One-pot four component domino strategy for the synthesis of novel spirooxindole pyrrolizine linked 1,2,3-triazoles *via* stereo- and regioselective [3+2] cycloaddition reaction in acidic Medium.

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1'-((1-(4-fluorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-6b,7,8,9-tetrahydro-6*H* spiro[chromeno[3,4-*a*]pyrrolizine-11,3'-indoline]-2',6(6*aH*,11*aH*)-dione (5a)



White solid; Yield = 89%; M.p.= 190-192; IR (CHCl₃) v/cm⁻¹ = 2965, 1756, 1516, 1461, 1227, 752; ¹H NMR (400MHz, DMSO-*d*₆) $\delta_{\rm H}$ = 7.76 (d, 1H, *J* = 6.87 Hz, Ar-H), 7.73-7.69 (m, 2H, Ar-H), 7.48 (s, 1H, Triazole), 7.42-7.34 (m, 3H, Ar-H), 7.17-7.13 (t, 1H, Ar-H), 7.05 (d, 1H, *J* = 7.63 Hz, Ar-H), 6.78 (d, 1H, *J* = 8.39, Ar-H), 6.62-6.59 (t, 1H, Ar-H), 6.47-6.44 (t, 1H, Ar-H), 6.05 (d, 1H, *J* = 7.63 Hz, Ar-H), 4.67-4.55 (q, 2H, -CH₂), 4.40-4.38 (dt, 1H, J = 3.41, 8.01 Hz, -CH), 4.14-4.11 (d, 1H, *J* = 11.45 Hz, -CH), 3.38-3.36 (dd, 1H, *J* = 11.45, 3.21, Hz, -CH), 3.17-3.13 (m, 1H, -CH₂), 2.58-2.55 (m, 1H, -CH₂), 2.34-2.28 (m, 1H, -CH₂), 1.86-1.77 (m, 2H, -CH₂), 1.63-1.57 (m, 1H, -CH₂); ¹³C NMR (100 MHz, DMSO-*d*₆) $\delta_{\rm C}$ = 175.3, 167.5, 161.7, 150.7, 143.2, 142.8, 132.9, 130.0, 128.2, 127.2, 126.6, 125.3, 123.0, 122.8, 122.6, 120.9, 117.4, 116.7, 116.2, 109.5, 76.0, 67.4, 50.3, 46.8, 42.8, 33.9, 32.7, 26.0; LCMS (ESI) *m/z* calcd for C₃₀H₂₄FN₅O₃ : 521.1865 [M⁺]; found: 522.1937 [M⁺+H].

1'-((1-(4-methoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-6b,7,8,9-tetrahydro-6*H*spiro[chromeno[3,4-*a*]pyrrolizine-11,3'-indoline]-2',6(6*aH*,11*aH*)-dione (5b)



White solid; Yield = 85%; M.p.= 173-175; IR (CHCl₃) v/cm⁻¹ = 2964, 1757, 1517, 1225, 1041, 754; ¹H NMR (400MHz, DMSO- d_6) δ_H = 7.76-7.75 (m, 1H, Ar-H), 7.54-7.53 (m, 2H, Ar-H), 7.37-7.33 (m, 1H, Ar-H), 7.28 (s, 1H, triazole), 7.14-7.12 (m, 2H, Ar-H), 7.08-7.06 (m, 1H, Ar-H), 7.03-7.01 (m, 1H, Ar-H), 6.80-6.78 (m, 1H, Ar-H), 6.63-6.59 (m, 1H, Ar-H), 6.48-6.44 (m, 1H, Ar-H), 6.07-6.05 (m, 1H, Ar-H), 4.66-4.53 (q, 2H, -CH₂), 4.37 (brs, 1H, -CH), 4.13-4.10 (m, 1H, -CH₂), 3.77 (s, 3H, -OCH₃), 3.43-3.31 (m, 1H, -CH₂), 3.14-3.11 (m, 1H, -CH₂), 2.55-2.54 (m, 1H, -CH₂), 2.33-2.27 (m, 1H, -CH₂), 1.90-1.75 (m, 2H, -CH₂), 1.62-1.57 (m, 1H, -CH₂); 13C NMR (100 MHz, DMSO- d_6) δ_C = 175.3, 167.5, 159.3, 150.7, 143.2, 142.6, 130.0, 129.7, 128.3, 127.2, 126.6, 125.3, 123.0, 122.5, 122.1, 120.6, 117.5, 116.2, 114.8, 109.5, 76.0, 67.4, 55.5, 50.4, 46.8, 42.8, 34.0, 32.7, 26.1; LCMS (ESI) *m/z* calcd for C₃₁H₂₇N₅O4 : 533.2065 [M⁺]; found: 534.2146 [M⁺+H].

1'-((1-(4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-6b,7,8,9-tetrahydro-6*H*-spiro[chromeno[3,4-*a*]pyrrolizine-11,3'-indoline]-2',6(6*aH*,11*aH*)-dione (5c)



Pale Yellow soli; Yield = 87%; M.p. = 212-214; IR (CHCl₃) v/cm⁻¹ = 2926, 1755, 1342, 1171, 752; ¹H NMR (400MHz, DMSO-*d*₆) $\delta_{\rm H}$ = 8.40 (d, 2H, *J* = 8.39 Hz, Ar-H), 8.01 (d, 2H, *J* = 9.16, Ar-H), 7.90 (s, 1H, triazole), 7.75 (d, 1H, *J* = 6.87, Ar-H), 7.39-7.36 (t, 1H, Ar-H), 7.17-7.10 (m, 2H, Ar-H), 6.77 (d, 1H, *J* = 7.63, Ar-H), 6.62-6.58 (t, 1H, Ar-H), 6.44-6.41 (t, 1H, Ar-H), 6.01 (d, 1H, *J* = 7.63, Ar-H), 4.68-4.58 (q, 2H, -CH₂), 4.38 (brs, 1H, -CH), 4.11-4.08 (m, 1H, -CH₂), 3.43-3.30 (m, 1H, -CH₂), 3.15-3.11 (m, 1H, -CH₂), 2.59-2.55 (m, 1H, -CH₂), 2.33-2.27 (m, 1H, -CH₂), 1.84-1.73 (m, 2H, -CH₂), 1.62-1.56 (m, 1H, -CH₂); ¹³C NMR (100 MHz, DMSO-*d*₆) $\delta_{\rm C}$ = 175.2, 167.5, 150.6, 146.7, 143.3, 143.1, 140.5, 130.0, 128.2, 127.1, 126.5, 125.5, 125.3, 122.9, 122.5, 121.2, 120.7, 117.3, 116.1, 109.6, 76.03, 67.5, 50.3, 46.8, 43.0, 33.7, 32.7, 26.0; LCMS (ESI) *m/z* calcd for C₃₀H₂₄N₆O₅ : 548.1811 [M⁺]; found: 549.1888 [M⁺+H].

1'-((1-p-tolyl-1*H*-1,2,3-triazol-4-yl)methyl)-6b,7,8,9-tetrahydro-6H-spiro[chromeno[3,4*a*]pyrrolizine-11,3'-indoline]-2',6(6*aH*,11*aH*)-dione (5d)



White solid; Yield = 80%; M.p. = 170-173; IR (CHCl₃) v/cm⁻¹= 2962, 1754, 1492, 1224, 1170, 751; ¹H NMR (400MHz, DMSO-*d*₆) $\delta_{\rm H}$ = 7.78-7.75 (m, 3H, Ar-H), 7.67-7.65 (m, 2H, Ar-H), 7.62 (s, 1H, triazole), 7.40-7.36 (t, 1H, Ar-H), 7.18-7.15 (t, 1H, Ar-H), 7.08 (d, 1H, *J* = 7.63 Hz, Ar-H), 6.80-6.79 (d, 1H, *J* = 7.63, Ar-H), 6.65-6.61 (t, 1H, Ar-H), 6.49-6.45 (t, 1H, Ar-H), 6.05 (d, 1H, *J* = 7.63 Hz, Ar-H), 4.68-4.57 (q, 2H, -CH₂), 4.39 (brs, 1H, -CH), 4.15-4.12 (m, 1H, -CH₂), 3.50-3.38 (m, 1H, -CH₂), 3.17-3.16 (m, 1H, -CH₂), 2.60-2.59 (m, 1H, -CH₂), 2.35-2.29 (m, 1H, -CH₂), 2.03 (s, 3H, -CH₃), 1.86-1.80 (m, 2H, -CH₂), 1.64-1.58 (m, 1H, -CH₂); ¹³C NMR (100 MHz, DMSO-*d*₆) $\delta_{\rm C}$ = 175.2, 167.5, 150.6, 143.2, 142.6, 138.4, 134.0, 130.1, 130.0, 128.2, 127.2, 126.5, 125.3, 123.0, 122.5, 123.0, 122.5, 120.4, 120.2, 117.4, 116.2, 109.5, 76.0, 67.4, 50.3, 46.8, 42.8, 33.9, 32.7, 26.0, 20.5; LCMS (ESI) *m*/*z* calcd for C₃₁H₂₇N₅O₃ : 517.2106 [M⁺]; found: 518.2180 [M⁺+H].

1'-((1-(7-chloroquinolin-4-yl)-1*H*-1,2,3-triazol-4-yl)methyl)-6b,7,8,9-tetrahydro-6*H*-spiro[chromeno[3,4-*a*]pyrrolizine-11,3'-indoline]-2',6(6*aH*,11*aH*)-dione (5e)



White solid; Yield = 84%; M.p. = 204-206; IR (CHCl₃) v/cm⁻¹= 2963, 1758, 1609, 1225, 1175, 755; ¹H NMR (400MHz, DMSO-*d*₆) $\delta_{\rm H}$ = 9.16-9.15 (m, 1H, Ar-H), 8.29 (s, 1H, Ar-H), 7.83 (d, 1H, *J* = 7.63 Hz, Ar-H), 7.79 (s, 1H, triazole), 7.67-7.66 (m, 1H, Ar-H), 7.46-7.42 (t, 1H, Ar-H) 7.36 (s, 1H, Ar-H), 7.24-7.20 (t, 1H, Ar-H), 7.12 (d, 1H, *J* = 7.63 Hz, Ar-H), 6.69 (d, 1H, *J* = 8.39, Ar-H), 6.39-6.30 (m, 2H, Ar-H), 6.12 (d, 1H, *J* = 7.63 Hz, Ar-H), 4.84-4.72 (q, 2H, - CH₂), 4.45-4.41 (m, 1H, -CH), 4.19-4.16 (m, 1H, -CH), 3.41-3.38 (m, 1H, -CH₂), 3.24-3.17 (m, 1H, -CH₂), 2.64-2.61 (m, 1H, -CH₂), 2.39- 2.32 (m, 1H, -CH₂), 1.91-1.78 (m, 1H, -CH₂), 1.68-1.62 (m, 1H, -CH₂); ¹³C NMR (100 MHz, DMSO-*d*₆) $\delta_{\rm C}$ = 175.3, 167.4, 152.3, 150.3, 150.8, 149.4, 143.1, 142.7, 139.9, 135.4, 130.1, 129.0, 128.2, 128.0, 127.2, 126.7, 125.2, 124.2, 122.9, 122.5, 120.1, 117.5, 117.0, 116.2, 109.4, 75.9, 67.4, 50.4, 46.7, 42.6, 33.9, 32.8, 30.5, 26.0; LCMS (ESI) *m/z* calcd for C₃₃H₂₅ClN₆O₃: 588.1671 [M⁺]; found: 589.1746 [M⁺+H].

1'-((1-(4-bromophenyl)-1H-1,2,3-triazol-4-yl)methyl)-6b,7,8,9-tetrahydro-6H-

spiro[chromeno[3,4-a]pyrrolizine-11,3'-indoline]-2',6(6aH,11aH)-dione (5f)



White solid; Yield = 88%; M.p. = 174-176; IR (CHCl₃) v/cm⁻¹= 2923, 1753, 1493, 1225, 1172, 753; ¹H NMR (400MHz, DMSO-*d*₆) $\delta_{\rm H}$ = 7.80 (d, 3H, *J* = 8.39, Ar-H), 7.69 (d, 2H, *J* = 9.16, Ar-H), 7.64 (s, 1H, triazole), 7.43-7.39 (t, 1H, Ar-H), 7.22-7.18 (t, 1H, Ar-H), 7.11 (d, 1H, *J* = 8.39 Hz, Ar-H), 6.81-6.79 (m, 1H, Ar-H), 6.69-6.65 (t, 1H, Ar-H), 6.52-6.49 (t, 1H, Ar-H), 6.09 (d, 1H, Ar-H), 4.71-4.60 (q, 2H, -CH₂), 4.45-4.42 (m, 1H, -CH), 4.16 (d, 1H, *J* = 11.4 Hz, -CH₂), 3.42-3.38 (m, 1H, Ar-H), 3.23- 3.16 (m, 1H, -CH₂), 2.63-2.60 (m, 1H, -CH₂), 2.39-2.32 (m, 1H, -CH₂), 1.90-1.78 (m, 2H, -CH₂), 1.70-1.61 (m, 1H, -CH₂); ¹³C NMR (100 MHz, DMSO-*d*₆) $\delta_{\rm C}$ = 175.2, 167.4, 150.6, 143.3, 142.8, 135.5, 132.7, 130.0, 128.1, 127.2, 126.5, 123.0, 122.5, 122.2, 121.4, 120.7, 117.3, 116.1, 109.5, 76.0, 67.4, 50.3, 46.7, 42.9, 33.8, 32.7, 26.0; LCMS (ESI) *m*/*z* calcd for C₃₀H₂₄ BrN₅O₃ : 581.1064 [M⁺]; found: 582.1138 [M⁺+H], 584.1123 [M⁺+(H+2)].

1'-((1-(4-fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3-hydroxy-6b,7,8,9-tetrahydro-6Hspiro[chromeno[3,4-a]pyrrolizine-11,3'-indoline]-2',6(6aH,11aH)-dione (5g)



White solid; Yield = 85%; M.p. = 172-174; IR (CHCl₃) v/cm⁻¹= 2924, 1715, 1514, 1231, 1163, 755; ¹H NMR (400MHz, DMSO-*d*₆) $\delta_{\rm H}$ = 9.48 (s, 1H, -OH), 7.82 (s, 1H, triazole), 7.78-7.73 (m, 3H, Ar-H), 7.41-7.37 (m, 3H, Ar-H), 7.19-7.16 (t, 1H, Ar-H), 7.06 (d, 1H, *J* = 7.63 Hz, Ar-H), 6.29 (s, 1H, Ar-H), 6.08 (d, 1H, *J* = 7.63 Hz, Ar-H), 6.00 (d, 1H, *J* = 8.39 Hz, Ar-H), 4.68 (s, 2H, -CH₂), 4.39 (m, 1H, -CH), 4.08-4.05 (m, 1H, -CH₂), 3.49-3.36 (m, 1H, -CH₂), 3.17 (brs, 1H, -CH₂), 2.59-2.56 (m, 1H, -CH₂), 2.34-2.30 (m, 1H, -CH₂), 1.86-1.76 (m, 2H, - CH₂), 1.65-1.61 (m, 1H, -CH₂); ¹³C NMR (100 MHz, DMSO-*d*₆) $\delta_{\rm C}$ = 175.5, 167.8, 162.9, 160.4, 157.6, 151.5, 143.4, 142.9, 132.8, 129.9, 128.0, 126.5, 125.5, 122.6, 122.5, 120.9, 116.8, 116.6, 110.9, 109.4, 107.3, 102.8, 75.6, 67.0, 50.3, 47.0, 42.2, 34.0, 32.8, 26.1; LCMS (ESI) *m/z* calcd for C₃₀H₂₄FN₅O₄: 537.1809 [M⁺]; found: 538.1884 [M⁺ +H].

1'-((1-(4-bromophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-3-hydroxy-6b,7,8,9-tetrahydro-6*H*-spiro[chromeno[3,4-*a*]pyrrolizine-11,3'-indoline]-2',6(6*aH*,11*aH*)-dione (5h)



White solid; Yield = 83%; M.p. = 174-177; IR (CHCl₃) v/cm⁻¹ = 2924, 1720, 1514, 1231, 1163, 758; ¹H NMR (400MHz, DMSO- d_6) $\delta_{\rm H}$ = 9.49 (s, 1H, OH), 7.87 (s, 1H, triazole), 7.76-7.74 (m, 3H, Ar-H), 7.69-7.67 (m, 2H, Ar-H), 7.40-7.36 (t, 1H, Ar-H), 7.19-7.15 (t, 1H, Ar-H), 7.05 (d, 1H, *J* = 8.39 Hz, Ar-H), 6.29 (s, 1H, Ar-H), 6.08 (d, 1H, *J* = 6.10 Hz, Ar-H), 5.99 (d, 1H, *J* = 8.01 Hz, Ar-H), 4.68 (s, 2H, -CH₂), 4.38 (brs, 1H, -CH), 4.07-4.04 (m, 1H, -CH), 3.46-3.43 (m, 1H, -CH), 3.16-3.13 (m, 1H, -CH₂), 2.58-2.55 (m, 1H, -CH₂), 2.36-2.30 (m, 1H, -CH₂), 1.92-1.75 (m, 2H,-CH₂), 1.67-1.55 (m, 1H, -CH₂); ¹³C NMR (100 MHz, DMSO- d_6) $\delta_{\rm C}$ = 175.4, 167.7, 157.5, 151.4, 143.3, 143.1, 135.6, 132.7, 129.9, 127.9, 126.5, 125.5, 122.4, 122.0, 121.3, 120.6, 110.8, 109.5, 107.4, 102.8, 75.67, 67.0, 50.3, 46.9, 42.3, 34.02, 32.8, 26.1; LCMS (ESI) *m/z* calcd for C₃₀H₂₄ BrN₅O₄ : 597.1003 [M⁺]; found: 598.1076 [M⁺ +H]; 600.1063 [M⁺+(H+2)].

3-hydroxy-1'-((1-(4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-6b,7,8,9-tetrahydro-6*H*-spiro[chromeno[3,4-*a*]pyrrolizine-11,3'-indoline]-2',6(6*aH*,11*aH*)-dione (5i)



Pale yellow solid; Yield = 86%; M.p. = 182-184; IR (CHCl₃) v/cm⁻¹= 2920, 1711, 1521, 1346, 1170, 752; 1H NMR (400MHz, DMSO- d_6) δ_H = 9.38 (s, 1H, -OH), 8.40 (d, 1H, *J* = 8.39 Hz, Ar-H), 8.06-8.05 (m, 1H, Ar-H), 8.02 (s, 1H, triazole), 7.77 (d, 1H, *J* = 7.35, Ar-H), 7.42-7.38 (t, 1H, Ar-H), 7.20-7.16 (t, 1H, Ar-H), 7.10 (d, 1H, *J* = 7.63 Hz, Ar-H), 6.25 (s, 1H, Ar-H), 6.04-

6.02 (m, 1H, Ar-H), 5.95-5.93 (m, 1H, Ar-H), 4.71 (s, 2H, -CH₂), 4.39 (brs, 1H, -CH), 4.06-4.03 (m, 1H, -CH), 3.49-3.40 (m, 1H, -CH₂), 3.17-3.18 (m, 1H, -CH₂), 2.58-2.52 (m, 1H, -CH₂), 2.34-2.32 (m, 1H, -CH₂), 1.87-1.78 (m, 2H, -CH₂), 1.65-1.61 (m, 1H, -CH₂); ¹³C NMR (100 MHz, DMSO- d_6) δ_C = 175.5, 167.7, 157.5, 151.4, 146.6, 143.5, 143.2, 140.5, 129.9, 127.9, 126.5, 125.5, 122.5, 121.1, 120.7, 110.7, 109.4, 107.3, 102.7, 75.6, 67.1, 50.3, 46.9, 42.3, 33.9, 32.8, 30.7, 26.1; LCMS (ESI) *m/z* calcd for C₃₀H₂₄ N₆O₆ : 564.1752 [M⁺]; found: 565.1825 [M⁺ +H].

3-hydroxy-1'-((1-p-tolyl-1*H*-1,2,3-triazol-4-yl)methyl)-6b,7,8,9-tetrahydro-6*H*-spiro[chromeno[3,4-*a*]pyrrolizine-11,3'-indoline]-2',6(6*aH*,11*aH*)-dione (5j)



White solid; Yield = 81%; M.p. = 173-175; IR (CHCl₃) v/cm⁻¹= 2924, 1713, 1515, 1166, 755; ¹H NMR (400MHz, DMSO- d_6) δ_H = 9.57 (s, 1H, -OH), 7.82 (s, 1H, triazole), 7.78 (d, 1H, J = 6.87 Hz, Ar-H), 7.58 (d, 1H, J = 8.39 Hz, Ar-H), 7.39-7.34 (m, 3H, Ar-H), 7.19-7.15 (t, 1H, Ar-H), 7.04 (d, 1H, J = 7.63 Hz, Ar-H), 6.33-6.31 (m, 1H, Ar-H), 6.14-6.11 (m, 1H, Ar-H), 6.04-6.02 (m, 1H, Ar-H), 4.71-4.63 (m, 2H,-CH₂), 4.41-4.36 (m, 1H, -CH), 4.09-4.06 (m, 1H, -CH), 3.33-3.32 (m, 1H, Ar-H), 3.19-3.13 (m, 1H, -CH₂), 2.57-2.54 (m, 1H, -CH₂), 2.35 (s, 3H, -CH₃), 2.32-2.30 (m, 1H, -CH₂), 1.87-1.75 (m, 2H, -CH₂), 1.67-1.56 (m, 1H, -CH₂); ¹³C NMR (100 MHz, DMSO- d_6) δ_C = 175.5, 167.7, 157.6, 151.5, 143.4, 142.8, 138.3, 134.0, 130.2. 129.9, 128.0, 126.5, 125.5, 122.4, 120.5, 119.9, 110.9, 109.4, 107.4, 102.9, 75.6, 67.0, 50.3, 47.0, 42.1, 34.1, 32.8, 30.7, 26.1, 20.6; LCMS (ESI) *m/z* calcd for C₃₁H₂₇ N₅O₄ : 533.2053 [M⁺]; found: 534.2127 [M⁺+H].

1'-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-3-hydroxy-6b,7,8,9-tetrahydro-6*H*-spiro[chromeno[3,4-*a*]pyrrolizine-11,3'-indoline]-2',6(6*aH*,11*aH*)-dione (5k)



White solid; Yield = 87%; M.p. = 175-177; IR (CHCl₃) v/cm⁻¹= 2923, 1712, 1498, 1169, 752; ¹H NMR (400MHz, DMSO-*d*₆) $\delta_{\rm H}$ = 9.48 (s, 1H, -OH), 7.87 (s, 1H, triazole), 7.78-7.74 (m, 3H, Ar-H), 7.62 (d, 1H, *J* = 8.77 Hz, Ar-H), 7.40-7.36 (t, 1H, Ar-H), 7.19-7.16 (t, 1H, Ar-H), 7.06 (d, 1H, *J* = 7.63 Hz, Ar-H), 6.32-6.26 (m, 1H, Ar-H), 6.09-6.07 (m, 1H, Ar-H), 5.99 (d, 1H, *J* = 8.39 Hz, Ar-H), 4.68 (s, 2H, -CH₂, 4.41-4.37 (m, 1H, -CH), 4.07-4.05 (d, 1H, *J* = 11.4 Hz, -CH), 3.30-3.29 (m, 1H, -CH₂), 3.19-3.13 (m, 1H, -CH₂), 2.58-2.55 (m, 1H, -CH₂), 2.36-2.30 (m, 1H, -CH₂), 1.88-1.76 (m, 2H, -CH₂), 1.68-1.59 (m, 1H, -CH₂); ¹³C NMR (100 MHz, DMSO-*d*₆) $\delta_{\rm C}$ = 175.5, 167.7, 157.5, 151.4, 143.3, 143.0, 135.0, 132.9, 129.8, 127.9, 126.5, 125.5, 122.4, 121.8, 120.7, 110.8, 109.4, 107.3, 102.8, 75.6, 67.0, 50.3, 46.9, 42.2, 34.0, 32.7, 26.1; LCMS (ESI) *m/z* calcd for C₃₀H₂₄ClN₅O₄: 553.1514 [M⁺]; found: 554.1587 [M⁺ +H]. 1'-((1-(7-chloroquinolin-4-yl)-1*H*-1,2,3-triazol-4-yl)methyl)-3-hydroxy-6b,7,8,9tetrahydro-6*H*-spiro[chromeno[3,4-*a*]pyrrolizine-11,3'-indoline]-2',6(6*aH*,11*aH*)-dione (5l)



White solid; Yield = 84%; M.p. = 185-187; IR (CHCl₃) v/cm⁻¹= 2931, 1712, 1609, 1462, 1160, 753; ¹H NMR (400MHz, DMSO-*d*₆) $\delta_{\rm H}$ = 9.19 (s, 1H, -OH), 9.10-9.09 (m, 1H, Ar-H), 8.25 (s, 1H, triazole), 7.80-7.78 (m, 2H, Ar-H), 7.74-7.71 (m, 1H, Ar-H), 7.62-7.61 (m, 1H, Ar-H), 7.53 (s, 1H, Ar-H), 7.43-7.39 (t, 1H, Ar-H), 7.22-7.18 (t,1H, Ar-H), 7.09 (d, 1H, *J* = 7.63 Hz, Ar-H), 6.17 (s, 1H, Ar-H), 5.97-5.88 (m, 2H, Ar-H), 4.86-4.75 (q, 2H, -CH₂), 4.47-4.33 (m, 1H, -CH), 4.06 (d, 1H, *J* = 11.4 Hz, -CH), 3.53-3.43 (m, 1H, -CH₂), 3.18-3.15 (m, 1H, -CH₂), 2.61-2.57 (m, 1H, -CH₂), 2.37-2.30 (m, 1H, -CH₂), 1.87-1.76 (m, 2H, -CH₂), 1.65-1.57 (m, 1H, -CH₂); ¹³C NMR (100 MHz, DMSO-*d*₆) $\delta_{\rm C}$ = 175.6, 167.8, 157.4, 152.4, 151.4, 149.3, 143.3, 142.8, 139.9, 135.2, 129.9, 128.8, 128.1, 127.9, 126.5, 125.4, 125.2, 124.4, 122.5, 120.3, 116.9, 110.9, 109.4, 107.3, 102.6, 75.6, 67.0, 50.4, 46.8, 42.3, 34.2, 32.8, 30.7, 26.1; LCMS (ESI) *m/z* calcd for C₃₃H₂₅ClN₆O₄: 604.1626 [M⁺]; found: 605.1700 [M⁺ +H].

2-bromo-1'-((1-(4-chlorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-6b,7,8,9-tetrahydro-6*H*-spiro[chromeno[3,4-*a*]pyrrolizine-11,3'-indoline]-2',6(6*aH*,11*aH*)-dione (5m)



White solid; Yield = 88%; M.p. = 215-216; IR (CHCl₃) v/cm⁻¹= 2931, 1760, 1475, 1167, 748; ¹H NMR (400MHz, DMSO-*d*₆) $\delta_{\rm H}$ = 7.83 (s, 1H, triazole), 7.80-7.77 (m, 2H, Ar-H), 7.65 (d, 1H, *J* = 8.39 Hz, Ar-H), 7.47-7.43 (t, 1H, Ar-H), 7.23-7.18 (m, 2H, Ar-H), 6.83-6.81 (m, 1H, Ar-H), 6.78-6.76 (m, 1H, Ar-H), 6.60 (s, 1H, Ar-H), 4.75-4.59 (q, 2H, -CH₂), 4.43 (brs, 1H, -CH), 4.14 (d, 1H, *J* = 11.4 Hz, -CH), 3.41-3.38 (m, 1H, -CH₂), 3.17-3.13 (m, 1H, -CH₂), 2.66-2.62 (m, 1H, -CH₂), 2.39-2.32 (m, 1H, -CH₂), 1.88-1.77 (m, 2H, -CH₂), 1.67-1.63 (m, 1H, -CH₂); ¹³C NMR (100 MHz, DMSO-*d*₆) $\delta_{\rm C}$ = 175.0, 167.0, 149.8, 143.1, 142.6, 135.1, 132.9, 130.7, 130.1, 129.7, 129.4, 126.5, 124.9, 122.6, 121.8, 120.8, 119.9, 118.3, 114.4, 109.7, 76.1, 67.6, 50.3, 46.3, 42.8, 33.7, 32.6, 26.0; LCMS (ESI) *m/z* calcd for C₃₀H₂₃ BrClN₅O₃ : 615.0680 [M⁺]; found: 616.0754 [M⁺ +H]; 618.0737 [M⁺+(H+2)].

2-bromo-1'-((1-(4-bromophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-6b,7,8,9-tetrahydro-6*H*-spiro[chromeno[3,4-*a*]pyrrolizine-11,3'-indoline]-2',6(6*aH*,11*aH*)-dione (5n)



White solid; Yield = 85%; M.p. = 177-179; IR (CHCl₃) v/cm⁻¹= 2928, 1758, 1610, 1489, 1223, 748; ¹H NMR (400MHz, DMSO- d_6) δ_H = 7.85 (s, 1H, triazole), 7.81-7.74 (m, 6H, Ar-H), 7.45-7.43 (t, 1H, ArH), 7.24-7.18 (m, 2H, Ar-H), 6.84-6.79 (m, 2H, Ar-H), 6.06 (s, 1H, Ar-H), 4.75-4.59 (q, 2H, -CH₂), 4.45-4.41 (m, 1H, -CH), 4.15 (d, 1H, *J* = 11.4 Hz, -CH), 3.42-3.41 (m, 1H, -CH₂), 3.19-3.14 (m, 1H, -CH₂), 2.66-2.62 (m, 1H, -CH₂), 2.39-2.34 (m, 1H, -CH₂), 1.89-1.78 (m, 2H, -CH₂), 1.70-1.62 (m, 1H, -CH₂); ¹³C NMR (100 MHz, DMSO- d_6) δ_C = 175.0, 167.0, 149.9, 143.1, 142.6, 135.5, 132.7, 130.7, 130.1, 129.4, 126.5, 124.9, 122.6, 122.0, 121.3, 120.8, 119.9, 118.3, 114.5, 109.7, 76.1, 67.6, 50.3, 46.3, 42.9, 33.8, 32.6, 26.0; LCMS (ESI) *m/z* calcd for C₃₀H₂₃ Br₂N₅O₃: 659.0167 [M⁺]; found: 660.0246 [M⁺+H]; 662.0232 [M⁺⁺(H+2)].

2-bromo-1'-((1-(7-chloroquinolin-4-yl)-1*H*-1,2,3-triazol-4-yl)methyl)-6b,7,8,9-tetrahydro-6*H*-spiro[chromeno[3,4-*a*]pyrrolizine-11,3'-indoline]-2',6(6*aH*,11*aH*)-dione (50)



White solid; Yield = 86%; M.p. = 174-176; IR (CHCl₃) v/cm⁻¹= 2969, 1761, 1609, 1476, 1224, 1174, 754; ¹H NMR (400MHz, DMSO- d_6) δ_H = 9.15-9.14 (m, 1H, Ar-H), 8.30-8.28(m, 1H, Ar-H), &.90 (d, 1H, J = 9.54 Hz, Ar-H), 7.83 (d, 1H, J = 7.63 Hz, Ar-H), 7.80-7.77 (dd, 1H, Ar-H), 7.72-7.71 (m, 1H, Ar-H), 7.59 (s, 1H, triazole), 7.49-7.45 (t, 1H, Ar-H), 7.26-7.22 (t, 1H, Ar-H), 7.16 (d, 1H, J = 7.63 Hz, Ar-H), 6.76 (d, 1H, J = 8.77 Hz, Ar-H), 6.64-6.62 (dd, 1H, Ar-H), 6.17-6.16 (m, 1H, Ar-H), 4.88-4.73 (q, 2H, -CH₂), 4.45-4.41 (m, 1H, -CH), 4.20-4.17 (m, 1H, -CH), 3.42-3.40 (m, 1H, -CH₂), 3.21-3.15 (m, 1H, -CH₂), 2.66-2.63 (m, 1H, -CH₂), 2.38-2.33 (m, 1H, -CH₂), 1.91-1.78 (m, 2H, -CH₂), 1.71-1.61 (m, 1H, -CH₂); ¹³C NMR (100 MHz, DMSO- d_6) δ_C = 175.1, 166.9, 152.3, 149.9, 149.3, 143.1, 142.6, 139.9, 135.4, 130.8, 130.2, 129.6, 129.0, 128.1, 126.7, 125.4, 124.8, 124.2, 122.7, 120.1, 120.0, 118.5, 116.8, 114.3, 109.5, 76.0, 67.5, 50.2, 46.3, 42.6, 33.9, 32.7, 26.0; LCMS (ESI) *m*/*z* calcd for C₃₃H₂₄ BrClN₆O₃ : 666.0775 [M⁺]; found: 667.0840 [M⁺+H]; 669.0842 [M⁺+(H+2)].

2-bromo-1'-((1-(4-methoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-6b,7,8,9-tetrahydro-6*H*-spiro[chromeno[3,4-*a*]pyrrolizine-11,3'-indoline]-2',6(6*aH*,11*aH*)-dione (5p)



White solid; Yield = 82%; M.p. = 185-187; IR (CHCl₃) v/cm⁻¹= 2966, 1710, 1610, 1516, 1170, 750; ¹H NMR (400MHz, DMSO-*d*₆) $\delta_{\rm H}$ = 7.79 (d, 1H, *J* = 7.63 Hz,Ar-H), 7.65 (d, 2H, *J* = 8.39 Hz, Ar-H), 7.55 (s, 1H, triazole,) 7.46-7.42 (t, 1H, Ar-H), 7.24-7.20 (t, 1H, Ar-H), 7.16 (d, 1H,

J = 8.39 Hz, Ar-H), 7.12 (d, 1H, J = 8.39 Hz, Ar-H), 6.84 (d, 1H, J = 8.39 Hz, Ar-H), 6.80-6.77 (dd, 1H, Ar-H), 6.11-6.10 (m, 1H, Ar-H), 4.75-4.59 (q, 2H, -CH₂), 4.45-4.41 (m, 1H, -CH), 4.17-4.15 (m, 1H, -CH), 3.82 (s, 3H, -OCH₃), 3.42-3.38 (dd, 1H, -CH₂), 3.20-3.14 (m, 1H, -CH₂), 2.66-2.62 (t, 1H, -CH₂), 2.39-2.33 (m, 1H, -CH₂), 1.90-1.78 (m, 2H, -CH₂), 1.71-1.62 (m, 1H, -CH) ¹³C NMR (100 MHz, DMSO- d_6) $\delta_C = 175.0$, 166.9, 159.2, 149.9, 143.2, 142.3, 130.8, 130.1, 129.7, 129.5, 126.5, 124.8, 122.6, 121.9, 120.5, 119.8, 118.3, 114.7, 114.4, 109.6, 76.1, 67.5, 55.5, 50.2, 46.3, 42.7, 33.9, 32.5, 30.6, 25.9; LCMS (ESI) *m/z* calcd for C₃₃H₂₄ BrClN₆O₃: 611.1161 [M⁺]; found: 612.1236 [M⁺+H]; 614.1219 [M⁺+(H+2)].

2-methyl-1'-((1-(4-methylphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)-3,3*a*-dihydro-2*H*-spiro[chromeno[3,4-*c*]pyrrole-1,3'-indoline]-2',4(9*bH*)-dione (5q)



Off-White solid; M.p.: 193-196 °C; Yield 71%; IR (CHCl₃, cm⁻¹) v/max: 3017, 1713, 1213, 739; ¹H NMR (400 MHz, DMSO, d_6) $\delta_{\rm H}$: 8.47 (s, 1H, ArH), 7.69-7.67 (m, 2H, ArH), 7.42-7.41(m, 1H, ArH), 7.37-7.32 (m, 3H, ArH), 7.27-7.25 (m, 2H, ArH),7.19-7.18 (m, 1H, ArH), 7.18-7.04 (m, 2H, ArH), 7.0-7.08 (m, 1H, ArH), 4.99-4.88 (m, 2H, N-CH₂), 4.20-4.17 (m, 1H, CH), 4.09- 4.04 (m, 1H, CH), 3.69-3.65 (m, 1H, CH), 3.26-3.22 (m, 1H, CH), 2.34 (s, 3H, CH₃), 1.91 (s, 3H, CH₃); ¹³C NMR (100 MHz, CDCl₃) ¹³C: 175.2, 166.3, 149.1, 143.1, 138.4, 134.2, 130.2, 128.4, 128.3, 128.0, 124.7, 124.0, 123.0, 122.0, 121.2, 119.8, 116.3, 109.2, 74.5, 72.3, 60.4, 60.1, 49.2, 33.8, 20.5; LCMS (ESI) m/z calcd. for C₂₉H₂₅N₅O₃: 491.1957, LCMS (ESI) found: 492.2036 [M+H]⁺.

2-methyl-1'-((1-(4-nitrophenyl)-1H-1,2,3-triazol-4-yl)methyl)-3,3a-dihydro-2H-

spiro[chromeno[3,4-c]pyrrole-1,3'-indoline]-2',4(9bH)-dione (5r).



Pale yellow solid; M.p.: 208-210 °C; Yield 78%; IR (CHCl₃, cm⁻¹) v/max: 2925, 1718, 1347, 754; ¹H NMR (400 MHz, DMSO, d_6) $\delta_{\rm H}$: 8.79 (s, 1H, ArH), 8.43-8.41 (m, 2H, ArH), 8.15-8.13 (m, 2H, ArH), 7.41-7.27(m, 4H, ArH), 7.17-7.09(m, 4H, ArH), 5.04-4.90(m, 2H, N-CH₂), 4.20-4.06(m, 2H, CH₂), 3.75-3.59 (m, 1H, CH), 3.26-3.24 (m, 1H, CH), 1.91 (s, 3H, CH₃); ¹³C NMR (100 MHz, DMS, d_6) ¹³C: 175.2, 166.3, 149.1, 146.7, 143.8, 143.0, 140.0, 129.5, 128.4, 128.3, 128.0, 125.6, 124.7, 121.9, 120.5, 109.2, 74.5, 72.3, 60.4, 60.1, 49.2, 33.9; LCMS (ESI) m/z calcd. for C₂₈H₂₂N₆O₅: 352.1652 [M⁺]; found: 523.1734 [M+H]⁺.

1-((1-(4-fluorophenyl)-1H-1,2,3-triazol-4-yl)methyl)indoline-2,3-dione (6a)



Yellow solid; M.p.: 174-177 °C; Yield 82%; IR (CHCl₃, cm⁻¹) v/max: 2923, 1737, 1611, 1231; ¹H NMR (400 MHz, CDCl₃) $\delta_{\rm H}$: 8.01 (s, 1H, ArH), 7.67-7.56 (m, 4H, ArH), 7.35-7.33 (m, 2H, ArH), 7.18-7.08 (m, 3H, ArH), 5.08 (s, 2H, OCH₂); ¹³C NMR (100 MHz, CDCl₃) ¹³C: 182.9, 150.0, 138.6, 125.4, 124.1, 122.5, 122.4, 117.5, 116.9, 116.7, 111.4, 35.3; LCMS (ESI) m/z calcd. for C₁₇H₁₁FN₄O₂: 322.08, LCMS (ESI) found: 323.0939 [M+H]⁺.





Figure 2. ¹³C NMR spectrum of compound 5a (100 MHz, DMSO).



Figure 3. Mass spectrum of compound 5a.

	Qu	alitative Com	pound Report		
Data File Sample Type Instrument Name Acq Method IRM Calibration Status Comment	MR2-104.d Sample Instrument 1 29.10.2014.m Success	Sample Name Position User Name Acquired Time DA Method	MR2-104 P182 Icmsdu-PC\admin 11-02-2015 12:38:34 Default.m		
Acquisition SW 6200 Version Q-Tr	0 series TOF/6500 series OF B.05.01 (B5125)	Into.			
Compound Table		-		MFG Diff	
Compound Label Cpd 1: C30 H24 F N5 O3	0.216 521.1865	C30 H24 F N5 O3	C30 H24 F N5 O3	(ppm) -0.33	C30 H24 F N5 O3
1.75 1.55 1.55 1.55 1.55 1.55 0.25 0 150 200 28 4FE MS Zoomed Spectrum x10 6 Cpd 1: C30 H24 F	([C 50 300 350 400 2 Count N5 03: +ESI MFE Spe 522,1937 ([C30 H24 F [N5 03]+1	30 H24 F N5 O3]+H)+ 150 500 550 600 650 s vs. Mass-to-Charge (m/z) ctrum (0.150-0.633 min) Fra- +I)+	700 750 800 850 90 g=135.0V MR2-104.d	0	
1.75 1.5					
1.75 1.75 1.25 1 0.75 0.25 0 490 495 500 505	(1) 510 515 520 525 530 Count	544.1756 C30 H24 F N5 O3]+Na)+ L. 535 540 545 550 555 560 s vs. Mass-to-Charge (m/z)	565 570 575 580 585 590	1 595	
1.75 1.75 1.25 1.25 0.5 0.25 0.490 495 500 505 MS Spectrum Peak List m/z z Abund	([510 515 520 525 530 Count Formula	544.1756 C30 H24 F N5 O3]+Na)+ 1. 535 540 545 550 555 560 5 vs. Mass-to-Charge (m/2) Ion	565 570 575 580 585 590	1 595	
1.75 1.75 1.25 1.25 1.25 0.5 0.25 0.490 495 500 505 MS Spectrum Peak List m/z z z Abund 522.1937 1 2 2	((510 515 520 525 530 Count 164009.25 C30 H24 F N5 164009.25 C30 H24 F N5	544,1756 C30 H24 F N5 03}+Na)+ 1 535 540 545 550 555 560 s vs. Mass-to-Charge (m/2) 10n 03 (M+H)+ 02	565 570 575 580 585 590	595	
1.75 1.75 1.75 1.25 1 0.75 0.25 0 490 495 500 505 502 2 490 495 502 2 490 495 522.1937 1 2 523.1969 524.1996 1	(1) 510 515 520 525 530 Count 515 520 525 530 Count 164009.25 C30 H24 F NS 773761.44 C30 H24 F NS 53769.71 C30 H24 F NS	544,1756 C30 H24 F N5 O3J+Na)+ 1. 535 540 545 550 555 560 s vs. Mass-to-Charge (m/z) 100 03 (M+H)+ 03 (M+H)+	565 570 575 580 585 590	595	
z z 1.75 .5 1.25 .1 0.75 .5 0.25 .25 0 .490 495 500 505 522.1937 1 2 523.1969 1 .5 525.2022 1 1	([5 510 515 520 525 530 Count 164009.25 C30 H24 F NS 727361.44 C30 H24 F NS 135769.71 C30 H24 F NS 138003, C30 H24 F NS	544.1756 C30 H24 F N5 03J+Na)+ Jr. 535 540 545 550 555 560 s vs. Mass-to-Charge (m/2) 100 03 (M+H)+ 03 (M+H)+ 03 (M+H)+ 03 (M+H)+	565 570 575 580 585 590	595	
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1.75	510 515 520 525 530 Count Formula 164003.25 C30 H24 F NS 133769.71 C30 H24 F NS 133769.71 C30 H24 F NS 134003. C30 H24 F NS 121300.64 C30 H24 F NS 56404.51 C30 H24 F NS 56404.51 C30 H24 F NS	544.1756 C30 H24 F N5 O3}+Na)+ J	565 570 575 580 585 590	595	
2 2 1.75 1.5 1.25 1 0.75 0.5 0.25 0 490 495 500 505 MS Spectrum P≥ak List m/z z Abund 523.1999 1 2 524.1996 1 552.5022 544.1756 1 545.178 550.187 1 560.1811 546.1811 1 560.197	(1 510 515 520 525 530 Count 164009.25 C30 H24 F NS 135769.71 C30 H24 F NS 189003. C30 H24 F NS 189003. C30 H24 F NS 56404.51 C30 H24 F NS 56404.51 C30 H24 F NS	544,1756 C30 H24 F N5 03J+Na)+ 1. 535 540 545 550 555 560 5 vs. Mass-to-Charge (m/z) 100 03 (M+H)+ 03 (M+H)+ 03 (M+H)+ 03 (M+H)+ 03 (M+Na)+ 03 (M+Na)+ 03 (M+Na)+ 03 (M+Ka)+	565 570 575 580 585 590	595	
z z 1.75 1.5 1.25 1 0.75 0.5 0.25 490 495 500 505 MS Spectrum Peak List m/z z Abund 522.1937 1 2 2 523.1969 1 5 5 524.1996 1 5 5 545.178 1 5 5 561.1531 1 1 1	((510 515 520 525 520 Count 510 515 520 525 520 773761.44 C30 124 F N5 184003.25 C30 124 F N5 184003.3 C30 124 F N5 184003.3 C30 124 F N5 19604.51 C30 124 F N5 10655.37 C30 124 F N5	544,1756 C30 H24 F N5 03}+Na)+ 1. 535 540 545 550 555 560 s vs. Mass-to-Charge (m/2) 100 03 (M+H)+ 03 (M+H)+ 03 (M+H)+ 03 (M+H)+ 03 (M+Na)+ 03 (M+K)+ 03 (M+K)+ 03 (M+K)+	- 565 570 575 580 585 590 - - - - - - - -	595	
n n 1.75 1.25 1 1 0.75 0.5 0.25 490 495 500 505 MS Spectrum Peak List m/z z Abund 522.1937 1 2 2 524.1936 1 525.2022 1 545.178 1 545.178 1 546.1811 1 560.1497 1 561.1531 1 562.1531 1	((510 515 520 525 530 Count 164009.25 C30 H24 F N5 135769.71 C30 H24 F N5 135769.71 C30 H24 F N5 13600.3 C30 H24 F N5 10665.37 C30 H24 F N5 10665.37 C30 H24 F N5 10665.37 C30 H24 F N5 10655.37 C30 H24 F N5 1067.31 C30 H24 F N5 1067.31 C30 H24 F N5	544,1756 C30 H24 F N5 03J+Na)+ 1. 535 540 545 550 555 560 s vs. Mass-to-Charge (m/2) 100 03 (M+H)+ 03 (M+H)+ 03 (M+H)+ 03 (M+H)+ 03 (M+Na)+ 03 (M+K)+ 03 (M+K)+ 03 (M+K)+	565 570 575 580 585 590	595	
z z 1.75 1.5 1.25 1 0.75 0.5 0.5 0.25 0 490 495 500 505 MS Spectrum Peak List m/z z Abund 522.197 1 252.31969 1 525.302 1 544.4756 1 546.4811 1 560.1497 1 561.1531 1 562.1513 1	((5 10 5 15 5 20 5 25 5 30 Count 164009.25 C30 H24 F N5 773761.44 C30 H24 F N5 135769.71 C30 H24 F N5 13603.C30 H24 F N5 10665.37 C30 H24 F N5 10665.37 C30 H24 F N5 10665.37 C30 H24 F N5 10665.37 C30 H24 F N5 5993.61 C30 H24 F N5	544,1756 C30 H24 F N5 O3J+Na)+ 1 555 540 545 550 555 560 s vs. Mass-to-Charge (m/2) 100 03 (M+H)+ 03 (M+H)+ 03 (M+H)+ 03 (M+H)+ 03 (M+Na)+ 03 (M+K)+ 03 (M+K)+ 03 (M+K)+	565 570 575 580 585 590	595	
1.75 1.75 1.25 1 0.75 0.5 0.5 0.75 <td>((5 510 515 520 525 530 Count 5 773761.44 C30 H24 F N5 773761.44 C30 H24 F N5 135769.71 C30 H24 F N5 13603.C30 H24 F N5 56404.51 C30 H24 F N5 56404.51 C30 H24 F N5 56404.51 C30 H24 F N5 5993.61 C30 H24 F N5</td> <td>544.1756 C30 H24 F N5 03HNa)* 1. 535 540 545 550 565 560 s vs. Mass-to-Charge (m/z) 03 (M+H)+ 03 (M+H)+ 03 (M+H)+ 03 (M+H)+ 03 (M+Na)+ 03 (M+Na)+ 03 (M+Na)+ 03 (M+K)+ 03 (M+K)+ 03 (M+K)+ 03 (M+K)+</td> <td>565 570 575 580 585 590</td> <td>595</td> <td></td>	((5 510 515 520 525 530 Count 5 773761.44 C30 H24 F N5 773761.44 C30 H24 F N5 135769.71 C30 H24 F N5 13603.C30 H24 F N5 56404.51 C30 H24 F N5 56404.51 C30 H24 F N5 56404.51 C30 H24 F N5 5993.61 C30 H24 F N5	544.1756 C30 H24 F N5 03HNa)* 1. 535 540 545 550 565 560 s vs. Mass-to-Charge (m/z) 03 (M+H)+ 03 (M+H)+ 03 (M+H)+ 03 (M+H)+ 03 (M+Na)+ 03 (M+Na)+ 03 (M+Na)+ 03 (M+K)+ 03 (M+K)+ 03 (M+K)+ 03 (M+K)+	565 570 575 580 585 590	595	

Figure 4. ¹H NMR spectrum of compound **5b** (400 MHz, DMSO).



Figure 5. ¹³C NMR spectrum of compound 5b (100 MHz, DMSO).



	Qual	litative Com	pound Repor	t	
Data File Sample Type Instrument Name Acq Method IRM Calibration Status Comment	MR2-106.d Sample Instrument 1 29.10.2014.m Success	Sample Name Position User Name Acquired Time DA Method	MR2-106 PIC9 Iomsdu-PC\admin 25-02-2015 15:47:14 Default.m		
Sample Group Acquisition SW 6200 see Version Q-TOF E	In ries TOF/6500 series 3.05.01 (85125)	fo.			
Compound Table	RT Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
	0.2 555.2005	C31 H27 N3 04	C31 H27 N5 04	-0.3	C31 H27 N5 O4
Compound Label m, Cpd 1: C31 H27 N5 O4 53	/z RT 4.2146 0.2	Algorithm Find by Molecular Fe	Mass ature 533.2065		
MEE MC Cooct					
v10.6 Cpd 1: C31 H27 N5 O	4: +ESI MFF Snectrum	(0.124-0.758 min) Ergo-	135 0V MR2-106 d		
1	([C31]	534.2146 H27 N5 O4]+H)+	133.0V MR2-100.0		
0.8					
0.6					
0.4					
0		11.			
150 200 250 3	00 350 400 450 5 Counts vs	00 550 600 650 70 Mass-to-Charge (m/z)	00 750 800 850 900 9	50	
MFE MS Zoomed Spectrum					
x10 6 Cpd 1: C31 H27 N5 O4	4: +ESI MFE Spectrum	(0.124-0.758 min) Frag=	135.0V MR2-106.d		
1. 0	[C31 H27 N5 O4]+H)+				
0.8					
0.6					
0.4	1	556.1957			
0.2	((C3	1 H27 N5 O4J+Na)+			
505 510 515 520 9	525 530 535 540 545	550 555 560 565 570	575 580 585 590 595 600	605	
MS Spectrum Peak List	Counts VS	. mass-to-onarge (m/z)			
m/z z Abund	Formula	Ion			
534.2146 1 12295 535.2176 1 4498	57.38 C31 H27 N5 O4 14.63 C31 H27 N5 O4	(M+H)+ (M+H)+	-		
536.2199 1 834	44.53 C31 H27 N5 O4	(M+H)+	1		
537 2216 1 110	13.69 C31 H27 N5 O4	(M+Na)+			
537.2216 1 115 556.1957 1 912	837.3 C31 H27 N5 O4	(M+Na)+	-		
537.2216 1 1153 556.1957 1 912 557.1992 1 311 558.2006 1 63	15.041C31 H27 N5 (14	(11110)#			
537.2216 1 1157 556.1957 1 912 557.1992 1 311 558.2006 1 633 572.1701 1 2475	16.04 C31 H27 N5 04 59.36 C31 H27 N5 04	(M+K)+			
537.2216 1 1151 556.1957 1 912 557.1992 1 311 558.2006 1 63 572.1701 1 247 573.1726 1 848 574.1717 1 33	16.04 C31 H27 N5 04 59.36 C31 H27 N5 04 80.12 C31 H27 N5 04 528.1 C31 H27 N5 04	(M+K)+ (M+K)+ (M+K)+			
537.2216 1 1151 556.1957 1 912 557.1992 1 311 558.2006 1 63 572.1701 1 247 573.1726 1 888 574.1717 1 30	10.04 C31 H27 N5 04 59.36 C31 H27 N5 04 80.12 C31 H27 N5 04 628.1 C31 H27 N5 04	(M+K)+ (M+K)+ (M+K)+			
537.2216 1 1151 556.1957 1 912 557.1992 1 311 558.2006 1 633 572.1701 1 247 573.1726 1 888 574.1717 1 38 574.1717 1 39	16.04 (C31 H27 N5 04 59.36 (C31 H27 N5 04 60.12 (C31 H27 N5 04 628.1 (C31 H27 N5 04	(M+K)+ (M+K)+ (M+K)+]		

Figure 6. Mass spectrum of compound 5b.





Figure 8. ¹³C NMR spectrum of compound 5c (100 MHz, DMSO).



÷ '	Qu	alitative Com	pound Repor	t		
Data File Sample Type Instrument Name Acq Method IRM Calibration Status Comment Sample Group	MR2 107.d Sample Instrument 1 29.10.2014.m Success	Sample Name Position User Name Acquired Time DA Method Info.	MR2 107 P2F3 Icmsdu-PC\admin 02-03-2015 14:47:35 Default.m			
Version Q-TO	* B.05.01 (B5125)					
Compound Table Compound Label	RT Mass	Formula	MEG Formula	MFG Diff		
Cpd 1: C30 H24 N6 O5	0.202 548.1811	C30 H24 N6 O5	C30 H24 N6 O5	(ppm) -0.57	C30 H24 N6 O5	
Compound Label n Cpd 1: C30 H24 N6 O5 5	7/z RT 49.1888 0.20	Algorithm 12 Find by Molecular Fea	Mass ture 548.1811			
MEE MS Spectrum						
x10.6 Cpd 1: C30 H24 N6 C	5: +ESI MEE Spectru	m (0 110 0 700) 5				
x10	vo. + Eor wir E Spectra	549.1888	35.0V MR2 107.d			
2.5	([C	230 H24 N6 O5]+H)+				
2-						
1.5						
1-						
0.5						
150 200 250	300 350 400 450	500 550 600 650 700	750 800 850 900 9	50		
MFE MS Zoomed Spectrum	Counts	vs. Mass-to-Charge (m/z)				
x10 6 Cpd 1: C30 H24 N6 O	5: +ESI MFE Spectrur	m (0 119-0 736 min) Front	E 0) (MD0 407 1			
	549.1888	aun.	10.0V MR2 107.0			
2.5	(1000 1124 100 05	1+11)+				
15						
1.5						
0.5		571.1704				
0		([0001124140003]+148	i)+			
	35 540 545 550 55 Counts v	55 560 565 570 575 5	80 585 590 595 600 6	05		
520 525 530 5						
520 525 530 53 MS Spectrum Peak List		and the second se				
520 525 530 53 MS Spectrum Peak List <i>m/z</i> z Abund	Formula	Ion				
520 525 530 53 MS Spectrum Peak List m/z z Abund 549.1888 1 305 550.1922 1 107913	Formula 9089 C30 H24 N6 O5 10.89 C30 H24 N6 O5	Ion (M+H)+ (M+H)+				
520 525 530 53 MS Spectrum Peak List x Abund 300 549,1888 1 300	Formula 9089 C30 H24 N6 O5 30.89 C30 H24 N6 O5 7.38 C30 H24 N6 O5	Ion (M+H)+ (M+H)+ (M+H)+				
520 525 530 53 MS Spectrum Peak List x Abund 549.1888 1 300 550.1922 1 110791 551.1945 1 2134 552.1969 1 3166 553.1976 1 3366	Formula 9089 C30 H24 N6 O5 30.89 C30 H24 N6 O5 7.38 C30 H24 N6 O5 8.63 C30 H24 N6 O5 1.44 C30 H24 N6 O5	Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+				
520 525 530 53 MS Spectrum Peak List z Abund 549.1888 1 300 550.1922 1 10791 551.1945 1 2134 552.1969 1 3166 553.1976 1 366 571.1204 1 15444	Formula 9089 C30 H24 N6 O5 30.89 C30 H24 N6 O5 7.38 C30 H24 N6 O5 8.63 C30 H24 N6 O5 1.44 C30 H24 N6 O5 0.63 C30 H24 N6 O5	Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+				
520 525 530 53 MS Spectrum Peak List z Abund 549.1888 1 300 550.1922 1 10791 551.1945 1 2134 552.169 1 3166 553.1976 1 366 571.1704 1 15444 572.1732 1 5174	Formula i9089 C30 H24 N6 OS 30.89 C30 H24 N6 OS 17.38 C30 H24 N6 OS 8.63 C30 H24 N6 OS 11.44 C30 H24 N6 OS 0.63 C30 H24 N6 OS 1.44 C30 H24 N6 OS 0.63 C30 H24 N6 OS 8.61 C30 H24 N6 OS 1.44 C30 H24 N6 OS 1.86 C30 H24 N6 OS	Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+				
520 525 530 52 MS Spectrum Peak List Z Abund 549.1888 1 300 550.1922 1 10791 551.1945 1 2134 552.169 1 3166 553.1976 1 3164 5721.1704 1 15444 572.1732 1 5174 573.1761 1 1086 574.1788 1 177	Formula 9088 C30 H24 N6 OS 30.89 C30 H24 N6 OS 17.38 C30 H24 N6 OS 14.4 C30 H24 N6 OS 14.4 C30 H24 N6 OS 14.4 C30 H24 N6 OS 0.63 C30 H24 N6 OS 0.63 C30 H24 N6 OS 0.63 C30 H24 N6 OS 0.61 C30 H24 N6 OS 1.66 C30 H24 N6 OS 5.42 C30 H24 N6 OS	Ion ((H+H)+ ((H+H)+ ((H+H)+ ((H+H)+ ((H+H)+ ((H+H)+ ((H+Na)+ ((H+Na)+ ((H+Na)+				
520 525 530 53 MS Spectrum Peak List z Abund 549.1888 1 300 550.1922 1 110791 551.1945 1 2134 552.1691 3166 3366 571.1704 1 15444 572.1732 1 5174 573.1761 1 1086 574.1788 1 171	Formula 99098 C30 H24 N6 OS 30.89 C30 H24 N6 OS 30.89 C30 H24 N6 OS 11.44 C30 H24 N6 OS 0.63 C30 H24 N6 OS 0.63 C30 H24 N6 OS 0.63 C30 H24 N6 OS 1.86 C30 H24 N6 OS 1.86 C30 H24 N6 OS 5.42 C30 H24 N6 OS	Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+				
520 525 530 53 MS Spectrum Peak List z Abund 549,1888 1 300 550,1922 1 10791 551,1945 1 2134 552,1969 1 316 571,1704 1 15444 572,1732 1 5174 574,1761 1 10981 574,1788 1 171	Formula 99098 C30 H24 N6 OS 30.89 C30 H24 N6 OS 30.89 C30 H24 N6 OS 11.44 C30 H24 N6 OS 0.63 C30 H24 N6 OS 0.63 C30 H24 N6 OS 0.63 C30 H24 N6 OS 8.61 C30 H24 N6 OS 1.86 C30 H24 N6 OS 5.42 C30 H24 N6 OS	Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+				
520 525 530 53 MS Spectrum Peak List x Abund 300 549.1888 1 300 300 550.1922 1 10791 301 551.1945 1 2134 306 553.1969 1 316 356 571.1704 1 15444 572.172 1517 573.1761 1 1064 574.1788 1 171 End Of Report 574.1788 1 171 574.1788 1 171	Formula 99098 C30 H24 N6 OS 30.89 C30 H24 N6 OS 30.81 C30 H24 N6 OS 11.44 C30 H24 N6 OS 0.63 C30 H24 N6 OS 0.63 C30 H24 N6 OS 1.66 C30 H24 N6 OS 1.66 C30 H24 N6 OS 5.42 C30 H24 N6 OS	Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+				
520 525 530 53 MS Spectrum Peak List /// /// // // // 549.1888 1 300	Formula 99089 C30 H24 N6 OS 30.89 C30 H24 N6 OS 30.81 C30 H24 N6 OS 11.44 C30 H24 N6 OS 0.63 C30 H24 N6 OS 0.63 C30 H24 N6 OS 1.66 C30 H24 N6 OS 1.66 C30 H24 N6 OS 5.42 C30 H24 N6 OS	Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+				
520 525 530 53 MS Spectrum Peak List /// /// // <th <="" td=""><td>Formula 99089 C30 H24 N6 OS 30.89 C30 H24 N6 OS 30.81 C30 H24 N6 OS 11.44 C30 H24 N6 OS 01.63 C30 H24 N6 OS 11.44 C30 H24 N6 OS 11.64 C30 H24 N6 OS 11.66 C30 H24 N6 OS 5.42 C30 H24 N6 OS</td><td>Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (M+Na)+</td><td></td><td></td><td></td></th>	<td>Formula 99089 C30 H24 N6 OS 30.89 C30 H24 N6 OS 30.81 C30 H24 N6 OS 11.44 C30 H24 N6 OS 01.63 C30 H24 N6 OS 11.44 C30 H24 N6 OS 11.64 C30 H24 N6 OS 11.66 C30 H24 N6 OS 5.42 C30 H24 N6 OS</td> <td>Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (M+Na)+</td> <td></td> <td></td> <td></td>	Formula 99089 C30 H24 N6 OS 30.89 C30 H24 N6 OS 30.81 C30 H24 N6 OS 11.44 C30 H24 N6 OS 01.63 C30 H24 N6 OS 11.44 C30 H24 N6 OS 11.64 C30 H24 N6 OS 11.66 C30 H24 N6 OS 5.42 C30 H24 N6 OS	Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (M+Na)+			
520 525 530 53 MS Spectrum Peak List m/z k list 300 549.1888 1 300 300 550.1922 1 10791 551.1945 2134 552.1969 1 316 553.1976 1 544 572.1720 1 1544 572.1721 1517 573.1761 1 1066 574.1788 1 171 End Of Report Find of the standard standa	Formula 99089 C30 H24 N6 OS 30.89 C30 H24 N6 OS 30.81 C30 H24 N6 OS 11.44 C30 H24 N6 OS 11.44 C30 H24 N6 OS 11.44 C30 H24 N6 OS 11.64 C30 H24 N6 OS 11.66 C30 H24 N6 OS 12.62 C30 H24 N6 OS 5.42 C30 H24 N6 OS	Ion (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (M+Na)+				

Figure 9. Mass spectrum of compound 5c.

Figure 10. ¹H NMR spectrum of compound 5d (400 MHz, DMSO).



Figure 11. ¹³C NMR spectrum of compound 5d (100 MHz, DMSO).



	lalitative Com	pound Repor	t	
Data File MR2 110.d Sample Type Sample Instrument Name Instrument 1 Acq Method 29.10.2014.m IRM Calibration Status Success	Sample Name Position User Name Acquired Time DA Method	MR2 110 P1E5 Icmsdu-PC\admin 09-03-2015 16:41:24 Default.m		
Sample Group Acquisition SW 6200 series TOF/6500 series Version Q-TOF B.05.01 (B5125)	Info.			
Compound Table		1		
Compound Label RT Mass Cpd 2: C31 H27 N5 O3 0.208 517.2106	Formula C31 H27 N5 O3	MFG Formula C31 H27 N5 O3	MFG Diff (ppm) 1.61	DB Formula C31 H27 N5 O3
Compound Label m/z RT Cpd 2: C31 H27 N5 O3 518.218 0.208	Algorithm Find by Molecular Feature	Mass 517.2106	,	
MFE MS Spectrum				
3.5- (10.31	um (0.124-0.541 min) Frag= 518.2180 H27 N5 O31+H1+	100.0V MR2 110.d		
3-	127 10 001+11)+			
2.5				
1.5				
0.5				
0	500 550 600 650 70	750 800 850 000 0		
Counts	vs. Mass-to-Charge (m/z)	730 800 830 900 9	50	
wto 5 Cod 2: C31 H27 N5 O3: +ESI MEE Sporter	m (0.124.0.541 min) 5			
3.5 518.2180	(0.124-0.541 min) Frag=1	00.0V MR2 110.d		
3- ([C31 H27 N5 O3]+H)+			
2.5				
1.5				
1.	540.1994 [C31 H27 N5 O3]+Na)+			
0.5				
490 495 500 505 510 515 520 525 5 Counts	530 535 540 545 550 555 vs. Mass-to-Charge (m/z)	560 565 570 575 580 5	85	
AS Spectrum Peak List				
z ADURD Formula 518.218 1 395118.97 C31 H27 N5 O3	Ion (M+H)+			
519.2207 1 133863.46 C31 H27 N5 O3	(M+H)+			
520.2229 1 25842.03 C31 H27 N5 O3 521.2249 1 3578.09 C31 H27 N5 O3	(M+H)+ (M+H)+			
540.1994 1 36566.13 C31 H27 N5 O3	(M+Na)+			
541.2023 1 13421.55 C31 H27 N5 O3	(M+Na)+			
543.2046 1 2610.42 C31 H27 N5 O3	(M+Na)+ (M+Na)+			
556.1736 1 16023.57 C31 H27 N5 O3	(M+K)+			
- End Of Report				

Figure 12. Mass spectrum of compound 5d.

Figure 13. ¹H NMR spectrum of compound 5e (400 MHz, DMSO).



Figure 14. ¹³C NMR spectrum of compound 5e (100 MHz, DMSO).



Figure 15. Mass spectrum of compound 5e.

		Qua	litative Com	pound Report		
Data File Sample Type Instrument Name Acq Method IRM Calibration Status Comment	MR2 11 Sample Instrun 29.10.2 Succas	11.d nent 1 2014.m s	Sample Name Position User Name Acquired Time DA Method	MR2 111 PIE3 Icmsdu-PC\admin 10-03-2015 15:06:06 Default.m		
Acquisition SW 620 Version Q-1	00 series TOF/0 FOF B.05.01 (E	6500 series 35125)				
Compound Table					MFG Diff	DD Famula
Compound Label	RT	Mass	Formula	MFG Formula C33 H25 CI N6 O3	(ppm) 0.93	C33 H25 CI N6 O3
Cpd 1: C33 H25 CI N6 O	3 0.205	588.1671	C33 H25 CI 10 05	0351125 01110 01		
Compound Label	m/z	RT	Algorithm	Mass		
Cpd 1: C33 H25 CI N6 O	3 589.1746	0.20	5 Find by Molecular Fi	Bature 588.1071		
MFE MS Spectrum	CI N6 O3: +E	ESI MFE Spec	ctrum (0.115-0.632 min) Fi	rag=100.0V MR2 111.d		
x10 5 0pd 1: 000 1120			589.1746 ((C33 H25 CLN6 O3]+H)	+		
4 -			([00011200110001]))			ŝ.
2					50 B C C C C C C C C C C C C C C C C C C	
2					1.000	
1			- .			
0 150 200	250 300 3	50 400 450) 500 550 600 650	700 750 800 850 900	950	
0 150 200	250 300 3	50 400 450 Counts) 500 550 600 650 s vs. Mass-to-Charge (m/z	700 750 800 850 900)	950	
MFE MS Zoomed Spectrum	250 300 3	50 400 450 Counts	500 550 600 650 s vs. Mass-to-Charge (m/z	700 750 800 850 900	950	
0	250 300 3 5 CI N6 O3: +	50 400 450 Counts ESI MFE Spe 589.(1746	0 500 550 600 650 s vs. Mass-to-Charge (m/z ctrum (0.115-0.632 min) F	700 750 800 850 900 ;) rag=100.0V MR2 111.d	950	
0 150 200 MFE MS Zoomed Spectrum x10 5 Cpd 1: C33 H25	250 300 3 5 CI N6 O3: + ([C33 H	50 400 450 Counts ESI MFE Spe 589.[1746 125 C N6 O3]	500 550 660 650 s vs. Mass-to-Charge (m/z ctrum (0.115-0.632 min) F	700 750 800 850 900) ;rag=100.0V MR2 111.d	950	
0 150 200 MFE MS Zoomed Spectrum x10 5 Cpd 1: C33 H28 5 4	250 300 3 5 CI N6 O3: + ([C33 H	50 400 450 Counts ESI MFE Spe 589.1746 125 C N6 O3]	500 550 600 650 s vs. Mass-to-Charge (m/z ctrum (0.115-0.632 min) F +H)+	7óo 75o 8óo 85o 9óo) rag=100.0V MR2 111.d	950	
0 - 150 200 MFE MS Zoomed Spectrum x10 5 Cpd 1: C33 H28 4- 3	250 300 3 5 CI N6 O3: + ([C33 H	50 400 450 Counts ESI MFE Spe 589.(1746 125 C N6 O3)) 500 550 600 650 s vs. Mass-to-Charge (m/z ctrum (0.115-0.632 min) F +H)+	700 750 800 850 900 ;) rag=100.0V MR2 111.d	950	
0 - 150 200 MFE MS Zoomed Spectrum x10 5 Cpd 1: C33 H28 4	250 300 3 5 CI N6 O3: + ([C33 H	50 400 450 Counts ESI MFE Spe 589.1746 125 C N6 03]) 500 550 600 650 s vs. Mass-to-Charge (m/z ctrum (0.115-0.632 min) F +H)+	700 750 800 850 900 ;) rag=100.0V MR2 111.d	950	
0 - 150 200 MFE MS Zoomed Spectrum x10 5 Cpd 1: C33 H28 4	250 300 3 5 CI N6 O3: + ([C33 H	50 400 45C Counts ESI MFE Spe 589./1746 125 C N6 O3)) 500 550 600 650 s vs. Mass-to-Charge (m/z ctrum (0.115-0.632 min) F +H)+ 611.1570 ([C33 H25 CI N6 03]+Na)	700 750 800 850 900 ;) rag=100.0V MR2 111.d	950	
0 - 150 200 MFE MS Zoomed Spectrum x10 5 Cpd 1: C33 H28 4	250 300 3 5 CI N6 O3: + ([C33 H	50 400 450 Counts 589.1746 125 C N6 03)) 500 550 600 650 s vs. Mass-to-Charge (m/z ctrum (0.115-0.632 min) F +H)+ ([C33 H25 CI N6 03]+Na) [11] 600 605 610 615 620	700 750 800 850 900) rag=100.0V MR2 111.d + 1 625 630 635 640 645 650	950	
0 - 150 200 MFE MS Zoomed Spectrum x10 5 Cpd 1: C33 H22 4	250 300 3 5 CI N6 O3: + ([C33 H	50 400 450 Counts 589.1746 125 C N6 03]- 585 590 595 Count) 500 550 600 650 s vs. Mass-to-Charge (m/z ctrum (0.115-0.632 min) F +H)+ ([C33 H25 Cl N6 O3]+Na) [1] 600 605 610 615 620 ts vs. Mass-to-Charge (m/	700 750 800 850 900) rag=100.0V MR2 111.d * L 625 630 635 640 645 650 z)	950	
0 MFE MS Zoomed Spectrum x10 5 Cpd 1: C33 H28 4 3 2 1 5 560 565 53 MS Spectrum Peak L	250 300 3 5 CI N6 03: + ([C33 H 70 575 580 ist	50 400 450 Count 581 MFE Spe 589,1746 225 C N6 03] 585 590 595 Count) 500 550 600 650 s vs. Mass-to-Charge (m/z ctrum (0.115-0.632 min) F +H)+ ([C33 H25 Cl N6 O3]+Na) [1] 600 605 610 615 620 ts vs. Mass-to-Charge (m/	700 750 800 850 900) rrag=100.0V MR2 111.d * L 625 630 635 640 645 650 z)	950	
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Figure 16. ¹H NMR spectrum of compound 5f (400 MHz, DMSO).

Figure 17. ¹³C NMR spectrum of compound 5f (100 MHz, DMSO).



<form></form>		Qual	itative Com	pound Report	:		
Simple Graph Concernent To (FISSO 3 and 10 and	Data File Sample Type Instrument Name Acq Method IRM Calibration Statu Comment	MR2 112.d Sample Instrument 1 29.10.2014.m Is Success	Sample Name Position User Name Acquired Time DA Method	MR2 112 P2F6 Icmsdu-PC\admin 13-03-2015 13:27:59 Default.m			
Compound Label m/z NT Algorithm Mass Cpd 1: C30 H24 Br N5 03 582.1138 0.201 Find by Molecular Feature S81.1064 MFE MS Spectrum S84.1123 (C30 H24 Br N5 03: +ESI MFE Spectrum (0.137-0.671 min) Frage-135.0V MR2 112.d 544.123 0 50 150 200 250 300 350 400 450 500 550 900 950 MFE MS Zoomed Spectrum (C30 H24 Br N5 03: +ESI MFE Spectrum (0.137-0.671 min) Frage-135.0V MR2 112.d 50 500 550 900 950 MFE MS Zoomed Spectrum (C30 H24 Br N5 03: +ESI MFE Spectrum (0.137-0.671 min) Frage-135.0V MR2 112.d 584.1123 (C30 H24 Br N5 03) +H)+ 50 555 560 560 560 500 <t< th=""><th>Compound Table Compound Label Cpd 1: C30 H24 Br I</th><th>6200 series TOF/6500 series Q-TOF B.05.01 (B5125)</th><th>Formula C30 H24 Br NS O3</th><th>MFG Formula C30 H24 Br N5 O3</th><th>MFG Diff (ppm) -0.28</th><th>DB Formula C30 H24 Br N5 O3</th></t<>	Compound Table Compound Label Cpd 1: C30 H24 Br I	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)	Formula C30 H24 Br NS O3	MFG Formula C30 H24 Br N5 O3	MFG Diff (ppm) -0.28	DB Formula C30 H24 Br N5 O3	
Compound Label m/z RT Algorithm Mass Cpd 1: C30 H24 Br NS 03 322.1138 0.201 Find by Molecular Feature S81.1064 MFE MS Spectrum x10 50 502.1128 100.117.0671 min) Frage135.0V MR2 112.4 x10 50 200 250 300 350 400 450 500.114.4 Find by Molecular Feature S81.1064 MFE MS Spectrum (C30 H24 Br NS 03: +ESI MFE Spectrum (0.137-0.671 min) Frage135.0V MR2 112.4 (C30 H24 Br NS 03: +ESI MFE Spectrum (0.137-0.671 min) Frage135.0V MR2 112.4 (C30 H24 Br NS 03: +ESI MFE Spectrum (0.137-0.671 min) Frage135.0V MR2 112.4 (C30 H24 Br NS 03) +H1)+ (C30 H24 Br NS 03) +H1)+ <td colspan<="" td=""><td></td><td></td><td></td><td></td><td></td><td></td></td>	<td></td> <td></td> <td></td> <td></td> <td></td> <td></td>						
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² ¹ ^{606.0933} ^{(C30 H24 Br N5 03)+Na)+ ¹ ¹ ¹ ^{550 555 560 565 570 575 580 585 590 695 600 605 610 615 620 625 630 635 640 645 650 655 ^{m/z} ^x ^{kbund} ^{fonmula} ^{fonmula} ^{m/z} ^{ssolital} ¹³¹ ¹⁶¹ ¹}}	1- 0 150 200 MFE MS Zoomed Spectra x10 5 Cpd 1: C30 H 6- 5- 4-	0 250 300 350 400 450 5 Counts vs H24 Br N5 O3: +ESI MFE Spectri 584,1123 ([C30 H24 Bi N5 O3]+H	550 550 600 650 7 5. Mass-to-Charge (m/z) um (0.137-0.671 min) Fr	700 750 800 850 900 1) rag=135.0V MR2 112.d	950		
 	1 0 150 20 MFE MS Zoomed Spectra x10 5 Cpd 1: C30 H 6 5 4 - 3	0 250 300 350 400 450 5 Counts vs H24 Br N5 03: +ESI MFE Spectru 584,1123 ([C30 H24 B1 N5 03]+H	5500 550 600 650 7 5. Mass-to-Charge (m/z) um (0.137-0.671 min) Fr	700 750 800 850 900 9) rag=135.0V MR2 112.d	950		
Image: Contract to the Contract of the	1 0 150 20 MFE MS Zoomed Spectra x10 5 Cpd 1: C30 H 6 5 4 3 2	0 250 300 350 400 450 5 Counts vs H24 Br N5 03; +ESI MFE Spectru 554,1123 ([C30 H24 Bit N5 03]+H	5500 550 600 650 7 s. Mass-to-Charge (m/z) um (0.137-0.671 min) Fr	7óo 75o 8óo 85o 9óo 9) rag=135.0V MR2 112.d	950		
U 1	1 0 150 200 MFE MS Zoomed Spectrr x10 5 Cpd 1: C30 H 6 5 4 - 3 2 - 1	0 250 300 350 400 450 5 Counts vs H24 Br N5 03: +ESI MFE Spectro 584, IT 123 ([C30 H24 Bt N5 03]+H	500 550 600 650 7 s. Mass-to-Charge (m/z) um (0.137-0.671 min) Fr)+	700 750 800 850 900 9) rag=135.0V MR2 112.d	360		
Counts vs. Mass-to-Charge (m/z) MS Spectrum Peak List m/z z Abund Formula Ion 582.1138 1 607489.61 C30 H24 Br N5 03 (M+H)+ 583.1164 1 200412.31 C30 H24 Br N5 03 (M+H)+ 584.1123 1 630141.5 C30 H24 Br N5 03 (M+H)+ 585.1146 1 35445.66 C30 H24 Br N5 03 (M+H)+ 586.1168 1 35445.66 C30 H24 Br N5 03 (M+H)+ 606.0933 1 22127.4 C30 H24 Br N5 03 (M+H0)+ 606.0933 1 22202.34 C30 H24 Br N5 03 (M+Na)+ 607.0966 1 7828.93 C30 H24 Br N5 03 (M+Na)+ 602.0668 1 6525.42 C30 H24 Br N5 03 (M+Na)+ 622.0668 1 6525.42 C30 H24 Br N5 03 (M+K)+ End Of Report End of Report Printed at: 13:38 on:13-03-2	1 0 150 200 MFE MS Zoomed Spectri x10 5 Cpd 1: C30 H 5 4 - 3 - 2 - 1 -	0 250 300 350 400 450 5 Counts vs H24 Br N5 03: +ESI MFE Spectra 554,1123 ([C30 H24 Bi N5 03]+H	500 550 600 650 7 s. Mass-to-Charge (m/z) um (0.137-0.671 min) Fr)+ 606.0933 30 H24 Br N5 03]+Na)+	700 750 800 850 900 9 rag=135.0V MR2 112.d	950		
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m/z z pound formula ion \$82.138 1 607498.61 C30 H24 Br N5 03 (M+H)+ \$83.1164 1 200412.31 C30 H24 Br N5 03 (M+H)+ \$84.1138 1 6030415. C30 H24 Br N5 03 (M+H)+ \$85.1164 1 200412.31 C30 H24 Br N5 03 (M+H)+ \$86.1168 1 93792.62 C30 H24 Br N5 03 (M+H)+ \$86.1168 1 35445.66 C30 H24 Br N5 03 (M+H)+ \$60.0952 1 2127.4 C30 H24 Br N5 03 (M+Ha)+ \$60.0933 1 22202.34 C30 H24 Br N5 03 (M+Na)+ \$607.0996 1 7828.93 C30 H24 Br N5 03 (M+Na)+ \$607.0996 1 7828.93 C30 H24 Br N5 03 (M+Na)+ \$607.0996 1 7828.93 C30 H24 Br N5 03 (M+Na)+ \$622.0668 1 6525.42 C30 H24 Br N5 03 (M+K)+ End Of Report End Of Report End of Report </td <td>1 0 150 20 MFE MS Zoamed Spectr x10 5 Cpd 1: C30 H 5 4 - 3 2 1 0 550 555 56</td> <td>0 250 300 350 400 450 5 Counts vs H24 Br N5 O3: +ESI MFE Spectri 584,1123 ([C30 H24 Br N5 O3]+H [] [] [] [] [] [] [] [] [] [] [] [] []</td> <td>5500 550 600 650 7 s. Mass-to-Charge (m/z) um (0.137-0.671 min) Fr)+ 606.0933 30 H24 Br N5 O3]+Na)+ 15 600 605 610 615 62 s. Mass-to-Charge (m/z)</td> <td>700 750 800 850 900 1 rag=135.0V MR2 112.d</td> <td>0 655</td> <td></td>	1 0 150 20 MFE MS Zoamed Spectr x10 5 Cpd 1: C30 H 5 4 - 3 2 1 0 550 555 56	0 250 300 350 400 450 5 Counts vs H24 Br N5 O3: +ESI MFE Spectri 584,1123 ([C30 H24 Br N5 O3]+H [] [] [] [] [] [] [] [] [] [] [] [] []	5500 550 600 650 7 s. Mass-to-Charge (m/z) um (0.137-0.671 min) Fr)+ 606.0933 30 H24 Br N5 O3]+Na)+ 15 600 605 610 615 62 s. Mass-to-Charge (m/z)	700 750 800 850 900 1 rag=135.0V MR2 112.d	0 655		
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S84.1123 1 630141.5 G30 H44 Br N5 0.3 (M+H)+ S85.1146 1 197799.26 G30 H24 Br N5 0.3 (M+H)+ S85.1168 1 3544.56 G30 H24 Br N5 0.3 (M+H)+ 604.0952 1 22127.4 G30 H24 Br N5 0.3 (M+Na)+ 605.0991 1 7483.77 C30 H24 Br N5 0.3 (M+Na)+ 605.0992 1 7483.77 C30 H24 Br N5 0.3 (M+Na)+ 605.0993 1 7483.77 C30 H24 Br N5 0.3 (M+Na)+ 607.0996 1 7828.93 C30 H24 Br N5 0.3 (M+Na)+ 602.0668 1 6525.42 C30 H24 Br N5 0.3 (M+K)+ End Of Report End Of Report Printed at: 13:38 on:13-03-2	MFE MS Zoomed Spectra x10 5 Cpd 1: C30 f 5 - 4 - 3 - 2 - 1 - 0 - 550 555 56 MS Spectrum Peal m/z z kb 582.1138 1	0 250 300 350 400 450 5 Counts vs m 124 Br N5 03: +ESI MFE Spectra 584,1123 ([C30 H24 Br N5 03]+H [], ([C3 0 565 570 575 580 585 590 59 Counts vs k List md Formula 607489.61 (20 H24 Br N5 03	500 550 600 660 7 s. Mass-to-Charge (m/z) um (0.137-0.671 min) Fr 1)+ 606.0933 30 H24 Br N5 03]+Na)+ 15 600 605 610 615 62 s. Mass-to-Charge (m/z) 10 n ((M+H)+	700 750 800 850 900 1 rag=135.0V MR2 112.d - - - - - - - - -	950		
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300-100 1 30445.00 CSD Inch of HO US (M+HD)+ 604.052 1 212274 C30 H24 Br NS 03 (M+Na)+ 605.093 1 7483.77 C30 H24 Br NS 03 (M+Na)+ 606.0933 1 22202.34 C30 H24 Br NS 03 (M+Na)+ 607.0966 1 7828.93 C30 H24 Br NS 03 (M+Na)+ 622.0668 1 6525.42 C30 H24 Br NS 03 (M+K)+ End Of Report End Of Report Printed at: 13:38 on:13-03-2	MFE MS Zoomed Spectri x10 5 Cpd 1: C30 H 5 6 4 - 3 - 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	0 250 300 350 400 450 5 Counts vs H24 Br N5 O3: +ESI MFE Spectru 554,1123 ([C30 H24 Br N5 O3]+H [] 0 565 570 575 580 685 590 59 Counts vs k List und Formula 607493.61 (30 H24 Br N5 O3 630141.5 (30 H24 Br N5 O3	500 550 600 650 7 s. Mass-to-Charge (m/z) um (0.137-0.671 min) Fr 006.0933 30 H24 Br N5 03]+Na)+ 11. 15 600 605 610 615 62 s. Mass-to-Charge (m/z) 10n (M+H)+ (M+H)+ (M+H)+	700 750 800 850 900 9 rag=135.0V MR2 112.d	950		
- 1 - 1 <td>MFE MS Zoomed Spectri x10 5 Cpd 1: C30 H 5 - 4 - 3 - 2 - 1 - 5 - 5 - 5 - 5 - 5 - 5 - 5 - 5 - 5 - 5</td> <td>0 250 300 350 400 450 6 Counts vs 124 Br N5 O3: +ESI MFE Spectri 554,1123 ((C30 H24 Br N5 O3)+H ((C30 H24 Br N5 O3)+H ((C30 H24 Br N5 O3) Counts vs clist und Formula 607480,61 (C30 H24 Br N5 O3) 200412.31 (C30 H24 Br N5 O3) 200412.01 (C30 H24 Br N5</td> <td>500 550 600 650 7 s. Mass-to-Charge (m/z) um (0.137-0.671 min) Fr 0060.0933 30 H24 Br N5 03]+Na)+ 11. 15 600 605 610 615 62 s. Mass-to-Charge (m/z) 10n (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+</td> <td>700 750 800 850 900 9 rag=135.0V MR2 112.d</td> <td>950</td> <td></td>	MFE MS Zoomed Spectri x10 5 Cpd 1: C30 H 5 - 4 - 3 - 2 - 1 - 5 - 5 - 5 - 5 - 5 - 5 - 5 - 5 - 5 - 5	0 250 300 350 400 450 6 Counts vs 124 Br N5 O3: +ESI MFE Spectri 554,1123 ((C30 H24 Br N5 O3)+H ((C30 H24 Br N5 O3)+H ((C30 H24 Br N5 O3) Counts vs clist und Formula 607480,61 (C30 H24 Br N5 O3) 200412.31 (C30 H24 Br N5 O3) 200412.01 (C30 H24 Br N5	500 550 600 650 7 s. Mass-to-Charge (m/z) um (0.137-0.671 min) Fr 0060.0933 30 H24 Br N5 03]+Na)+ 11. 15 600 605 610 615 62 s. Mass-to-Charge (m/z) 10n (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+	700 750 800 850 900 9 rag=135.0V MR2 112.d	950		
606.0933 1 22202.34 C30 H24 Br NS 03 (M+Na)+ 607.0956 1 7828.93 C30 H24 Br NS 03 (M+Na)+ 622.0668 1 6525.42 C30 H24 Br NS 03 (M+K)+ End Of Report End Of Report Printed at: 13:38 on:13-03-2	$\begin{array}{c} 1\\ 0\\ \hline \\ 150 & 20 \end{array}$ MFE MS Zoomed Spectric x10 5 Cpd 1: C30 H 5 - - - - - - - - - - - - -	0 250 300 350 400 450 5 Counts vs m 124 Br N5 O3: +ESI MFE Spectr. 584,1123 ((C30 H24 Br N5 O3)+H (C30 H24 Br N5 O3)+H (C30 H24 Br N5 O3) (C0 565 570 575 580 585 590 59 Counts vs k List und Formula 607489.61 C30 H24 Br N5 O3 197799.26 C30 H24 Br N5 O3	500 550 600 650 7 s. Mass-to-Charge (m/z) um (0.137-0.671 min) Fr)+ 606.0933 30 H24 Br N5 O3]+Na)+ <u>1.1.</u> 55 600 605 610 615 62 s. Mass-to-Charge (m/z) 10 m (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+	700 750 800 850 900 1 rag=135.0V MR2 112.d	950		
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End Of Report	1 0 150 200 MFE MS Zoomed Spectra x10 5 6 5 4 3 2 1 0 550 555 56 MS Spectrum Peal m/z z Ab 583.1164 1 588.1146 1	0 250 300 350 400 450 5 Counts vs m 124 Br N5 03: +ESI MFE Spectro 584,1123 ([C30 H24 Br N5 03]+H ([C30 H24 Br N5 03]+H ([C30 H24 Br N5 03] 0 565 570 575 580 585 590 59 Counts vs k List 07489,61 C30 H24 Br N5 03 20012.31 (23 H24 Br N5 03 20012.31 (23 H24 Br N5 03 20141.51 (23 H24 Br N5 03 20141.51 (23 H24 Br N5 03 22127.4 (23 H24 Br N5 03 22127.4 (23 H24 Br N5 03 22127.4 (23 H24 Br N5 03 7483.77 (23 H24 Br N5 03 7483.77 (23 H24 Br N5 03 7282.93) (23 H24 Br N5 03	500 550 600 660 7 s. Mass-to-Charge (m/z) um (0.137-0.671 min) Fr 0 10 124 Br N5 03]+Na)+ 1,1 15 600 605 610 615 62 s. Mass-to-Charge (m/z) 10 m (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+	700 750 800 850 900 9 rag=135.0V MR2 112.d	0 655		
Anilent Technologies Dogo 1 of 1 Drintod at 13:38 on 13-03-0	MFE MS Zoomed Spectra x10 5 Cpd 1: C30 H 5 4 3 2 1 55 55 5 5 4 3 2 1 55 55 55 55 55 55 55 55 55	0 250 300 350 400 450 6 Counts vs 124 Br N5 O3: +ESI MFE Spectri 584,1723 ((C30 H24 Br N5 O3)+H ((C30 H24 Br N5 O3)+H ((C30 H24 Br N5 O3)+H ((C30 H24 Br N5 O3) 200412.31 C30 H24 Br N5 O3 200412.31 C30 H24 Br N5 O3 201424 C30 H24 Br N5 O3 2121274 (C30 H24 Br N5 O3) 221274 (C30 H24 Br N5 O3) 22202.34 (C30 H24 Br N5 O3) 22202.	500 550 600 660 7 s. Mass-to-Charge (m/z) um (0.137-0.671 min) Fr 0060.0933 30 H24 Br N5 03]+Na)+ <u>11.</u> 15 600 605 610 615 625 s. Mass-to-Charge (m/z) 10n (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+K)+ (M+K)+	700 750 800 850 900 9	0 655		
Anilent Technologies Dogo 1 of 1 Drintod at 13:38 on 13-03-0	MFE MS Zoomed Spectric x10 5 5 5 4 3 2 1 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5 5	0 250 300 350 400 450 5 Counts vs m 124 Br N5 O3: +ESI MFE Spectri 584,1123 ((C30 H24 Br N5 O3)+H ((C30 H24 Br N5 O3)+H ((C30 H24 Br N5 O3)+H ((C30 H24 Br N5 O3)+H (C30 H24 Br N5 O3) 200412.31 (C30 H24 Br N5 O3) 197799.26 (C30 H24 Br N5 O3) 197799.27 (C30 H24 Br N5 O3) 197799.28 (C30 H24 Br N5 O3) 19728.29 (C30 H24 Br N5 O3) 192127.4 (C30 H24 Br N5 O3) 19728.29 (C30 H24 Br N5 O3) 19729.29 (C30 H24 Br N5 O3) 19729.29 (C30 H24 Br N5 O3) 19729.20 (C30 H24 Br N5 O3) 19720.20 (C30 H24 Br N5 O3) 19720	500 550 600 650 7 s. Mass-to-Charge (m/z) um (0.137-0.671 min) Fr)+ 606.0933 30 H24 Br N5 O3]+Na)+ <u>1.1.</u> 15 600 605 610 615 62 s. Mass-to-Charge (m/z) 10 m (M+H)+	700 750 800 850 900 1 rag=135.0V MR2 112.d	950		
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Anilant Technologies Days 1 of 1 Drinted at: 12:38 on:13-03-3	MFE MS Zoomed Spectri x10 5 Cpd 1: C30 H 5 5 5 5 5 5 5 5 5 5 5 5 5	0 250 300 350 400 450 5 Counts vs m 124 Br N5 O3: +ESI MFE Spectri 584,1123 ((C30 H24 Br N5 O3)+H ((C30 H24 Br N5 O3)+H ((C30 H24 Br N5 O3) 200412,31 (C30 H24 Br N5 O3) 200412,31 (C30 H24 Br N5 O3) 200412,31 (C30 H24 Br N5 O3) 35445.66 (C30 H24 Br N5 O3) 35445.66 (C30 H24 Br N5 O3) 35445.66 (C30 H24 Br N5 O3) 22127,4 (C30 H24 Br N5 O3) 22202,34 (C30 H24 Br N5 O3) 7282,93 (C30 H24 Br N5 O3)	Image: Solution of the second secon	700 750 800 850 900 1 rag=135.0V MR2 112.d	0 655		
Printed at: 13:38 on 14-14-1	MFE MS Zoomed Spectri x10 5 Cpd 1: C30 f 5 - 4 - 3 - 2 - 1 - 0 - 55 55 56 MS Spectrum Peal <i>m/z</i> z Ab 583.1164 1 584.1123 1 583.1146 1 584.1123 1 585.1146 1 604.0952 1 605.0933 1 607.0966 1	0 250 300 350 400 450 5 Counts vs m 124 Br N5 O3: +ESI MFE Spectri 584,1123 ((C30 H24 Br N5 O3)+H (C30 H24 Br N5 O3)+H (C30 H24 Br N5 O3) 0 565 570 575 580 585 590 59 Counts vs k List md Formula 607489.61 (23 H24 Br N5 O3) 200412.31 (23 H24 Br N5 O3) 200412.31 (23 H24 Br N5 O3) 35445.66 (23 H24 Br N5 O3) 35445.66 (23 H24 Br N5 O3) 22127.47 (230 H24 Br N5 O3) 22202.34 (230 H24 Br N5 O3) 7483.77 (230 H24 Br N5 O3) 72829.93 (230 H24 Br N5 O3)	500 550 600 660 7 5. Mass-to-Charge (m/z) um (0.137-0.671 min) Fr 1)+ 606.0933 30 H24 Br N5 03]+Na)+ 1,1. 15 600 605 610 615 62 5. Mass-to-Charge (m/z) 10 (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (M+K)+ (M+K)+	700 750 800 850 900 1 rag=135.0V MR2 112.d	0 655		

Figure 18. Mass spectrum of compound 5f.

Figure 19. ¹H NMR spectrum of compound 5g (400 MHz, DMSO).



Figure 20. ¹³C NMR spectrum of compound 5g (100 MHz, DMSO).



1	Qualita	tive Com	oound Report		
	Data File MR2 113.d Sample Sample Instrument Name Instrument 1 Acq Method 29.10.2014.m IRM Calibration Status Success Comment Success	Sample Name Position User Name Acquired Time DA Method	MR2 113 PIA5 Icmsdu-PC\admin 18-03-2015 16:01:58 Default.m		
	Sample Group Info. Acquisition SW 6200 series TOF/6500 series Version Q-TOF B.05.01 (B5125)				
	Compound Table	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
	Compound Label RT Mass Cpd 1: C30 H24 F N5 O4 0.201 537.1809	C30 H24 F N5 O4	C30 H24 F N5 O4	0.56	C30 H24 F N5 O4
	MFE MS Spectrum x10 5 Cpd 1: C30 H24 F N5 O4: +ESI MFE Spectrum (52	0.112-0.663 min) Fra	ag=135.0V MR2 113.d		
	8- ([C30 H24	F N5 O4]+H)+			i.
	- 6 - 4 -				
	2 269.5975	-			
	0 ([C30 H24 F N5 (24)+2+)+2 150 200 250 300 350 400 450 500 Counts vs. M) 550 600 650 Mass-to-Charge (m/z	700 750 800 850 900)	950	
	MFE MS Zoomed Spectrum x10 5 Cpd 1: C30 H24 F N5 O4: +ESI MFE Spectrum	(0.112-0.663 min) Fr	ag=135.0V MR2 113.d		
	8		([C30 H24 F N5 O4]+H)+		
	6				
	2-				
	0 260 280 300 320 340 360 380 400 Counts vs.) 420 440 460 4 Mass-to-Charge (m/	80 500 520 540 560 58 z)	30 600	
	MS Spectrum Peak List	Ion			
	538.1884 1 950648.06 C30 H24 F N5 O4 539.191 1 327333.77 C30 H24 F N5 O4	(M+H)+ (M+H)+ (M+H)+			
	540.1932 1 58603.3 C30 H24 F N5 04 541.1967 1 8883.83 C30 H24 F N5 04 560.1690 1 47683 37 C30 H24 F N5 04	(M+H)+ (M+Na)+			
	560.1089 1 +/063.37 C30 124 1 103 04 561.1714 1 16294.88 C30 H24 F N5 04 562.1743 1 .3366.76 C30 H24 F N5 04	(M+Na)+ (M+Na)+			
	576.1442 1 5366.76 C30 H2 F N5 O4 577.1461 1 6087.59 C30 H24 F N5 O4	(M+K)+ (M+K)+			
	578.1443 1 2456.83 C30 H24 F N5 O4	(M+K)+			
	End Of Report				

Figure 21. Mass spectrum of compound 5g.

Figure 22. ¹H NMR spectrum of compound 5h (400 MHz, DMSO).



Figure 23. ¹³C NMR spectrum of compound 5h (100 MHz, DMSO).



Qualita	tive Com	pound Report		
Data File MR2 115.d Sample Type Sample Instrument Name Instrument 1 Acq Method 29.10.2014.m IRM Calibration Status Surcess Comment Surcess	Sample Name Position User Name Acquired Time DA Method	MR2 115 P1E7 Icmsdu-PC\admin 23-03-2015 14:58:15 Default.m		
Sample Group Info. Acquisition SW 6200 series TOF/6500 series Version Q-TOF B.05.01 (B5125)				
Compound Label PT Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C30 H24 Br N5 O4 0.231 597.1003 C	30 H24 Br N5 O4	C30 H24 Br N5 O4	1.39	C30 H24 Br N5 O4
MFE MS Spectrum x10 5 Cpd 1: C30 H24 Br N5 O4: +ESI MFE Spectrum (2 5	0.155-0.439 min) Fr 600.1063	ag=135.0V MR2 115.d		
2.5 - ([C:	80 H24 Br N5 O4]+H)+		
1.5-	-			
0.5	550 600 650	700 750 800 850 900	950	
MFE MS Zoomed Spectrum	0 155 0 420 min) 5	20-125 0V MP2 115 d		
x10 5 CPa 1: C30 H24 Br N5 04: +E31 MrE 2 pectrum 2.5- ([C30 H24 Br N5 04]+H)+ 2-	0.155-0.459 mm) Pi	ag-133.00 Minz 113.0		
1.5				
0.5	622.0874 24 Br N5 O4]+Na)+	1.		
570 575 580 585 590 595 600 605 610 61 Counts vs. M	5 620 625 630 635 ass-to-Charge (m/z	640 645 650 655 660 665	670	
m/z z Abund Formula	Ion			
598.1076 1 260365.76 C30 H24 Br N5 O4 599.1104 1 86919.08 C30 H24 Br N5 O4	(M+H)+ (M+H)+			
600.1063 1 267695.66 C30 H24 Br N5 O4	(M+H)+			
601.1086 1 85347.78 C30 H24 Br N5 O4 602.1109 1 16283.39 C30 H24 Br N5 O4	(M+H)+ (M+H)+			
620.0895 1 31524.26 C30 H24 Br N5 O4	(M+Na)+			
622.0874 1 34032.5 C30 H24 Br N5 O4	(M+Na)+			
623.0898 1 11215.73 C30 H24 Br N5 O4	(M+Na)+ (M+K)+			
638.0618 1 12442.79 C30 H24 Br N5 04 638.0618 1 13566.82 C30 H24 Br N5 04	(M+K)+			
End Of Report				

Figure 24. Mass spectrum of compound 5h.

Figure 25. ¹H NMR spectrum of compound 5i (400 MHz, DMSO).



Figure 26. ¹³C NMR spectrum of compound 5i (100 MHz, DMSO).



 Qualitative Compound Report
Data File MR2 116.d Sample Name MR2 116 Sample Type Sample Position P182 Instrument Name Instrument I User Name Icmsdu-PC\admin Acq Method 29.10.2014.m Acquired Time 24-03-2015 15:02:39 IRM Calibration Status Success DA Method Default.m
Sample Group Info. Acquisition SW 62d0 series TOF/6500 series Version Q-TOF B.05.01 (B5125)
Compound Table
Compound Label RT Mass Formula MFG Formula (ppm) DB Formula Cpd 1: C30 H24 N6 06 0.218 564.1752 C30 H24 N6 06 C30 H24 N6 06 1 C30 H24 N6 06
Compound Label m/z RT Algorithm Mass Cpd 1: C30 H24 N6 06 565.1825 0.218 Find by Molecular Feature 564.1752
MFE MS Spectrum
x10 5 Cpd 1: C30 H24 N6 O6: +ESI MFE Spectrum (0.158-0.575 min) Frag=135.0V MR2 116.d
2 ([C30 H24 N6 O6]+H)+
1.5
1
0.5
150 200 250 300 350 400 450 500 550 600 650 700 750 800 850 900 950 Counts vs. Mass-to-Charge (m/z)
MFE MS Zoomed Spectrum
x10 3 Cpd 1. C30 H24 NO C6. 4C31 MHC 3pectrum (0.156-0.575 min) Frag=135.0V MH2 116.0
2- ((C30 H24 No Obj+H)+
1.5
1
0.5 - ([C30 H24 N6 O6]+Na)+
Counts vs. Mass-to-Charge (m/z)
m/s spectrum reak LIST
565.1825 1 230437.3 C30 H24 N6 O6 (M+H)+ 566.1854 1 75612.29 C30 H24 N6 O6 (M+H)+
567.1882 1 16111.56 C30 H24 N6 O6 (M+H)+
So8.19 1 Z518.15 C30 H24 N6 (M+H)+ 587.1636 1 20233.27 C30 H24 N6 (M+Na)+
588.1674 1 7167.26 C30 H24 N6 O6 (M+Na)+ 589.1695 1 1511.29 C30 H24 N6 O6 (M+Na)+
603.1388 1 8183.46 C30 H24 N6 O6 (M+K)+
604.1419 1 3165.61 C30 H24 N6 (M+K)+ 605.1396 1 1389.25 C30 H24 N6 (M+K)+
End Of Report

Figure 27. Mass spectrum of compound 5i.

Figure 28. ¹H NMR spectrum of compound 5j (400 MHz, DMSO).



Figure 29. ¹³C NMR spectrum of compound 5j (100 MHz, DMSO).



				Oua	alitative Con	nound Dana		
					intuitive com	проина керо	rt	
	Data Fi	le	MR2	-117.d	Comula No.			
	Sample	Туре	Sam	ple	Sample Name Position	MR2-117		
	Instrun	nent Name	Instr	ument 1	User Name	PIFI (cmsdu-PC)admin		
	IRM Cal	libration Status	29.1	0.2014.m	Acquired Time	30-03-2015 14:49:56		
	Comme	nt	Suce	855	DA Method	Default.m		
	Sample	Group						
	Acquisit	ion SW 6	200 series TOF	/6500 series	nro.			
		Q	2-10F B.05.01	(85125)				
	Compo	und Table						
	Con	pound Label	RT	Mass	Formula	MFG Formula	MFG Diff	
		u 1. C31 H27 N5 C	0.216	533.2053	C31 H27 N5 O4	C31 H27 N5 O4	(ppm) 1.83	C31 H27 N5 O4
	Compos	und Lab al						
	Cpd 1: C	31 H27 N5 O4	<i>m/z</i> 534.2127	RT 0.216	Algorithm	Mass		
	L				ind by Holecular rea	iture 533.2053		
	MFE MS Sp	ectrum						
	x10 6	Cpd 1: C31 H27 I	N5 04: +ESI	MFE Spectrum	(0.139-0.423 min) Frag=1	35.0V MR2-117.d		
	0.0			([C31 I	534.2127 127 N5 O4]+H)+			
	0.0							
	0.6							
	0.4							
	0.2	267	7.6105		-			
	04	([C31 H27	N5 04]+2H)+	2				
		130 200 25	0 300 350	400 450 50 Counts vs.	00 550 600 650 700 Mass-to-Charge (m/z)	750 800 850 900 95	50	
	MFE MS Zoo	med Spectrum						
	×10 6 Cr	od 1: C31 H27 N	5 O4: +ESI M	FE Spectrum (0	0.139-0.423 min) Frag=13	5.0V MR2-117.d		
	0.8					534.2127 ([C31 H27 N5 O4]+H)+		
	0.0							
	0.6							
	0.4							
	0.2							
	0	260 280 20						
		200 200 300	J 320 340	360 380 400 Counts vs. M	420 440 460 480 5 Mass-to-Charge (m/z)	00 520 540 560 580	600	
L.	IS Spectro	um Peak List						
É	267.6105	Abund	4900.18 C31	H27 N5 O4	Ion			
F	534.2127	1 106	9358.63 C31	H27 N5 04	(M+2H)+2 (M+H)+			
F	535.2156	1 38	4592.12 C31	127 N5 O4	(M+H)+			
F	537.2188		4633.38 C31 0999 57 C31 0	127 N5 04	(M+H)+			
F	556.1935	1	70343.2 C31 H	127 N5 04	(M+H)+ (M+N=)+			
H	557.1969	1	25307.9 C31 H	127 N5 O4	(M+Na)+			
F	572.1676	1 1	5238.03 C31 H	27 N5 04	(M+Na)+			
	573.1708	1 6	5048.69 C31 H	27 N5 04	(M+K)+ (M+K)+			
	End Of Pen	t			(interpreted)			
	- nu or rtept	AC						
1	AnilantTa	abralasias						

Figure 30. Mass spectrum of compound 5j.

Figure 31. ¹H NMR spectrum of compound 5k (400 MHz, DMSO).



Figure 32. ¹³C NMR spectrum of compound 5k (100 MHz, DMSO).



	Qual	itative Com	pound Report		
Data File Sampie Type Instrument Name	MR2-118.d Sample Instrument 1	Sample Name Position User Name	MR2-118 P2-A6		
Acq Method IRM Calibration Status Comment	29.10.2014.m Success	Acquired Time DA Method	31-03-2015 15:05:03 Default.m		
Sample Group Acquisition SW 6200 Version Q-TO	In series TOF/6500 series F B.05.01 (B5125)	lfo.			
Compound Table				MFG Diff	
Compound Label Cpd 4: C30 H24 CI N5 O4	RT Mass 0.215 553.1514	Formula C30 H24 Cl N5 O4	MFG Formula C30 H24 CI N5 O4	(ppm) E 0.55 C30	B Formula H24 Cl N5 O4
Compound Label Cpd 4: C30 H24 Cl N5 O4	<i>m/z</i> RT 554.1587 0.215	Algorithm Find by Molecular Fe	Mass eature 553.1514		
MFE MS Spectrum					
x10 6 1.6 1.4	N5 O4: +ESI MFE Spectr ([C3)	rum (0.139-0.723 min) Fr 554.1587 0 H24 C(N5 O4]+H)+	ag=135.0V MR2-118.d		i.
1.2					
0.6 -		-			
0.2 0 ([C30 H24 C 150 200 256	7.5832 CI N5 O4]+2H)+2 0 300 350 400 450 Counts V	500 550 600 650 7	700 750 800 850 900	950	
MFE MS Zoomed Spectrum		(0.400.0.700			
MFE MS Zoomed Spectrum x10 6 Cpd 4: C30 H24 C 1.6 1.4	I N5 O4: +ESI MFE Spect	rum (0.139-0.723 min) F	rag=135.0V MR2-118.d 554.1587 . ([C30 H24 C N5 O4]+H)+		
MFE MS Zoomed Spectrum x10 6 Cpd 4: C30 H24 C 1.6 1.4 1.2 1	I N5 O4: +ESI MFE Spect	rum (0.139-0.723 min) F	rag=135.0V MR2-118.d 554.j587 , ([C30 H24 Cl N5 O4]+H)+		
MFE MS Zoomed Spectrum x10 6 1.6 1.4 1.2 1 0.8 0.6	I N5 O4: +ESI MFE Spect	rum (0.139-0.723 min) F	rag=135.0V MR2-118.d 554,if587 , ([C30 H24 Cl N5 O4]+H)+		
MFE MS Zoomed Spectrum x10 6 Cpd 4: C30 H24 Cl 1.4 1.2 1 0.8 0.6 0.4 0.2	I N5 O4: +ESI MFE Spect	rum (0.139-0.723 min) F	rag=135.0V MR2-118.d 554.J587 ([C30 H24 Cl N5 O4]+H)+		
MFE MS Zoomed Spectrum x10 6 1.6 1.4 1.2 0.8 0.6 0.4 0.2 0 260 280 300	I N5 O4: +ESI MFE Spect 320 340 360 380 400 Counts	rum (0.139-0.723 min) F 1 (0.139-0.723 min) F 2 (0.139-0.723 min) F	rag=135.0V MR2-118.d 554.J587 ([C30 H24 Cl N5 O4]+H)+ ([C30 520 540 560 580 60	0 620	
MFE MS Zoomed Spectrum x10 6 Cpd 4: C30 H24 Cl 1.6 1.4 1.2 0 260 280 300 MS Spectrum Peak List m/z z Abund	I N5 O4: +ESI MFE Spect 320 340 360 380 400 Counts E	rum (0.139-0.723 min) F 0. 420 440 460 480 vs. Mass-to-Charge (m/a Ion	rag=135.0V MR2-118.d 554.1587 . ([C30 H24 Cl N5 O4]+H)+ 500 520 540 560 580 60	10 620	
MFE MS Zoomed Spectrum x10 6 Cpd 4: C30 H24 C 1.6 1.4 1.2 0 260 280 300 MS Spectrum Peak List m/z z Abund 554.1587 1 1 554.1587 1	320 340 360 380 400 Counts Formula 664031.63 (20 H24 CI NS C 584651.57 (20 H24 CI NS C	rum (0.139-0.723 min) F) 420 440 450 480 1 vs. Mass-to-Charge (m/a Ion (M+H)+)4 ((M+H)+	rag=135.0V MR2-118.d 554.1587 . ([C30 H24 Cl N5 O4]+H)+ 500 520 540 560 580 6(0 620	
MFE MS Zoomed Spectrum x10 6 1.6 1.4 1.2 0 260 280 300 MS Spectrum Peak List m/z z Abund 554.1587 1 1 556.1581 1	320 340 360 380 400 Counts 664031.63 C30 H24 CI NS C 584651.57 (C30 H24 CI NS C 644284.2 (C30 H24 CI NS C 644284.2 (C30 H24 CI NS C	rum (0.139-0.723 min) F) 420 440 450 480 3 vs. Mass-to-Charge (m/a Ion 4 (M+H)+ 34 (M+H)+ 34 (M+H)+	rag=135.0V MR2-118.d 554.1587 ([C30 H24 Cl N5 O4]+H)+ 500 520 540 560 580 6(0 620	
MFE MS Zoomed Spectrum x10 6 1.6 1.4 1.2 0.8 0.6 0.4 0.2 0 260 280 300 MS Spectrum Peak List <u>m/z z Abund</u> 554.1587 1 1 555.1618 1 555.1518 1 557.1592 1 557.1592 1	320 340 360 380 400 Counts Formula 664031.63 C30 H24 CI NS C 584651.57 (C30 H24 CI NS C 644284.2 C30 H24 CI NS C 644284.2 C30 H24 CI NS C 644284.2 C30 H24 CI NS C	rum (0, 139-0, 723 min) F) 420 440 450 480 3 vs. Mass-to-Charge (m/2 Kon 4 (M+H)+ 34 (M+H)+ 34 (M+H)+ 34 (M+H)+ 34 (M+H)+	rag=135.0V MR2-118.d 554.1587 ([C30 H24 Cl N5 O4]+H)+ 500 520 540 560 580 6(0 620	
MFE MS Zoomed Spectrum x10 6 1.6 1.4 1.2 1 0.8 0.6 0.4 0.2 0 260 280 300 MS Spectrum Peak List <u>m/z z Abund</u> 554.1587 1 1 555.1618 1 555.1618 1 555.1618 1 555.1628 1 557.1592 1 557.1592 1 556.1588 1 576.1402 1	320 340 360 380 400 Counts Formula 664031.63 C30 H24 Cl NS C 584651.57 C30 H24 Cl NS C 644284.2 C30 H24 Cl NS C 644284.2 C30 H24 Cl NS C 191171.93 C30 H24 Cl NS C 120598.38 C30 H24 Cl NS C 120598.38 C30 H24 Cl NS C	rum (0, 139-0, 723 min) F) 420 440 450 480 3 ys, Mass-to-Charge (m/z 4 (M+H)+ 4 (rag=135.0V MR2-118.d 554.1587 ([C30 H24 Cl N5 O4]+H)+ 500 520 540 560 580 6(0 620	
MFE MS Zoomed Spectrum x10 6 1.6 1.4 1.2 1 0.8 0.6 0.4 0.2 260 280 300 MS Spectrum Peak List <u>m/z z Abund</u> 554.1587 1 1 555.1518 1 555.1518 1 557.1592 1 557.1592 1 557.1592 1 577.1429 1 577.1429 1	320 340 360 380 400 Counts Formula 664031.63 C30 H24 Cl N5 C 584651.57 C30 H24 Cl N5 C 644284.2 C30 H24 Cl N5 C 644284.2 C30 H24 Cl N5 C 191171.93 C30 H24 Cl N5 C 120598.38 C30 H24 Cl N5 C 41761.82 C30 H24 Cl N5 C 41761.82 C30 H24 Cl N5 C	rum (0, 139-0, 723 min) F) 420 440 450 480 3 vs. Mass-to-Charge (m/z 100 (M+H)+ 14	rag=135.0V MR2-118.d 554.1587 ([C30 H24 Cl N5 O4]+H)+ 500 520 540 560 580 6(0 620	
MFE MS Zoomed Spectrum x10 6 1.6 1.4 1.2 1 0.8 0.6 0.4 0.2 0 260 280 300 MS Spectrum Peak List m/z z Abund 554.1587 1 1 555.1618 1 555.1618 1 555.1618 1 555.1618 1 555.1618 1 556.1575 1 557.1592 1 557.1592 1 557.1592 1 557.1402 1 577.1429 1 577.1429 1 577.1388 1 579.1398 1	320 340 360 380 400 Counts Formula 664031.63 C30 H24 Cl NS C 584651.57 C30 H24 Cl NS C 644284.2 C30 H24 Cl NS C 644284.2 C30 H24 Cl NS C 644284.2 C30 H24 Cl NS C 120598.38 C30 H24 Cl NS C 41761.82 C30 H24 Cl NS C 41761.82 C30 H24 Cl NS C 41473.36 C30 H24 Cl NS C 14473.36 C30 H24 Cl NS C	rum (0, 139-0, 723 min) F) 420 440 450 480 3 vs. Mass-to-Charge (m/z 100 (M+H)+ 14	rag=135.0V MR2-118.d 554.1587 ([C30 H24 Cl N5 O4]+H)+ 500 520 540 560 580 6(0 620	
MFE MS Zoomed Spectrum x10 6 1.6 1.4 1.2 0.8 0.6 0.4 0.2 0 260 280 300 MS Spectrum Peak List m/z z Abund 554.1587 1 1 555.1575 1 557.1592 1 558.1588 1 577.1429 1 578.1388 1 578.1388 1 578.1388 1 578.1389 1 578.1499 1 578.1499 1 578.1499 1 578.1	I N5 O4: +ESI MFE Spect 320 340 360 380 400 Counts Formula 664031.63 C30 H24 CI N5 C 544551.57 C30 H24 CI N5 C 644284, 230 H24 CI N5 C 191171.93 C30 H24 CI N5 C 10593.83 C30 H24 CI N5 C 41761.82 C30 H24 CI N5 C 41473.46 C30 H24 CI N5 C 14473.46 C30 H24 CI N5 C 16267.15 C30 H24 CI N5 C	rum (0.139-0.723 min) F 0 420 440 450 480 1 vs. Mass-to-Charge (m/2 10 (M+H)+ 14 (M+	rag=135.0V MR2-118.d 554.1587 ([C30 H24 Cl N5 O4]+H)+ 500 520 540 560 580 60	0 620	

Figure 33. Mass spectrum of compound 5k.

Figure 34. ¹H NMR spectrum of compound 5l (400 MHz, DMSO).



Figure 35. ¹³C NMR spectrum of compound 5l (100 MHz, DMSO).



Figure 36. Mass spectrum of compound 5l.

				Qu	alita	tive Com	pound R	eport			
Data Fil	e		MR21 Samp	19.d		Sample Name	MR2119 P2-D8				
Instrum	ent Name		Instru	ment 1		User Name					
Acq Met	hod	habua	29.10	.2014.m		Acquired Time	06-04-2015 15:07	7:06			
Comme Sample Acquisit Version	nt Group ion SW	6200 Q-TC	I series TOF, DF B.05.01 (/6500 series B5125)	Info.						
Compo	ound Tabl	le							MFG Diff		
Co	mpound La	abel	RT 0.201	Mass	6 03	Formula	MFG For	mula	(ppm)	C33 H25 CL	N6 04
Сра	1: C33 H25	U 110 U4	0.201	004.102		3 H25 CI NO 04	055 1125 0	110 04	0.00	635 1125 61	1001
MFE MS	Spectrum	33 H25 CI	I N6 Q4: +I	-SI MEE Sr	pectrum (0	132-0.549 min) Fr	ag=135.0V MR21				
×10 °	Cpu I. C	331123 01	1140 04. 11		605.170)	ag 100.00 militzi	10.0			
3.5				([C33 H	125 CI N6	O4]+H)+					i.
3	-										
2.5											
1.5	(1C3	303.0 3 H25 CU	0888 N6 041+2F	1)+2							
1	1 (100	120 011	10041.21	1)-2		-					
0.5	-				1.						
0	2	00 30	20 400) 500 Cour	600 nts vs. Ma	700 800 ss-to-Charge (m/z)	900 1000	1100	1200		
MFE MS	Zoomed Sp	ectrum									
×10 5	Cpd 1: C	33 H25 CI	I N6 O4: +I	ESI MFE Sp	bectrum (0	.132-0.549 min) Fr	ag=135.0V MR21	19.d			
4	-		(IC33)	605.1700 H25 CI N6 C	041+H)+						
3.5			(loss .								
2.5											
2											
1.5								1200	2200		
0.5								(2M	-3306 +H)+		
C	300	400	500	600	700	800 900	1000 1	100 120	00		
MC Co	o okuumo D	ank Link		Cou	nts vs. Ma	ss-to-Charge (m/z)					
ms sp m/z	z	Abund	Form	nula		Ion					
30:	8.0888 2	12147	74.15 C33 I	125 CI N6 O4		(M+2H)+2					
30.	3.5903 2 1.0887 2	4537	74.37 C33 1	125 CI N6 O4		(M+2H)+2 (M+2H)+2					
	1.5894 2	159	954.8 C33 I	125 CI N6 O4		(M+2H)+2					
	505.17 1	43532	22.53 C33	125 CI N6 O4		(M+H)+					
60	7.1688 1	16086	01.73 C33	125 CI N6 04		(M+H)+ (M+H)+					
60	3.1704 1	523	32.37 C33	125 CI N6 04		(M+H)+					
62	7.1516 1	2756	66.45 C33 I	125 CI N6 04		(M+Na)+					
62	3.1631 1	1116	58.31 C33	H25 CI N6 O4		I(M+Na)+					
End	Of Report	-									





Figure 38. ¹³C NMR spectrum of compound 5m (100 MHz, DMSO).



-	4		Qua	litative Com	pound Report	:	
	Data File Sample Type Instrument Name Acq Method IRM Calibration Status Comment	mr21 Samj Instr 29.11 Succ	.20.d ple ument 1 0.2014.m ess	Sample Name Position User Name Acquired Time DA Method	mr2120 P1-89 08-04-2015 15:46:12 Default.m		
	Sample Group Acquisition SW 620 Version Q-T	0 series TO OF B.05.01) F/6500 series (B5125)	Info.			
	Compound Table					MEG Diff	
	Compound Label	RT	Mass	Formula	MFG Formula	(ppm)	DB Formula
	Cpd 1: C30 H23 Br Cl N5 O3	0.201	615.068	C30 H23 Br CI N5 O3	C30 H23 Br Cl N5 O3	-1.24	C30 H23 Br Cl N5 O3
	Compound Label Cpd 1: C30 H23 Br Cl N5 O3	<i>m/z</i> 616.075	RT 4 0.20	Algorithm 1 Find by Molecular Fe	Mass ature 615.068		
	4 3 2 1 0 ([C36 H20 Cl3 N 200 300 MFE MS Zoomed Spectrum x10 5 Cpd 1: C30 H23 E 5 4 3-	([C: 13 O]+2H)- 400 3r CI N5 O	30 H23 Br CI NS +2 500 600 Counts 3: +ESI MFE Sp	5 O3 +H)+ 700 800 900 100 vs. Mass-to-Charge (m/z) pectrum (0.133-0.434 min)	0 1100 1200 1300 14 Frag=135.0V mr2120.d 618.0737 ([C30 H23 Br CI N5 O3]+I	400 H)+	
	2- 1- 300 320 340 MS Spectrum Peak List m/z z Abund	0 360 380 t Fon) 400 420 440 Counts mula) 460 480 500 520 540 vs. Mass-to-Charge (m/z) Ion	560 580 600 620 640 66	50 680	
	616.0754 1 3892 617.078 1 126 618.0737 1 5315 619.076 1 1691 620.072 1 1448 621.074 1 423 623.073 1 88 638.057 1 204 640.0547 1 224	34.99 C30 3467.1 C30 314.63 C30 13.11 C30 358.24 C30 302.93 C30 953.18 C30 480.07 C30 444.42 C30	H23 Br Cl N5 03 H23 Br Cl N5 03	(M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+			
	641.0576 1 96	544.03 C30	H23 Br Cl N5 O3	8 (M+Na)+			
			And in case of the local division of the loc				

Figure 39. Mass spectrum of compound 5m.





Figure 41. ¹³C NMR spectrum of compound 5n (100 MHz, DMSO).



а I	Qualita	ative Comp	ound Report		
Data File Sampie Type Instrument Name Acq Method IRM (calibration Status Comment Sample Group Acquisition SW 6200 se	MR2 121.d Sample Instrument 1 29.10.2014.m Success Info. refes TOF/6500 series o co p. (75125)	Sample Name M Position P User Name Acquired Time 1 DA Method D	IR2 121 1-D6 0-04-2015 15:40:23 Þefault.m		
Compound Table Compound Label Cpd 1: C30 H23 Br2 N5 03	RT Mass 0.2 659.0167	Formula C30 H23 Br2 N5 O3	MFG Formula C30 H23 Br2 N5 O3	MFG Diff (ppm) 0.08	DB Formula C30 H23 Br2 N5 O3
Compound Label n Cpd 1: C30 H23 Br2 N5 6	<i>m/z</i> RT 560.0246 0.2	Algorithm Find by Molecular Fea	Mass ture 659.0167		
×10 5 Cpd 1: C30 H23 Brz	662.0232 ([C30 H23 Br2 N5	2 O3]+H)+			
1		-		1/00	
1 200 300 MFE MS Zaomed Spectrum x10 5 Cpd 1: C30 H23 Br 4 3 2 1	400 500 60 70 Counts vs -2 N5 03: +ESI MFE Spect 662,0232 (IC30 H23 Br2 N5 C	0 800 900 100 Mass-to-Charge (m/2) um (0.139-0.606 min) F)3]+H)+ 684.0044 ((C30 H23 Br2 N50	0 1100 1200 1300 rag=135.0V MR2 121.d 3]+Na)+	1400	
1 200 300 MFE MS Zaomed Spectrum x10 5 Cpd 1: C30 H23 Br 4 3 6 630 635 640 MS Spectrum Peak List m/z z Abud	400 500 600 70 Counts vs 2 N5 03: +ESI MFE Spectr 662,2232 ([C30 H23 Br2 N5 C 645 650 655 660 665 Counts v 645 650 655 660 665	0 800 900 1000 Mass-to-Charge (m/2) um (0.139-0.606 min) F 3]+H)+ 684.0044 ((C30 H23 Br2 N5 O (C30 H23 Br2 N5 O (C30 H23 Br2 N5 O (14+H)+	0 1100 1200 1300 rag=135.0V MR2 121.d h3]+Na)+	1400	
1 200 300 MFE MS Zoomed Spectrum x10 5 Cpd 1: C30 H23 Br 4 3 2- 1 0 630 635 640 MS Spectrum Peak List m/z z Abund 660.0276 1 2244 661.0272 1 2493 662.0252 1 446 664.0281 1 2493 665.0271 1 146 665.0271 1 199 665.0256 1 142 668.0025 1 109 668.0025 1 109 668.0025 1 109 668.0025 1 100	400 500 600 70 Counts vs (C30 H23 Br2 N5 C3 (C30 H23 Br2 N5 C3) (C30 H23 Br2 N5 C3	0 800 900 100 Mass-to-Charge (m/2) um (0.139-0.606 min) F 33]+H)+ ((C30 H23 Br2 N50 (C30 H23 Br2 N50 (H4+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+Na)+ (M+Na)+	0 1100 1200 1300 rag=135.0V MR2 121.d r3]+Na)+	715 720	
1 200 300 MFE MS Zaomed Spectrum x10 5 Cpd 1: C30 H23 Br 3 - - 1 - - - 3 - - - 1 - - - - 3 - - - - 4 - - - - - 1 -	400 500 600 70 Counts vs (C30 H23 Br2 N5 03 (C30 H23 Br2 N5 03)	0 800 900 100 Mass-to-Charge (m/2) um (0.139-0.606 min) F 33]+H)+ ((C30 H23 Gr2 N5 O L1) 670 675 680 685 6 s. Mass-to-Charge (m/2) (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+	0 1100 1200 1300 rag=135.0V MR2 121.d 23]+Na)+ 30 695 700 705 710 1	1400	

Figure 42. Mass spectrum of compound 5n.

Figure 43. ¹H NMR spectrum of compound 50 (400 MHz, DMSO).



Figure 44. ¹³C NMR spectrum of compound 50 (100 MHz, DMSO).



		Qual	itative Com	pound Repor	t	
Data File Sample Type Instrument Name Acq Method IRM Calibration Status Comment Sample Group Acquisition SW	MR2 12 Sample Instrum 29.10.21 Success 6200 series TOF/6	2.d ent 1 014.m Int 500 series	Sample Name Position User Name Acquired Time DA Method	MR2 122 P1-E1 13-04-2015 15:52:20 Default.m		
Compound Table	Q 101 0.00101 (0.					
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 5: C33 H24 Br Cl N6	03 0.215	666.0775	C33 H24 Br Cl N6 O3	C33 H24 Br CI N6 O3	1.05	C33 H24 Br Cl N6 O
x10 5 Cpd 5: C33 H2 2-	24 Br CI N6 O3: +	ESI MFE Spec 669. ([C33 H24 Br (strum (0.149-0.616 min) 0824 DI N6 O3]+H)+	Frag=135.0V MR2 122.d		
([C33 H24 F 1- 0.5-	335.0452 Br Cl N6 O3]+2H)+2	-			
MFE MS Zoomed Spectrum x10 5 Cpd 5: C33 H2 2- 1.5- 1- 0.5-	n 24 Br Cl N6 O3: +	ESI MFE Spec	Mass-to-Charge (m/z)	Frag=135.0V MR2 122.d 669.0824 ([C33 H24 Br C] N6 O3	+H)+	
MS Spectrum Peak I	0 380 400 420 List	440 460 480 9 Counts vs	500 520 540 560 580 . Mass-to-Charge (m/z)	600 620 640 660 680 700	720	
m/z z Abun 334.0456 2 1 334.0457 2 1 335.0452 2 1 335.0452 2 1 335.0454 2 1 366.0445 2 1 667.084 1 1 668.0865 1 1 620.024 1 2	Formul 82129.80 C33 H2 32007.80 C33 H2 13420.75 C33 H2 42762.4 C33 H2 35855.03 C33 H2 173635.7 C33 H2 64503.74 C33 H2 64503.74 C33 H2 9202.80 C33 H2	Ia 4 Br Cl N6 O3 4 Br Cl N6 O3	Ion (M+2H)+2 (M+2H)+2 (M+2H)+2 (M+2H)+2 (M+H)+ (M+H)+ (M+H)+ (M+H)+ (M+H)+			
671.081 1	66975.23 C33 H24	+ br CI N6 03 4 Br CI N6 03	(M+H)+ (M+H)+			
End Of Report						

Figure 45. Mass spectrum of compound 50.

Figure 46. ¹H NMR spectrum of compound 5p (400 MHz, DMSO).



Figure 47. ¹³C NMR spectrum of compound 5p (100 MHz, DMSO).



	Quali	tative Com	pound Report		
Data File Sample Type Instrument Name Acq Method IRM Calibration Status Comment	MR2 123.d Sample Instrument 1 29.10.2014.m Sutcess	Sample Name Position User Name Acquired Time DA Method	MR2 123 P1-C6 15-04-2015 15:44:30 Default.m		
Sample Group Acquisition SW 6200 Version Q-TO	Inf series TOF/6500 series IF B.05.01 (B5125)	ю.			
Compound Table Compound Label Cpd 1: C31 H26 Br N5 O4	RT Mass 0.211 611.1161	Formula C31 H26 Br N5 O4	MFG Formula C31 H26 Br N5 O4	MFG Diff (ppm) 1.16	DB Formula C31 H26 Br N5 O4
Compound Label Cpd 1: C31 H26 Br N5 O4	<i>m/z</i> RT 612.1236 0.211	Algorithm Find by Molecular F	Mass eature 611.1161		
MFE MS Spectrum					
x10 5 Cpd 1: C31 H26 Br 1.75 1.5 1.25	r N5 O4: +ESI MFE Spectro 614.1219 ([C31 H26 Br N5 O4	um (0.130-0.463 min) F 4]+H)+	rag=135.0V MR2 123.d		
1 0.75 0.5	77				
0.25 0 (M+2H) 200 300	400 500 600 70 Counts vi	00 800 900 10 s. Mass-to-Charge (m/z	00 1100 1200 1300 14 z)	400	
MFE MS Zoomed Spectrum x10 5 Cpd 1: C31 H26 B 1.75- 1.5-	r N5 O4: +ESI MFE Spectr	um (0.130-0.463 min) F	Frag=135.0V MR2 123.d 614.1219 ([C31 H26 Br N5 O4]+H)+	
1.25 1- 0.75 0.5- 307.5637					
0.25 (M+2H)+2 0 280 300 320 340	0 360 380 400 420 440 Counts v	460 480 500 520 54 s. Mass-to-Charge (m/	40 560 580 600 620 640 6 z)	60 680	
MS Spectrum Peak List	t Formula	Ion (M+2H)+2			
307.5637 2 26 612.1236 1 1810 613.1261 1 620 614.1219 1 1875 615.1244 1 615	040.88 C31 H26 Br N5 O4 093.92 C31 H26 Br N5 O4 522.66 C31 H26 Br N5 O4 510.21 C31 H26 Br N5 O4	(M+H)+ (M+H)+ (M+H)+ (M+H)+			
616.1271 1 12 634.107 1 7 635.1117 1 29 636.1039 1 82 637.1076 1 28	2329.5 C31 H26 Br N5 O4 7974.2 C31 H26 Br N5 O4 667.69 C31 H26 Br N5 O4 216.11 C31 H26 Br N5 O4 898.56 C31 H26 Br N5 O4	(M+H)+ (M+Na)+ (M+Na)+ (M+Na)+ (M+Na)+			
End Of Report					

Figure 48. Mass spectrum of compound 5p.

Figure 49. ¹H NMR spectrum of compound 5q (400 MHz, DMSO).



Figure 50. ¹³C NMR spectrum of compound 5q (100 MHz, DMSO).





Figure 51. Mass spectrum of compound 5q.

Figure 52. ¹H NMR spectrum of compound 5r (400 MHz, DMSO).



Figure 53. ¹³C NMR spectrum of compound 5r (100 MHz, DMSO).



Figure 54. Mass spectrum of compound 5r.

Data File Sample Type Instrument Name Acq Method IRM Calibration Status Comment	MR2-NC Sample Instrum 29.10.2 Success	02.d xent 1 014.m	Sample Name Position User Name Acquired Time DA Method	MR2-NO2 P1-C1 SMILY 24-11-2015 15:00:20 Default.m		
Sample Group Acquisition SW 6200) series TOF/6	In 5500 series	ifo.			
Compound Table	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 22: C28 H22 N6 05	11	522.1662	C28 H22 N6 05	C28 H22 N6 05	-1.98	C28 H22 N6 U5
and the second		DT	Algorithm	Mass		
Compound Label	m/7					
Compound Label Cpd 22: C28 H22 N6 O5	<i>m/z</i> 523.1734	11	Find by Molecular Fe	ature 522.1662		
Compound Label Cpd 22: C28 H22 N6 O5 MFE MS Spectrum	<i>m/z</i> 523.1734	11	Find by Molecular Fe	ature 522.1662		
Compound Label Cpd 22: C28 H22 N6 O5 MFE MS Spectrum x10 4 Cpd 22: C28 H22 1.4 1.2 1.2 1	<i>m/z</i> 523.1734 N6 O5: +ES	I MFE Spectru 523.1 ([C28 H22 14	Find by Molecular Fe Find by Molecular Fe m (# 8-23) Frag=135.0\ 734 6 O5]+H)+	ature 522.1662 / MR2-NO2.d		

Formula	'C ₃₄ H ₂₇ Cl ₃ N ₆ O ₃ '
Formula weight (g)	673.97
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system, space group Triclinic	Monoclinic, P21/n
Unit cell dimensions	a = 17.3297(8) Å alpha = 90.00 deg.
	b = 9.1210(6) Å beta = 92.608(4) deg.
	c = 20.2870(10) Å gamma = 90.00 deg.
Volume	3203.3(3)A ³
Z	4 g/cm ³
Absorption coefficient	0.332 mm ⁻¹
F(000)	1224
Crystal size	0.04 X 0.03 X 0.01 mm
Theta range for data collection	3.17 to 21.36 deg
Limiting indices	-19<=h<=20, -9<=k<=10, -24<=l<=19
Completeness to theta	99.9%
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	1.00000 and 0.86823
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	5632/0/411
Goodness-of-fit on F ² Final R indices [I>2sigma(I)]	0.955 R1 = 0.1009, wR2 = 0.2792
R indices (all data)	R1 = 0.1793, $wR2 = 0.3310$
Largest diff. peak and hole	0.60 and -0.54 e.A ⁻³

 Table 1: Crystal data and structure refinement information for the title compound 5e.

The crystal structure shows that spiro carbon of *N*-propargyl isatin and pyrrolizine ring deviates by an angle 110.26° (Fig. 55a). The compound reveals two types of interactions, namely,

intermolecular and intramolecular hydrogen bonding (Table 2). The intermolecular H-bonding stabilized the molecule by C4-H4...Cl2 and C20-H20A...N6 and C16-H16...N2 with a distance of 2.912, 2.594 and 2.700 Å, respectively (Fig. 55b). The structure also involves intramolecular hydrogen bonding interaction between the C7-H7...O1, C24-H24...C22, C1-H1...C19, C17-H17...C20 and C20-H20B...O3 with a distance of 2.683, 2.822, 2.880, 2.865 and 2.563 Å respectively (Fig. 55c).







(b)

55



Figure 55: (a) View of crystal 5e shown along b axis; (b) Intermolecular hydrogen bonding interactions in the crystal of 5e; (c) Intramolecular hydrogen bonding in the crystal 5e.

Table 2: Intermolecular and intramolecular hydrogen bonding geometries of 5e

D-HA	D-H (Å)	HA (Å)	DA (Å)	D-HA (°)
С7-Н7О3	0.98	2.52	2.9946 (2)	109
C20-H20AN6 ⁱ	0.97	2.59	3.5498 (2)	171
C26-H26N3 ⁱⁱ	0.93	2.56	3.0629 (2)	115
C34-H34AO1	0.97	2.59	3.5393 (2)	166

Note: D, Donor; A, Acceptor; Symmetry code: i) -x, 1-y, -z; ii) 1/2-x, -1/2+y, 1/2-z.