Electronic Supplementary Information

Design, synthesis, antibacterial and insecticidal activities of novel *N*-phenylpyrazole fraxinellone hybrid compounds

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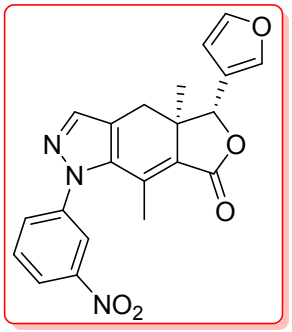
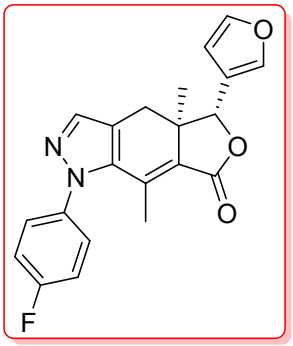
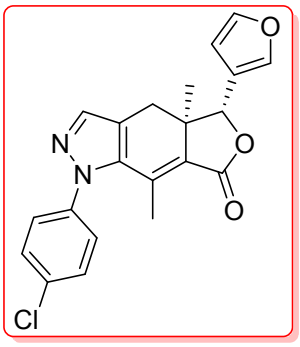
Spectra data for compounds 4e-t.



Data for ***4e***: Yellow solid, yield: 84%, purity: 98%, mp: 201-203 ^{o}C; $[\alpha]^{20}_{D}$ = -29^{o} (*c* 3.8 mg/mL, $CHCl_3$); IR cm^{-1} (KBr): 3089, 2926, 1740, 1630, 1531, 1350, 1217, 1162, 1025; ^{1}H NMR (400 MHz, $CDCl_3$) *δ*: 8.33 (d, *J* = 9.2 Hz, 2H, -Ph), 7.68-7.76 (m, 2H, -Ph), 7.62 (s, 1H, -C*H*=N-), 7.54 (s, 1H, H-2′), 7.49 (t, *J* = 1.6 Hz, 1H, H-5′), 6.40 (d, *J* = 0.8 Hz, 1H, H-4′), 5.21 (s, 1H, H-8), 2.83-2.91 (m, 2H, H-6), 2.10 (s, 3H, H-10), 0.95 (s, 3H, H-11); ^{13}C NMR (100 MHz, $CDCl_3$) *δ*: 168.5, 148.5, 143.8, 141.3, 140.0, 139.6, 139.2, 133.9, 131.7, 130.5, 130.1, 123.5, 121.0, 119.9, 108.5, 82.6, 44.9, 30.5, 18.5, 14.7. HRMS (ESI): Calcd for $C_{21}H_{18}O_5N_3$ ($[M+H]^+$), 392.1241; Found, 392.1239.

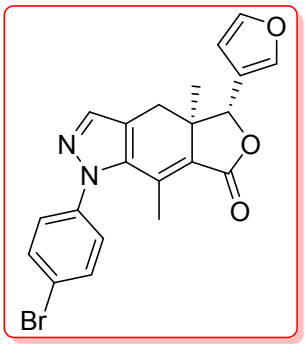


Data for ***4f***: Pale yellow solid, yield: 65%, purity: 96%, mp: 224-225 ^{o}C; $[\alpha]^{20}_{D}$ = -1^{o} (*c* 3.4 mg/mL, $CHCl_3$); IR cm^{-1} (KBr): 3134, 2974, 2929, 1740, 1513, 1160, 1033; ^{1}H NMR (400 MHz, $CDCl_3$) *δ*: 7.55 (s, 1H, -C*H*=N-), 7.52 (s, 1H, H-2′), 7.48 (t, *J* = 1.6 Hz, 1H, H-5′), 7.37-7.40 (m, 1H, -Ph), 7.16-7.20 (m, 2H, -Ph), 6.39 (d, *J* = 0.8 Hz, 1H, H-4′), 5.19 (s, 1H, H-8), 2.80-2.88 (m, 2H, H-6), 2.05 (s, 3H, H-10), 0.90 (s, 3H, H-11); HRMS (ESI): Calcd for $C_{21}H_{18}O_3N_2F$ ($[M+H]^+$), 365.1296; Found, 365.1295.

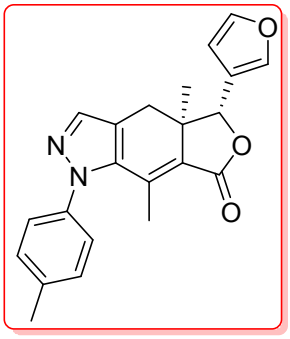


Data for ***4g****:* Yellow solid, yield: 66%, purity: 99%, mp: 197-199 ^{o}C; $[\alpha]^{20}_{D}$ = 17^{o} (*c* 3.8 mg/mL, $CHCl_3$); IR cm^{-1} (KBr): 2967,

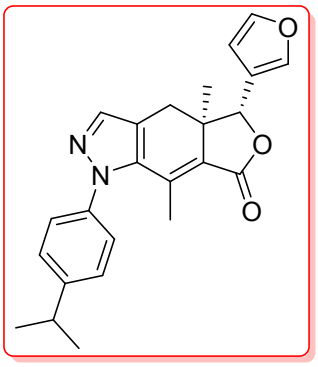
2925, 2893, 1737, 1627, 1497, 1160, 1032; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.56 (s, 1H, -C*H*=N-), 7.52 (s, 1H, H-2′), 7.48 (t, *J* = 1.6 Hz, 1H, H-5′), 7.46 (d, *J* = 9.6 Hz, 2H, -Ph), 7.34 (d, *J* = 8.8 Hz, 2H, -Ph), 6.39 (d, *J* = 1.2 Hz, 1H, H-4′), 5.19 (s, 1H, H-8), 2.79-2.88 (m, 2H, H-6), 2.08 (s, 3H, H-10), 0.91 (s, 3H, H-11); HRMS (ESI): Calcd for $C_{21}H_{18}O_3N_2Cl$ ([M+H]$^+$), 381.1000; Found, 381.0999, $C_{21}H_{18}O_3N_2{}^{37}Cl$ ([M+H]$^+$), 383.0971, Found, 381.0970.



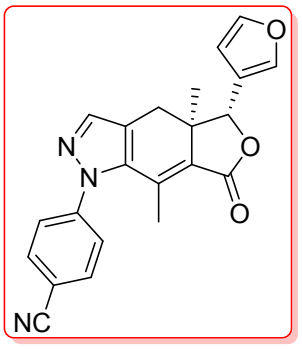
Data for ***4h***: Brown solid, yield: 84%, purity: 96%, mp: 188-190 ^{o}C; $[\alpha]^{20}_D$ = 16^o (*c* 5.0 mg/mL, $CHCl_3$); IR cm^{-1} (KBr): 3070, 2967, 2923, 2891, 1739, 1626, 1492, 1217, 1160, 1033; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.61 (d, *J* = 8.8 Hz, 2H, -Ph), 7.56 (s, 1H, -C*H*=N-), 7.52 (s, 1H, H-2′), 7.48 (t, *J* = 1.6 Hz, 1H, H-5′), 7.28 (d, *J* = 8.4 Hz, 2H, -Ph), 6.39 (d, *J* = 0.8 Hz, 1H, H-4′), 5.19 (s, 1H, H-8), 2.79-2.88 (m, 2H, H-6), 2.08 (s, 3H, H-10), 0.91 (s, 3H, H-11); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 168.7, 143.8, 140.0, 139.4, 139.3, 138.4, 134.9, 132.4, 129.8, 127.5, 122.9, 119.9, 119.1, 108.5, 82.6, 44.9, 30.5, 18.5, 14.5. HRMS (ESI): Calcd for $C_{21}H_{18}O_3N_2Br$ ([M+H]$^+$), 425.0495; Found, 425.0494, $C_{21}H_{18}O_3N_2{}^{81}Br$ ([M+H]$^+$), 427.0475; Found, 427.0474.



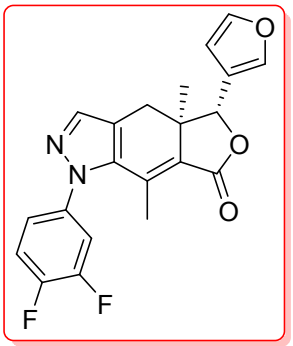
Data for ***4i***: White solid, yield: 76%, purity: 99%, mp: 232-234 ^{o}C; $[\alpha]^{20}_D$ = -5^o (*c* 3.1 mg/mL, $CHCl_3$); IR cm^{-1} (KBr): 3134, 2974, 2929, 1740, 1629, 1513, 1211, 1160, 1033; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.54 (s, 1H, -C*H*=N-), 7.52 (s, 1H, H-2′), 7.48 (d, *J* = 2.0 Hz, 1H, H-5′), 7.26-7.27 (m, 4H, -Ph), 6.39 (d, *J* = 1.2, 1H, H-4′), 5.18 (s, 1H, H-8), 2.79-2.88 (m, 2H, H-6), 2.43 (s, 3H, -C*H*$_3$), 2.05 (s, 3H, H-10), 0.90 (s, 3H, H-11).



Data for ***4j***: Pale yellow solid, yield: 73%, purity: 99%, mp: 206-208 °C; $[\alpha]^{20}_{D}$ = 14° (*c* 3.4 mg/mL, $CHCl_3$); IR cm^{-1} (KBr): 3124, 2959, 2927, 1745, 1629, 1513, 1161, 1024; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.53 (s, 1H, -C*H*=N-), 7.52 (s, 1H, H-2'), 7.48 (t, *J* = 1.6 Hz, 1H, H-5'), 7.28-7.33 (m, 4H, -Ph), 6.39 (d, *J* = 0.8 Hz, 1H, H-4'), 5.18 (d, *J* = 2.8 Hz, 1H, H-8), 2.95-3.02 (m, 1H, -C*H*$(CH_3)_2$), 2.79-2.88 (m, 2H, H-6), 2.05 (s, 3H, H-10), 1.30 (s, 3H, -CH_3), 1.28 (s, 3H, -CH_3), 0.91 (s, 3H, H-11); HRMS (ESI): Calcd for $C_{24}H_{25}O_3N_2$ ($[M+H]^+$), 389.1860; Found, 389.1858.

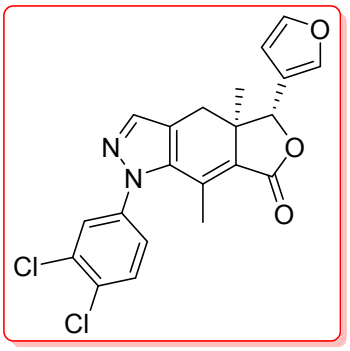


Data for ***4k***: Yellow solid, yield: 86%, purity: 99%, mp: 187-189 °C; $[\alpha]^{20}_{D}$ = 22° (*c* 2.3 mg/mL, $CHCl_3$); IR cm^{-1} (KBr): 3089, 2956, 2922, 2226, 1739, 1632, 1605, 1510, 1215, 1160, 1033; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.79 (d, *J* = 8.4 Hz, 2H, -Ph), 7.62 (s, 1H, -C*H*=N-), 7.54 (d, *J* = 8.4 Hz, 2H, -Ph), 7.53 (s, 1H, H-2'), 7.49 (t, *J* = 1.6 Hz, 1H, H-5'), 6.39 (d, *J* = 0.8 Hz, 1H, H-4'), 5.20 (s, 1H, H-8), 2.81-2.89 (m, 2H, H-6), 2.11 (s, 3H, H-10), 0.92 (s, 3H, H-11); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 168.5, 143.8, 143.6, 140.0, 139.6, 139.4, 134.1, 133.2, 130.5, 126.3, 120.2, 119.8, 117.8, 112.6, 108.4, 82.6, 44.9, 30.5, 18.5, 14.9. HRMS (ESI): Calcd for $C_{22}H_{18}O_3N_3$ ($[M+H]^+$), 372.1343; Found, 372.1342.

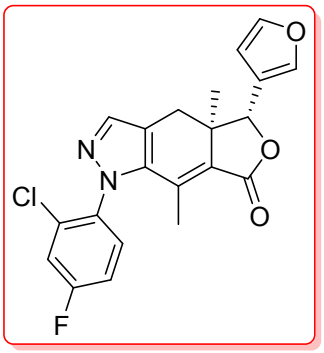


Data for ***4l***: White solid, yield: 87%, purity: 99%, mp: 198-200 °C; $[\alpha]^{20}_{D}$ = -4° (*c* 3.8 mg/mL, $CHCl_3$); IR cm^{-1} (KBr): 3134, 2968,

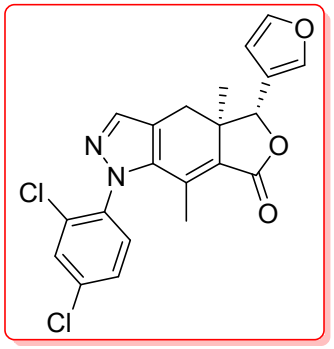
2931, 1741, 1633, 1520, 1158, 1033; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.55 (s, 1H, -C*H*=N-), 7.52 (s, 1H, H-2′), 7.48 (t, *J* = 1.6 Hz, 1H, H-5′), 7.27-7.34 (m, 2H, -Ph), 7.13-7.16 (m, 1H, -Ph), 6.39 (d, *J* = 1.2 Hz, 1H, H-4′), 5.19 (s, 1H, H-8), 2.79-2.88 (m, 2H, H-6), 2.10 (s, 3H, H-10), 0.91 (s, 3H, H-11); HRMS (ESI): Calcd for $C_{21}H_{17}O_3N_2F_2$ ([M+H]$^+$), 383.1202; Found, 383.1200.



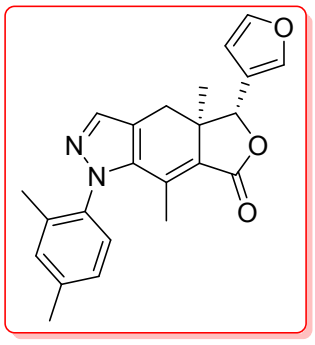
Data for ***4m***: Pale yellow solid, yield: 71%, purity: 99%, mp: 204-206 ^{o}C; $[\alpha]^{20}_D = 3^o$ (*c* 3.0 mg/mL, $CHCl_3$); IR cm^{-1} (KBr): 3071, 2966, 2925, 1746, 1628, 1486, 1216, 1132, 1032; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.55-7.58 (m, 3H, -Ph and -C*H*=N-), 7.52 (s, 1H, H-2′), 7.48 (d, *J* = 1.6 Hz, 1H, H-5′), 7.25-7.27 (m, 1H, -Ph), 6.39 (d, *J* = 1.2 Hz, 1H, H-4′), 5.19 (d, *J* = 2.8 Hz, 1H, H-8), 2.80-2.88 (m, 2H, H-6), 2.12 (s, 3H, H-10), 0.91 (s, 3H, H-11); HRMS (ESI): Calcd for $C_{21}H_{17}O_3N_2Cl_2$ ([M+H]$^+$), 415.0611; Found, 415.0609, $C_{21}H_{17}O_3N_2{}^{37}Cl_2$ ([M+H]$^+$), 419.0552; Found, 419.0552.



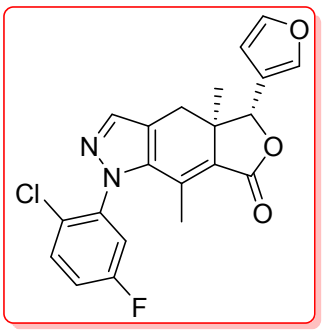
Data for ***4n***: Pale yellow solid, yield: 80%, purity: 98%, mp: 176-178 ^{o}C; $[\alpha]^{20}_D = 10^o$ (*c* 5.8 mg/mL, $CHCl_3$); IR cm^{-1} (KBr):3118, 3063, 2965, 2926, 1737, 1633, 1508, 1169, 1022; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.59-7.63 (m, 2H, -Ph and -C*H*=N-), 7.52 (s, 1H, H-2′), 7.48 (t, *J* = 1.6 Hz, 1H, H-5′), 7.08-7.36 (m, 2H, -Ph), 6.38 (s, 1H, H-4′), 5.19 (s, 1H, H-8), 2.79-2.94 (m, 2H, H-6), 2.00 (s, 3H, H-10), 0.89 (s, 3H, H-11); HRMS (ESI): Calcd for $C_{21}H_{17}O_3N_2ClF$ ([M+H]$^+$), 399.0906; Found, 399.0905, $C_{21}H_{17}O_3N_2{}^{37}ClF$ ([M+H]$^+$), 401.0877; Found, 401.0875.



Data for ***4o***: Orange solid, yield: 77%, purity: 97%, mp: 202-204 °C; $[\alpha]^{20}_{D}$ = 23° (*c* 3.8 mg/mL, $CHCl_3$); IR cm^{-1} (KBr): 3143, 2967, 1740, 1633, 1498, 1217, 1160, 1028; ^{1}H NMR (400 MHz, $CDCl_3$) *δ*: 7.56-7.61 (m, 2H, -Ph and -C*H*=N-), 7.53-7.54 (m, 1H, -Ph), 7.52 (s, 1H, H-2'), 7.48 (d, *J* = 1.6 Hz, 1H, H-5'), 6.38 (s, 1H, H-4'), 5.19 (d, *J* = 2.8 Hz, 1H, H-8), 2.79-2.90 (m, 2H, H-6), 2.01 (s, 3H, H-10), 0.89 (s, 3H, H-11); HRMS (ESI): Calcd for $C_{21}H_{17}O_3N_2Cl_2$ ($[M+H]^+$), 415.0611; Found, 415.0609, $C_{21}H_{17}O_3N_2{}^{37}Cl_2$ ($[M+H]^+$), 419.0552; Found, 419.0552.

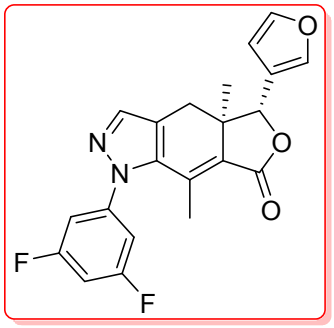


Data for ***4p***: Pale yellow solid, yield: 82%, purity: 99%, mp: 173-175 °C; $[\alpha]^{20}_{D}$ = 40° (*c* 2.3 mg/mL, $CHCl_3$); IR cm^{-1} (KBr): 3117, 2963, 2923, 1741, 1631, 1508, 1216, 1159, 1023; ^{1}H NMR (400 MHz, $CDCl_3$) *δ*: 7.55 (s, 1H, -C*H*=N-), 7.51 (s, 1H, H-2'), 7.47 (t, *J* = 1.6 Hz, 1H, H-5'), 6.96-7.33 (m, 3H, -Ph), 6.39 (s, 1H, H-4'), 5.18 (s, 1H, H-8), 2.78-2.90 (m, 2H, H-6), 2.39 (s, 3H, -CH_3), 1.92 (s, 3H, H-10), 1.83 (s, 3H, -CH_3), 0.89 (s, 3H, H-11); HRMS (ESI): Calcd for $C_{23}H_{23}O_3N_2$ ($[M+H]^+$), 375.1703; Found, 375.1702.

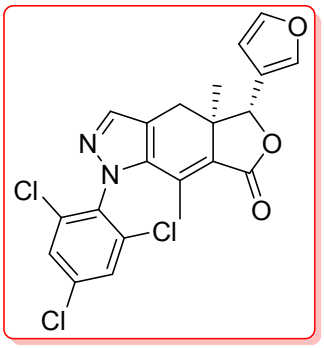


Data for ***4q***: White solid, yield: 76%, purity: 99%, mp: 161-162 °C; $[\alpha]^{20}_{D}$ = 12° (*c* 3.5 mg/mL, $CHCl_3$); IR cm^{-1} (KBr): 2972, 2924, 1753, 1643, 1447, 1218, 1159, 1021; ^{1}H NMR (400 MHz, $CDCl_3$) *δ*: 7.55-7.62 (m, 1H, -Ph and -C*H*=N-), 7.46-7.52 (m, 3H,

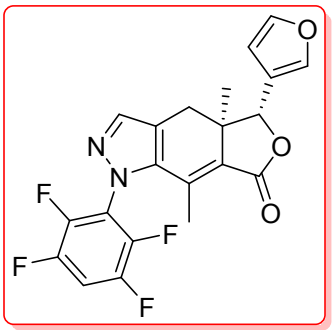
-Ph and H-2', 5'), 7.06-7.41 (m, 2H, -Ph), 6.39 (s, 1H, H-4'), 5.19 (s, 1H, H-8), 2.79-2.94 (m, 2H, H-6), 2.03 (s, 3H, H-10), 0.89 (s, 3H, H-11); HRMS (ESI): Calcd for $C_{21}H_{17}O_3N_2ClF$ ([M+H]$^+$), 399.0906; Found, 399.0905, $C_{21}H_{17}O_3N_2{}^{37}ClF$ ([M+H]$^+$), 401.0877; Found, 401.0876.



Data for ***4r***: Pale yellow solid, yield: 90%, purity: 99%, mp: 177-179 ^{o}C; $[\alpha]^{20}_D$ = 0.4^o (*c* 3.0 mg/mL, $CHCl_3$); IR cm^{-1} (KBr): 3117, 2974, 2929, 1738, 1620, 1217, 1163, 1121, 1026; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.58 (s, 1H, -C*H*=N-), 7.53 (s, 1H, H-2'), 7.48 (t, *J* = 1.6 Hz, 1H, H-5'), 7.27-7.34 (m, 2H, -Ph), 6.91-7.00 (m, 3H, -Ph), 6.39 (d, *J* = 0.8 Hz, 1H, H-4'), 5.20 (s, 1H, H-8), 2.80-2.88 (m, 2H, H-6), 2.16 (s, 3H, H-10), 0.92 (s, 3H, H-11); HRMS (ESI): Calcd for $C_{21}H_{17}O_3N_2F_2$ ([M+H]$^+$), 383.1202; Found, 383.1201.

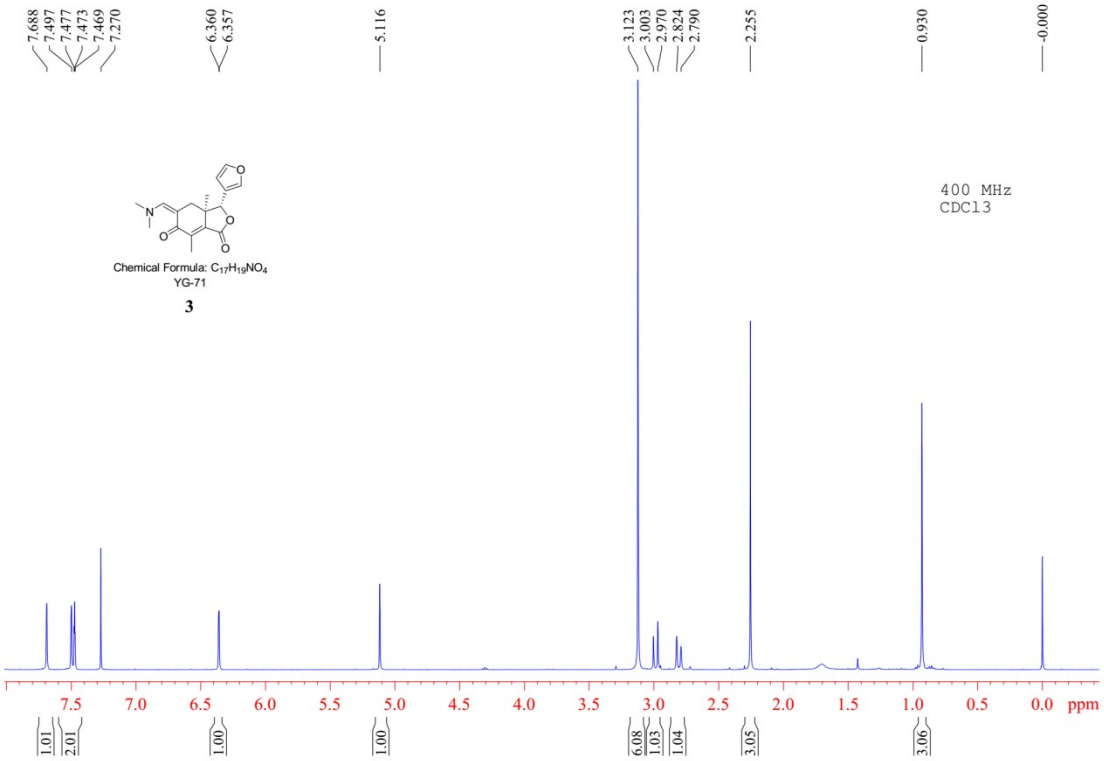


Data for ***4s***: Pale yellow solid, yield: 82%, purity: 99%, mp: 174-176 ^{o}C; $[\alpha]^{20}_D$ = 19^o (*c* 3.6 mg/mL, $CHCl_3$); IR cm^{-1} (KBr): 3116, 2962, 2926, 1740, 1638, 1377, 1216, 1158, 1022; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.67 (m, 1H, -C*H*=N-), 7.55 (d, *J* = 2.0 Hz, 1H, -Ph), 7.52 (s, 1H, H-2'), 7.47 (t, *J* = 2.0 Hz, 1H, H-5'), 6.38 (d, *J* = 1.2 Hz, 1H, H-4'), 5.21 (s, 1H, H-8), 2.79-2.94 (m, 2H, H-6), 2.01 (s, 3H, H-10), 0.87 (s, 3H, H-11); HRMS (ESI): Calcd for $C_{21}H_{16}O_3N_2Cl_3$ ([M+H]$^+$), 449.0221; Found, 449.0218, $C_{21}H_{16}O_3N_2{}^{37}Cl_3$ ([M+H]$^+$), 455.0133; Found, 455.0130.



Data for ***4t***: White solid, yield: 83%, purity: 99%, mp: 71-73 ^{o}C; $[\alpha]^{20}_{D}$ = 17^{o} (*c* 2.5 mg/mL, $CHCl_3$); IR cm^{-1} (KBr): 3069, 2965, 2925, 1746, 1640, 1513, 1278, 1165, 1024; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.71 (m, 1H, -C*H*=N-), 7.52 (s, 1H, H-2'), 7.48 (t, *J* = 1.6 Hz, 1H, H-5'), 7.32-7.34 (m, 1H, -Ph), 6.39 (d, *J* = 1.2 Hz, 1H, H-4'), 5.21 (s, 1H, H-8), 2.81-2.92 (m, 2H, H-6), 2.13 (s, 3H, H-10), 0.89 (s, 3H, H-11); HRMS (ESI): Calcd for $C_{21}H_{15}O_3N_2F_4$ ($[M+H]^+$), 419.1013; Found, 419.1012.

The spectrum ^{1}H NMR/^{13}C NMR, HPLC and HRMS of compounds 3, 4a-t:



High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : D162168

Sample Serial Number: YG-71 compound **3**

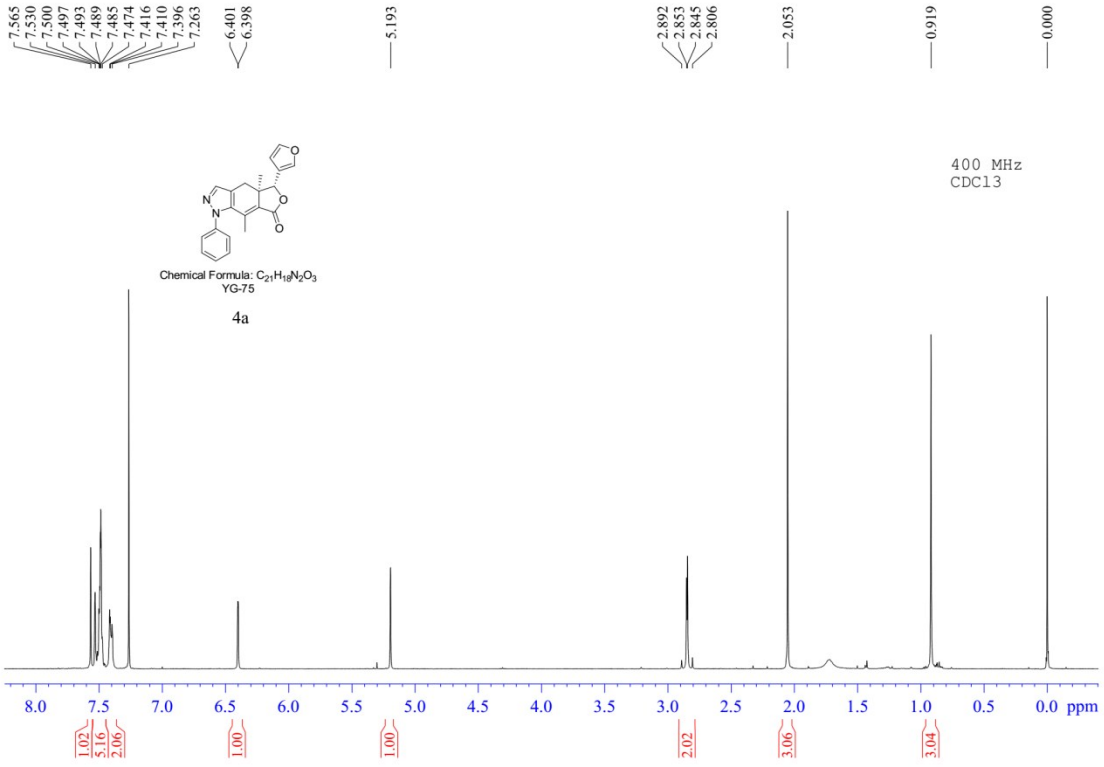
Operator : 001 Date: 2016/08/27

Operation Mode: DART Positive

Elemental composition search on mass 302.14

m/z= 297.14-307.14

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
302.1387	302.1387	0.05	8.5	$C_{17}H_{20}O_4N$
	302.1400	-4.38	13.5	$C_{18}H_{16}N_5$
	302.1373	4.49	9.0	$C_{15}H_{18}O_3N_4$



High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : D162169

Sample Serial Number: YG-75 compound **4a**

Operator : 001 Date: 2016/08/27

Operation Mode: DART Positive

Elemental composition search on mass 347.14

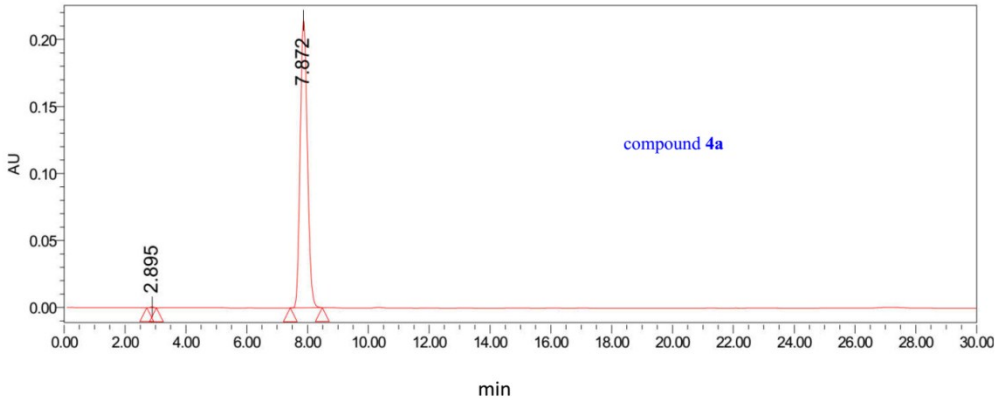
m/z= 342.14-352.14

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
347.1390	347.1390	-0.11	13.5	$C_{21}H_{19}O_3N_2$
	347.1377	3.76	14.0	$C_{19}H_{17}O_2N_5$

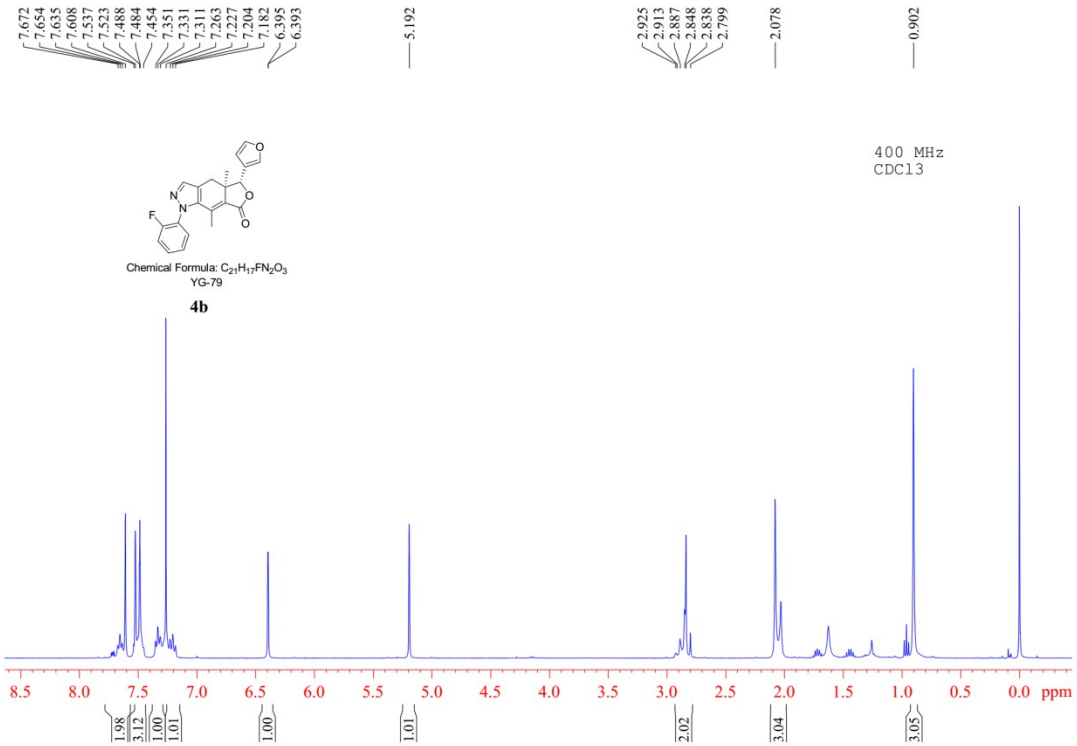
Empower 3 SOFTWARE

Waters Reports

Sample Information			
Sample Name	YG-75	Collector	System
Sample Type	Standard	Collection Method Group	YG
Bottle Number	6	Collection Time	2016/12/27 16:38:45 CST
Number of Injections	1	Processing Date	2016/12/27 19:28:48 CST
Injection Volume	10.00 ul	Processing Method	1
Run Time	30.0 Minutes	Channel Name	W2489 ChA 254nm



Name	Retention Time (min)	Area (μV*s)	% Area	Height (μV)
1	2.895	5570	0.16	617
2	7.872	3511086	99.84	214889



High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : D162171

Sample Serial Number: YG-79 compound **4b**

Operator : 001 Date: 2016/08/27

Operation Mode: DART Positive

Elemental composition search on mass 365.13

m/z= 360.13-370.13

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
365.1296	365.1296	-0.02	13.5	$C_{21}H_{18}O_3N_2F$
	365.1294	0.53	10.0	$C_{16}H_{17}O_3N_5F_2$
	365.1291	1.22	8.0	$C_{18}H_{23}O_5NS$
	365.1291	1.23	13.5	$C_{17}H_{17}N_8S$
	365.1301	-1.36	0.5	$C_{10}H_{23}O_6N_4F_2S$
	365.1301	-1.41	1.0	$C_7H_{20}O_9N_7F$
	365.1290	1.71	-0.5	$C_{11}H_{25}O_{13}$
	365.1290	1.72	5.0	$C_{10}H_{19}O_8N_7$
	365.1289	1.77	4.5	$C_{13}H_{22}O_5N_4FS$
	365.1303	-1.90	9.5	$C_{14}H_{18}ON_8FS$

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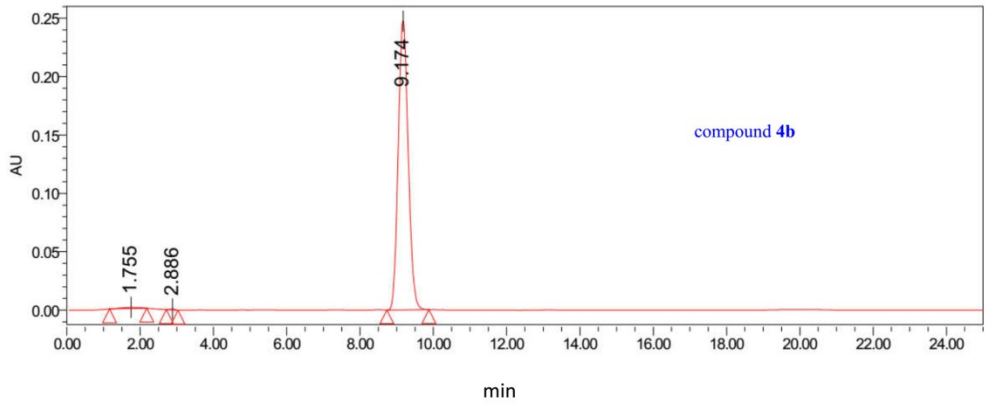
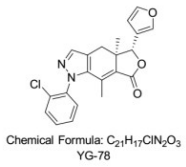
Waters Reports

Sample Information			
Sample Name	YG-79	Collector	System
Sample Type	Standard	Collection Method Group	YG
Bottle Number	3	Collection Time	2016/12/26 20:44:33 CST
Number of Injections	1	Processing Date	2016/12/27 19:10:54 CST
Injection Volume	10.00 *ul*	Processing Method	1
Run Time	25.0 Minutes	Channel Name	W2489 ChA 254nm

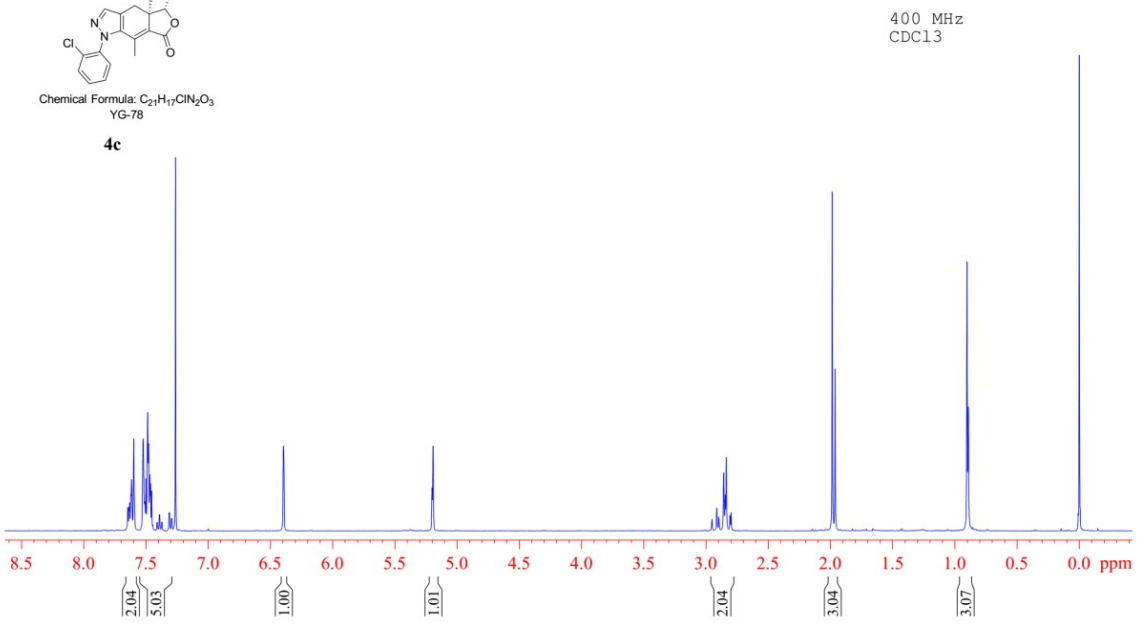


Name	Retention Time (min)	Area (μV*s)	% Area	Height (μV)
1	1.755	38336	0.81	1023
2	2.886	8285	0.17	834
3	9.174	4692061	99.02	247759



Chemical Formula: $C_{21}H_{17}ClN_2O_3$
YG-78

4c



High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : D162170

Sample Serial Number: YG-78 compound **4c**

Operator : 001 Date: 2016/08/27

Operation Mode: DART Positive

Elemental composition search on mass 381.10

m/z= 376.10-386.10

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
381.1000	381.1000	-0.17	13.5	$C_{21}H_{18}O_3N_2Cl$
	381.0996	1.10	18.0	$C_{24}H_{15}O_4N$
	381.1009	-2.41	23.0	$C_{25}H_{11}N_5$
	381.0987	3.35	14.0	$C_{19}H_{16}O_2N_5Cl$
	381.0982	4.63	18.5	$C_{22}H_{13}O_3N_4$

For $C_{21}H_{18}O_3N_2{}^{37}Cl$ ($[M+H]^+$):

High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : D162170

Sample Serial Number: YG-78 compound **4c**

Operator : 001 Date: 2016/08/27

Operation Mode: DART Positive

Elemental composition search on mass 383.10

m/z= 378.10-388.10

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
383.0970	383.0971	-0.15	13.5	$C_{21}H_{18}O_3N_2{}^{37}Cl$
	383.0958	3.36	14.0	$C_{19}H_{16}O_2N_5{}^{37}Cl$

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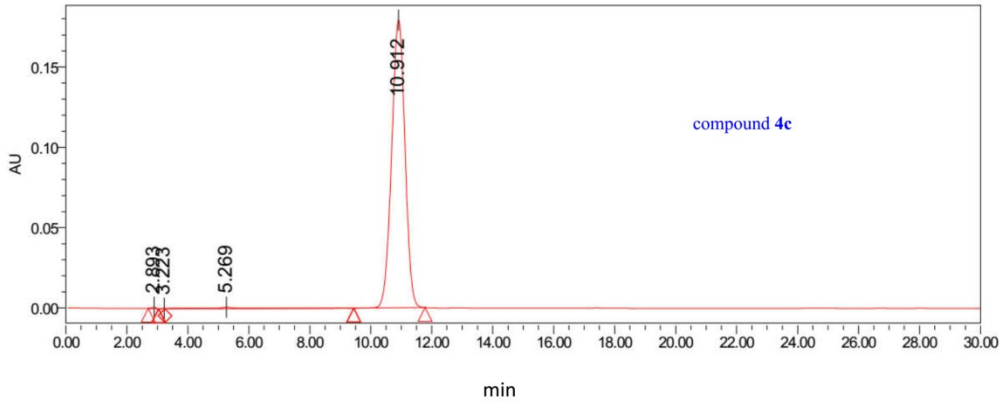
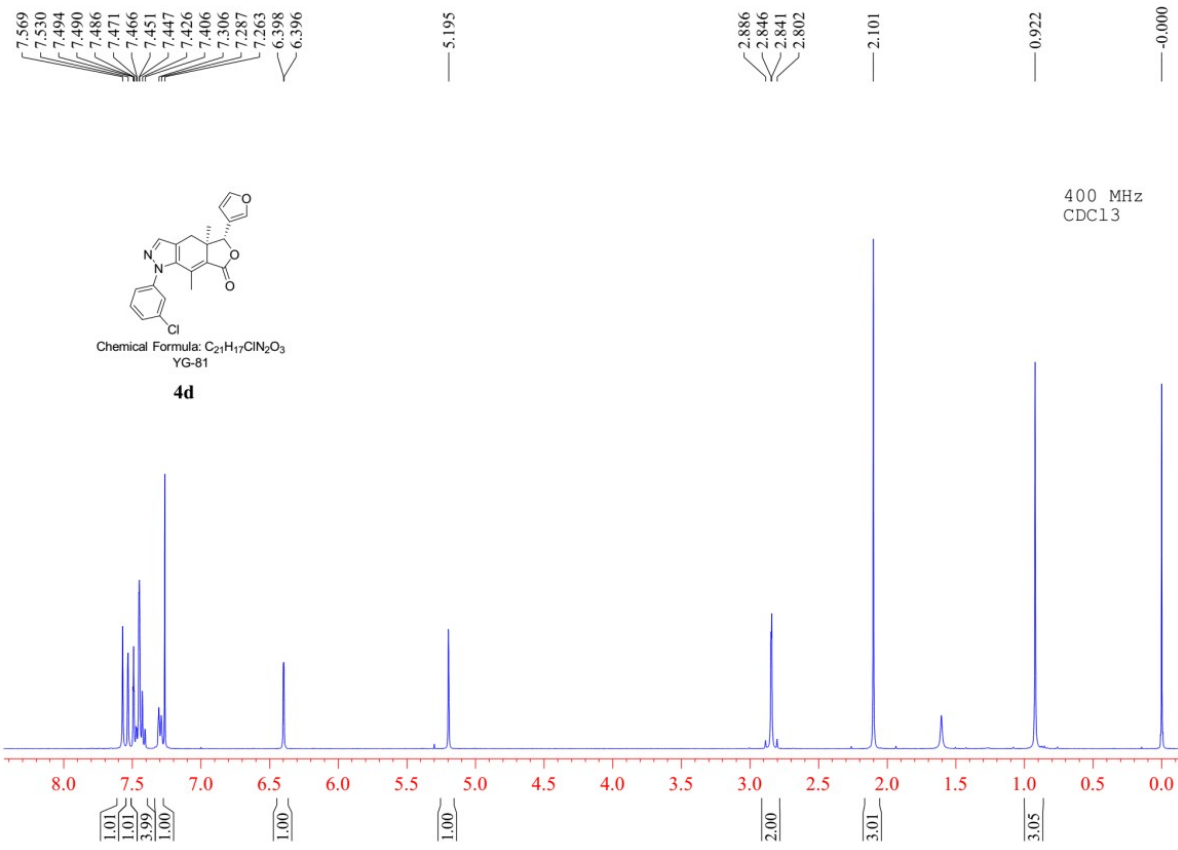
Waters Reports

Sample Information			
Sample Name	YG-78	Collector	System
Sample Type	Standard	Collection Method Group	YG
Bottle Number	2	Collection Time	2016/12/26 20:10:46 CST
Number of Injections	1	Processing Date	2016/12/27 19:09:35 CST
Injection Volume	10.00 *u*l	Processing Method	1
Run Time	30.0 Minutes	Channel Name	W2489 ChA 254nm



Name	Retention Time (min)	Area (μV*s)	% Area	Height (μV)
1	2.893	8240	0.15	818
2	3.223	2122	0.04	230
3	5.269	78565	1.42	905
4	10.912	5449392	98.39	179257



High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : D162173

Sample Serial Number: YG-81 compound **4d**

Operator : 001 Date: 2016/08/27

Operation Mode: DART Positive

Elemental composition search on mass 381.10

m/z= 376.10-386.10

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
381.0999	381.1000	-0.25	13.5	$C_{21}H_{18}O_3N_2Cl$
	381.0996	1.02	18.0	$C_{24}H_{15}O_4N$
	381.1009	-2.48	23.0	$C_{25}H_{11}N_5$
	381.0987	3.27	14.0	$C_{19}H_{16}O_2N_5Cl$
	381.0982	4.55	18.5	$C_{22}H_{13}O_3N_4$

For $C_{21}H_{18}O_3N_2{}^{37}Cl$ ($[M+H]^+$):

High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : D162173

Sample Serial Number: YG-81 compound **4d**

Operator : 001 Date: 2016/08/27

Operation Mode: DART Positive

Elemental composition search on mass 383.10

m/z= 378.10-388.10

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
383.0971	383.0971	0.06	13.5	$C_{21}H_{18}O_3N_2{}^{37}Cl$
	383.0958	3.57	14.0	$C_{19}H_{16}O_2N_5{}^{37}Cl$

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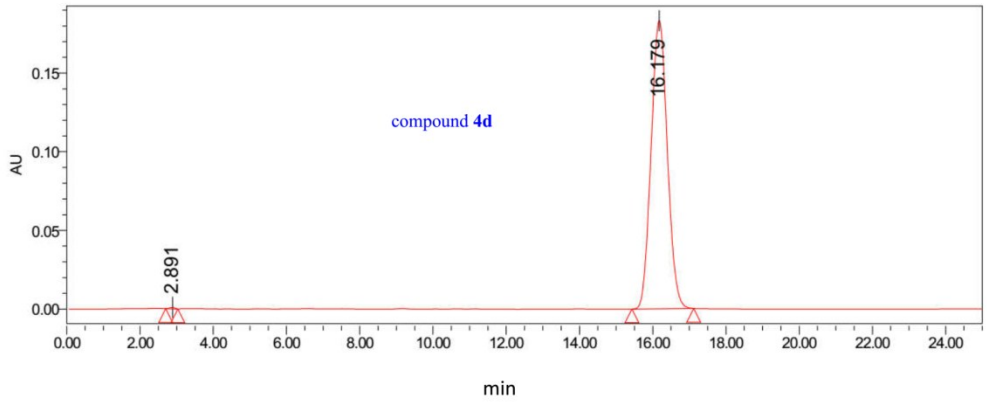
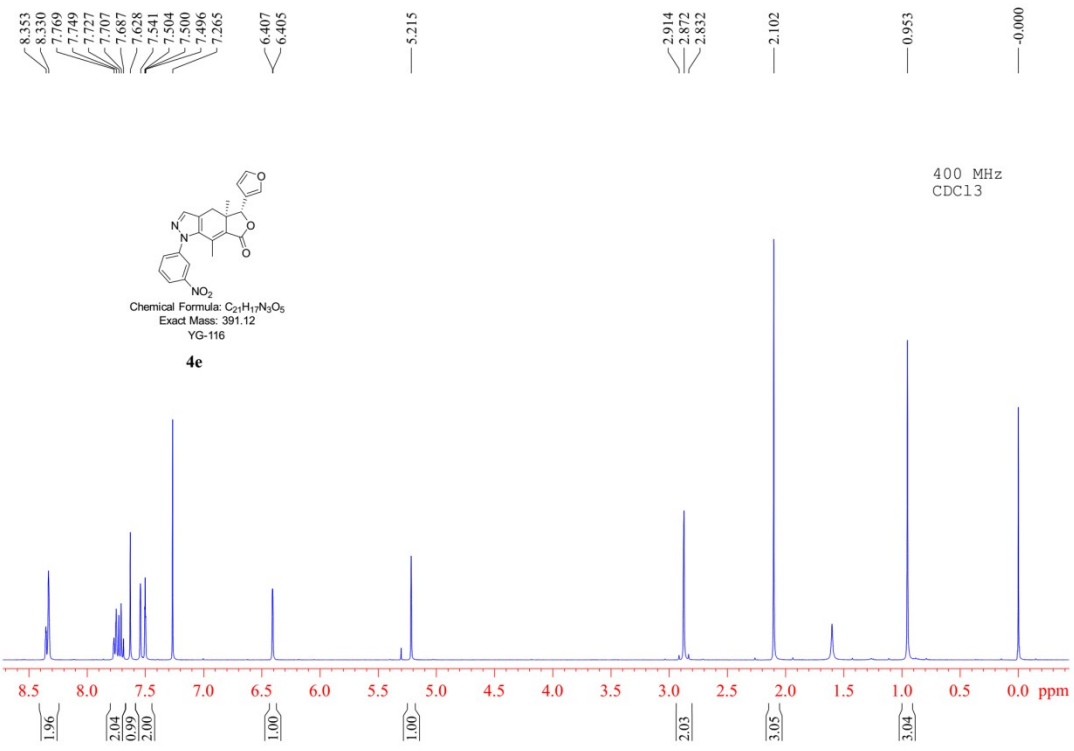
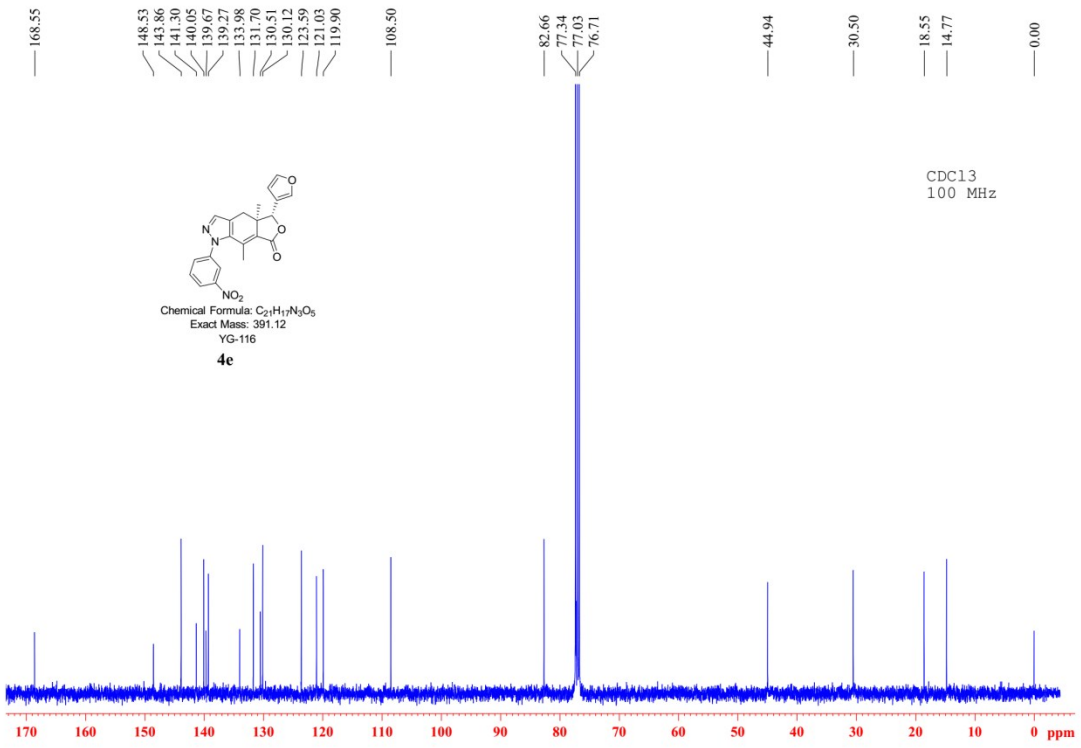
Waters Reports

Sample Information			
Sample Name	YG-81	Collector	System
Sample Type	Standard	Collection Method Group	YG
Bottle Number	5	Collection Time	2016/12/26 21:35:52 CST
Number of Injections	1	Processing Date	2016/12/27 19:13:40 CST
Injection Volume	10.00 ul	Processing Method	1
Run Time	25.0 Minutes	Channel Name	W2489 ChA 254nm



Name	Retention Time (min)	Area (μV*s)	% Area	Height (μV)
1	2.891	9385	0.17	937
2	16.179	5654915	99.83	183206





High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : D162188

Sample Serial Number: YG-116 compound **4e**

Operator : 001 Date: 2016/08/27

Operation Mode: DART Positive

Elemental composition search on mass 392.12

m/z= 387.12-397.12

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
392.1239	392.1241	-0.55	14.5	$C_{21}H_{18}O_5N_3$

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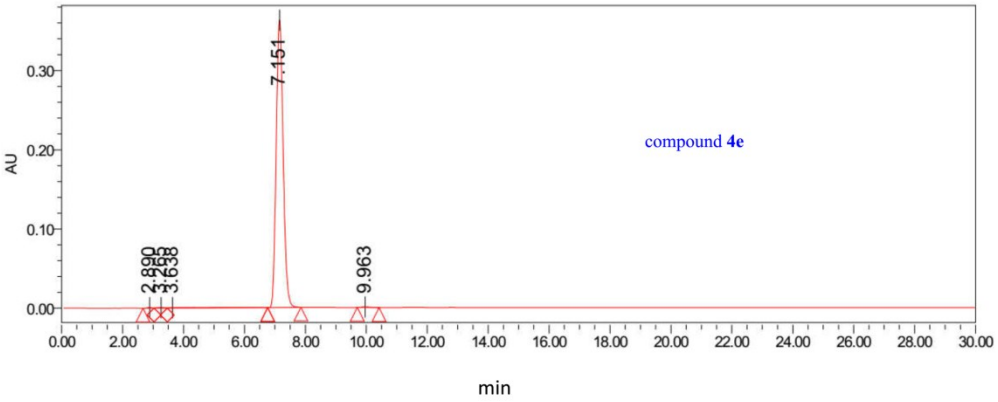
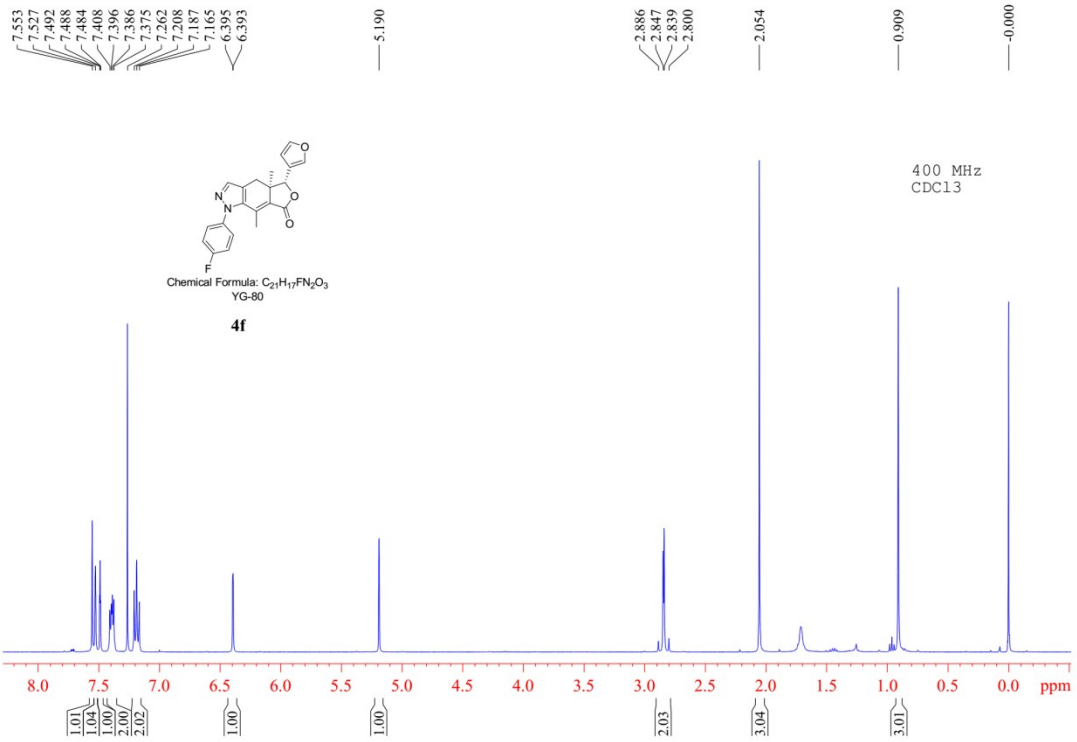
Waters Reports

Sample Information			
Sample Name	YG-116	Collector	System
Sample Type	Standard	Collection Method Group	YG
Bottle Number	1	Collection Time	2016/12/26 19:16:47 CST
Number of Injections	1	Processing Date	2016/12/27 19:07:39 CST
Injection Volume	10.00 ul	Processing Method	1
Run Time	30.0 Minutes	Channel Name	W2489 ChA 254nm



Name	Retention Time (min)	Area (μV*s)	% Area	Height (μV)
1	2.890	7829	0.13	683
2	3.265	10967	0.19	639
3	3.638	67913	1.16	675
4	7.151	5732627	98.28	362854
5	9.963	13494	0.23	667



High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : D162172

Sample Serial Number: YG-80 compound **4f**

Operator : 001 Date: 2016/08/27

Operation Mode: DART Positive

Elemental composition search on mass 365.13

m/z= 360.13-370.13

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
365.1295	365.1296	-0.27	13.5	$C_{21}H_{18}O_3N_2F$
	365.1294	0.28	10.0	$C_{16}H_{17}O_3N_5F_2$
	365.1291	0.97	8.0	$C_{18}H_{23}O_5NS$
	365.1291	0.99	13.5	$C_{17}H_{17}N_8S$
	365.1290	1.46	-0.5	$C_{11}H_{25}O_{13}$
	365.1290	1.47	5.0	$C_{10}H_{19}O_8N_7$
	365.1289	1.52	4.5	$C_{13}H_{22}O_5N_4FS$
	365.1301	-1.61	0.5	$C_{10}H_{23}O_6N_4F_2S$
	365.1301	-1.66	1.0	$C_7H_{20}O_9N_7F$
	365.1288	2.02	1.5	$C_5H_{18}O_8N_{10}F$

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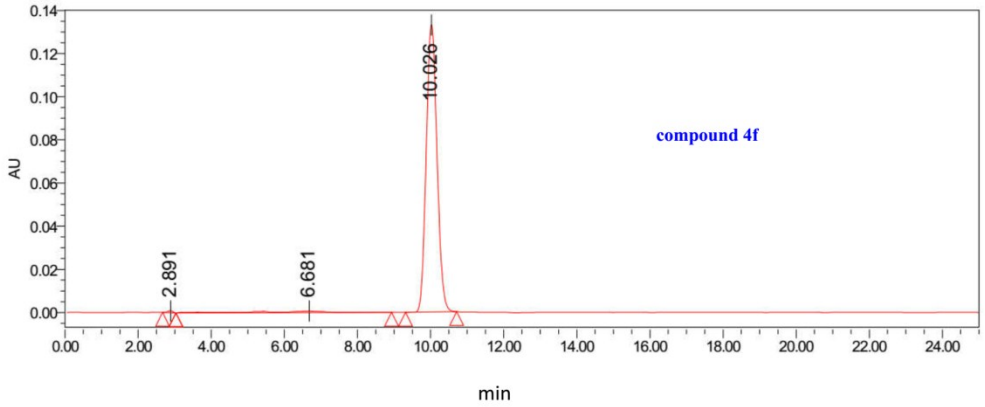
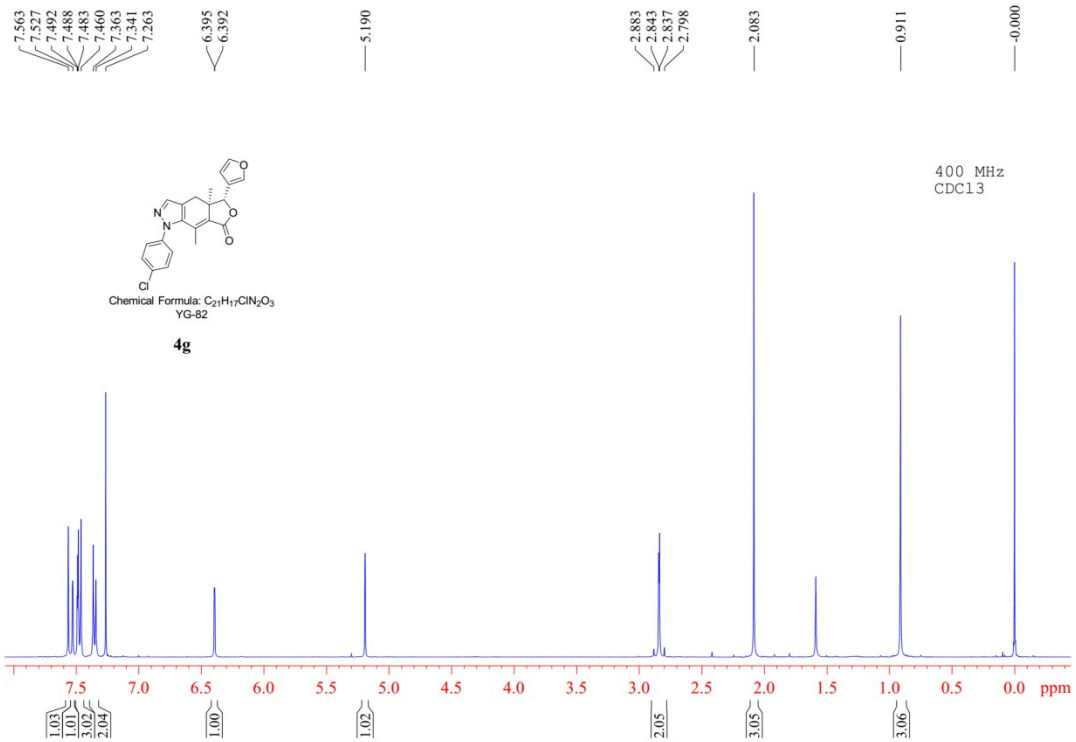
Waters Reports

Sample Information			
Sample Name	YG-80	Collector	System
Sample Type	Standard	Collection Method Group	YG
Bottle Number	4	Collection Time	2016/12/26 21:10:13 CST
Number of Injections	1	Processing Date	2016/12/27 19:12:24 CST
Injection Volume	10.00 ul	Processing Method	1
Run Time	25.0 Minutes	Channel Name	W2489 ChA 254nm



Name	Retention Time (min)	Area (μV*s)	% Area	Height (μV)
1	2.891	9122	0.32	886
2	6.681	91850	3.26	696
3	10.026	2717344	96.42	133336



High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : D162174

Sample Serial Number: YG-82 compound **4g**

Operator : 001 Date: 2016/08/27

Operation Mode: DART Positive

Elemental composition search on mass 381.10

m/z= 376.10-386.10

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
381.0999	381.1000	-0.36	13.5	$C_{21}H_{18}O_3N_2Cl$
	381.0996	0.92	18.0	$C_{24}H_{15}O_4N$
	381.1009	-2.59	23.0	$C_{25}H_{11}N_5$
	381.0987	3.16	14.0	$C_{19}H_{16}O_2N_5Cl$
	381.0982	4.44	18.5	$C_{22}H_{13}O_3N_4$

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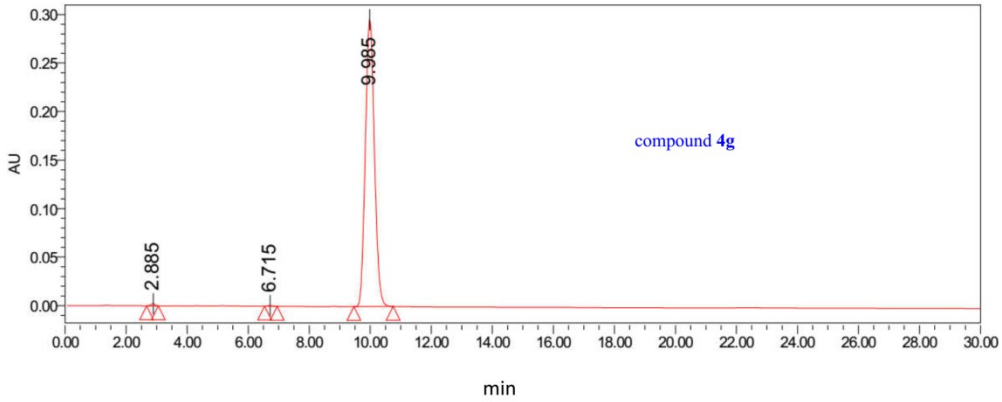
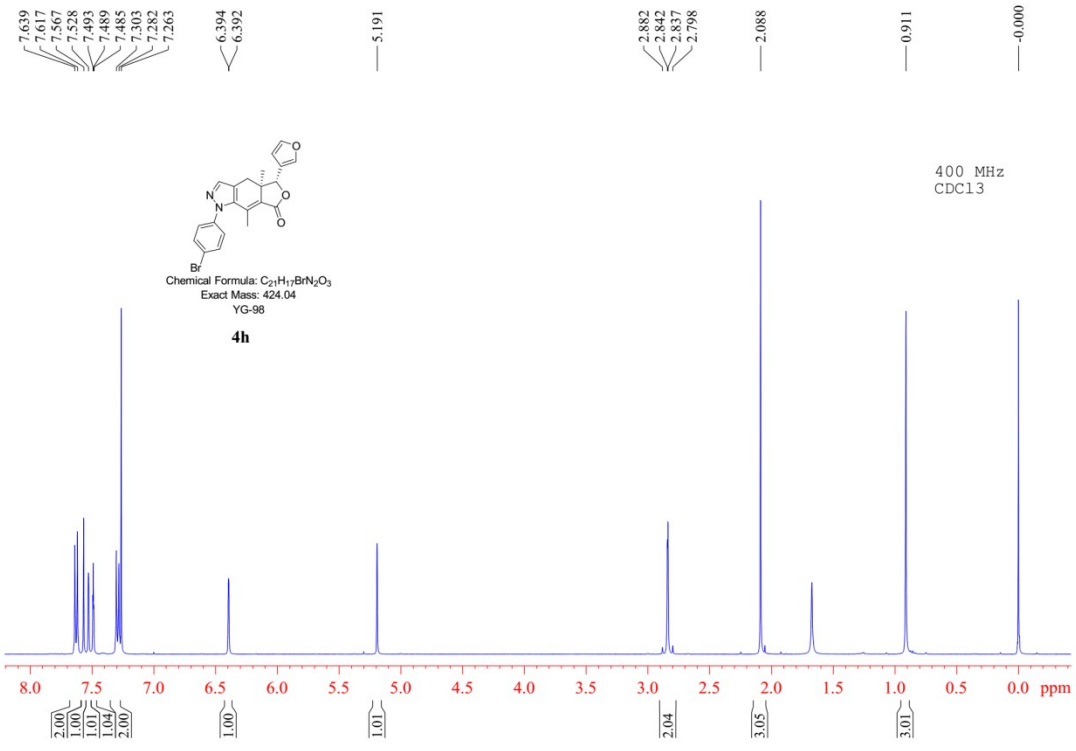
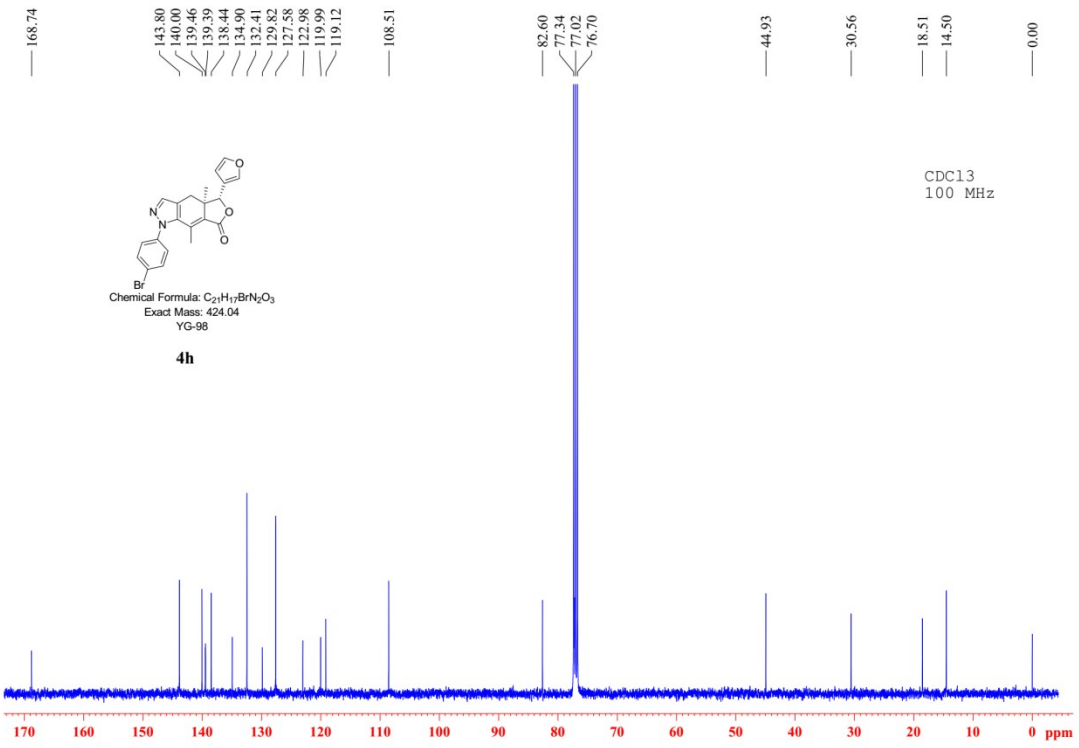
Waters Reports

Sample Information			
Sample Name	YG-82	Collector	System
Sample Type	Standard	Collection Method Group	YG
Bottle Number	7	Collection Time	2016/12/27 11:05:51 CST
Number of Injections	1	Processing Date	2016/12/27 19:24:52 CST
Injection Volume	10.00 *ul*	Processing Method	1
Run Time	30.0 Minutes	Channel Name	W2489 ChA 254nm



Name	Retention Time (min)	Area (μV*s)	% Area	Height (μV)
1	2.885	19882	0.32	2083
2	6.715	6414	0.10	477
3	9.985	6094798	99.57	295816





High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : D162187

Sample Serial Number: YG-98 compound **4h**

Operator : 001 Date: 2016/08/27

Operation Mode: DART Positive

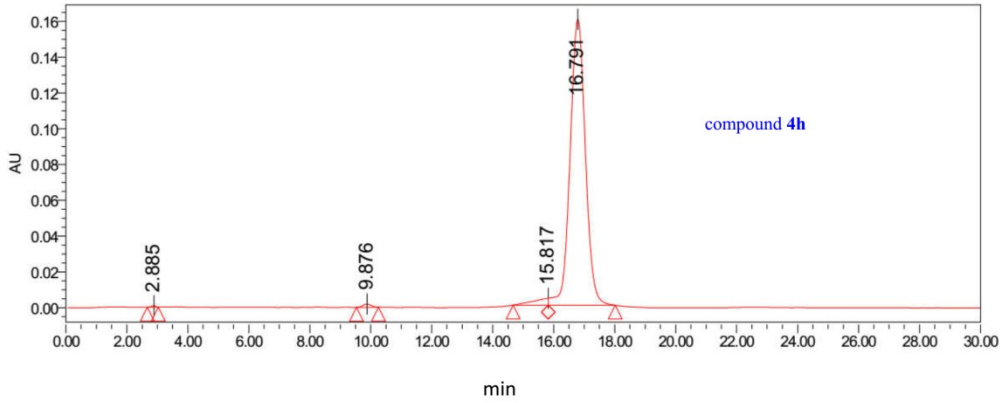
Elemental composition search on mass 425.05

m/z= 420.05-430.05

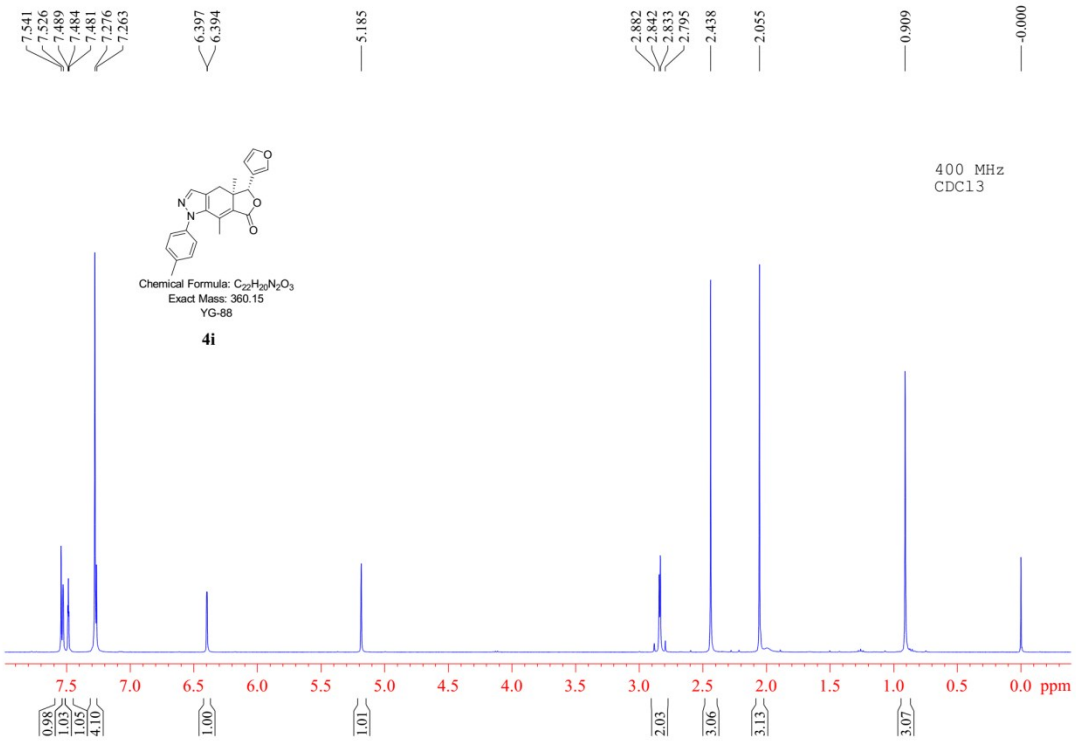
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
425.0494	425.0495	-0.24	13.5	$C_{21}H_{18}O_3N_2Br$
	425.0482	2.92	14.0	$C_{19}H_{16}O_2N_5Br$

Waters Reports

Sample Information			
Sample Name	YG-98	Collector	System
Sample Type	Standard	Collection Method Group	YG
Bottle Number	20	Collection Time	2016/12/27 5:27:33 CST
Number of Injections	1	Processing Date	2016/12/27 19:22:19 CST
Injection Volume	10.00 *ul*	Processing Method	1
Run Time	30.0 Minutes	Channel Name	W2489 ChA 254nm

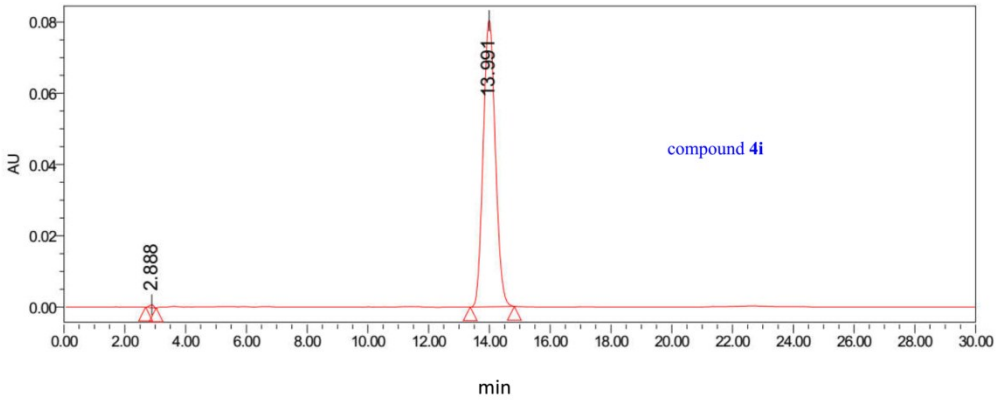


Name	Retention Time (min)	Area (μV*s)	% Area	Height (μV)
1	2.885	9350	0.16	933
2	9.876	35079	0.61	1811
3	15.817	132794	2.31	3879
4	16.791	5578026	96.92	159822

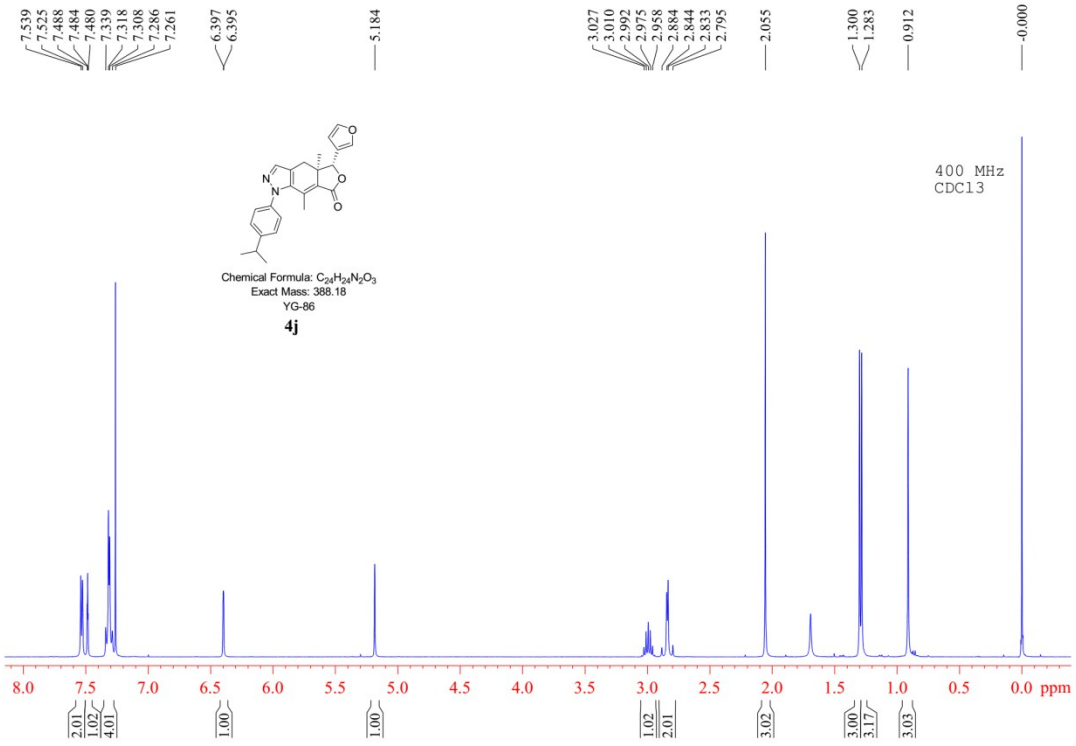


Waters Reports

Sample Information			
Sample Name	YG-88	Collector	System
Sample Type	Standard	Collection Method Group	YG
Bottle Number	13	Collection Time	2016/12/27 1:52:53 CST
Number of Injections	1	Processing Date	2016/12/27 19:18:05 CST
Injection Volume	10.00 *ul*	Processing Method	1
Run Time	30.0 Minutes	Channel Name	W2489 ChA 254nm



Name	Retention Time (min)	Area (μV*s)	% Area	Height (μV)
1	2.888	7888	0.35	773
2	13.991	2235850	99.65	80371



High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : D162178

Sample Serial Number: YG-86 compound **4j**

Operator : 001 Date: 2016/08/27

Operation Mode: DART Positive

Elemental composition search on mass 389.19

m/z= 384.19-394.19

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
389.1858	389.1860	-0.54	13.5	$C_{24}H_{25}O_3N_2$
	389.1846	2.91	14.0	$C_{22}H_{23}O_2N_5$

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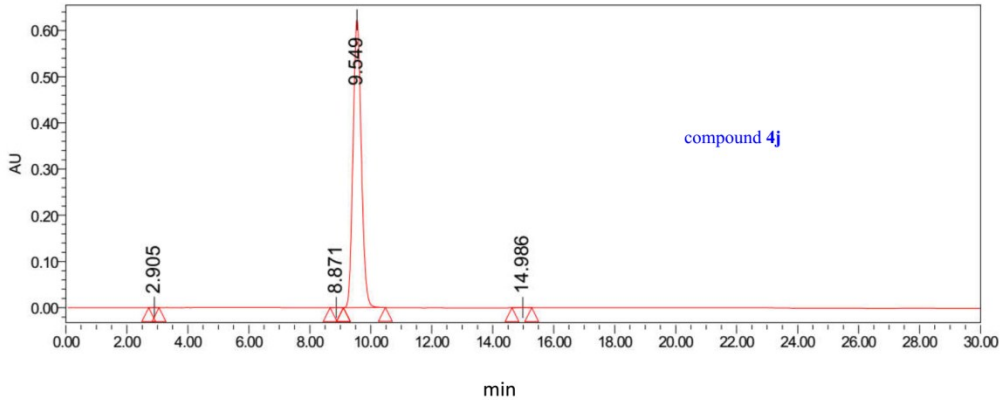
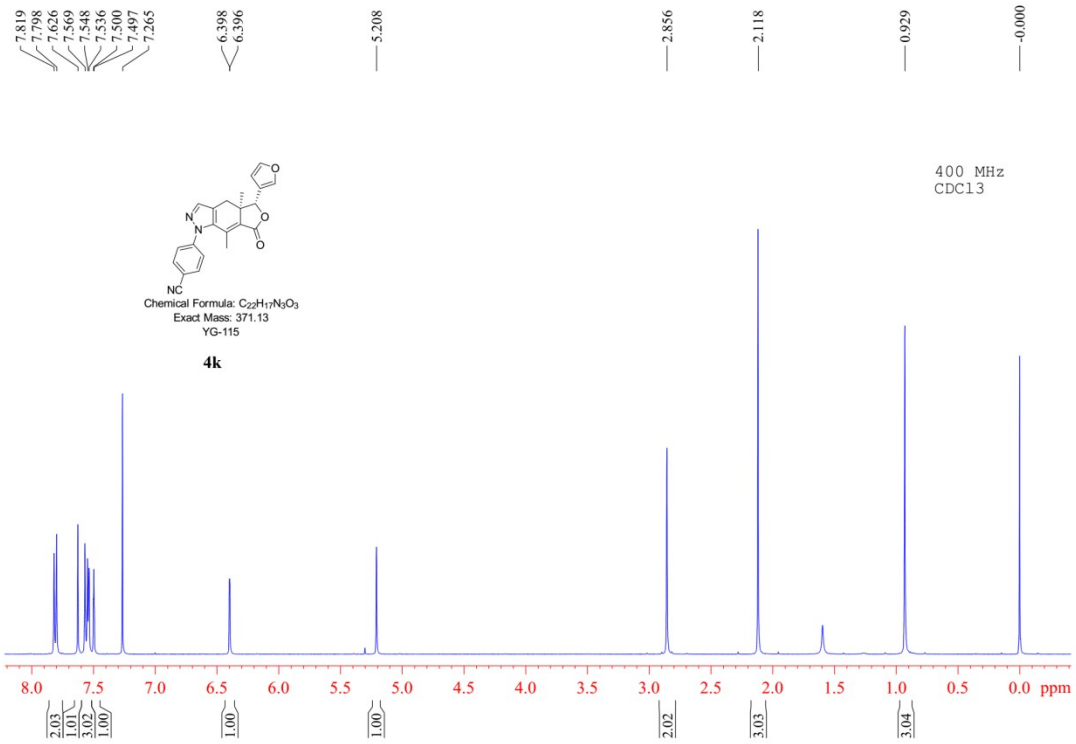
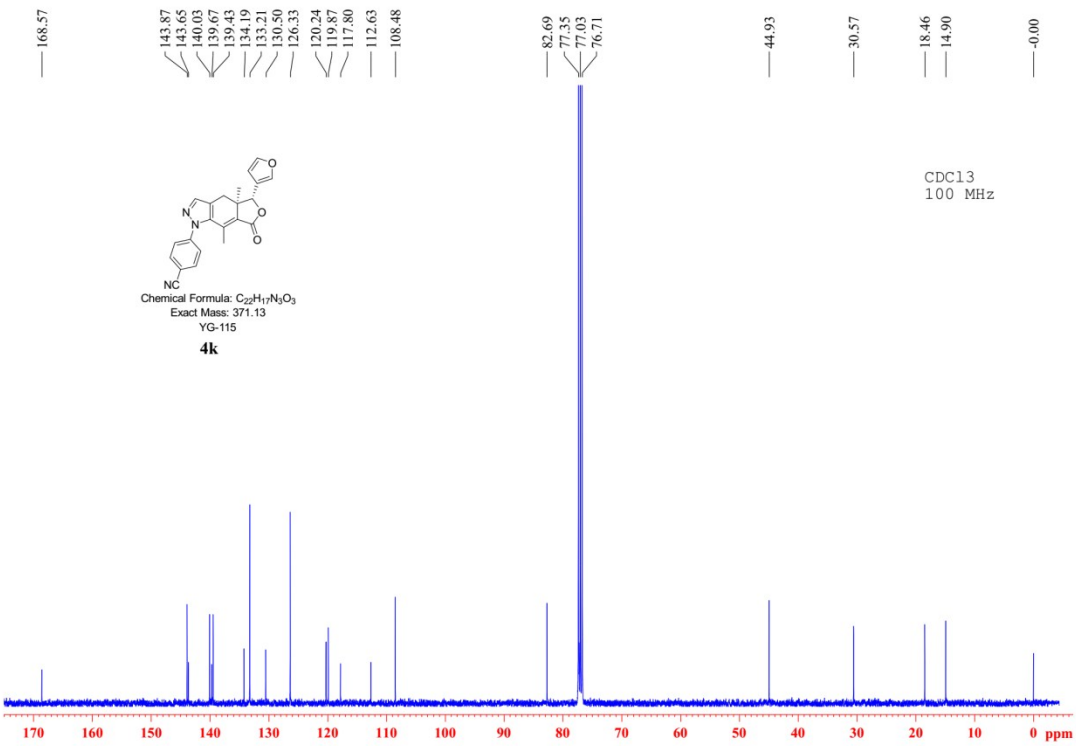
Waters Reports

Sample Information			
Sample Name	YG-86	Collector	System
Sample Type	Standard	Collection Method Group	YG
Bottle Number	11	Collection Time	2016/12/27 13:00:12 CST
Number of Injections	1	Processing Date	2016/12/27 19:25:41 CST
Injection Volume	10.00 ul	Processing Method	1
Run Time	30.0 Minutes	Channel Name	W2489 ChA 254nm



Name	Retention Time (min)	Area (μV*s)	% Area	Height (μV)
1	2.905	7649	0.06	886
2	8.871	6980	0.06	508
3	9.549	11744304	99.72	622853
4	14.986	18325	0.16	821


7.819
7.798
7.626
7.569
7.548
7.536
7.500
7.497
7.265
6.398
6.396
5.208
2.856
2.118
0.929
-0.000
400 MHz
CDCl3
Chemical Formula: C22H17N3O3
Exact Mass: 371.13
YG-115
4k
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0 ppm
2.03
1.01
3.02
1.00
1.00
1.00
2.02
3.03
3.04


168.57
143.87
143.65
140.03
139.67
139.43
134.19
133.21
130.50
126.33
120.24
119.87
117.80
112.63
108.48
82.69
77.35
77.03
76.71
44.93
30.57
18.46
14.90
-0.00
CDCl3
100 MHz
Chemical Formula: C22H17N3O3
Exact Mass: 371.13
YG-115
4k
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0 ppm

High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : D162189

Sample Serial Number: YG-115 compound **4k**

Operator : 001 Date: 2016/08/27

Operation Mode: DART Positive

Elemental composition search on mass 372.13

m/z= 367.13-377.13

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
372.1342	372.1343	-0.21	15.5	$C_{22}H_{18}O_3N_3$
	372.1356	-3.82	15.0	$C_{24}H_{20}O_4$

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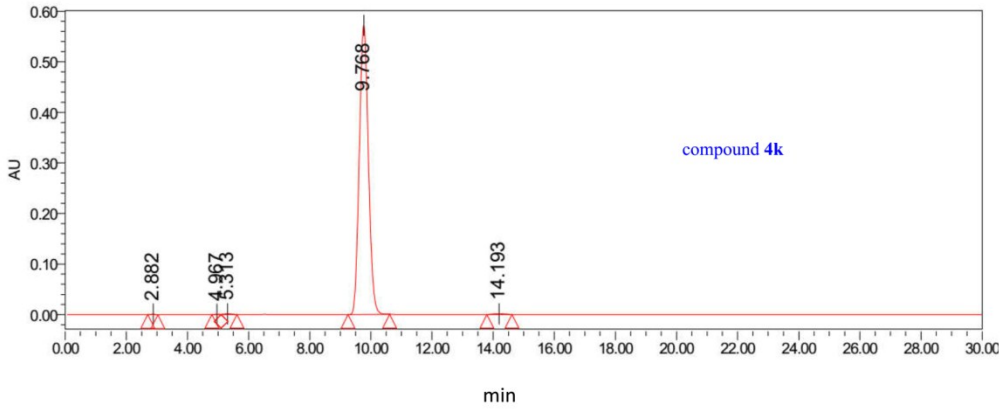
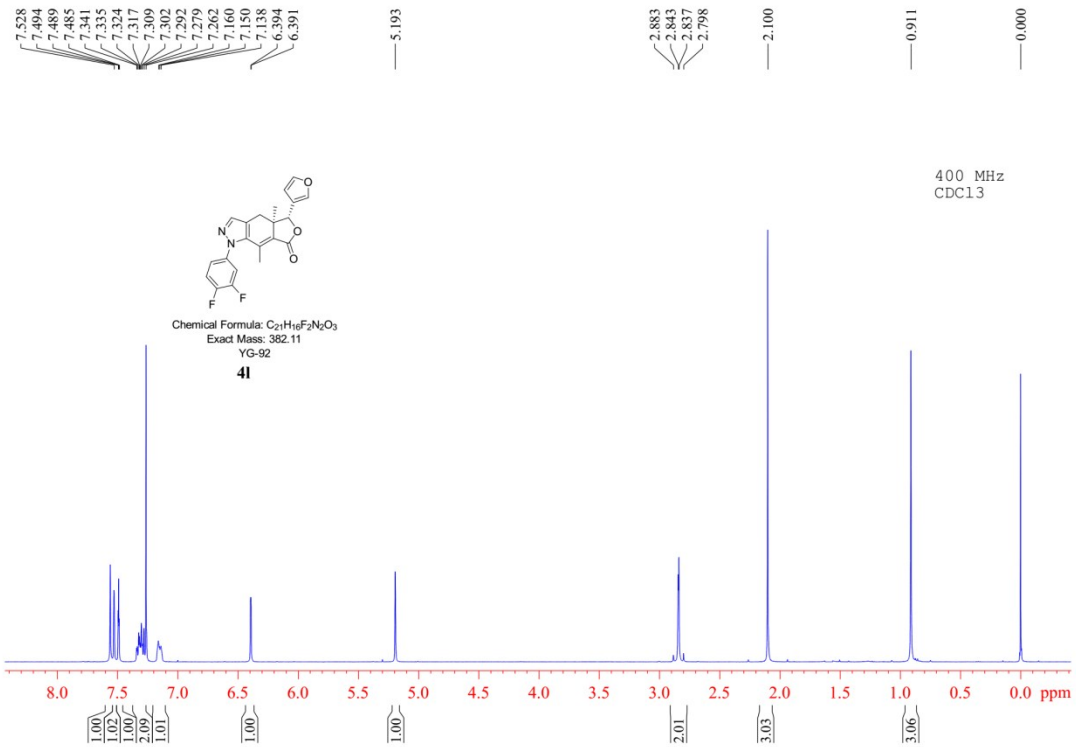
Waters Reports

Sample Information			
Sample Name	YG-115	Collector	System
Sample Type	Standard	Collection Method Group	YG
Bottle Number	21	Collection Time	2016/12/27 5:58:14 CST
Number of Injections	1	Processing Date	2016/12/27 19:22:49 CST
Injection Volume	10.00 ul	Processing Method	1
Run Time	30.0 Minutes	Channel Name	W2489 ChA 254nm



Name	Retention Time (min)	Area (μV*s)	% Area	Height (μV)
1	2.882	7953	0.07	809
2	4.967	4434	0.04	413
3	5.313	19130	0.16	1326
4	9.768	11815158	99.42	572010
5	14.193	36878	0.31	1450



High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : D162181

Sample Serial Number: YG-92 compound **4l**

Operator : 001 Date: 2016/08/27

Operation Mode: DART Positive

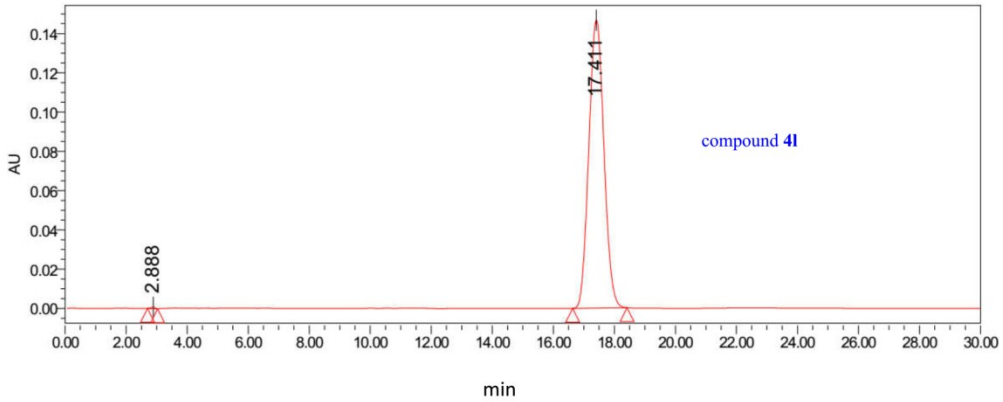
Elemental composition search on mass 383.12

m/z= 378.12-388.12

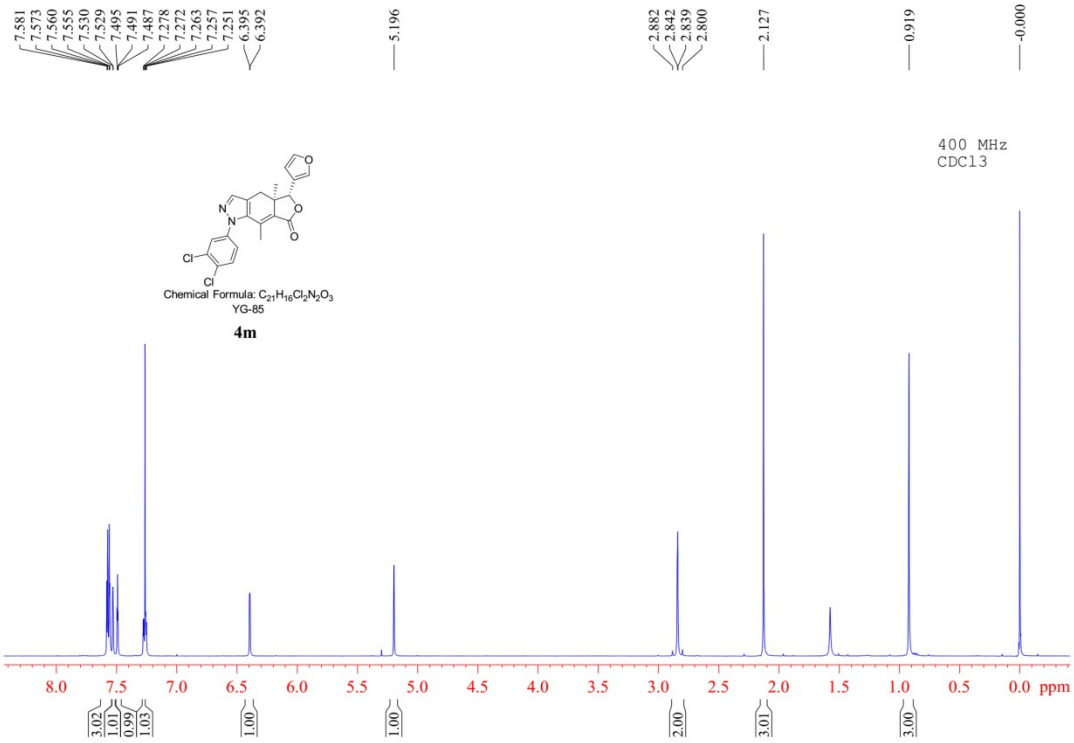
m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
383.1200	383.1202	-0.35	13.5	$C_{21}H_{17}O_3N_2F_2$
	383.1190	2.63	17.5	$C_{24}H_{16}O_2N_2F$
	383.1188	3.15	14.0	$C_{19}H_{15}O_2N_5F_2$

Waters Reports

Sample Information			
Sample Name	YG-92	Collector	System
Sample Type	Standard	Collection Method Group	YG
Bottle Number	17	Collection Time	2016/12/27 3:55:35 CST
Number of Injections	1	Processing Date	2016/12/27 19:20:47 CST
Injection Volume	10.00 ul	Processing Method	1
Run Time	30.0 Minutes	Channel Name	W2489 ChA 254nm



Name	Retention Time (min)	Area (μV*s)	% Area	Height (μV)
1	2.888	7474	0.15	755
2	17.411	5037494	99.85	146794



High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : D162177

Sample Serial Number: YG-85 compound **4m**

Operator : 001 Date: 2016/08/27

Operation Mode: DART Positive

Elemental composition search on mass 415.06

m/z= 410.06-420.06

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
415.0609	415.0611	-0.37	13.5	$C_{21}H_{17}O_3N_2Cl_2$
	415.0606	0.80	18.0	$C_{24}H_{14}O_4NCl$
	415.0614	-1.25	27.5	$C_{28}H_7ON_4$
	415.0601	1.98	22.5	$C_{27}H_{11}O_5$
	415.0619	-2.42	23.0	$C_{25}H_{10}N_5Cl$
	415.0597	2.86	14.0	$C_{19}H_{15}O_2N_5Cl_2$
	415.0592	4.04	18.5	$C_{22}H_{12}O_3N_4Cl$
	415.0628	-4.48	27.0	$C_{30}H_9O_2N$

For $C_{21}H_{17}O_3N_2{}^{37}Cl_2$ ($[M+H]^+$):

High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : D162177

Sample Serial Number: YG-85 compound **4m**

Operator : 001 Date: 2016/08/27

Operation Mode: DART Positive

Elemental composition search on mass 419.06

m/z= 414.06-424.06

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
419.0552	419.0552	-0.06	13.5	$C_{21}H_{17}O_3N_2{}^{37}Cl_2$
	419.0564	-2.87	26.5	$C_{27}H_7O_2N_4$
	419.0538	3.15	14.0	$C_{19}H_{15}O_2N_5{}^{37}Cl_2$
	419.0537	3.53	22.0	$C_{24}H_9O_5N_3$

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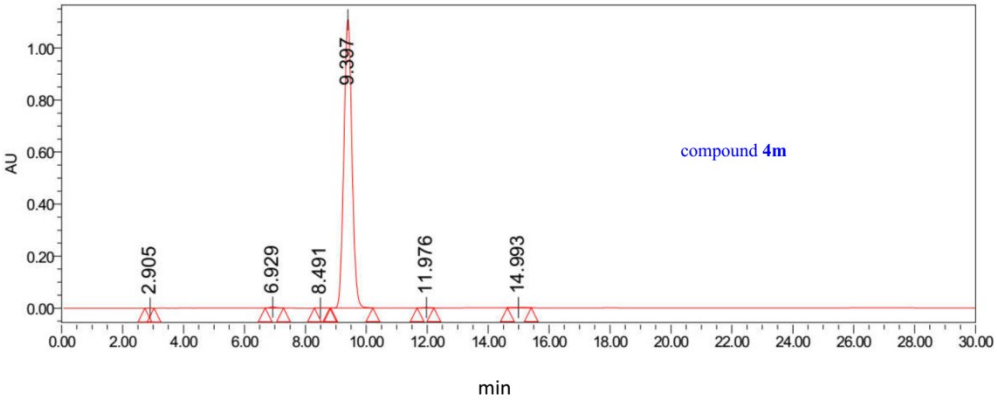
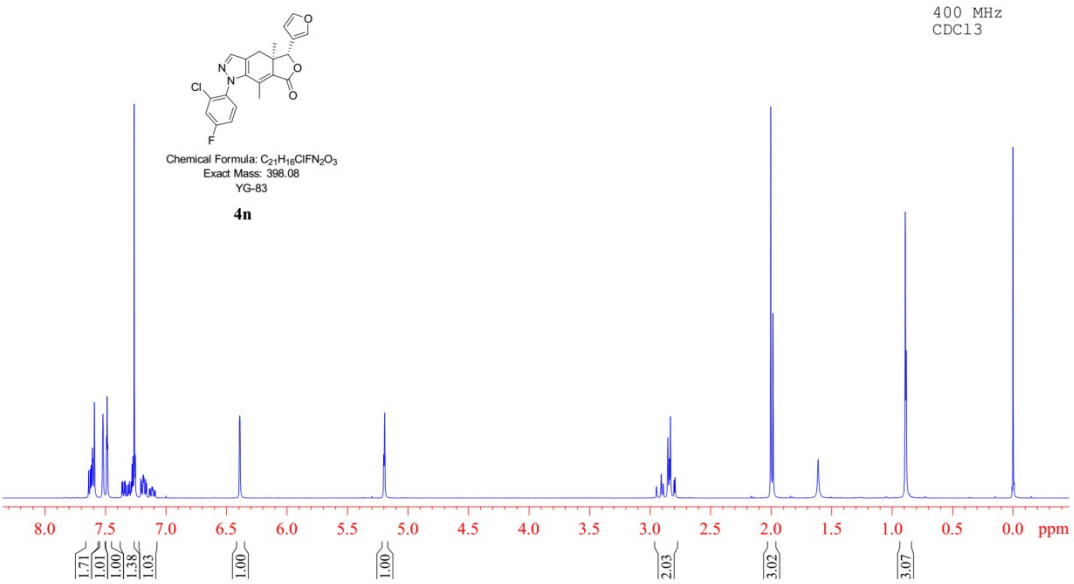
Waters Reports

Sample Information			
Sample Name	YG-85	Collector	System
Sample Type	Standard	Collection Method Group	YG
Bottle Number	10	Collection Time	2016/12/27 13:30:57 CST
Number of Injections	1	Processing Date	2016/12/27 19:26:19 CST
Injection Volume	10.00 *ul*	Processing Method	1
Run Time	30.0 Minutes	Channel Name	W2489 ChA 254nm



Name	Retention Time (min)	Area (μV*s)	% Area	Height (μV)
1	2.905	4693	0.02	552
2	6.929	55169	0.27	3971
3	8.491	6601	0.03	437
4	9.397	20448675	99.46	1108935
5	11.976	13442	0.07	737
6	14.993	30670	0.15	1228



High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : D162180

Sample Serial Number: YG-83 compound **4n**

Operator : 001 Date: 2016/08/27

Operation Mode: DART Positive

Elemental composition search on mass 399.09

m/z= 394.09-404.09

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
399.0905	399.0906	-0.39	13.5	$C_{21}H_{17}O_3N_2ClF$
	399.0901	0.83	18.0	$C_{24}H_{14}O_4NF$
	399.0895	2.48	17.5	$C_{24}H_{16}O_2N_2Cl$
	399.0915	-2.52	23.0	$C_{25}H_{10}N_5F$
	399.0893	2.98	14.0	$C_{19}H_{15}O_2N_5ClF$
	399.0917	-3.02	26.5	$C_{30}H_{11}N_2$
	399.0890	3.70	22.0	$C_{27}H_{13}O_3N$
	399.0888	4.20	18.5	$C_{22}H_{12}O_3N_4F$

For $C_{21}H_{17}O_3N_2{}^{37}ClF$ ([M+H]$^+$):

High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : D162180

Sample Serial Number: YG-83 compound **4n**

Operator : 001 Date: 2016/08/27

Operation Mode: DART Positive

Elemental composition search on mass 401.09

m/z= 396.09-406.09

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
401.0875	401.0877	-0.44	13.5	$C_{21}H_{17}O_3N_2{}^{37}ClF$
	401.0880	-1.36	17.5	$C_{21}H_{13}O_5N_4$
	401.0865	2.41	17.5	$C_{24}H_{16}O_2N_2{}^{37}Cl$
	401.0863	2.91	14.0	$C_{19}H_{15}O_2N_5{}^{37}ClF$
	401.0862	3.34	13.5	$C_{24}H_{20}{}^{37}Cl_2F$
	401.0855	4.92	5.0	$C_{13}H_{21}O_5N_5{}^{37}Cl_2$

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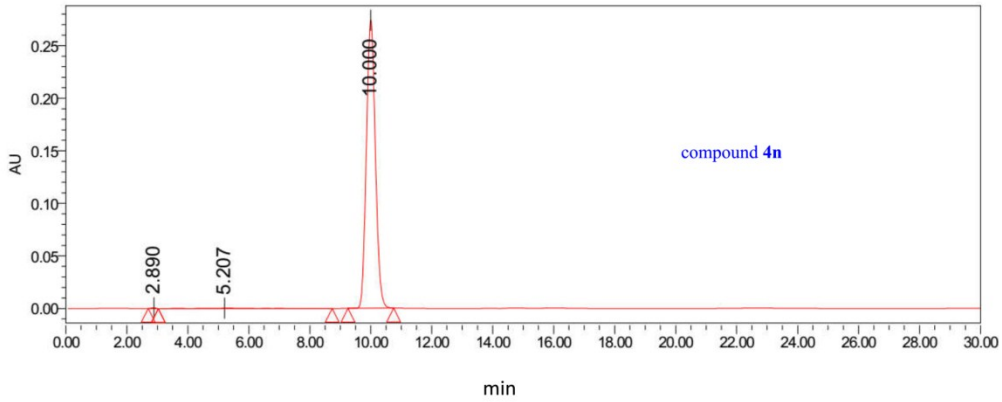
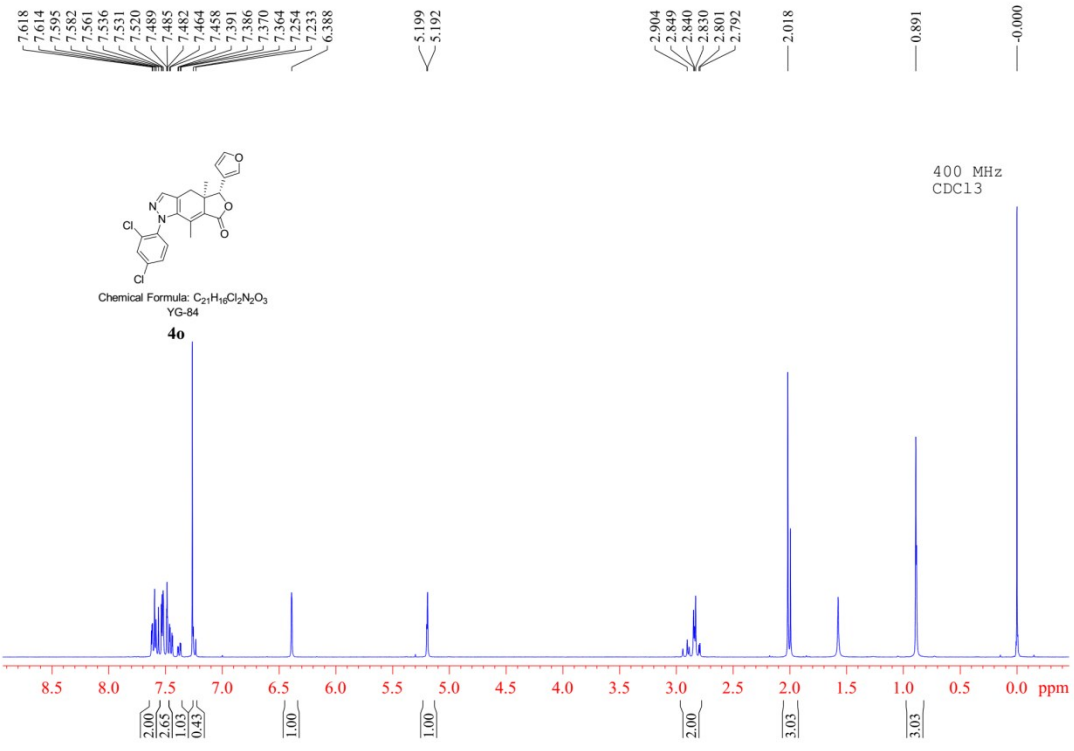
Waters Reports

Sample Information			
Sample Name	YG-83	Collector	System
Sample Type	Standard	Collection Method Group	YG
Bottle Number	8	Collection Time	2016/12/26 23:19:38 CST
Number of Injections	1	Processing Date	2016/12/27 19:14:44 CST
Injection Volume	10.00 *ul*	Processing Method	1
Run Time	30.0 Minutes	Channel Name	W2489 ChA 254nm



Name	Retention Time (min)	Area (μV*s)	% Area	Height (μV)
1	2.890	7872	0.14	792
2	5.207	60523	1.07	376
3	10.000	5598605	98.79	273865



High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : D162176

Sample Serial Number: YG-84 compound **4o**

Operator : 001 Date: 2016/08/27

Operation Mode: DART Positive

Elemental composition search on mass 415.06

m/z= 410.06-420.06

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
415.0609	415.0611	-0.35	13.5	$C_{21}H_{17}O_3N_2Cl_2$
	415.0606	0.83	18.0	$C_{24}H_{14}O_4NCl$
	415.0614	-1.22	27.5	$C_{28}H_7ON_4$
	415.0601	2.00	22.5	$C_{27}H_{11}O_5$
	415.0619	-2.40	23.0	$C_{25}H_{10}N_5Cl$
	415.0597	2.89	14.0	$C_{19}H_{15}O_2N_5Cl_2$
	415.0592	4.06	18.5	$C_{22}H_{12}O_3N_4Cl$
	415.0628	-4.46	27.0	$C_{30}H_9O_2N$

For $C_{21}H_{17}O_3N_2{}^{37}Cl_2$ ($[M+H]^+$):

High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : D162176

Sample Serial Number: YG-84 compound **4o**

Operator : 001 Date: 2016/08/27

Operation Mode: DART Positive

Elemental composition search on mass 419.06

m/z= 414.06-424.06

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
419.0552	419.0552	0.01	13.5	$C_{21}H_{17}O_3N_2{}^{37}Cl_2$
	419.0564	-2.80	26.5	$C_{27}H_7O_2N_4$
	419.0538	3.22	14.0	$C_{19}H_{15}O_2N_5{}^{37}Cl_2$
	419.0537	3.60	22.0	$C_{24}H_9O_5N_3$

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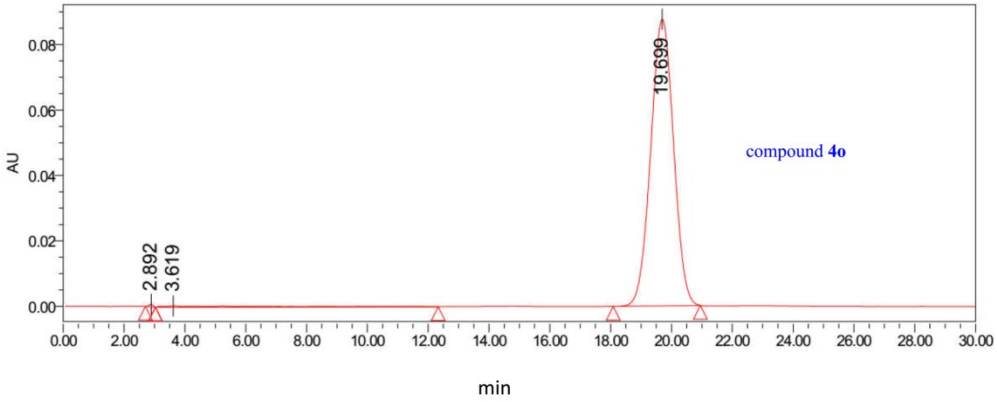
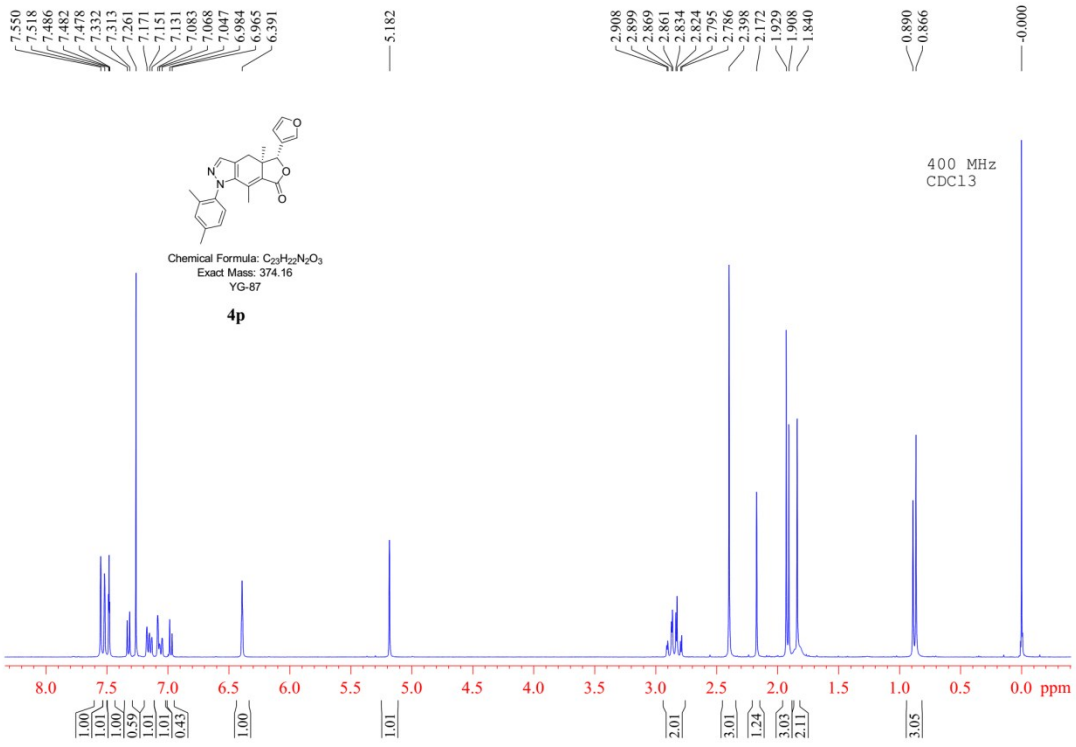
Waters Reports

Sample Information			
Sample Name	YG-84	Collector	System
Sample Type	Standard	Collection Method Group	YG
Bottle Number	9	Collection Time	2016/12/26 23:50:15 CST
Number of Injections	1	Processing Date	2016/12/27 19:15:39 CST
Injection Volume	10.00 *ul*	Processing Method	1
Run Time	30.0 Minutes	Channel Name	W2489 ChA 254nm



Name	Retention Time (min)	Area (μV*s)	% Area	Height (μV)
1	2.892	7767	0.17	779
2	3.619	110334	2.35	422
3	19.699	4579598	97.49	87594



High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : D162179

Sample Serial Number: YG-87 compound **4p**

Operator : 001 Date: 2016/08/27

Operation Mode: DART Positive

Elemental composition search on mass 375.17

m/z= 370.17-380.17

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
375.1702	375.1703	-0.29	13.5	$C_{23}H_{23}O_3N_2$
	375.1690	3.29	14.0	$C_{21}H_{21}O_2N_5$

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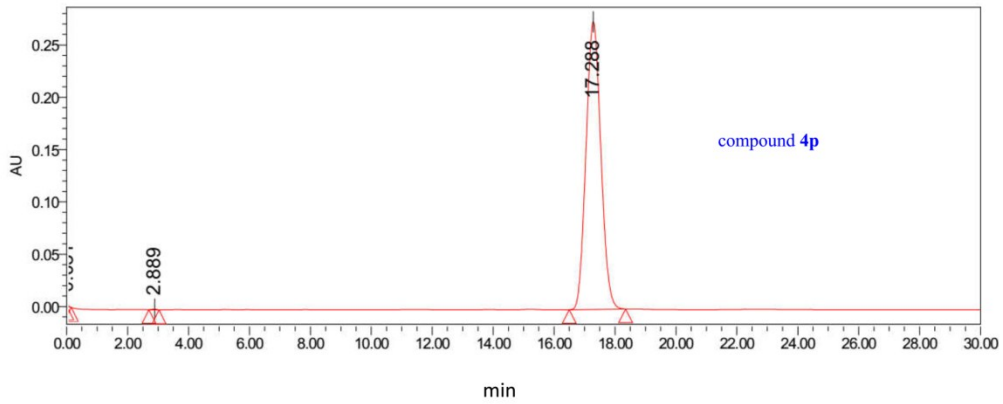
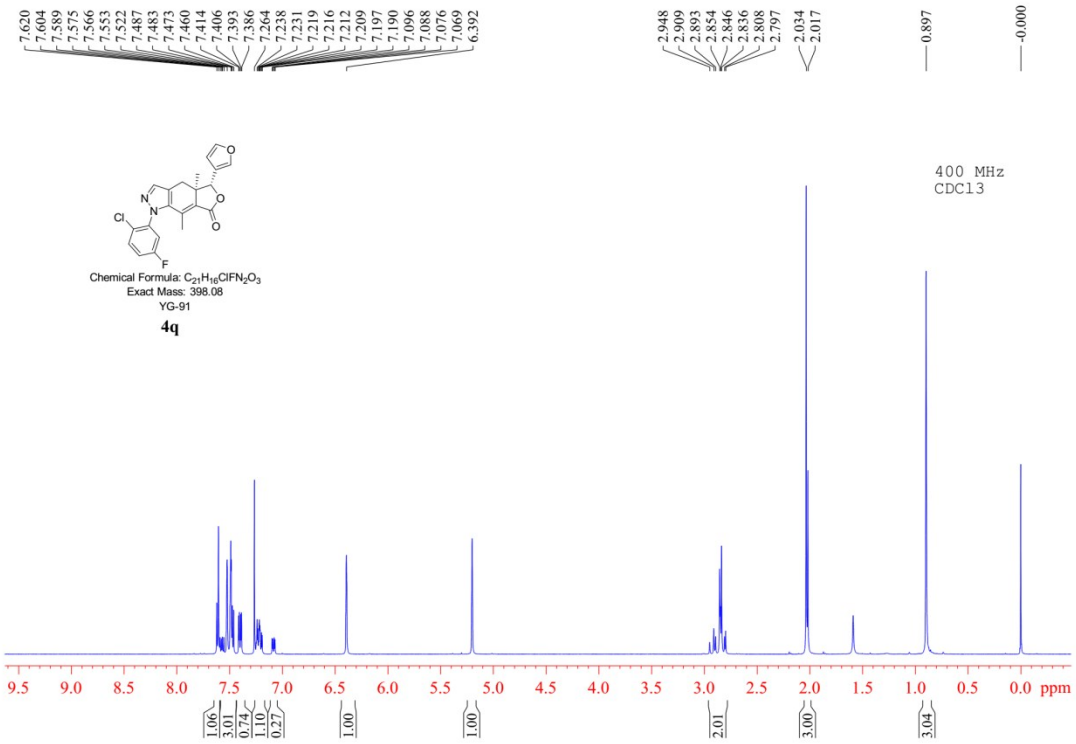
Waters Reports

Sample Information			
Sample Name	YG-87	Collector	System
Sample Type	Standard	Collection Method Group	YG
Bottle Number	12	Collection Time	2016/12/27 1:22:11 CST
Number of Injections	1	Processing Date	2016/12/27 19:17:25 CST
Injection Volume	10.00 ul	Processing Method	1
Run Time	30.0 Minutes	Channel Name	W2489 ChA 254nm



Name	Retention Time (min)	Area (μV*s)	% Area	Height (μV)
1	0.031	394	0.04	986
2	2.889	7868	0.08	784
3	17.288	9289227	99.87	274895



High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : D162183

Sample Serial Number: YG-91 compound **4q**

Operator : 001 Date: 2016/08/27

Operation Mode: DART Positive

Elemental composition search on mass 399.09

m/z= 394.09-404.09

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
399.0905	399.0906	-0.34	13.5	$C_{21}H_{17}O_3N_2ClF$
	399.0901	0.88	18.0	$C_{24}H_{14}O_4NF$
	399.0915	-2.47	23.0	$C_{25}H_{10}N_5F$
	399.0895	2.53	17.5	$C_{24}H_{16}O_2N_2Cl$
	399.0917	-2.97	26.5	$C_{30}H_{11}N_2$
	399.0893	3.03	14.0	$C_{19}H_{15}O_2N_5ClF$
	399.0890	3.75	22.0	$C_{27}H_{13}O_3N$
	399.0888	4.25	18.5	$C_{22}H_{12}O_3N_4F$

For $C_{21}H_{17}O_3N_2{}^{37}ClF$ ([M+H]$^+$):

High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : D162183

Sample Serial Number: YG-91 compound **4q**

Operator : 001 Date: 2016/08/27

Operation Mode: DART Positive

Elemental composition search on mass 401.09

m/z= 396.09-406.09

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
401.0876	401.0877	-0.19	13.5	$C_{21}H_{17}O_3N_2{}^{37}ClF$
	401.0880	-1.11	17.5	$C_{21}H_{13}O_5N_4$
	401.0865	2.66	17.5	$C_{24}H_{16}O_2N_2{}^{37}Cl$
	401.0863	3.16	14.0	$C_{19}H_{15}O_2N_5{}^{37}ClF$
	401.0862	3.59	13.5	$C_{24}H_{20}{}^{37}Cl_2F$
	401.0895	-4.86	9.0	$C_{18}H_{21}O_3N_3{}^{37}Cl_2$

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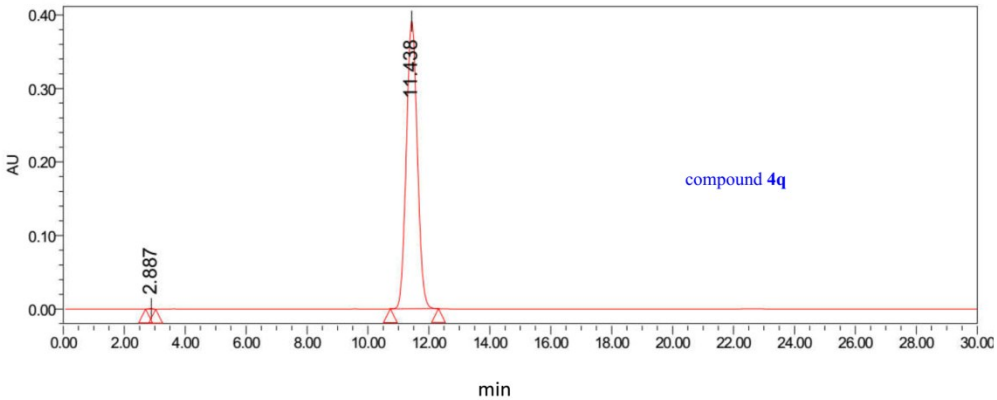
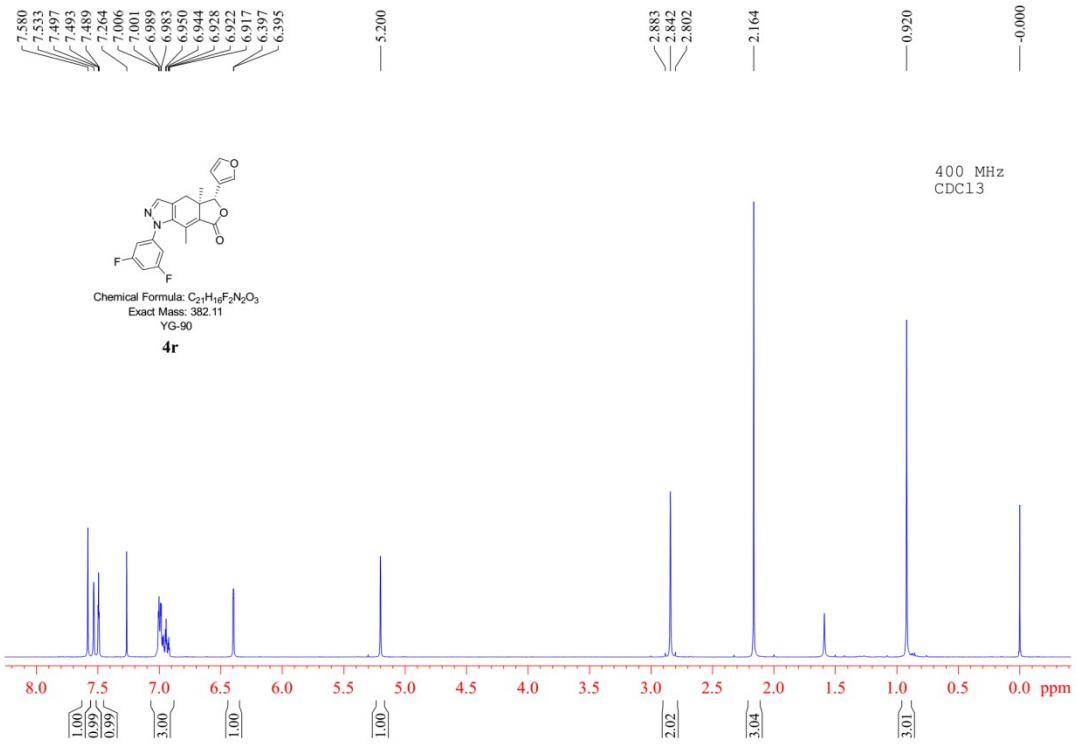
Waters Reports

Sample Information			
Sample Name	YG-91	Collector	System
Sample Type	Standard	Collection Method Group	YG
Bottle Number	16	Collection Time	2016/12/27 3:24:53 CST
Number of Injections	1	Processing Date	2016/12/27 19:20:07 CST
Injection Volume	10.00 ul	Processing Method	1
Run Time	30.0 Minutes	Channel Name	W2489 ChA 254nm



Name	Retention Time (min)	Area (μV*s)	% Area	Height (μV)
1	2.887	7662	0.08	762
2	11.438	9829269	99.92	391530



High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : D162182

Sample Serial Number: YG-90 compound **4r**

Operator : 001 Date: 2016/08/27

Operation Mode: DART Positive

Elemental composition search on mass 383.12

m/z= 378.12-388.12

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
383.1201	383.1202	-0.17	13.5	$C_{21}H_{17}O_3N_2F_2$
	383.1190	2.81	17.5	$C_{24}H_{16}O_2N_2F$
	383.1188	3.33	14.0	$C_{19}H_{15}O_2N_5F_2$

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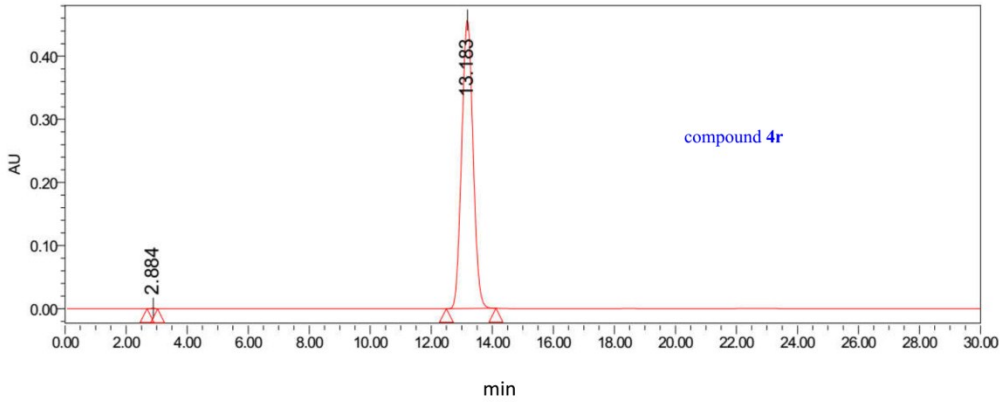
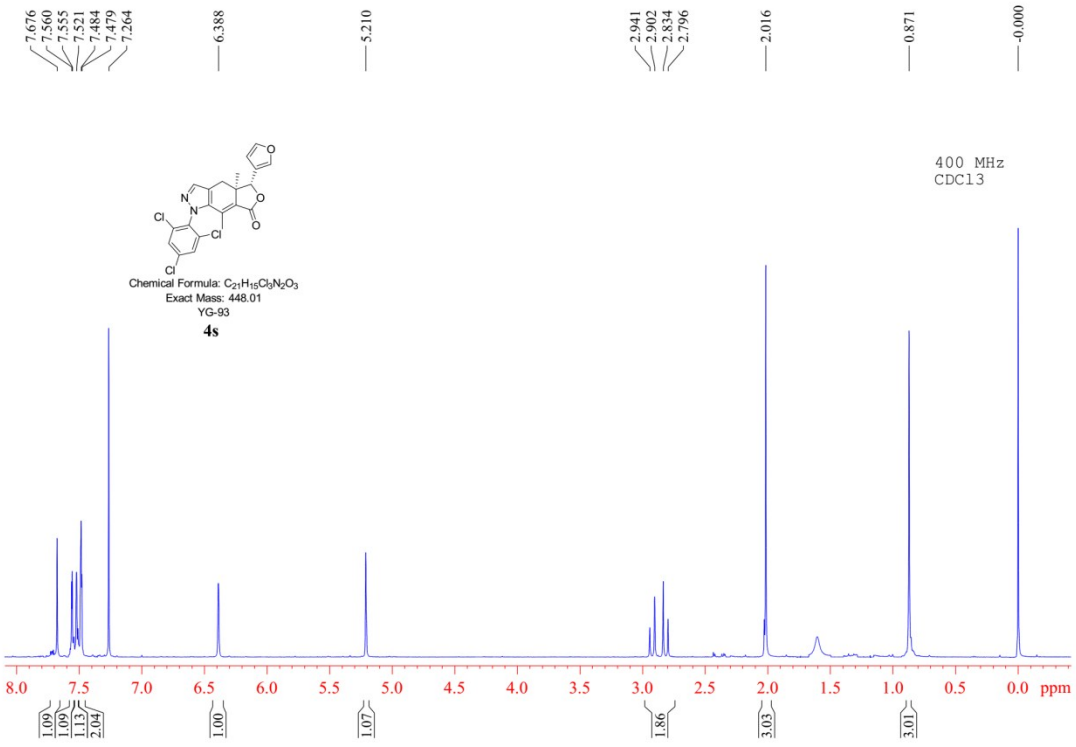
Waters Reports

Sample Information			
Sample Name	YG-90	Collector	System
Sample Type	Standard	Collection Method Group	YG
Bottle Number	15	Collection Time	2016/12/27 2:54:14 CST
Number of Injections	1	Processing Date	2016/12/27 19:19:38 CST
Injection Volume	10.00 *ul*	Processing Method	1
Run Time	30.0 Minutes	Channel Name	W2489 ChA 254nm



Name	Retention Time (min)	Area (μV*s)	% Area	Height (μV)
1	2.884	7950	0.07	785
2	13.183	11834021	99.93	456910



High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : D162185

Sample Serial Number: YG-93 compound **4s**

Operator :001 Date: 2016/08/27

Operation Mode: DART Positive

Elemental composition search on mass 449.02

m/z= 444.02-454.02

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
449.0218	449.0216	0.30	18.0	$C_{24}H_{13}O_4NCl_2$
	449.0219	-0.34	10.0	$C_{16}H_{15}O_3N_5Cl_3F$
	449.0214	0.75	14.5	$C_{19}H_{12}O_4N_4Cl_2F$
	449.0221	-0.78	13.5	$C_{21}H_{16}O_3N_2Cl_3$
	449.0211	1.39	22.5	$C_{27}H_{10}O_5Cl$
	449.0225	-1.59	27.5	$C_{28}H_6ON_4Cl$
	449.0209	1.83	19.0	$C_{22}H_9O_5N_3ClF$
	449.0208	2.21	14.0	$C_{19}H_{14}O_2N_5Cl_3$
	449.0228	-2.24	14.0	$C_{21}H_{14}O_5NCl_2F$
	449.0230	-2.68	23.0	$C_{25}H_9N_5Cl_2$

For $C_{21}H_{16}O_3N_2{}^{37}Cl_3$ ($[M+H]^+$):

High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : D162185

Sample Serial Number: YG-93 compound **4s**

Operator : 001 Date: 2016/08/27

Operation Mode: DART Positive

Elemental composition search on mass 455.01

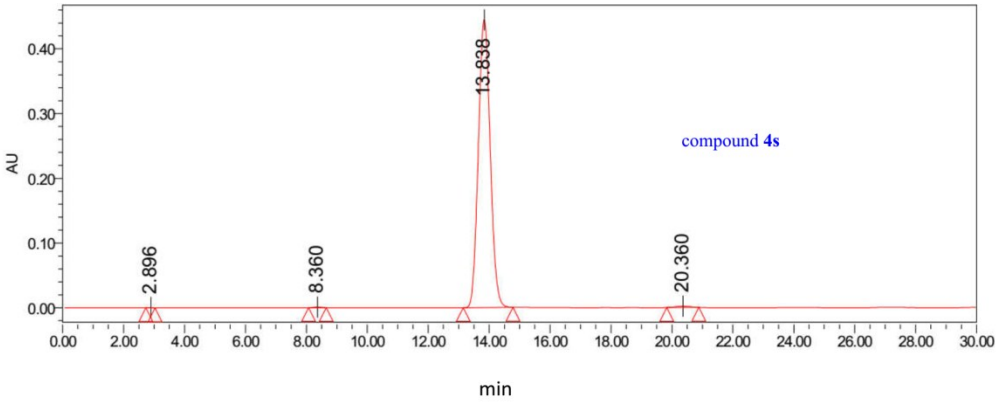
m/z= 450.01-460.01

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
455.0130	455.0133	-0.58	13.5	$C_{21}H_{16}O_3N_2{}^{37}Cl_3$
	455.0119	2.38	14.0	$C_{19}H_{14}O_2N_5{}^{37}Cl_3$
	455.0117	2.73	22.0	$C_{24}H_8O_5N_3{}^{37}Cl$
	455.0144	-3.16	26.5	$C_{27}H_6O_2N_4{}^{37}Cl$

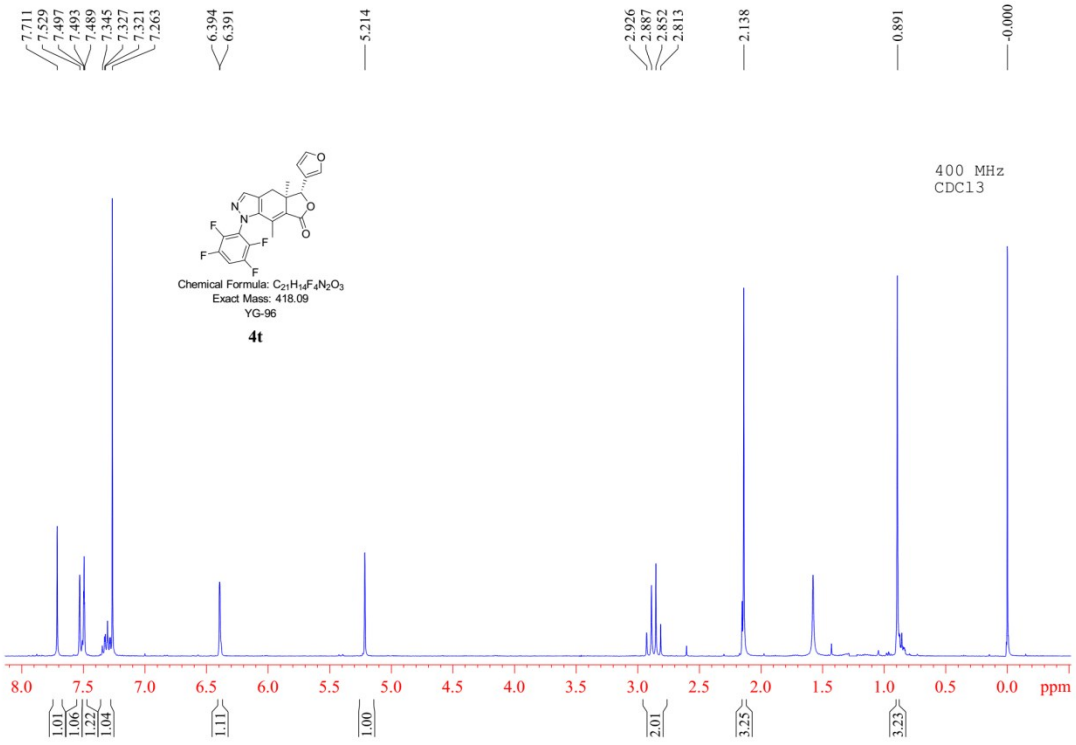
Empower 3 SOFTWARE

Waters Reports

Sample Information			
Sample Name	YG-93	Collector	System
Sample Type	Standard	Collection Method Group	YG
Bottle Number	18	Collection Time	2016/12/27 14:56:30 CST
Number of Injections	1	Processing Date	2016/12/27 19:27:45 CST
Injection Volume	10.00 ul	Processing Method	1
Run Time	30.0 Minutes	Channel Name	W2489 ChA 254nm



Name	Retention Time (min)	Area (μV*s)	% Area	Height (μV)
1	2.896	3918	0.03	426
2	8.360	17664	0.15	1106
3	13.838	12020529	99.29	444621
4	20.360	64229	0.53	1917



High Resolution MS DATA REPORT

Instrument: Thermo Fisher Scientific LTQ FT Ultra

Card Serial Number : D162186

Sample Serial Number: YG-96 compound **4t**

Operator : 001 Date: 2016/08/27

Operation Mode: DART Positive

Elemental composition search on mass 419.10

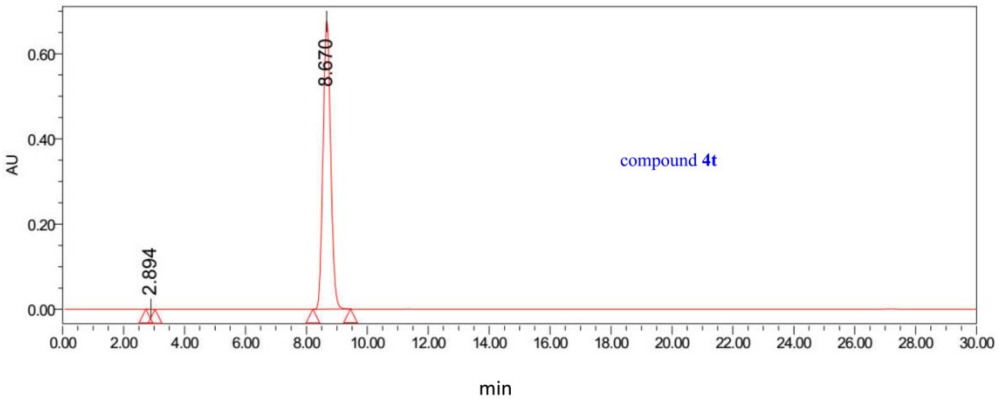
m/z= 414.10-424.10

m/z	Theo. Mass	Delta (ppm)	RDB equiv.	Composition
419.1012	419.1013	-0.29	21.0	$C_{24}H_{13}O_3N_5$
	419.1013	-0.39	13.5	$C_{21}H_{15}O_3N_2F_4$
	419.1002	2.34	17.5	$C_{24}H_{14}O_2N_2F_3$
	419.1000	2.82	14.0	$C_{19}H_{13}O_2N_5F_4$
	419.1024	-3.02	17.0	$C_{21}H_{14}O_4N_5F$
	419.1026	-3.49	20.5	$C_{26}H_{15}O_4N_2$

Empower 3 SOFTWARE

Waters Reports

Sample Information			
Sample Name	YG-96	Collector	System
Sample Type	Standard	Collection Method Group	YG
Bottle Number	19	Collection Time	2016/12/27 15:57:51 CST
Number of Injections	1	Processing Date	2016/12/27 19:28:15 CST
Injection Volume	10.00 ul	Processing Method	1
Run Time	30.0 Minutes	Channel Name	W2489 ChA 254nm



Name	Retention Time (min)	Area (μV*s)	% Area	Height (μV)
1	2.894	4476	0.04	498
2	8.670	11914933	99.96	676592