Supporting Information

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Synthesis of Novel Fused Chromone-Pyrimidine Hybrids and 2, 4, 5-Trisubstituted Pyrimidine Derivatives via the ANRORC Rearrangement

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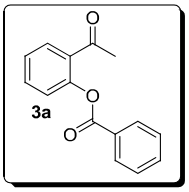
Contents

1. General

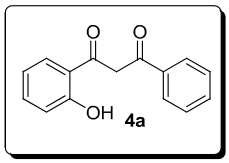
Dry solvents were purchased from chemical suppliers and used without further purification. Analytical thin-layer chromatography (TLC) was performed on commercially available Merck TLC Silica gel 60 F_{254}. Silica gel column chromatography was performed on silica gel 60 (spherical 100-200 μm). IR spectra 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.

***Experimental Procedure for the Preparation of 2-acetylphenyl benzoate (3a)*:**



To a stirred solution of 2-hydoxy acetophenone (**1a)** (2 g, 14.68 mmol) in pyridine (3 ml) was added benzoyl chloride (**2a**) (2.9 g, 20.56 mmol) at 0 ^{0}C and the reaction mixture was stirred at RT for 1h. The progress of the reaction was monitored by TLC (5% Ethyl acetate in petroleum ether) showed completion of the reaction. After completion of the reaction; the reaction mixture was poured in to ice cold 1N HCl (70 ml) and stirred at RT for 2 h. The solid was filtered and washed with water and dried under vacuum to give the crude product. The crude product was washed with *n*-pentane to afford the pure compound **3a** (3 g, 85%) as an off white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.22 (d, 2H), 7.87 (d, 1H), 7.68 (m, 1H), 7.56 (m, 3H), 7.39 (t, 1H), 7.25 (m, 1H), 2.54 (s, 3H). MS (EI): *m/z* 240 (M+1,100).

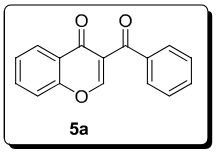
Experimental Procedure for the Preparation of 1-(2-hydroxyphenyl)-3- phenylpropane-1,3-dione (4a):



To a stirred solution of compound **3a** (2.7g, 11.25mmol) in pyridine (10 ml) was added NaOH powder (675 mg, 16.87 mmol) at 50 ^{0}C and the reaction mixture was stirred at the same temperature for 1h. The reaction mixture became thick solid. The progress of the reaction was monitored by TLC (10% Ethyl acetate in petroleum ether) showed completion of the reaction. After completion of the reaction; the reaction mixture was acidified with 20 % acetic acid solution and stirred at RT for 3 h. The yellow coloured solid was filtered and washed with water and dried under vacuum to afford the pure compound **4a** (2.4 g, 90%) as a yellow coloured solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 15.54 (s, 1H), 12.09 (s, 1H), 7.93 (m, 2H), 7.78 (dd, 1H), 7.75 (m, 1H), 7.50 (m, 3H), 7.01 (dd, 1H), 6.90 (t, 1H), 6.85 (s, 1H). MS (EI): *m/z* 240 (M+1,100).

(Note: compound 4 1H-NMR shows keto enol form)

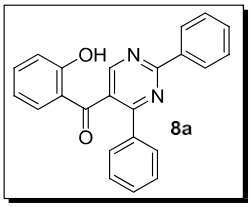
Experimental Procedure for the Preparation of 3-benzoyl-4H- chromen- 4-one (5a):



To a stirred solution of compound **4a** (6 g, 25.00 mmol) in toluene (60 ml) was added DMF-DMA (17 ml, 75.00 mmol) at 5 ^{0}C and the reaction mixture was

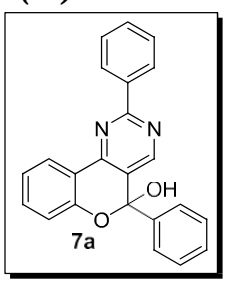
heated to 80 ^{0}C for 1h. The progress of the reaction was monitored by TLC (10% Ethyl acetate in petroleum ether) showed completion of the reaction. After completion of the reaction; the reaction mixture was evaporated to afford the crude compound which was purified by silica gel column chromatography (15 % EtOAc/petroleum ether) to gave the pure compound **5a** (5.5 g, 88%) as an off white solid. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.38 (m, 2H), 7.87 (dd, 2H), 7.76 (t, 1H), 7.57 (m, 2H), 7.48 (m, 3H). MS (EI): *m/z* 250 (M+1,100).

2, 4-diphenylpyrimidin-5-yl)(2-hydroxyphenyl)methanone (8a):



25 % NaOMe (0.8 ml, 3.6 mmol) in methanol was taken in methanol under N2 atm, to this compound **6a** (0.313 g, 2.00 mmol) was added at RT and stirred for 5 min. Then compound **5a** was added and stirred the reaction mixture at RT for 16 h. The progress of the reaction was monitored by TLC (20% Ethyl acetate in petroleum ether) showed completion of the reaction. After completion of the reaction; the reaction mixture evaporated to afford the crude compound which was purified by silica gel column chromatography (5 % EtOAc/petroleum ether) to gave the pure compound **8a** (0.150 g, 21%) as an off white solid. M.p. 129-133 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 11.90 (s, 1H), 8.87 (s, 1H),8.64 (m, 2H), 7.76 (dd, 2H),7.56 (m, 3H), 7.39 (m, 4H), 7.36 (d, 1H), 7.01 (dd, 1H), 6.72 (t, 1H). IR (KBr, cm^{-1}): 3227, 3058, 1971, 1621, 1549, 1419, 1332, 1240, 922, 742, 692. ^{13}C NMR (100 MHz, DMSO-d6) = 196.3, 163.3, 159.3, 156.9, 136.8, 136.8, 136.5, 136.0, 131.4, 130.9, 130.2, 130.2, 129.0, 129.0, 128.8, 128.4, 128.4, 128.1, 128.1, 122.3, 122.3, 119.3, 117.3. MS (EI): *m/z* 352 (M+1,100), HRMS: (ESI): Calcd for: $C_{23}H_{16}N_2O_2$ [M+H]: 353.1212; Found: 353.1320

Experimental Procedure for the Preparation of 2, 5-diphenyl-5H-chromeno [4, 3-d] pyrimidin-5-ol (7a):



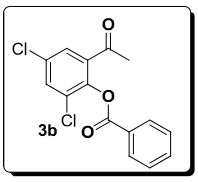
Elution of the column with 10% EtOAc/petroleum ether to gave the pure compound **7a** (0.400 g**,** 57%**)** as an off white solid. M.p. 171-175 °C. ^{1}H

NMR (400 MHz, DMSO-d6): δ = 8.52 (m, 3H), 8.31 (d, 2H), 7.62 (m, 6H), 7.48 (m, 3H), 7.27 (t, 1H), 7.17 (d, 1H). IR (KBr, cm^{-1}): 3469, 3169, 1757, 1598, 1552, 1418, 1048, 957, 753, 692. ^{13}C NMR (100 MHz, CD_3COCD_3) = 164.8, 156.6, 155.8, 154.5, 142.5, 138.4, 131.7, 131.9, 134.5, 131.9, 129.8, 129.7, 129.5, 129.1, 127.9, 126.2, 125.8, 125.3, 123.2, 121.0, 120.8, 119.1, 99.9. MS (EI): *m/z* 352 (M+1,100), HRMS: (ESI): Calcd for: $C_{23}H_{16}N_2O_2$ [M+H]: 353.1212; Found: 353.1316

We confirmed the compounds 7a & 8a by 1H-NMR, N^{15}-HMBC, NOE, HMBC, HSQC, LC-MS and HRMS data

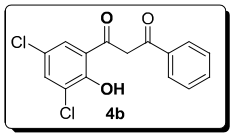
Note: Similarly we prepared the compounds (**1 to 20**) using the above general procedures in quantitative yield.

2-acetyl-4, 6-dichlorophenyl benzoate (3b):



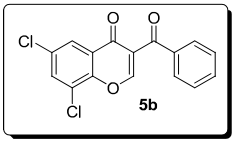
^1H NMR (400 MHz, $CDCl_3$): δ = 8.21 (dd, 2H), 7.60 (m, 3H), 7.50(m, 2H), 2.52 (s, 3H). MS (EI): *m/z* 307 (M-1,100).

1-(3,5-dichloro-2-hydroxyphenyl)-3-phenylpropane-1,3-dione(4b):



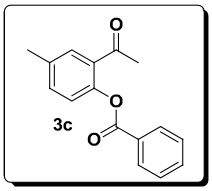
^1H NMR (400 MHz, $CDCl_3$): δ = 15.3 (s, 1H), 12.72 (d, 2H), 7.95 (m, 2H), 7.60 (m, 6H), 6.77 (s, 1H), 2.65 (s, 2H). MS (EI): *m/z* 307 (M+1,100). (Note: compound 4a 1H-NMR showed keto enol form)

3-benzoyl-6,8-dichloro-4H-chromen-4-one (5b):



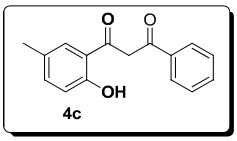
^1H NMR (400 MHz, $CDCl_3$): δ = 8.33 (s, 1H), 8.12 (d, 1H), 7.83 (m, 2H), 7.79 (d, 1H), 7.62 (m, 1H), 7.48 (m, 2H). MS (EI): *m/z* 318 (M+1,100).

2-acetyl-4-methylphenyl benzoate (3c):



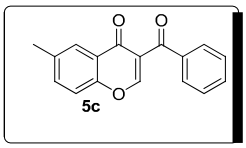
^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.21 (m, 2H), 7.65 (m, 2H), 7.52 (m, 2H), 7.37 (m, 1H), 7.12 (d, 1H), 2.52 (s, 3H).2.42 (s, 3H). MS (EI): *m/z* 254 (M-1,100).

1-(2-hydroxy-5-methylphenyl)-3-phenylpropane-1,3-dione (4c):



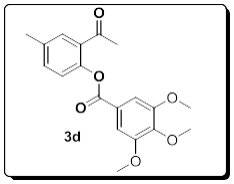
^{1}H NMR (400 MHz, $CDCl_3$): δ = 15.6 (s, 1H), 11.90 (s, 1H), 7.94 (d, 2H), 7.51 (m, 5H), 7.27 (m, 1H), 6.92 (d, 1H), 2.3 (s, 3H). MS (EI): *m/z* 254 (M+1,100) (Note: compound 4a 1H-NMR shows keto enol form)

3-benzoyl-6-methyl-4H-chromen-4-one (5c):



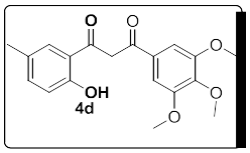
^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.27 (s, 1H), 8.04 (d, 1H), 7.85 (m, 2H), 7.57 (m, 2H), 7.44 (m, 3H), 2.47 (s, 3H). MS (EI): *m/z* 264 (M+1,100).

2-acetyl-4-methylphenyl 3, 4, 5-trimethoxybenzoate (3d):



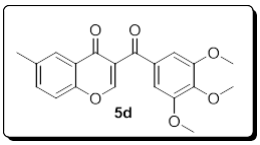
^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.65 (d, 1H), 7.46 (s, 2H), 7.38 (m, 1H), 7.12 (d, 1H), 3.94 (s, 9H). 2.54 (s, 3H), 2.42 (s, 3H). MS (EI): *m/z* 344 (M-1,100).

1-(2-hydroxy-5-methylphenyl)-3-(3,4,5-trimethoxyphenyl)propane-1,3-dione (4d):



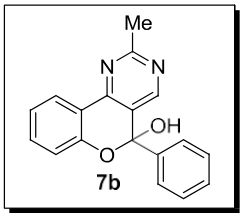
^{1}H NMR (400 MHz, $CDCl_3$): δ = 15.92 (s, 1H), 11.9 (s, 1H), 7.50 (d, 1H), 7.27 (d, 1H), 7.20 (m, 2H), 6.95 (m, 1H), 6.7 (d, 1H), 3.95 (s, 9H). 2.25 (s, 3H). MS (EI): *m/z* 344 (M+1,100). (Note: compound 4a 1H-NMR shows keto enol form)

6-methyl-3-(3,4,5-trimethoxybenzoyl)-4H-chromen-4-one (5d):



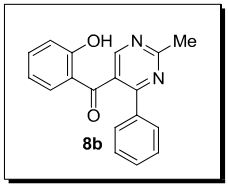
^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.23 (s, 1H), 8.04 (d, 1H), 7.54 (m, 1H), 7.45 (d, 1H), 7.13 (s, 2H), 3.93 (s, 3H). 3.86 (s, 6H), 2.48 (s, 3H). MS (EI): *m/z* 354 (M+1,100).

2-methyl-5-phenyl-5H-chromeno [4, 3-d] pyrimidin-5-ol (7b):



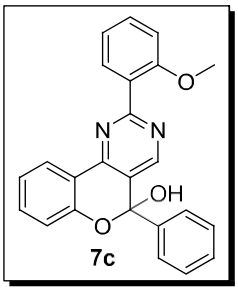
M.p. 207-211 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ = 8.28 (d, 1H), 8.27 (s, 1H), 8.17 (s, 1H), 7.55 (m, 3H), 7.45 (m, 3H), 7.20 (t, 1H), 7.11 (d, 1H), 2.68 (s, 3H). IR (KBr, cm^{-1}): 3061, 2781, 2604, 1823, 1600, 1582, 1427, 1232, 1056, 944, 761, 696. ^{13}C NMR (100 MHz, DMSO-d6) = 167.4, 154.9, 154.4, 152.5, 141.4, 133.5, 128.9, 128.7, 128.5, 128.1, 126.6, 124.48, 124.3, 122.6, 119.0, 117.9, 98.6, 25.7. MS (EI): *m/z* 290 (M+1,100), HRMS: (ESI): Calcd for $C_{18}H_{14}N_2O_2$ [M+H]: 291.1055; Found: 291.1155.

(2-hydroxyphenyl)(2-methyl-4-phenylpyrimidin-5-yl) methanone (8b):



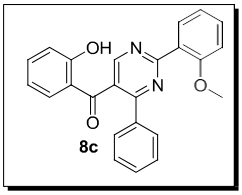
M.p. 104-108 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 11.84 (s, 1H), 8.72 (s, 1H), 7.62 (d, 2H), 7.43 (t, 1H), 7.30 (m, 3H), 7.17 (d, 1H), 6.95 (d, 1H), 6.68 (t, 1H), 2.90 (s, 3H). IR (KBr, cm^{-1}): 3400, 3051, 2921, 1967, 1821, 1627, 1427, 1031, 925, 796, 752, 694. ^{13}C NMR (100 MHz, CDCl3) = 200.5, 169.4, 163.8, 163.0, 156.6, 137.3, 136.6, 132.5, 130.5, 130.1, 128.9, 128.8, 128.7, 127.7, 119.3, 119.9, 118.4, 26.3. MS (EI): *m/z* 290 (M+1,100), HRMS: (ESI): Calcd for $C_{18}H_{14}N_2O_2$ [M+H]: 291.1055; Found: 291.1121.

2-(2-methoxyphenyl)-5-phenyl-5H-chromeno [4, 3-d] pyrimidin-5-ol (7c):



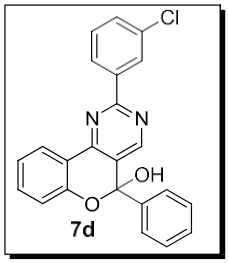
M.p. 181-185 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ = 8.30 (m, 3H), 7.76 (m, 3H), 7.50 (t, 1H), 7.48 (m, 4H), 7.20 (m, 3H), 7.07 (t, 1H), 3.79 (s, 3H). IR (KBr, cm^{-1}): 3237, 3067, 2943, 2837, 2622, 1956, 1817, 1579, 1389, 1258, 1227, 1047, 1023, 966, 946, 749, 699. ^{13}C NMR (100 MHz, DMSO-d6) = 165.0, 157.4, 154.8, 154.4, 152.6, 141.3, 133.6, 131.0, 130.9, 128.8, 128.2, 128.2, 128.2, 128.1, 126.7, 124.6, 124.5, 122.1, 120.2, 119.1, 117.9, 112.4, 98.6, 55.8. MS (EI): *m/z* 382 (M+1,100), HRMS: (ESI): Calcd for $C_{24}H_{18}N_2O_3$ [M+H]: 383.1317; Found: 383.1849.

(2-hydroxyphenyl)(2-(2-methoxyphenyl)-4-phenylpyrimidin-5-yl) methanone (8c):



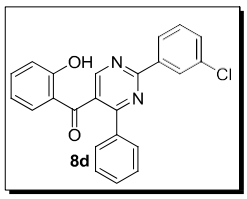
M.p. 90-94 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 11.90 (s, 1H), 8.91 (s, 1H), 7.95 (m, 1H), 7.70 (m, 2H), 7.49 (m, 2H), 7.37 (m, 4H), 7.17 (m, 2H), 7.02 (d, 1H), 6.72 (t, 1H).3.96 (s, 3H). IR (KBr, cm^{-1}): 3422, 3039, 2926, 2837, 1623, 1425, 1248, 1025, 926, 772, 746, 691. ^{13}C NMR (100 MHz, CDCl3) = 200.6, 166.4, 163.8, 163.1, 158.1, 156.6, 137.3, 136.8, 132.7, 132.1, 131.7, 130.5, 129.2, 128.7, 128.5, 127.9, 127.5, 127.5, 120.7, 119.4, 119.2, 118.5, 112.2, 56.1. MS (EI): *m/z* 382 (M+1,100), HRMS: (ESI): Calcd for $C_{24}H_{18}N_2O_3$ [M+H]: 383.1317; Found: 383.1379.

2-(3-chlorophenyl)-5-phenyl-5H-chromeno [4, 3-d] pyrimidin-5-ol (7d):



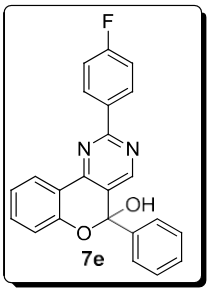
M.p. 157-161 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ = 8.50 (m, 3H), 8.21 (d, 2H), 7.60 (m, 5H), 7.46 (m, 3H), 7.28 (t, 1H), 7.18 (d, 1H). IR (KBr, cm^{-1}): 3068, 2925, 2764, 2609, 1955, 1571, 1385, 1225, 1047, 973, 751, 699. ^{13}C NMR (100 MHz, DMSO-d6) = 161.6, 155.5, 154.6, 153.2, 141.2, 138.9, 133.9, 133.6, 130.8, 130.7, 128.8, 128.8, 128.1, 128.1, 127.4, 126.6, 126.5, 125.6, 124.8, 122.2, 118.9, 117.9, 98.6. MS (EI): *m/z* 386 (M+1,100), HRMS: (ESI): Calcd for $C_{23}H_{15}ClN_2O_2$ [M+H]: 387.0822; Found: 387.0938.

(2-(3-chlorophenyl)-4-phenylpyrimidin-5-yl)(2-hydroxyphenyl)methanone (8d):



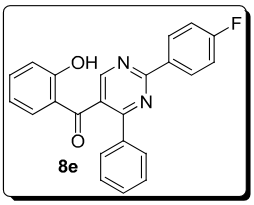
M.p. 121-125 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 11.86 (s, 1H), 8.87 (s, 1H), 8.62 (d, 1H), 8.51 (m, 1H), 7.73 (m, 2H), 7.48 (m, 6H), 7.24 (m, 1H), 7.00 (d, 1H), 6.70 (t, 1H). IR (KBr, cm^{-1}): 3061, 3033, 2383, 1943, 1893, 1680, 1550, 1421, 1217, 926, 755, 677. ^{13}C NMR (100 MHz, CDCl3) = 200.3, 164.1, 163.8, 163.1, 157.2, 138.5, 137.4, 136.6, 134.8, 132.5, 131.4, 130.8, 129.9, 129.9, 129.1, 129.0, 128.8, 128.7, 128.5, 126.8, 119.3, 119.2, 118.5. MS (EI): *m/z* 386 (M+1,100), HRMS: (ESI): Calcd for $C_{23}H_{15}ClN_2O_2$ [M+H]: 387.0822; Found: 387.0919.

2-(4-fluorophenyl)-5-phenyl-5H-chromeno [4, 3-d] pyrimidin-5-ol (7e):



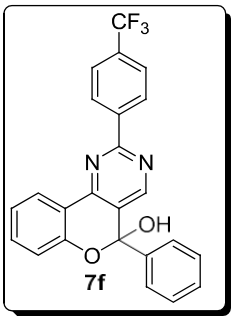
M.p. 182-186 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ = 8.57 (m, 2H), 8.49 (m, 1H), 8.29 (s, 2H), 7.62 (m, 3H), 7.45 (m, 3H), 7.41 (m, 2H).7.27 (t, 1H), 7.16 (d, 1H). IR (KBr, cm^{-1}): 3533, 3413, 2770, 2607, 1895, 1578, 1393, 1228, 1034, 950, 759, 690. ^{13}C NMR (100 MHz, DMSO-d6) = 165.3, 162.9 (C-F), 162.1, 155.4, 154.6, 153.1, 141.3, 133.8, 133.3, 133.3, 130.4, 130.3, 128.8, 128.1, 126.6, 125.0, 124.7, 122.1, 119.0, 117.9, 115.7, 115.5, 98.6. MS (EI): *m/z* 370 (M+1,100), HRMS: (ESI): Calcd for $C_{23}H_{15}FN_2O_2$ [M+H]: 371.1118; Found: 371.1231.

(2-(4-fluorophenyl)-4-phenylpyrimidin-5-yl)(2-hydroxyphenyl)methanone (8e):



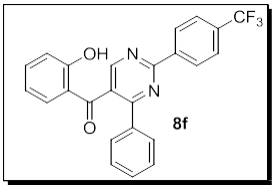
M.p. 166-170 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 11.88 (s, 1H), 8.85 (s, 1H), 8.64 (m, 2H), 7.72 (m, 2H), 7.40 (m, 4H), 7.25 (m, 3H), 7.00 (d, 1H), 6.70 (t, 1H). IR (KBr, cm^{-1}): 3455, 3066, 3028, 1907, 1610, 1557, 1423, 1330, 1217, 924, 758, 677. ^{13}C NMR (100 MHz, CDCl3) = 200.5, 166.4, 164.1, 164.0, 163.9, 163.0 (C-F), 157.2, 137.3, 136.8, 132.9, 132.9, 132.5, 131.0, 130.9, 130.7, 129.1, 128.7, 128.0, 119.4, 119.1, 118.5, 115.8, 115.6. MS (EI): *m/z* 370 (M+1,100), HRMS: (ESI): Calcd for $C_{23}H_{15}FN_2O_2$ [M+H]: 371.1118; Found: 371.1272.

5-phenyl-2-(4-(trifluoromethyl)phenyl)-5H-chromeno [4, 3-d] pyrimidin-5-ol (7f):



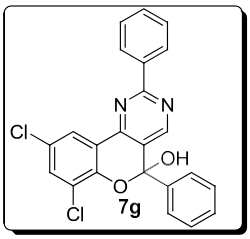
M.p. 184-188 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ = 8.71 (d, 2H), 8.52 (m, 1H), 8.36 (d, 2H), 7.94 (d, 2H), 7.63 (m, 3H), 7.46 (m, 3H), 7.29 (t, 1H), 7.18 (t, 1H). IR (KBr, cm^{-1}): 3528, 3065, 2922, 1807, 1578, 1391, 1323, 1126, 950, 855, 762, 694. ^{13}C NMR (100 MHz, DMSO-d6) = 161.6, 155.6, 154.6, 153.3, 141.2, 140.5, 133.9, 131.0 (C-F), 130.7, 130.5, 128.8, 128.6, 128.5, 128.1, 126.6, 125.8, 125.6, 125.2, 124.7 (C-F_3), 123.0, 122.2, 118.9, 118.0, 98.6. MS (EI): *m/z* 420 (M+1,100), HRMS: (ESI): Calcd for $C_{24}H_{15}F_3N_2O_2$ [M+H]: 421.1086; Found: 421.1137.

(2-hydroxyphenyl)(4-phenyl-2-(4-(trifluoromethyl)phenyl)pyrimidin-5-yl)methanone (8f):



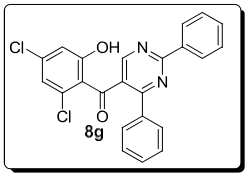
M.p. 194-198 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 11.85 (s, 1H), 8.90 (s, 1H), 8.74 (d, 2H), 7.76 (m, 4H), 7.40 (m, 4H), 7.24 (m, 1H), 7.02 (d, 1H), 6.71 (t, 1H). IR (KBr, cm^{-1}): 3233, 3064, 3034, 2928, 1628, 1553, 1423, 1320, 1111, 926, 856, 662. ^{13}C NMR (100 MHz, CDCl3) = 200.3, 164.1, 163.7, 163.1, 157.3, 139.9, 137.5, 136.6, 133.1, 132.8, 132.4, 130.8 (C-F), 129.1, 129.0, 128.8, 128.8, 128.8, 125.6 (C-F_3), 125.6, 125.3, 122.6, 119.3, 119.2, 118.6. MS (EI): *m/z* 420 (M+1,100), HRMS: (ESI): Calcd for $C_{24}H_{15}F_3N_2O_2$ [M+H]: 421.1086; Found: 421.1143.

7, 9-dichloro-2, 5-diphenyl-5H-chromeno [4, 3-d] pyrimidin-5-ol (7g):



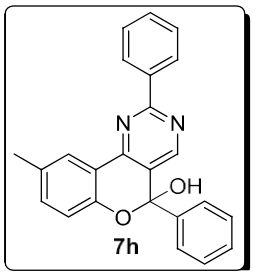
M.p. 210-213 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ = 8.72 (s, 1H), 8.54 (m, 2H), 8.45 (m, 2H), 7.91 (d, 1H), 7.63 (m, 2H), 7.57 (m, 3H), 7.48 (m, 3H). IR (KBr, cm^{-1}): 3439, 3172, 3066, 2920, 1579, 1533, 1442, 1228, 1045, 952, 771, 692. ^{13}C NMR (100 MHz, DMSO-d6) = 163.4, 161.5, 156.0, 151.5, 149.2, 147.6, 140.5, 136.3, 132.7, 131.4, 129.1, 128.8, 128.5, 128.4, 128.3, 128.1, 128.1, 126.6, 126.6, 126.1, 123.1, 122.9, 121.9. MS (EI): *m/z* 420 (M+1,100), HRMS: (ESI): Calcd for $C_{23}H_{14}Cl_2N_2O_2$ [M+H]: 421.0432; Found: 421.0483.

(2,4-dichloro-6-hydroxyphenyl)(2,4-diphenylpyrimidin-5-yl)methanone (8g):



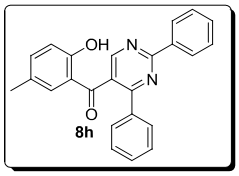
M.p. 123-127 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 12.26 (s, 1H), 8.91 (s, 1H), 8.64 (m, 2H), 7.68 (m, 2H), 7.55 (m, 3H), 7.45 (m, 4H), 7.06 (d, 1H). IR (KBr, cm^{-1}): 3330, 3063, 2923, 2853, 1625, 1551, 1424, 1316, 1220, 967, 866, 740, 683. ^{13}C NMR (100 MHz, CDCl3) = 199.7, 165.7, 164.4, 157.5, 157.2, 136.7, 136.5, 136.4, 131.9, 131.0, 129.9, 129.1, 128.9, 128.9, 128.9, 128.9, 128.8, 128.7, 127.2, 124.0, 123.6, 120.2. MS (EI): *m/z* 420 (M+1,100), HRMS: (ESI): Calcd for $C_{23}H_{14}Cl_2N_2O_2$ [M+H]: 421.0432; Found: 421.0549.

9-methyl-2,5-diphenyl-5H-chromeno [4, 3-d] pyrimidin-5-ol (7h):



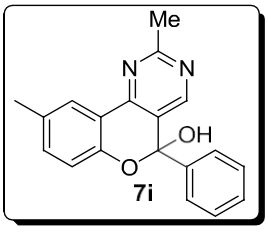
M.p. 186-190 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ = 8.52 (m, 2H), 8.29 (m, 2H), 8.22 (s, 1H), 7.60 (m, 5H), 7.40 (m, 4H), 7.05 (d, 1H), 2.42 (s, 3H). IR (KBr, cm^{-1}): 3181, 3060, 2914, 2855, 2767, 1899, 1582, 1436, 1228, 1034, 764, 693. ^{13}C NMR (100 MHz, DMSO-d6) = 163.0, 155.3, 153.2, 152.5, 141.4, 136.8, 134.5, 131.0, 128.7, 128.7, 128.6, 128.6, 128.1, 127.9, 127.9, 126.6, 125.2, 125.2, 124.5, 124.4, 118.8, 117.8, 98.5, 20.3. MS (EI): *m/z* 366 (M+1,100), HRMS: (ESI): Calcd for $C_{24}H_{18}N_2O_2$ [M+H]: 367.1368; Found: 367.0568.

(2,4-diphenylpyrimidin-5-yl)(2-hydroxy-5-methylphenyl)methanone (8h):



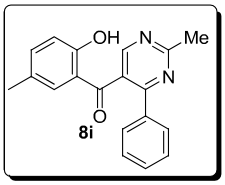
M.p. 110 -114 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 11.73 (s, 1H), 8.87 (s, 1H), 8.64 (m, 2H), 7.74 (m, 2H), 7.55 (m, 3H), 7.40 (m, 3H), 7.01 (d, 1H), 7.015 (s, 1H), 6.95 (d, 1H), 2.09 (s, 3H). IR (KBr, cm^{-1}): 3057, 2920, 2861, 1634, 1550, 1478, 1334, 1242, 1197, 952, 740, 684. ^{13}C NMR (100 MHz, CDCl3) = 200.3, 165.1, 164.1, 161.1, 157.3, 138.4, 137.0, 136.7, 132.1, 132.3, 132.4, 131.5, 131.6, 129.1, 128.7, 128.7, 128.7, 128.7, 128.6, 128.4, 128.2, 119.0, 118.2, 20.1. MS (EI): *m/z* 366 (M+1,100), HRMS: (ESI): Calcd for $C_{24}H_{18}N_2O_2$ [M+H]: 367.1368; Found: 367.1483.

2,9-dimethyl-5-phenyl-5H-chromeno [4, 3-d] pyrimidin-5-ol (7i):



M.p. 226-230 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ = 8.08 (m, 3H), 7.54 (m, 2H), 7.40 (m, 4H), 7.02 (d, 1H), 2.67 (s, 3H), 2.36 (s, 3H). IR (KBr, cm^{-1}): 3179, 3065, 2920, 2855, 1623, 1563, 1447, 1046, 962, 761, 699. ^{13}C NMR (100 MHz, DMSO-d6) = 167.3, 154.8, 152.7, 152.4, 141.5, 134.2, 131.0, 128.7, 128.6, 128.6, 128.0, 126.6, 124.4, 124.2, 118.7, 117.7, 98.5, 25.7, 20.2. MS (EI): *m/z* 304 (M+1,100), HRMS: (ESI): Calcd for $C_{19}H_{16}N_2O_2$ [M+H]: 305.1212; Found: 305.1272.

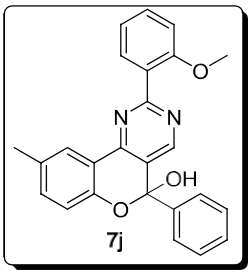
(2-hydroxy-5-methylphenyl)(2-methyl-4-phenylpyrimidin-5-yl)methanone (8i):



M.p. 152-156 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 11.67 (s, 1H), 8.71 (s, 1H), 7.60 (m, 2H), 7.35 (m, 3H), 7.25 (m, 1H), 6.94 (s, 1H), 6.90 (d, 1H),

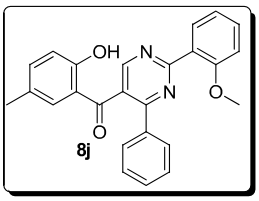
2.90 (s, 3H), 2.10 (s, 3H). IR (KBr, cm^{-1}): 3439, 3052, 2919, 1637, 1555, 1430, 1328, 1195, 953, 840, 745, 692. ^{13}C NMR (100 MHz, CDCl3) = 200.2, 169.4, 164.0, 161.0, 156.7, 138.4, 136.8, 132.1, 130.1, 128.9, 128.8, 128.8, 128.7, 128.3, 127.8, 118.9, 118.2, 26.3, 20.1. MS (EI): *m/z* 304 (M+1,100), HRMS: (ESI): Calcd for $C_{19}H_{16}N_2O_2$ [M+H]: 305.1212; Found: 305.1298.

2-(2-methoxyphenyl)-9-methyl-5-phenyl-5H-chromeno [4 ,3-d] pyrimidin-5-ol (7j):



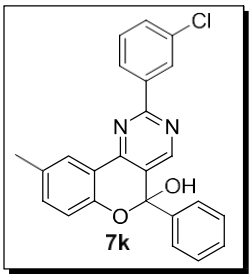
M.p. 150-154 °C. ^1H NMR (400 MHz, DMSO-d6): δ = 8.20 (d, 2H), 8.09 (s, 1H), 7.61 (m, 3H), 7.30 (m, 8H), 3.90 (s, 3H), 2.40 (s, 3H). IR (KBr, cm^{-1}): 3500, 3176, 3055, 2924, 2839, 1585, 1446, 1396, 1249, 960, 754, 692. ^{13}C NMR (100 MHz, DMSO-d6) = 165.0, 157.3, 154.7, 152.8, 152.4, 141.4, 134.3, 131.0, 130.9, 130.8, 128.7, 128.7, 128.4, 128.2, 128.1, 126.6, 124.6, 124.4, 120.2, 118.8, 117.8, 112.3, 98.5, 55.7, 20.2. MS (EI): *m/z* 396 (M+1,100), HRMS: (ESI): Calcd for $C_{25}H_{20}N_2O_3$ [M+H]: 397.1474; Found: 397.1591.

(2-hydroxy-5-methylphenyl)(2-(2-methoxyphenyl)-4-phenylpyrimidin-5-yl)methanone (8j):



^1H NMR (400 MHz, $CDCl_3$): δ = 11.67 (s, 1H), 8.90 (s, 1H), 7.98 (d, 1H), 7.69 (d, 2H), 7.48 (t,1H), 7.35 (m, 3H), 7.25 (m, 1H), 7.12 (m, 3H), 6.91 (d, 1H), 3.97 (s, 3H), 2.10 (s, 3H). IR (KBr, cm^{-1}): 3448, 3055, 2922, 2364, 1653, 1558, 1479, 1323, 1136, 942, 750, 686. ^{13}C NMR (100 MHz, CDCl3) = 200.3, 164.0, 161.1, 158.2, 156.7, 138.5, 137.0, 132.3, 132.2, 131.8, 131.7, 130.4, 130.3, 129.1, 128.6, 128.5, 128.4, 128.4, 127.7, 120.8, 119.0, 118.3, 112.3, 56.2, 20.2. MS (EI): *m/z* 396 (M+1,100), HRMS: (ESI): Calcd for $C_{25}H_{20}N_2O_3$ [M+H]: 397.1474; Found: 397.1567.

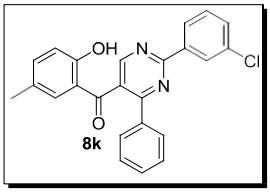
2-(3-chlorophenyl)-9-methyl-5-phenyl-5H-chromeno [4, 3-d] pyrimidin-5-ol (7k):



M.p. 190-194 °C. ^1H NMR (400 MHz, DMSO-d6): δ = 8.50 (m, 2H), 8.30 (m, 3H), 7.63 (m, 4H), 7.45 (m, 4H), 7.07 (d, 1H), 2.42 (s, 3H). IR (KBr, cm^{-1}): 3205, 3072, 2920, 1581, 1446, 1388, 1220, 1037, 987, 763, 756,

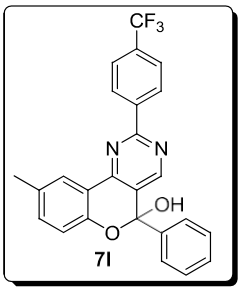
692. ^{13}C NMR (100 MHz, DMSO-d6) = 161.6, 155.4, 153.4, 152.5, 141.3, 138.9, 134.7, 133.6, 131.2, 130.8, 130.7, 128.8, 128.7, 128.1, 128.1, 127.3, 126.6, 126.5, 125.7, 124.5, 118.6, 117.8, 98.5, 20.3. MS (EI): *m/z* 400 (M+1,100), HRMS: (ESI): Calcd for $C_{24}H_{17}ClN_2O_2$ [M+H]: 401.0979; Found: 401.1052.

(2-(3-chlorophenyl)-4-phenylpyrimidin-5-yl)(2-hydroxy-5-methylphenyl)methanone (8k):



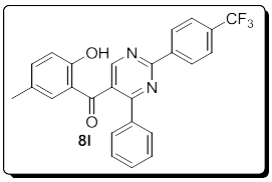
M.p. 158-162 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 11.63 (s, 1H), 8.87 (s, 1H), 8.63 (t, 1H), 8.52 (m, 1H), 7.72 (m, 2H), 7.51 (m, 2H), 7.41 (m, 3H), 7.23 (d, 1H), 6.98 (d, 1H), 6.91 (d, 1H), 2.05 (s, 3H). IR (KBr, cm^{-1}): 3034, 2920, 2854, 1674, 1593, 1425, 1336, 1209, 954, 831, 752, 688. ^{13}C NMR (100 MHz, CDCl3) = 200.1, 164.2, 163.8, 161.1, 157.3, 138.6, 136.7, 134.9, 134.9, 132.0, 131.4, 130.7, 129.9, 129.1, 128.7, 128.7, 128.6, 128.6, 128.4, 128.4, 126.8, 118.9, 118.3, 20.2. MS (EI): *m/z* 400 (M+1,100), HRMS: (ESI): Calcd for $C_{24}H_{17}ClN_2O_2$ [M+H]: 401.0979; Found: 401.1035.

9-methyl-5-phenyl-2-(4-(trifluoromethyl)phenyl)-5H-chromeno [4, 3-d] pyrimidin-5-ol (7l):



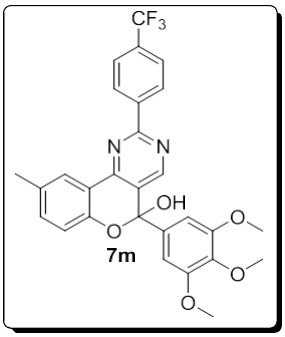
M.p. 178-181 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ = 8.71 (d, 2H), 8.36 (s, 1H), 8.30 (m, 2H), 7.93 (d, 2H), 7.63 (m, 2H), 7.44 (m, 4H), 7.07 (d, 1H) 2.42 (s, 3H). IR (KBr, cm^{-1}): 3568, 3215, 3066, 2926, 2862, 1583, 1323, 1238, 1166, 964, 761, 692. ^{13}C NMR (100 MHz, DMSO-d6) = 163.0, 155.5, 154.0, 152.0, 140.4, 140.2, 134.8, 132.5, 132.3, 129.4 (C-F), 128.6, 128.6, 128.5, 128.5, 128.5, 125.4, 125.1, 125.0, 124.5 (C-F_3), 123.0, 118.9, 118.0, 98.6, 53.4, 20.8. MS (EI): *m/z* 434 (M+1,100), HRMS: (ESI): Calcd for $C_{25}H_{17}F_3N_2O_2$ [M+H]: 435.1242; Found: 435.1340.

(2-hydroxy-5-methylphenyl)(4-phenyl-2-(4-(trifluoromethyl)phenyl)pyrimidin-5 yl)methanone(8l):



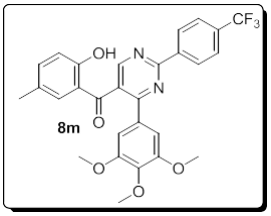
M.p. 156-160 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 11.69 (s, 1H), 8.90 (s, 1H), 8.75 (d, 2H), 7.80 (d, 2H), 7.77 (d, 2H), 7.40 (m, 3H), 7.25 (m, 1H), 7.00 (m, 2H), 2.10 (s, 3H). IR (KBr, cm^{-1}): 3446, 3057, 2920, 1627, 1550, 1421, 1327, 1193, 1008, 952, 823, 678. ^{13}C NMR (100 MHz, CDCl3) = 196.0, 163.1, 161.8, 157.4, 156.9, 140.2, 137.2, 136.6, 131.7, 131.3, 131.2, 131.0 (C-F), 130.7, 130.4, 129.0, 128.8, 128.7, 128.5, 128.1, 125.8, 125.2, (C-F_3) 123.0, 121.7, 117.3, 19.6. MS (EI): *m/z* 434 (M+1,100), HRMS: (ESI): Calcd for $C_{25}H_{17}F_3N_2O_2$ [M+H]: 435.1242; Found: 435.1335.

9-methyl-2-(4-(trifluoromethyl)phenyl)-5-(3,4,5-trimethoxyphenyl)-5H-chromeno[4,3-d] pyrimidin-5-ol (7m):



M.p. 201 -205 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ = 8.72 (d, 2H), 8.37 (s, 1H), 8.32 (d, 1H), 8.18 (s, 1H), 7.94 (d, 2H), 7.42 (m, 1H), 7.09 (d, 1H), 6.91 (s, 2H), 3.75 (s, 6H), 3.71 (s, 3H), 2.50 (s, 3H). IR (KBr, cm^{-1}): 3431, 3290, 2931, 2831, 1944, 1602, 1552, 1454, 1120, 957, 723, 682. ^{13}C NMR (100 MHz, DMSO-d6) = 161.0, 155.5, 153.3, 152.5, 152.4, 140.6, 137.7, 136.6, 134.6, 131.3 (C-F), 130.1, 128.6, 125.9, 128.8, 128.8, 125.7, 125.7, 125.6, 124.4 (C-F_3), 124.4, 118.8, 118.0, 104.4, 98.3, 60.0, 55.9, 55.8, 20.3. MS (EI): *m/z* 524 (M+1,100), HRMS: (ESI): Calcd for $C_{28}H_{23}F_3N_2O_5$ [M+H]: 525.1559; Found: 524.1588.

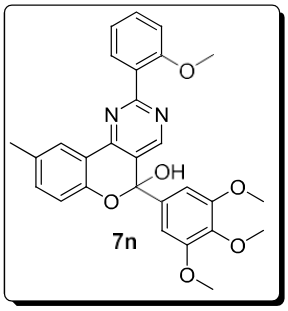
(2-hydroxy-5-methylphenyl)(2-(4-(trifluoromethyl)phenyl)-4-(3,4,5 trimethoxyphenyl)pyrimidin-5-yl)methanone (8m):



M.p. 170-174 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 11.69 (s, 1H), 8.90 (s, 1H), 8.74 (d, 2H), 7.81 (d, 2H), 7.25 (s, 1H), 7.00 (m, 4H), 3.83 (s, 3H), 3.77 (s, 6H), 2.09 (s, 3H). IR (KBr, cm^{-1}): 3415, 2949, 2360, 1620, 1597, 1546, 1415, 1325, 1242, 854, 731, 663. ^{13}C NMR (100 MHz, CDCl3) = 200.5, 165.8, 163.6, 163.4, 157.1, 153.4, 140.3, 139.9, 138.8, 133.1, 132.8, 131.7, 131.6 (C-F), 128.9, 128.7, 128.5, 128.4, 125.6, 125.6, 125.3 (C-F_3), 122.6, 119.0, 118.3, 106.5, 60.8, 56.0, 56.0, 20.1. MS (EI): *m/z* 524

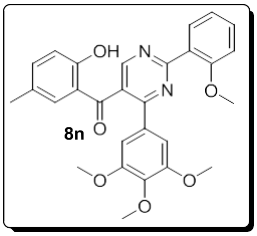
(M+1,100), HRMS: (ESI): Calcd for $C_{28}H_{23}F_3N_2O_5$ [M+H]: 525.1559; Found: 525.1664.

2-(2-methoxyphenyl)-9-methyl-5-(3,4,5-trimethoxyphenyl)-5H-chromeno[4,3-d]pyrimidin-5-ol (7n):



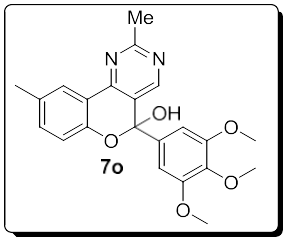
M.p. 117-121 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ = 8.94 (s, 1H), 8.29 (s, 2H), 7.62 (m, 1H), 7.50 (m, 1H), 7.39 (m, 1H), 7.19 (d, 1H), 7.09 (m, 2H), 6.90 (s, 2H), 3.78 (s, 9H), 3.70 (s, 3H), 2.37 (s, 3H). IR (KBr, cm^{-1}): 3186, 2929, 1707, 1625, 1597, 1490, 1246, 1122, 948, 858, 752, 659. ^{13}C NMR (100 MHz, DMSO-d6) = 165.0, 157.3, 154.7, 152.6, 152.4, 152.4, 152.3, 137.7, 136.8, 134.2, 131.1, 131.0, 130.8, 128.6, 124.5, 124.4, 124.3, 120.2, 119.0, 117.9, 112.4, 104.4, 98.5, 60.0, 55.9, 55.8, 55.7, 20.3. MS (EI): *m/z* 486 (M+1,100), HRMS: (ESI): Calcd for $C_{28}H_{26}N_2O_6$ [M+H]: 487.1791; Found: 487.1874.

(2-hydroxy-5-methylphenyl)(2-(2-methoxyphenyl)-4-(3,4,5-trimethoxyphenyl)pyrimidin-5-yl)methanone (8n):



M.p. 78-81°C. ^{1}H NMR (400 MHz, DMSO-d6): δ = 10.77 (s, 1H), 8.94 (s, 1H), 7.78 (d, 1H), 7.52 (s, 1H), 7.25 (m, 3H), 7.11 (s, 1H), 6.80 (m, 3H), 6.85 (s, 3H), 3.65 (s, 9H), 2.16 (s, 3H). IR (KBr, cm^{-1}): 3415, 2927, 2837, 1724, 1658, 1591, 1413, 1328, 1240, 825, 752, 651. ^{13}C NMR (100 MHz, DMSO-d6) = 196.9, 164.9, 162.1, 157.7, 157.4, 156.0, 152.6, 138.9, 138.9, 137.1, 132.2, 131.4, 131.1, 130.0, 128.0, 128.0, 127.6, 127.6, 121.6, 120.3, 117.2, 112.6, 106.6, 59.9, 55.8, 55.6, 55.5, 19.6. MS (EI): *m/z* 486 (M+1,100), HRMS: (ESI): Calcd for $C_{28}H_{26}N_2O_6$ [M+H]: 487.1791; Found: 487.1902.

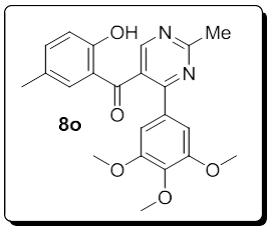
2,9-dimethyl-5-(3,4,5-trimethoxyphenyl)-5H-chromeno [4, 3-d] pyrimidin-5-ol (7o):



M.p. 167-172 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ = 8.07 (m, 3H), 7.37 (m, 1H), 7.05 (d, 1H), 6.83 (s, 2H), 3.70 (s, 6H), 3.65 (s, 3H), 2.65 (s, 3H), 2.39 (s, 3H). IR (KBr, cm^{-1}): 3205, 2929, 2729, 1587, 1560, 1413, 1236,

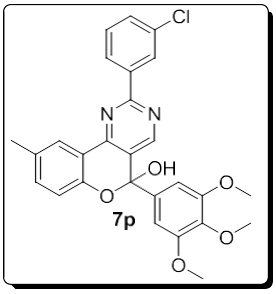
1128, 964, 837, 792, 632. ^{13}C NMR (100 MHz, DMSO-d6) = 167.2, 154.8, 152.5, 152.5, 152.3, 152.3, 137.6, 136.9, 134.1, 131.0, 124.3, 124.2, 118.9, 117.9, 104.4, 104.4, 98.3, 60.0, 55.8, 55.8, 25.7, 20.2. MS (EI): *m/z* 394 (M+1,100), HRMS: (ESI): Calcd for $C_{22}H_{22}N_2O_5$ [M+H]: 395.1529, Found: 395.1644.

(2-hydroxy-5-methylphenyl)(2-methyl-4-(3,4,5-trimethoxyphenyl)pyrimidin-5-yl)methanone (8o):



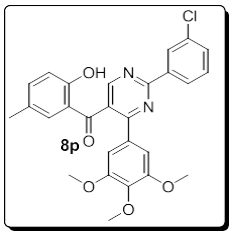
M.p. 117-120 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 11.64 (s, 1H), 8.72 (s, 1H), 7.20 (m, 1H), 6.87 (m, 4H), 3.80 (s, 3H), 3.70 (s, 6H), 2.90 (s, 3H), 2.10 (s, 3H). IR (KBr, cm^{-1}): 3280, 3059, 2929, 1707, 1629, 1564, 1423, 1382, 1294, 950, 788, 655. ^{13}C NMR (100 MHz, CDCl3) = 200.7, 169.3, 163.2, 160.7, 156.5, 153.4, 153.3, 140.0, 138.5, 131.9, 131.7, 128.3, 127.6, 119.1, 118.2, 106.3, 106.3, 60.7, 56.0, 56.0, 26.3, 20.1. MS (EI): *m/z* 394 (M+1,100), HRMS: (ESI): Calcd for $C_{22}H_{22}N_2O_5$ [M+H]: 395.1529, Found: 395.1610.

2-(3-chlorophenyl)-9-methyl-5-(3,4,5-trimethoxyphenyl)-5H-chromeno[4,3-d]pyrimidin-5-ol (7p):



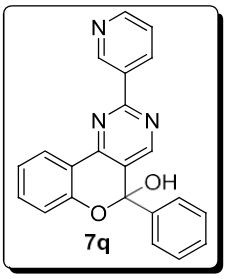
M.p. 148-152 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ = 8.50 (m, 2H), 8.30 (m, 2H), 8.16 (s, 1H), 7.64 (m, 2H), 7.41 (m, 1H), 7.08 (d, 1H), 6.90 (d, 2H), 3.76 (s, 6H), 3.70 (s, 3H), 2.44 (s, 3H). IR (KBr, cm^{-1}): 3387, 2987, 2357, 2144, 1967, 1687, 1585, 1402, 1327, 1232, 908, 597. ^{13}C NMR (100 MHz, DMSO-d6) =161.5, 155.4, 153.2, 153.2, 152.5, 152.4, 139.0, 137.7, 136.7, 134.5, 133.6, 131.3, 130.8, 130.7, 127.3, 126.5, 125.7, 124.5, 118.8, 118.0, 104.4, 104.4, 88.3, 60.0, 55.9, 55.8, 20.6. MS (EI): *m/z* 490 (M+1,100), HRMS: (ESI): Calcd for $C_{27}H_{23}ClN_2O_5$ [M+H]: 491.1295, Found: 491.1375.

(2-(3-chlorophenyl)-4-(3,4,5-trimethoxyphenyl)pyrimidin-5-yl)(2-hydroxy-5-methylphenyl)methanone (8p):



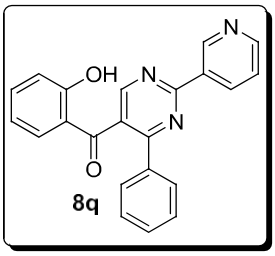
M.p. 168-172 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 11.70 (s, 1H), 8.85 (s, 1H), 8.62 (s, 1H), 8.51 (d, 1H), 7.50 (m, 2H), 7.22 (m, 1H), 6.96 (s, 2H), 6.89, (m, 2H), 3.82 (s, 9H), 2.05 (s, 3H). IR (KBr, cm^{-1}): 3768, 3059, 2841, 2368, 1843, 1728, 1614, 1556, 1490, 1328, 932, 667. ^{13}C NMR (100 MHz, CDCl3) = 200.5, 163.7, 163.4, 160.8, 157.0, 153.4, 153.40, 140.3, 138.7, 138.5, 134.9, 131.8, 131.6, 131.5, 129.9, 128.7, 128.5, 128.5, 126.7, 119.1, 118.3, 106.5, 106.5, 60.8, 56.1, 56.1, 20.1. MS (EI): *m/z* 490 (M+1,100), HRMS: (ESI): Calcd for $C_{27}H_{23}ClN_2O_5$ [M+H]: 491.1295, Found: 491.1910.

5-phenyl-2-(pyridin-3-yl)-5H-chromeno[4,3-d]pyrimidin-5-ol (7q):



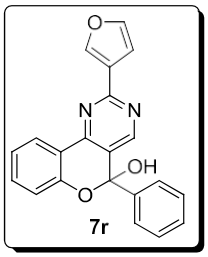
M.p. 217-221 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ = 9.65 (d, 1H), 8.86 (m, 1H), 8.79 (m, 1H), 8.53 (m, 1H), 8.35 (s, 2H), 7.62 (m, 4H).7.47 (m, 3H), 7.29 (t, 1H), 7.17 (d, 1H). IR (KBr, cm^{-1}): 3271, 3084, 2378, 2614, 1680, 1568, 1384, 1246, 1193, 956, 761, 609. ^{13}C NMR (100 MHz, TFA-d) = 189.6, 170.3, 167.9, 162.4, 161.6, 158.6, 150.6, 147.0, 146.3, 142.5, 142.0, 138.1, 136.4, 134.4, 133.4, 130.9, 129.2, 128.3, 122.7, 121.8, 120.8, 113.4. MS (EI): *m/z* 353 (M+1,100), HRMS: (ESI): Calcd for $C_{22}H_{15}N_3O_2$ [M+H]: 354.1164, Found: 354.1246.

(2-hydroxyphenyl)(4-phenyl-2-(pyridin-3-yl)pyrimidin-5-yl)methanone (8q):



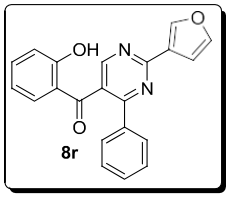
M.p. 166-170 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ = 10.78 (s, 1H), 9.64 (m, 1H), 9.00 (s, 1H), 8.84 (m, 2H), 7.69 (m, 3H), 7.53 (m, 1H), 7.39 (m, 4H), 6.84 (m, 2H). IR (KBr, cm^{-1}): 3084, 2567, 2380, 1633, 1558, 1531, 1423, 1384, 1192, 929, 759, 692. ^{13}C NMR (100 MHz, TFA-d) = 202.1, 170.4, 164.2, 164.1, 158.5, 148.9, 145.4, 144.5, 141.8, 141.8, 138.3, 136.5, 135.2, 134.9, 138.8, 131.7, 131.5, 130.4, 123.3, 121.0, 120.6, 113.3. MS (EI): *m/z* 353 (M+1,100), HRMS: (ESI): Calcd for $C_{22}H_{15}N_3O_2$ [M+H]: 354.1164, Found: 354.1237.

2-(furan-3-yl)-5-phenyl-5H-chromeno[4,3-d]pyrimidin-5-ol (7r):



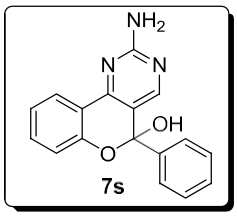
M.p. 200-204 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ = 8.54 (m, 1H), 8.43 (m, 1H), 8.25 (s, 1H), 8.20 (s, 1H), 7.85 (m, 1H), 7.60 (m, 3H).7.44 (m, 3H), 7.24 (m, 1H), 7.14 (m, 2H). IR (KBr, cm^{-1}): 3151, 3118, 3088, 2763, 2376, 1963, 1598, 1494, 1240, 958, 756, 694. ^{13}C NMR (100 MHz, DMSO-d6) =160.1, 155.3, 154.5, 152.9, 145.3, 144.7, 141.4, 133.7, 128.7, 128.7, 128.1, 126.6, 126.5, 126.5, 124.7, 124.5, 122.0, 118.9, 117.9, 109.4, 98.7. MS (EI): *m/z* 342 (M+1,100), HRMS: (ESI): Calcd for $C_{21}H_{14}N_2O_3$ [M+H]: 343.1004, Found: 343.1089.

(2-(furan-3-yl)-4-phenylpyrimidin-5-yl)(2-hydroxyphenyl)methanone (8r):



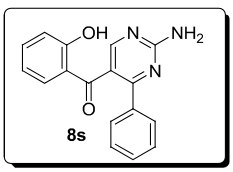
M.p. 105-109 °C. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 11.87 (s, 1H), 8.77 (s, 1H), 8.40 (m, 1H), 7.69 (m, 2H), 7.55 (m, 1H), 7.30 (m, 4H), 7.24 (m, 1H), 7.17 (m, 1H), 7.00 (m, 1H), 6.695 (m, 1H). IR (KBr, cm^{-1}): 3138, 3049, 2378, 1625, 1550, 1438, 1307, 1238, 1151, 925, 763, 686. ^{13}C NMR (100 MHz, CDCl3) = 200.4, 164.0, 163.0, 161.9, 157.1, 145.9, 144.1, 137.2, 136.7, 132.5, 130.6, 129.1, 128.7, 128.7, 127.6, 126.6, 126.6, 119.4, 119.1, 118.4, 109.5. MS (EI): *m/z* 342 (M+1,100), HRMS: (ESI): Calcd for $C_{21}H_{14}N_2O_3$ [M+H]: 343.1004, Found: 343.1086.

2-amino-5-phenyl-5H-chromeno[4,3-d]pyrimidin-5-ol (7s):



M.p. 190-194 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ = 8.14 (m, 1H), 7.85 (s, 1H), 7.68 (s, 1H), 7.56 (m, 2H), 7.48 (m, 1H), 7.41 (m, 4H).7.16 (t, 1H), 7.07 (d, 2H). IR (KBr, cm^{-1}): 3583, 3321, 2725, 2650, 1687, 1598, 1467, 1394, 1197, 948, 765, 690. ^{13}C NMR (100 MHz, DMSO-d6) = 160.4, 156.0, 155.2, 152.3, 141.6, 132.3, 128.4, 128.4, 128.0, 126.7, 124.7, 121.9, 119.0, 118.7, 117.4, 116.7, 98.8. MS (EI): *m/z* 291 (M+1,100), HRMS: (ESI): Calcd for $C_{17}H_{13}N_3O_2$ [M+H]: 292.1008, Found: 292.1090.

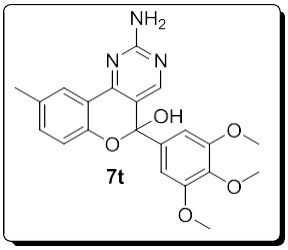
(2-amino-4-phenylpyrimidin-5-yl)(2-hydroxyphenyl)methanone (8s):



M.p. 250-254 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ = 10.96 (s, 1H), 8.37 (s, 1H), 7.31 (m, 9H), 6.78 (m, 2H). IR (KBr, cm^{-1}): 3414, 3323, 2719,

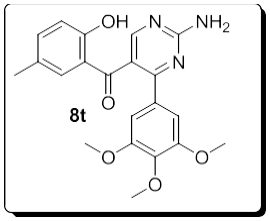
2376, 1685, 1629, 1570, 1481, 1242, 918, 758, 698. ^{13}C NMR (100 MHz, TFA-d) = .198.8, 172.7, 157.6, 155.7, 141.6, 137.7, 136.3, 134.7, 134.6, 134.2, 133.8, 132.5, 131.8, 131.6, 123.4, 123.3, 120.8. MS (EI): *m/z* 291 (M+1,100), HRMS: (ESI): Calcd for $C_{17}H_{13}N_3O_2$ [M+H]: 292.1008, Found: 292.1085.

2-amino-9-methyl-5-(3,4,5-trimethoxyphenyl)-5H-chromeno[4,3-d]pyrimidin-5-ol (7t):



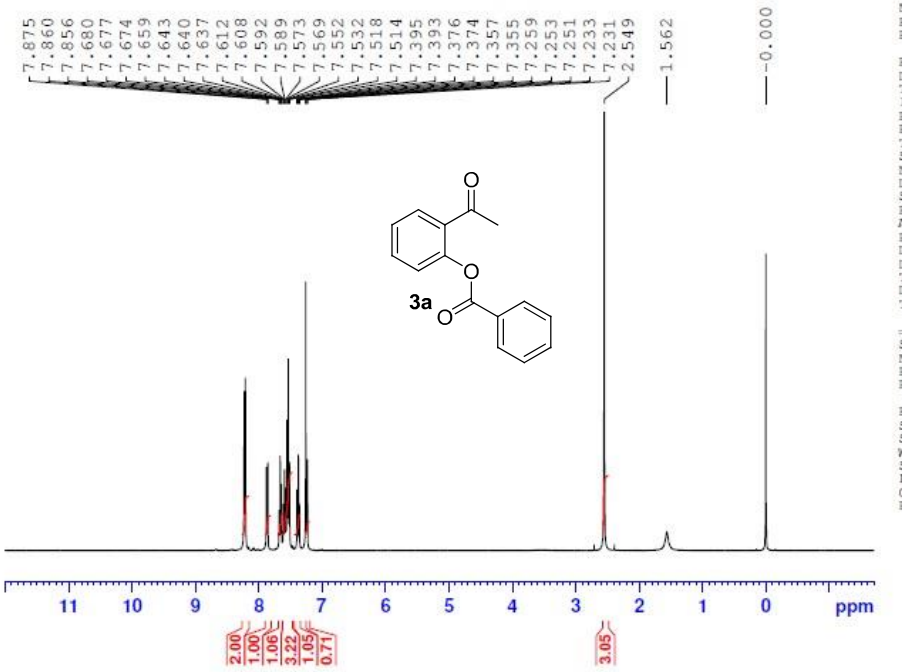
M.p. 162-166 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ = 7.95 (d, 1H), 7.67 (d, 2H), 7.29 (m, 1H), 6.96 (d, 1H), 6.83 (m, 4H), 3.75 (s, 3H), 3.65 (s, 6H), 2.45 (s, 3H). IR (KBr, cm^{-1}): 3421, 3325, 3180, 2933, 1647, 1589, 1562, 1458, 1327, 999, 742, 655. ^{13}C NMR (100 MHz, DMSO-d6) = 192.7, 163.4, 163.2, 156.2, 153.4, 152.6, 152.2, 137.8, 137.4, 133.2, 124.0, 119.4, 117.6, 106.9, 104.3, 98.8, 59.9, 55.8, 55.7, 20.3, 19.8. MS (EI): *m/z* 395 (M+1,100), HRMS: (ESI): Calcd for $C_{21}H_{21}N_3O_5$ [M+H]: 396.1481, Found: 396.1552.

(2-amino-4-(3,4,5-trimethoxyphenyl)pyrimidin-5-yl)(2-hydroxy-5-methylphenyl)methanone (8t):



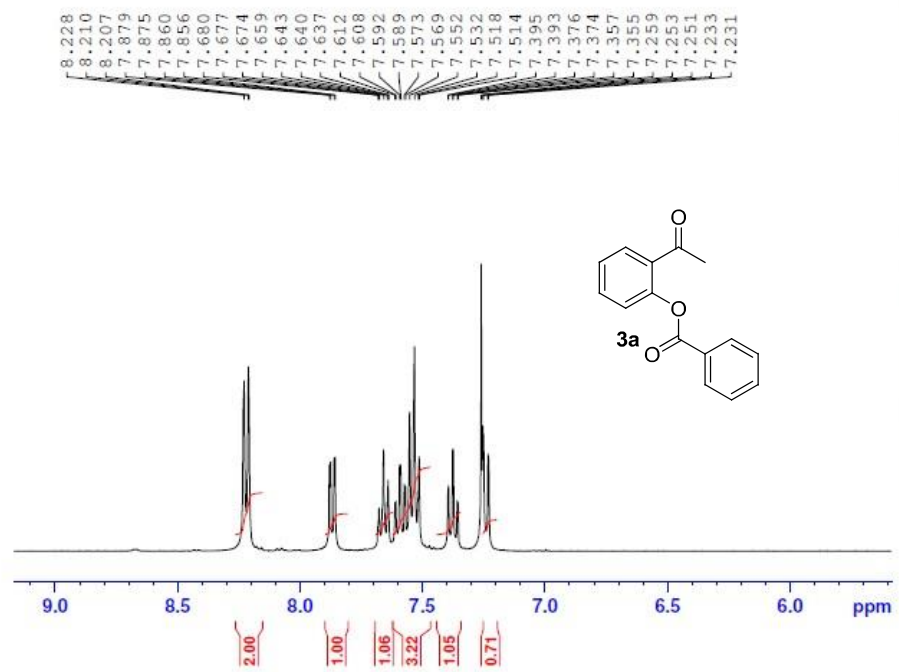
M.p. 186-190 °C. ^{1}H NMR (400 MHz, DMSO-d6): δ = 10.87 (s, 1H), 8.45 (s, 1H), 7.45 (s, 2H), 7.10 (m, 1H), 6.98 (d, 1H), 6.67 (m, 3H), 3.37 (s, 6H), 3.57 (s, 3H), 2.05 (s, 3H). IR (KBr, cm^{-1}): 3456, 3348, 3230, 2943, 1629, 1564, 1477, 1334, 1228, 972, 746, 659. ^{13}C NMR (100 MHz, CDCl3) = 200.6, 166.2, 163.2, 163.5, 159.6, 157.4, 153.3, 140.0, 137.9, 137.3, 132.5, 132.0, 128.0, 122.1, 119.6, 118.0, 106.3, 60.9, 56.2, 55.0, 20.3. MS (EI): *m/z* 395 (M+1,100), HRMS: (ESI): Calcd for $C_{21}H_{21}N_3O_5$ [M+H]: 396.1481, Found: 396.1557.

GVK-SAM-1-PAGE-48




```
Current Data Parameters
NAME          511511B5364
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20151123
Time                9.24
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32050
SOLVENT            CDC13
NS                     8
DS                     2
SWH             8012.820 Hz
FIDRES          0.250010 Hz
AQ              1.9999200 sec
RG                162.54
DW                62.400 usec
DE                 6.50 usec
TE                298.2 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            400.1300098 MHz
WDW                   EM
SSB       0
LB                 0.50 Hz
GB        0
PC                 1.00
```

GVK-SAM-1-PAGE-48



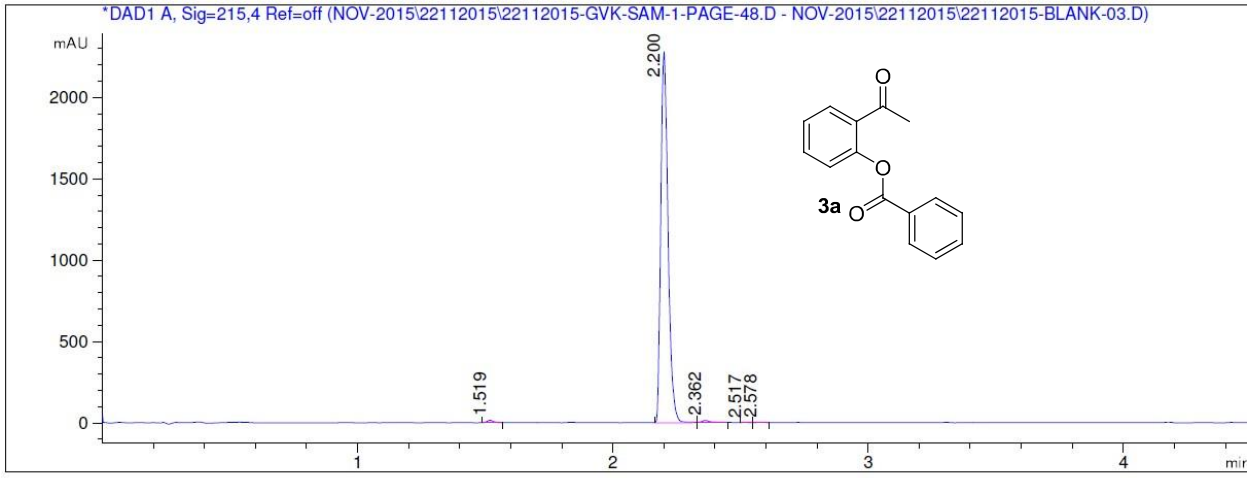

```
Current Data Parameters
NAME          511511B5364
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20151123
Time                9.24
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32050
SOLVENT            CDC13
NS                     8
DS                     2
SWH             8012.820 Hz
FIDRES          0.250010 Hz
AQ              1.9999200 sec
RG                162.54
DW                62.400 usec
DE                 6.50 usec
TE                298.2 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            400.1300098 MHz
WDW                   EM
SSB       0
LB                 0.50 Hz
GB        0
PC                 1.00
```

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

LCMS REPORT

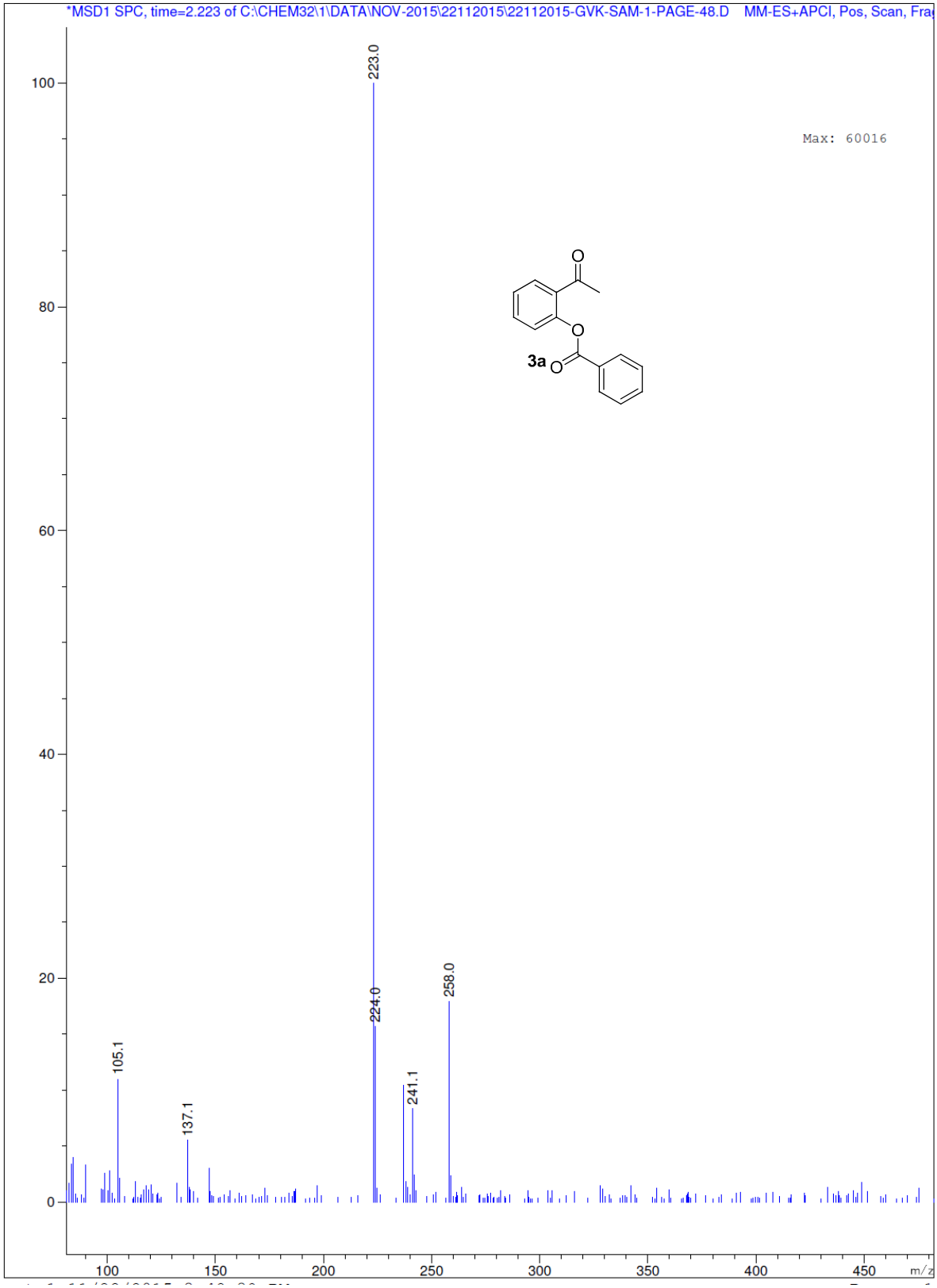
Sample Name :GVK-SAM-1-PAGE-48 Vial position :P1-A-09
Date of Analysis:22/11/2015;3:41:50 PM Injection Vol: 0.5 µL
Acq. Method->C:\CHEM32\1\METHODS\RND-FA- 4.5 MIN_1.M Instrument ID:ANL-MCL5-LCMS-001

Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: A1: 0.1 % FA IN WATER B1: 0.1%FA IN ACN
Gradient: Time (min) /%B1: 0/3, 0.3/3, 2.8/98,4.0/98,4.2/3,4.5/3
Column Flow Rate: 0.6 ml/min

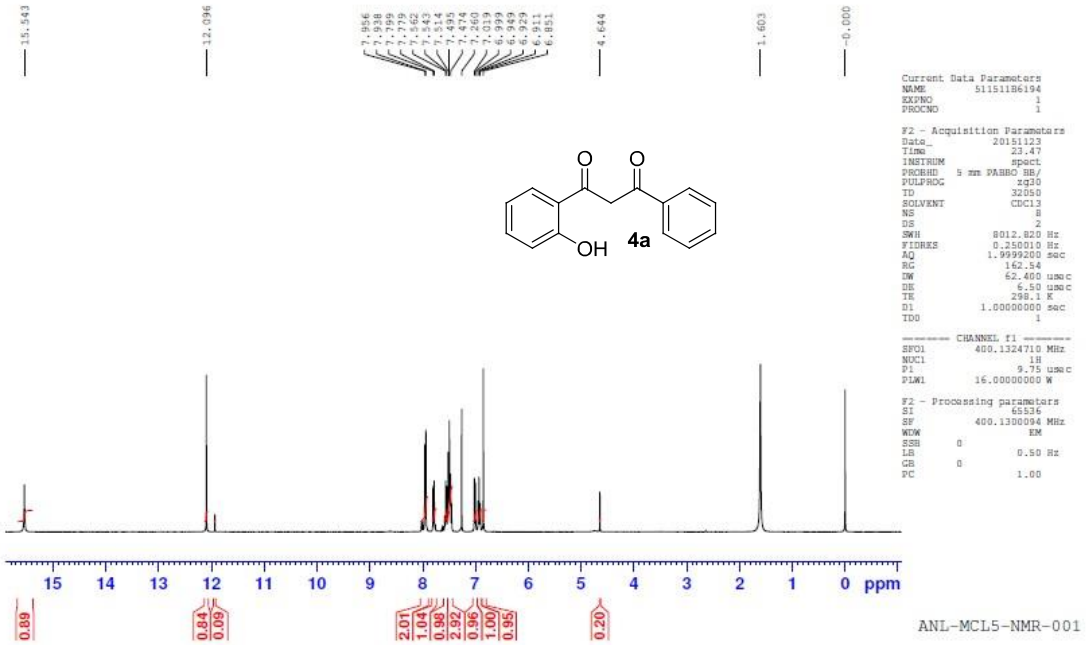


Pea No	RT min	Area	Area %
1	1.52	26.994	0.590
2	2.20	4511.067	98.619
3	2.36	33.537	0.733
4	2.52	0.887	0.019
5	2.58	1.737	0.038

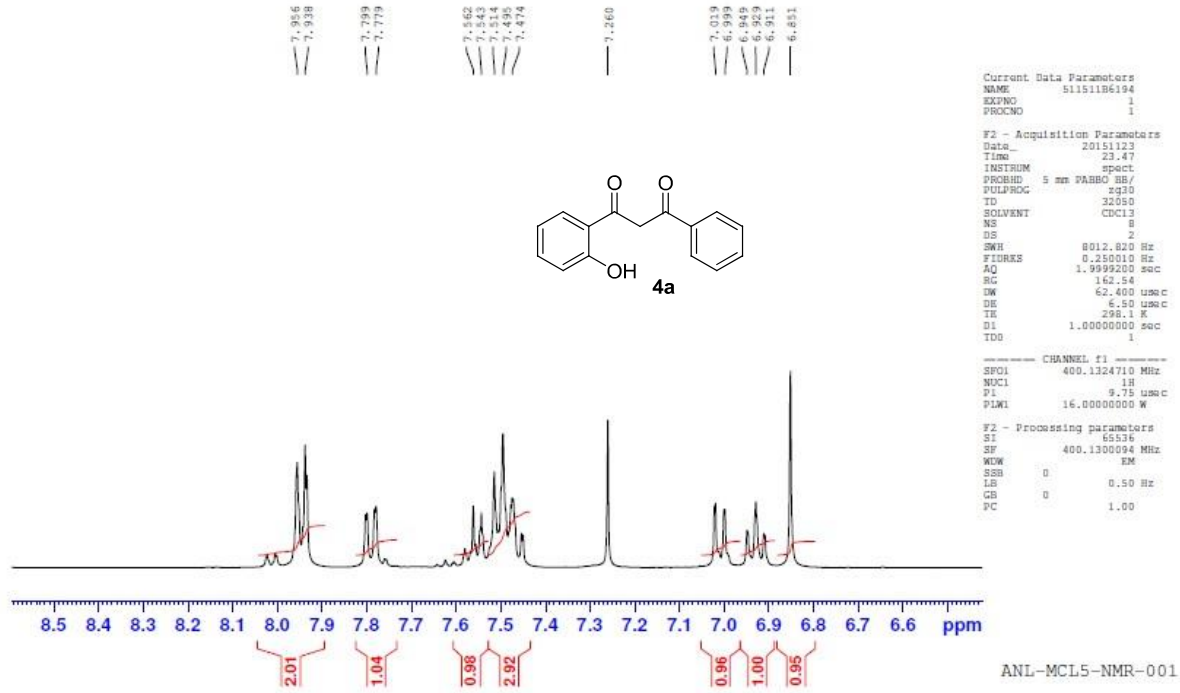
MS Spectrum


*MSD1 SPC, time=2.223 of C:\CHEM32\1\DATA\NOV-2015\22112015\22112015-GVK-SAM-1-PAGE-48.D MM-ES+APCI, Pos, Scan, Fra
Max: 60016
223.0
224.0
258.0
105.1
137.1
241.1
3a
100
80
60
40
20
0
100
150
200
250
300
350
400
450
m/z

GVK-SAM-1-PAGE-49



GVK-SAM-1-PAGE-49

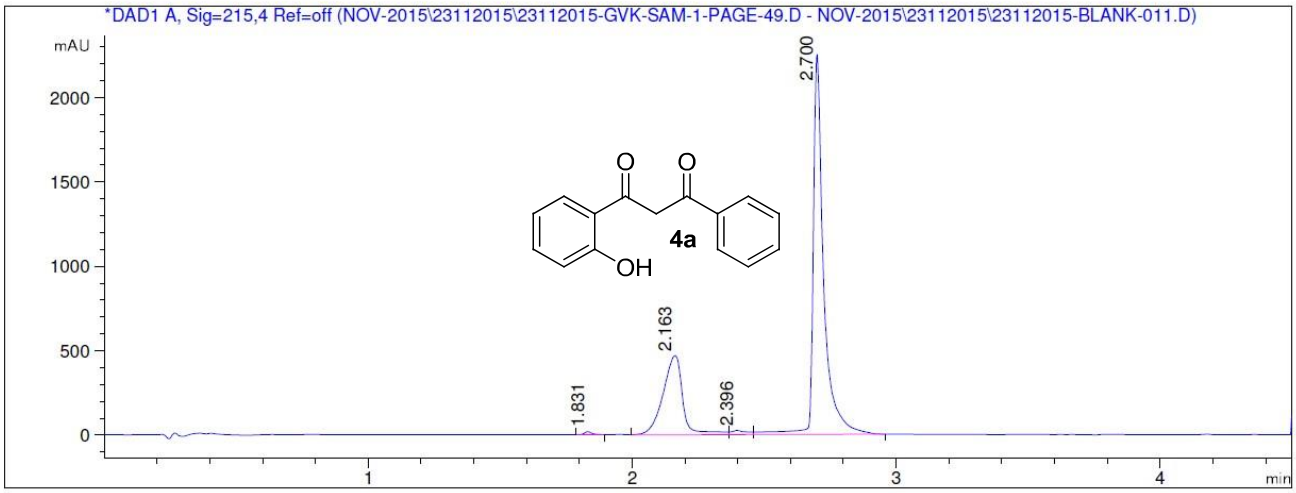


GVK BIOSCIENCES PVT. LTD.
MEDICINAL CHEMISTRY LABORATORY - ANALYTICAL RESEARCH

LCMS REPORT

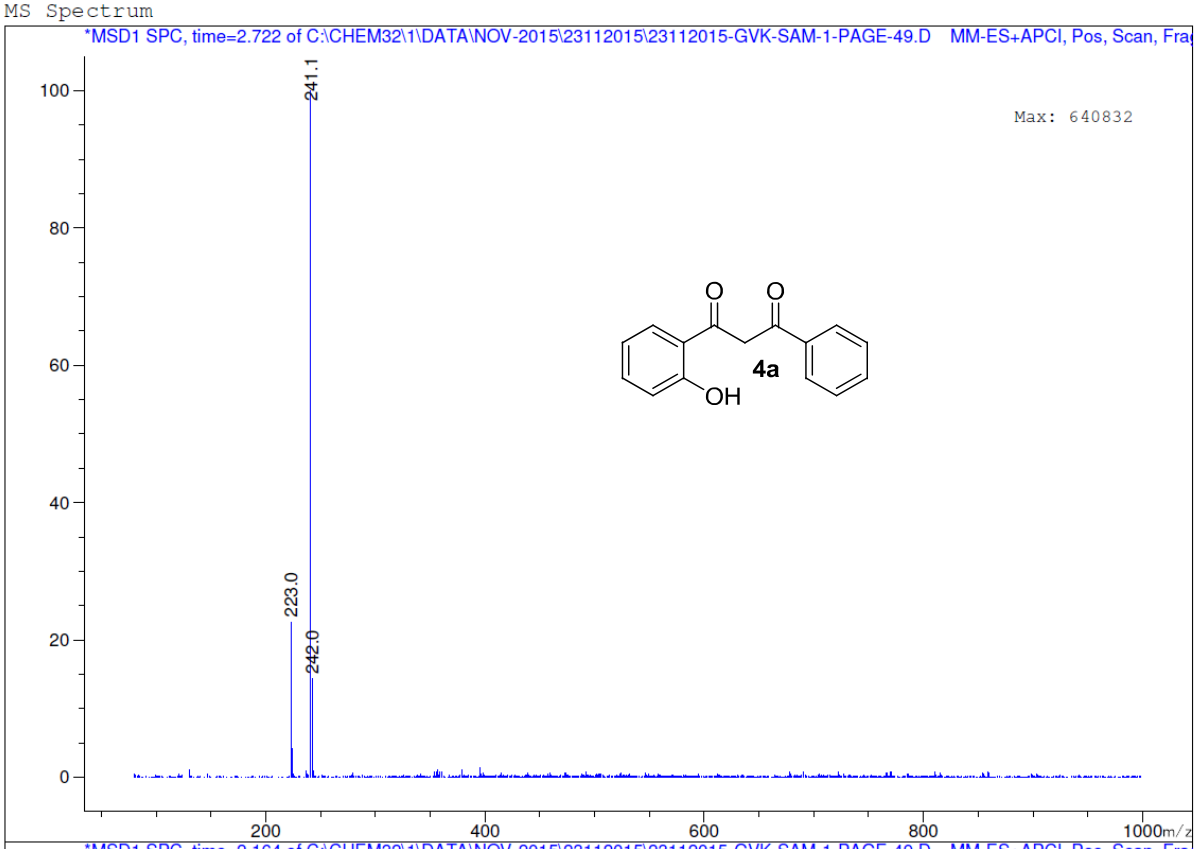
Sample Name :GVK-SAM-1-PAGE-49 Vial position :P2-F-03
Date of Analysis:24/11/2015;12:07:44 AM Injection Vol: 0.5 µL
Acq. Method->C:\CHEM32\1\METHODS\RND-FA- 4.5 MIN_1.M Instrument ID:ANL-MCL5-LCMS-001

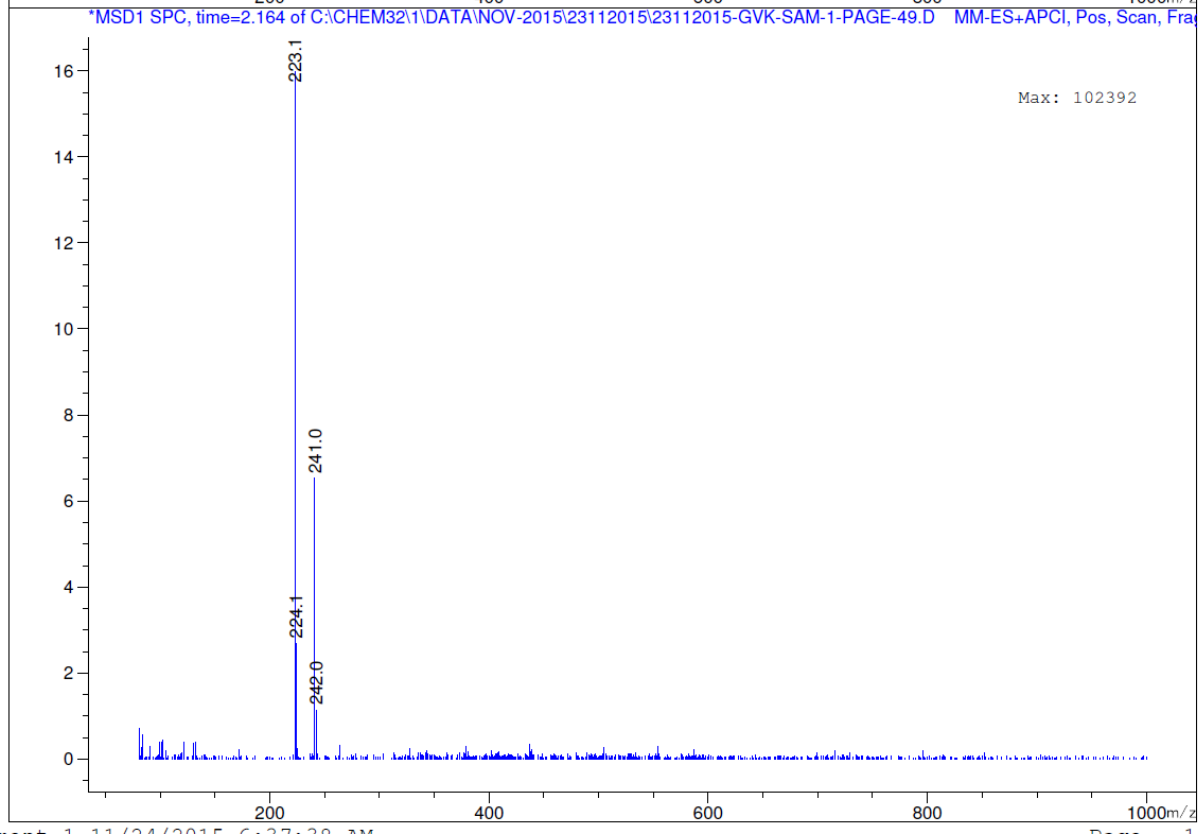
Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: A1: 0.1 % FA IN WATER B1: 0.1%FA IN ACN
Gradient: Time (min) /%B1: 0/3, 0.3/3, 2.8/98,4.0/98,4.2/3,4.5/3
Column Flow Rate: 0.6 ml/min



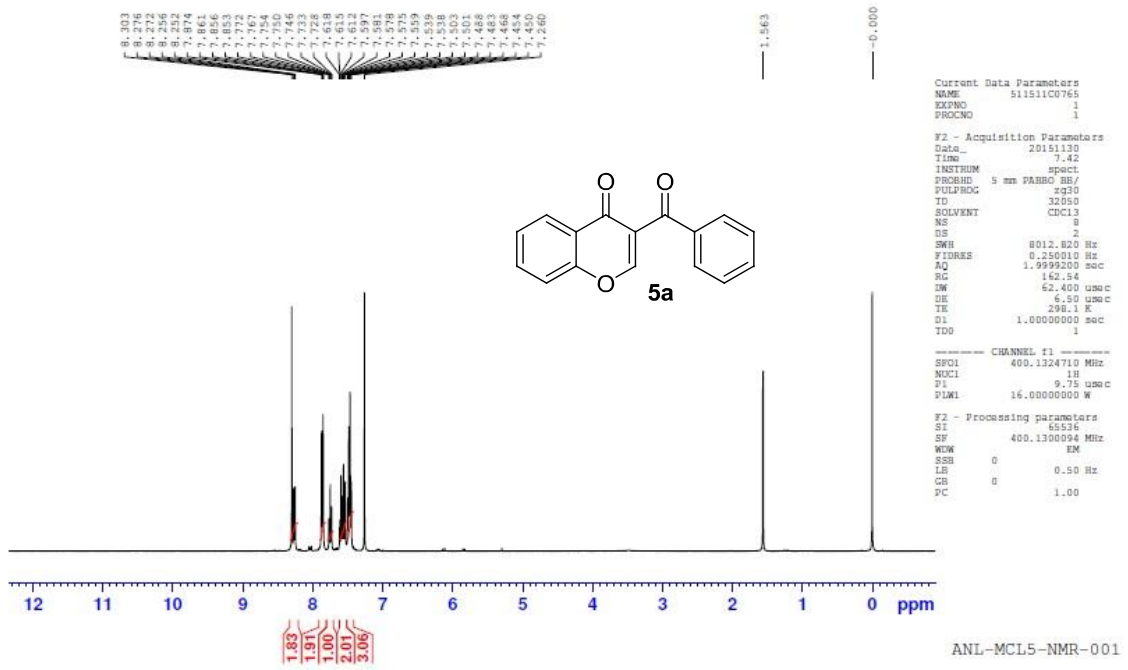
Pea No	RT min	Area	Area %
1	1.83	38.113	0.433
2	2.16	2449.560	27.832
3	2.40	101.074	1.148
4	2.70	6212.585	70.587

MS Spectrum


*MSD1 SPC, time=2.722 of C:\CHEM32\1\DATA\NOV-2015\23112015\23112015-GVK-SAM-1-PAGE-49.D MM-ES+APCI, Pos, Scan, Fra
Max: 640832
241.1
223.0
242.0
O
O
OH
4a
100
80
60
40
20
0
200
400
600
800
1000m/z

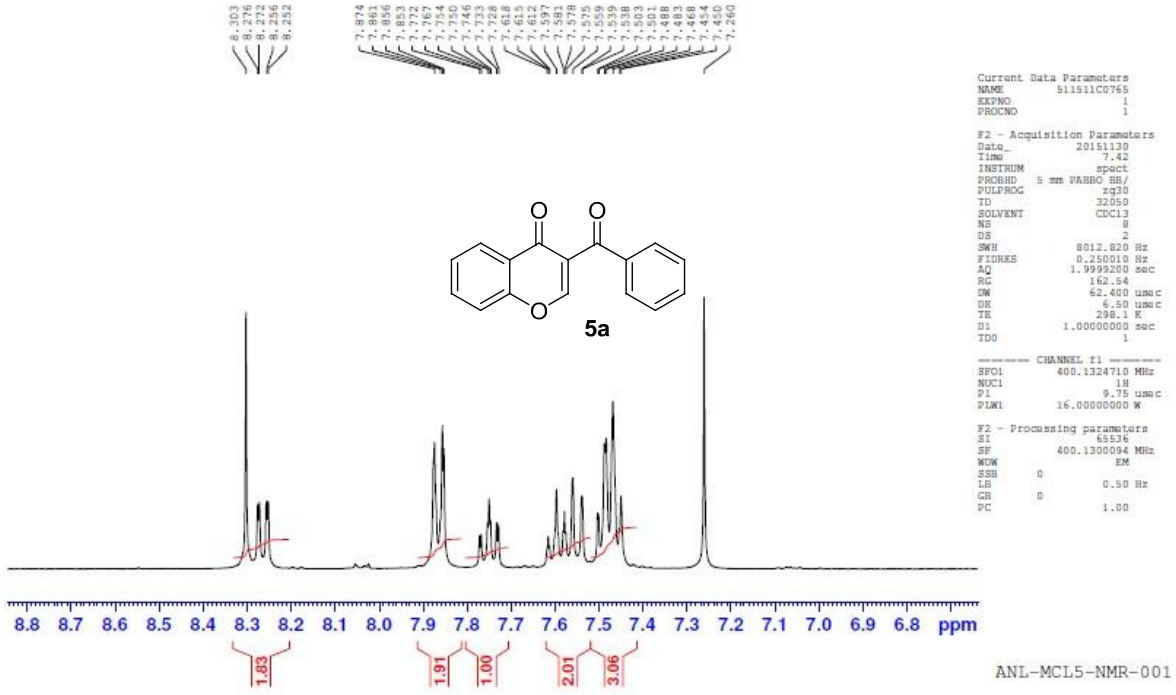

*MSD1 SPC, time=2.164 of C:\CHEM32\1\DATA\NOV-2015\23112015\23112015-GVK-SAM-1-PAGE-49.D MM-ES+APCI, Pos, Scan, Fra
Max: 102392
223.1
241.0
224.1
242.0
16
14
12
10
8
6
4
2
0
200
400
600
800
1000m/z

GVK-SAM-1-PAGE-53



ANL-MCL5-NMR-001

GVK-SAM-1-PAGE-53



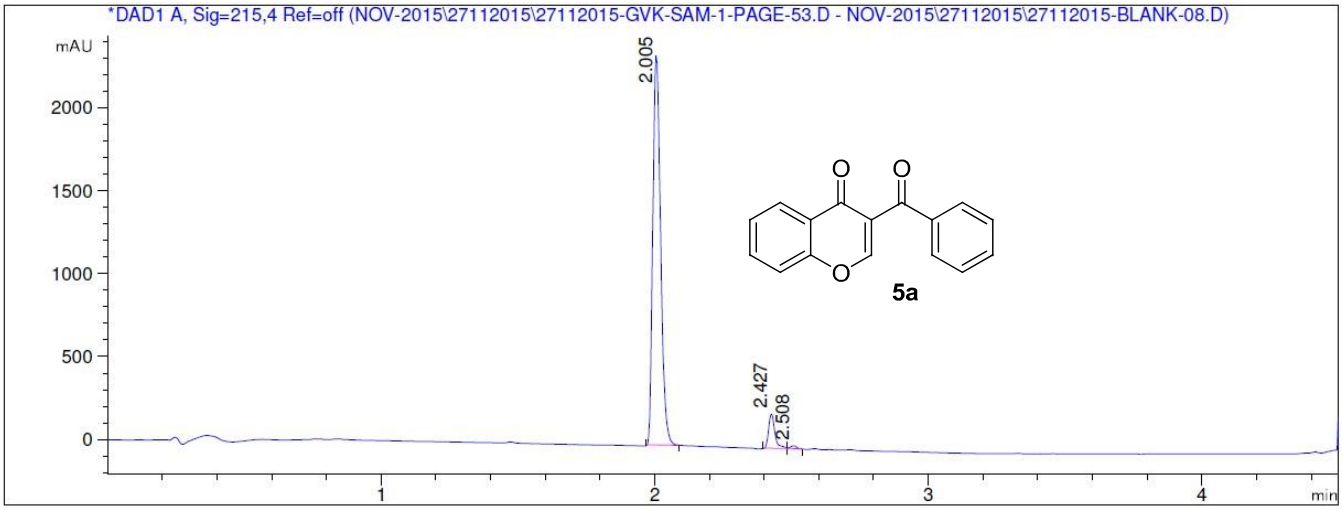
ANL-MCL5-NMR-001

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

LCMS REPORT

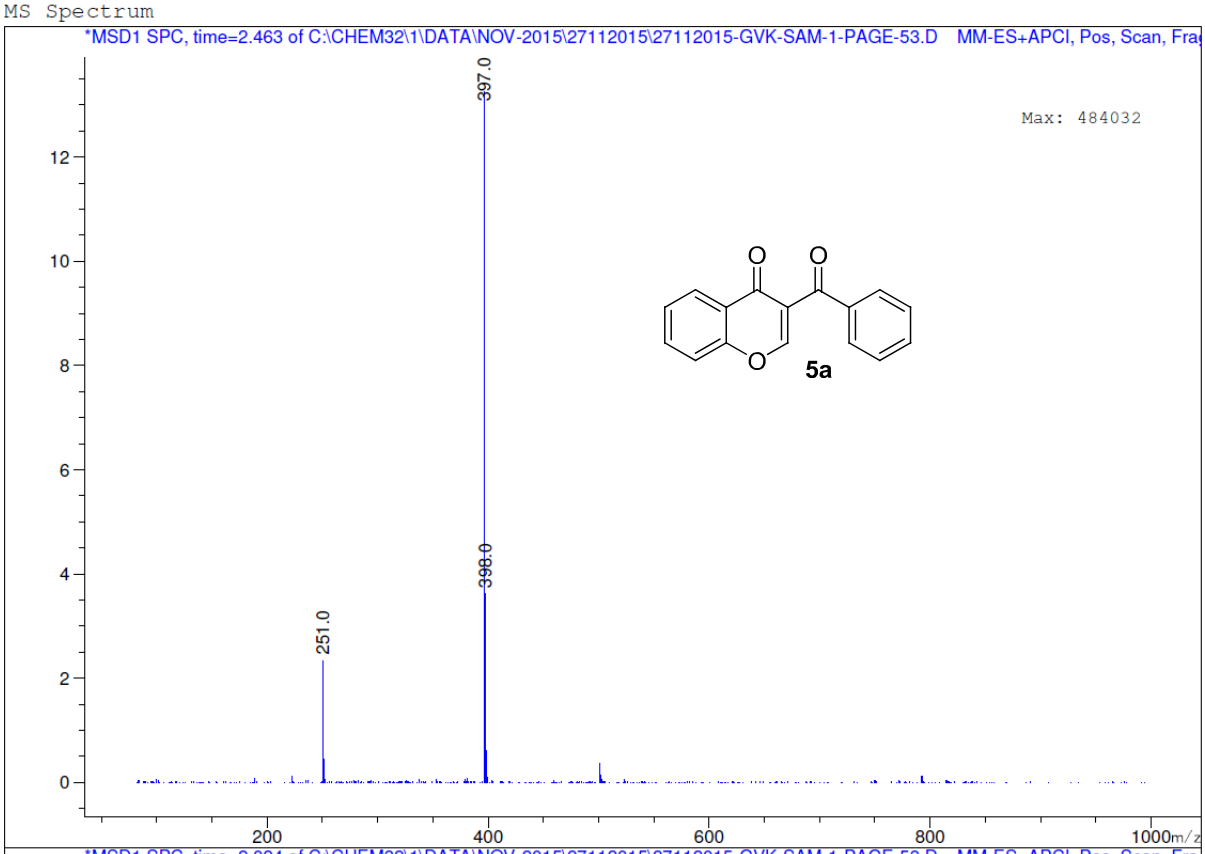
>Sample Name: GVK-SAM-1-PAGE-53 Vial position :P2-C-08
Date of Analysis:27/11/2015;10:26:02 PM Injection Vol :0.5 µL
Acq. Method :C:\CHEM32\1\METHODS\RND-FA- 4.5 MIN_1.M Instrument ID :ANL-MCL5-LCMS-001

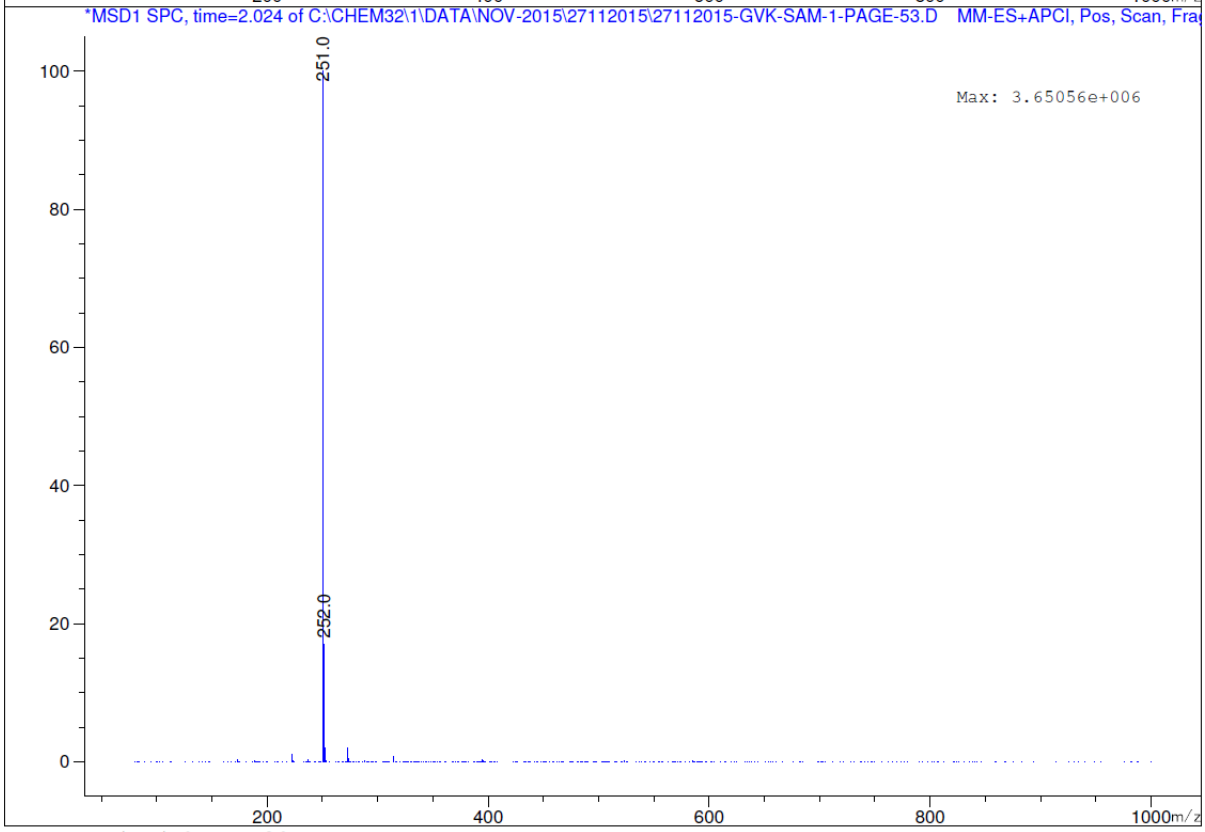
Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: A1: 0.1 % FA IN WATER B1: 0.1%FA IN ACN
Gradient: Time (min) /%B1:0/3, 0.3/3, 2.8/98,4.0/98,4.2/3,4.5/3
Column Flow Rate: 0.6 ml/min



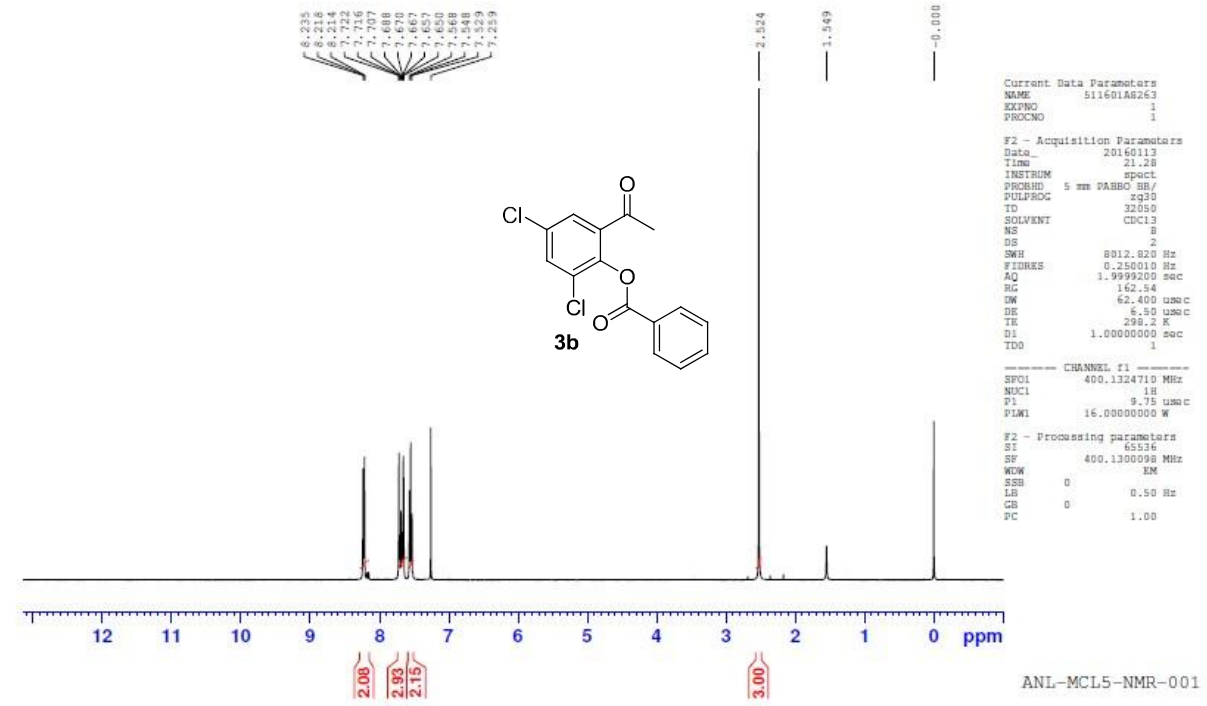
Pea No	RT min	Area	Area %
1	2.01	4.649e3	92.884
2	2.43	330.261	6.598
3	2.51	25.904	0.518

MS Spectrum


*MSD1 SPC, time=2.463 of C:\CHEM32\1\DATA\NOV-2015\27112015\27112015-GVK-SAM-1-PAGE-53.D MM-ES+APCI, Pos, Scan, Frag
Max: 484032
397.0
398.0
251.0
O
O
O
5a
m/z


*MSD1 SPC, time=2.024 of C:\CHEM32\1\DATA\NOV-2015\27112015\27112015-GVK-SAM-1-PAGE-53.D MM-ES+APCI, Pos, Scan, Frag
Max: 3.65056e+006
251.0
252.0
m/z

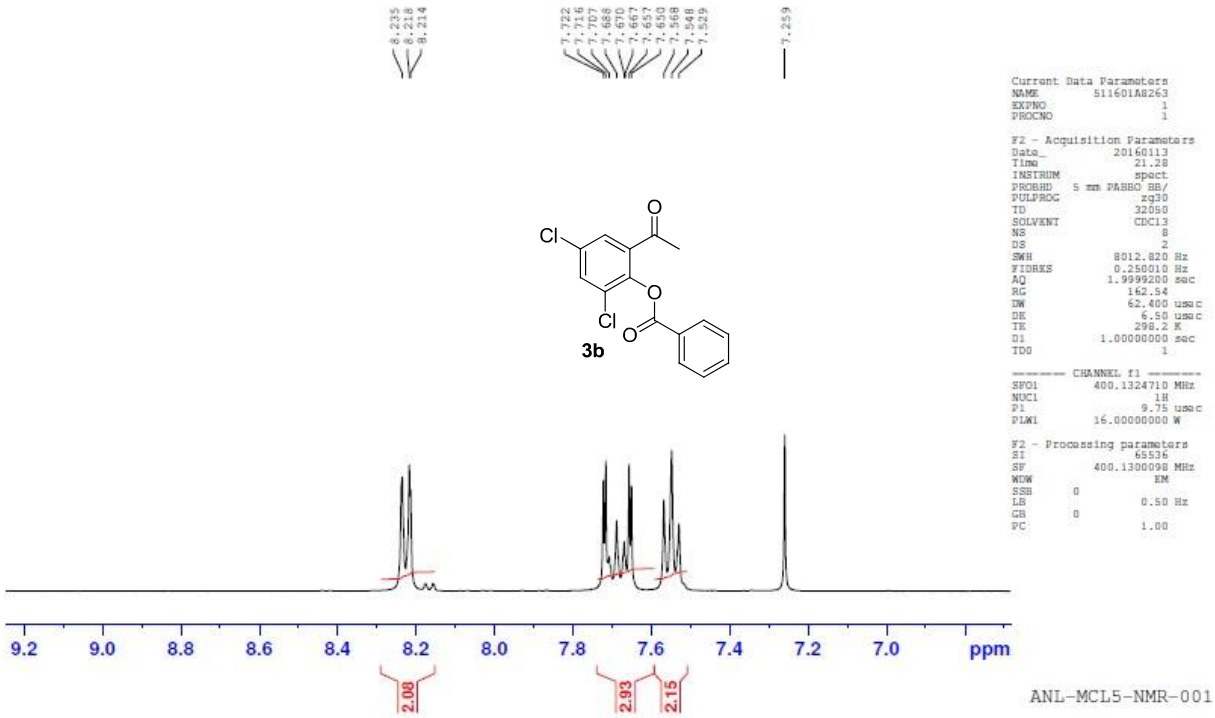
GVK-SAM-5-PAGE-2




```
Current Data Parameters
NAME          511601A8263
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20160113
Time              21.28
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                32050
SOLVENT           CDCl3
NS                    8
DS                    2
SWH            8012.820 Hz
FIDRES         0.250010 Hz
AQ             1.9999200 sec
RG               162.54
DW              62.400 usec
DE               6.50 usec
TE              298.2 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            400.1300098 MHz
WDW                   EM
SSB       0
LB                0.50 Hz
GB        0
PC                1.00
```

ANL-MCL5-NMR-001

GVK-SAM-5-PAGE-2




```
Current Data Parameters
NAME          511601A8263
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20160113
Time              21.28
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                32050
SOLVENT           CDCl3
NS                    8
DS                    2
SWH            8012.820 Hz
FIDRES         0.250010 Hz
AQ             1.9999200 sec
RG               162.54
DW              62.400 usec
DE               6.50 usec
TE              298.2 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            400.1300098 MHz
WDW                   EM
SSB       0
LB                0.50 Hz
GB        0
PC                1.00
```

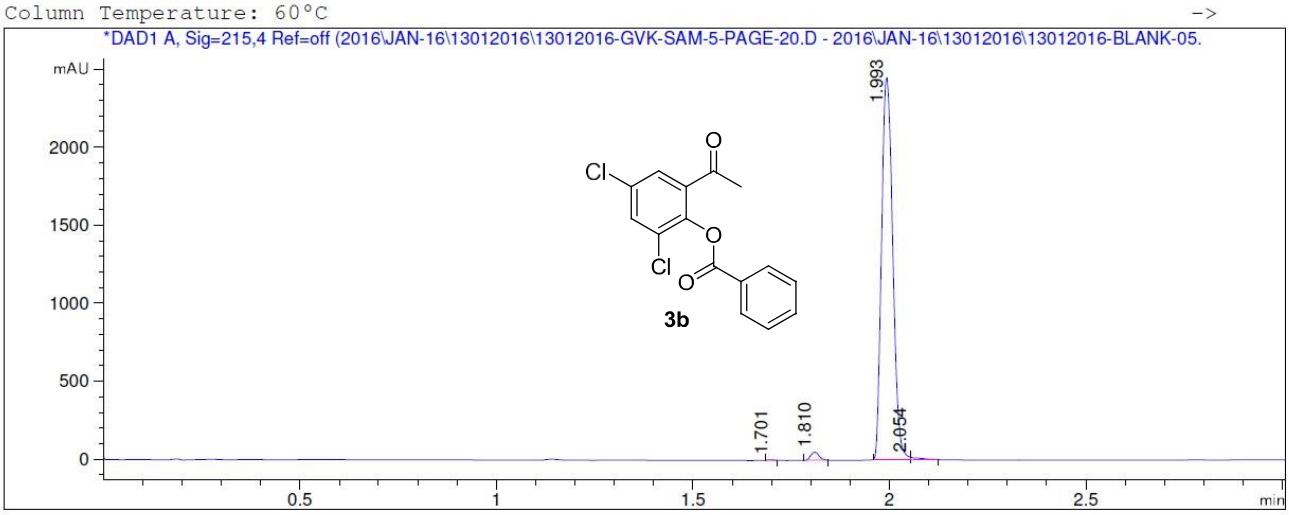
ANL-MCL5-NMR-001

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

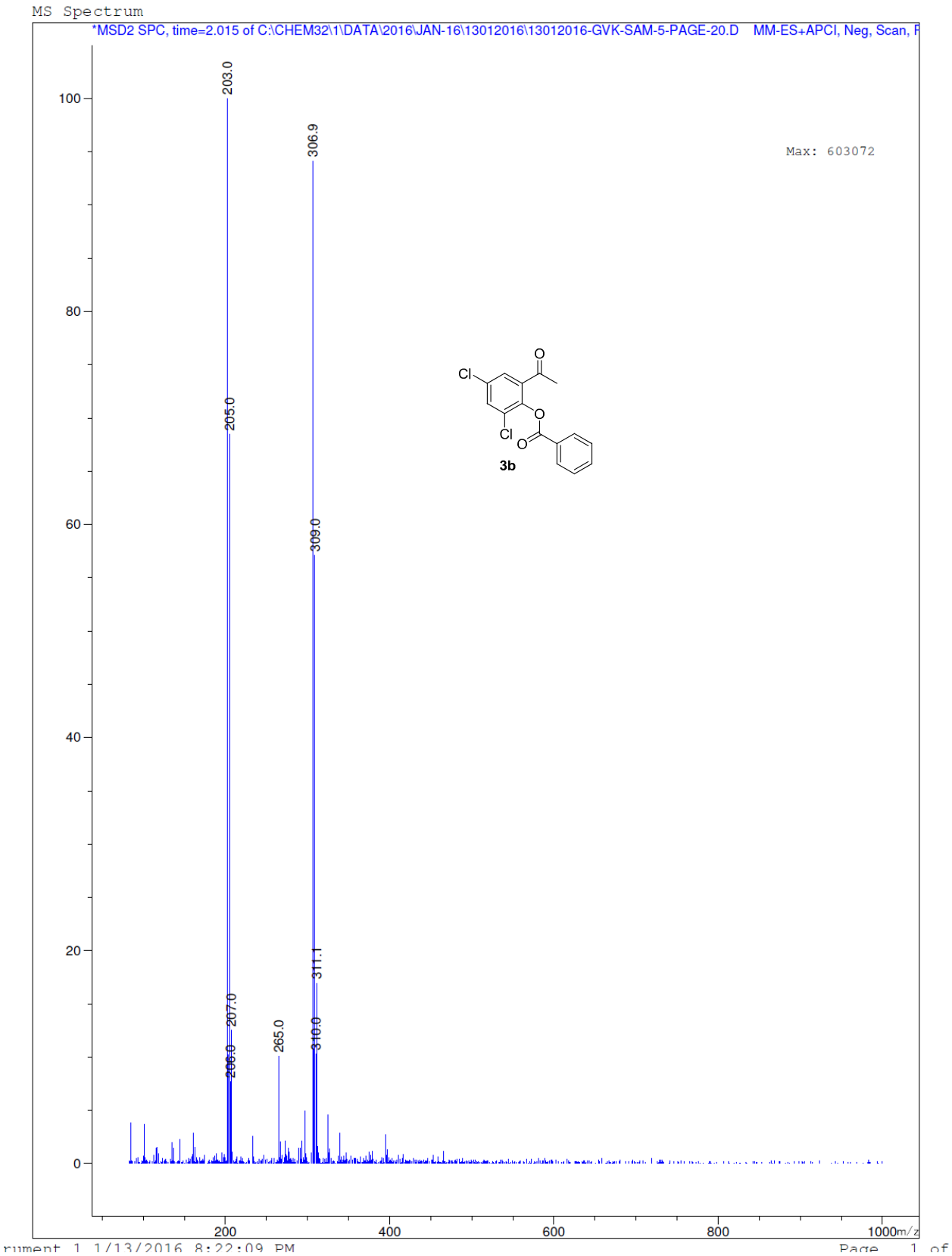
LCMS REPORT

Sample Name :GVK-SAM-5-PAGE-20 Vial position :P1-F-06
Date of Analysis:1/13/2016 8:16:12 PM Injection Vol :0.500µl
Acq. Method :C:\CHEM32\1\METHODS\RND-FA- 3.0 MIN.M Instrument ID :ANL-MCL5-LCMS-001

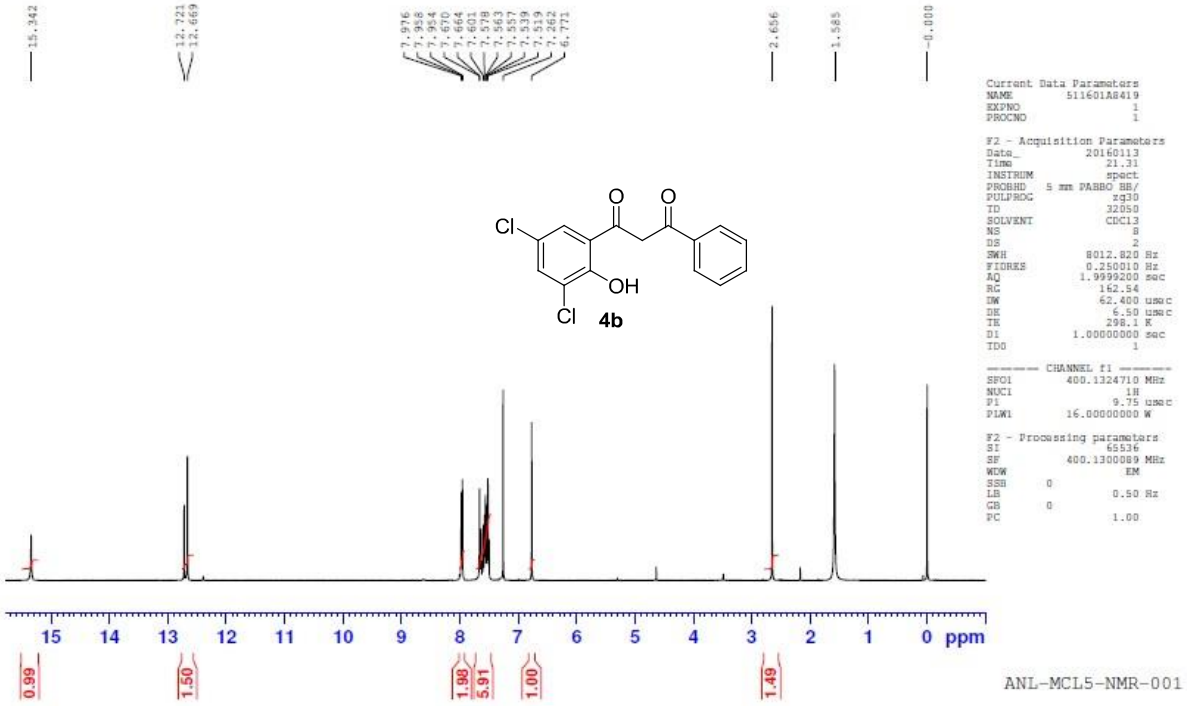
RND-FA-3.0 MIN.M
Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: B1: 0.1 % FA IN WATER A1: 0.1%FA IN ACN
Gradient: Time (min) /%A1: 0/2, 0.3/2, 2.3/98,2.8/98,2.8/2,3.0/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 60°C ->



Pea No	RT min	Area	Area %
1	1.70	4.561	0.092
2	1.81	74.941	1.513
3	1.99	4848.227	97.914
4	2.05	23.772	0.480

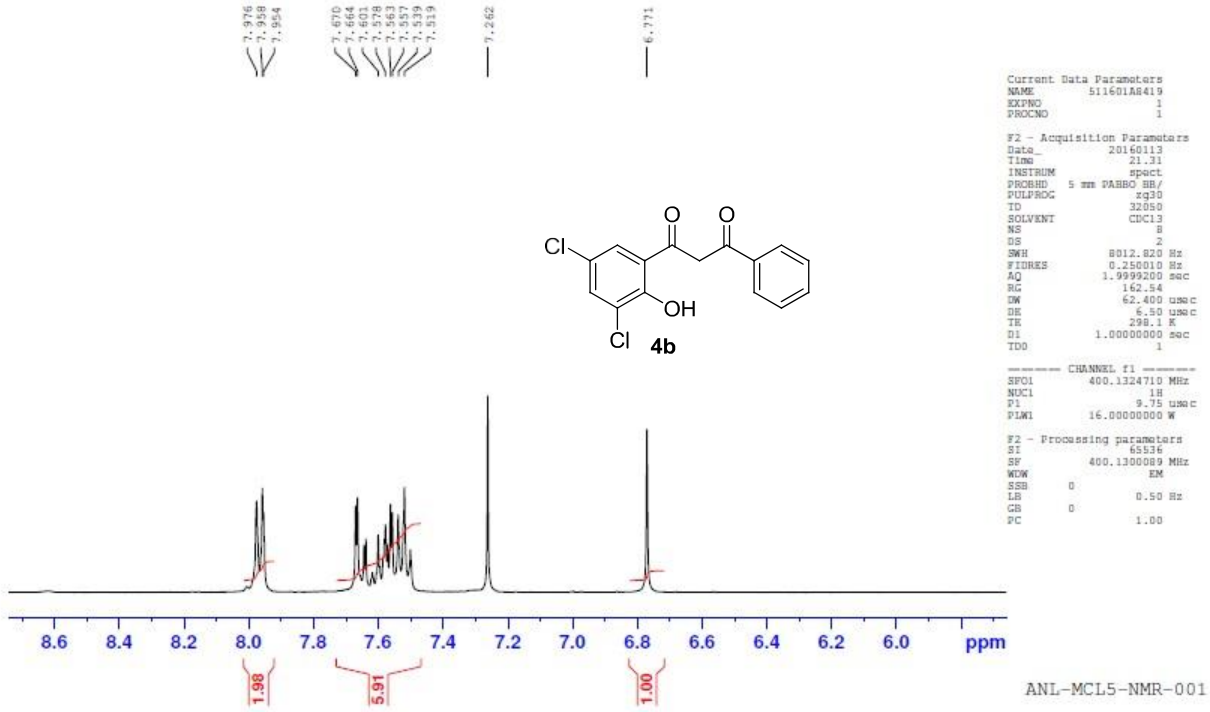

MS Spectrum
*MSD2 SPC, time=2.015 of C:\CHEM32\1\DATA\2016\JAN-16\13012016\13012016-GVK-SAM-5-PAGE-20.D MM-ES+APCI, Neg, Scan, F
Max: 603072
203.0
306.9
205.0
309.0
311.1
207.0
265.0
310.0
206.0
100
80
60
40
20
0
200
400
600
800
1000m/z
Cl
Cl
O
O
O
3b
rument 1 1/13/2016 8:22:09 PM
Page 1 of

GVK-SAM-5-PAGE-22



ANL-MCL5-NMR-001

GVK-SAM-5-PAGE-22



ANL-MCL5-NMR-001

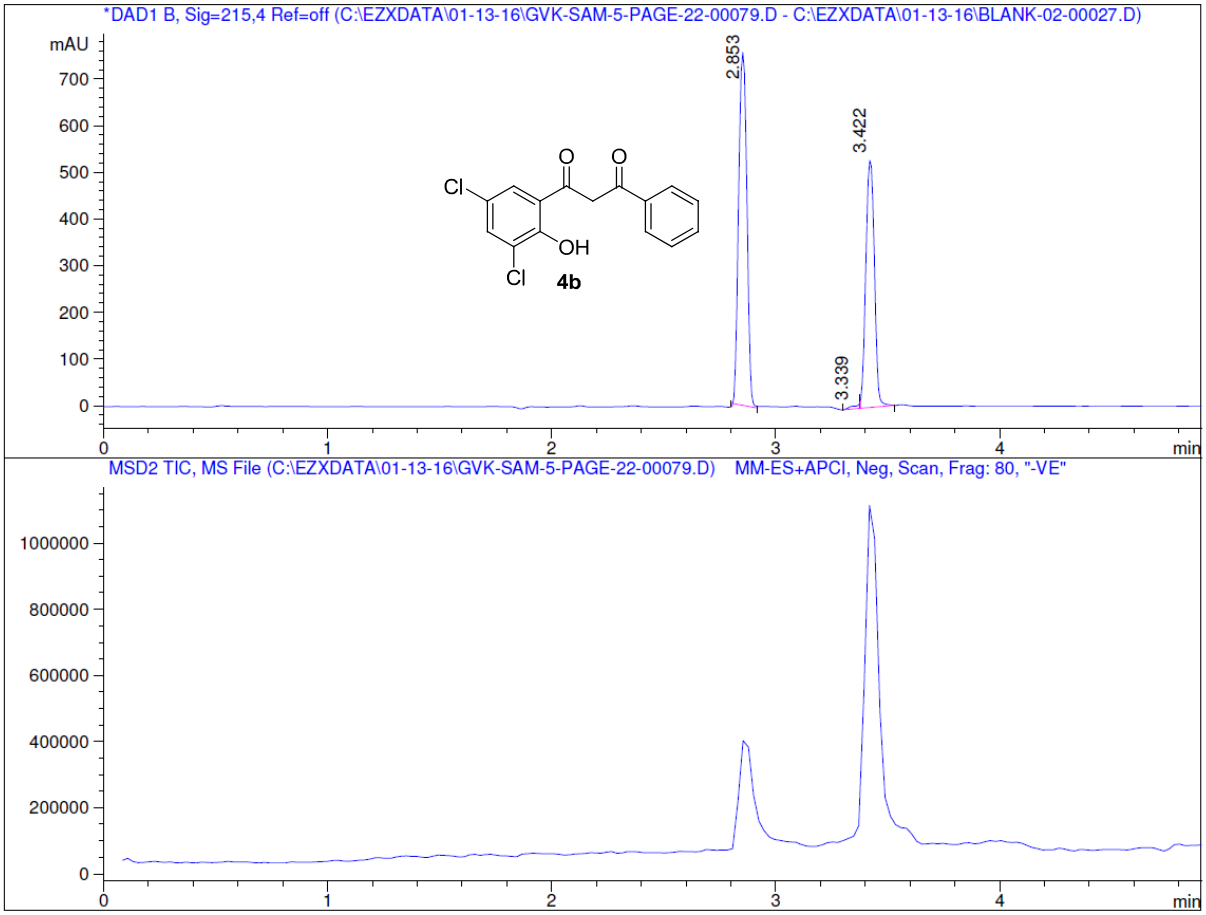
GVK BIOSCIENCES PVT. LTD.
MEDICINAL CHEMISTRY LABORATORY-ANALYTICAL RESEARCH

ELSD-MS REPORT

Date of Analysis:13/01/2016;9:22:15 PM Vial Position :Vial 80
Sample Name :GVK-SAM-5-PAGE-22 Injection Vol : 3.000µl
Acq. Method :C:\CHEM32\1\METHODS\RND X-BRIDGE 5->Instrument ID :ANL-MCL2-LCMS-002

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 : Ambient
Flow rate : 2.0 ml/min

->

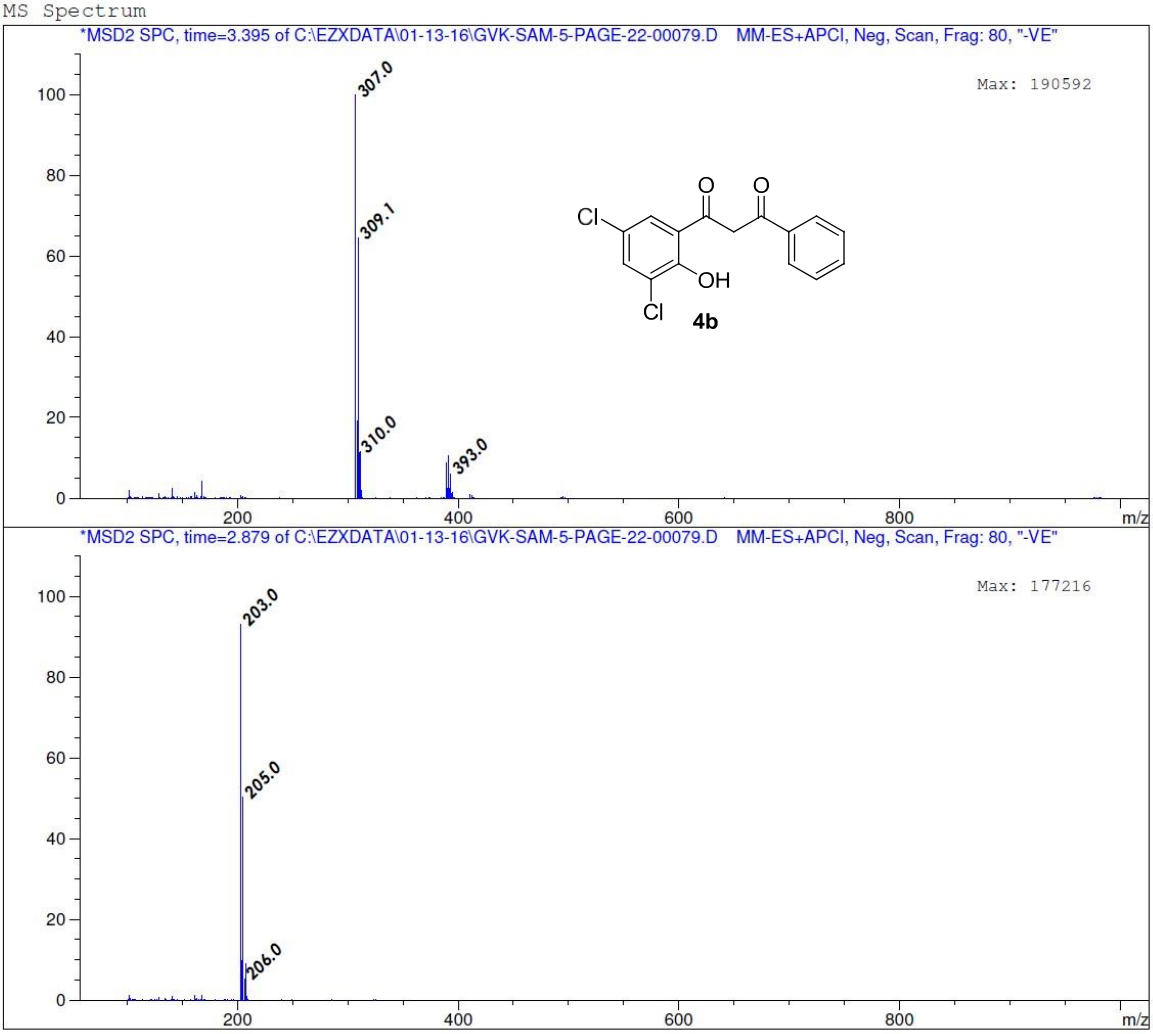


DAD1 B, Sig=215,4 Ref=->

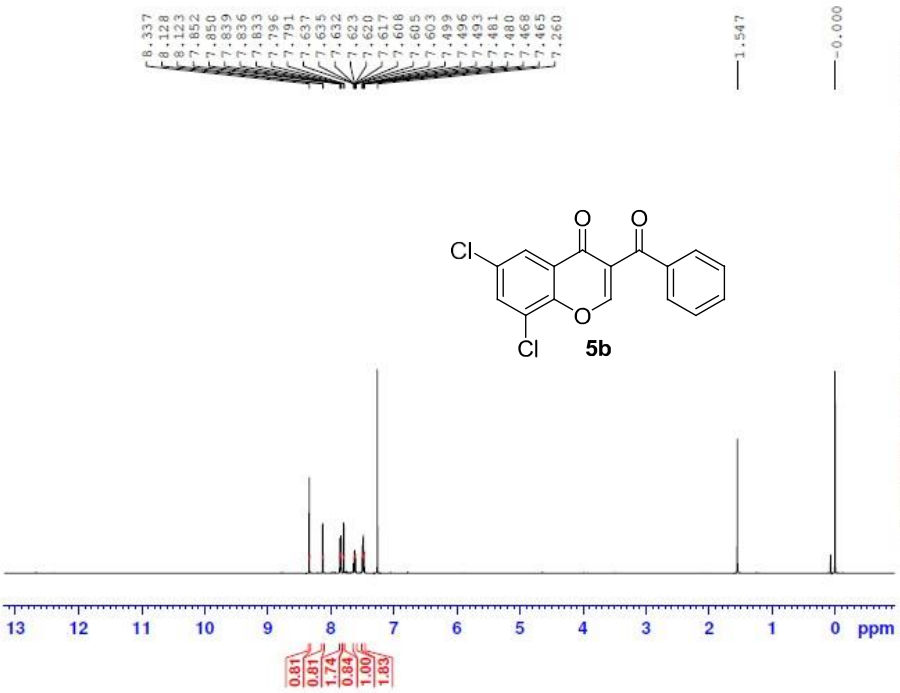
PEAK No	RT min	Area	Area %
1	2.853	1924.310	57.399
2	3.339	26.579	0.793
3	3.422	1401.637	41.808

```
Print of window 80: MS Spectrum
Data File  : C:\EZXDATA\01-13-16\GVK-SAM-5-PAGE-22-00079.D
Sample Name : GVK-SAM-5-PAGE-22
======================================================================
Acq. Operator   : ESAMPLE
Acq. Instrument : INSTRUMENT 1                    Location : Vial 80
Injection Date  : 1/13/2016 9:22:15 PM                 Inj :   1
                                                 Inj Volume : 3.000 µl
Acq. Method     : C:\CHEM32\1\METHODS\RND X-BRIDGE 5.0 MI
Last changed    : 1/13/2016 9:20:46 PM by ESAMPLE
                  (modified after loading)
Analysis Method : C:\CHEM32\1\METHODS\RND X-BRIDGE 5.0 MIN.M
Last changed    : 1/11/2016 7:27:38 PM by D SUNDARA RAO
Method Info     : 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 : Ambient
                  Flow rate : 2.0 ml/min

Sample Info     : Easy-Access Method: 'RND X-BRIDGE 5.0 MIN'

Additional Info : Peak(s) manually integrated
```

MS Spectrum



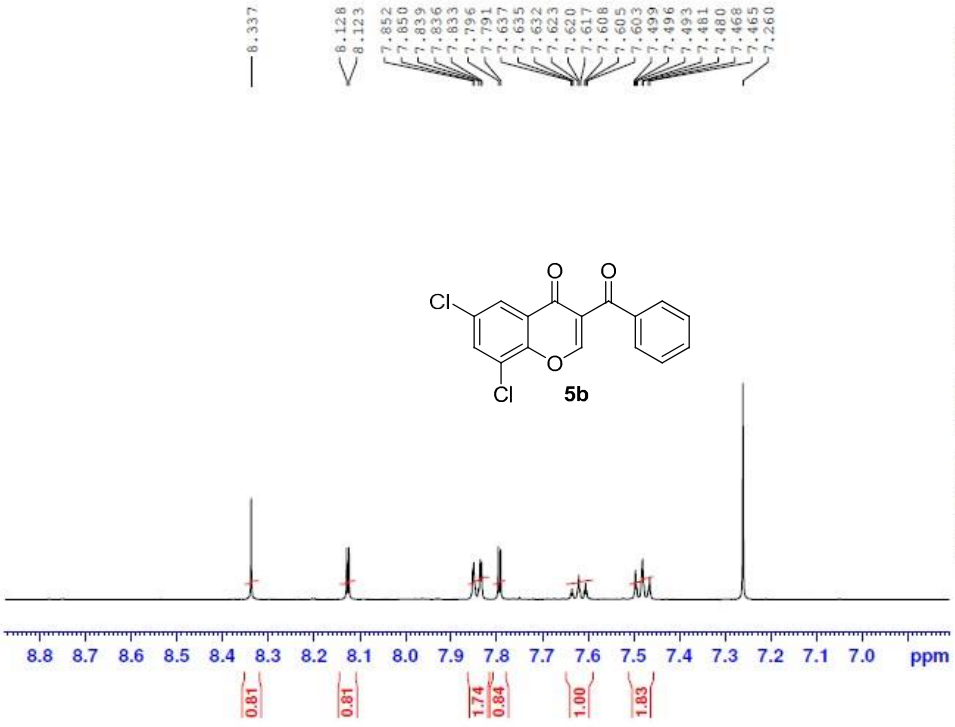
GVK-SAM-5-Page-23-NP




```
Current Data Parameters
NAME          511601A9893
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_              20160118
Time                 17.29
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      8
DS                      0
SWH            10000.000 Hz
FIDRES         0.152588 Hz
AQ             3.2767999 sec
RG                 157.05
DW                 50.000 usec
DE                  6.50 usec
TE                 298.1 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          500.1330885 MHz
NUC1                    1H
P1                  10.00 usec
PLW1          24.00000000 W

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

ANL-MCL5-NMR-002

GVK-SAM-5-Page-23-NP



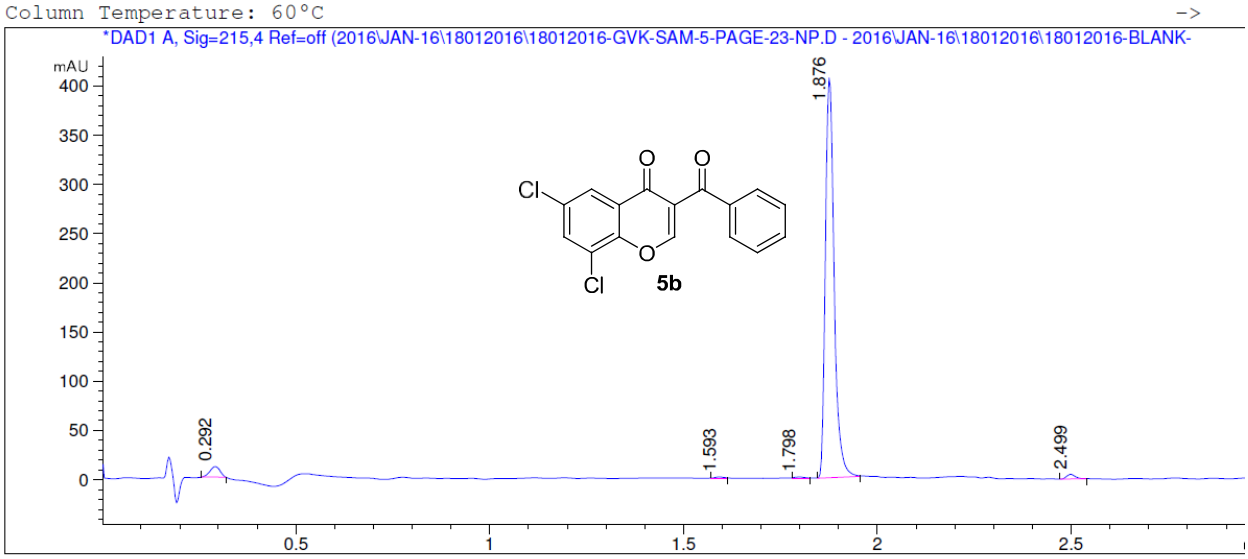

```
Current Data Parameters
NAME          511601A9893
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_              20160118
Time                 17.29
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      8
DS                      0
SWH            10000.000 Hz
FIDRES         0.152588 Hz
AQ             3.2767999 sec
RG                 157.05
DW                 50.000 usec
DE                  6.50 usec
TE                 298.1 K
D1             1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          500.1330885 MHz
NUC1                    1H
P1                  10.00 usec
PLW1          24.00000000 W

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

ANL-MCL5-NMR-002

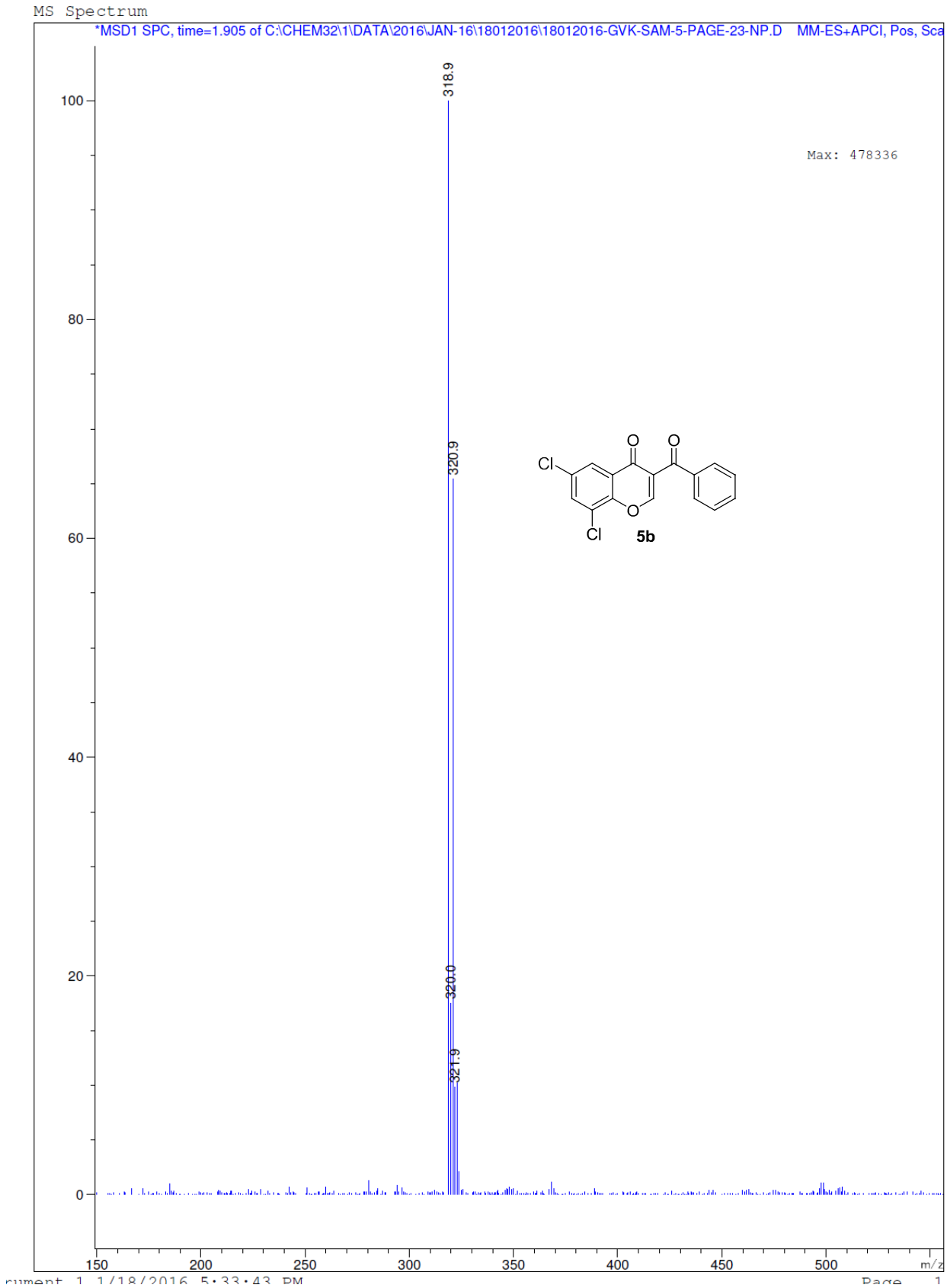
GVK BIOSCIENCES PVT. LTD.
MEDICINAL CHEMISTRY LABORATORY - ANALYTICAL RESEARCH
LCMS REPORT

Sample Name :GVK-SAM-5-PAGE-23-NP	Vial position :P1-C-06
Date of Analysis:1/18/2016 5:26:08 PM	Injection Vol :0.500µl
Acq. Method :C:\CHEM32\1\METHODS\RND-FA- 3.0 MIN.M	Instrument ID :ANL-MCL5-LCMS-001

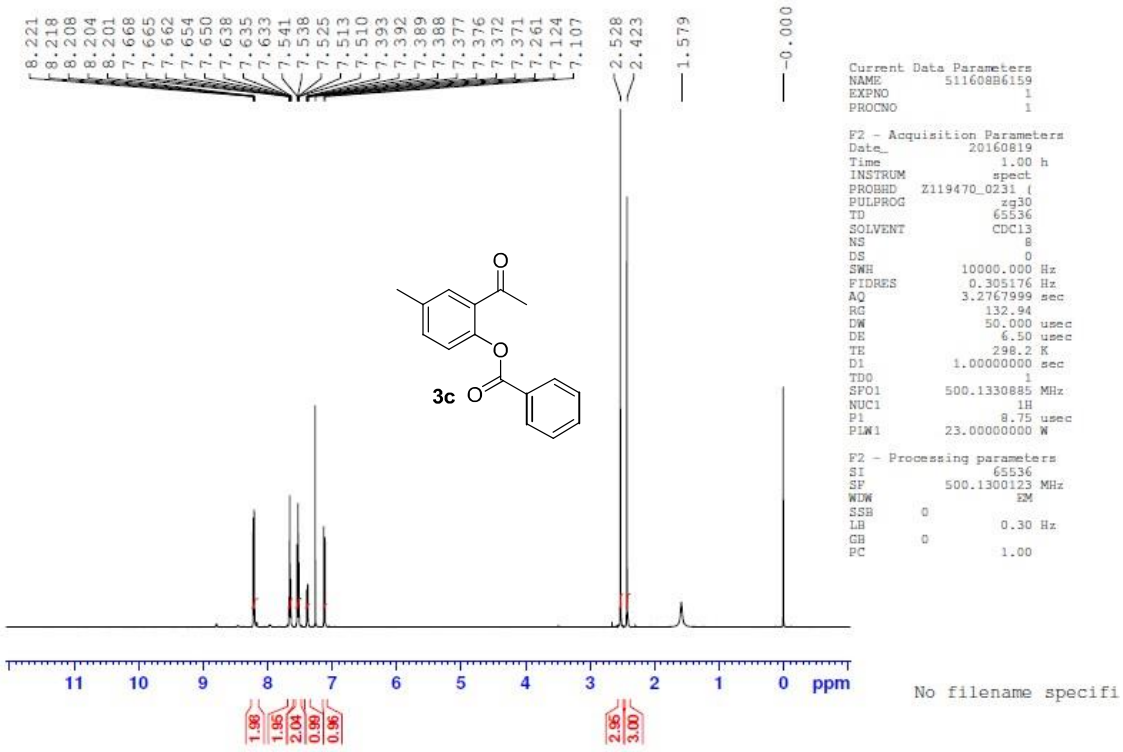
Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: B1: 0.1 % FA IN WATER A1: 0.1%FA IN ACN
Gradient: Time (min) /%A1: 0/2, 0.3/2, 2.3/98,2.8/98,2.81/2,3.0/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 60°C ->



Pea No	RT min	Area	Area %
1	0.29	19.215	2.862
2	1.59	2.370	0.353
3	1.80	2.309	0.344
4	1.88	640.507	95.406
5	2.50	6.950	1.035


MS Spectrum
*MSD1 SPC, time=1.905 of C:\CHEM32\1\DATA\2016\JAN-16\18012016\18012016-GVK-SAM-5-PAGE-23-NP.D MM-ES+APCI, Pos, Sca
Max: 478336
318.9
320.9
320.0
321.9
100
80
60
40
20
0
150
200
250
300
350
400
450
500
m/z
Cl
Cl
O
O
O
5b

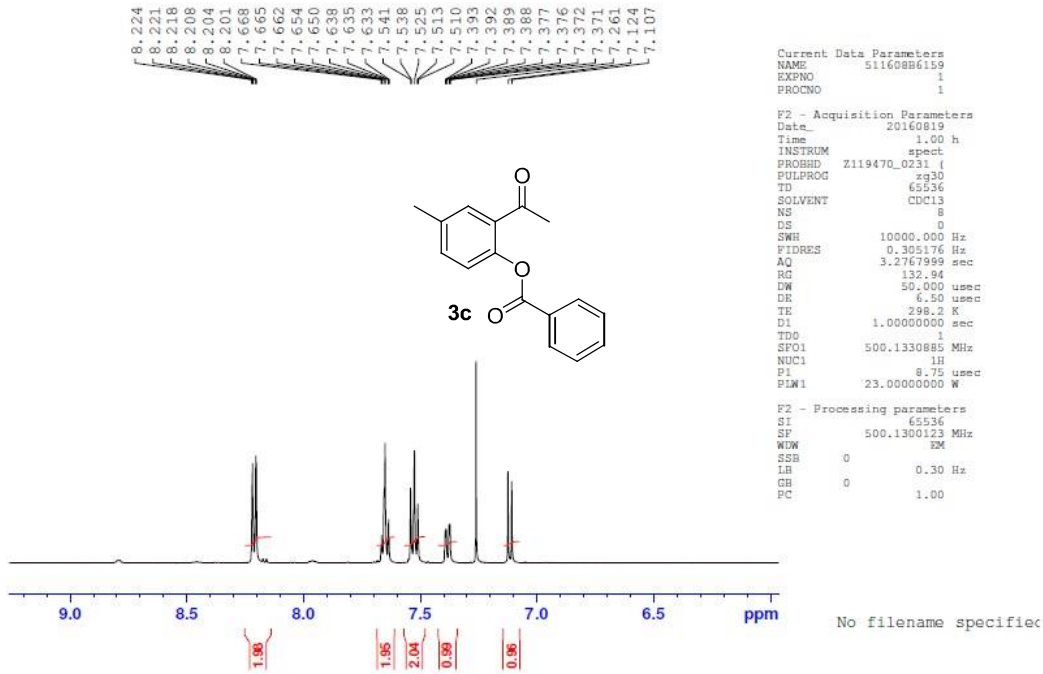
GVK-SAM-6-page-19




```
Current Data Parameters
NAME          511608B6159
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20160819
Time                1.00 h
INSTRUM            spect
PROBHD    Z119470_0231 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     0
SWH            10000.000 Hz
FIDRES             0.305176 Hz
AQ                 3.2767999 sec
RG                   132.94
DW                  50.000 usec
DE                   6.50 usec
TE                  298.2 K
D1              1.00000000 sec
TD0                    1
SFO1           500.1330885 MHz
NUC1                  1H
P1                   8.75 usec
PLW1           23.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.1300123 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

No filename specifi

GVK-SAM-6-page-19



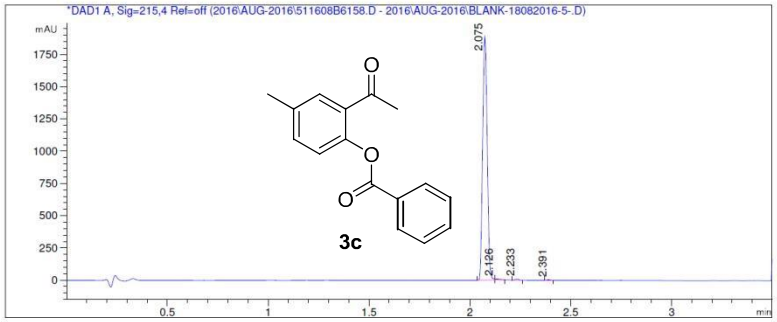

```
Current Data Parameters
NAME          511608B6159
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20160819
Time                1.00 h
INSTRUM            spect
PROBHD    Z119470_0231 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     0
SWH            10000.000 Hz
FIDRES             0.305176 Hz
AQ                 3.2767999 sec
RG                   132.94
DW                  50.000 usec
DE                   6.50 usec
TE                  298.2 K
D1              1.00000000 sec
TD0                    1
SFO1           500.1330885 MHz
NUC1                  1H
P1                   8.75 usec
PLW1           23.00000000 W

F2 - Processing parameters
SI                 65536
SF            500.1300123 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

No filename specifiec

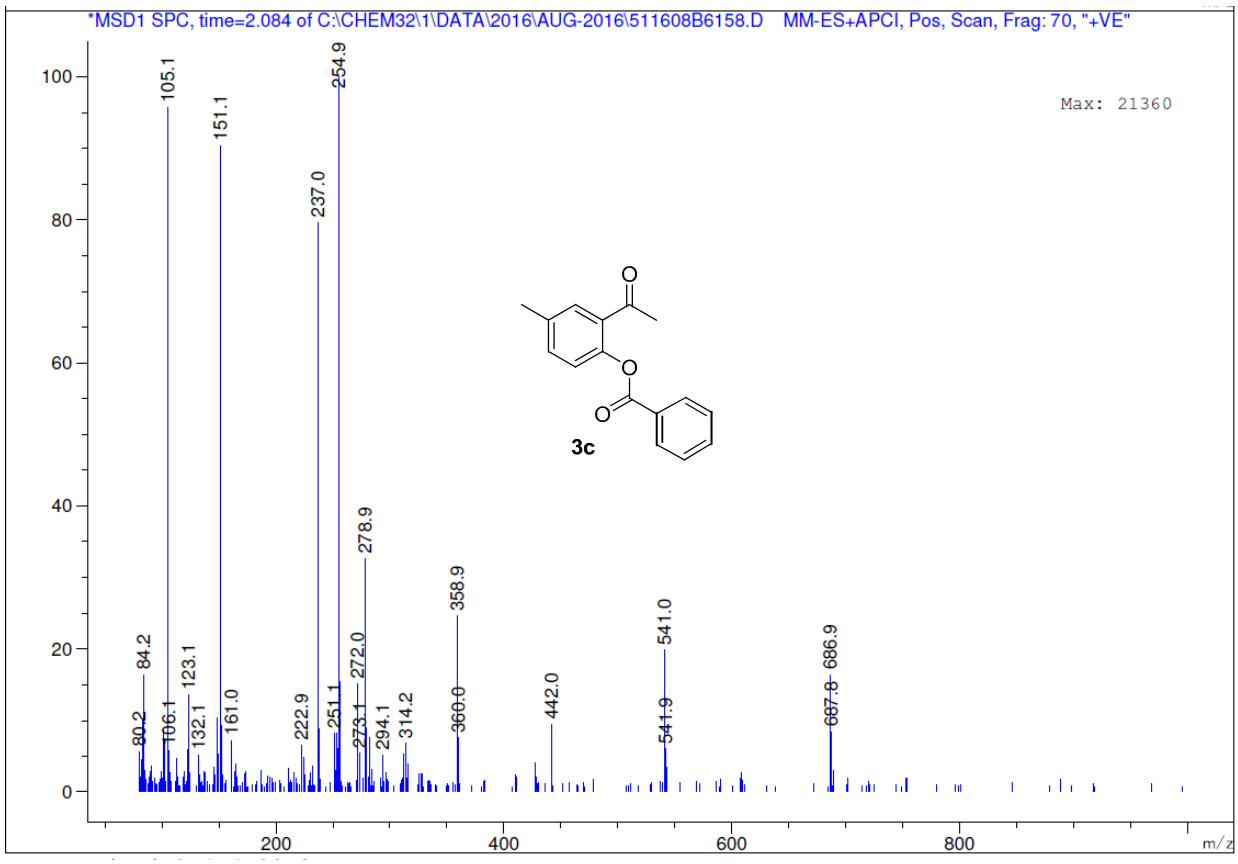
GVK BIOSCIENCES PVT. LTD.
MEDICINAL CHEMISTRY LABORATORY - ANALYTICAL RESEARCH
LCMS REPORT

Sample Name : GVK-SAM-6-page-19 Vial position : P1-E-04
Date of Analysis :8/18/2016 10:07:07 PM Injection Vol :0.500µl
Acq. Method :C:\CHEM32\1\METHODS\RND-FA- 3.5 MIN.M Instrument ID :ANL-MCL5-LCMS-001

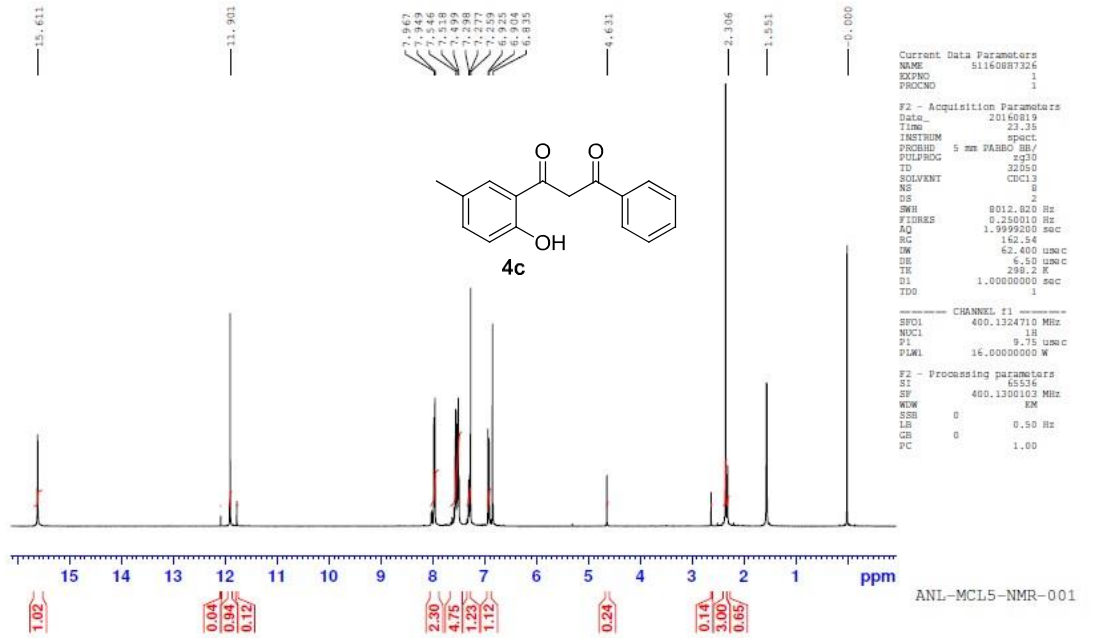
RND-FA-3.5 MIN.M
Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: B1: 0.1 % FA IN WATER A1: 0.1%FA IN ACN
Gradient: Time (min) /%A1: 0/2, 0.4/2, 2.8/98,3.4/98,3.41/2,3.5/2
Column Flow Rate: 0.6 ml/min
Column Temperature: 60°C



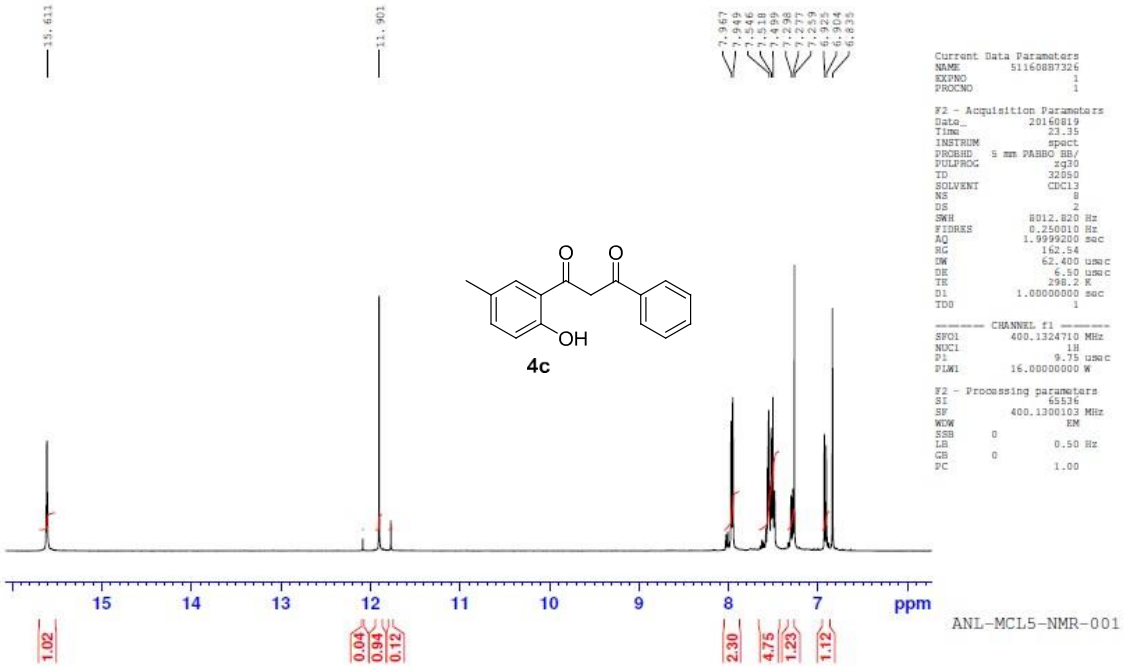
Peak No	RT min	Area	Area %
1	2.07	2982.400	98.966



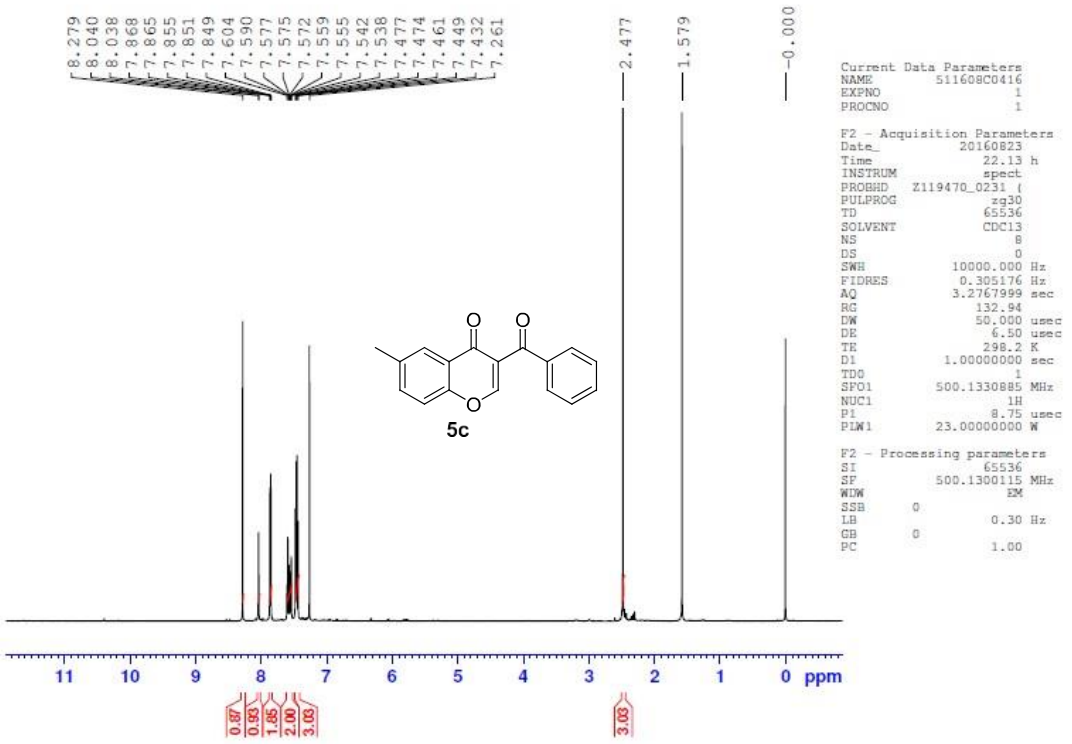
GVK-SAM-6-page-20



GVK-SAM-6-page-20



GVK-SAM-6-Page-21

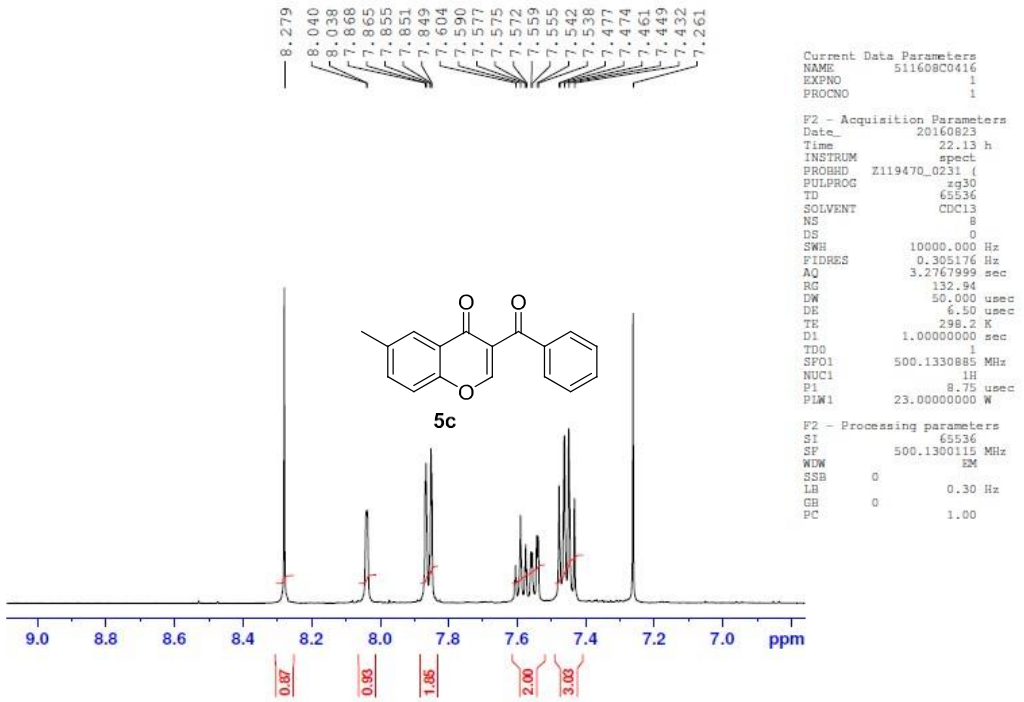


Current Data Parameters
NAME 511608C0416
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160823
Time 22.13 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 132.94
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.1330885 MHz
NUC1 1H
P1 8.75 usec
PLW1 23.00000000 W

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

GVK-SAM-6-Page-21



Current Data Parameters
NAME 511608C0416
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160823
Time 22.13 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 132.94
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.1330885 MHz
NUC1 1H
P1 8.75 usec
PLW1 23.00000000 W

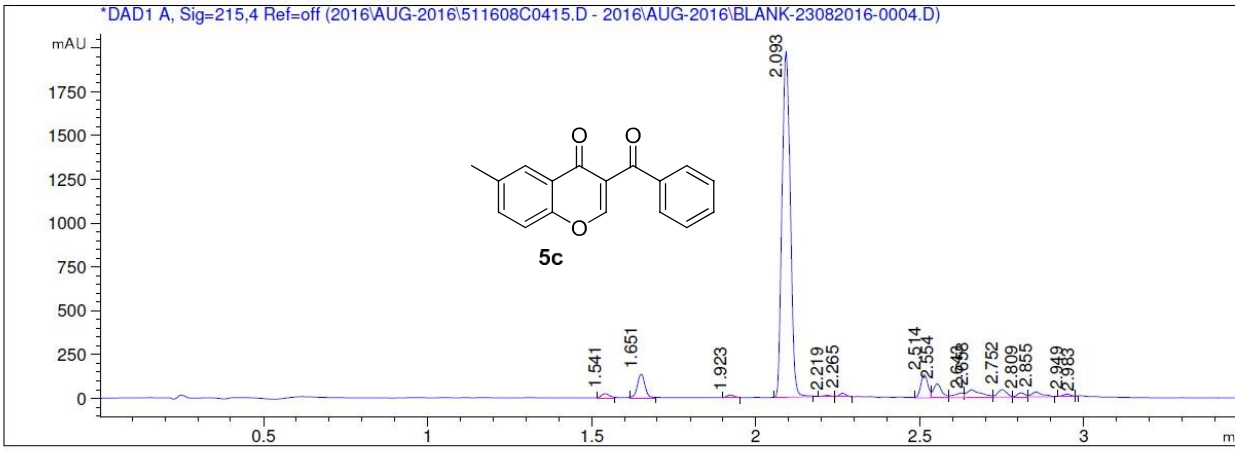
F2 - Processing parameters
SI 65536
SF 500.1300115 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

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

LCMS REPORT

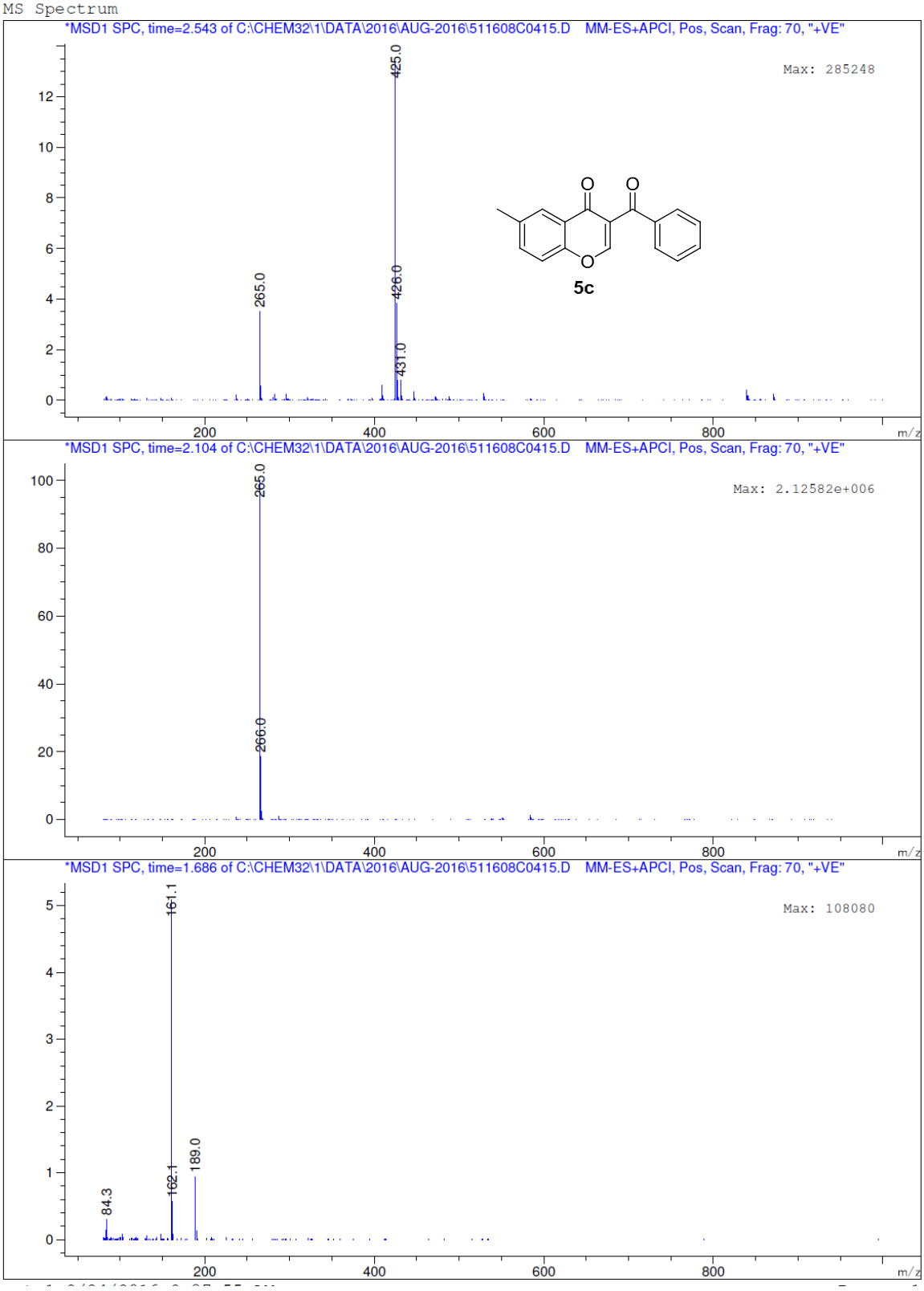
Sample Name :GVK-SAM-6-PAGE-21 Vial position :P1-D-03
Date of Analysis:23/08/2016;10:08:44 PM Injection Vol: 0.5 µL
Acq. Method->C:\CHEM32\1\METHODS\RND-FA- 3.5 MIN.M Instrument ID:ANL-MCL5-LCMS-001
C:\CHEM32\1\DATA\2016\AUG-2016\511608C0415.D

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, 0.4/2, 2.8/98,3.4/98,3.41/2,3.5/2
Column Flow Rate: 0.6 ml/min
Column Temperature: 60°C

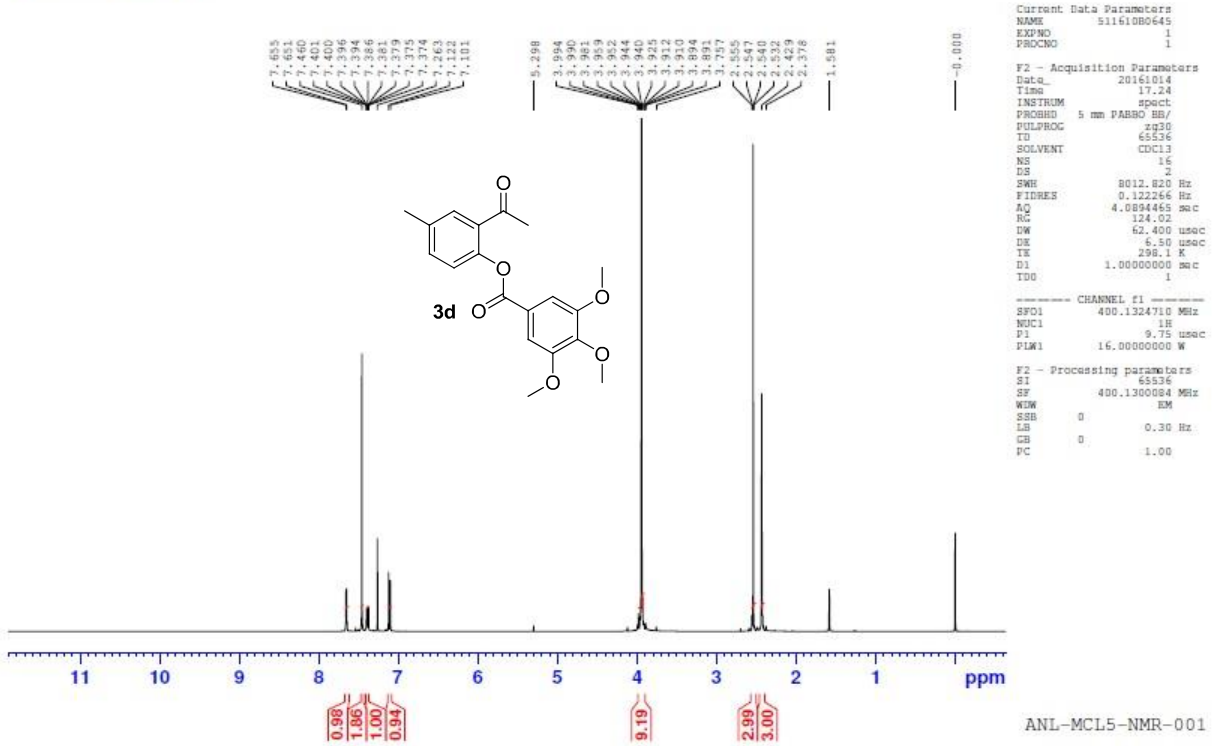


Peak No	RT min	Area	Area %
1	1.54	44.779	0.989
2	1.65	223.081	4.927
3	1.92	23.121	0.511
4	2.09	3469.248	76.615
5	2.22	11.679	0.258
6	2.27	25.128	0.555
7	2.51	202.877	4.480
8	2.55	139.298	3.076
9	2.64	53.813	1.188
10	2.66	129.655	2.863
11	2.75	84.176	1.859
12	2.81	38.810	0.857
13	2.85	63.456	1.401
14	2.95	17.925	0.396
15	2.98	1.093	0.024

MS Spectrum


*MSD1 SPC, time=2.543 of C:\CHEM32\1\DATA\2016\AUG-2016\511608C0415.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 285248
425.0
426.0
265.0
431.0
5c
*MSD1 SPC, time=2.104 of C:\CHEM32\1\DATA\2016\AUG-2016\511608C0415.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 2.12582e+006
265.0
266.0
*MSD1 SPC, time=1.686 of C:\CHEM32\1\DATA\2016\AUG-2016\511608C0415.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 108080
161.1
189.0
162.1
84.3
m/z

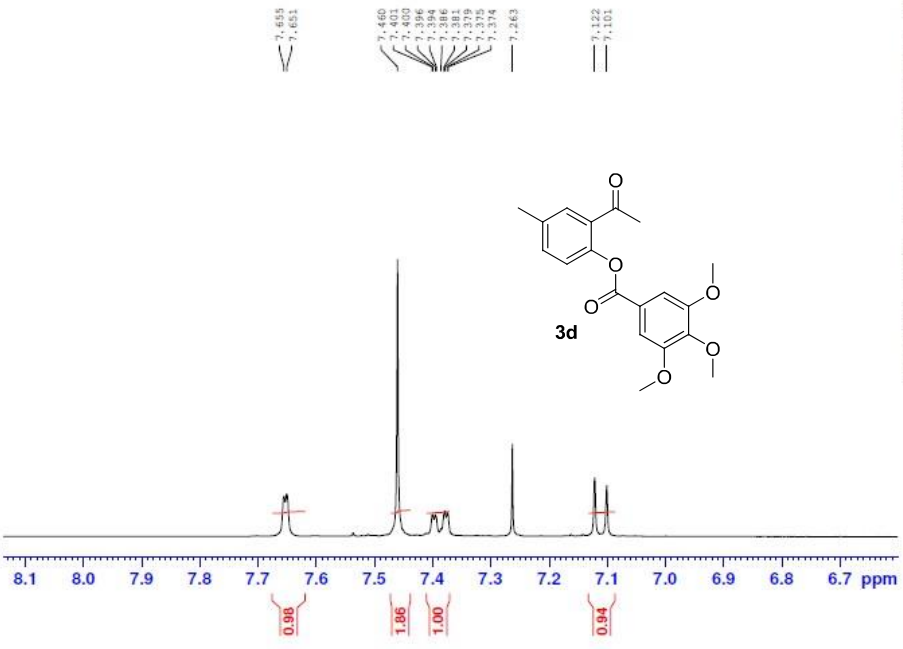
GVK-SAM-6-page-35




```
Current Data Parameters
NAME          511610B0645
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Data_           20161014
Time              17.24
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              124.02
DW              62.400 usec
DE               6.50 usec
TE              298.1 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          400.1300084 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

ANL-MCL5-NMR-001

GVK-SAM-6-page-35

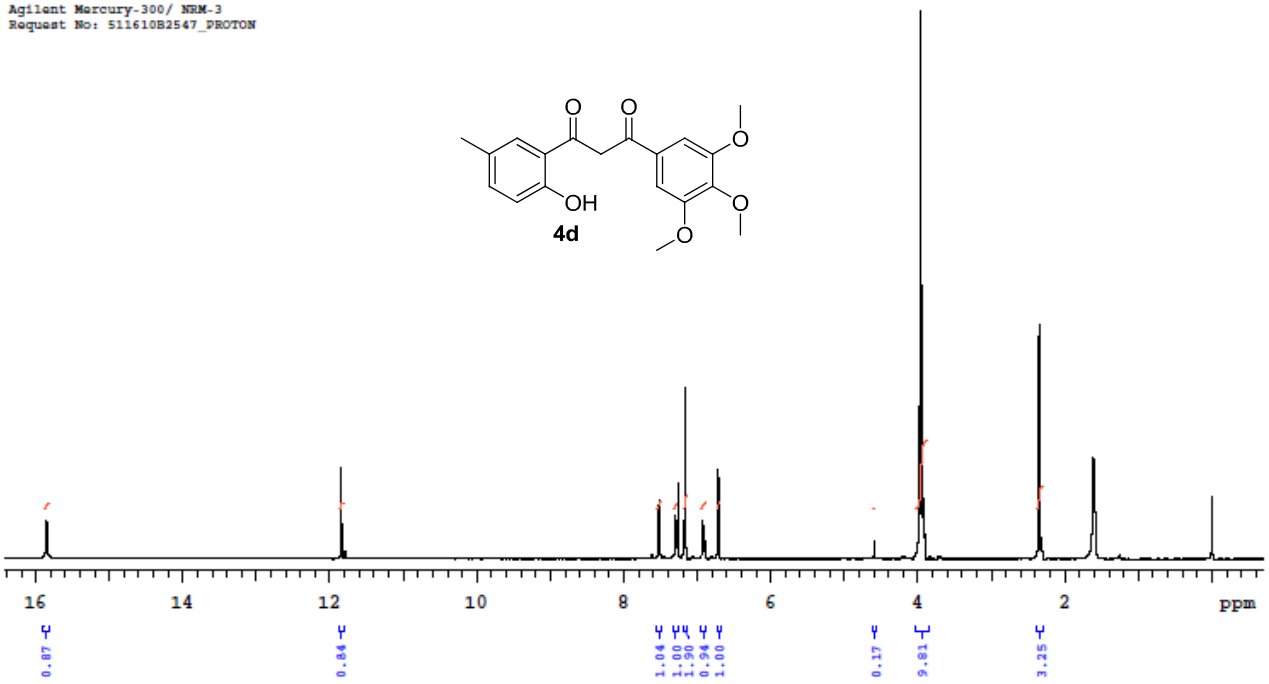



```
Current Data Parameters
NAME          511610B0645
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Data_           20161014
Time              17.24
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              124.02
DW              62.400 usec
DE               6.50 usec
TE              298.1 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          400.1300084 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   1.00
```

ANL-MCL5-NMR-001

Sample Name:
GVK-SAM-6-page-35a

Solvent: cdcl3
Date: Oct 18 2016
Agilent Mercury-300/ NMR-3
Request No: 511610B2547_PROTON



4d

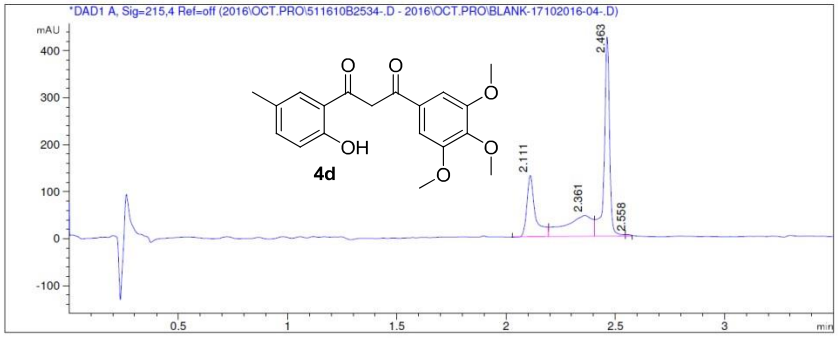
Plotname: 511610B2547_PROTON_01_plot01

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

Sample Name : GVK-SAM-6-page-35a Vial position : P2-A-07
Date of Analysis :10/17/2016 9:33:52 PM Injection Vol :0.100µl
Acq. Method :C:\CHEM32\1\METHODS\RND-FA- 3.5 MIN.M Instrument ID :ANL-MCL5-LCMS-001

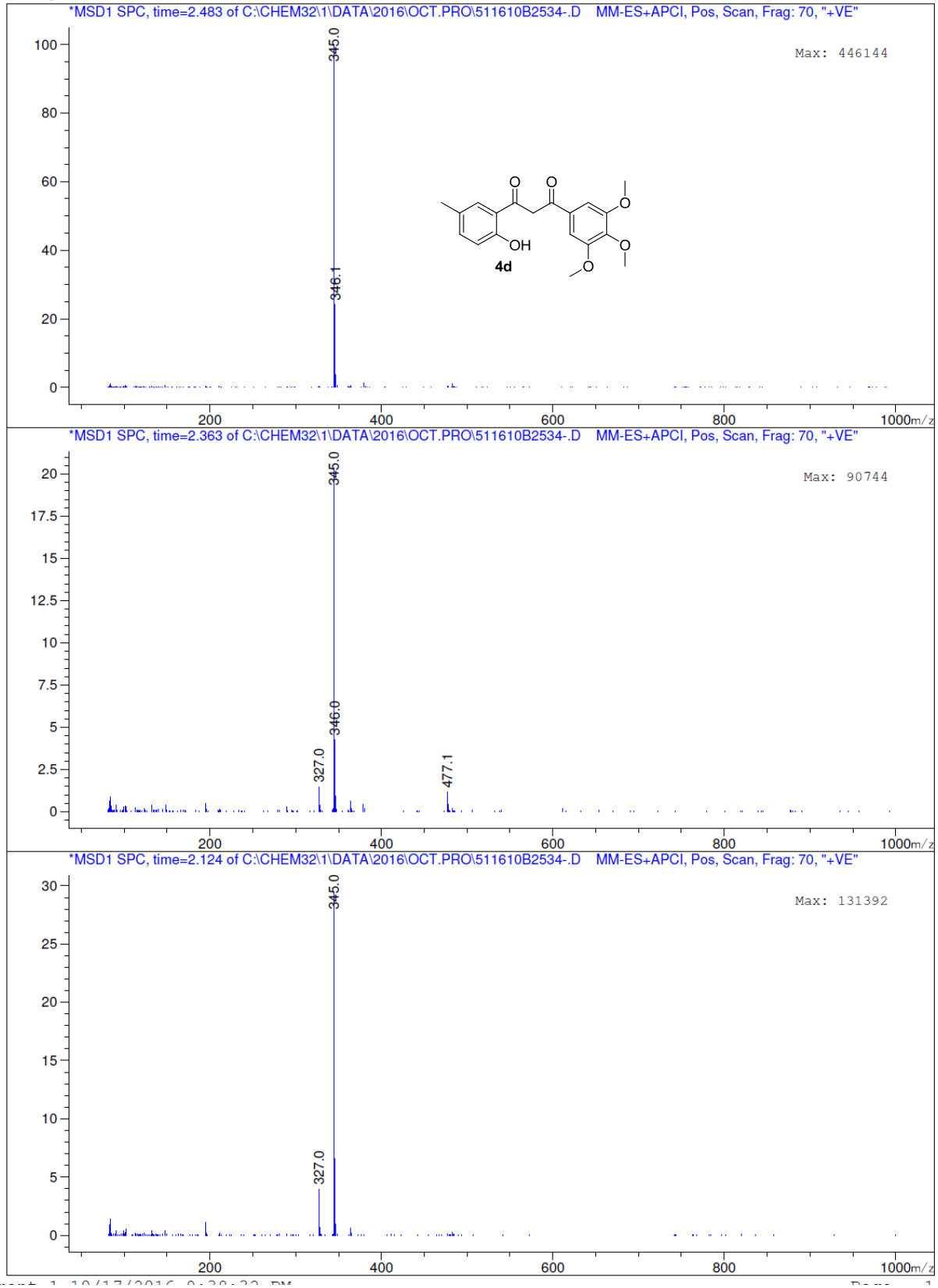
RND-FA-3.5 MIN.M
Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: B1: 0.1 % FA IN WATER A1: 0.1%FA IN ACN
Gradient: Time (min) /%A1: 0/2, 0.4/2, 2.6/98,3.1/98,3.11/2,3.5/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 60°C

->

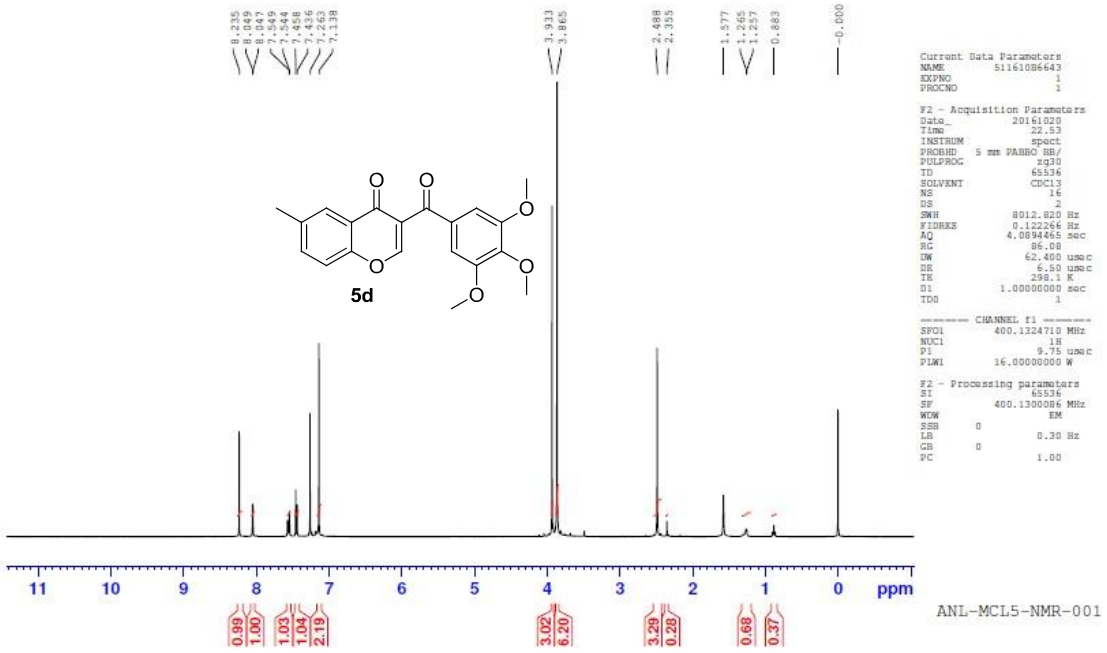


Pea No	RT min	Area	Area %
1	2.11	349.020	23.886
2	2.36	383.745	26.263
3	2.46	723.847	49.538
4	2.56	4.569	0.313

MS Spectrum

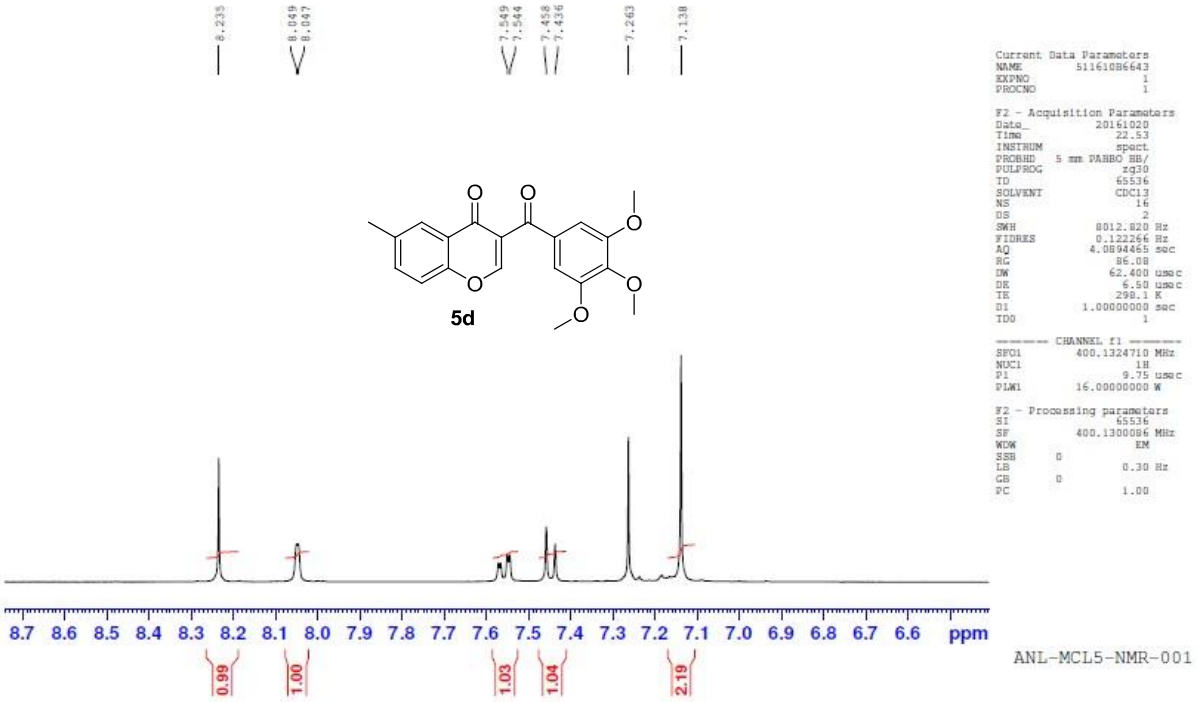

*MSD1 SPC, time=2.483 of C:\CHEM32\1\DATA\2016\OCT.PRO\511610B2534-.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 446144
345.0
346.1
4d
*MSD1 SPC, time=2.363 of C:\CHEM32\1\DATA\2016\OCT.PRO\511610B2534-.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 90744
345.0
346.0
327.0
477.1
*MSD1 SPC, time=2.124 of C:\CHEM32\1\DATA\2016\OCT.PRO\511610B2534-.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 131392
345.0
327.0
m/z

GVK-SAM-6-page-36



ANL-MCL5-NMR-001

GVK-SAM-6-page-36



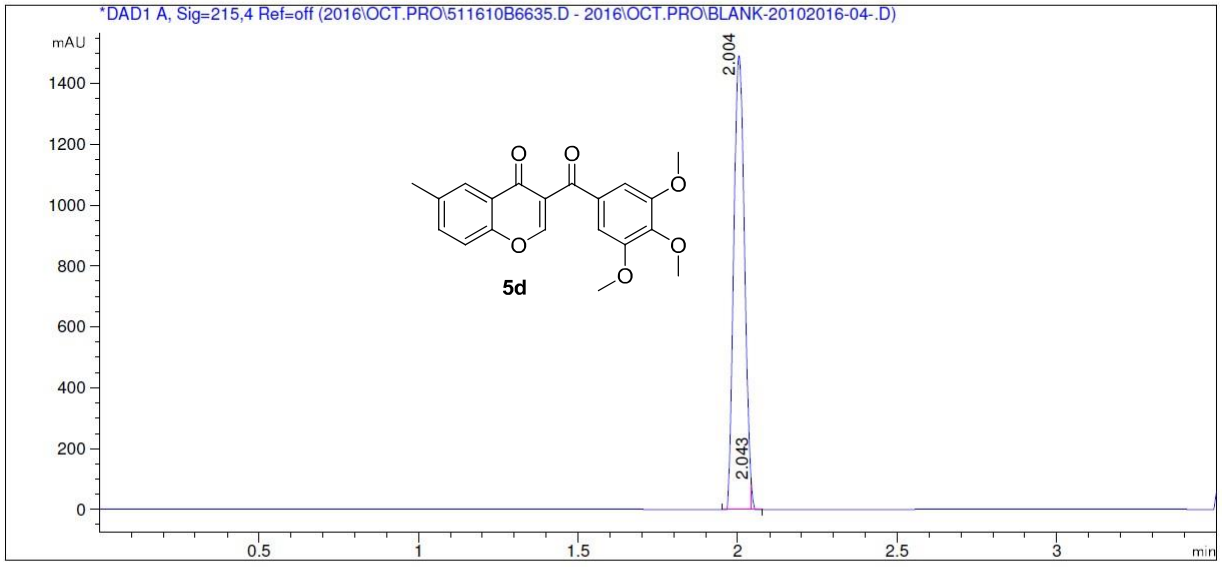
ANL-MCL5-NMR-001

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

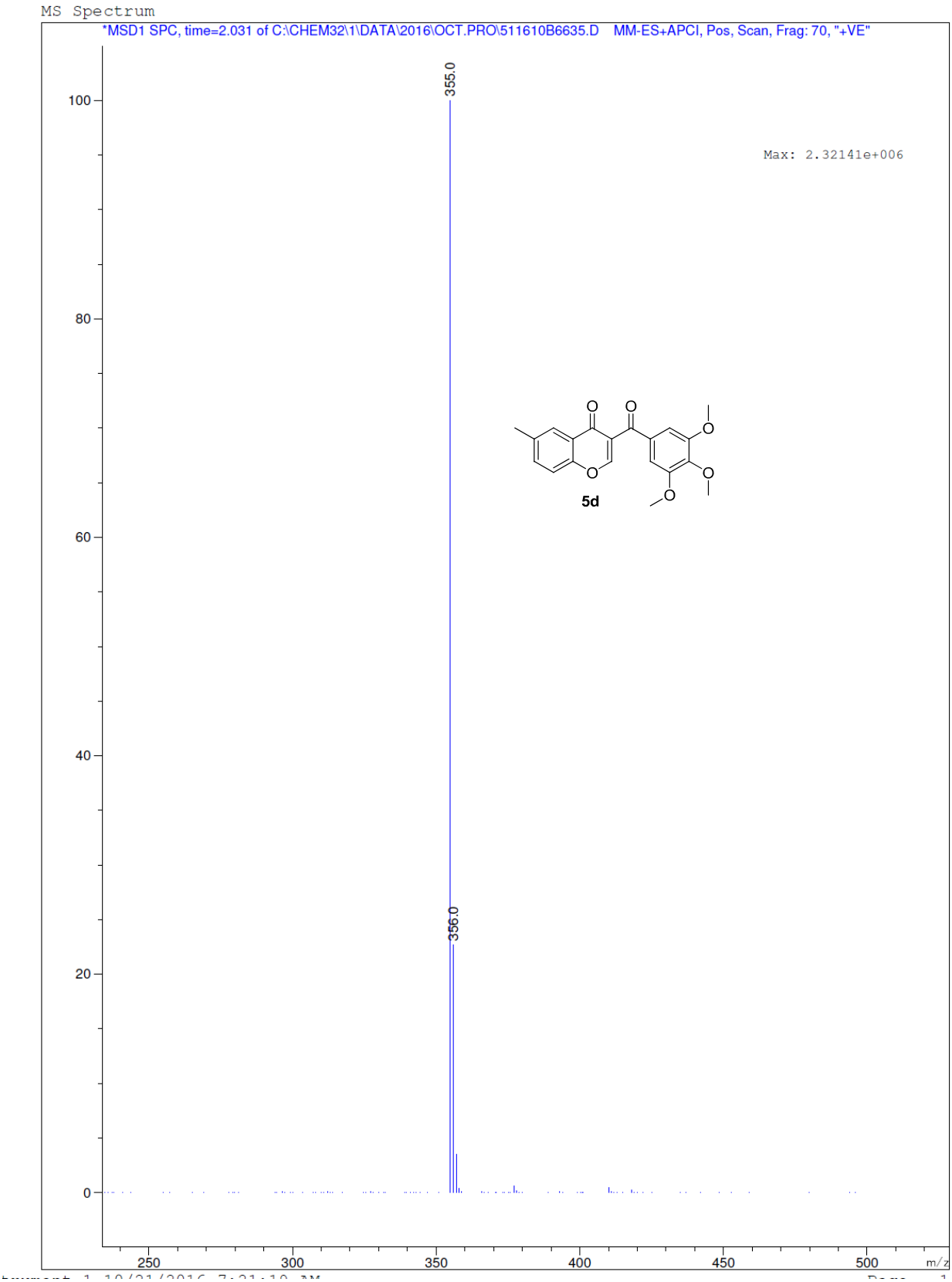
Sample Name :GVK-DU-SAM-6-PAGE-36 Vial position : P1-E-09
Date of Analysis :10/20/2016 11:40:33 PM Injection Vol : 0.500uL
Acq. Method :C:\CHEM32\1\METHODS\RND-FA- 3.5 MIN.M Instrument ID :ANL-MCL5-LCMS-001

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, 0.4/2, 2.6/98,3.1/98,3.11/2,3.5/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 60°C

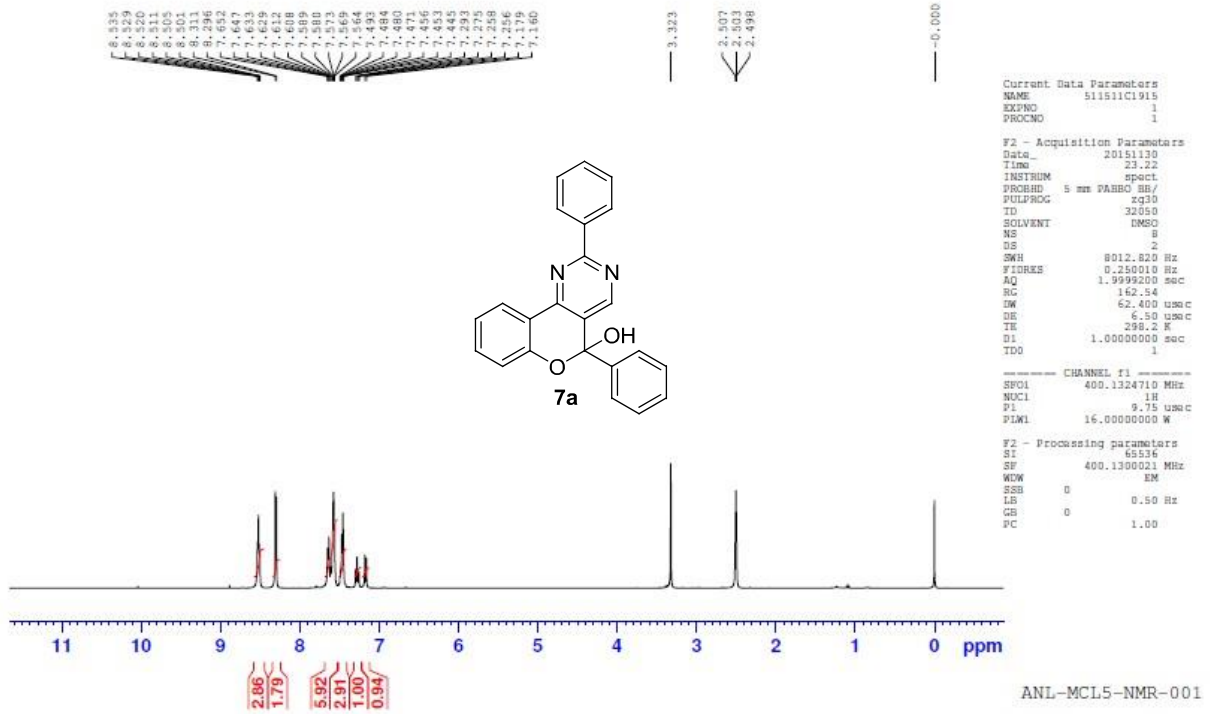
->



Peak No	RT min	Area	Area %
1	2.00	3489.687	99.514
2	2.04	17.050	0.486


MS Spectrum
*MSD1 SPC, time=2.031 of C:\CHEM32\1\DATA\2016\OCT.PRO\511610B6635.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 2.32141e+006
355.0
356.0
5d
100
80
60
40
20
0
250
300
350
400
450
500
m/z

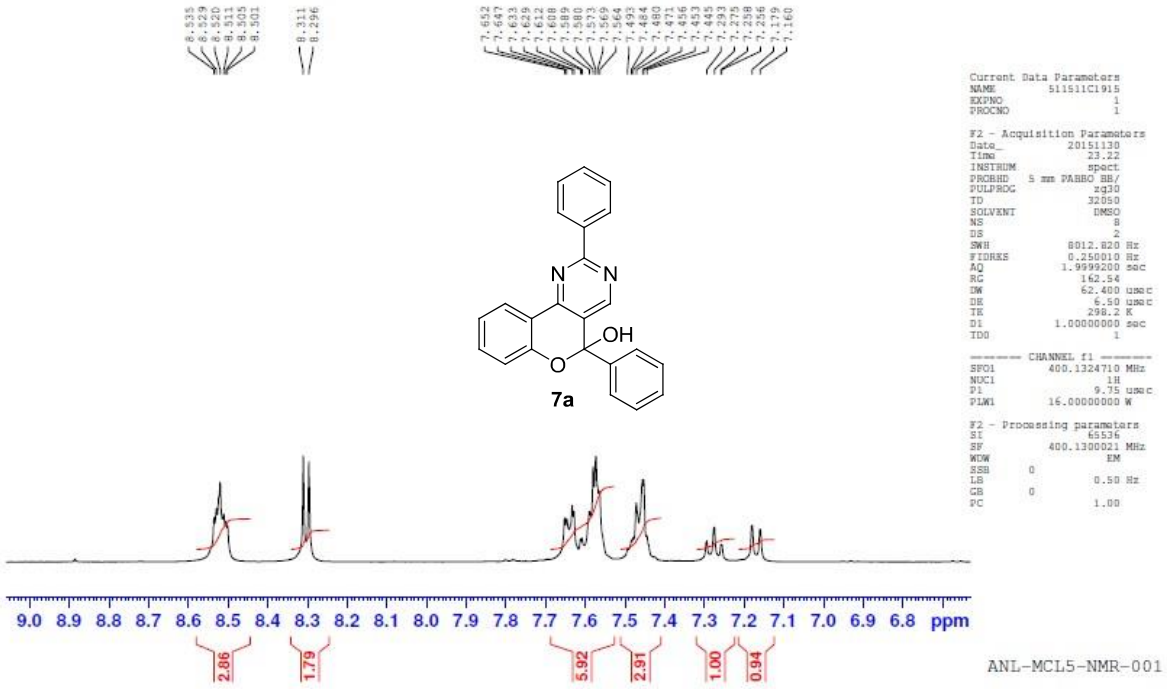
GVK-SAM-1-PAGE-54P




```
Current Data Parameters
NAME          511511C1915
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_          20151130
Time              23.22
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32050
SOLVENT           DMSO
NS                   8
DS                   2
SWH           8012.820 Hz
FIDRES        0.250010 Hz
AQ            1.9999200 sec
RG              162.54
DW               62.400 usec
DE                6.50 usec
TE              298.2 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          400.1300021 MHz
WDW               EM
SSB       0
LB                0.50 Hz
GB        0
PC                1.00
```

ANL-MCL5-NMR-001

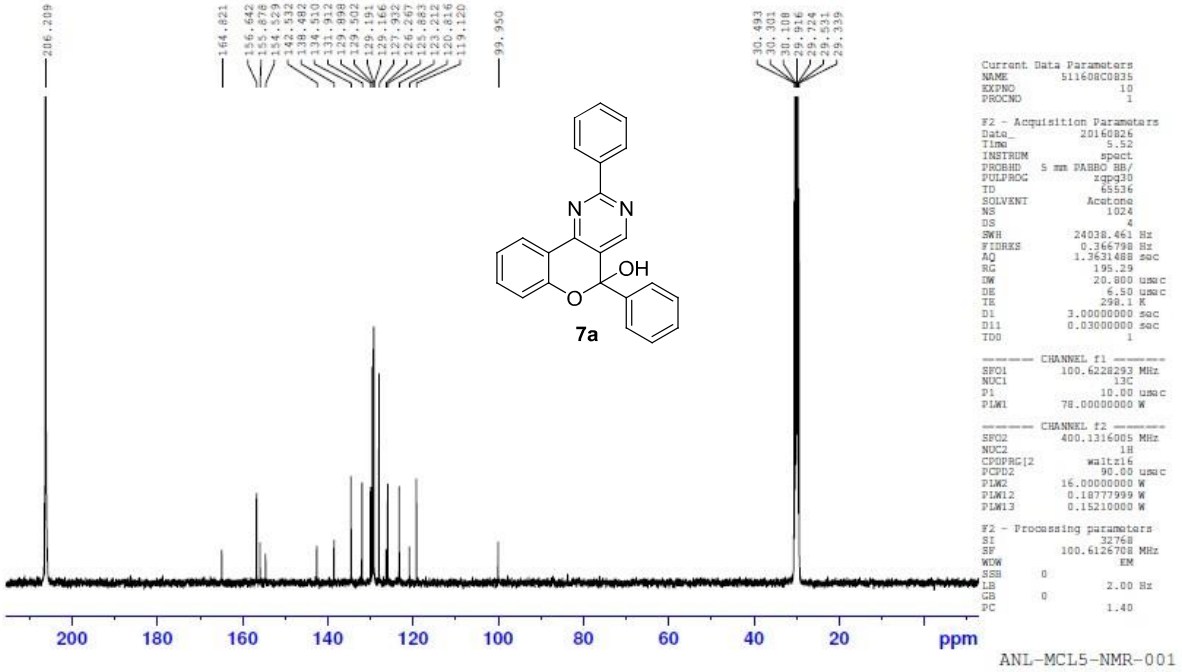
GVK-SAM-1-PAGE-54P



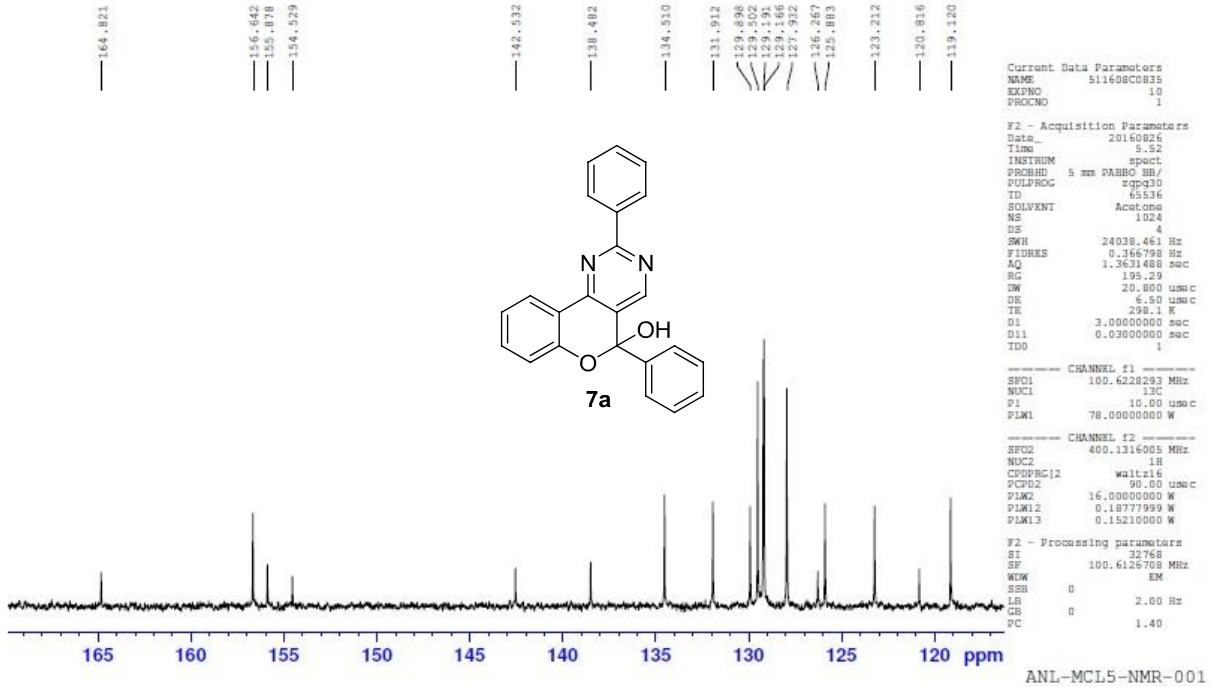

```
Current Data Parameters
NAME          511511C1915
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_          20151130
Time              23.22
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32050
SOLVENT           DMSO
NS                   8
DS                   2
SWH           8012.820 Hz
FIDRES        0.250010 Hz
AQ            1.9999200 sec
RG              162.54
DW               62.400 usec
DE                6.50 usec
TE              298.2 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          400.1300021 MHz
WDW               EM
SSB       0
LB                0.50 Hz
GB        0
PC                1.00
```

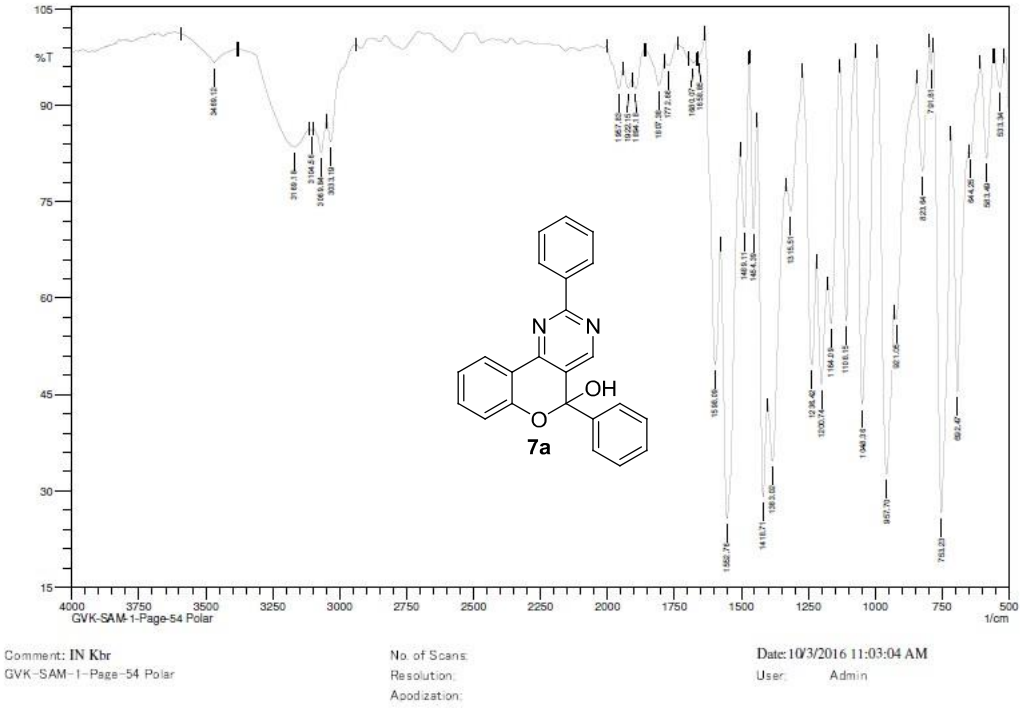
ANL-MCL5-NMR-001

GVK-SAM-1-PAGE-54POLAR

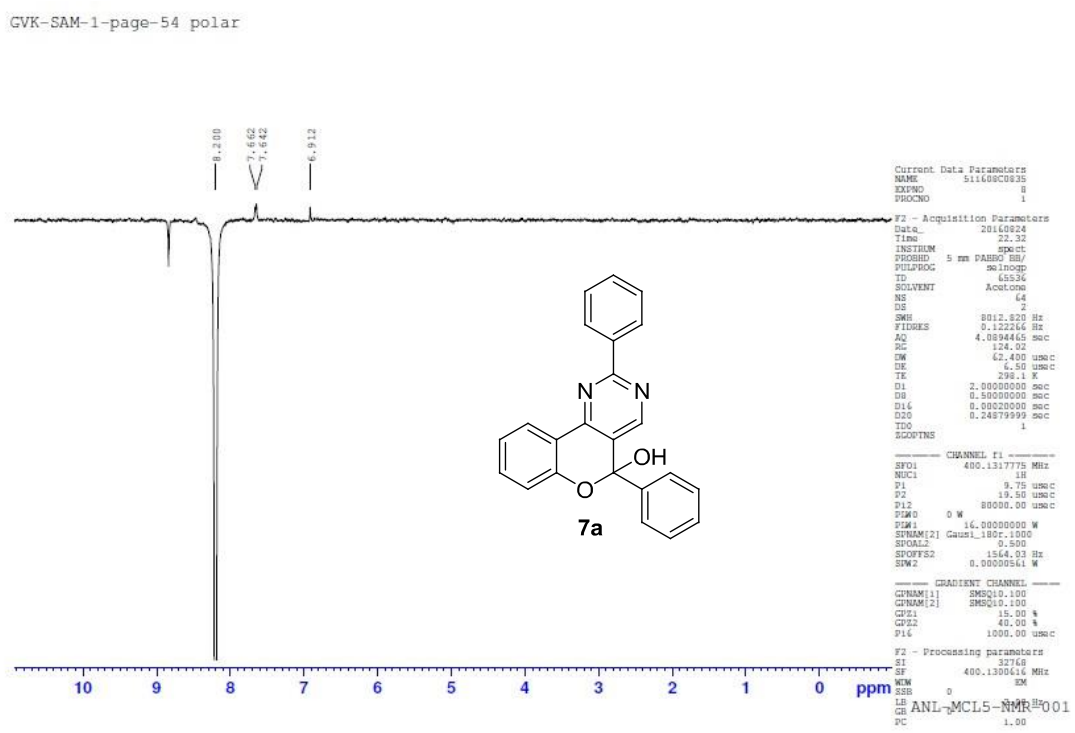


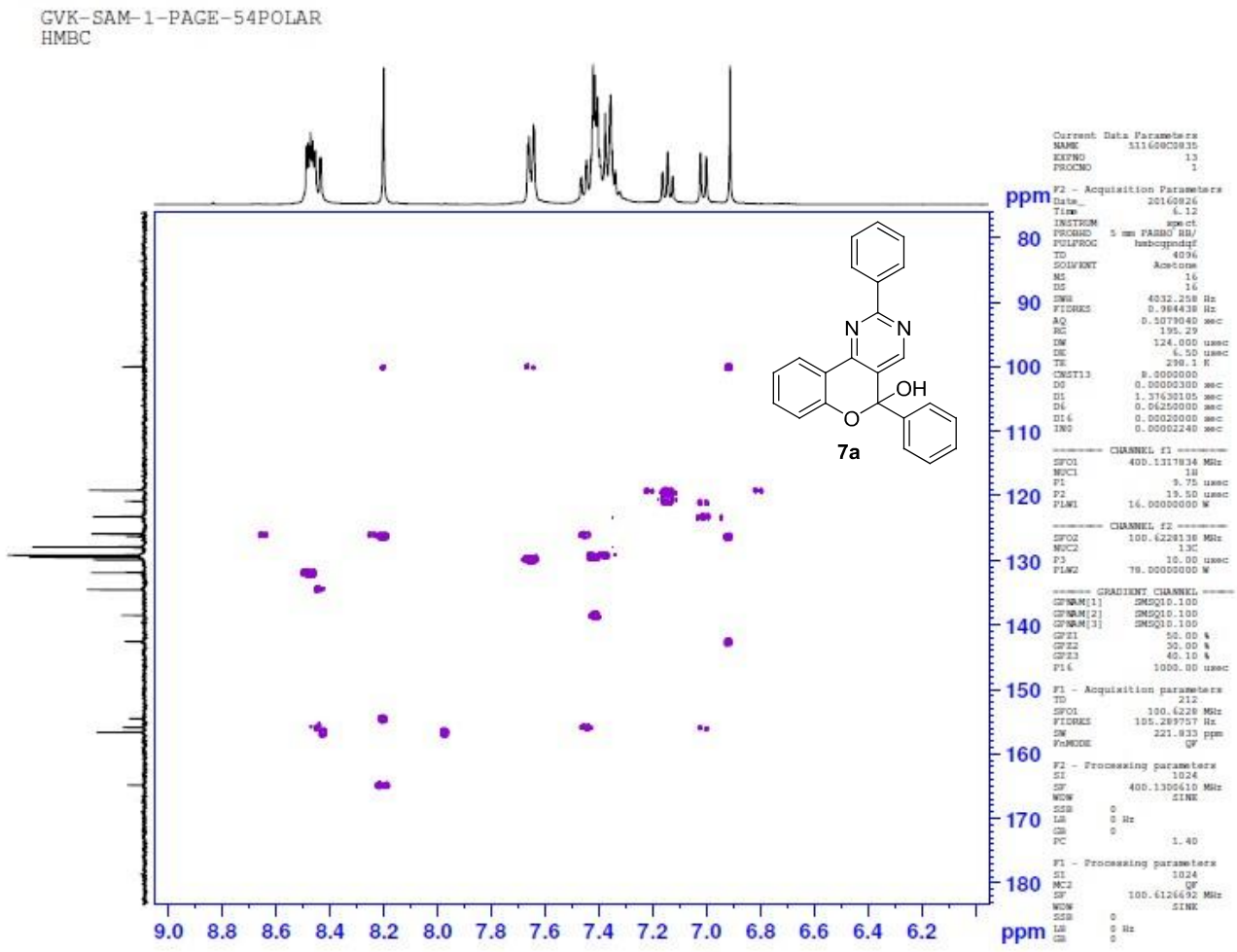
GVK-SAM-1-PAGE-54POLAR

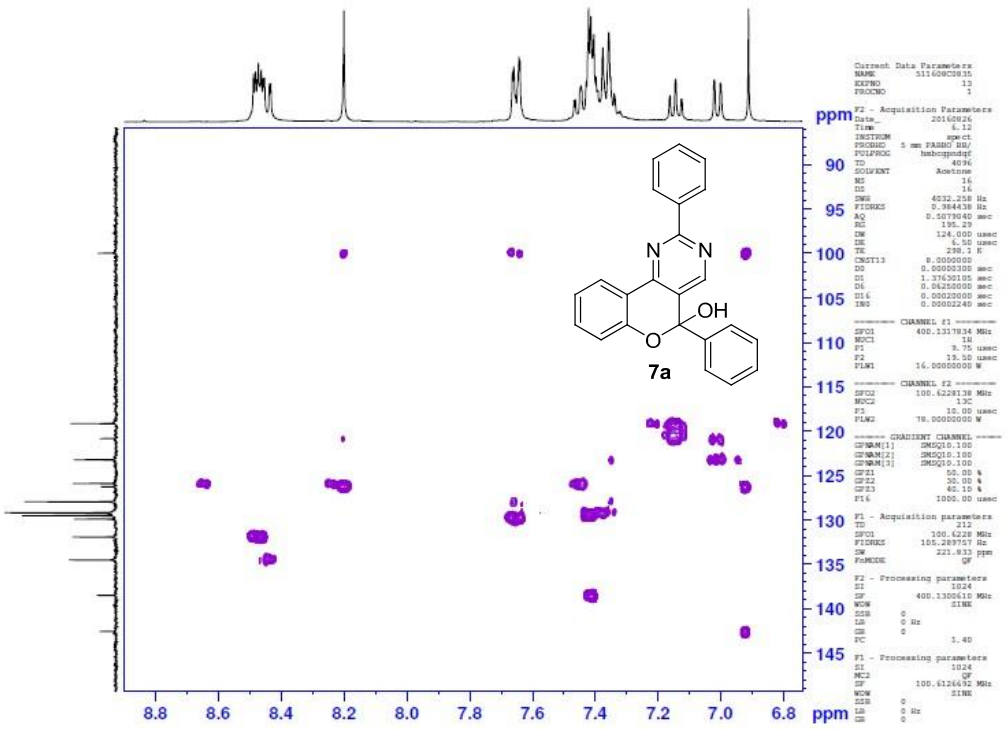


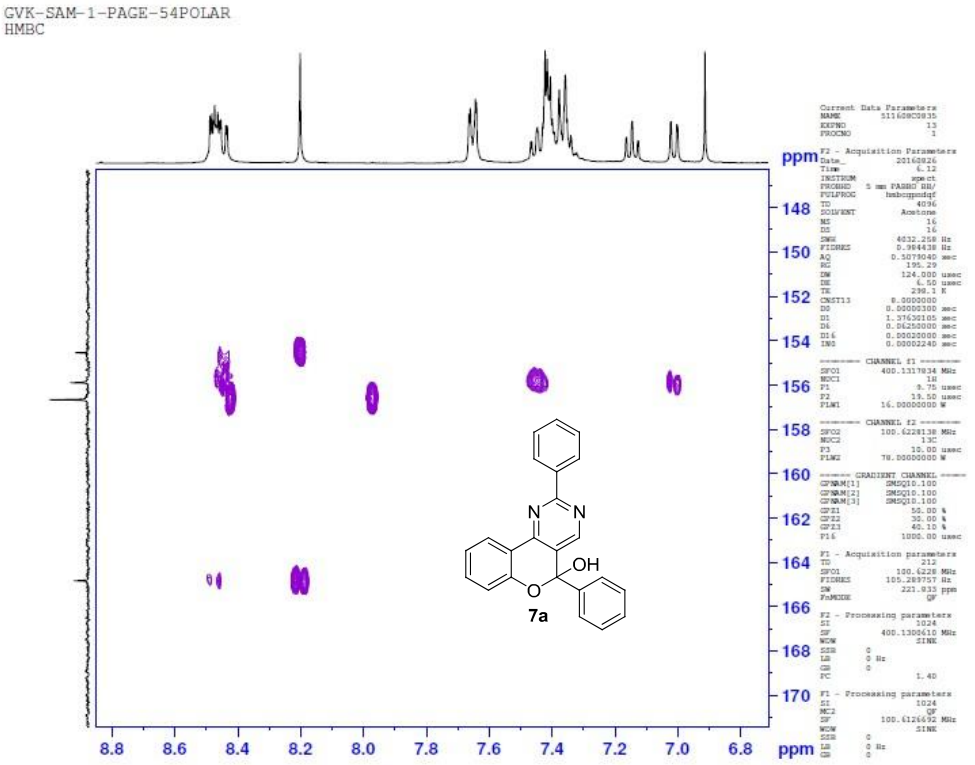


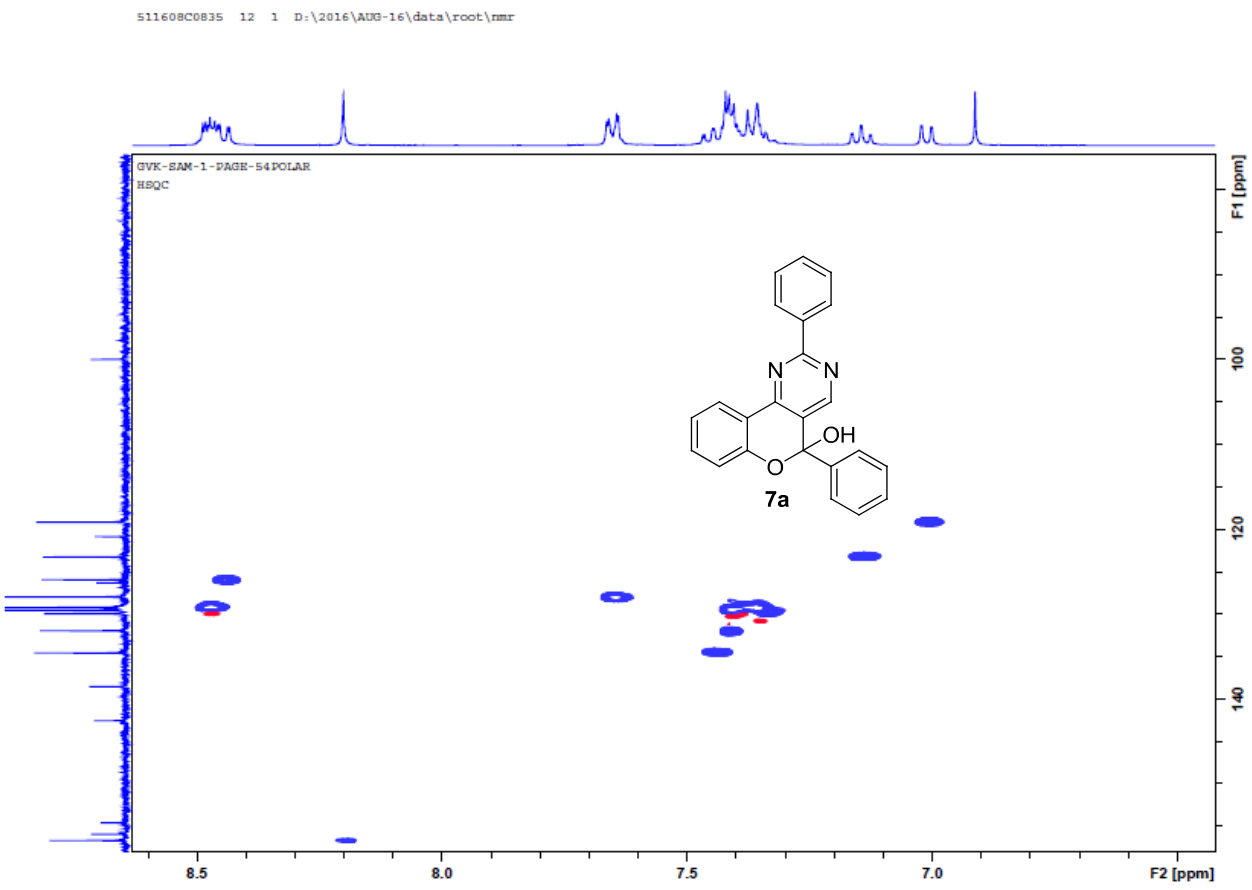
Compound 7a Structure Confirmation data:

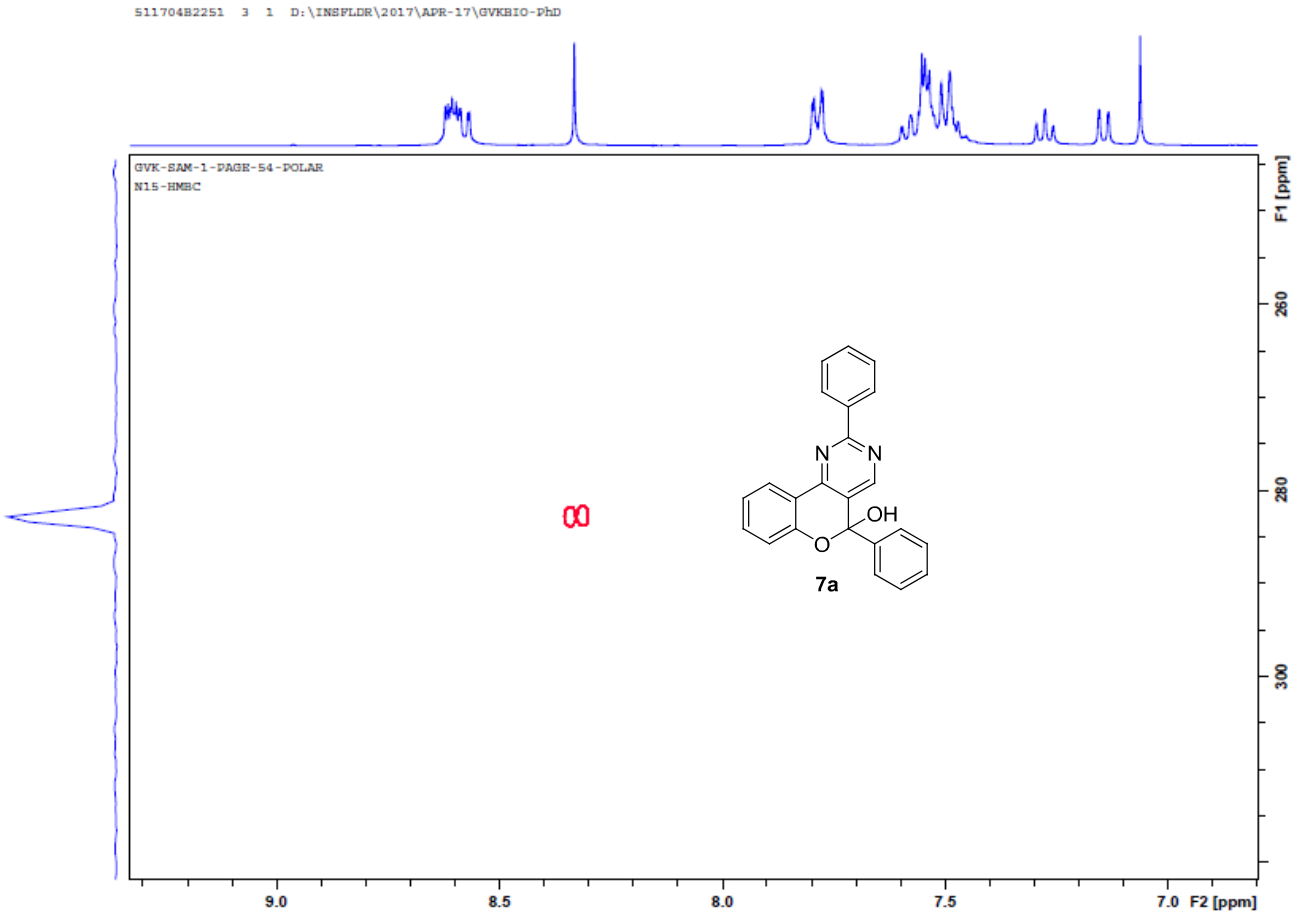



GVK-SAM-1-PAGE-54POLAR
HMBC
N
N
OH
O
7a
ppm
9.0 8.8 8.6 8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2
80 90 100 110 120 130 140 150 160 170 180


GVK-SAM-1-PAGE-54POLAR
HMBC
7a
ppm


GVK-SAM-1-PAGE-54POLAR
HMBC
7a
ppm


511608C0835 12 1 D:\2016\AUG-16\data\root\nmr
GVK-SAM-1-PAGE-54POLAR
HSQC
N
N
OH
O
7a
F1 [ppm]
100
120
140
8.5
8.0
7.5
7.0
F2 [ppm]


511704B2251 3 1 D:\INSFLDR\2017\APR-17\GVKBIO-PhD
GVK-SAM-1-PAGE-54-POLAR
N15-HMBC
N
N
OH
O
7a
F1 [ppm]
260
280
300
9.0
8.5
8.0
7.5
7.0 F2 [ppm]

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

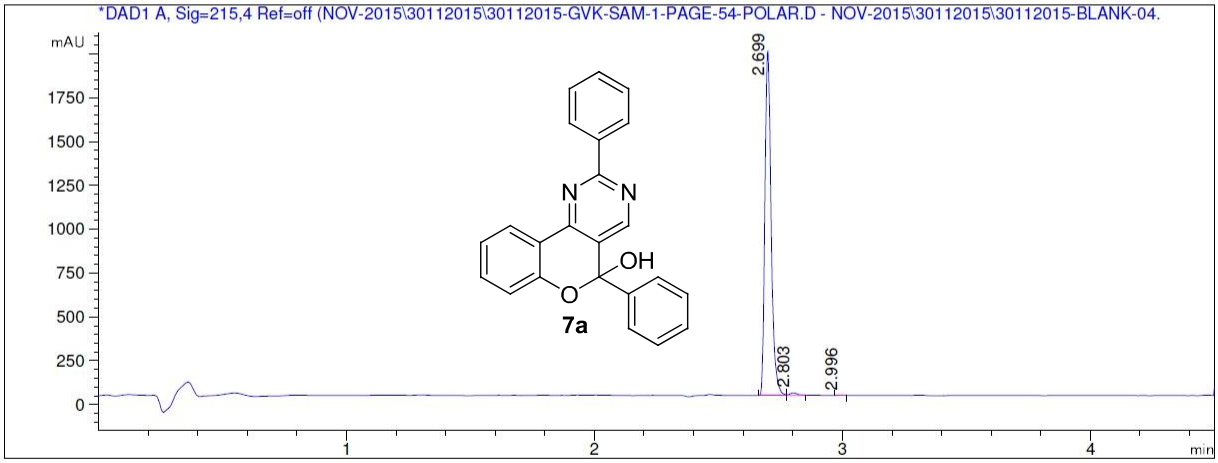
LCMS REPORT

==========

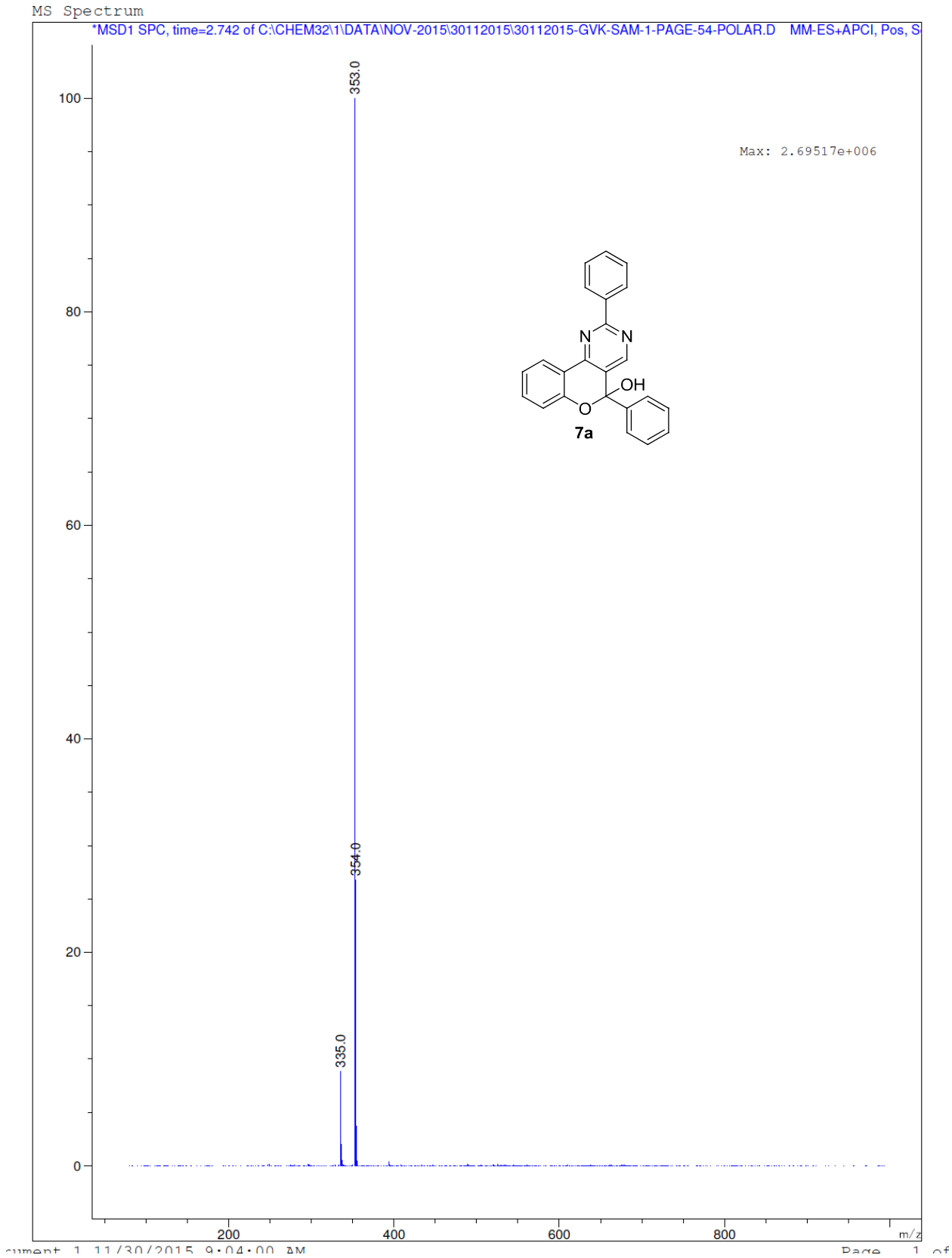
>Sample Name: GVK-SAM-1-PAGE-54-POLAR Vial position :P1-B-02
Date of Analysis:30/11/2015;8:54:03 AM Injection Vol :0.5 µL
Acq. Method :C:\CHEM32\1\METHODS\RND-FA- 4.5 MIN_1.M Instrument ID :ANL-MCL5-LCMS-001

==========

Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: A1: 0.1 % FA IN WATER B1: 0.1%FA IN ACN
Gradient: Time (min) /%B1:0/3, 0.3/3, 2.8/98,4.0/98,4.2/3,4.5/3
Column Flow Rate: 0.6 ml/min



Peak No	RT min	Area	Area %
1	2.70	3.440e3	98.934
2	2.80	32.269	0.928
3	3.00	4.805	0.138

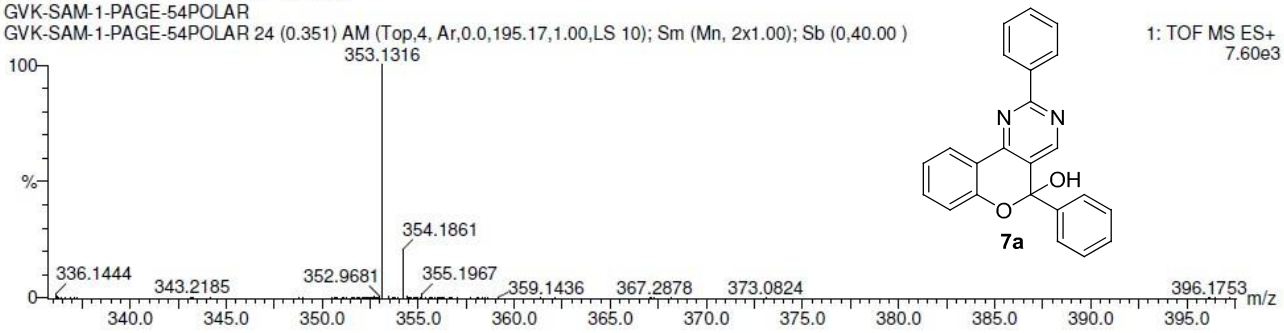

MS Spectrum
*MSD1 SPC, time=2.742 of C:\CHEM32\1\DATA\NOV-2015\30112015\30112015-GVK-SAM-1-PAGE-54-POLAR.D MM-ES+APCI, Pos, S
Max: 2.69517e+006
353.0
354.0
335.0
100
80
60
40
20
0
200
400
600
800
m/z
N
N
OH
O
7a

Single Mass Analysis

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

Monoisotopic Mass, Even Electron Ions
4 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-23 H: 0-17 N: 0-2 O: 0-2

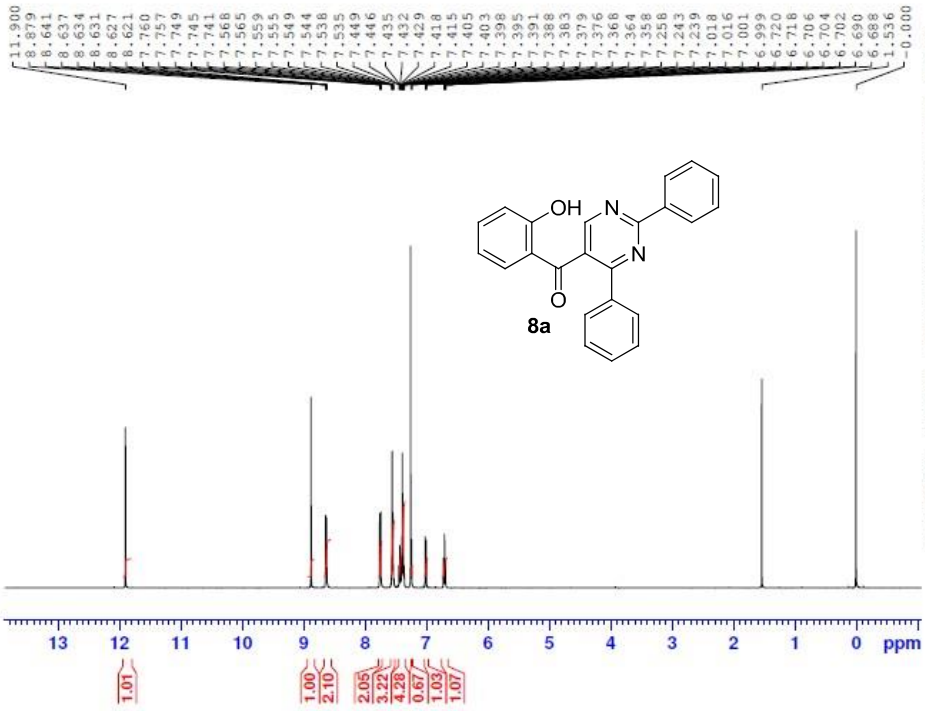
GVK-SAM-1-PAGE-54POLAR
GVK-SAM-1-PAGE-54POLAR 24 (0.351) AM (Top,4, Ar,0.0,195.17,1.00,LS 10); Sm (Mn, 2x1.00); Sb (0,40.00)



7a

Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
353.1316	353.1290	2.6	7.4	16.5	277.0	C23 H17 N2 O2

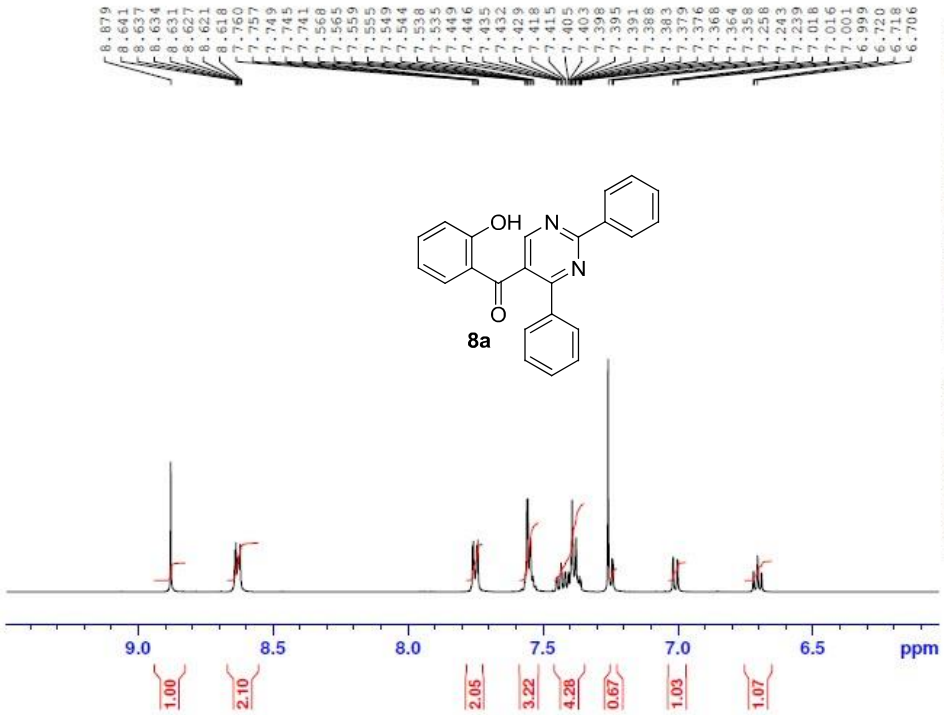
GVK-SAM-1-PAGE-54NP




```
Current Data Parameters
NAME          511511C1269
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20151130
Time               10.30
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDC13
NS                     8
DS                     0
SWH          10000.000 Hz
FIDRES           0.152588 Hz
AQ           3.2767999 sec
RG                132.94
DW                50.000 usec
DE                 6.50 usec
TE                299.9 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 =======
SFO1         500.1330885 MHz
NUC1                   1H
P1                 10.00 usec
PLW1        24.00000000 W

F2 - Processing parameters
SI                 65536
SF           500.1300139 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

ANL-MCL5-NMR-002

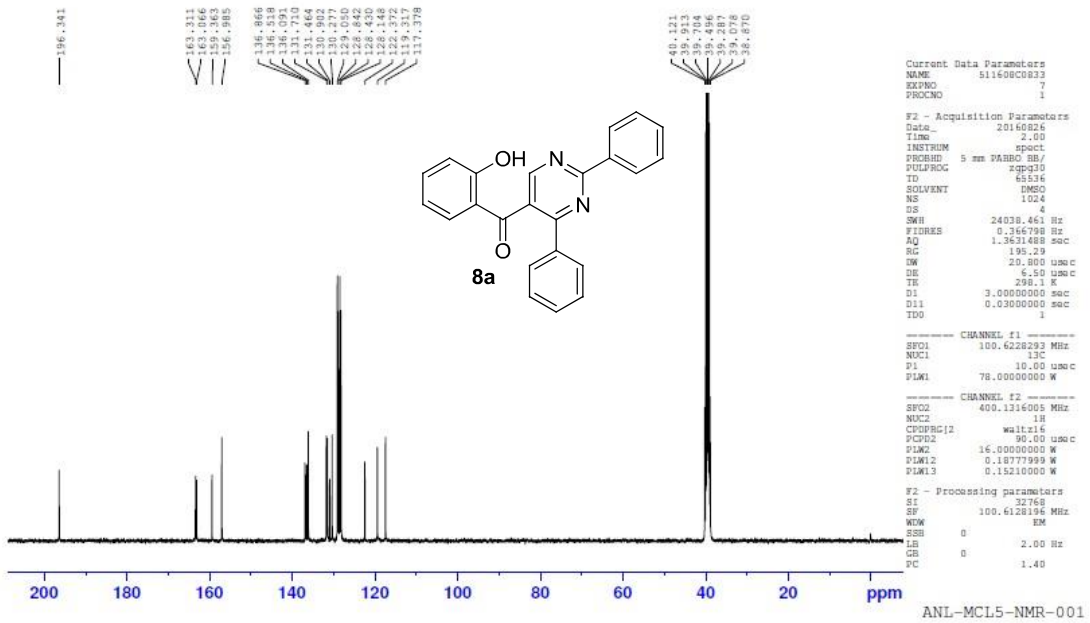
GVK-SAM-1-PAGE-54NP




```
Current Data Parameters
NAME          511511C1269
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20151130
Time               10.30
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDC13
NS                     8
DS                     0
SWH          10000.000 Hz
FIDRES           0.152588 Hz
AQ           3.2767999 sec
RG                132.94
DW                50.000 usec
DE                 6.50 usec
TE                299.9 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 =======
SFO1         500.1330885 MHz
NUC1                   1H
P1                 10.00 usec
PLW1        24.00000000 W

F2 - Processing parameters
SI                 65536
SF           500.1300139 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

ANL-MCL5-NMR-002

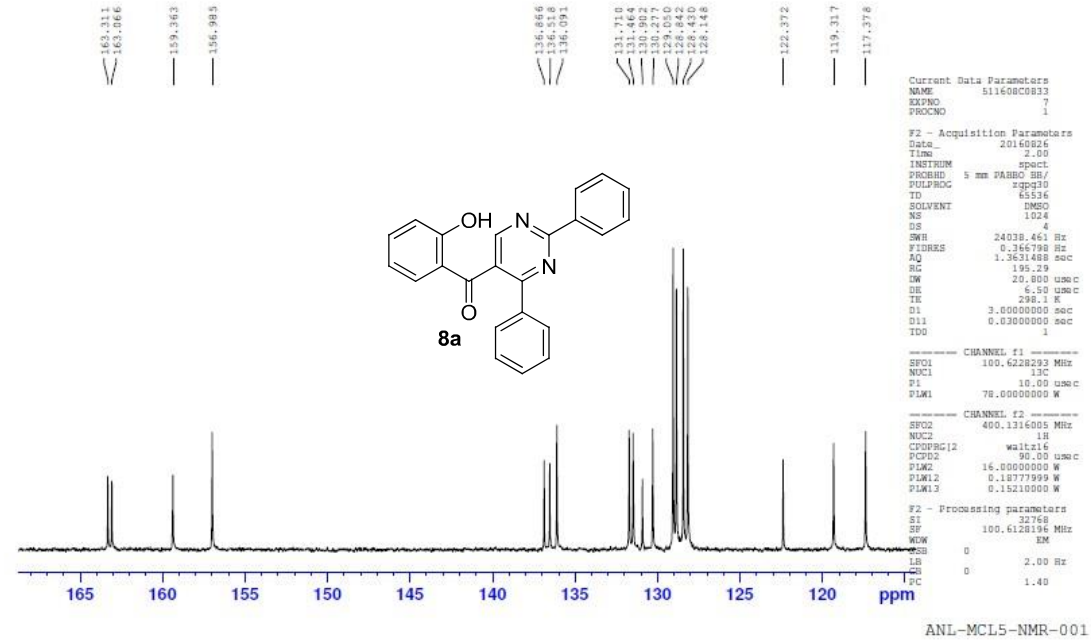
GVK-SAM-1-PAGE-54-NON-POLAR




```
Current Data Parameters
NAME          511608C0833
EXPNO                   7
PROCNO                  1

F2 - Acquisition Parameters
Date_         20160826
Time               2.00
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG        zgpg30
TD              65536
SOLVENT          DMSO
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              298.1 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          100.6128196 MHz
WDW                 EM
SSB                  0
LB                2.00 Hz
GB                   0
PC                1.40
```

ANL-MCL5-NMR-001

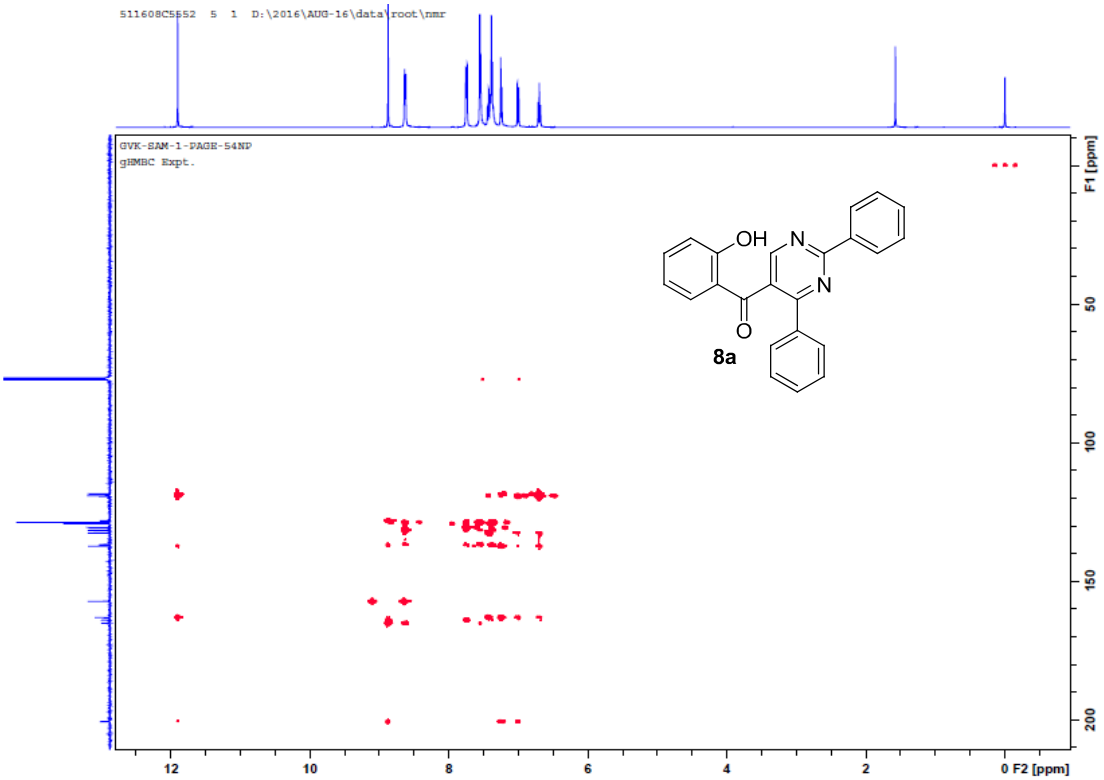
GVK-SAM-1-PAGE-54-NON-POLAR

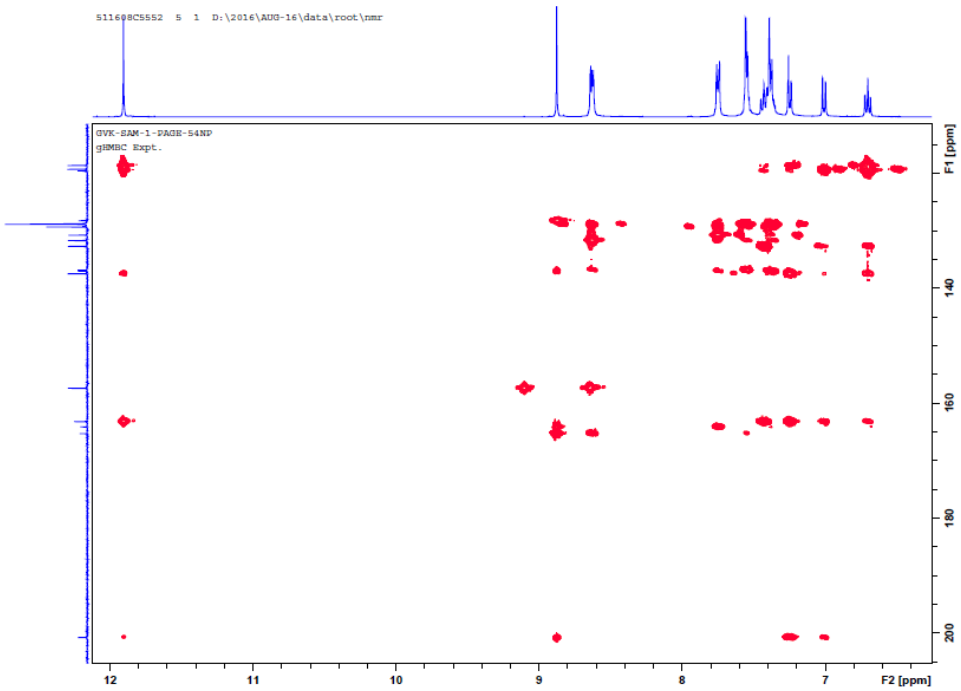


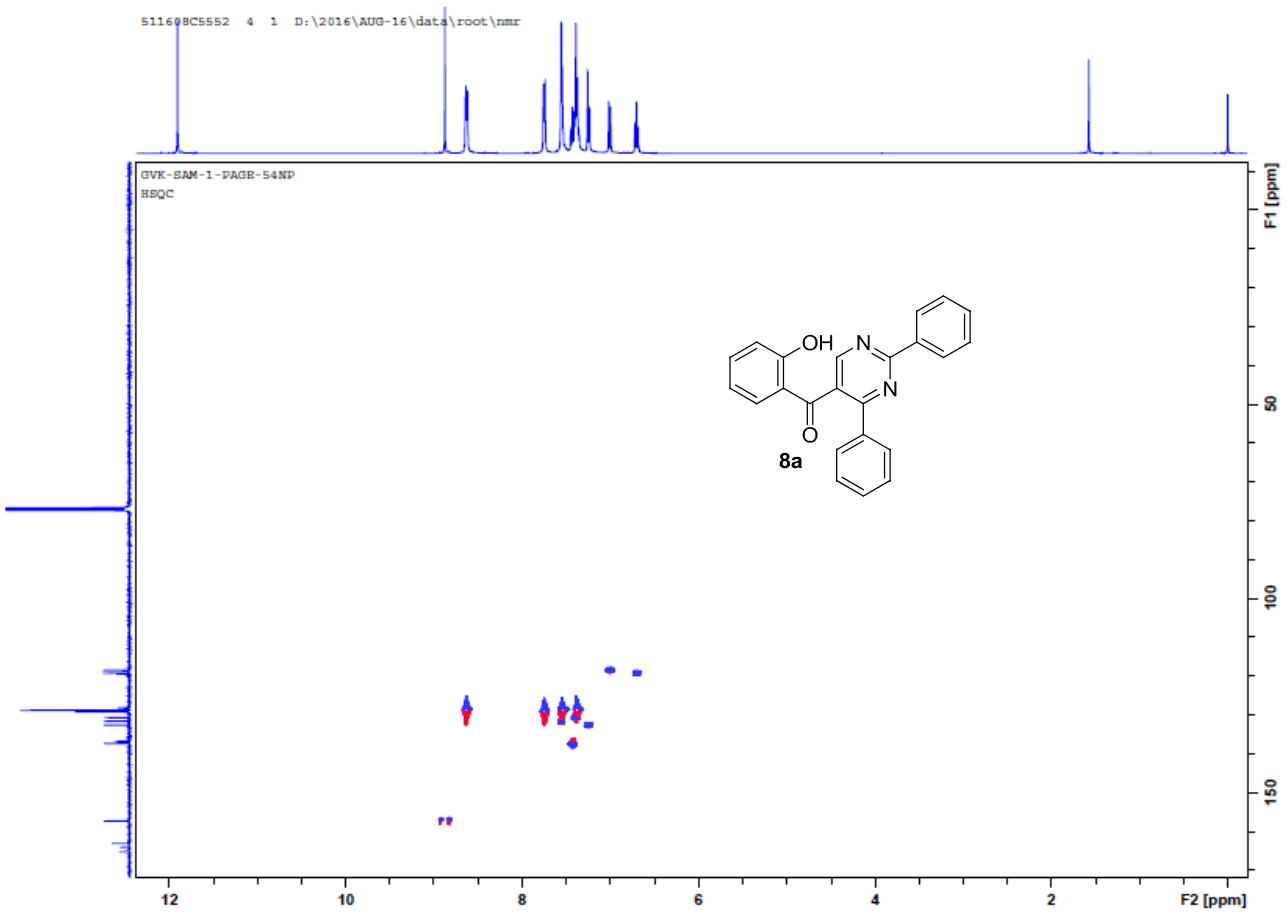

```
Current Data Parameters
NAME          511608C0833
EXPNO                   7
PROCNO                  1

F2 - Acquisition Parameters
Date_         20160826
Time               2.00
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG        zgpg30
TD              65536
SOLVENT          DMSO
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              298.1 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          100.6128196 MHz
WDW                 EM
SSB                  0
LB                2.00 Hz
GB                   0
PC                1.40
```

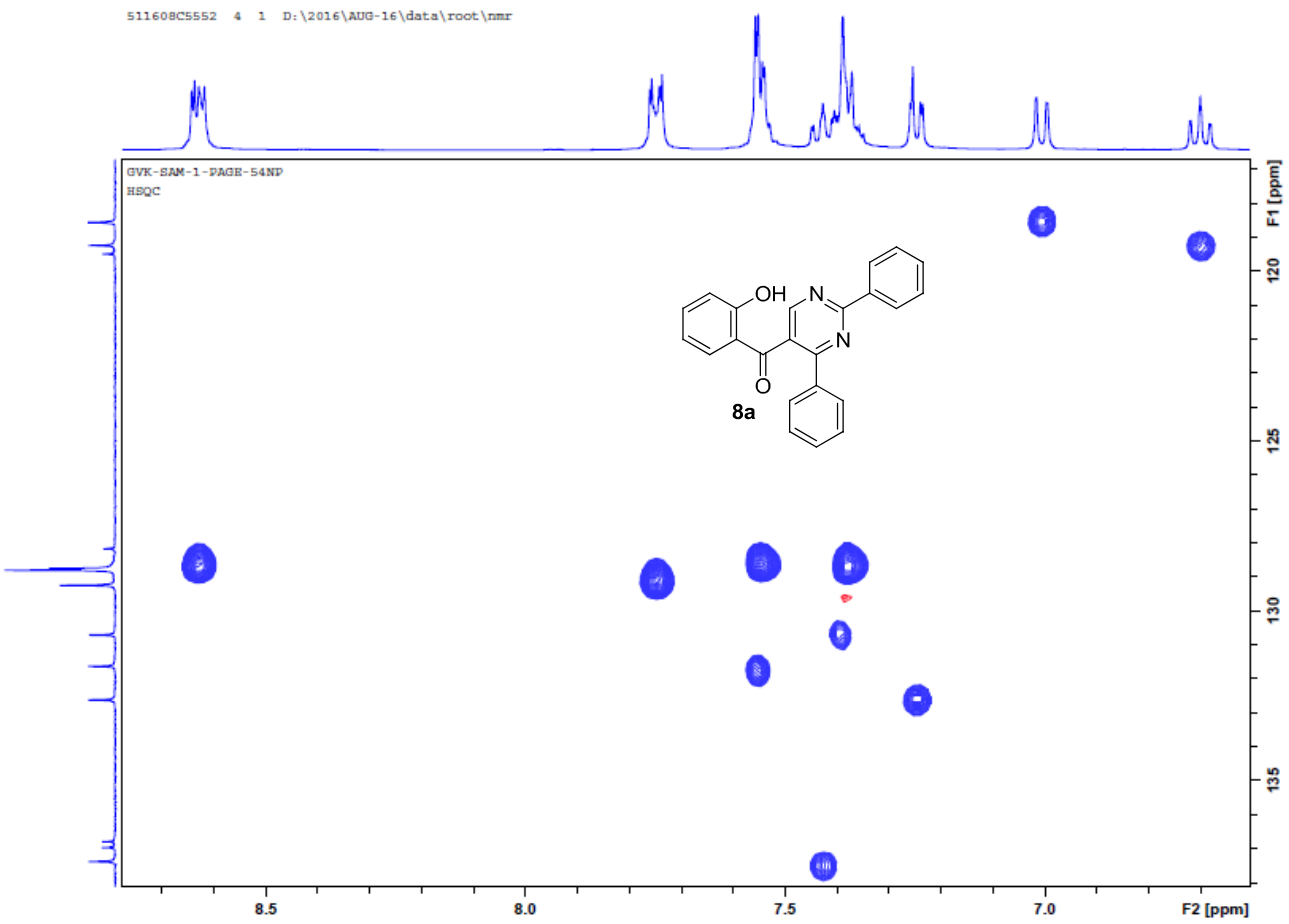
ANL-MCL5-NMR-001

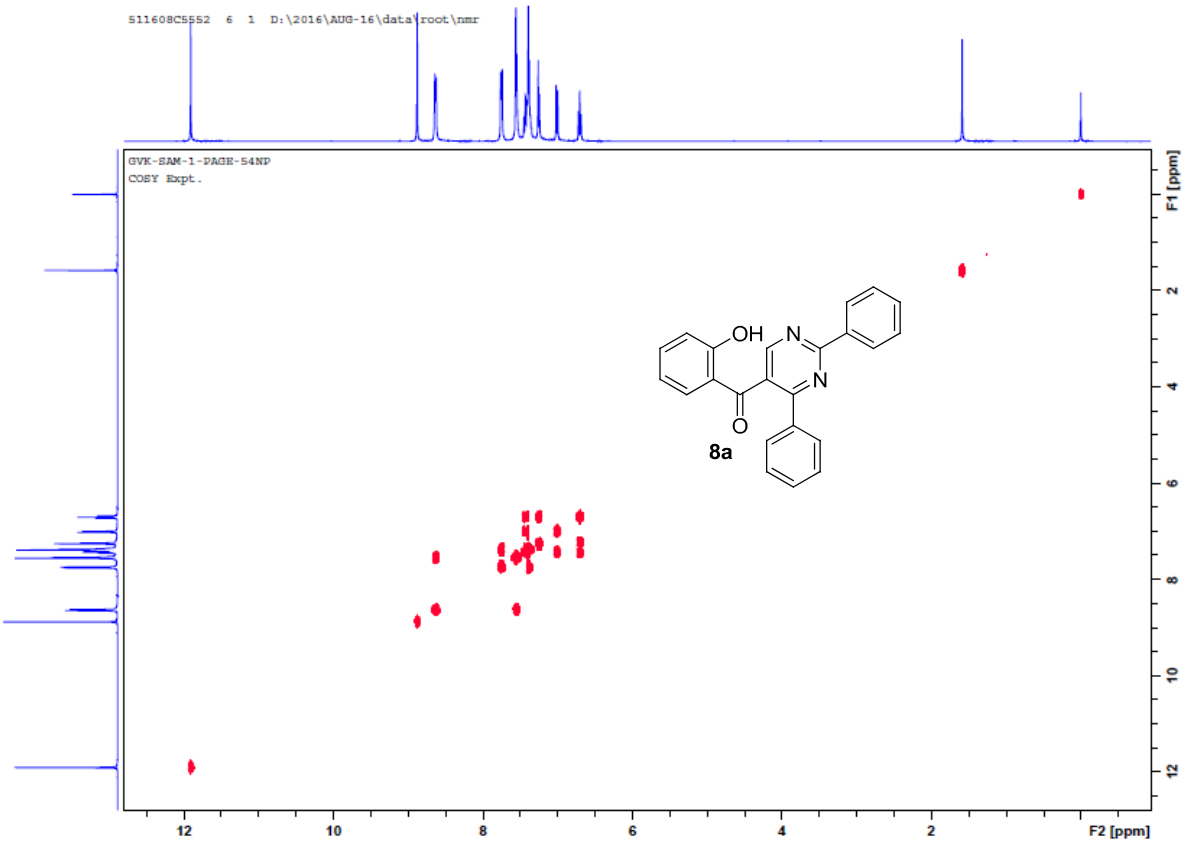
Compound **8a** Structure Confirmation data:

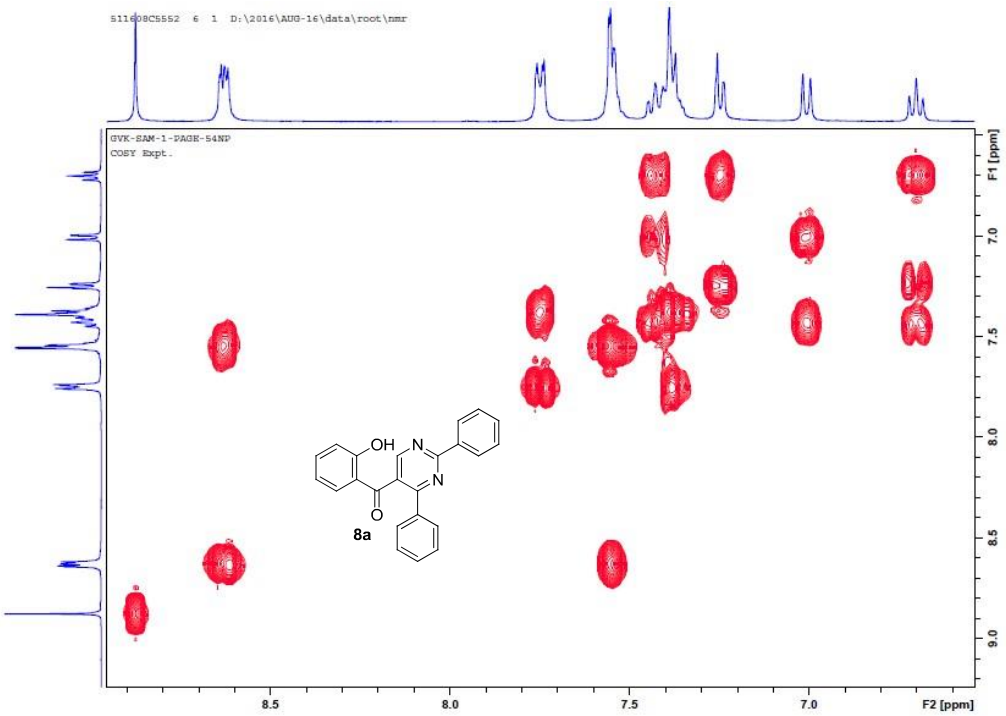


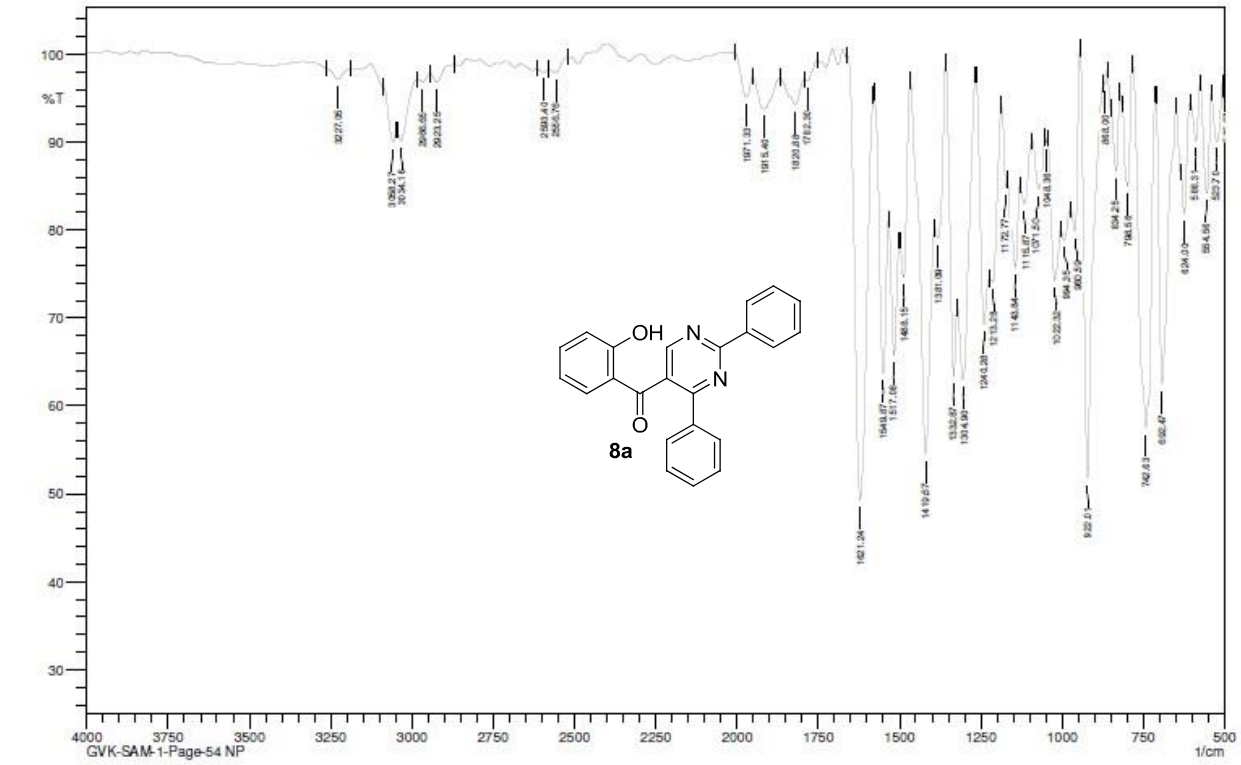



511608C5552 4 1 D:\2016\AUG-16\data\root\nmr
GVK-SAM-1-PAGE-54NP
HSQC
OH
N
N
O
8a
F1 [ppm]
50
100
150
12
10
8
6
4
2
F2 [ppm]


511608C5552 4 1 D:\2016\AUG-16\data\root\nmr
GVK-SAM-1-PAGE-54NP
HSQC
OH
N
N
O
8a
F1 [ppm]
120
125
130
135
8.5
8.0
7.5
7.0
F2 [ppm]


511608C5552 6 1 D:\2016\AUG-16\data\root\nmr
GVK-SAM-1-PAGE-54NP
COSY Expt.
OH
N
N
O
8a
F1 [ppm]
F2 [ppm]
12
10
8
6
4
2


511608C5552 6 1 D:\2016\AUG-16\data\root\nmr
GVK-SAM-1-PAGE-54NP
COSY Expt.
OH
N
N
O
8a
F1 [ppm]
F2 [ppm]
8.5
8.0
7.5
7.0
9.0



Comment: IN Kbr
GVK-SAM-1-Page-54 NP

No. of Scans:
Resolution:
Apodization:

Date: 10/3/2016 11:07:57 AM
User: Admin

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

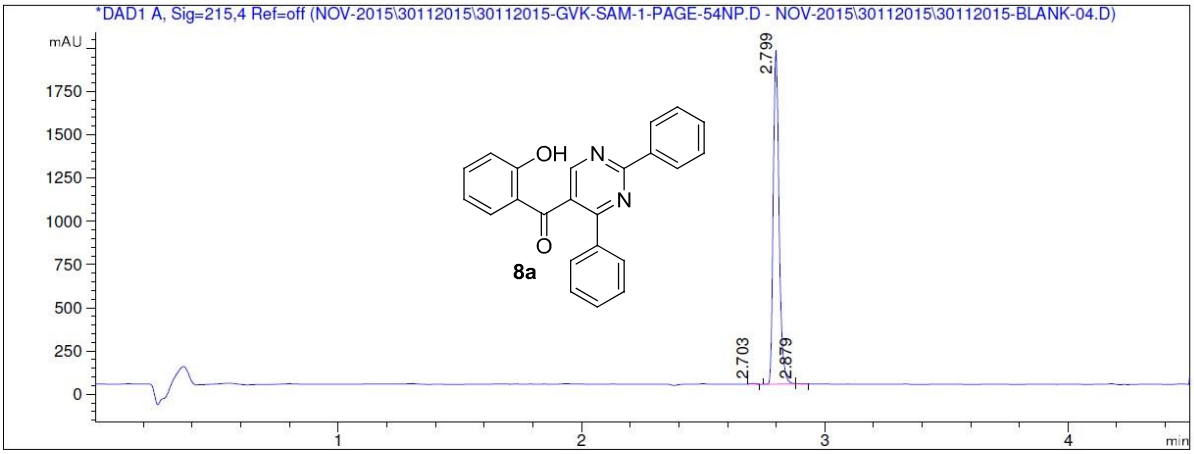
LCMS REPORT

==========

>Sample Name: GVK-SAM-1-PAGE-54NP Vial position :P1-B-01
Date of Analysis:30/11/2015;8:48:21 AM Injection Vol :0.5 µL
Acq. Method :C:\CHEM32\1\METHODS\RND-FA- 4.5 MIN_1.M Instrument ID :ANL-MCL5-LCMS-001

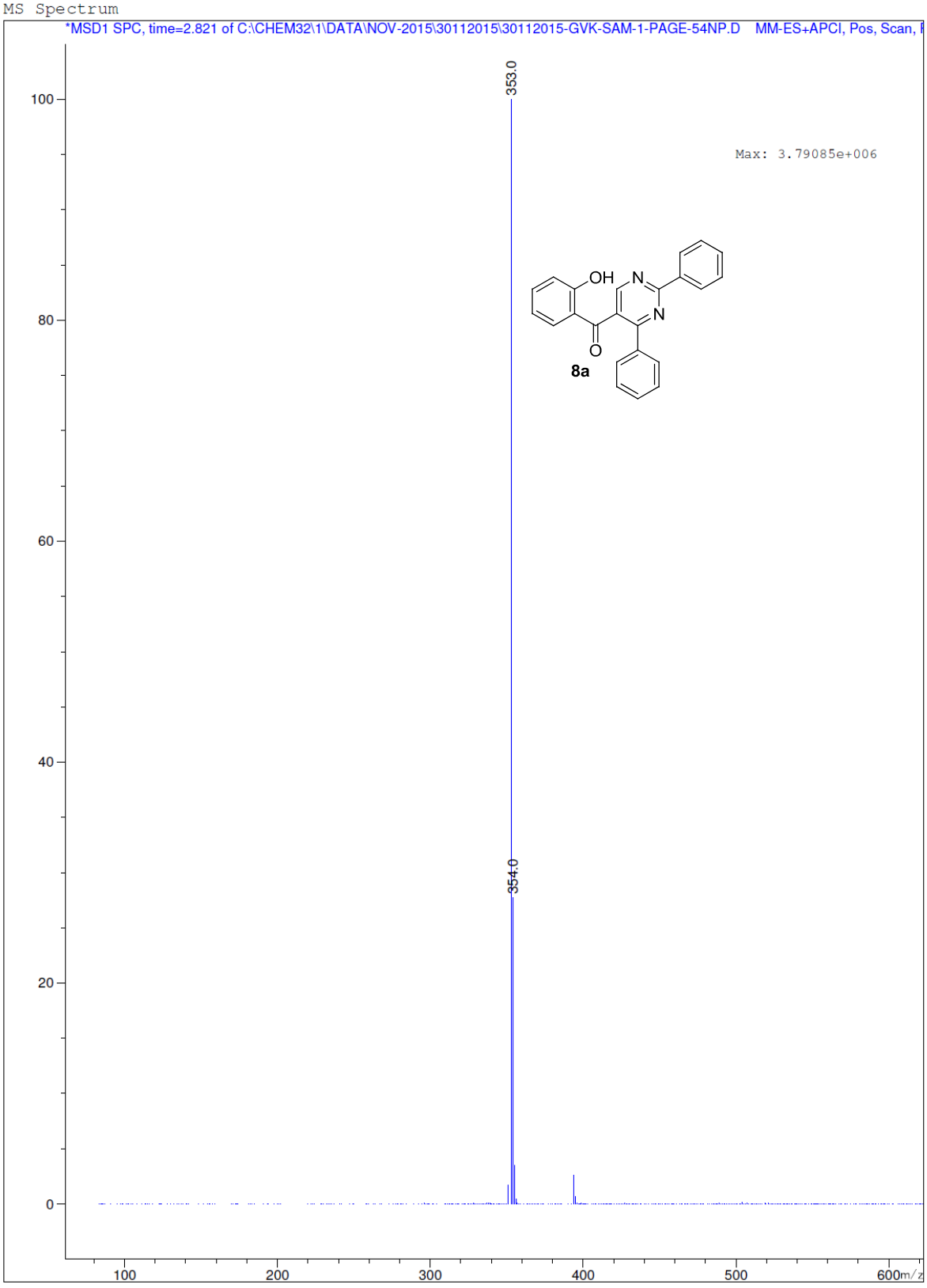
==========

Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: A1: 0.1 % FA IN WATER B1: 0.1%FA IN ACN
Gradient: Time (min) /%B1:0/3, 0.3/3, 2.8/98,4.0/98,4.2/3,4.5/3
Column Flow Rate: 0.6 ml/min



Peak No	RT min	Area	Area %
1	2.70	6.437	0.200
2	2.80	3.213e3	99.692
3	2.88	3.482	0.108

MS Spectrum

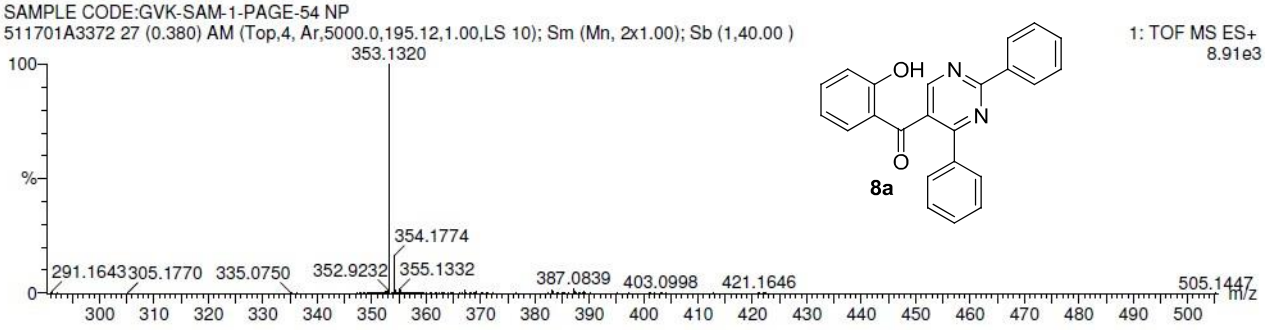

*MSD1 SPC, time=2.821 of C:\CHEM32\1\DATA\NOV-2015\30112015\30112015-GVK-SAM-1-PAGE-54NP.D MM-ES+APCI, Pos, Scan,
Max: 3.79085e+006
353.0
354.0
OH
N
N
O
8a
100
80
60
40
20
0
100
200
300
400
500
600m/z

Single Mass Analysis

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

Monoisotopic Mass, Even Electron Ions
4 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-23 H: 0-17 N: 0-2 O: 0-2

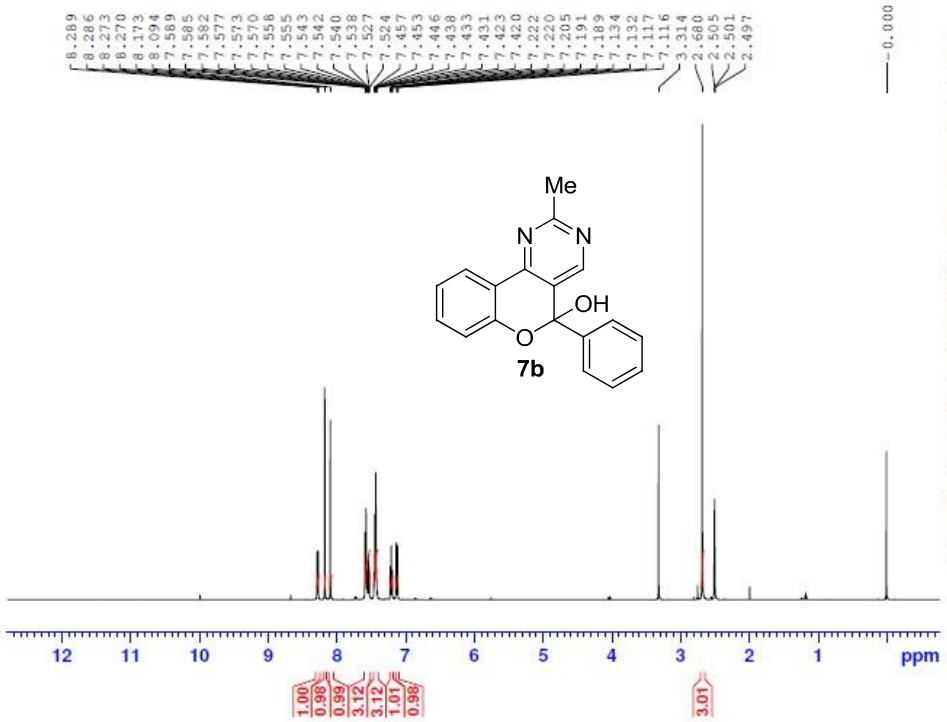
SAMPLE CODE:GVK-SAM-1-PAGE-54 NP
511701A3372 27 (0.380) AM (Top,4, Ar,5000.0,195.12,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)



8a

Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
353.1320	353.1290	3.0	8.5	16.5	376.4	C23 H17 N2 O2

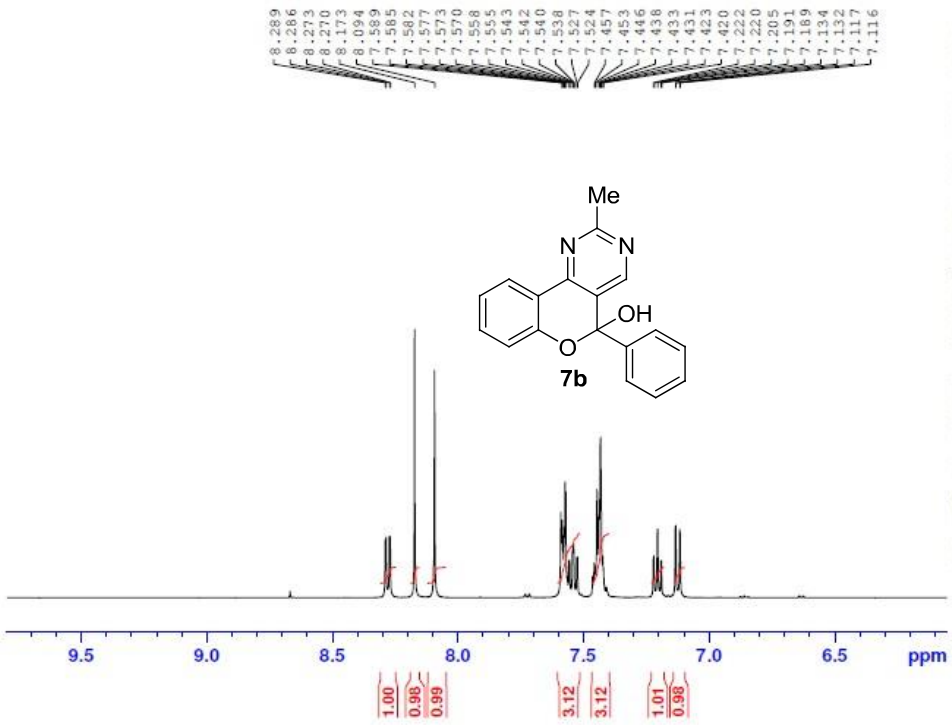
GVK-SAM-1-PAGE-63P




```
Current Data Parameters
NAME          511512A5812
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20151209
Time                6.51
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                     8
DS                     0
SWH          10000.000 Hz
FIDRES           0.152588 Hz
AQ            3.2767999 sec
RG                118.49
DW                50.000 usec
DE                 6.50 usec
TE                300.4 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 =======
SFO1         500.1330885 MHz
NUC1                   1H
P1                 10.00 usec
PLW1        24.00000000 W

F2 - Processing parameters
SI                 65536
SF           500.1300045 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

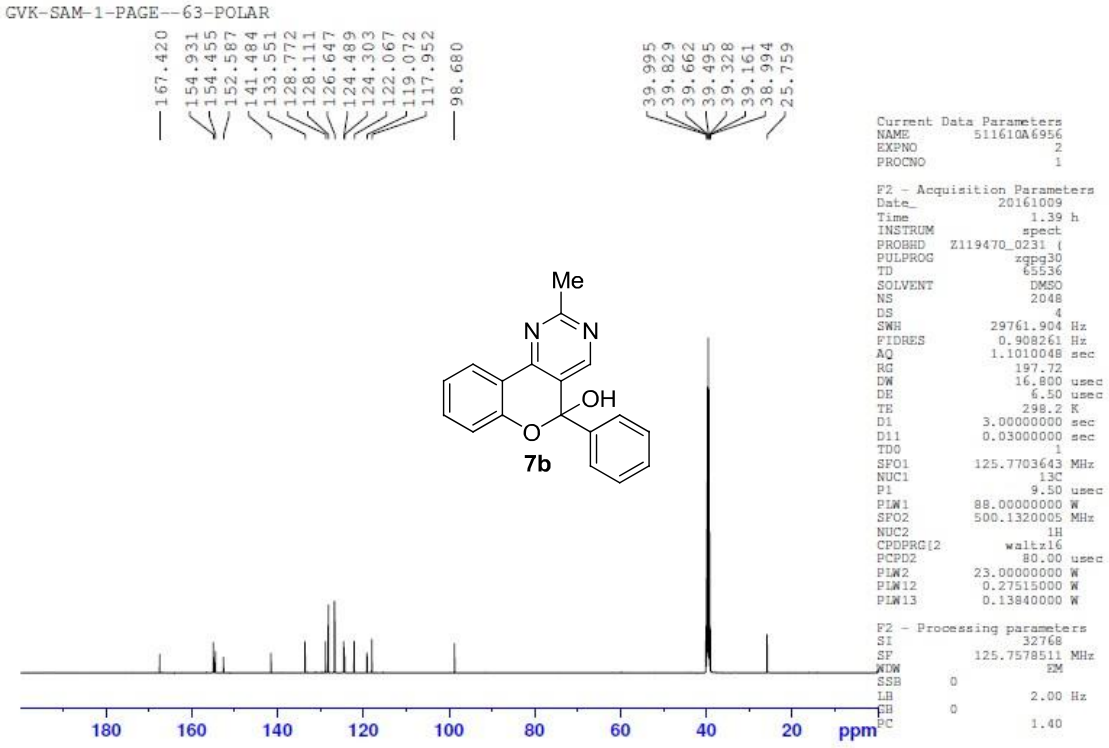
ANL-MCL5-NMR-002

GVK-SAM-1-PAGE-63P




```
Current Data Parameters
NAME          511512A5812
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20151209
Time                6.51
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT             DMSO
NS                     8
DS                     0
SWH          10000.000 Hz
FIDRES           0.152588 Hz
AQ            3.2767999 sec
RG                118.49
DW                50.000 usec
DE                 6.50 usec
TE                300.4 K
D1           1.00000000 sec
TD0                    1

======== CHANNEL f1 =======
SFO1         500.1330885 MHz
NUC1                   1H
P1                 10.00 usec
PLW1        24.00000000 W

F2 - Processing parameters
SI                 65536
SF           500.1300045 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

ANL-MCL5-NMR-002


GVK-SAM-1-PAGE--63-POLAR
167.420
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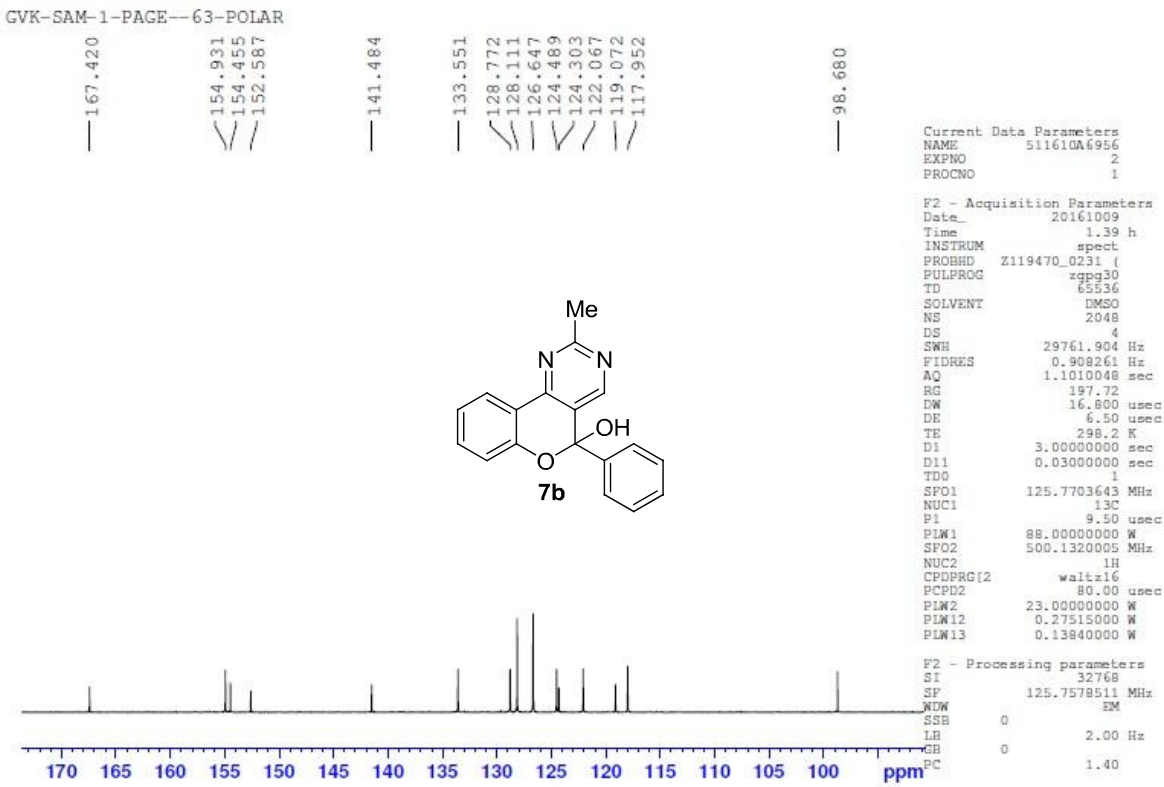
154.455
152.587
141.484
133.551
128.772
128.111
126.647
124.489
124.303
122.067
119.072
117.952
98.680
39.995
39.829
39.662
39.495
39.328
39.161
38.994
25.759
Me
N
N
OH
O
7b
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME 511610A6956
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161009
Time 1.39 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 298.2 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7578511 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40


GVK-SAM-1-PAGE--63-POLAR
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124.489
124.303
122.067
119.072
117.952
98.680
Me
N
N
OH
O
7b
170
165
160
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150
145
140
135
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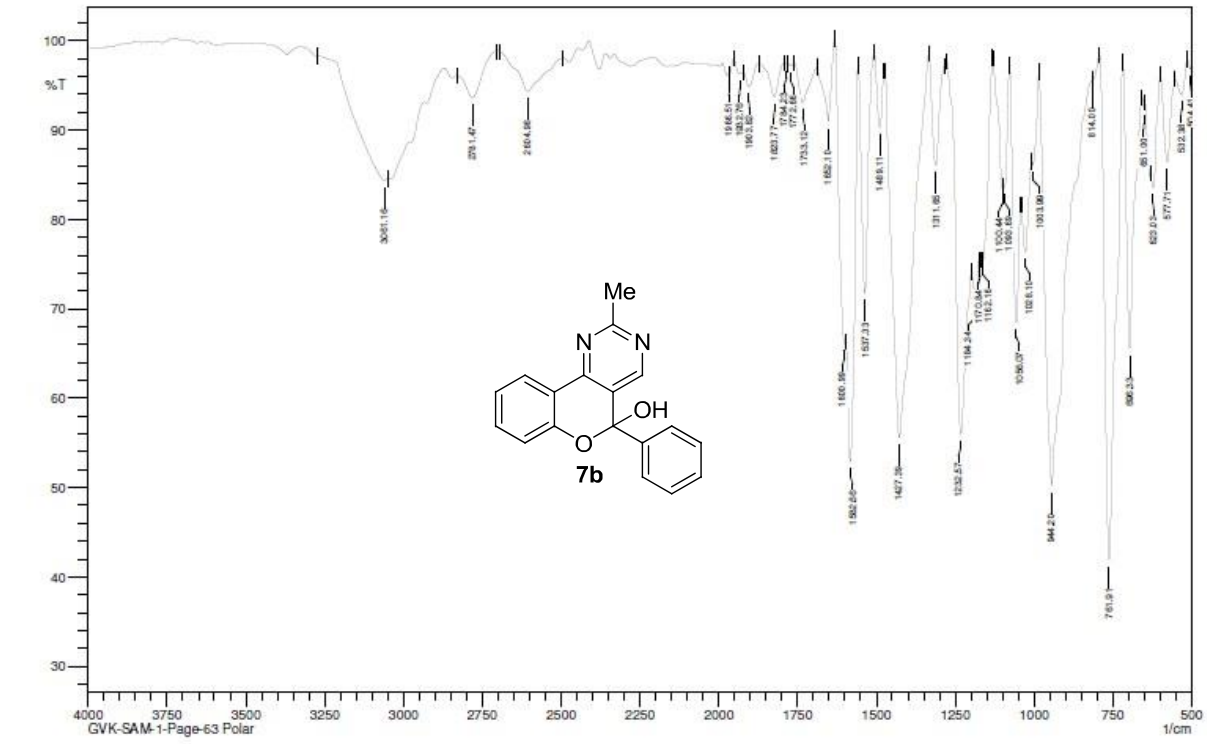
125
120
115
110
105
100
ppm
Current Data Parameters
NAME 511610A6956
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161009
Time 1.39 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2048
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 298.2 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7578511 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40



Comment: IN Kbr
GVK-SAM-1-Page-63 Polar

No. of Scans:
Resolution:
Apodization:

Date: 10/3/2016 11:20:36 AM
User: Admin

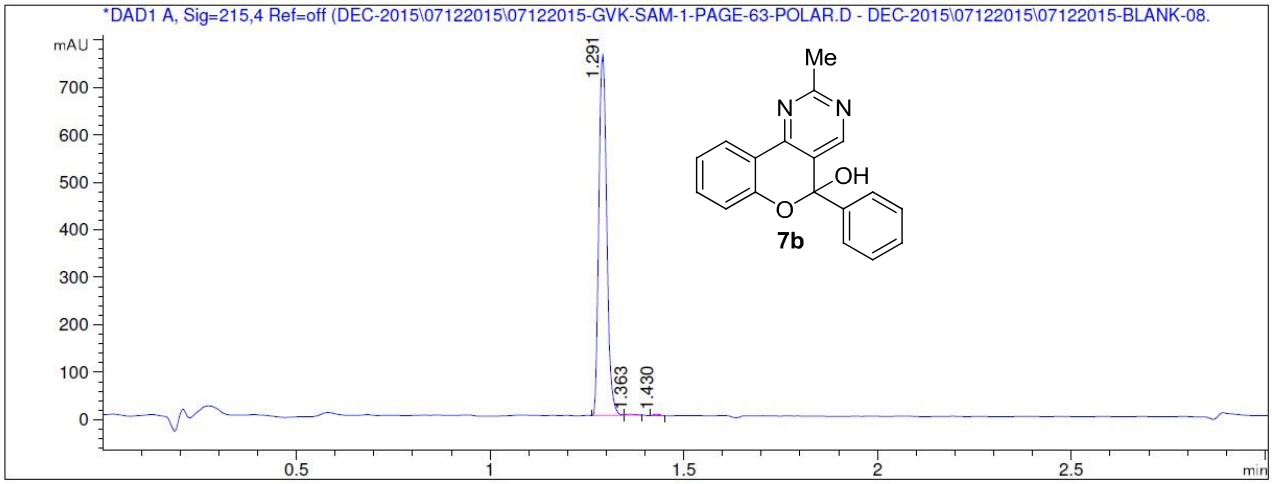
GVK BIOSCIENCES PVT. LTD.
MEDICINAL CHEMISTRY LABORATORY - ANALYTICAL RESEARCH

LCMS REPORT

Sample Name: GVK-SAM-1-PAGE-63-POLAR Vial position :P1-B-01
Date of Analysis:07/12/2015;7:40:15 PM Injection Vol :0.5 µL
Acq. Method :C:\CHEM32\1\METHODS\RND-FA- 3.0 MIN.M Instrument ID :ANL-MCL5-LCMS-001

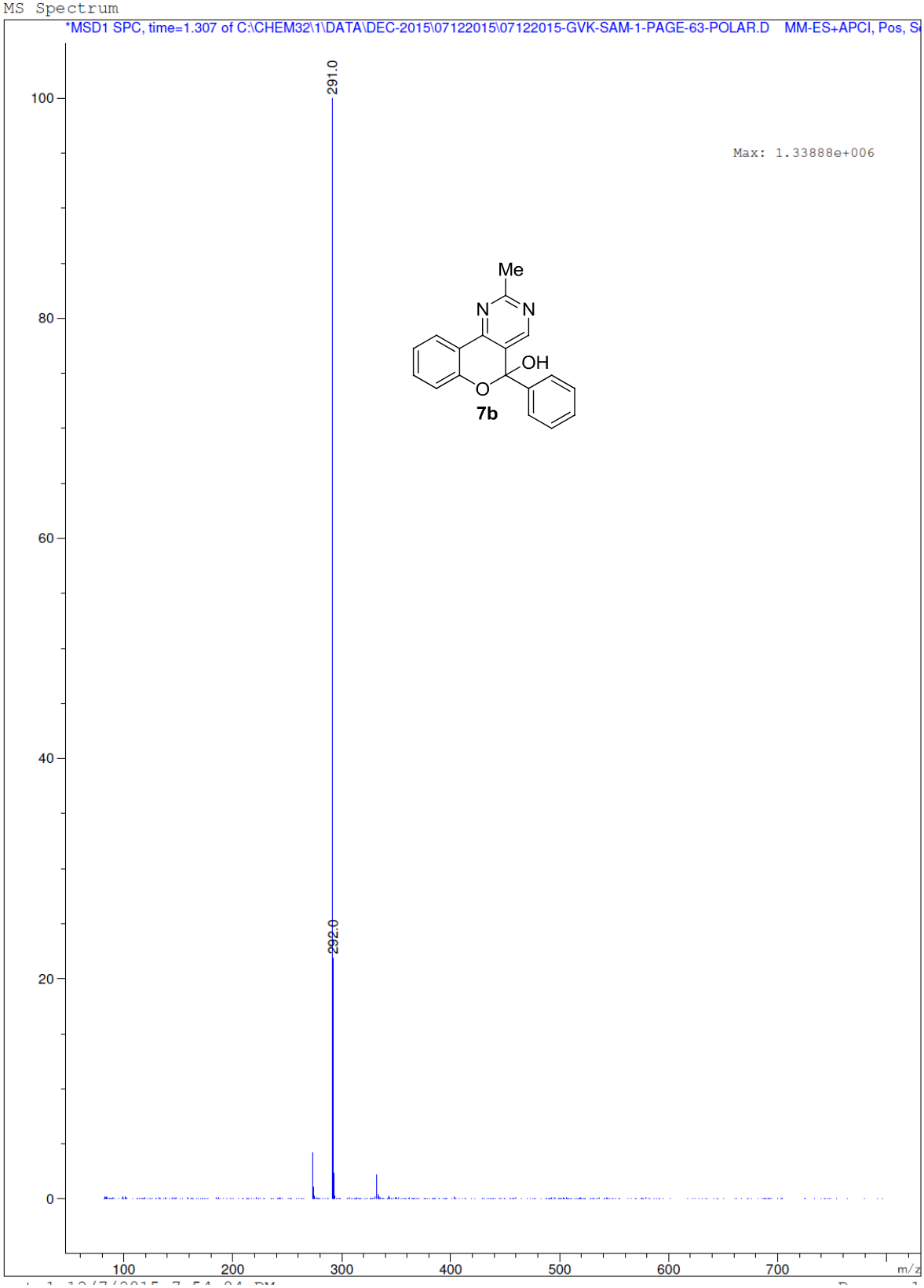
Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: A1: 0.1 % FA IN WATER B1: 0.1%FA IN ACN
Gradient: Time (min) /%B1:0/2, 0.2/2, 1.8/98,2.6/98,2.61/2,3.0/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 45°C

->



Pea No	RT min	Area	Area %
1	1.29	1.079e3	99.445
2	1.36	2.687	0.248
3	1.43	3.336	0.308

MS Spectrum


*MSD1 SPC, time=1.307 of C:\CHEM32\1\DATA\DEC-2015\07122015\07122015-GVK-SAM-1-PAGE-63-POLAR.D MM-ES+APCI, Pos, S
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292.0
Max: 1.33888e+006
Me
N
N
OH
O
7b
100
80
60
40
20
0
100
200
300
400
500
600
700
m/z

Elemental Composition Report **Page 1**

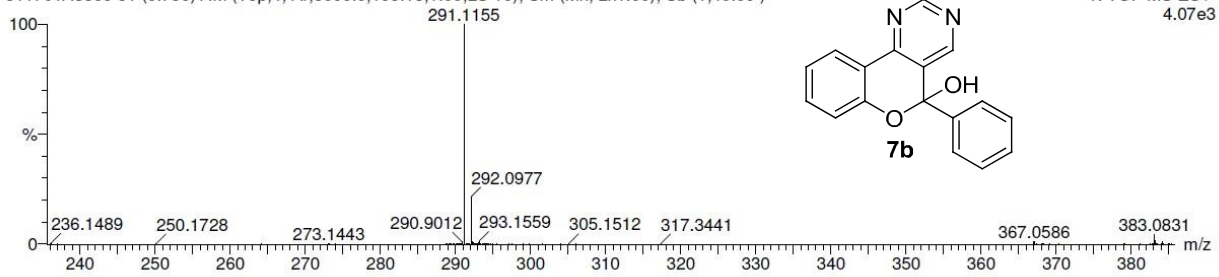
Single Mass Analysis

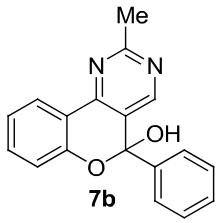
Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
4 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-18 H: 0-15 N: 0-2 O: 0-2

SAMPLE CODE:GVK-SAM-1-PAGE-63 POLAR
511701A3369 51 (0.750) AM (Top,4, Ar,5000.0,195.13,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

1: TOF MS ES+
4.07e3

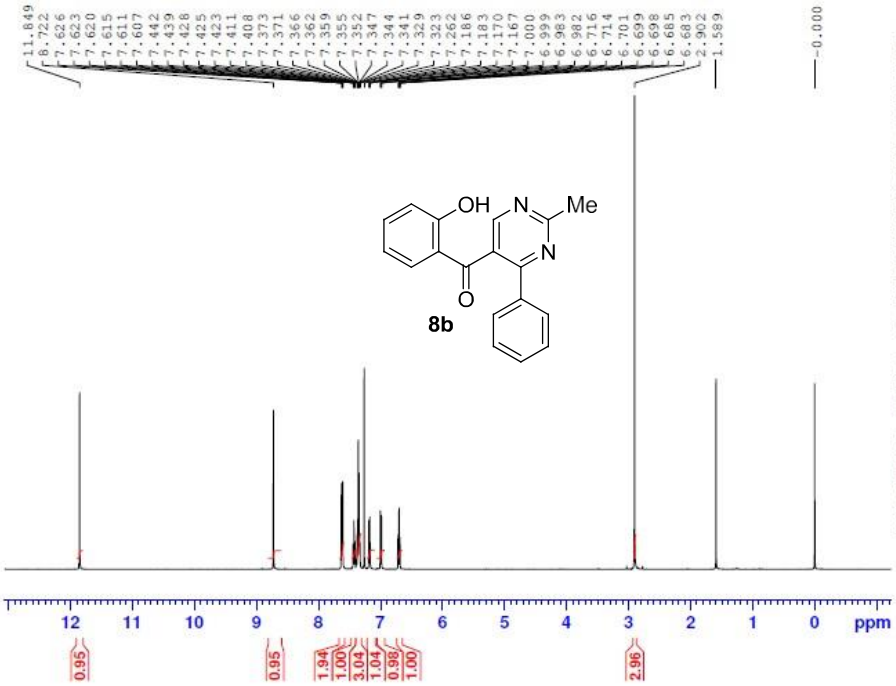




7b

Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
291.1155	291.1134	2.1	7.2	12.5	54.4	C18 H15 N2 O2

GVK-SAM-1-PAGE-63NP

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Current Data Parameters
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EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
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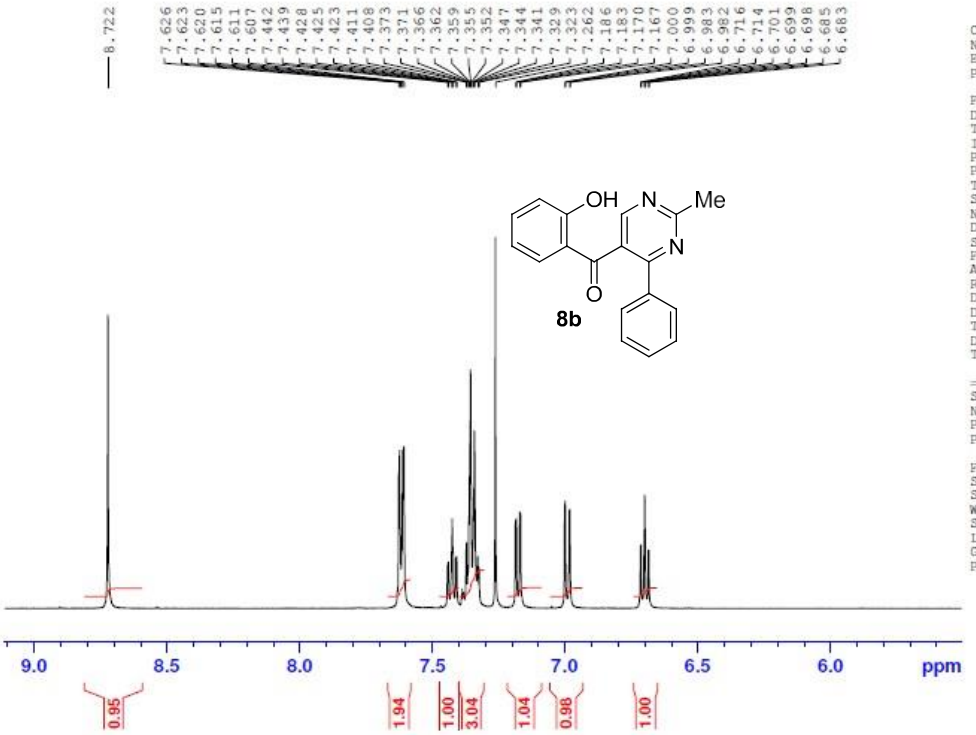
Time               18.21
INSTRUM            spect
PROBHD  5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    8
DS                    0
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG               118.49
DW               50.000 usec
DE                6.50 usec
TE               296.6 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 =======
SFO1         500.1330885 MHz
NUC1               1H
P1               10.00 usec
PLW1        24.00000000 W

F2 - Processing parameters
SI                65536
SF           500.1300119 MHz
WDW                EM
SSB       0
LB               0.30 Hz
GB        0
PC               1.00
```

ANL-MCL5-NMR-002

GVK-SAM-1-PAGE-63NP




```
Current Data Parameters
NAME          511512A5244
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_           20151207
Time               18.21
INSTRUM            spect
PROBHD  5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                    8
DS                    0
SWH           10000.000 Hz
FIDRES        0.152588 Hz
AQ            3.2767999 sec
RG               118.49
DW               50.000 usec
DE                6.50 usec
TE               296.6 K
D1            1.00000000 sec
TD0                   1

======== CHANNEL f1 =======
SFO1         500.1330885 MHz
NUC1               1H
P1               10.00 usec
PLW1        24.00000000 W

F2 - Processing parameters
SI                65536
SF           500.1300119 MHz
WDW                EM
SSB       0
LB               0.30 Hz
GB        0
PC               1.00
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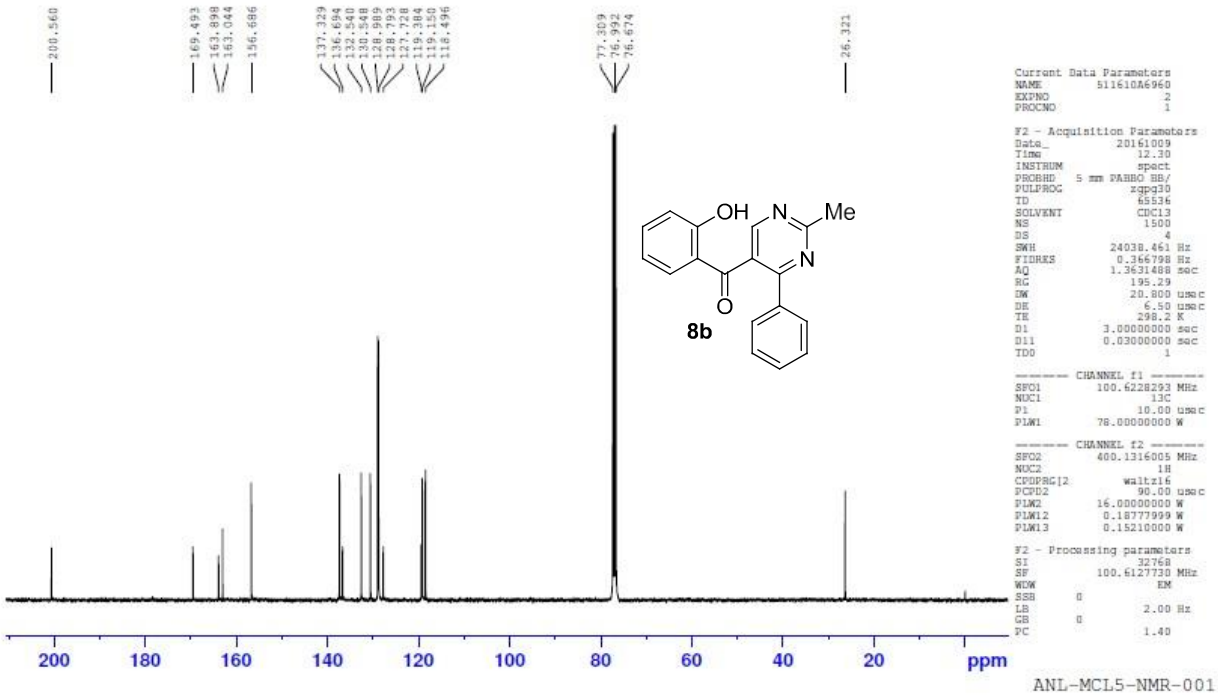
ANL-MCL5-NMR-002

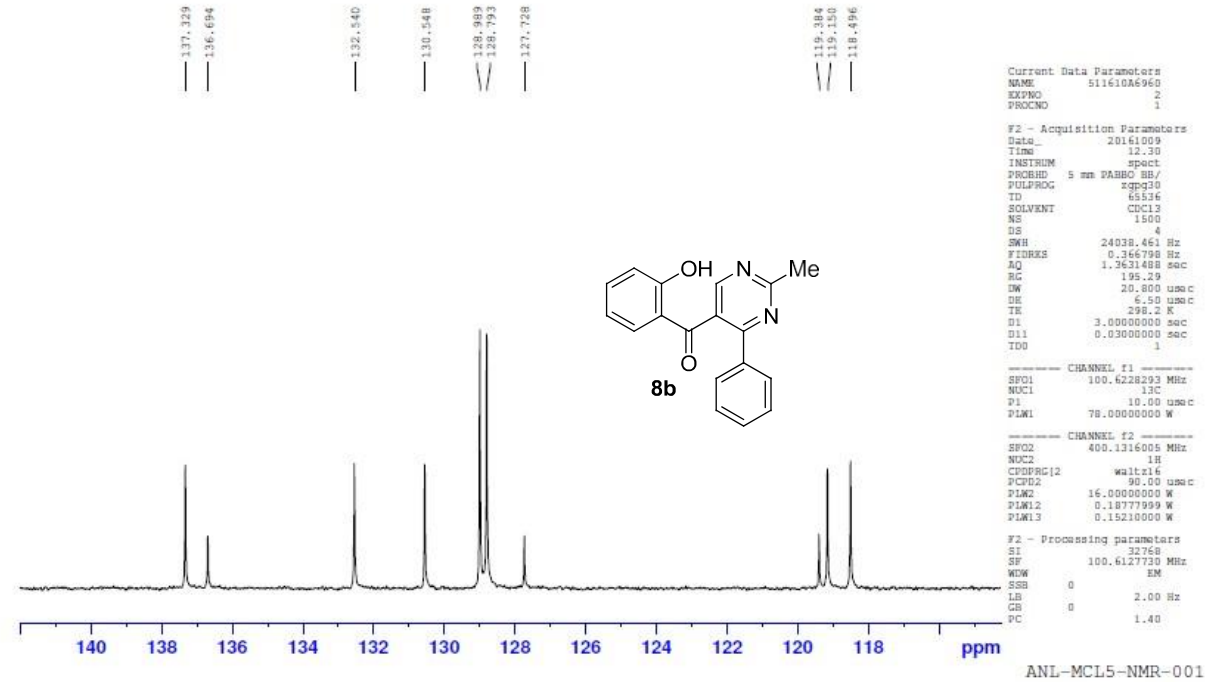
GVK-SAM-1-page-63NP




```
Current Data Parameters
NAME          511610A6960
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20161009
Time               12.30
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1500
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                298.2 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          100.6127730 MHz
WDW                   EM
SSB       0
LB                 2.00 Hz
GB        0
PC                 1.40
```

ANL-MCL5-NMR-001

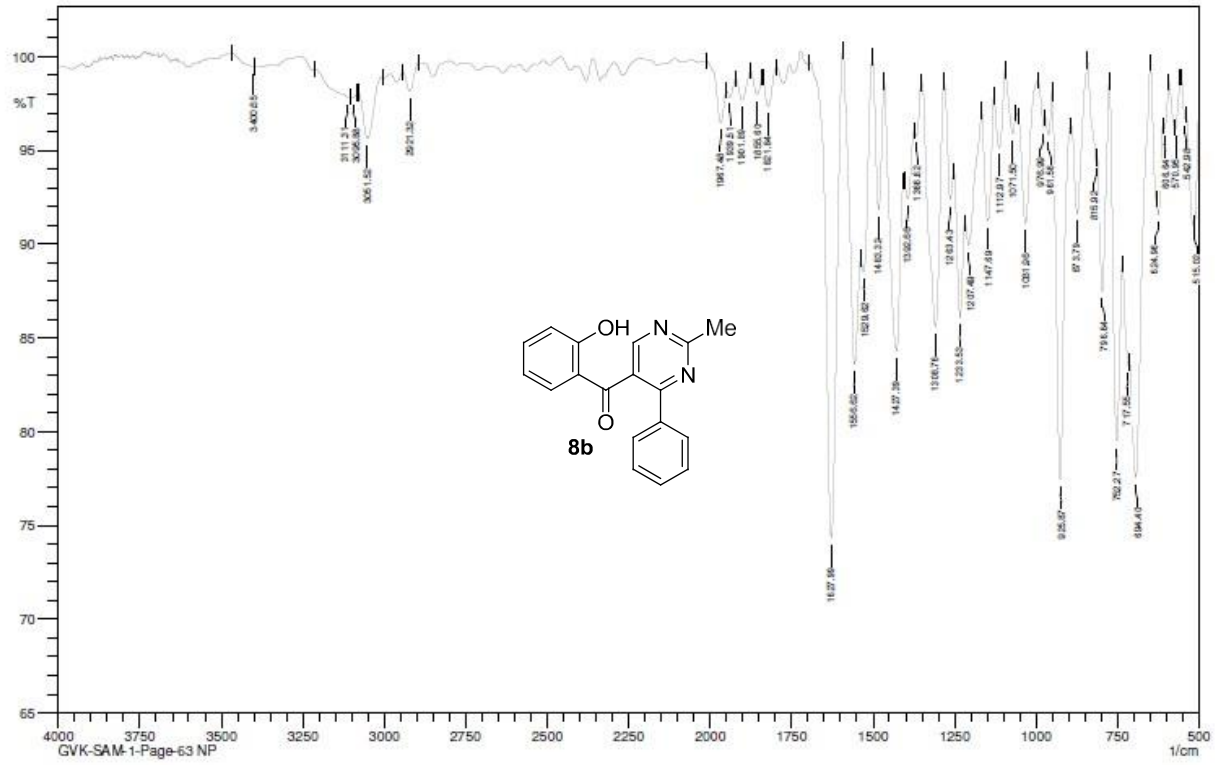
GVK-SAM-1-page-63NP




```
Current Data Parameters
NAME          511610A6960
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20161009
Time               12.30
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1500
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                298.2 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          100.6127730 MHz
WDW                   EM
SSB       0
LB                 2.00 Hz
GB        0
PC                 1.40
```

ANL-MCL5-NMR-001

SHIMADZU



Comment: IN Kbr
GVK-SAM-1-Page-63 NP

No. of Scans:
Resolution:
Apodization:

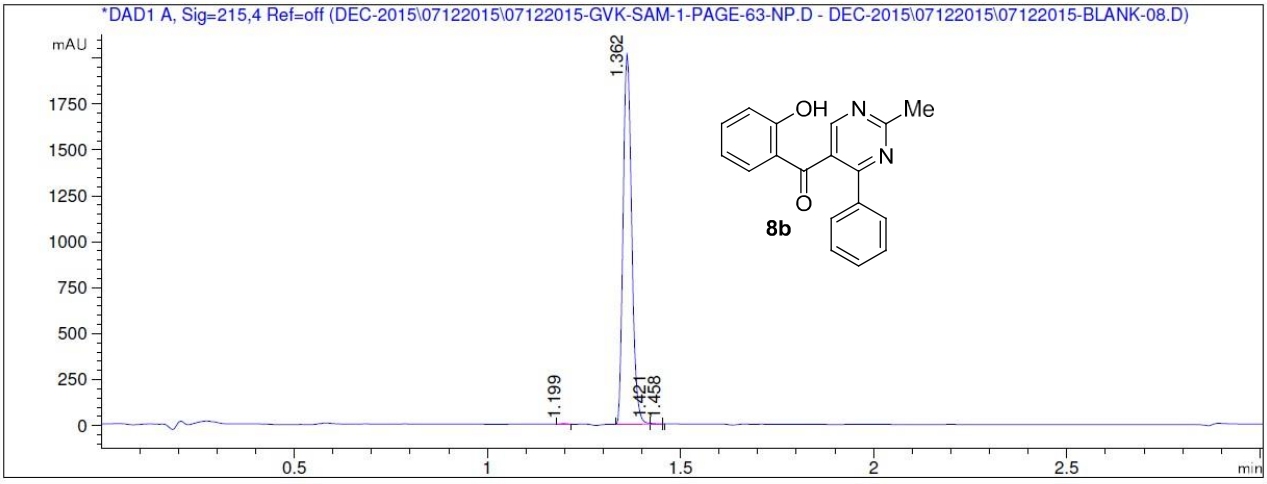
Date: 10/3/2016 11:00:48 AM
User: Admin

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

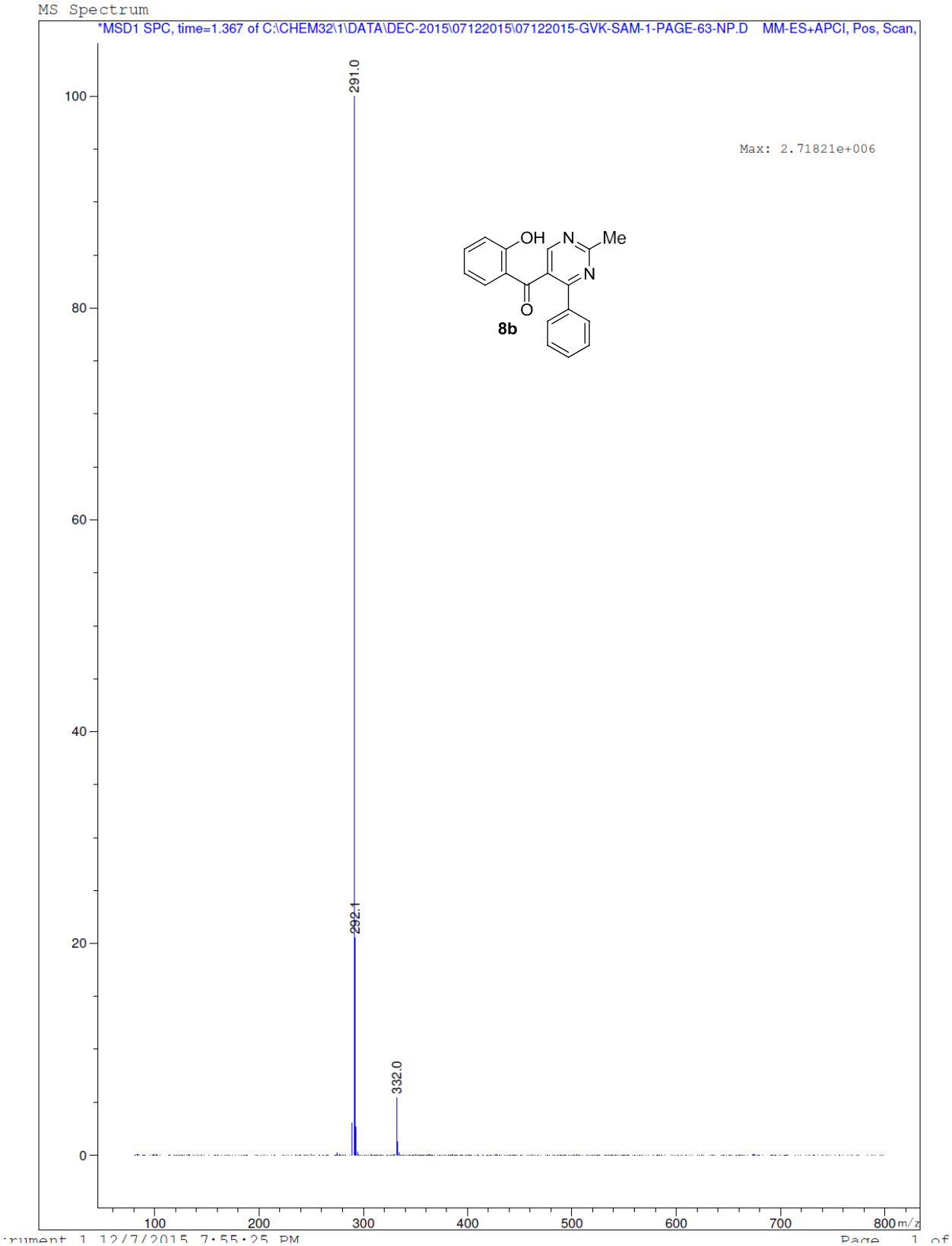
LCMS REPORT

Sample Name: GVK-SAM-1-PAGE-63-NP Vial position :P1-B-02
Date of Analysis:07/12/2015;7:44:12 PM Injection Vol :0.5 µL
Acq. Method :C:\CHEM32\1\METHODS\RND-FA- 3.0 MIN.M Instrument ID :ANL-MCL5-LCMS-001

Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: A1: 0.1 % FA IN WATER B1: 0.1%FA IN ACN
Gradient: Time (min) /%B1:0/2, 0.2/2, 1.8/98,2.6/98,2.61/2,3.0/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 45°C



Peak No	RT min	Area	Area %
1	1.20	4.608	0.147
2	1.36	3.118e3	99.735
3	1.42	3.541	0.113
4	1.46	0.125	0.004


MS Spectrum
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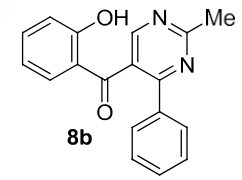
Max: 2.71821e+006
291.0
292.1
332.0
OH
N
Me
N
O
8b
100
80
60
40
20
0
100
200
300
400
500
600
700
800 m/z

Single Mass Analysis

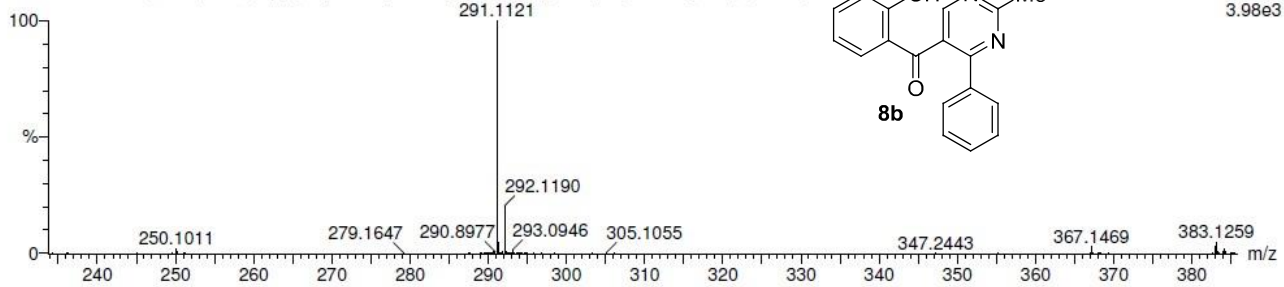
Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
4 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-18 H: 0-15 N: 0-2 O: 0-2
SAMPLE CODE:GVK-SAM-1-PAGE-63 NP
511701A3370 64 (0.945) AM (Top,4, Ar,5000.0,195.10,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)



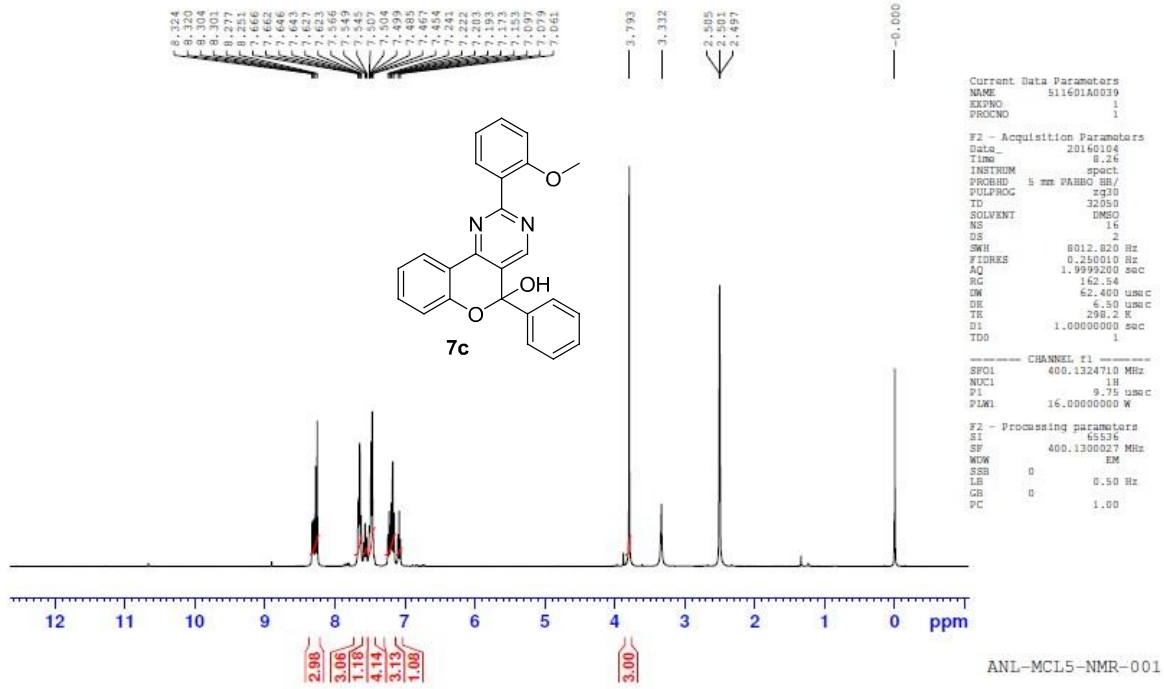
8b

1: TOF MS ES+
3.98e3



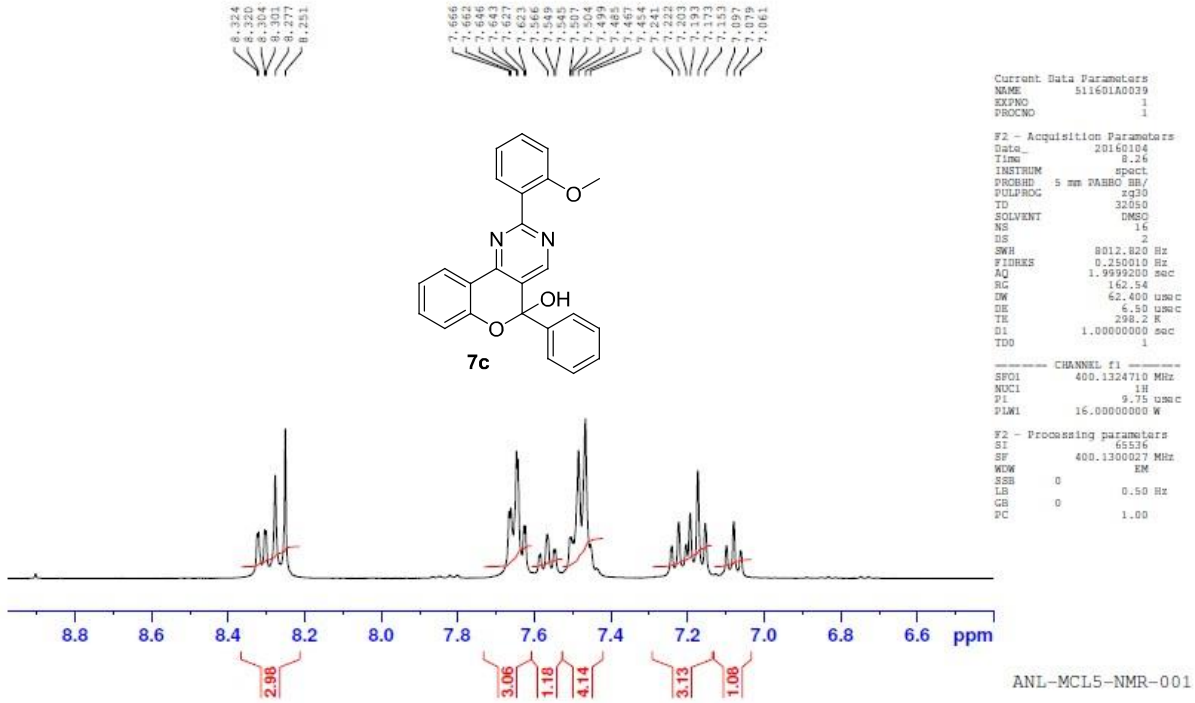
Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
291.1121	291.1134	-1.3	-4.5	12.5	33.5	C18 H15 N2 O2

GVK-SAM-5-PAGE-13P

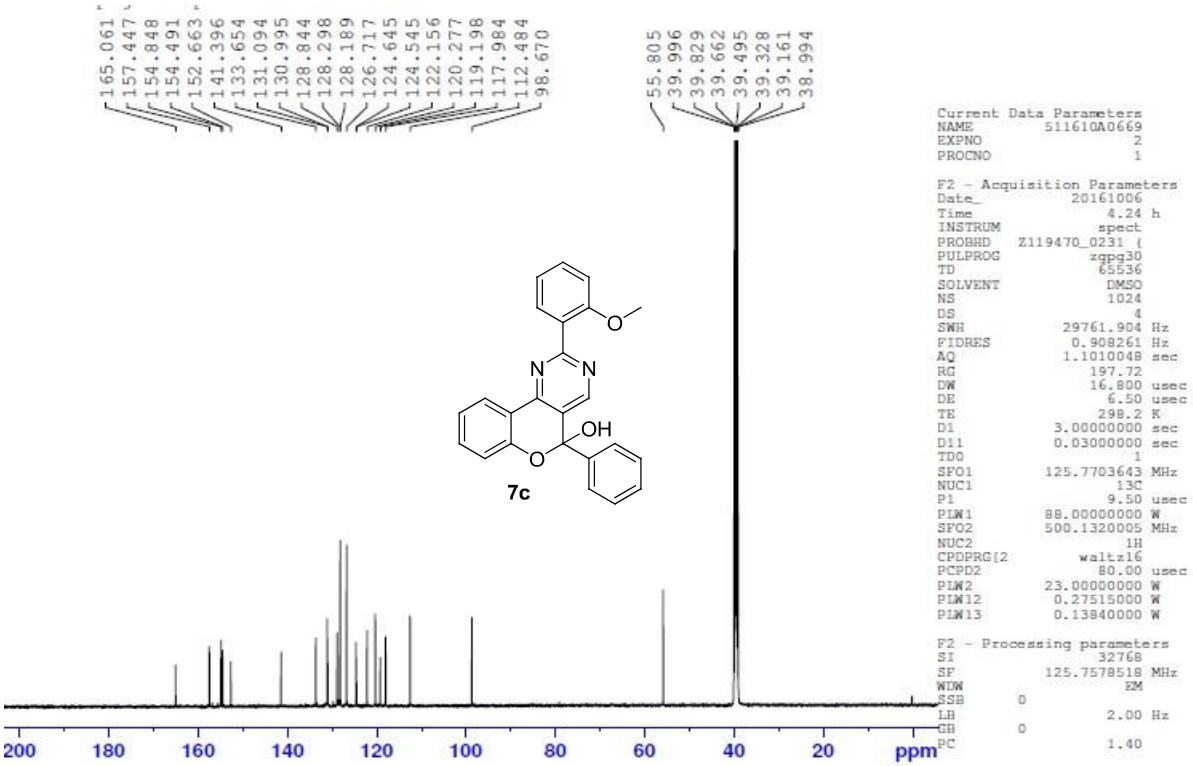


ANL-MCL5-NMR-001

GVK-SAM-5-PAGE-13P



ANL-MCL5-NMR-001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154.491
152.663
141.396
133.654
131.094
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128.844
128.298
128.189
126.717
124.645
124.545
122.156
120.277
119.198
117.984
112.484
98.670
55.805
39.996
39.829
39.662
39.495
39.328
39.161
38.994
O
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N
OH
O
7c
200
180
160
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100
80
60
40
20
ppm
Current Data Parameters
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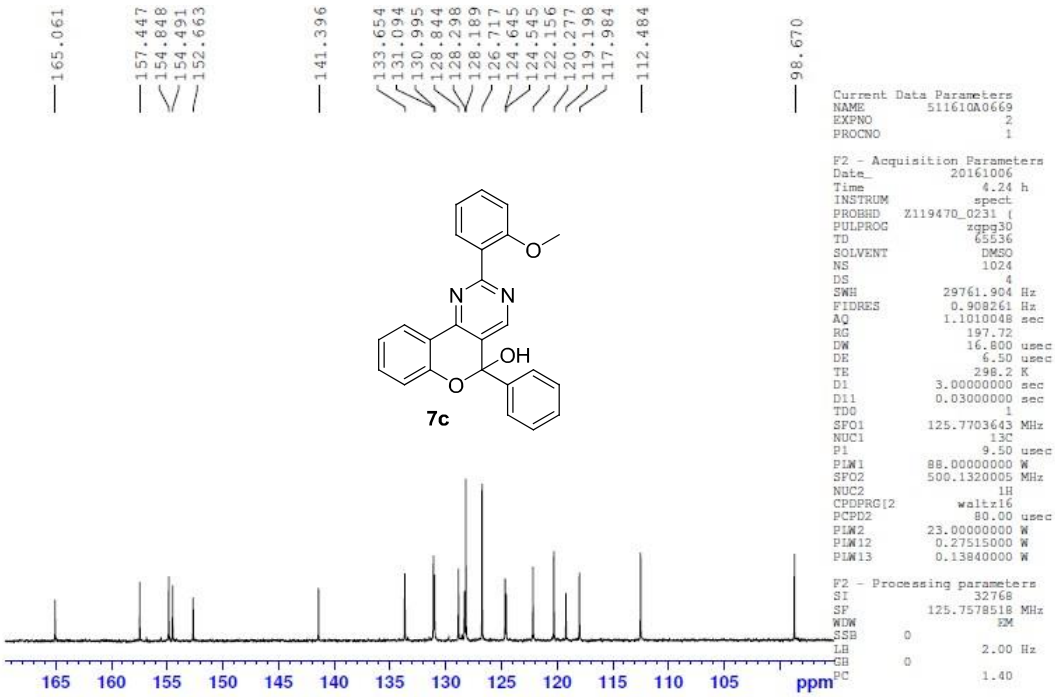
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161006
Time 4.24 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 298.2 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7578518 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40


165.061
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154.491
152.663
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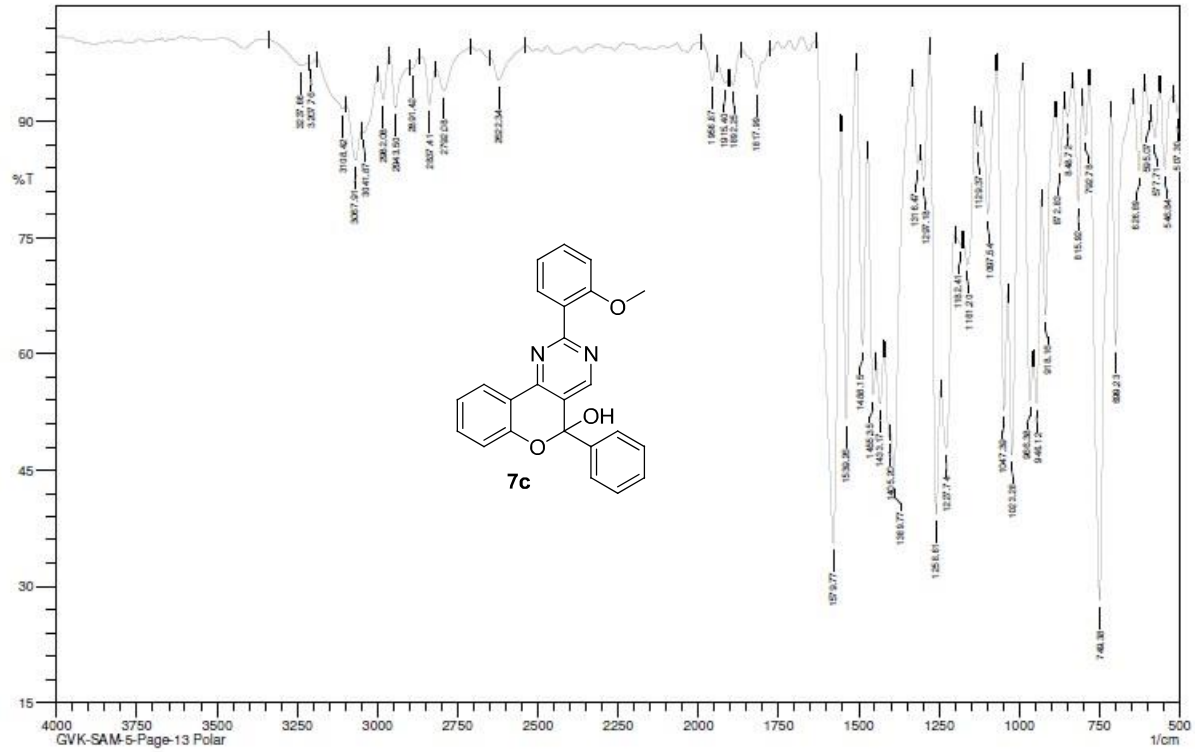
130.995
128.844
128.298
128.189
126.717
124.645
124.545
122.156
120.277
119.198
117.984
112.484
98.670
O
N
N
OH
O
7c
165
160
155
150
145
140
135
130
125
120
115
110
105
ppm
Current Data Parameters
NAME 511610A0669
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161006
Time 4.24 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 298.2 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7578518 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

SHIMADZU



7c

Comment: IN Kbr
GVK-SAM-5-Page-13 Polar

No. of Scans:
Resolution:
Apodization:

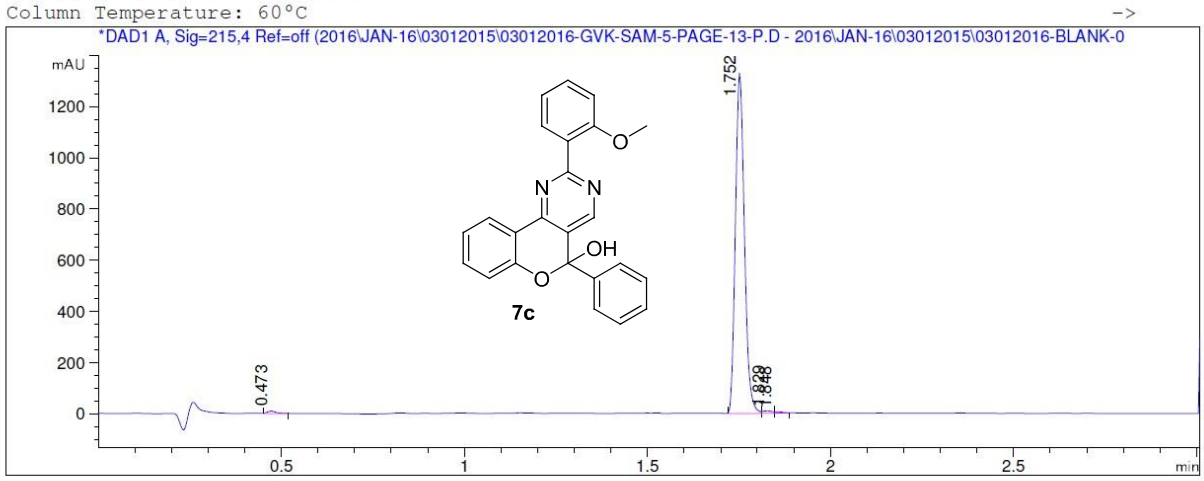
Date: 10/3/2016 10:54:16 AM
User: Admin

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

LCMS REPORT

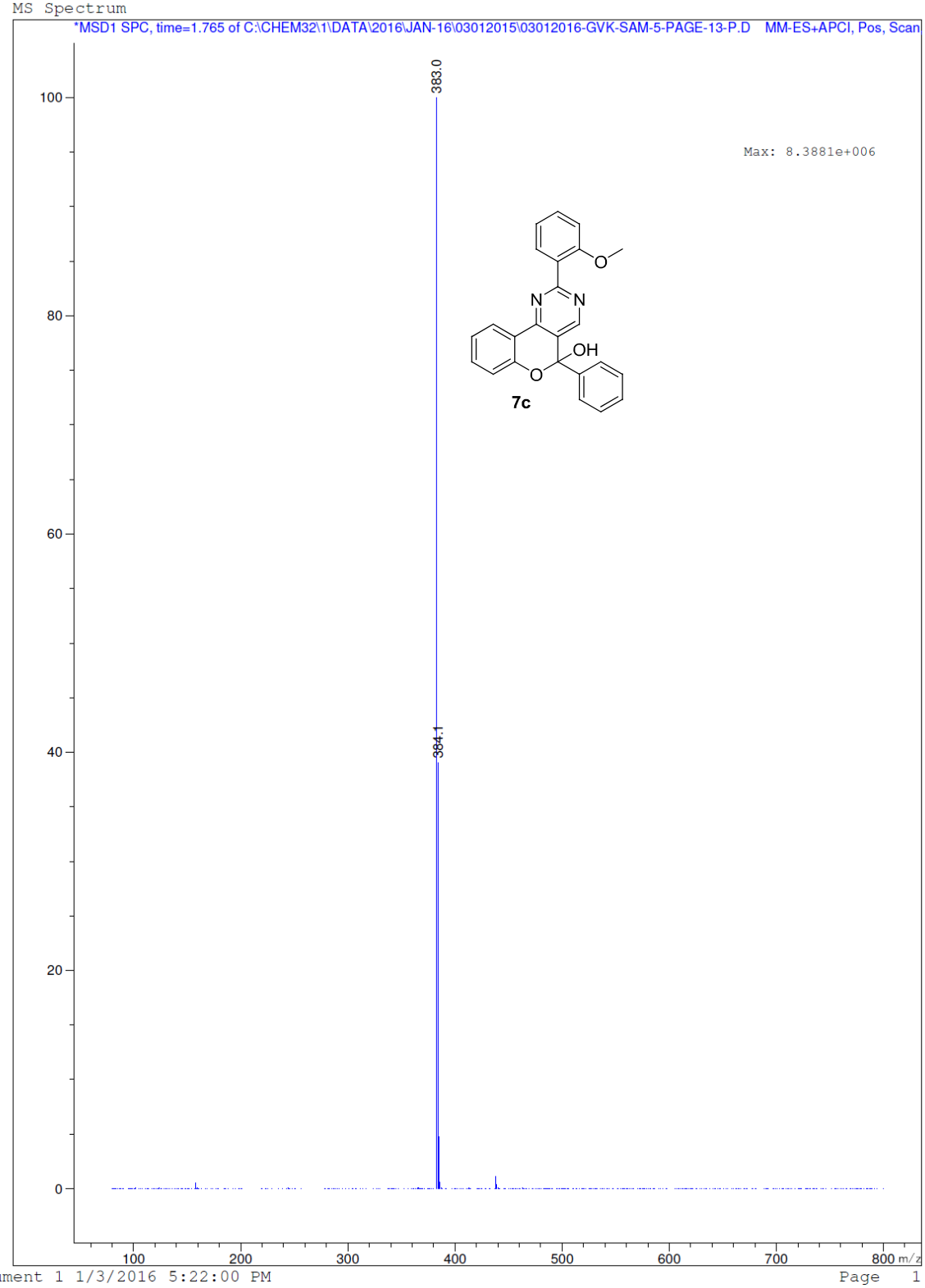
Sample Name :GVK-SAM-5-PAGE-13-P Vial position :P1-A-06
Date of Analysis:1/3/2016 4:37:03 PM Injection Vol :0.5 µL
Acq. Method :C:\CHEM32\1\METHODS\RND-FA- 3.0 MIN-1.M Instrument ID :ANL-MCL5-LCMS-001

RND-FA-3.0 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, 0.3/2, 2.3/98,2.8/98,2.81/2,3.0/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 60°C ->



Pea No	RT min	Area	Area %
1	0.47	16.177	0.702
2	1.75	2264.565	98.259
3	1.83	16.899	0.733
4	1.85	7.049	0.306

MS Spectrum



rument 1 1/3/2016 5:22:00 PM Page 1 o

Elemental Composition Report

Single Mass Analysis

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

Selected filters: None

Monoisotopic Mass, Even Electron Ions

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

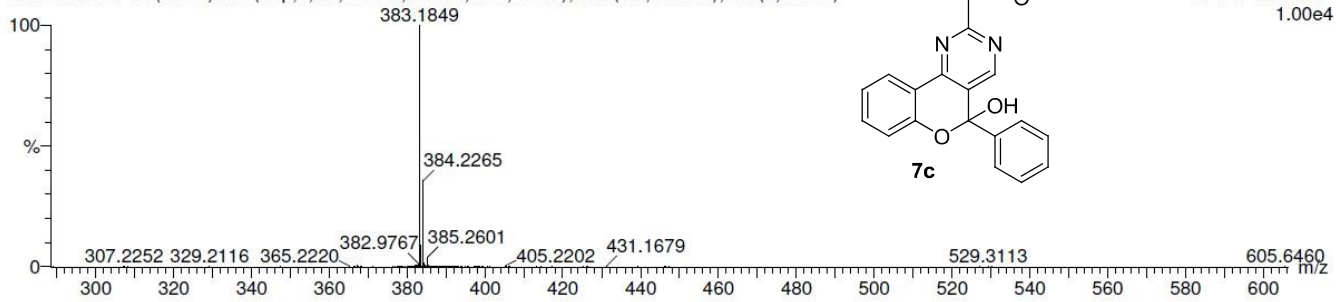
Elements Used:

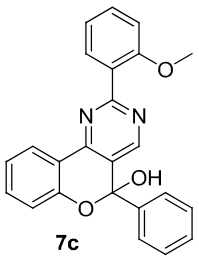
C: 0-24 H: 0-19 N: 0-2 O: 0-3

SAMPLE CODE:GVK-SAM-5-PAGE-13 POLAR

511701A2181 18 (0.258) AM (Top,4, Ar,5000.0,195.18,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

1: TOF MS ES+
1.00e4

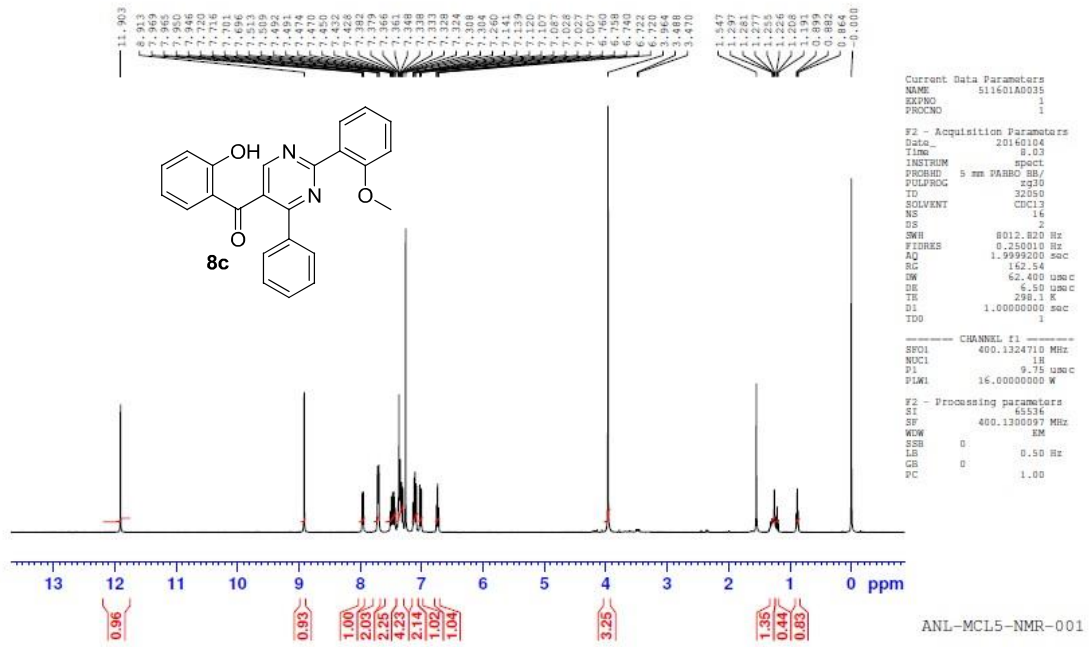




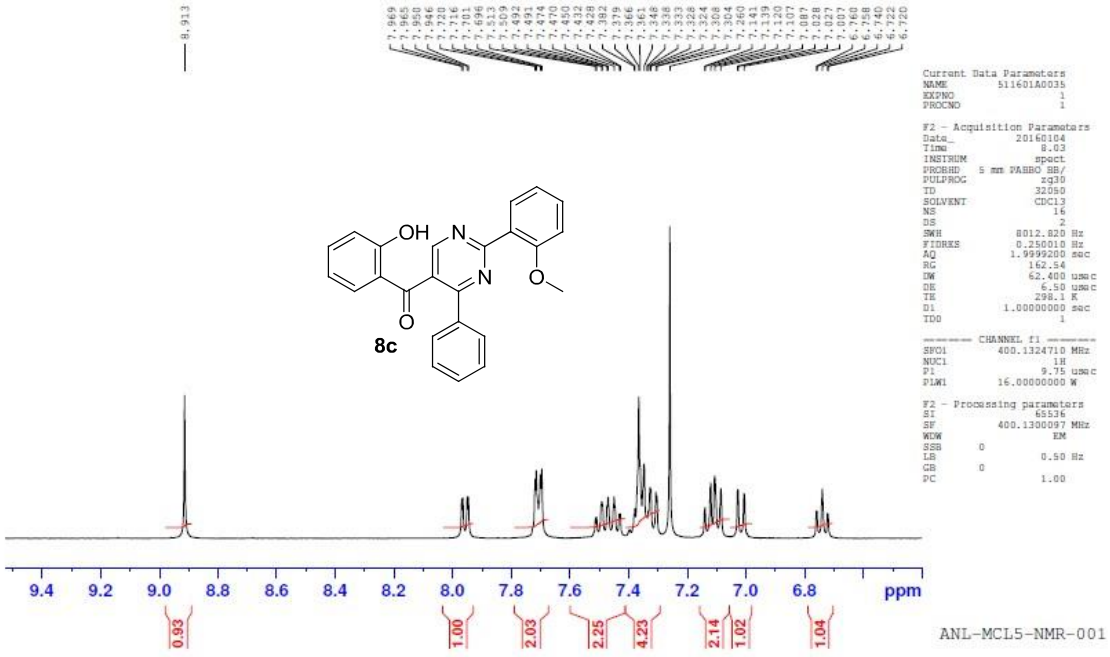
7c

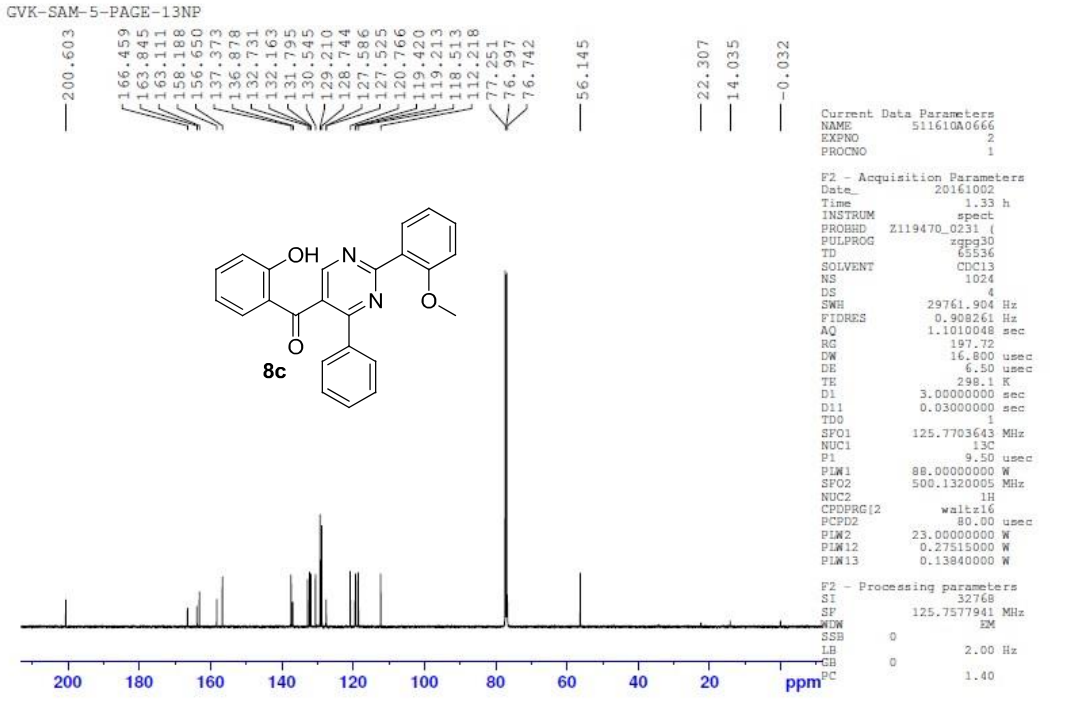
Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
383.1849	383.1396	45.3	118.2	16.5	1023.1	C24 H19 N2 O3

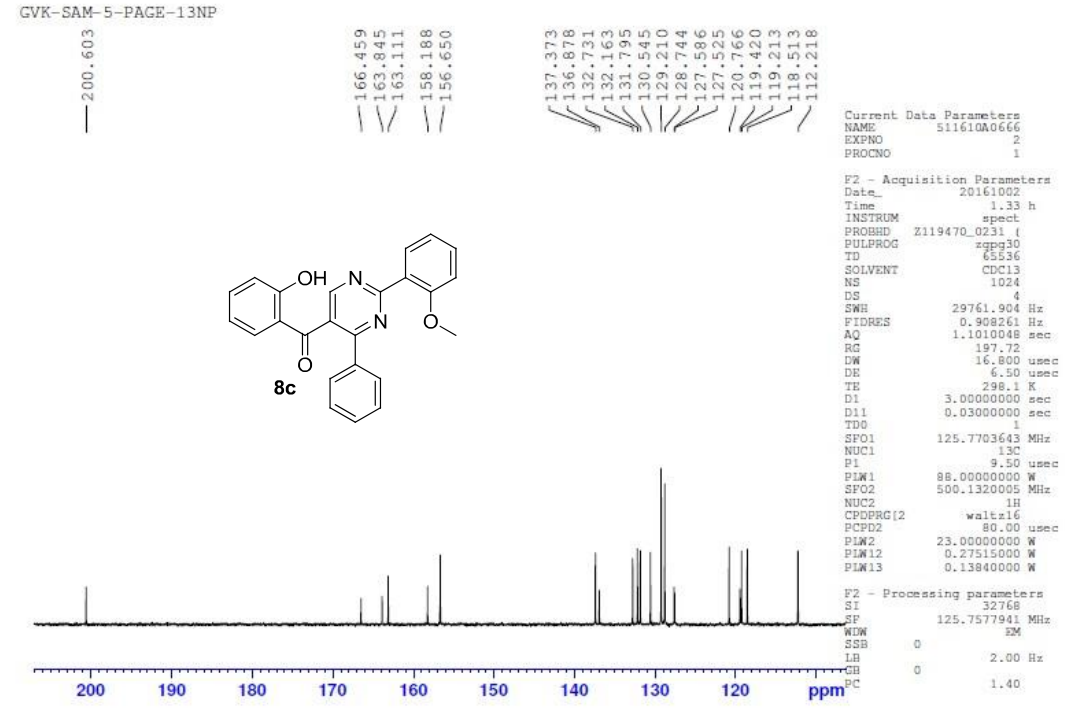
GVK-SAM-5-PAGE-13NP

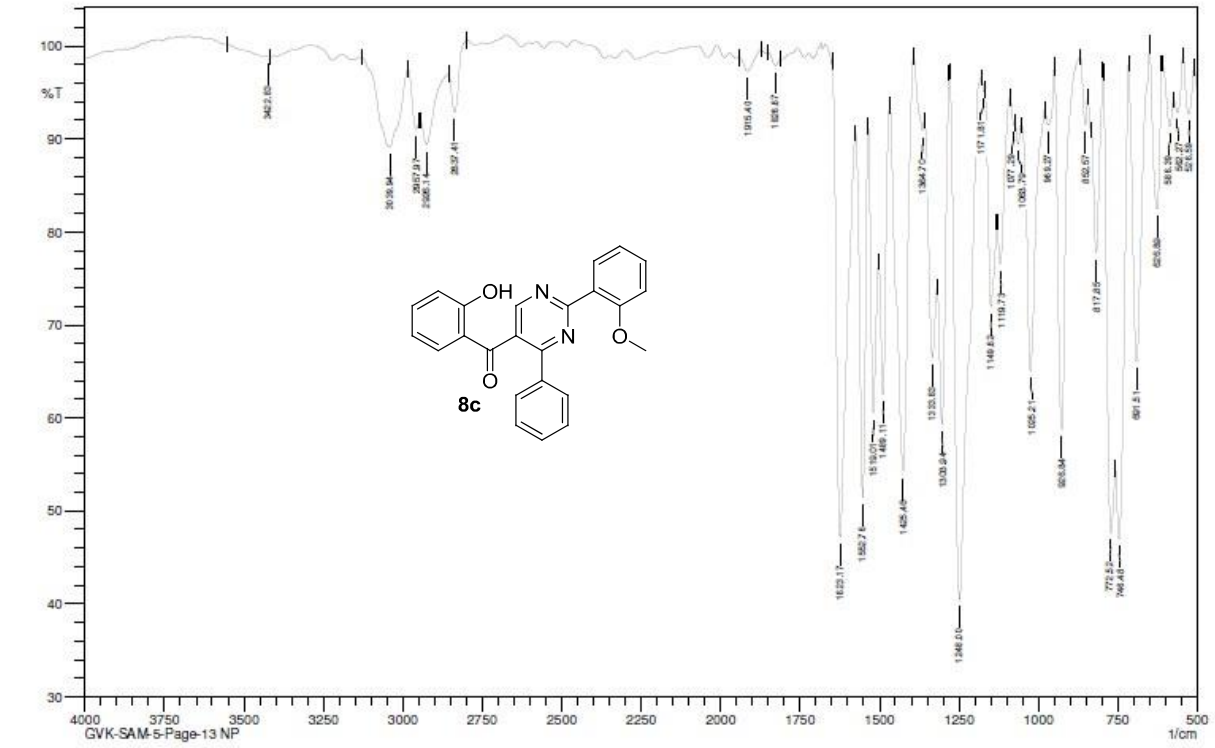


GVK-SAM-5-PAGE-13NP




GVK-SAM-5-PAGE-13NP
200.603
166.459
163.845
163.111
158.188
156.650
137.373
136.878
132.731
132.163
131.795
130.545
129.210
128.744
127.586
127.525
120.766
119.420
119.213
118.513
112.218
77.251
76.997
76.742
56.145
22.307
14.035
0.032
OH
N
N
O
O
8c
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME 511610A0666
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161002
Time 1.33 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 298.1 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7577941 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40


GVK-SAM-5-PAGE-13NP
200.603
166.459
163.845
163.111
158.188
156.650
137.373
136.878
132.731
132.163
131.795
130.545
129.210
128.744
127.586
127.525
120.766
119.420
119.213
118.513
112.218
OH
N
N
O
O
8c
200
190
180
170
160
150
140
130
120
ppm
Current Data Parameters
NAME 511610A0666
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161002
Time 1.33 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 298.1 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7577941 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40



Comment: IN Kbr
GVK-SAM-5-Page-13 NP

No. of Scans:
Resolution:
Apodization:

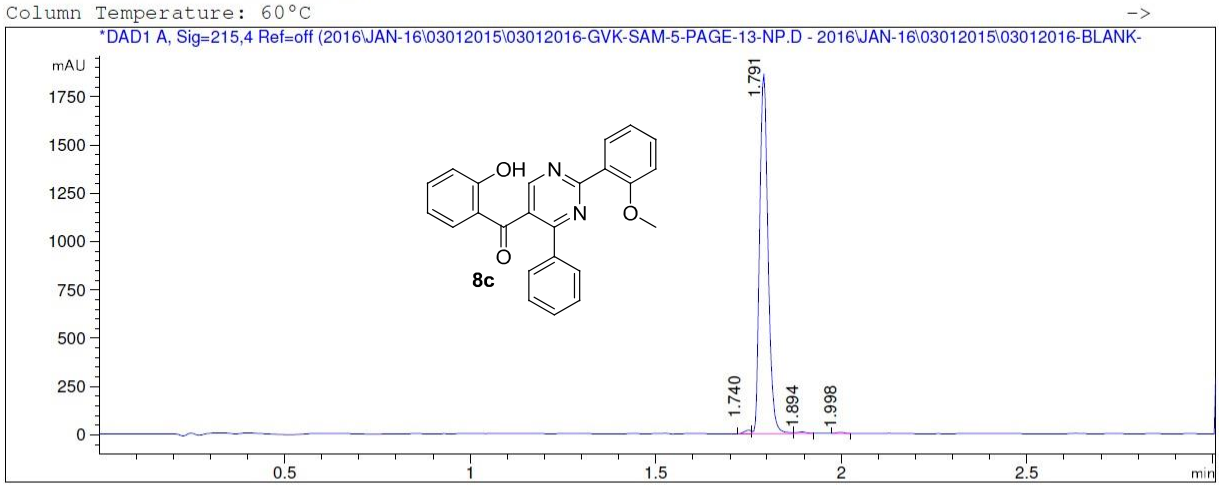
Date: 10/3/2016 10:51:14 AM
User: Admin

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

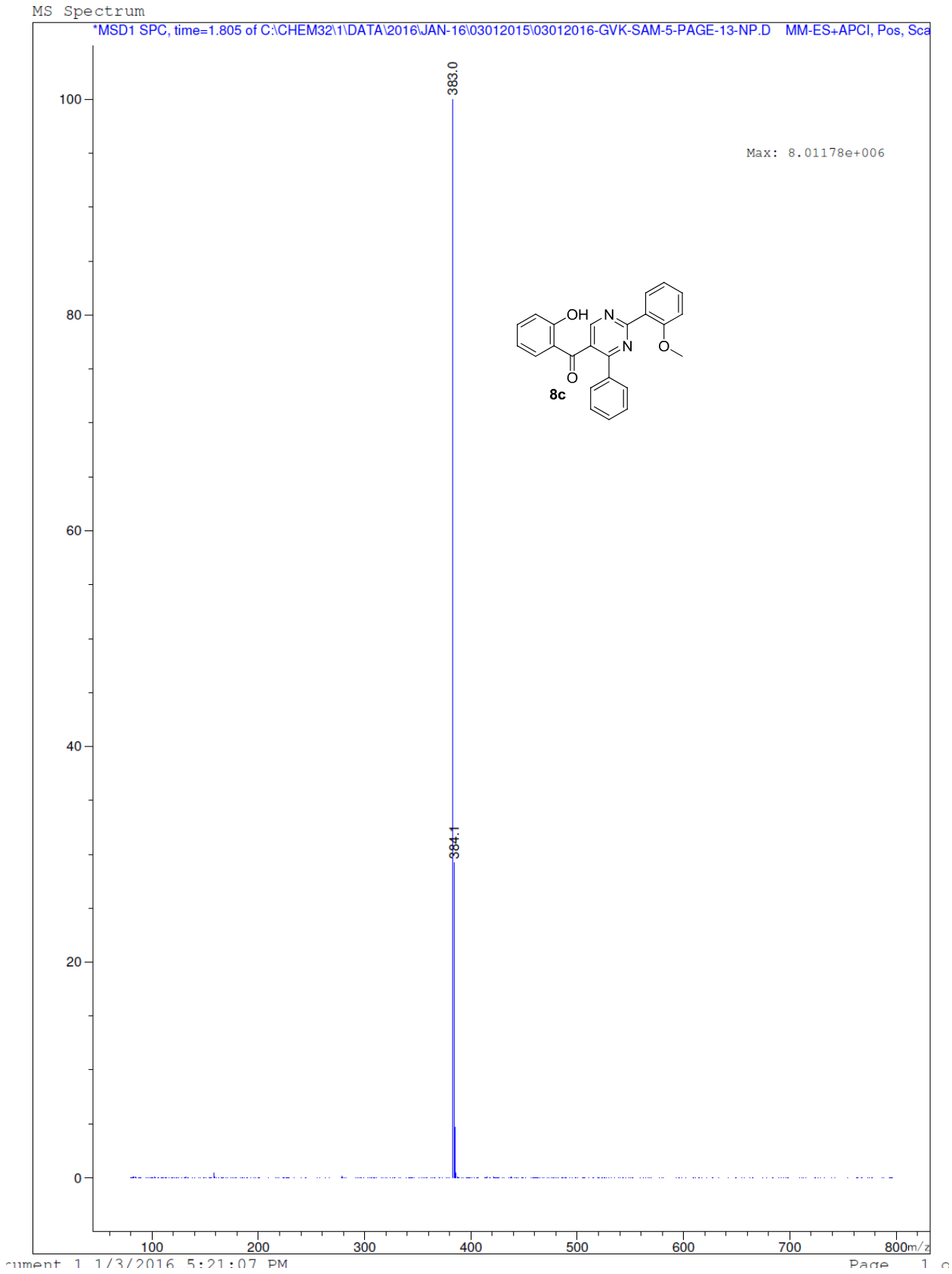
LCMS REPORT

Sample Name :GVK-SAM-5-PAGE-13-NP Vial position :P1-A-05
Date of Analysis:1/3/2016 4:33:04 PM Injection Vol :0.5 µL
Acq. Method :C:\CHEM32\1\METHODS\RND-FA- 3.0 MIN-1.M Instrument ID :ANL-MCL5-LCMS-001

RND-FA-3.0 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, 0.3/2, 2.3/98,2.8/98,2.81/2,3.0/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 60°C ->



Peak No	RT min	Area	Area %
1	1.74	25.287	0.851
2	1.79	2926.346	98.514
3	1.89	12.057	0.406
4	2.00	6.796	0.229


MS Spectrum
*MSD1 SPC, time=1.805 of C:\CHEM32\1\DATA\2016\JAN-16\03012015\03012016-GVK-SAM-5-PAGE-13-NP.D MM-ES+APCI, Pos, Sca
383.0
384.1
Max: 8.01178e+006
OH
N
N
O
O
8c
100
80
60
40
20
0
100
200
300
400
500
600
700
800m/z

Elemental Composition Report

Single Mass Analysis

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

Selected filters: None

Monoisotopic Mass, Even Electron Ions

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

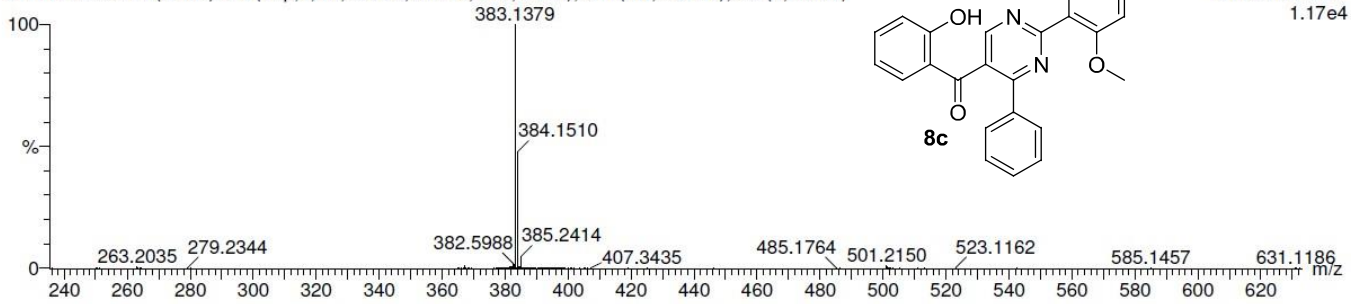
Elements Used:

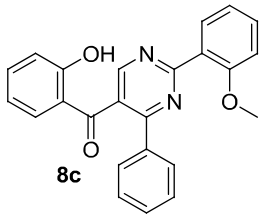
C: 0-24 H: 0-19 N: 0-2 O: 0-3

SAMPLE CODE:GVK-SAM-5-PAGE-13NP

511701A2190 34 (0.483) AM (Top,4, Ar,5000.0,195.18,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

1: TOF MS ES+
1.17e4

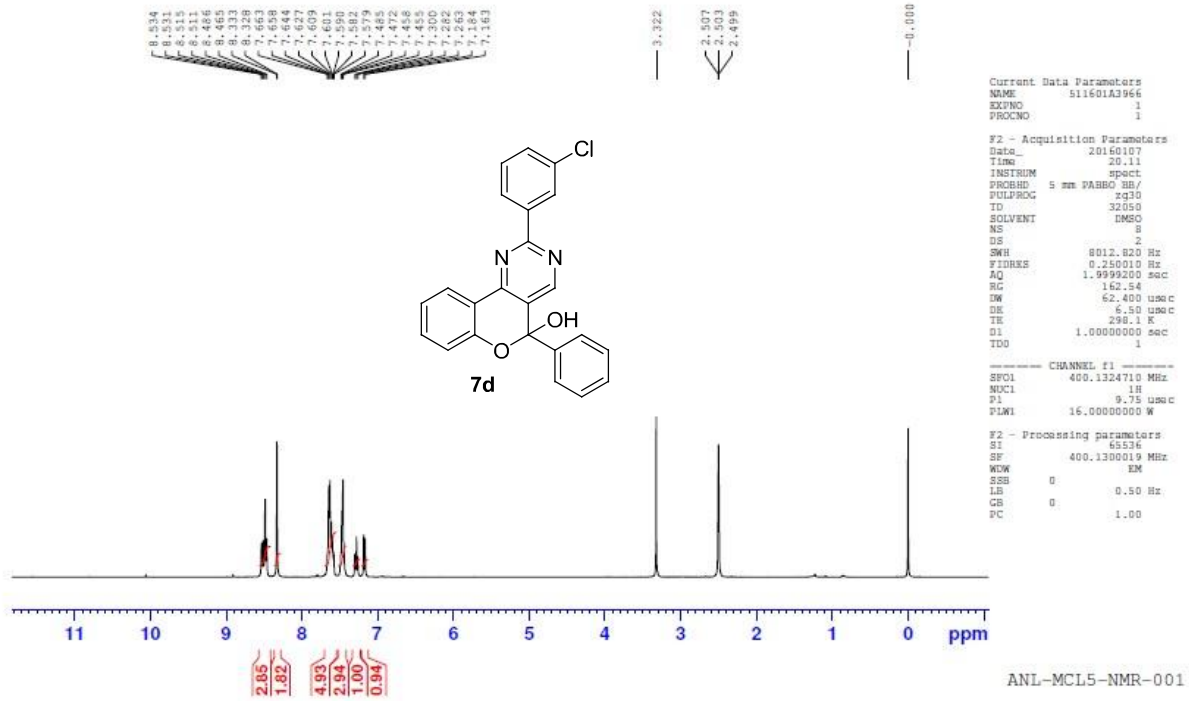




8c

Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
383.1379	383.1396	-1.7	-4.4	16.5	526.4	C24 H19 N2 O3

GVK-SAM-5-PAGE-14-POLAR-1



Current Data Parameters
NAME 511601A3966
EXPNO 1
PROCNO 1

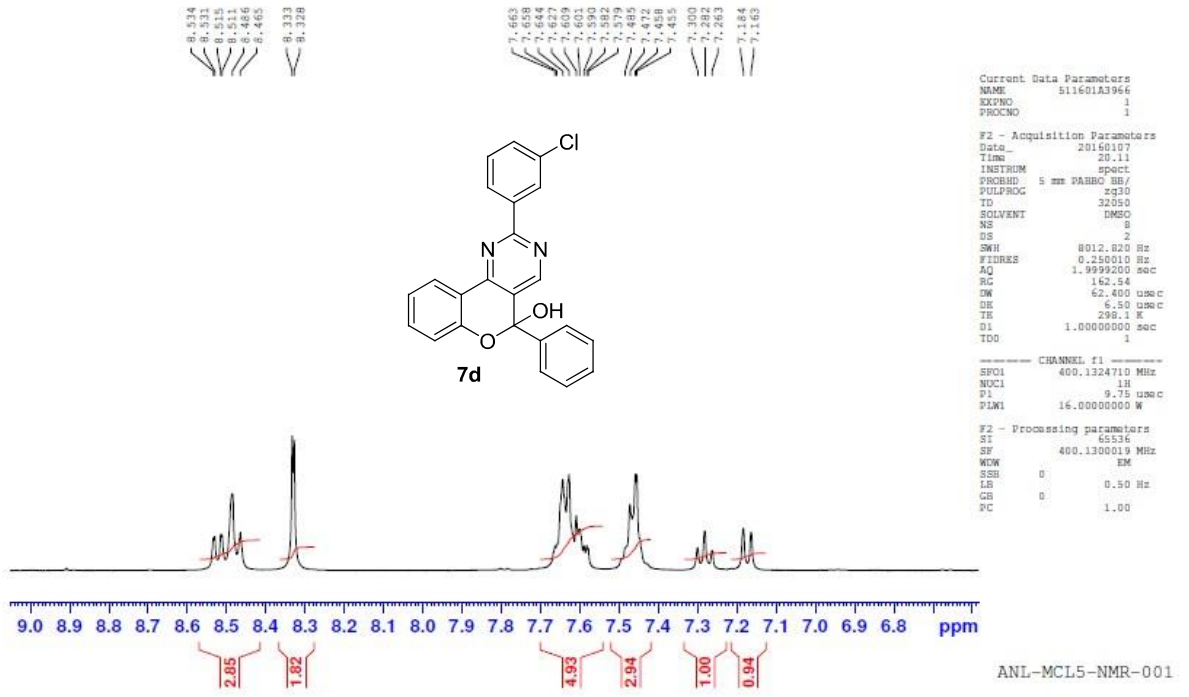
F2 - Acquisition Parameters
Date_ 20160107
Time 20.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32050
SOLVENT DMSO
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.250010 Hz
AQ 1.9999200 sec
RG 162.54
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 65536
SF 400.1300019 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00

ANL-MCL5-NMR-001

GVK-SAM-5-PAGE-14-POLAR-1



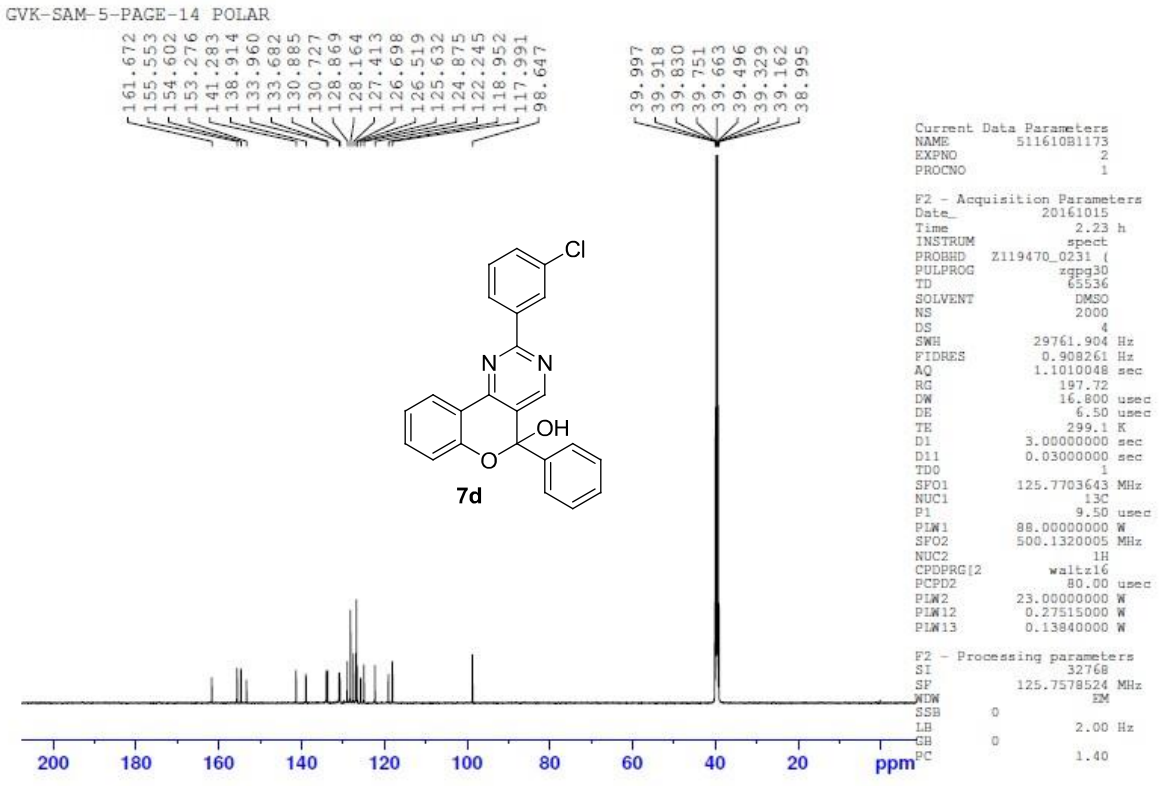
Current Data Parameters
NAME 511601A3966
EXPNO 1
PROCNO 1

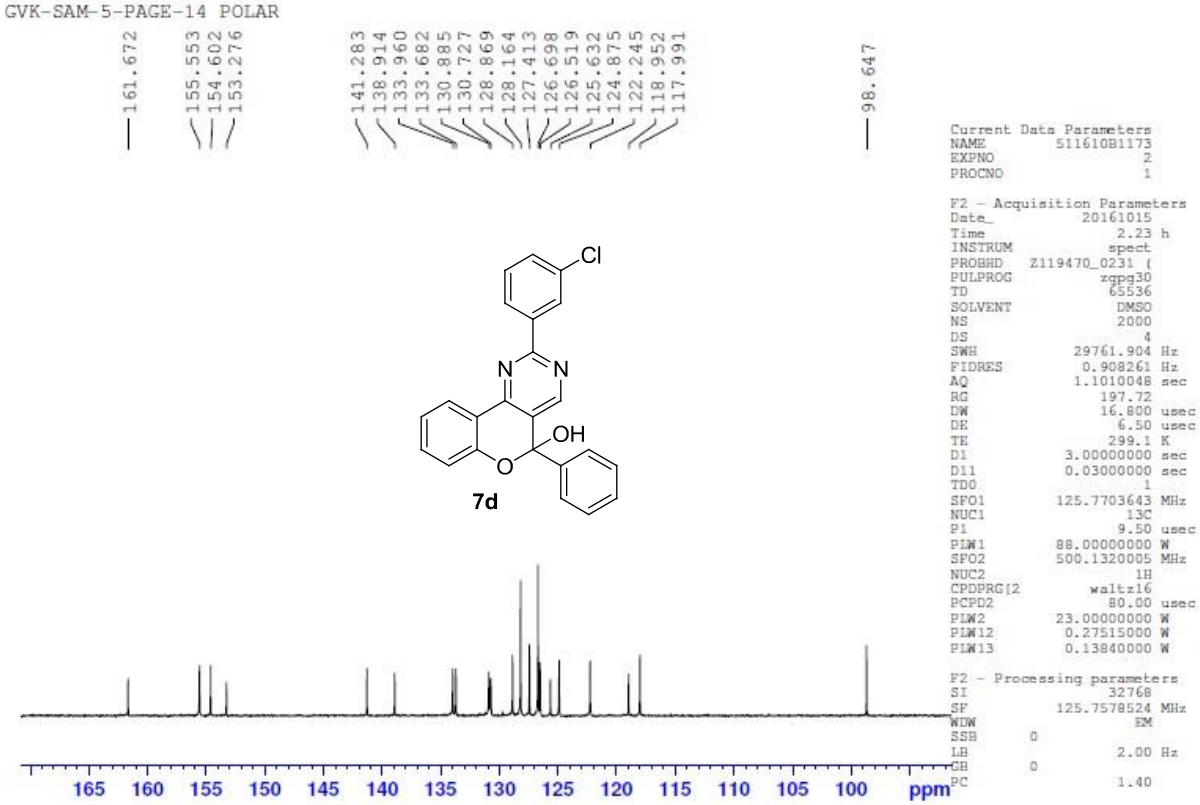
F2 - Acquisition Parameters
Date_ 20160107
Time 20.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32050
SOLVENT DMSO
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.250010 Hz
AQ 1.9999200 sec
RG 162.54
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

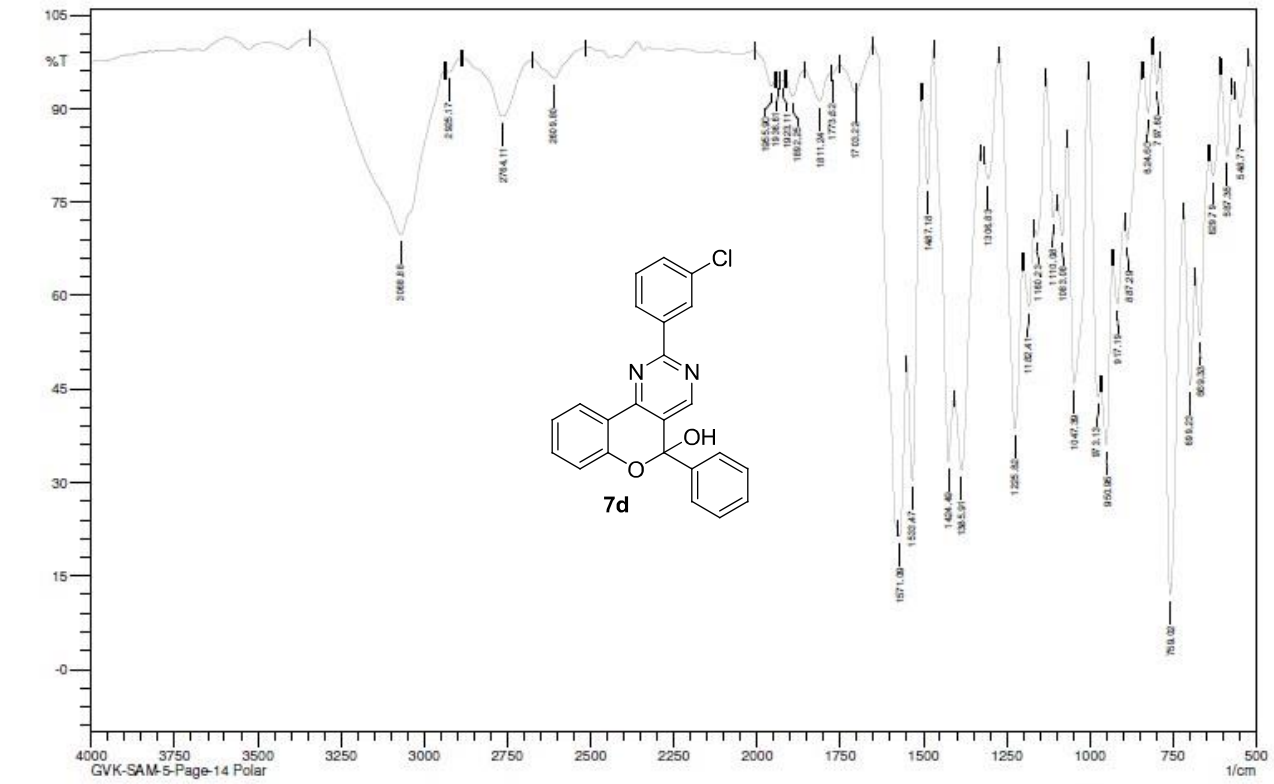
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 9.75 usec
PLW1 16.00000000 W

F2 - Processing parameters
SI 65536
SF 400.1300019 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00

ANL-MCL5-NMR-001


GVK-SAM-5-PAGE-14 POLAR
161.672
155.553
154.602
153.276
141.283
138.914
133.960
133.682
130.885
130.727
128.869
128.164
127.413
126.698
126.519
125.632
124.875
122.245
118.952
117.991
98.647
39.997
39.918
39.830
39.751
39.663
39.496
39.329
39.162
38.995
Cl
N
N
OH
O
7d
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME 511610B1173
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161015
Time 2.23 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2000
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 299.1 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7578524 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40


GVK-SAM-5-PAGE-14 POLAR
161.672
155.553
154.602
153.276
141.283
138.914
133.960
133.682
130.885
130.727
128.869
128.164
127.413
126.698
126.519
125.632
124.875
122.245
118.952
117.991
98.647
Cl
N
N
OH
O
7d
165
160
155
150
145
140
135
130
125
120
115
110
105
100
ppm
Current Data Parameters
NAME 511610B1173
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161015
Time 2.23 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2000
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 299.1 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7578524 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40



Comment: IN Kbr
GVK-SAM-5-Page-14 Polar

No. of Scans:
Resolution:
Apodization:

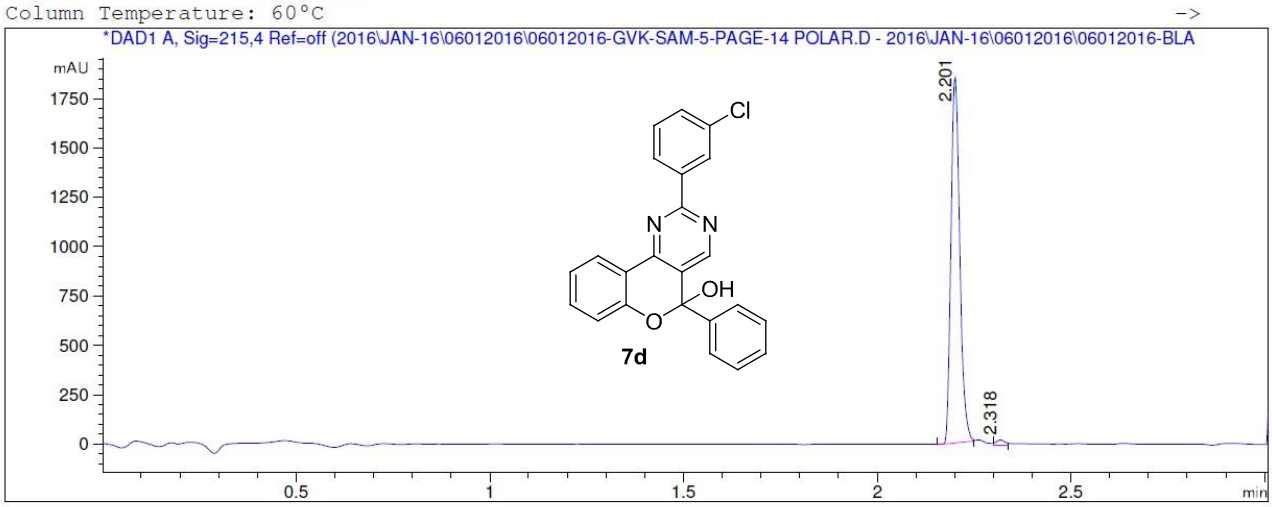
Date: 10/3/2016 11:17:13 AM
User: Admin

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

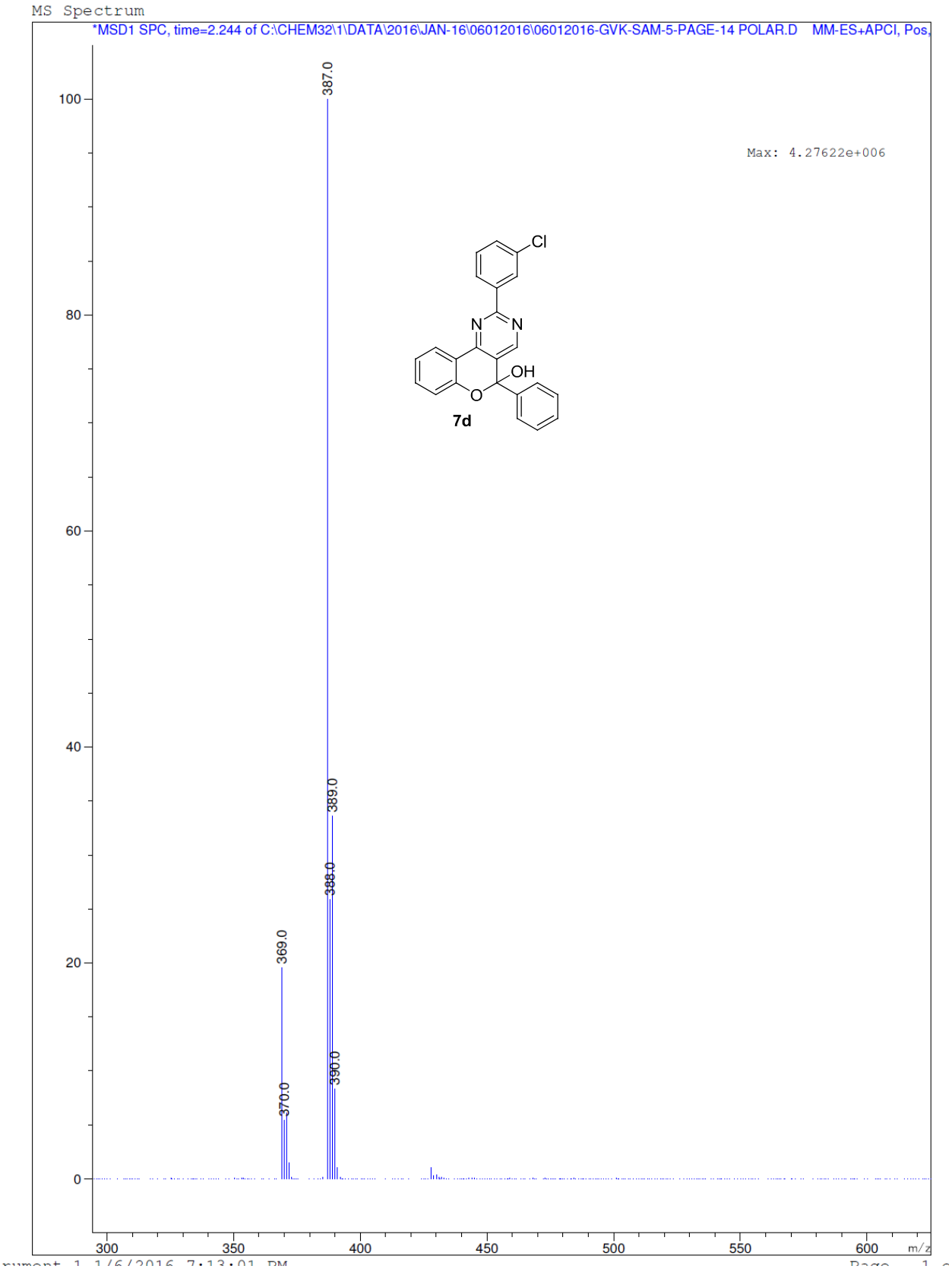
LCMS REPORT

Sample Name :GVK-SAM-5-PAGE-14 POLAR Vial position :P1-B-08
Date of Analysis:1/6/2016 7:08:06 PM Injection Vol :0.500µl
Acq. Method :C:\CHEM32\1\METHODS\RND-FA- 3.0 MIN-1.M Instrument ID :ANL-MCL5-LCMS-001

RND-FA-3.0 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, 0.3/2, 2.3/98,2.8/98,2.81/2,3.0/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 60°C ->



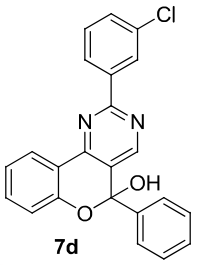
Pea No	RT min	Area	Area %
1	2.20	2935.549	98.782
2	2.32	36.196	1.218


MS Spectrum
*MSD1 SPC, time=2.244 of C:\CHEM32\1\DATA\2016\JAN-16\06012016\06012016-GVK-SAM-5-PAGE-14 POLAR.D MM-ES+APCI, Pos,
Max: 4.27622e+006
387.0
389.0
388.0
369.0
390.0
370.0
Cl
N
N
OH
O
7d
100
80
60
40
20
0
300
350
400
450
500
550
600
m/z

Elemental Composition Report **Page 1**

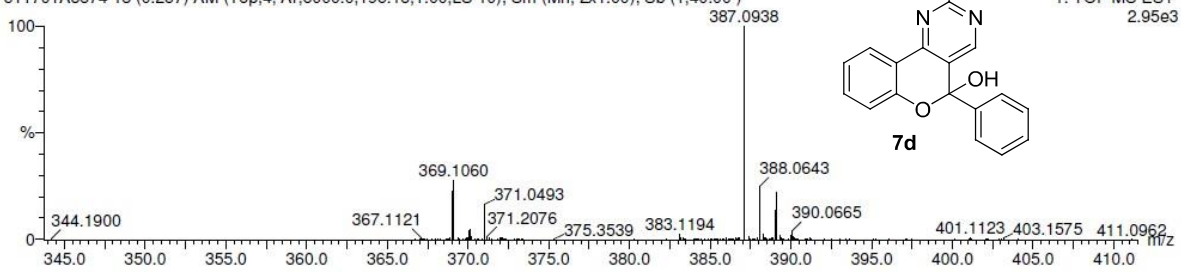
Single Mass Analysis
Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-23 H: 0-16 N: 0-2 O: 0-2 Cl: 0-1
SAMPLE CODE:GVK-SAM-5-PAGE-14 POLAR
511701A3374 18 (0.257) AM (Top,4, Ar,5000.0,195.13,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)



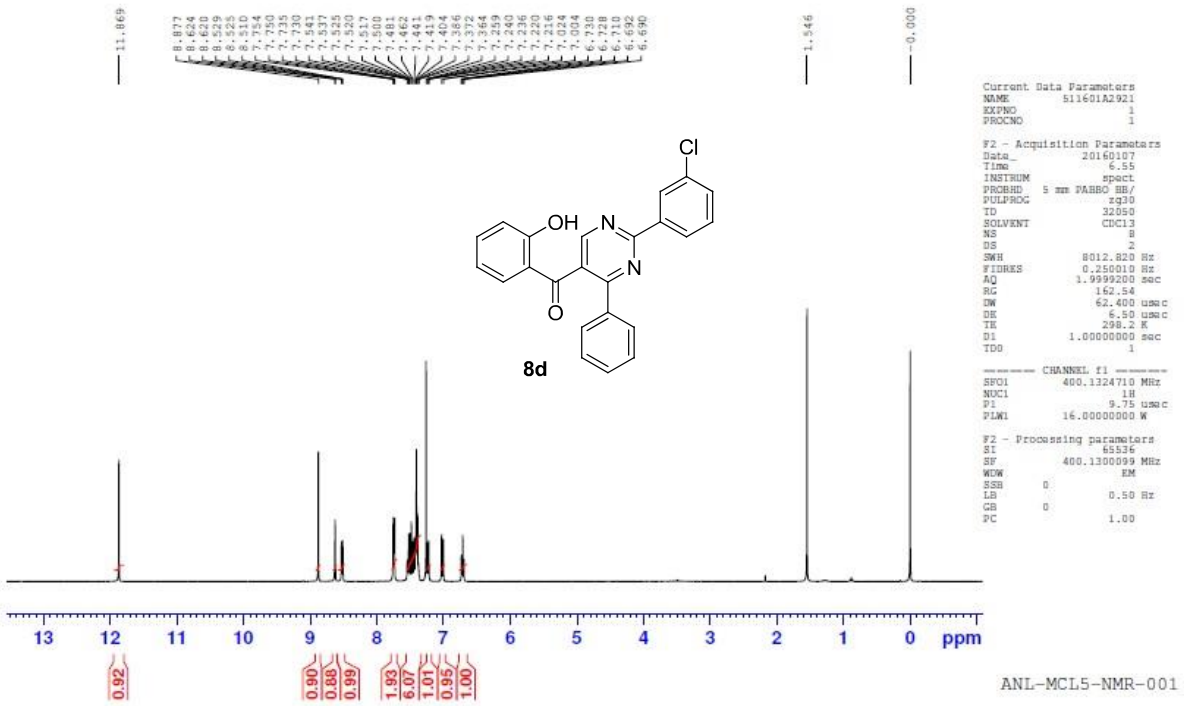
7d

1: TOF MS ES+
2.95e3



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
387.0938	387.0900	3.8	9.8	16.5	111.8	C23 H16 N2 O2 Cl

GVK-SAM-5-PAGE-14

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Current Data Parameters
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EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Data_           20160107
Time                6.55
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32050
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             8012.820 Hz
FIDRES          0.250010 Hz
AQ              1.9999200 sec
RG                162.54
DW                62.400 usec
DE                 6.50 usec
TE                298.2 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            400.1300099 MHz
WDW                   EM
SSB       0
LB                 0.50 Hz
GB        0
PC                 1.00
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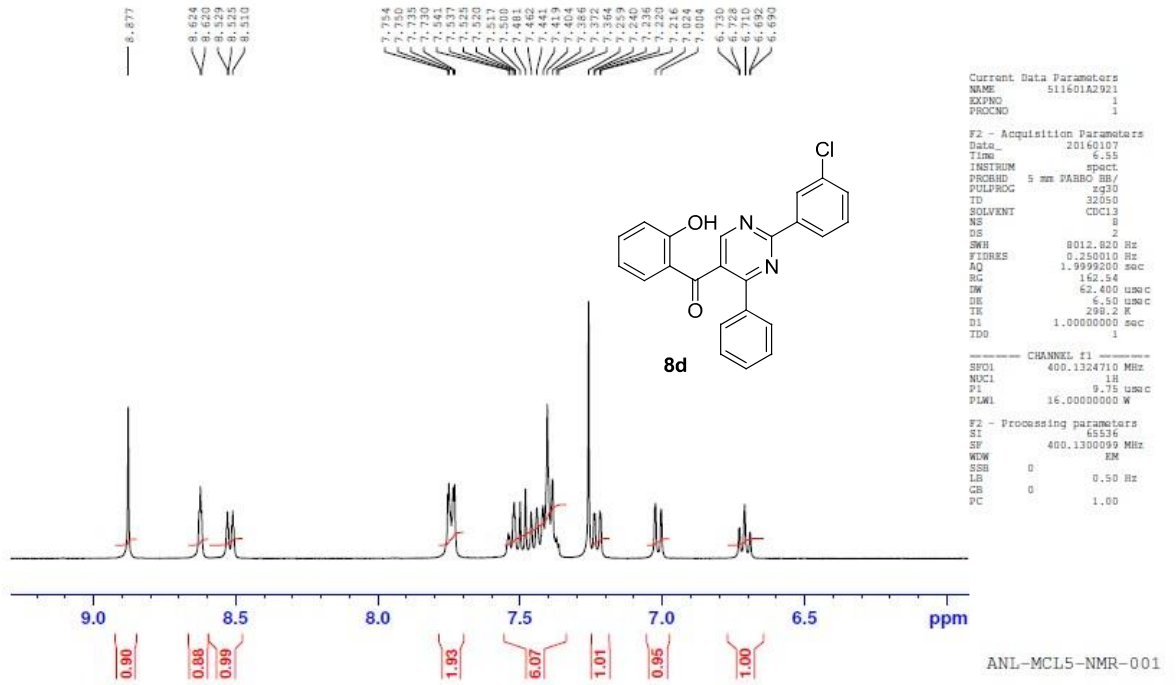
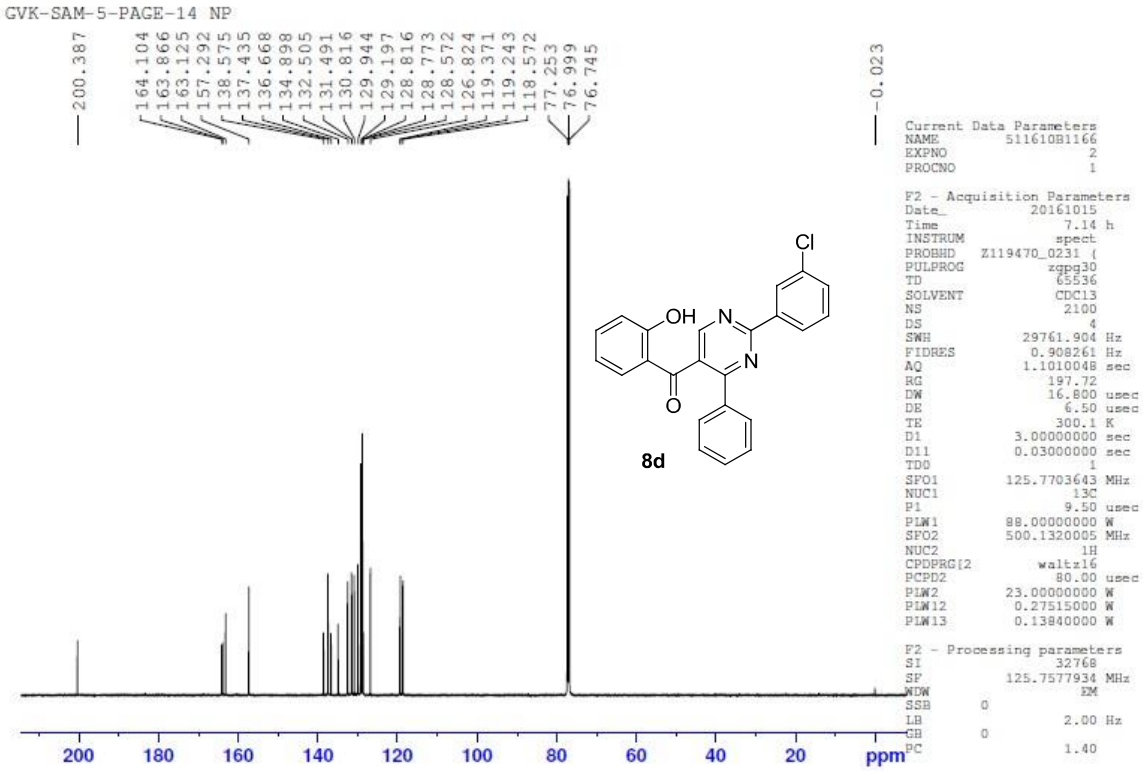
ANL-MCL5-NMR-001

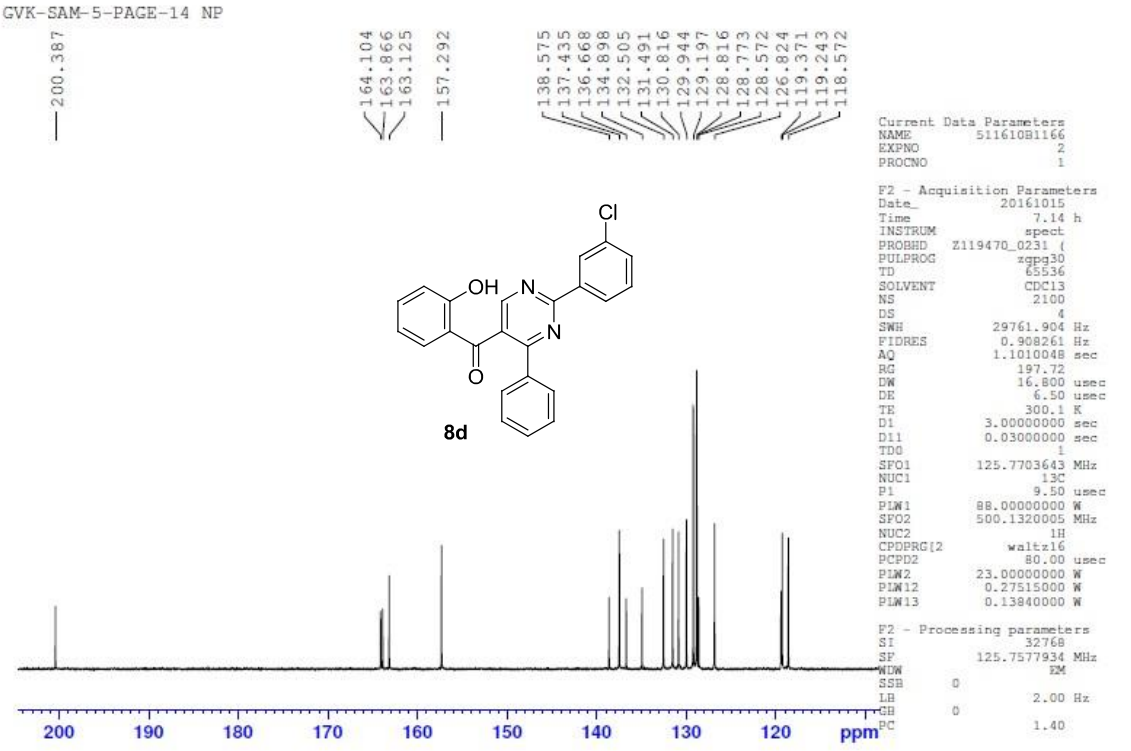
GVK-SAM-5-PAGE-14

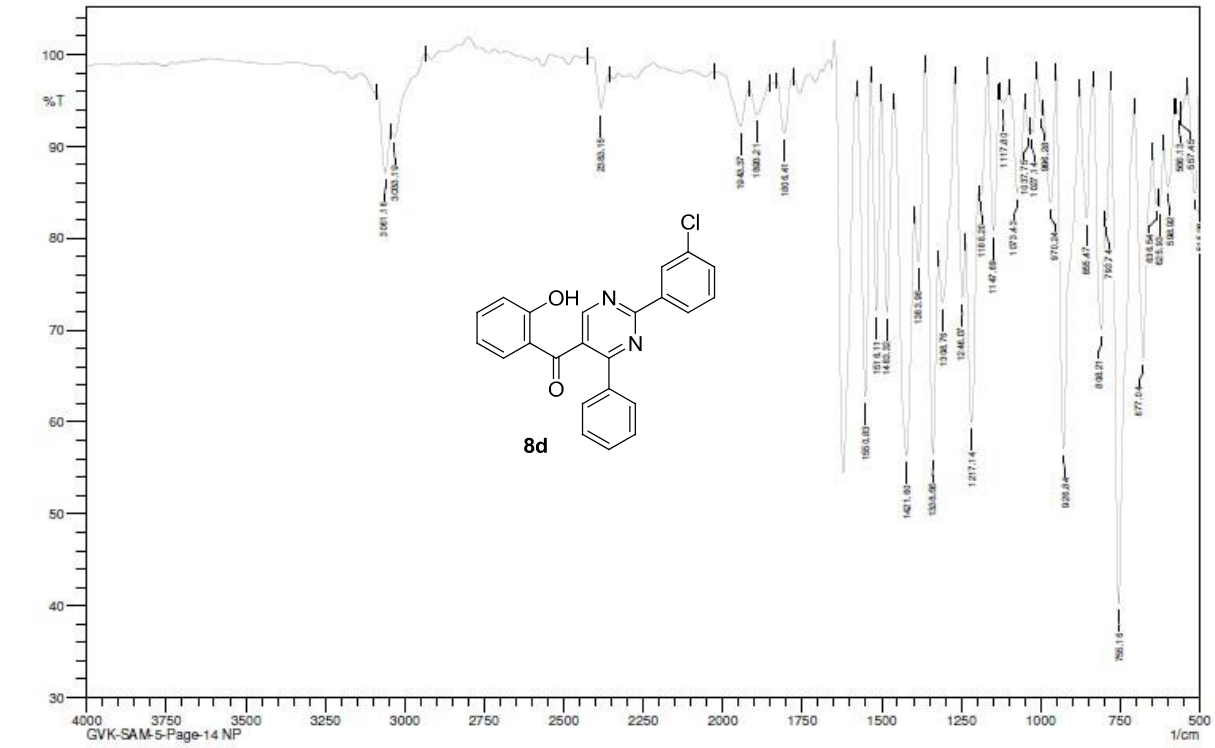



```
Current Data Parameters
NAME          511601A2921
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Data_           20160107
Time                6.55
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 32050
SOLVENT            CDCl3
NS                     8
DS                     2
SWH             8012.820 Hz
FIDRES          0.250010 Hz
AQ              1.9999200 sec
RG                162.54
DW                62.400 usec
DE                 6.50 usec
TE                298.2 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            400.1300099 MHz
WDW                   EM
SSB       0
LB                 0.50 Hz
GB        0
PC                 1.00
```

ANL-MCL5-NMR-001


GVK-SAM-5-PAGE-14 NP
200.387
164.104
163.866
163.125
157.292
138.575
137.435
136.668
134.898
132.505
131.491
130.816
129.944
129.197
128.816
128.773
128.572
126.824
119.371
119.243
118.572
77.253
76.999
76.745
0.023
Cl
OH
N
N
O
8d
Current Data Parameters
NAME 511610B1166
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161015
Time 7.14 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2100
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 300.1 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7577934 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


GVK-SAM-5-PAGE-14 NP
200.387
164.104
163.866
163.125
157.292
138.575
137.435
136.668
134.898
132.505
131.491
130.816
129.944
129.197
128.816
128.773
128.572
126.824
119.371
119.243
118.572
Cl
OH
N
N
O
8d
Current Data Parameters
NAME 511610B1166
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161015
Time 7.14 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2100
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 300.1 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7577934 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
200
190
180
170
160
150
140
130
120
ppm



Comment: IN Kbr
GVK-SAM-5-Page-14 NP

No. of Scans:
Resolution:
Apodization:

Date: 10/3/2016 11:26:47 AM
User: Admin

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

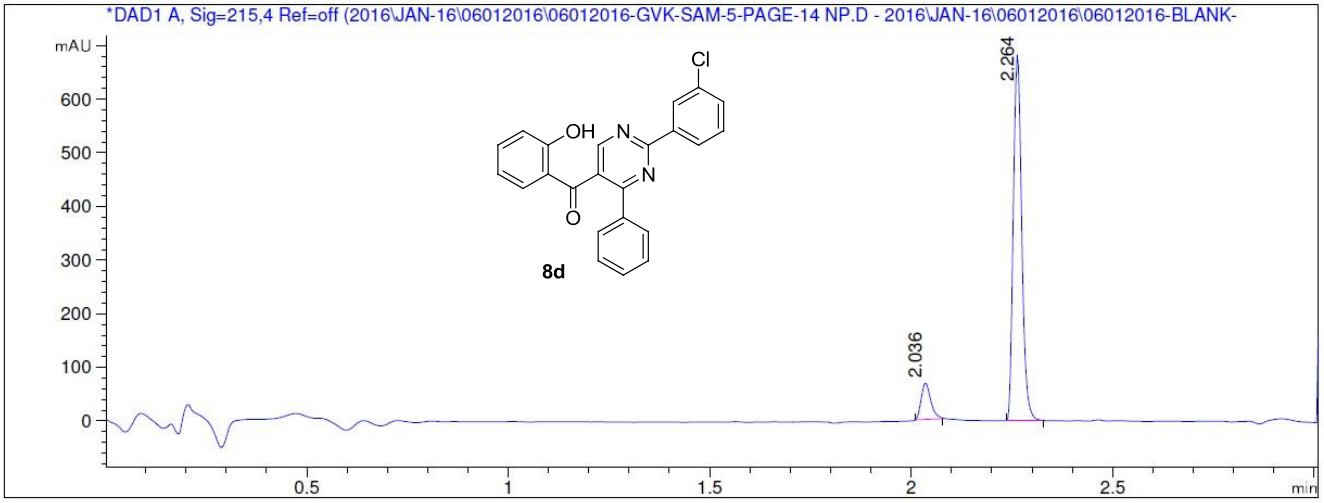
LCMS REPORT

==========

Sample Name :GVK-SAM-5-PAGE-14 NP Vial position :P1-C-01
Date of Analysis:1/6/2016 7:15:59 PM Injection Vol :0.300µl
Acq. Method :C:\CHEM32\1\METHODS\RND-FA- 3.0 MIN-1.M Instrument ID :ANL-MCL5-LCMS-001

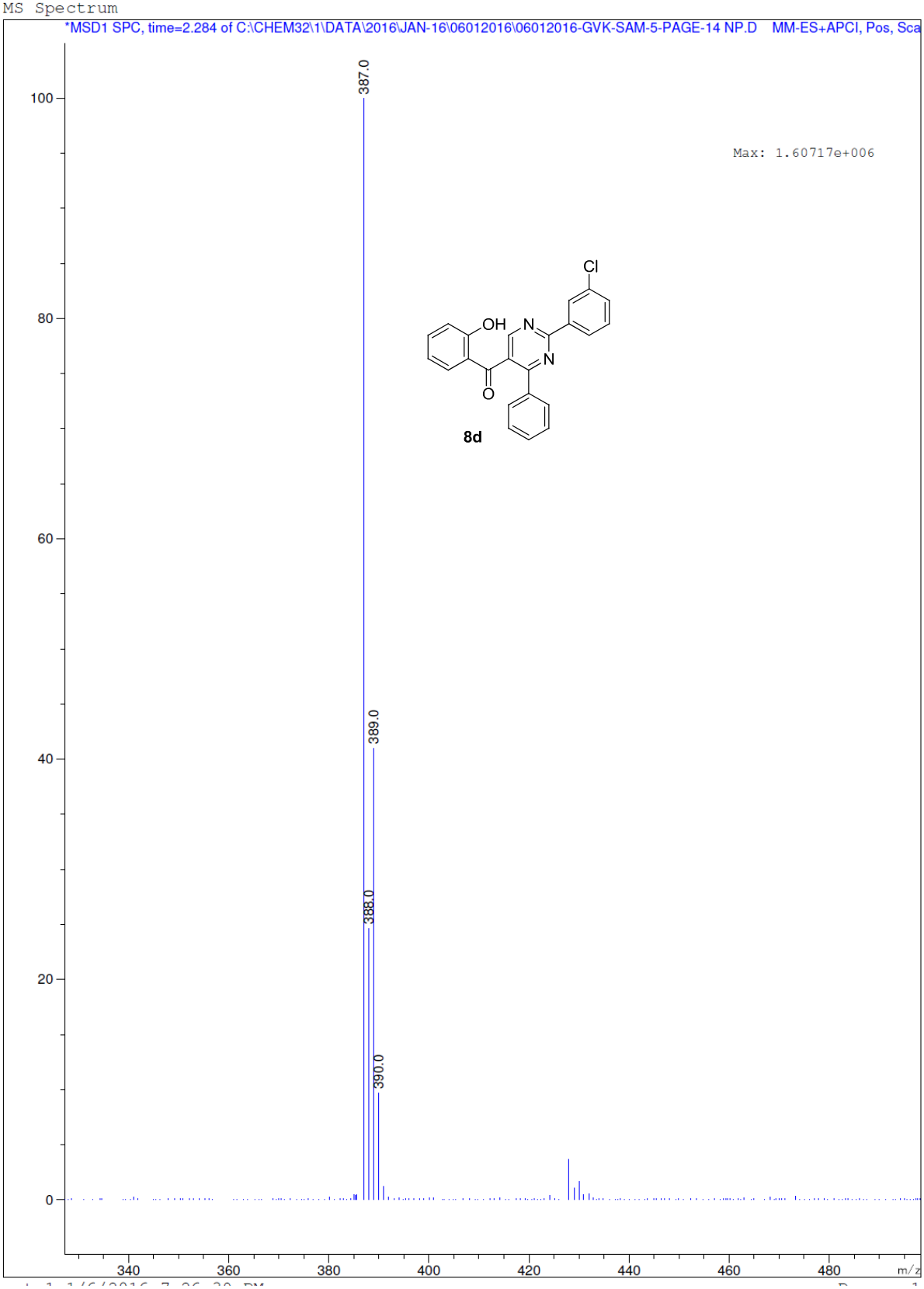
==========

RND-FA-3.0 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, 0.3/2, 2.3/98,2.8/98,2.81/2,3.0/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 60°C ->



Pea No	RT min	Area	Area %
1	2.04	112.299	10.138
2	2.26	995.449	89.862

MS Spectrum

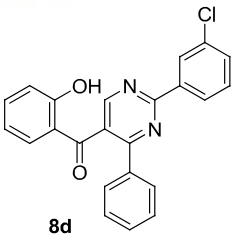

*MSD1 SPC, time=2.284 of C:\CHEM32\1\DATA\2016\JAN-16\06012016\06012016-GVK-SAM-5-PAGE-14 NP.D MM-ES+APCI, Pos, Sca
Max: 1.60717e+006
387.0
389.0
388.0
390.0
Cl
OH
N
N
O
8d
100
80
60
40
20
0
340
360
380
400
420
440
460
480
m/z

Single Mass Analysis

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

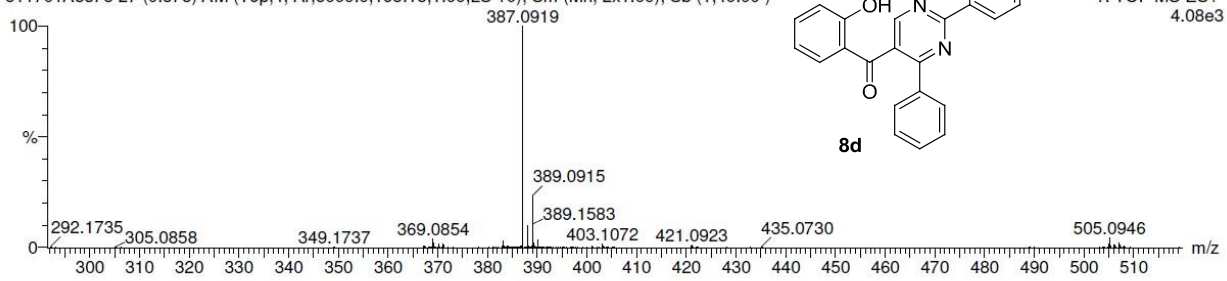
Monoisotopic Mass, Even Electron Ions
12 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-23 H: 0-16 N: 0-2 O: 0-2 Cl: 0-1

SAMPLE CODE:GVK-SAM-5-PAGE-14NP
511701A3375 27 (0.378) AM (Top,4, Ar,5000.0,195.15,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)



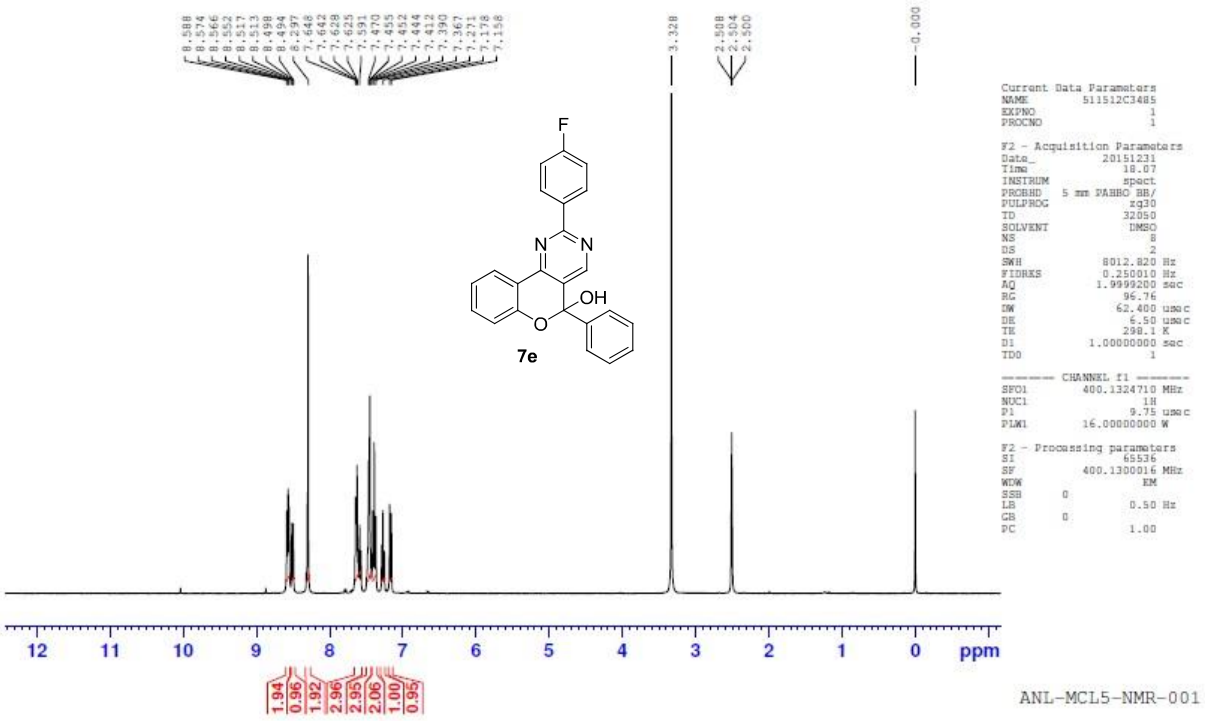
8d

1: TOF MS ES+
4.08e3



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
387.0919	387.0900	1.9	4.9	16.5	356.8	C23 H16 N2 O2 Cl

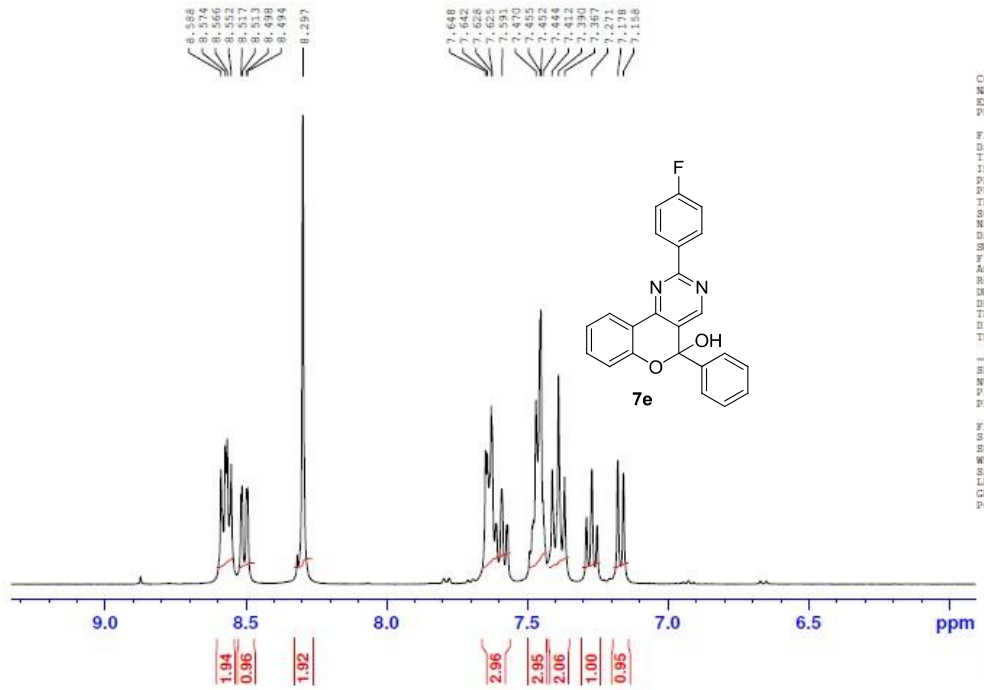
GVK-SAM-5-PAGE-15POLAR




```
Current Data Parameters
NAME          511512C3485
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_              20151231
Time                 18.07
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  32050
SOLVENT              DMSO
NS                      8
DS                      2
SWH               8012.820 Hz
FIDRES            0.250010 Hz
AQ                1.9999200 sec
RG                   96.76
DW                  62.400 usec
DE                   6.50 usec
TE                  298.1 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              400.1300016 MHz
WDW                     EM
SSB                     0
LB                   0.50 Hz
GB                      0
PC                   1.00
```

ANL-MCL5-NMR-001

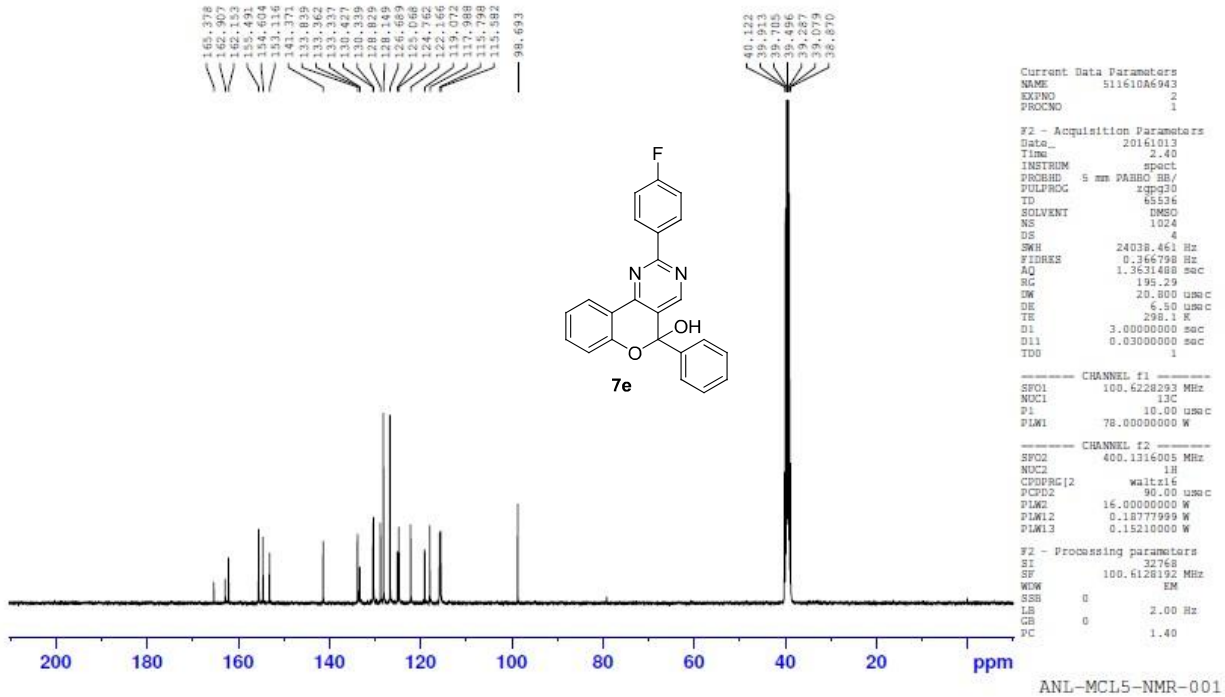
GVK-SAM-5-PAGE-15POLAR




```
Current Data Parameters
NAME          511512C3485
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_              20151231
Time                 18.07
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  32050
SOLVENT              DMSO
NS                      8
DS                      2
SWH               8012.820 Hz
FIDRES            0.250010 Hz
AQ                1.9999200 sec
RG                   96.76
DW                  62.400 usec
DE                   6.50 usec
TE                  298.1 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              400.1300016 MHz
WDW                     EM
SSB                     0
LB                   0.50 Hz
GB                      0
PC                   1.00
```

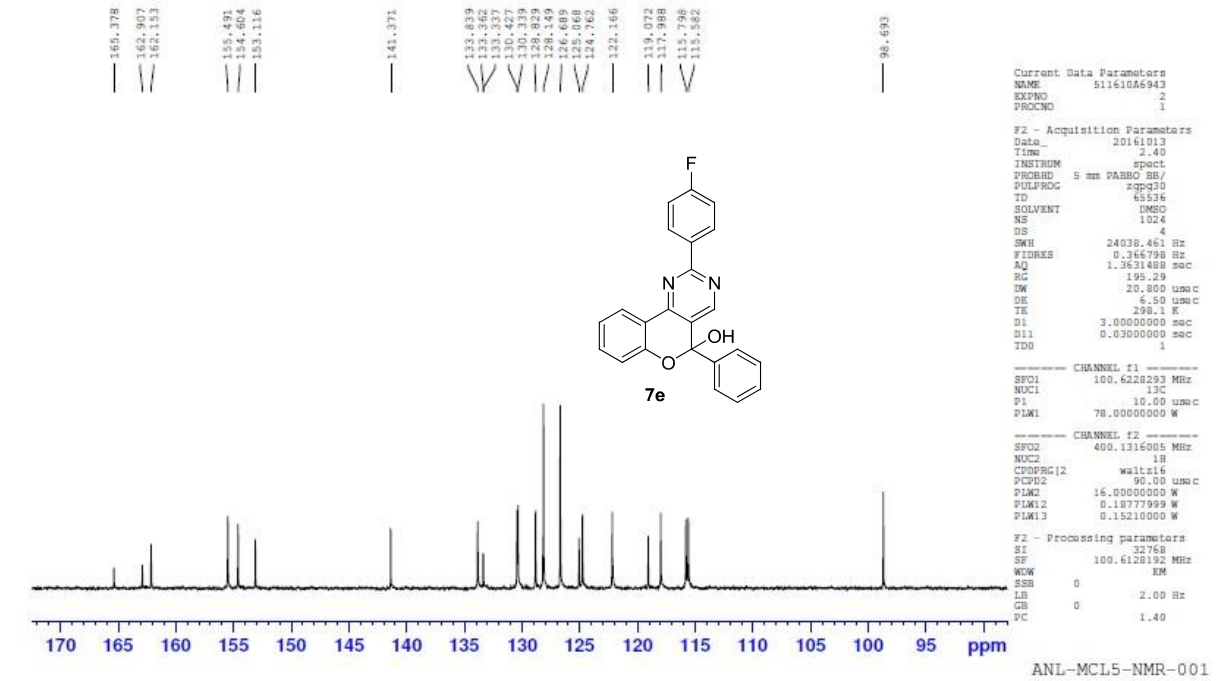
ANL-MCL5-NMR-001

GVK-SAM-5-PAGE-15 POLAR

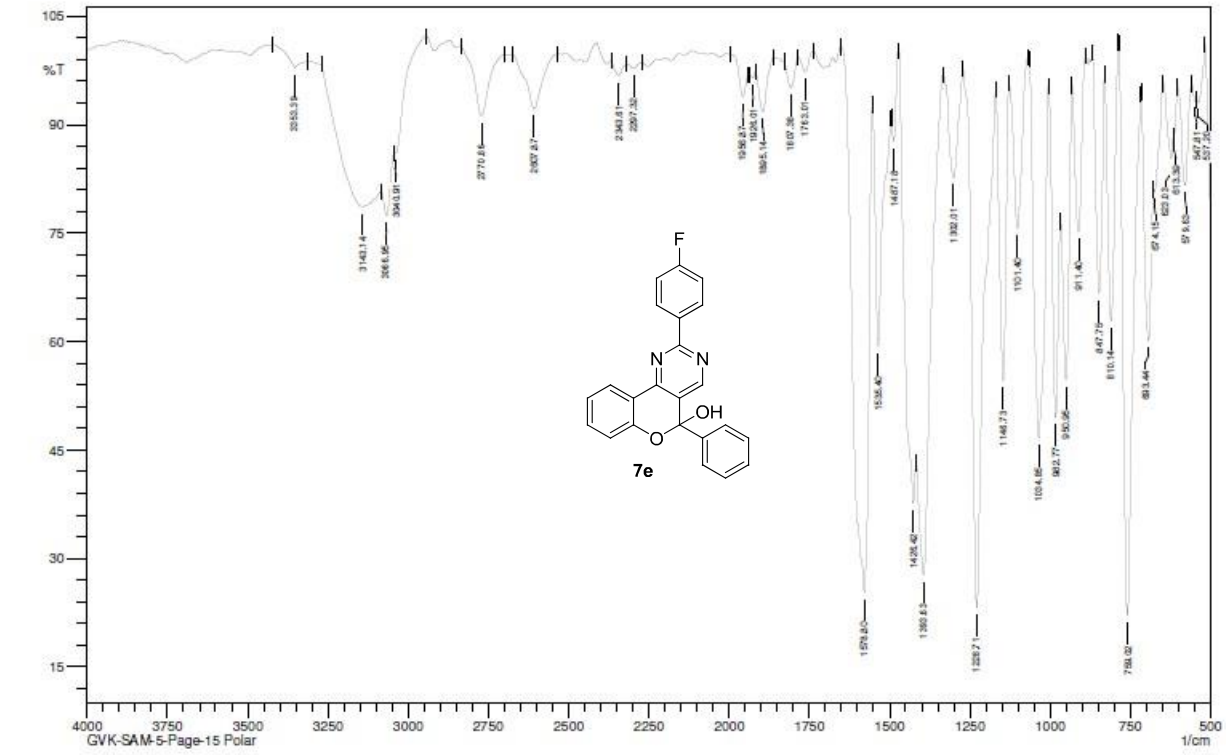


ANL-MCL5-NMR-001

GVK-SAM-5-PAGE-15 POLAR



ANL-MCL5-NMR-001



Comment: IN Kbr
GVK-SAM-5-Page-15 Polar

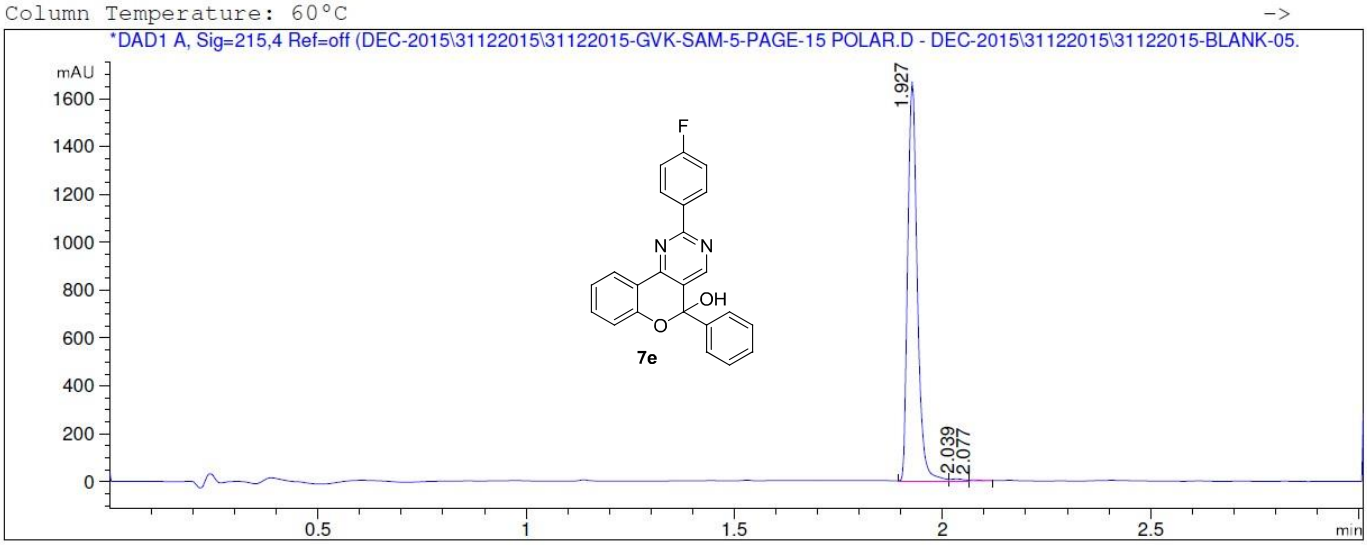
No. of Scans:
Resolution:
Apodization:

Date: 10/3/2016 11:14:50 AM
User: Admin

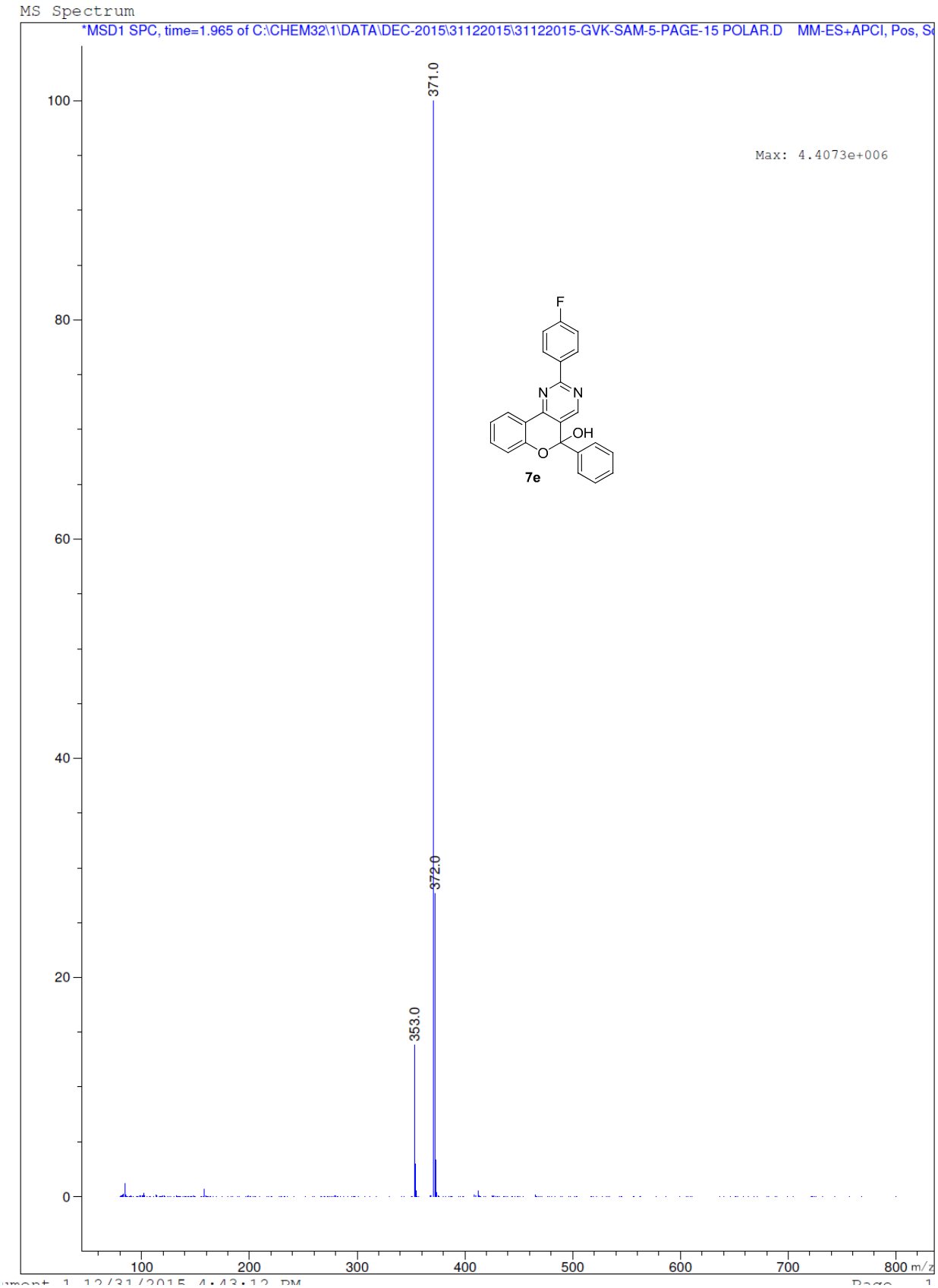
GVK BIOSCIENCES PVT. LTD.
MEDICINAL CHEMISTRY LABORATORY - ANALYTICAL RESEARCH

LCMS REPORT

```
================================================================================
Sample Name     :GVK-SAM-5-PAGE-15 POLAR                    Vial position  :P2-A-05
Date of Analysis:12/31/2015    4:31:47 PM                  Injection Vol  :0.5   µL
Acq. Method     :C:\CHEM32\1\METHODS\RND-FA- 3.0 MIN-1.M   Instrument ID  :ANL-MCL5-LCMS-001

================================================================================
RND-FA-3.0 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, 0.3/2, 2.3/98,2.8/98,2.81/2,3.0/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 60°C                                                    ->
```



Pea No	RT min	Area	Area %
1	1.93	2655.073	99.221
2	2.04	15.650	0.585
3	2.08	5.207	0.195


MS Spectrum
*MSD1 SPC, time=1.965 of C:\CHEM32\1\DATA\DEC-2015\31122015\31122015-GVK-SAM-5-PAGE-15 POLAR.D MM-ES+APCI, Pos, S
Max: 4.4073e+006
371.0
372.0
353.0
F
N
N
OH
O
7e
100
80
60
40
20
0
100
200
300
400
500
600
700
800 m/z

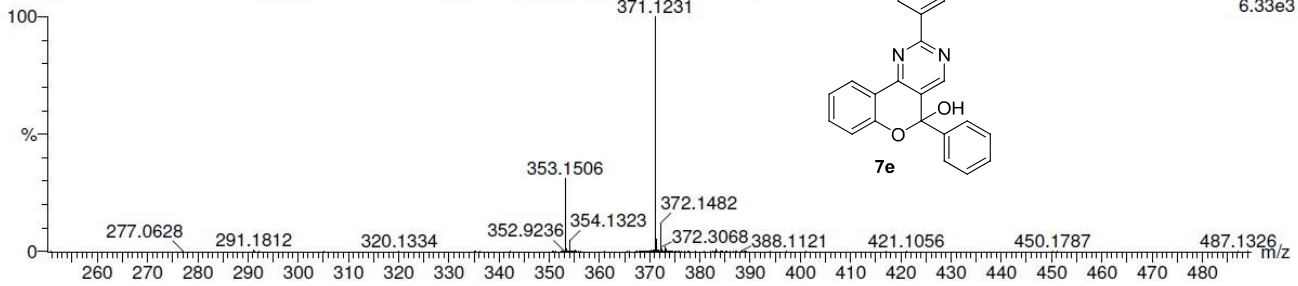
Single Mass Analysis

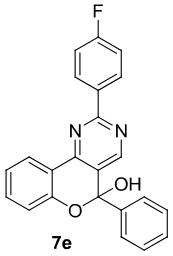
Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
10 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-23 H: 0-16 N: 0-2 O: 0-2 F: 0-1

SAMPLE CODE:GVK-SAM-5-PAGE-15 POLAR
511701A3367 21 (0.285) AM (Top,4, Ar,5000.0,195.14,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

1: TOF MS ES+
6.33e3

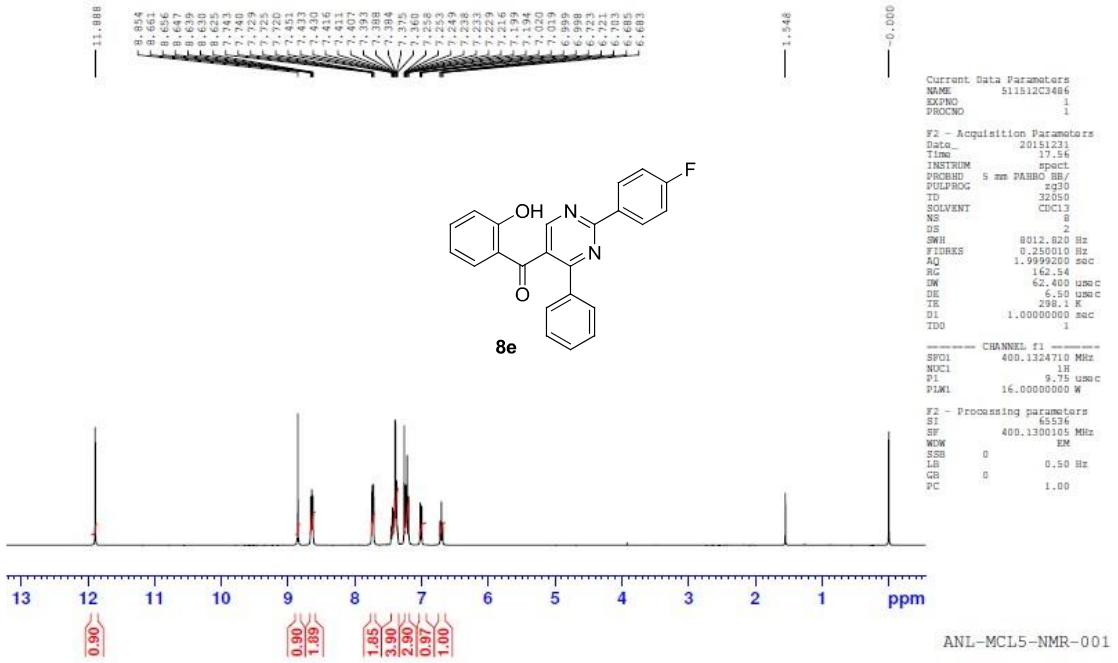




7e

Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
371.1231	371.1196	3.5	9.4	16.5	407.5	C23 H16 N2 O2 F

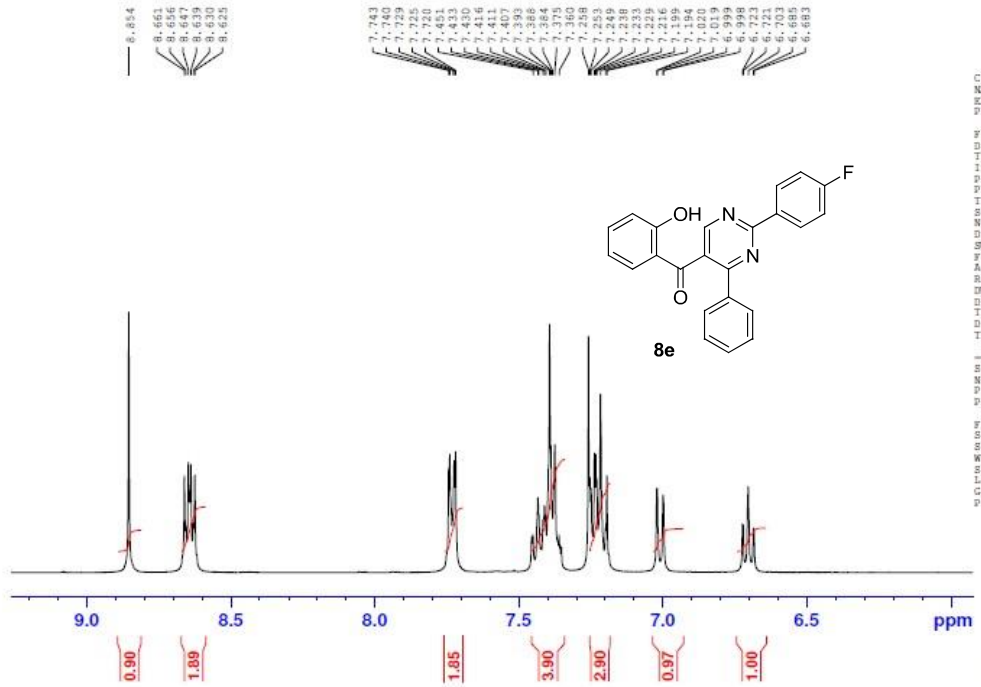
GVK-SAM-5-PAGE-15NP




```
Current Data Parameters
NAME                  511512C3486
EXPNO                           1
PROCNO                          1

F2 - Acquisition Parameters
Date_                    20151231
Time                        17.56
INSTRUM                     spect
PROBHD    5 mm PABBO BB/
PULPROG                     zg30
TD                         32050
SOLVENT                    CDCl3
NS                             8
DS                             2
SWH                     8012.820 Hz
FIDRES                  0.250010 Hz
AQ                      1.9999200 sec
RG                         162.54
DW                         62.400 usec
DE                          6.50 usec
TE                         298.1 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                    400.1300105 MHz
WDW                           EM
SSB                 0
LB                          0.50 Hz
GB                  0
PC                          1.00
```

ANL-MCL5-NMR-001

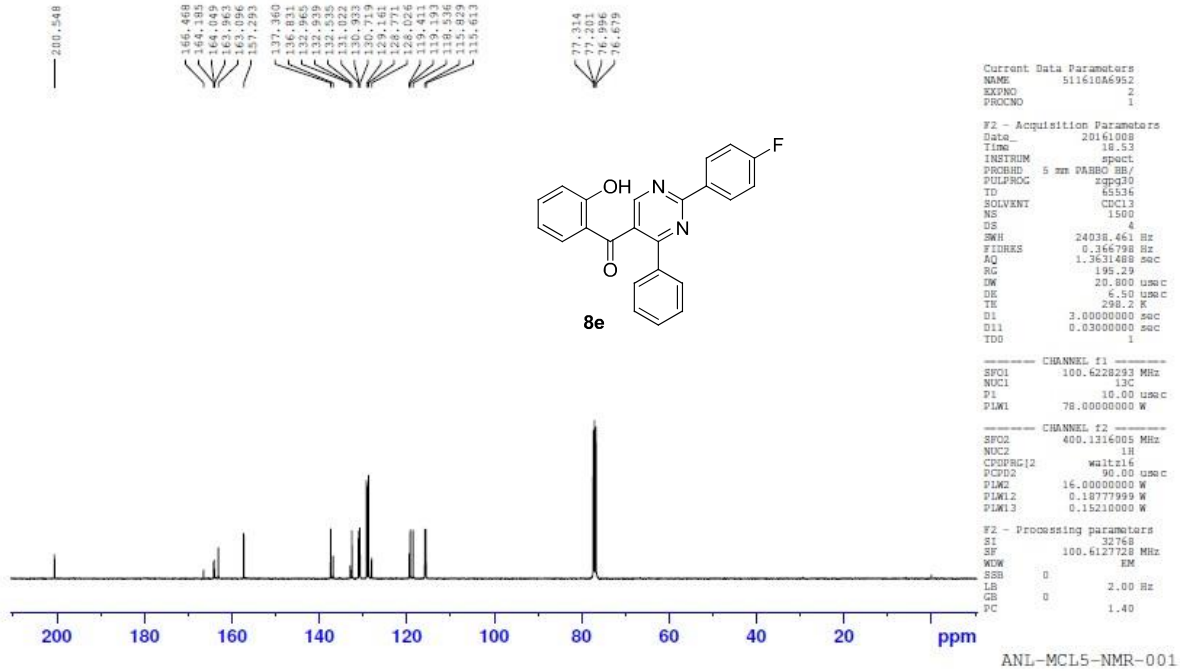
GVK-SAM-5-PAGE-15NP




```
Current Data Parameters
NAME                  511512C3486
EXPNO                           1
PROCNO                          1

F2 - Acquisition Parameters
Date_                    20151231
Time                        17.56
INSTRUM                     spect
PROBHD    5 mm PABBO BB/
PULPROG                     zg30
TD                         32050
SOLVENT                    CDCl3
NS                             8
DS                             2
SWH                     8012.820 Hz
FIDRES                  0.250010 Hz
AQ                      1.9999200 sec
RG                         162.54
DW                         62.400 usec
DE                          6.50 usec
TE                         298.1 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                    400.1300105 MHz
WDW                           EM
SSB                 0
LB                          0.50 Hz
GB                  0
PC                          1.00
```

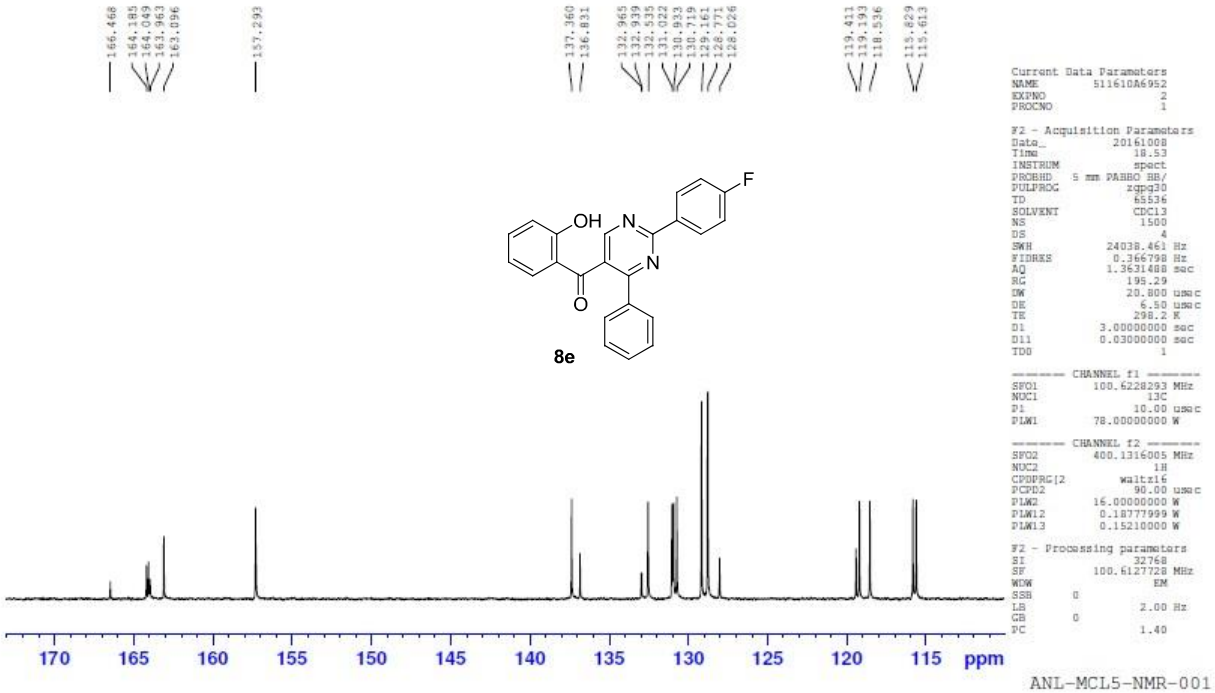
ANL-MCL5-NMR-001

GVK-SAM-5-page-15 NP



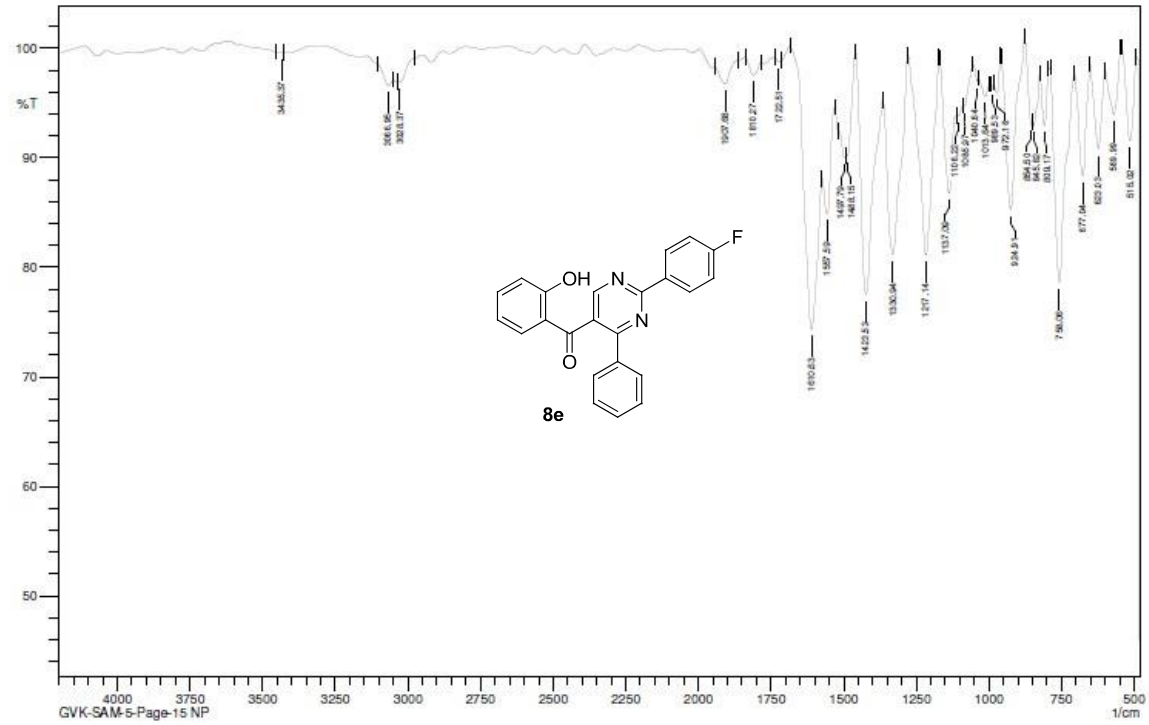
ANL-MCL5-NMR-001

GVK-SAM-5-page-15 NP



ANL-MCL5-NMR-001

SHIMADZU



8e

Comment: IN Kbr
$(IR Spectrum|DESCRIPTION)

No. of Scans:
Resolution:
Apodization:

Date: 10/3/2016 10:57:49 AM
User: Admin

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

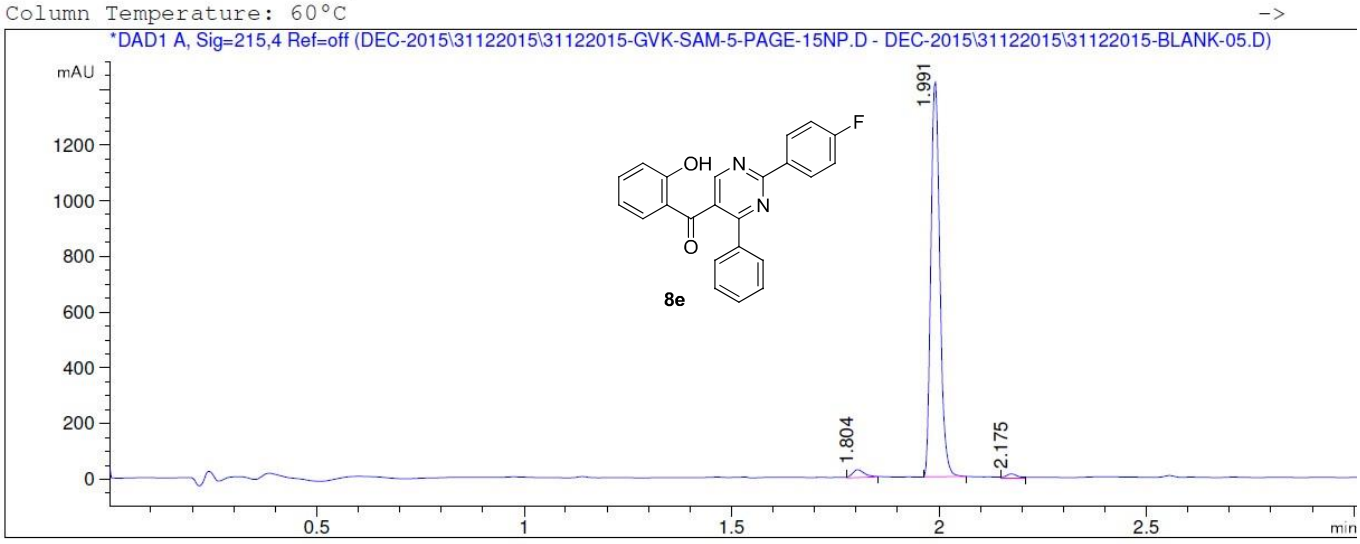
LCMS REPORT

==========

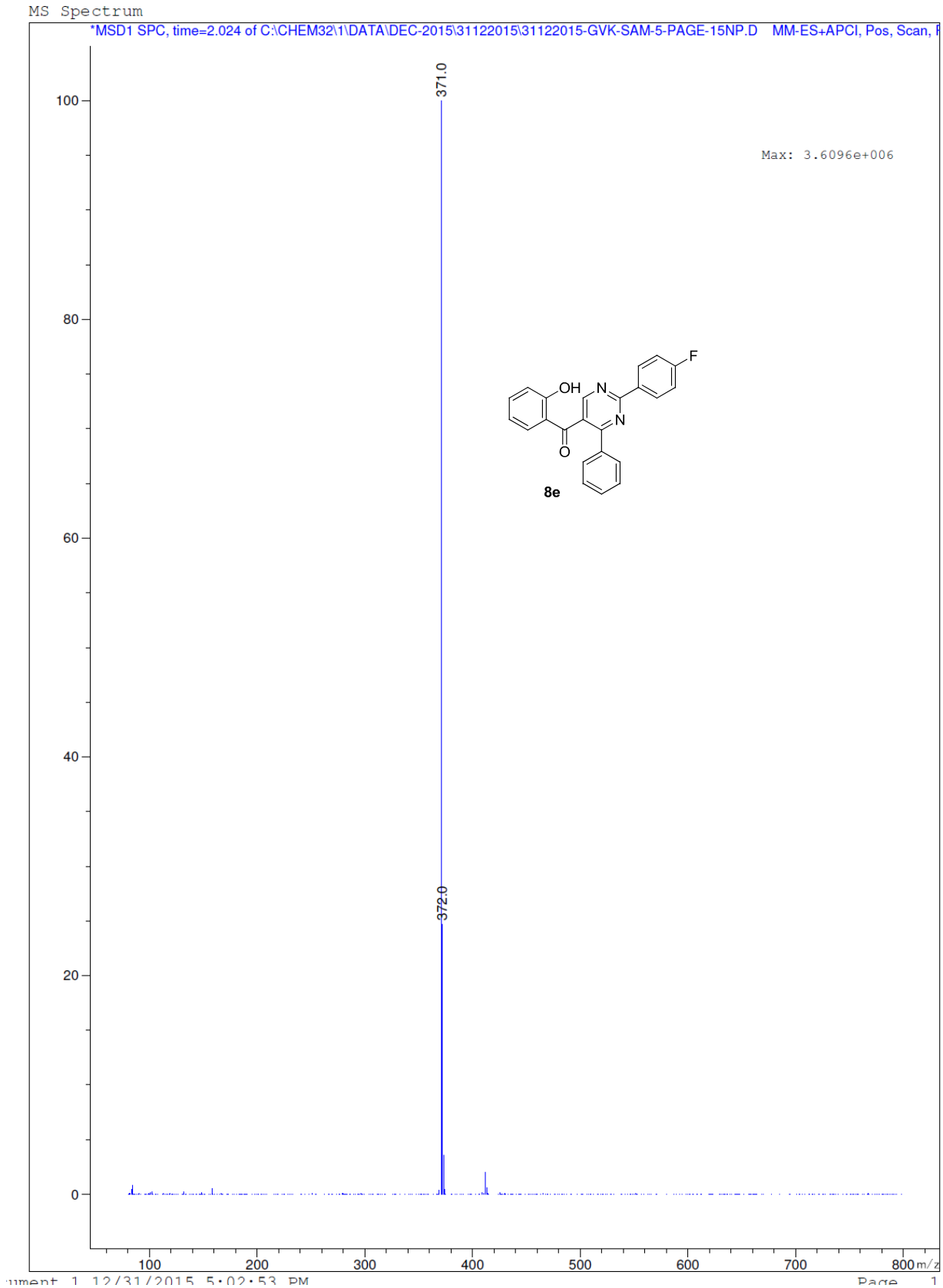
Sample Name :GVK-SAM-5-PAGE-15NP Vial position :P2-A-08
Date of Analysis:12/31/2015 4:51:27 PM Injection Vol :0.5 µL
Acq. Method :C:\CHEM32\1\METHODS\RND-FA- 3.0 MIN-1.M Instrument ID :ANL-MCL5-LCMS-001

==========

RND-FA-3.0 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, 0.3/2, 2.3/98,2.8/98,2.81/2,3.0/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 60°C ->



Peak No	RT min	Area	Area %
1	1.80	58.451	2.621
2	1.99	2144.079	96.133
3	2.17	27.788	1.246

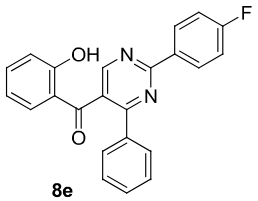

MS Spectrum
*MSD1 SPC, time=2.024 of C:\CHEM32\1\DATA\DEC-2015\31122015\31122015-GVK-SAM-5-PAGE-15NP.D MM-ES+APCI, Pos, Scan,
371.0
372.0
Max: 3.6096e+006
OH
N
N
O
F
8e
100
80
60
40
20
0
100
200
300
400
500
600
700
800
m/z

Elemental Composition Report

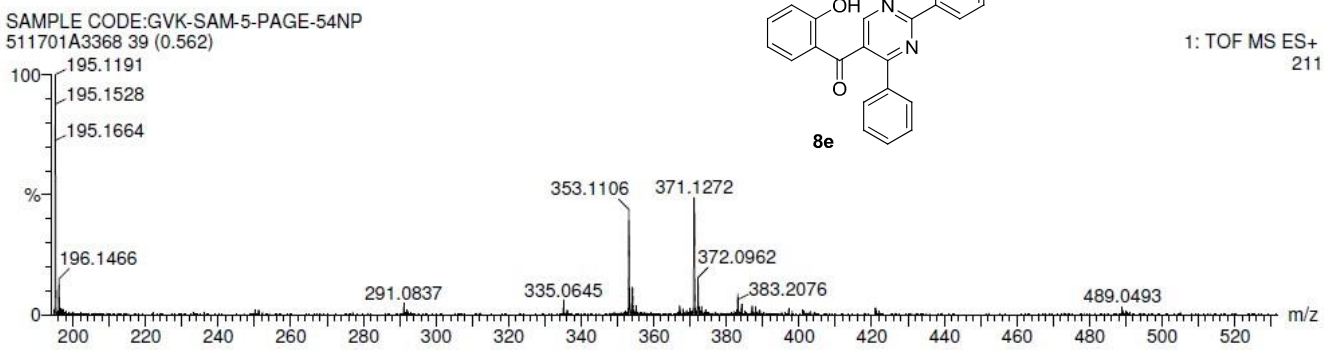
Single Mass Analysis

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

Monoisotopic Mass, Even Electron Ions
10 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-23 H: 0-16 N: 0-2 O: 0-2 F: 0-1

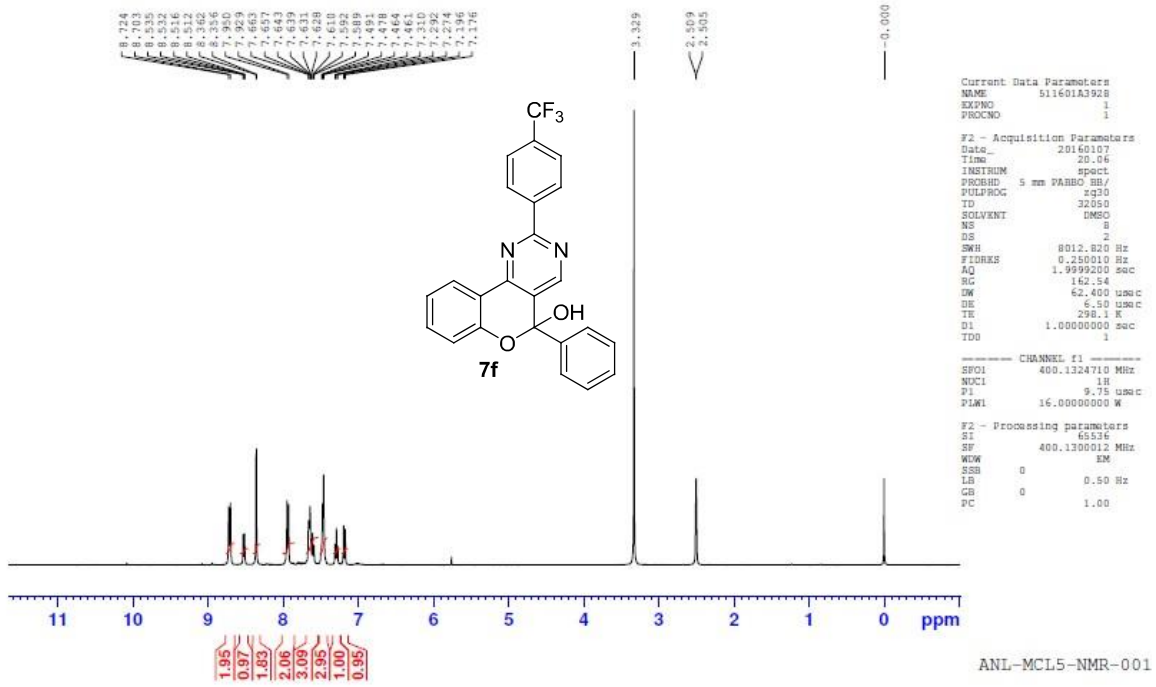


8e



Minimum:				-1.5	
Maximum:		5.0	1000.0	50.0	
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**Formula**
371.1272	371.1196	7.6	20.5	16.5	C23 H16 N2 O2 F

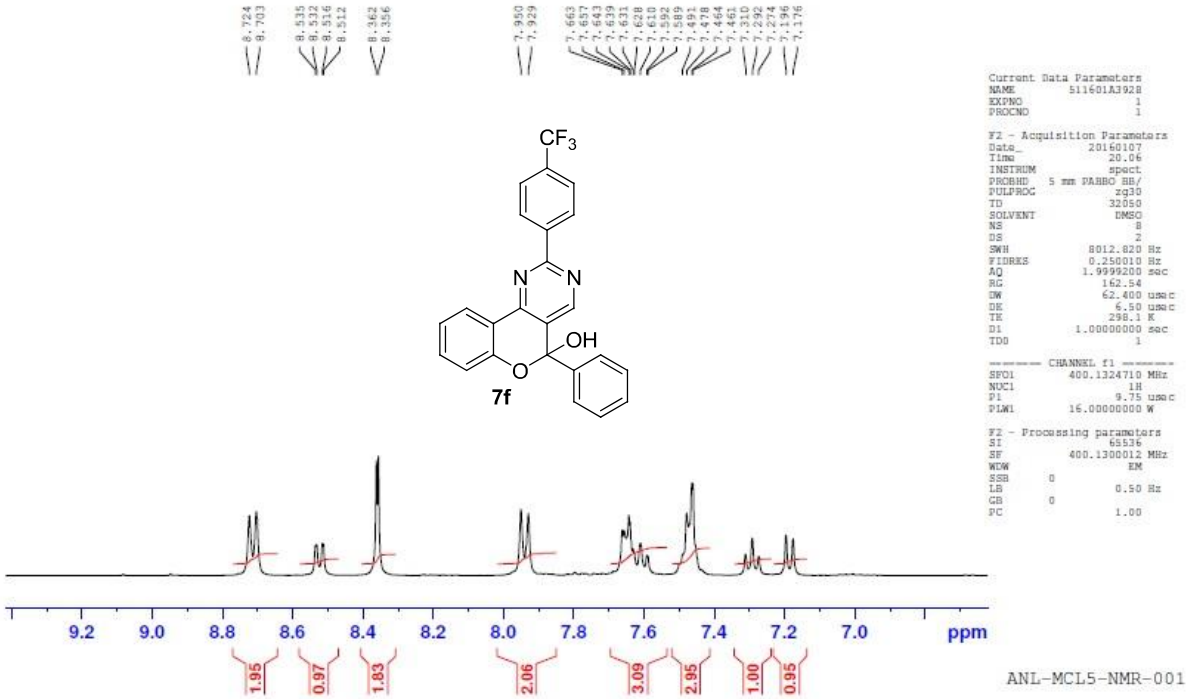
GVK-SAM-5-PAGE-17POLAR




```
Current Data Parameters
NAME          511601A3928
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_              20160107
Time_                 20.06
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG               zg30
TD                   32050
SOLVENT              DMSO
NS                       8
DS                       2
SWH               8012.820 Hz
FIDRES            0.250010 Hz
AQ                1.9999200 sec
RG                   162.54
DW                  62.400 usec
DE                   6.50 usec
TE                  298.1 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               400.1300012 MHz
WDW                        EM
SSB                      0
LB                    0.50 Hz
GB                       0
PC                    1.00
```

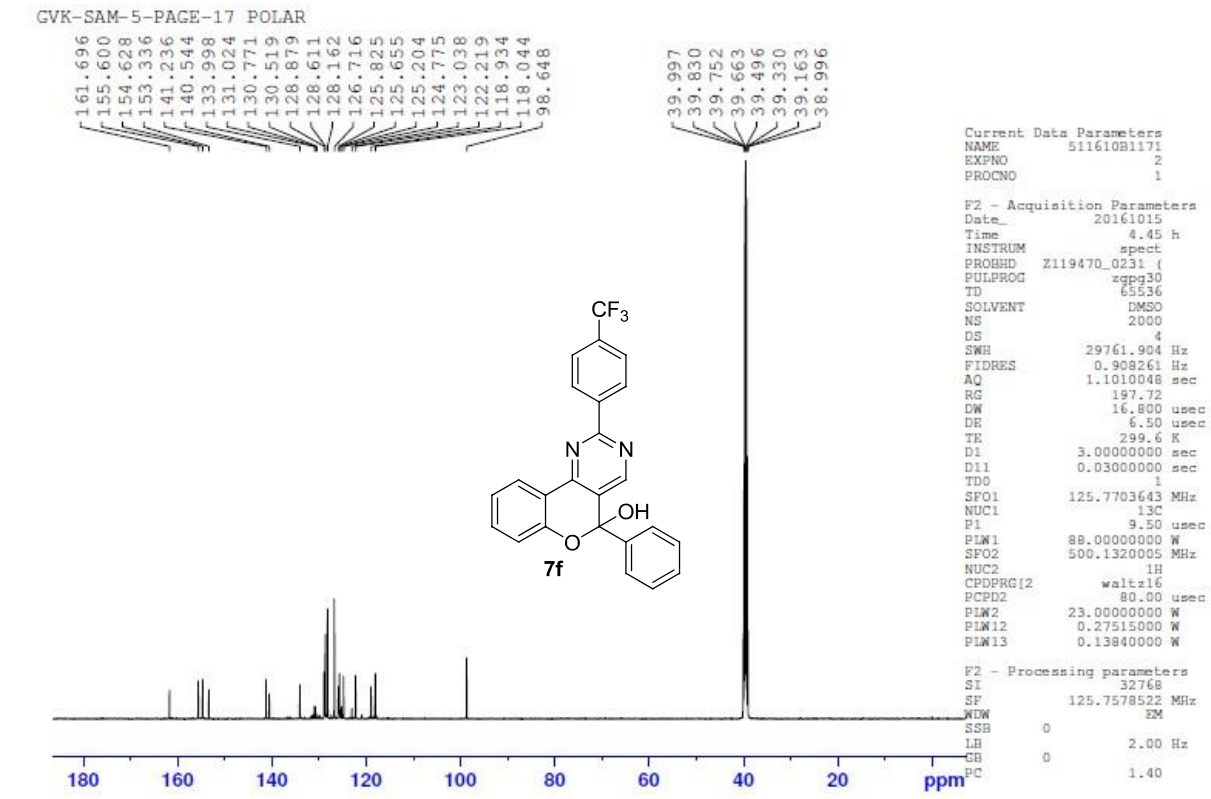
ANL-MCL5-NMR-001

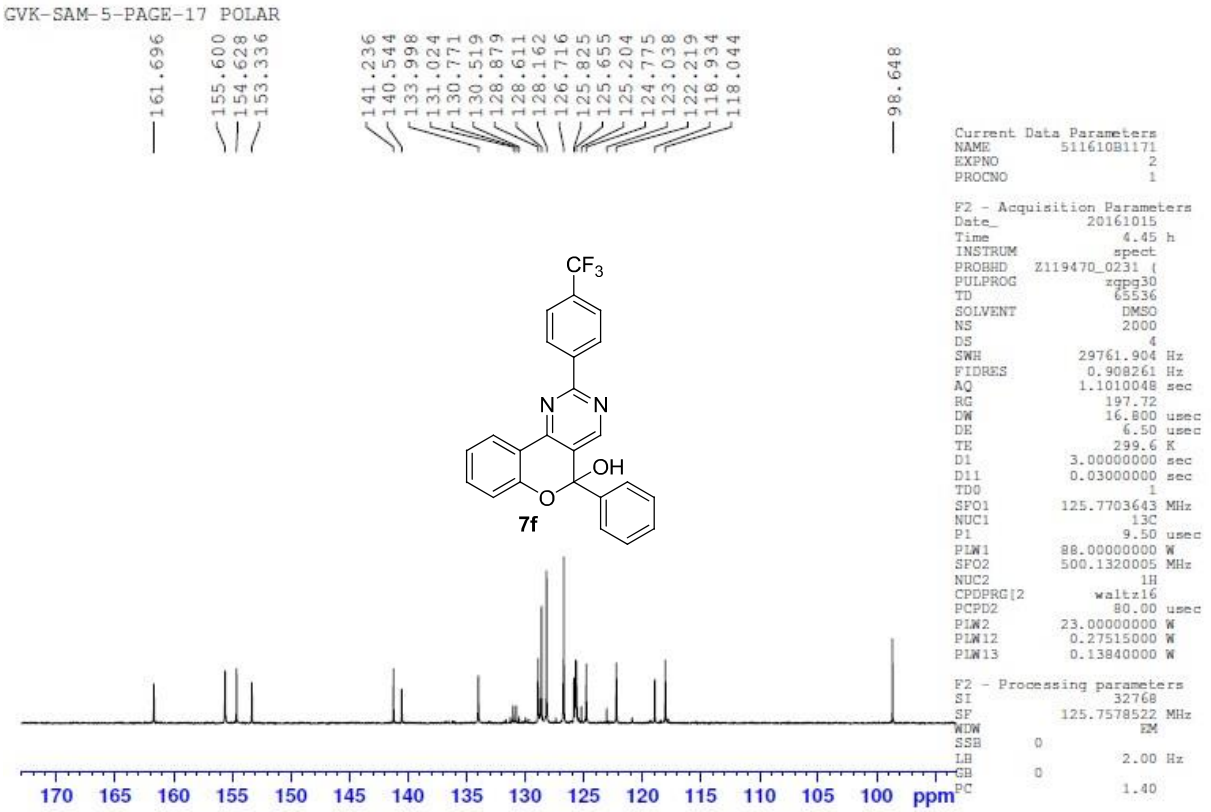
GVK-SAM-5-PAGE-17POLAR



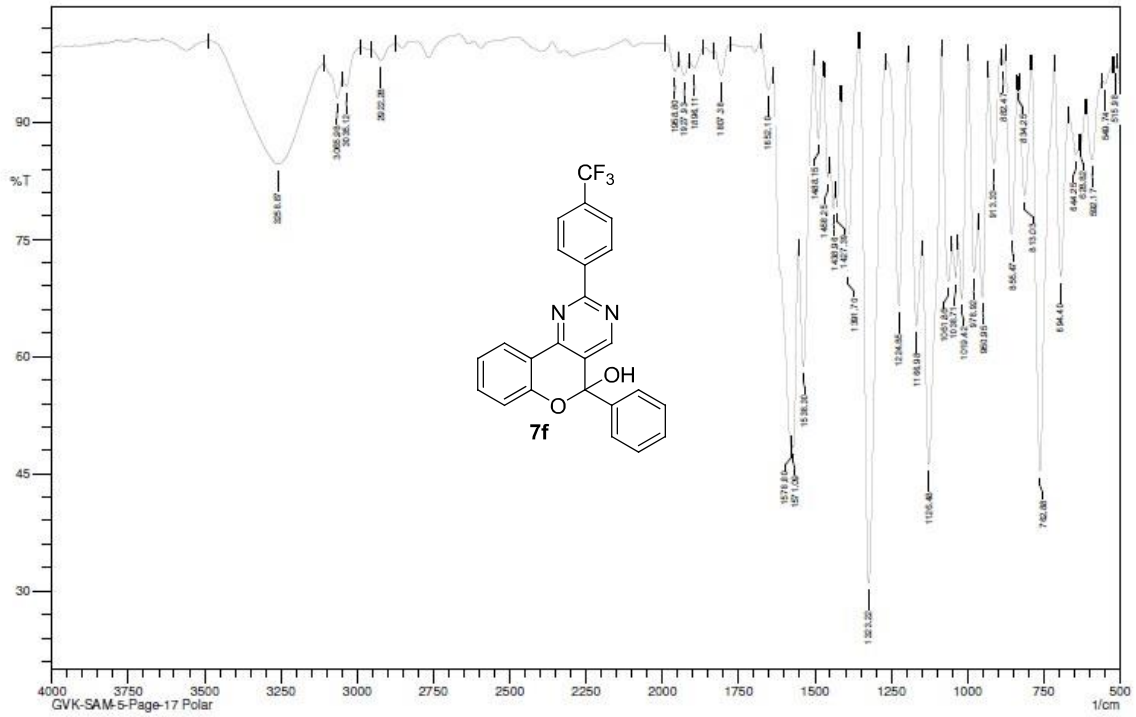

```
Current Data Parameters
NAME          511601A3928
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_              20160107
Time_                 20.06
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG               zg30
TD                   32050
SOLVENT              DMSO
NS                       8
DS                       2
SWH               8012.820 Hz
FIDRES            0.250010 Hz
AQ                1.9999200 sec
RG                   162.54
DW                  62.400 usec
DE                   6.50 usec
TE                  298.1 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               400.1300012 MHz
WDW                        EM
SSB                      0
LB                    0.50 Hz
GB                       0
PC                    1.00
```

ANL-MCL5-NMR-001


GVK-SAM-5-PAGE-17 POLAR
161.696
155.600
154.628
153.336
141.236
140.544
133.998
131.024
130.771
130.519
128.879
128.611
128.162
126.716
125.825
125.655
125.204
124.775
123.038
122.219
118.934
118.044
98.648
39.997
39.830
39.752
39.663
39.496
39.330
39.163
38.996
CF3
N
N
OH
O
7f
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME 511610B1171
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161015
Time 4.45 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2000
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 299.6 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7578522 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40


GVK-SAM-5-PAGE-17 POLAR
161.696
155.600
154.628
153.336
141.236
140.544
133.998
131.024
130.771
130.519
128.879
128.611
128.162
126.716
125.825
125.655
125.204
124.775
123.038
122.219
118.934
118.044
98.648
CF3
N
N
OH
O
7f
170
165
160
155
150
145
140
135
130
125
120
115
110
105
100
ppm
Current Data Parameters
NAME 511610B1171
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161015
Time 4.45 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 2000
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 299.6 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7578522 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

SHIMADZU



Comment: IN Kbr
GVK-SAM-5-Page-17 Polar

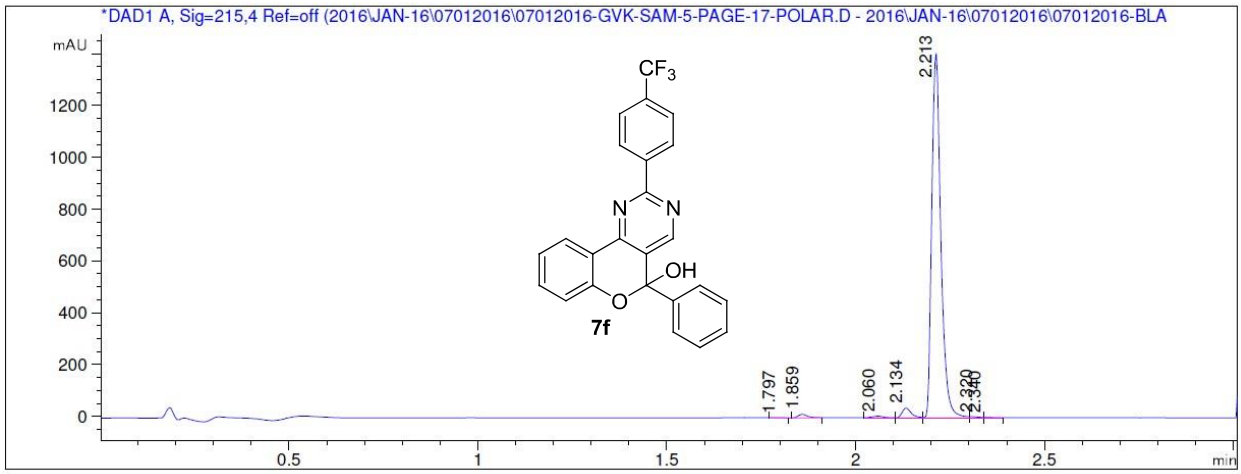
No. of Scans:
Resolution:
Apodization:

Date: 10/3/2016 11:22:47 AM
User: Admin

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

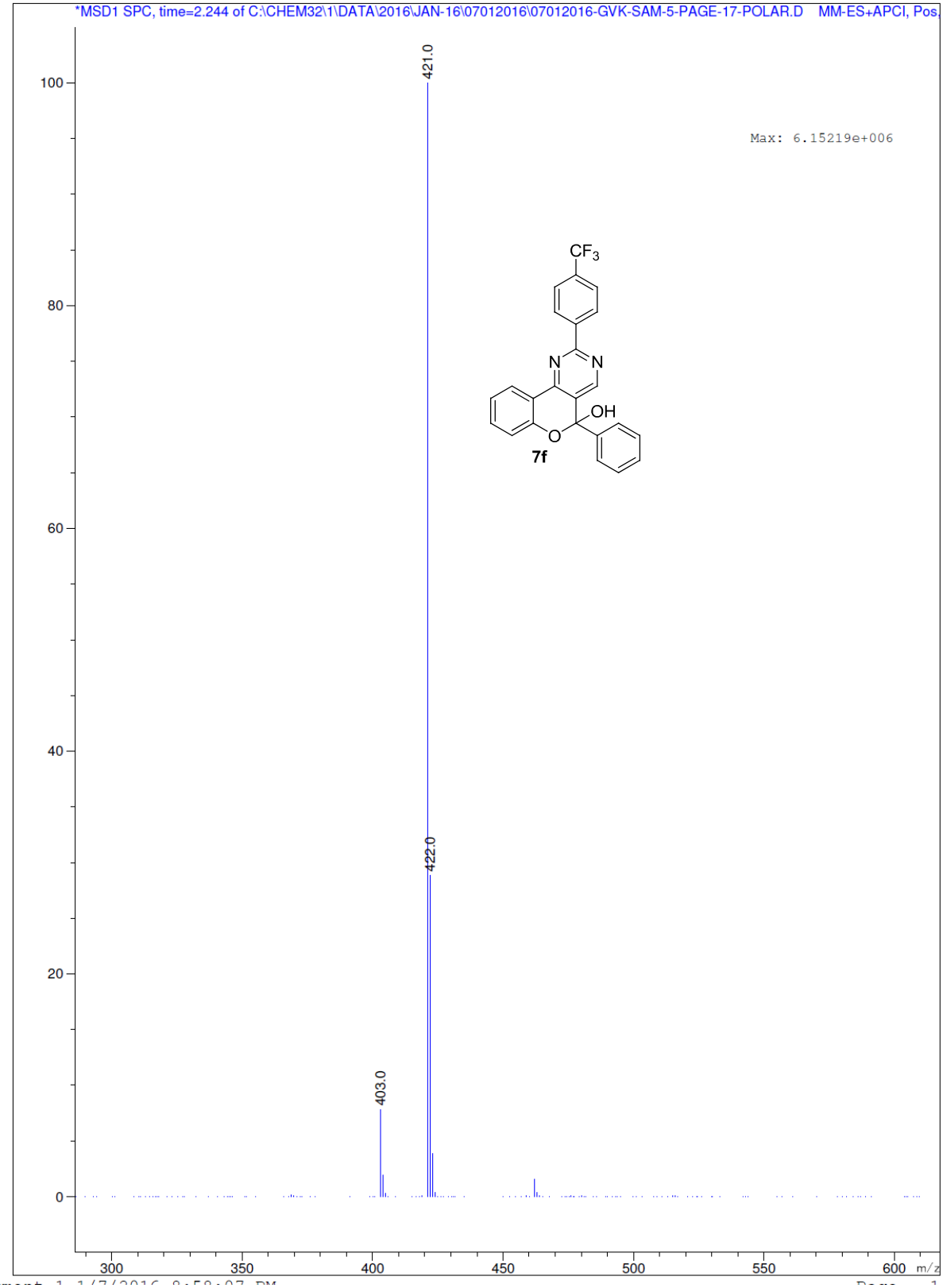
LCMS REPORT

```
================================================================================================
Sample Name     :GVK-SAM-5-PAGE-17-POLAR                          Vial position  :P1-C-09
Date of Analysis:07/01/2016;8:31:49 PM                            Injection Vol:  0.5   µL
Acq. Method->C:\CHEM32\1\METHODS\RND-FA- 3.0 MIN-1.M          Instrument ID:ANL-MCL5-LCMS-001

================================================================================================
RND-FA-3.0 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, 0.3/2, 2.3/98,2.8/98,2.81/2,3.0/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 60°C                                                                    ->
```



Peak No	RT min	Area	Area %
1	1.80	1.435	0.058
2	1.86	22.242	0.904
3	2.06	13.475	0.548
4	2.13	62.808	2.553
5	2.21	2351.906	95.617
6	2.32	6.271	0.255
7	2.34	1.567	0.064

MS Spectrum


*MSD1 SPC, time=2.244 of C:\CHEM32\1\DATA\2016\JAN-16\07012016\07012016-GVK-SAM-5-PAGE-17-POLAR.D MM-ES+APCI, Pos,
Max: 6.15219e+006
421.0
422.0
403.0
CF3
N
N
OH
O
7f
100
80
60
40
20
0
300
350
400
450
500
550
600
m/z

Single Mass Analysis

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

Selected filters: None

Monoisotopic Mass, Even Electron Ions

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

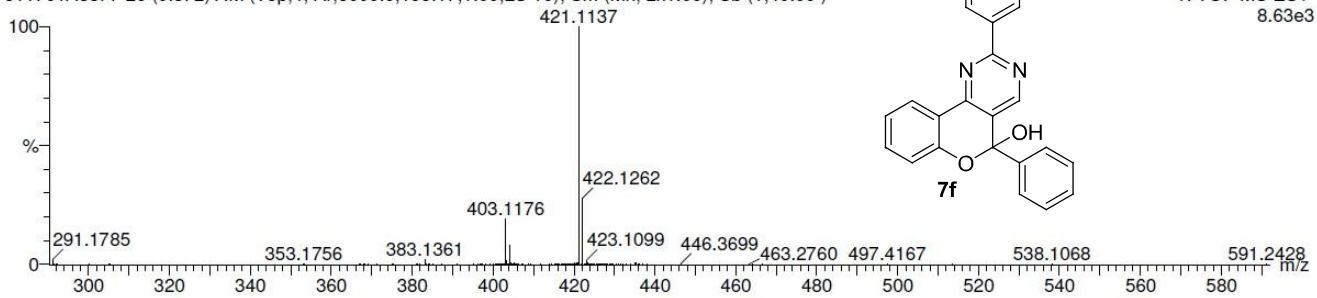
Elements Used:

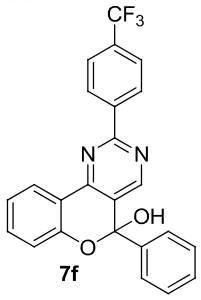
C: 0-24 H: 0-16 N: 0-2 O: 0-2 F: 0-3

SAMPLE CODE:GVK-SAM-5-PAGE-17 POLAR

511701A3377 26 (0.372) AM (Top,4, Ar,5000.0,195.17,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

1: TOF MS ES+
8.63e3

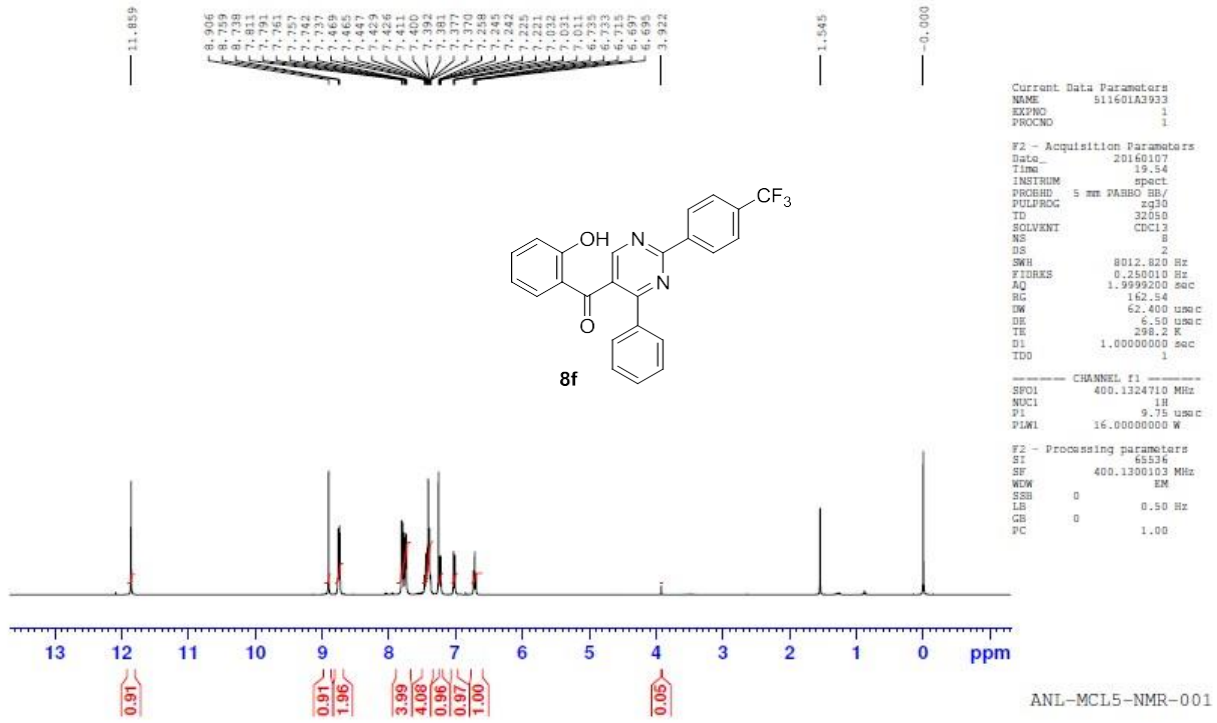




7f

Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
421.1137	421.1164	-2.7	-6.4	16.5	150.2	C24 H16 N2 O2 F3

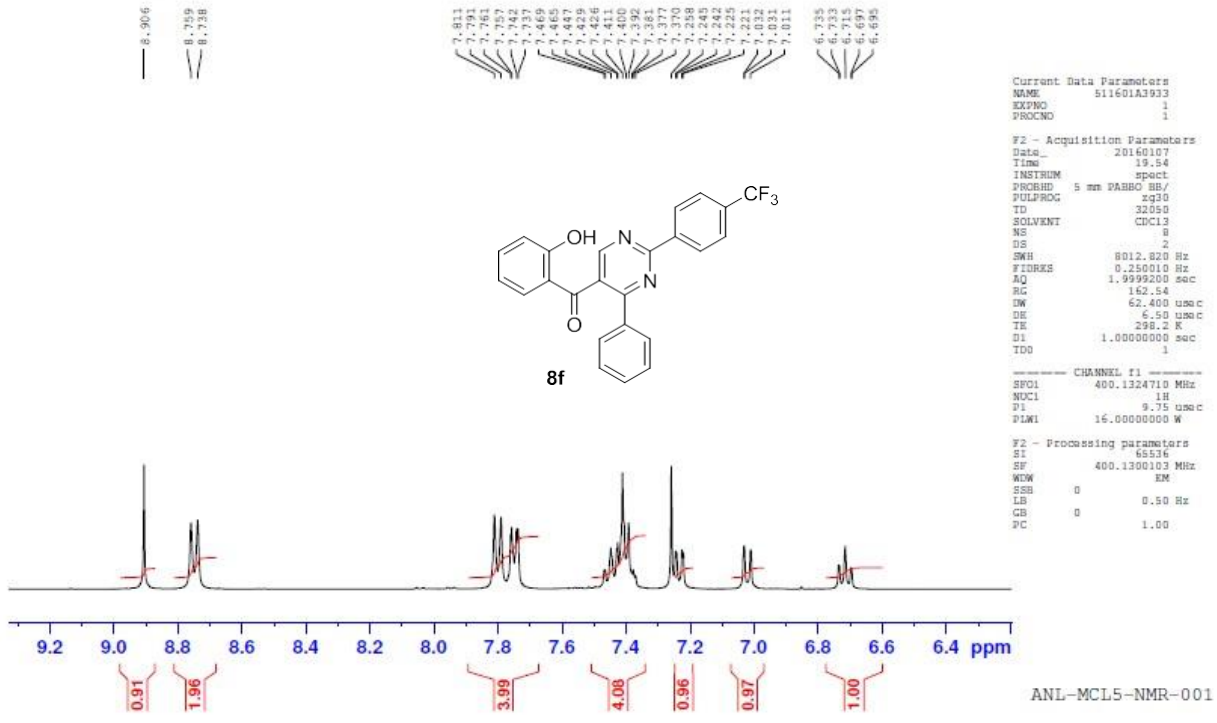
GVK-SAM-5-PAGE-17-NONPOLAR




```
Current Data Parameters
NAME          511601A3933
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Data_           20160107
TIME              19.54
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32050
SOLVENT          CDCl3
NS                   8
DS                   2
SWH           8012.820 Hz
FIDRES        0.250010 Hz
AQ            1.9999200 sec
RG              162.54
DW             62.400 usec
DE              6.50 usec
TE              298.2 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          400.1300103 MHz
WDW                EM
SSB       0
LB              0.50 Hz
GB        0
PC              1.00
```

ANL-MCL5-NMR-001

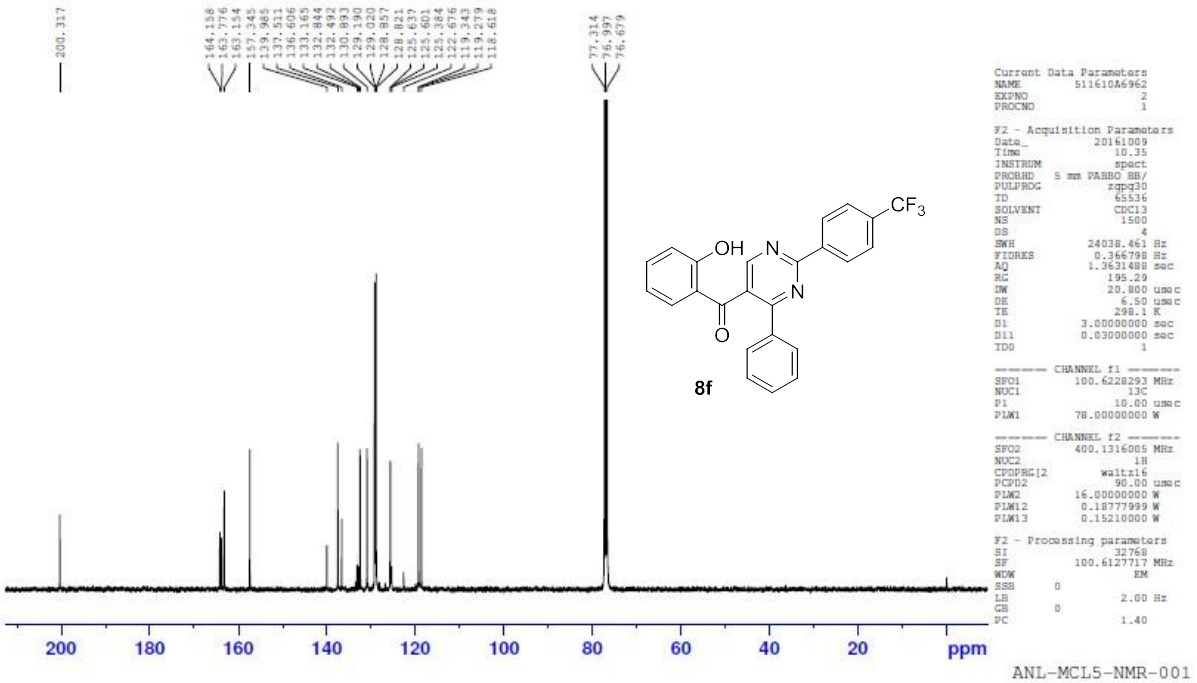
GVK-SAM-5-PAGE-17-NONPOLAR




```
Current Data Parameters
NAME          511601A3933
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Data_           20160107
TIME              19.54
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               32050
SOLVENT          CDCl3
NS                   8
DS                   2
SWH           8012.820 Hz
FIDRES        0.250010 Hz
AQ            1.9999200 sec
RG              162.54
DW             62.400 usec
DE              6.50 usec
TE              298.2 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          400.1300103 MHz
WDW                EM
SSB       0
LB              0.50 Hz
GB        0
PC              1.00
```

ANL-MCL5-NMR-001

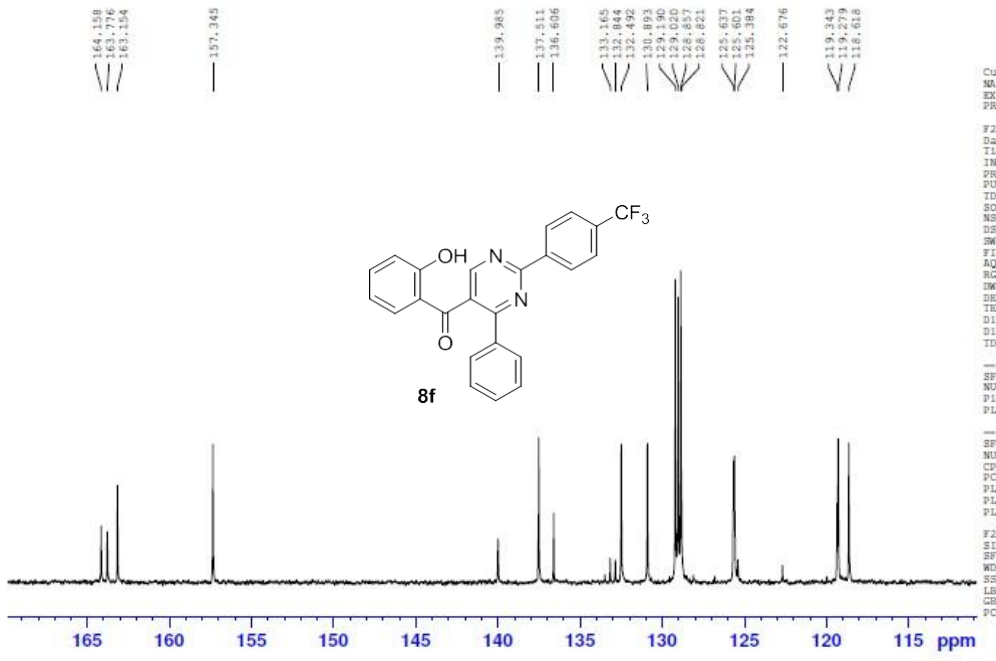
GVK-SAM-5-page-17NP




```
Current Data Parameters
NAME          511610A6962
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20161009
Time              10.35
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT           CDCl3
NS                 1500
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              298.1 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          100.6127717 MHz
WDW                   EM
SSB       0
LB                 2.00 Hz
GB        0
PC                 1.40
```

ANL-MCL5-NMR-001

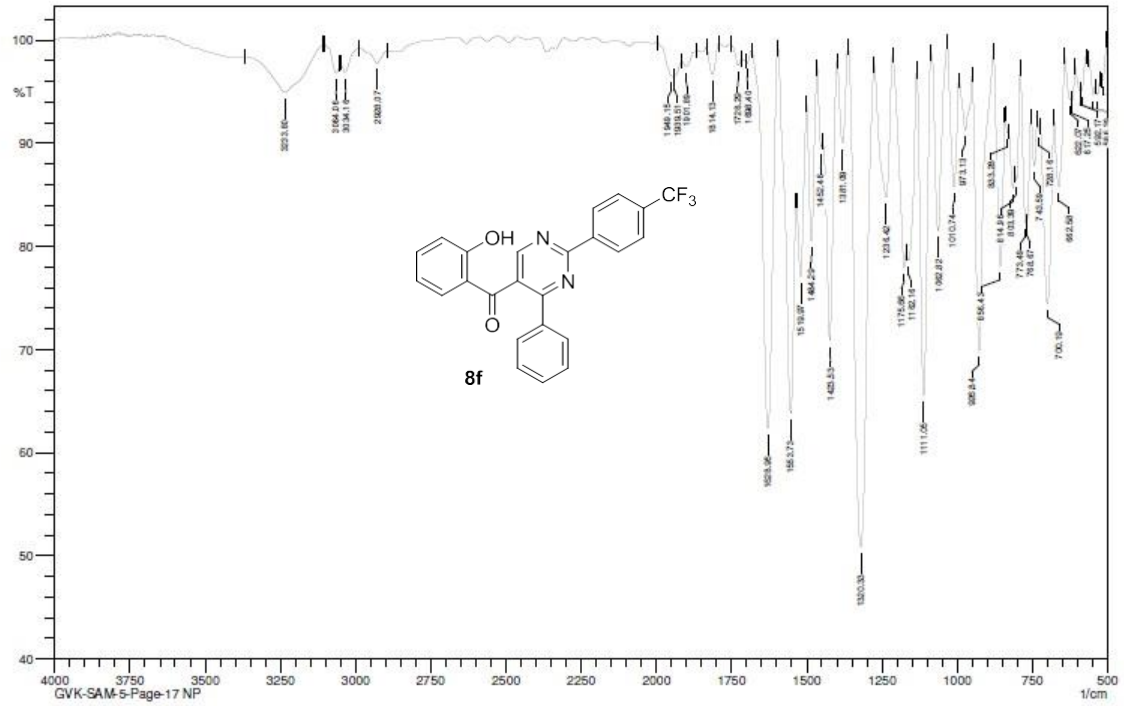
GVK-SAM-5-page-17NP




```
Current Data Parameters
NAME          511610A6962
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20161009
Time              10.35
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT           CDCl3
NS                 1500
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              298.1 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          100.6127717 MHz
WDW                   EM
SSB       0
LB                 2.00 Hz
GB        0
PC                 1.40
```

ANL-MCL5-NMR-001

SHIMADZU



8f

Comment: IN Kbr
GVK-SAM-5-Page-17 NP

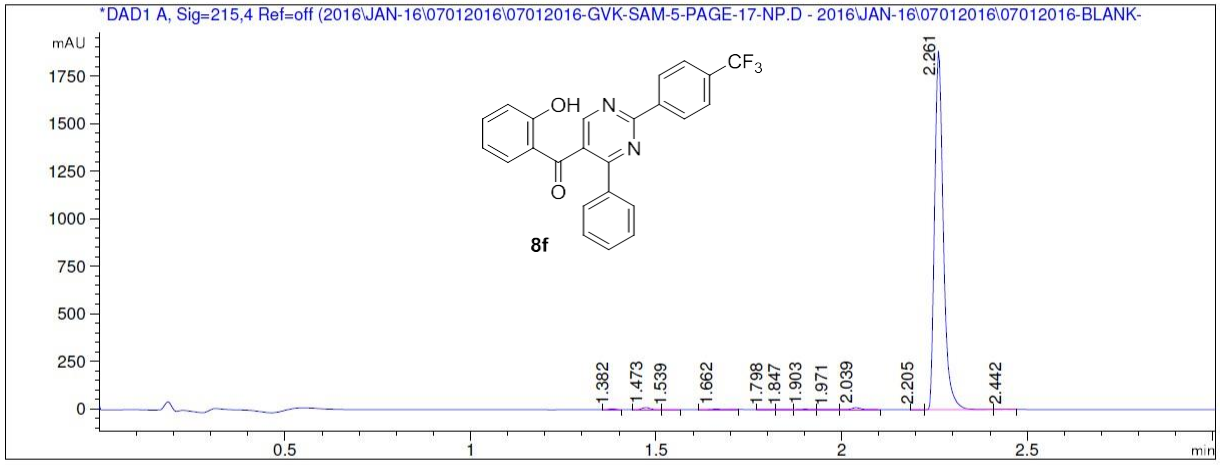
No. of Scans:
Resolution:
Apodization:

Date: 10/3/2016 11:05:38 AM
User: Admin

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

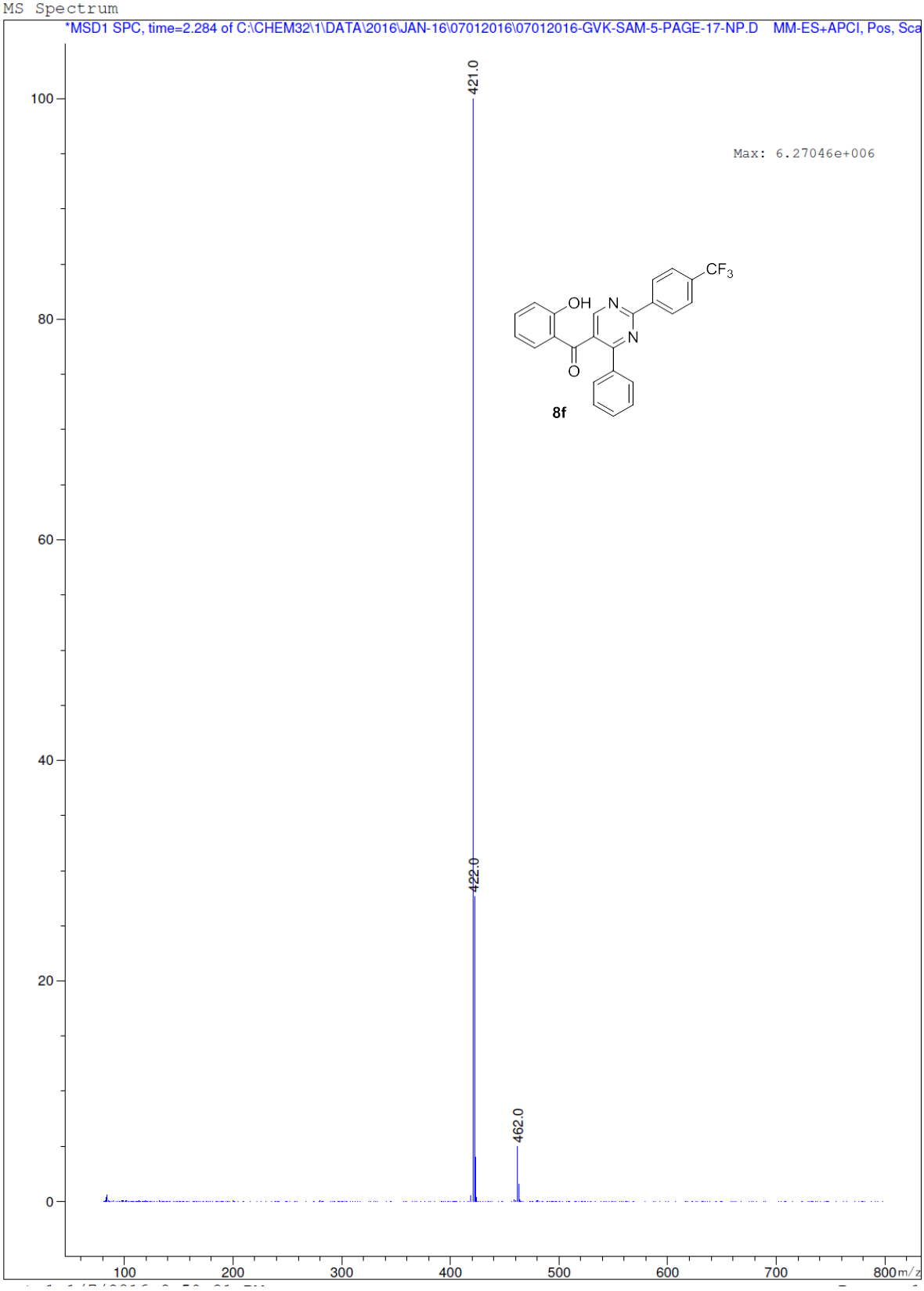
LCMS REPORT

```
================================================================================
Sample Name     :GVK-SAM-5-PAGE-17-NP                    Vial position  :P1-D-01
Date of Analysis:07/01/2016;8:35:46 PM                   Injection Vol:  0.5   µL
Acq. Method->C:\CHEM32\1\METHODS\RND-FA- 3.0 MIN-1.M     Instrument ID:ANL-MCL5-LCMS-001

================================================================================
RND-FA-3.0 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, 0.3/2, 2.3/98,2.8/98,2.81/2,3.0/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 60°C                                                    ->
```



Pea No	RT min	Area	Area %
1	1.38	5.918	0.187
2	1.47	17.465	0.553
3	1.54	1.538	0.049
4	1.66	6.057	0.192
5	1.80	1.733	0.055
6	1.85	1.112	0.035
7	1.90	3.855	0.122
8	1.97	3.328	0.105
9	2.04	19.808	0.627
10	2.20	0.961	0.030
11	2.26	3094.609	97.965
12	2.44	2.494	0.079

MS Spectrum


*MSD1 SPC, time=2.284 of C:\CHEM32\1\DATA\2016\JAN-16\07012016\07012016-GVK-SAM-5-PAGE-17-NP.D MM-ES+APCI, Pos, Sca
Max: 6.27046e+006
421.0
422.0
462.0
OH
N
N
O
CF3
8f
100
80
60
40
20
0
100
200
300
400
500
600
700
800 m/z

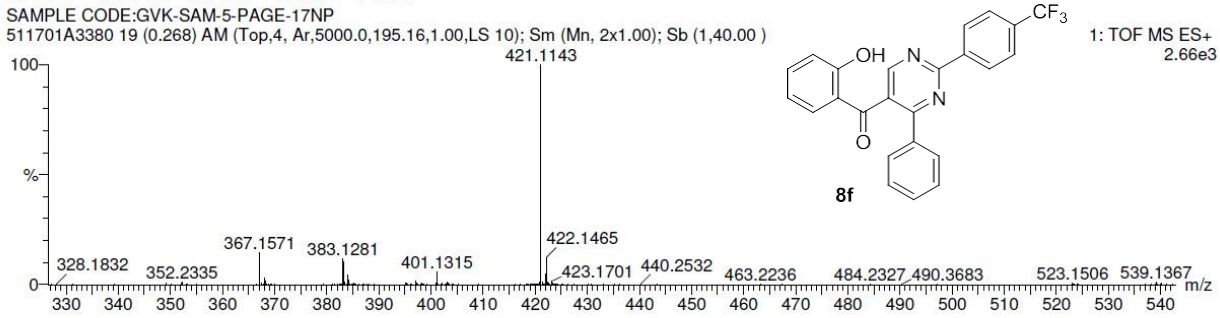
Elemental Composition Report **Page 1**

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

Monoisotopic Mass, Even Electron Ions
27 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-24 H: 0-16 N: 0-2 O: 0-2 F: 0-3

SAMPLE CODE:GVK-SAM-5-PAGE-17NP
511701A3380 19 (0.268) AM (Top,4, Ar,5000.0,195.16,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

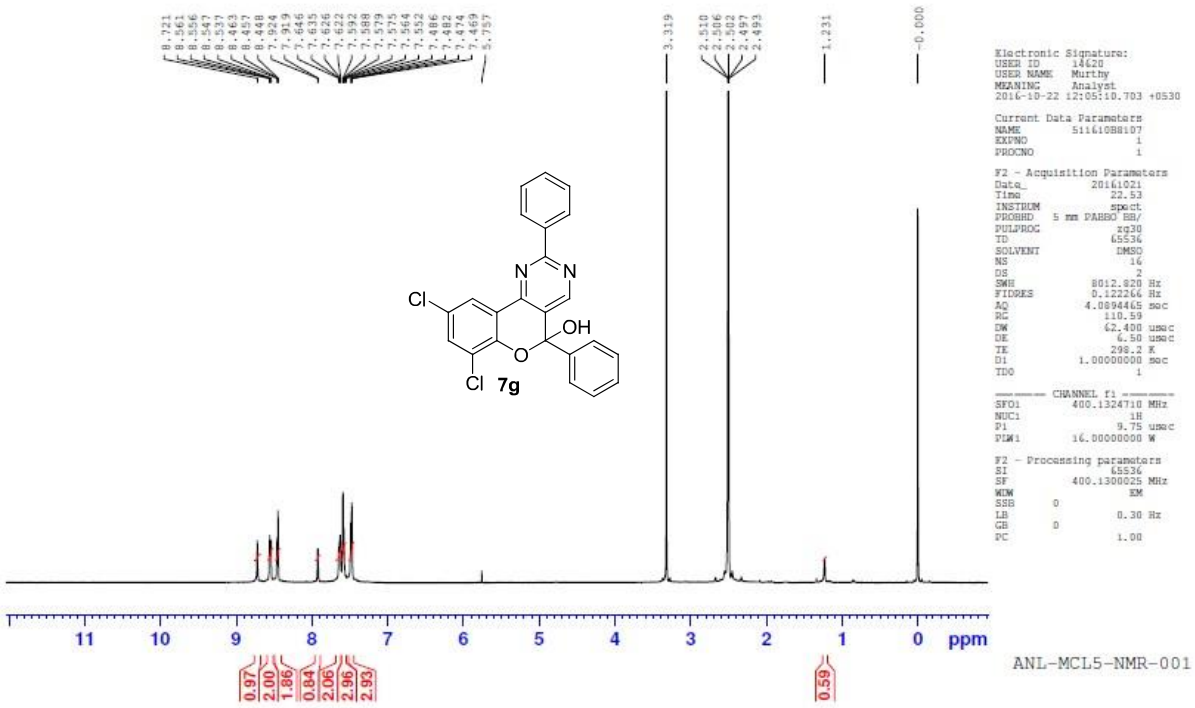
1: TOF MS ES+
2.66e3



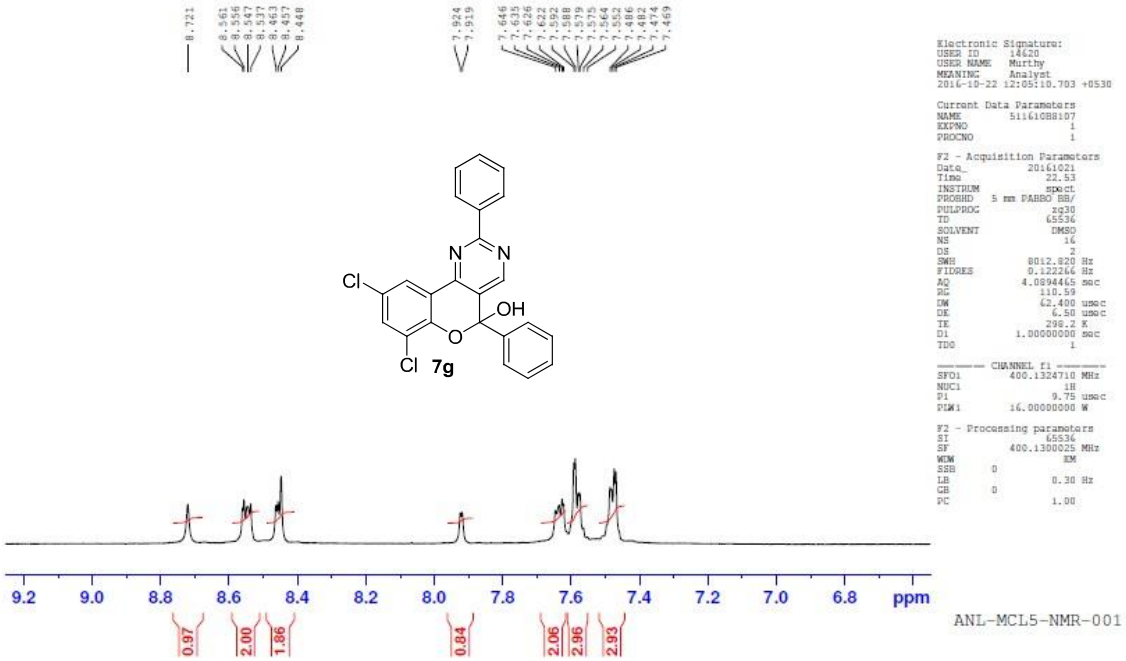
8f

Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
421.1143	421.1164	-2.1	-5.0	16.5	205.7	C24 H16 N2 O2 F3

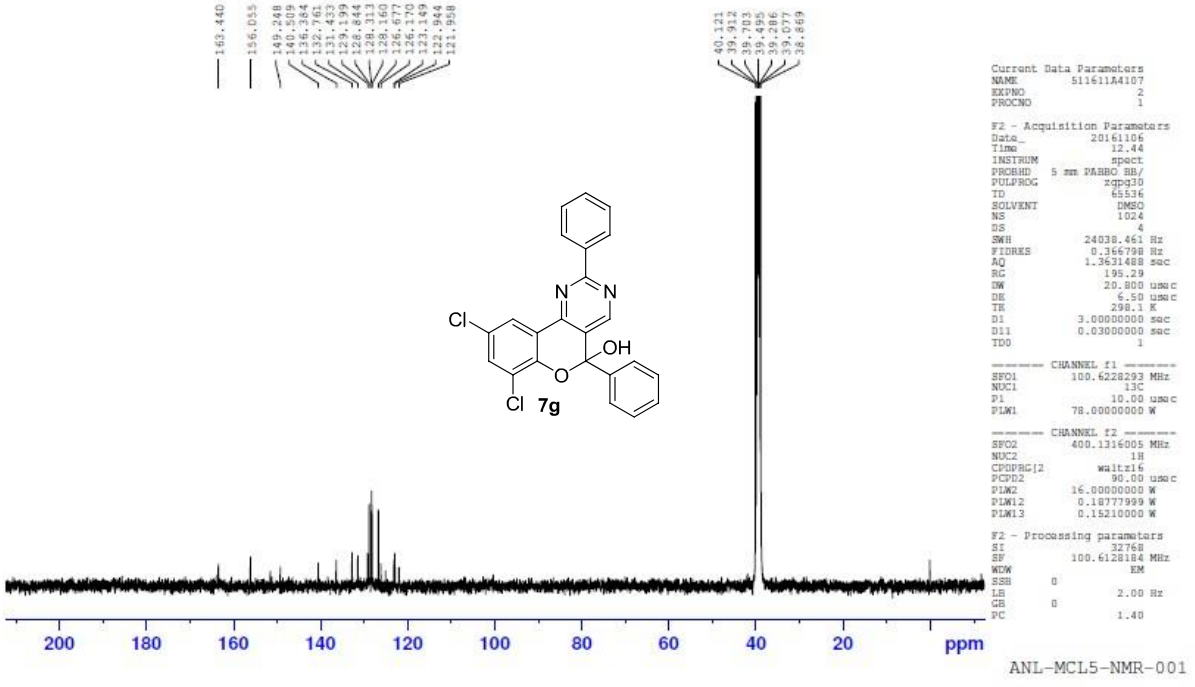
GVK-SAM-6-PAGE-4-POLAR



GVK-SAM-6-PAGE-4-POLAR

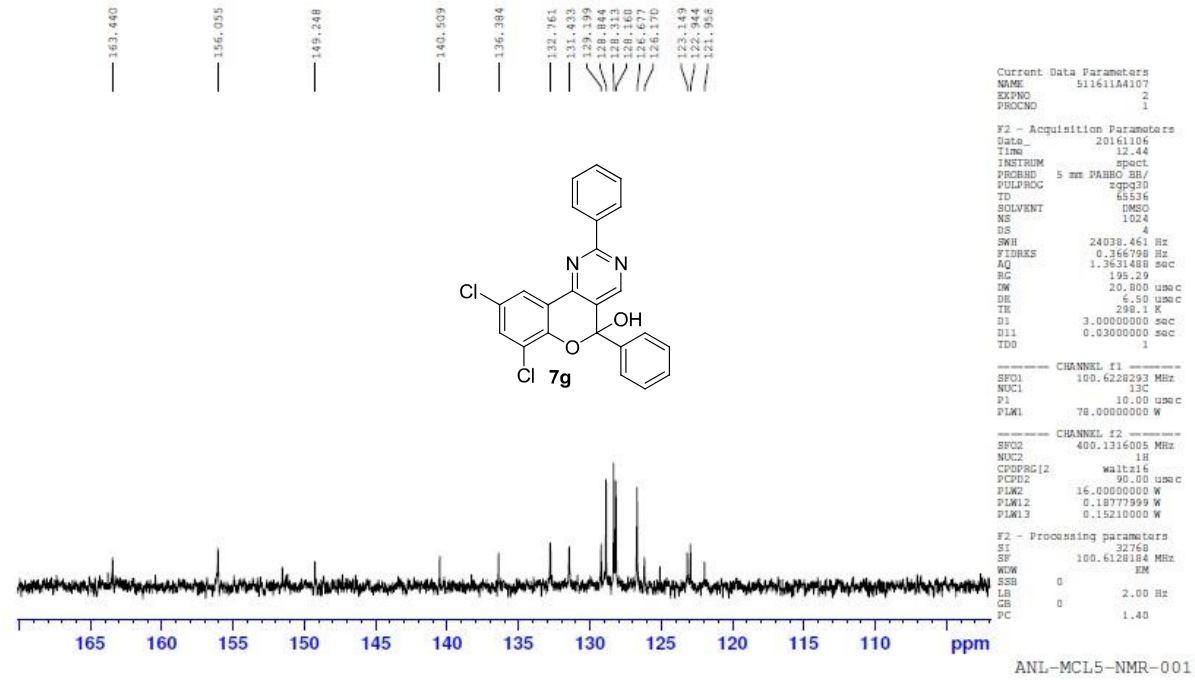


GVK-SAM-6-page-4 polar



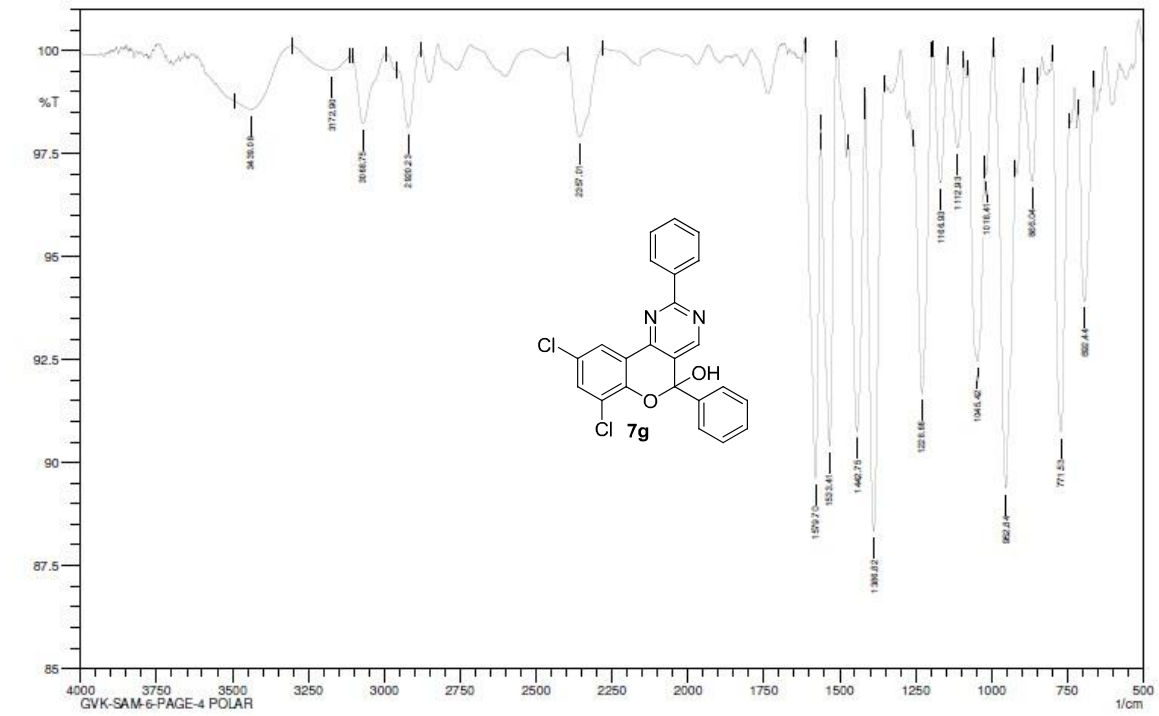
ANL-MCL5-NMR-001

GVK-SAM-6-page-4 polar



ANL-MCL5-NMR-001

SHIMADZU



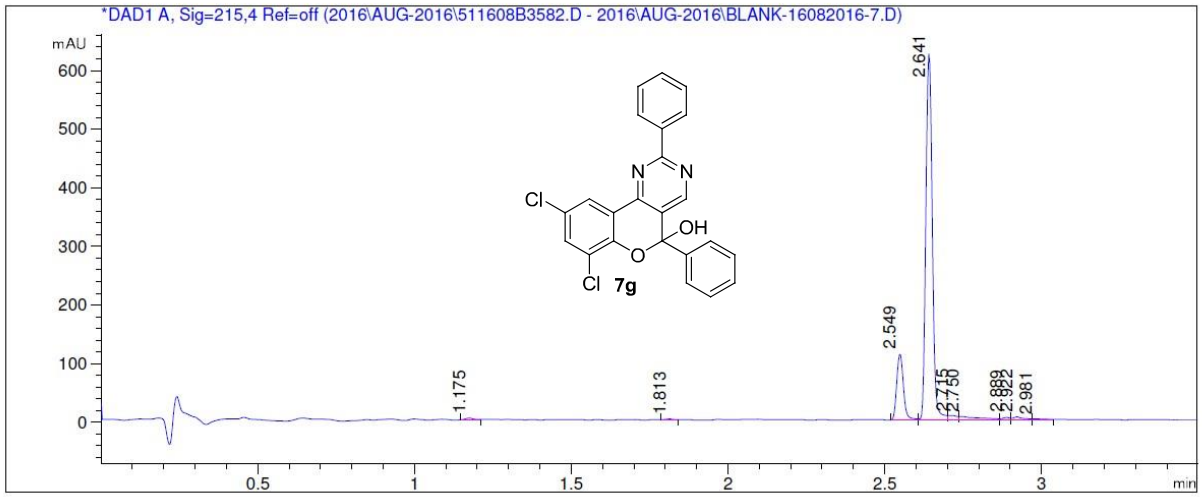
Comment: IN Kbr
GVK-SAM-6-PAGE-4 POLAR

No. of Scans:
Resolution:
Apodization:

Date: 11/15/2016 10:45:15 AM
User: Admin

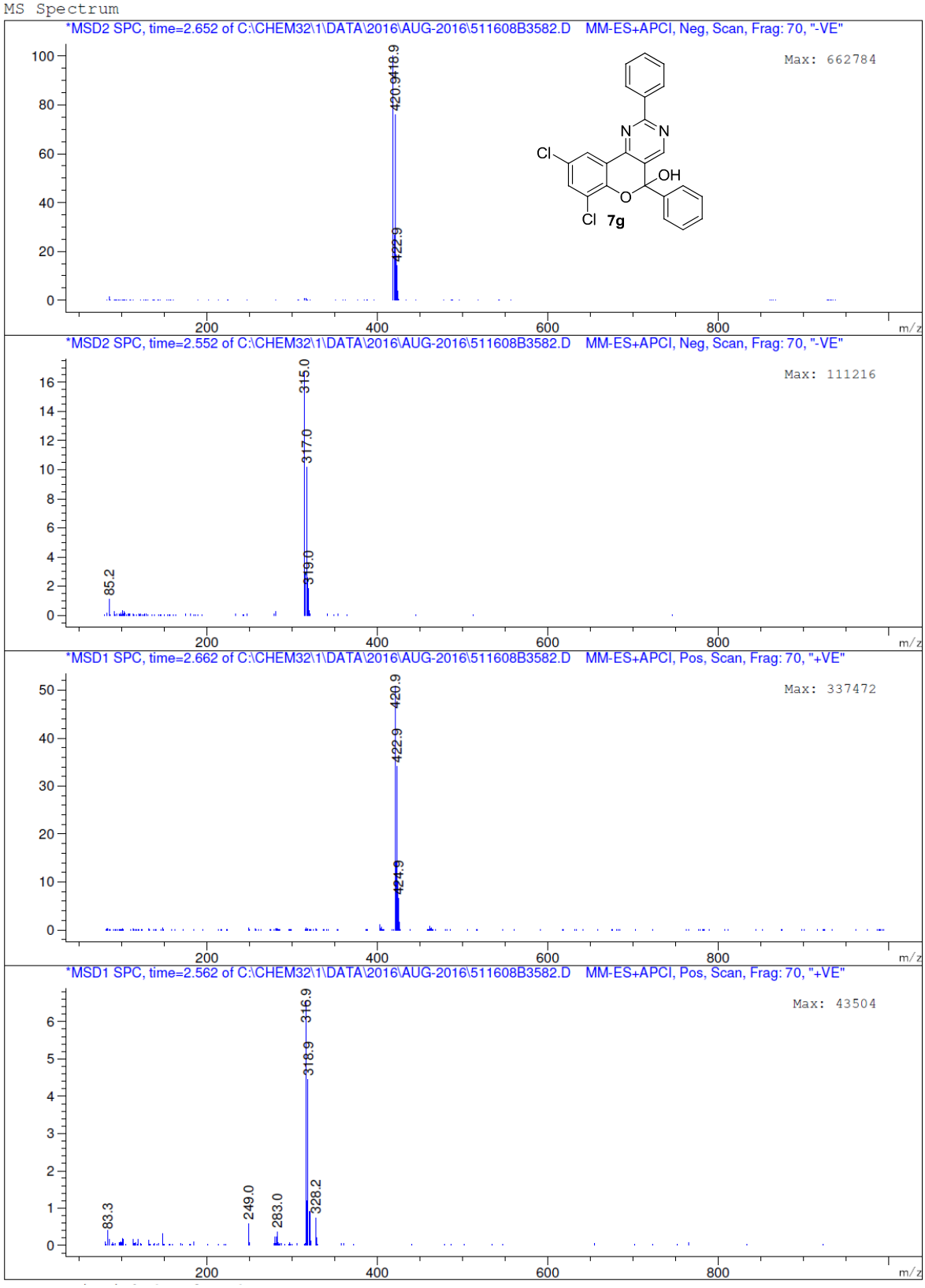
GVK BIOSCIENCES PVT. LTD.
MEDICINAL CHEMISTRY LABORATORY - ANALYTICAL RESEARCH
LCMS REPORT

```
================================================================================================
Sample Name      :GVK-SAM-6-PAGE-4POLAR                        Vial position  : P1-C-02
Date of Analysis :8/16/2016        9:08:01 PM                  Injection Vol  :0.500µl
Acq. Method      :C:\CHEM32\1\METHODS\RND-FA- 3.5 MIN.M        Instrument ID  :ANL-MCL5-LCMS-001
================================================================================================
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, 0.4/2, 2.8/98,3.4/98,3.41/2,3.5/2
Column Flow Rate: 0.6 ml/min
Column Temperature: 60°C
                                                                                          ->
```



Pea No	RT min	Area	Area %
1	1.17	4.740	0.416
2	1.81	1.947	0.171
3	2.55	167.448	14.705
4	2.64	904.193	79.406
5	2.71	14.294	1.255
6	2.75	24.465	2.149
7	2.89	6.521	0.573
8	2.92	11.155	0.980
9	2.98	3.929	0.345

MS Spectrum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Max: 662784
420.9
418.9
422.9
Cl
N
N
OH
O
Cl
7g
*MSD2 SPC, time=2.552 of C:\CHEM32\1\DATA\2016\AUG-2016\511608B3582.D MM-ES+APCI, Neg, Scan, Frag: 70, "-VE"
Max: 111216
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317.0
319.0
85.2
*MSD1 SPC, time=2.662 of C:\CHEM32\1\DATA\2016\AUG-2016\511608B3582.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 337472
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Max: 43504
316.9
318.9
328.2
249.0
283.0
83.3
m/z

Elemental Composition Report

Single Mass Analysis

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

Selected filters: None

Monoisotopic Mass, Even Electron Ions

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

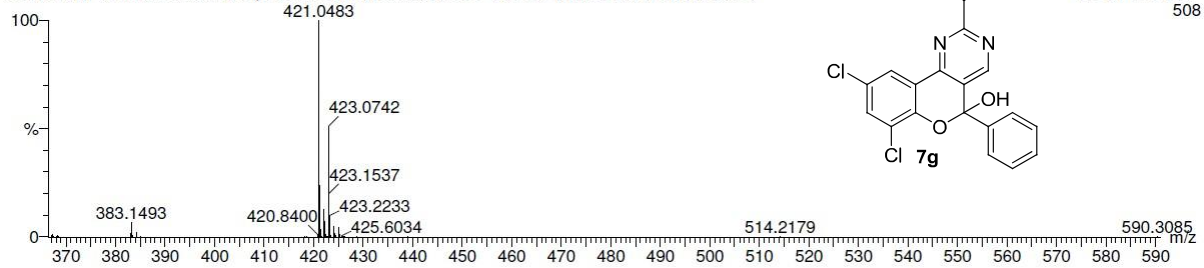
Elements Used:

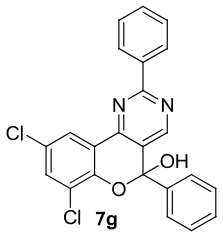
C: 0-23 H: 0-15 N: 0-2 O: 0-2 Cl: 0-2

SAMPLE CODE:GVK-SAM-6-PAGE-4 POLAR

511701A2143 38 (0.552) AM (Top,4, Ar,5000.0,195.18,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

1: TOF MS ES+
508

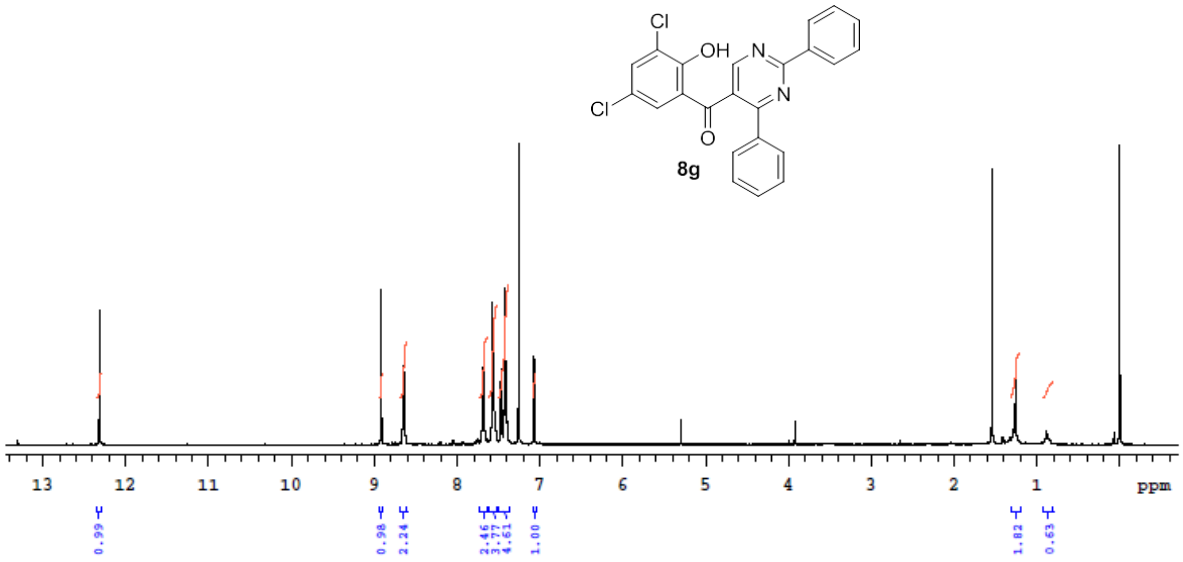




Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
421.0483	421.0511	-2.8	-6.7	16.5	28.6	C23 H15 N2 O2 Cl2

Sample Name:
GVK-SAM-6-PAGE-4ND

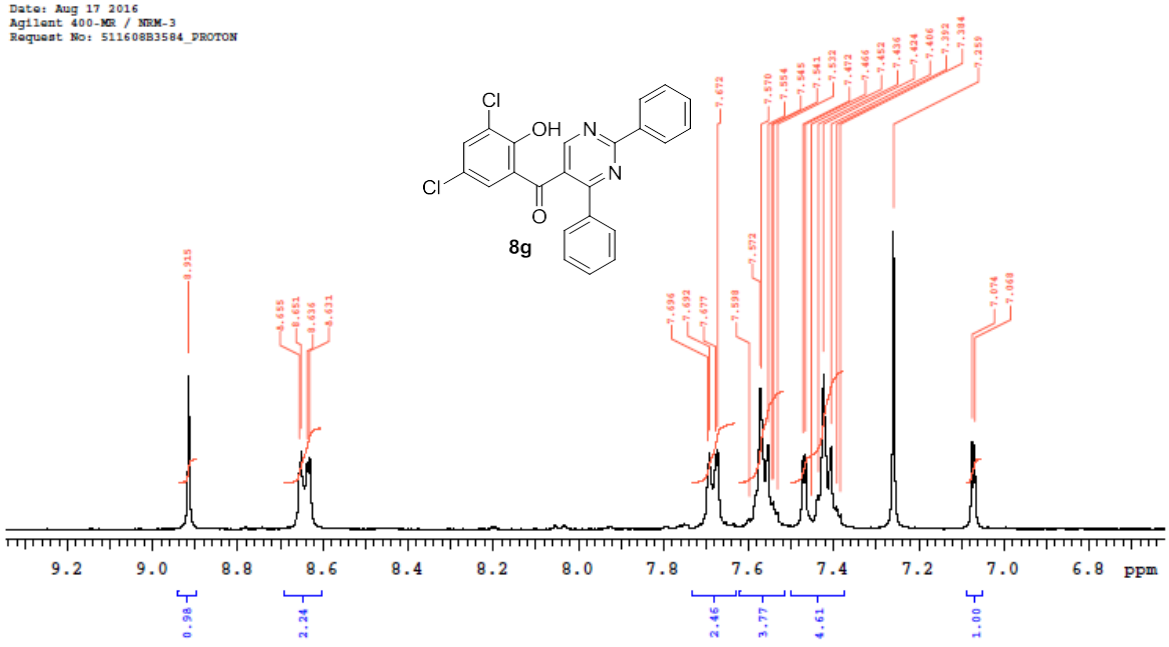
Solvent: cdcl3
Date: Aug 17 2016
Agilent 400-MR / NRM-3
Request No: 511608B3584_PROTON



Plotname: 511608B3584_PROTON_01_plot01

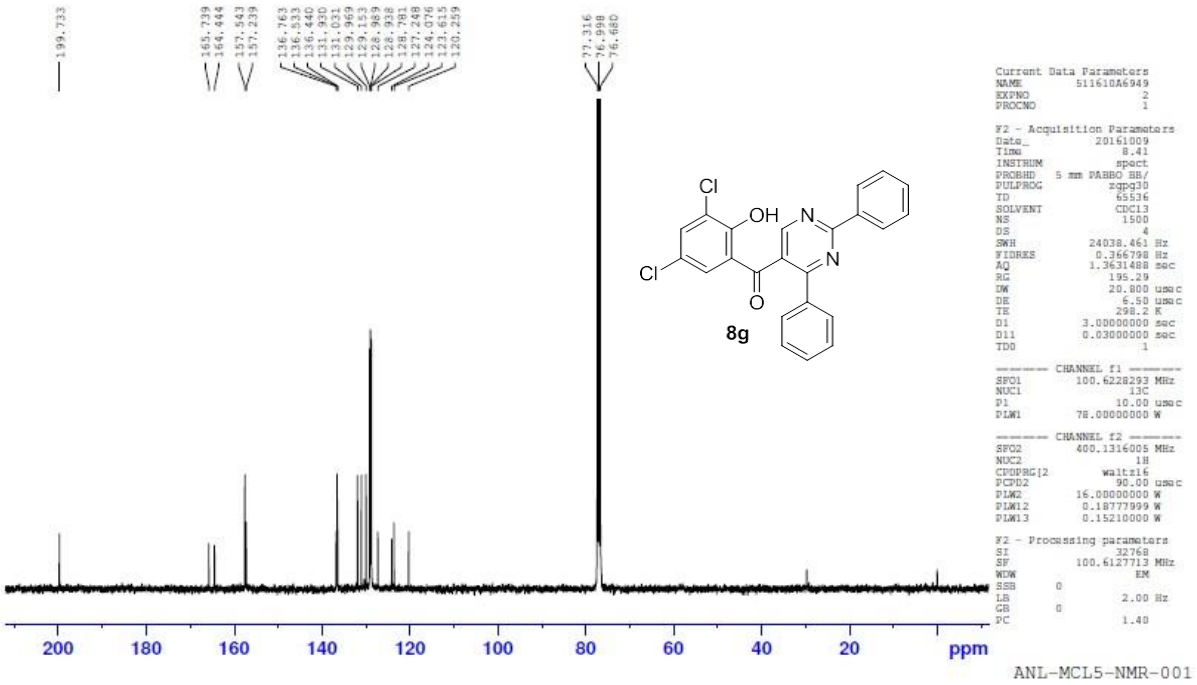
Sample Name:
GVK-SAM-6-PAGE-4ND

Solvent: cdcl3
Date: Aug 17 2016
Agilent 400-MR / NRM-3
Request No: 511608B3584_PROTON



Plotname: 511608B3584_PROTON_01_plot02

GVK-SAM-6-page-4NP

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Current Data Parameters
NAME          511610A6949
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20161009
Time                8.41
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                1500
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               298.2 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          100.6127713 MHz
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LB                 2.00 Hz
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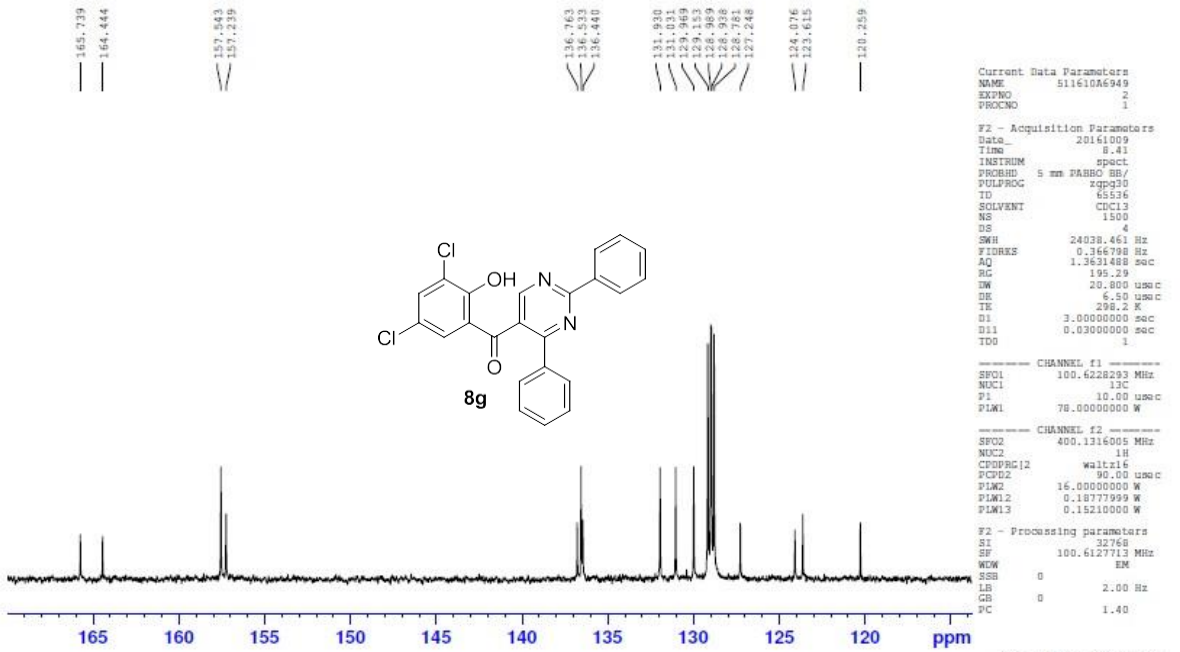
ANL-MCL5-NMR-001

GVK-SAM-6-page-4NP

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Current Data Parameters
NAME          511610A6949
EXPNO                   2
PROCNO                  1

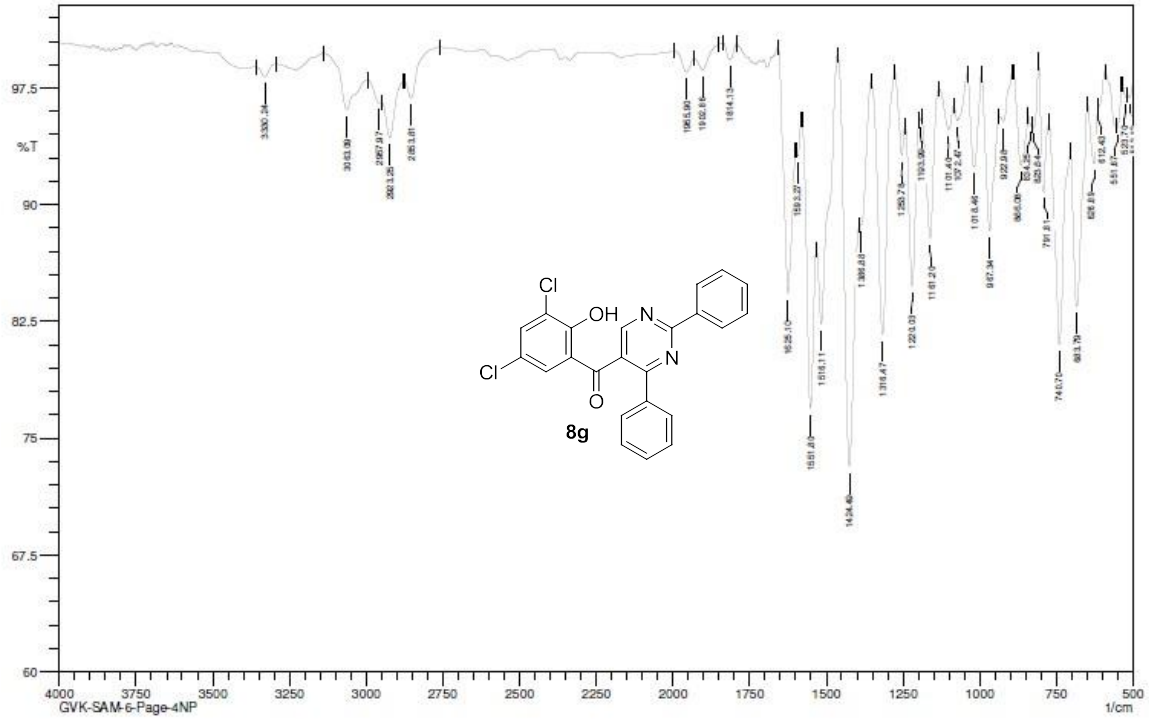
F2 - Acquisition Parameters
Date_           20161009
Time                8.41
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                1500
DS                   4
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG               195.29
DW               20.800 usec
DE                6.50 usec
TE               298.2 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          100.6127713 MHz
WDW                EM
SSB                0
LB                 2.00 Hz
GB                 0
PC                 1.40
```

ANL-MCL5-NMR-001



Comment: IN Kbr
$(IR Spectrum|DESCRIPTION)

No. of Scans:
Resolution:
Apodization:

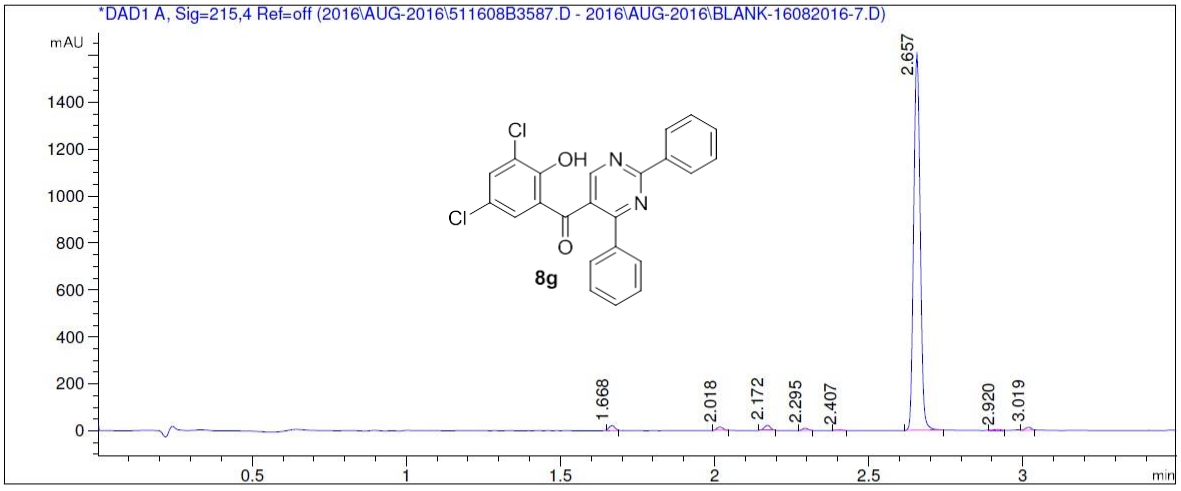
Date: 10/3/2016 9:35:27 AM
User: Admin

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

Sample Name :GVK-SAM-6-PAGE-4NP Vial position : P1-B-07
Date of Analysis :8/16/2016 8:41:20 PM Injection Vol :0.500µl
Acq. Method :C:\CHEM32\1\METHODS\RND-FA- 3.5 MIN.M Instrument ID :ANL-MCL5-LCMS-001

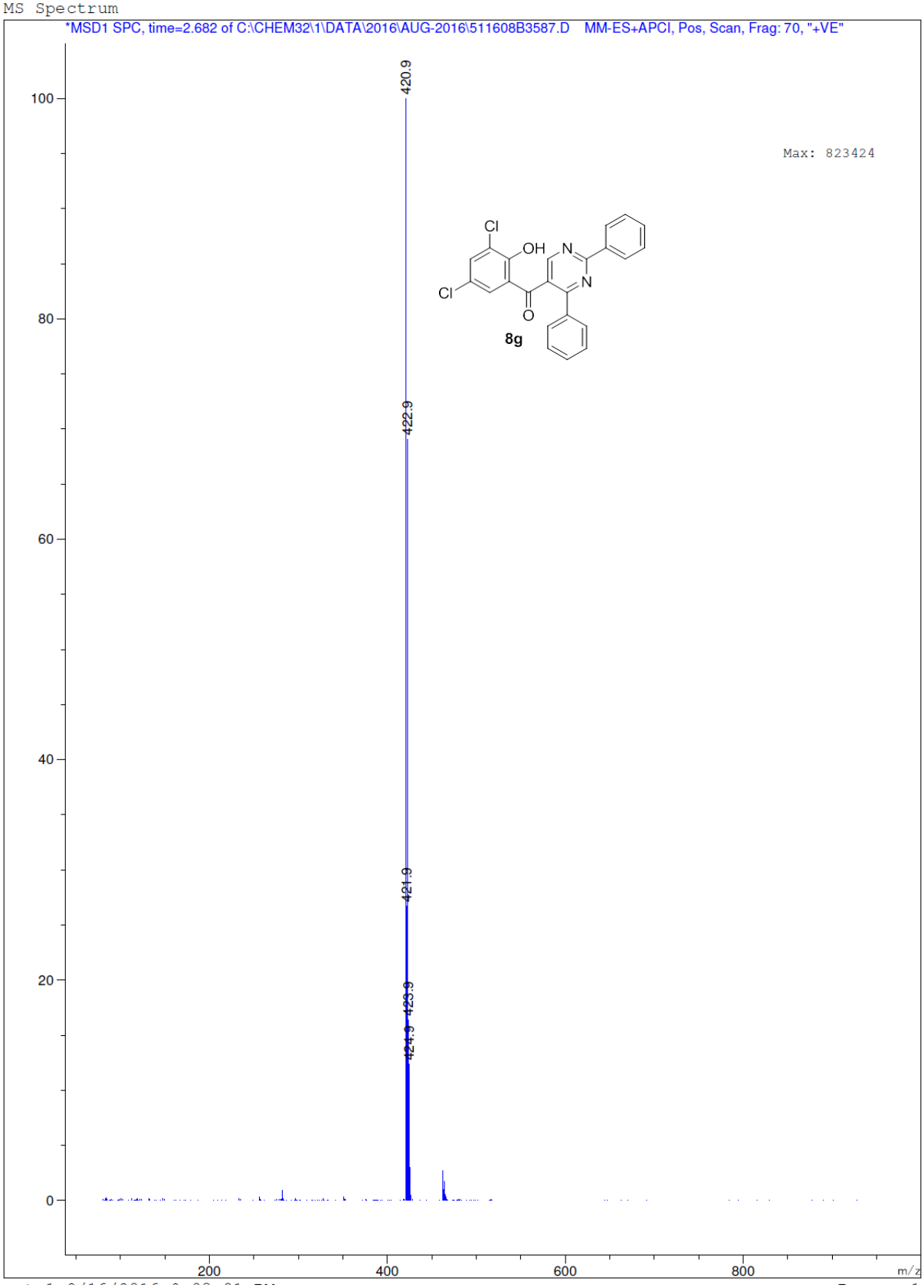
RND-FA-3.5 MIN.M
Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: B1: 0.1 % FA IN WATER A1: 0.1%FA IN ACN
Gradient: Time (min) /%A1: 0/2, 0.4/2, 2.8/98,3.4/98,3.41/2,3.5/2
Column Flow Rate: 0.6 ml/min
Column Temperature: 60°C

->



Peak No	RT min	Area	Area %
1	1.67	29.772	1.196
2	2.02	17.808	0.716
3	2.17	23.815	0.957
4	2.29	10.580	0.425
5	2.41	2.399	0.096
6	2.66	2376.283	95.479
7	2.92	9.834	0.395
8	3.02	18.317	0.736

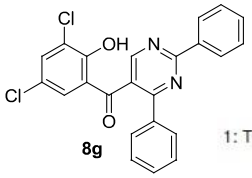
MS Spectrum


*MSD1 SPC, time=2.682 of C:\CHEM32\1\DATA\2016\AUG-2016\511608B3587.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 823424
420.9
422.9
421.9
423.9
424.9
Cl
OH
N
N
Cl
O
8g
100
80
60
40
20
0
200
400
600
800
m/z

Elemental Composition Report **Page 1**

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

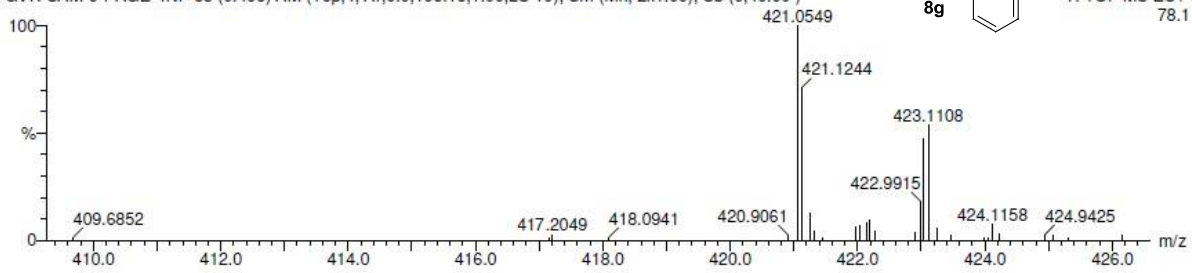
Monoisotopic Mass, Odd and Even Electron Ions
21 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-23 H: 0-15 N: 0-2 O: 0-2 Cl: 0-2



8g

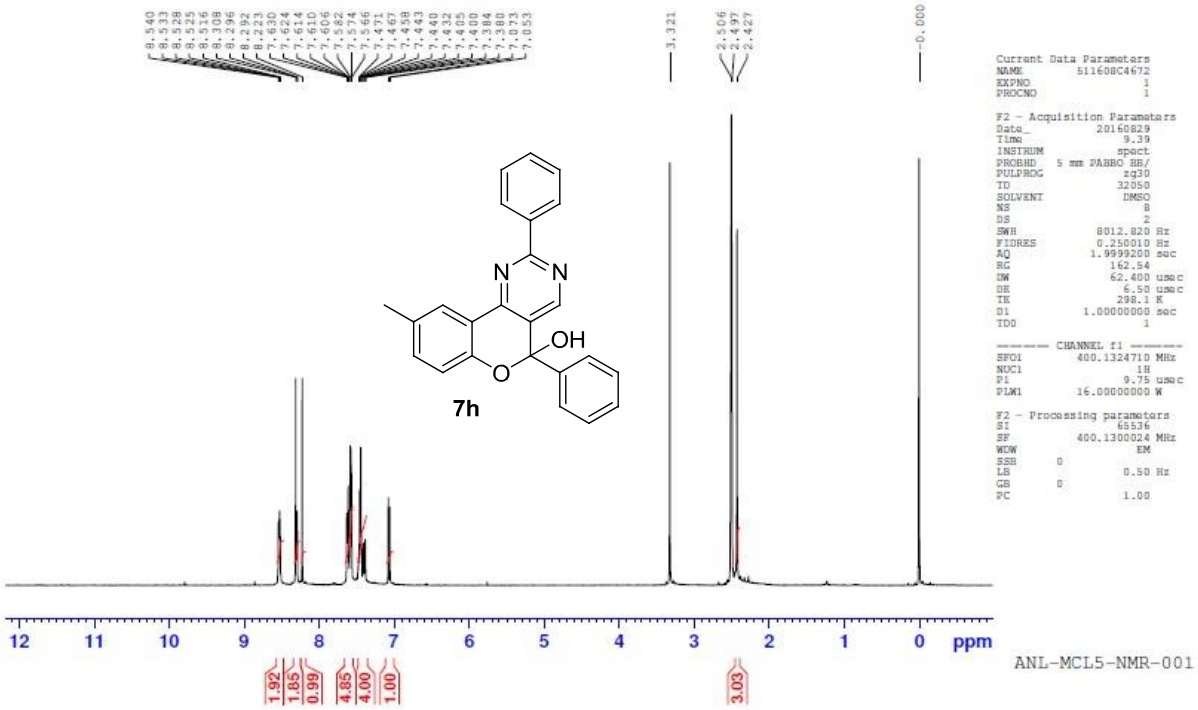
GVK-SAM-6-PAGE-4NP
GVK-SAM-6-PAGE-4NP 35 (0.493) AM (Top,4, Ar,0.0,195.18,1.00,LS 10); Sm (Mn, 2x1.00); Sb (0,40.00)

1: TOF MS ES+
78.1

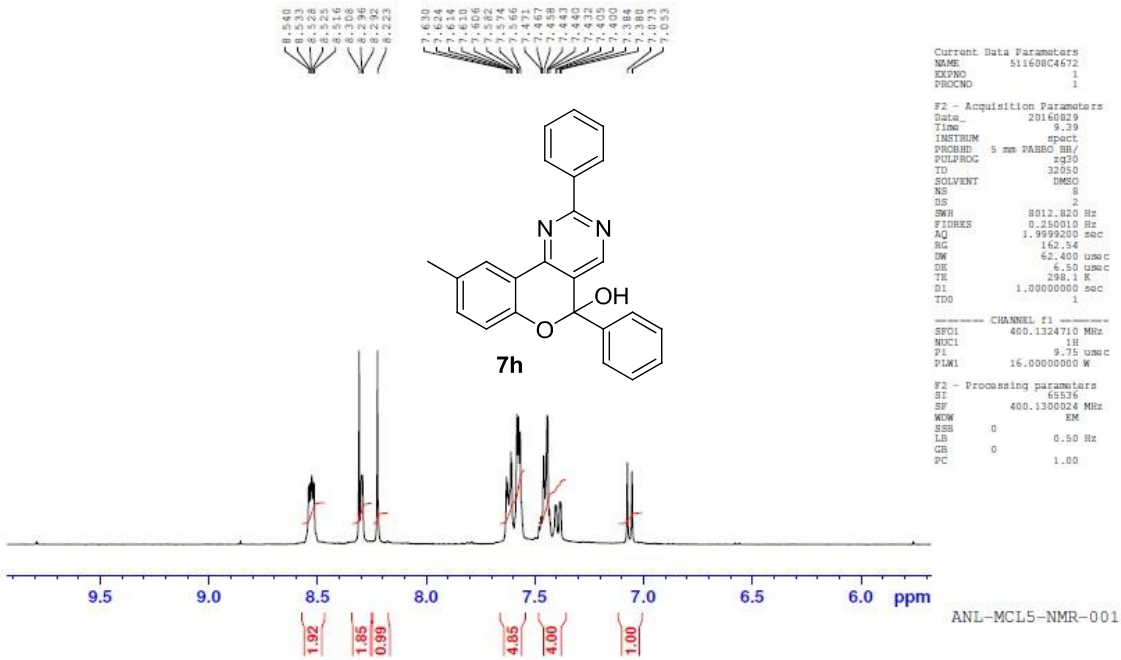


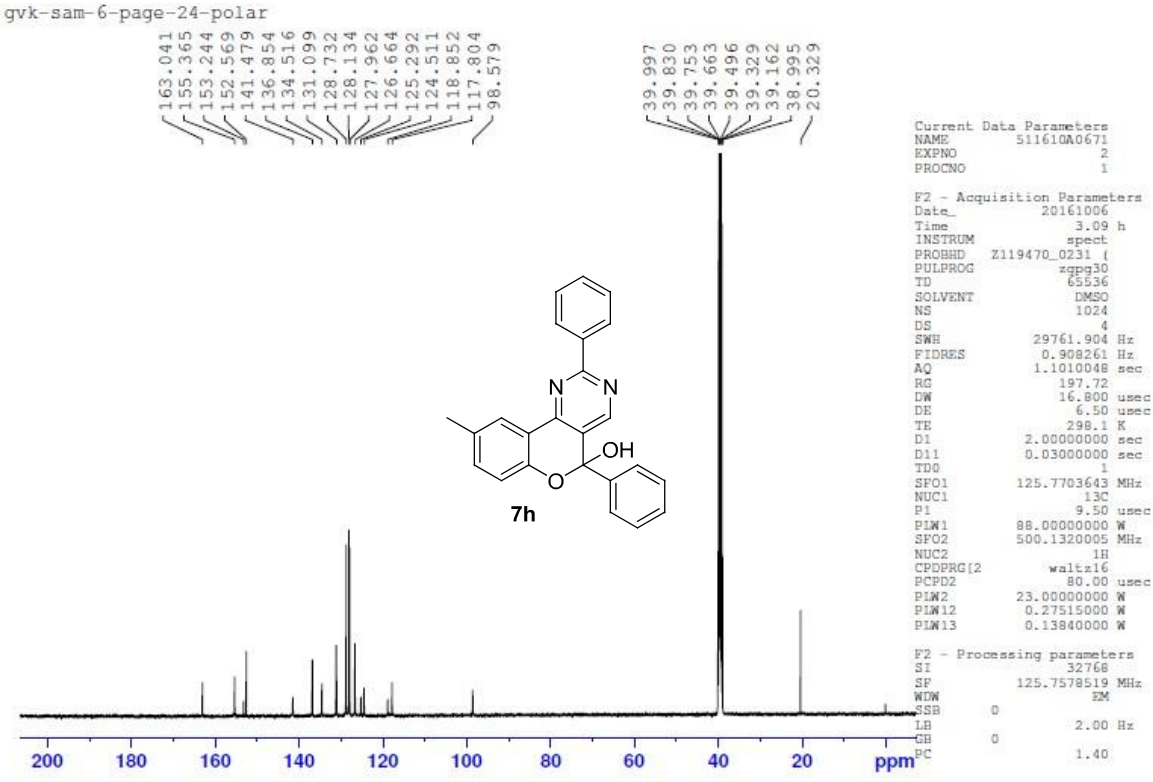
Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
421.0549	421.0511	3.8	9.0	16.5	11.3	C23 H15 N2 O2 Cl2

GVK-SAM-6-PAGE-24 POLAR



GVK-SAM-6-PAGE-24 POLAR




gvk-sam-6-page-24-polar
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153.244
152.569
141.479
136.854
134.516
131.099
128.732
128.134
127.962
126.664
125.292
124.511
118.852
117.804
98.579
39.997
39.830
39.753
39.663
39.496
39.329
39.162
38.995
20.329
OH
7h
200
180
160
140
120
100
80
60
40
20
ppm
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NAME 511610A0671
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161006
Time 3.09 h
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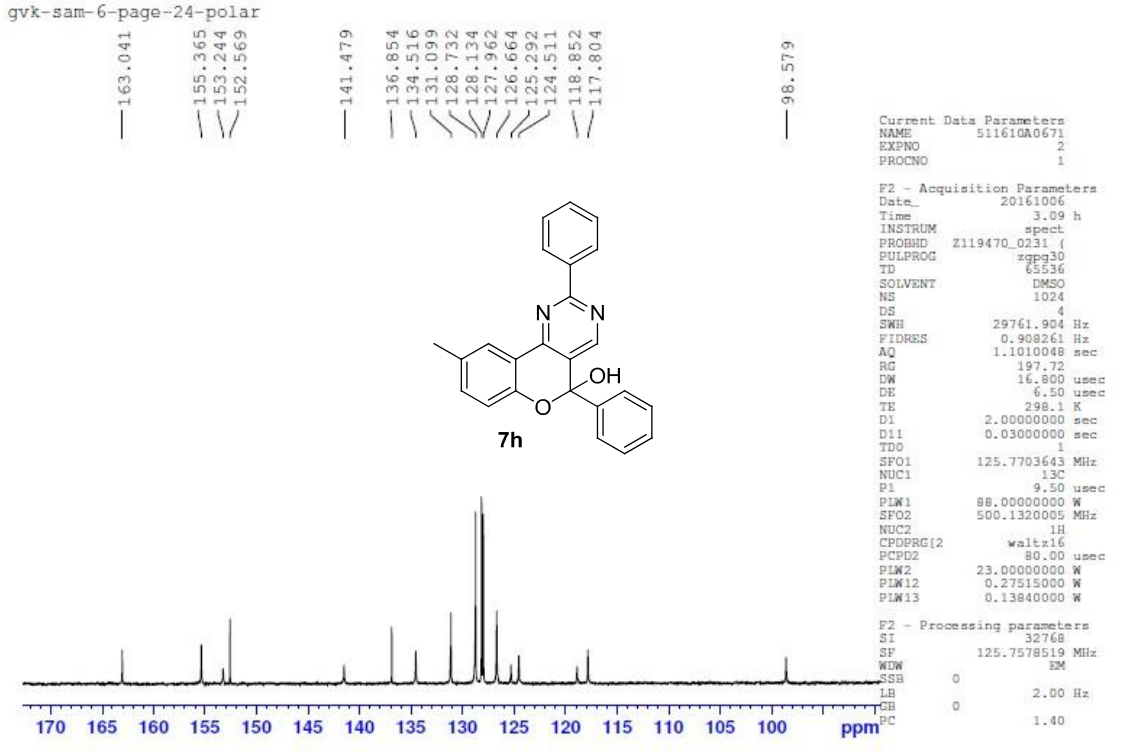
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7578519 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40


gvk-sam-6-page-24-polar
163.041
155.365
153.244
152.569
141.479
136.854
134.516
131.099
128.732
128.134
127.962
126.664
125.292
124.511
118.852
117.804
98.579
OH
7h
170
165
160
155
150
145
140
135
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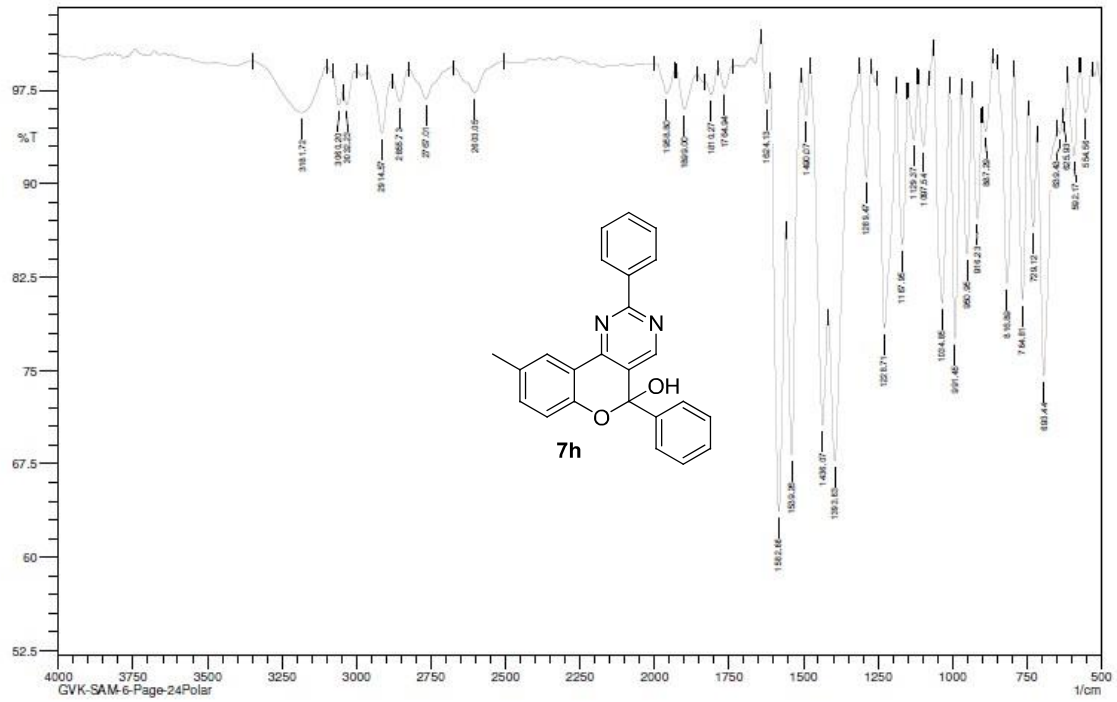
125
120
115
110
105
100
ppm
Current Data Parameters
NAME 511610A0671
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161006
Time 3.09 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 298.1 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7578519 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

SHIMADZU



7h

Comment: IN Kbr
GVK-SAM-6-Page-24Polar

No. of Scans:
Resolution:
Apodization:

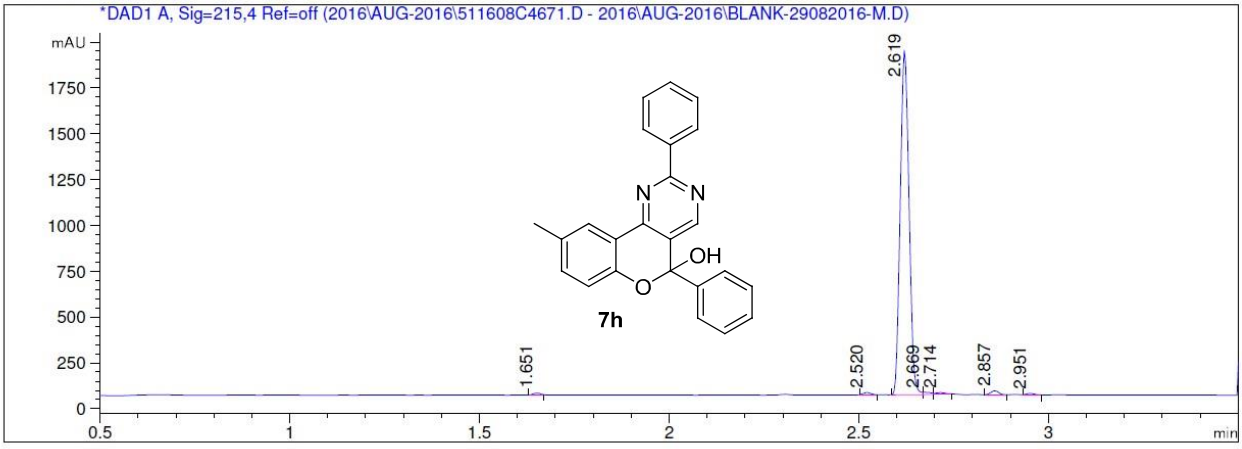
Date: 10/3/2016 9:58:45 AM
User: Admin

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

LCMS REPORT

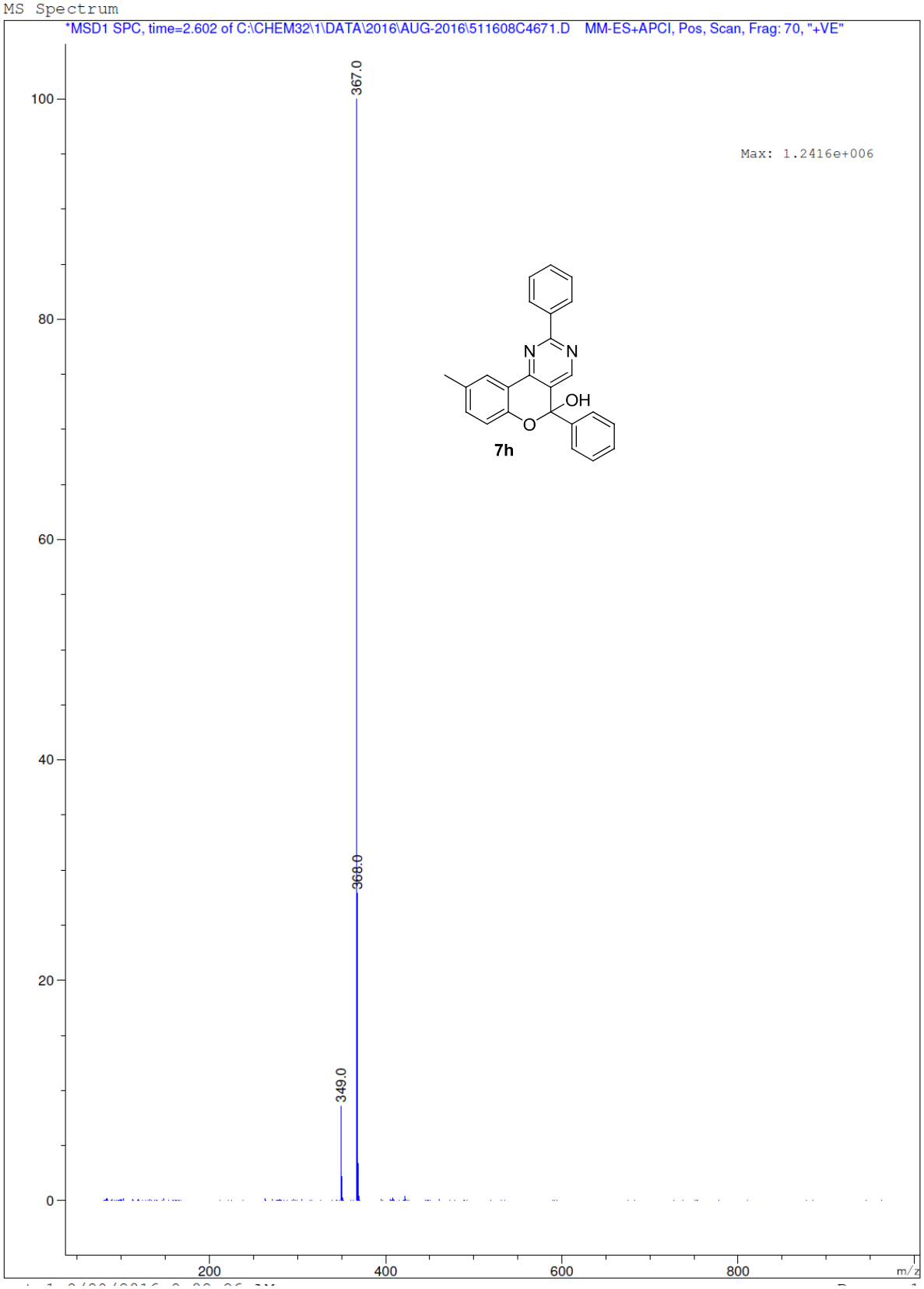
Sample Name :GVK-SAM-6-PAGE-24POLAR Vial position :P1-A-06
Date of Analysis:29/08/2016;7:45:10 AM Injection Vol: 0.5 µL
Acq. Method->C:\CHEM32\1\METHODS\RND-FA- 3.5 MIN.M Instrument ID:ANL-MCL5-LCMS-001
C:\CHEM32\1\DATA\2016\AUG-2016\511608C4671.D

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, 0.4/2, 2.8/98,3.4/98,3.41/2,3.5/2
Column Flow Rate: 0.6 ml/min
Column Temperature: 60°C ->



Peak No	RT min	Area	Area %
1	1.65	16.331	0.521
2	2.52	20.588	0.657
3	2.62	3020.892	96.350
4	2.67	15.544	0.496
5	2.71	18.607	0.593
6	2.86	35.877	1.144
7	2.95	7.499	0.239

MS Spectrum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Max: 1.2416e+006
367.0
368.0
349.0
100
80
60
40
20
0
200
400
600
800
m/z
N
N
OH
O
7h

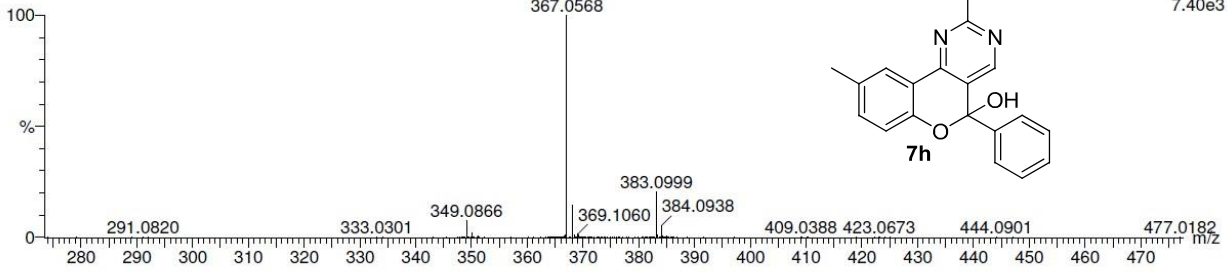
Single Mass Analysis

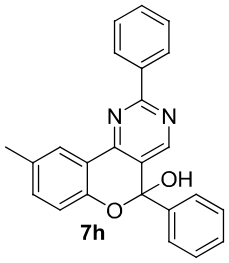
Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
4 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-24 H: 0-19 N: 0-2 O: 0-2

SAMPLE CODE:GVK-SAM-6-PAGE-24 POLAR
511701A2151 31 (0.452) AM (Top,4, Ar,5000.0,195.14,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

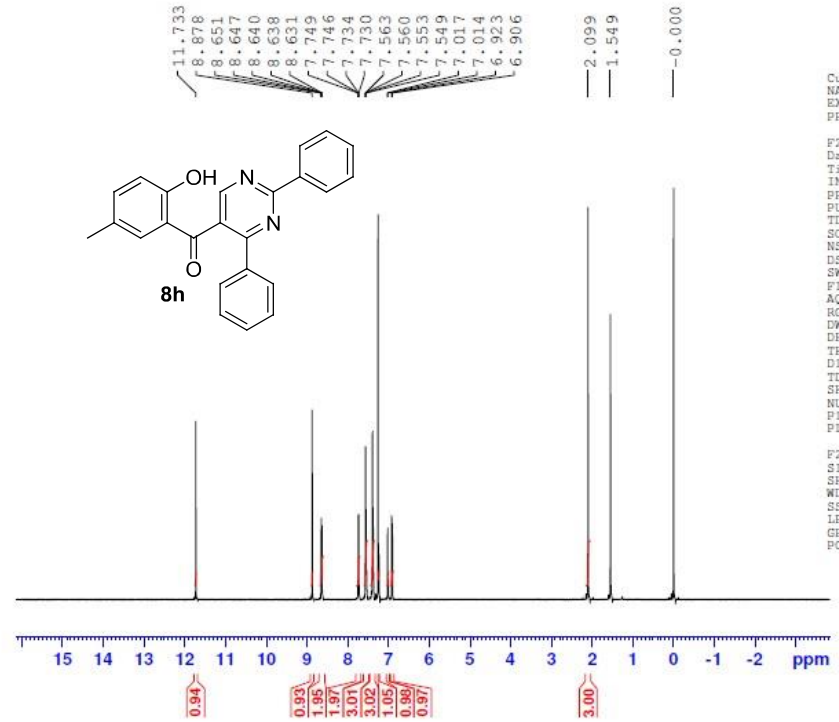
1: TOF MS ES+
7.40e3





Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
367.0568	367.1447	-87.9	-239.5	16.5	1717.9	C24 H19 N2 O2

GVK-SAM-6-page-24NP

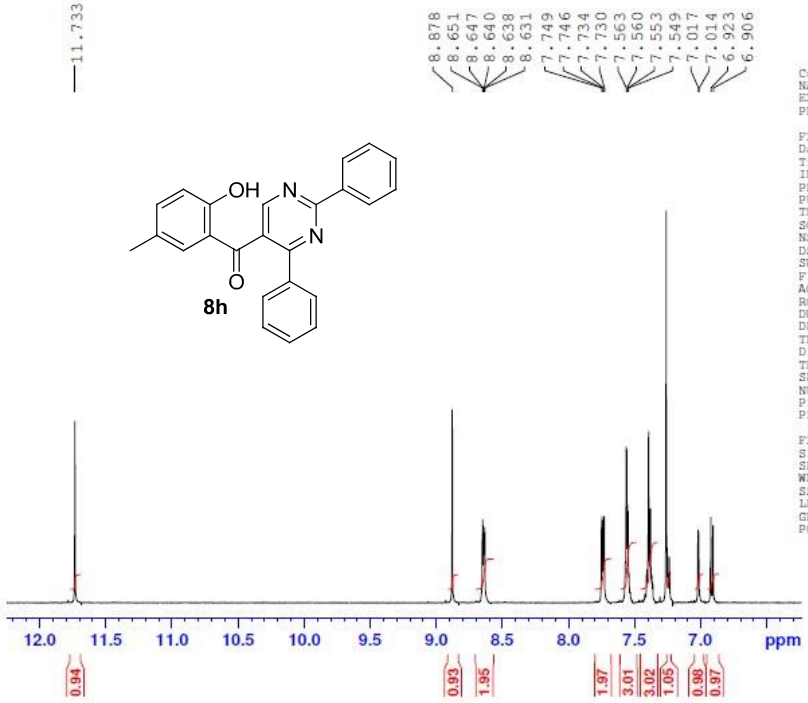



```
Current Data Parameters
NAME          511608C4670
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20160829
Time                10.30 h
INSTRUM              spect
PROBHD   Z119470_0231 (
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      8
DS                      0
SWH           10000.000 Hz
FIDRES            0.305176 Hz
AQ             3.2767999 sec
RG                 157.05
DW                50.000 usec
DE                 6.50 usec
TE                298.2 K
D1             1.00000000 sec
TD0                     1
SFO1          500.1330885 MHz
NUC1                   1H
P1                  8.75 usec
PLW1          23.00000000 W

F2 - Processing parameters
SI                  65536
SF            500.1300127 MHz
WDW                    EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

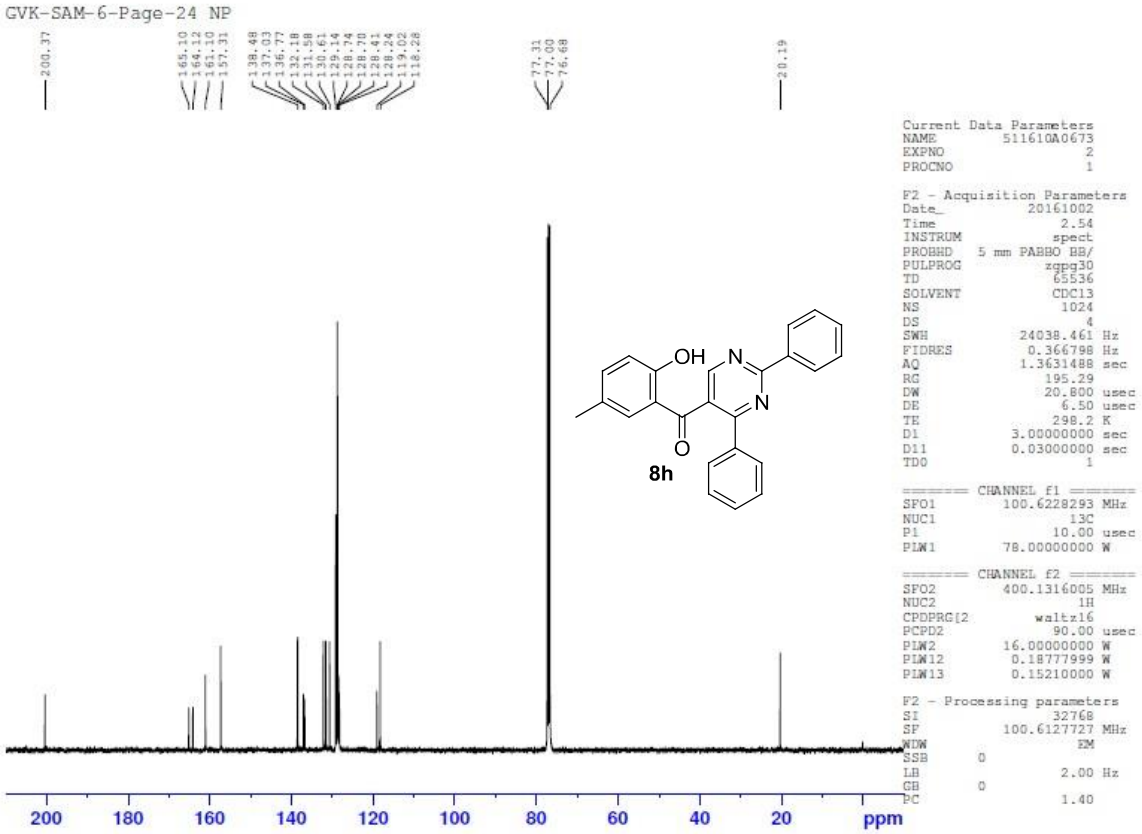
GVK-SAM-6-page-24NP




```
Current Data Parameters
NAME          511608C4670
EXPNO                   1
PROCNO                  1

F2 - Acquisition Parameters
Date_            20160829
Time                10.30 h
INSTRUM              spect
PROBHD   Z119470_0231 (
PULPROG              zg30
TD                  65536
SOLVENT             CDCl3
NS                      8
DS                      0
SWH           10000.000 Hz
FIDRES            0.305176 Hz
AQ             3.2767999 sec
RG                 157.05
DW                50.000 usec
DE                 6.50 usec
TE                298.2 K
D1             1.00000000 sec
TD0                     1
SFO1          500.1330885 MHz
NUC1                   1H
P1                  8.75 usec
PLW1          23.00000000 W

F2 - Processing parameters
SI                  65536
SF            500.1300127 MHz
WDW                    EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



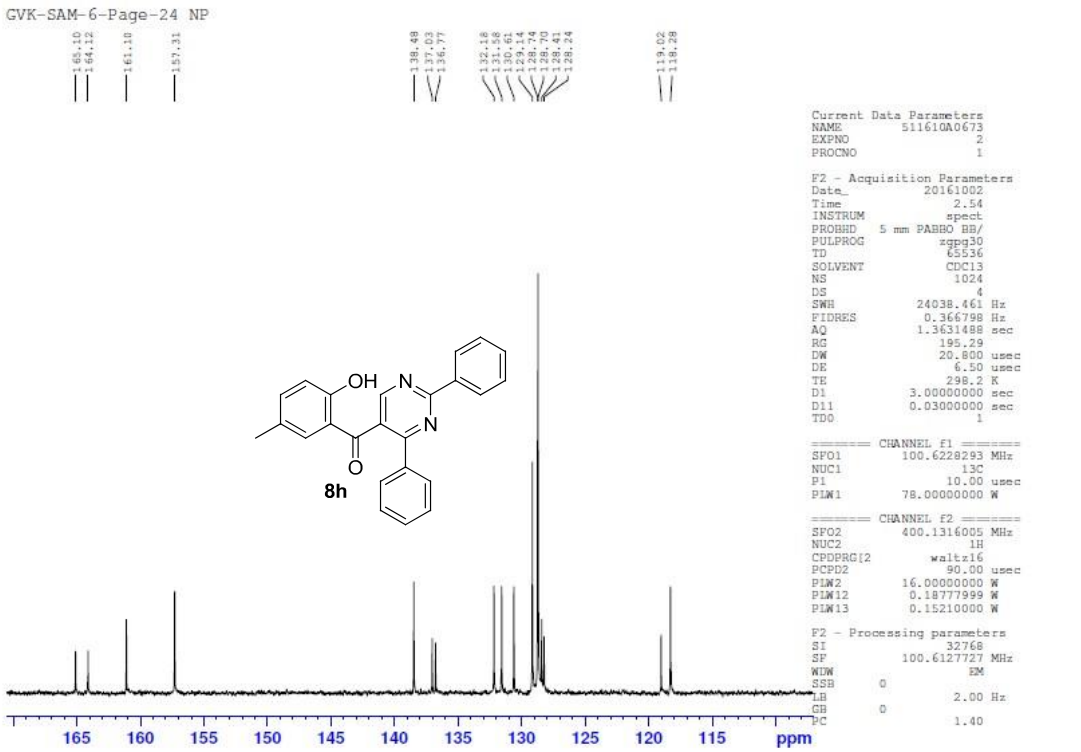
Current Data Parameters
NAME 511610A0673
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161002
Time 2.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
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 298.2 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 100.6127727 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40



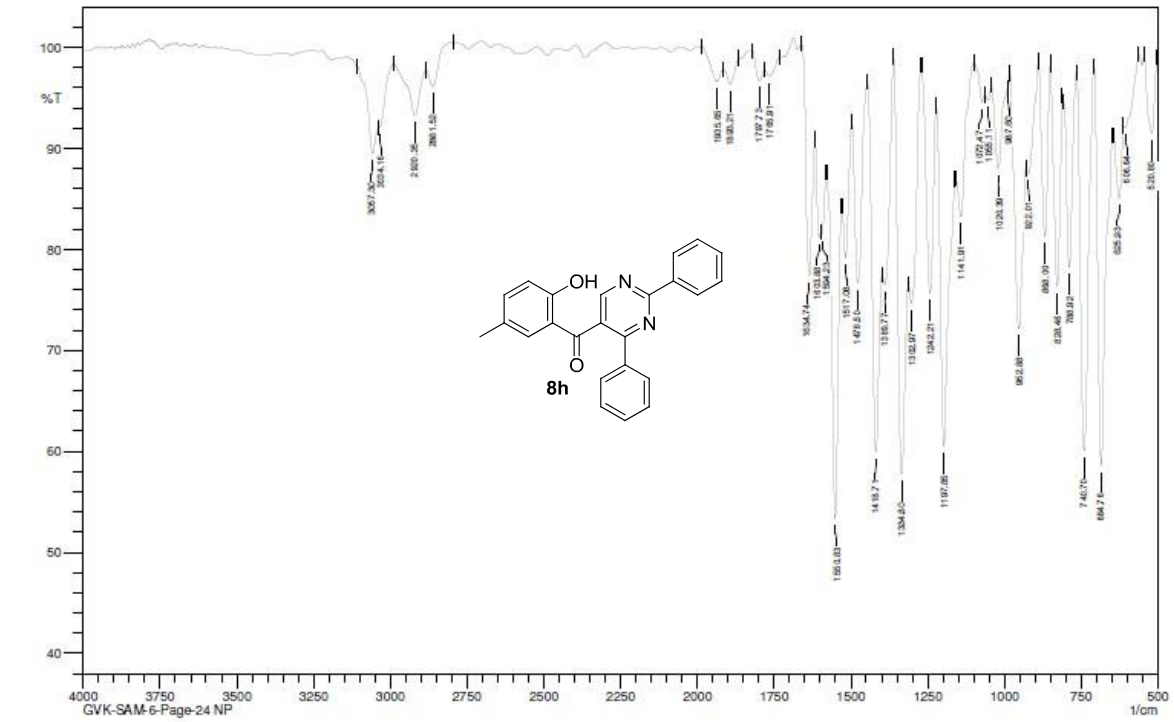
Current Data Parameters
NAME 511610A0673
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161002
Time 2.54
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
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 298.2 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 100.6127727 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40



Comment: IN Kbr
GVK-SAM-6-Page-24 NP

No. of Scans:
Resolution:
Apodization:

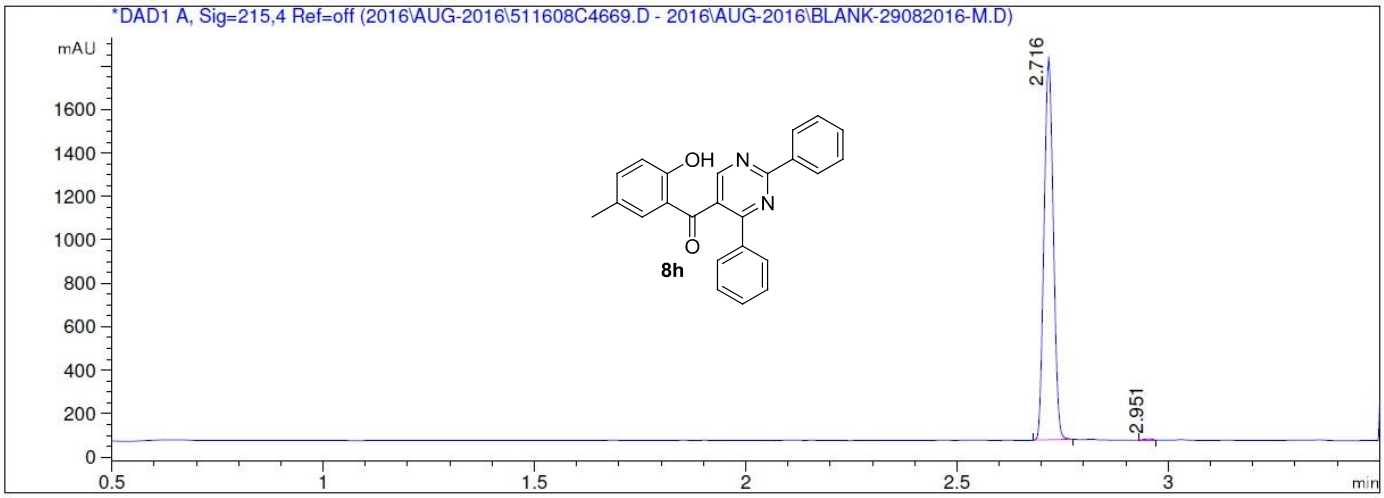
Date: 10/3/2016 10:48:45 AM
User: Admin

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

LCMS REPORT

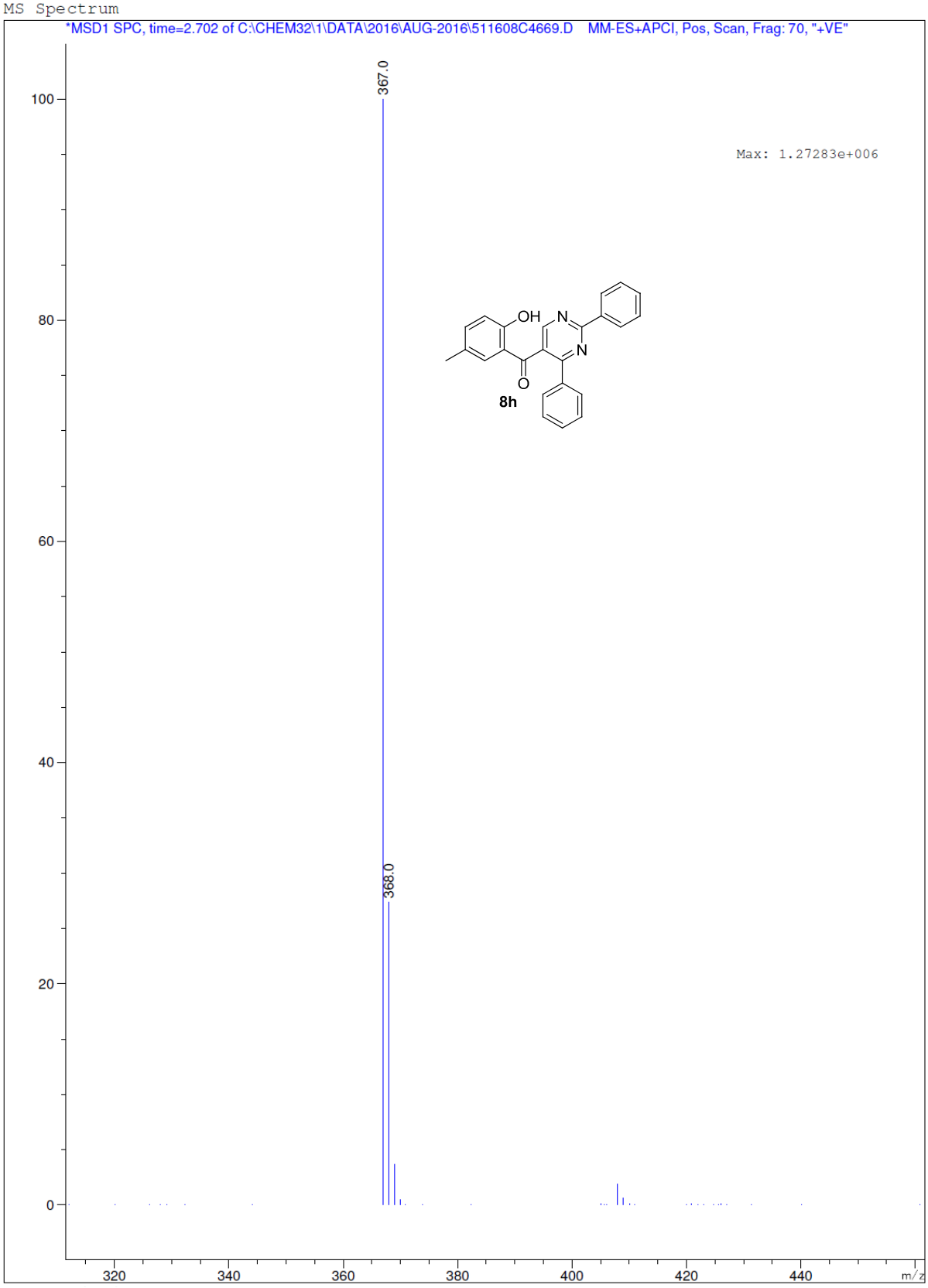
Sample Name :GVK-SAM-6-PAGE-24NP Vial position :P1-A-05
Date of Analysis:29/08/2016;7:40:43 AM Injection Vol: 0.5 µL
Acq. Method->C:\CHEM32\1\METHODS\RND-FA- 3.5 MIN.M Instrument ID:ANL-MCL5-LCMS-001
C:\CHEM32\1\DATA\2016\AUG-2016\511608C4669.D

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, 0.4/2, 2.8/98,3.4/98,3.41/2,3.5/2
Column Flow Rate: 0.6 ml/min
Column Temperature: 60°C ->



Pea No	RT min	Area	Area %
1	2.72	2670.468	99.745
2	2.95	6.838	0.255

MS Spectrum


*MSD1 SPC, time=2.702 of C:\CHEM32\1\DATA\2016\AUG-2016\511608C4669.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 1.27283e+006
367.0
368.0
OH
N
N
O
8h
100
80
60
40
20
0
320
340
360
380
400
420
440
m/z

Elemental Composition Report

Single Mass Analysis

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

Selected filters: None

Monoisotopic Mass, Even Electron Ions

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

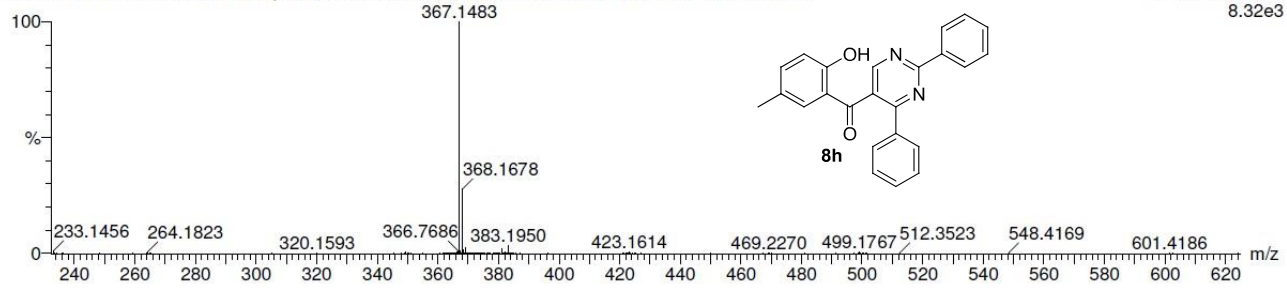
Elements Used:

C: 0-24 H: 0-19 N: 0-2 O: 0-2

SAMPLE CODE:GVK-SAM-6-PAGE-24 NP

511701A2184 32 (0.464) AM (Top,4, Ar,5000.0,195.18,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

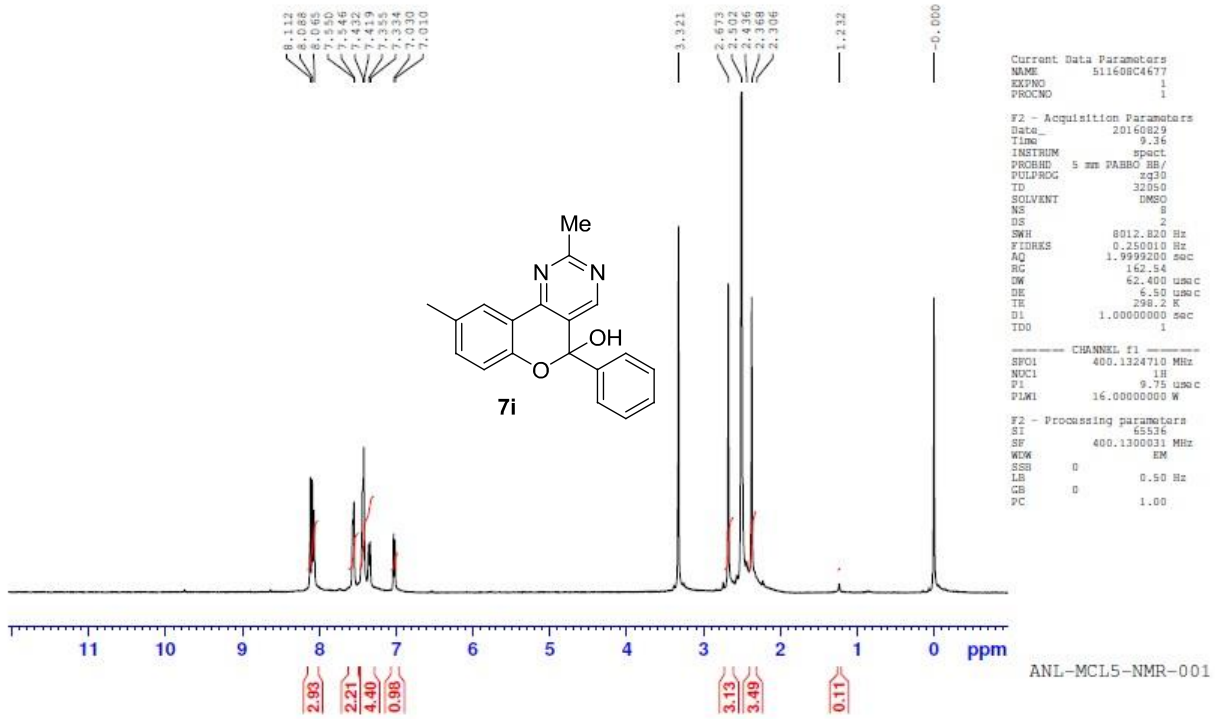
1: TOF MS ES+
8.32e3



8h

Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
367.1483	367.1447	3.6	9.8	16.5	80.4	C24 H19 N2 O2

GVK-SAM-6-PAGE-25 POLAR



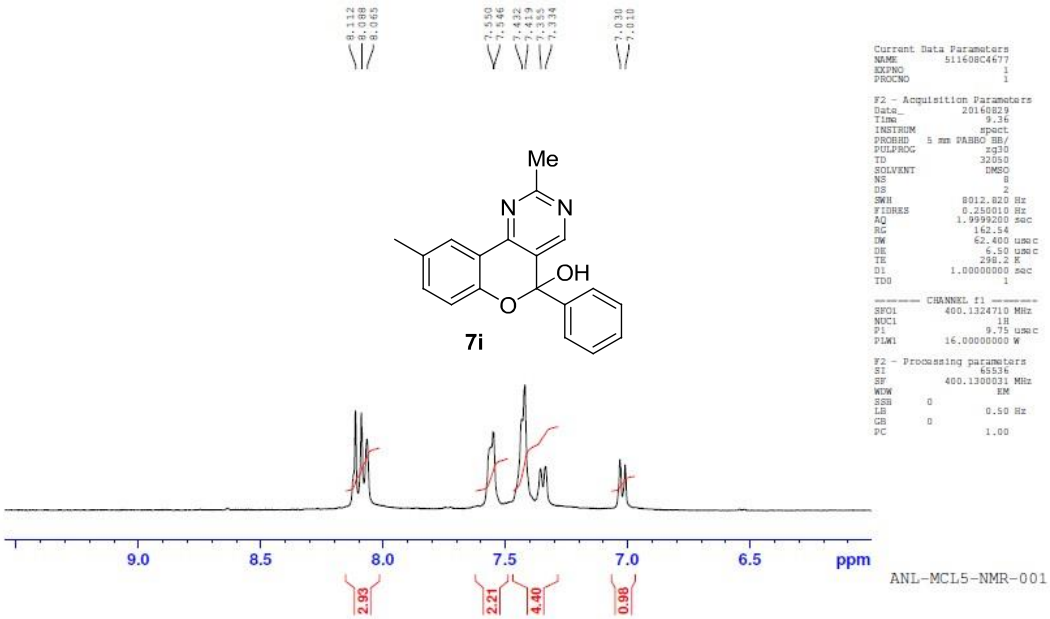
Current Data Parameters
NAME 511608C4677
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160829
Time 9.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32050
SOLVENT DMSO
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.250010 Hz
AQ 1.9999200 sec
RG 162.54
DW 62.400 usec
DE 6.50 usec
TE 298.2 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 400.1300031 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00

GVK-SAM-6-PAGE-25 POLAR

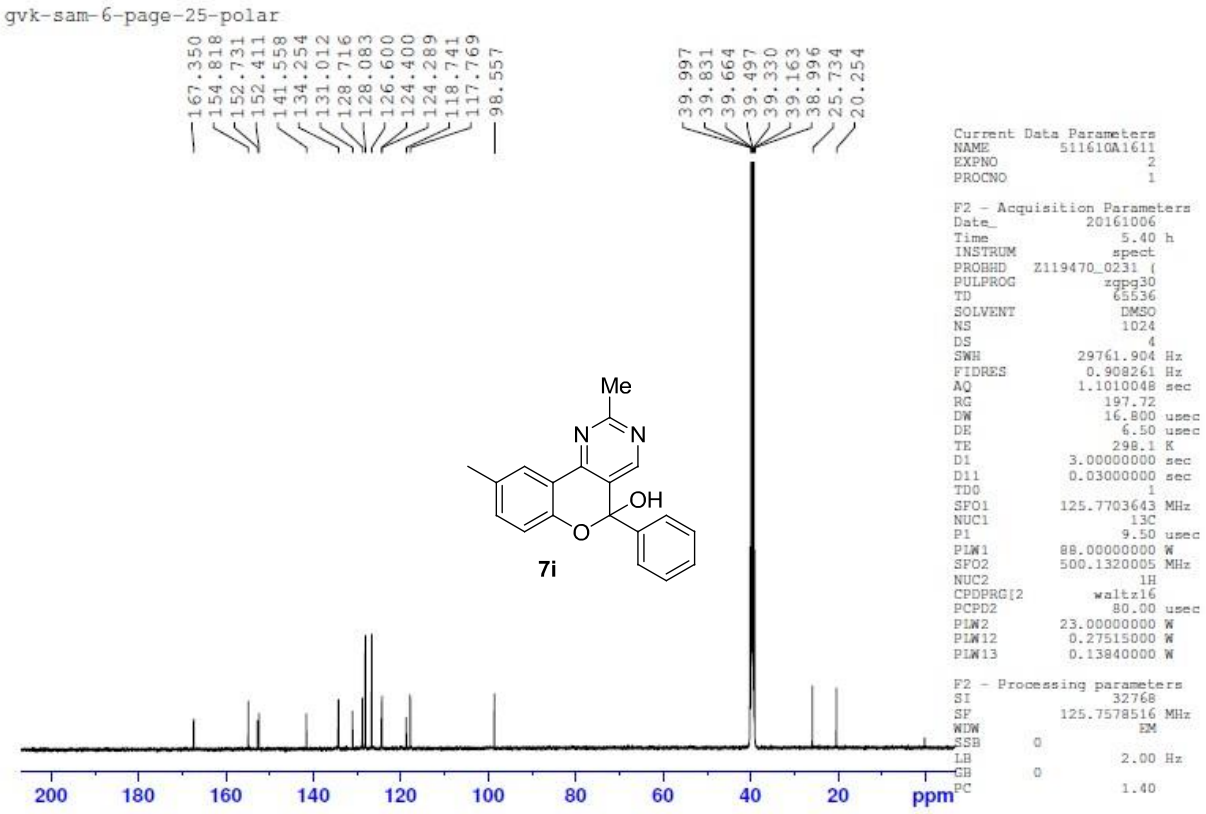


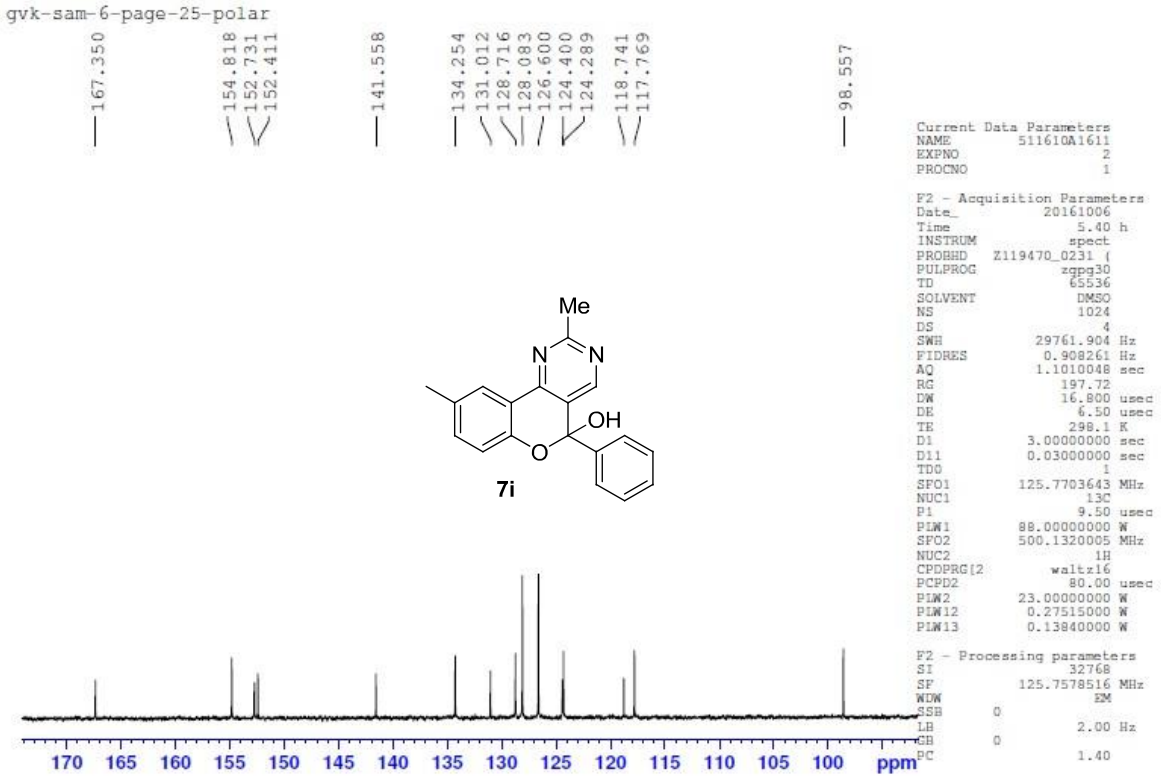
Current Data Parameters
NAME 511608C4677
EXPNO 1
PROCNO 1

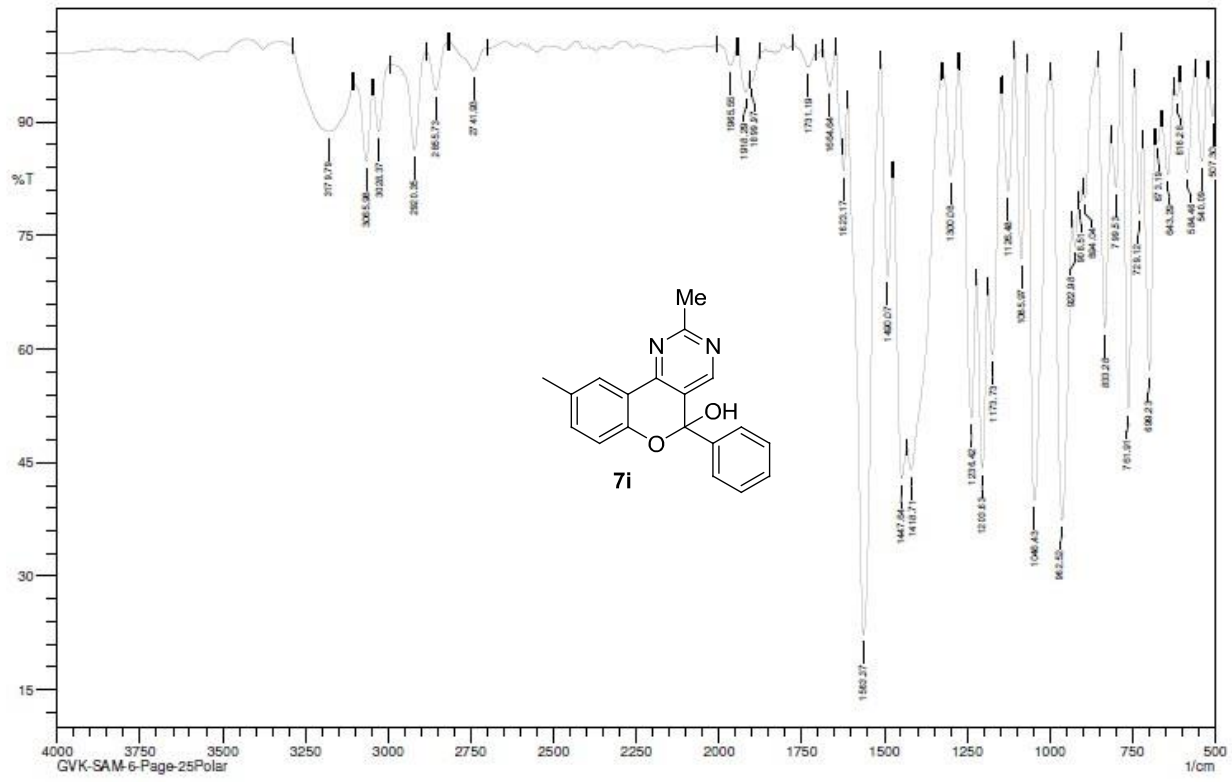
F2 - Acquisition Parameters
Date_ 20160829
Time 9.36
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32050
SOLVENT DMSO
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.250010 Hz
AQ 1.9999200 sec
RG 162.54
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 65536
SF 400.1300031 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00


gvk-sam-6-page-25-polar
167.350
154.818
152.731
152.411
141.558
134.254
131.012
128.716
128.083
126.600
124.400
124.289
118.741
117.769
98.557
39.997
39.831
39.664
39.497
39.330
39.163
38.996
25.734
20.254
Me
N
N
OH
O
7i
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME 511610A1611
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161006
Time 5.40 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 298.1 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7578516 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40


gvk-sam-6-page-25-polar
167.350
154.818
152.731
152.411
141.558
134.254
131.012
128.716
128.083
126.600
124.400
124.289
118.741
117.769
98.557
Me
N
N
OH
O
7i
170
165
160
155
150
145
140
135
130
125
120
115
110
105
100
ppm
Current Data Parameters
NAME 511610A1611
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161006
Time 5.40 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 298.1 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7578516 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40



Comment: IN Kbr
GVK-SAM-6-Page-25Polar

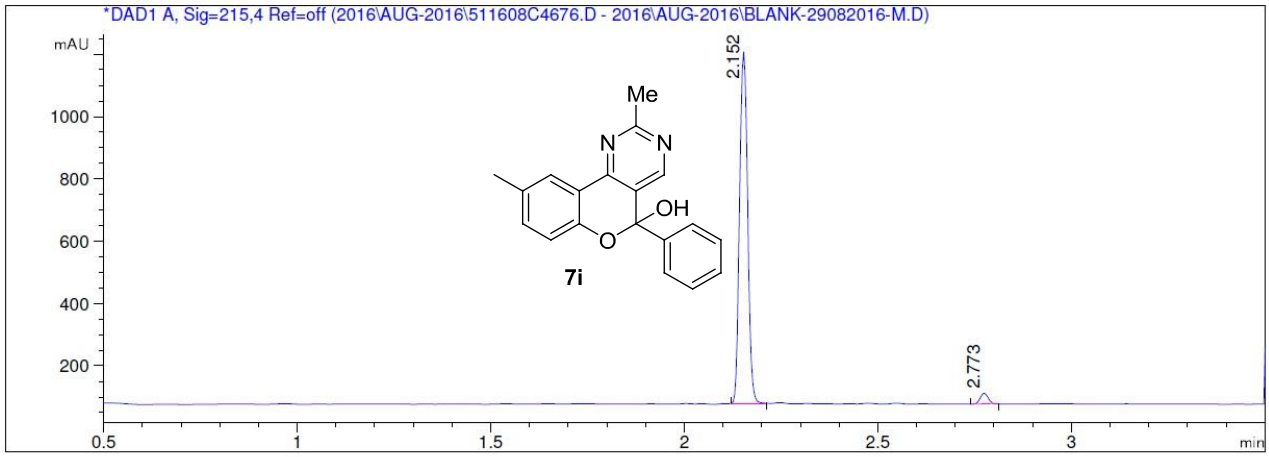
No. of Scans:
Resolution:
Apodization:

Date: 10/3/2016 9:47:58 AM
User: Admin

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

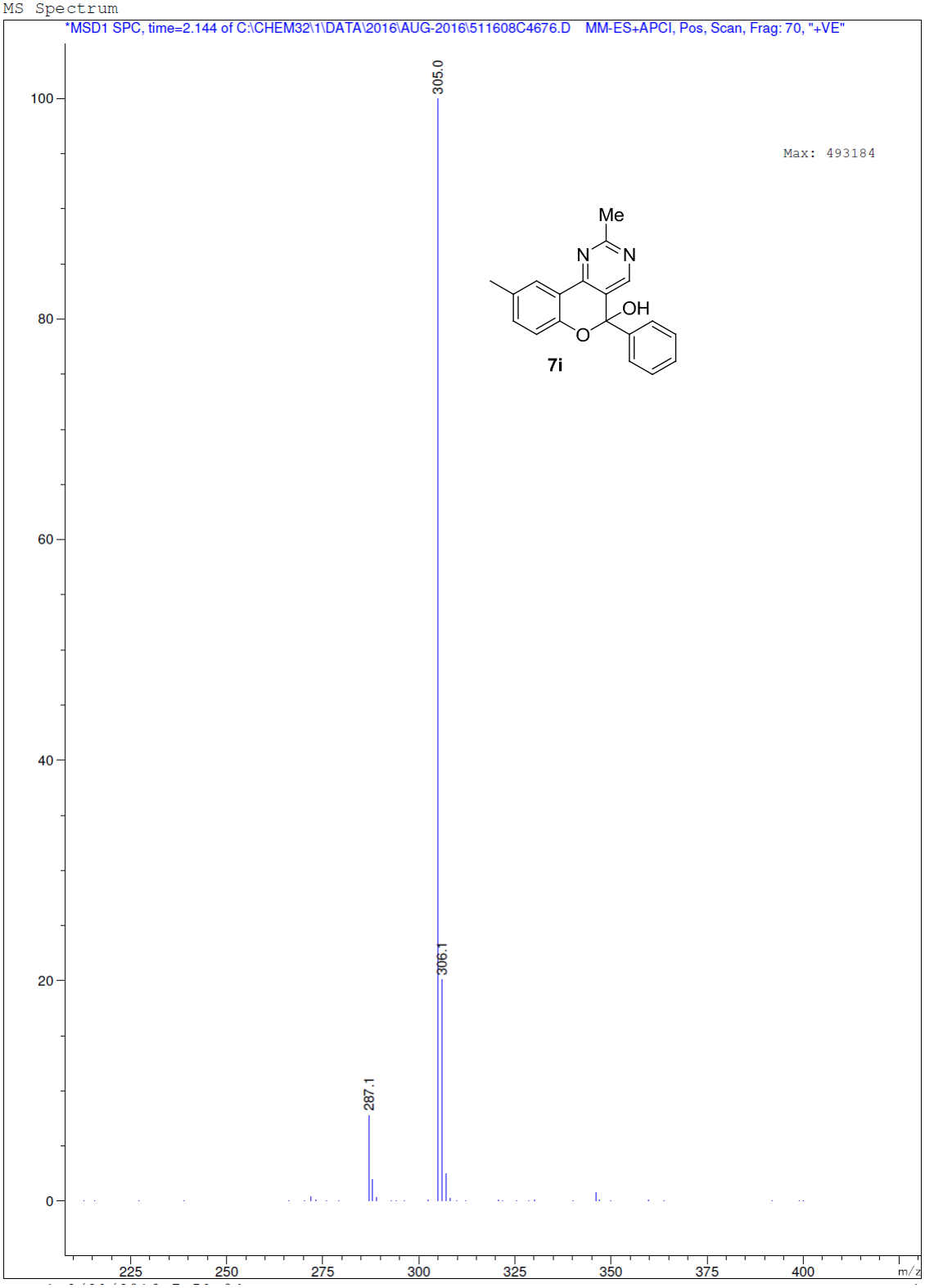
LCMS REPORT

```
================================================================================
Sample Name     :GVK-SAM-6-PAGE-25POLAR                    Vial position  :P1-A-04
Date of Analysis:29/08/2016;7:36:17 AM                     Injection Vol:  0.5   µL
Acq. Method->C:\CHEM32\1\METHODS\RND-FA- 3.5 MIN.M     Instrument ID:ANL-MCL5-LCMS-001
C:\CHEM32\1\DATA\2016\AUG-2016\511608C4676.D
================================================================================
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, 0.4/2, 2.8/98,3.4/98,3.41/2,3.5/2
Column Flow Rate: 0.6 ml/min
Column Temperature: 60°C                                                    ->
```



Pea No	RT min	Area	Area %
1	2.15	1631.143	97.189
2	2.77	47.183	2.811

MS Spectrum


*MSD1 SPC, time=2.144 of C:\CHEM32\1\DATA\2016\AUG-2016\511608C4676.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 493184
305.0
306.1
287.1
Me
N
N
OH
O
7i
100
80
60
40
20
0
225
250
275
300
325
350
375
400
m/z

Elemental Composition Report

Single Mass Analysis

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

Selected filters: None

Monoisotopic Mass, Even Electron Ions

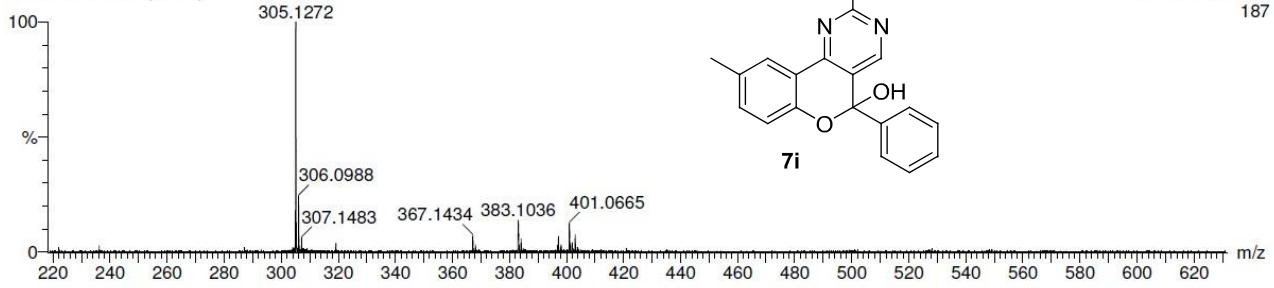
29 formula(e) evaluated with 19 results within limits (up to 1 closest results for each mass)

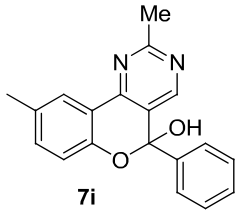
Elements Used:

C: 0-24 H: 0-18 N: 0-2 O: 0-2 Cl: 0-1

SAMPLE CODE:GVK-SAM-6-PAGE-25POLAR

511701A2130 39 (0.564)

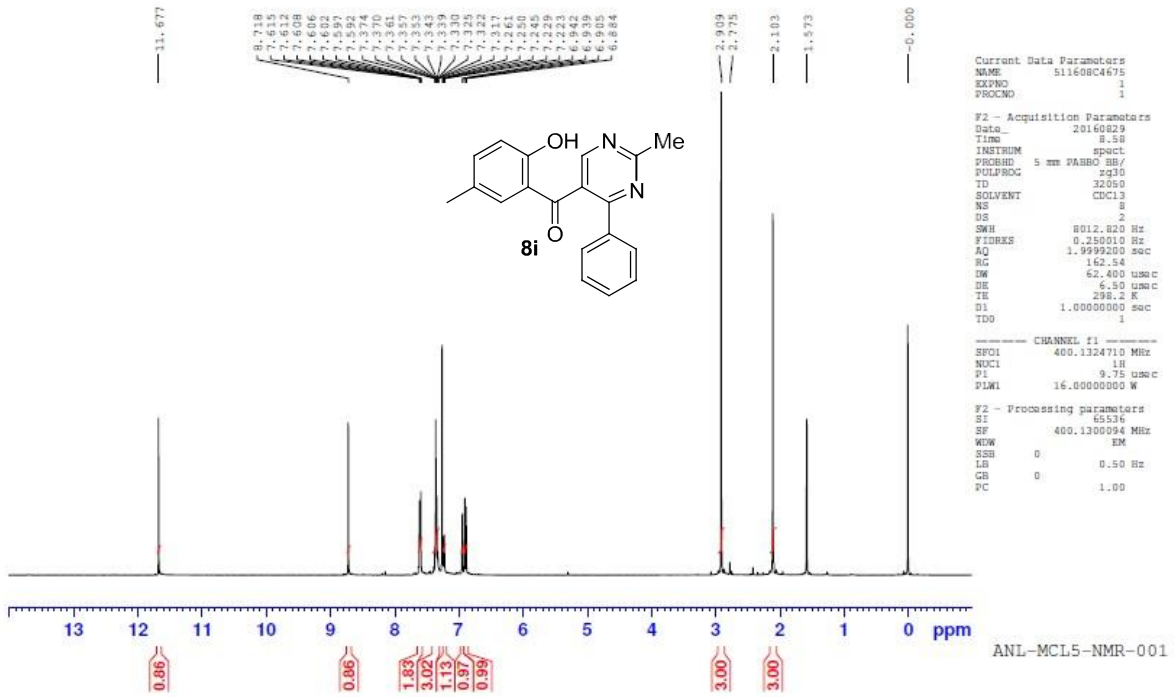




7i

Minimum:				-1.5	
Maximum:		5.0	1000.0	50.0	
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**Formula**
305.1272	305.1290	-1.8	-5.9	12.5	C19 H17 N2 O2

GVK-SAM-6-page-25 NP



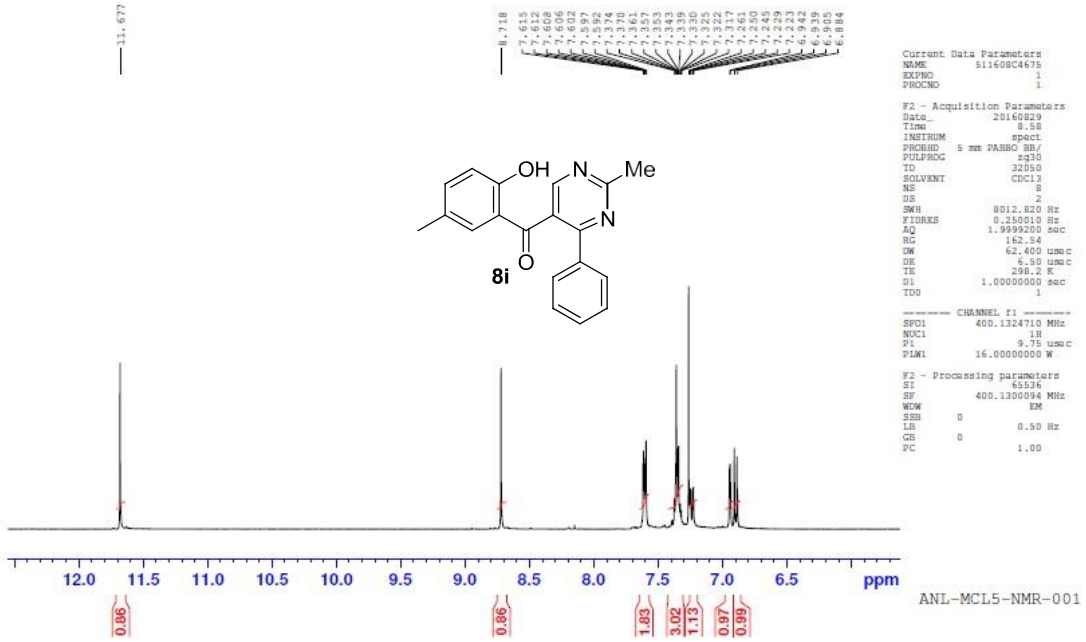
Current Data Parameters
NAME 511608C4675
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160829
Time 8.58
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32050
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.250010 Hz
AQ 1.9999200 sec
RG 162.54
DW 62.400 usec
DE 6.50 usec
TE 298.2 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 400.1300094 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00

GVK-SAM-6-page-25 NP

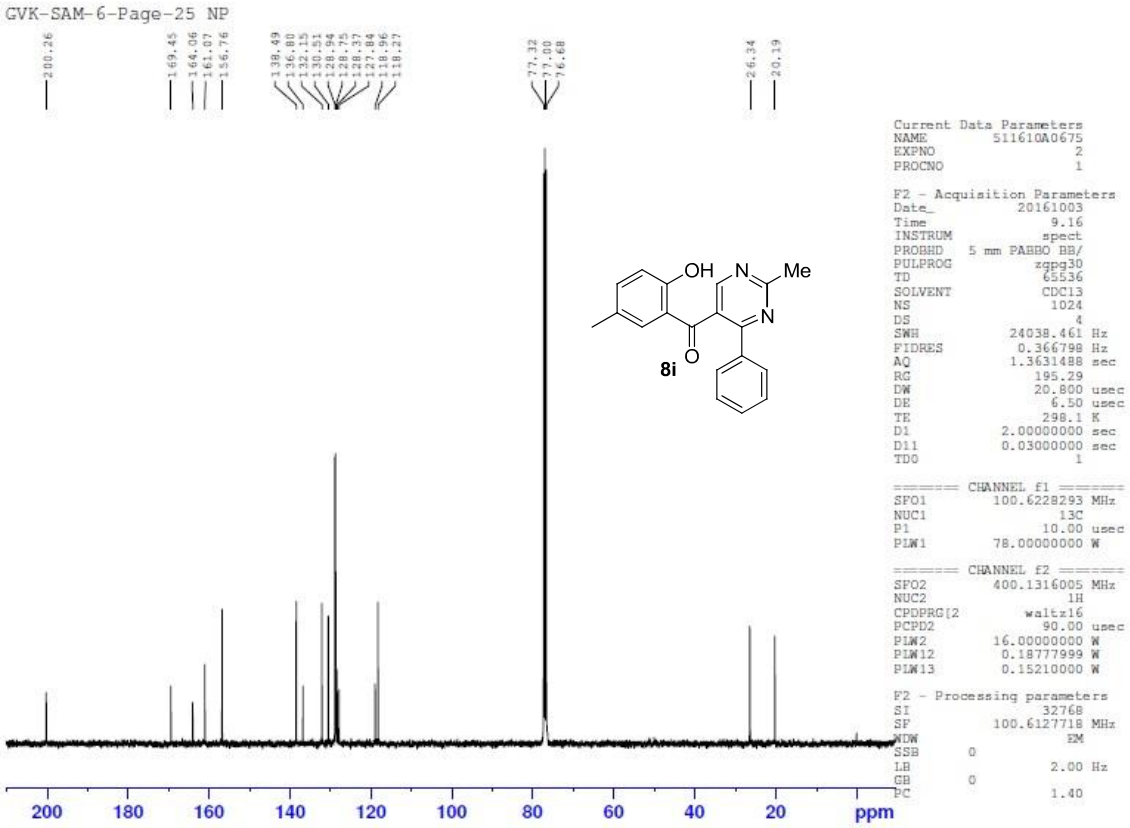


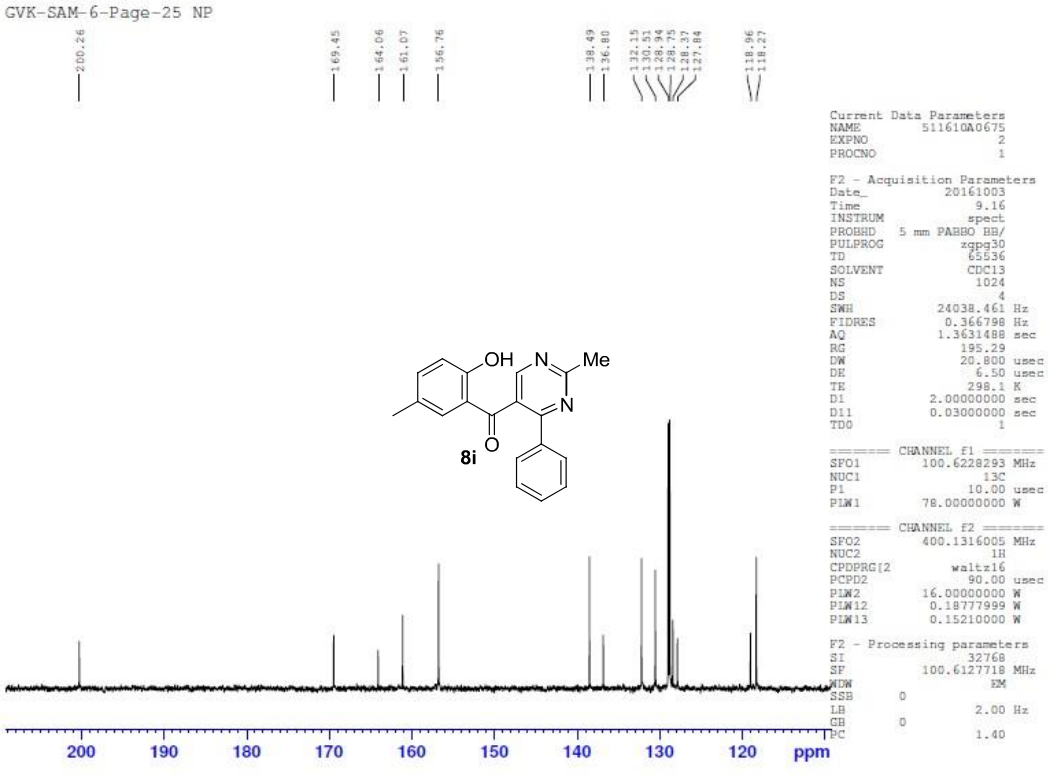
Current Data Parameters
NAME 511608C4675
EXPNO 1
PROCNO 1

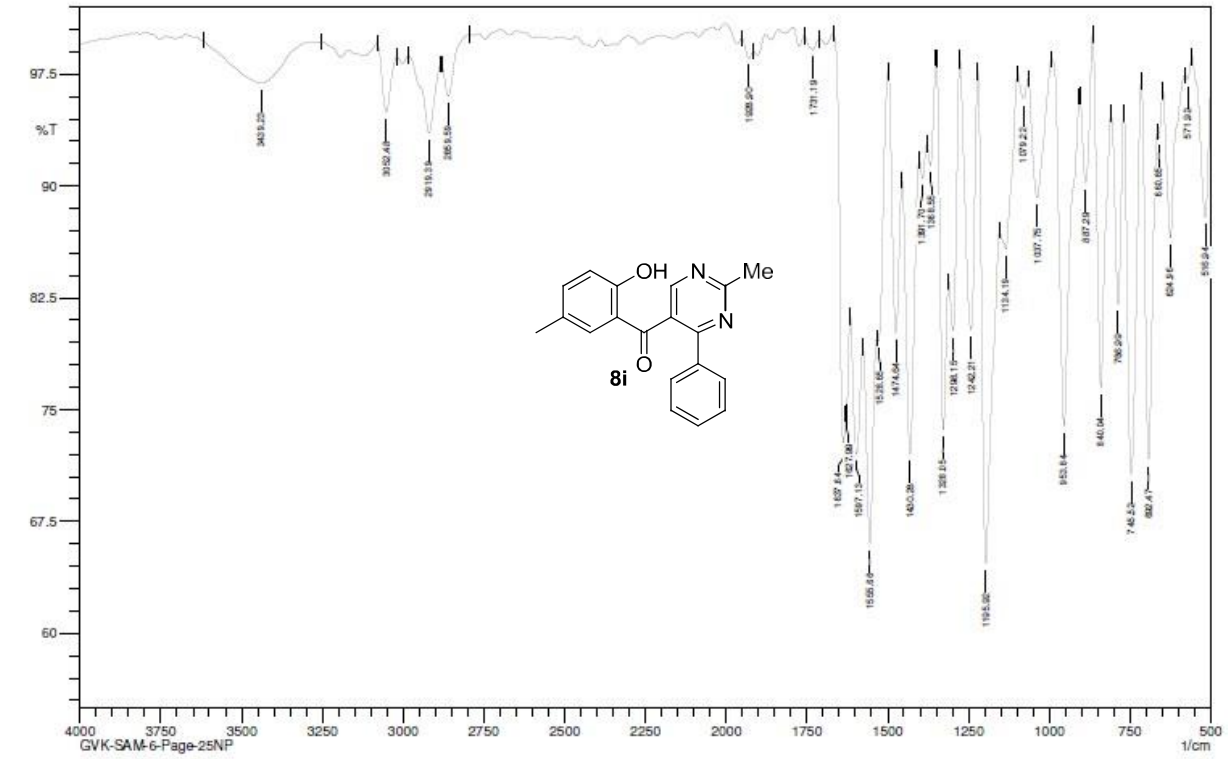
F2 - Acquisition Parameters
Date_ 20160829
Time 8.58
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 32050
SOLVENT CDCl3
NS 8
DS 2
SWH 8012.820 Hz
FIDRES 0.250010 Hz
AQ 1.9999200 sec
RG 162.54
DW 62.400 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 65536
SF 400.1300094 MHz
WDW EM
SSB 0
LB 0.50 Hz
GB 0
PC 1.00


GVK-SAM-6-Page-25 NP
200.26
169.45
164.06
161.07
156.76
138.49
136.80
132.15
130.51
128.94
128.75
128.37
127.84
118.96
118.27
77.32
77.00
76.68
26.34
20.19
OH
N
Me
N
O
8i
Current Data Parameters
NAME 511610A0675
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161003
Time 9.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
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 298.1 K
D1 2.00000000 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 100.6127718 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


GVK-SAM-6-Page-25 NP
200.26
169.45
164.06
161.07
156.76
138.49
136.80
132.15
130.51
128.94
128.75
128.37
127.84
118.96
118.27
OH
N
Me
N
O
8i
Current Data Parameters
NAME 511610A0675
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161003
Time 9.16
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT CDC13
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 298.1 K
D1 2.00000000 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 100.6127718 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
200
190
180
170
160
150
140
130
120
ppm



Comment: IN Kbr
GVK-SAM-6-Page-25NP

No. of Scans:
Resolution:
Apodization:

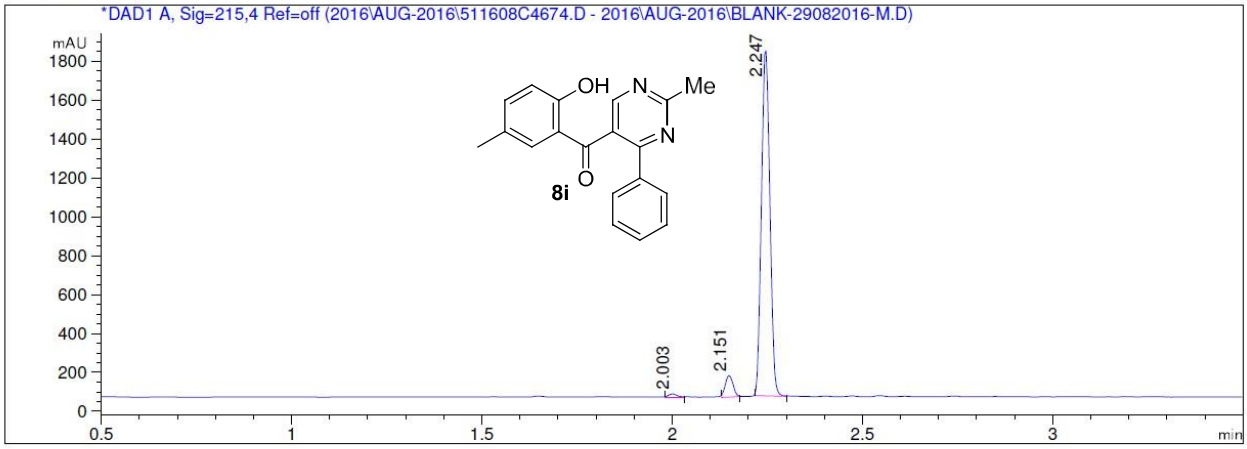
Date: 10/3/2016 9:41:52 AM
User: Admin

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

LCMS REPORT

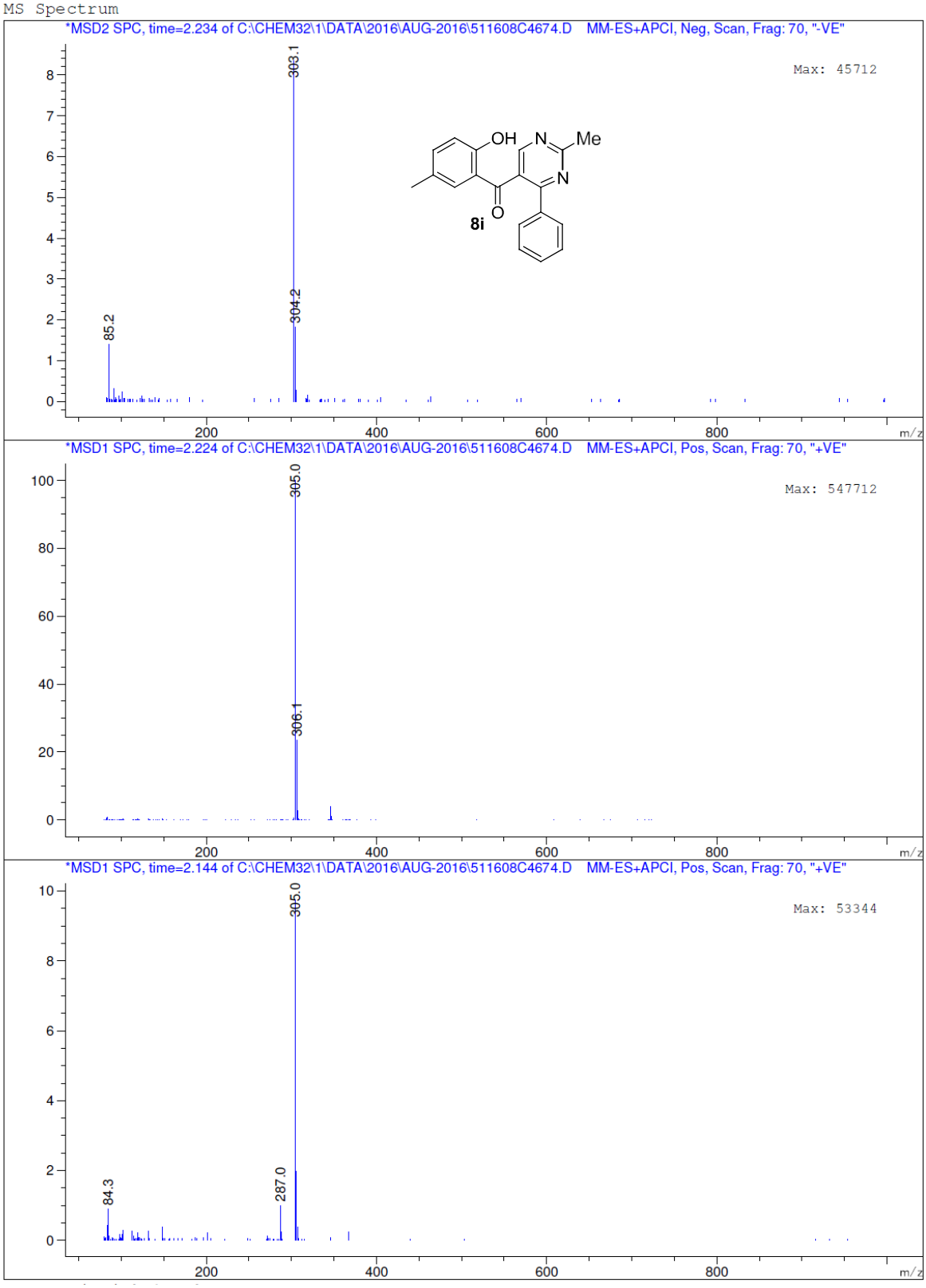
Sample Name :GVK-SAM-6-PAGE-25NP Vial position :P1-A-08
Date of Analysis:29/08/2016;7:54:04 AM Injection Vol: 0.5 µL
Acq. Method->C:\CHEM32\1\METHODS\RND-FA- 3.5 MIN.M Instrument ID:ANL-MCL5-LCMS-001
C:\CHEM32\1\DATA\2016\AUG-2016\511608C4674.D

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, 0.4/2, 2.8/98,3.4/98,3.41/2,3.5/2
Column Flow Rate: 0.6 ml/min
Column Temperature: 60°C ->



Peak No	RT min	Area	Area %
1	2.00	36.412	1.238
2	2.15	156.837	5.333
3	2.25	2747.358	93.428

MS Spectrum

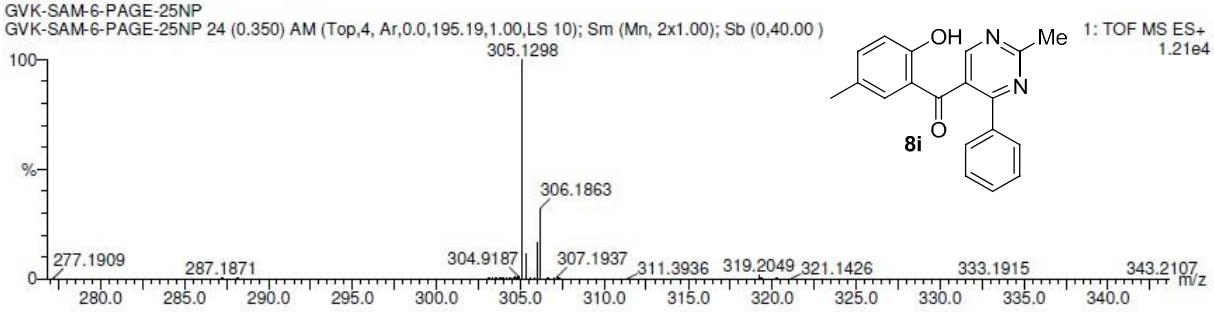

*MSD2 SPC, time=2.234 of C:\CHEM32\1\DATA\2016\AUG-2016\511608C4674.D MM-ES+APCI, Neg, Scan, Frag: 70, "-VE"
Max: 45712
303.1
304.2
85.2
OH
N
Me
N
O
8i
m/z
*MSD1 SPC, time=2.224 of C:\CHEM32\1\DATA\2016\AUG-2016\511608C4674.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 547712
305.0
306.1
m/z
*MSD1 SPC, time=2.144 of C:\CHEM32\1\DATA\2016\AUG-2016\511608C4674.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 53344
305.0
287.0
84.3
m/z

Elemental Composition Report **Page 1**

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

Monoisotopic Mass, Even Electron Ions
4 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-19 H: 0-17 N: 0-2 O: 0-2

GVK-SAM-6-PAGE-25NP
GVK-SAM-6-PAGE-25NP 24 (0.350) AM (Top,4, Ar,0.0,195.19,1.00,LS 10); Sm (Mn, 2x1.00); Sb (0,40.00)



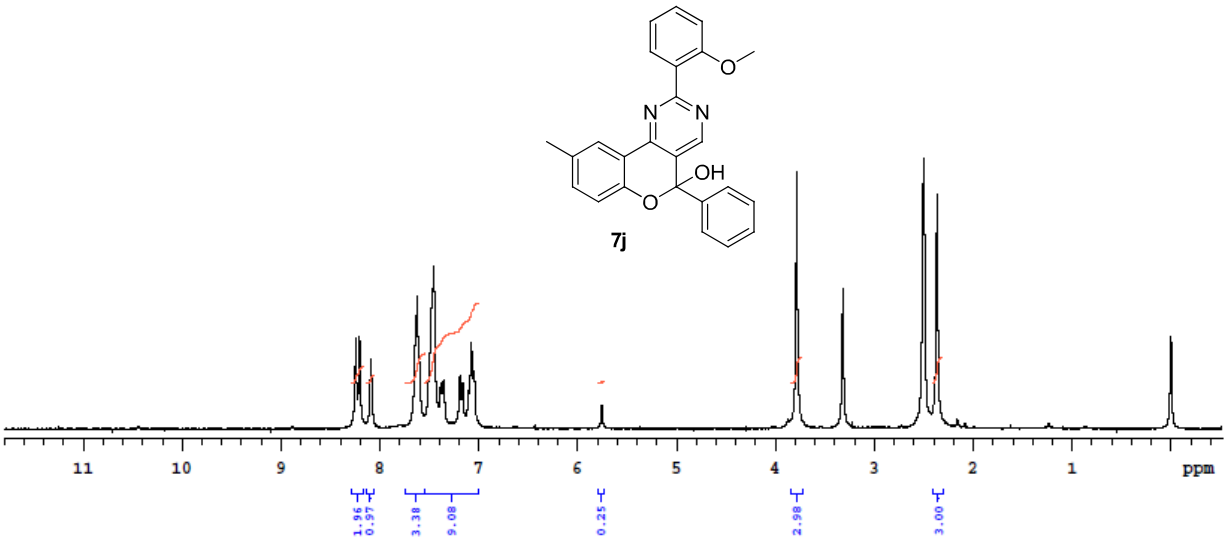
8i

Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
305.1298	305.1290	0.8	2.6	12.5	837.8	C19 H17 N2 O2

Sample Name:

GVK-SAM-6-page-32 polar

Solvent: dmso
Date: Sep 26 2016
Agilent Vnmrs300 / NRM-3
Request No: 511609B9959_PROTON



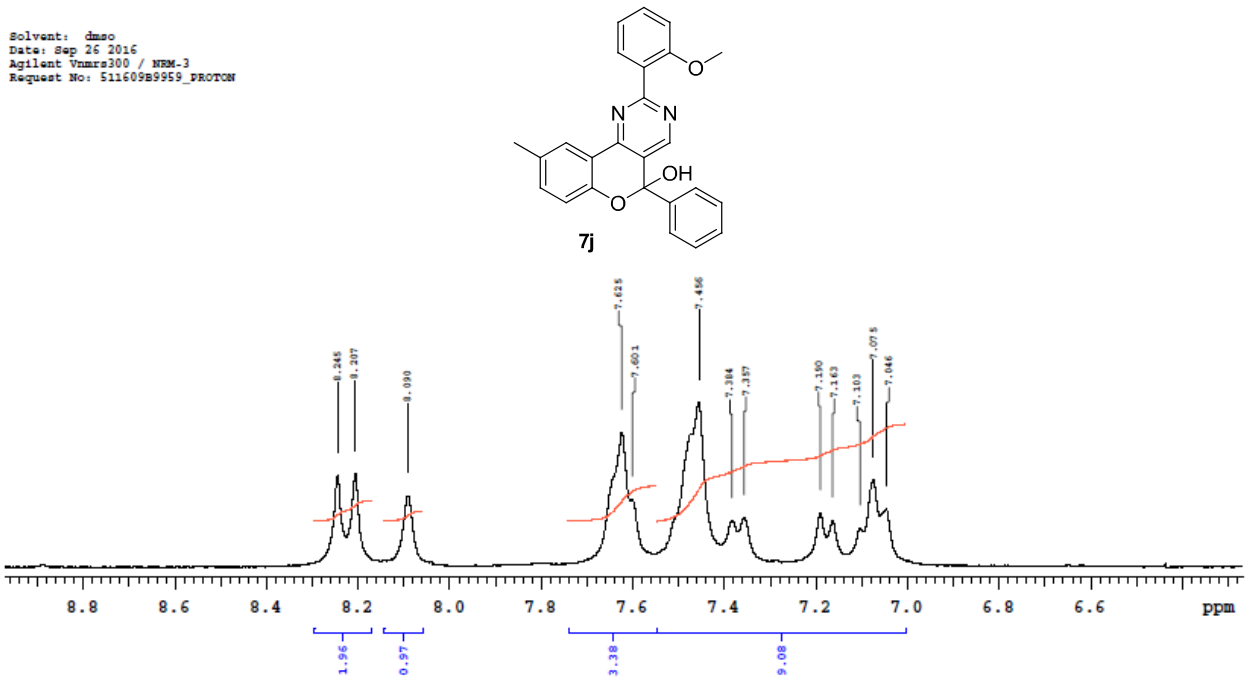
7j

Plotname: 511609B9959_PROTON_01_plot01

Sample Name:

GVK-SAM-6-page-32 polar

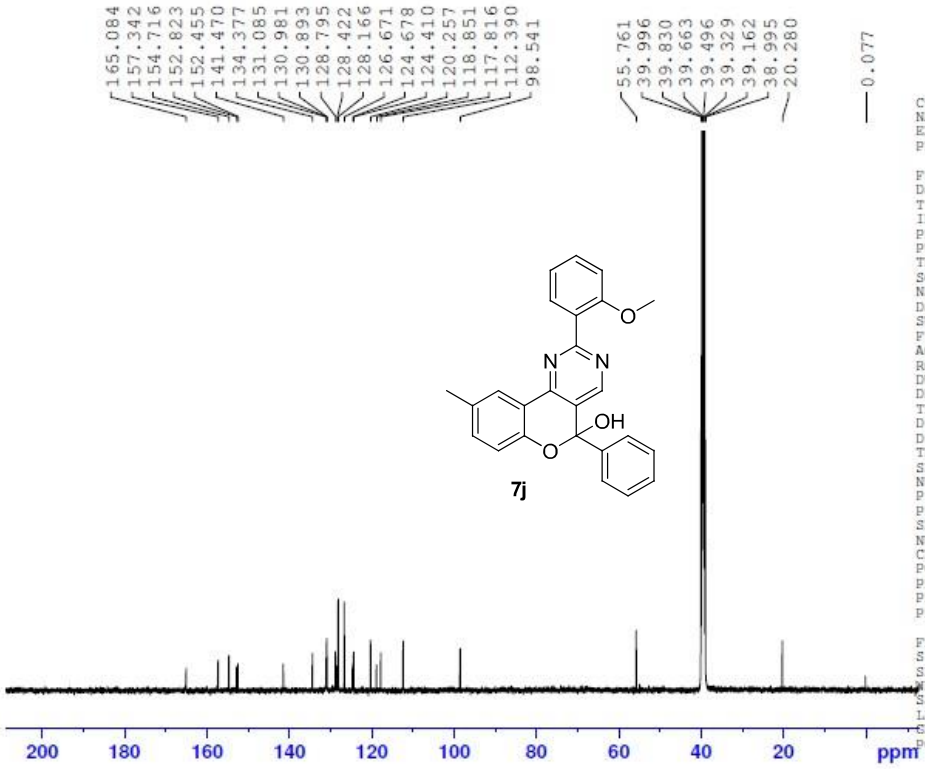
Solvent: dmso
Date: Sep 26 2016
Agilent Vnmrs300 / NRM-3
Request No: 511609B9959_PROTON



7j

Plotname: 511609B9959_PROTON_01_plot02

GVK-SAM-6-PAGE-32POLAR

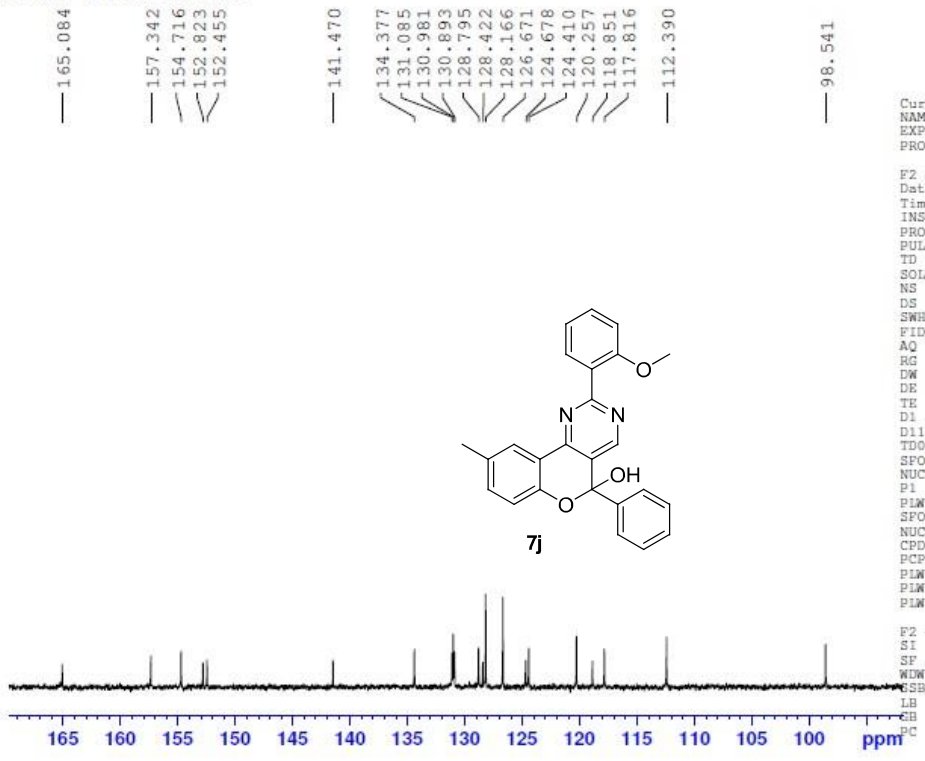



```
Current Data Parameters
NAME          511610B8494
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20161025
Time                6.31 h
INSTRUM            spect
PROBHD    Z119470_0231 (
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                  851
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                197.72
DW                16.800 usec
DE                 6.50 usec
TE                298.2 K
D1            3.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P1                 9.50 usec
PLW1         88.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2         23.00000000 W
PLW12         0.27515000 W
PLW13         0.13840000 W

F2 - Processing parameters
SI                 32768
SF          125.7578519 MHz
WDW                   EM
SSB       0
LB                 2.00 Hz
GB        0
PC                 1.40
```

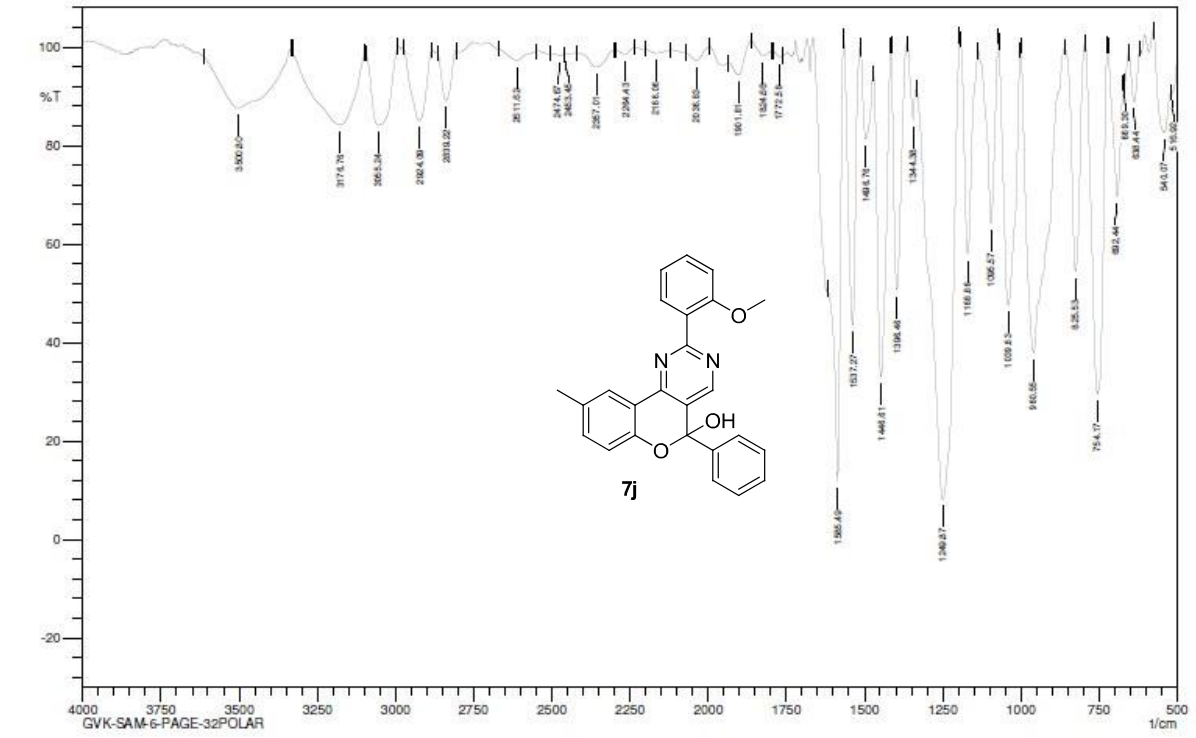
GVK-SAM-6-PAGE-32POLAR




```
Current Data Parameters
NAME          511610B8494
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20161025
Time                6.31 h
INSTRUM            spect
PROBHD    Z119470_0231 (
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                  851
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                197.72
DW                16.800 usec
DE                 6.50 usec
TE                298.2 K
D1            3.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        125.7703643 MHz
NUC1                13C
P1                 9.50 usec
PLW1         88.00000000 W
SFO2        500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2         23.00000000 W
PLW12         0.27515000 W
PLW13         0.13840000 W

F2 - Processing parameters
SI                 32768
SF          125.7578519 MHz
WDW                   EM
SSB       0
LB                 2.00 Hz
GB        0
PC                 1.40
```



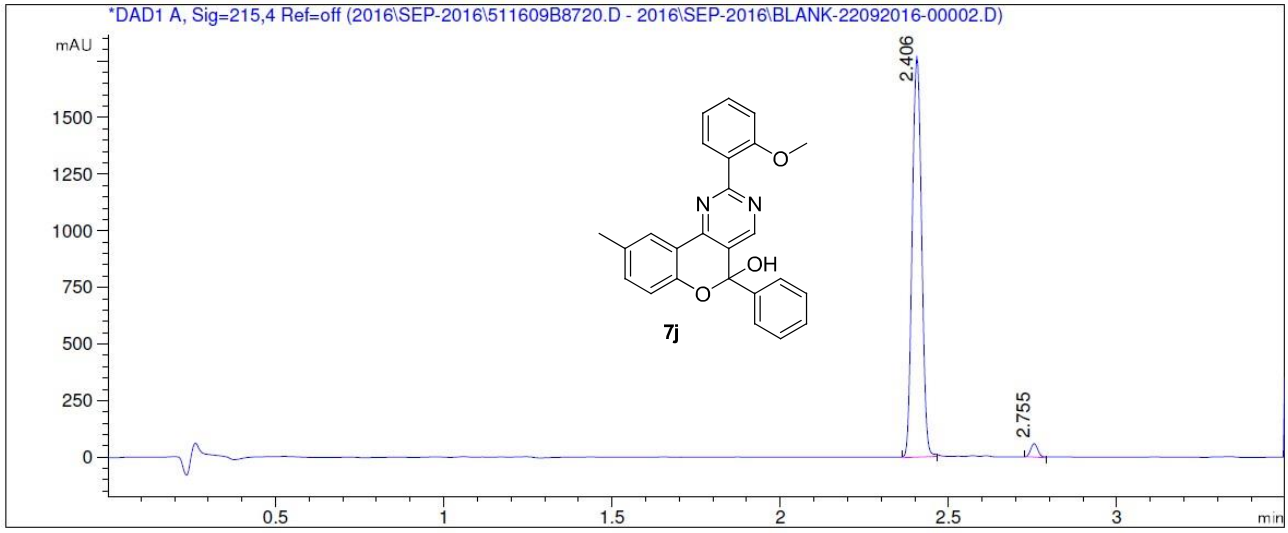
Comment: IN Kbr
GVK-SAM-6-PAGE-32POLAR

No. of Scans:
Resolution:
Apodization:

Date: 11/15/2016 9:35:12 AM
User: Admin

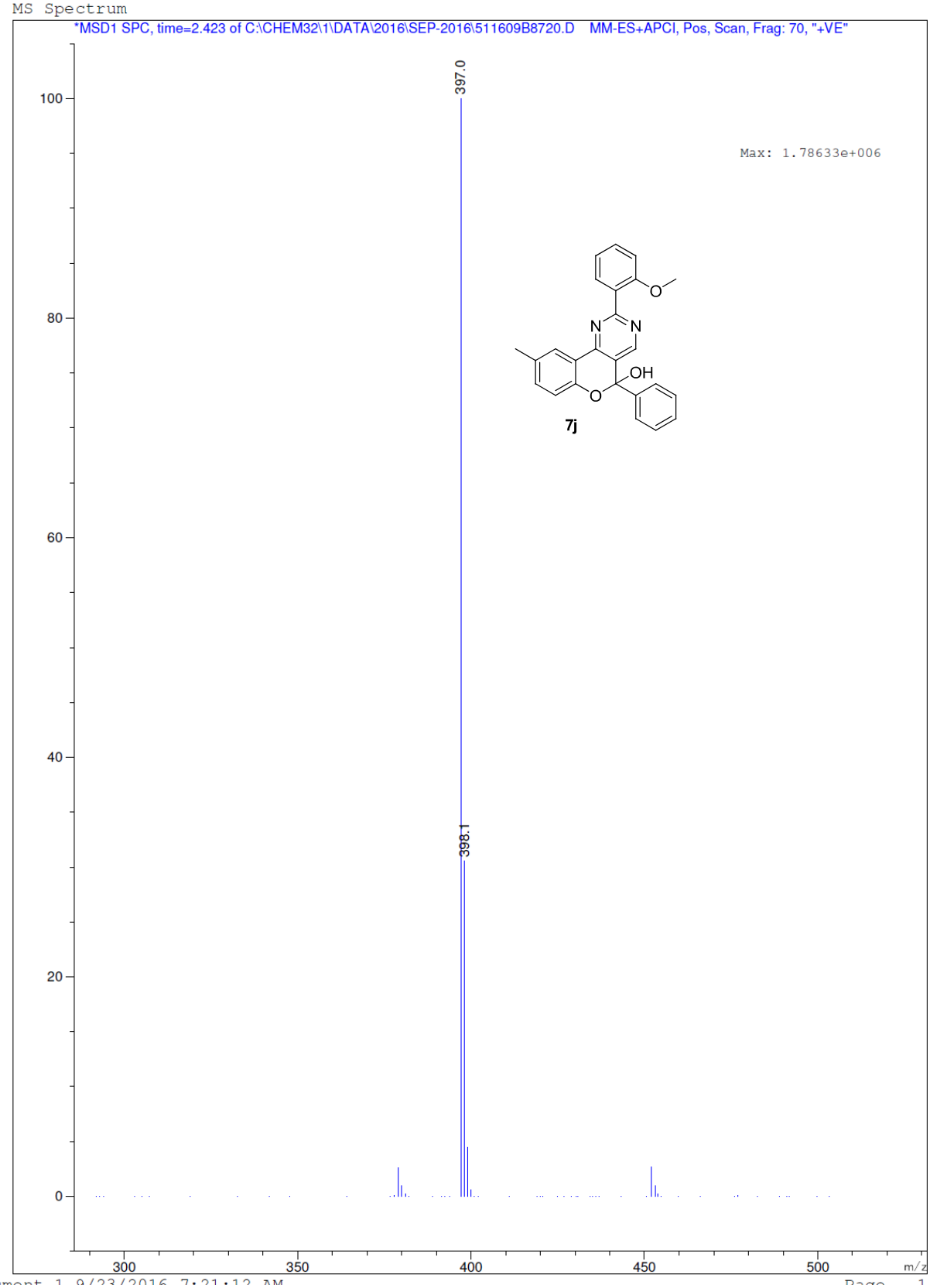
GVK BIOSCIENCES PVT. LTD.
MEDICINAL CHEMISTRY LABORATORY - ANALYTICAL RESEARCH
LCMS REPORT

```
================================================================================================
Sample Name      :GVK-SAM-6-PAGE-32P                          Vial position  : P1-B-06
Date of Analysis :9/22/2016        9:38:10 PM              Injection Vol  :0.500µl
Acq. Method      :C:\CHEM32\1\METHODS\RND-FA- 3.5 MIN.M     Instrument ID  :ANL-MCL5-LCMS-001
================================================================================================
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, 0.4/2, 2.8/98,3.4/98,3.41/2,3.5/2
Column Flow Rate: 0.6 ml/min
Column Temperature: 60°C
                                                                                            ->
================================================================================================
```



Pea No	RT min	Area	Area %
1	2.41	3376.333	97.437
2	2.75	88.805	2.563

MS Spectrum



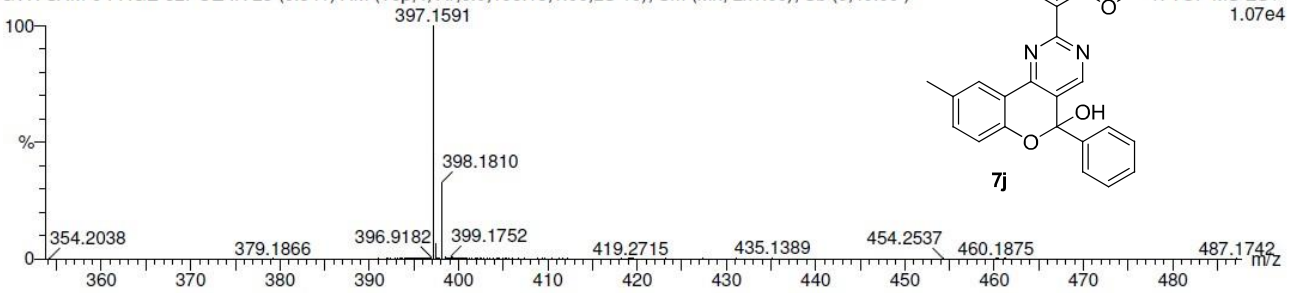
7j

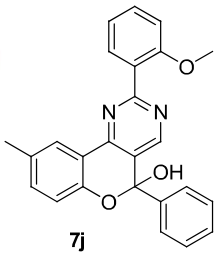
Single Mass Analysis

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

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: 0-25 H: 0-21 N: 0-2 O: 0-3

GVK-SAM-6-PAGE-32POLAR
GVK-SAM-6-PAGE-32POLAR 23 (0.341) AM (Top,4, Ar,0.0,195.18,1.00,LS 10); Sm (Mn, 2x1.00); Sb (0,40.00)



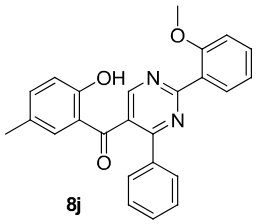


7j

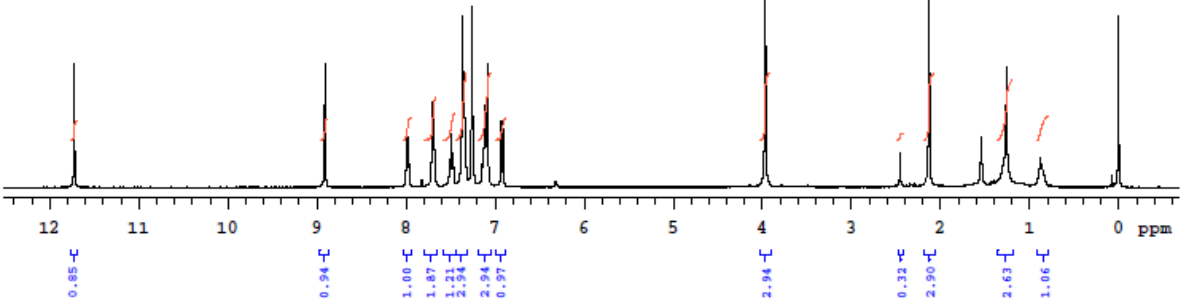
Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
397.1591	397.1552	3.9	9.8	16.5	737.7	C25 H21 N2 O3

Sample Name:
GVKSAM-6-PAGE-32-NON-POLAR

Solvent: cdcl3
Date: Nov 11 2016
Agilent 400-MR / NRM-3
Request No: 511611B0350_PROTON



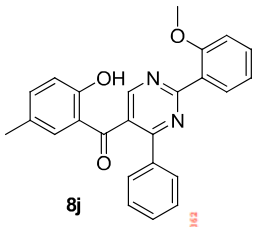
8j



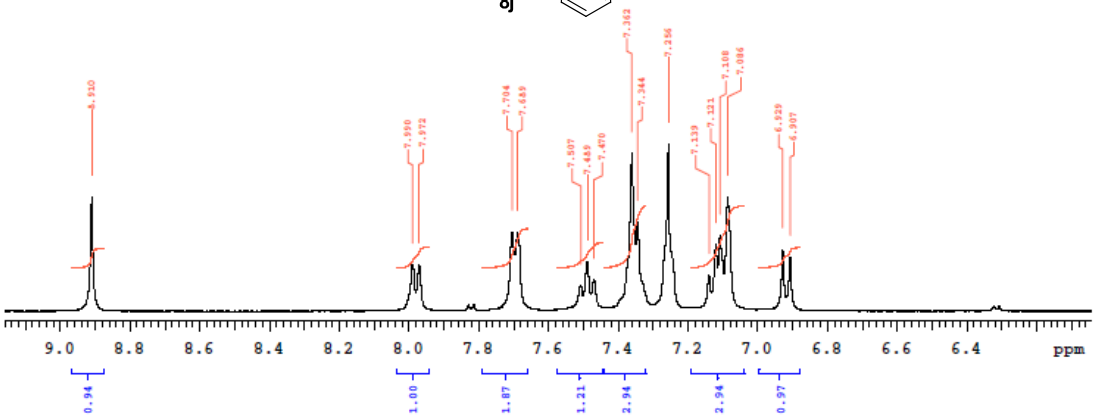
Plotname: 511611B0350_PROTON_01_plot01

Sample Name:
GVKSAM-6-PAGE-32-NON-POLAR

Solvent: cdcl3
Date: Nov 11 2016
Agilent 400-MR / NRM-3
Request No: 511611B0350_PROTON

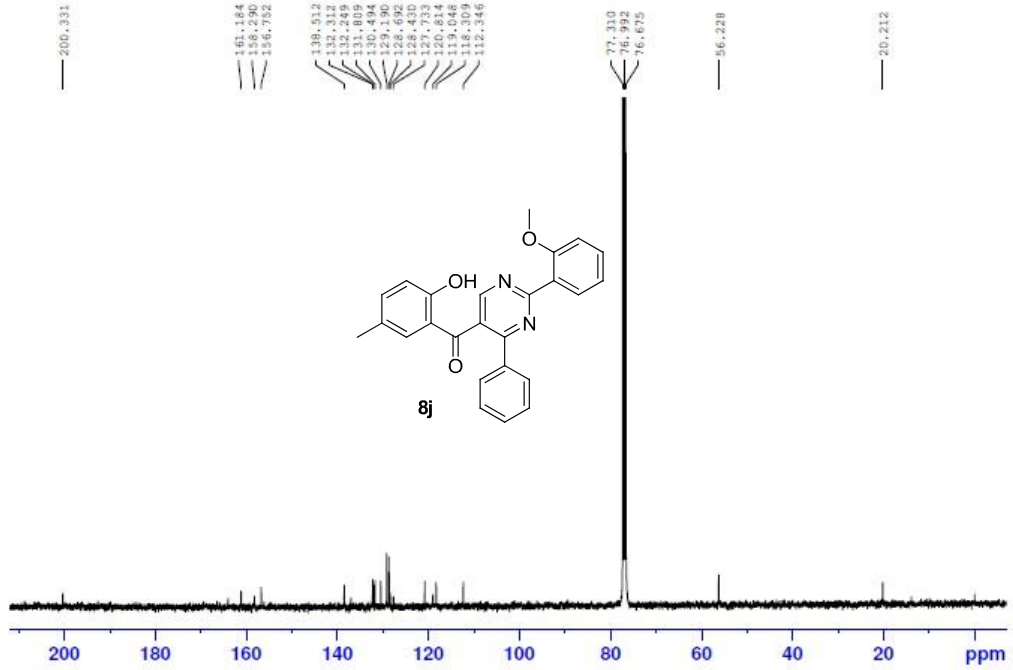


8j



Plotname: 511611B0350_PROTON_01_plot02

GVK-SAM-6-page-32NP




```
Current Data Parameters
NAME          511611C4411
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20161130
Time              2.23
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

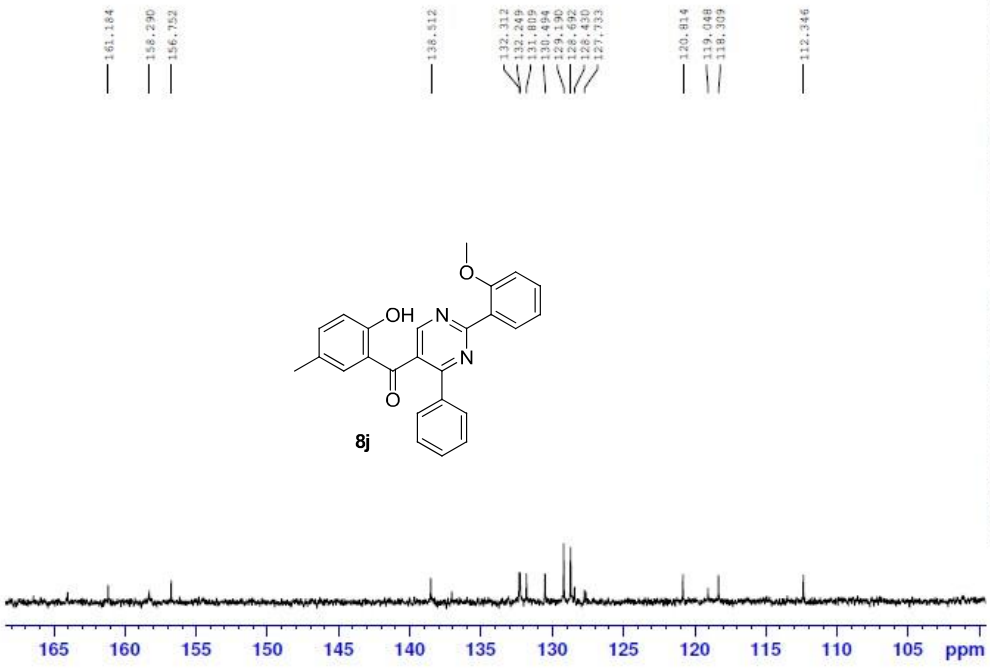
======== CHANNEL f1 ========
SFO1        100.6228293 MHz
NUC1              13C
P1              10.00 usec
PLW1        78.00000000 W

======== 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          100.6127695 MHz
WDW                 EM
SSB       0
LB              2.00 Hz
GB        0
PC              1.40
```

ANL-MCL5-NMR-001

GVK-SAM-6-page-32NP




```
Current Data Parameters
NAME          511611C4411
EXPNO                   2
PROCNO                  1

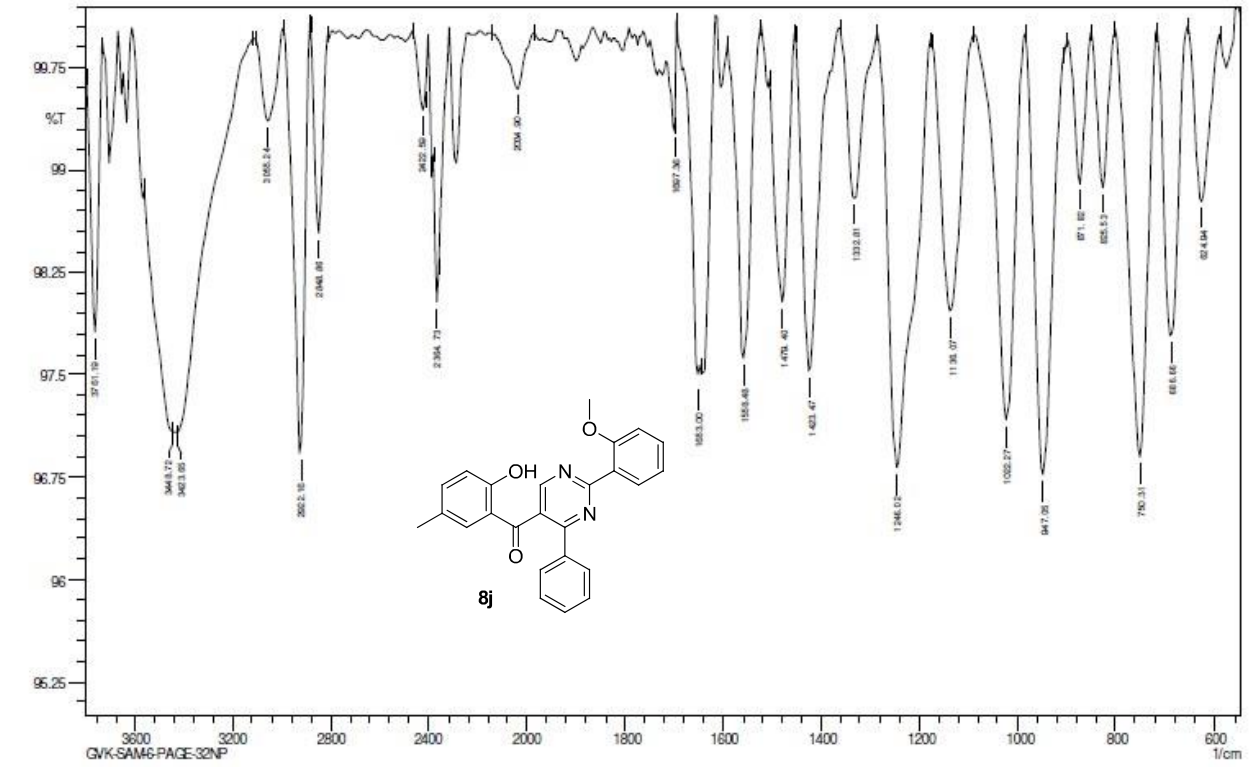
F2 - Acquisition Parameters
Date_           20161130
Time              2.23
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                1024
DS                   4
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            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          100.6127695 MHz
WDW                 EM
SSB       0
LB              2.00 Hz
GB        0
PC              1.40
```

ANL-MCL5-NMR-001



Comment: IN Kbr
GVK-SAM-6-PAGE-32NP

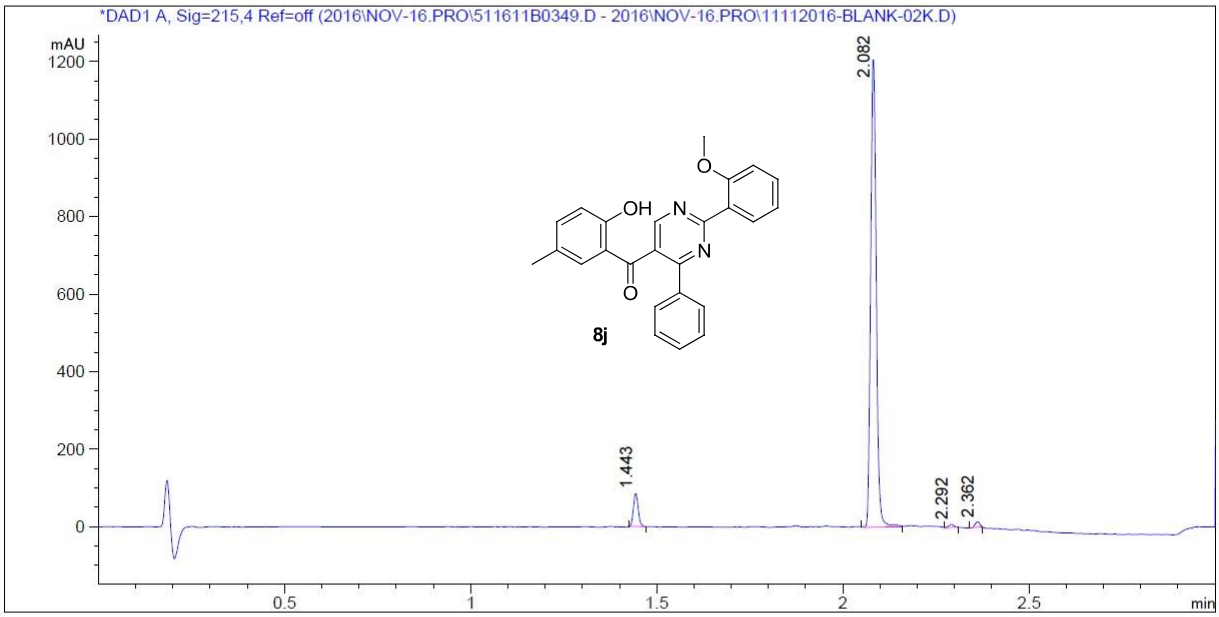
No. of Scans;
Resolution;
Apodization;

Date:11/29/2016 9:27:28 AM
User; Admin

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

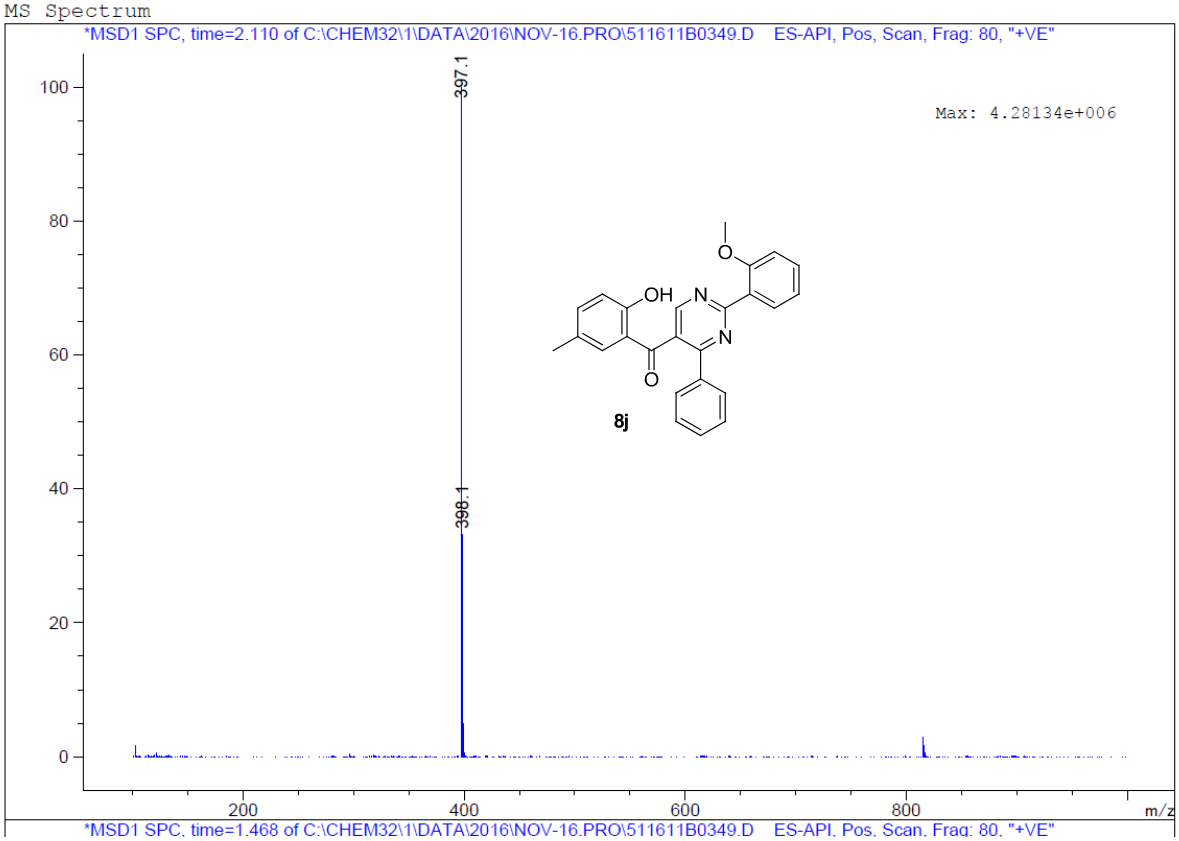
```
================================================================================================
Date of Analysis: 11/11/2016   9:39:55 PM            Vial Position  :P1-B-09
Acq. Method     :    RND-FA-3.0-MIN                  Injection Vol : 0.500       ul
                                                     Instrument ID  :ANL-MCL3-LCMS-003
Sample Name     : GVK-SAM-6-PAGE-32NONPOLAR
================================================================================================
 GVK_LCMS_18

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



Pea No	RT min	Area	Area %
1	1.443	76.327	5.607
2	2.082	1265.604	92.963
3	2.292	7.439	0.546
4	2.362	12.033	0.884

MS Spectrum

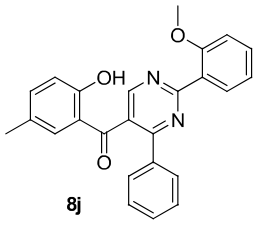

*MSD1 SPC, time=2.110 of C:\CHEM32\1\DATA\2016\NOV-16.PRO\511611B0349.D ES-API, Pos, Scan, Frag: 80, "+VE"
Max: 4.28134e+006
397.1
398.1
100
80
60
40
20
0
200
400
600
800
m/z
OH
N
N
O
O
8j
*MSD1 SPC, time=1.468 of C:\CHEM32\1\DATA\2016\NOV-16.PRO\511611B0349.D ES-API, Pos, Scan, Frag: 80, "+VE"

Single Mass Analysis

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

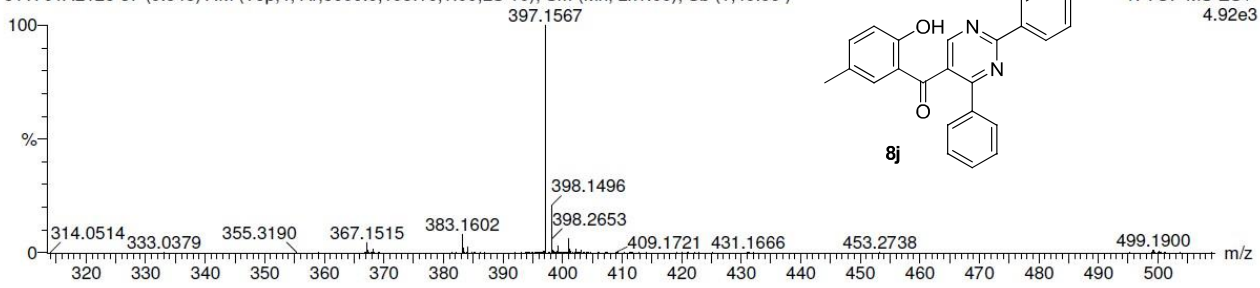
Monoisotopic Mass, Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 1 best isotopic matches for each mass)
Elements Used:
C: 0-25 H: 0-21 N: 0-2 O: 0-3

SAMPLE CODE:GVK-SAM-6-PAGE-32NP
511701A2125 37 (0.545) AM (Top,4, Ar,5000.0,195.16,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)



8j

1: TOF MS ES+
4.92e3

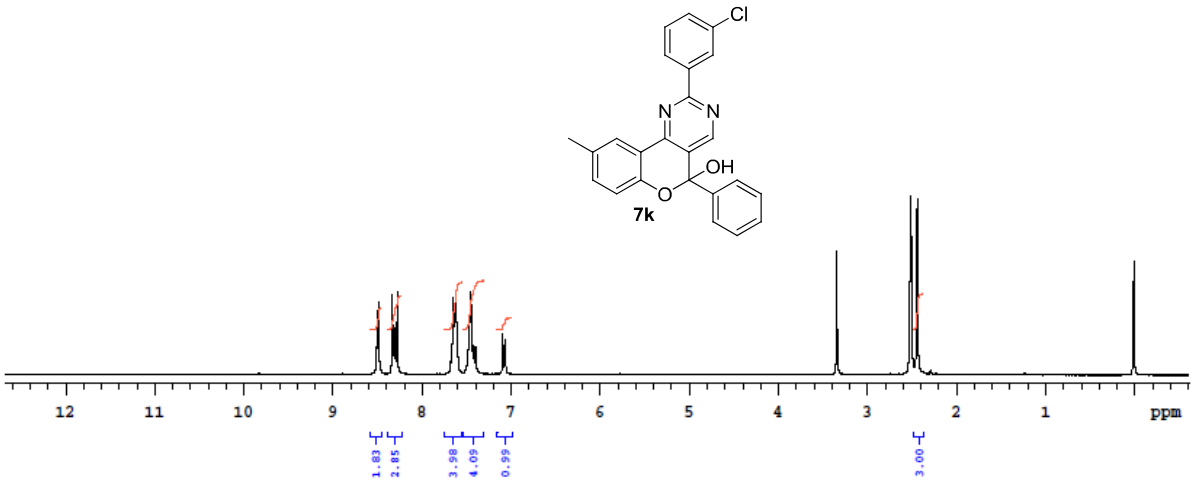


Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
397.1567	397.1552	1.5	3.8	16.5	87.1	C25 H21 N2 O3

Sample Name:

GVK-SAM-6-PAGE-33-POLAR

Solvent: dmso
Date: Sep 27 2016
Agilent Vnmrs300 / NRM-3
Request No: 511609C1657_PROTON

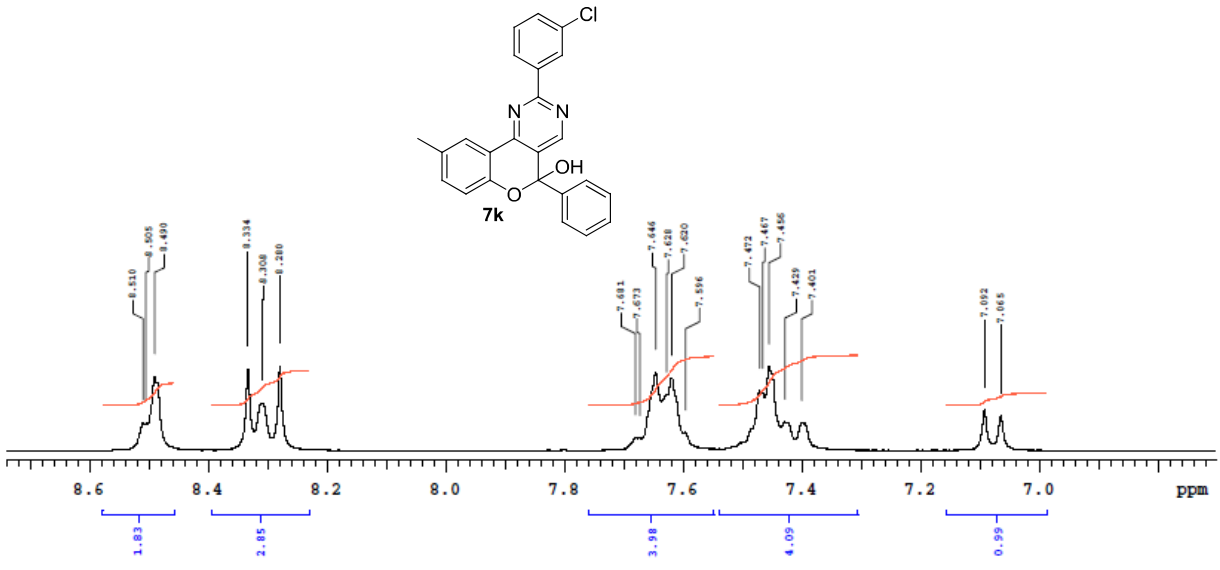


Plotname: 511609C1657_PROTON_01_plot01

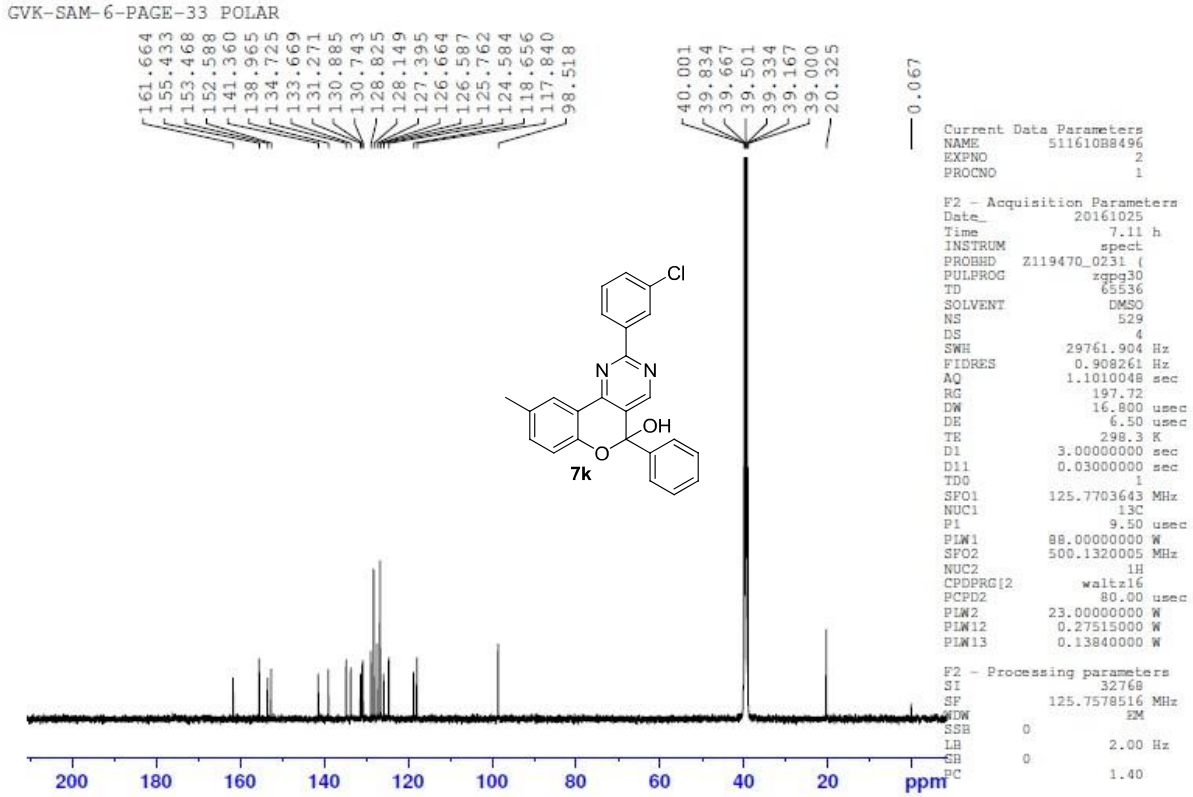
Sample Name:

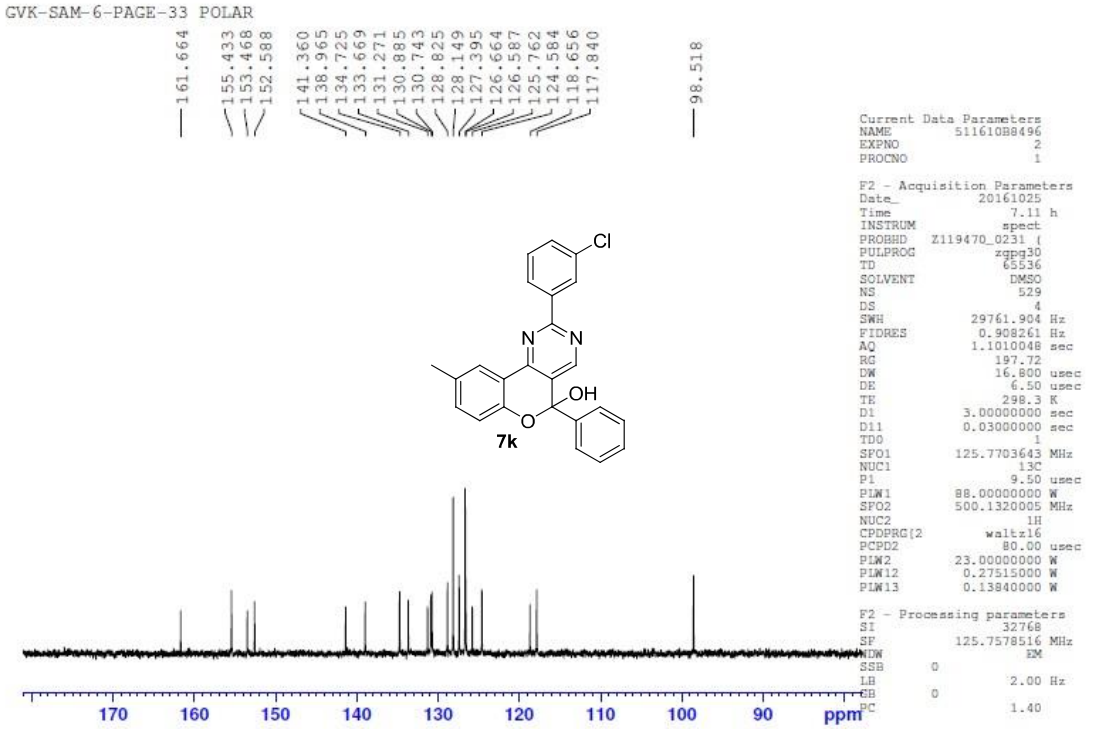
GVK-SAM-6-PAGE-33-POLAR

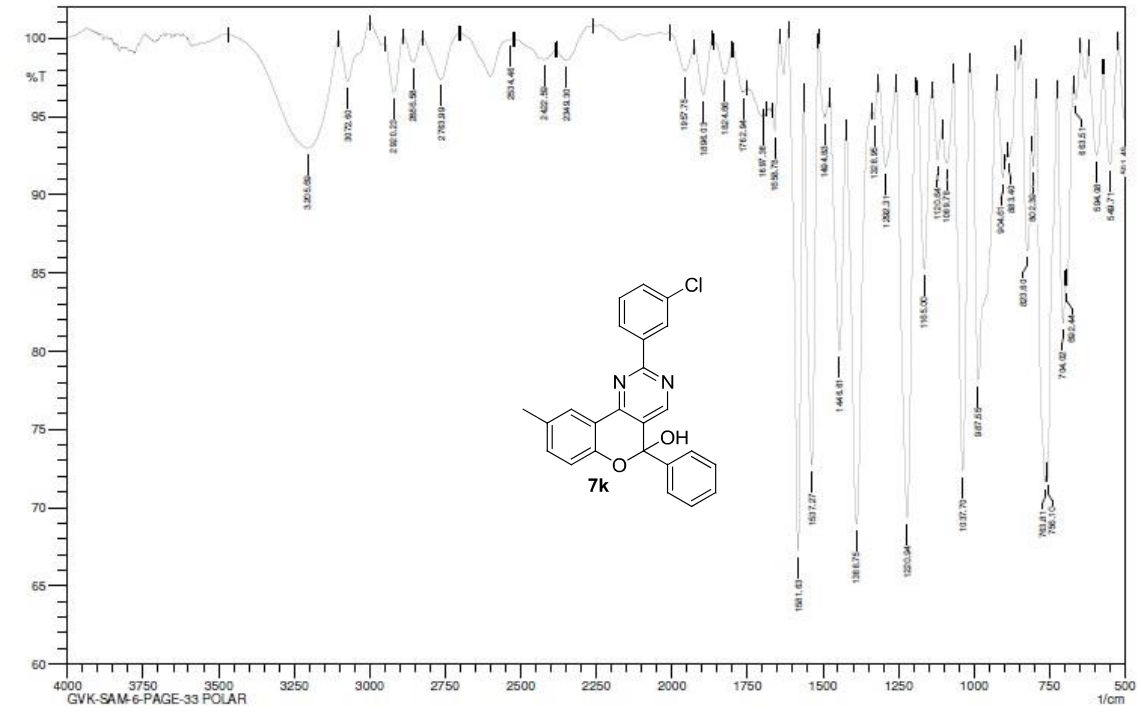
Solvent: dmso
Date: Sep 27 2016
Agilent Vnmrs300 / NRM-3
Request No: 511609C1657_PROTON



Plotname: 511609C1657_PROTON_01_plot02


GVK-SAM-6-PAGE-33 POLAR
161.664
155.433
153.468
152.588
141.360
138.965
134.725
133.669
131.271
130.885
130.743
128.825
128.149
127.395
126.664
126.587
125.762
124.584
118.656
117.840
98.518
40.001
39.834
39.667
39.501
39.334
39.167
39.000
20.325
0.067
Cl
N
N
OH
O
7k
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME 511610B8496
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161025
Time 7.11 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 529
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 298.3 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7578516 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40


GVK-SAM-6-PAGE-33 POLAR
161.664
155.433
153.468
152.588
141.360
138.965
134.725
133.669
131.271
130.885
130.743
128.825
128.149
127.395
126.664
126.587
125.762
124.584
118.656
117.840
98.518
Cl
N
N
OH
O
7k
170
160
150
140
130
120
110
100
90
ppm
Current Data Parameters
NAME 511610B8496
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161025
Time 7.11 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 529
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 298.3 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7578516 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40



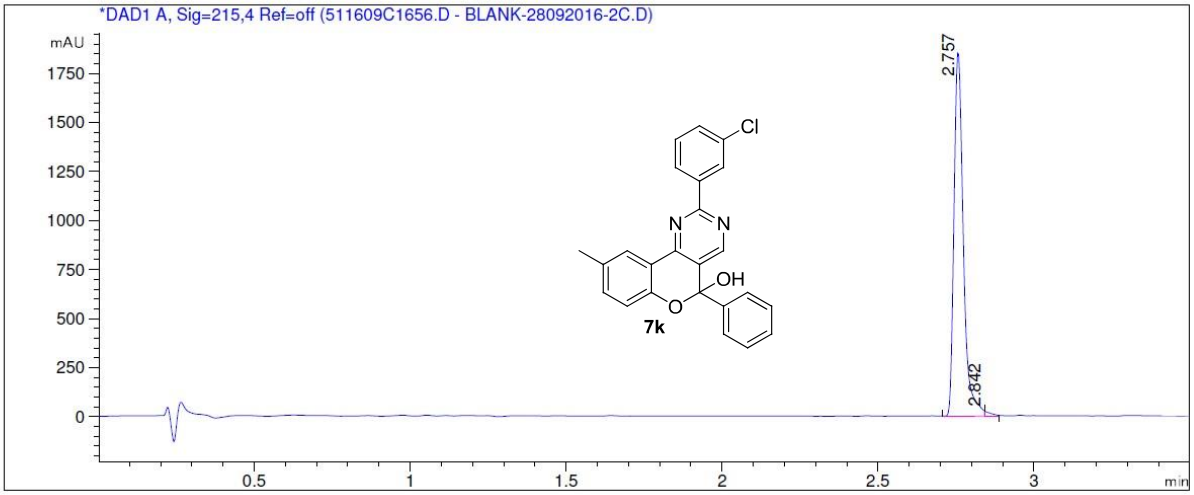
omment: IN Kbr
VK-SAM-6-PAGE-33 POLAR

No. of Scans:
Resolution:
Apodization:

Date: 11/15/2016 10:12:19 AM
User: Admin

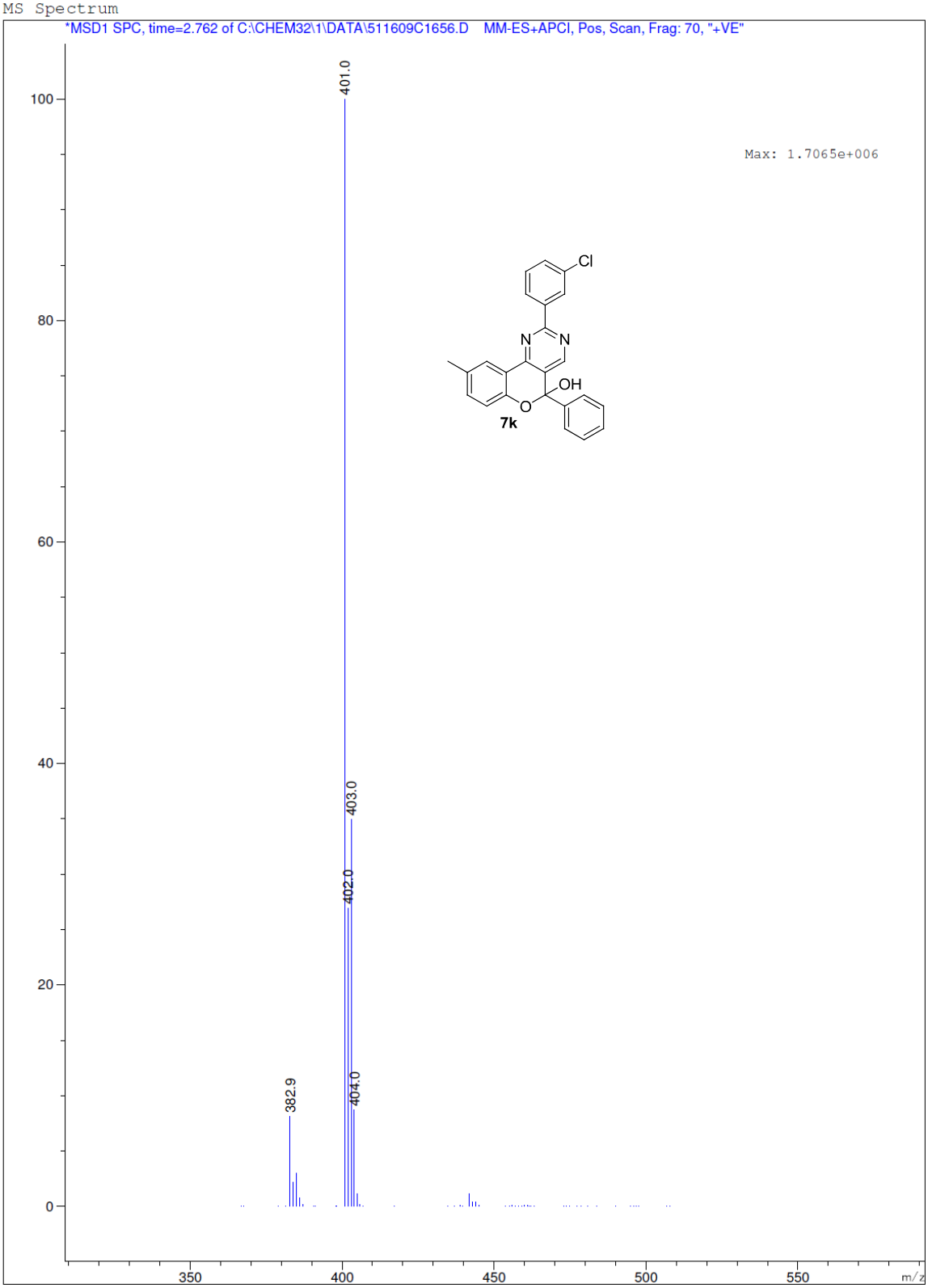
GVK BIOSCIENCES PVT. LTD.
MEDICINAL CHEMISTRY LABORATORY - ANALYTICAL RESEARCH
LCMS REPORT

```
================================================================================================
Sample Name      :GVK-SAM-6-33POLAR                          Vial position  : P1-A-01
Date of Analysis :9/28/2016        8:11:26 AM              Injection Vol  :0.500µl
Acq. Method      :C:\CHEM32\1\METHODS\RND-FA- 3.5 MIN.M     Instrument ID  :ANL-MCL5-LCMS-001
================================================================================================
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, 0.4/2, 2.8/98,3.4/98,3.41/2,3.5/2
Column Flow Rate: 0.6 ml/min
Column Temperature: 60°C
                                                                                            ->
================================================================================================
```



Pea No	RT min	Area	Area %
1	2.76	3894.532	99.152
2	2.84	33.301	0.848

MS Spectrum


*MSD1 SPC, time=2.762 of C:\CHEM32\1\DATA\511609C1656.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 1.7065e+006
401.0
403.0
402.0
404.0
382.9
Cl
N
N
OH
O
7k
100
80
60
40
20
0
350
400
450
500
550
m/z

Elemental Composition Report

Single Mass Analysis

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

Selected filters: None

Monoisotopic Mass, Even Electron Ions

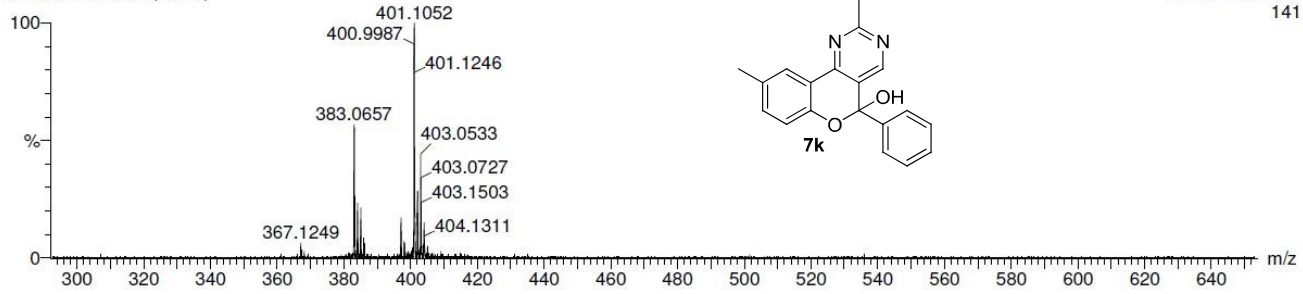
12 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)

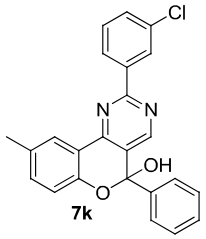
Elements Used:

C: 0-24 H: 0-18 N: 0-2 O: 0-2 Cl: 0-1

SAMPLE CODE:GVK-SAM-6-PAGE-33POLAR

511701A2120 22 (0.330)

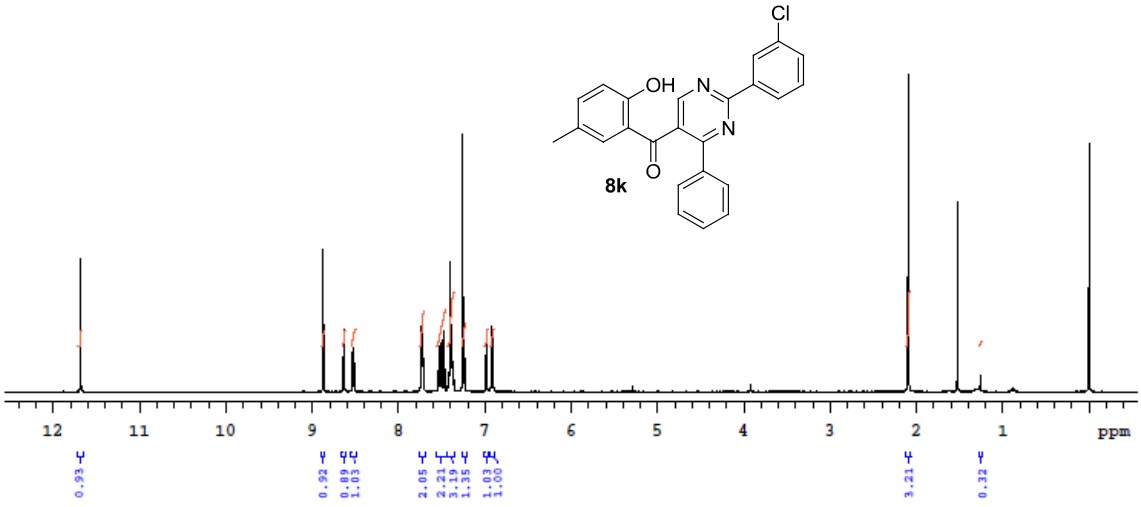




Minimum:				-1.5	
Maximum:		5.0	1000.0	50.0	
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**Formula**
401.1052	401.1057	-0.5	-1.2	16.5	C24 H18 N2 O2 Cl

Sample Name:
GVK-SAM-6-PAGE-33NP

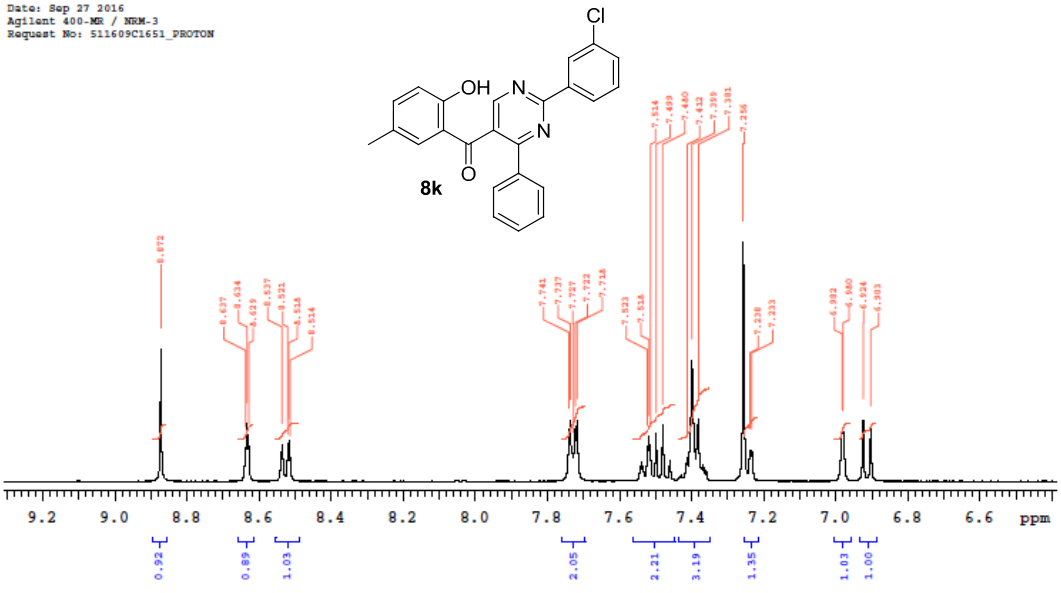
Solvent: cdcl3
Date: Sep 27 2016
Agilent 400-MR / NRM-3
Request No: 511609C1651_PROTON



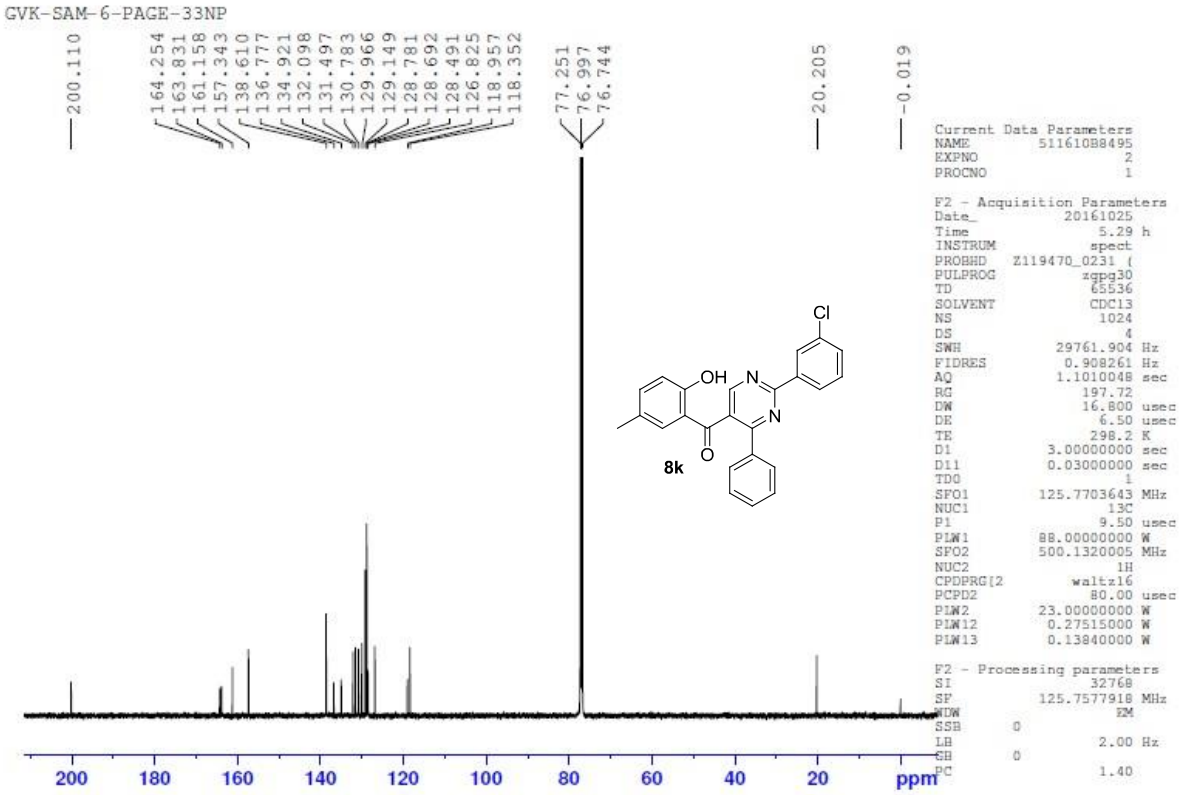
Plotname: 511609C1651_PROTON_01_plot01

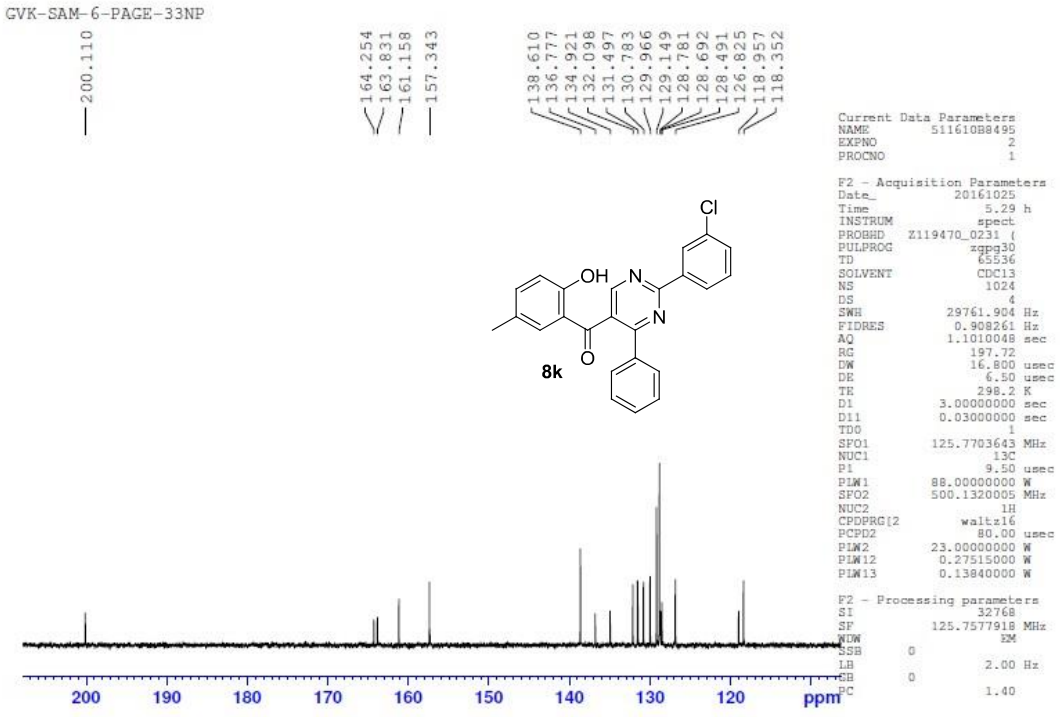
Sample Name:
GVK-SAM-6-PAGE-33NP

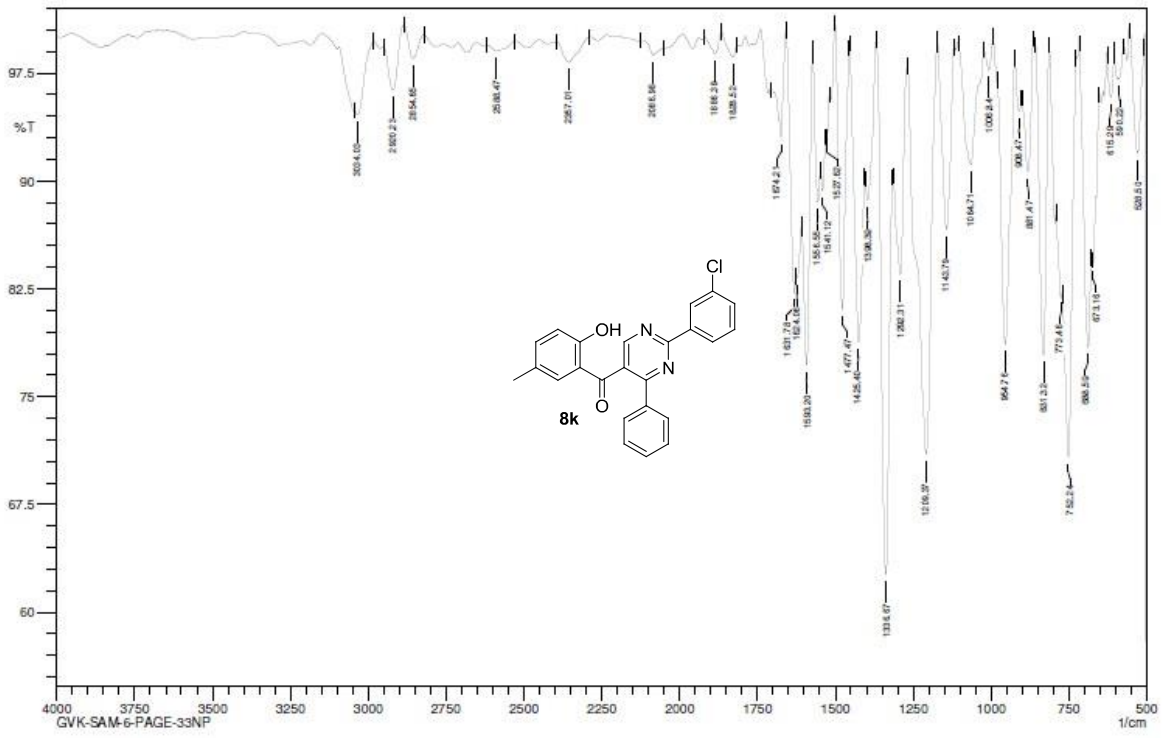
Solvent: cdcl3
Date: Sep 27 2016
Agilent 400-MR / NRM-3
Request No: 511609C1651_PROTON



Plotname: 511609C1651_PROTON_01_plot02


GVK-SAM-6-PAGE-33NP
200.110
164.254
163.831
161.158
157.343
138.610
136.777
134.921
132.098
131.497
130.783
129.966
129.149
128.781
128.692
128.491
126.825
118.957
118.352
77.251
76.997
76.744
20.205
-0.019
Cl
OH
N
N
O
8k
Current Data Parameters
NAME 511610B8495
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161025
Time 5.29 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 298.2 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7577918 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


GVK-SAM-6-PAGE-33NP
200.110
164.254
163.831
161.158
157.343
138.610
136.777
134.921
132.098
131.497
130.783
129.966
129.149
128.781
128.692
128.491
126.825
118.957
118.352
Cl
OH
N
N
O
8k
Current Data Parameters
NAME 511610B8495
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161025
Time 5.29 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 298.2 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7577918 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40
200
190
180
170
160
150
140
130
120
ppm



Comment: IN Kbr
GVK-SAM-6-PAGE-33NP

No. of Scans:
Resolution:
Apodization:

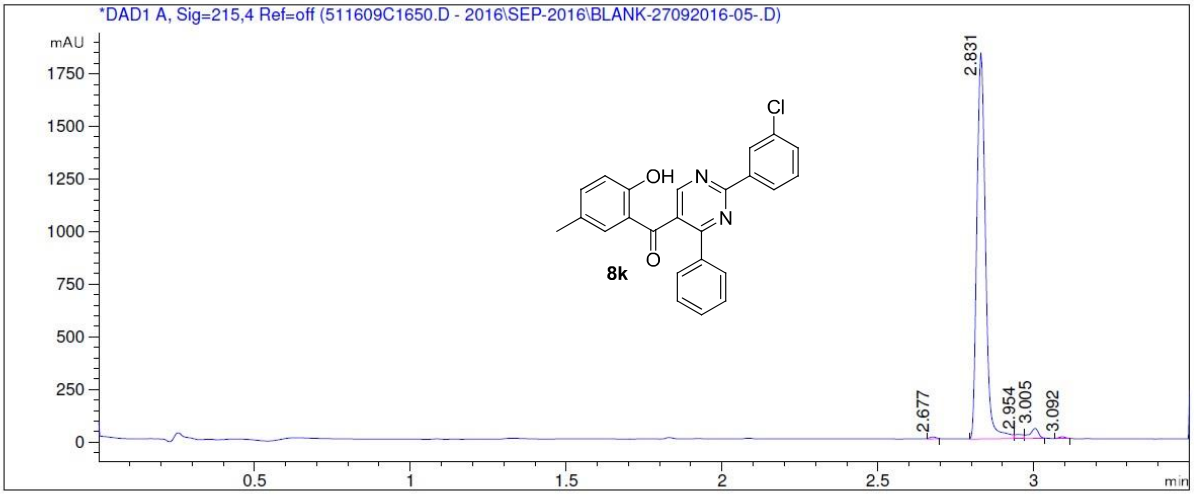
Date: 11/15/2016 10:05:13 AM
User: Admin

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

Sample Name :GVK-SAM-6-PAGE-33NP Vial position : P2-E-03
Date of Analysis :9/27/2016 11:17:46 PM Injection Vol :0.500µl
Acq. Method :C:\CHEM32\1\METHODS\RND-FA- 3.5 MIN.M Instrument ID :ANL-MCL5-LCMS-001

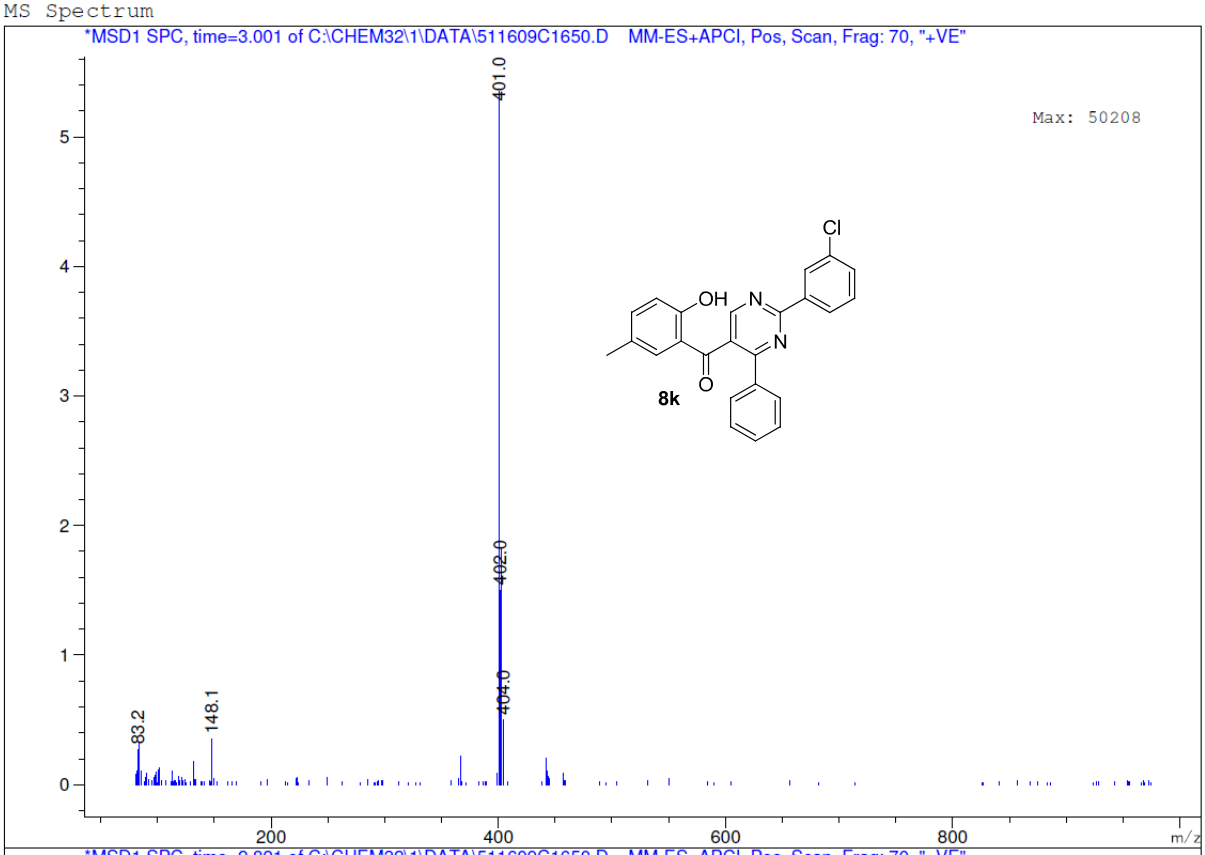
RND-FA-3.5 MIN.M
Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: B1: 0.1 % FA IN WATER A1: 0.1%FA IN ACN
Gradient: Time (min) /%A1: 0/2, 0.4/2, 2.8/98,3.4/98,3.41/2,3.5/2
Column Flow Rate: 0.6 ml/min
Column Temperature: 60°C

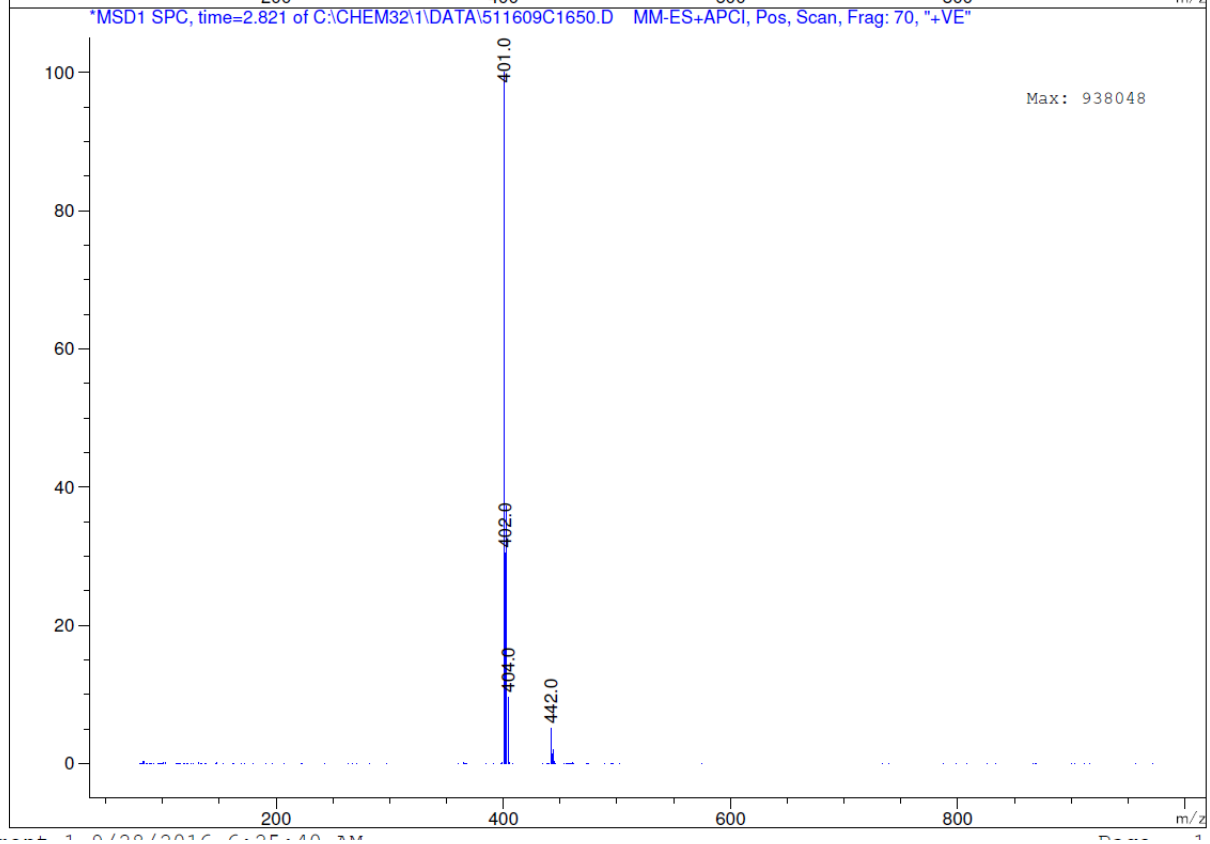
->



Peak No	RT min	Area	Area %
1	2.68	13.615	0.375
2	2.83	3474.404	95.638
3	2.95	37.733	1.039
4	3.00	92.649	2.550
5	3.09	14.459	0.398

MS Spectrum


*MSD1 SPC, time=3.001 of C:\CHEM32\1\DATA\511609C1650.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 50208
401.0
402.0
404.0
83.2
148.1
Cl
OH
N
N
O
8k
m/z


*MSD1 SPC, time=2.821 of C:\CHEM32\1\DATA\511609C1650.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 938048
401.0
402.0
404.0
442.0
m/z

Elemental Composition Report

Single Mass Analysis

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

Selected filters: None

Monoisotopic Mass, Even Electron Ions

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

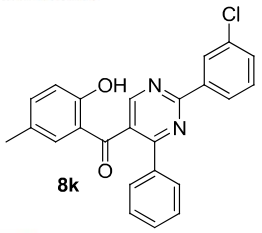
Elements Used:

C: 0-24 H: 0-18 N: 0-2 O: 0-2 Cl: 0-1

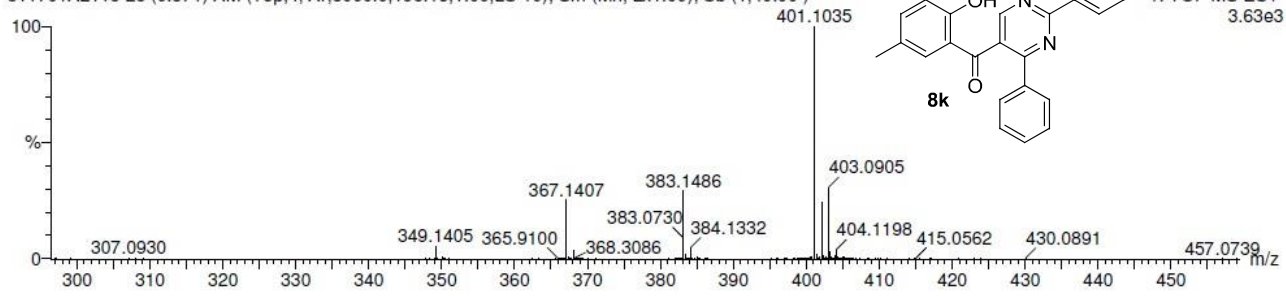
SAMPLE CODE:GVK-SAM-6-PAGE-33NP

511701A2115 26 (0.371) AM (Top,4, Ar,5000.0,195.15,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

1: TOF MS ES+
3.63e3



8k

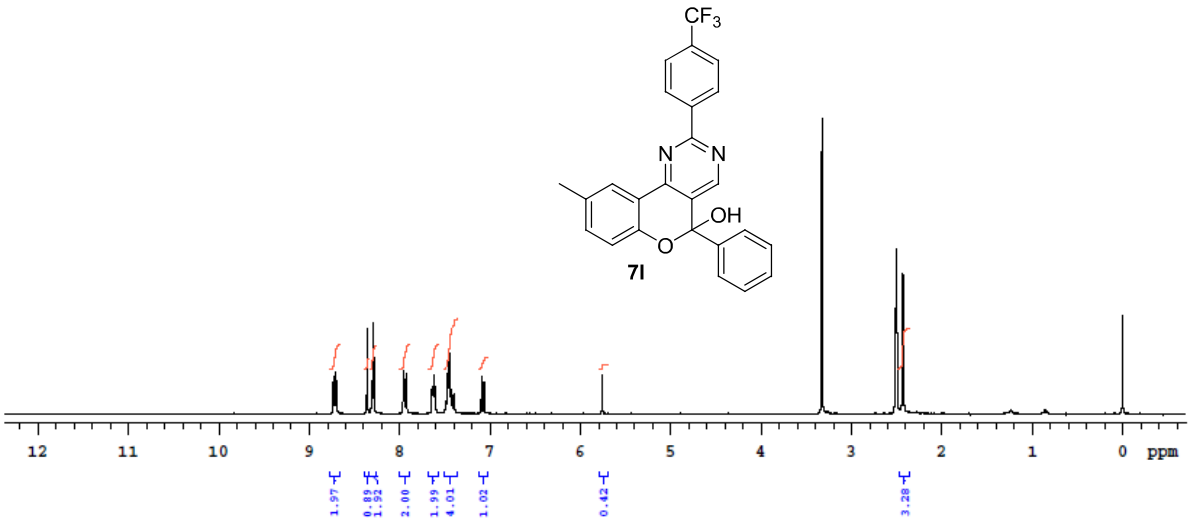


Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
401.1035	401.1057	-2.2	-5.5	16.5	20.6	C24 H18 N2 O2 Cl

Sample Name:

GVK-SAM-6-PAGE-34P

Solvent: dmso
Date: Oct 1 2016
Agilent Vnmrs300 / NRM-3
Request No: 511610A0384_PROTON

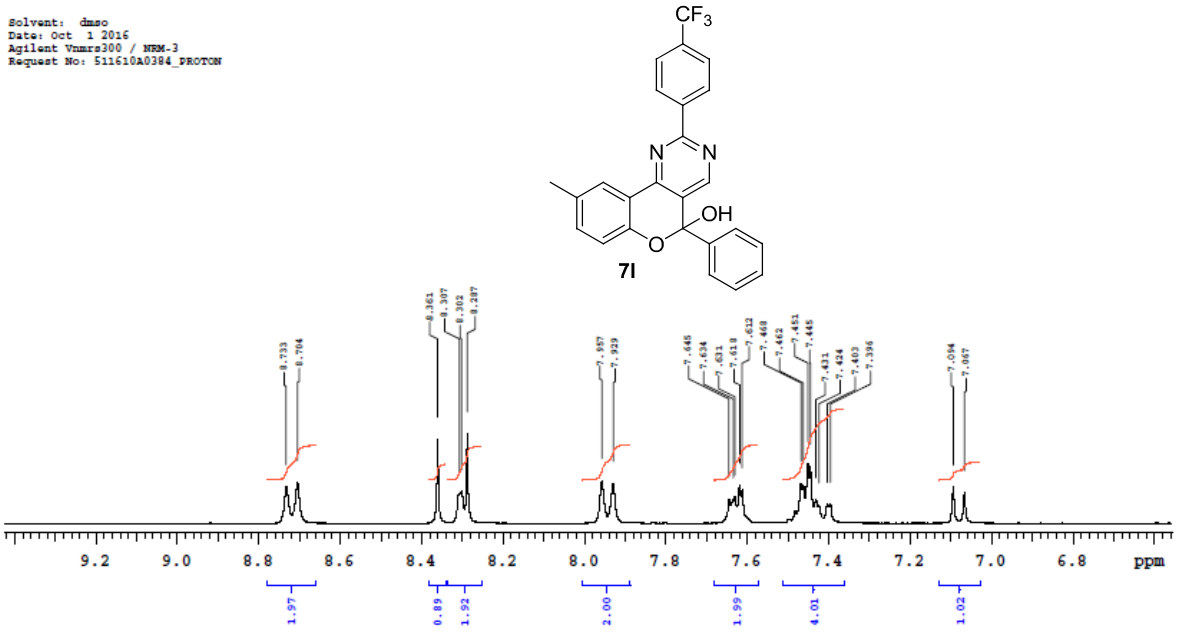


Plotname: 511610A0384_PROTON_01_plot01

Sample Name:

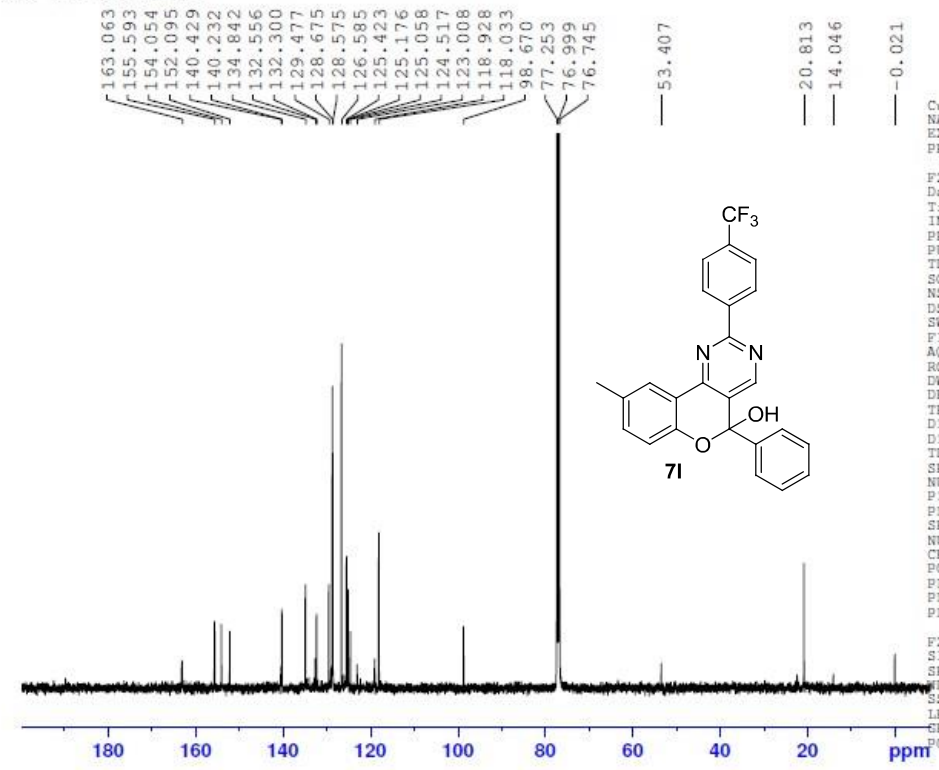
GVK-SAM-6-PAGE-34P

Solvent: dmso
Date: Oct 1 2016
Agilent Vnmrs300 / NRM-3
Request No: 511610A0384_PROTON



Plotname: 511610A0384_PROTON_01_plot02

GVK-SAM-6-PAGE-34P

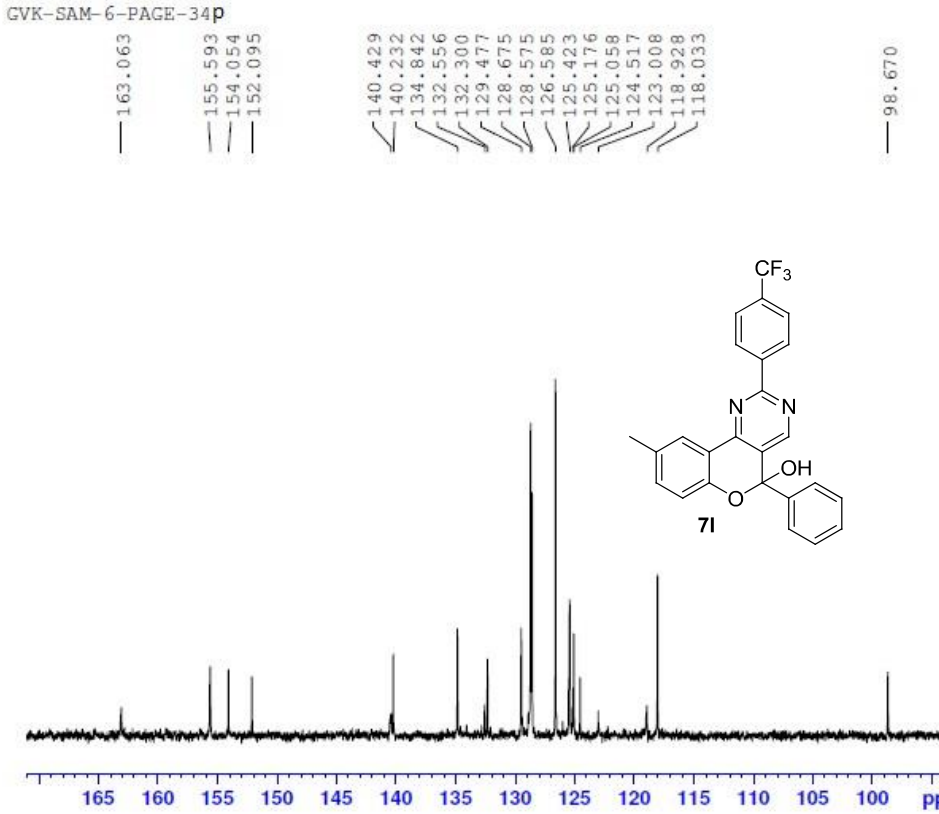


Current Data Parameters
NAME 511610B8493
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161025
Time 4.15 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 299.0 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W

F2 - Processing parameters
SI 32768
SF 125.7577918 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

GVK-SAM-6-PAGE-34P

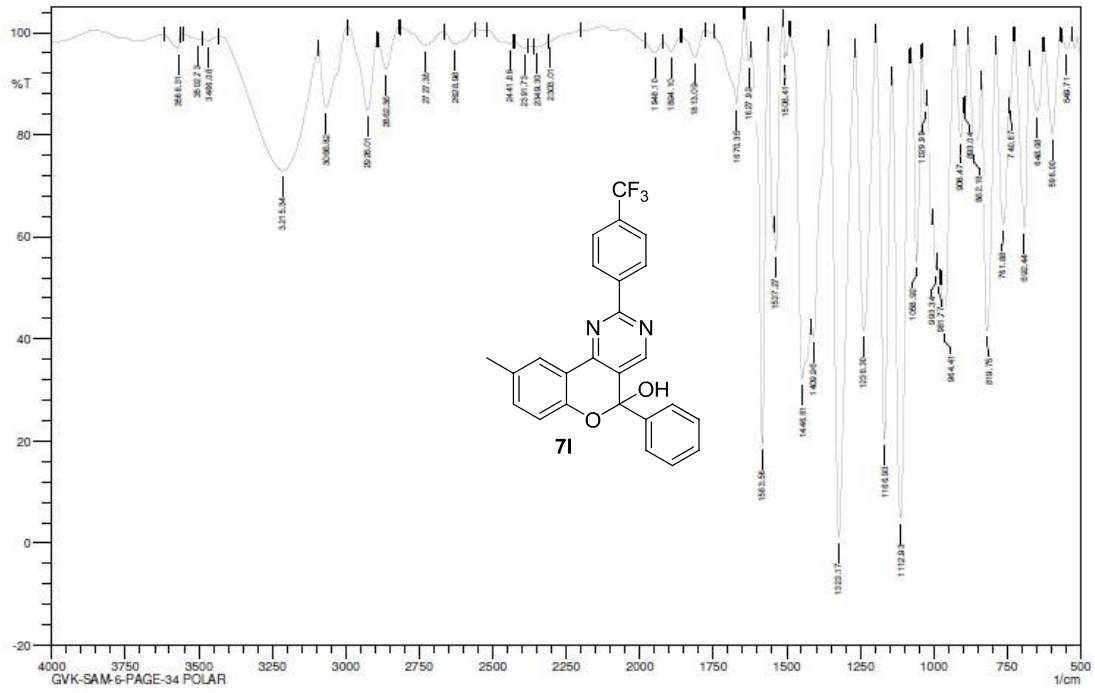


Current Data Parameters
NAME 511610B8493
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161025
Time 4.15 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 299.0 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W

F2 - Processing parameters
SI 32768
SF 125.7577918 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

SHIMADZU



7l

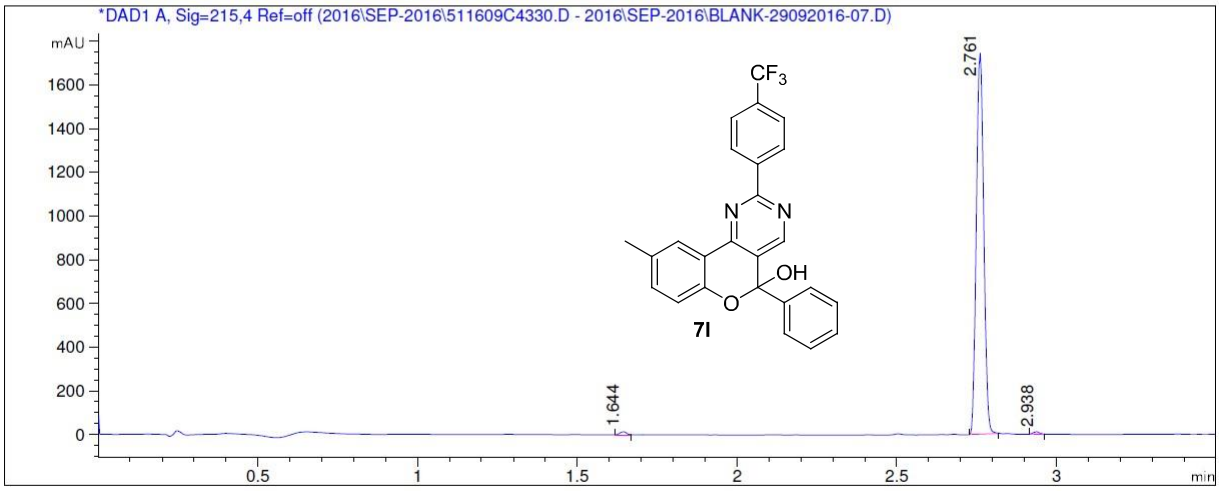
Comment: IN Kbr
GVK-SAM-6-PAGE-34 POLAR

No. of Scans:
Resolution:
Apodization:

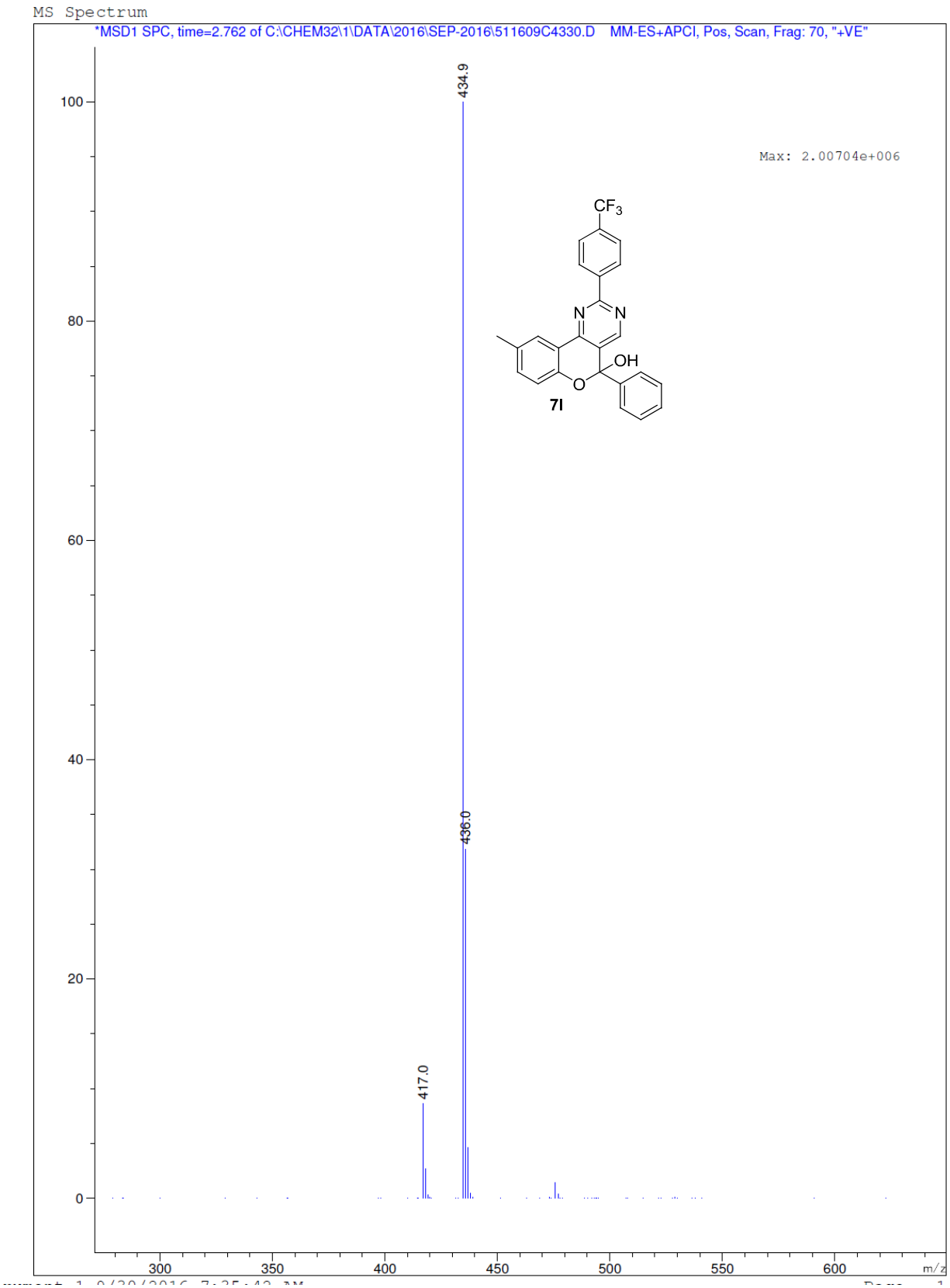
Date: 11/15/2016 10:37:13 AM
User: Admin

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

```
================================================================================================
Sample Name      : GVK-SAM-6-page-34 Polar                    Vial position  : P1-D-08
Date of Analysis :9/29/2016         11:28:34 PM             Injection Vol  :0.500µl
Acq. Method      :C:\CHEM32\1\METHODS\RND-FA- 3.5 MIN.M     Instrument ID  :ANL-MCL5-LCMS-001
================================================================================================
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, 0.4/2, 2.6/98,3.1/98,3.11/2,3.5/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 60°C
                                                                                              ->
================================================================================================
```



Peak No	RT min	Area	Area %
1	1.64	22.159	0.776
2	2.76	2814.225	98.617
3	2.94	17.300	0.606


MS Spectrum
*MSD1 SPC, time=2.762 of C:\CHEM32\1\DATA\2016\SEP-2016\511609C4330.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 2.00704e+006
434.9
436.0
417.0
CF3
N
N
OH
O
7l
100
80
60
40
20
0
300
350
400
450
500
550
600
m/z

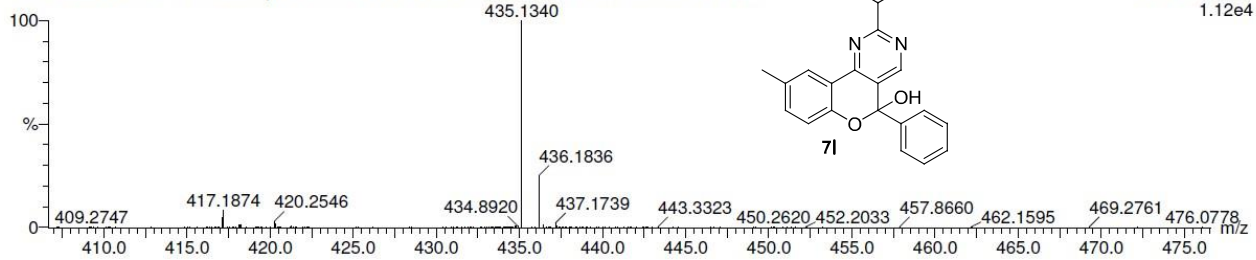
Elemental Composition Report

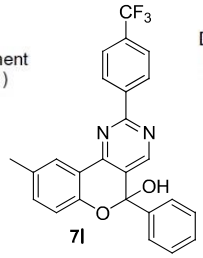
Single Mass Analysis

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

Monoisotopic Mass, Even Electron Ions
27 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-25 H: 0-18 N: 0-2 O: 0-2 F: 0-3

GVK-SAM-6-PAGE-34POLAR
GVK Bio sciences (pvt)Ltd
Analytical Research and Development
Date of analysis:25-Mar-201721:14:06
Instru ment ID:ANL-MCL3-LCMS-001
511703C0744 20 (0.277) AM (Top,4, Ar,0.0,195.11,1.00,LS 10); Sm (Mn, 2x1.00); Sb (0,40.00)
1: TOF MS ES+
1.12e4

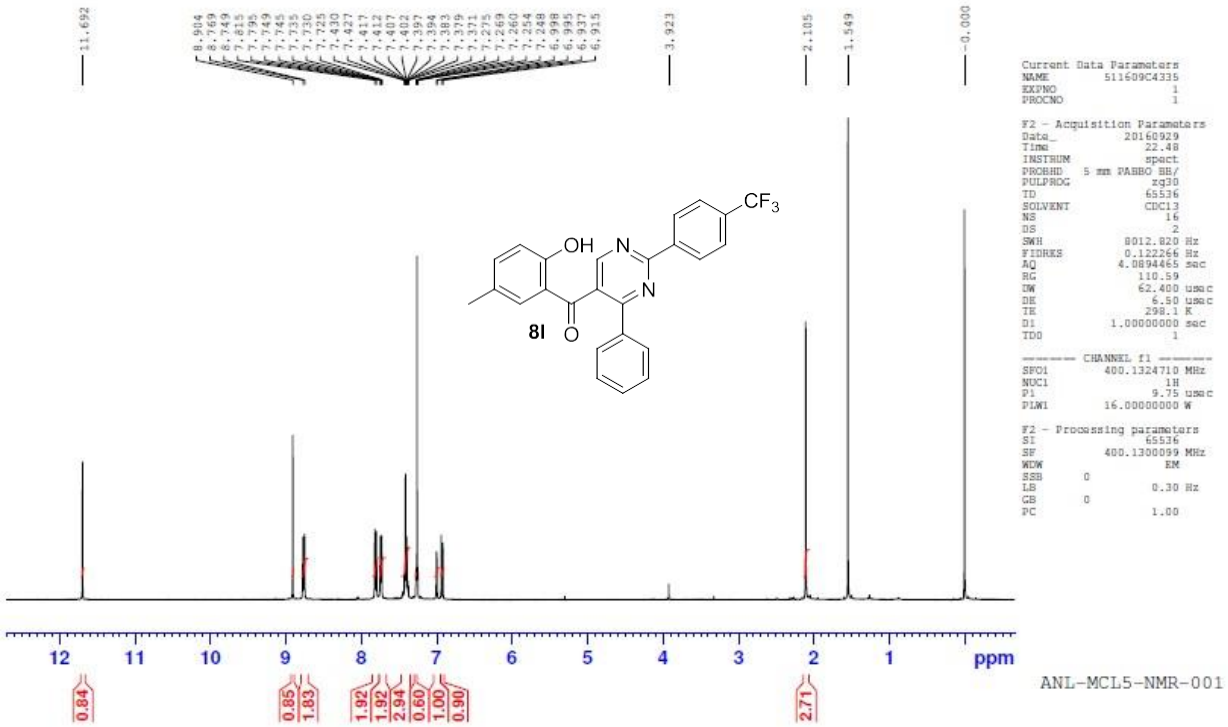




7l

Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
435.1340	435.1320	2.0	4.6	16.5	275.0	C25 H18 N2 O2 F3

GVK-SAM-6-page-34NP



Current Data Parameters
NAME 511609C4335
EXPNO 1
PROCNO 1

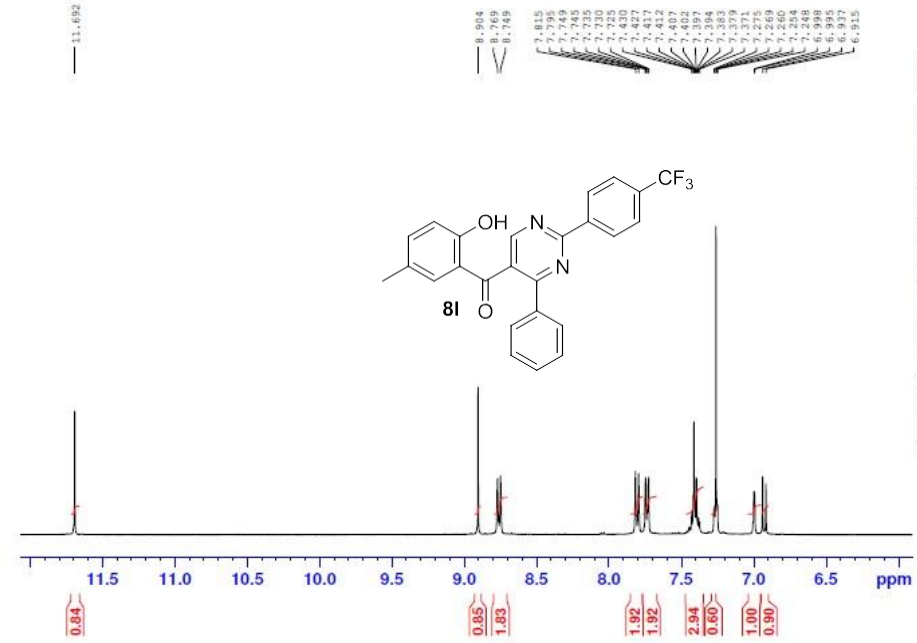
F2 - Acquisition Parameters
Date_ 20160929
Time 22.48
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 110.59
DW 62.400 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1

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

F2 - Processing parameters
SI 65536
SF 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

ANL-MCL5-NMR-001

GVK-SAM-6-page-34NP



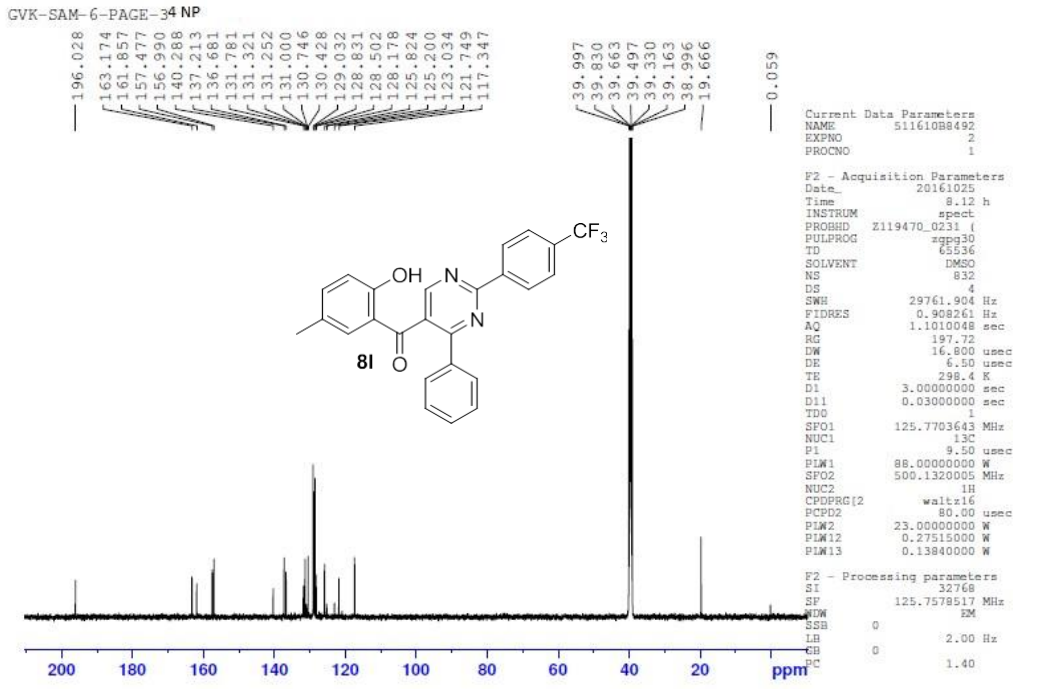
Current Data Parameters
NAME 511609C4335
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20160929
Time 22.48
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 298.1 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 400.1300099 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

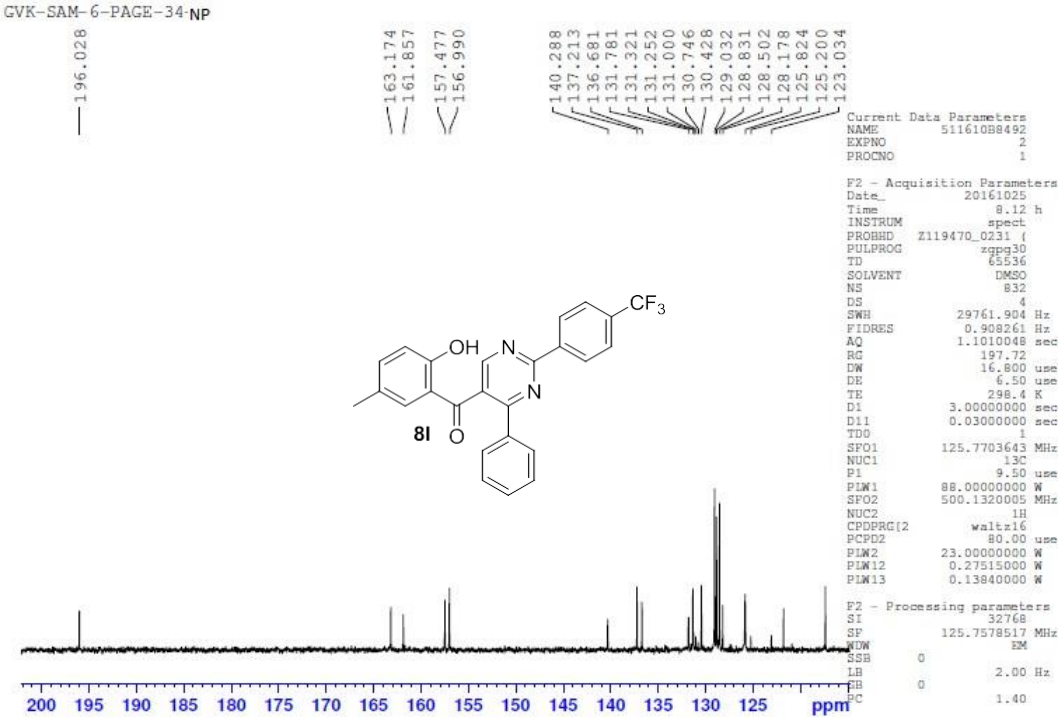
ANL-MCL5-NMR-001



Current Data Parameters
NAME 511610B8492
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161025
Time 8.12 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 832
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 298.4 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W

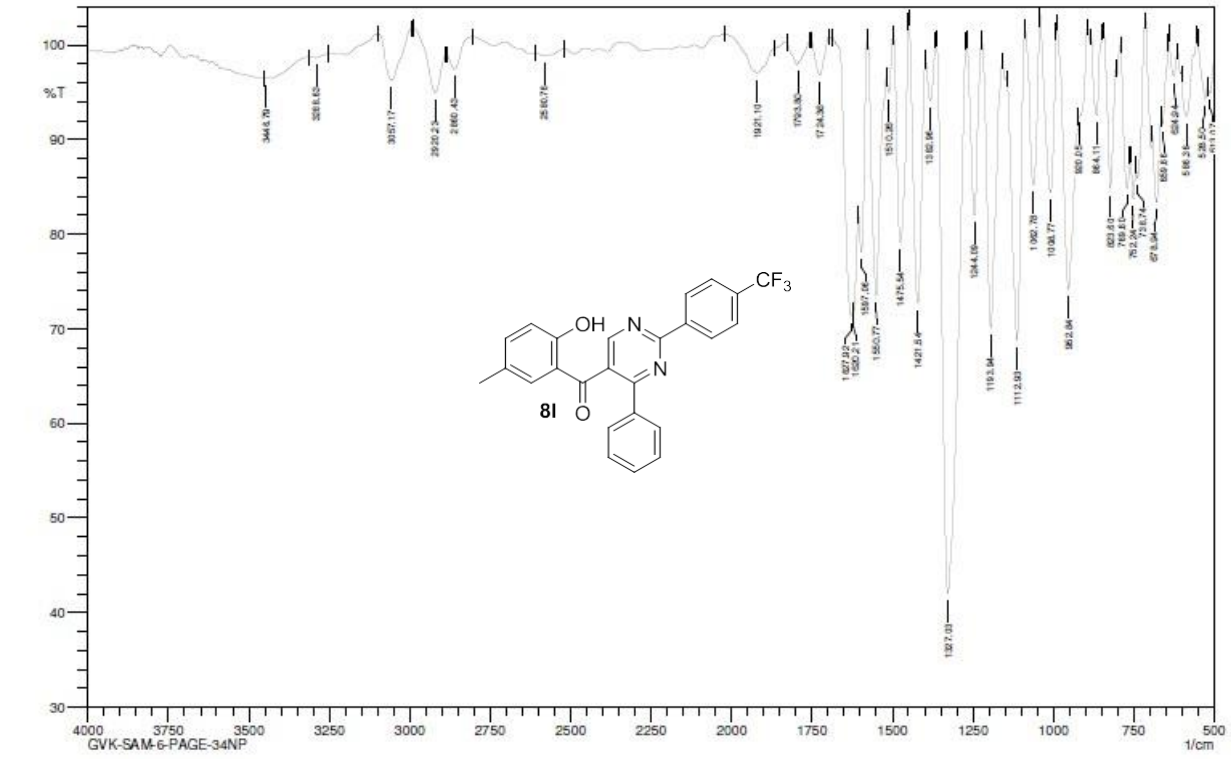
F2 - Processing parameters
SI 32768
SF 125.7578517 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40



Current Data Parameters
NAME 511610B8492
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161025
Time 8.12 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 832
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 use
DE 6.50 use
TE 298.4 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 use
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 use
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W

F2 - Processing parameters
SI 32768
SF 125.7578517 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40



Comment: IN Kbr
GVK-SAM-6-PAGE-34NP

No. of Scans:
Resolution:

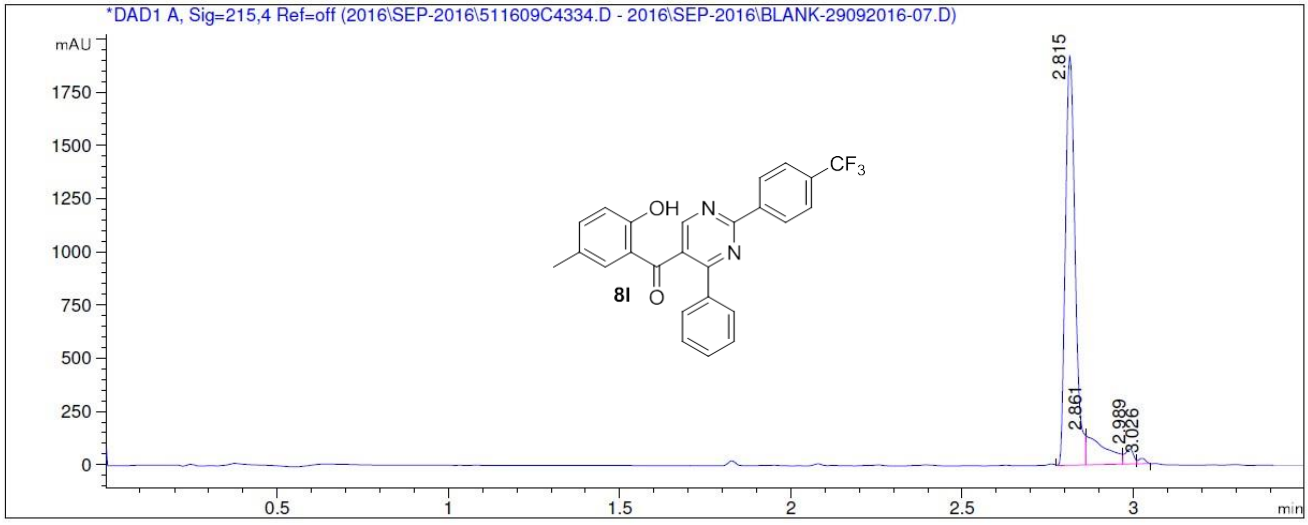
Date: 11/15/2016 10:18:51 AM
User: Admin

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

Sample Name : GVK-SAM-6-page-34NP Vial position : P1-D-04
Date of Analysis :9/29/2016 11:10:47 PM Injection Vol :0.500µl
Acq. Method :C:\CHEM32\1\METHODS\RND-FA- 3.5 MIN.M Instrument ID :ANL-MCL5-LCMS-001

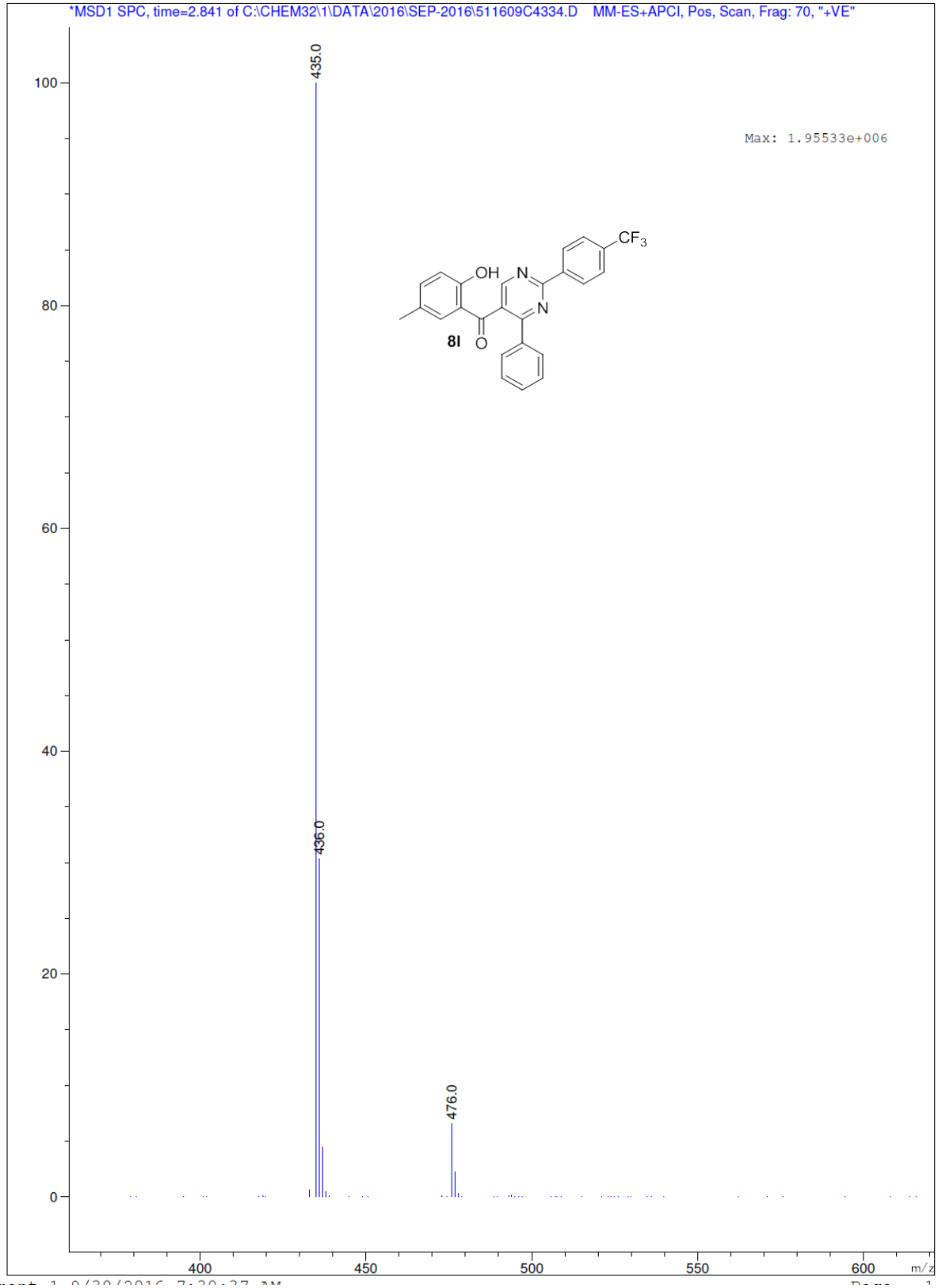
RND-FA-3.5 MIN.M
Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: B1: 0.1 % FA IN WATER A1: 0.1%FA IN ACN
Gradient: Time (min) /%A1: 0/2, 0.4/2, 2.6/98,3.1/98,3.11/2,3.5/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 60°C

->



Peak No	RT min	Area	Area %
1	2.81	3797.606	84.422
2	2.86	543.713	12.087
3	2.99	121.975	2.712
4	3.03	35.061	0.779

MS Spectrum

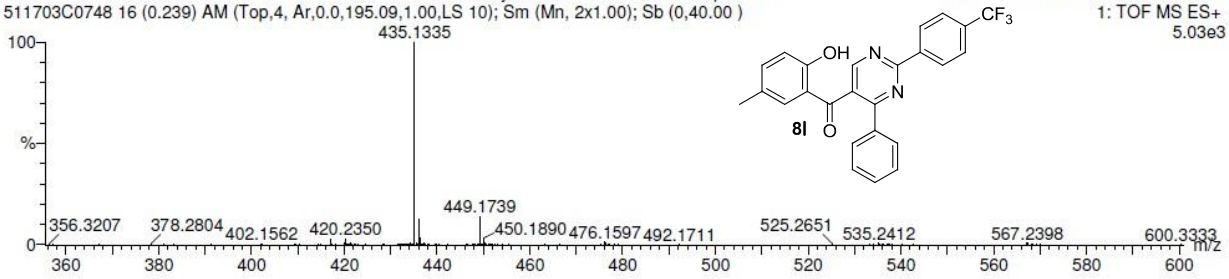

*MSD1 SPC, time=2.841 of C:\CHEM32\1\DATA\2016\SEP-2016\511609C4334.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 1.95533e+006
435.0
436.0
476.0
OH
N
N
O
CF3
8l
100
80
60
40
20
0
400
450
500
550
600
m/z

Single Mass Analysis

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

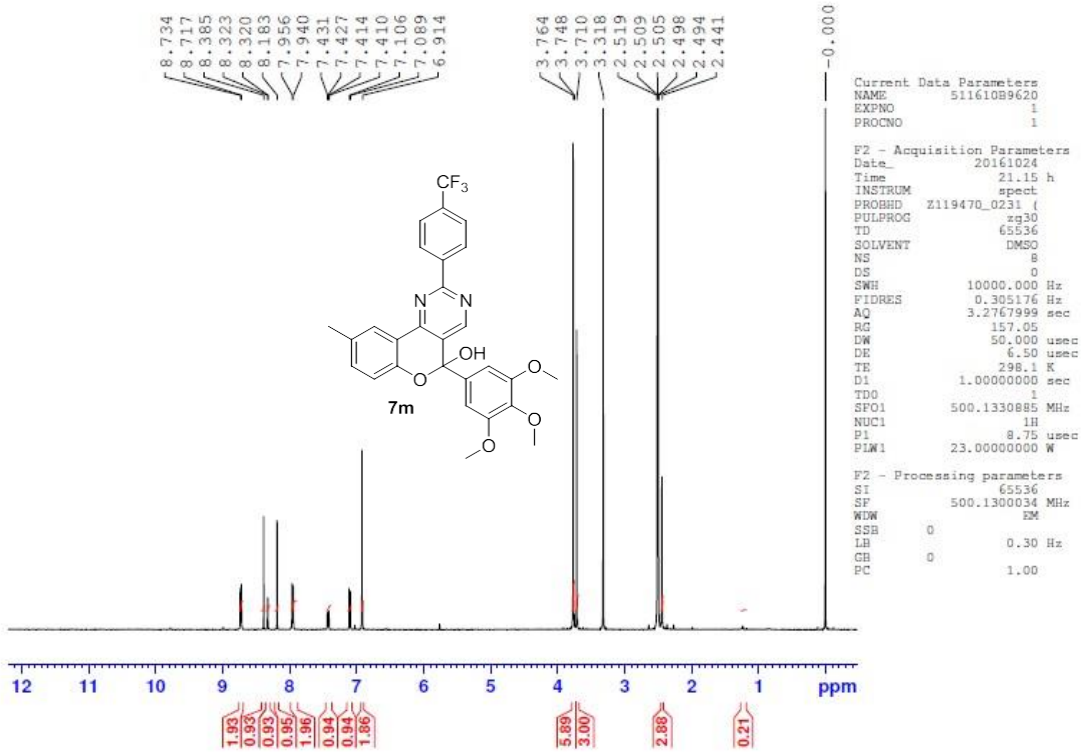
Monoisotopic Mass, Even Electron Ions
27 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-25 H: 0-18 N: 0-2 O: 0-2 F: 0-3

GVK-SAM-6-PAGE-34NP
GVK Bio sciences (pvt)Ltd
Analytical Research and Development
Date of analysis:25-Mar-201721:18:49
Instru ment ID:ANL-MCL3-LCMS-001
511703C0748 16 (0.239) AM (Top,4, Ar,0.0,195.09,1.00,LS 10); Sm (Mn, 2x1.00); Sb (0,40.00)
1: TOF MS ES+
5.03e3



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
435.1335	435.1320	1.5	3.4	16.5	533.7	C25 H18 N2 O2 F3

GVK-SAM-6-PAGE-37-POLAR

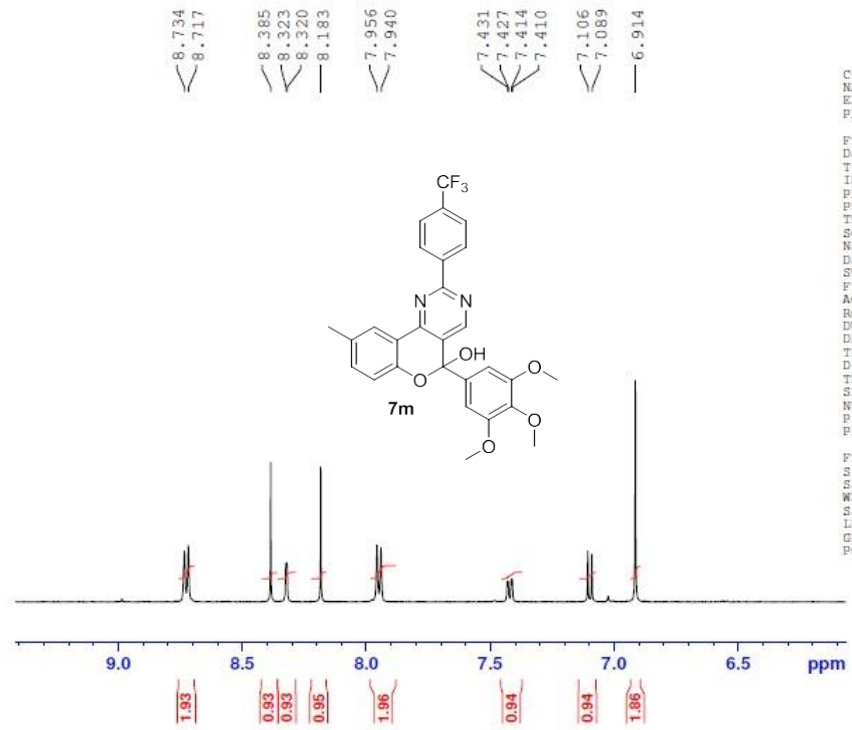


Current Data Parameters
NAME 511610B9620
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161024
Time 21.15 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 157.05
DW 50.000 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.1330885 MHz
NUC1 1H
P1 8.75 usec
PLW1 23.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1300034 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

GVK-SAM-6-PAGE-37-POLAR

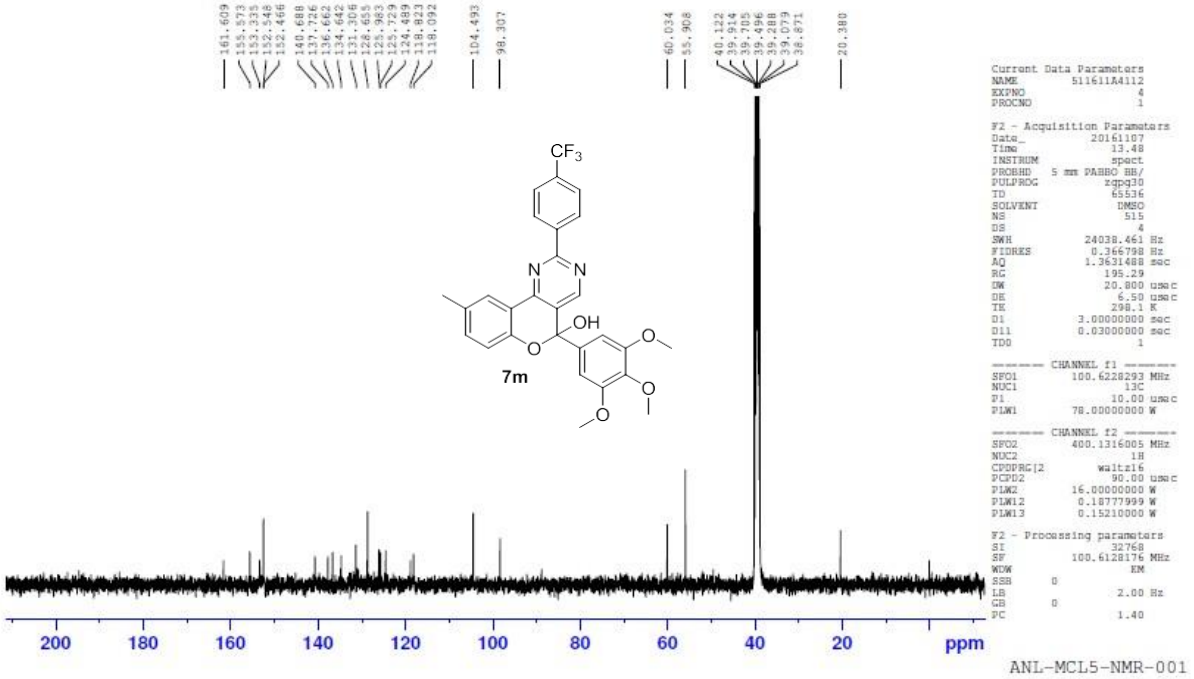


Current Data Parameters
NAME 511610B9620
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161024
Time 21.15 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 157.05
DW 50.000 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.1330885 MHz
NUC1 1H
P1 8.75 usec
PLW1 23.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1300034 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

GVK-SAM-6-page-37 polar




```
Current Data Parameters
NAME          511611A4112
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_          20161107
Time              13.48
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT           DMSO
NS                  515
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              298.1 K
D1              3.00000000 sec
D11             0.03000000 sec
TD0                   1

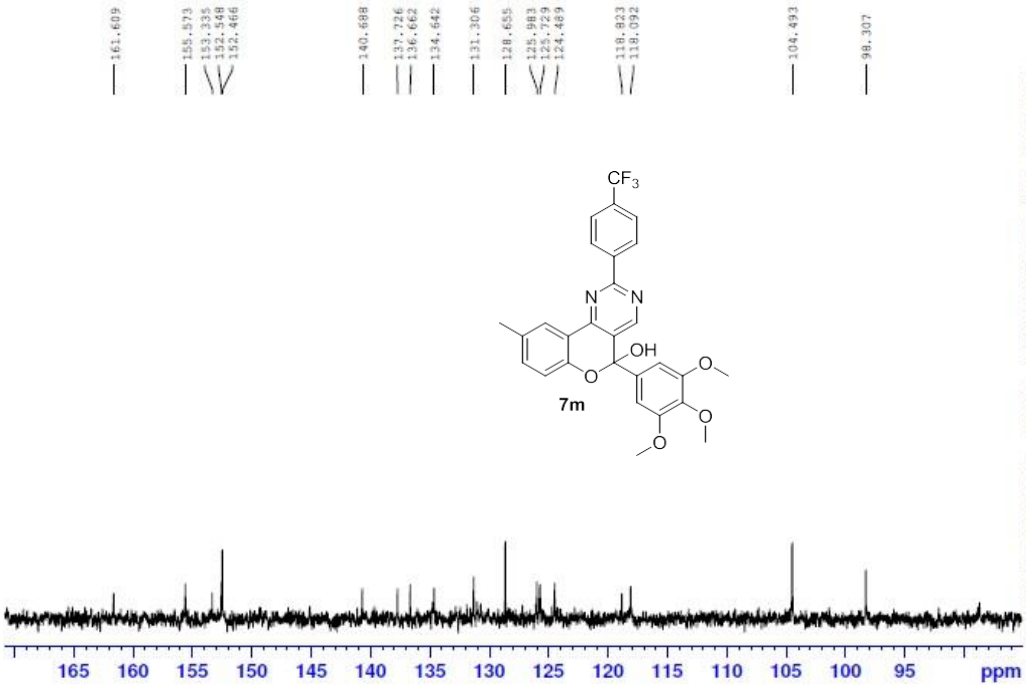
======== CHANNEL f1 ========
SFO1         100.6228293 MHz
NUC1               13C
P1               10.00 usec
PLW1          78.00000000 W

======== 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           100.6128176 MHz
WDW                  EM
SSB      0
LB               2.00 Hz
GB       0
PC               1.40
```

ANL-MCL5-NMR-001

GVK-SAM-6-page-37 polar




```
Current Data Parameters
NAME          511611A4112
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_          20161107
Time              13.48
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT           DMSO
NS                  515
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              298.1 K
D1              3.00000000 sec
D11             0.03000000 sec
TD0                   1

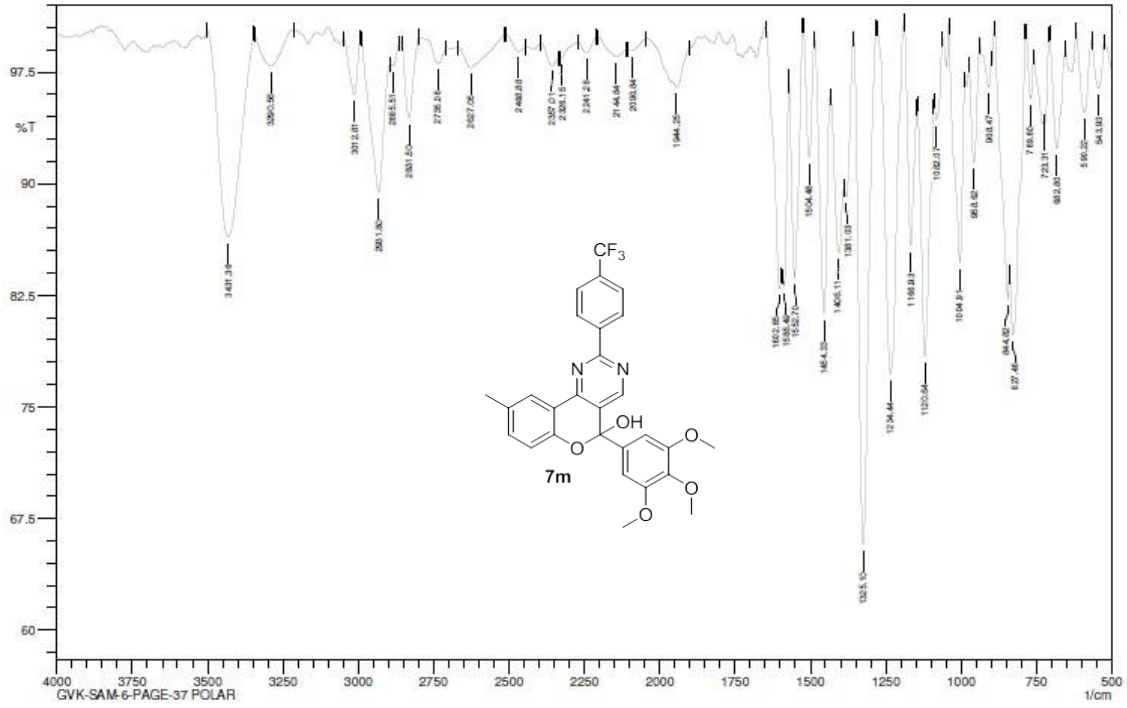
======== CHANNEL f1 ========
SFO1         100.6228293 MHz
NUC1               13C
P1               10.00 usec
PLW1          78.00000000 W

======== 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           100.6128176 MHz
WDW                  EM
SSB      0
LB               2.00 Hz
GB       0
PC               1.40
```

ANL-MCL5-NMR-001

SHIMADZU



Comment: IN Kbr
GVK-SAM-6-PAGE-37 POLAR

No. of Scans:
Resolution:
Apodization:

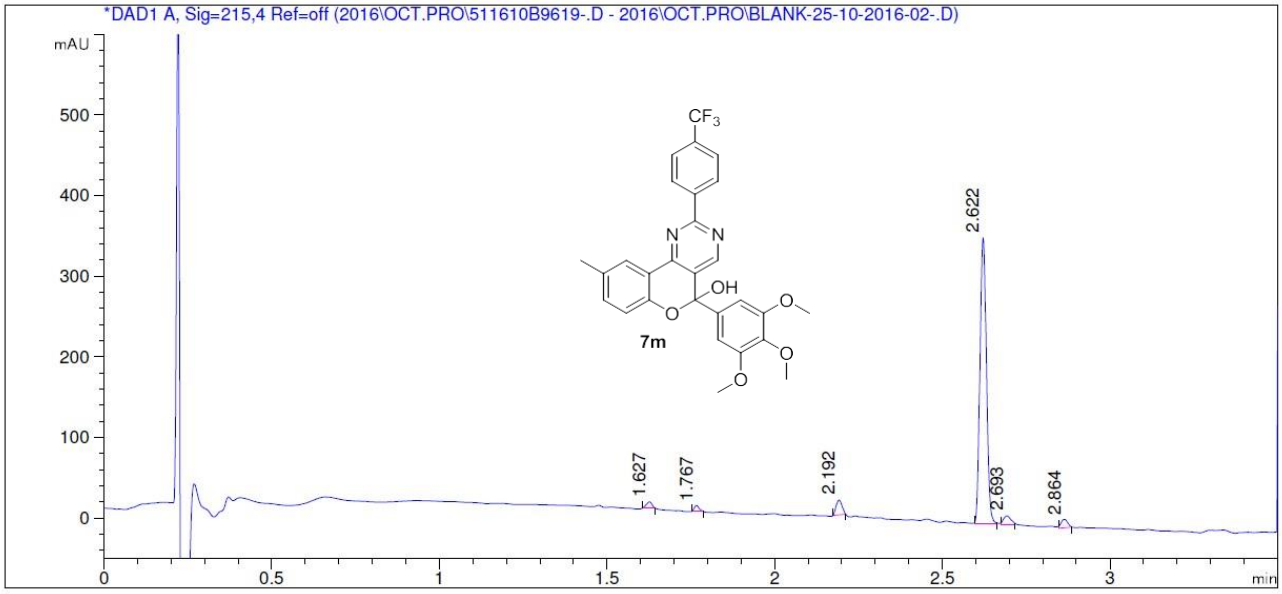
Date: 11/15/2016 11:02:35 AM
User: Admin

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

Sample Name : GVK-SAM-6-page-37 polar Vial position : P2-A-01
Date of Analysis :10/25/2016 9:35:40 AM Injection Vol : 3.000uL
Acq. Method :C:\CHEM32\1\METHODS\RND-FA- 3.5 MIN.M Instrument ID :ANL-MCL5-LCMS-001

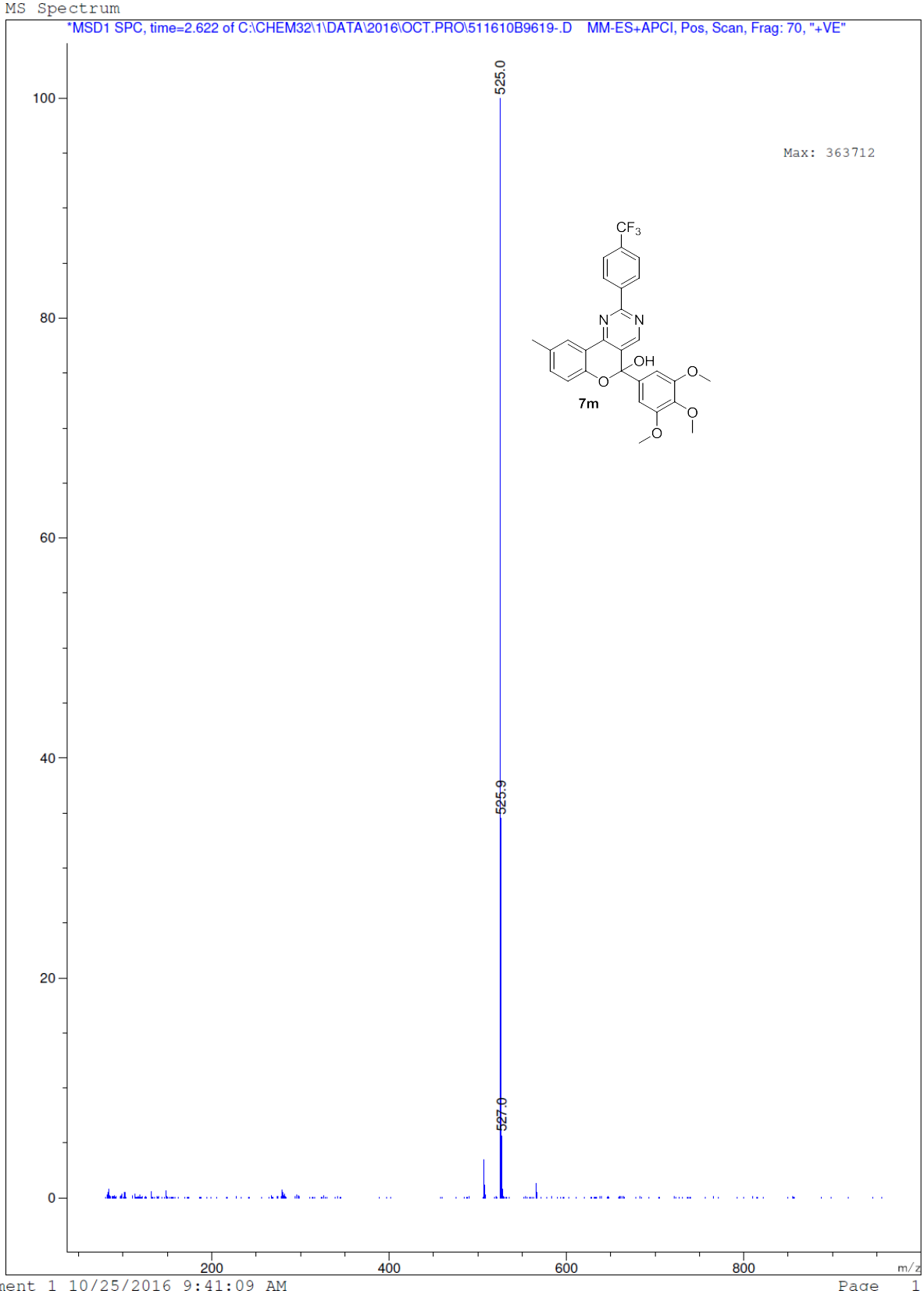
RND-FA-3.5 MIN.M
Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: B1: 0.1 % FA IN WATER A1: 0.1%FA IN ACN
Gradient: Time (min) /%A1: 0/2, 0.4/2, 2.6/98,3.1/98,3.11/2,3.5/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 60°C

->



Pea No	RT min	Area	Area %
1	1.63	10.113	1.845
2	1.77	6.889	1.257
3	2.19	22.396	4.085
4	2.62	476.022	86.830
5	2.69	18.523	3.379
6	2.86	14.277	2.604

MS Spectrum



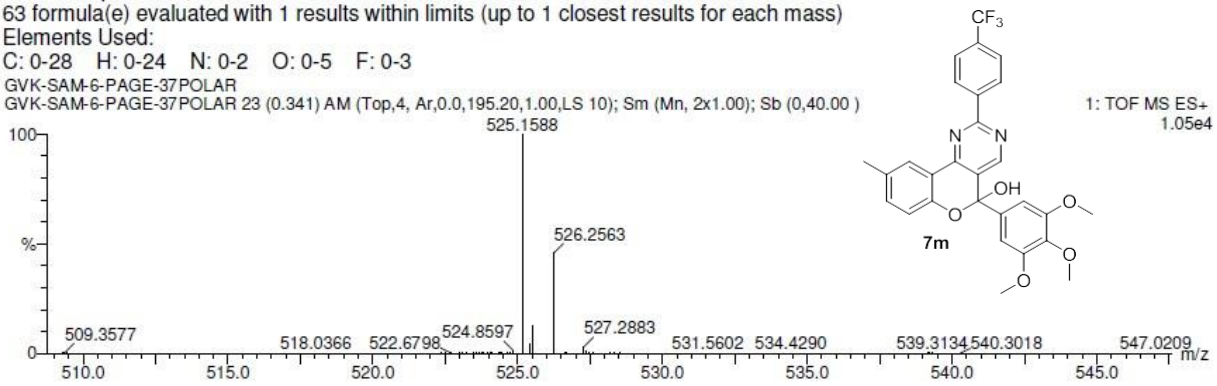
:rument 1 10/25/2016 9:41:09 AM Page 1 o:

Elemental Composition Report **Page 1**

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

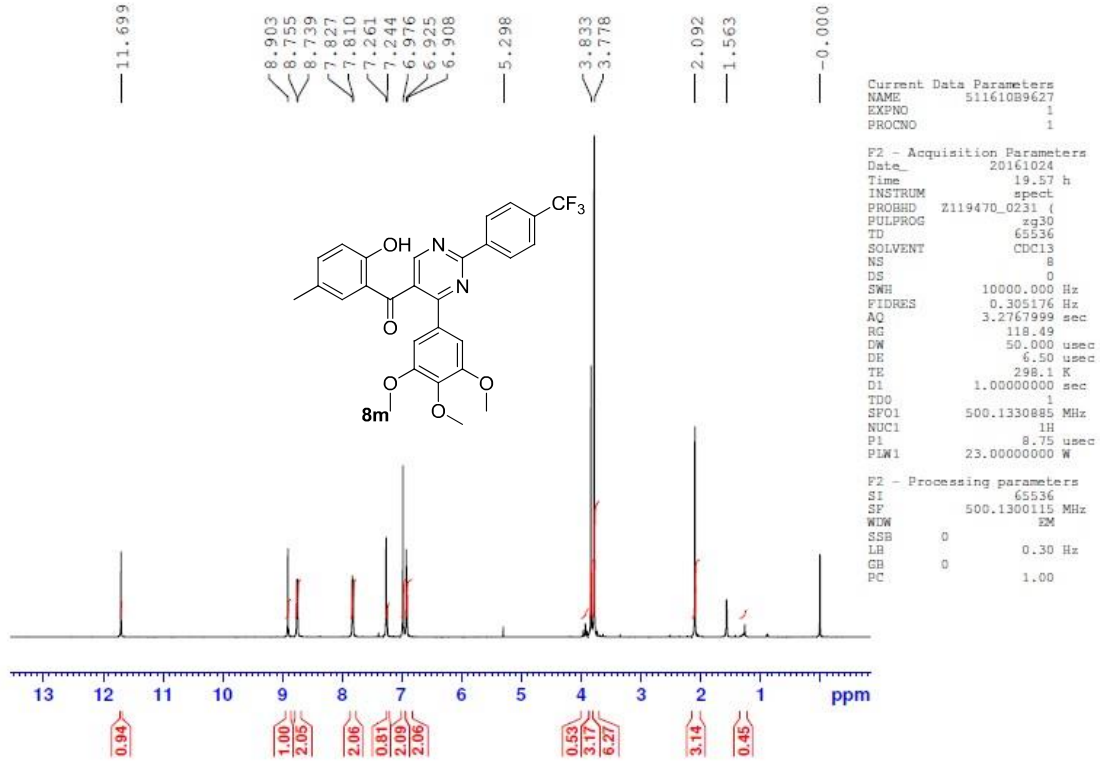
Monoisotopic Mass, Even Electron Ions
63 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-28 H: 0-24 N: 0-2 O: 0-5 F: 0-3

GVK-SAM-6-PAGE-37POLAR
GVK-SAM-6-PAGE-37POLAR 23 (0.341) AM (Top,4, Ar,0.0,195.20,1.00,LS 10); Sm (Mn, 2x1.00); Sb (0,40.00)



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
525.1588	525.1637	-4.9	-9.3	16.5	817.4	C28 H24 N2 O5 F3

GVK-SAM-6-page-37 NP

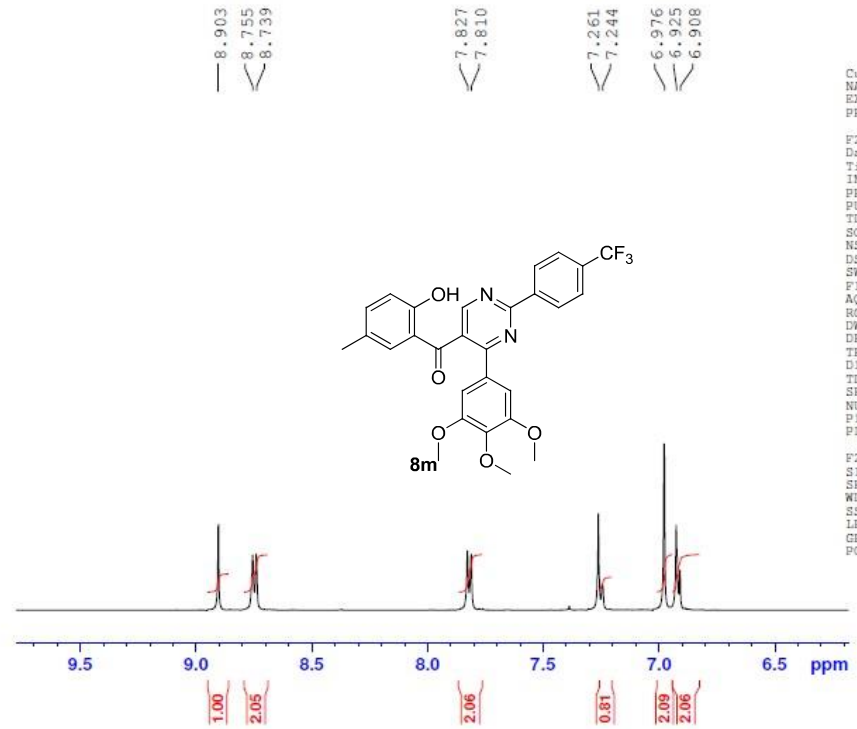


Current Data Parameters
NAME 511610B9627
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161024
Time 19.57 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 118.49
DW 50.000 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.1330885 MHz
NUC1 1H
P1 8.75 usec
PLW1 23.00000000 W

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

GVK-SAM-6-page-37 NP

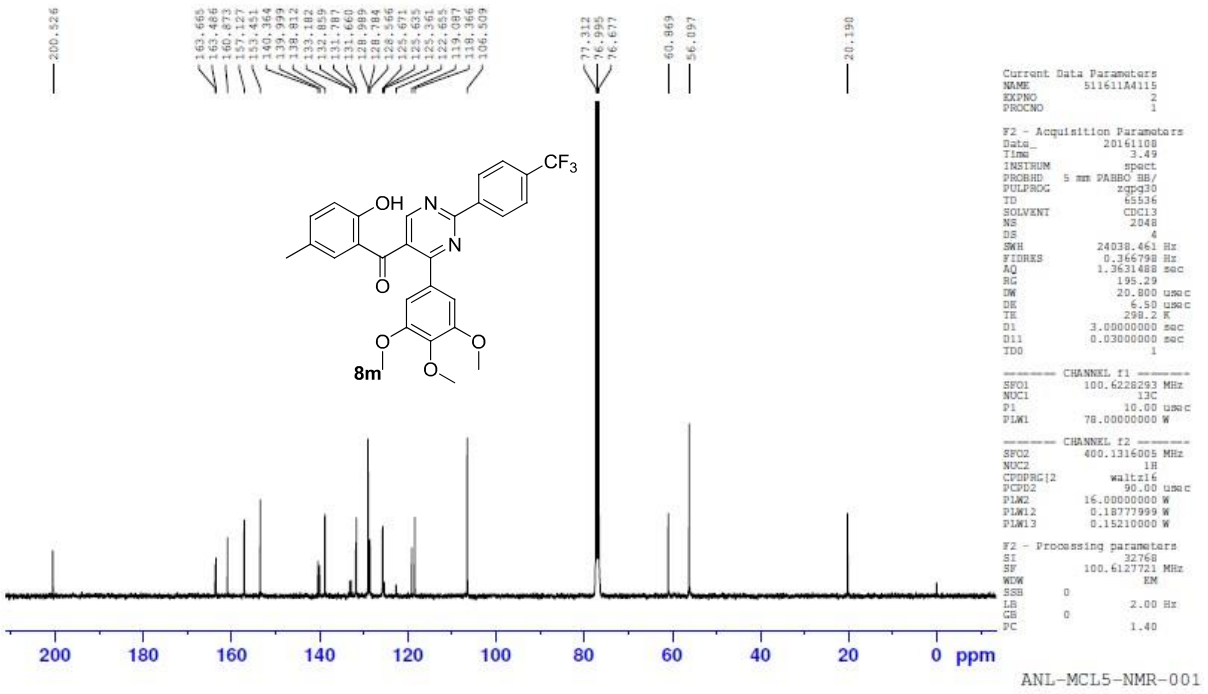


Current Data Parameters
NAME 511610B9627
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161024
Time 19.57 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 118.49
DW 50.000 usec
DE 6.50 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
SFO1 500.1330885 MHz
NUC1 1H
P1 8.75 usec
PLW1 23.00000000 W

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

GVK-SAM-6PAGE-37NP




```
Current Data Parameters
NAME          511611A4115
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_          20161108
Time               3.49
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                2048
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              298.2 K
D1          3.00000000 sec
D11         0.03000000 sec
TD0                  1

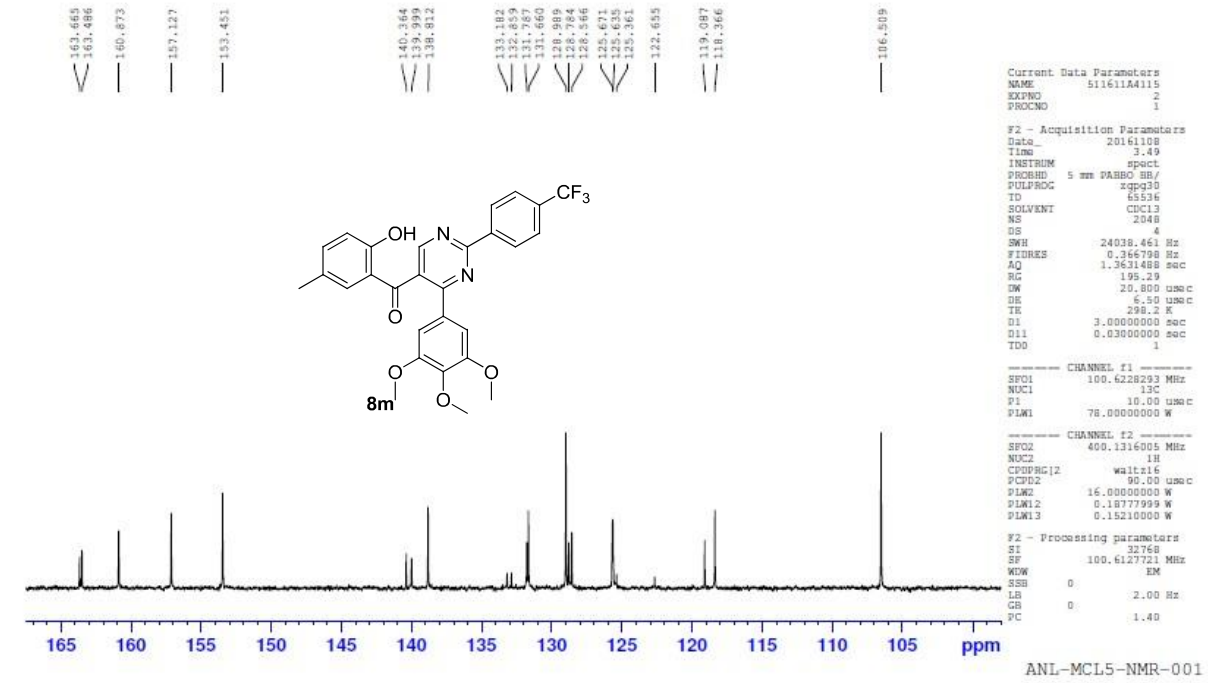
======== CHANNEL f1 ========
SFO1       100.6228293 MHz
NUC1              13C
P1              10.00 usec
PLW1       78.00000000 W

======== 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         100.6127721 MHz
WDW                   EM
SSB       0
LB                2.00 Hz
GB        0
PC                1.40
```

ANL-MCL5-NMR-001

GVK-SAM-6PAGE-37NP




```
Current Data Parameters
NAME          511611A4115
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_          20161108
Time               3.49
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT          CDCl3
NS                2048
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              298.2 K
D1          3.00000000 sec
D11         0.03000000 sec
TD0                  1

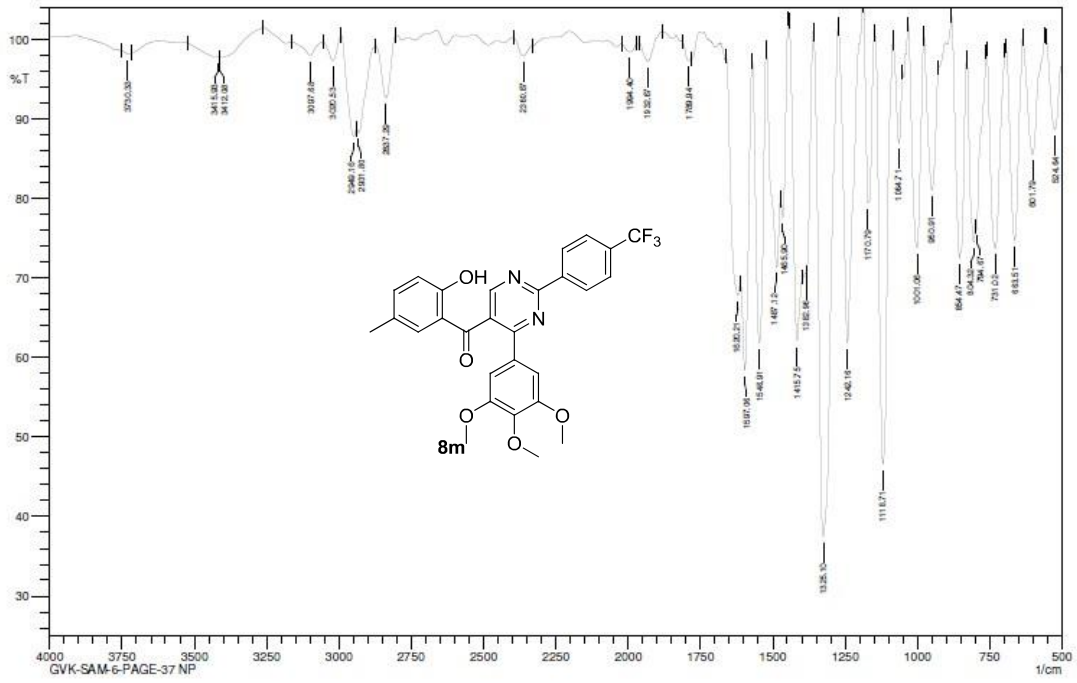
======== CHANNEL f1 ========
SFO1       100.6228293 MHz
NUC1              13C
P1              10.00 usec
PLW1       78.00000000 W

======== 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         100.6127721 MHz
WDW                   EM
SSB       0
LB                2.00 Hz
GB        0
PC                1.40
```

ANL-MCL5-NMR-001

SHIMADZU



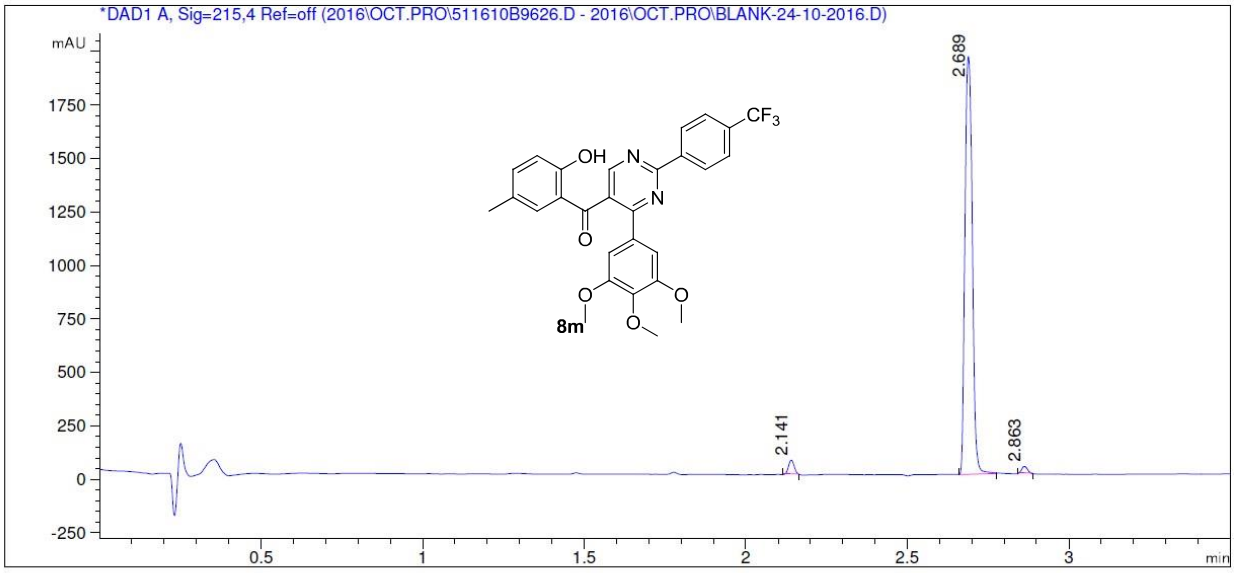
Comment: IN Kbr
GVK-SAM-6-PAGE-37 NP

No. of Scans:
Resolution:
Apodization:

Date: 11/15/2016 11:09:14 AM
User: Admin

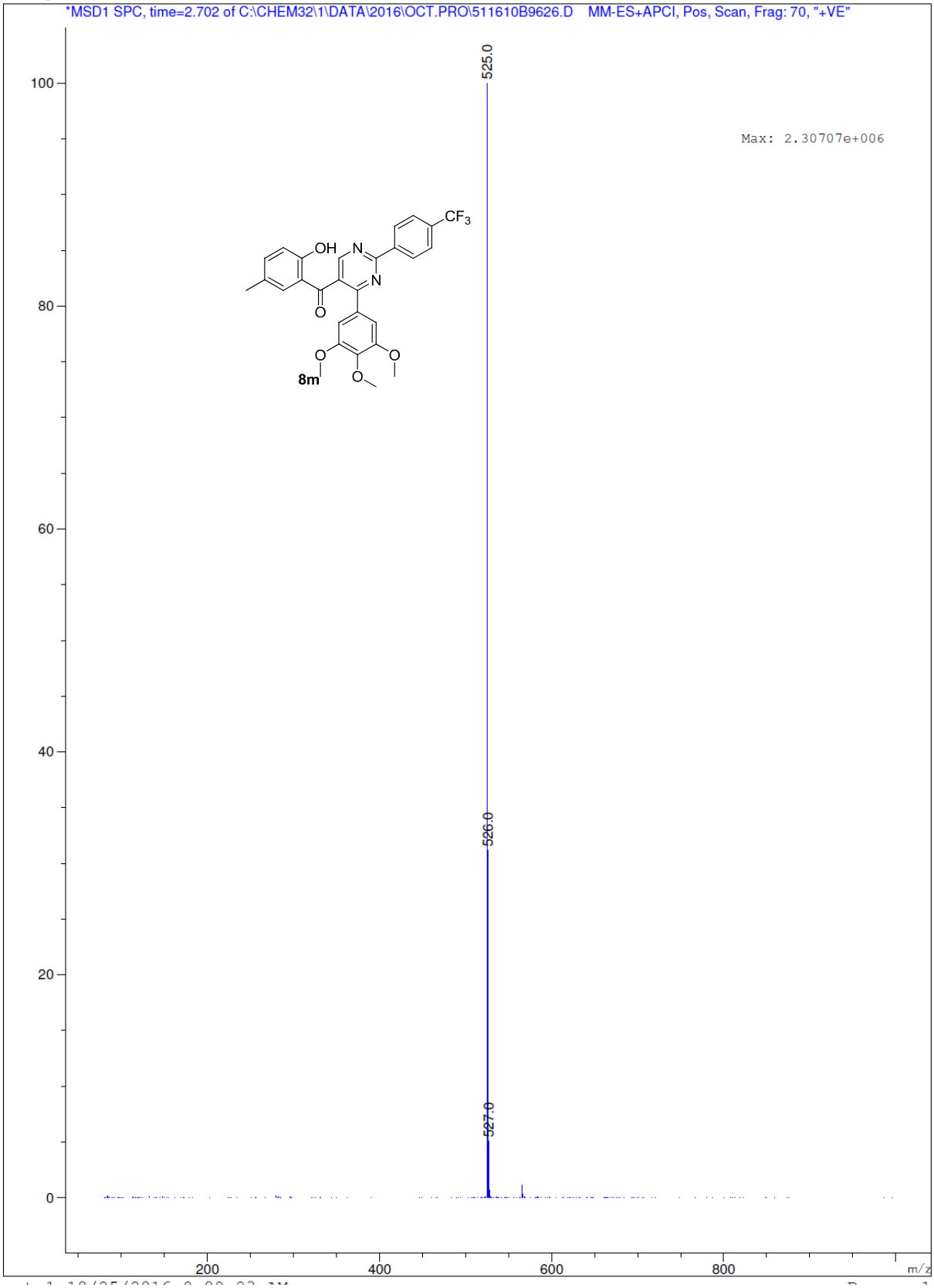
GVK BIOSCIENCES PVT. LTD.
MEDICINAL CHEMISTRY LABORATORY - ANALYTICAL RESEARCH
LCMS REPORT

```
================================================================================================
Sample Name      : GVK-SAM-6-page-37 NP                          Vial position  : P2-A-03
Date of Analysis :10/24/2016        11:30:31 PM              Injection Vol  :     0.300uL
Acq. Method      :C:\CHEM32\1\METHODS\RND-FA- 3.5 MIN.M     Instrument ID  :ANL-MCL5-LCMS-001
================================================================================================
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, 0.4/2, 2.6/98,3.1/98,3.11/2,3.5/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 60°C
                                                                                          ->
================================================================================================
```



Peak No	RT min	Area	Area %
1	2.14	74.539	2.330
2	2.69	3090.920	96.618
3	2.86	33.640	1.052

MS Spectrum


*MSD1 SPC, time=2.702 of C:\CHEM32\1\DATA\2016\OCT.PRO\511610B9626.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 2.30707e+006
525.0
526.0
527.0
100
80
60
40
20
0
200
400
600
800
m/z
OH
N
N
O
CF3
O
O
O
8m

Elemental Composition Report

Single Mass Analysis

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

Selected filters: None

Monoisotopic Mass, Odd and Even Electron Ions

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

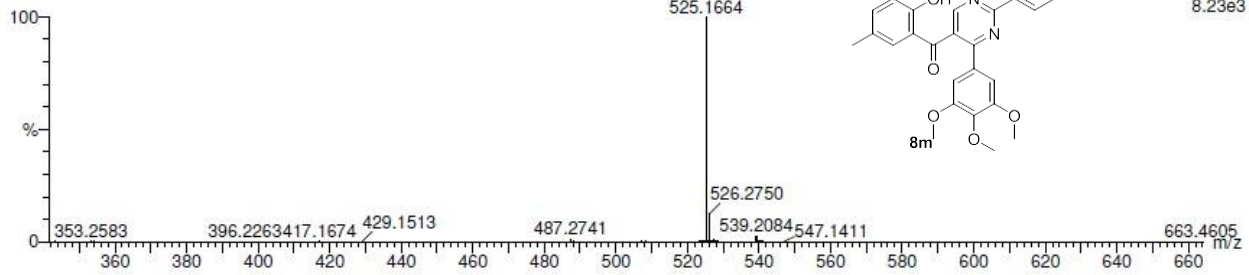
Elements Used:

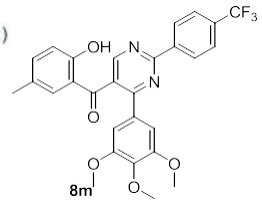
C: 0-28 H: 0-24 N: 0-2 O: 0-5 F: 0-3

GVK-SAM-6-PAGE-37NP

GVK-SAM-6-PAGE-37NP 21 (0.287) AM (Top,4, Ar,0.0,195.18,1.00,LS 10); Sm (Mn, 2x1.00); Sb (0,40.00)

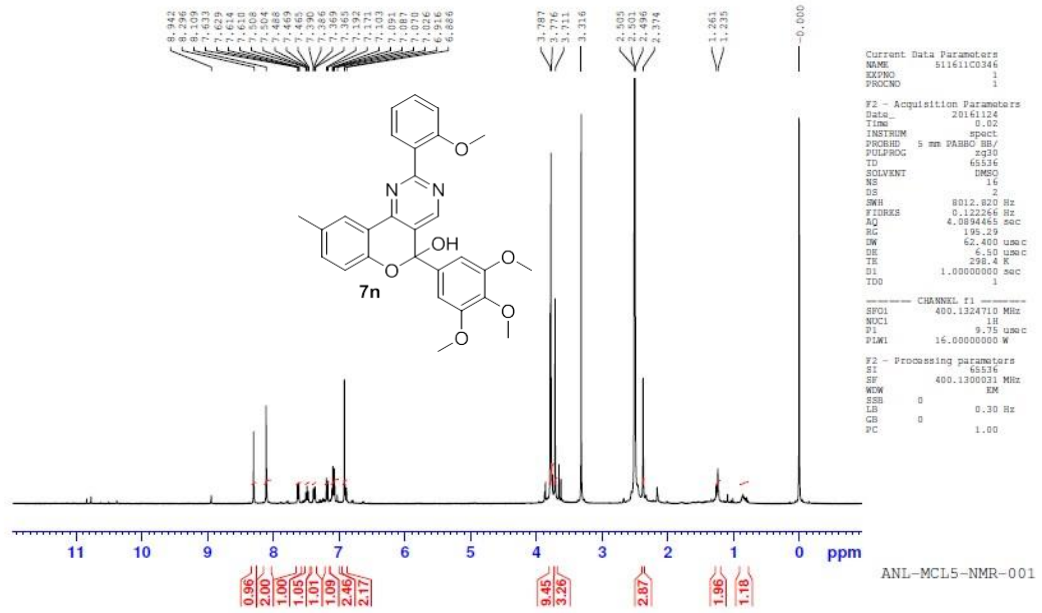
1: TOF MS ES+
8.23e3



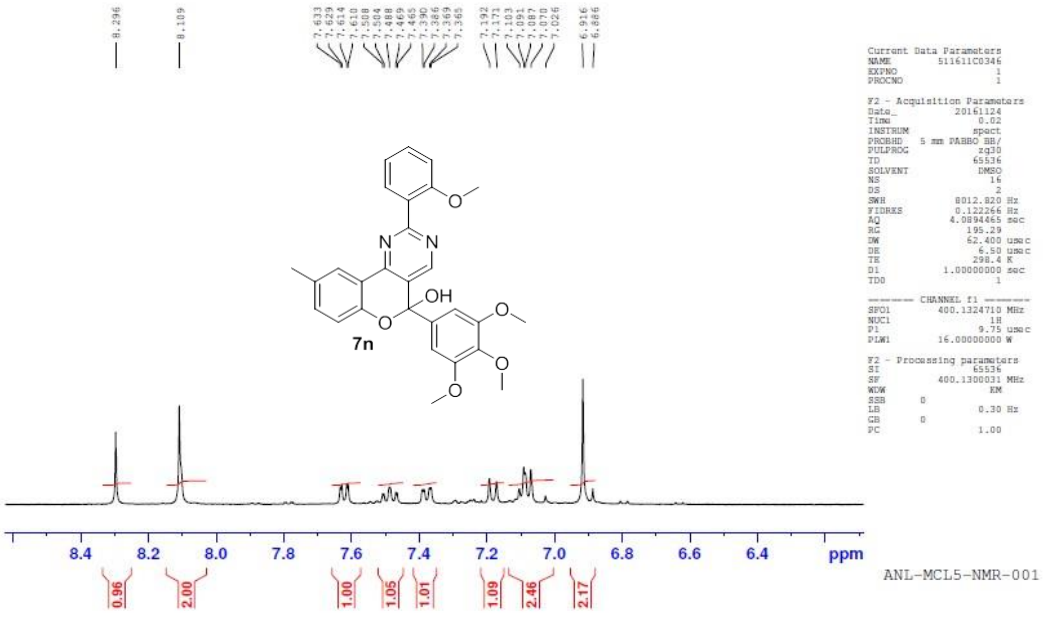


Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
525.1664	525.1637	2.7	5.1	16.5	1203.7	C28 H24 N2 O5 F3

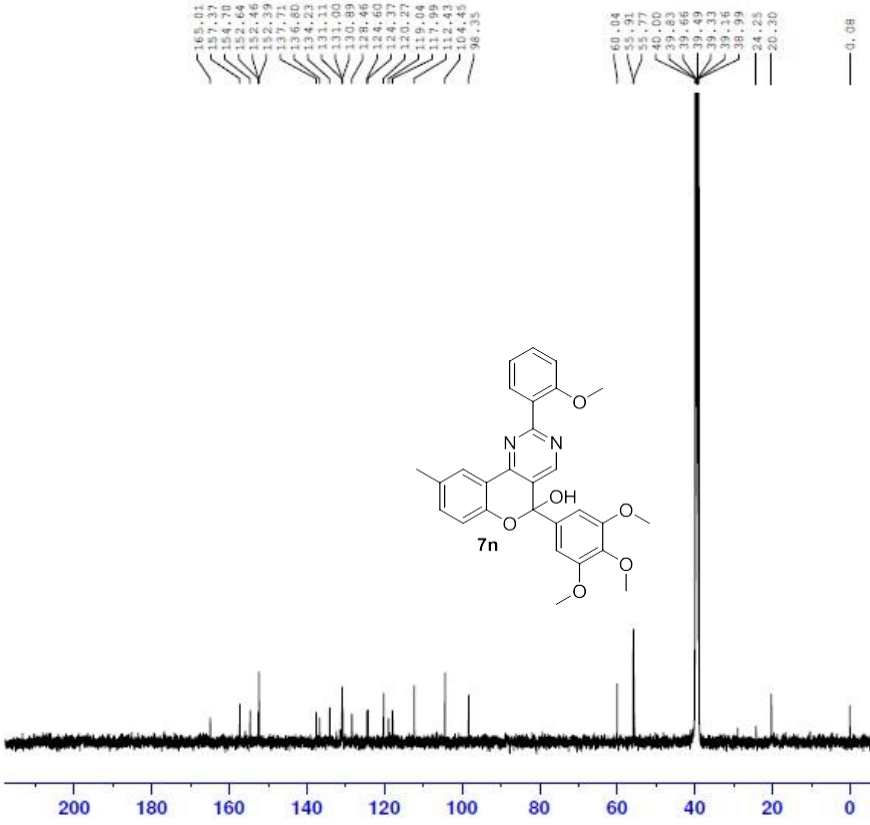
GVK-SAM-6-PAGE-38-P1



GVK-SAM-6-PAGE-38-P1



GVK-SAM-6-PAGE-38P-I

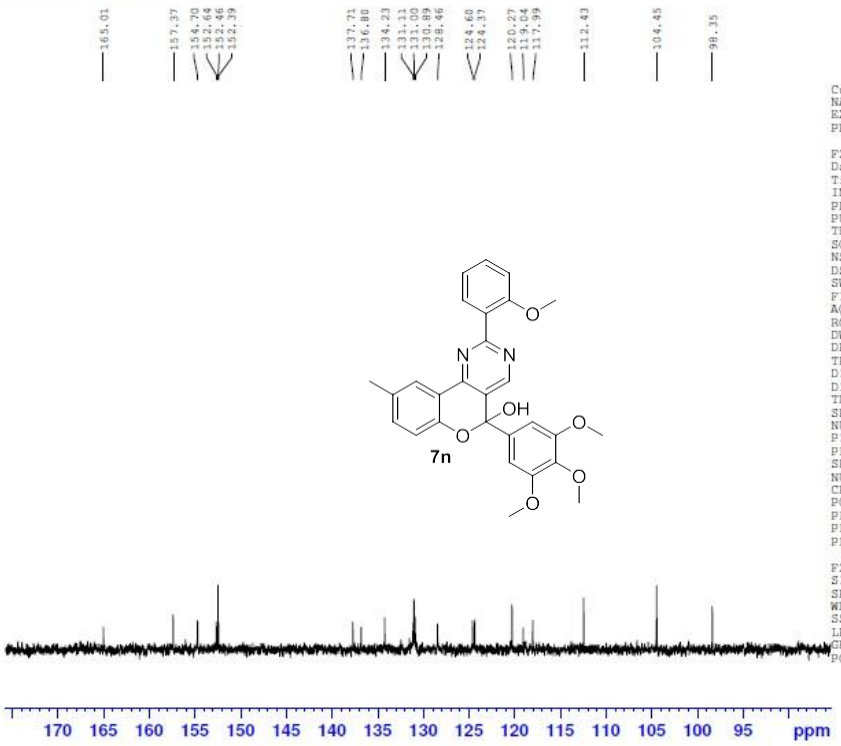



```
Current Data Parameters
NAME          511611B4302
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20161119
Time               20.15 h
INSTRUM             spect
PROBHD   Z119470_0231 (
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 1024
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                197.72
DW                16.800 usec
DE                 6.50 usec
TE                298.3 K
D1            3.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         125.7703643 MHz
NUC1                13C
P1                 9.50 usec
PLW1         88.00000000 W
SFO2         500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         23.00000000 W
PLW12         0.27515000 W
PLW13         0.13840000 W

F2 - Processing parameters
SI                 32768
SF          125.7578519 MHz
WDW                   EM
SSB       0
LB                 2.00 Hz
GB        0
PC                 1.40
```

GVK-SAM-6-PAGE-38P-I

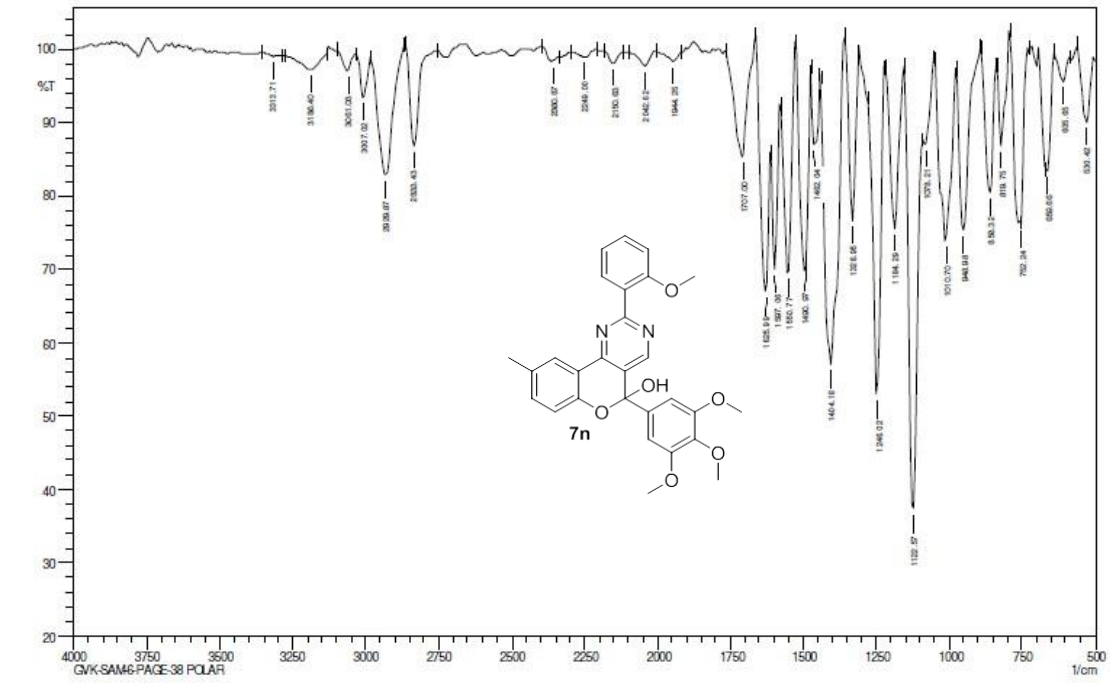



```
Current Data Parameters
NAME          511611B4302
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20161119
Time               20.15 h
INSTRUM             spect
PROBHD   Z119470_0231 (
PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 1024
DS                    4
SWH           29761.904 Hz
FIDRES         0.908261 Hz
AQ             1.1010048 sec
RG                197.72
DW                16.800 usec
DE                 6.50 usec
TE                298.3 K
D1            3.00000000 sec
D11           0.03000000 sec
TD0                    1
SFO1         125.7703643 MHz
NUC1                13C
P1                 9.50 usec
PLW1         88.00000000 W
SFO2         500.1320005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2         23.00000000 W
PLW12         0.27515000 W
PLW13         0.13840000 W

F2 - Processing parameters
SI                 32768
SF          125.7578519 MHz
WDW                   EM
SSB       0
LB                 2.00 Hz
GB        0
PC                 1.40
```

SHIMADZU



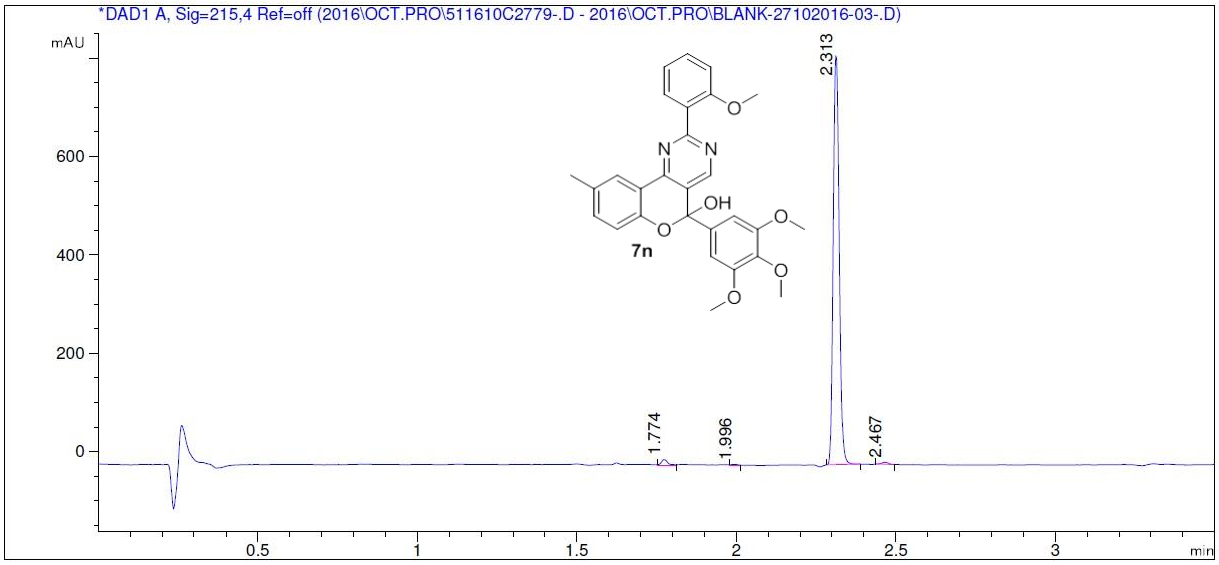
Comment: IN Kbr
G:\VK-SAM-6-PAGE-38 POLAR

No. of Scans;
Resolution;

Date:11/15/2016 12:09:15 PM
User; Admin

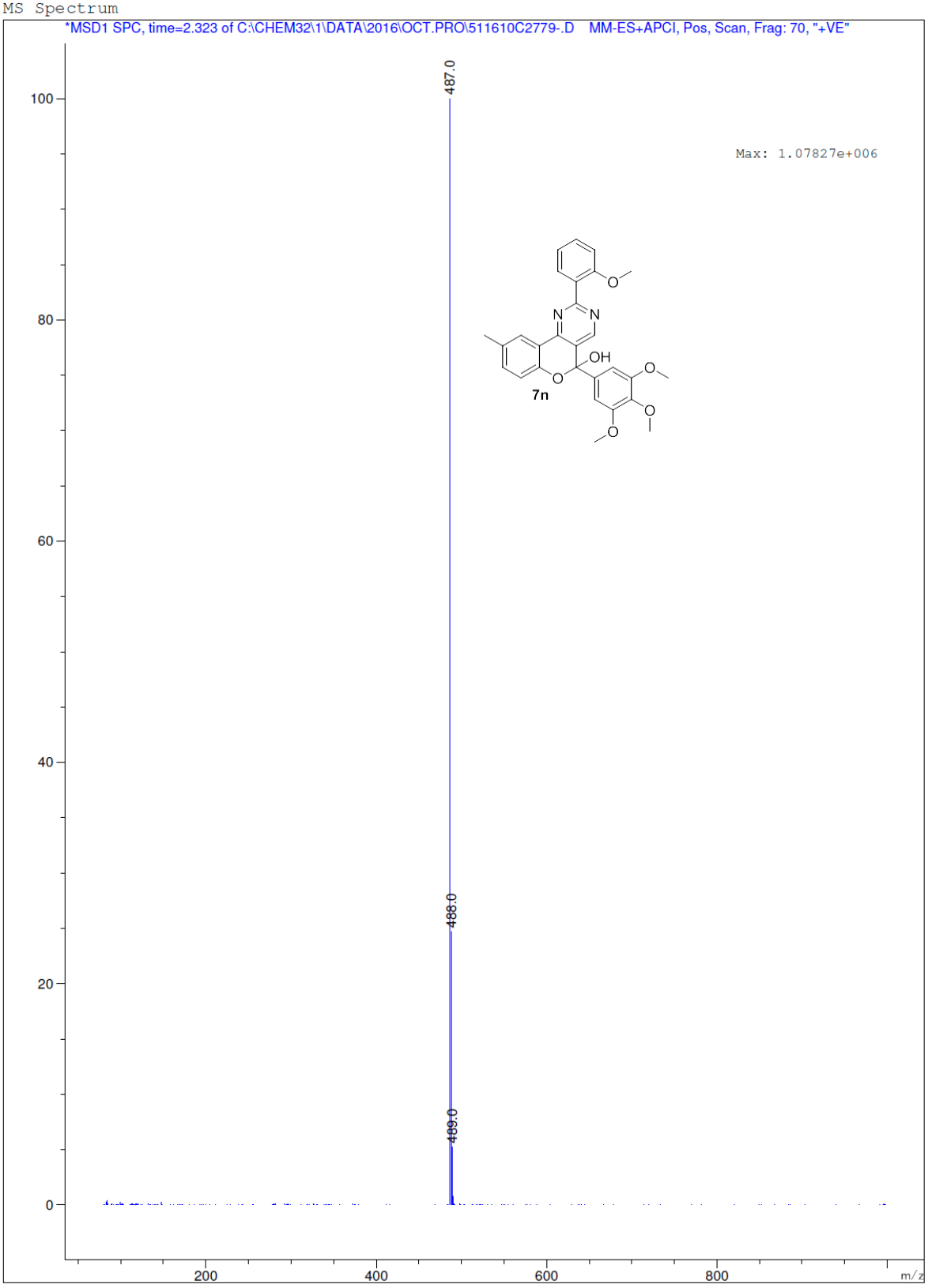
GVK BIOSCIENCES PVT. LTD.
MEDICINAL CHEMISTRY LABORATORY - ANALYTICAL RESEARCH
LCMS REPORT

```
================================================================================================
Sample Name      : GVK-SAM-6-PAGE-38POLAR                    Vial position  : P1-C-09
Date of Analysis :10/27/2016        1:42:41 PM              Injection Vol  :     0.100uL
Acq. Method      :C:\CHEM32\1\METHODS\RND-FA- 3.5 MIN.M     Instrument ID  :ANL-MCL5-LCMS-001
================================================================================================
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, 0.4/2, 2.6/98,3.1/98,3.11/2,3.5/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 60°C
                                                                                          ->
================================================================================================
```



Pea No	RT min	Area	Area %
1	1.77	14.051	1.277
2	2.00	1.395	0.127
3	2.31	1079.401	98.103
4	2.47	5.430	0.494

MS Spectrum

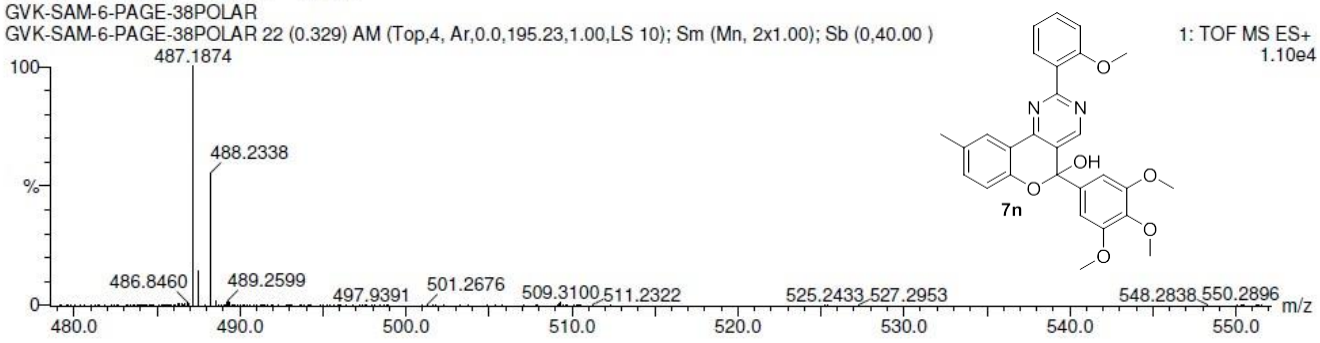

*MSD1 SPC, time=2.323 of C:\CHEM32\1\DATA\2016\OCT.PRO\511610C2779-.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 1.07827e+006
487.0
488.0
489.0
100
80
60
40
20
0
200
400
600
800
m/z
N
N
OH
O
O
O
O
O
7n

Single Mass Analysis

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

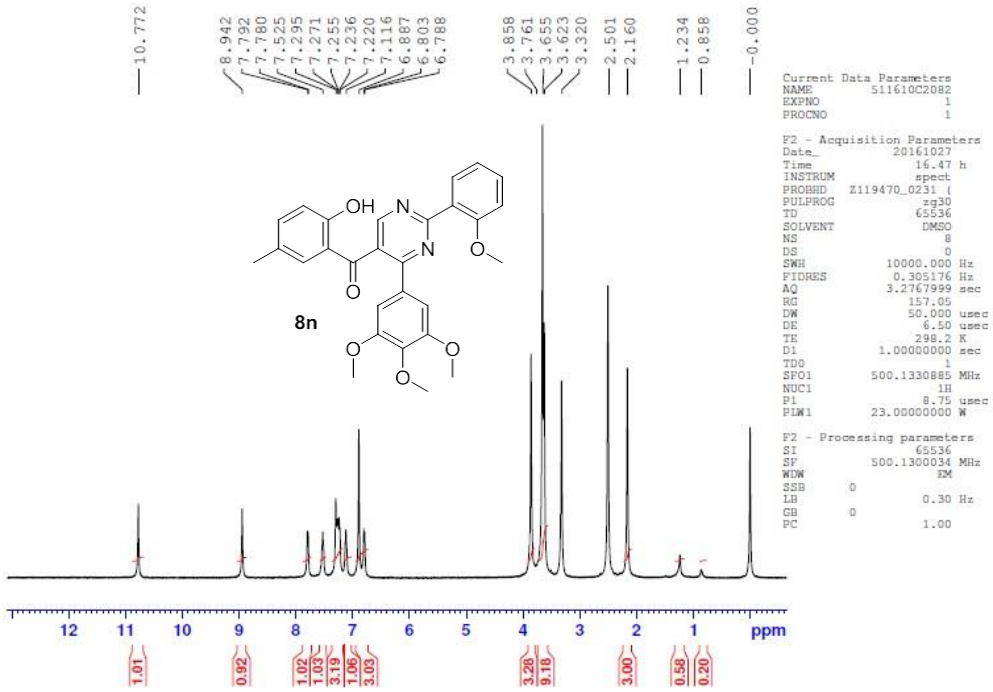
Monoisotopic Mass, Even Electron Ions
16 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-28 H: 0-27 N: 0-2 O: 0-6

GVK-SAM-6-PAGE-38POLAR
GVK-SAM-6-PAGE-38POLAR 22 (0.329) AM (Top,4, Ar,0.0,195.23,1.00,LS 10); Sm (Mn, 2x1.00); Sb (0,40.00)



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
487.1874	487.1869	0.5	1.0	16.5	1381.7	C28 H27 N2 O6

GVK-SAM-6-PAGE-38POLAR

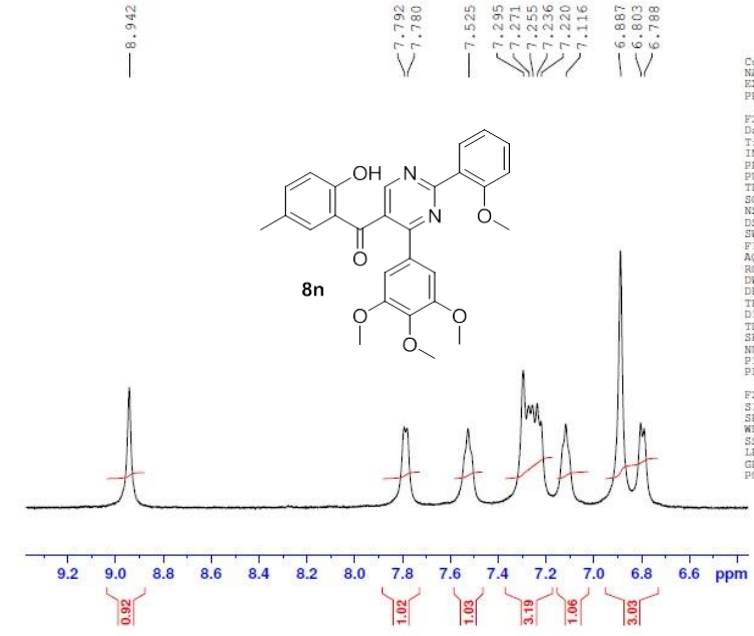


Current Data Parameters
NAME 511610C2082
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161027
Time 16.47 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 157.05
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.1330885 MHz
NUC1 1H
P1 8.75 usec
PLW1 23.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1300034 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

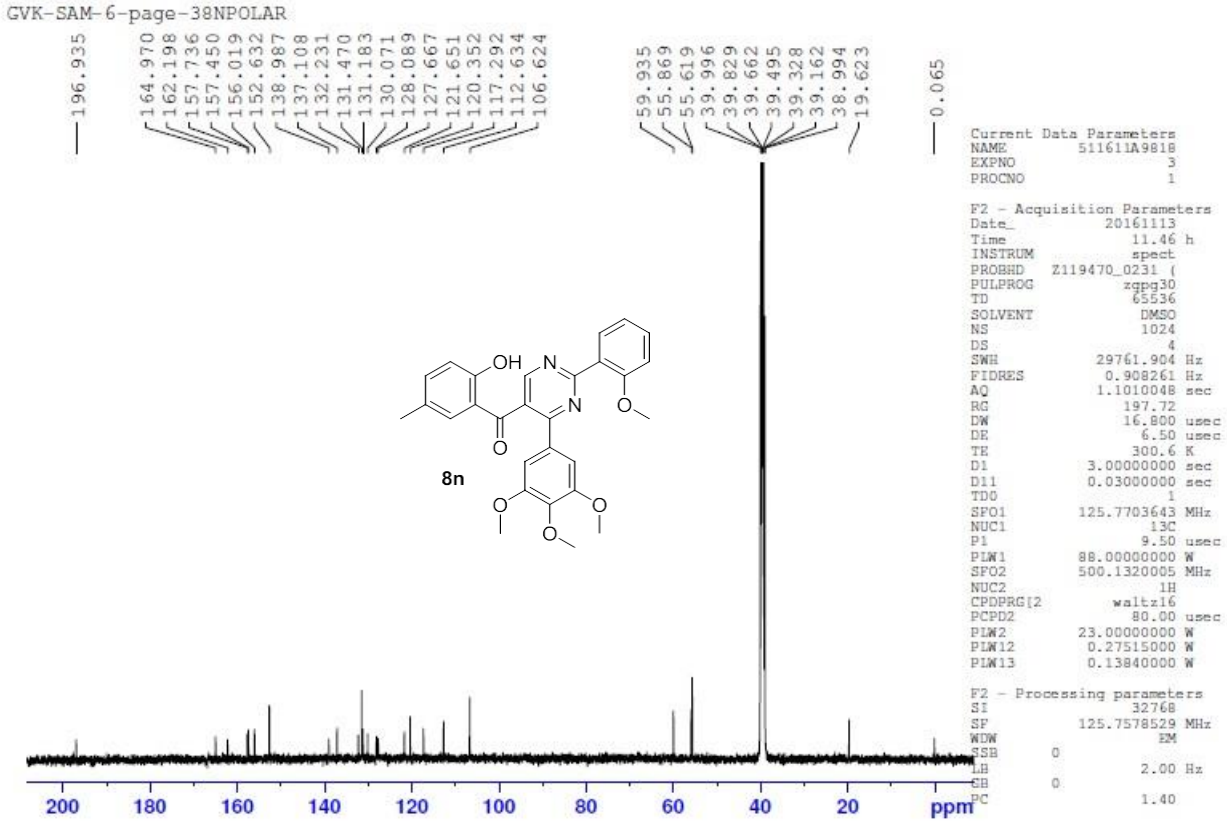
GVK-SAM-6-PAGE-38POLAR



Current Data Parameters
NAME 511610C2082
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161027
Time 16.47 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 157.05
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.1330885 MHz
NUC1 1H
P1 8.75 usec
PLW1 23.00000000 W

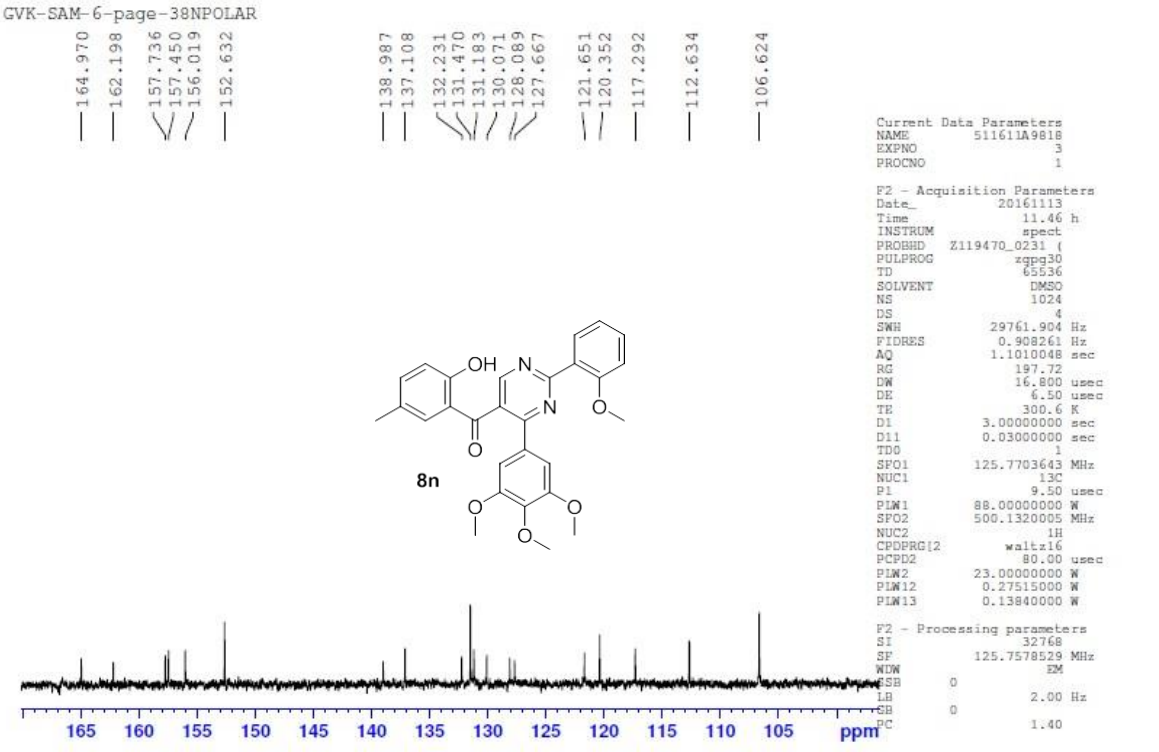
F2 - Processing parameters
SI 65536
SF 500.1300034 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00




```
Current Data Parameters
NAME          511611A9818
EXPNO                   3
PROCNO                  1

F2 - Acquisition Parameters
Date_           20161113
Time               11.46 h
INSTRUM             spect
PROBHD   Z119470_0231 (
PULPROG           zgpg30
TD                 65536
SOLVENT              DMSO
NS                   1024
DS                      4
SWH            29761.904 Hz
FIDRES          0.908261 Hz
AQ             1.1010048 sec
RG                 197.72
DW                 16.800 usec
DE                  6.50 usec
TE                 300.6 K
D1            3.00000000 sec
D11           0.03000000 sec
TD0                     1
SFO1         125.7703643 MHz
NUC1                  13C
P1                  9.50 usec
PLW1         88.00000000 W
SFO2         500.1320005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2         23.00000000 W
PLW12         0.27515000 W
PLW13         0.13840000 W

F2 - Processing parameters
SI                  32768
SF           125.7578529 MHz
WDW                    EM
SSB          0
LB                 2.00 Hz
GB           0
PC                 1.40
```

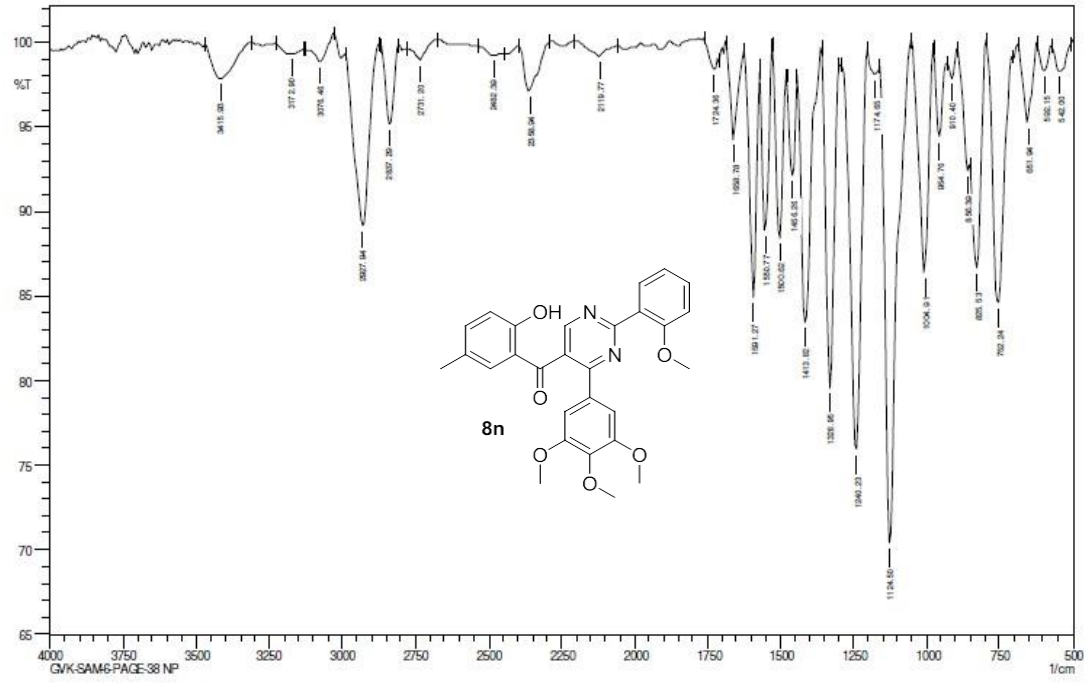



```
Current Data Parameters
NAME          511611A9818
EXPNO                   3
PROCNO                  1

F2 - Acquisition Parameters
Date_           20161113
Time               11.46 h
INSTRUM             spect
PROBHD   Z119470_0231 (
PULPROG           zgpg30
TD                 65536
SOLVENT              DMSO
NS                   1024
DS                      4
SWH            29761.904 Hz
FIDRES          0.908261 Hz
AQ             1.1010048 sec
RG                 197.72
DW                 16.800 usec
DE                  6.50 usec
TE                 300.6 K
D1            3.00000000 sec
D11           0.03000000 sec
TD0                     1
SFO1         125.7703643 MHz
NUC1                  13C
P1                  9.50 usec
PLW1         88.00000000 W
SFO2         500.1320005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2         23.00000000 W
PLW12         0.27515000 W
PLW13         0.13840000 W

F2 - Processing parameters
SI                  32768
SF           125.7578529 MHz
WDW                    EM
SSB          0
LB                 2.00 Hz
GB           0
PC                 1.40
```

SHIMADZU



8n

Comment: IN Kbr
G\K-SAM-6-PAGE-38 NP

No. of Scans;
Resolution;
Apodization;

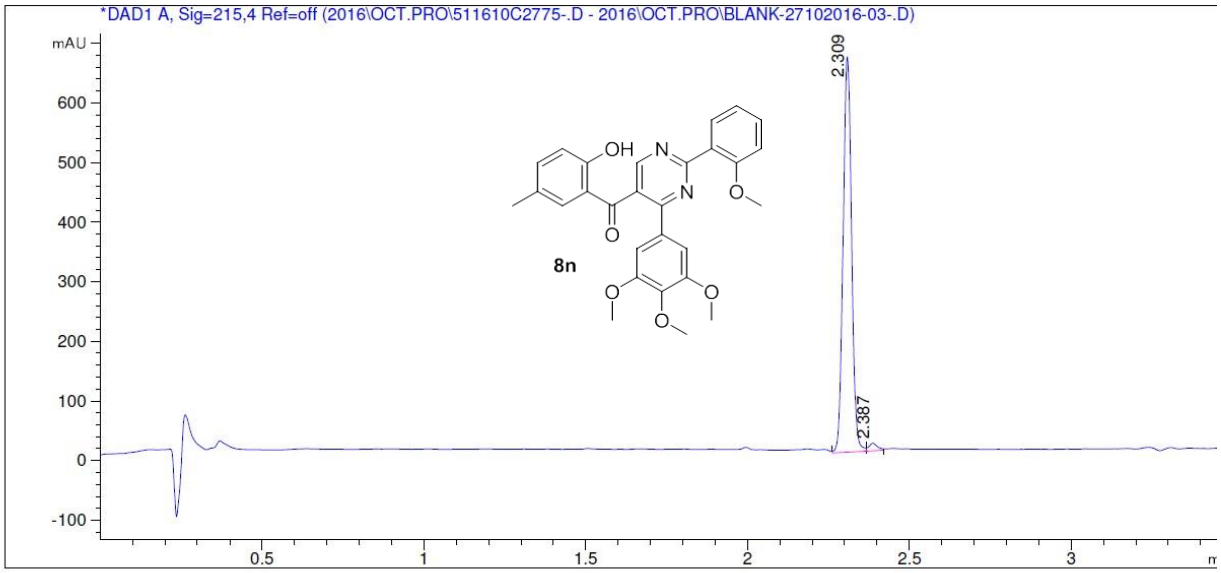
Date:11/15/2016 12:02:08 PM
User; Admin

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

Sample Name : GVK-SAM-6-PAGE-38NP Vial position : P1-C-07
Date of Analysis :10/27/2016 1:33:54 PM Injection Vol : 0.100uL
Acq. Method :C:\CHEM32\1\METHODS\RND-FA- 3.5 MIN.M Instrument ID :ANL-MCL5-LCMS-001

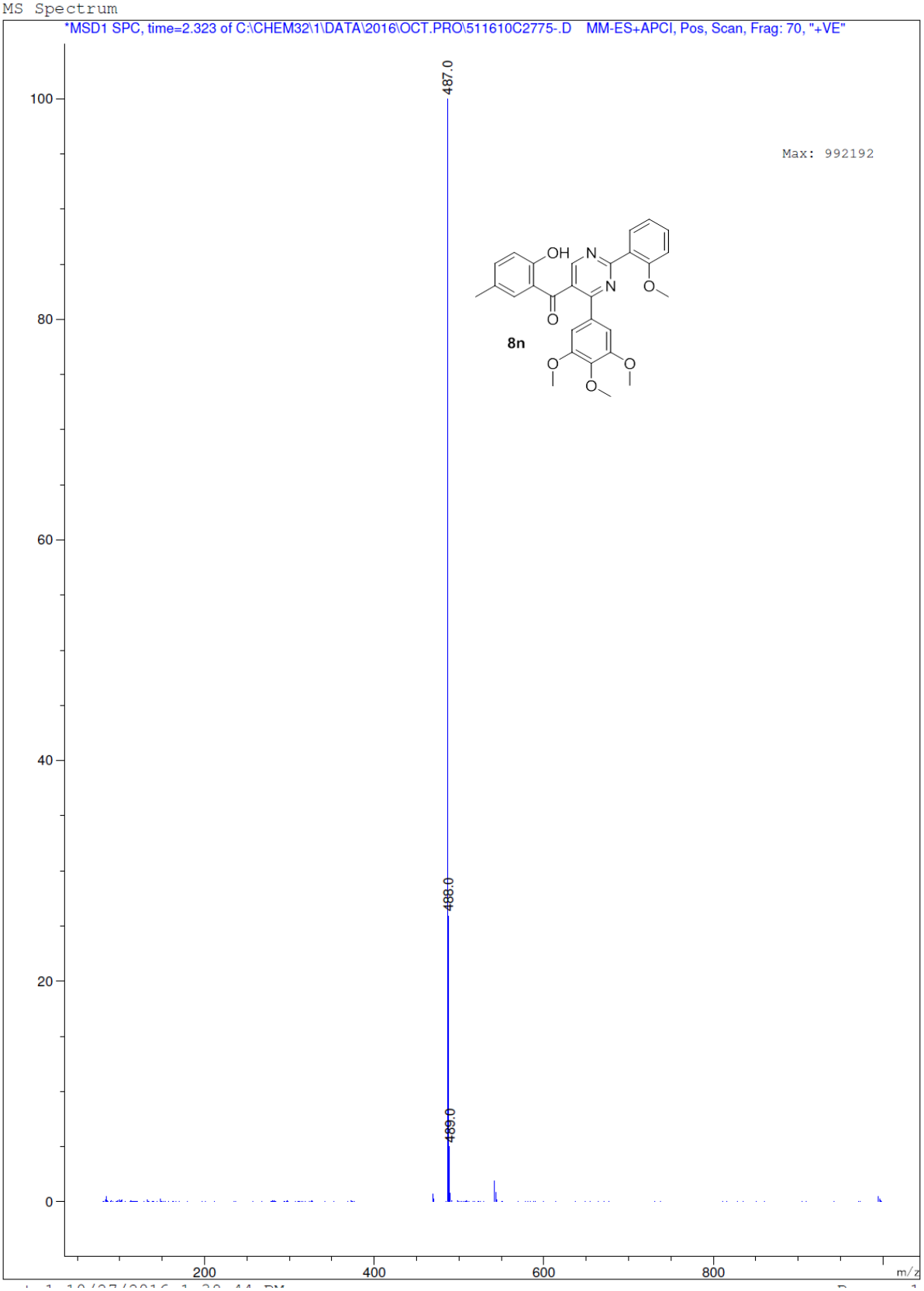
RND-FA-3.5 MIN.M
Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: B1: 0.1 % FA IN WATER A1: 0.1%FA IN ACN
Gradient: Time (min) /%A1: 0/2, 0.4/2, 2.6/98,3.1/98,3.11/2,3.5/2
Column Flow Rate: 0.8 ml/min
Column Temperature: 60°C

->



Pea No	RT min	Area	Area %
1	2.31	1208.406	98.092
2	2.39	23.501	1.908

MS Spectrum

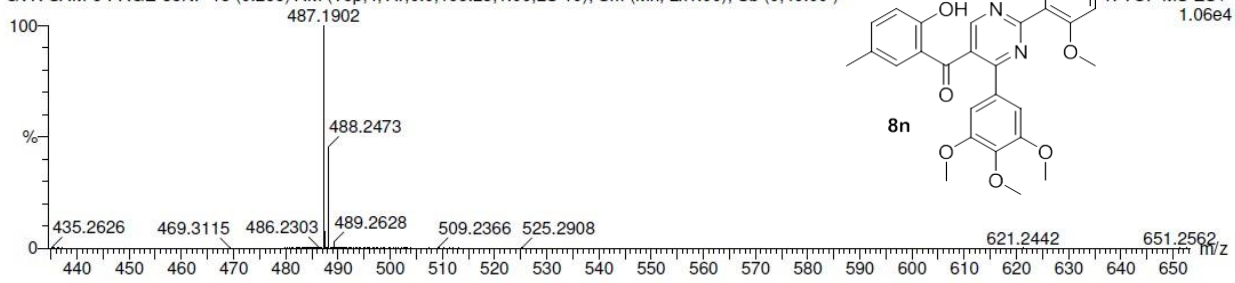

*MSD1 SPC, time=2.323 of C:\CHEM32\1\DATA\2016\OCT.PRO\511610C2775-.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 992192
487.0
488.0
489.0
8n
100
80
60
40
20
0
200
400
600
800
m/z

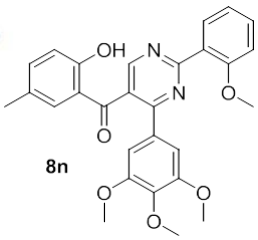
Single Mass Analysis

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

Monoisotopic Mass, Even Electron Ions
16 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-28 H: 0-27 N: 0-2 O: 0-6

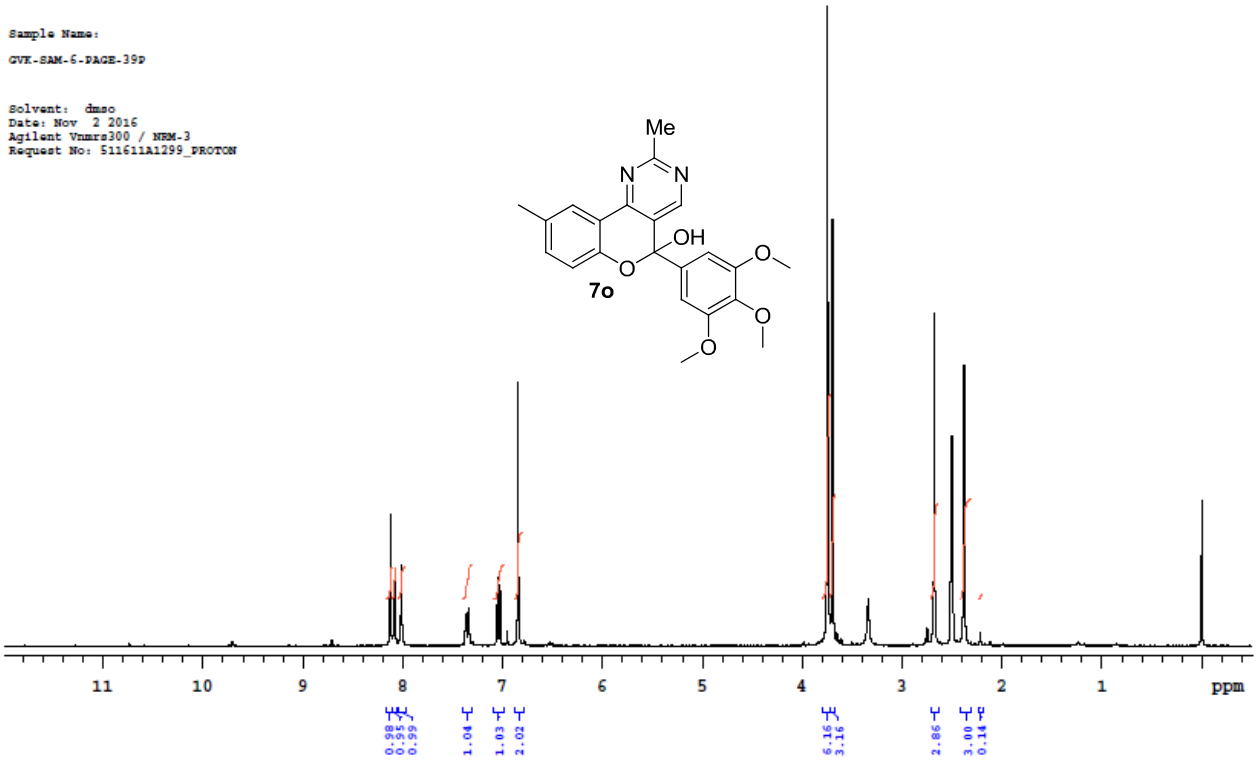
GVK-SAM-6-PAGE-38NP
GVK-SAM-6-PAGE-38NP 18 (0.256) AM (Top,4, Ar,0.0,195.23,1.00,LS 10); Sm (Mn, 2x1.00); Sb (0,40.00)

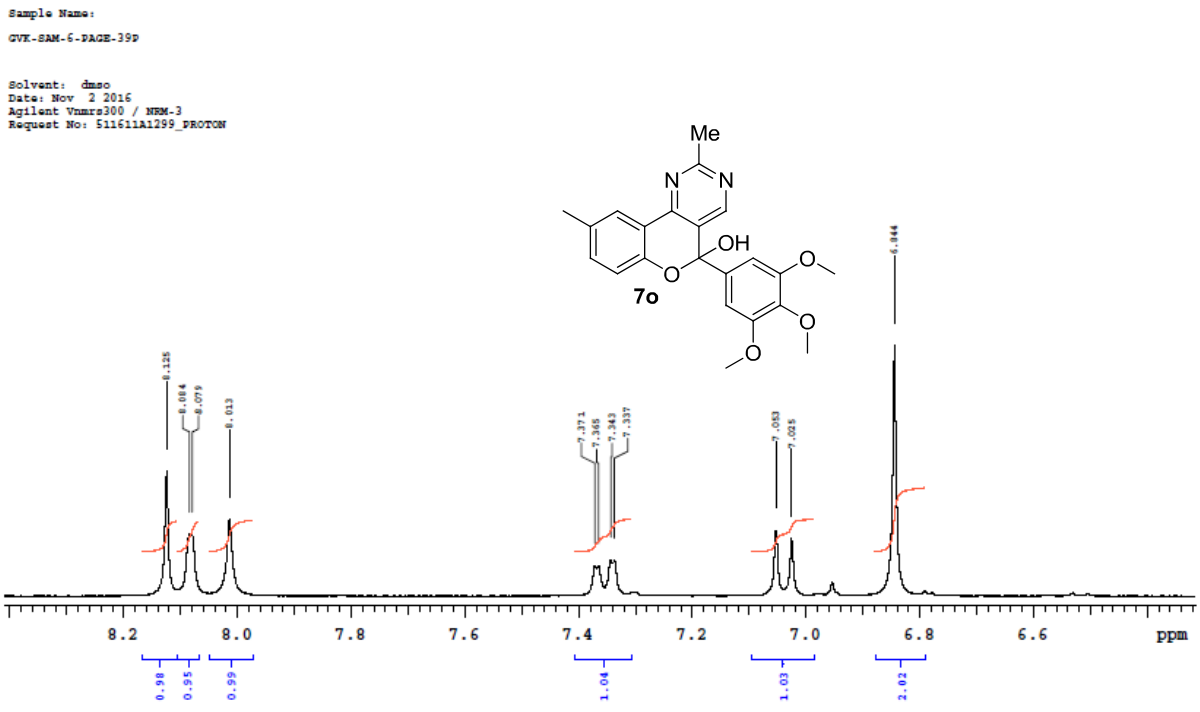




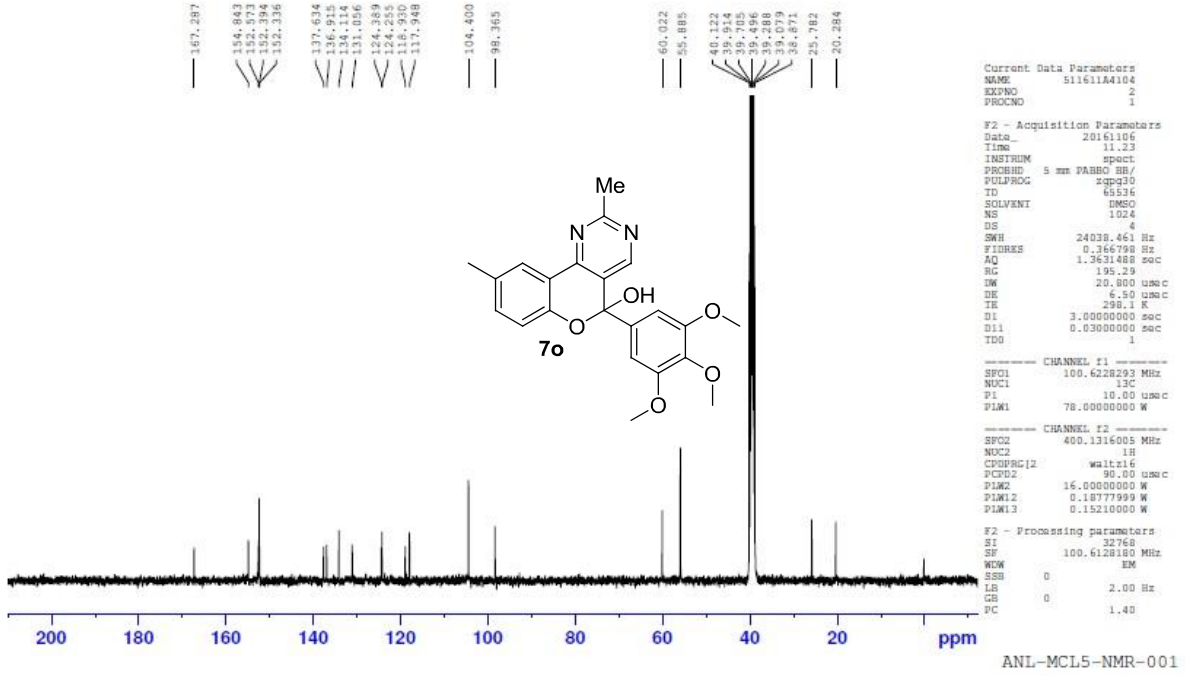
8n

Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
487.1902	487.1869	3.3	6.8	16.5	637.8	C28 H27 N2 O6


Sample Name:
GVK-SAM-6-PAGE-39P
Solvent: dmso
Date: Nov 2 2016
Agilent Vnmrs300 / NRM-3
Request No: 511611A1299_PROTON
Me
N
N
OH
O
O
O
O
7o
11
10
9
8
7
6
5
4
3
2
1
ppm
0.98
0.95
0.99
1.04
1.03
2.02
6.16
3.16
2.86
3.00
0.14


Sample Name:
GVK-SAM-6-PAGE-39P
Solvent: dmso
Date: Nov 2 2016
Agilent Vnmrs300 / NRM-3
Request No: 511611A1299_PROTON
Me
N
N
OH
O
O
O
O
7o
8.125
8.084
8.079
8.013
7.371
7.368
7.343
7.337
7.053
7.028
6.844
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
ppm
0.98
0.95
0.99
1.04
1.03
2.02

GVK-SAM-6-page-39 polar




```
Current Data Parameters
NAME          511611A4104
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Data_           20161106
Time              11.23
INSTRUM           spect
PROBHD  5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT           DMSO
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              298.1 K
D1          3.00000000 sec
D11         0.03000000 sec
TD0                  1

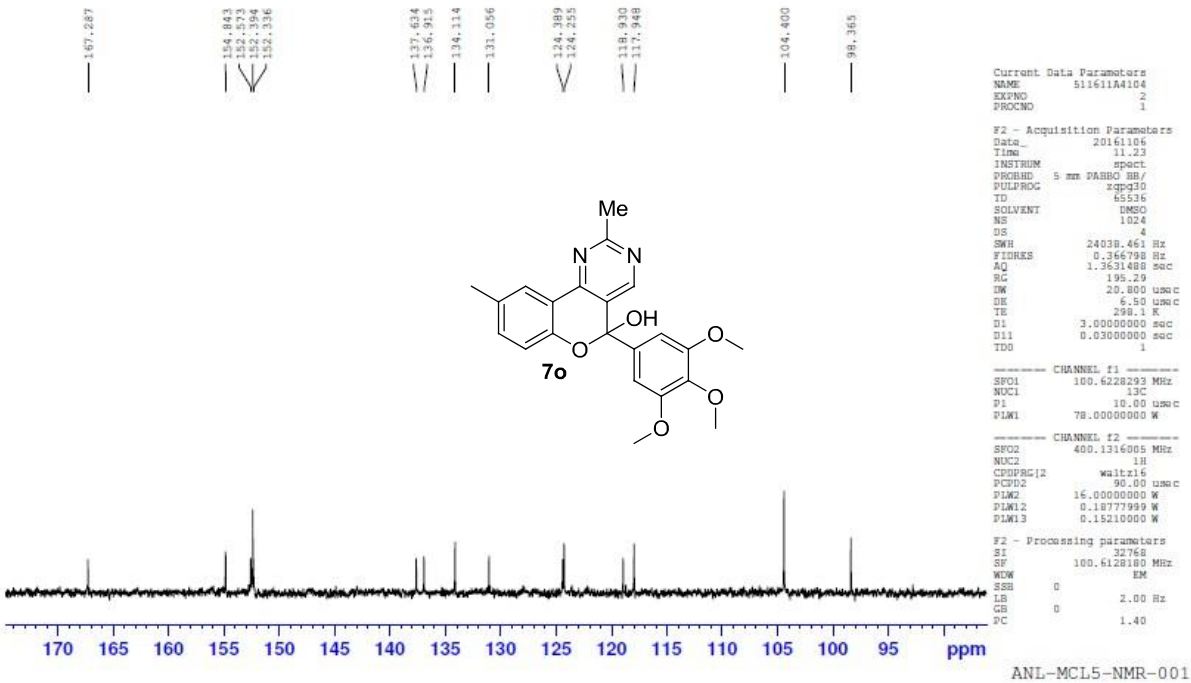
======== CHANNEL f1 ========
SFO1        100.6228293 MHz
NUC1               13C
P1               10.00 usec
PLW1        78.00000000 W

======== 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          100.6128180 MHz
WDW                EM
SSB       0
LB              2.00 Hz
GB        0
PC              1.40
```

ANL-MCL5-NMR-001

GVK-SAM-6-page-39 polar




```
Current Data Parameters
NAME          511611A4104
EXPNO                   2
PROCNO                  1

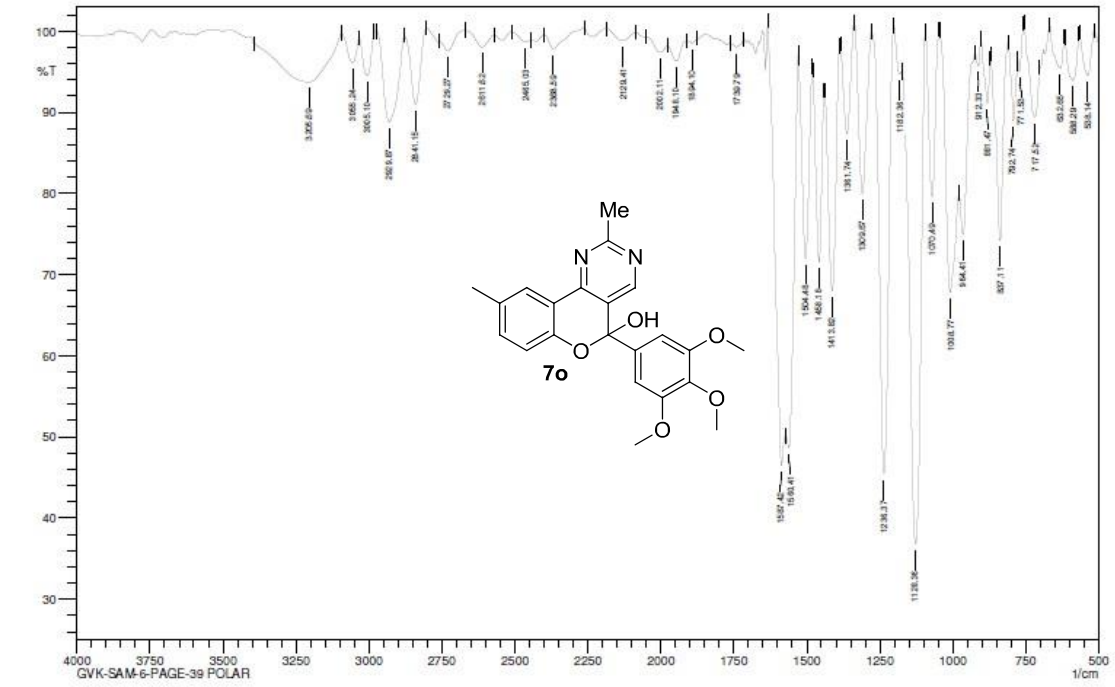
F2 - Acquisition Parameters
Data_           20161106
Time              11.23
INSTRUM           spect
PROBHD  5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT           DMSO
NS                1024
DS                   4
SWH          24038.461 Hz
FIDRES        0.366798 Hz
AQ            1.3631488 sec
RG              195.29
DW             20.800 usec
DE              6.50 usec
TE              298.1 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          100.6128180 MHz
WDW                EM
SSB       0
LB              2.00 Hz
GB        0
PC              1.40
```

ANL-MCL5-NMR-001



Comment: IN Kbr
GVK-SAM-6-PAGE-39 POLAR

No. of Scans:
Resolution:
Apodization:

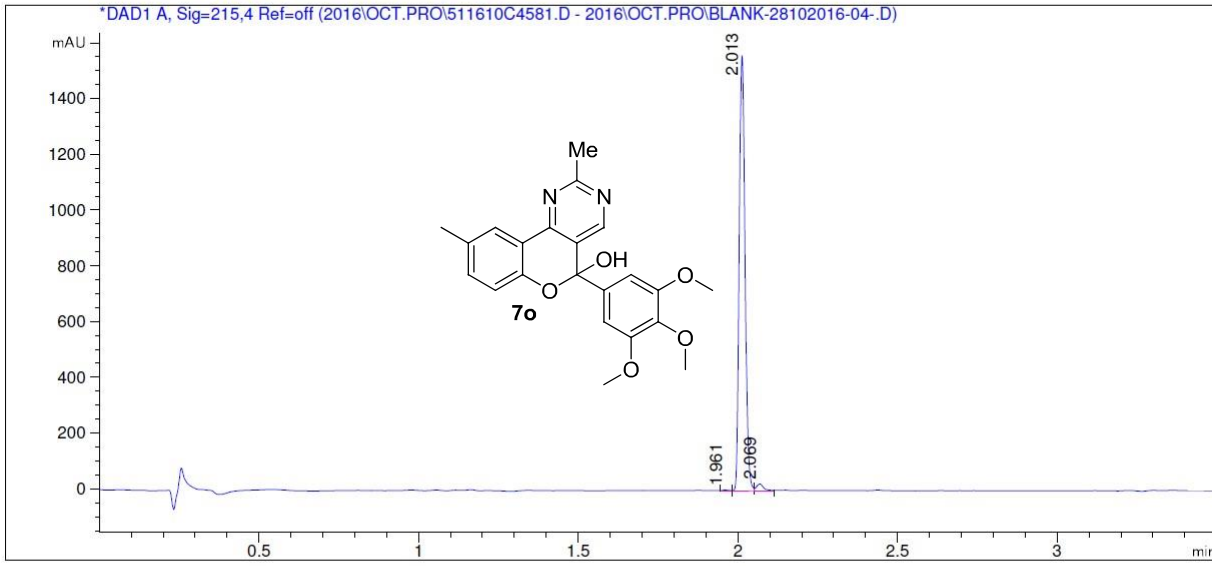
Date: 11/15/2016 10:56:26 AM
User: Admin

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

Sample Name :GVK-SAM-6-PAGE-39-POLAR Vial position : P1-A-08
Date of Analysis :10/28/2016 6:55:06 PM Injection Vol : 0.300uL
Acq. Method :C:\CHEM32\1\METHODS\RND-FA- 3.5 MIN.M Instrument ID :ANL-MCL5-LCMS-001

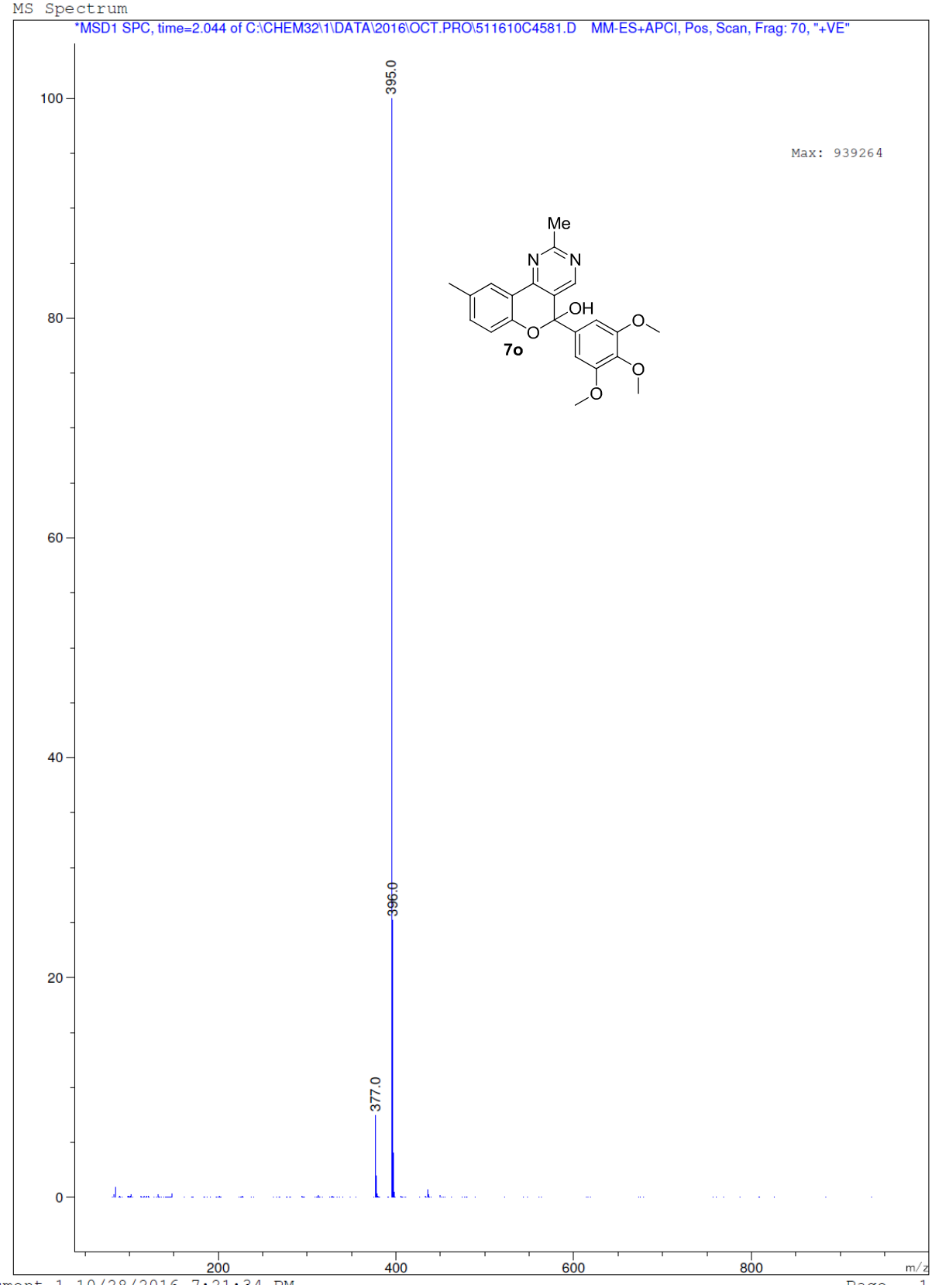
RND-FA-3.5 MIN.M
Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: B1: 0.1 % FA IN WATER A1: 0.1%FA IN ACN
Gradient: Time (min) /%A1: 0/2, 0.4/2, 2.8/98,3.4/98,3.41/2,3.5/2
Column Flow Rate: 0.6 ml/min
Column Temperature: 60°C

->



Peak No	RT min	Area	Area %
1	1.96	5.811	0.287
2	2.01	1978.339	97.813
3	2.07	38.432	1.900

MS Spectrum


*MSD1 SPC, time=2.044 of C:\CHEM32\1\DATA\2016\OCT.PRO\511610C4581.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 939264
395.0
396.0
377.0
100
80
60
40
20
0
200
400
600
800
m/z
Me
N
N
OH
O
O
O
O
7o

Elemental Composition Report

Single Mass Analysis

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

Selected filters: None

Monoisotopic Mass, Even Electron Ions

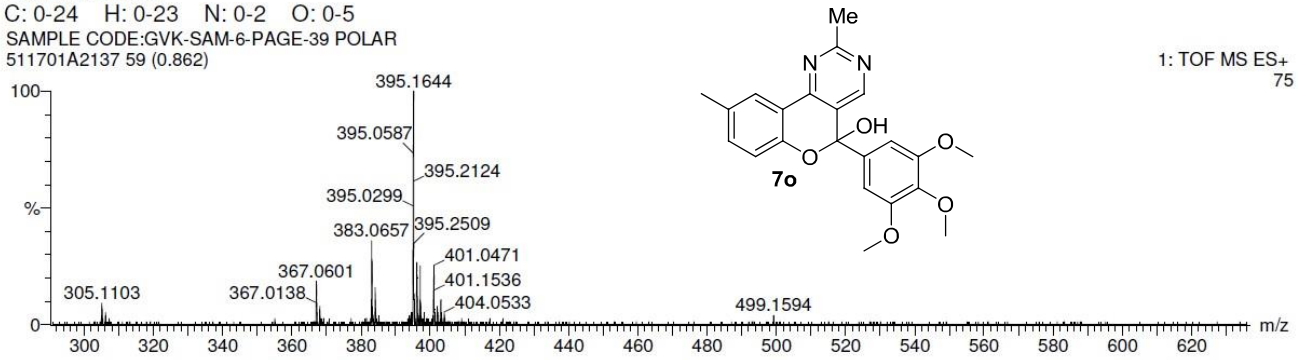
12 formula(e) evaluated with 3 results within limits (up to 1 closest results for each mass)

Elements Used:

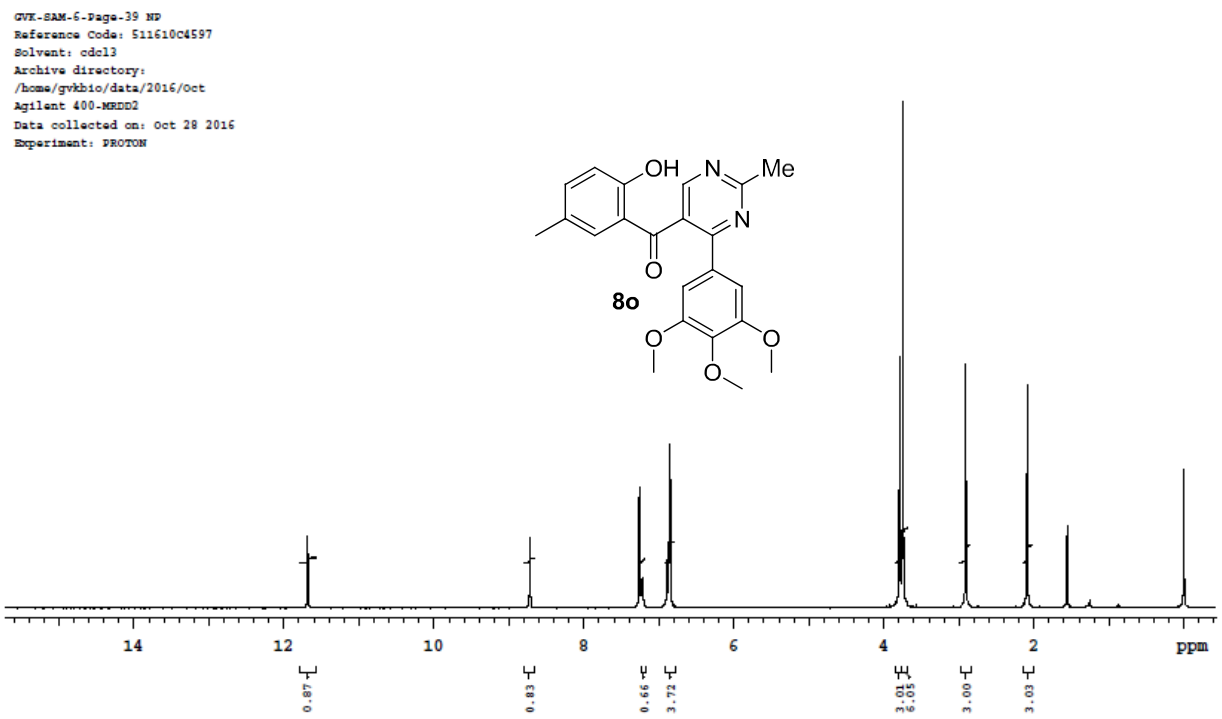
C: 0-24 H: 0-23 N: 0-2 O: 0-5

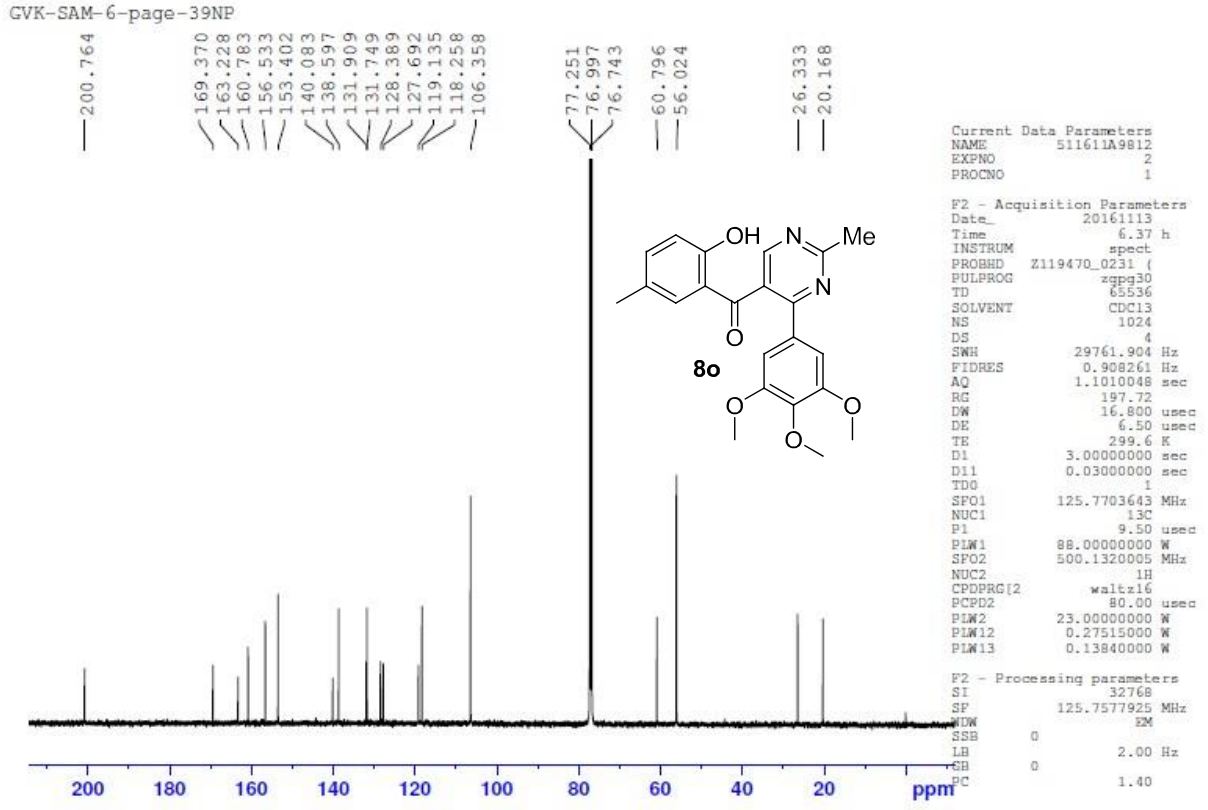
SAMPLE CODE:GVK-SAM-6-PAGE-39 POLAR

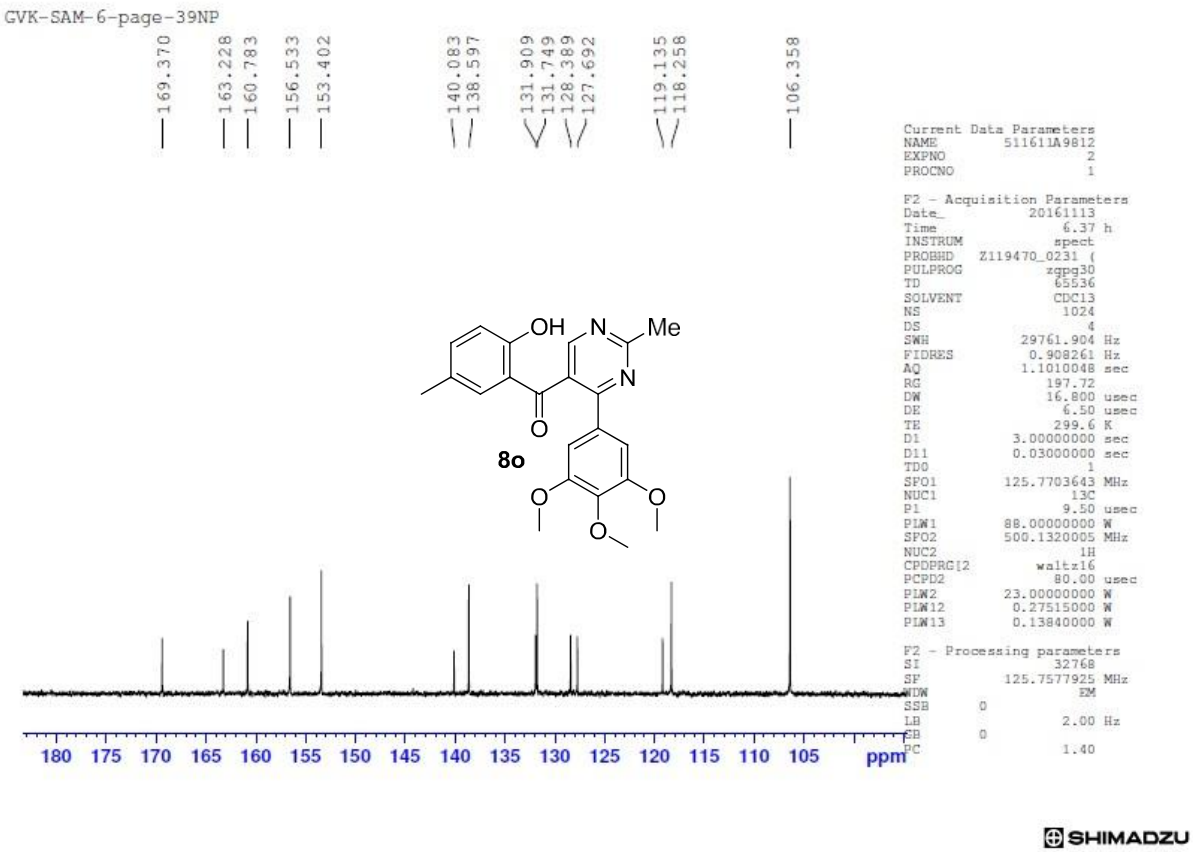
511701A2137 59 (0.862)



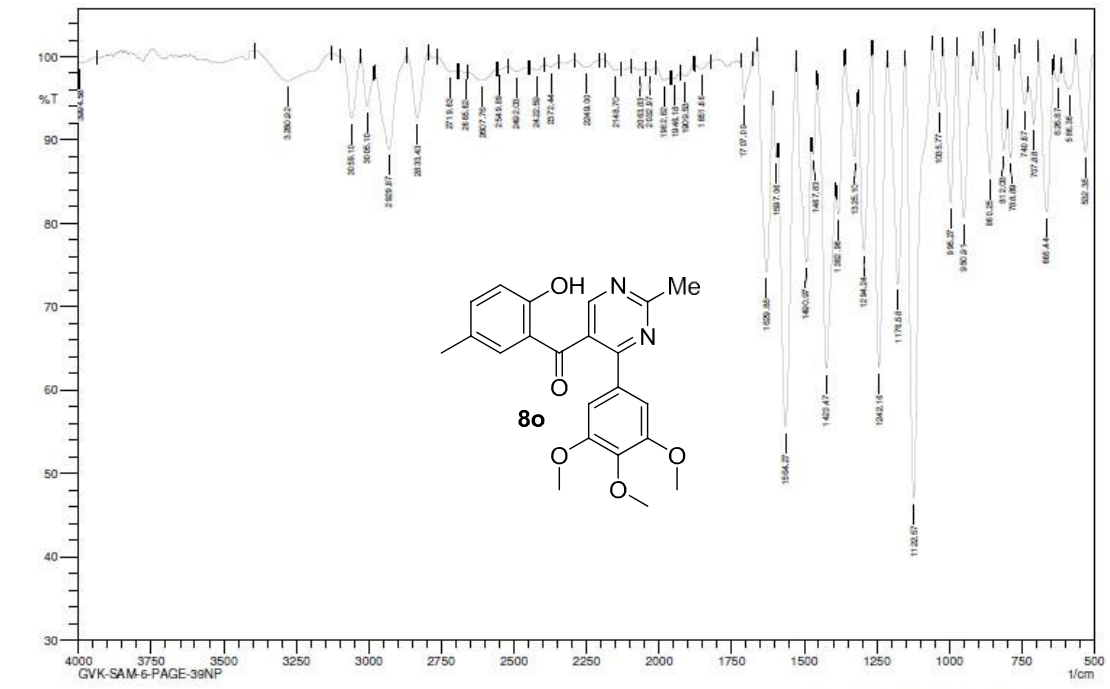
Minimum:				-1.5	
Maximum:		5.0	1000.0	50.0	
Mass	Calc. Mass	mDa	PPM	DBE	Formula
395.1644	395.1607	3.7	9.4	12.5	C22 H23 N2 O5


GVK-SAM-6-Page-39 NP
Reference Code: 511610C4597
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2016/Oct
Agilent 400-MRDD2
Data collected on: Oct 28 2016
Experiment: PROTON
OH
N
Me
N
O
8o
O
O
O
14
12
10
8
6
4
2
ppm
0.87
0.83
0.66
3.72
3.01
6.05
3.00
3.03


GVK-SAM-6-page-39NP
200.764
169.370
163.228
160.783
156.533
153.402
140.083
138.597
131.909
131.749
128.389
127.692
119.135
118.258
106.358
77.251
76.997
76.743
60.796
56.024
26.333
20.168
OH
N
Me
N
O
8o
O
O
O
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME 511611A9812
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161113
Time 6.37 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 299.6 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7577925 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40



SHIMADZU



Comment: IN Kbr
GVK-SAM-6-PAGE-39NP

No. of Scans:
Resolution:
Apodization:

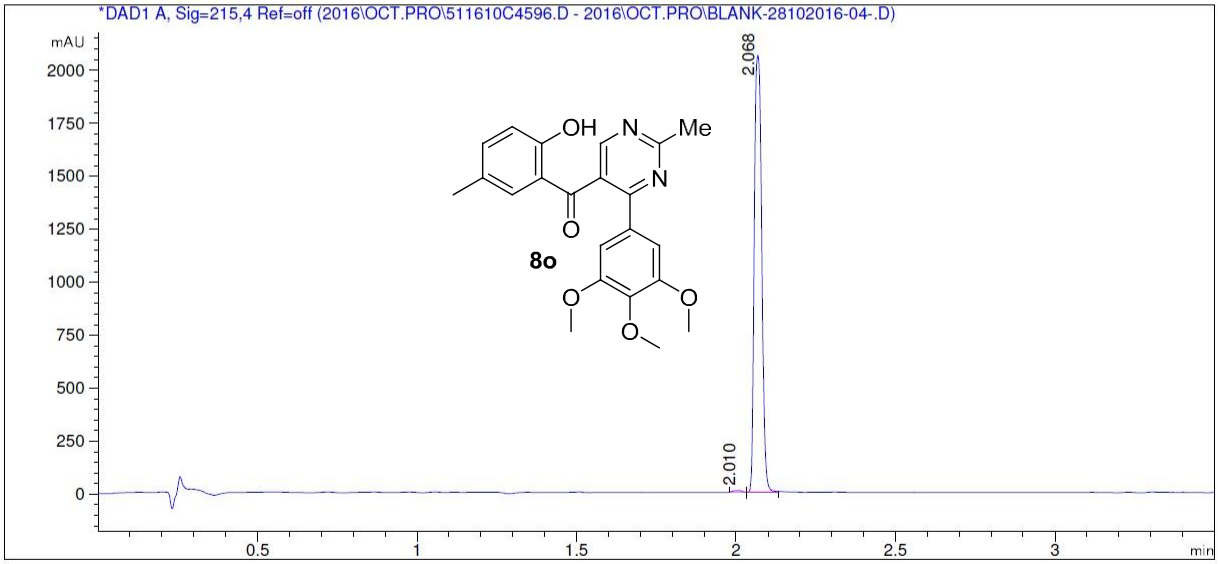
Date: 11/15/2016 11:15:55 AM
User: Admin

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

Sample Name :GVK-SAM-6-PAGE-39NP Vial position : P1-A-09
Date of Analysis :10/28/2016 7:08:34 PM Injection Vol : 0.300uL
Acq. Method :C:\CHEM32\1\METHODS\RND-FA- 3.5 MIN.M Instrument ID :ANL-MCL5-LCMS-001

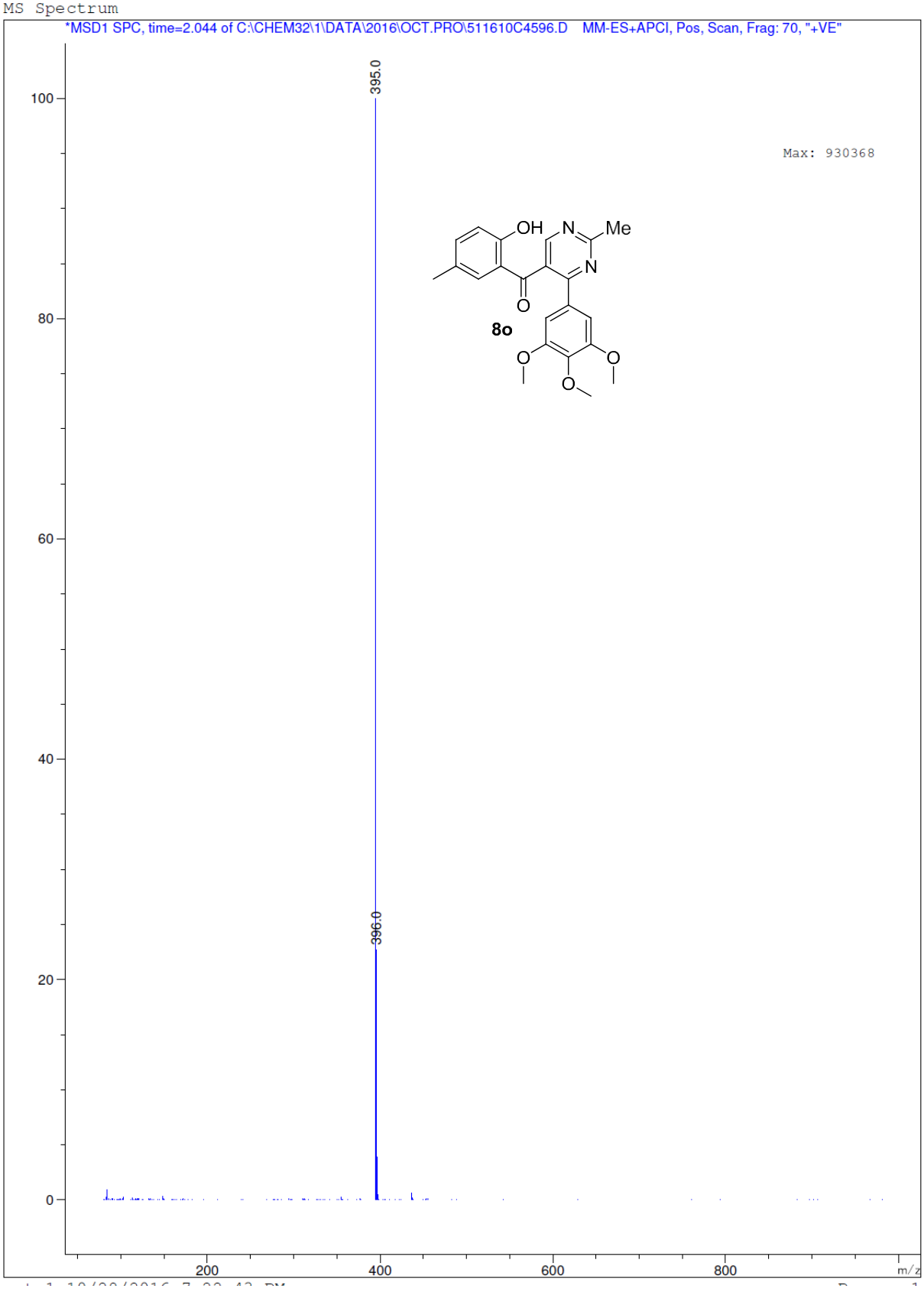
RND-FA-3.5 MIN.M
Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: B1: 0.1 % FA IN WATER A1: 0.1%FA IN ACN
Gradient: Time (min) /%A1: 0/2, 0.4/2, 2.8/98,3.4/98,3.41/2,3.5/2
Column Flow Rate: 0.6 ml/min
Column Temperature: 60°C

->



Pea No	RT min	Area	Area %
1	2.01	11.331	0.339
2	2.07	3333.982	99.661

MS Spectrum

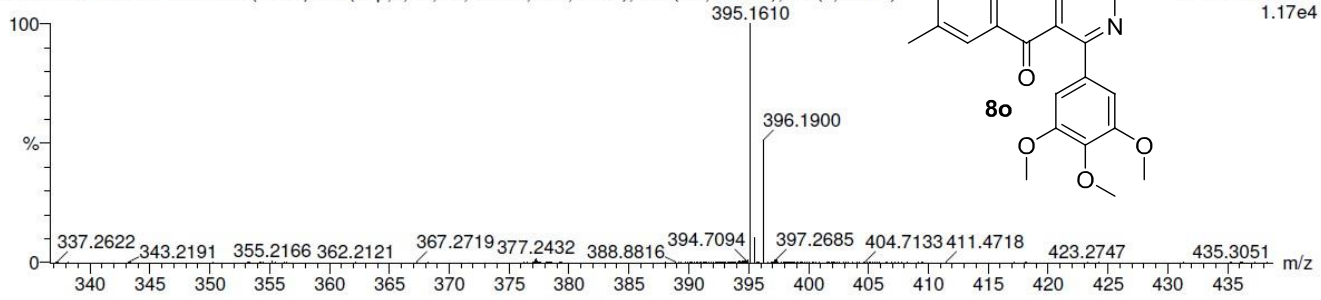

*MSD1 SPC, time=2.044 of C:\CHEM32\1\DATA\2016\OCT.PRO\511610C4596.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 930368
395.0
396.0
OH
N
Me
N
O
8o
O
O
O
100
80
60
40
20
0
200
400
600
800
m/z

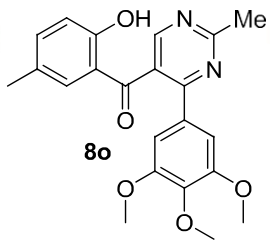
Single Mass Analysis

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

Monoisotopic Mass, Even Electron Ions
13 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-22 H: 0-23 N: 0-2 O: 0-5

GVK-SAM-6-PAGE-39NP
GVK-SAM-6-PAGE-39NP 23 (0.340) AM (Top,4, Ar,0.0,195.18,1.00,LS 10); Sm (Mn, 2x1.00); Sb (0,40.00)

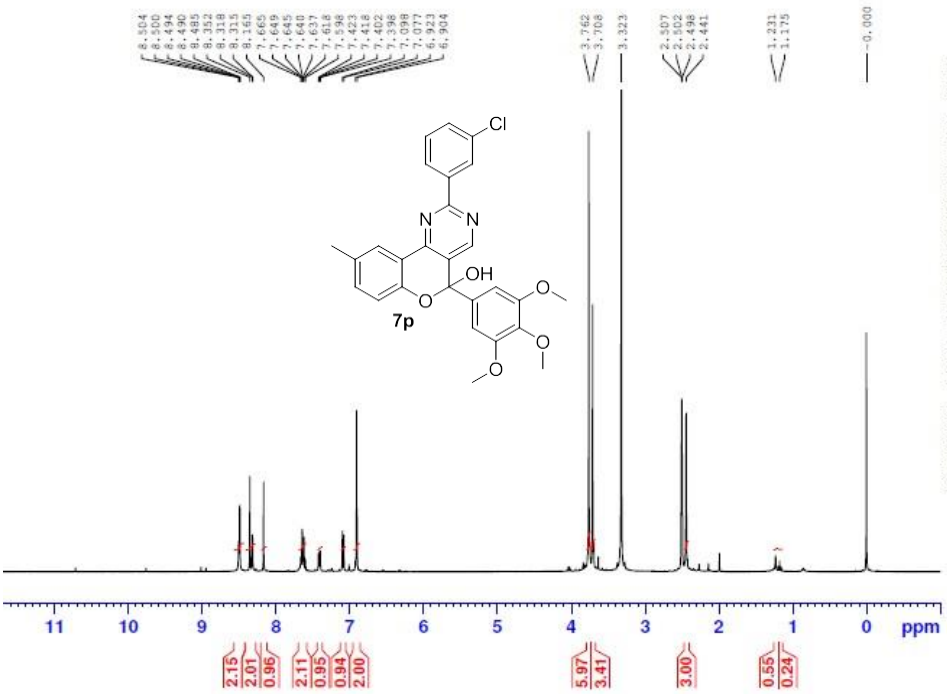




8o

Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
395.1610	395.1607	0.3	0.8	12.5	1503.1	C22 H23 N2 O5

-GVK-POLAR-40




```
Current Data Parameters
NAME          511611A0565
EXPNO                   1
PROCNO                  1

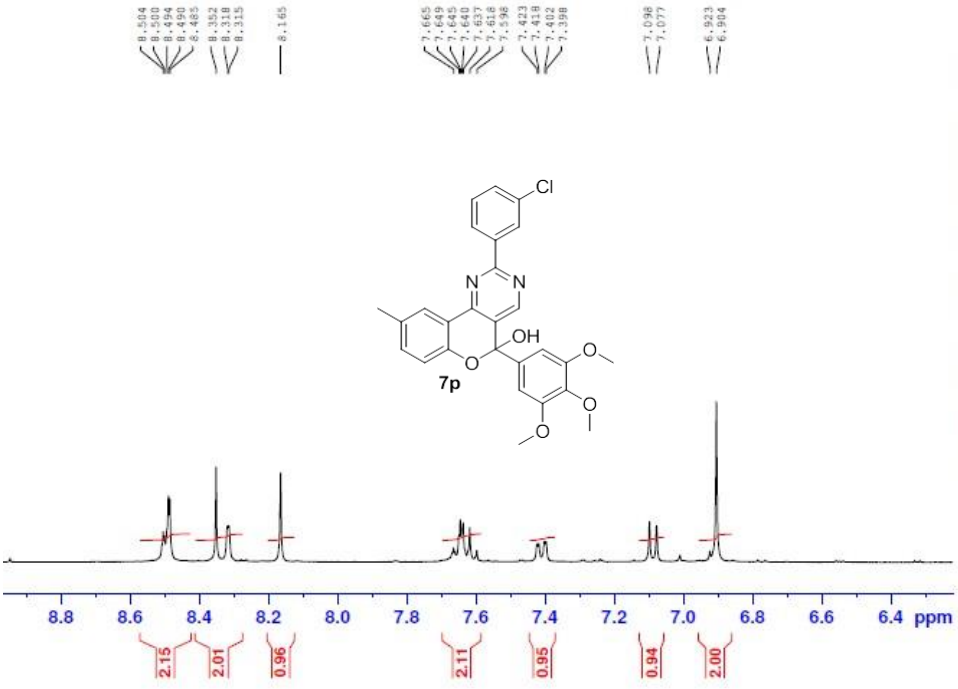
F2 - Acquisition Parameters
Date_              20161102
Time                 15.48
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                     16
DS                      2
SWH               8012.820 Hz
FIDRES               0.122266 Hz
AQ                4.0894465 sec
RG                   175.18
DW                  62.400 usec
DE                   6.50 usec
TE                  298.1 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              400.1300025 MHz
WDW                    EM
SSB          0
LB                   0.30 Hz
GB           0
PC                   1.00
```

ANL-MCL5-NMR-001

-GVK-POLAR-40




```
Current Data Parameters
NAME          511611A0565
EXPNO                   1
PROCNO                  1

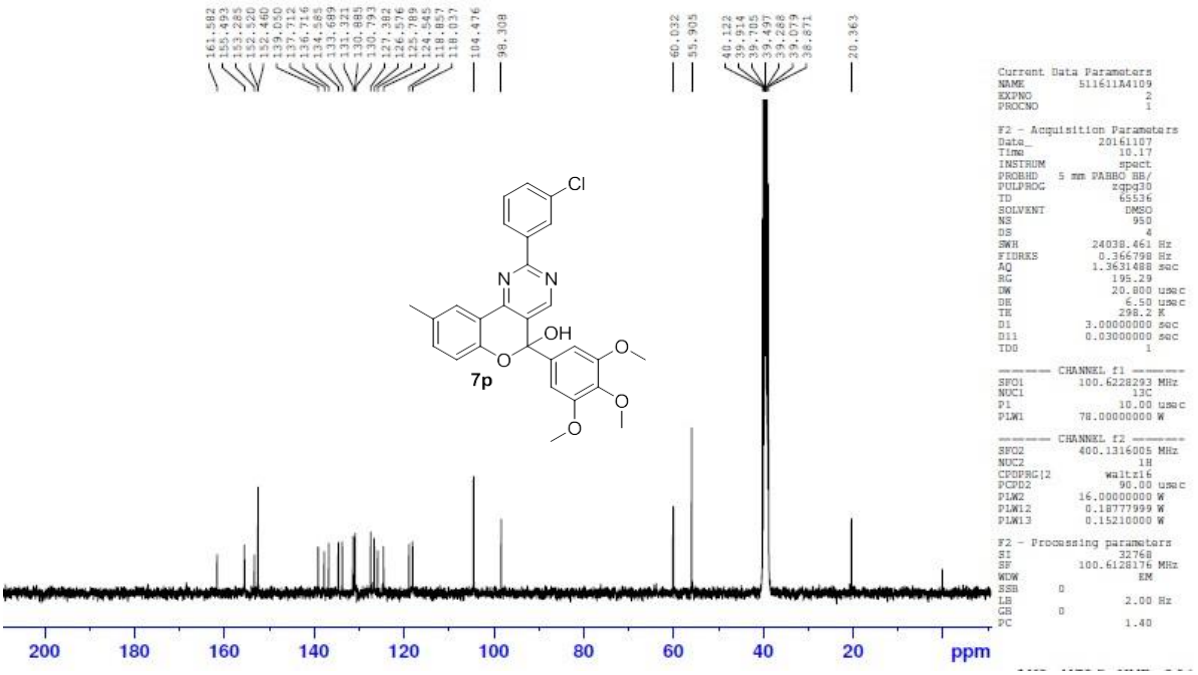
F2 - Acquisition Parameters
Date_              20161102
Time                 15.48
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                     16
DS                      2
SWH               8012.820 Hz
FIDRES               0.122266 Hz
AQ                4.0894465 sec
RG                   175.18
DW                  62.400 usec
DE                   6.50 usec
TE                  298.1 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              400.1300025 MHz
WDW                    EM
SSB          0
LB                   0.30 Hz
GB           0
PC                   1.00
```

ANL-MCL5-NMR-001

GVK-polar-40



Current Data Parameters
NAME 511611A4109
EXPNO 2
PROCNO 1

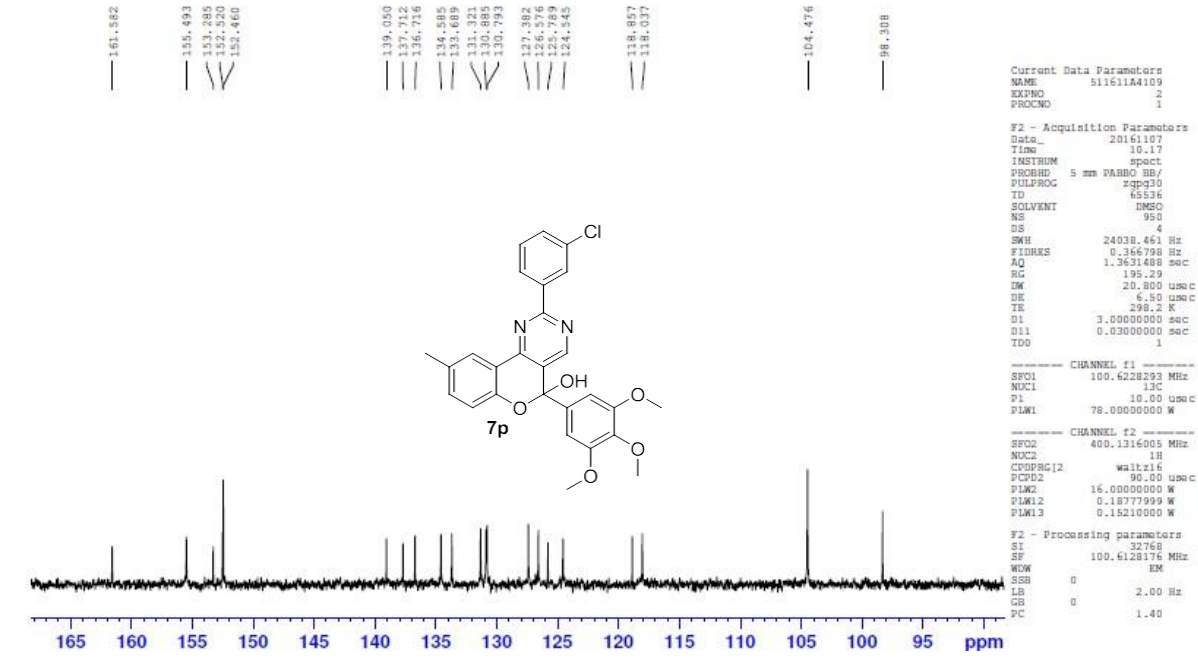
F2 - Acquisition Parameters
Date_ 20161107
Time 10.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 950
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631488 sec
RG 195.29
DW 20.800 usec
DE 6.50 usec
TE 298.2 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1

====== 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 100.6128176 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

GVK-polar-40



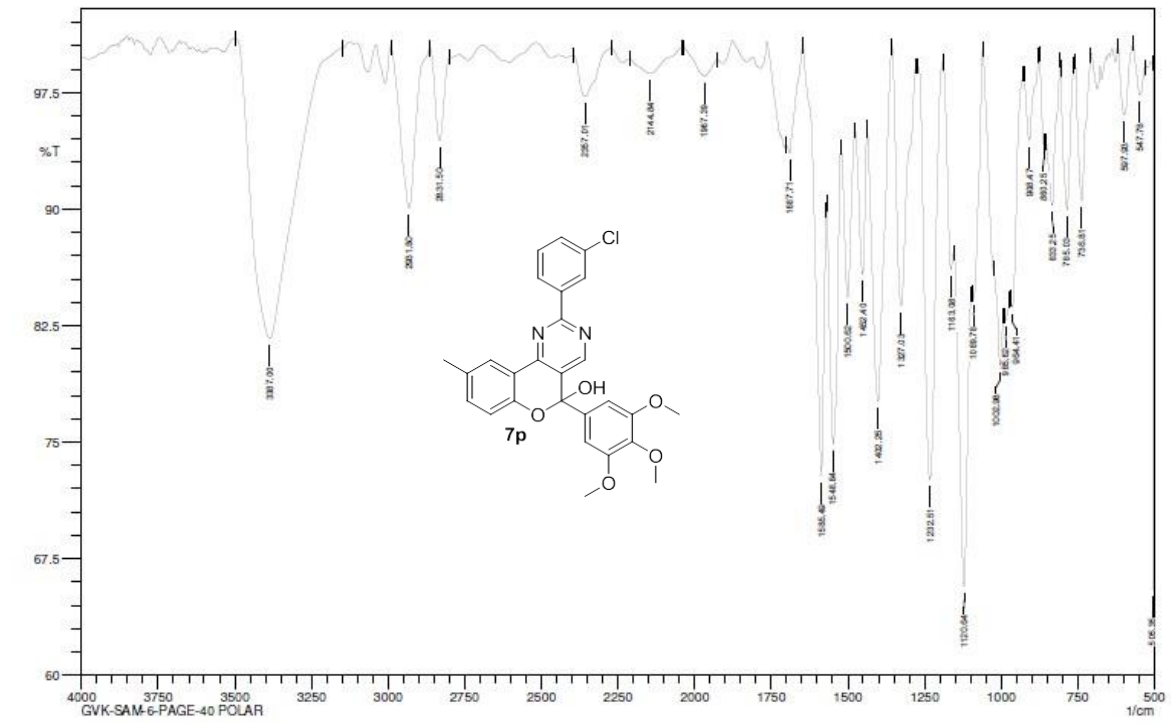
Current Data Parameters
NAME 511611A4109
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161107
Time 10.17
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 950
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 298.2 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 100.6128176 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

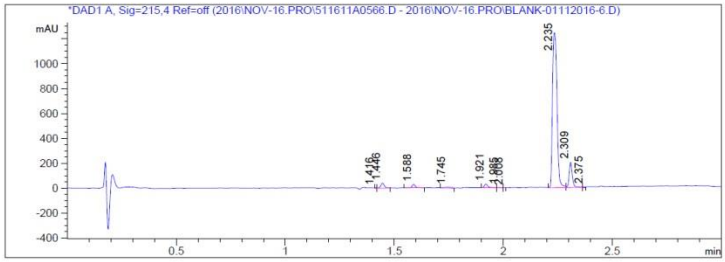


Comment: IN Kbr
GVK-SAM-6-PAGE-40 POLAR

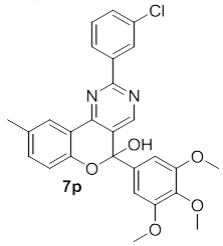
No. of Scans:
Resolution:
Apodization:

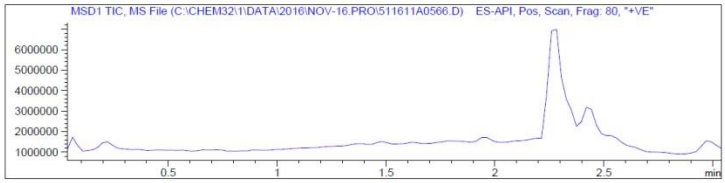
Date: 11/15/2016 10:50:31 AM
User: Admin

```
================================================================================
Date of Analysis:11/1/2016                      Vial Position  :P1-D-01
 SAMPLE NAME :          -GVK-POLAR              Injection Vol : 0.500          ul
                                                Instrument ID  :ANL-MCL3-LCMS-003
Acq. Method     :  RND-FA-3.0-MIN
================================================================================
Acq. Method Conditions: RND-FA-3.0-MIN
Column: Acquity UPLC BEH C18 (50mmx2.1 mm, 1.7µm)
Mobile Phase: B: 0.1% Formic Acid in Water, A: 0.1% Formic Acid in Acetonitrile
Gradient: Time (min)/ %A:  0/3, 0.4/3,2.2/98, 2.6/98, 2.61/3, 3.0/3
Column Temp: 60°C, Flow Rate: 0.8ml/min
```

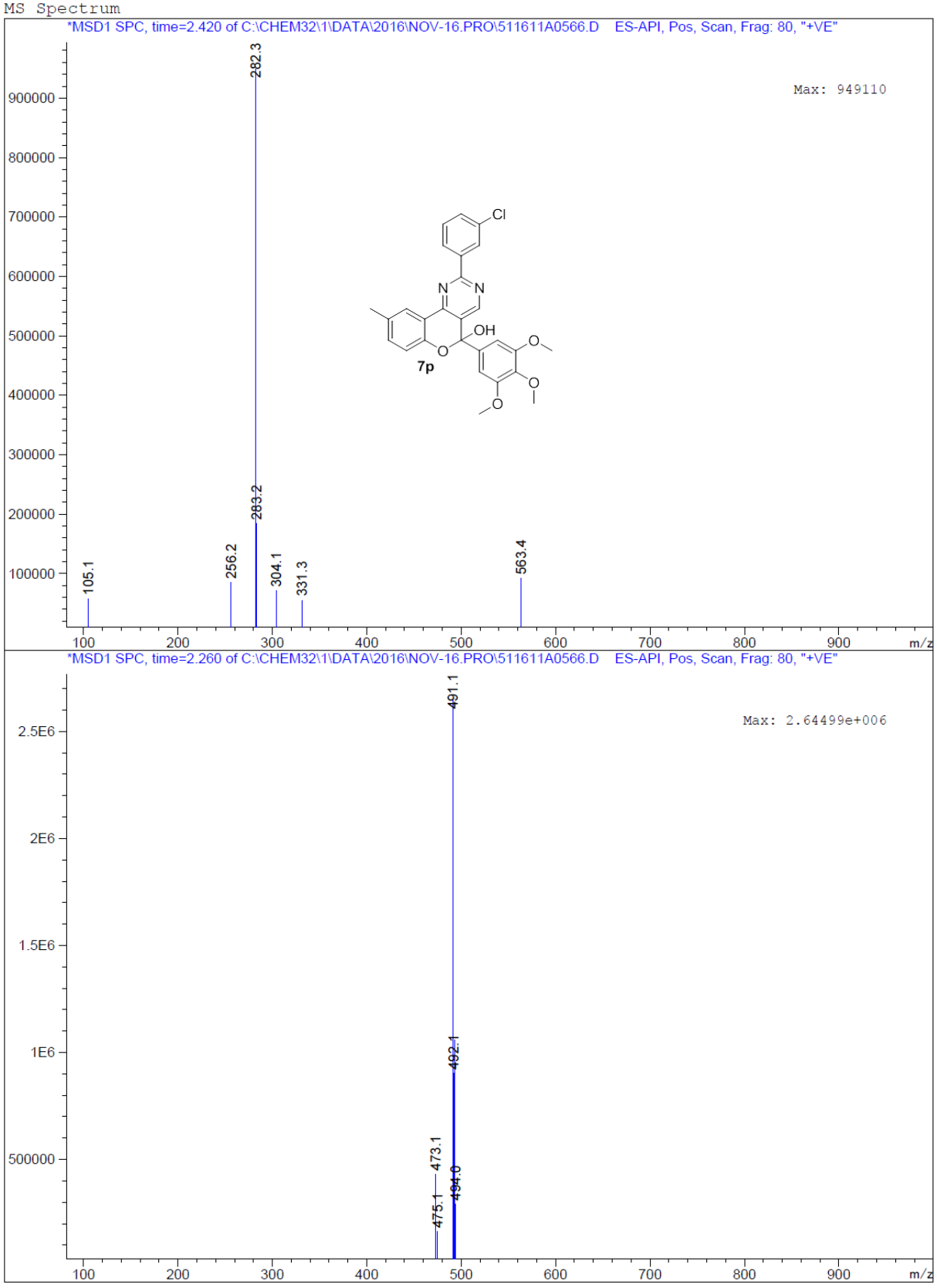


Pea No	RT min	Area	Area %
1	1.416	1.503	0.070
2	1.446	44.283	2.074
3	1.588	32.571	1.525
4	1.745	17.623	0.825
5	1.921	32.087	1.503
6	1.985	3.856	0.181
7	2.008	1.284	0.060
8	2.235	1786.399	83.655
9	2.309	212.363	9.945
10	2.375	3.465	0.162





MS Spectrum

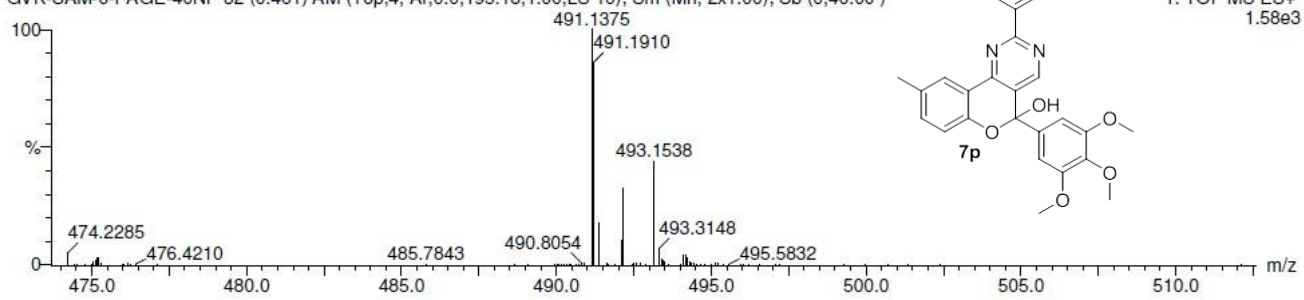

*MSD1 SPC, time=2.420 of C:\CHEM32\1\DATA\2016\NOV-16.PRO\511611A0566.D ES-API, Pos, Scan, Frag: 80, "+VE"
Max: 949110
282.3
283.2
105.1
256.2
304.1
331.3
563.4
Cl
N
N
OH
O
O
O
O
7p
*MSD1 SPC, time=2.260 of C:\CHEM32\1\DATA\2016\NOV-16.PRO\511611A0566.D ES-API, Pos, Scan, Frag: 80, "+VE"
Max: 2.64499e+006
491.1
492.1
473.1
494.0
475.1
m/z

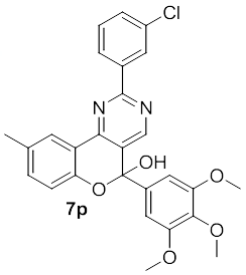
Single Mass Analysis

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

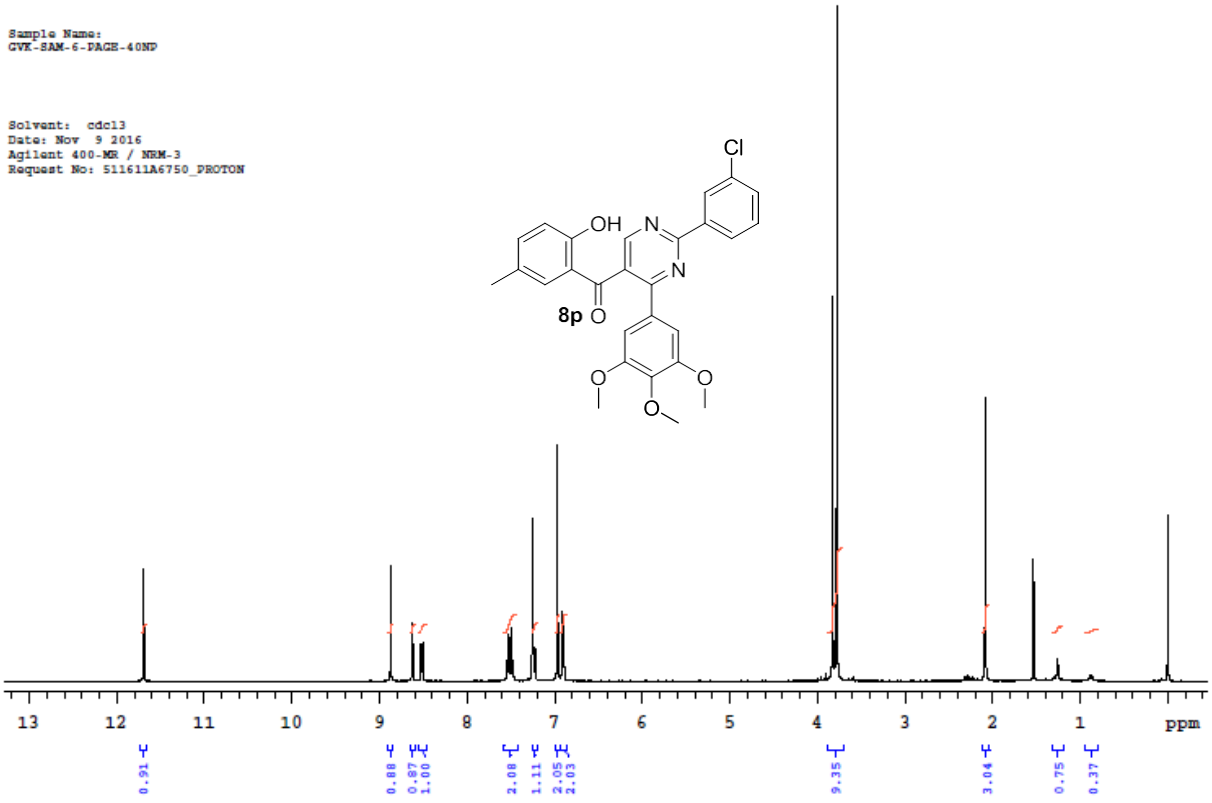
Monoisotopic Mass, Even Electron Ions
30 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-27 H: 0-24 N: 0-2 O: 0-5 Cl: 0-1

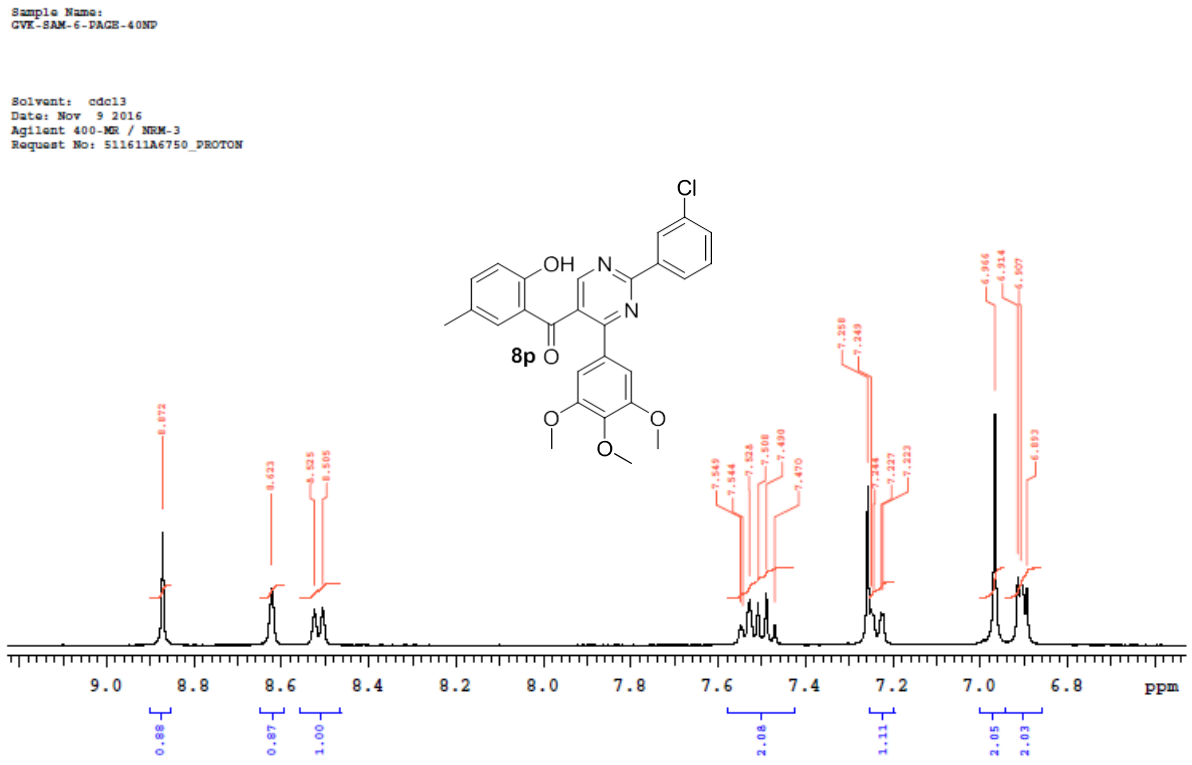
GVK-SAM-6-PAGE-40NP
GVK-SAM-6-PAGE-40NP 32 (0.461) AM (Top,4, Ar,0.0,195.18,1.00,LS 10); Sm (Mn, 2x1.00); Sb (0,40.00)

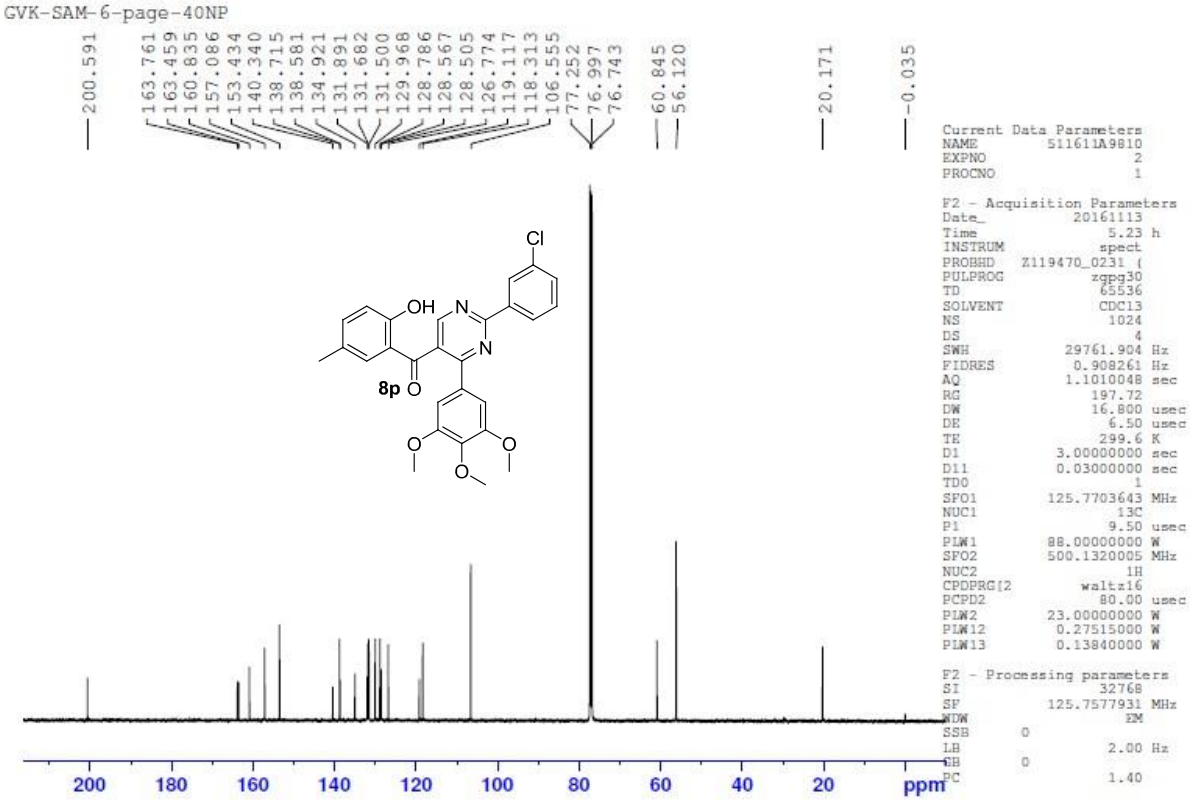


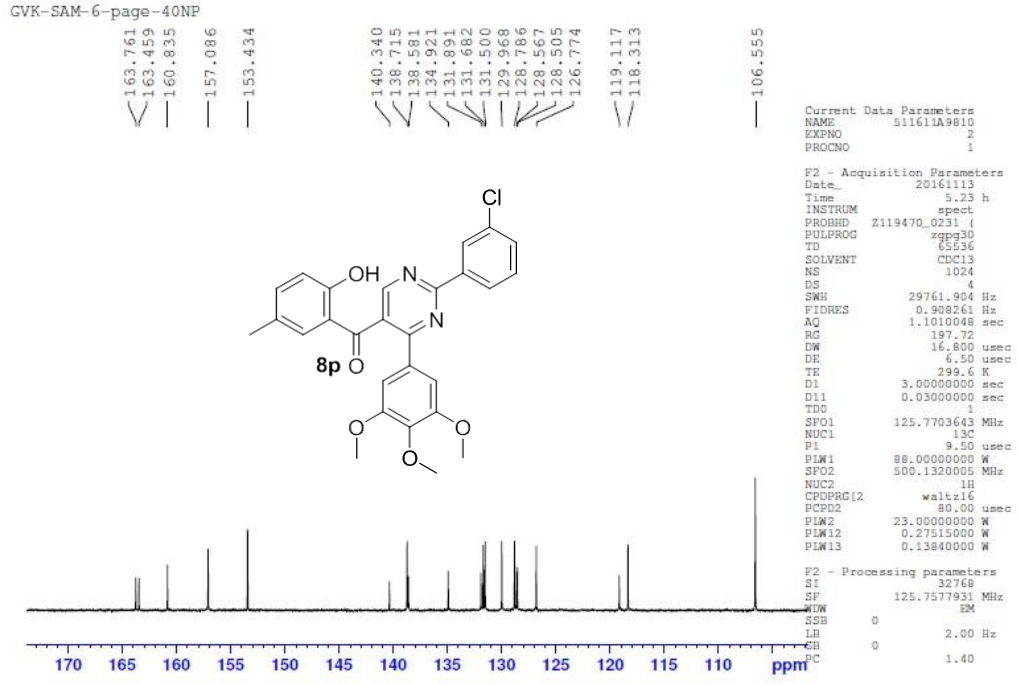


Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
491.1375	491.1374	0.1	0.2	16.5	8.0	C27 H24 N2 O5 Cl

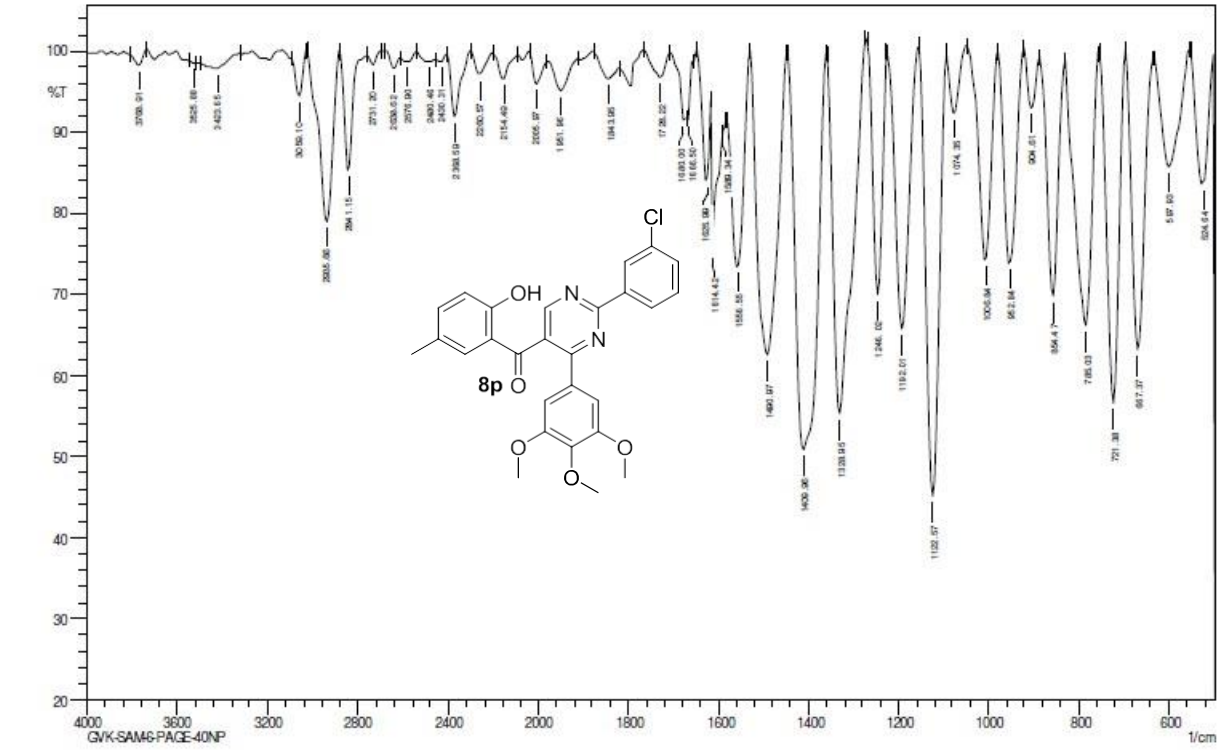

Sample Name:
GVK-SAM-6-PAGE-40ND
Solvent: cdcl3
Date: Nov 9 2016
Agilent 400-MR / NRM-3
Request No: 511611A6750_PROTON
Cl
OH
N
N
8p O
O
O
O
13
12
11
10
9
8
7
6
5
4
3
2
1
ppm
0.91
0.88
0.87
1.00
2.08
1.11
2.05
2.03
9.35
3.04
0.75
0.37


Sample Name:
GVK-SAM-6-PAGE-40ND
Solvent: cdcl3
Date: Nov 9 2016
Agilent 400-MR / NRM-3
Request No: 511611A6750_PROTON
Cl
OH
N
N
8p O
O
O
O
8.872
8.623
8.525
8.505
7.569
7.544
7.528
7.508
7.490
7.470
7.258
7.249
7.241
7.227
7.223
6.946
6.934
6.907
6.893
9.0
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
ppm
0.88
0.87
1.00
2.08
1.11
2.05
2.03


GVK-SAM-6-page-40NP
200.591
163.761
163.459
160.835
157.086
153.434
140.340
138.715
138.581
134.921
131.891
131.682
131.500
129.968
128.786
128.567
128.505
126.774
119.117
118.313
106.555
77.252
76.997
76.743
60.845
56.120
20.171
-0.035
Cl
OH
N
N
8p O
O
O
O
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME 511611A9810
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161113
Time 5.23 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 299.6 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7577931 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40


GVK-SAM-6-page-40NP
163.761
163.459
160.835
157.086
153.434
140.340
138.715
138.581
134.921
131.891
131.682
131.500
129.968
128.786
128.567
128.505
126.774
119.117
118.313
106.555
Cl
OH
N
N
8p O
O
O
O
170
165
160
155
150
145
140
135
130
125
120
115
110
ppm
Current Data Parameters
NAME 511611A9810
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161113
Time 5.23 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT CDC13
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 299.6 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7577931 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

SHIMADZU



Comment: IN Kbr
GVK-SAM-6-PAGE-40NP

No. of Scans;
Resolution;

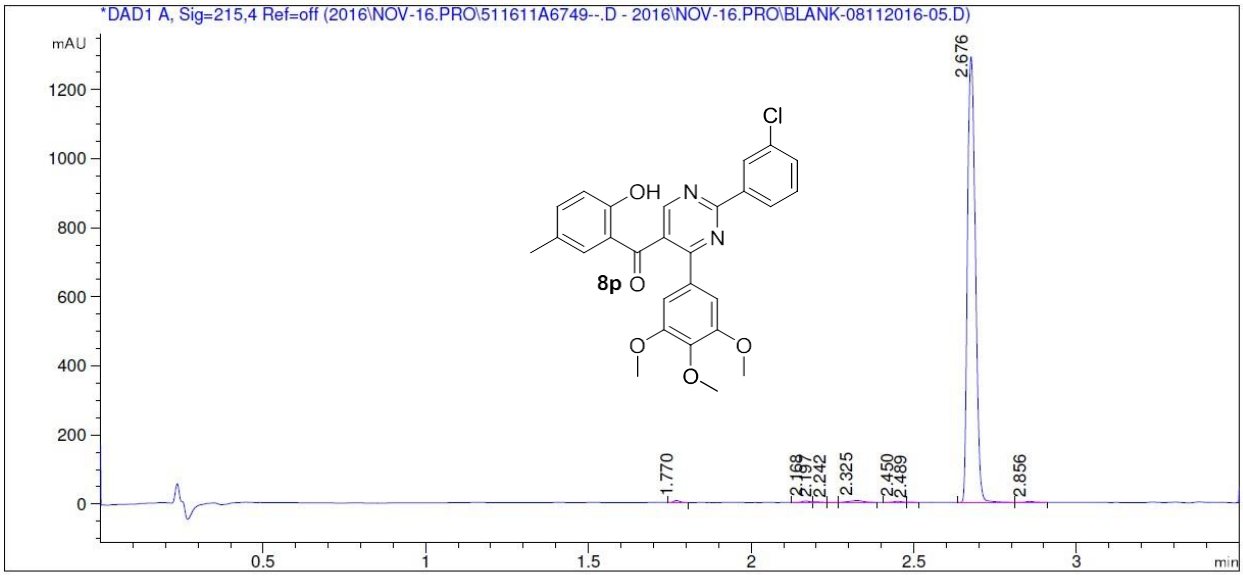
Date:11/29/2016 9:32:19 AM
User; Admin

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

Sample Name :GVK-SAM-6-PAGE-40NP Vial position : P1-C-05
Date of Analysis :11/8/2016 9:52:42 PM Injection Vol : 0.500uL
Acq. Method :C:\CHEM32\1\METHODS\RND-FA- 3.5 MIN.M Instrument ID :ANL-MCL5-LCMS-001

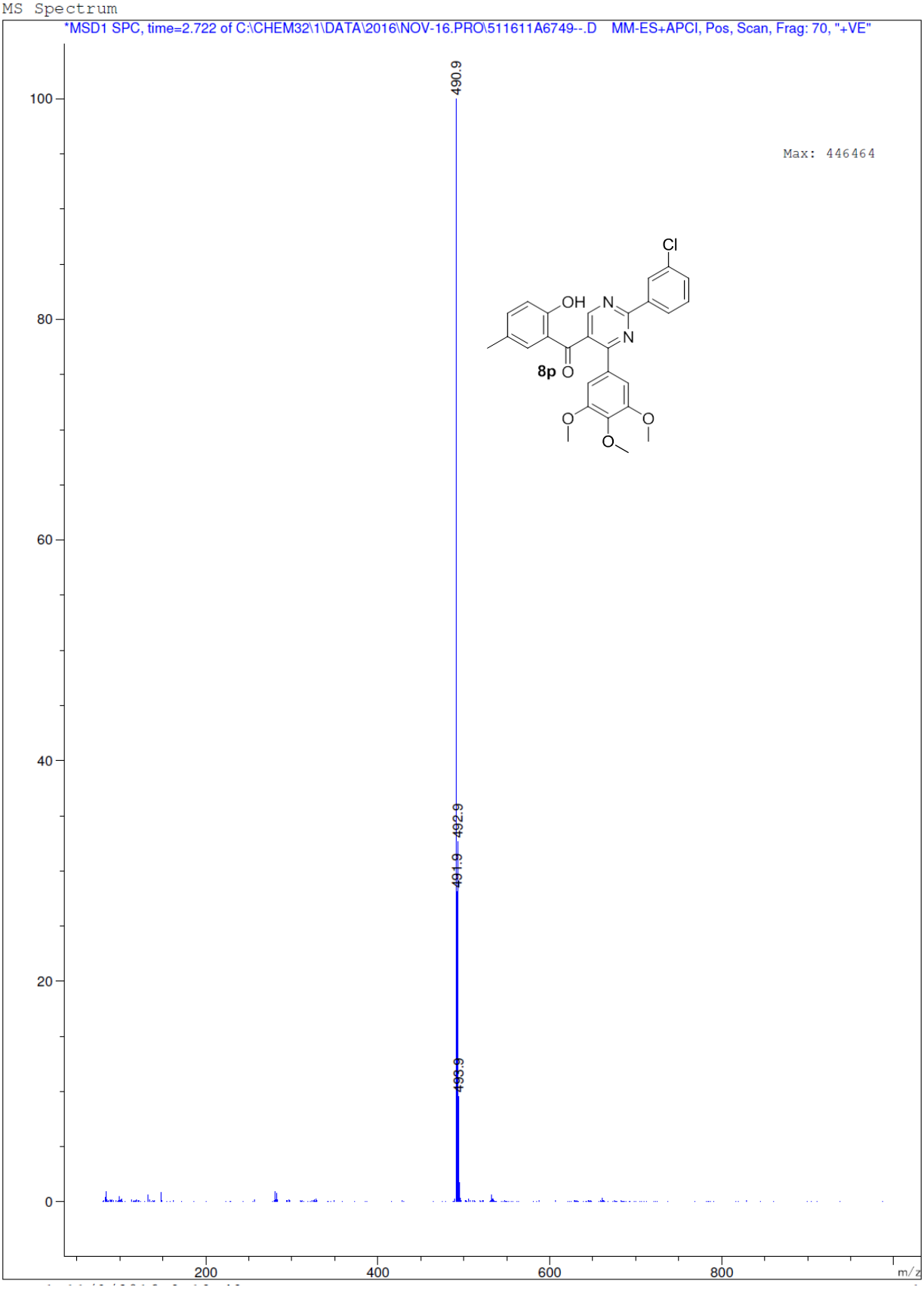
RND-FA-3.5 MIN.M
Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7um)
Mobile Phase: B1: 0.1 % FA IN WATER A1: 0.1%FA IN ACN
Gradient: Time (min) /%A1: 0/2, 0.4/2, 2.8/98,3.4/98,3.41/2,3.5/2
Column Flow Rate: 0.6 ml/min
Column Temperature: 60°C

->



Pea No	RT min	Area	Area %
1	1.77	8.143	0.366
2	2.17	8.699	0.391
3	2.20	3.617	0.162
4	2.24	1.274	0.057
5	2.32	16.844	0.757
6	2.45	6.183	0.278
7	2.49	1.282	0.058
8	2.68	2172.804	97.600
9	2.86	7.396	0.332

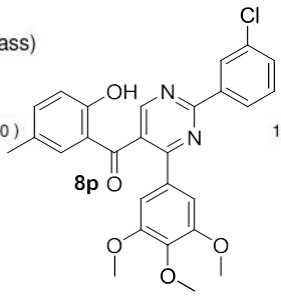
MS Spectrum


*MSD1 SPC, time=2.722 of C:\CHEM32\1\DATA\2016\NOV-16.PRO\511611A6749--.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 446464
490.9
492.9
491.9
493.9
8p
Cl
OH
N
N
O
O
O
O
100
80
60
40
20
0
200
400
600
800
m/z

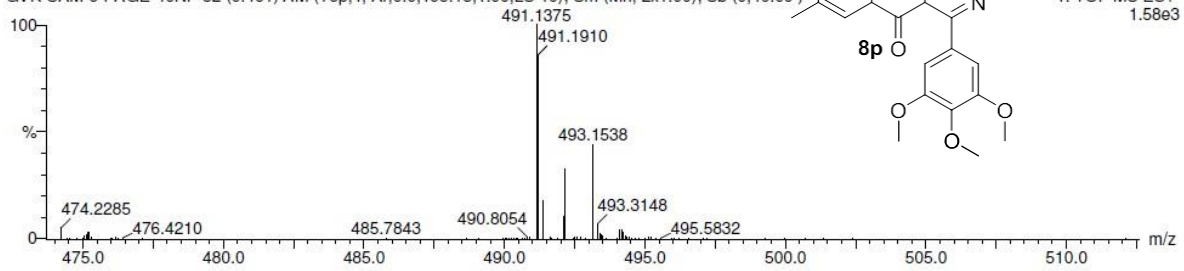
Elemental Composition Report **Page 1**

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

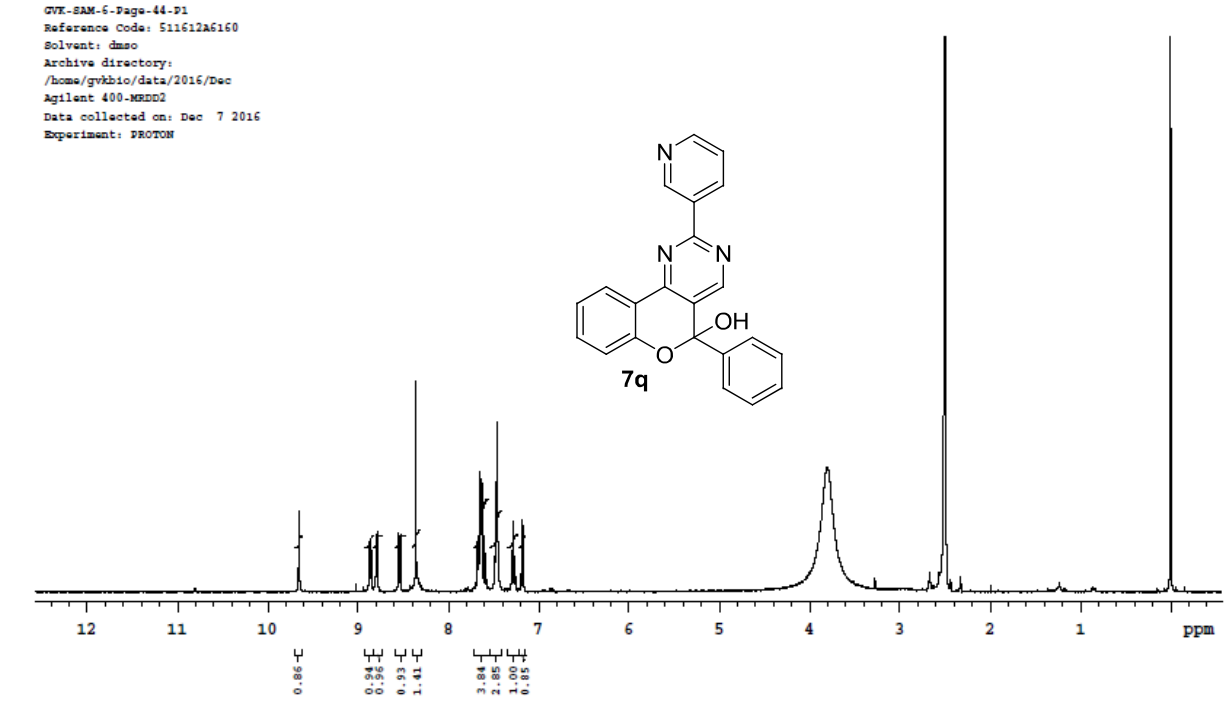
Monoisotopic Mass, Even Electron Ions
30 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-27 H: 0-24 N: 0-2 O: 0-5 Cl: 0-1
GVK-SAM-6-PAGE-40NP
GVK-SAM-6-PAGE-40NP 32 (0.461) AM (Top,4, Ar,0.0,195.18,1.00,LS 10); Sm (Mn, 2x1.00); Sb (0,40.00)

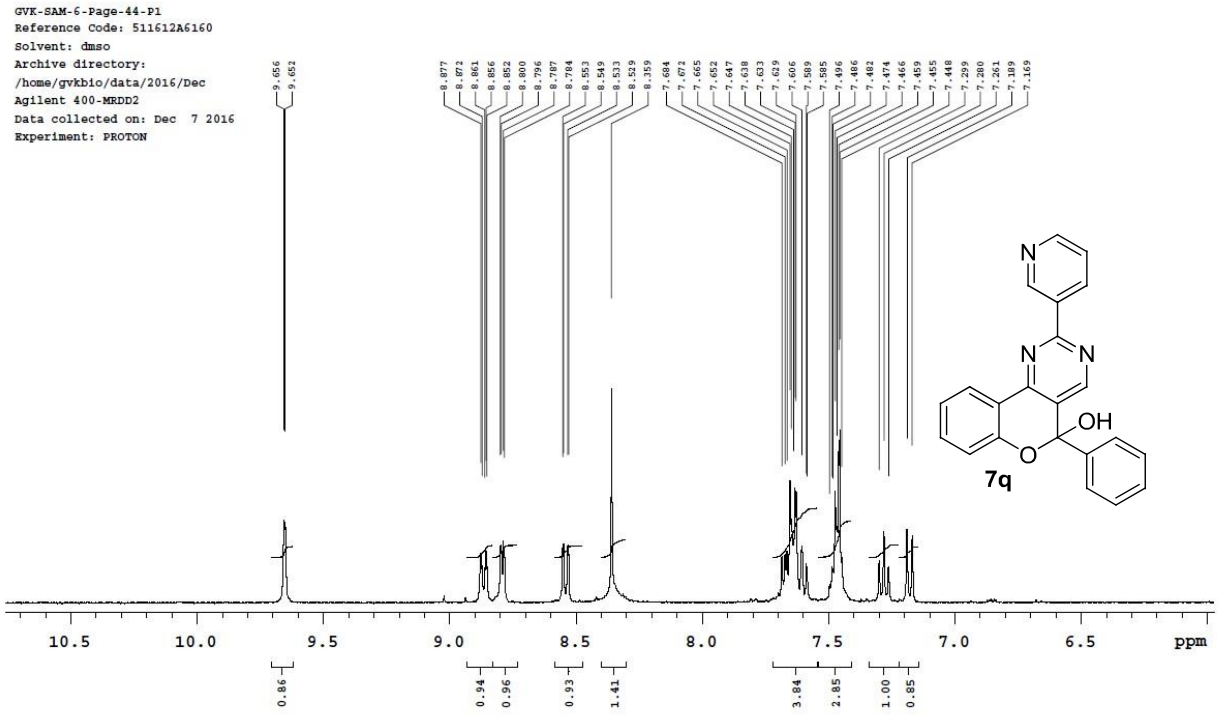


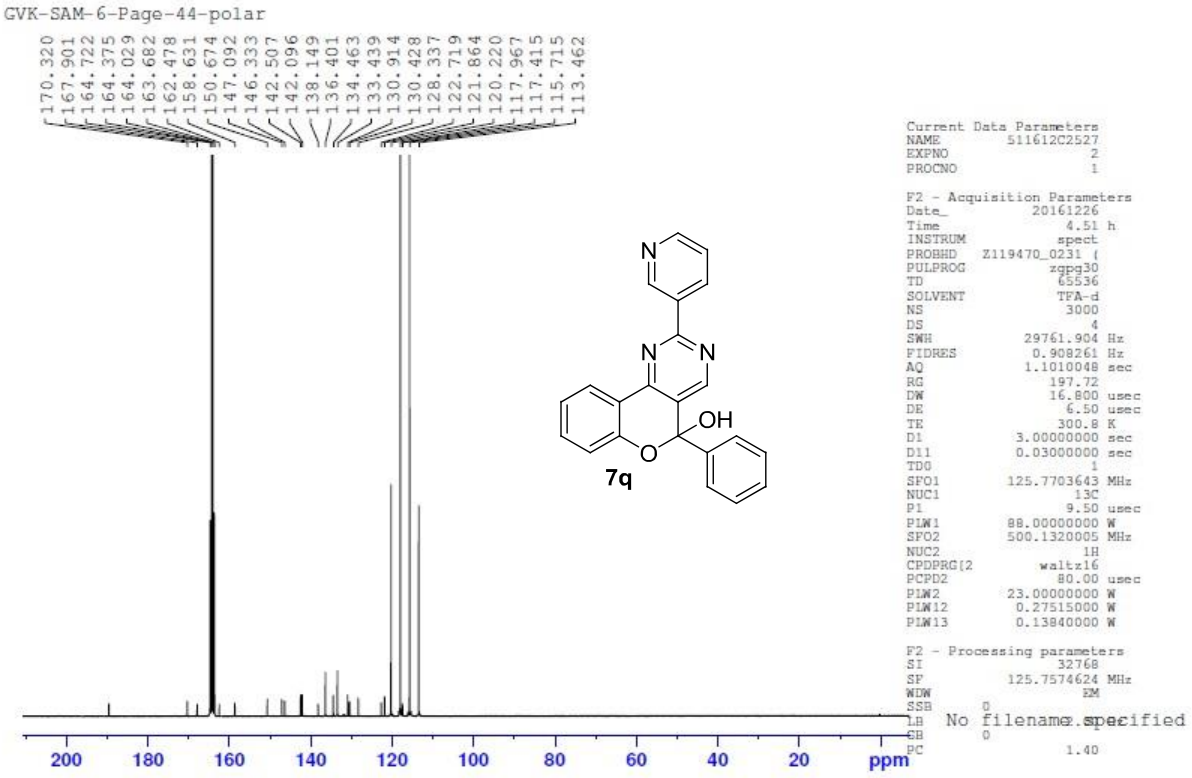
1: TOF MS ES+
1.58e3

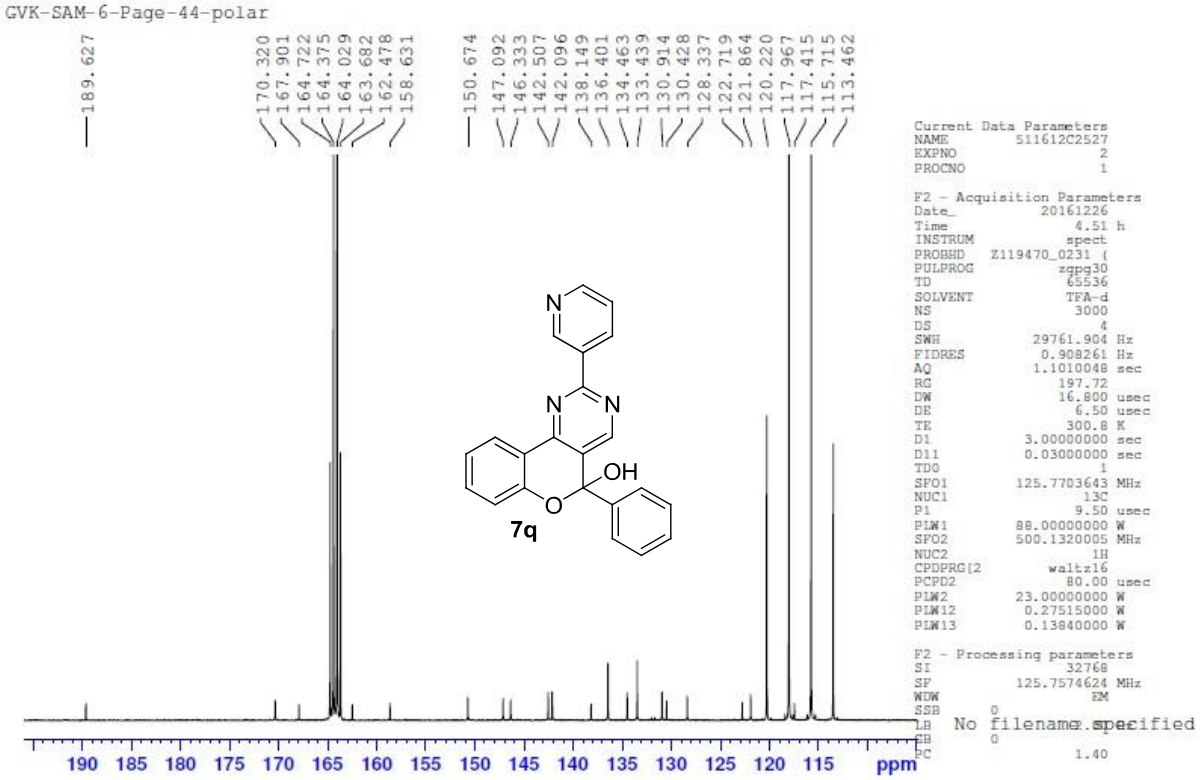


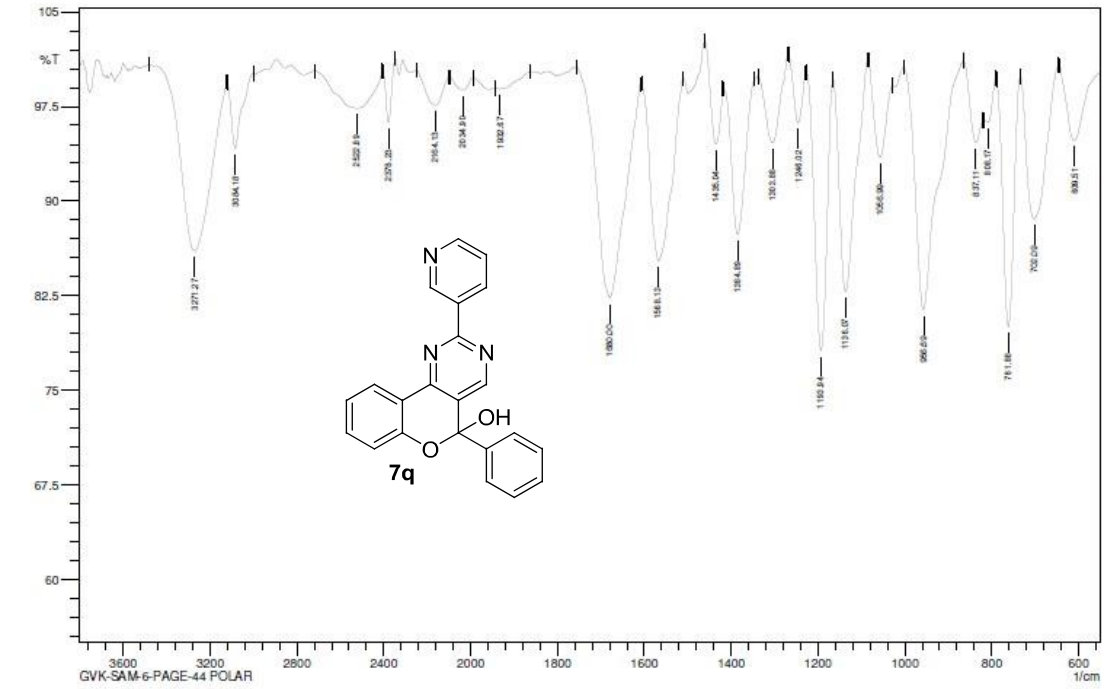
Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
491.1375	491.1374	0.1	0.2	16.5	8.0	C27 H24 N2 O5 Cl


GVK-SAM-6-Page-44-P1
Reference Code: 511612A6160
Solvent: dmso
Archive directory:
/home/gvkbio/data/2016/Dec
Agilent 400-MRDD2
Data collected on: Dec 7 2016
Experiment: PROTON
N
N
N
OH
O
7q
12
11
10
9
8
7
6
5
4
3
2
1
ppm
0.86
0.94
0.96
0.93
1.41
3.84
2.85
1.00
0.85


GVK-SAM-6-Page-44-P1
Reference Code: 511612A6160
Solvent: dmso
Archive directory:
/home/gvkbio/data/2016/Dec
Agilent 400-MRDD2
Data collected on: Dec 7 2016
Experiment: PROTON
9.656
9.652
8.877
8.872
8.861
8.856
8.852
8.800
8.796
8.787
8.784
8.553
8.549
8.533
8.529
8.359
7.684
7.672
7.665
7.652
7.647
7.638
7.633
7.629
7.606
7.589
7.585
7.496
7.486
7.482
7.474
7.466
7.459
7.455
7.448
7.299
7.280
7.261
7.189
7.169
N
N
N
OH
O
7q
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
ppm
0.86
0.94
0.96
0.93
1.41
3.84
2.85
1.00
0.85


GVK-SAM-6-Page-44-polar
170.320
167.901
164.722
164.375
164.029
163.682
162.478
158.631
150.674
147.092
146.333
142.507
142.096
138.149
136.401
134.463
133.439
130.914
130.428
128.337
122.719
121.864
120.220
117.967
117.415
115.715
113.462
N
N
N
OH
O
7q
Current Data Parameters
NAME 511612C2527
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161226
Time 4.51 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT TFA-d
NS 3000
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 300.8 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7574624 MHz
WDW EM
SSB 0
LB No filename specified
GB 0
PC 1.40
200 180 160 140 120 100 80 60 40 20 ppm


GVK-SAM-6-Page-44-polar
189.627
170.320
167.901
164.722
164.375
164.029
163.682
162.478
158.631
150.674
147.092
146.333
142.507
142.096
138.149
136.401
134.463
133.439
130.914
130.428
128.337
122.719
121.864
120.220
117.967
117.415
115.715
113.462
N
N
N
OH
O
7q
Current Data Parameters
NAME 511612C2527
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161226
Time 4.51 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT TFA-d
NS 3000
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 300.8 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7574624 MHz
WDW EM
SSB 0
LB No filename specified
GB 0
PC 1.40
190 185 180 175 170 165 160 155 150 145 140 135 130 125 120 115 ppm



Comment: IN Kbr
GVK-SAM-6-PAGE-44 POLAR

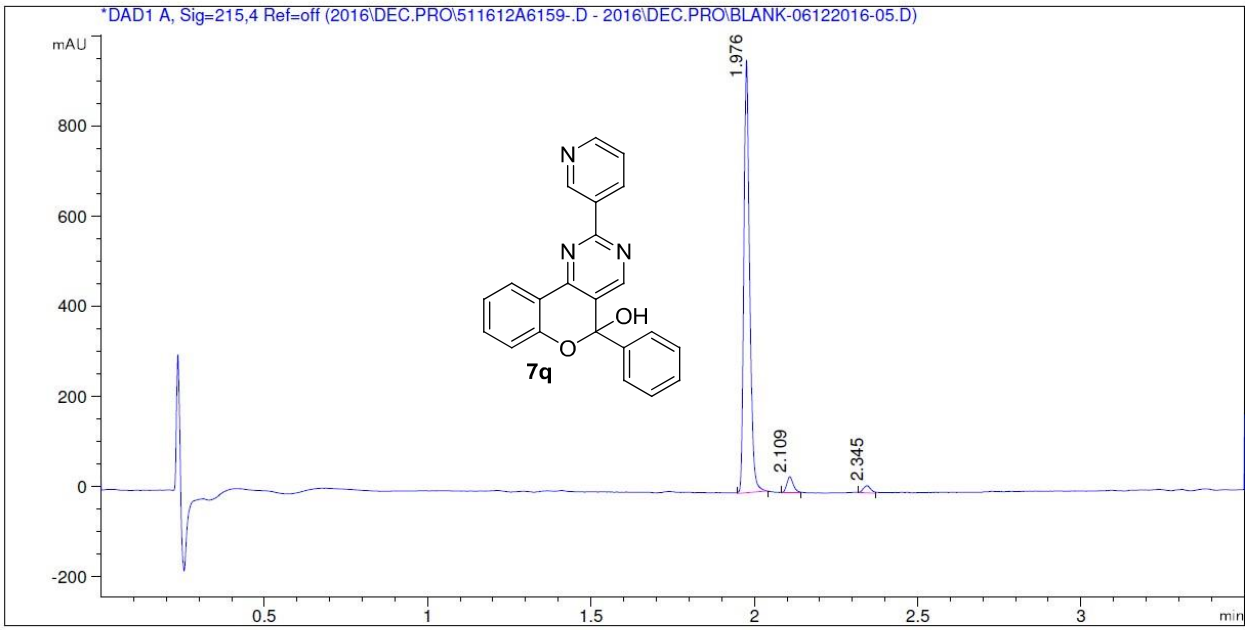
No. of Scans:
Resolution:
Apodization:

Date: 12/22/2016 11:43:06 AM
User: Admin

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

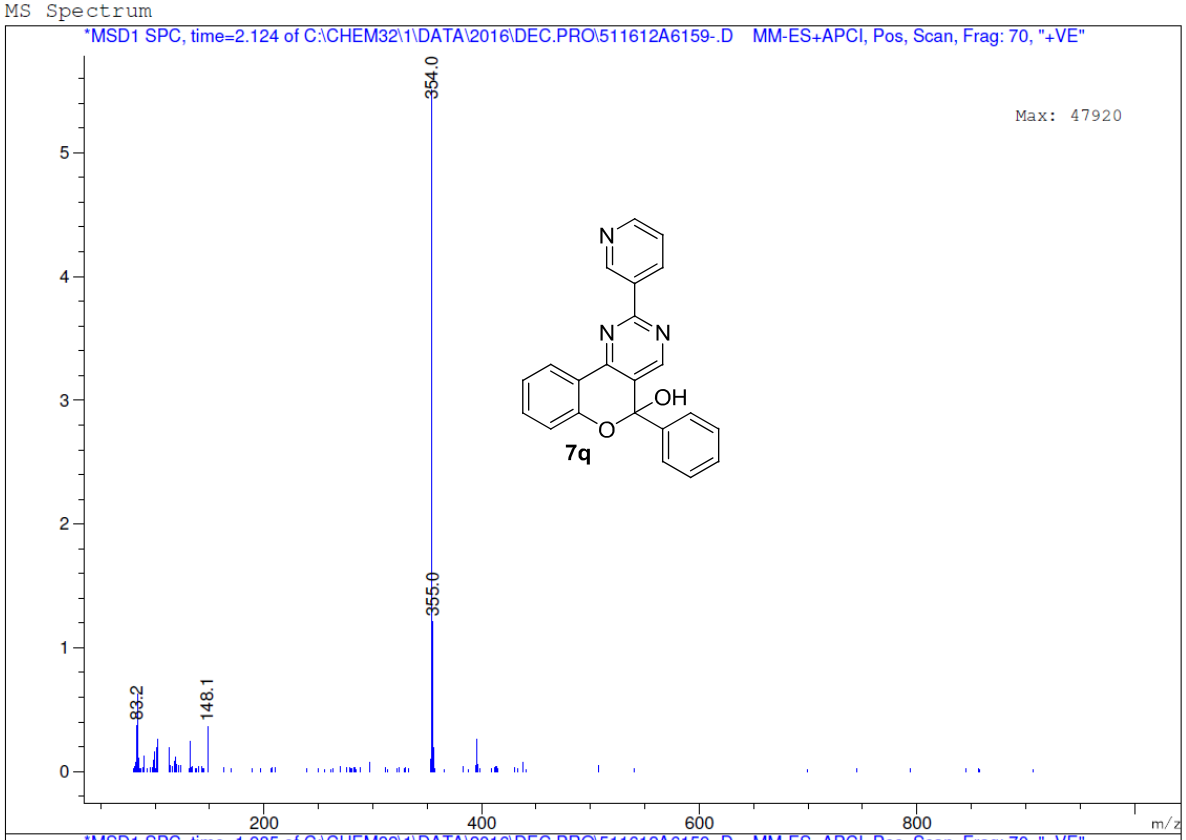
Vial position : P2-C-01
Date of Analysis :12/7/2016 9:46:58 PM Injection Vol : 2.000uL
Acq. Method :C:\CHEM32\1\METHODS\RND-FA- 3.5 MIN.M Instrument ID :ANL-MCL5-LCMS-001
Sample Name : GVK-SAM-6-PAGE-44P1

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, 0.4/2, 2.8/98,3.4/98,3.41/2,3.5/2
Column Flow Rate: 0.6 ml/min
Column Temperature: 60°C ->



Pea No	RT min	Area	Area %
1	1.98	1171.845	94.393
2	2.11	45.472	3.663
3	2.34	24.131	1.944

MS Spectrum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Max: 47920
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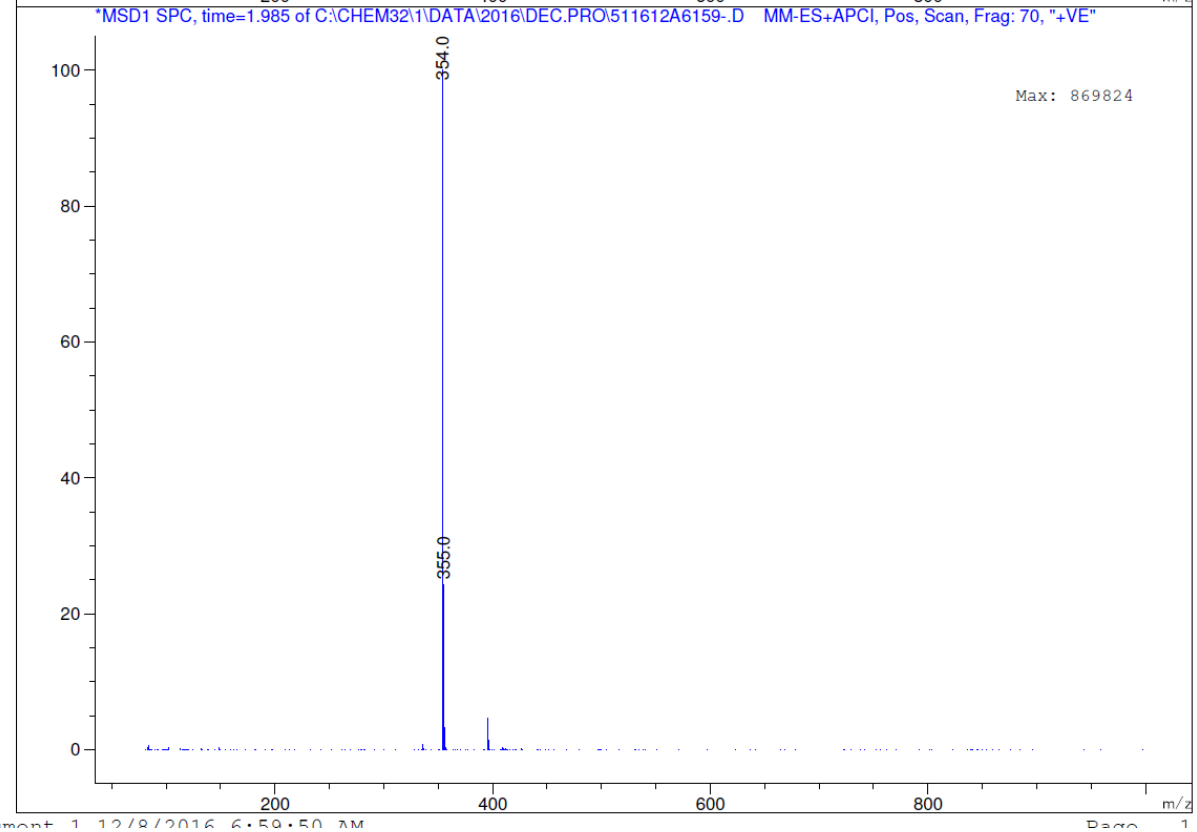
355.0
83.2
148.1
OH
O
7q
m/z


*MSD1 SPC, time=1.985 of C:\CHEM32\1\DATA\2016\DEC.PRO\511612A6159-.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 869824
354.0
355.0
m/z

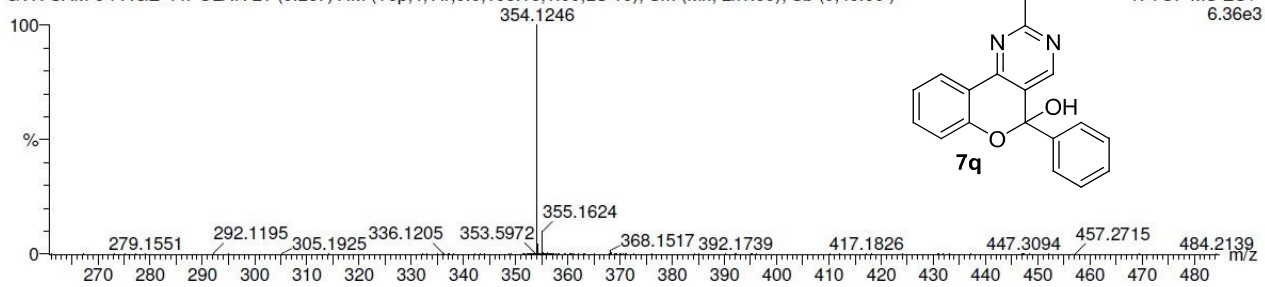
Single Mass Analysis

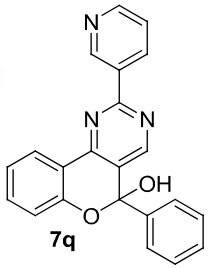
Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

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: 0-22 H: 0-16 N: 0-3 O: 0-2

GVK-SAM-6-PAGE-44POLAR
GVK-SAM-6-PAGE-44POLAR 21 (0.287) AM (Top,4, Ar,0.0,195.16,1.00,LS 10); Sm (Mn, 2x1.00); Sb (0,40.00)

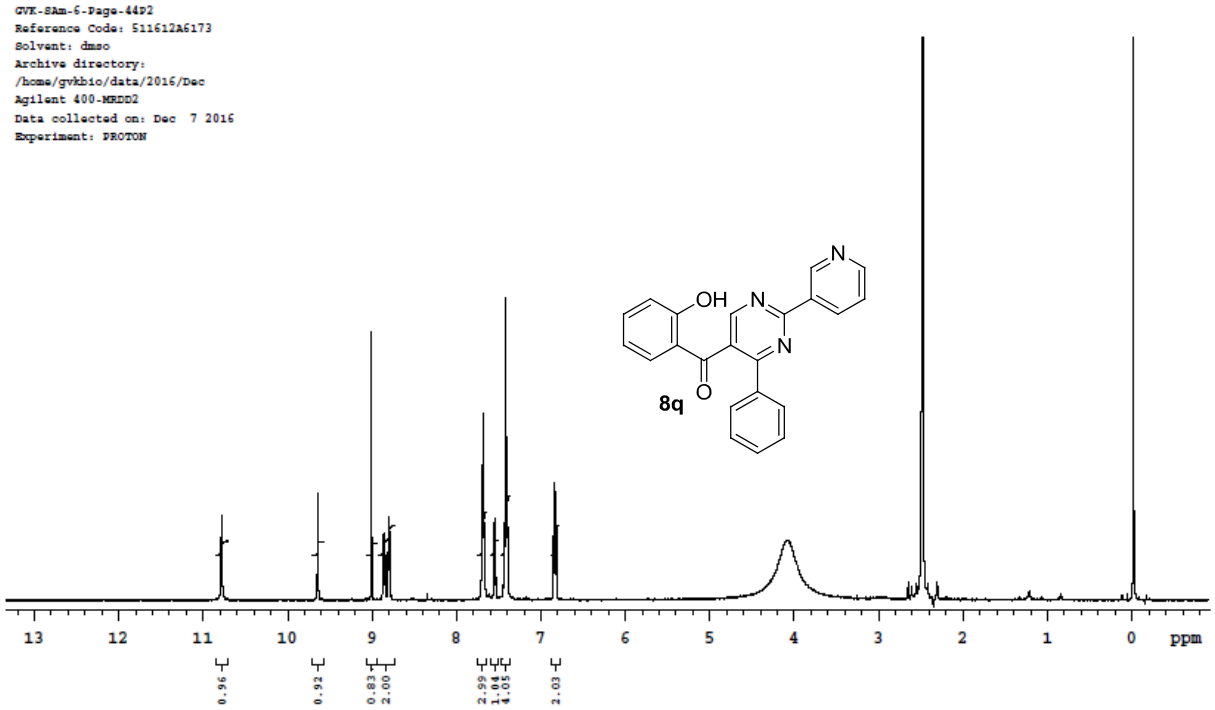
1: TOF MS ES+
6.36e3

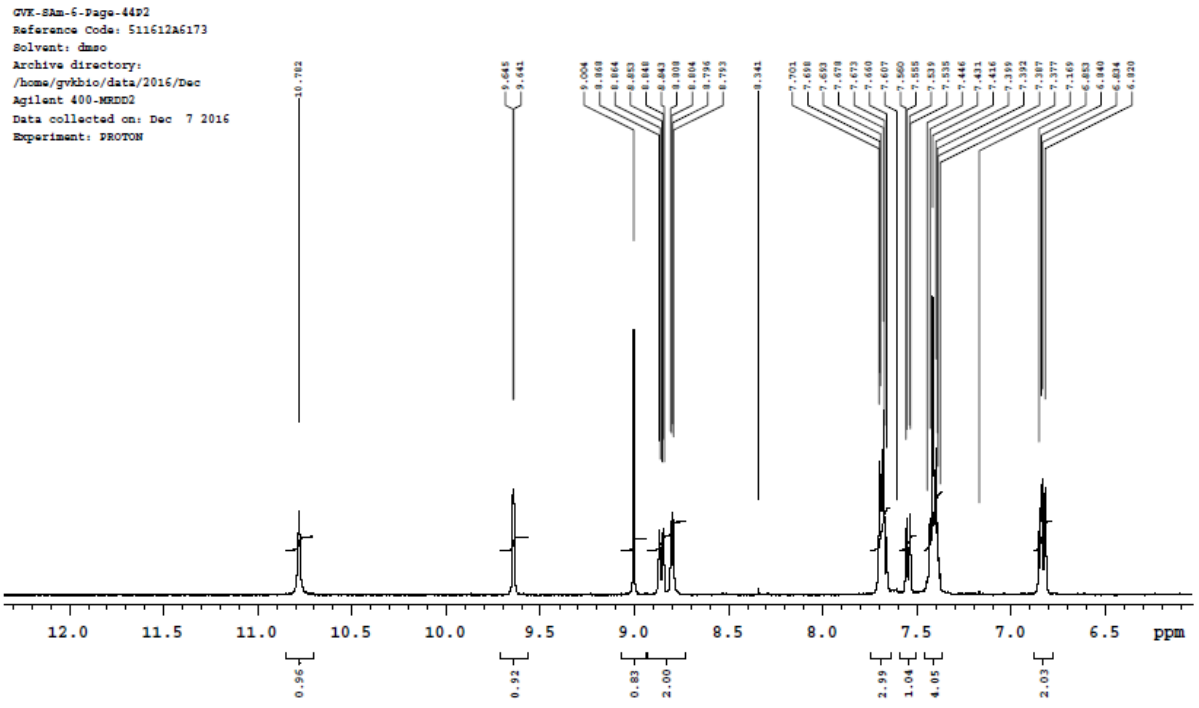


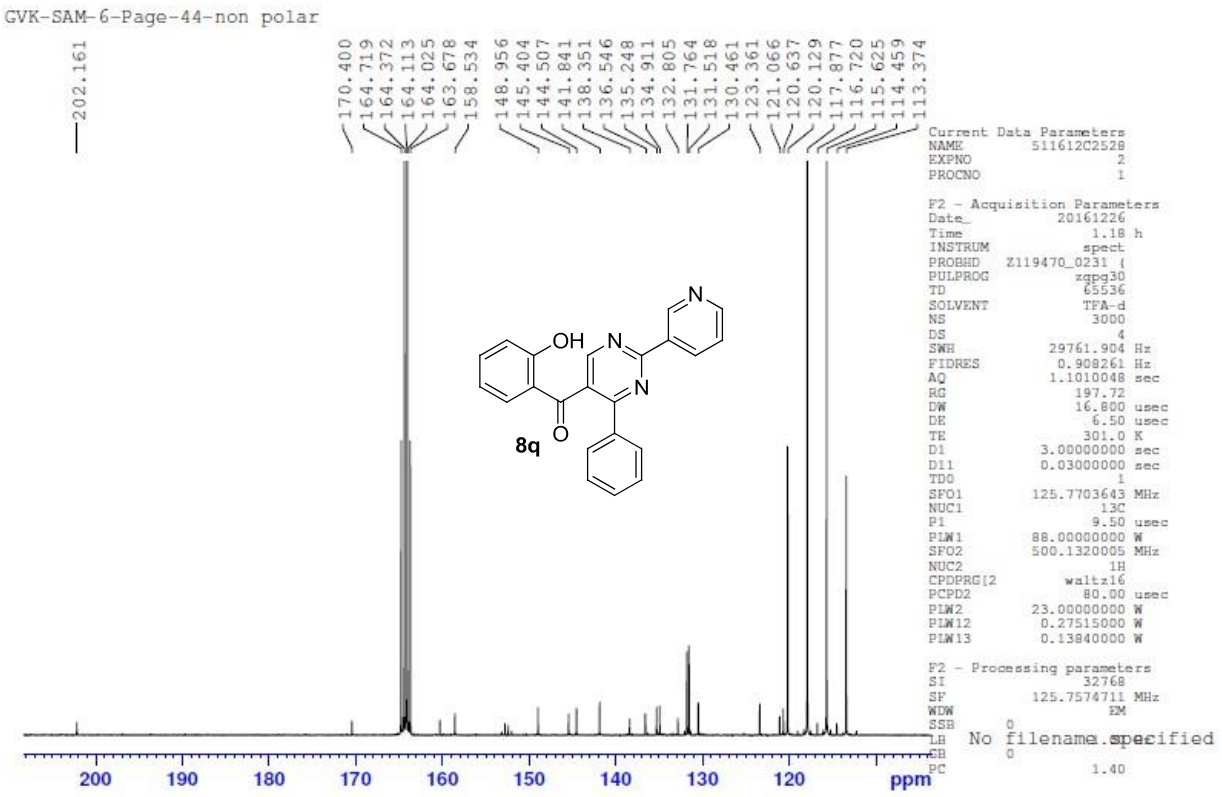


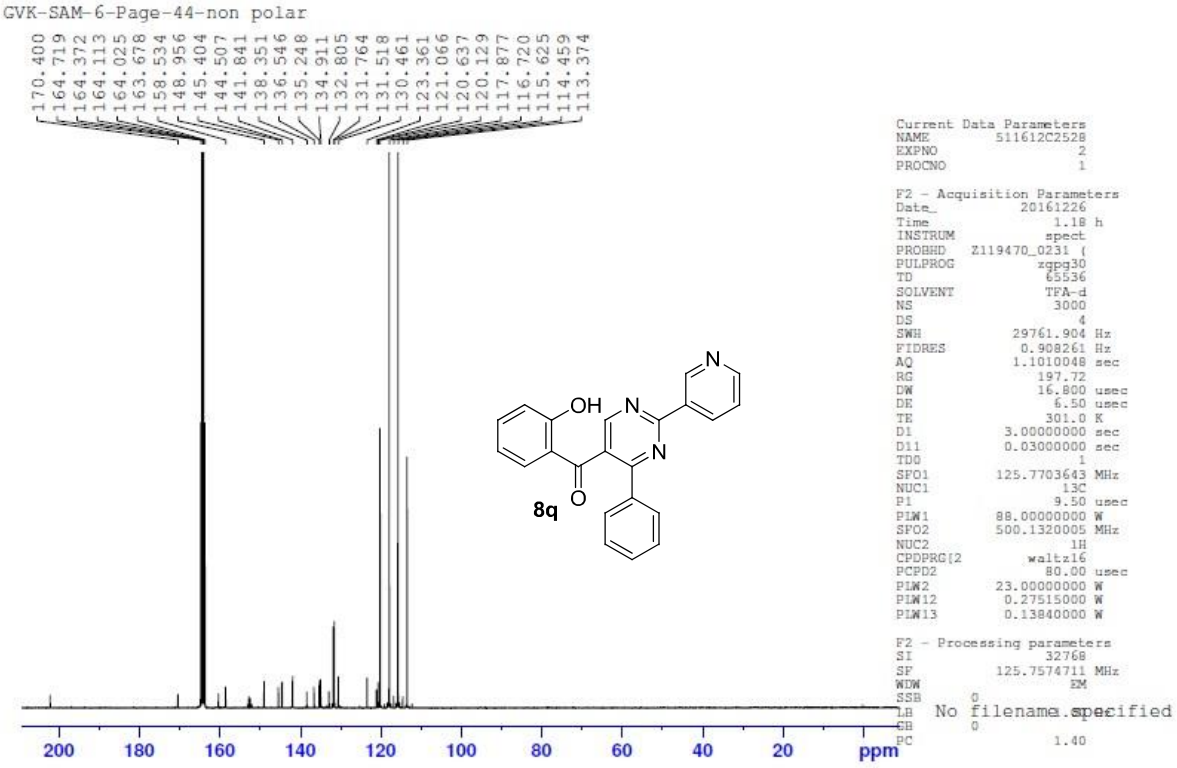
7q

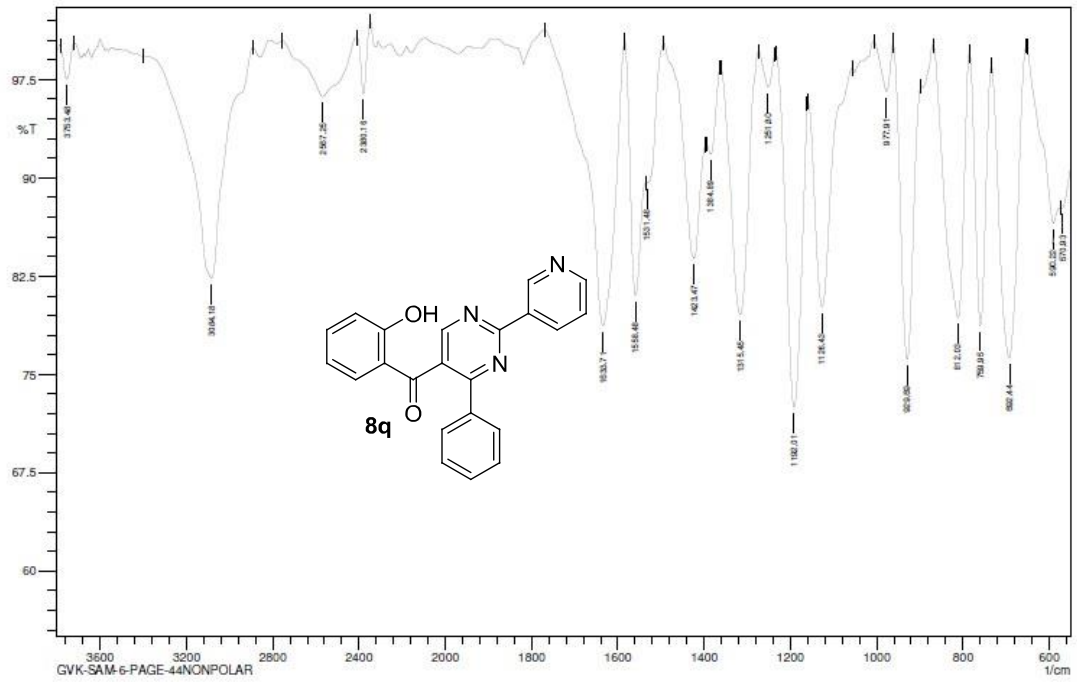
Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
354.1246	354.1243	0.3	0.8	16.5	687.7	C22 H16 N3 O2


GVK-SAm-6-Page-44P2
Reference Code: 511612A6173
Solvent: dmso
Archive directory:
/home/gvkbio/data/2016/Dec
Agilent 400-MRDD2
Data collected on: Dec 7 2016
Experiment: PROTON
OH
N
N
N
O
8q
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.96
0.92
0.83
2.00
2.59
1.04
4.05
2.03


GVK-SAm-6-Page-44P2
Reference Code: 511612A6173
Solvent: dmso
Archive directory:
/home/gvkbio/data/2016/Dec
Agilent 400-MRDD2
Data collected on: Dec 7 2016
Experiment: PROTON
10.782
9.645
9.641
9.004
8.868
8.864
8.853
8.848
8.843
8.808
8.804
8.796
8.793
8.341
7.701
7.698
7.693
7.678
7.673
7.660
7.607
7.560
7.555
7.539
7.535
7.446
7.431
7.416
7.399
7.392
7.387
7.377
7.169
6.853
6.840
6.824
6.820
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
ppm
0.96
0.92
0.83
2.00
2.59
1.04
4.05
2.03


GVK-SAM-6-Page-44-non polar
202.161
170.400
164.719
164.372
164.113
164.025
163.678
158.534
148.956
145.404
144.507
141.841
138.351
136.546
135.248
134.911
132.805
131.764
131.518
130.461
123.361
121.066
120.637
120.129
117.877
116.720
115.625
114.459
113.374
OH
N
N
N
O
8q
Current Data Parameters
NAME 511612C2528
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161226
Time 1.18 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT TFA-d
NS 3000
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 301.0 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7574711 MHz
WDW EM
SSB 0
LB 1
GB 0
PC 1.40
No filename specified
200
190
180
170
160
150
140
130
120
ppm


GVK-SAM-6-Page-44-non polar
170.400
164.719
164.372
164.113
164.025
163.678
158.534
148.956
145.404
144.507
141.841
138.351
136.546
135.248
134.911
132.805
131.764
131.518
130.461
123.361
121.066
120.637
120.129
117.877
116.720
115.625
114.459
113.374
OH
N
N
N
O
8q
Current Data Parameters
NAME 511612C2528
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161226
Time 1.18 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT TFA-d
NS 3000
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 301.0 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7574711 MHz
WDW EM
SSB 0
LB 1
GB 0
PC 1.40
No filename specified
200
180
160
140
120
100
80
60
40
20
ppm



Comment: IN Kbr
GVK-SAM-6-PAGE-44NONPOLAR

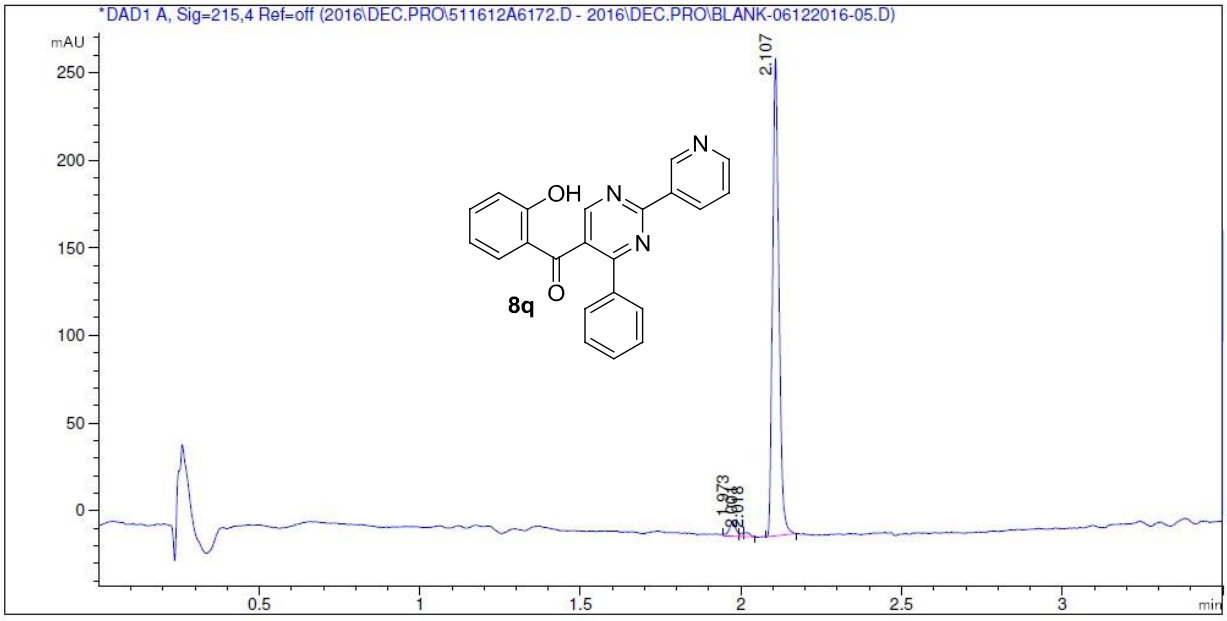
No. of Scans:
Resolution:
Apodization:

Date: 12/22/2016 11:34:09 AM
User: Admin

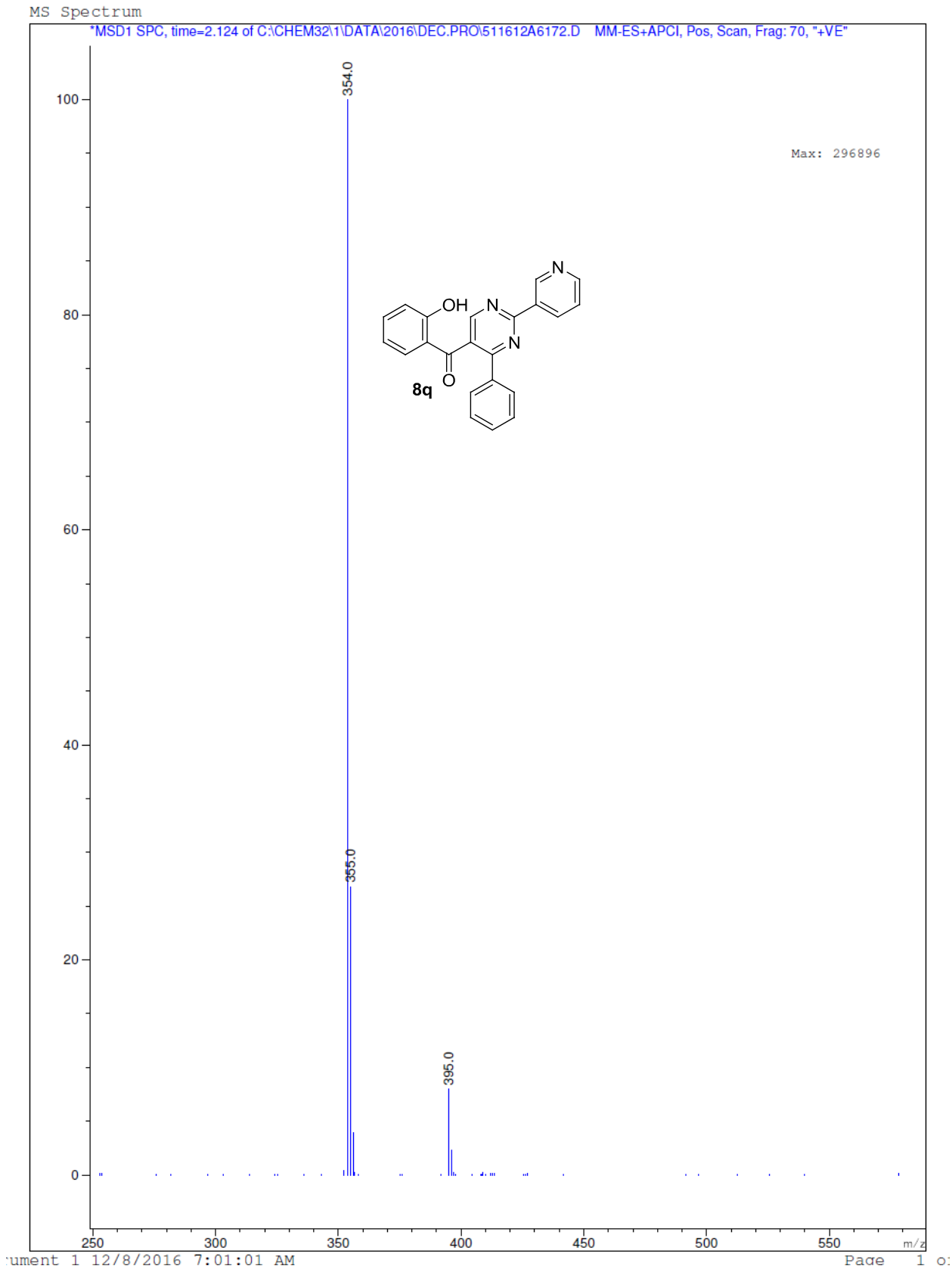
GVK BIOSCIENCES PVT. LTD.
MEDICINAL CHEMISTRY LABORATORY - ANALYTICAL RESEARCH
LCMS REPORT

Vial position : P2-C-02
Date of Analysis :12/7/2016 9:51:46 PM Injection Vol : 0.300uL
Acq. Method :C:\CHEM32\1\METHODS\RND-FA- 3.5 MIN.M Instrument ID :ANL-MCL5-LCMS-001
Sample Name : GVK-SAM-6-PAGE-44P2

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, 0.4/2, 2.8/98,3.4/98,3.41/2,3.5/2
Column Flow Rate: 0.6 ml/min
Column Temperature: 60°C ->



Pea No	RT min	Area	Area %
1	1.97	11.699	2.999
2	2.00	1.353	0.347
3	2.02	3.040	0.779
4	2.11	374.036	95.875

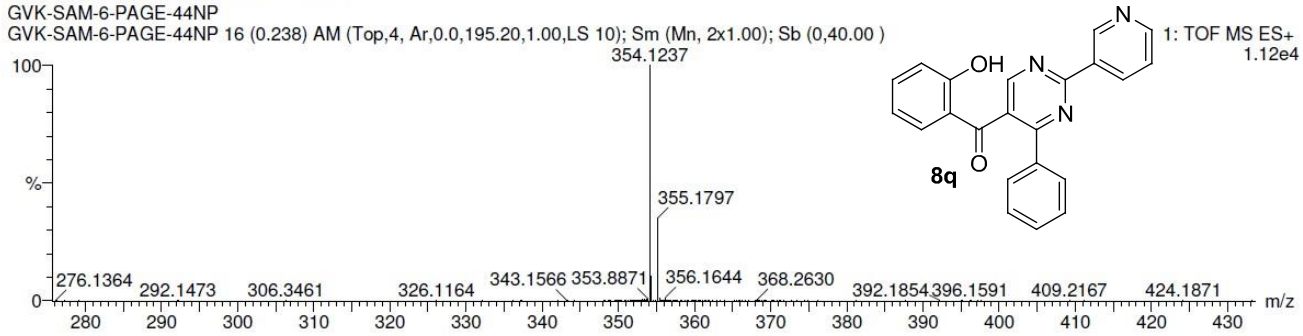

MS Spectrum
*MSD1 SPC, time=2.124 of C:\CHEM32\1\DATA\2016\DEC.PRO\511612A6172.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
Max: 296896
354.0
355.0
395.0
OH
N
N
N
O
8q
100
80
60
40
20
0
250
300
350
400
450
500
550
m/z
ument 1 12/8/2016 7:01:01 AM
Page 1 o

Single Mass Analysis

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

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: 0-22 H: 0-16 N: 0-3 O: 0-2

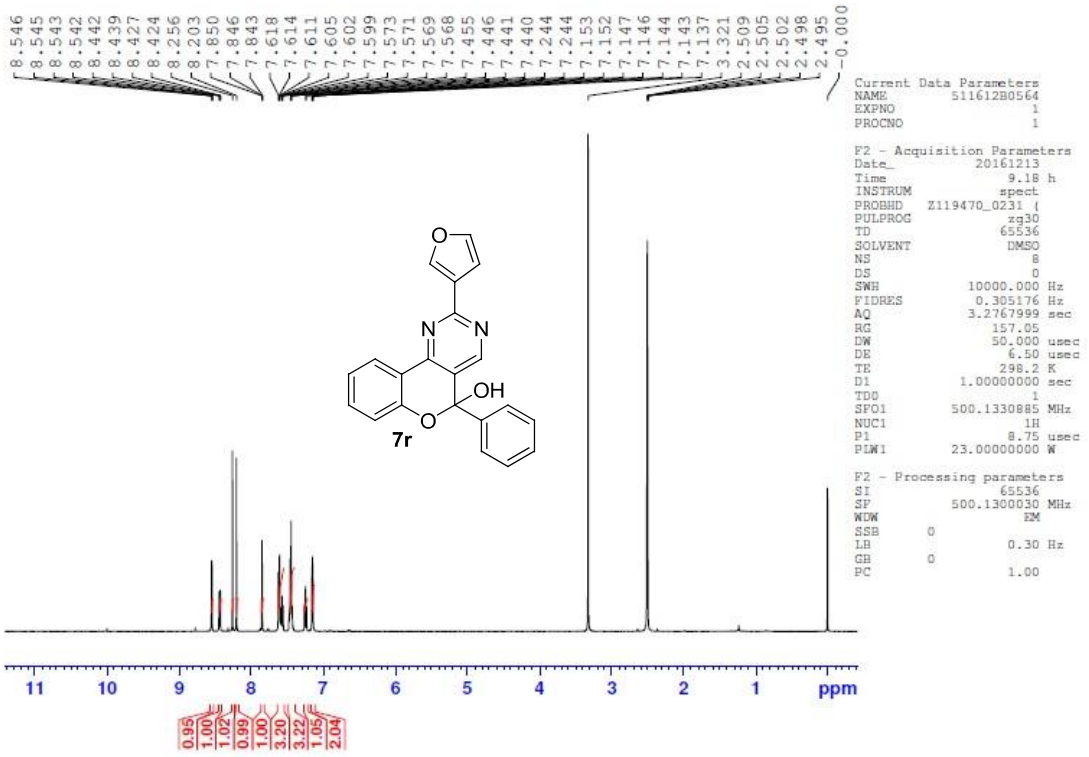
GVK-SAM-6-PAGE-44NP
GVK-SAM-6-PAGE-44NP 16 (0.238) AM (Top,4, Ar,0.0,195.20,1.00,LS 10); Sm (Mn, 2x1.00); Sb (0,40.00)



8q

Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
354.1237	354.1243	-0.6	-1.7	16.5	678.0	C22 H16 N3 O2

GVK-SAM-6-PAGE-47 POLAR

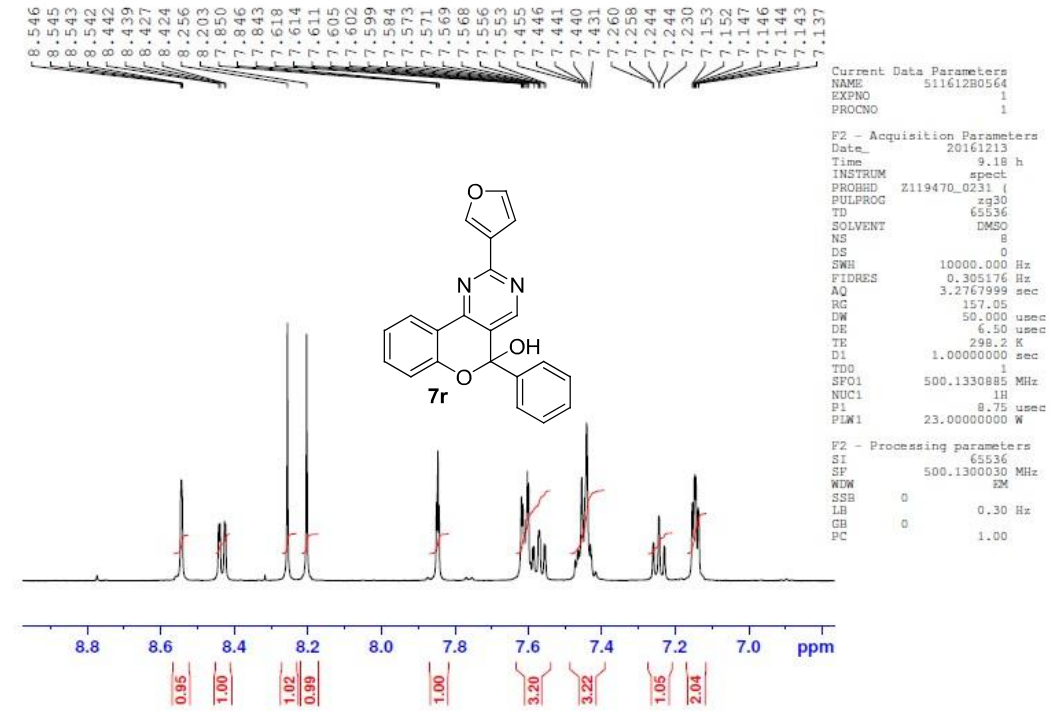


Current Data Parameters
NAME 511612B0564
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161213
Time 9.18 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 157.05
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.1330885 MHz
NUC1 1H
P1 8.75 usec
PLW1 23.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1300030 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

GVK-SAM-6-PAGE-47 POLAR

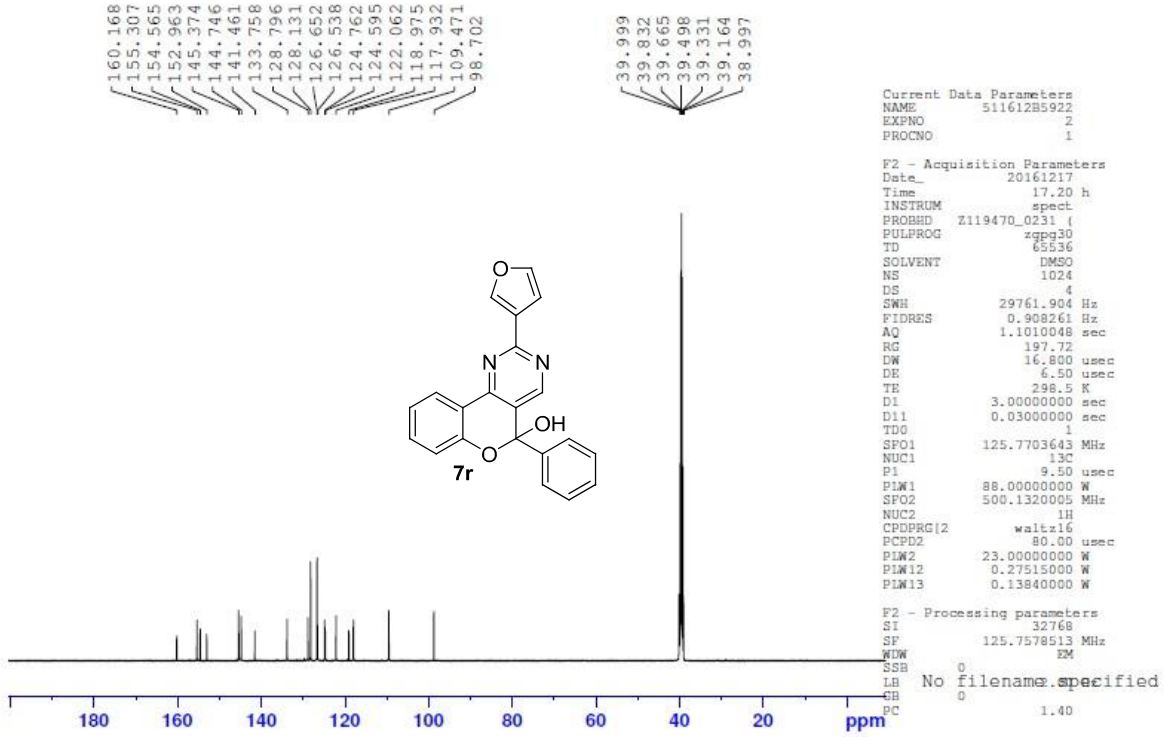


Current Data Parameters
NAME 511612B0564
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20161213
Time 9.18 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 8
DS 0
SWH 10000.000 Hz
FIDRES 0.305176 Hz
AQ 3.2767999 sec
RG 157.05
DW 50.000 usec
DE 6.50 usec
TE 298.2 K
D1 1.00000000 sec
TD0 1
SFO1 500.1330885 MHz
NUC1 1H
P1 8.75 usec
PLW1 23.00000000 W

F2 - Processing parameters
SI 65536
SF 500.1300030 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

GVK-SAM-6-PAGE-47 POLAR

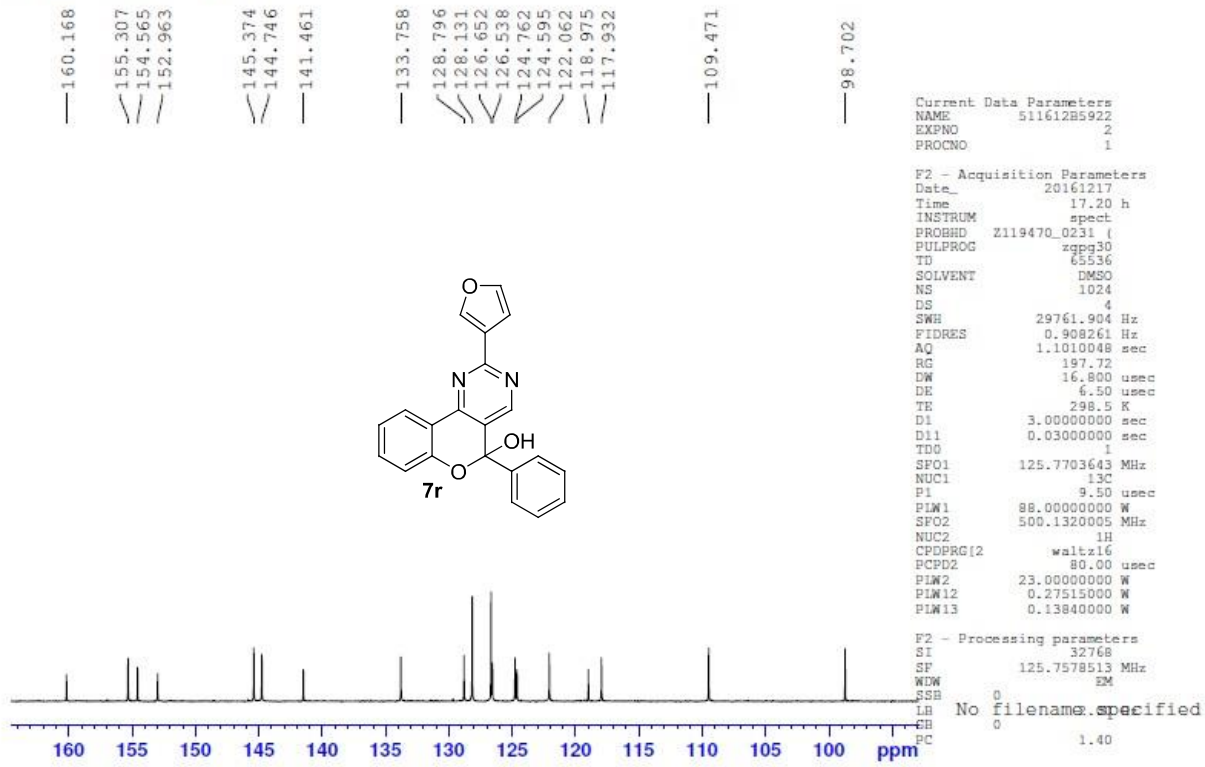



```
Current Data Parameters
NAME          511612B5922
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20161217
Time               17.20 h
INSTRUM             spect
PROBHD    Z119470_0231 (
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                  1024
DS                     4
SWH            29761.904 Hz
FIDRES          0.908261 Hz
AQ              1.1010048 sec
RG                 197.72
DW                 16.800 usec
DE                  6.50 usec
TE                 298.5 K
D1              3.00000000 sec
D11             0.03000000 sec
TD0                    1
SFO1           125.7703643 MHz
NUC1                  13C
P1                  9.50 usec
PLW1           88.00000000 W
SFO2           500.1320005 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2           23.00000000 W
PLW12           0.27515000 W
PLW13           0.13840000 W

F2 - Processing parameters
SI                  32768
SF            125.7578513 MHz
WDW                    EM
SSB                    0
LB   No filename specified
GB                     0
PC                  1.40
```

GVK-SAM-6-PAGE-47 POLAR

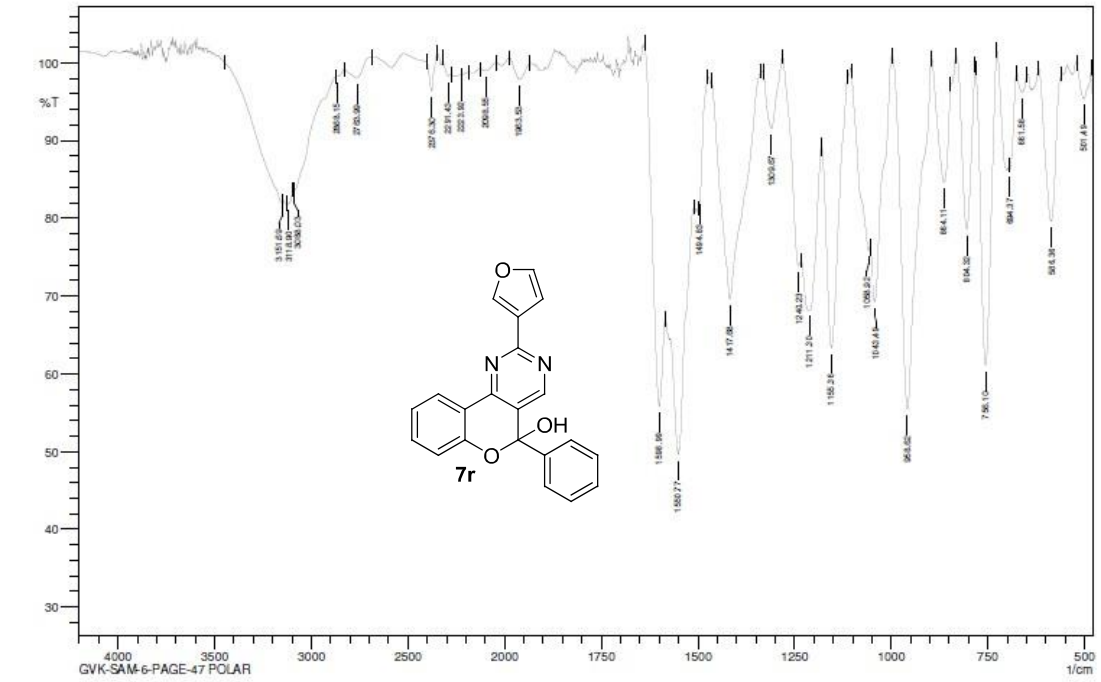



```
Current Data Parameters
NAME          511612B5922
EXPNO                   2
PROCNO                  1

F2 - Acquisition Parameters
Date_           20161217
Time               17.20 h
INSTRUM             spect
PROBHD    Z119470_0231 (
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                  1024
DS                     4
SWH            29761.904 Hz
FIDRES          0.908261 Hz
AQ              1.1010048 sec
RG                 197.72
DW                 16.800 usec
DE                  6.50 usec
TE                 298.5 K
D1              3.00000000 sec
D11             0.03000000 sec
TD0                    1
SFO1           125.7703643 MHz
NUC1                  13C
P1                  9.50 usec
PLW1           88.00000000 W
SFO2           500.1320005 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2           23.00000000 W
PLW12           0.27515000 W
PLW13           0.13840000 W

F2 - Processing parameters
SI                  32768
SF            125.7578513 MHz
WDW                    EM
SSB                    0
LB   No filename specified
GB                     0
PC                  1.40
```

SHIMADZU



Comment: IN Kbr
GVK-SAM-6-PAGE-47 POLAR

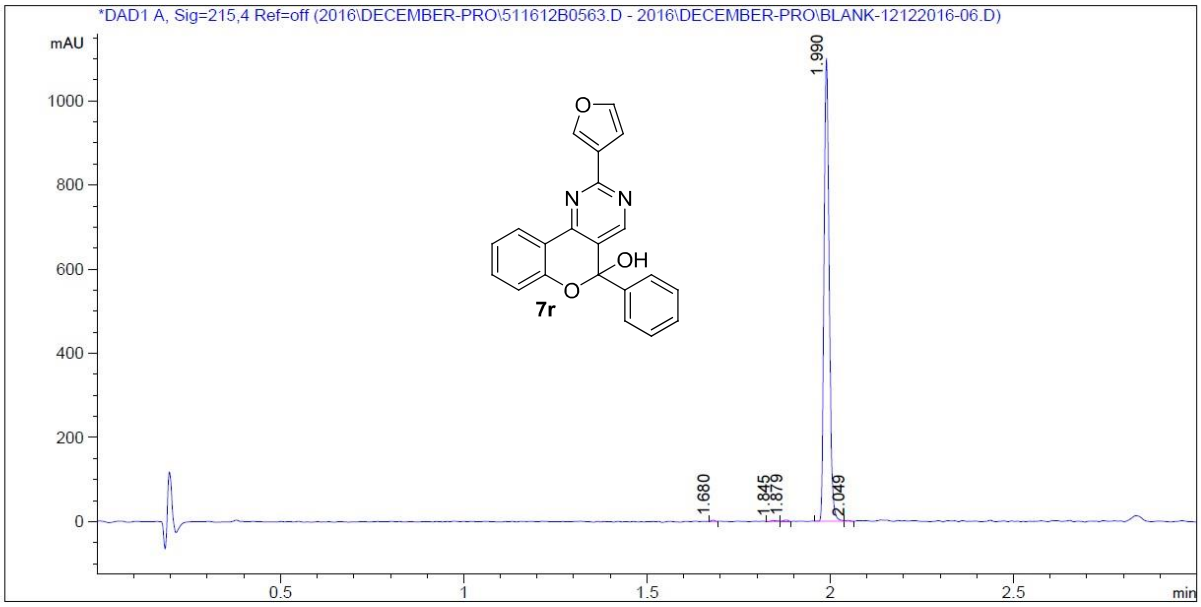
No. of Scans:
Resolution:
Apodization:

Date: 12/22/2016 11:36:54 AM
User: Admin

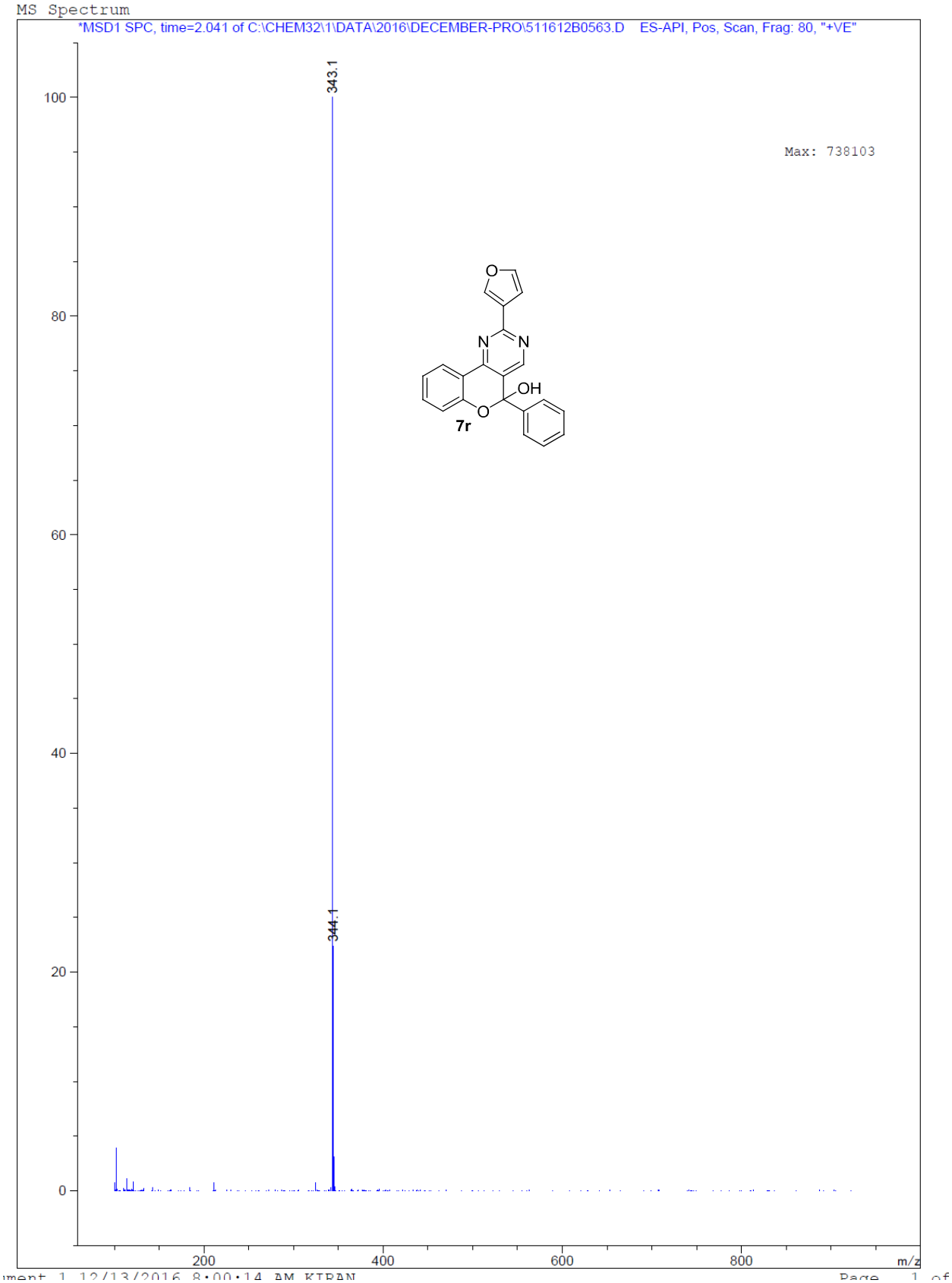
MEDICINAL CHEMISTRY LABORATORY - ANALYTICAL RESEARCH

```
================================================================================================
Date of Analysis: 12/12/2016   9:55:06 PM            Vial Position  :P1-E-04
Acq. Method     :   RND-FA-3.0-MIN                   Injection Vol : 0.500       ul
                                                     Instrument ID  :ANL-MCL3-LCMS-003
Sample Name     :GVK-SAM-6-PAGE-47-POLAR
================================================================================================
 GVK_LCMS_18

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



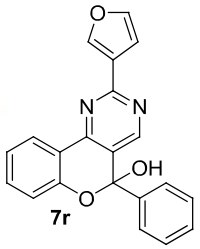
Peak No	RT min	Area	Area %
1	1.680	2.073	0.191
2	1.845	2.534	0.233
3	1.879	2.702	0.248
4	1.990	1078.659	99.161
5	2.049	1.820	0.167


MS Spectrum
*MSD1 SPC, time=2.041 of C:\CHEM32\1\DATA\2016\DECEMBER-PRO\511612B0563.D ES-API, Pos, Scan, Frag: 80, "+VE"
343.1
344.1
Max: 738103
7r
100
80
60
40
20
0
200
400
600
800
m/z

Single Mass Analysis

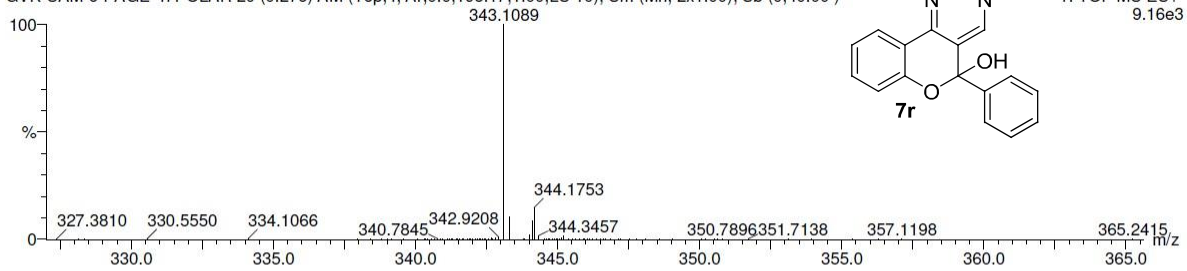
Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

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: 0-21 H: 0-15 N: 0-2 O: 0-3
GVK-SAM-6-PAGE-47POLAR
GVK-SAM-6-PAGE-47POLAR 20 (0.276) AM (Top,4, Ar,0.0,195.17,1.00,LS 10); Sm (Mn, 2x1.00); Sb (0,40.00)



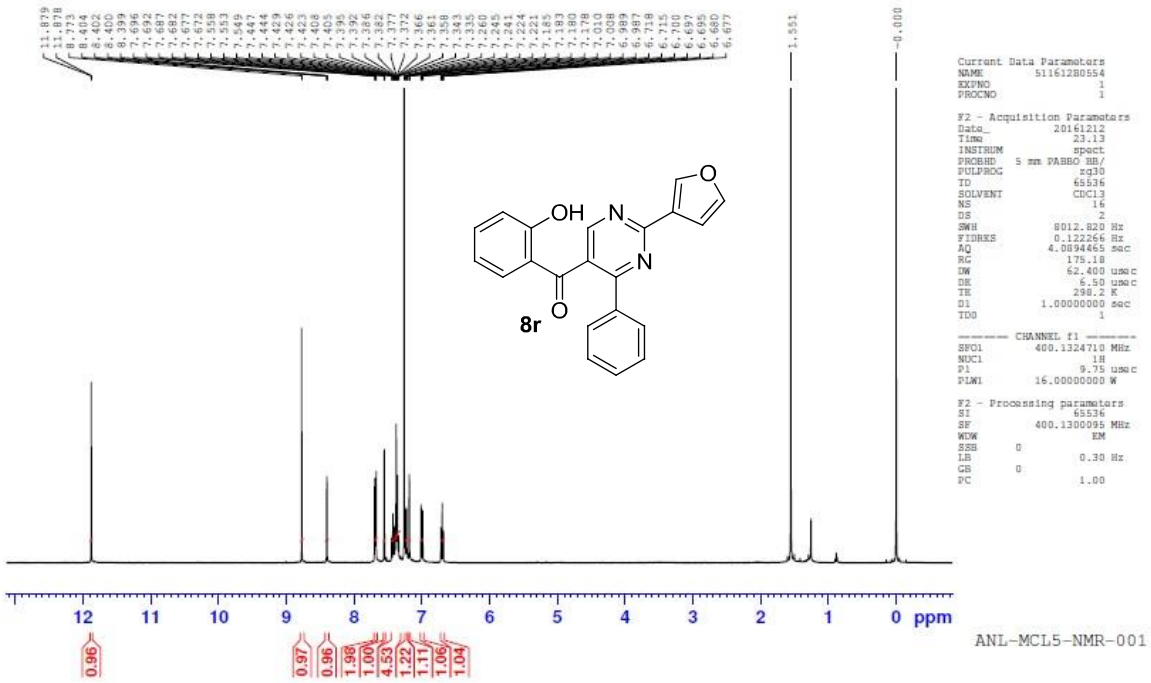
7r

1: TOF MS ES+
9.16e3

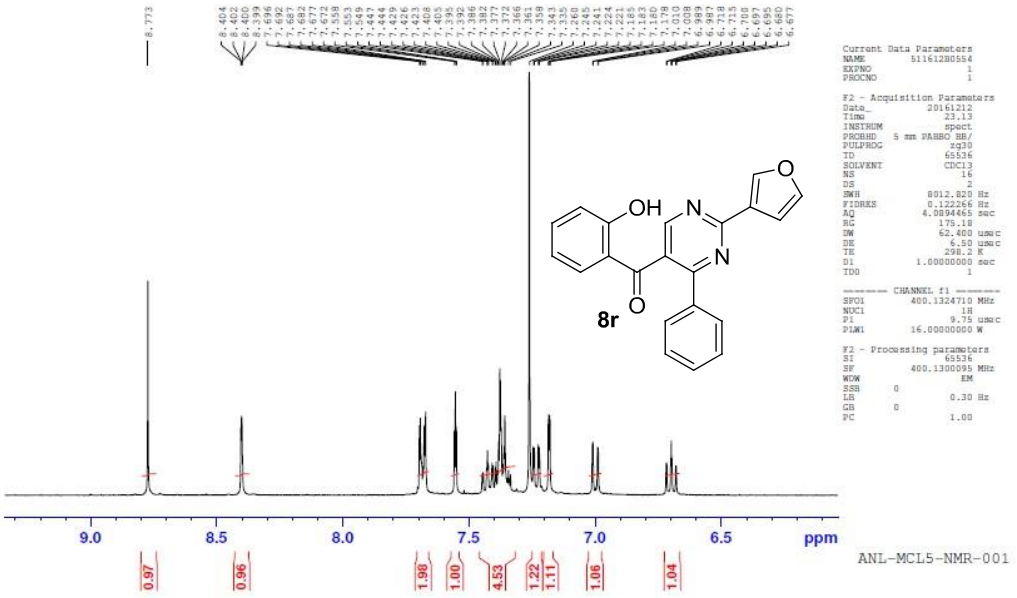


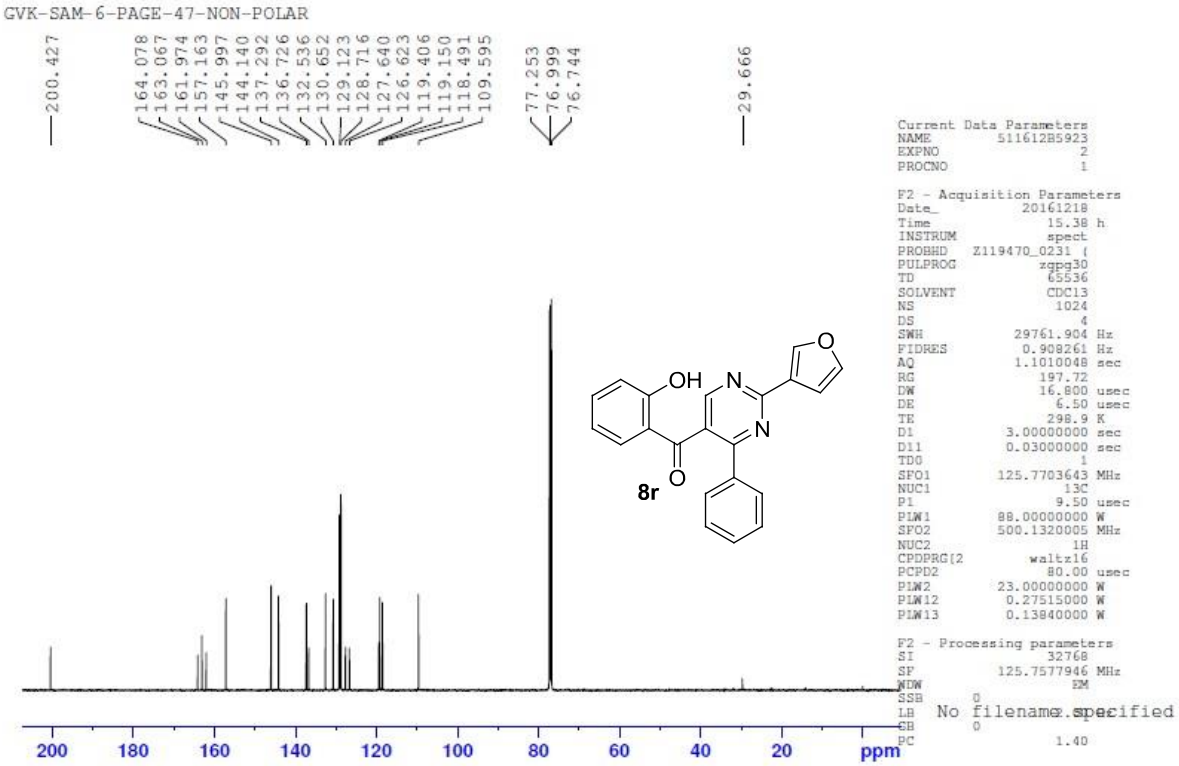
Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
343.1089	343.1083	0.6	1.7	15.5	435.3	C21 H15 N2 O3

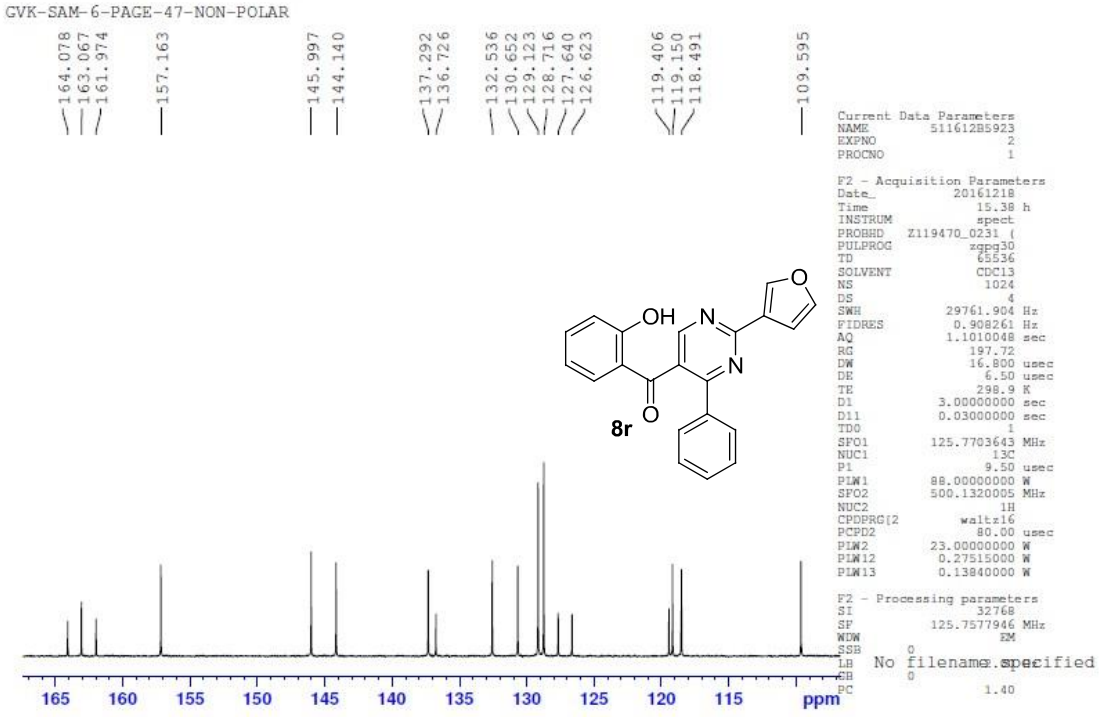
gvk-sam-6-page-47np

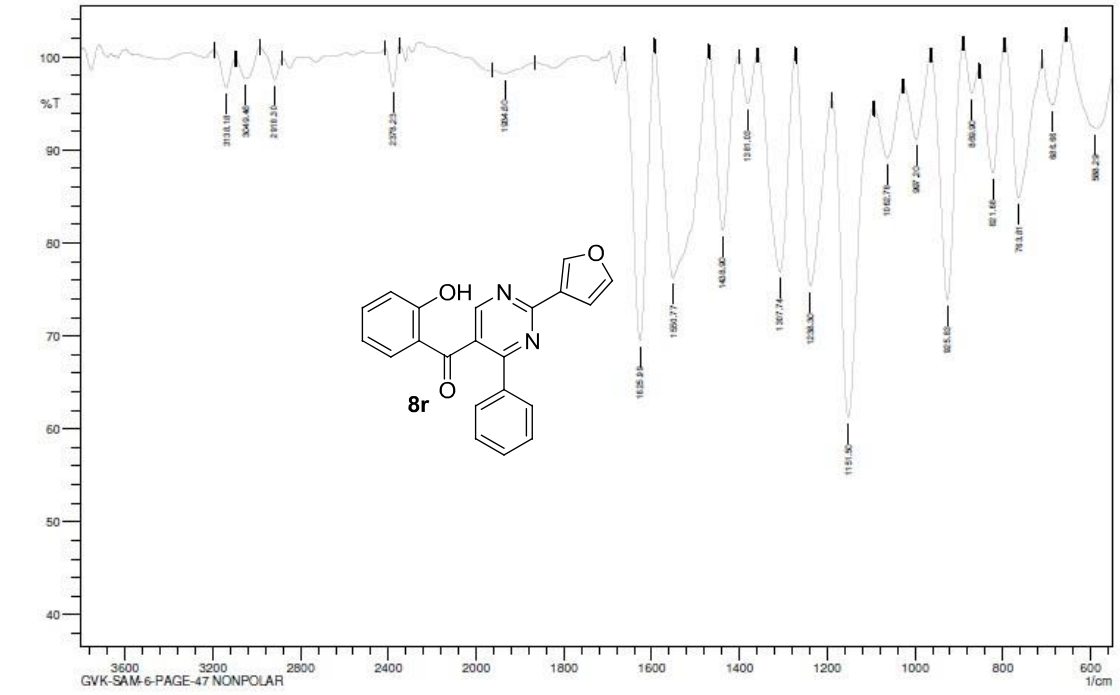


gvk-sam-6-page-47np




GVK-SAM-6-PAGE-47-NON-POLAR
200.427
164.078
163.067
161.974
157.163
145.997
144.140
137.292
136.726
132.536
130.652
129.123
128.716
127.640
126.623
119.406
119.150
118.491
109.595
77.253
76.999
76.744
29.666
OH
N
N
O
O
8r
200
180
160
140
120
100
80
60
40
20
ppm
Current Data Parameters
NAME 511612B5923
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161218
Time 15.38 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 298.9 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7577946 MHz
WDW EM
SSB 0
LB No filename specified
GB 0
PC 1.40


GVK-SAM-6-PAGE-47-NON-POLAR
164.078
163.067
161.974
157.163
145.997
144.140
137.292
136.726
132.536
130.652
129.123
128.716
127.640
126.623
119.406
119.150
118.491
109.595
OH
N
N
O
O
8r
165
160
155
150
145
140
135
130
125
120
115
ppm
Current Data Parameters
NAME 511612B5923
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161218
Time 15.38 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 298.9 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7577946 MHz
WDW EM
SSB 0
LB No filename specified
GB 0
PC 1.40



Comment: IN Kbr
GVK-SAM-6-PAGE-47 NONPOLAR

No. of Scans:
Resolution:
Apodization:

Date: 12/22/2016 11:26:18 AM
User: Admin

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

LCMS REPORT

==========

Sample Name :GVK-SAM-6-PAGE-47-NP Vial Position :P1-A-01
Date of Analysis: 13/12/2016; 5:37:18 PM Injection Vol :0.3 µL
Acq. Method :RND-FA-3.5-MIN Instrument ID :ANL-MCL5-LCMS-001

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GVK_LCMS_31

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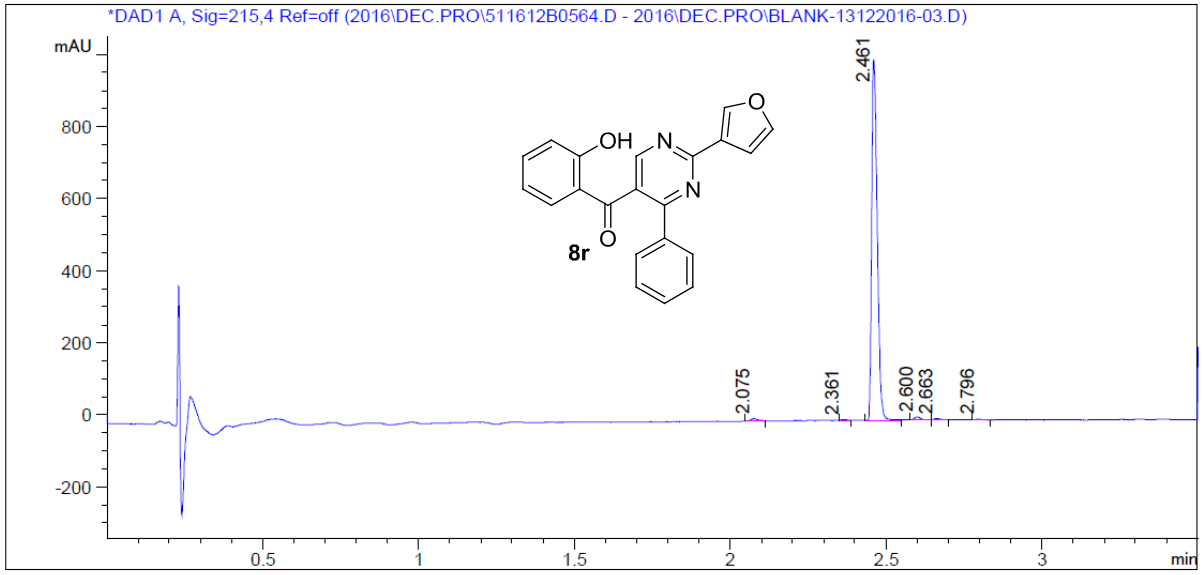
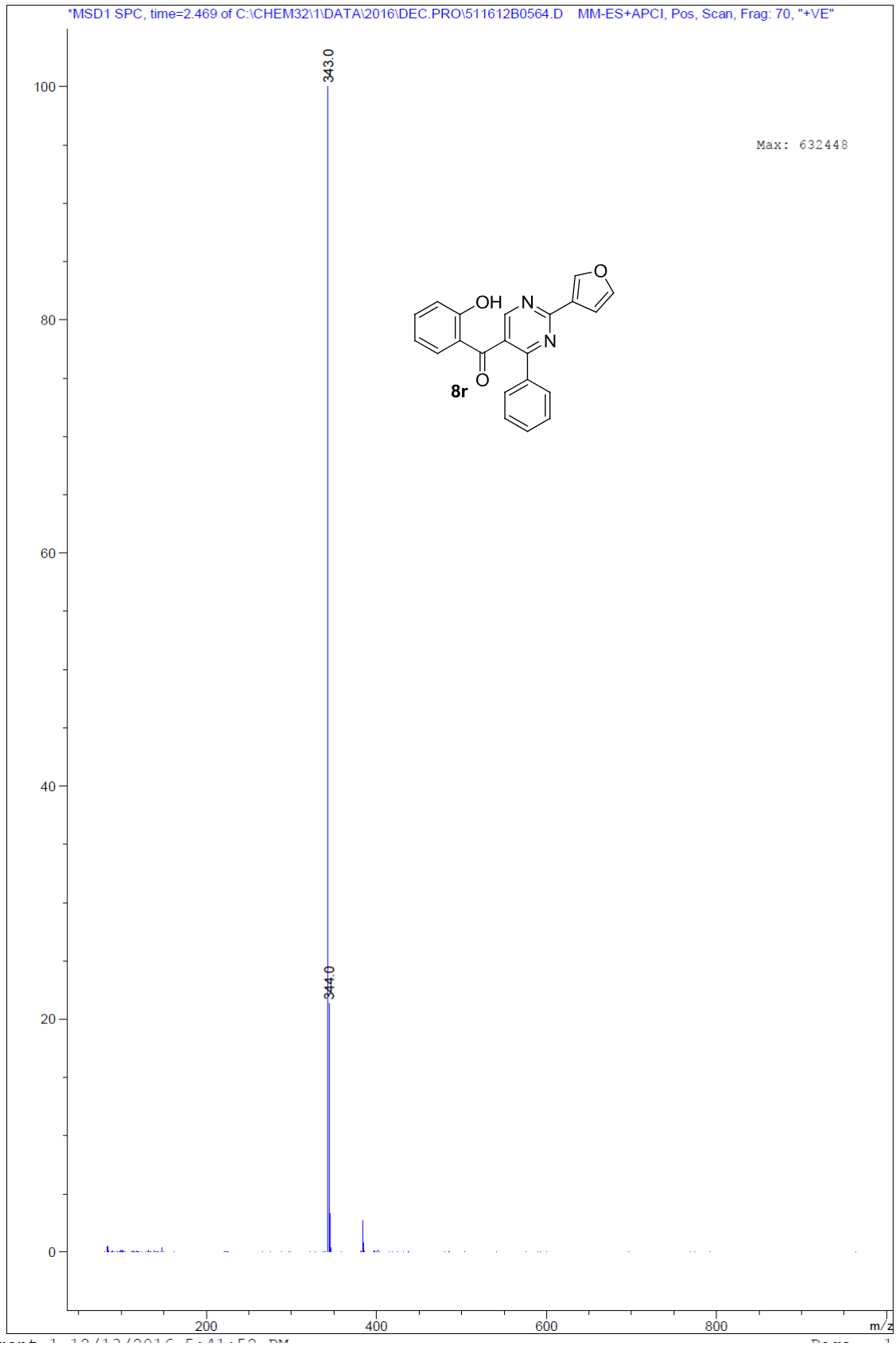


Pea No	RT min	Area	Area %
1	2.08	10.457	0.824
2	2.36	2.451	0.193
3	2.46	1.236e3	97.377
4	2.60	12.624	0.995
5	2.66	5.219	0.411
6	2.80	2.543	0.200

MS Spectrum

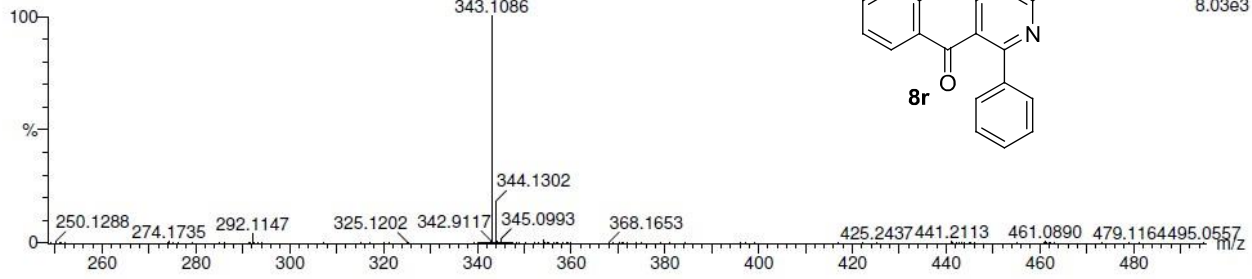

*MSD1 SPC, time=2.469 of C:\CHEM32\1\DATA\2016\DEC.PRO\511612B0564.D MM-ES+APCI, Pos, Scan, Frag: 70, "+VE"
343.0
344.0
Max: 632448
OH
N
N
O
O
8r
100
80
60
40
20
0
200
400
600
800
m/z

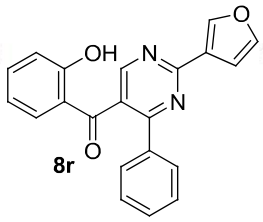
Single Mass Analysis

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

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: 0-21 H: 0-15 N: 0-2 O: 0-3

GVK-SAM-6-PAGE-47NP
GVK-SAM-6-PAGE-47NP 26 (0.370) AM (Top,4, Ar,0.0,195.17,1.00,LS 10); Sm (Mn, 2x1.00); Sb (0,40.00)

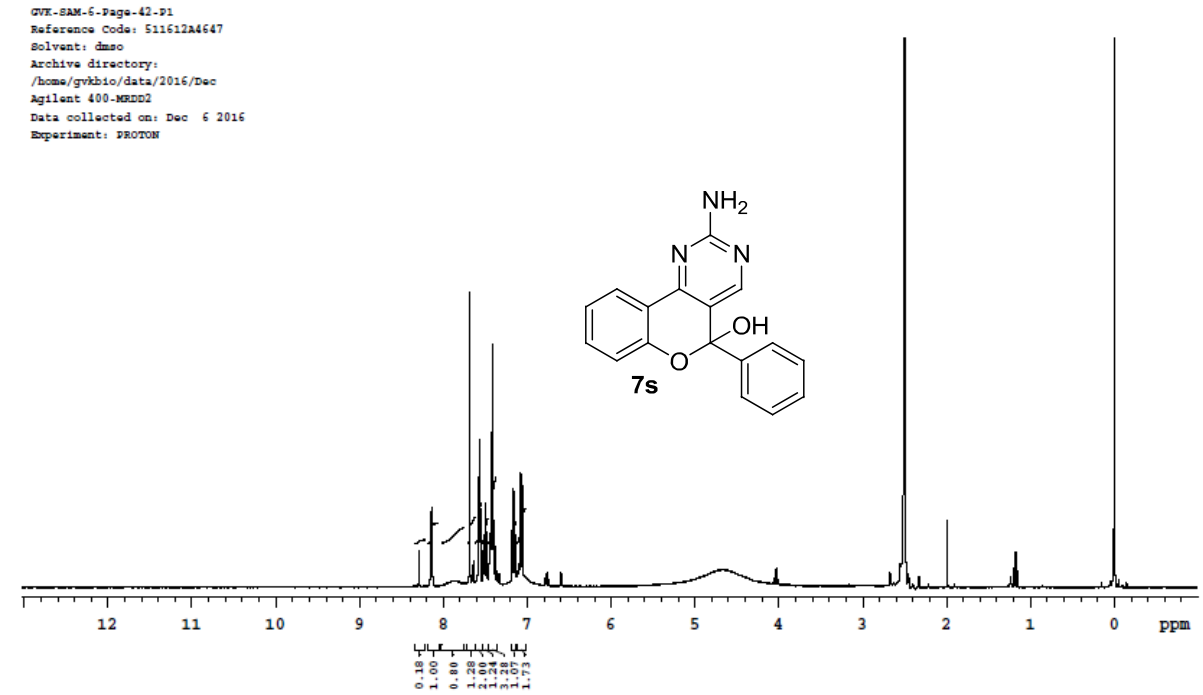


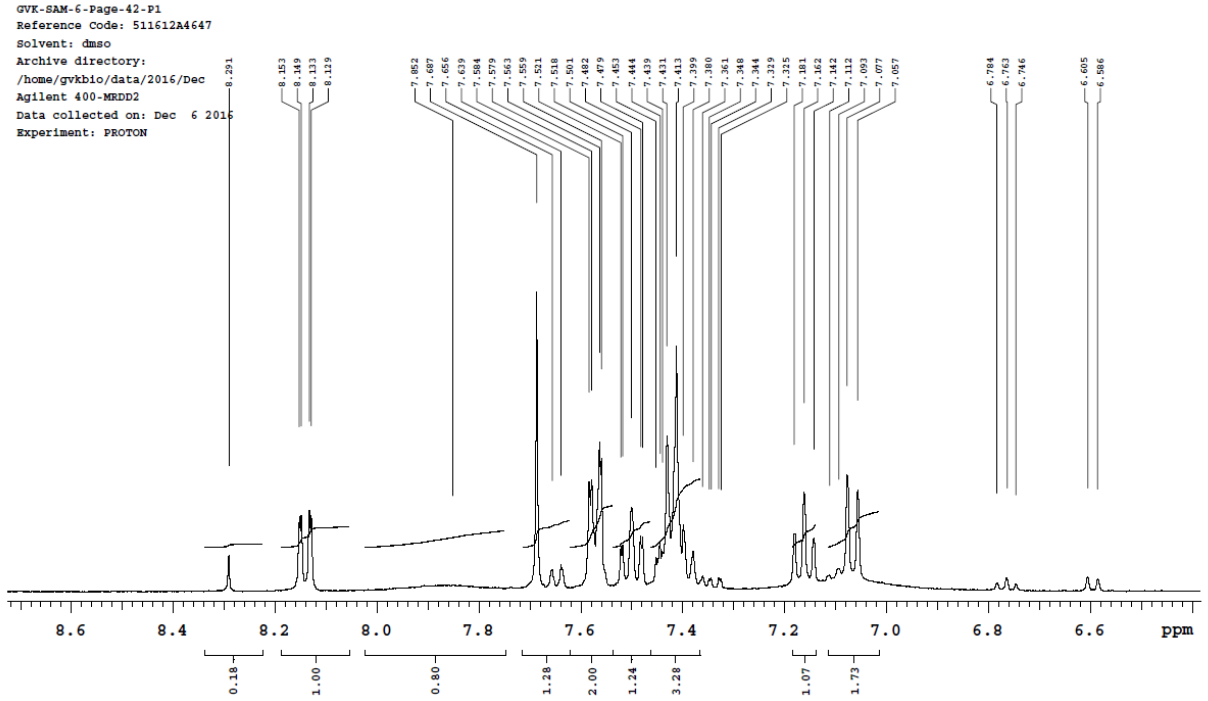


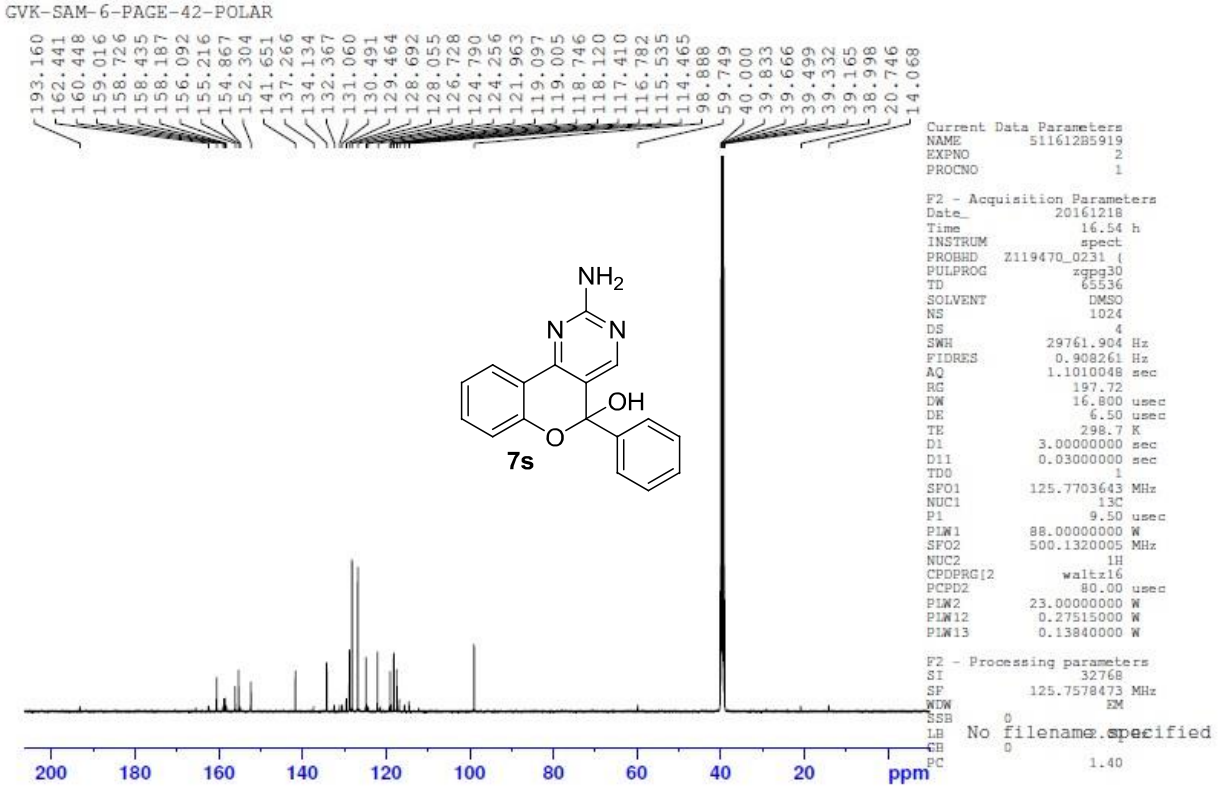
8r

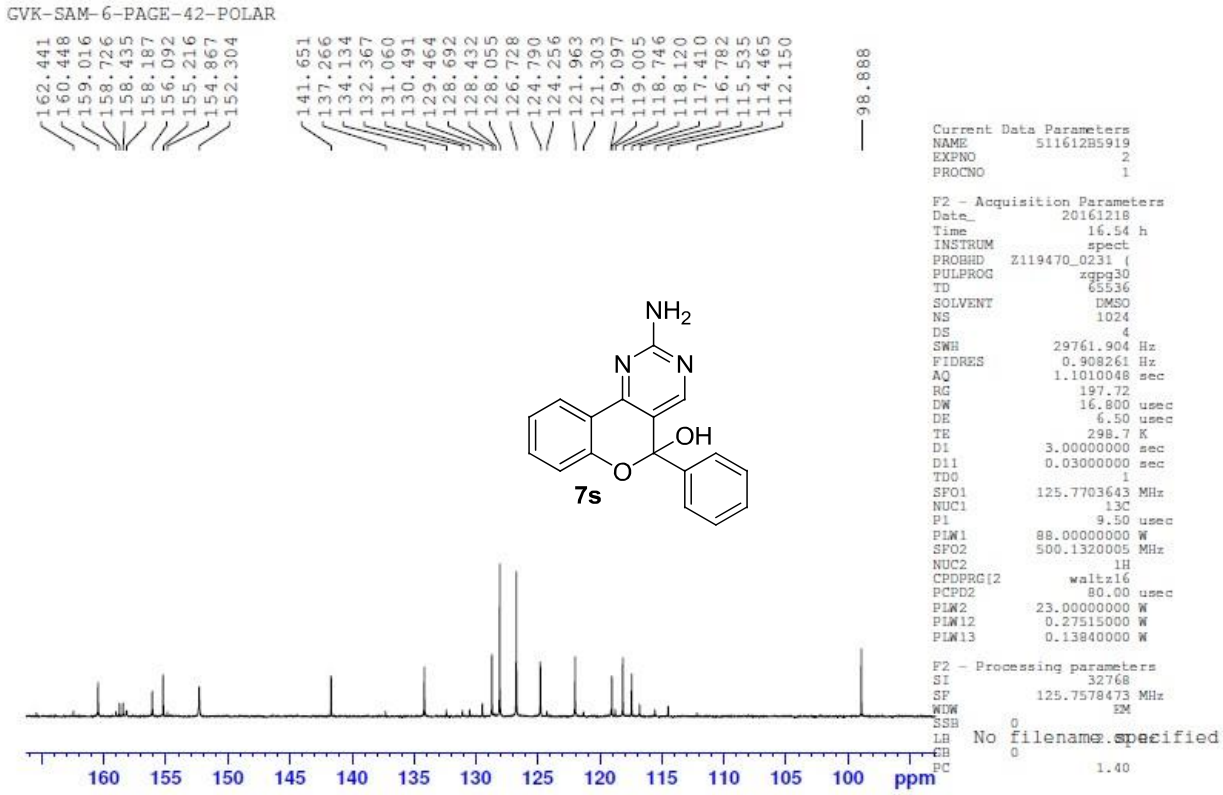
1: TOF MS ES+
8.03e3

Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
343.1086	343.1083	0.3	0.9	15.5	126.0	C21 H15 N2 O3

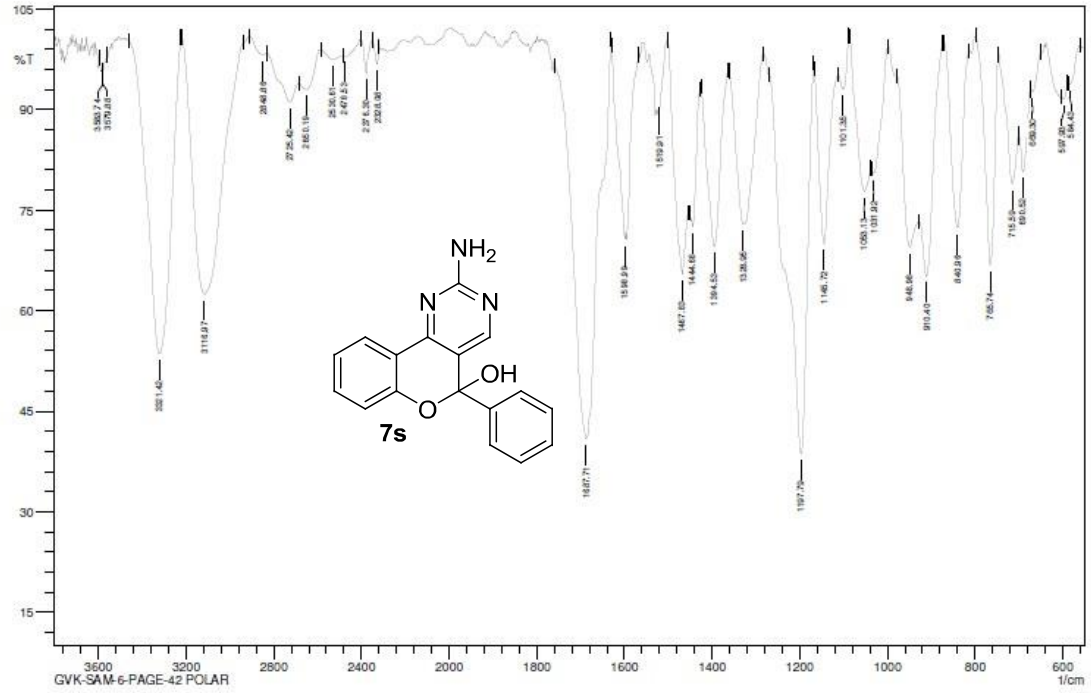

GVK-SAM-6-Page-42-P1
Reference Code: 511612A4647
Solvent: dmso
Archive directory:
/home/gvkbio/data/2016/Dec
Agilent 400-MRDD2
Data collected on: Dec 6 2016
Experiment: PROTON
NH2
N
N
OH
O
7s
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.18
1.00
0.80
1.28
2.00
1.24
3.28
1.07
1.73


GVK-SAM-6-Page-42-P1
Reference Code: 511612A4647
Solvent: dmso
Archive directory:
/home/gvkbio/data/2016/Dec
Agilent 400-MRDD2
Data collected on: Dec 6 2016
Experiment: PROTON
8.291
8.153
8.149
8.133
8.129
7.852
7.687
7.656
7.639
7.584
7.579
7.563
7.559
7.521
7.518
7.501
7.482
7.479
7.453
7.444
7.439
7.431
7.413
7.399
7.380
7.361
7.348
7.344
7.329
7.325
7.181
7.162
7.142
7.112
7.093
7.077
7.057
6.784
6.763
6.746
6.605
6.586
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
ppm
0.18
1.00
0.80
1.28
2.00
1.24
3.28
1.07
1.73


GVK-SAM-6-PAGE-42-POLAR
193.160
162.441
160.448
159.016
158.726
158.435
158.187
156.092
155.216
154.867
152.304
141.651
137.266
134.134
132.367
131.060
130.491
129.464
128.692
128.055
126.728
124.790
124.256
121.963
119.097
119.005
118.746
118.120
117.410
116.782
115.535
114.465
98.888
59.749
40.000
39.833
39.666
39.499
39.332
39.165
38.998
20.746
14.068
NH2
N
N
OH
O
7s
Current Data Parameters
NAME 511612B5919
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161218
Time 16.54 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 298.7 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7578473 MHz
WDW EM
SSB 0
LB No filename specified
GB 0
PC 1.40
200
180
160
140
120
100
80
60
40
20
ppm


GVK-SAM-6-PAGE-42-POLAR
162.441
160.448
159.016
158.726
158.435
158.187
156.092
155.216
154.867
152.304
141.651
137.266
134.134
132.367
131.060
130.491
129.464
128.692
128.432
128.055
126.728
124.790
124.256
121.963
121.303
119.097
119.005
118.746
118.120
117.410
116.782
115.535
114.465
112.150
98.888
NH2
N
N
OH
O
7s
Current Data Parameters
NAME 511612B5919
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161218
Time 16.54 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 1024
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 298.7 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7578473 MHz
WDW EM
SSB 0
LB No filename specified
GB 0
PC 1.40
160
155
150
145
140
135
130
125
120
115
110
105
100
ppm

SHIMADZU



Comment: IN Kbr
GVK-SAM-6-PAGE-42 POLAR

No. of Scans:
Resolution:
Apodization:

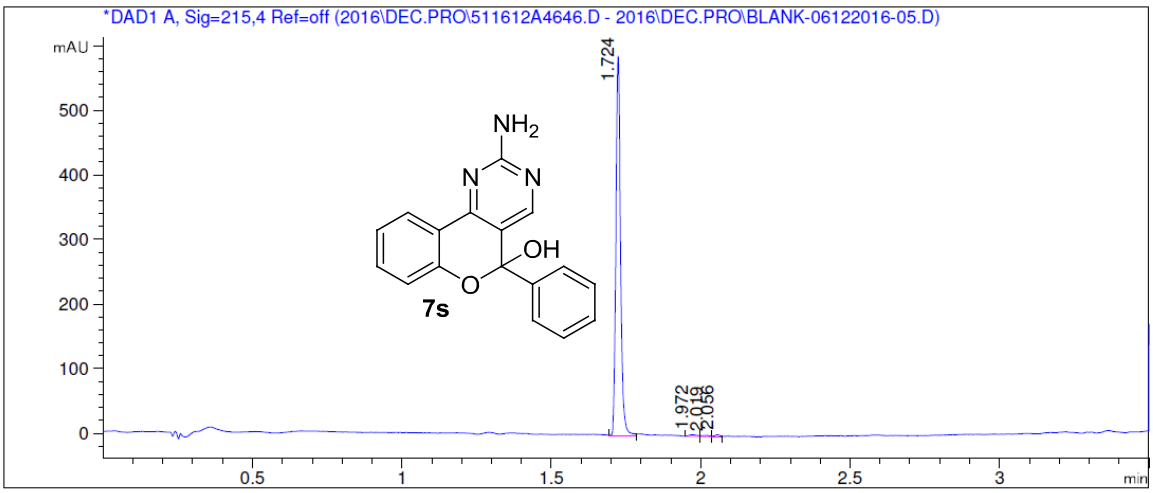
Date: 12/22/2016 11:40:06 AM
User: Admin

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

LCMS REPORT

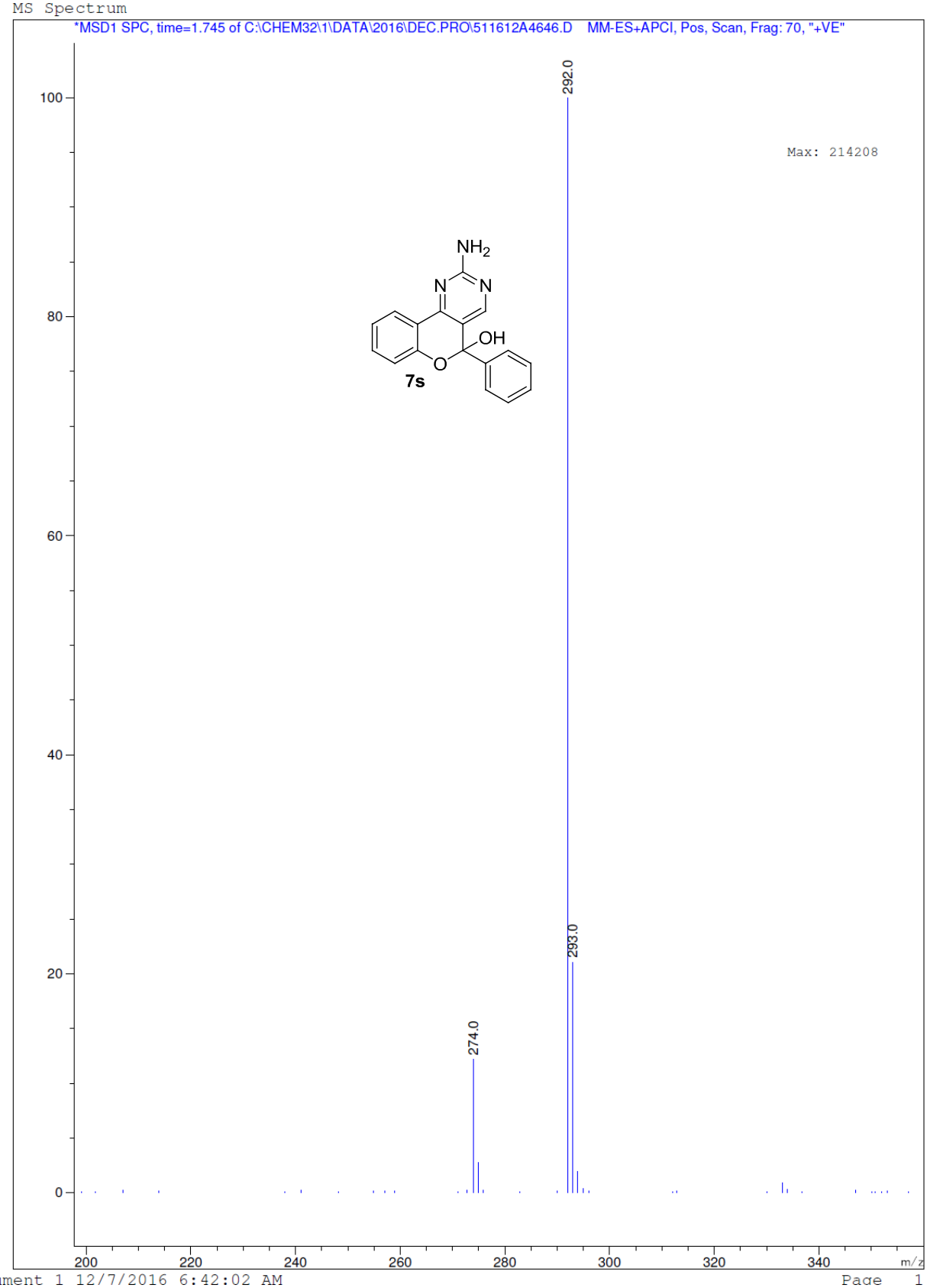
Sample Name : GVK-SAM-6-PAGE-12-P1 Vial Position :P1-B-09
Date of Analysis: 06/12/2016; 9:24:45 PM Injection Vol :Actual ->
Acq. Method :RND-FA-3.5-MIN Instrument ID :ANL-MCL5-LCMS-001

GVK_LCMS_31



Pea No	RT min	Area	Area %
1	1.72	627.993	98.146
2	1.97	4.990	0.780
3	2.02	3.045	0.476
4	2.06	3.830	0.599

MS Spectrum



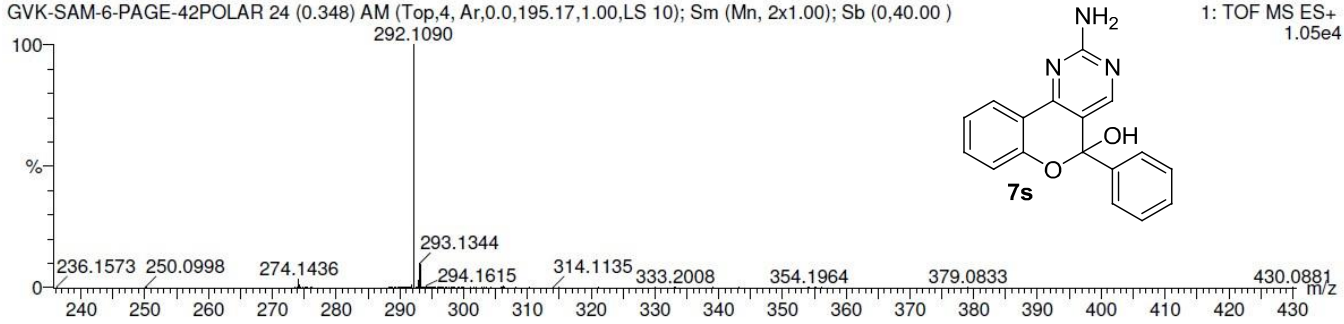
ument 1 12/7/2016 6:42:02 AM Page 1 o

Single Mass Analysis

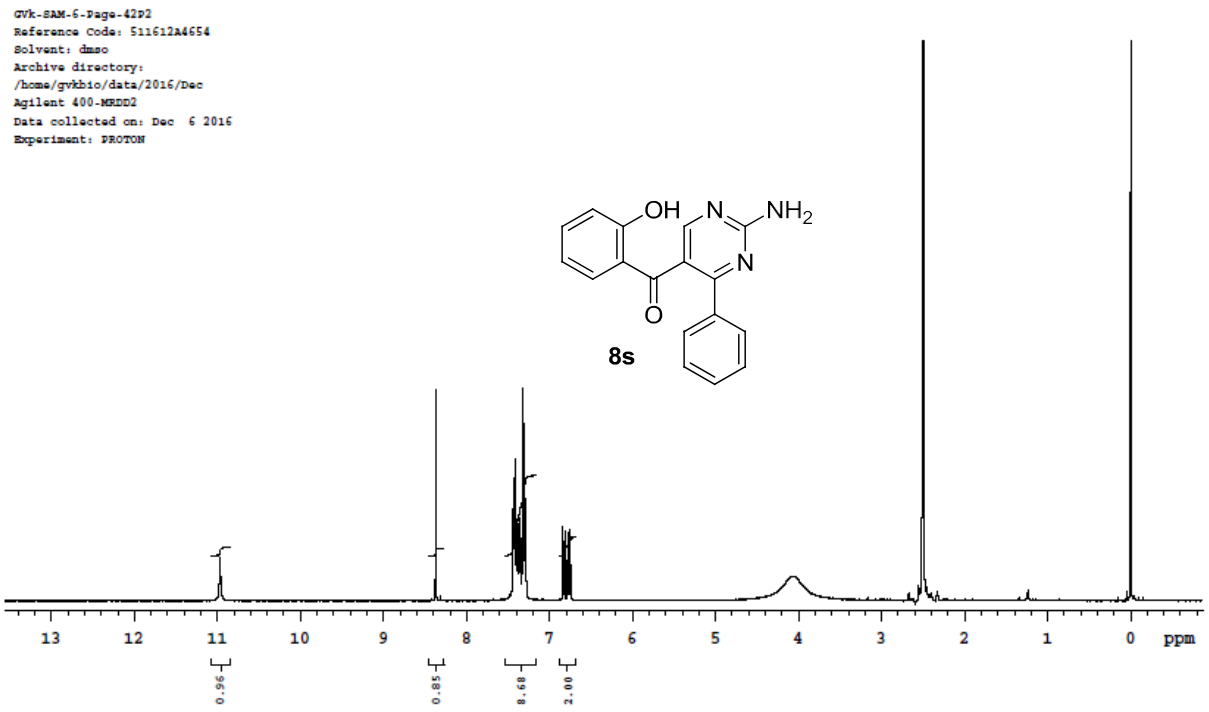
Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

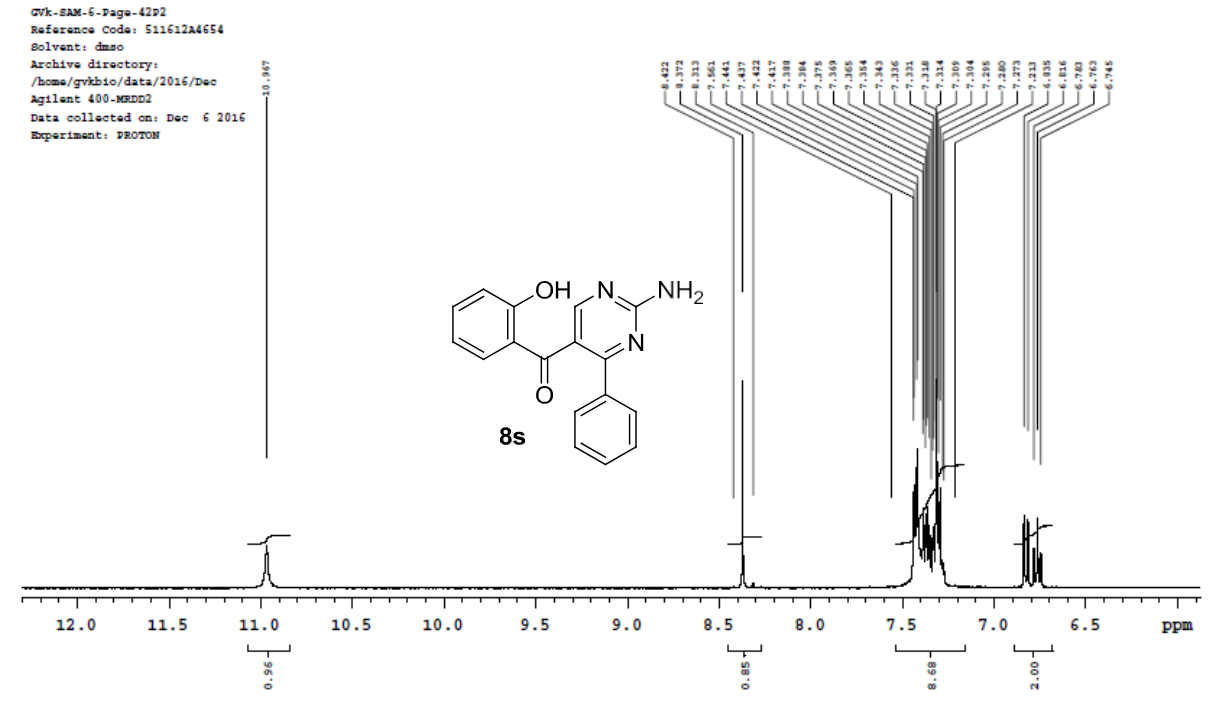
Monoisotopic Mass, Even Electron Ions
7 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-17 H: 0-14 N: 0-3 O: 0-2

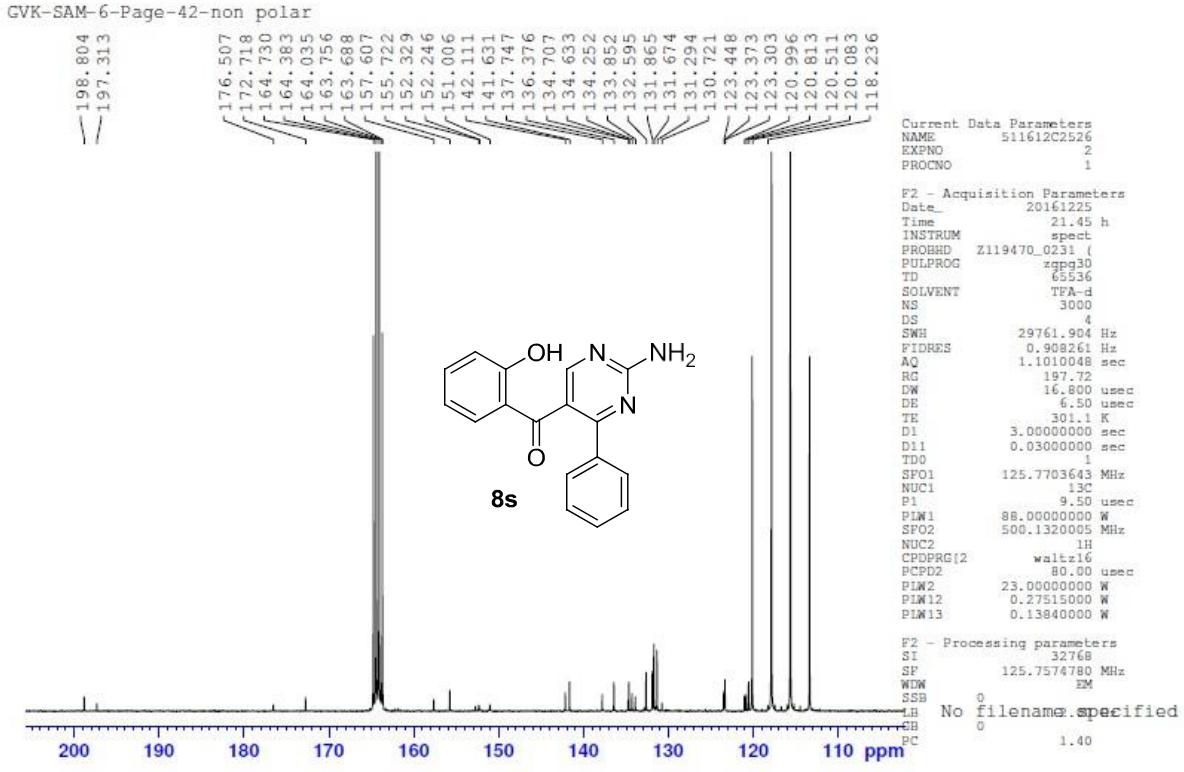
GVK-SAM-6-PAGE-42POLAR
GVK-SAM-6-PAGE-42POLAR 24 (0.348) AM (Top,4, Ar,0.0,195.17,1.00,LS 10); Sm (Mn, 2x1.00); Sb (0,40.00)



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	**Calc. Mass**	**mDa**	**PPM**	**DBE**	**i-FIT**	**Formula**
292.1090	292.1086	0.4	1.4	12.5	600.0	C17 H14 N3 O2


GVk-SAM-6-Page-42P2
Reference Code: 511612A4654
Solvent: dmso
Archive directory:
/home/gvkbio/data/2016/Dec
Agilent 400-MRDD2
Data collected on: Dec 6 2016
Experiment: PROTON
OH
N
NH2
N
O
8s
13
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
0.96
0.85
8.68
2.00


GVk-SAM-6-Page-42P2
Reference Code: 511612A4654
Solvent: dmso
Archive directory:
/home/gvkbio/data/2016/Dec
Agilent 400-MRDD2
Data collected on: Dec 6 2016
Experiment: PROTON
10.967
OH
N
NH2
N
O
8s
12.0
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
ppm
0.96
0.85
8.68
2.00


GVK-SAM-6-Page-42-non polar
198.804
197.313
176.507
172.718
164.730
164.383
164.035
163.756
163.688
157.607
155.722
152.329
152.246
151.006
142.111
141.631
137.747
136.376
134.707
134.633
134.252
133.852
132.595
131.865
131.674
131.294
130.721
123.448
123.373
123.303
120.996
120.813
120.511
120.083
118.236
OH
N
NH2
N
O
8s
Current Data Parameters
NAME 511612C2526
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20161225
Time 21.45 h
INSTRUM spect
PROBHD Z119470_0231 (
PULPROG zgpg30
TD 65536
SOLVENT TFA-d
NS 3000
DS 4
SWH 29761.904 Hz
FIDRES 0.908261 Hz
AQ 1.1010048 sec
RG 197.72
DW 16.800 usec
DE 6.50 usec
TE 301.1 K
D1 3.00000000 sec
D11 0.03000000 sec
TD0 1
SFO1 125.7703643 MHz
NUC1 13C
P1 9.50 usec
PLW1 88.00000000 W
SFO2 500.1320005 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 23.00000000 W
PLW12 0.27515000 W
PLW13 0.13840000 W
F2 - Processing parameters
SI 32768
SF 125.7574780 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
No filename specified
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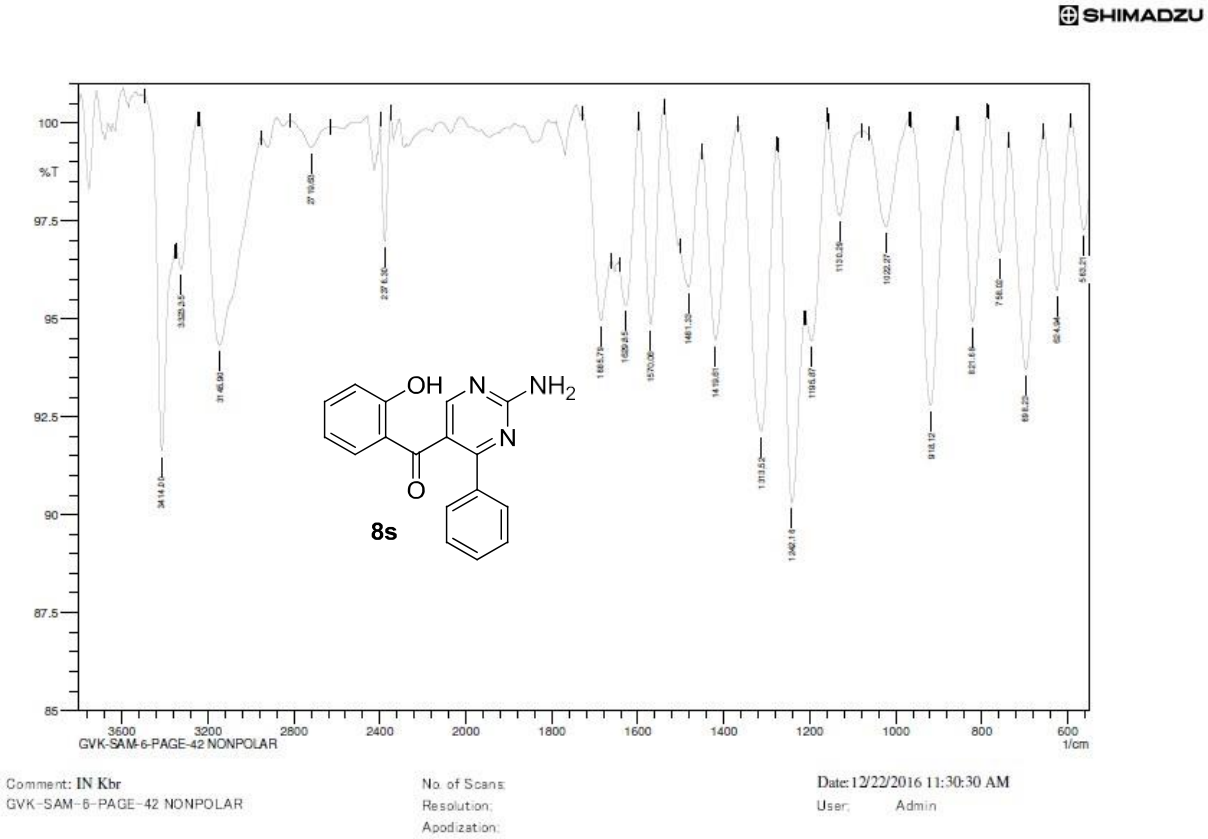
190
180
170
160
150
140
130
120
110 ppm


SHIMADZU
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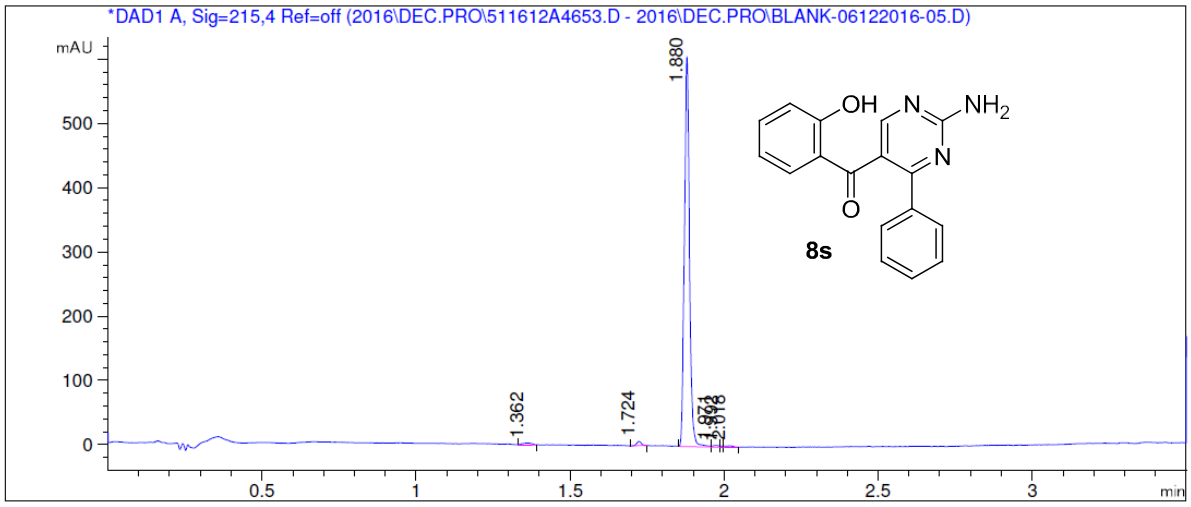
%T
97.5
95
92.5
90
87.5
85
3600
3200
2800
2400
2000
1800
1600
1400
1200
1000
800
600
1/cm
GVK-SAM-6-PAGE-42 NONPOLAR
OH
N
NH2
N
O
8s
Comment: IN Kbr
GVK-SAM-6-PAGE-42 NONPOLAR
No. of Scans:
Resolution:
Apodization:
Date: 12/22/2016 11:30:30 AM
User: Admin

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

LCMS REPORT

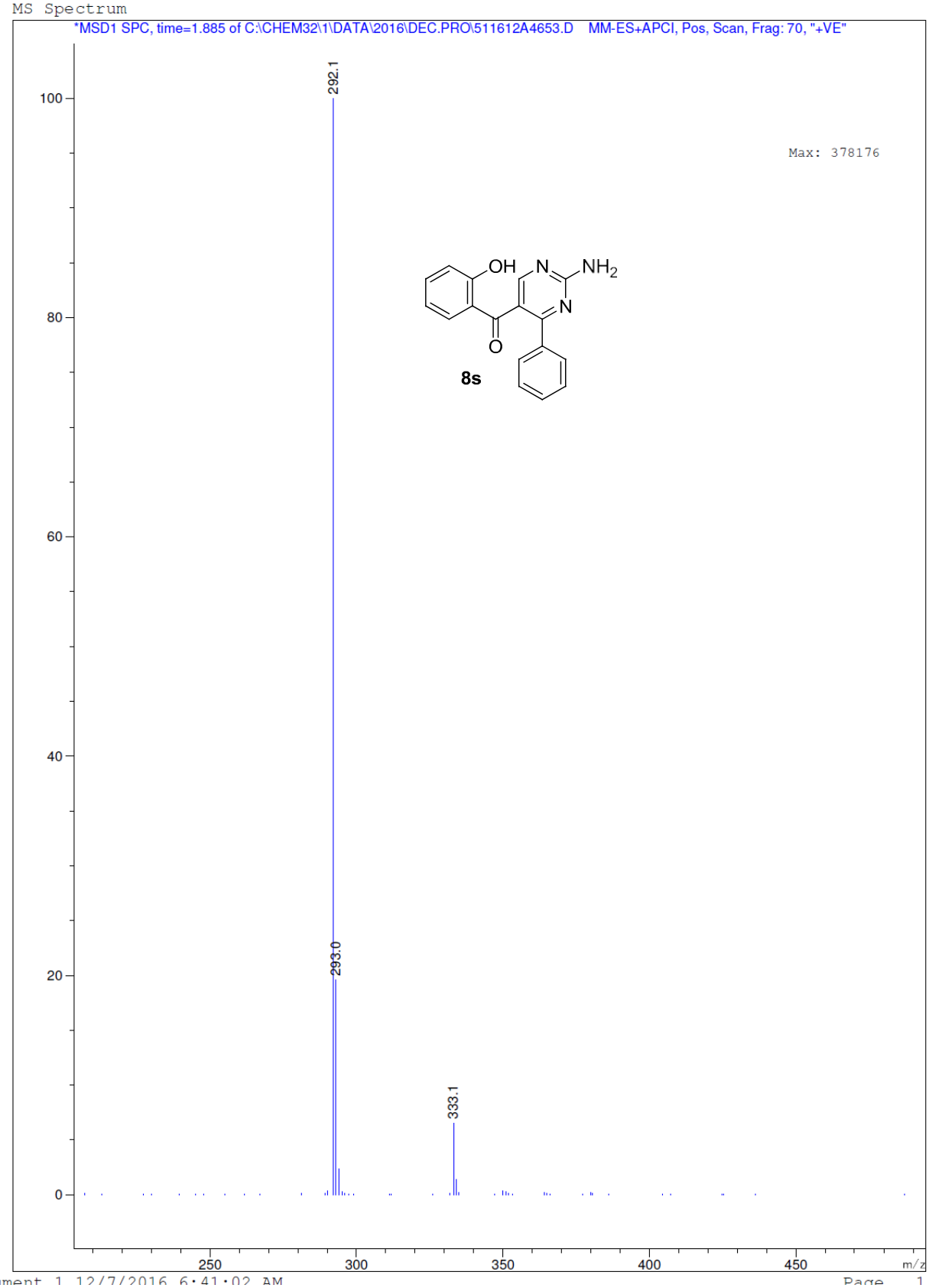
Sample Name : GVK-SAM-6-PAGE-12-P2 Vial Position :P1-B-08
Date of Analysis: 06/12/2016; 9:20:06 PM Injection Vol :Actual ->
Acq. Method :RND-FA-3.5-MIN Instrument ID :ANL-MCL5-LCMS-001

GVK_LCMS_31



Pea No	RT min	Area	Area %
1	1.36	6.958	0.962
2	1.72	6.374	0.882
3	1.88	699.856	96.807
4	1.97	3.814	0.528
5	1.99	1.216	0.168
6	2.02	4.720	0.653

MS Spectrum



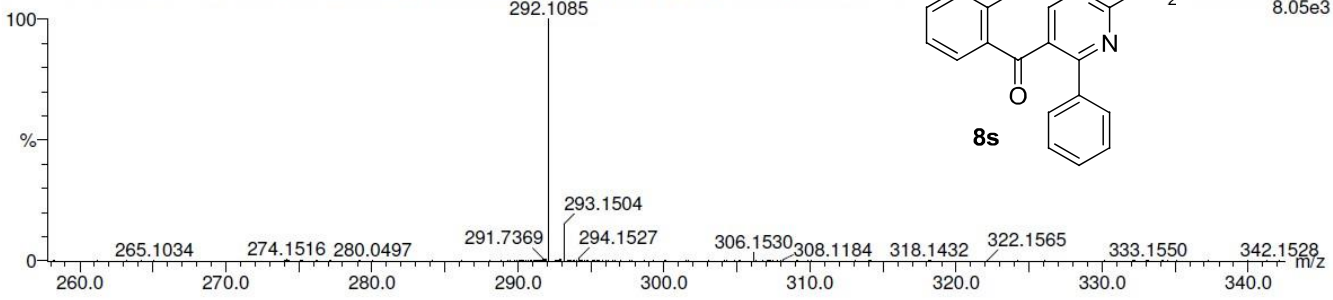
rument 1 12/7/2016 6:41:02 AM Page 1

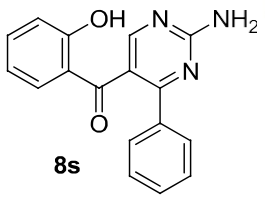
Single Mass Analysis

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

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: 0-14 N: 0-3 O: 0-2

GVK-SAM-6-PAGE-42NP
GVK-SAM-6-PAGE-42NP 24 (0.348) AM (Top,4, Ar,0.0,195.15,1.00,LS 10); Sm (Mn, 2x1.00); Sb (0,40.00)





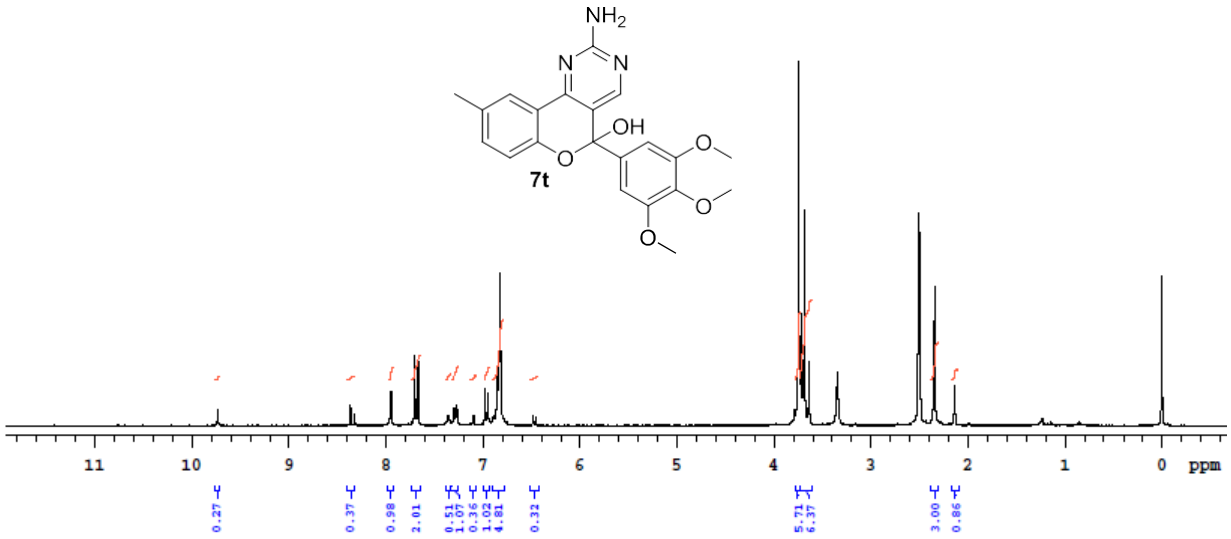
8s

Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
292.1085	292.1086	-0.1	-0.3	12.5	204.3	C17 H14 N3 O2

Sample Name:

GVK-SAM-6-PAGE-41-P1

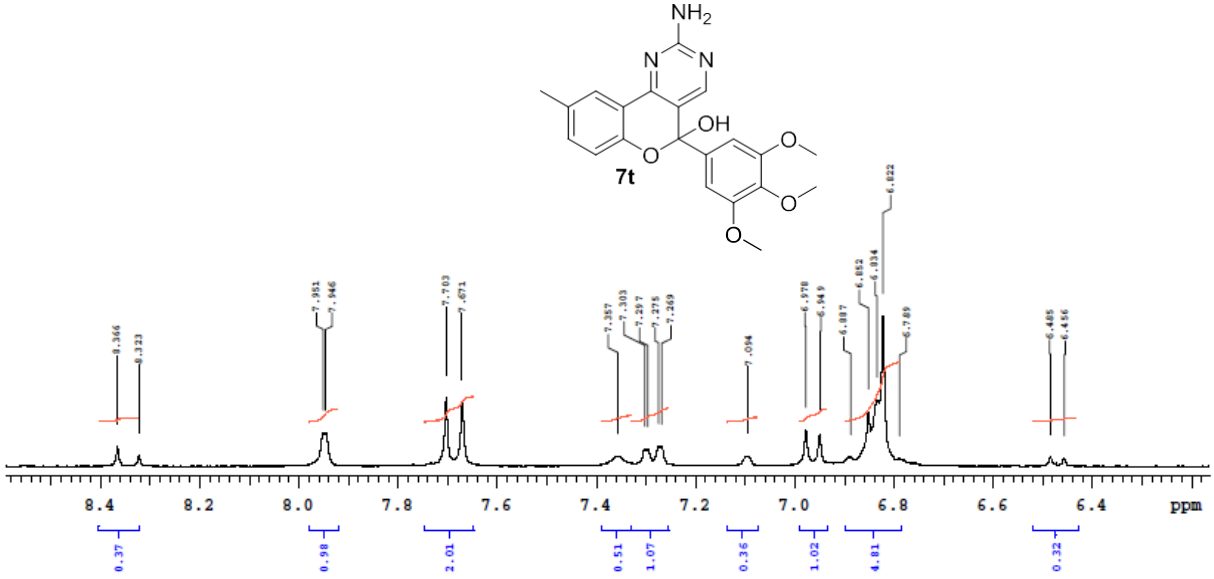
Solvent: dmso
Date: Nov 24 2016
Agilent Vnmrs300 / NRM-3
Request No: 511611C1695_PROTON

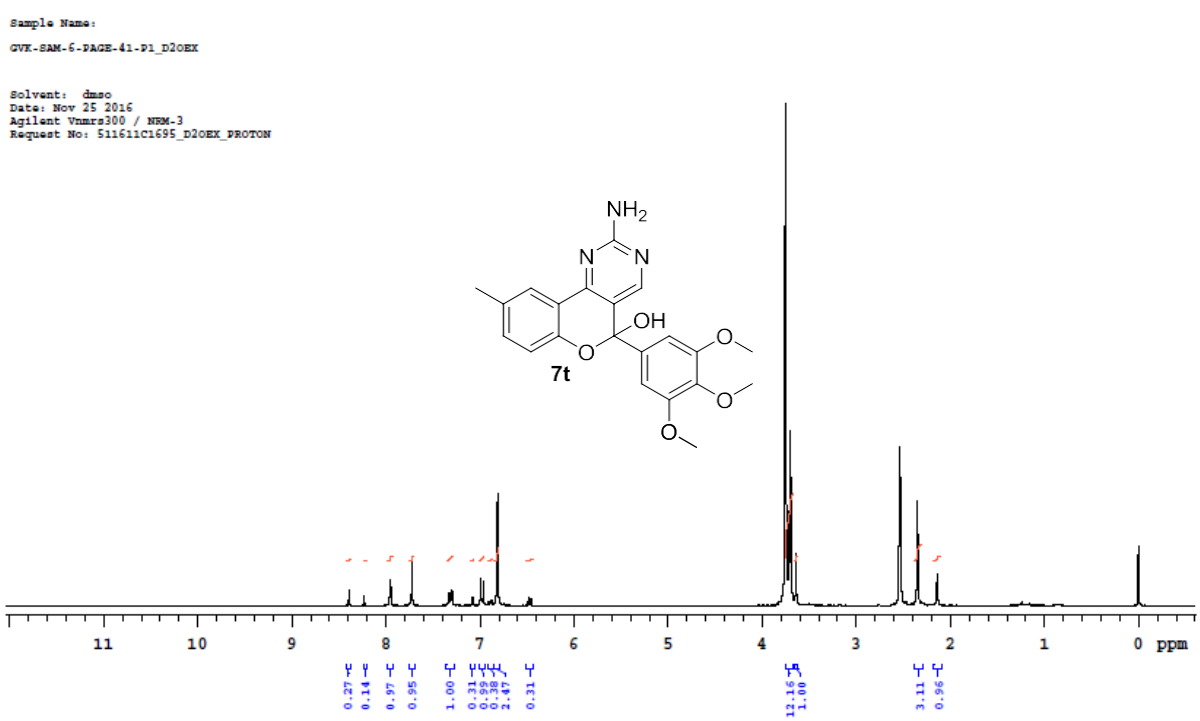


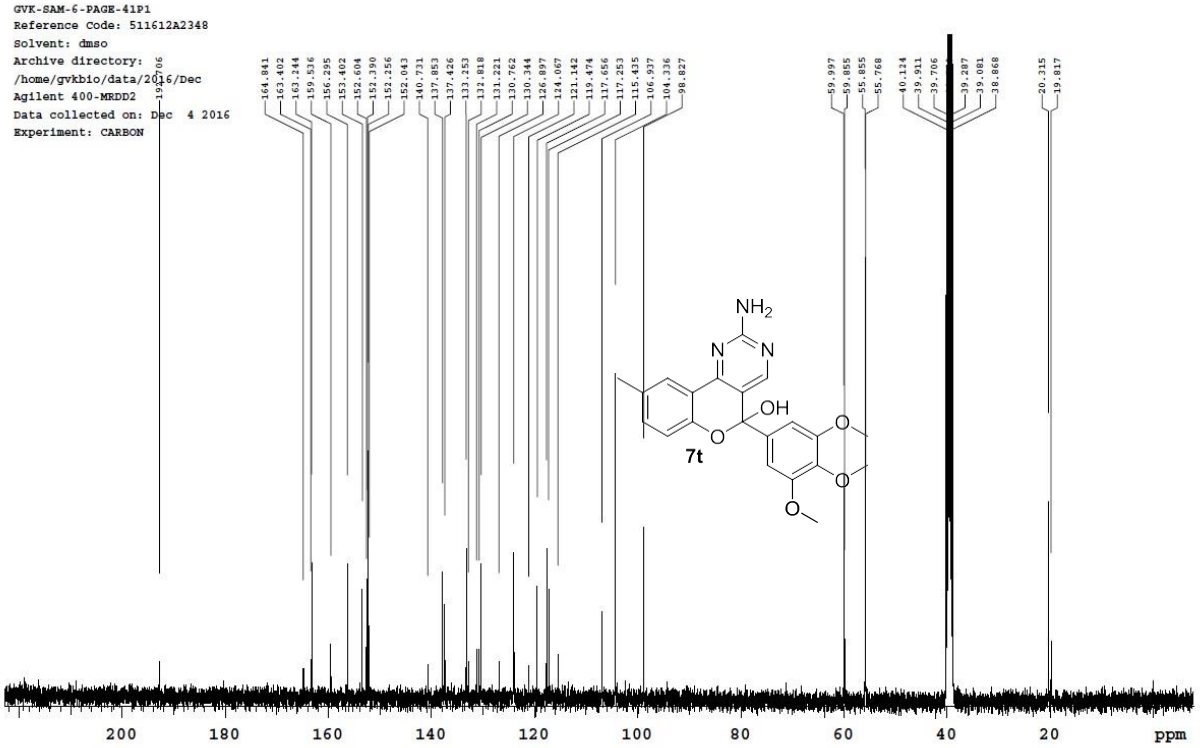
Sample Name:

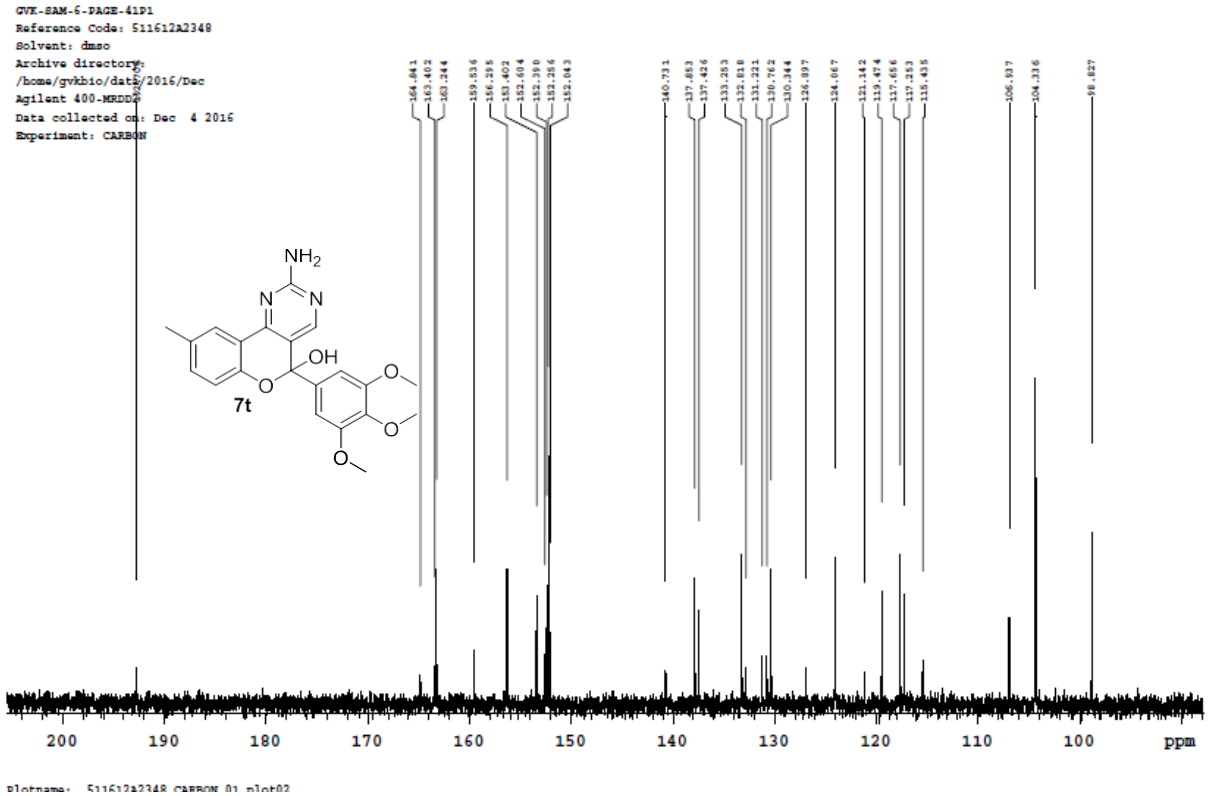
GVK-SAM-6-PAGE-41-P1

Solvent: dmso
Date: Nov 24 2016
Agilent Vnmrs300 / NRM-3
Request No: 511611C1695_PROTON

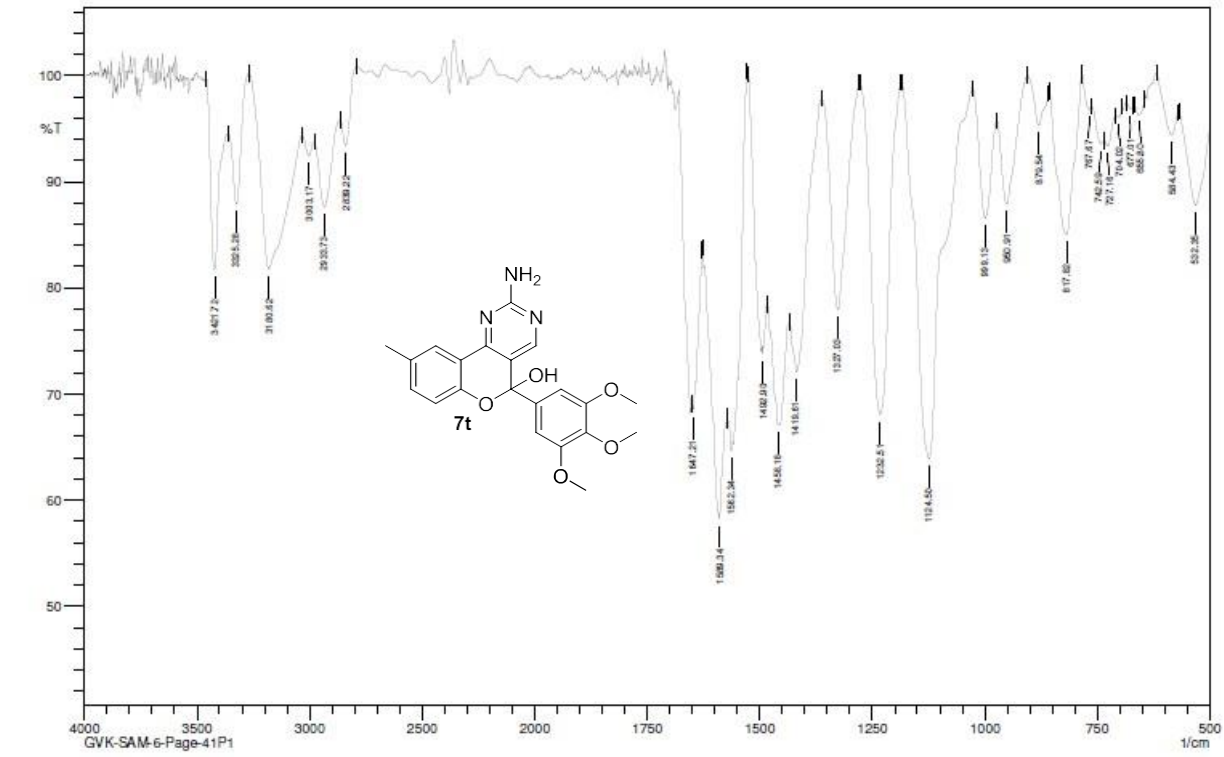



Sample Name:
GVK-SAM-6-PAGE-41-P1_D2OEX
Solvent: dmso
Date: Nov 25 2016
Agilent Vnmrs300 / NRM-3
Request No: 511611C1695_D2OEX_PROTON
NH2
N
N
OH
O
O
O
O
7t
11
10
9
8
7
6
5
4
3
2
1
0 ppm
0.27
0.14
0.97
0.95
1.00
0.31
0.99
0.89
2.47
0.31
12.16
1.00
3.11
0.96


GVK-SAM-6-PAGE-41P1
Reference Code: 511612A2348
Solvent: dmso
Archive directory:
/home/gvkbio/data/2016/Dec
Agilent 400-MRDD2
Data collected on: Dec 4 2016
Experiment: CARBON
164.841
163.402
163.244
159.536
156.295
153.402
152.604
152.390
152.256
152.043
140.731
137.853
137.426
133.253
132.818
131.221
130.762
130.344
126.897
124.067
121.142
119.474
117.656
117.253
115.435
106.937
104.336
98.827
59.997
59.855
55.855
55.768
40.124
39.911
39.706
39.287
39.081
38.868
20.315
19.817
NH2
N
N
OH
O
O
O
O
7t
200
180
160
140
120
100
80
60
40
20
ppm


GVK-SAM-6-PAGE-41P1
Reference Code: 511612A2348
Solvent: dmso
Archive directory:
/home/gvkbio/data/2016/Dec
Agilent 400-MRDD2
Data collected on: Dec 4 2016
Experiment: CARBON
164.841
163.402
163.244
159.536
156.295
153.402
152.604
152.390
152.256
152.043
140.731
137.853
137.426
133.253
132.818
131.221
130.762
130.344
126.897
124.067
121.142
119.474
117.656
117.253
115.435
106.937
104.336
98.827
NH2
N
N
OH
O
O
O
O
7t
200
190
180
170
160
150
140
130
120
110
100
ppm

SHIMADZU



Comment: IN Kbr
GVK-SAM-6-Page-41P1

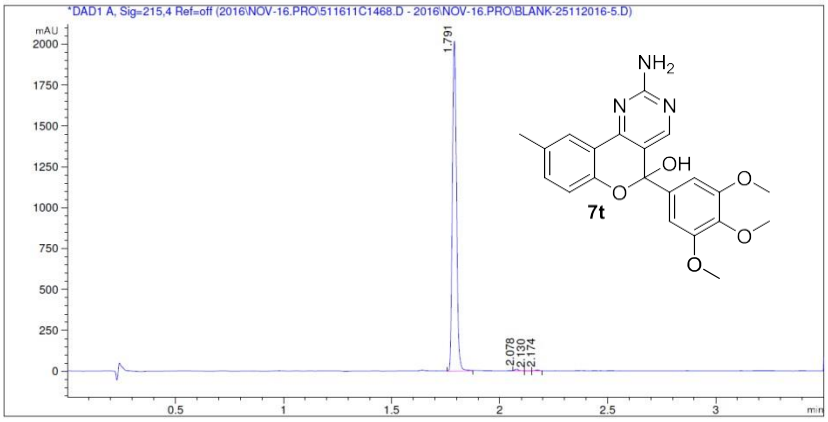
No. of Scans:
Resolution:
Apodization:

Date: 12/5/2016 12:40:13 PM
User: Admin

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

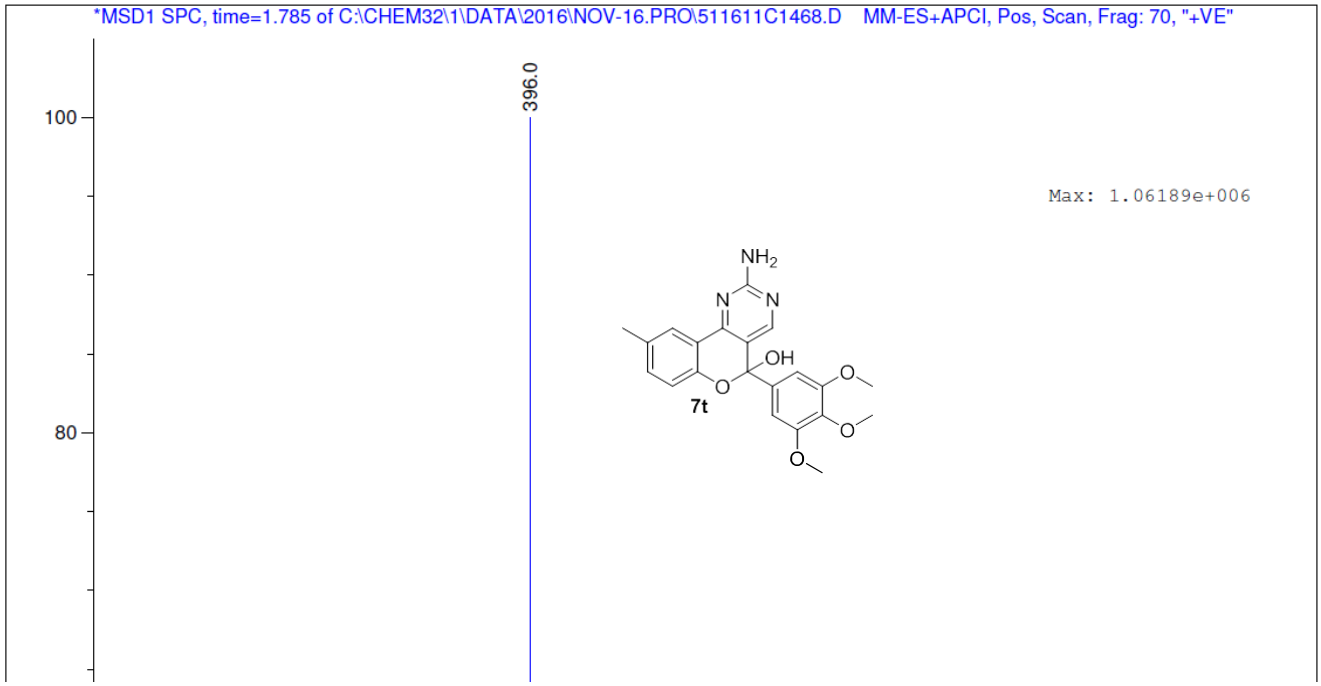
Sample Name : SAM-6-page-41 P1 Vial position : P1-C-09
Date of Analysis :11/25/2016 8:09:36 PM Injection Vol : 0.300uL
Acq. Method :C:\CHEM32\1\METHODS\RND-FA- 3.5 MIN.M Instrument ID :ANL-MCL5-LCMS-001

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, 0.4/2, 2.8/98,3.4/98,3.41/2,3.5/2
Column Flow Rate: 0.6 ml/min
Column Temperature: 60°C ->



Pea No	RT min	Area	Area %
1	1.79	2707.164	98.964
2	2.08	17.055	0.623
3	2.13	1.838	0.067
4	2.17	9.437	0.345

MS Spectrum

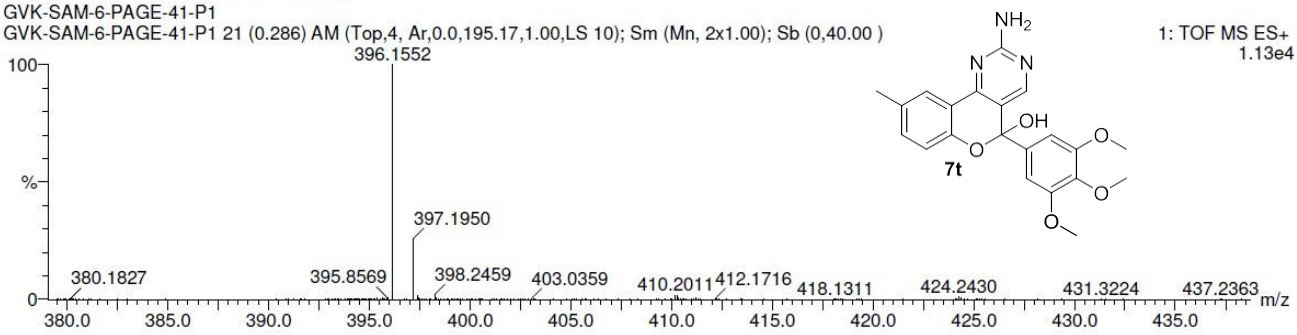


Single Mass Analysis

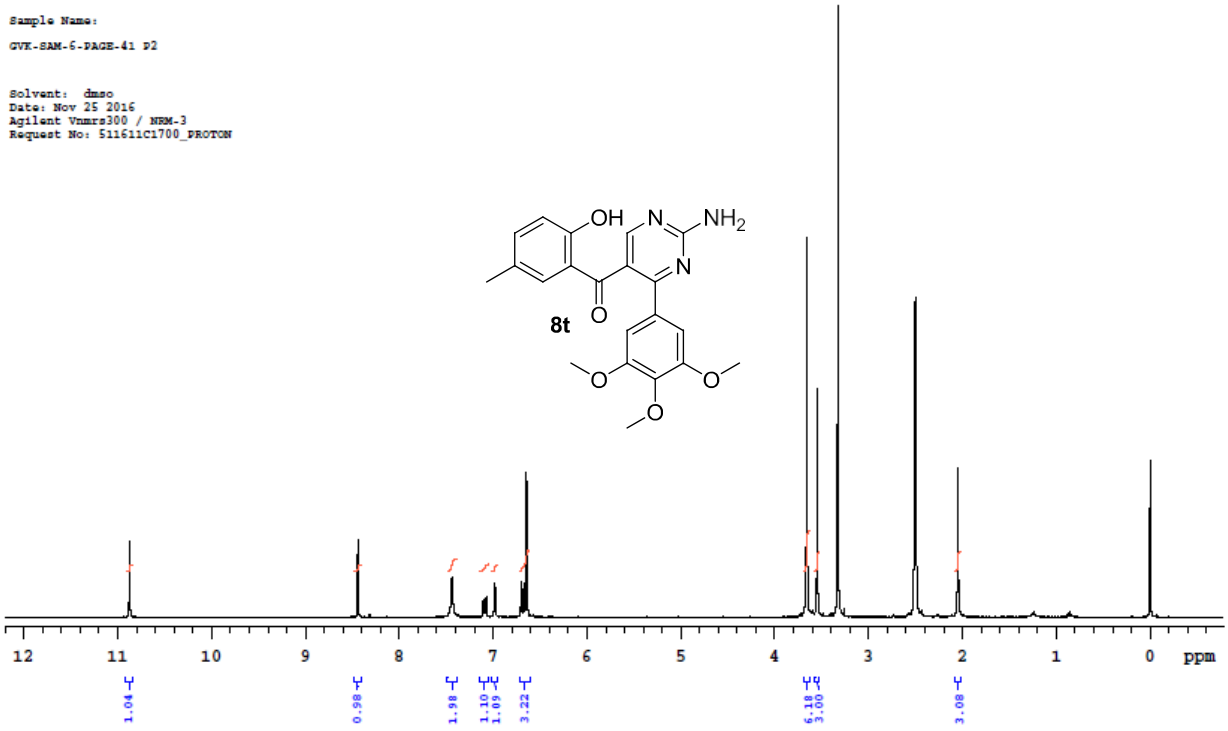
Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

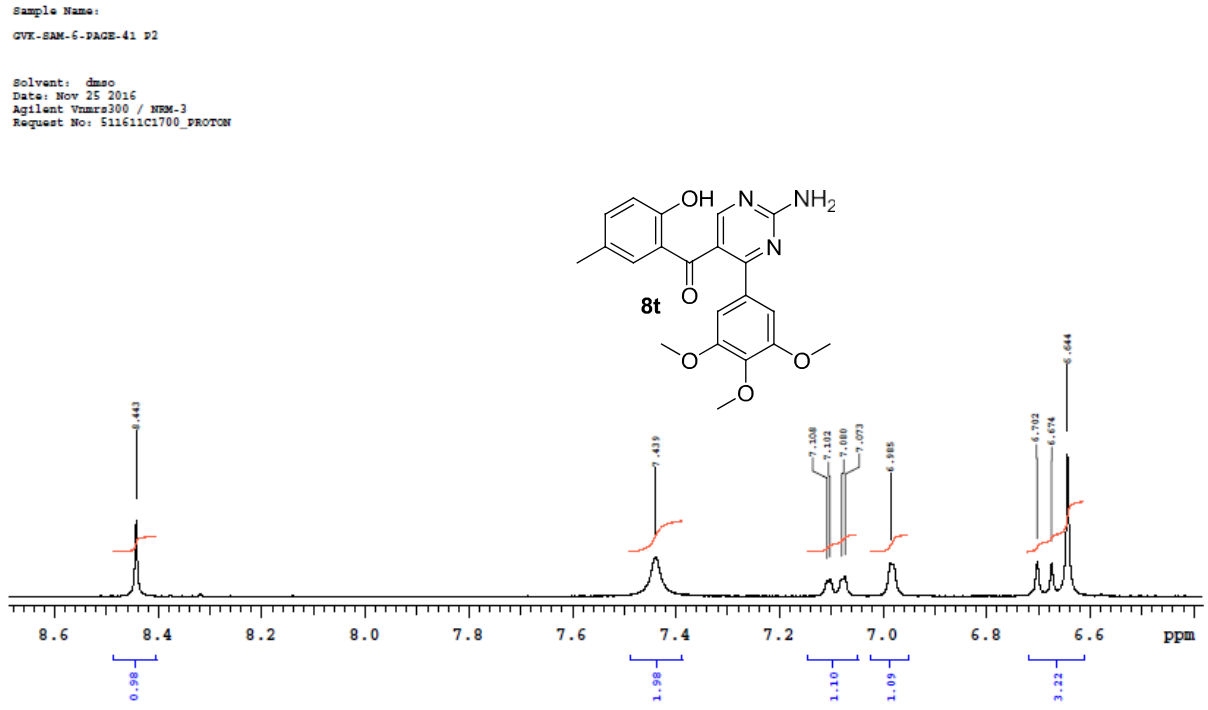
Monoisotopic Mass, Even Electron Ions
19 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-21 H: 0-22 N: 0-3 O: 0-5

GVK-SAM-6-PAGE-41-P1
GVK-SAM-6-PAGE-41-P1 21 (0.286) AM (Top,4, Ar,0.0,195.17,1.00,LS 10); Sm (Mn, 2x1.00); Sb (0,40.00)



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
396.1552	396.1559	-0.7	-1.8	12.5	246.4	C21 H22 N3 O5

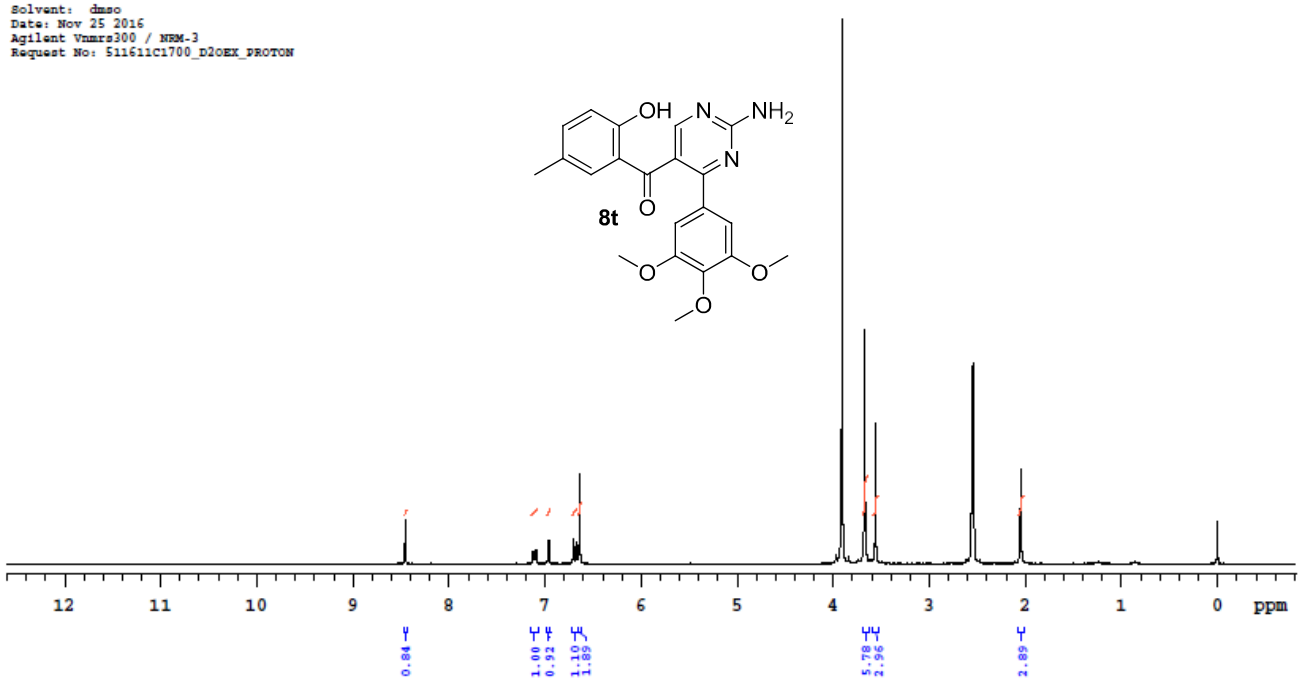

Sample Name:
GVK-SAM-6-PAGE-41 P2
Solvent: dmso
Date: Nov 25 2016
Agilent Vnmrs300 / NRM-3
Request No: 511611C1700_PROTON
OH
N
NH2
N
O
8t
O
O
O
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm
1.04
0.98
1.98
1.10
1.09
3.22
6.18
3.00
3.08

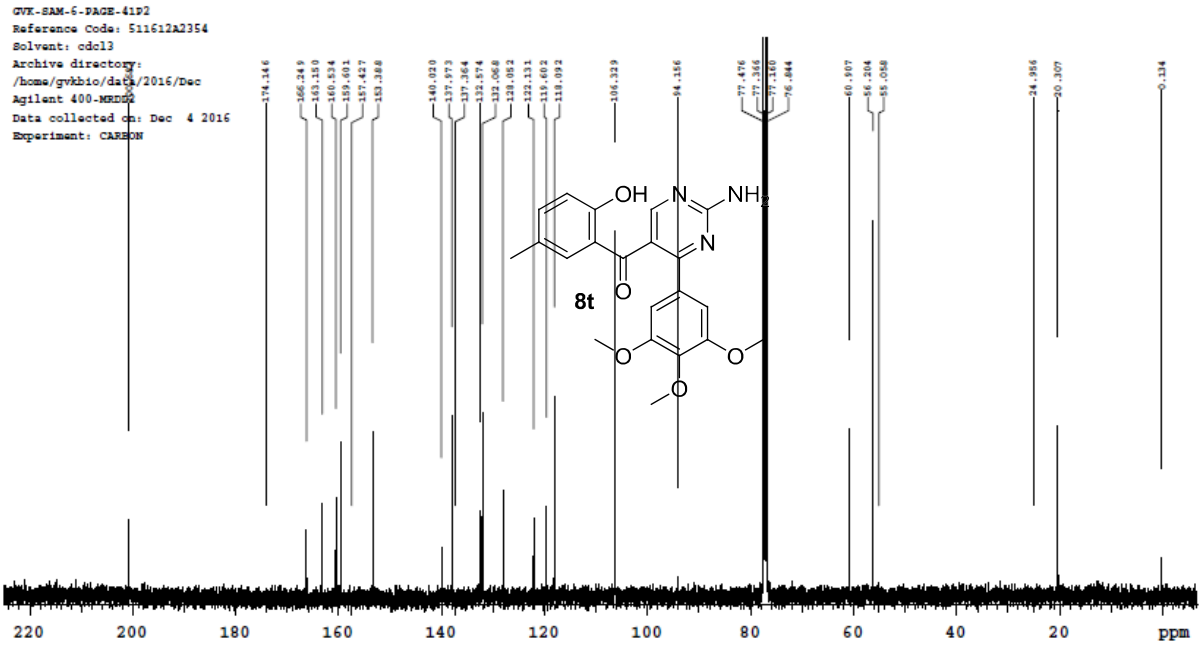

Sample Name:
GVK-SAM-6-PAGE-41 P2
Solvent: dmso
Date: Nov 25 2016
Agilent Vnmrs300 / NRM-3
Request No: 511611C1700_PROTON
OH
N
NH2
N
O
8t
O
O
O
8.443
7.439
7.108
7.102
7.080
7.073
6.985
6.702
6.674
6.644
8.6
8.4
8.2
8.0
7.8
7.6
7.4
7.2
7.0
6.8
6.6
ppm
0.98
1.98
1.10
1.09
3.22

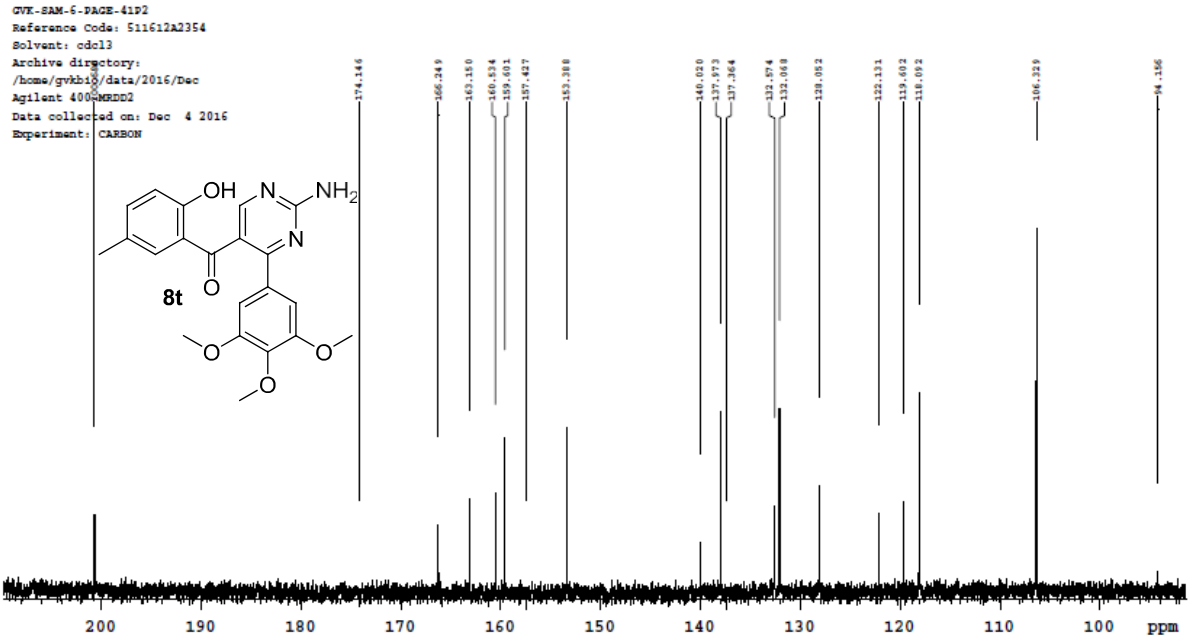
Sample Name:

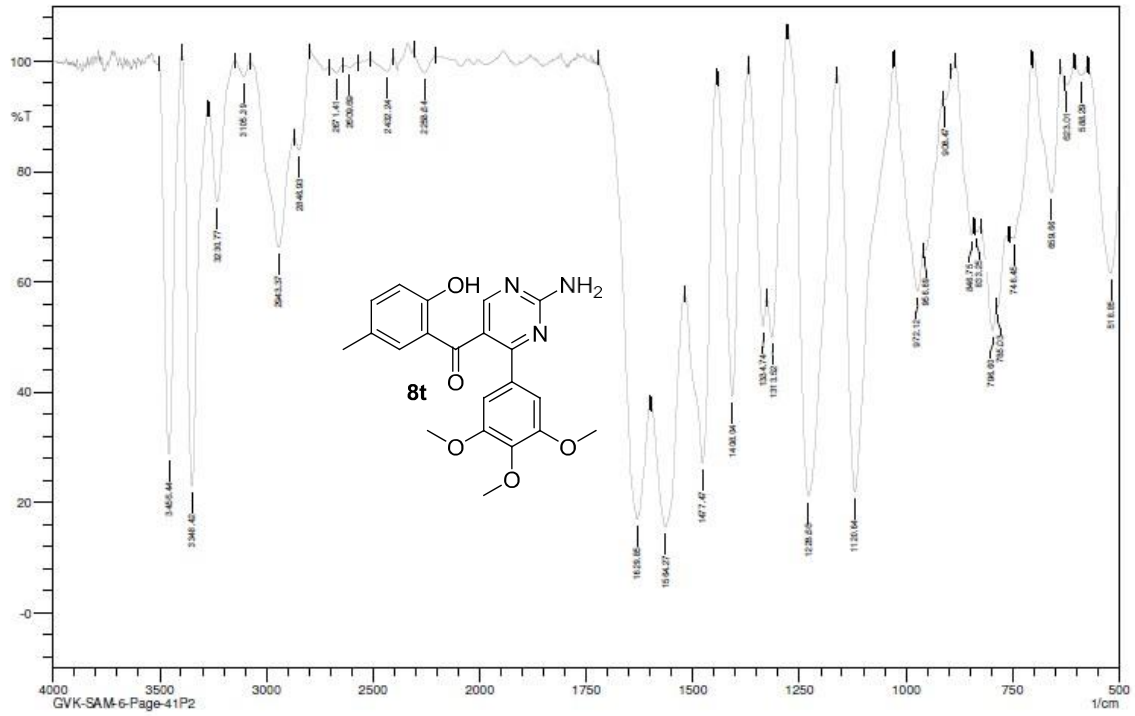
GVK-SAM-6-PAGE-41-P2_D2OEX

Solvent: dmso
Date: Nov 25 2016
Agilent Vnmrs300 / NEM-3
Request No: 511611C1700_D2OEX_PROTON




GVK-SAM-6-PAGE-41P2
Reference Code: 511612A2354
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2016/Dec
Agilent 400-MRDD2
Data collected on: Dec 4 2016
Experiment: CARBON
OH
N
NH2
N
O
8t
O
O
O
220
200
180
160
140
120
100
80
60
40
20
ppm


GVK-SAM-6-PAGE-41P2
Reference Code: 511612A2354
Solvent: cdcl3
Archive directory:
/home/gvkbio/data/2016/Dec
Agilent 400-MRDD2
Data collected on: Dec 4 2016
Experiment: CARBON
OH
N
NH2
N
O
8t
O
O
O
200
190
180
170
160
150
140
130
120
110
100
ppm


SHIMADZU
%T
100
80
60
40
20
0
4000
3500
3000
2500
2000
1750
1500
1250
1000
750
500
1/cm
GVK-SAM-6-Page-41P2
OH
N
NH2
N
O
O
O
O
8t
Comment: IN Kbr
GVK-SAM-6-Page-41P2
No. of Scans:
Resolution:
Apodization:
Date: 12/5/2016 12:42:23 PM
User: Admin

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

```
================================================================================================
Date of Analysis: 11/25/2016   12:21:39 AM          Vial Position  :P1-E-05
Acq. Method     :    RND-FA-3.0-MIN                 Injection Vol : 0.500       ul
                                                    Instrument ID  :ANL-MCL3-LCMS-003
Sample Name     :GVK-SAM-6-PAGE-41-P2
================================================================================================
 GVK_LCMS_18

================================================================================================
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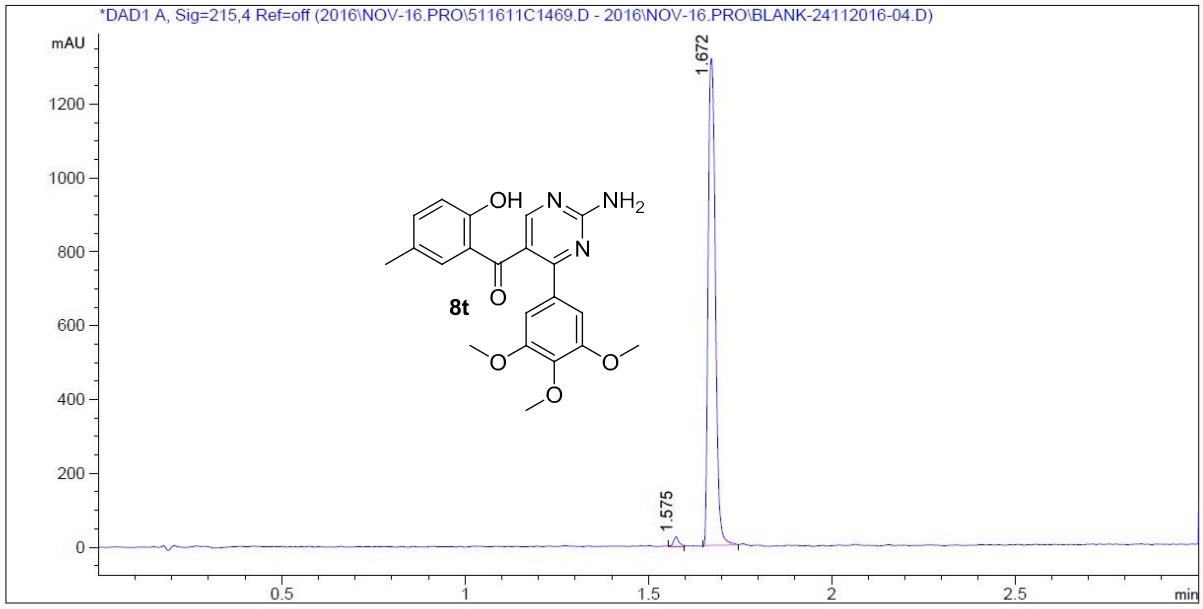
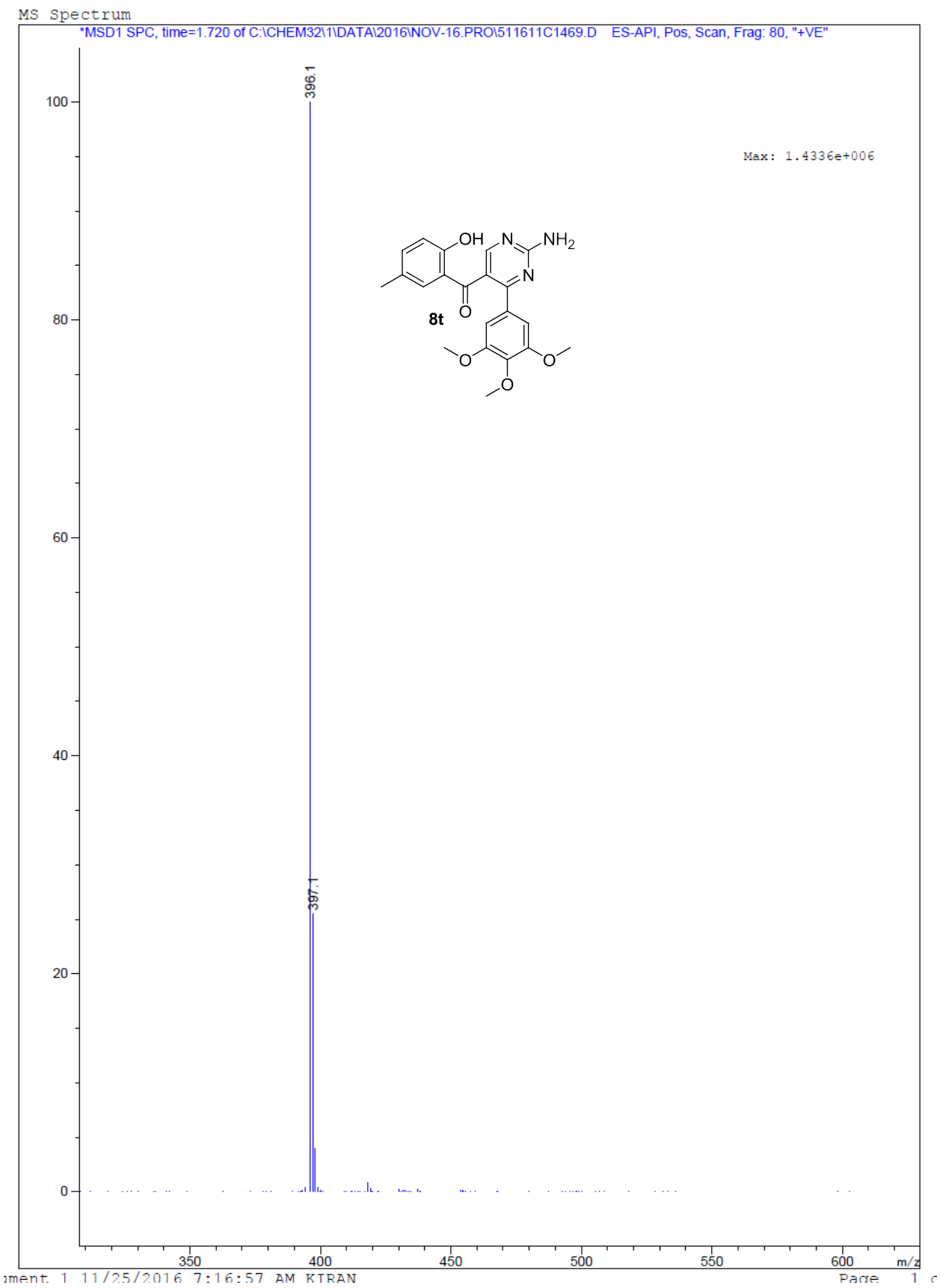


Pea No	RT min	Area	Area %
1	1.575	26.498	1.450
2	1.672	1801.219	98.550

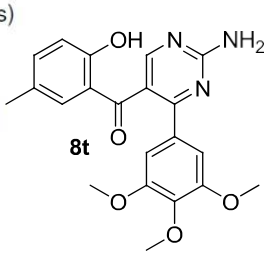

MS Spectrum
*MSD1 SPC, time=1.720 of C:\CHEM32\1\DATA\2016\NOV-16.PRO\511611C1469.D ES-API, Pos, Scan, Frag: 80, "+VE"
396.1
397.1
Max: 1.4336e+006
OH
N
NH2
N
O
8t
O
O
O
100
80
60
40
20
0
350
400
450
500
550
600
m/z

Single Mass Analysis

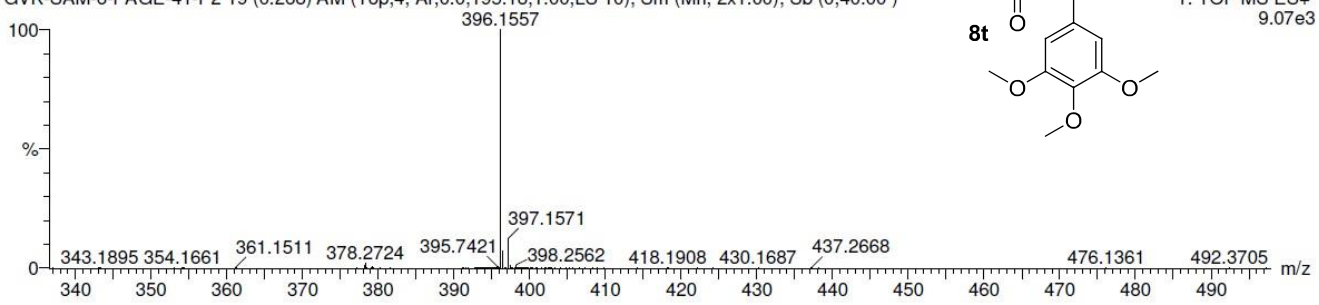
Tolerance = 1000.0 PPM / DBE: min = -1.5, max = 50.0
Selected filters: None

Monoisotopic Mass, Even Electron Ions
19 formula(e) evaluated with 1 results within limits (up to 1 closest results for each mass)
Elements Used:
C: 0-21 H: 0-22 N: 0-3 O: 0-5

GVK-SAM-6-PAGE-41-P2
GVK-SAM-6-PAGE-41-P2 19 (0.268) AM (Top,4, Ar,0.0,195.18,1.00,LS 10); Sm (Mn, 2x1.00); Sb (0,40.00)



1: TOF MS ES+
9.07e3



Minimum:				-1.5		
Maximum:		5.0	1000.0	50.0		
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	Formula
396.1557	396.1559	-0.2	-0.5	12.5	573.7	C21 H22 N3 O5