

## Supplementary Information for:

### Development of quinazolinone derivatives as modulators of virulence factors of *Pseudomonas aeruginosa* cystic fibrosis strains

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HRMS spectrum of compound **7a**

HRMS spectrum of compound **11a**

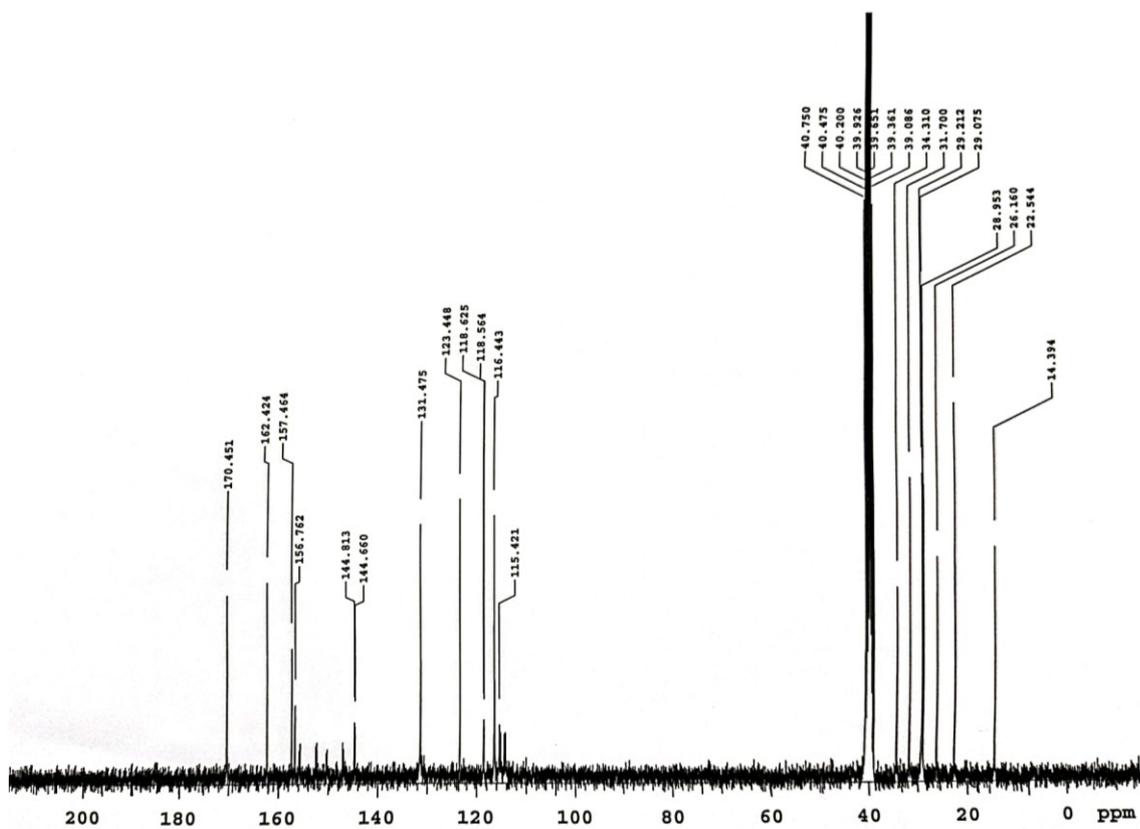
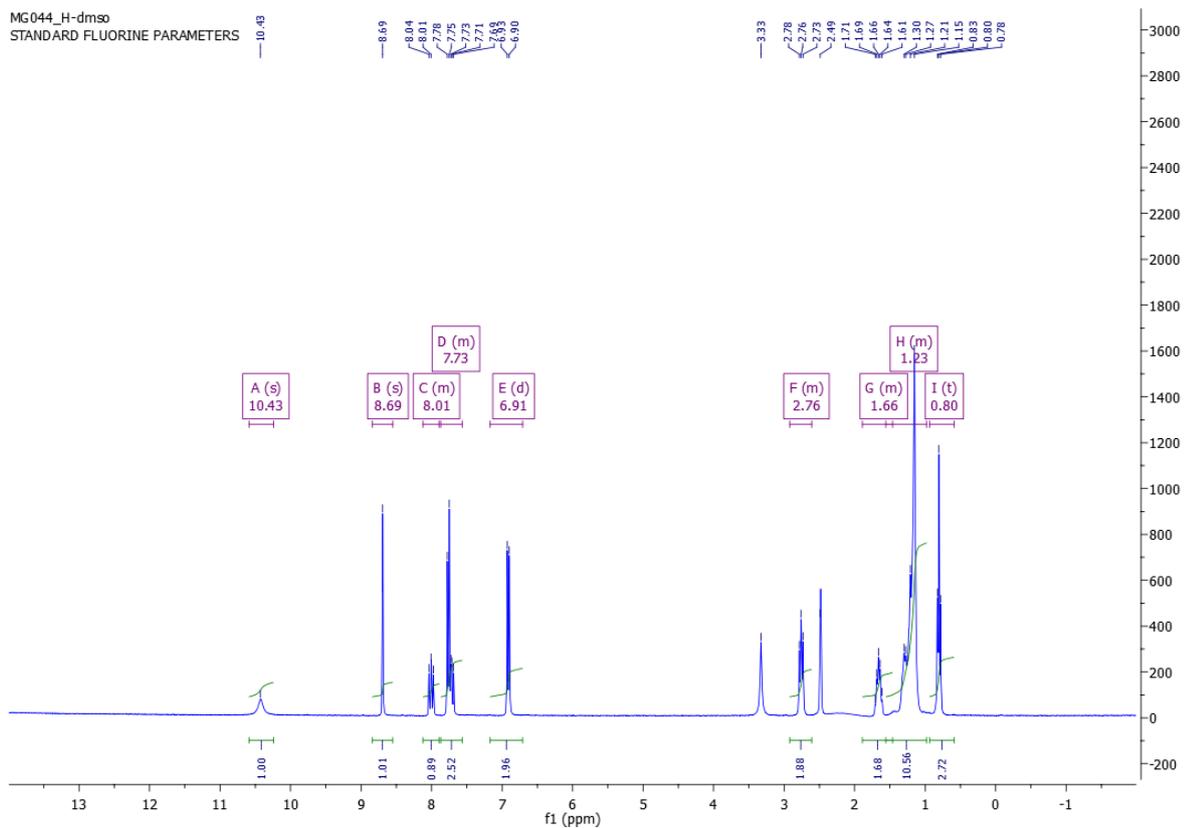
HRMS spectrum of compound **11b**

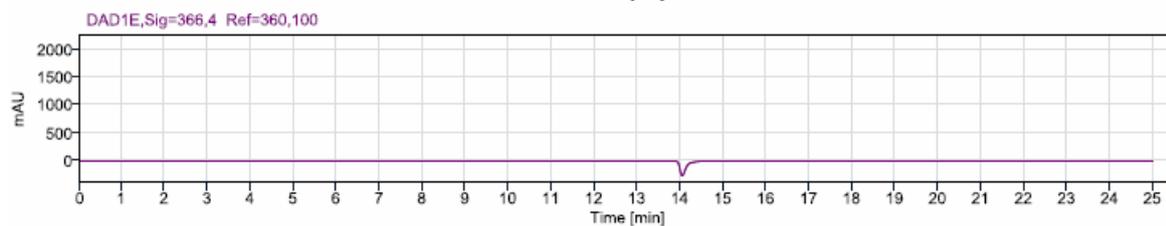
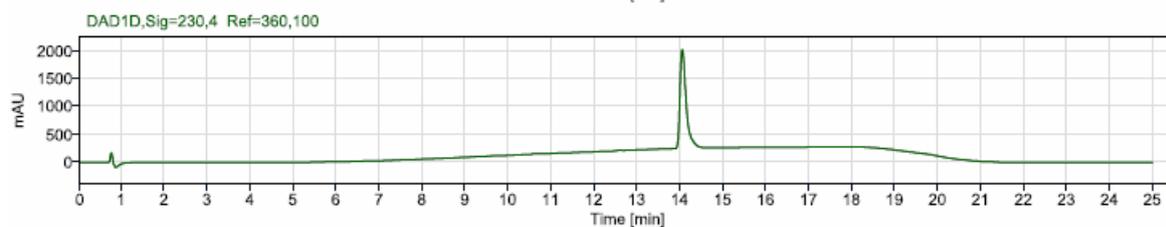
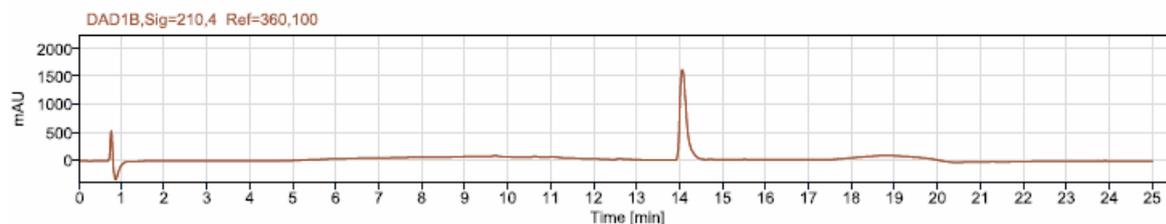
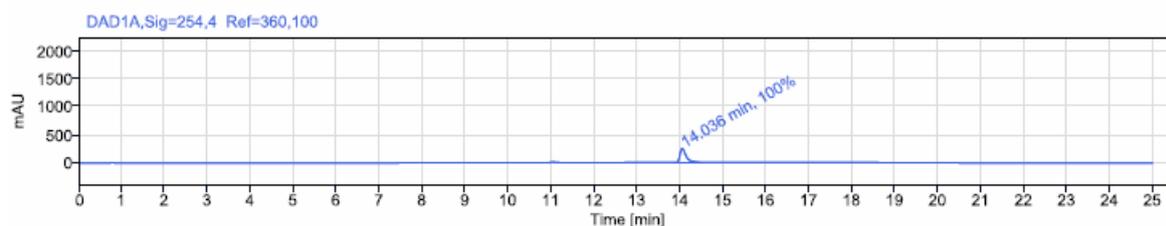
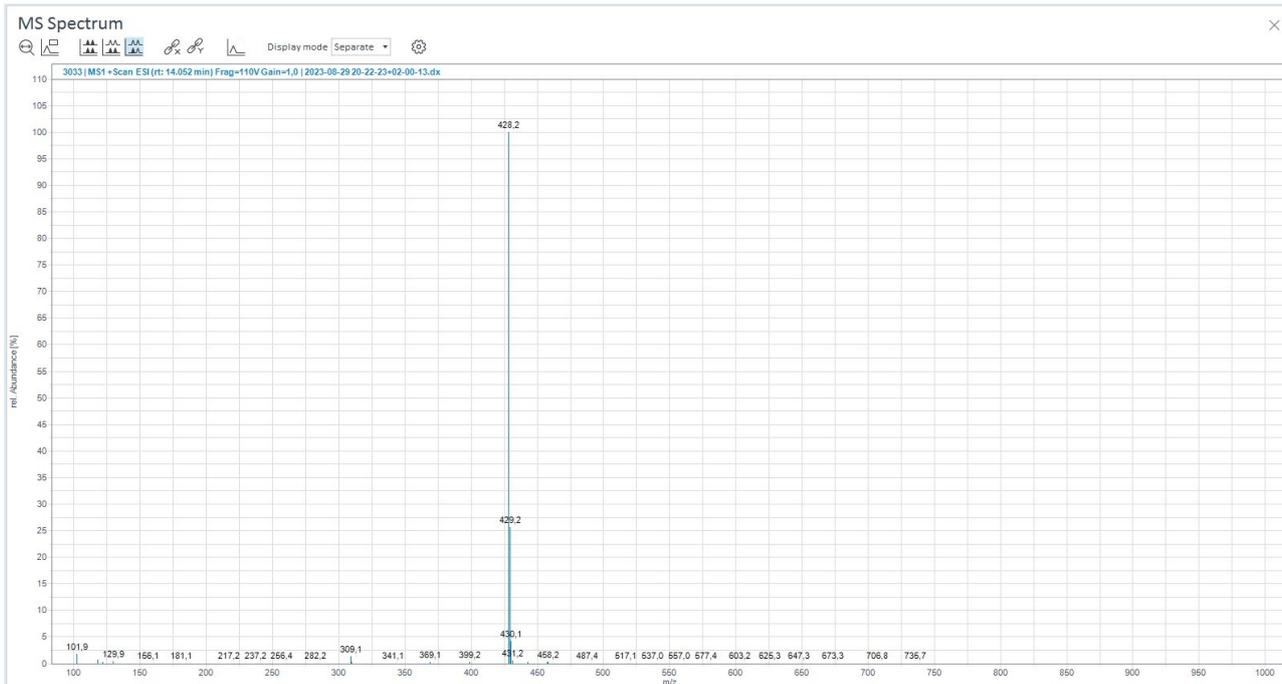
HRMS spectrum of compound **11c**

HRMS spectrum of compound **11d**

# $^1\text{H}$ , $^{13}\text{C}$ NMR and HPLC/MS spectra of compound 7a

MG044\_H-dmsd  
STANDARD FLUORINE PARAMETERS

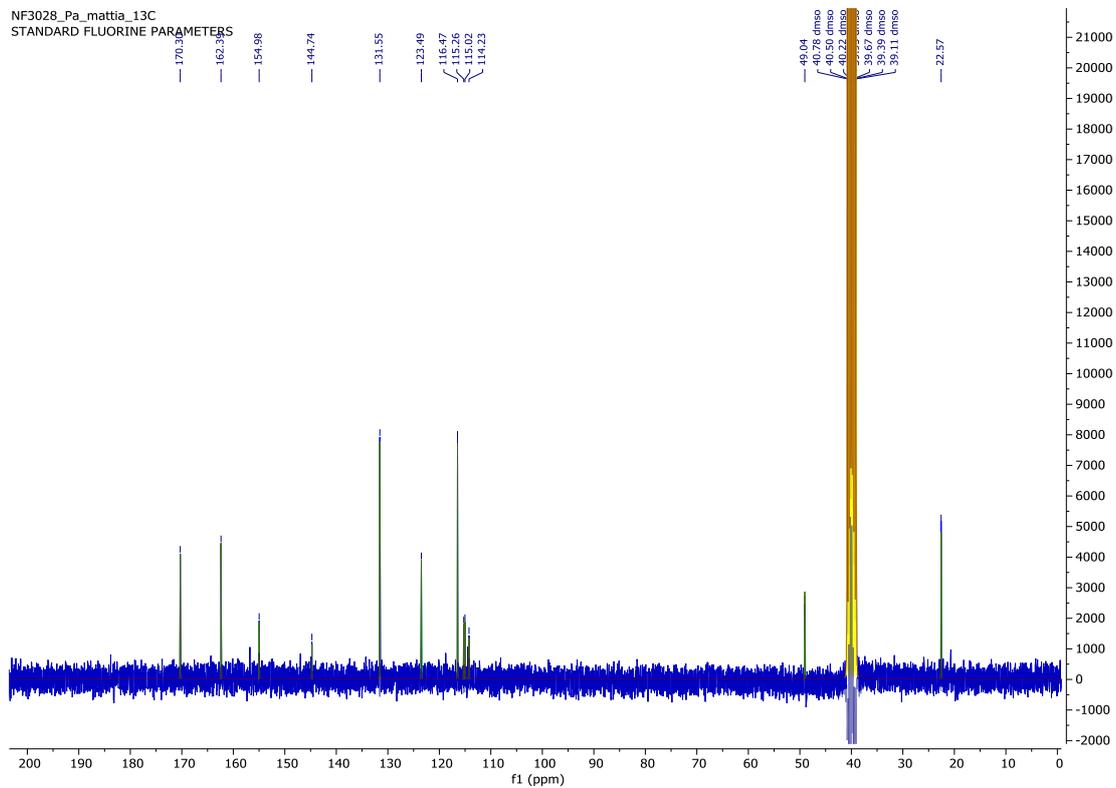
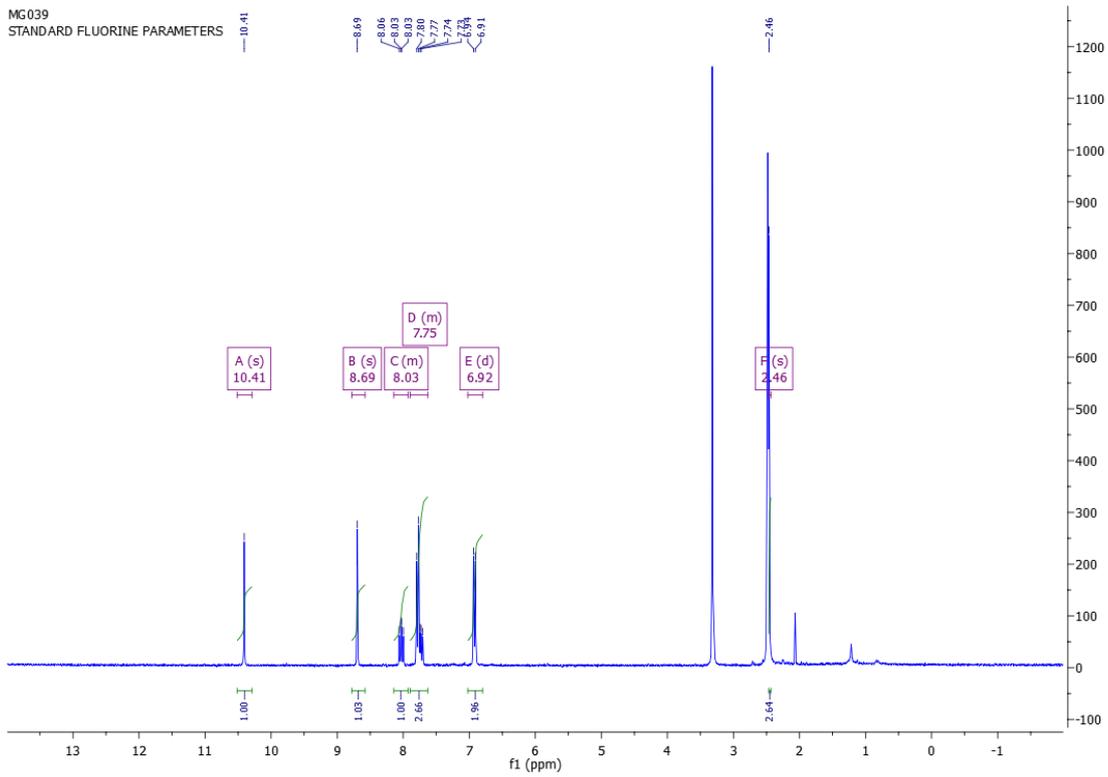


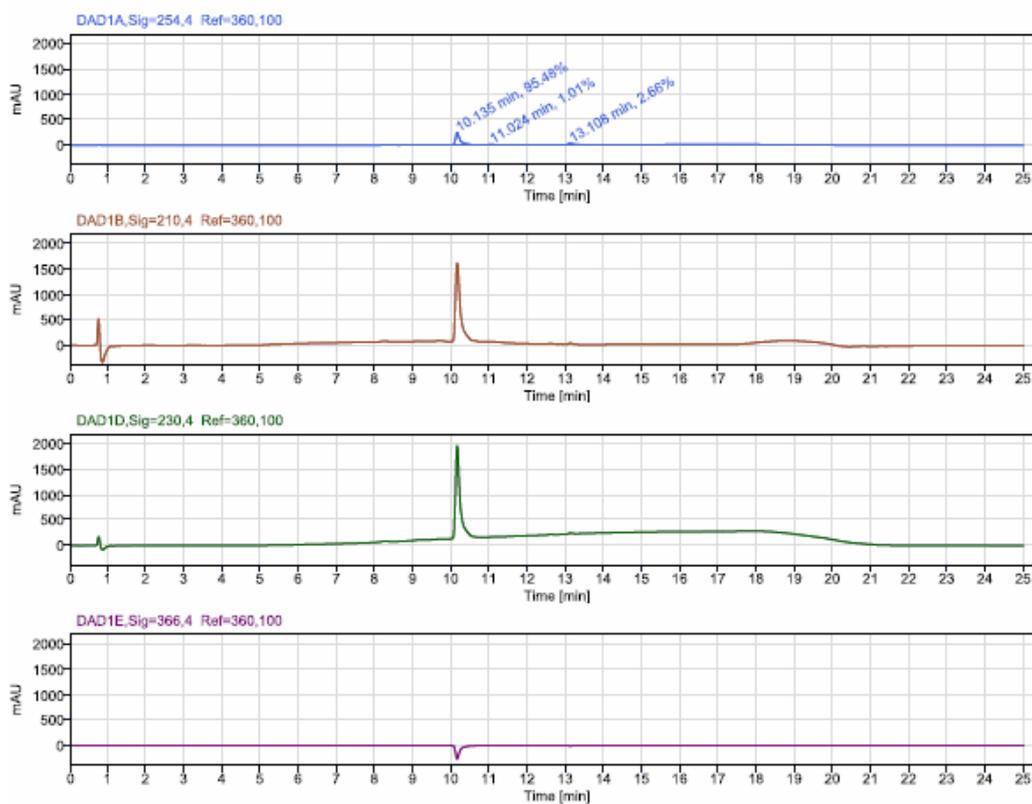
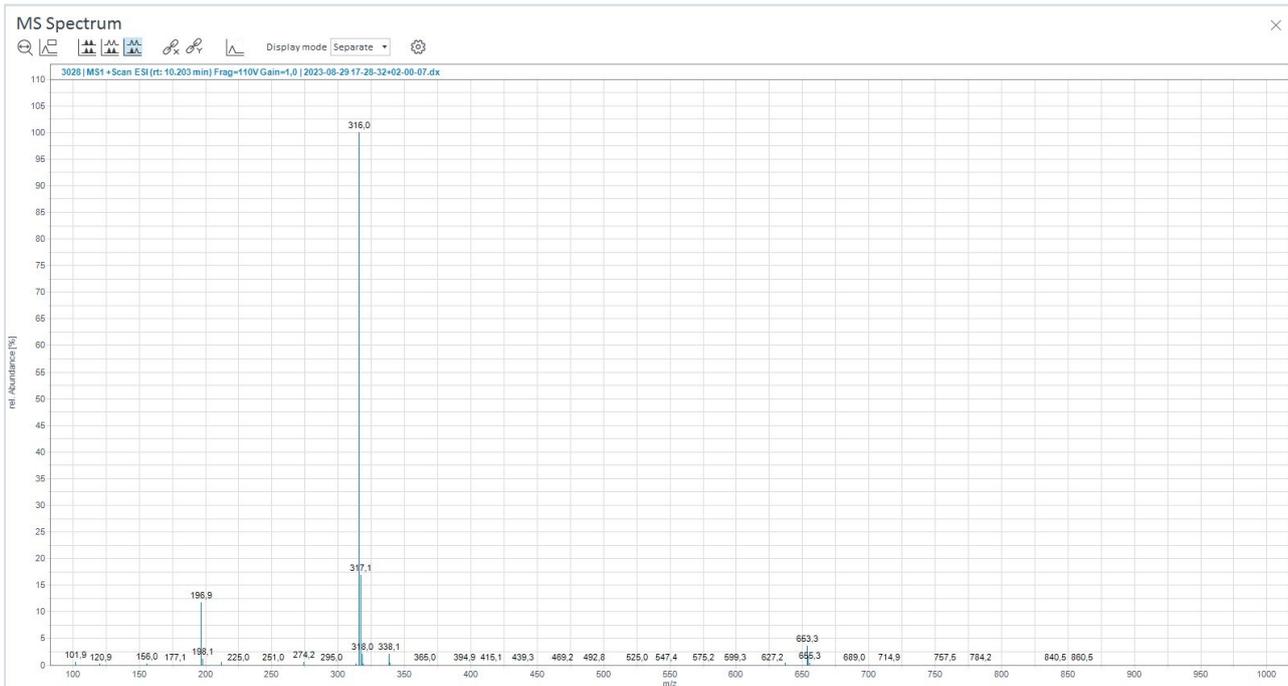


### Peak Results (Area Percent at least 1%)

RT (min)	Signal Description	Width (min)	Area	Height	Area%
14.036	DAD1A, Sig=254,4 Ref=360,100	0.610	2456.4	246.2	100.00
14.056	MS1 +TIC SCAN ESI Frag=110V Gain=1.0	0.792	17266573.7	992387.3	100.00

# <sup>1</sup>H, <sup>13</sup>C NMR and HPLC/MS spectra of compound 7b

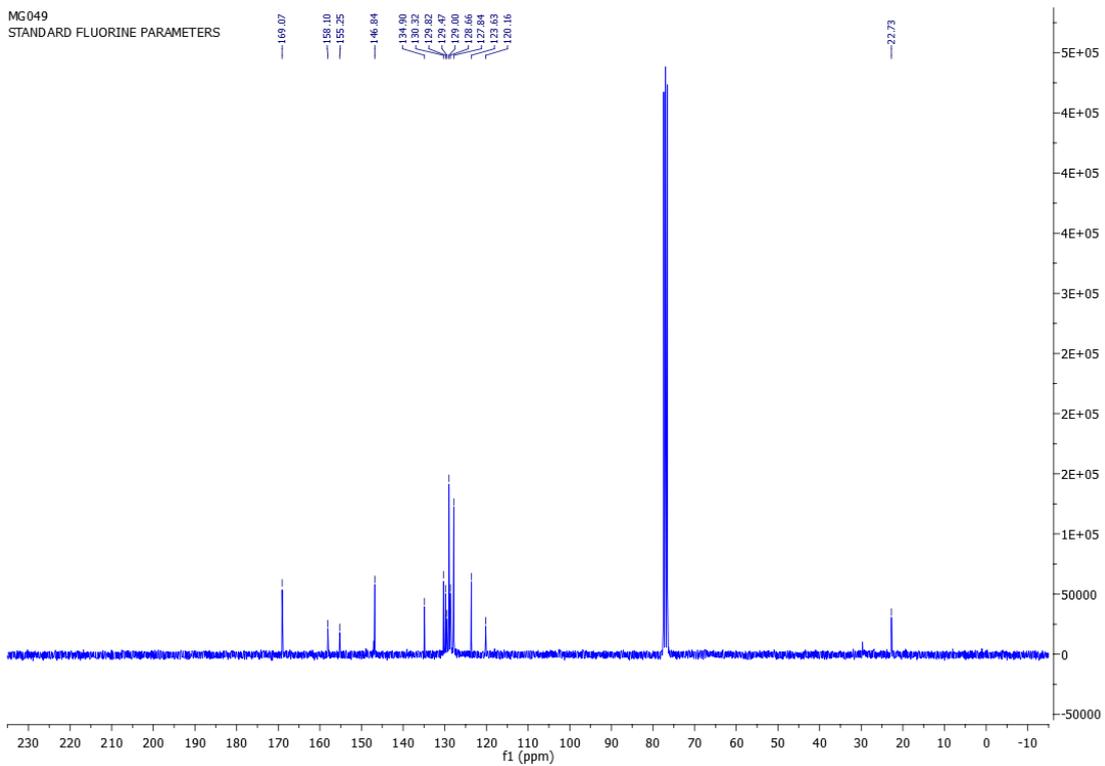
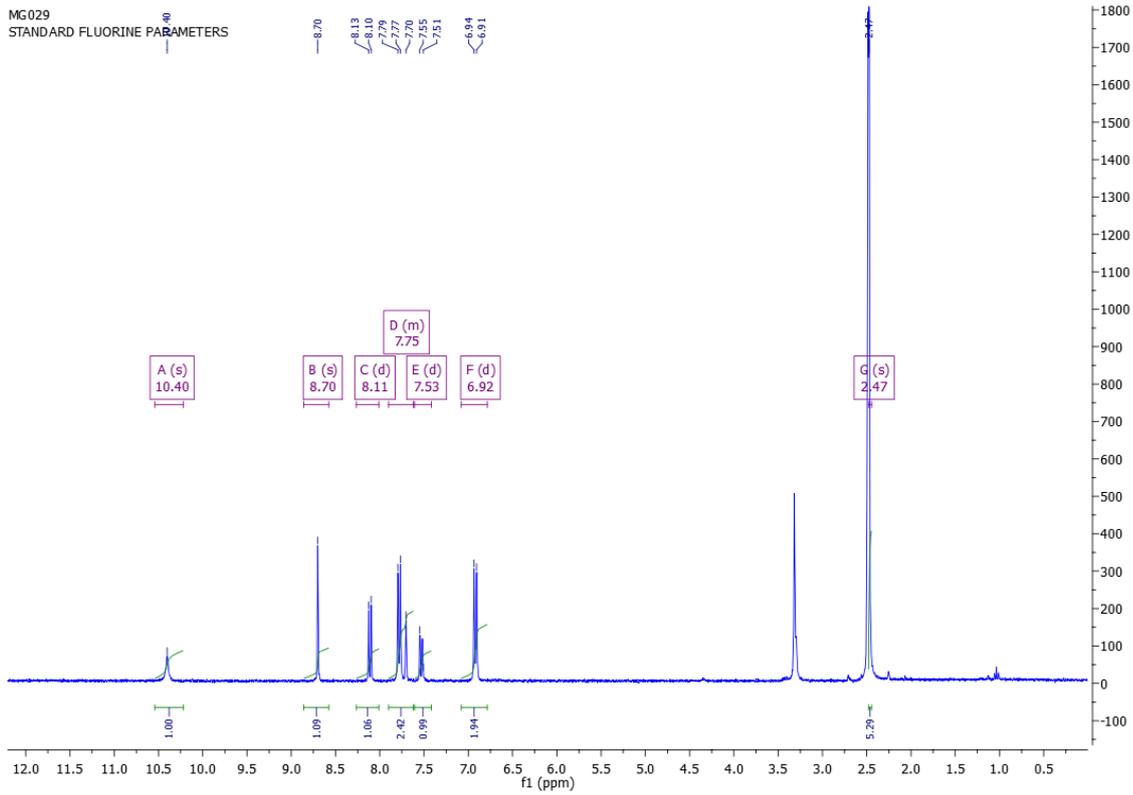


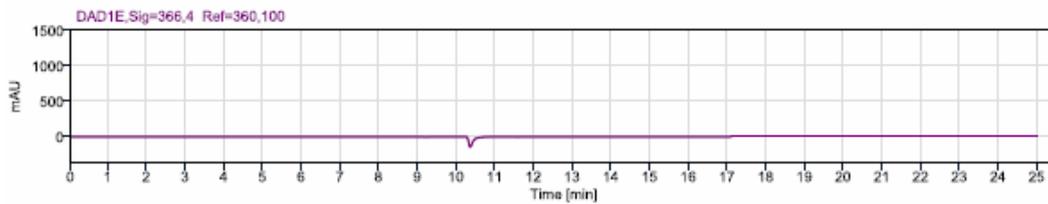
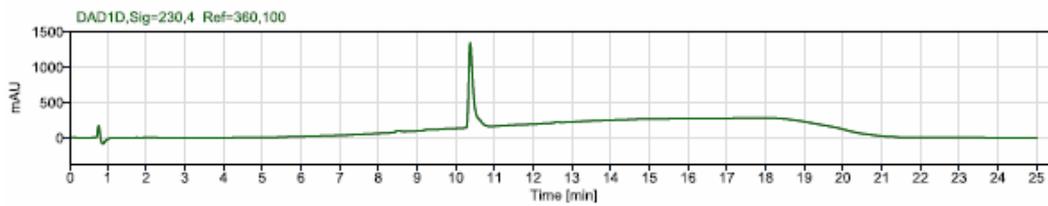
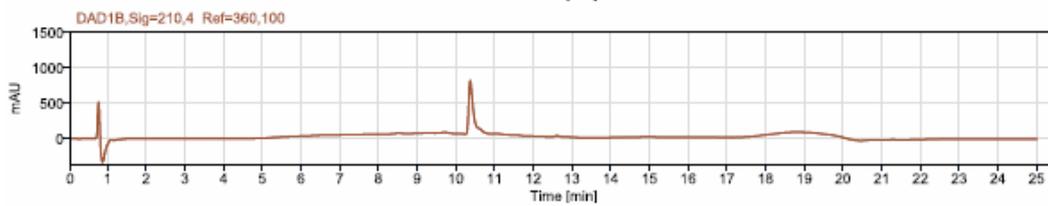
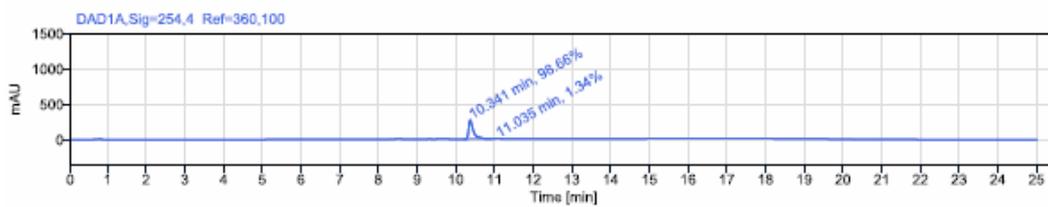
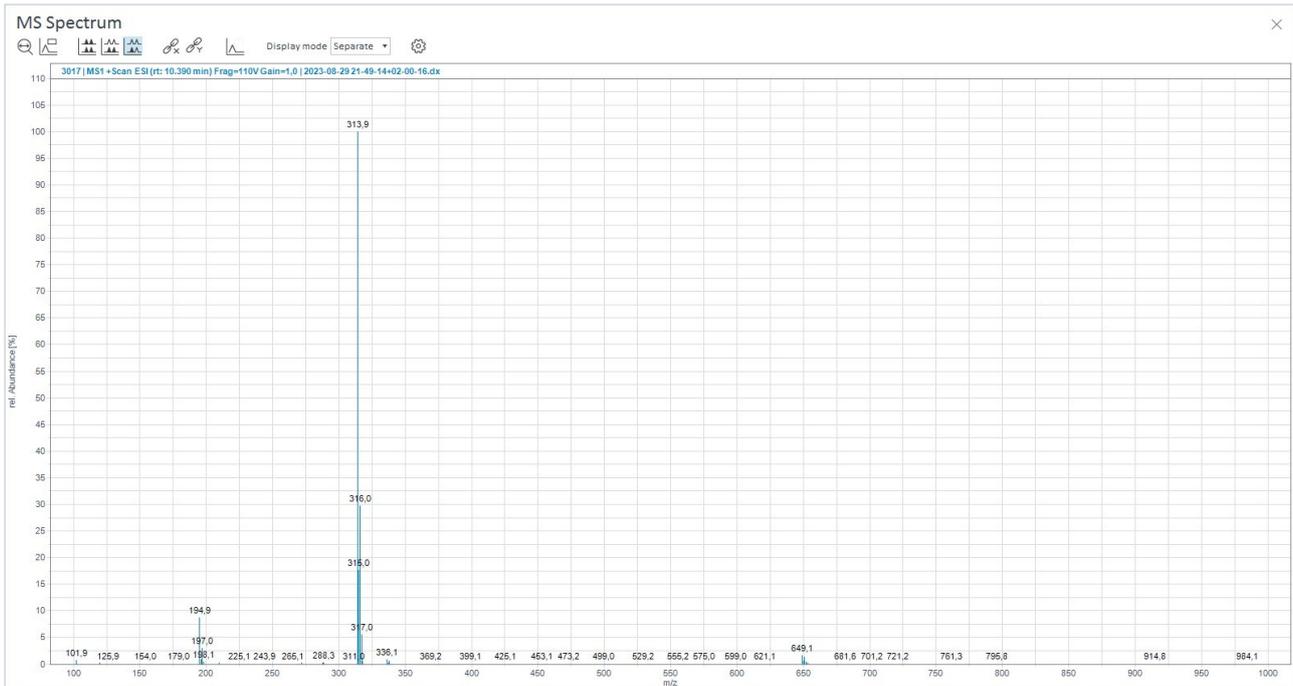


Peak Results (Area Percent at least 1%)

RT (min)	Signal Description	Width (min)	Area	Height	Area%
10.135	DAD1A, Sig=254,4 Ref=360,100	0.957	2041,4	241,0	95,48
10.203	MS1 +TIC SCAN ESI Frag=110V Gain=1.0	0.875	26574503,5	1687708,2	100,00
11.024	DAD1A, Sig=254,4 Ref=360,100	0.134	21,5	4,4	1,01
13.108	DAD1A, Sig=254,4 Ref=360,100	0.146	56,9	12,5	2,66

# <sup>1</sup>H, <sup>13</sup>C NMR and HPLC/MS spectra of compound 7c

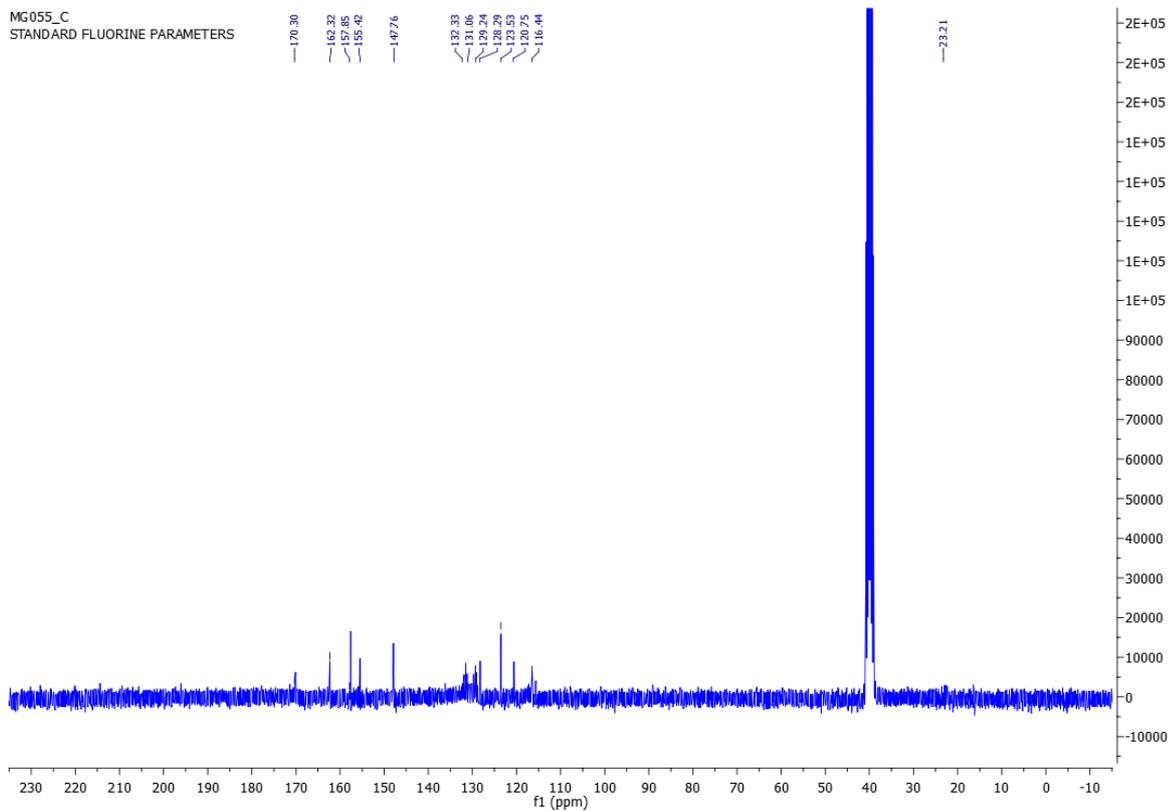
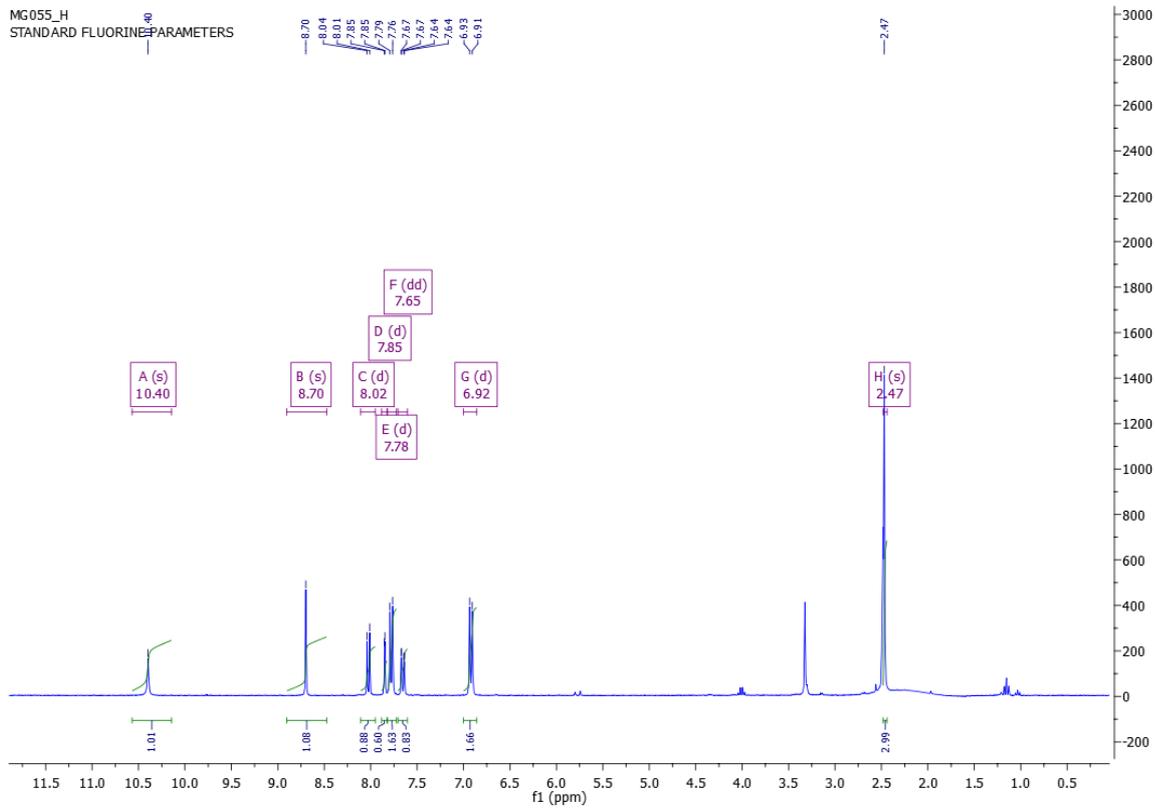


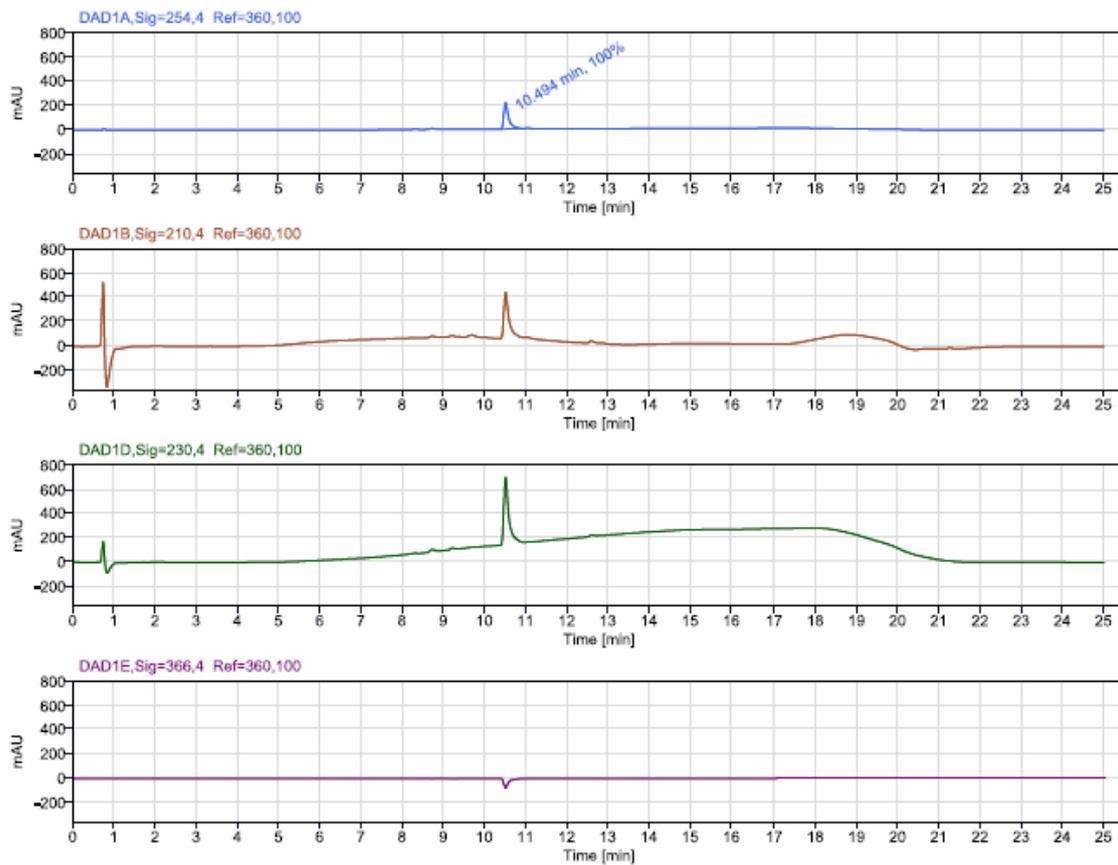
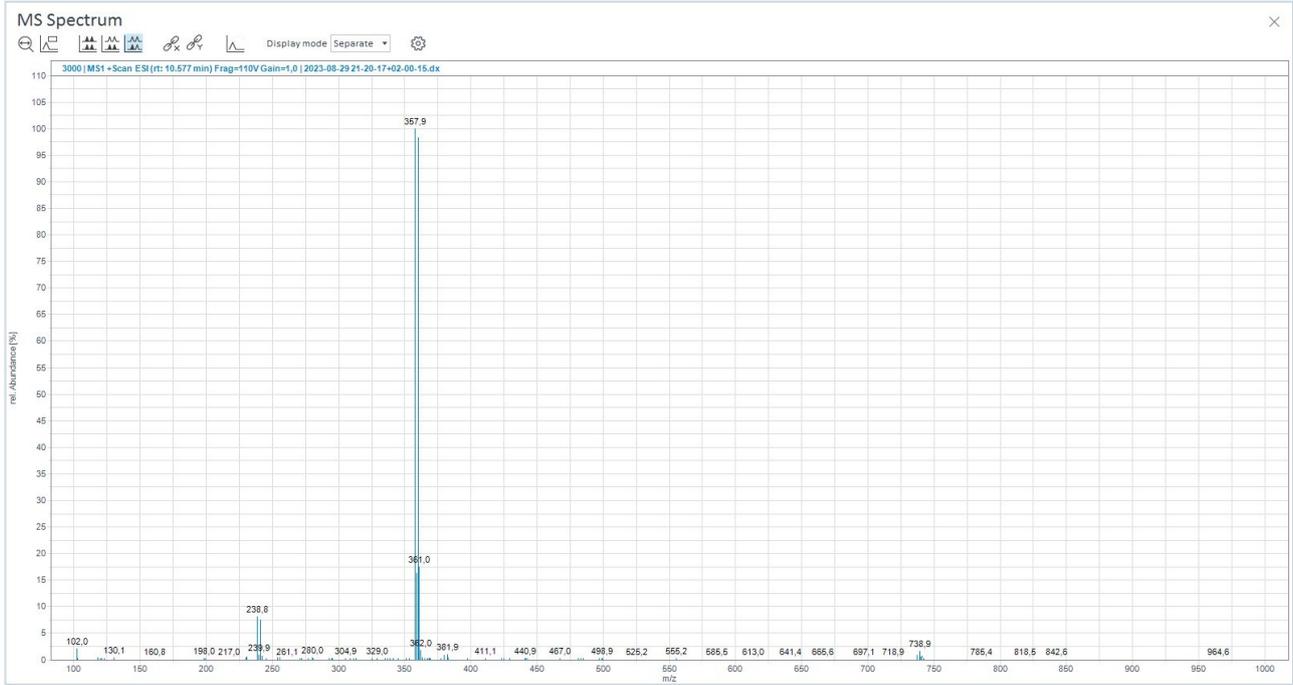


**Peak Results (Area Percent at least 1%)**

RT (min)	Signal Description	Width (min)	Area	Height	Area%
10,341	DAD1A,Sig=254,4 Ref=360,100	0,700	2307,3	272,2	98,66
10,398	MS1 +TIC SCAN ESI Frag=110V Gain=1.0	0,446	18242039,3	1526702,9	100,00
11,035	DAD1A,Sig=254,4 Ref=360,100	0,198	31,3	4,7	1,34

# <sup>1</sup>H, <sup>13</sup>C NMR and HPLC/MS spectra of compound 7d

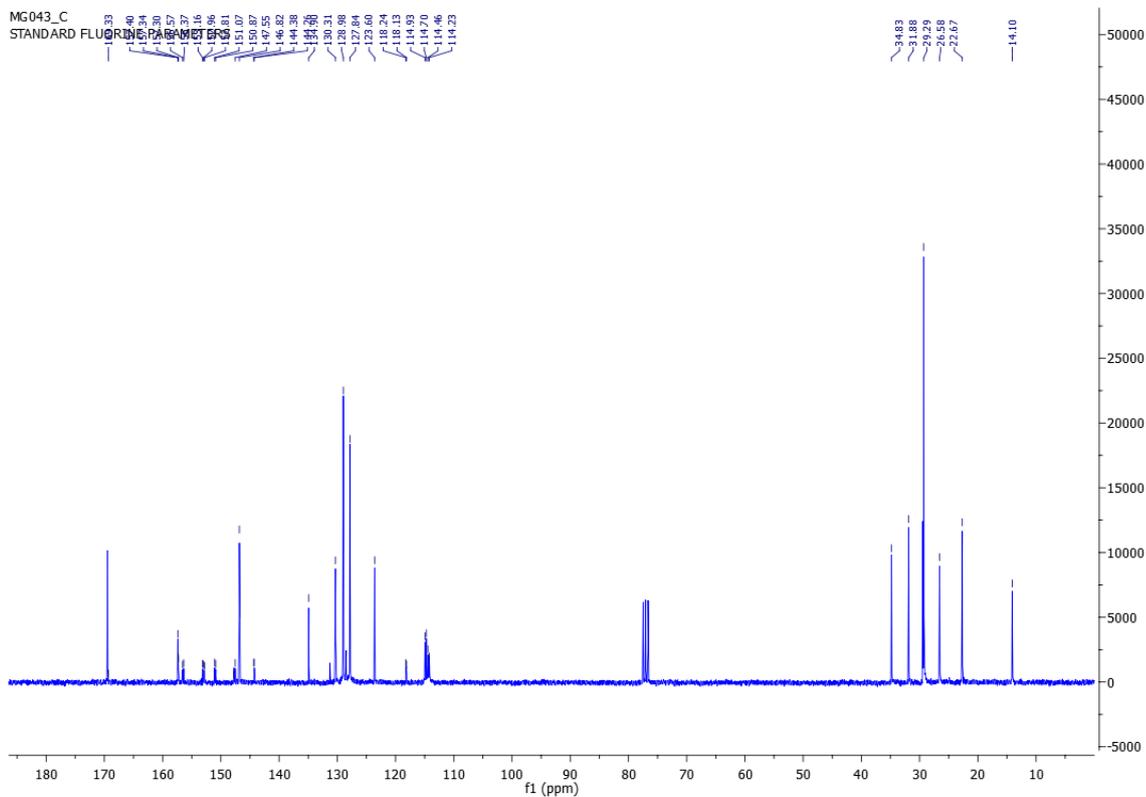
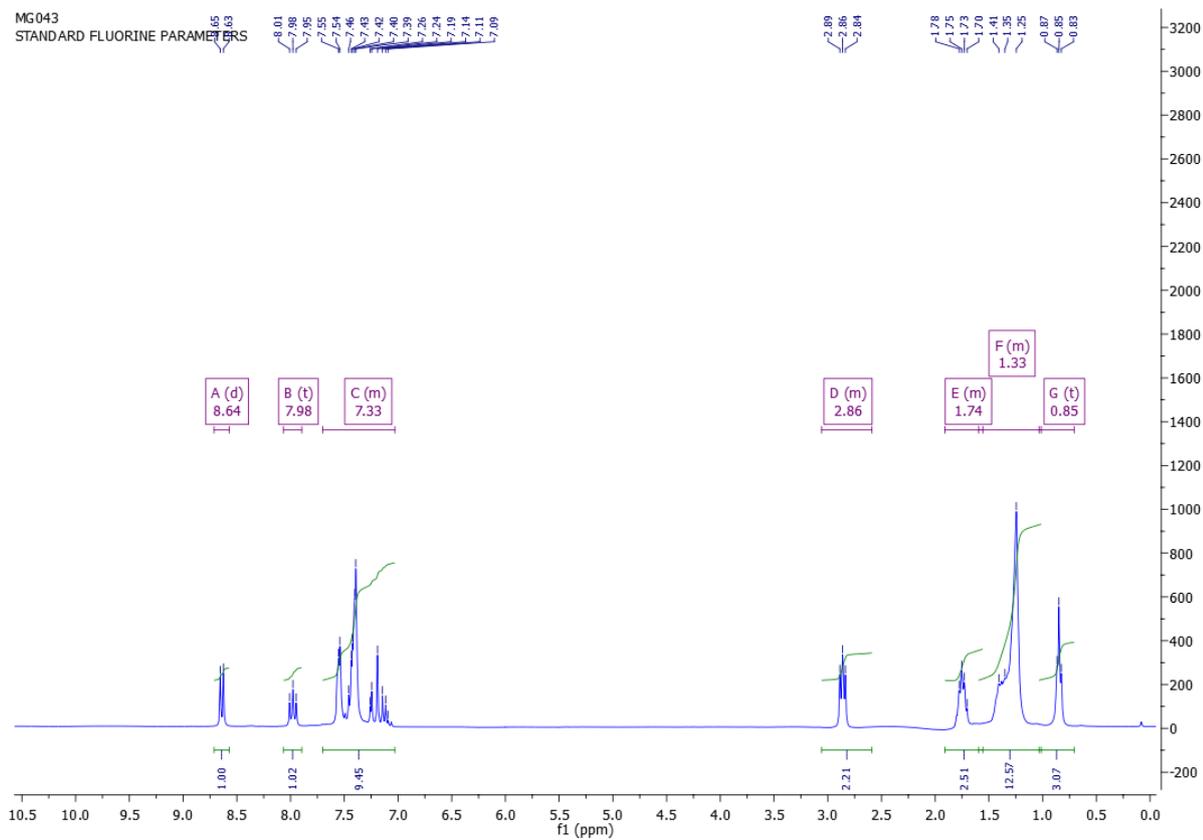


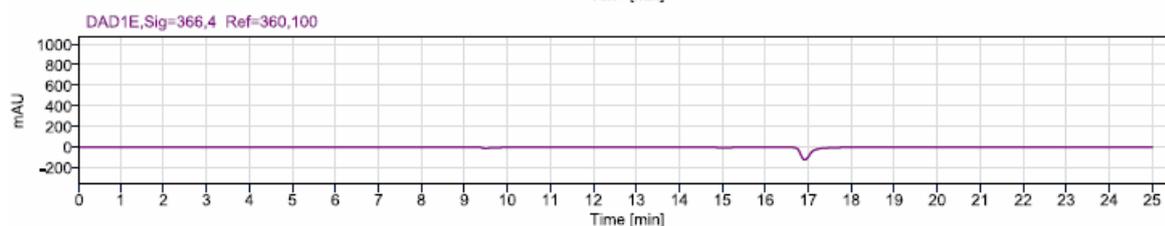
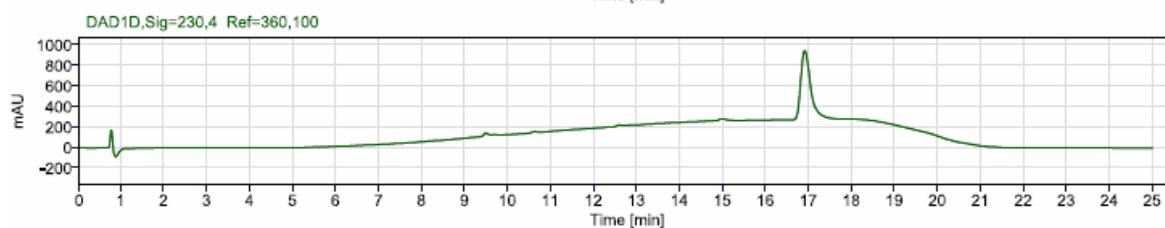
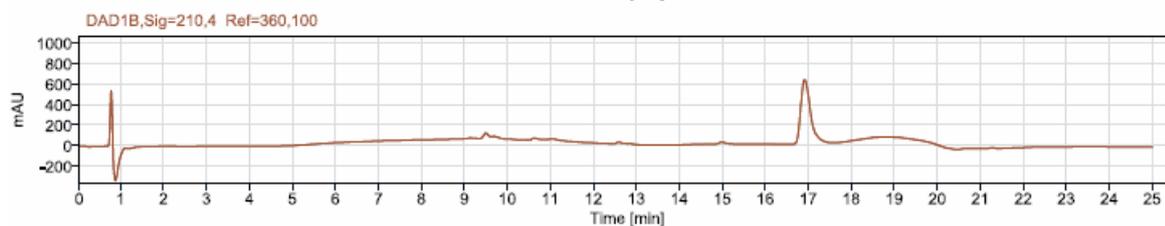
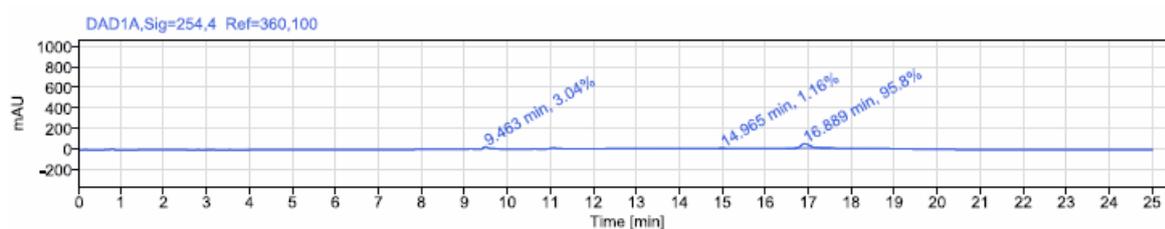
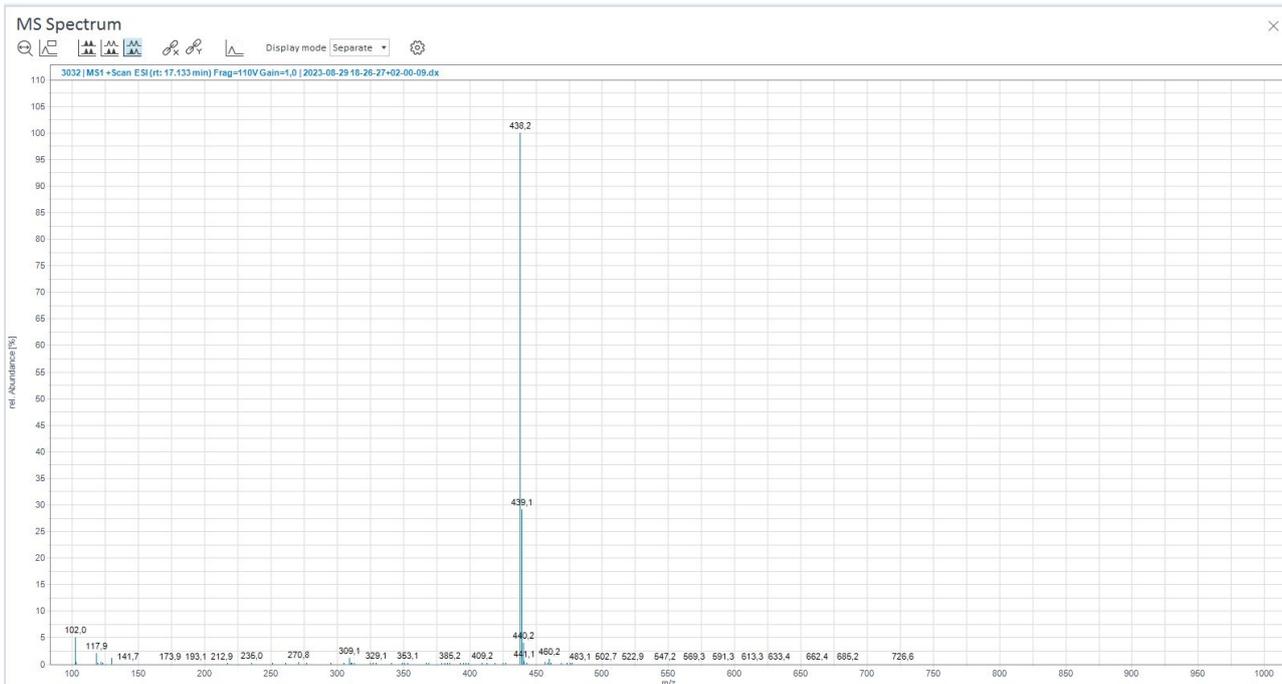


**Peak Results (Area Percent at least 1%)**

RT (min)	Signal Description	Width (min)	Area	Height	Area%
10.494	DAD1A, Sig=254,4 Ref=360,100	0.599	1748.6	216.8	100.00
10.571	MS1 +TIC SCAN ESI Frag=110V Gain=1.0	0.159	5198269.9	994096.1	100.00

# <sup>1</sup>H, <sup>13</sup>C NMR and HPLC/MS spectra of compound 8a

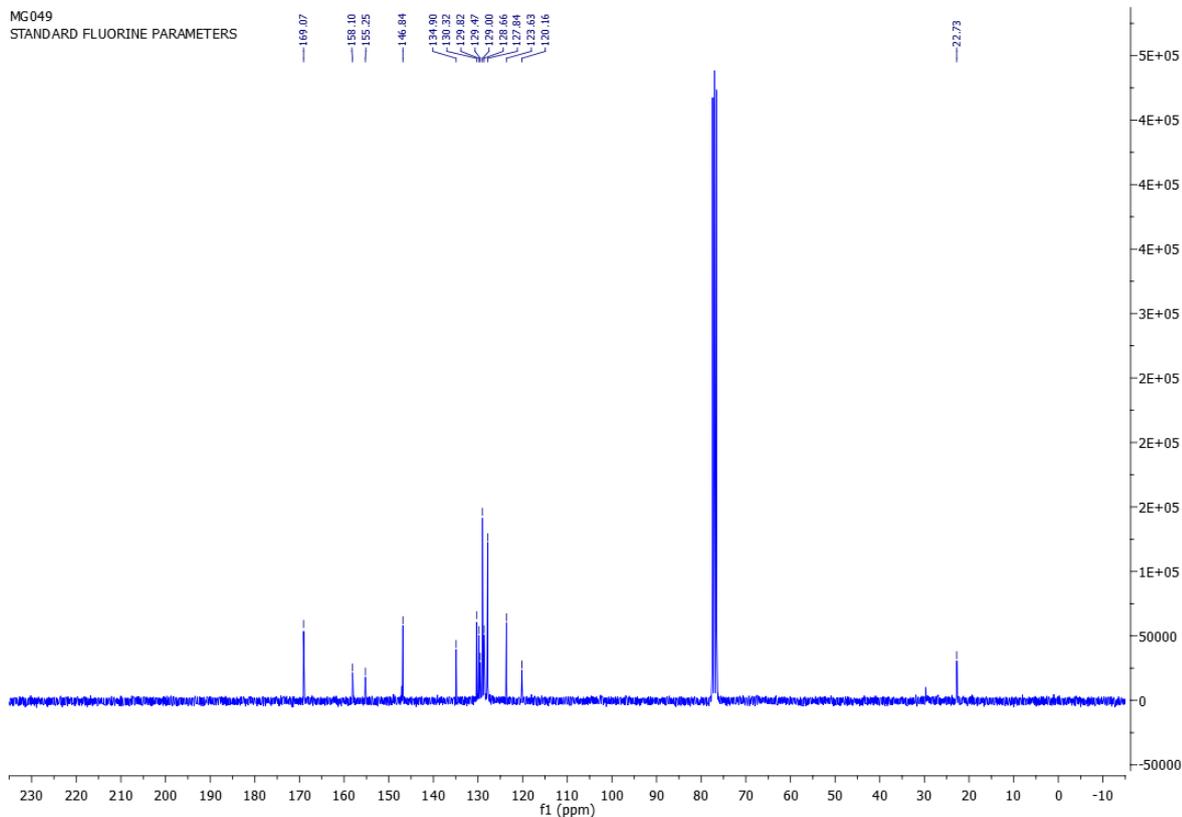
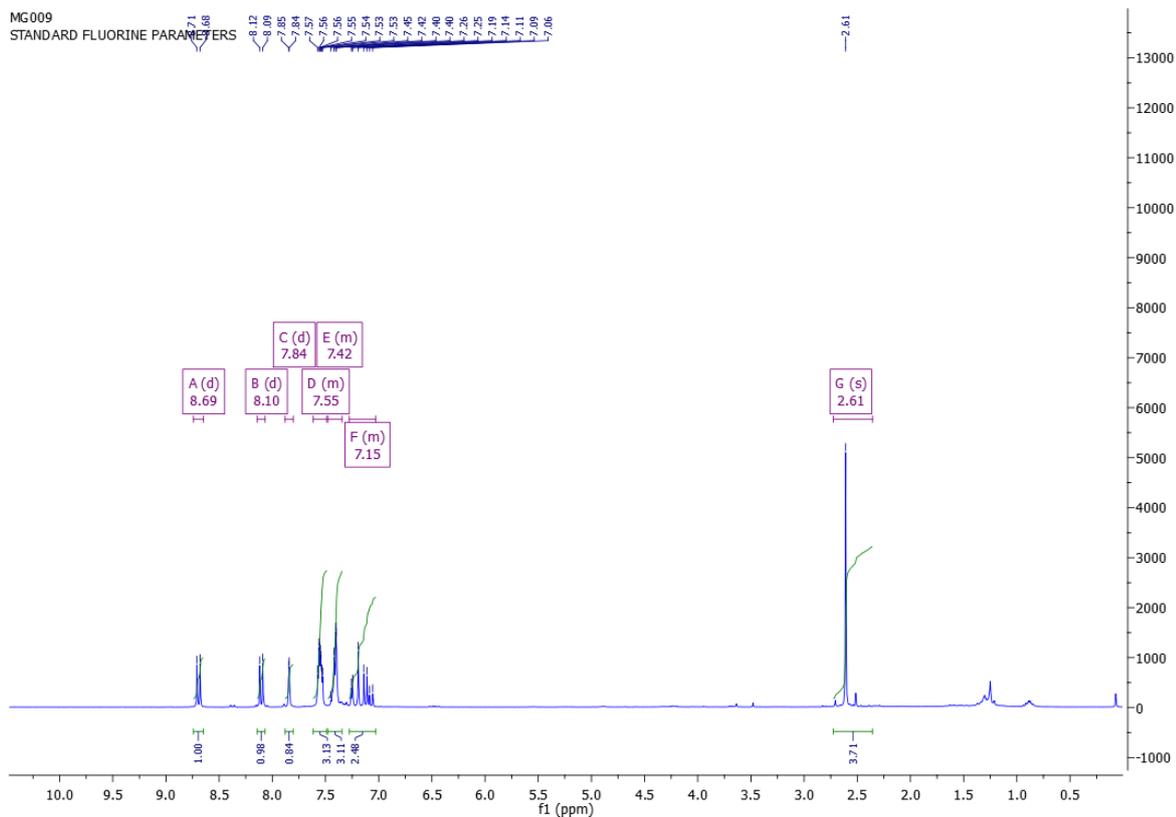


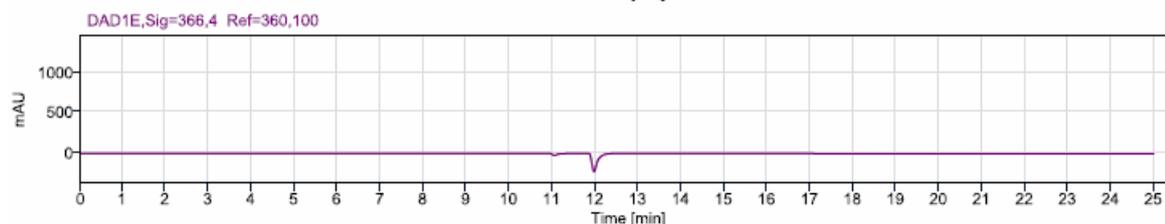
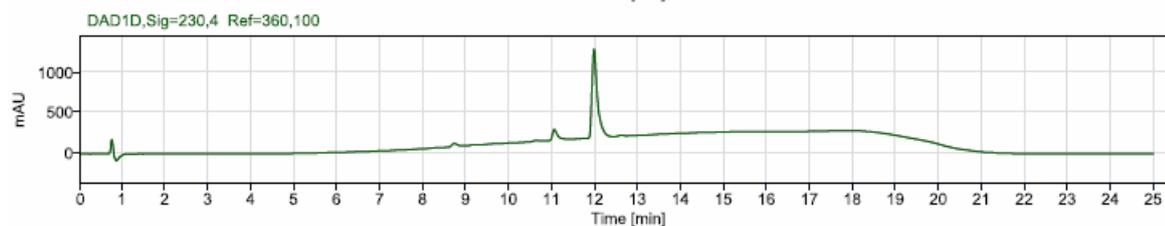
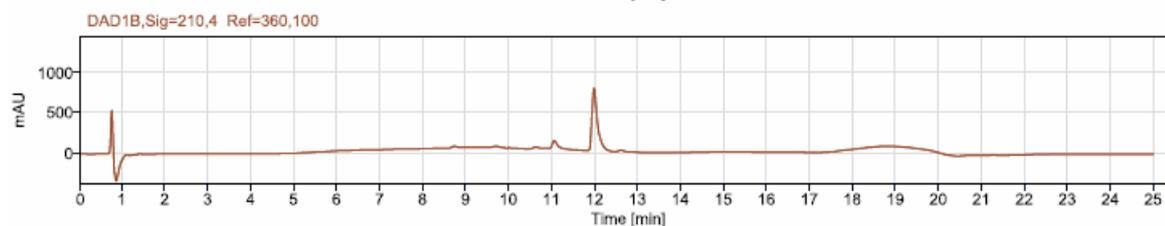
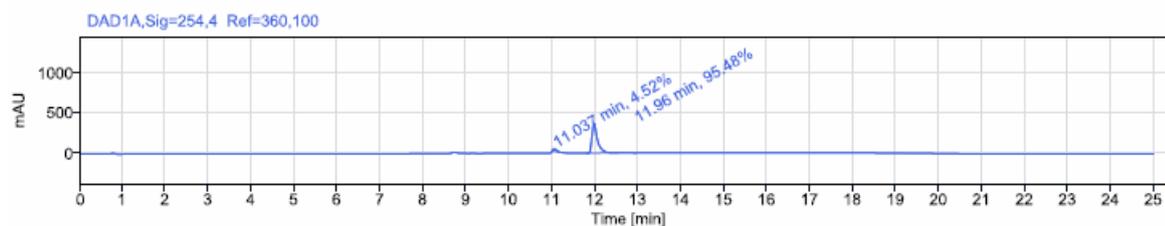
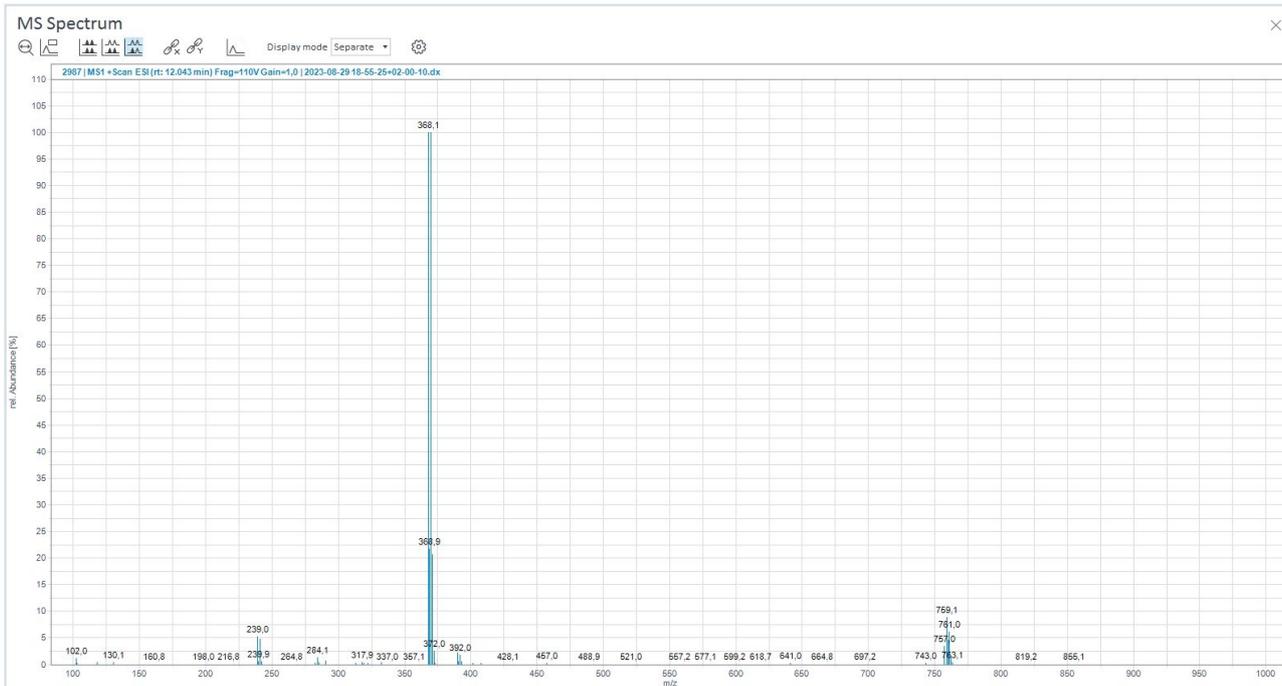


### Peak Results (Area Percent at least 1%)

RT (min)	Signal Description	Width (min)	Area	Height	Area%
9.463	DAD1A, Sig=254,4 Ref=360,100	0.088	21.4	7.0	3.04
14.965	DAD1A, Sig=254,4 Ref=360,100	0.171	8.2	1.2	1.16
16.889	DAD1A, Sig=254,4 Ref=360,100	1,046	674,7	43,3	95,80
17.135	MS1 +TIC SCAN ESI Frag=110V Gain=1.0	0.563	7460209.7	319982.3	100.00

# <sup>1</sup>H, <sup>13</sup>C NMR and HPLC/MS spectra of compound 8b

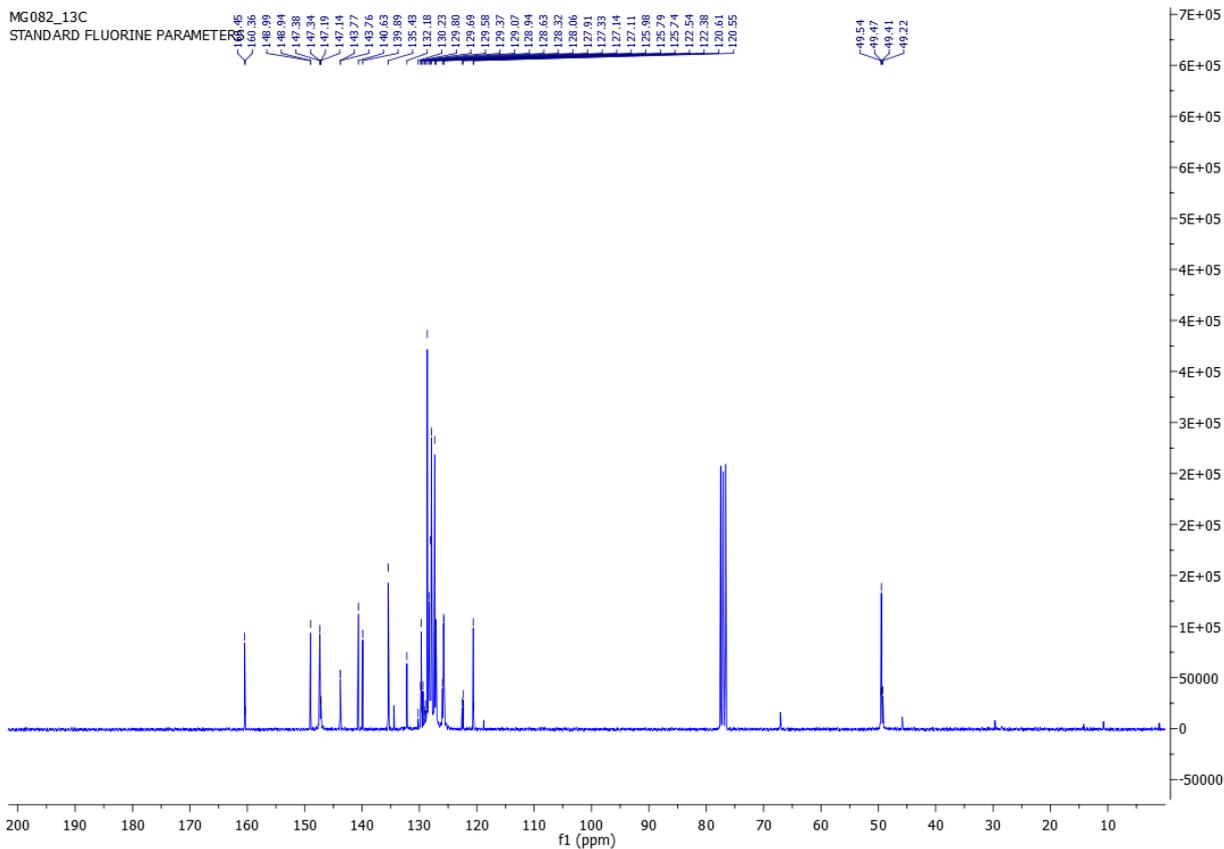
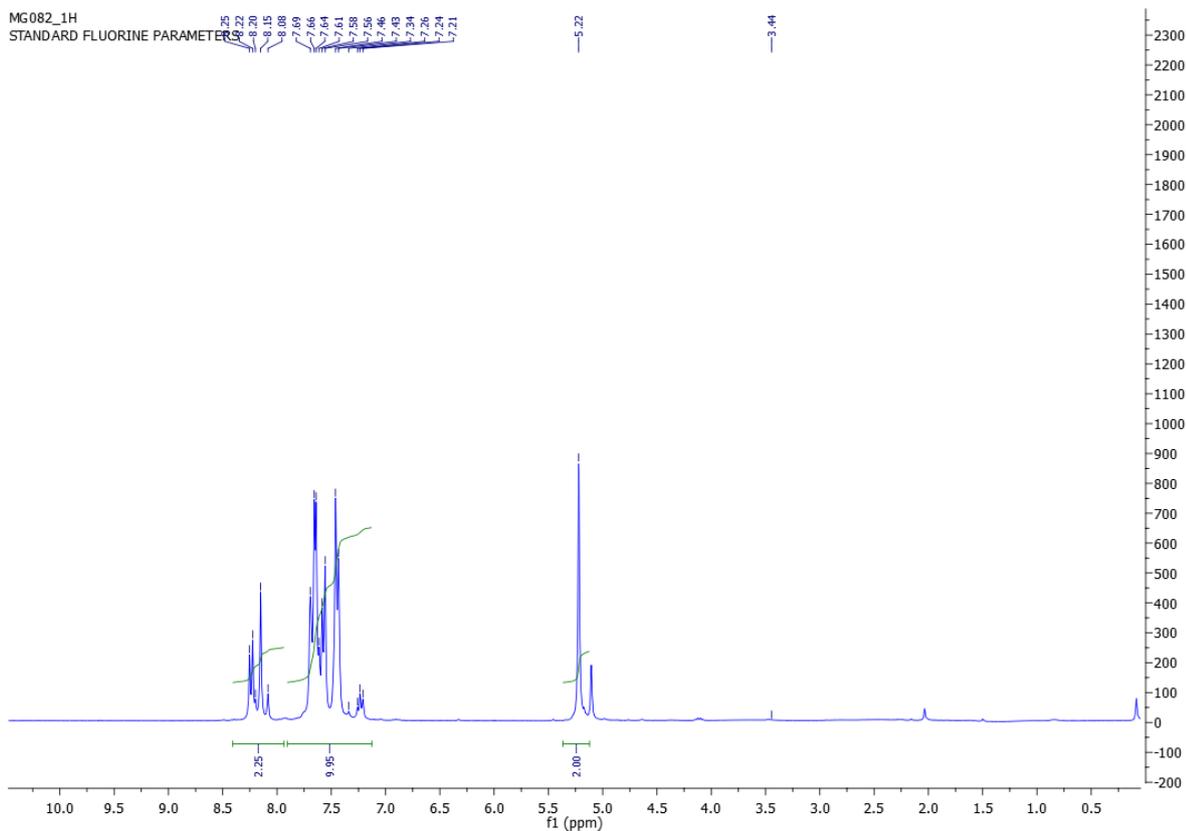


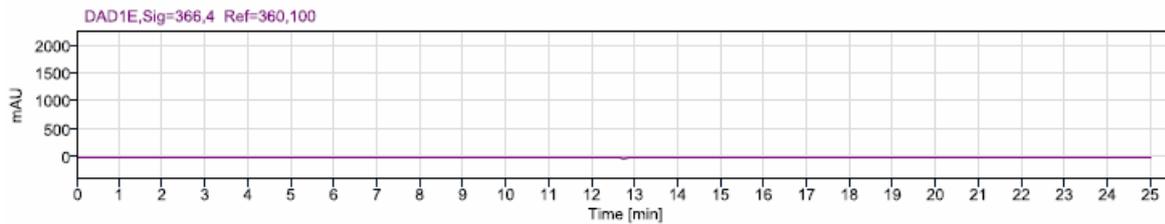
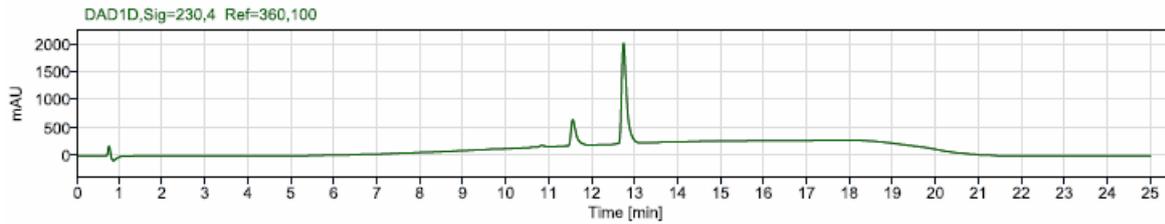
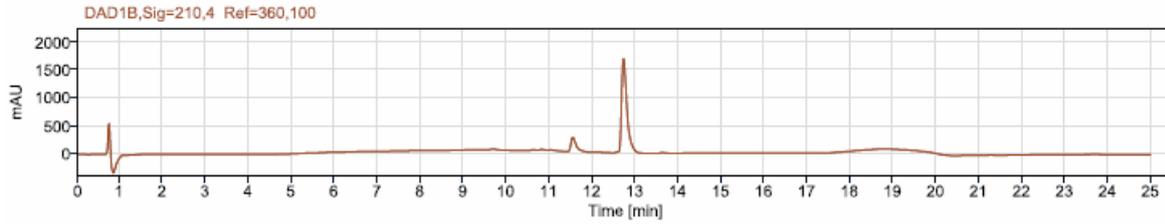
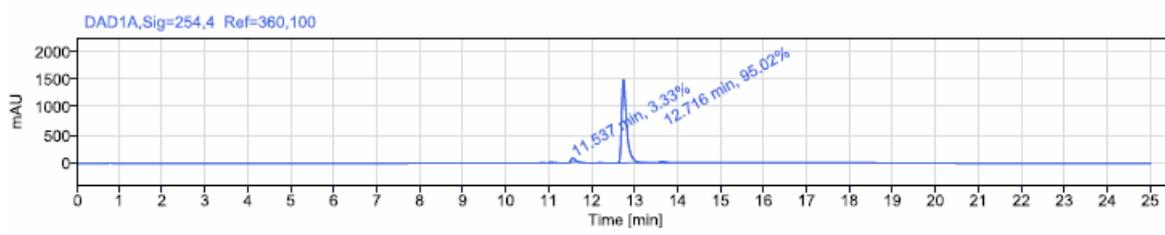
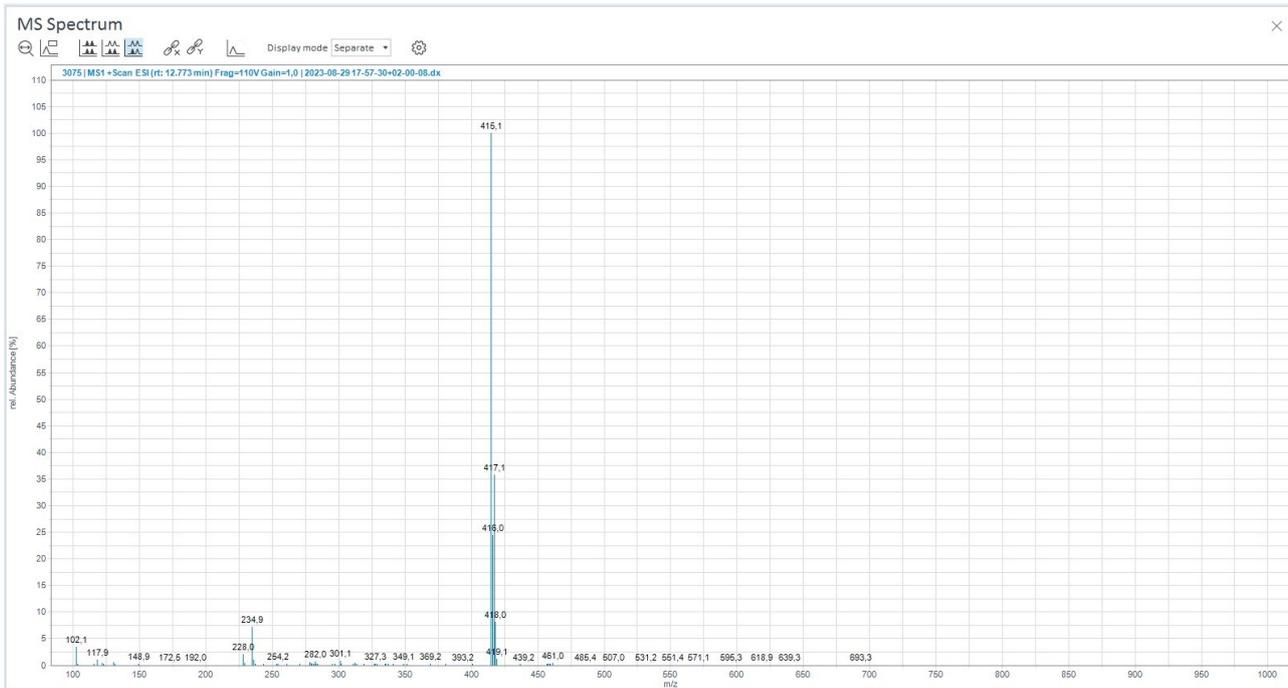


**Peak Results (Area Percent at least 1%)**

RT (min)	Signal Description	Width (min)	Area	Height	Area%
11.037	DAD1A, Sig=254,4 Ref=360,100	0.158	153.6	31.0	4.52
11.960	DAD1A, Sig=254,4 Ref=360,100	0.746	3241.3	364.8	95.48
12.040	MS1 +TIC SCAN ESI Frag=110V Gain=1,0	0.698	25124082,9	1714932,0	100,00

# <sup>1</sup>H, <sup>13</sup>C NMR and HPLC/MS spectra of compound 9

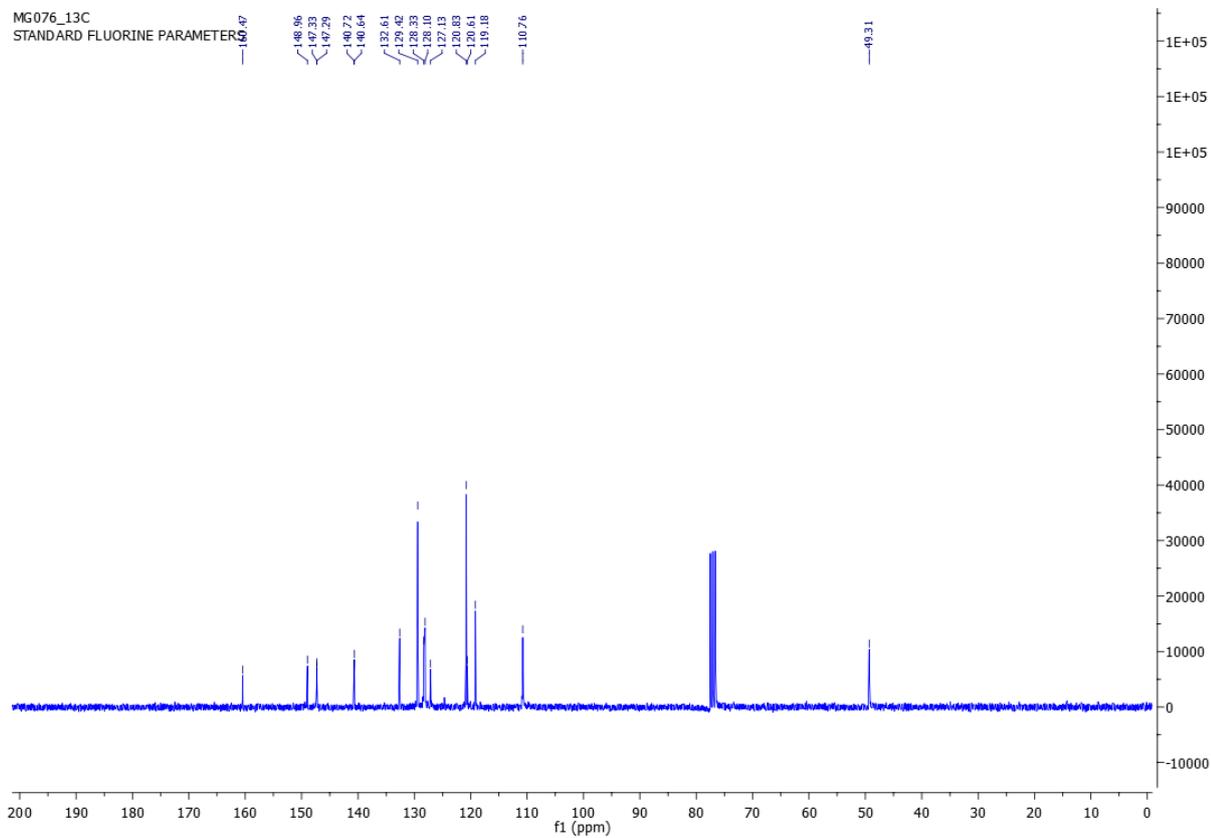
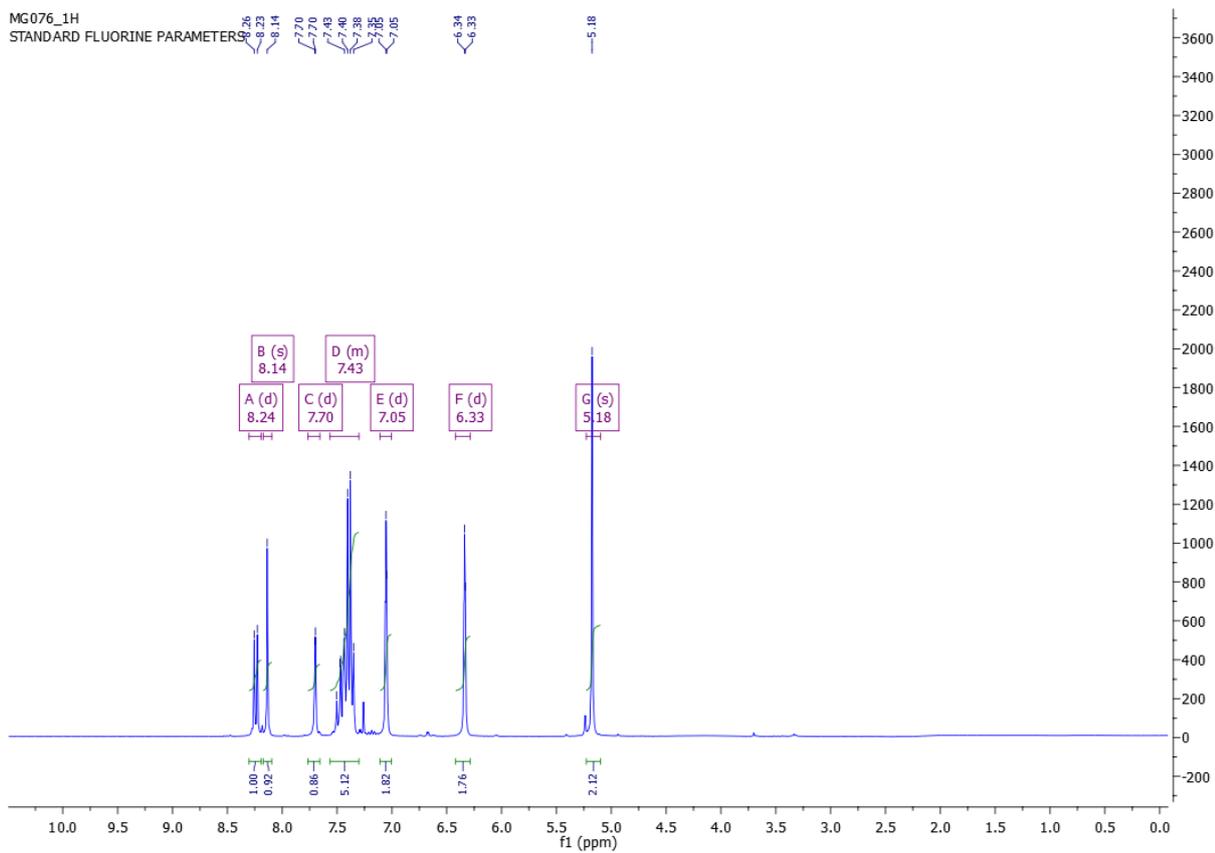




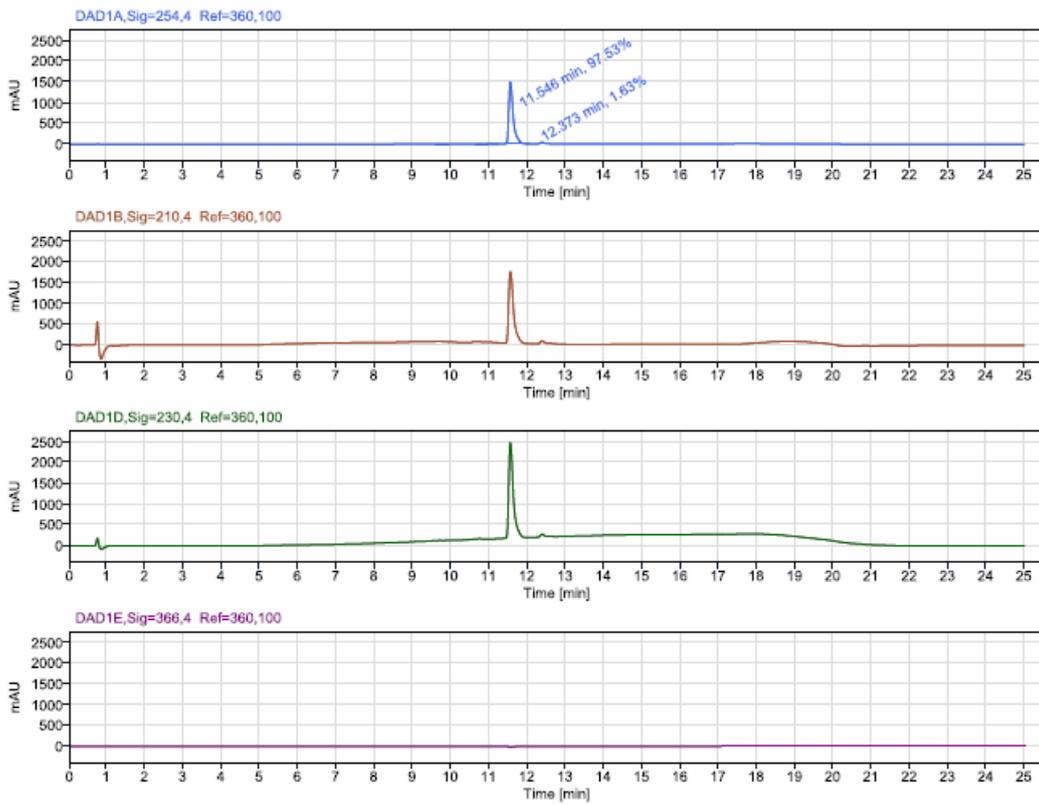
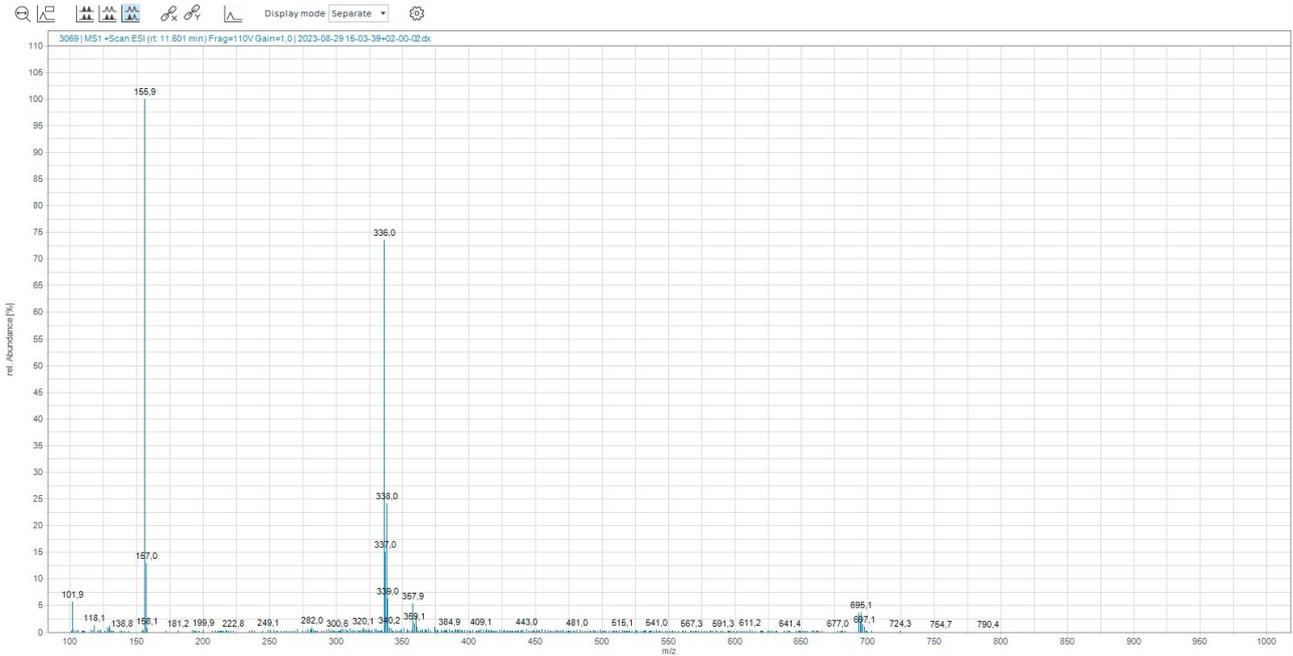
**Peak Results (Area Percent at least 1%)**

RT (min)	Signal Description	Width (min)	Area	Height	Area%
11.537	DAD1A, Sig=254,4 Ref=360,100	0.187	421.6	71.6	3.33
12.716	DAD1A, Sig=254,4 Ref=360,100	0.720	12036.0	1486.7	95.02
12.781	MS1 + TIC SCAN ESI Frag=110V Gain=1.0	0.580	9926186.2	876734.5	100.00

# <sup>1</sup>H, <sup>13</sup>C NMR and HPLC/MS spectra of compound 10



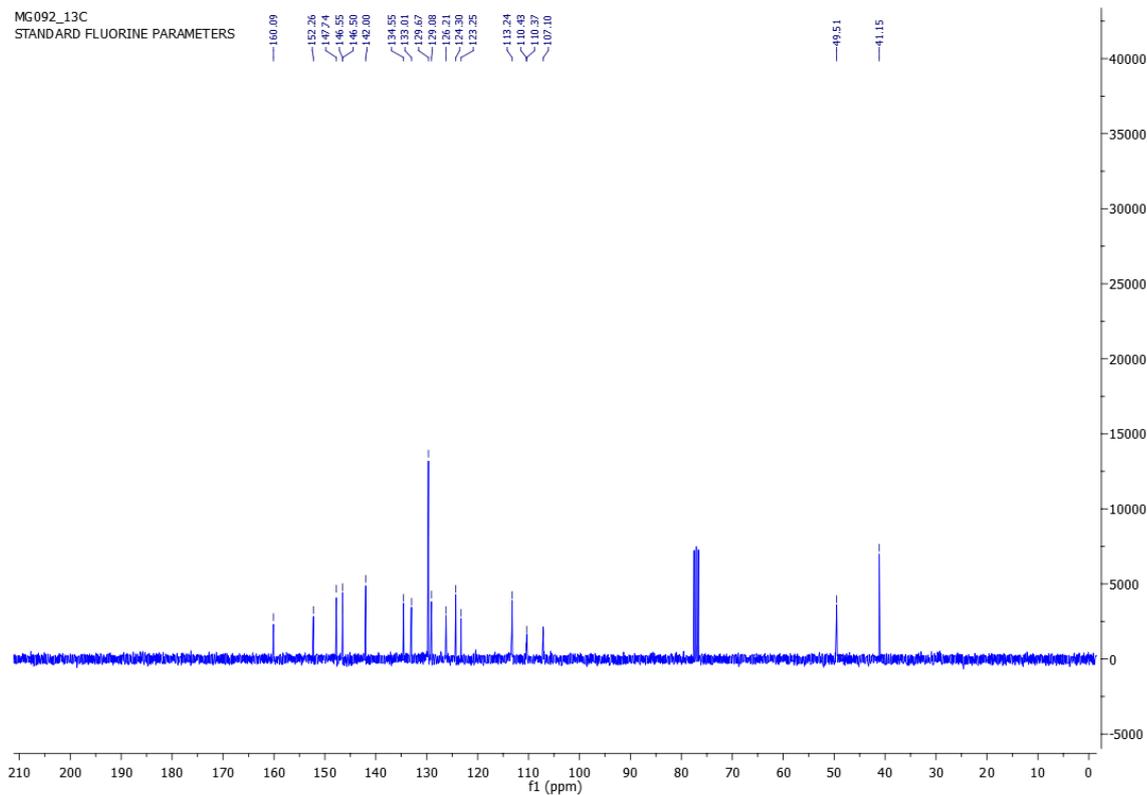
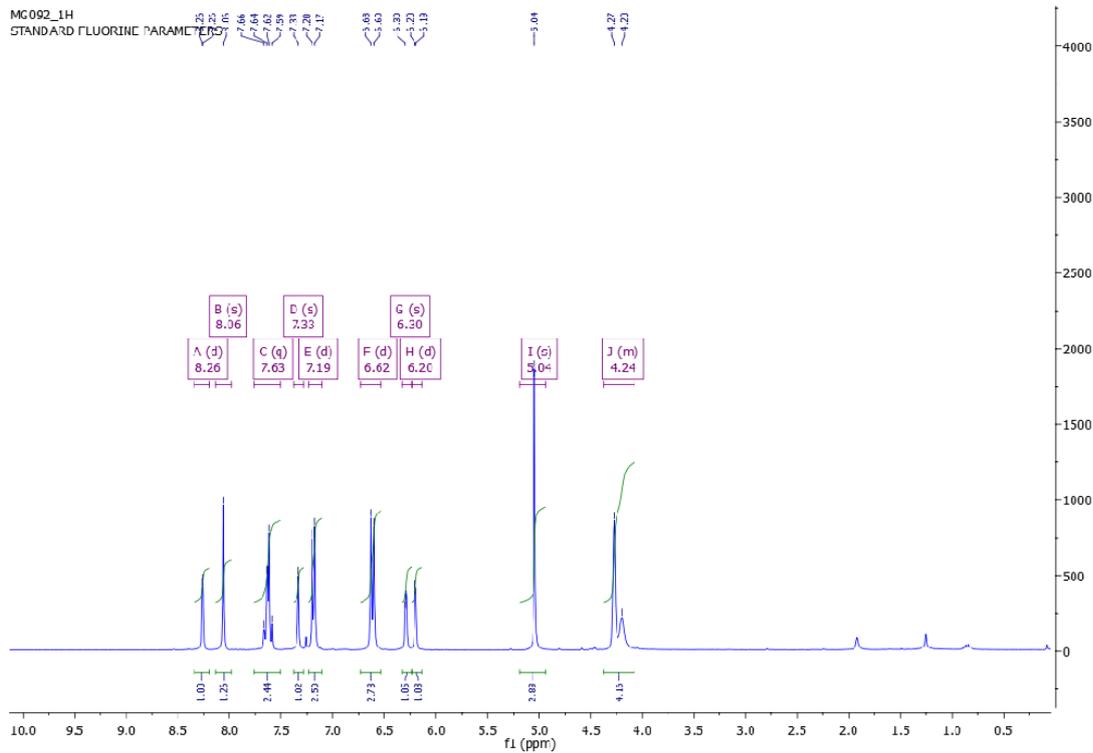
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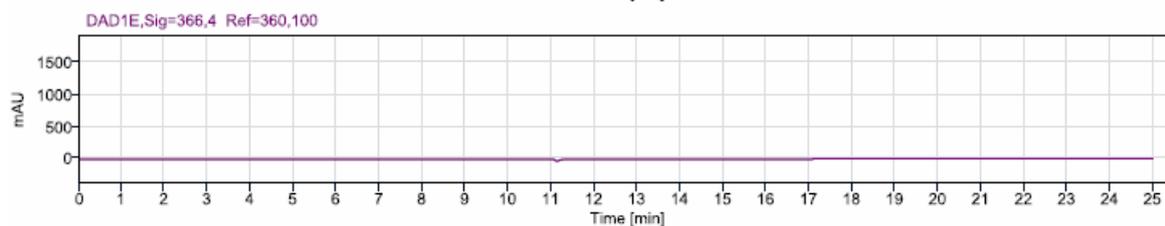
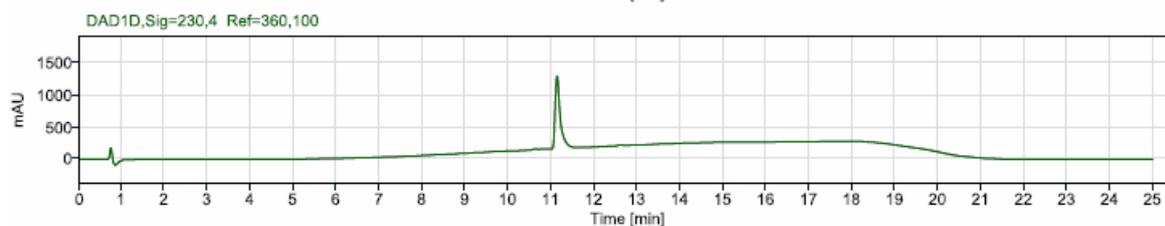
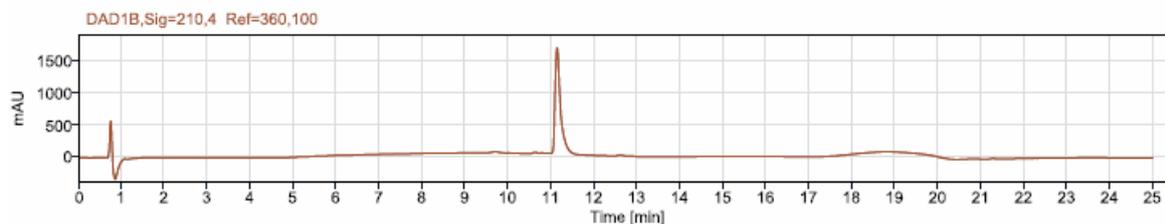
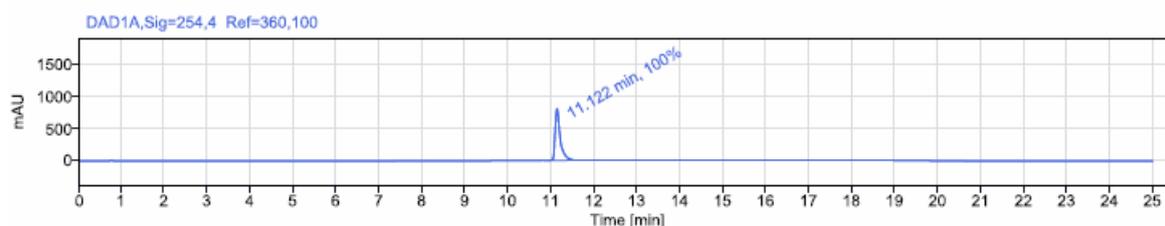
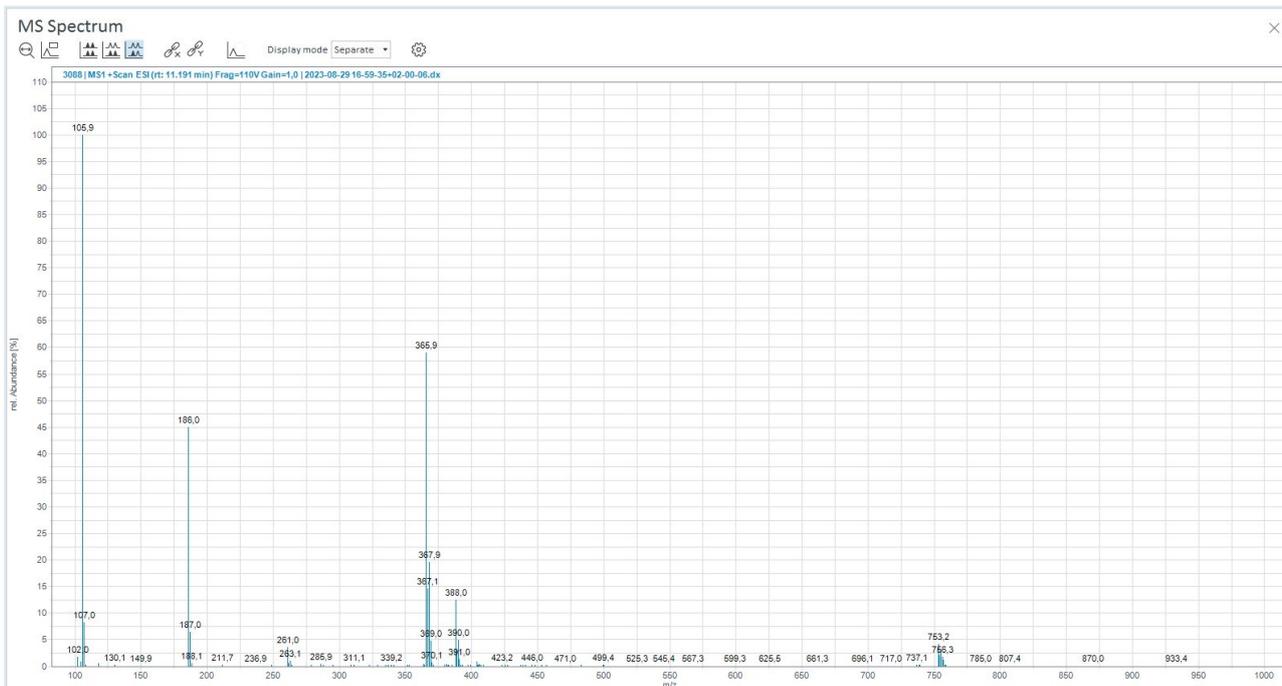


## Peak Results (Area Percent at least 1%)

RT (min)	Signal Description	Width (min)	Area	Height	Area%
11.546	DAD1A, Sig=254,4 Ref=360,100	0.600	12079.4	1498.3	97.53
11.598	MS1 +TIC SCAN ESI Frag=110V Gain=1.0	0.309	4466372.3	433691.7	100.00
12.373	DAD1A, Sig=254,4 Ref=360,100	0.198	202.4	32.6	1.63

# <sup>1</sup>H, <sup>13</sup>C NMR and HPLC/MS spectra of compound 11a

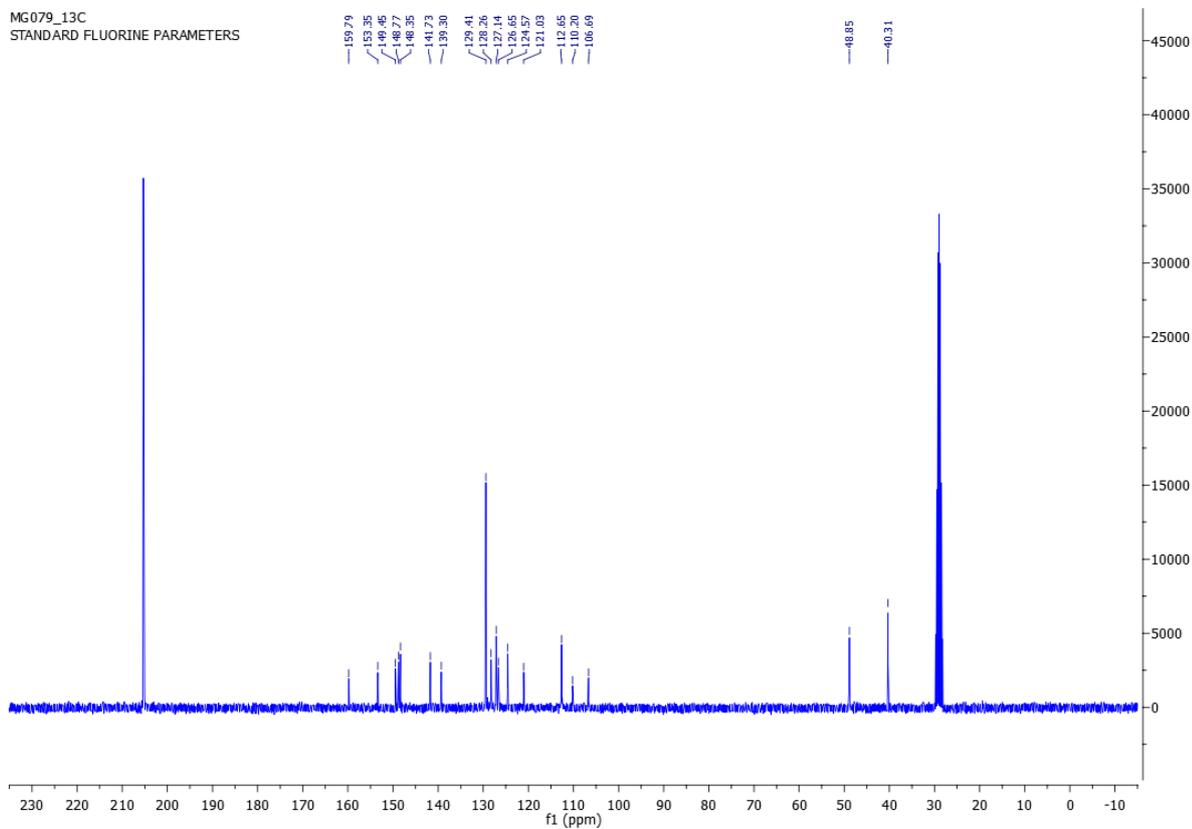
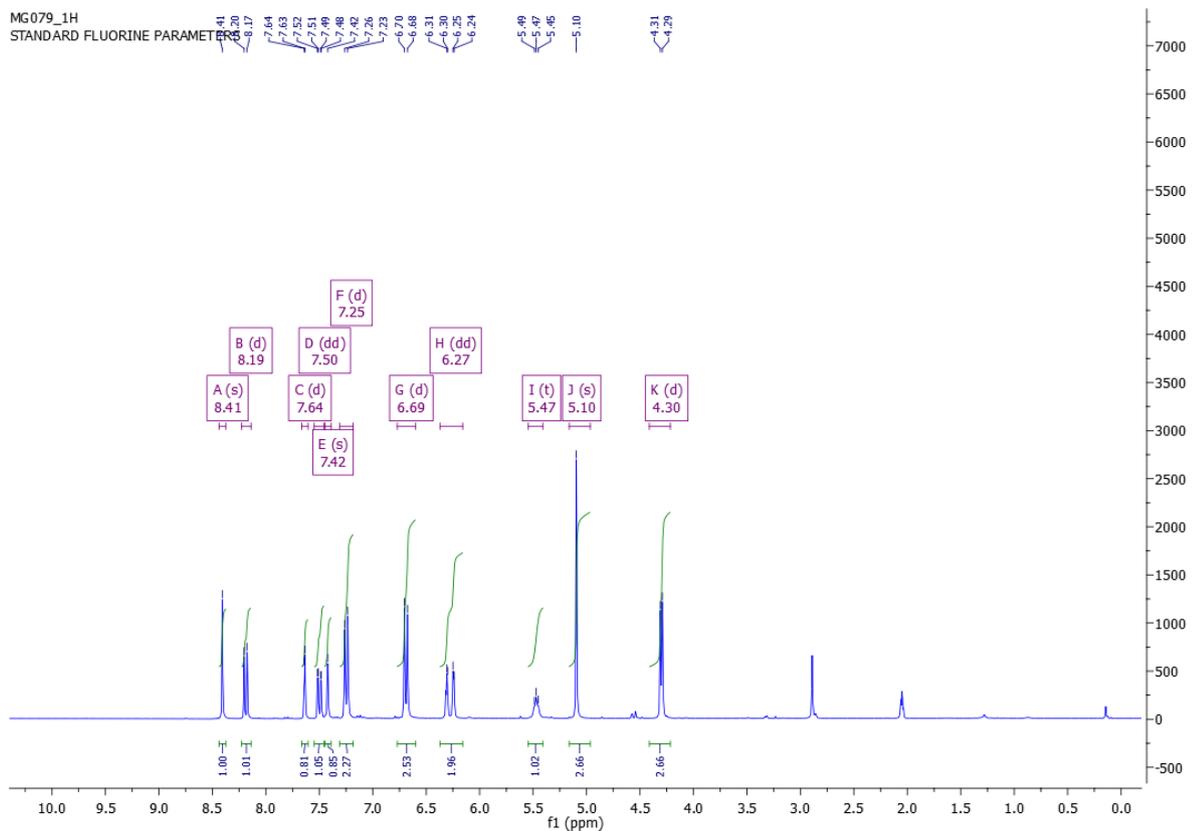




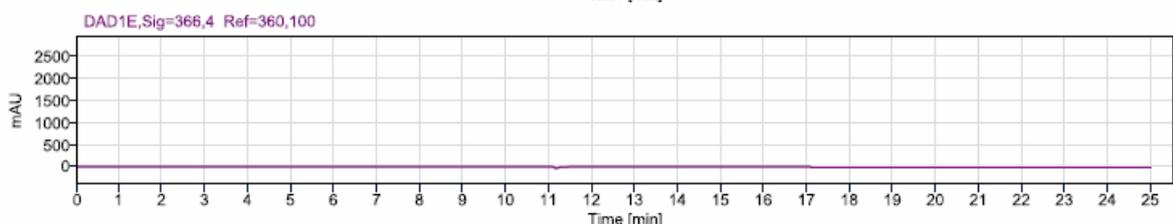
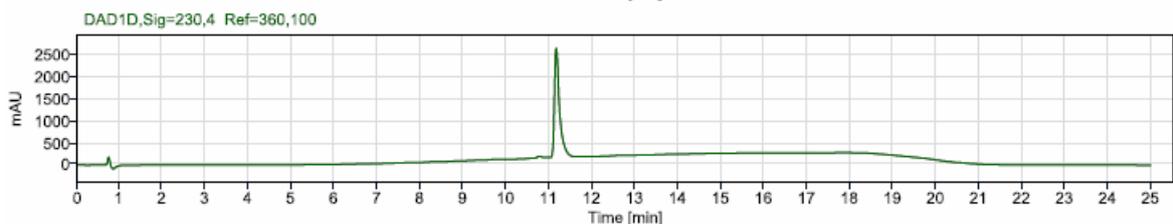
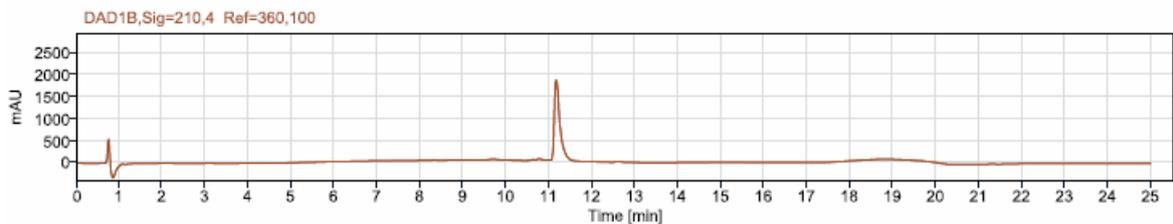
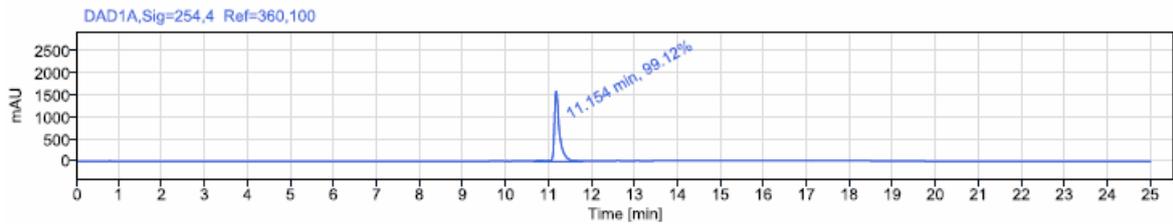
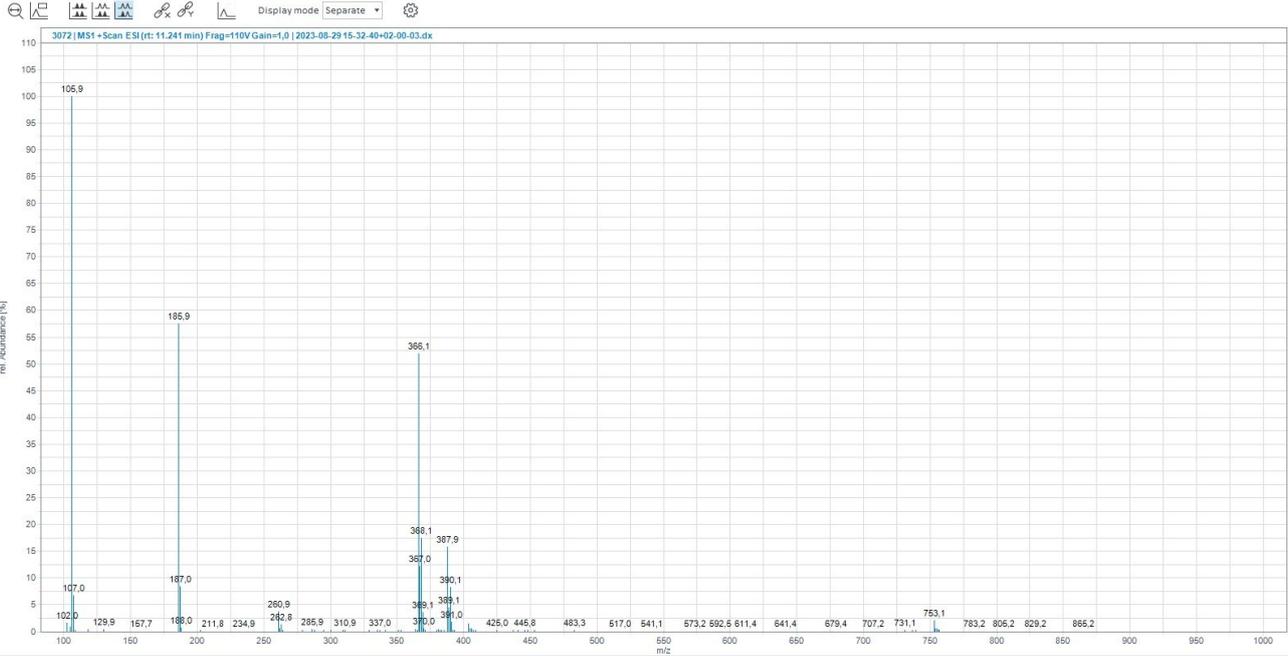
**Peak Results (Area Percent at least 1%)**

RT (min)	Signal Description	Width (min)	Area	Height	Area%
11.122	DAD1A, Sig=254,4 Ref=360,100	0.744	6527.2	799.6	100.00
11.194	MS1 +TIC SCAN ESI Frag=110V Gain=1.0	0.641	13906450.8	1242457.4	100.00

# $^1\text{H}$ , $^{13}\text{C}$ NMR and HPLC/MS spectra of compound 11b



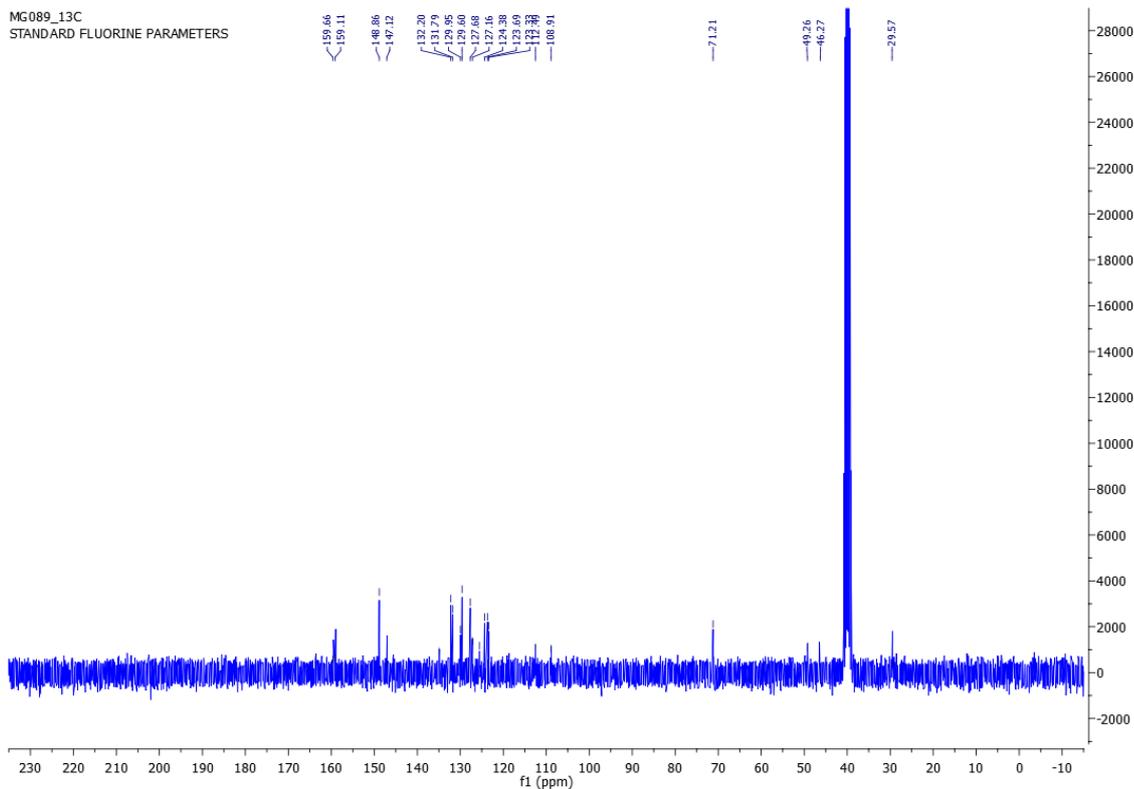
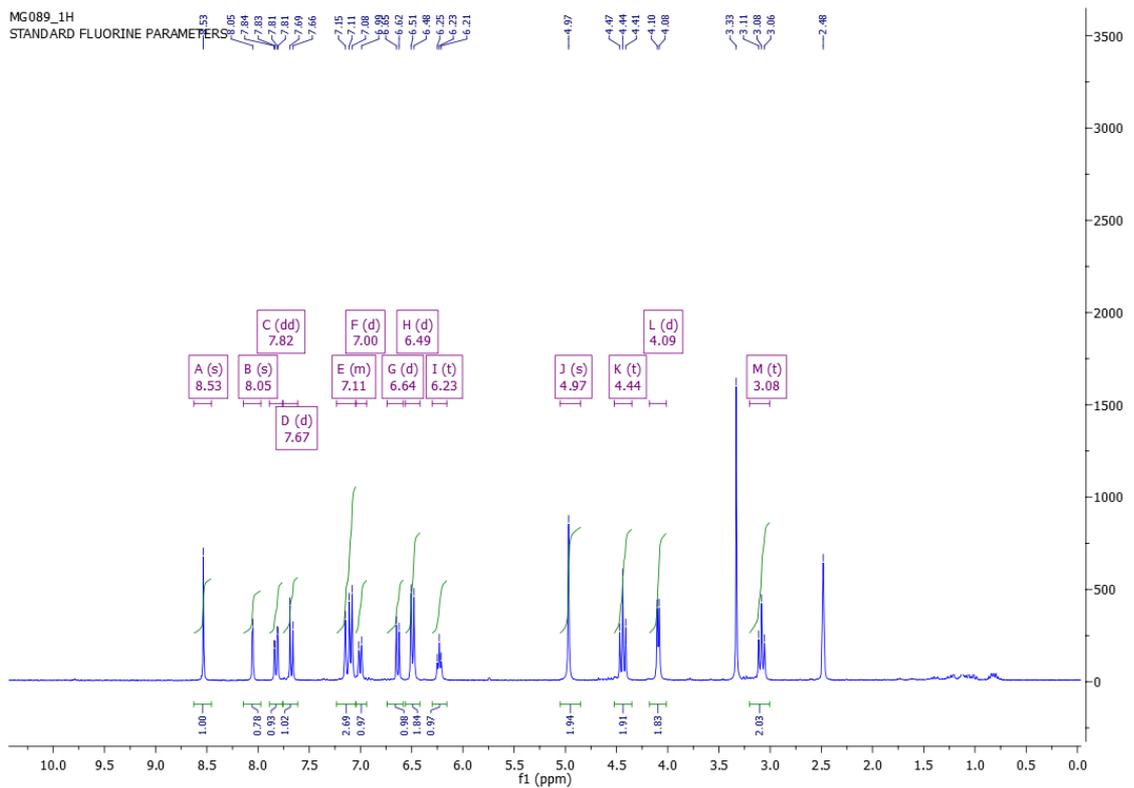
MS Spectrum

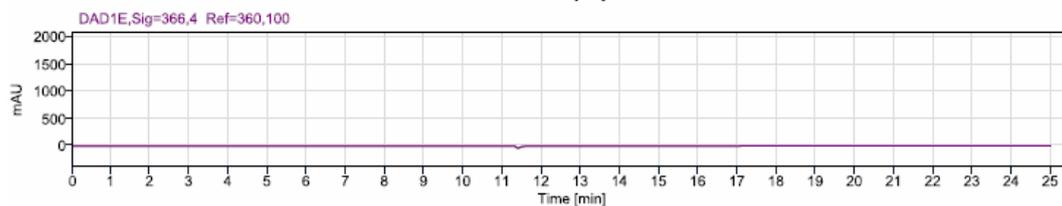
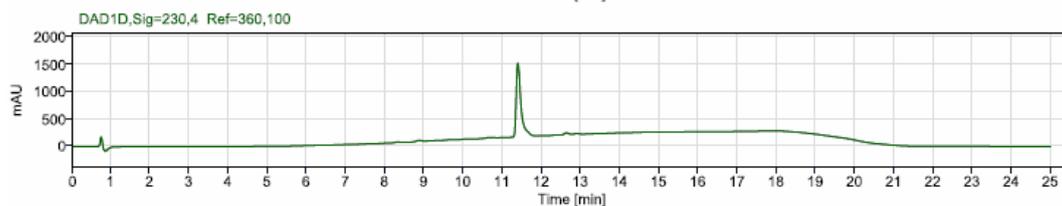
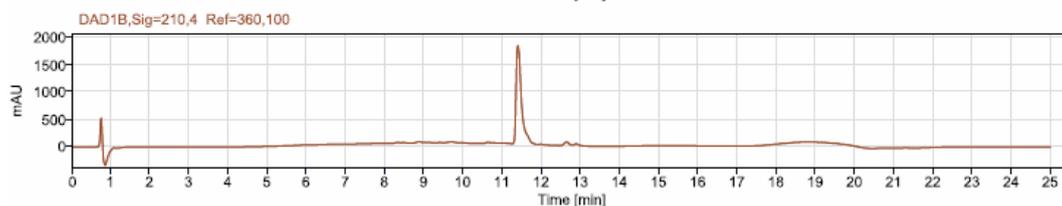
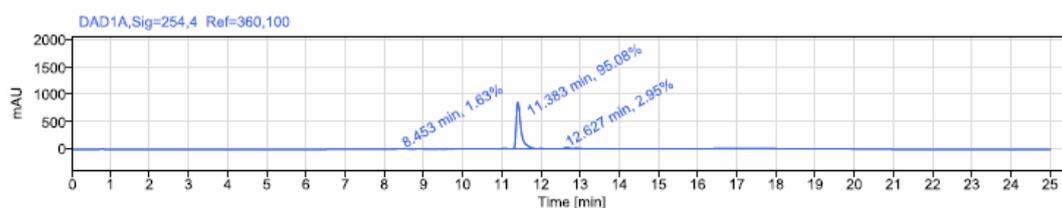
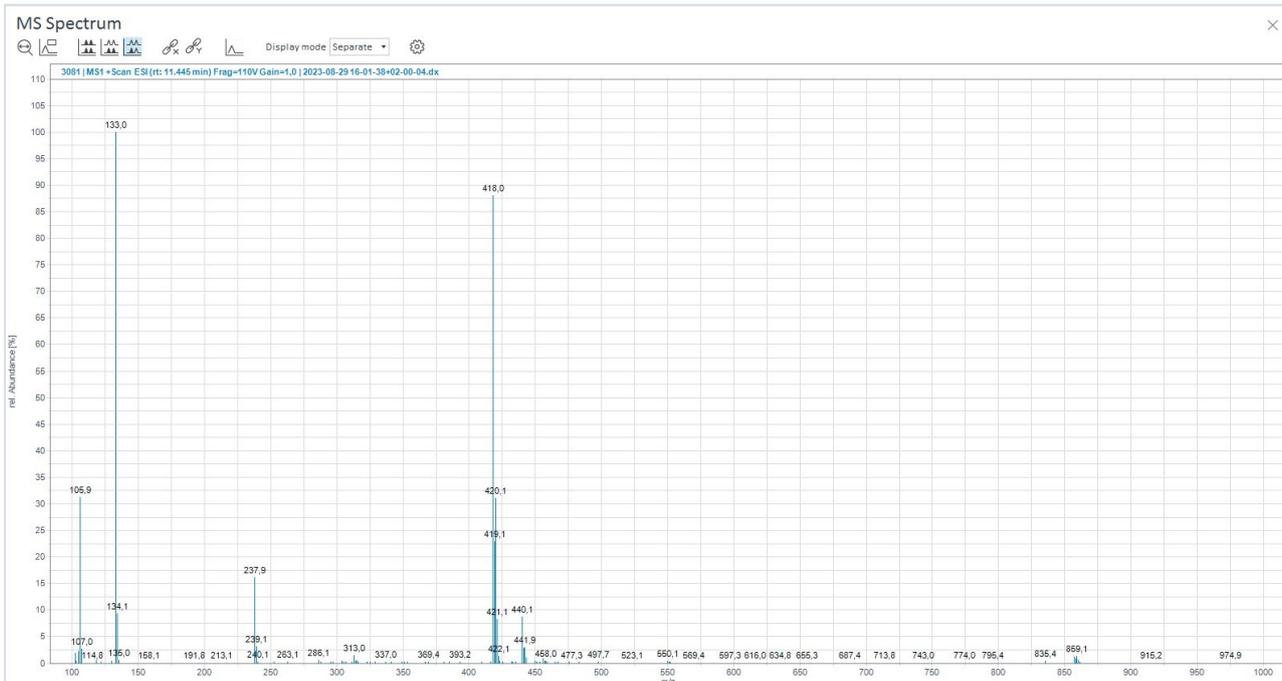


Peak Results (Area Percent at least 1%)

RT (min)	Signal Description	Width (min)	Area	Height	Area%
11.154	DAD1A,Sig=254,4 Ref=360,100	0.862	12972.6	1597.1	99.12
11.237	MS1 +TIC SCAN ESI Frag=110V Gain=1.0	0.245	7000609.1	954160.4	100.00

# $^1\text{H}$ , $^{13}\text{C}$ NMR and HPLC/MS spectra of compound 11c

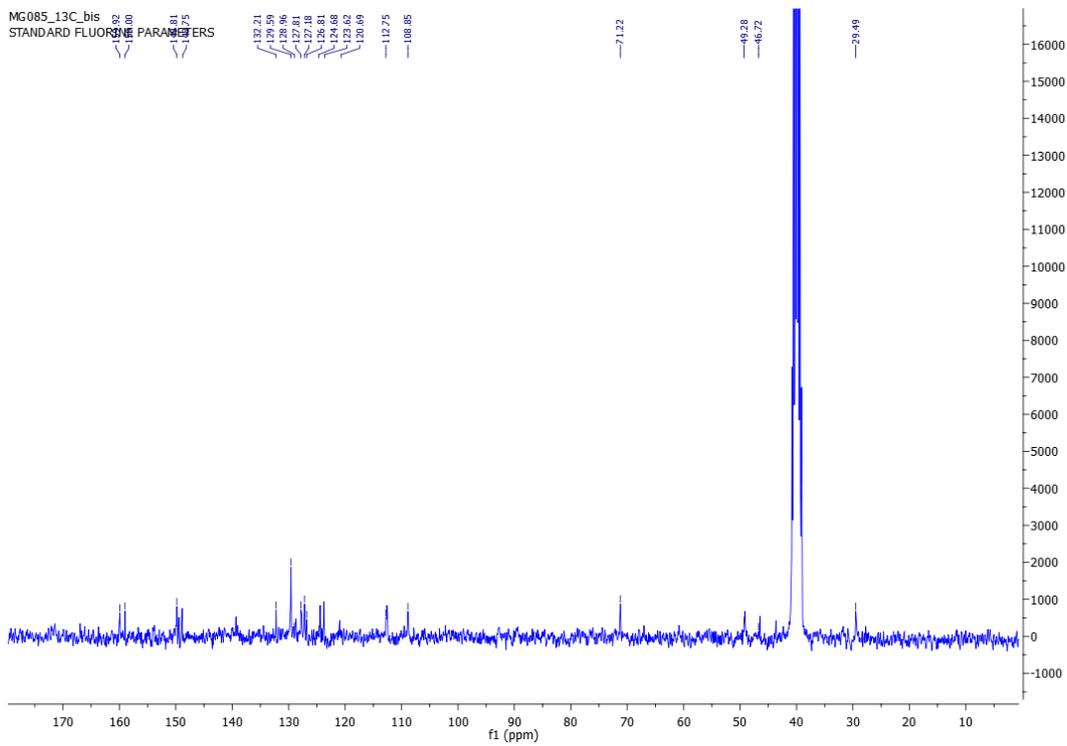
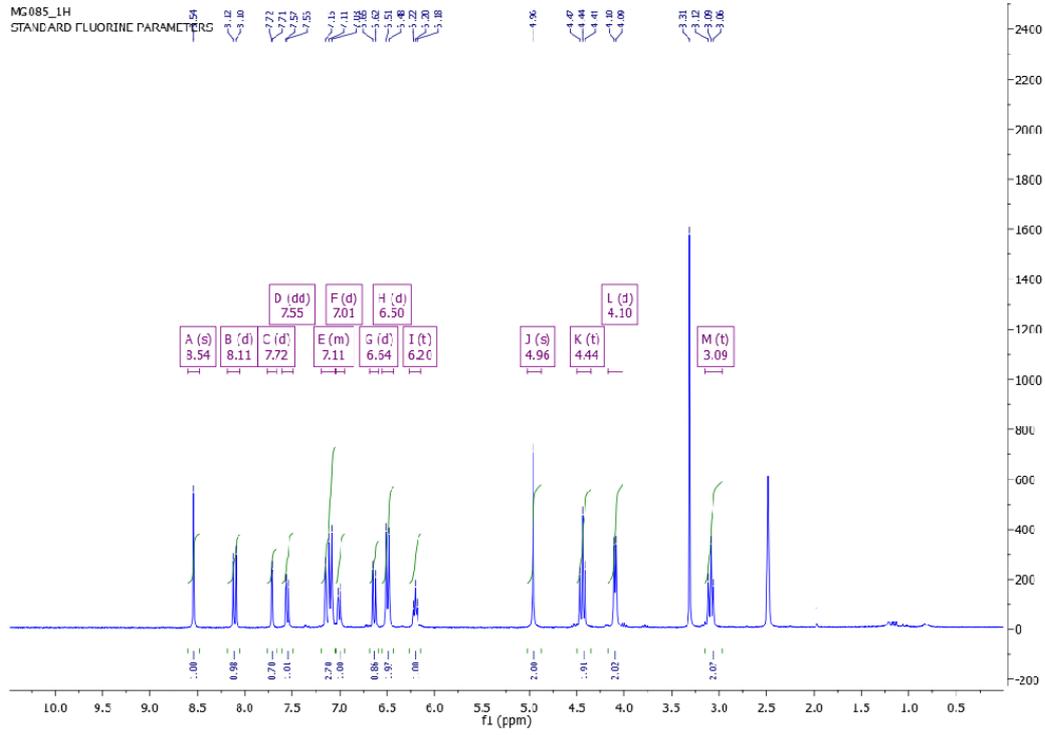


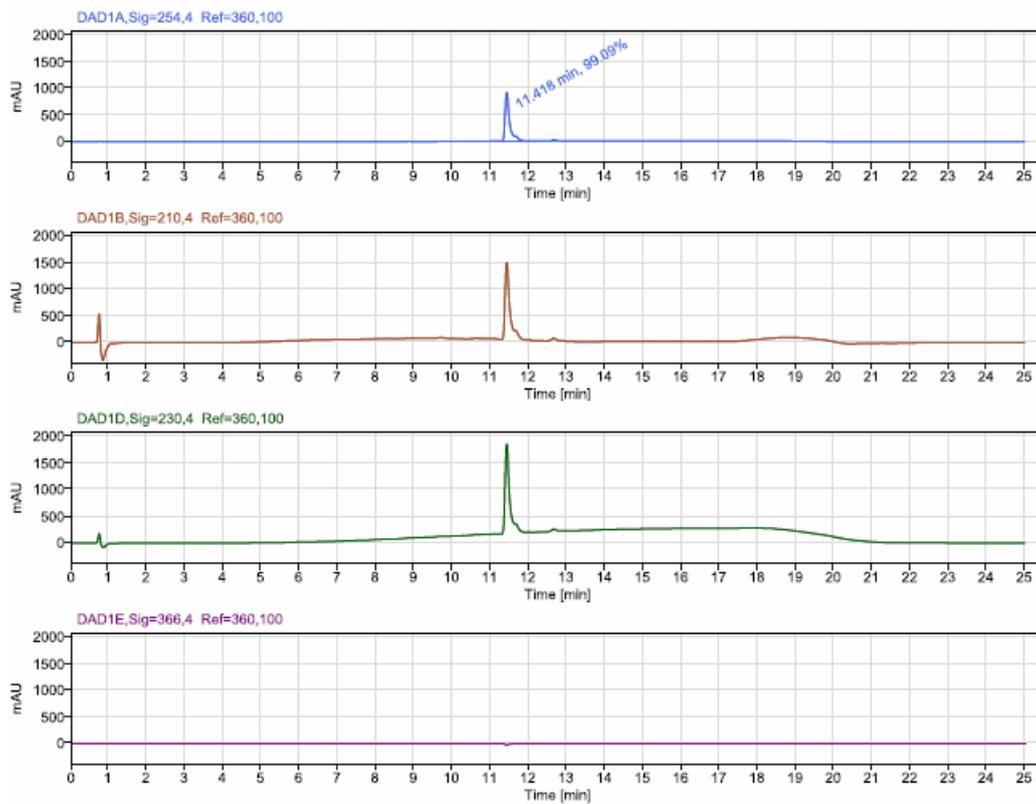
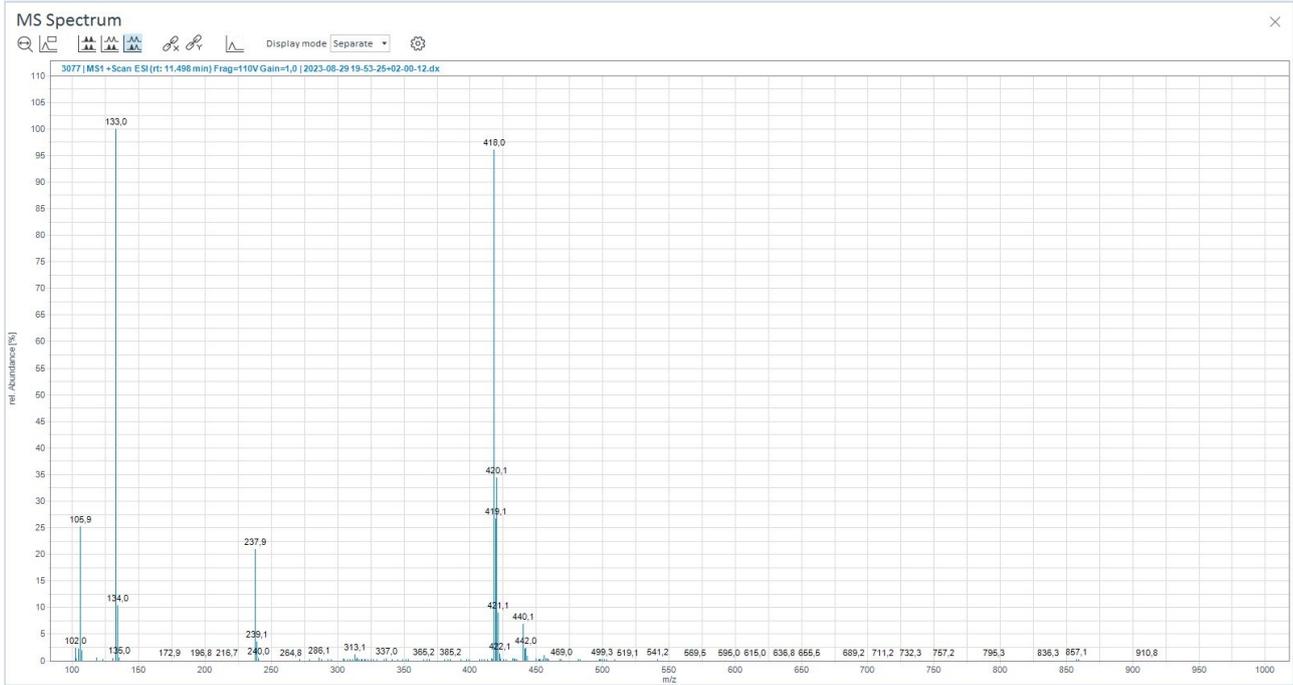


**Peak Results (Area Percent at least 1%)**

RT (min)	Signal Description	Width (min)	Area	Height	Area%
8.453	DAD1A, Sig=254,4 Ref=360,100	0.937	122.9	6.7	1.63
11.383	DAD1A, Sig=254,4 Ref=360,100	0.829	7149.8	855.5	95.08
11.450	MS1 +TIC SCAN ESI Frag=110V Gain=1,0	0,666	18189544,3	1504397,8	100,00
12.627	DAD1A, Sig=254,4 Ref=360,100	0.757	221.9	18.7	2.95

# <sup>1</sup>H, <sup>13</sup>C NMR and HPLC/MS spectra of compound 11d

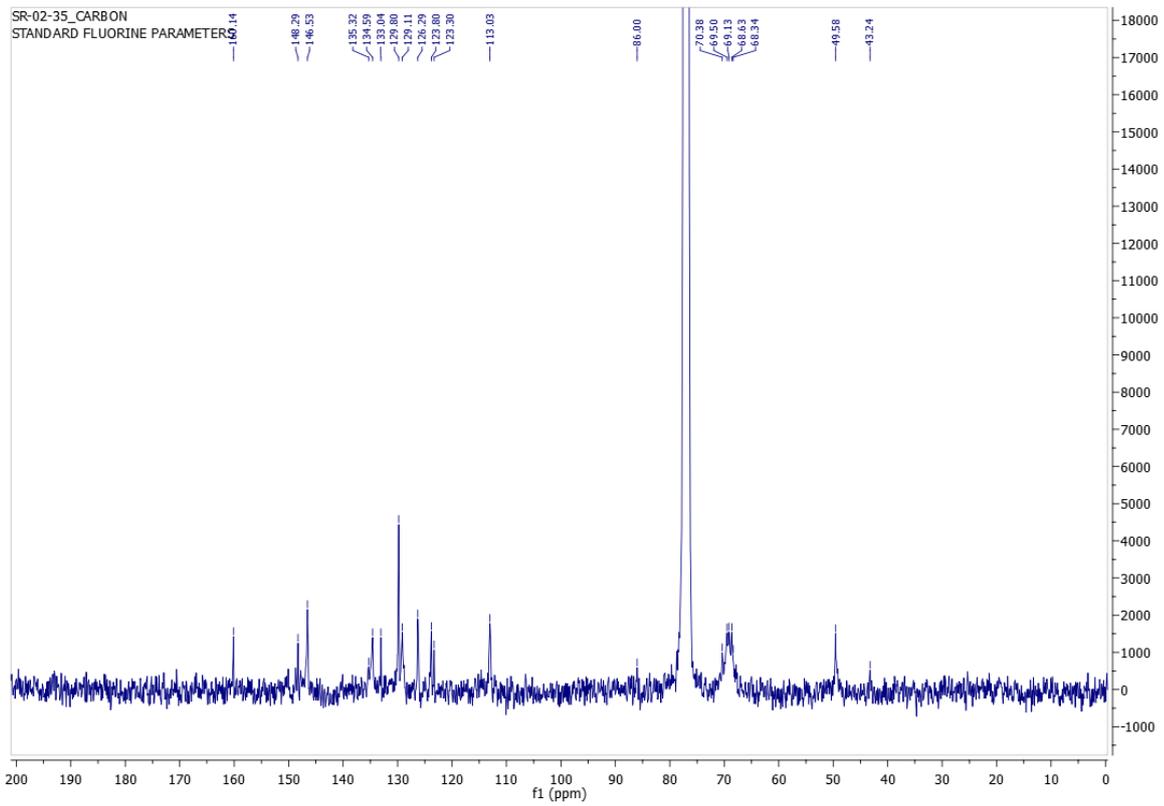
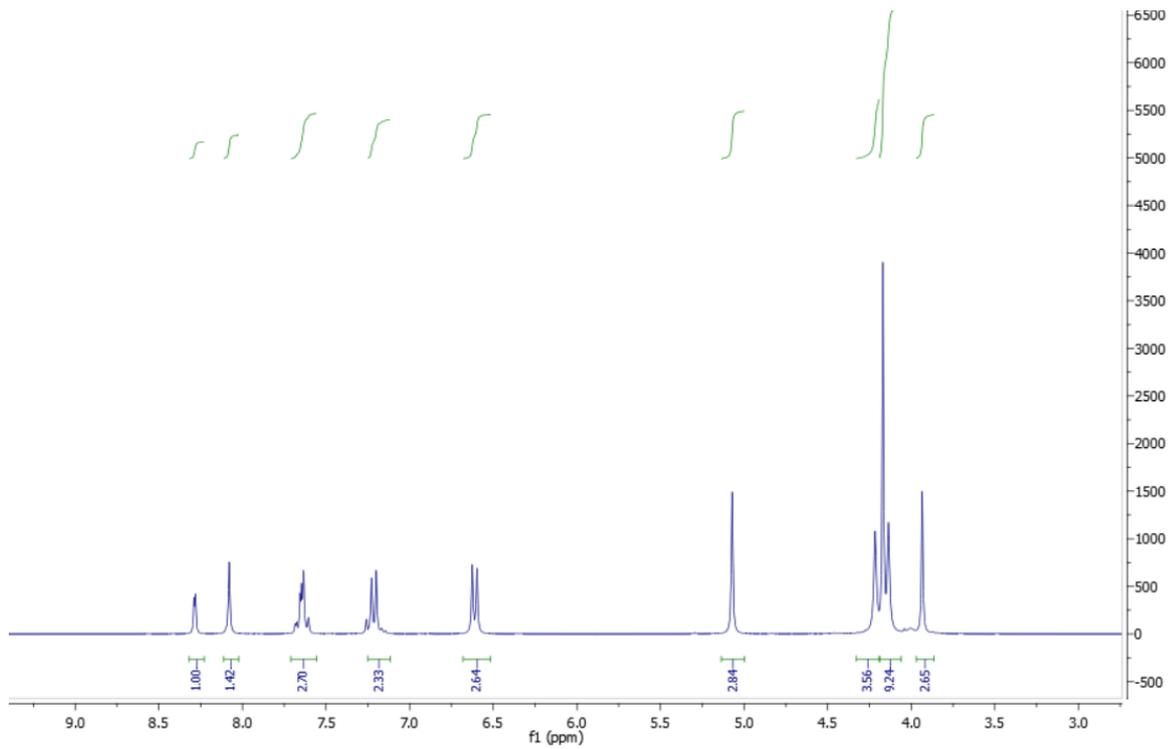


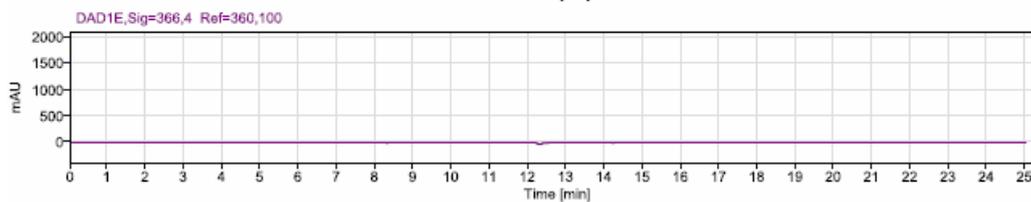
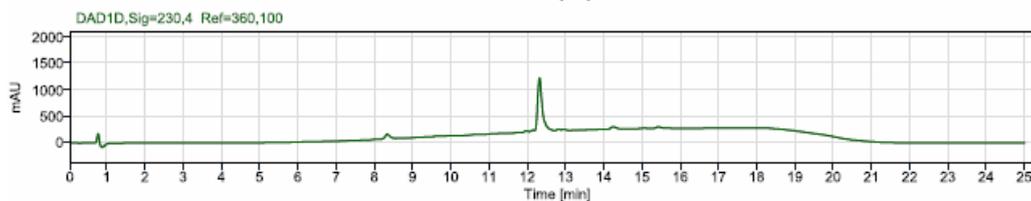
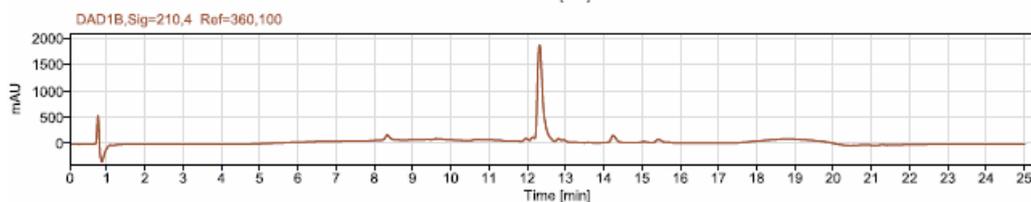
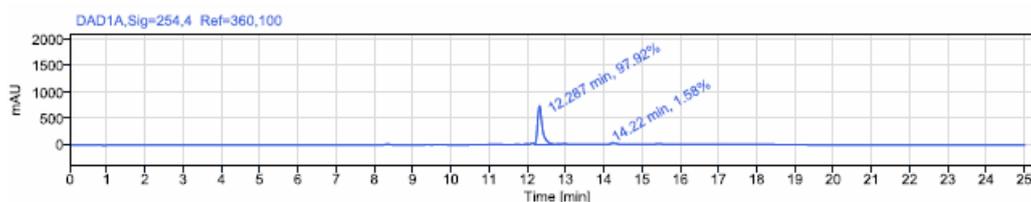
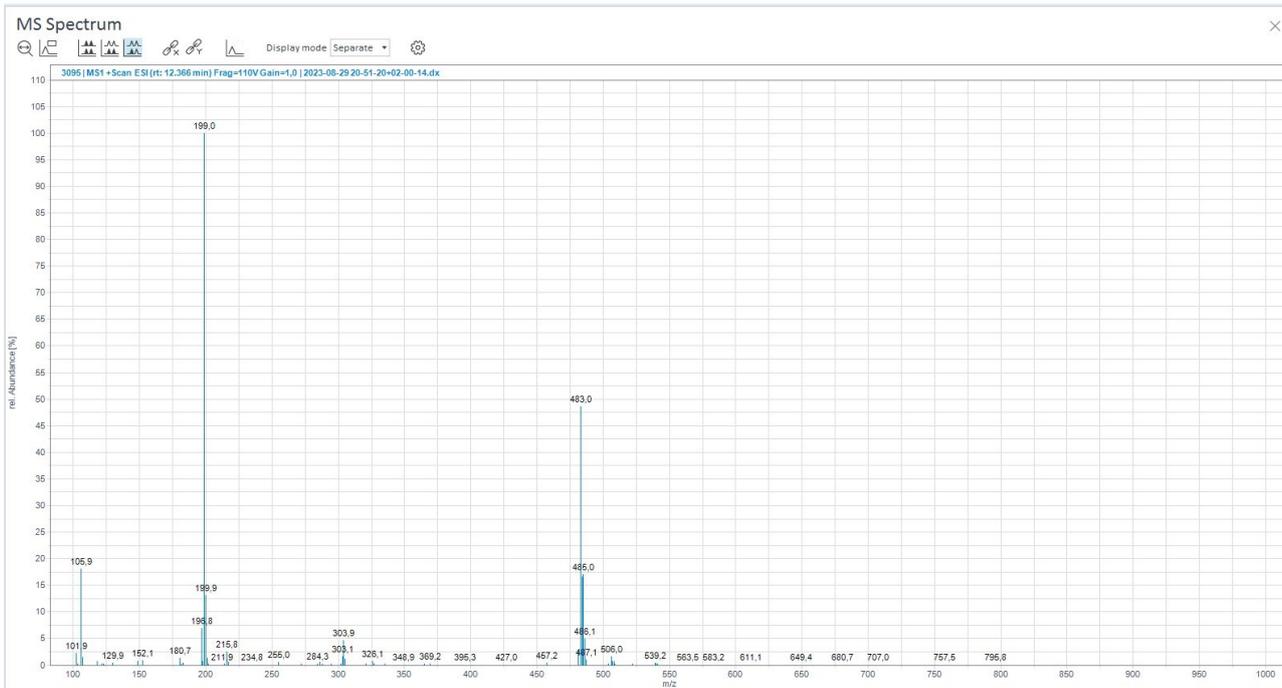


**Peak Results (Area Percent at least 1%)**

RT (min)	Signal Description	Width (min)	Area	Height	Area%
11.418	DAD1A,Sig=254,4 Ref=360,100	0.916	7954.0	921.1	99.09
11.494	MS1 +TIC SCAN ESI Frag=110V Gain=1.0	0.334	14399325.7	1429202.5	100.00

**$^1\text{H}$ ,  $^{13}\text{C}$  NMR and HPLC/MS spectra of compound 11e**



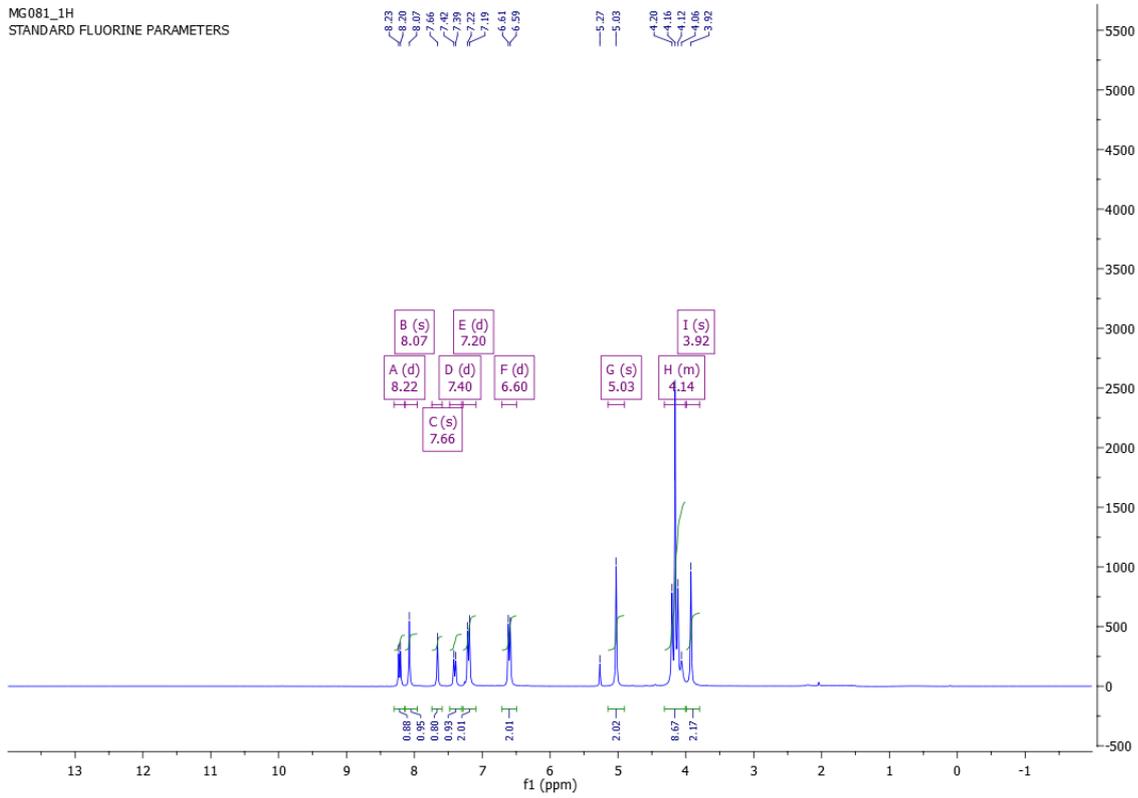


**Peak Results (Area Percent at least 1%)**

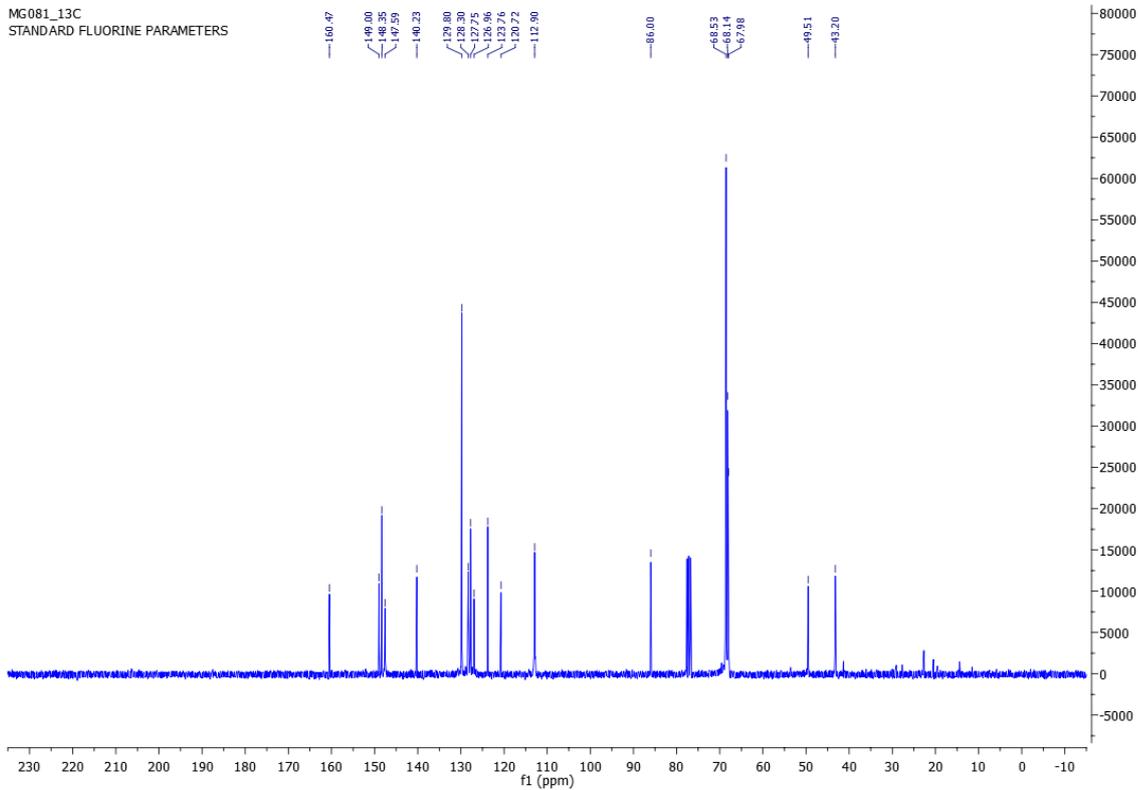
RT (min)	Signal Description	Width (min)	Area	Height	Area%
12.287	DAD1A, Sig=254,4 Ref=360,100	0.524	6154.9	729.0	97.92
12.366	MS1 +TIC SCAN ESI Frag=110V Gain=1.0	0.184	6862495.4	896087.9	100.00
14.220	DAD1A, Sig=254,4 Ref=360,100	0.158	99.4	17.2	1.58

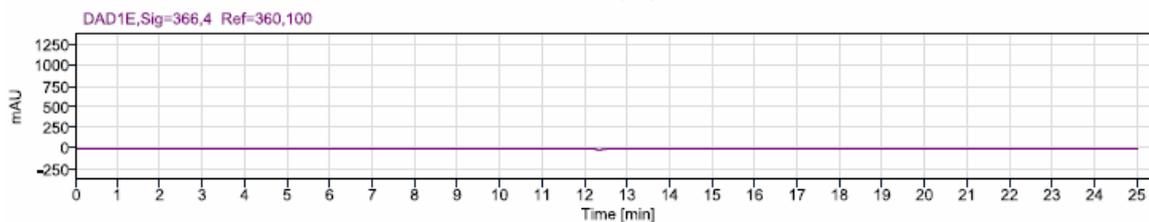
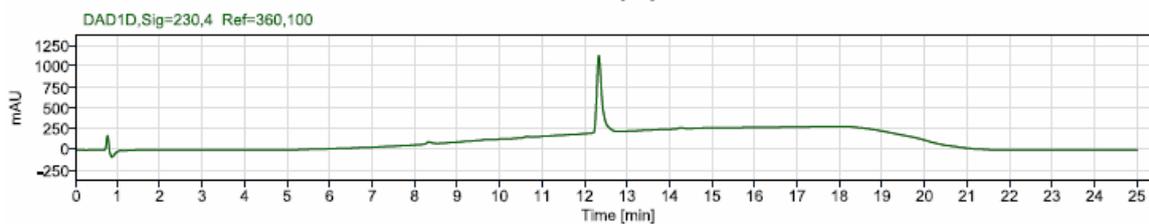
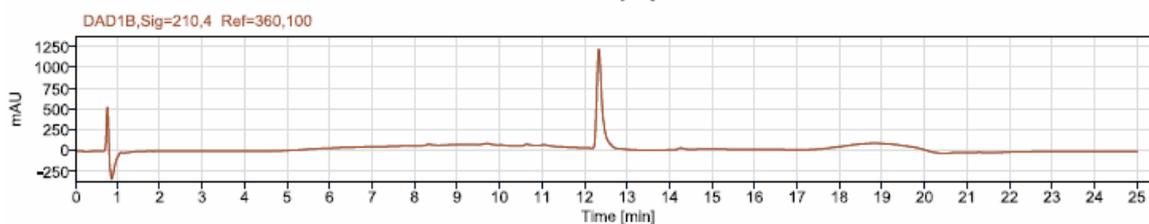
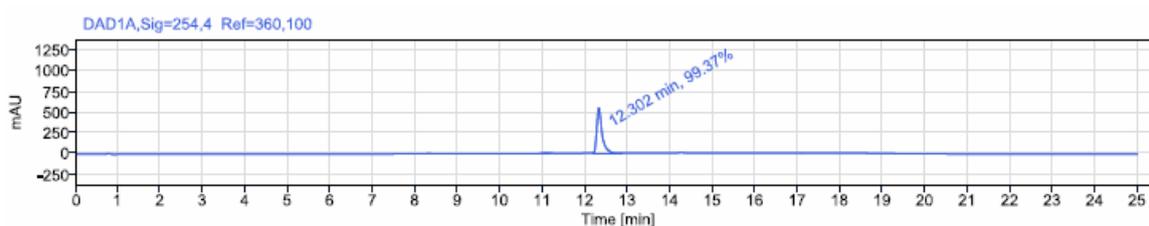
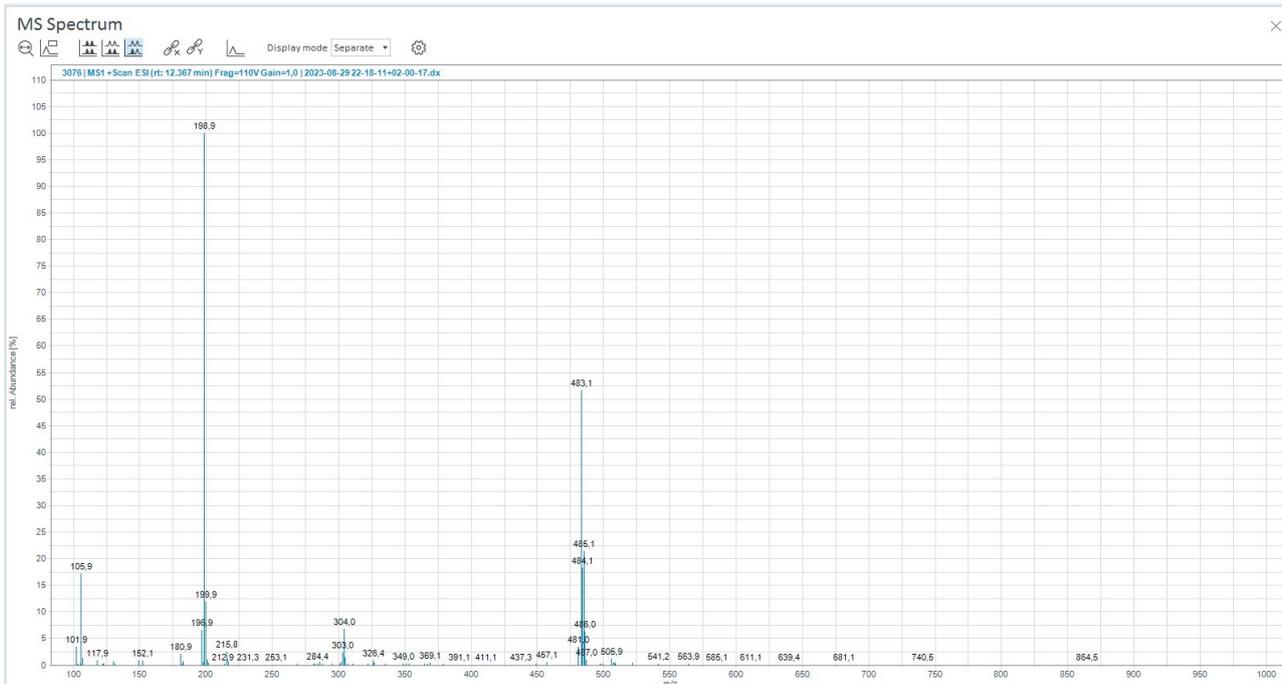
# <sup>1</sup>H, <sup>13</sup>C NMR and HPLC/MS spectra of compound 11f

MG081\_1H  
STANDARD FLUORINE PARAMETERS



MG081\_13C  
STANDARD FLUORINE PARAMETERS

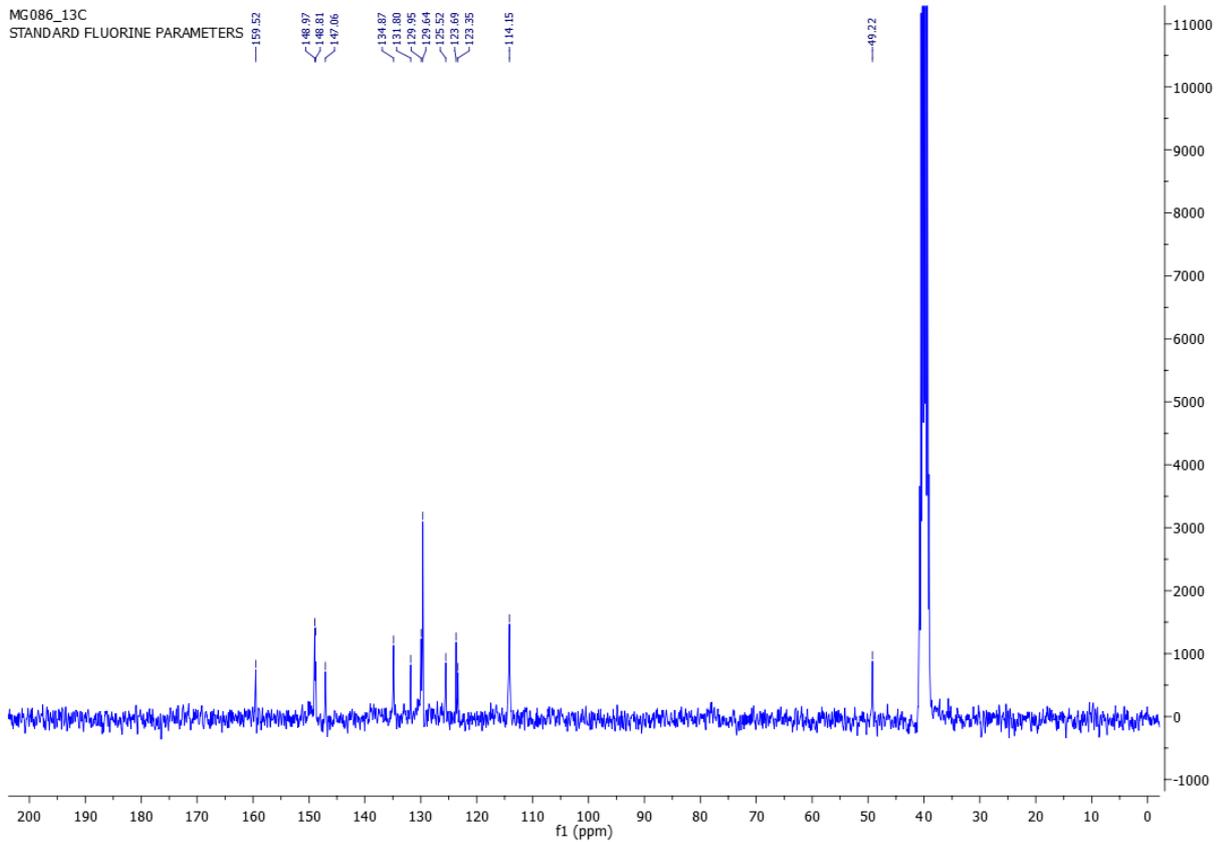
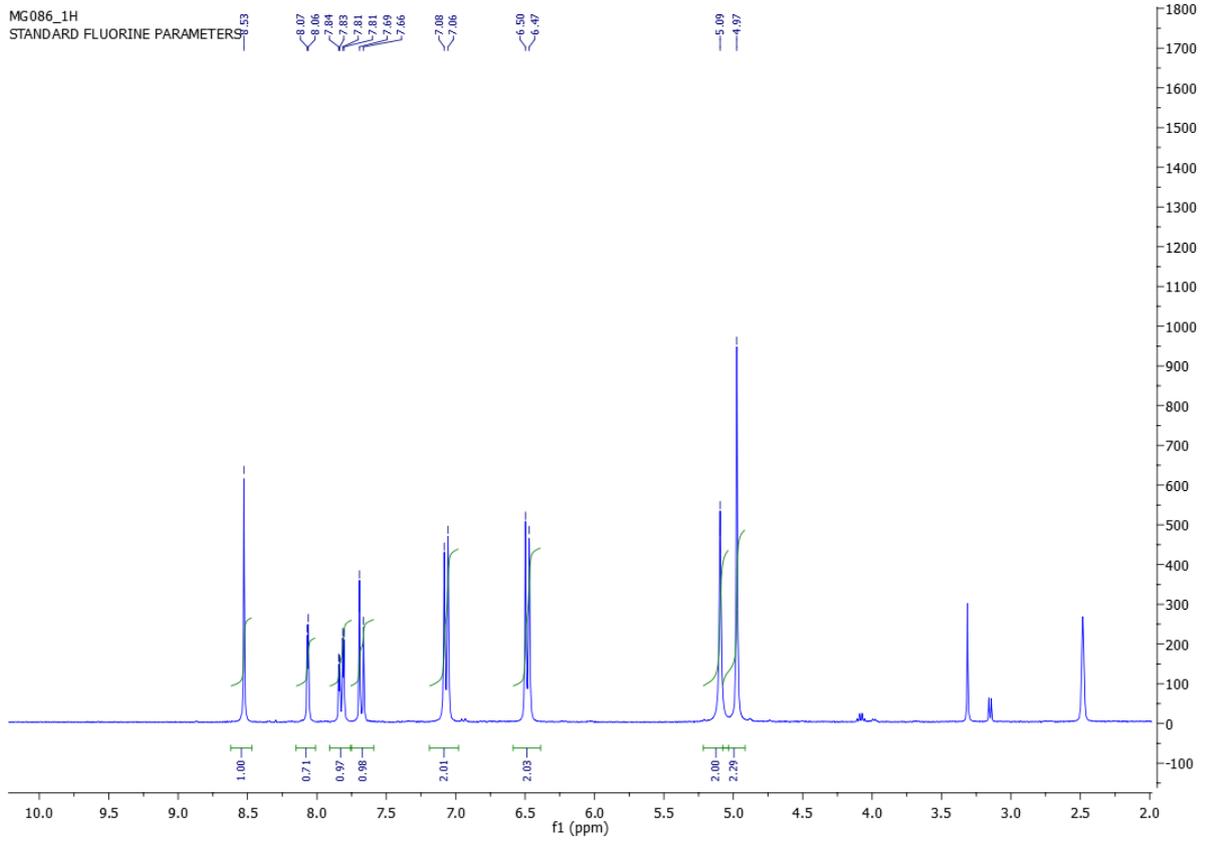


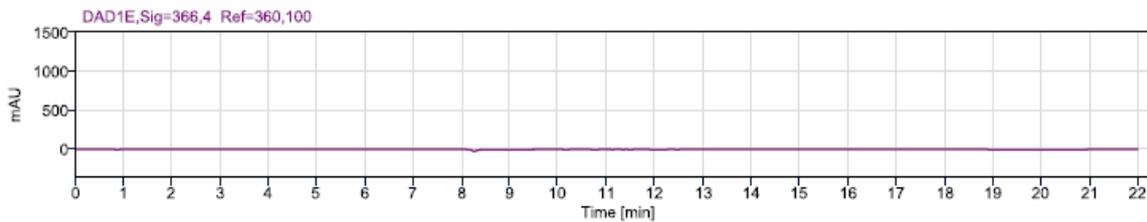
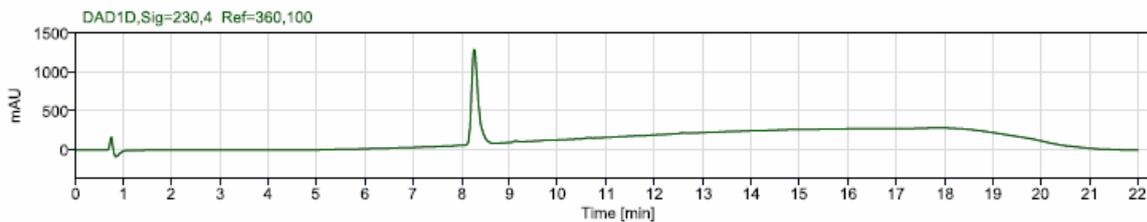
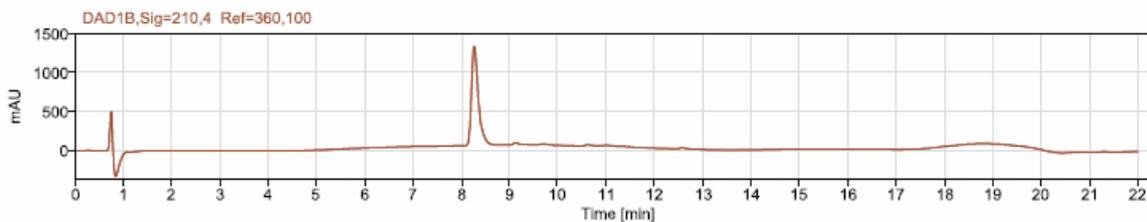
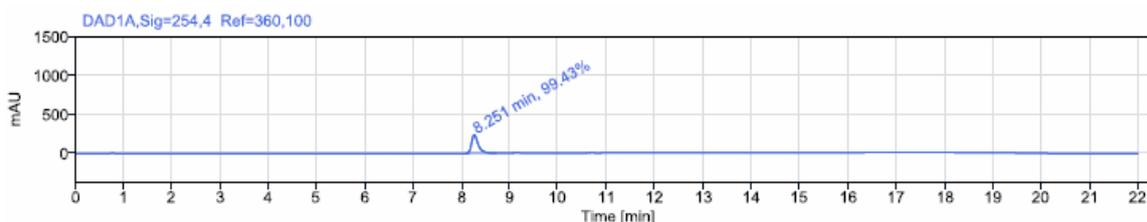
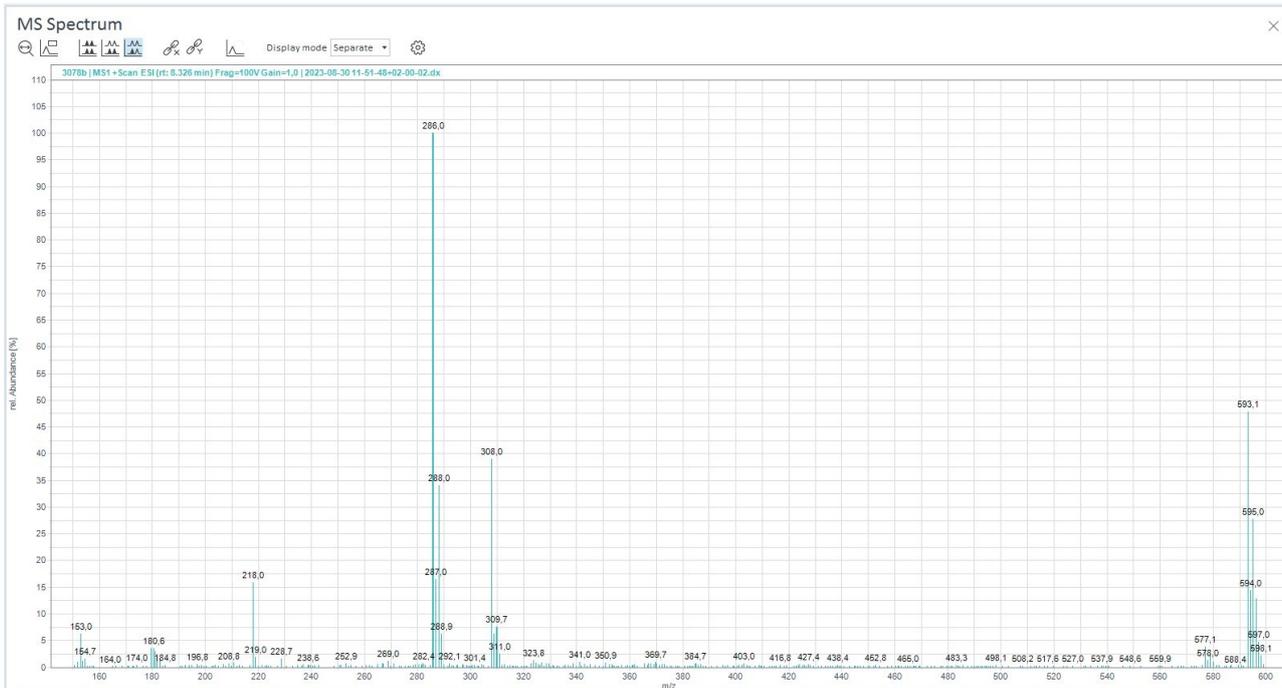


**Peak Results (Area Percent at least 1%)**

RT (min)	Signal Description	Width (min)	Area	Height	Area%
12.302	DAD1A, Sig=254,4 Ref=360,100	0.669	4656.8	541.3	99.37
12.364	MS1 +TIC SCAN ESI Frag=110V Gain=1.0	0.106	1641912.5	363973.6	100.00

# $^1\text{H}$ , $^{13}\text{C}$ NMR and HPLC/MS spectra of compound 22a

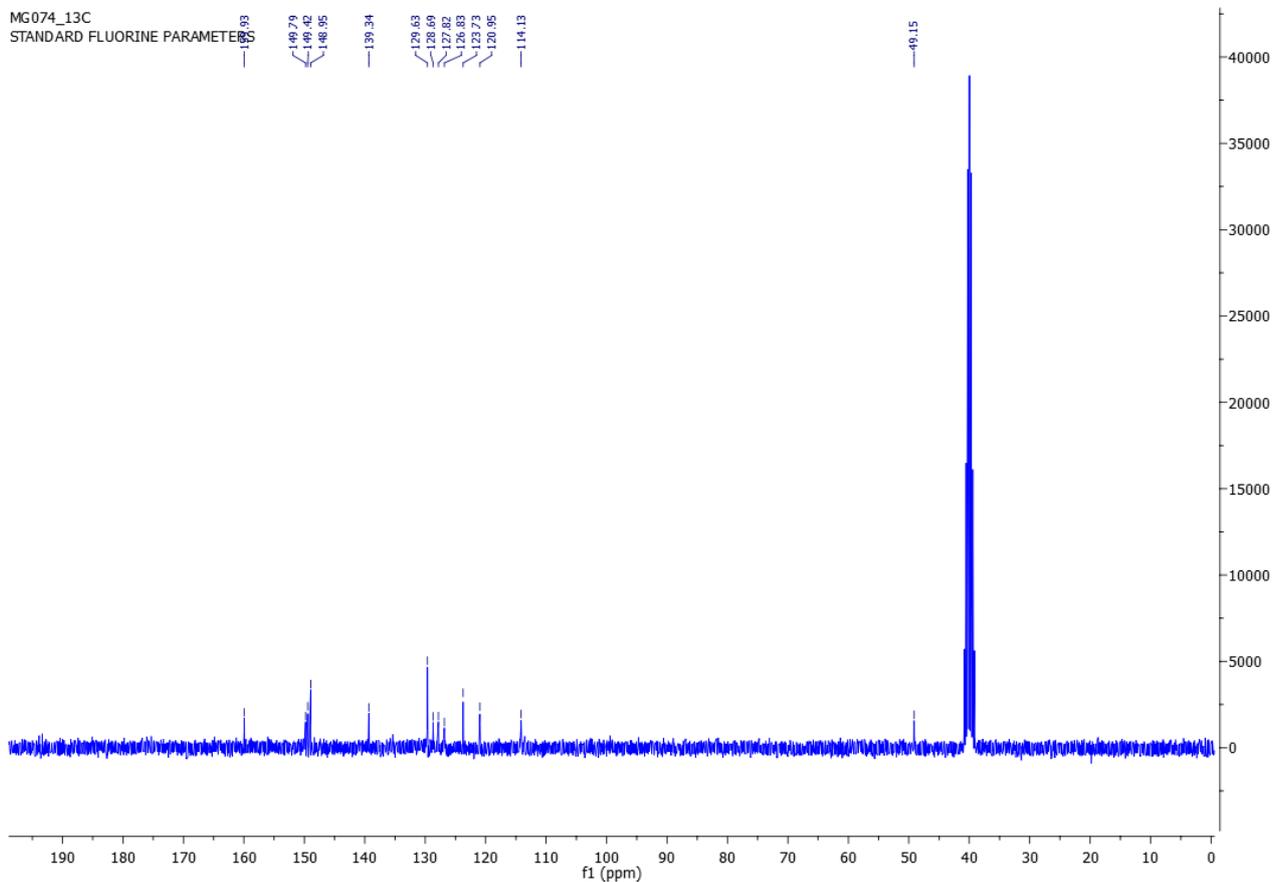
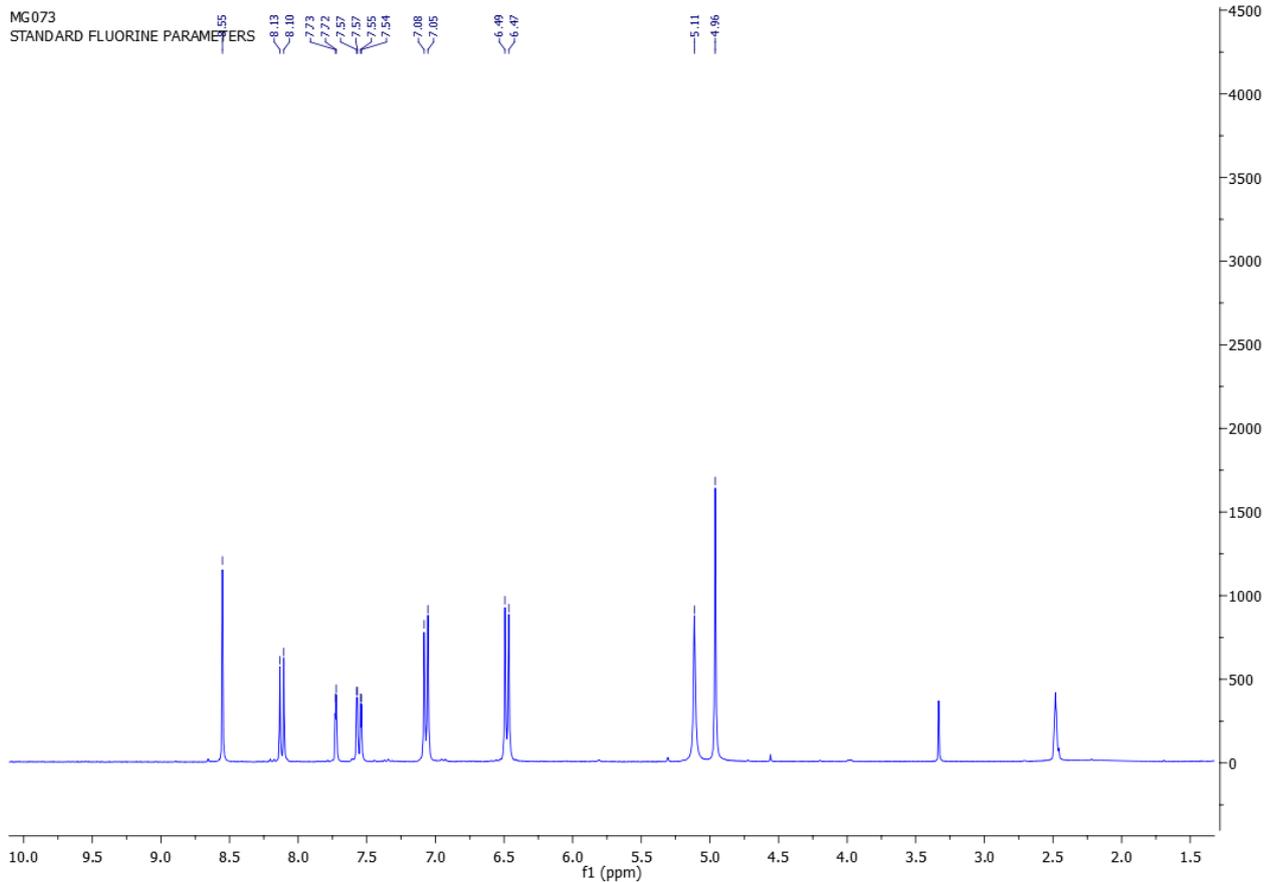


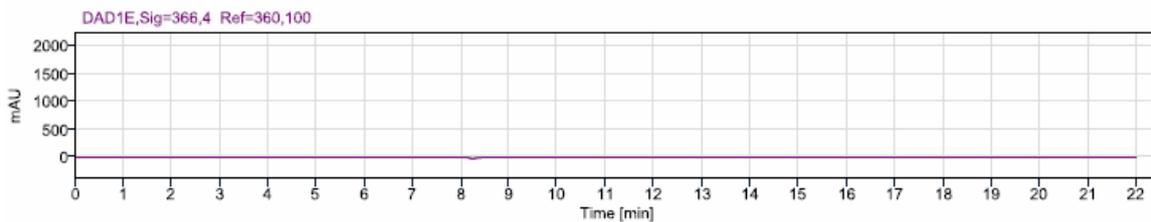
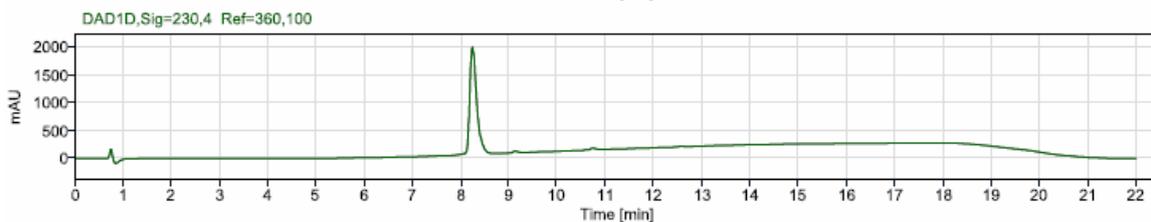
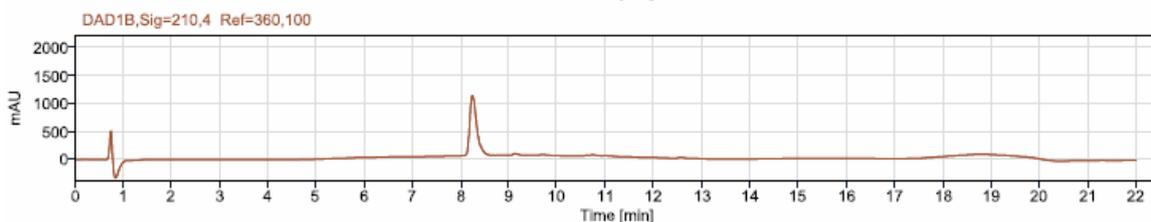
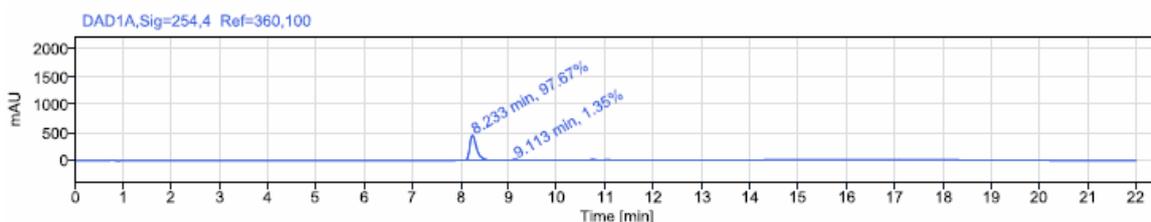
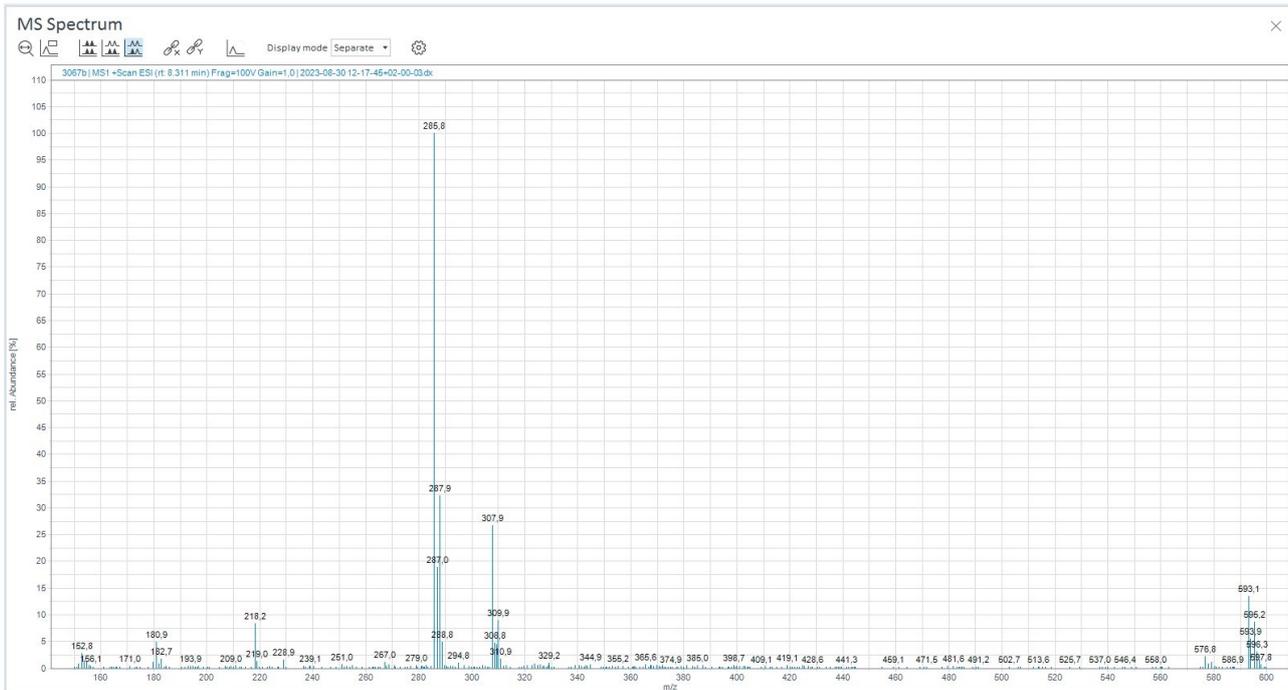


**Peak Results (Area Percent at least 1%)**

RT (min)	Signal Description	Width (min)	Area	Height	Area%
8.251	DAD1A, Sig=254,4 Ref=360,100	0.663	2282.5	239.0	99.43
8.324	MS1 +TIC SCAN ESI Frag=100V Gain=1.0	0.418	3273900.3	329227.4	100.00
8.326	MS1 +TIC SIM ESI Frag=100V Gain=1.0	0.461	948102.5	83126.0	100.00
8.361	MS1 -TIC SCAN ESI Frag=100V Gain=1.0	0.676	268240.5	18259.0	100.00

# <sup>1</sup>H, <sup>13</sup>C NMR and HPLC/MS spectra of compound 22b



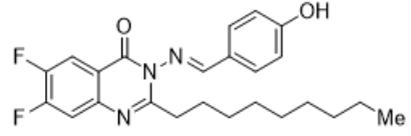
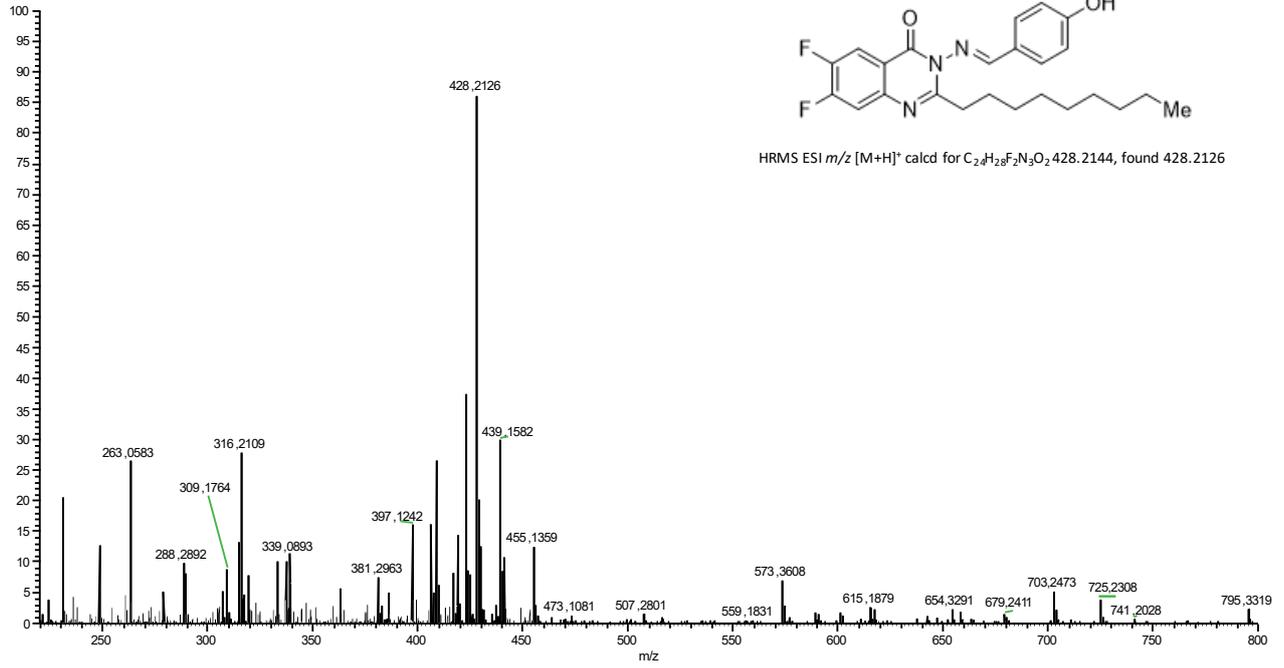


**Peak Results (Area Percent at least 1%)**

RT (min)	Signal Description	Width (min)	Area	Height	Area%
8.233	DAD1A, Sig=254,4 Ref=360,100	0.740	4456.3	450.0	97.67
8.304	MS1 +TIC SIM ESI Frag=100V Gain=1.0	1.183	1243736.5	101700.5	100.00
8.309	MS1 +TIC SCAN ESI Frag=100V Gain=1.0	0.718	3806960.1	301412.0	100.00
9.113	DAD1A, Sig=254,4 Ref=360,100	0.142	61.7	13.0	1.35

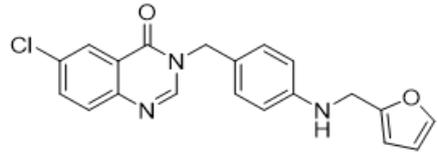
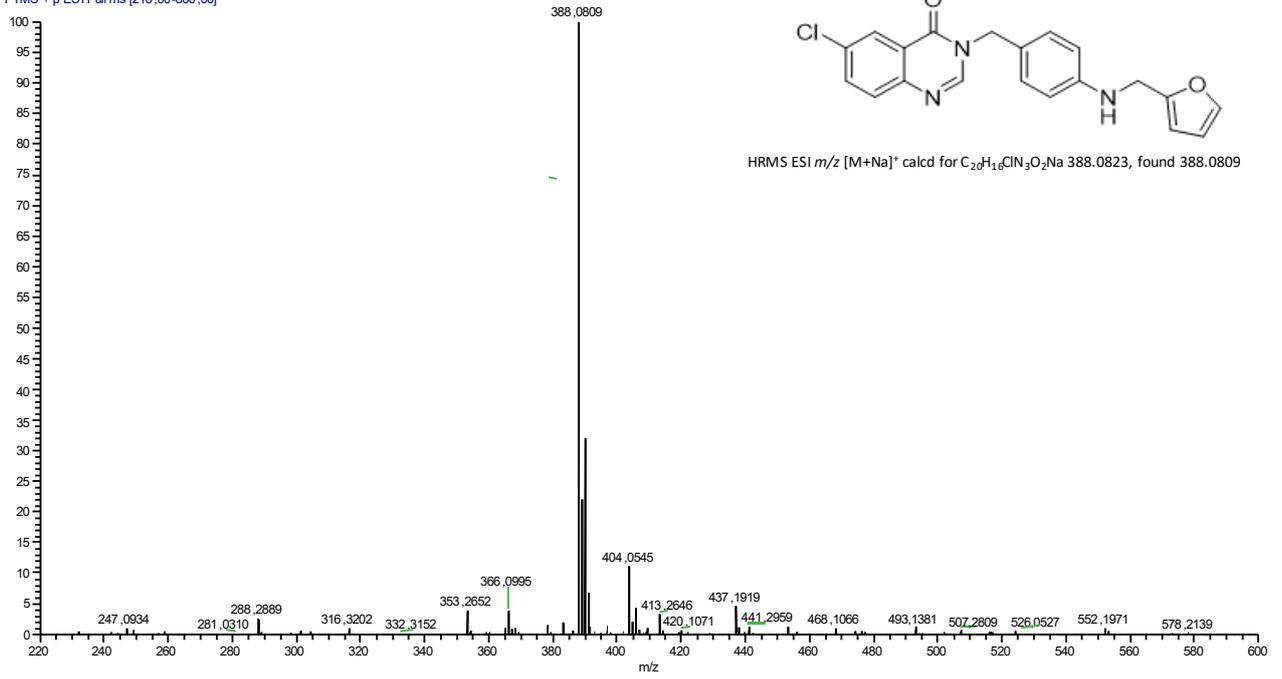
# HRMS spectrum of compound 7a

NF3033 #18 RT: 0.14 AV: 1 NL: 9,38E6  
T: FTMS + p ESI Full ms [216.00-900.00]



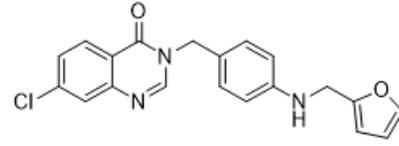
# HRMS spectrum of compound 11a

NF3088 #33 RT: 0.26 AV: 1 NL: 5.92E7  
T: FTMS + p ESI Full ms [216.00-800.00]



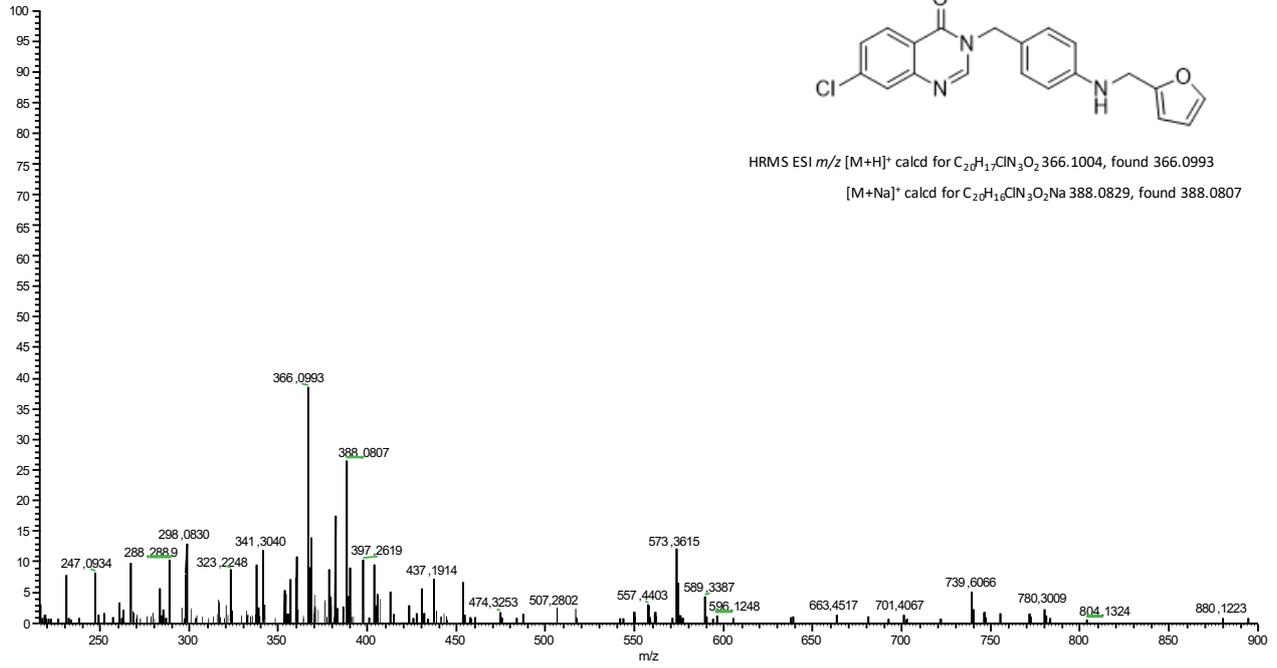
# HRMS spectrum of compound 11b

NF3072 #83 RT: 0.65 AV: 1 NL: 2.53E6  
T: FTMS + p ESI Full ms [216.00-900.00]



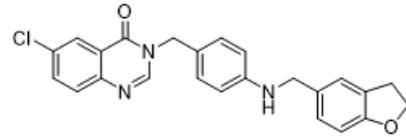
HRMS ESI  $m/z$   $[M+H]^+$  calcd for  $C_{20}H_{17}ClN_3O_2$  366.1004, found 366.0993

$[M+Na]^+$  calcd for  $C_{20}H_{16}ClN_3O_2Na$  388.0829, found 388.0807

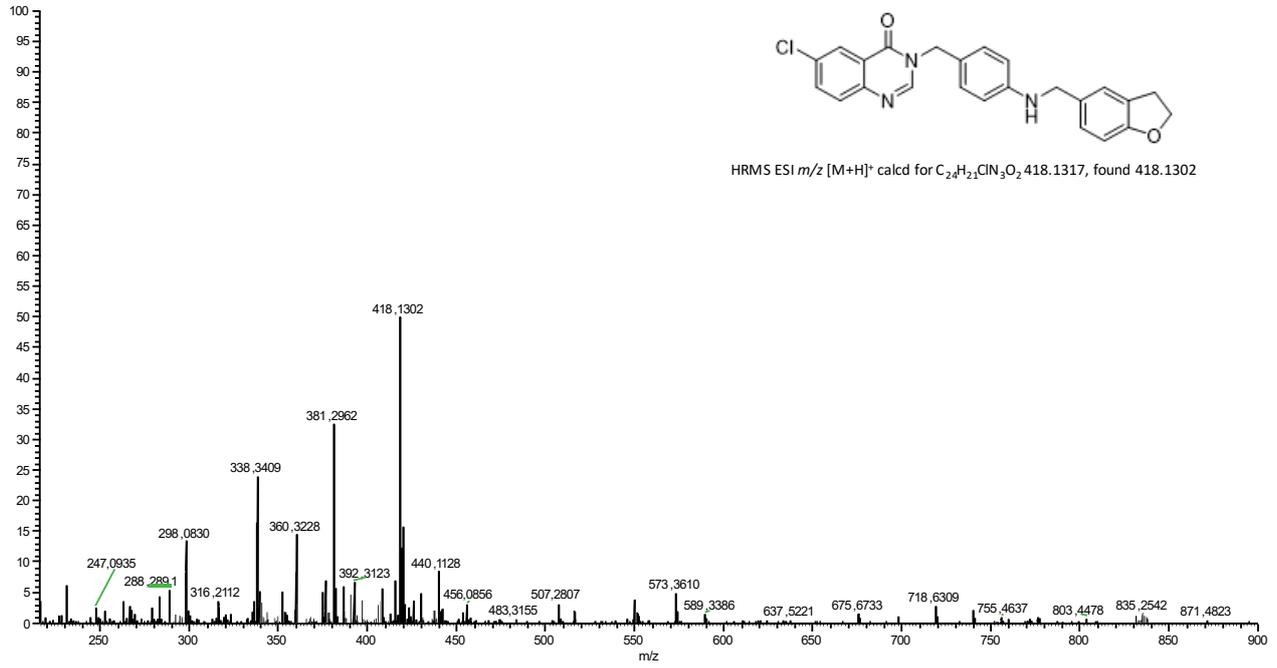


# HRMS spectrum of compound 11c

NF3081 BIS H20 #2 RT:0.01 AV: 1 NL: 8,31E6  
T: FTMS + p ESI Full ms [216.00-900.00]

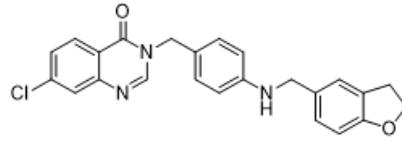


HRMS ESI  $m/z$   $[M+H]^+$  calcd for  $C_{24}H_{21}ClN_3O_2$  418.1317, found 418.1302



# HRMS spectrum of compound 11d

NF3077 #38 RT: 0.30 AV: 1 NL: 4,26E6  
T: FTMS + p ESI Full ms [216.00-800.00]



HRMS ESI  $m/z$   $[M+H]^+$  calcd for  $C_{24}H_{21}ClN_3O_2$  418.1317, found 418.1304

