Supporting Information

New Journal of Chemistry

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

M. Sambaiah\textsuperscript{a,b}, K. Raghavulu\textsuperscript{a}, K. Shiva Kumar \textsuperscript{b}, Satyanarayana Yennam \textsuperscript{a} & Manoranjana Behera* \textsuperscript{a}

\textsuperscript{a}Chemistry services, GVK Biosciences Pvt. Ltd., Survey No’s: 125 (part) & 126, IDA Mallapur, Hyderabad-500076, Telangana State, India

\textsuperscript{b}Department of Chemistry, GITAM University, Hyderabad Campus, Rudraram Village, patancheru Mandal, Sangareddy Dist., 502329, Telangana state, India

E-mail: Manoranjana.behera@gvkbio.com; Tel: +040 67483507

Contents

1. General 2

2. General Experimental procedure for compounds 3a&7a 3-5

3. Analytical Data for compounds 3b-5d 5-6

4. Analytical Data for compounds 7b-8t 7-19

5. Spectral data 20-298
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 F254. 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-hydroxy acetophenone (1a) (2 g, 14.68 mmol) in pyridine (3 ml) was added benzoyl chloride (2a) (2.9 g, 20.56 mmol) at 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 °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 °C and the reaction mixture was
heated to 80°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\(_3\)): \(\delta = 8.38\ (m, 2H), 7.87\ (dd, 2H), 7.76\ (t, 1H), 7.57\ (m, 2H), 7.48\ (m, 3H).\) MS (EI): \(m/2\) 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\(_3\)): \(\delta = 11.90\ (s, 1H), 8.87\ (s, 1H), 8.64\ (m, 2H), 7.76\ (dd, 2H), 7.56\ (m, 3H), 7.39\ (m, 4H), 7.01\ (dd, 1H), 6.72\ (t, 1H).\) IR (KBr, cm\(^{-1}\)): 3227, 3058, 1971, 1621, 1549, 1419, 1332, 1240, 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, 128.1, 128.1, 122.3, 119.3, 117.3. MS (EI): \(m/2\) 352 (M+1,100), HRMS: (ESI): Calcd for: C\(_{23}\)H\(_{16}\)N\(_2\)O\(_2\) [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): \(\delta = 8.52\) (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\(_3\)COCD\(_3\)) = 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):

We confirmed the compounds 7a & 8a by 1H-NMR, \(^{15}\)N-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):

\[\text{\(1^H\) NMR (400 MHz, CDCl}_3\): } \delta = 8.21 \ (dd, 2H), \ 7.60 \ (m, \ 3H), \ 7.50 (m, \ 2H), \ 2.52 \ (s, \ 3H). \text{ MS (EI): } m/z \ 307 \ (M-1,100).\]

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

\[\text{\(1^H\) NMR (400 MHz, CDCl}_3\): } \delta = 15.3 \ (s, \ 1H), \ 12.72 \ (d, \ 2H), \ 7.95 (m, \ 2H), \ 7.60 \ (m, \ 6H), \ 6.77 \ (s, \ 1H), \ 2.65 \ (s, \ 2H). \text{ MS (EI): } m/z \ 307 \ (M+1,100). \text{ (Note: compound 4a 1H-NMR showed keto enol form)}\]

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

\[\text{\(1^H\) NMR (400 MHz, CDCl}_3\): } \delta = 8.33 \ (s, \ 1H), \ 8.12 \ (d, \ 1H), \ 7.83 (m, \ 2H), \ 7.79 \ (d, \ 1H), \ 7.62 \ (m, \ 1H), \ 7.48 \ (m, \ 2H). \text{ MS (EI): } m/z \ 318 \ (M+1,100).\]

2-acetyl-4-methylphenyl benzoate (3c):
$^1$H NMR (400 MHz, CDCl$_3$): $\delta =$ 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$_3$): $\delta =$ 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$_3$): $\delta =$ 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$_3$): $\delta =$ 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$_3$): $\delta =$ 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$_3$): $\delta =$ 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$_2$O$_2$ [M+H]: 291.1055; Found: 291.1155.

**2-(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, CDCl$_3$) = 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$_2$O$_2$ [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, 1566, 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, 128.1, 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$_2$O$_3$ [M+H]: 383.1317; Found: 383.1849.

**2-(2-hydroxyphenyl)(2-(2-methoxyphenyl)-4-phenylpyrimidin-5-yl) methanone (8c):**
M.p. 90-94 °C. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ = 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, CDCl$_3$) = 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$_2$O$_3$ [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-d$_6$): $\delta$ = 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, 2926, 2764, 2609, 1955, 1571, 1385, 1225, 1047, 973, 751, 699. $^{13}$C NMR (100 MHz, DMSO-d$_6$) = 161.6, 155.5, 154.6, 153.2, 141.2, 138.9, 133.9, 133.6, 130.8, 130.7, 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$_2$O$_2$ [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$_3$): $\delta$ = 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, CDCl$_3$) = 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$_2$O$_2$ [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$_2$O$_2$ [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), 7.00 (d, 1H), 6.70 (t, 1H). IR (KBr, cm$^{-1}$): 3455, 3066, 3028, 1907, 1610, 1557, 1423, 1330, 1217, 924, 677. $^{13}$C NMR (100 MHz, CDCl$_3$) = 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$_2$O$_2$ [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$_3$N$_2$O$_2$ [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$_3$): $\delta$ = 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, CDCl$_3$) = 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$_3$N$_2$O$_2$ [M+H]: 421.1086; Found: 421.1143.

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

![Image of 7g](image)

M.p. 210-213 °C. $^1$H NMR (400 MHz, DMSO-d$_6$): $\delta$ = 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-d$_6$) = 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$_2$N$_2$O$_2$ [M+H]: 421.0432; Found: 421.0483.

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

![Image of 8g](image)

M.p. 123-127 °C. $^1$H NMR (400 MHz, CDCl$_3$): $\delta$ = 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, CDCl$_3$) = 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, 128.7, 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$_2$N$_2$O$_2$ [M+H]: 421.0432; Found: 421.0549.

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

7, 9-dichloro-2, 5-diphenyl-5H-chromeno [4, 3-d] pyrimidin-5-ol (7g):
M.p. 186-190 °C. \(^1\)H NMR (400 MHz, DMSO-d6): \(\delta = 8.52\) (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. \(^1^3\)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\(_2\)O\(_2\) [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\(_3\)): \(\delta = 11.73\) (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, 1570, 1478, 1334, 1242, 1197, 952, 740, 684. \(^1^3\)C NMR (100 MHz, CDCl\(_3\)) = 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, 128.6, 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\(_2\)O\(_2\) [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): \(\delta = 8.08\) (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. \(^1^3\)C NMR (100 MHz, DMSO-d6) = 167.3, 154.8, 152.7, 152.4, 141.5, 134.2, 131.0, 128.7, 128.6, 128.0, 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\(_2\)O\(_2\) [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\(_3\)): \(\delta = 11.67\) (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), 6.87 (d, 1H), 6.65 (d, 1H), 6.34 (d, 1H), 6.27 (s, 1H), 5.80 (s, 1H), 5.77 (s, 1H), 4.07 (s, 3H), 3.80 (s, 3H), 3.74 (s, 3H), 2.83 (s, 3H). IR (KBr, cm\(^{-1}\)): 3432, 3068, 3036, 2929, 2855, 1628, 1564, 1446, 1399, 1046, 963, 747, 696. \(^1^3\)C NMR (100 MHz, CDCl\(_3\)) = 167.2, 155.3, 153.5, 153.2, 141.5, 134.2, 131.0, 128.7, 128.6, 128.0, 126.6, 124.4, 124.2, 118.7, 117.7, 98.5, 25.7, 20.2. MS (EI): \(m/z\) 326 (M+1,100), HRMS: (ESI): Calcd for C\(_{24}\)H\(_{18}\)N\(_2\)O\(_2\) [M+H]: 367.1368; Found: 367.1483.
2.90 (s, 3H), 2.10 (s, 3H). IR (KBr, cm⁻¹): 3439, 3052, 2919, 1637, 1555, 1430, 1328, 1195, 953, 840, 745, 692. ¹³C 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, 128.7, 128.3, 127.8, 118.9, 118.2, 26.3, 20.1. MS (EI): m/z 304 (M+1,100), HRMS: (ESI): Calcd for C₁₀H₁₆N₂O₂ [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. ¹³C 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, 128.4, 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 C₂₅H₂₀N₂O₃ [M+H]: 397.1474; Found: 397.1591.

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

¹H NMR (400 MHz, CDCl₃): 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. ¹³C 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 C₂₅H₂₀N₂O₃ [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, 153.4, 152.5, 141.3, 138.9, 134.7, 133.6, 131.2, 130.8, 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$_2$O$_2$ [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, CDCl$_3$) = 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, 128.4, 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$_2$O$_2$ [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), 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, 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$_3$N$_2$O$_2$ [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$_3$): $\delta$ = 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, CDCl$_3$) = 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$_3$N$_2$O$_2$ [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-d$_6$): $\delta$ = 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-d$_6$) = 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$_3$N$_2$O$_5$ [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$_3$): $\delta$ = 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, CDCl$_3$) = 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$_{33}$F$_{2}$N$_{2}$O$_{5}$ [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-d$_6$): $\delta$ = 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, 1424, 1122, 948, 858, 752, 659. $^{13}$C NMR (100 MHz, DMSO-d$_6$) = 165.0, 157.3, 154.7, 152.6, 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$_{2}$O$_{6}$ [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-d$_6$): $\delta$ = 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-d$_6$) = 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$_{2}$O$_{6}$ [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-d$_6$): $\delta$ = 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, 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$_{2}$O$_{5}$ [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$_3$): $\delta$ = 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, CDCl$_3$) = 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$_{2}$O$_{5}$ [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): $\delta$ = 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$_{2}$O$_{5}$ [M+H]: 491.1295, Found: 491.1375.

(2-(3-chlorophenyl)-4-(3,4,5-trimethoxyphenyl)pyrimidin-5-yl)(2-hydroxy-5-methylphenyl)methanone (8p):
5-phenyl-2-(pyridin-3-yl)-5H-chromeno[4,3-d]pyrimidin-5-ol (7q):

M.p. 217-221 °C. 1H NMR (400 MHz, DMSO-d6): δ = 9.65 (d, 1H), 8.86 (m, 1H), 8.79 (m, 1H), 8.53 (m, 1H), 8.35 (m, 1H), 7.62 (m, 4H), 7.29 (t, 1H), 7.17 (d, 1H). IR (KBr, cm⁻¹): 3271, 3084, 2378, 2614, 1680, 1568, 1531, 1423, 1384, 1344, 1334, 1309, 1292, 1283, 1227, 1218, 1208, 1134. MS (EI): m/z 353 (M+1,100), HRMS: (ESI): Calcd for C22H15N3O2 [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. 1H 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. 13C 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 C22H15N3O2 [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, 1H), 7.14 (m, 2H). IR (KBr, cm$^{-1}$): 3151, 3118, 3088, 2763, 1934, 1598, 1494, 1440, 1337, 1287, 128.7, 128.1, 126.6, 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$_2$O$_3$ [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, 1625, 1550, 1438, 1307, 1238, 1151, 925, 763, 686. $^{13}$C NMR (100 MHz, CDCl$_3$) = 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$_2$O$_3$ [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$_3$O$_2$ [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\(_3\)O\(_2\) [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): \(\delta = 7.95\) (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, 1598, 1562, 1458, 1334, 1228, 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\(_3\)O\(_5\) [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): \(\delta = 10.87\) (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\(_3\)O\(_5\) [M+H]: 396.1481, Found: 396.1557.
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, 1.7µm)
Mobile Phase: A1: 0.1 % FA IN WATER B1: 0.1% FA IN ACN
Gradient: Time (min) /%B1: 0/3, 0.3/3, 2.8/98, 4.0/98, 4.2/3, 4.5/3
Column Flow Rate: 0.6 ml/min

<table>
<thead>
<tr>
<th>Peak</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.52</td>
<td>26.994</td>
<td>0.590</td>
</tr>
<tr>
<td>2</td>
<td>2.20</td>
<td>4511.067</td>
<td>98.619</td>
</tr>
<tr>
<td>3</td>
<td>2.36</td>
<td>33.537</td>
<td>0.733</td>
</tr>
<tr>
<td>4</td>
<td>2.52</td>
<td>0.887</td>
<td>0.019</td>
</tr>
<tr>
<td>5</td>
<td>2.58</td>
<td>1.737</td>
<td>0.038</td>
</tr>
</tbody>
</table>
Sample Name : GVK-SAM-1-PAGE-49
Date of Analysis: 24/11/2015; 12:07:44 AM
Acq. Method->C:\CHEM32\1\METHODS\RND-FA- 4.5 MIN_1.M
Vial position : P2-F-03
Injection Vol: 0.5 µL
Instrument ID: ANL-MCL5-LCMS-001

Column: ACQUITY UPLC BEH C18 (50mm × 2.1mm, 1.7µm)
Mobile Phase: A1: 0.1% FA IN WATER B1: 0.1%FA IN ACN
Gradient: Time (min) / %B1: 0/3, 0.3/3, 2.8/98, 4.0/98, 4.2/3, 4.5/3
Column Flow Rate: 0.6 ml/min

<table>
<thead>
<tr>
<th>Peak</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.83</td>
<td>38.113</td>
<td>0.433</td>
</tr>
<tr>
<td>2</td>
<td>2.16</td>
<td>2499.560</td>
<td>27.832</td>
</tr>
<tr>
<td>3</td>
<td>2.40</td>
<td>101.074</td>
<td>1.148</td>
</tr>
<tr>
<td>4</td>
<td>2.70</td>
<td>6212.585</td>
<td>70.587</td>
</tr>
</tbody>
</table>
Sample Name: GVK-SAM-1-PAGE-53
Vial position : E2-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, 1.7µm)
Mobile Phase: A1: 0.1 % FA IN WATER B1: 0.1%FA IN ACN
Gradient: Time (min) /%B1:0/3, 0.3/3, 2.8/98, 4.0/98, 4.2/3, 4.5/3
Column Flow Rate: 0.6 ml/min

<table>
<thead>
<tr>
<th>Peak</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>No</td>
<td>min</td>
<td>------</td>
<td>--------</td>
</tr>
<tr>
<td>------</td>
<td>-----</td>
<td>------</td>
<td>--------</td>
</tr>
<tr>
<td>1</td>
<td>2.01</td>
<td>4.649e3</td>
<td>92.884</td>
</tr>
<tr>
<td>2</td>
<td>2.43</td>
<td>330.261</td>
<td>6.598</td>
</tr>
<tr>
<td>3</td>
<td>2.51</td>
<td>25.904</td>
<td>0.518</td>
</tr>
</tbody>
</table>

[Graph of a molecule with peaks labeled]
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, 1.7µm)  
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

<table>
<thead>
<tr>
<th>Pea</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>--</td>
<td>--</td>
<td>--</td>
<td>--</td>
</tr>
<tr>
<td>1</td>
<td>1.70</td>
<td>4.561</td>
<td>0.092</td>
</tr>
<tr>
<td>2</td>
<td>1.81</td>
<td>74.941</td>
<td>1.513</td>
</tr>
<tr>
<td>3</td>
<td>1.99</td>
<td>4848.227</td>
<td>97.914</td>
</tr>
<tr>
<td>4</td>
<td>2.05</td>
<td>23.772</td>
<td>0.480</td>
</tr>
</tbody>
</table>

Date of Analysis: 13/01/2016; 9:22:15 PM
Vial Position: Vial 80
Sample Name: GVK-SAM-5-PAGE-22
Injection Vol: 3.000 µl
Acq. Method: C:\CHEM32\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

<table>
<thead>
<tr>
<th>PEAK No</th>
<th>RT min</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.853</td>
<td>1924.310</td>
<td>57.399</td>
</tr>
<tr>
<td>2</td>
<td>3.339</td>
<td>26.579</td>
<td>0.793</td>
</tr>
<tr>
<td>3</td>
<td>3.422</td>
<td>1401.637</td>
<td>41.808</td>
</tr>
</tbody>
</table>

Graphs showing chromatograms and mass spectra.
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, 1.7µm)
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

<table>
<thead>
<tr>
<th>Peak</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.29</td>
<td>19.21</td>
<td>2.862</td>
</tr>
<tr>
<td>2</td>
<td>1.59</td>
<td>2.370</td>
<td>0.353</td>
</tr>
<tr>
<td>3</td>
<td>1.80</td>
<td>2.309</td>
<td>0.344</td>
</tr>
<tr>
<td>4</td>
<td>1.88</td>
<td>640.507</td>
<td>95.406</td>
</tr>
<tr>
<td>5</td>
<td>2.50</td>
<td>6.950</td>
<td>1.035</td>
</tr>
</tbody>
</table>
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

Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7µm)
Mobile Phase: B1: 0.1 % FA IN WATER A1: 0.1%FA IN ACN
Gradient: Time (min) /%A1: 0/2, 0.4/2, 2.8/98, 3.4/98, 3.8/41/2, 3.5/2
Column Flow Rate: 0.6 ml/min
Column Temperature: 60°C

<table>
<thead>
<tr>
<th>Pea</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.54</td>
<td>44.779</td>
<td>0.989</td>
</tr>
<tr>
<td>2</td>
<td>1.65</td>
<td>223.081</td>
<td>4.927</td>
</tr>
<tr>
<td>3</td>
<td>1.92</td>
<td>23.121</td>
<td>0.511</td>
</tr>
<tr>
<td>4</td>
<td>2.09</td>
<td>3469.248</td>
<td>76.615</td>
</tr>
<tr>
<td>5</td>
<td>2.22</td>
<td>11.679</td>
<td>0.258</td>
</tr>
<tr>
<td>6</td>
<td>2.27</td>
<td>25.128</td>
<td>0.555</td>
</tr>
<tr>
<td>7</td>
<td>2.51</td>
<td>202.877</td>
<td>4.480</td>
</tr>
<tr>
<td>8</td>
<td>2.55</td>
<td>139.298</td>
<td>3.076</td>
</tr>
<tr>
<td>9</td>
<td>2.64</td>
<td>53.813</td>
<td>1.188</td>
</tr>
<tr>
<td>10</td>
<td>2.66</td>
<td>129.655</td>
<td>2.863</td>
</tr>
<tr>
<td>11</td>
<td>2.75</td>
<td>84.176</td>
<td>1.859</td>
</tr>
<tr>
<td>12</td>
<td>2.81</td>
<td>38.810</td>
<td>0.857</td>
</tr>
<tr>
<td>13</td>
<td>2.85</td>
<td>63.456</td>
<td>1.401</td>
</tr>
<tr>
<td>14</td>
<td>2.95</td>
<td>17.925</td>
<td>0.396</td>
</tr>
<tr>
<td>15</td>
<td>2.98</td>
<td>1.093</td>
<td>0.024</td>
</tr>
</tbody>
</table>
Sample Name: [GSK Name]
Date of Analysis: [02/17/2016]
Vial position: [F2-A-07]
Sample ID: [GSK Sample Id]
Acq. Method: [LC/MS/MS] [Method Name]
Injection Vol: [9.000 µl]
Instrument ID: [ARL-MCL5-ICMS-001]

Column: [ACQUITY UPLC BEH C18 (50mm x 1.7m, 1.7µm)]
Mobile Phases: B: [0.1% FA in WATER] A: [0.1%FA in ACN]
Gradient: Time (min) / %A: [0/0, 0.4/2, 2.6/98,3.1/98,3.3/2,3.5/2]
Column Temperature: [60°C]
Column Flow Rate: [0.8 ml/min]

<table>
<thead>
<tr>
<th>Peak</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>4a</td>
<td>2.11</td>
<td>349.020</td>
<td>23.886</td>
</tr>
<tr>
<td>5d</td>
<td>2.36</td>
<td>383.745</td>
<td>26.263</td>
</tr>
<tr>
<td>4d</td>
<td>2.46</td>
<td>723.847</td>
<td>49.538</td>
</tr>
<tr>
<td>5d</td>
<td>2.56</td>
<td>4.569</td>
<td>0.313</td>
</tr>
</tbody>
</table>
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\RNO-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

<table>
<thead>
<tr>
<th>Peak</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>12.00</td>
<td>3489.687</td>
<td>99.514</td>
</tr>
<tr>
<td>2</td>
<td>12.04</td>
<td>17.050</td>
<td>0.486</td>
</tr>
</tbody>
</table>
Compound 7a Structure Confirmation data:
Sample Name: CVK-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\METHODS\RND-FA- 4.5 MIN_1.M
Instrument ID: ANL-MCL5-LCMS-001

Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7μm)
Mobile Phase: A1: 0.1 % FA IN WATER B1: 0.1%FA IN ACN
Gradient: Time (min) / A1: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
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 closest results for each mass)
Elements Used:
C: 0-23  H: 0-17  N: 0-2  O: 0-2

GVK-SAM-1-PAGE-64POLAR
GVK-SAM-1-PAGE-64POLAR 24 (0.361) AM (Top,4, Ar,0,0,195.17,1.00,1.00,LS 10); Sm (Mn,2xt.00); Sb (0,40.00)

Minimum:
Maximum: 5.0  1000.0  -1.5

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>1-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>353.1316</td>
<td>353.1290</td>
<td>2.6</td>
<td>7.4</td>
<td>16.5</td>
<td>277.0</td>
<td>C23 H17 N2 O2</td>
</tr>
</tbody>
</table>

1: TOF MS ES+ 7.60e3
Compound 8a Structure Confirmation data:
Sample Name: GVK-SAM-1-PAGE-54NP
Vial position: P1-E-01
Date of Analysis: 30/11/2015 8:48:21 AM
Injection Vol: 0.5 µL
Acq. Method: C:\CHEM32\METHODS\RND-FA-4.5 MIN_1.M
Instrument ID: iANL-MCL5-LCMS-001

Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7µm)
Mobile Phase: A1: 0.1% FA IN WATER, B1: 0.1% FA IN ACN
Gradient: Time (min) /%B1: 0/3, 0.3/3, 2.3/98, 4.0/98, 4.2/3, 4.5/3
Column Flow Rate: 0.6 mL/min

<table>
<thead>
<tr>
<th>Pea</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>2.70</td>
<td>6.437</td>
<td>0.200</td>
</tr>
<tr>
<td>2</td>
<td>2.80</td>
<td>3.213e3</td>
<td>99.692</td>
</tr>
<tr>
<td>3</td>
<td>2.88</td>
<td>3.482</td>
<td>0.108</td>
</tr>
</tbody>
</table>

\[N\]
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)

Minimum:  5.0  1000.0  50.0
Maxumum:  -1.5

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>1-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>353.1320</td>
<td>353.1290</td>
<td>3.0</td>
<td>8.5</td>
<td>16.5</td>
<td>376.4</td>
<td>C23 H17 N2 O2</td>
</tr>
</tbody>
</table>
Sample Name: GVK-SAM-1-PAGE-63-POLAR
Vial position: F1-B-01
Date of Analysis: 07/12/2015; 7:40:15 PM
Injection Vol: 0.5 µL
Acq. Method: C:\CHEM32\METHOD\RND-FA- 3.0 MIN.M
Instrument ID: ANL-MCL5-LCMS-001

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

<table>
<thead>
<tr>
<th>Peak</th>
<th>RT (min)</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.29</td>
<td>1.079e3</td>
<td>99.445</td>
</tr>
<tr>
<td>2</td>
<td>1.36</td>
<td>2.687</td>
<td>0.248</td>
</tr>
<tr>
<td>3</td>
<td>1.43</td>
<td>3.336</td>
<td>0.308</td>
</tr>
</tbody>
</table>

[Chemical structure image]
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 S1 (0.750) AM (Top, 4, Ar, 5000, 0, 195.13, 1.00, LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>1-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>291.1155</td>
<td>291.1154</td>
<td>2.1</td>
<td>7.2</td>
<td>12.5</td>
<td>54.4</td>
<td>C18 H15 N2 O2</td>
</tr>
</tbody>
</table>

1: TOF MS ES+ 4.07e3
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, 1.7µm)  
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

<table>
<thead>
<tr>
<th>Peak</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.20</td>
<td>4.608</td>
<td>0.147</td>
</tr>
<tr>
<td>2</td>
<td>1.36</td>
<td>13.118e3</td>
<td>99.735</td>
</tr>
<tr>
<td>3</td>
<td>1.42</td>
<td>3.541</td>
<td>0.113</td>
</tr>
<tr>
<td>4</td>
<td>1.46</td>
<td>0.125</td>
<td>0.004</td>
</tr>
</tbody>
</table>
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 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 (0.94e5) AM (Top4, Ar, 5000.0, 195.10, 1.00, LS 10); Sm (M, 2x1.00); Sb (1.40.00)

![Chemical Structure]

Minimum: 291.1121
Maximum: 291.1134

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>291.1121</td>
<td>291.1134</td>
<td>-1.3</td>
<td>-4.5</td>
<td>12.5</td>
<td>33.5</td>
<td>C18 H15 N2 O2</td>
</tr>
</tbody>
</table>

1: TOF MS ES+ 3.98e5
Sample Name: GVK-SAM-5-PAGE-13-P
Vial position: P1-A-06
Date of Analysis: 1/3/2016 4:17:03 PM
Injection Vol: 0.5 μL
Acq. Method: C:\CHEM32\METHODS\RND-FA-3.0 MIN-1.M
Instrument ID: ANL-Mc15-LCMS-001

RND-FA-3.0 MIN.M
Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7μm)
Mobile Phase: B1: 0.1 % FA IN WATER A1: 0.1%FA IN ACN
Gradient: Time (min) /%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

<table>
<thead>
<tr>
<th>Pea</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0.47</td>
<td>16.177</td>
<td>0.702</td>
</tr>
<tr>
<td>2</td>
<td>1.75</td>
<td>2264.565</td>
<td>98.259</td>
</tr>
<tr>
<td>3</td>
<td>1.83</td>
<td>16.899</td>
<td>0.733</td>
</tr>
<tr>
<td>4</td>
<td>1.85</td>
<td>7.049</td>
<td>0.306</td>
</tr>
</tbody>
</table>
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
511701A21B1 18 (0.256) AM (Top, 4, Ar, 5000, 0.195, 1.10, LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

Minimum:  5.0  1000.0  50.0
Maximum:  -1.5

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>383.1849</td>
<td>383.1396</td>
<td>45.3</td>
<td>118.2</td>
<td>16.5</td>
<td>1023.1</td>
<td>C24 H19 N2 O3</td>
</tr>
</tbody>
</table>

1: TOF MS ES+ 1.0064
Sample Name: GVK-SAM-5-PAGE-13-NP
Date of Analysis: 1/3/2016 4:33:04 PM
Injection Vol: 0.5 µL
Vial position: P1-A-05
Acq. Method: C:\CHEM32\1\METHODS\RND-FA-3.0 MIN-1.M
Instrument ID: ANL-MCL5-LCMS-001

Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7µm)
Mobile Phase: B1: 0.1% FA IN WATER A1: 0.1% FA IN ACN
Gradient: Time (min) /%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

<table>
<thead>
<tr>
<th>Pea</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>1.74</td>
<td>25.287</td>
<td>0.851</td>
</tr>
<tr>
<td>2</td>
<td>1.79</td>
<td>2926.346</td>
<td>98.514</td>
</tr>
<tr>
<td>3</td>
<td>1.89</td>
<td>12.057</td>
<td>0.406</td>
</tr>
<tr>
<td>4</td>
<td>2.00</td>
<td>6.796</td>
<td>0.229</td>
</tr>
</tbody>
</table>
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 )

Minimum:
Maximum:
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
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: 0.500ul
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: ACQUTY UFLC 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

<table>
<thead>
<tr>
<th>Pea</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>No</td>
<td>min</td>
<td>-------</td>
<td>--------</td>
</tr>
<tr>
<td>-----</td>
<td>----</td>
<td>------</td>
<td>--------</td>
</tr>
<tr>
<td>1</td>
<td>2.20</td>
<td>2935.549</td>
<td>98.782</td>
</tr>
<tr>
<td>2</td>
<td>2.32</td>
<td>36.196</td>
<td>1.218</td>
</tr>
</tbody>
</table>
## 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: 0-23  H: 0-16  N: 0-2  O: 0-2  Cl: 0-1
SAMPLE CODE: GWK-SAM-S-PAGE-14 POLAR
511701AS374 18 (9.257) AM (Top,A,At:3000.0,195.13,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1.40.00)

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>307.0938</td>
<td>307.0900</td>
<td>3.8</td>
<td>9.6</td>
<td>16.5</td>
<td>121.0</td>
<td>C23 H16 N2 O2 Cl</td>
</tr>
</tbody>
</table>
Sample Name: GVK-SAM-5-PAGE-14 NP
Vial position: Fl-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, 1.7µm)
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

<table>
<thead>
<tr>
<th>Pea</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>2.04</td>
<td>112.299</td>
<td>10.138</td>
</tr>
<tr>
<td>2</td>
<td>2.26</td>
<td>995.449</td>
<td>89.862</td>
</tr>
</tbody>
</table>

---
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: 0-23  H: 0-16  N: 0-2  O: 0-2  Cl: 0-1
SAMPLE CODE:GVIK-SAM-5-PAGE-14NP
511701A337527 (0.37S) AM (Top4, Ar,0000.0,195.15,1.00,LS 10): Sm (Mn, 2x1.00); Sb (1,40.00 )

Minimum: -1.5
Maximum: 1.9

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>1-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>387.0919</td>
<td>387.0900</td>
<td>1.9</td>
<td>4.9</td>
<td>16.5</td>
<td>356.8</td>
<td>C23 H16 N2 O2 Cl</td>
</tr>
</tbody>
</table>
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\rund-fa-3.0 min-1.m
instrument id : anl-mcl5-lcms-001

rund-fa-3.0 min.m

column: acquity uplc beh c18 (50mmx2.1mm, 1.7µm)
mobile phase: b1: 0.1% fa in water a1: 0.1% fa in acn
gradient: time (min) /%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


<table>
<thead>
<tr>
<th>peak</th>
<th>rt</th>
<th>area</th>
<th>area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.93</td>
<td>2655.073</td>
<td>99.221</td>
</tr>
<tr>
<td>2</td>
<td>2.04</td>
<td>15.650</td>
<td>0.585</td>
</tr>
<tr>
<td>3</td>
<td>2.08</td>
<td>5.207</td>
<td>0.195</td>
</tr>
</tbody>
</table>
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

SAMPLE CODE: GVK-SAM-5-PAGE-15 POLAR
511701A367 21 (0.285) AM (Top, 4, Ar, 5000.0, 195.14, 1.00, LS 10); Sm (Mn, 2x1.00); Sb (1.40.00)

Minimum: 371.1231
Maximum: 5.0 1000.0 50.0

Mass  Calc. Mass  mDa  PPM  DBE  1-FIT  Formula
371.1231  371.1296  3.5  9.4  16.5  407.5  C23 H16 N2 O2 F

1: TOF MS ES+  6.33e3
**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, 1.7μm)  
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

---

<table>
<thead>
<tr>
<th>Peak</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.80</td>
<td>58.451</td>
<td>2.621</td>
</tr>
<tr>
<td>2</td>
<td>1.99</td>
<td>2144.079</td>
<td>96.133</td>
</tr>
<tr>
<td>3</td>
<td>2.17</td>
<td>27.788</td>
<td>1.246</td>
</tr>
</tbody>
</table>

---

DAD1 A. Sig.-215.4 Ref-off (DEC-20153112201531122015-GVK-SAM-5-PAGE-15NP.D - DEC-20153112201531122015-BLANK-05.D)
**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

SAMPLE CODE: GVK: SAM 5-PAGE-54NP
511701A3368 39 (0.562)

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>371.1272</td>
<td>371.1196</td>
<td>7.6</td>
<td>20.5</td>
<td>16.5</td>
<td>C23 H16 N2 O2 F</td>
</tr>
</tbody>
</table>

Minimum: 5.0 1000.0 50.0
Maximum: -1.5
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: 0.24  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)

Minimum:  
Maximum:  
Mass  Calc. Mass  mDa  PPM  DBE  1-FIT  Formula
421.1137  421.1164  -2.7  -6.4  16.5  150.2  C24 H16 N2 O2 F3

1: TOF MS ES+ 8.63e3
<table>
<thead>
<tr>
<th>Pea</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.38</td>
<td>5.918</td>
<td>0.187</td>
</tr>
<tr>
<td>2</td>
<td>1.47</td>
<td>17.465</td>
<td>0.553</td>
</tr>
<tr>
<td>3</td>
<td>1.54</td>
<td>3.148</td>
<td>0.049</td>
</tr>
<tr>
<td>4</td>
<td>1.66</td>
<td>6.057</td>
<td>0.192</td>
</tr>
<tr>
<td>5</td>
<td>1.80</td>
<td>1.733</td>
<td>0.055</td>
</tr>
<tr>
<td>6</td>
<td>1.85</td>
<td>1.112</td>
<td>0.035</td>
</tr>
<tr>
<td>7</td>
<td>1.90</td>
<td>3.855</td>
<td>0.122</td>
</tr>
<tr>
<td>8</td>
<td>1.97</td>
<td>3.328</td>
<td>0.105</td>
</tr>
<tr>
<td>9</td>
<td>2.04</td>
<td>19.808</td>
<td>0.627</td>
</tr>
<tr>
<td>10</td>
<td>2.20</td>
<td>0.961</td>
<td>0.030</td>
</tr>
<tr>
<td>11</td>
<td>2.26</td>
<td>30.946</td>
<td>97.365</td>
</tr>
<tr>
<td>12</td>
<td>2.44</td>
<td>2.494</td>
<td>0.079</td>
</tr>
</tbody>
</table>
**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: 0-24  H: 0-16  N: 0-2  O: 0-2  F: 0-3

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

511701A338119 (0.266) AM (Top,4, At,5000.0,195.16,1,0,0,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>1-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>421.1143</td>
<td>421.1164</td>
<td>-2.1</td>
<td>-5.0</td>
<td>16.5</td>
<td>205.7</td>
<td>C24 H16 N2 O2 F3</td>
</tr>
</tbody>
</table>
Sample Name: GVK-SAM-6-PAGE-4POLAR
Vial position: P1-C-02
Date of Analysis: 8/16/2016 9:08:01 PM
Injection Vol: 0.500ul
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

<table>
<thead>
<tr>
<th>Peak</th>
<th>RT (min)</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.17</td>
<td>4.740</td>
<td>0.416</td>
</tr>
<tr>
<td>2</td>
<td>1.81</td>
<td>1.947</td>
<td>0.171</td>
</tr>
<tr>
<td>3</td>
<td>2.55</td>
<td>167.448</td>
<td>14.705</td>
</tr>
<tr>
<td>4</td>
<td>2.64</td>
<td>904.193</td>
<td>79.406</td>
</tr>
<tr>
<td>5</td>
<td>2.71</td>
<td>14.294</td>
<td>1.255</td>
</tr>
<tr>
<td>6</td>
<td>2.75</td>
<td>24.465</td>
<td>2.149</td>
</tr>
<tr>
<td>7</td>
<td>2.89</td>
<td>6.521</td>
<td>0.573</td>
</tr>
<tr>
<td>8</td>
<td>2.92</td>
<td>11.155</td>
<td>0.980</td>
</tr>
<tr>
<td>9</td>
<td>2.98</td>
<td>3.929</td>
<td>0.345</td>
</tr>
</tbody>
</table>
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:

SAMPLE CODE: SPK-SAM-6-PAGE-4 POLAR
511701A2143 36 (0,552) AM (Top,4, Ar.5000,0,195.16,1,00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  Formula
421.0493 421.0511  -2.8  -6.7  16.5  28.6  C23 H15 N2 O2 Cl2
Sample Name  : GVK-SAM-6-PAGE-4NP  Vial position : F1-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, 1.7µm)  
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  

<table>
<thead>
<tr>
<th>Peak</th>
<th>RT (min)</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.67</td>
<td>29.772</td>
<td>1.196</td>
</tr>
<tr>
<td>2</td>
<td>2.02</td>
<td>17.808</td>
<td>0.716</td>
</tr>
<tr>
<td>3</td>
<td>2.17</td>
<td>23.815</td>
<td>0.957</td>
</tr>
<tr>
<td>4</td>
<td>2.29</td>
<td>10.580</td>
<td>0.425</td>
</tr>
<tr>
<td>5</td>
<td>2.41</td>
<td>2.399</td>
<td>0.096</td>
</tr>
<tr>
<td>6</td>
<td>2.66</td>
<td>2376.283</td>
<td>95.479</td>
</tr>
<tr>
<td>7</td>
<td>2.92</td>
<td>9.834</td>
<td>0.395</td>
</tr>
<tr>
<td>8</td>
<td>3.02</td>
<td>18.317</td>
<td>0.736</td>
</tr>
</tbody>
</table>

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
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

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); Sn (Mn, 2x1.00); Sb (0,40.00)

Minimum: 5.0
Maximum: 1000.0

Mass  Calc. Mass    mDa  PPM  DBE  1-FIT  Formula
421.0549  421.0541  3.8  9.0  16.5  11.3  C23 H15 N2 O2 C12

1: TOF MS ES+
78.1
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\METHOD\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, 1.7µm)
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

<table>
<thead>
<tr>
<th>Peak</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.65</td>
<td>16.33</td>
<td>0.521</td>
</tr>
<tr>
<td>2</td>
<td>2.52</td>
<td>20.588</td>
<td>0.657</td>
</tr>
<tr>
<td>3</td>
<td>2.62</td>
<td>3020.892</td>
<td>96.350</td>
</tr>
<tr>
<td>4</td>
<td>2.67</td>
<td>15.544</td>
<td>0.496</td>
</tr>
<tr>
<td>5</td>
<td>2.71</td>
<td>18.607</td>
<td>0.593</td>
</tr>
<tr>
<td>6</td>
<td>2.86</td>
<td>35.877</td>
<td>1.144</td>
</tr>
<tr>
<td>7</td>
<td>2.95</td>
<td>7.499</td>
<td>0.239</td>
</tr>
</tbody>
</table>

146
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 POLAR
511701A2151 31 (0.452) AM (Top,4, Ar:5000.0,195.14,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1.40, 0.00)

Minimum:
-1.5

Maximum:
5.0  1000.0  50.0

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>Form</th>
<th>1-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>367.0568</td>
<td>367.1447</td>
<td>-87.9</td>
<td>-239.5</td>
<td>16.5</td>
<td>1717.9</td>
<td>C24 H19 N2 O2</td>
<td></td>
</tr>
</tbody>
</table>
Sample Name: GVK-SAM-6-PAGE-24NF  
Vial position: F1-A-05  
Date of Analysis: 29/08/2016, 7:40:43 AM  
Injection Vol: 0.5 μL  
Acq. Method: C:\CHEM32\METHODS\RND-FA-3.5 MIN.M  
Instrument ID: ANL-MCL5-LCMS-001  
C:\CHEM32\DATA\2016\AUG-2016\511608C4669.D

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

<table>
<thead>
<tr>
<th>Pea</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.72</td>
<td>2670.468</td>
<td>99.745</td>
</tr>
<tr>
<td>2</td>
<td>2.95</td>
<td>6.838</td>
<td>0.255</td>
</tr>
</tbody>
</table>
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, 0, 195.18, 1.00, LS 10); Sm (Mn, 2x1.00); Sb (1.40.00)

Minimum:  367.1483
Maximum:  367.1477

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
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\METHODS\RND-FA-3.5 MIN.M
Instrument ID: ANL-MCL5-LCMS-001
C:\CHEM32\DATA\2016\AUG-2016\S11608C4676.D

Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7μm)
Mobile Phase: B1: 0.1% FA IN WATER A1: 0.1% FA IN ACN
Gradient: Time (min) /%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

<table>
<thead>
<tr>
<th>Peak</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.15</td>
<td>1631.143</td>
<td>97.189</td>
</tr>
<tr>
<td>2</td>
<td>2.77</td>
<td>47.183</td>
<td>2.811</td>
</tr>
</tbody>
</table>

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
511701A213039 (0.564)

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>305.1272</td>
<td>305.1290</td>
<td>-1.8</td>
<td>-5.9</td>
<td>12.5</td>
<td>C19 H17 N2 O2</td>
</tr>
</tbody>
</table>

Minimum: 5.0
Maximum: 1000.0

1: TOF MS ES+ 187
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\METHODS\RND-FA-3.5 MIN.M  
Instrument ID: ANL-MCL5-LCMS-001  
C:\CHEM32\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, 2.8/95, 3.4/98, 3.41/2, 3.5/2  
Column Flow Rate: 0.6 ml/min  
Column Temperature: 60°C  

<table>
<thead>
<tr>
<th>Pea</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>---</td>
<td>---</td>
<td>------</td>
<td>--------</td>
</tr>
<tr>
<td>1</td>
<td>2.00</td>
<td>36.412</td>
<td>1.238</td>
</tr>
<tr>
<td>2</td>
<td>2.15</td>
<td>156.837</td>
<td>5.333</td>
</tr>
<tr>
<td>3</td>
<td>2.25</td>
<td>2747.358</td>
<td>93.428</td>
</tr>
</tbody>
</table>
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(s) 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-S-PAGE-25NP 166
GVK-SAM-S-PAGE-25NP 04 (0.350) AM (Top, Ar,0.0,195,19,1.00,1.00,LS 10); Sm (M, 2x1.00); Sb (0.40,0.0)

Minimum:  5.0  1000.0  50.0
Maximum:  1.5

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-32P  Vial position : E1-A-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 (50nmx2.1mm, 1.7μm)
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

<table>
<thead>
<tr>
<th>Peak</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.41</td>
<td>3376.333</td>
<td>97.437</td>
</tr>
<tr>
<td>2</td>
<td>2.75</td>
<td>88.805</td>
<td>2.563</td>
</tr>
</tbody>
</table>

---

*DAD1 A, Sig=215.4 Ref-off (2016-SEP-2016/1609B6720.D - 2016-SEP-2016/BLANK-22062016-00002.D)*
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
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, 0.0, 0.0, 0.0, 1.00, LS 10); Sm (Min, 2x1.00); Sb (0,40.00)

Minimum: 397.1591  397.1552  3.9  9.8  16.5  737.7  C25 H21 N2 O3
Analysis Method: RND-FA-3.0-MN  Injection Vol: 0.500 ul
Sample Name: GVK-SAM-6-PAGE-32NONPOLAR

<table>
<thead>
<tr>
<th>Peak</th>
<th>RT (min)</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.443</td>
<td>763.32</td>
<td>5.607</td>
</tr>
<tr>
<td>2</td>
<td>2.082</td>
<td>1265.604</td>
<td>92.963</td>
</tr>
<tr>
<td>3</td>
<td>2.292</td>
<td>7.439</td>
<td>0.546</td>
</tr>
<tr>
<td>4</td>
<td>2.362</td>
<td>12.033</td>
<td>0.884</td>
</tr>
</tbody>
</table>
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: 0.25  H: 0.21  N: 0.2  O: 0.3
SAMPLE CODE:GIVK-SAM-6-PAGE-32NP
511701A212S 37 (0.545) AM (Top,4, Ar,5000.0,195.16,1.00,LS 10); Sm (Mn, 2x1.00); Sb (1,40.00)

Minimum: 1.5
Maximum: 5.0  1000.0  50.0

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>1-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>397.1567</td>
<td>397.1552</td>
<td>1.5</td>
<td>3.8</td>
<td>16.5</td>
<td>87.1</td>
<td>C25 H21 N2 O3</td>
</tr>
</tbody>
</table>
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

<table>
<thead>
<tr>
<th>Pea</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>No</td>
<td>min</td>
<td>----------</td>
<td>--------</td>
</tr>
<tr>
<td>1</td>
<td>2.76</td>
<td>3894.532</td>
<td>99.152</td>
</tr>
<tr>
<td>2</td>
<td>2.84</td>
<td>33.301</td>
<td>0.848</td>
</tr>
</tbody>
</table>

**DAD1 A, Sig=215,4 Ref-off (511609C1656.D - BLANK-28092016-2C.D)**
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:  401.1052  -1.5
Maximum:  401.1057   50.0

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>401.1052</td>
<td>401.1057</td>
<td>-0.5</td>
<td>-1.2</td>
<td>16.5</td>
<td>C24 H18 N2 O2 Cl</td>
</tr>
</tbody>
</table>
Sample Name: GVK-SAM-6-PAGE-33NP
Vial position: F2-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, 1.7µm)
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

>
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

Minimum:  5.0  1000.0  50.0
Maximum:  -1.5

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-PIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>401.1035</td>
<td>401.1057</td>
<td>-2.2</td>
<td>-5.5</td>
<td>16.5</td>
<td>20.6</td>
<td>C24 H18 N2 O2 Cl</td>
</tr>
</tbody>
</table>
Sample Name: GVK-SAM-6-page-34 Polar
Date of Analysis: 9/29/2016 11:28:34 PM
Injection Vol: 0.500µl
Acq. Method: C:\CHEM32\METHODS\RND-FA-3.5 MIN.M
Instrument ID: ANL-MCL5-LCMS-001

RND-FA-3.5 MIN.M
Column: ACQUITY UFLC BEH C18 (50mmx2.1mm, 1.7µm)
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

---

<table>
<thead>
<tr>
<th>Pea</th>
<th>RT (min)</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.64</td>
<td>22.15</td>
<td>0.776</td>
</tr>
<tr>
<td>2</td>
<td>2.26</td>
<td>2814.225</td>
<td>98.617</td>
</tr>
<tr>
<td>3</td>
<td>2.94</td>
<td>17.300</td>
<td>0.606</td>
</tr>
</tbody>
</table>

---
**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 Bio sciences (pvt)Ltd
Analytical Research and Development

Date of analysis: 25-Mar-2017 11:14:06
Instrum ent ID: ANL-MCL3-LCMS-001
1: TOF MS ES+
1.12e4

**Experimental Data**

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>1-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>435.1340</td>
<td>435.1320</td>
<td>2.0</td>
<td>4.6</td>
<td>16.5</td>
<td>275.0</td>
<td>C25 H18 N2 O2 F3</td>
</tr>
</tbody>
</table>
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

Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7µm)
Mobile Phase: B1: 0.1% FA IN WATER A1: 0.1%FA IN ACN
Gradient: Time (min) /%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

<table>
<thead>
<tr>
<th>Peak</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.81</td>
<td>3797.606</td>
<td>84.422</td>
</tr>
<tr>
<td>2</td>
<td>2.86</td>
<td>543.713</td>
<td>12.087</td>
</tr>
<tr>
<td>3</td>
<td>2.99</td>
<td>121.975</td>
<td>2.712</td>
</tr>
<tr>
<td>4</td>
<td>3.03</td>
<td>35.061</td>
<td>0.779</td>
</tr>
</tbody>
</table>

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:

GVK Bio sciences (pvt) Ltd
Analytical Research and Development

Date of analysis: 25-Mar-2017 18:49
Instrument ID: ANL-MCL3-LCMS-001
1: TOF MS ES+
5.03e5

Minimum: 121
Maximum: 5000.0

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBK</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>435.1335</td>
<td>435.1320</td>
<td>1.5</td>
<td>3.4</td>
<td>16.5</td>
<td>533.7</td>
<td>C25 H18 N2 O2 F3</td>
</tr>
</tbody>
</table>
Sample Name: GVK-SAM-6-page-37 polar  
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  

<table>
<thead>
<tr>
<th>Peak</th>
<th>RT (min)</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.63</td>
<td>10.11</td>
<td>1.845</td>
</tr>
<tr>
<td>2</td>
<td>2.19</td>
<td>6.889</td>
<td>1.257</td>
</tr>
<tr>
<td>3</td>
<td>2.62</td>
<td>22.396</td>
<td>4.085</td>
</tr>
<tr>
<td>4</td>
<td>2.69</td>
<td>476.022</td>
<td>86.630</td>
</tr>
<tr>
<td>5</td>
<td>2.86</td>
<td>18.523</td>
<td>3.379</td>
</tr>
<tr>
<td>6</td>
<td>2.86</td>
<td>14.277</td>
<td>2.604</td>
</tr>
</tbody>
</table>

*DA T A, Sig=215,4 Ref-off (2016/OCT.PRO/51161089619-D - 2016/OCT.PRO/BLANK-25-10-2016-02-D)*
**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
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-S-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)

![Chemical Structure](image)

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>525.1588</td>
<td>525.1637</td>
<td>-4.9</td>
<td>-9.3</td>
<td>16.5</td>
<td>817.4</td>
<td>C28 H24 N2 O5 F3</td>
</tr>
</tbody>
</table>

Minimum: 1
Maximum: 5.0 1000.0 50.0
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: B: 0.1 % FA IN WATER  A: 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

<table>
<thead>
<tr>
<th>Pea</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>2.14</td>
<td>74.539</td>
<td>2.330</td>
</tr>
<tr>
<td>2</td>
<td>2.69</td>
<td>3090.920</td>
<td>96.618</td>
</tr>
<tr>
<td>3</td>
<td>2.86</td>
<td>33.640</td>
<td>1.052</td>
</tr>
</tbody>
</table>
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

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>1-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>525.1664</td>
<td>525.1637</td>
<td>2.7</td>
<td>5.1</td>
<td>16.5</td>
<td>1203.7</td>
<td>C28 H24 N2 O5 F3</td>
</tr>
</tbody>
</table>

Minimum: 5.0  1000.0  50.0
Maximum: -1.5
Sample Name: GVK-SAM-6-PAGE-38POLAR  
Vial position: F1-C-09
Date of Analysis: 10/27/2016  1:42:41 PM  
Injection Vol: 0.100uL
Acq. Method: C:\CHEM32\METHODS\RND-FA-3.5 MIN.M
Instrument ID: ANL-MCLS-LCMS-001

RND-FA-3.5 MIN.M
Column: ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7μm)
Mobile Phase: B1: 0.1% FA IN WATER  A1: 0.1%FA IN ACN
Gradient: Time (min) /%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

---

![Graph](image)

<table>
<thead>
<tr>
<th>Pea</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.77</td>
<td>14.05</td>
<td>1.27</td>
</tr>
<tr>
<td>2</td>
<td>2.00</td>
<td>1.395</td>
<td>0.127</td>
</tr>
<tr>
<td>3</td>
<td>2.31</td>
<td>1079.401</td>
<td>98.103</td>
</tr>
<tr>
<td>4</td>
<td>2.47</td>
<td>5.430</td>
<td>0.494</td>
</tr>
</tbody>
</table>

---
# 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

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-5-PAGE-38POLAR**

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>1-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>487.1874</td>
<td>487.1869</td>
<td>0.5</td>
<td>1.0</td>
<td>16.5</td>
<td>1381.7</td>
<td>C28 H27 N2 O6</td>
</tr>
</tbody>
</table>
Sample Name: GVK-SAM-6-PAGE-38HP
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

<table>
<thead>
<tr>
<th>Peak</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.31</td>
<td>1209.406</td>
<td>98.092</td>
</tr>
<tr>
<td>2</td>
<td>2.39</td>
<td>23.501</td>
<td>1.908</td>
</tr>
</tbody>
</table>
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
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 (0.40,0.0)

Minimum:  1.0  1000.0  50.0
Maximum: 5.0

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-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\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

<table>
<thead>
<tr>
<th>Peak</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.96</td>
<td>5.811</td>
<td>0.287</td>
</tr>
<tr>
<td>2</td>
<td>2.01</td>
<td>1978.339</td>
<td>97.613</td>
</tr>
<tr>
<td>3</td>
<td>2.07</td>
<td>38.432</td>
<td>1.900</td>
</tr>
</tbody>
</table>
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(a) 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: 395.1644 mass 395.1607
Maximum: 5.0 1000.0 50.0

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>395.1644</td>
<td>395.1607</td>
<td>3.7</td>
<td>9.4</td>
<td>12.5</td>
<td>C22 H23 N2 O5</td>
</tr>
</tbody>
</table>
Sample Name: GVK-SAM-6-PAGE-39MF
Vial position: F1-A-09
Date of Analysis: 10/28/2016 7:08:34 PM
Injection Vol: 0.300μL
Acq. Method: C:\CHEM32\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, 1.7μm)
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

<table>
<thead>
<tr>
<th>Peak</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.01</td>
<td>11.331</td>
<td>0.339</td>
</tr>
<tr>
<td>2</td>
<td>2.07</td>
<td>3333.982</td>
<td>99.661</td>
</tr>
</tbody>
</table>
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

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>395.1610</td>
<td>395.1607</td>
<td>0.3</td>
<td>0.8</td>
<td>12.5</td>
<td>1503.1</td>
<td>C22 H23 N2 O5</td>
</tr>
</tbody>
</table>
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
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.S-PAGE-10NP
GVK.SAM.S-PAGE-10NP

Minimum:  5.0  1000.0  50.0
Maximum:  

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

1: TOF MS ES+ 1.58e3
Sample Name: GVK-SAM-6-PAGE-40NF  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: %B: 0.1% FA IN WATER A1: 0.1%FA IN ACN
Gradient: Time (min) /%B: 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

<table>
<thead>
<tr>
<th>Pea</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>No</td>
<td>min</td>
<td>------</td>
<td>------</td>
</tr>
<tr>
<td>-----</td>
<td>-----</td>
<td>--------</td>
<td>--------</td>
</tr>
<tr>
<td>1</td>
<td>1.77</td>
<td>8.143</td>
<td>0.366</td>
</tr>
<tr>
<td>2</td>
<td>2.17</td>
<td>8.699</td>
<td>0.391</td>
</tr>
<tr>
<td>3</td>
<td>2.20</td>
<td>3.617</td>
<td>0.162</td>
</tr>
<tr>
<td>4</td>
<td>2.24</td>
<td>1.274</td>
<td>0.057</td>
</tr>
<tr>
<td>5</td>
<td>2.32</td>
<td>16.844</td>
<td>0.757</td>
</tr>
<tr>
<td>6</td>
<td>2.45</td>
<td>6.138</td>
<td>0.278</td>
</tr>
<tr>
<td>7</td>
<td>2.49</td>
<td>1.282</td>
<td>0.058</td>
</tr>
<tr>
<td>8</td>
<td>2.68</td>
<td>2172.804</td>
<td>97.600</td>
</tr>
<tr>
<td>9</td>
<td>2.86</td>
<td>7.396</td>
<td>0.332</td>
</tr>
</tbody>
</table>
**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
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

![Chemical Structure](image)

**Minimum:**
**Maximum:**

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>1-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>491.1375</td>
<td>491.1374</td>
<td>0.1</td>
<td>0.2</td>
<td>16.5</td>
<td>0.0</td>
<td>C27 H24 N2 O5 Cl</td>
</tr>
</tbody>
</table>
Date of Analysis : 12/7/2016 9:46:58 PM  Injection Vol : 2.000uL
Acq. Method : C:\CHEM32\METHODS\RND-FA- 3.5 MIN.M  Instrument ID : ANL-MCL5-LCMS-001
Sample Name : GVK-SAM-6-PAGE-44P1

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

<table>
<thead>
<tr>
<th>Peak</th>
<th>RT (min)</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.98</td>
<td>1171.845</td>
<td>94.393</td>
</tr>
<tr>
<td>2</td>
<td>2.11</td>
<td>45.472</td>
<td>3.663</td>
</tr>
<tr>
<td>3</td>
<td>2.34</td>
<td>24.131</td>
<td>1.944</td>
</tr>
</tbody>
</table>
**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 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,0,0,0,195,16,1.00, LS 10); Sm (Mn, 2x1.00); Sb (0,40.00)

![Chemical Structure](image)

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>354.1246</td>
<td>354.1243</td>
<td>0.3</td>
<td>0.8</td>
<td>16.5</td>
<td>687.7</td>
<td>C22 H16 N3 O2</td>
</tr>
</tbody>
</table>

Minimum: -1.5

Maximum: 5.0

1: TOF MS ES+

6.36e3
**LCMS REPORT**

**Vial position:** P2-C-02

**Date of Analysis:** 12/7/2016

**Injection Vol:** 0.300μL

**Acq. Method:** C:\CHEM32\METHODS\RND-FA-3.5 MIN.M

**Sample Name:** CVK-SAM-6-PACE-44P2

**Instrument ID:** ANL-MCL5-LCMS-001

---

**RND-FA-3.5 MIN.M**

**Column:** ACQUITY UPLC BEH C18 (50mmx2.1mm, 1.7μm)

**Mobile Phase:** B1: 0.1% FA IN WATER A1: 0.1%FA IN ACN

**Gradient:** Time (min) /%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

---

**DAD1 A: S Ig-215,4 Ref-off (2016\DEC\PRO511612A0172.D - 2016\DEC\PROBLANK-06122016-05.D)**

<table>
<thead>
<tr>
<th>Peak</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.97</td>
<td>11.699</td>
<td>2.999</td>
</tr>
<tr>
<td>2</td>
<td>2.00</td>
<td>1.353</td>
<td>0.347</td>
</tr>
<tr>
<td>3</td>
<td>2.02</td>
<td>3.040</td>
<td>0.779</td>
</tr>
<tr>
<td>4</td>
<td>2.11</td>
<td>374.036</td>
<td>95.875</td>
</tr>
</tbody>
</table>

---

259
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

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>1-PIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>354.1237</td>
<td>354.1243</td>
<td>-0.6</td>
<td>-1.7</td>
<td>16.5</td>
<td>678.0</td>
<td>C22 H16 N3 O2</td>
</tr>
</tbody>
</table>
Sample Name: GVK-SAM-6-PAGE-47-POLAR

<table>
<thead>
<tr>
<th>Peak</th>
<th>RT (min)</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.680</td>
<td>2.073</td>
<td>0.191</td>
</tr>
<tr>
<td>2</td>
<td>1.845</td>
<td>2.524</td>
<td>0.233</td>
</tr>
<tr>
<td>3</td>
<td>1.879</td>
<td>2.702</td>
<td>0.249</td>
</tr>
<tr>
<td>4</td>
<td>1.990</td>
<td>1.078659</td>
<td>99.161</td>
</tr>
<tr>
<td>5</td>
<td>2.049</td>
<td>1.620</td>
<td>0.167</td>
</tr>
</tbody>
</table>
### 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 closest results for each mass)

Elements Used:
C: 0.21  H: 0.15  N: 0.2  O: 0.3

GVK-SAM-6-PAGE-4TPOLAR
GVK-SAM-6-PAGE-4TPOLAR 20 (0.276) AM (Top,4,Ar,0,0,195.17,1.00,LS 10); Sm (Mn, 2x1.00); Sb (0.40.00)

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>343.1089</td>
<td>343.1083</td>
<td>0.6</td>
<td>1.7</td>
<td>15.5</td>
<td>435.3</td>
<td>C21 H15 N2 O3</td>
</tr>
</tbody>
</table>
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

<table>
<thead>
<tr>
<th>Pea</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>2.08</td>
<td>10.457</td>
<td>0.824</td>
</tr>
<tr>
<td>2</td>
<td>2.36</td>
<td>2.451</td>
<td>0.193</td>
</tr>
<tr>
<td>3</td>
<td>2.46</td>
<td>1.236e3</td>
<td>97.377</td>
</tr>
<tr>
<td>4</td>
<td>2.60</td>
<td>12.624</td>
<td>0.995</td>
</tr>
<tr>
<td>5</td>
<td>2.66</td>
<td>5.219</td>
<td>0.411</td>
</tr>
<tr>
<td>6</td>
<td>2.80</td>
<td>2.543</td>
<td>0.200</td>
</tr>
</tbody>
</table>
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, 196.171.00, LS 10); Sm (Mn, 2x1.00); Sb (0.40.000)

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>1-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>343.1086</td>
<td>343.1083</td>
<td>0.3</td>
<td>0.9</td>
<td>15.5</td>
<td>126.0</td>
<td>C21 H15 N2 O3</td>
</tr>
</tbody>
</table>
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

<table>
<thead>
<tr>
<th>Peak</th>
<th>RT (min)</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.72</td>
<td>627,993</td>
<td>98.146</td>
</tr>
<tr>
<td>2</td>
<td>1.97</td>
<td>4,990</td>
<td>0.780</td>
</tr>
<tr>
<td>3</td>
<td>2.02</td>
<td>3.045</td>
<td>0.476</td>
</tr>
<tr>
<td>4</td>
<td>2.06</td>
<td>3.830</td>
<td>0.599</td>
</tr>
</tbody>
</table>
**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 closest results for each mass)

Elements Used:
C: 0-17  H: 0-14  N: 0-3  O: 0-2

GVK-SAM-8-PAGE-42POLAR

GVK-SAM-9-PAGE-42POLAR 24 (0.348) AM (Tap,4,Ar,0,0,195.17,1.00,LS 10); Sm (Mn, 2x1.00); Sb (0.40.00)

![Chemical Structure](image)

1: TOF MS ES+ 1.05e4

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>292.1090</td>
<td>292.1086</td>
<td>0.4</td>
<td>1.4</td>
<td>12.5</td>
<td>600.0</td>
<td>C17 H14 N3 O2</td>
</tr>
</tbody>
</table>

Minimum: 5.0  1000.0  50.0

Maximum:

Minimum: 5.0  1000.0  50.0

Maximum:
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

<table>
<thead>
<tr>
<th>Pea</th>
<th>RT</th>
<th>Area</th>
<th>Area %</th>
</tr>
</thead>
<tbody>
<tr>
<td>No</td>
<td>min</td>
<td>------</td>
<td>--------</td>
</tr>
<tr>
<td>1</td>
<td>1.36</td>
<td>6.958</td>
<td>0.962</td>
</tr>
<tr>
<td>2</td>
<td>1.72</td>
<td>6.374</td>
<td>0.882</td>
</tr>
<tr>
<td>3</td>
<td>1.88</td>
<td>699.856</td>
<td>96.807</td>
</tr>
<tr>
<td>4</td>
<td>1.97</td>
<td>3.814</td>
<td>0.528</td>
</tr>
<tr>
<td>5</td>
<td>1.99</td>
<td>1.216</td>
<td>0.168</td>
</tr>
<tr>
<td>6</td>
<td>2.02</td>
<td>4.720</td>
<td>0.653</td>
</tr>
</tbody>
</table>
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 )

Minimum:  
Maximum:  
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
**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, 0.195, 1.17, 1.00; LS 10); Sm (Mn, 2x1.00); Sb (0.40.00)

![Chemical Structure](image)

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-PIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>396.1552</td>
<td>396.1559</td>
<td>-0.7</td>
<td>-1.8</td>
<td>12.5</td>
<td>246.4</td>
<td>C21H22N3O5</td>
</tr>
<tr>
<td>Pea</td>
<td>RT</td>
<td>Area</td>
<td>Area %</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-----</td>
<td>-----</td>
<td>-------</td>
<td>---------</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>No</td>
<td>min</td>
<td>------</td>
<td>---------</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>1.575</td>
<td>26.450</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>2</td>
<td>1.672</td>
<td>190.1219</td>
<td>96.550</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Acq. Method: ANL-FR-3.0-MIN  Injection Vol: 0.500 ul
Sample Name: GVK-SAM-6-PAGE-41-P2
Instrument ID: ANL-MCL3-LCMS-003

GVK_LCMS_18
### 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

![Chemical Structure](image)

<table>
<thead>
<tr>
<th>Mass</th>
<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>396.1557</td>
<td>396.1559</td>
<td>-0.2</td>
<td>-0.5</td>
<td>12.5</td>
<td>573.7</td>
<td>C21 H22 N3 O5</td>
</tr>
</tbody>
</table>

Minimum:  1.5
Maximum:  5.0  1000.0  50.0