Facile synthesis of Triphenylenes and Triphenylene/Phenanthrene fused heteroaromatics

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Supporting Information

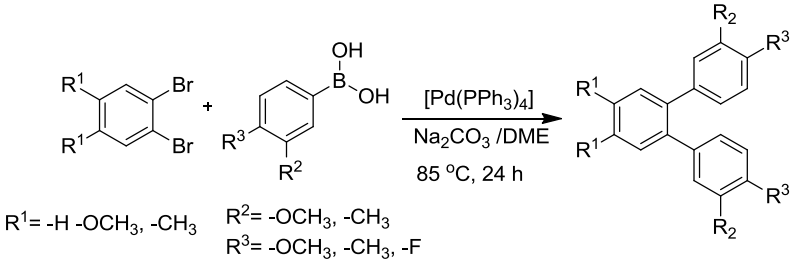
Contents

1. **General Information**. NMR instrument (300 MHz) was used to record ^{1}H and ^{13}C NMR spectra in deuterated solvents with residual protonated solvent signals as an internal reference. ^{1}H NMR's data is reported as follows: chemical shift (δ, ppm), multiplicity (s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet), integration, coupling constant (Hz). ^{13}C NMR's data is recorded in terms of chemical shift (δ, ppm). FT-IR Spectrometer was used to record infrared spectra and are reported in frequency of absorption. MS-TOF mass spectrometer and ESI mass spectrometer were used to record low resolution and high-resolution mass spectra. Column chromatographic separations were carried out on silica gel (100–200 mesh). Cerium(IV) ammonium nitrate was purchased from Sigma-Aldrich and used without further purification. In all reaction, dry solvents were used. All starting materials were prepared according to the known literature procedure.

2. Preparation and Characterization Data of Scholl Precursors

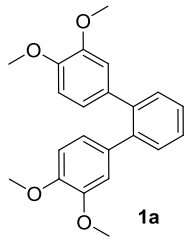
2.1 Preparation of *o*-terphenyls derivatives

Various *o*-terphenyls derivatives (**1a-i**) were prepared by very well-known Suzuki-Miyaura coupling reaction.[1]



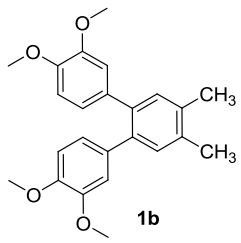
1,2-dibromobenzene (0.5 g, 2.12 mmol), 3,4-dimethoxyphenylboronic acid (1.2 g, 6.36 mmol) and $Pd(PPh_3)_4$ (11 mg) were taken in 20 mL DME. To this, solution of Na_2CO_3 (1.5 g) in water (4 ml) was added. The resulting suspension was degassed and heated at 85 ^oC for 24 h under N_2 atmosphere. After that, the reaction mixture was cooled to room temperature, to this water was added and the compound was extracted with ethylacetate, dried over Na_2SO_4. The solvent was concentrated under reduced pressure and compound was purified by column chromatography on silica gel with EtOAc and hexane (2:8) as eluent to afford compound *o*-terrphenyl **1a** as white solid, yield 667 mg (90%).

3,3",4,4"-tetramethoxy-*o*-terphenyl (1a).



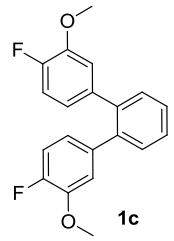
Compound **1a** was synthesized according to the reported procedure.[1] ^1H NMR matching to the reported literature.[2]

3,3",4,4"-tetramethoxy-4',5',-dimethyl-1,1,2,1"-terphenyl (1b).



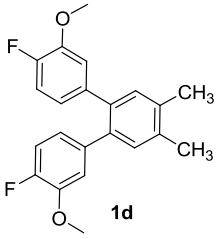
Compound **1b** was synthesized according to the reported procedure.[1] ^1H NMR matching to the reported literature.[2]

4,4''-difluoro-3,3''-dimethoxy-1,1':2',1''-terphenyl (1c).



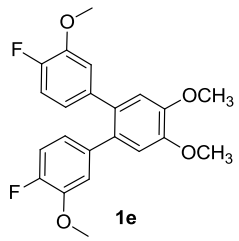
White solid, yield 621 mg, 90%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.43 (s, 4H), 6.99 (dd, *J* = 11.1, 8.4 Hz, 2H), 6.77-6.73 (m, 2H), 6.65 (d, *J* = 8.3 Hz, 2H), 3.63 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 151.5 (d, *J* = 246.0 Hz), 147.0 (d, *J* = 10.8 Hz), 139.8, 137.8 (d, *J* = 4.0 Hz), 130.5, 127.9, 122.0 (d, *J* = 6.7 Hz), 115.73 (d, *J* = 18.3 Hz), 115.4, 56.1. GC-MS (m/z): 326.2 [M+].

4,4''-difluoro-3,3''-dimethoxy-4',5'-dimethyl-1,1':2',1''-terphenyl (1d).



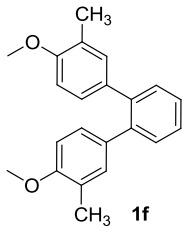
White solid, yield 603 mg, 90 %. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.23 (s, 2H), 6.98 (dd, *J* = 11.2, 8.3 Hz, 2H), 6.77 – 6.72 (m, 2H), 6.66 (dd, *J* = 8.3, 1.5 Hz, 2H), 3.64 (s, 6H), 2.37 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 151.4 (d, *J* = 245.6 Hz), 146.9 (d, *J* = 10.8 Hz), 137.8 (d, *J* = 3.9 Hz), 137.2, 136.4, 131.7, 121.9 (d, *J* = 6.6 Hz), 115.7, 115.5, 56.1, 19.5. GC-MS (m/z): 354.3 [M+].

4,4''-difluoro-3,3'',4',5'-tetramethoxy-1,1':2',1''-terphenyl (1e).



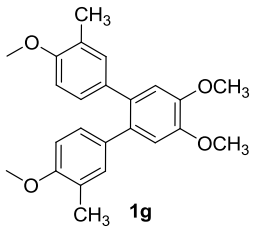
White solid, yield 587 mg, 90%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 6.98 (dd, *J* = 11.2, 8.3 Hz, 2H), 6.93 (s, 2H), 6.77-6.72 (m, 2H), 6.62 (dd, *J* = 8.2, 1.8 Hz, 2H), 3.95 (s, 6H), 3.62 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 151.4 (d, $J_{C,F}$ = 246 Hz), 148.6, 147.0 (d, $J_{C,F}$ = 10.8 Hz), 137.8 (d, $J_{C,F}$ = 4.0 Hz),, 132.3, 122.0 (d, $J_{C,F}$ = 6.6 Hz), 115.8 (d, *J* = 3.8 Hz), 115.6, 113.6, 56.2, 56.2. GC-MS (m/z): 386.2 [M+].

4,4''-dimethoxy-3,3''-dimethyl-1,1':2',1''-terphenyl (1f).



White solid, yield 606 mg, 90% .^{1}H NMR (300 MHz, $CDCl_3$): δ 7.38-7.42 (m, 4H), 7.02 (s, 2H), 6.88-6.91 (m, 2H), 6.67 (d, *J* = 9 Hz, 2H), 3.81 (s, 6H), 2.17 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 156.5, 140.4, 133.9, 132.2, 130.7, 128.4, 127.0, 125.9, 109.5, 55.3, 16.3. GC-MS (m/z): 318.3 [M+].

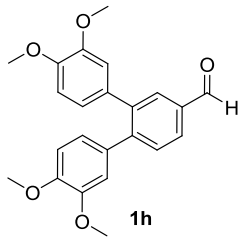
4,4',4'',5'-tetramethoxy-3,3''-dimethyl-1,1':2',1''-terphenyl (1g).



1g

White solid, yield 587 mg, 92%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 6.99 (s, 2H), 6.85-6.89 (m, 4H), 6.66 (s, 1H), 6.64 (s, 1H), 3.93 (s, 6H), 3.80 (s, 6H), 2.16 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 156.3, 147.9, 133.8, 132.8, 132.1, 128.4, 125.9, 113.8, 109.5, 56.1, 55.4, 16.3. GC-MS (m/z): 378.0 [M+].

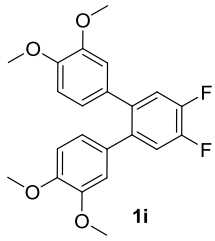
3,3'',4,4''-tetramethoxy-[1,1':2',1''-terphenyl]-4'-carbaldehyde (1h).



1h

White solid, yield 716 mg, 90%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 10.06 (s, 1H), 7.91 (s, 1H), 7.87 (d, *J* = 7.9 Hz, 1H), 7.58 (d, *J* = 7.9 Hz, 1H), 6.79 (d, *J* = 3.6 Hz, 4H), 6.61 (s, 2H), 3.86 (s, 6H), 3.62 (s, 3H), 3.60 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 192.0, 148.6, 148.6, 148.6, 148.4, 146.4, 141.1, 135.4, 133.2, 133.1, 131.9, 131.2, 128.3, 122.0, 113.3, 113.3, 111.1, 111.0, 77.6, 77.2, 76.7, 55.9, 55.9, 55.8. HRMS-ESI: $[M+Na]^+$, Calcd. For $C_{23}H_{22}NaO_5$ 401.1359; found 401.1366.

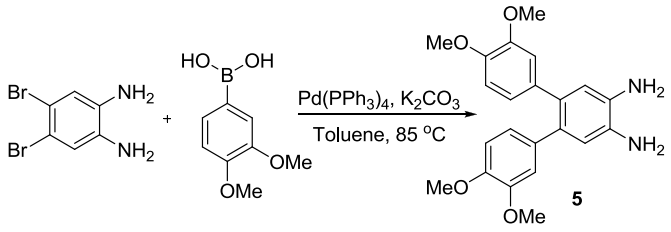
4',5'-difluro-3,3'',4,4''-tetramethoxy-1,1':2',1''-terphenyl (**1i**).



1i

White solid, yield 653 mg, 92%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.34 - 7.26 (m, 1H), 7.24 (s, 1H), 6.74 (dt, *J* = 8.2, 4.9 Hz, 4H), 6.55 (d, *J* = 1.7 Hz, 2H), 3.93 (s, 6H), 3.68 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 150.9 (d, *J* = 14.6 Hz), 148.3 (d, *J* = 18.7 Hz), 147.5 (d, *J* = 14.5 Hz), 136.9 (t, *J* = 4.6 Hz), 132.5, 121.9, 118.9 (dd, *J* = 10.7, 7.2 Hz), 113.2, 110.9, 55.9, 55.8. HRMS-ESI: $[M+Na]^+$, Calcd. For $C_{22}H_{20}F_2NaO_4$ 409.1227; found 409.1273.

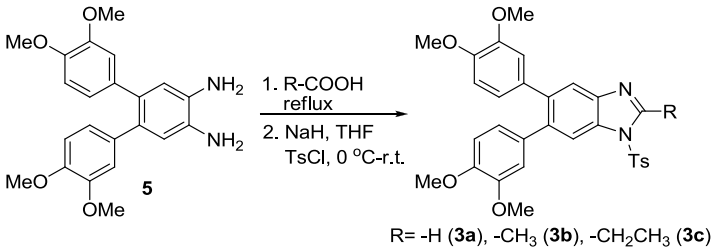
2.2 Preparation of compound 5 : [3]



5

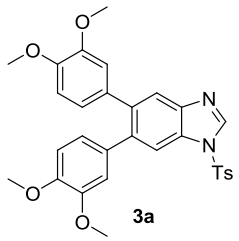
4, 5-dibromo-1, 2-phenylenediamine (1.0 g, 3.76 mmol), 3,4-dimethoxyphenylboronic acid (1.7 g, 9.4 mmol) and $Pd(PPh_3)_4$ (0.11 g, 0.094 mmol) were taken in 60 mL toluene. To this 15 ml of 2M K_2CO_3 aqueous solution was added. The resulting suspension was degassed and heated at 85 ^oC for 24 h under N_2 atmosphere. After that, the reaction mixture was cooled to room temperature, to this water was added and the compound was extracted with ethylacetate, dried over Na_2SO_4. The solvent was concentrated under reduced pressure and compound was purified by column chromatography on silica gel with EtOAc and hexane (9:1) as eluent to afford compound **5** as brown solid, yield 800 mg, 55%.

2.3 General procedure for the preparation of compound 3a, 3b and 3c: [4]



Compound **5** (0.2 g) was taken in formic acid (4 ml) and refluxed for 16 h. The reaction mixture was cooled to room temperature; water was added and extracted with dichloromethane. The solvent was removed under reduced pressure and compound was purified by column chromatography on silica gel with EtOAc and hexane (8:2) as eluent. After that, the compound was subjected for *N*-tosylation according to the literature procedure[4(b)] to afford the compound **3a** as a white solid, yield 215 mg, 75%. Similarly, we prepared compound **3b** and **3c** by taking acetic acid and propanoic acid respectively.

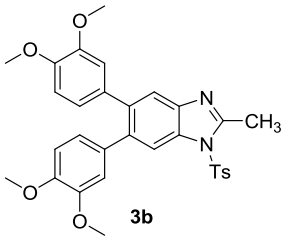
5,6-bis(3,4-dimethoxyphenyl)-1-tosyl-1*H*-benzo[*d*]imidazole (3a).



White solid, yield 215 mg, 75%. ^1H NMR (300 MHz, $CDCl_3$): δ 8.40 (s, 1H),7.92 (s, 1H), 7.91 (d, *J*= 6 Hz, 2H) 7.80 (s, 1H), 7.32 (d, *J* = 9 Hz, 2H), 6.82 (s, 2H), 6.67 (s, 2H), 6.56 (s, 2H), 3.89 (s, 3H), 3.85 (s, 3H), 3.59 (s, 6H), 2.40 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 148.5, 148.3, 148.1, 146.4, 143.5, 141.9, 138.8, 138.1, 134.8, 134.3, 134.1, 130.5, 130.2, 127.5, 122.3, 122.3, 122.2, 114.1, 113.9, 113.8, 111.1,56.1, 56.0, 55.9, 55.8, 21.8. HRMS

ESI: $[M+Na]^+$, Calcd. For $C_{30}H_{28}N_2NaO_6S$ 567.1560; found 567.1553.

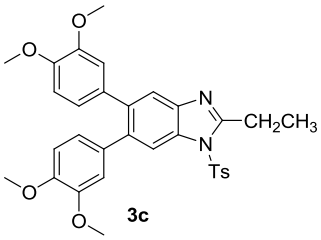
5,6-bis(3,4-dimethoxyphenyl)-2-methyl-1-tosyl-1*H*-benzo[*d*]imidazole (3b).



3b

White solid, yield 220 mg, 75%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.06 (s, 1H), 7.84 (d, *J* = 9 Hz, 2H), 7.66 (s, 1H), 7.32 (d, *J* = 9 Hz, 2H), 6.84 (s, 2H), 6.77 (s, 2H), 6.59 (s, 2H), 3.88 (s, 3H), 3.85 (s, 3H), 3.60 (s, 6H), 2.83 (s, 3H), 2.41 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 152.2, 148.4, 148.4, 148.1, 147.9, 146.2, 141.4, 137.8, 137.8, 135.6, 134.6, 134.3, 132.7, 130.4, 127.0, 122.3, 122.2, 120.9, 114.8, 114.2, 113.9, 111.03, 56.1, 56.0, 55.9, 55.8, 21.8, 17.1. HRMS ESI: $[M+H]^+$, Calcd. for $C_{31}H_{31}N_2O_6S$ 559.1897; found 559.1899.

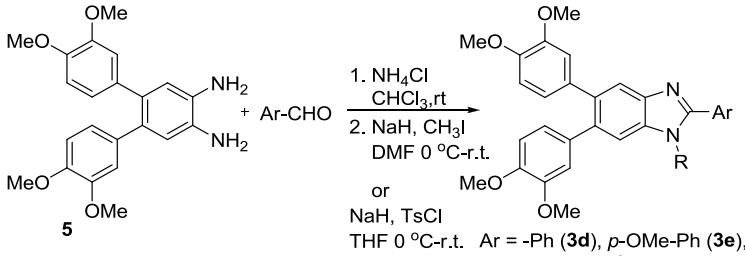
5,6-bis(3,4-dimethoxyphenyl)-2-ethyl-1-tosyl-1*H*-benzo[*d*]imidazole (3c).



3c

White solid, yield 210 mg, 70%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.07 (s, 1H) , 7.83 (d, *J* = 9 Hz, 2H), 7.72 (s, 1H), 7.31 (d, *J* = 9 Hz, 2H), 6.83 (s, 2H), 6.76 (s, 2H), 6.59 (s, 2H), 3.88 (s, 3H), 3.85 (s, 3H), 3.59 (s, 6H), 3.21 (q, *J* = 6 Hz, 2H), 2.40 (s, 3H), 1.46 (t, *J* = 6 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 157.1, 148.4, 148.1, 147.9, 146.0, 141.4, 137.8, 137.7, 135.8, 134.6, 134.4, 130.4, 127.0, 122.3, 122.2, 121.1, 115.0, 114.2, 113.9, 111.0, 56.0, 56.0, 55.9, 55.8, 23.6, 21.8, 11.9. HRMS ESI: $[M+H]^+$, Calcd. for $C_{32}H_{33}N_2O_6S$ 573.2054; found 573.2058.

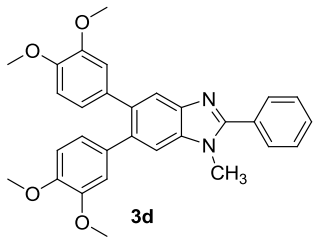
2.4 General procedure for the preparation of compound 3d-i: [5]



Ar = -Ph (**3d**), *p*-OMe-Ph (**3e**), *p*-F-Ph (**3f**), *p*-CF_3-Ph (**3g**), *p*-NO_2-Ph (**3h**), thiophene (**3i**)

Aromatic aldehyde (1.0 equiv) was added to a stirred solution of compound **5** (300 mg, mmol), and ammonium chloride (4.0 equiv) in chloroform (5 ml) for five minutes at room temperature. The resulting reaction mixture was stirred at room temperature for 4 h. The compound was extracted with dichloromethane and the organic layer washed with H_2O (10 ml). The compound was purified by column chromatography on silica gel with EtOAc and hexane (8:2) as eluent. Further, the compound was subjected for *N*-methylation[5(b)] (**3d**-**3f** and **3i**) or *N*-tosylation[4(b)] (**3g** and **3h**).

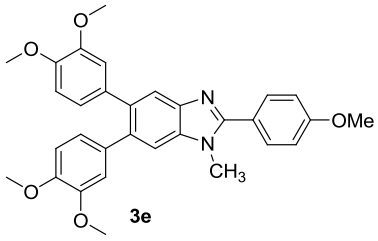
5,6-bis(3,4-dimethoxyphenyl)-1-methyl-2-phenyl-1*H*-benzo[*d*]imidazole (3d).



3d

White solid, yield 165 mg, 65%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.91, 7.83, 7.82, 7.81, 7.57, 7.56, 7.55, 7.44, 6.88, 6.85, 6.83, 6.82, 6.80, 6.77, 6.66, 6.65, 3.94, 3.88, 3.87, 3.62. ^{13}C NMR (75 MHz, $CDCl_3$): δ 154.5, 148.4, 148.4, 148.0, 147.8, 141.7, 136.6, 135.3, 135.0, 130.3, 129.6, 129.0, 122.4, 122.0, 120.9, 114.2, 111.2, 111.0, 56.1, 56.0, 55.9, 55.8, 32.1. HRMS ESI: $[M+H]^+$, Calcd. for $C_{30}H_{29}N_2O_4$ 481.2122; found 481.2122.

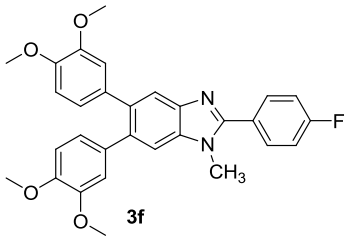
5,6-bis(3,4-dimethoxyphenyl)-2-(4-methoxyphenyl)-1-methyl-1*H*-benzo[*d*]imidazole (3e).



3e

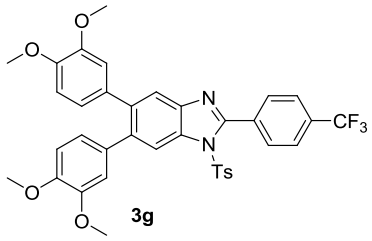
White solid, yield 174 mg, 65%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.86 (s, 1H), 7.76 (d, *J* = 8 Hz, 2H), 7.40 (s, 1H), 7.06 (d, *J* = 8 Hz, 2H), 6.85-6.80 (m, 4H), 6.67 (s, 1H), 6.65 (s, 1H), 3.90 (s, 3H), 3.89 (s, 6H), 3.87 (s, 6H), 3.61 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 161.0, 154.6, 148.3, 148.2, 147.8, 142.1, 136.0, 135.9, 135.8, 135.3, 135.1, 130.9, 122.3, 122.1, 120.7, 114.3, 114.1, 110.9, 55.9, 55.9, 55.8, 55.7, 55.4, 31.9. HRMS ESI: $[M+H]^+$, Calcd. for $C_{31}H_{31}N_2O_5$; 511.2227 found 511.2216.

5,6-bis(3,4-dimethoxyphenyl)-2-(4-fluorophenyl)-1-methyl-1*H*-benzo[*d*]imidazole (3f).



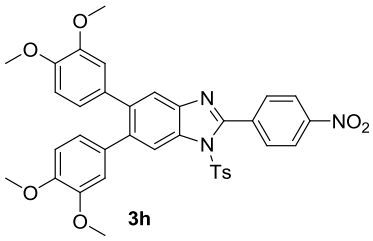
White solid, yield 157 mg, 60%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.88 (s, 1H), 7.83-7.79 (m, 2H), 7.44 (s, 1H), 7.29-7.26 (m, 2H), 6.90-6.86 (m, 4H), 6.84-6.66 (m, 2H), 3.91 (s, 3H), 3.89 (s, 3H), 3.88 (s, 3H), 3.63 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 165.5, 162.2, 153.8, 148.4, 148.4, 142.9, 142.4, 136.4, 136.0, 135.1, 131.6, 131.5, 126.5, 122.4, 122.2, 121.1, 116.2, 116.0, 114.2, 111.2, 111.0, 56.1, 56.0, 55.9, 55.8, 32.0. HRMS ESI: $[M+H]^+$, Calcd. for $C_{30}H_{28}F_1N_2O_4$ 499.2028; found 499.2032.

5,6-bis(3,4-dimethoxyphenyl)-1-tosyl-2-(4-(trifluoromethyl)phenyl)-1*H*-benzo[*d*]imidazole (3g).



Yellow solid, yield 217 mg, 60%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.24 (s, 1H), 7.78-7.72 (m, 5H), 7.38 (d, *J* = 9 Hz, 2H), 7.15 (d, *J* = 9 Hz, 2H),6.69- 6.79 (m, 2H), 6.63 (s, 2H), 6.62-6.61 (m, 2H), 3.90 (s, 3H), 3.86 (s, 3H), 3.63(s, 3H), 3.61 (s, 3H), 2.37 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 153.0, 148.6, 148.5, 148.3, 148.2, 146.2, 142.0, 139.1, 138.8, 135.1, 134.4, 134.1, 133.3, 131.4, 130.0, 127.2, 124.8 (q, *J* = 3.75 Hz), 122.4, 122.2, 121.8, 116.4, 114.2, 113.9, 111.2, 111.1. HRMS ESI: $[M+H]^+$, Calcd. for $C_{37}H_{32}F_3N_2O_6S$ 689.1928; found 689.1929.

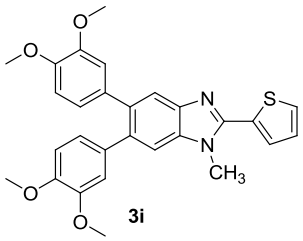
5,6-bis(3,4-dimethoxyphenyl)-2-(4-nitrophenyl)-1-tosyl-1*H*-benzo[*d*]imidazole (3h).



Yellow solid; yield 192 mg, 55%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.34 (d, *J* = 8.9 Hz, 2H), 8.22 (s, 1H), 7.85 (d, *J* = 8.9 Hz, 2H), 7.78 (s, 1H), 7.41 (d, *J* = 8.4 Hz, 2H), 7.18 (d, *J* = 8.1 Hz, 2H), 6.98 – 6.81 (m, 2H), 6.79 (s, 2H), 6.69 – 6.53 (m, 2H), 3.90 (s, 3H), 3.86 (s, 3H), 3.62 (s, 3H), 3.60 (s, 3H), 2.37 (s, 2H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 152.2, 149.2, 148.6,

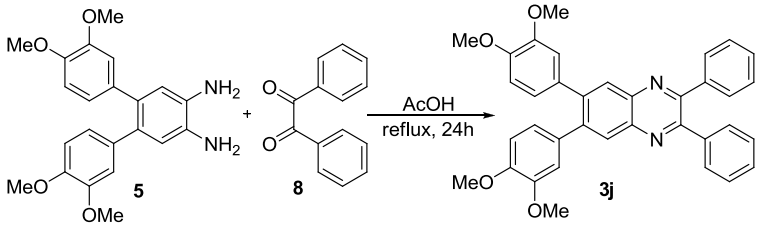
148.6, 148.4, 148.2, 146.5, 142.0, 139.5, 139.0, 136.4, 135.0, 134.2, 133.9, 133.3, 132.1, 130.2, 127.1, 123.0, 122.4, 122.2, 122.0, 116.4, 114.2, 113.9, 111.2, 111.1, 56.1, 56.0, 56.0, 55.9, 21.8. HRMS ESI: $[M+H]^+$, Calcd. for $C_{36}H_{32}N_3O_8S$ 666.1904; found 666.1895.

5,6-bis(3,4-dimethoxyphenyl)-1-methyl-2-(thiophen-2-yl)-1*H*-benzo[*d*]imidazole (3i).



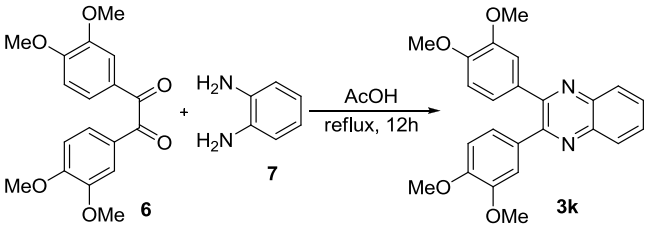
Solid, yield 153 mg, 61%. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.85 (s, 1H), 7.62 (d, *J* = 3.0 Hz, 1H), 7.54 (d, *J* = 6.0 Hz, 1H), 7.38 (s, 1H), 7.24 – 7.20 (m, 1H), 6.87 – 6.76 (m, 4H), 6.66 – 6.63 (m, 2H), 4.03 (s, 3H), 3.87 (s, 3H), 3.86 (s, 3H), 3.61 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 148.9, 148.4, 148.3, 147.8, 147.6, 142.4, 136.3, 136.2, 136.0, 135.3, 135.0, 132.6, 128.8, 128.1, 128.0, 122.4, 122.1, 121.0, 114.1, 110.9, 56.0, 56.0, 55.9, 55.8, 32.0. HRMS ESI: $[M+H]^+$, Calcd. for $C_{28}H_{27}N_2O_4S$ 487.1686; found 487.1693.

2.5 Preparation of 6,7-bis(3,4-dimethoxyphenyl)-2,3-diphenylquinoxaline (3j).[3]



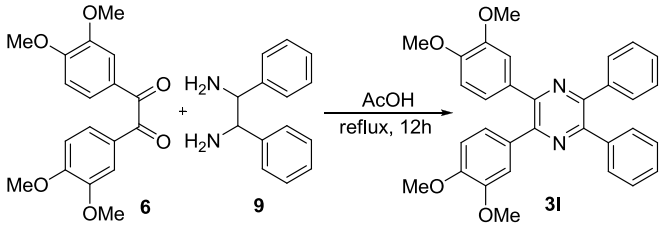
Compound **8** (1.0 equiv.) and **5** (1.2 equiv.) was taken in acetic acid as a solvent and the resulting reaction mixture was refluxed for 24 h. The reaction mixture was cooled to room temperature, as this water was added and extracted with dichloromethane. The resulting solution was dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography over silica gel with ethylacetate and hexane as eluent to afford the desired product **3j** as yellow solid in 87 % yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.23 (s, 2H), 7.53-7.56 (m, 4H), 7.34-7.36 (m, 6H), 6.91-675 (m, 6H), 3.89 (s, 6H), 3.66 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 153.8, 148.6, 148.5, 143.2, 140.6, 139.3, 133.3, 130.0, 129.0, 128.4, 122.4, 113.6, 111.1, 56.0, 55.9. HRMS ESI: $[M+Na]^+$, Calcd. for $C_{36}H_{30}N_2NaO_4$ 577.2097; found 577.2093.

2.6 Preparation of 2,3-bis(3,4-dimethoxyphenyl)quinoxaline (3k).[3]



Compound **6** (1.0 equiv) and benzene-1,2-diamine (1.2 equiv) was taken in acetic acid as a solvent and the resulting reaction mixture was refluxed for 16 h. The reaction mixture was cooled to room temperature, as this water was added and extracted with dichloromethane. The resulting solution was dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography over silica gel with ethylacetate and hexane as eluent to afford the desired product **3k** as yellow solid in 85 % yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.15 (dd, *J* = 6 Hz, *J* = 3 Hz,, 2H), 7.76 (dd, *J* = 6 Hz, *J* = 3 Hz,, 2H), 7.11-713 (m, 4H), 6.86 (d, *J* = 9 Hz, 2H), 3.90 (s, 6H), 3.76 (s, 6H). NMR (75 MHz, $CDCl_3$): δ 153.1, 149.9, 148.9, 141.2, 132.0, 129.8, 129.2, 123.0, 113.1, 111.0, 56.1, 56.0. HRMS ESI: $[M+H]^+$, Calcd. for $C_{24}H_{23}N_2O_4$ 403.1652; found 403.1656.

2.7 Preparation of 2,3-bis(3,4-dimethoxyphenyl)-5,6-diphenylpyrazine (3l). [3]

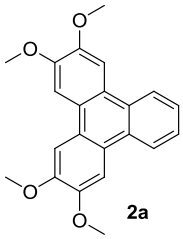


Compound **6** (1.0 equiv) and **9** (1.2 equiv) was taken in acetic acid as a solvent and the resulting reaction mixture was refluxed for 24h. The reaction mixture was cooled to room temperature, as this water was added and extracted with dichloromethane. The resulting solution was dried over Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography over silica gel with ethylacetate and hexane as eluent to afford the desired product **3l** as yellow solid in 85 % yield. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.66 (s, 4H), 7.35 (s, 6H), 7.28 (s, 4H), 6.86 (s, 2H), 3.92 (s, 6H), 3.76 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 149.7, 148.8, 147.9, 147.7, 138.8, 131.4, 130.0, 128.6, 128.4, 122.9, 113.1, 111.0, 56.1, 56.0. HRMS ESI: $[M+H]^+$, Calcd. for $C_{32}H_{29}N_2O_4$ 505.2122; found 505.2120.

3. General Procedure for the oxidative cyclodehydrogenation of Scholl Precursors (A)

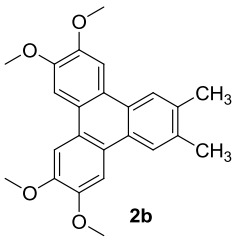
o-terphenyl **1a** (35 mg, 0.1 mmol) was taken in 2ml dry acetonitrile and ceric(IV) ammonium nitrate (109.6 mg, 0.2 mmol) was added under nitrogen gas atmosphere. The reaction immediately turns to green and the progress of the reaction was monitored by TLC. After completion of the reaction, the reaction mixture was passed through a pad of celite and washed with dichloromethane. The filtrate was concentrated under reduced pressure. The compound was purified by column chromatography on silica gel using EtOAc and hexane as eluent to afford cyclized product **2a**.

2,3,6,7-tetramethoxytriphenylene (2a) .



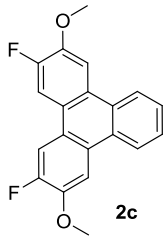
According to the general procedure A, Compound **2a** was prepared from **1a**. Yield: 27 mg, 81%; solid, mp 175-177 ^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.47 (dd, *J* = 6Hz, *J* = 3 Hz, 2H), 7.97 (s, 2H) 7.75 (s, 2H), 7.59 (dd, *J* = 6 Hz, *J* = 3 Hz, 2H), 4.12 (s, 12H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 149.6, 149.1, 129.0, 126.2, 124.1, 123.7, 123.0, 104.9, 104.5, 56.2, 56.1. HRMS ESI: $[M+H]^+$, Calcd. for $C_{22}H_{21}O_4$ 349.1434; found 349.1441. IR (KBr) cm^{-1}: 3492, 2931, 1616, 1513, 1460, 1411, 1263, 1214, 1158, 1048, 846, 785, 752.

2,3,6,7-tetramethoxy-10,11-dimethyltriphenylene (2b).



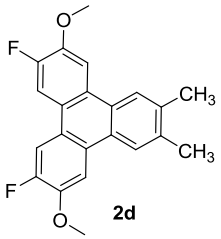
Prepared according to the general procedure A, Yield: 29 mg, 79%; white solid, mp 234-236^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.18 (s, 2H), 7.92 (s, 2H), 7.73 (s, 2H), 4.12 (s, 6H), 4.10 (s, 6H), 2.52 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 149.1, 148.9, 135.2, 127.2, 123.7, 123.6, 123.4, 104.6, 104.4, 56.2, 56.1, 20.4. HRMS ESI: $[M+H]^+$, Calcd. for $C_{24}H_{25}O_4$ 377.1747; found 377.1733. IR (KBr) cm^{-1}: 2916, 2825, 1603, 1503, 1465, 1301, 1245, 1134, 888, 770, 608.

3,6-difluoro-2,7-dimethoxytriphenylene (2c).



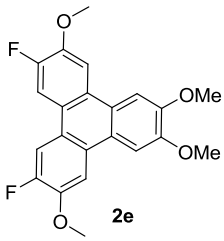
Prepared according to the general procedure A, Yield: 15 mg, 47%; white solid, mp 160-162 ^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.46 (q, 2H), 8.01 (s, 1H), 7.98 (s, 1H), 7.94 (s, 1H) , 7.90 (s, 1H), 7.66 (q, 2H), 4.10 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.1 (d, $J_{C,F}$ = 246.7 Hz), 147.3 (d, $J_{C,F}$ = 12 Hz), 129.0, 127.1, 126.2, 123.7, 123.4, 109.6 (d, $J_{C,F}$ = 19.5 Hz), 106.6, 56.4. ESI: $[M+Na]^+$, Calcd. for $C_{20}H_{14}F_2$ NaO_2 347.0860 ; found 347.0809. IR (KBr) cm^{-1}: 3556, 2929, 2360, 1516, 1403, 1314, 1221, 1117,850, 771.

2,11-difluoro-3,10-dimethoxy-6,7-dimethyltriphenylene (2d).



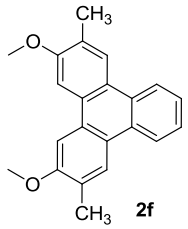
Prepared according to the general procedure A, Yield: 17 mg, 50%; white solid 170-172 ^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.10 (s, 2H), 7.92 (s, 1H), 7.90 (d, J = 3Hz, 2H), 7.85(s, 1H), 4.10 (s, 6H), 2.51 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 150.8 (d, $J_{C,F}$ = 246.0 Hz), 147.2 (d, $J_{C,F}$ = 12 Hz), 136.2, 127.1, 126.2, 123.8, 123.4, 109.5 (d, $J_{C,F}$ = 19.5 Hz), 106.5, 56.5, 20.4. HRMS ESI: $[M+Na]^+$, Calcd. for $C_{22}H_{18}F_2NaO_2$ 375.1167; found 375.1177. IR (KBr) cm^{-1}: 3461, 2977, 2941, 1602, 1509, 1454, 1403, 1270, 1207, 1117, 855, 776, 718.

2,11-difluoro-3,6,7,10-tetramethoxytriphenylene (2e).



Prepared according to the general procedure A, Yield: 31 mg, 82%; solid, mp 186-188 ^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.71 (s, 1H), 7.67 (s, 1H), 7.61 (s, 1H), 7.58 (s, 1H) , 7.57 (s, 2H), 4.10 (s, 6H), 4.07 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 150.5 (d, $J_{C,F}$ = 245.2 Hz), 149.4, 147.1 (d, $J_{C,F}$ = 12 Hz), 125.8, 123.3, 122.9, 109.5 (d, $J_{C,F}$ = 19.5 Hz), 106.2, 104.6, 56.5, 56.2. HRMS ESI: $[M+H]^+$, Calcd. for $C_{22}H_{19}F_2O_4$ 385.1246; found 385.1244. IR (KBr) cm^{-1}: IR (KBr) cm^{-1}: 3465, 2975, 2925, 2359, 1609, 1505, 1445, 1405, 1278, 1207, 1117, 855, 816 716.

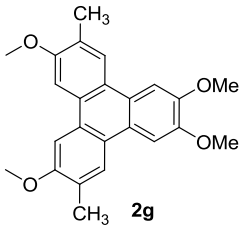
3,6-dimethoxy-2,7-dimethyltriphenylene (2f).



2f

Prepared according to the general procedure A, Yield: 29 mg, 90%; white solid, mp 160-162 ^{o}C.^{1}H NMR (300 MHz, $CDCl_3$): δ 8.53 (dd, *J* = 6, *J* = 3 Hz, 2H), 8.37 (s, 2H), 7.75 (s, 2H), 7.56 (dd, *J* = 6 Hz, *J* = 3 Hz, 2H), 4.05 (s, 6H), 2.47 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 157.6, 129.2, 128.9, 127.3, 126.0, 125.5, 123.5, 122.8, 102.4, 55.5, 17.0. HRMS ESI: $[M+H]^+$, Calcd. for $C_{22}H_{20}O_2$ 317.1536; found 317.1534. IR (KBr) cm^{-1}: 3001, 2943, 2916, 2838, 2360, 1605, 1503, 1469, 1300, 1242, 1134, 1028, 775, 606.

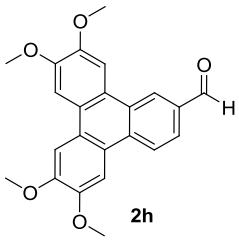
2,3,7,10-tetramethoxy-6,11-dimethyltriphenylene (2g).



2g

Prepared according to the general procedure A, Yield: 18 mg, 50%; solid, mp 182-185^{o}C.^{1}H NMR (300 MHz, $CDCl_3$): δ 8.22 (s, 2H), 7.89 (s, 2H), 7.81 (s, 2H), 4.13 (s, 6H), 4.08 (s, 6H), 2.49 (s, 6H).). ^{13}C NMR (75 MHz, $CDCl_3$): δ 156.9, 148.7, 128.5, 127.3, 124.9, 123.4, 123.2, 104.3, 102.5, 56.2, 55.6, 17.0. HRMS ESI: $[M+H]^+$, Calcd. for $C_{24}H_{25}O_4$ 377.1547; found 377.1549. IR (KBr) cm^{-1}: 3465, 2933, 2363, 1616, 1513, 1460, 1263, 1214, 1048, 846, 785.

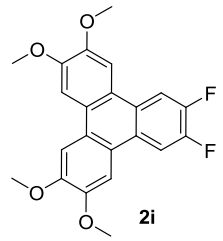
6,7,10,11-tetramethoxytriphenylene-2-carbaldehyde (2h).



2h

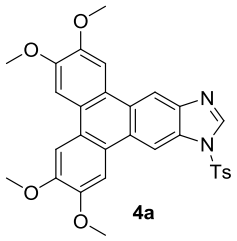
Prepared according to the general procedure A, Yield: 28 mg, 74%; yellow solid, mp 193-195 ^{o}C.. ^{1}H NMR (300 MHz, DMSO-d_6): δ 10.29 (s, 1H), 9.32 (s, 1H), 8.92 (d, *J*=9, 1H), 8.23 (s, 1H), 8.18 (s, 1H), 8.02 (d, *J*=9, 3H), 4.07-4.04 (m, 12H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 193.1, 150.6, 149.9, 149.2, 149.0, 146.3, 133.7, 132.6, 128.7, 128.2, 125.0, 124.4, 123.8, 123.3, 122.5, 122.0, 105.8, 105.4, 105.1, 56.0, 55.9, 55.8. HRMS ESI: $[M+H]^+$, Calcd. for $C_{23}H_{20}O_5$ 377.1384; found 377.1387. IR (KBr) cm^{-1}: 3446, 2959, 2834, 1695, 1598, 1516, 1463, 1255, 1140, 1023, 836, 761.

2,3-difluoro-6,7,10,11-tetramethoxytriphenylene (2i).



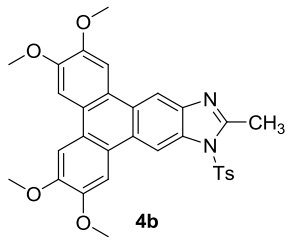
Prepared according to the general procedure A, Yield: 28 mg,74%; white solid, mp 192-194 ^{o}C. ^{1}H NMR (300 MHz, DMSO-d_6): δ 8.74 (t, J = 10.9 Hz, 2H), 7.96 (s, 2H), 7.91 (s, 2H), 4.03 (s, 3H), 4.01 (s, 3H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 149.6, 149.0, 126.0 (t, J = 3.8 Hz), 123.5, 121.8, 111.9 – 111.2 (m), 105.5, 104.8, 55.9. HRMS ESI: $[M+H]^+$, Calcd. for $C_{22}H_{19}F_2O_4$ 385.1245; found 385.1248. IR (KBr, cm^{-1}): 3462, 2933, 1614, 1512, 1418, 1378, 1265, 1157, 1056, 862, 768.

2,3,6,7-tetramethoxy-10-tosyl-10*H*-tripenyleno[2,3-*d*]imidazole (4a).



Prepared according to the general procedure A, Yield: 40 mg, 75%; white solid, mp 179-181 ^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.71 (d, J = 6 Hz, 2H), 8.45 (s, 1H), 7.92 – 7.88 (m, 4H), 7.70 (d, J = 6 Hz, 2H), 7.28 – 7.25 (m, 2H), 4.17 – 4.09 (m, 12H), 2.32 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 149.9, 149.6, 149.1, 149.0, 146.4, 143.2, 143.0, 134.9, 130.5, 130.1, 127.7, 127.2, 127.1, 124.3, 123.6, 123.3, 114.4, 105.5, 105.4, 105.0, 104.6, 104.5, 56.2, 56.1, 29.8, 21.7. HRMS ESI: $[M+H]^+$, Calcd. for $C_{30}H_{27}N_2O_6S$ 543.1584; found 543.1583. IR (KBr, cm^{-1}): 3465, 2928, 1618, 1515, 1460, 1324, 1248, 1168, 1048, 868.

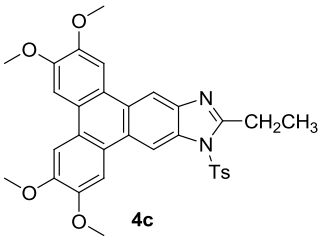
2,3,6,7-tetramethoxy-11-methyl-10-tosyl-10*H*-triphenyleno[2,3-*d*]imidazole (4b).



Prepared according to the general procedure A, Yield: 45 mg, 83%; white solid, mp 178-182 ^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.01 (s, 1H), 8.63 (s, 1H), 8.01 (s, 1H), 7.94 (s, 1H), 7.82 (dd, J = 14.2, 7.2 Hz, 4H), 7.28 (s, 2H), 4.19 (s, 3H), 4.17 (s, 3H), 4.15 (s, 3H), 4.11 (s, 3H), 2.87 (s, 3H), 2.37 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 153.6, 149.7, 149.6, 149.1, 146.2, 141.2, 135.8, 132.9, 130.4, 127.0, 126.8, 124.1, 123.8, 123.6, 112.9, 106.7, 105.4, 105.0, 104.7, 104.6, 56.3, 56.1, 21.8, 17.3. HRMS ESI: $[M+H]^+$,

Calcd. for $C_{31}H_{29}N_2O_6S$ 557.1740; found 557.1739. IR (KBr, cm^{-1}): 3456, 2929, 2361, 1609, 1512, 1466, 1375, 1248, 1161, 1031, 862, 667, 589.

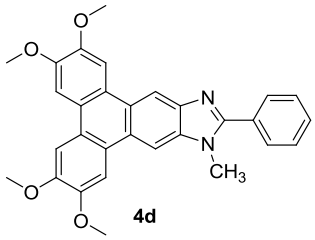
11-ethyl-2,3,6,7-tetramethoxy-10-tosyl-10*H*-triphenyleno[2,3-*d*]imidazole (4c).



4c

Prepared according to the general procedure A, Yield: 47 mg, 83%; white solid,mp 181-183 °C. ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.09 (s, 1H), 8.75 (s, 1H), 8.06 (s, 1H), 7.98 (s, 1H), 7.90 – 7.69 (m, 4H), 7.27 (s, 2H), 4.19 (s, 3H), 4.16 (s, 3H), 4.14 (s, 3H), 4.09 (s, 3H), 3.22 (q, *J* = 7.3 Hz, 2H), 2.36 (s, 3H), 1.51 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 158.4, 149.7, 149.5, 149.1, 146.1, 141.2, 135.9, 135.4, 133.0, 130.4, 127.0, 126.8, 124.1, 123.8, 123.6, 116.1, 113.1, 106.8, 105.4, 104.9, 104.7, 104.5, 56.3, 56.0, 23.8, 21.8, 11.4. HRMS ESI: $[M+H]^+$, Calcd. for $C_{32}H_{31}N_2O_6S$ 571.1897; found 571.1916. IR (KBr, cm^{-1}): 3457, 2931, 2361, 1599, 1515, 1460, 1371, 1250, 1166, 1032, 860, 808, 668, 585.

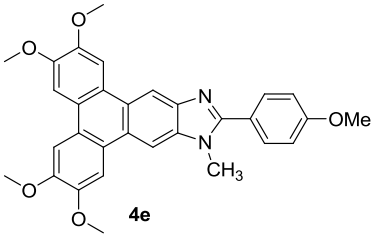
2,3,6,7-tetramethoxy-10-methyl-11-phenyl-10*H*-triphenyleno[2,3-*d*]imidazole (4d).



4d

Prepared according to the general procedure A, Yield: 37 mg, 80%, solid, mp 182-185 °C. ^{1}H NMR (300 MHz, DMSO-d_6): δ 9.07 (s, 1H), 8.84 (s, 1H), 8.32 (s, 1H), 8.25 (s, 1H), 8.01 (d, *J* = 6.0 Hz, 4H), 7.64 (d, *J* = 6.0 Hz, 3H), 4.14 (s, 3H), 4.10 (s, 3H), 4.08-4.06 (m, 9H). ^{13}C NMR (75 MHz, DMSO-d_6): δ 155.4, 149.1, 148.8, 148.8, 148.8, 142.2, 136.8, 130.2, 129.8, 129.3, 128.7, 125.2, 124.8, 123.9, 123.6, 123.0, 122.5, 112.5, 106.1, 105.4, 103.5, 56.0, 55.9, 55.9, 55.7, 32.2. HRMS ESI: $[M+H]^+$, Calcd. for $C_{30}H_{27}N_2O_4$ 479.1965; found 479.1965. IR (KBr, cm^{-1}): 3462, 2922, 2362, 1618, 1521, 1410, 1265, 1165, 1350, 1032, 868, 745.

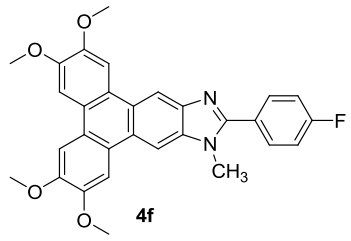
2,3,6,7-tetramethoxy-11-(4-methoxyphenyl)-10-methyl-10*H*-triphenyleno[2,3-*d*]imidazole (4e).



4e

Prepared according to the general procedure A, Yield: 38 mg ,75%; solid, mp 220-222 ^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.87 (s, 1H), 8.16 (s, 1H), 8.06 (s, 1H), 7.89 (s, 1H), 7.82 (d, *J* = 9 Hz, 2H), 7.74 (s, 2H), 7.08 (d, *J* = 6, 2H), 4.11 (s, 12H), 3.99 (s, 3H), 3.91 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 161.4, 149.2, 149.1, 148.8, 131.2, 125.8, 124.5, 124.0, 123.8, 123.0, 114.4, 112.4, 105.2, 104.7, 104.6, 101.9, 56.3, 56.3, 56.2, 56.0, 55.6, 32.3. HRMS ESI: $[M+H]^+$, Calcd. for $C_{31}H_{29}N_2O_5$ 509.2071; found 509.2064. IR (KBr, cm^{-1}): 3446, 2928, 2361, 1618, 1509, 1465, 1244, 1162, 1347, 1025, 866.

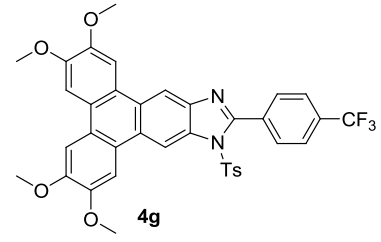
11-(4-fluorophenyl)-2,3,6,7-tetramethoxy-10-methyl-10*H*-triphenyleno[2,3-*d*]imidazole (4f).



4f

Prepared according to the general procedure A, Yield: 38 mg, 78%; solid, mp 224-226 ^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.90 (s, 1H), 8.21 (s, 1H), 8.08 (s, 1H), 7.93 (s, 1H), 7.89-7.85 (m, 2H), 7.77 (s, 2H), 7.27 (m, 2H), 4.12 (s, 12H), 4.00 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 165.6, 162.3, 155.3, 149.3, 149.1, 148.8, 142.4, 136.6, 131.7, 131.6, 126.3, 126.1, 125.9, 124.5, 124.0, 123.9, 123.1, 116.3, 116.0, 112.8, 105.2, 104.7, 102.0, 56.3, 56.2, 56.0, 32.2. HRMS ESI: $[M+H]^+$, Calcd. for $C_{30}H_{26}FN_2O_4$ 497.1871; found 497.1870. IR (KBr, cm^{-1}): 3455, 2932, 2361, 1615, 1515, 1465, 1367, 1250, 1166, 1350, 1032, 860, 668.

2,3,6,7-tetramethoxy-10-tosyl-11-(4-(trifluoromethyl)phenyl)-10*H*-triphenyleno[2,3-*d*]imidazole (4g).

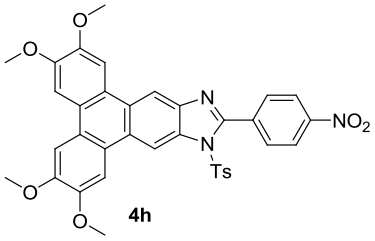


4g

Prepared according to the general procedure A, Yield: 40 mg, 60%; yellow solid, mp 196-198 ^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$): δ 9.14 (s, 1H), 8.71 (s, 1H), 8.01 (s, 1H), 7.90 (d, *J* =

7.90 Hz, 3H), 7.77 (d, *J* = 9 Hz, 4H), 7.28 (d, *J* = 9 Hz, 2H), 7.04 (d, *J* = 9 Hz, 2H), 4.18 (s, 3H), 4.15 (s, 3H), 4.13 (s, 3H), 4.08 (s, 3H), 2.26 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 154.7, 149.9, 149.8, 149.2, 149.2, 146.2, 141.8, 134.8, 133.6, 133.4, 132.9, 131.6, 130.0, 128.0, 127.8, 126.9, 124.8, 124.8, 124.3, 123.8, 123.6, 123.5, 113.9, 108.7, 105.4, 105.0, 104.6, 104.5, 56.3, 56.0, 24.9, 21.7. HRMS ESI: $[M+H]^+$, Calcd. for $C_{37}H_{30}F_3N_2O_6S$ 687.1771; found 687.1780. IR (KBr, cm^{-1}): 3467, 2927, 2361, 1618, 1518, 1465, 1326, 1264, 1163, 843 669, 589.

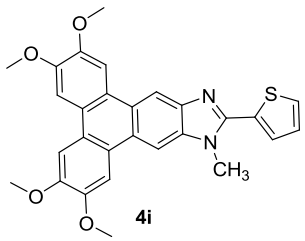
2,3,6,7-tetramethoxy-11-(4-nitrophenyl)-10-tosyl-10*H*-triphenyleno[2,3-*d*]imidazole (4h).



4h

Prepared according to the general procedure A, Yield: 39 mg, 60%; yellow solid, mp 216-220 ^{o}C.^{1}H NMR (300 MHz, $CDCl_3$): δ 9.10 (s, 1H), 8.69 (s, 1H), 8.38 (s, 1H), 8.35 (s, 1H), 8.00-7.90 (m, 3H), 7.89 (s, 1H), 7.74 (d, *J* = 6 Hz, 2H), 7.29 (d, *J* = 9 Hz, 2H), 7.04 (d, *J* = 9 Hz, 2H), 4.18 (s, 3H), 4.15 (s, 3H), 4.13 (s, 3H), 4.08 (s, 3H), 2.26 (s, 3H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 153.9, 150.0, 149.8, 149.2, 149.2, 146.4, 141.8, 136.2, 134.7, 133.3, 132.3, 130.1, 128.2, 127.9, 126.8, 124.3, 123.8, 123.5, 123.4, 123.0, 114.0, 108.6, 105.3, 105.0, 104.5, 104.4, 56.3, 56.0, 21.7. HRMS ESI: $[M+H]^+$, Calcd. for $C_{36}H_{30}N_3O_8S$ 664.1748; found 664.1723. IR (KBr, cm^{-1}): 3461, 2924, 2362, 1709, 1617, 1521, 1409, 1354, 1265, 1085, 845, 666.

2,3,6,7-tetramethoxy-11-(thiophen-2-yl)-10-tosyl-10*H*-triphenyleno[2,3-*d*]imidazole (4i).

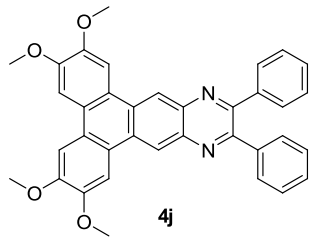


4i

Prepared according to the general procedure A, Yield: 35 mg, 75%; yellow solid, mp 195-197^{o}C. ^{1}H NMR (300 MHz, $CDCl_3$): δ 8.80 (s, 1H), 8.05 (s, 1H), 7.99 (s, 1H), 7.82 (s, 1H), 7.70 (s, 2H), 7.63 (d, *J* = 3.5 Hz, 1H), 7.57 (d, *J* = 5.0 Hz, 1H), 7.21 (dd, *J* = 10.4, 6.4 Hz, 1H), 4.07 (m, 15H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 150.2, 149.2, 149.0, 148.7, 142.2, 136.5, 132.6, 129.8, 129.3, 128.4, 128.2, 126.0, 125.9, 124.3, 123.8, 123.7, 123.0, 115.5,

112.5, 105.0, 104.5, 104.4, 101.6, 56.2, 56.1, 56.0, 32.1. HRMS ESI: $[M+H]^+$, Calcd. for $C_{28}H_{25}N_2O_4S$; 485.1530 found 485.1515. IR (KBr, cm^{-1}): 3445, 2933, 2361, 1615, 1517, 1408, 1344, 1262, 1023, 844.

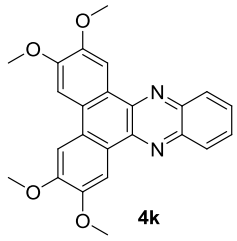
2,3,6,7-tetramethoxy-11,12-diphenylphenanthro[9,10-*g*]quinoxaline (4j).



4j

Prepared according to the general procedure A, Yield: 42 mg, 78%; yellow solid, mp 246-248 ^oC.^1H NMR (300 MHz, $CDCl_3$): δ 9.18 (s, 2H), 8.12 (s, 2H), 7.73 (s, 2H), 7.57-7.60 (m, 4H), 7.38-7.40 (m, 6H), 4.13 (s, 12H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 154.0, 150.5, 149.3, 139.5, 139.0, 131.7, 130.0, 129.0, 128.5, 124.8, 123.1, 122.3, 106.0, 104.8, 56.3. HRMS ESI: $[M+H]^+$, Calcd. for $C_{36}H_{29}N_2O_4$ 553.2122; found 553.2123. IR (KBr, cm^{-1}): 3461, 2927, 2362, 1618, 1518, 1414, 1326, 1266, 1165, 1044, 841, 770.

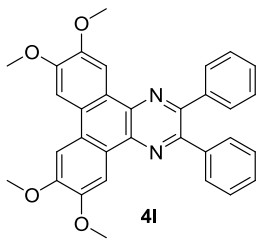
2,3,6,7-tetramethoxydibenzo[*a,c*]phenazine (4k).



4k

Prepared according to the general procedure A, , Yield: 30 mg, 75%; yellow solid, mp 224-226 ^oC. ^1H NMR (300 MHz, $CDCl_3$): δ 8.69 (s, 1H), 8.28 (dd, *J* = 6.4, 3.4 Hz, 1H), 7.82 (dd, *J* = 6.5, 3.4 Hz, 1H), 7.55 (s, 2H), 4.19 (s, 6H), 4.12 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 151.7, 149.2, 141.7, 141.6, 129.3, 129.1, 126.3, 123.8, 107.1, 103.8, 56.3, 56.2. HRMS ESI: $[M+H]^+$, Calcd. for $C_{24}H_{21}N_2O_4$ 401.1496; found 401.1505. IR (KBr) cm^{-1}: 3446, 2927, 2361, 1605, 1512, 1455, 1258, 1144, 1025, 860, 780.

6,7,10,11-tetramethoxy-2,3-diphenyldibenzo[*f,h*]quinoxaline (4l).

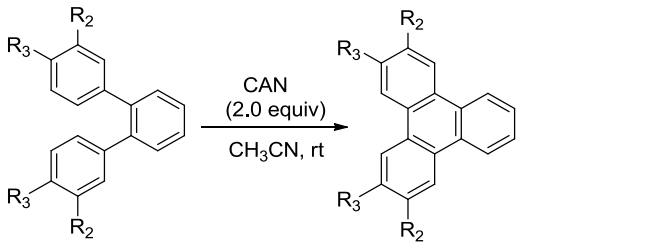


4l

Prepared according to the general procedure A, Yield: 37 mg, 75%; yellow solid, mp 188-192 ^oC. ^1H NMR (300 MHz, $CDCl_3$): δ 8.71 (s, 2H), 7.76 (s, 2H), 7.66-7.69 (m, 4H), 7.38-7.39 (m,

6H), 4.16 (s, 6H), 4.15 (s, 6H). ^{13}C NMR (75 MHz, $CDCl_3$): δ 151.3, 150.4, 149.4, 139.8, 138.0, 130.3, 128.6, 128.3, 126.1, 123.9, 106.4, 103.8, 56.3. HRMS ESI: $[M+H]^+$, Calcd. for $C_{32}H_{27}N_2O_4$ 503.1965; found 503.1911. IR (KBr) cm^{-1}: 3438, 2927, 2361, 1605, 1514, 1451, 1348, 1256, 1167, 1023, 859, 769.

4. Screening of CAN mediated Scholl reaction of *o*-terphenyls (with or without –OMe substitution):

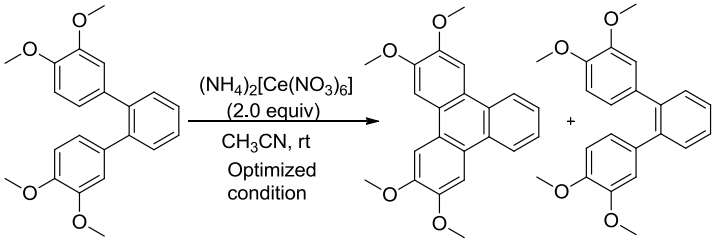


$R_2 = R_3 = -H$; (0% yield)
$R_2 = -OMe$, $R_3 = -H$; (0% yield)
$R_2 = -H$, $R_3 = -OMe$; (0% yield)

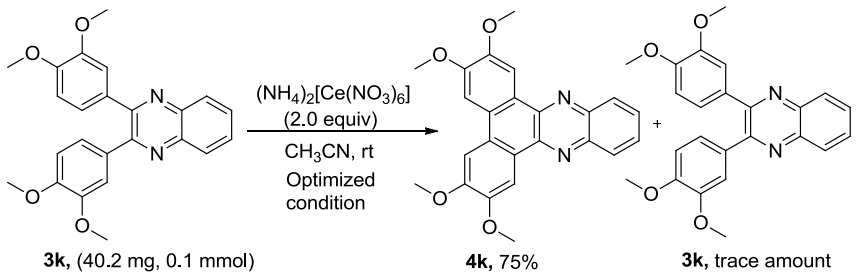
5. Comparison of CAN mediated Scholl reaction with $FeCl_3$ mediated Scholl Reaction:

To compare the reactivity of CAN mediated Scholl reaction with the literature reported $FeCl_3$ oxidative cyclization protocol, we have run cyclization reaction for the substrates **1a** and **3k** under both condition. The experimental procedure and results are summarized below:

(i) CAN mediated Scholl reaction of substrate **1a** and **3k** under optimized reaction condition:

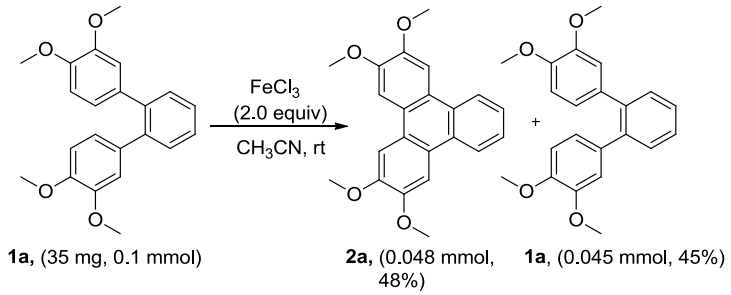


1a, (35 mg, 0.1 mmol) **2a,** 81% **1a**, 0%



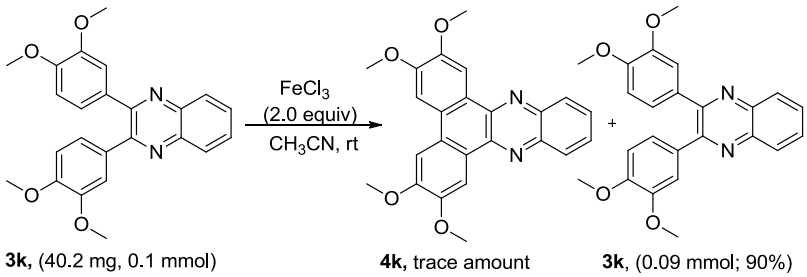
(ii) $FeCl_3$ mediated Scholl reaction of substrate **1a** and **3k**

o-terphenyl **1a** (35 mg, 0.1 mmol) was taken in 2ml dry acetonitrile and anhydrous $FeCl_3$ (32.4 mg, 0.2 mmol) was added under nitrogen gas atmosphere. The reaction immediately turns to green and then light yellow, and we observed 40-45% conversion of product within 10 min of the progress of the reaction. After 2 h, the reaction mixture was quenched with water (5 ml) and the compound was extracted with ethylacetae and organic layer was dried over Na_2SO_4. The organic layer was concentrated under reduced pressure. The compound was purified by column chromatography on silica gel using EtOAc and hexane (3:7) as eluent to afford as cyclized product **2a** (yield 48%) as well as starting material **1a (**yield 45%**)**. This result is consistent with the result reported by Rathore et. al. in which they used $FeCl_3$ in CH_2Cl_2 solvent at 0 ^oC.[6]



Compound **3k** (40.2 mg, 0.1 mmol) was taken in 2 ml dry acetonitrile and $FeCl_3$ (32.4 mg, 0.2 mmol) was added under nitrogen gas atmosphere. The reaction turns to yellow and the progress of the reaction was monitored by TLC. After 2 h, we observed trace amount of yellow spot (**4k**), prolonging the reaction time did not improved the conversion of the product. Therefore, the reaction was quenched with water (5 ml) and compound was extracted with ethylacetate, dried over Na_2SO_4 and concentrated under reduced pressure.

The compound was purified by column chromatography on silica gel using EtOAc and hexane as eluent to afford only starting material **3k** (90%).

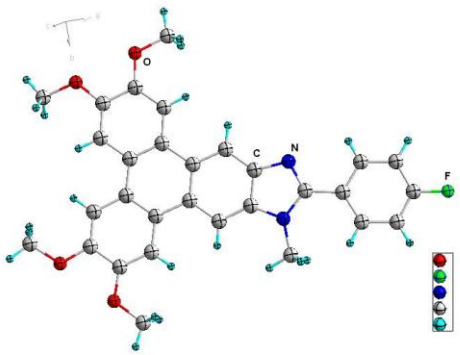


3k, (40.2 mg, 0.1 mmol) **4k,** trace amount **3k**, (0.09 mmol; 90%)

6. References:

1. (*a*) A. Suzuki, *Chem. Commun.,* 2005, 4759; (*b*) J. Hassan, M. Sevignon, C. Gozzi, E. Schulz and M. Lemaire, *Chem. Rev.,* 2002, **102**, 1359.
2. L. Zhai, R. Shukla and R. Rathore, *Org. Lett.,* 2009, **11**, 3474.
3. B. Gao, M. Wang, Y. Cheng, L. Wang, X. Jing and F. Wang, *J. Am. Chem. Soc.,* 2008, **130**, 8297.
4. (*a*) H. Thakuria and G. Das, *ARKIVOC* 2008, (**xv**), 321-328; (*b*) C. W. Williams, R. Shenje and S. France, *J. org. Chem.*, 2016, **81**, 8253.
5. (*a*) D. Nannapaneni, A. V. Gupta, M. Reddy and R. C. Sarva, *Journal of Young Pharmacists* 2010, **2**, 273; (b) B. M. Trost, J. Xie and J. D. Sieber*, J. Am. Chem. Soc.,* 2011, **133**, 20611.
6. L. Zhai, R. Shukla, S. H. Wadumethrige and R. Rathore, *J. Org. Chem.,* 2010, **75**, 4748.

7. Single Crystal X-ray structure of compound 4f



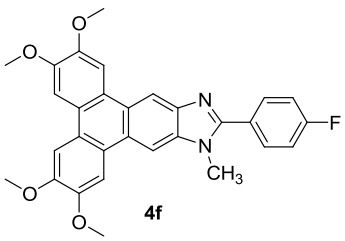
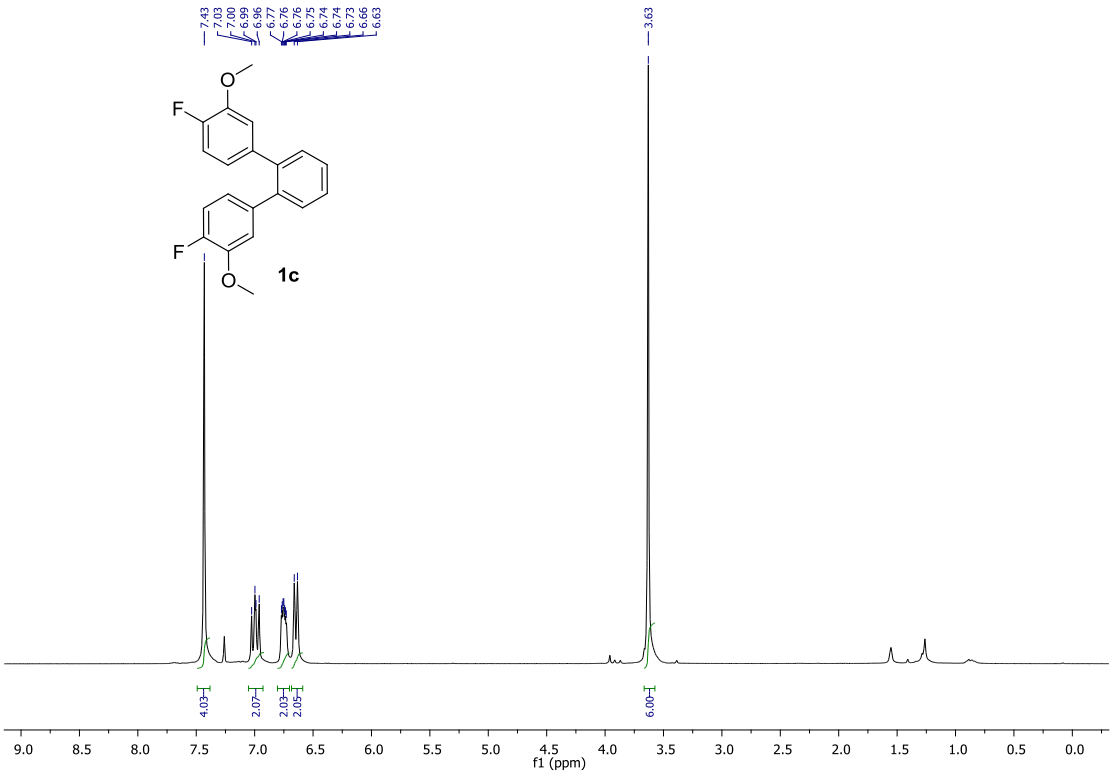
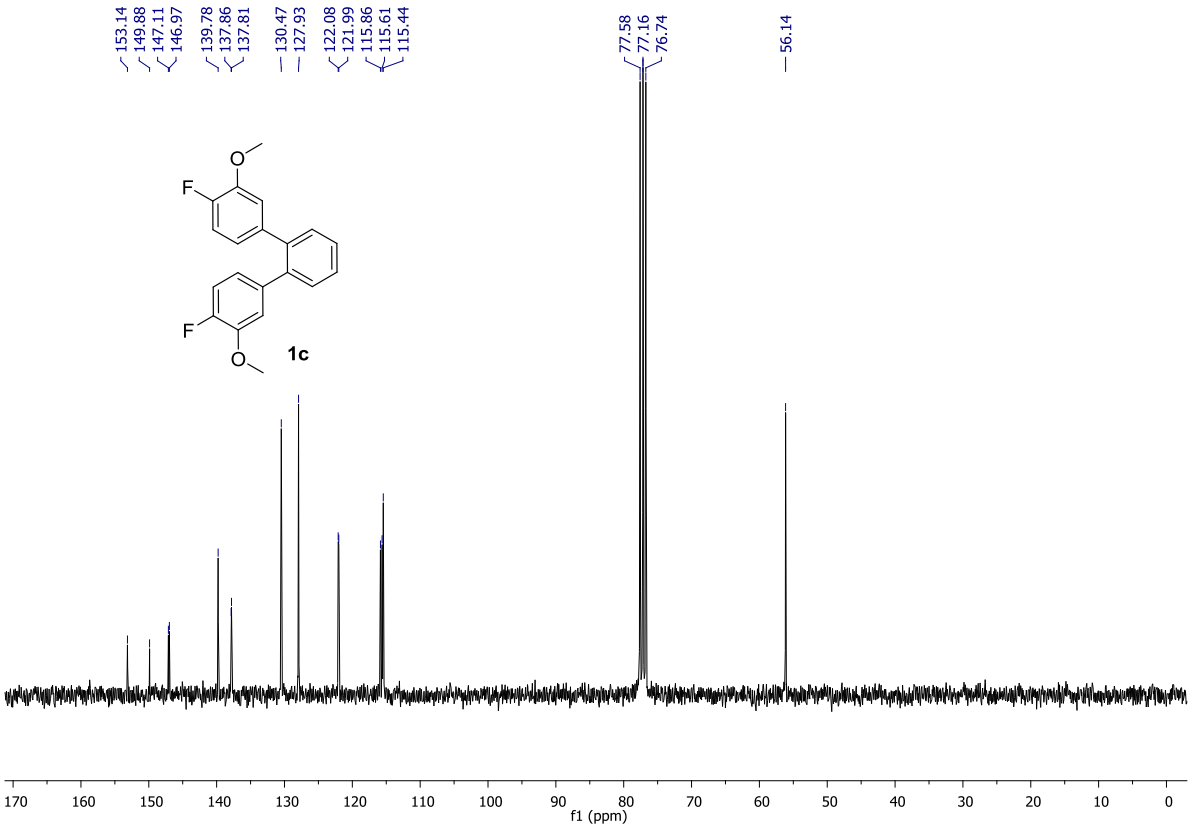
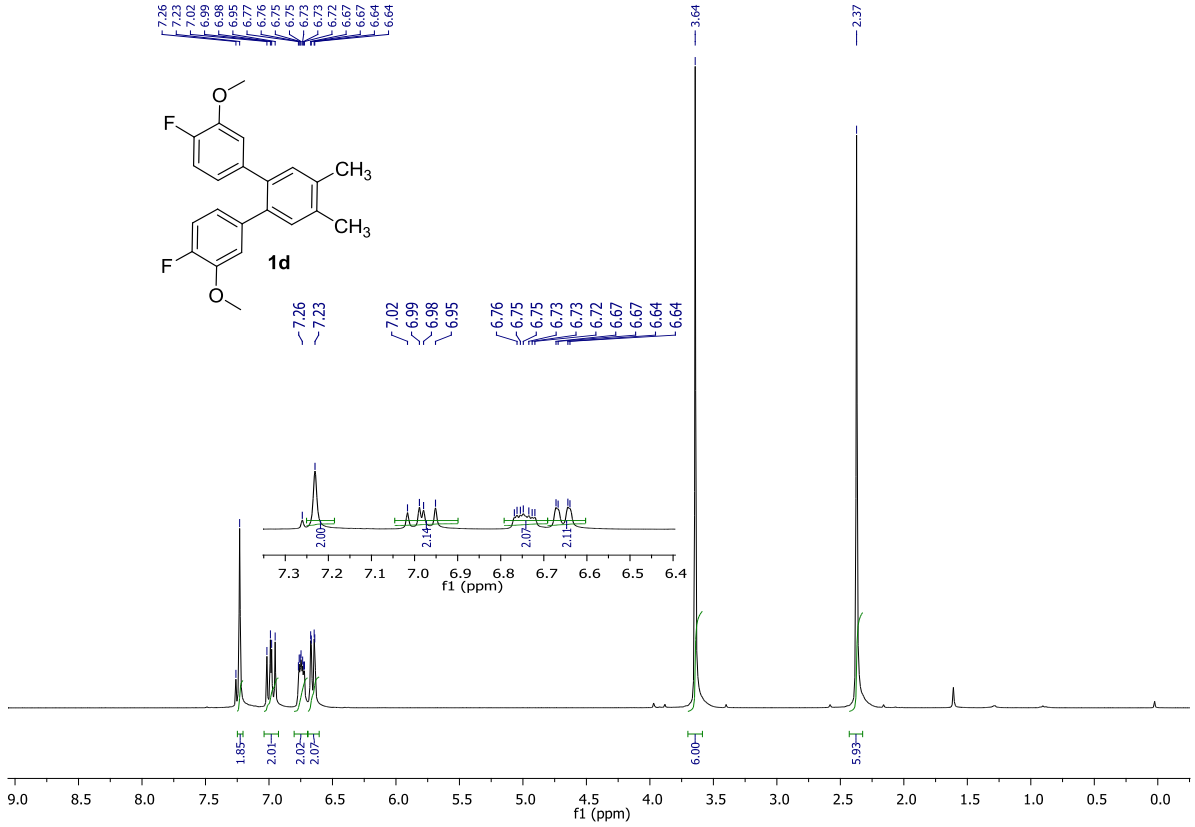


Figure S1. Molecular structure of compound **4f**. Thermal ellipsoids are drawn at the 50% probability level.

8. Copies of ^{1}H and ^{13}C NMR Spectra



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7.23
7.02
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6.98
6.95
6.77
6.76
6.75
6.75
6.73
6.73
6.72
6.67
6.67
6.64
6.64
3.64
2.37
O
F
CH3
CH3
F
O
1d
7.26
7.23
7.02
6.99
6.98
6.95
6.76
6.75
6.75
6.73
6.73
6.72
6.67
6.67
6.64
6.64
2.00
2.14
2.07
2.11
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
6.5
6.4
f1 (ppm)
1.85
2.01
2.02
2.07
6.00
5.93
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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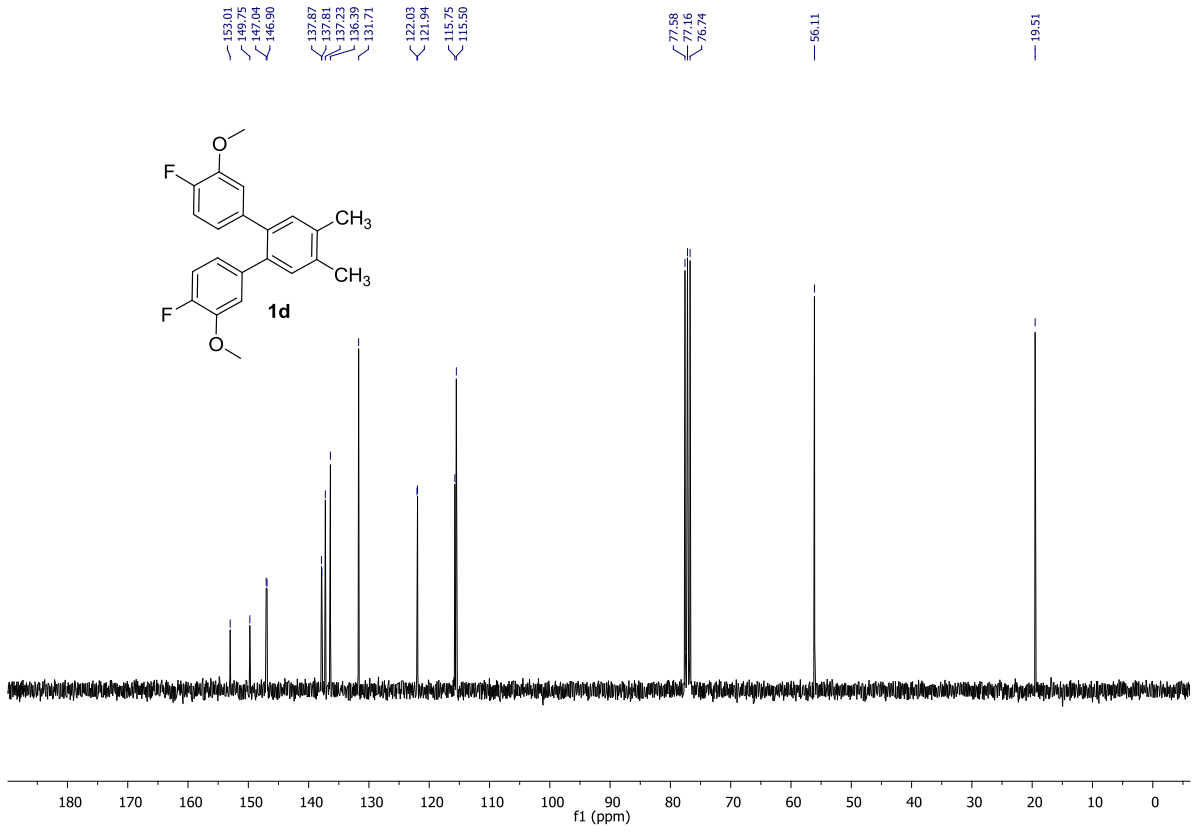
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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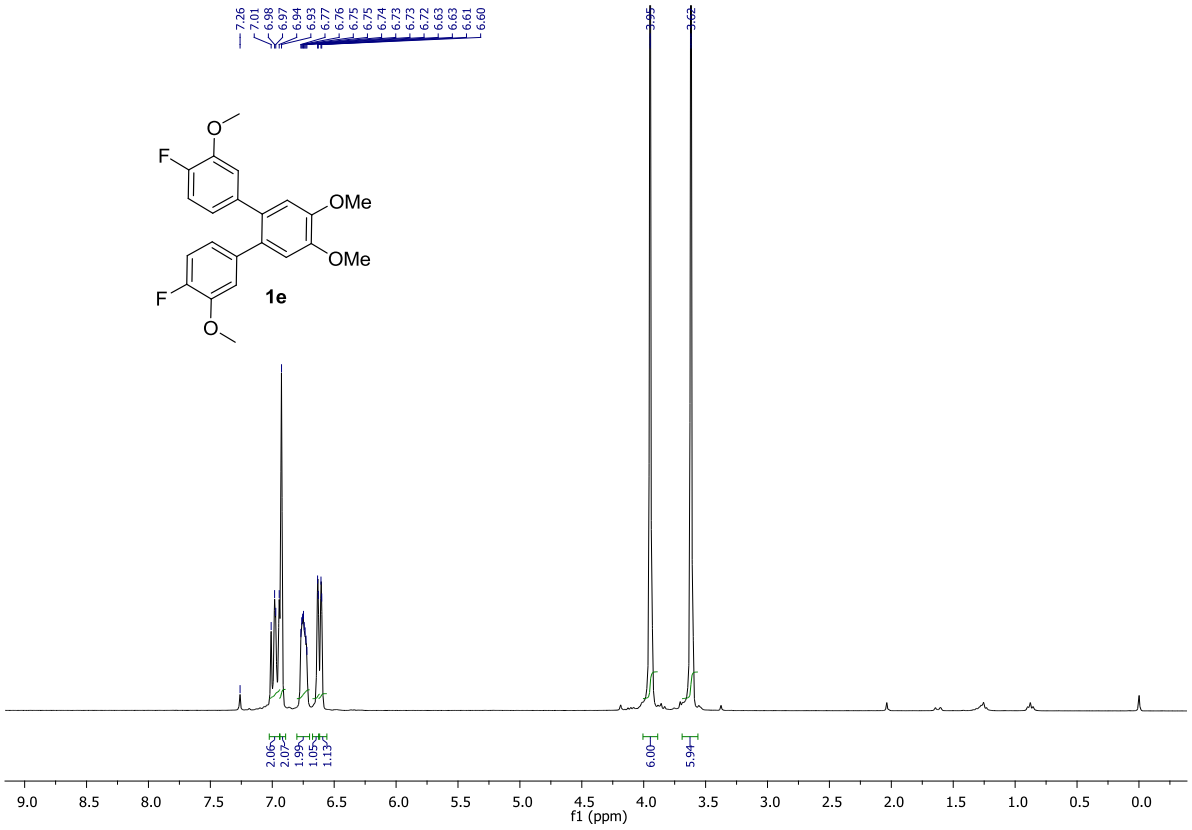
136.39
131.71
122.03
121.94
115.75
115.50
77.58
77.16
76.74
56.11
19.51
O
F
CH3
CH3
F
O
1d
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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6.93
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6.76
6.75
6.75
6.74
6.73
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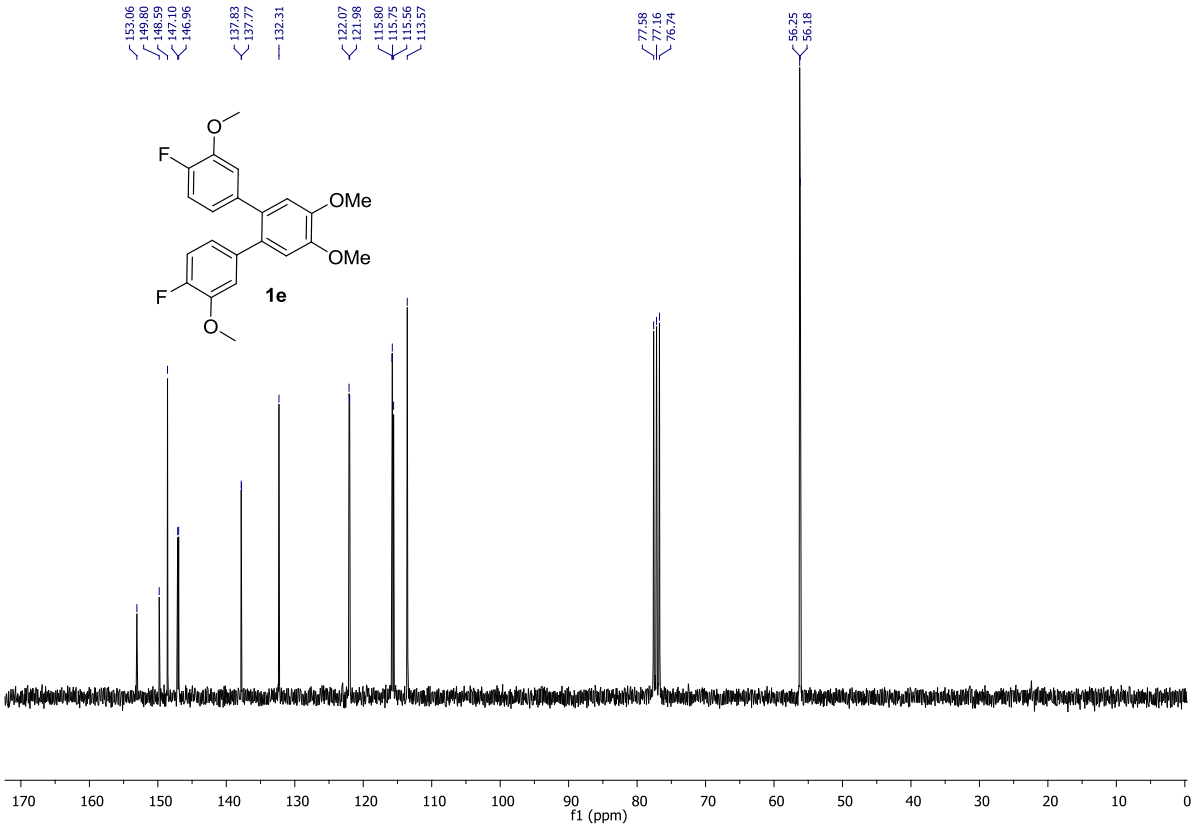
6.72
6.63
6.63
6.61
6.60
3.95
3.62
F
O
OMe
OMe
F
O
1e
2.06
2.07
1.99
1.05
1.13
6.00
5.94
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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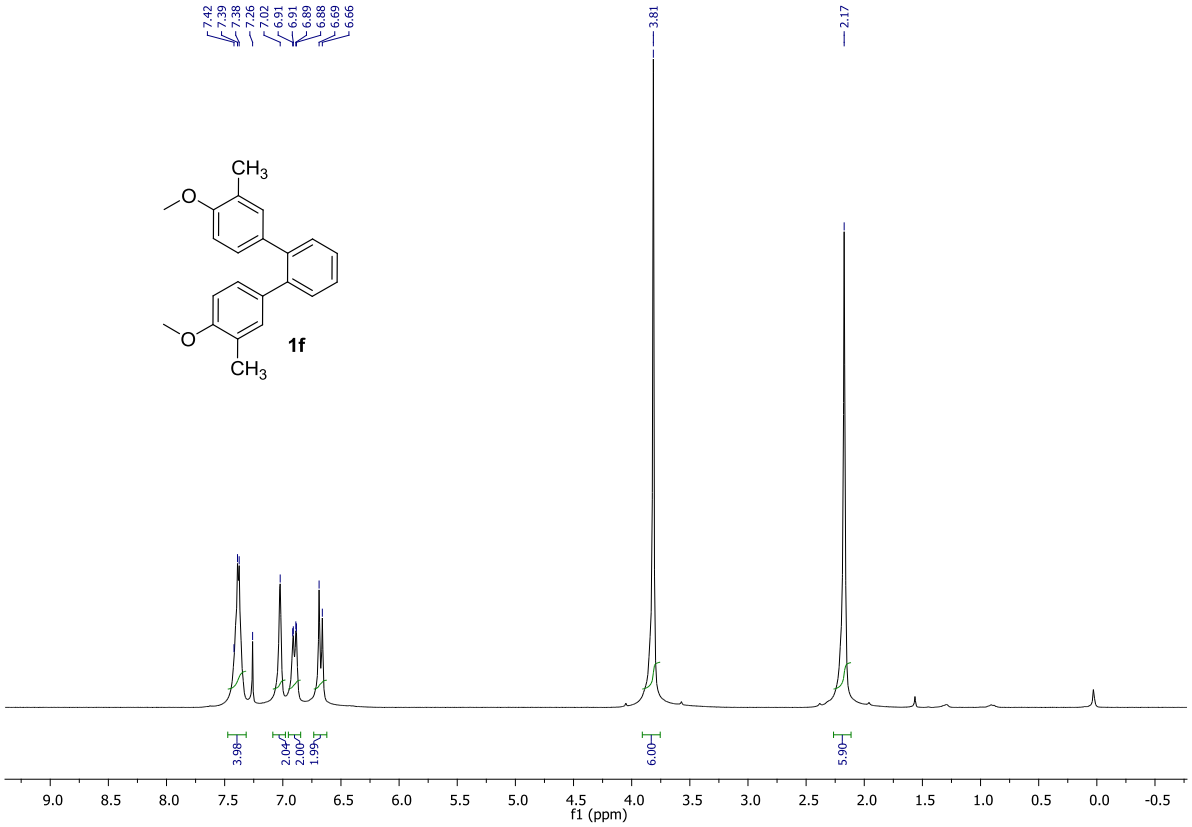
148.59
147.10
146.96
137.83
137.77
132.31
122.07
121.98
115.80
115.75
115.56
113.57
77.58
77.16
76.74
56.25
56.18
F
O
OMe
OMe
F
O
1e
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.39
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7.25
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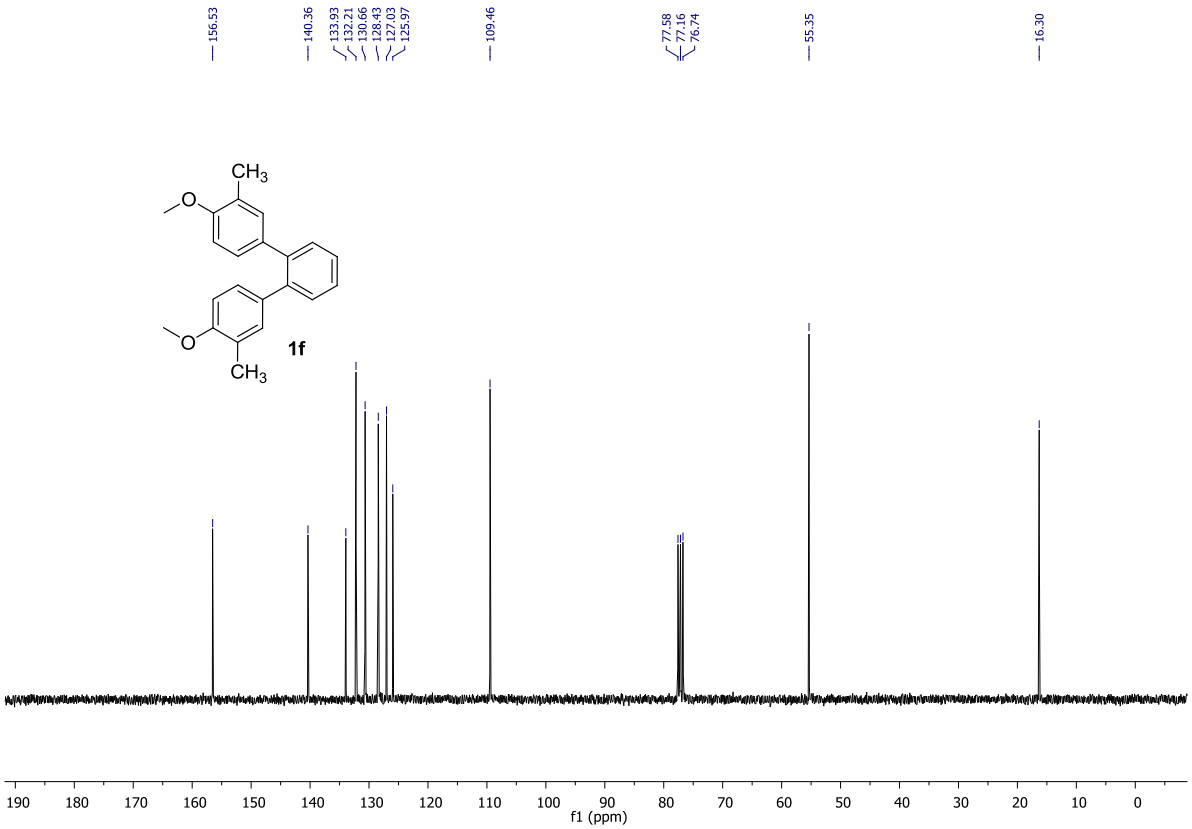
6.91
6.91
6.89
6.88
6.69
6.66
3.81
2.17
CH3
O
O
CH3
1f
3.98
2.04
2.00
1.99
6.00
5.90
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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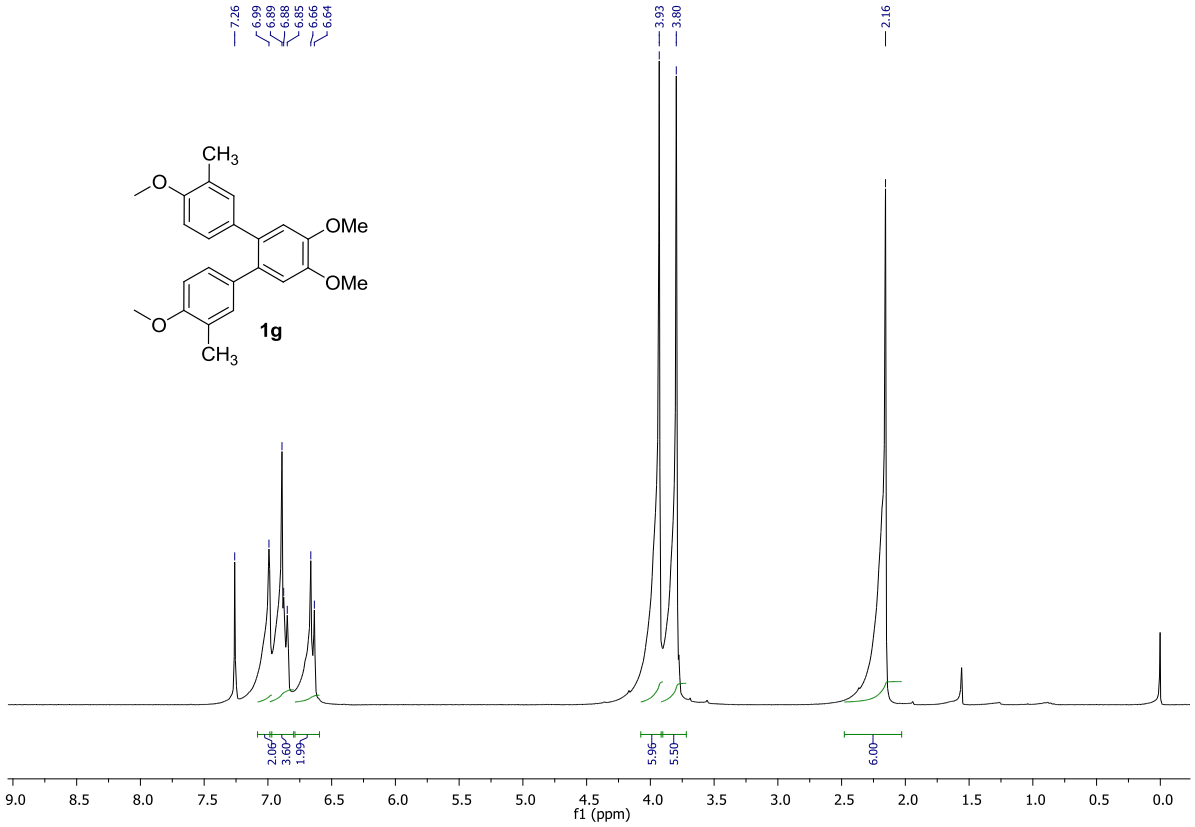
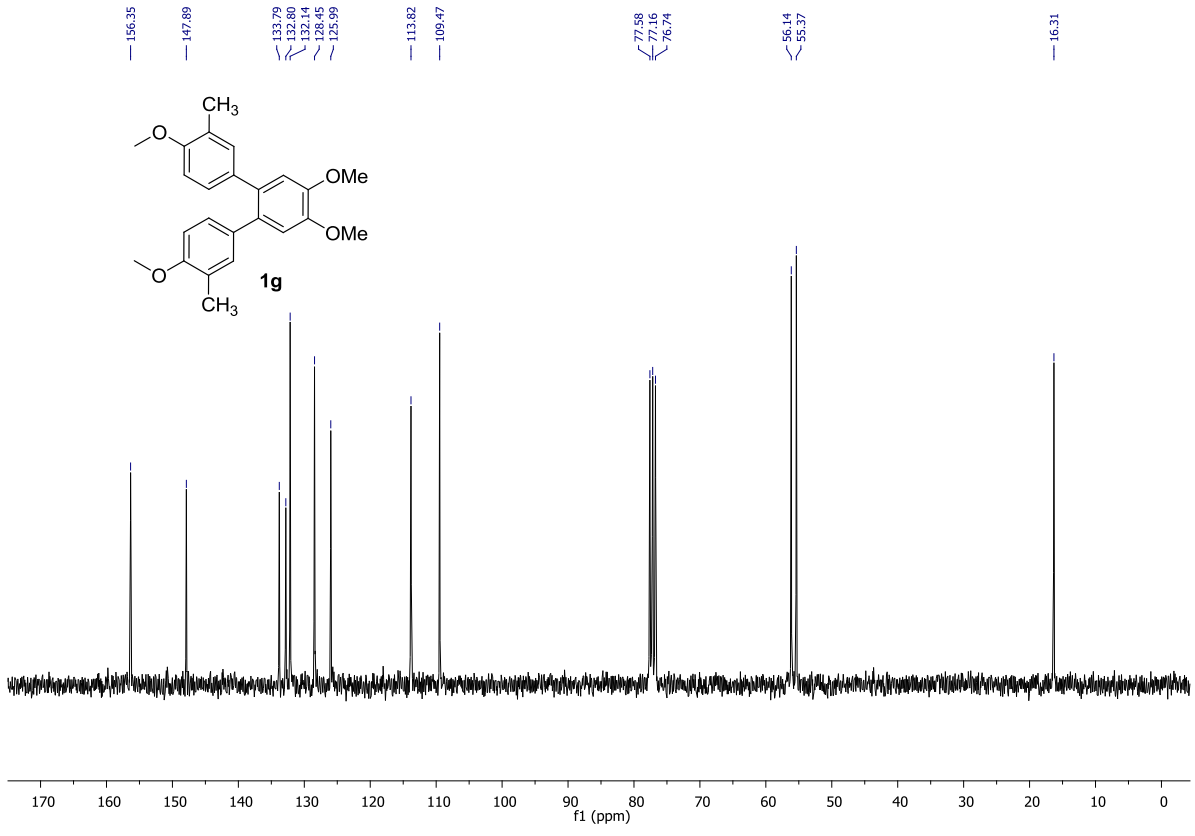
140.36
133.93
132.21
130.66
128.43
127.03
125.97
109.46
77.58
77.16
76.74
55.35
16.30
CH3
O
O
CH3
1f
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.26
6.99
6.89
6.88
6.85
6.66
6.64
3.93
3.80
2.16
CH3
O
OMe
OMe
O
CH3
1g
2.06
3.60
1.99
5.96
5.50
6.00
9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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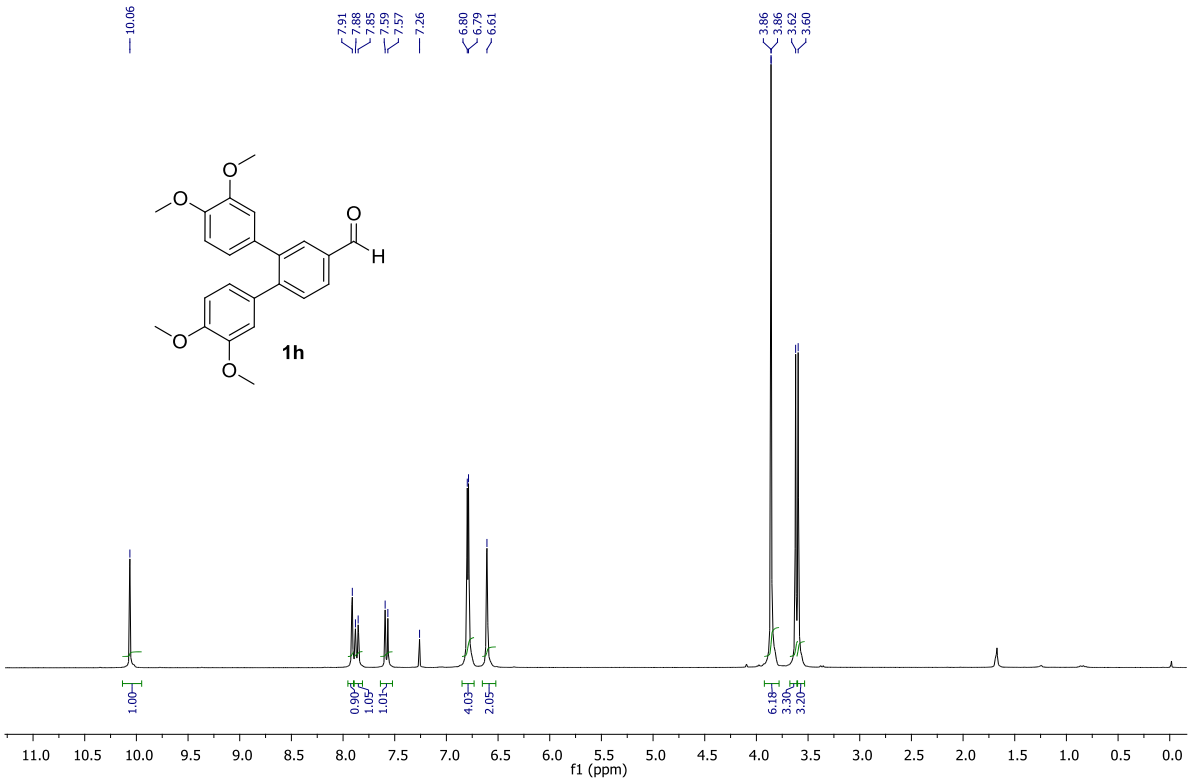
128.45
125.99
113.82
109.47
77.58
77.16
76.74
56.14
55.37
16.31
CH3
O
OMe
OMe
O
CH3
1g
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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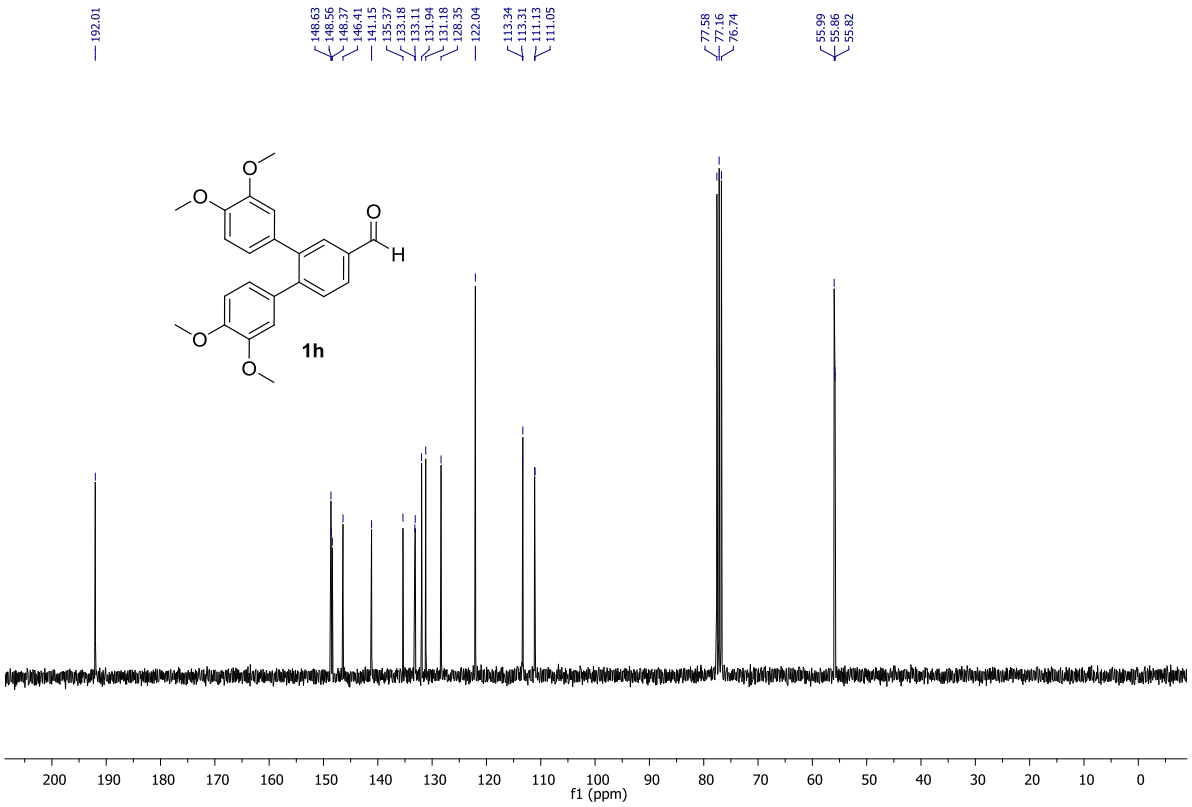
7.91
7.88
7.85
7.59
7.57
7.26
6.80
6.79
6.61
3.86
3.86
3.62
3.60
1h
1.00
0.90
1.05
1.01
4.03
2.05
6.18
3.30
3.20
f1 (ppm)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135.37
133.18
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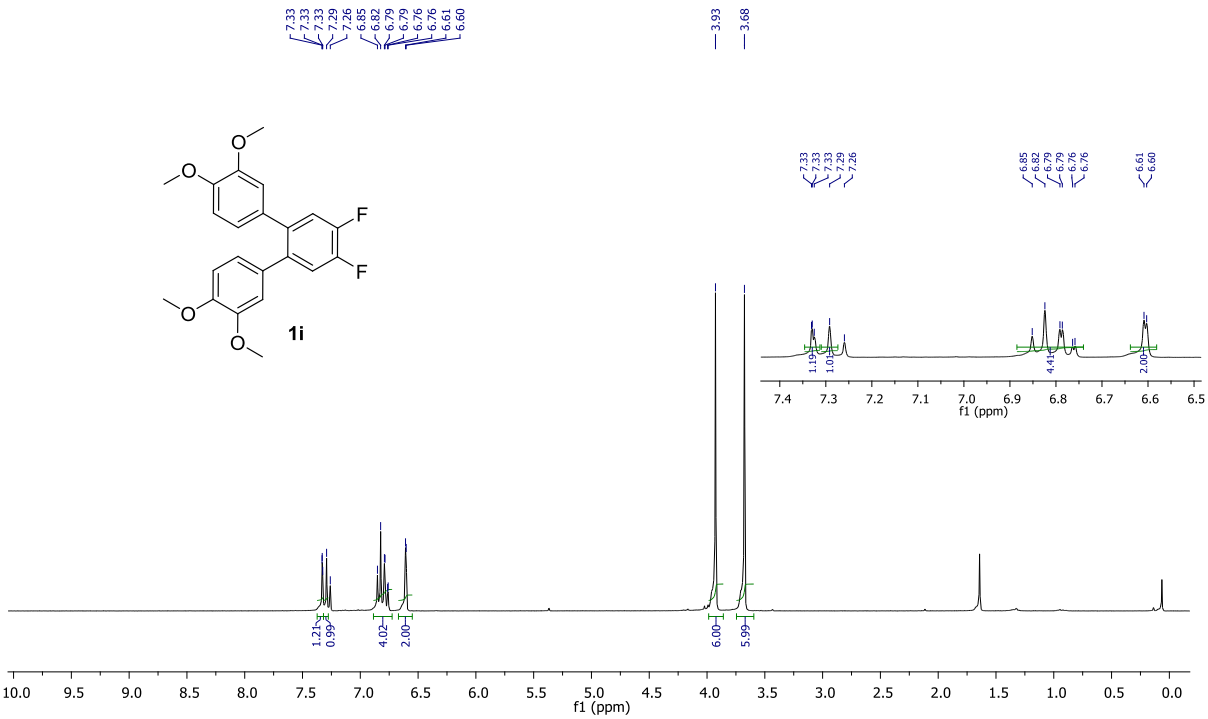
131.94
131.18
128.35
122.04
113.34
113.31
111.13
111.05
77.58
77.16
76.74
55.99
55.86
55.82
1h
f1 (ppm)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7.33
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7.29
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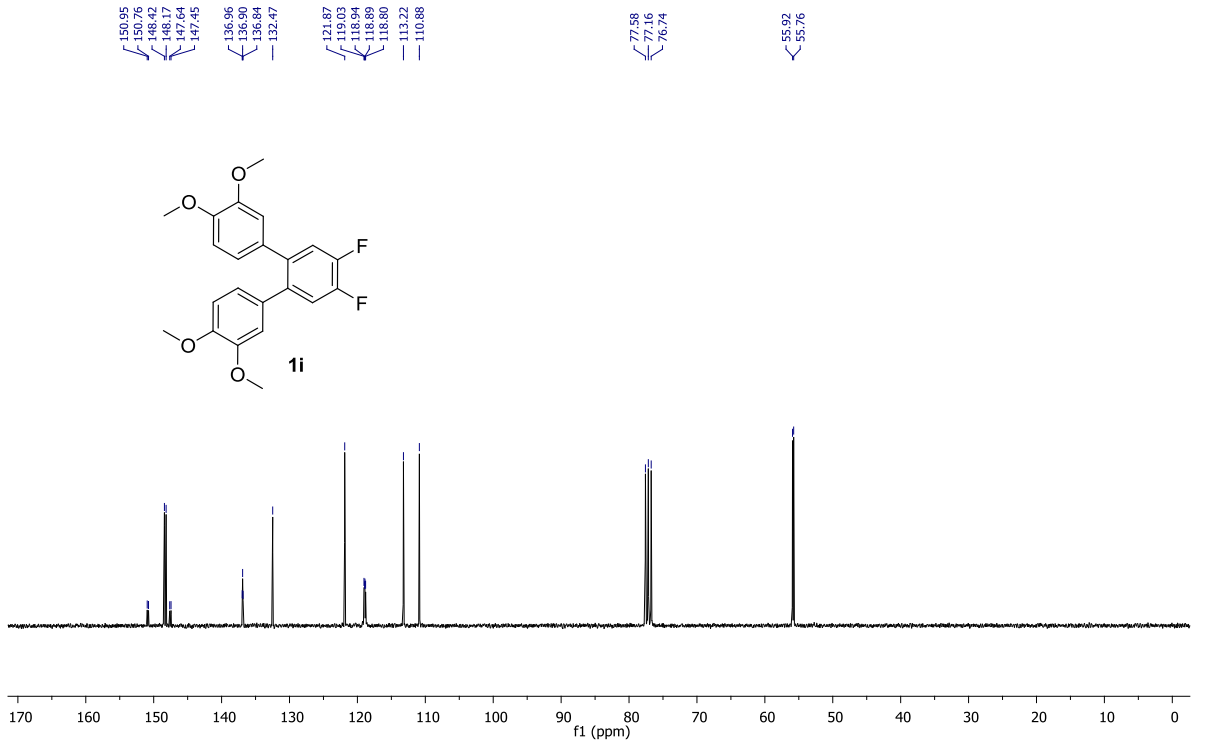
6.85
6.82
6.79
6.79
6.76
6.76
6.61
6.60
3.93
3.68
F
F
1i
1.21
0.99
4.02
2.00
6.00
5.99
f1 (ppm)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147.45
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136.90
136.84
132.47
121.87
119.03
118.94
118.89
118.80
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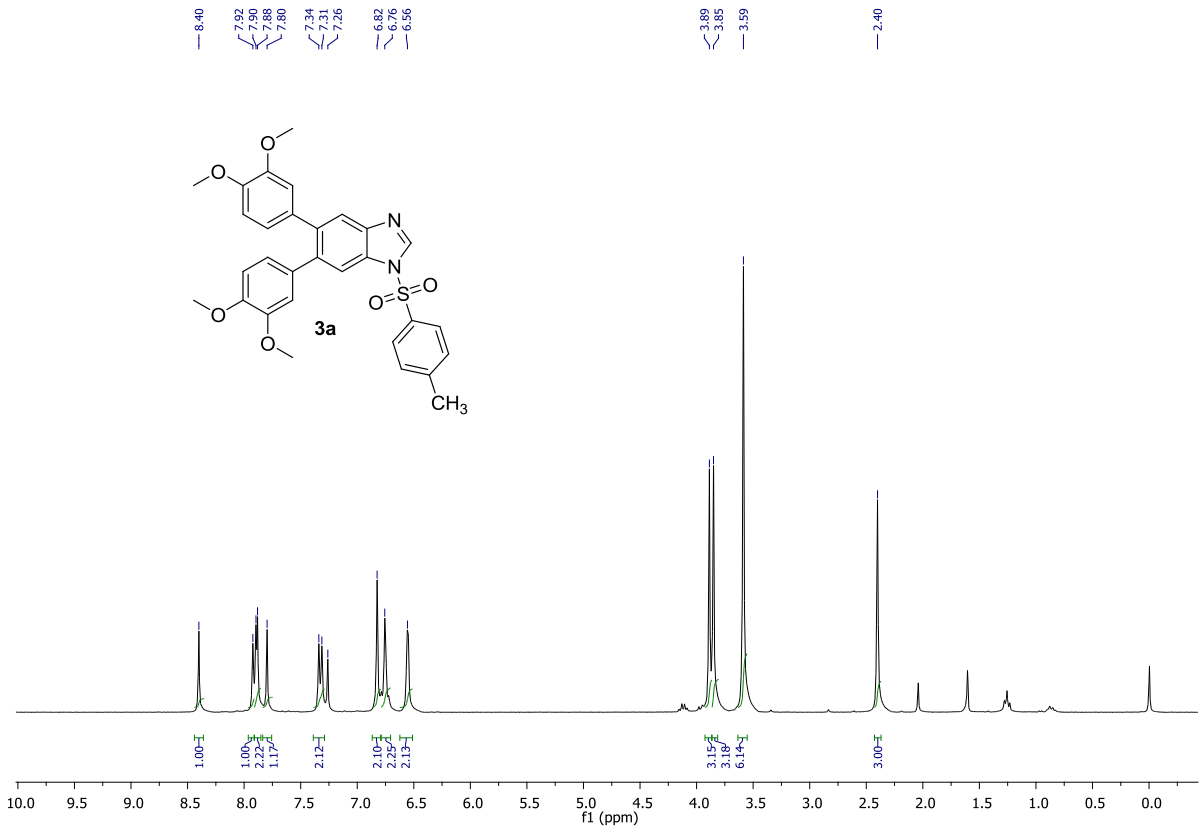
110.88
77.58
77.16
76.74
55.92
55.76
F
F
1i
f1 (ppm)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7.34
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7.26
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6.76
6.56
3.89
3.85
3.59
2.40
3a
1.00
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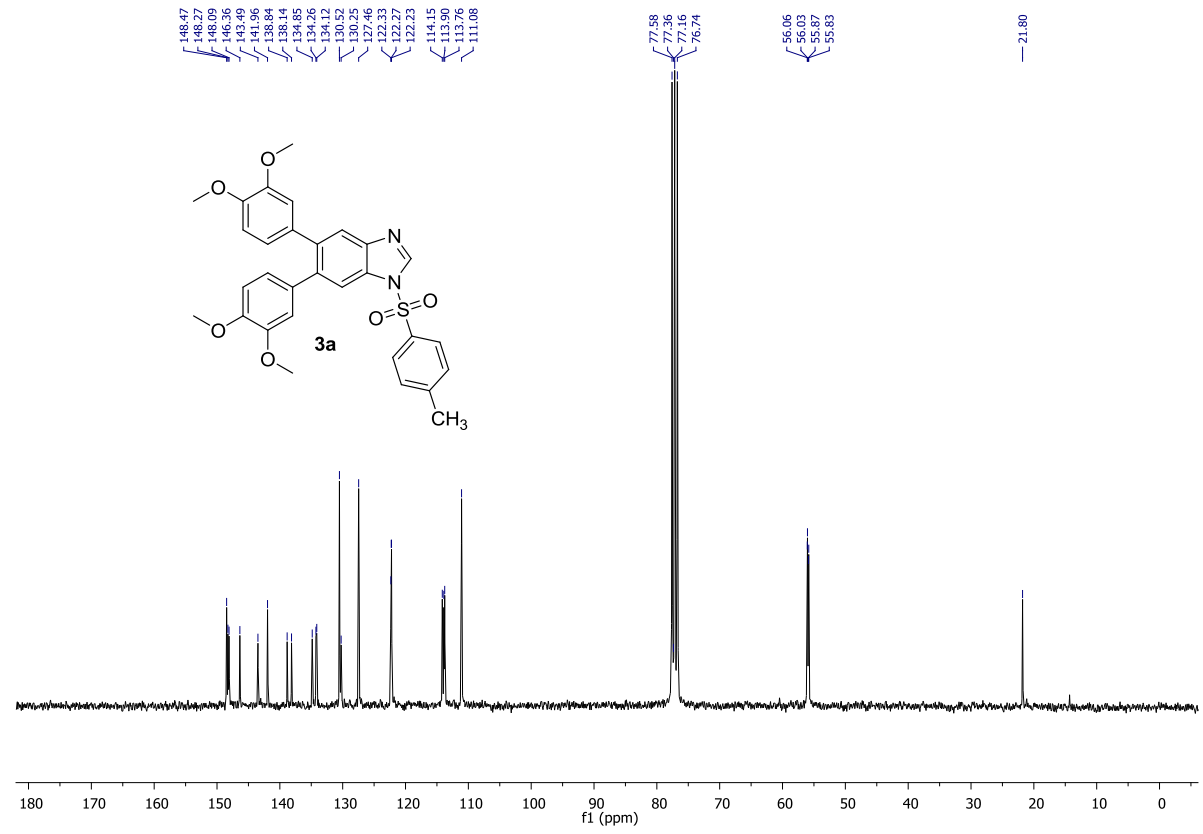
2.25
2.13
3.15
3.18
6.14
3.00
f1 (ppm)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138.14
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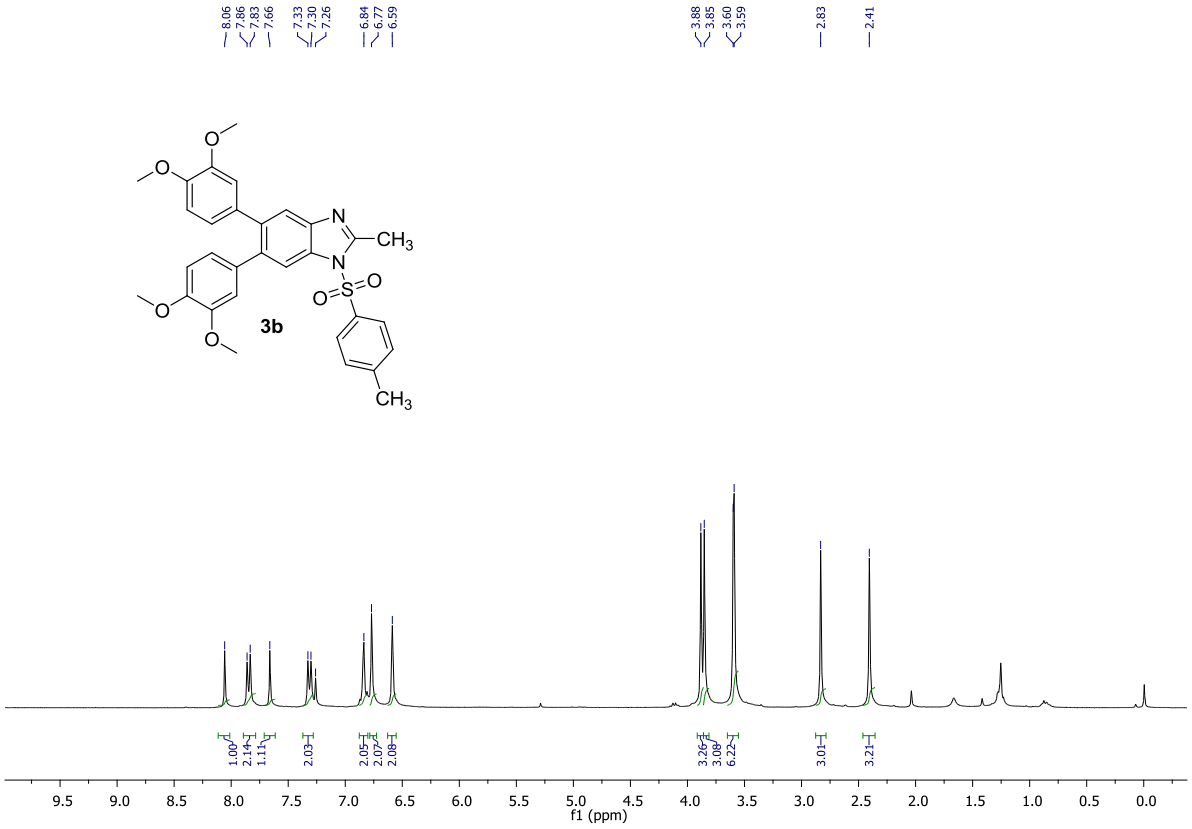
134.26
134.12
130.52
130.25
127.46
122.33
122.27
122.23
114.15
113.90
113.76
111.08
77.58
77.36
77.16
76.74
56.06
56.03
55.87
55.83
21.80
3a
f1 (ppm)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7.86
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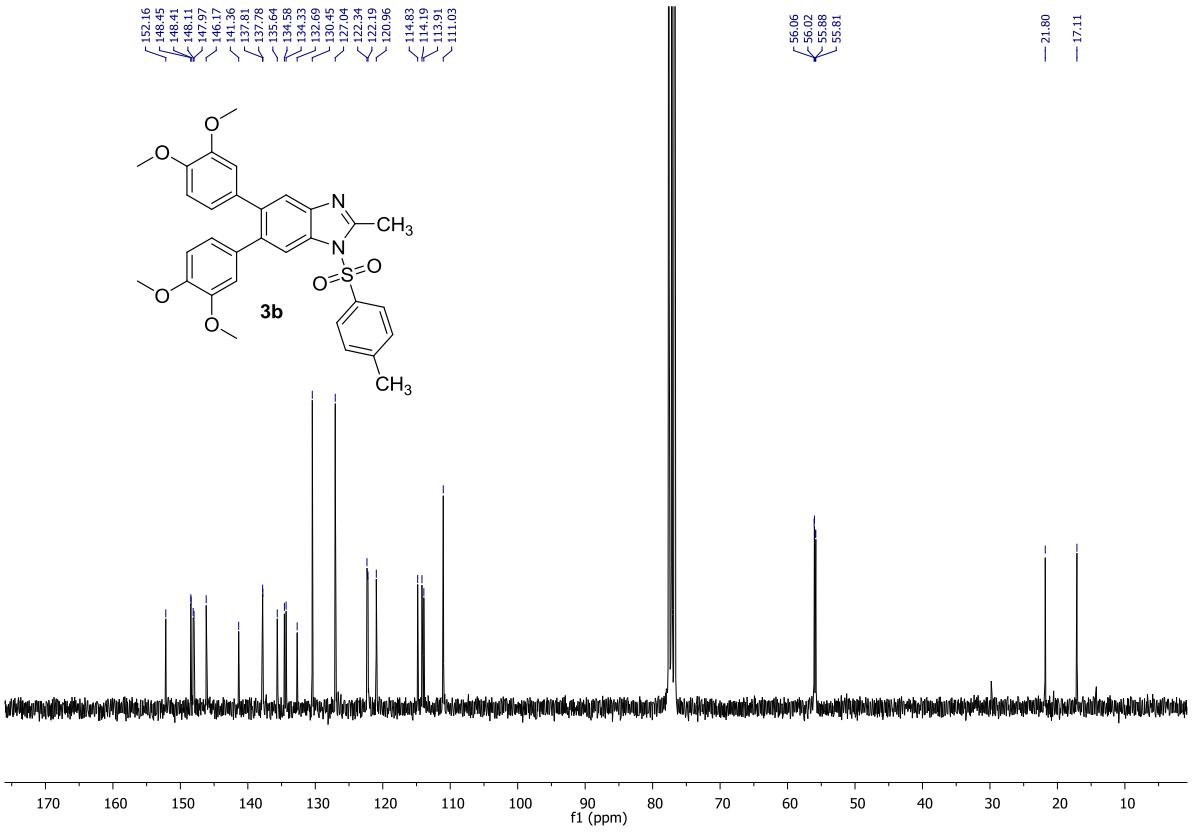
7.30
7.26
6.84
6.77
6.59
3.88
3.85
3.60
3.59
2.83
2.41
3b
1.00
2.14
1.11
2.03
2.05
2.07
2.08
3.26
3.08
6.22
3.01
3.21
f1 (ppm)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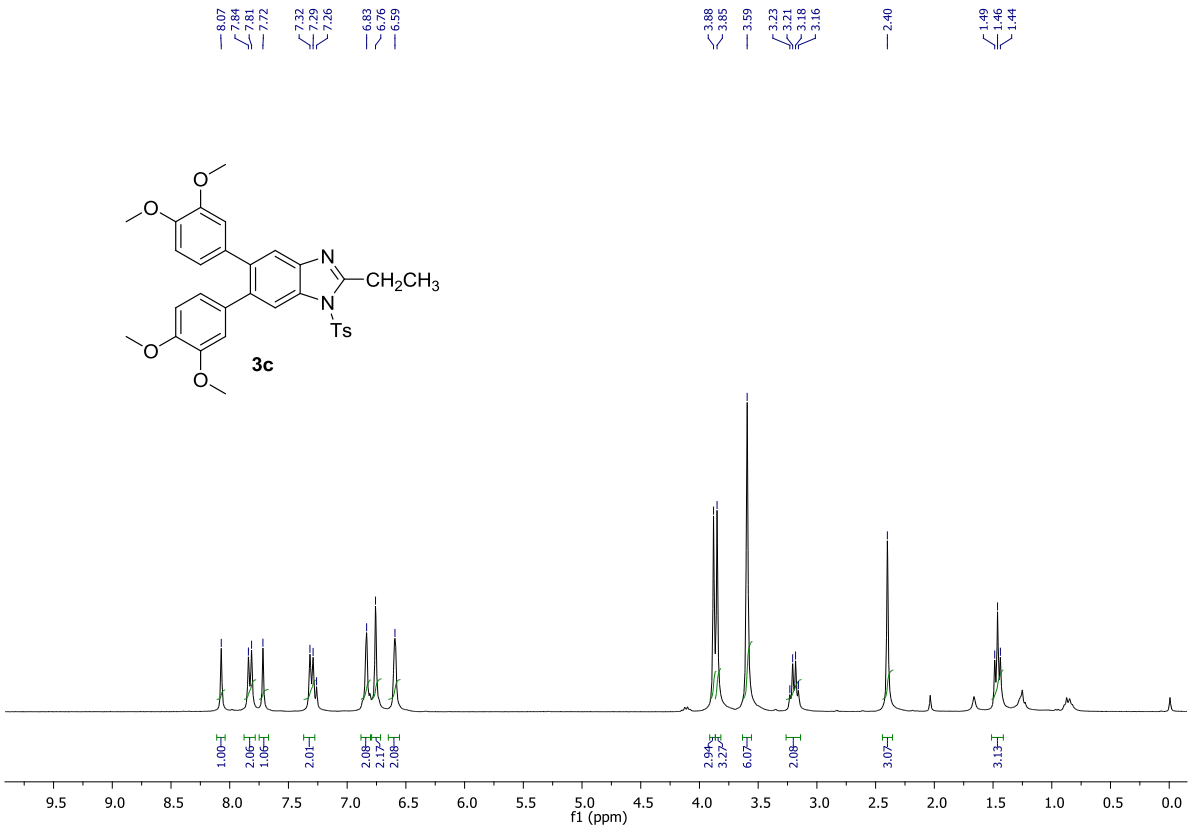
134.33
132.69
130.45
127.04
122.34
122.19
120.96
114.83
114.19
113.91
111.03
56.06
56.02
55.88
55.81
21.80
17.11
3b
f1 (ppm)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7.26
6.83
6.76
6.59
3.88
3.85
3.59
3.23
3.21
3.18
3.16
2.40
1.49
1.46
1.44
O
O
O
O
N
N
CH2CH3
Ts
3c
1.00
2.06
1.06
2.01
2.08
2.17
2.08
2.94
3.27
6.07
2.08
3.07
3.13
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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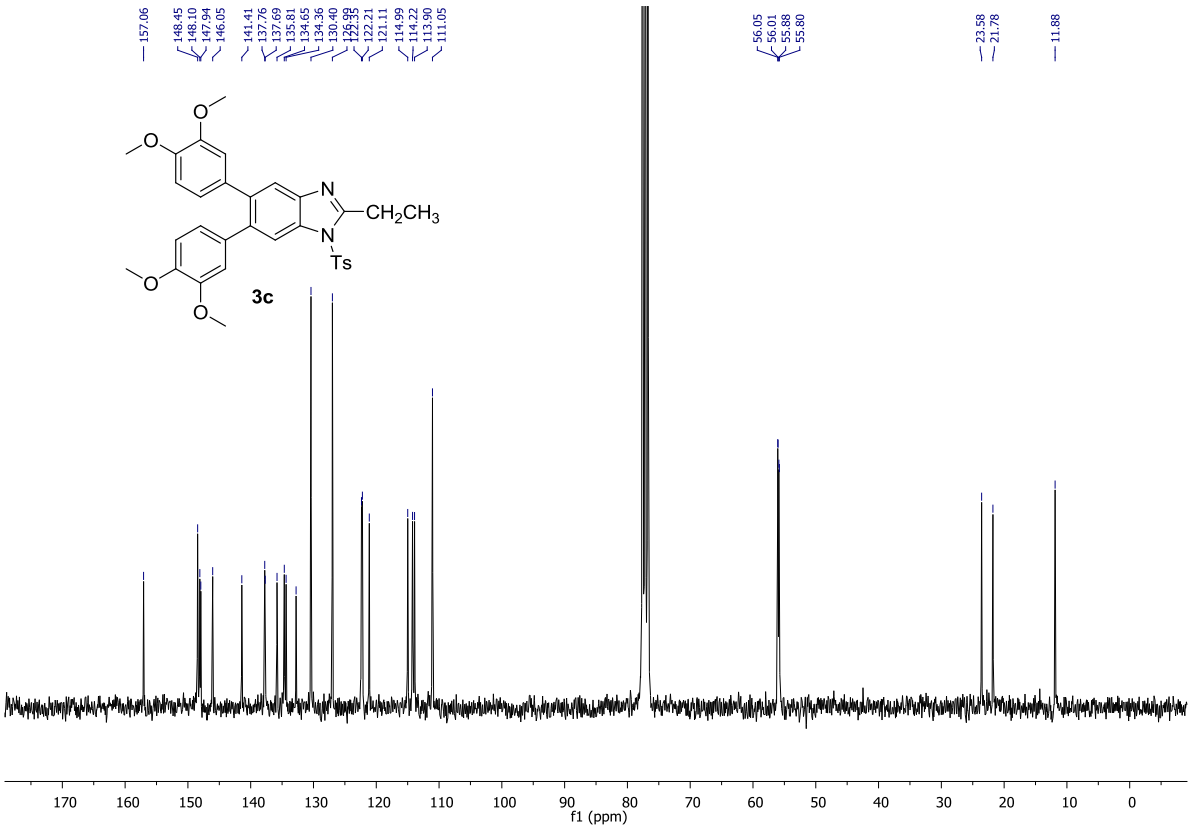
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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148.10
147.94
146.05
141.41
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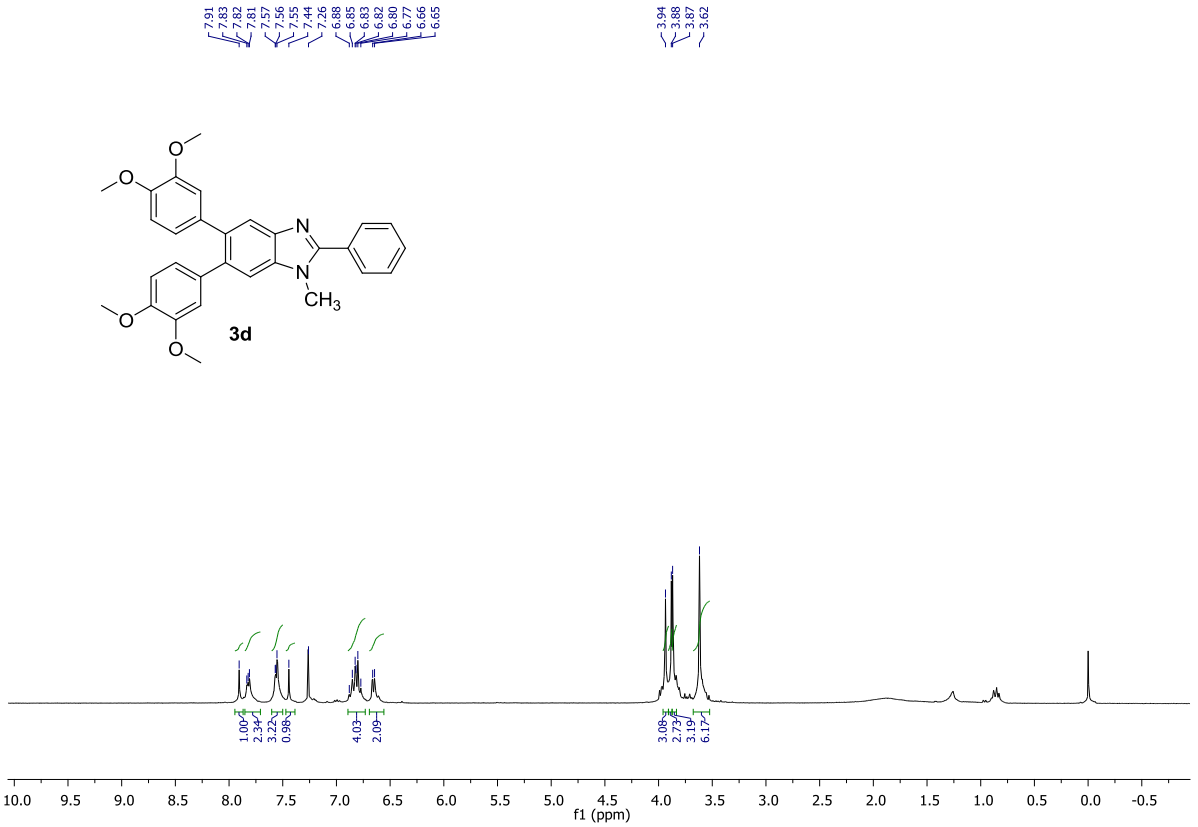
137.69
135.81
134.65
134.36
130.40
122.21
121.11
114.99
114.22
113.90
111.05
56.05
56.01
55.88
55.80
23.58
21.78
11.88
O
O
O
O
N
N
CH2CH3
Ts
3c
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.44
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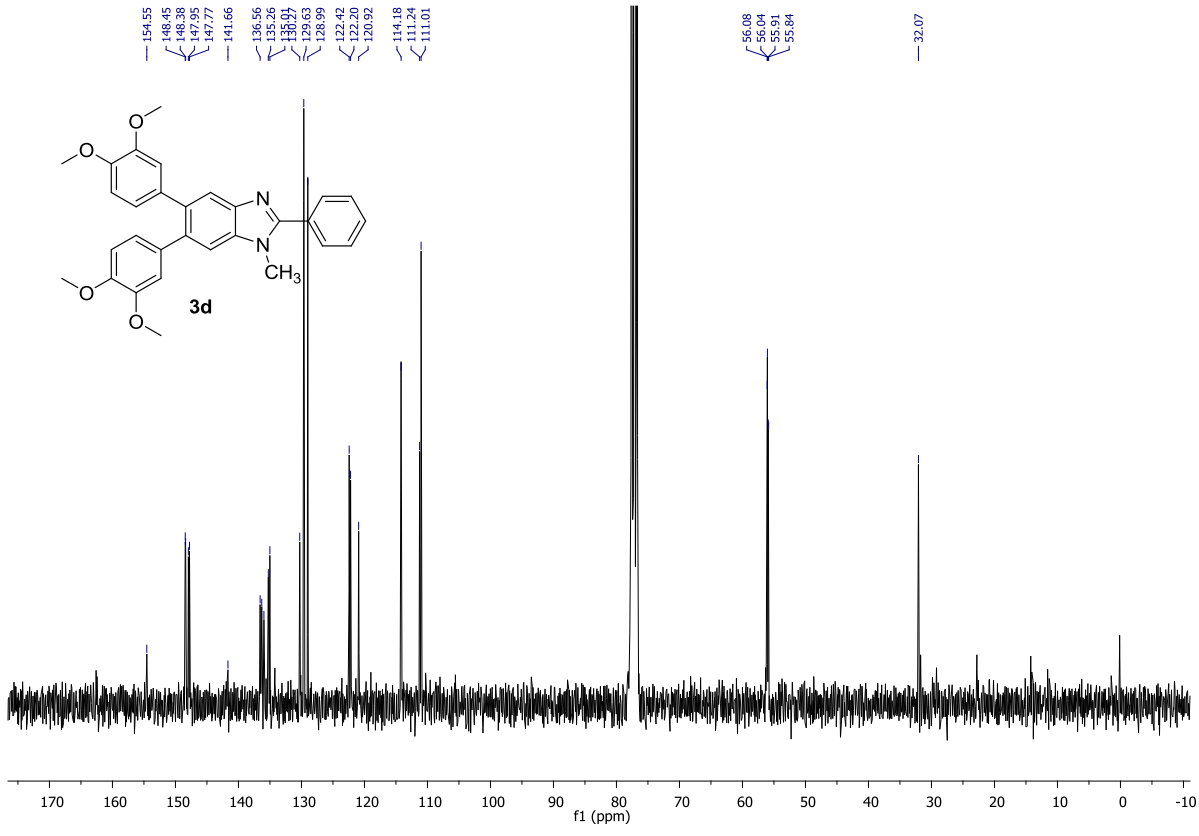
6.88
6.85
6.83
6.82
6.80
6.77
6.66
6.65
3.94
3.88
3.87
3.62
3d
1.00
2.34
3.22
0.98
4.03
2.09
3.08
2.73
3.19
6.17
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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129.63
128.99
122.42
122.20
120.92
114.18
111.24
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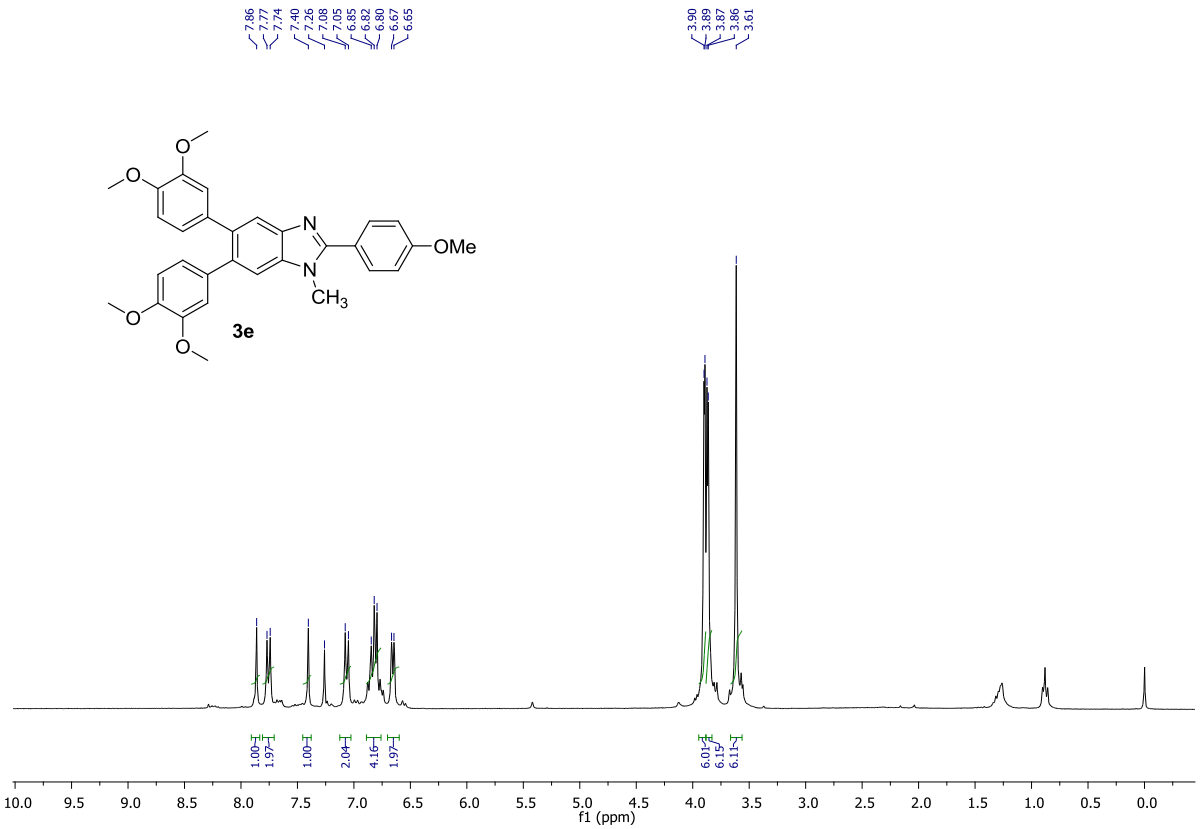
55.91
55.84
32.07
3d
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)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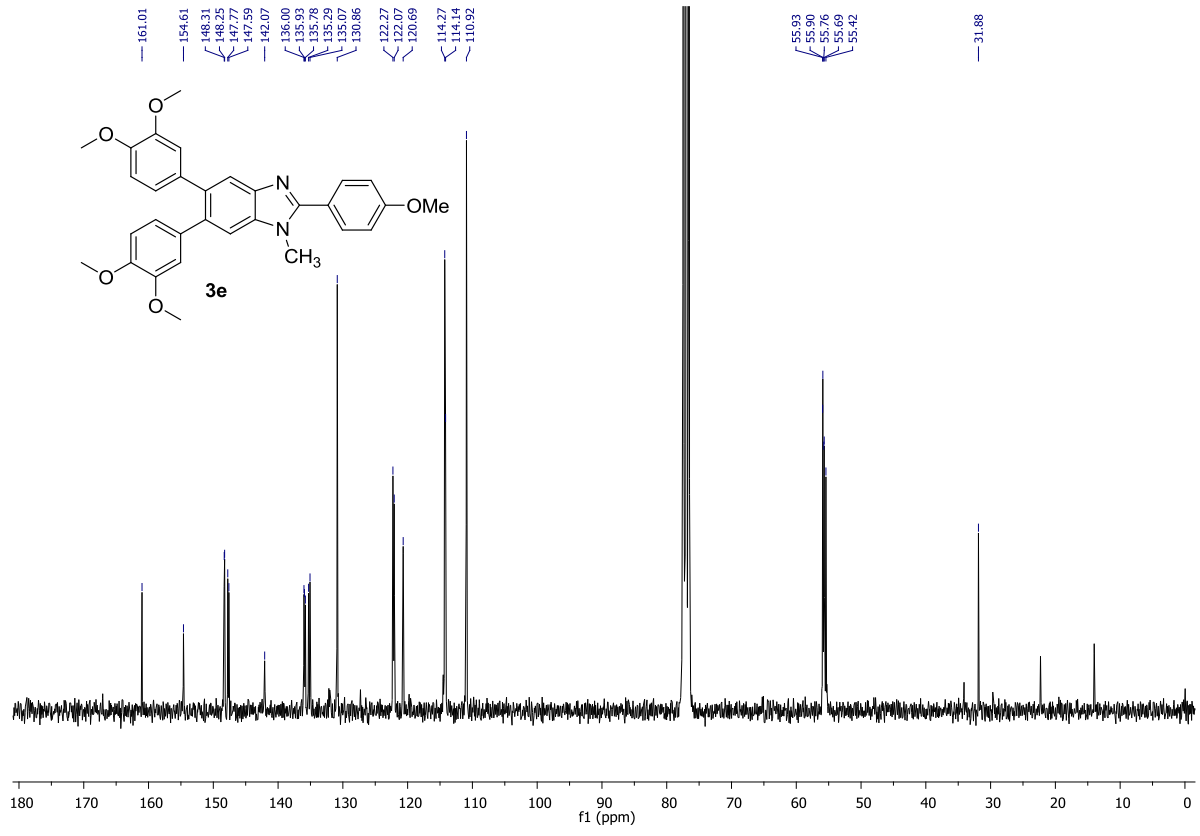
7.74
7.40
7.26
7.08
7.05
6.85
6.82
6.80
6.67
6.65
3.90
3.89
3.87
3.86
3.61
OMe
N
N
CH3
O
3e
1.00
1.97
1.00
2.04
4.16
1.97
6.01
6.15
6.11
f1 (ppm)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136.00
135.93
135.78
135.29
135.07
130.86
122.27
122.07
120.69
114.27
114.14
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55.93
55.90
55.76
55.69
55.42
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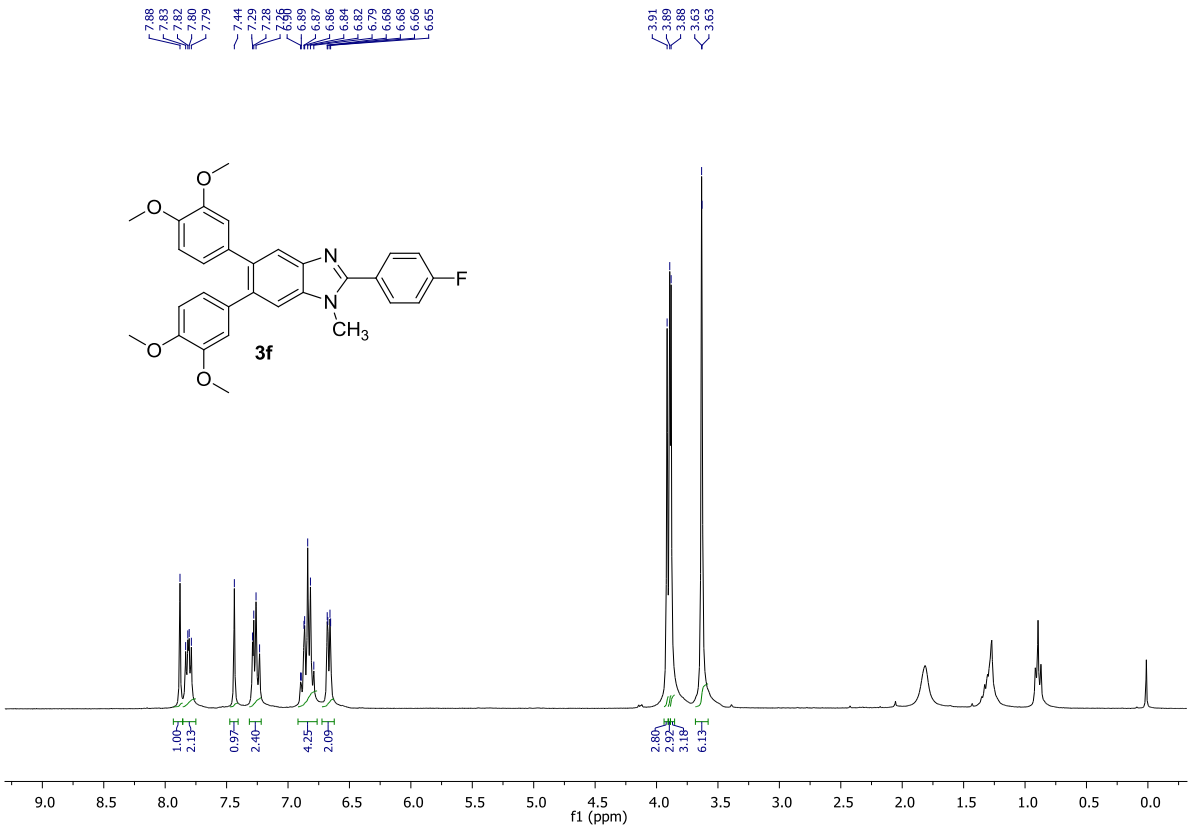
OMe
N
N
CH3
O
3e
f1 (ppm)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7.29
7.28
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6.87
6.86
6.84
6.82
6.79
6.68
6.68
6.66
6.65
3.91
3.89
3.88
3.63
3.63
O
O
O
O
N
N
CH3
F
3f
1.00
2.13
0.97
2.40
4.25
2.09
2.80
2.92
3.18
6.13
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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4.5
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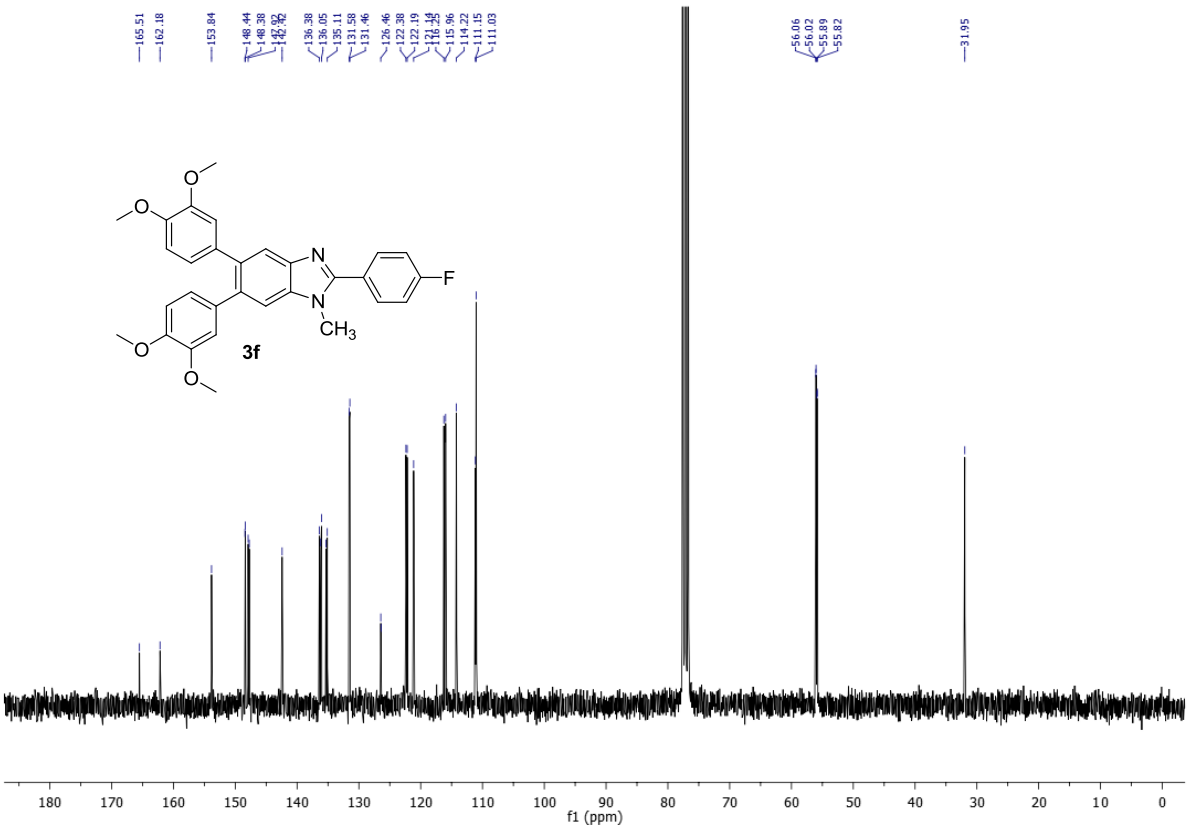
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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136.38
136.05
135.11
131.58
131.46
126.46
122.38
122.19
115.96
114.22
111.15
111.03
56.06
56.02
55.89
55.82
31.95
O
O
O
O
N
N
CH3
F
3f
180
170
160
150
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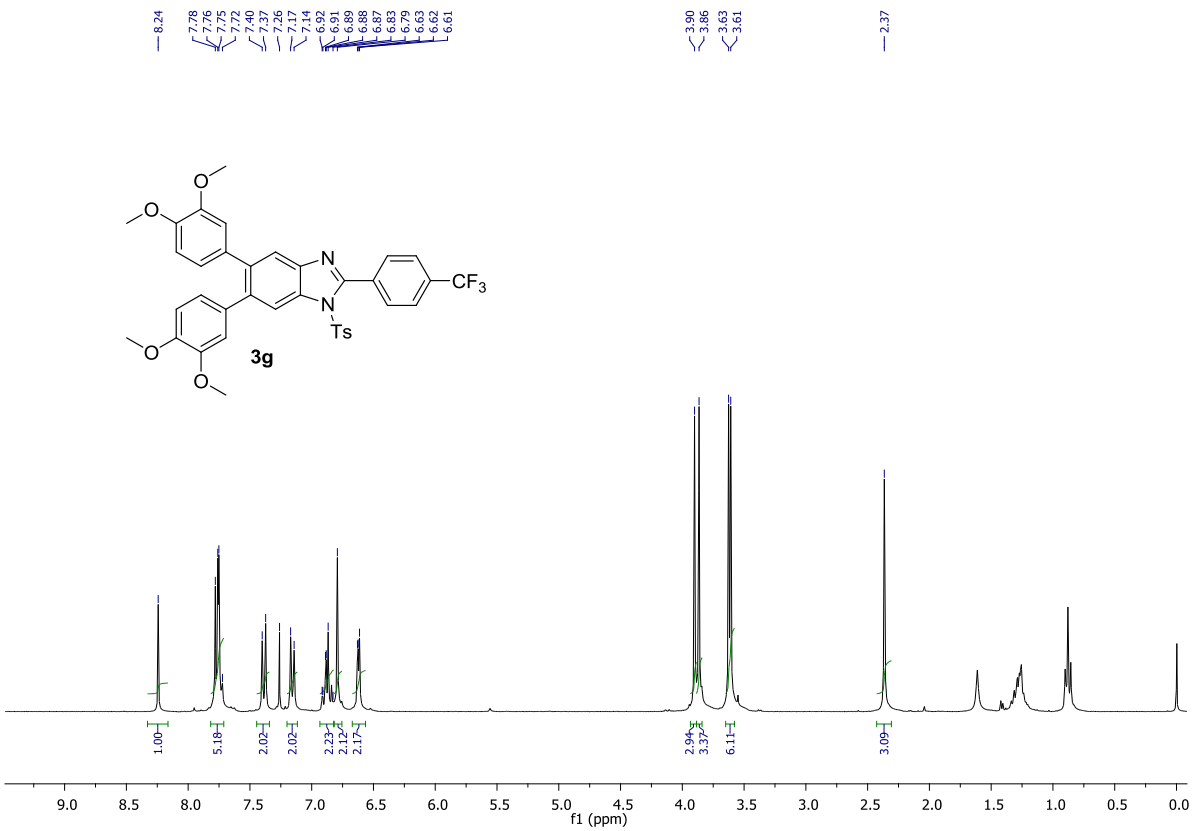
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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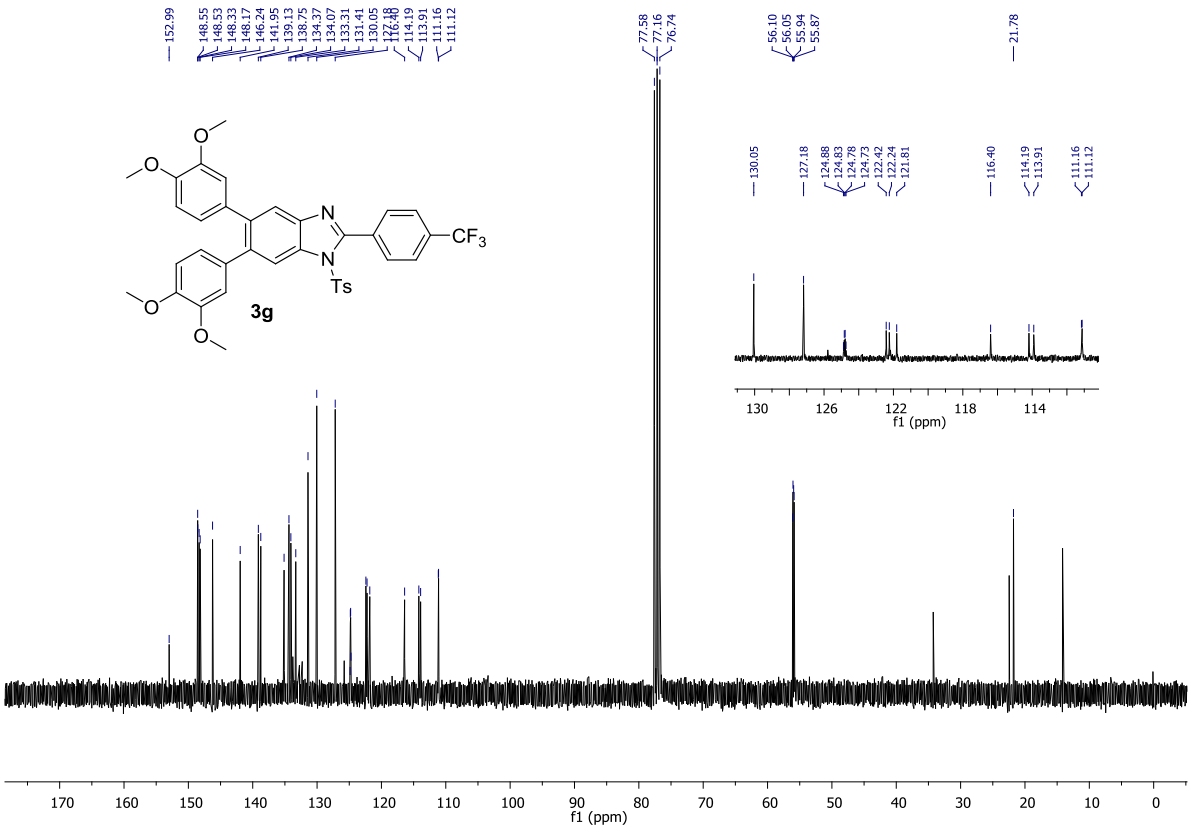
7.40
7.37
7.26
7.17
7.14
6.92
6.91
6.89
6.88
6.87
6.83
6.79
6.63
6.62
6.61
3.90
3.86
3.63
3.61
2.37
O
O
O
O
N
N
Ts
CF3
3g
1.00
5.18
2.02
2.02
2.23
2.12
2.17
2.94
3.37
6.11
3.09
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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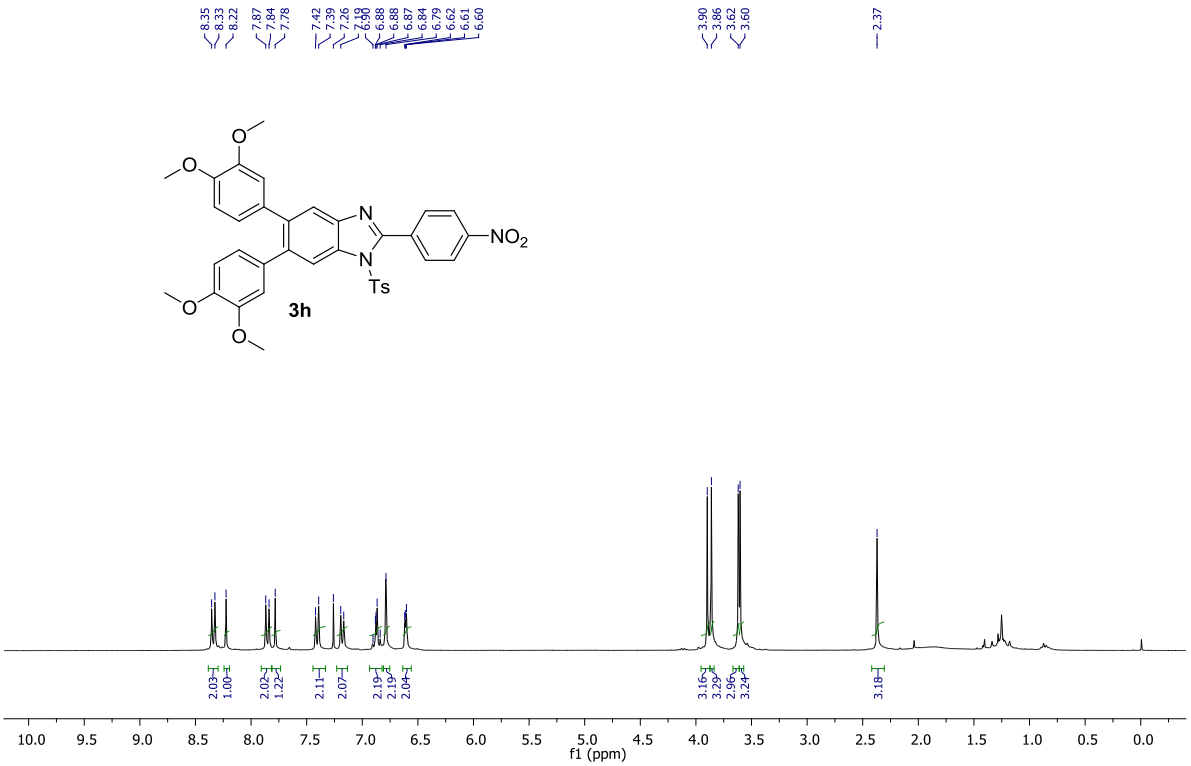
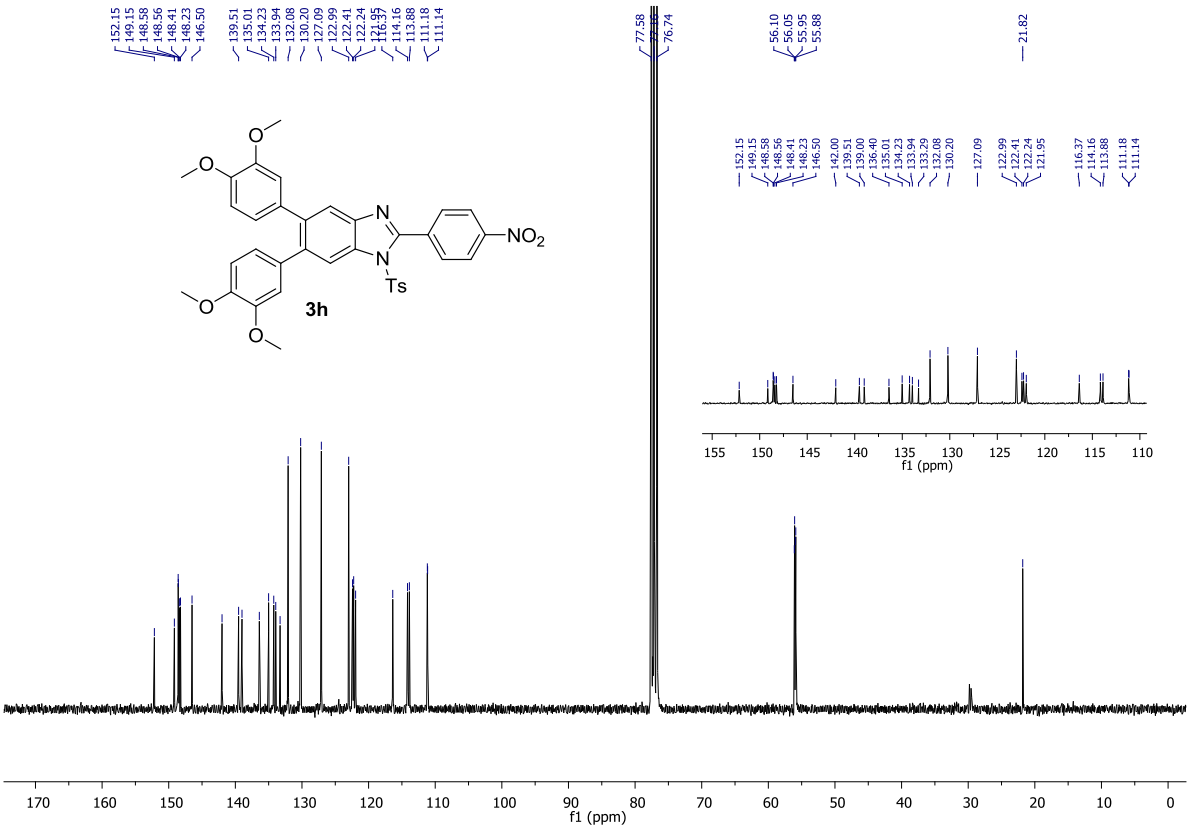
148.55
148.53
148.33
148.17
146.24
141.95
139.13
138.75
134.37
134.07
133.31
131.41
130.05
127.18
116.40
114.19
113.91
111.16
111.12
77.58
77.16
76.74
56.10
56.05
55.94
55.87
21.78
130.05
127.18
124.88
124.83
124.78
124.73
122.42
122.24
121.81
116.40
114.19
113.91
111.16
111.12
O
O
O
O
N
N
Ts
CF3
3g
130
126
122
118
114
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.35
8.33
8.22
7.87
7.84
7.78
7.42
7.39
7.26
7.19
6.90
6.88
6.87
6.84
6.79
6.62
6.61
6.60
3.90
3.86
3.62
3.60
2.37
O
O
O
O
N
N
Ts
NO2
3h
2.03
1.00
2.02
1.22
2.11
2.07
2.19
2.19
2.04
3.16
3.29
2.96
3.24
3.18
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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148.23
146.50
139.51
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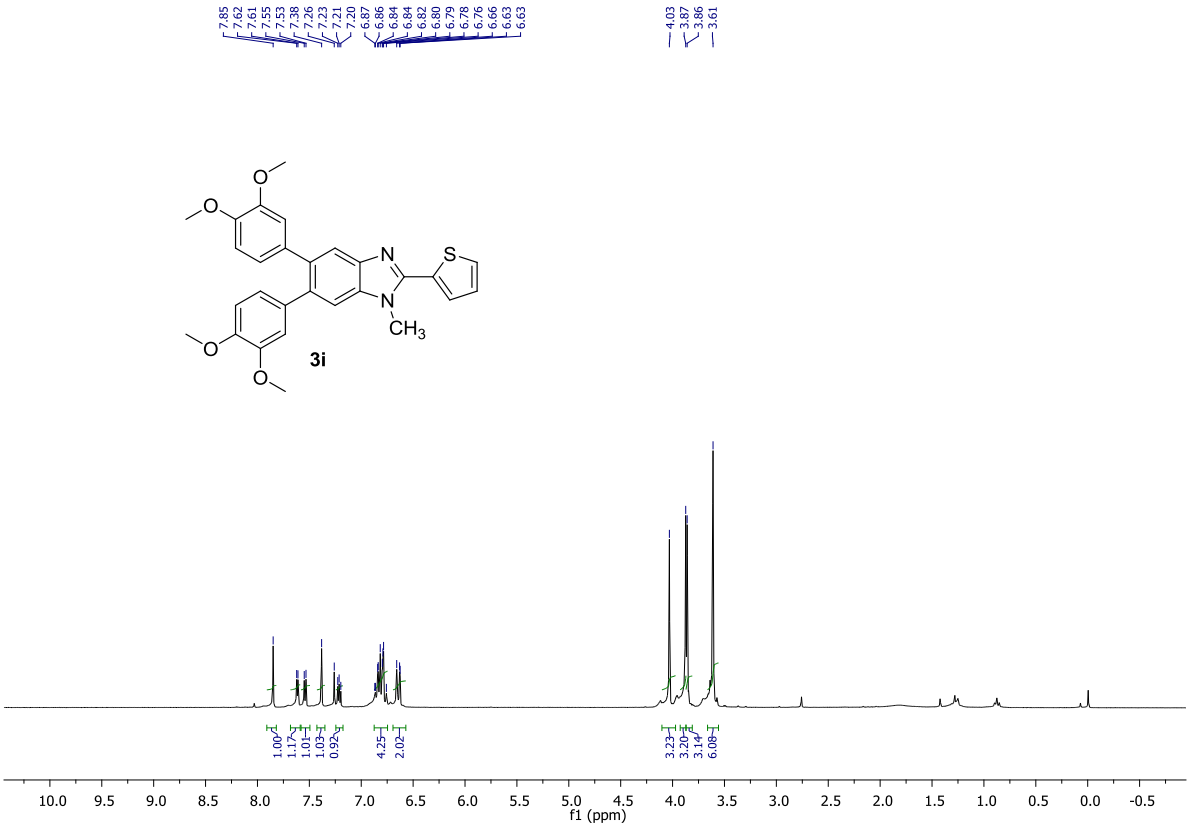
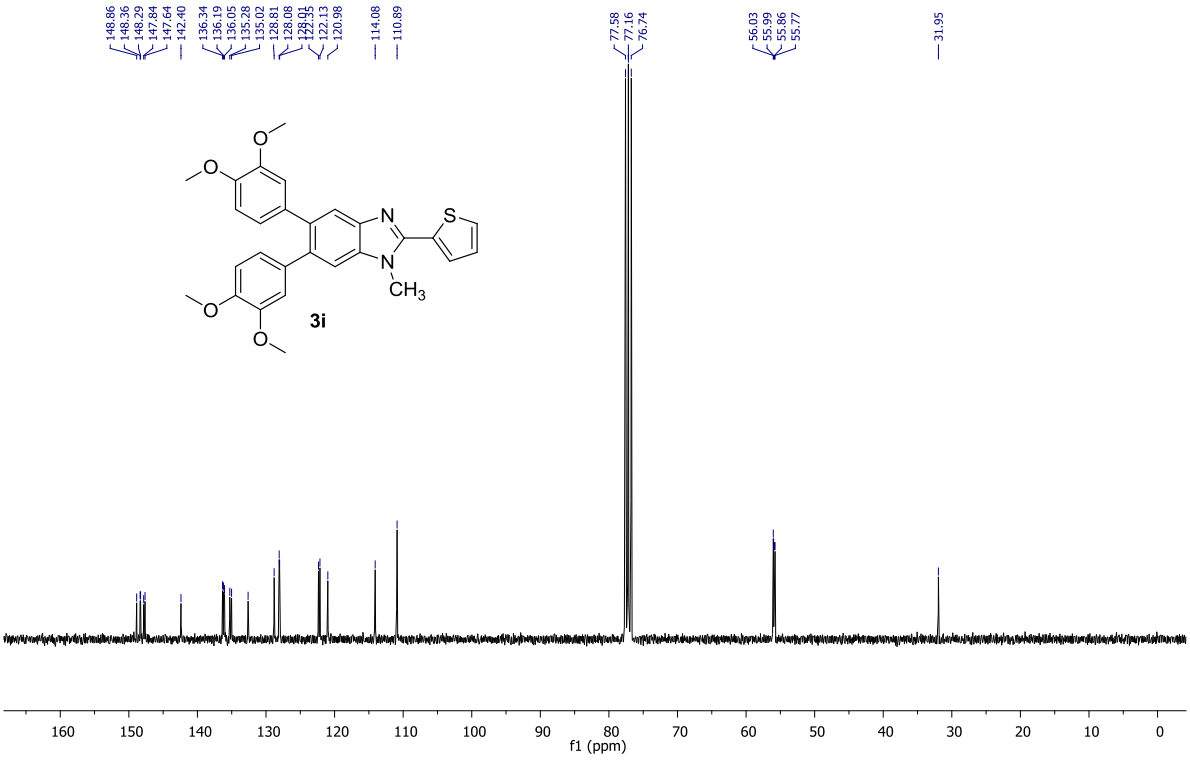
134.23
133.94
132.08
130.20
127.09
122.99
122.41
122.24
116.37
114.16
113.88
111.18
111.14
77.58
77.16
76.74
56.10
56.05
55.95
55.88
21.82
O
O
O
O
N
N
Ts
NO2
3h
142.00
139.51
139.00
136.40
135.01
134.23
133.94
133.29
132.08
130.20
127.09
122.99
122.41
122.24
121.95
116.37
114.16
113.88
111.18
111.14
155
150
145
140
135
130
125
120
115
110
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


7.85
7.62
7.61
7.55
7.53
7.38
7.26
7.23
7.21
7.20
6.87
6.86
6.84
6.84
6.82
6.80
6.79
6.78
6.76
6.66
6.63
6.63
4.03
3.87
3.86
3.61
O
O
O
O
N
S
N
CH3
3i
1.00
1.17
1.01
1.03
0.92
4.25
2.02
3.23
3.20
3.14
6.08
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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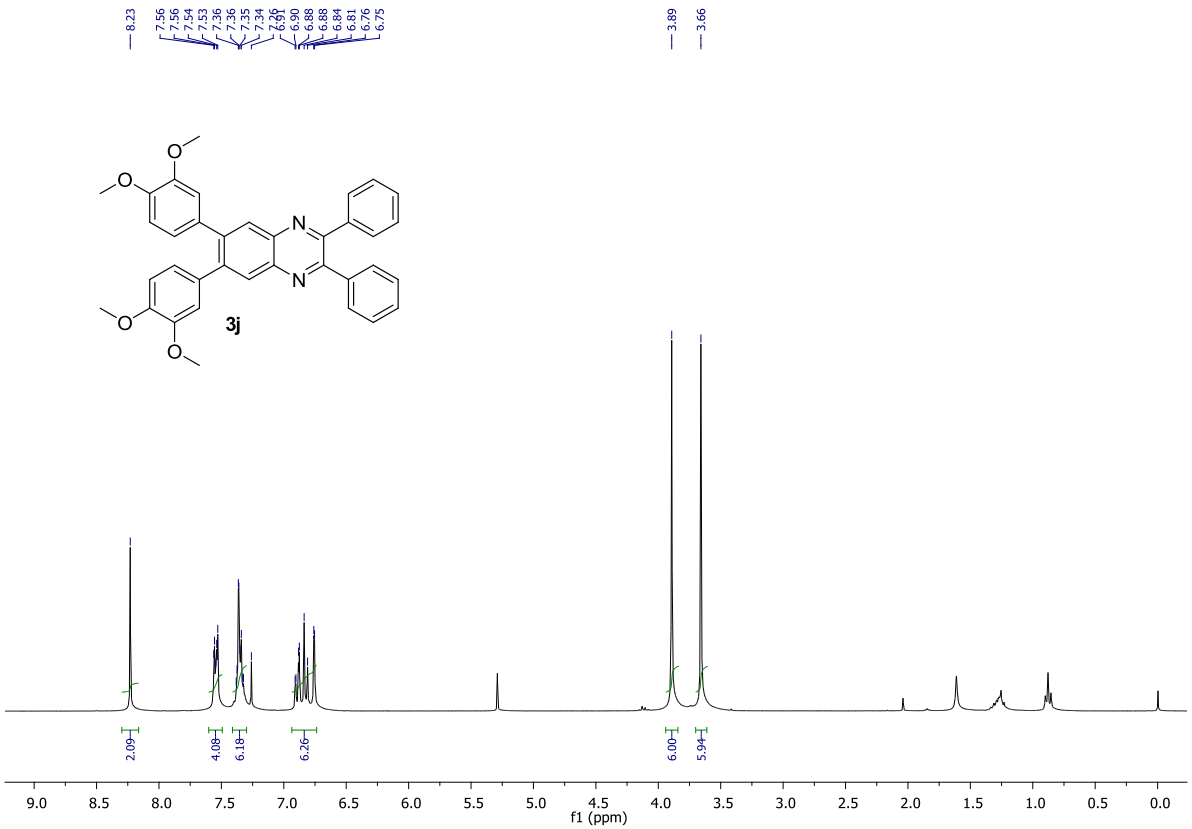
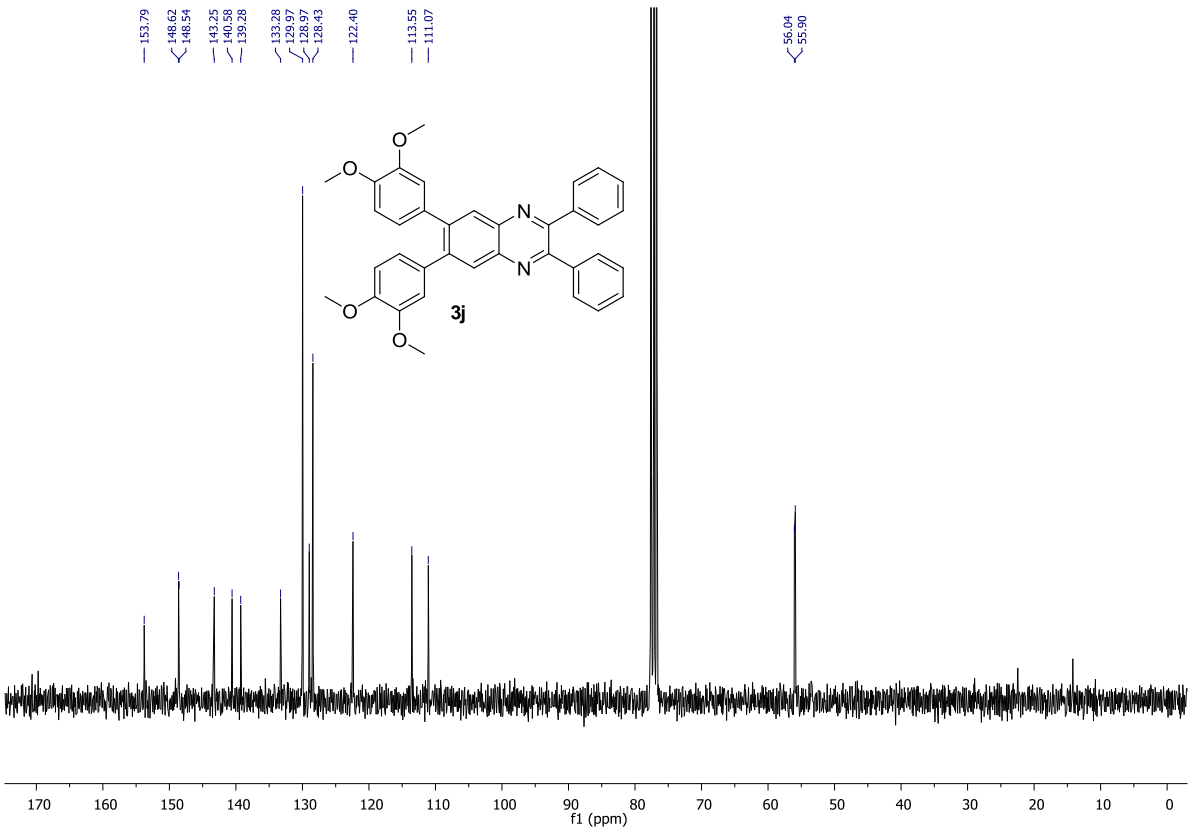
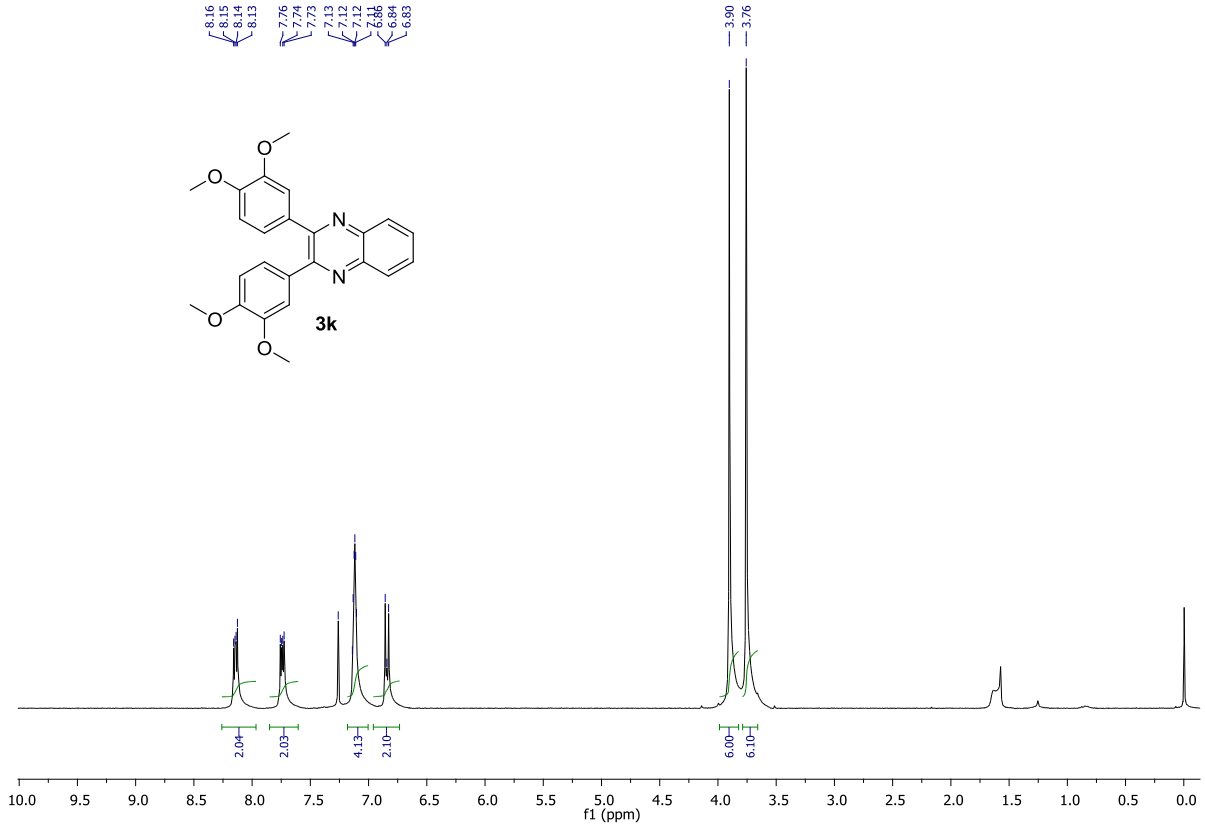
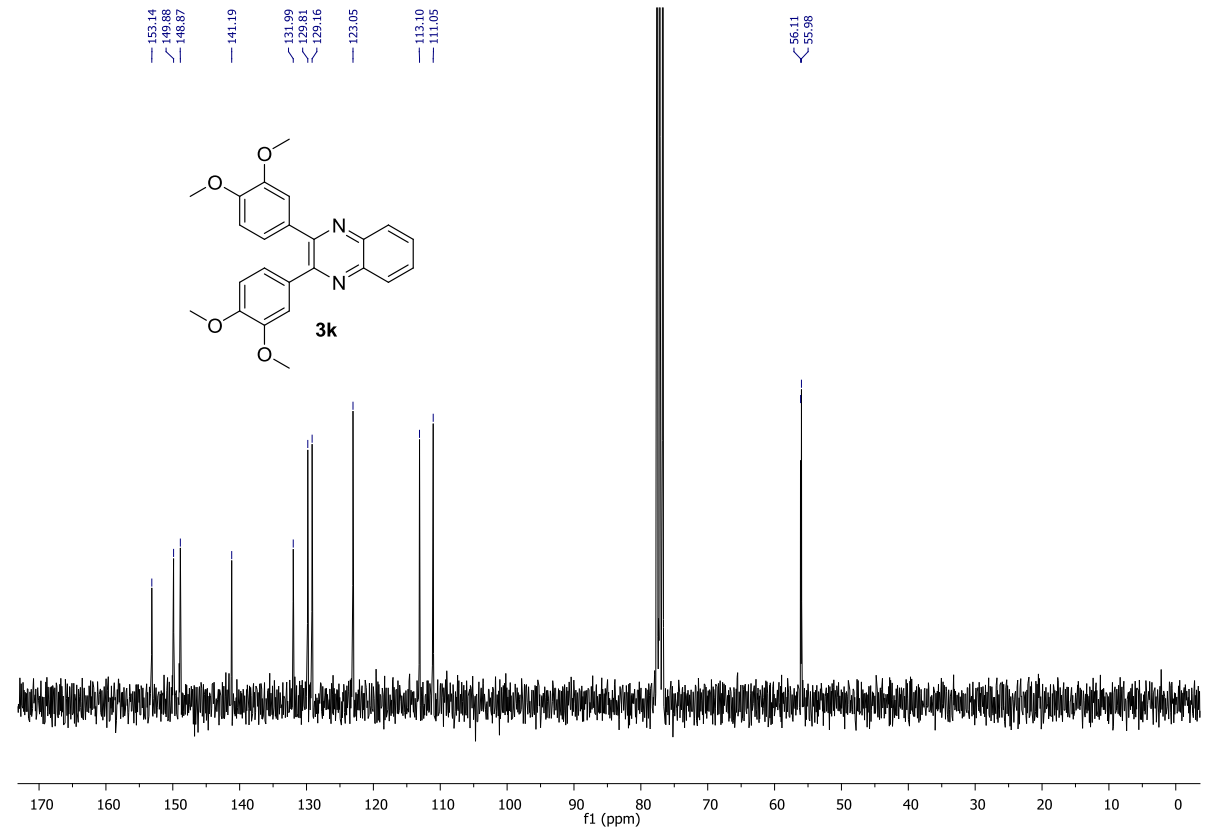
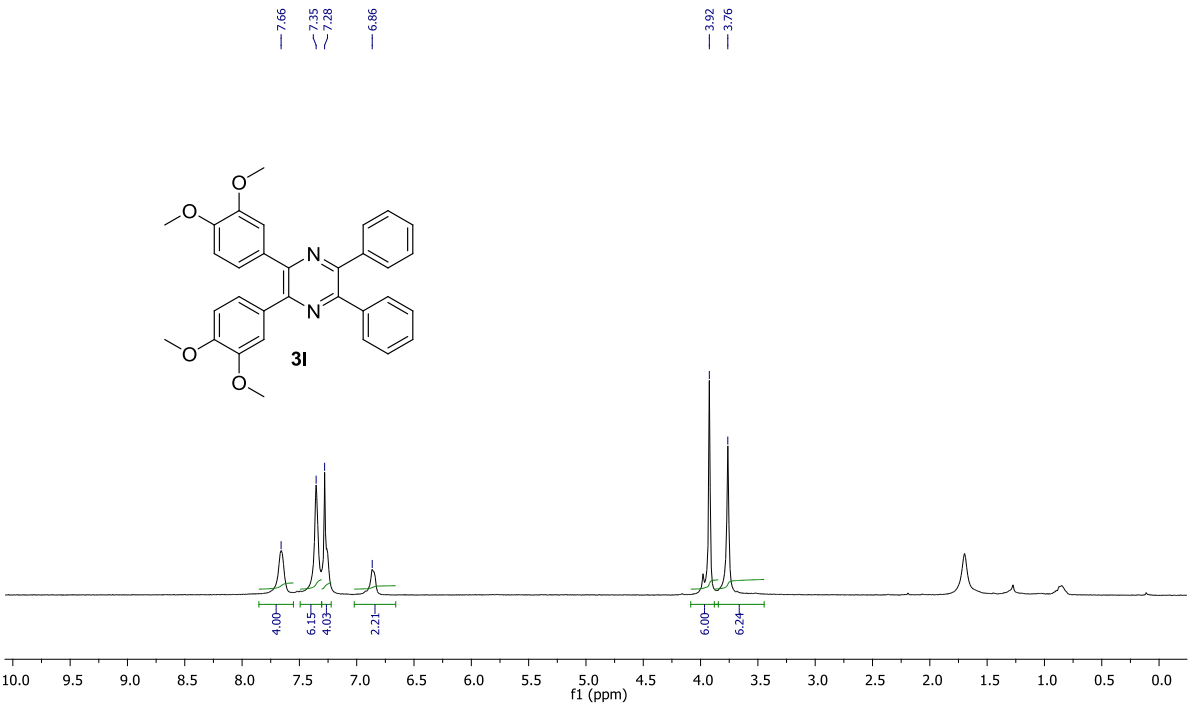
148.29
147.84
147.64
142.40
136.34
136.19
136.05
135.28
135.02
128.81
128.08
128.01
122.35
122.13
120.98
114.08
110.89
77.58
77.16
76.74
56.03
55.99
55.86
55.77
31.95
O
O
O
O
N
S
N
CH3
3i
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

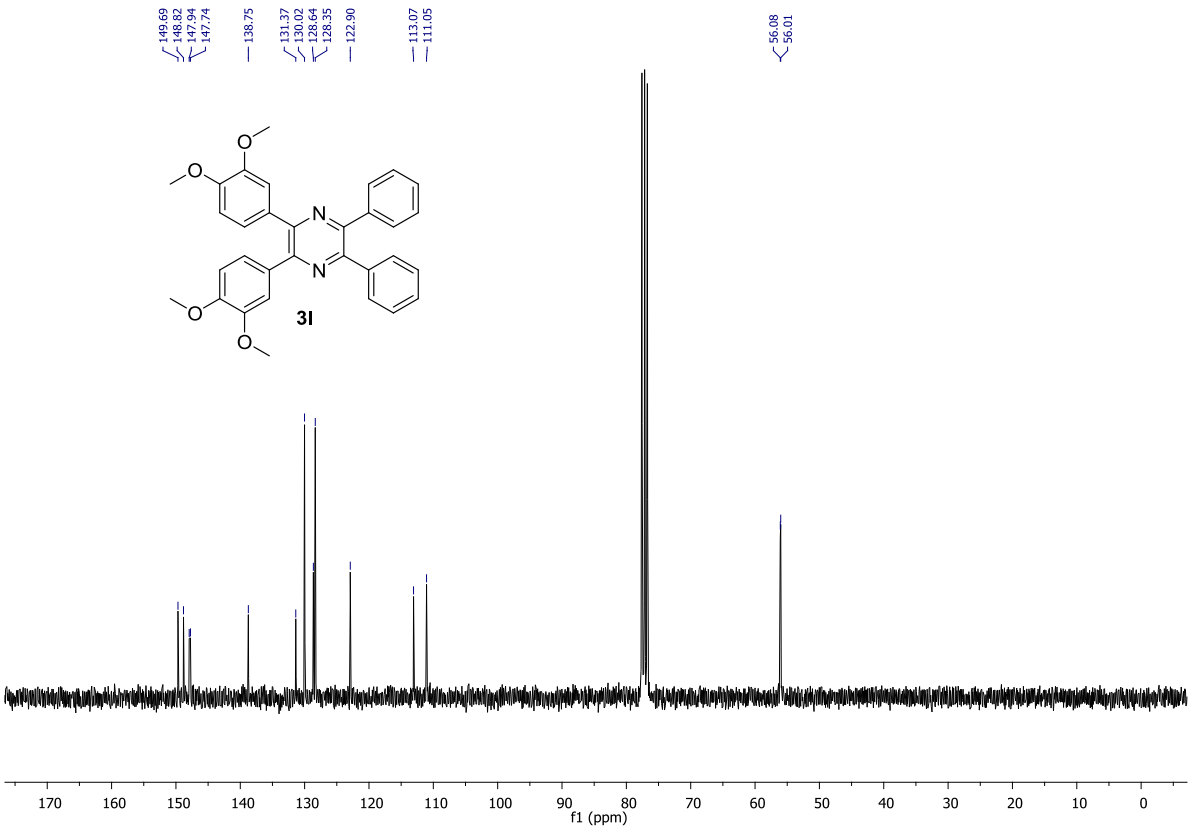

8.23
7.56
7.56
7.54
7.53
7.36
7.35
7.34
7.26
6.91
6.90
6.88
6.88
6.84
6.81
6.76
6.75
3.89
3.66
3j
2.09
4.08
6.18
6.26
6.00
5.94
f1 (ppm)


153.79
148.62
148.54
143.25
140.58
139.28
133.28
129.97
128.97
128.43
122.40
113.55
111.07
56.04
55.90
3j
f1 (ppm)


8.16
8.15
8.14
8.13
7.76
7.74
7.73
7.13
7.12
7.12
7.11
6.86
6.84
6.83
3.90
3.76
3k
2.04
2.03
4.13
2.10
6.00
6.10
f1 (ppm)


153.14
149.88
148.87
141.19
131.99
129.81
129.16
123.05
113.10
111.05
56.11
55.98
3k
f1 (ppm)


7.66
7.35
7.28
6.86
3.92
3.76
3l
4.00
6.15
4.03
2.21
6.00
6.24
f1 (ppm)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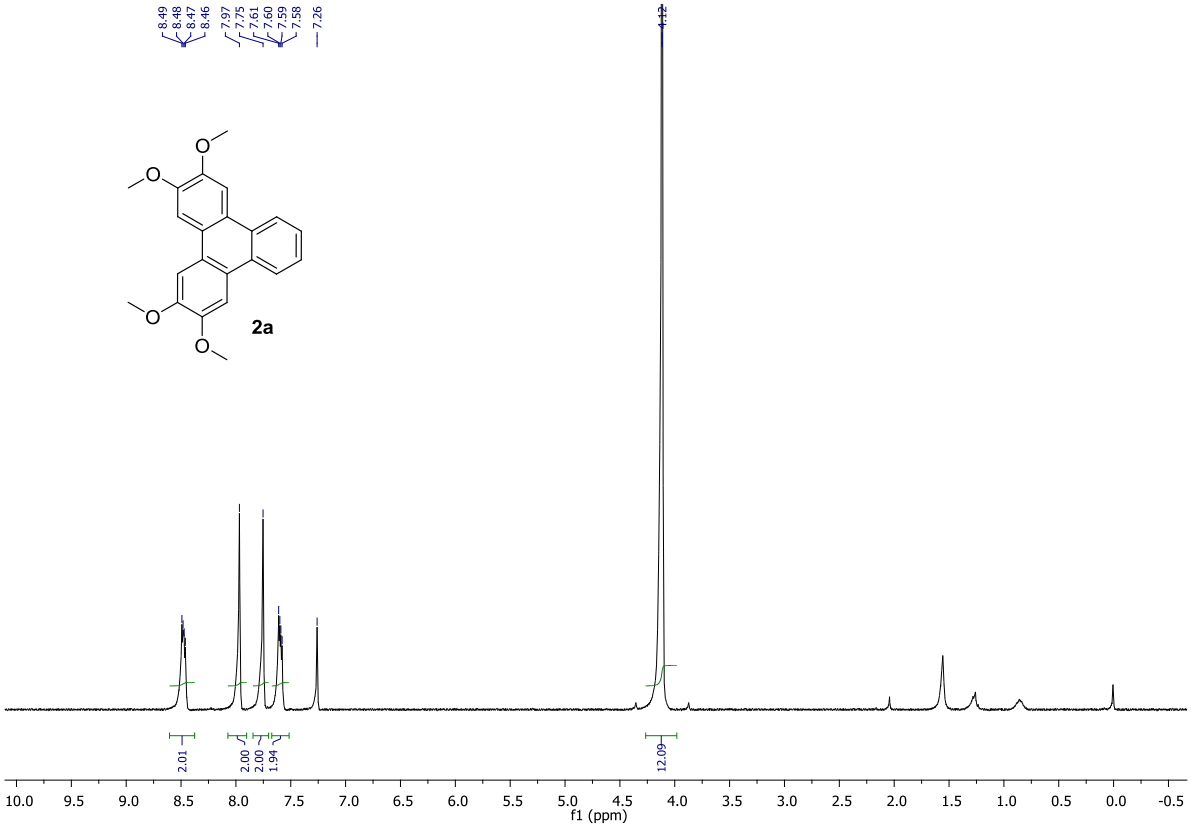
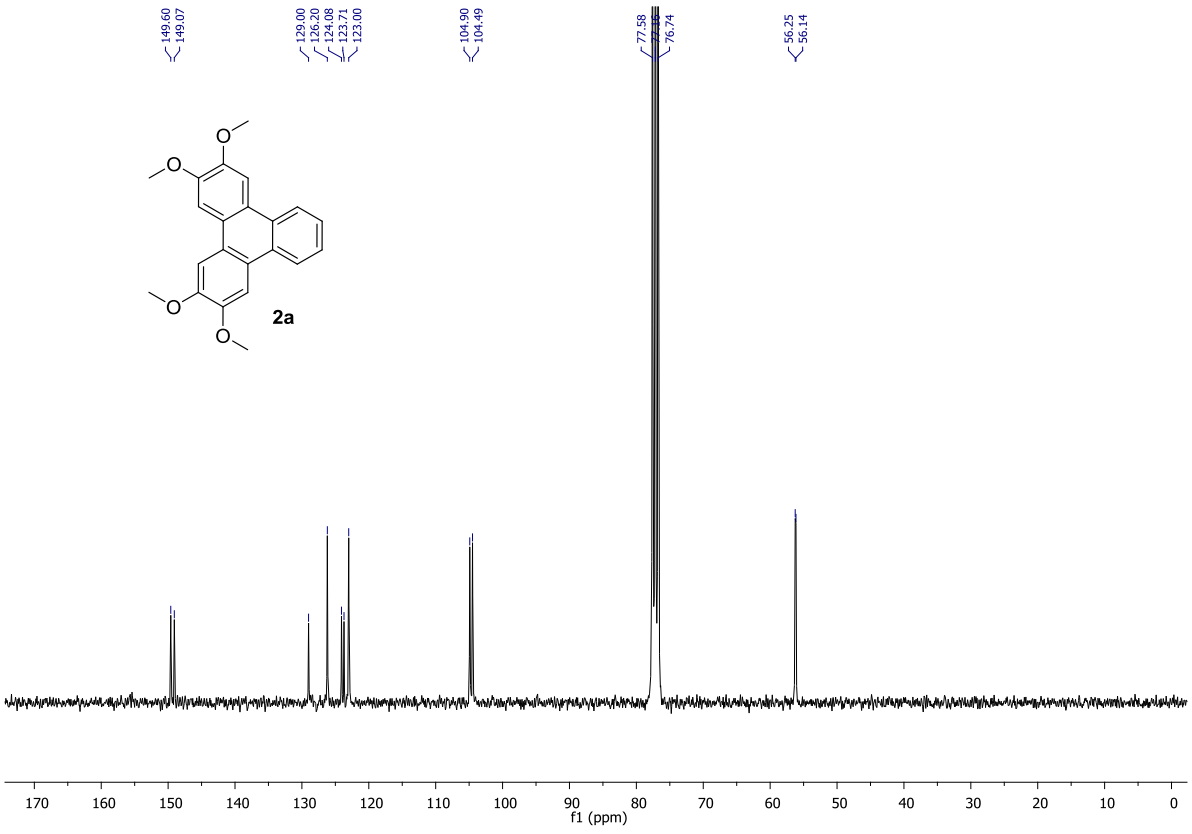
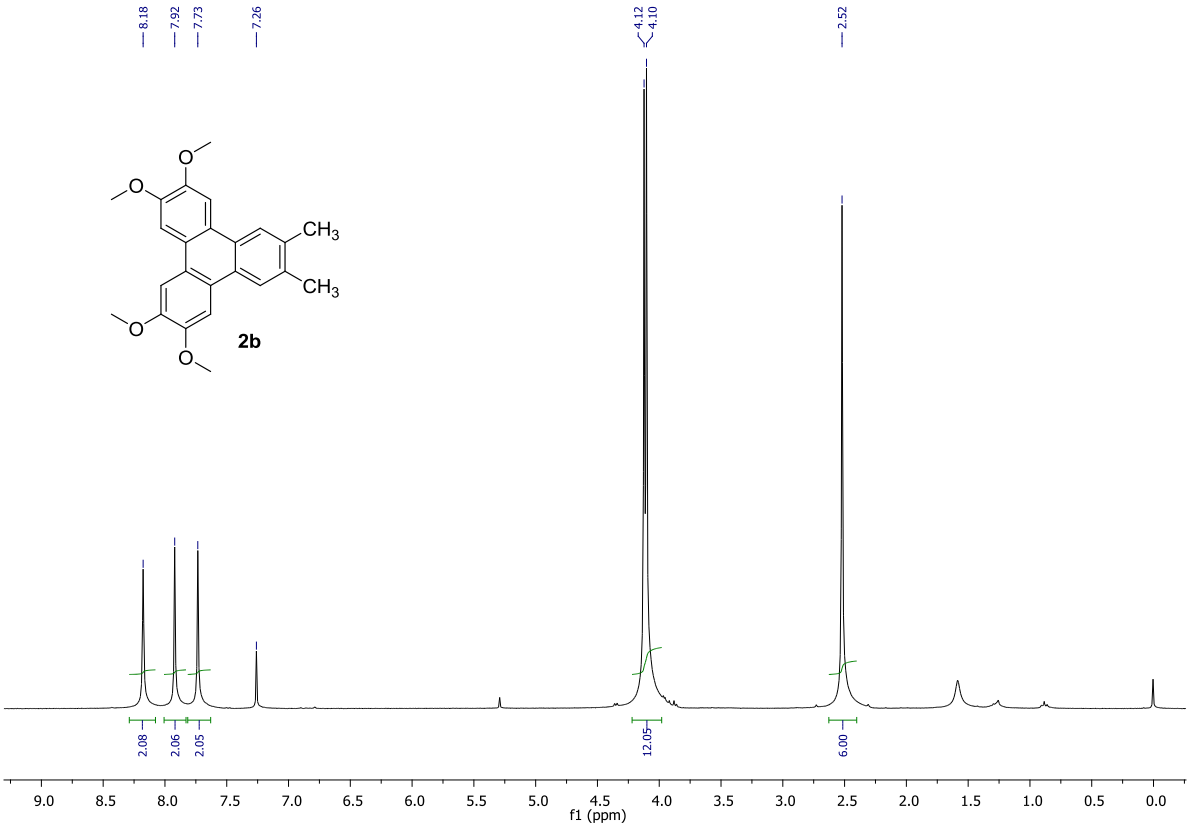
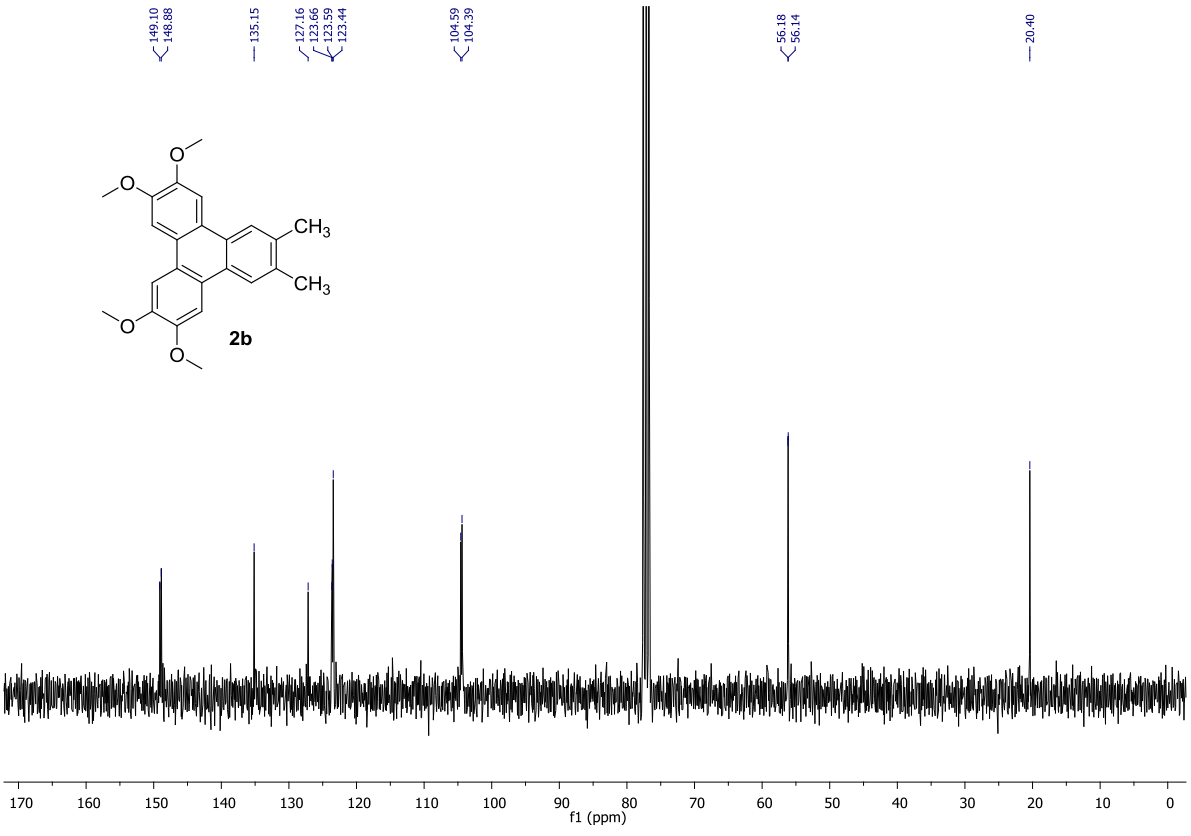
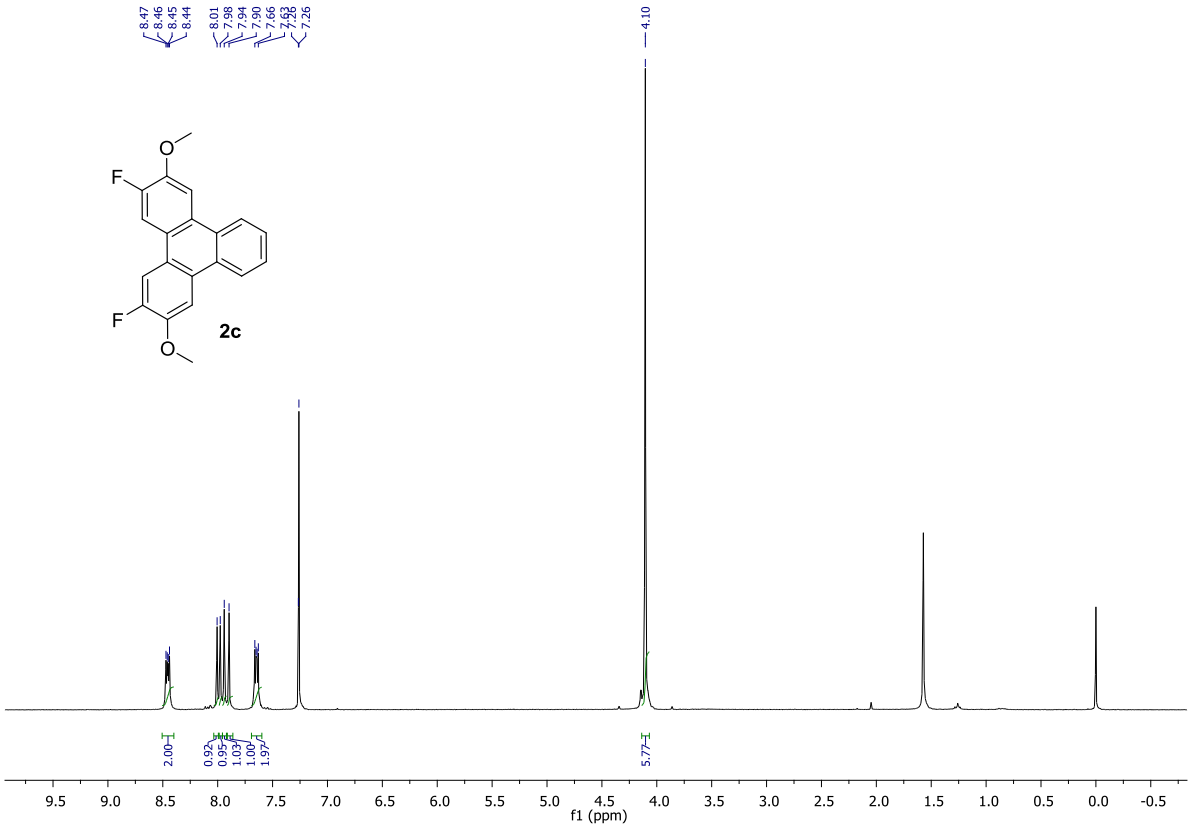
148.82
147.94
147.74
138.75
131.37
130.02
128.64
128.35
122.90
113.07
111.05
56.08
56.01
3l
f1 (ppm)

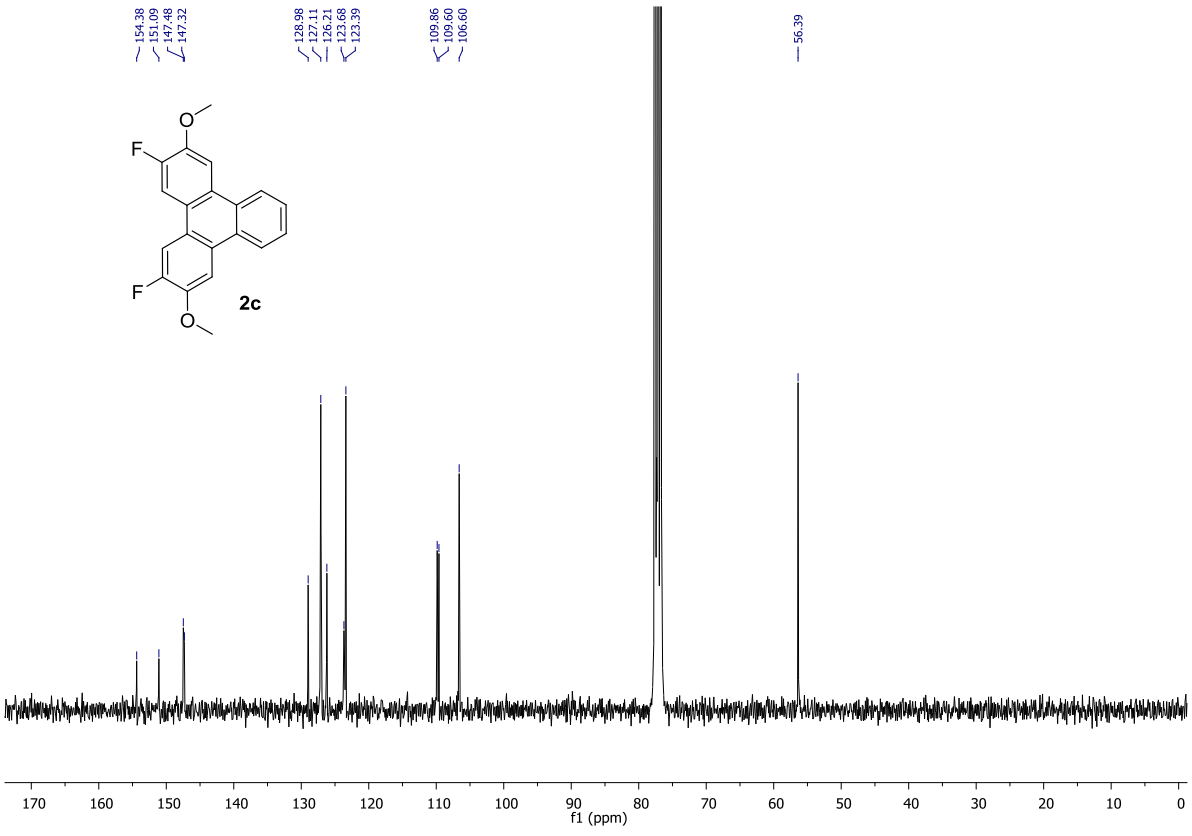

8.49
8.48
8.47
8.46
7.97
7.75
7.61
7.60
7.59
7.58
7.26
4.12
2a
2.01
2.00
2.00
1.94
12.09
f1 (ppm)

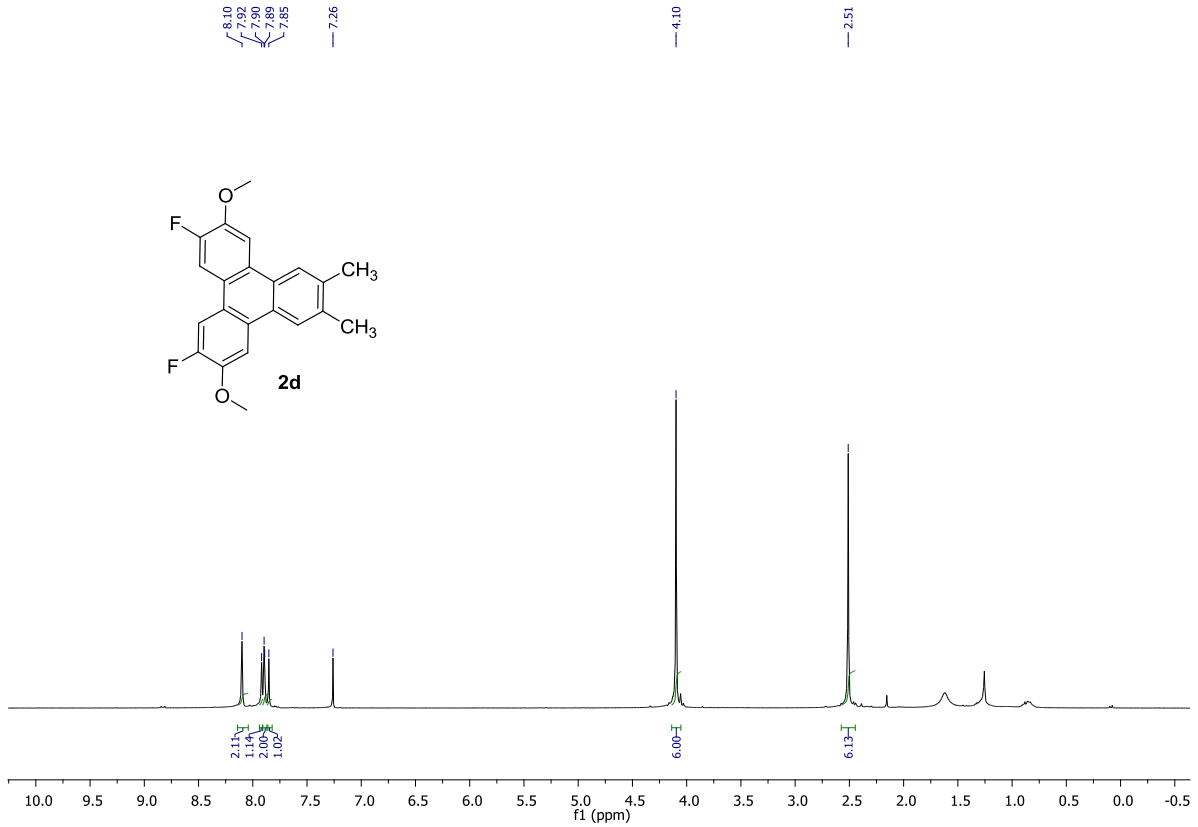

149.60
149.07
129.00
126.20
124.08
123.71
123.00
104.90
104.49
77.58
76.74
56.25
56.14
2a
f1 (ppm)

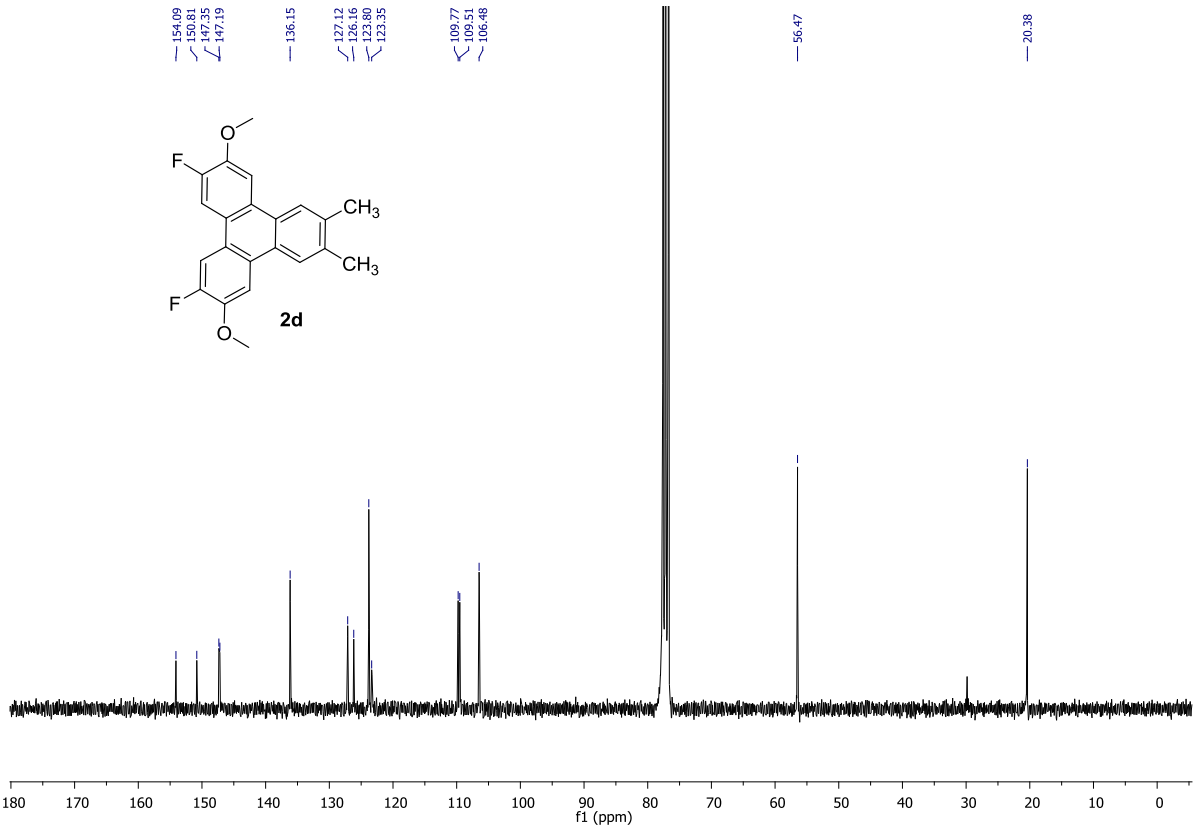

8.18
7.92
7.73
7.26
4.12
4.10
2.52
O
O
O
O
CH3
CH3
2b
2.08
2.06
2.05
12.05
6.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


149.10
148.88
135.15
127.16
123.66
123.59
123.44
104.59
104.39
56.18
56.14
20.40
O
O
O
O
CH3
CH3
2b
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.47
8.46
8.45
8.44
8.01
7.98
7.94
7.90
7.66
7.63
7.26
7.26
4.10
F
O
F
O
2c
2.00
0.92
0.95
1.03
1.00
1.97
5.77
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


154.38
151.09
147.48
147.32
128.98
127.11
126.21
123.68
123.39
109.86
109.60
106.60
56.39
F
O
F
O
2c
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.10
7.92
7.90
7.89
7.85
7.26
4.10
2.51
F
O
CH3
CH3
F
O
2d
2.11
1.14
2.00
1.02
6.00
6.13
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)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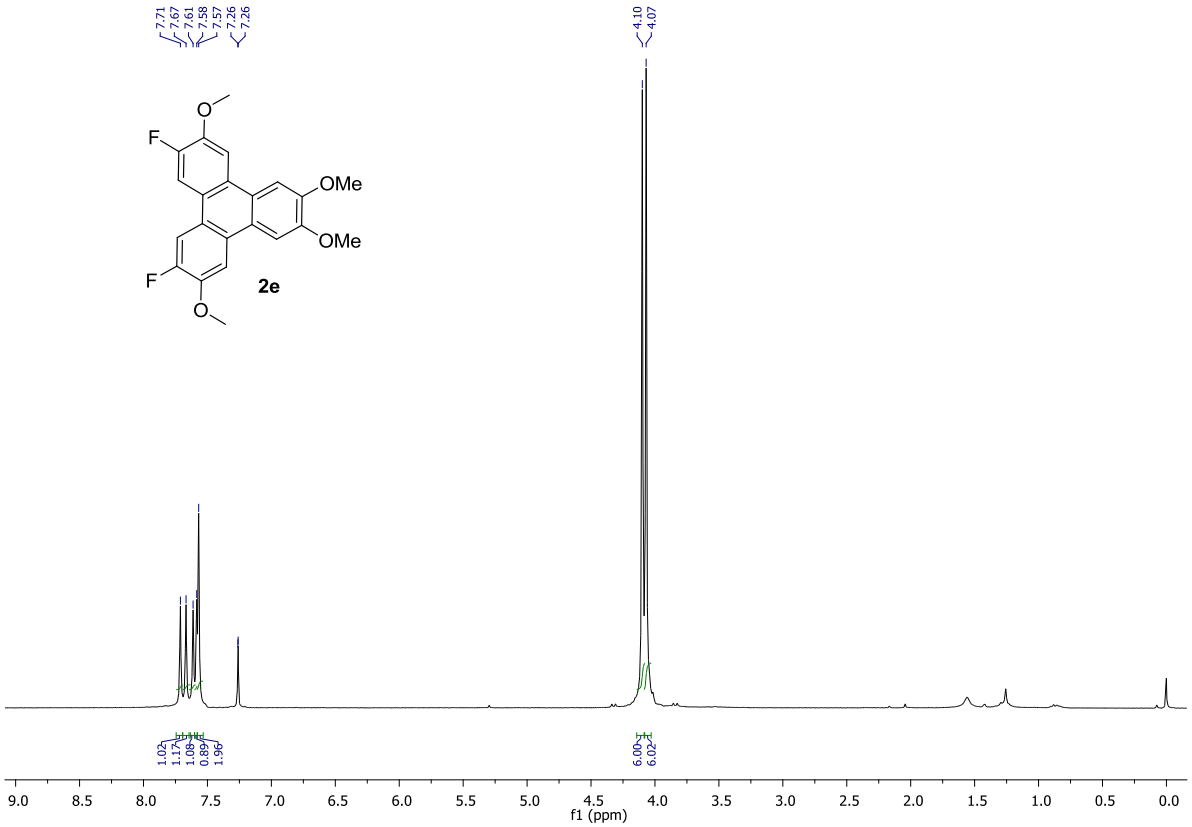
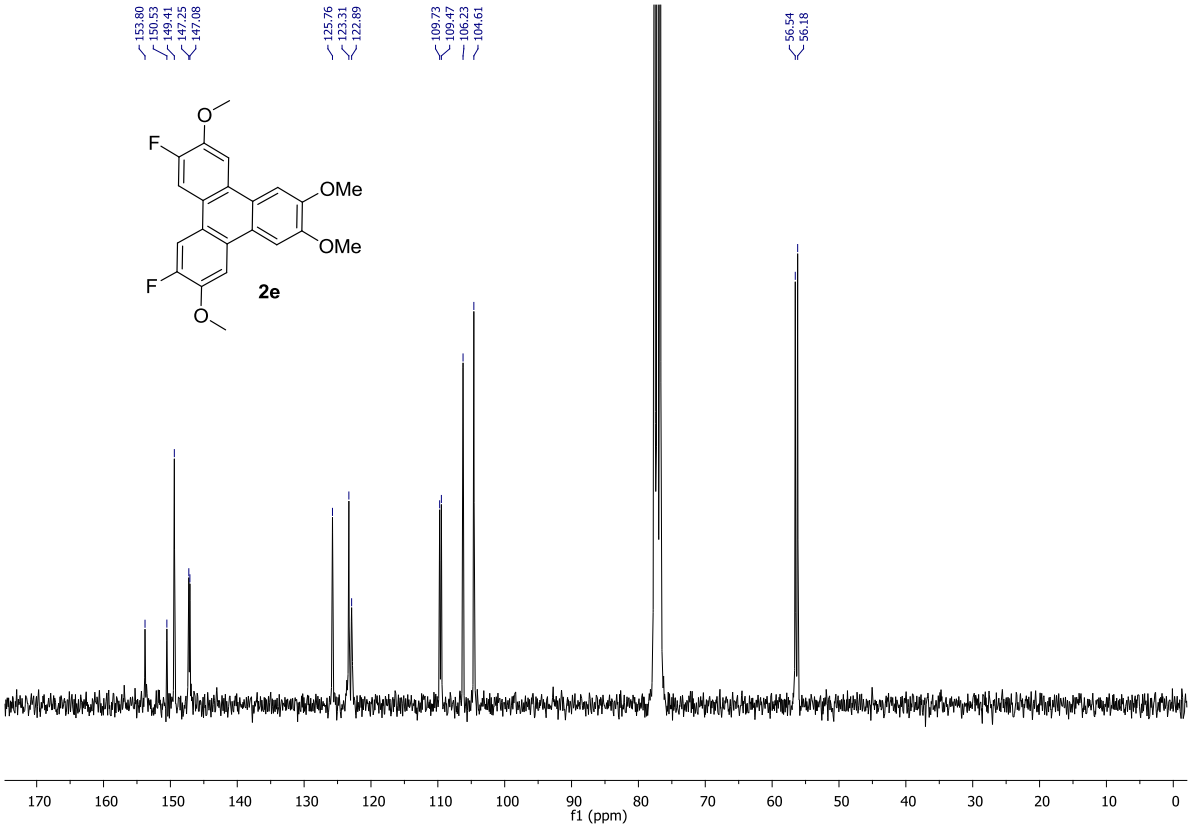
150.81
147.35
147.19
136.15
127.12
126.16
123.80
123.35
109.77
109.51
106.48
56.47
20.38
F
O
CH3
CH3
F
O
2d
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


7.71
7.67
7.61
7.58
7.57
7.26
7.26
4.10
4.07
O
F
OMe
OMe
F
O
2e
1.02
1.17
1.08
0.89
1.96
6.00
6.02
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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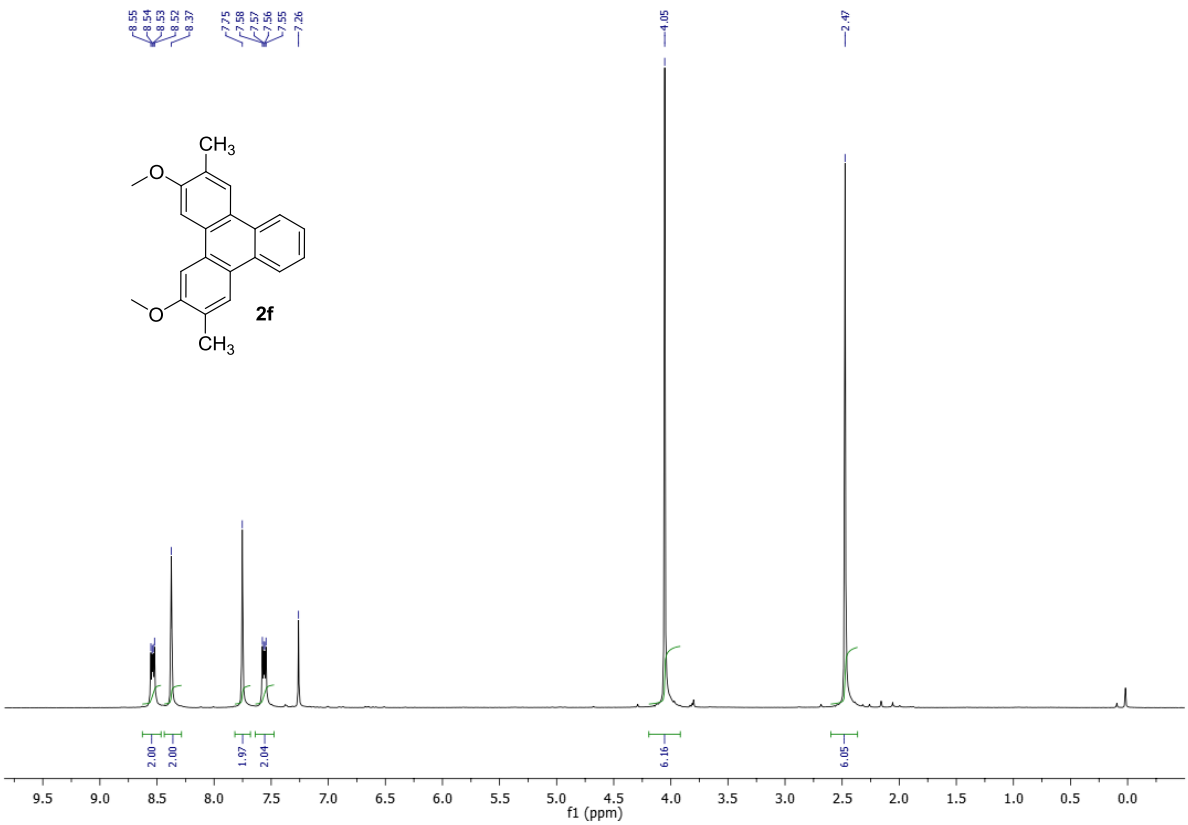
150.53
149.41
147.25
147.08
125.76
123.31
122.89
109.73
109.47
106.23
104.61
56.54
56.18
O
F
OMe
OMe
F
O
2e
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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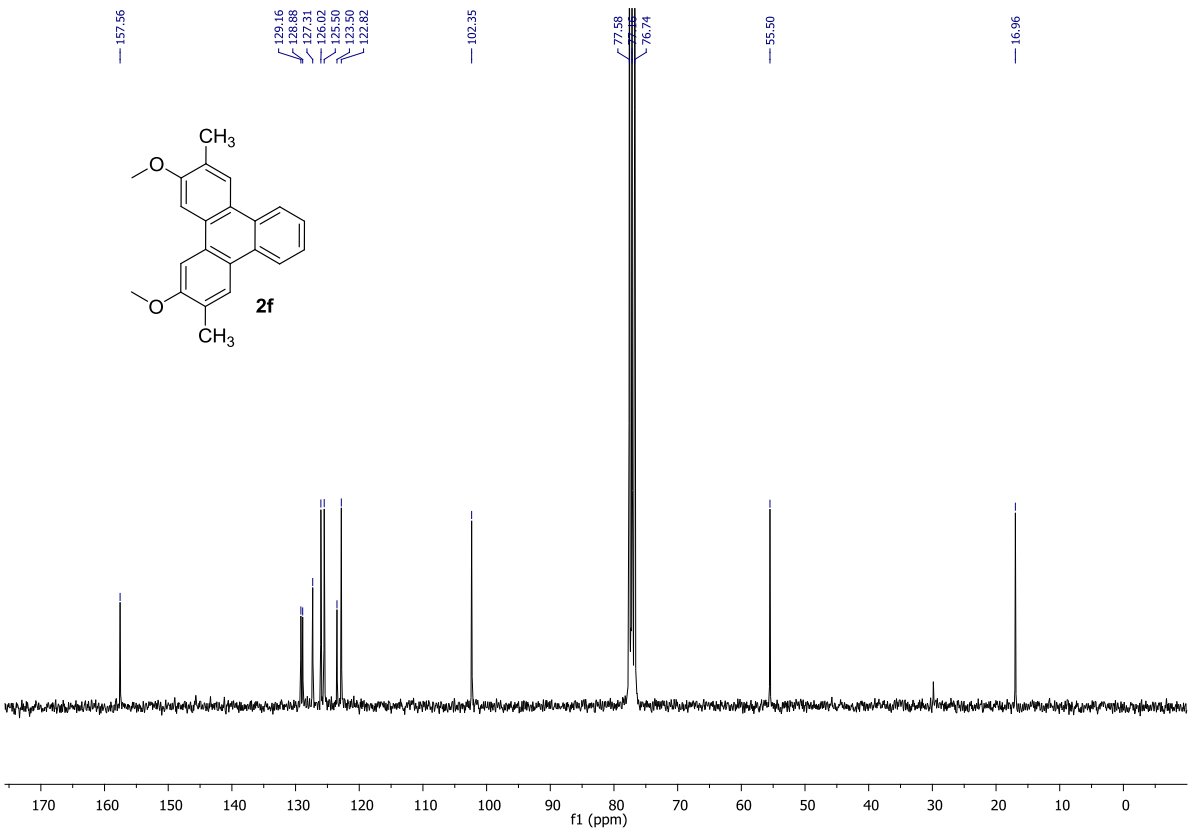
8.54
8.53
8.52
8.37
7.75
7.58
7.57
7.56
7.55
7.26
4.05
2.47
CH3
O
O
CH3
2f
2.00
2.00
1.97
2.04
6.16
6.05
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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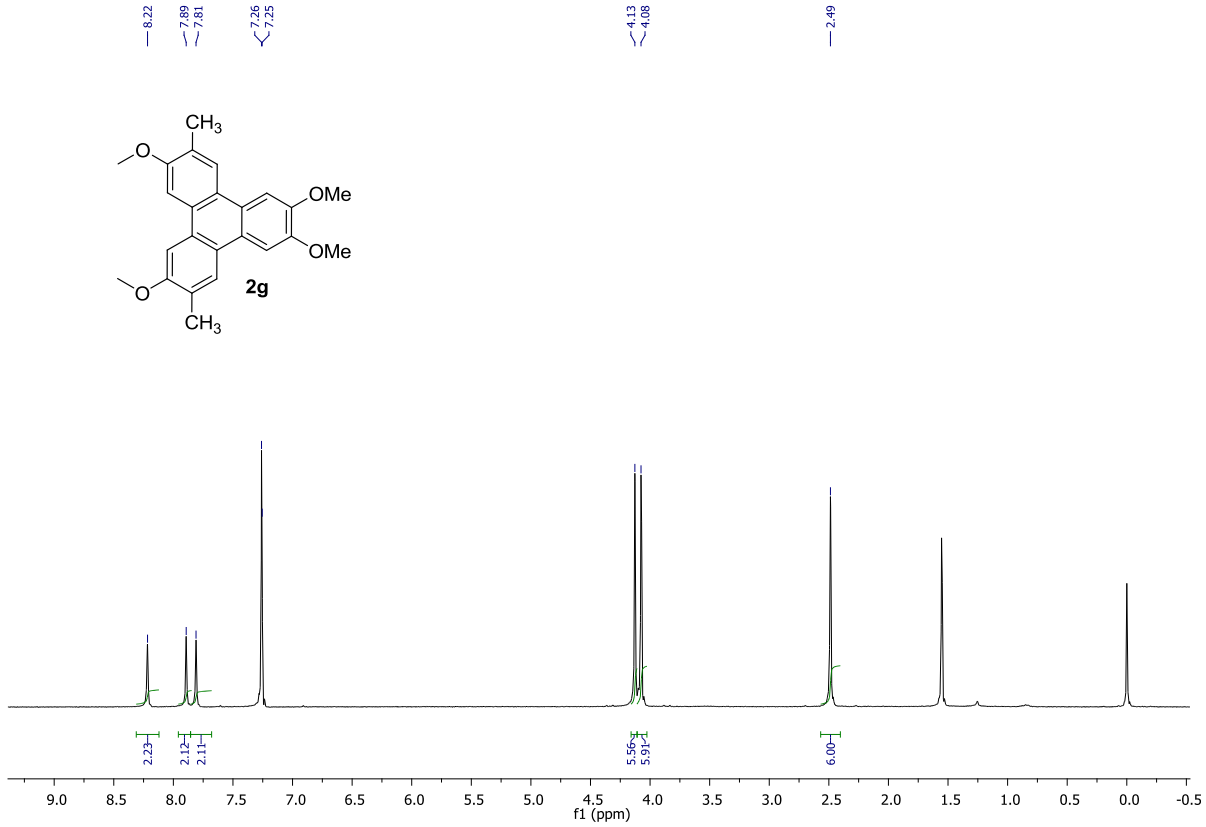
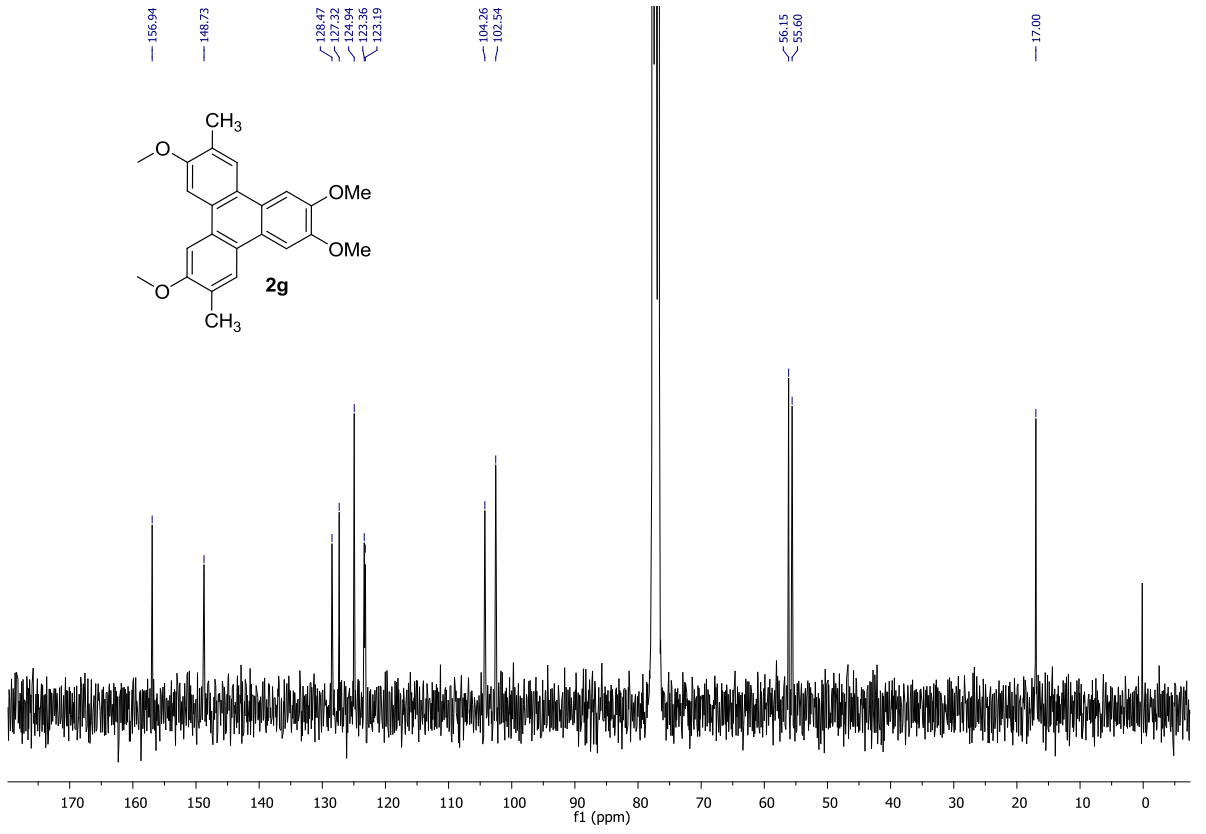
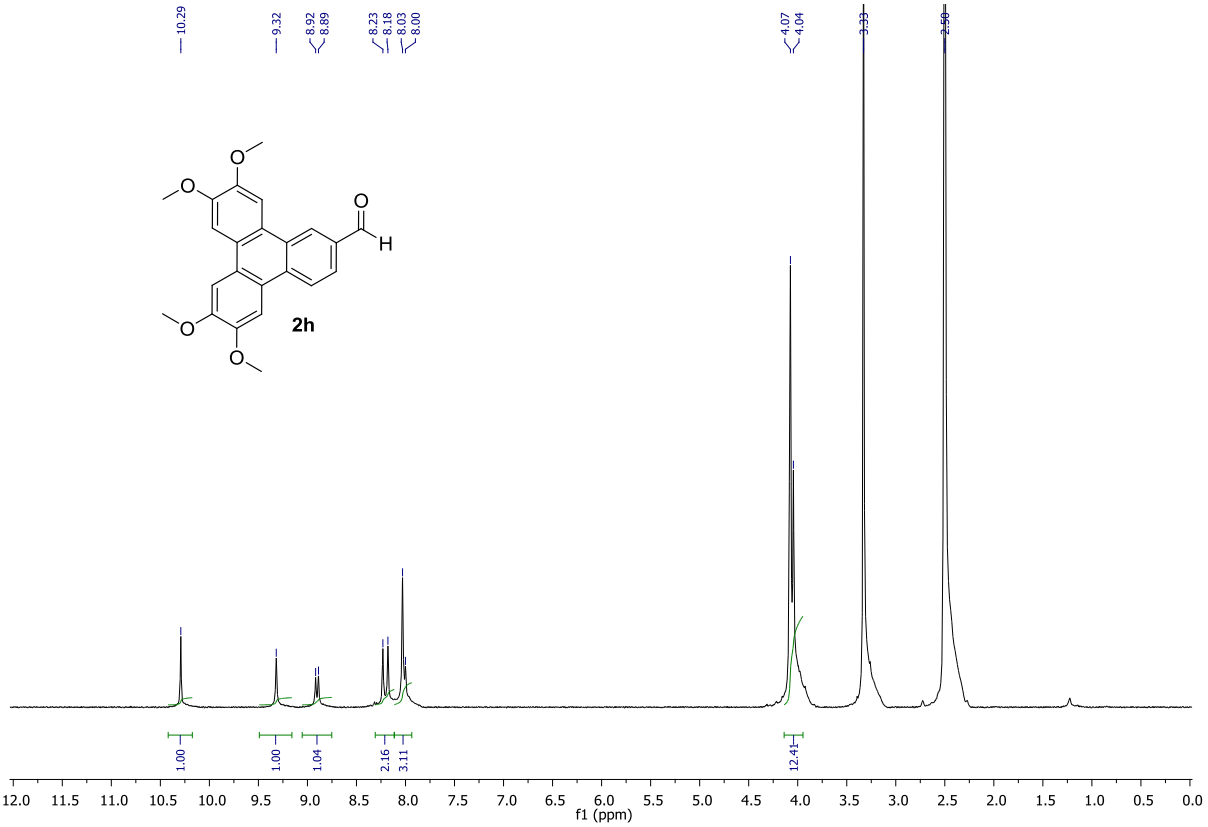
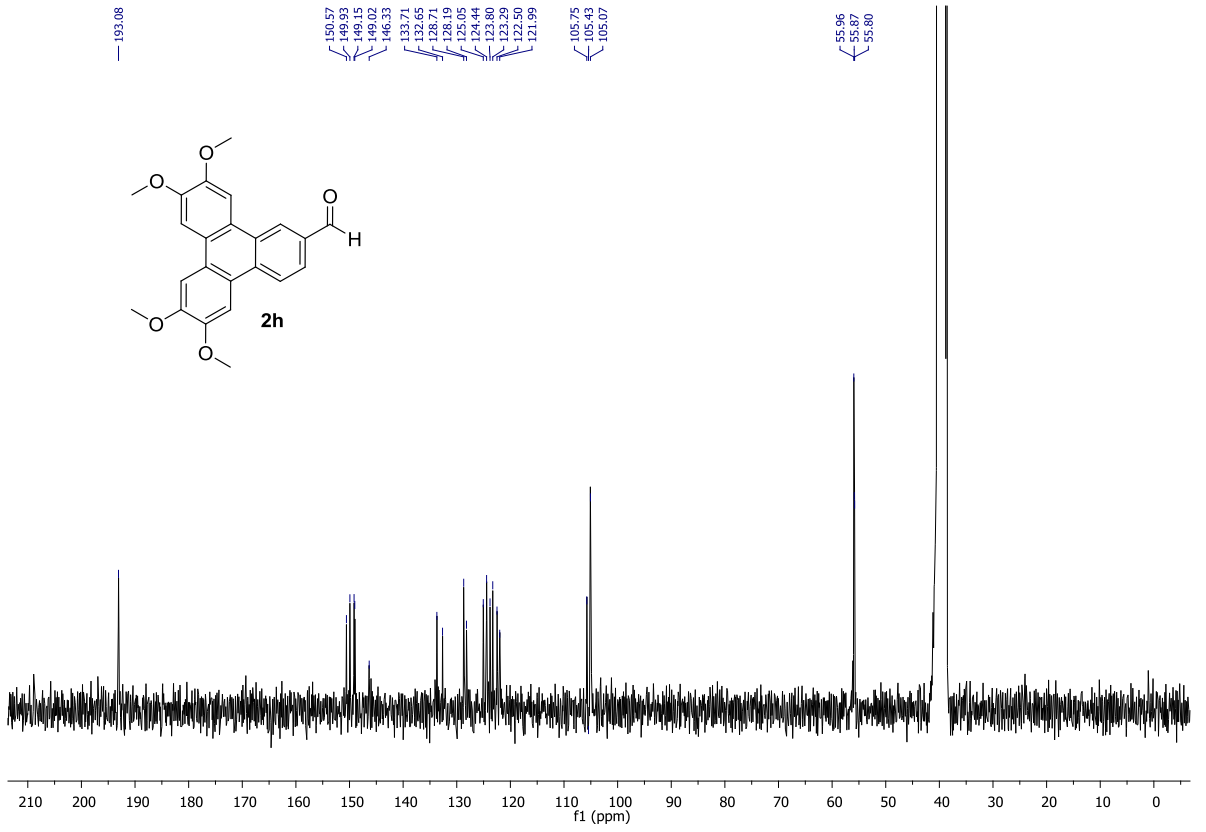
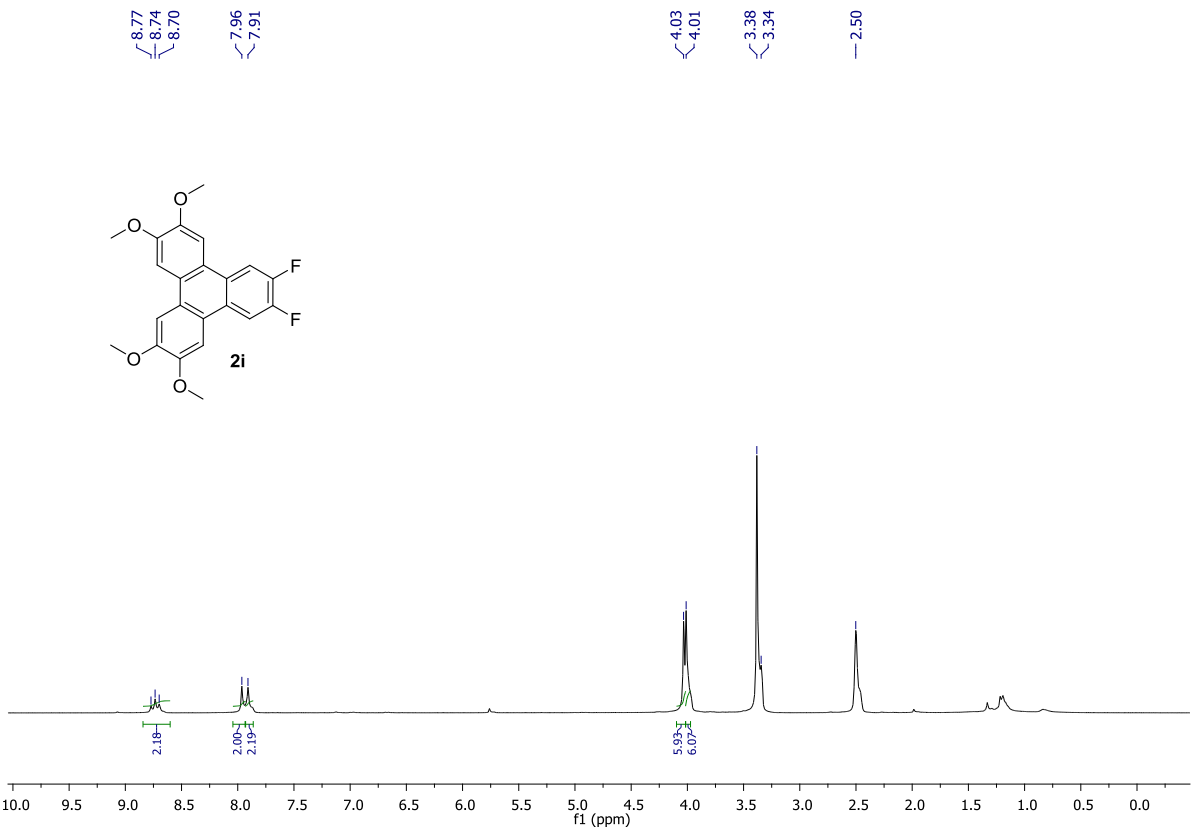
129.16
128.88
127.31
126.02
125.50
123.50
122.82
102.35
77.58
77.16
76.74
55.50
16.96
CH3
O
O
CH3
2f
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


8.22
7.89
7.81
7.26
7.25
4.13
4.08
2.49
CH3
O
OMe
OMe
O
CH3
2g
2.23
2.12
2.11
5.56
5.91
6.00
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)


156.94
148.73
128.47
127.32
124.94
123.36
123.19
104.26
102.54
56.15
55.60
17.00
CH3
O
OMe
OMe
O
CH3
2g
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


10.29
9.32
8.92
8.89
8.23
8.18
8.03
8.00
4.07
4.04
3.33
2.50
O
O
O
O
H
2h
1.00
1.00
1.04
2.16
3.11
12.41
12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


193.08
150.57
149.93
149.15
149.02
146.33
133.71
132.65
128.71
128.19
125.05
124.44
123.80
123.29
122.50
121.99
105.75
105.43
105.07
55.96
55.87
55.80
O
O
O
O
H
2h
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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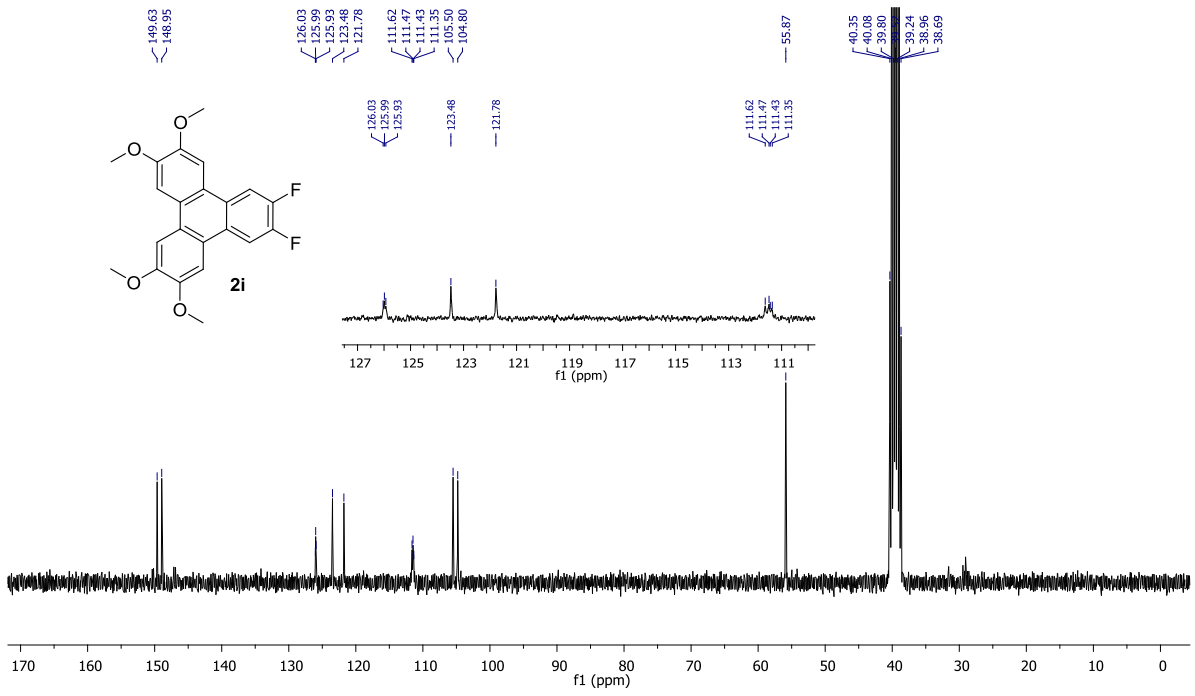
8.74
8.70
7.96
7.91
4.03
4.01
3.38
3.34
2.50
F
F
O
O
O
O
2i
2.18
2.00
2.19
5.93
6.07
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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148.95
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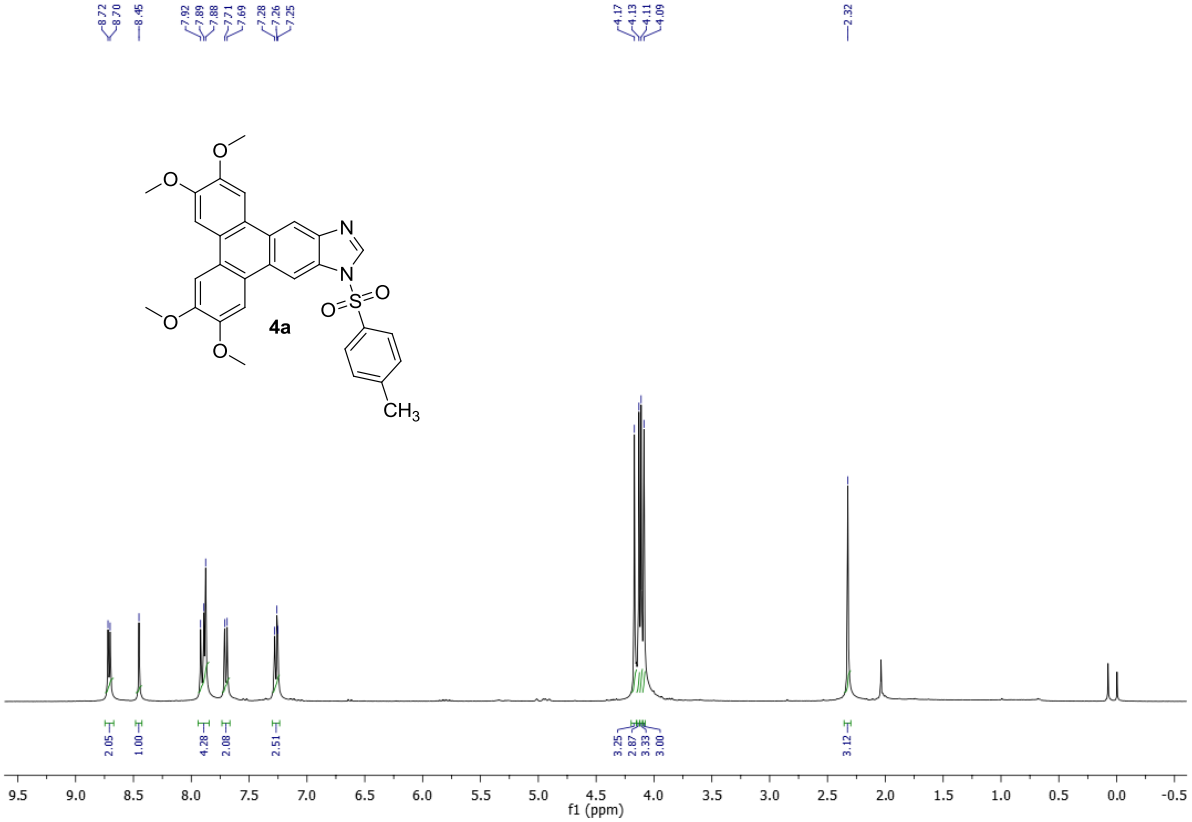
125.93
123.48
121.78
111.62
111.47
111.43
111.35
105.50
104.80
55.87
40.35
40.08
39.80
39.24
38.96
38.69
F
F
O
O
O
O
2i
127
125
123
121
119
117
115
113
111
f1 (ppm)
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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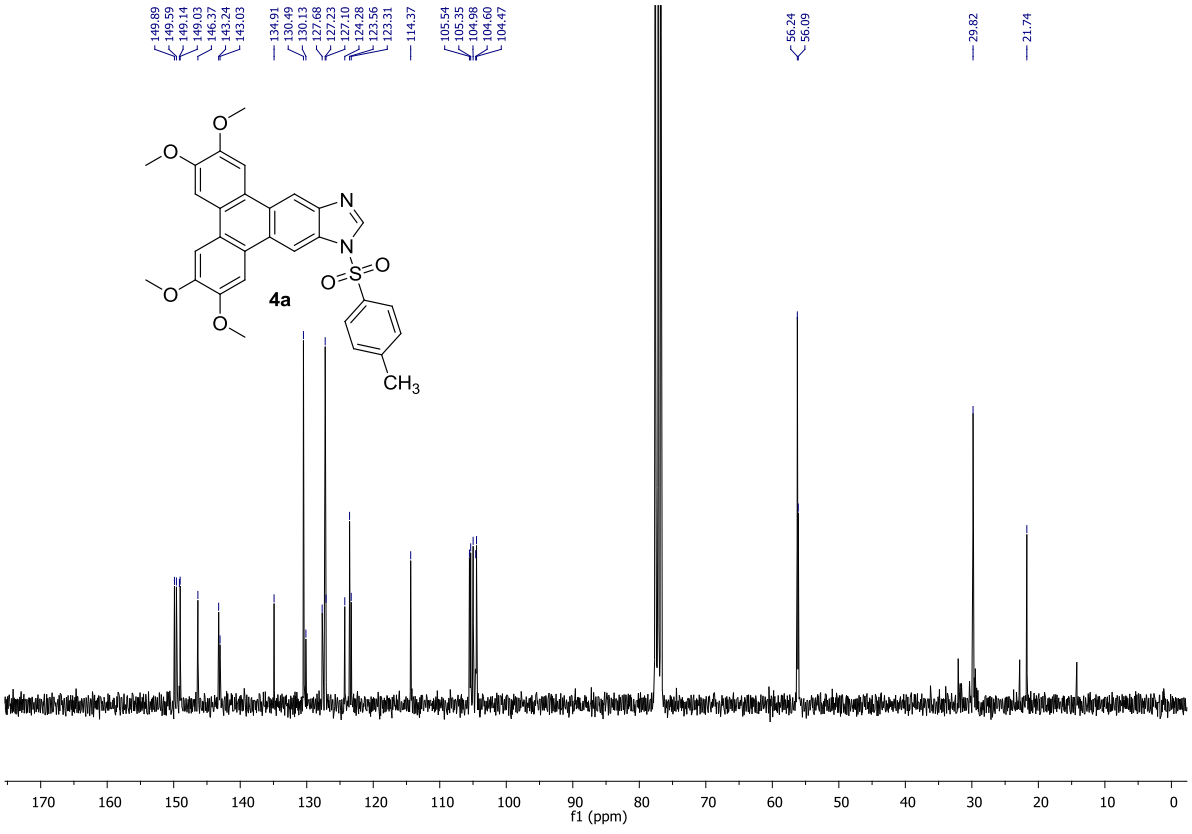
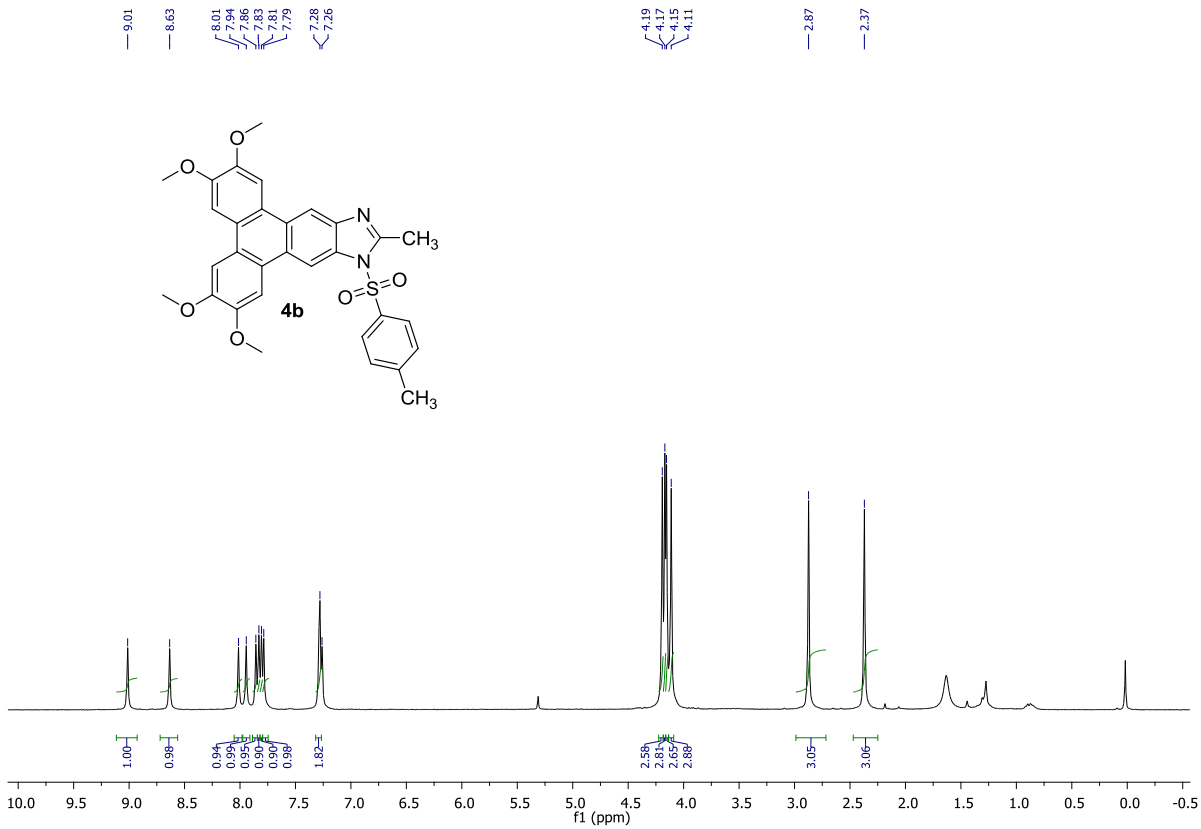
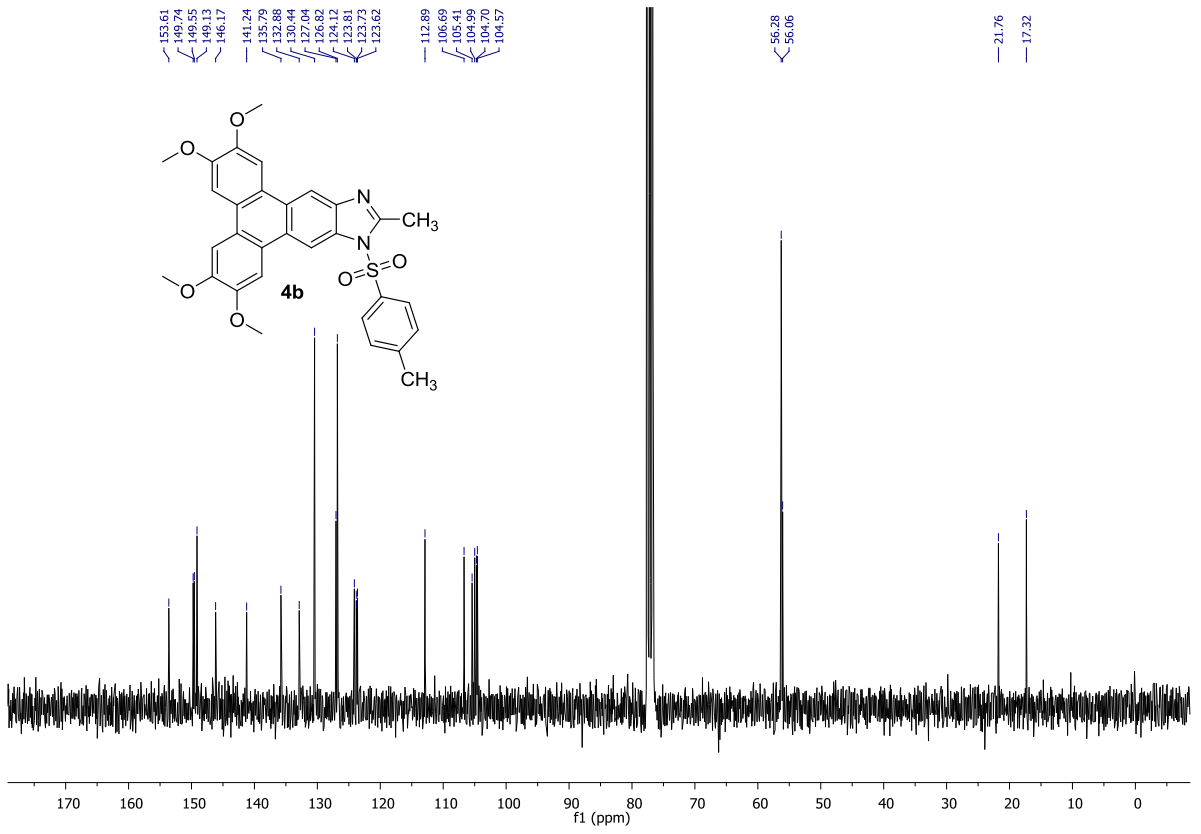
8.70
8.45
7.92
7.89
7.88
7.71
7.69
7.28
7.26
7.25
4.17
4.13
4.11
4.09
2.32
4a
2.05
1.00
4.28
2.08
2.51
3.25
2.87
3.33
3.00
3.12
f1 (ppm)


149.89
149.59
149.14
149.03
146.37
143.24
143.03
134.91
130.49
130.13
127.68
127.23
127.10
124.28
123.56
123.31
114.37
105.54
105.35
104.98
104.60
104.47
56.24
56.09
29.82
21.74
4a
f1 (ppm)


9.01
8.63
8.01
7.94
7.86
7.83
7.81
7.79
7.28
7.26
4.19
4.17
4.15
4.11
2.87
2.37
4b
1.00
0.98
0.94
0.99
0.95
0.90
0.90
0.98
1.82
2.58
2.81
2.65
2.89
3.05
3.06
f1 (ppm)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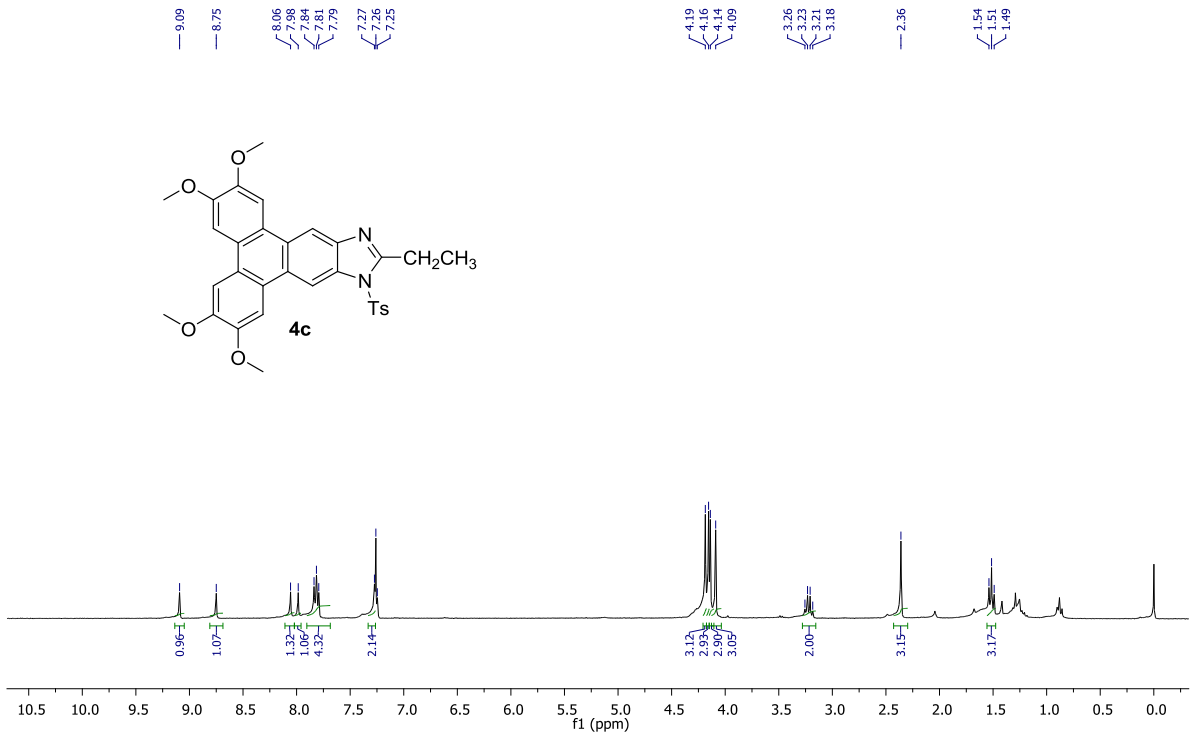
141.24
135.79
132.88
130.44
127.04
126.82
124.12
123.81
123.73
123.62
112.89
106.69
105.41
104.99
104.70
104.57
56.28
56.06
21.76
17.32
4b
f1 (ppm)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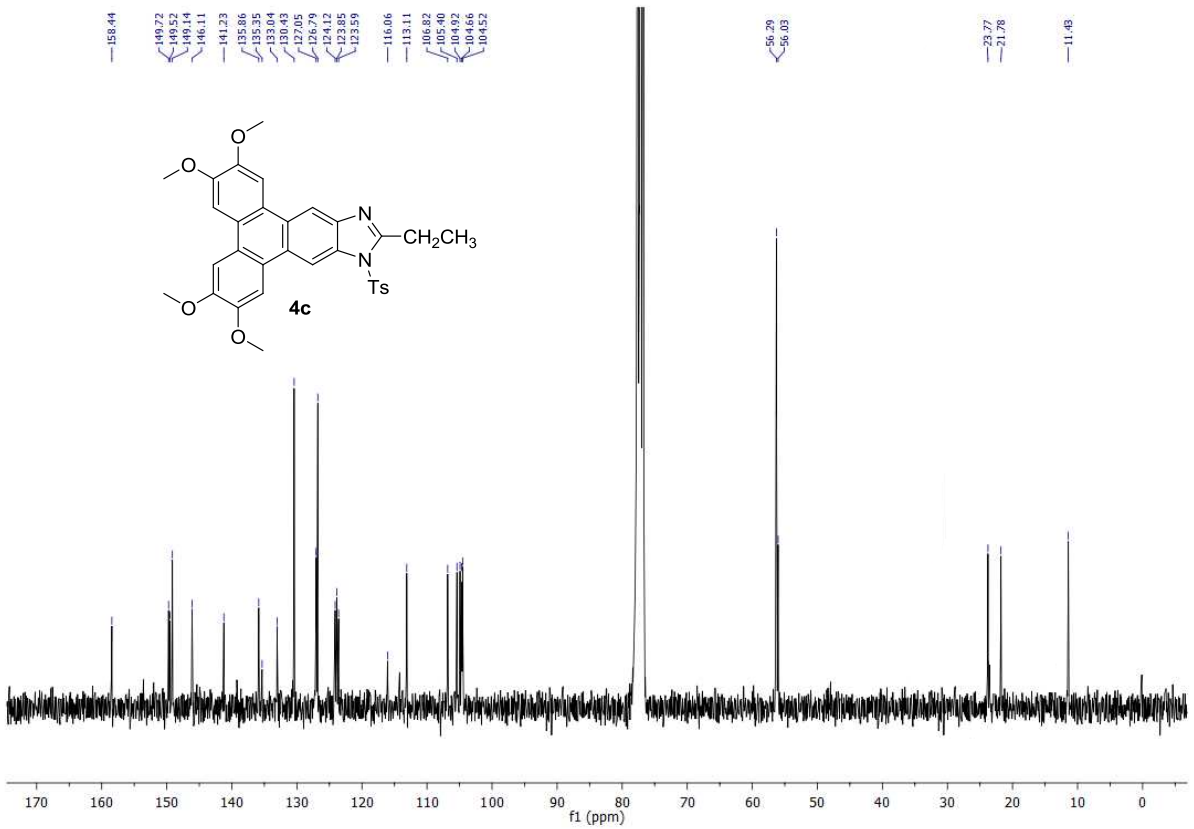
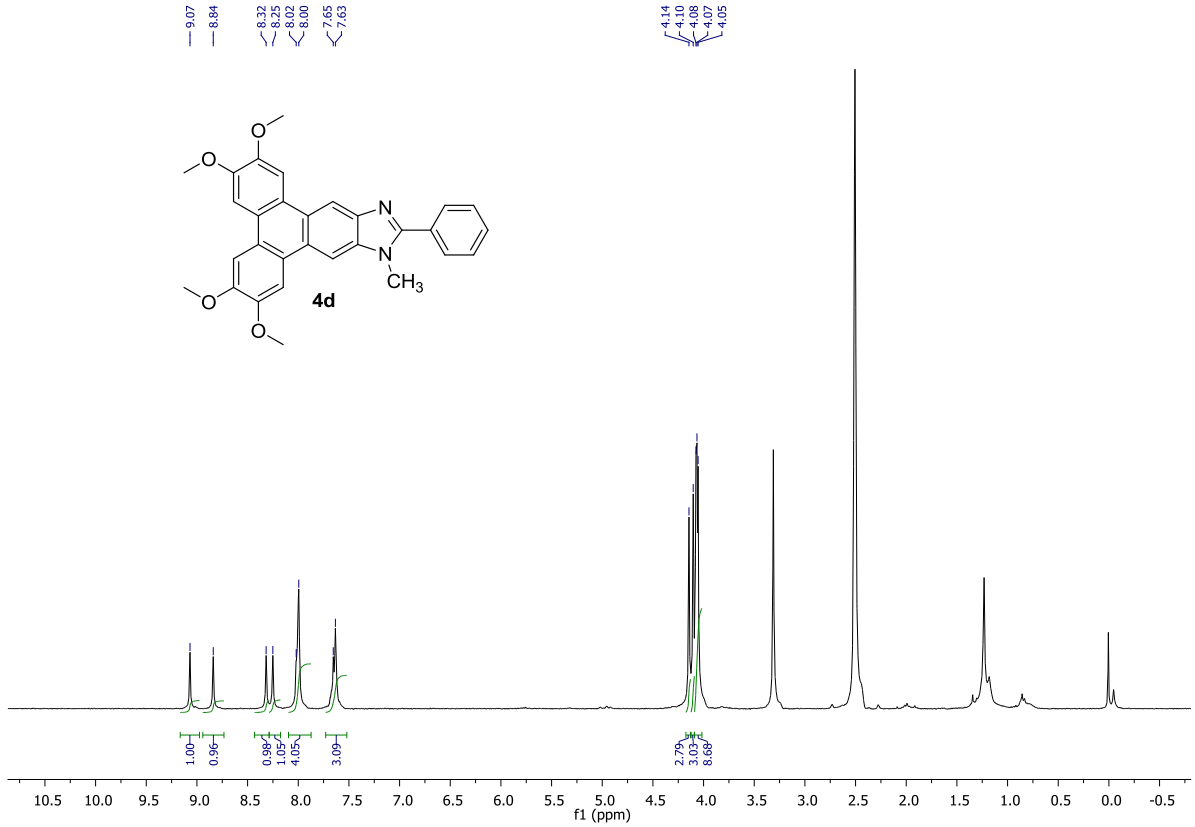
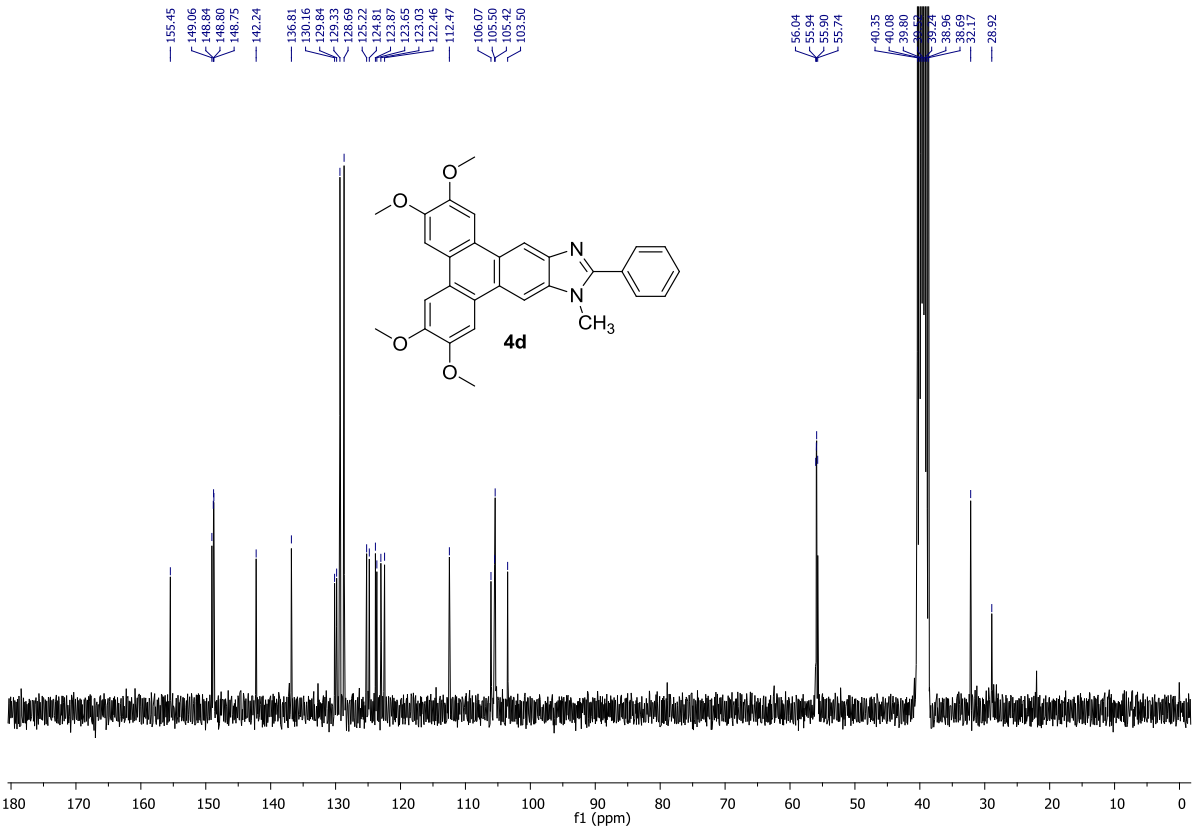
8.75
8.06
7.98
7.84
7.81
7.79
7.27
7.26
7.25
4.19
4.16
4.14
4.09
3.26
3.23
3.21
3.18
2.36
1.54
1.51
1.49
O
O
O
O
N
N
CH2CH3
Ts
4c
0.96
1.07
1.32
1.06
4.32
2.14
3.12
2.93
2.90
3.05
2.00
3.15
3.17
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


158.44
149.72
149.52
149.14
146.11
141.23
135.86
135.35
133.04
130.43
127.05
126.79
124.12
123.85
123.59
116.06
113.11
106.82
105.40
104.92
104.66
104.52
56.29
56.03
23.77
21.78
11.43
O
O
O
O
N
N
CH2CH3
Ts
4c
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


9.07
8.84
8.32
8.25
8.02
8.00
7.65
7.63
4.14
4.10
4.08
4.07
4.05
4d
1.00
0.96
0.98
1.05
4.05
3.09
2.79
3.03
8.68
f1 (ppm)


155.45
149.06
148.84
148.80
148.75
142.24
136.81
130.16
129.84
129.33
128.69
125.22
124.81
123.87
123.65
123.03
122.46
112.47
106.07
105.50
105.42
103.50
56.04
55.94
55.90
55.74
40.35
40.08
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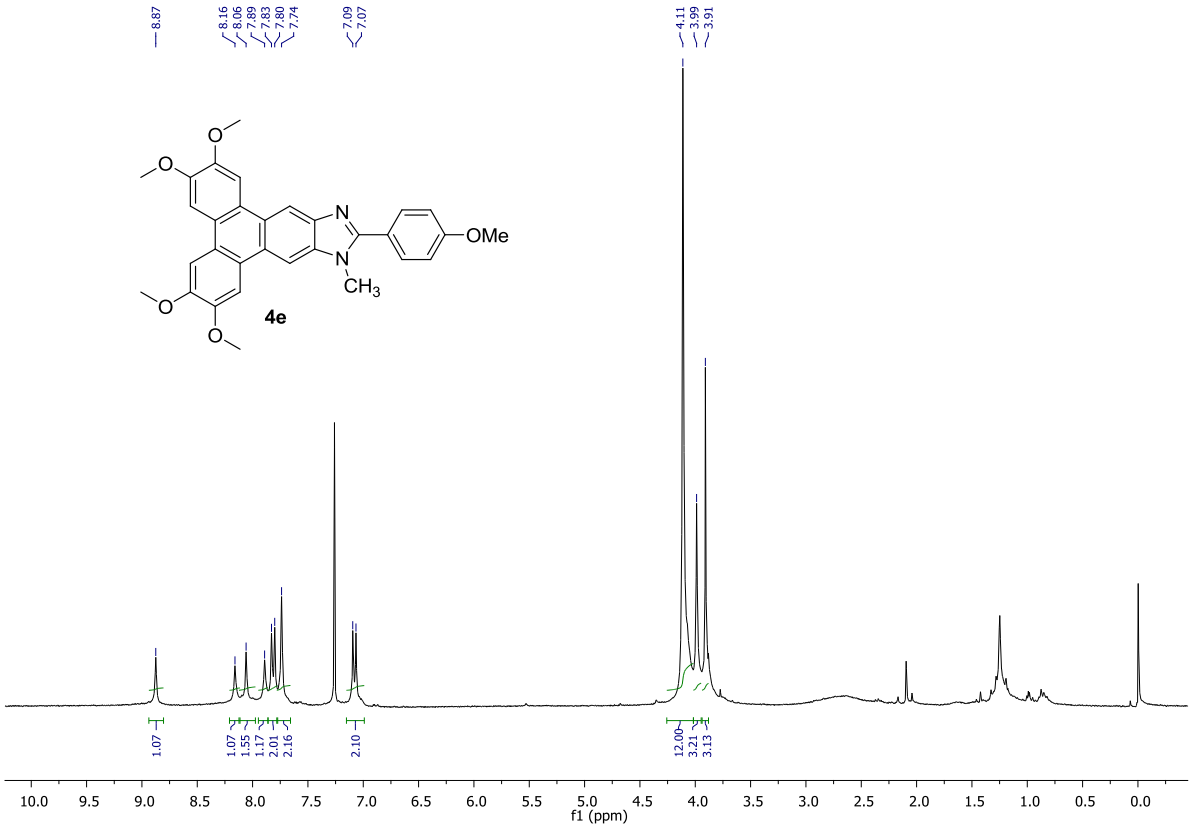
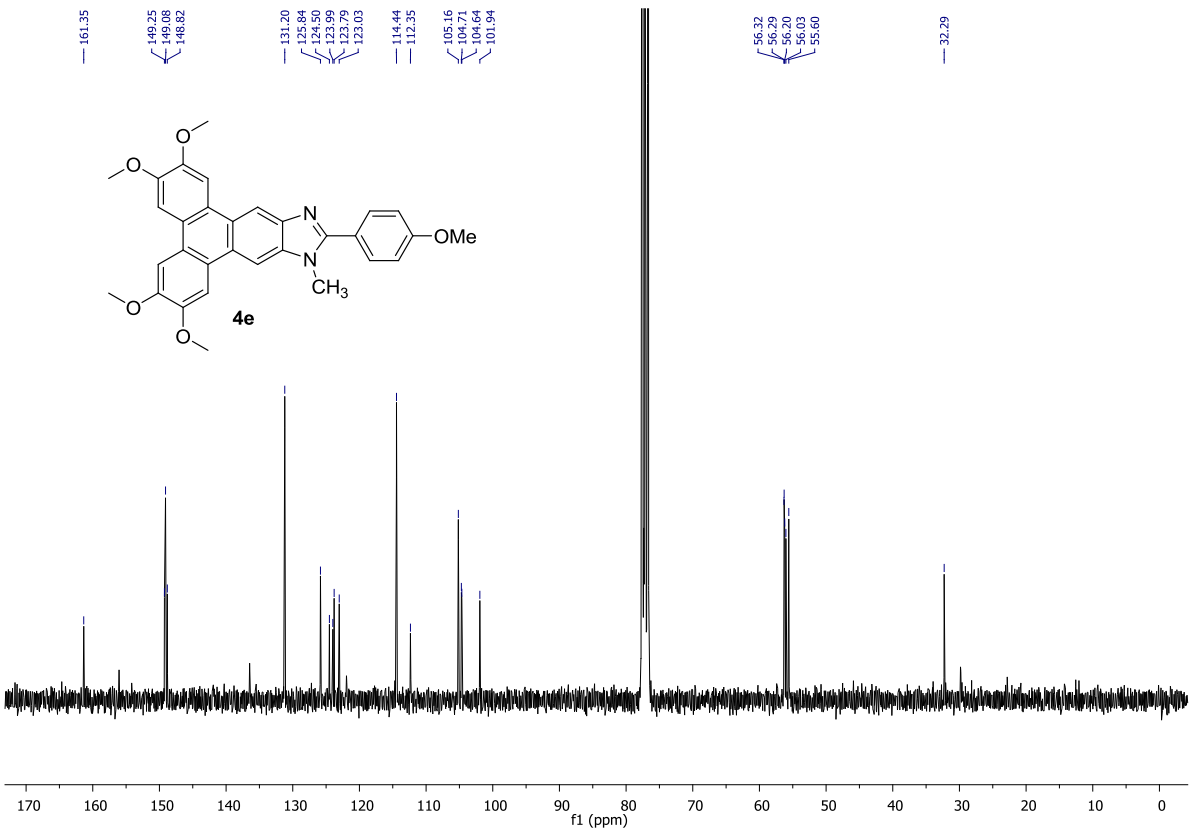
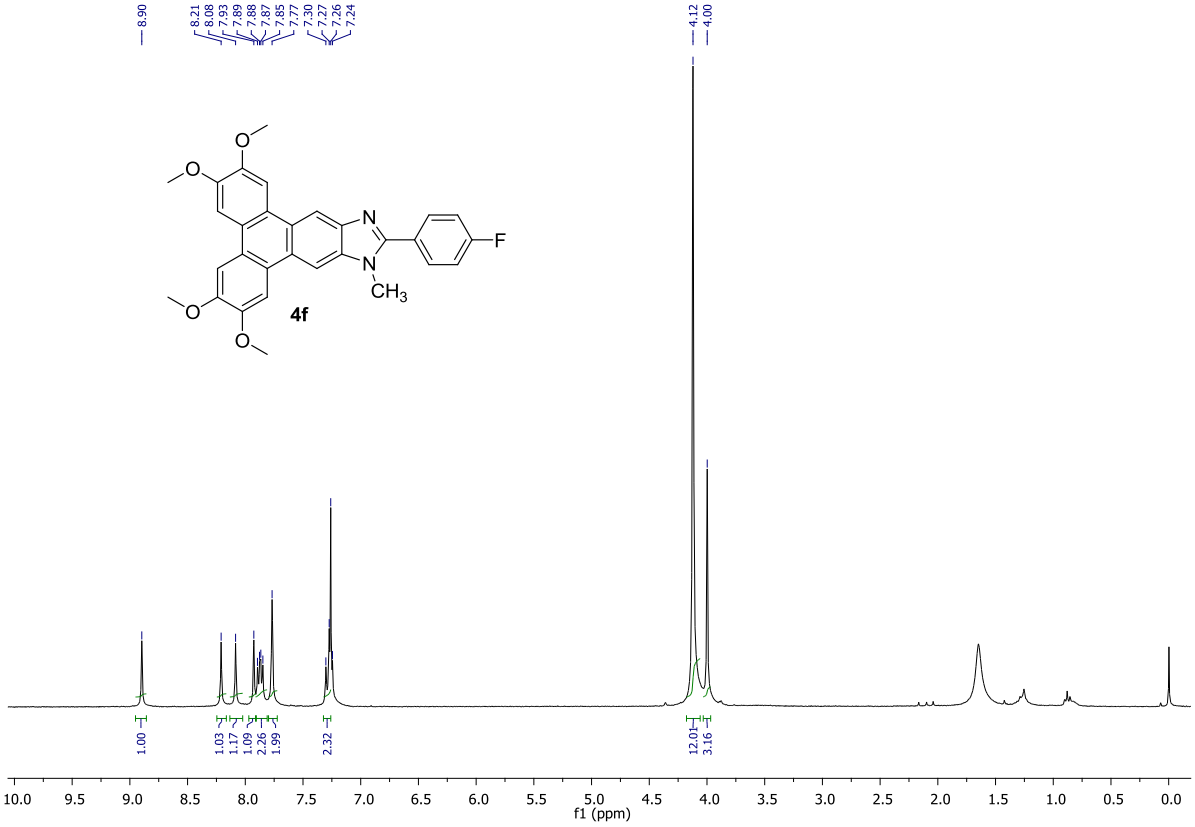
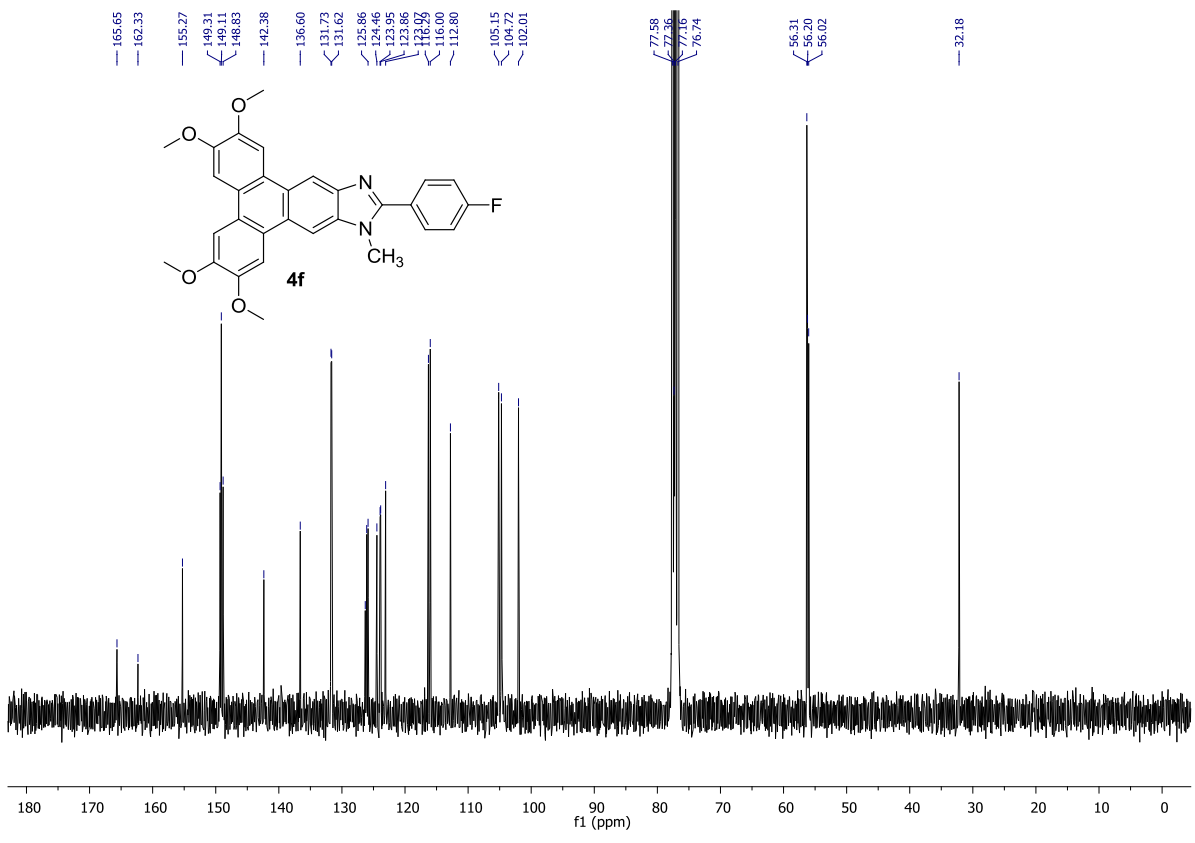
38.69
32.17
28.92
4d
f1 (ppm)


8.87
8.16
8.06
7.89
7.83
7.80
7.74
7.09
7.07
4.11
3.99
3.91
OMe
CH3
4e
1.07
1.07
1.55
1.17
2.01
2.16
2.10
12.00
3.21
3.13
f1 (ppm)


161.35
149.25
149.08
148.82
131.20
125.84
124.50
123.99
123.79
123.03
114.44
112.35
105.16
104.71
104.64
101.94
56.32
56.29
56.20
56.03
55.60
32.29
OMe
CH3
4e
f1 (ppm)


8.90
8.21
8.08
7.93
7.89
7.88
7.87
7.85
7.77
7.30
7.27
7.26
7.24
4.12
4.00
O
O
O
O
N
N
CH3
F
4f
1.00
1.03
1.17
1.09
2.26
1.99
2.32
12.01
3.16
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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155.27
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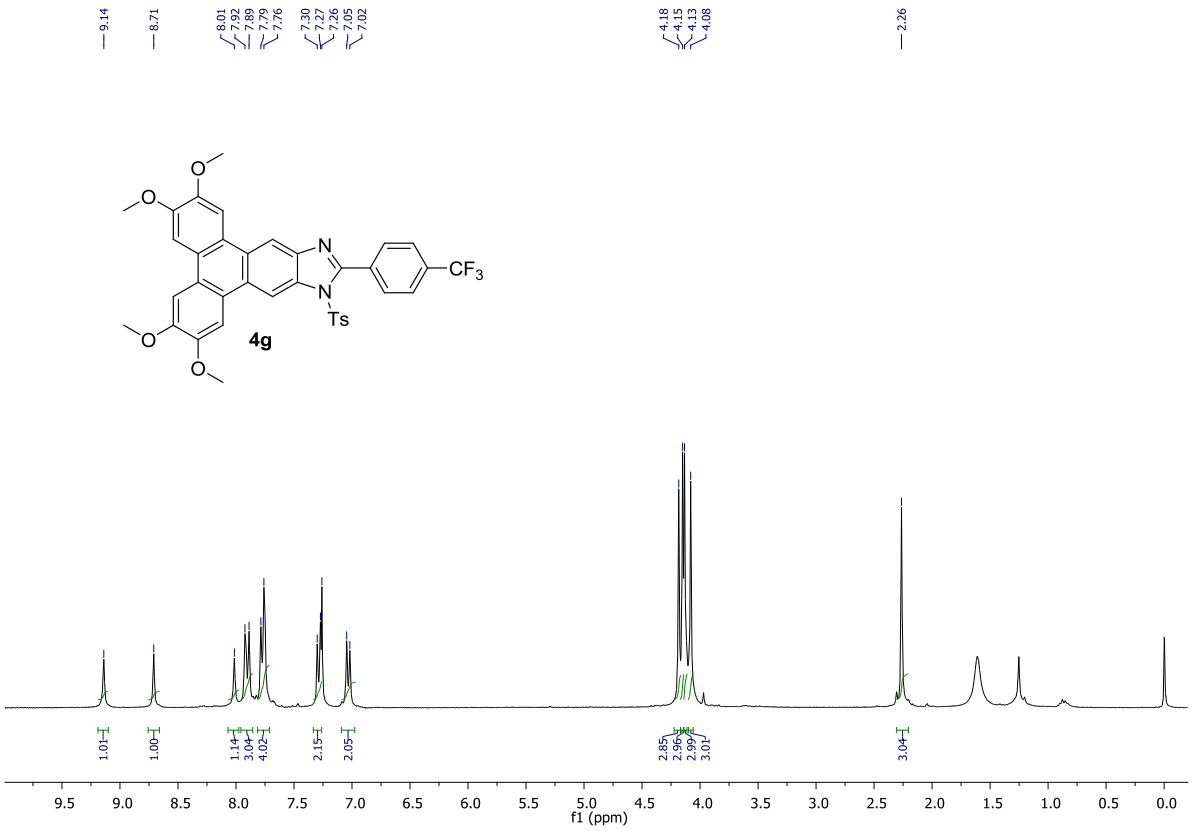
149.11
148.83
142.38
136.60
131.73
131.62
125.86
124.46
123.95
123.86
123.07
116.29
116.00
112.80
105.15
104.72
102.01
77.58
77.36
77.16
76.74
56.31
56.20
56.02
32.18
O
O
O
O
N
N
CH3
F
4f
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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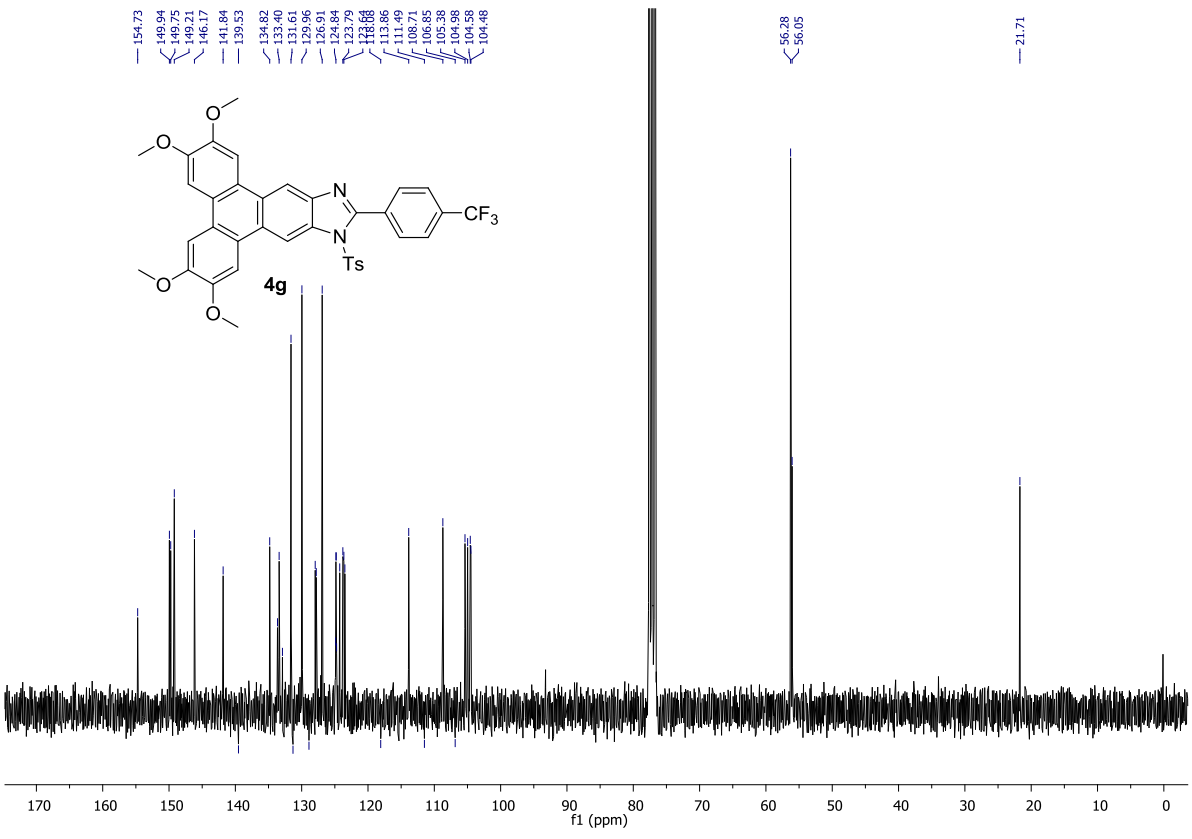
8.01
7.92
7.89
7.79
7.76
7.30
7.27
7.26
7.05
7.02
4.18
4.15
4.13
4.08
2.26
O
O
O
O
N
N
Ts
CF3
4g
1.01
1.00
1.14
3.04
4.02
2.15
2.05
2.85
2.96
2.99
3.01
3.04
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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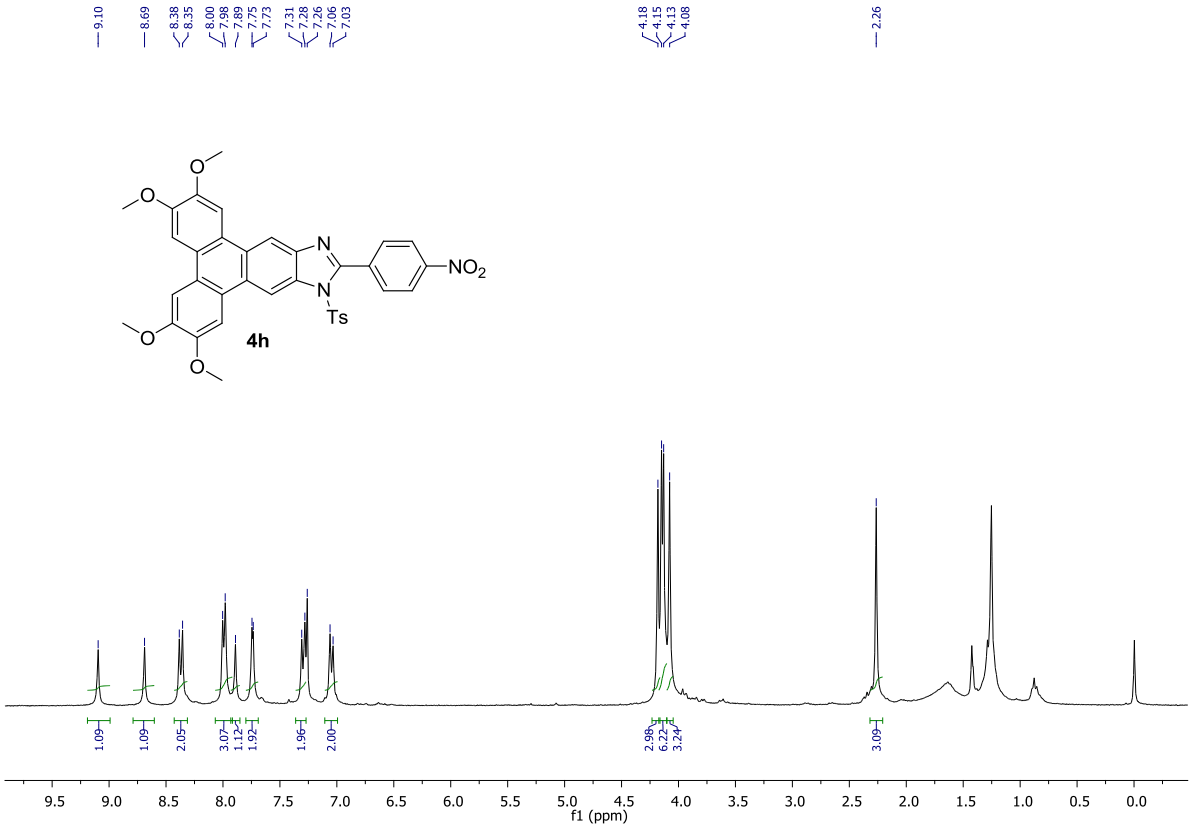
149.21
146.17
141.84
139.53
134.82
133.40
131.61
129.96
126.91
124.84
123.79
113.86
111.49
108.71
106.85
105.38
104.98
104.58
104.48
56.28
56.05
21.71
O
O
O
O
N
N
Ts
CF3
4g
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


9.10
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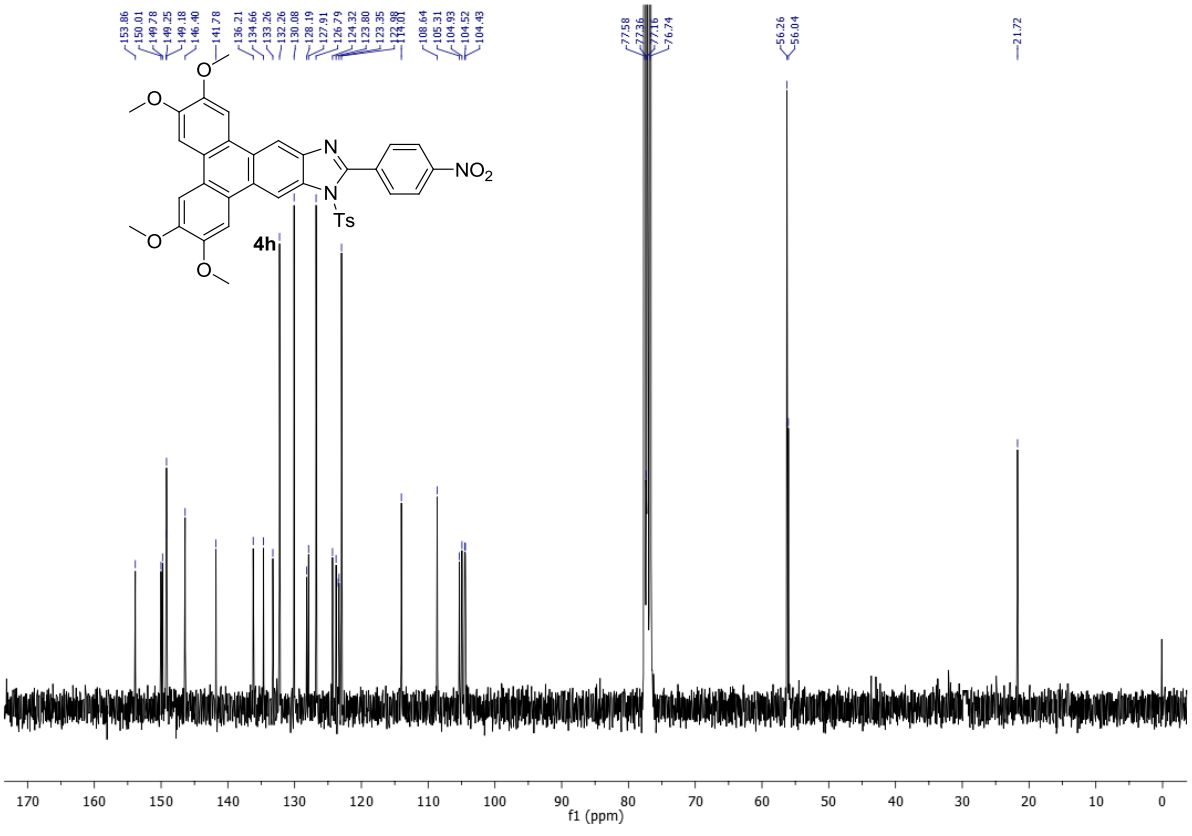
8.38
8.35
8.00
7.98
7.89
7.75
7.73
7.31
7.28
7.26
7.06
7.03
4.18
4.15
4.13
4.08
2.26
O
O
O
O
N
N
NO2
Ts
4h
1.09
1.09
2.05
3.07
1.12
1.92
1.96
2.00
2.98
6.22
3.24
3.09
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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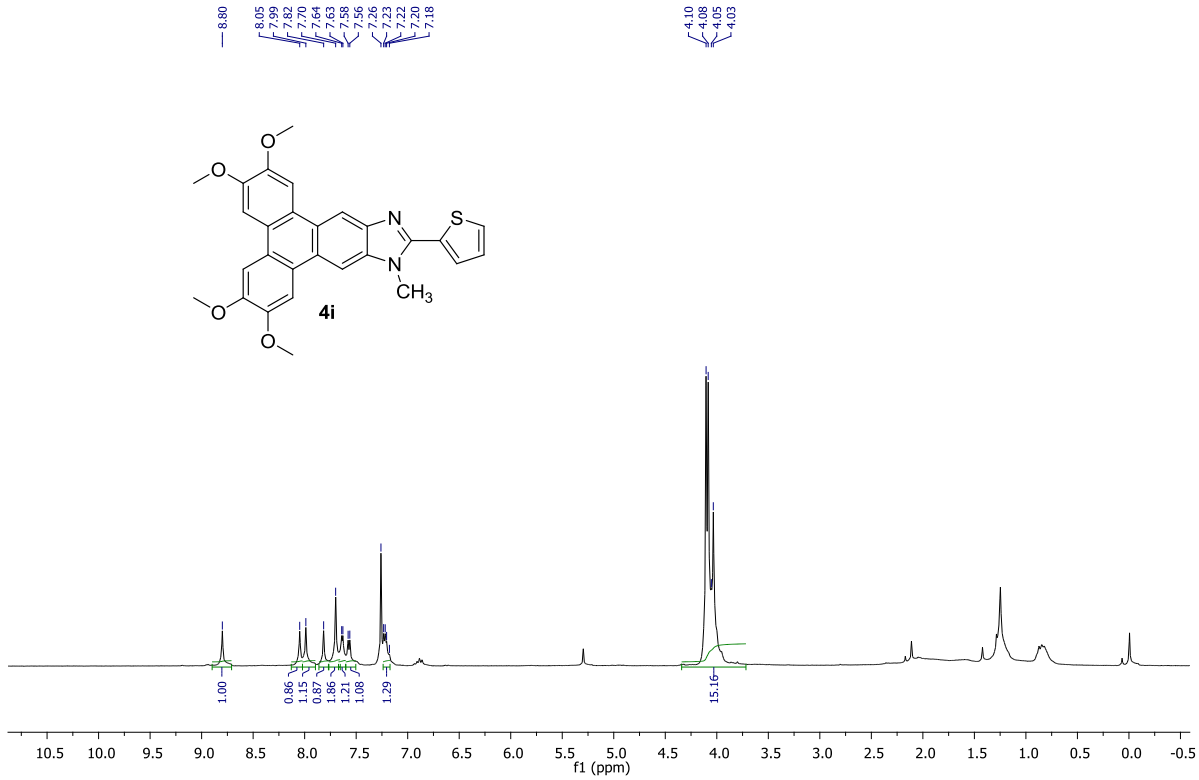
141.78
136.21
134.66
133.26
132.26
130.08
128.19
127.91
126.79
124.32
123.80
123.35
108.64
105.31
104.93
104.52
104.43
77.58
77.36
77.16
76.74
56.26
56.04
21.72
O
O
O
O
N
N
NO2
Ts
4h
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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8.05
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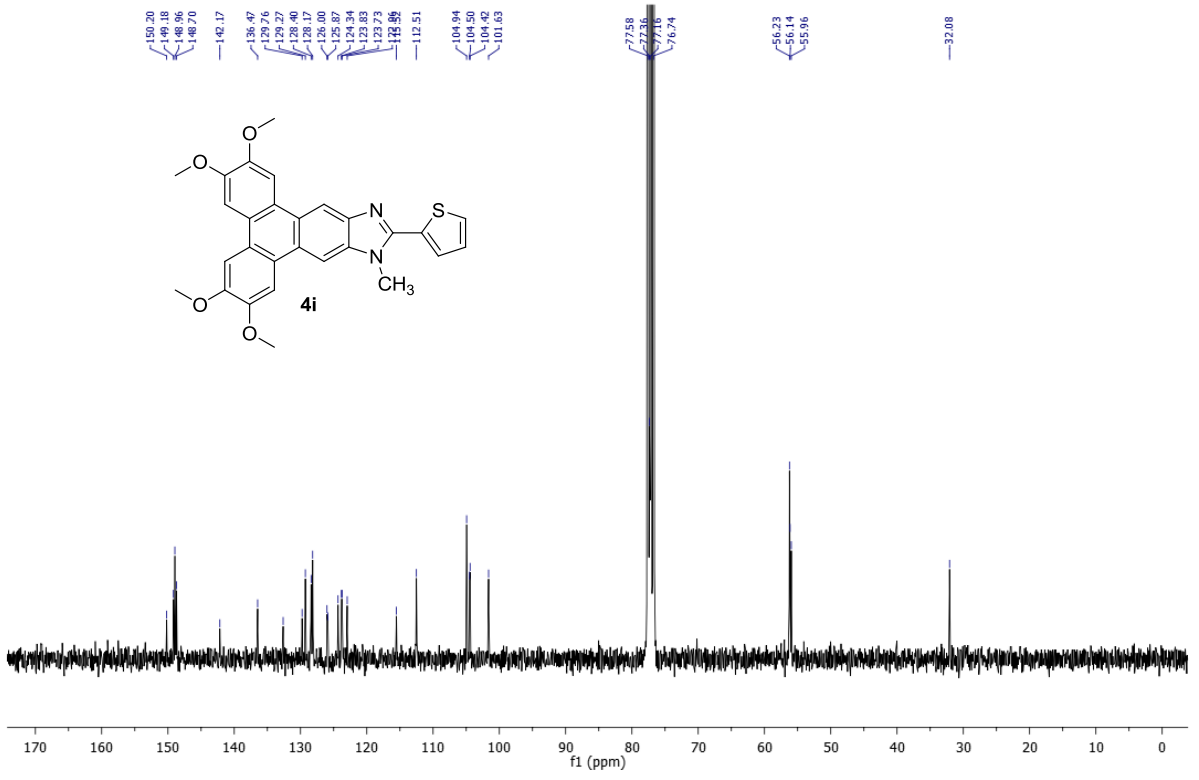
7.70
7.64
7.63
7.58
7.56
7.26
7.23
7.22
7.20
7.18
4.10
4.08
4.05
4.03
4i
1.00
0.86
1.15
0.87
1.86
1.21
1.08
1.29
15.16
f1 (ppm)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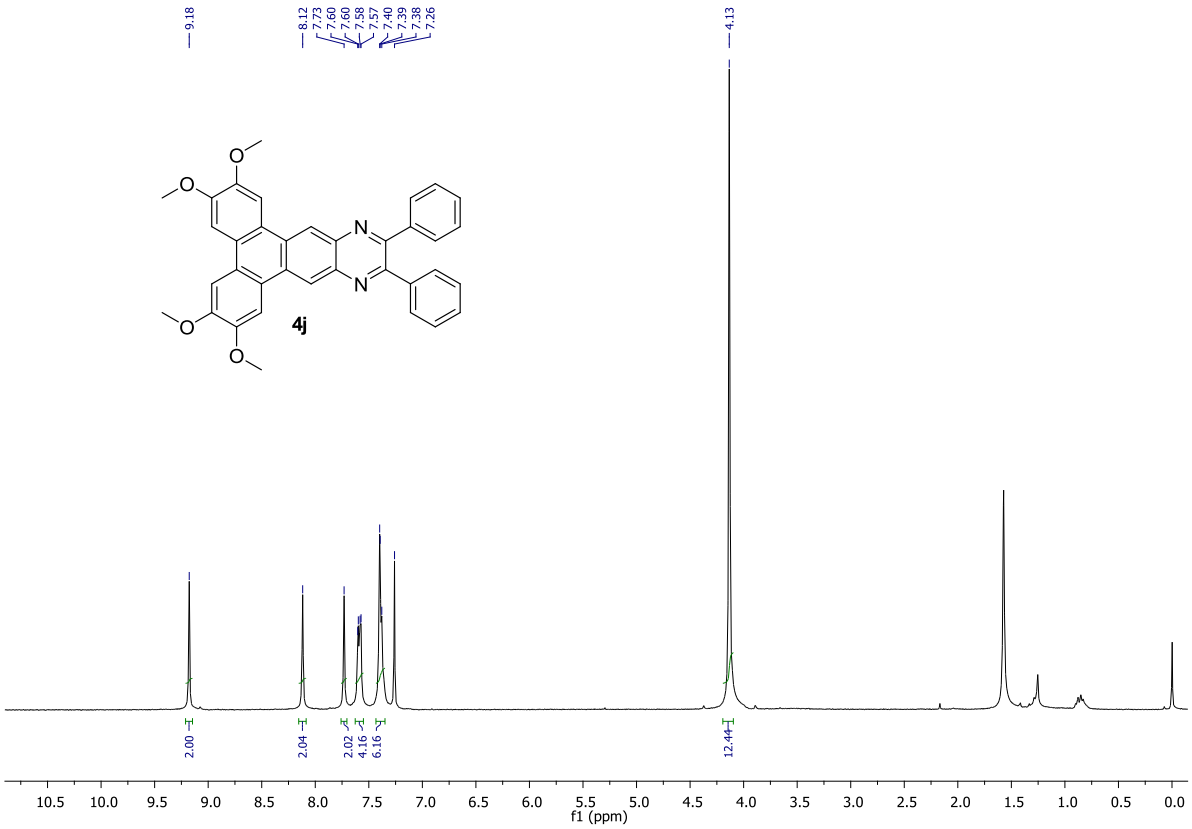
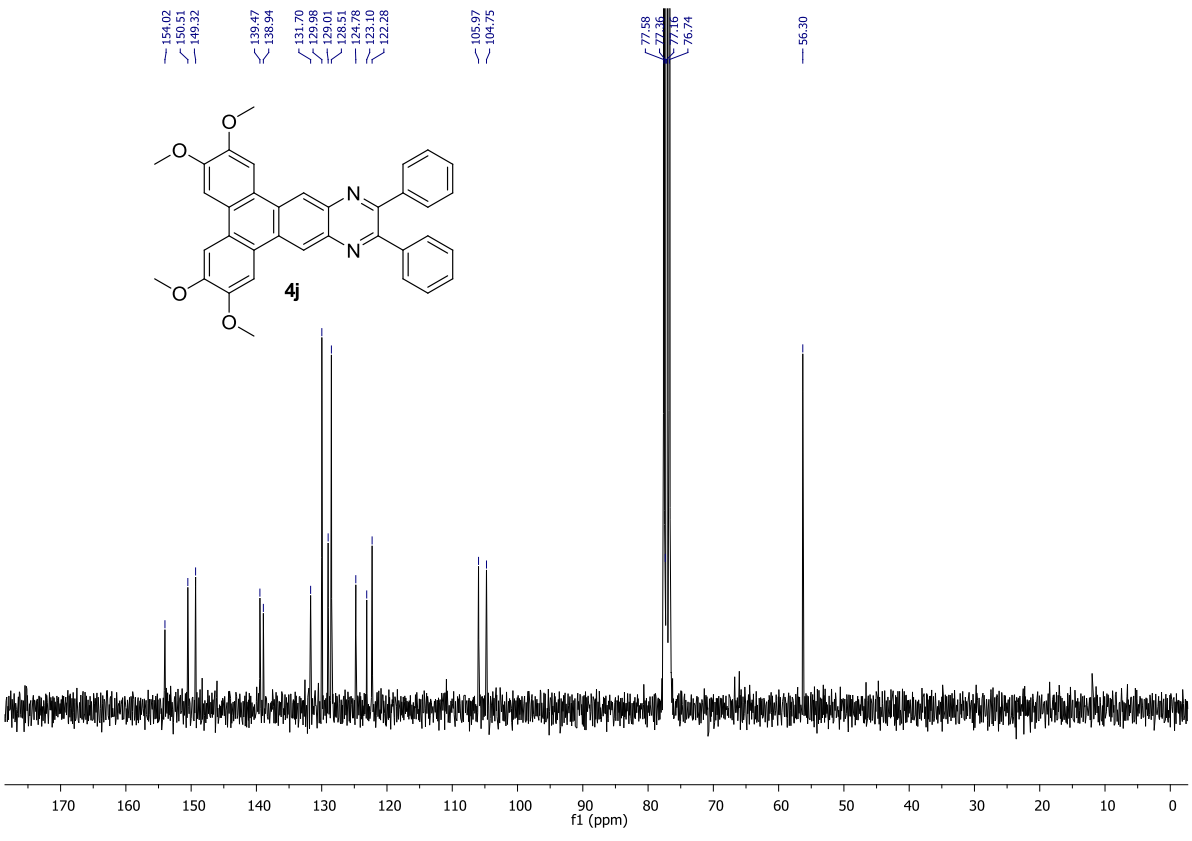
149.18
148.96
148.70
142.17
136.47
129.76
129.27
128.40
128.17
126.00
125.87
124.34
123.83
123.73
112.51
104.94
104.50
104.42
101.63
77.58
77.36
77.16
76.74
56.23
56.14
55.96
32.08
4i
f1 (ppm)


9.18
8.12
7.73
7.60
7.60
7.58
7.57
7.40
7.39
7.38
7.26
4.13
4j
2.00
2.04
2.02
4.16
6.16
12.44
f1 (ppm)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149.32
139.47
138.94
131.70
129.98
129.01
128.51
124.78
123.10
122.28
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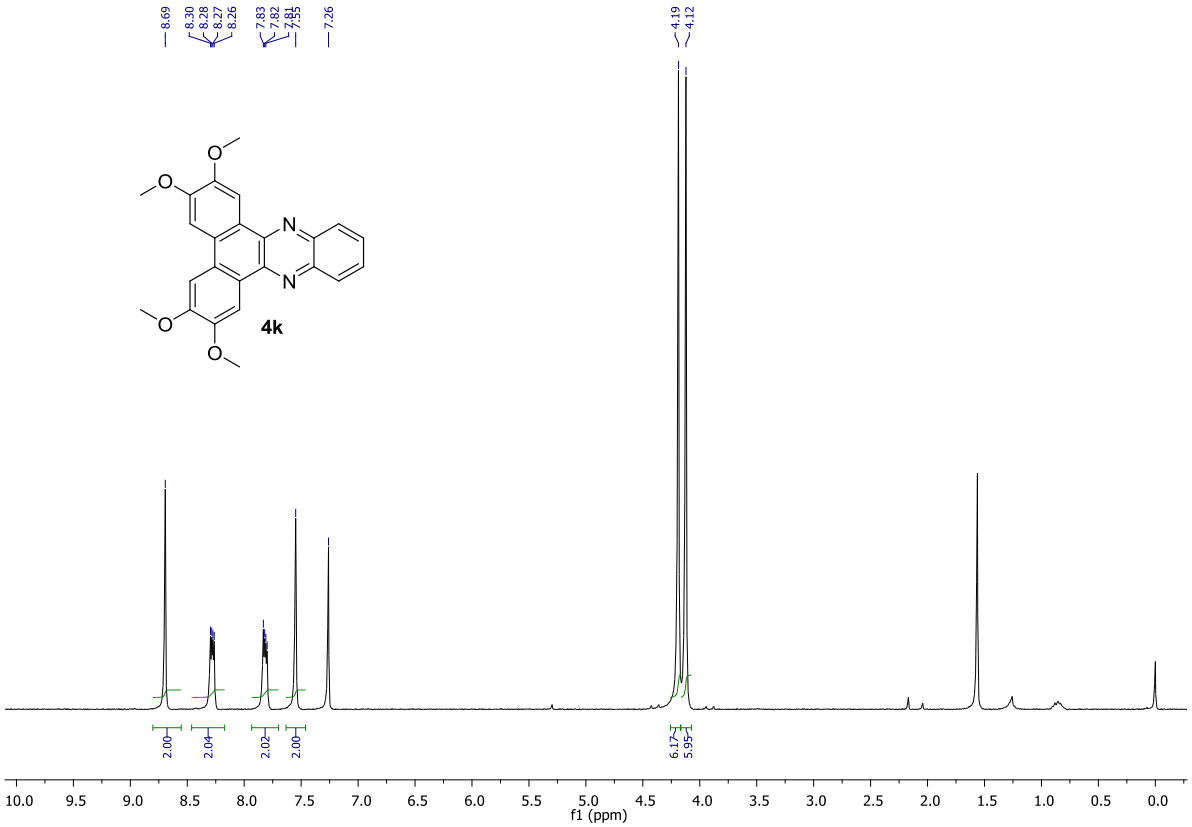
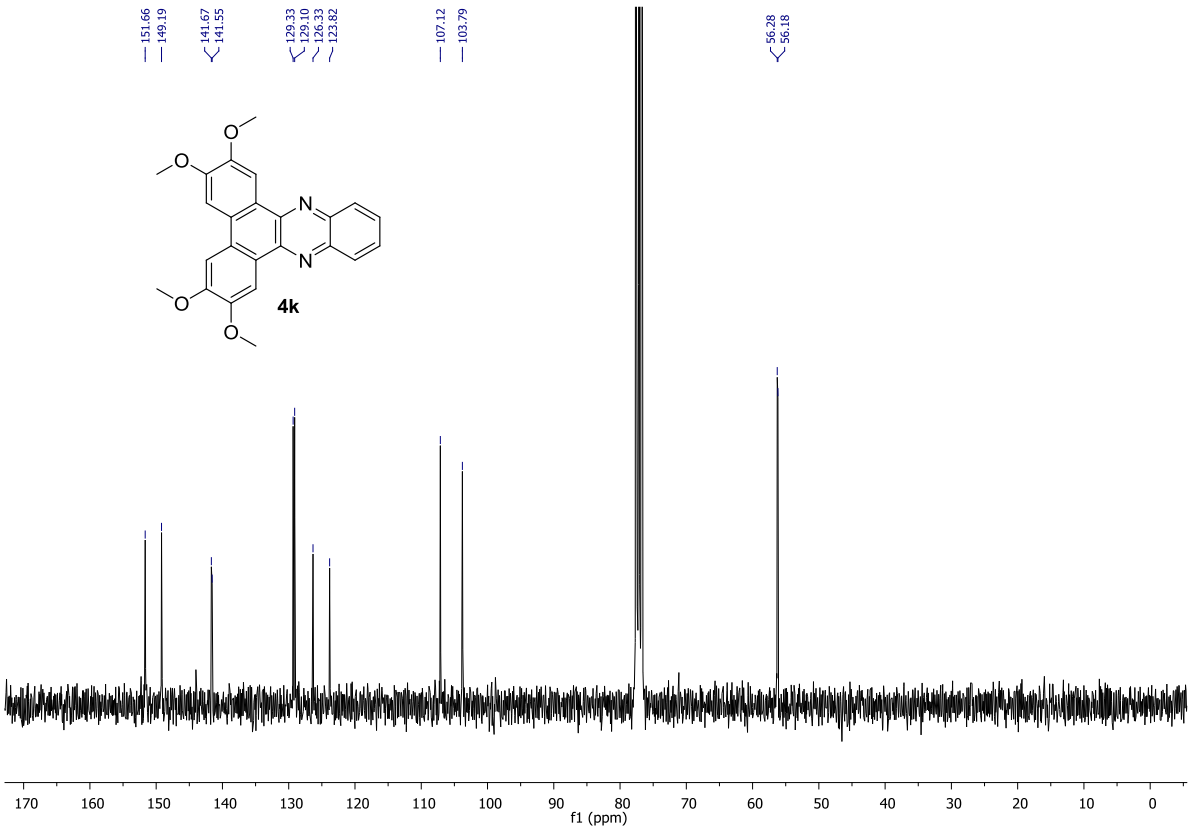
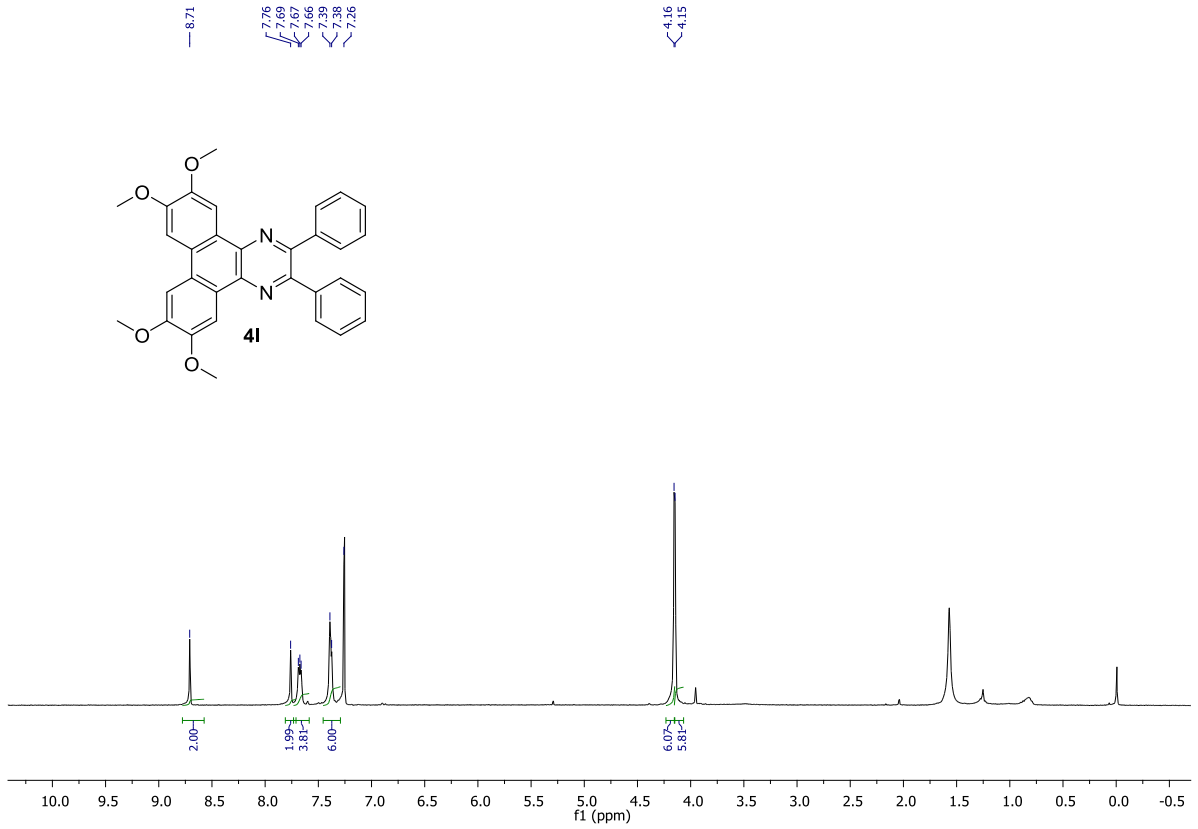
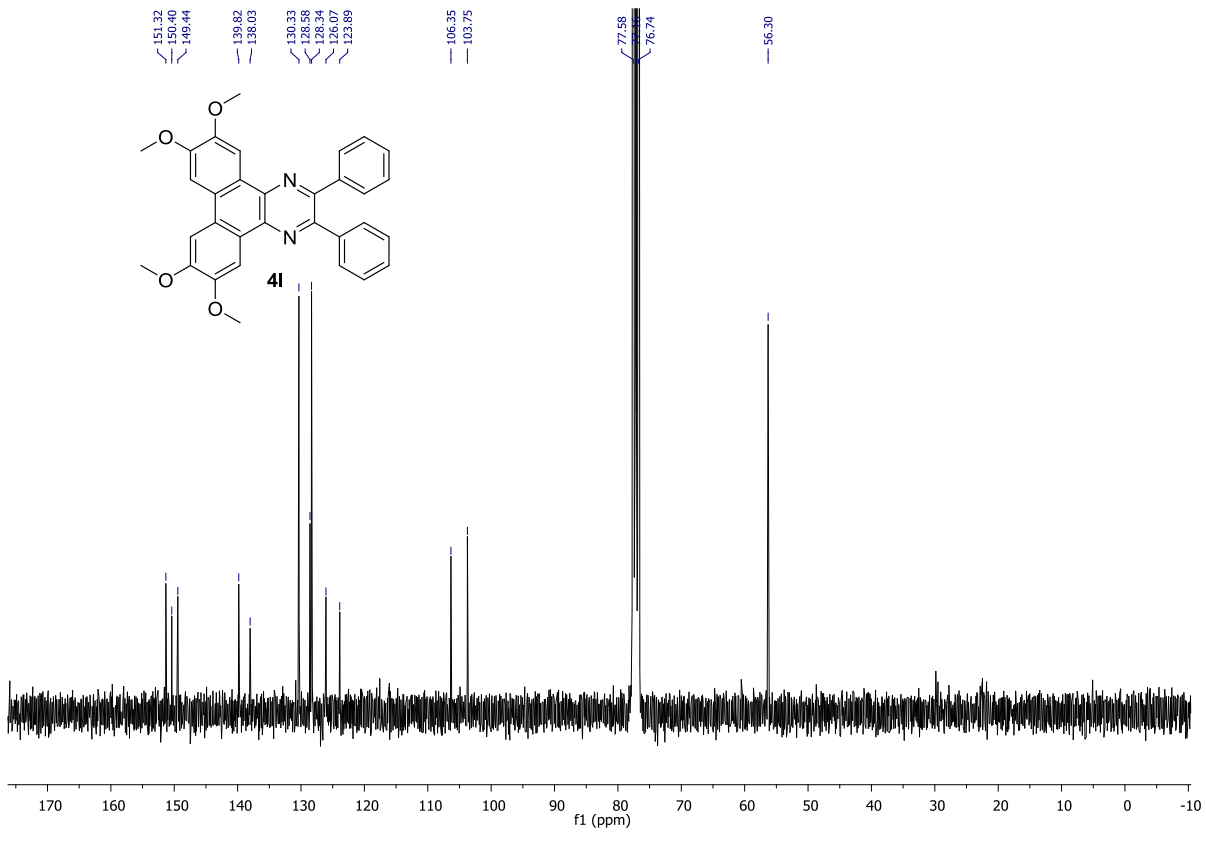
77.36
77.16
76.74
56.30
4j
f1 (ppm)


8.69
8.30
8.28
8.27
8.26
7.83
7.82
7.81
7.55
7.26
4.19
4.12
4k
2.00
2.04
2.02
2.00
6.17
5.95
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


151.66
149.19
141.67
141.55
129.33
129.10
126.33
123.82
107.12
103.79
56.28
56.18
4k
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


8.71
7.76
7.69
7.67
7.66
7.39
7.38
7.26
4.16
4.15
4l
2.00
1.99
3.81
6.00
6.07
5.81
f1 (ppm)


151.32
150.40
149.44
139.82
138.03
130.33
128.58
128.34
126.07
123.89
106.35
103.75
77.58
76.74
56.30
4l
f1 (ppm)