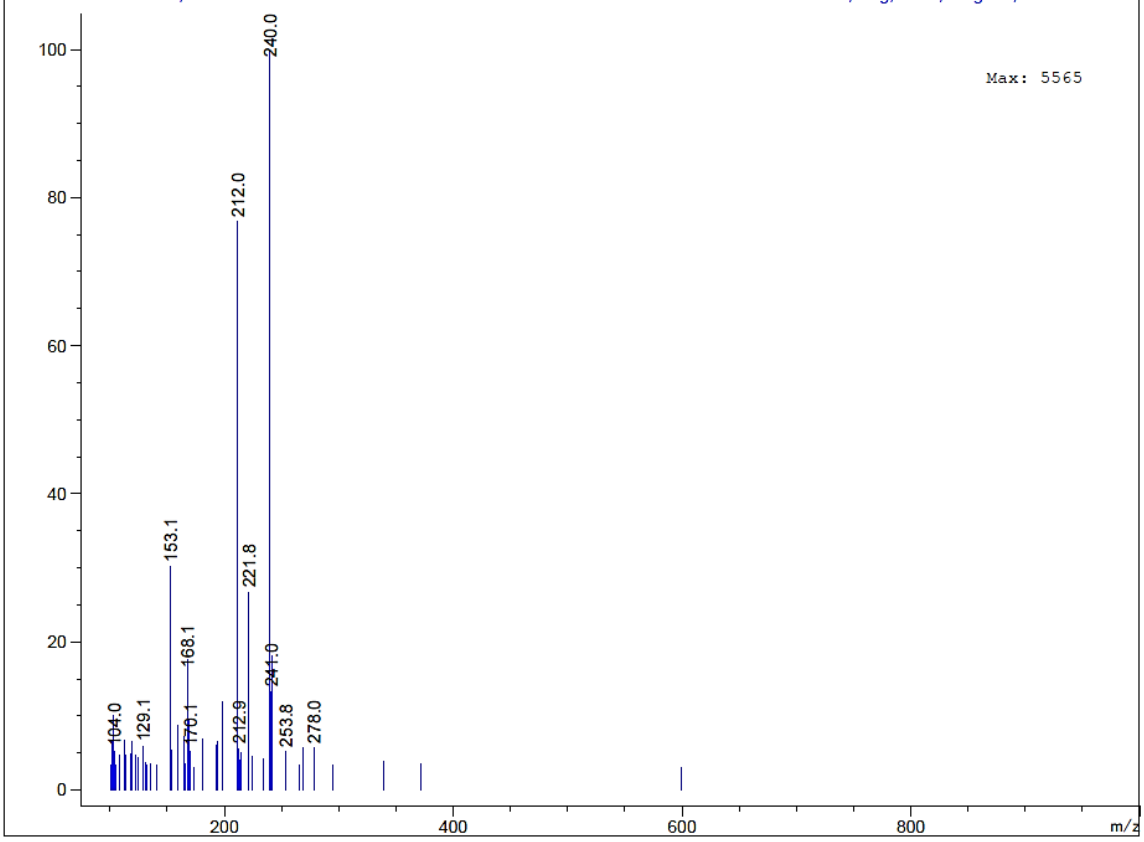
DAD1 A, Sig=215,4 Ref=off

Peak No	RT min	Height	Area	Area %
1	1.73	226.759	255.540	93.604
2	1.93	8.123	7.803	2.858
3	1.95	4.543	5.591	2.048
4	2.06	1.190	0.587	0.215
5	2.08	3.118	3.479	1.274

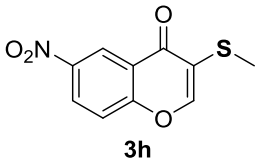
MS Spectrum



3h



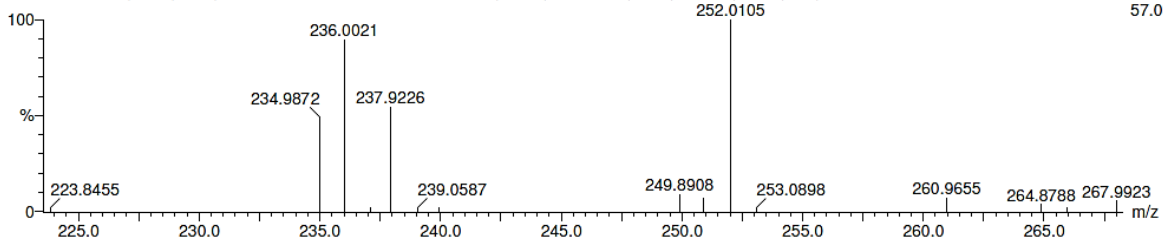
Single Mass Analysis (displaying only valid results)
Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None



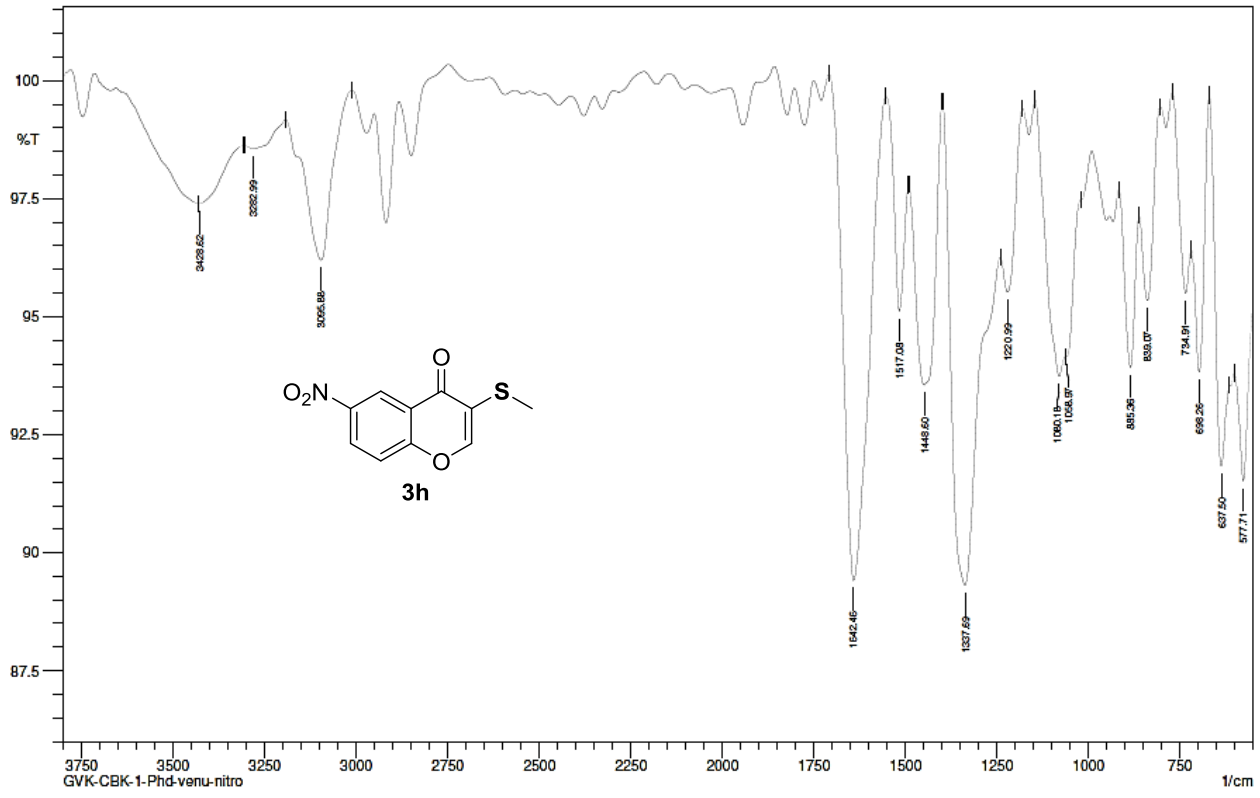
3h

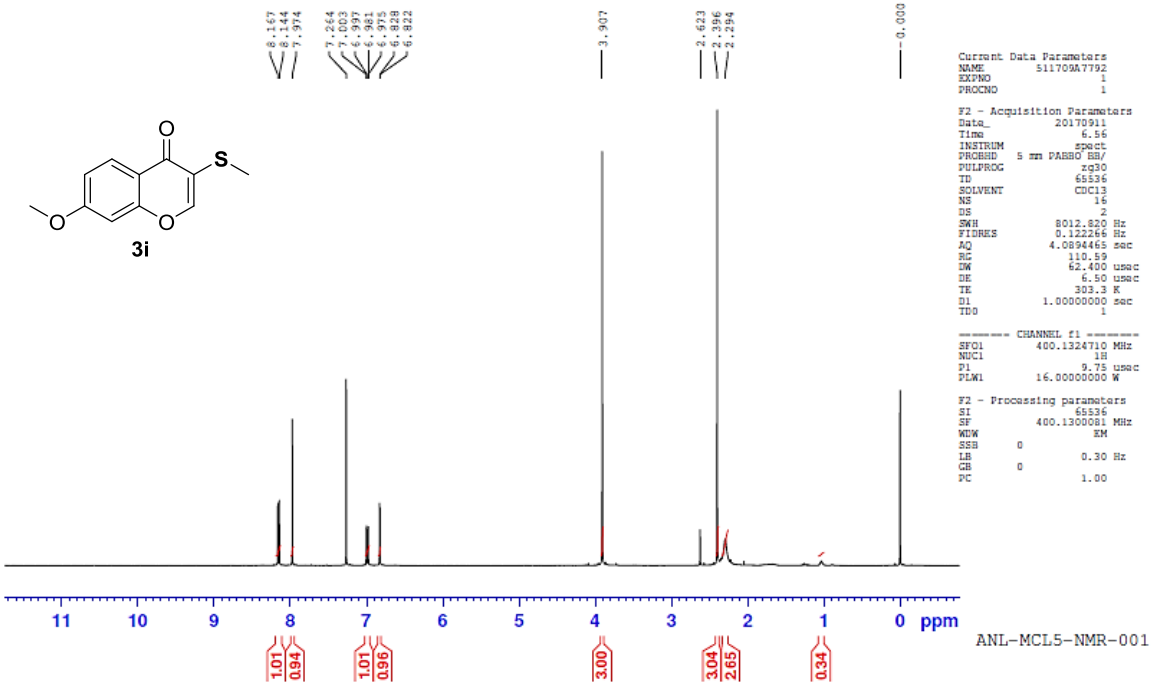
Monoisotopic Mass, Odd and Even Electron Ions
18 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-10 H: 0-8 N: 0-1 O: 0-4 S: 0-1

GVK-CBK-Phd-29
GVK Bio sciences (pvt)Ltd
Analytical Research and Development
Date of analysis:08-Dec-201716:02:57
Instru ment ID:ANL-MCL3-LCMS-001
511712A8095 8 (0.326) AM (Cen,2, 50.00, Ar,5.0,194.98,1.00,LS 5); Sm (Mn, 5x2.00); Sb (1,40.00); Cm (2:22)
1: TOF MS ES+
57.0



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
236.0021	236.0018	0.3	1.3	8.5	31.0	C10 H6 N O4 S






```
Current Data Parameters
NAME          511709A7792
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_              20170911
Time                  6.56
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                     16
DS                      2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894465 sec
RG                  110.59
DW                  62.400 usec
DE                   6.50 usec
TE                  303.3 K
D1               1.00000000 sec
TD0                     1

====== CHANNEL f1 =======
SFO1            400.1324710 MHz
NUC1                    1H
P1                   9.75 usec
PLW1            16.00000000 W

F2 - Processing parameters
SI                  65536
SF              400.1300081 MHz
WDW                    EM
SSB                 0
LB                   0.30 Hz
GB                  0
PC                   1.00
```


```
Current Data Parameters
NAME          511709B4411
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_              20170916
Time                  7.19 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               3.00000000 sec
D11              0.03000000 sec
TD0                     1
SFO1            125.7703643 MHz
NUC1                   13C
P1                  10.00 usec
PLW1            79.88800049 W
SFO2            500.1320005 MHz
NUC2                    1H
CPDPRG[2            waltz16
PCPD2                80.00 usec
PLW2            20.38699913 W
PLW12            0.31854999 W
PLW13            0.16023000 W

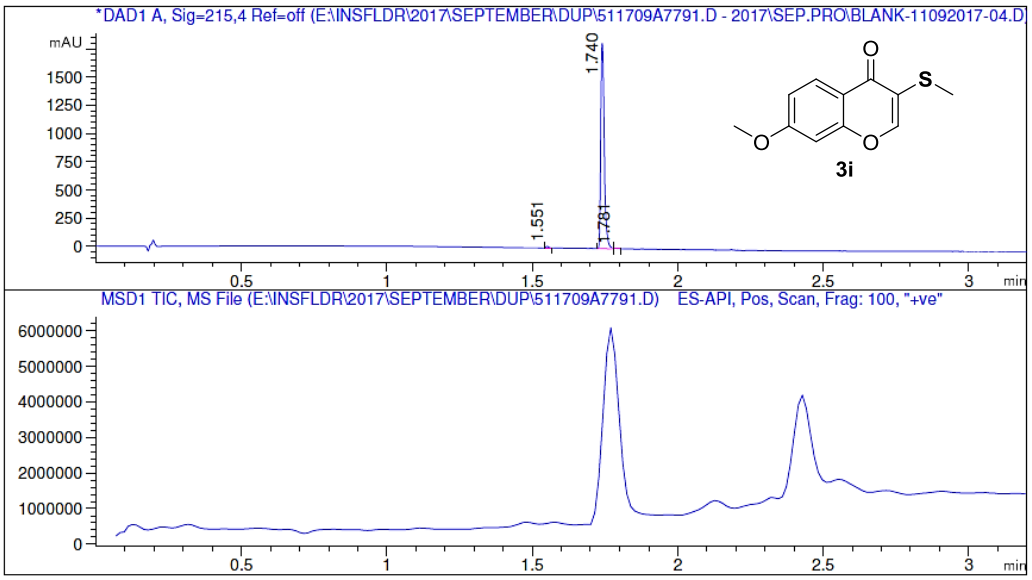
F2 - Processing parameters
SI                  32768
SF              125.7577948 MHz
WDW                    EM
SSB                 0
LB                   2.00 Hz
GB                  0
PC                   1.40
```

GVK BIO SCIENCES PVT LTD

LC/MS REPORT

Date of Analysis : 9/9/2017 TIME : 2:21:41 PM Vial position: P1-B-08
Sample Name : GVK-RK-009-70 Injection Vol: 0.300 µL
Acq. Method : C:\Chem32\1\METHODS\RND-FA-3.2-MIN.M Instrument Name:ANL-MCL5-LCMS-002

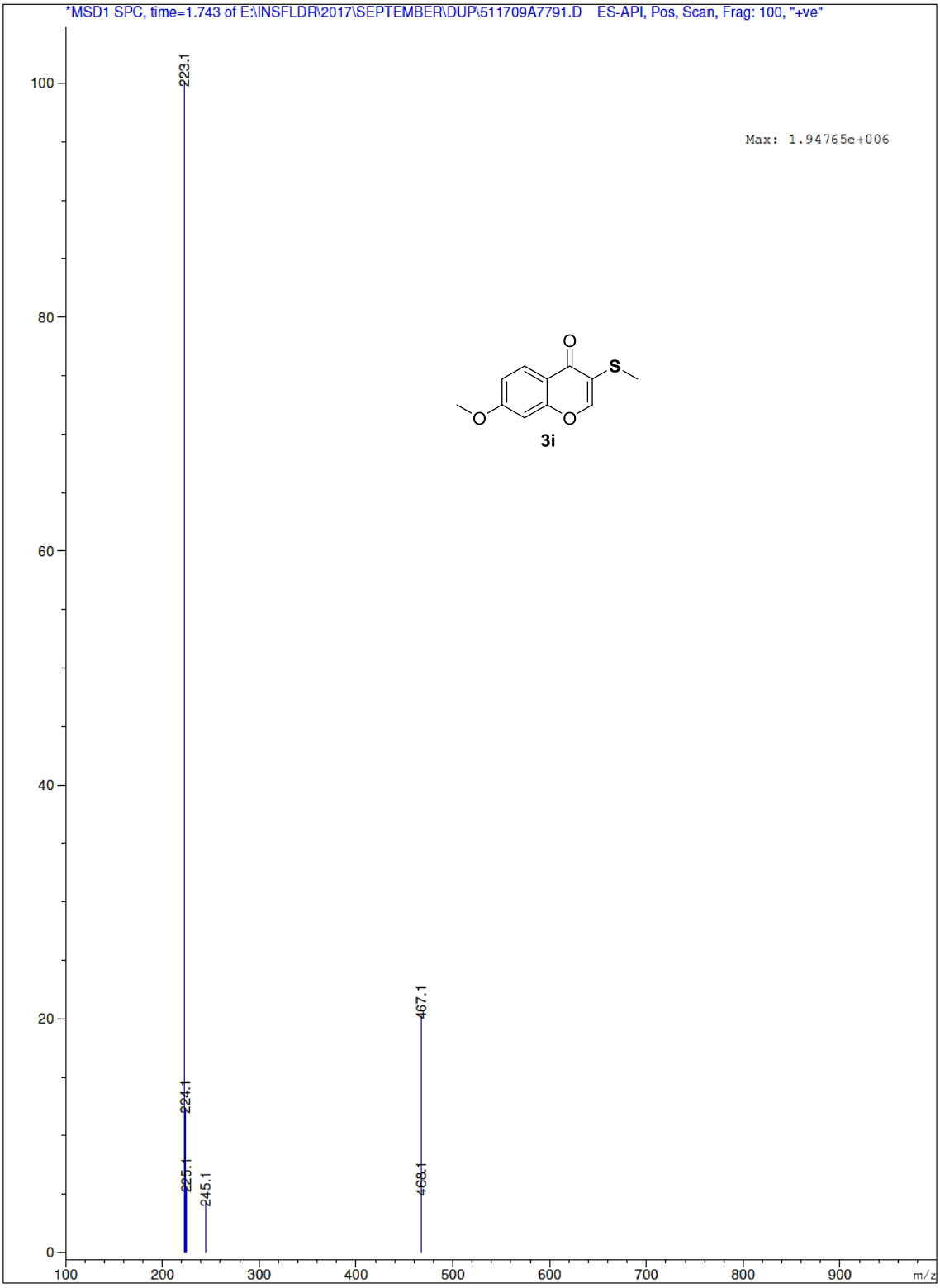
Acq Method Conditions : RND-FA-3.2-MIN
Column : Aquity UPLC BEH C18 (50mmx2.1 mm,1.7um)
Mobile phase:A: 0.1% of Formic Acid in Water,B: 0.1% of Formic acid in Acetonitrile
Gradient : Time(min)/ %B 0/2,0.2/2,1.5/98,2.6/98,2.61/2,3.2/2
Column temparature :45 C,Flow rate :0.8 ml/mn



DAD1 A, Sig=215,4 Ref=off

PEAK No	RT min	Height	Area	Area %
1	1.551	17.216	14.191	0.922
2	1.740	1.825e3	1520.469	98.798
3	1.781	5.329	4.314	0.280

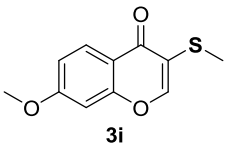
MS Spectrum


*MSD1 SPC, time=1.743 of E:\INSFLDR\2017\SEPTEMBER\DUP\511709A7791.D ES-API, Pos, Scan, Frag: 100, "+ve"
Max: 1.94765e+006
223.1
224.1
225.1
245.1
467.1
468.1
O
S
O
O
3i
100
80
60
40
20
0
100
200
300
400
500
600
700
800
900
m/z

Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None



3i

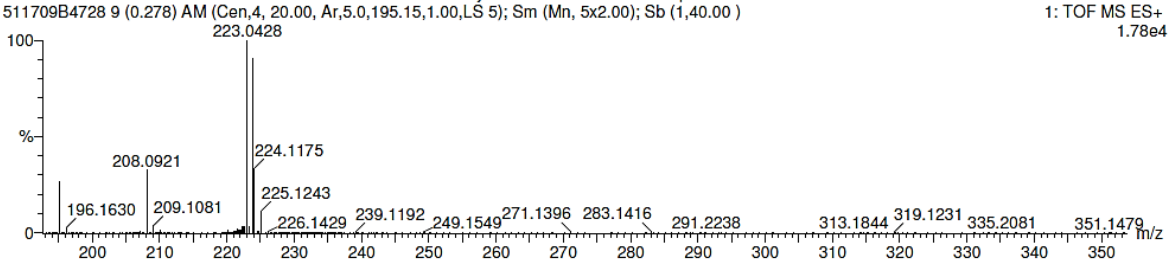
Monoisotopic Mass, Odd and Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-11 H: 0-11 O: 0-3 S: 0-1

GVK-RK-009-70

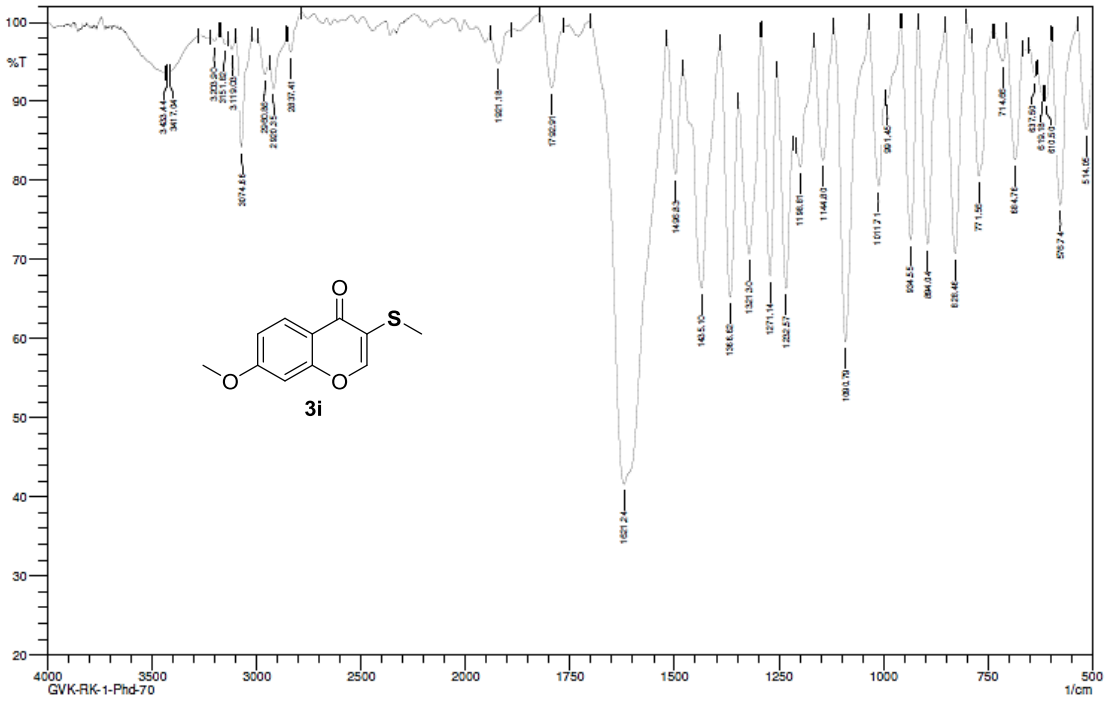
GVK Bio sciences (pvt)Ltd
Analytical Research and Development

Date of analysis:04-Oct-201715:56:29
Instru ment ID:ANL-MCL3-LCMS-001
1: TOF MS ES+
1.78e4

511709B4728 9 (0.278) AM (Cen,4, 20.00, Ar,5.0,195.15,1.00,LS 5); Sm (Mn, 5x2.00); Sb (1,40.00)



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
223.0428	223.0429	-0.1	-0.4	6.5	58596.0	C11 H11 O3 S

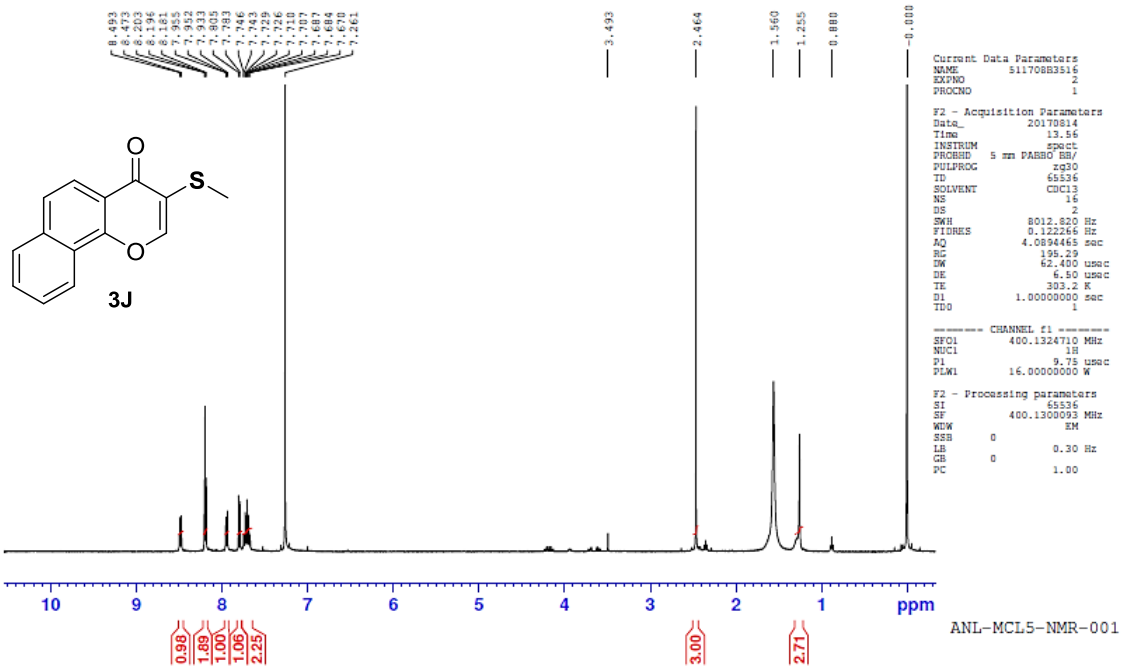


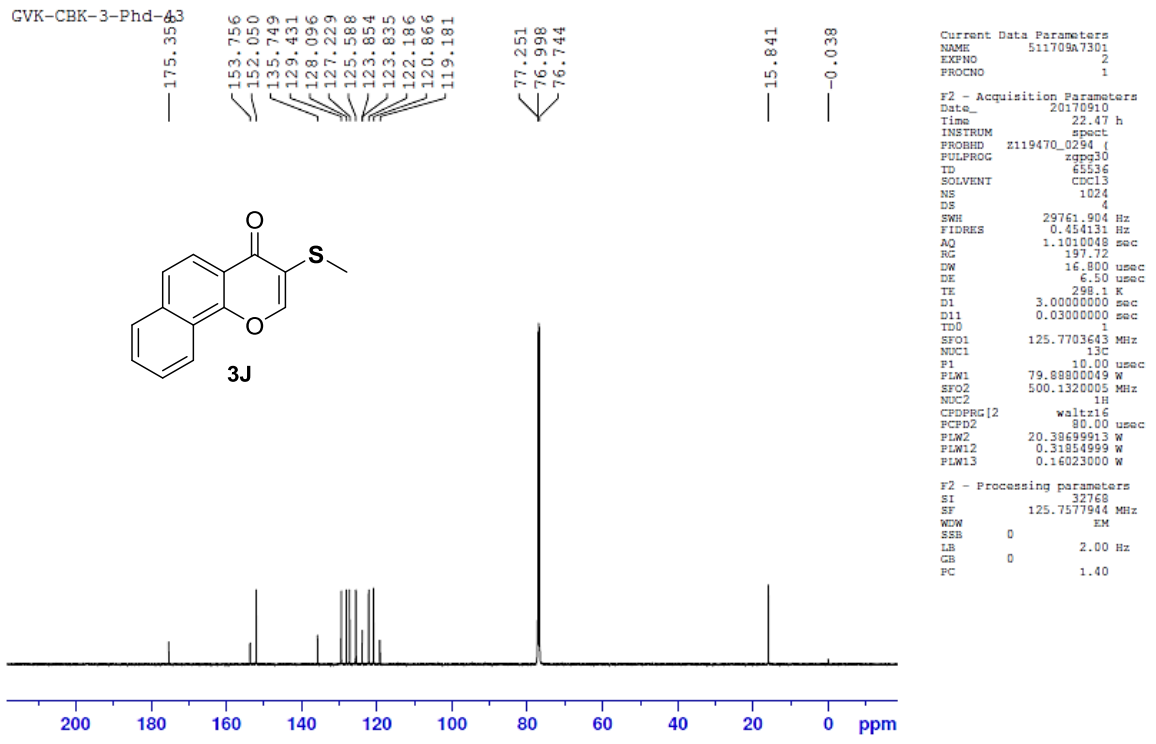
3i

Comment: IN Kbr
GVK-RK-1-Phd-70

No. of Scans:
Resolution:
Apodization:

Date: 1/10/2018 11:53:16 AM
User: Admin

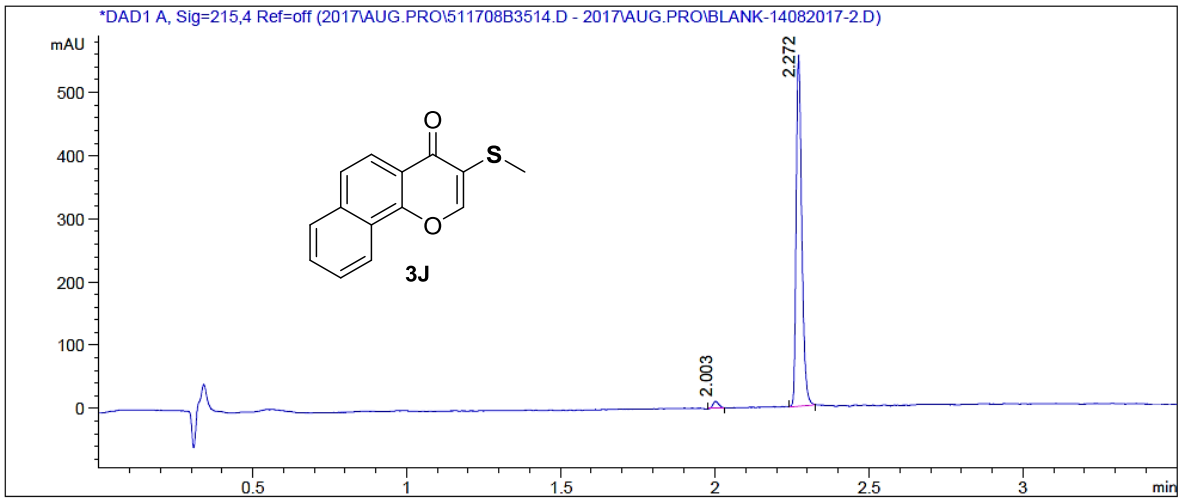

3J
ANL-MCL5-NMR-001
ppm


GVK-CBK-3-Phd-13
3J
ppm

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

```
Vial position   : P1-D-06
Date of Analysis : 8/14/2017          2:17:57 PM          Injection Vol   : 0.300uL
Acq. Method      : RND-FA-3.5mns                          Instrument ID   : ANL-MCL5-LCMS-0
Sample Name      : GVK-CBK-3-Phd-43
```

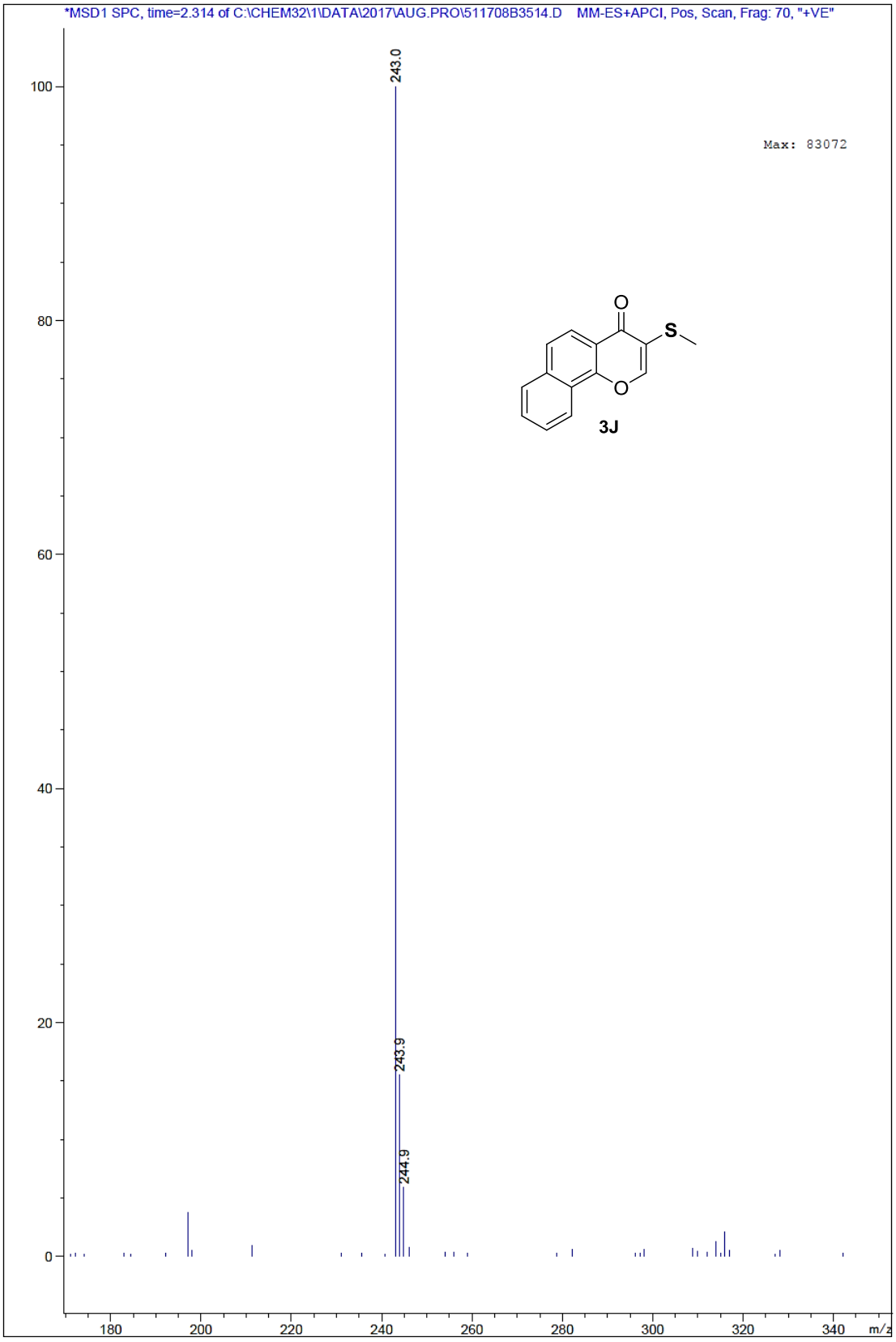
RND-FA-3.5 MIN.M
Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: B1: 0.1 % FA IN WATER A1: 0.1%FA IN ACN
Gradient: Time (min) /%A1: 0/2, 0.2/2, 2.3/98,3.4/98,3.41/2,3.5/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 50°C ->



DAD1 A, Sig=215,4 Ref=off

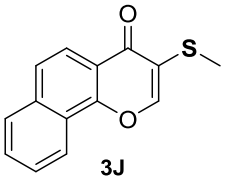
Peak No	RT min	Height	Area	Area %
1	2.00	11.467	15.421	2.160
2	2.27	555.519	698.488	97.840

MS Spectrum


*MSD1 SPC, time=2.314 of C:\CHEM32\1\DATA\2017\AUG.PRO\511708B3514.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 83072
243.0
243.9
244.9
O
S
O
3J
100
80
60
40
20
0
180
200
220
240
260
280
300
320
340
m/z

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None



3J

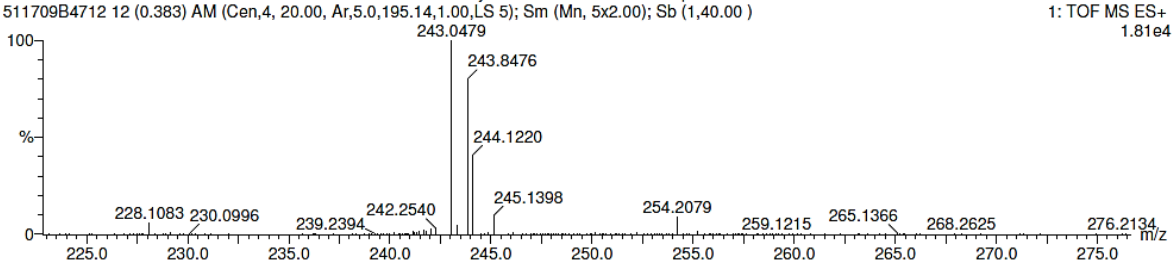
Monoisotopic Mass, Odd and Even Electron Ions
5 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-14 H: 0-11 O: 0-2 S: 0-1

GVK-CBK-1-43

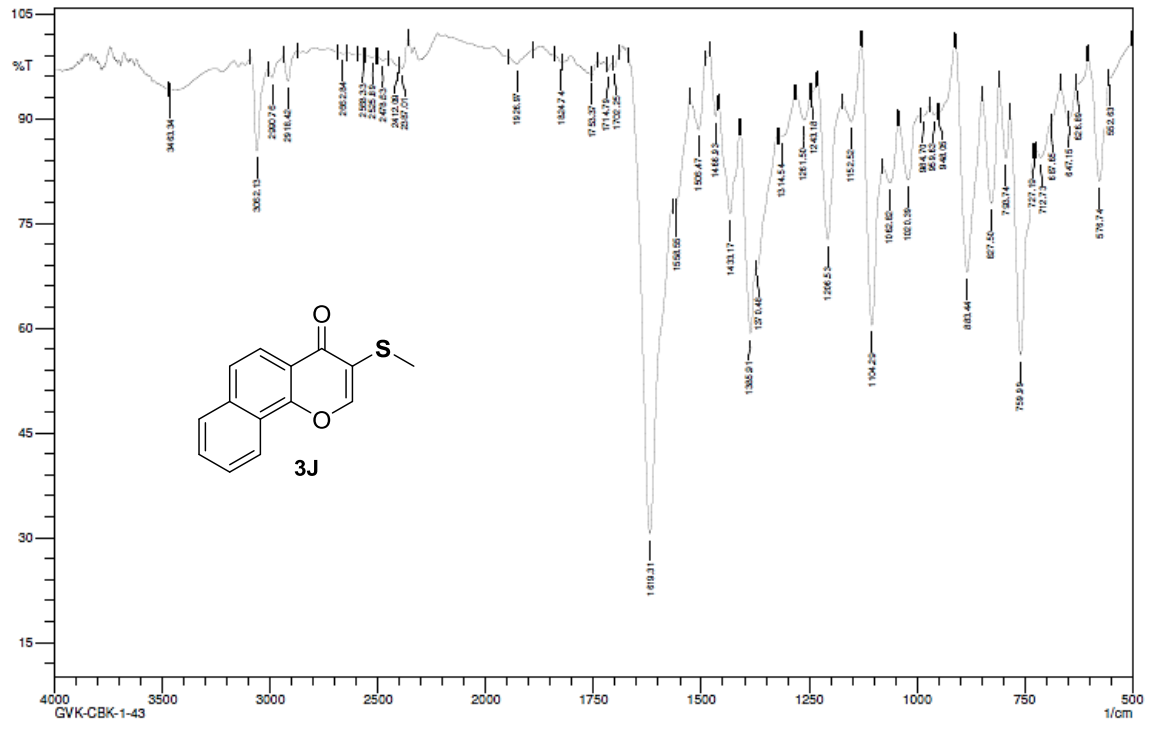
GVK Bio sciences (pvt)Ltd
Analytical Research and Development

Date of analysis:04-Oct-201715:13:06
Instru ment ID:ANL-MCL3-LCMS-001
1: TOF MS ES+
1.81e4

511709B4712 12 (0.383) AM (Cen,4, 20.00, Ar,5.0,195.14,1.00,LS 5); Sm (Mn, 5x2.00); Sb (1,40.00)



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
243.0479	243.0480	-0.1	-0.4	9.5	33012.7	C14 H11 O2 S

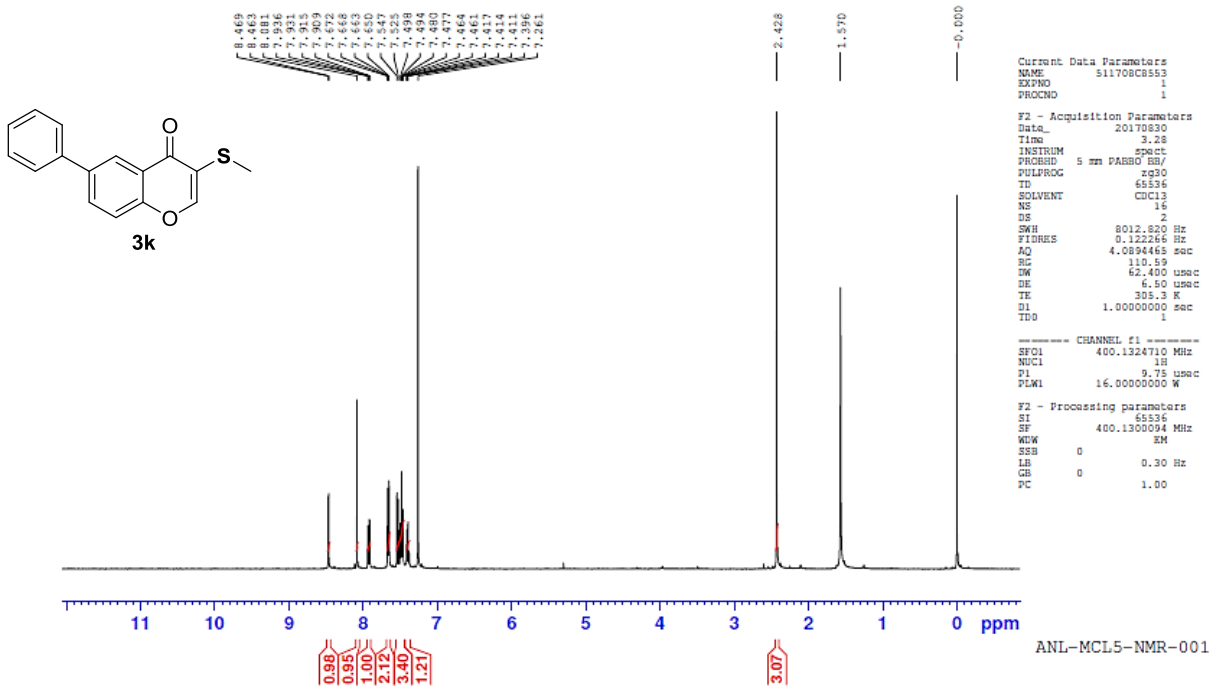


3J

Comment: IN Kbr
GVK-CBK-1-43

No. of Scans:
Resolution:
Apodization:

Date:9/13/2017 12:27:12 PM
User: Admin

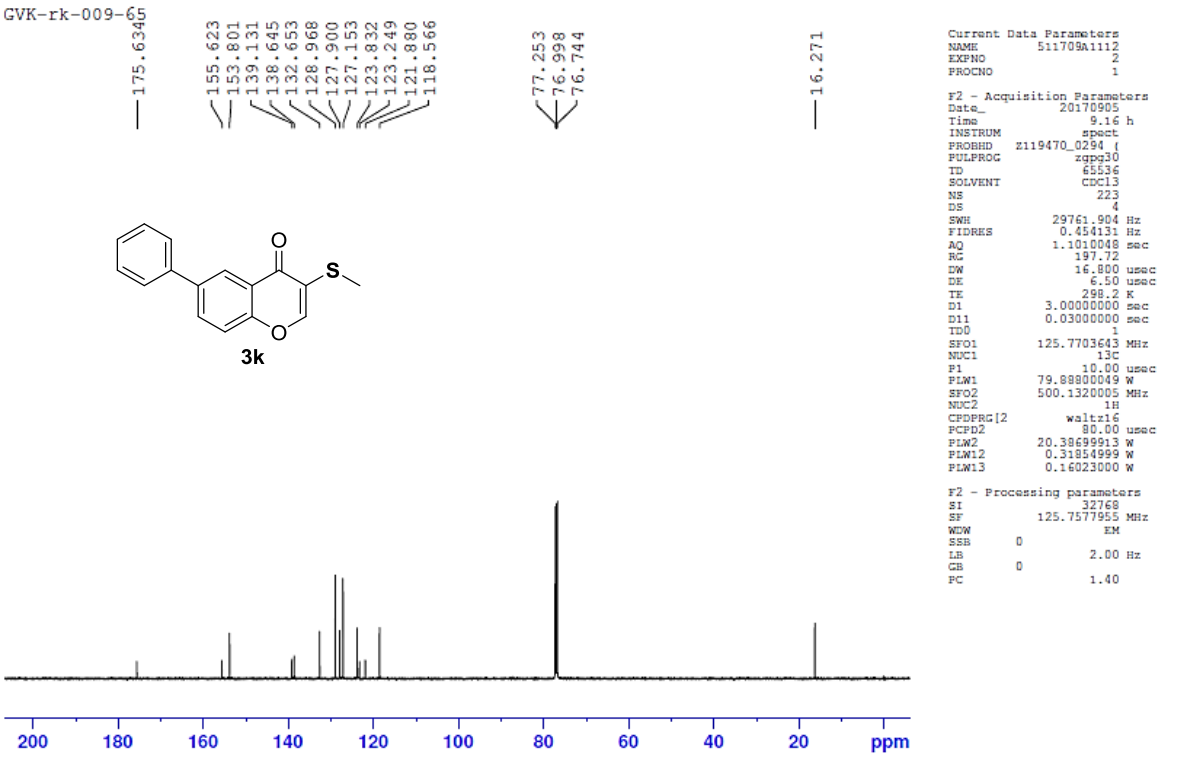



```
Current Data Parameters
NAME          511708CB553
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Data_           20170830
Time                3.28
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           8012.820 Hz
FIDRES        0.122266 Hz
AQ            4.0894465 sec
RG                110.59
DW               62.400 usec
DE                6.50 usec
TE               305.3 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        400.1324710 MHz
NUC1                   1H
P1                  9.75 usec
PLW1        16.00000000 W

F2 - Processing parameters
SI                 65536
SF          400.1300094 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```




```
Current Data Parameters
NAME          511709A1112
EXPNO                   2
PROCNO                  1

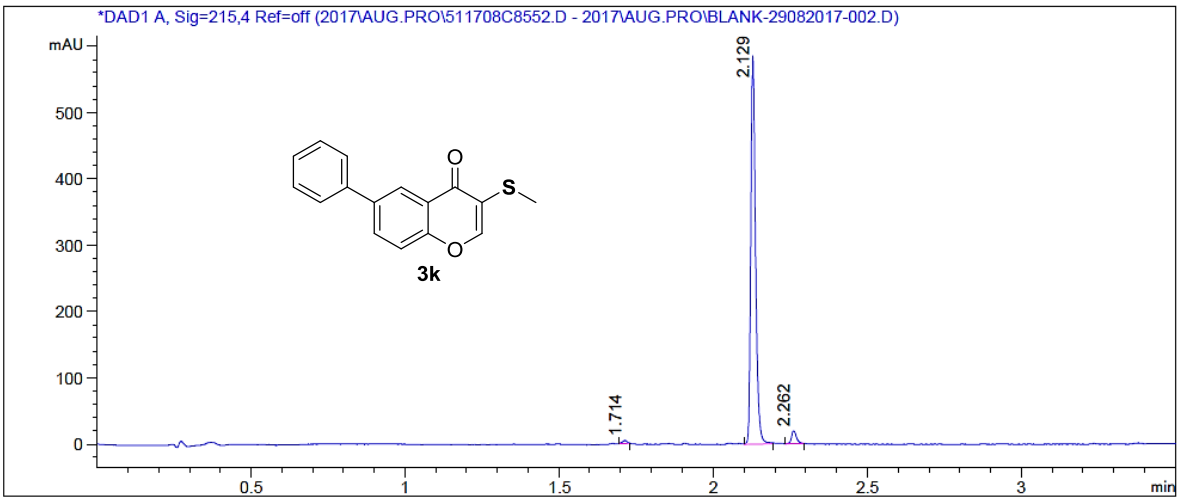
F2 - Acquisition Parameters
Data_           20170905
Time                9.16 h
INSTRUM             spect
PROBHD   Z119470_0294 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   223
DS                     4
SWH          29761.904 Hz
FIDRES        0.454131 Hz
AQ            1.1010048 sec
RG                197.72
DW               16.800 usec
DE                6.50 usec
TE               298.2 K
D1            3.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1        125.7703643 MHz
NUC1                  13C
P1                 10.00 usec
PLW1        79.88800049 W
SFO2        500.1320005 MHz
NUC2                   1H
CPDPRG[2           waltz16
PCPD2              80.00 usec
PLW2        20.38699913 W
PLW12        0.31854999 W
PLW13        0.16023000 W

F2 - Processing parameters
SI                 32768
SF          125.7577955 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.40
```

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

Vial position : P1-E-06
Date of Analysis : 8/29/2017 10:09:22 PM Injection Vol : 0.300uL
Acq. Method : RND-FA-3.5mns Instrument ID : ANL-MCL5-LCMS-0
Sample Name : GVK-RK-009-65

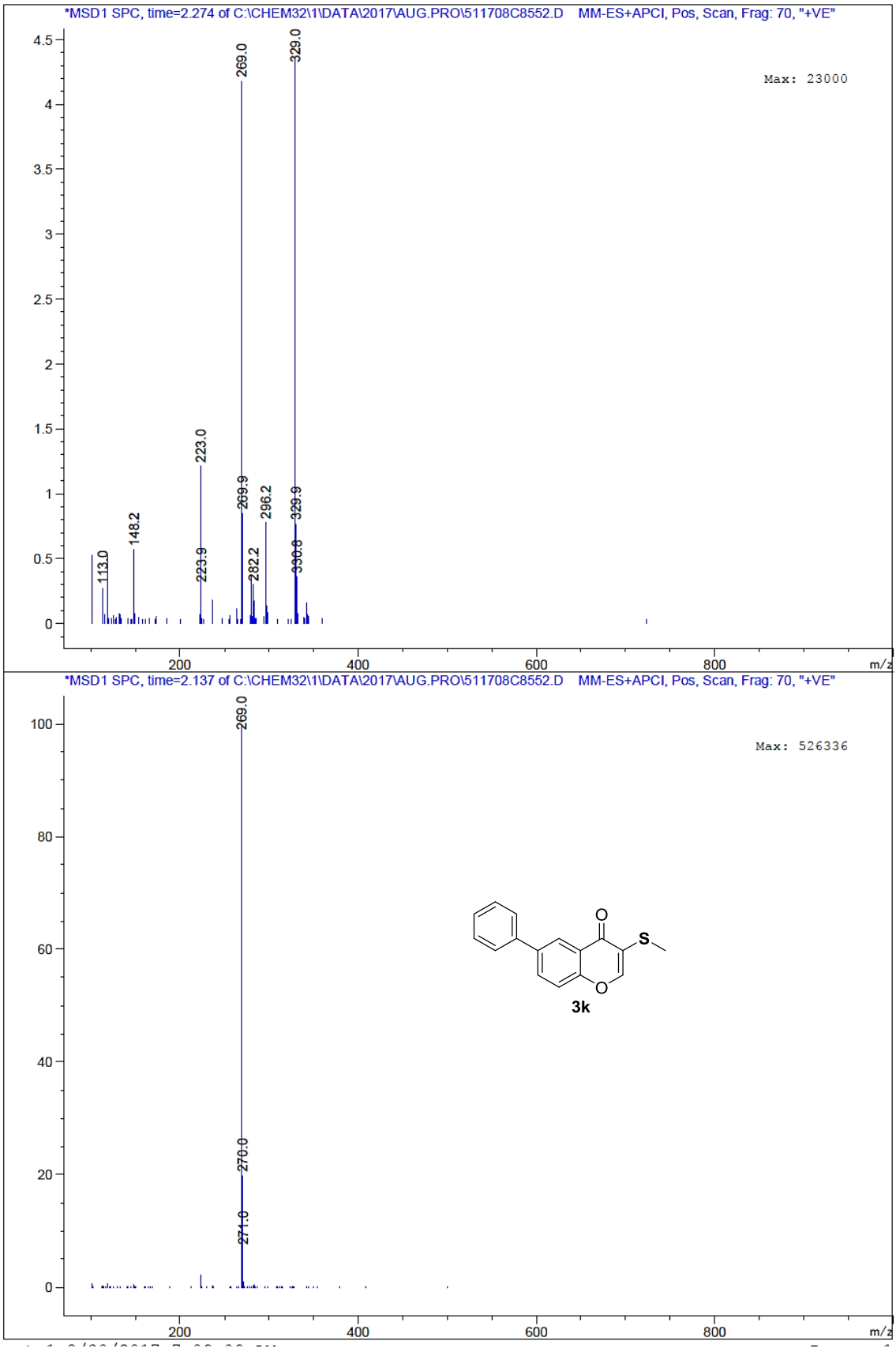
RND-FA-3.5 MIN.M
Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: B1: 0.1 % FA IN WATER A1: 0.1%FA IN ACN
Gradient: Time (min) /%A1: 0/2, 0.2/2, 2.3/98,3.4/98,3.41/2,3.5/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 50°C ->



DAD1 A, Sig=215,4 Ref=off

Peak No	RT min	Height	Area	Area %
1	1.71	4.843	5.243	0.803
2	2.13	588.426	626.218	95.912
3	2.26	19.589	21.446	3.285

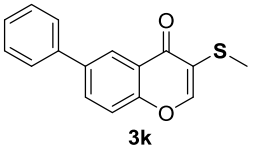
MS Spectrum


*MSD1 SPC, time=2.274 of C:\CHEM32\1\DATA\2017\AUG.PRO\511708C8552.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 23000
269.0
329.0
223.0
269.9
296.2
329.9
148.2
113.0
223.9
282.2
330.8
m/z
*MSD1 SPC, time=2.137 of C:\CHEM32\1\DATA\2017\AUG.PRO\511708C8552.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 526336
269.0
270.0
271.0
O
S
O
3k
m/z

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None



3k

Monoisotopic Mass, Even Electron Ions

5 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)

Elements Used:

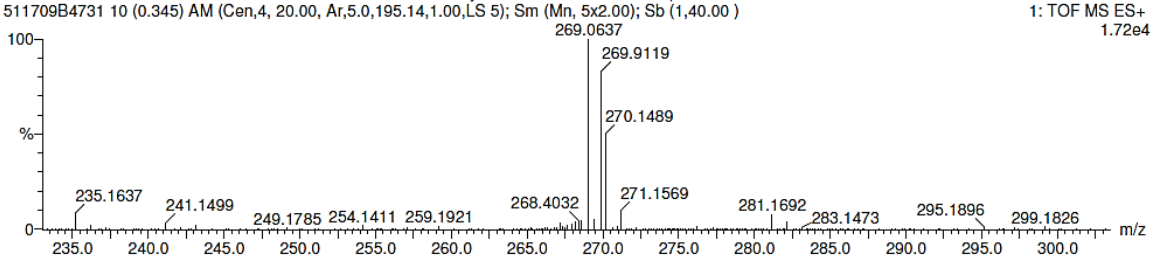
C: 0-16 H: 0-13 O: 0-2 S: 0-1

GVK-RK-009-65

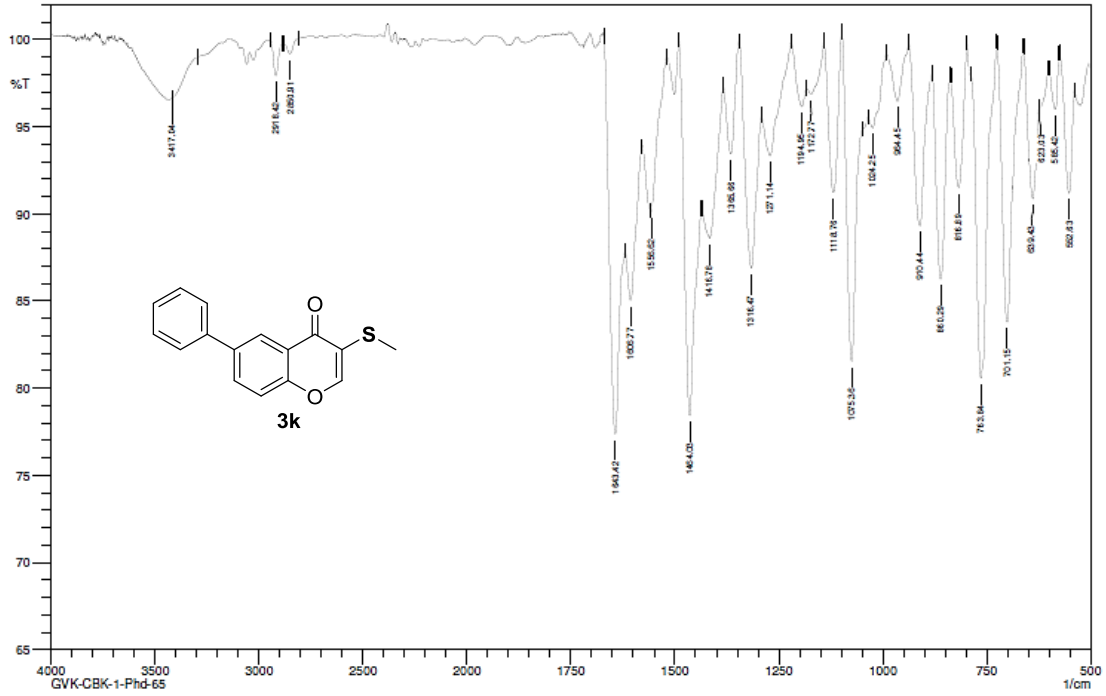
GVK Bio sciences (pvt)Ltd
Analytical Research and Development

Date of analysis:04-Oct-201715:35:58
Instru ment ID:ANL-MCL3-LCMS-001
1: TOF MS ES+
1.72e4

511709B4731 10 (0.345) AM (Cen,4, 20.00, Ar,5.0,195.14,1.00,LS 5); Sm (Mn, 5x2.00); Sb (1,40.00)



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
269.0637	269.0636	0.1	0.4	10.5	17759.7	C16 H13 O2 S

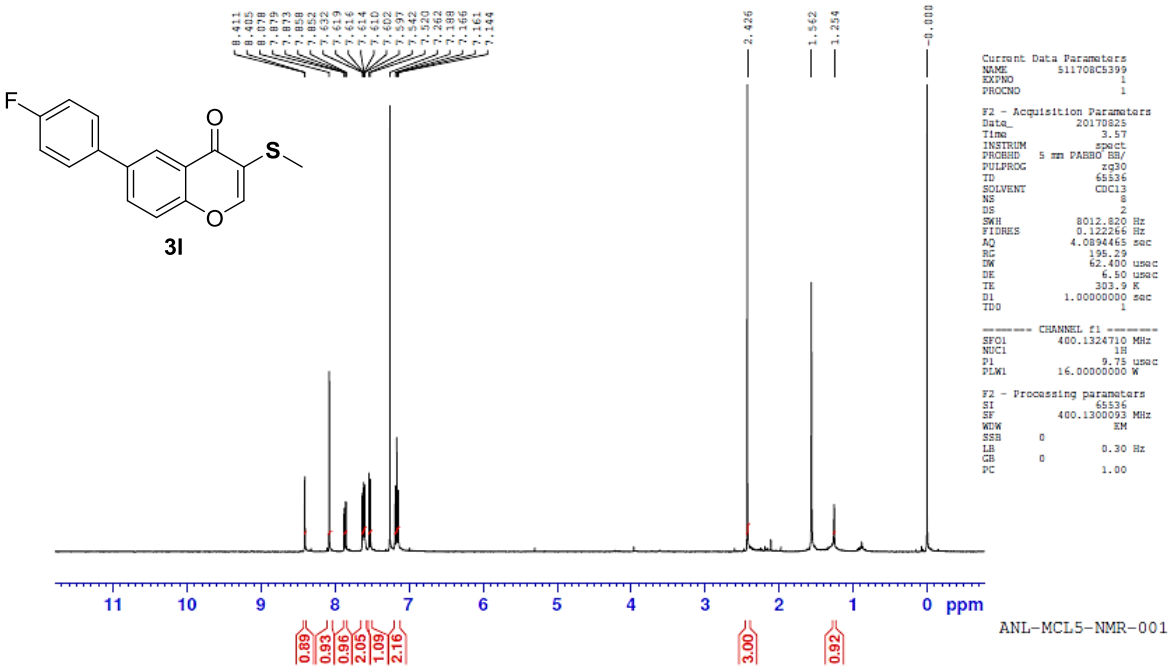


3k

Comment: IN Kbr
GVK-CBK-1-Phd-65

No. of Scans:
Resolution:
Apodization:

Date: 1/10/2018 11:45:30 AM
User: Admin

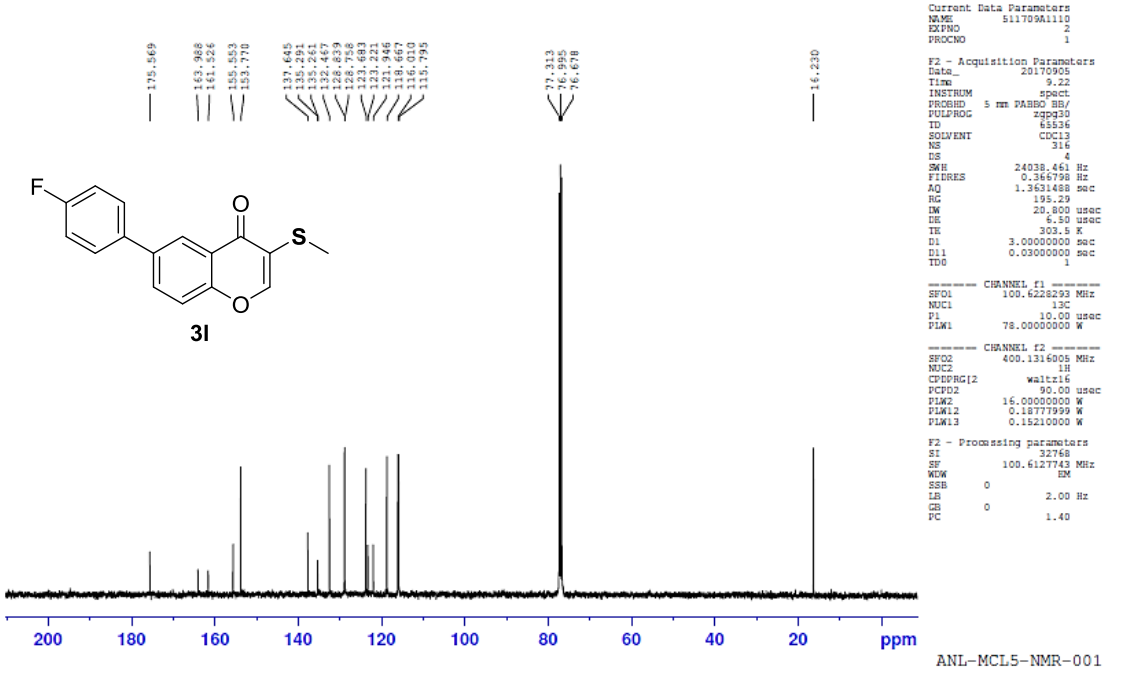



```
Current Data Parameters
NAME          511708C5399
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Data_           20170825
Time                3.57
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ              4.0894465 sec
RG                 195.29
DW                62.400 usec
DE                 6.50 usec
TE                303.9 K
D1              1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                  1H
P1                 9.75 usec
PLW1          16.00000000 W

F2 - Processing parameters
SI                 65536
SF            400.1300093 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



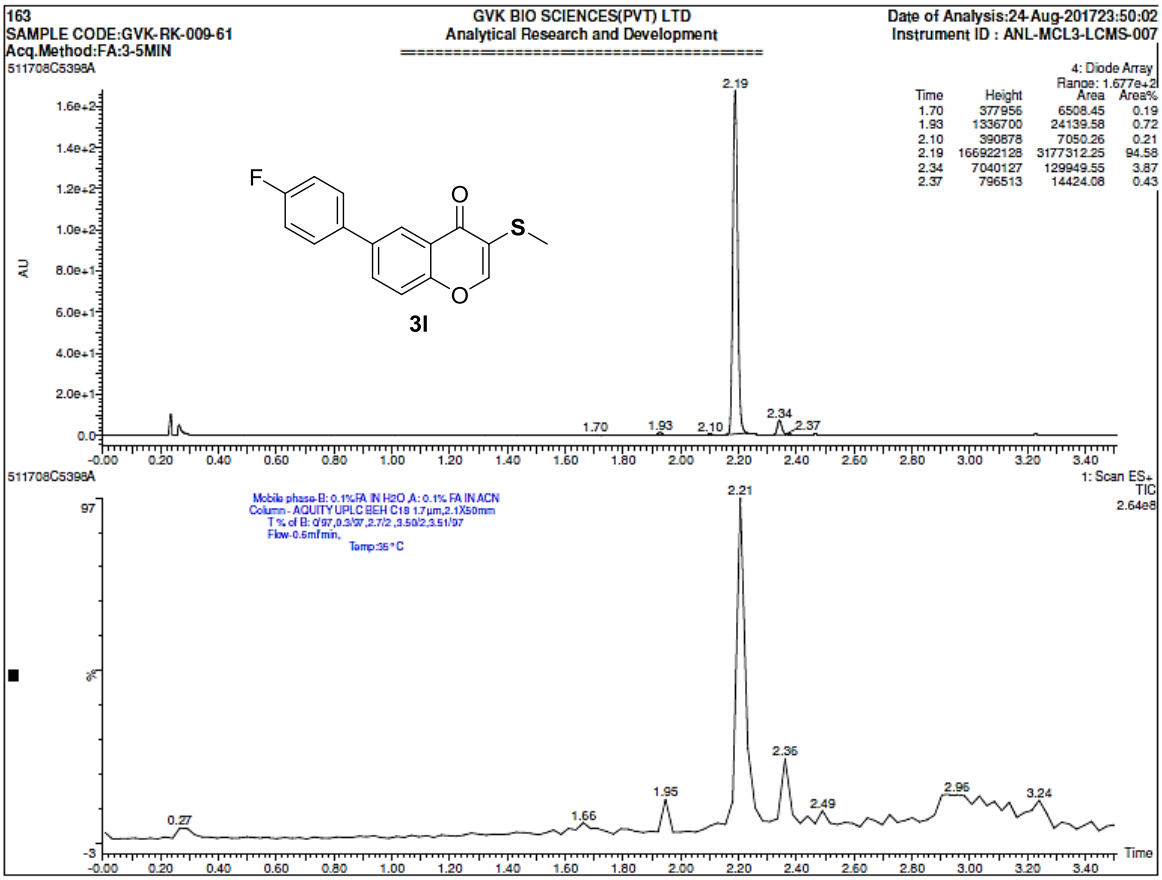

```
Current Data Parameters
NAME          511709A1110
EXPNO                   2
PROCNO                  1

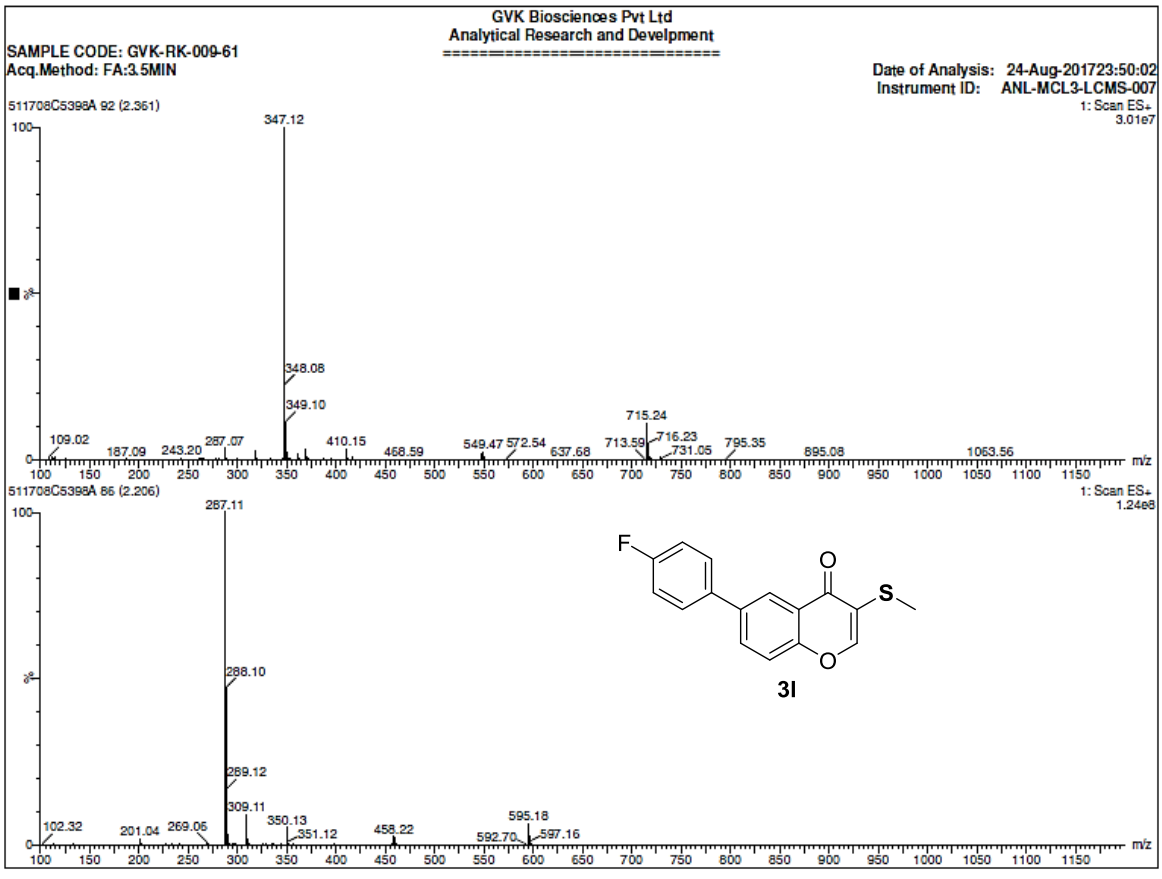
F2 - Acquisition Parameters
Data_           20170905
Time                9.22
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   316
DS                     4
SWH            24038.461 Hz
FIDRES          0.366798 Hz
AQ              1.3631488 sec
RG                 195.29
DW                20.800 usec
DE                 6.50 usec
TE                303.5 K
D1              3.00000000 sec
D11             0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1          100.6228293 MHz
NUC1                  13C
P1                10.00 usec
PLW1          78.00000000 W

======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2          16.00000000 W
PLW12          0.18777999 W
PLW13          0.15210000 W

F2 - Processing parameters
SI                 32768
SF            100.6127743 MHz
WDW                   EM
SSB       0
LB                 2.00 Hz
GB        0
PC                 1.40
```

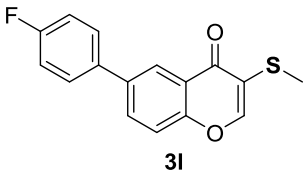

163
SAMPLE CODE:GVK-RK-009-61
Acq.Method:FA:3-5MIN
GVK BIO SCIENCES(PVT) LTD
Analytical Research and Development
Date of Analysis:24-Aug-201723:50:02
Instrument ID : ANL-MCL3-LCMS-007
511708C5398A
4: Diode Array
Range: 1.677e+2
Time Height Area Area%
1.70 377956 6508.45 0.19
1.93 1336700 24139.58 0.72
2.10 390878 7050.26 0.21
2.19 166922128 3177312.25 94.58
2.34 7040127 129949.55 3.87
2.37 796513 14424.08 0.43
AU
2.19
1.70
1.93
2.10
2.34
2.37
F
O
S
O
3I
511708C5398A
1: Scan ES+
TIC
2.64e8
Mobile phase-B: 0.1%FA IN H2O ,A: 0.1% FA IN ACN
Column - AQUITY UPLC BEH C18 1.7µm,2.1X50mm
T % of B: 0/97,0.3/97,2.7/2 ,3.50/2,3.51/97
Flow-0.6ml/min,
Temp:35 °C
%
2.21
0.27
1.66
1.95
2.36
2.49
2.96
3.24
Time


GVK Biosciences Pvt Ltd
Analytical Research and Development
SAMPLE CODE: GVK-RK-009-61
Acq.Method: FA:3.5MIN
Date of Analysis: 24-Aug-201723:50:02
Instrument ID: ANL-MCL3-LCMS-007
511708C5398A 92 (2.361)
1: Scan ES+
3.01e7
347.12
348.08
349.10
715.24
716.23
m/z
511708C5398A 86 (2.206)
1: Scan ES+
1.24e8
287.11
288.10
289.12
309.11
595.18
F
O
S
O
3I

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None



3l

Monoisotopic Mass, Odd and Even Electron Ions

10 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)

Elements Used:

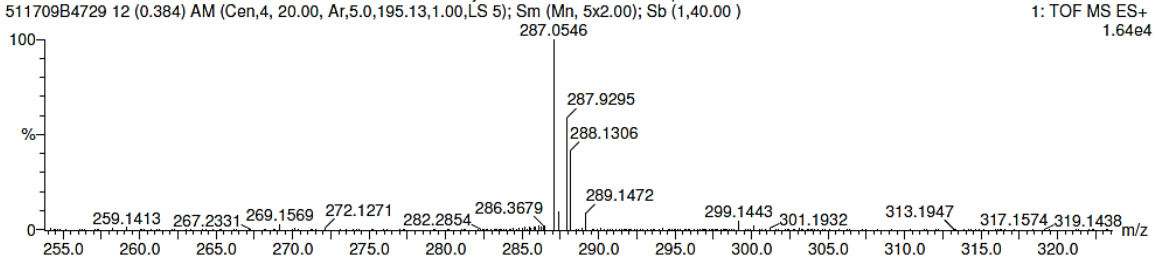
C: 0-16 H: 0-12 O: 0-2 F: 0-1 S: 0-1

GVK-RK-009-61

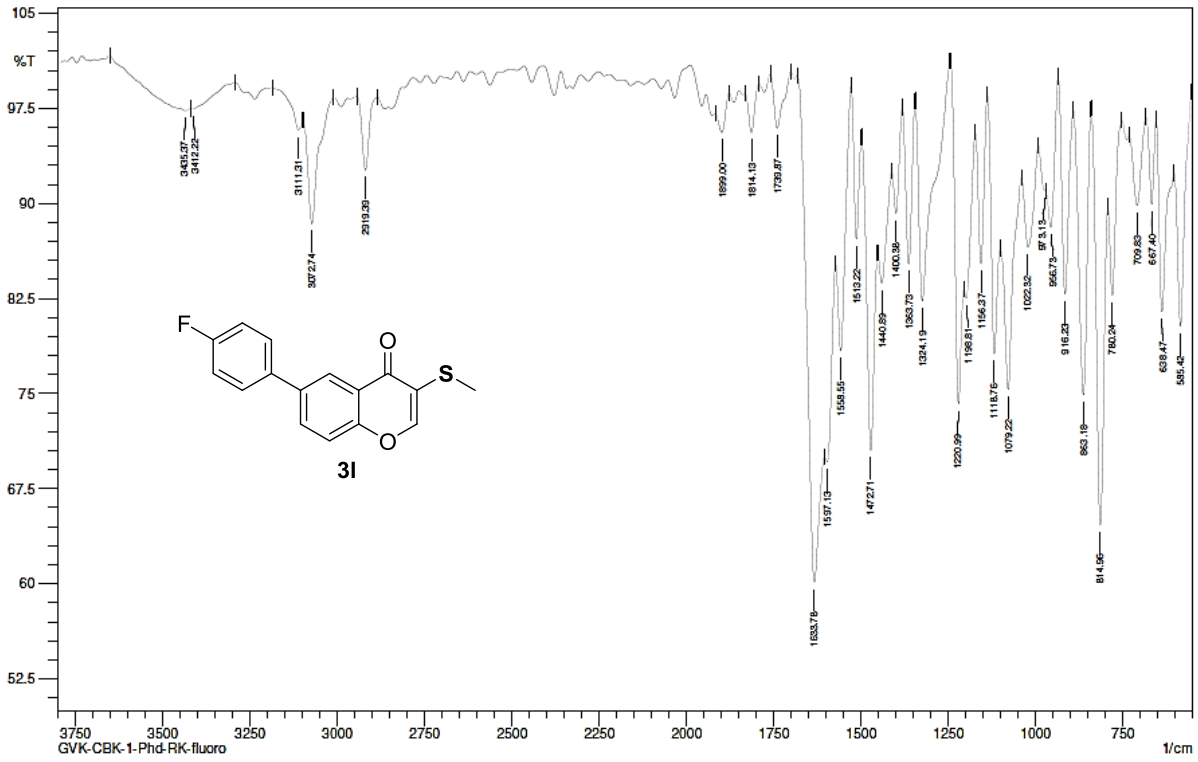
GVK Bio sciences (pvt)Ltd
Analytical Research and Development

Date of analysis:04-Oct-201715:38:17
Instru ment ID:ANL-MCL3-LCMS-001
1: TOF MS ES+
1.64e4

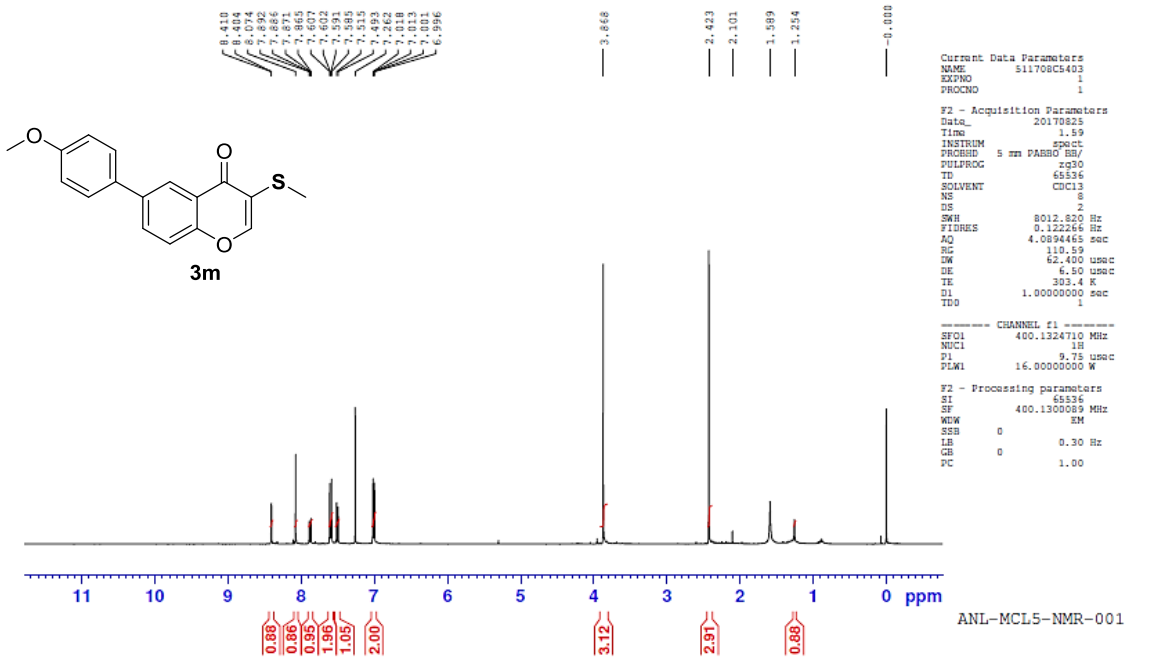
511709B4729 12 (0.384) AM (Cen,4, 20.00, Ar,5.0,195.13,1.00,LS 5); Sm (Mn, 5x2.00); Sb (1,40.00)



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
287.0546	287.0542	0.4	1.4	10.5	7797.3	C16 H12 O2 F S



3l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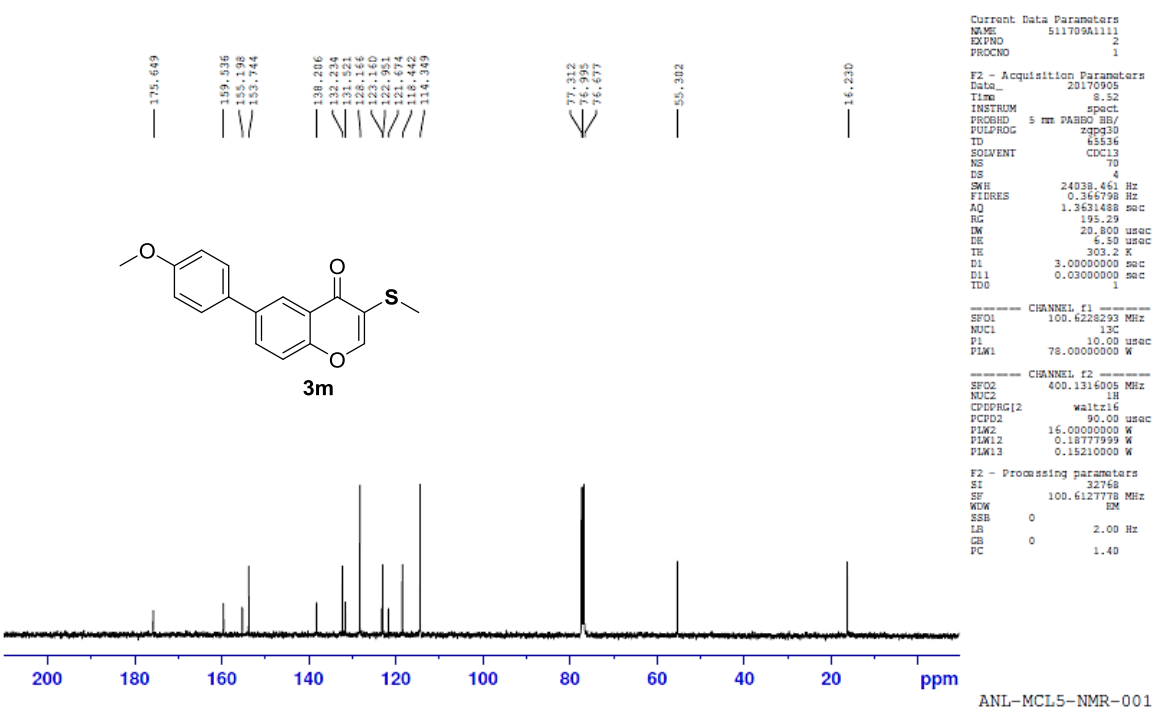
8.404
8.074
7.892
7.886
7.871
7.865
7.607
7.602
7.591
7.585
7.515
7.493
7.262
7.018
7.013
7.001
6.996
3.868
2.423
2.101
1.589
1.254
0.000
O
O
S
O
3m
Current Data Parameters
NAME 511708C5403
EXPNO 1
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170825
Time 1.59
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 110.59
DW 62.400 usec
DE 6.50 usec
TE 303.4 K
D1 1.00000000 sec
TD0 1
CHANNEL f1
SFO1 400.1324710 MHz
NUC1 1H
P1 9.75 usec
PLW1 16.00000000 W
F2 - Processing parameters
SI 65536
SF 400.1300089 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
11 10 9 8 7 6 5 4 3 2 1 0 ppm
0.88 0.86 0.95 1.96 1.05 2.00 3.12 2.91 0.88
ANL-MCL5-NMR-001


175.649
159.536
155.198
153.744
138.206
132.234
131.521
128.566
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122.951
121.674
118.442
114.349
77.312
76.995
76.677
55.382
16.230
O
O
S
O
3m
Current Data Parameters
NAME 511709A1111
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20170905
Time 8.52
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 70
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 195.29
DW 20.800 usec
DE 6.50 usec
TE 303.2 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
CHANNEL f1
SFO1 100.6228293 MHz
NUC1 13C
P1 10.00 usec
PLW1 78.00000000 W
CHANNEL f2
SFO2 400.1316005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 16.00000000 W
PLW12 0.18777999 W
PLW13 0.15210000 W
F2 - Processing parameters
SI 32768
SF 100.6127778 MHz
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SSB 0
LB 2.00 Hz
GB 0
PC 1.40
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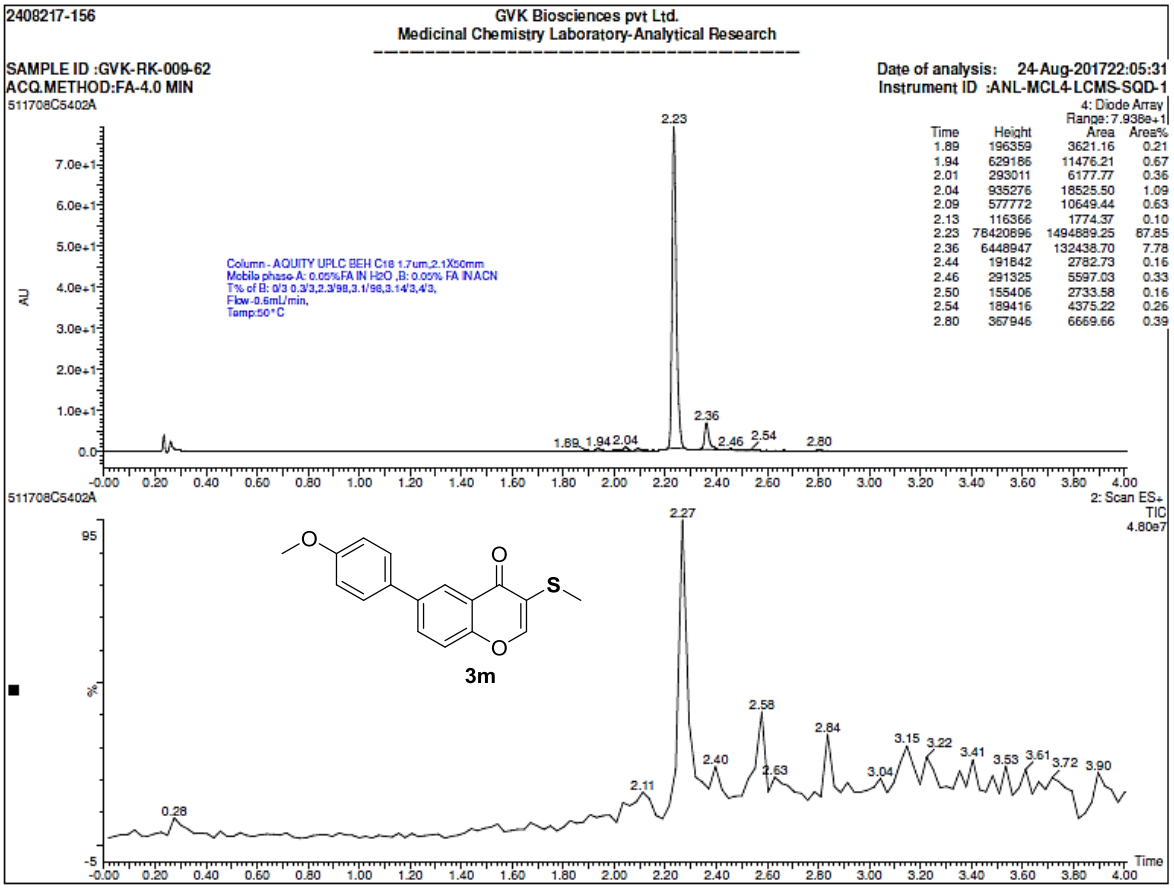
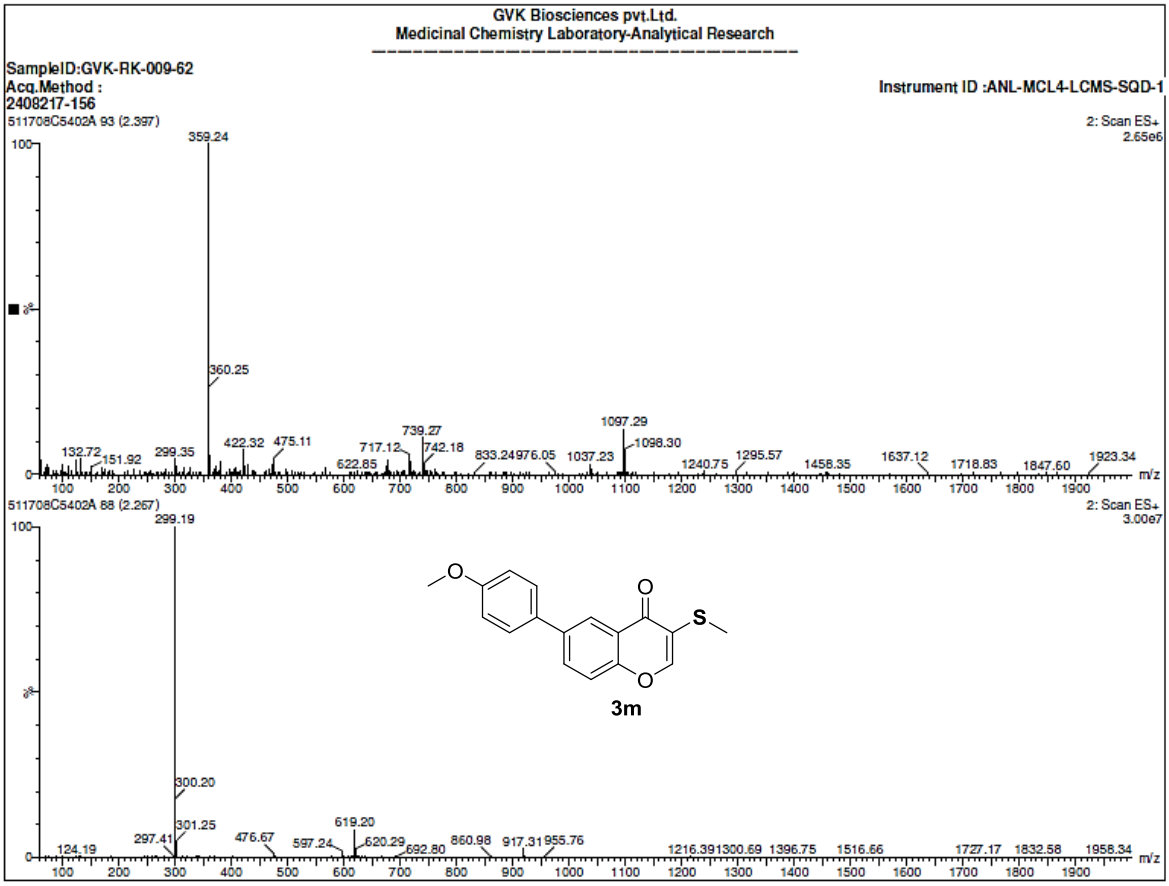
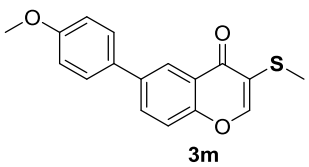
ANL-MCL5-NMR-001


2408217-156
GVK Biosciences pvt Ltd.
Medicinal Chemistry Laboratory-Analytical Research
SAMPLE ID :GVK-RK-009-62
ACQ.METHOD:FA-4.0 MIN
Date of analysis: 24-Aug-201722:05:31
Instrument ID :ANL-MCL4-LCMS-SQD-1
511708C5402A
4: Diode Array
Range: 7.936e+1
Time Height Area Area%
1.89 196359 3621.16 0.21
1.94 629186 11476.21 0.67
2.01 293011 6177.77 0.36
2.04 935276 18525.50 1.09
2.09 577772 10649.44 0.63
2.13 116366 1774.37 0.10
2.23 78420896 1494889.25 87.85
2.36 6448947 132438.70 7.78
2.44 191842 2782.73 0.16
2.46 291325 5597.03 0.33
2.50 155406 2733.58 0.16
2.54 189416 4375.22 0.26
2.80 367946 6669.66 0.39
Column - AQUITY UPLC BEH C18 1.7um,2.1X50mm
Mobile phase-A: 0.05%FA IN H2O ,B: 0.05% FA IN ACN
T% of B: 0/3 0.3/3,2.3/98,3.1/98,3.14/3,4/3,
Flow-0.6mL/min,
Temp:50°C
AU
2.23
1.89 1.94 2.04 2.36 2.46 2.54 2.80
511708C5402A
2: Scan ES+
TIC
4.80e7
%
2.27
0.28 2.11 2.40 2.53 2.58 2.84 3.04 3.15 3.22 3.41 3.53 3.61 3.72 3.90
Time
3m


GVK Biosciences pvt.Ltd.
Medicinal Chemistry Laboratory-Analytical Research
SampleID:GVK-RK-009-62
Acq.Method :
2408217-156
Instrument ID :ANL-MCL4-LCMS-SQD-1
511708C5402A 93 (2.397)
2: Scan ES+
2.65e6
359.24
360.25
132.72 151.92 299.35 422.32 475.11 622.85 717.12 739.27 742.18 833.24 976.05 1037.23 1097.29 1098.30 1240.75 1295.57 1458.35 1637.12 1718.83 1847.60 1923.34
m/z
511708C5402A 88 (2.267)
2: Scan ES+
3.00e7
299.19
300.20
124.19 297.41 301.25 476.67 597.24 619.20 620.29 692.80 860.98 917.31 955.76 1216.39 1300.69 1396.75 1516.66 1727.17 1832.58 1958.34
3m

Single Mass Analysis
Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None



3m

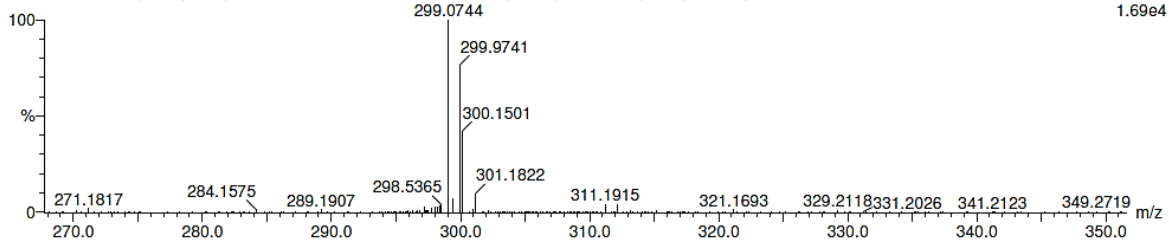
Monoisotopic Mass, Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-17 H: 0-15 O: 0-3 S: 0-1

GVK-RK-009-62

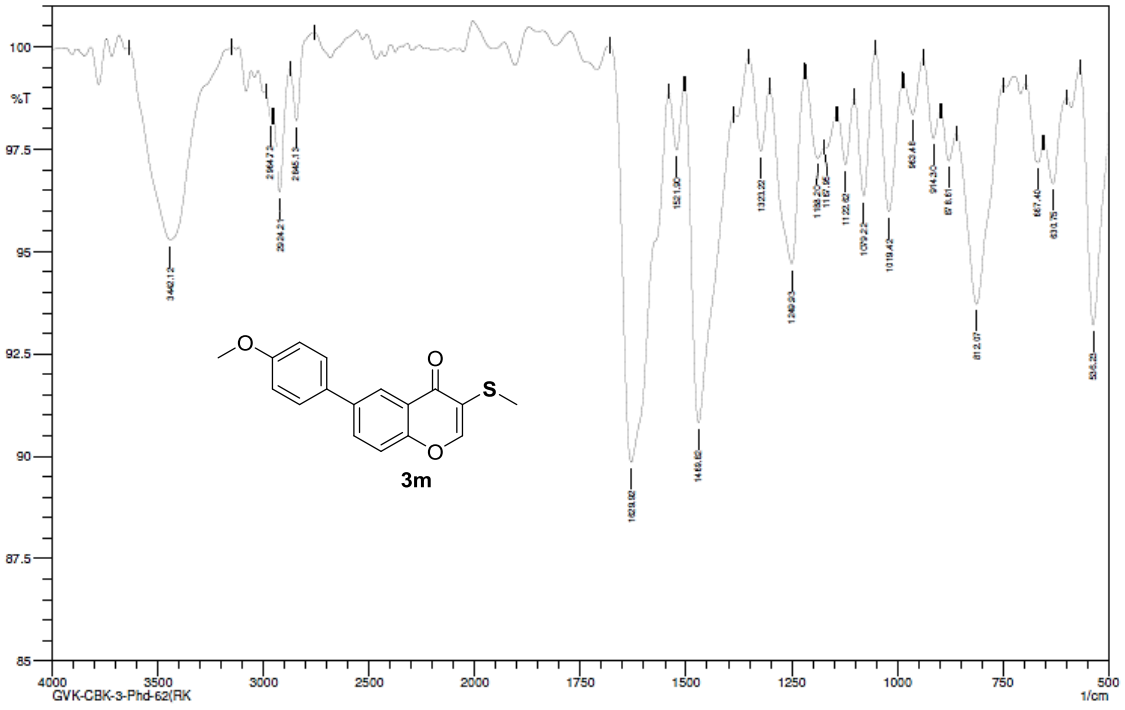
GVK Bio sciences (pvt)Ltd
Analytical Research and Development

Date of analysis:04-Oct-201715:40:38
Instru ment ID:ANL-MCL3-LCMS-001
1: TOF MS ES+
1.69e4

511709B4730 10 (0.346) AM (Cen,4, 20.00, Ar,5.0,195.13,1.00,LS 5); Sm (Mn, 5x2.00); Sb (1,40.00)



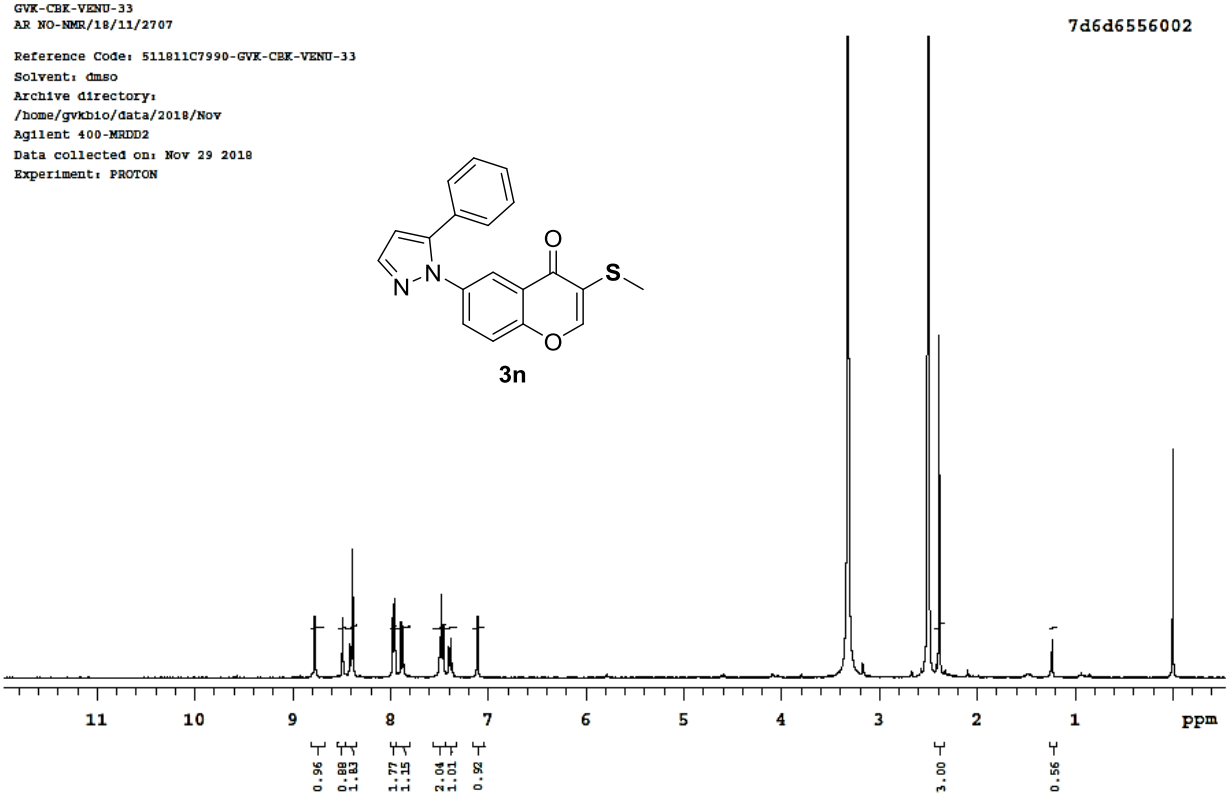
Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
299.0744	299.0742	0.2	0.7	10.5	8182.5	C17 H15 O3 S

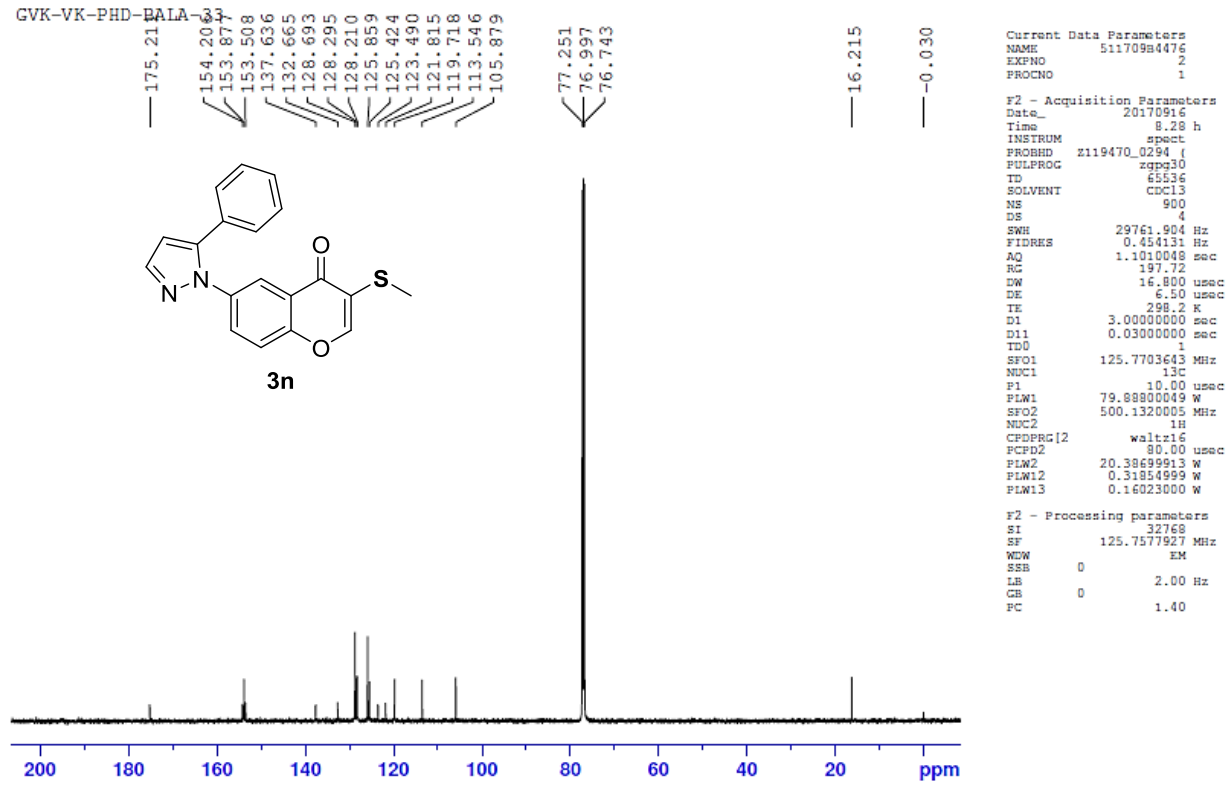


Comment: IN Kbr
GVK-CBK-3-Phd-62(RK

No. of Scans:
Resolution:
Apodization:

Date: 3/2/2018 10:32:32 AM
User: Admin





Current Data Parameters
NAME 511709B4476
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20170916
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INSTRUM spect
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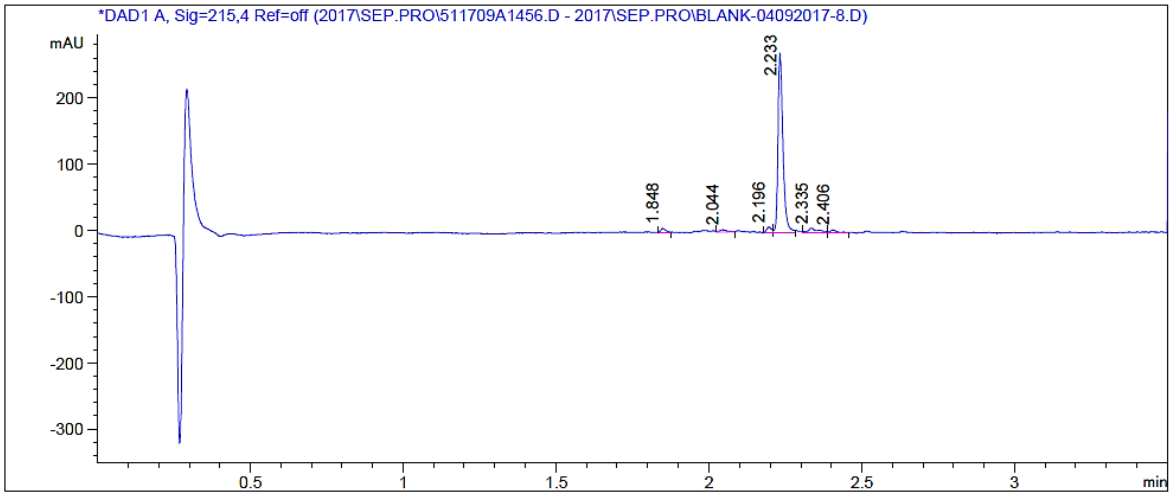
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 900
DS 4
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 298.2 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 10.00 usec
PLW1 79.88800049 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 20.38699913 W
PLW12 0.31854999 W
PLW13 0.16023000 W

F2 - Processing parameters
SI 32768
SF 125.7577927 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

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

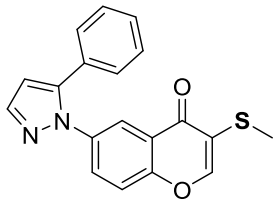
Vial position : P1-A-04
Date of Analysis : 9/4/2017 1:48:16 PM Injection Vol : 0.300uL
Acq. Method : RND-FA-3.5mns Instrument ID : ANL-MCL5-LCMS-0(
Sample Name : GVK-PHD-VK-BALA-33-1

RND-FA-3.5 MIN.M
Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: B1: 0.1 % FA IN WATER A1: 0.1%FA IN ACN
Gradient: Time (min) /%A1: 0/2, 0.2/2, 2.3/98,3.4/98,3.41/2,3.5/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 50°C ->



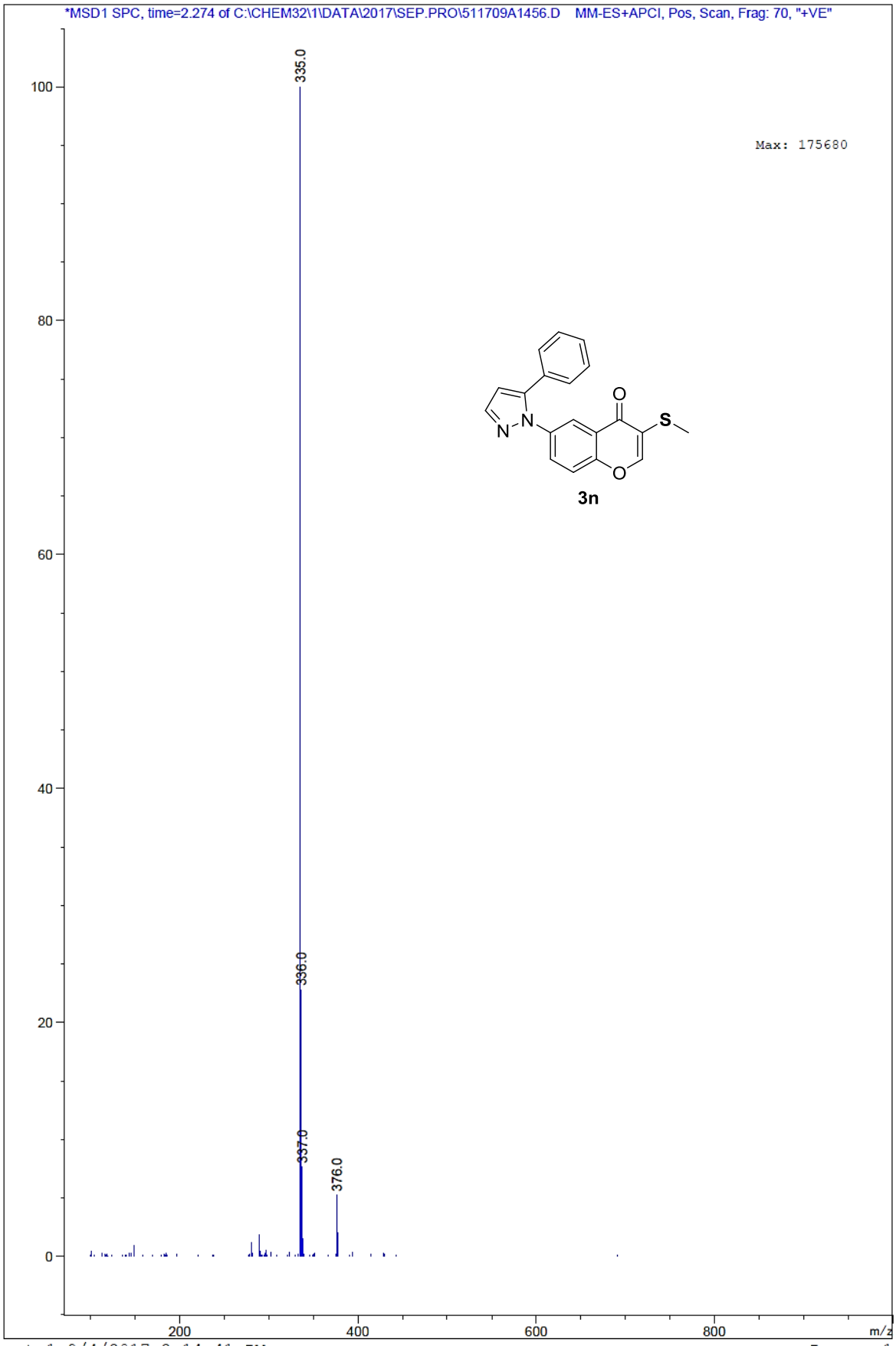
DAD1 A, Sig=215,4 Ref=off

Peak No	RT min	Height	Area	Area %
1	1.85	6.014	6.647	1.897
2	2.04	3.392	5.959	1.700
3	2.20	8.162	8.844	2.524
4	2.23	269.243	310.176	88.506
5	2.34	6.675	13.655	3.896
6	2.41	3.693	5.177	1.477

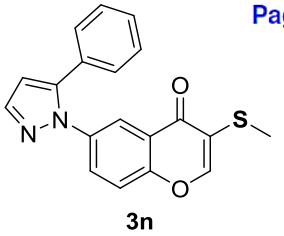


3n

MS Spectrum


*MSD1 SPC, time=2.274 of C:\CHEM32\1\DATA\2017\SEP.PRO\511709A1456.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 175680
335.0
336.0
337.0
376.0
100
80
60
40
20
0
200
400
600
800
m/z
O
N
N
S
O
3n

Elemental Composition Report



3n

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

12 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)

Elements Used:

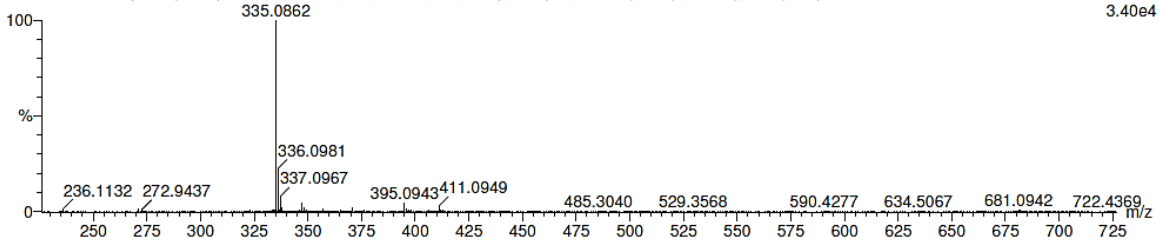
C: 0-19 H: 0-15 N: 0-2 O: 0-2 S: 0-1

GVK-CBK-1-Phd-33

GVK Bio sciences (pvt)Ltd
Analytical Research and Development

Date of analysis:19-Feb-201811:50:51
Instru ment ID:ANL-MCL3-LCMS-001
1: TOF MS ES+
3.40e4

511802B3851- 9 (0.369) AM (Cen,2, 50.00, Ar,5.0,195.09,1.00,LS 5); Sm (Mn, 5x2.00); Sb (1,40.00); Cm (4:18)



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
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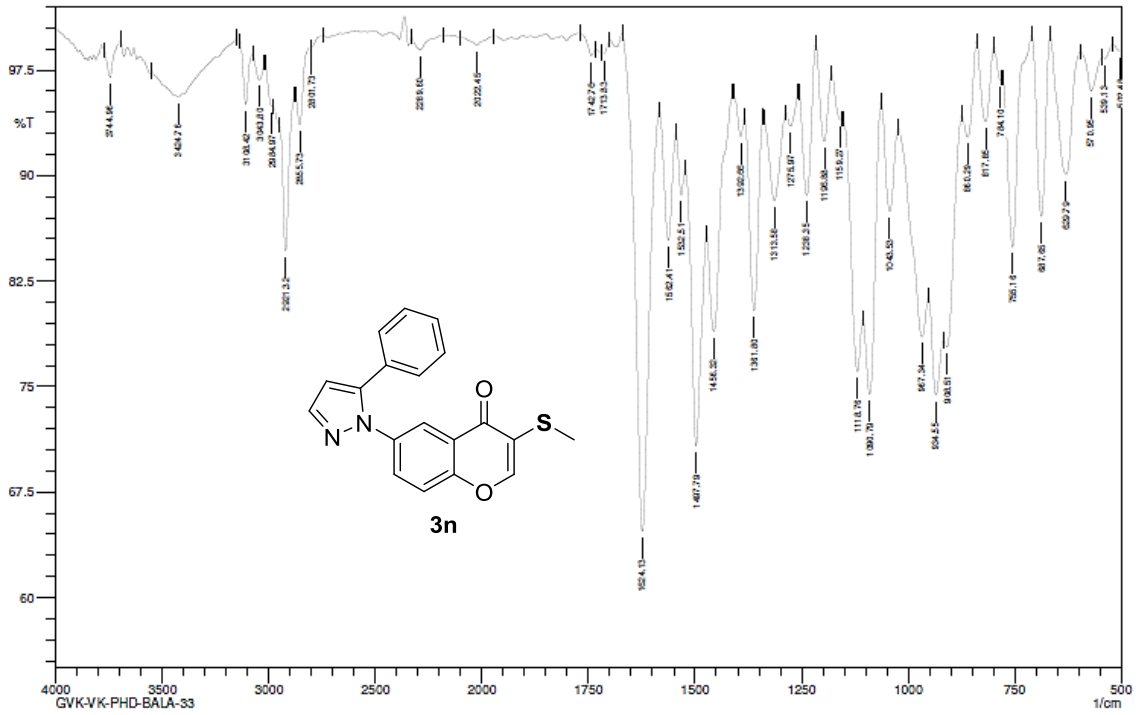
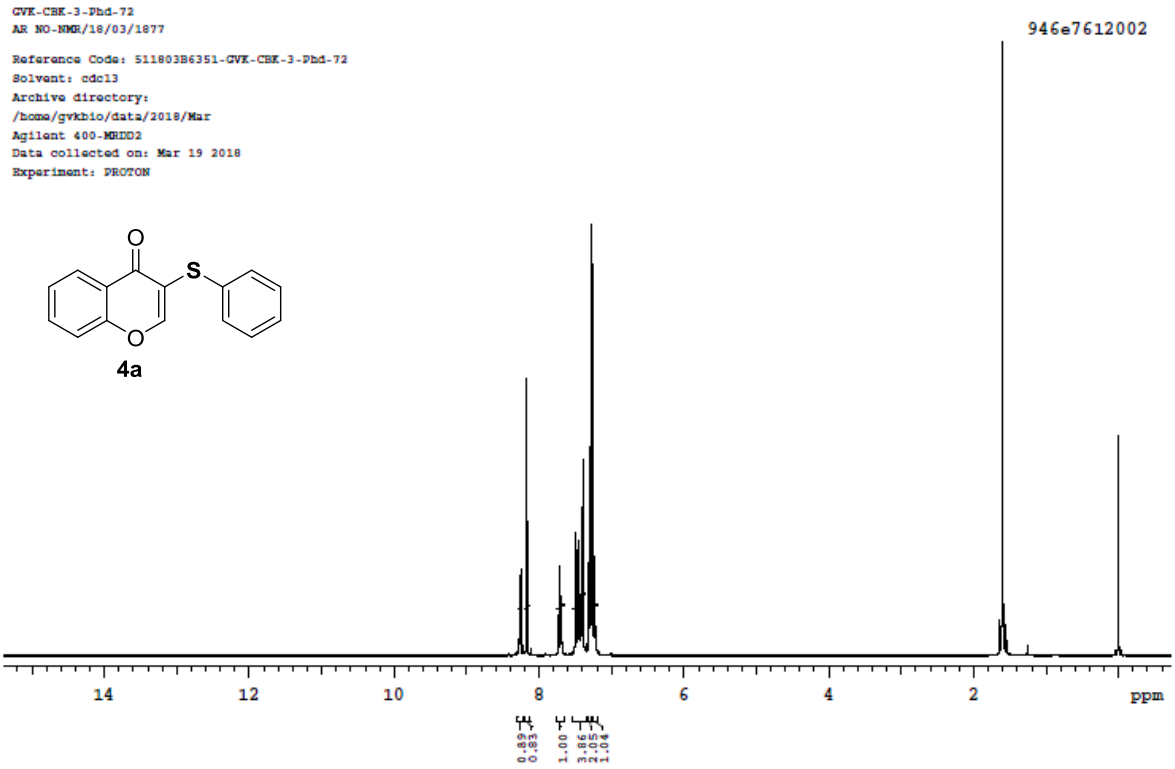


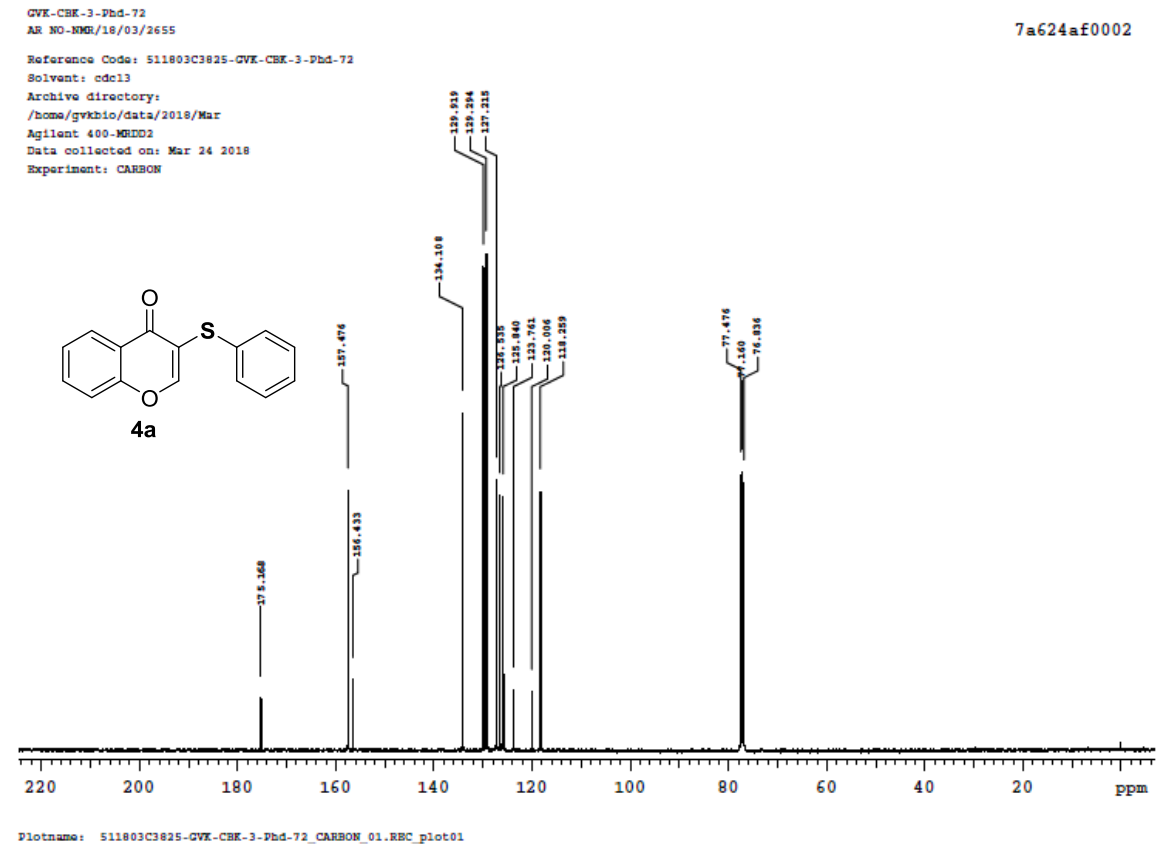
3n

Comment: IN Kbr
GVK-VK-PHD-BALA-33

No. of Scans:
Resolution:
Apodization:

Date:9/18/2017 6:17:56 PM
User: Admin


GVK-CBK-3-Phd-72
AR NO-NMR/18/03/1877
946e7612002
Reference Code: 511803B6351-GVK-CBK-3-Phd-72
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2018/Mar
Agilent 400-MRDD2
Data collected on: Mar 19 2018
Experiment: PROTON
4a
14
12
10
8
6
4
2
ppm
0.89
0.83
1.00
3.86
2.05
1.04


GVK-CBK-3-Phd-72
AR NO-NMR/18/03/2655
7a624af0002
Reference Code: 511803C3825-GVK-CBK-3-Phd-72
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2018/Mar
Agilent 400-MRDD2
Data collected on: Mar 24 2018
Experiment: CARBON
4a
175.168
157.476
156.433
134.108
129.919
129.294
127.215
126.538
125.840
123.741
120.006
118.259
77.476
77.160
76.836
220
200
180
160
140
120
100
80
60
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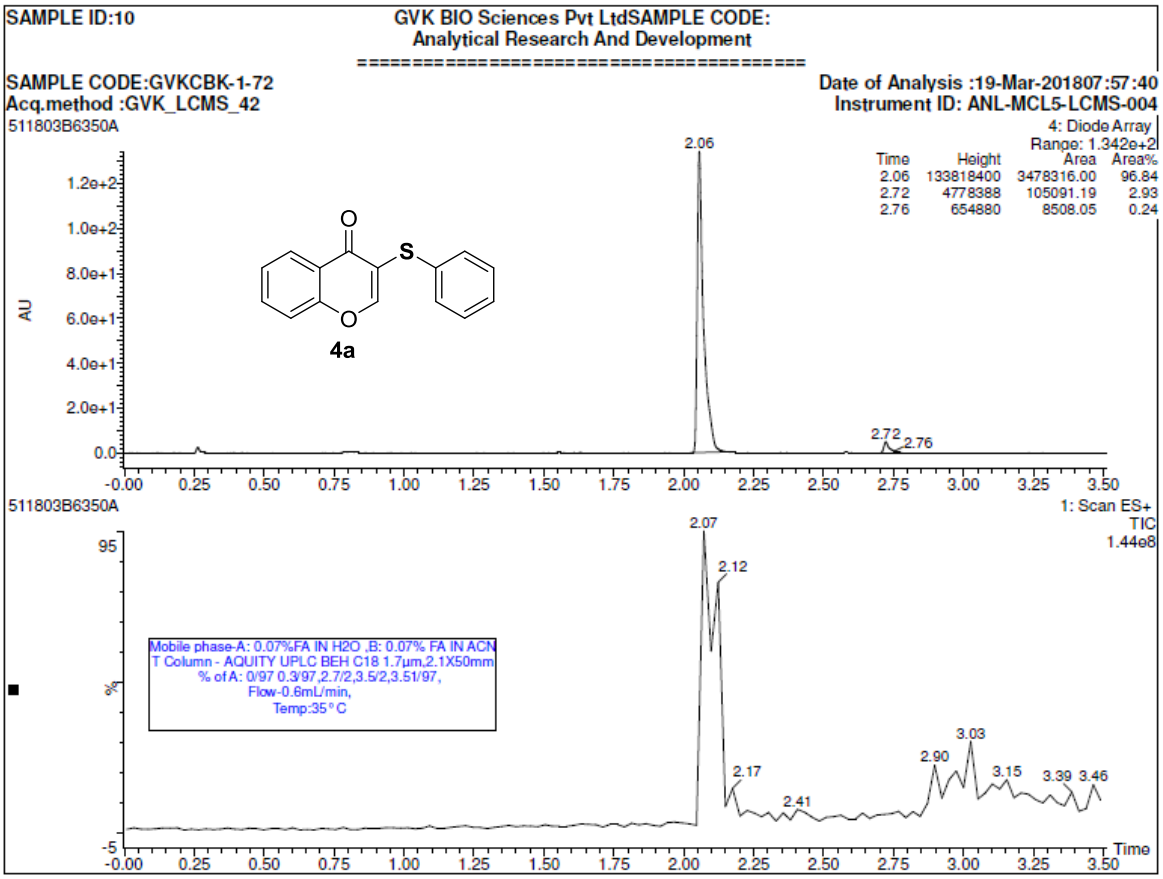
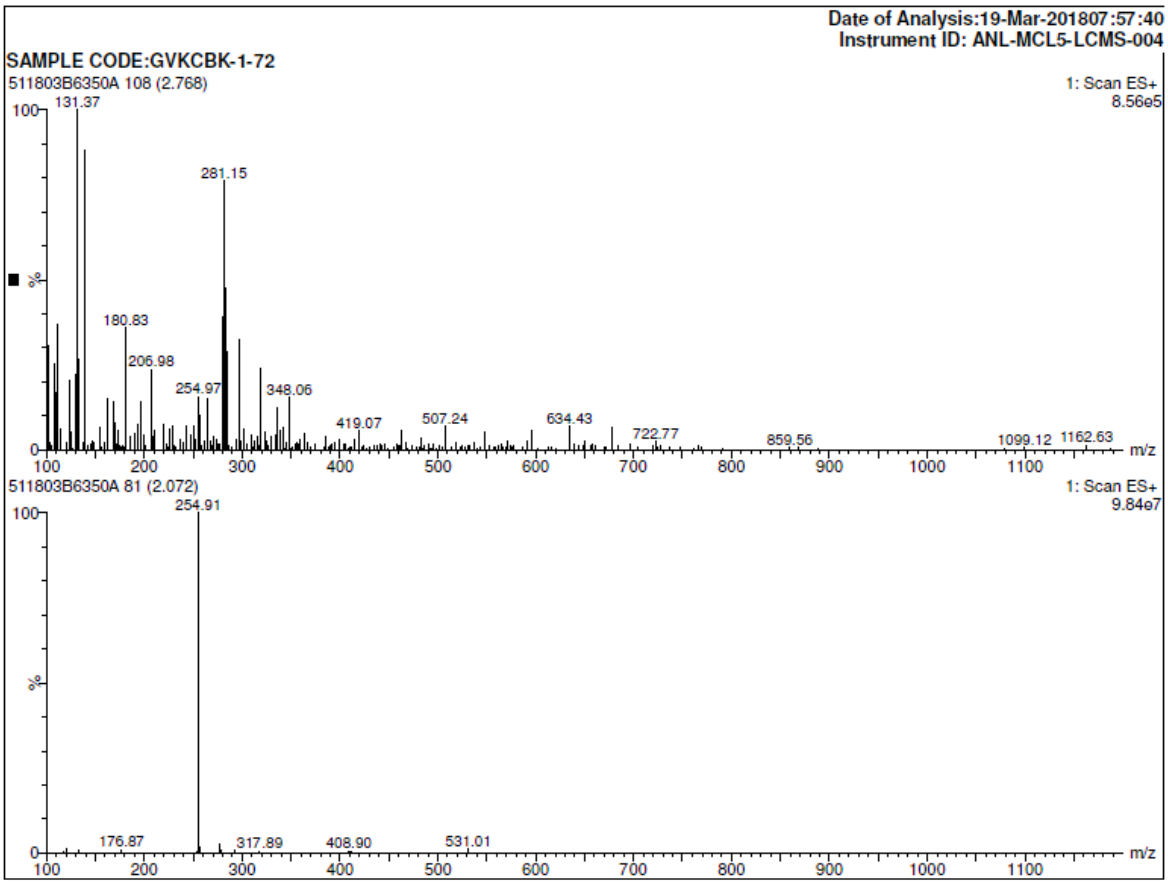
20
ppm
Plotname: 511803C3825-GVK-CBK-3-Phd-72_CARBON_01.REC_plot01


SAMPLE ID:10
GVK BIO Sciences Pvt LtdSAMPLE CODE:
Analytical Research And Development
SAMPLE CODE:GVKCBK-1-72
Acq.method :GVK_LCMS_42
Date of Analysis :19-Mar-201807:57:40
Instrument ID: ANL-MCL5-LCMS-004
511803B6350A
4: Diode Array
Range: 1.342e+2
Time Height Area Area%
2.06 133818400 3478316.00 96.84
2.72 4778388 105091.19 2.93
2.76 654880 8508.05 0.24
AU
4a
2.06
2.72
2.76
511803B6350A
1: Scan ES+
TIC
1.44e8
Mobile phase-A: 0.07%FA IN H2O ,B: 0.07% FA IN ACN
T Column - AQUITY UPLC BEH C18 1.7µm,2.1X50mm
% of A: 0/97 0.3/97,2.7/2,3.5/2,3.51/97,
Flow-0.6mL/min,
Temp:35°C
2.07
2.12
2.17
2.41
2.90
3.03
3.15
3.39
3.46
Time

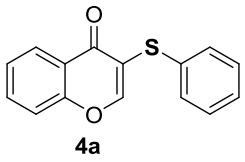

Date of Analysis:19-Mar-201807:57:40
Instrument ID: ANL-MCL5-LCMS-004
SAMPLE CODE:GVKCBK-1-72
511803B6350A 108 (2.768)
1: Scan ES+
8.56e5
131.37
281.15
180.83
206.98
254.97
348.06
419.07
507.24
634.43
722.77
859.56
1099.12
1162.63
m/z
511803B6350A 81 (2.072)
1: Scan ES+
9.84e7
254.91
176.87
317.89
408.90
531.01
m/z

Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None



4a

Monoisotopic Mass, Odd and Even Electron Ions

5 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

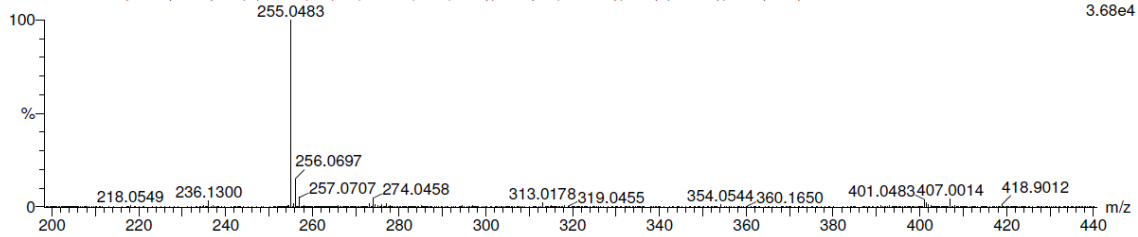
C: 0-15 H: 0-11 O: 0-2 S: 0-1

GVK-CBK-1-72

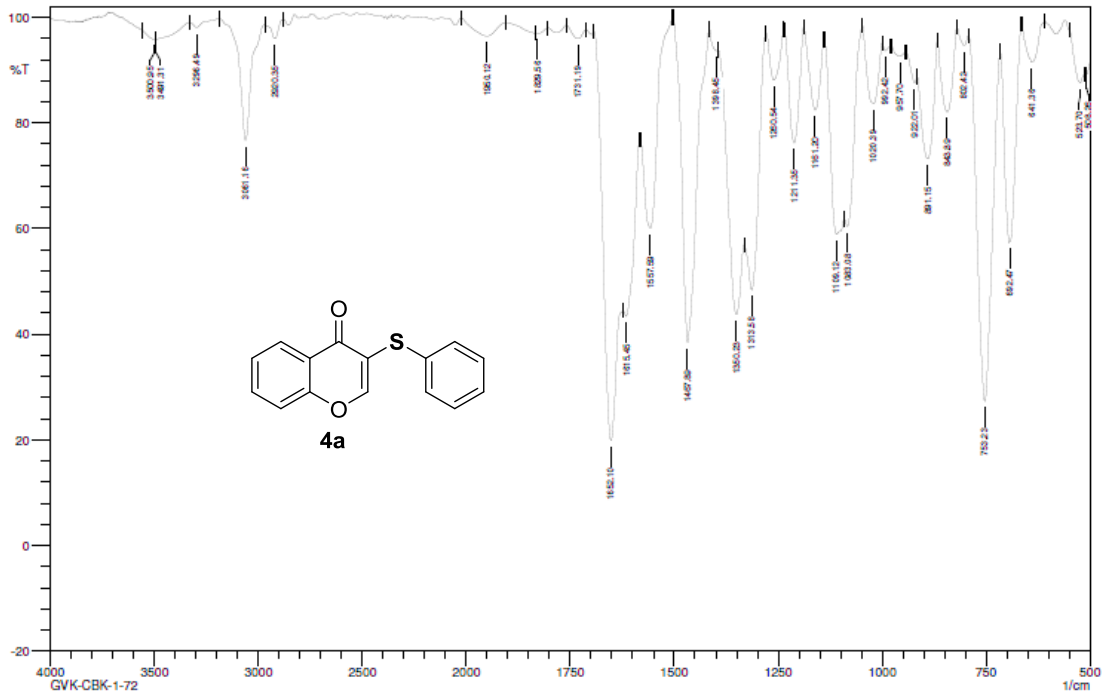
GVK Bio sciences (pvt)Ltd
Analytical Research and Development

Date of analysis:11-Apr-201816:11:09
Instru ment ID:ANL-MCL3-LCMS-001
1: TOF MS ES+
3.68e4

511846B3882 7 (0.282) AM (Cen,2, 50.00, Ar,5.0,195.10,1.00,LS 5); Sm (Mn, 5x2.00); Sb (1,40.00); Cm (4:14)



Minimum:				-1.5		
Maximum:		50.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
255.0483	255.0480	0.3	1.2	10.5	264.0	C15 H11 O2 S



4a

Comment: IN Kbr
GVK-CBK-1-72

No. of Scans:
Resolution:
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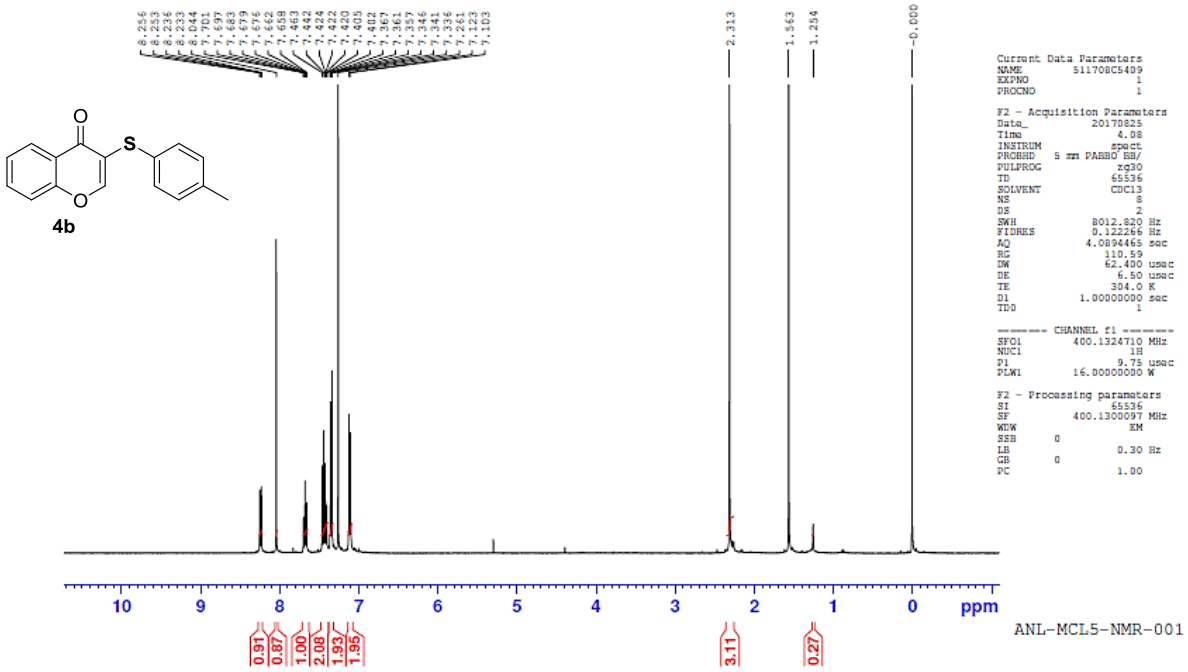
User: Admin

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Current Data Parameters
NAME          511708C5409
EXPNO                   1
PROCNO                  1

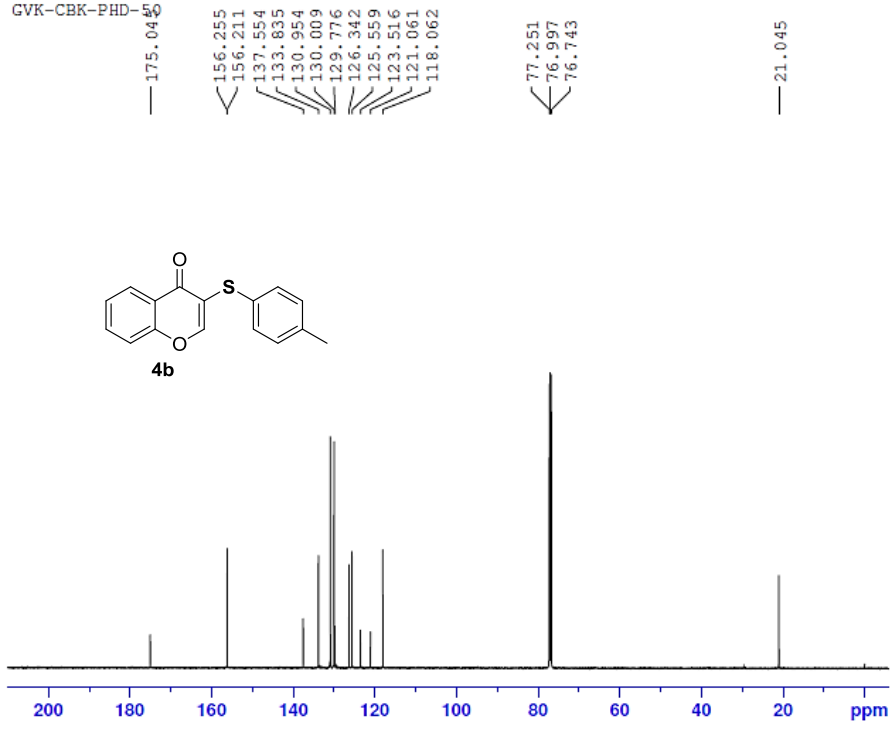
F2 - Acquisition Parameters
Date_              20170825
Time                   4.08
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDCl3
NS                       8
DS                       2
SWH               8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894465 sec
RG                   110.59
DW                  62.400 usec
DE                   6.50 usec
TE                  304.0 K
D1                1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1            400.1324710 MHz
NUC1                      1H
P1                     9.75 usec
PLW1           16.00000000 W

F2 - Processing parameters
SI                       65536
SF              400.1300097 MHz
WDW                         EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

ANL-MCL5-NMR-001

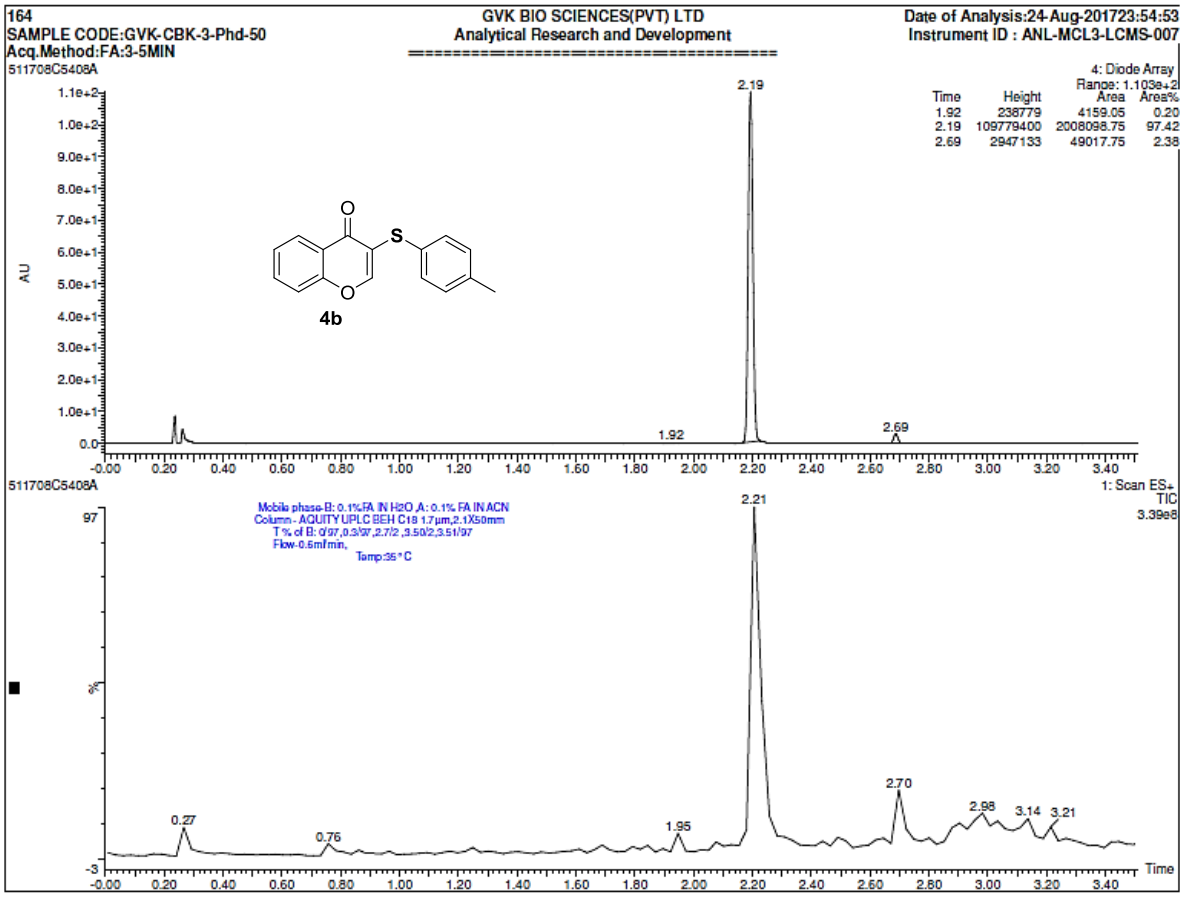
GVK-CBK-PHD-50

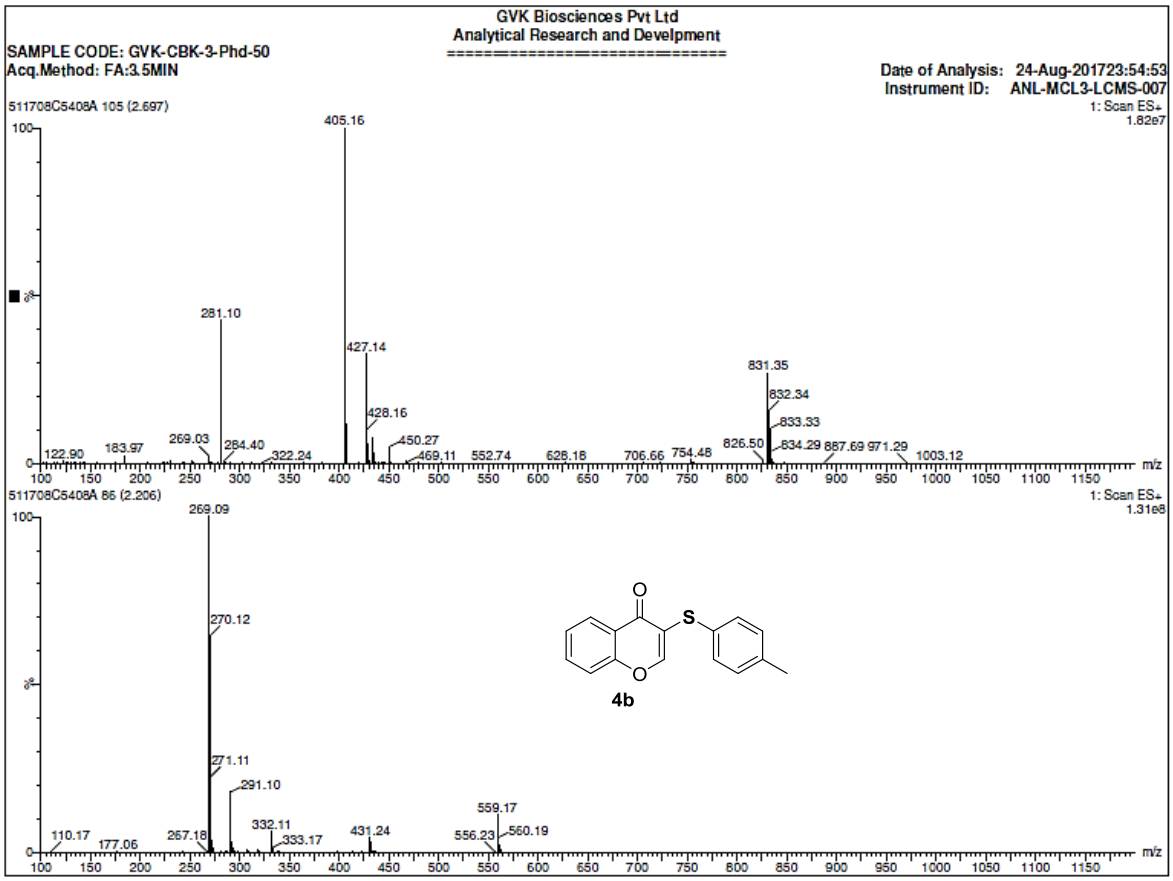



```
Current Data Parameters
NAME          511710C6615
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_              20171029
Time                  15.22 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                3.00000000 sec
D11               0.03000000 sec
TD0                      1
SFO1            125.7703643 MHz
NUC1                     13C
P1                   10.00 usec
PLW1             79.88800049 W
SFO2            500.1320005 MHz
NUC2                     1H
CPDPRG[2            waltz16
PCPD2                80.00 usec
PLW2            20.38699913 W
PLW12            0.31854999 W
PLW13            0.16023000 W

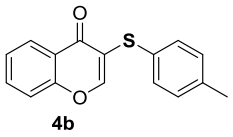
F2 - Processing parameters
SI                       32768
SF              125.7577963 MHz
WDW                         EM
SSB          0
LB                     2.00 Hz
GB           0
PC                     1.40
```


164
SAMPLE CODE:GVK-CBK-3-Phd-50
Acq.Method:FA:3-5MIN
GVK BIO SCIENCES(PVT) LTD
Analytical Research and Development
Date of Analysis:24-Aug-201723:54:53
Instrument ID : ANL-MCL3-LCMS-007
511708C5408A
4: Diode Array
Range: 1.103e+2
Time Height Area Area%
1.92 238779 4159.05 0.20
2.19 109779400 2008098.75 97.42
2.69 2947133 49017.75 2.38
AU
2.19
1.92
2.69
4b
511708C5408A
1: Scan ES+
TIC
3.39e8
Mobile phase-B: 0.1%FA IN H2O ,A: 0.1% FA IN ACN
Column - AQUITY UPLC BEH C18 1.7µm,2.1X50mm
T % of B: 0/97,0.3/97,2.7/2 ,3.50/2,3.51/97
Flow-0.6ml/min,
Temp:35°C
2.21
0.27
0.76
1.95
2.70
2.98
3.14
3.21
Time


GVK Biosciences Pvt Ltd
Analytical Research and Develpment
SAMPLE CODE: GVK-CBK-3-Phd-50
Acq.Method: FA:3.5MIN
Date of Analysis: 24-Aug-201723:54:53
Instrument ID: ANL-MCL3-LCMS-007
511708C5408A 105 (2.697)
1: Scan ES+
1.82e7
405.16
281.10
427.14
428.16
831.35
832.34
833.33
m/z
511708C5408A 86 (2.206)
1: Scan ES+
1.31e8
269.09
270.12
271.11
291.10
559.17
4b

Single Mass Analysis (displaying only valid results)

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None



4b

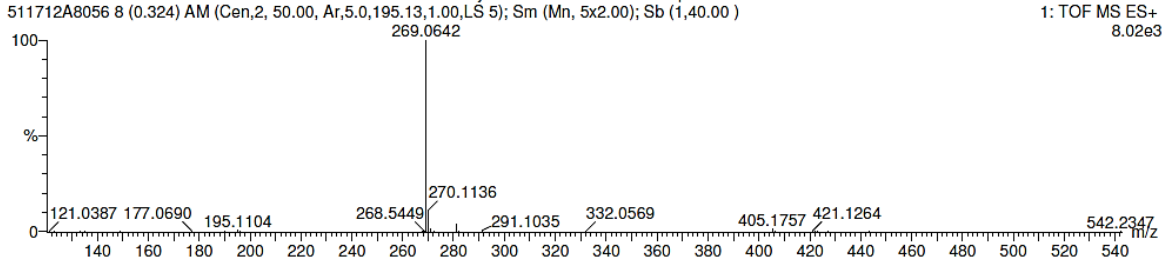
Monoisotopic Mass, Odd and Even Electron Ions
5 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-16 H: 0-13 O: 0-2 S: 0-1

GVK-CBK-Phd-50

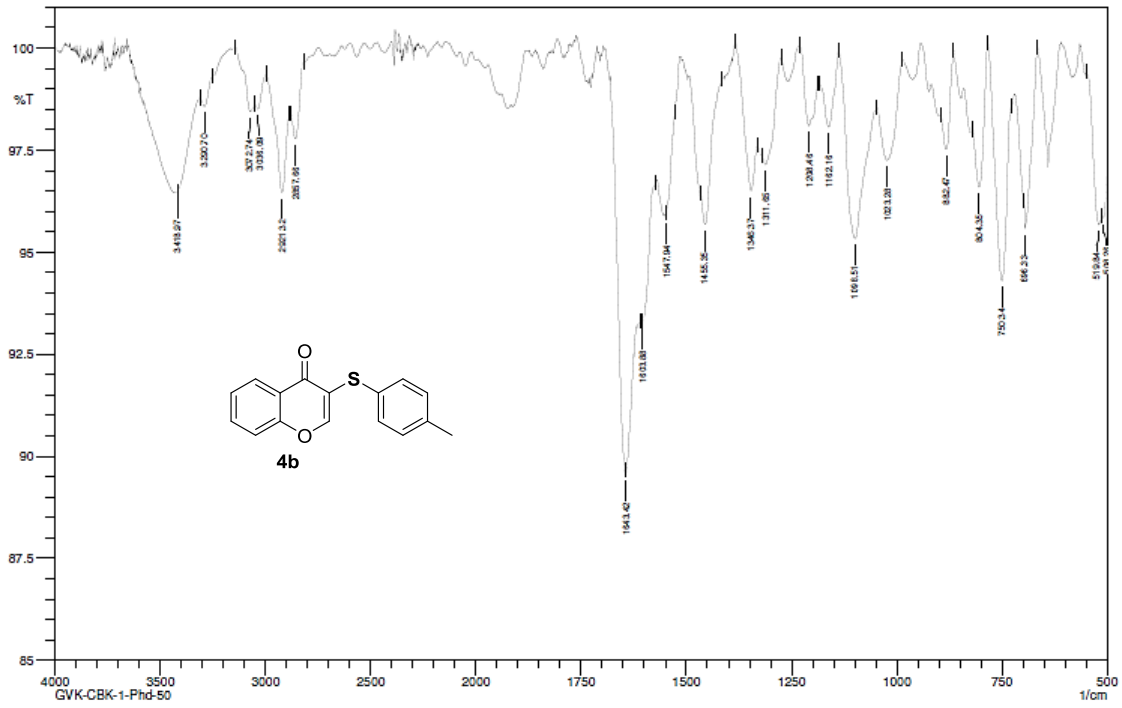
GVK Bio sciences (pvt)Ltd
Analytical Research and Development

Date of analysis:08-Dec-201716:17:50
Instru ment ID:ANL-MCL3-LCMS-001
1: TOF MS ES+
8.02e3

511712A8056 8 (0.324) AM (Cen,2, 50.00, Ar,5.0,195.13,1.00,LS 5); Sm (Mn, 5x2.00); Sb (1,40.00)



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
269.0642	269.0636	0.6	2.2	10.5	845.6	C16 H13 O2 S



4b

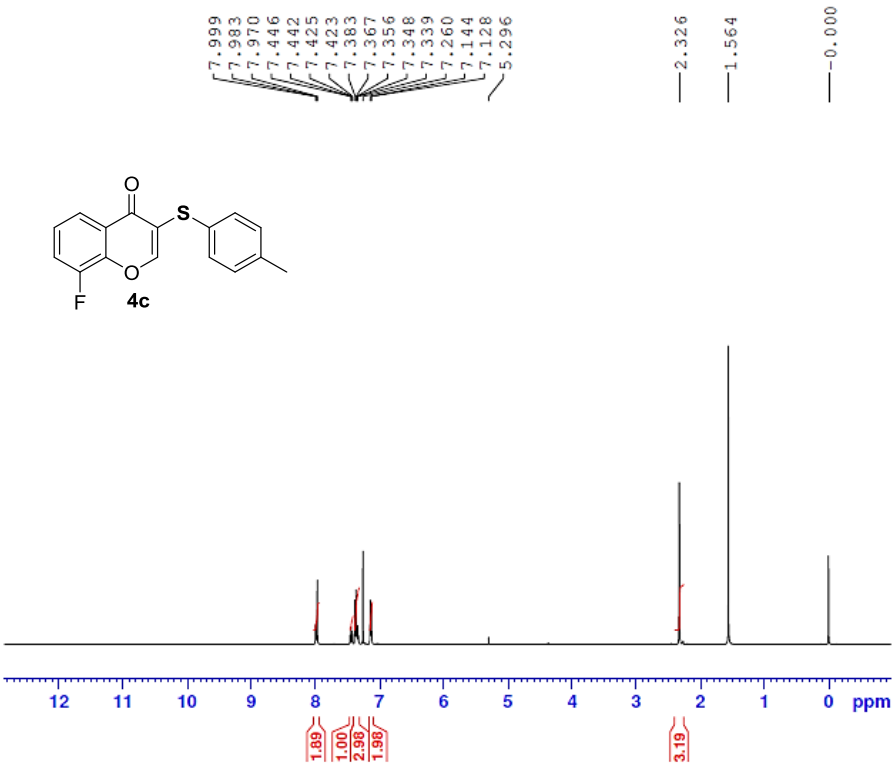
GVK-CBK-1-Phd-50

Comment: IN Kbr
GVK-CBK-1-Phd-50

No. of Scans:
Resolution:
Apodization:

Date: 12/22/2017 10:48:57 AM
User: Admin

GVK-CBK-1-51

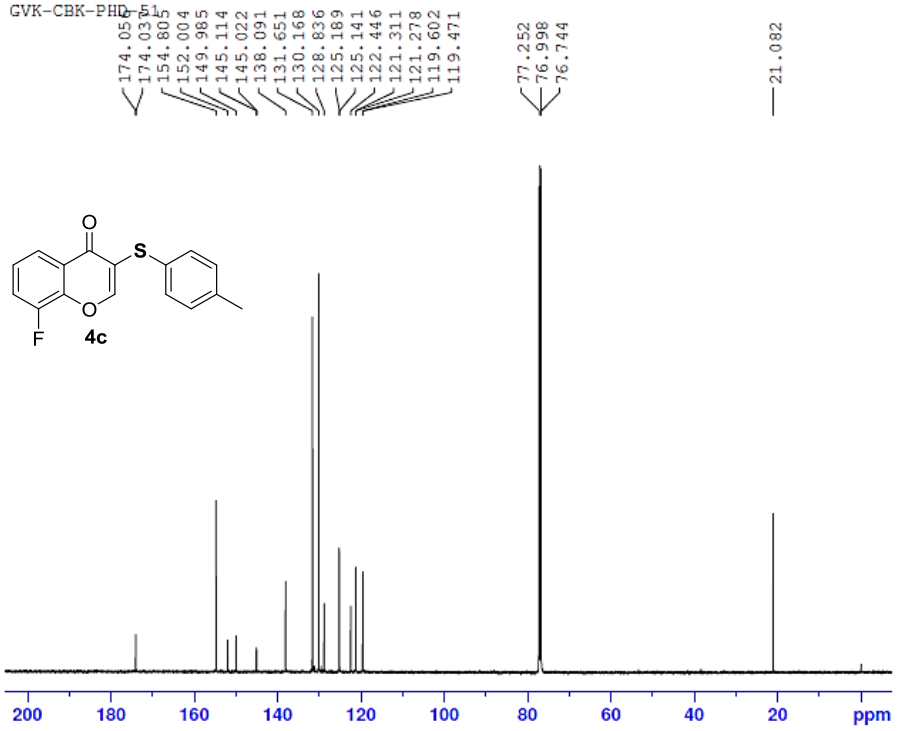



```
Current Data Parameters
NAME          511708c5775
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20170828
Time                8.35 h
INSTRUM             spect
PROBHD    Z119470_0294 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH            10000.000 Hz
FIDRES             0.152588 Hz
AQ              3.2767999 sec
RG                 197.72
DW                 50.000 usec
DE                  6.50 usec
TE                303.1 K
D1             1.00000000 sec
TD0                    1
SFO1           500.1330883 MHz
NUC1                  1H
P1                 10.00 usec
PLW1           20.38699913 W

F2 - Processing parameters
SI                 65536
SF           500.1300116 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

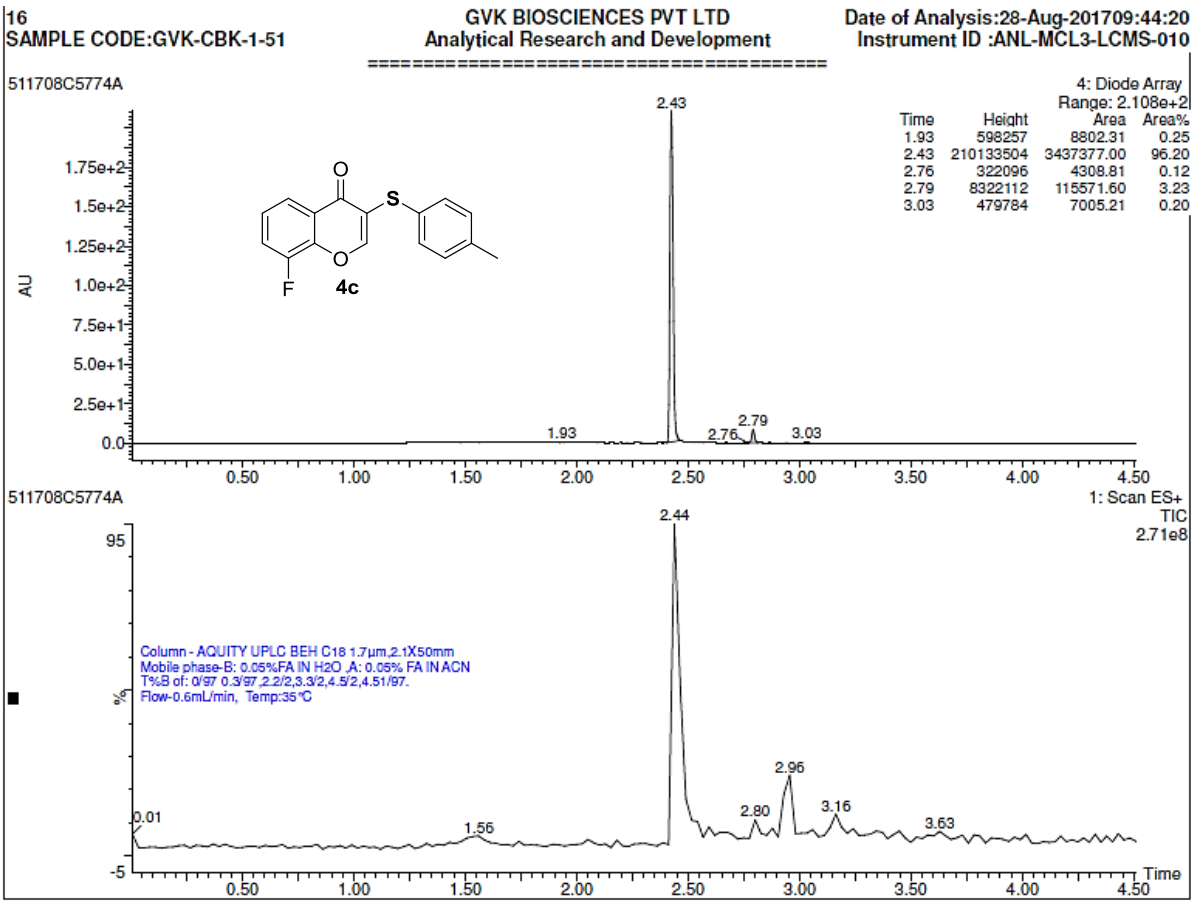
GVK-CBK-PHD-51

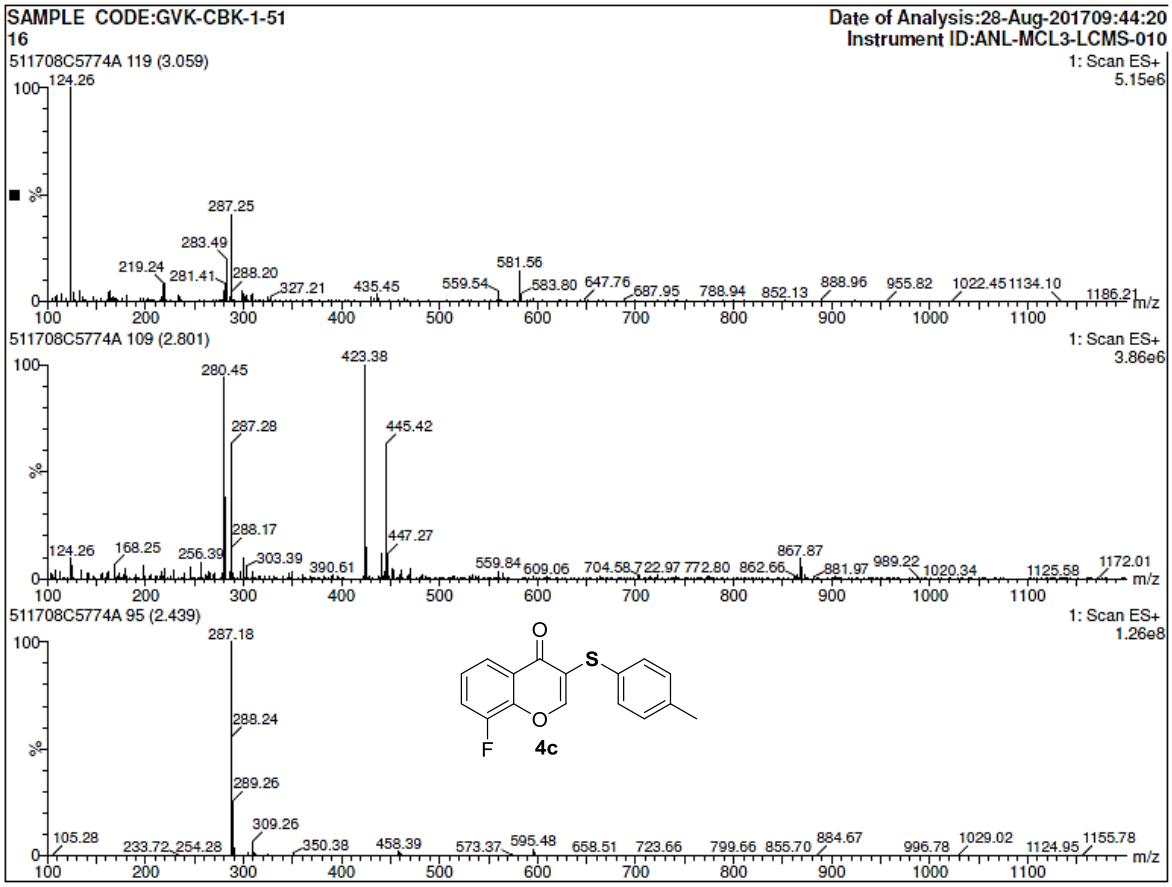



```
Current Data Parameters
NAME          511710c6616
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20171029
Time               14.07 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             3.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1           125.7703643 MHz
NUC1                  13C
P1                 10.00 usec
PLW1           79.88800049 W
SFO2           500.1320005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2           20.38699913 W
PLW12           0.31854999 W
PLW13           0.16023000 W

F2 - Processing parameters
SI                 32768
SF           125.7577954 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.40
```

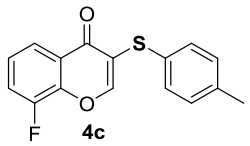

16
SAMPLE CODE:GVK-CBK-1-51
GVK BIOSCIENCES PVT LTD
Analytical Research and Development
Date of Analysis:28-Aug-201709:44:20
Instrument ID :ANL-MCL3-LCMS-010
511708C5774A
4: Diode Array
Range: 2.108e+2
Time Height Area Area%
1.93 598257 8802.31 0.25
2.43 210133504 3437377.00 96.20
2.76 322096 4308.81 0.12
2.79 8322112 115571.60 3.23
3.03 479784 7005.21 0.20
AU
2.43
1.93
2.76
2.79
3.03
4c
511708C5774A
1: Scan ES+
TIC
2.71e8
Column - ACUITY UPLC BEH C18 1.7µm,2.1X50mm
Mobile phase-B: 0.05%FA IN H2O ,A: 0.05% FA IN ACN
T%B of: 0/97 0.3/97 ,2.2/2,3.3/2,4.5/2,4.51/97.
Flow-0.6mL/min, Temp:35°C
2.44
2.96
2.80
3.16
3.63
1.56
0.01
Time


SAMPLE CODE:GVK-CBK-1-51
16
Date of Analysis:28-Aug-201709:44:20
Instrument ID:ANL-MCL3-LCMS-010
511708C5774A 119 (3.059)
1: Scan ES+
5.15e6
124.26
287.25
283.49
219.24
281.41
288.20
327.21
435.45
559.54
581.56
583.80
647.76
687.95
788.94
852.13
888.96
955.82
1022.45
1134.10
1186.21
m/z
511708C5774A 109 (2.801)
1: Scan ES+
3.86e6
423.38
280.45
287.28
445.42
288.17
447.27
124.26
168.25
256.39
303.39
390.61
559.84
609.06
704.58
722.97
772.80
862.66
867.87
881.97
989.22
1020.34
1125.58
1172.01
m/z
511708C5774A 95 (2.439)
1: Scan ES+
1.26e8
287.18
288.24
289.26
309.26
105.28
233.72
254.28
350.38
458.39
573.37
595.48
658.51
723.66
799.66
855.70
884.67
996.78
1029.02
1124.95
1155.78
m/z
4c

Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None



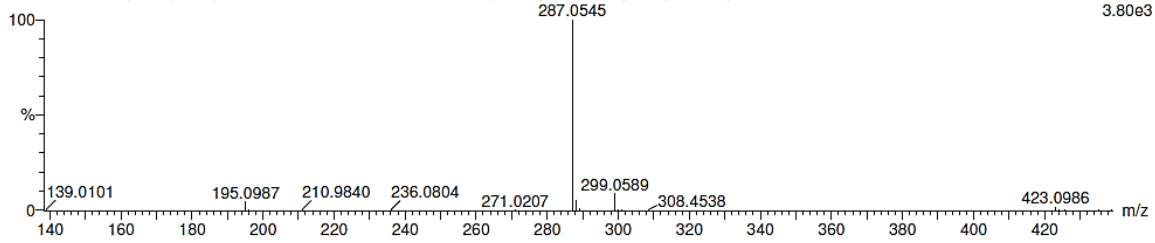
Monoisotopic Mass, Odd and Even Electron Ions
10 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-16 H: 0-12 O: 0-2 F: 0-1 S: 0-1

GVK-CBK-Phd-51

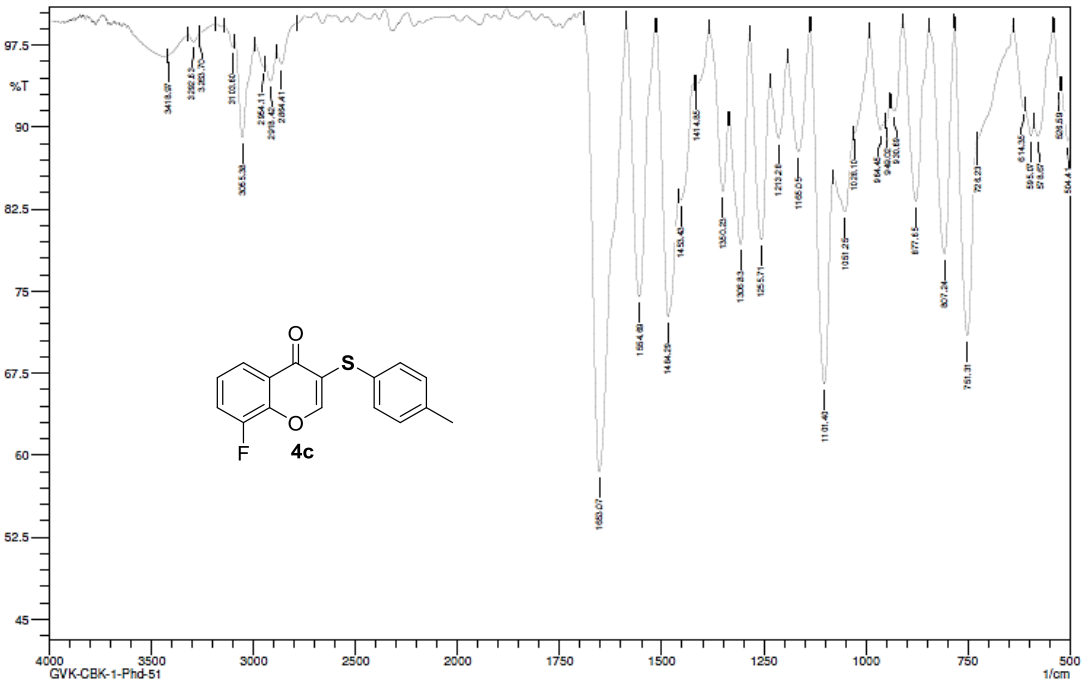
GVK Bio sciences (pvt)Ltd
Analytical Research and Development

Date of analysis:08-Dec-201715:55:45
Instru ment ID:ANL-MCL3-LCMS-001
1: TOF MS ES+
3.80e3

511712A8035 8 (0.330) AM (Cen,2, 80.00, Ar,5.0,195.09,1.00,LS 5); Sm (Mn, 5x2.00); Sb (1,40.00)



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
287.0545	287.0542	0.3	1.0	10.5	748.4	C16 H12 O2 F S



Comment: IN Kbr
GVK-CBK-1-Phd-51

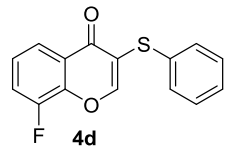
No. of Scans:
Resolution:
Apodization:

Date: 12/22/2017 12:36:58 PM
User: Admin

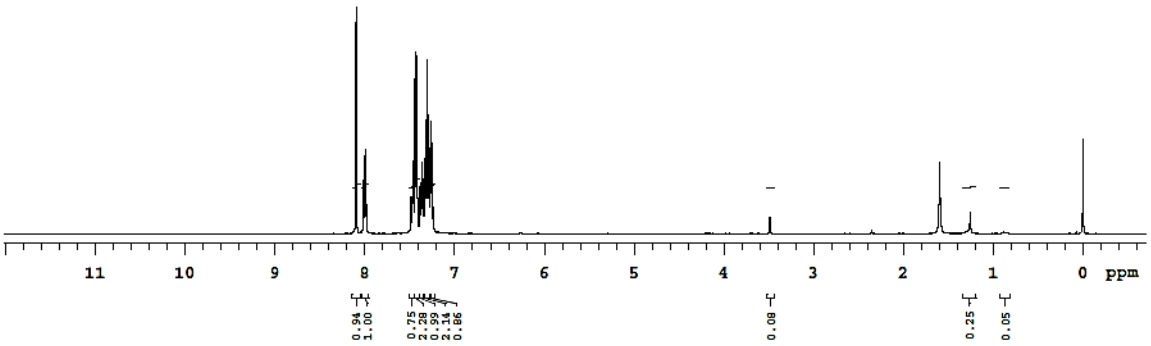
GVK-CBK-1-Phd-73
AR NO-NMR/18/11/2708

38ef5487002

Reference Code: 511811C7994-GVK-CBK-1-Phd-73
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2018/Nov
Agilent 400-MRDD2
Data collected on: Nov 29 2018
Experiment: PROTON



4d

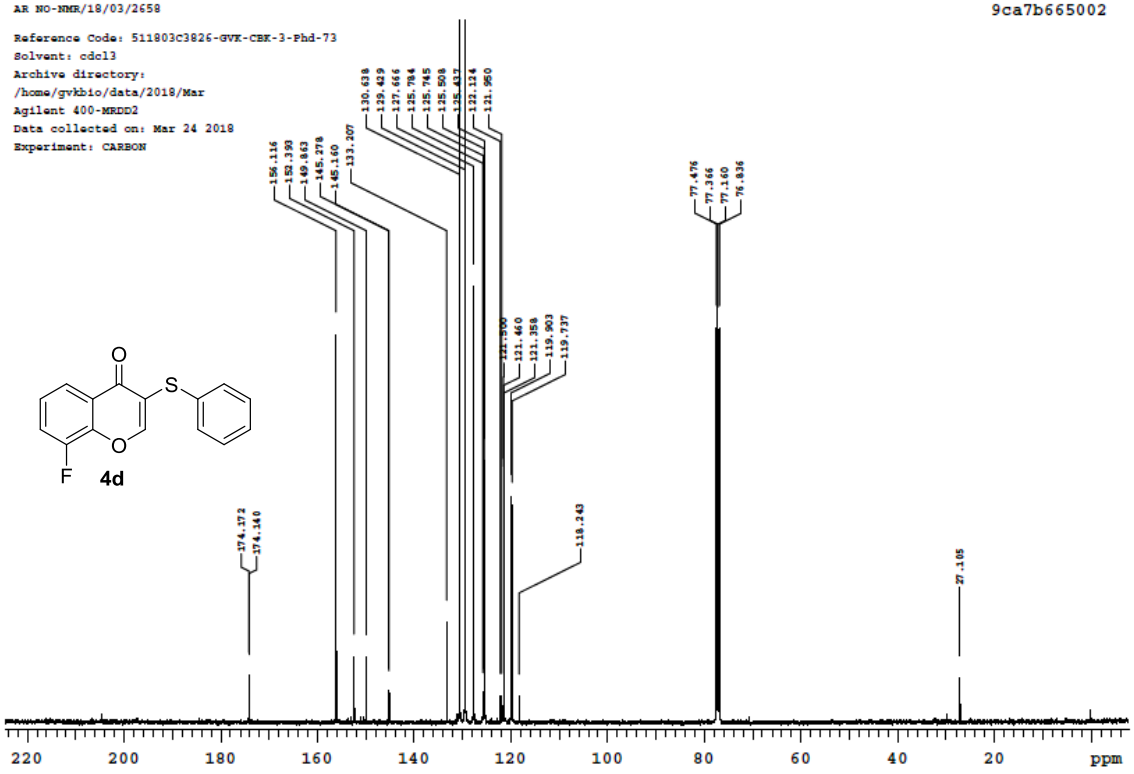


GVK-CBK-3-Phd-73
AR NO-NMR/18/03/2658

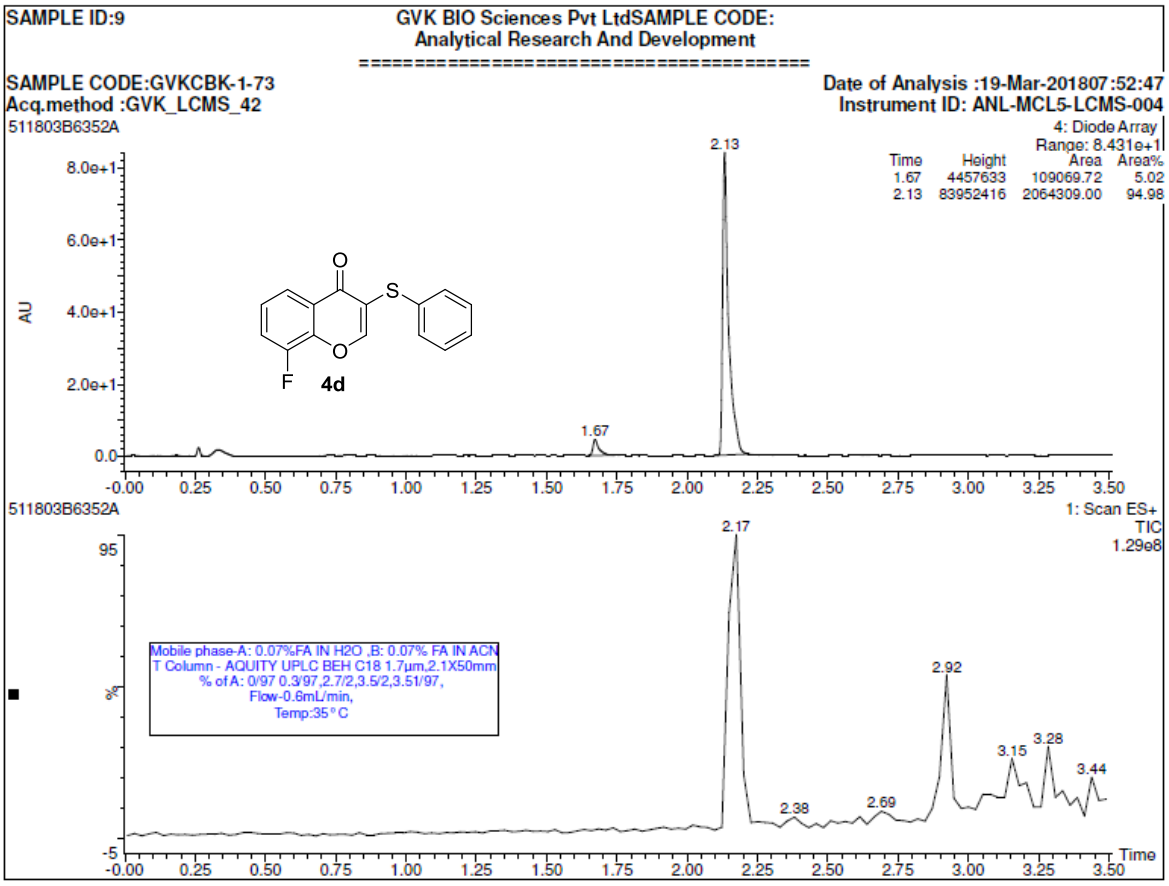
9ca7b665002

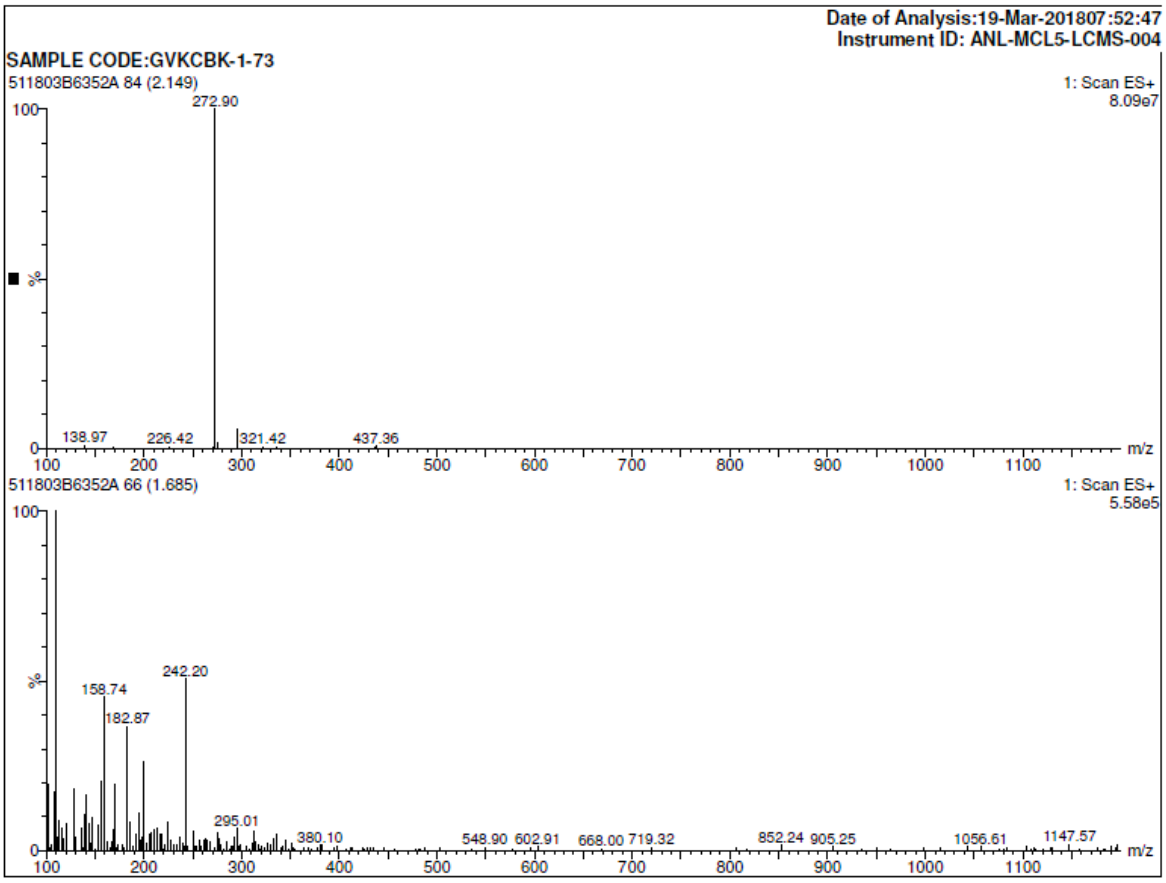
Reference Code: 511803C3826-GVK-CBK-3-Phd-73
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2018/Mar
Agilent 400-MRDD2
Data collected on: Mar 24 2018
Experiment: CARBON

4d

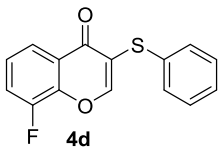


Plotname: 511803C3826-GVK-CBK-3-Phd-73 CARBON 01.REC plot01


SAMPLE ID:9
GVK BIO Sciences Pvt LtdSAMPLE CODE:
Analytical Research And Development
SAMPLE CODE:GVKCBK-1-73
Acq.method :GVK_LCMS_42
Date of Analysis :19-Mar-201807:52:47
Instrument ID: ANL-MCL5-LCMS-004
511803B6352A
4: Diode Array
Range: 8.431e+1
Time Height Area Area%
1.67 4457633 109069.72 5.02
2.13 83952416 2064309.00 94.98
AU
2.13
1.67
4d
511803B6352A
1: Scan ES+
TIC
1.29e8
Mobile phase-A: 0.07%FA IN H2O ,B: 0.07% FA IN ACN
T Column - AQUITY UPLC BEH C18 1.7µm,2.1X50mm
% of A: 0/97 0.3/97,2.7/2,3.5/2,3.51/97,
Flow-0.6mL/min,
Temp:35°C
2.17
2.92
3.15
3.28
3.44
2.38
2.69
%
Time


Date of Analysis:19-Mar-201807:52:47
Instrument ID: ANL-MCL5-LCMS-004
SAMPLE CODE:GVKCBK-1-73
511803B6352A 84 (2.149)
1: Scan ES+
8.09e7
272.90
138.97
226.42
321.42
437.36
m/z
511803B6352A 66 (1.685)
1: Scan ES+
5.58e5
242.20
158.74
182.87
295.01
380.10
548.90 602.91 668.00 719.32
852.24 905.25
1056.61
1147.57
m/z

Elemental Composition Report



Single Mass Analysis (displaying only valid results)

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

10 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

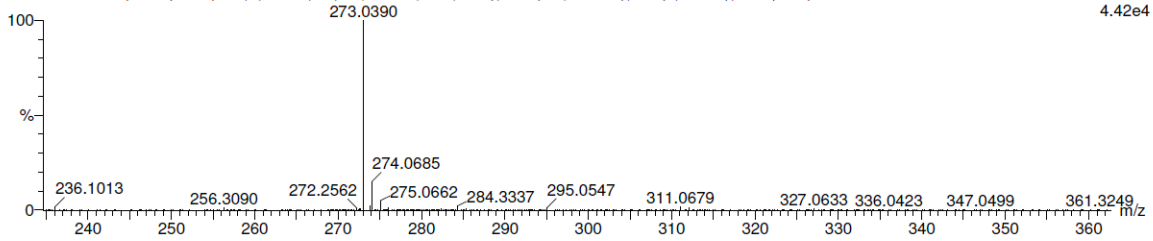
C: 0-15 H: 0-10 O: 0-2 F: 0-1 S: 0-1

GVK-CBK-1-73

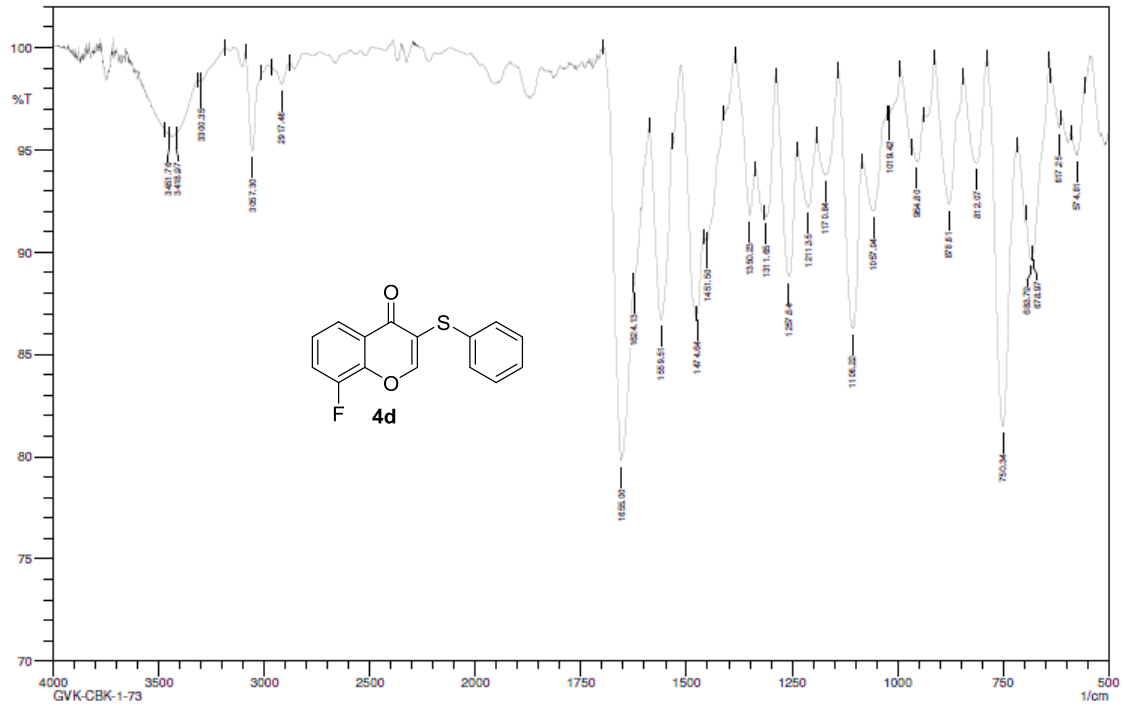
GVK Bio sciences (pvt)Ltd
Analytical Research and Development

Date of analysis:13-Apr-201815:06:28
Instru ment ID:ANL-MCL3-LCMS-001
1: TOF MS ES+
4.42e4

511848B3883 7 (0.285) AM (Cen,2, 50.00, Ar,5.0,195.11,1.00,LS 5); Sm (Mn, 5x2.00); Sb (1,40.00); Cm (5:13)



Minimum:				-1.5		
Maximum:		50.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
273.0390	273.0386	0.4	1.5	10.5	414.9	C15 H10 O2 F S

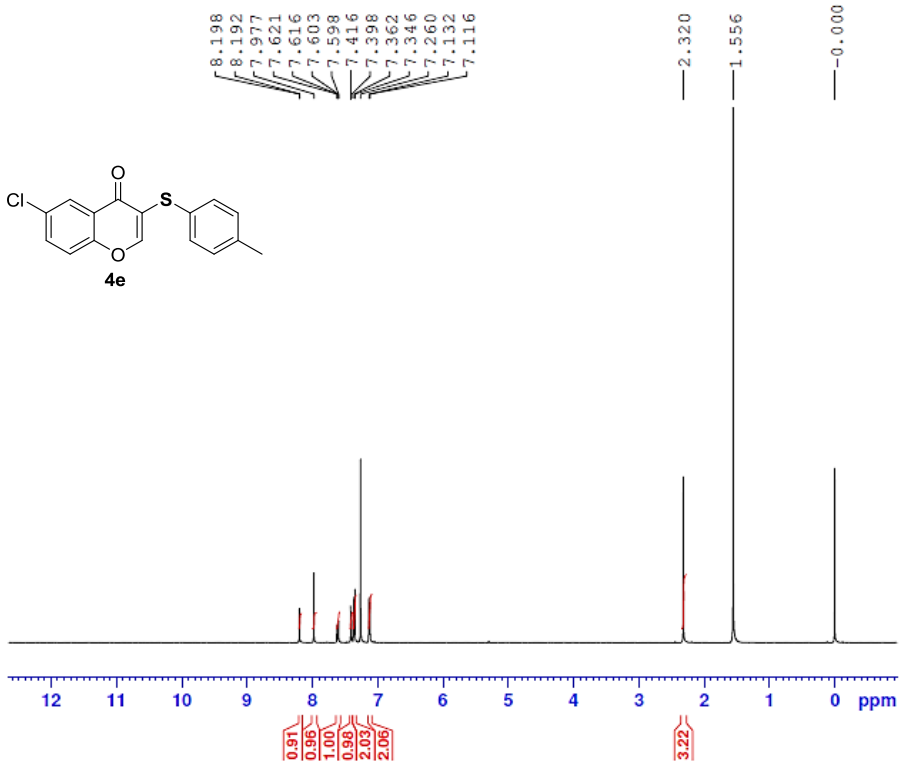


Comment: IN Kbr
GVK-CBK-1-73

No. of Scans:
Resolution:

Date:4/2/2018 1:16:11 PM
User: Admin

GVK-CBK-1-52

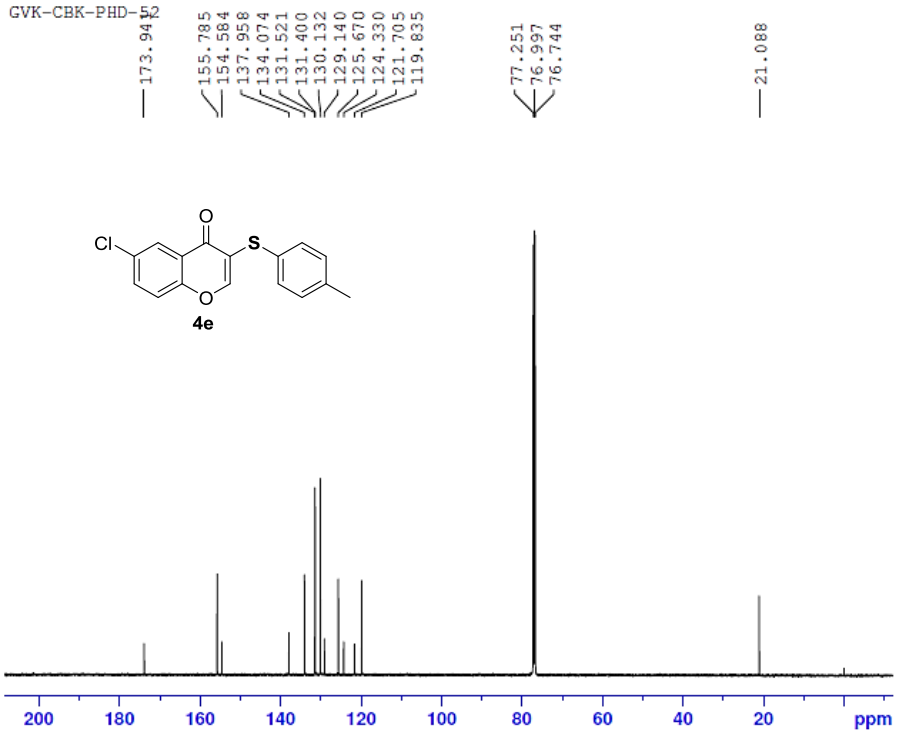



```
Current Data Parameters
NAME          511708C5773
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20170828
Time                8.42 h
INSTRUM             spect
PROBHD    Z119470_0294 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES            0.152588 Hz
AQ             3.2767999 sec
RG                 197.72
DW                50.000 usec
DE                 6.50 usec
TE                 303.1 K
D1             1.00000000 sec
TD0                    1
SFO1          500.1330883 MHz
NUC1                  1H
P1                 10.00 usec
PLW1          20.38699913 W

F2 - Processing parameters
SI                 65536
SF            500.1300116 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  1.00
```

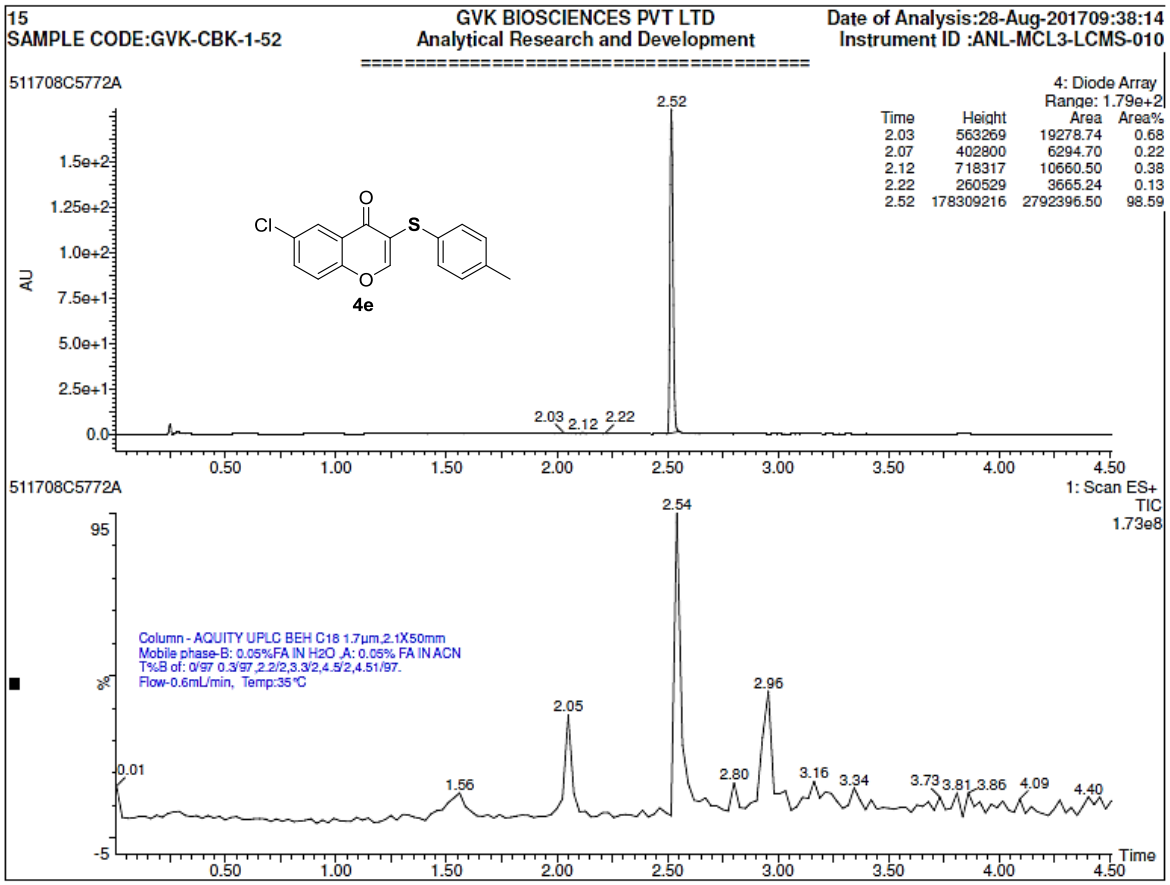
GVK-CBK-PHD-52

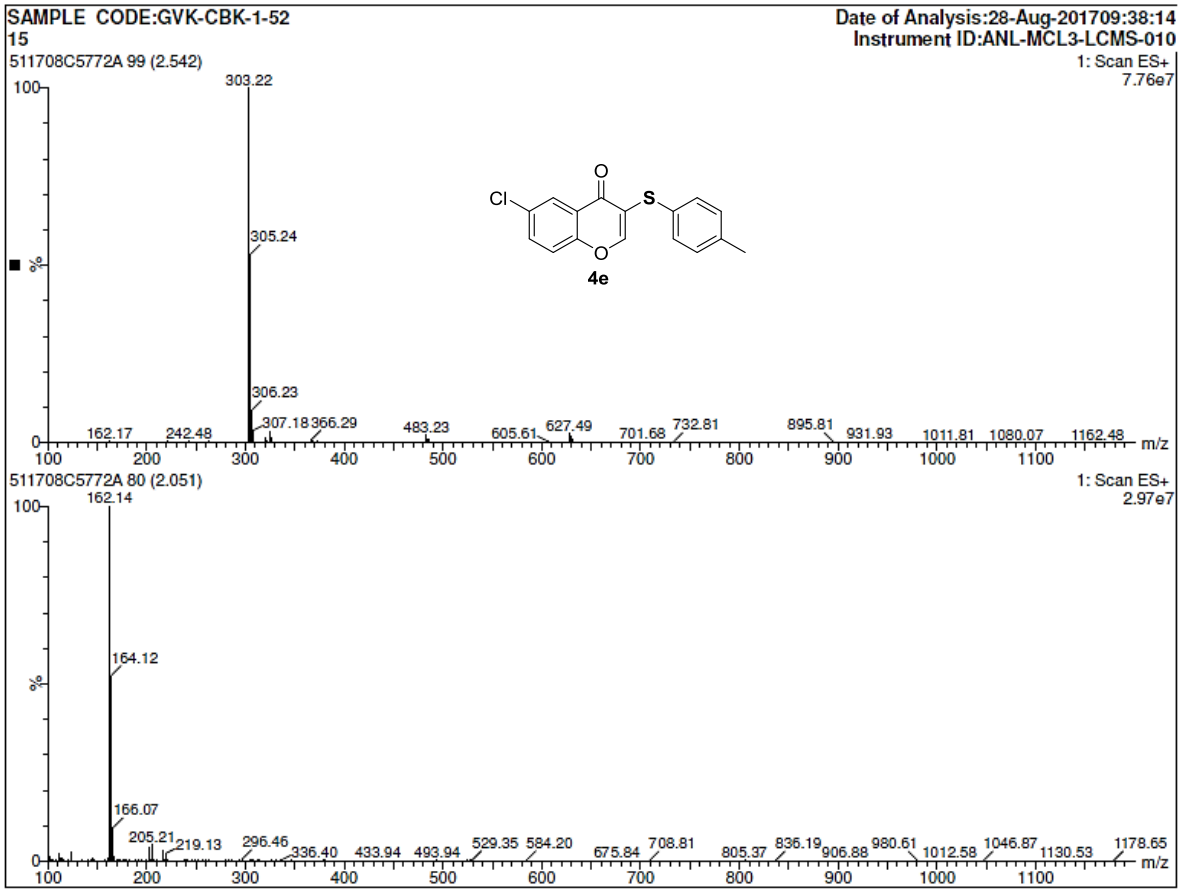



```
Current Data Parameters
NAME          511710C6618
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20171029
Time               16.36 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                 298.1 K
D1             3.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1          125.7703643 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          79.88800049 W
SFO2          500.1320005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2          20.38699913 W
PLW12          0.31854999 W
PLW13          0.16023000 W

F2 - Processing parameters
SI                 32768
SF            125.7577936 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.40
```

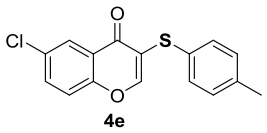

15
SAMPLE CODE:GVK-CBK-1-52
GVK BIOSCIENCES PVT LTD
Analytical Research and Development
Date of Analysis:28-Aug-201709:38:14
Instrument ID :ANL-MCL3-LCMS-010
511708C5772A
4: Diode Array
Range: 1.79e+2
Time Height Area Area%
2.03 563269 19278.74 0.68
2.07 402800 6294.70 0.22
2.12 718317 10660.50 0.38
2.22 260529 3665.24 0.13
2.52 178309216 2792396.50 98.59
AU
2.52
2.03
2.12
2.22
4e
511708C5772A
1: Scan ES+
TIC
1.73e8
Column - AQUITY UPLC BEH C18 1.7µm,2.1X50mm
Mobile phase-B: 0.05%FA IN H2O ,A: 0.05% FA IN ACN
T%B of: 0/97 0.3/97 ,2.2/2,3.3/2,4.5/2,4.51/97.
Flow-0.6mL/min, Temp:35°C
2.54
2.96
2.05
0.01
1.56
2.80
3.16
3.34
3.73
3.81
3.86
4.09
4.40
Time


SAMPLE CODE:GVK-CBK-1-52
15
Date of Analysis:28-Aug-201709:38:14
Instrument ID:ANL-MCL3-LCMS-010
511708C5772A 99 (2.542)
1: Scan ES+
7.76e7
303.22
305.24
306.23
307.18
162.17
242.48
366.29
483.23
605.61
627.49
701.68
732.81
895.81
931.93
1011.81
1080.07
1162.48
m/z
4e
511708C5772A 80 (2.051)
1: Scan ES+
2.97e7
162.14
164.12
166.07
205.21
219.13
296.46
336.40
433.94
493.94
529.35
584.20
675.84
708.81
805.37
836.19
906.88
980.61
1012.58
1046.87
1130.53
1178.65
m/z

Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None



4e

Monoisotopic Mass, Odd and Even Electron Ions
11 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-16 H: 0-12 O: 0-2 S: 0-1 Cl: 0-1

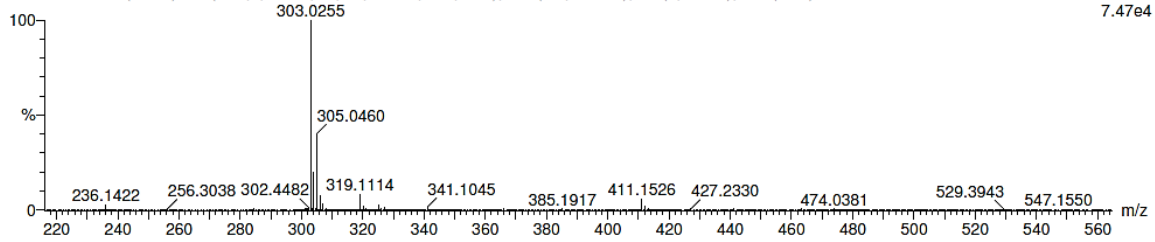
GVK-CBK-1-Phd-52

GVK Bio sciences (pvt)Ltd
Analytical Research and Development

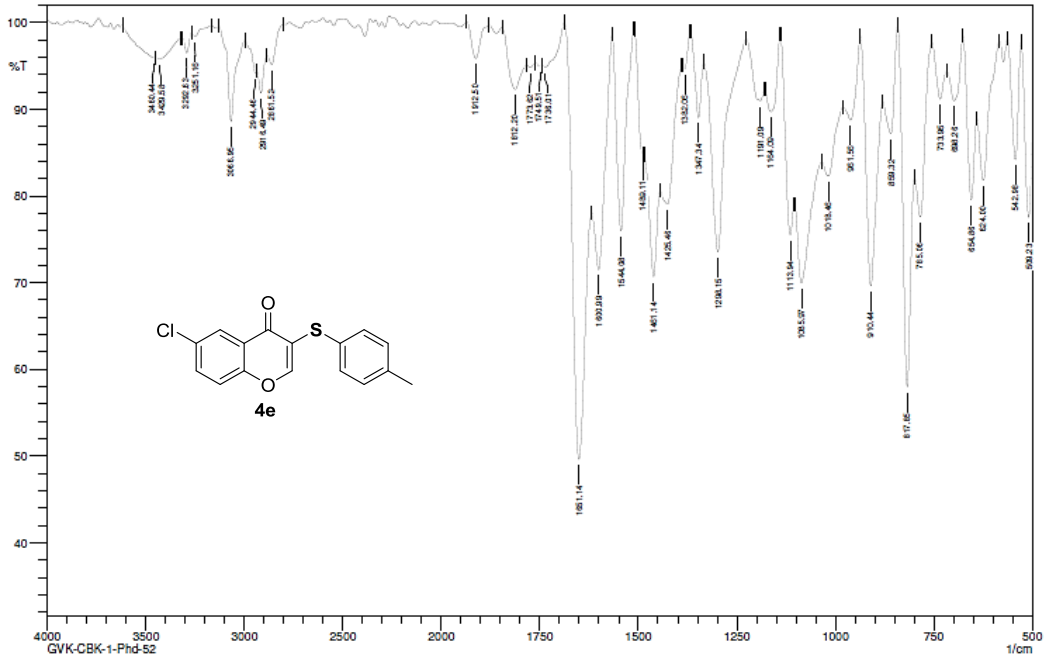
Date of analysis:16-Feb-201815:29:15
Instru ment ID:ANL-MCL3-LCMS-001

511802B3837 8 (0.325) AM (Cen,2, 50.00, Ar,5.0,195.10,1.00,LS 5); Sm (Mn, 5x2.00); Sb (1,40.00); Cm (5:16)

1: TOF MS ES+
7.47e4



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
303.0255	303.0247	0.8	2.6	10.5	917.1	C16 H12 O2 S Cl



4e

Comment: IN Kbr
GVK-CBK-1-Phd-52

No. of Scans:
Resolution:
Apodization:

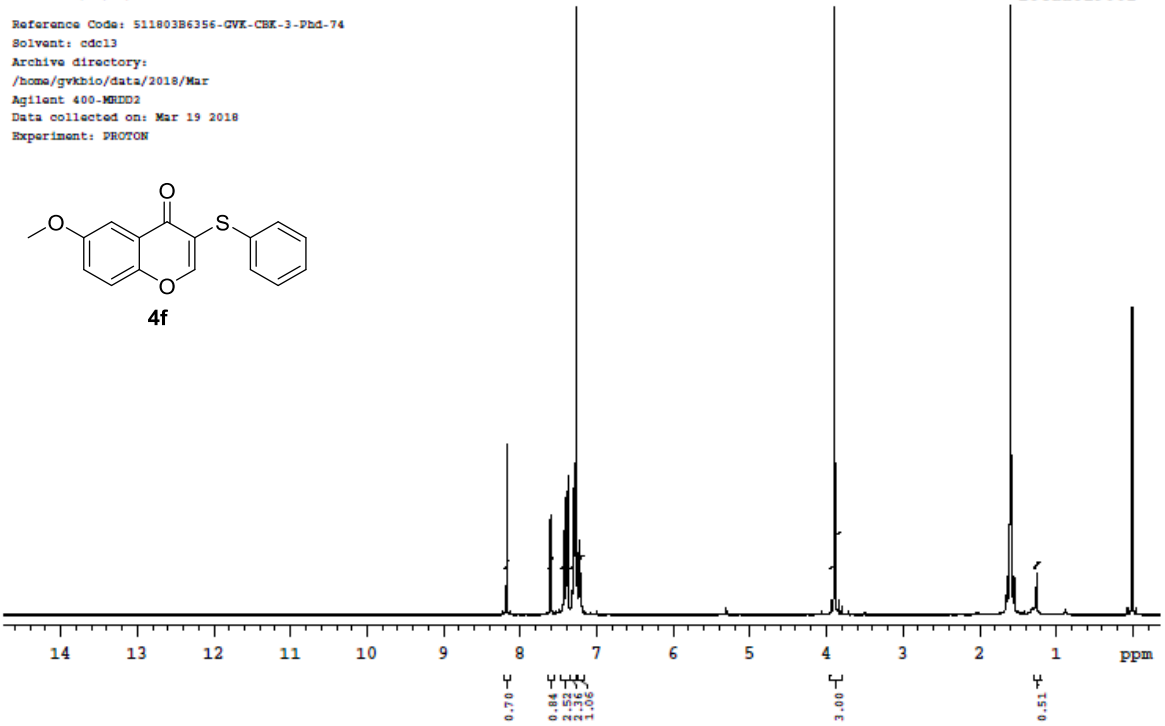
Date: 12/22/2017 11:57:54 AM
User: Admin

GVK-CBK-3-Phd-74
AR NO-NMR/18/03/1879

Reference Code: 511803B6356-GVK-CBK-3-Phd-74
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2018/Mar
Agilent 400-MRDD2
Data collected on: Mar 19 2018
Experiment: PROTON

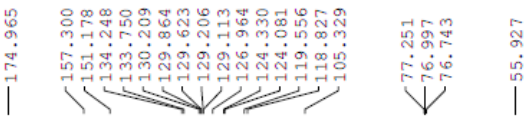
164da619002

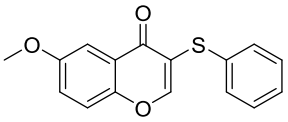
4f



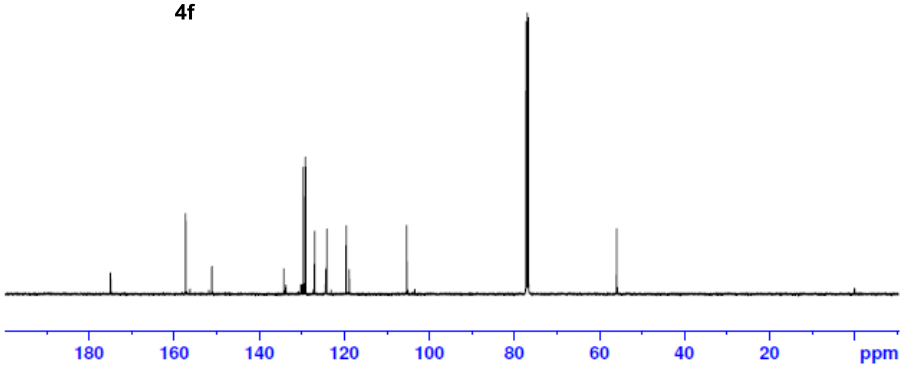
Plotname: 511803B6356-GVK-CBK-3-Phd-74_PROTON_01.REC_plot01

GVK-CBK-3-Phd-74





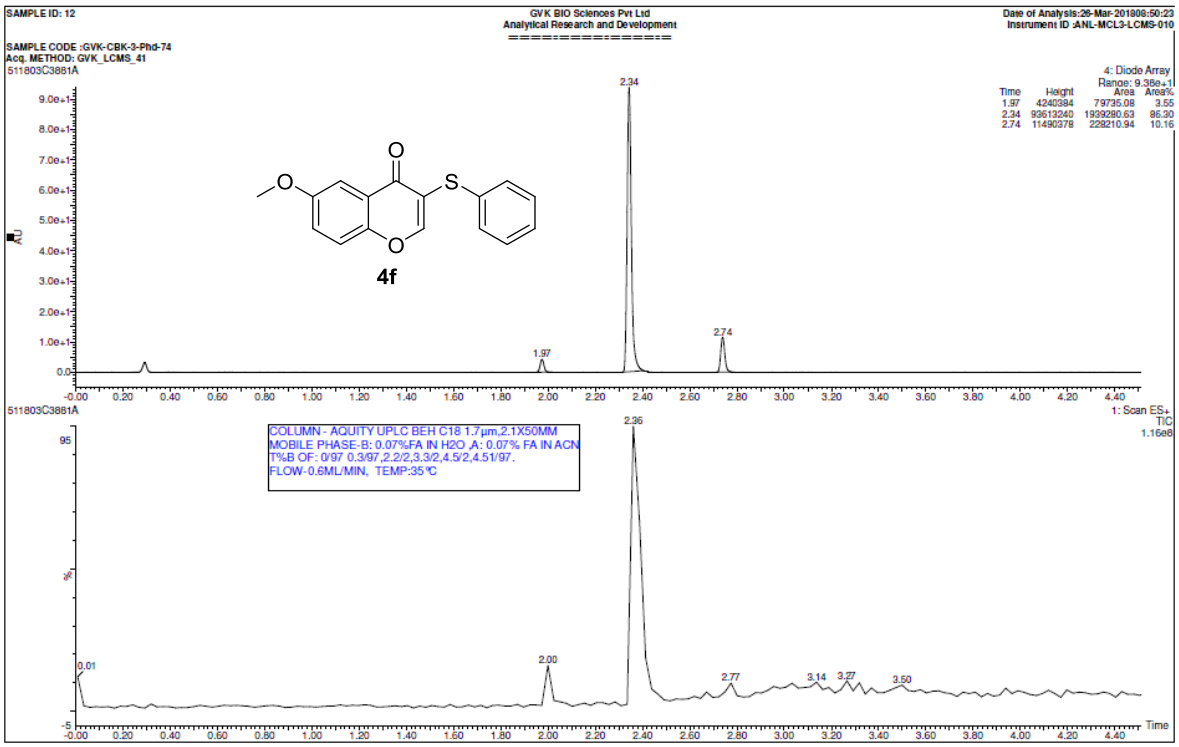
4f

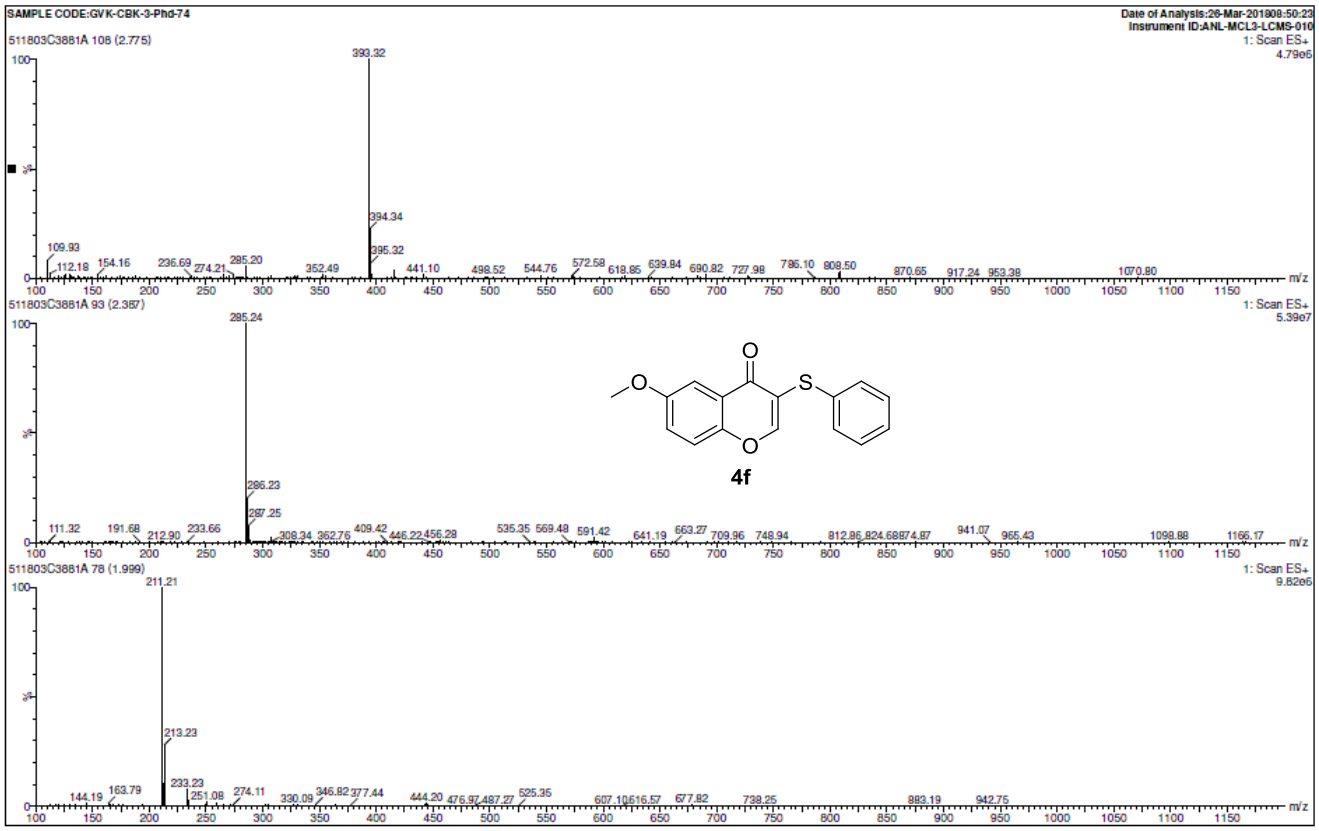


Current Data Parameters
NAME 511803b0374
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20180331
Time 10.27 h
INSTRUM spect
PROBHD Z119470_0294 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 480
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 298.3 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 10.00 usec
PLW1 79.88800049 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 90.00 usec
PLW2 20.38699913 W
PLW12 0.25169000 W
PLW13 0.16023000 W

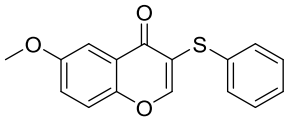
F2 - Processing parameters
SI 32768
SF 125.7577945 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40


SAMPLE ID: 12
GVK BIO Sciences Pvt Ltd
Analytical Research and Development
Date of Analysis:26-Mar-201808:50:23
Instrument ID :ANL-MCL3-LCMS-010
SAMPLE CODE :GVK-CBK-3-Phd-74
Acq. METHOD: GVK_LCMS_41
511803C3881A
4: Diode Array
Range: 9.36e+1
Time Height Area Area%
1.97 4240394 79735.08 3.55
2.34 93613240 1939280.63 86.30
2.74 11490378 228210.94 10.16
2.34
1.97
2.74
4f
511803C3881A
1: Scan ES+
TIC
1.16e8
COLUMN - AQUITY UPLC BEH C18 1.7µm,2.1X50MM
MOBILE PHASE-B: 0.07%FA IN H2O ,A: 0.07% FA IN ACN
T%B OF: 0/97 0.3/97,2.2/2,3.3/2,4.5/2,4.51/97.
FLOW-0.6ML/MIN, TEMP:35°C
2.36
0.01
2.00
2.77
3.14
3.27
3.50
Time


SAMPLE CODE:GVK-CBK-3-Phd-74
Date of Analysis:26-Mar-201808:50:23
Instrument ID:ANL-MCL3-LCMS-010
511803C3881A 108 (2.775)
1: Scan ES+
4.79e6
393.32
394.34
395.32
511803C3881A 93 (2.387)
1: Scan ES+
5.39e7
285.24
286.23
287.25
4f
511803C3881A 78 (1.999)
1: Scan ES+
9.82e6
211.21
213.23
233.23
m/z

Single Mass Analysis (displaying only valid results)

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None



4f

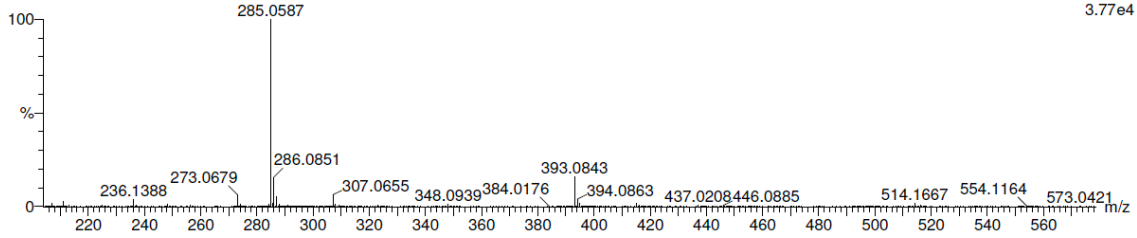
Monoisotopic Mass, Odd and Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-16 H: 0-13 O: 0-3 S: 0-1

GVK-CBK-1-74

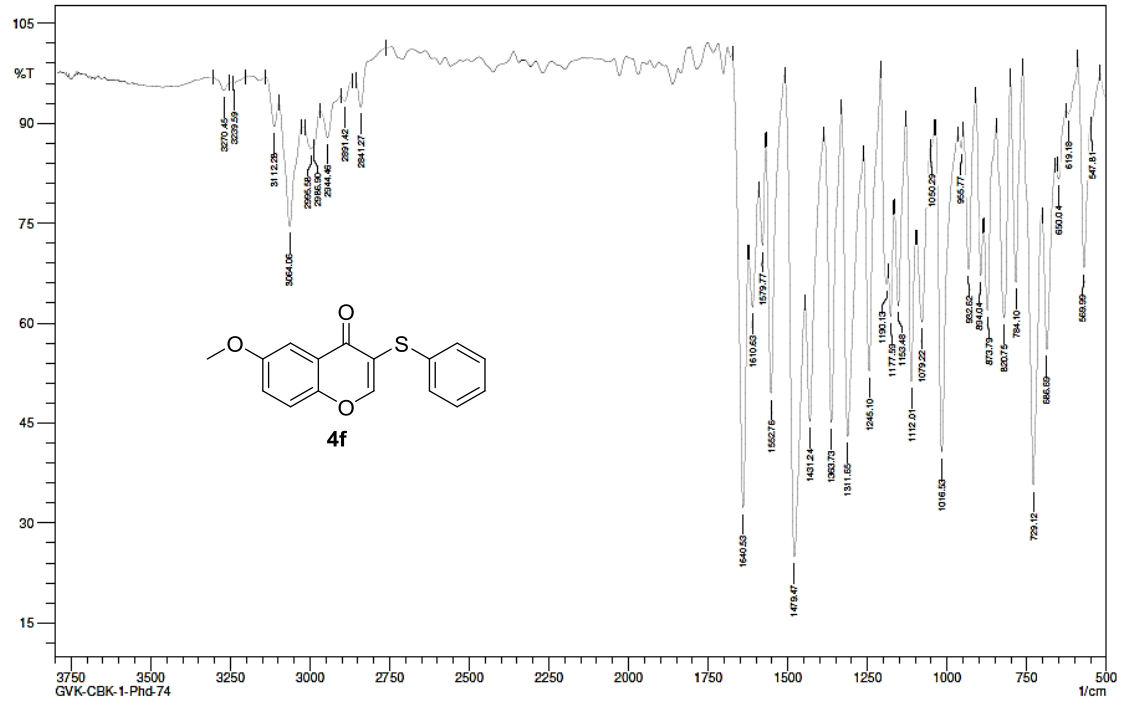
GVK Bio sciences (pvt)Ltd
Analytical Research and Development

Date of analysis:11-Apr-201816:04:11
Instru ment ID:ANL-MCL3-LCMS-001
1: TOF MS ES+
3.77e4

511843B3886 7 (0.281) AM (Cen,2, 50.00, Ar,5.0,195.11,1.00,LS 5); Sm (Mn, 5x2.00); Sb (1,40.00); Cm (4:13)



Minimum:				-1.5		
Maximum:		50.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
285.0587	285.0585	0.2	0.7	10.5	319.5	C16 H13 O3 S

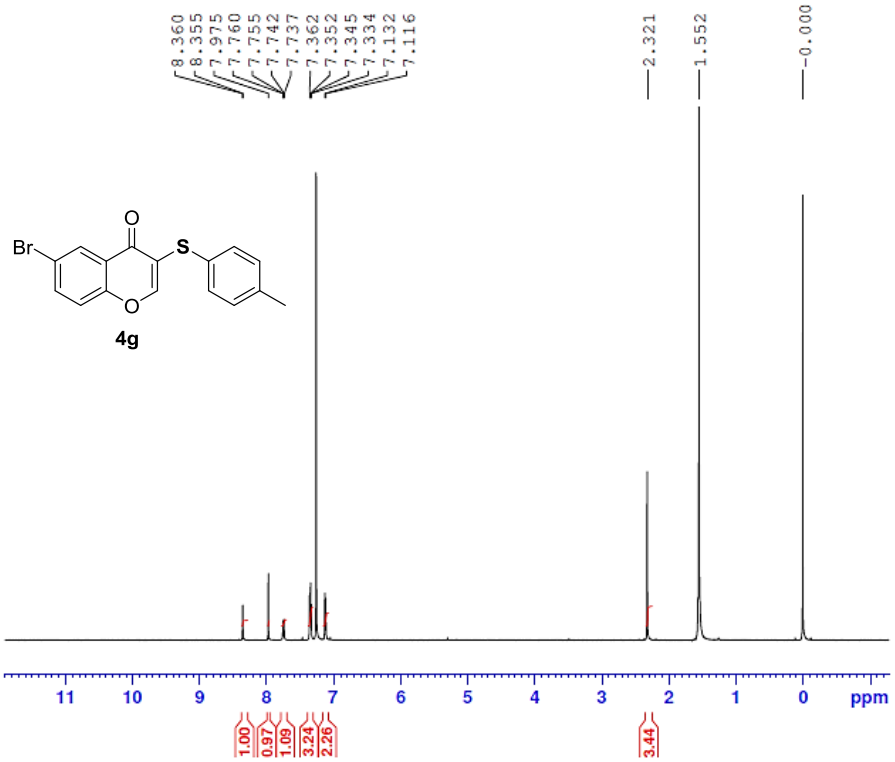


Comment: **IN Kbr**
GVK-CBK-1-Phd-74

No. of Scans;
Resolution;

Date: 11/30/2018 4:38:06 PM
User; Admin

GVK-CBK-1-53

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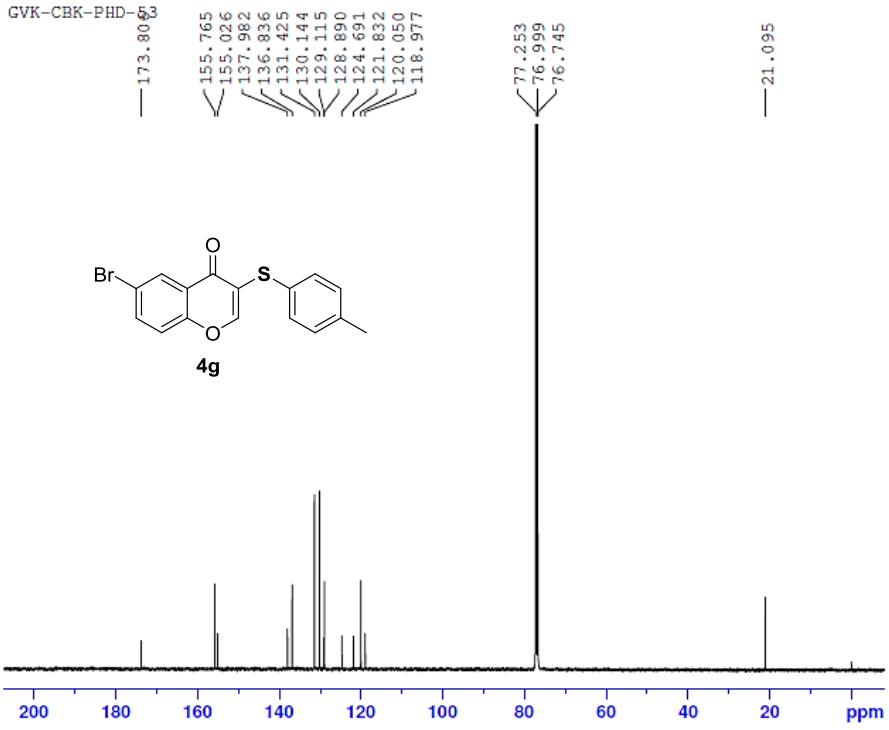
Current Data Parameters
NAME          511708c5771
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20170828
Time                8.31 h
INSTRUM            spect
PROBHD    Z119470_0294 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           10000.000 Hz
FIDRES            0.152588 Hz
AQ             3.2767999 sec
RG                 197.72
DW                 50.000 usec
DE                  6.50 usec
TE                303.1 K
D1             1.00000000 sec
TD0                    1
SFO1          500.1330883 MHz
NUC1                  1H
P1                 10.00 usec
PLW1          20.38699913 W

F2 - Processing parameters
SI                 65536
SF            500.1300115 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

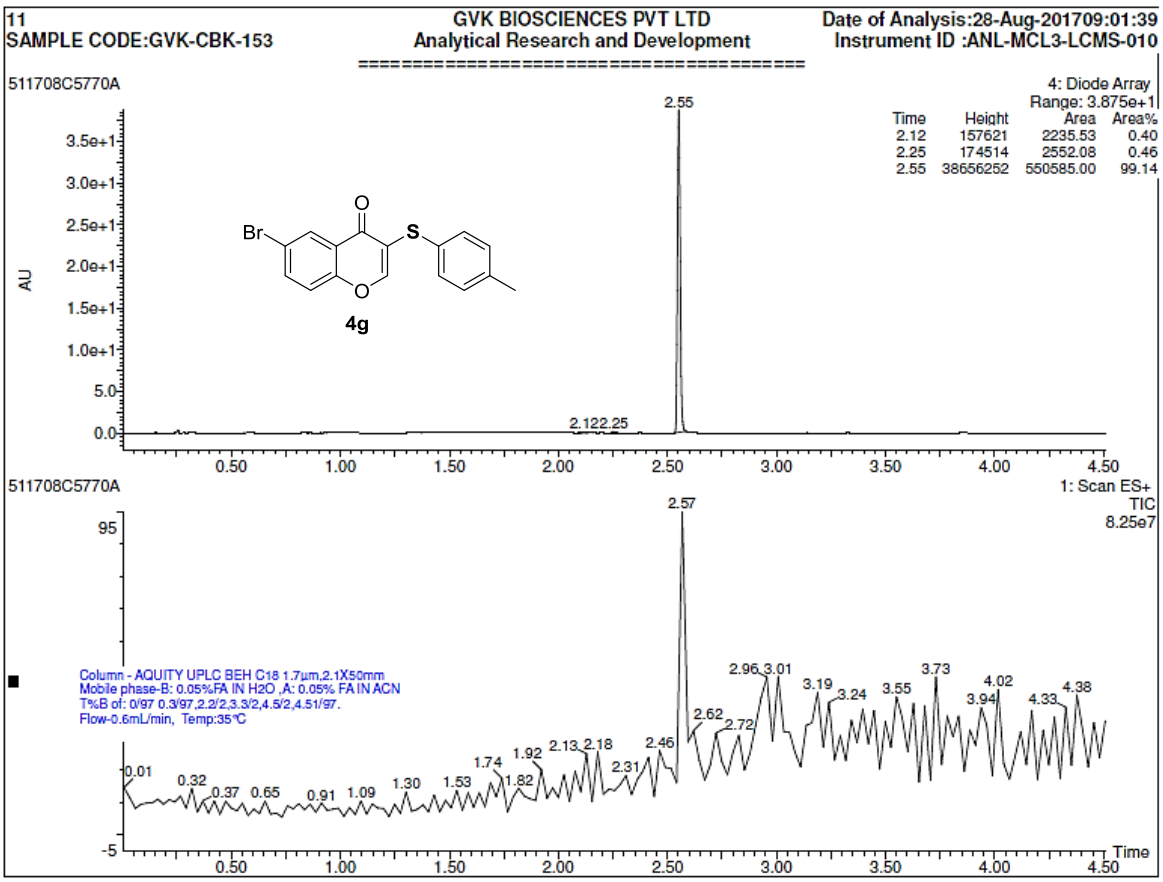
GVK-CBK-PHD-53

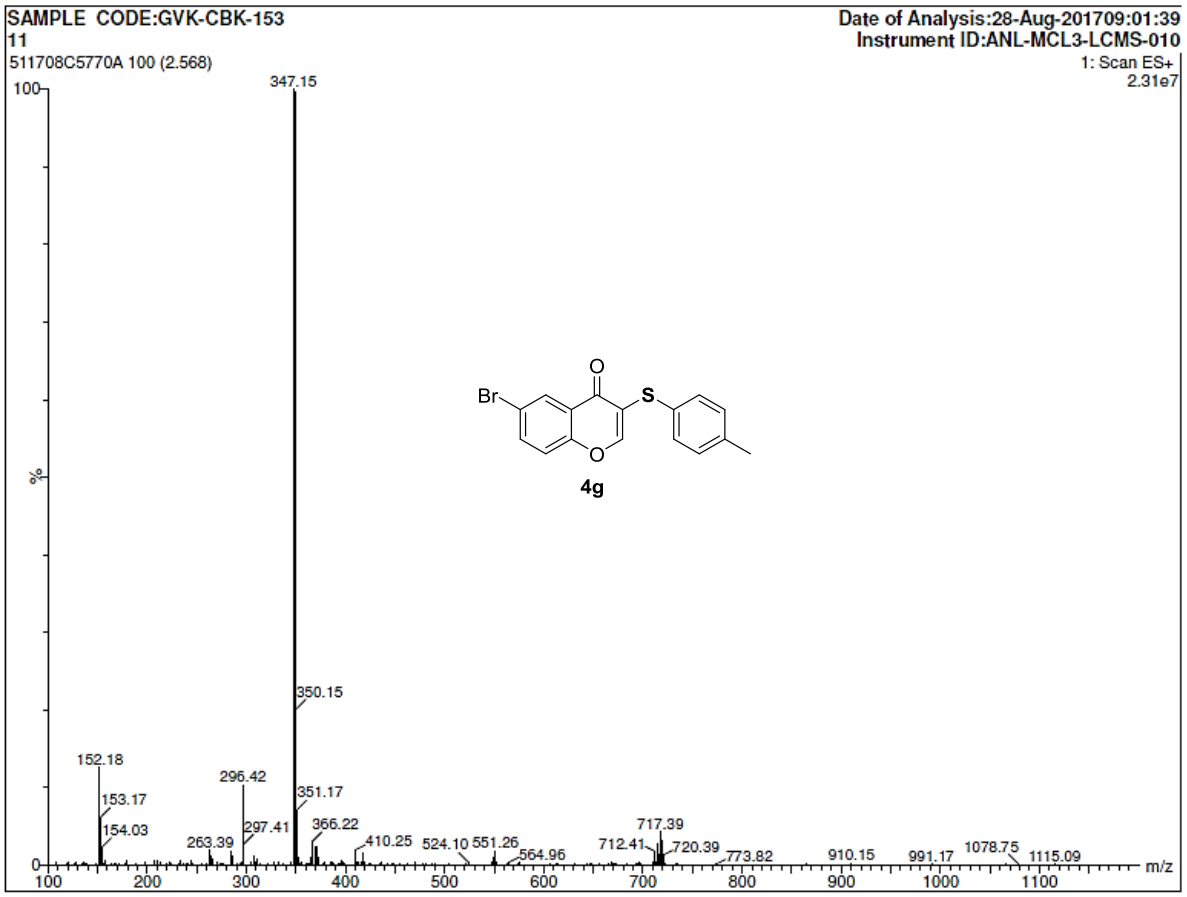



```
Current Data Parameters
NAME          511710c6619
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20171029
Time               17.52 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             3.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1          125.7703643 MHz
NUC1                  13C
P1                 10.00 usec
PLW1          79.88800049 W
SFO2          500.1320005 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2          20.38699913 W
PLW12          0.31854999 W
PLW13          0.16023000 W

F2 - Processing parameters
SI                 32768
SF            125.7577927 MHz
WDW                   EM
SSB       0
LB                 2.00 Hz
GB        0
PC                 1.40
```

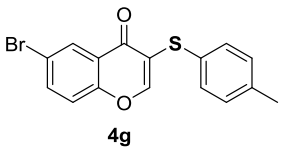

11
SAMPLE CODE:GVK-CBK-153
GVK BIOSCIENCES PVT LTD
Analytical Research and Development
Date of Analysis:28-Aug-201709:01:39
Instrument ID :ANL-MCL3-LCMS-010
511708C5770A
4: Diode Array
Range: 3.875e+1
Time Height Area Area%
2.12 157621 2235.53 0.40
2.25 174514 2552.08 0.46
2.55 38656252 550585.00 99.14
AU
2.55
2.122.25
4g
511708C5770A
1: Scan ES+
TIC
8.25e7
Column - AQUITY UPLC BEH C18 1.7µm,2.1X50mm
Mobile phase-B: 0.05%FA IN H2O ,A: 0.05% FA IN ACN
T%B of: 0/97 0.3/97,2.2/2,3.3/2,4.5/2,4.51/97.
Flow-0.6mL/min, Temp:35°C
2.57
Time


SAMPLE CODE:GVK-CBK-153
11
Date of Analysis:28-Aug-201709:01:39
Instrument ID:ANL-MCL3-LCMS-010
511708C5770A 100 (2.568)
1: Scan ES+
2.31e7
%
347.15
350.15
4g
m/z

Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

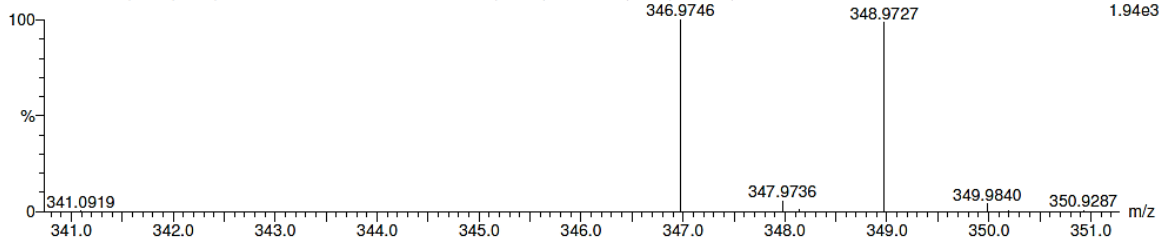


4g

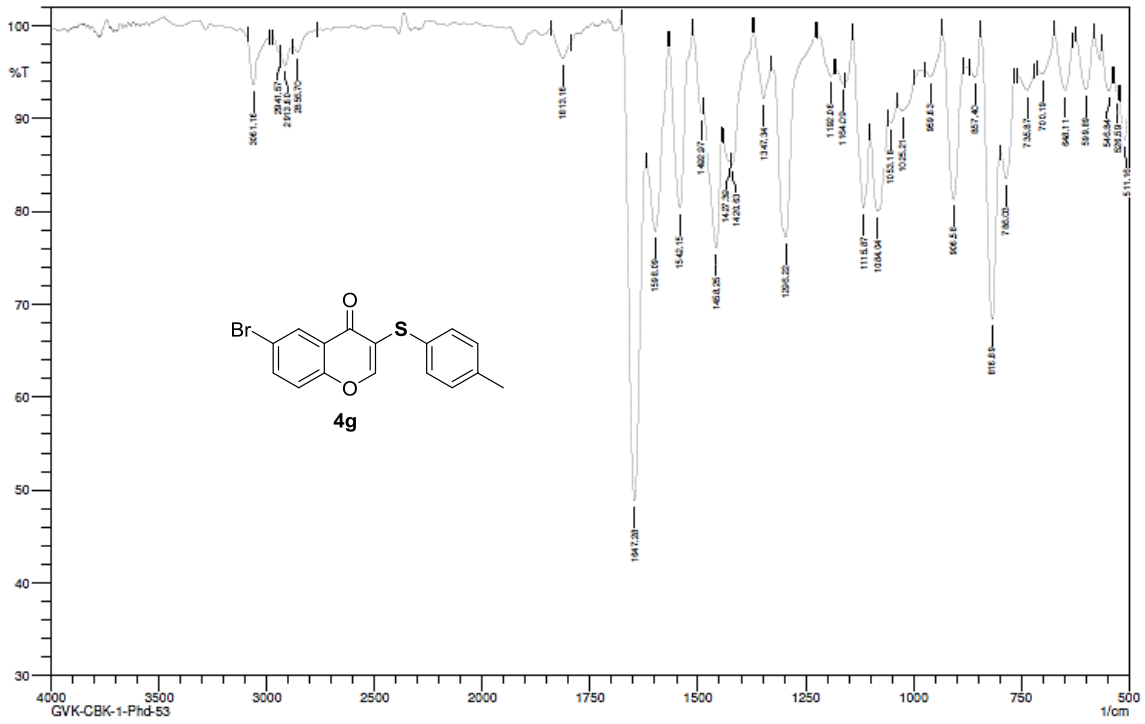
Monoisotopic Mass, Odd and Even Electron Ions
11 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-16 H: 0-12 O: 0-2 S: 0-1 Br: 0-1

GVK-CBK-Phd-53 | GVK Bio sciences (pvt)Ltd, Analytical Research and Development | Date of analysis:08-Dec-201716:08:27

511712A8065 8 (0.323) AM (Cen,2, 80.00, Ar,5.0,195.09,1.00,LS 5); Sm (Mn, 5x2.00); Sb (1,40.00) | Instru ment ID:ANL-MCL3-LCMS-001 | 1: TOF MS ES+ | 1.94e3



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
346.9746	346.9741	0.5	1.4	10.5	239.1	C16 H12 O2 S Br



4g

Comment: IN Kbr
GVK-CBK-1-Phd-53

No. of Scans:
Resolution:
Apodization:

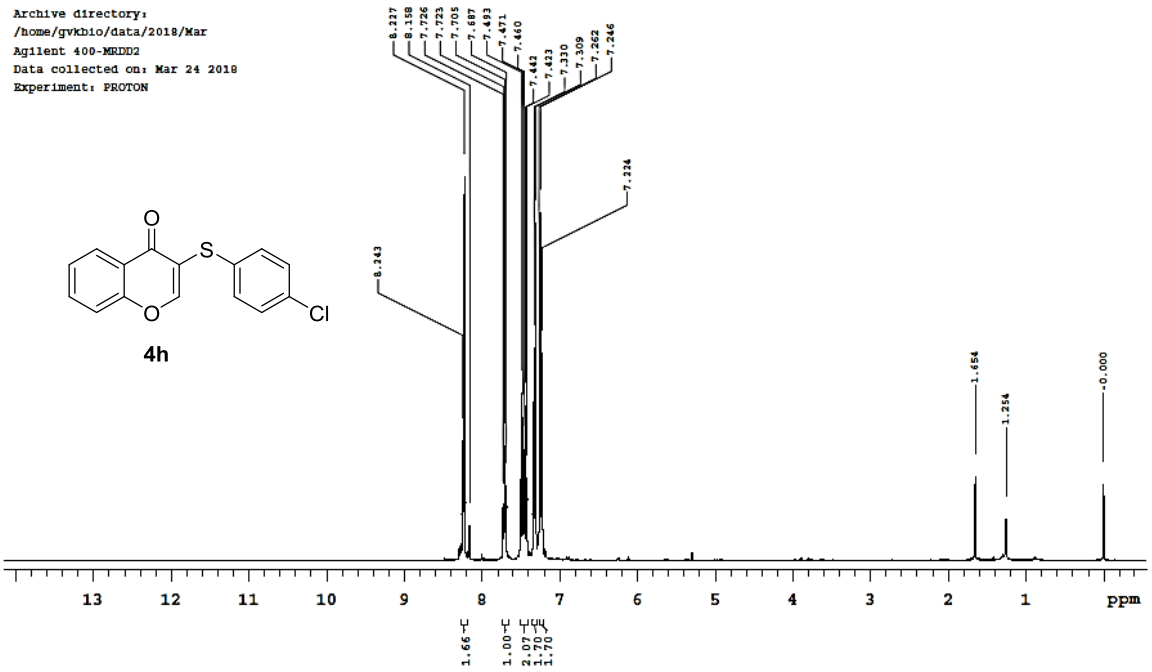
Date: 12/22/2017 12:31:22 PM
User: Admin

GVK-CBK-3-Phd-75
AR NO-NMR/18/03/2656

6a17bc29002

Reference Code: 511803C3827-GVK-CBK-3-Phd-75
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2018/Mar
Agilent 400-MRDD2
Data collected on: Mar 24 2018
Experiment: PROTON

4h

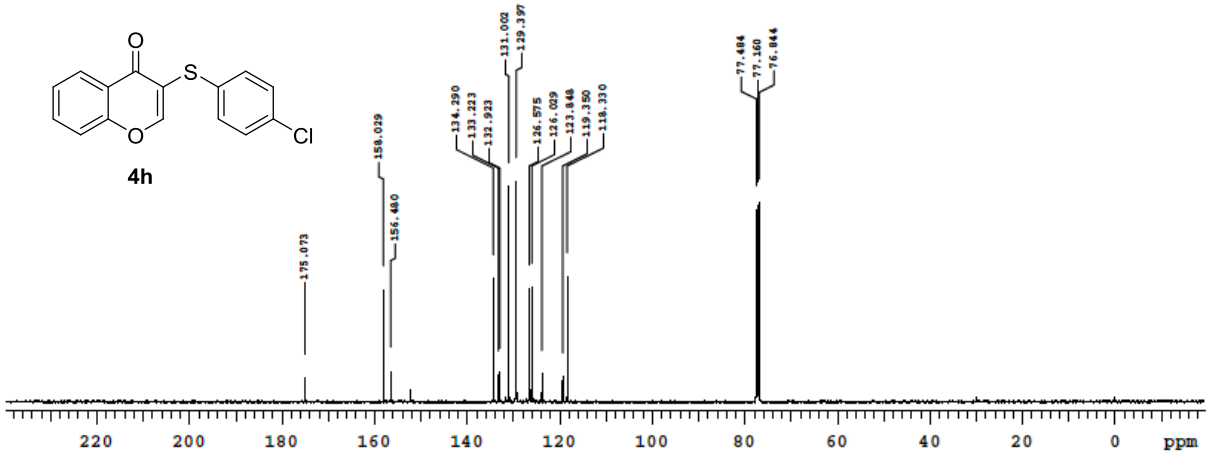


GVK-CBK-3-Phd-75
AR NO-NMR/18/03/2656

fdb063e3002

Reference Code: 511803C3827-GVK-CBK-3-Phd-75
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2018/Mar
Agilent 400-MRDD2
Data collected on: Mar 24 2018
Experiment: CARBON

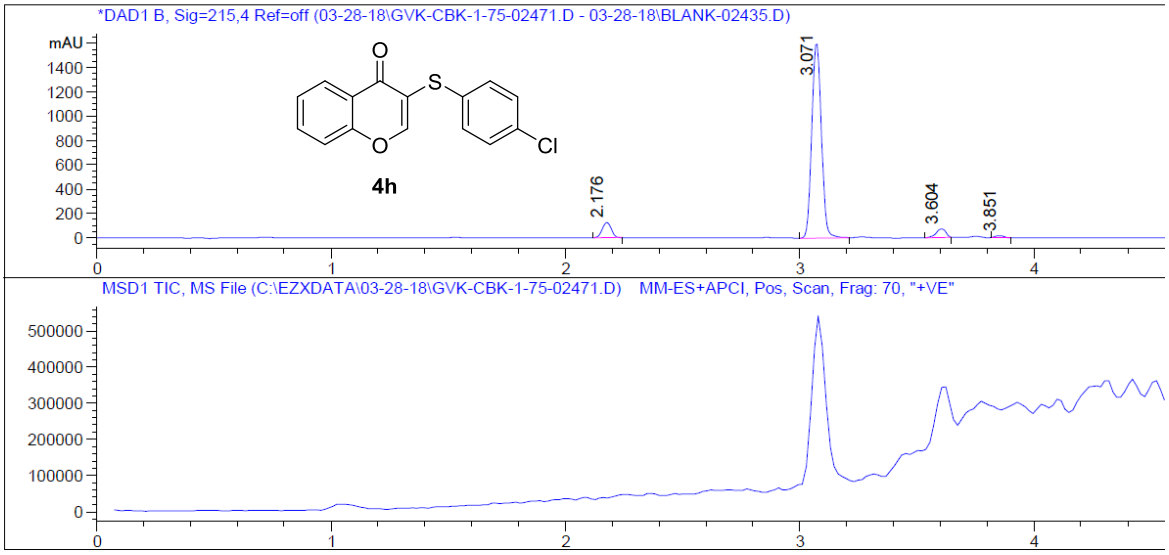
4h



Plotname: 511803C3827-GVK-CBK-3-Phd-75_CARBON_01.REC_plot01

```
================================================================================
Data file       : C:\EZXDATA\03-28-18\GVK-CBK-1--> Vial position:  Vial 56
                                                   Instrument Name:ANL-MCL2-LCMS-002
Injection Date  : 28-Mar-2018    03:32:00 PM       Injection Vol:             4.000
Sample Name     :   GVK-CBK-1-75
================================================================================
  Acq. Method Conditions: RND X-Bridge 5.0 Min
  COLUMN : X-BRIDGE C18 (4.6mm x 75mm) 3.5 µm
  MOBILE PHASE A: 10mM Ammonium Acetate in water, B 100% ACN
  Gradient : % of B 0.0/10,0.2/10,2.5/75,3.0/100,4.8/100,5.0/10
  Column Temp : 35° C
  Flow rate : 2.0 ml/min

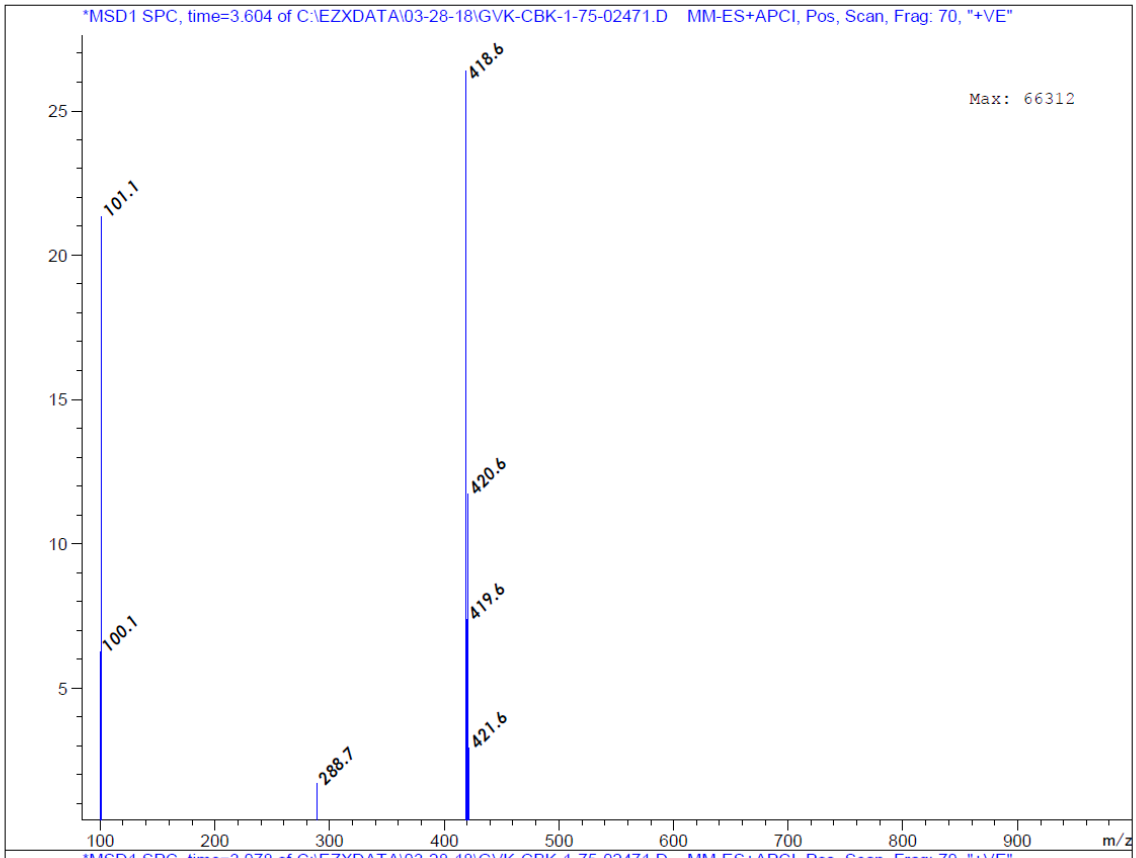
================================================================================->
```

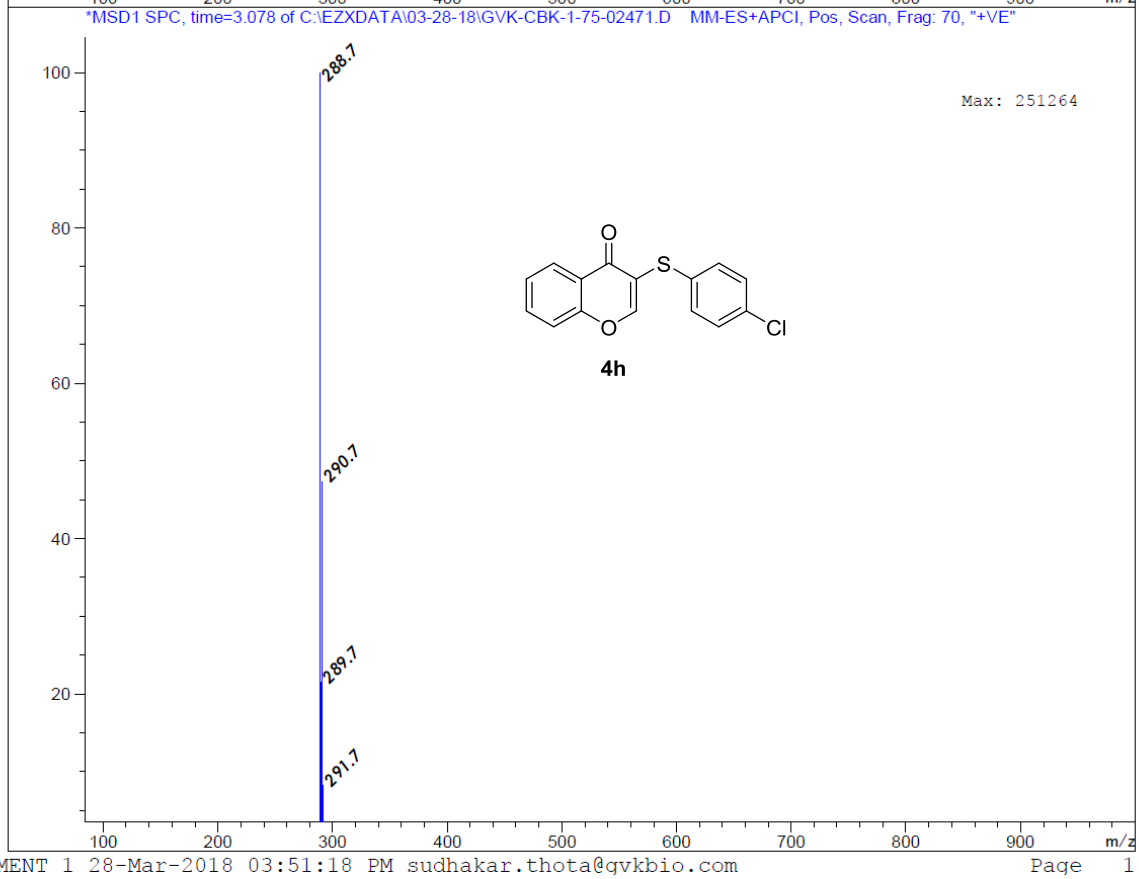


DAD1 B, Sig=215,4 Ref=off

PEAK No	RT min	Area	Area %
1	2.176	338.080	6.548
2	3.071	4565.847	88.432
3	3.604	212.711	4.120
4	3.851	46.480	0.900

MS Spectrum





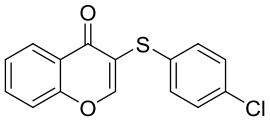
TRUMENT 1 28-Mar-2018 03:51:18 PM sudhakar.thota@gvkbio.com Page 1 o

Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None



4h

Monoisotopic Mass, Odd and Even Electron Ions

11 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

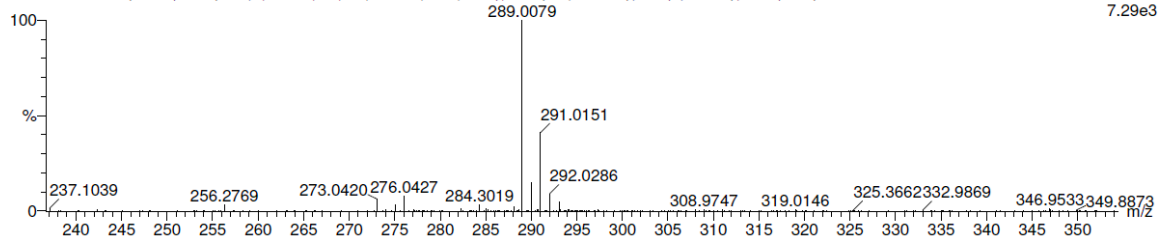
C: 0-15 H: 0-10 O: 0-2 S: 0-1 Cl: 0-1

GVK-CBK-1-75

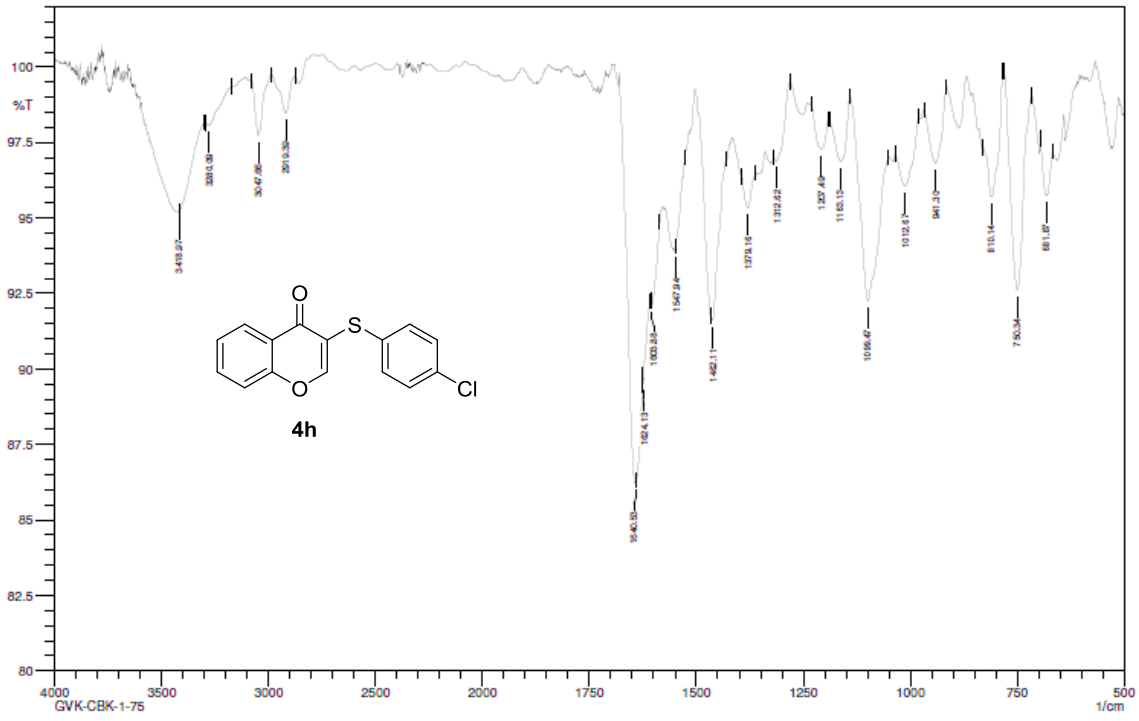
GVK Bio sciences (pvt)Ltd
Analytical Research and Development

Date of analysis:11-Apr-201816:08:58
Instru ment ID:ANL-MCL3-LCMS-001
1: TOF MS ES+
7.29e3

511845B3887 7 (0.285) AM (Cen,2, 50.00, Ar,5.0,195.09,1.00,LS 5); Sm (Mn, 5x2.00); Sb (1,40.00); Cm (5:10)



Minimum:				-1.5		
Maximum:		50.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
289.0079	289.0090	-1.1	-3.8	10.5	34.5	C15 H10 O2 S Cl

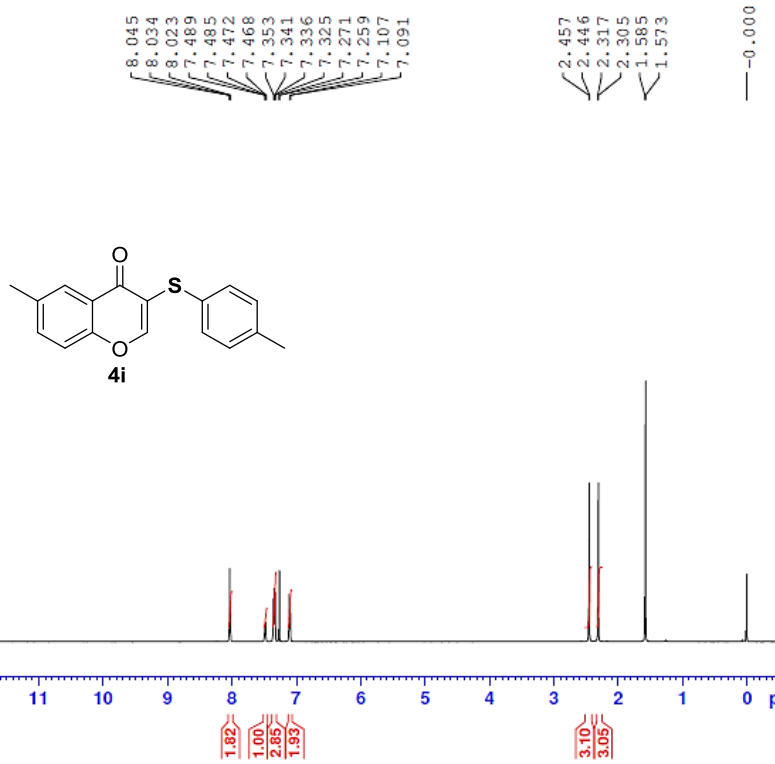


Comment: IN Kbr
GVK-CBK-1-75

No. of Scans:
Resolution:
Apodization:

Date: 4/2/2018 1:07:44 PM
User: Admin

GVK-CBK-1-54



Current Data Parameters
NAME 511708c5769
EXPNO 1
PROCNO 1

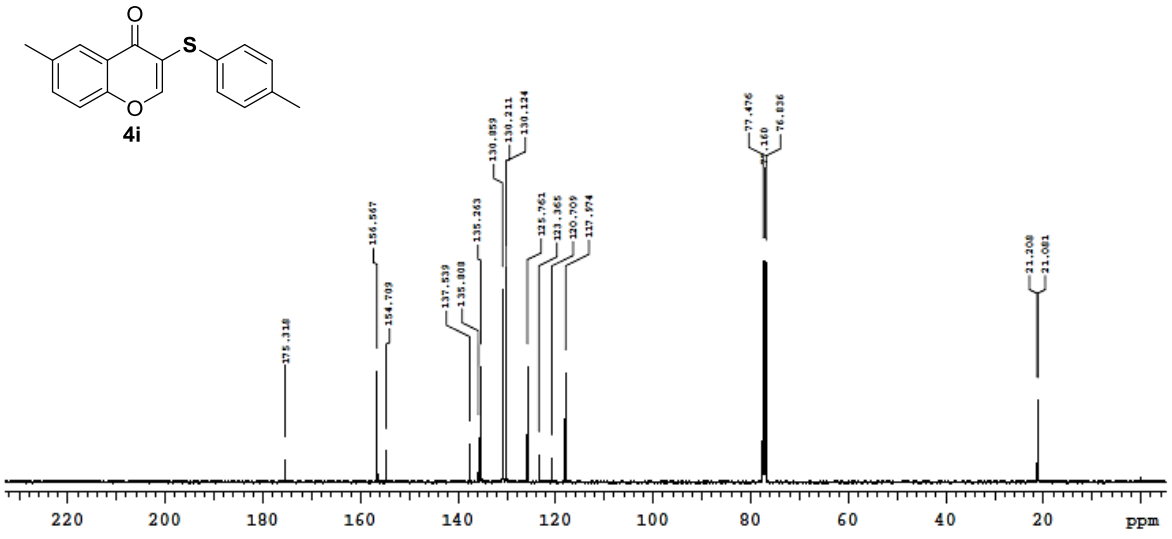
F2 - Acquisition Parameters
Date_ 20170828
Time 8.39 h
INSTRUM spect
PROBHD Z119470_0294 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 10000.000 Hz
FIDRES 0.152588 Hz
AQ 3.2767999 sec
RG 174.8
DW 50.000 usec
DE 6.50 usec
TE 303.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.1330883 MHz
NUC1 1H
P1 10.00 usec
PLW1 20.38699913 W

F2 - Processing parameters
SI 65536
SF 500.1300112 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

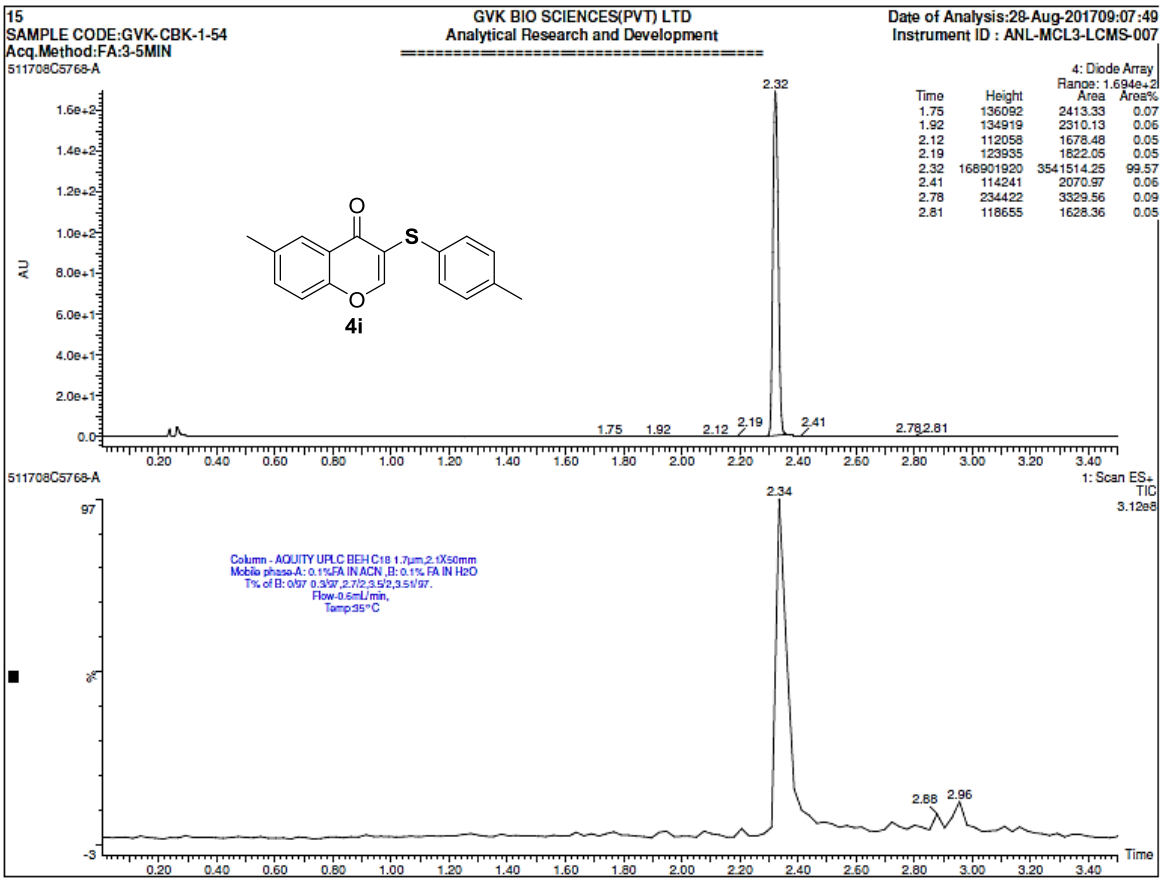
GVK-CBK-1-Phd-54
AR NO-NMR/17/12/0956

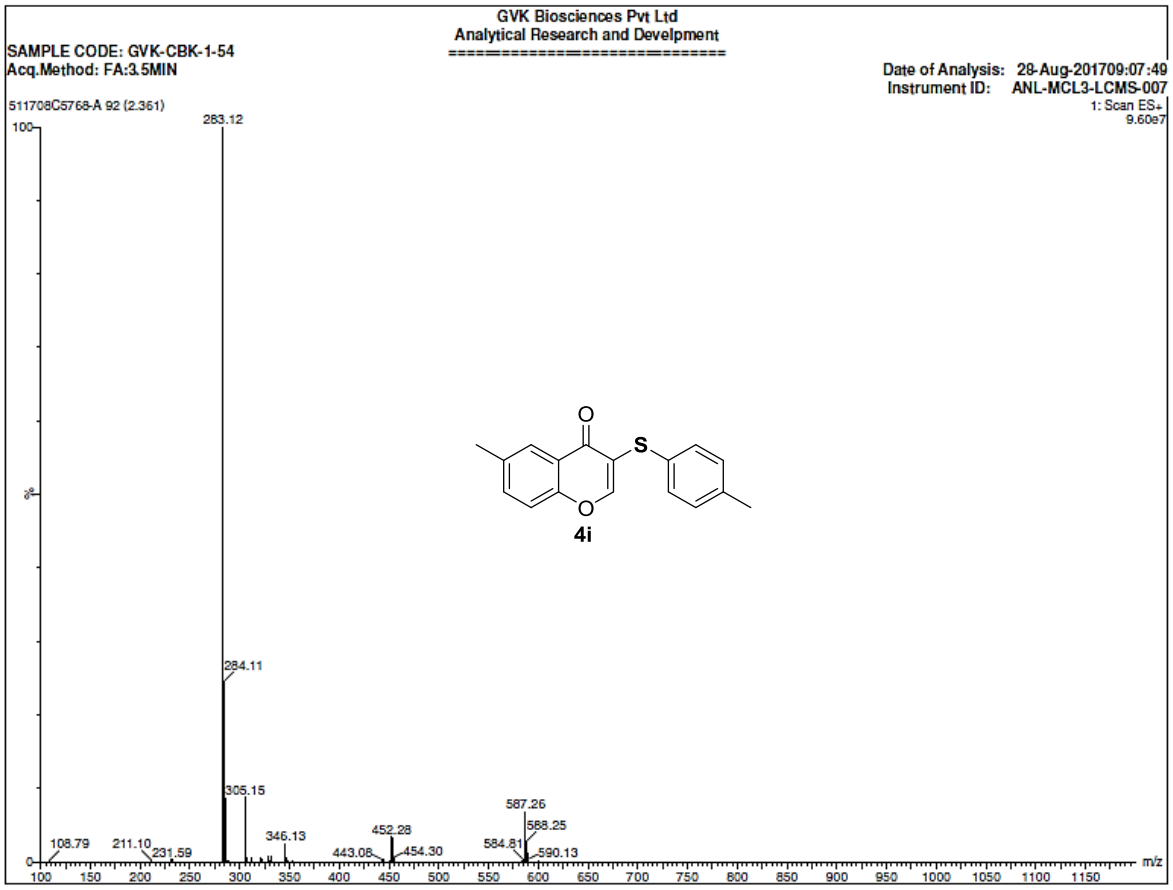
a3fa4469002

Reference Code: 511712A8165-GVK-CBK-1-Phd-54
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2017/Dec
Agilent 400-MRDD2
Data collected on: Dec 9 2017
Experiment: CARBON



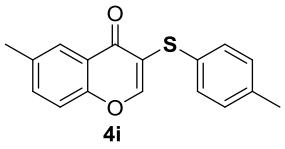
Plotname: 511712A8165-GVK-CBK-1-Phd-54_CARBON_01.REC_plot01


15
SAMPLE CODE:GVK-CBK-1-54
Acq.Method:FA:3-5MIN
GVK BIO SCIENCES(PVT) LTD
Analytical Research and Development
Date of Analysis:28-Aug-201709:07:49
Instrument ID : ANL-MCL3-LCMS-007
511708C5768-A
4: Diode Array
Range: 1.694e+2
Time Height Area Area%
1.75 136092 2413.33 0.07
1.92 134919 2310.13 0.06
2.12 112058 1678.48 0.05
2.19 123935 1822.05 0.05
2.32 168901920 3541514.25 99.57
2.41 114241 2070.97 0.06
2.78 234422 3329.56 0.09
2.81 118655 1628.36 0.05
AU
4i
511708C5768-A
1: Scan ES+
TIC
3.12e8
Column - ACQUITY UPLC BEH C18 1.7µm,2.1X50mm
Mobile phase-A: 0.1%FA IN ACN ,B: 0.1% FA IN H2O
T% of B: 0/97 0.3/97,2.7/2,3.5/2,3.51/97.
Flow-0.6mL/min,
Temp:35°C
Time


GVK Biosciences Pvt Ltd
Analytical Research and Develpment
SAMPLE CODE: GVK-CBK-1-54
Acq.Method: FA:3.5MIN
Date of Analysis: 28-Aug-201709:07:49
Instrument ID: ANL-MCL3-LCMS-007
511708C5768-A 92 (2.361)
1: Scan ES+
9.60e7
4i
m/z

Single Mass Analysis (displaying only valid results)

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None



4i

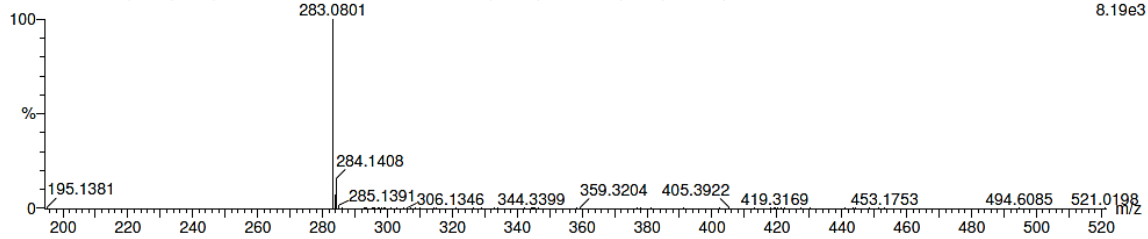
Monoisotopic Mass, Odd and Even Electron Ions
5 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-17 H: 0-15 O: 0-2 S: 0-1

GVK-CBK-Phd-54

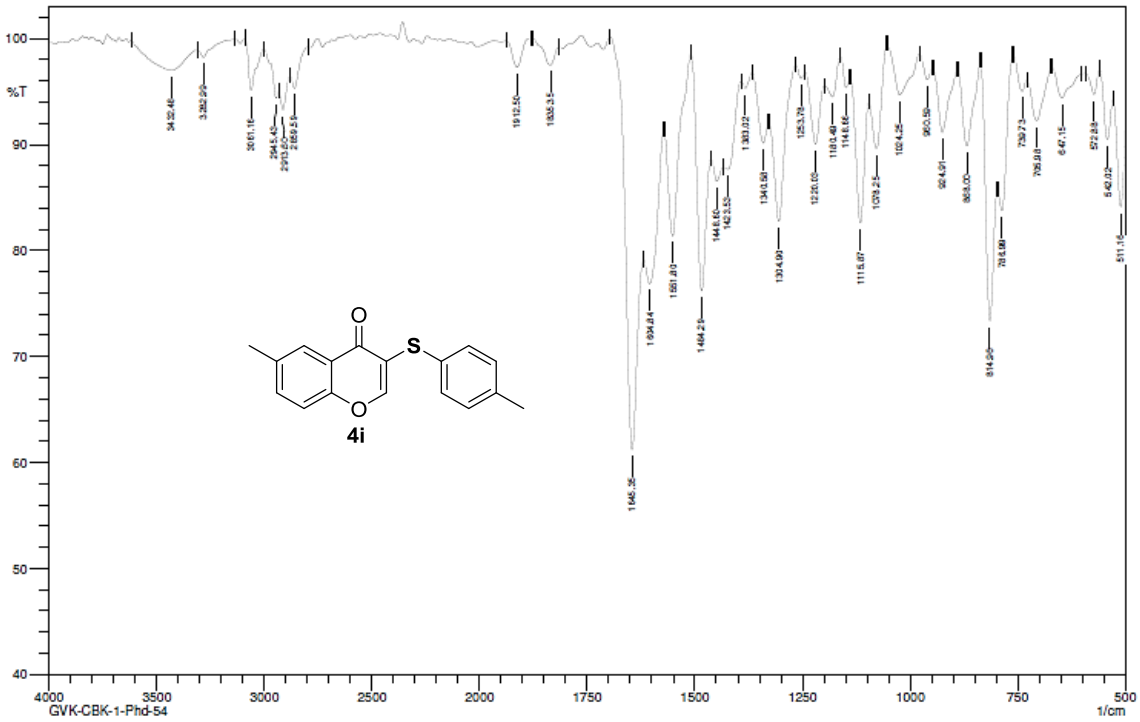
GVK Bio sciences (pvt)Ltd
Analytical Research and Development

Date of analysis:08-Dec-201715:53:13
Instru ment ID:ANL-MCL3-LCMS-001
1: TOF MS ES+
8.19e3

511712A8067 8 (0.326) AM (Cen,2, 80.00, Ar,5.0,195.12,1.00,LS 5); Sm (Mn, 5x2.00); Sb (1,40.00)



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
283.0801	283.0793	0.8	2.8	10.5	746.4	C17 H15 O2 S



4i

GVK-CBK-1-Phd-54

Comment: IN Kbr
GVK-CBK-1-Phd-54

No. of Scans:
Resolution:
Apodization:

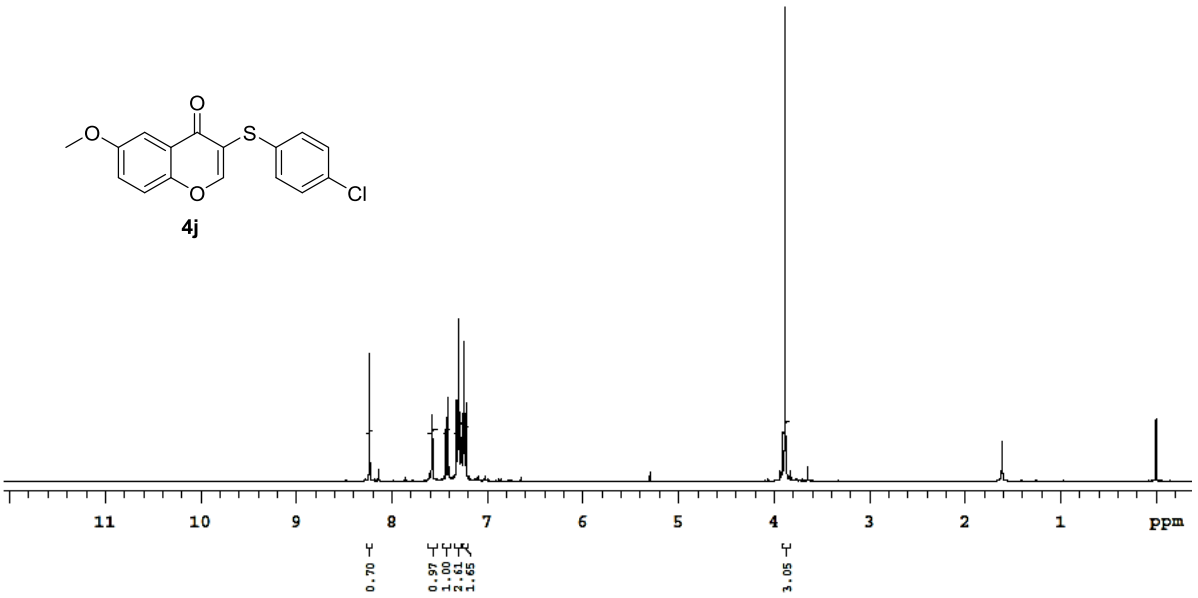
Date: 12/22/2017 12:18:50 PM
User: Admin

GVK-CBK-3-Phd-76
AR NO-NMR/18/03/2657

43b0a046002

Reference Code: 511803C3828-GVK-CBK-3-Phd-76
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2018/Mar
Agilent 400-MRDD2
Data collected on: Mar 24 2018
Experiment: PROTON

4j

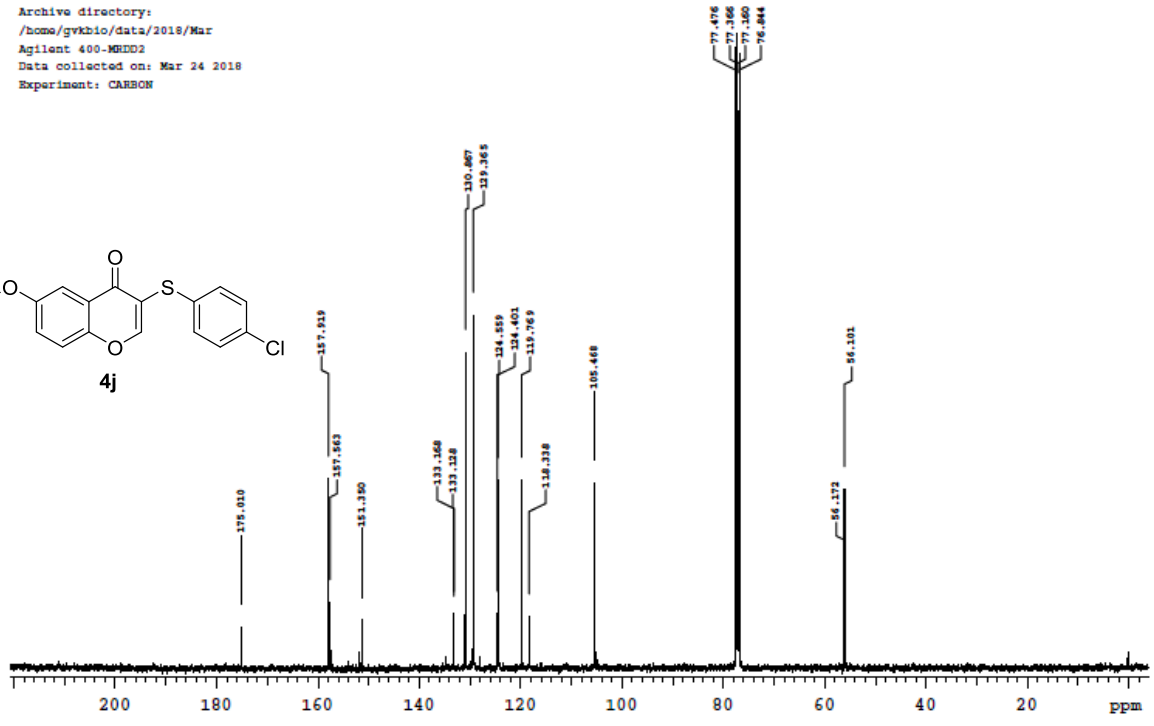


GVK-CBK-3-Phd-76
AR NO-NMR/18/03/2657

43981d3e002

Reference Code: 511803C3828-GVK-CBK-3-Phd-76
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2018/Mar
Agilent 400-MRDD2
Data collected on: Mar 24 2018
Experiment: CARBON

4j



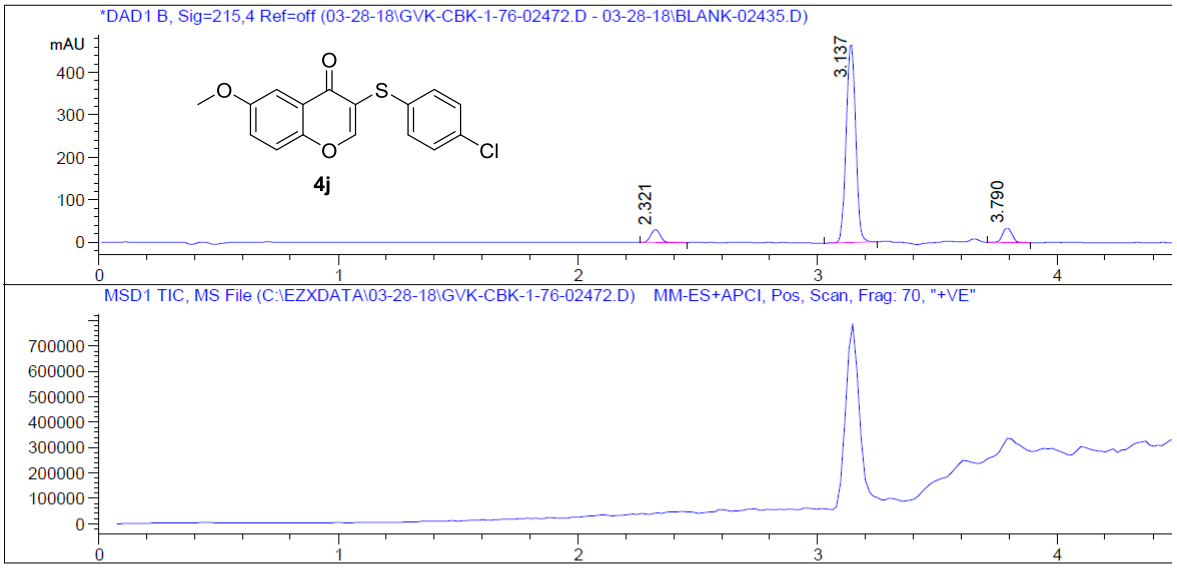
Plotname: 511803C3828-GVK-CBK-3-Phd-76_CARBON_01.REC_plot01

GVK BIO SCIENCES PVT LTD

LC/MS REPORT

```
================================================================================
Data file       : C:\EZXDATA\03-28-18\GVK-CBK-1--> Vial position:  Vial 57
                                                  Instrument Name:ANL-MCL2-LCMS-002
Injection Date  : 28-Mar-2018    03:40:11 PM      Injection Vol:            4.000
Sample Name     :   GVK-CBK-1-76
================================================================================
  Acq. Method Conditions: RND X-Bridge 5.0 Min
  COLUMN : X-BRIDGE C18 (4.6mm x 75mm) 3.5 µm
  MOBILE PHASE A: 10mM Ammonium Acetate in water, B 100% ACN
  Gradient : % of B 0.0/10,0.2/10,2.5/75,3.0/100,4.8/100,5.0/10
  Column Temp : 35° C
  Flow rate : 2.0 ml/min

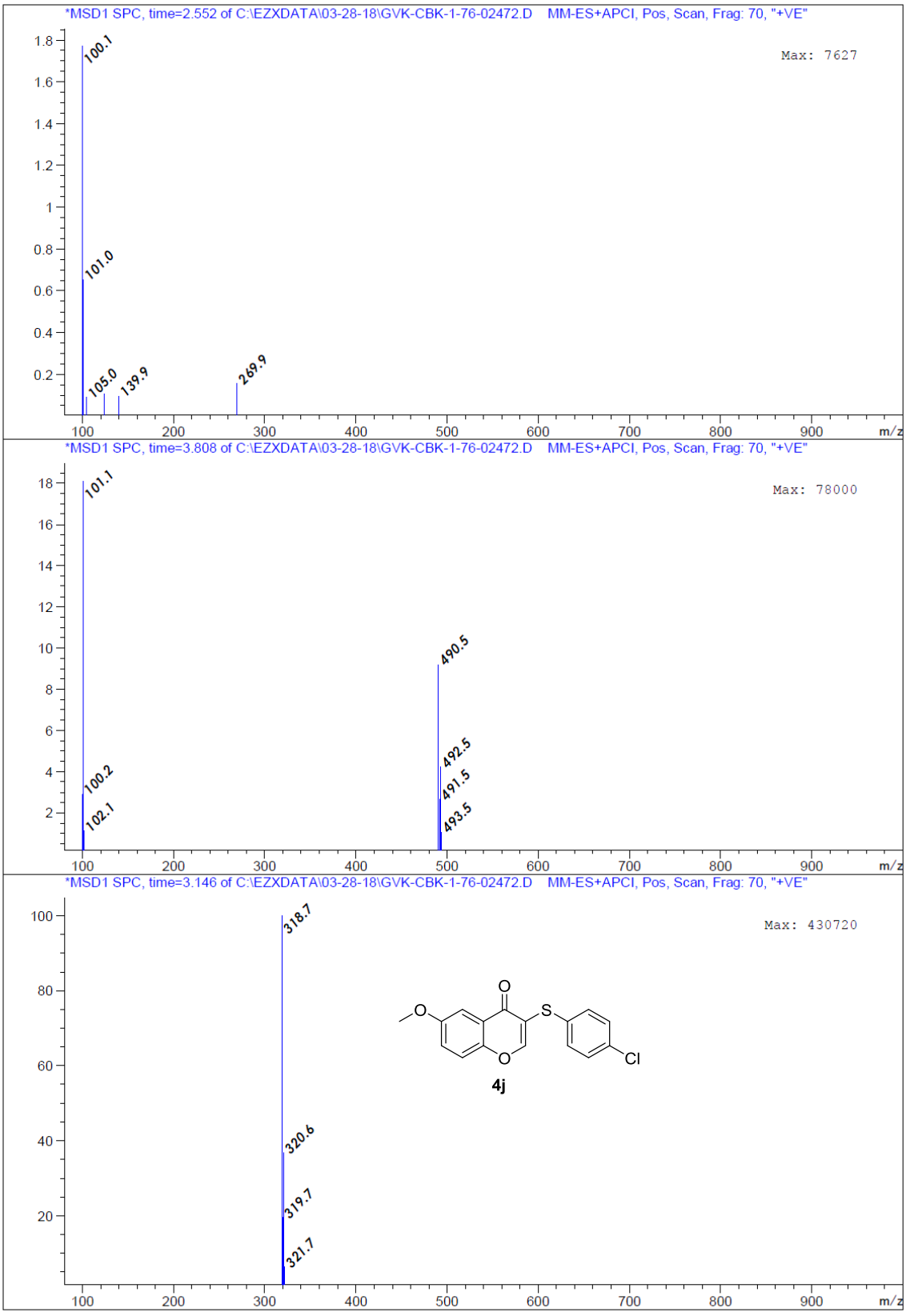
================================================================================
```



DAD1 B, Sig=215,4 Ref=off

PEAK No	RT min	Area	Area %
1	2.321	85.025	5.777
2	3.137	1295.772	88.041
3	3.790	90.990	6.182

MS Spectrum

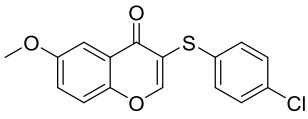

*MSD1 SPC, time=2.552 of C:\EZXDATA\03-28-18\GVK-CBK-1-76-02472.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 7627
100.1
101.0
105.0
139.9
269.9
*MSD1 SPC, time=3.808 of C:\EZXDATA\03-28-18\GVK-CBK-1-76-02472.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 78000
101.1
100.2
102.1
490.5
492.5
491.5
493.5
*MSD1 SPC, time=3.146 of C:\EZXDATA\03-28-18\GVK-CBK-1-76-02472.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 430720
318.7
320.6
319.7
321.7
O
O
S
O
Cl
4j
m/z

Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0

Selected filters: None



4j

Monoisotopic Mass, Odd and Even Electron Ions

15 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)

Elements Used:

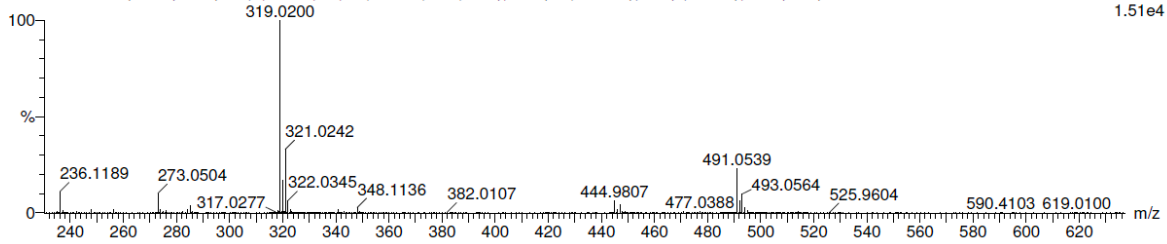
C: 0-16 H: 0-12 O: 0-3 S: 0-1 Cl: 0-1

GVK-CBK-1-76

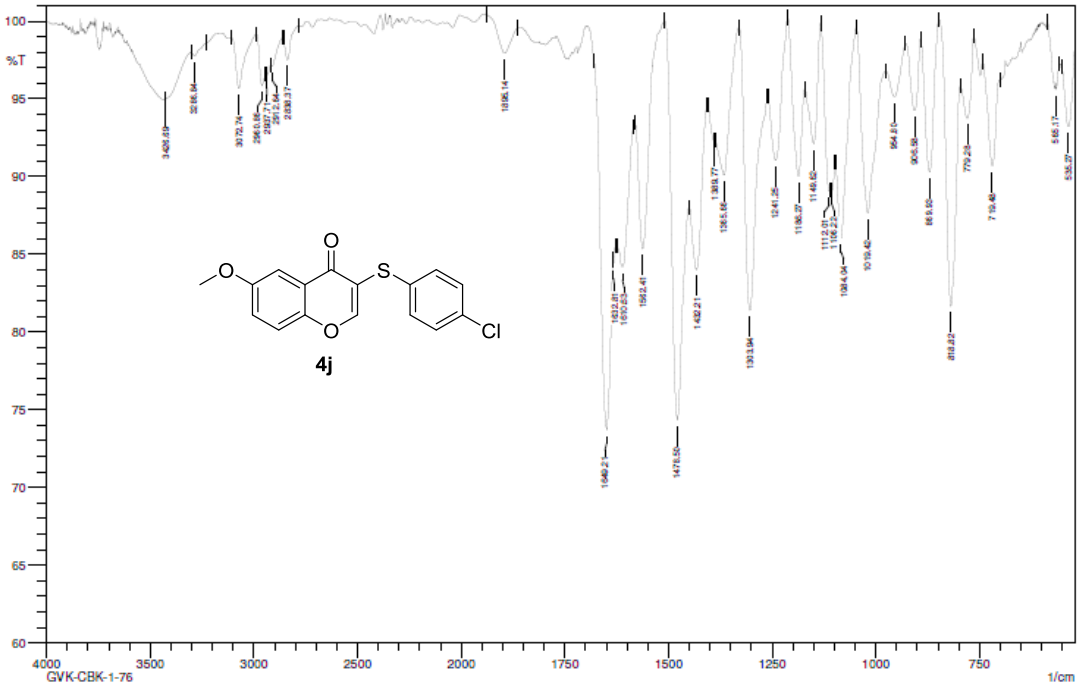
GVK Bio sciences (pvt)Ltd
Analytical Research and Development

Date of analysis:11-Apr-201816:06:29
Instru ment ID:ANL-MCL3-LCMS-001
1: TOF MS ES+
1.51e4

511844B3888 7 (0.281) AM (Cen,2, 50.00, Ar,5.0,195.09,1.00,LS 5); Sm (Mn, 5x2.00); Sb (1,40.00); Cm (4:15)



Minimum:				-1.5		
Maximum:		50.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
319.0200	319.0196	0.4	1.3	10.5	67.8	C16 H12 O3 S Cl



Comment: IN Kbr
GVK-CBK-1-76

No. of Scans:
Resolution:
Apodization:

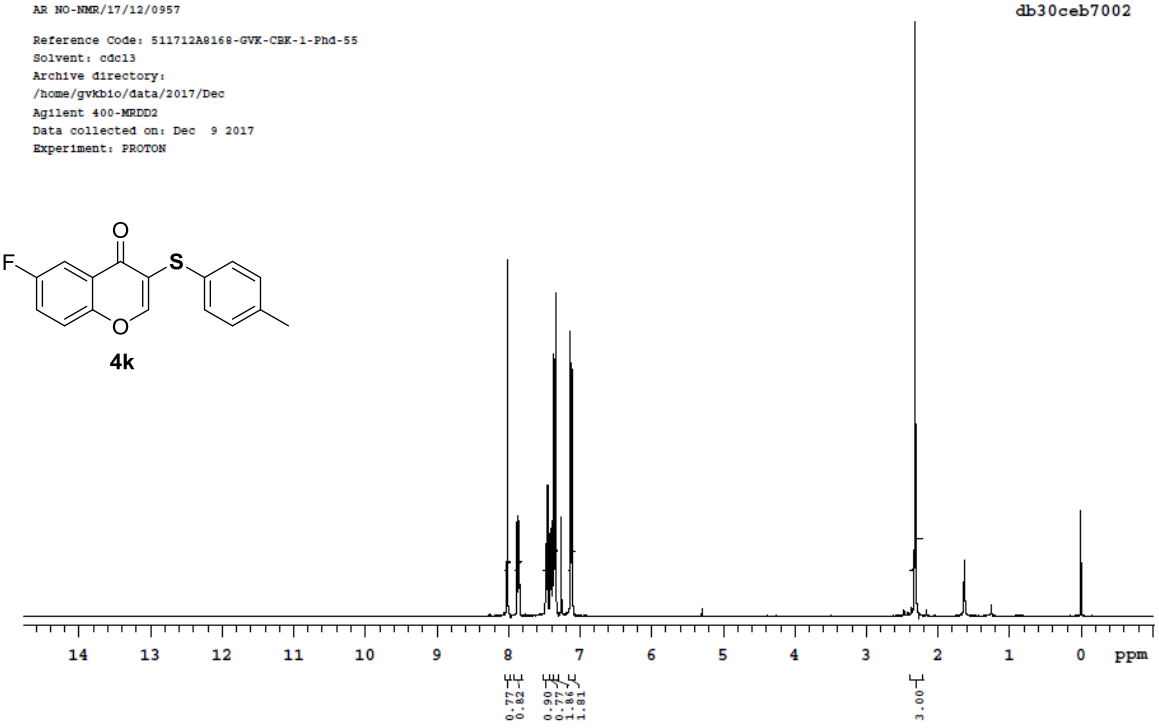
Date: 4/2/2018 1:19:32 PM
User: Admin

GVK-CBK-1-Phd-55
AR NO-NMR/17/12/0957

db30ceb7002

Reference Code: 511712A8168-GVK-CBK-1-Phd-55
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2017/Dec
Agilent 400-MRDD2
Data collected on: Dec 9 2017
Experiment: PROTON

4k

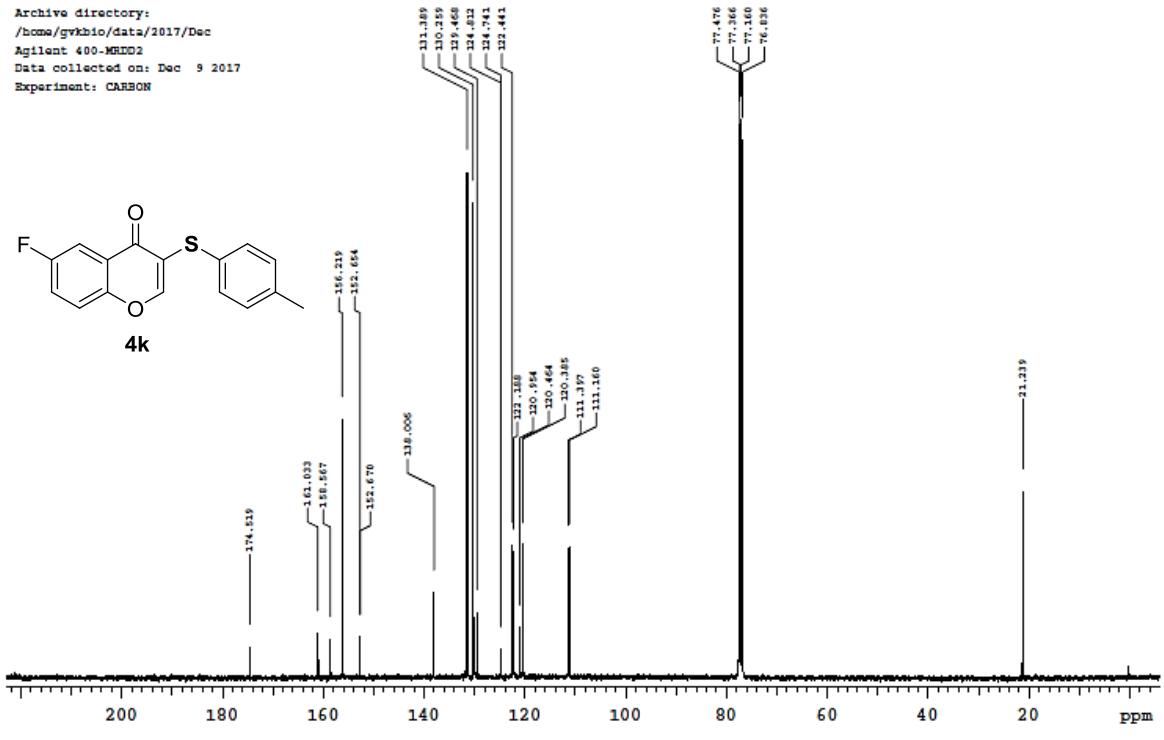


GVK-CBK-1-Phd-55
AR NO-NMR/17/12/0957

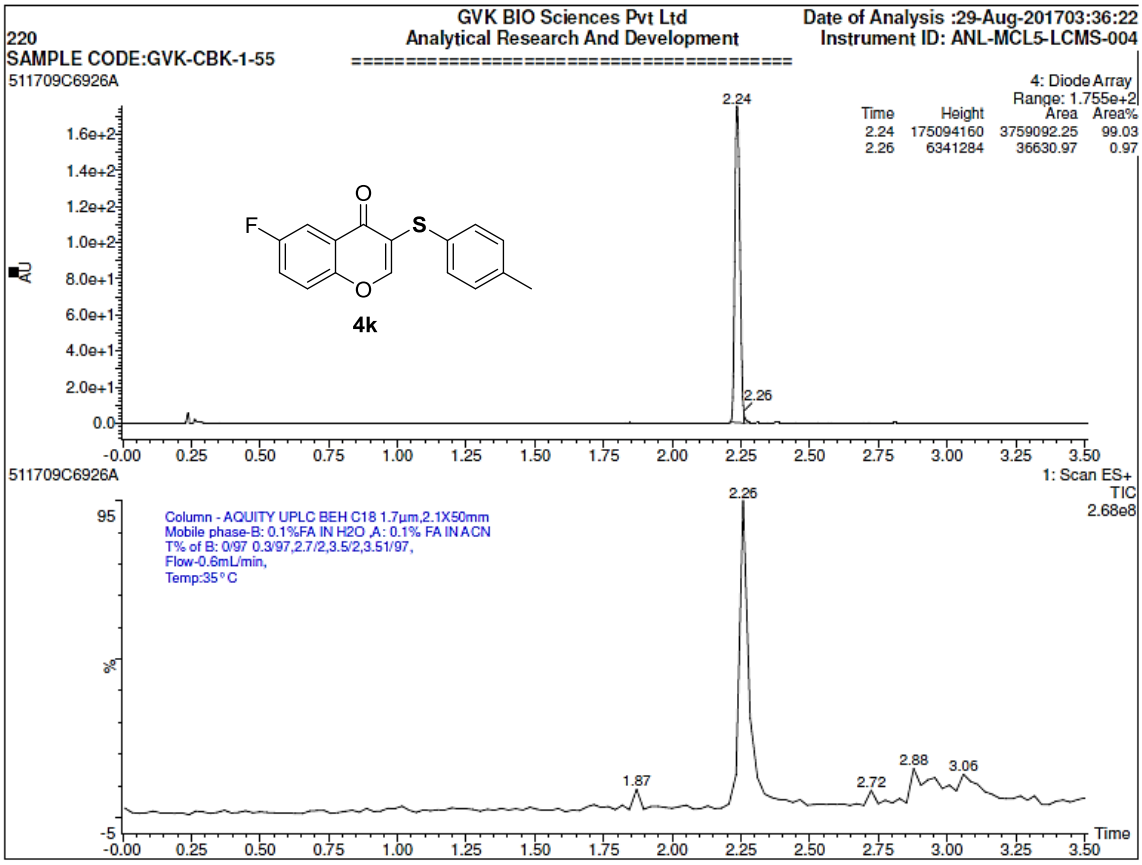
b72c0a28002

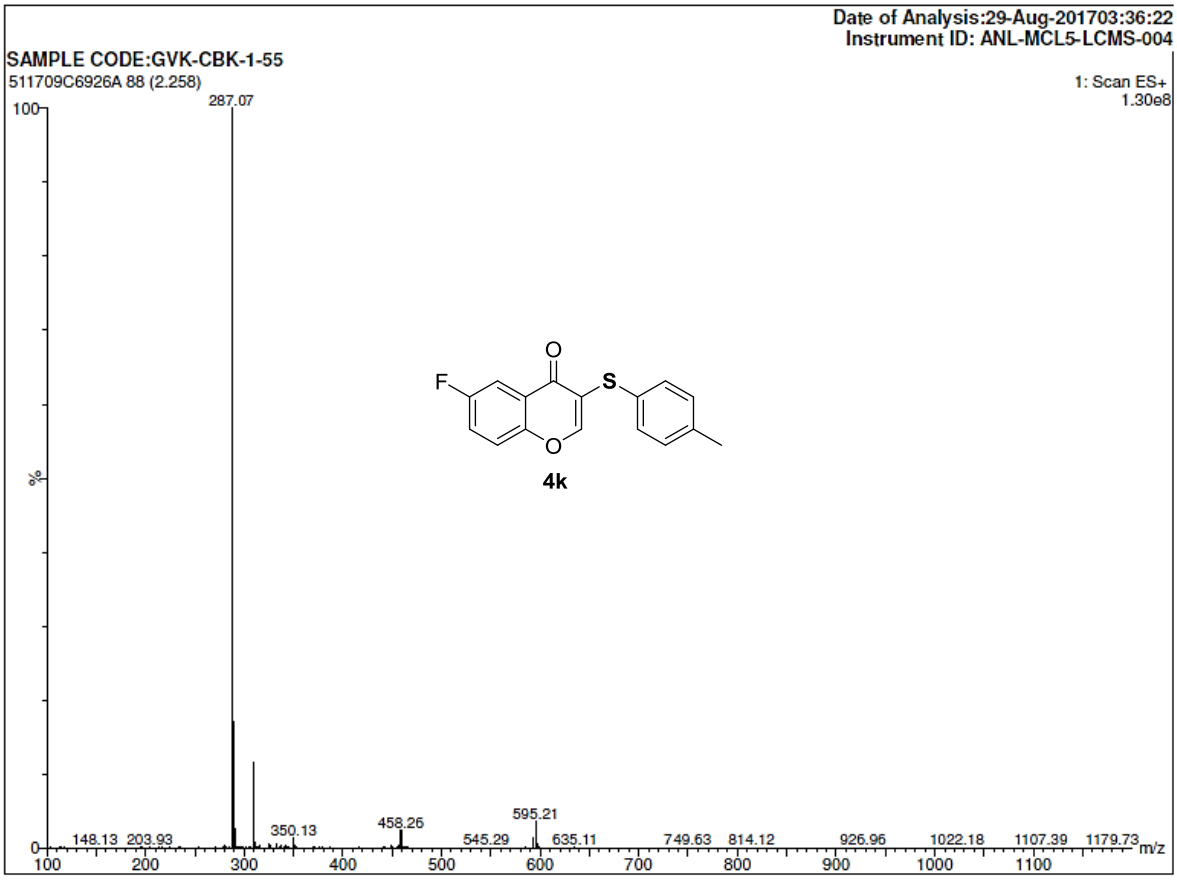
Reference Code: 511712A8168-GVK-CBK-1-Phd-55
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2017/Dec
Agilent 400-MRDD2
Data collected on: Dec 9 2017
Experiment: CARBON

4k



Plotname: 511712A8168-GVK-CBK-1-Phd-55_CARBON_01.REC_plot01

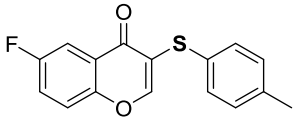

GVK BIO Sciences Pvt Ltd
Analytical Research And Development
Date of Analysis :29-Aug-201703:36:22
Instrument ID: ANL-MCL5-LCMS-004
220
SAMPLE CODE:GVK-CBK-1-55
511709C6926A
4: Diode Array
Range: 1.755e+2
Time Height Area Area%
2.24 175094160 3759092.25 99.03
2.26 6341284 36630.97 0.97
2.24
2.26
AU
4k
511709C6926A
1: Scan ES+
TIC
2.68e8
Column - AQUITY UPLC BEH C18 1.7µm,2.1X50mm
Mobile phase-B: 0.1%FA IN H2O ,A: 0.1% FA IN ACN
T% of B: 0/97 0.3/97,2.7/2,3.5/2,3.51/97,
Flow-0.6mL/min,
Temp:35°C
1.87
2.72
2.88
3.06
Time


Date of Analysis:29-Aug-201703:36:22
Instrument ID: ANL-MCL5-LCMS-004
SAMPLE CODE:GVK-CBK-1-55
511709C6926A 88 (2.258)
1: Scan ES+
1.30e8
287.07
4k
148.13
203.93
350.13
458.26
595.21
545.29
635.11
749.63
814.12
926.96
1022.18
1107.39
1179.73
m/z

Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None



4k

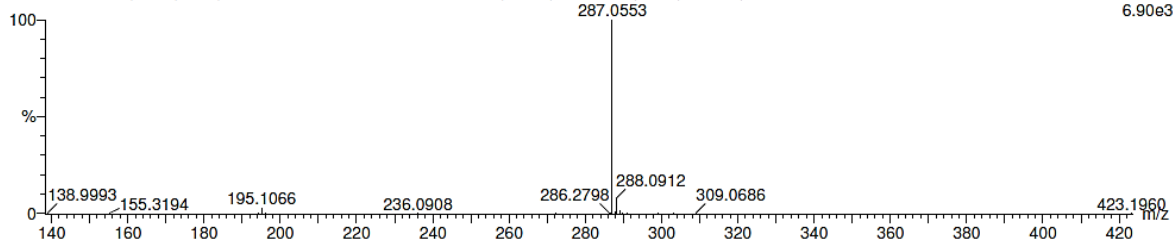
Monoisotopic Mass, Odd and Even Electron Ions
10 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-16 H: 0-12 O: 0-2 F: 0-1 S: 0-1

GVK-CBK-Phd-55

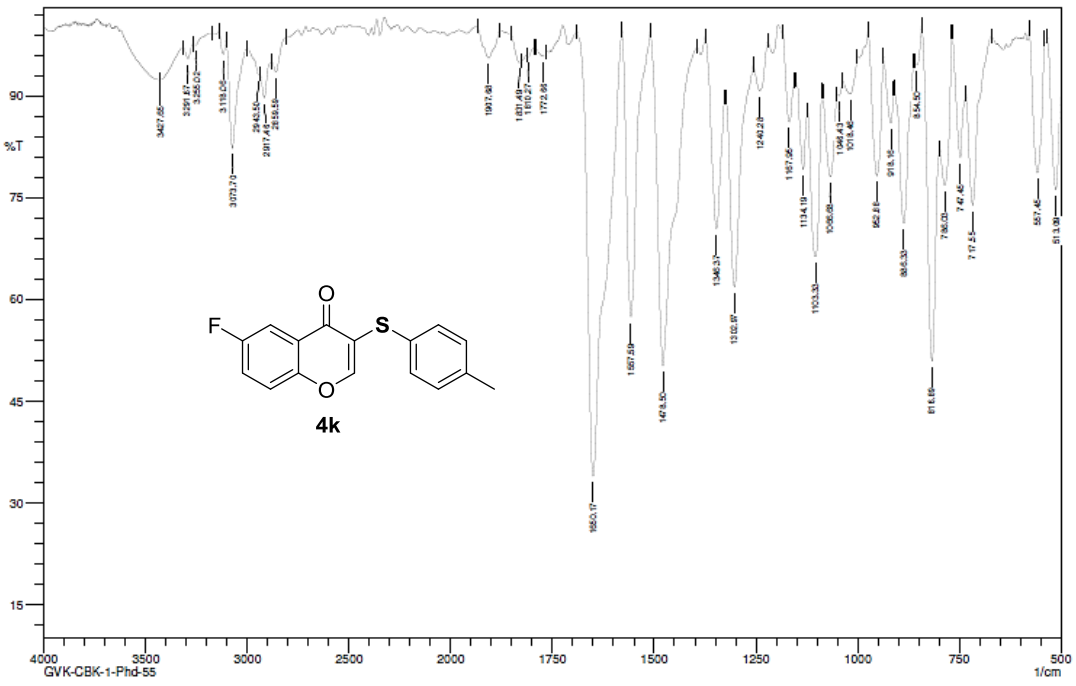
GVK Bio sciences (pvt)Ltd
Analytical Research and Development

Date of analysis:08-Dec-201716:13:09
Instru ment ID:ANL-MCL3-LCMS-001
1: TOF MS ES+
6.90e3

511712A8071 8 (0.326) AM (Cen,2, 50.00, Ar,5.0,195.12,1.00,LS 5); Sm (Mn, 5x2.00); Sb (1,40.00)



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
287.0553	287.0542	1.1	3.8	10.5	904.9	C16 H12 O2 F S



Comment: IN Kbr
GVK-CBK-1-Phd-55

No. of Scans:
Resolution:
Apodization:

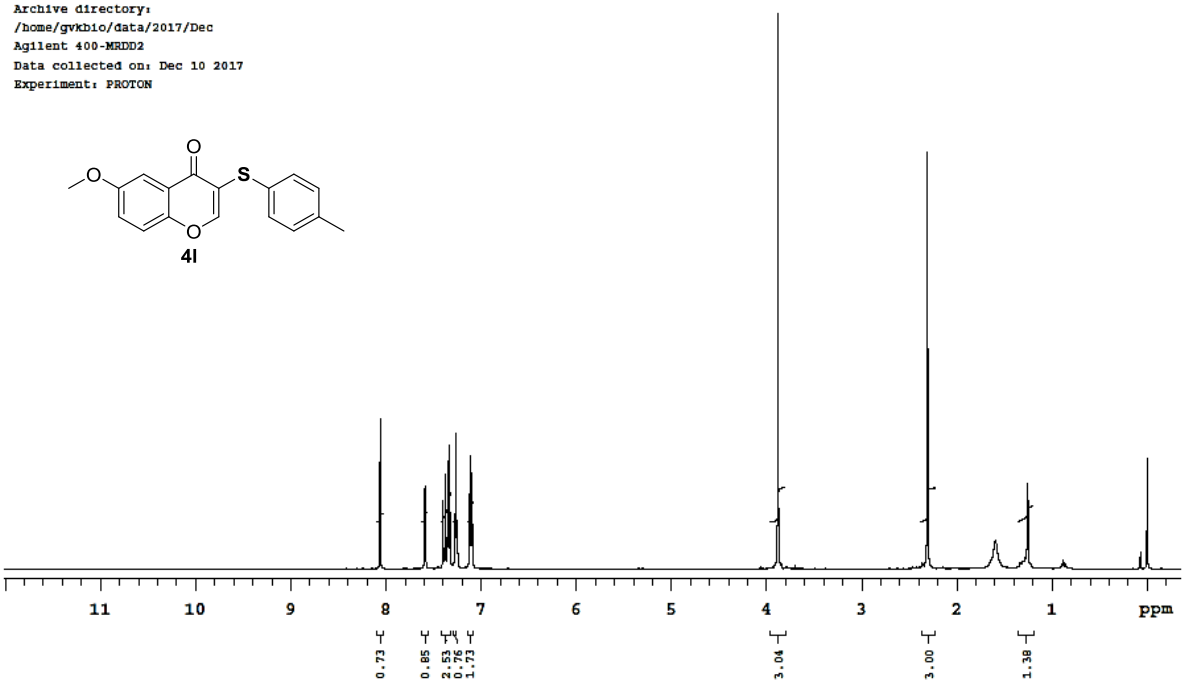
Date: 12/22/2017 12:26:31 PM
User: Admin

GVK-CEK-1-Phd-56
AR NO-NMR/17/12/0961

e73984cb004

Reference Code: 511712A8170-GVK-CEK-1-Phd-56
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2017/Dec
Agilent 400-MRDD2
Data collected on: Dec 10 2017
Experiment: PROTON

4l

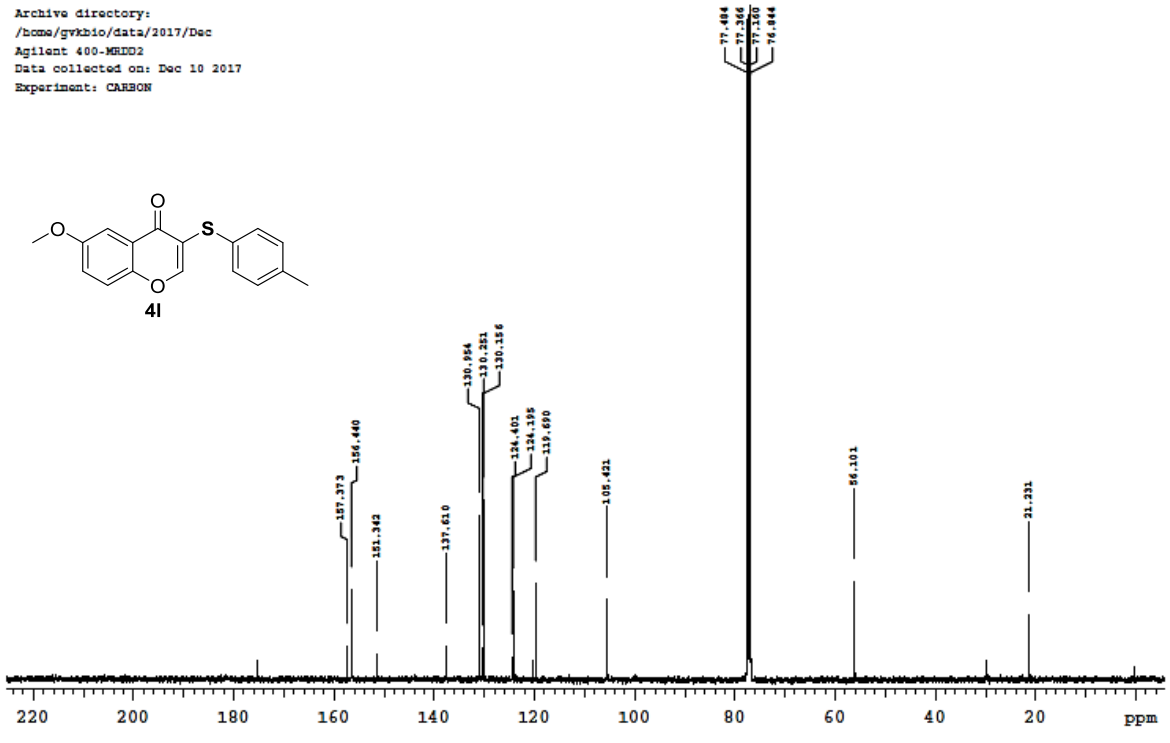


GVK-CEK-1-Phd-56
AR NO-NMR/17/12/0961

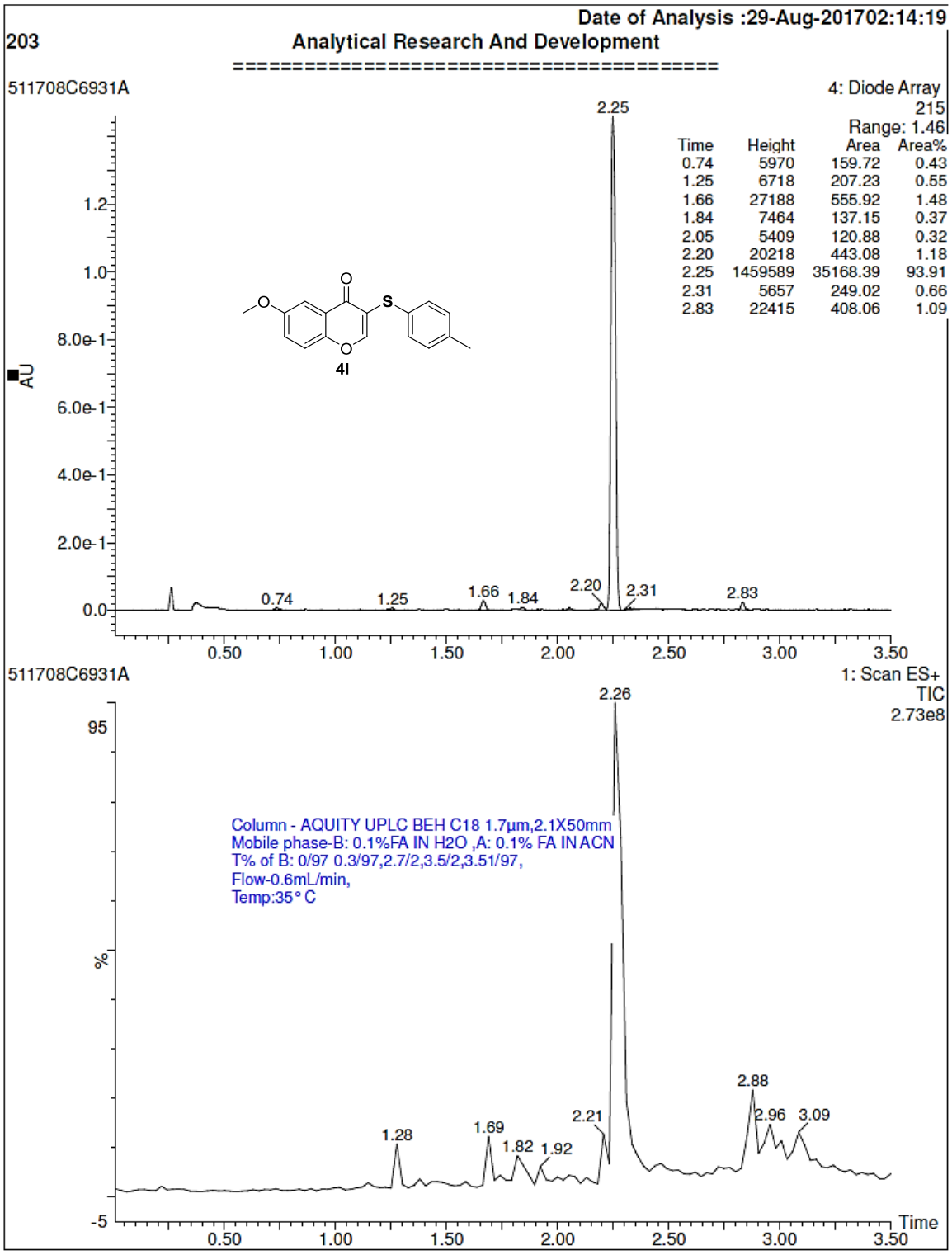
ff69db74002

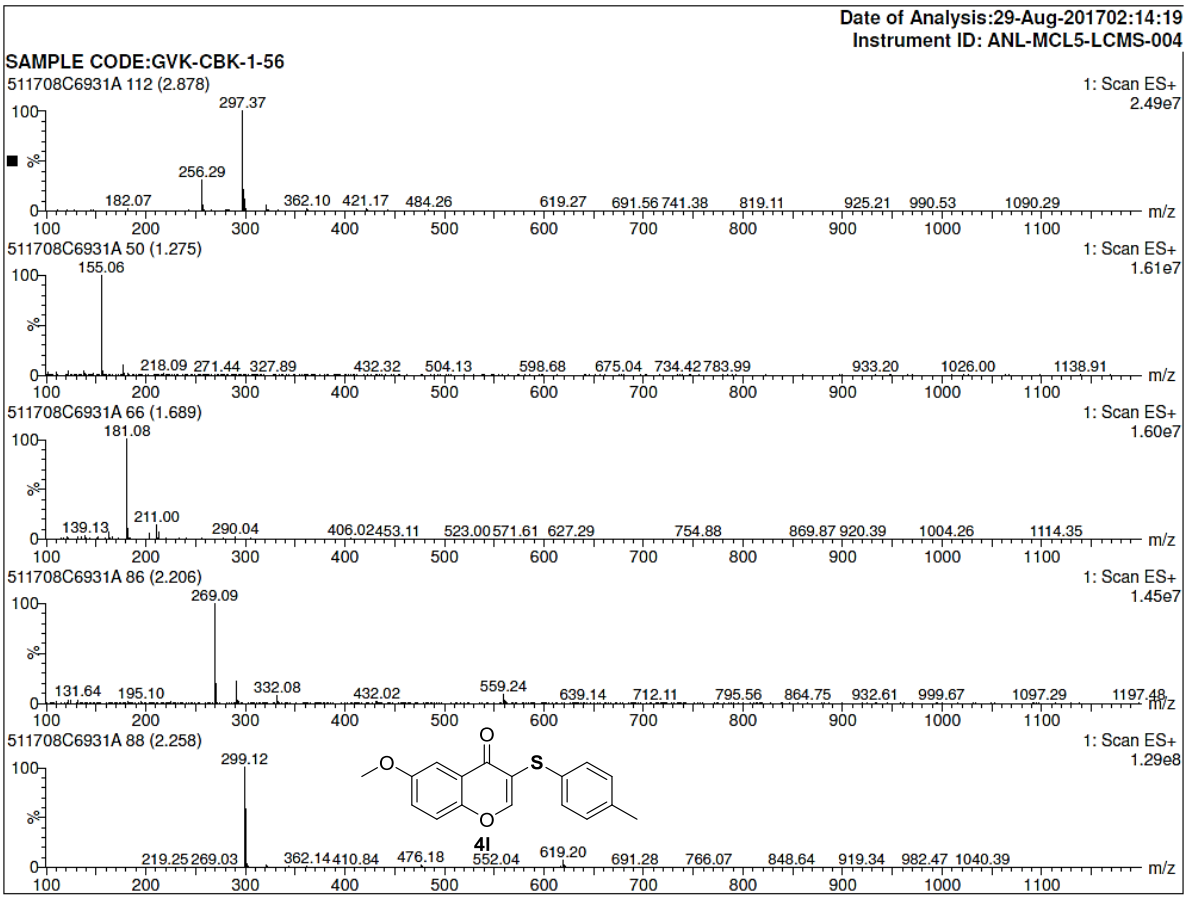
Reference Code: 511712A8170-GVK-CEK-1-Phd-56
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2017/Dec
Agilent 400-MRDD2
Data collected on: Dec 10 2017
Experiment: CARBON

4l



Plotname: 511712A8170-GVK-CEK-1-Phd-56_CARBON_01.RRC plot01

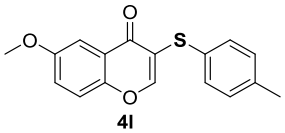

Date of Analysis :29-Aug-201702:14:19
203
Analytical Research And Development
511708C6931A
4: Diode Array
215
Range: 1.46
Time Height Area Area%
0.74 5970 159.72 0.43
1.25 6718 207.23 0.55
1.66 27188 555.92 1.48
1.84 7464 137.15 0.37
2.05 5409 120.88 0.32
2.20 20218 443.08 1.18
2.25 1459589 35168.39 93.91
2.31 5657 249.02 0.66
2.83 22415 408.06 1.09
4l
AU
2.25
0.74
1.25
1.66
1.84
2.20
2.31
2.83
511708C6931A
1: Scan ES+
TIC
2.73e8
Column - AQUITY UPLC BEH C18 1.7µm,2.1X50mm
Mobile phase-B: 0.1%FA IN H2O ,A: 0.1% FA IN ACN
T% of B: 0/97 0.3/97,2.7/2,3.5/2,3.51/97,
Flow-0.6mL/min,
Temp:35° C
%
2.26
1.28
1.69
1.82
1.92
2.21
2.88
2.96
3.09
Time


Date of Analysis:29-Aug-201702:14:19
Instrument ID: ANL-MCL5-LCMS-004
SAMPLE CODE:GVK-CBK-1-56
511708C6931A 112 (2.878)
1: Scan ES+
2.49e7
297.37
256.29
182.07
362.10 421.17 484.26
619.27
691.56 741.38
819.11
925.21
990.53
1090.29
m/z
511708C6931A 50 (1.275)
1: Scan ES+
1.61e7
155.06
218.09 271.44 327.89
432.32
504.13
598.68
675.04 734.42 783.99
933.20
1026.00
1138.91
m/z
511708C6931A 66 (1.689)
1: Scan ES+
1.60e7
181.08
139.13
211.00
290.04
406.02 453.11
523.00 571.61 627.29
754.88
869.87 920.39
1004.26
1114.35
m/z
511708C6931A 86 (2.206)
1: Scan ES+
1.45e7
269.09
131.64
195.10
332.08
432.02
559.24
639.14
712.11
795.56
864.75
932.61
999.67
1097.29
1197.48
m/z
511708C6931A 88 (2.258)
1: Scan ES+
1.29e8
299.12
O
O
S
O
4l
219.25 269.03
362.14 410.84
476.18
552.04
619.20
691.28
766.07
848.64
919.34
982.47 1040.39
m/z
100
200
300
400
500
600
700
800
900
1000
1100

Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None



4l

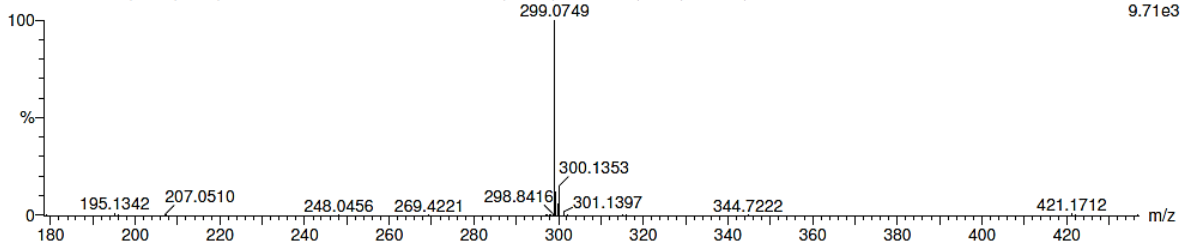
Monoisotopic Mass, Odd and Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-17 H: 0-15 O: 0-3 S: 0-1

GVK-CBK-Phd-56

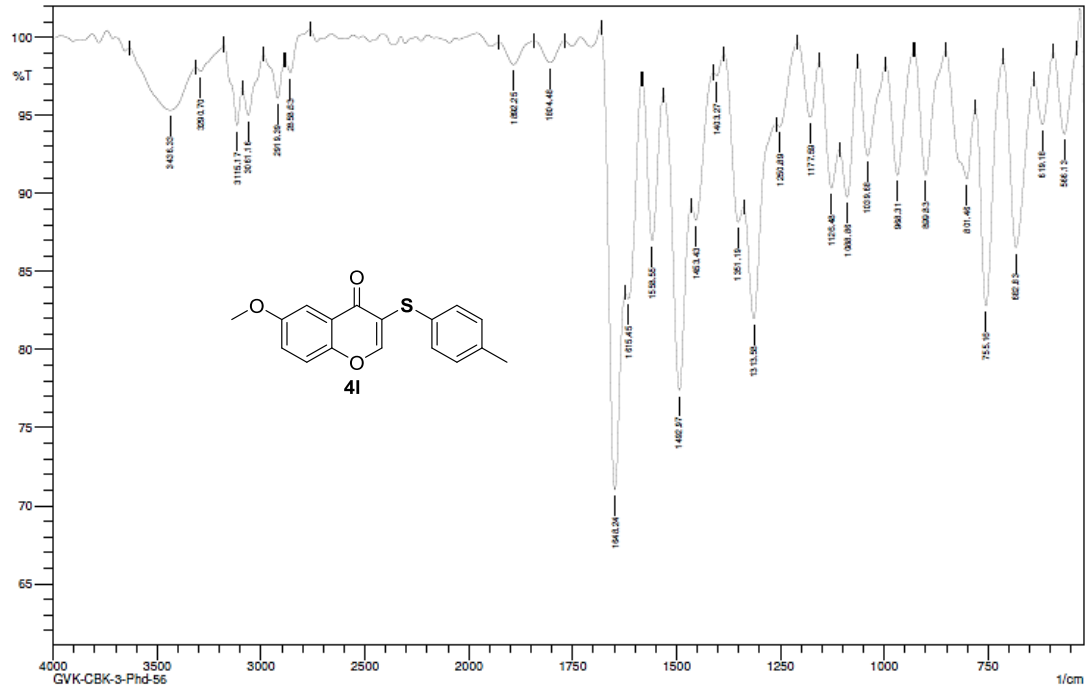
GVK Bio sciences (pvt)Ltd
Analytical Research and Development

Date of analysis:08-Dec-201716:22:30
Instru ment ID:ANL-MCL3-LCMS-001
1: TOF MS ES+
9.71e3

511712A8073 9 (0.370) AM (Cen,2, 50.00, Ar,5.0,195.13,1.00,LS 5); Sm (Mn, 5x2.00); Sb (1,40.00)



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
299.0749	299.0742	0.7	2.3	10.5	939.5	C17 H15 O3 S

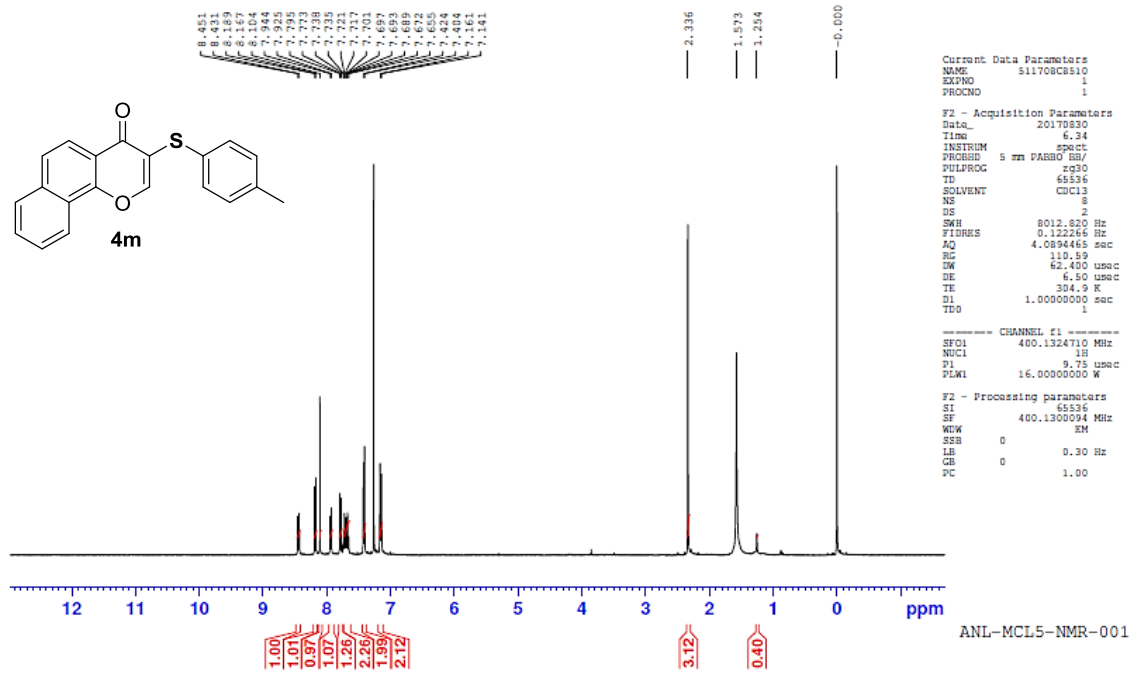


Comment: IN Kbr
GVK-CBK-3-Phd-56

No. of Scans:
Resolution:
Apodization:

Date:3/2/2018 10:27:04 AM
User: Admin

GVK-CBK-3-Phd-57

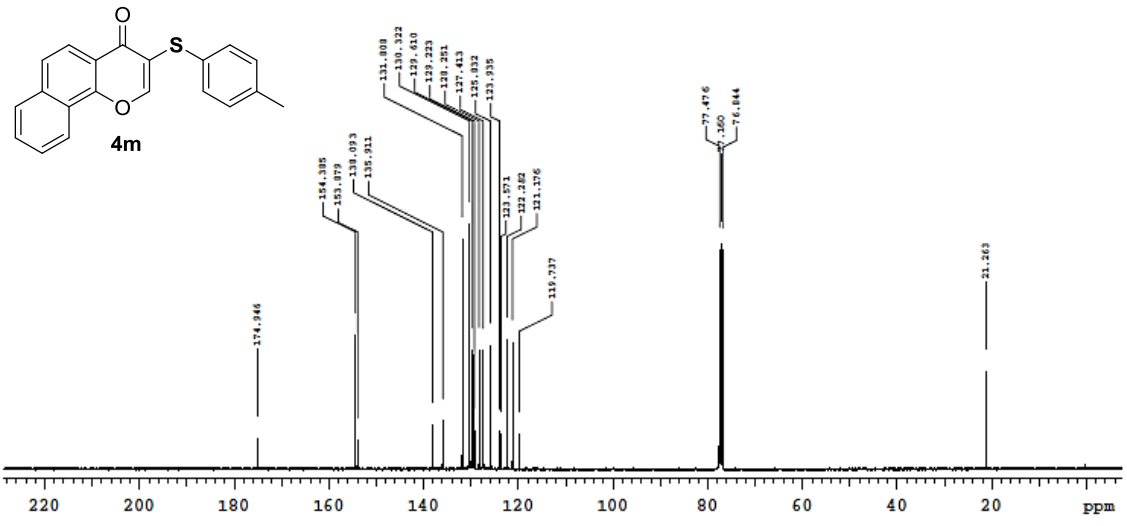


ANL-MCL5-NMR-001

GVK-CBK-1-Phd-57
AR NO-NMR/17/12/0958

60f0ef6c002

Reference Code: 511712A8171-GVK-CBK-1-Phd-57
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2017/Dec
Agilent 400-MRDD2
Data collected on: Dec 9 2017
Experiment: CARBON

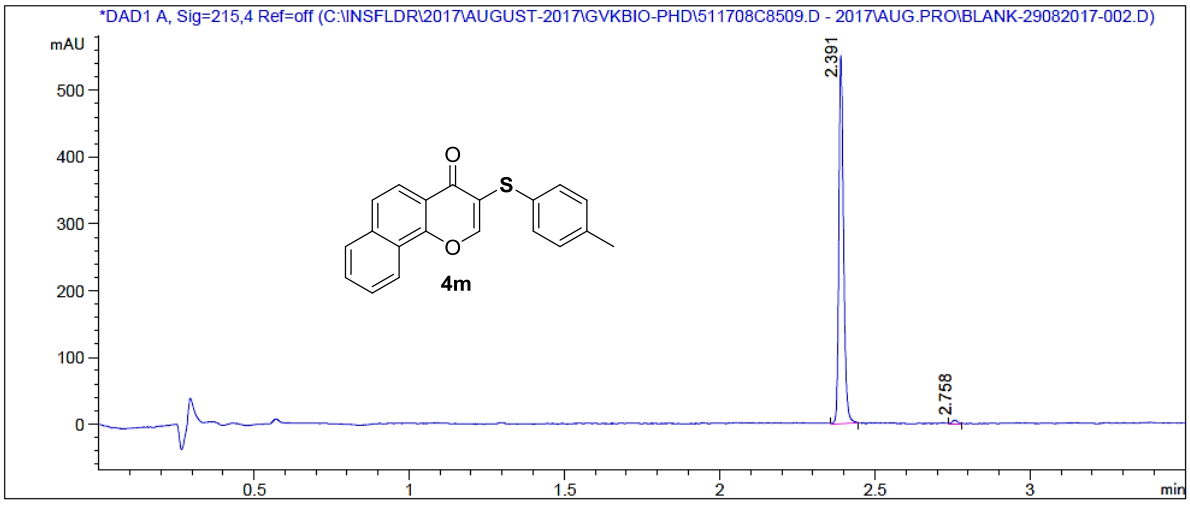


Plotname: 511712A8171-GVK-CBK-1-Phd-57_CARBON_01.REC_plot01

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

Vial position : P2-E-02
Date of Analysis : 8/30/2017 2:02:41 AM Injection Vol : 0.300uL
Acq. Method : RND-FA-3.5mns Instrument ID : ANL-MCL5-LCMS-(
Sample Name : GVK-CBK-1-57

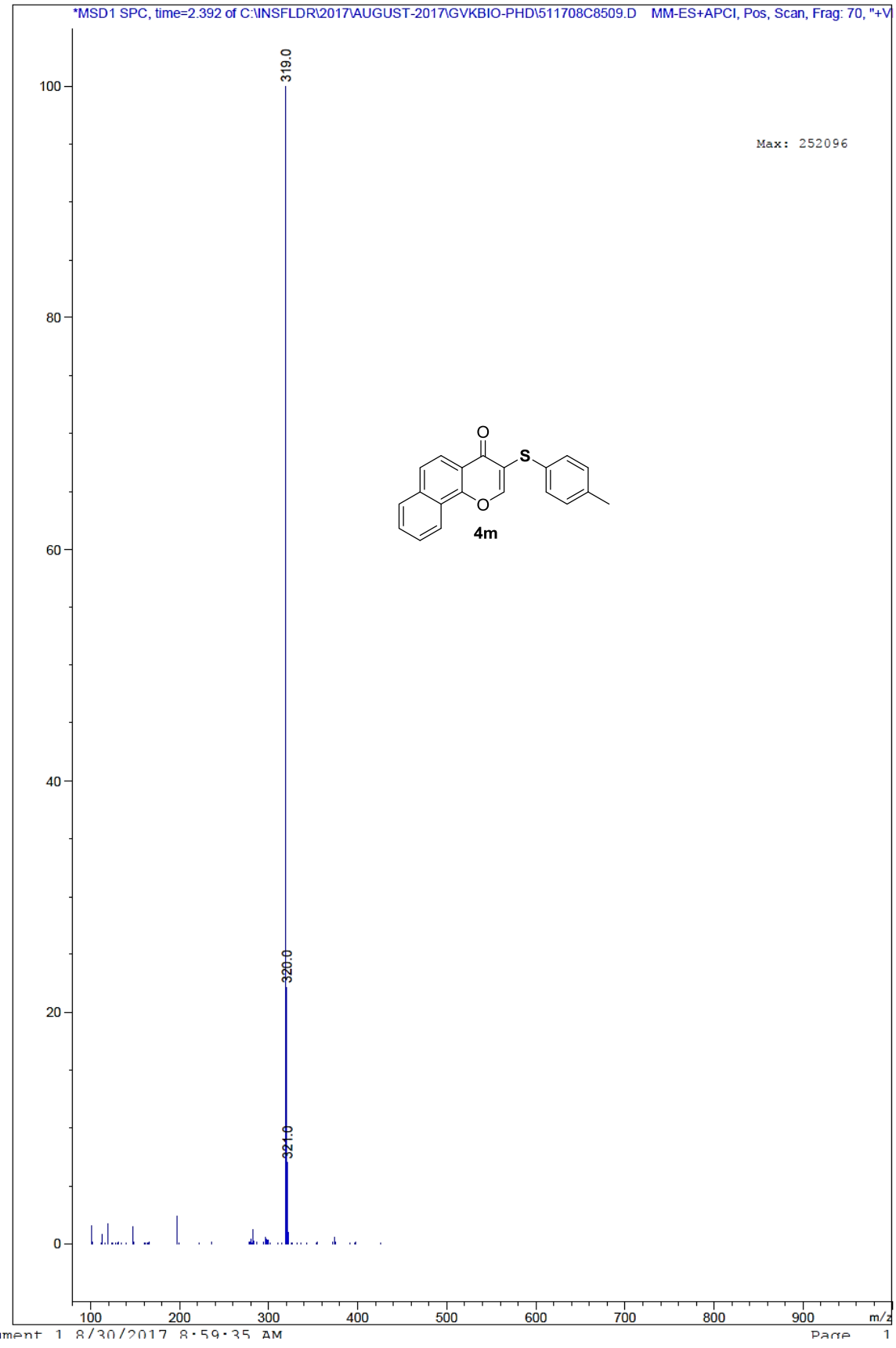
RND-FA-3.5 MIN.M
Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: B1: 0.1 % FA IN WATER A1: 0.1%FA IN ACN
Gradient: Time (min) /%A1: 0/2, 0.2/2, 2.3/98,3.4/98,3.41/2,3.5/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 50°C ->



DAD1 A, Sig=215,4 Ref=off

Pea No	RT min	Height	Area	Area %
1	2.39	553.595	577.247	98.947
2	2.76	5.197	6.142	1.053

MS Spectrum

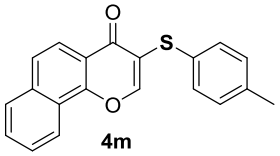


ument 1 8/30/2017 8:59:35 AM Page 1 of

Elemental Composition Report

Single Mass Analysis

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None



4m

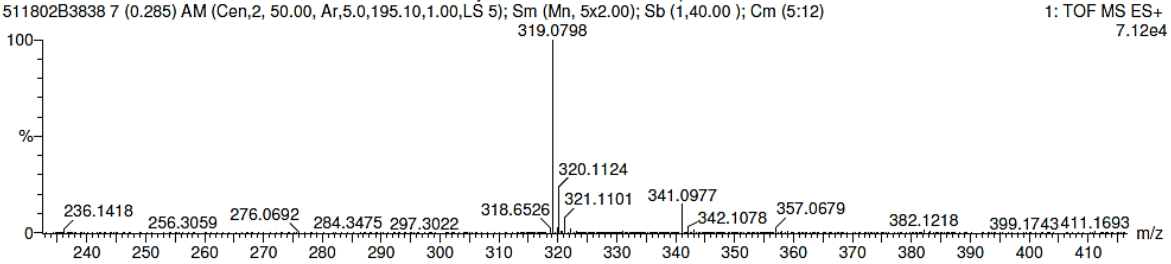
Monoisotopic Mass, Odd and Even Electron Ions
3 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-20 H: 0-15 O: 0-2 S: 0-1

GVK-CBK-1-Phd-57

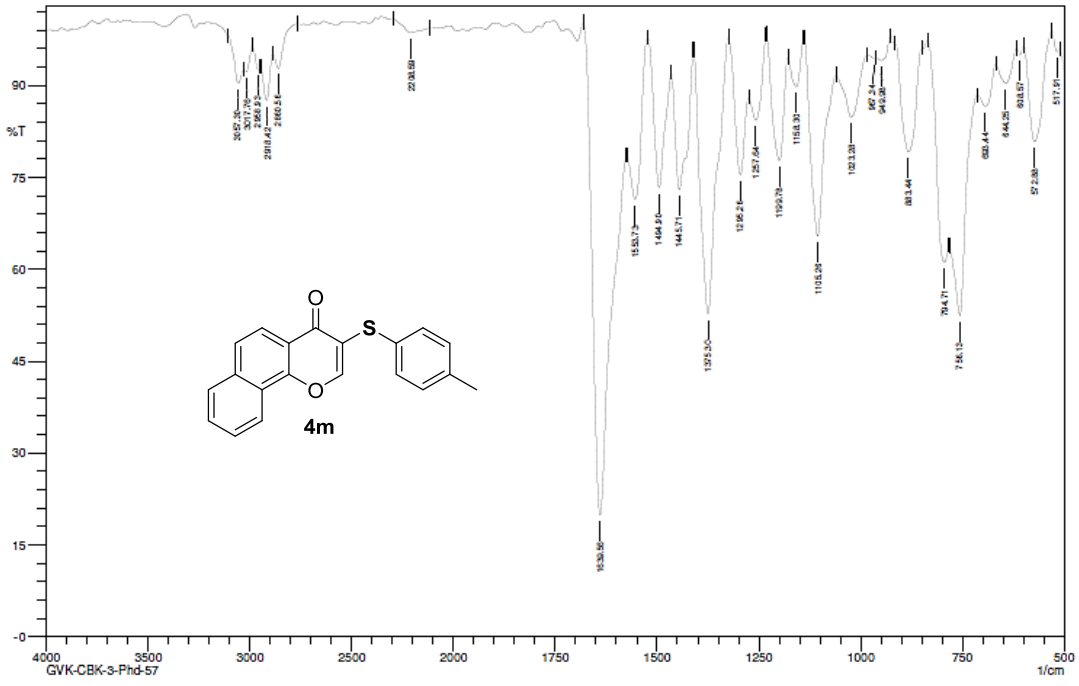
GVK Bio sciences (pvt)Ltd
Analytical Research and Development

Date of analysis:16-Feb-201815:26:55
Instru ment ID:ANL-MCL3-LCMS-001
1: TOF MS ES+
7.12e4

511802B3838 7 (0.285) AM (Cen,2, 50.00, Ar,5.0,195.10,1.00,LS 5); Sm (Mn, 5x2.00); Sb (1,40.00); Cm (5:12)



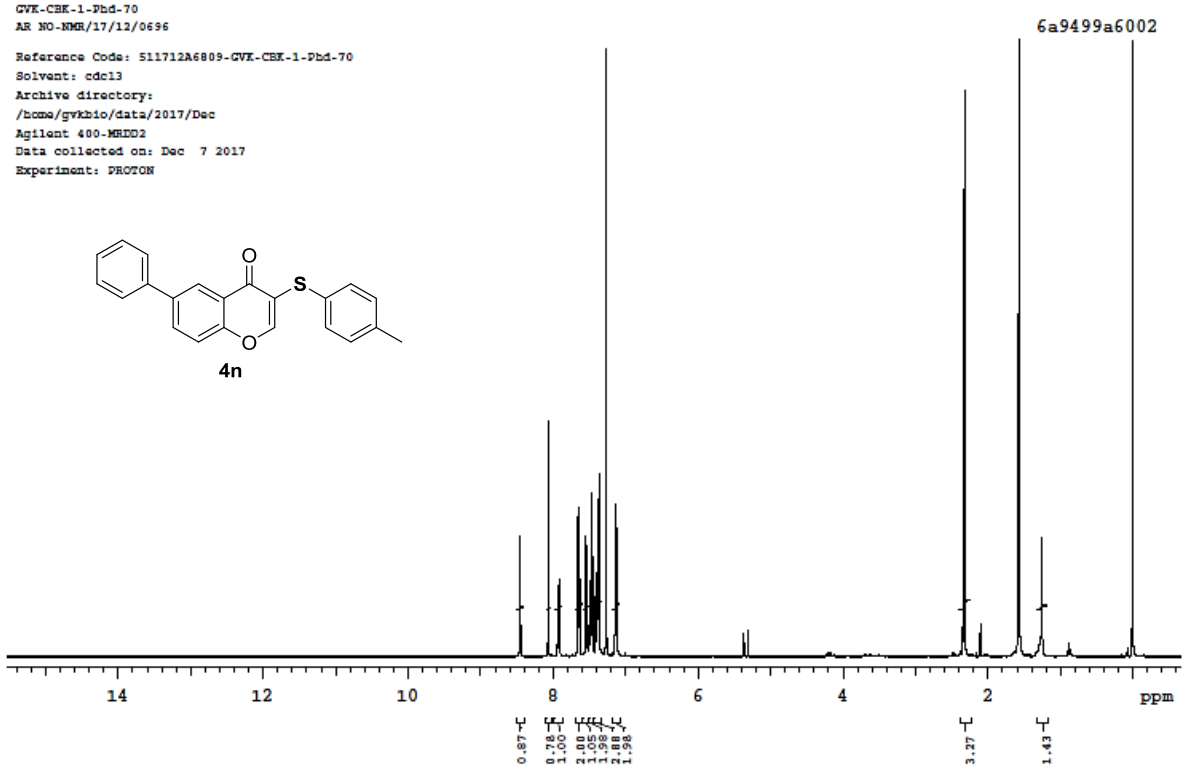
Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
319.0798	319.0793	0.5	1.6	13.5	549.2	C20 H15 O2 S

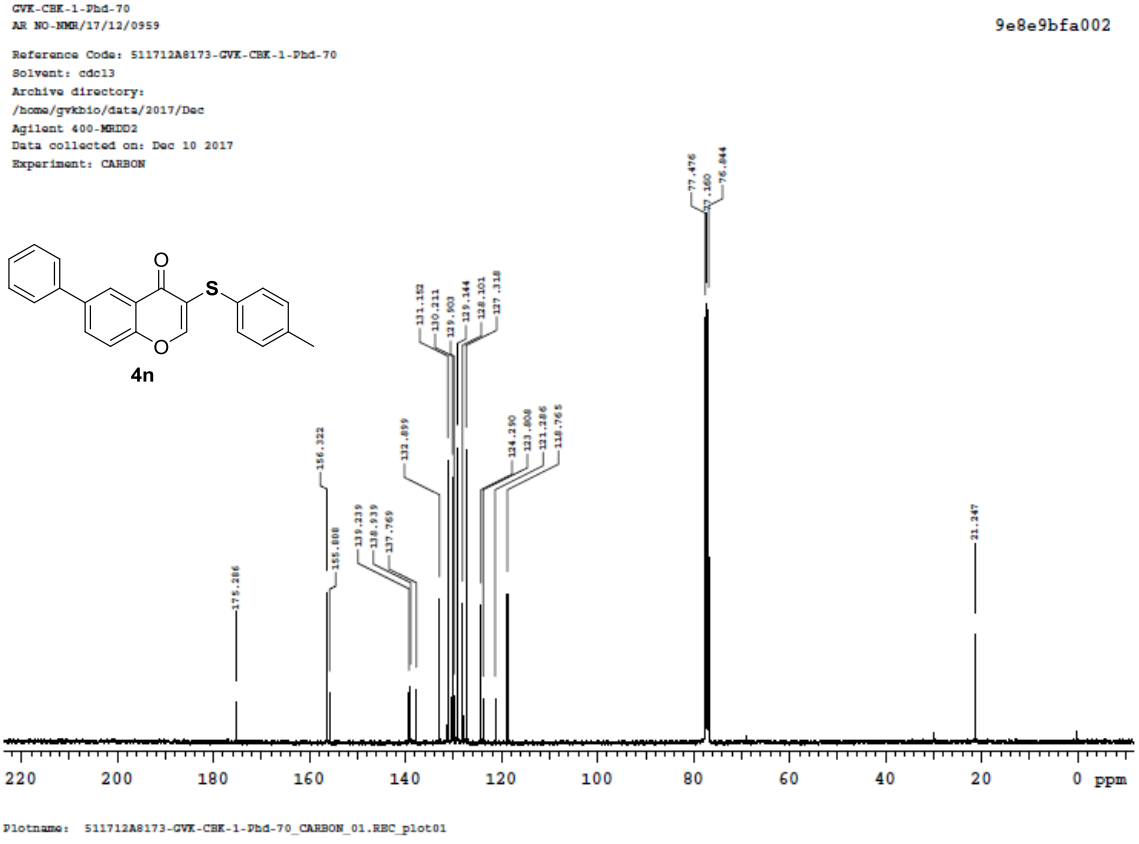


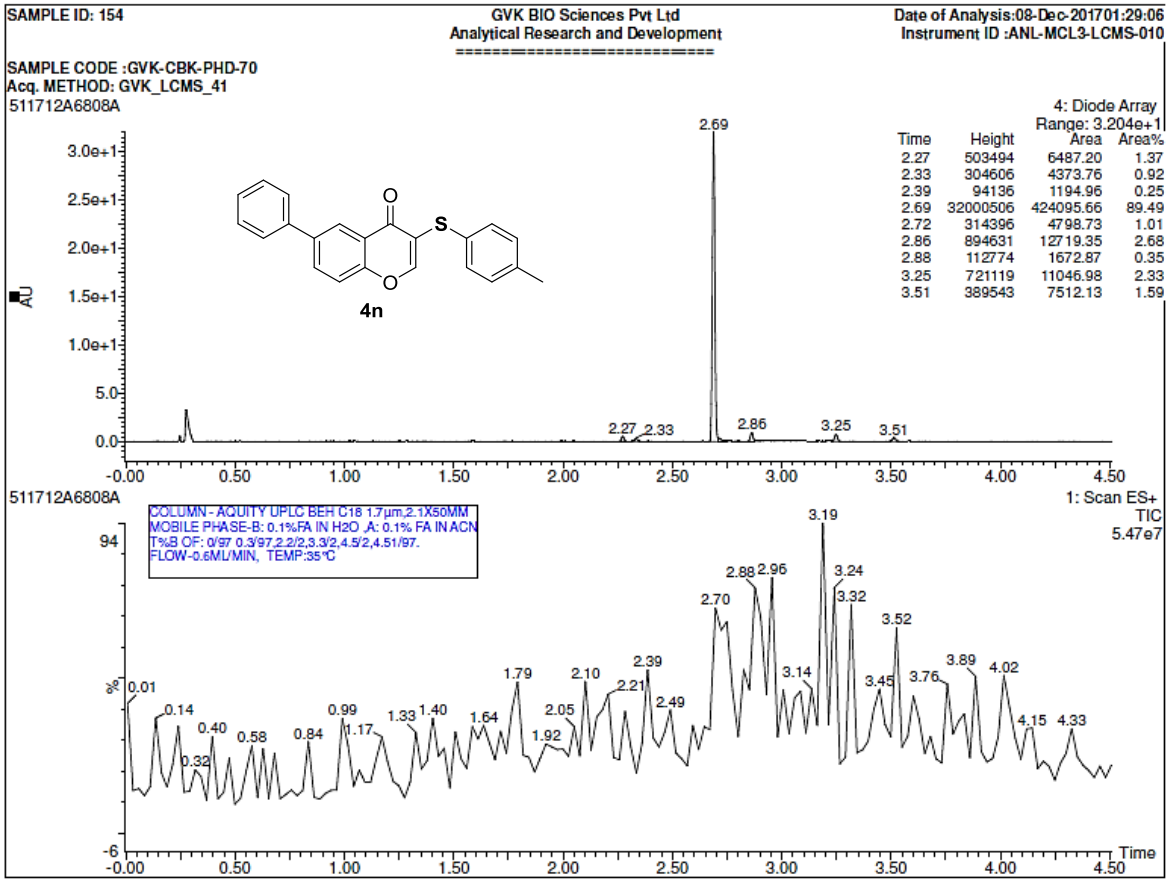
Comment: IN Kbr
GVK-CBK-3-Phd-57

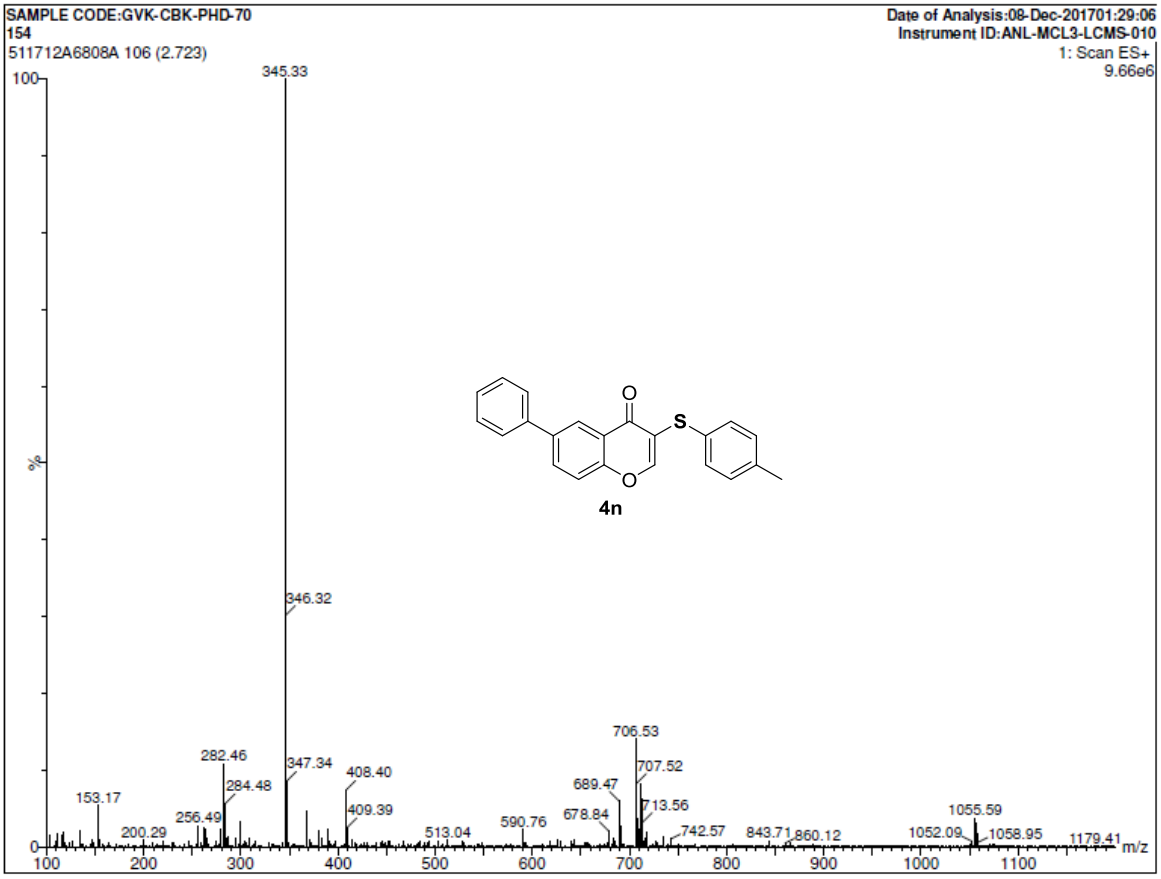
No. of Scans:
Resolution:
Apodization:

Date: 1/22/2018 12:16:19 PM
User: Admin


GVK-CBK-1-Phd-70
AR NO-NMR/17/12/0696
Reference Code: 511712A6809-GVK-CBK-1-Phd-70
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2017/Dec
Agilent 400-MRDD2
Data collected on: Dec 7 2017
Experiment: PROTON
6a9499a6002
4n
14
12
10
8
6
4
2
ppm


GVK-CBK-1-Phd-70
AR NO-NMR/17/12/0959
Reference Code: 511712A8173-GVK-CBK-1-Phd-70
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2017/Dec
Agilent 400-MRDD2
Data collected on: Dec 10 2017
Experiment: CARBON
9e8e9bfa002
4n
220
200
180
160
140
120
100
80
60
40
20
0 ppm
Plotname: 511712A8173-GVK-CBK-1-Phd-70_CARBON_01.REC_plot01

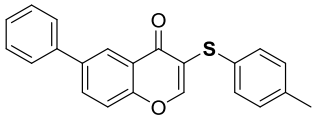

SAMPLE ID: 154
GVK BIO Sciences Pvt Ltd
Analytical Research and Development
Date of Analysis:08-Dec-201701:29:06
Instrument ID :ANL-MCL3-LCMS-010
SAMPLE CODE :GVK-CBK-PHD-70
Acq. METHOD: GVK_LCMS_41
511712A6808A
4: Diode Array
Range: 3.204e+1
Time Height Area Area%
2.27 503494 6487.20 1.37
2.33 304606 4373.76 0.92
2.39 94136 1194.96 0.25
2.69 32000506 424095.66 89.49
2.72 314396 4798.73 1.01
2.86 894631 12719.35 2.68
2.88 112774 1672.87 0.35
3.25 721119 11046.98 2.33
3.51 389543 7512.13 1.59
AU
4n
511712A6808A
1: Scan ES+
TIC
5.47e7
COLUMN - AQUITY UPLC BEH C18 1.7µm,2.1X50MM
MOBILE PHASE-B: 0.1%FA IN H2O ,A: 0.1% FA IN ACN
T%B OF: 0/97 0.3/97,2.2/2,3.3/2,4.5/2,4.51/97.
FLOW-0.6ML/MIN, TEMP:35°C
%
Time


SAMPLE CODE:GVK-CBK-PHD-70
154
Date of Analysis:08-Dec-201701:29:06
Instrument ID:ANL-MCL3-LCMS-010
511712A6808A 106 (2.723)
1: Scan ES+
9.66e6
%
4n
m/z

Elemental Composition Report

Single Mass Analysis (displaying only valid results)

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None



4n

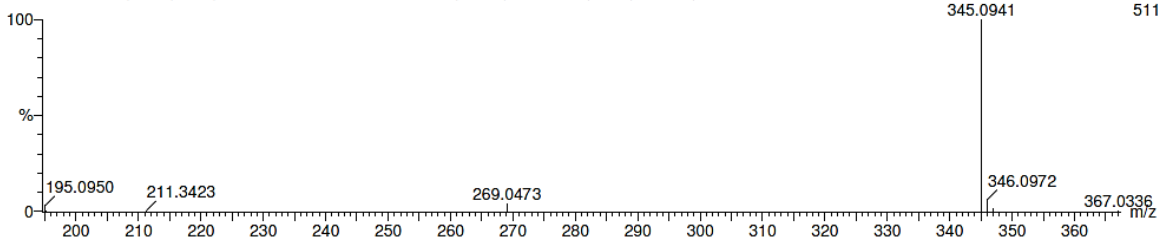
Monoisotopic Mass, Even Electron Ions
3 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-22 H: 0-17 O: 0-2 S: 0-1

GVK-CBK-Phd-70

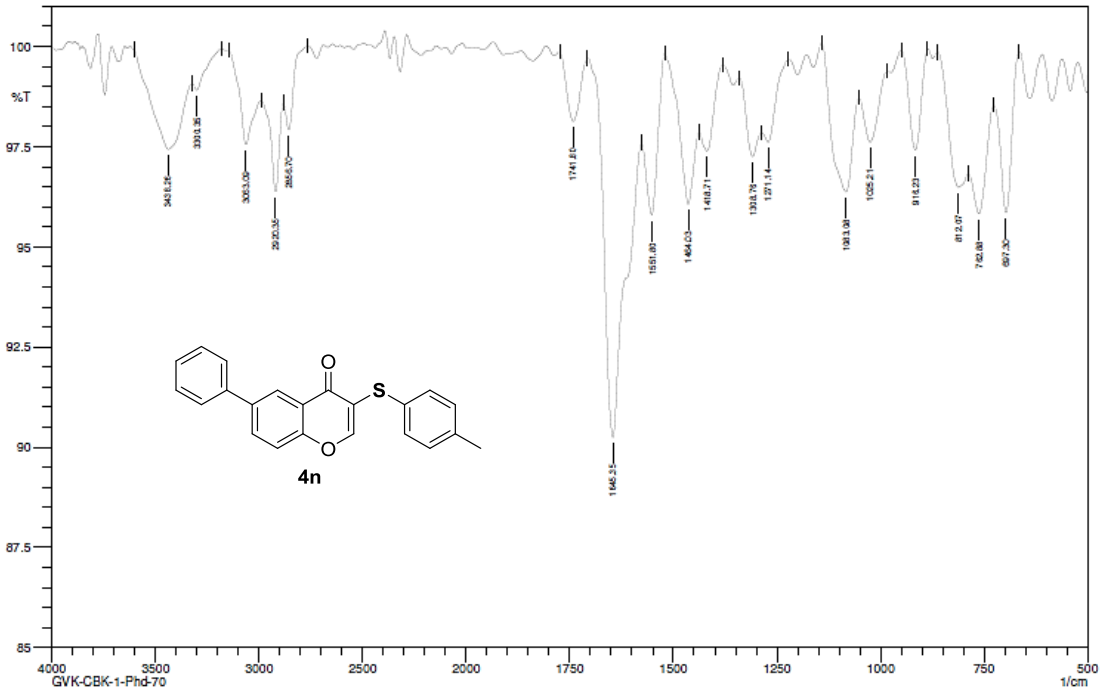
GVK Bio sciences (pvt)Ltd
Analytical Research and Development

Date of analysis:08-Dec-201716:20:13
Instru ment ID:ANL-MCL3-LCMS-001
2: TOF MS ES+

511712A8084 9 (0.354) AM (Cen,2, 50.00, Ar,5.0,195.10,1.00); Sm (Mn, 5x2.00); Sb (1,40.00)



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
345.0941	345.0949	-0.8	-2.3	14.5	106.0	C22 H17 O2 S

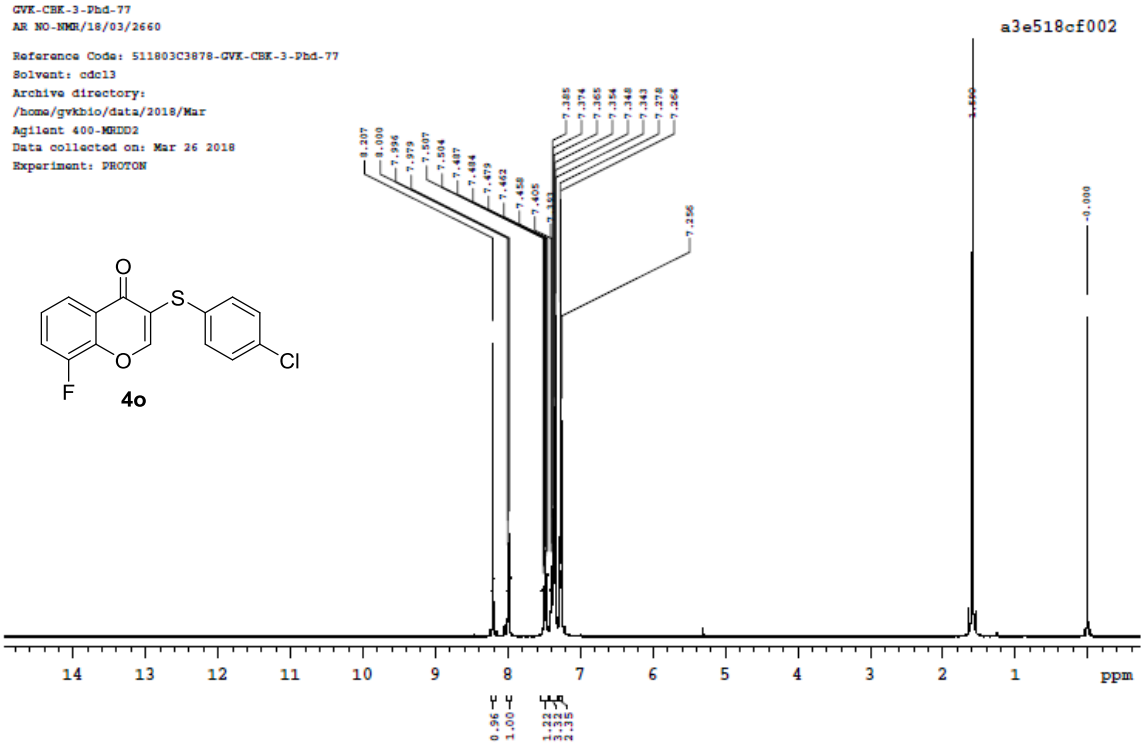


4n

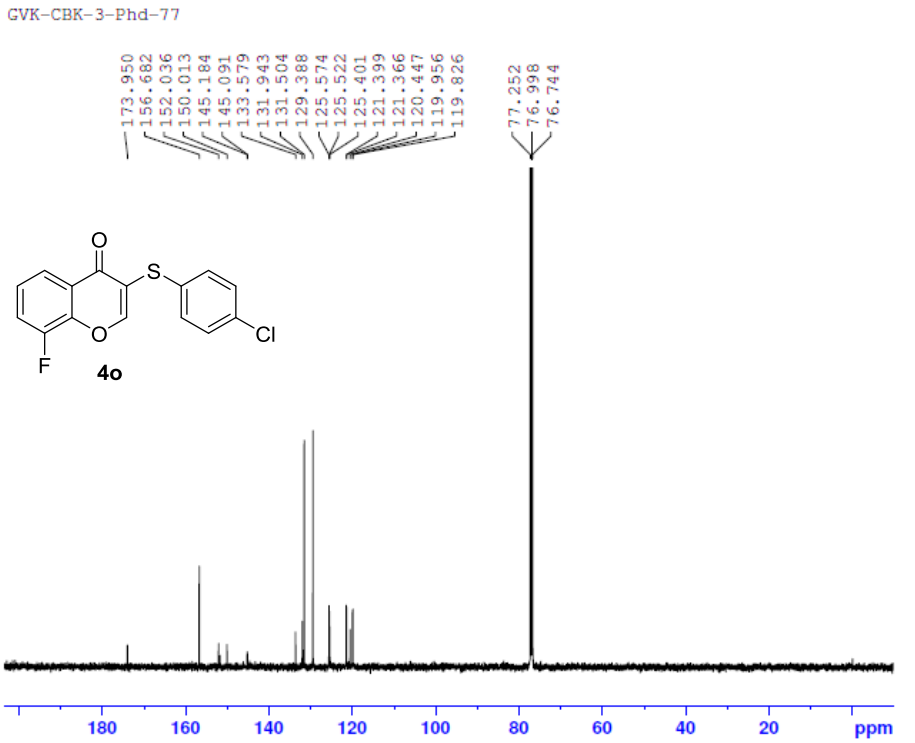
Comment: IN Kbr
GVK-CBK-1-Phd-70

No. of Scans:
Resolution:
Apodization:

Date: 1/10/2018 11:59:31 AM
User: Admin



Plotname: 511803C3878-GVK-CBK-3-Phd-77_PROTON_01.REC_plot01

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Current Data Parameters
NAME          511803D0375
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_              20180331
Time                  9.48 h
INSTRUM              spect
PROBHD    z119470_0294 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   256
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             3.00000000 sec
D11            0.03000000 sec
TD0                    1
SFO1           125.7703643 MHz
NUC1                  13c
P1                 10.00 usec
PLW1           79.88800049 W
SFO2           500.1320005 MHz
NUC2                  1H
CPDPRG[2           waltz16
PCPD2              90.00 usec
PLW2           20.38699913 W
PLW12           0.25169000 W
PLW13           0.16023000 W

F2 - Processing parameters
SI                 32768
SF             125.7577936 MHz
WDW                   EM
SSB                    0
LB                  2.00 Hz
GB                     0
PC                  1.40
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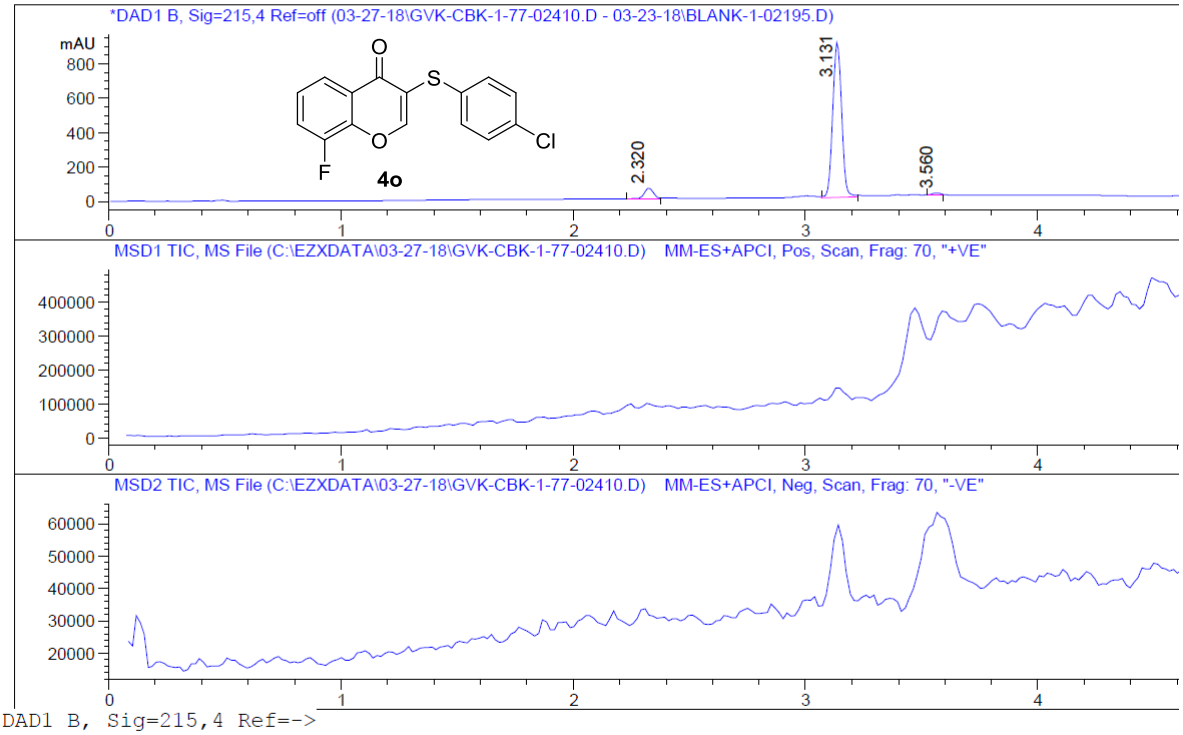
LC/MS REPORT

```
================================================================================
Data file       :C:\EZXDATA\03-27-18\GVK-CBK-1-77-02410.D
Injection Date  :27-Mar-2018     08:25:15 PM              Vial position:  Vial 84
Sample Name :    BIAT-005554C(BI01700605)- ->             Instrument Name:ANL-MCL2-LCMS-0
                                                        Injection Vol::       4.000
================================================================================
```

GVK_LCMS_19

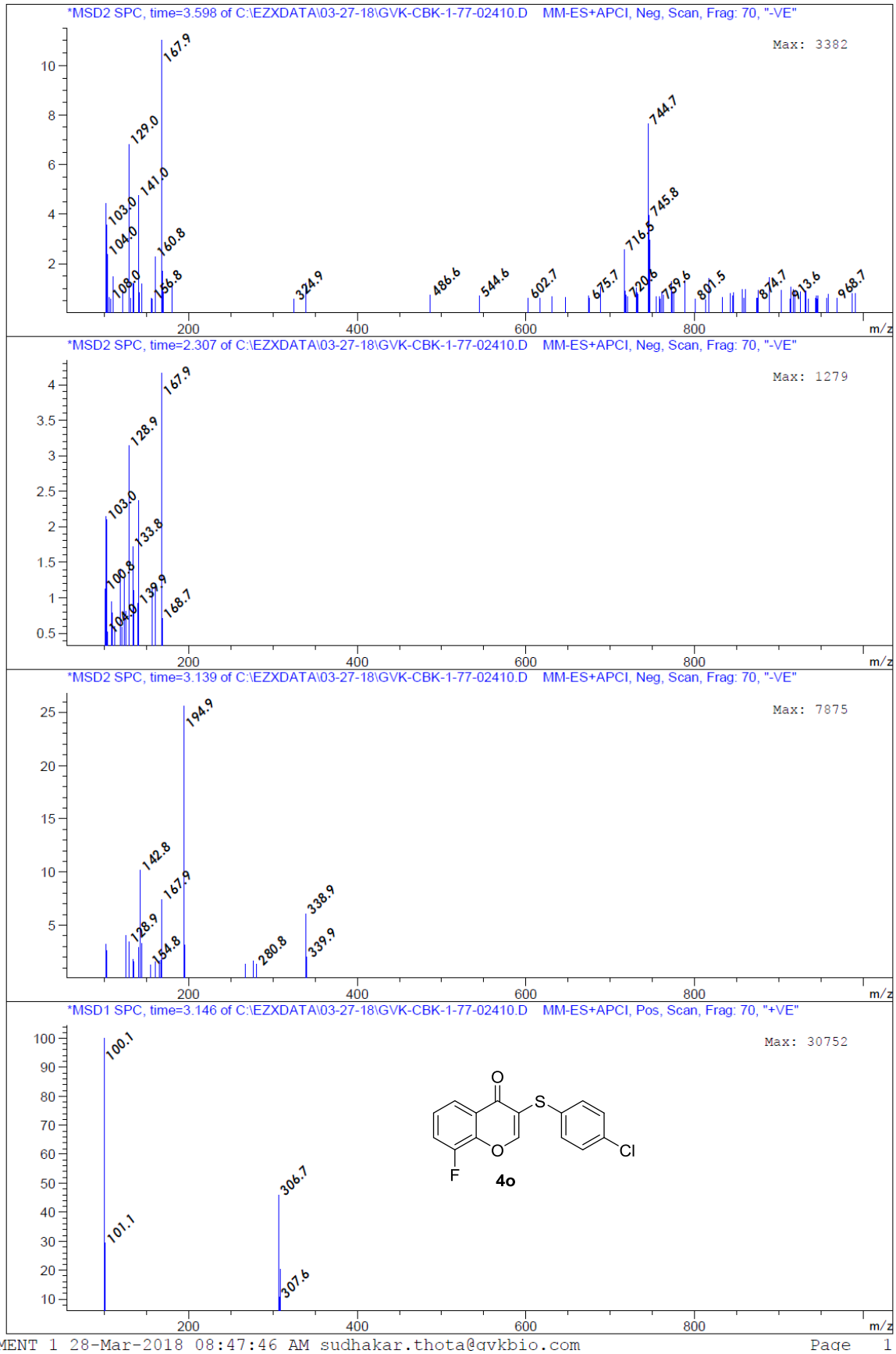
```
================================================================================
```



DAD1 B, Sig=215,4 Ref=->

PEAK No	RT min	Area	Area %
1	2.320	219.153	8.040
2	3.131	2479.407	90.966
3	3.560	27.080	0.994

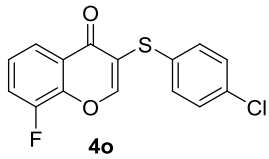
MS Spectrum



RUMENT 1 28-Mar-2018 08:47:46 AM sudhakar.thota@gvkbio.com Page 1 o

Single Mass Analysis (displaying only valid results)

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None



4o

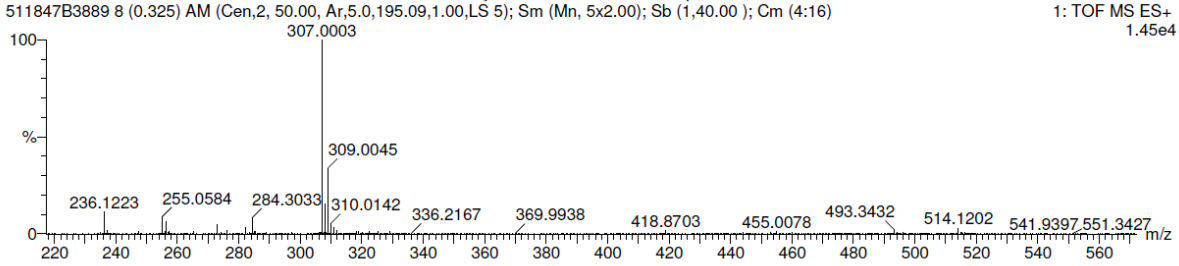
Monoisotopic Mass, Odd and Even Electron Ions
22 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-15 H: 0-9 O: 0-2 F: 0-1 S: 0-1 Cl: 0-1

GVK-CBK-1-77

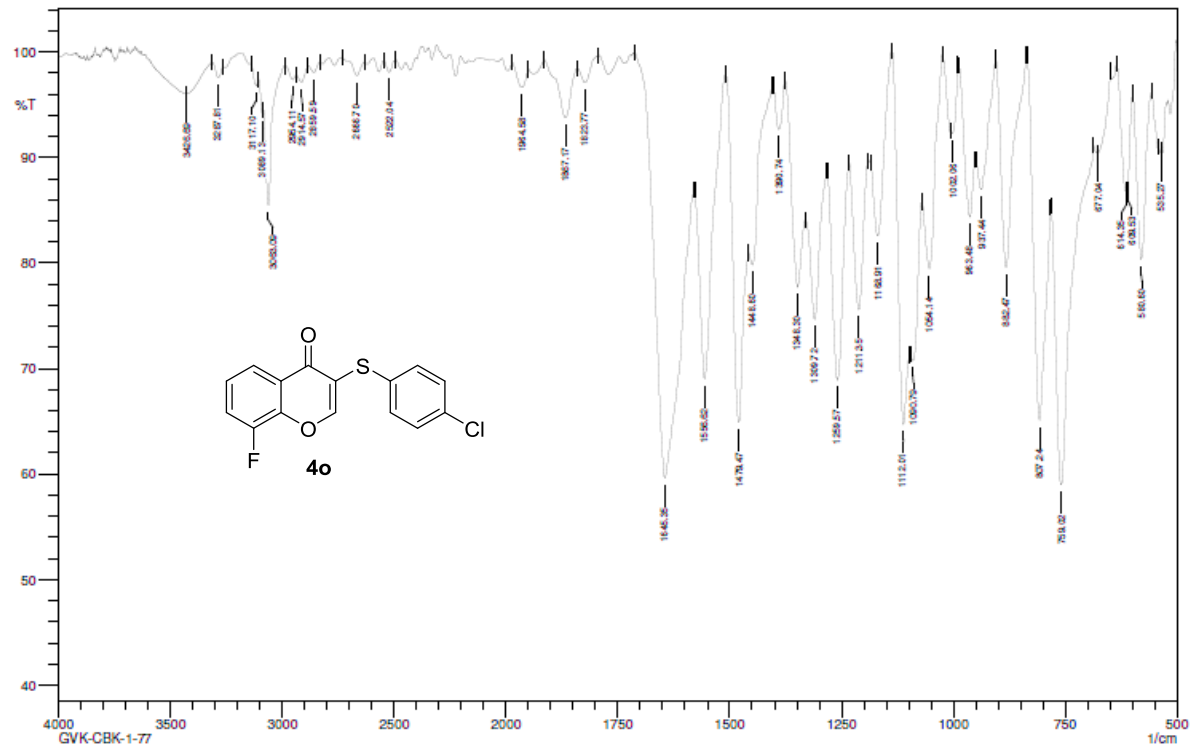
GVK Bio sciences (pvt)Ltd
Analytical Research and Development

Date of analysis:11-Apr-201816:13:30
Instru ment ID:ANL-MCL3-LCMS-001
1: TOF MS ES+
1.45e4

511847B3889 8 (0.325) AM (Cen,2, 50.00, Ar,5.0,195.09,1.00,LS 5); Sm (Mn, 5x2.00); Sb (1,40.00); Cm (4:16)



Minimum:				-1.5		
Maximum:		50.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
307.0003	306.9996	0.7	2.3	10.5	54.1	C15 H9 O2 F S Cl



omment: IN Kbr
VK-CBK-1-77

No. of Scans:
Resolution:
Apodization:

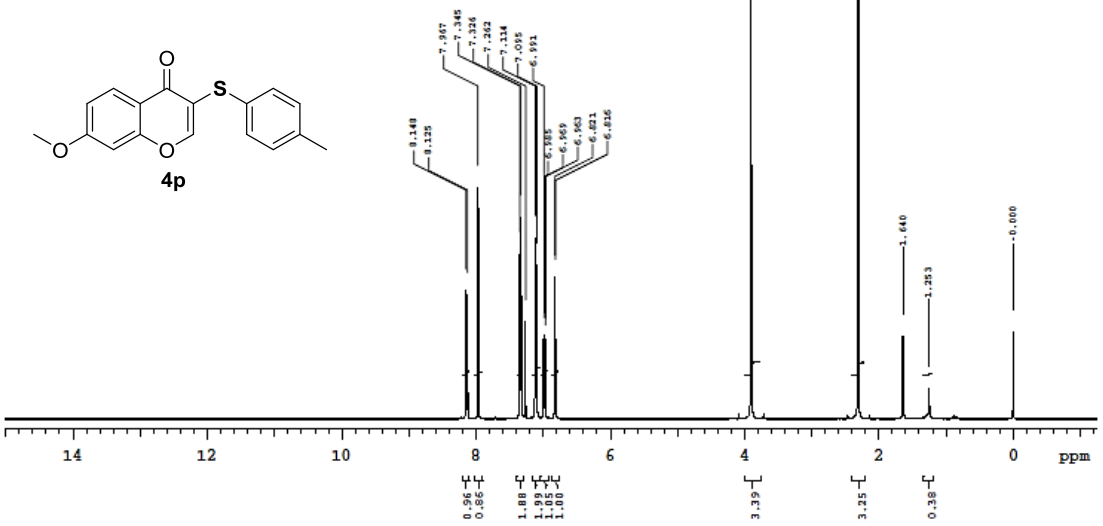
Date: 4/2/2018 1:11:11 PM
User: Admin

GVK-CBK-1-Phd-71
AR NO-NMR/17/12/0960

c762fe3e002

Reference Code: 511712A8174-GVK-CBK-1-Phd-71
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2017/Dec
Agilent 400-MRDD2
Data collected on: Dec 10 2017
Experiment: PROTON

4p

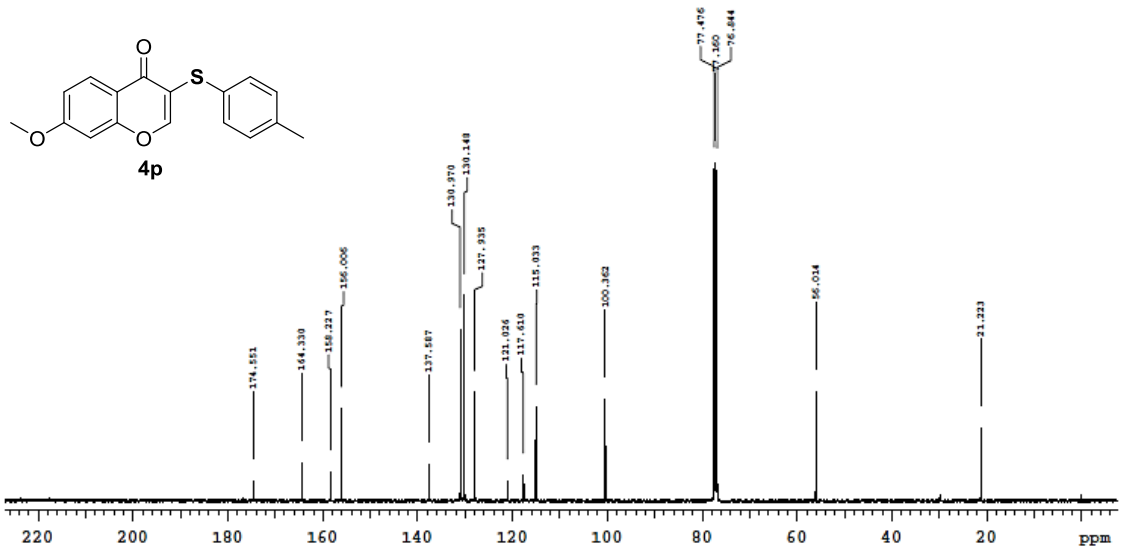


GVK-CBK-1-Phd-71
AR NO-NMR/17/12/0960

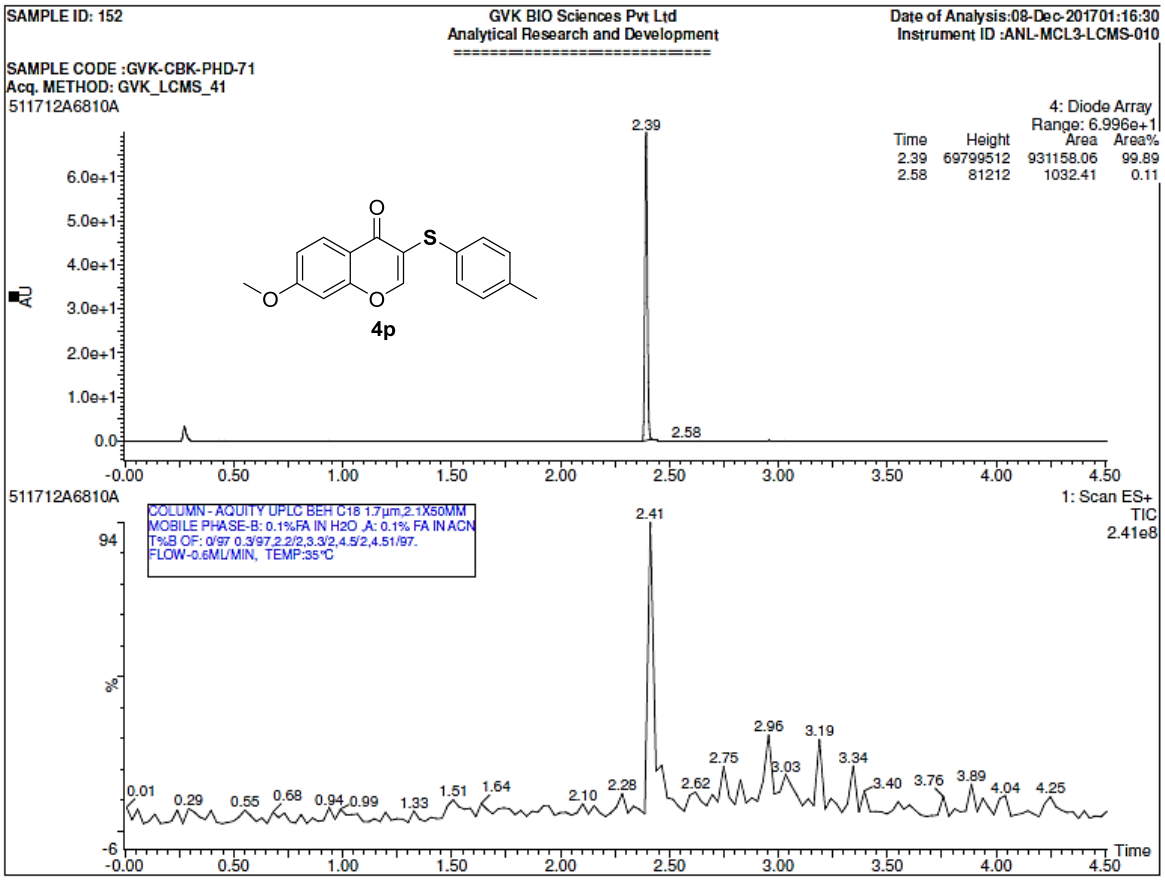
8e7bf3dd002

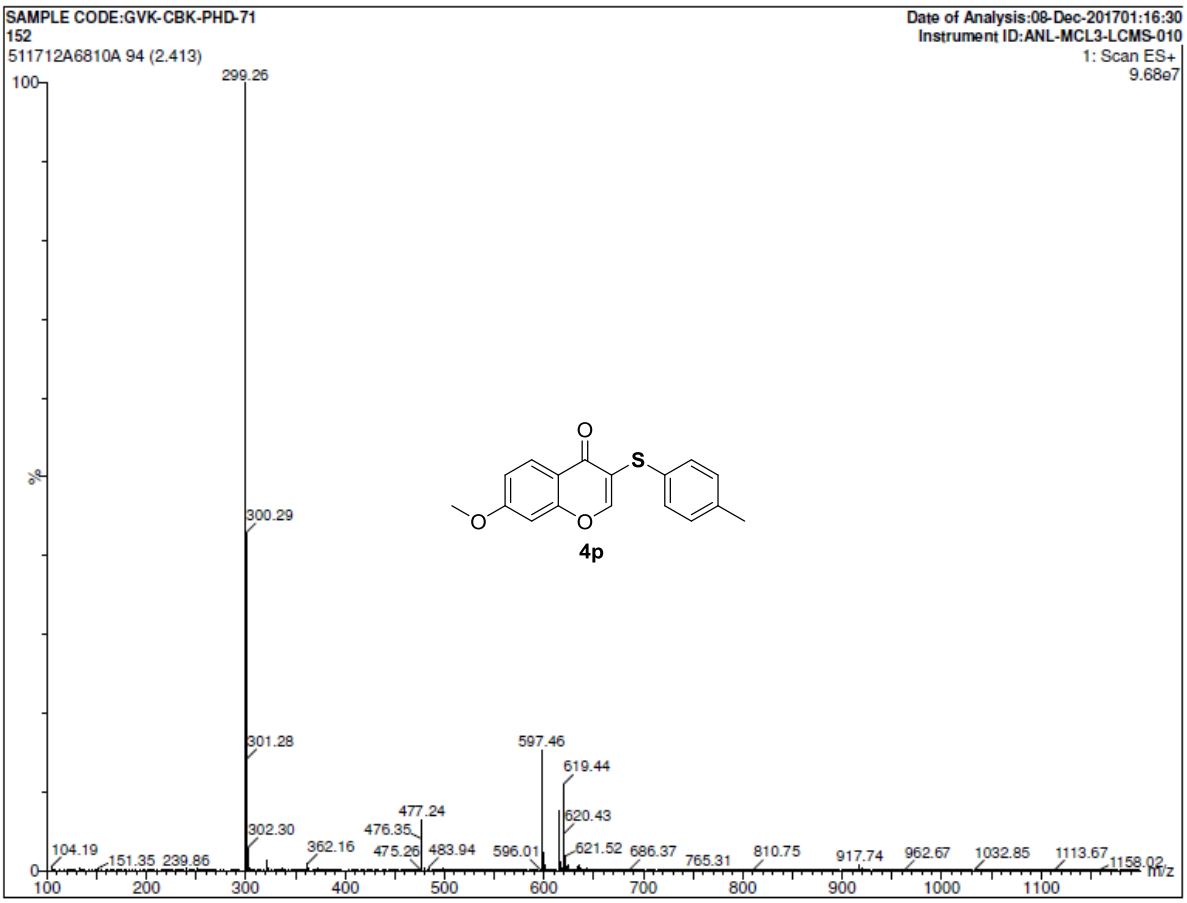
Reference Code: 511712A8174-GVK-CBK-1-Phd-71
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2017/Dec
Agilent 400-MRDD2
Data collected on: Dec 10 2017
Experiment: CARBON

4p



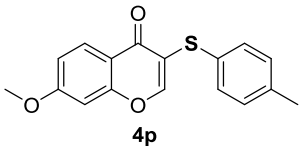
Plotname: 511712A8174-GVK-CBK-1-Phd-71_CARBON_01.REC_plot01


SAMPLE ID: 152
GVK BIO Sciences Pvt Ltd
Analytical Research and Development
Date of Analysis:08-Dec-201701:16:30
Instrument ID :ANL-MCL3-LCMS-010
SAMPLE CODE :GVK-CBK-PHD-71
Acq. METHOD: GVK_LCMS_41
511712A6810A
4: Diode Array
Range: 6.996e+1
Time Height Area Area%
2.39 69799512 931158.06 99.89
2.58 81212 1032.41 0.11
4p
AU
2.39
2.58
511712A6810A
1: Scan ES+
TIC
2.41e8
COLUMN - ACQUITY UPLC BEH C18 1.7µm,2.1X50MM
MOBILE PHASE-B: 0.1%FA IN H2O ,A: 0.1% FA IN ACN
T%B OF: 0/97 0.3/97,2.2/2,3.3/2,4.5/2,4.51/97.
FLOW-0.6ML/MIN, TEMP:35°C
2.41
Time


SAMPLE CODE:GVK-CBK-PHD-71
152
Date of Analysis:08-Dec-201701:16:30
Instrument ID:ANL-MCL3-LCMS-010
511712A6810A 94 (2.413)
1: Scan ES+
9.68e7
4p
299.26
300.29
301.28
597.46
619.44
620.43
477.24
476.35
475.26
302.30
362.16
483.94
596.01
621.52
686.37
765.31
810.75
917.74
962.67
1032.85
1113.67
1158.02
104.19
151.35
239.86
m/z

Single Mass Analysis (displaying only valid results)

Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None



4p

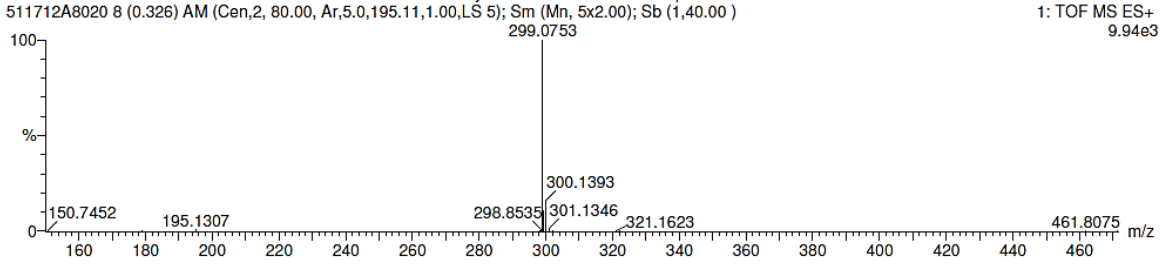
Monoisotopic Mass, Odd and Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-17 H: 0-15 O: 0-3 S: 0-1

GVK-CBK-Phd-71

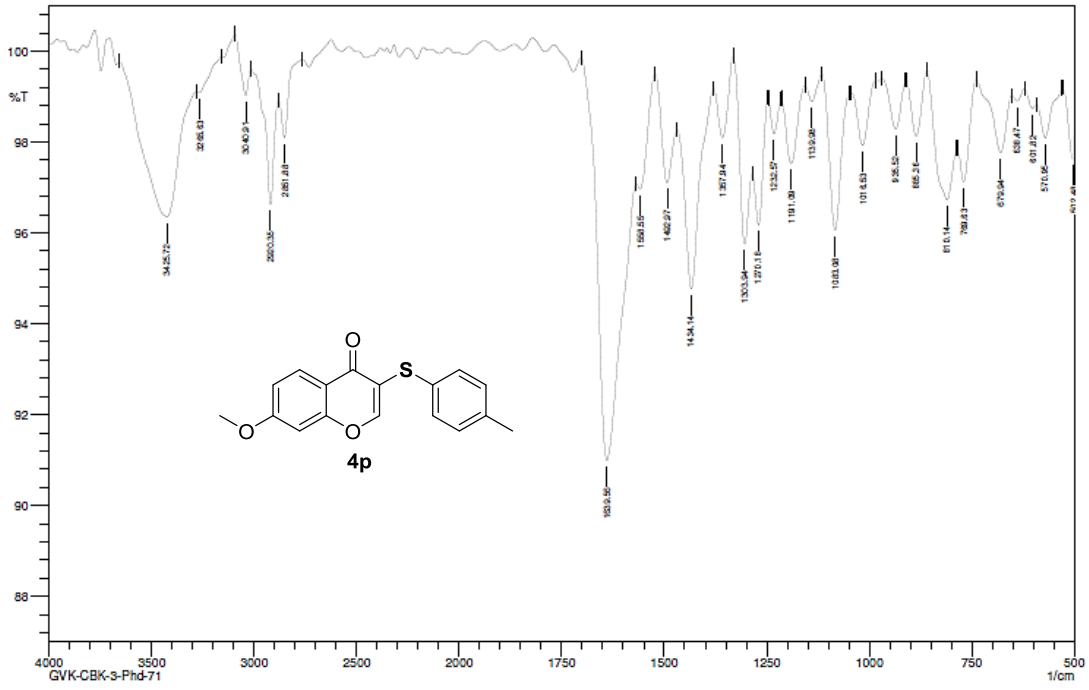
GVK Bio sciences (pvt)Ltd
Analytical Research and Development

Date of analysis:08-Dec-201716:00:26
Instru ment ID:ANL-MCL3-LCMS-001
1: TOF MS ES+
9.94e3

511712A8020 8 (0.326) AM (Cen,2, 80.00, Ar,5.0,195.11,1.00,LS 5); Sm (Mn, 5x2.00); Sb (1,40.00)



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
299.0753	299.0742	1.1	3.7	10.5	999.6	C17 H15 O3 S



Comment: IN Kbr
GVK-CBK-3-Phd-71

No. of Scans:
Resolution:
Apodization:

Date: 1/22/2018 12:11:07 PM
User: Admin