Supporting Information for:

A Friedländer route to 5,7-Diazapentacenes

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Experimental details

1,5-dibromo-2,4-dinitrobenzene 11: 1,3-Dibromobenzene (**10**, 7.0 g, 29.7 mmol) was slowly added to a stirring mixture of concentrated sulfuric acid (6.5 mL) and fuming nitric acid (6.5 mL), while being cooled in an ice bath. 1,3-dibromobenzene was added slowly so as to maintain a temperature of 10-20 ^{o}C. After the addition was complete, the temperature was maintained at 35 ^{o}C for 3 h. The reaction mixture was then poured onto crushed ice. The solid precipitate formed was collected by filtration, and washed several times with water. The solid was then dissolved in a mixture of absolute ethanol (90 mL) and acetone (20 mL), the solution filtered and cooled in the fridge overnight. The crystals collected were washed with cold ethanol to give **11** (6.73 g, 20.7 mmol) as a bright yellow solid with a yield of 70%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.47 (1H, s), 8.24 (1H, s). ^{13}C NMR (100 MHz, $CDCl_3$) δ 119.86, 122.88, 141.39, 149.47.

1,5-di(hept-1-yn-1-yl)-2,4-dinitrobenzene 12 In a sealed flask, **11** (0.200 g, 0.61 mmol), $Pd(PPh_3)_4$ (0.036 g, 0.03 mmol) and CuI (0.012 g, 0.06 mmol) were added and purged with N_2 for 5 min. After which, degassed 1-heptyne (0.17 mL), THF (8 mL) and Et_3N (0.43 mL) were added. The mixture was then stirred at room temperature for 7h. The reaction mixture was then filtered through Celite, redissolved in diethyl ether, washed two times with NH_4Cl (10% aqueous solution), then dried over $MgSO_4$ and concentrated. Purification via column chromatography (Hexane: Et_2O = 9:1) gave **12** (0.172 g, 0.482 mmol) as a brown oil with a yield of 78%. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.71 (1H, s, CH), 7.76 (1H, s, CH), 2.53 (4H, t, J = 7.07 Hz, ≡-CH_2), 1.67 (4H, m), 1.50-1.35 (8H, m), 0.94 (6H, t, J = 7.07Hz). ^{13}C NMR (400 MHz, $CDCl_3$) δ 147.07 (C-NO_2), 141.03 (CH), 123.82 ((Ar)C-≡), 121.52 (CH), 105.91 (≡C-), 74.94 ((≡C-), 31.02 (≡-CH_2), 27.72, 22.14, 20.06, 13.91 (CH_3). HRMS (ESI): [M + H]+ calcd for $C_{20}H_{25}N_2O_4$ m/z 357.1814, found m/z 357.1813 (correct isotope distribution)

1,1'-(4,6-diamino-1,3-phenylene)bis(heptan-1-one) 8 A solution of **12** (3.75 g, 10.52 mmol) in 15ml of EtOH was added to a solution of $SnCl_2$*$2H_2O$ (25.2 g, 112 mmol) in EtOH (70 mL) and stirred at 70 ^{o}C for 4h under nitrogen. The reaction mixture was quenched with 5% aq Na_2CO_3 (400 mL), mixed with 500 ml of EtOAc, and 50g of Celite, and filtered. The organic layer was separated, dried over $MgSO_4$, then concentrated. Purification via column chromatography (Hexane: EtOAc = 2:1) gave **8** as a yellow solid (2.1 g, 6.32 mmol, 60%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.32 (1H, s, CH), 6.58 (4H, br. s, NH_2), 5.66 (1H, s, CH), 2.86 (4H, t, J = 7.58 Hz, C(O)-CH_2), 1.73 (4H, m), 1.41-1.26 (12H, m), 0.91 (6H, t, J = 7.07 Hz, CH_3). ^{13}C NMR (100 MHz, $CDCl_3$) □ 200.85 (CO), 154.63 (C-NH_2), 138.69 (CH), 110.51 (C-C=O), 98,65 (CH), 38.69 (CH_2-C=O), 31.73 (CH_2), 29.26 (CH_2), 25.65 (CH_2), 22.55 (CH_2), 14.04 (CH_3). HRMS (ESI): [M + H]+ calcd for $C_{20}H_{33}N_2O_2$ m/z 333.2537, found m/z 333.2535 (correct isotope distribution)

12,14-dihexyl-1,2,3,4,8,9,10,11-octahydroquinolino[3,2-b]acridine 7a. 8 (0.503 g, 1.51 mmol), EtOH (10 mL) and 37% wt HCl (0.30 mL, 3.62 mmol) were added into a sealed flask and purged with N_2 for 5 min. Cyclohexanone (**9**, 0.38 mL, 3.82 mmol) was added and the reaction was stirred at 75 ^oC for 20h. The reaction mixture was cooled down to room temperature, then quenched with 5% aqueous NaOH solution. The organic layer was then extracted, washing several times with CH_2Cl_2, the organic fraction was dried over $MgSO_4$ then filtered. Purification via flash chromatography (CH_2Cl_2: EtOAc: Et_3N = 1:1:0.1) gave **7a** (0.497 g, 0.92 mmol) as a yellow solid with a yield of 73%.^{1}H NMR (400 MHz, $CDCl_3$) δ 8.64 (1H, s, CH), 8.55 (1H, s, CH), 3.16 (8H, m), 2.98 (4H, t, J = 5.81, CH_2), 1.96 (8H, m), 1.71-1.65 (4H, m), 1.65-1.54 (4H, m), 1.43-1.34 (8H, m), 0.93 (6H, t, J = 7.07 Hz) ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.01, 144.89, 144.73, 127.41, 124.69, 117.89, 35.07, 31.78, 30.19, 27.97, 23.24, 22.70, 14.05. HRMS (ESI): [M + H]+ calcd for $C_{32}H_{45}N_2$ m/z 457.3577, found m/z 457.3582 (correct isotope distribution)

7,9-dihexyl-5,6,10,11-tetrahydrobenzo[h]benzo[7,8]quinolino[3,2-b]acridine 7b. 8 (0.203 g, 0.61 mmol), EtOH (5 mL) and 37% wt HCl (0.18 mL, 2.00 mmol) were added into a sealed flask and purged with N_2 for 5 min. a-Tetralone (0.17ml, 1.28 mmol). was added and the reaction was stirred at 75 ^oC for 20h. The reaction mixture was cooled down to room temperature, then quenched with 5% aqueous NaOH solution. The mixture was then extracted with dichloromethane (DCM), the organic fraction was dried over $MgSO_4$, then filtered and evaporated. Recrystallization from EtOH gave **7b** as a yellow solid (0.176 g, 0.32 mmol, 52%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.96 (1H, s, CH), 8.70 (2H, d, J = 7.58 Hz, CH), 8.61 (1H, s, CH), 7.47 (2H, m, CH), 7.41 (2H, m, CH), 7.30 (2H, d, J = 7.33 Hz, CH), 3.27 (2H, m, CH_2), 3.19 (2H, t, J = 5.81), 3.04 (2H, m, CH_2), 1.78 (2H, m, CH_2), 1.60 (2H, m, CH_2), 1.46 – 1.34 (4H, m, CH_2), 0.94 (6H, t, J = 7.07 Hz). ^{13}C NMR

(100 MHz, $CDCl_3$) δ = 154.24, 145.87, 143.62, 139.59, 135.36, 129.75, 129.39, 127.63, 127.52, 127.29, 126.93, 125.57, 118.29, 31.84, 30.16, 30.01, 28.46, 28.29, 25.61, 22.74, 14.10. HRMS (ESI): [M + H]+ calcd for $C_{40}H_{45}N_2$ m/z 553.3577, found m/z 553.3579 (correct isotope distribution)

1,1'-(4,6-dihexyl-2,8-dimethylpyrido[3,2-g]quinoline-3,7-diyl)bis(ethan-1-one) 7c. Obtained by reaction of **8** with acetylacetone employing the same procedure as for **7b** in 51% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.73 (1H, s, N-C=C(H)-C-N), 8.65 (1H, s, CH), 3.02 (4H, m, CH2), 2.70 (3H, s, CH3-CO), 2.65 (3H, s, CH3-Ar), 1.77 (4H, m, CH2), 1.53 (4H, m, CH2), 1.28 – 1.43 (8H, m, CH2), 0.91 (6H, t, J = 7.07 Hz, CH3). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 206.10 (CO), 155.27, 146.25, 143.10, 135.17, 128.24, 123.76, 120.10, 32.68, 31.59, 31.42, 30.21, 30.08, 24.19, 22.61, 13.99. HRMS (ESI): [M + H]+ calcd for $C_{30}H_{41}N_2O_2$ m/z 461.3163, found m/z 461.3166 (correct isotope distribution)

6-amino-7-hexanoyl-9-hexyl-3,4-dihydroacridin-1(2H)-one 7d. Obtained from reaction of **8** with 1,3-cyclohxedione employing the same procedure as for **7b** with 32% yield, recrystallized from hexane/EtOH. ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.70 (1H, s, N-C=C(H)-C-N), 7.01 (1H, s, CH), 6.42 (2H, br. s., NH2), 3.46 (2H, m, CH2), 3.16 (2H, t, J = 6.06 Hz, CH2), 3.09 (2H, t, J = 7.33 Hz, CH2), 2.75 (2H, t, J = 6.32 Hz, CH2), 2.15 (2H, m, CH2), 1.56 – 1.85 (6H, m, CH2), 1.32 – 1.48 (10H, m, CH2), 0.88 – 0.96 (6H, m, 2CH3). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 203.32, 199.27, 166.23, 156.13, 151.18, 151.10, 131.95, 121.89, 121.30, 118.51, 110.54, 41.09, 39.82, 35.34, 31.66, 31.63, 31.41, 30.07, 29.15, 28.94, 25.25, 22.66, 22.53, 21.09, 14.06, 13.99. HRMS (ESI): [M + H]+ calcd for $C_{26}H_{37}N_2O_2$ m/z 409.2850, found m/z 409.2861 (correct isotope distribution)

13,15-dihexylbenzo[4,5]furo[3,2-b]benzofuro[2',3':5,6]pyrido[3,2-g]quinoline 7e. Obtained from reaction of 8 with benzofuranone employing the same procedure as for **7b** with 45% yield, purified using column chromatography (Hex:EtOAc = 2:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.26 (1H, s, N-C=C(H)-C-N), 8.77 (1H, s, CH), 8.45 (2H, d, J = 7.58 Hz, CH), 7.65 (2H, t, J = 7.58 Hz, CH), 7.55 (2H, J = 8.08 Hz, CH), 7.47 (2H, m, CH), 3.48 (4H, t, J = 7.83 Hz, CH2), 1.94 (4H, m, CH2), 1.58 (4H, m, CH2), 1.22 – 1.46 (8H, m, CH2), 0.92 (6H, t, J = 6.82 Hz, CH3). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 160.05, 149.11, 145.77, 144.37, 131.52, 128.72, 126.34, 124.80, 123.43, 123.25, 122.90, 118.13, 112.06. HRMS (ESI): [M + H]+ calcd for $C_{36}H_{37}N_2O_2$ m/z 529.2850, found m/z 529.2862 (correct isotope distribution)

Attempted dehydrogenation of 7a and 7b:

7a 12,14-dihexyl-1,2,3,4,8,9,10,11-octahydroquinolino[3,2-b]acridine (**7a**, 0.2 g, 0.439 mmol) and Pd/C (0.047 g, 0.439 mmol) were added to a flask, connected to a reflux condenser and bubble counter and were purged in N_2 for 5min. Ph_2O (5 mL) was added and the reaction mixture was heated at 200 ^{o}C for 24h. The reaction mixture was quenched with $CHCl_3$ (30 mL), 10 % HCl (20 mL) and aq NaOH was added till the mixture was alkaline. The organic layer was extracted, washed with water and DCM several times. TLC only showed spots of Ph_2O and no trace of the desired product.

7b: 7b (0.167 g, 0.366 mmol) and Pd/C (0.040 g, 0.376 mmol) were added to a flask, connected to a bubble counter and were purged in N_2 for 5min. Ph_2O (4.2 mL) was added and the reaction mixture was heated at 175 ^{o}C for 24h. The reaction mixture was filtered through celite, washed with DCM, and the filtrate evaporated. After which Hexane was added, and left in the freezer for

1h. Then, the mixture was filtered and the brown residue (0.030 g) was obtained. NMR showed a complex mixture of oligomers.

4,6-dihexyl-2,3,7,8-tetraphenylpyrido[3,2-g]quinoline (17a). The procedure is representative for synthesis of **17a-c**. A mixture of **8** (499mg, 1.5 mmol), **16a** (648mg, 3.3 mmol, 2.2eq) and TsOH*H_2O (628mg, 3.3 mmol, 2.2 mmol) was stirred at 105°C under nitrogen for 1h. Cooled down to room temperature, quenched with aqueous ammonia, extracted with DCM, dried over $MgSO_4$, and then evaporated. Recrystallization from ethanol afforded 294mg (0.45 mmol) of **17a** (30% yield).

^{1}H NMR (400 MHz, $CDCl_3$) δ =9.13 (1H, s, N-C=C(H)-C-N), 8.88 (1H, s, CH), 7.39 – 7.44 (4H, m, Ph), 7.29 – 7.36 (4H, m, Ph), 7.19 – 7.25 (10H, m, Ph), 3.11 (4H, m, Ar-CH2), 1.76 (4H, m, CH2), 1.38 (4H, m, CH2), 1.23 (8H, m, CH2), 0.85 (6H, t, J = 6.82 Hz, CH3). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 160.93, 146.68, 146.18, 141.28, 138.99, 133.28, 130.59, 130.04, 129.84, 127.98, 127.68, 127.53, 127.07, 125.10, 120.45, 31.40, 31.10, 30.00, 29.92, 22.50, 13.97. HRMS (ESI): [M + H]+ calcd for $C_{48}H_{49}N_2$ m/z 653.3890, found m/z 653.3905 (correct isotope distribution)

2,8-bis(3,4-dimethoxyphenyl)-4,6-dihexyl-3,7-diphenylpyrido[3,2-g]quinoline (17b).

Obtained by recrystallization from ethanol with 33% yield.

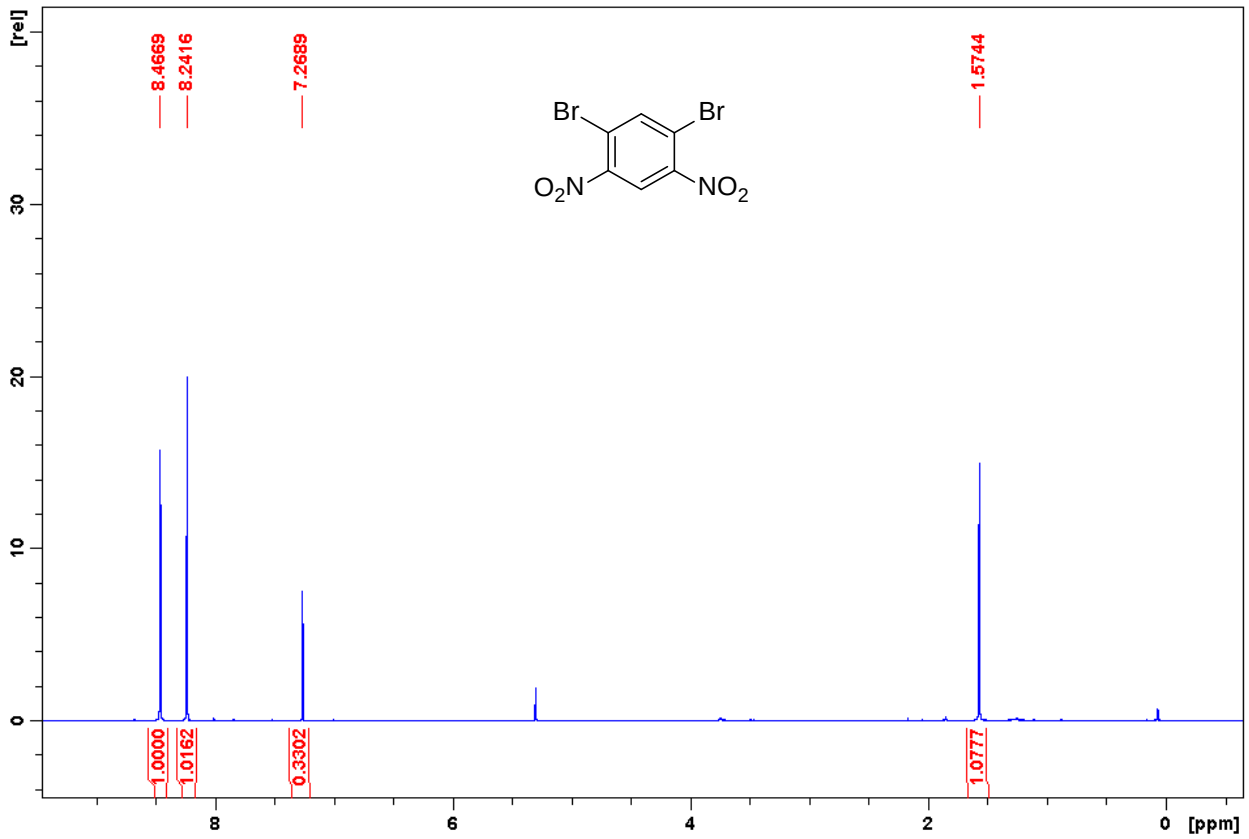
^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.08 (1H, s, N-C=C(H)-C-N), 8.84 (1H, s, CH), 7.30 – 7.40 (6H, m, Ph), 7.22 – 7.26 (4H, m, Ph), 7.17 (2H, dd, J1 = 8.34 Hz, J2 = 2.02 Hz, 2H, CH), 6.85 (2H, d, J = 2.02 Hz), 6.80 (2H, d, J = 8.34 Hz, CH), 3.87 (6H, s, OCH3), 3.63 (6H, s, OCH3), 3.09 (4H, m, Ar-CH2), 1.74 (4H, m, CH2), 1.37 (4H, m, CH2), 1.23 (8H, m, CH2), 0.84 (6H, t, J = 6.82 Hz, CH3). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 159.96, 148.83, 147.73, 146.70, 146.26, 139.47, 133.82,

133.04, 130.58, 129.58, 128.20, 127.12, 124.92, 123.16, 120.38, 113.49, 110.48, 55.79, 55.60, 31.39, 31.08, 29.99, 29.90, 22.49, 13.96. HRMS (ESI): [M + H]+ calcd for $C_{52}H_{57}N_2O_4$ m/z 773.4324, found m/z 773.4313 (correct isotope distribution)

2,3,7,8-tetrakis(3,4-dimethoxyphenyl)-4,6-dihexylpyrido[3,2-g]quinoline (17c). Purified using column chromatography (DCM : EtOAc 1:1). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.06 (1H, s, N-C=C(H)-C-N), 8.82 (1H, s, CH), 7.12 (2H, dd, J1 = 8.34 Hz, J2 = 2.02 Hz, CH), 6.97 (2H, d, J = 2.02 Hz, CH), 6.88 (2H, d, J = 8.34 Hz), 6.76 – 6.83 (4H, m, 2CH), 6.72 (2H, m, CH), 3.93 (6H, s, OCH3), 3.87 (6H, s, OCH3), 3.75 (6H, s, OCH3), 3.70 (6H, s, OCH3), 3.13 (4H, m, Ar-CH2), 1.78 (4H, m, CH2), 1.42 (4H, m, CH2), 1.26 (12H, m, CH2), 0.86 (6H, t, J = 6.82 Hz, CH3). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 160.93, 146.68, 146.18, 141.28, 138.99, 133.28, 130.59, 130.04, 129.84, 127.98, 127.53, 127.07, 125.10, 120.45, 31.40, 31.10, 30.00, 29.92, 22.50, 13.97. HRMS (ESI): [M + H]+ calcd for $C_{56}H_{65}N_2O_8$ m/z 893.4735, found m/z 893.4752 (correct isotope distribution)

20,22-dihexyl-2,3,6,7,13,14,17,18-octamethoxydibenzo[a,c]dibenzo[5,6:7,8]quinolino[2,3-i]acridine (18b). BF_3*Et_2O (1.21ml, 9.4mmol, 9.1 eq of BF_3) was added to a mixture of **17b** (772mg, 1.0 mmol), [Bis(trifluoroacetoxy)iodo]benzene (PIFA, 1871mg, 4,4mmol, 4,4 eq) and 8ml of anhydrous DCM at +5°C under nitrogen. Then the mixture was stirred for 2h at +15°C. After quenching with saturated aqueous Na_2CO_3 solution, the organic compounds were extracted with DCM. The organic fraction was dried with $MgSO_4$ and evaporated. Column chromatography (DCM : EtOAc : Et_3N = 9:1:0.2) afforded 214 mg of the product as a red solid (28% yield). ^{1}H NMR (400 MHz, CD_2Cl_2 + CF_3COOH) δ = 9.61 (1H, s, N-C=C(H)-C-N), 9.53 (1H, s, CH), 8.56

(2H, d, J = 7.58, CH), 8.41 (2H, d, J = 8.08), 8.34 (2H, s, CH), 8.00 (2H, s, CH), 7.94 (2H, m, CH), 7.83 (2H, m, CH), 4.25 (6H, s, OCH3), 4.21 (4H, m, CH2), 4.12 (6H, s, OCH3), 2.17 (4H, m, CH2), 1.68 (4H, m, CH2), 1.34 – 1.48 (8H, m, CH2), 0.92 (6H, t, J = 7.07 Hz, CH3). ^{13}C NMR (100 MHz, CD_2Cl_2 + CF_3COOH) δ = 159.15, 158.57, 152.16, 147.39, 136.71, 134.49, 131.61, 131.01, 130.61, 128.77, 127.47, 126.67, 126.39, 125.14, 125.11, 117.12, 109.72, 107.43, 106.31, 57.42, 57.18, 34.65, 33.58, 31.97, 30.37, 23.17, 14.27. HRMS (ESI): [M + H]+ calcd for $C_{52}H_{53}N_2O_4$ m/z 769.4005, found m/z 769.4014 (correct isotope distribution)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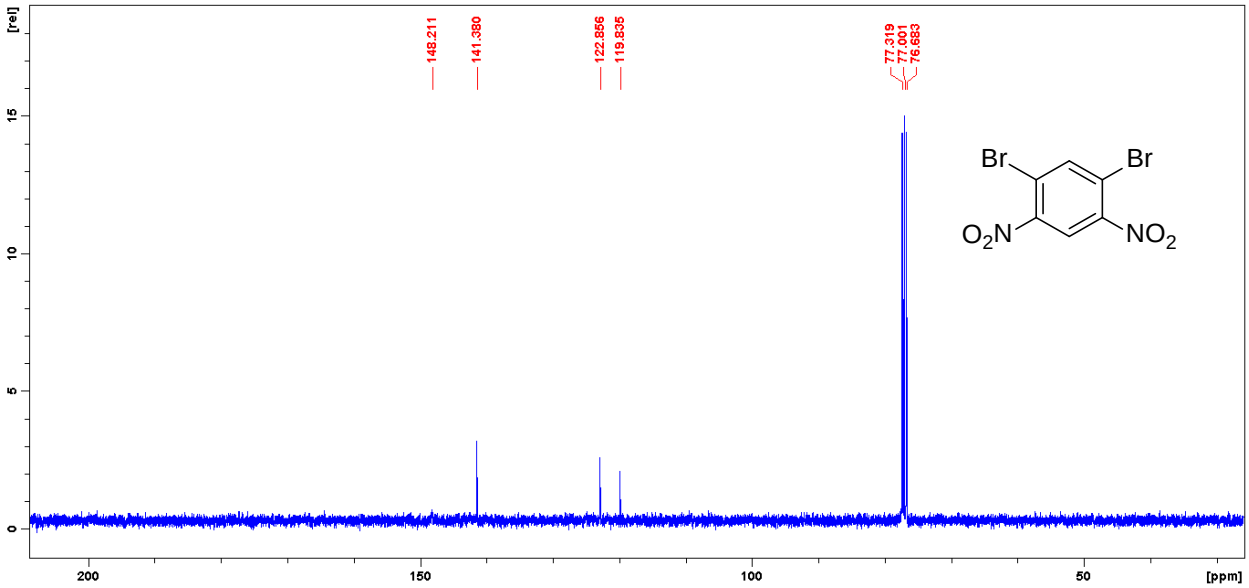
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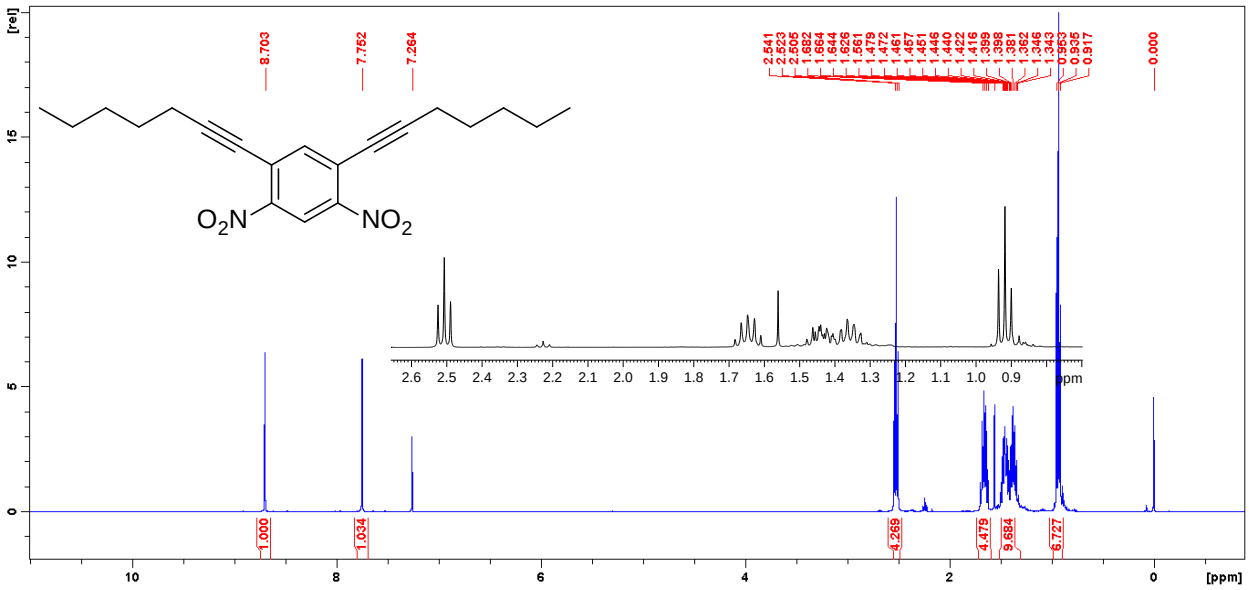
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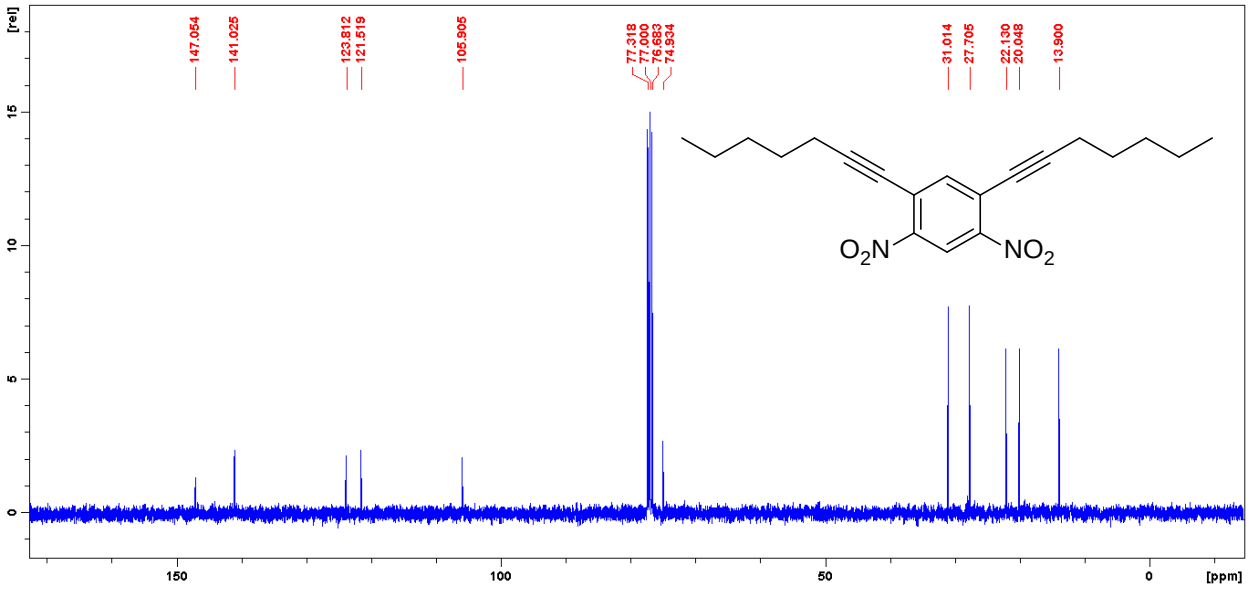
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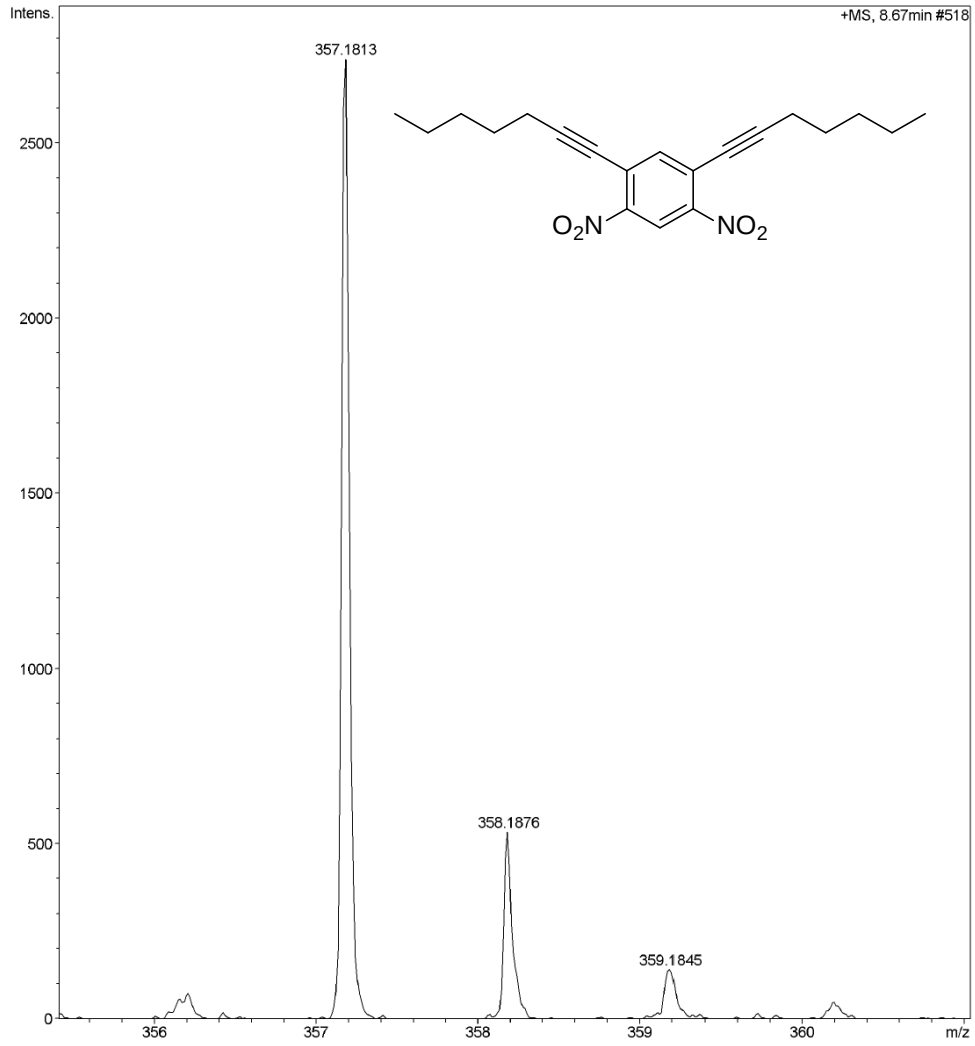
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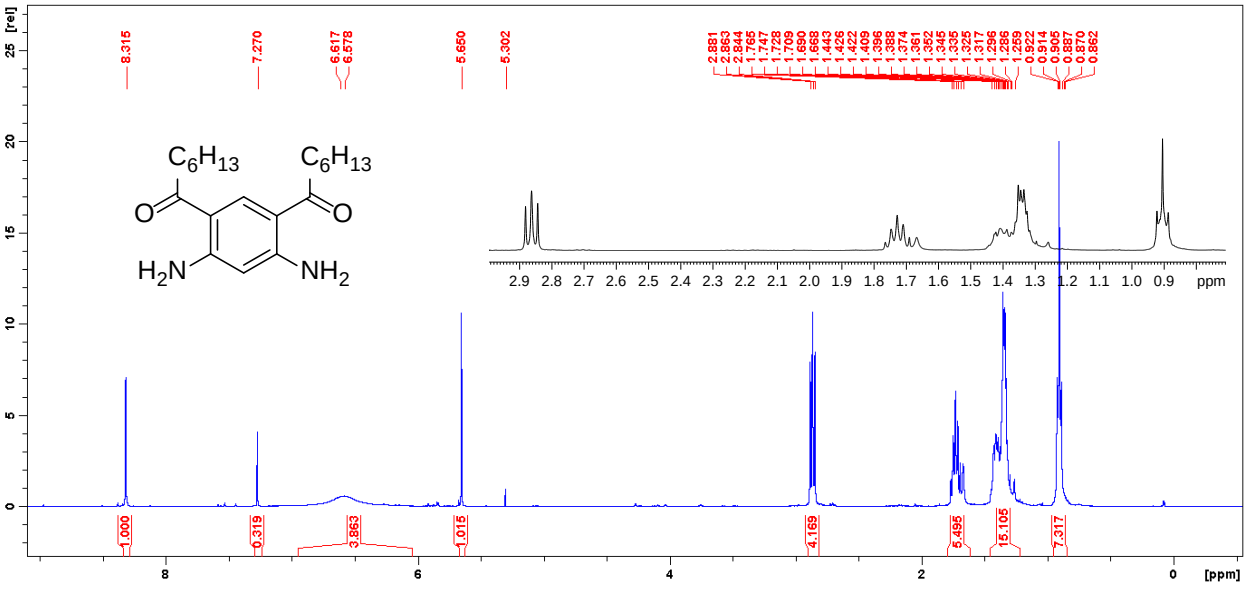
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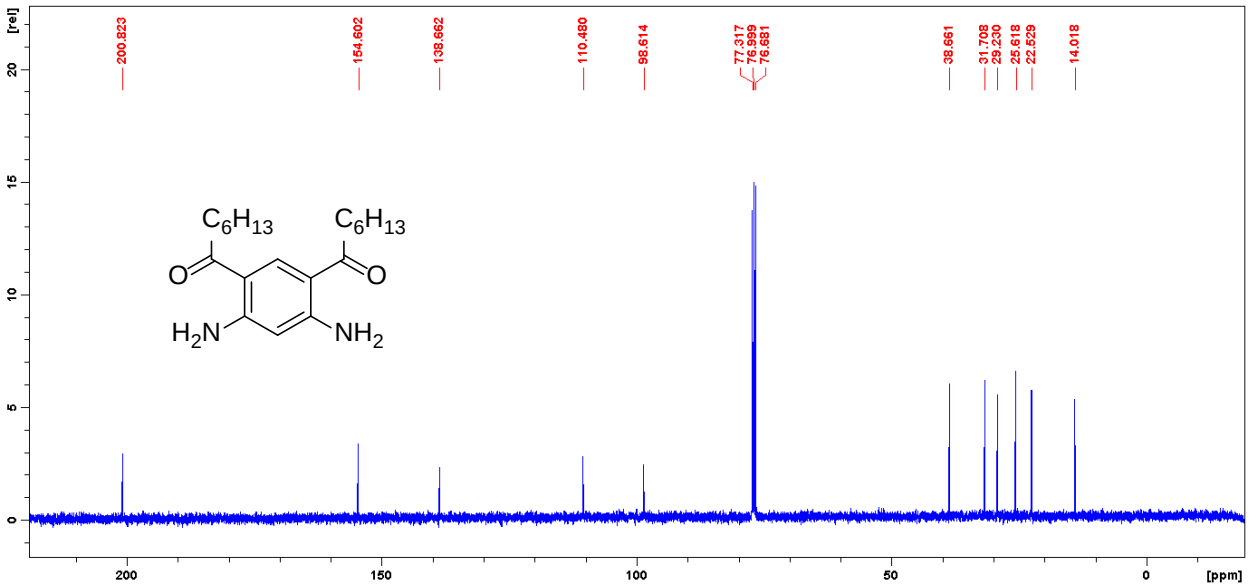
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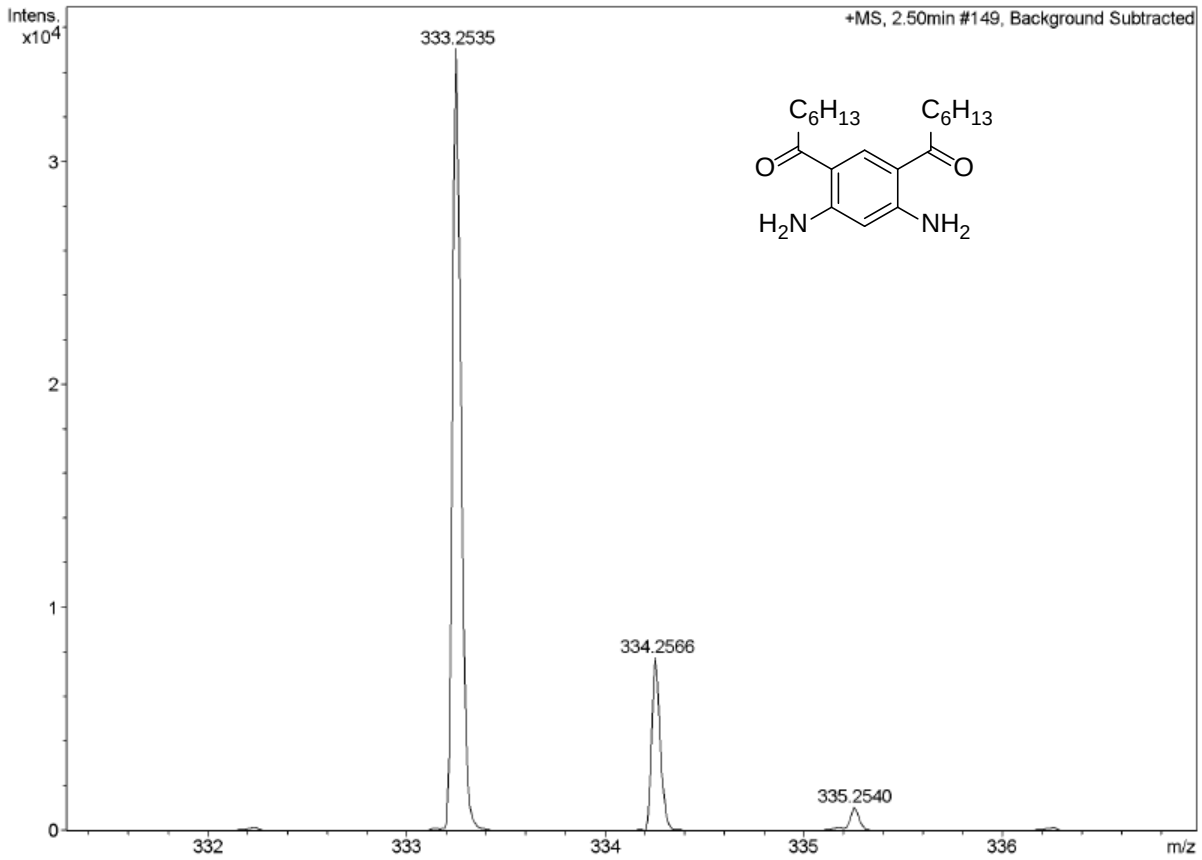
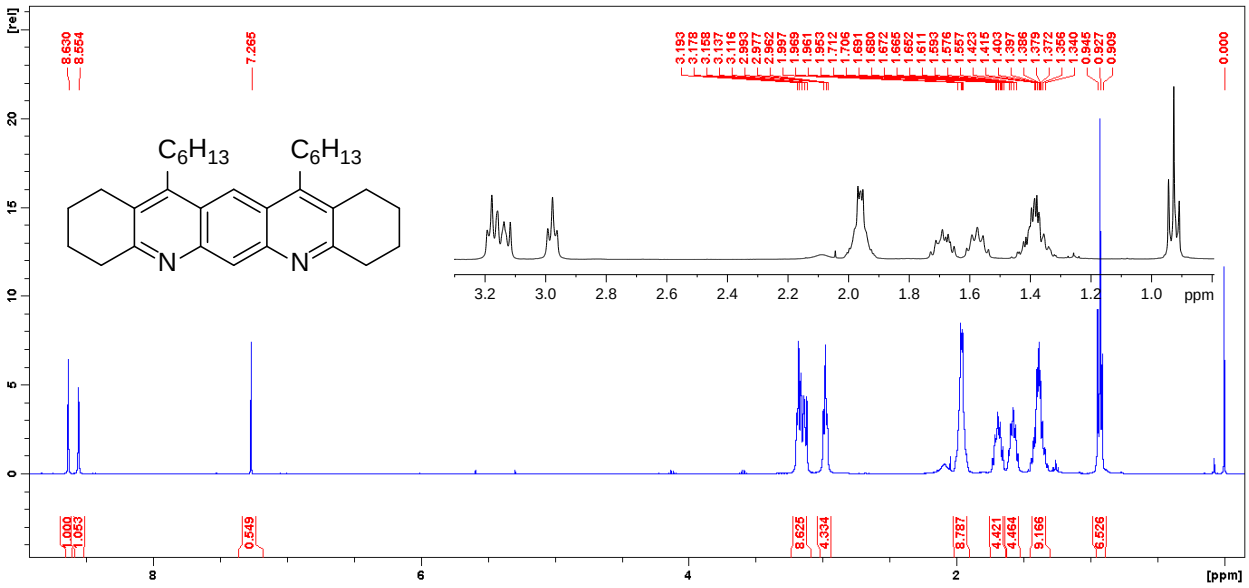
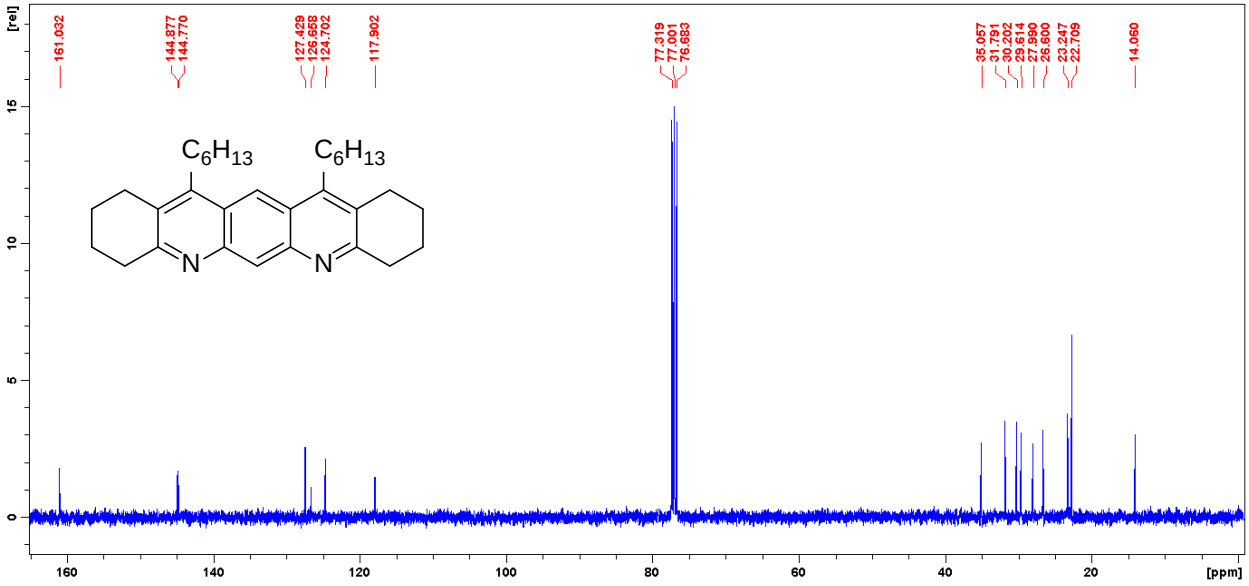
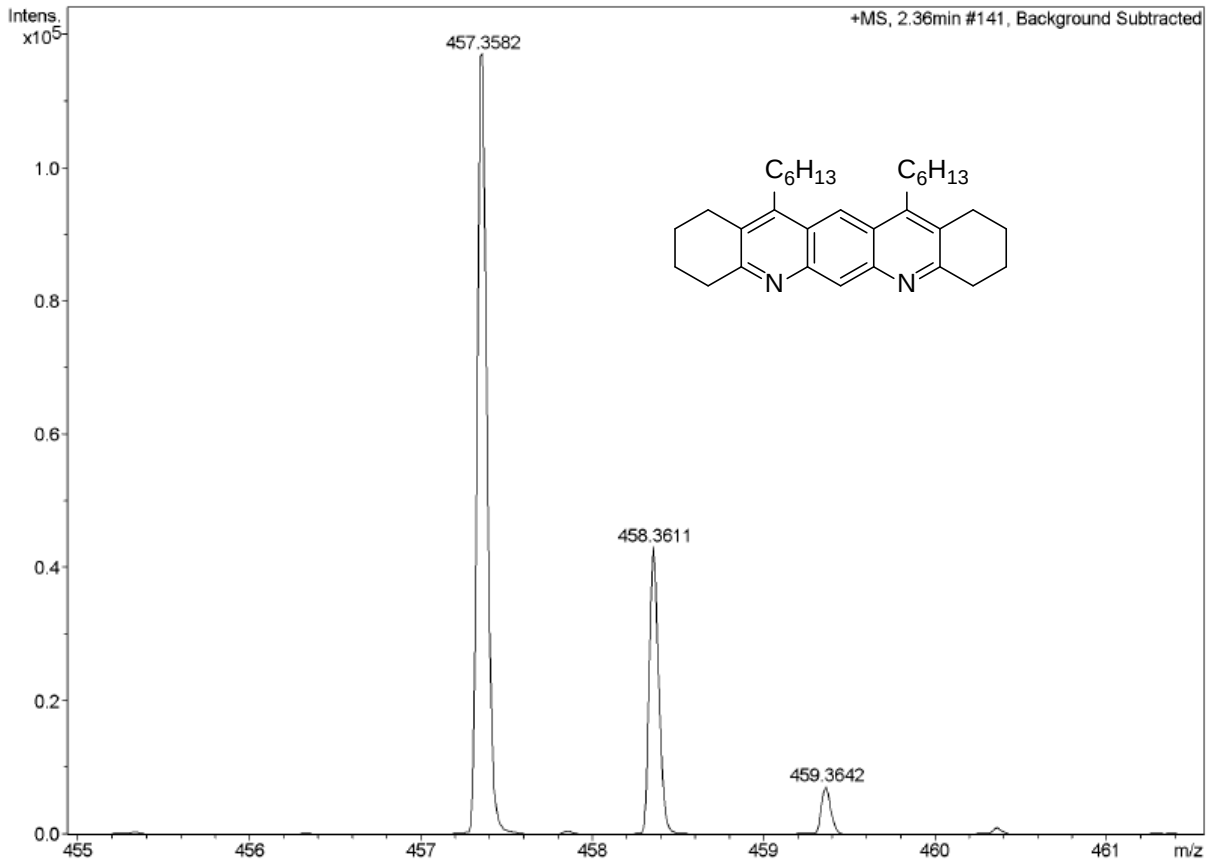
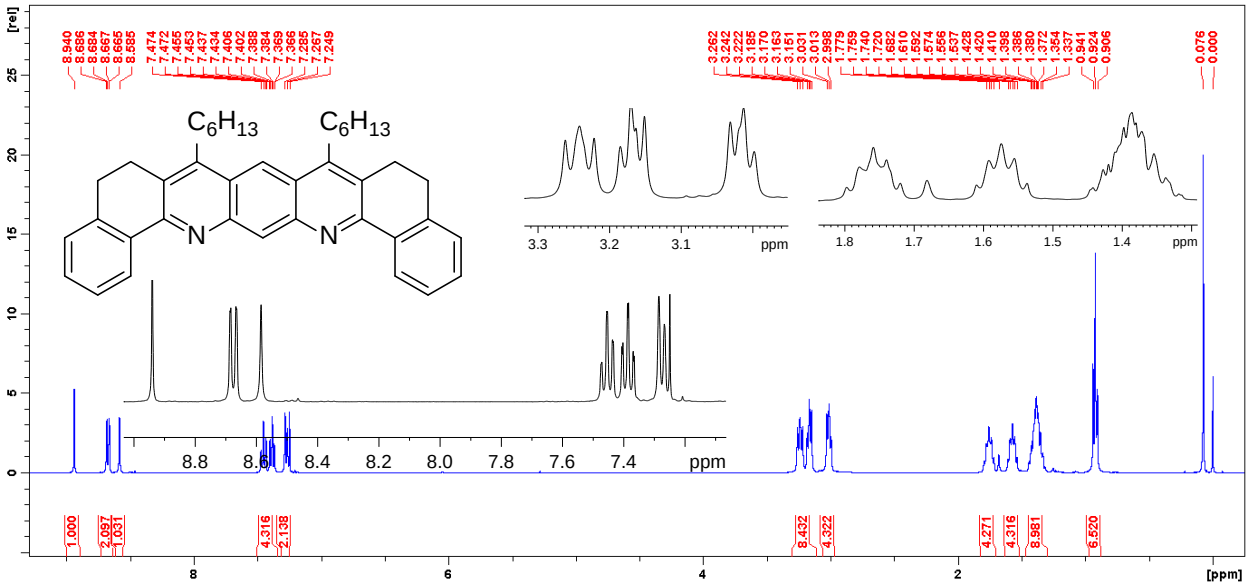
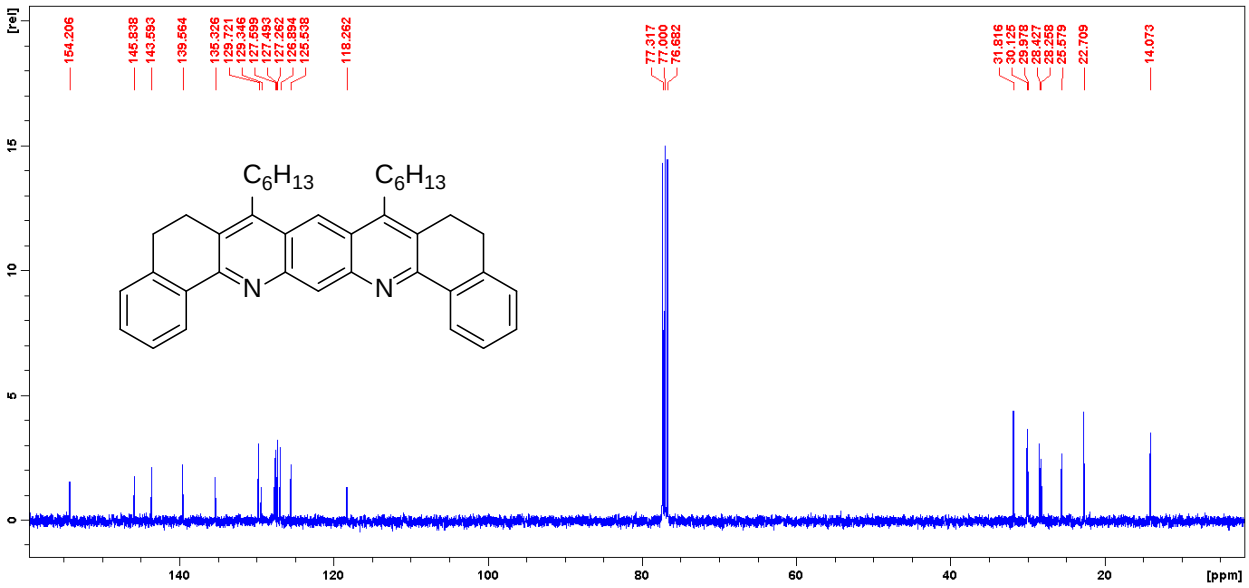

Intens.
x10^4
+MS, 2.50min #149, Background Subtracted
333.2535
334.2566
335.2540
C_6H_{13}
C_6H_{13}
O
O
H_2N
NH_2
m/z

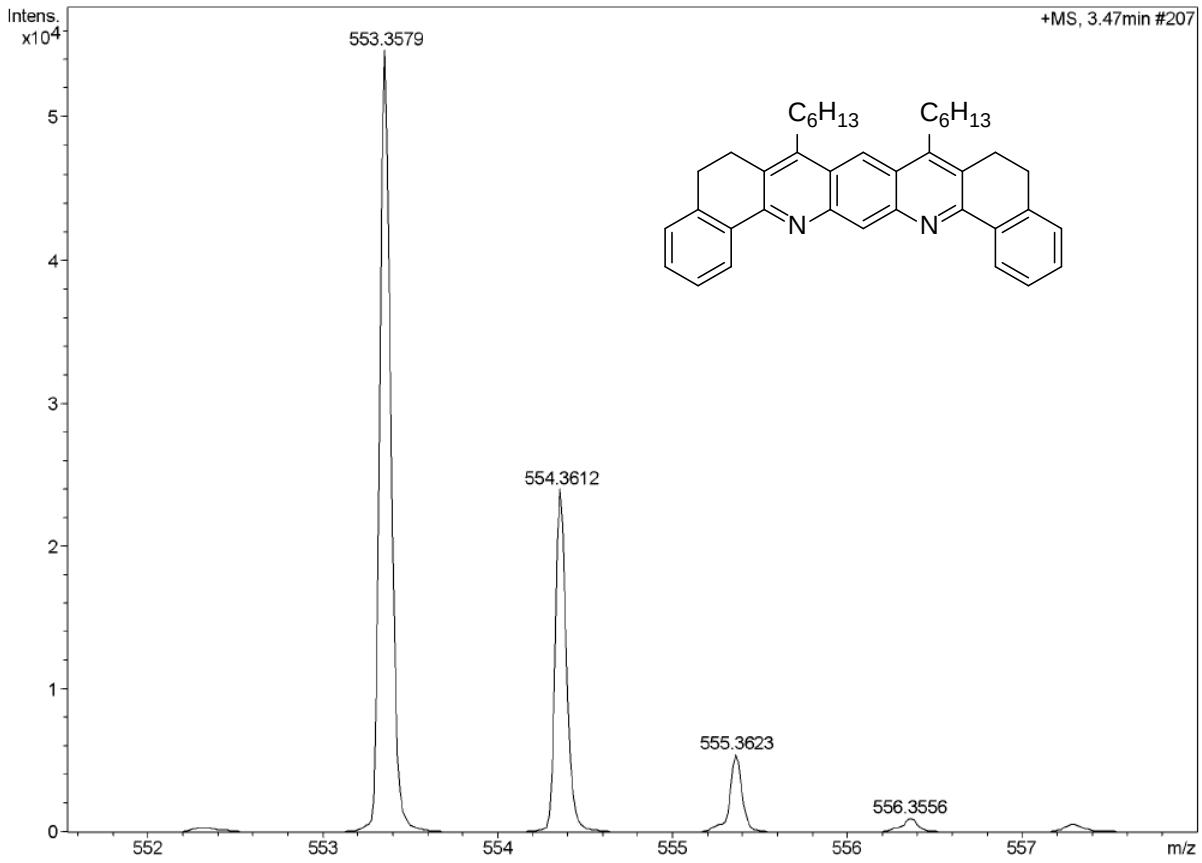

[rel]
8.630
8.554
7.265
3.193
3.178
3.168
3.137
3.115
2.993
2.977
2.962
1.997
1.969
1.961
1.953
1.712
1.706
1.691
1.680
1.672
1.665
1.652
1.611
1.593
1.576
1.557
1.423
1.415
1.403
1.397
1.386
1.379
1.372
1.356
1.340
0.945
0.927
0.909
0.000
C6H13
C6H13
N
N
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
ppm
1.000
1.053
0.549
8.625
4.334
8.787
4.421
4.464
9.166
6.526
8
6
4
2
[ppm]

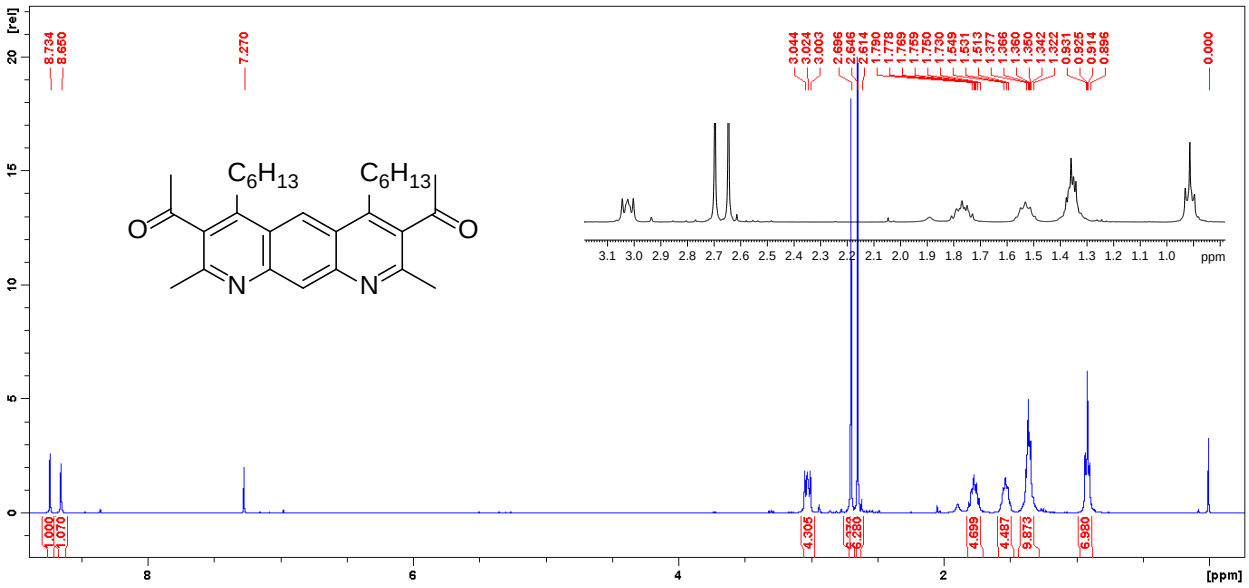

[rel]
161.032
144.877
144.770
127.429
126.858
124.702
117.902
77.319
77.001
76.683
35.057
31.791
30.202
29.614
27.990
26.600
23.247
22.709
14.060
C6H13
C6H13
N
N
160
140
120
100
80
60
40
20
[ppm]

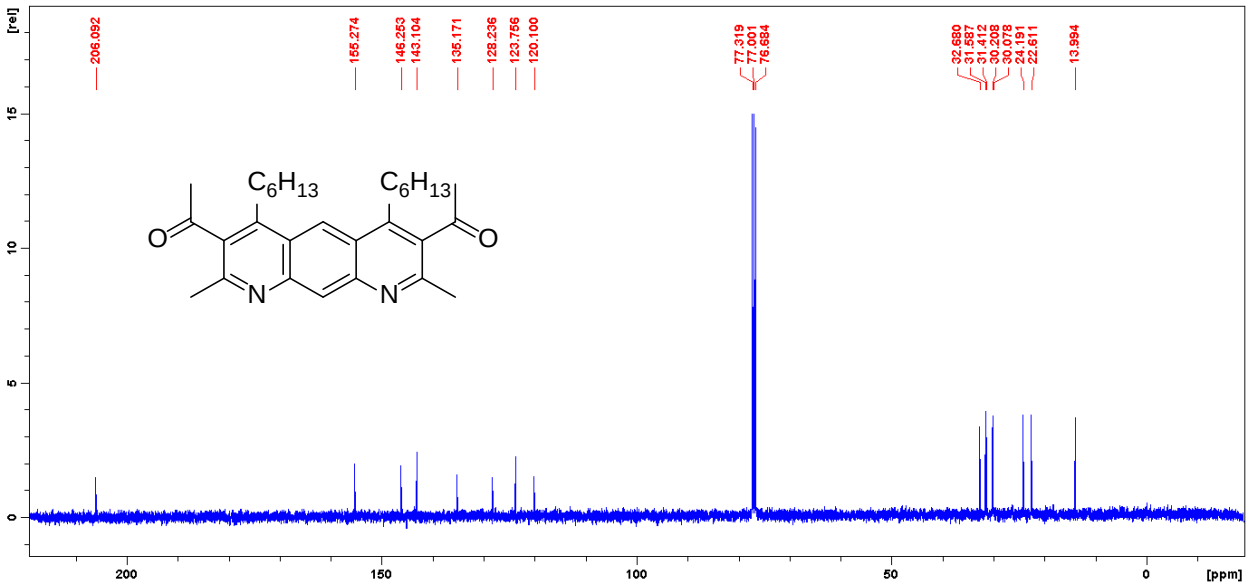

Intens.
x10^5
+MS, 2.36min #141, Background Subtracted
457.3582
458.3611
459.3642
C6H13
C6H13
N
N
0.0
0.2
0.4
0.6
0.8
1.0
455
456
457
458
459
460
461
m/z

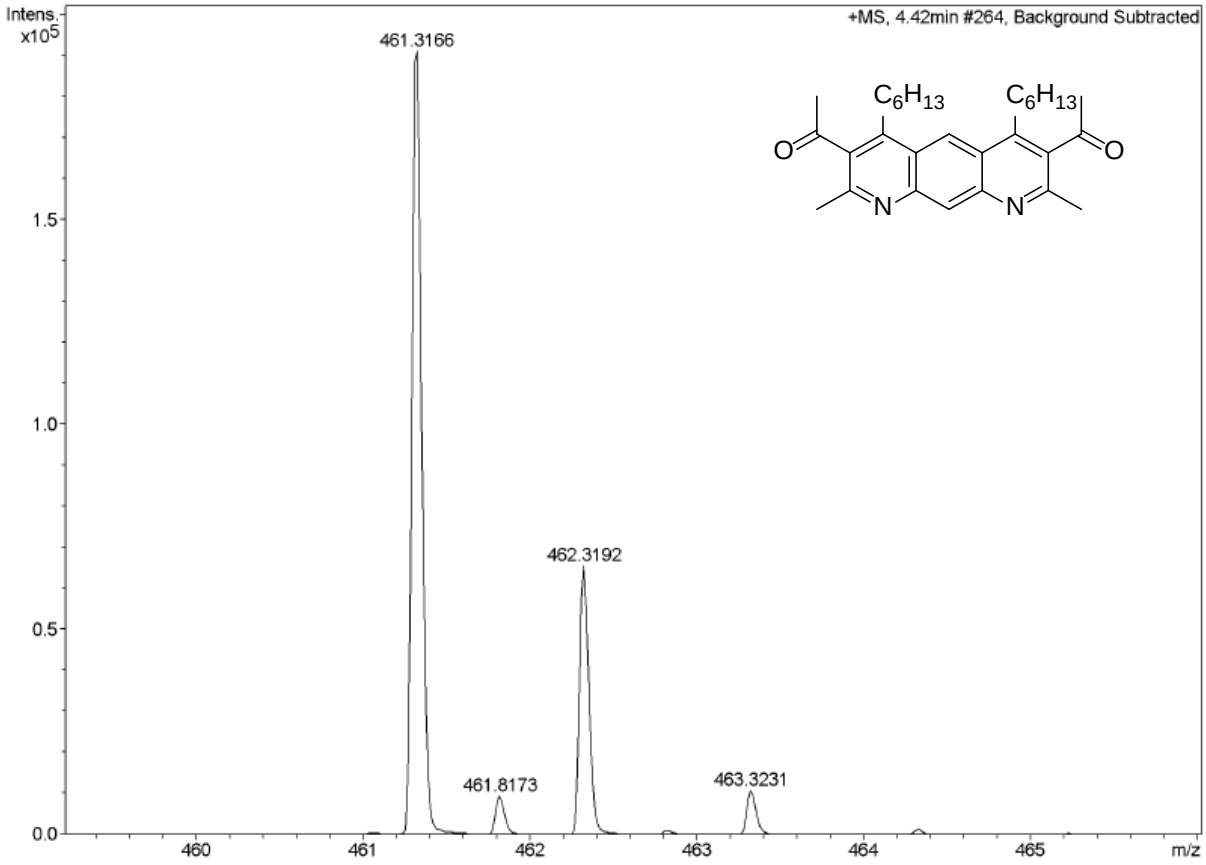

[rel]
C6H13
C6H13
N
N
8.8
8.6
8.4
8.2
8.0
7.8
7.6
7.4
ppm
3.3
3.2
3.1
ppm
1.8
1.7
1.6
1.5
1.4
ppm
[ppm]

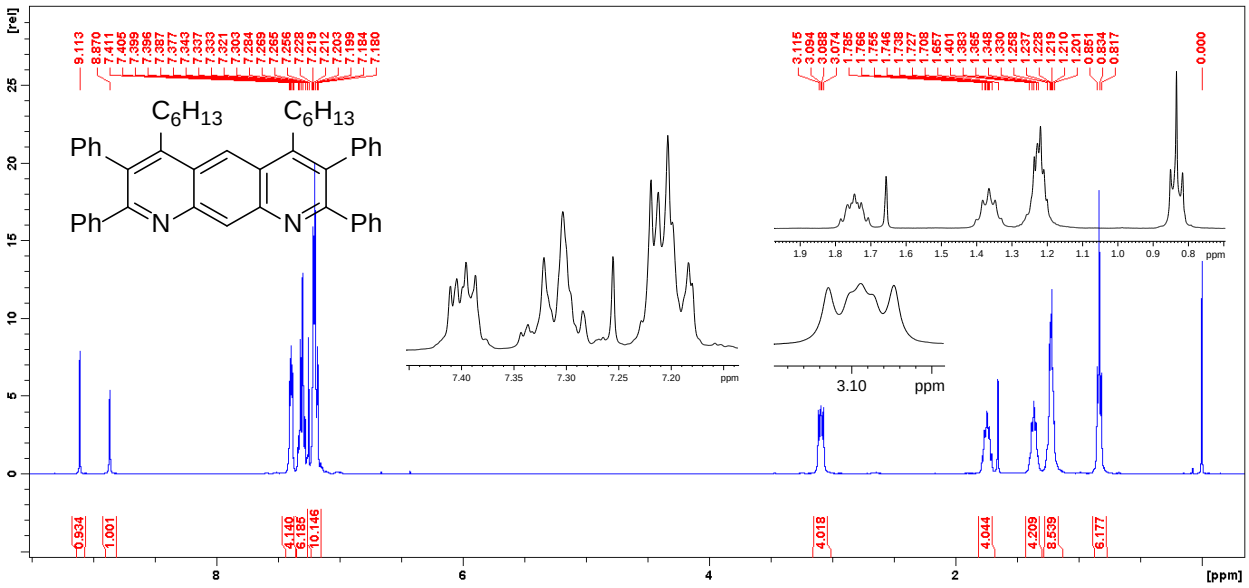

[rel]
154.206
145.838
143.593
139.564
135.326
129.721
129.346
127.596
127.493
127.262
126.894
125.538
118.262
77.317
77.000
76.682
31.816
30.125
29.978
28.427
28.258
25.579
22.709
14.073
C_6H_{13}
C_6H_{13}
N
N
140
120
100
80
60
40
20
[ppm]

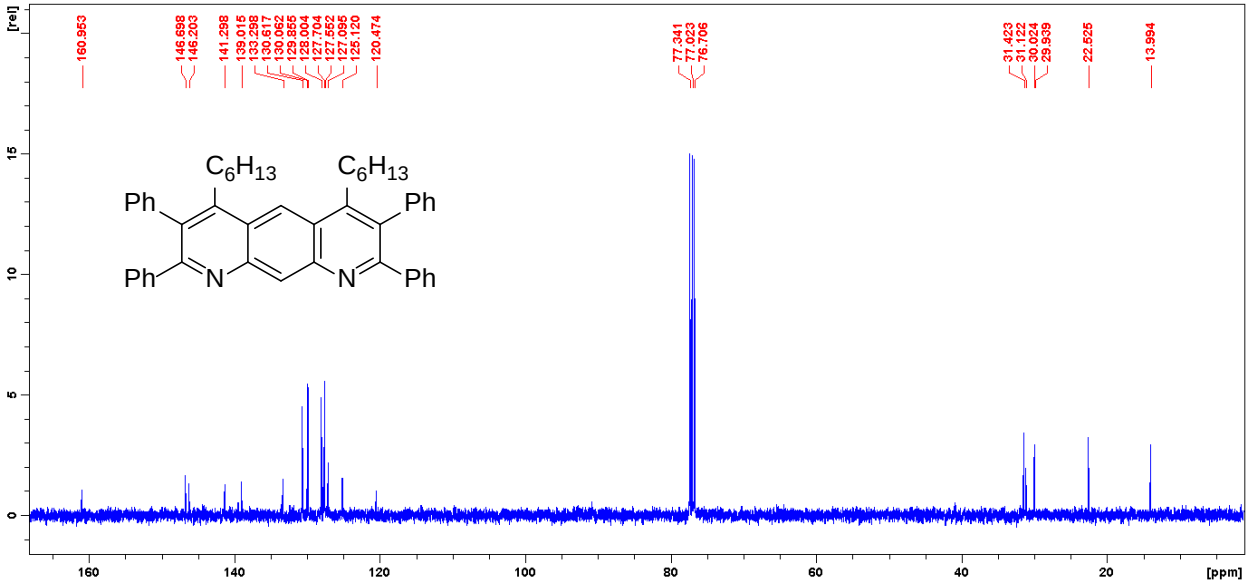

Intens.
x10^4
+MS, 3.47min #207
553.3579
554.3612
555.3623
556.3556
C_6H_{13}
C_6H_{13}
N
N
552
553
554
555
556
557
m/z

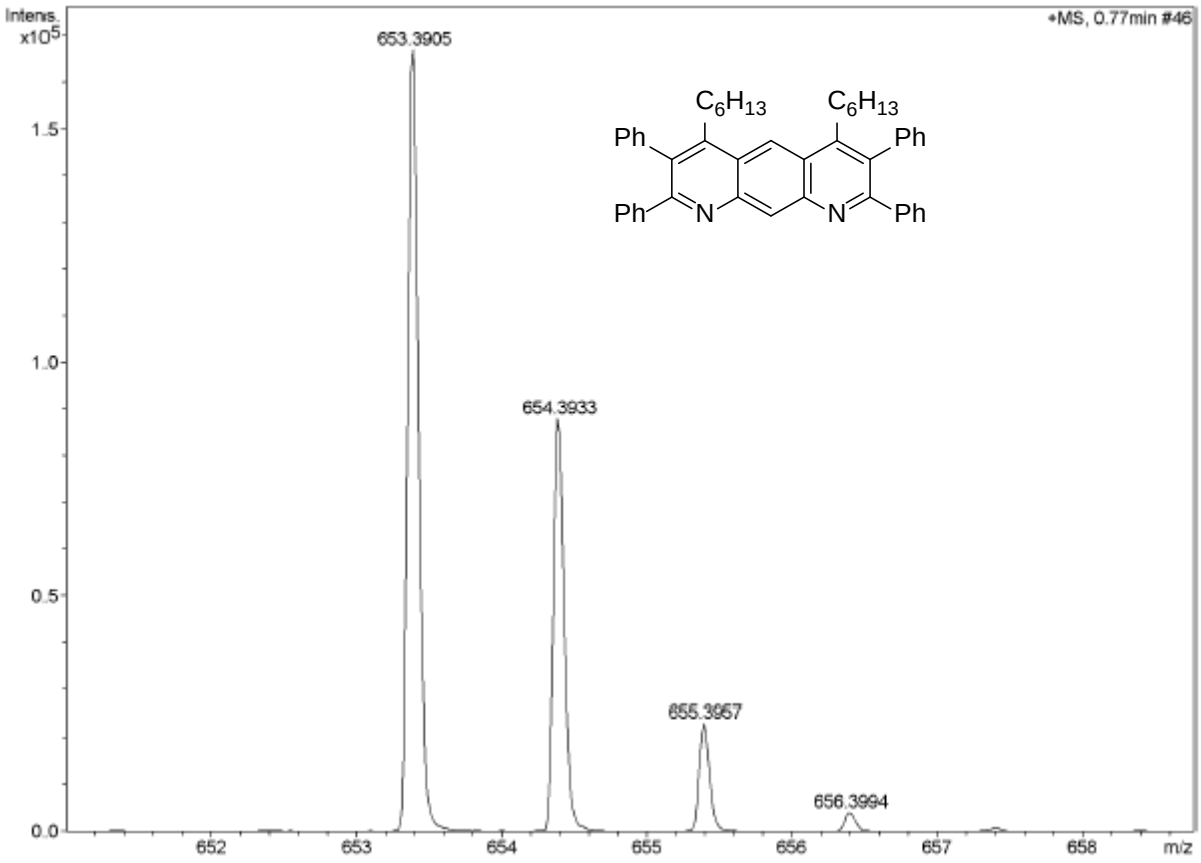

[rel]
8.734
8.650
7.270
3.044
3.024
3.003
2.696
2.646
2.614
1.790
1.778
1.769
1.759
1.750
1.730
1.549
1.531
1.513
1.377
1.366
1.360
1.350
1.342
1.322
0.931
0.925
0.914
0.896
0.000
C_6H_{13}
C_6H_{13}
O
O
N
N
ppm
1.000
1.070
4.305
6.230
6.250
4.699
4.487
9.873
6.980
[ppm]

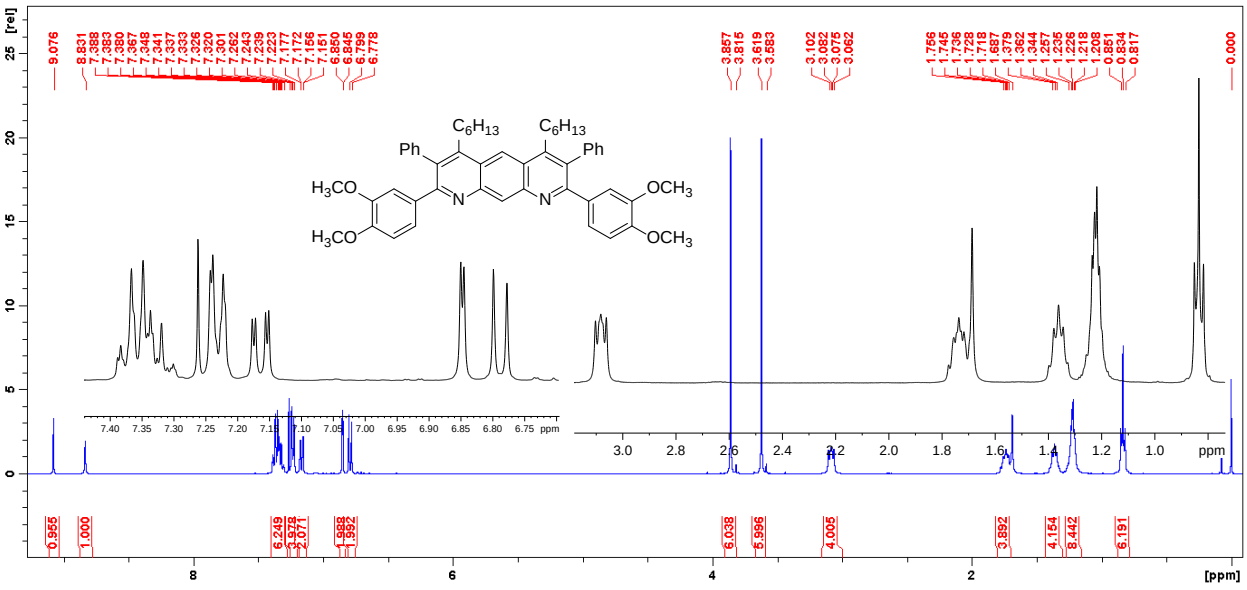

[rel]
206.092
155.274
146.253
143.104
135.171
128.236
123.756
120.100
77.319
77.001
76.684
32.680
31.697
31.412
30.208
30.078
24.191
22.611
13.994
C_6H_{13}
C_6H_{13}
O
O
N
N
[ppm]

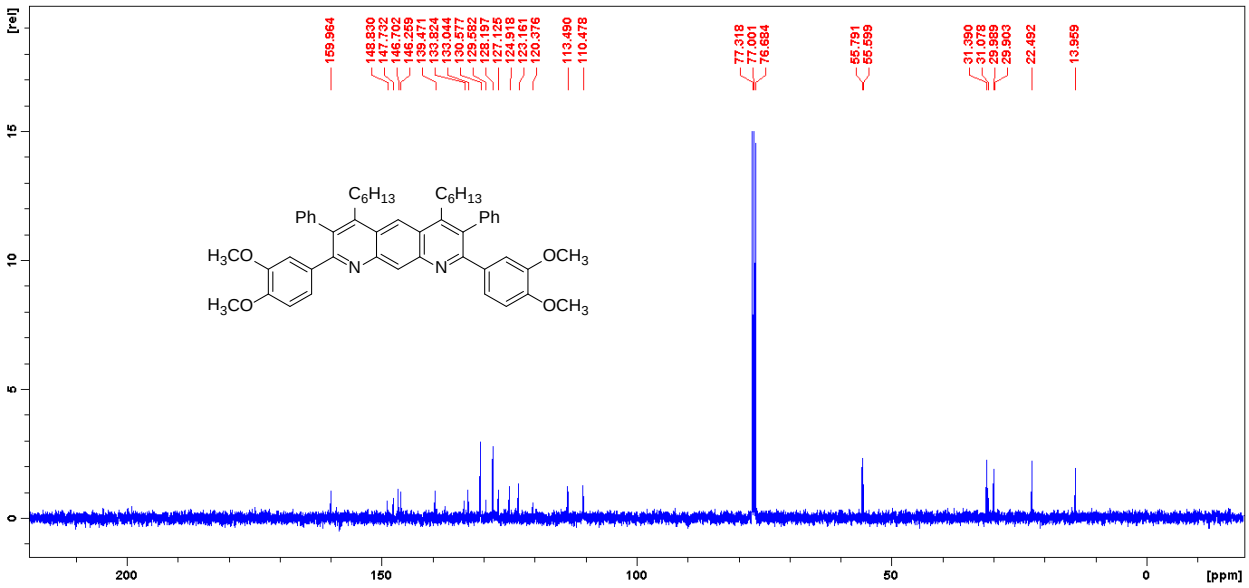

Intens.
x10^5
+MS, 4.42min #264, Background Subtracted
461.3166
462.3192
461.8173
463.3231
C6H13
C6H13
O
O
N
N
1.5
1.0
0.5
0.0
460
461
462
463
464
465
m/z

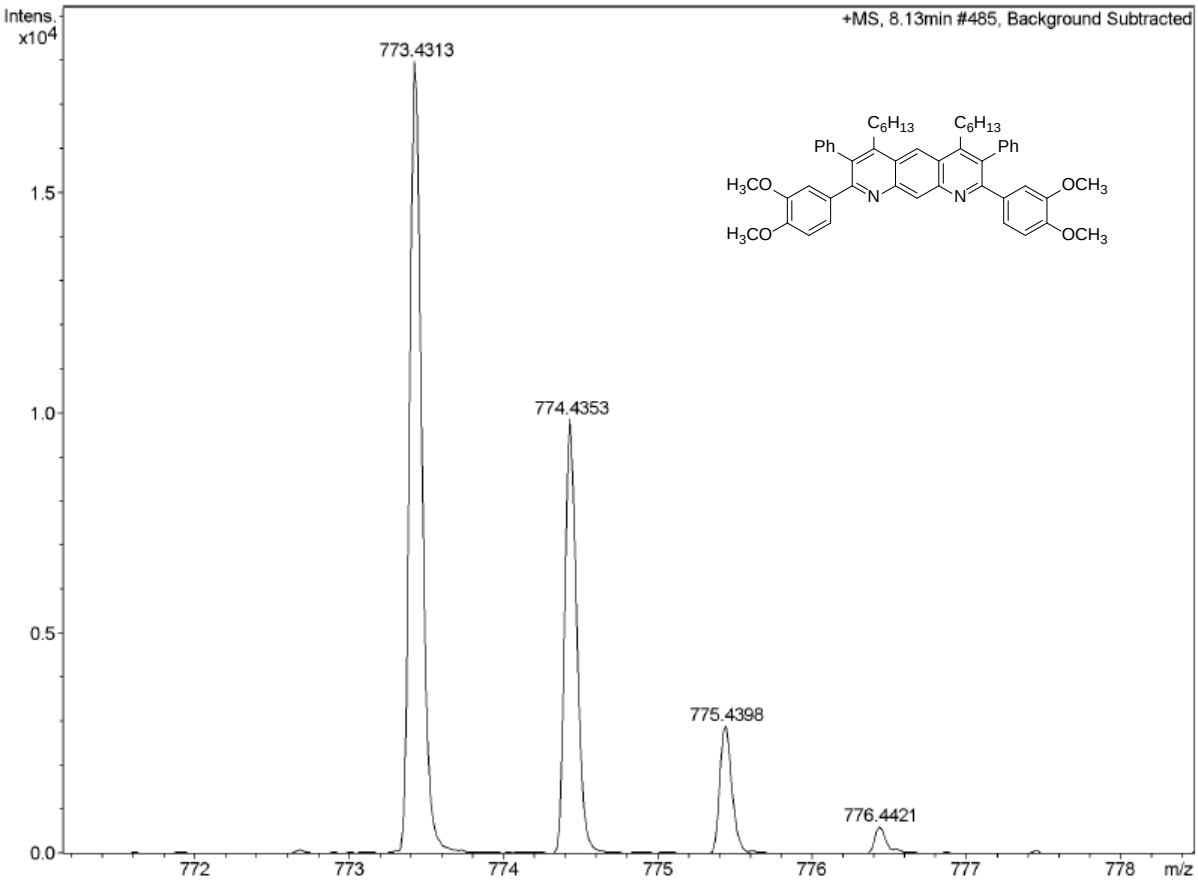

[rel]
9.113
8.870
7.411
7.405
7.399
7.396
7.387
7.377
7.343
7.337
7.333
7.321
7.303
7.284
7.269
7.265
7.256
7.228
7.219
7.212
7.203
7.199
7.184
7.180
3.115
3.094
3.088
3.074
1.785
1.766
1.755
1.746
1.738
1.727
1.708
1.657
1.401
1.383
1.365
1.348
1.330
1.258
1.237
1.228
1.219
1.210
1.201
0.851
0.834
0.817
0.000
C6H13
C6H13
Ph
Ph
Ph
Ph
N
N
7.40
7.35
7.30
7.25
7.20
ppm
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1.0
0.9
0.8
ppm
3.10
ppm
0.934
1.001
4.140
6.185
10.146
4.018
4.044
4.209
8.539
6.177
8
6
4
2
[ppm]

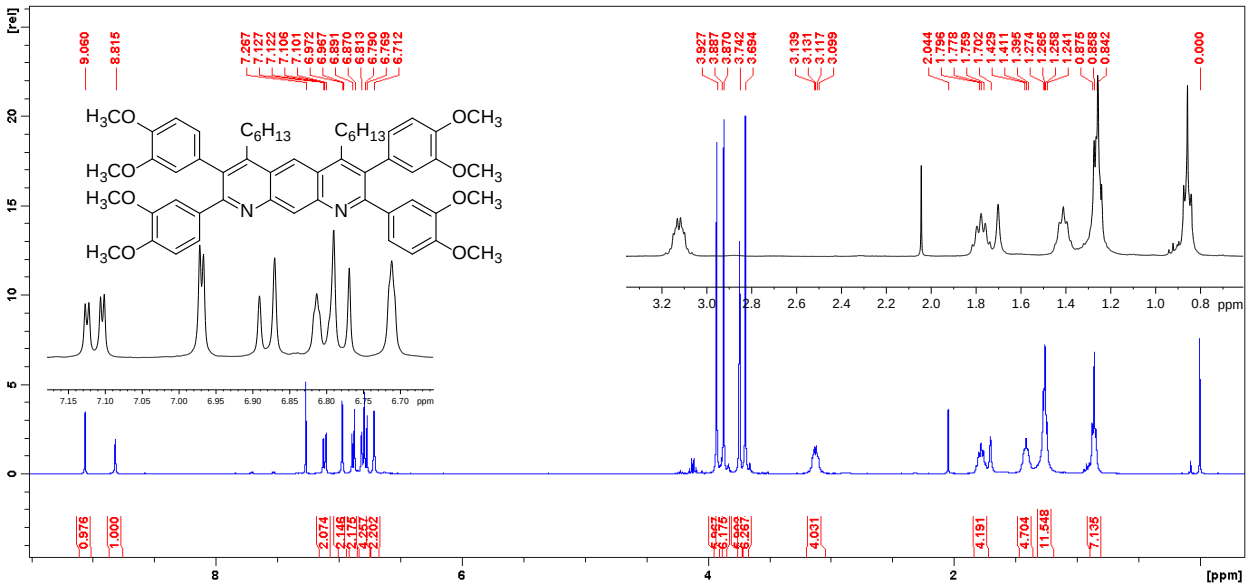

[rel]
160.953
146.698
146.203
141.298
139.015
133.298
130.617
130.062
129.855
128.004
127.704
127.552
127.095
126.120
120.474
77.341
77.023
76.706
31.423
31.122
30.024
29.939
22.525
13.994
C6H13
C6H13
Ph
Ph
Ph
Ph
N
N
160
140
120
100
80
60
40
20
[ppm]

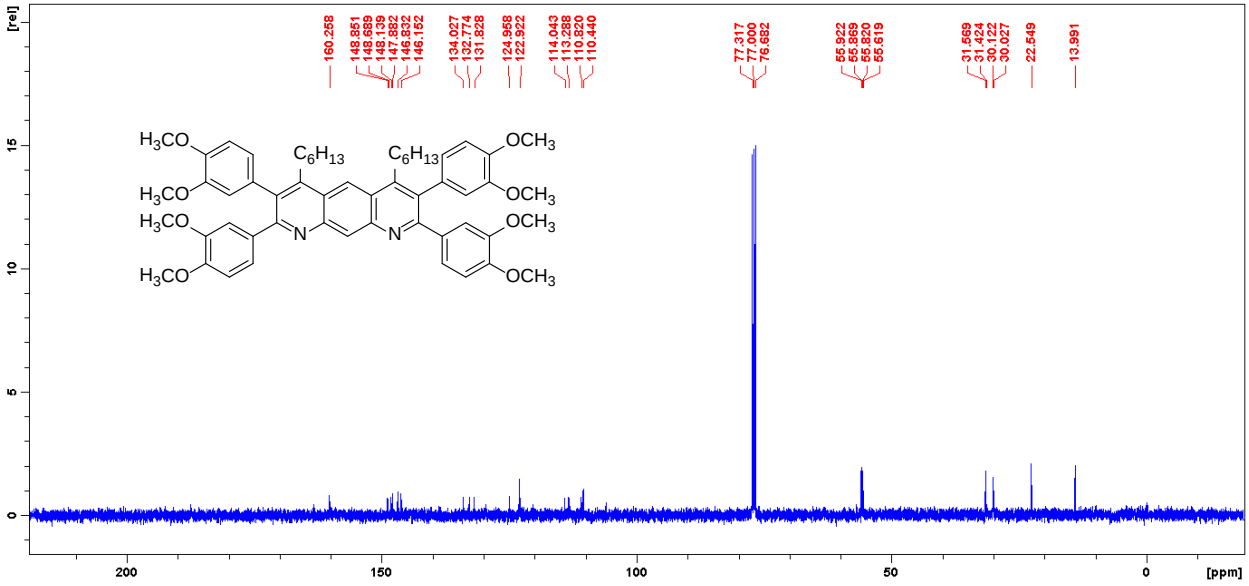

Intens.
x10^5
+MS, 0.77min #46
653.3905
654.3933
655.3967
656.3994
1.5
1.0
0.5
0.0
652
653
654
655
656
657
658
m/z
C6H13
C6H13
Ph
Ph
Ph
Ph
N
N

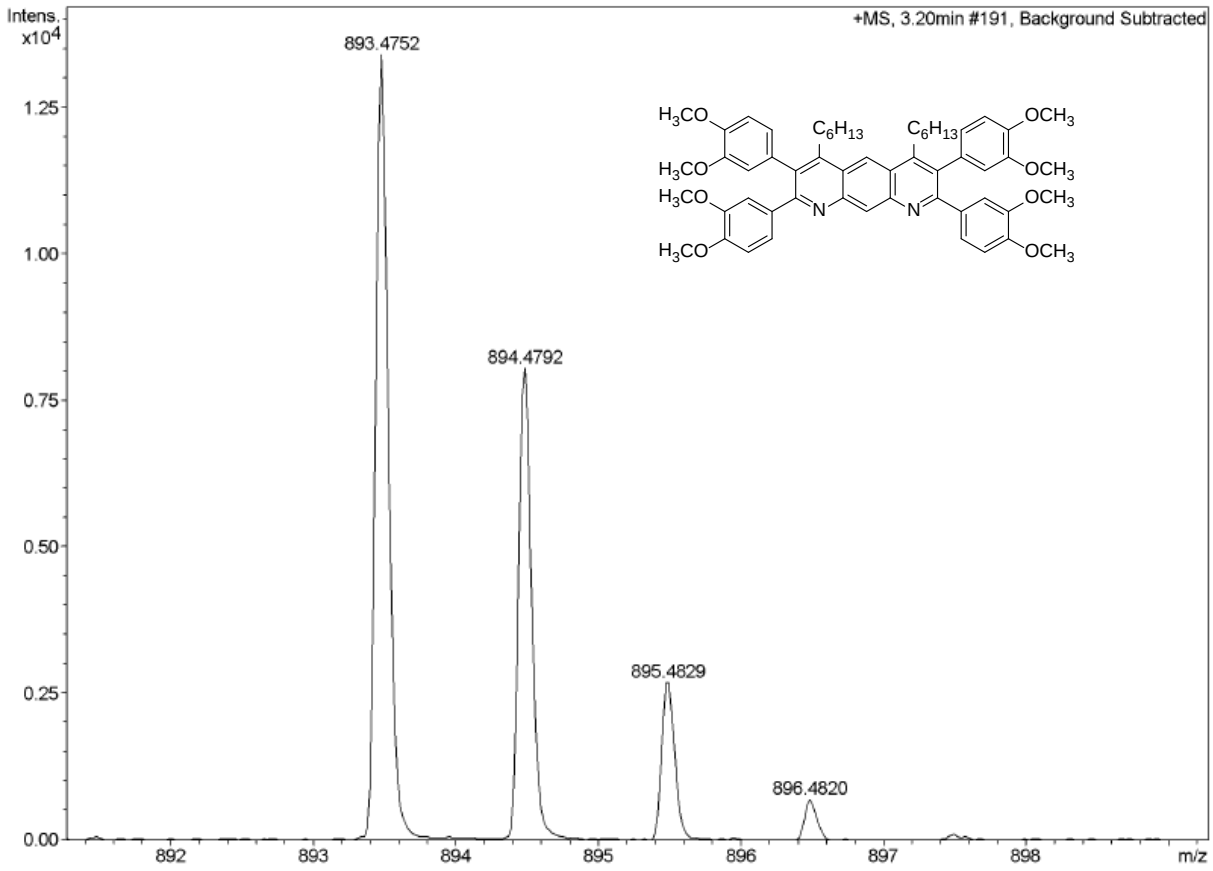

[rel]
25
20
15
10
5
0
9.076
8.831
7.388
7.383
7.380
7.367
7.348
7.341
7.337
7.333
7.326
7.320
7.301
7.262
7.243
7.239
7.223
7.177
7.172
7.166
7.151
6.850
6.845
6.799
6.778
3.857
3.815
3.619
3.583
3.102
3.082
3.075
3.062
1.766
1.745
1.736
1.728
1.718
1.687
1.379
1.362
1.344
1.257
1.235
1.226
1.218
1.208
0.851
0.834
0.817
0.000
C6H13
C6H13
Ph
Ph
H3CO
H3CO
OCH3
OCH3
N
N
7.40 7.35 7.30 7.25 7.20 7.15 7.10 7.05 7.00 6.95 6.90 6.85 6.80 6.75 ppm
3.0 2.8 2.6 2.4 2.2 2.0 1.8 1.6 1.4 1.2 1.0 ppm
0.965
1.000
6.249
3.978
2.071
1.988
1.992
6.038
5.996
4.005
3.892
4.154
8.442
6.191
8
6
4
2
[ppm]

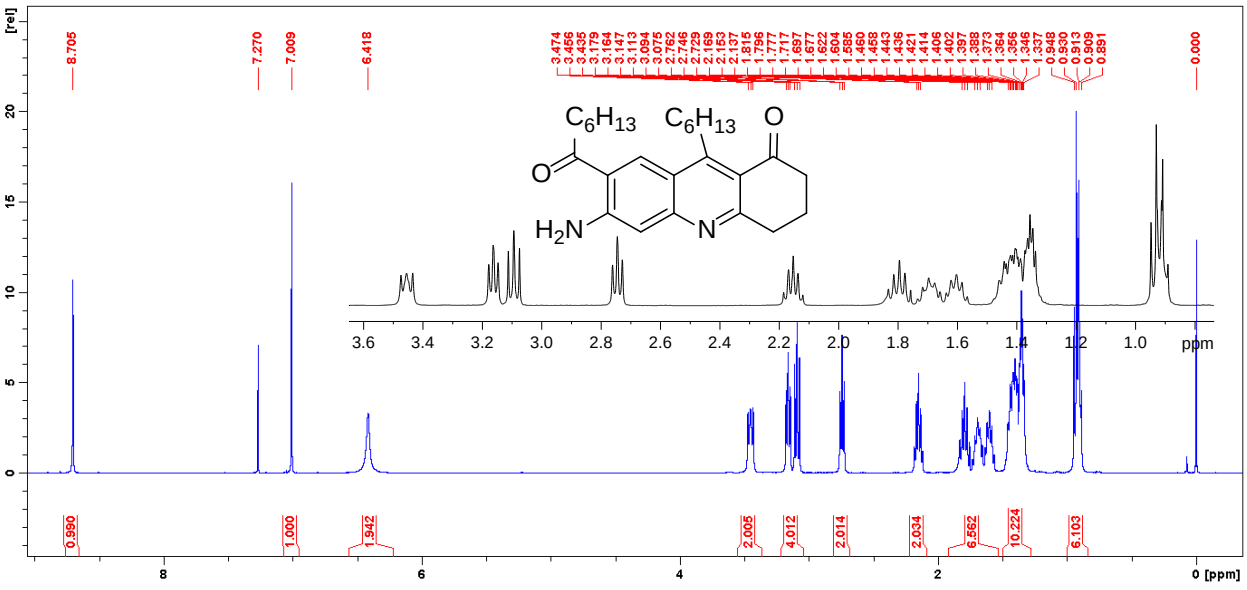

[rel]
159.964
148.830
147.732
146.702
146.259
139.471
133.824
133.044
130.577
129.582
128.197
127.125
124.918
123.191
120.376
113.490
110.478
77.318
77.001
76.684
55.791
55.599
31.390
31.078
29.989
29.903
22.492
13.959
C_6H_{13}
C_6H_{13}
Ph
Ph
H_3CO
H_3CO
OCH_3
OCH_3
N
N
200
150
100
50
0
[ppm]

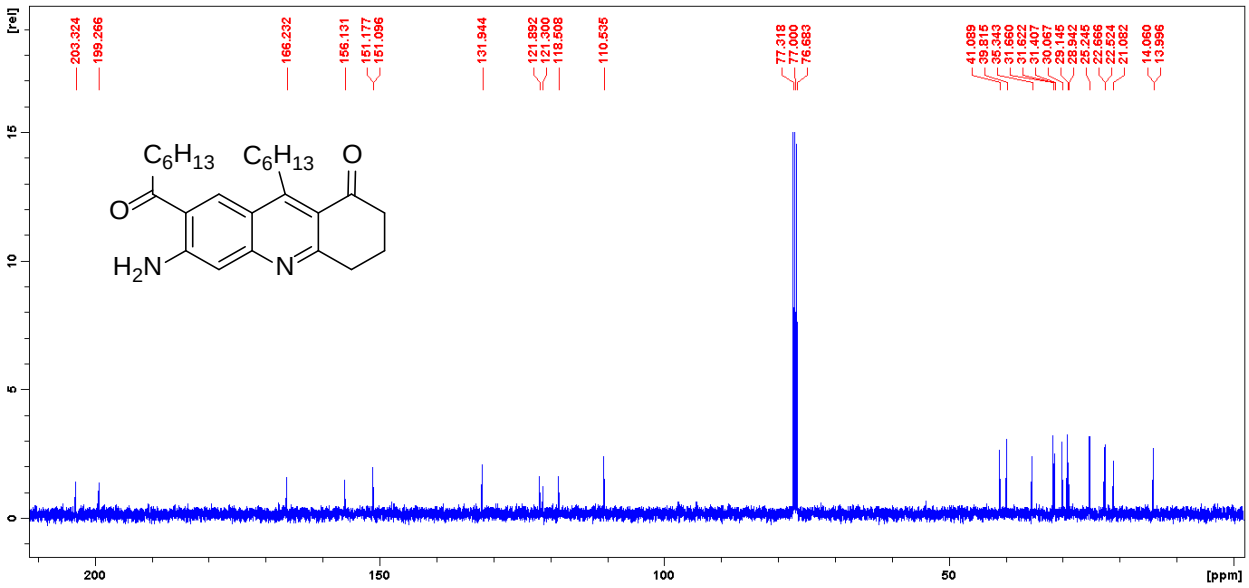

Intens.
x10^4
+MS, 8.13min #485, Background Subtracted
773.4313
774.4353
775.4398
776.4421
C_6H_{13}
C_6H_{13}
Ph
Ph
H_3CO
H_3CO
OCH_3
OCH_3
N
N
m/z

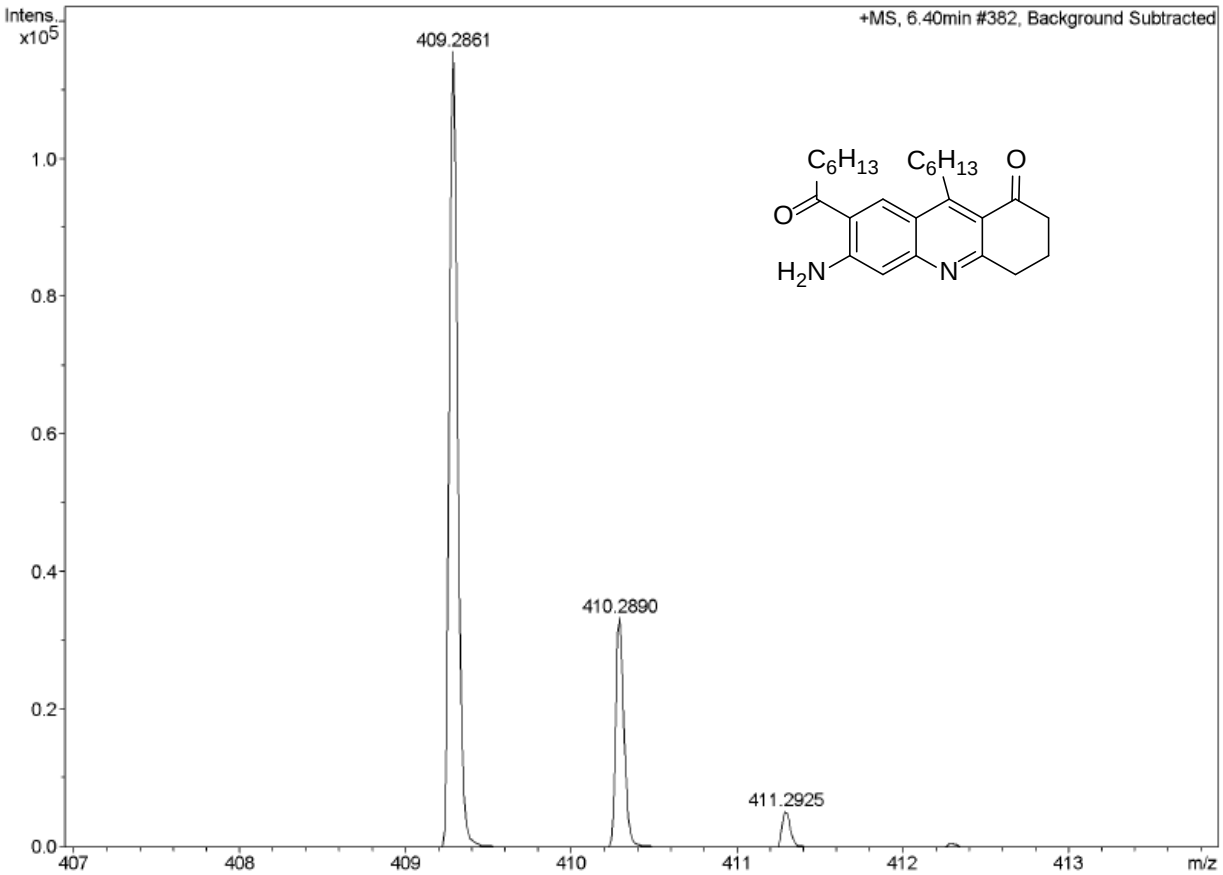

[rel]
9.060
8.815
7.267
7.127
7.122
7.106
7.101
6.972
6.967
6.891
6.870
6.813
6.790
6.769
6.712
3.927
3.887
3.870
3.742
3.694
3.139
3.131
3.117
3.099
2.044
1.796
1.778
1.759
1.702
1.429
1.411
1.395
1.274
1.265
1.258
1.241
0.875
0.858
0.842
0.000
H_3CO
C_6H_{13}
OCH_3
N
0.976
1.000
2.074
2.146
2.115
4.247
2.202
4.031
4.191
4.704
11.548
7.135
[ppm]

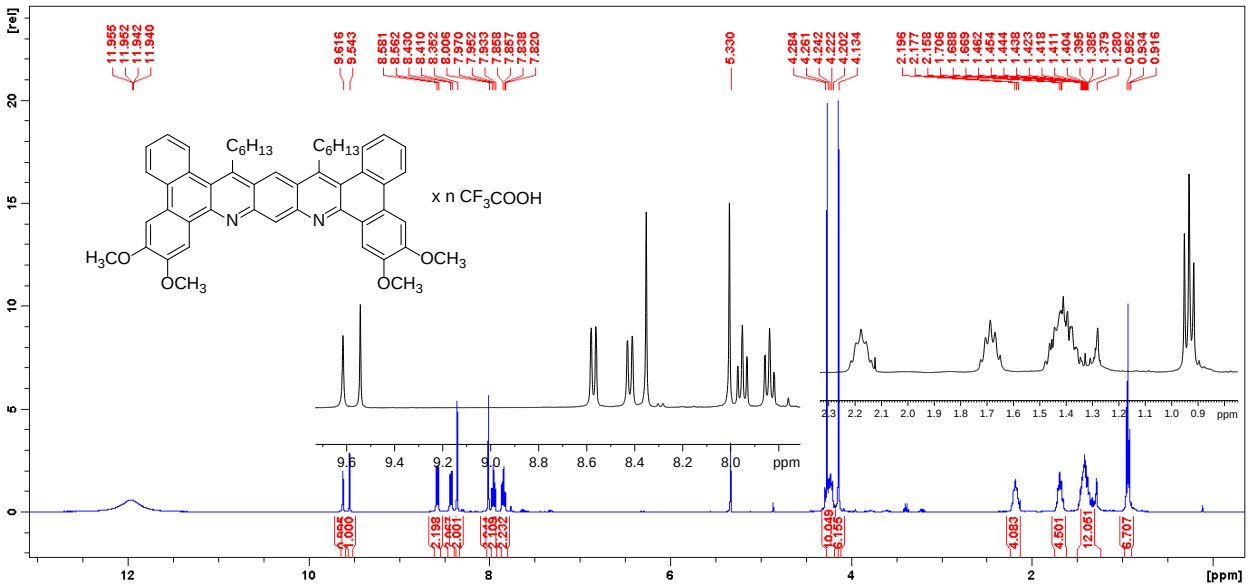

[rel]
160.268
148.851
148.639
148.139
147.882
146.832
146.152
134.027
132.774
131.828
124.958
122.922
114.043
113.288
110.320
110.440
77.317
77.000
76.682
55.922
55.889
55.820
55.619
31.569
31.424
30.122
30.027
22.549
13.991
H_3CO
C_6H_{13}
OCH_3
N
[ppm]

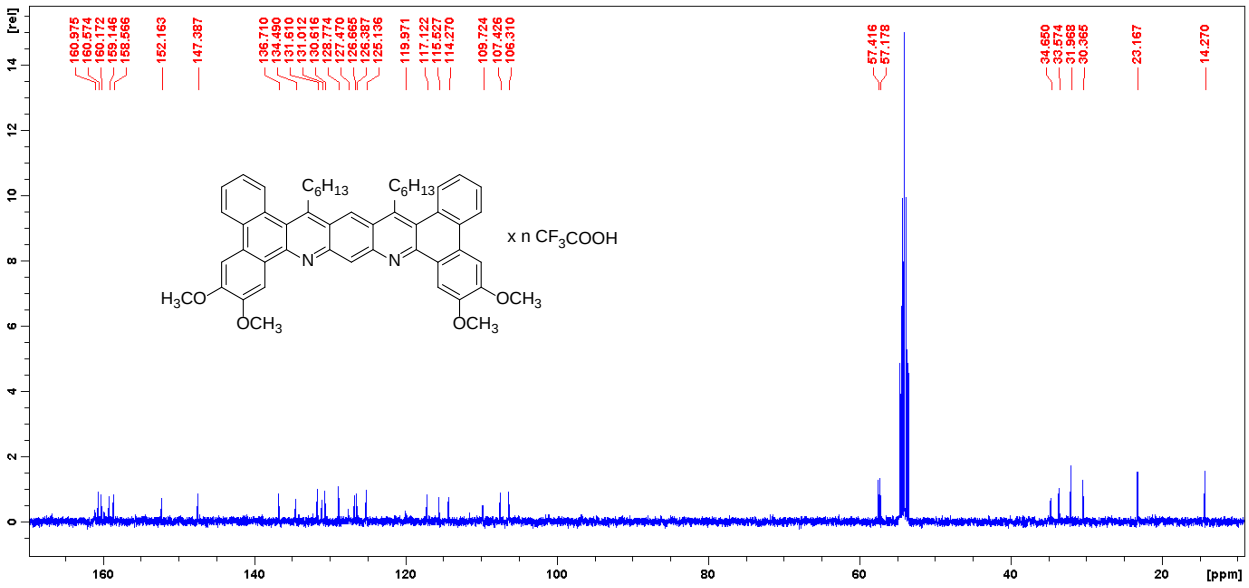

Intens.
x10^4
+MS, 3.20min #191, Background Subtracted
893.4752
894.4792
895.4829
896.4820
1.25
1.00
0.75
0.50
0.25
0.00
892
893
894
895
896
897
898
m/z
H3CO
OCH3
C6H13
N

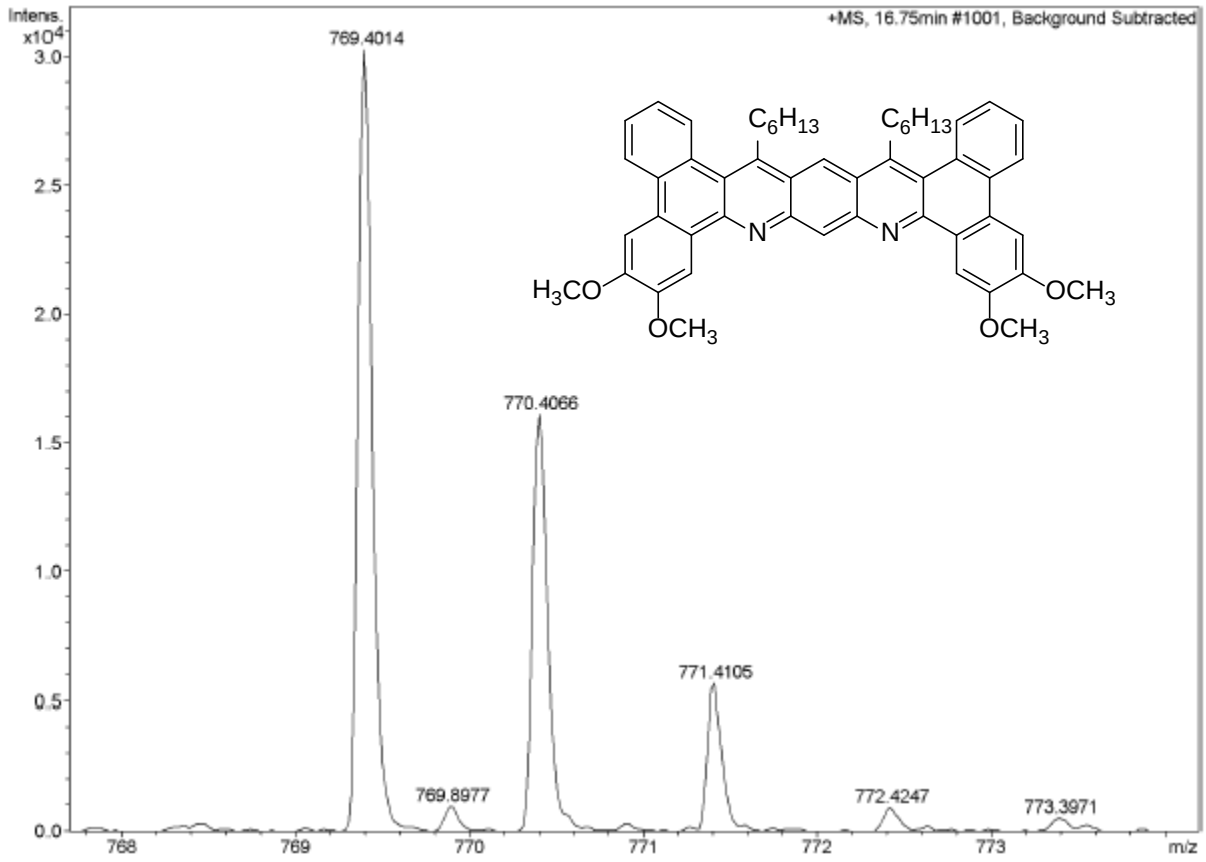

[rel]
8.705
7.270
7.009
6.418
0.000
C6H13
O
H2N
N
3.6
3.4
3.2
3.0
2.8
2.6
2.4
2.2
2.0
1.8
1.6
1.4
1.2
1.0
ppm
0.990
1.000
1.942
2.005
4.012
2.014
2.034
6.562
10.224
6.103
8
6
4
2
0 [ppm]

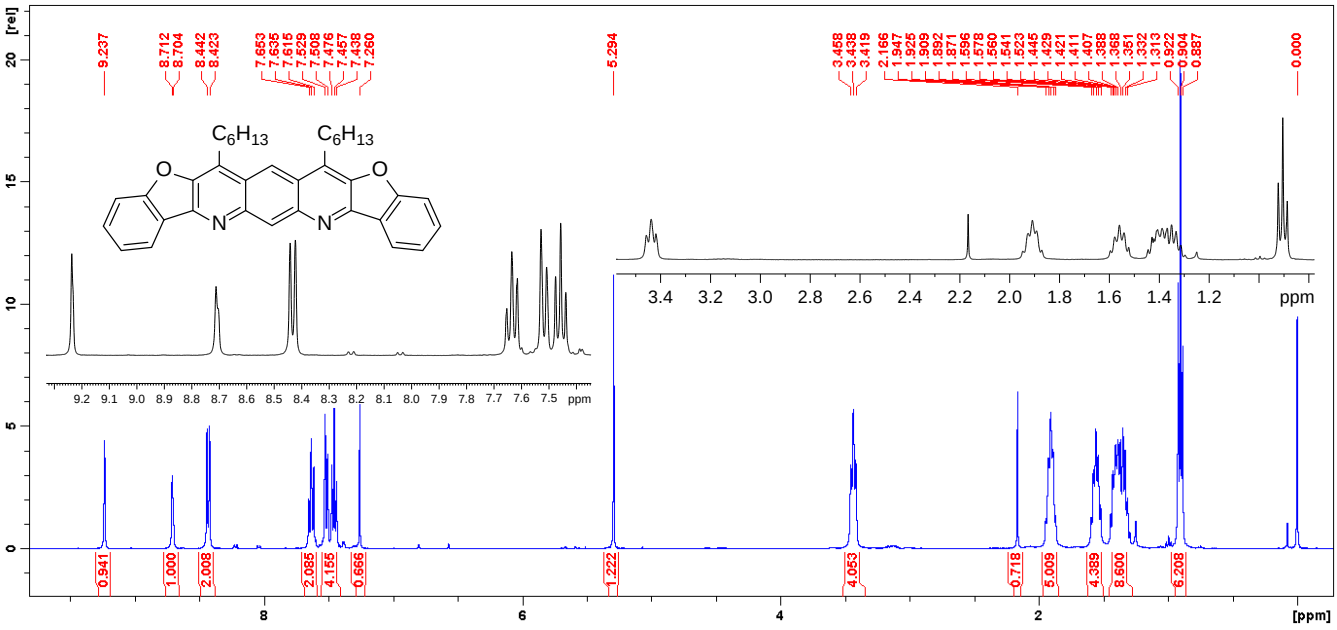

[rel]
203.324
199.266
166.232
156.131
151.177
151.096
131.944
121.892
121.300
118.508
110.535
77.318
77.000
76.683
41.089
39.815
35.343
31.650
31.622
31.407
30.067
29.145
28.942
25.245
22.686
22.524
21.052
14.060
13.996
C_6H_{13}
C_6H_{13}
O
O
H_2N
N
200
150
100
50
[ppm]

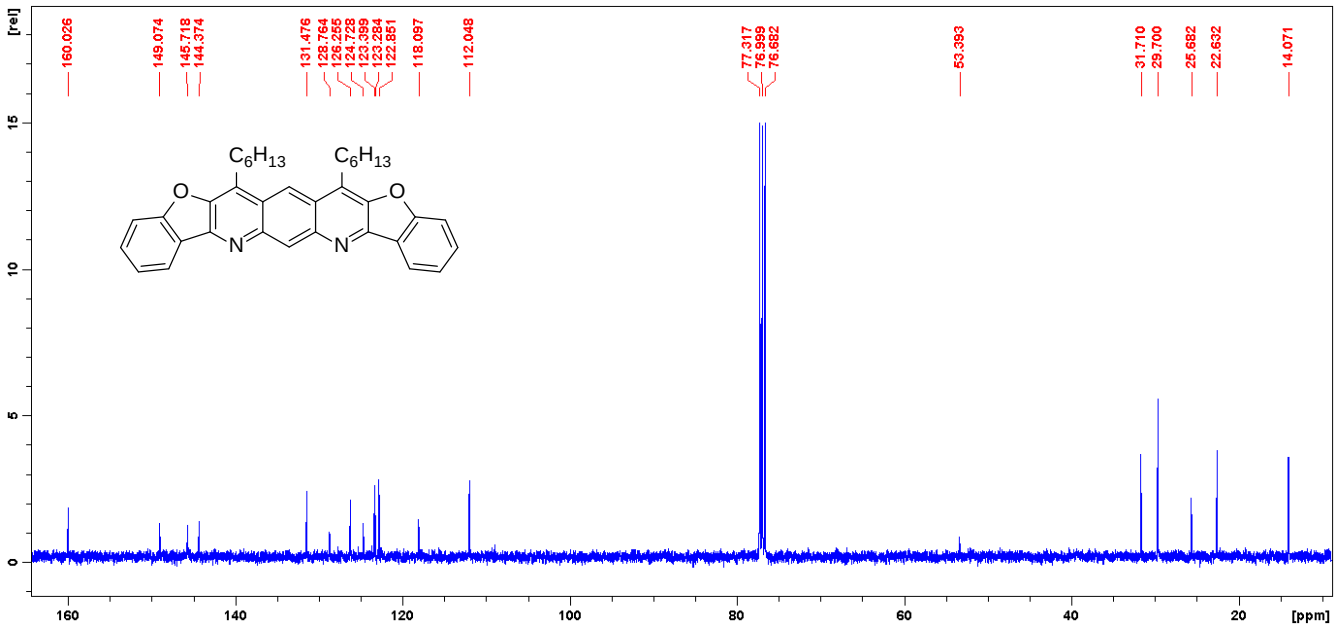

Intens.
x10^5
+MS, 6.40min #382, Background Subtracted
409.2861
410.2890
411.2925
C_6H_{13}
C_6H_{13}
O
O
H_2N
N
m/z

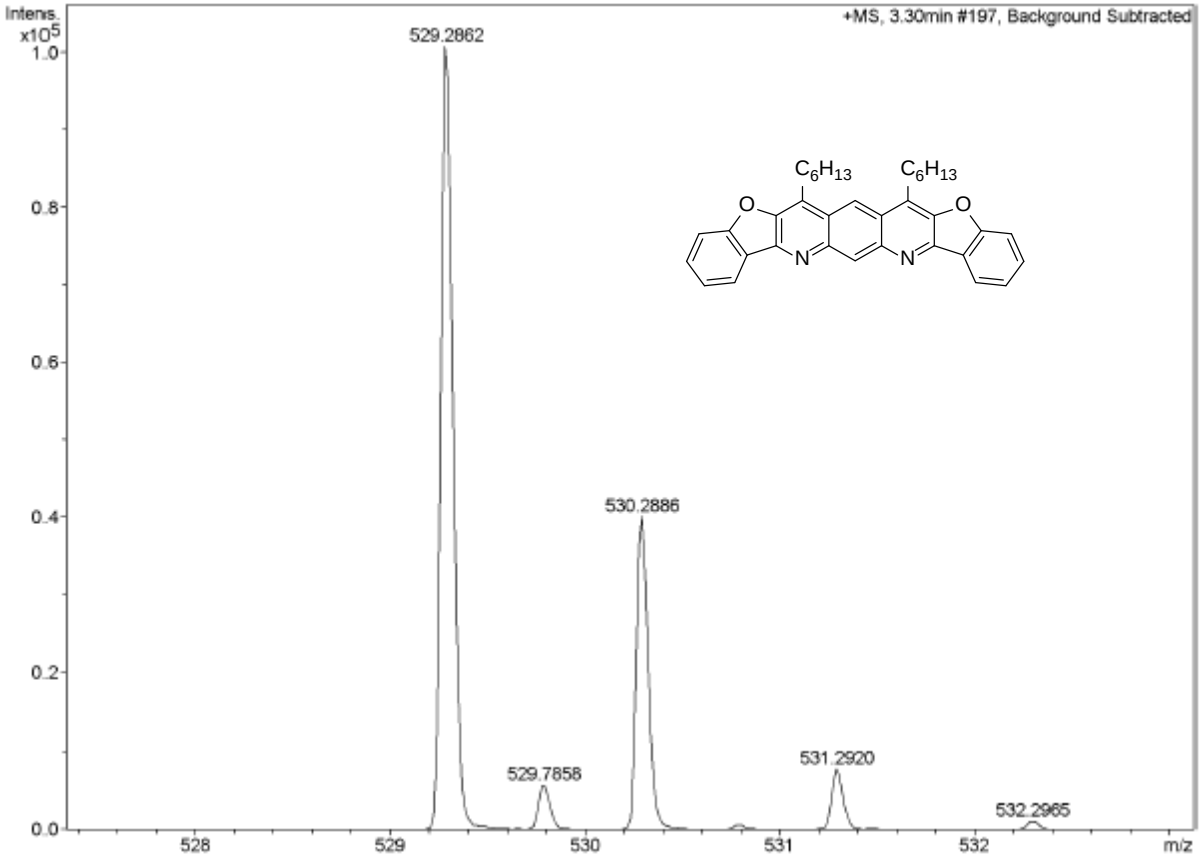

[rel]
11.955
11.952
11.942
11.940
9.616
9.543
8.581
8.562
8.430
8.410
8.352
8.006
7.970
7.962
7.933
7.858
7.857
7.838
7.820
5.330
4.284
4.261
4.242
4.222
4.202
4.134
2.196
2.177
2.155
1.706
1.688
1.669
1.462
1.454
1.444
1.438
1.423
1.418
1.411
1.401
1.395
1.385
1.379
1.280
0.952
0.934
0.916
C6H13
C6H13
x n CF3COOH
H3CO
OCH3
OCH3
OCH3
ppm
[ppm]

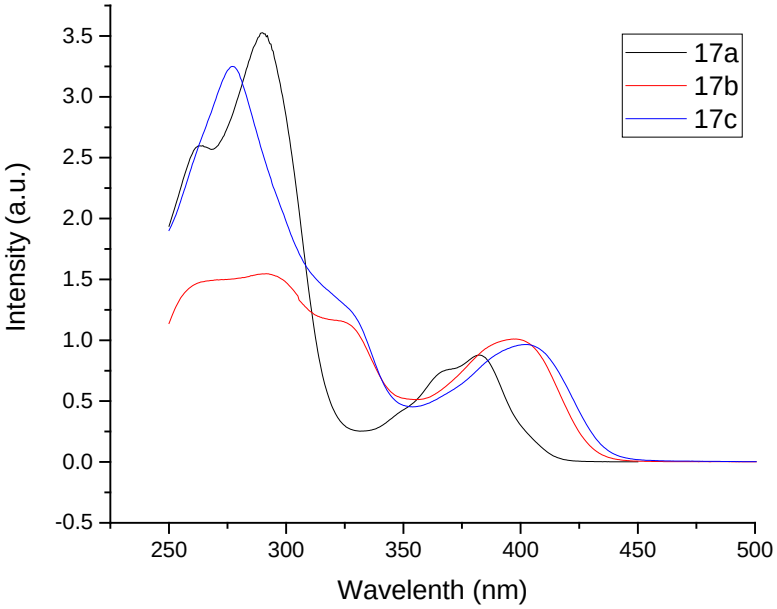

[rel]
160.875
160.574
160.172
159.146
158.866
152.163
147.387
136.710
134.490
131.610
131.012
130.616
128.774
127.870
126.669
126.387
125.136
119.971
117.122
115.527
114.270
109.724
107.426
106.310
57.416
57.178
34.650
33.574
31.968
30.385
23.167
14.270
C6H13
C6H13
x n CF3COOH
H3CO
OCH3
OCH3
OCH3
[ppm]

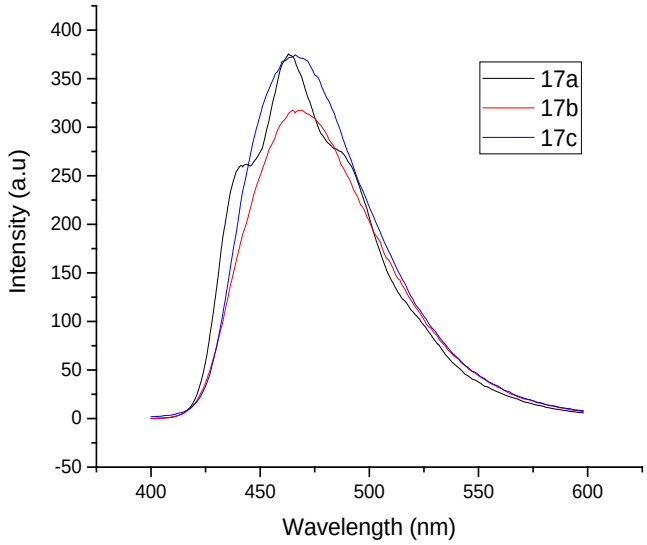

Intens.
x10^4
+MS, 16.75min #1001, Background Subtracted
769.4014
770.4066
771.4105
769.8977
772.4247
773.3971
m/z
C6H13
C6H13
H3CO
OCH3
OCH3
OCH3
N
N


[rel]
ppm
[ppm]
C6H13
C6H13
O
O
N
N


[rel]
160.026
149.074
145.718
144.374
131.476
128.764
126.255
124.728
123.399
123.284
122.851
118.097
112.048
77.317
76.999
76.682
53.393
31.710
29.700
25.682
22.632
14.071
C_6H_{13}
C_6H_{13}
O
O
N
N
15
10
5
0
160
140
120
100
80
60
40
20
[ppm]


Intens.
x10^5
+MS, 3.30min #197, Background Subtracted
529.2862
530.2886
529.7858
531.2920
532.2965
C_6H_{13}
C_6H_{13}
O
O
N
N
1.0
0.8
0.6
0.4
0.2
0.0
528
529
530
531
532
m/z





UV Vis (top) and photoluminescence (bottom) spectra of 17a-c (5 x 10^{-5} M in chloroform)