Electronic Supplementary Material (ESI) for RSC Advances.

An efficient, green synthesis of novel regioselective and stereoselective indan-1,3-diones grafted spirooxindolopyrrolizidines linked 1,2,3-triazoles *via* one-pot five-component using PEG-400.

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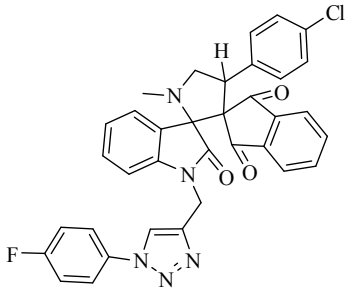
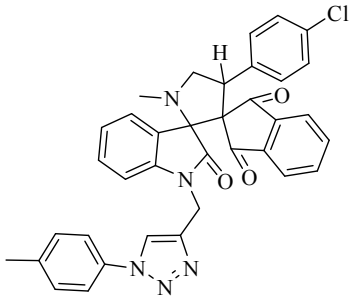
Spectral data

1-*N*-methyl-spiro[2.3']-1'-*N*-((1-(4-fluorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)oxindole-spiro[3.2'']-indan-1,3-dione- (4-chlorophenyl)-pyrrolidine (6a)



Pale Yellow solid; Yield = 85%; M.p: 202-205 ^{o}C ; IR (KBr) ν/cm^{-1}= 2946, 1717, 1515, 1453, 1357, 1233, 1049, 847; ^{1}H NMR (400MHz, DMSO-d_6) δ_H : 8.64 (s, 1H, Ar-H), 7.92-7.89 (m, 2H, Ar-H), 7.68-7.64 (m, 3H, Ar-H), 7.51-7.49 (m, 1H, Ar-H), 7.44-7.40 (m, 2H, Ar-H), 7.10-7.07 (m, 2H, Ar-H), 7.04-7.02 (m, 1H, Ar-H), 6.92-6.89 (m, 4H, Ar-H), 6.75-6.71 (m, 1H, Ar-H), 5.05-5.01 (m, 1H, C-H), 4.97-4.91 (m, 2H, N-CH_2), 4.01-3.97 (m, 1H, C-H), 3.61-3.56 (m, 1H, C-H), 2.08 (s, 3H, N-CH_3); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C: 197.3, 196.5, 173.4, 162.9, 161.1, 160.4, 143.0, 142.7, 142.0, 140.7, 136.9, 136.3, 133.1, 132.1, 130.4, 130.1, 124.9, 122.7, 122.7, 122.5, 122.4, 122.2, 121.9, 116.8, 115.2, 115.0, 109.6, 76.8, 69.6, 55.8, 45.2, 34.6, 34.5; LCMS (ESI) *m/z* calcd for $C_{35}H_{25}FClN_5O_3$: 618.1705 [M^+]; found: 619.1709 [M^+ +H].

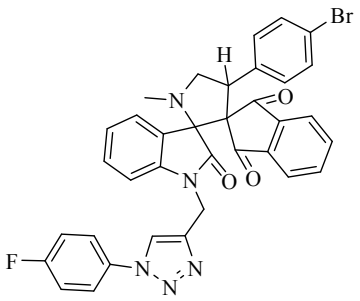
1-*N*-methyl-spiro[2.3']-1'-*N*-((1-(4-methylphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)oxindole-spiro[3.2'']-indan-1,3-dione- (4-chlorophenyl)-pyrrolidine (6b).



Pale Yellow solid; Yield: 80%; M.p: 196-197^{o}C; IR (KBr) ν/ cm^{-1} = 2928, 1717, 1611, 1515, 1463, 1217, 767; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H : 8.58 (s, 1H, Ar-H), 7.74-7.72 (m,2H,Ar-H), 7.69-7.64 (m, 3H, Ar-H), 7.50-7.48 (m, 1H, Ar-H), 7.37 (d, 2H, *J*= 8.54 Hz, Ar-H), 7.19-7.02 (m, 5H, Ar-H), 6.90 (d, 2H, *J*=8.54 Hz, Ar-H), 6.74-6.71 (m, 1H, Ar-H), 5.04-5.00 (m, 1H, C-H), 4.96-4.89 (m, 2H, N-CH_2), 4.02-3.98 (m, 1H, C-H), 3.62-3.57 (m, 1H, C-H), 2.34 (s, 3H, Ar-CH_3), 2.09 (s, 3H, N-CH_3); ^{13}C NMR

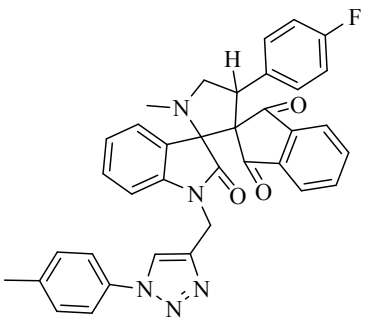
(100 MHz, DMSO) δ_C : 197.2, 196.2, 173.3, 142.7, 142.7, 142.0, 140.7, 138.4, 136.9, 136.3, 135.1, 134.3, 131.8, 130.3, 130.2, 130.1, 128.3, 124.8, 122.7, 122.6, 122.5, 122.1, 121.4, 119.9, 109.6, 76.8, 69.4, 55.6, 45.0, 34.6, 34.5; LCMS (ESI) *m/z* calcd for $C_{36}H_{28}ClN_5O_3$: 614.1953 [M^+]; found: 614.1947 [M^+ +H].

1-*N*-methyl-spiro[2.3']-1'-*N*-((1-(4-fluorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)oxindole-spiro[3.2'']-indan-1,3-dione- (4-bromophenyl)-pyrrolidine (6c).



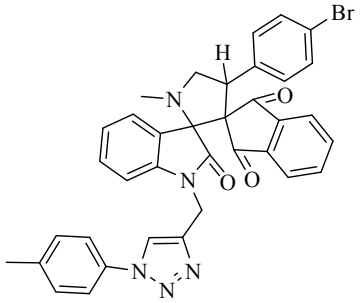
Pale Yellow Solid; Yield: 83%; M.p: 195-199 ^oC; IR (KBr) ν/cm^{-1} = 2932, 1715, 1522, 1492, 1224, 1047, 845; ^1H NMR (400 MHz, DMSO-d_6) δ_H : 8.63 (s, 1H, Ar-H), 7.92-7.89 (m, 2H, Ar-H), 7.70-7.64 (m, 3H, Ar-H), 7.51-7.49 (m, 1H, Ar-H), 7.45-7.41 (m, 2H, Ar-H), 7.29-7.27 (m, 2H, Ar-H), 7.06-7.04 (m, 1H, Ar-H), 7.02-6.99 (m, 2H, Ar-H), 6.92-6.89 (m, 2H, Ar-H), 6.75-6.71 (m, 1H, Ar-H), 5.02- 4.97 (m, 1H, C-H), 4.95-4.90 (m, 2H, N-CH_2), 4.01-3.97 (m, 1H, C-H), 3.62-3.57 (m, 1H, C-H), 2.46 (s, 3H, N-CH_3); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C: 197.3, 196.3, 173.3, 162.2, 161.6, 159.8, 142.9, 142.7, 141.1, 140.7, 136.3, 136.3, 133.0, 133.0, 130.3, 130.0, 124.9, 122.7, 122.6, 122.4, 122.3, 122.1, 121.8, 116.9, 116.6, 115.0, 109.5, 76.7, 69.5, 55.4, 45.1, 34.6, 34.4; LCMS (ESI) *m/z* calcd for $C_{35}H_{25}BrFN_5O_3$: 662.1198 [M^+]; found: 664.1185 [M^+ +H], 666.1242 [(M^++H) +2].

1-*N*-methyl-spiro[2.3']-1'-*N*-((1-(4-methylphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)oxindole-spiro[3.2'']-indan-1,3-dione- (4-fluorophenyl)-pyrrolidine (6d).



Pale Yellow Solid; Yield: 82%; M.p: 212-214; IR (KBr) ν/ cm^{-1} = 2925, 1718, 1605, 1465, 1239, 1046; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H = 8.58 (s, 1H, Ar-H), 7.74-7.72 (m, 2H, Ar-H), 7.67-7.63 (m, 3H, Ar-H), 7.50-7.48 (m, 1H, Ar-H), 7.38-7.36 (m, 2H, Ar-H), 7.11-7.07 (m, 2H, Ar-H), 7.04-7.02 (m, 1H, Ar-H), 6.92-6.90 (m, 4H, Ar-H), 6.75-6.71 (m, 1H, Ar-H), 5.05-5.01 (m, 1H, C-H), 4.96-4.90 (m, 2H, N-CH_2), 4.02-3.98 (m, 1H, C-H), 3.61-3.57 (m, 1H, C-H), 2.34 (s, 3H, Ar-CH_3), 2.09 (s, 3H, NCH_3); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C = 197.3, 196.3, 173.4, 161.1, 142.8, 142.7, 142.0, 140.7, 138.4, 136.9, 136.3, 134.3, 132.1, 130.4, 130.3, 130.0, 124.9, 122.7, 122.4, 122.1, 121.4, 119.9, 115.1, 109.6, 76.7, 69.5, 55.8, 45.1, 34.6, 34.5, 20.5; HRMS (ESI) *m/z* calcd for $C_{36}H_{28}FN_5O_3$: 598.2249 [M^+]; found: 598.2241 [M^++H], 600.2299 [(M^++H) +2].

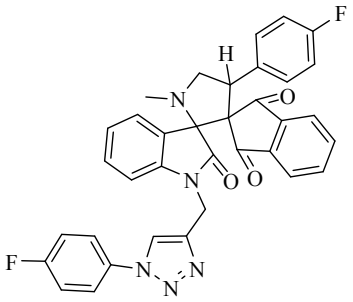
1-*N*-methyl-spiro[2.3']-1'-*N*-((1-(4-methylphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)oxindole-spiro[3.2'']-indan-1,3-dione- (4-bromophenyl)-pyrrolidine (6e).



Pale Yellow solid; Yield: 81%; M.p: 226-228^{o}C; IR (KBr) ν/ cm^{-1} = 2926, 1719, 1611, 1466, 1242, 1171, 578; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H = 8.60 (s, 1H, Ar-H), 7.77-7.75 (m, 2H, Ar-H), 7.70-7.68 (m, 3H, Ar-H), 7.52-7.50 (m, 1H, Ar-H), 7.41-7.39 (m, 2H, Ar-H), 7.09-7.07 (m, 2H, Ar-H), 7.05-7.02 (m, 3H, Ar-H), 6.94-6.92 (m, 2H, Ar-H), 6.77-6.73 (m, 1H, Ar-H), 5.05-5.03 (m, 1H, C-H), 5.01-4.92 (m, 2H, N-CH_2), 4.05-4.00 (m, 1H, C-H), 3.65-3.60 (m, 1H, C-H), 2.37 (s, 3H, Ar-CH_3), 2.11 (s, 3H, N-CH_3); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C= 197.1, 196.2, 173.3, 142.7, 142.7, 141.9, 141.9, 140.7,

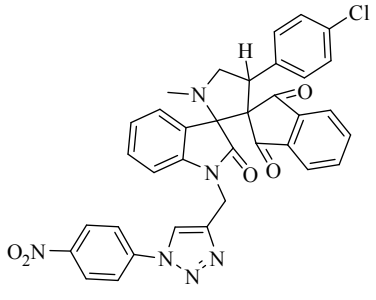
138.4, 137.0, 136.3, 135.5, 134.2, 131.2, 130.6, 130.3, 130.1, 124.8, 122.7, 122.6, 122.5, 122.2, 121.4, 120.4, 119.9, 109.6, 76.9, 69.3, 55.5, 45.0, 34.6, 34.5, 20.5; LCMS (ESI) *m/z* calcd. for $C_{36}H_{28}BrN_5O_3$: 658.1448 [M^+]; found: 658.1455 [M^+ +H], 660.1428 [(M^+ +H) +2].

1-*N*-methyl-spiro[2.3']-1'-*N*-((1-(4-fluorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)oxindole-spiro[3.2'']-indan-1,3-dione- (4-fluorophenyl)-pyrrolidine (6f).



Pale Yellow Solid; Yield: 84%; M.p: 186-188; IR (KBr) ν/cm^{-1}= 2947, 1719, 1604, 1473, 1249, 1032; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H: 8.64 (s, 1H, Ar-H), 7.94-7.89 (m, 2H, Ar-H), 7.68-7.62 (m, 3H, Ar-H), 7.51-7.49 (m, 1H, Ar-H), 7.45-7.40 (m, 3H, Ar-H),7.11-7.07 (m, 2H, Ar-H), 7.04-7.02 (m, 1H, Ar-H), 6.93-6.89 (m, 3H, Ar-H), 6.75-6.71 (m, 1H, Ar-H), 5.06-5.01 (m, 1H, C-H), 4.97-4.91 (m, 2H, N-CH_2), 4.02-3.98 (m, 1H, C-H), 3.62-3.57 (m, 1H, C-H), 2.09 (s, 3H, N-CH_3); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C: 197.3, 196.3, 173.3, 162.2, 161.6, 159.8, 142.9, 142.7, 141.9, 140.7, 136.8, 136.3, 133.0, 132.0, 130.3, 130.0, 124.9, 122.7, 122.6, 122.4, 122.1, 121.8, 116.9, 116.6, 115.0, 109.5, 76.7, 69.5, 55.8, 45.1, 34.6, 34.4; LCMS (ESI) *m/z* calcd. for $C_{35}H_{25}F_2N_5O_3$: 602.1998 [M^+]; found: 602.1998 [M^++H].

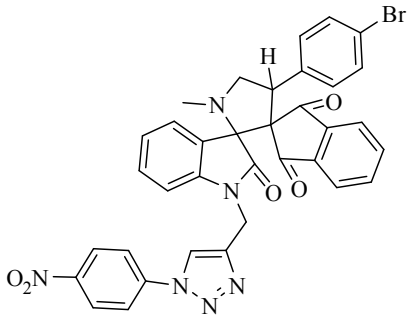
1-*N*-methyl-spiro[2.3']-1'-*N*-((1-(4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)oxindole-spiro[3.2'']-indan-1,3-dione- (4-chlorophenyl)-pyrrolidine (6g).



Pale Yellow Solid; Yield: 82%; M.p: 199-202^{o}C; IR (KBr) ν/cm^{-1}= 2939, 1717, 1609, 1525, 1491, 1342, 750; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H = 8.88 (s, 1H, Ar-H), 8.43-8.41 (m, 2H, Ar-H), 8.21-8.18

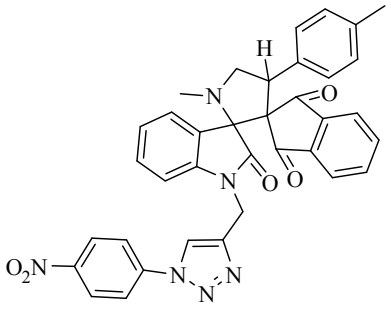
(m, 2H, Ar-H), 7.71-7.67 (m, 2H, Ar-H), 7.65-7.63(m, 2H, Ar-H, 7.52-7.51 (m, 1H, Ar-H), 7.15-7.13 (m, 2H, Ar-H), 7.07-7.05 (m, 2H, Ar-H), 6.94-6.90 (m, 2H, Ar-H), 6.75-6.71 (m, 1H, Ar-H), 5.04-5.02 (m, 1H, C-H), 4.99-4.96 (m, 2H, N-CH_2), 4.02-3.98 (m, 1H, C-H), 3.62-3.57 (m, 1H, C-H), 2.09 (s, 3H, N-CH_3) ; ^{13}C NMR (100 MHz, DMSO-d_6) δ_C = 197.1, 196.1, 173.3, 146.7, 143.5, 142.6, 141.9, 140.6, 136.9, 136.2, 135.0, 131.8, 130.2, 130.0, 128.2, 125.6, 124.8, 122.6, 122.1, 120.6, 109.5, 76.7, 69.4, 55.5, 45.0, 34.5, 34.4; LCMS (ESI) *m/z* calcd. for $C_{35}H_{25}ClN_6O_5$: 645.1648 [M^+]; found: 645.1636 [M^+ +H], 647.1629 [(M^+ +H) +2].

1-*N*-methyl-spiro[2.3']-1'-*N*-((1-(4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)oxindole-spiro[3.2'']-indan-1,3-dione- (4-bromophenyl)-pyrrolidine (6h).



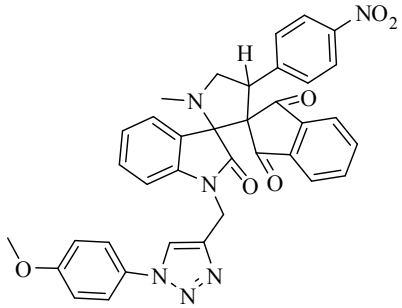
Pale Yellow Solid; Yield: 86%; M.p: 200-203^{o}C; IR (KBr) ν/cm^{-1} = 2924, 1717, 1599, 1341, 1261, 1167, 750; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H = 8.88 (s, 1H, Ar-H), 8.44-8.41 (m, 2H, Ar-H), 8.21-8.19 (m, 2H, Ar-H), 7.70-7.64 (m, 3H, Ar-H), 7.53-7.51 (m, 1H, Ar-H), 7.29-7.27 (m, 2H, Ar-H), 7.07-7.03 (m, 1H, Ar-H), 7.01-6.99 (m, 2H, Ar-H), 6.94-6.90 (m, 2H, Ar-H), 6.75-6.71 (m, 1H, Ar-H), 5.06-5.02 (m, 1H, C-H), 4.99-4.94 (m, 2H, N-CH_2), 4.02-3.98 (m, 1H, C-H), 3.62-3.57 (m, 1H, C-H), 2.09 (s, 1H, N-CH_3); ^{13}C NMR(100 MHz, DMSO-d_6) δ_C = 197.1, 196.1, 173.3, 146.7, 143.5, 142.6, 141.9, 140.7, 136.9, 136.9, 136.3, 135.5, 131.1, 130.5, 130.0, 125.6, 124.8, 122.6, 122.1, 120.6, 120.3, 109.5, 76.8, 69.3, 55.5, 45.0, 34.5, 34.4; LCMS (ESI) *m/z* calcd. for $C_{35}H_{25}BrN_6O_5$: 689.1143 [M^+]; found: 691.1128 [(M^+ +H) +2].

1-*N*-methyl-spiro[2.3']-1'-*N*-((1-(4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)oxindole-spiro[3.2'']-indan-1,3-dione- (4-methylphenyl)-pyrrolidine (6i).



Pale Yellow Solid; Yield: 79%; M.p: 185-187°C; IR (KBr) ν/cm^{-1} = 2924, 1717, 1599, 1524, 1341, 1261, 1109; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H = 8.89 (s, 1H, Ar-H), 8.44-8.42 (m, 2H, Ar-H), 8.21-8.19 (m, 2H, Ar-H), 7.69-7.61 (m, 3H, Ar-H), 7.52-7.50 (m, 1H, Ar-H), 7.06-7.02 (m, 1H, Ar-H), 6.93-6.91 (m, 4H, Ar-H), 6.88-6.86 (m, 2H, Ar-H), 6.75-6.71 (m, 1H, Ar-H), 5.03-5.02 (m, 1H, C-H), 4.99-4.94 (m, 2H, N-CH_2), 4.02-3.98 (m, 1H, C-H), 3.57-3.53 (m, 1H, C-H), 2.09 (s, 3H, Ar-CH_3), 2.05 (s, 3H, N-CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ_C : 198.9, 196.9, 174.3, 147.2, 144.7, 142.7, 142.5, 141.3, 141.2, 136.9, 135.9, 135.1, 132.5, 130.0, 128.9, 128.7, 126.0, 125.5, 123.3, 122.9, 122.8, 122.1, 121.5, 120.3, 108.8, 70.3, 56.5, 47.2, 35.2, 20.8; LCMS (ESI) *m/z* calcd. for $C_{36}H_{28}N_6O_5$: 625.2185 [M^+]; found: 625.2185 [M^+ +H].

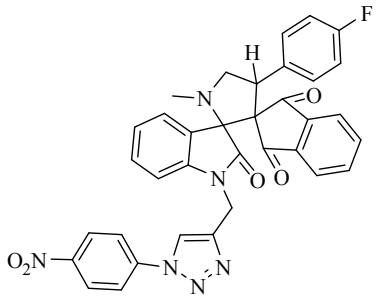
1-*N*-methyl-spiro[2.3']-1'-*N*-((1-(4-methoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)oxindole-spiro[3.2'']-indan-1,3-dione- (4-nitrophenyl)-pyrrolidine (6j).



Pale Yellow solid; Yield: 87%; M.p: 174-178°C; IR (KBr) ν/cm^{-1} = 2946, 1717, 1515, 1453, 1357, 1233, 1049; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H = 8.53 (s, 1H, Ar-H), 7.97-7.95 (m, 2H, Ar-H), 7.78-7.75 (m, 2H, Ar-H), 7.69-7.63 (m, 3H, Ar-H), 7.50-7.48 (m, 1H, Ar-H), 7.35-7.33 (m, 2H, Ar-H), 7.12-7.10 (m, 2H, Ar-H), 7.05-7.02 (m, 1H, Ar-H), 6.93-6.88 (m, 2H, Ar-H), 6.75-6.71 (m, 1H, Ar-H), 5.17-5.12 (m, 1H, C-H), 5.01-4.89 (m, 2H, N-CH_2), 4.11-4.07 (m, 1H, C-H), 3.78 (s, 3H, O-CH_3), 3.70-3.65 (m, 1H, C-H), 2.10 (s, 3H, N-CH_3); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C = 197.4, 196.4, 173.4, 161.6, 146.9, 146.2, 142.9, 142.7, 142.7, 142.0, 140.7, 136.8, 136.2, 133.0, 129.9, 129.4, 124.9, 122.9, 122.8,

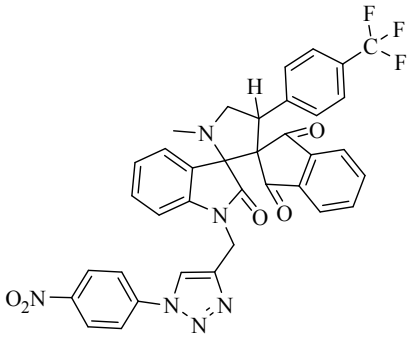
122.6, 122.3, 122.1, 121.9, 121.8, 116.7, 109.5, 108.5, 107.9, 100.8, 76.7, 69.5, 55.9, 55.7, 34.5, 34.4; LCMS (ESI) *m/z* calcd. for $C_{36}H_{28}N_6O_6$: 641.2143 [M^+]; found: 641.2135 [M^+ +H].

1-*N*-methyl-spiro[2.3']-1'-*N*-((1-(4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)oxindole-spiro[3.2'']-indan-1,3-dione- (4-fluorophenyl)-pyrrolidine (6k).



Pale Yellow solid, Yield: 82%; M.p: 199-203°C; IR (KBr) ν/cm^{-1} = 2939, 1742, 1609, 1560, 1466, 1343, 1229, 1162; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H = 8.90 (s, 1H, Ar-H), 8.44-8.42 (m, 2H, Ar-H), 8.21-8.19 (m, 2H, Ar-H), 7.70-7.63 (m, 3H, Ar-H), 7.53-7.51(m, 1H, Ar-H), 7.10-7.03 (m, 3H, Ar-H), 6.94-6.92 (m, 2H, Ar-H), 6.91-6.89 (m, 2H, Ar-H), 6.75-6.72 (m, 1H, Ar-H), 5.06-5.02 (m, 1H, C-H), 5.00-4.95 (m, 2H, N-CH_2), 4.01-3.97 (m, 1H, C-H), 3.61-3.56 (m, 1H, C-H), 2.09 (s, 3H, N-CH_3); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C = 197.3, 196.3, 173.4, 161.1, 146.7, 143.6, 142.7, 142.0, 140.7, 136.9, 136.3, 132.0, 130.4, 130.1, 125.7, 124.9, 122.8, 122.6, 122.6, 122.2, 120.6, 115.1, 109.6, 76.7, 69.5, 55.8, 45.2, 34.6, 34.4; LCMS (ESI) *m/z* calcd. for $C_{36}H_{28}FN_6O_6$: 629.1943 [M^+]; found: 629.1929 [M^+ +H], 631.1984 [(M^+ +H) +2].

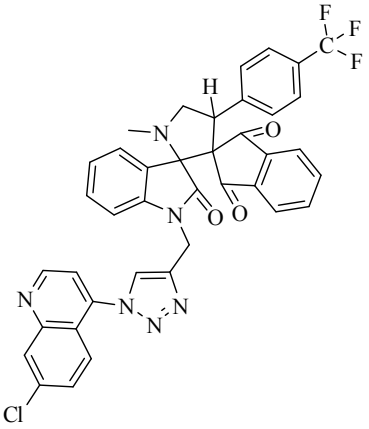
1-*N*-methyl-spiro[2.3']-1'-*N*-((1-(4-nitrophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)oxindole-spiro[3.2'']-indan-1,3-dione- (4-(trifluoromethyl)phenyl)-pyrrolidine (6l).



Pale Yellow Solid; Yield: 87%; M.p: 174-178°C; IR (KBr) ν/cm^{-1} = 2938, 1717, 1611, 1523, 1313, 1233, 1129, 855; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H = 8.92 (s, 1H, Ar-H), 8.47-8.44 (m, 2H, Ar-H),

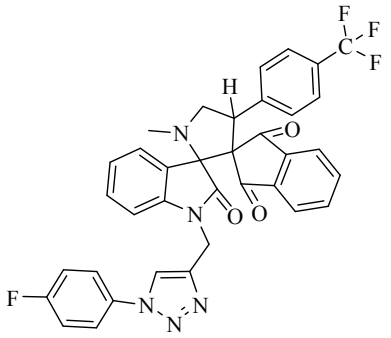
8.24-8.22 (m, 2H, Ar-H), 7.70-7.65 (m, 3H, Ar-H), 7.56-7.54 (m, 1H, Ar-H), 7.50-7.48 (m, 2H, Ar-H), 7.31-7.29 (m, 2H, Ar-H), 7.10-7.06 (m, 1H, Ar-H), 6.98-6.93 (m, 2H, Ar-H), 6.78-6.75 (m, 1H, Ar-H), 5.16-5.11 (m, 1H, C-H), 5.07-4.97 (m, 2H, N-CH_2), 4.12-4.08 (m, 1H, C-H), 3.71-3.66 (m, 1H, C-H), 2.14 (s, 3H, N-CH_3); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C = 196.9, 196.0, 173.3, 146.7, 143.4, 142.6, 141.9, 141.1, 140.7, 140.6, 136.9, 136.3, 133.6, 130.1, 129.2, 127.9, 127.5, 125.6, 125.1, 124.8, 122.6, 122.4, 122.20, 120.6, 109.5, 76.9, 69.4, 55.4, 45.1, 34.6, 34.4; LCMS (ESI) *m/z* calcd. for $C_{36}H_{25}F_3N_6O_5$: 679.1911[M^+]; found: 679.1893 [M^++H].

1-*N*-methyl-spiro[2.3']-1'-*N*-((1-(7-choloroquinoline)-1*H*-1,2,3-triazol-4-yl)methyl)oxindole-spiro[3.2'']-indan-1,3-dione- (4-(trifluoromethyl)phenyl)-pyrrolidine (6m).



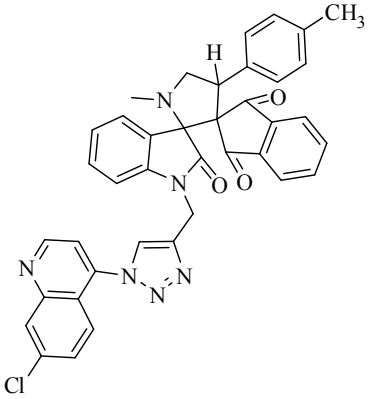
Pale Yellow Solid; Yield: 80%; M.p: 148-151^{o}C; IR (KBr) ν/cm^{-1} = 2946, 1717, 1515, 1453, 1357, 1233, 1049, 847; ^{1}HNMR (400MHz, DMSO-d_6) δ_H = 9.13-9.11(m, 1H, Ar-H), 8.70 (s, 1H, Ar-H), 8.25-8.24 (m, 1H, Ar-H), 7.96-7.93 (m, 1H, Ar-H), 7.81-7.80 (m, 1H, Ar-H), 7.75-7.73 (m, 1H, Ar-H), 7.68-7.63 (m, 4H, Ar-H) , 7.49-7.45(m, 3H, Ar-H , 7.27-7.25 (m, 2H, Ar-H), 7.08-7.06 (m, 1H, Ar-H), 7.00-6.98 (m, 1H, Ar-H), 6.92-6.90 (m, 1H, Ar-H), 6.77-6.73 (m, 1H, Ar-H), 5.12-5.10 (m, 1H, C-H), 5.06-4.99 (m, 2H, N-CH_2), 4.09-4.05 (m, 1H, C-H), 3.67-3.62 (m, 1H, C-H), 2.11 (s, 3H, N-CH_3); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C = 197.1, 196.2, 173.3, 152.5, 149.4, 142,7, 142.7, 142.0, 141.2, 140.7, 140.5, 137.1, 136.5, 135.5, 130.3, 129.3, 129.1, 128.2, 125.9, 125.8, 125.3, 125.0, 124.8, 122.8, 122.7, 122.6, 122.4, 120.4, 117.2, 77.1, 69.5, 55.6, 45.1, 34.7, 28.3; LCMS (ESI) *m/z* calcd. for $C_{39}H_{26}ClF_3N_6O_3$: 719.1780 [M^+]; found: 719.1749 [M^+ +H], 721.1742 [(M^+ +H) +2].

1-*N*-methyl-spiro[2.3']-1'-*N*-((1-(4-fluorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)oxindole-spiro[3.2'']-indan-1,3-dione- (4- (trifluoromethyl)phenyl)-pyrrolidine (6n).



Pale Yellow solid; Yield: 85%; M.p: 162-166°C; IR (KBr) ν/cm^{-1} = 2939, 1744, 1609, 1516, 1487, 1169; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H = 8.64 (s, 1H, Ar-H), 7.93-7.89 (m, 2H, Ar-H), 7.68-7.64 (m, 2H, Ar-H), 7.50-7.40 (m, 6H, Ar-H), &.28-7.26 (m, 2H, Ar-H), 7.06-7.02 (m, 1H, Ar-H), 6.92-6.89 (m, 2H, Ar-H), 6.74-6.71 (m, 1H, Ar-H), 5.13-5.08 (m, 1H, C-H), 5.00-4.90 (m, 2H, N-CH_2), 4.09-4.05 (m, 1H, C-H), 3.67-3.62 (m, 1H, C-H), 2.10 (s, 3H, N-CH_3); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C = 196.9, 196.0, 173.3, 142.9, 142.7, 141.9, 141.2, 140.6, 137.0, 136.4, 133.1, 130.1, 129.2, 125.2, 124.87, 123.4, 122.7, 122.6, 122.4, 122.2, 121.9, 116.8, 109.6, 76.9, 69.4, 56.0, 55.4, 45.1, 34.6, 34.4; LCMS (ESI) *m/z* calcd. for $C_{36}H_{25}F_4N_5O_3$: 652.1966 [M^+]; found: 652.1963 [M^+ +H], 654.2019 [(M^+ +H) +2].

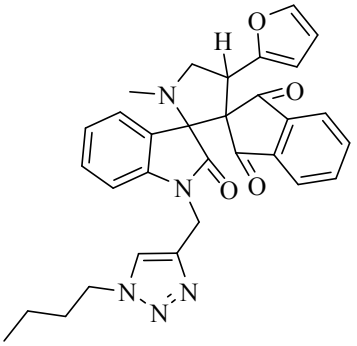
1-*N*-methyl-spiro[2.3']-1'-*N*-((1-(7-choloroquinoline)-1*H*-1,2,3-triazol-4-yl)methyl)oxindole-spiro[3.2'']-indan-1,3-dione- (4-methylphenyl)-pyrrolidine (6o).



Pale Yellow solid; Yield: 74%; M.p: 133-135°C; IR (KBr) ν/ cm^{-1} = 2861, 1711, 1614, 1467, 1352, 1173, 757; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H = 9.14-9.13 (m, 1H, Ar-H), 8.70 (s, 1H, Ar-H), 8.26-8.25 (m, 1H, Ar-H), 7.95-7.93 (m, 1H, Ar-H), 7.81-7.80 (m, 1H, Ar-H), 7.75-7.72 (m, 1H, Ar-H), 7.67-7.61 (m, 3H, Ar-H), 7.48-7.46 (m, 1H, Ar-H), 7.09-7.05 (m, 1H, Ar-H), 6.98-6.97 (m, 1H, Ar-H), 6.93-6.91 (m, 3H, Ar-H), 6.88-6.86 (m, 2H, Ar-H), 6.76-6.72 (m, 1H, Ar-H), 5.06-5.03 (m, 1H, C-H), 5.01-4.95 (m, 2H, N-CH_2), 4.03-3.98 (m, 1H, C-H), 3.57-3.53 (m, 1H, C-H), 2.10 (s, 3H, CH_3), 2.04 (s, 3H, N-CH_3); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C = 197.6, 196.4, 173.5, 152.5, 149.4, 147.0, 142.7, 142.1,

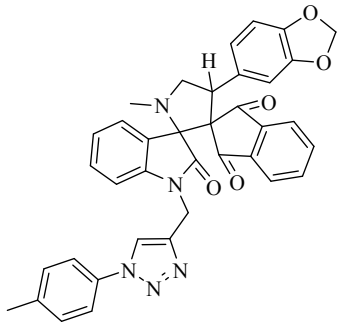
140.7, 140.3, 136.8, 136.4, 136.2, 135.5, 132.8, 130.0, 129.0, 128.9, 128.3, 128.2, 125.8, 125.2, 124.9, 122.6, 122.5, 122.2, 120.4, 117.1, 109.7, 99.4, 98.6, 81.4, 76.8, 69.6, 55.8, 45.5, 34.7, 34.5, 20.4; LCMS (ESI) *m/z* calcd. for $C_{39}H_{29}ClN_6O_3$: 665.2062 [M^+]; found: 666.2060 [M^+ +H].

1-*N*-methyl-spiro[2.3']-1'-*N*-((1-(n-butylazide)-1*H*-1,2,3-triazol-4-yl)methyl)oxindole-spiro[3.2'']-indan-1,3-dione- (furfuraldehyde)-pyrrolidine (6p).



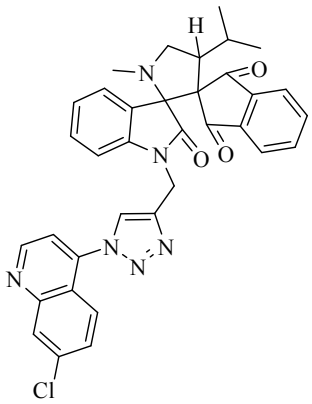
Pale Yellow Solid; Yield: 80%; M.p: 184-188°C; IR (KBr) ν/cm^{-1} = 2924, 1717, 1610, 1465, 1339, 1265, 765, 720; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H = 7.89 (s, 1H, Ar-H), 7.75-7.68 (m, 3H, Ar-H), 7.65-7.63 (m, 1H, Ar-H), 7.11 (s, 1H, Ar-H), 7.01-6.98 (t, 1H, Ar-H), 6.85-6.78 (dd, 2H, Ar-H), 6.70-6.67 (t, 1H, Ar-H), 6.15-6.11 (m, 2H, Ar-H), 4.97-4.92 (t, 1H, -CH), 4.88-4.78 (q, 2H, $-CH_2$), 4.31-4.29 (t, 2H,$-NCH_2$), 3.86-3.82 (t, 1H, -CH), 3.60-3.56 (t, 1H, -CH), 1.71-1.67 (m, 2H, $-CH_2$), 1.16-1.07 (m, 2H, $-CH_2$), 0.78-0.75 (t, 3H, $-CH_3$); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C = 197.1, 196.3, 173.7, 151.5, 143.2, 142.7, 142.0, 141.3, 137.2, 136.6, 130.5, 125.1, 123.7, 123.2, 122.9, 122.3, 111.0, 110.2, 107.6, 79.9, 67.8, 55.1, 49.3, 35.2, 34.7, 32.3, 30.8, 19.6, 13.5; LCMS (ESI) *m/z* calcd. for $C_{31}H_{29}N_5O_4$: 536.2289 [M^+]; found: 536.2290 [M^+ +H].

.**1-*N*-methyl-spiro[2.3']-1'-*N*-((1-(4-fluorophenyl)-1*H*-1,2,3-triazol-4-yl)methyl)oxindole-spiro[3.2'']-indan-1,3-dione-(piperonal)-pyrrolidine (6q).**



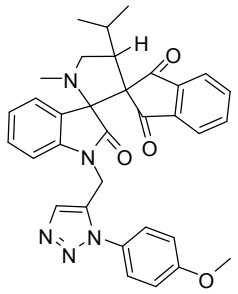
Pale Yellow Solid; Yield: 86%; M.p: 182-186°C; IR (KBr) ν/cm^{-1} = 2944, 1717, 1609, 1468, 1348, 1234, 1169, 1042; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H = 8.65 (s, 1H, Ar-H), 7.99-7.88 (m, 3H, Ar-H), 7.71-7.68 (m, 3H, Ar-H), 7.55-7.52 (m, 1H, Ar-H), 7.47-7.43 (m, 3H, Ar-H), 7.09-7.05 (m, 1H, Ar-H), 6.96-6.92 (m, 2H, Ar-H), 6.77-6.74 (m, 1H, Ar-H), 6.66-6.61 (m, 2H, Ar-H), 6.51-6.49 (m, 1H, Ar-H), 5.86-5.84 (m, 2H, O-CH_2-O) , 5.05-5.03 (m, 1H, C-H), 4.99-4,97 (m, 2H, N-CH_2), 3,99-3.95 (m, 1H, C-H), 3.60-3.55 (m, 1H, C-H), 2.11 (s, 3H, N-CH_3); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C = 197.4, 196.4, 173.4, 146.9, 146.2, 142.9, 142.7, 142.0, 140.7, 136.8, 136.2, 133.0, 129.9, 129.4, 124.9, 122.9, 122.8, 122.6, 122.4, 122.3, 122.2, 122.1, 121.9, 121.8,116.9, 116.6, 109.5, 108.5, 107.9, 100.8, 76.7, 69.5, 55.9, 45.7, 34.5, 34.4; LCMS (ESI) *m/z* calcd. for $C_{36}H_{26}FN_5O_5$: 628.1991 [M$^+$]; found: 628.1975 [M$^+$ +H].

1-*N*-methyl-spiro[2.3']-1'-*N*-((1-(7-chloroquinoline)-1*H*-1,2,3-triazol-4-yl)methyl)oxindole-spiro[3.2'']-indan-1,3-dione-(isobutyl)-pyrrolidine (6r).



Pale Yellow Solid; Yield: 78%; M.p: 190-193°C; IR (KBr) ν/cm^{-1}= 2967, 1727, 1621, 1458, 1344, 1263, 1173, 1026, 765; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H = 9.13-9.12 (m, 1H, Ar-H), 8.64 (s, 1H, Ar-H), 8.24-8.21 (m, 1H, Ar-H), 7.96-7.94 (m, 1H, Ar-H, 7.82-7.63 (m, 5H, Ar-H), 7.43-7.41 (m, 1H, Ar-H), 7.04-7.00 (m, 1H, Ar-H), 6.93-6.91 (m, 1H, Ar-H), 6.83-6.81 (m, 1H, Ar-H), 6.70-6.67 (m, 1H, Ar-H), 5.03-4.88 (m, 2H, CH_2), 3.45-3.38 (m, 2H, CH_2), 2.45 (m, 1H, -CH), 1.99 (s, 3H, NCH_3), 1.76-1.68 (brs, 1H, -CH), 0.87-0.81 (m, 3H, CH_3), 0.25-0.23 (m, 3H, CH_3); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C = 197.8, 197.2, 173.4, 152.4, 149.3, 142.6, 142.5, 141.7, 140.3, 136.5, 136.0, 135.3, 129.9, 128.9, 128.1, 125.8, 125.2, 124.5, 122.6, 122.5, 122.4, 121.9, 120.3, 117.0, 109.4, 77.5, 67.2, 57.7, 47.9, 34.6, 34.2, 29.1, 21.8, 21.7; LCMS (ESI) *m/z* calcd. for $C_{35}H_{29}ClN_6O_3$: 617.2062 [M$^+$]; found: 617.2055 [M$^+$ +H].

1-*N*-methyl-spiro[2.3']-1'-*N*-((1-(4-methoxyphenyl)-1*H*-1,2,3-triazol-4-yl)methyl)oxindole-spiro[3.2'']-indan-1,3-dione- (isobutyl)-pyrrolidine (6s).



Pale Yellow Solid; Yield: 74%; M.p: 204-206^{o}C; IR (KBr) ν/cm^{-1} = 2933, 1726, 1601, 1468, 1343, 1263, 1169, 767; ^{1}H NMR (400 MHz, DMSO-d_6) δ_H = 8.45 (s, 1H, Ar-H), 7.81-7.74 (m, 4H, Ar-H), 7.68-7.65 (m, 1H, Ar-H), 7.43-7.41 (m, 1H, Ar-H), 7.12-7.10 (m, 2H, Ar-H), 7.00-6.96 (m, 1H, Ar-H), 6.84-6.79 (m, 2H, Ar-H), 6.68-6.64 (m, 1H, Ar-H), 4.92-4.77 (m, 2H, -CH_2), 3.82-3.80 (m, 1H, C-H), 3.78 (s, 3H, O-CH_3), 3.45-3.36 (m, 2H, -CH_2), 1.96 (s, 3H, N-CH_3), 1.76-1.70 (m, 1H, C-H), 0.83-0.82 (m, 3H, -CH_3), 0.26-0.24 (m, 3H, -CH_3); ^{13}C NMR (100 MHz, DMSO-d_6) δ_C = 197.8, 197.2, 173.3, 159.3, 142.6, 142.5, 141.7, 140.3, 136.6, 136.1, 129.9, 124.6, 122.6, 122.5, 122.3, 121.9, 121.7, 121.4, 114.9, 109.3, 77.5, 67.2, 57.7, 55.5, 47.8, 34.6, 34.3, 29.1, 21.9, 21.7; LCMS (ESI) *m/z* calcd. for $C_{33}H_{31}N_5O_4$: 562.2449 [M^+]; found: 562.2461 [M^+ +H].

Figure 1. ^{1}H NMR spectrum of compound **6a** (400 MHz, $CDCl_3$)

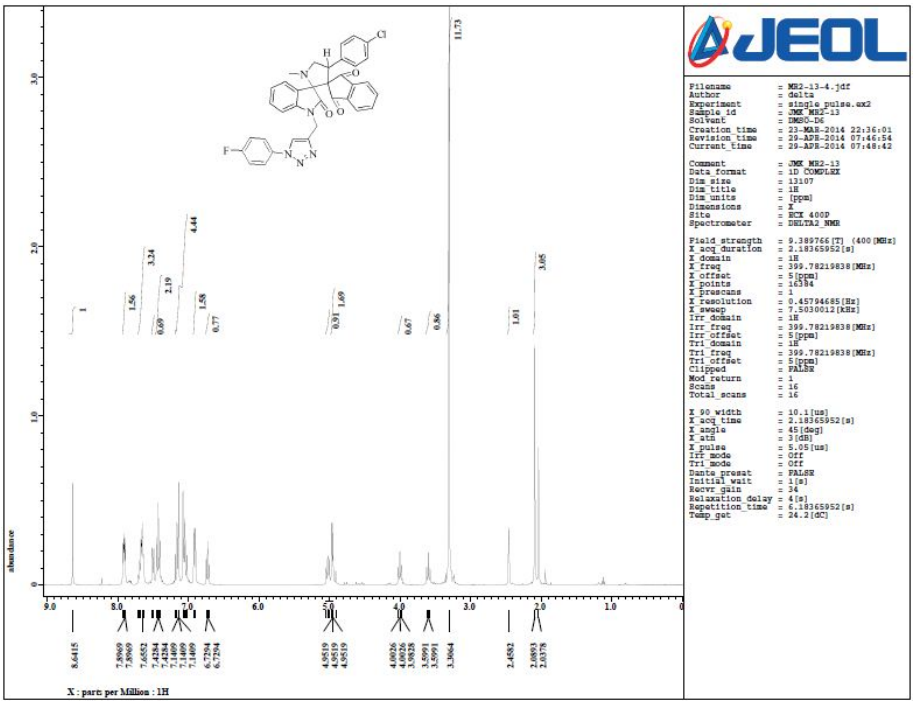


Figure 2. ^{13}C NMR spectrum of compound **6a** (100 MHz, $CDCl_3$).

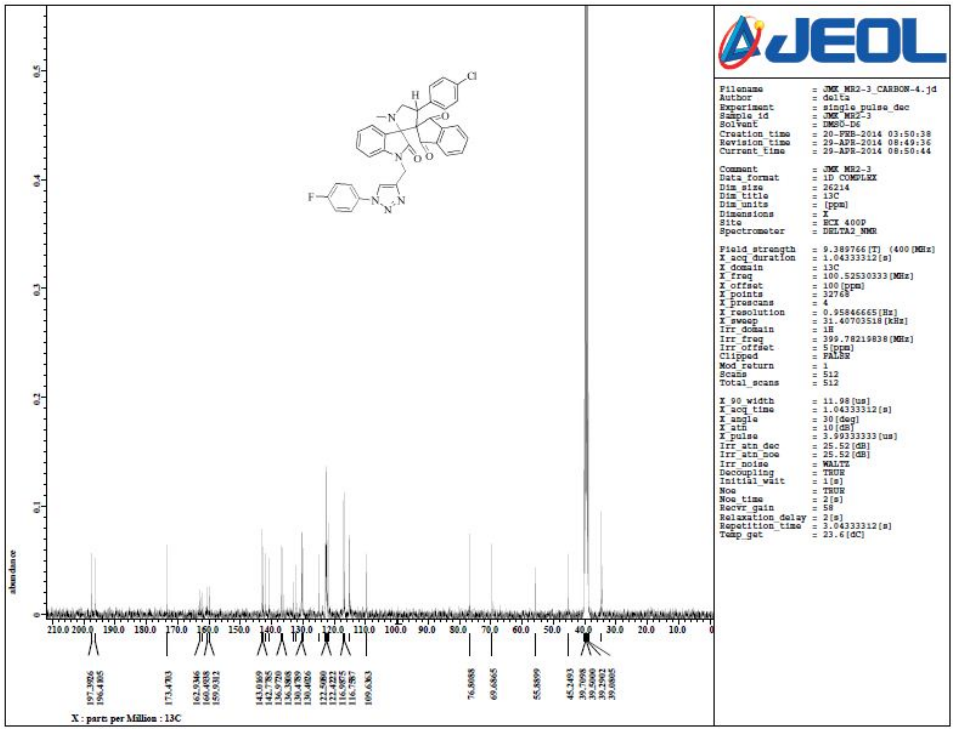


Figure 3. Mass spectrum of compound **6a**.

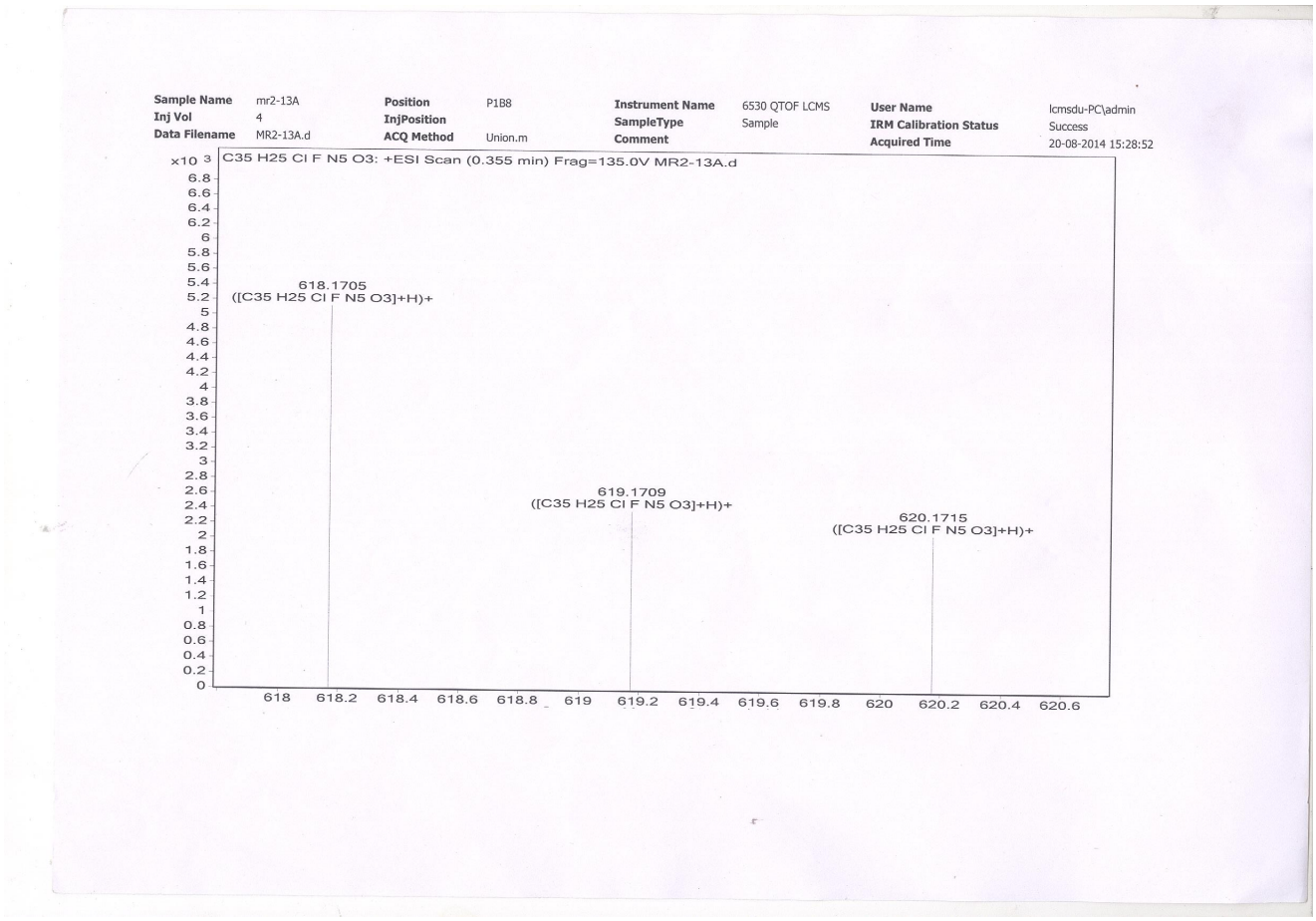


Figure 4. ^{1}H NMR spectrum of compound **6b** (400 MHz, $CDCl_3$)

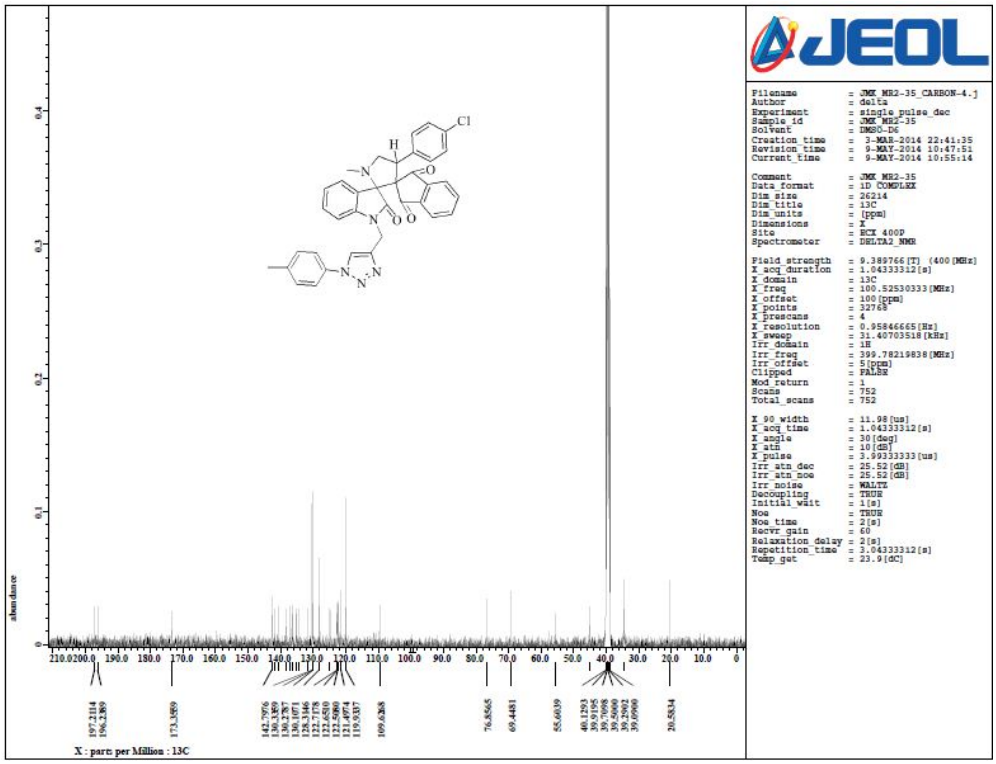


Figure 5. ^{13}C NMR spectrum of compound **6b** (100 MHz, $CDCl_3$).

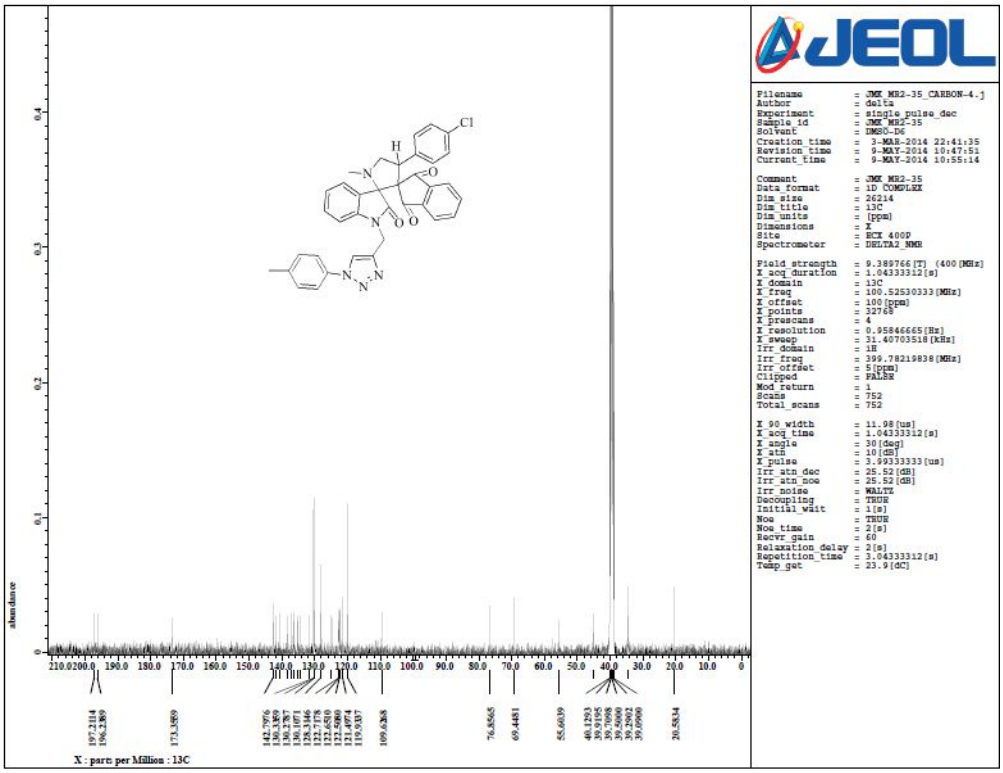
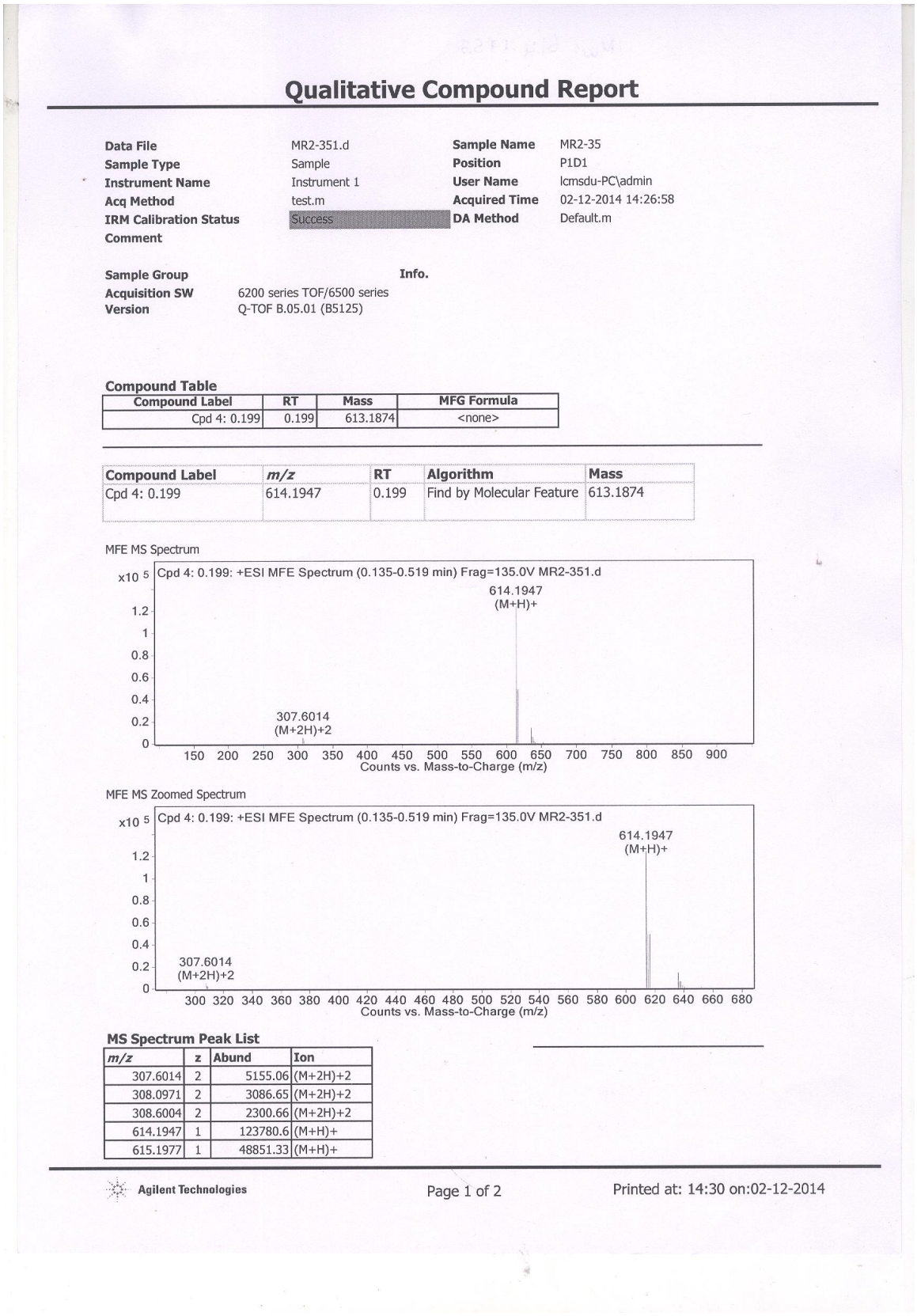


Figure 6. Mass spectrum of compound **6b.**



Qualitative Compound Report

Data File	MR2-351.d	**Sample Name**	MR2-35
Sample Type	Sample	**Position**	P1D1
Instrument Name	Instrument 1	**User Name**	lcmsdu-PC\admin
Acq Method	test.m	**Acquired Time**	02-12-2014 14:26:58
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**

Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	MFG Formula
Cpd 4: 0.199	0.199	613.1874	<none>

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: 0.199	614.1947	0.199	Find by Molecular Feature	613.1874

MFE MS Spectrum

MFE MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund	Ion
307.6014	2	5155.06	(M+2H)+2
308.0971	2	3086.65	(M+2H)+2
308.6004	2	2300.66	(M+2H)+2
614.1947	1	123780.6	(M+H)+
615.1977	1	48851.33	(M+H)+

Figure 7. ^{1}H NMR spectrum of compound **6c** (400 MHz, $CDCl_3$)

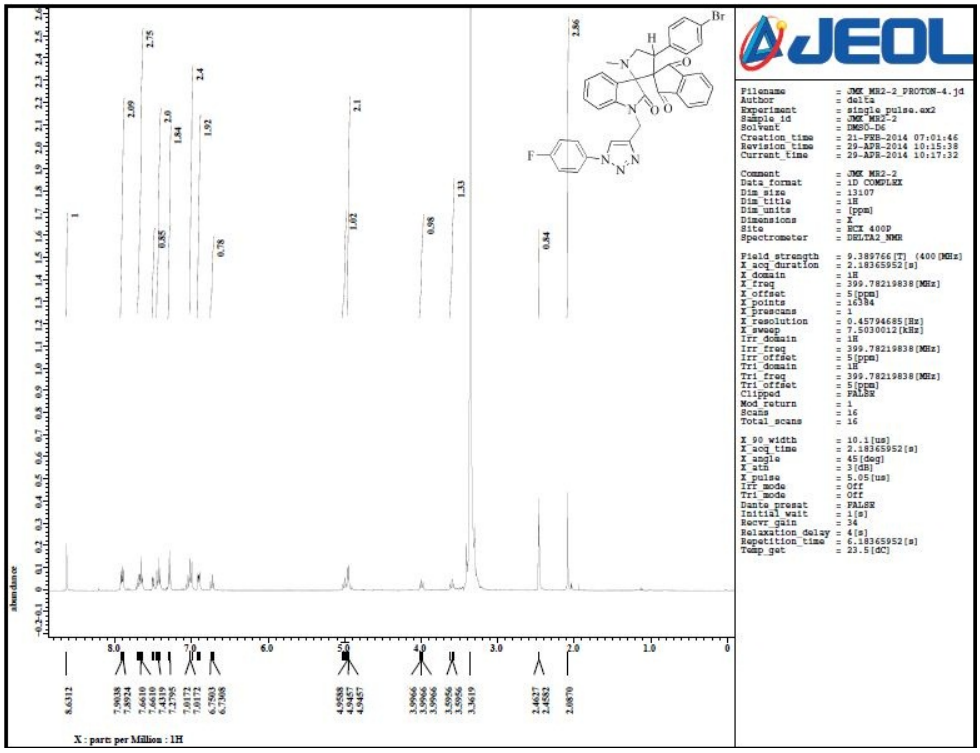


Figure 8. ^{13}C NMR spectrum of compound **6c** (100 MHz, $CDCl_3$).

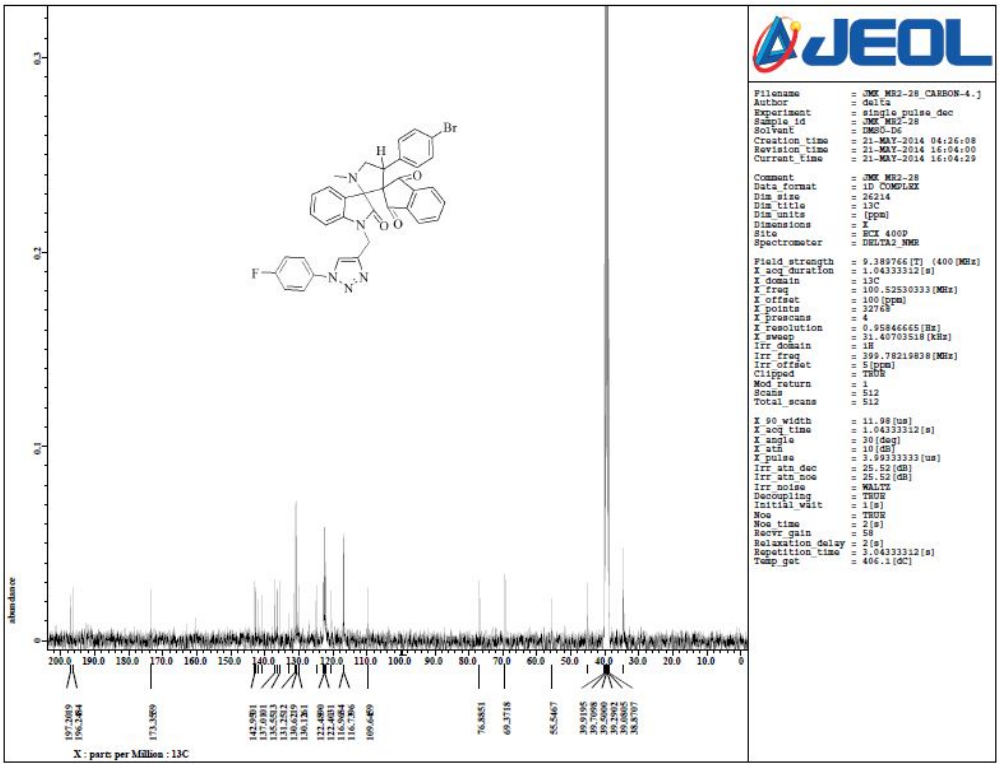
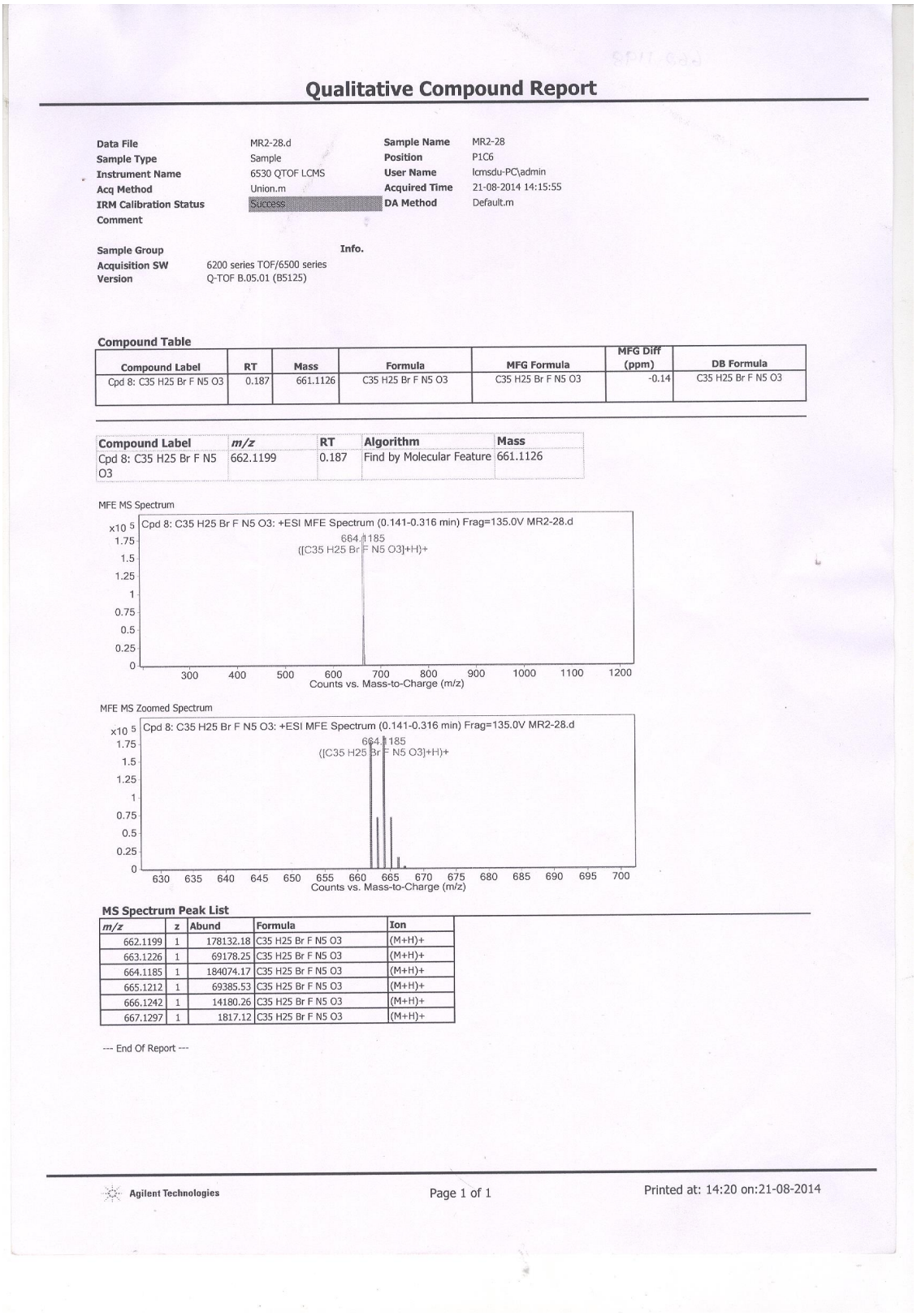


Figure 9. Mass spectrum of compound **6c**.



Qualitative Compound Report

Data File	MR2-28.d	**Sample Name**	MR2-28
Sample Type	Sample	**Position**	P1C6
Instrument Name	6530 QTOF LCMS	**User Name**	lcmsdu-PC\admin
Acq Method	Union.m	**Acquired Time**	21-08-2014 14:15:55
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 8: C35 H25 Br F N5 O3	0.187	661.1126	C35 H25 Br F N5 O3	C35 H25 Br F N5 O3	-0.14	C35 H25 Br F N5 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 8: C35 H25 Br F N5 O3	662.1199	0.187	Find by Molecular Feature	661.1126

MFE MS Spectrum

MFE MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
662.1199	1	178132.18	C35 H25 Br F N5 O3	(M+H)+
663.1226	1	69178.25	C35 H25 Br F N5 O3	(M+H)+
664.1185	1	184074.17	C35 H25 Br F N5 O3	(M+H)+
665.1212	1	69385.53	C35 H25 Br F N5 O3	(M+H)+
666.1242	1	14180.26	C35 H25 Br F N5 O3	(M+H)+
667.1297	1	1817.12	C35 H25 Br F N5 O3	(M+H)+

--- End Of Report ---

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Figure 10. ^{1}H NMR spectrum of compound **6d** (400 MHz, $CDCl_3$).

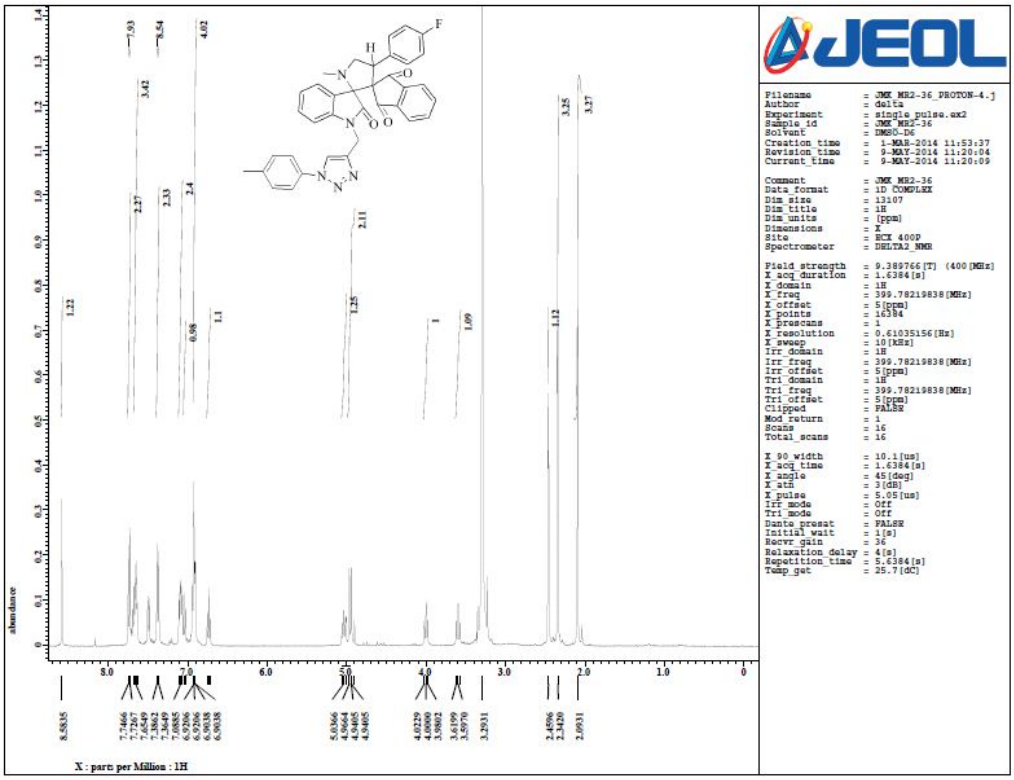


Figure 11. ^{13}C NMR spectrum of compound **6d** (100 MHz, $CDCl_3$).

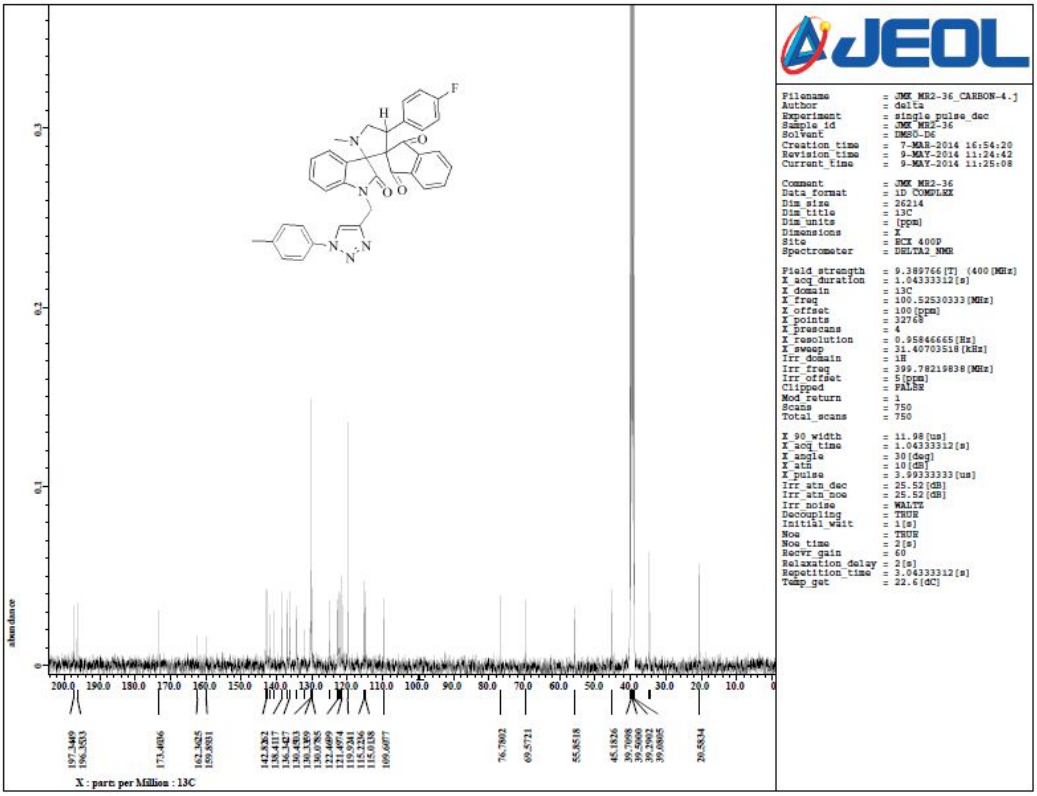
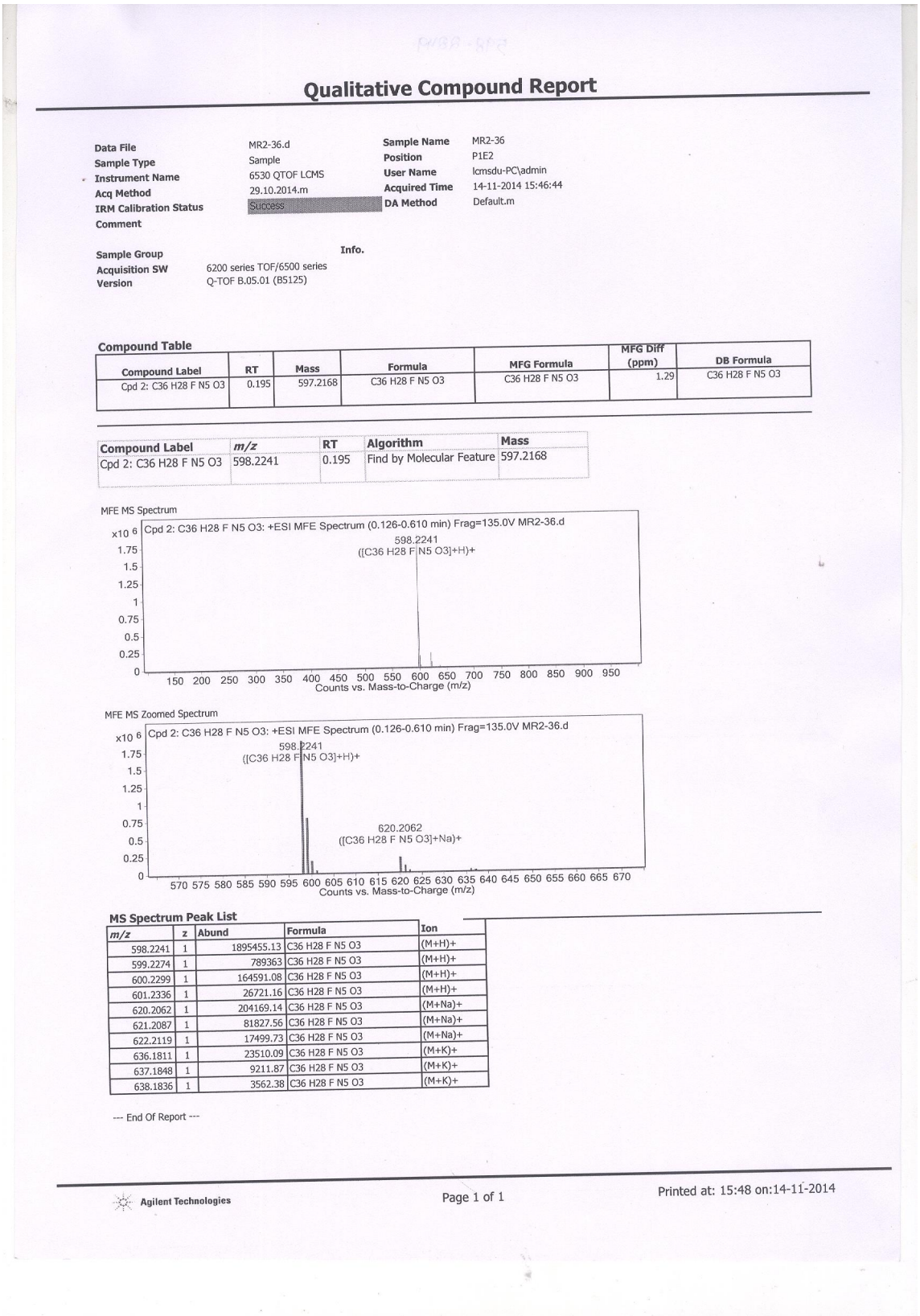


Figure 12. Mass spectrum of compound **6d**.



Qualitative Compound Report

Data File	MR2-36.d	**Sample Name**	MR2-36
Sample Type	Sample	**Position**	P1E2
Instrument Name	6530 QTOF LCMS	**User Name**	lcmsdu-PC\admin
Acq Method	29.10.2014.m	**Acquired Time**	14-11-2014 15:46:44
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Info.

Sample Group	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C36 H28 F N5 O3	0.195	597.2168	C36 H28 F N5 O3	C36 H28 F N5 O3	1.29	C36 H28 F N5 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 2: C36 H28 F N5 O3	598.2241	0.195	Find by Molecular Feature	597.2168

MFE MS Spectrum

MFE MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
598.2241	1	1895455.13	C36 H28 F N5 O3	(M+H)+
599.2274	1	789363	C36 H28 F N5 O3	(M+H)+
600.2299	1	164591.08	C36 H28 F N5 O3	(M+H)+
601.2336	1	26721.16	C36 H28 F N5 O3	(M+H)+
620.2062	1	204169.14	C36 H28 F N5 O3	(M+Na)+
621.2087	1	81827.56	C36 H28 F N5 O3	(M+Na)+
622.2119	1	17499.73	C36 H28 F N5 O3	(M+Na)+
636.1811	1	23510.09	C36 H28 F N5 O3	(M+K)+
637.1848	1	9211.87	C36 H28 F N5 O3	(M+K)+
638.1836	1	3562.38	C36 H28 F N5 O3	(M+K)+

--- End Of Report ---

Figure 13. ^{1}H NMR spectrum of compound **6e** (400 MHz, $CDCl_3$).

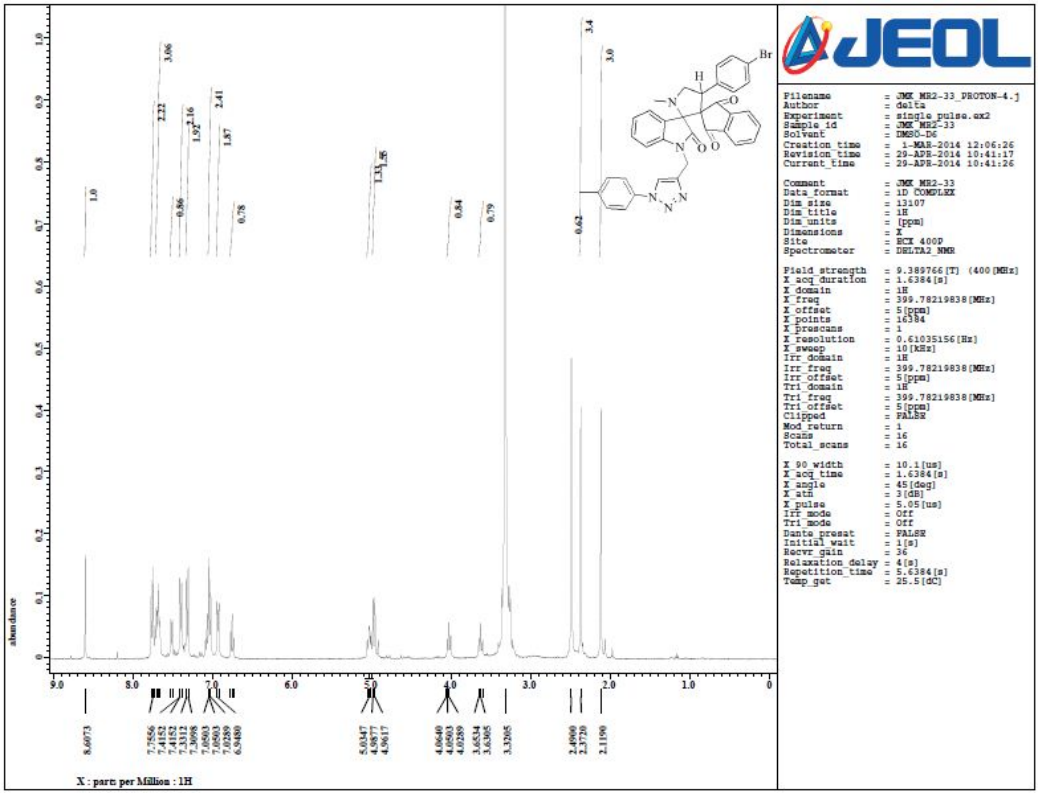


Figure 14. ^{13}C NMR spectrum of compound **6e** (100 MHz, $CDCl_3$).

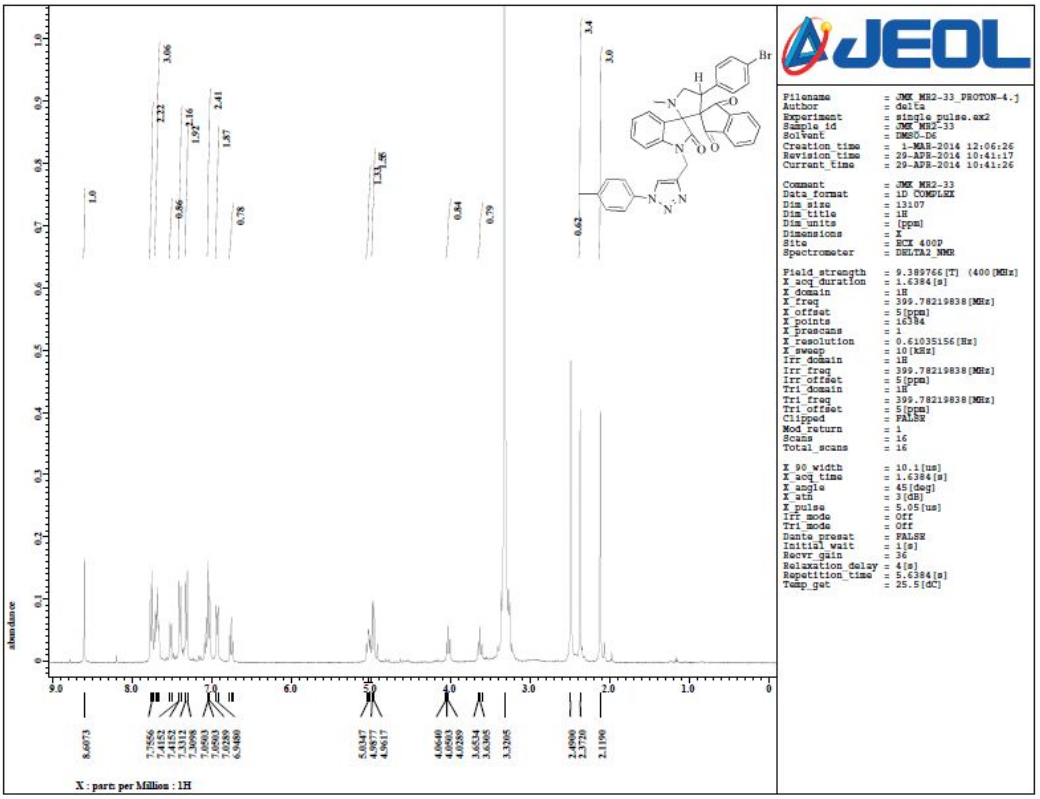


Figure 15. Mass spectrum of compound **6e**.

Qualitative Analysis Report

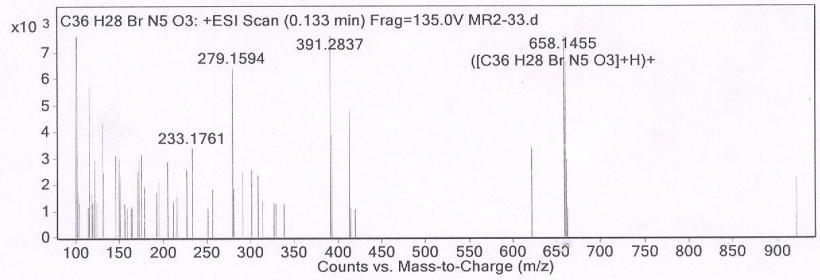
Data Filename	MR2-33.d	**Sample Name**	MR2-33
Sample Type	Sample	**Position**	P2F8
Instrument Name	6530 QTOF LCMS	**User Name**	lcmsdu-PC\admin
Acq Method	Union.m	**Acquired Time**	25-08-2014 14:28:25
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**

Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
100.0766		9123.3		
101.0716	1	44205.87		
115.0867		5695.14		
130.1588		4265.27		
279.1594	1	6384.01		
391.2837	1	13524.75		
392.2878	1	3873.17		
413.2669	1	4776.41		
658.1455	1	7614.94	C36 H28 Br N5 O3	(M+H)+
660.1428	1	6655.56	C36 H28 Br N5 O3	(M+H)+

--- End Of Report ---

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Figure 16. ^{1}H NMR spectrum of compound **6f** (400 MHz, $CDCl_3$).

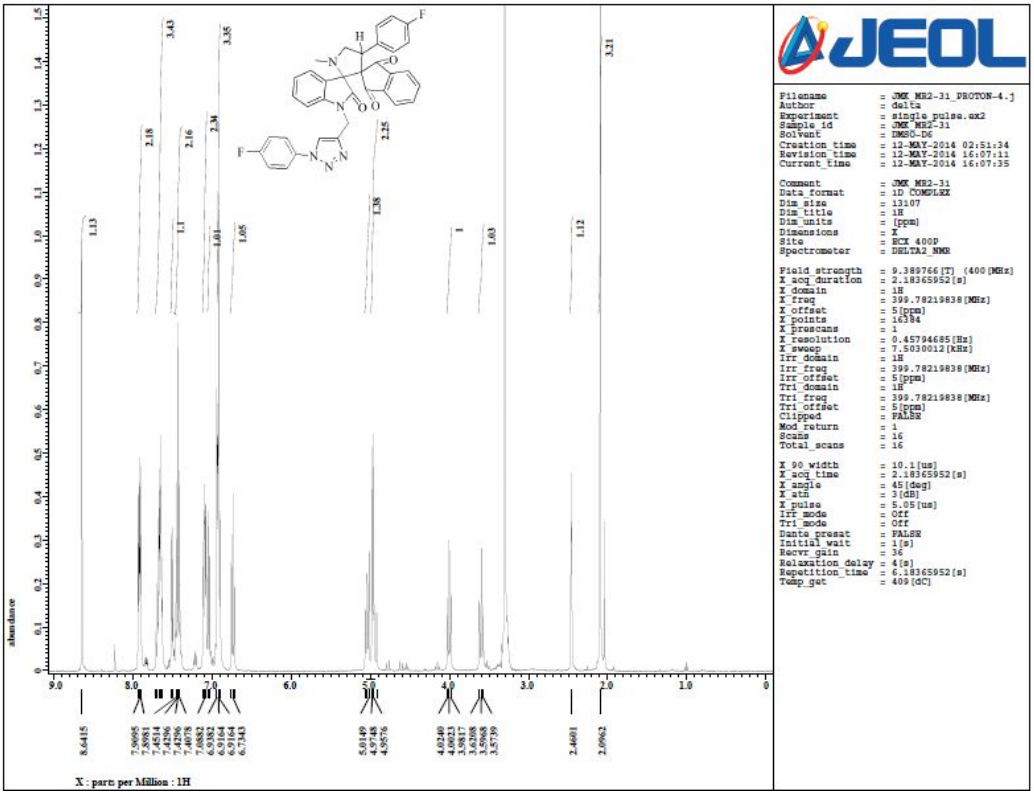


Figure 17. ^{13}C NMR spectrum of compound **6f** (100 MHz, $CDCl_3$).

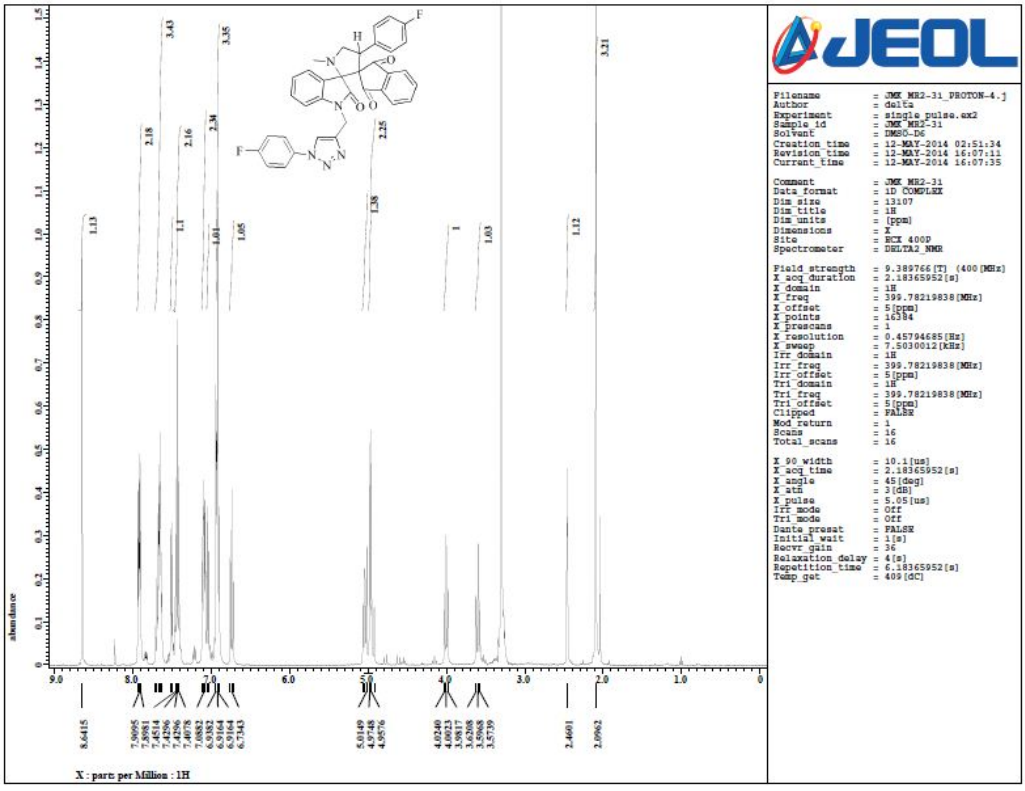


Figure 18. Mass spectrum of compound **6f**.

Qualitative Analysis Report

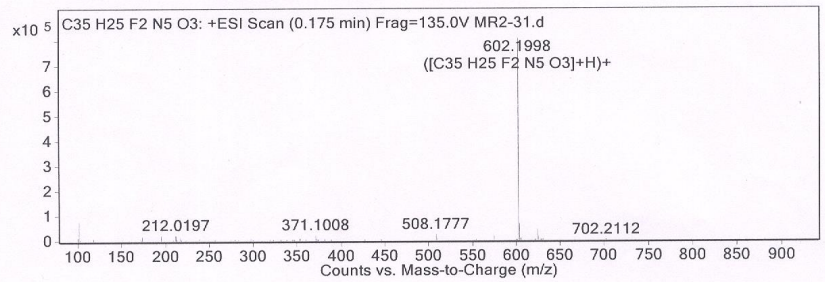
Data Filename	MR2-31.d	**Sample Name**	MR2-31
Sample Type	Sample	**Position**	P2F1
Instrument Name	6530 QTOF LCMS	**User Name**	lcmsdu-PC\admin
Acq Method	Union.m	**Acquired Time**	22-08-2014 15:06:31
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**

Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI



Peak List

m/z	z	Abund	Formula	Ion
101.0711	1	78428.48		
195.1223	1	21677.83		
212.0197	1	22925.09		
371.1008	1	22882.1		
508.1777	1	25707.01		
602.1998	1	810350.81	C35 H25 F2 N5 O3	(M+H)+
603.2031	1	324834.75	C35 H25 F2 N5 O3	(M+H)+
604.2059	1	66396.16	C35 H25 F2 N5 O3	(M+H)+
624.1814	1	44522.64		
625.1845	1	18550.19		

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Figure 19. ^{1}H NMR spectrum of compound **6g** (400 MHz, $CDCl_3$).

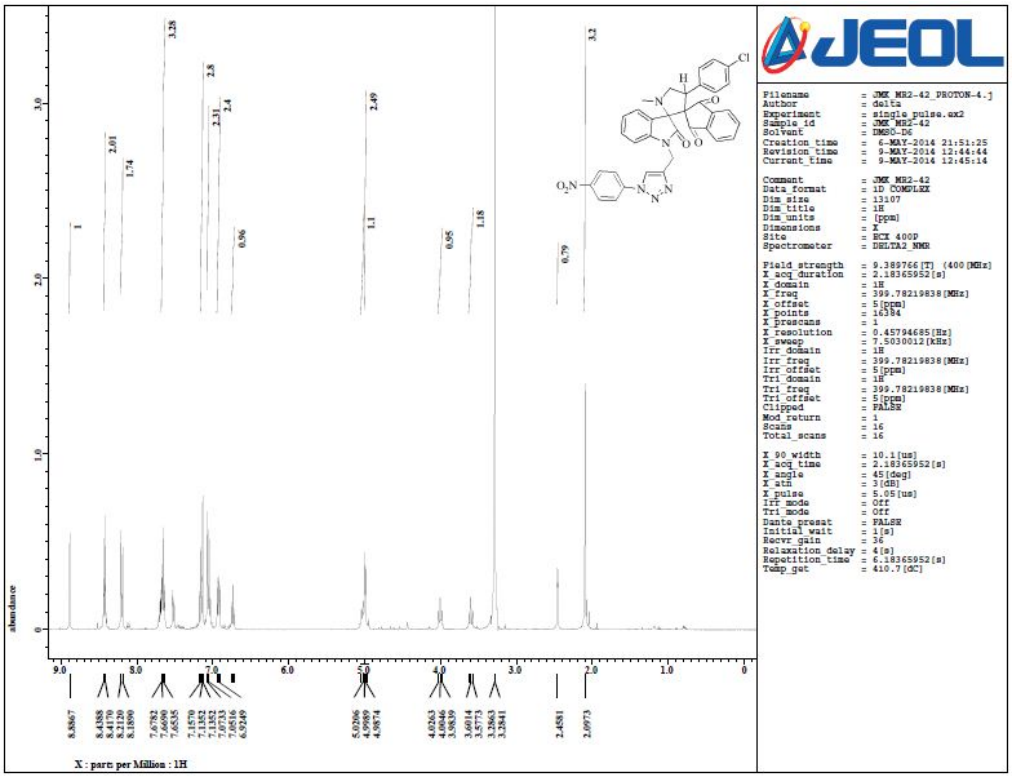


Figure 20. ^{13}C NMR spectrum of compound **6g** (100 MHz, $CDCl_3$).

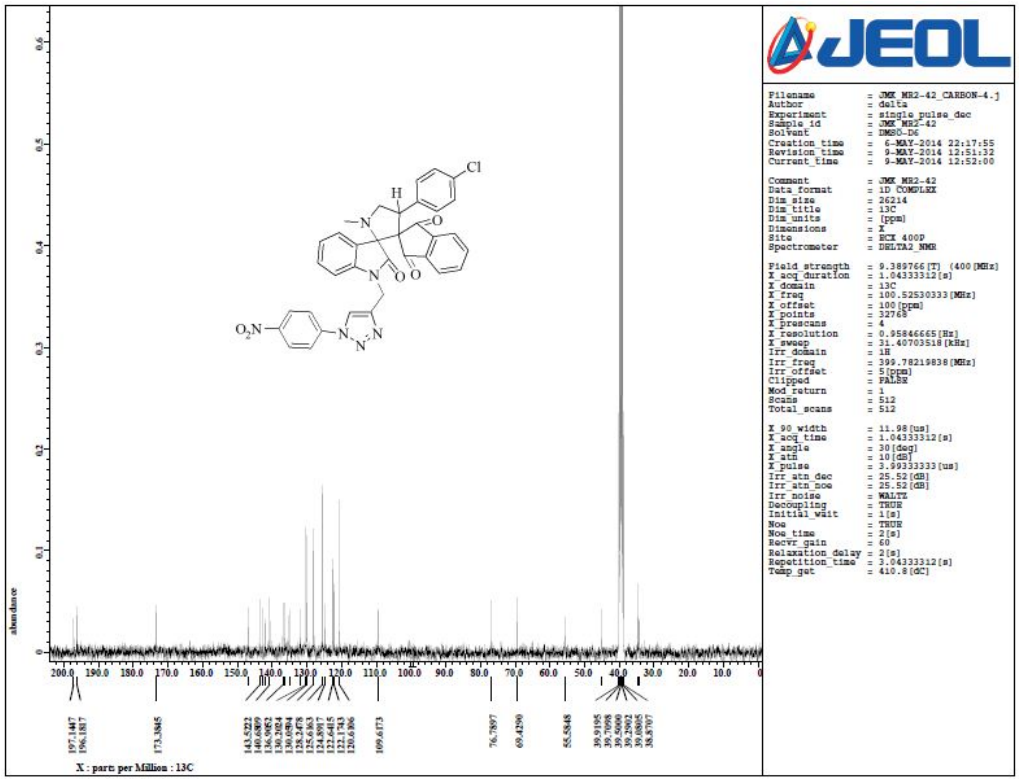
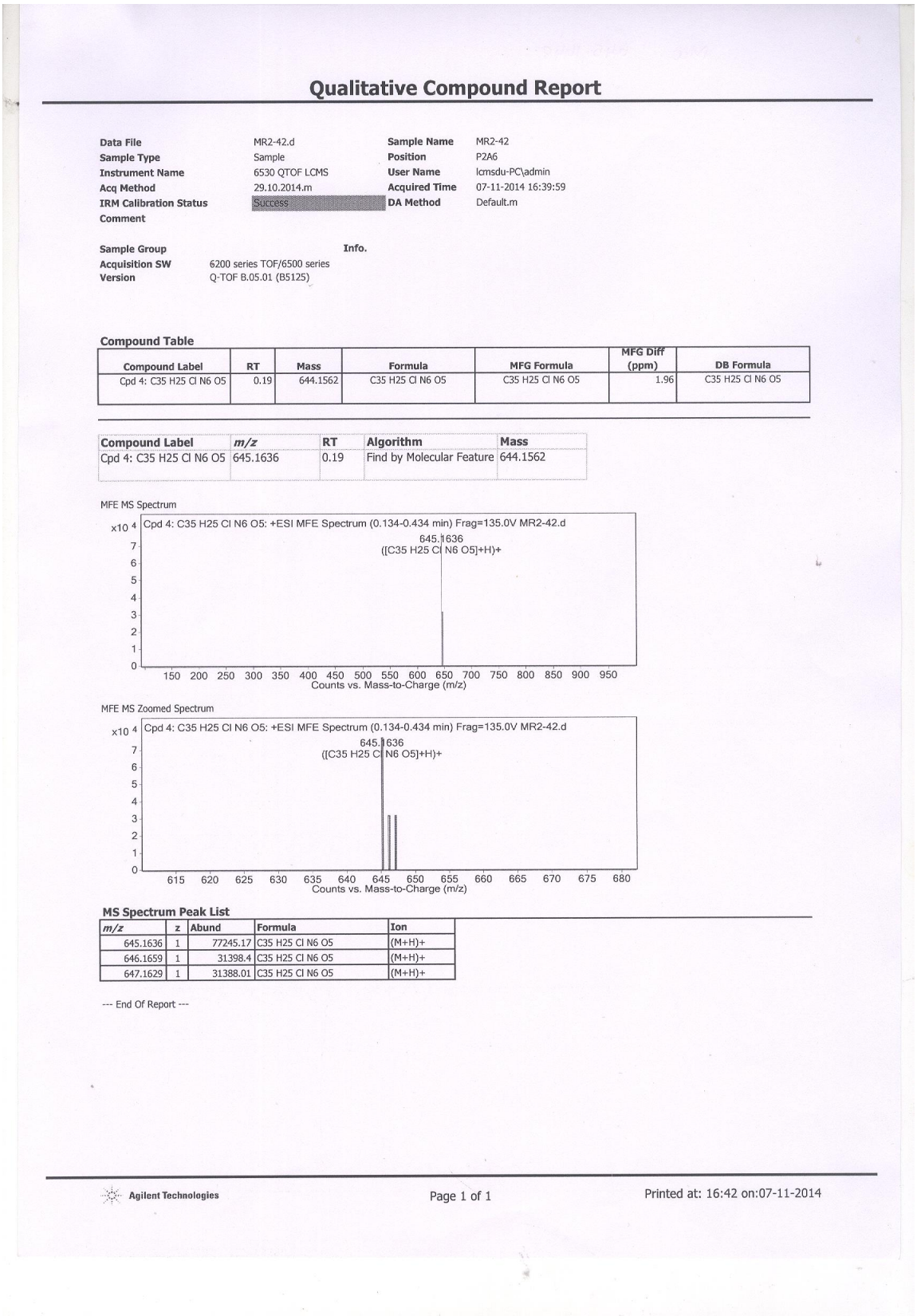


Figure 21. Mass spectrum of compound **6g**.



Qualitative Compound Report

Data File	MR2-42.d	**Sample Name**	MR2-42
Sample Type	Sample	**Position**	P2A6
Instrument Name	6530 QTOF LCMS	**User Name**	lcmsdu-PC\admin
Acq Method	29.10.2014.m	**Acquired Time**	07-11-2014 16:39:59
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C35 H25 Cl N6 O5	0.19	644.1562	C35 H25 Cl N6 O5	C35 H25 Cl N6 O5	1.96	C35 H25 Cl N6 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C35 H25 Cl N6 O5	645.1636	0.19	Find by Molecular Feature	644.1562

MFE MS Spectrum

MFE MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
645.1636	1	77245.17	C35 H25 Cl N6 O5	(M+H)+
646.1659	1	31398.4	C35 H25 Cl N6 O5	(M+H)+
647.1629	1	31388.01	C35 H25 Cl N6 O5	(M+H)+

--- End Of Report ---

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Figure 22. ^{1}H NMR spectrum of compound **6h** (400 MHz, $CDCl_3$).

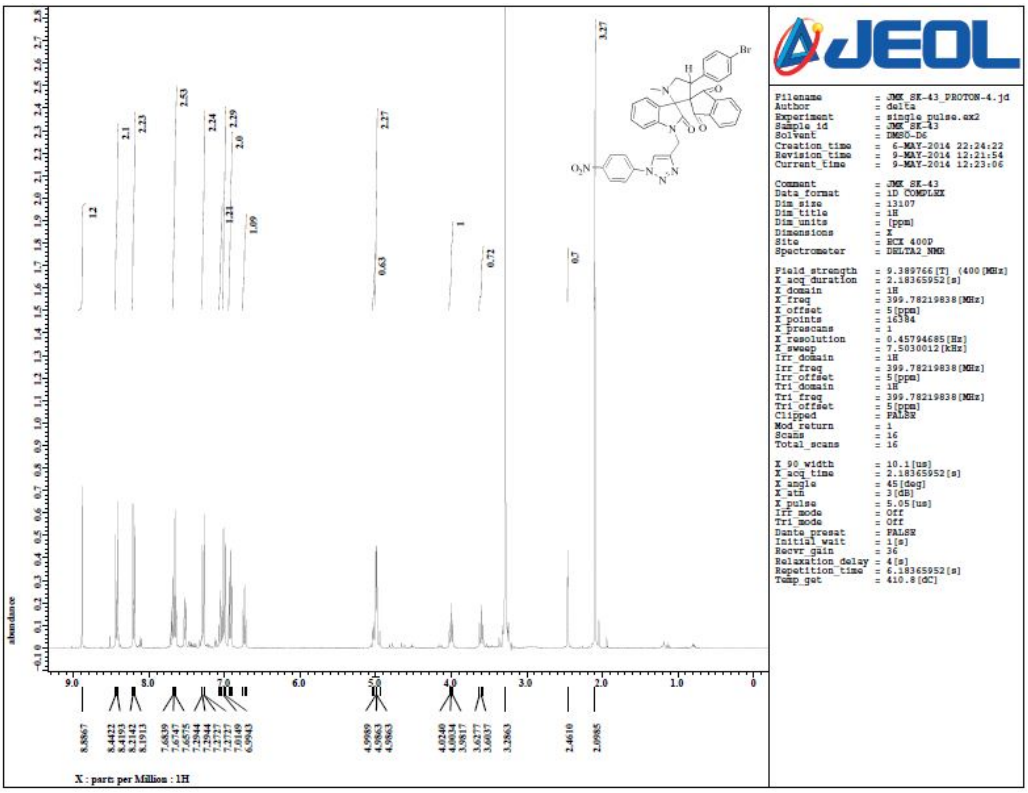


Figure 23. ^{13}C NMR spectrum of compound **6h** (100 MHz, $CDCl_3$).

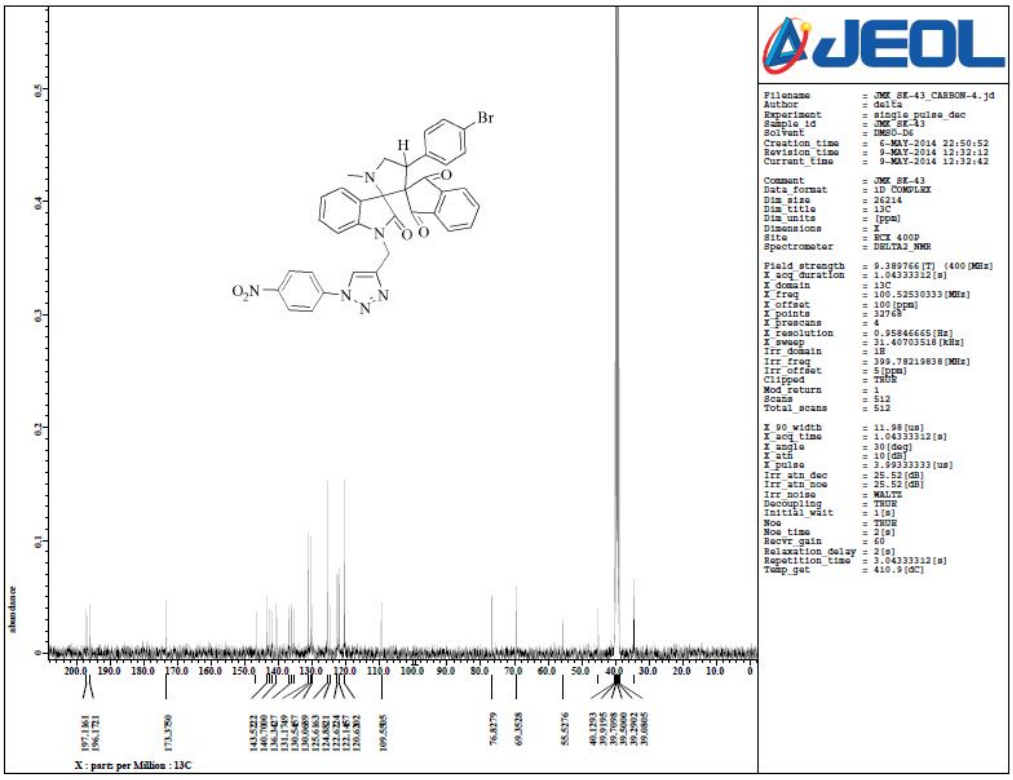
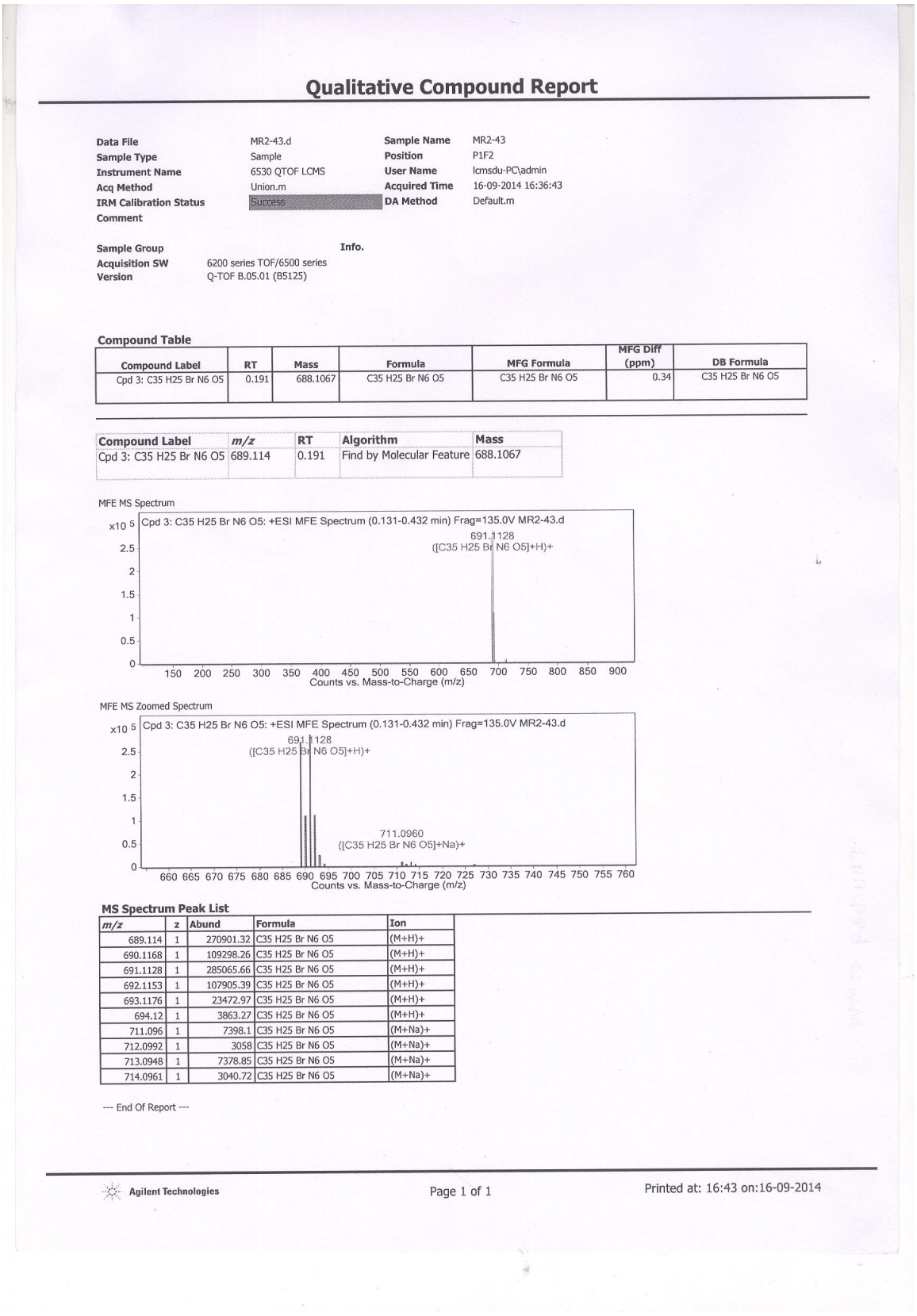


Figure 24. Mass spectrum of compound **6h**.



Qualitative Compound Report

Data File	MR2-43.d	**Sample Name**	MR2-43
Sample Type	Sample	**Position**	P1F2
Instrument Name	6530 QTOF LCMS	**User Name**	lcmsdu-PC\admin
Acq Method	Union.m	**Acquired Time**	16-09-2014 16:36:43
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C35 H25 Br N6 O5	0.191	688.1067	C35 H25 Br N6 O5	C35 H25 Br N6 O5	0.34	C35 H25 Br N6 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C35 H25 Br N6 O5	689.114	0.191	Find by Molecular Feature	688.1067

MFE MS Spectrum

MFE MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
689.114	1	270901.32	C35 H25 Br N6 O5	(M+H)+
690.1168	1	109298.26	C35 H25 Br N6 O5	(M+H)+
691.1128	1	285065.66	C35 H25 Br N6 O5	(M+H)+
692.1153	1	107905.39	C35 H25 Br N6 O5	(M+H)+
693.1176	1	23472.97	C35 H25 Br N6 O5	(M+H)+
694.12	1	3863.27	C35 H25 Br N6 O5	(M+H)+
711.096	1	7398.1	C35 H25 Br N6 O5	(M+Na)+
712.0992	1	3058	C35 H25 Br N6 O5	(M+Na)+
713.0948	1	7378.85	C35 H25 Br N6 O5	(M+Na)+
714.0961	1	3040.72	C35 H25 Br N6 O5	(M+Na)+

--- End Of Report ---

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Figure 25. ^{1}H NMR spectrum of compound **6i** (400 MHz, $CDCl_3$).

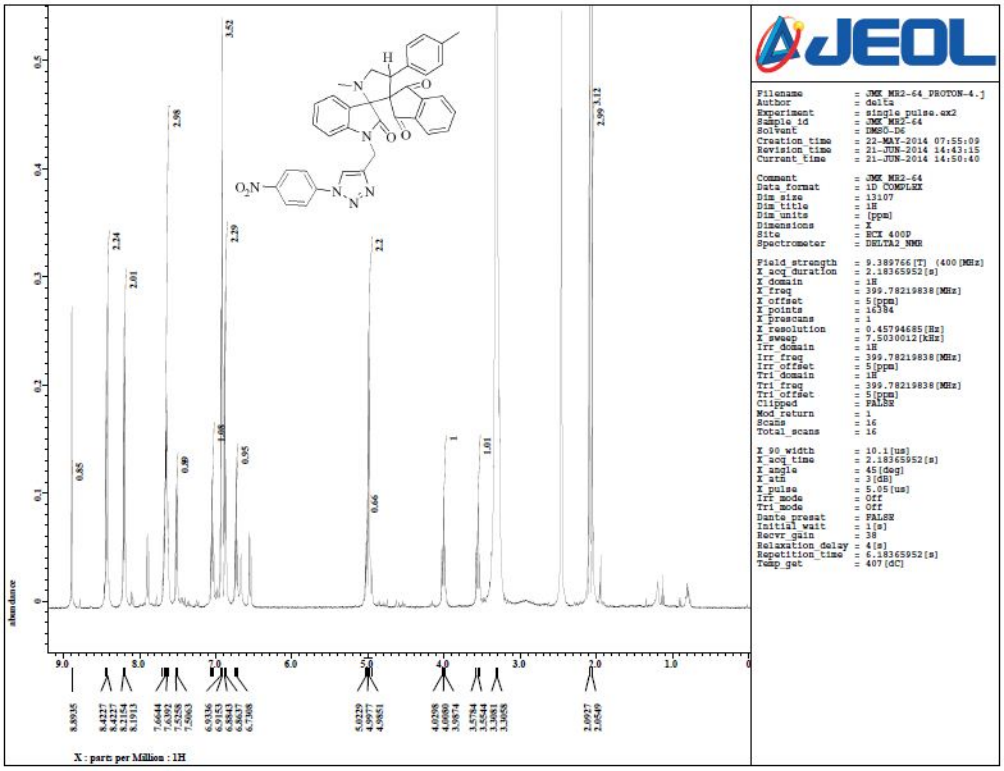


Figure 26. ^{13}C NMR spectrum of compound **6i** (100 MHz, $CDCl_3$).

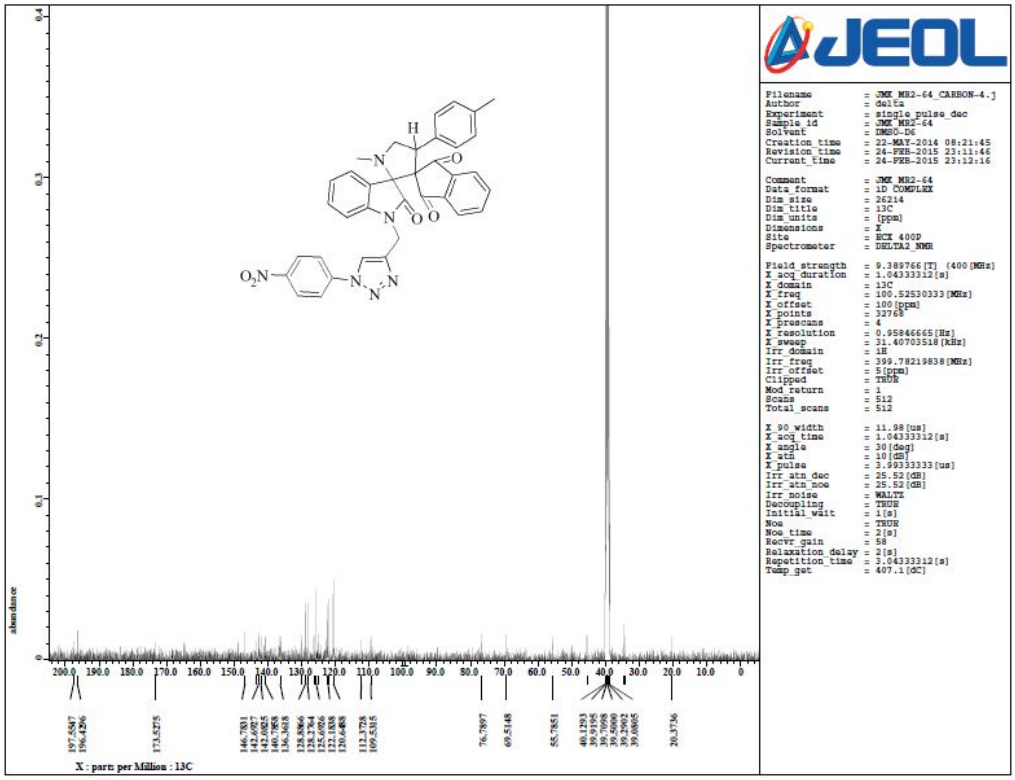
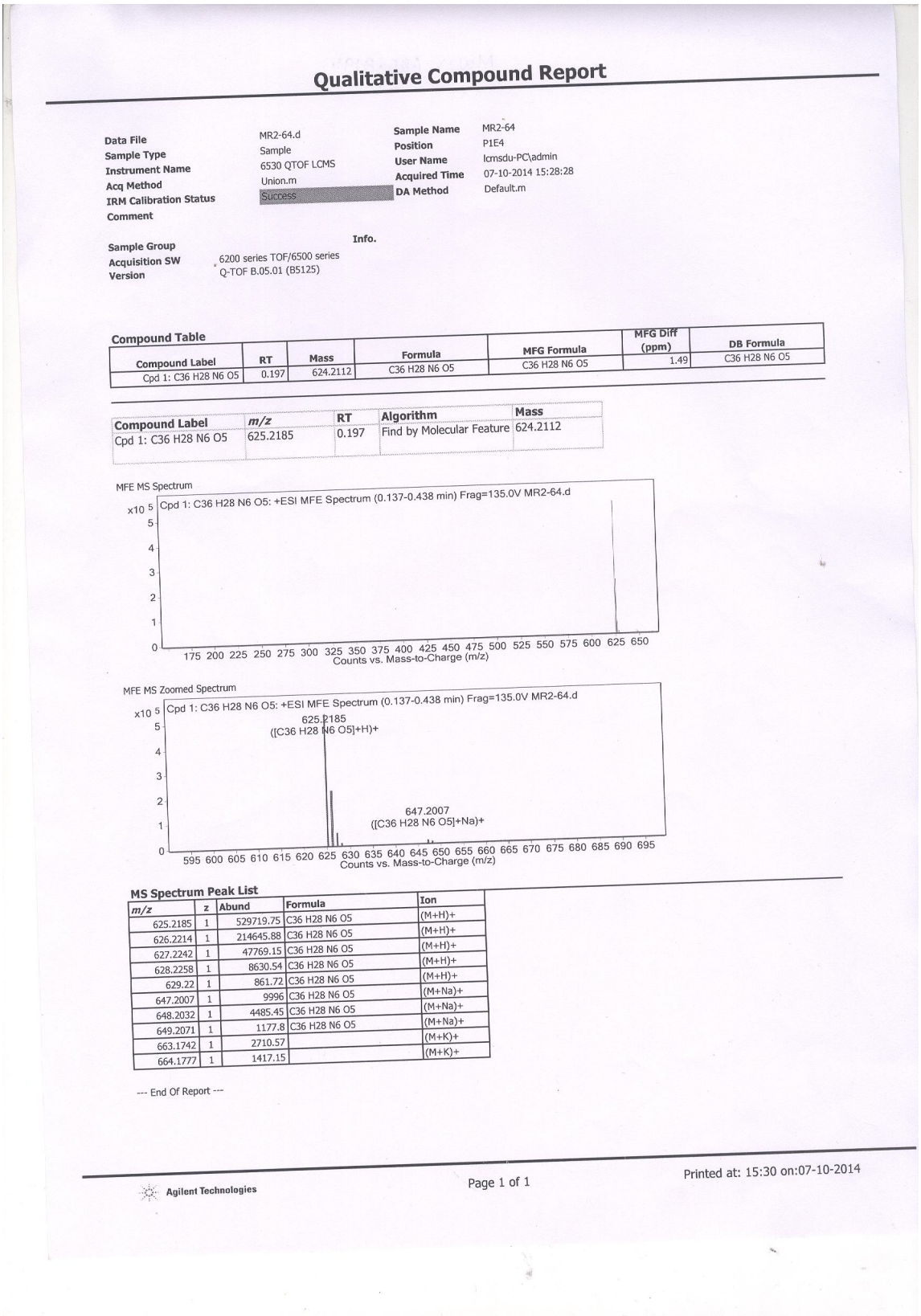


Figure 27. Mass spectrum of compound **6i**.



Qualitative Compound Report

Data File	MR2-64.d	**Sample Name**	MR2-64
Sample Type	Sample	**Position**	P1E4
Instrument Name	6530 QTOF LCMS	**User Name**	lcmsdu-PC\admin
Acq Method	Union.m	**Acquired Time**	07-10-2014 15:28:28
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Info.

Sample Group	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C36 H28 N6 O5	0.197	624.2112	C36 H28 N6 O5	C36 H28 N6 O5	1.49	C36 H28 N6 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C36 H28 N6 O5	625.2185	0.197	Find by Molecular Feature	624.2112

MFE MS Spectrum

MFE MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
625.2185	1	529719.75	C36 H28 N6 O5	(M+H)+
626.2214	1	214645.88	C36 H28 N6 O5	(M+H)+
627.2242	1	47769.15	C36 H28 N6 O5	(M+H)+
628.2258	1	8630.54	C36 H28 N6 O5	(M+H)+
629.22	1	861.72	C36 H28 N6 O5	(M+H)+
647.2007	1	9996	C36 H28 N6 O5	(M+Na)+
648.2032	1	4485.45	C36 H28 N6 O5	(M+Na)+
649.2071	1	1177.8	C36 H28 N6 O5	(M+Na)+
663.1742	1	2710.57		(M+K)+
664.1777	1	1417.15		(M+K)+

--- End Of Report ---

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Figure 28. ^{1}H NMR spectrum of compound **6j** (400 MHz, $CDCl_3$).

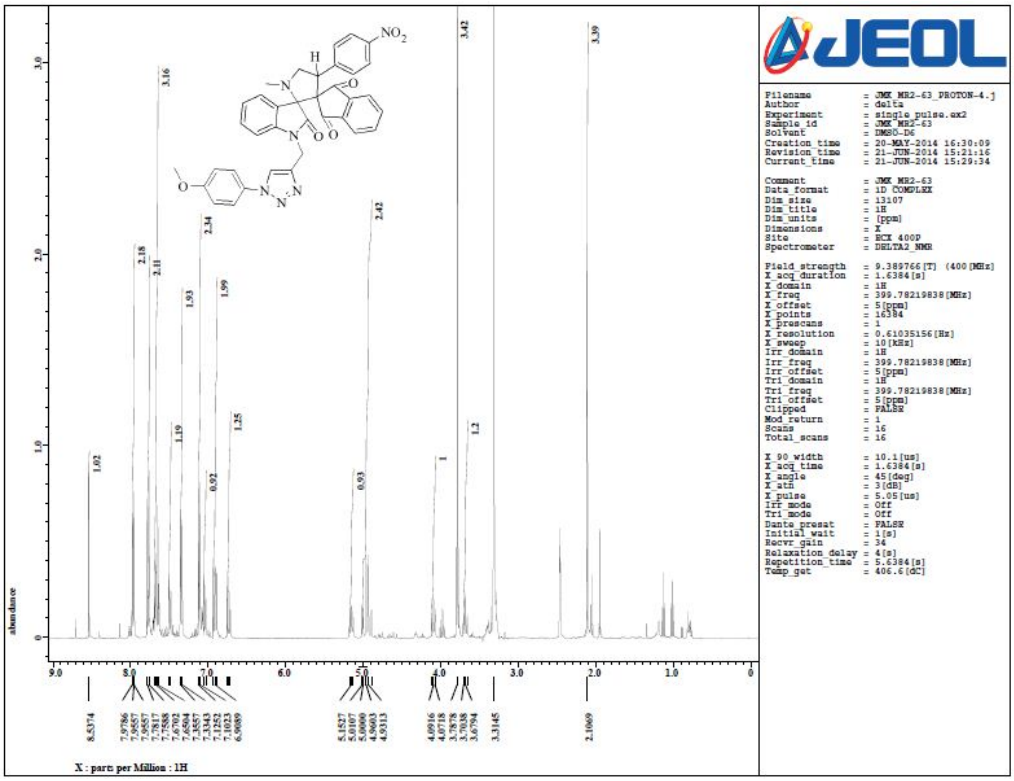


Figure 29. ^{13}C NMR spectrum of compound **6j** (100 MHz, $CDCl_3$).

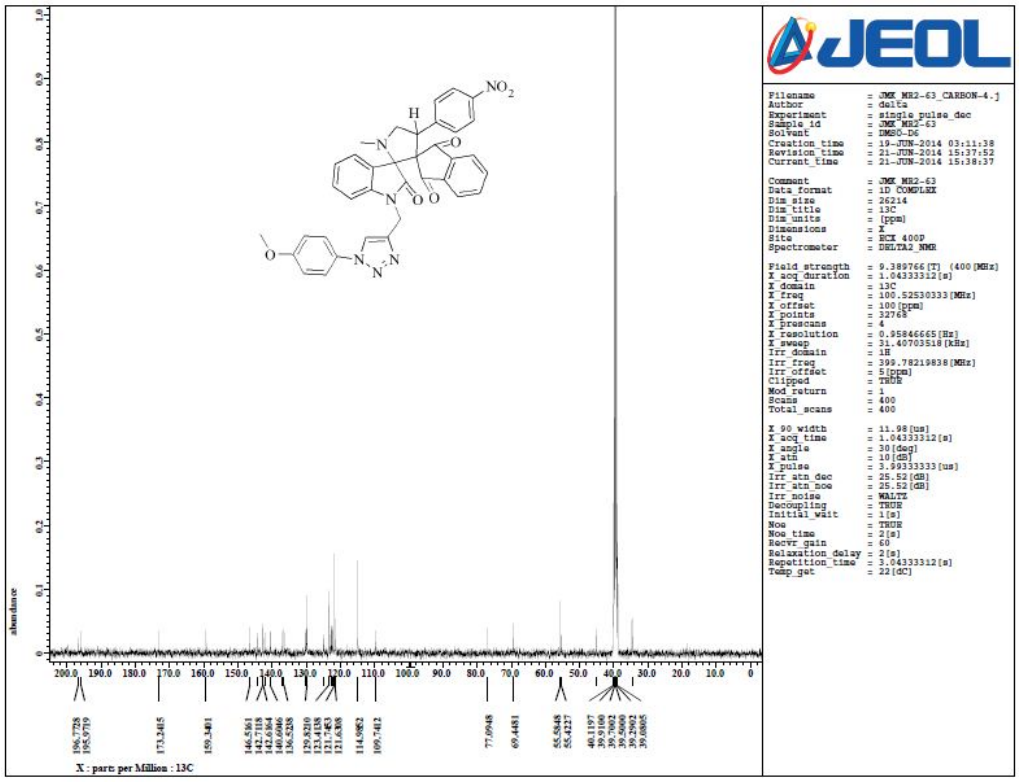
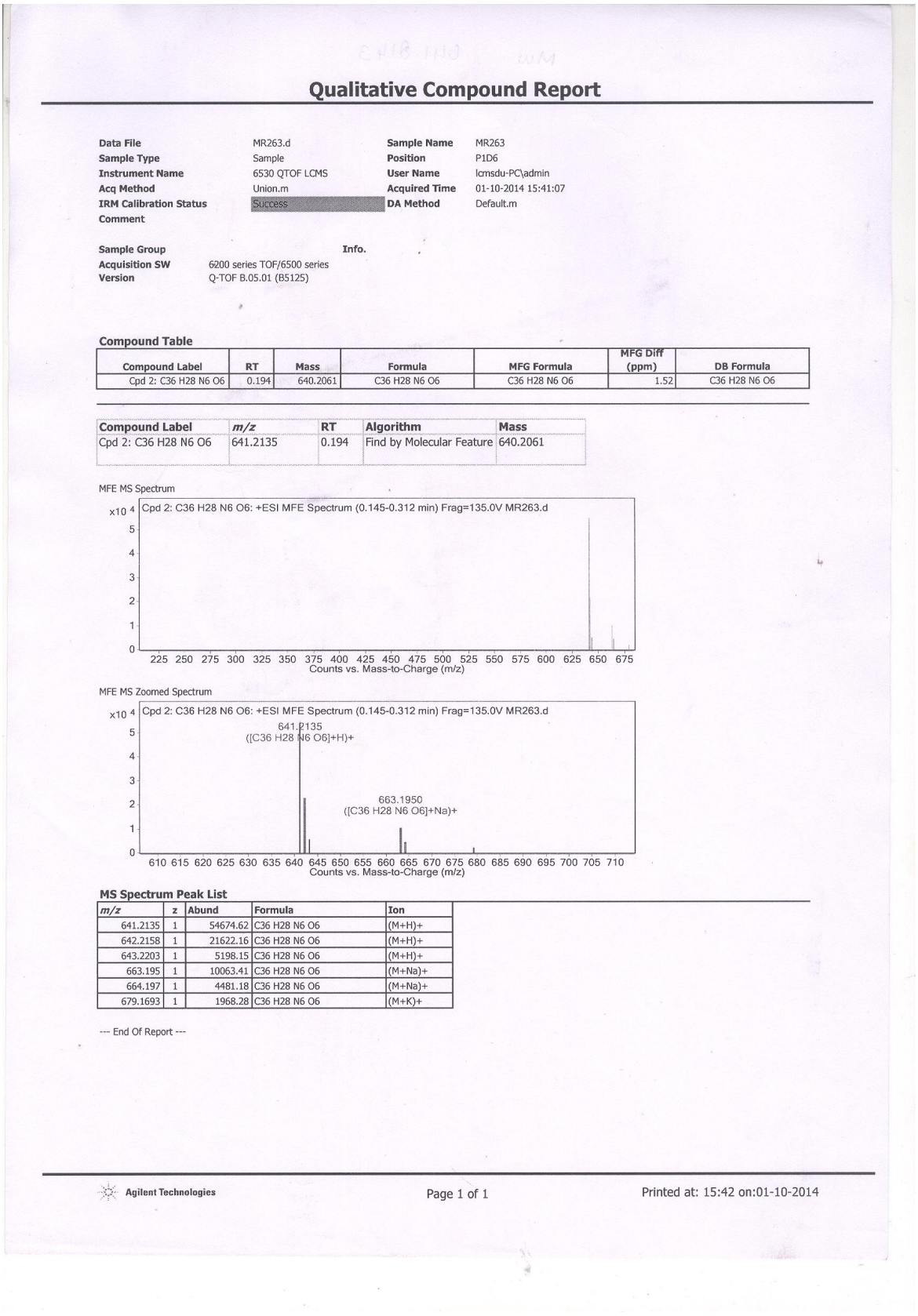


Figure 30. Mass spectrum of compound **6j**.



Qualitative Compound Report

Data File	MR263.d	**Sample Name**	MR263
Sample Type	Sample	**Position**	P1D6
Instrument Name	6530 QTOF LCMS	**User Name**	lcmsdu-PC\admin
Acq Method	Union.m	**Acquired Time**	01-10-2014 15:41:07
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C36 H28 N6 O6	0.194	640.2061	C36 H28 N6 O6	C36 H28 N6 O6	1.52	C36 H28 N6 O6

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 2: C36 H28 N6 O6	641.2135	0.194	Find by Molecular Feature	640.2061

MFE MS Spectrum

MFE MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
641.2135	1	54674.62	C36 H28 N6 O6	(M+H)+
642.2158	1	21622.16	C36 H28 N6 O6	(M+H)+
643.2203	1	5198.15	C36 H28 N6 O6	(M+H)+
663.195	1	10063.41	C36 H28 N6 O6	(M+Na)+
664.197	1	4481.18	C36 H28 N6 O6	(M+Na)+
679.1693	1	1968.28	C36 H28 N6 O6	(M+K)+

--- End Of Report ---

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Figure 31. ^{1}H NMR spectrum of compound **6k** (400 MHz, $CDCl_3$).

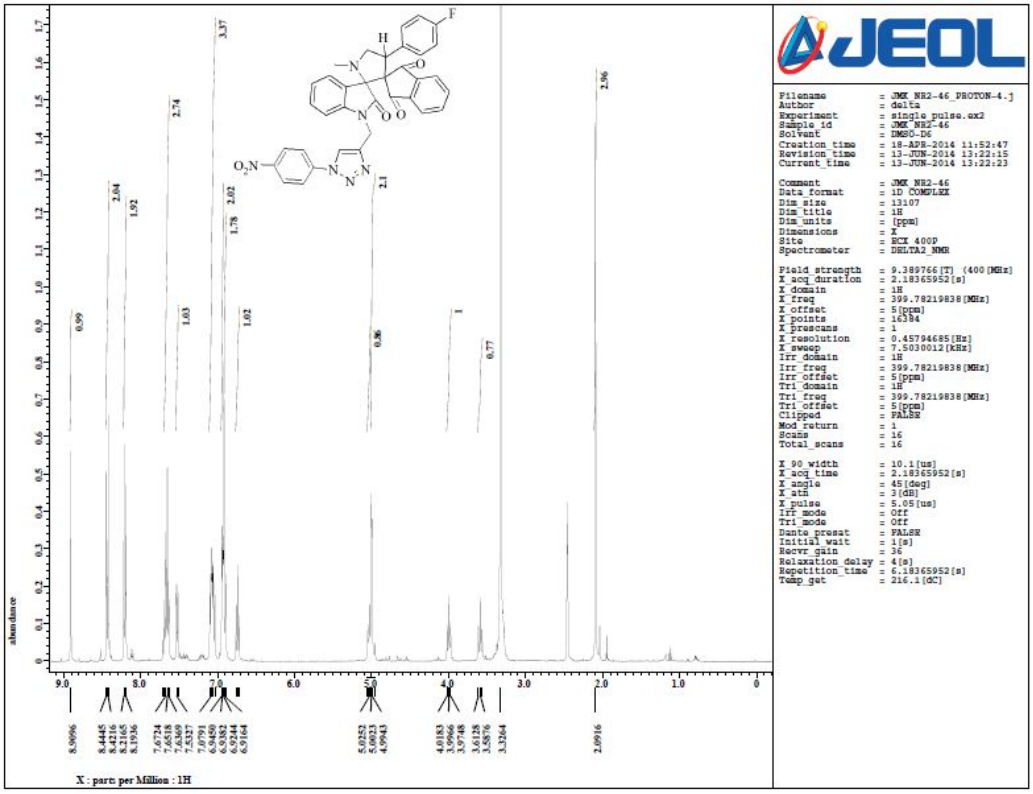


Figure 22. ^{13}C NMR spectrum of compound **6k** (100 MHz, $CDCl_3$).

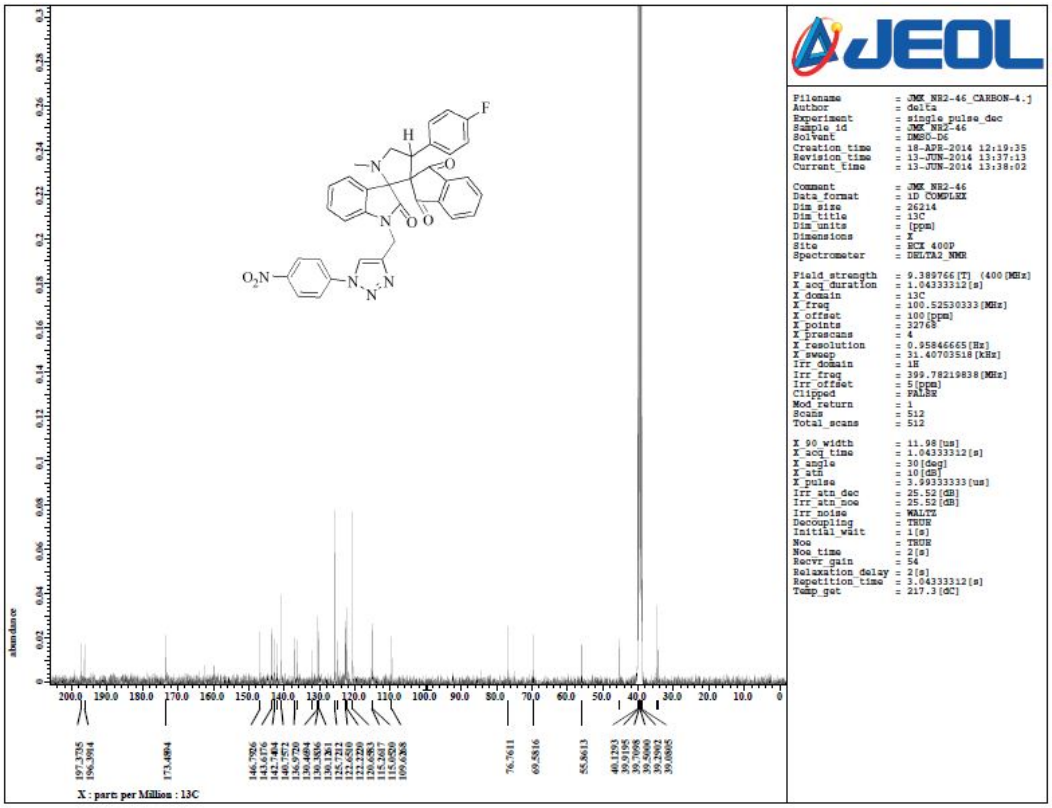


Figure 33. Mass spectrum of compound **6k.**

Qualitative Compound Report

Data File	MR 8 46.d	**Sample Name**	MR 8 46
Sample Type	Sample	**Position**	P1B7
Instrument Name	6530 QTOF LCMS	**User Name**	lcmsdu-PC\admin
Acq Method	Union.m	**Acquired Time**	17-09-2014 16:04:45
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

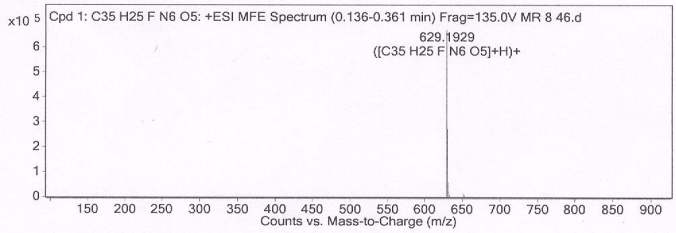
Sample Group **Info.**
Acquisition SW 6200 series TOF/6500 series
Version Q-TOF B.05.01 (B5125)

Compound Table

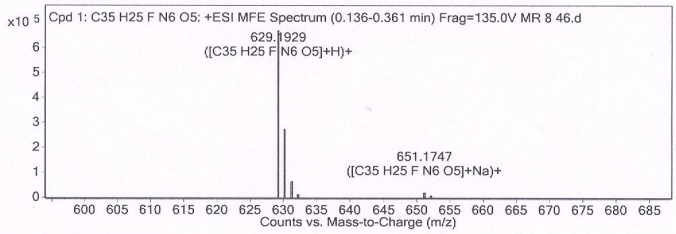
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C35 H25 F N6 O5	0.192	628.1856	C35 H25 F N6 O5	C35 H25 F N6 O5	2.32	C35 H25 F N6 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C35 H25 F N6 O5	629.1929	0.192	Find by Molecular Feature	628.1856

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
629.1929	1	667126.31	C35 H25 F N6 O5	(M+H)+
630.1959	1	271727.07	C35 H25 F N6 O5	(M+H)+
631.1984	1	59004.89	C35 H25 F N6 O5	(M+H)+
632.2007	1	9900.89	C35 H25 F N6 O5	(M+H)+
633.2016	1	590.9	C35 H25 F N6 O5	(M+H)+
651.1747	1	17979.07	C35 H25 F N6 O5	(M+Na)+
652.1776	1	7126.53	C35 H25 F N6 O5	(M+Na)+
653.1795	1	1654.49	C35 H25 F N6 O5	(M+Na)+

--- End Of Report ---

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Figure 34. ^{1}H NMR spectrum of compound **6l** (400 MHz, $CDCl_3$).

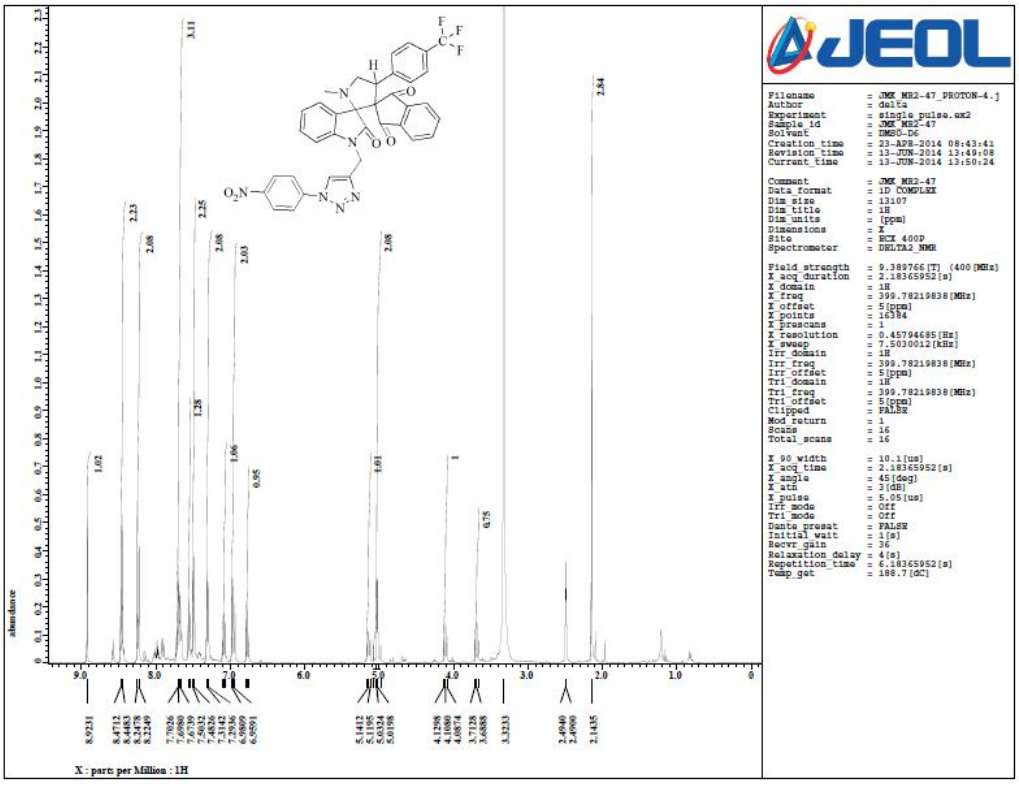


Figure 35. ^{13}C NMR spectrum of compound **6l** (100 MHz, $CDCl_3$).

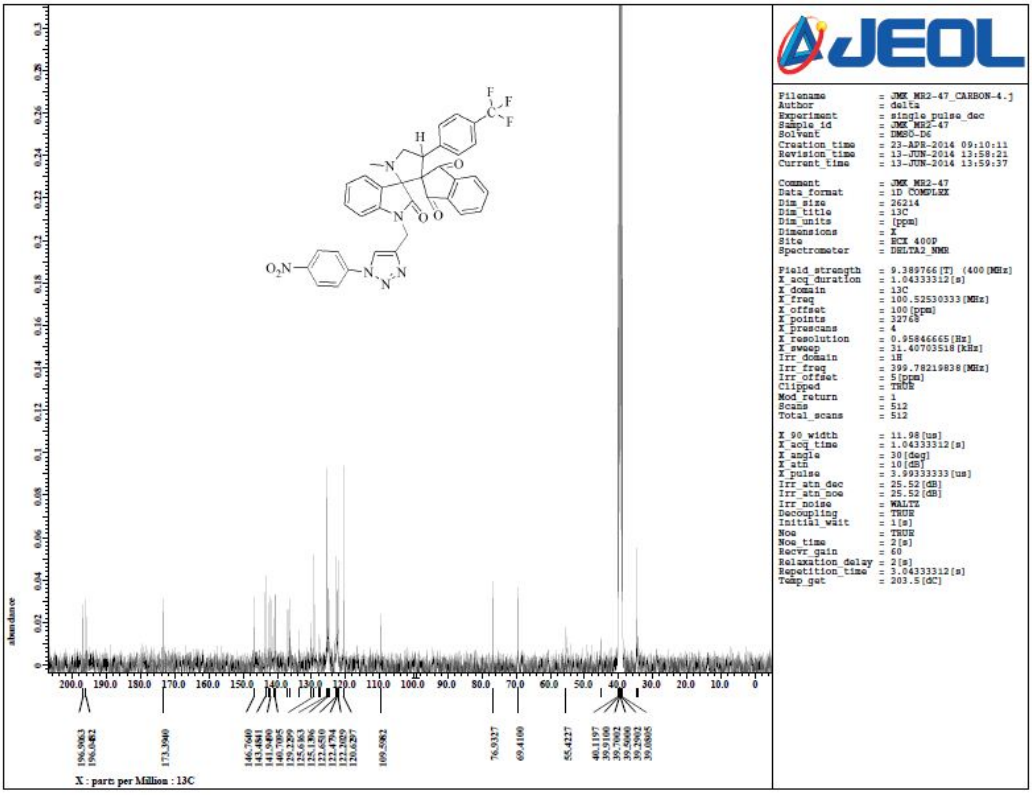
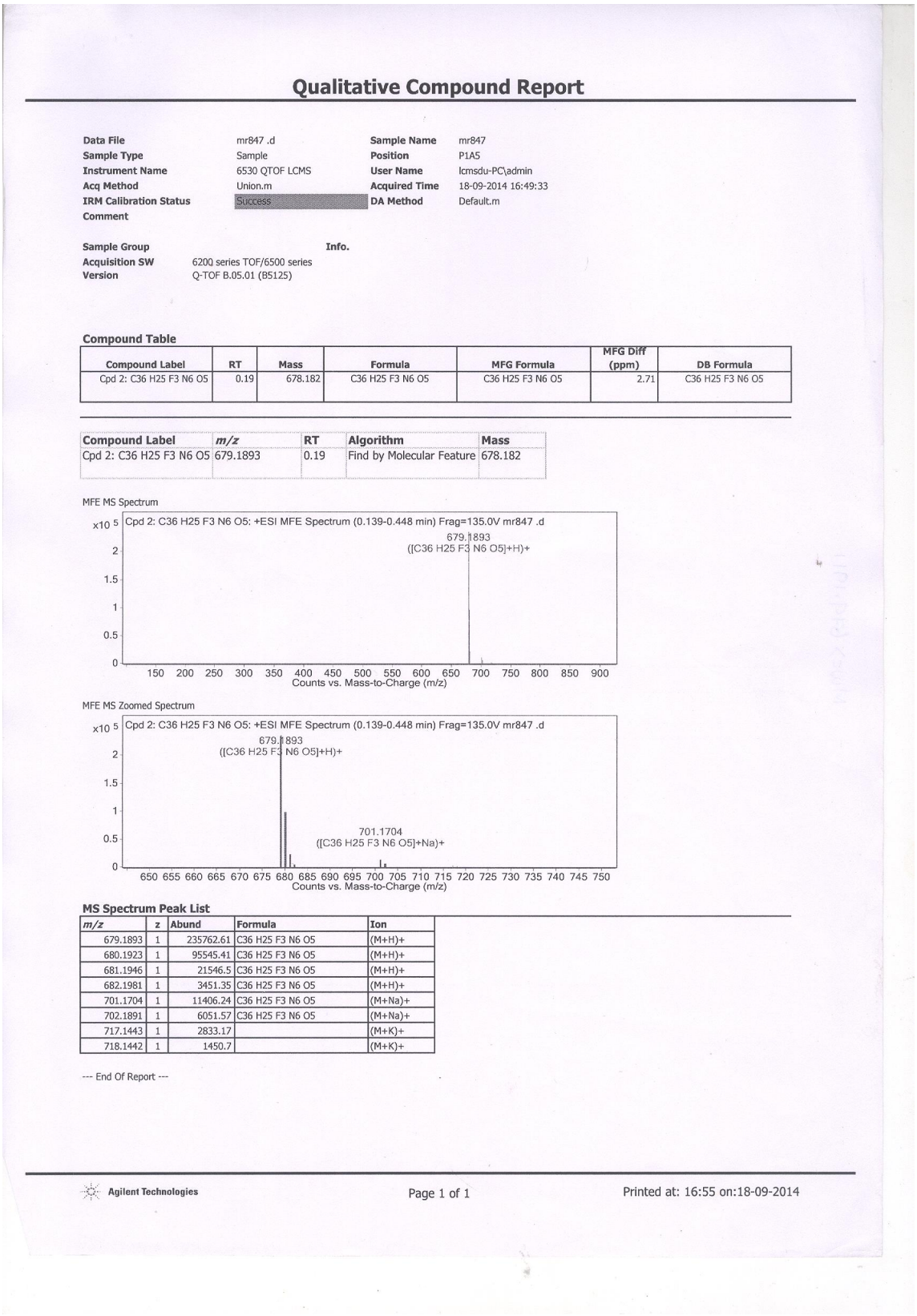


Figure 36. Mass spectrum of compound **6l.**



Qualitative Compound Report

Data File	mr847 .d	**Sample Name**	mr847
Sample Type	Sample	**Position**	P1A5
Instrument Name	6530 QTOF LCMS	**User Name**	lcmsdu-PC\admin
Acq Method	Union.m	**Acquired Time**	18-09-2014 16:49:33
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 2: C36 H25 F3 N6 O5	0.19	678.182	C36 H25 F3 N6 O5	C36 H25 F3 N6 O5	2.71	C36 H25 F3 N6 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 2: C36 H25 F3 N6 O5	679.1893	0.19	Find by Molecular Feature	678.182

MFE MS Spectrum

MFE MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
679.1893	1	235762.61	C36 H25 F3 N6 O5	(M+H)+
680.1923	1	95545.41	C36 H25 F3 N6 O5	(M+H)+
681.1946	1	21546.5	C36 H25 F3 N6 O5	(M+H)+
682.1981	1	3451.35	C36 H25 F3 N6 O5	(M+H)+
701.1704	1	11406.24	C36 H25 F3 N6 O5	(M+Na)+
702.1891	1	6051.57	C36 H25 F3 N6 O5	(M+Na)+
717.1443	1	2833.17		(M+K)+
718.1442	1	1450.7		(M+K)+

--- End Of Report ---

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Figure 37. ^{1}H NMR spectrum of compound **6m** (400 MHz, $CDCl_3$).

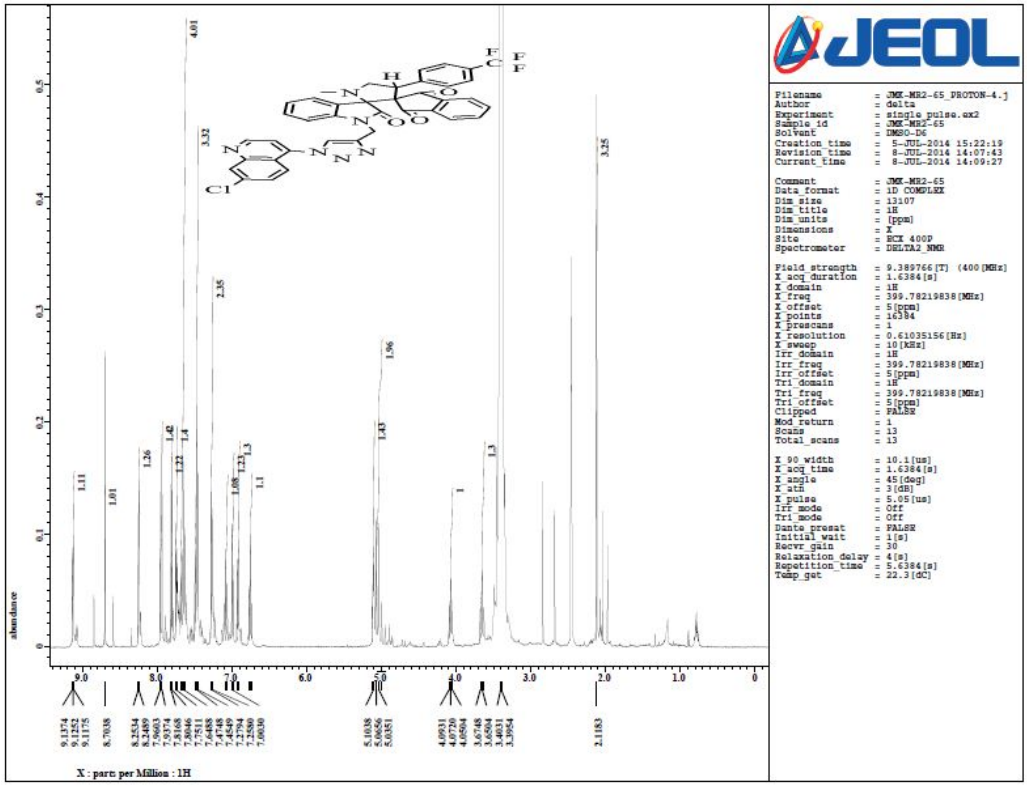


Figure 38. ^{13}C NMR spectrum of compound **6m** (100 MHz, $CDCl_3$).

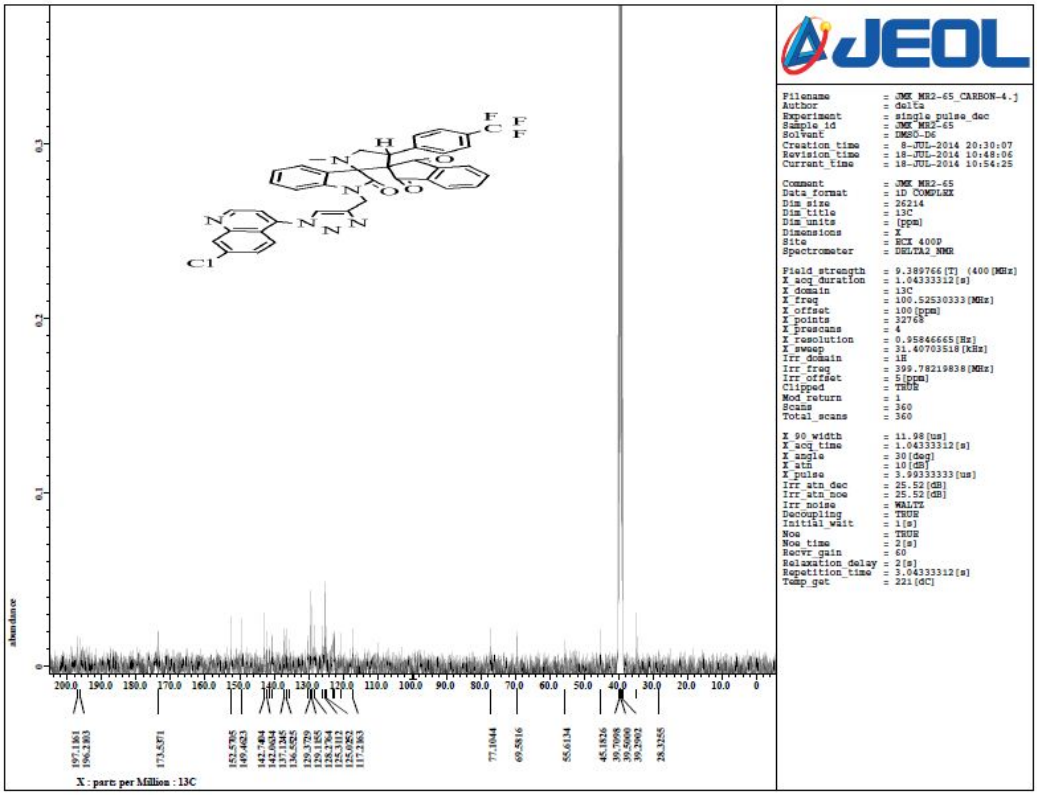


Figure 39. Mass spectrum of compound **6m.**

Qualitative Compound Report

Data File	MR2-65.d	**Sample Name**	MR2-65
Sample Type	Sample	**Position**	P2C1
Instrument Name	6530 QTOF LCMS	**User Name**	Icmsdu-PC\admin
Acq Method	29.10.2014.m	**Acquired Time**	12-11-2014 16:35:41
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

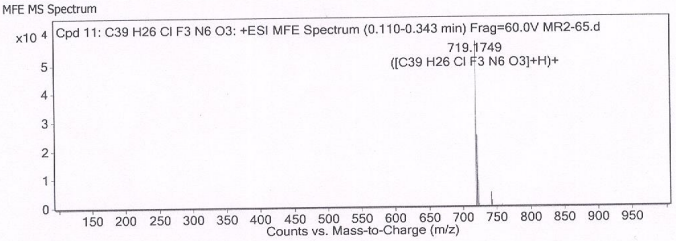
Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

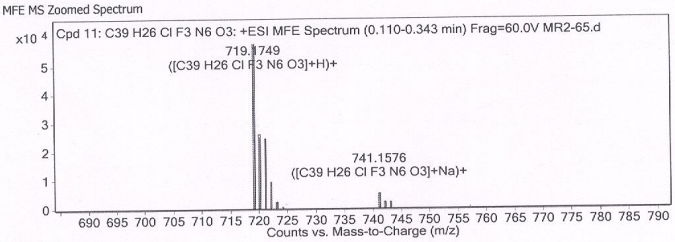
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 11: C39 H26 Cl F3 N6 O3	0.191	718.1677	C39 H26 Cl F3 N6 O3	C39 H26 Cl F3 N6 O3	4.14	C39 H26 Cl F3 N6 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 11: C39 H26 Cl F3 N6 O3	719.1749	0.191	Find by Molecular Feature	718.1677

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
719.1749	1	57633.35	C39 H26 Cl F3 N6 O3	(M+H)+
720.1782	1	24933.35	C39 H26 Cl F3 N6 O3	(M+H)+
721.1742	1	24690.04	C39 H26 Cl F3 N6 O3	(M+H)+
722.1767	1	9021.09	C39 H26 Cl F3 N6 O3	(M+H)+
723.1796	1	2610.7	C39 H26 Cl F3 N6 O3	(M+H)+
724.1743	1	564.64	C39 H26 Cl F3 N6 O3	(M+H)+
741.1576	1	4729.36	C39 H26 Cl F3 N6 O3	(M+Na)+
742.1588	1	2368.46	C39 H26 Cl F3 N6 O3	(M+Na)+
743.1537	1	2087.69	C39 H26 Cl F3 N6 O3	(M+Na)+
757.1271	1	627.78		(M+K)+

--- End Of Report ---

Figure 40. ^{1}H NMR spectrum of compound **6n** (400 MHz, $CDCl_3$).

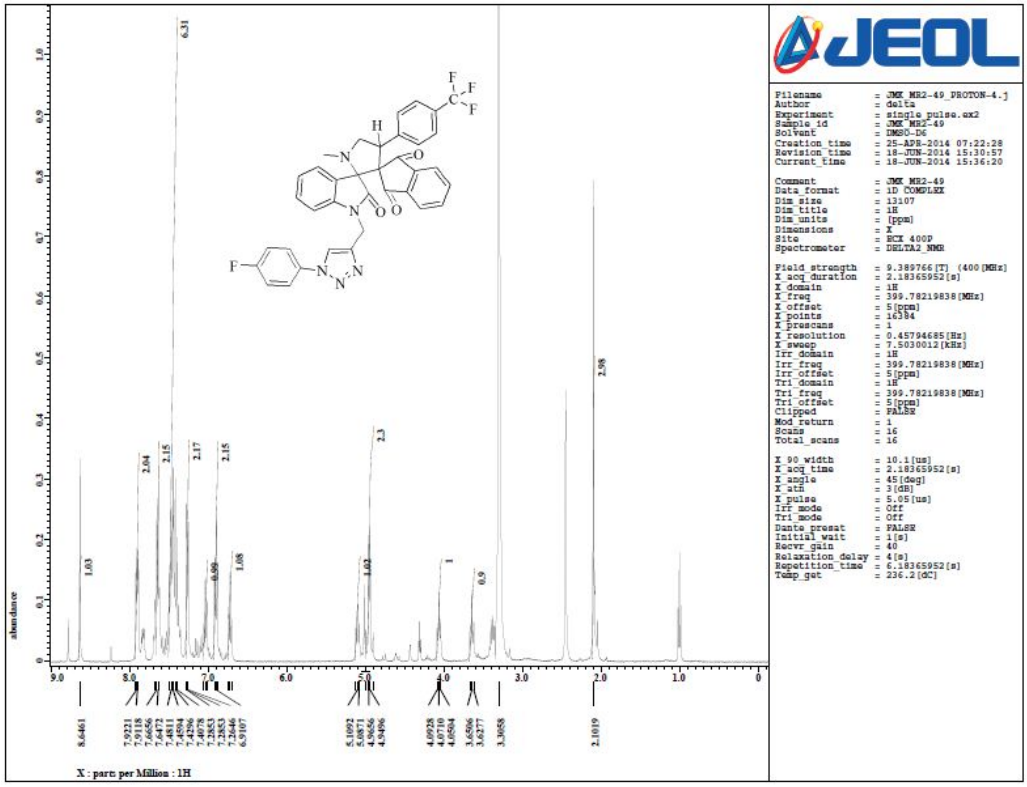


Figure 41. ^{13}C NMR spectrum of compound **6n** (100 MHz, $CDCl_3$).

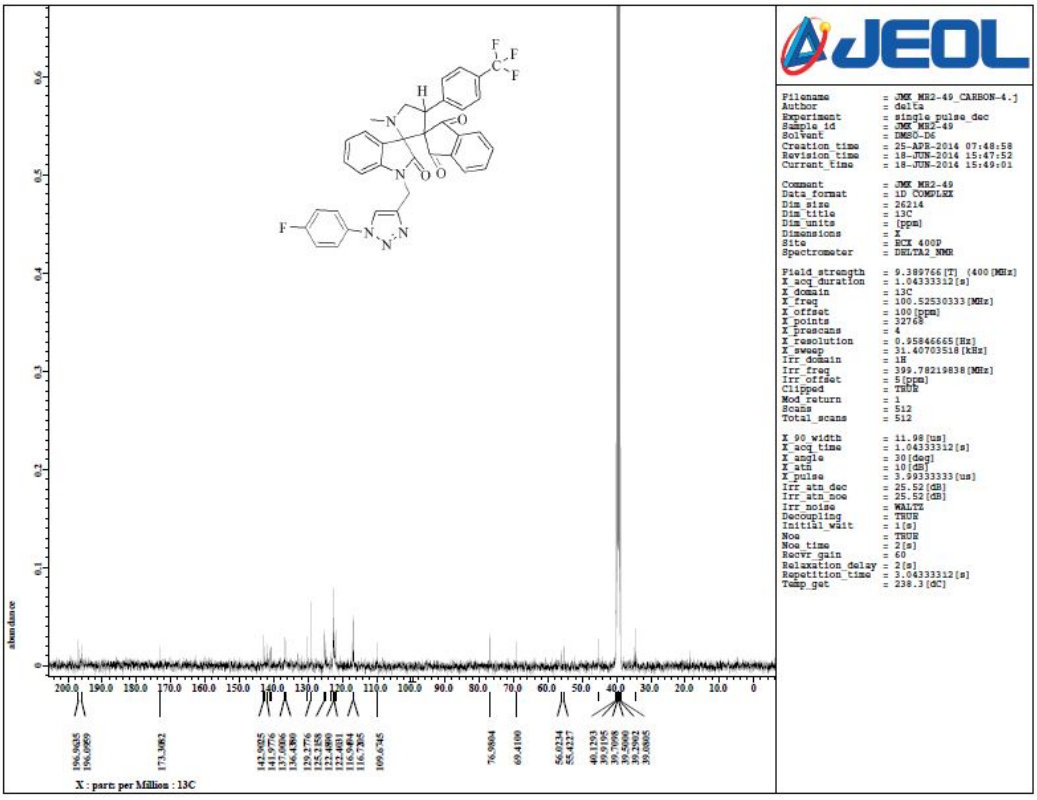
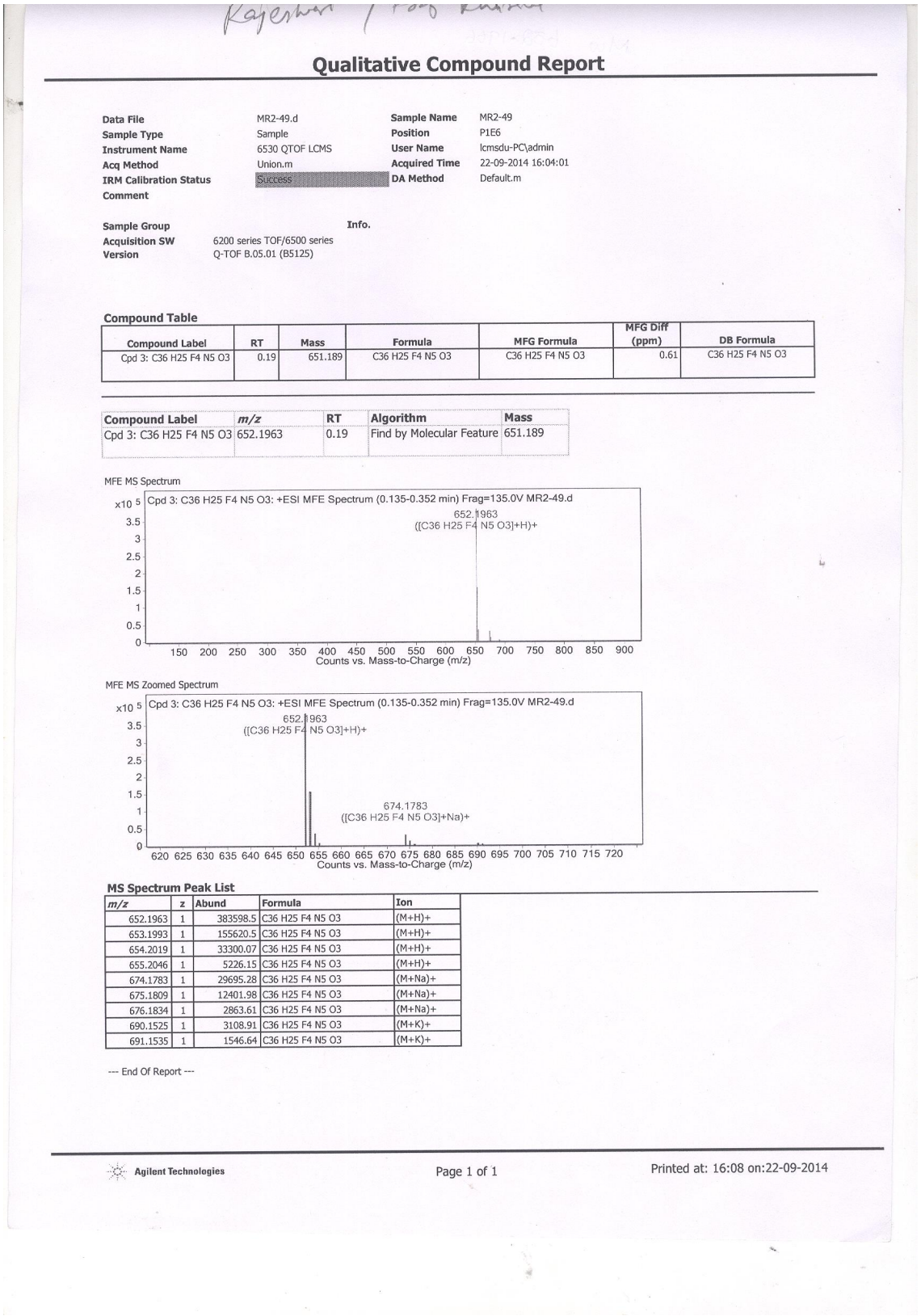


Figure 42. Mass spectrum of compound **6n.**



Qualitative Compound Report

Data File	MR2-49.d	**Sample Name**	MR2-49
Sample Type	Sample	**Position**	P1E6
Instrument Name	6530 QTOF LCMS	**User Name**	lcmsdu-PC\admin
Acq Method	Union.m	**Acquired Time**	22-09-2014 16:04:01
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 3: C36 H25 F4 N5 O3	0.19	651.189	C36 H25 F4 N5 O3	C36 H25 F4 N5 O3	0.61	C36 H25 F4 N5 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 3: C36 H25 F4 N5 O3	652.1963	0.19	Find by Molecular Feature	651.189

MFE MS Spectrum

MFE MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
652.1963	1	383598.5	C36 H25 F4 N5 O3	(M+H)+
653.1993	1	155620.5	C36 H25 F4 N5 O3	(M+H)+
654.2019	1	33300.07	C36 H25 F4 N5 O3	(M+H)+
655.2046	1	5226.15	C36 H25 F4 N5 O3	(M+H)+
674.1783	1	29695.28	C36 H25 F4 N5 O3	(M+Na)+
675.1809	1	12401.98	C36 H25 F4 N5 O3	(M+Na)+
676.1834	1	2863.61	C36 H25 F4 N5 O3	(M+Na)+
690.1525	1	3108.91	C36 H25 F4 N5 O3	(M+K)+
691.1535	1	1546.64	C36 H25 F4 N5 O3	(M+K)+

--- End Of Report ---

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Figure 43. ^{1}H NMR spectrum of compound **6o** (400 MHz, $CDCl_3$).

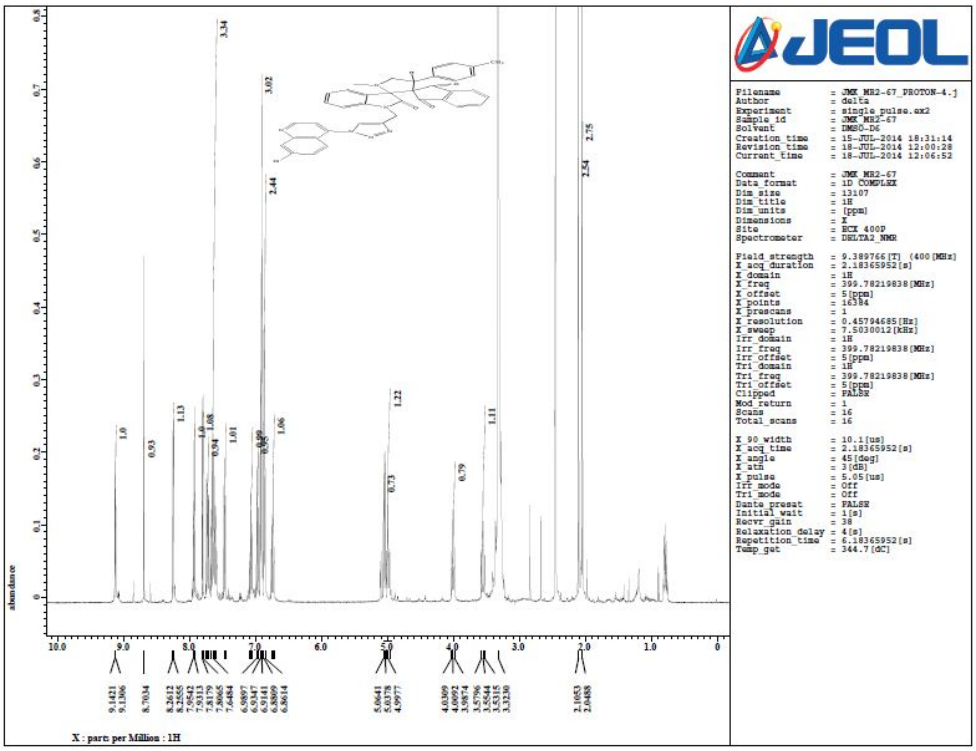


Figure 44. ^{13}C NMR spectrum of compound **6o** (100 MHz, $CDCl_3$).

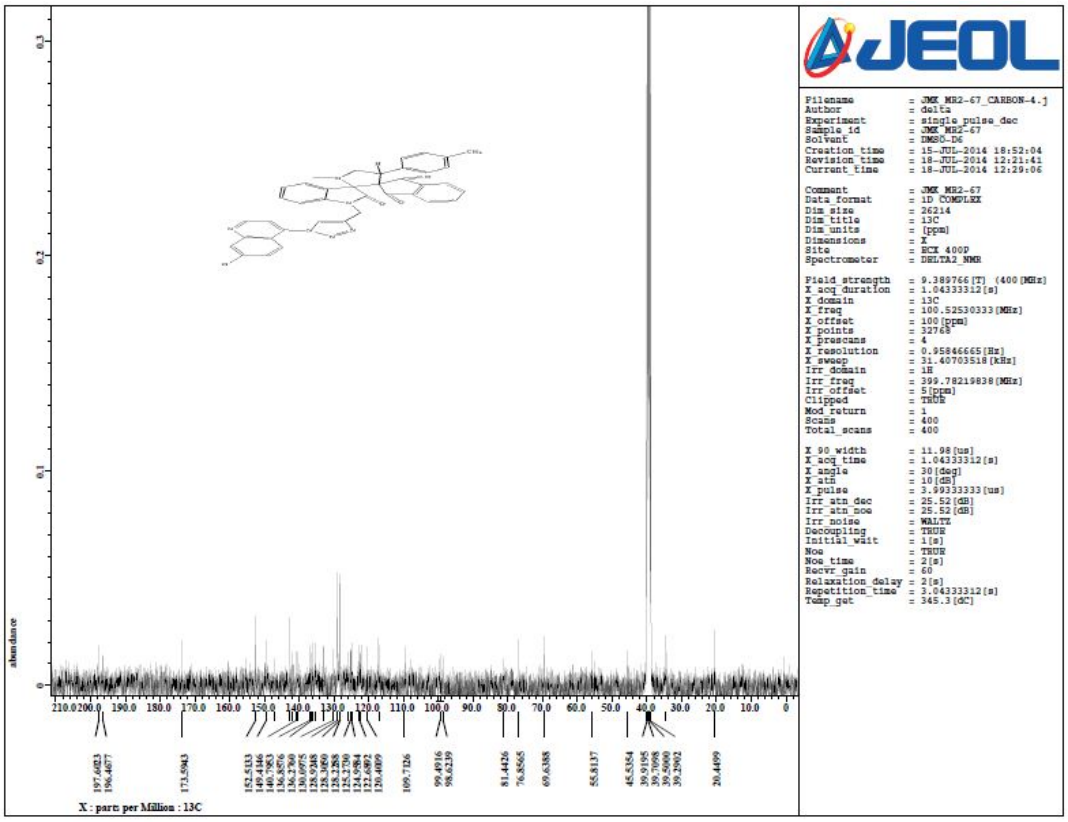


Figure 45. Mass spectrum of compound **6o.**

Qualitative Compound Report

Data File	MR2-61.d	**Sample Name**	MR2-61
Sample Type	Sample	**Position**	P1B4
Instrument Name	6530 QTOF LCMS	**User Name**	lcmsdu-PC\admin
Acq Method	Union.m	**Acquired Time**	10-10-2014 12:40:53
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

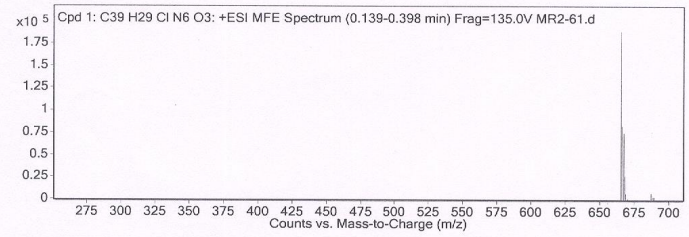
Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

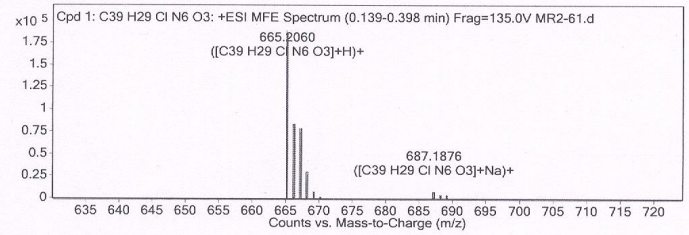
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C39 H29 Cl N6 O3	0.195	664.1987	C39 H29 Cl N6 O3	C39 H29 Cl N6 O3	0.35	C39 H29 Cl N6 O3

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C39 H29 Cl N6 O3	665.206	0.195	Find by Molecular Feature	664.1987

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
665.206	1	188601.8	C39 H29 Cl N6 O3	(M+H)+
666.2091	1	82161.49	C39 H29 Cl N6 O3	(M+H)+
667.2056	1	74877.61	C39 H29 Cl N6 O3	(M+H)+
668.2065	1	27574.62	C39 H29 Cl N6 O3	(M+H)+
669.2094	1	6519.29	C39 H29 Cl N6 O3	(M+H)+
670.2112	1	499.81	C39 H29 Cl N6 O3	(M+H)+
687.1876	1	6652.68	C39 H29 Cl N6 O3	(M+Na)+
688.1909	1	3195.84	C39 H29 Cl N6 O3	(M+Na)+
689.1882	1	2824.59	C39 H29 Cl N6 O3	(M+Na)+

--- End Of Report ---

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Printed at: 12:42 on:10-10-2014

Figure 46. ^{1}H NMR spectrum of compound **6p** (400 MHz, $CDCl_3$).

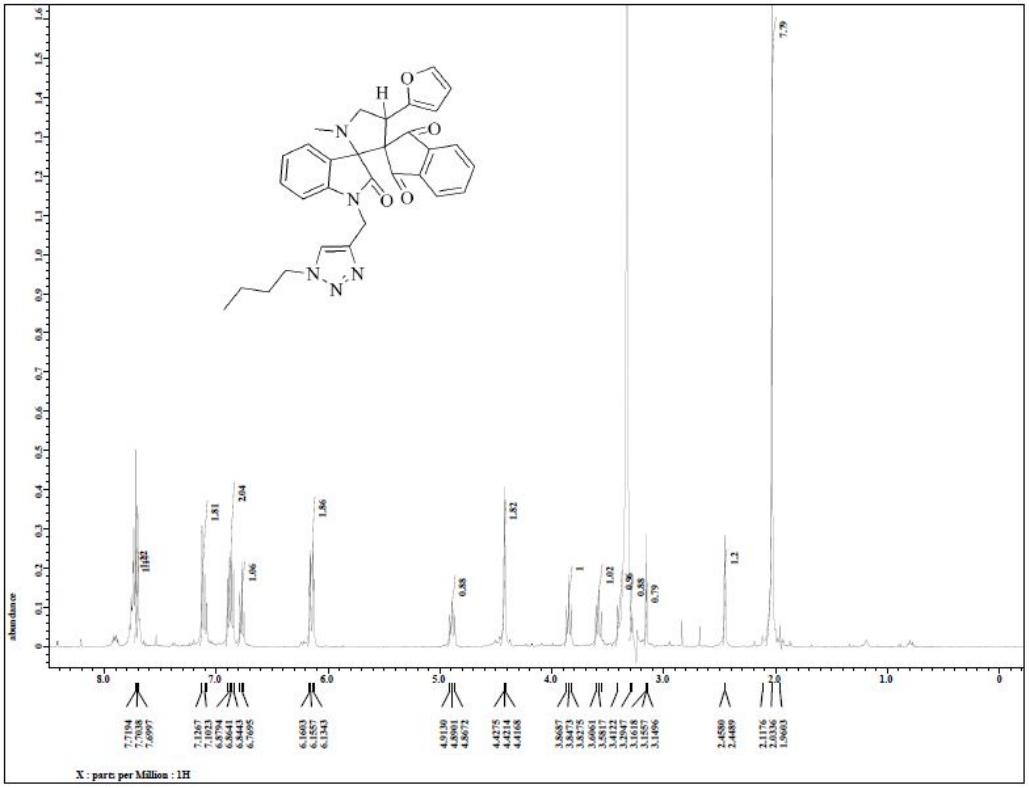


Figure 47. ^{13}C NMR spectrum of compound **6p** (100 MHz, $CDCl_3$).

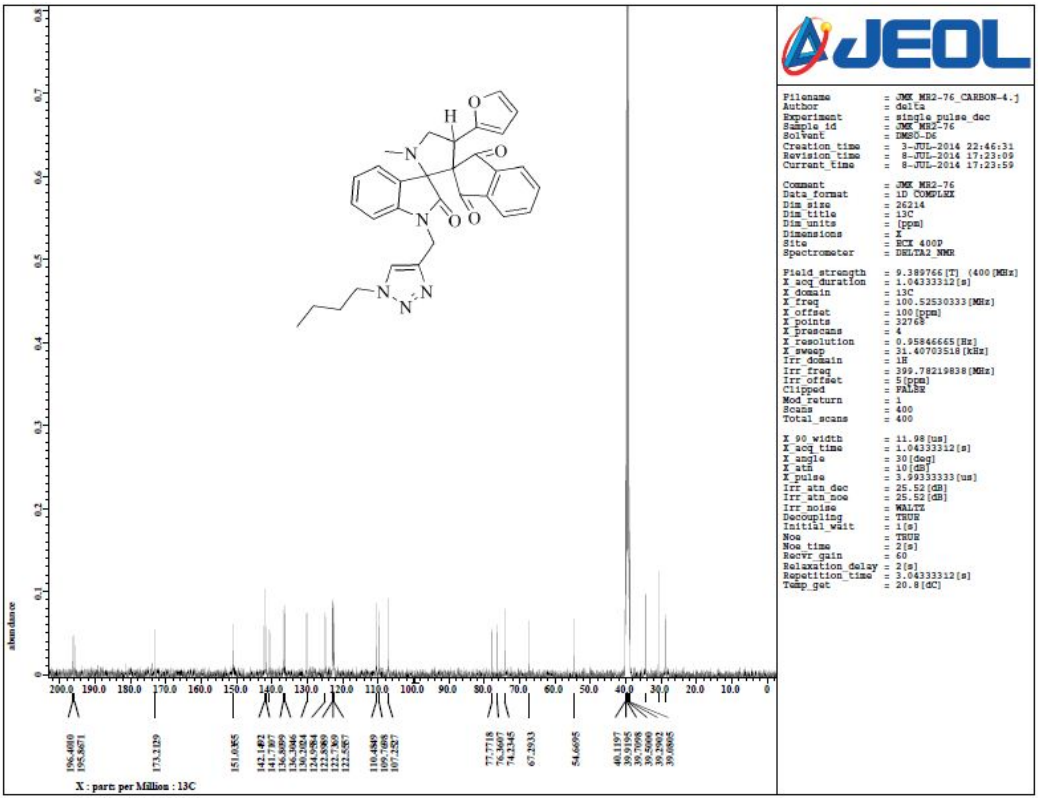
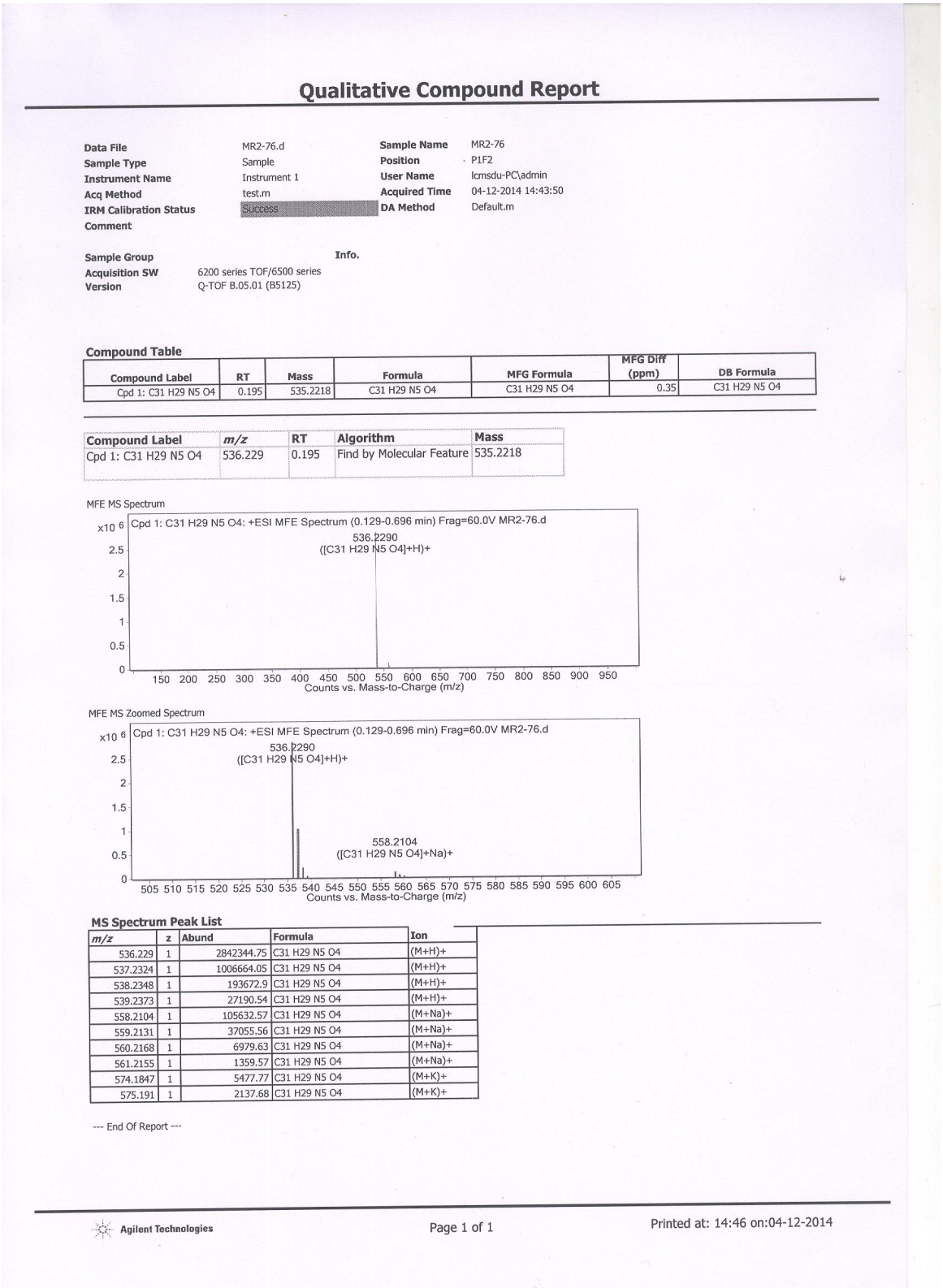


Figure 48. Mass spectrum of compound **6p.**



Qualitative Compound Report

Data File	MR2-76.d	**Sample Name**	MR2-76
Sample Type	Sample	**Position**	P1F2
Instrument Name	Instrument 1	**User Name**	lcmsdu-PC\admin
Acq Method	test.m	**Acquired Time**	04-12-2014 14:43:50
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Info.

Sample Group	
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C31 H29 N5 O4	0.195	535.2218	C31 H29 N5 O4	C31 H29 N5 O4	0.35	C31 H29 N5 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C31 H29 N5 O4	536.229	0.195	Find by Molecular Feature	535.2218

MFE MS Spectrum

MFE MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
536.229	1	2842344.75	C31 H29 N5 O4	(M+H)+
537.2324	1	1006664.05	C31 H29 N5 O4	(M+H)+
538.2348	1	193672.9	C31 H29 N5 O4	(M+H)+
539.2373	1	27190.54	C31 H29 N5 O4	(M+H)+
558.2104	1	105632.57	C31 H29 N5 O4	(M+Na)+
559.2131	1	37055.56	C31 H29 N5 O4	(M+Na)+
560.2168	1	6979.63	C31 H29 N5 O4	(M+Na)+
561.2155	1	1359.57	C31 H29 N5 O4	(M+Na)+
574.1847	1	5477.77	C31 H29 N5 O4	(M+K)+
575.191	1	2137.68	C31 H29 N5 O4	(M+K)+

--- End Of Report ---

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Figure 49. ^{1}H NMR spectrum of compound **6q** (400 MHz, $CDCl_3$).

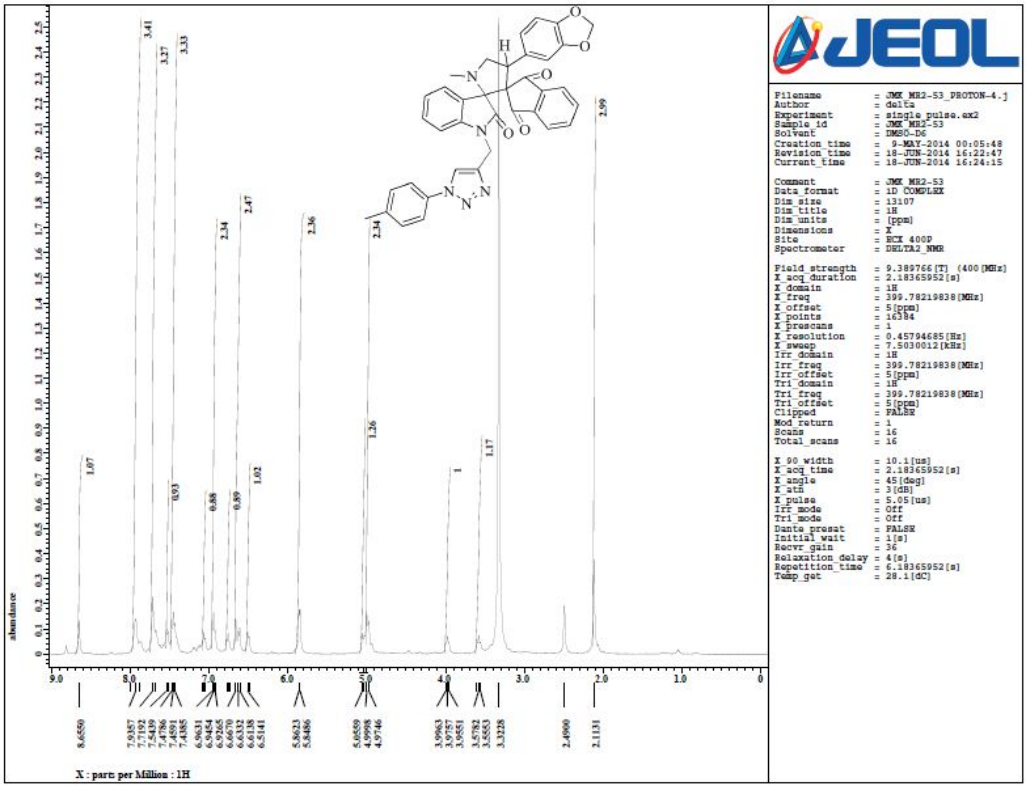


Figure 50. ^{13}C NMR spectrum of compound **6q** (100 MHz, $CDCl_3$).

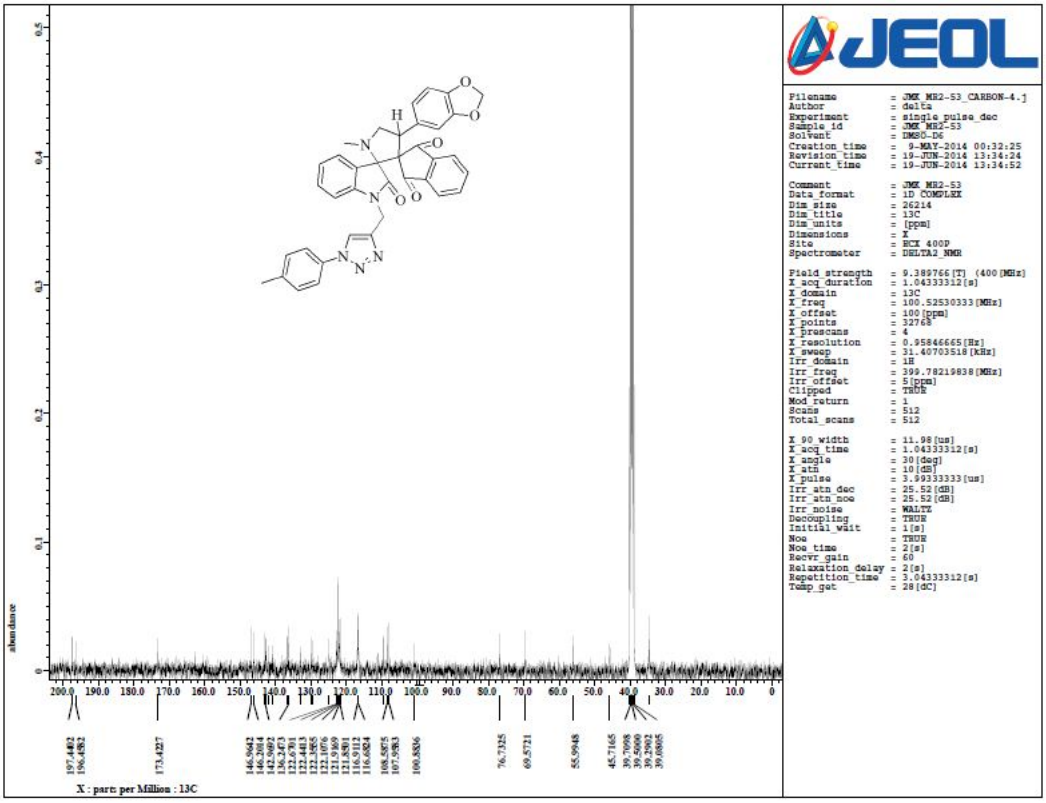


Figure 51. Mass spectrum of compound **6q.**

Qualitative Compound Report

Data File	MR253.d	**Sample Name**	MR253
Sample Type	Sample	**Position**	P1D4
Instrument Name	6530 QTOF LCMS	**User Name**	lcmsdu-PC\admin
Acq Method	Union.m	**Acquired Time**	29-09-2014 15:33:13
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**

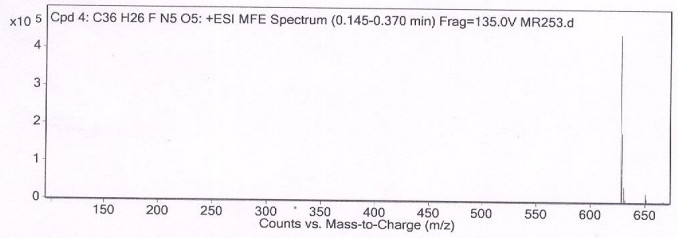
Acquisition SW Version 6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

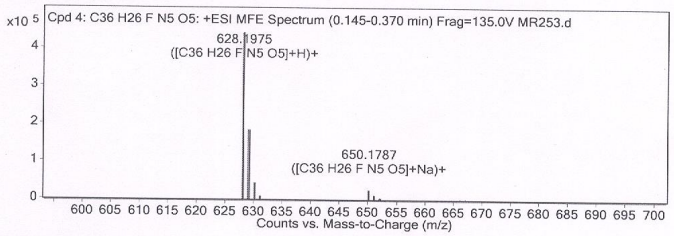
Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 4: C36 H26 F N5 O5	0.195	627.1901	C36 H26 F N5 O5	C36 H26 F N5 O5	2.77	C36 H26 F N5 O5

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 4: C36 H26 F N5 O5	628.1975	0.195	Find by Molecular Feature	627.1901

MFE MS Spectrum



MFE MS Zoomed Spectrum



MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
628.1975	1	441321.63	C36 H26 F N5 O5	(M+H)+
629.2002	1	181113.28	C36 H26 F N5 O5	(M+H)+
630.2031	1	40516.81	C36 H26 F N5 O5	(M+H)+
631.2056	1	6920.64	C36 H26 F N5 O5	(M+H)+
632.2038	1	434.69	C36 H26 F N5 O5	(M+H)+
650.1787	1	23264.71	C36 H26 F N5 O5	(M+Na)+
651.1825	1	9438.3	C36 H26 F N5 O5	(M+Na)+
652.1861	1	2355.08	C36 H26 F N5 O5	(M+Na)+
666.1534	1	2142.88		(M+K)+
667.1596	1	1206.02		(M+K)+

--- End Of Report ---

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Figure 52. ^{1}H NMR spectrum of compound **6r** (400 MHz, $CDCl_3$).

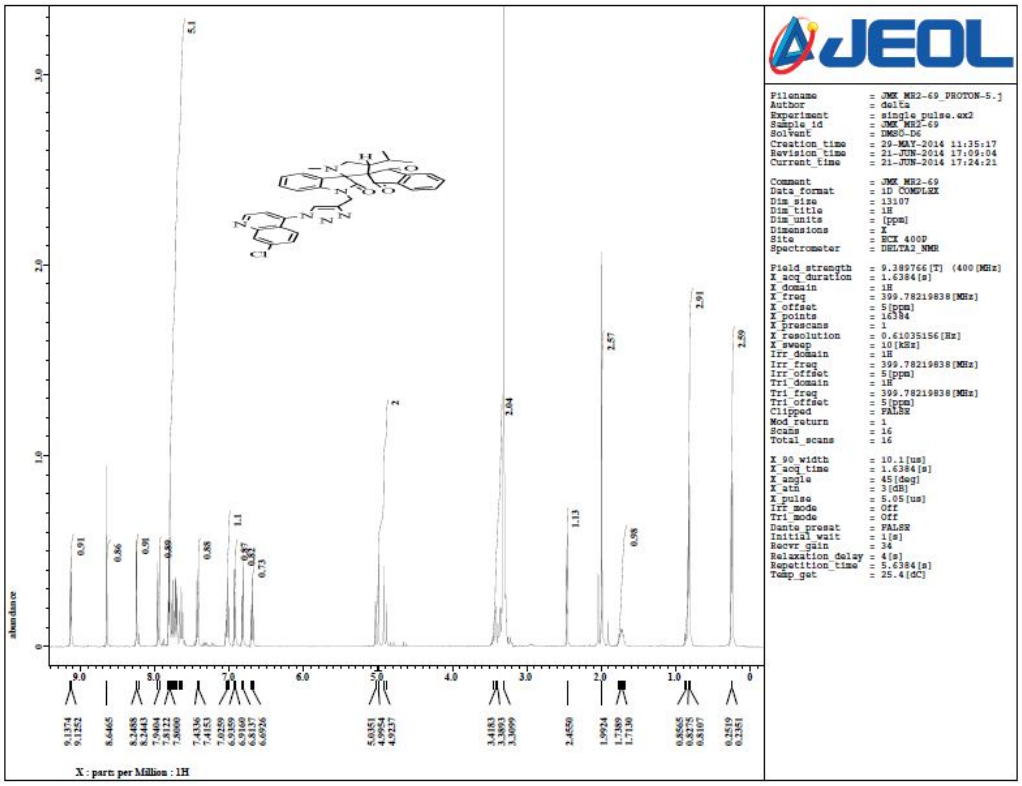


Figure 53. ^{13}C NMR spectrum of compound **6r** (100 MHz, $CDCl_3$).

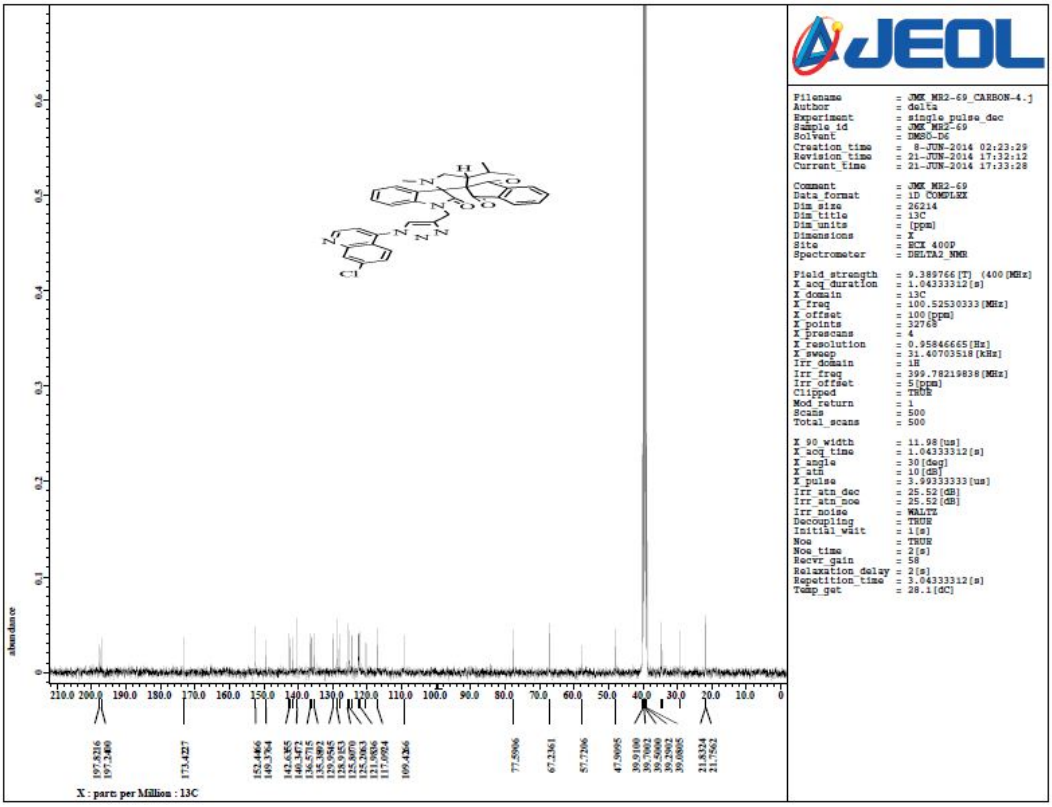
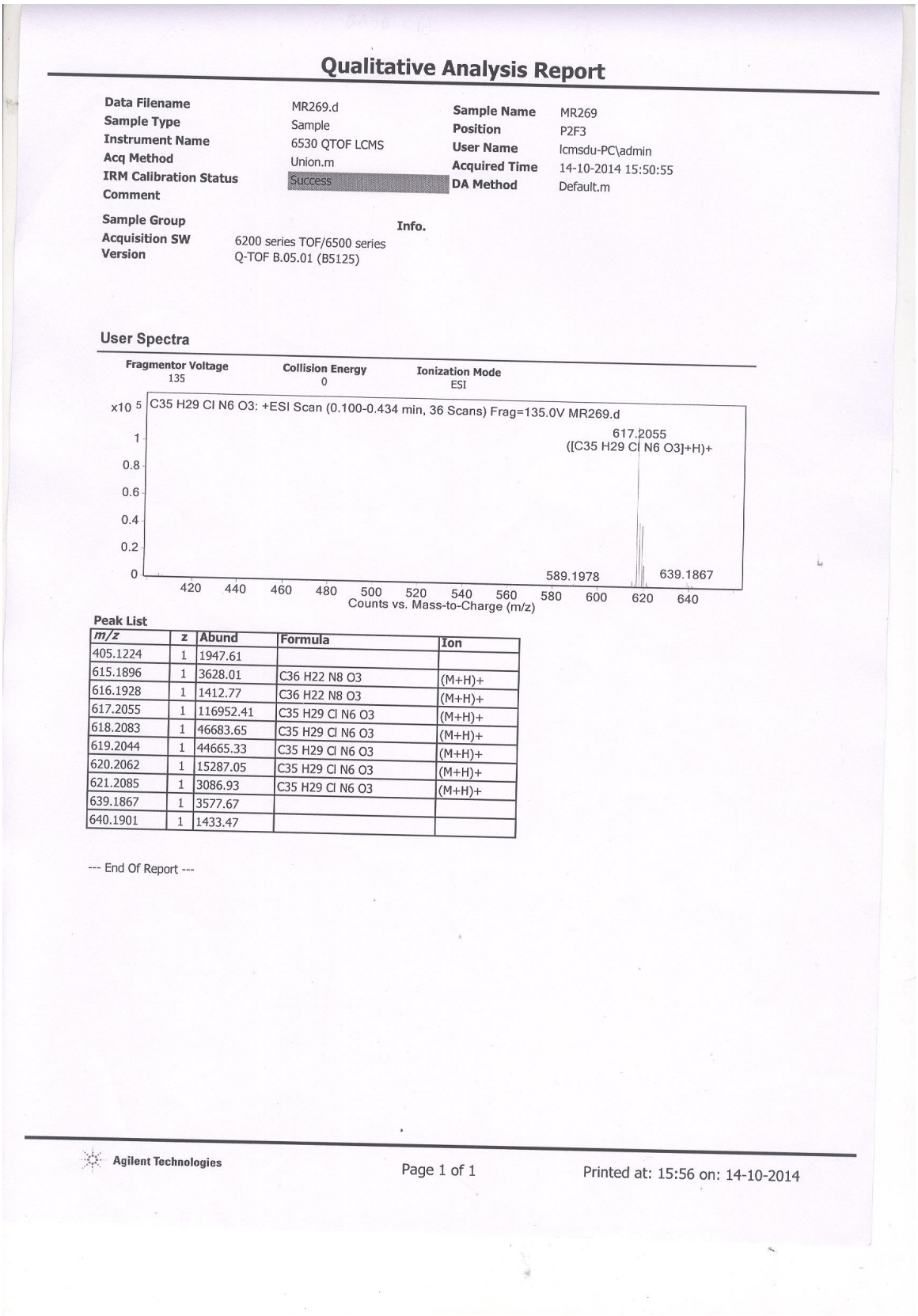


Figure 54. Mass spectrum of compound **6r.**



Qualitative Analysis Report

Data Filename	MR269.d	**Sample Name**	MR269
Sample Type	Sample	**Position**	P2F3
Instrument Name	6530 QTOF LCMS	**User Name**	lcmsdu-PC\admin
Acq Method	Union.m	**Acquired Time**	14-10-2014 15:50:55
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group **Info.**

Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

User Spectra

Fragmentor Voltage	Collision Energy	Ionization Mode
135	0	ESI

Peak List

m/z	z	Abund	Formula	Ion
405.1224	1	1947.61		
615.1896	1	3628.01	C36 H22 N8 O3	(M+H)+
616.1928	1	1412.77	C36 H22 N8 O3	(M+H)+
617.2055	1	116952.41	C35 H29 Cl N6 O3	(M+H)+
618.2083	1	46683.65	C35 H29 Cl N6 O3	(M+H)+
619.2044	1	44665.33	C35 H29 Cl N6 O3	(M+H)+
620.2062	1	15287.05	C35 H29 Cl N6 O3	(M+H)+
621.2085	1	3086.93	C35 H29 Cl N6 O3	(M+H)+
639.1867	1	3577.67		
640.1901	1	1433.47		

--- End Of Report ---

Figure 55. ^{1}H NMR spectrum of compound **6s** (400 MHz, $CDCl_3$).

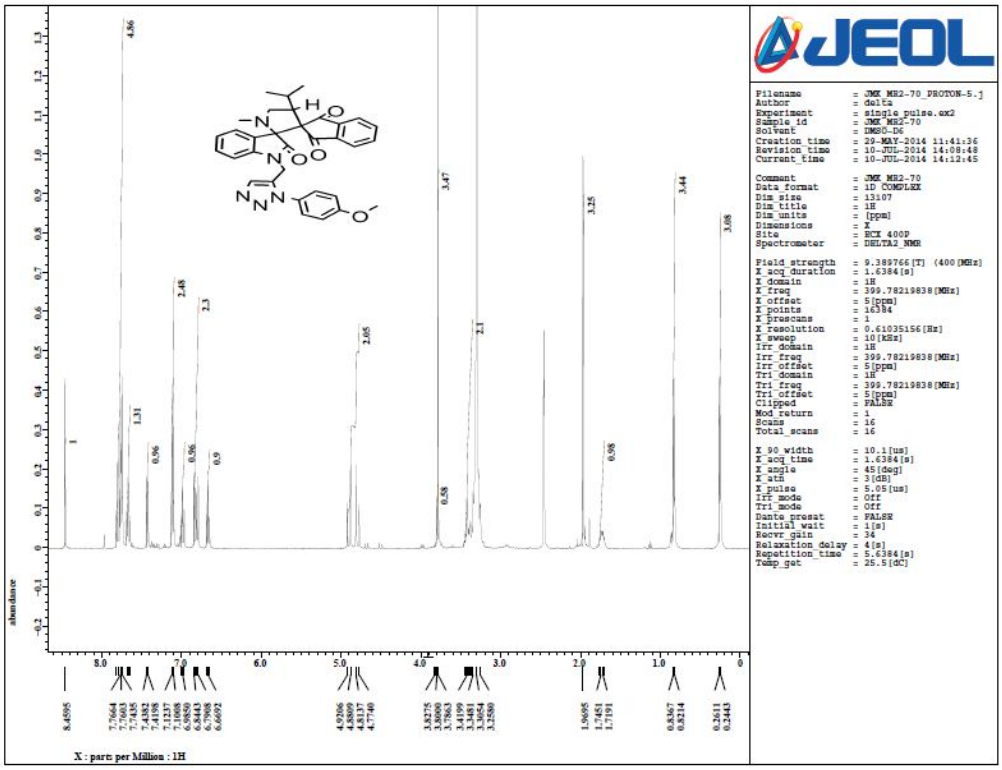


Figure 56. ^{13}C NMR spectrum of compound **6s** (100 MHz, $CDCl_3$).

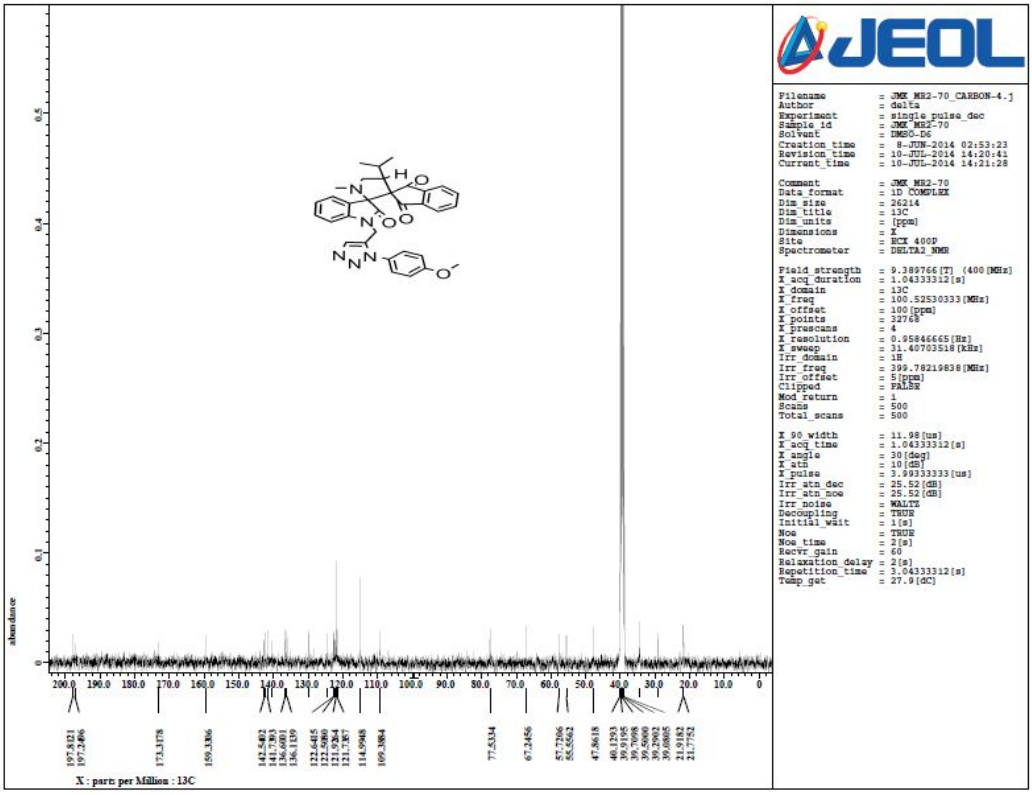
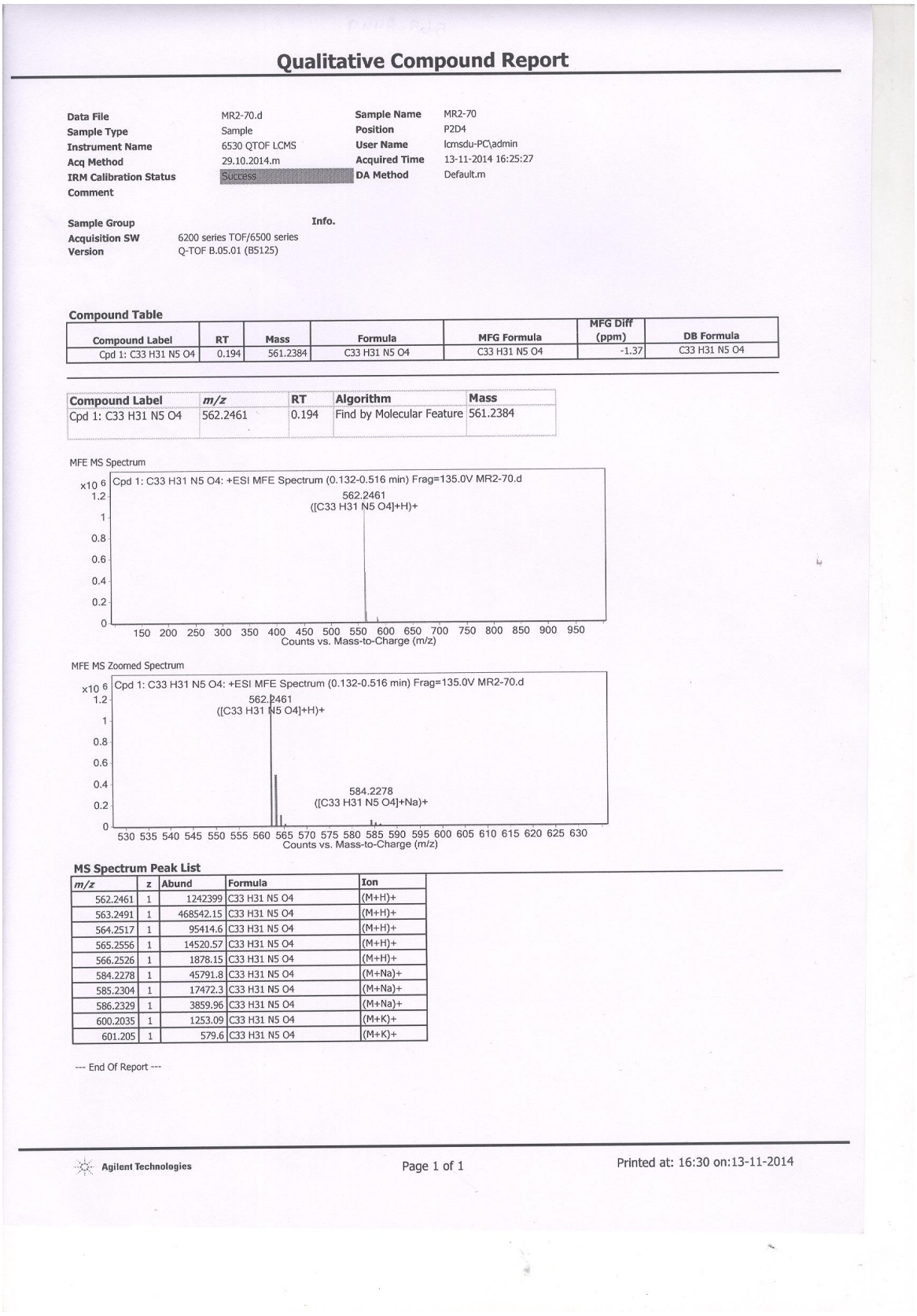


Figure 57. Mass spectrum of compound **6s.**



Qualitative Compound Report

Data File	MR2-70.d	**Sample Name**	MR2-70
Sample Type	Sample	**Position**	P2D4
Instrument Name	6530 QTOF LCMS	**User Name**	lcmsdu-PC\admin
Acq Method	29.10.2014.m	**Acquired Time**	13-11-2014 16:25:27
IRM Calibration Status	Success	**DA Method**	Default.m
Comment			

Sample Group	**Info.**
Acquisition SW Version	6200 series TOF/6500 series Q-TOF B.05.01 (B5125)

Compound Table

Compound Label	RT	Mass	Formula	MFG Formula	MFG Diff (ppm)	DB Formula
Cpd 1: C33 H31 N5 O4	0.194	561.2384	C33 H31 N5 O4	C33 H31 N5 O4	-1.37	C33 H31 N5 O4

Compound Label	*m/z*	RT	Algorithm	Mass
Cpd 1: C33 H31 N5 O4	562.2461	0.194	Find by Molecular Feature	561.2384

MFE MS Spectrum

MFE MS Zoomed Spectrum

MS Spectrum Peak List

m/z	z	Abund	Formula	Ion
562.2461	1	1242399	C33 H31 N5 O4	(M+H)+
563.2491	1	468542.15	C33 H31 N5 O4	(M+H)+
564.2517	1	95414.6	C33 H31 N5 O4	(M+H)+
565.2556	1	14520.57	C33 H31 N5 O4	(M+H)+
566.2526	1	1878.15	C33 H31 N5 O4	(M+H)+
584.2278	1	45791.8	C33 H31 N5 O4	(M+Na)+
585.2304	1	17472.3	C33 H31 N5 O4	(M+Na)+
586.2329	1	3859.96	C33 H31 N5 O4	(M+Na)+
600.2035	1	1253.09	C33 H31 N5 O4	(M+K)+
601.205	1	579.6	C33 H31 N5 O4	(M+K)+

--- End Of Report ---

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