

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**

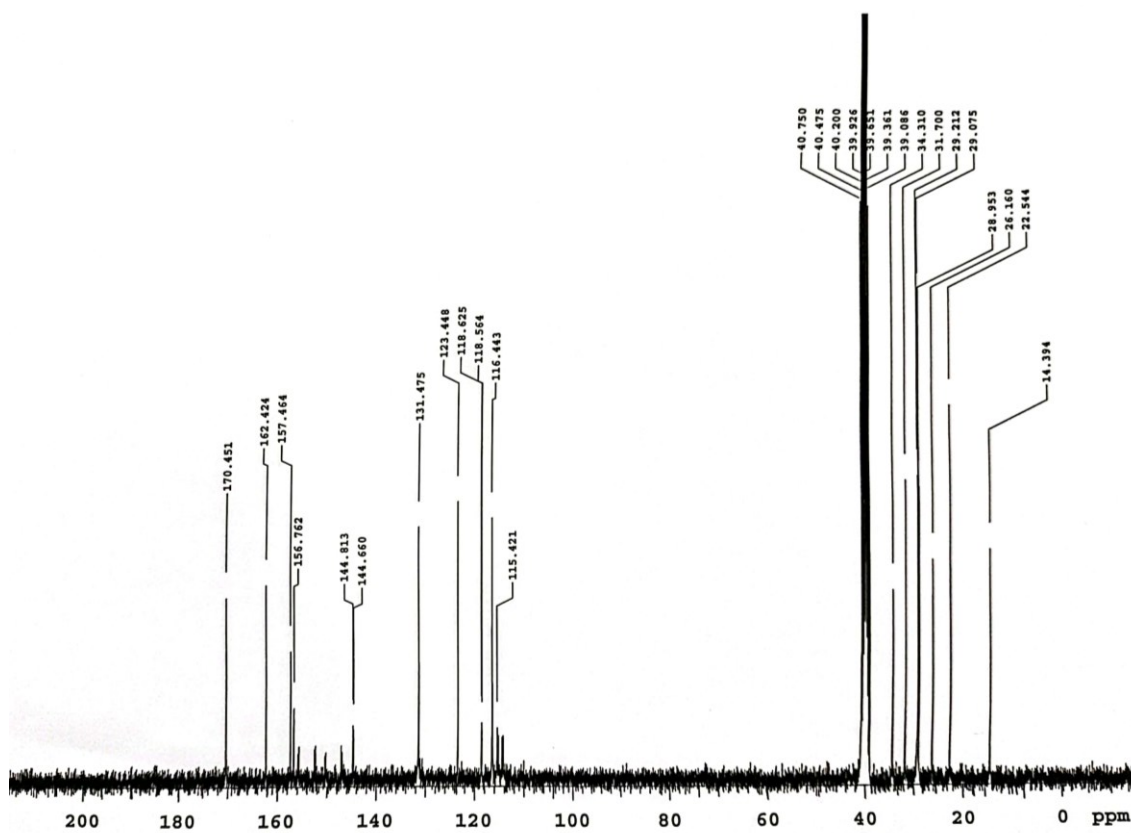
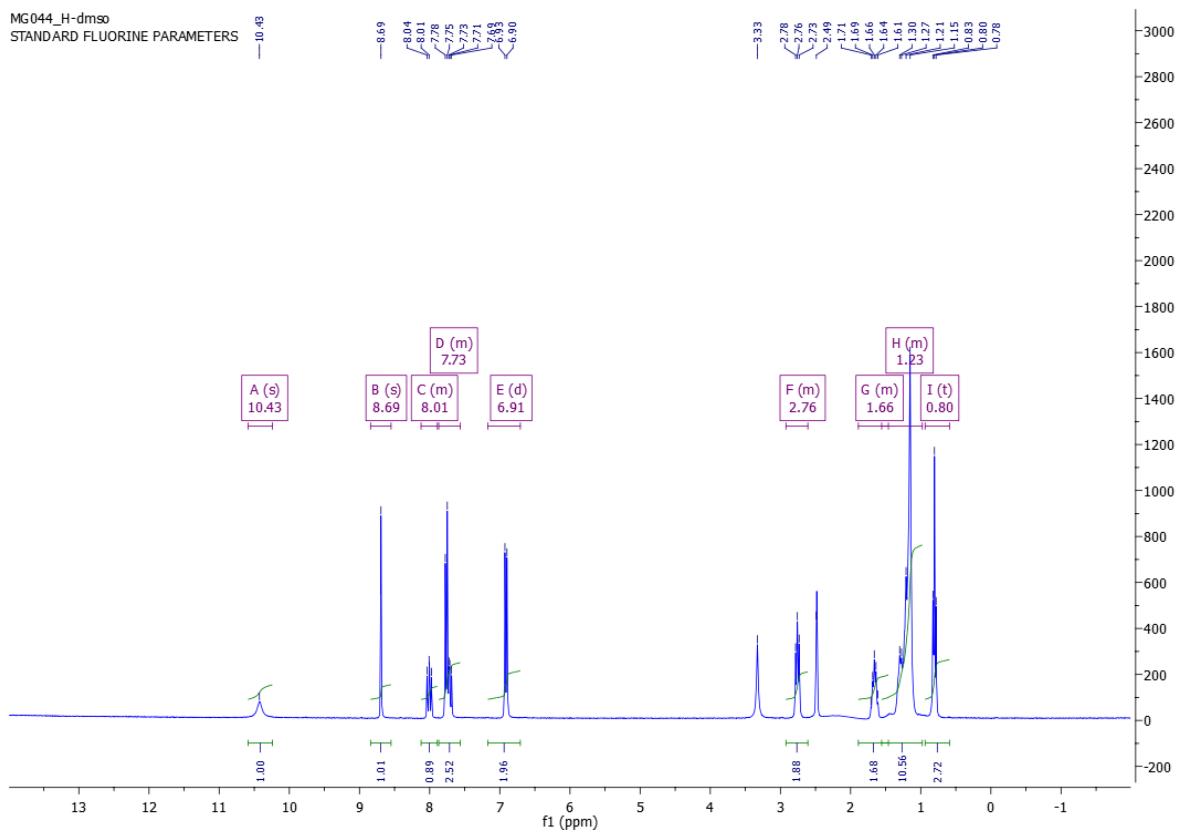
HRMS spectrum of compound **11b**

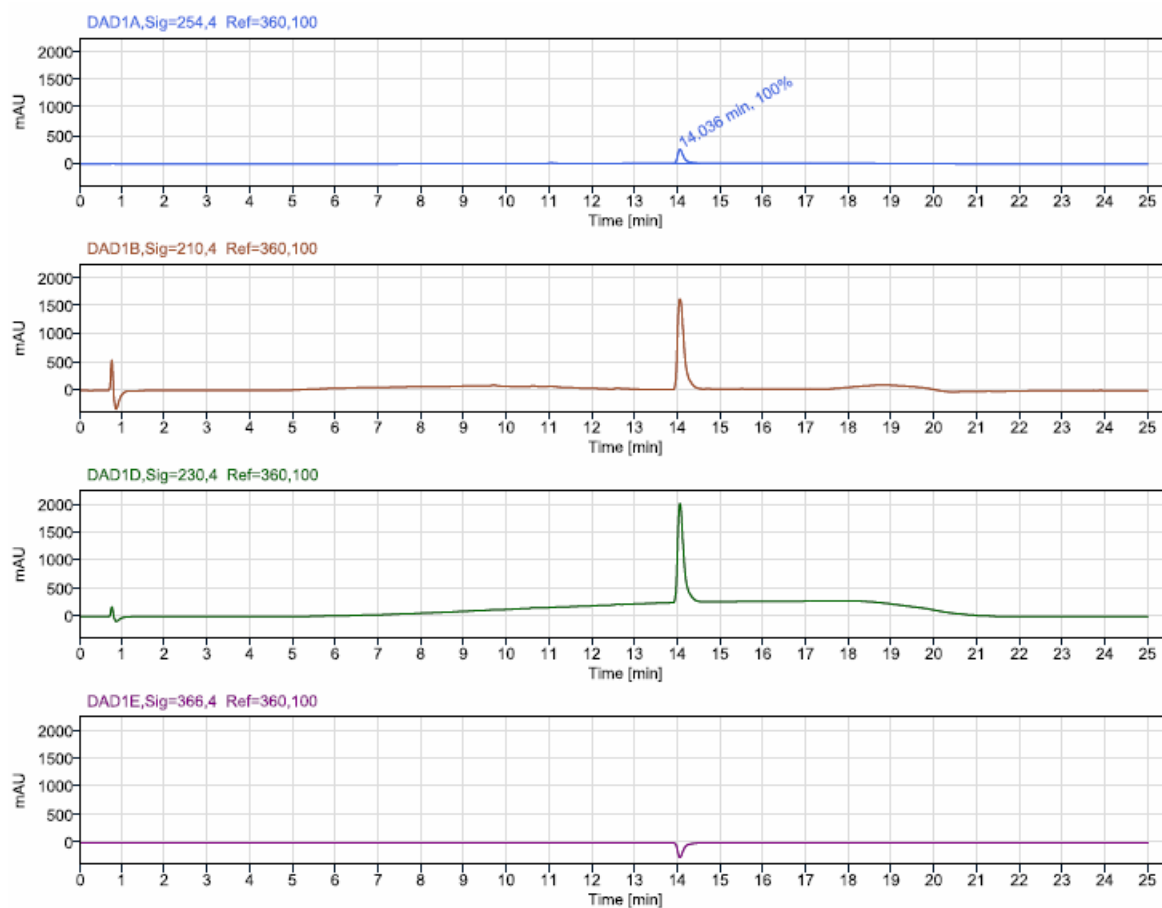
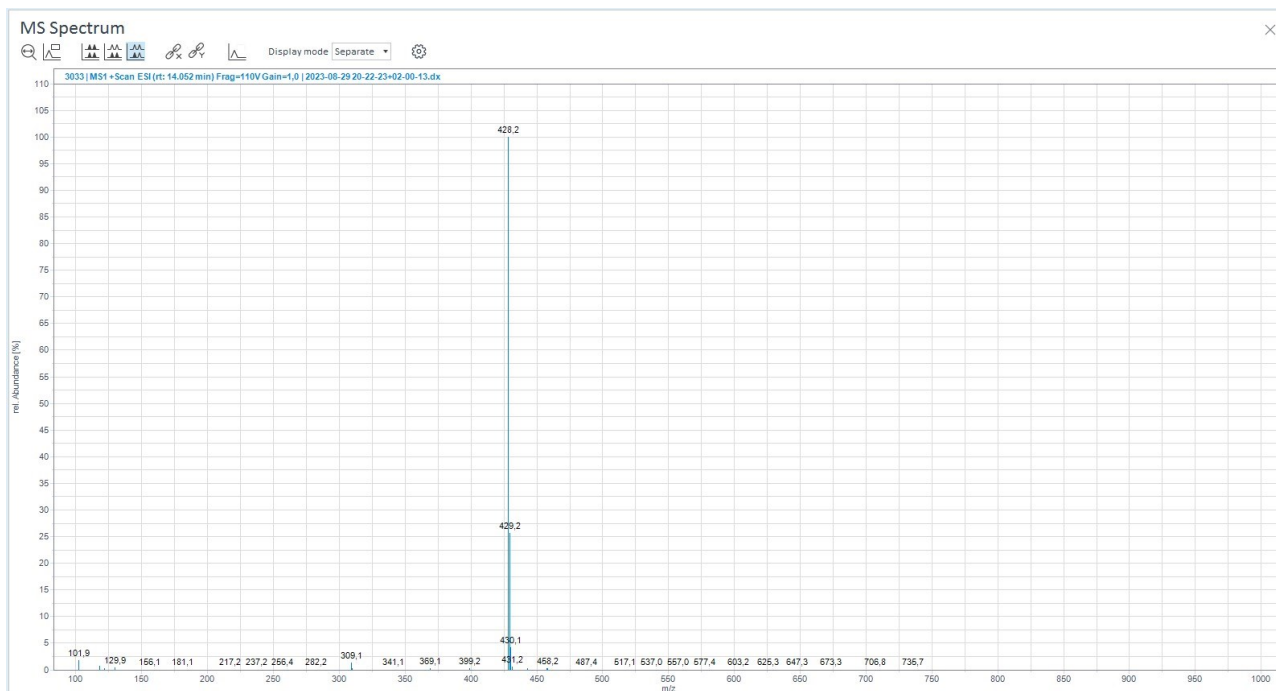
HRMS spectrum of compound **11c**

HRMS spectrum of compound **11d**

¹H, ¹³C NMR and HPLC/MS spectra of compound 7a

MG044_H-dmsd
STANDARD FLUORINE PARAMETERS

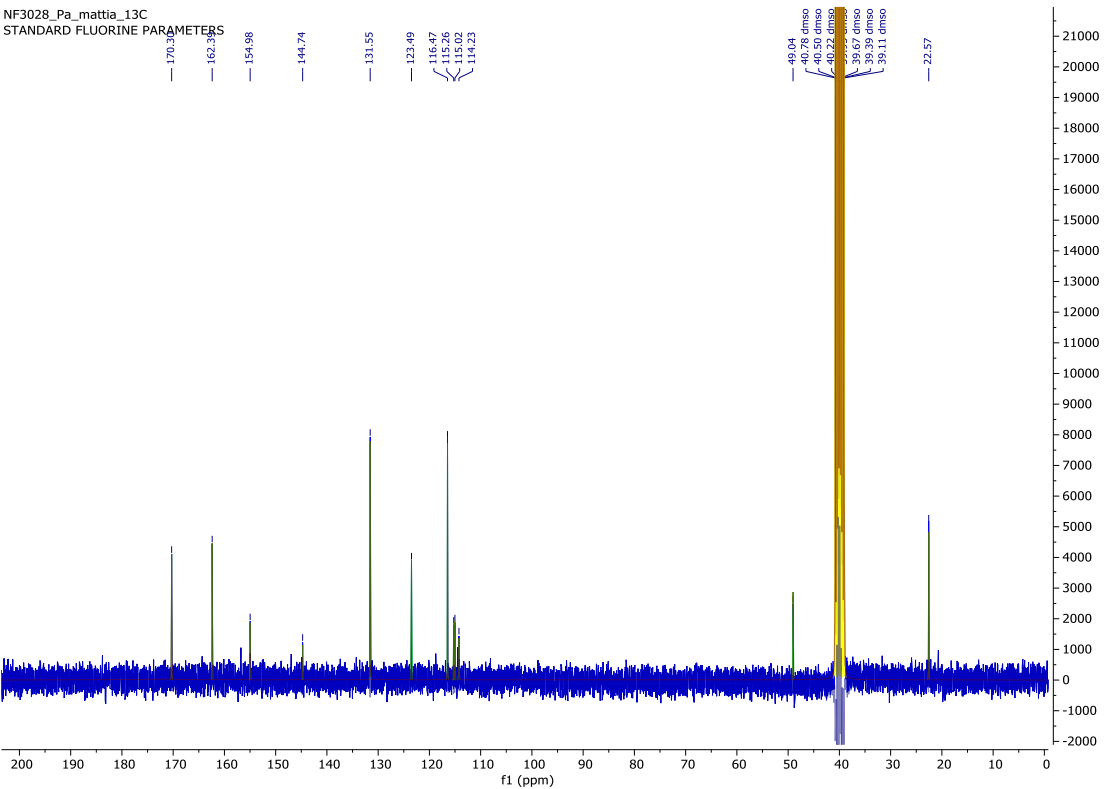
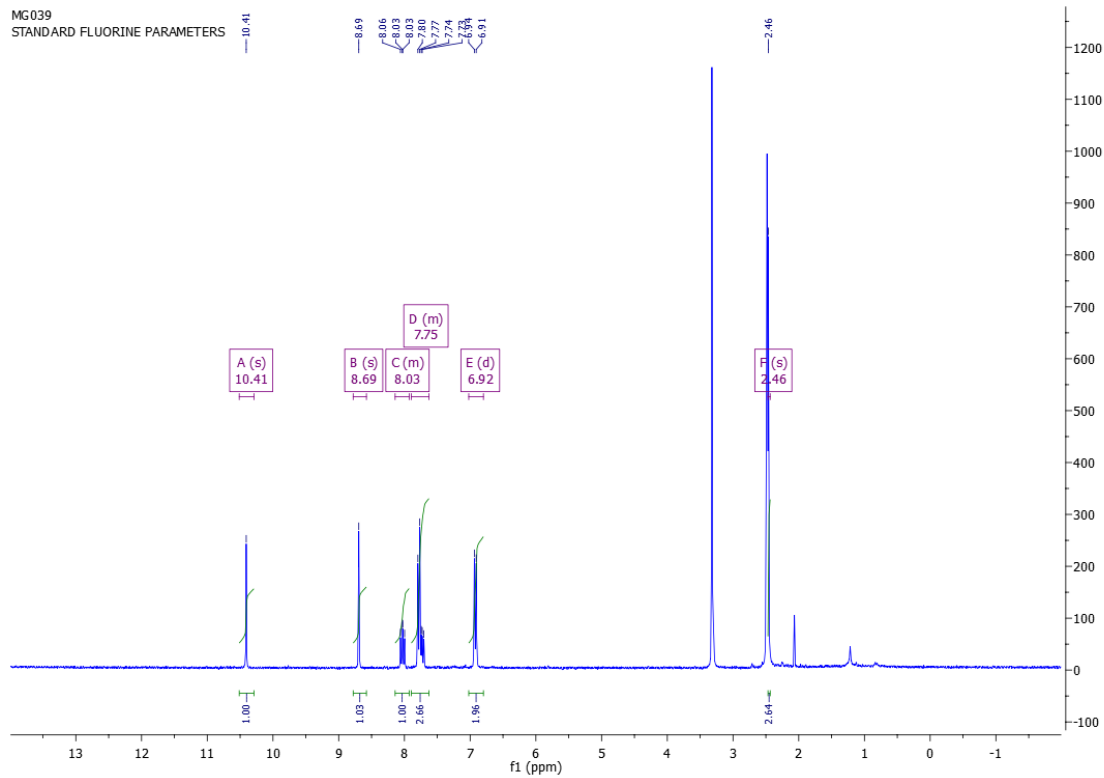


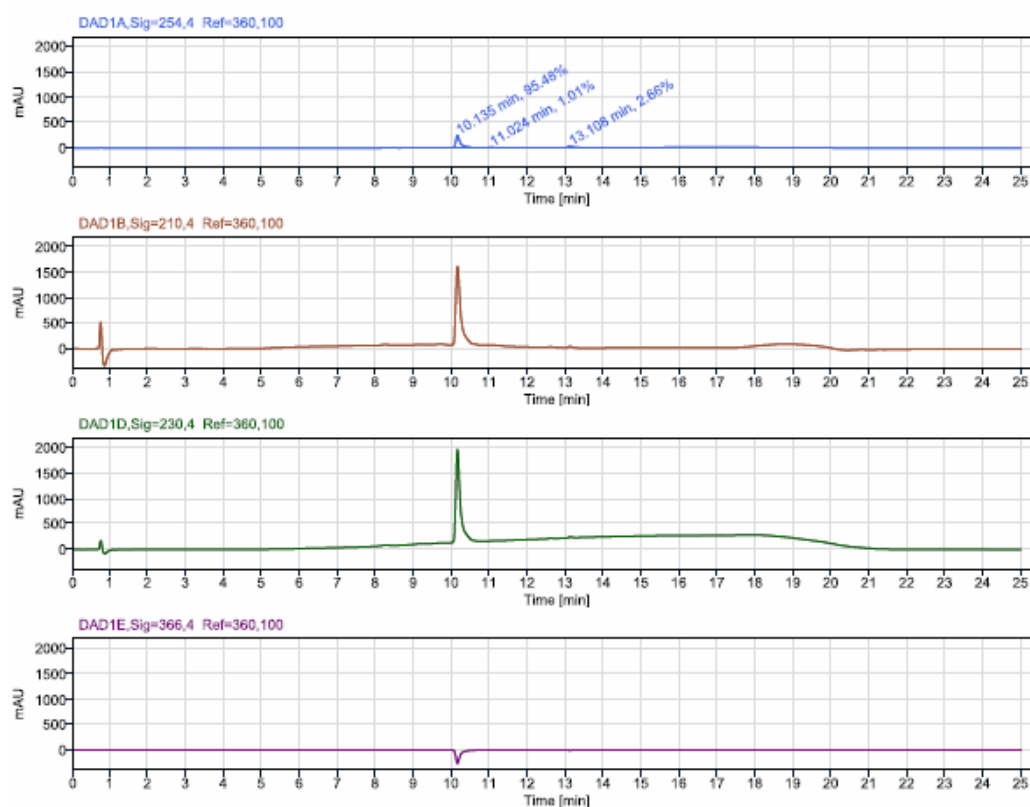
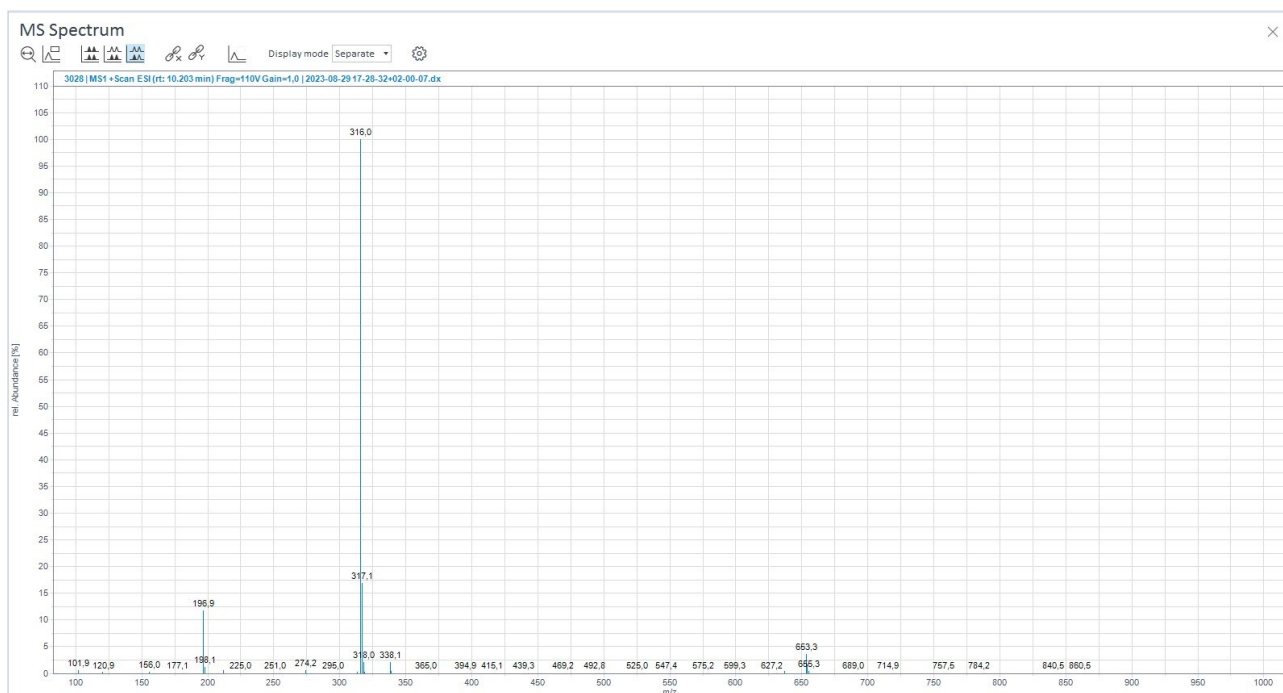


Peak Results (Area Percent at least 1%)

| RT (min) | Signal Description | Width (min) | Area | Height | Area% |
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| 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 |

¹H, ¹³C NMR and HPLC/MS spectra of compound 7b

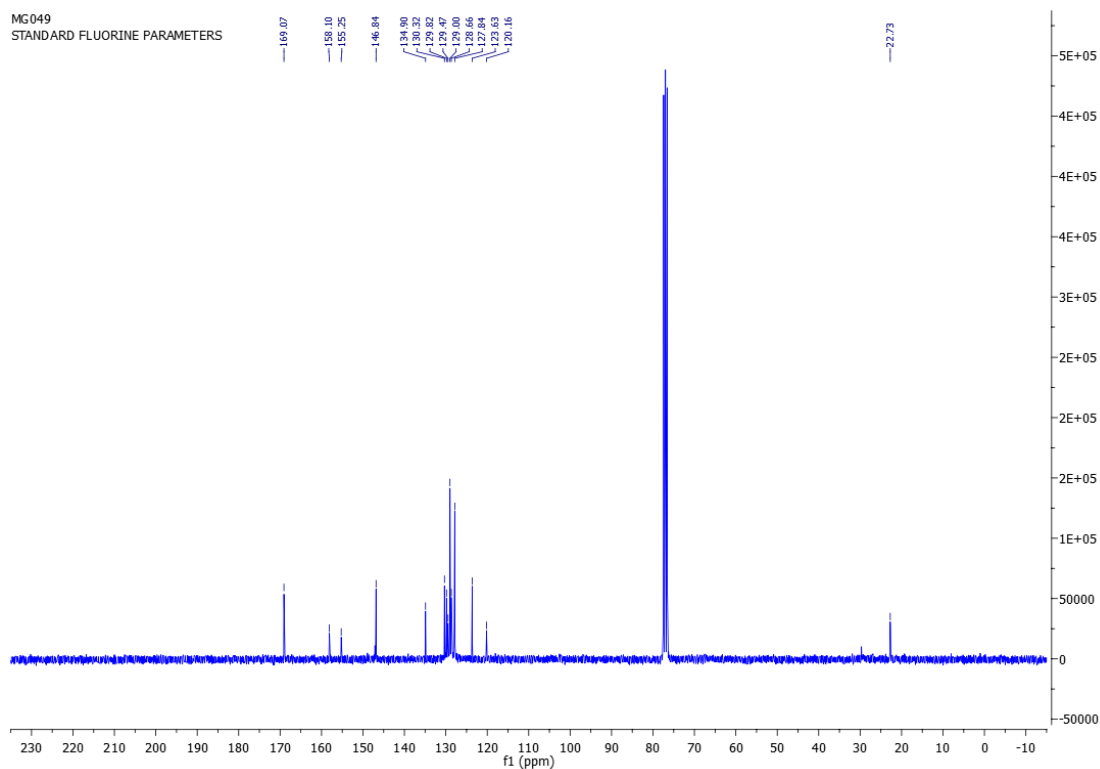
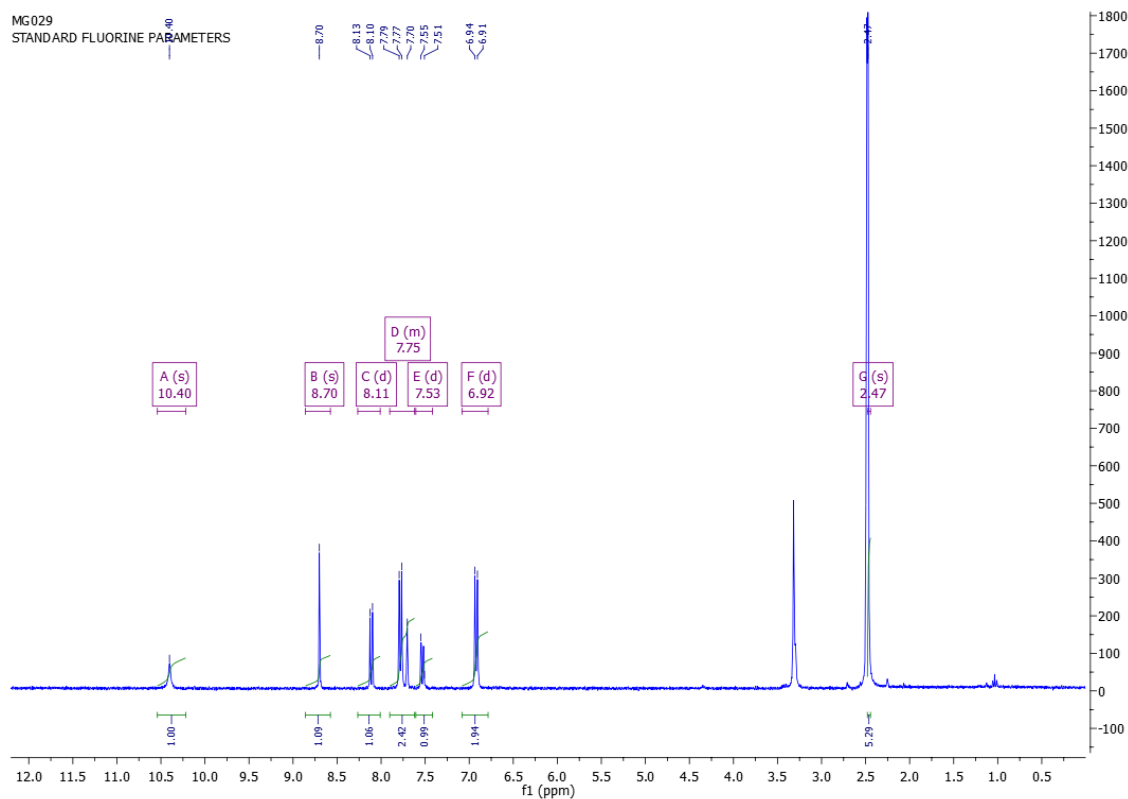


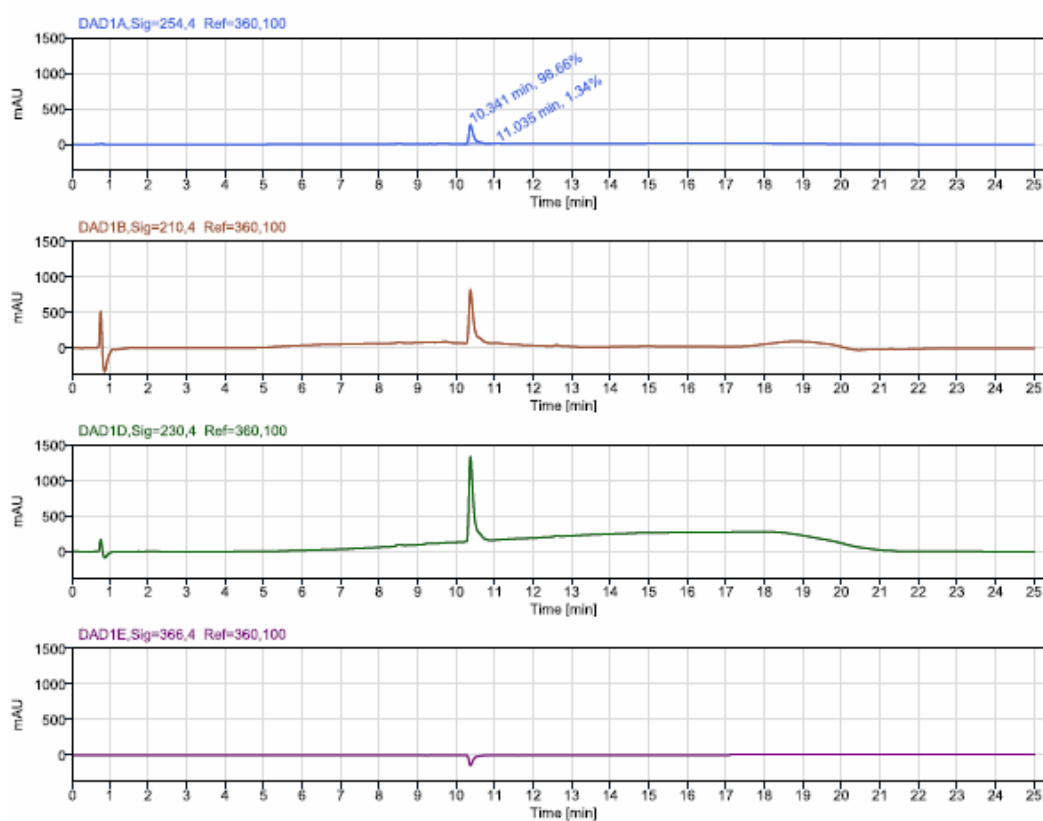
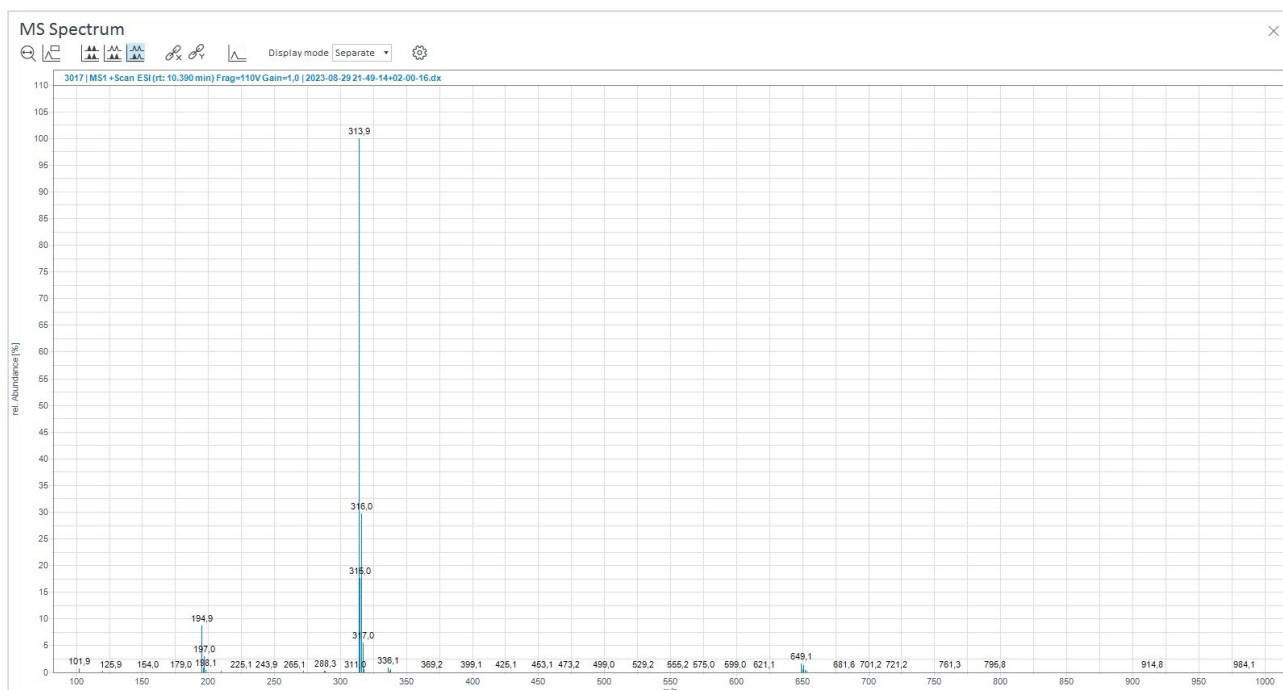


Peak Results (Area Percent at least 1%)

| RT (min) | Signal Description | Width (min) | Area | Height | Area% |
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| 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 |

¹H, ¹³C NMR and HPLC/MS spectra of compound 7c

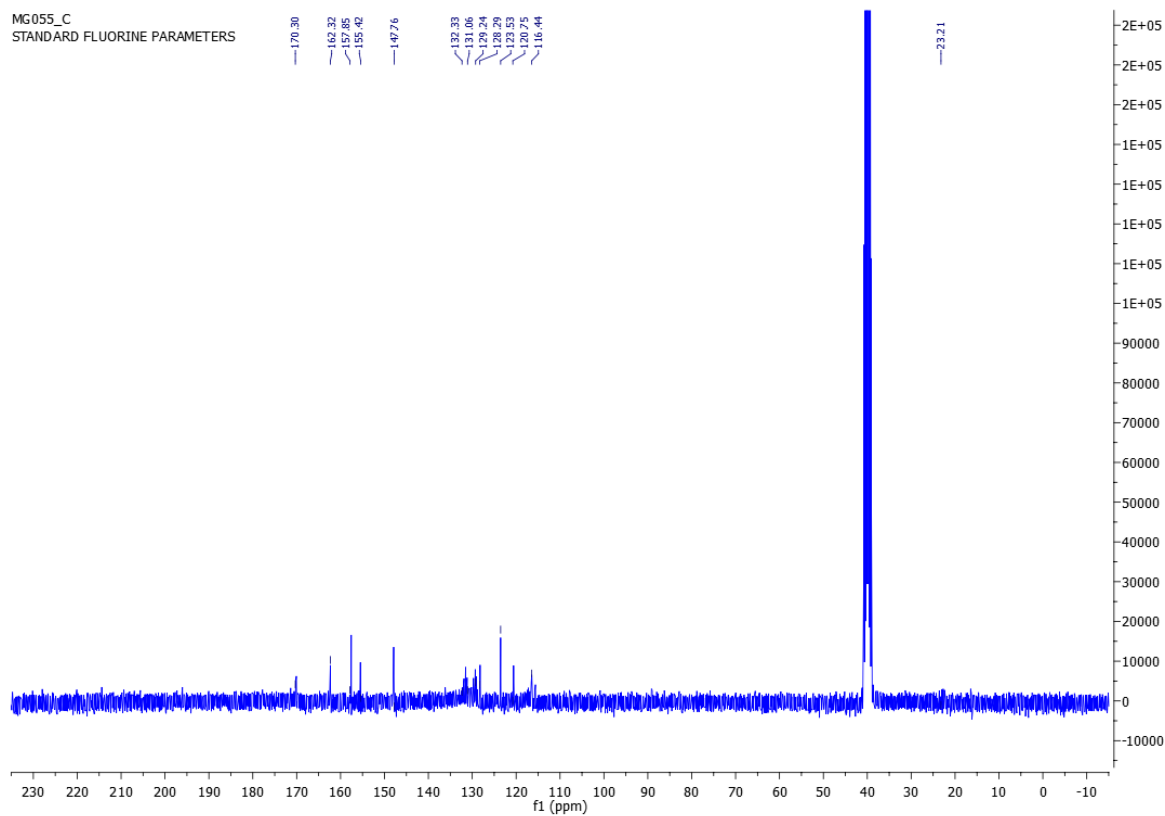
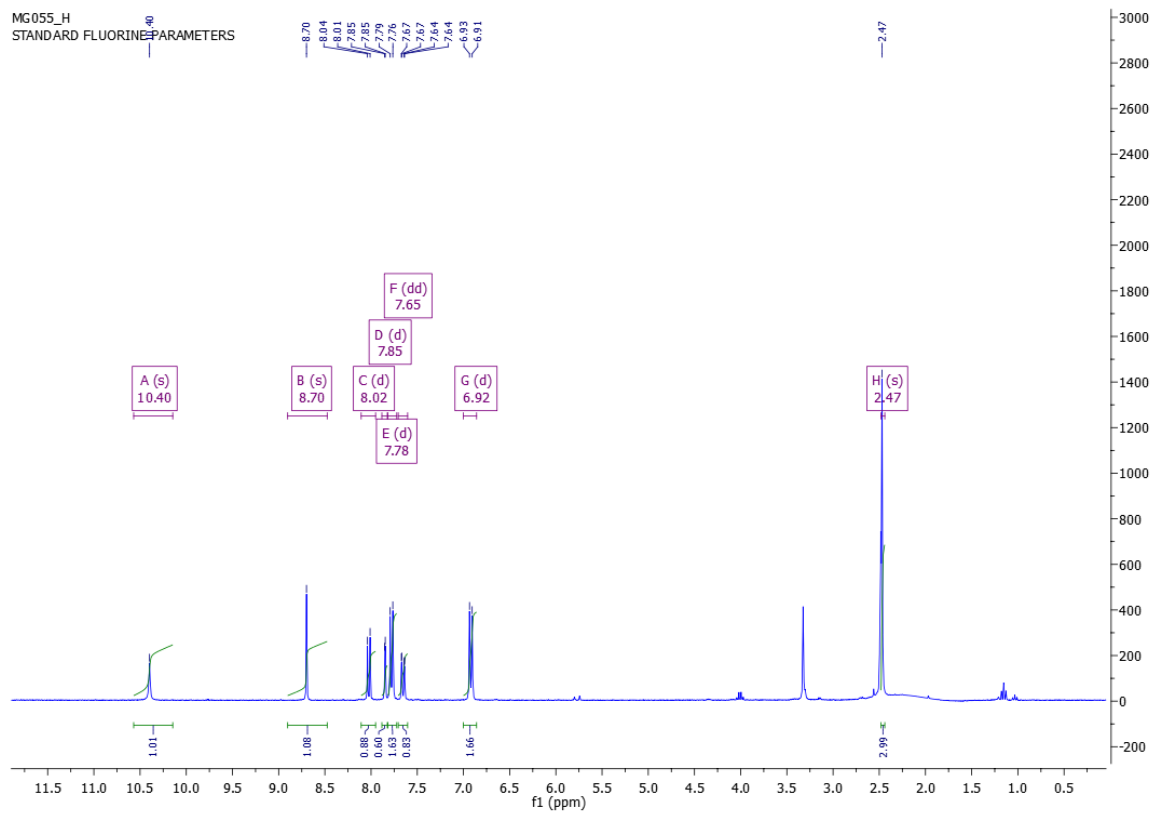


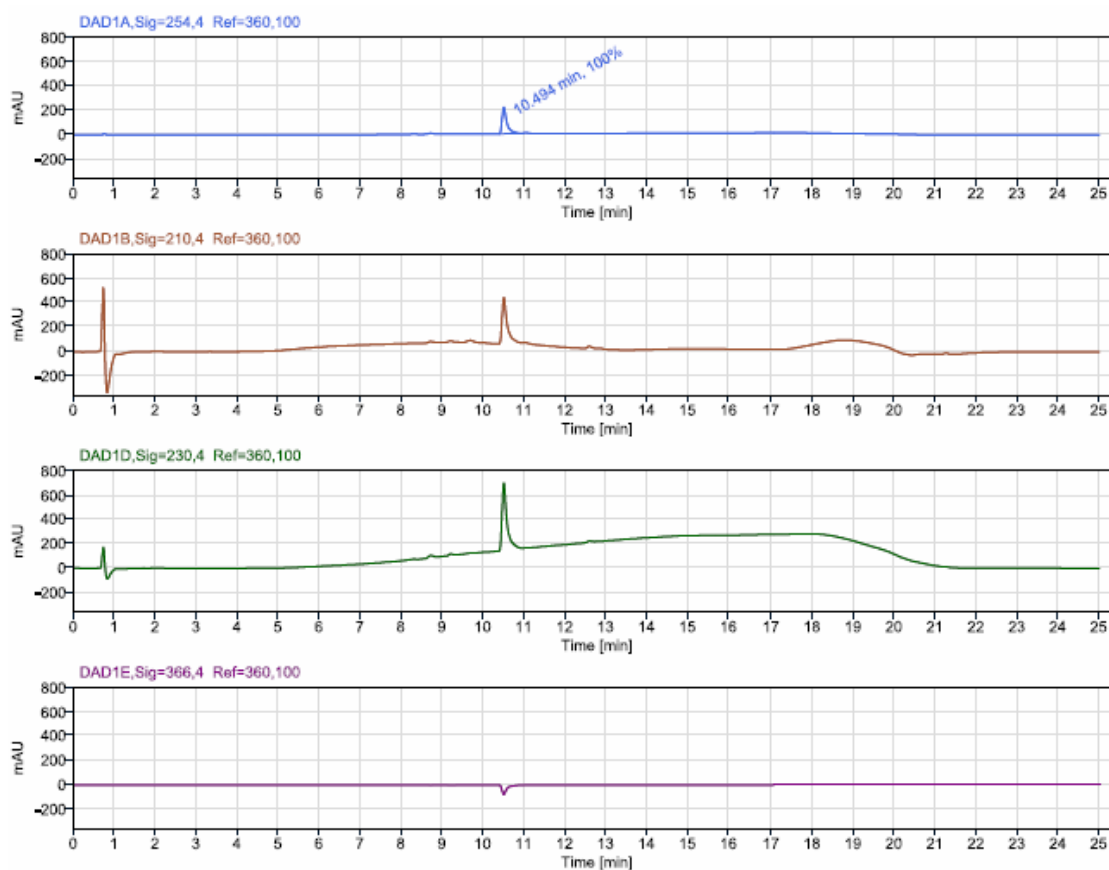
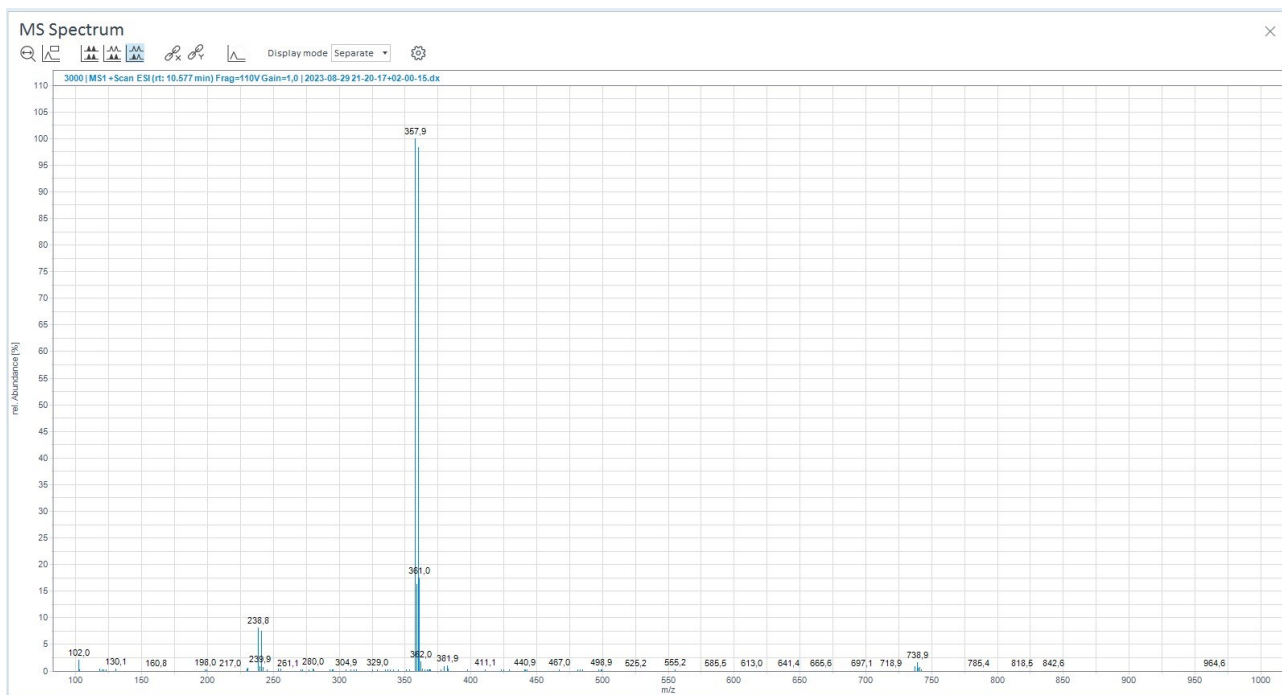


Peak Results (Area Percent at least 1%)

| RT (min) | Signal Description | Width (min) | Area | Height | Area% |
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| 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 |

¹H, ¹³C NMR and HPLC/MS spectra of compound 7d

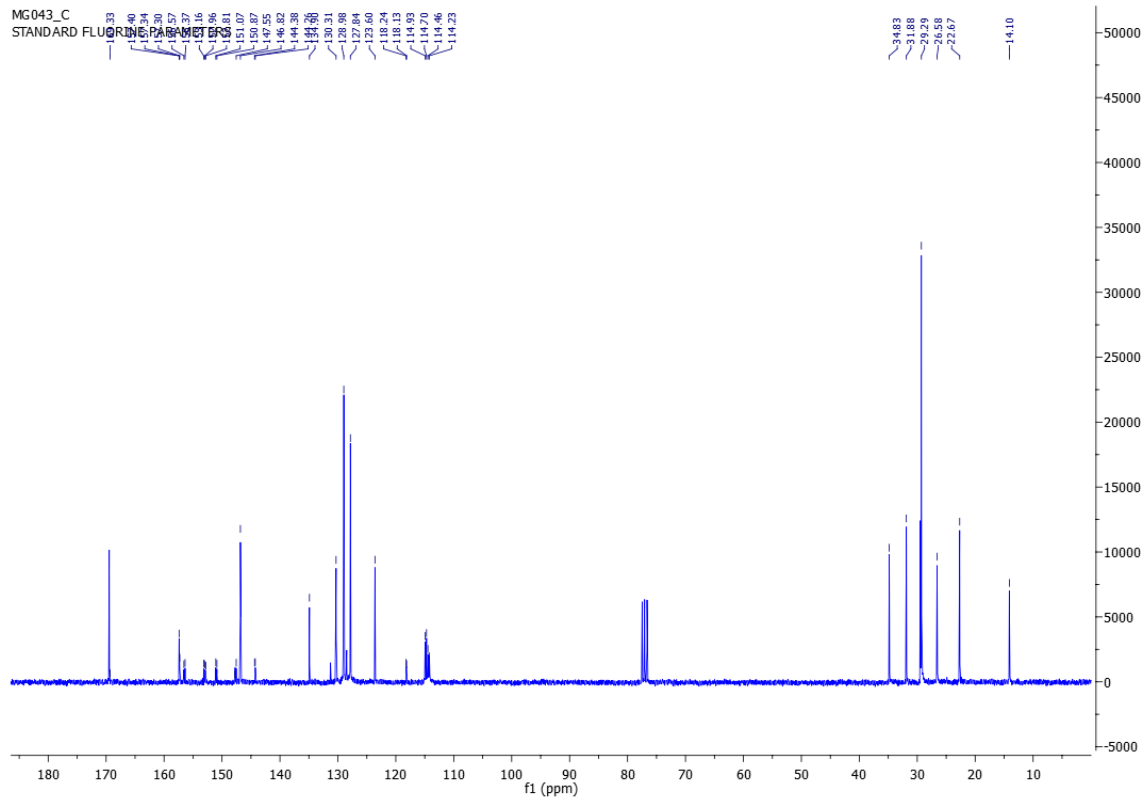
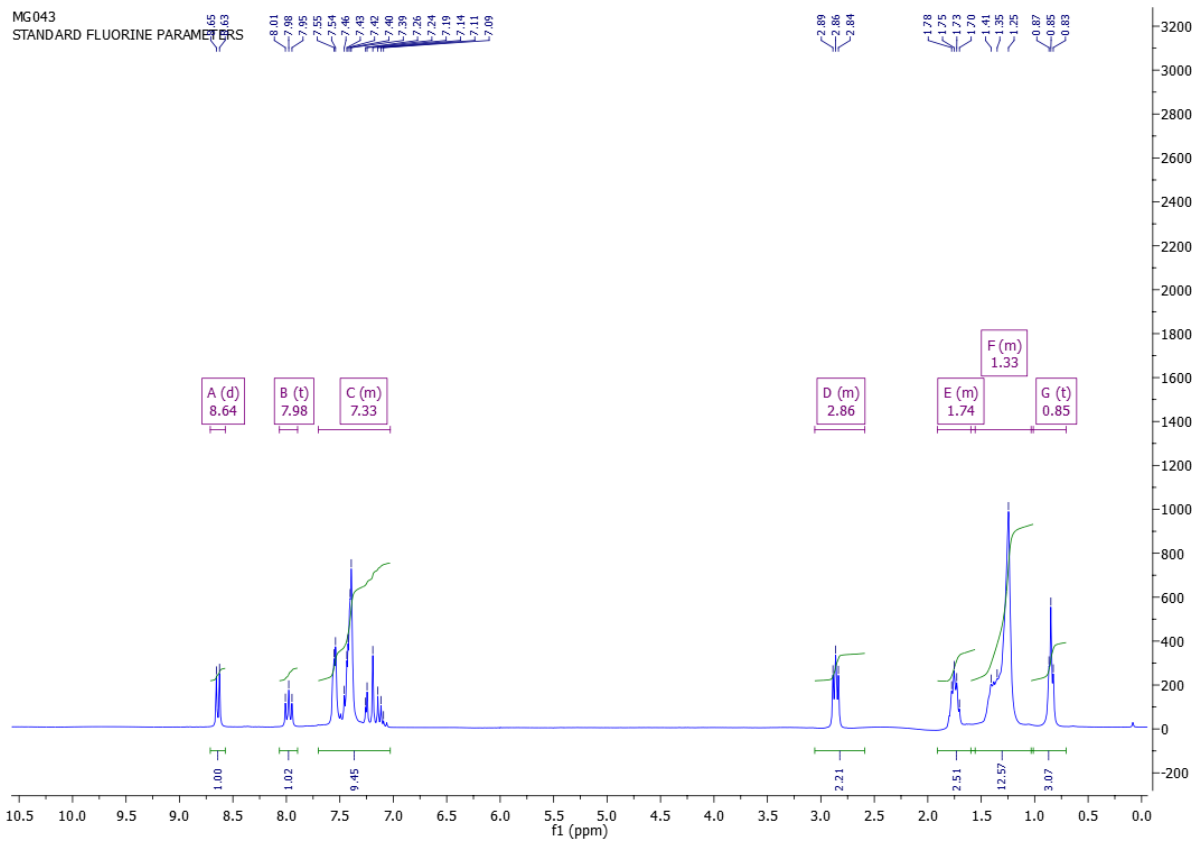


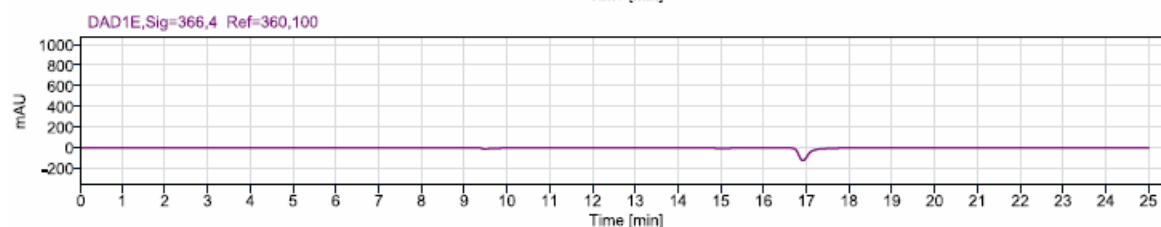
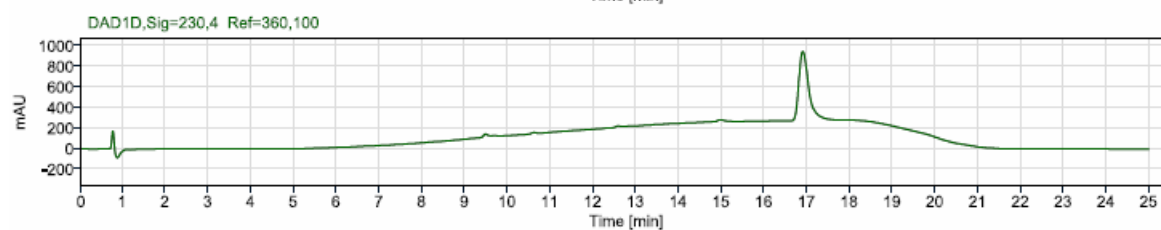
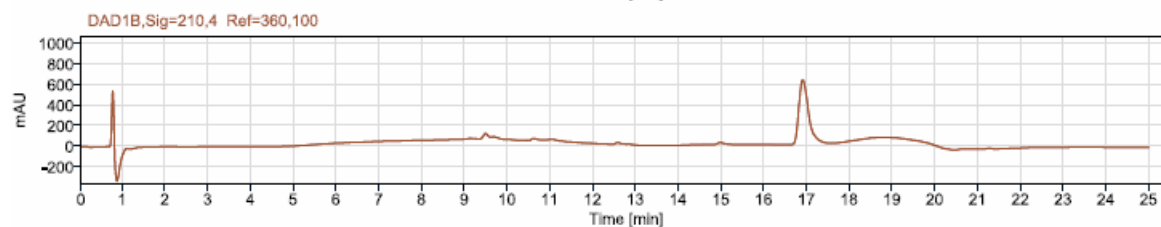
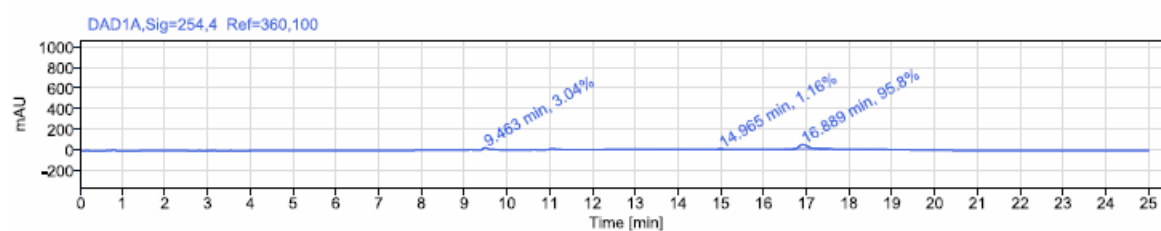
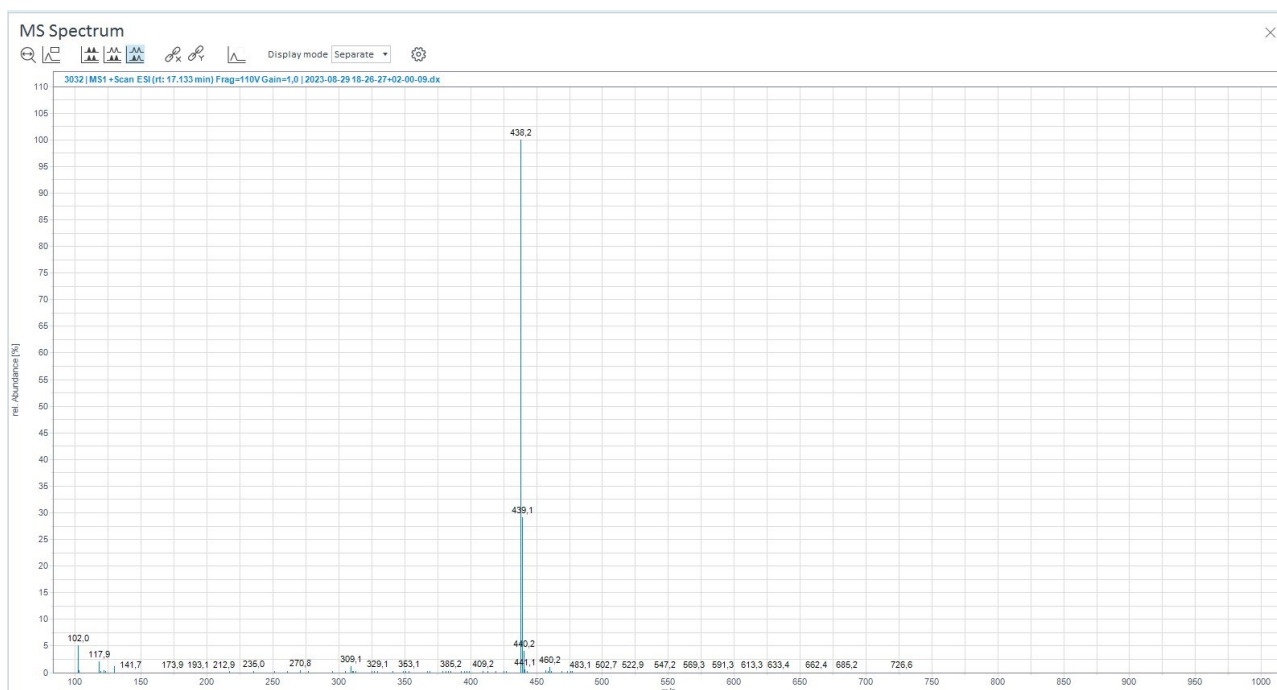


Peak Results (Area Percent at least 1%)

| 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 |

¹H, ¹³C NMR and HPLC/MS spectra of compound 8a

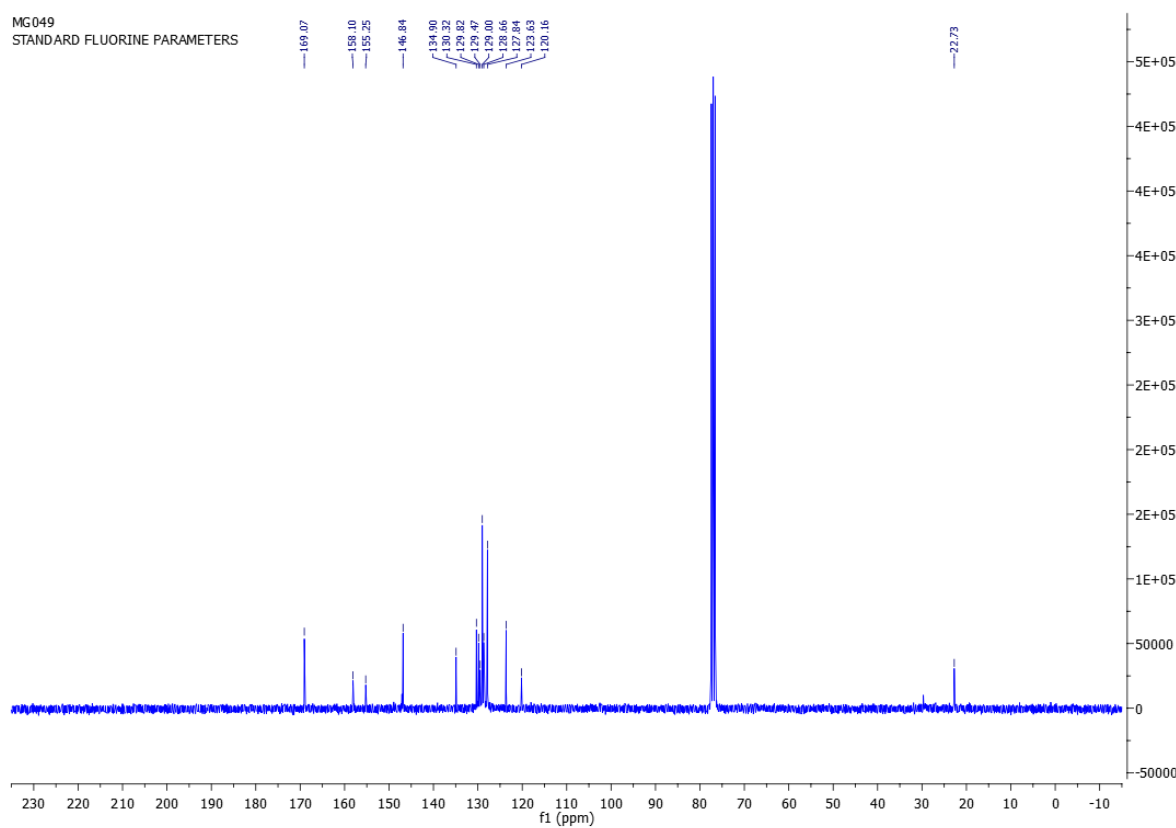
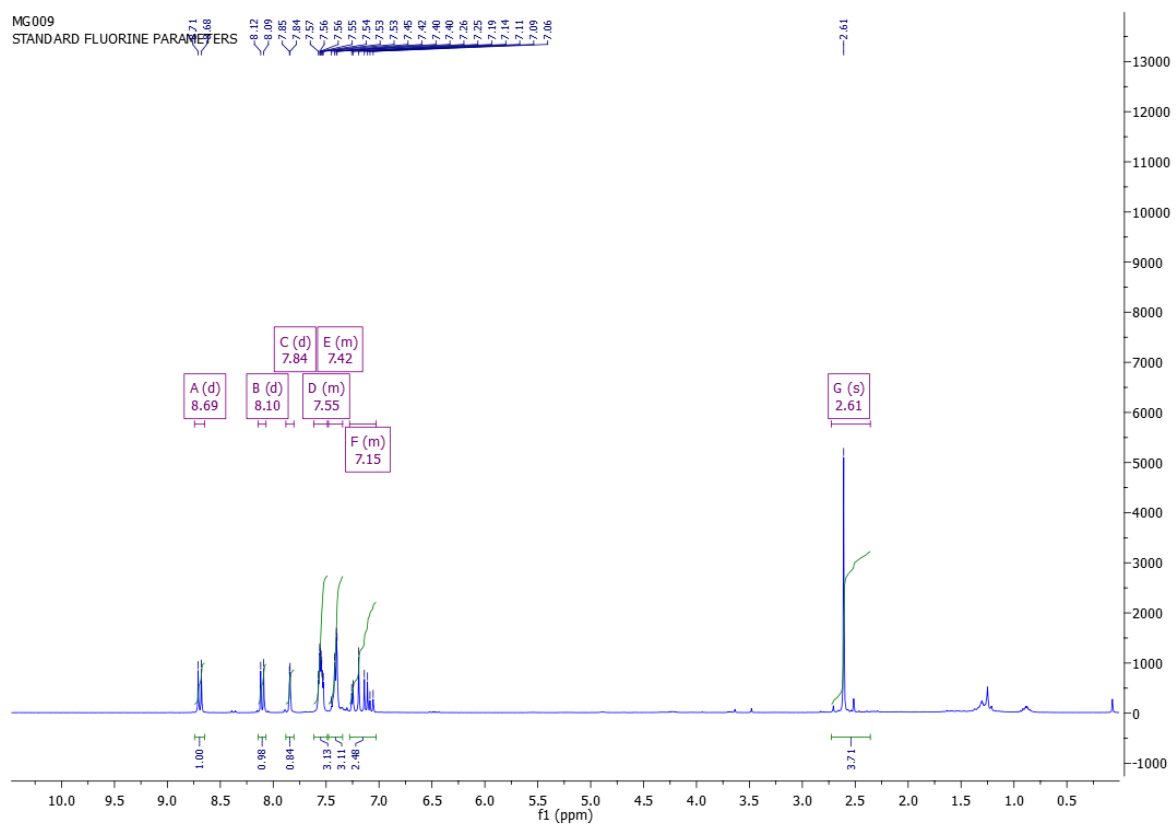


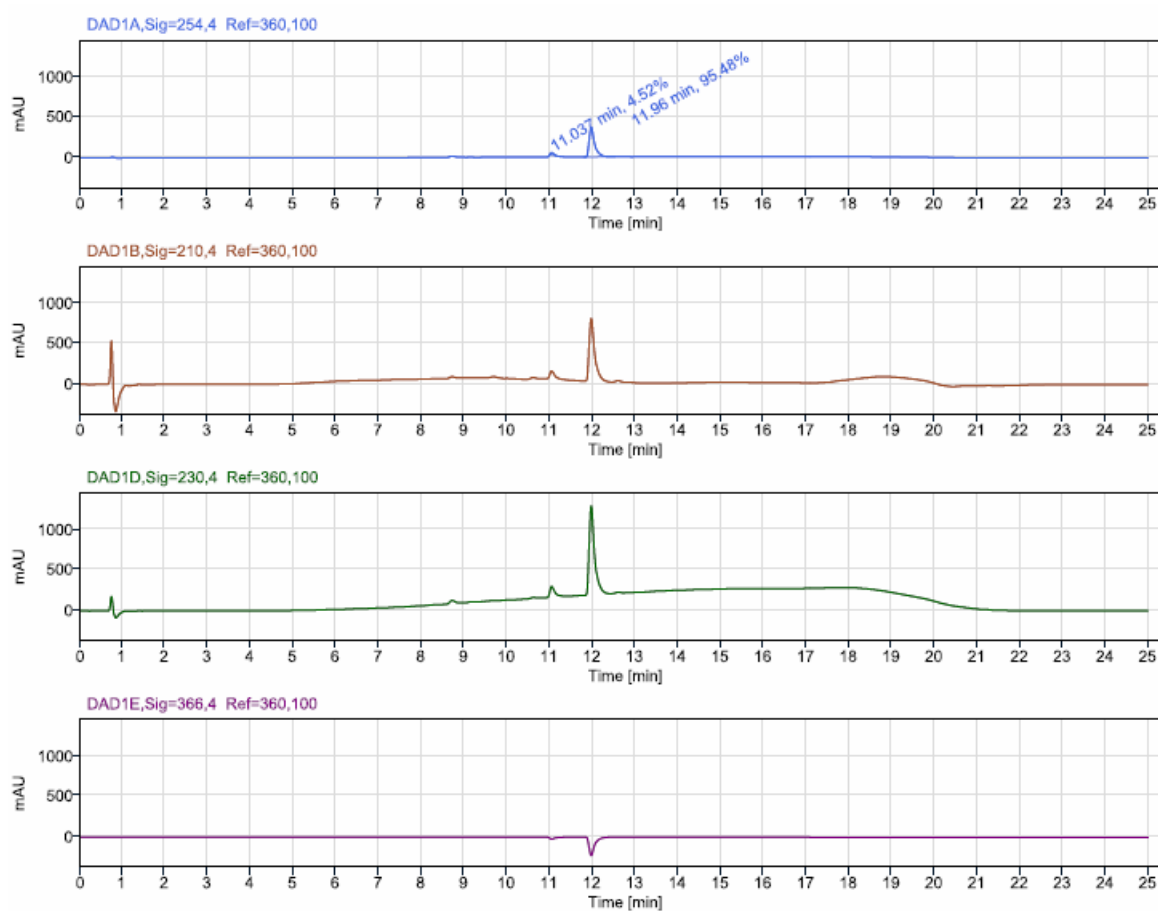
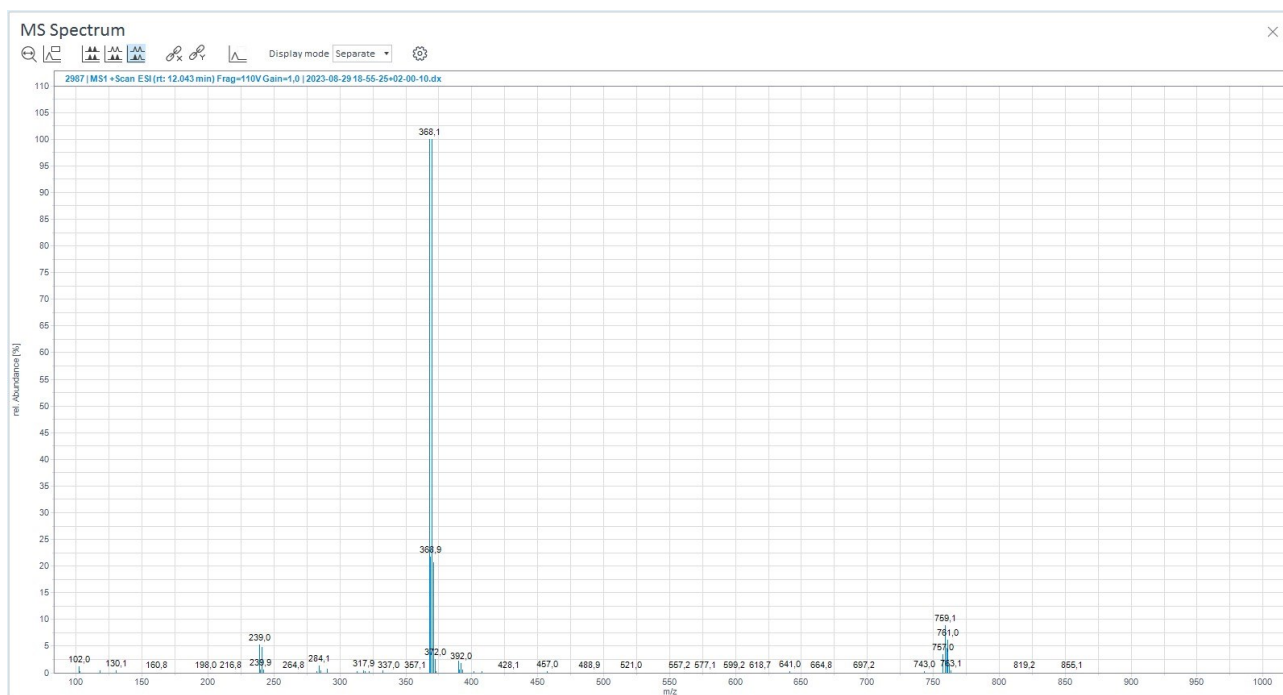


Peak Results (Area Percent at least 1%)

| 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 |

¹H, ¹³C NMR and HPLC/MS spectra of compound 8b





Peak Results (Area Percent at least 1%)

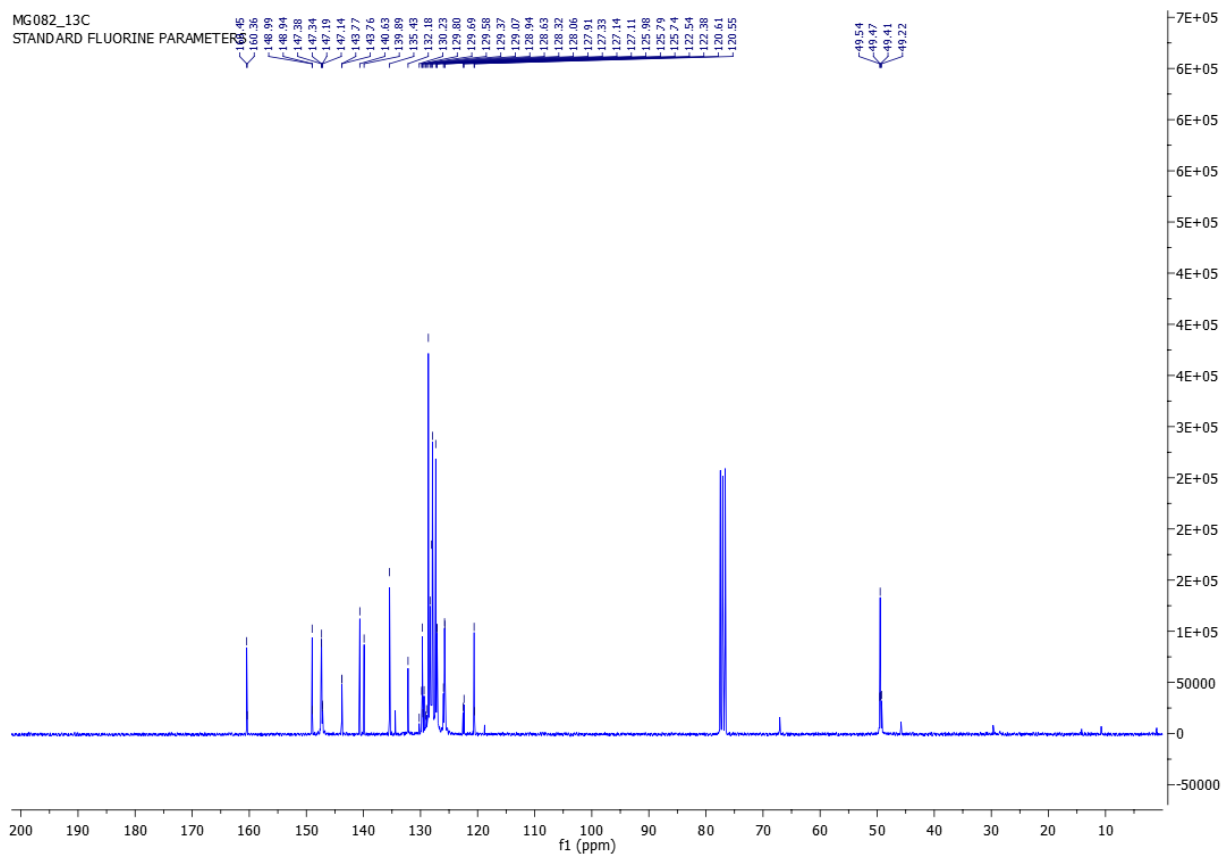
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|----------|--------------------------------------|-------------|------------|-----------|--------|
| 11.037 | DAD1A, Sig=254,4 Ref=360,100 | 0.158 | 153.6 | 31.0 | 4.52 |
| 11.960 | DAD1A, Sig=254,4 Ref=360,100 | 0.746 | 3241.3 | 364.8 | 95.48 |
| 12.040 | MS1 +TIC SCAN ESI Frag=110V Gain=1,0 | 0.698 | 25124082,9 | 1714932,0 | 100,00 |

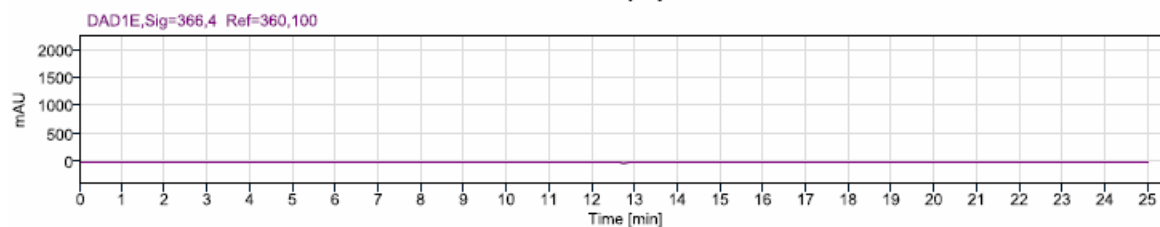
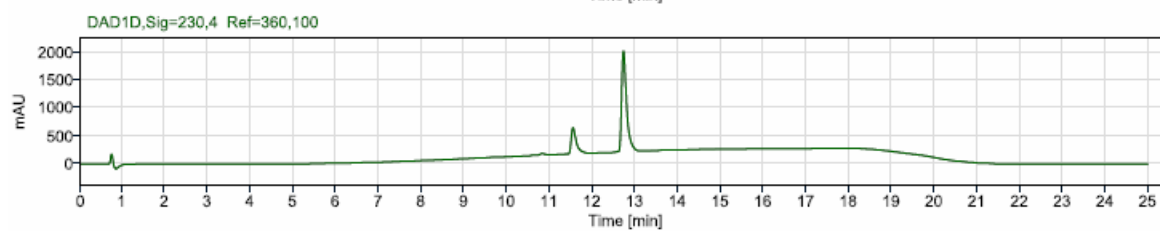
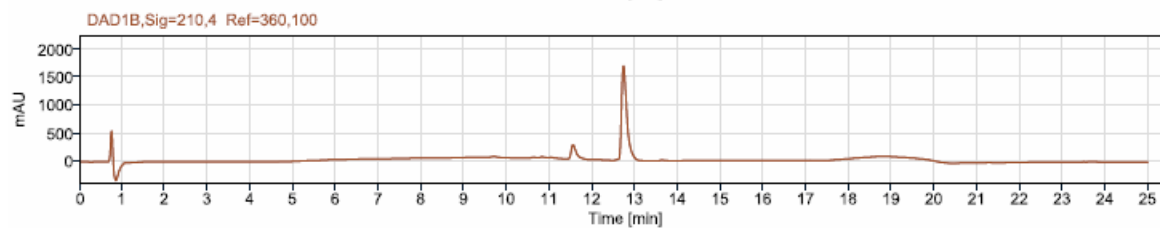
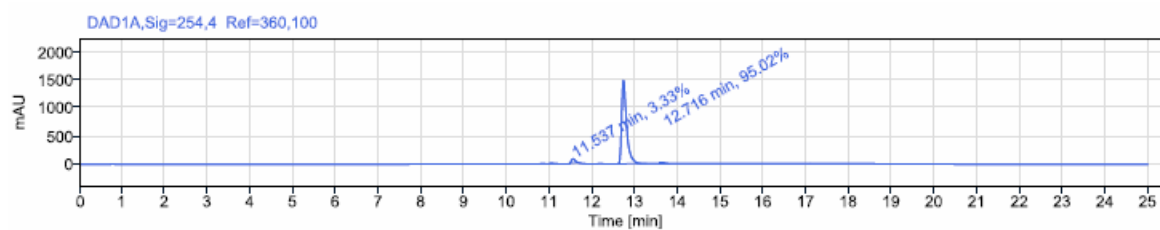
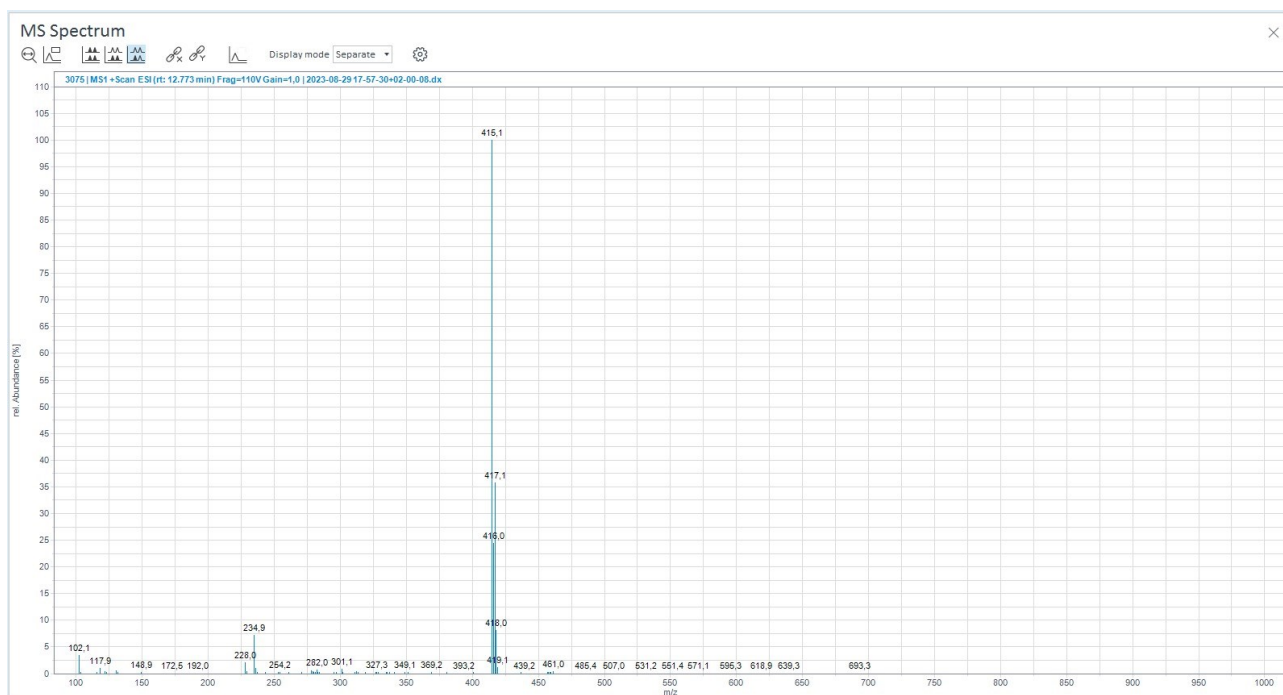
MG082_1H
STANDARD FLUORINE PARAMETER

8.25
8.22
8.20
8.15
8.08
7.69
7.66
7.64
7.61
7.58
7.56
7.46
7.38
7.34
7.26
7.24
7.21
5.22
3.44

2.25
9.95
2.00

f1 (ppm)

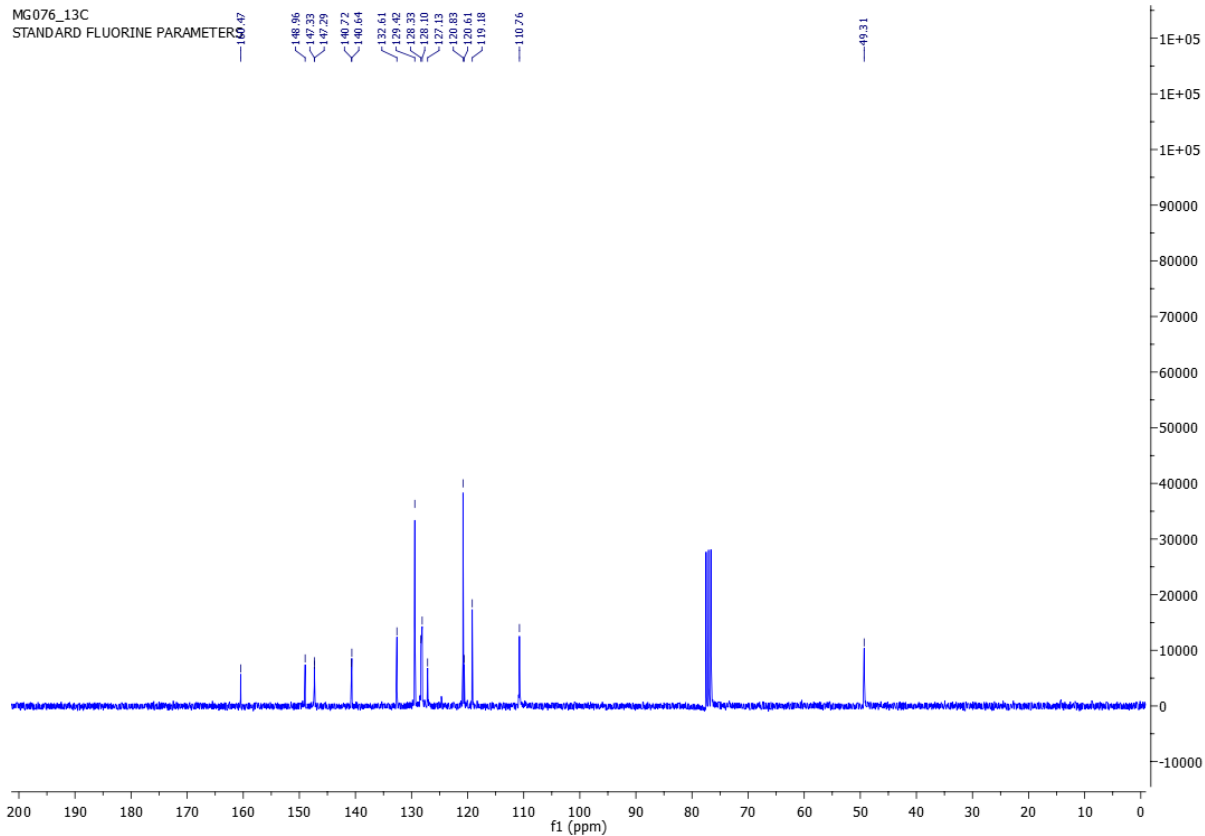
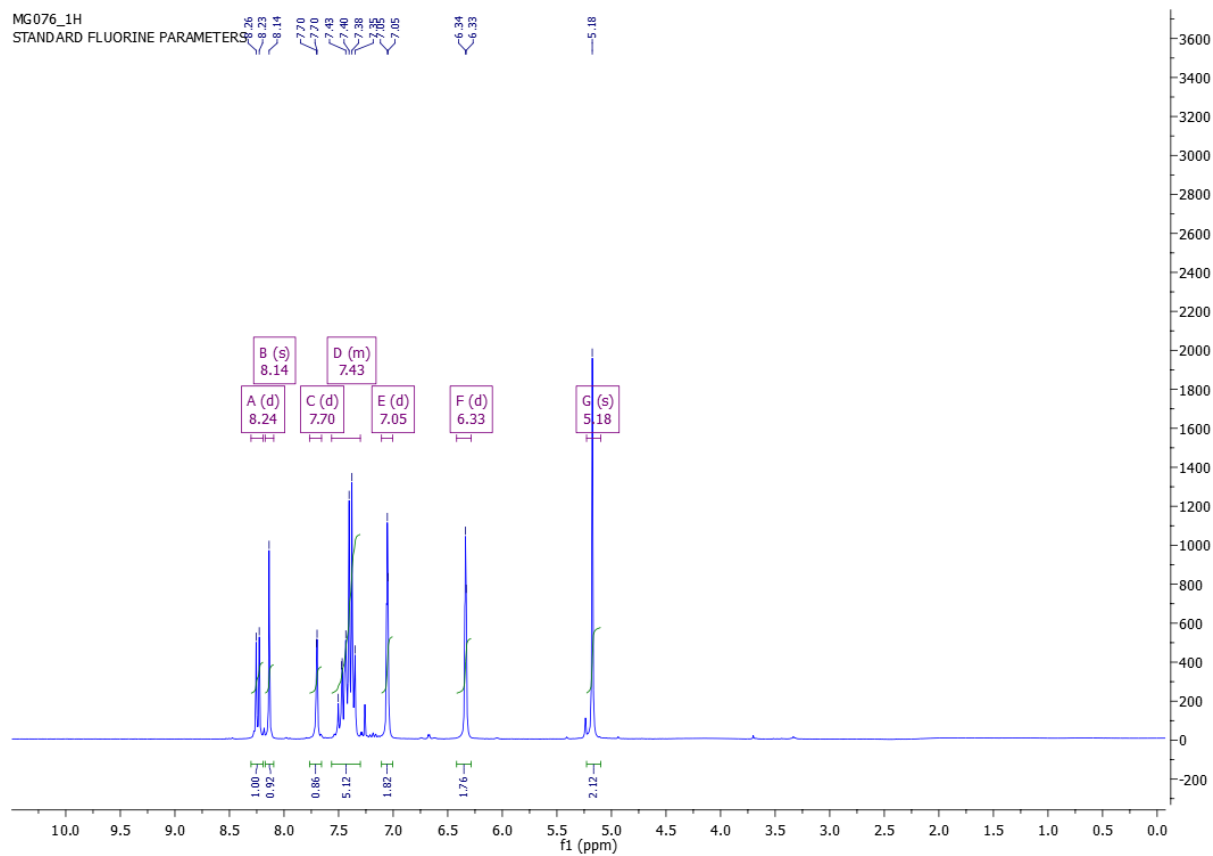


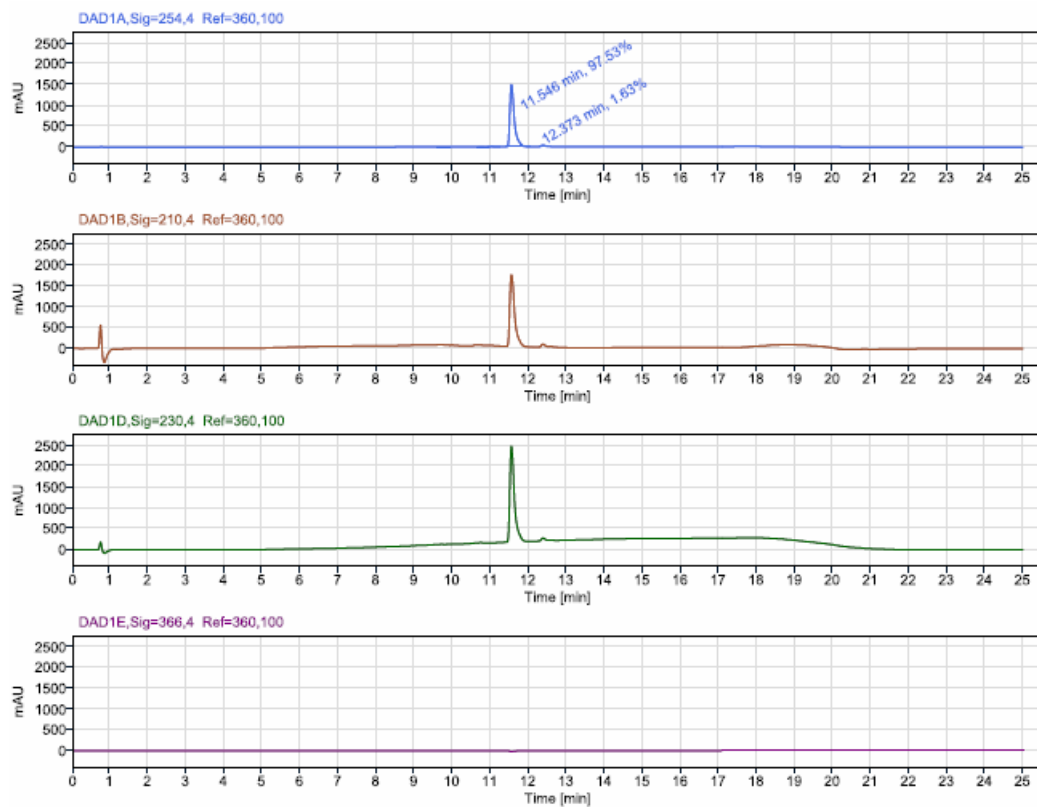
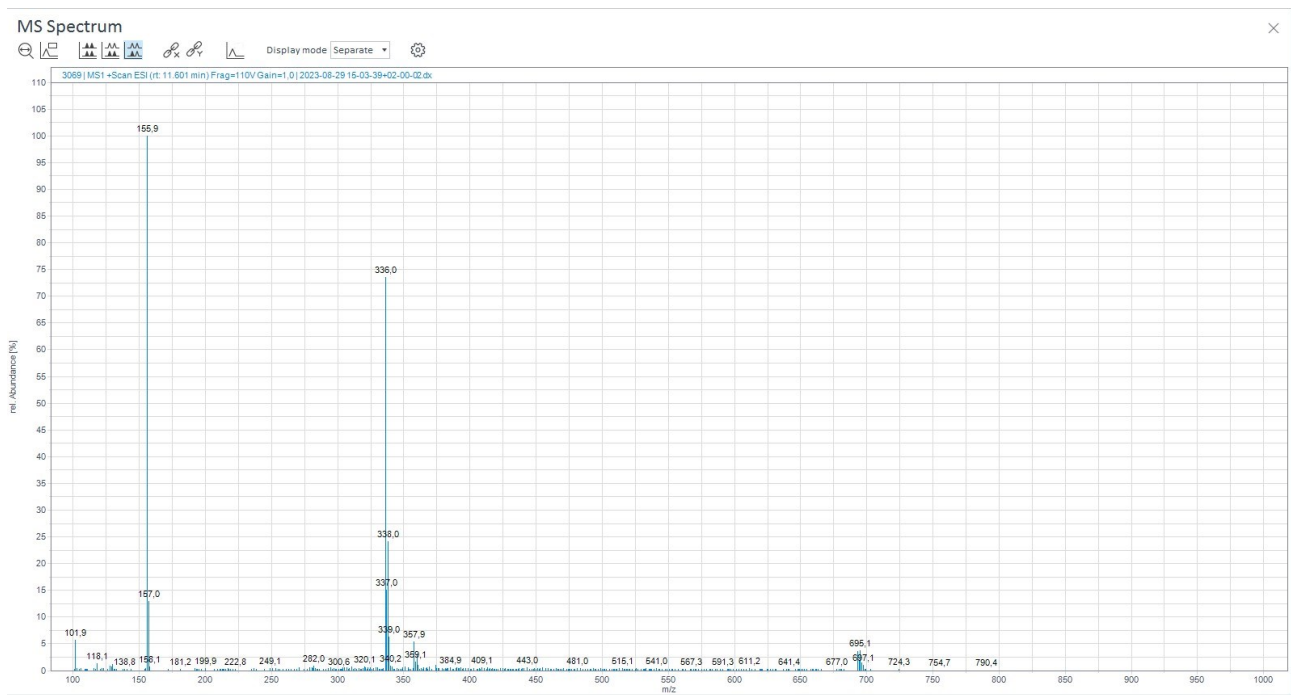


Peak Results (Area Percent at least 1%)

| 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 |

¹H, ¹³C NMR and HPLC/MS spectra of compound 10

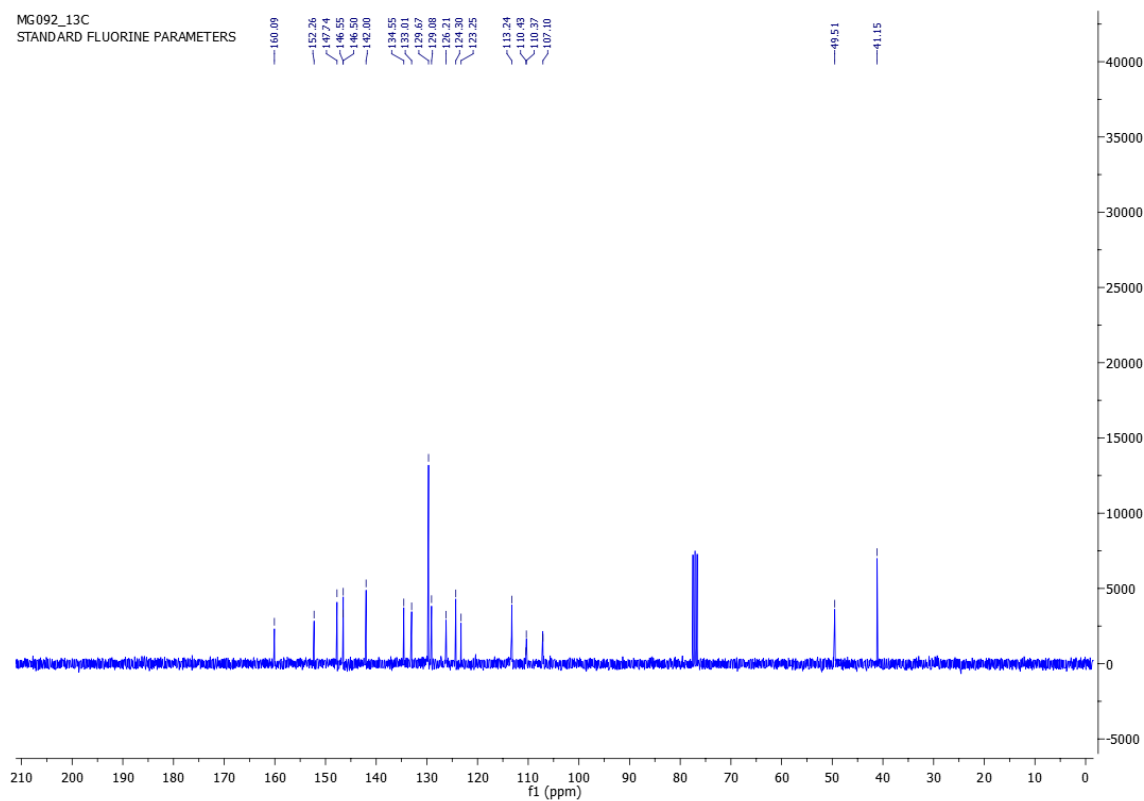
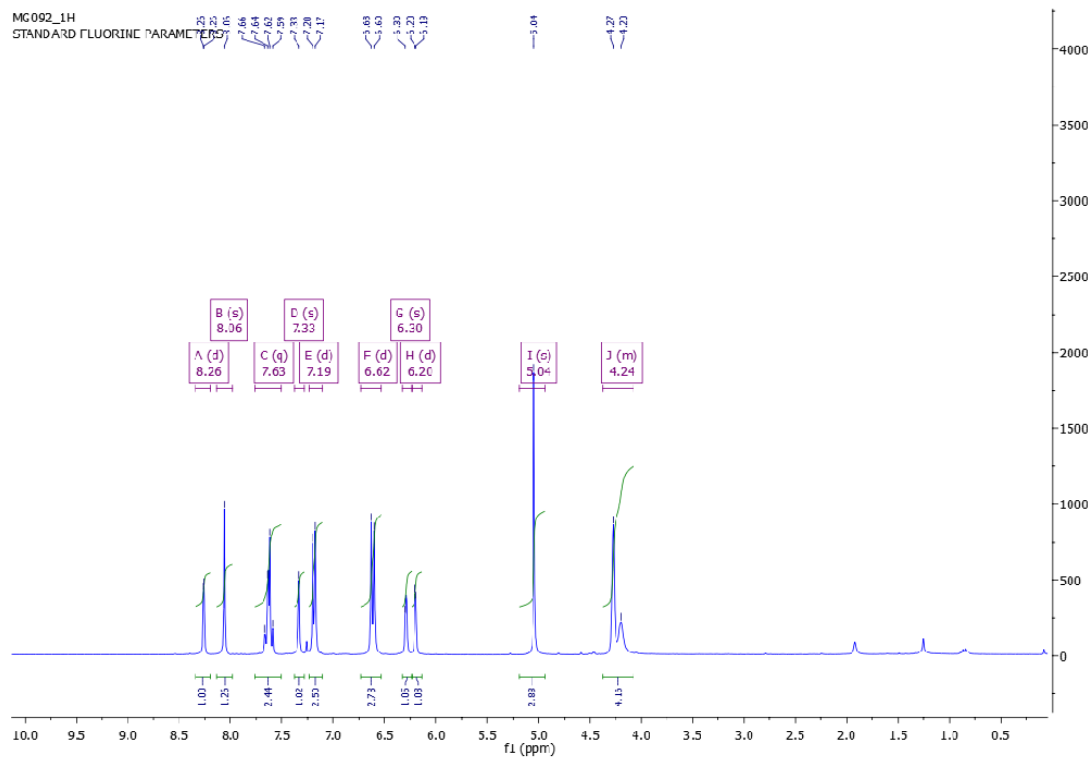


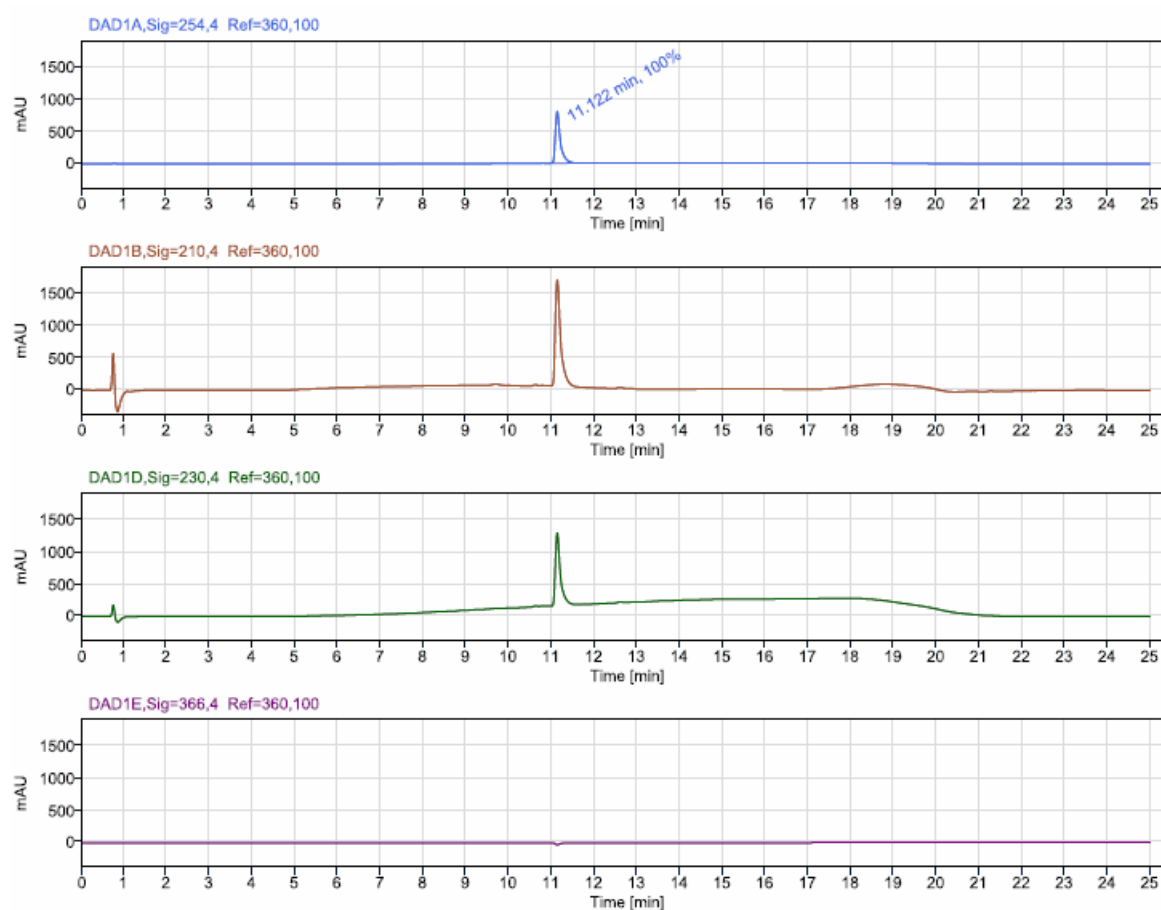
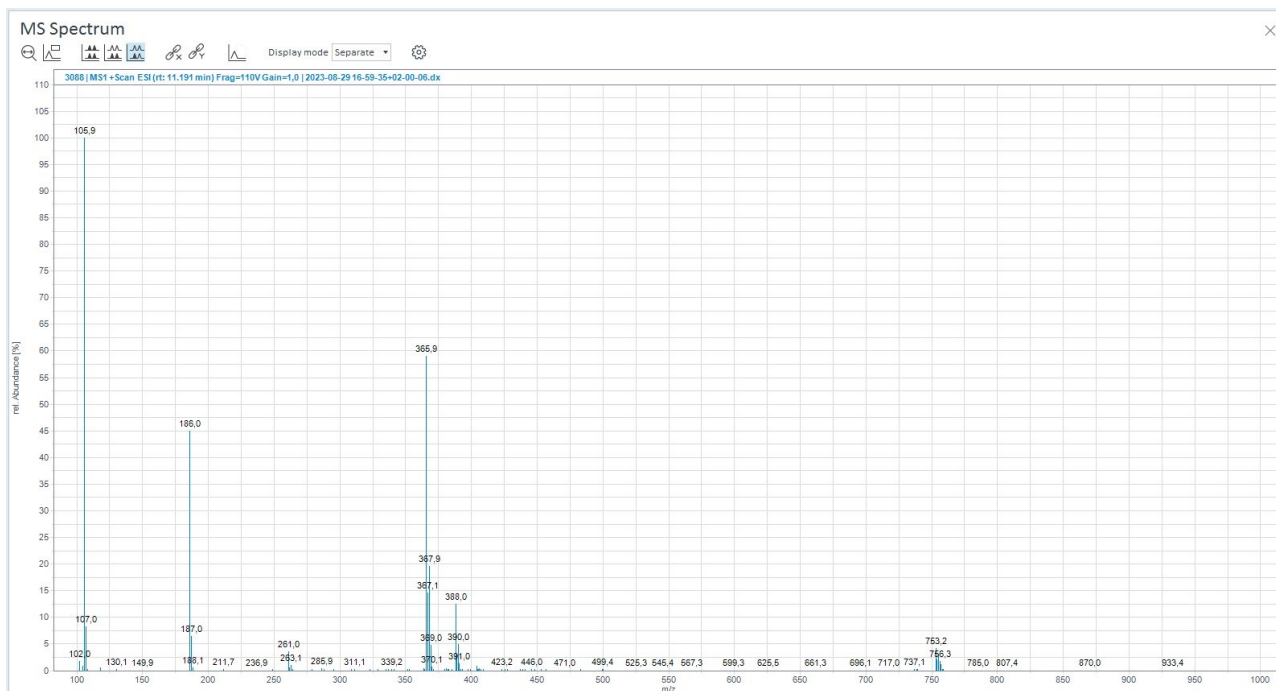


Peak Results (Area Percent at least 1%)

| 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 |

^1H , ^{13}C NMR and HPLC/MS spectra of compound 11a

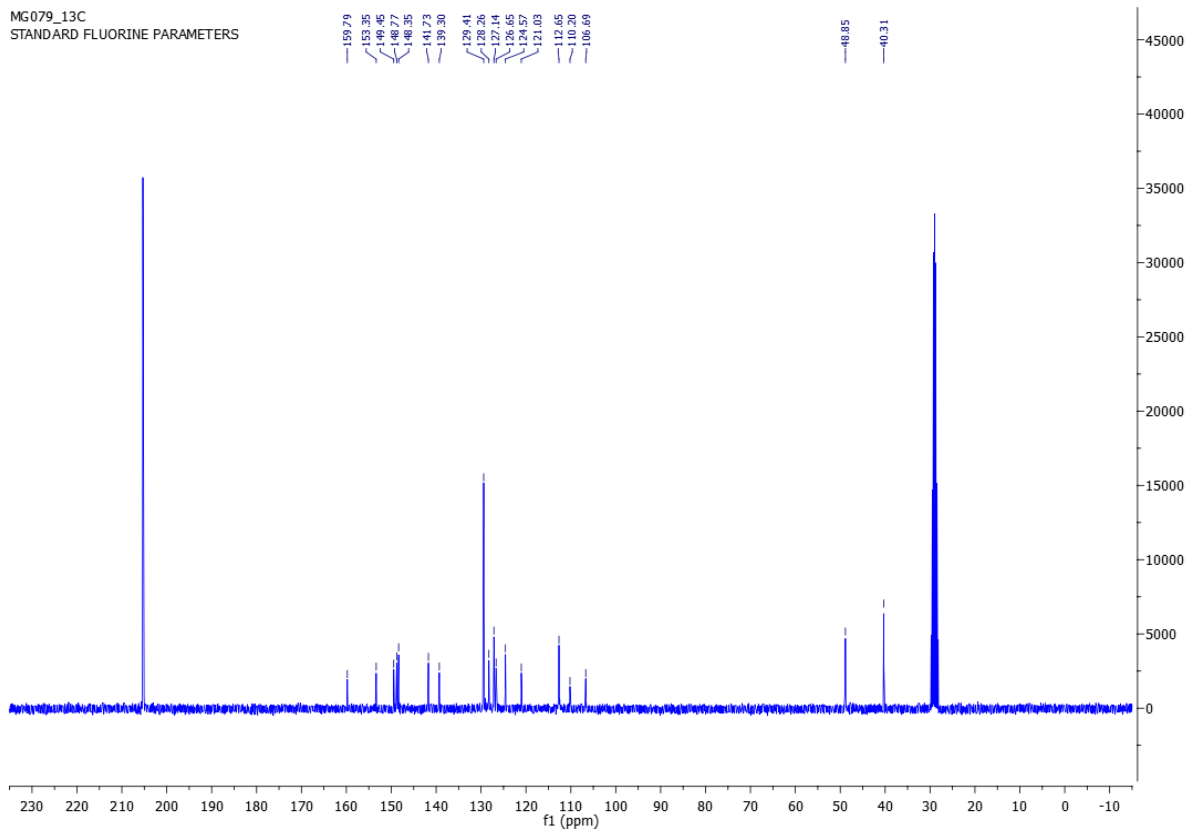
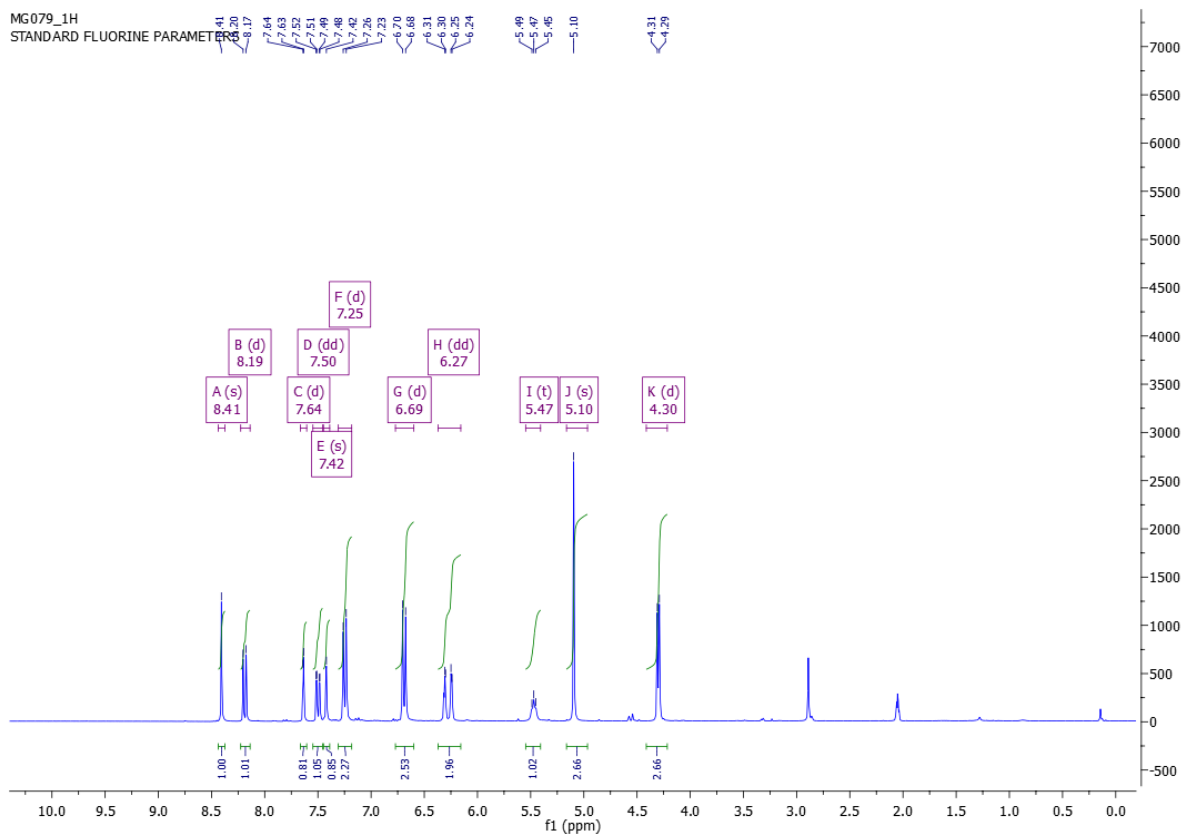




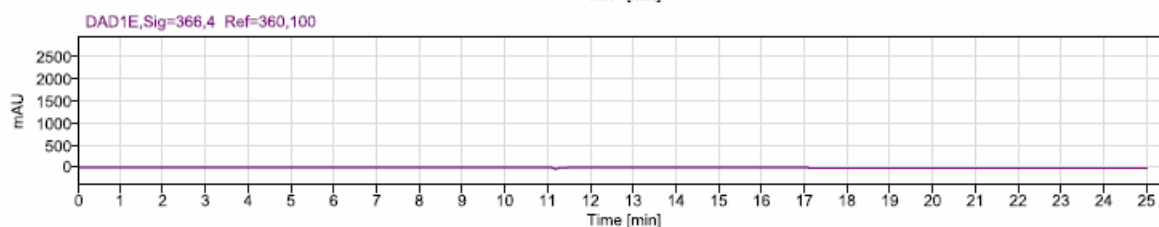
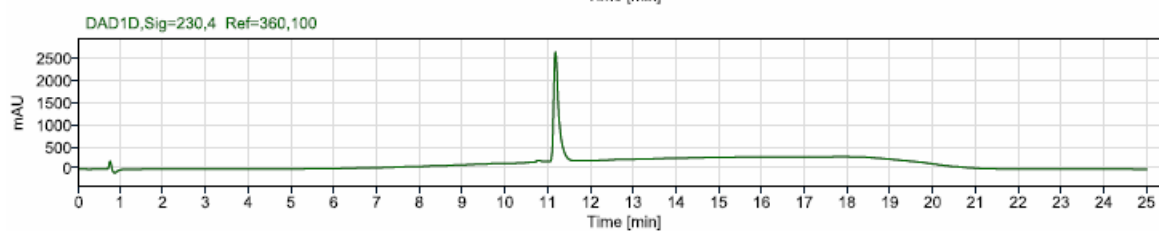
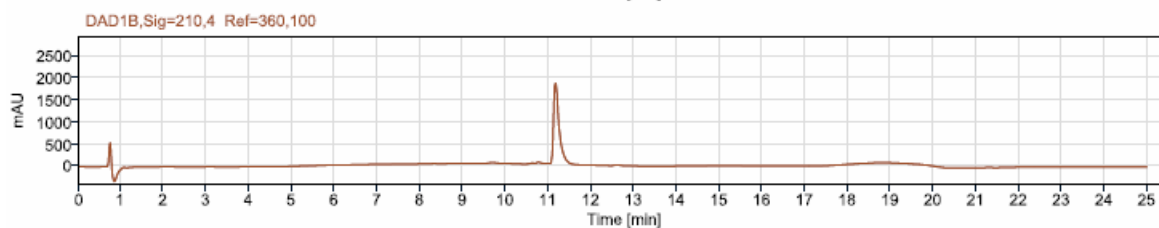
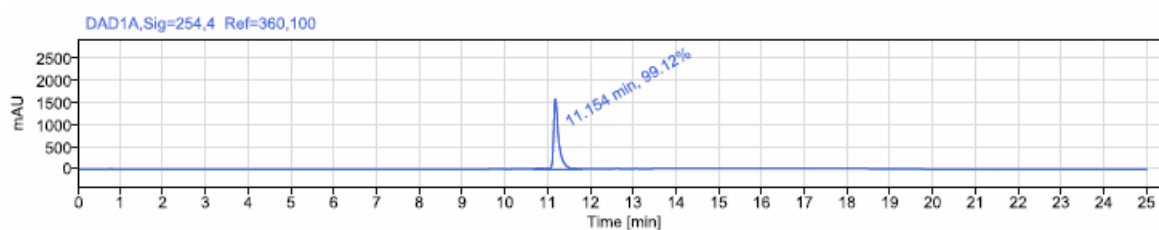
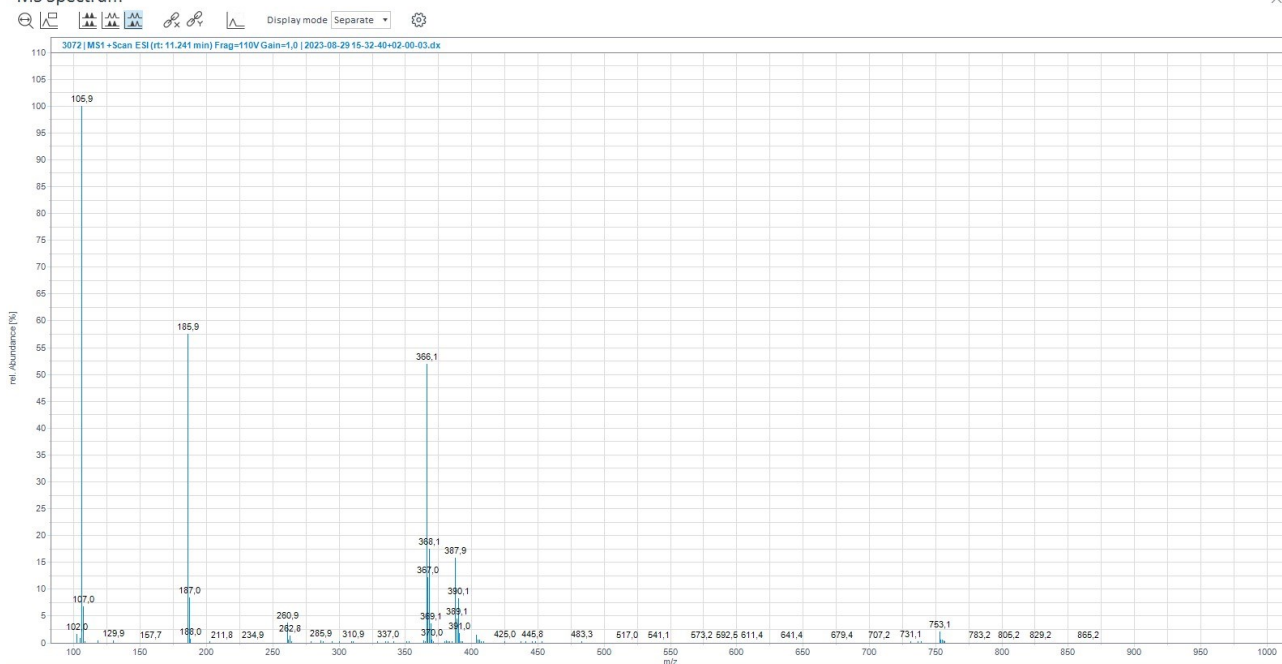
Peak Results (Area Percent at least 1%)

| 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 |

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



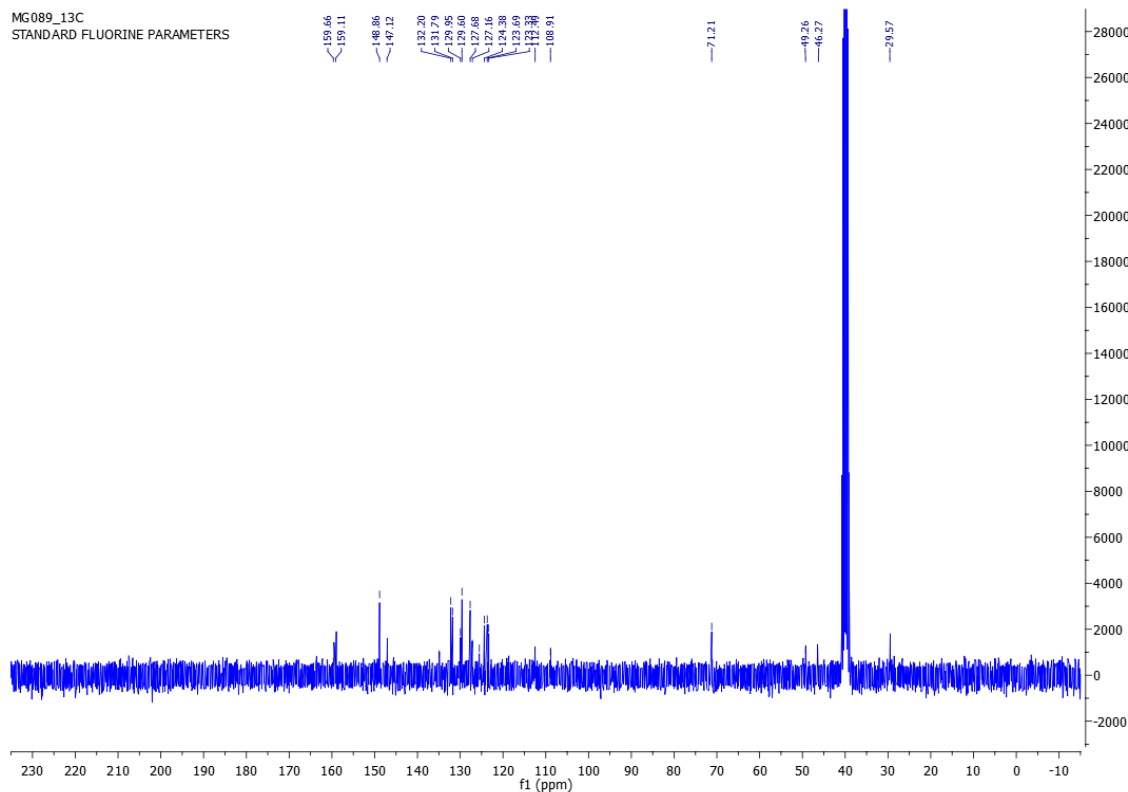
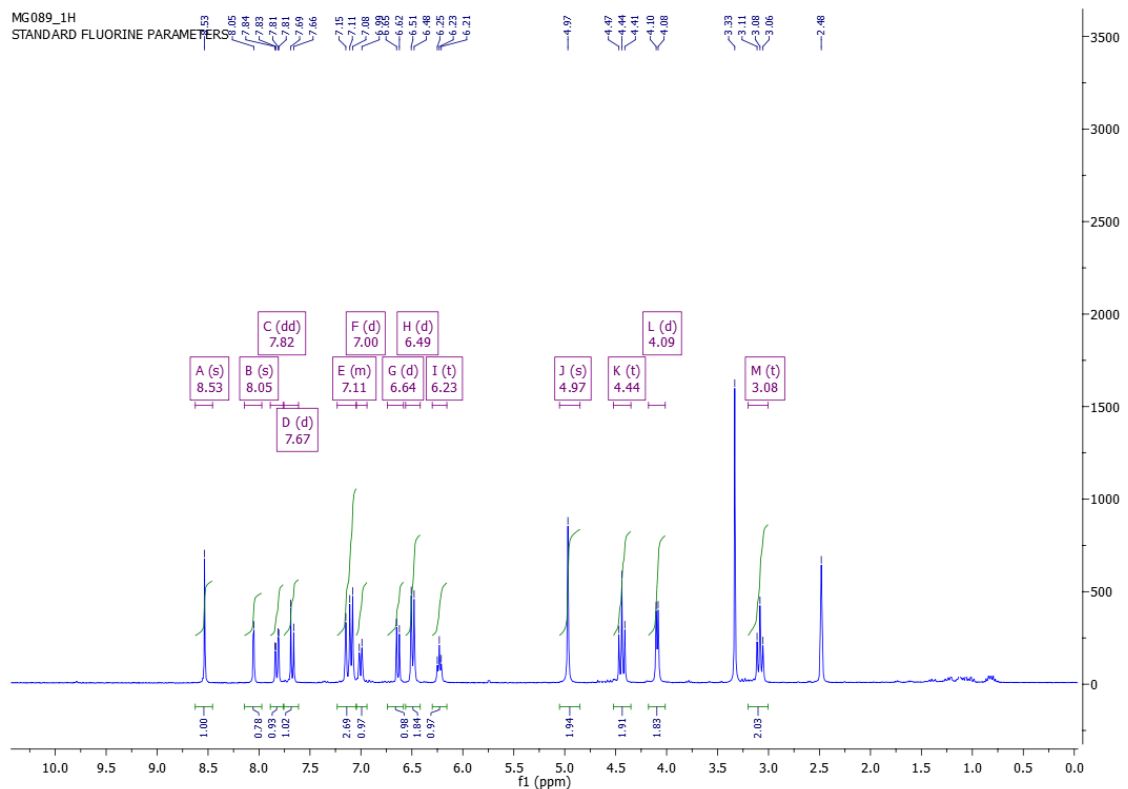
MS Spectrum

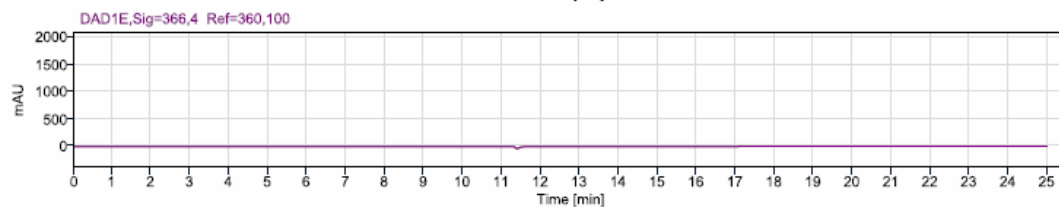
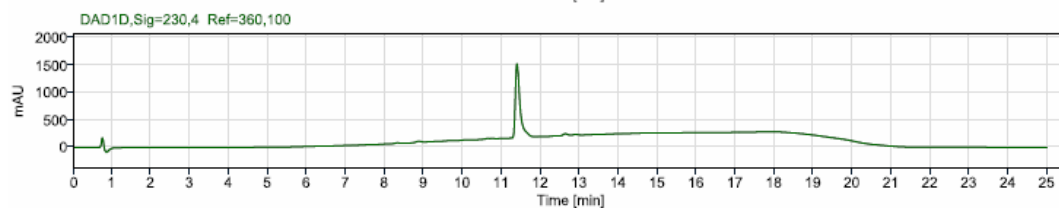
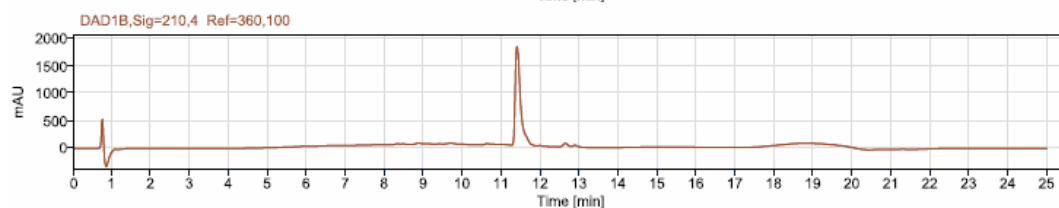
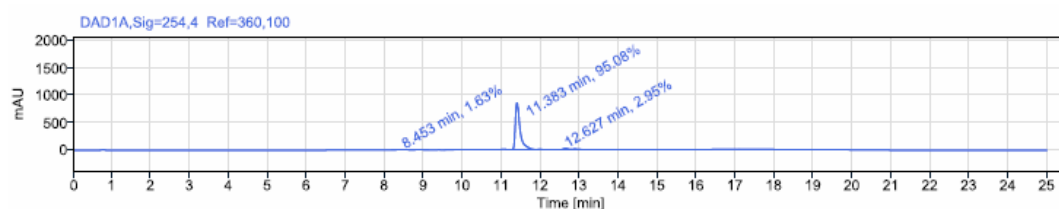
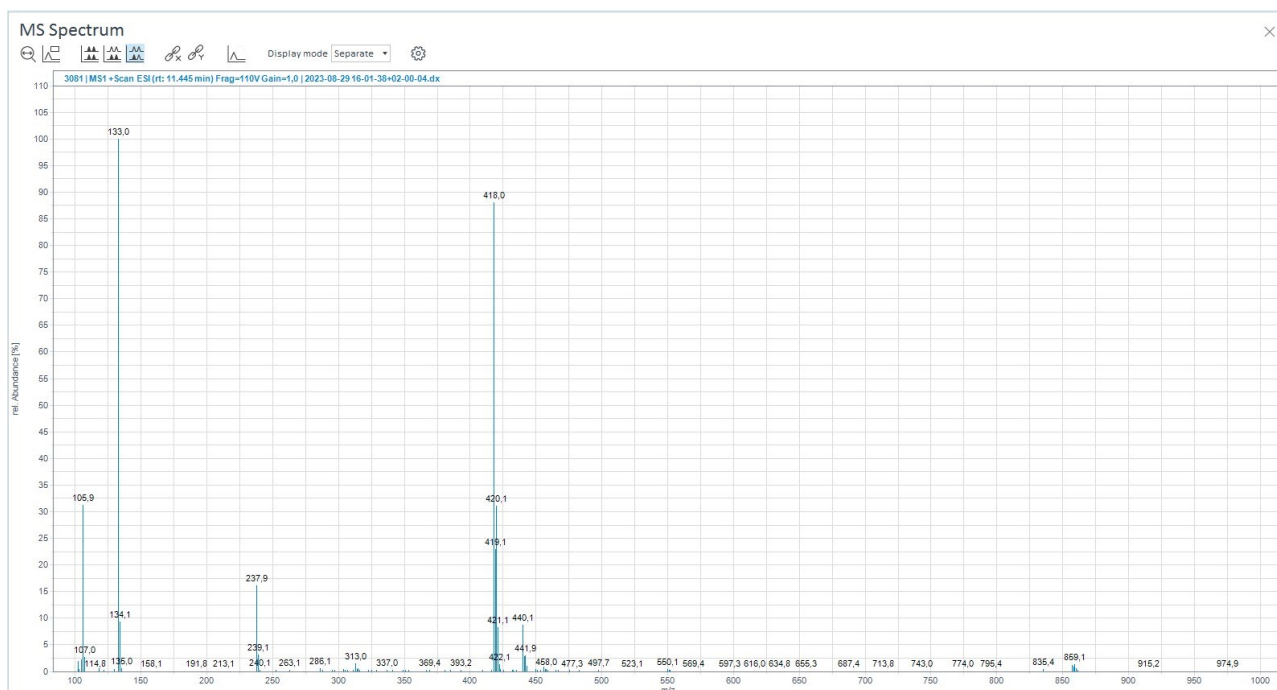


Peak Results (Area Percent at least 1%)

| 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 |

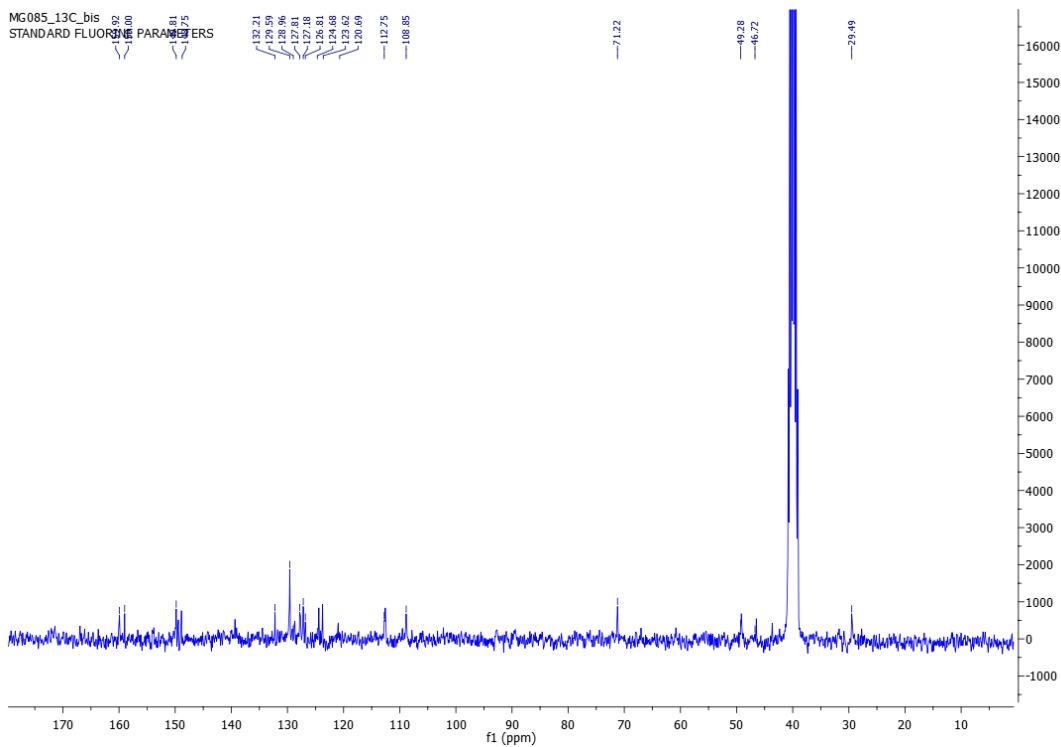
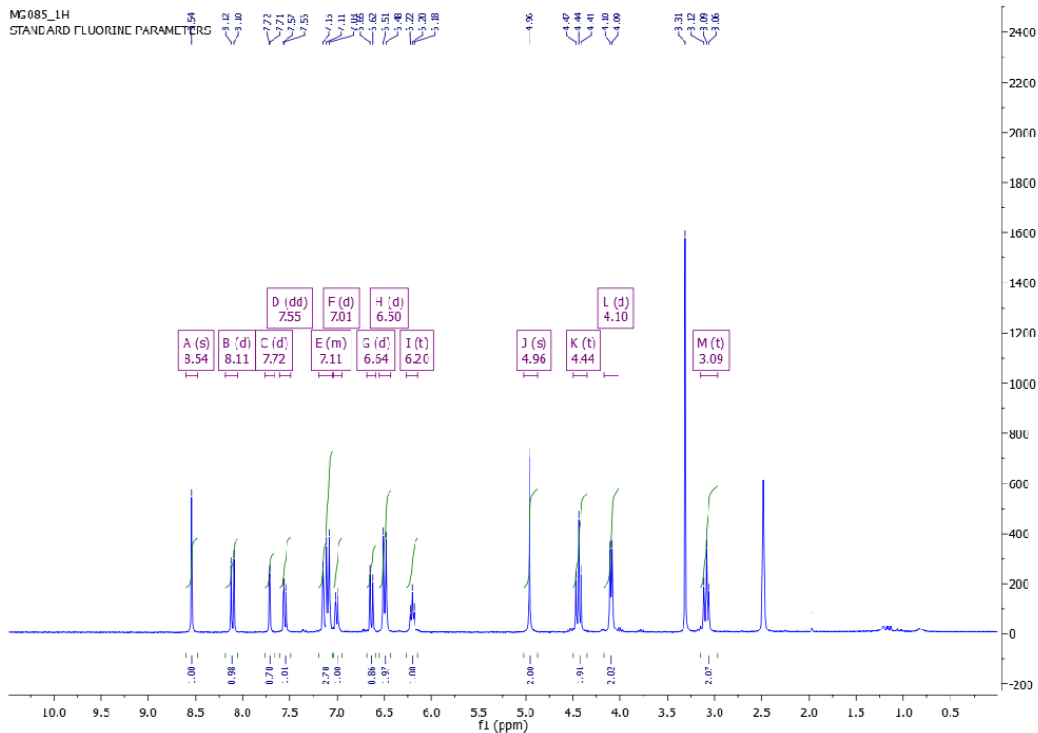
¹H, ¹³C NMR and HPLC/MS spectra of compound 11c

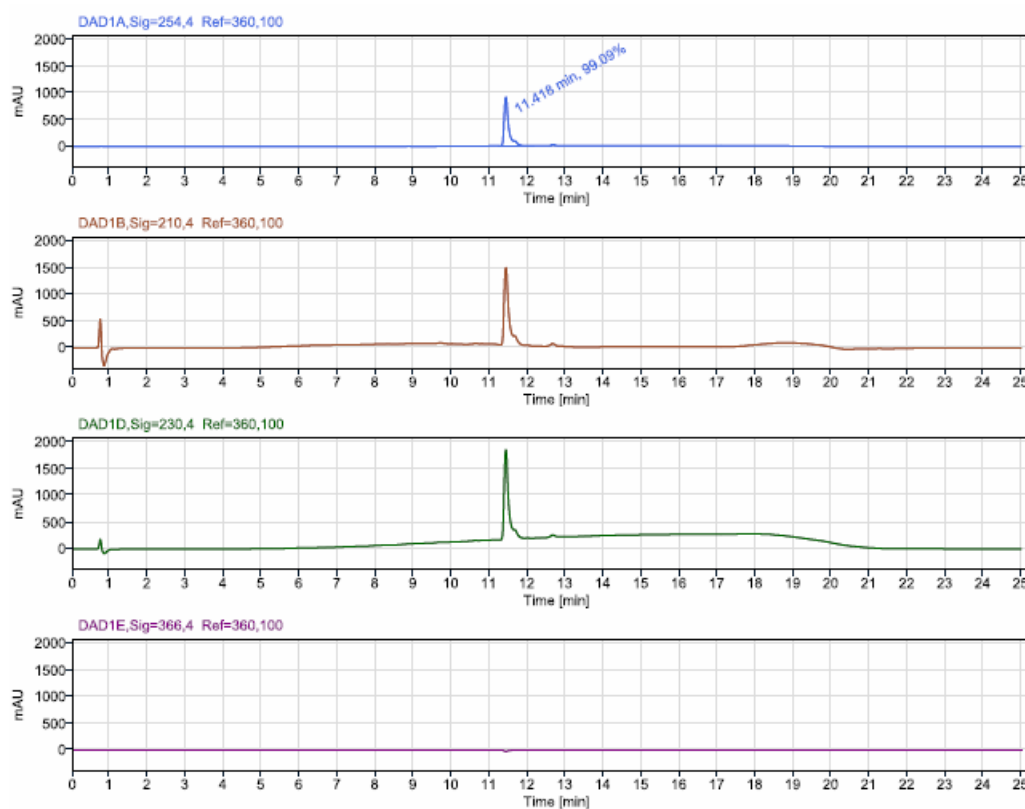
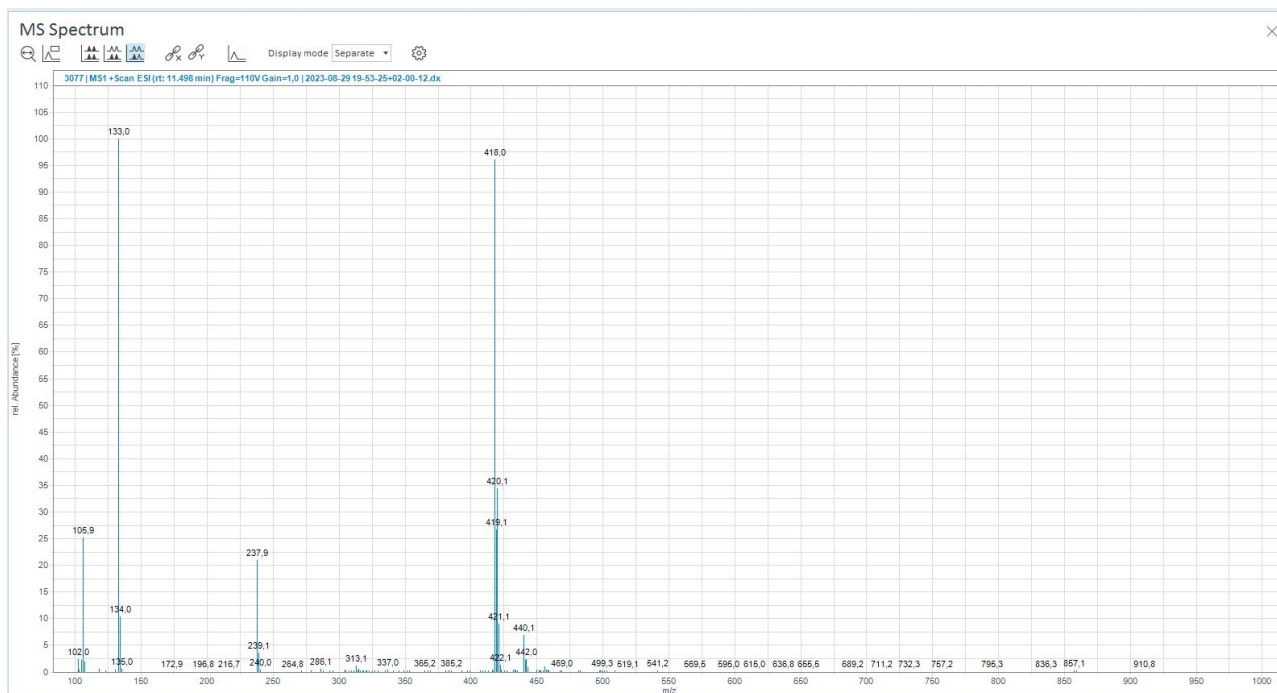




Peak Results (Area Percent at least 1%)

| 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 |

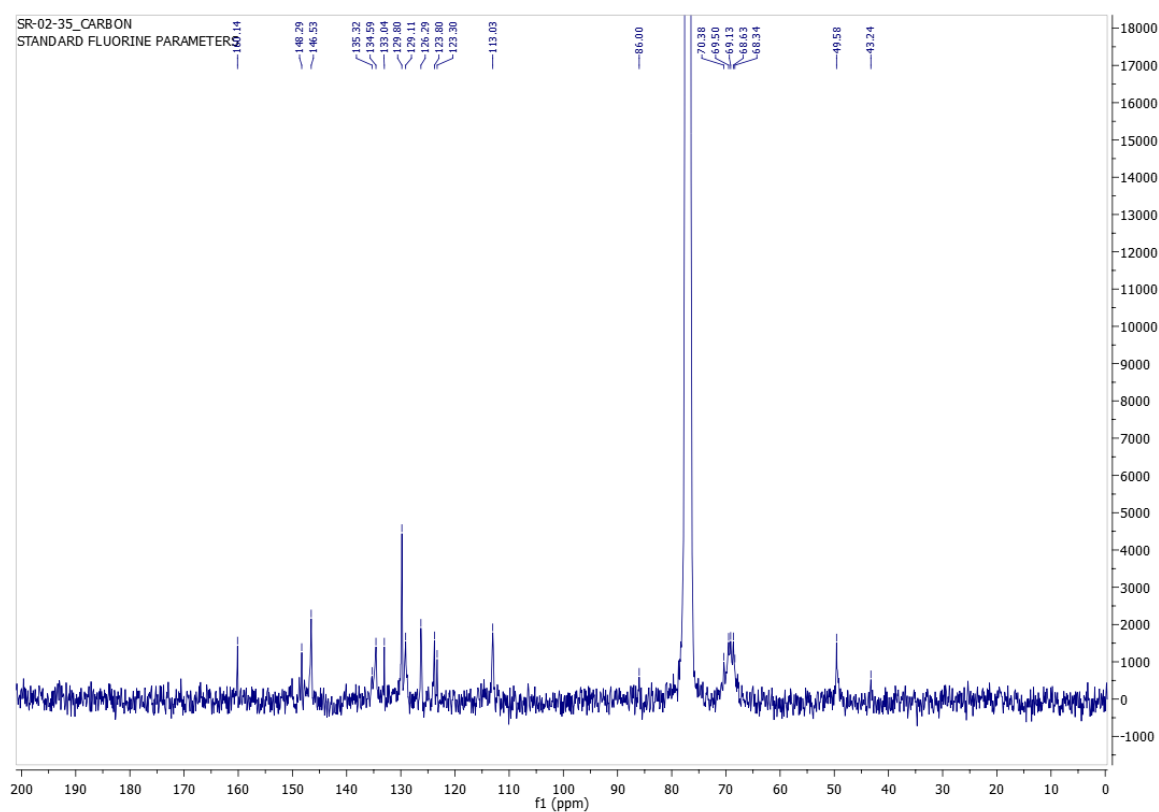
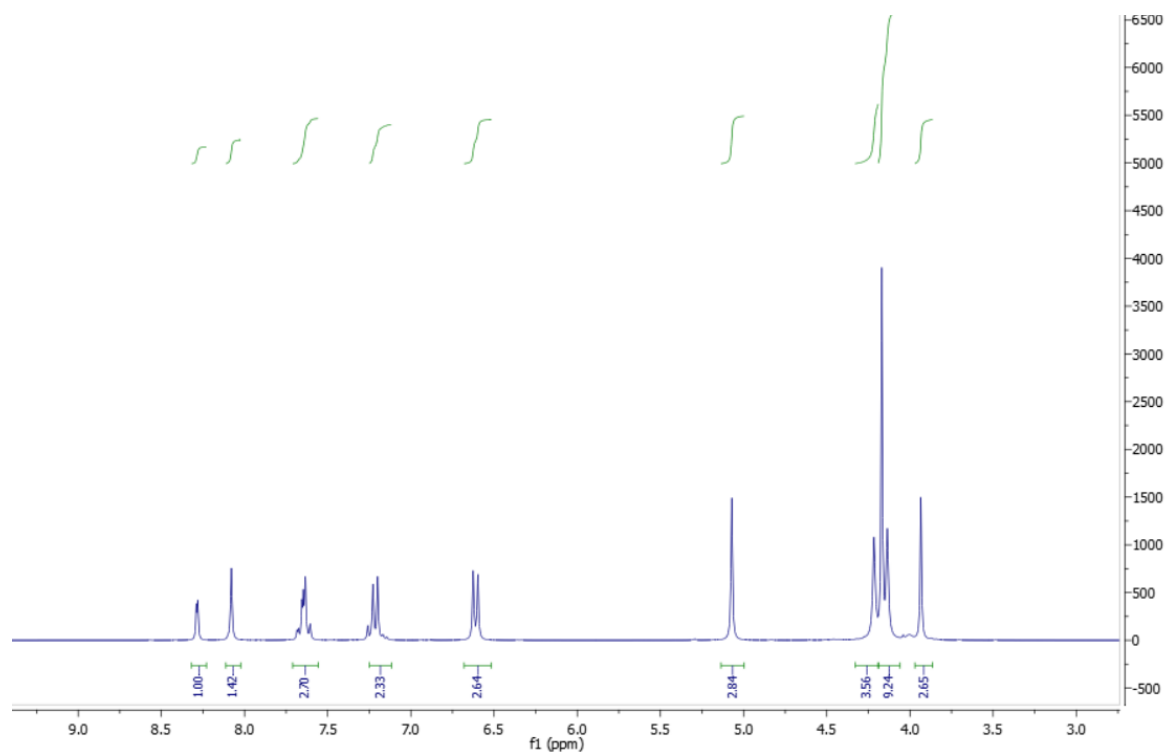
¹H, ¹³C NMR and HPLC/MS spectra of compound 11d

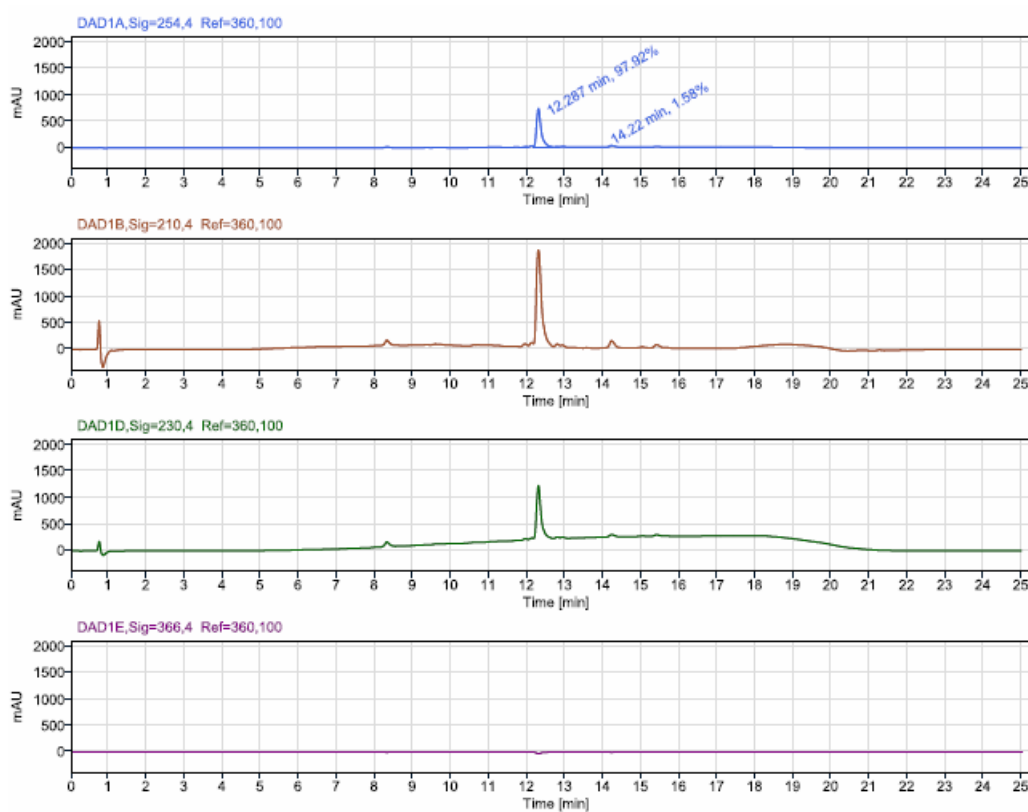
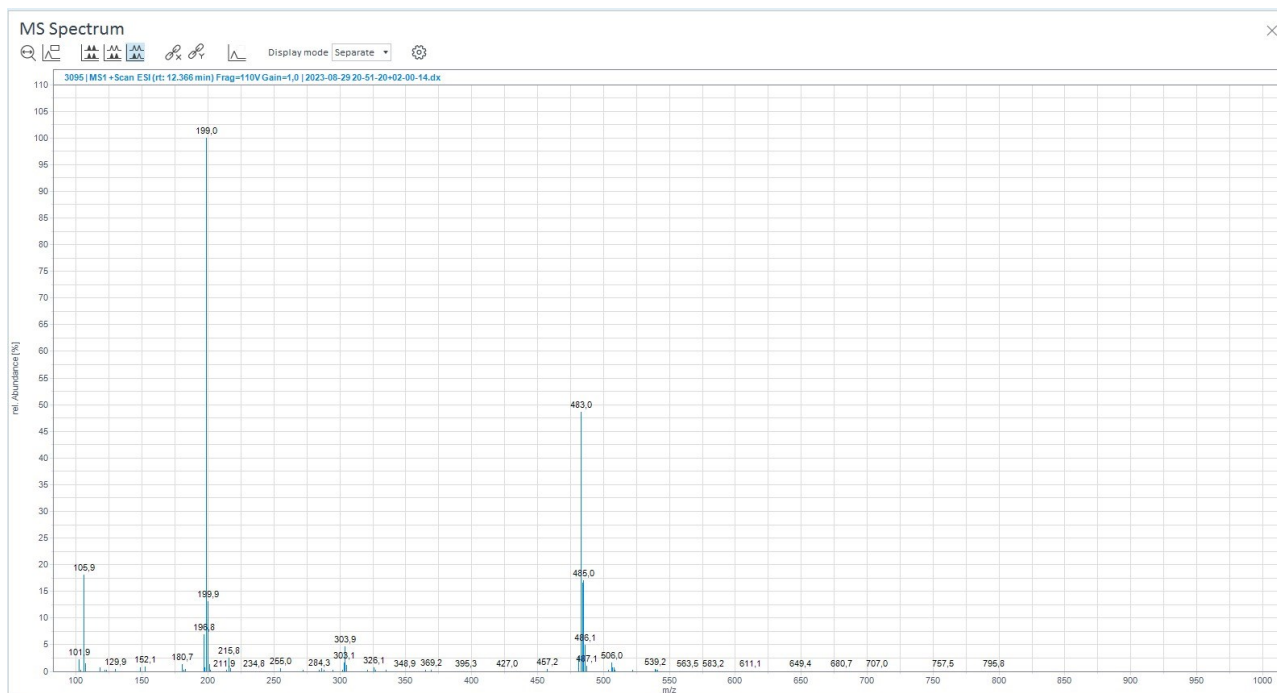


Peak Results (Area Percent at least 1%)

| 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 |

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

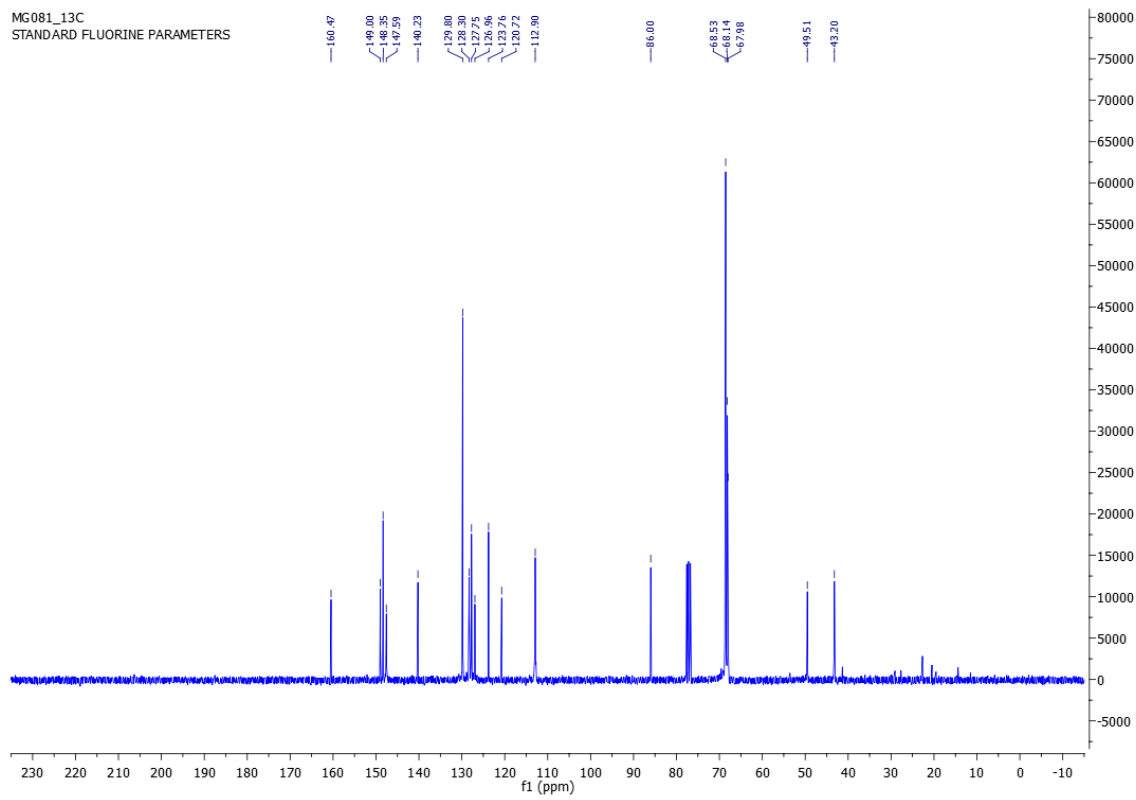
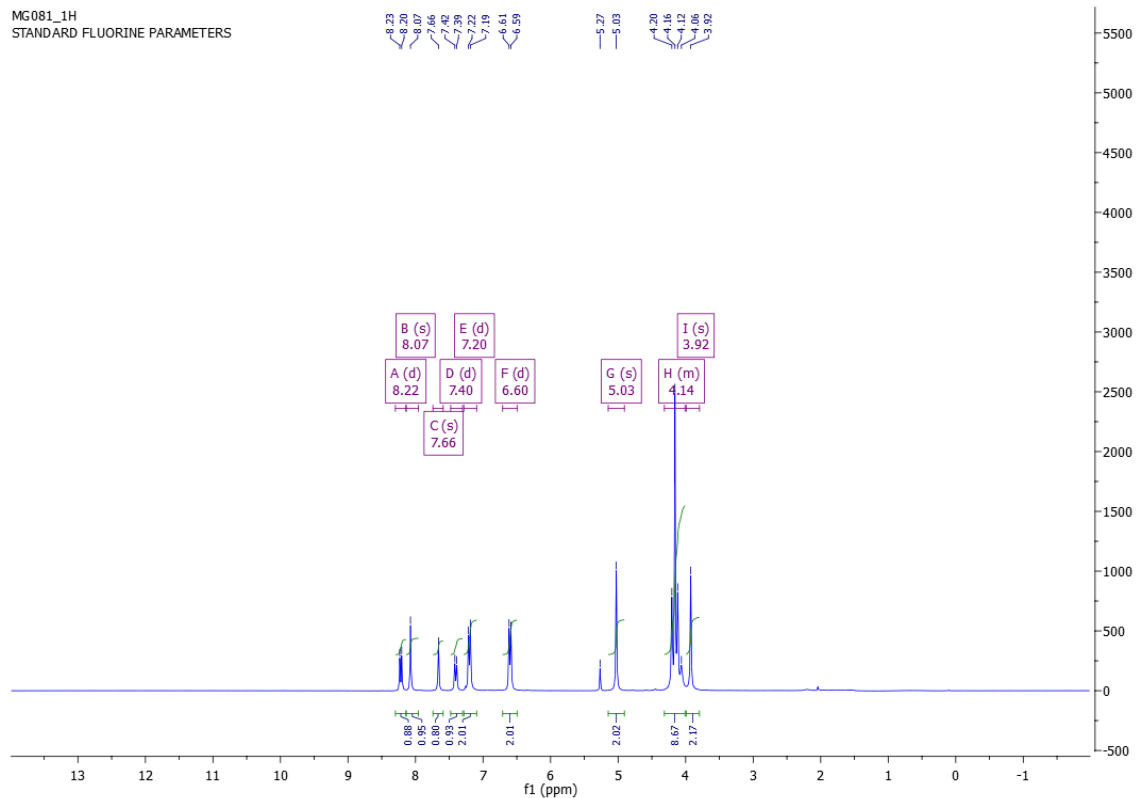


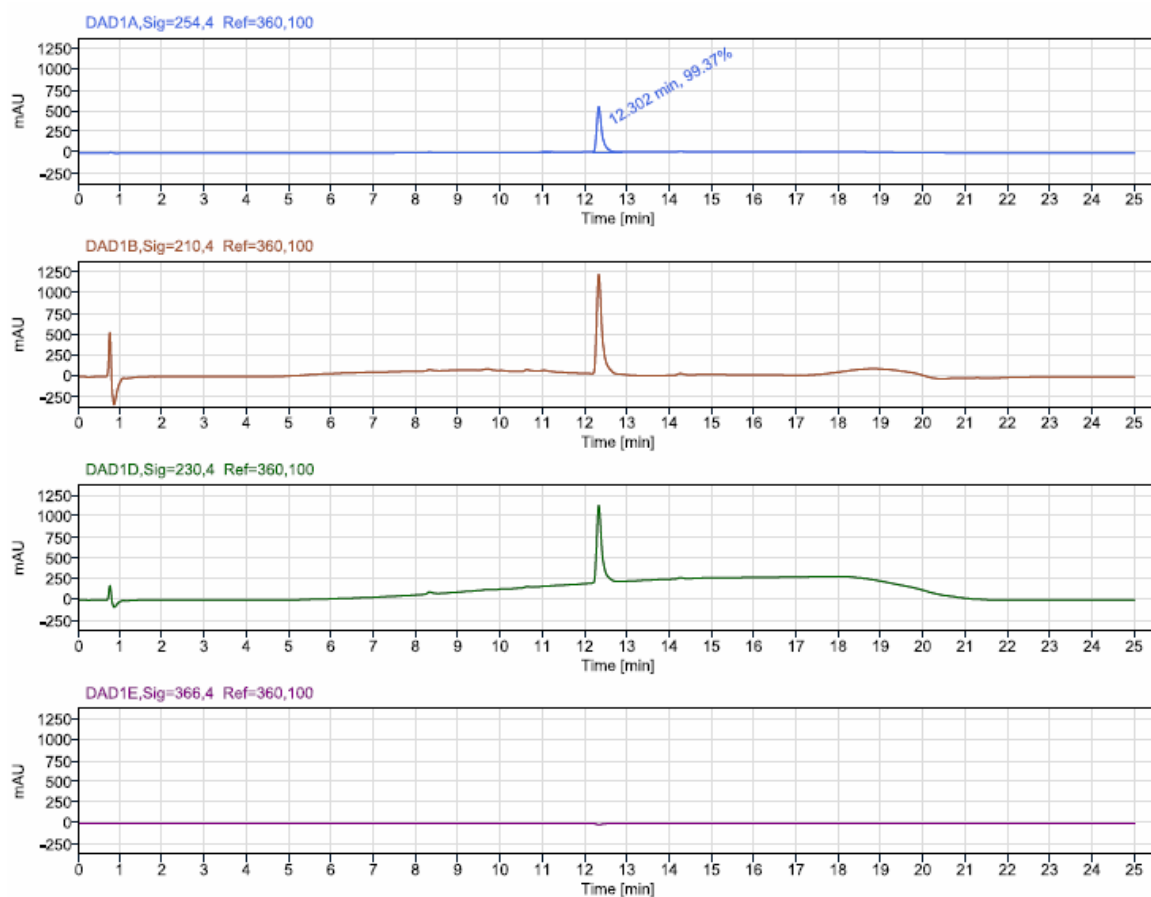
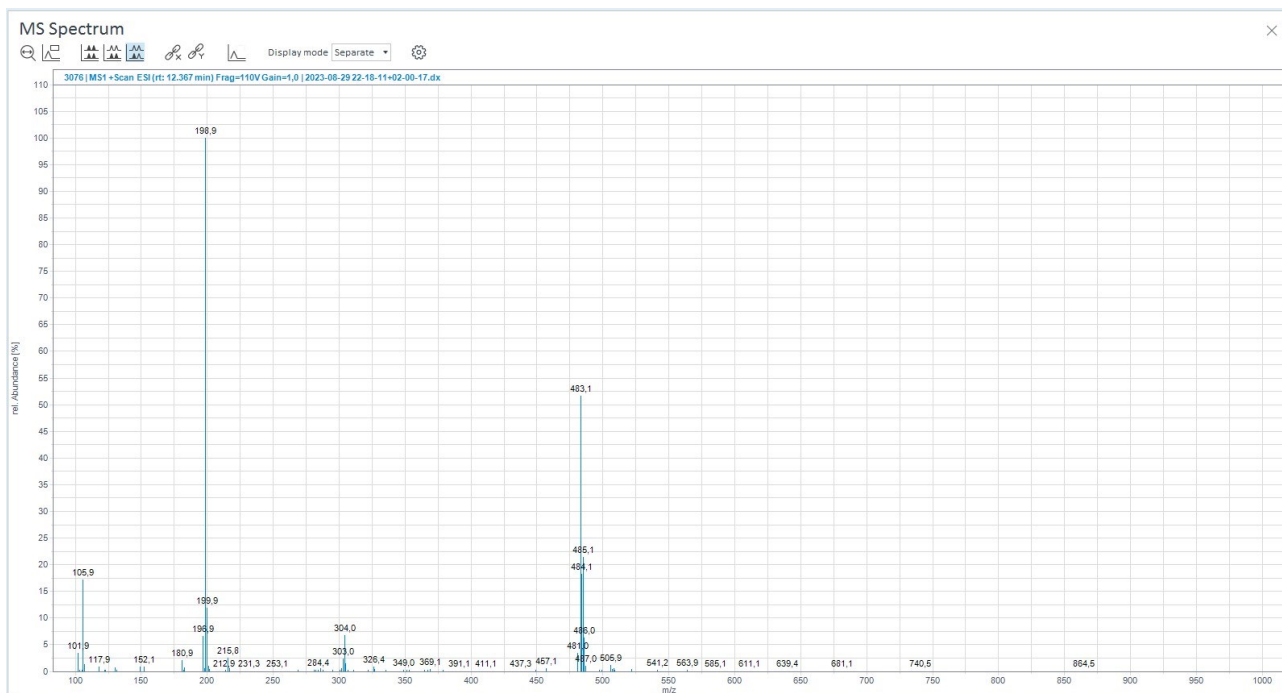


Peak Results (Area Percent at least 1%)

| 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 |

¹H, ¹³C NMR and HPLC/MS spectra of compound 11f

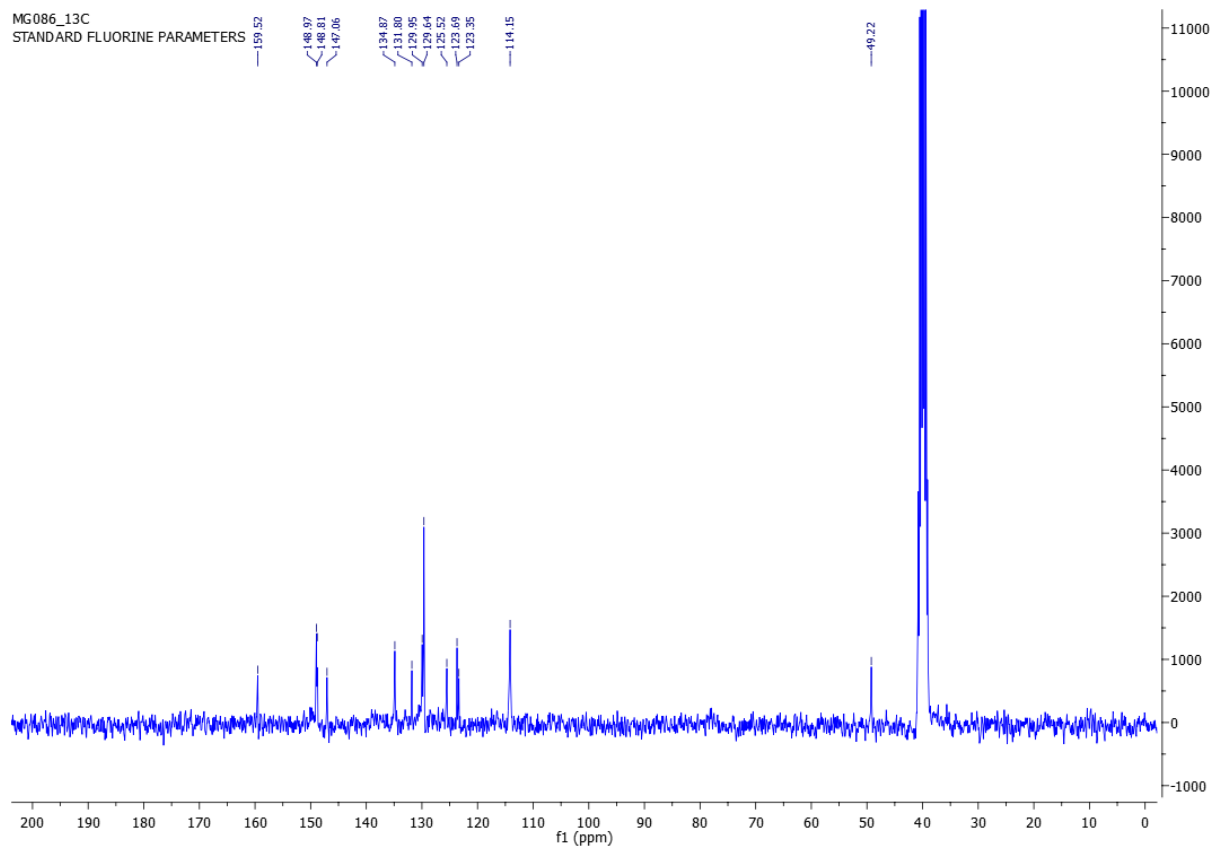
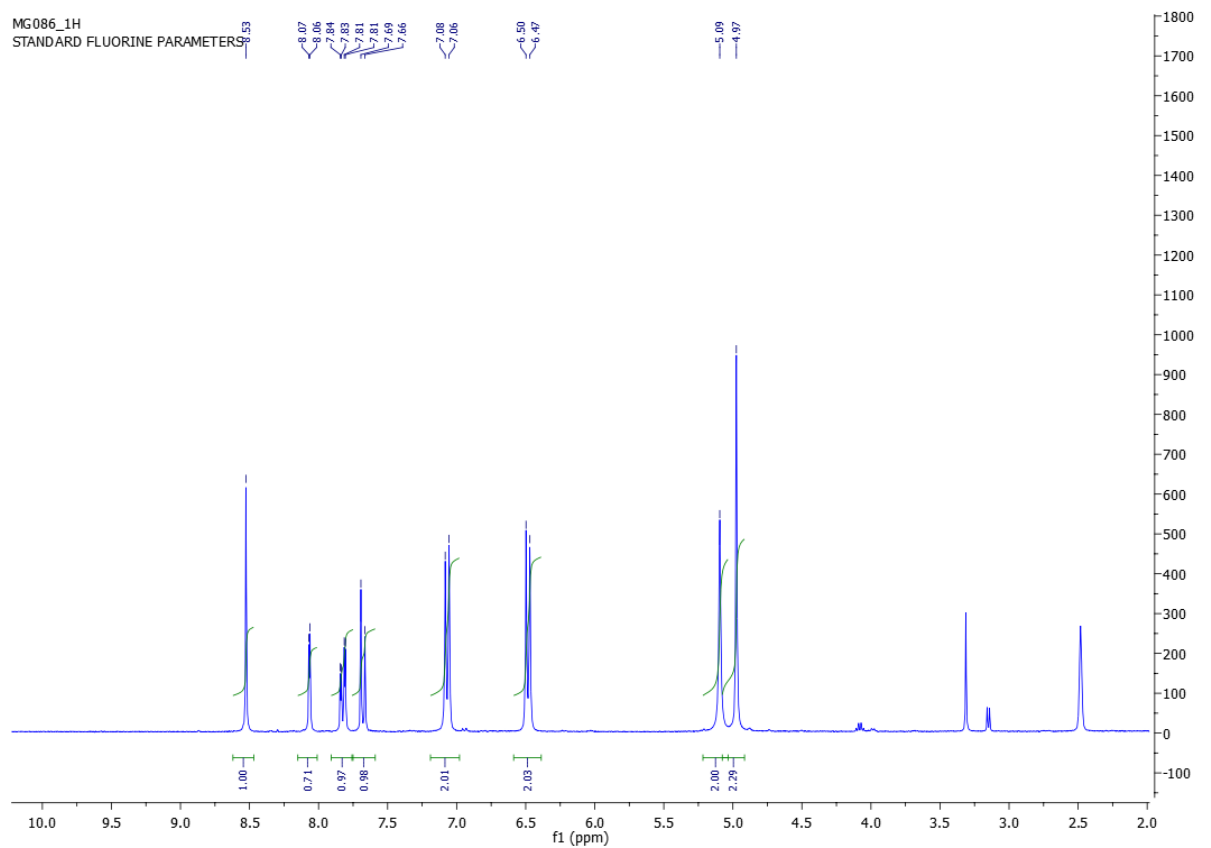


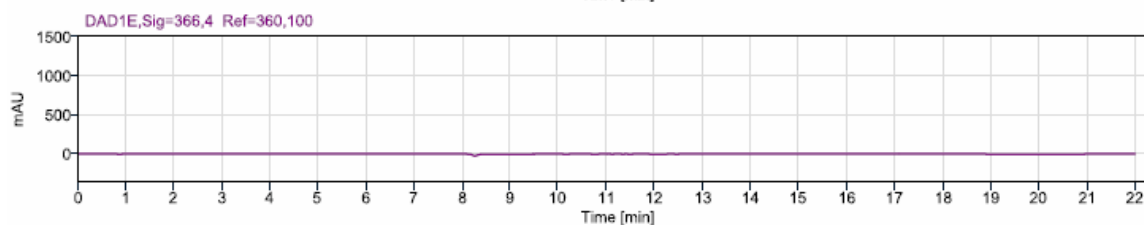
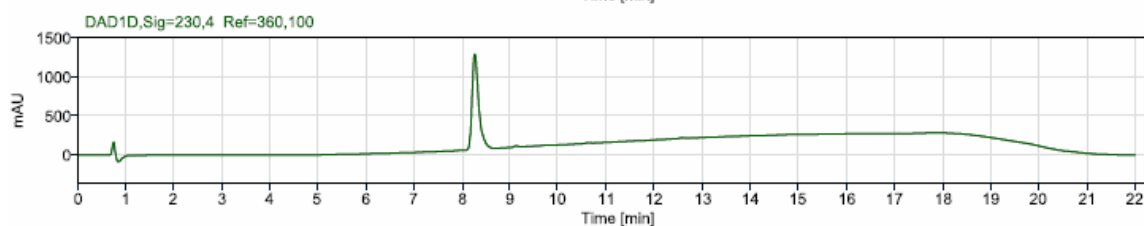
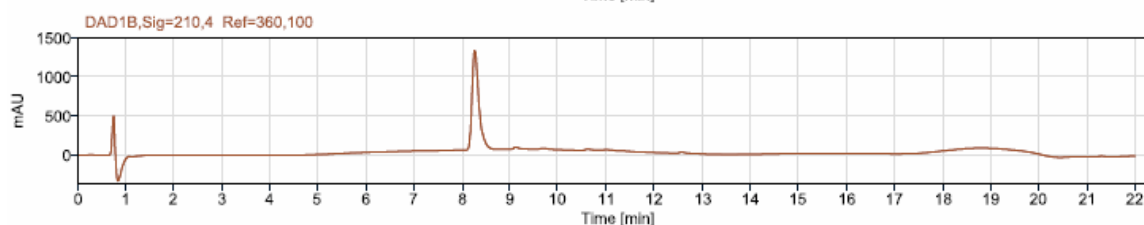
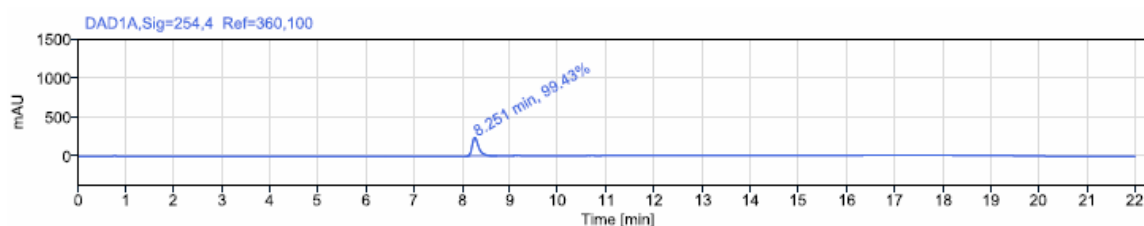
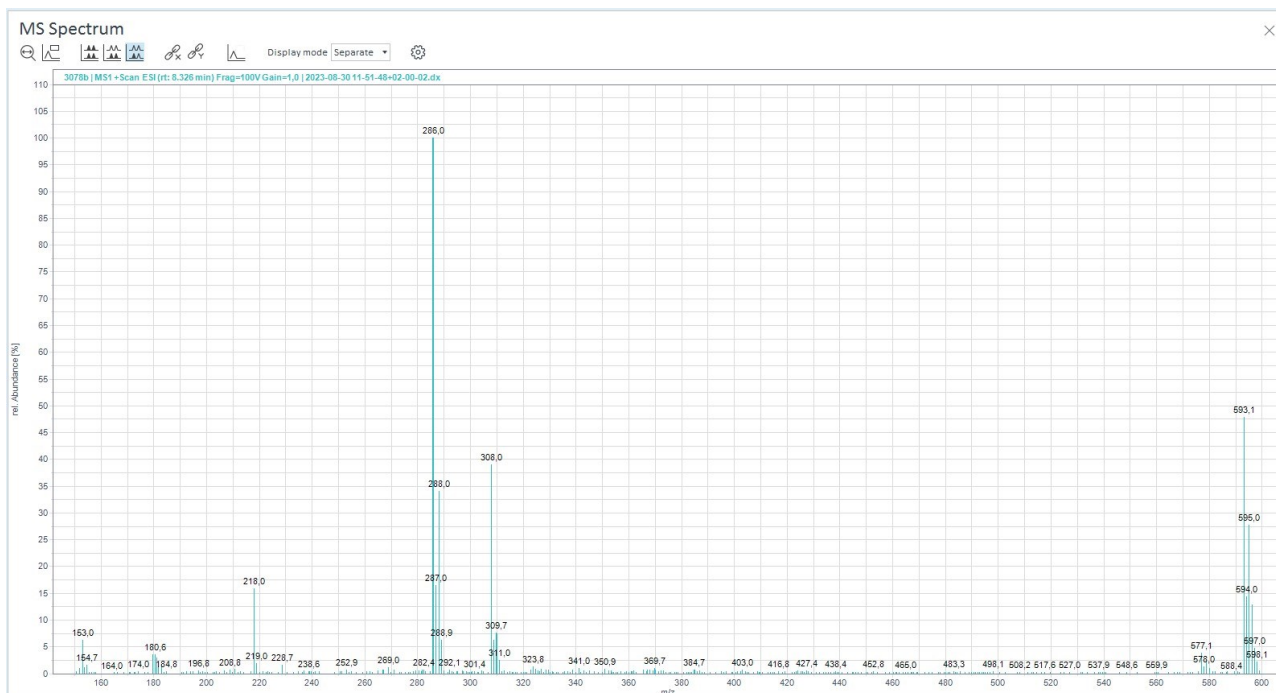


Peak Results (Area Percent at least 1%)

| 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 |

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

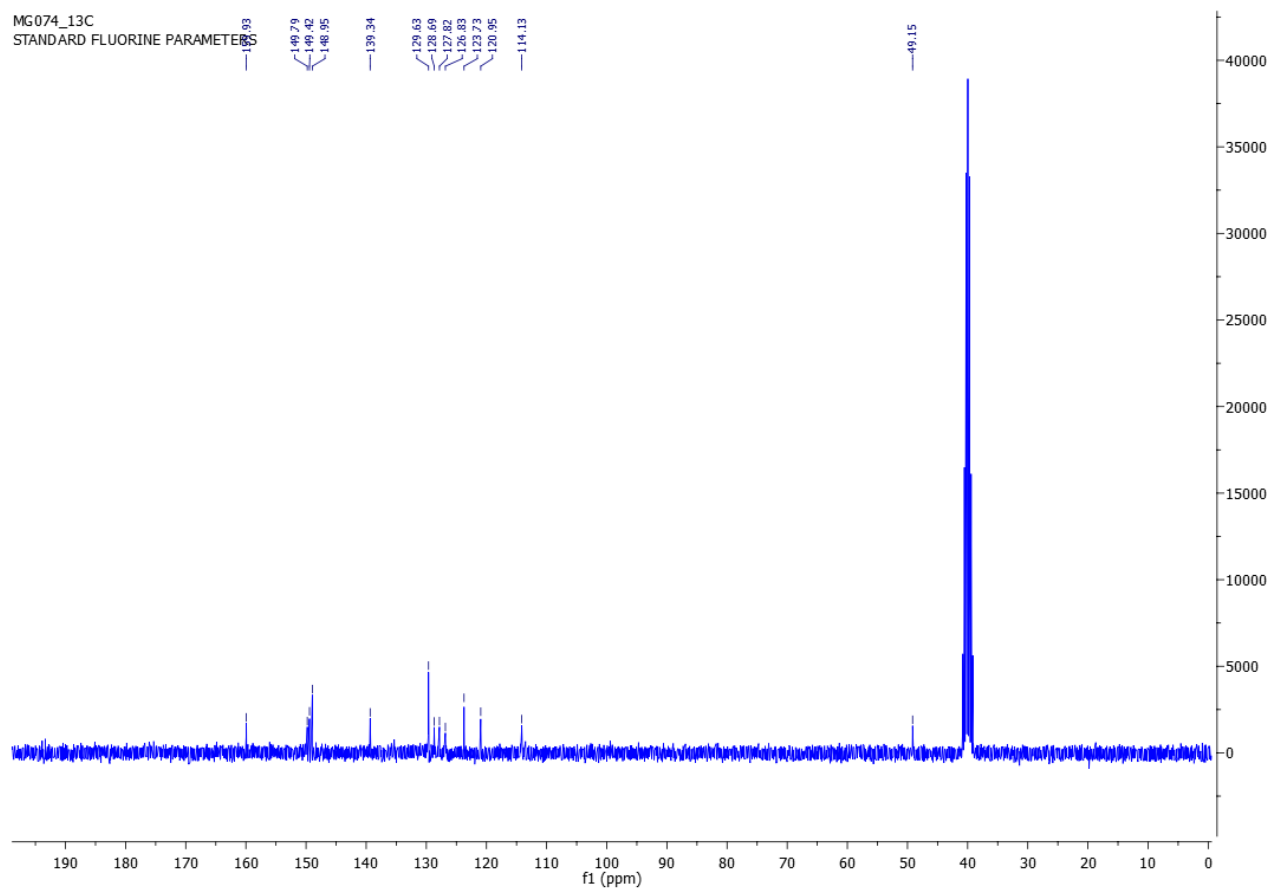
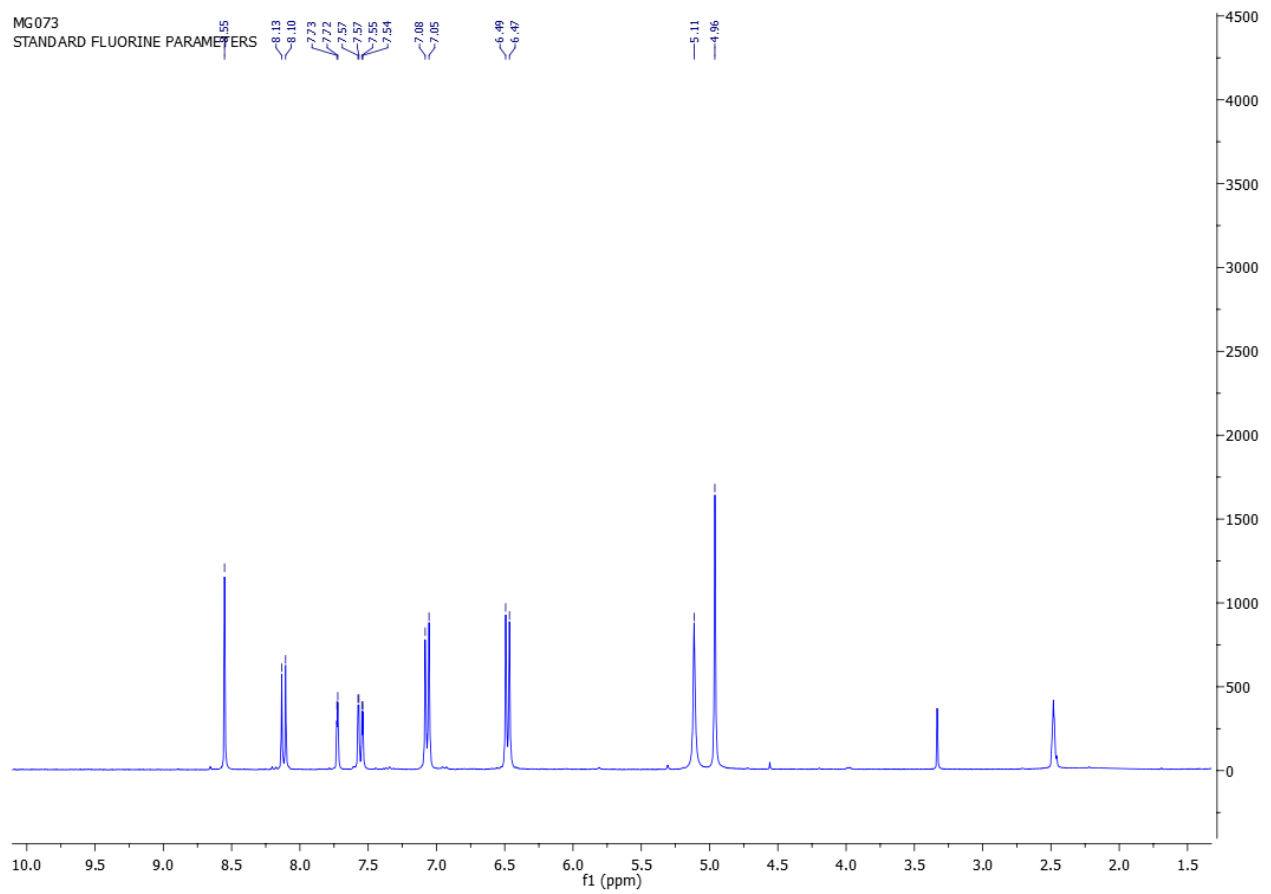


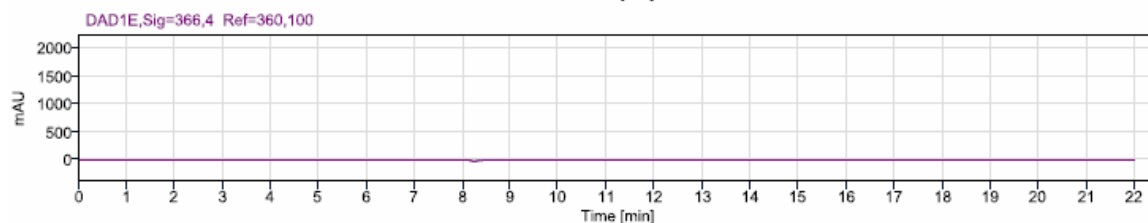
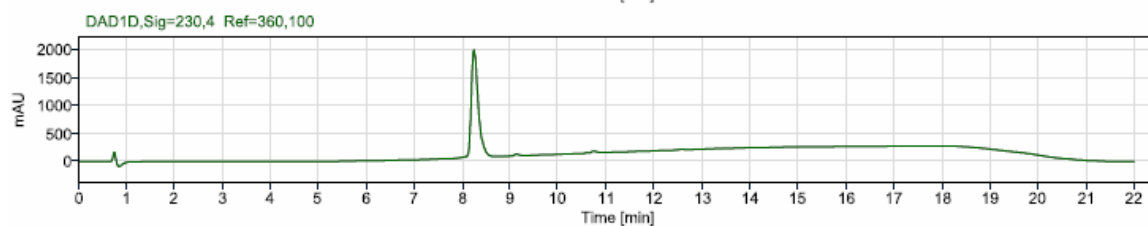
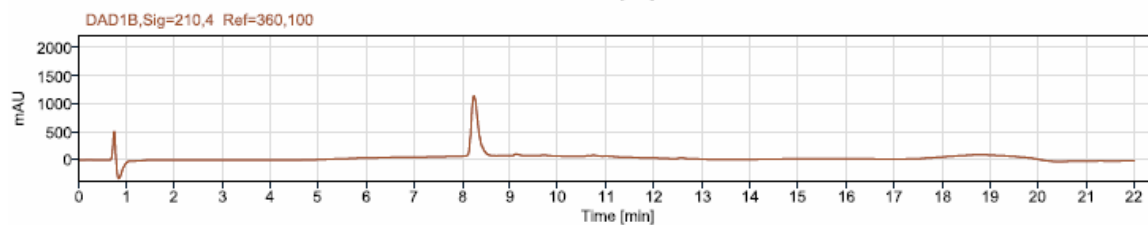
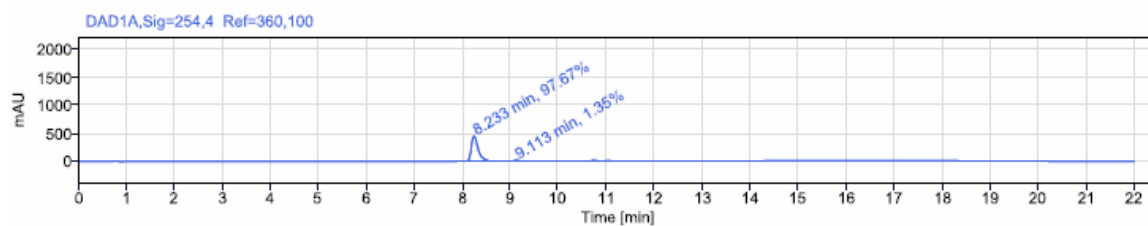
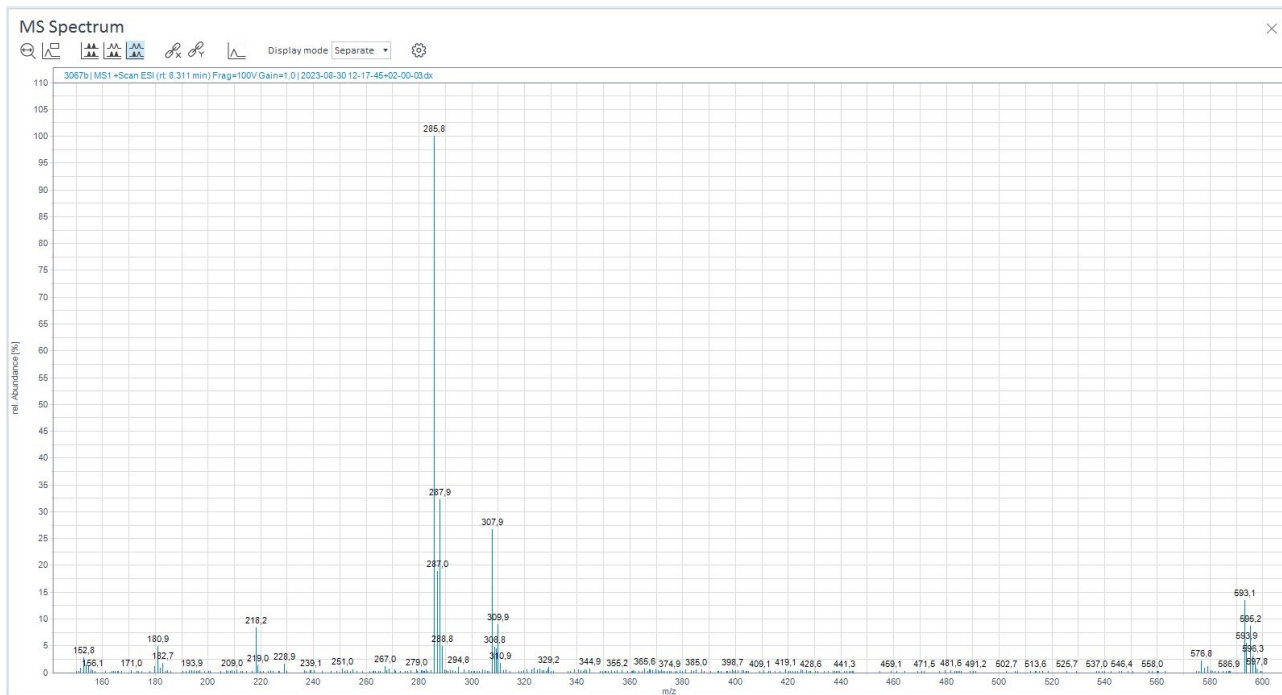


Peak Results (Area Percent at least 1%)

| 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 |

¹H, ¹³C NMR and HPLC/MS spectra of compound 22b



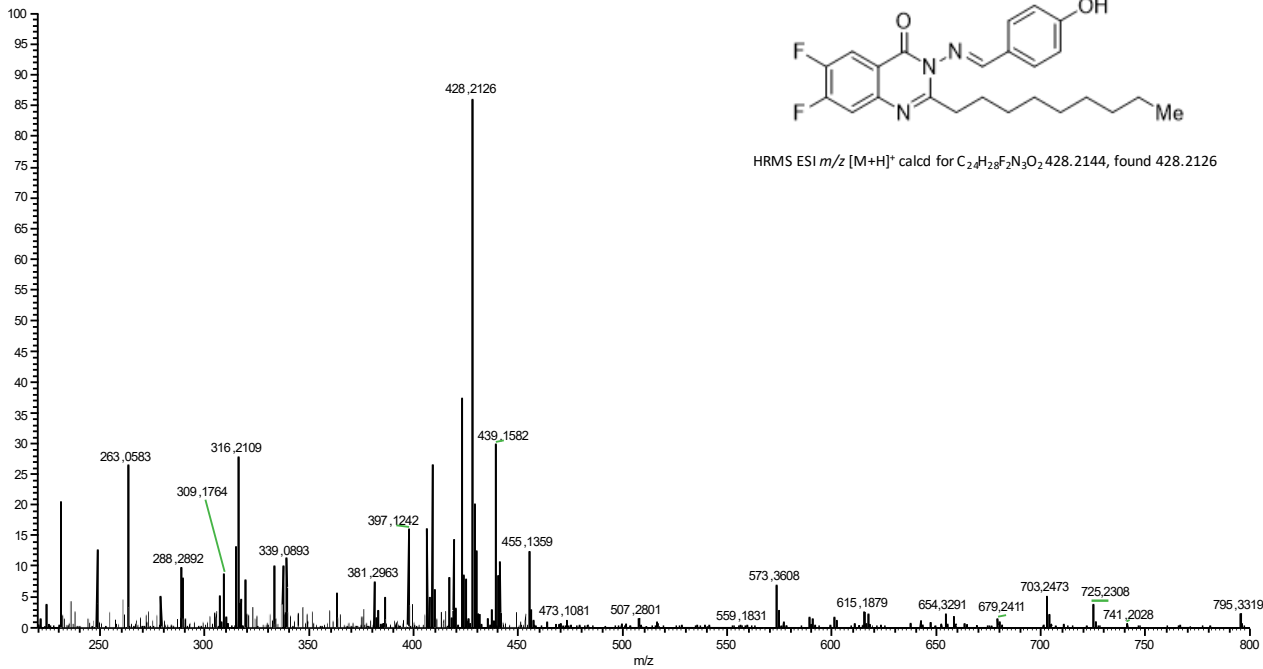


Peak Results (Area Percent at least 1%)

| 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 |

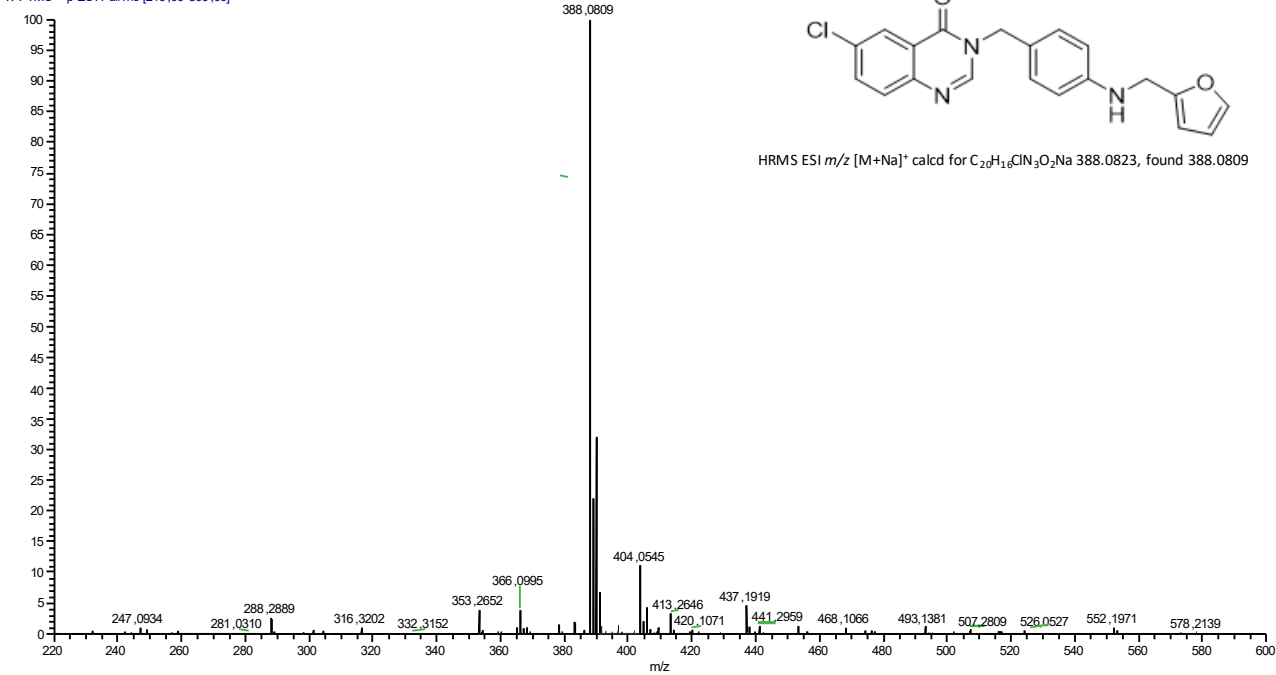
HRMS spectrum of compound 7a

NF3033 #18 RT: 0.14 AV: 1 NL: 9.38E6
T: FTMS + p ESI Full ms [216.00-900.00]



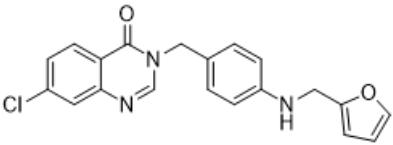
HRMS spectrum of compound 11a

NF3088 #33 RT: 0.26 AV: 1 NL: 5.92E7
T: FTMS + p ESI Full ms [216,00-800,00]

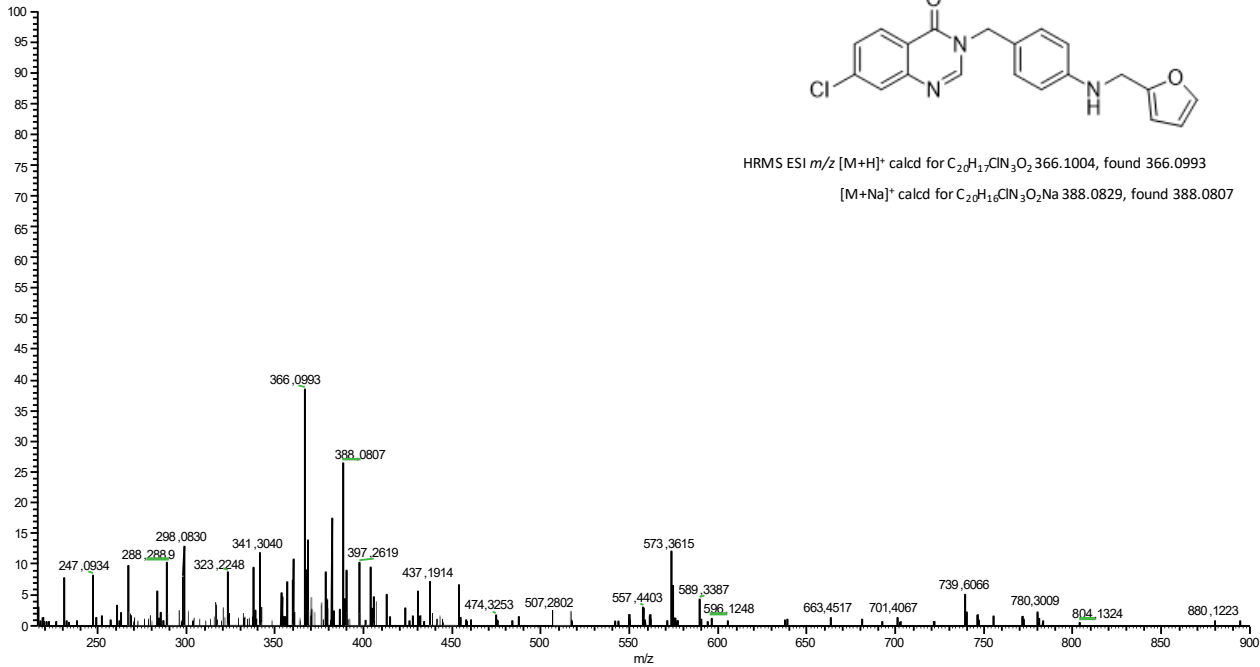


HRMS spectrum of compound 11b

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

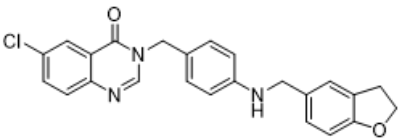


HRMS ESI m/z $[M+H]^+$ calcd for $C_{20}H_{17}ClN_3O_2$ 366.1004, found 366.0993
 $[M+Na]^+$ calcd for $C_{20}H_{16}ClN_3O_2Na$ 388.0829, found 388.0807

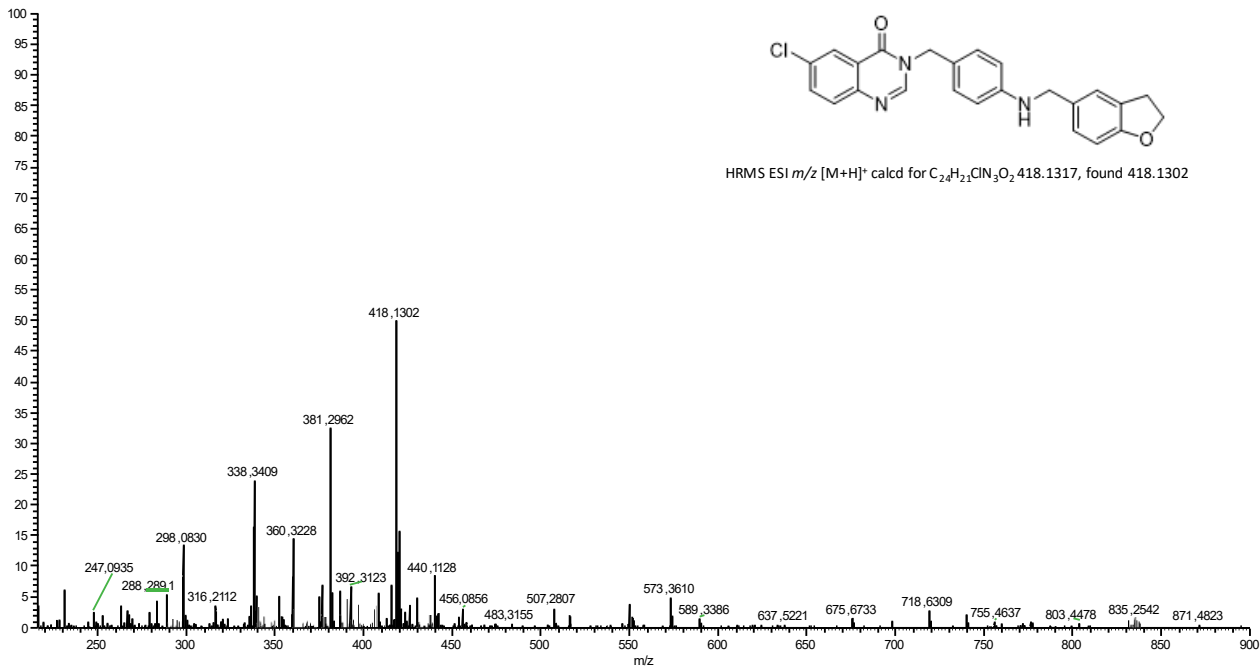


HRMS spectrum of compound 11c

NF3081 BIS H2O #2 RT:0.01 AV: 1 NL: 8,31E6
T: FTMS + p ESI Full ms [216,00-900,00]

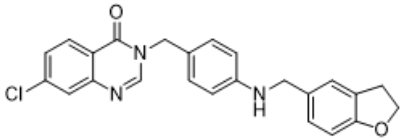


HRMS ESI m/z $[M+H]^+$ calcd for $C_{24}H_{21}ClN_3O_2$ 418.1317, found 418.1302



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

