Supporting Information

Transition-Metal-Free [4+2] Cycloaddition of Diaryliodonium salts Accessing Phenazine, Phenothiazine, Phenoxazine and Dioxane Derivatives

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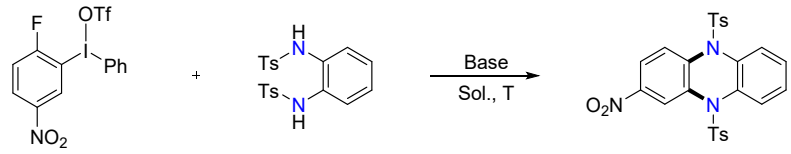
1. General Information

All reactions were monitored by thin layer chromatography (TLC) using Macherey-Nagel 0.20 mm silica gel 60 plates. Flash column chromatography was performed on silica gel 60 (particle size 300-400 mesh ASTM, purchased from Taizhou, China). ^{1}H, ^{13}C, ^{19}F spectra were recorded with, JEOL • JNM-ECZL600G instrument. All ^{1}H NMR data are reported in δ units, parts per million (ppm), and were measured relative to the residual proton signal in the deuterated solvent at 7.26 ppm ($CDCl_3$) and 2.50 ppm (DMSO-d_6). All ^{13}C NMR spectra are decoupled and reported in ppm relative to the solvent signal at 77.16 ppm ($CDCl_3$) and 39.52 ppm (DMSO-d_6). High-resolution mass spectra HRMS (ESI-TOF) were recorded on Brucker microtof. Compounds were visualized by irradiation with UV light, or stained with iodine/silica gel, or potassium permanganate. Preparatory thin-layer chromatography (Prep-TLC) was performed on silica gel GF with UV 254 (20 × 20 cm, 1000 microns, from Yantai Jiang you Silica Gel Development Co., Ltd.) and visualized with UV light.

Materials. Reaction solvents THF and toluene were distilled over sodium and stored under nitrogen atmosphere. While DCM, Dioxane and CH_3CN was distilled over CaH_2 and stored under nitrogen atmosphere. All diaryliodonium salts **1** in the article were known and prepared according to the previously reported procedures.[1] All ambident nucleophile **2** in the article were known and prepared according to the previously reported procedures.[2] [3] [4] All other commercial reagents and solvents were purchased from Energy-Chemical Ltd, and used as received unless otherwise noted.

2. Detailed Optimization Studies

Table S1. Screening of reaction conditions for synthesis of 3.[a]



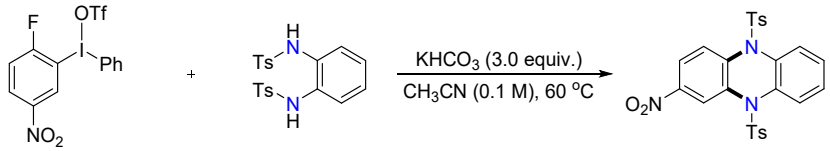
1 **2** **3**

Entry	2a	Base	Sol.	T (°C)	3a (%)[b]
1	2.0 eq.	$KHCO_3$ (3.0 eq.)	Tol	60	Trace
2	2.0 eq.	$KHCO_3$ (3.0 eq.)	DCE	60	28
3	2.0 eq.	$KHCO_3$ (3.0 eq.)	Dioxane	60	66
4	2.0 eq.	$KHCO_3$ (3.0 eq.)	THF	60	40
5	2.0 eq.	$KHCO_3$ (3.0 eq.)	DMSO	60	43
6	2.0 eq.	$KHCO_3$ (3.0 eq.)	DMF	60	45
7	2.0 eq.	$KHCO_3$ (3.0 eq.)	$CHCl_3$	60	Trace
8	2.0 eq.	$KHCO_3$ (3.0 eq.)	ACN	60	88
9	1.2 eq.	$KHCO_3$ (3.0 eq.)	ACN	60	56
10	1.5 eq.	$KHCO_3$ (3.0 eq.)	ACN	60	74
11	2.0 eq.	K_2CO_3 (3.0 eq.)	ACN	60	46
12	2.0 eq.	^{t}BuOK (3.0 eq.)	ACN	60	Trace
13	2.0 eq.	Cs_2CO_3 (3.0 eq.)	ACN	60	12
14	2.0 eq.	DBU(3.0 eq.)	ACN	60	48
15	2.0 eq.	DMAP (3.0 eq.)	ACN	60	Trace
16	2.0 eq.	DABCO (3.0 eq.)	ACN	60	56
17	2.0 eq.	NaH (3.0 eq.)	ACN	60	15
18	2.0 eq.	$KHCO_3$ (1.0 eq.)	ACN	60	70
19	2.0 eq.	$KHCO_3$ (2.0 eq.)	ACN	60	77
20	2.0 eq.	$KHCO_3$ (4.0 eq.)	ACN	60	88
21	2.0 eq.	$KHCO_3$ (5.0 eq.)	ACN	60	89
22	2.0 eq.	$KHCO_3$ (3.0 eq.)	ACN	25	Trace
23	2.0 eq.	$KHCO_3$ (3.0 eq.)	ACN	40	78
24	2.0 eq.	$KHCO_3$ (3.0 eq.)	ACN	80	85

[a] Reaction conditions: **1** (0.1 mmol), **2** (x mmol), base (y equiv), solvent (0.1 M), T, 12 h. [b] ^{1}H NMR yields using 1,3,5-trimethoxybenzene as internal standard.

3. Experimental Procedures

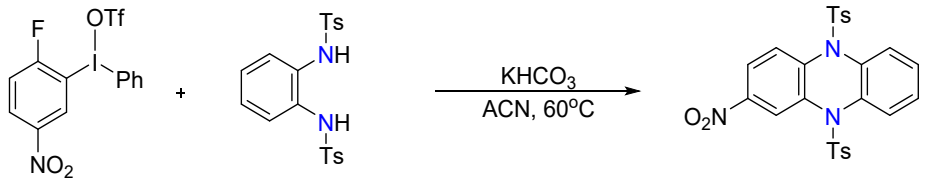
a) General procedure for 3



1 **2** **3**

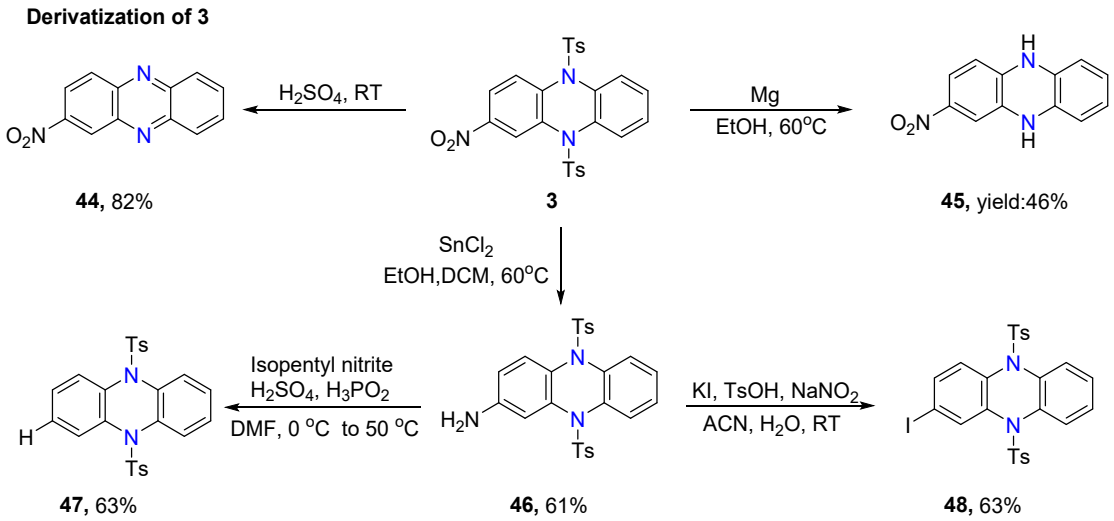
Added diaryliodonium salts **1** (49.6 mg, 0.1 mmol, 1.0equiv), *o*-phenylenediamine derivatives **2** (0.2 mmol, 2.0 equiv) and $KHCO_3$ (30 mg, 0.3 mmol, 3.0 equiv) in 1.0 mL of Acetonitrile and the mixture was allowed to stir for 12 h at 60 °C. Until the reaction was complete as indicated by TLC. The reaction mixture was then quenched with H_2O, extracted with dichloromethane (3×5 mL) and the combined organic layers were dried over Na_2SO_4, and concentrated in vacuo. The resulting crude product was purified by flash column chromatography on silica gel to obtain product **3**.

b) Gram scale synthesis and late-stage functionalization



1 **2** **3,** 63%(1.32g)

Added diaryliodonium salt **1** (1.97 g, 4 mmol, 1.0 equiv), o-phenylenediamine derivatives **2** (3.33 g, 8 mmol, 2.0 equiv) and $KHCO_3$(1.2 g, 12mmol, 3.0 equiv) in 30 mL of Acetonitrile and the mixture was allowed to stir for 16 h at 60 °C. Until the reaction was complete as indicated by TLC. The reaction mixture was then quenched with H_2O, extracted with dichloromethane (3×80 mL) and the combined organic layers were dried over Na_2SO_4, and concentrated in vacuo. The resulting crude product was purified by flash column chromatography on silica gel to obtain product **3** (1.32g, 63%).



Synthesis of 2-nitrophenazine (44)

Added **3** (53.5 mg, 0.1 mmol, 1.0 equiv) in 2 mL of sulfuric acid and the mixture was allowed to stir for 12 h at room temperature. Until the reaction was complete as indicated by TLC. The reaction mixture was slowly poured into ice water, extracted with dichloromethane (3×5 mL) and the combined organic layers were dried over Na_2SO_4, and concentrated in vacuo. The resulting crude product was purified by flash column chromatography on silica gel to obtain product **44** (18.4 mg, 82%).

Synthesis of 2-nitro-5,10-dihydrophenazine (45)

Added **3** (53.5 mg, 0.1 mmol, 1.0 equiv), magnesium ribbon (24 mg, 1.0 mmol, 10.0 equiv) in 2 mL of ethanol and the mixture was allowed to stir for 12 h at 60 °C. Until the reaction was complete as indicated by TLC. The reaction mixture was then quenched with H_2O, extracted with dichloromethane (3×5 mL) and the combined organic layers were dried over Na_2SO_4, and concentrated in vacuo. The resulting crude product was purified by flash column chromatography on silica gel to obtain product **45** (10.4 mg, 46%).

Synthesis of 5,10-ditosyl-5,10-dihydrophenazin-2-amine (46)

Added **3** (535.1 mg, 1.0 mmol) in 20 mL of ethyl alcohol followed by dropwise addition of 5M $SnCl_2$ solution (5 ml) at 60 °C and the mixture was allowed to stir for 3 h at 60 °C, until the reaction was complete as indicated by TLC. The reaction mixture was quenched with H_2O and adjusted to pH 10.5 with KOH. The solution was extracted with Ethyl ether (3×30 mL) and the

combined organic layers were dried over Na_2SO_4, and concentrated in vacuo. The resulting crude product was purified by flash column chromatography on silica gel to obtain product **46** (308.1 mg, 61%).

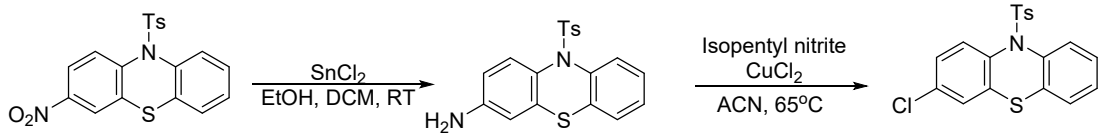
Synthesis of 5,10-ditosyl-5,10-dihydrophenazine (47)

Added **46** (101.0 g, 0.2 mmol, 1.0 equiv) to 2ml DMF. The mixture was cooled to 0 °C, then add sulfuric acid (122.5 mg, 1.25 mmol, 6.25 equiv) and isopentyl nitrite (21.1 mg, 0.38 mmol, 1.9 equiv). After stirring for 1h at 0 °C, phosphinic acid (68 mg, 1.03 mmol, 5.16 equiv) was added carefully. Upon complete addition of the reagents, the mixture was allowed to 50 °C where it was stirred for 4 hours. Until the reaction was complete as indicated by TLC. The reaction mixture was quenched with H_2O, extracted with CH_2Cl_2 (3×5 mL) and the combined organic layers were dried over Na_2SO_4, and concentrated in vacuo. The resulting crude product was purified by flash column chromatography on silica gel to obtain product **47** (61.75 mg, 63%).

Synthesis of 2-iodo-5,10-ditosyl-5,10-dihydrophenazine (48)

Added **46** (101.0 mg, 0.2 mmol, 1.0equiv) and *p*-toluenesulfonic acid monohydrate (114.1 mg, 3.0 equiv) in acetonitrile (3 mL). The reaction was cooled to 0 °C before a solution of $NaNO_2$ (27.6 mg, 2.0 equiv) and KI (58 mg, 2.5 equiv) in water (1 mL) was added drop wise. Upon complete addition of the reagents, the mixture was allowed to reach room temperature where it was stirred for 24 hours. Until the reaction was complete as indicated by TLC. The reaction mixture was quenched with H_2O, extracted with CH_2Cl_2 (3×10 mL) and the combined organic layers were dried over Na_2SO_4, and concentrated in vacuo. The resulting crude product was purified by flash column chromatography on silica gel to obtain product **48** (77.6 mg, 63%).

Derivatization of 40



40 **49**, 88% **50,** 84%

Synthesis of 10-tosyl-10H-phenothiazin-3-amine (49)

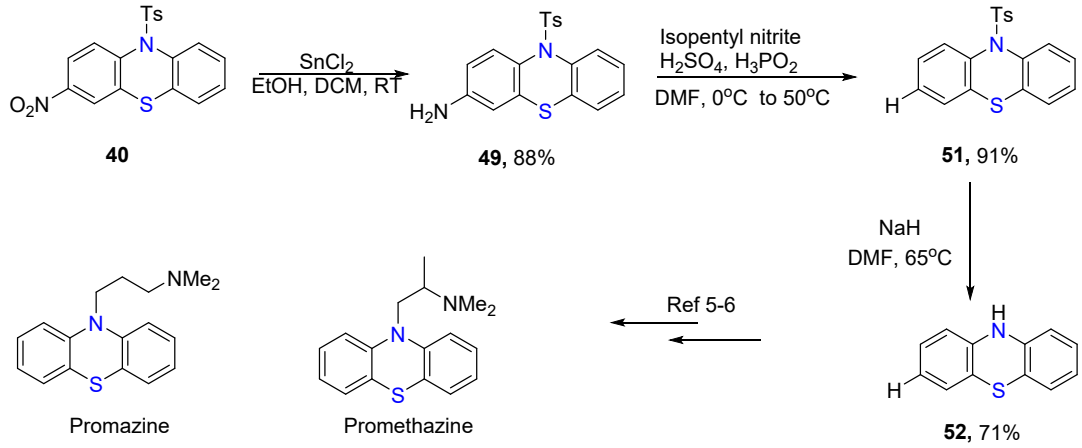
Added **40** (398.0 mg, 1.0 mmol) in 20 mL of ethyl alcohol followed by dropwise addition of 5M $SnCl_2$ solution (5 ml) at rt and the mixture was allowed to stir for 6 h at room temperature,

until the reaction was complete as indicated by TLC. The reaction mixture was quenched with H_2O and adjusted to pH 10.5 with KOH. The solution was extracted with ethyl ether (3×30 mL) and the combined organic layers were dried over Na_2SO_4, and concentrated in vacuo. The resulting crude product was purified by flash column chromatography on silica gel to obtain product **49** (323.8 mg, 88%).

Synthesis of 3-chloro-10-tosyl-10H-phenothiazine (50)

Added $CuCl_2$ (101.0 g, 0.24 mmol, 1.2 equiv) and isopentyl nitrite (21.1 mg, 0.38 mmol, 1.9 equiv.) to 2.0 ml dry acetonitrile under nitrogen atmosphere. Then add **49** (73.6 mg, 0.2 mmol, 1.0 equiv) at 65 °C and the mixture was allowed to stir for 1 h at 65 °C. Until the reaction was complete as indicated by TLC. The reaction mixture was quenched with H_2O, extracted with CH_2Cl_2 (3×5 mL) and the combined organic layers were dried over Na_2SO_4, and concentrated in vacuo. The resulting crude product was purified by flash column chromatography on silica gel to obtain product **50** (65.0 mg, 84%).

Total synthesis of Promazine and Promethazine



Synthesis of 10-tosyl-10H-phenothiazine (51)

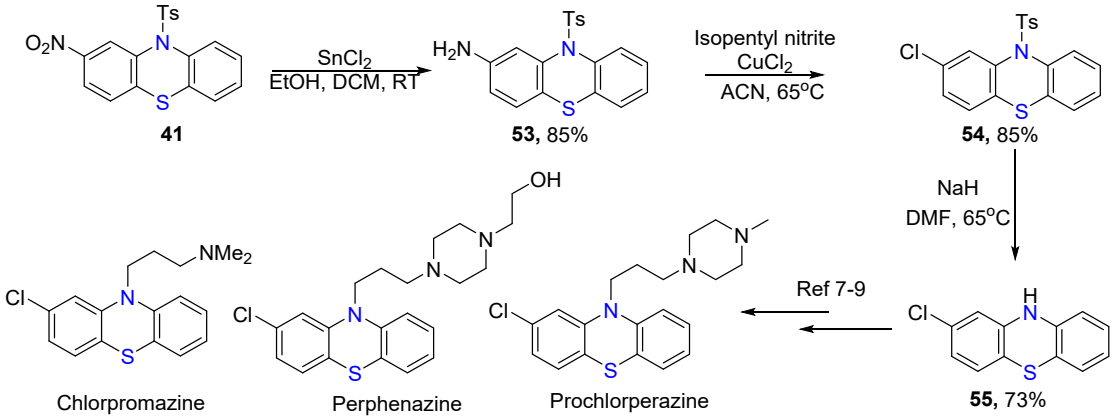
Added **49** (73.6 g, 0.2 mmol, 1.0 equiv) to 2ml DM. The mixture was cooled to 0 °C, then add sulfuric acid (122.5 mg, 1.25 mmol, 6.25 equiv) and Isopentyl nitrite (21.1 mg, 0.38 mmol, 1.9 equiv). After stirring for 1h at 0 °C, phosphinic acid (68 mg, 1.03 mmol, 5.16 equiv) was added carefully. The reaction was warmed to 50 °C and maintained at this temperature until gas evolution ceased (4 h). Until the reaction was complete as indicated by TLC. The reaction mixture was quenched with H_2O, extracted with CH_2Cl_2 (3×5 mL) and the combined organic layers were

dried over Na_2SO_4, and concentrated in vacuo. The resulting crude product was purified by flash column chromatography on silica gel to obtain product **51** (64.3 mg, 91%).

Synthesis of 10H-phenothiazine (52)

To a suspension solution of NaH (0.4 mmol, 2.0 equiv) in dry DMA (1.0 mL) was added dropwise the solution of **51** (70.6 mg, 0.2 mmol, 1 equiv) in dry DMA (0.5mL) by syringe. Then the mixture was heated at 65 °C Until the reaction was complete as indicated by TLC. The reaction mixture was quenched with H_2O, extracted with CH_2Cl_2 (3×5 mL) and the combined organic layers were dried over Na_2SO_4, and concentrated in vacuo. The resulting crude product was purified by flash column chromatography on silica gel to obtain product **52** (28.3 mg, 71%). Compound **52** can be converted into Promazine [5] and Promethazine [6] as described in previous literature.

Total synthesis of Perphenazine, Chlorpromazine, and Prochlorperazine



Synthesis of 10-tosyl-10H-phenothiazin-2-amine (53)

Added **41** (398.0 mg, 1.0 mmol) in 20 mL of ethyl alcohol followed by dropwise addition of 5M $SnCl_2$ solution (5 ml) at rt and the mixture was allowed to stir for 6 h at room temperature, until the reaction was complete as indicated by TLC. The reaction mixture was quenched with H_2O and adjusted to pH 10.5 with KOH. The solution was extracted with ethyl ether (3×30 mL) and the combined organic layers were dried over Na_2SO_4, and concentrated in vacuo. The resulting crude product was purified by flash column chromatography on silica gel to obtain product **53** (312.8 mg, 85%).

Synthesis of 2-chloro-10-tosyl-10H-phenothiazine (54)

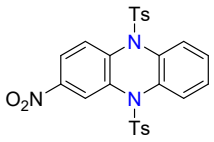
Added $CuCl_2$ (101.0 g, 0.24 mmol, 1.2 equiv) and isopentyl nitrite (21.1 mg, 0.38 mmol, 1.9 equiv) to 2ml dry acetonitrile under nitrogen atmosphere. Then add **53** (73.6 mg, 0.2 mmol, 1.0 equiv) at 65 ^oC and the mixture was allowed to stir for 1 h at 65 ^oC. Until the reaction was complete as indicated by TLC. The reaction mixture was quenched with H_2O, extracted with CH_2Cl_2 (3×5 mL) and the combined organic layers were dried over Na_2SO_4, and concentrated in vacuo. The resulting crude product was purified by flash column chromatography on silica gel to obtain product **54** (65.8 mg, 85%).

Synthesis of 2-chloro-10H-phenothiazine (55)

To a suspension solution of NaH (0.4 mmol, 2.0 equiv) in dry DMA (1.0 mL) was added dropwise the solution of **54** (77.4 mg, 0.2 mmol, 1 equiv) in dry DMA (0.5mL) by syringe. Then the mixture was heated at 65 ^oC Until the reaction was complete as indicated by TLC. The reaction mixture was quenched with H_2O, extracted with CH_2Cl_2 (3×5 mL) and the combined organic layers were dried over Na_2SO_4, and concentrated in vacuo. The resulting crude product was purified by flash column chromatography on silica gel to obtain product **55** (34.1 mg, 73%). Compound **55** can be converted into Perphenazine [7] Chlorpromazine [8], and Prochlorperazine [9] as described in previous literature

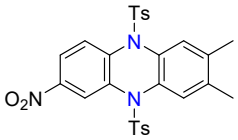
4. Analytical data of New Compounds

2-Nitro-5,10-ditosyl-5,10-dihydrophenazine (3)



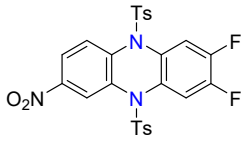
The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 2:1 to afford **3** as brown solid (47.0 mg, 88% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.26 (s, 1H), 8.09 (d, *J* = 9.0 Hz, 1H), 7.57 – 7.51 (m, 5H), 7.44 – 7.40 (m, 2H), 7.32 – 7.26 (m, 6H), 2.44 (s, 3H), 2.43 (s, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 145.7, 145.32, 145.30, 141.1, 136.5, 136.3, 135.4, 134.3, 133.9, 130.6, 130.6, 127.4, 127.3, 127.2, 126.9, 125.3, 125.1, 124.8, 121.8, 120.9, 21.80, 21.79. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{26}H_{20}N_3O_6S_2$ ([M - H]$^-$), 534.0799 found, 534.0796.

2,3-Dimethyl-7-nitro-5,10-ditosyl-5,10-dihydrophenazine (4)



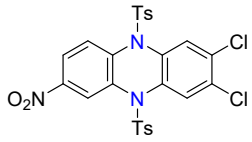
The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 2:1 to afford **4** as brown solid (34.4 mg, 61% yield), TLC: Rf = 0.27 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.23 (s, 1H), 8.05 (d, *J* = 9.0 Hz, 1H), 7.54 – 7.51 (m, 4H), 7.31 – 7.28 (m, 4H), 7.18 (d, *J* = 8.4 Hz, 2H), 2.44 (s, 3H), 2.43 (s, 3H), 2.24 (s, 3H), 2.23 (s, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 145.6, 145.14, 145.12, 141.3, 136.7, 136.4, 136.3, 136.2, 135.6, 131.8, 131.3, 130.5, 127.3, 127.0, 126.0, 125.4, 125.0, 121.7, 120.8, 21.80, 21.79, 19.9, 19.8. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{28}H_{24}N_3O_6S_2$ ([M - H]$^-$), 562.1112 found, 562.1110.

2,3-Difluoro-7-nitro-5,10-ditosyl-5,10-dihydrophenazine (5)



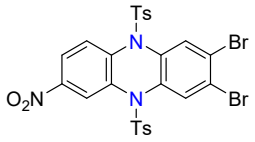
The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 2:1 to afford **5** as brown solid (36.0 mg, 63% yield), TLC: Rf = 0.25 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.22 (s, 1H), 8.11 (d, *J* = 9.0 , 1H), 7.57 – 7.50 (m, 5H), 7.35 – 7.30 (m, 4H), 7.28 – 7.24 (m, 2H), 2.45 (d, *J* = 8.4 Hz, 6H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 149.7 – 149.5 (m), 148.0 – 147.9 (m), 146.0, 145.81, 145.80, 140.4, 135.82, 135.80, 135.0, 130.81, 130.78, 130.7 – 130.6 (m), 130.4 – 130.3 (m), 127.3, 127.1, 125.3, 122.2, 120.8, 114.2 (d, *J* = 21.14 Hz), 113.9 (d, *J* = 21.14 Hz). 113.85, 113.84, 21.82, 21.81. **^{19}F NMR** (565 MHz, Chloroform-d) δ -135.6 – -135.8 (m), -135.8 – -135.9 (m). **HRMS** (ESI-TOF) (m/z): Calcd for $C_{26}H_{18}F_2N_3O_6S_2$ ([M - H]$^-$), 570.0611 found, 570.0608.

2,3-Dichloro-7-nitro-5,10-ditosyl-5,10-dihydrophenazine (6)



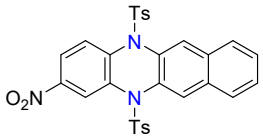
The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 30:1 to afford **6** as yellow solid (38.6 mg, 64% yield), TLC: Rf = 0.25 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.21 (s, 1H), 8.10 (d, *J* = 9.0 Hz, 1H), 7.56 – 7.49 (m, 7H), 7.36 – 7.31 (m, 4H), 2.45 (s, 3H), 2.44 (s, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 146.0, 145.9, 145.8, 140.3, 135.8, 134.9, 133.7, 133.4, 131.44, 131.39, 130.82, 130.79, 127.3, 127.1, 126.5, 126.1, 125.3, 122.2, 120.7, 21.9, 21.8. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{26}H_{18}Cl_2N_3O_6S_2$ ([M - H]$^-$), 602.0020 found, 602.0018.

2,3-Dibromo-7-nitro-5,10-ditosyl-5,10-dihydrophenazine (7)



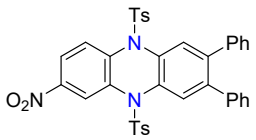
The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 2:1 to afford **7** as brown solid (45.6 mg, 66% yield), TLC: Rf = 0.24 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.20 (s, 1H), 8.10 (d, *J* = 9.0 Hz, 1H), 7.69 (s, 1H), 7.64 (s, 1H), 7.55 (d, *J* = 8.4, 3H), 7.52 (d, *J* = 8.4 Hz, 2H), 7.33 (d, *J* = 8.4 Hz, 4H), 2.46 (s, 3H), 2.44 (s, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 146.0, 145.86, 145.85, 140.3, 135.8, 135.7, 135.0, 134.3, 134.1, 130.81, 130.78, 129.5, 129.2, 127.4, 127.2, 125.3, 123.22, 123.18, 122.17, 120.7, 21.86, 21.85. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{26}H_{18}Br_2N_3O_6S_2$ ([M - H]$^-$), 689.9009 found, 689.9007.

2-Nitro-5,12-ditosyl-5,12-dihydrobenzo[b]phenazine (8)



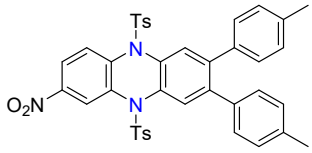
The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 30:1 to afford **8** as yellow solid (28.7 mg, 49% yield), TLC: Rf = 0.24 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.33 (s, 1H), 8.11 (d, *J* = 9.0 Hz, 1H), 7.86 (d, *J* = 7.2 Hz, 2H), 7.80 – 7.76 (m, 2H), 7.62 (d, *J* = 9.0 Hz, 1H), 7.57 – 7.54 (m, 4H), 7.51 – 7.48 (m, 2H), 7.30 (t, *J* = 8.4 Hz, 4H), 2.44 (s, 3H), 2.43 (s, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 145.7, 145.34, 145.33, 140.9, 136.6, 136.5, 135.2, 132.5, 132.1, 131.7, 131.6, 130.64, 130.62, 128.0, 127.3, 127.18, 127.14, 127.2, 125.4, 123.4, 122.8, 121.9, 121.0, 21.82, 21.81. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{30}H_{22}N_3O_6S_2$ ([M - H]$^-$), 584.0956 found, 584.0954.

7-Nitro-2,3-diphenyl-5,10-ditosyl-5,10-dihydrophenazine (9)



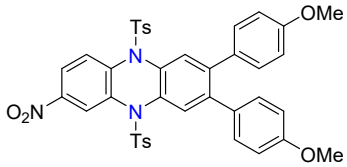
The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 2:1 to afford **9** as yellow solid (52.2 mg, 76% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.29 (s, 1H), 8.10 (d, *J* = 9.0 Hz, 1H), 7.63 – 7.58 (m, 5H), 7.50 (s, 2H), 7.32 (t, *J* = 8.4 Hz, 4H), 7.24 – 7.20 (m, 6H), 7.10 – 7.07 (m, 4H), 2.44 (s, 3H), 2.43 (s, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 145.7, 145.38, 145.36, 141.1, 139.82, 139.77, 139.7, 136.4, 136.3, 135.4, 133.3, 132.9, 130.59, 130.58, 129.87, 129.86, 128.21, 128.19, 127.4, 127.29, 127.27, 127.2, 127.1, 126.7, 125.1, 121.9, 120.7, 21.79, 21.78. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{38}H_{28}N_3O_6S_2$ ([M - H]$^-$), 686.1425 found, 686.1423.

7-Nitro-2,3-di-p-tolyl-5,10-ditosyl-5,10-dihydrophenazine (10)



The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 2:1 to afford **10** as yellow solid (43.6 mg, 61% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.28 (s, 1H), 8.09 (d, *J* = 9.0 Hz, 1H), 7.62 – 7.57 (m, 5H), 7.46 (s, 2H), 7.31 (t, *J* = 8.4 Hz, 4H), 7.04 – 7.01 (m, 4H), 6.99 – 6.97 (m, 4H), 2.44 (s, 3H), 2.43 (s, 3H), 2.32 (s, 3H), 2.32 (s, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 145.7, 145.30, 145.29, 141.1, 139.73, 139.65, 137.03, 136.97, 136.94, 136.93, 136.5, 136.3, 135.5, 133.1, 132.7, 130.57, 130.56, 129.69, 129.68, 128.94, 128.93, 127.4, 127.2, 127.1, 126.6, 125.1, 121.8, 120.7, 21.79, 21.78, 21.3. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{40}H_{32}N_3O_6S_2$ ([M - H]$^-$), 714.1738 found, 714.1736.

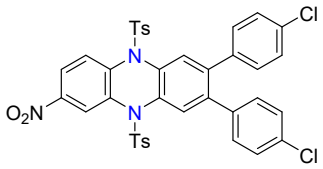
2,3-Bis(4-methoxyphenyl)-7-nitro-5,10-ditosyl-5,10-dihydrophenazine(11)



The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 2:1 to afford **11** as yellow solid (22.4 mg, 57% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.28 (s, 1H), 8.08 (d, *J* = 9.0 Hz, 1H), 7.61 – 7.56 (m, 5H), 7.43 (s, 2H), 7.33 – 7.30 (m, 4H), 7.03 – 6.98 (m, 4H), 6.79 – 6.73 (m, 4H), 3.79 (s, 3H), 3.78 (s, 3H), 2.44 (s, 3H), 2.43 (s, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 158.88, 158.87, 145.7, 145.31, 145.29, 141.11, 139.3, 139.2, 136.5, 136.3, 135.4, 132.9, 132.5, 132.4, 132.30, 131.0, 130.57, 130.56, 127.4, 127.2, 127.0, 126.5, 125.0, 121.8, 120.7, 113.72,

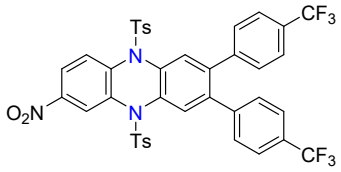
113.70, 55.34, 55.33, 21.79, 21.78. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{40}H_{32}N_3O_8S_2$ ([M - H]$^-$), 746.1636 found, 746.1634.

2,3-Bis(4-chlorophenyl)-7-nitro-5,10-ditosyl-5,10-dihydrophenazine(12)



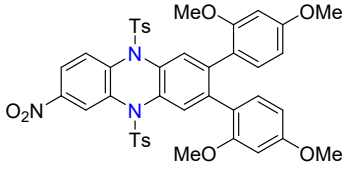
The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 2:1 to afford **12** as yellow solid (54.4 mg, 72% yield), TLC: Rf = 0.25 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.27 (s, 1H), 8.09 (d, *J* = 9.0 Hz, 1H), 7.58 (t, *J* = 7.8 Hz, 5H), 7.44 (s, 2H), 7.32 (t, *J* = 8.4 Hz, 4H), 7.23 – 7.20 (m, 4H), 7.02 – 6.99 (m, 4H), 2.44 (s, 3H), 2.43 (s, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 145.8, 145.54, 145.52, 140.9, 138.4, 138.3, 137.94, 137.89, 136.6, 136.1, 135.3, 133.8, 133.73, 133.72, 133.4, 131.1, 130.7, 130.6, 128.7, 128.6, 127.4, 127.2, 127.1, 126.6, 125.1, 122.0, 120.7, 21.81, 21.80. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{38}H_{26}Cl_2N_3O_6S_2$ ([M - H]$^-$), 754.0646 found, 754.0644.

7-Nitro-5,10-ditosyl-2,3-bis(4-(trifluoromethyl)phenyl)-5,10-dihydrophenazine(13)



The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 2:1 to afford **13** as yellow solid (37.9 mg, 46% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.27 (s, 1H), 8.11 (d, *J* = 9.0 Hz, 1H), 7.61 – 7.57 (m, 5H), 7.52 – 7.49 (m, 6H), 7.35 – 7.31 (m, 4H), 7.21 – 7.18 (m, 4H), 2.45 (s, 3H), 2.44 (s, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 145.8, 145.61, 145.59, 142.9, 140.7, 138.2, 138.1, 136.11, 136.05, 135.2, 134.2, 133.8, 130.7, 130.6, 130.09, 130.08, 127.33, 127.29, 127.1, 126.9, 125.5 – 125.4 (m), 125.1, 124.9, 123.1, 122.0, 120.6, 21.8. **^{19}F NMR** (565 MHz, Chloroform-d) δ -62.43. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{40}H_{26}F_6N_3O_6S_2$ ([M - H]$^-$), 822.1173 found, 822.1171.

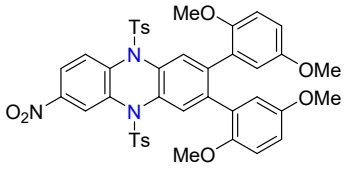
2,3-Bis(2,4-dimethoxyphenyl)-7-nitro-5,10-ditosyl-5,10-dihydrophenazine(14)



The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 2:1 to afford **14** as yellow solid (52.5 mg, 65% yield), TLC: Rf = 0.21 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.23 (s, 1H), 8.05 (d, *J* = 9.0 Hz, 1H), 7.58 (d, *J* = 8.4 Hz, 4H), 7.48 (d, *J* = 9.0 Hz, 1H), 7.46 (s, 1H), 7.43 (s, 1H), 7.30 – 7.27

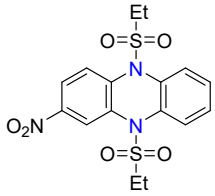
(m, 4H), 6.92 – 6.89 (m, 2H), 6.36 – 6.30 (m, 4H), 3.78 (s, 3H), 3.77 (s, 3H), 3.50 (s, 3H), 3.48 (s, 3H), 2.42 (s, 3H), 2.42 (s, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 160.3, 157.23, 157.21, 145.6, 145.1, 145.0, 141.3, 137.5, 137.4, 136.8, 136.5, 135.5, 132.3, 131.9, 131.8, 131.7, 130.48, 130.47, 127.7, 127.3, 127.02, 126.99, 124.99, 122.3, 122.2, 121.7, 120.7, 104.1, 98.4, 98.4, 55.46, 55.45, 55.3, 55.2, 21.80, 21.78. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{42}H_{36}N_3O_{10}S_2$ ([M - H]$^-$), 806.1848 found, 806.1846.

2,3-Bis(2,5-dimethoxyphenyl)-7-nitro-5,10-ditosyl-5,10-dihydrophenazine(15)



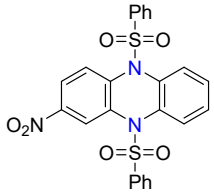
The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 2:1 to afford **15** as yellow solid (42.8 mg, 53% yield), TLC: Rf = 0.22 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.25 (s, 1H), 8.07 (d, *J* = 9.0 Hz, 1H), 7.60 (d, *J* = 8.4 Hz, 4H), 7.54 – 7.48 (m, 3H), 7.29 (d, *J* = 8.4, 4H), 6.74 – 6.66 (m, 4H), 6.60 (s, 2H), 3.61 (s, 3H), 3.60 (s, 3H), 3.48 (s, 3H), 3.47 (s, 3H), 2.43 (s, 3H), 2.42 (s, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 153.2, 150.61, 150.59, 145.6, 145.2, 145.1, 141.2, 137.2, 137.1, 136.7, 136.4, 135.5, 132.7, 132.3, 130.50, 130.49, 129.8, 129.7, 127.5, 127.3, 127.1, 126.8, 124.9, 121.7, 120.7, 117.0, 116.9, 114.10, 114.07, 111.9, 55.90, 55.89, 21.77, 21.76. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{42}H_{36}N_3O_{10}S_2$ ([M - H]$^-$), 806.1848 found, 806.1846.

5,10-Bis(ethylsulfonyl)-2-nitro-5,10-dihydrophenazine(16)



The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 2:1 to afford **16** as yellow solid (31.2 mg, 76% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.28 (s, 1H), 8.17 (d, *J* = 9.0 Hz, 1H), 7.67 (d, *J* = 9.0 Hz, 1H), 7.55 (s, 1H), 7.47 (s, 1H), 7.36 (s, 2H), 3.49 (q, *J* = 7.8 Hz, 2H), 3.42 (q, *J* = 7.8 Hz, 2H), 1.57 (t, *J* = 7.2 Hz, 3H), 1.51 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 146.2, 141.8, 136.4, 135.0, 134.8, 128.1, 128.0, 126.1, 125.5, 125.4, 122.4, 121.1, 50.0, 49.6, 8.2, 8.1. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{16}H_{16}N_3O_6S_2$ ([M - H]$^-$), 410.0486 found, 410.0484.

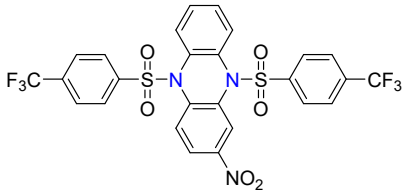
2-Nitro-5,10-bis(phenylsulfonyl)-5,10-dihydrophenazine(17)



The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 30:1 to afford **17** as yellow solid (42.6 mg, 84% yield),

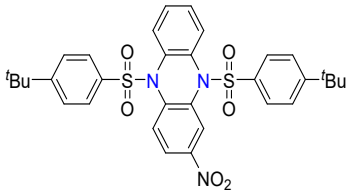
TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.27 (s, 1H), 8.11 (d, *J* = 9.0 Hz, 1H), 7.67 – 7.63 (m, 6H), 7.56 – 7.51 (m, 5H), 7.46 – 7.43 (m, 1H), 7.43 – 7.40 (m, 1H), 7.31 – 7.27 (m, 2H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 145.9, 141.0, 139.5, 139.2, 135.4, 134.3, 134.10, 134.08, 133.9, 130.1, 130.0, 127.6, 127.5, 127.2, 126.9, 125.4, 125.2, 124.8, 122.00, 120.9.**HRMS** (ESI-TOF) (m/z): Calcd for $C_{24}H_{16}N_3O_6S_2$ ([M - H]$^-$), 506.0486 found, 506.0484.

2-Nitro-5,10-bis((4-(trifluoromethyl)phenyl)sulfonyl)-5,10-dihydrophenazine(18)



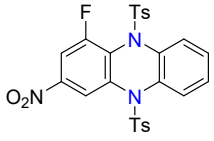
The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 30:1 to afford **18** as yellow solid (36.0 mg, 56% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.28 (s, 1H), 8.17 (d, *J* = 9.0 Hz, 1H), 7.80 – 7.75 (m, 8H), 7.54 (d, *J* = 9.0 Hz, 1H), 7.43 – 7.34 (m, 4H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 146.2, 142.6, 142.3, 140.7, 136.0, 135.7, 135.3, 134.1, 133.7, 128.1, 128.0, 127.8, 127.5, 127.41, 127.37 (q, *J* = 3.6 Hz), 127.3, 125.6, 125.0, 124.06, 124.02, 122.5, 122.3, 122.2, 121.1. **^{19}F NMR** (565 MHz, Chloroform-d) δ -63.22. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{26}H_{14}F_6N_3O_6S_2$ ([M - H]$^-$), 642.0234 found, 642.0232.

5,10-Bis((4-(tert-butyl)phenyl)sulfonyl)-2-nitro-5,10-dihydrophenazine(19)



The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 2:1 to afford **19** as yellow solid (44.6 mg, 72% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.28 (s, 1H), 8.09 (d, *J* = 9.0 Hz, 1H), 7.55 – 7.50 (m, 9H), 7.47 – 7.44 (m, 1H), 7.44 – 7.41 (m, 1H), 7.31 – 7.27 (m, 2H), 1.33 (s, 9H), 1.32 (s, 9H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 158.1, 145.8, 141.1, 136.5, 136.1, 135.5, 134.3, 134.0, 127.4, 127.3, 127.1, 127.0, 126.6, 125.4, 125.2, 124.8, 121.8, 120.9, 35.4, 31.12, 31.11. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{32}H_{32}N_3O_6S_2$ ([M - H]$^-$), 618.1738 found, 618.1738.

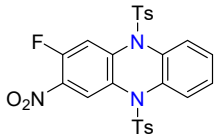
1-Fluoro-3-nitro-5,10-ditosyl-5,10-dihydrophenazine(20)



The crude was purified by flash chromatography using Petroleum ether/

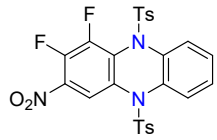
Dichloromethane 2:1 to afford **20** as yellow solid (40.4 mg, 73% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.39 (s, 1H), 7.92 (d, *J* = 9.6 Hz, 1H), 7.74 (d, *J* = 8.4 Hz, 2H), 7.67 (d, *J* = 8.4 Hz, 1H), 7.57 (d, *J* = 8.4 Hz, 2H), 7.34 – 7.30 (m, 3H), 7.26 (d, *J* = 8.4 Hz, 2H), 7.23 (t, *J* = 7.8 Hz, 1H), 7.12 (d, *J* = 7.8 Hz, 1H), 2.46 (s, 3H), 2.39 (s, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 156.5, 154.8, 146.1(d, *J* = 10.6 Hz), 145.5, 145.4, 138.9(d, *J* = 3.0 Hz,), 136.7, 135.5, 135.0, 134.1, 130.49, 130.48(d, *J* = 3.0 Hz), 130.1, 130.1, 130.0, 128.29, 128.26, 128.0, 127.9, 127.4, 125.6, 124.7, 116.3(d, *J* = 3.0 Hz), 110.1, 109.9, 21.8. **^{19}F NMR** (565 MHz, Chloroform-d) δ -110.68. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{26}H_{19}FN_3O_6S_2$ ([M - H]$^-$), 552.0705 found, 552.0703.

2-Fluoro-3-nitro-5,10-ditosyl-5,10-dihydrophenazine(21)



The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 2:1 to afford **21** as yellow solid (34.8 mg, 63% yield), TLC: Rf = 0.24 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.16 (d, *J* = 7.2 Hz, 1H), 7.57 – 7.55 (m, 2H), 7.49 – 7.46 (m, 3H), 7.35 – 7.32 (m, 3H), 7.30 – 7.25 (m, 5H), 2.44 (s, 3H), 2.44 (s, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 154.7, 152.9, 145.6, 145.5, 142.14, 142.07, 136.6, 135.5, 134.6(d, *J* = 7.6 Hz), 134.2, 133.2, 130.7, 130.6, 130.5 (d, *J* = 3.0 Hz), 127.6, 127.4, 127.3, 126.8, 126.1, 124.0, 123.3, 113.8, 113.7, 21.81, 21.80. **^{19}F NMR** (565 MHz, Chloroform-d) δ -116.41. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{26}H_{19}FN_3O_6S_2$ ([M - H]$^-$), 552.0705 found, 552.0703.

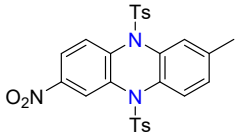
1,2-Difluoro-3-nitro-5,10-ditosyl-5,10-dihydrophenazine(22)



The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 2:1 to afford **22** as yellow solid (28.0 mg, 49% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.27 (d, *J* = 4.8 Hz, 1H), 7.78 (d, *J* = 8.4 Hz, 2H), 7.71 (d, *J* = 8.4 Hz, 1H), 7.53 (d, *J* = 8.4 Hz, 2H), 7.36 – 7.32 (m, 3H), 7.26 – 7.25 (m, 3H), 7.25 – 7.21 (m, 1H), 7.05 (d, *J* = 7.8 Hz, 1H), 2.47 (s, 3H), 2.39 (s, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 145.64, 145.58, 136.8, 135.84-135.82(m), 135.1, 134.5, 134.0, 132.79-132.77(m), 130.5, 130.2, 129.19-129.17(m), 128.34, 128.31, 128.2, 128.0, 127.7, 126.2, 124.2, 116.8, 21.8. **^{19}F NMR** (565 MHz, Chloroform-d) δ -133.21 (d, *J* = 21.5 Hz), -141.46 (d, *J* = 28.0 Hz). **HRMS** (ESI-TOF) (m/z): Calcd for

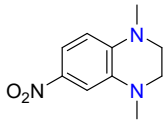
$C_{26}H_{18}F_2N_3O_6S_2$ ([M - H]$^-$), 570.0611 found, 570.0608.

2-Methyl-7-nitro-5,10-ditosyl-5,10-dihydrophenazine(23)



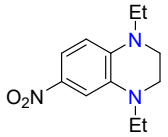
The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 2:1 to afford **23** as yellow solid (33.5 mg, 61% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-*d*) δ 8.31 – 8.26 (m, 1H), 8.14 – 8.07 (m, 1H), 7.56 (d, *J* = 8.4 Hz, 4H), 7.35 – 7.33 (m, 4H), 7.11 (t, *J* = 7.8 Hz, 1H), 2.49 – 2.46 (m, 6H), 2.40 – 2.37 (m, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 145.7, 145.6, 145.3, 145.23, 145.19, 145.17, 141.3, 141.1, 137.7, 137.66, 136.7, 136.6, 136.4, 136.3, 135.6, 135.4, 134.1, 133.7, 131.7, 131.3, 130.6, 128.2, 128.1, 127.2, 127.98, 126.95, 125.8, 125.2, 125.1, 125.0, 124.9, 124.3, 121.8, 121.7, 120.9, 120.88, 21.79, 21.79, 21.77, 21.33, 21.26. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{27}H_{22}N_3O_6S_2$ ([M - H]$^-$), 548.0956 found, 548.0954.

1,4-Dimethyl-6-nitro-1,2,3,4-tetrahydroquinoxaline(24)



The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 30:1 to afford **24** as red solid (18.2 mg, 88% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 7.70 (d, *J* = 9.0 Hz, 1H), 7.32 (s, 1H), 6.38 (d, *J* = 9.0 Hz, 1H), 3.56 – 3.53 (m, 2H), 3.29 – 3.26 (m, 2H), 3.02 (s, 3H), 2.92 (s, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 142.5, 138.2, 135.4, 117.3, 107.5, 105.5, 49.9, 48.4, 39.5, 39.1. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{10}H_{12}N_3O_2$ ([M - H]-), 206.0935 found, 206.0933.

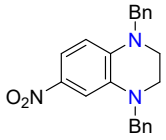
1,4-Diethyl-6-nitro-1,2,3,4-tetrahydroquinoxaline(25)



The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 30:1 to afford **25** as red solid (150.4 mg, 64% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 7.68 – 7.59 (m, 1H), 7.37 (s, 1H), 6.42 (d, *J* = 9.0 Hz, 1H), 3.52 – 3.49 (m, 2H), 3.43 (q, *J* = 7.2 Hz, 2H), 3.37 (q, *J* = 7.2 Hz, 2H), 3.30 – 3.26 (m, 2H), 1.22 – 1.18 (m, 6H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 141.4, 137.9, 133.8, 116.7, 107.7, 105.6, 47.33, 46.0, 45.5,

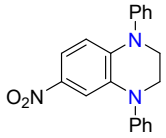
45.0, 10.8, 10.1. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{12}H_{16}N_3O_2$ ([M - H]$^-$), 234.1248 found, 234.1245.

1,4-Dibenzyl-6-nitro-1,2,3,4-tetrahydroquinoxaline(26)



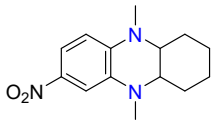
The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 1:1 to afford **26** as red solid (13.3 mg, 37% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 1:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 7.61 (d, *J* = 9.0 Hz, 1H), 7.51 (s, 1H), 7.37 – 7.32 (m, 6H), 7.31 – 7.28 (m, 2H), 7.24 – 7.22 (m, 2H), 6.45 (d, *J* = 9.0 Hz, 1H), 4.61 (s, 2H), 4.49 (s, 2H), 3.61 – 3.58 (m, 2H), 3.35 – 3.32 (m, 2H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 141.88, 138.4, 137.1, 136.5, 134.6, 129.1, 129.0, 127.8, 127.7, 126.7, 117.1, 108.8, 106.5, 55.4, 55.3, 48.9, 45.9. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{22}H_{20}N_3O_2$ ([M - H]$^-$), 358.1561 found, 358.1558.

6-Nitro-1,4-diphenyl-1,2,3,4-tetrahydroquinoxaline(27)



The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 1:1 to afford **27** as red solid (13.2 mg, 40% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 9.02 (s, 1H), 8.31 (d, *J* = 9.0 Hz, 1H), 8.21 – 8.13 (m, 1H), 7.58 – 7.52 (m, 1H), 7.42 (d, *J* = 8.4 Hz, 1H), 7.37 (t, *J* = 7.8 Hz, 1H), 7.27 (s, 2H), 7.24 – 7.20 (m, 2H), 6.81 – 6.77 (m, 1H), 6.59 – 6.54 (m, 2H), 4.58 (t, *J* = 6.0 Hz, 2H), 3.73 (t, *J* = 6.0 Hz, 2H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 146.8, 143.9, 141.7, 141.1, 129.8, 127.7, 123.2, 122.8, 121.9, 121.27, 121.25, 118.5, 117.5, 113.0, 109.7, 108.6, 42.6. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{20}H_{16}N_3O_2$ ([M - H]$^-$), 330.1248 found, 330.1246.

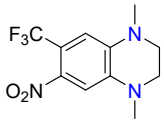
5,10-Dimethyl-7-nitro-1,2,3,4,4a,5,10,10a-octahydrophenazine(28)



The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 30:1 to afford **28** as red solid (22.4 mg, 56% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 7.73 (d, *J* = 9.0 Hz, 1H), 7.42 (s, 1H), 6.44 (d, *J* = 9.0 Hz, 1H), 3.14 – 3.10 (m, 1H), 2.99 (s, 3H), 2.82 (s, 3H), 2.66 – 2.62 (m, 1H), 2.33 – 2.27 (m, 2H), 1.93 – 1.83 (m, 2H),

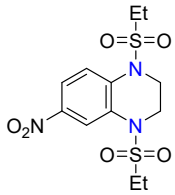
1.37 – 1.24 (m, 4H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 144.7, 138.1, 137.7, 117.8, 108.7, 106.4, 63.3, 60.6, 34.5, 33.2, 30.4, 29.8, 24.6, 24.1. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{14}H_{18}N_3O_2$ ([M - H]$^-$), 260.1405 found, 260.1403.

1,4-Dimethyl-6-nitro-7-(trifluoromethyl)-1,2,3,4-tetrahydroquinoxaline(29)



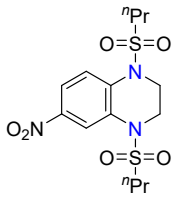
The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 30:1 to afford **29** as red solid (19.0 mg, 69% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 7.14 (s, 1H), 6.65 (s, 1H), 3.49 (t, *J* = 4.8 Hz, 2H), 3.38 (t, *J* = 4.8 Hz, 2H), 3.02 (s, 3H), 2.96 (s, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 139.33, 137.16, 123.23 (q, *J* = 271.5 Hz), 115.01 (q, *J* = 33.1 Hz), 106.95, 106.86 (q, *J* = 33.1 Hz), 49.01, 48.15, 39.07, 39.04. **^{19}F NMR** (565 MHz, Chloroform-d) δ -58.1. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{11}H_{11}F_3N_3O_2$ ([M - H]$^-$), 274.0809 found, 274.0807.

1,4-Bis(ethylsulfonyl)-6-nitro-1,2,3,4-tetrahydroquinoxaline(30)



The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 1:1 to afford **30** as red solid (20.0 mg, 55% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.43 (s, 1H), 7.99 (d, *J* = 9.0 Hz, 1H), 7.90 (d, *J* = 9.0 Hz, 1H), 4.00 – 3.97 (m, 2H), 3.90 – 3.87 (m, 2H), 3.23 – 3.17 (m, 4H), 1.99 – 1.84 (m, 4H), 1.11 (t, *J* = 7.8 Hz, 3H), 1.07 (t, *J* = 7.8 Hz, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 143.5, 135.4, 128.5, 121.2, 120.4, 118.9, 55.3, 54.3, 46.3, 45.0, 17.2, 17.0, 13.0, 12.9. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{12}H_{16}N_3O_6S_2$ ([M - H]$^-$), 362.0486 found, 362.0484.

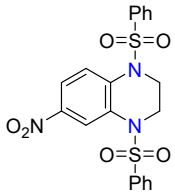
6-Nitro-1,4-bis(propylsulfonyl)-1,2,3,4-tetrahydroquinoxaline(31)



The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 1:1 to afford **31** as red solid (20.7 mg, 53% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 1:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.42 (s, 1H), 8.00 (d, *J* = 9.0 Hz, 1H), 7.90 (d, *J* = 9.0 Hz, 1H), 4.02 – 4.00 (m, 2H), 3.91 – 3.89 (m, 2H), 3.32 – 3.25 (m, 4H), 1.49 (t, *J* = 7.2 Hz, 3H), 1.42 (t, *J* = 7.2 Hz, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 143.6, 135.5, 128.6, 121.2, 120.5, 119.0, 48.2,

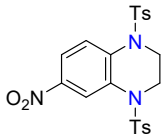
47.2, 46.6, 45.2, 8.2, 8.0. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{14}H_{20}N_3O_6S_2$ ([M - H]$^-$), 390.0799 found, 390.0797.

6-Nitro-1,4-bis(phenylsulfonyl)-1,2,3,4-tetrahydroquinoxaline(32)



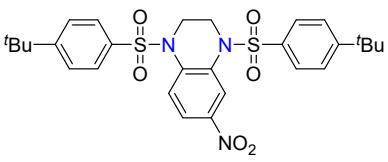
The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 1:1 to afford **32** as red solid (27.5 mg, 60% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 1:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.68 (s, 1H), 7.98 (d, *J* = 9.0 Hz, 1H), 7.94 (d, *J* = 9.0 Hz, 1H), 7.64 – 7.60 (m, 4H), 7.59 – 7.56 (m, 2H), 7.49 – 7.45 (m, 4H), 3.69 – 3.65 (m, 4H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 143.9, 138.1, 138.0, 134.2, 134.1, 134.0, 129.99, 129.8, 128.1, 127.4, 127.1, 122.6, 119.9, 119.1, 44.2, 43.5. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{20}H_{16}N_3O_6S_2$ ([M - H]$^-$), 458.0486 found, 458.0484.

6-Nitro-1,4-ditosyl-1,2,3,4-tetrahydroquinoxaline(33)



The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 1:1 to afford **33** as red solid (32.1 mg, 66% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 1:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.67 (s, 1H), 7.98 (d, *J* = 9.0 Hz, 1H), 7.92 (d, *J* = 9.0 Hz, 1H), 7.52 – 7.45 (m, 4H), 7.26 – 7.24 (m, 4H), 3.65 – 3.60 (m, 4H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 145.4, 145.2, 143.7, 135.1, 135.1, 133.9, 130.34, 130.33, 128.0, 127.4, 127.2, 122.5, 119.7, 119.0, 43.9, 43.2, 21.7. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{22}H_{20}N_3O_6S_2$ ([M - H]$^-$), 486.0799 found, 486.0797.

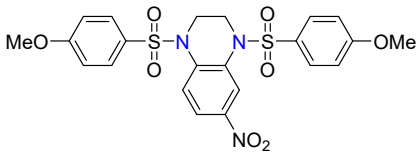
1,4-Bis((4-(tert-butyl)phenyl)sulfonyl)-6-nitro-1,2,3,4-tetrahydroquinoxaline(34)



The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 1:1 to afford **34** as red solid (31.4 mg, 55% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 1:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.64 (s, 1H), 7.96 – 7.92 (m, 2H), 7.59 (d, *J* = 9.0 Hz, 2H), 7.55 (d, *J* = 9.0 Hz, 2H), 7.50 (t, *J* = 8.4 Hz, 4H), 3.69 – 3.63 (m, 4H), 1.32 (s, 9H), 1.32 (s, 9H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 158.4, 158.3, 143.7, 135.2,

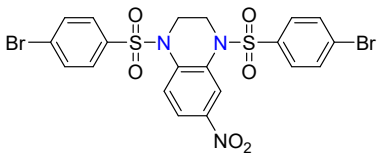
135.11, 134.2, 128.1, 127.3, 127.0, 126.9, 126.8, 122.4, 119.8, 119.2, 44.2, 43.5, 35.47, 35.46, 31.11, 31.10. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{28}H_{32}N_3O_6S_2$ ([M - H]$^-$), 570.1738 found, 570.1736.

1,4-Bis((4-methoxyphenyl)sulfonyl)-6-nitro-1,2,3,4-tetrahydroquinoxaline(35)



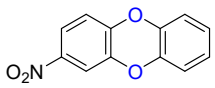
The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 1:1 to afford **35** as red solid (26.4 mg, 51% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 1:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.68 (s, 1H), 7.99 (d, *J* = 9.0 Hz, 1H), 7.93 – 7.90 (m, 1H), 7.54 – 7.48 (m, 4H), 6.91 – 6.88 (m, 4H), 3.86 (s,6H), 3.68 – 3.62 (m, 4H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 164.1, 164.0, 143.8, 134.0, 129.7, 129.43, 129.35, 128.2, 122.6, 119.7, 119.0, 114.93, 114.92, 55.9, 44.0, 43.3. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{22}H_{20}N_3O_8S_2$ ([M - H]$^-$), 518.0697 found, 518.0695.

1,4-Bis((4-bromophenyl)sulfonyl)-6-nitro-1,2,3,4-tetrahydroquinoxaline(36)



The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 1:1 to afford **36** as red solid (38.1 mg, 62% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 1:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.64 (s, 1H), 7.97 (s, 2H), 7.64 – 7.62 (m, 4H), 7.49 (d, *J* = 8.4 Hz, 2H), 7.45 (d, *J* = 8.4 Hz, 2H), 3.76 – 3.70 (m, 4H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 144.11, 136.93, 133.89, 133.19, 133.17, 129.7, 129.6, 128.9, 128.6, 122.7, 120.2, 119.0, 44.6, 44.0. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{20}H_{14}Br_2N_3O_6S_2$ ([M - H]$^-$), 613.8696 found, 613.8694.

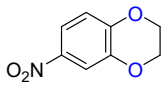
2-Nitrodibenzo[b,e][1,4]dioxine(37)



The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 3:1 to afford **37** as yellow solid (10.8 mg, 47% yield), TLC: Rf = 0.24 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 7.82 (d, *J* = 9.0 Hz, 1H), 7.73 (s, 1H), 6.98 – 6.94 (m, 2H), 6.92 (d, *J* = 9.0 Hz, 1H), 6.90 – 6.87

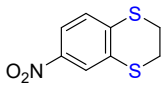
(m, 2H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 147.8, 142.3, 141.12, 141.06, 130.6, 125.3, 124.9, 120.2, 116.81, 116.79, 116.6, 112.6. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{12}H_6NO_4$ ([M - H]$^-$), 228.0302 found, 228.0308.

6-Nitro-2,3-dihydrobenzo[b][1,4]dioxine(38)



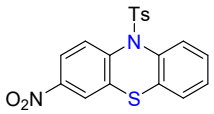
The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 3:1 to afford **38** as yellow solid (7.3 mg, 40% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 7.80 – 7.76 (m, 2H), 6.94 (d, *J* = 7.8 Hz, 1H), 4.37 – 4.34 (m, 2H), 4.32 – 4.30 (m, 2H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 149.4, 143.2, 141.9, 117.8, 117.4, 113.6, 64.8, 64.2. **HRMS** (ESI-TOF) (m/z): Calcd for $C_8H_6NO_4$ ([M - H]$^-$), 180.0302 found, 180.0309.

6-Nitro-2,3-dihydrobenzo[b][1,4]dithiine(39)



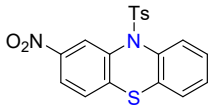
The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 3:1 to afford **39** as yellow solid (8.7 mg, 41% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.02 (s, 1H), 7.81 (d, *J* = 9.0 Hz, 1H), 7.24 (d, *J* = 9.0 Hz, 1H), 3.40 – 3.37 (m, 2H), 3.32 – 3.29 (m, 2H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 145.0, 140.2, 132.0, 128.7, 123.8, 119.9, 29.3, 28.0. **HRMS** (ESI-TOF) (m/z): Calcd for $C_8H_6NO_2S_2$ ([M - H]$^-$), 211.9845 found, 211.9843.

3-Nitro-10-tosyl-10H-phenothiazine(40) [10]



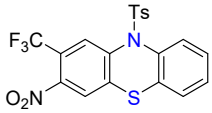
The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 2:1 to afford **40** as yellow solid (23.1 mg, 58% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.16 (d, *J* = 9.0 Hz, 1H), 8.00 (s, 1H), 7.88 (d, *J* = 9.0 Hz, 1H), 7.76 (d, *J* = 8.4 Hz, 1H), 7.41 – 7.38 (m, 1H), 7.28 (t, *J* = 7.8 Hz, 1H), 7.16 – 7.13 (m, 3H), 7.09 (d, *J* = 8.4 Hz, 2H), 2.39 (s, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 146.7, 145.0, 141.9, 135.8, 135.3, 135.2, 131.4, 130.6, 130.0, 129.9, 128.4, 128.2, 127.7, 127.2, 122.3, 122.2, 21.8. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{19}H_{13}N_2O_4S_2$ ([M - H]$^-$), 397.0322 found, 397.0320.

2-Nitro-10-tosyl-10H-phenothiazine(41) [11]



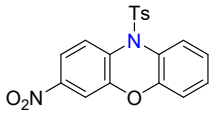
The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 2:1 to afford **41** as yellow solid (13.9 mg, 35% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.56 (s, 1H), 8.09 (d, *J* = 8.4 Hz, 1H), 7.78 (d, *J* = 8.4 Hz, 1H), 7.41 (t, *J* = 7.8 Hz, 1H), 7.28 (t, *J* = 7.8 Hz, 1H), 7.25 (d, *J* = 8.4 Hz, 1H), 7.15 – 7.12 (m, 3H), 7.08 (d, *J* = 8.4 Hz, 2H), 2.39 (s, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 147.1, 144.9, 142.1, 136.7, 135.7, 135.0, 131.0, 130.3, 129.7, 128.5, 128.3, 127.88, 127.07, 127.05, 125.2, 122.6, 21.8. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{19}H_{13}N_2O_4S_2$ ([M - H]$^-$), 397.0322 found, 397.0320.

3-Nitro-10-tosyl-2-(trifluoromethyl)-10H-phenothiazine(42)



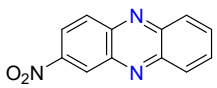
The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 2:1 to afford **42** as yellow solid (26.1 mg, 56% yield), TLC: Rf = 0.24 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.12 (s, 1H), 7.77 (d, *J* = 7.8 Hz, 1H), 7.66 (s, 1H), 7.43 (d, *J* = 8.4 Hz, 1H), 7.32 – 7.30 (m, 1H), 7.17 – 7.15 (m, 2H), 7.14 – 7.11 (m, 3H), 2.41 (s, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 145.4, 139.9, 139.8, 135.4, 134.6, 130.2, 130.1, 129.9, 129.4 (q, *J* = 5.4 Hz), 128.72, 128.68, 127.6, 127.2, 123.5, 122.59, 122.56, 122.4, 120.8, 21.8. **^{19}F NMR** (565 MHz, Chloroform-d) δ -59.56. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{20}H_{12}F_3N_2O_4S_2$ ([M - H]$^-$), 465.0196 found, 465.0194.

3-Nitro-10-tosyl-10H-phenoxazine(43) [12]



The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 2:1 to afford **43** as yellow solid (24.1 mg, 63% yield), TLC: Rf = 0.24 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 8.02 (d, *J* = 9.0 Hz, 1H), 7.82 (d, *J* = 9.0 Hz, 1H), 7.69 (d, *J* = 7.8 Hz, 1H), 7.67 (s, 1H), 7.26 – 7.20 (m, 2H), 7.09 – 7.06 (m, 2H), 6.98 (d, *J* = 8.4 Hz, 2H), 6.85 (d, *J* = 7.8 Hz, 1H), 2.37 (s, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 151.3, 150.2, 147.2, 145.4, 132.7, 132.5, 129.65, 129.1, 128.6, 127.9, 127.7, 125.6, 124.9, 119.0, 116.6, 112.1, 21.8. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{19}H_{13}N_2O_5S$ ([M - H]$^-$), 381.0551 found, 381.0549.

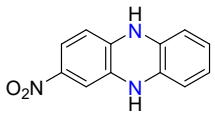
2-Nitrophenazine(44)



The crude was purified by flash chromatography using Dichloromethane to

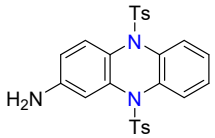
afford **44** as yellow solid (18.5 mg, 82% yield), TLC: Rf = 0.26 (Dichloromethane) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 9.21 (s, 1H), 8.57 (d, *J* = 9.0 Hz, 1H), 8.42 – 8.39 (m, 1H), 8.32 – 8.28 (m, 2H), 7.99 – 7.93 (m, 2H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 148.3, 145.1, 145.0, 144.8, 141.8, 132.9, 132.1, 131.8, 130.2, 130.1, 126.9, 123.4. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{12}H_6N_3O_2$ ([M - H]$^-$), 224.0466 found, 224.0464.

2-Nitro-5,10-dihydrophenazine(45)



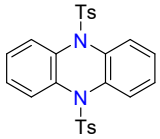
The crude was purified by flash chromatography using Dichloromethane to afford **45** as yellow solid (10.4 mg, 46% yield), TLC: Rf = 0.26 (Dichloromethane) [UV]. **^{1}H NMR** (600 MHz, DMSO-d6) δ 8.05 (d, *J* = 8.4 Hz, 1H), 7.97 (d, *J* = 9.0 Hz, 1H), 7.90 (d, *J* = 9.0 Hz, 1H), 7.79 – 7.72 (m, 1H), 7.68 – 7.61 (m, 1H), 7.45 (d, *J* = 9.0 Hz, 1H), 6.92 (s, 1H), 6.49 (s, 2H). **^{13}C NMR** (150 MHz, DMSO-d6) δ 151.1, 145.8, 143.2, 139.8, 139.4, 130.19, 130.16, 129.3, 128.1, 127.2, 126.8, 101.2. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{12}H_8N_3O_2$ ([M - H]-), 226.0622 found, 226.0620.

5,10-Ditosyl-5,10-dihydrophenazin-2-amine(46)



The crude was purified by flash chromatography using Dichloromethane to afford **46** as brown solid (30.8 mg, 61% yield), TLC: Rf = 0.26 (Dichloromethane) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 7.53 (d, *J* = 8.4 Hz, 2H), 7.45 – 7.41 (m, 3H), 7.26 (d, *J* = 7.8 Hz, 2H), 7.24 – 7.14 (m, 6H), 6.61 (s, 1H), 6.53 (d, *J* = 8.4 Hz, 1H), 2.40 (s, 3H), 2.39 (s, 3H). ^{13}C NMR (150 MHz, Chloroform-*d*) δ 144.7, 143.9, 140.7, 136.5, 135.8, 130.4, 130.2, 129.9, 129.83, 129.75, 129.5, 128.4, 127.44, 127.36, 126.7, 124.2, 120.4, 21.8, 21.7. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{26}H_{22}N_3O_4S_2$ ([M - H]-), 504.1057 found, 504.1055.

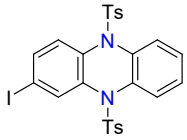
5,10-Ditosyl-5,10-dihydrophenazine(47)



The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 2:1 to afford **47** as yellow solid (30.8 mg, 63% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 7.50 (d, *J* = 8.4 Hz, 2H), 7.43 – 7.38 (m, 2H), 7.26 (d, *J* = 8.4 Hz, 2H), 7.24 – 7.20 (m, 2H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 144.5, 137.2, 135.0, 130.3, 126.9, 126.7,

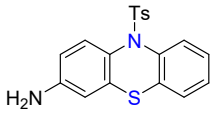
125.1, 21.7. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{26}H_{21}N_2O_4S_2$ ([M - H]$^-$), 489.0948 found, 489.0946.

2-Iodo-5,10-ditosyl-5,10-dihydrophenazine(48)



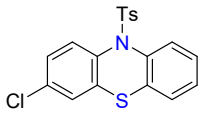
The crude was purified by flash chromatography using Petroleum ether/ Ethyl acetate 2:1 to afford **48** as white solid (38.8 mg, 63% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 7.75 (s, 1H), 7.54 – 7.47 (m, 5H), 7.40 – 7.35 (m, 2H), 7.27 (d, *J* = 8.4 Hz, 4H), 7.23 – 7.20 (m, 2H), 7.09 (d, *J* = 8.4 Hz, 1H), 2.42 (s, 6H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 91.6, 91.5, 83.8, 83.4, 82.8, 82.5, 81.9, 81.3, 81.2, 80.8, 77.2, 73.9, 73.71, 73.68, 73.6, 73.0, 72.0, 71.6. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{26}H_{20}IN_2O_4S_2$ ([M - H]$^-$), 614.9915 found, 614.9913.

10-Tosyl-10H-phenothiazin-3-amine(49)



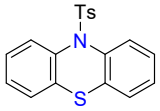
The crude was purified by flash chromatography using Dichloromethane to afford **49** as brown solid (32.4 mg, 88% yield), TLC: Rf = 0.24 (Dichloromethane) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 7.70 (d, *J* = 7.8 Hz, 1H), 7.49 (d, *J* = 8.4 Hz, 1H), 7.32 – 7.28 (m, 1H), 7.19 (t, *J* = 7.8 Hz, 1H), 7.14 (d, *J* = 8.4 Hz, 2H), 7.08 (d, *J* = 7.8 Hz, 1H), 7.04 (d, *J* = 7.8 Hz, 2H), 6.62 – 6.59 (m, 1H), 6.38 (s, 1H), 2.37 (s, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 146.1, 144.0, 136.5, 136.1, 134.1, 133.1, 130.8, 130.1, 129.3, 127.9, 127.6, 127.1, 126.9, 126.4, 114.1, 112.2, 21.8. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{19}H_{15}N_2O_2S_2$ ([M - H]$^-$), 367.0580 found, 367.0578.

3-Chloro-10-tosyl-10H-phenothiazine(50)



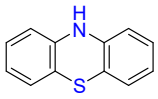
The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 2:1 to afford **50** as yellow solid (32.5 mg, 84% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 7.75 (s, 1H), 7.72 (d, *J* = 8.4 Hz, 1H), 7.36 – 7.32 (m, 1H), 7.23 (t, *J* = 7.8 Hz, 1H), 7.20 (d, *J* = 8.4 Hz, 1H), 7.16 (d, *J* = 7.8 Hz, 2H), 7.11 (d, *J* = 7.8 Hz, 1H), 7.06 (d, *J* = 7.8 Hz, 2H), 7.03 (d, *J* = 8.4 Hz, 1H), 2.38 (s, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 144.5, 136.0, 135.9, 135.0, 134.7, 133.6, 132.3, 131.1, 130.2, 129.6, 128.0, 127.8, 127.7, 127.5, 127.0, 126.6, 21.8. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{19}H_{13}ClNO_2S_2$ ([M - H]$^-$), 386.0082 found, 386.0080.

10-Tosyl-10H-phenothiazine(51)



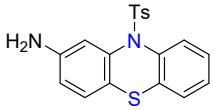
The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 2:1 to afford **51** as yellow solid (32.1 mg, 91% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 7.75 (d, *J* = 7.8 Hz, 2H), 7.35 – 7.31 (m, 2H), 7.22 (t, *J* = 7.8 Hz, 2H), 7.14 (d, *J* = 8.4 Hz, 2H), 7.11 (d, *J* = 7.8 Hz, 2H), 7.04 (d, *J* = 8.4 Hz, 2H), 2.37 (s, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 144.2, 136.2, 136.0, 133.2, 130.1, 129.4, 127.8, 127.7, 127.3, 127.0, 21.7. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{19}H_{14}NO_2S_2$ ([M - H]$^-$), 352.0471 found, 352.0469.

10H-Phenothiazine(52)



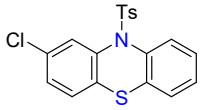
The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 5:1 to afford **52** as white solid (14.1 mg, 71% yield), TLC: Rf = 0.29 (Petroleum ether/ Dichloromethane 5:1) [UV]. **^{1}H NMR** (600 MHz, DMSO-d6) δ 8.58 (s, 1H), 6.98 (t, *J* = 7.8 Hz, 2H), 6.90 (d, *J* = 7.8 Hz, 2H), 6.75 (t, *J* = 7.8 Hz, 2H), 6.68 (d, *J* = 7.8 Hz, 2H). **^{13}C NMR** (150 MHz, DMSO-d6) δ 142.1, 127.6, 126.3, 121.8, 116.4, 114.5. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{12}H_8NS$ ([M - H]$^-$), 198.0383 found, 198.0381.

10-Tosyl-10H-phenothiazin-2-amine(53)



The crude was purified by flash chromatography using Dichloromethane to afford **53** as brown solid (31.3 mg, 85% yield), TLC: Rf = 0.26 (Dichloromethane) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 7.70 (d, *J* = 8.0 Hz, 1H), 7.29 (t, *J* = 7.8 Hz, 1H), 7.21 – 7.17 (m, 3H), 7.12 (s, 1H), 7.10 (d, *J* = 7.8 Hz, 1H), 7.05 (d, *J* = 7.8 Hz, 2H), 6.88 (d, *J* = 8.4 Hz, 1H), 2.37 (s, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 146.1, 144.1, 137.3, 136.4, 136.2, 134.3, 130.1, 129.4, 127.8, 127.7, 127.6, 127.0, 126.9, 121.0, 116.7, 115.0, 21.8. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{19}H_{15}N_2O_2S_2$ ([M - H]$^-$), 367.0580 found, 367.0578.

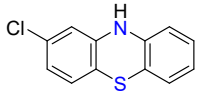
2-Chloro-10-tosyl-10H-phenothiazine(54)



The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 2:1 to afford **54** as yellow solid (32.9 mg, 85% yield), TLC: Rf = 0.26 (Petroleum ether/ Dichloromethane 2:1) [UV]. **^{1}H NMR** (600 MHz, Chloroform-d) δ 7.75 (s, 1H), 7.72 (d, *J* = 7.8 Hz, 1H), 7.35 (t, *J* = 7.8 Hz, 1H), 7.24 (t, *J* = 7.2 Hz, 1H), 7.20 (d, *J* = 8.4 Hz, 1H), 7.16 (d, *J* = 8.4 Hz, 2H), 7.11 (d, *J* = 7.8 Hz, 1H), 7.06 (d, *J* = 7.8 Hz, 2H), 7.03 (d, *J* = 8.4 Hz, 1H), 2.38 (s, 3H). **^{13}C NMR** (150 MHz, Chloroform-d) δ 144.5, 137.0, 136.0, 135.7,

132.9, 132.7, 131.8, 130.15, 130.14, 129.5, 128.0, 127.8, 127.62, 127.58, 127.1, 21.8. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{19}H_{13}ClNO_2S_2$ ([M - H]$^-$), 386.0082 found, 386.0080.

2-Chloro-10H-phenothiazine(55)

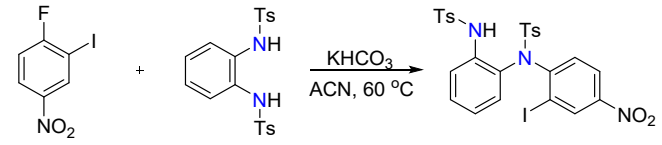


The crude was purified by flash chromatography using Petroleum ether/ Dichloromethane 5:1 to afford **55** as white solid (17.0 mg, 73% yield), TLC: Rf = 0.28 (Petroleum ether/ Dichloromethane 5:1) [UV]. **^{1}H NMR** (600 MHz, DMSO-d6) δ 8.76 (s, 1H), 7.00 (t, *J* = 7.8 Hz, 1H), 6.92 – 6.89 (m, 2H), 6.77 (t, *J* = 8.4 Hz, 2H), 6.69 (s, 1H), 6.66 (d, *J* = 7.8 Hz, 1H). **^{13}C NMR** (150 MHz, DMSO-d6) δ 143.6, 141.2, 131.9, 127.9, 127.5, 126.4, 122.5, 121.3, 116.1, 115.6, 114.8, 113.8. **HRMS** (ESI-TOF) (m/z): Calcd for $C_{12}H_7ClNS$ ([M - H]$^-$), 231.9993 found, 231.9998.

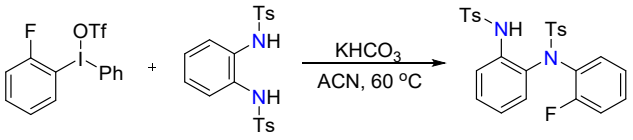
4. Mechanistic investigation

4.1 Controlled experiments

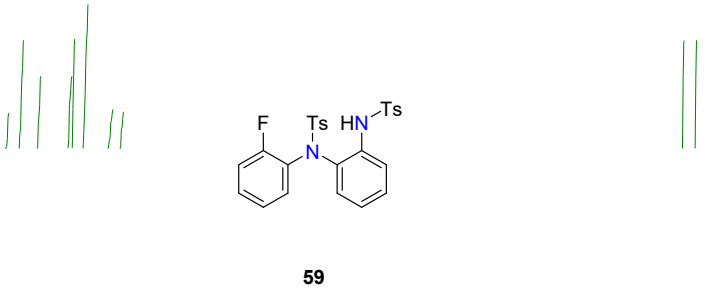
To clarify the sequence of two consecutive nucleophilic substitutions during the cycloaddition reaction of the diaryliodonium salt, several controlled experiments were performed. When fluoroaromatic **56** was subjected to the reaction conditions, no cycloaddition product **3** or any other substituted products were observed. In contrast, nitro-free iodonium salt **58** smoothly afforded **59**, indicating that C-F bond cleavage requires synergistic activation by the nitro group and the hypervalent iodine center.



56 **2** **57,** n.d.



58 **2** **59,** 20%



59

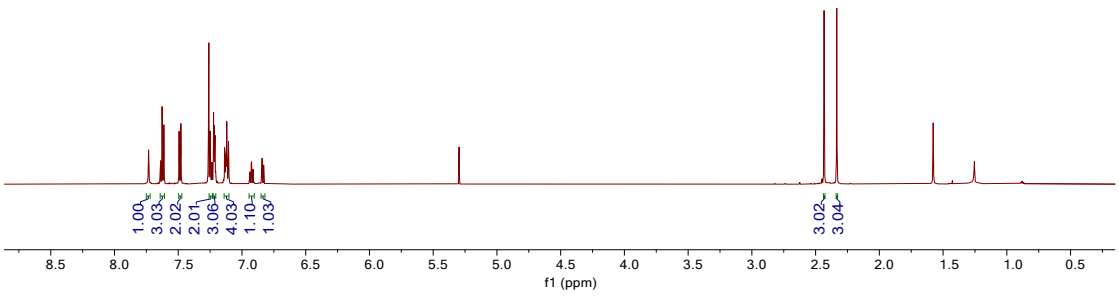
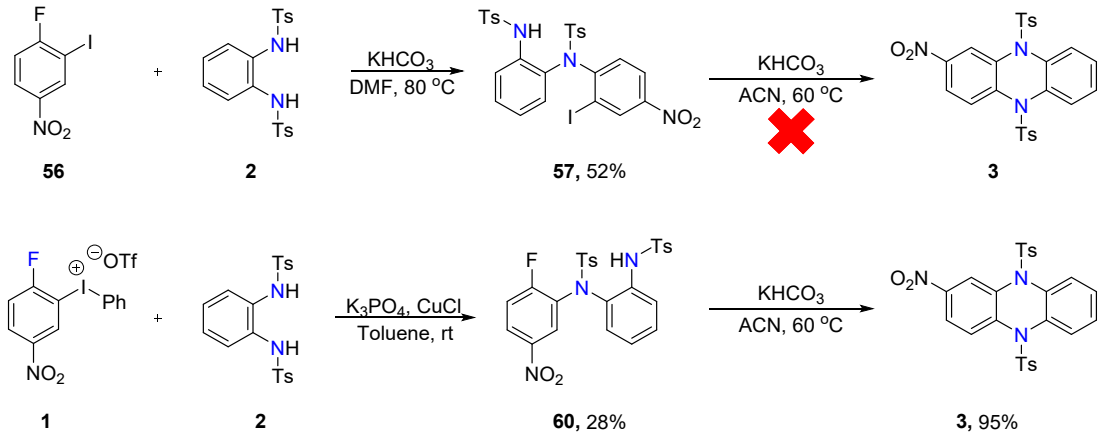


Fig. S1 ^{1}H NMR data of **59**

Further, in order to prove the first step of cyclization reaction. We attempted the independent synthesis of the two divergent intermediates, **57** and **60**. Notably, intermediate **57**, isolated during optimization, could not be converted to **3**, suggesting significant kinetic or thermodynamic barriers. If the iodonium salt participates in the reaction first, compound **60** is likely to be the key intermediate of this reaction. Notably, using the synthesized compound **60** directly as the substrate under standard conditions can yield the target product **3**, indicating that this may be another reaction pathway.



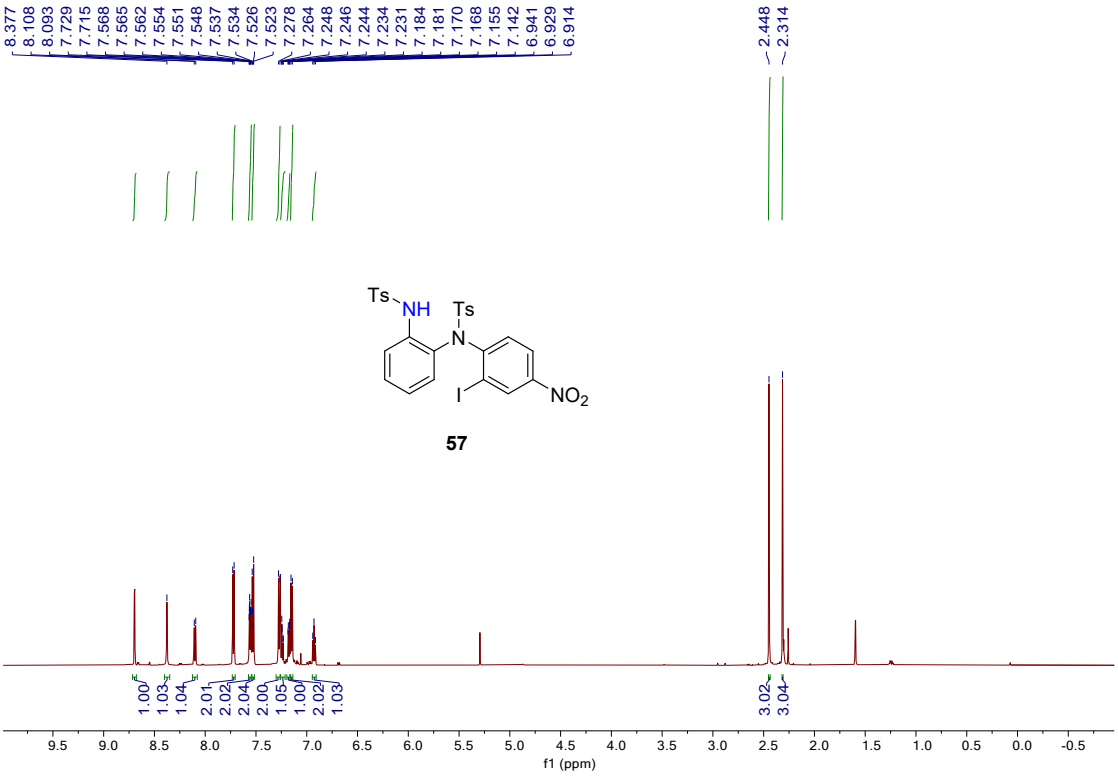


Fig. S2 ^{1}H NMR data of **57**

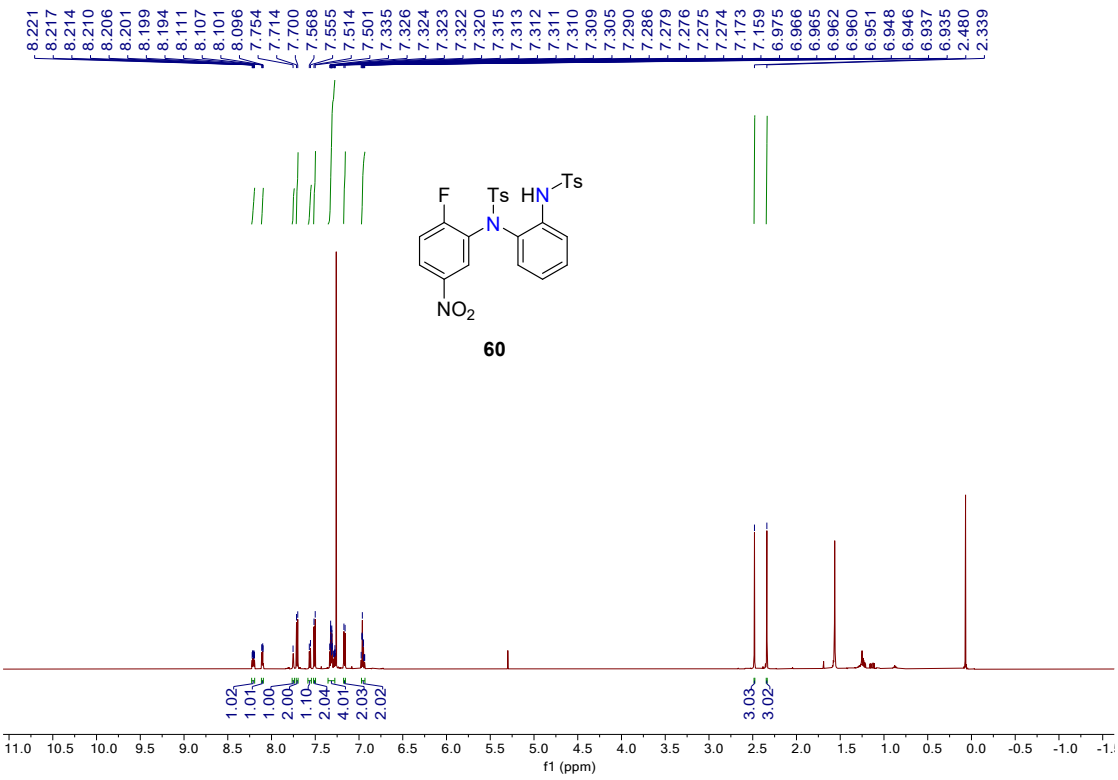


Fig. S3 ^{1}H NMR data of **60**

Overall, these control experiments indicate the importance of electron-withdrawing groups in

the iodized salt, which play a crucial role in promoting the reaction, and the nucleophilic substitution in the initial step should be associated with the cleavage of the C-F or C-I bond. These experimental results are aligning with findings from previous studies [1], [13-15]

5. References

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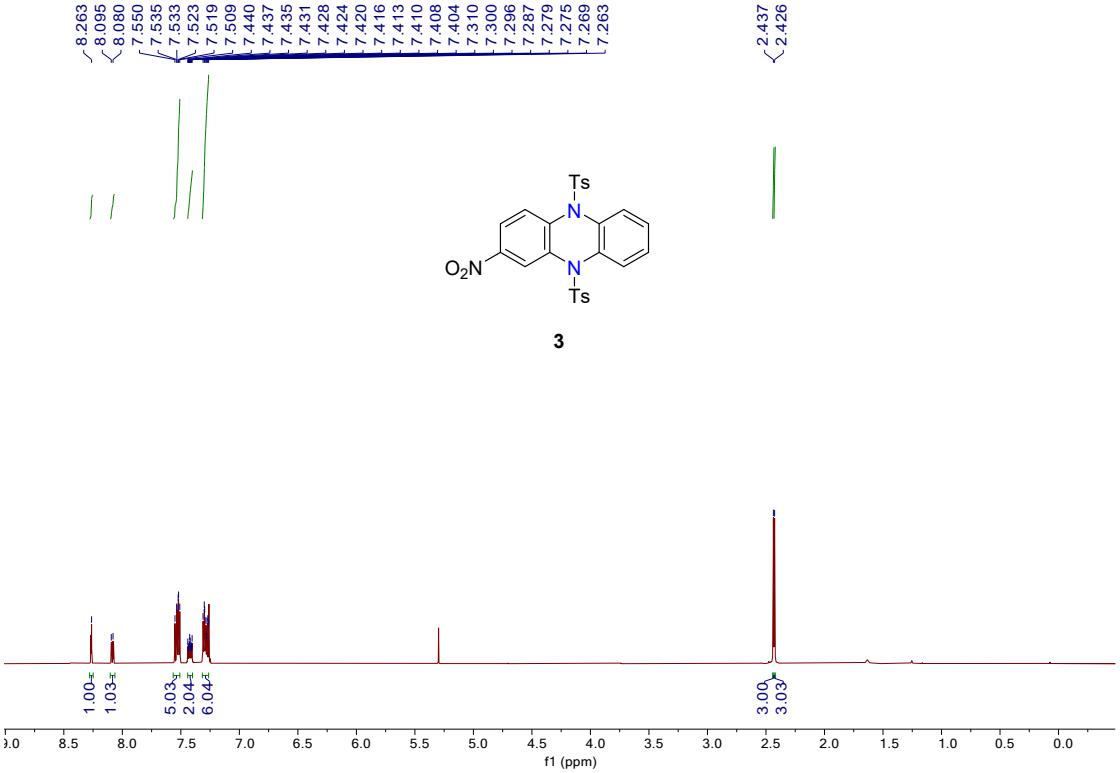
6. ^{1}H, ^{13}C, ^{19}F Spectra of New Compounds



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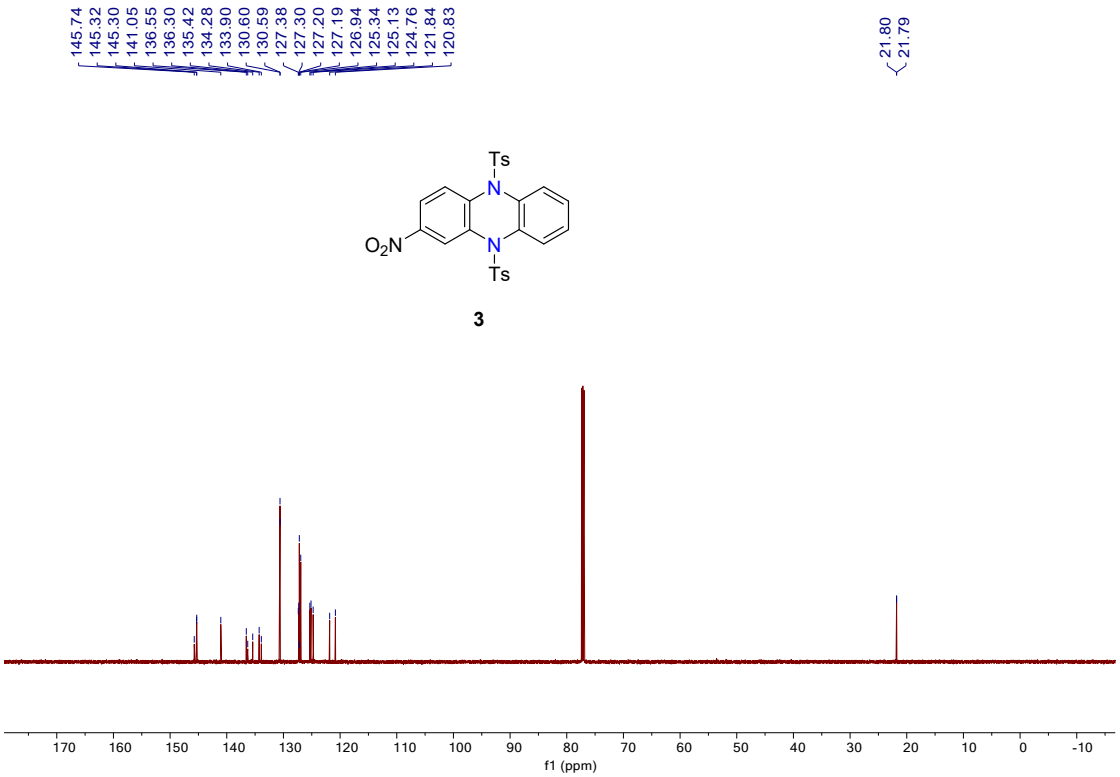

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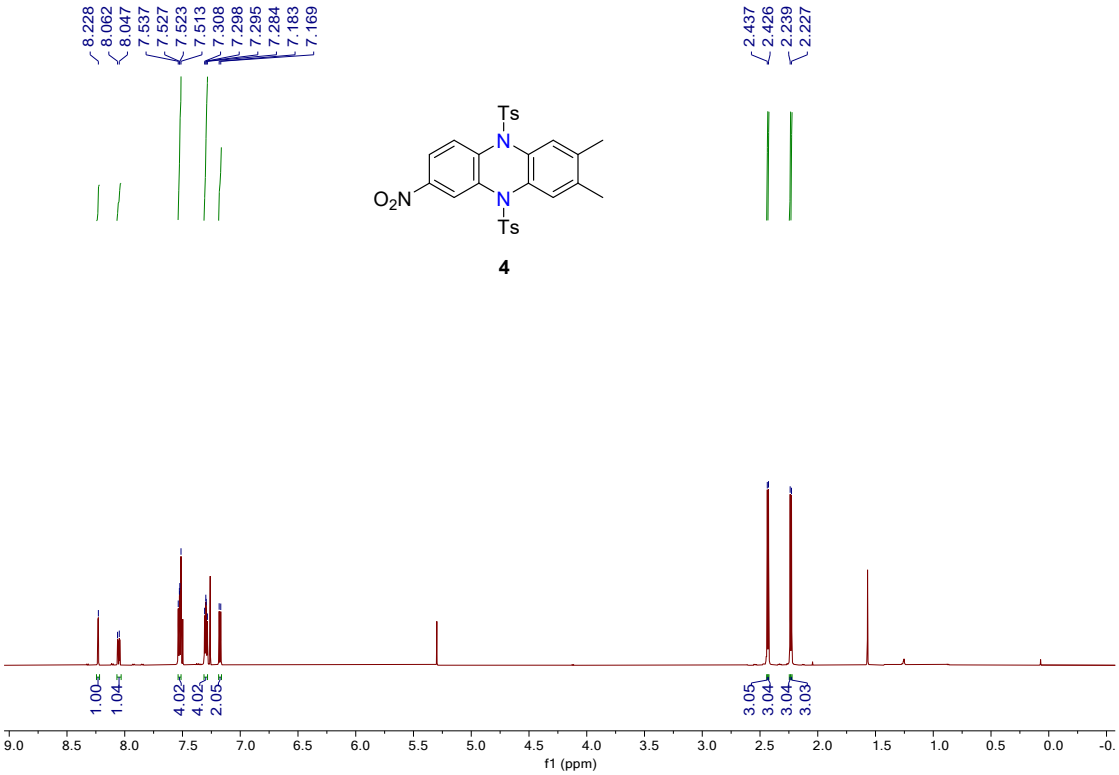
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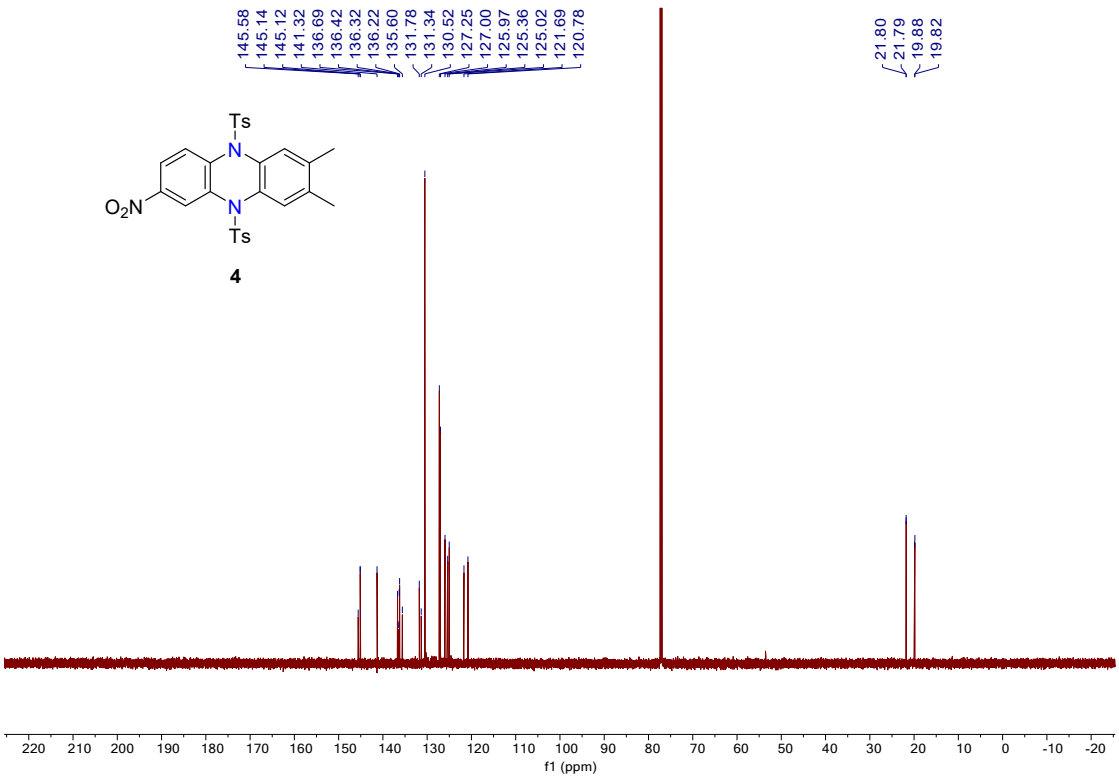
8.047
7.537
7.527
7.523
7.513
7.308
7.298
7.295
7.284
7.183
7.169
2.437
2.426
2.239
2.227
Ts
N
O2N
N
Ts
4
1.00
1.04
4.02
4.02
2.05
3.05
3.04
3.04
3.03
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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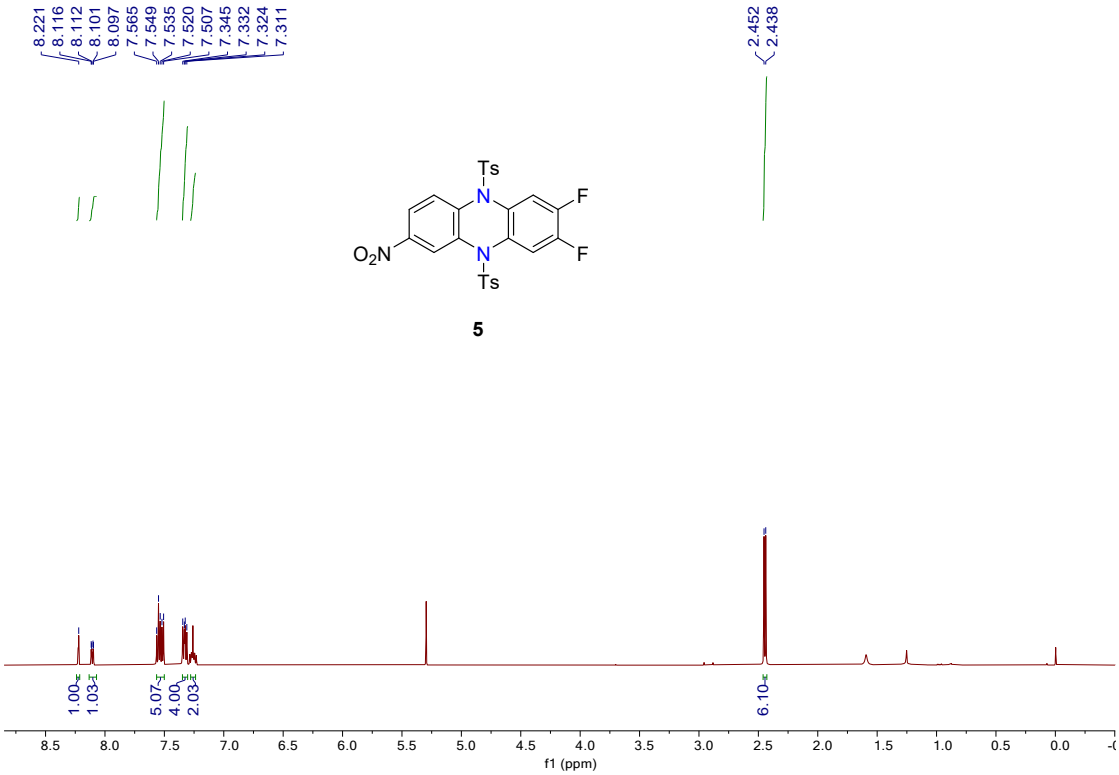
145.14
145.12
141.32
136.69
136.42
136.32
136.22
135.60
131.78
131.34
130.52
127.25
127.00
125.97
125.36
125.02
121.69
120.78
21.80
21.79
19.88
19.82
Ts
N
O2N
N
Ts
4
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)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8.116
8.112
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8.097
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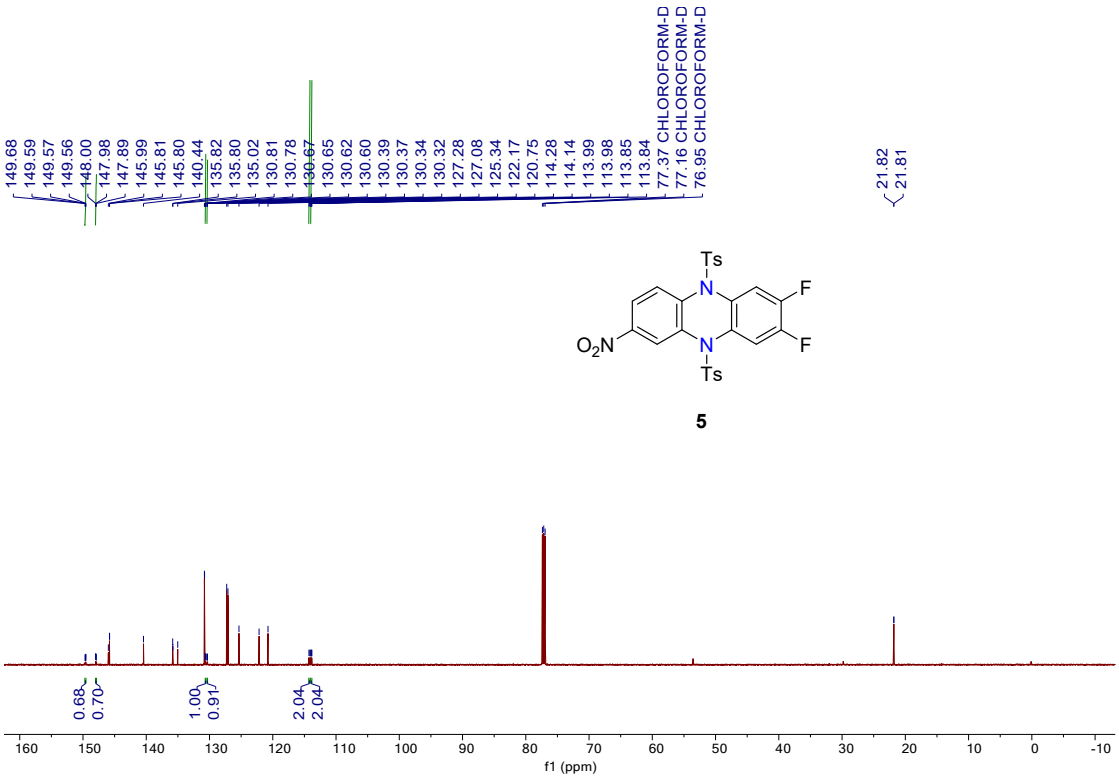
7.549
7.535
7.520
7.507
7.345
7.332
7.324
7.311
2.452
2.438
Ts
N
F
O2N
N
F
Ts
1.00
1.03
5.07
4.00
2.03
6.10
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

5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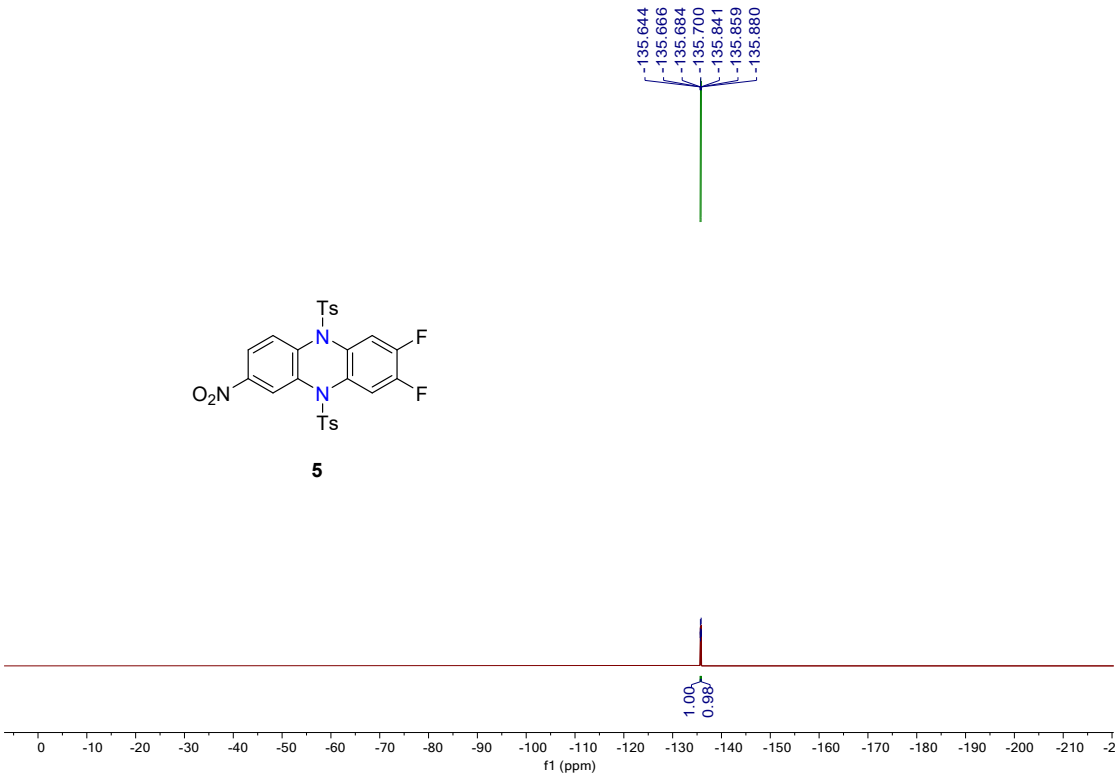
135.80
135.02
130.81
130.78
130.67
130.65
130.62
130.60
130.39
130.37
130.34
130.32
127.28
127.08
125.34
122.17
120.75
114.28
114.14
113.99
113.98
113.85
113.84
77.37 CHLOROFORM-D
77.16 CHLOROFORM-D
76.95 CHLOROFORM-D
21.82
21.81
Ts
N
F
O2N
N
F
Ts
0.68
0.70
1.00
0.91
2.04
2.04
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

5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Ts
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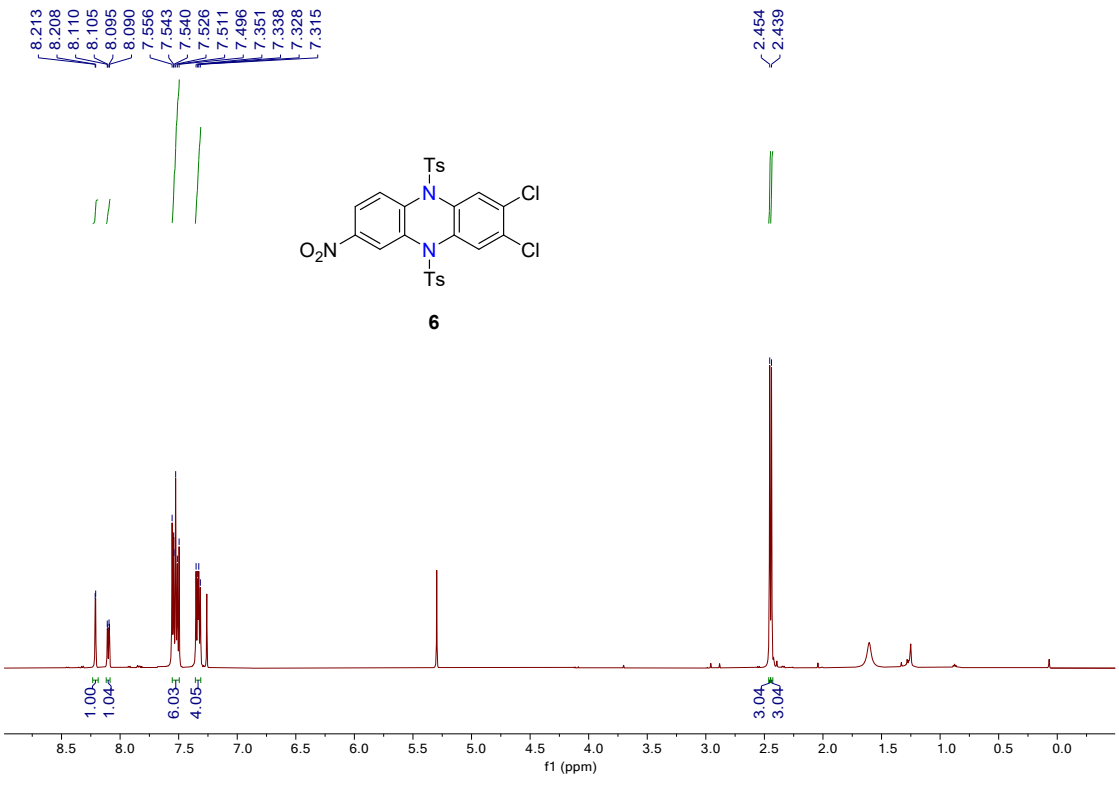
F
O2N
N
F
Ts
1.00
0.98
f1 (ppm)

5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8.090
7.556
7.543
7.540
7.526
7.511
7.496
7.351
7.338
7.328
7.315
2.454
2.439
Ts
N
Cl
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N
Cl
Ts
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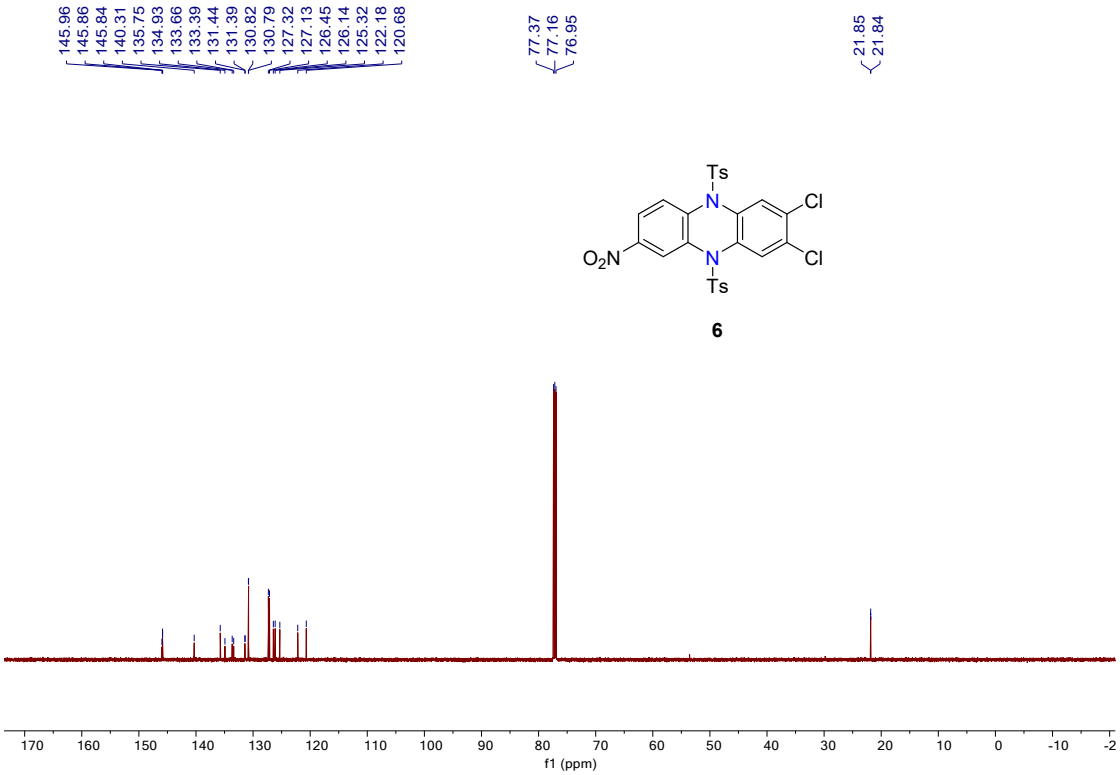
6.03
4.05
3.04
3.04
f1 (ppm)

6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133.66
133.39
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131.39
130.82
130.79
127.32
127.13
126.45
126.14
125.32
122.18
120.68
77.37
77.16
76.95
21.85
21.84
Ts
N
Cl
O2N
N
Cl
Ts
170
160
150
140
130
120
110
100
90
80
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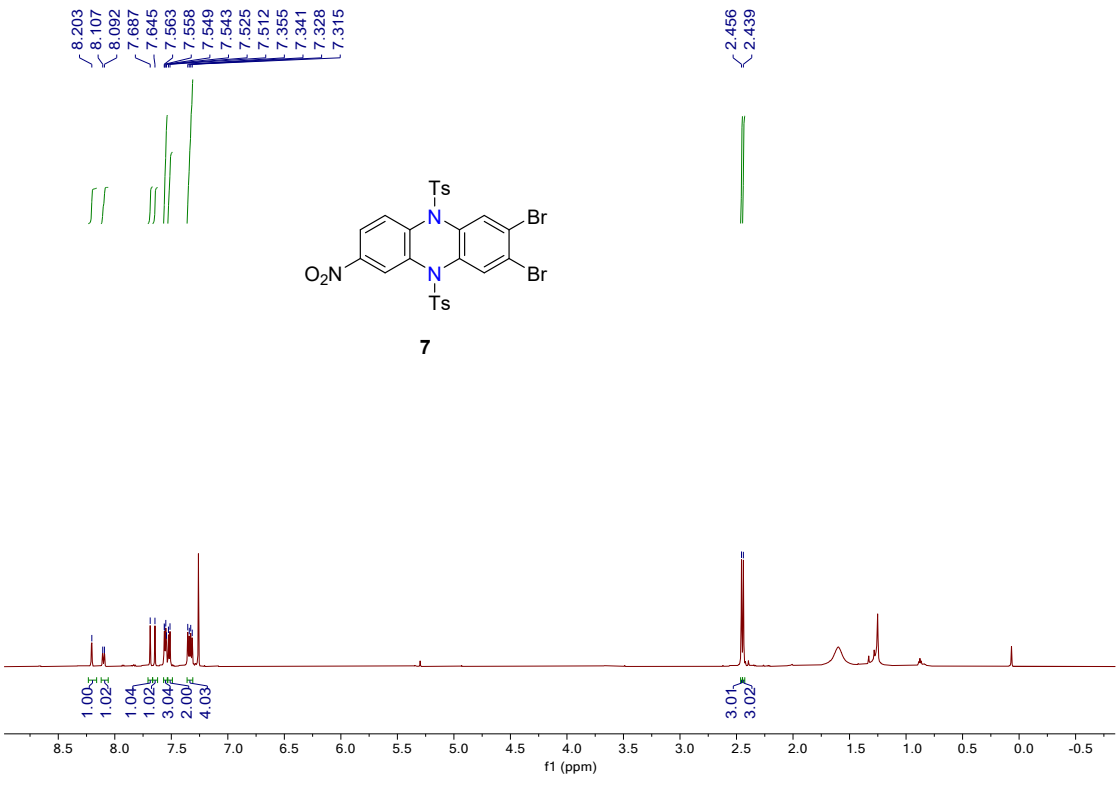
60
50
40
30
20
10
0
-10
-2
f1 (ppm)

6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7.315
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Ts
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Br
O2N
N
Br
Ts
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1.04
1.02
3.04
2.00
4.03
3.01
3.02
8.5
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7.0
6.5
6.0
5.5
5.0
4.5
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1.5
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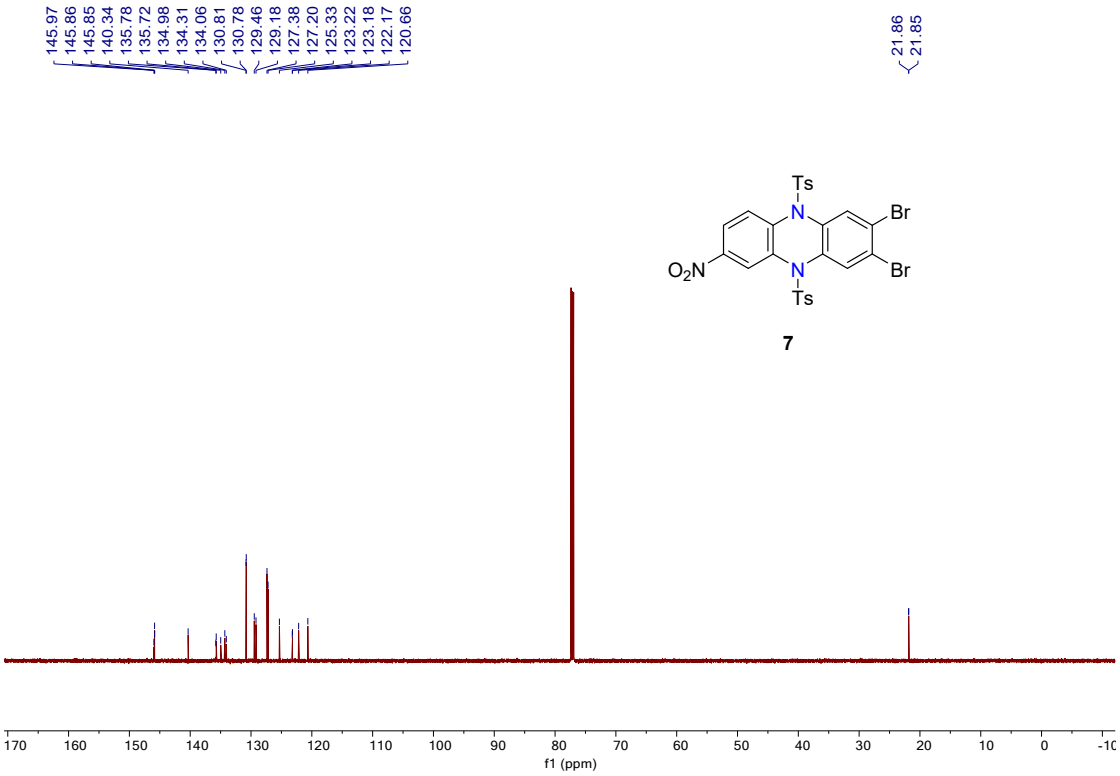
f1 (ppm)

7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134.31
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129.18
127.38
127.20
125.33
123.22
123.18
122.17
120.66
21.86
21.85
Ts
N
Br
O2N
N
Br
Ts
170
160
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100
90
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70
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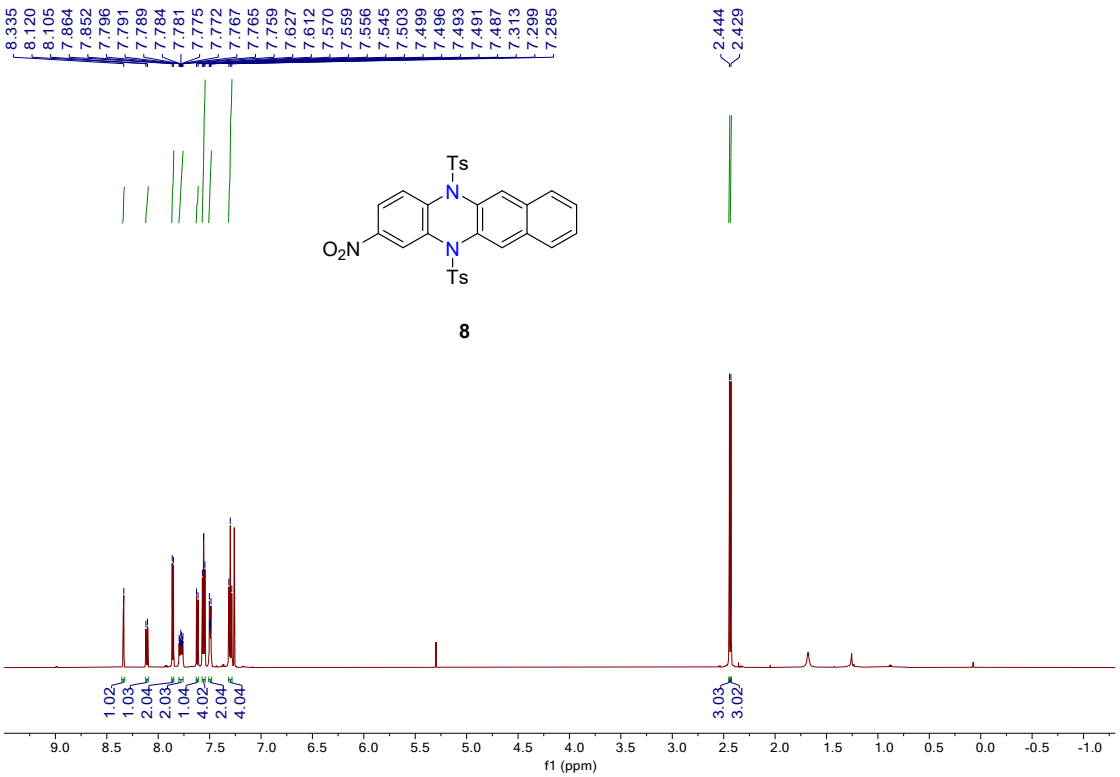
50
40
30
20
10
0
-10
f1 (ppm)

7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7.765
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7.499
7.496
7.493
7.491
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Ts
N
O2N
N
Ts
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1.03
2.04
2.03
1.04
4.02
2.04
4.04
3.03
3.02
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8.5
8.0
7.5
7.0
6.5
6.0
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5.0
4.5
4.0
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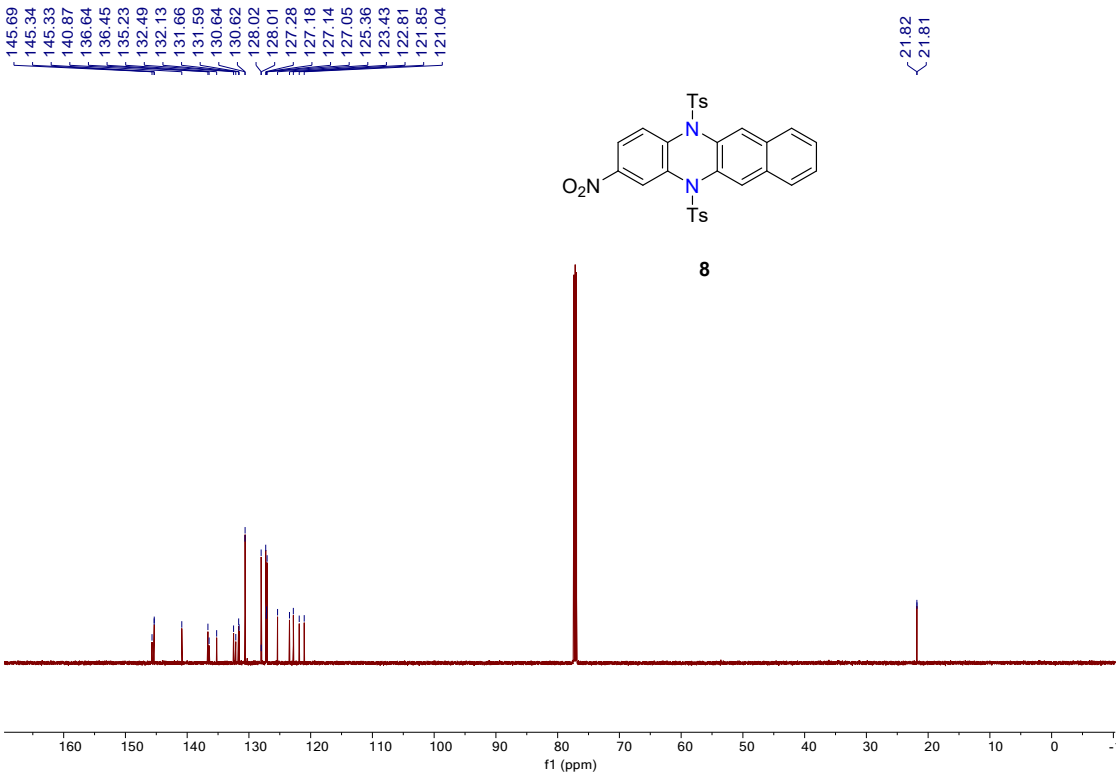
-1.0
f1 (ppm)

8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132.49
132.13
131.66
131.59
130.64
130.62
128.02
128.01
127.28
127.18
127.14
127.05
125.36
123.43
122.81
121.85
121.04
21.82
21.81
Ts
N
O2N
N
Ts
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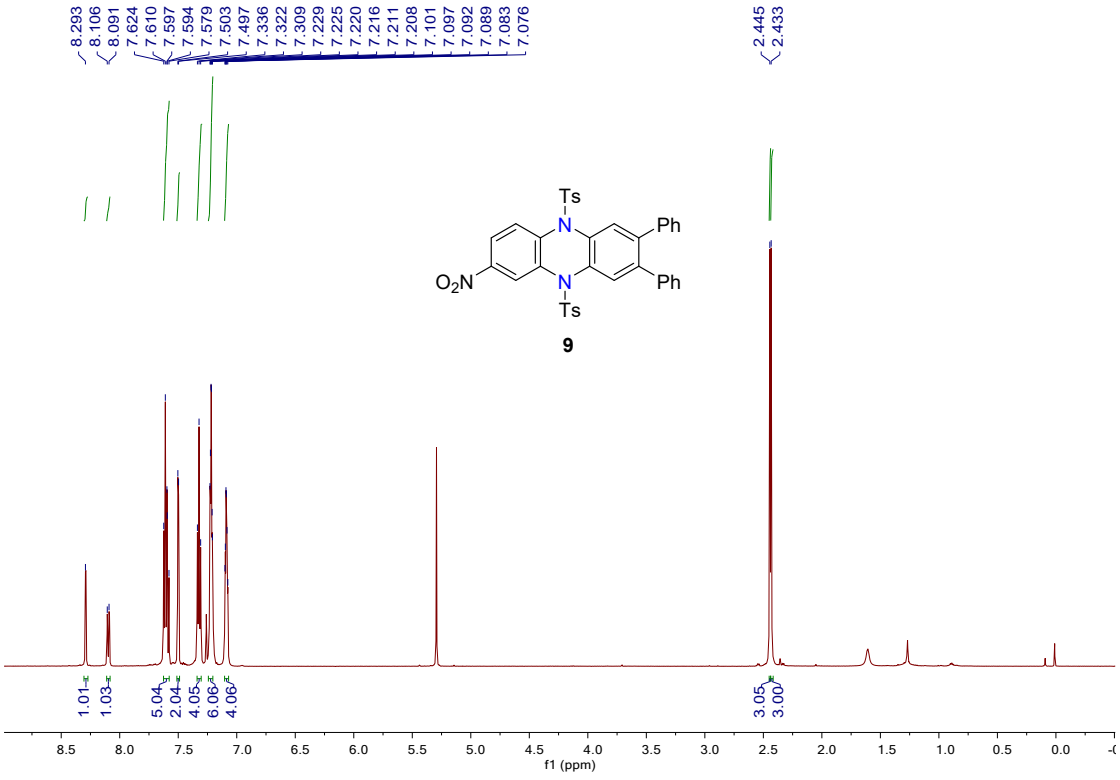
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

8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7.216
7.211
7.208
7.101
7.097
7.092
7.089
7.083
7.076
2.445
2.433
Ts
N
Ph
O2N
N
Ph
Ts
1.01
1.03
5.04
2.04
4.05
6.08
4.06
3.05
3.00
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)

9


145.72
145.38
145.36
141.05
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139.77
139.74
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133.32
132.91
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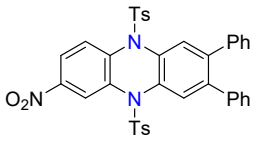
120.73


21.79
21.78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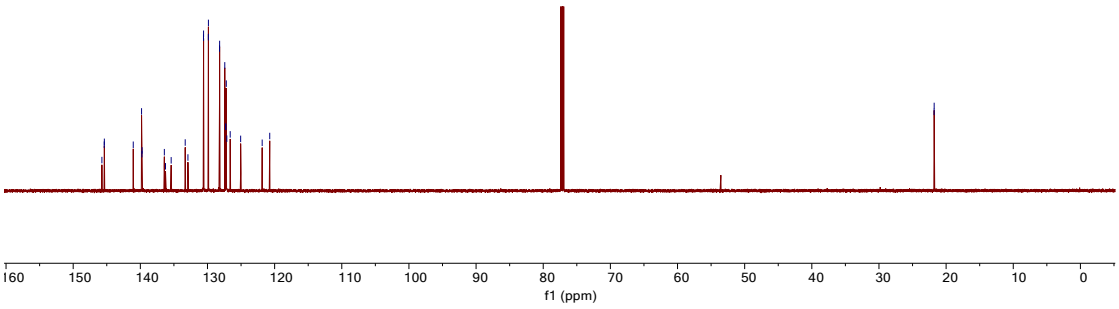
Ph
O2N
N
Ph
Ts

9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150
140
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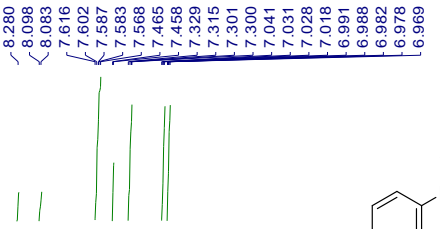
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.301
7.300
7.041
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7.028
7.018
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6.982
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6.969


2.442
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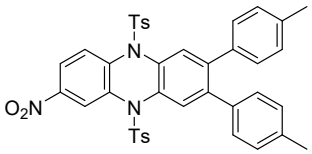
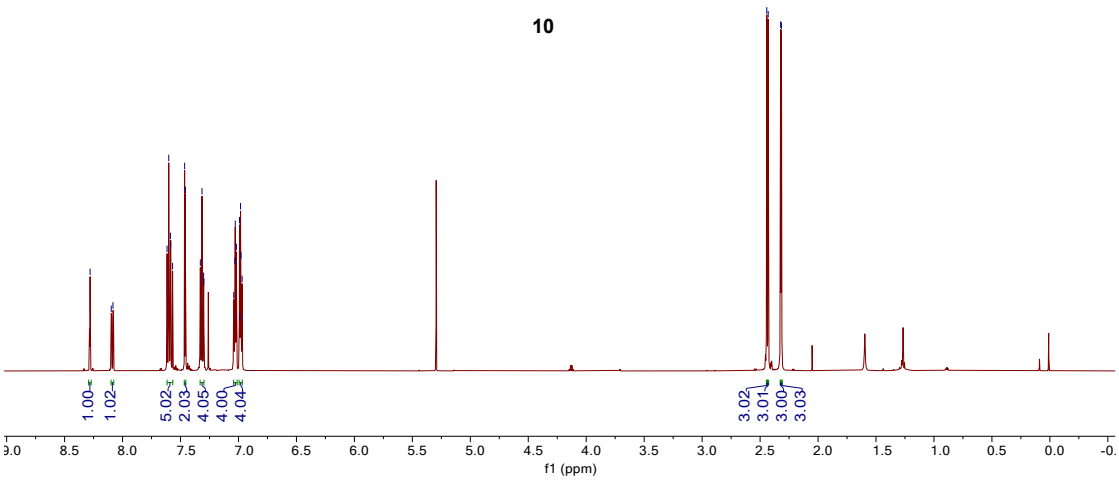
2.316


Ts
N
O2N
N
Ts

10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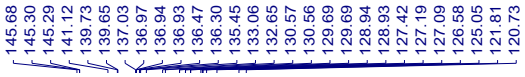
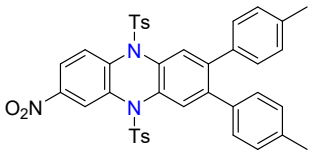
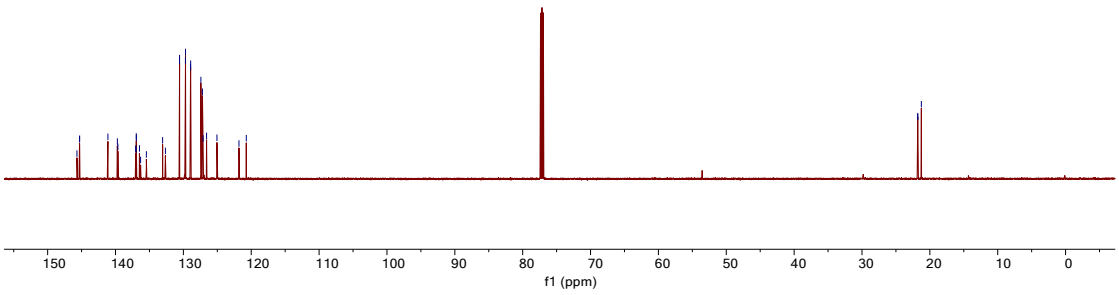
4.05
4.00
4.04
3.02
3.01
3.00
3.03
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)


145.68
145.30
145.29
141.12
139.73
139.65
137.03
136.97
136.94
136.93
136.47
136.30
135.45
133.06
132.65
130.57
130.56
129.69
129.69
128.94
128.93
127.42
127.19
127.09
126.58
125.05
121.81
120.73


21.79
21.78
21.25


Ts
N
O2N
N
Ts

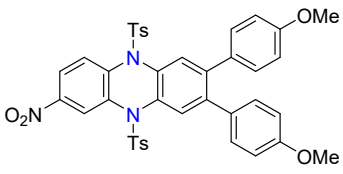
10


150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

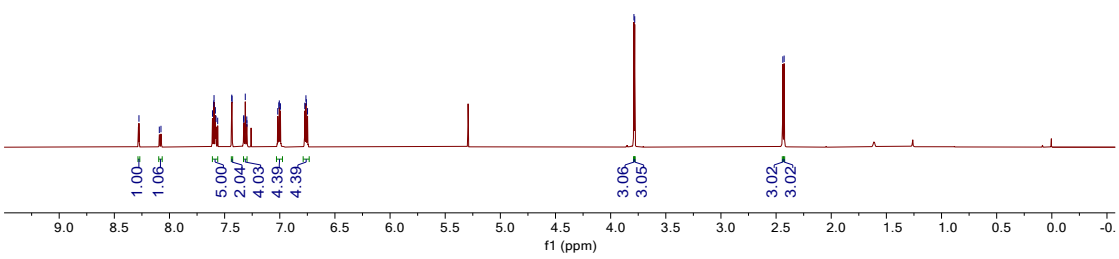

8.277
8.092
8.077
7.610
7.598
7.596
7.584
7.578
7.563
7.435
7.433
7.327
7.326
7.313
7.299
7.298
7.019
7.009
7.004
6.994
6.773
6.763
6.759
6.748

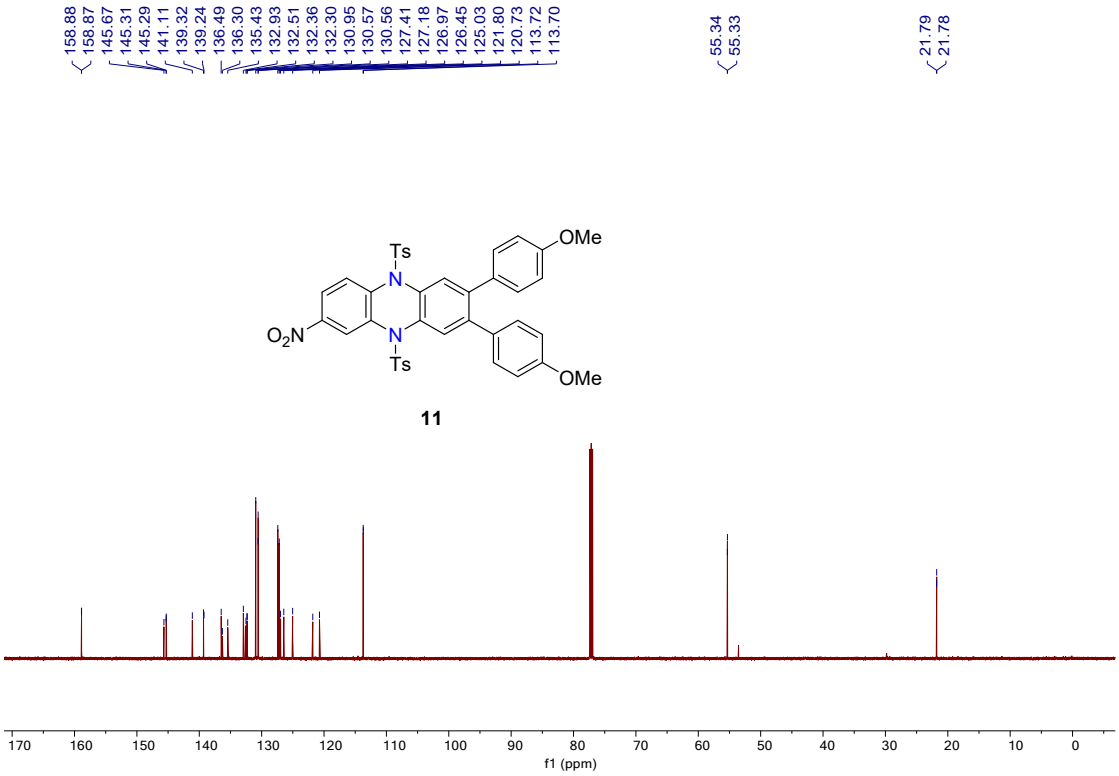

3.789
3.782


2.439
2.427

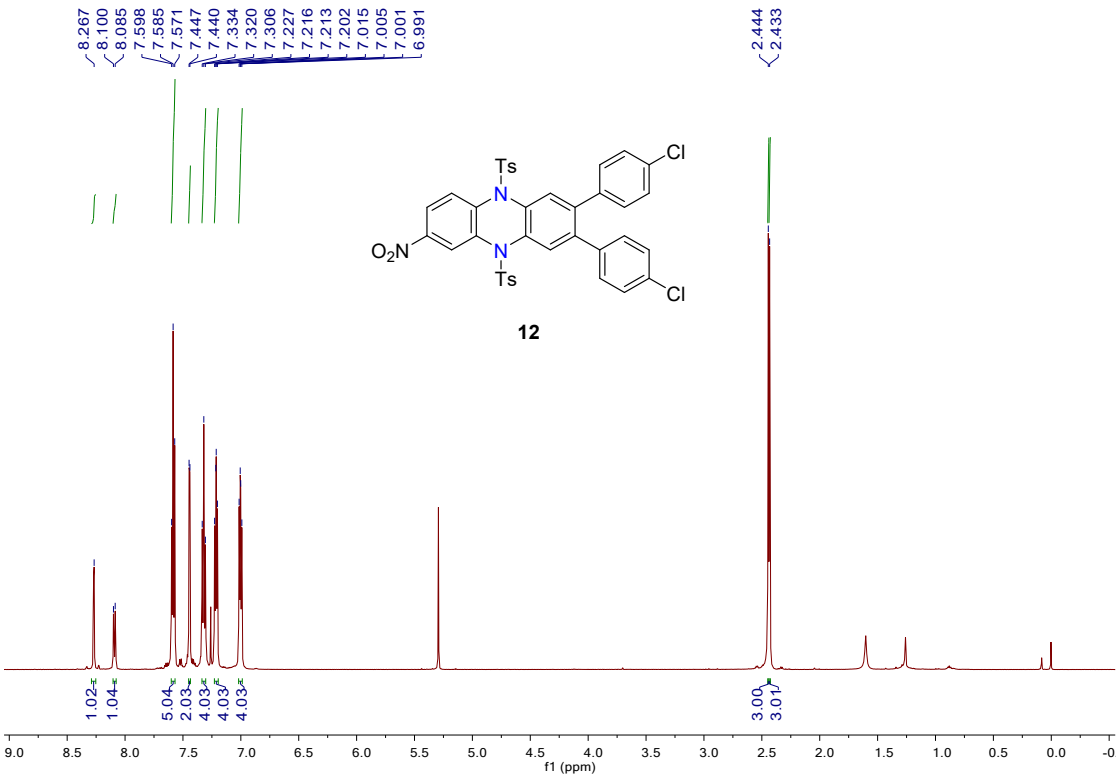

Ts
N
OMe
O2N
N
Ts
OMe

11

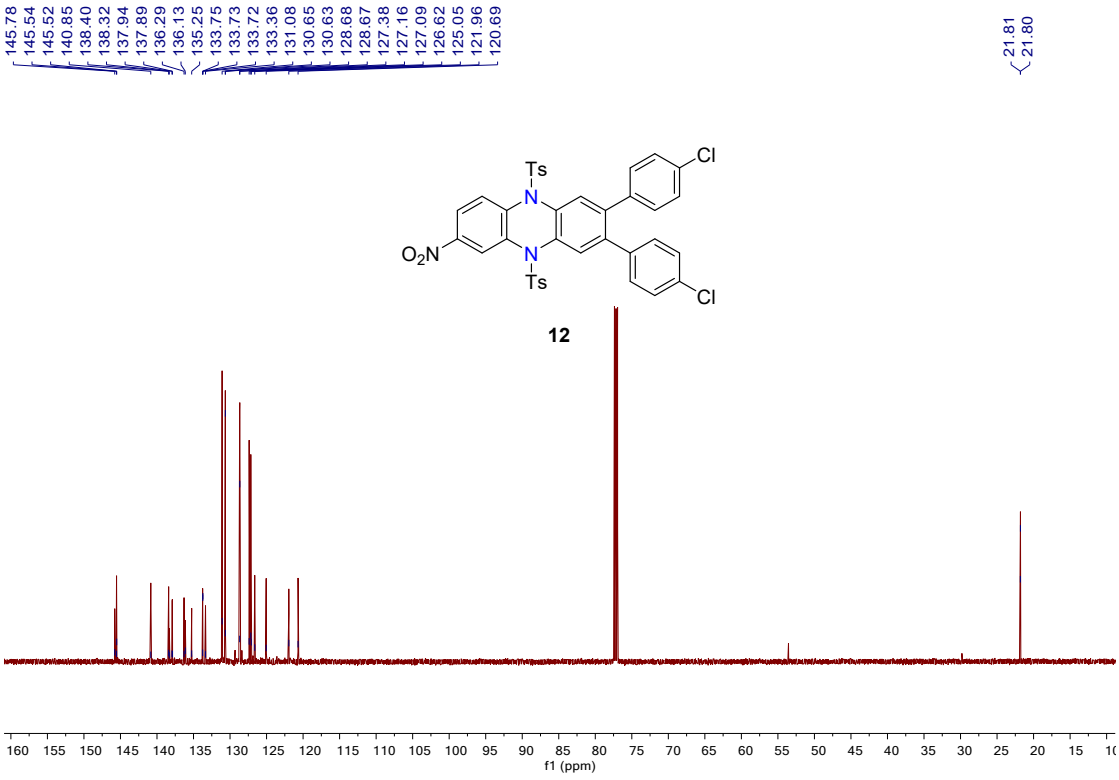

1.00
1.06
5.00
2.04
4.03
4.39
4.39
3.06
3.05
3.02
3.02
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)


158.88
158.87
145.67
145.31
145.29
141.11
139.32
139.24
136.49
136.30
135.43
132.93
132.51
132.36
132.30
130.95
130.57
130.56
127.41
127.18
126.97
126.45
125.03
121.80
120.73
113.72
113.70
55.34
55.33
21.79
21.78
Ts
N
N
Ts
O2N
OMe
OMe
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

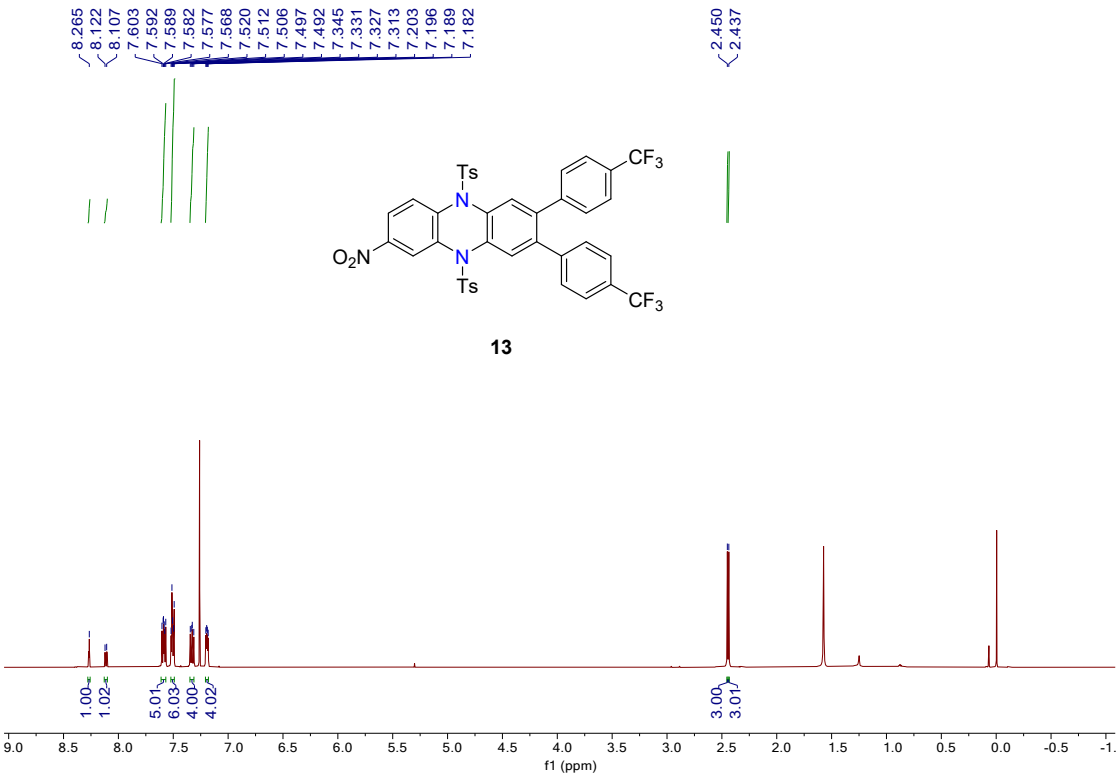
11


8.267
8.100
8.085
7.598
7.585
7.571
7.447
7.440
7.334
7.320
7.306
7.227
7.216
7.213
7.202
7.015
7.005
7.001
6.991
2.444
2.433
Ts
N
N
Ts
O2N
Cl
Cl
1.02
1.04
5.04
2.03
4.03
4.03
3.00
3.01
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
f1 (ppm)

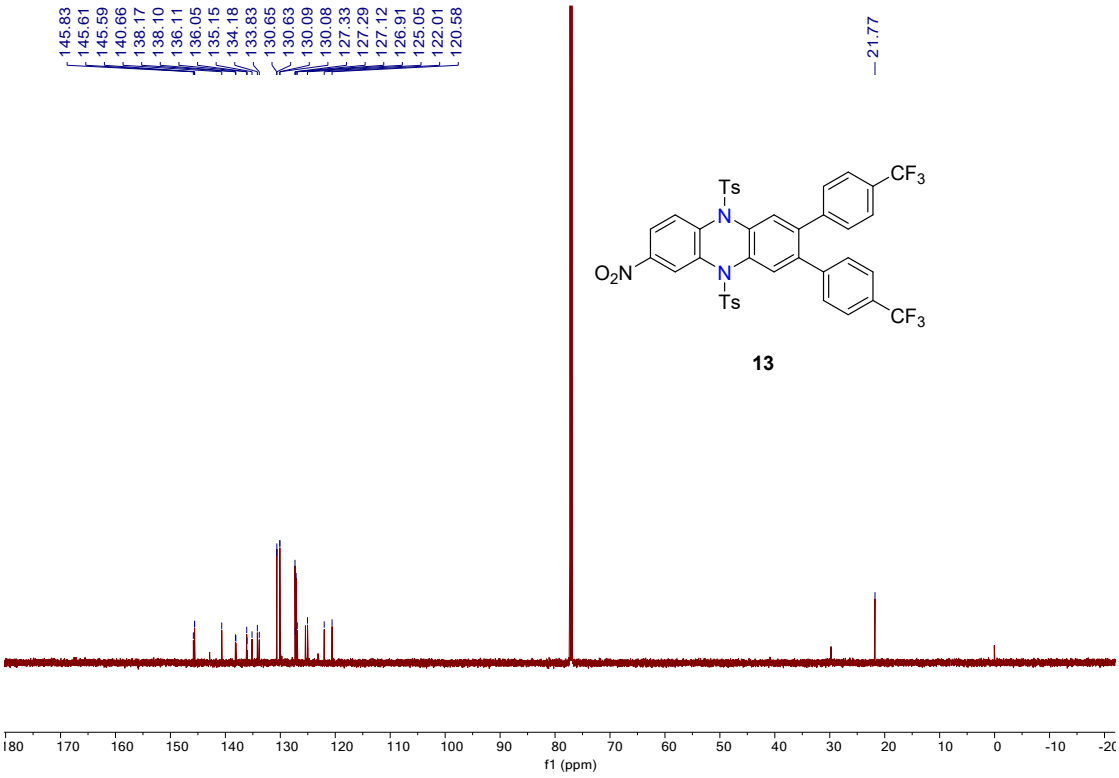
12


145.78
145.54
145.52
140.85
138.40
138.32
137.94
137.89
136.29
136.13
135.25
133.75
133.73
133.72
133.36
131.08
130.65
130.63
128.68
128.67
127.38
127.16
127.09
126.62
125.05
121.96
120.69
21.81
21.80
Ts
N
O2N
N
Ts
Cl
Cl
160 155 150 145 140 135 130 125 120 115 110 105 100 95 90 85 80 75 70 65 60 55 50 45 40 35 30 25 20 15 10
f1 (ppm)

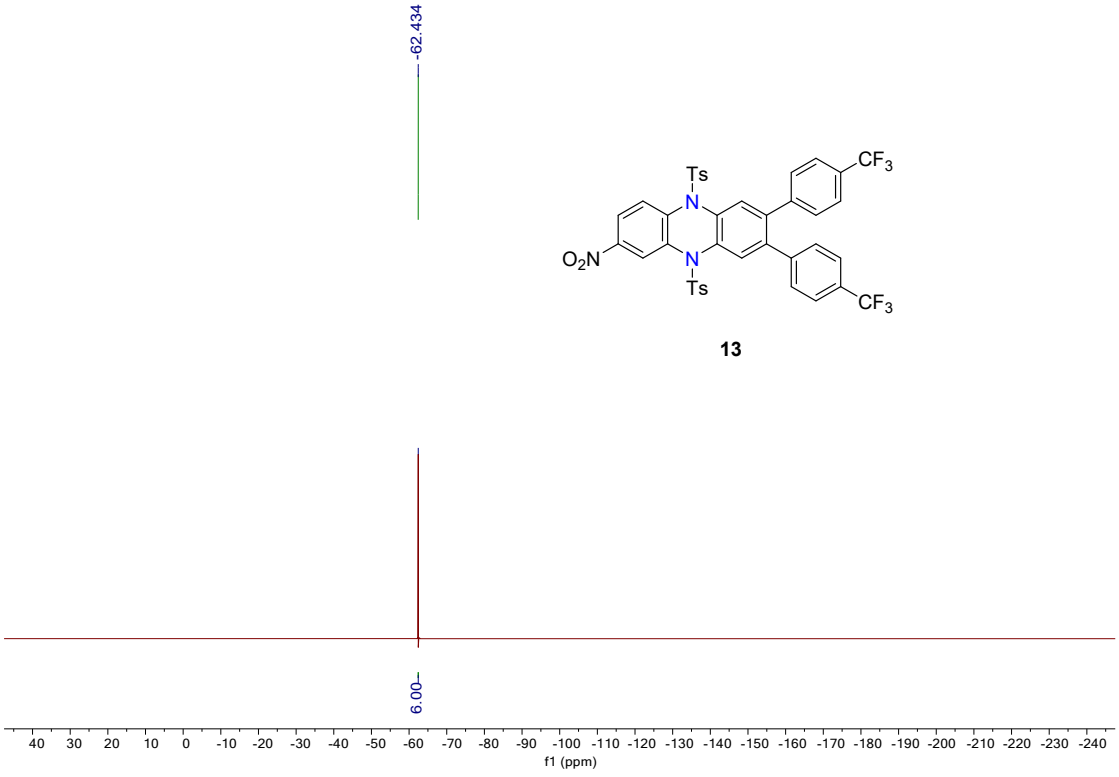
12


8.265
8.122
8.107
7.603
7.592
7.589
7.582
7.577
7.568
7.520
7.512
7.506
7.497
7.492
7.345
7.331
7.327
7.313
7.203
7.196
7.189
7.182
2.450
2.437
Ts
N
O2N
N
Ts
CF3
CF3
1.00
1.02
5.01
6.03
4.00
4.02
3.00
3.01
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 -1.
f1 (ppm)

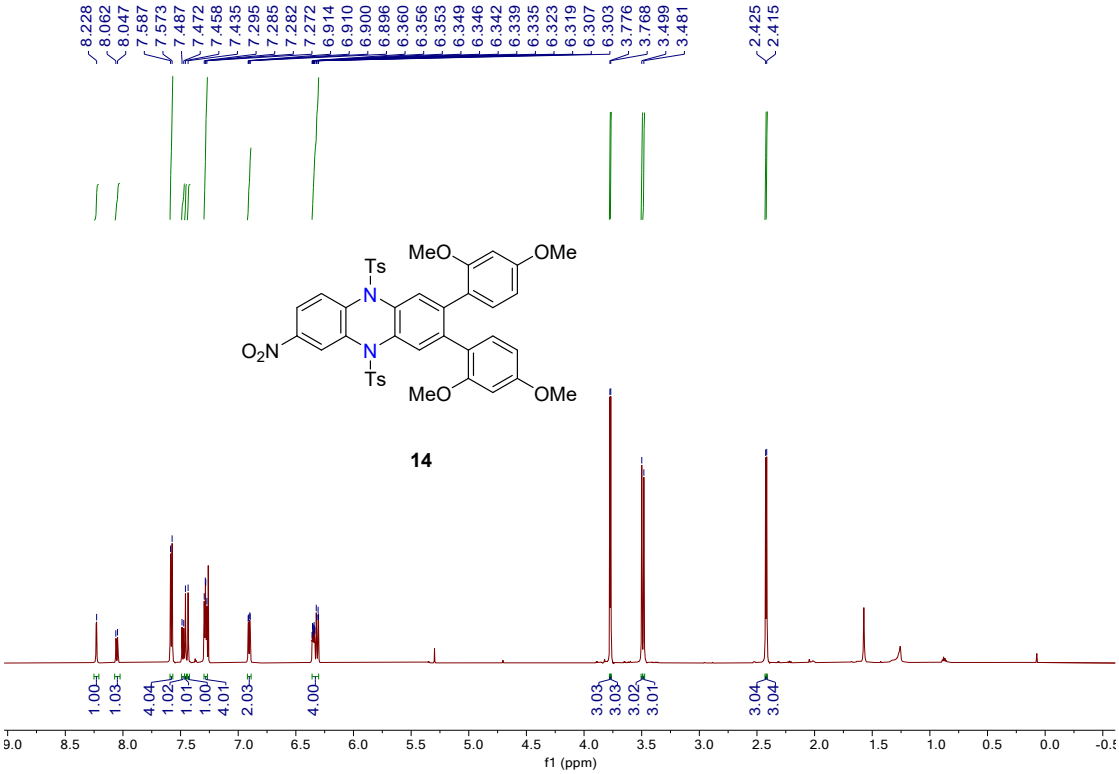
13

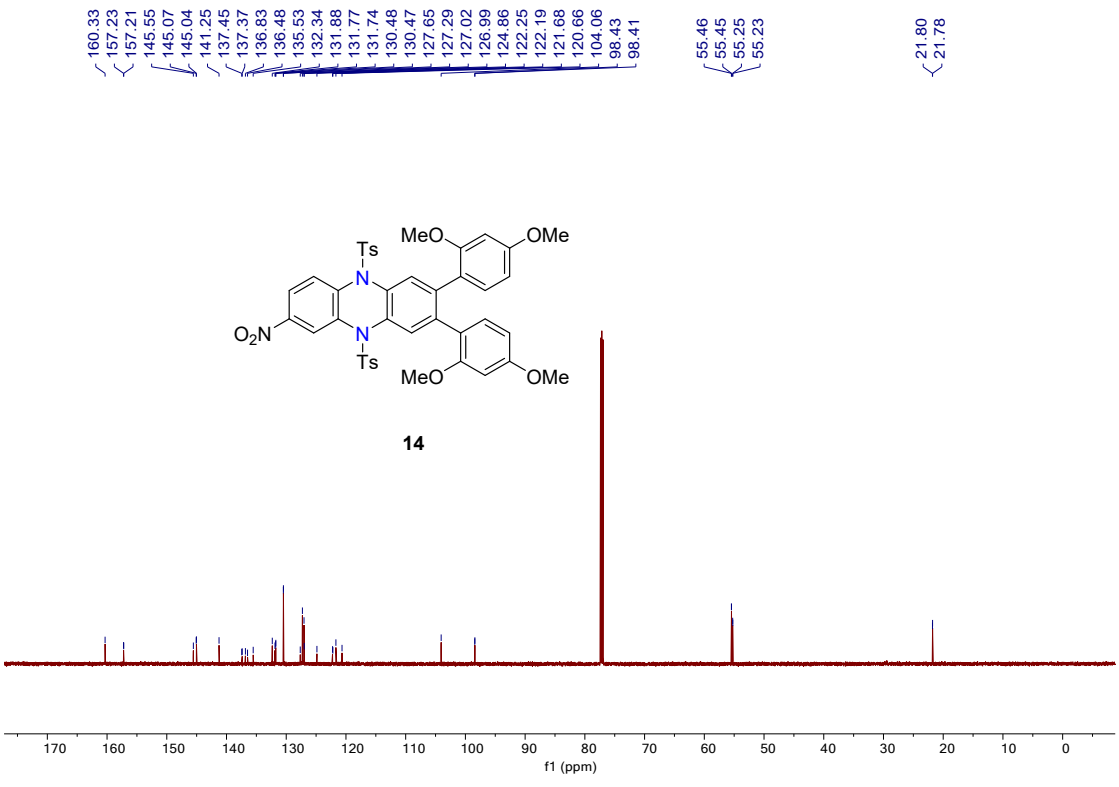

145.83
145.61
145.59
140.66
138.17
138.10
136.11
136.05
135.15
134.18
133.83
130.65
130.63
130.09
130.08
127.33
127.29
127.12
126.91
125.05
122.01
120.58
21.77
Ts
N
N
Ts
O2N
CF3
CF3
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)

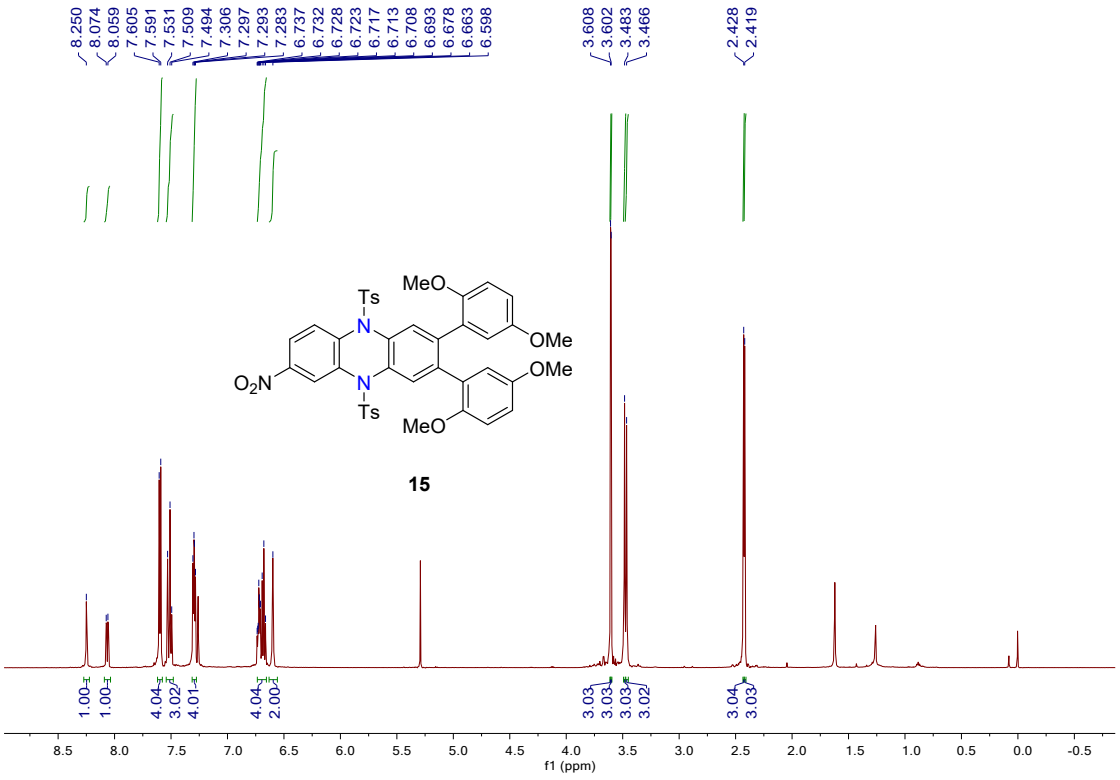
13

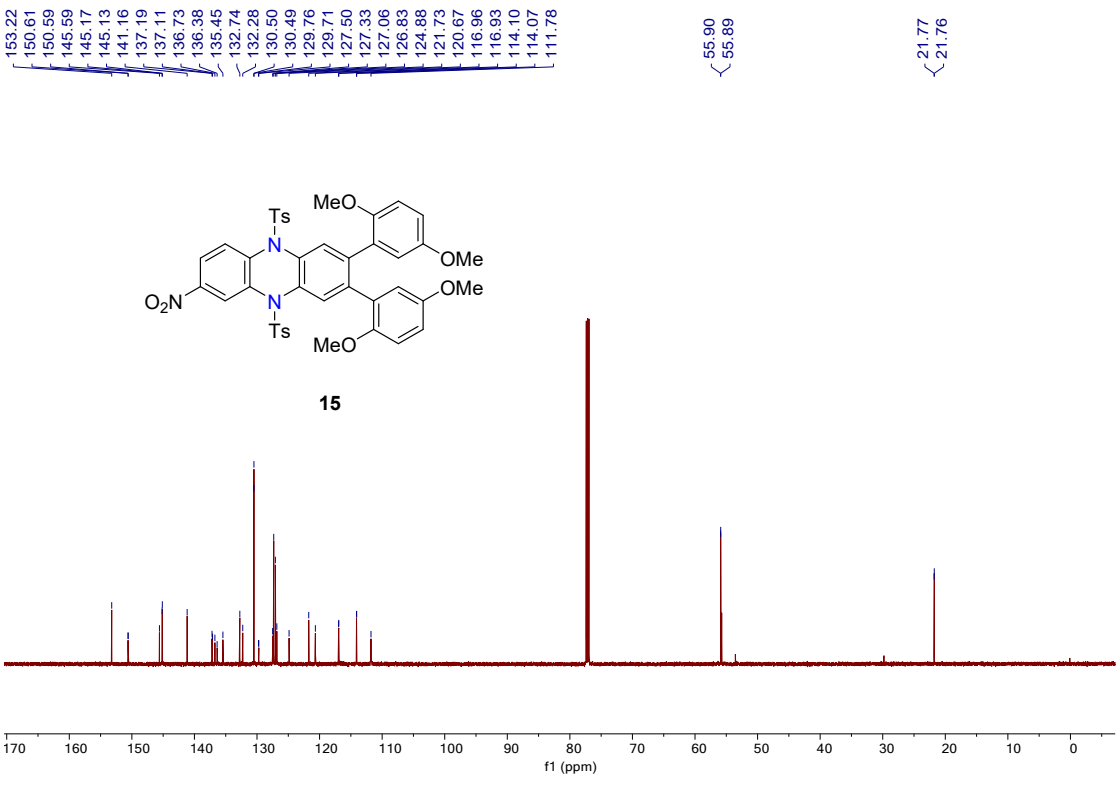

-62.434
Ts
N
N
Ts
O2N
CF3
CF3
6.00
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240
f1 (ppm)

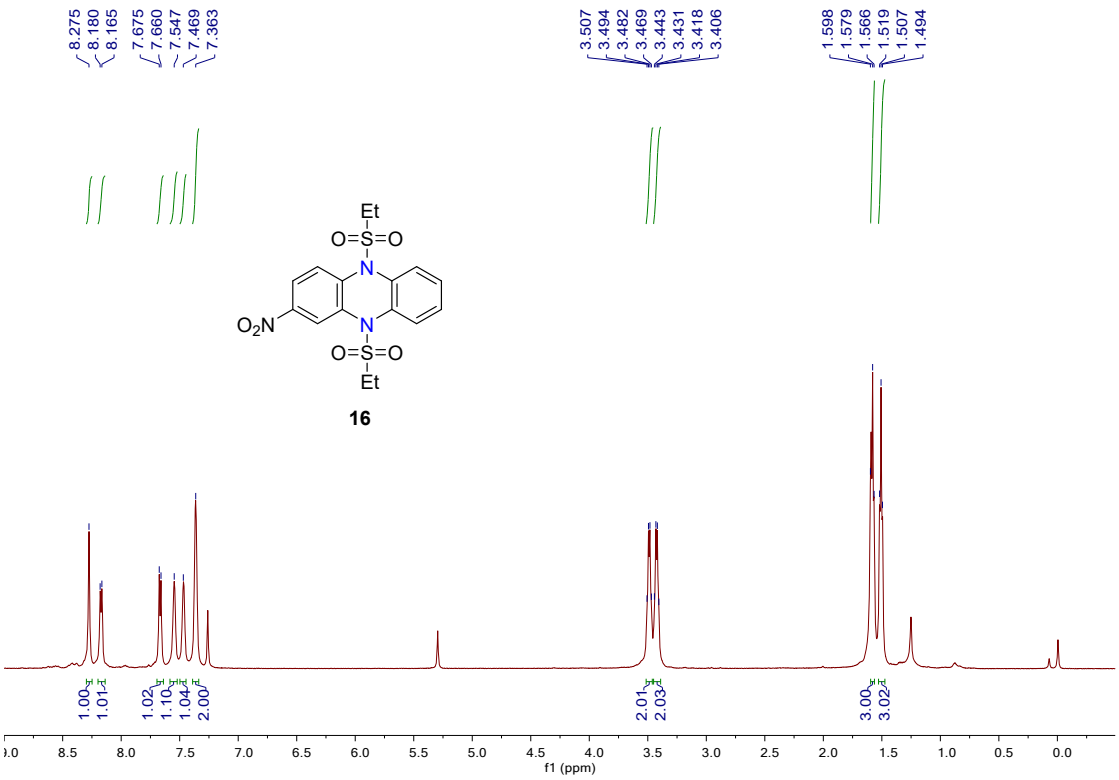
13

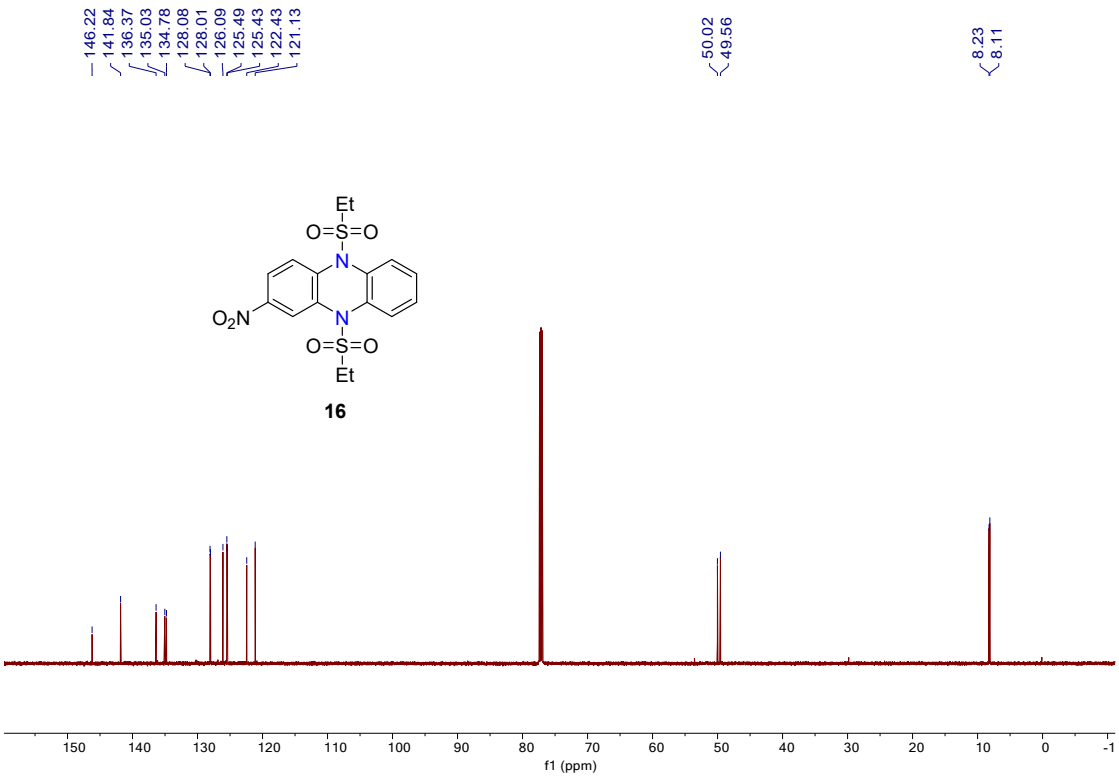

8.228
8.062
8.047
7.587
7.573
7.487
7.472
7.458
7.435
7.295
7.285
7.282
7.272
6.914
6.910
6.900
6.896
6.360
6.356
6.353
6.349
6.346
6.342
6.339
6.335
6.323
6.319
6.307
6.303
3.776
3.768
3.499
3.481
2.425
2.415
MeO
OMe
Ts
N
O2N
N
Ts
MeO
OMe
14
1.00
1.03
4.04
1.02
1.01
1.00
4.01
2.03
4.00
3.03
3.03
3.02
3.01
3.04
3.04
f1 (ppm)

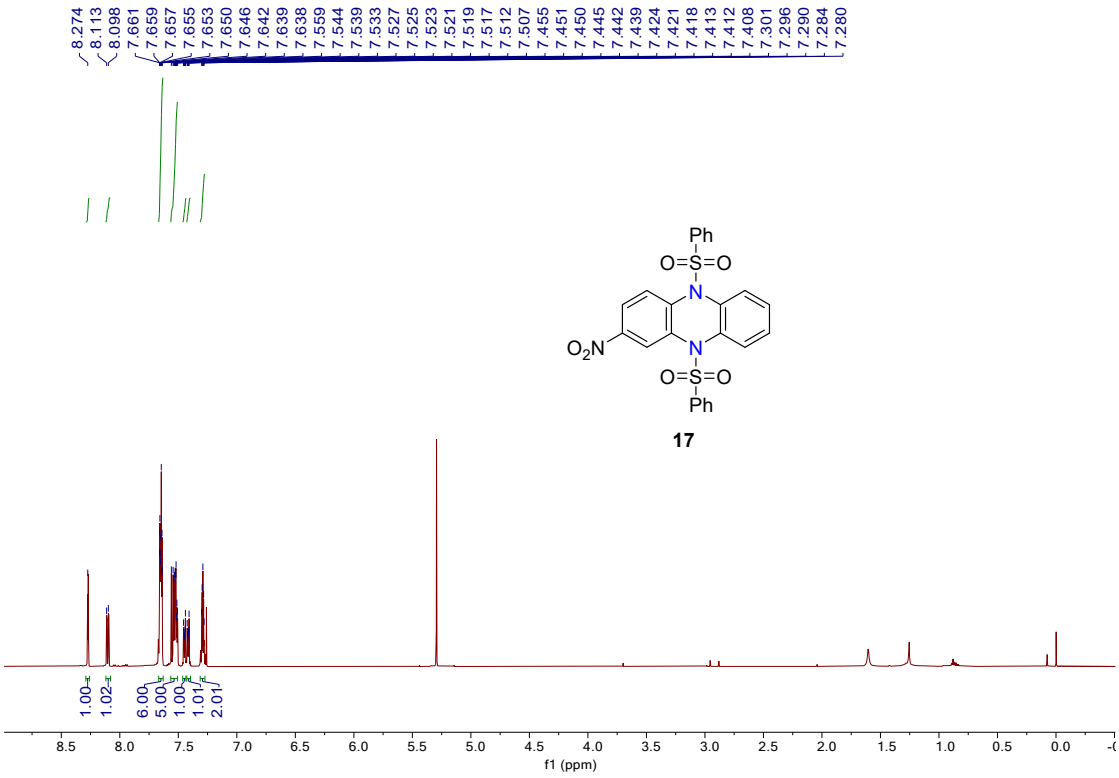

160.33
157.23
157.21
145.55
145.07
145.04
141.25
137.45
137.37
136.83
136.48
135.53
132.34
131.88
131.77
131.74
130.48
130.47
127.65
127.29
127.02
126.99
124.86
122.25
122.19
121.68
120.66
104.06
98.43
98.41
55.46
55.45
55.25
55.23
21.80
21.78
MeO
OMe
Ts
N
O2N
N
Ts
MeO
OMe
14
f1 (ppm)


8.250
8.074
8.059
7.605
7.591
7.531
7.509
7.494
7.306
7.297
7.293
7.283
6.737
6.732
6.728
6.723
6.717
6.713
6.708
6.693
6.678
6.663
6.598
3.608
3.602
3.483
3.466
2.428
2.419
MeO
OMe
OMe
MeO
Ts
N
N
Ts
O2N
15
1.00
1.00
4.04
3.02
4.01
4.04
2.00
3.03
3.03
3.03
3.02
3.04
3.03
f1 (ppm)

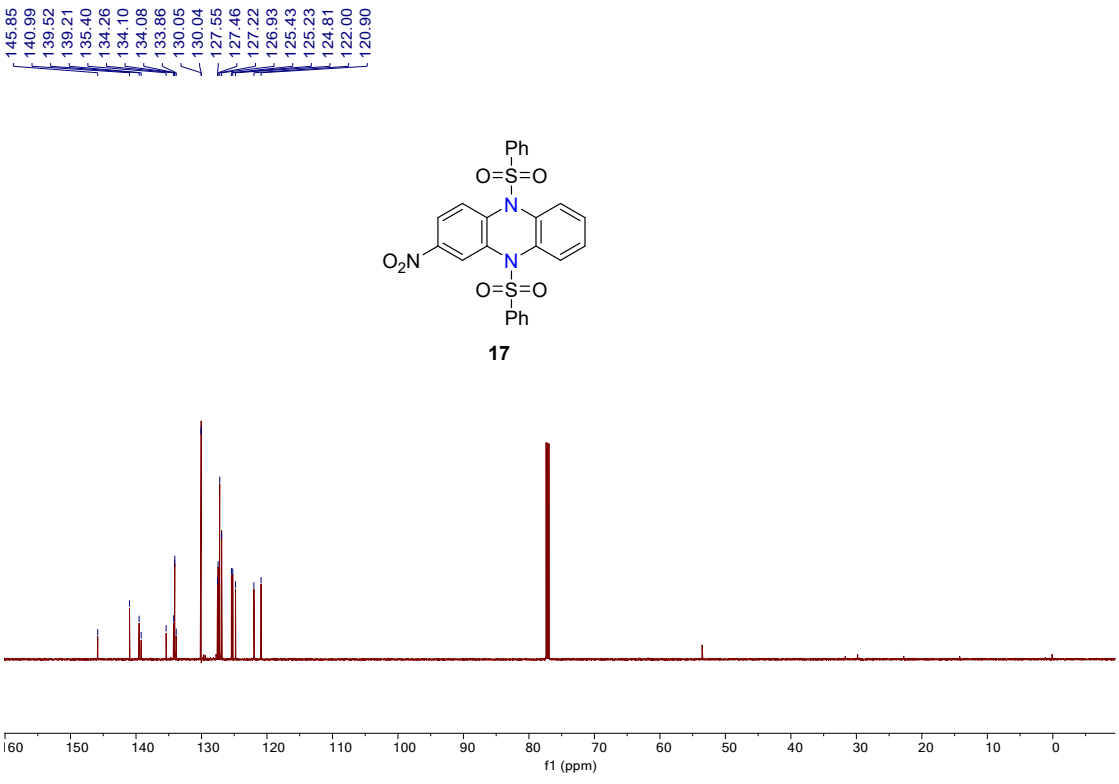

153.22
150.61
150.59
145.59
145.17
145.13
141.16
137.19
137.11
136.73
136.38
135.45
132.74
132.28
130.50
130.49
129.76
129.71
127.50
127.33
127.06
126.83
124.88
121.73
120.67
116.96
116.93
114.10
114.07
111.78
55.90
55.89
21.77
21.76
MeO
OMe
OMe
MeO
Ts
N
N
Ts
O2N
15
f1 (ppm)


8.275
8.180
8.165
7.675
7.660
7.547
7.469
7.363
3.507
3.494
3.482
3.469
3.443
3.431
3.418
3.406
1.598
1.579
1.566
1.519
1.507
1.494
Et
O=S=O
N
O2N
N
O=S=O
Et
16
1.00
1.01
1.02
1.10
1.04
2.00
2.01
2.03
3.00
3.02
f1 (ppm)


146.22
141.84
136.37
135.03
134.78
128.08
128.01
126.09
125.49
125.43
122.43
121.13
50.02
49.56
8.23
8.11
Et
O=S=O
N
O2N
N
O=S=O
Et
16
f1 (ppm)

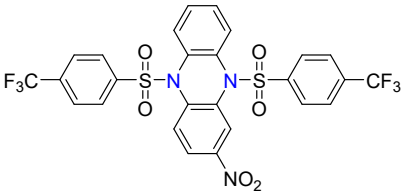

8.274
8.113
8.098
7.661
7.659
7.657
7.655
7.653
7.650
7.646
7.642
7.639
7.638
7.559
7.544
7.539
7.533
7.527
7.525
7.523
7.521
7.519
7.517
7.512
7.507
7.455
7.451
7.450
7.445
7.442
7.439
7.424
7.421
7.418
7.413
7.412
7.408
7.301
7.296
7.290
7.284
7.280
Ph
O=S=O
N
O2N
N
O=S=O
Ph
1.00
1.02
6.00
5.00
1.00
1.01
2.01
f1 (ppm)

17

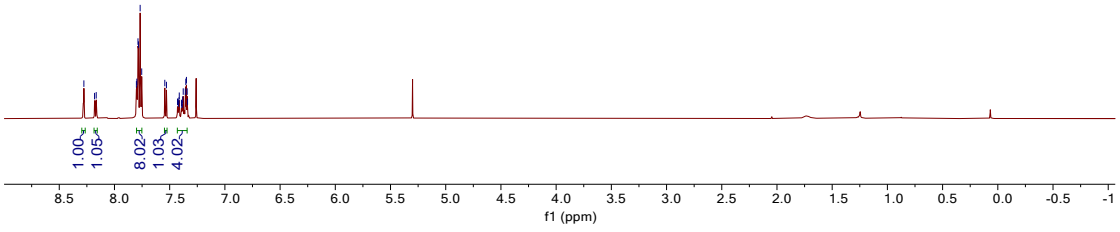

145.85
140.99
139.52
139.21
135.40
134.26
134.10
134.08
133.86
130.05
130.04
127.55
127.46
127.22
126.93
125.43
125.23
124.81
122.00
120.90
Ph
O=S=O
N
O2N
N
O=S=O
Ph
f1 (ppm)

17

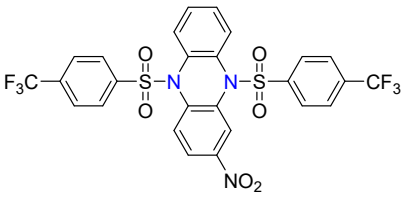

8.277
8.180
8.165
7.801
7.797
7.787
7.783
7.767
7.753
7.544
7.529
7.429
7.425
7.419
7.416
7.413
7.393
7.390
7.387
7.382
7.377
7.359
7.354
7.348
7.342
7.338


F3C
CF3
NO2

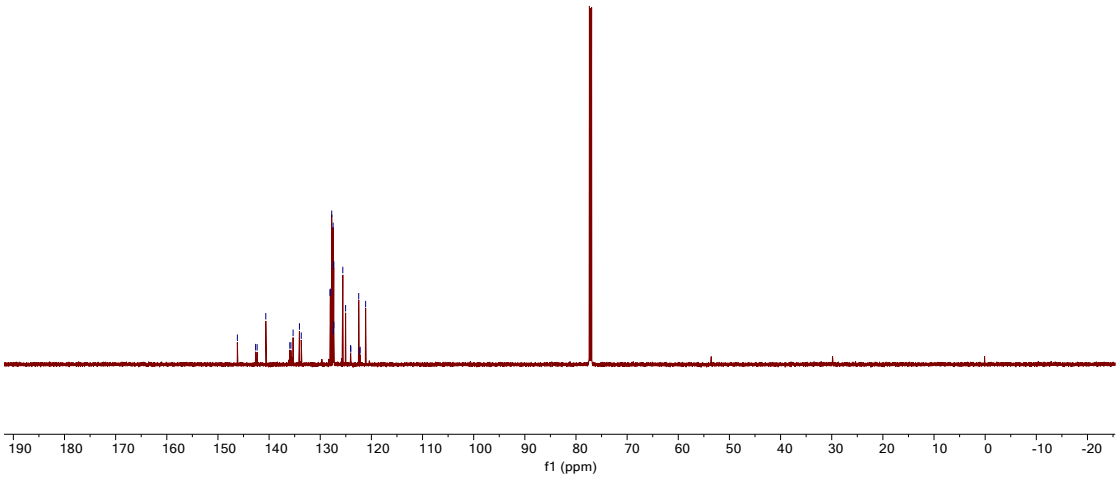
18

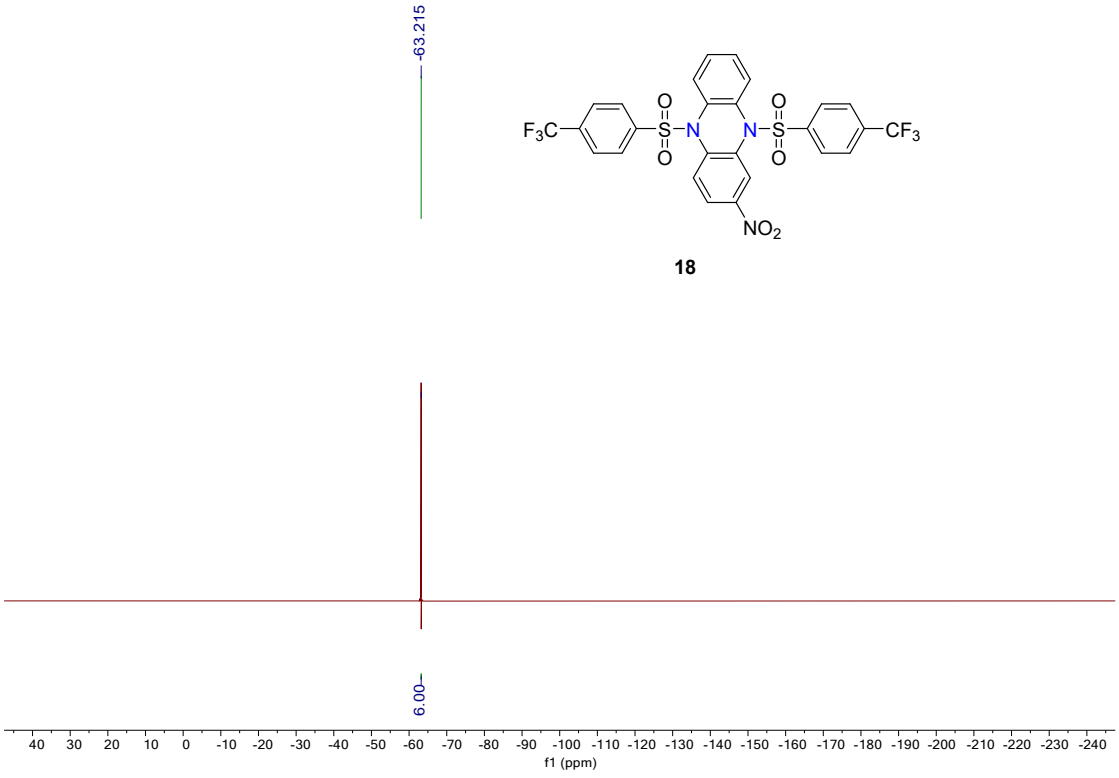

1.00
1.05
8.02
1.03
4.02
f1 (ppm)


146.20
142.64
142.34
140.65
135.95
135.73
135.31
134.07
133.71
128.10
128.02
127.76
127.49
127.41
127.38
127.36
127.33
125.59
125.04
124.06
124.02
122.48
122.25
122.21
121.13

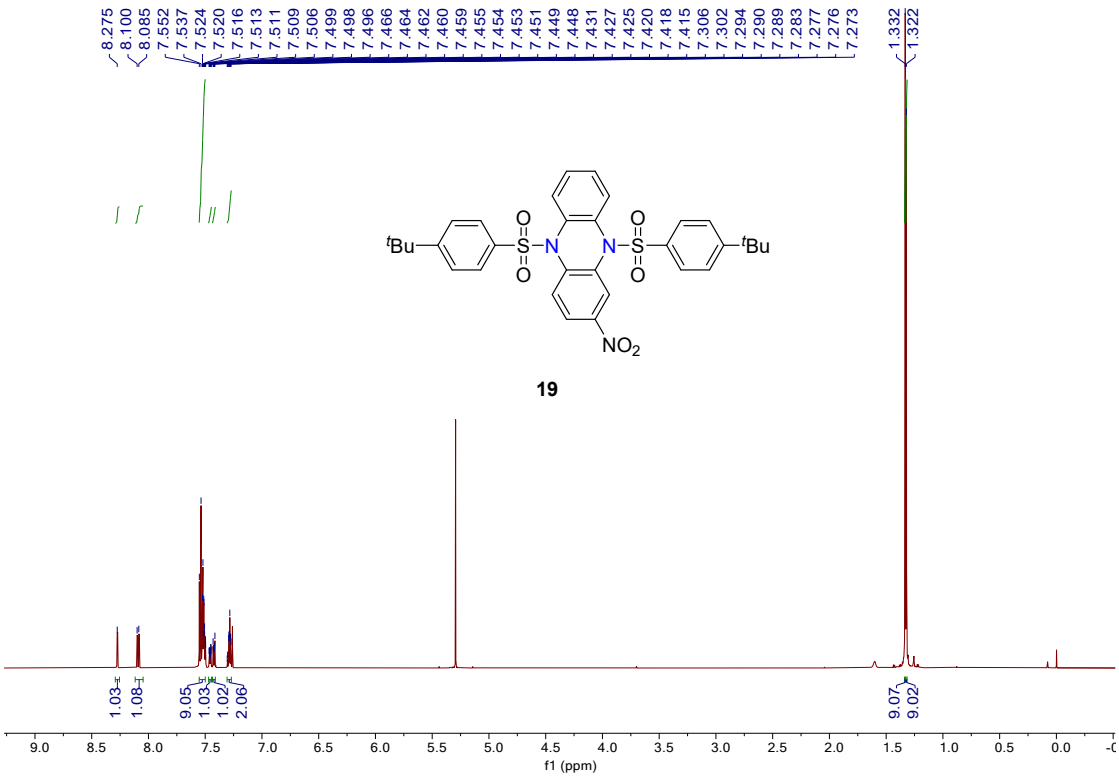

F3C
CF3
NO2

18

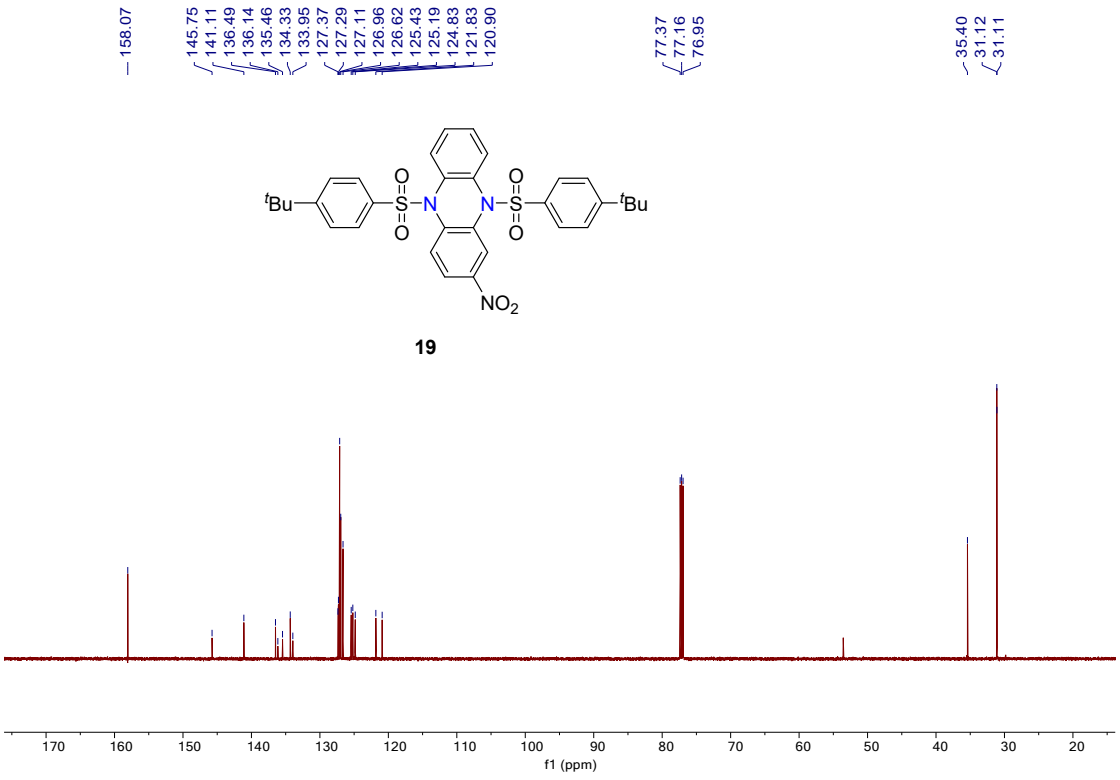

f1 (ppm)

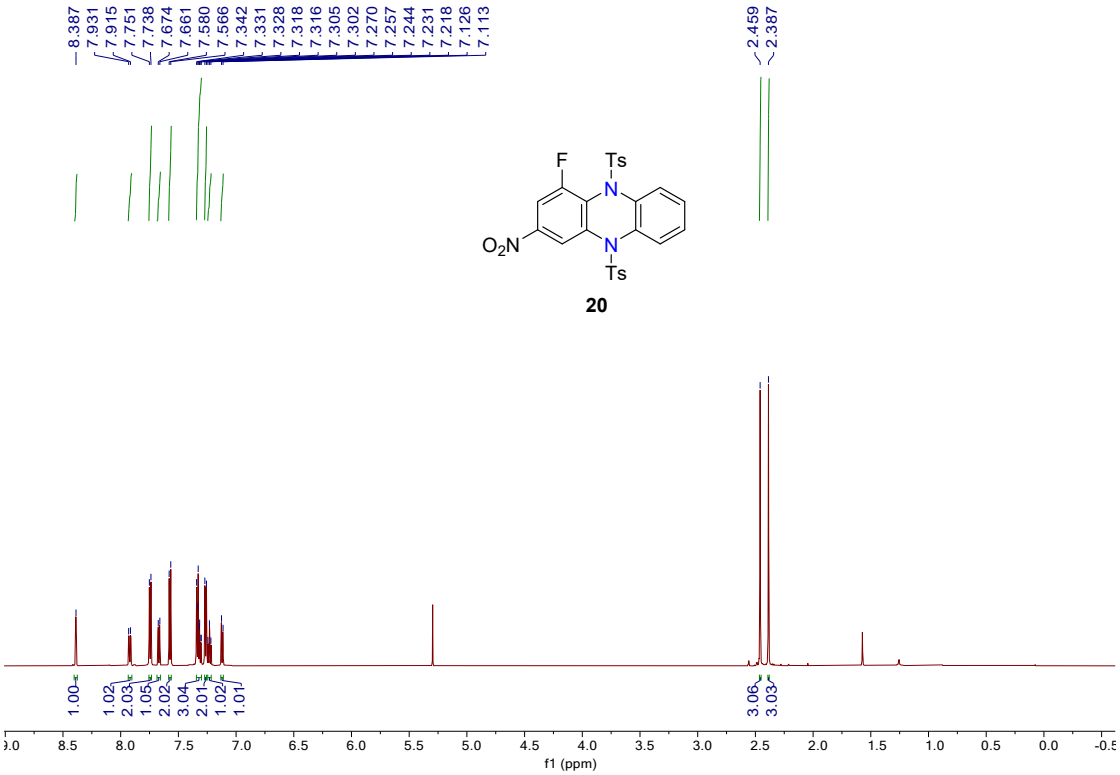

-63.215
F3C
CF3
NO2
6.00
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240
f1 (ppm)

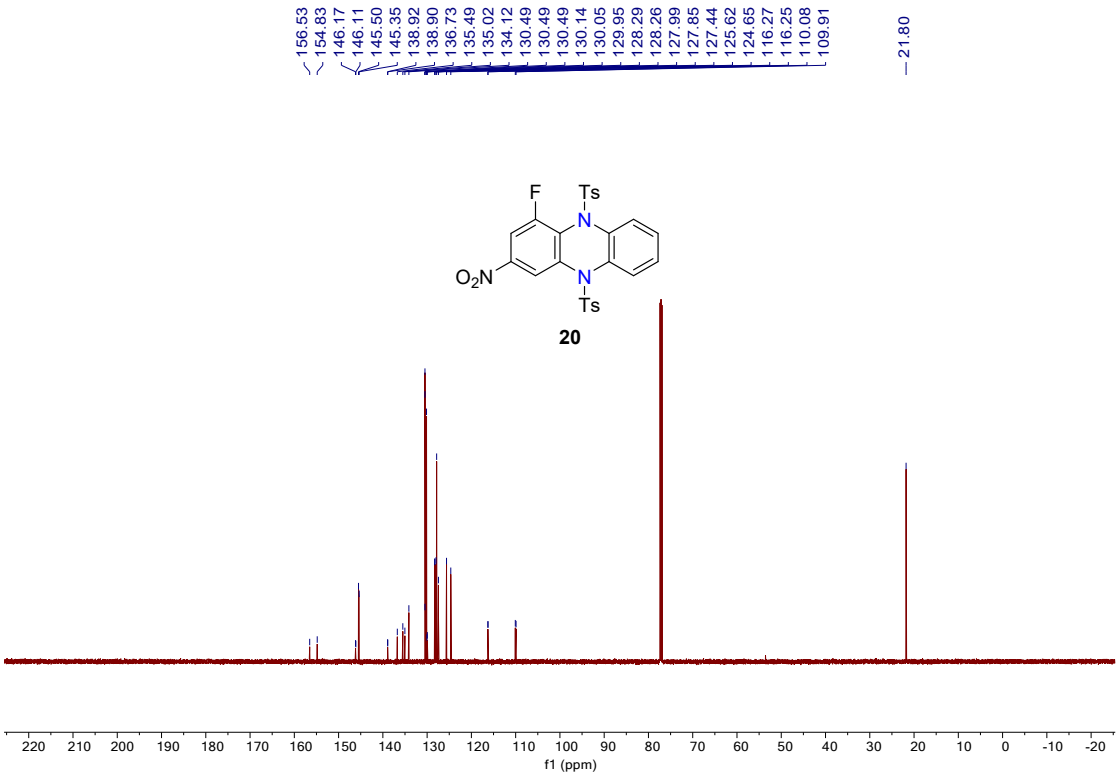
18

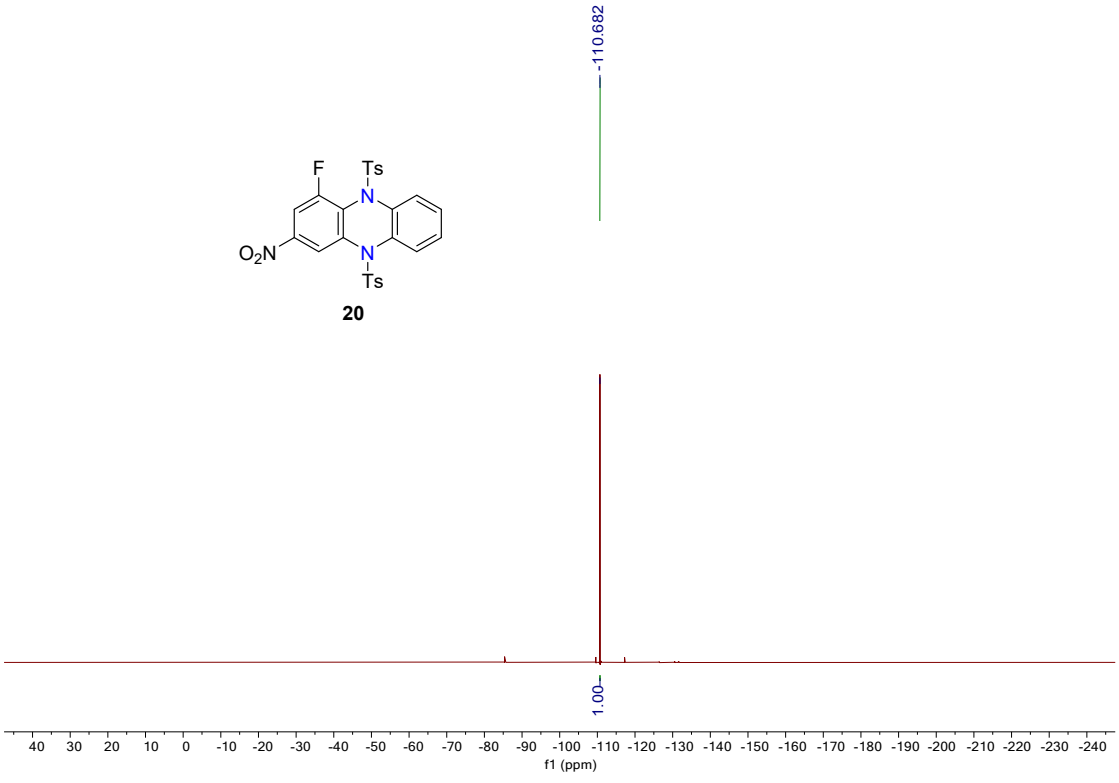

8.275
8.100
8.085
7.552
7.537
7.524
7.520
7.516
7.513
7.511
7.509
7.506
7.499
7.498
7.496
7.466
7.464
7.462
7.460
7.459
7.455
7.454
7.453
7.451
7.449
7.448
7.431
7.427
7.425
7.420
7.418
7.415
7.306
7.302
7.294
7.290
7.289
7.283
7.277
7.276
7.273
1.332
1.322
tBu
tBu
NO2
1.03
1.08
9.05
1.03
1.02
2.06
9.07
9.02
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)

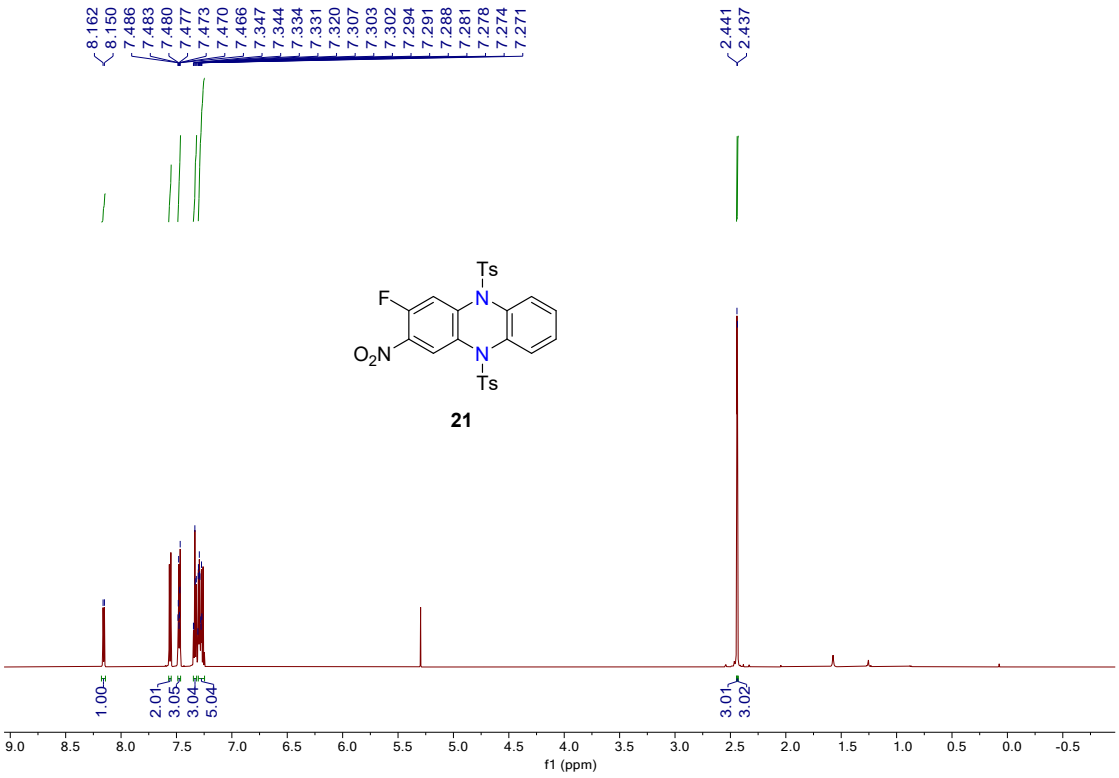
19

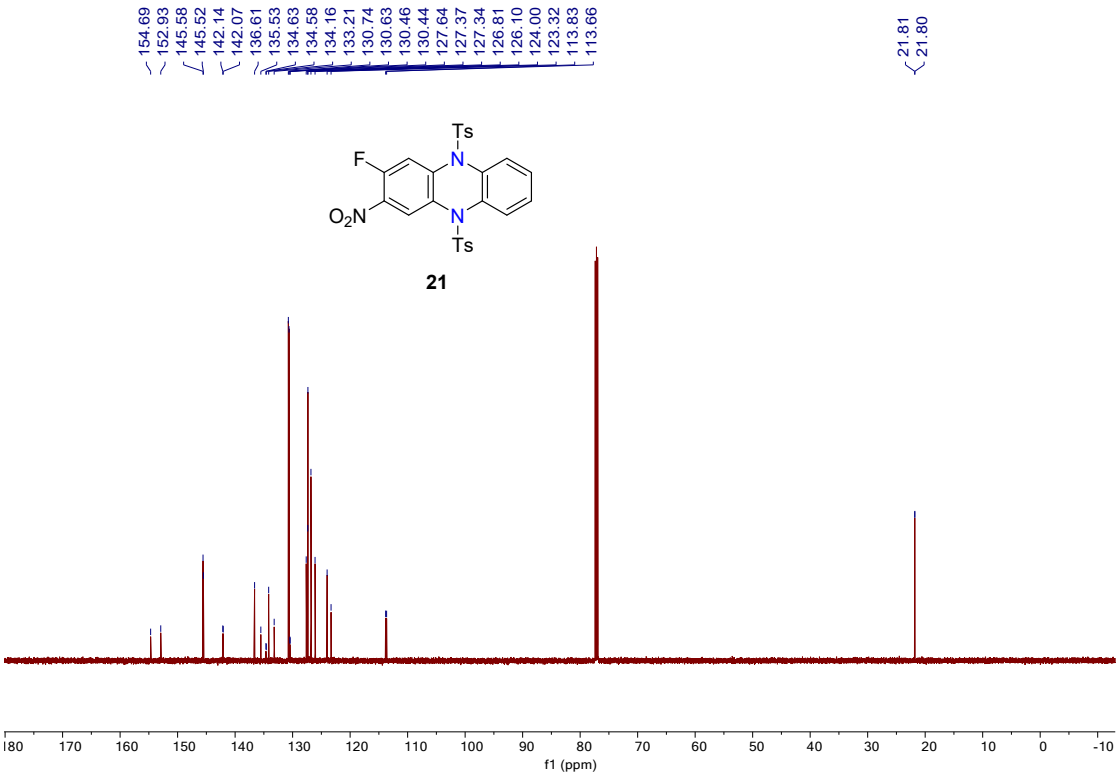

158.07
145.75
141.11
136.49
136.14
135.46
134.33
133.95
127.37
127.29
127.11
126.96
126.62
125.43
125.19
124.83
121.83
120.90
77.37
77.16
76.95
35.40
31.12
31.11
tBu
tBu
NO2
19
f1 (ppm)

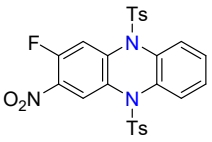

8.387
7.931
7.915
7.751
7.738
7.674
7.661
7.580
7.566
7.342
7.331
7.328
7.318
7.316
7.305
7.302
7.270
7.257
7.244
7.231
7.218
7.126
7.113
2.459
2.387
F
Ts
N
O2N
Ts
20
1.00
1.02
2.03
1.05
2.02
3.04
2.01
1.02
1.01
3.06
3.03
f1 (ppm)


156.53
154.83
146.17
146.11
145.50
145.35
138.92
138.90
136.73
135.49
135.02
134.12
130.49
130.49
130.49
130.14
130.05
129.95
128.29
128.26
127.99
127.85
127.44
125.62
124.65
116.27
116.25
110.08
109.91
21.80
F
Ts
N
O2N
N
Ts
20
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20
f1 (ppm)


-110.682
F
Ts
N
O2N
N
Ts
20
1.00
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240
f1 (ppm)

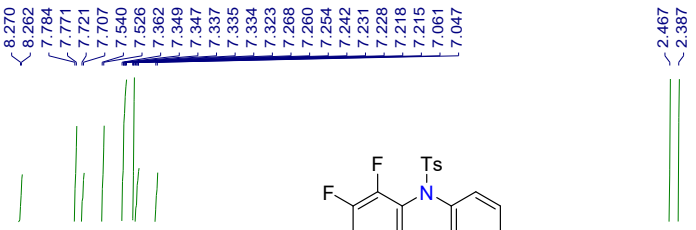

8.162
8.150
7.486
7.483
7.480
7.477
7.473
7.470
7.466
7.347
7.344
7.334
7.331
7.320
7.307
7.303
7.302
7.294
7.291
7.288
7.281
7.278
7.274
7.271
2.441
2.437
Ts
F
N
O2N
N
Ts
21
1.00
2.01
3.05
3.04
5.04
3.01
3.02
f1 (ppm)


154.69
152.93
145.58
145.52
142.14
142.07
136.61
135.53
134.63
134.58
134.16
133.21
130.74
130.63
130.46
130.44
127.64
127.37
127.34
126.81
126.10
124.00
123.32
113.83
113.66
21.81
21.80
Ts
F
N
O2N
N
Ts
21
f1 (ppm)


Ts
F
N
O_2N
N
Ts

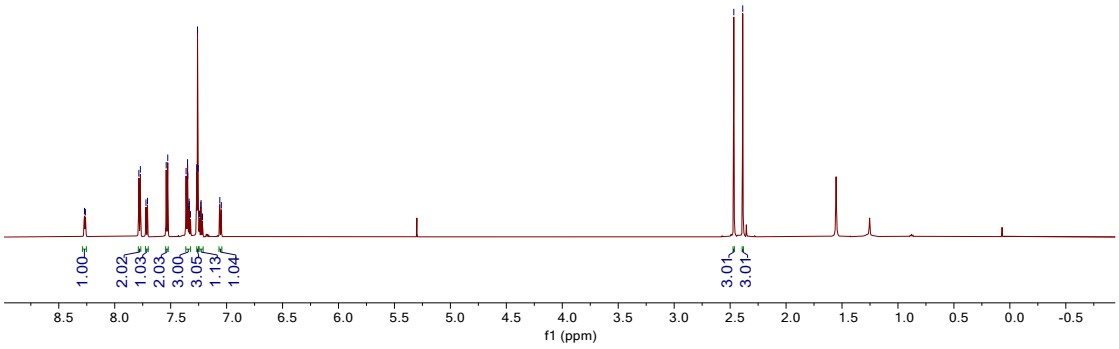
21

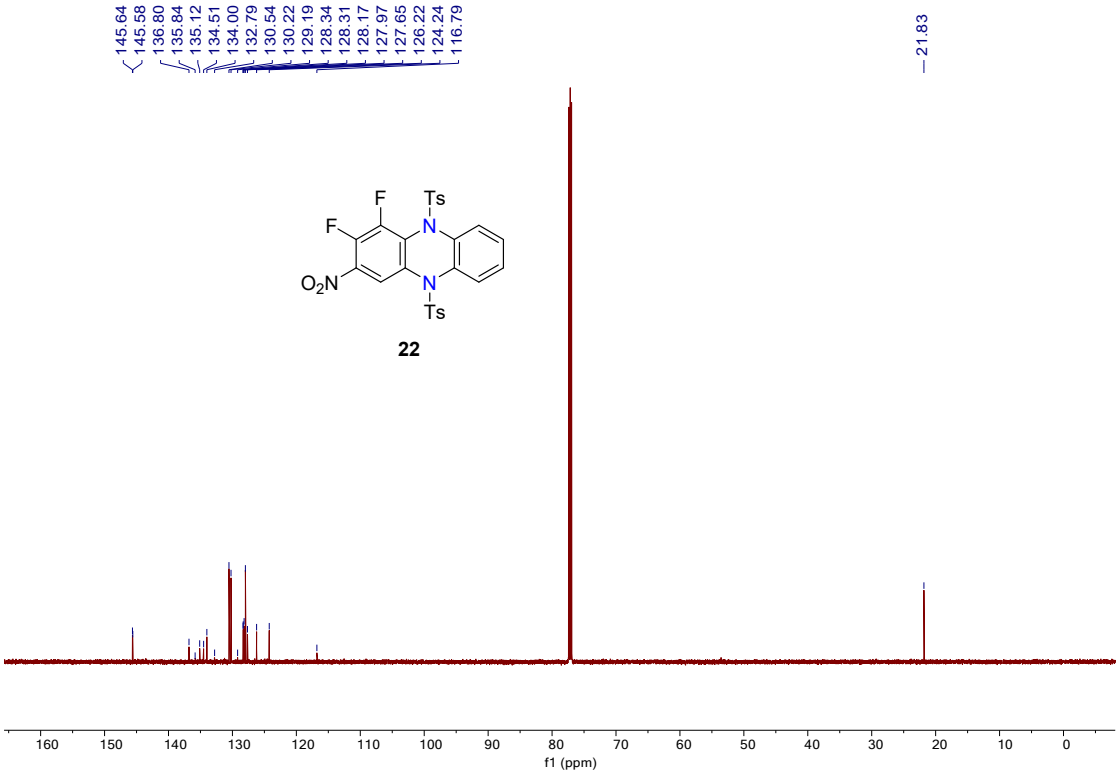
-116.412
1.00
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240
f1 (ppm)


8.270
8.262
7.784
7.771
7.721
7.707
7.540
7.526
7.362
7.349
7.347
7.337
7.335
7.334
7.323
7.268
7.260
7.254
7.242
7.231
7.228
7.218
7.215
7.061
7.047
2.467
2.387

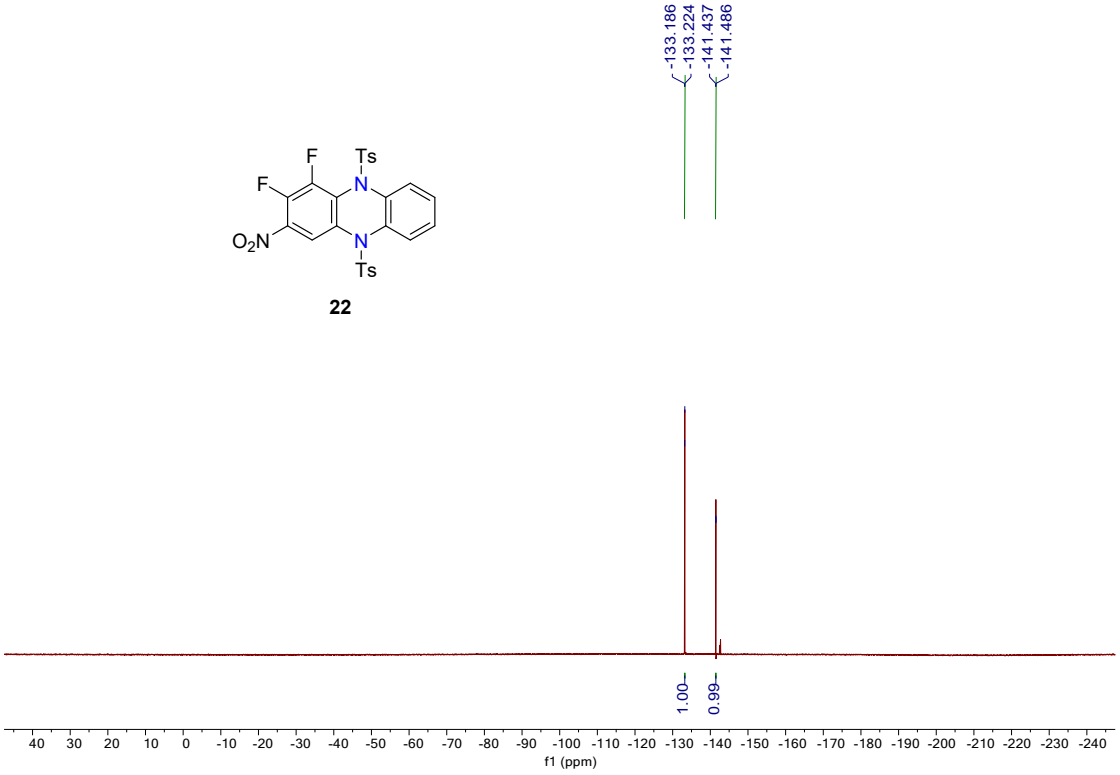
F
Ts
F
N
O_2N
N
Ts

22

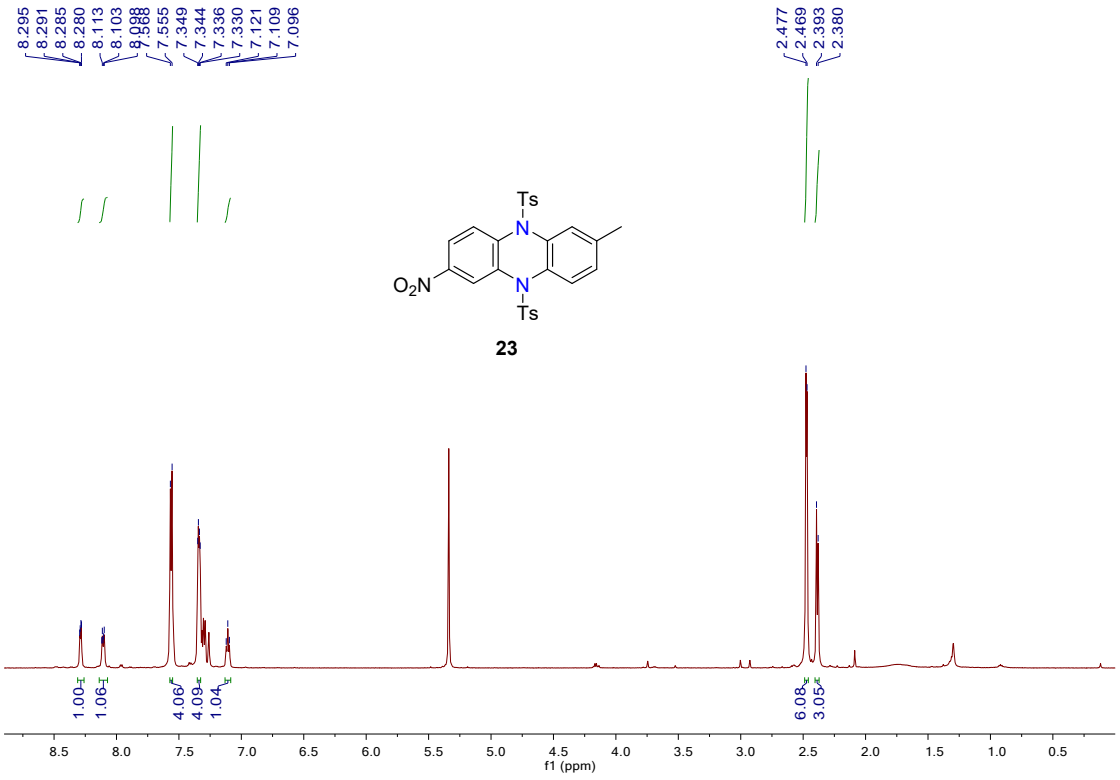

1.00
2.02
1.03
2.03
3.00
3.05
1.13
1.04
3.01
3.01
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


145.64
145.58
136.80
135.84
135.12
134.51
134.00
132.79
130.54
130.22
129.19
128.34
128.31
128.17
127.97
127.65
126.22
124.24
116.79
21.83
F
Ts
F
N
O2N
N
Ts
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

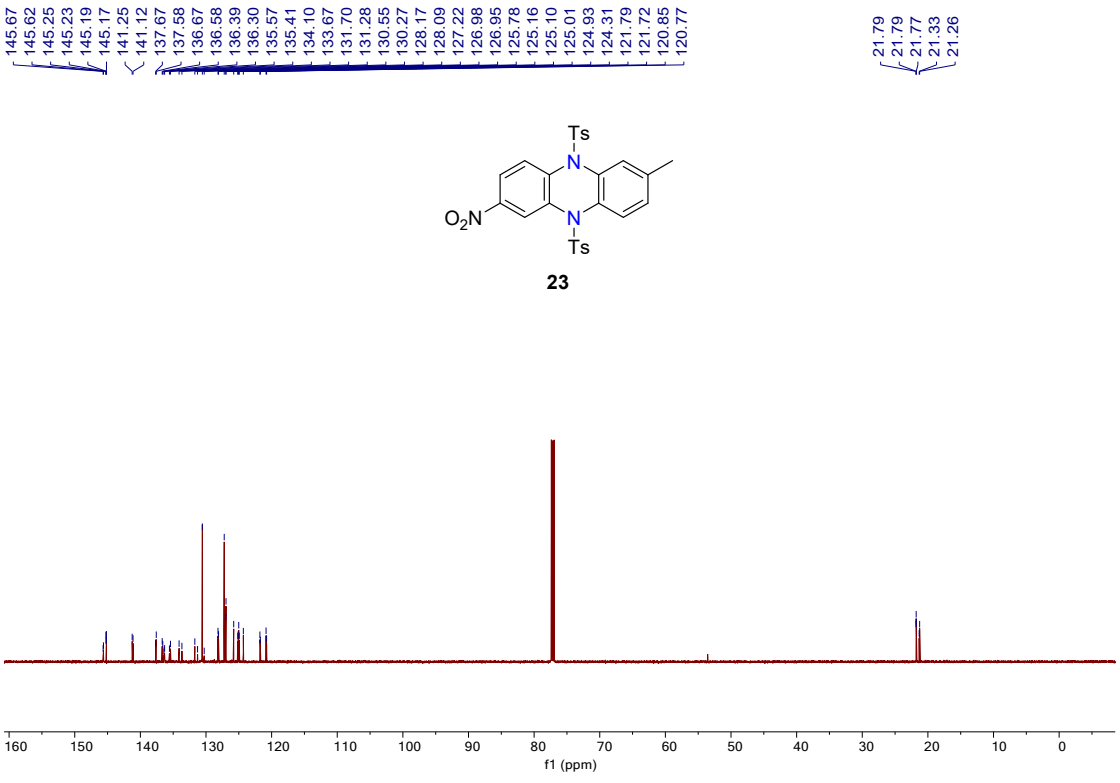
22


-133.186
-133.224
-141.437
-141.486
F
Ts
F
N
O2N
N
Ts
1.00
0.99
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
-180
-190
-200
-210
-220
-230
-240
f1 (ppm)

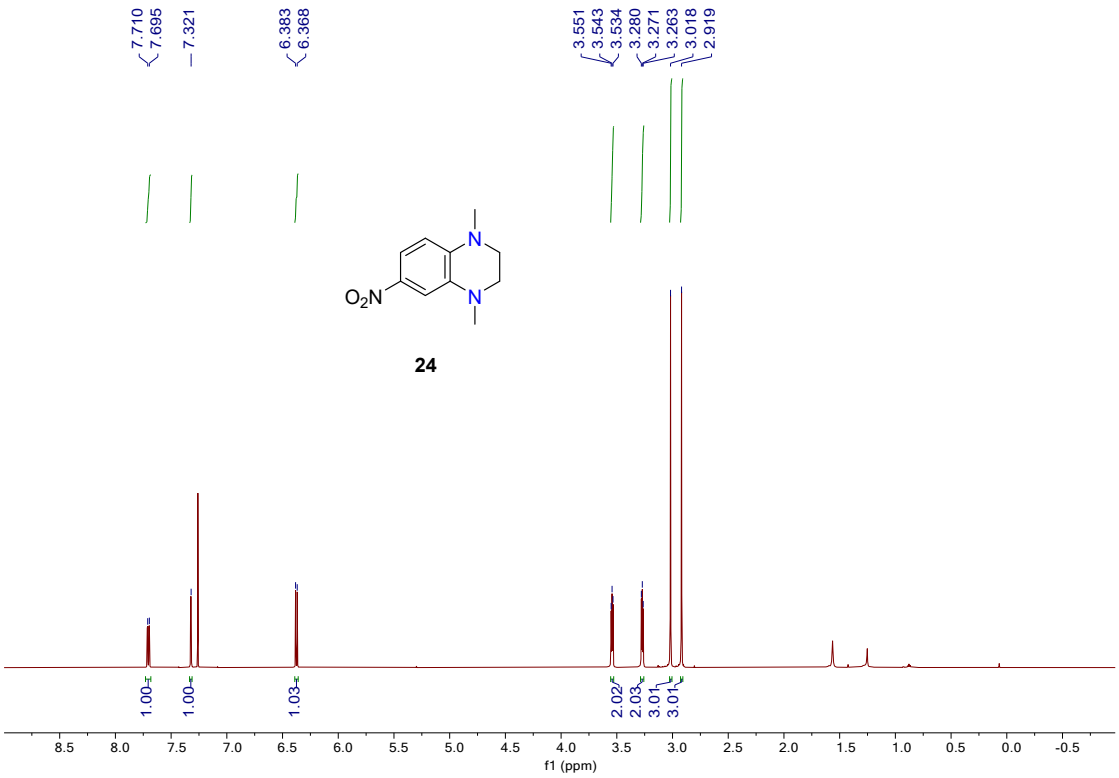
22

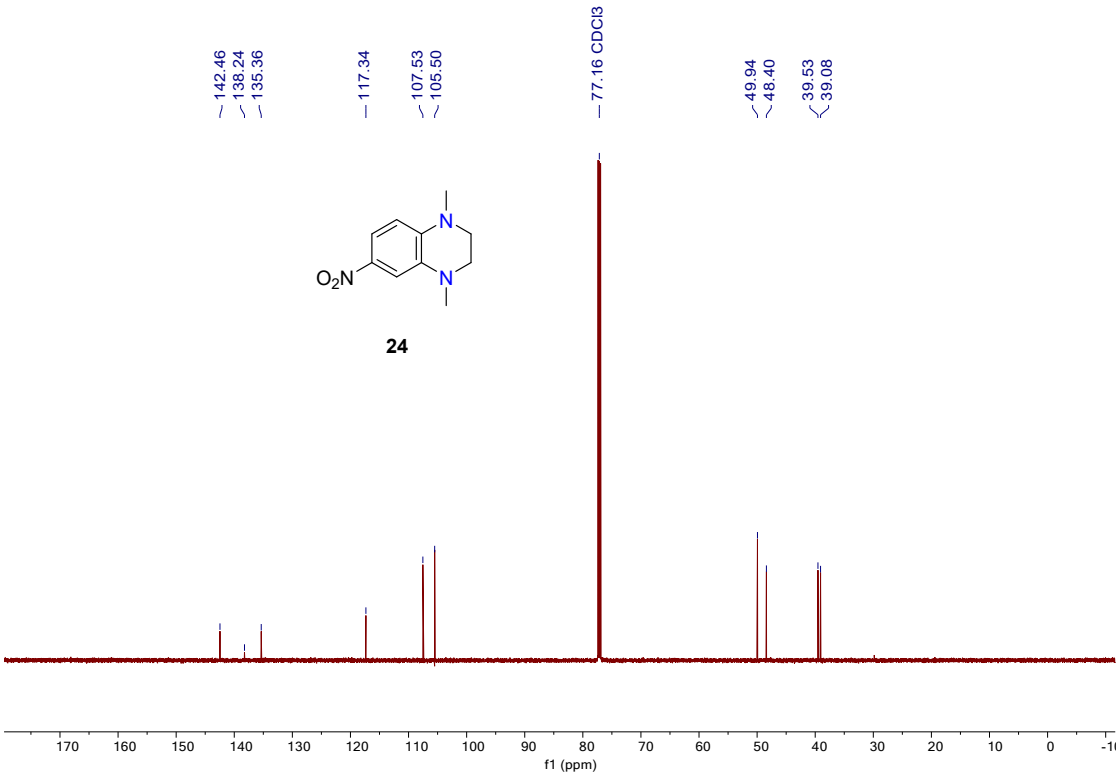

8.295
8.291
8.285
8.280
8.113
8.103
7.555
7.349
7.344
7.336
7.330
7.121
7.109
7.096
2.477
2.469
2.393
2.380
Ts
N
O2N
N
Ts
1.00
1.06
4.06
4.09
1.04
6.08
3.05
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

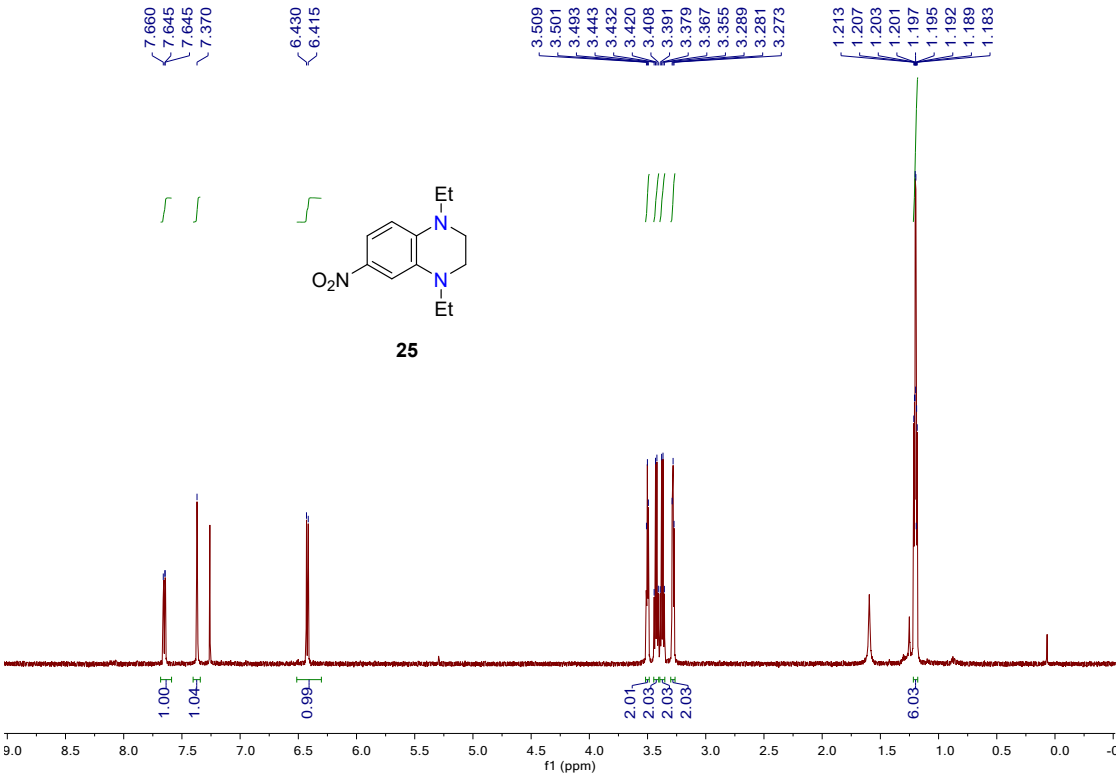
23


145.67
145.62
145.25
145.23
145.19
145.17
141.25
141.12
137.67
137.58
136.67
136.58
136.39
136.30
135.57
135.41
134.10
133.67
131.70
131.28
130.55
130.27
128.17
128.09
127.22
126.98
126.95
125.78
125.16
125.10
125.01
124.93
124.31
121.79
121.72
120.85
120.77
21.79
21.79
21.77
21.33
21.26
Ts
N
O2N
N
Ts
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

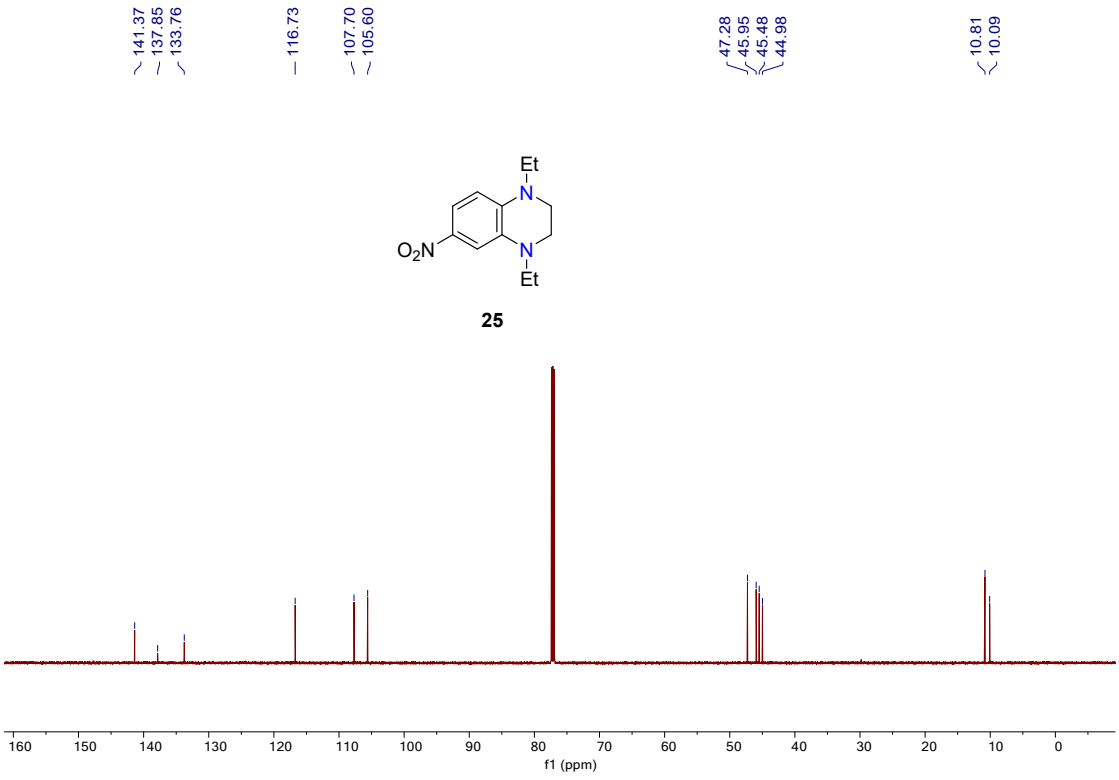
23


7.710
7.695
7.321
6.383
6.368
3.551
3.543
3.534
3.280
3.271
3.263
3.018
2.919
O2N
N
N
24
1.00
1.00
1.03
2.02
2.03
3.01
3.01
f1 (ppm)

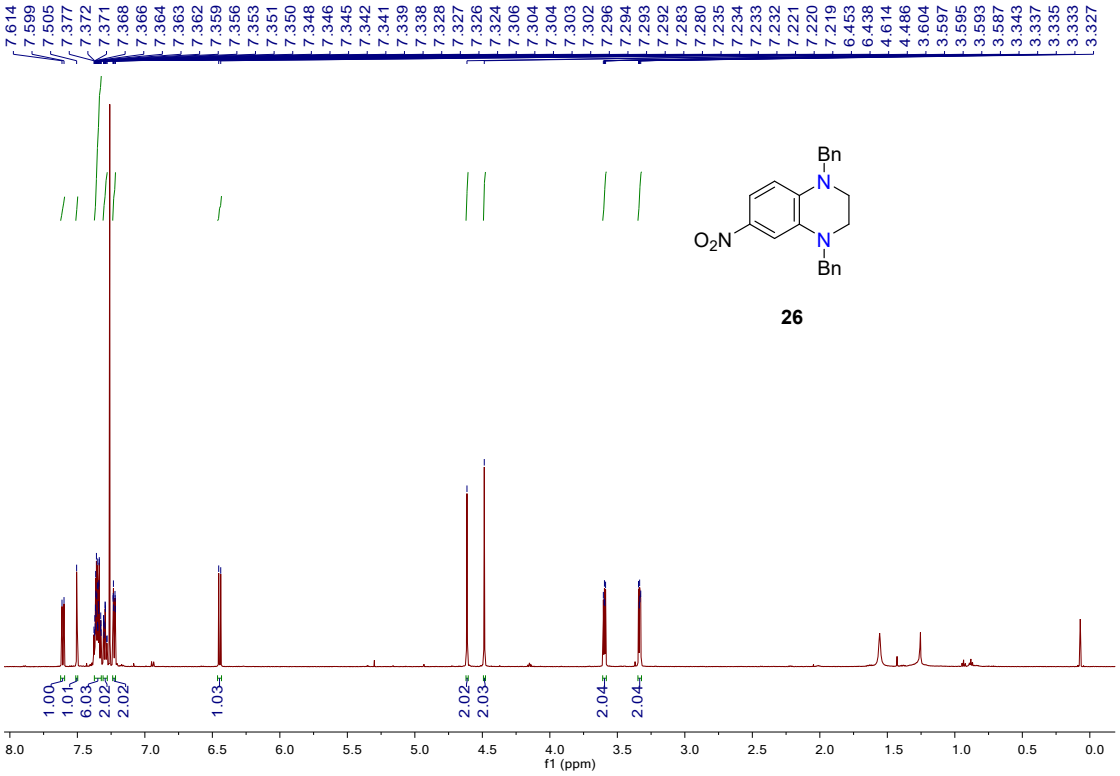

142.46
138.24
135.36
117.34
107.53
105.50
77.16 CDCl3
49.94
48.40
39.53
39.08
O2N
N
N
24
f1 (ppm)

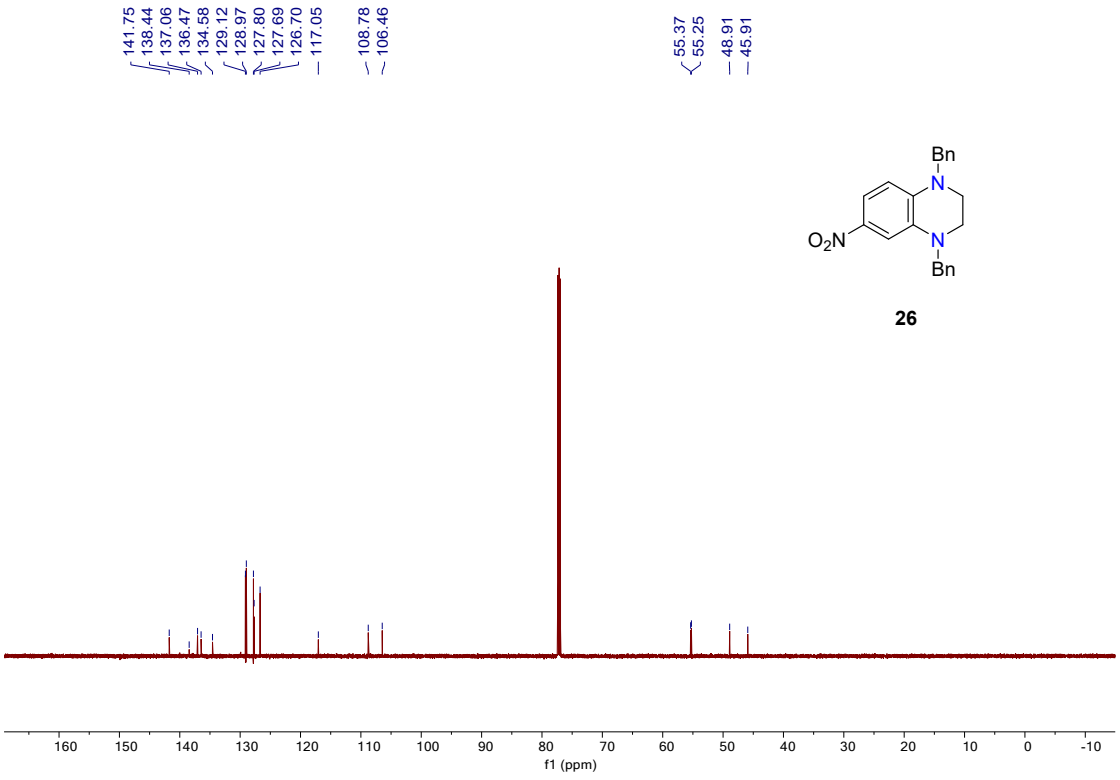

7.660
7.645
7.645
7.370
6.430
6.415
3.509
3.501
3.493
3.443
3.432
3.420
3.408
3.391
3.379
3.367
3.355
3.289
3.281
3.273
1.213
1.207
1.203
1.201
1.197
1.195
1.192
1.189
1.183
Et
N
O2N
N
Et
1.00
1.04
0.99
2.01
2.03
2.03
2.03
6.03
f1 (ppm)

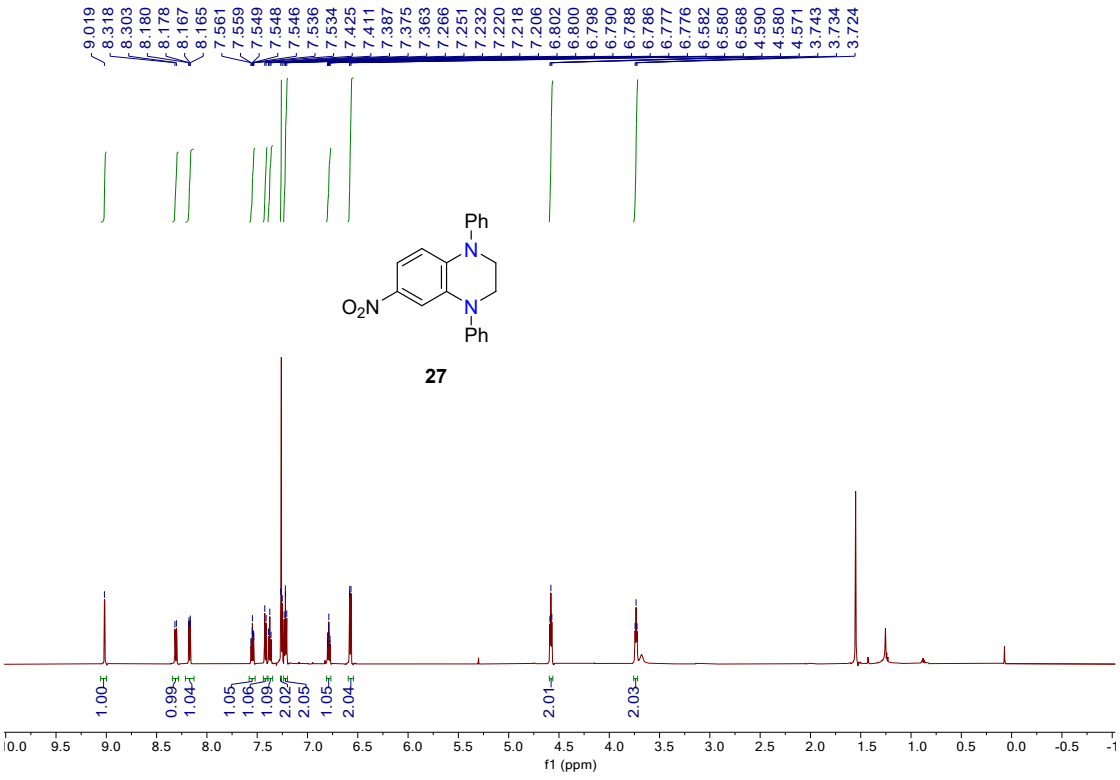
25


141.37
137.85
133.76
116.73
107.70
105.60
47.28
45.95
45.48
44.98
10.81
10.09
Et
N
O2N
N
Et
f1 (ppm)

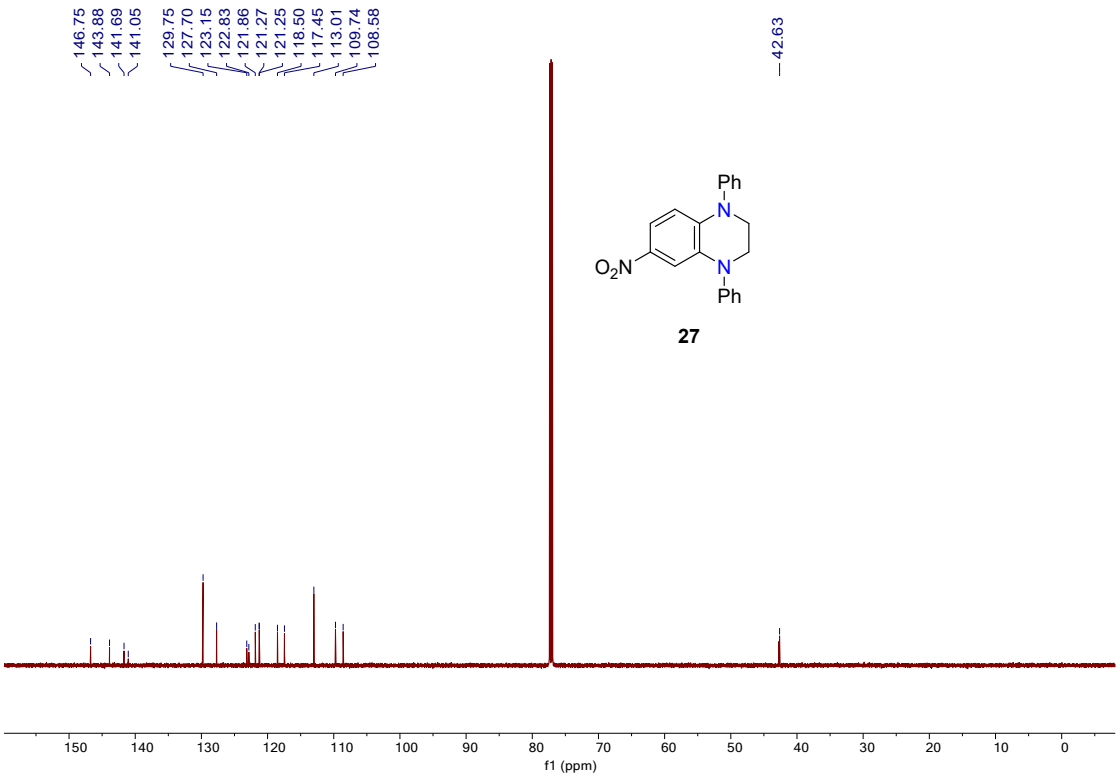
25


7.614
7.599
7.505
7.377
7.372
7.371
7.368
7.366
7.364
7.363
7.362
7.359
7.356
7.353
7.351
7.350
7.348
7.346
7.345
7.342
7.341
7.339
7.338
7.328
7.327
7.326
7.324
7.306
7.304
7.304
7.303
7.302
7.296
7.294
7.293
7.292
7.283
7.280
7.235
7.234
7.233
7.232
7.221
7.220
7.219
6.453
6.438
4.614
4.486
3.604
3.597
3.595
3.593
3.587
3.343
3.337
3.335
3.333
3.327
Bn
N
O2N
N
Bn
26
1.00
1.01
6.03
2.02
2.02
1.03
2.02
2.03
2.04
2.04
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)

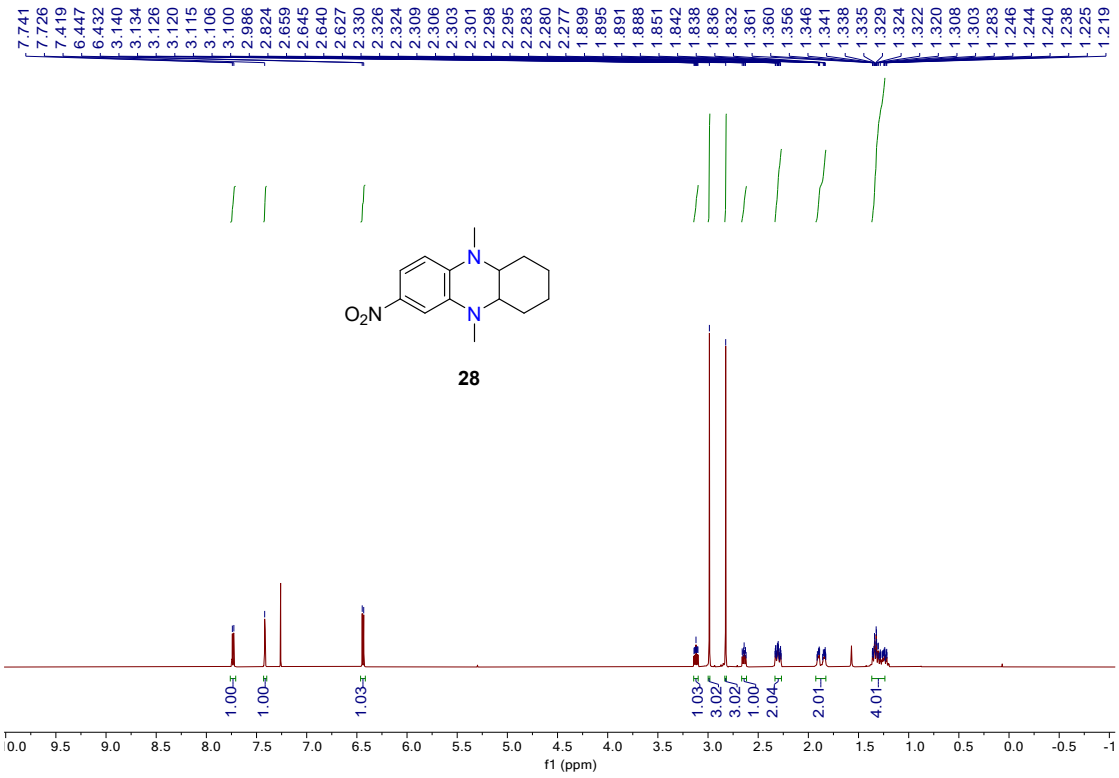

141.75
138.44
137.06
136.47
134.58
129.12
128.97
127.80
127.69
126.70
117.05
108.78
106.46
55.37
55.25
48.91
45.91
Bn
N
O2N
N
Bn
26
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

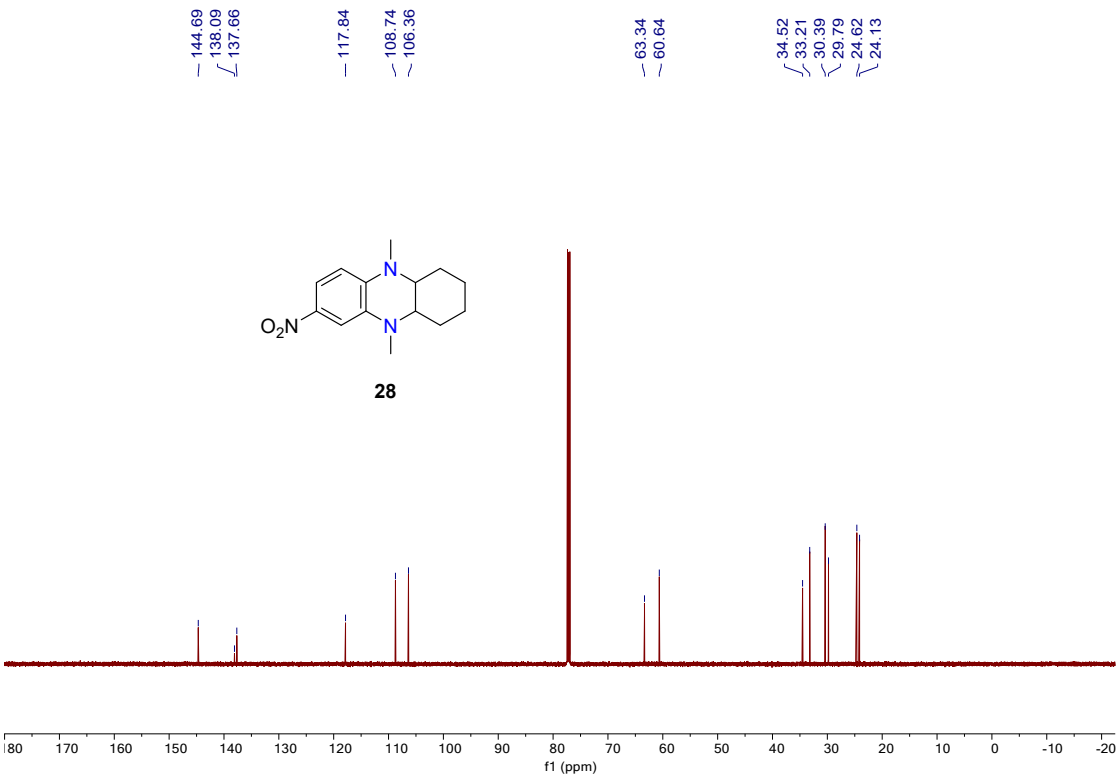

9.019
8.318
8.303
8.180
8.178
8.167
8.165
7.561
7.559
7.549
7.548
7.546
7.536
7.534
7.425
7.411
7.387
7.375
7.363
7.266
7.251
7.232
7.220
7.218
7.206
6.802
6.800
6.798
6.790
6.788
6.786
6.777
6.776
6.582
6.580
6.568
4.590
4.580
4.571
3.743
3.734
3.724
Ph
N
O2N
N
Ph
1.00
0.99
1.04
1.05
1.06
1.09
2.02
2.05
1.05
2.04
2.01
2.03
f1 (ppm)

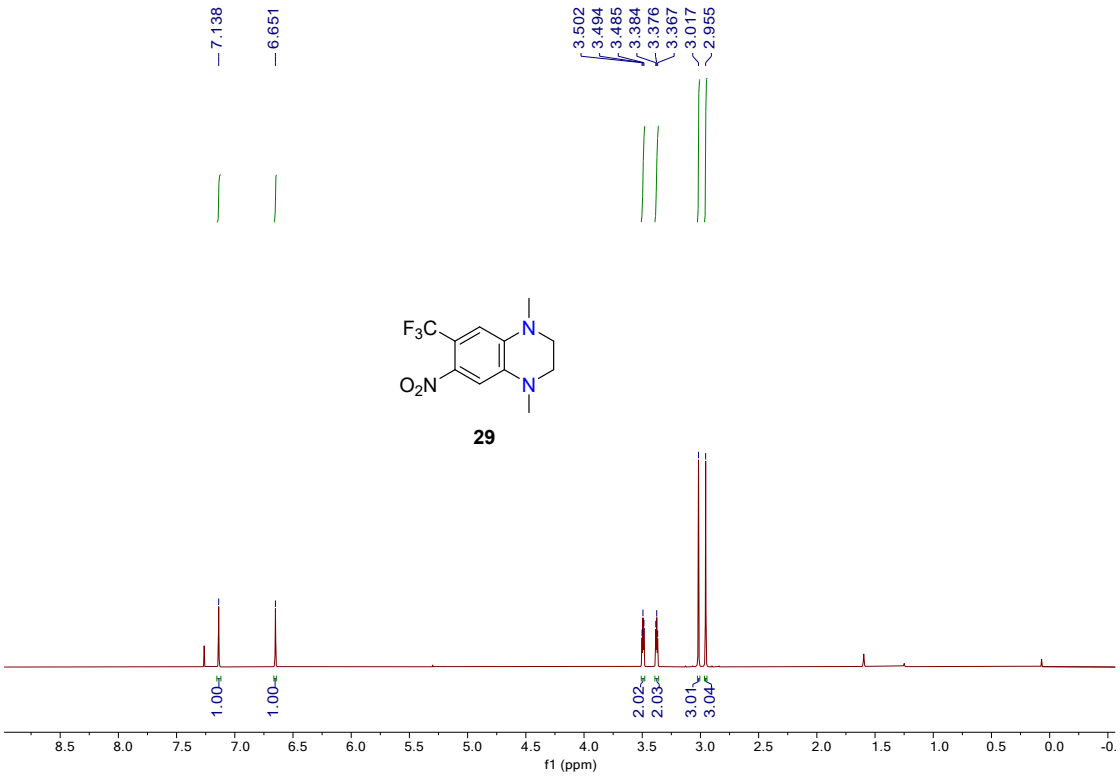
27

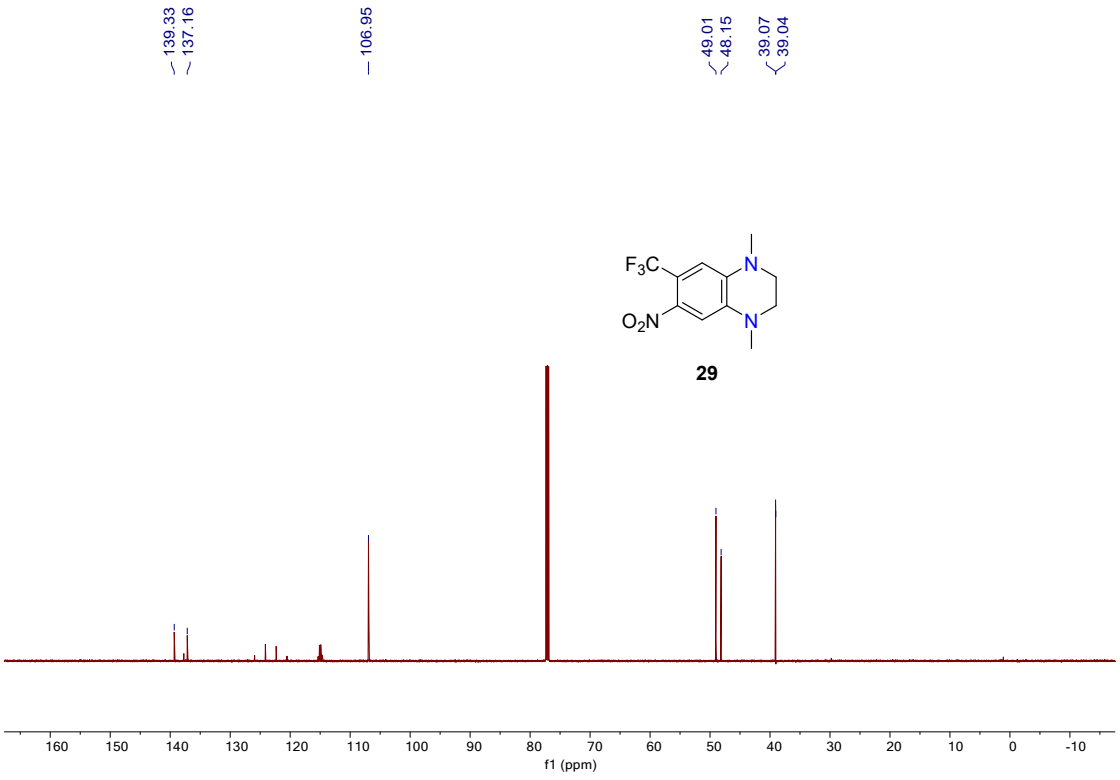

146.75
143.88
141.69
141.05
129.75
127.70
123.15
122.83
121.86
121.27
121.25
118.50
117.45
113.01
109.74
108.58
42.63
Ph
N
O2N
N
Ph
f1 (ppm)

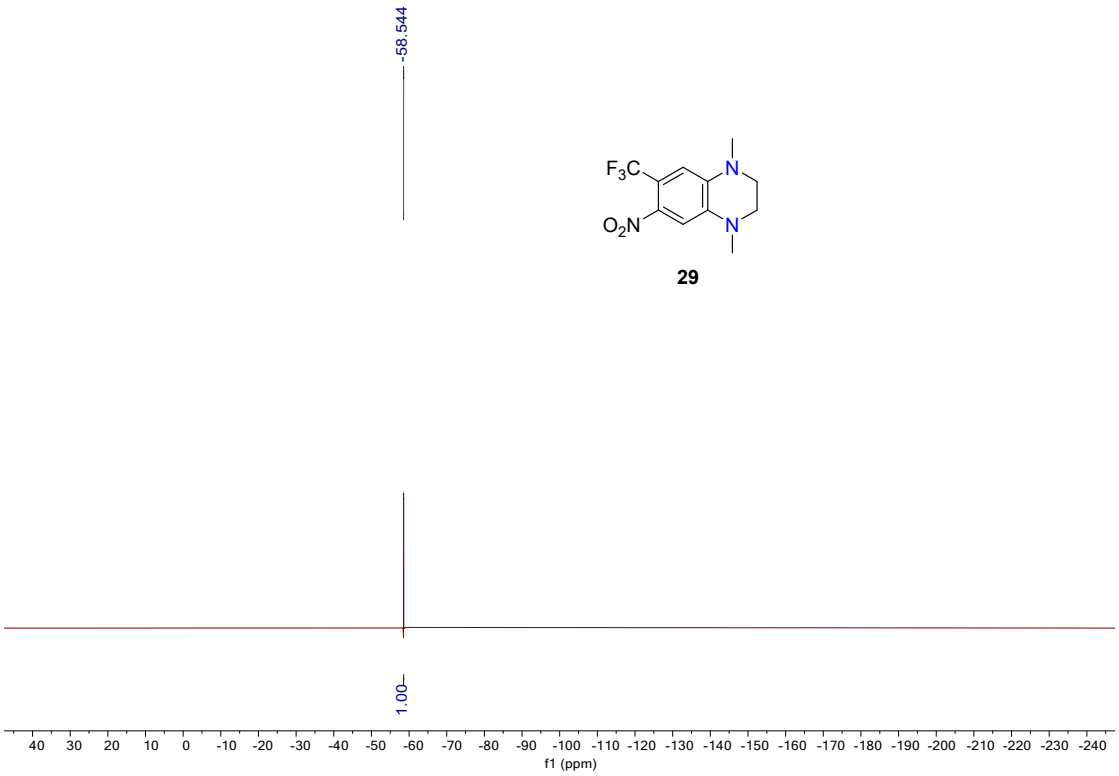
27


7.741
7.726
7.419
6.447
6.432
3.140
3.134
3.126
3.120
3.115
3.106
3.100
2.986
2.824
2.659
2.645
2.640
2.627
2.330
2.326
2.324
2.309
2.306
2.303
2.301
2.298
2.295
2.283
2.280
2.277
1.899
1.895
1.891
1.888
1.851
1.842
1.838
1.836
1.832
1.361
1.360
1.356
1.346
1.341
1.338
1.335
1.329
1.324
1.322
1.320
1.308
1.303
1.283
1.246
1.244
1.240
1.238
1.225
1.219
O2N
N
N
28
1.00
1.00
1.03
1.03
3.02
3.02
1.00
2.04
2.01
4.01
f1 (ppm)

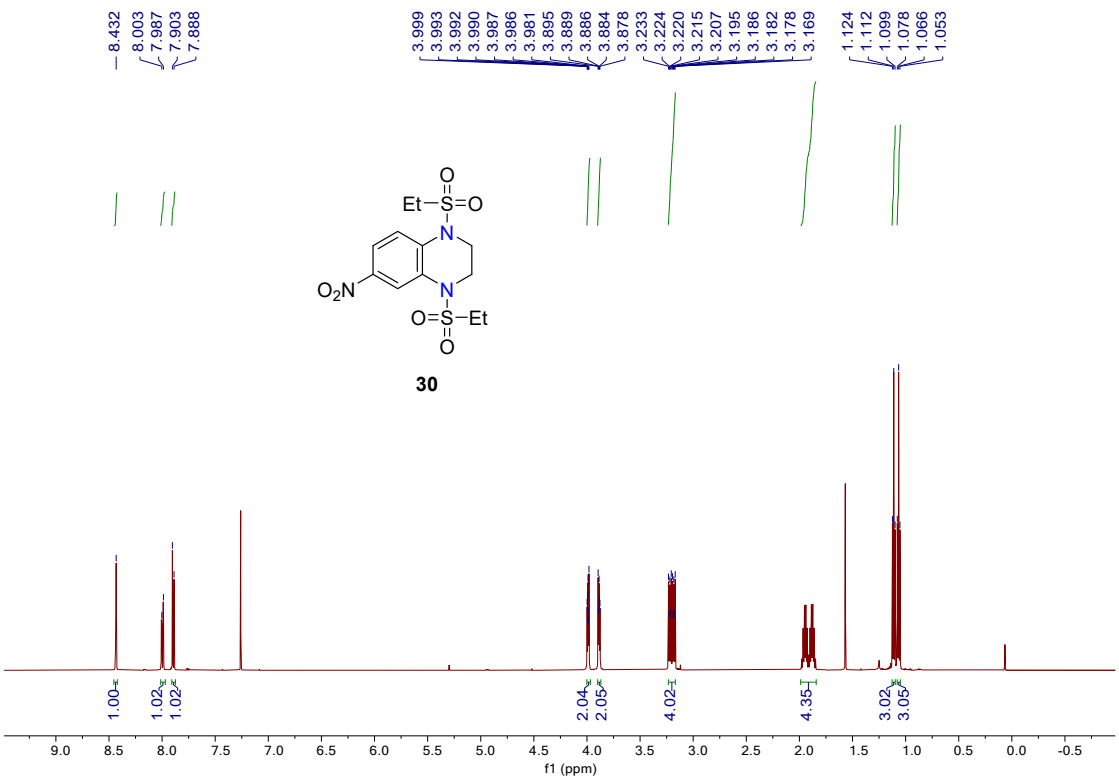

144.69
138.09
137.66
117.84
108.74
106.36
63.34
60.64
34.52
33.21
30.39
29.79
24.62
24.13
O2N
N
N
28
f1 (ppm)


7.138
6.651
3.502
3.494
3.485
3.384
3.376
3.367
3.017
2.955
F3C
O2N
N
N
29
1.00
1.00
2.02
2.03
3.01
3.04
f1 (ppm)

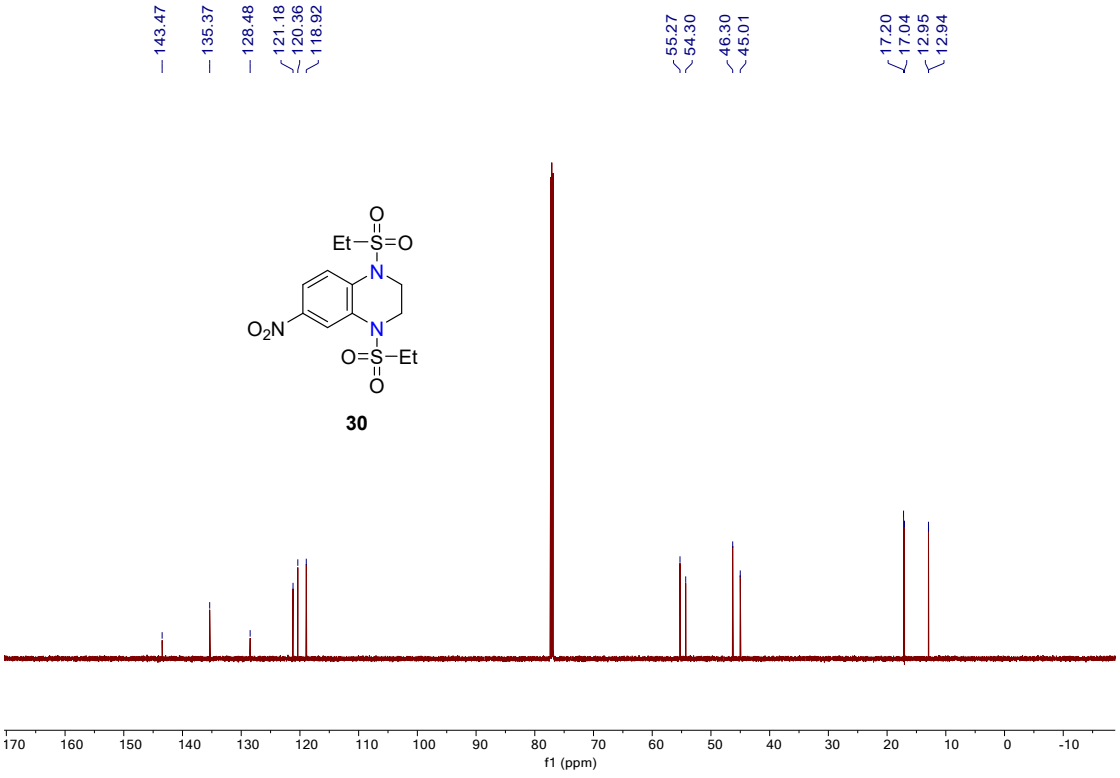

139.33
137.16
106.95
49.01
48.15
39.07
39.04
F3C
O2N
N
N
29
f1 (ppm)


-58.544
1.00
40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240
f1 (ppm)

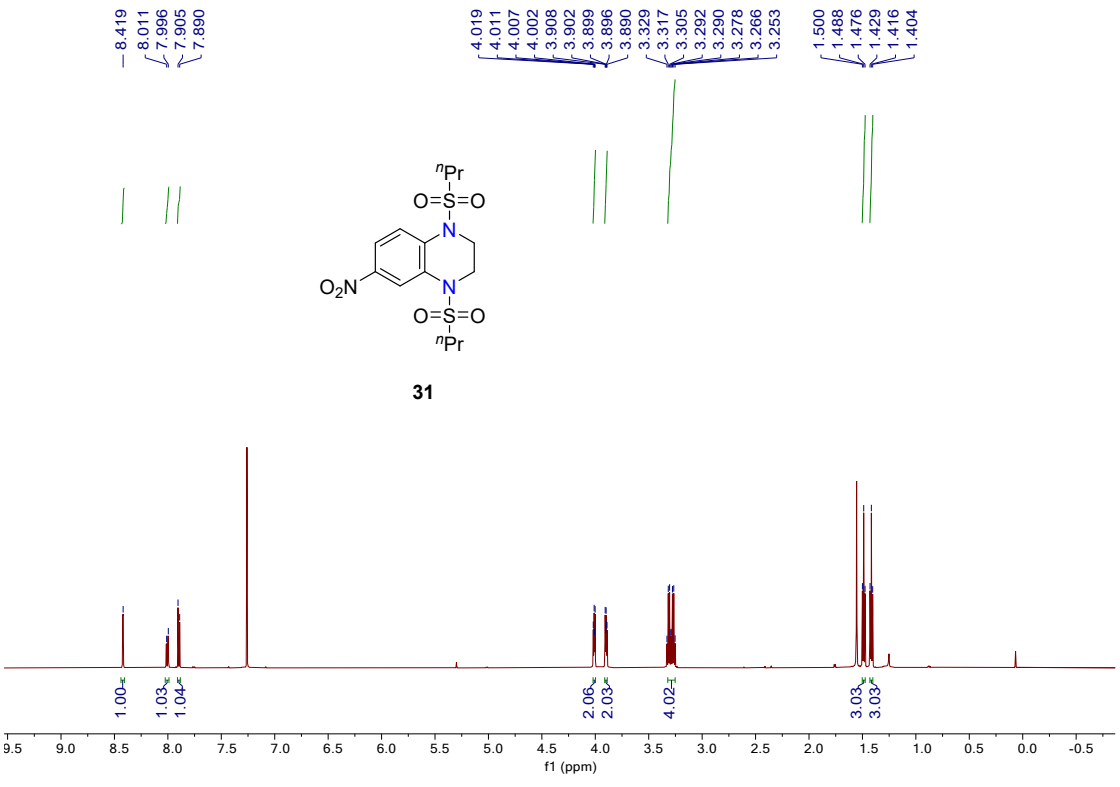
29


8.432
8.003
7.987
7.903
7.888
3.999
3.993
3.992
3.990
3.987
3.986
3.981
3.895
3.889
3.886
3.884
3.878
3.233
3.224
3.220
3.215
3.207
3.195
3.186
3.182
3.178
3.169
1.124
1.112
1.099
1.078
1.066
1.053
1.00
1.02
1.02
2.04
2.05
4.02
4.35
3.02
3.05
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)

30


143.47
135.37
128.48
121.18
120.36
118.92
55.27
54.30
46.30
45.01
17.20
17.04
12.95
12.94
Et—S=O
O
N
O2N
N
O=S—Et
O
f1 (ppm)

30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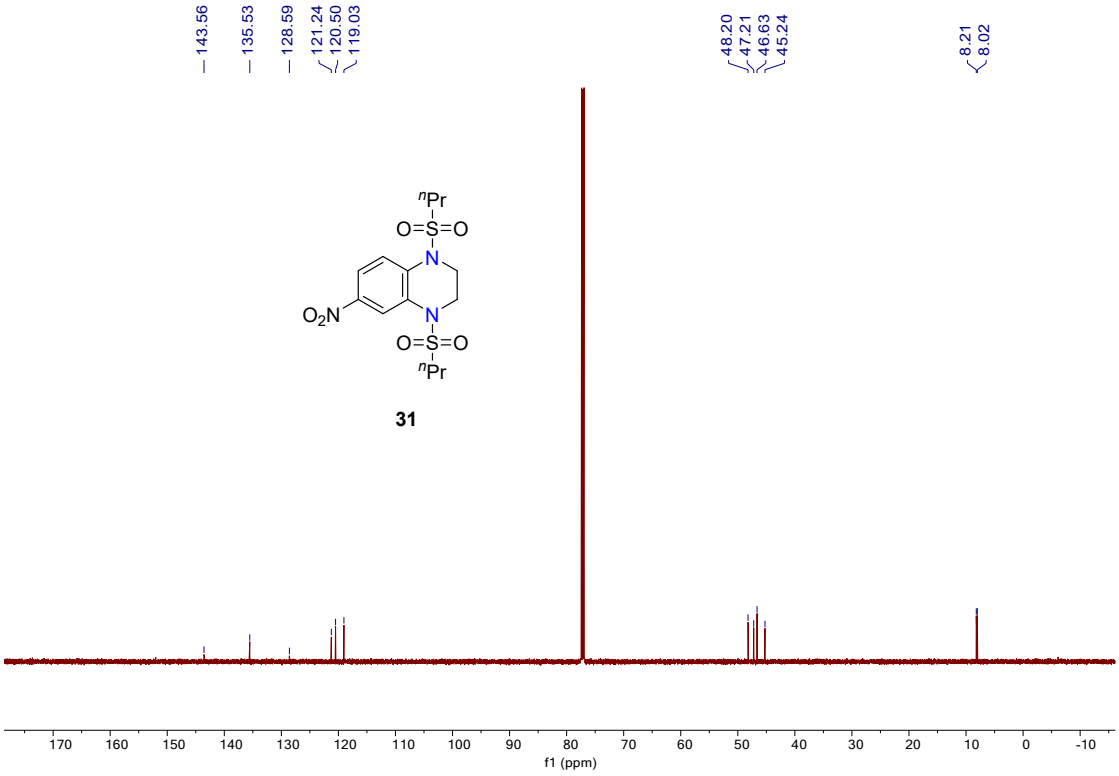
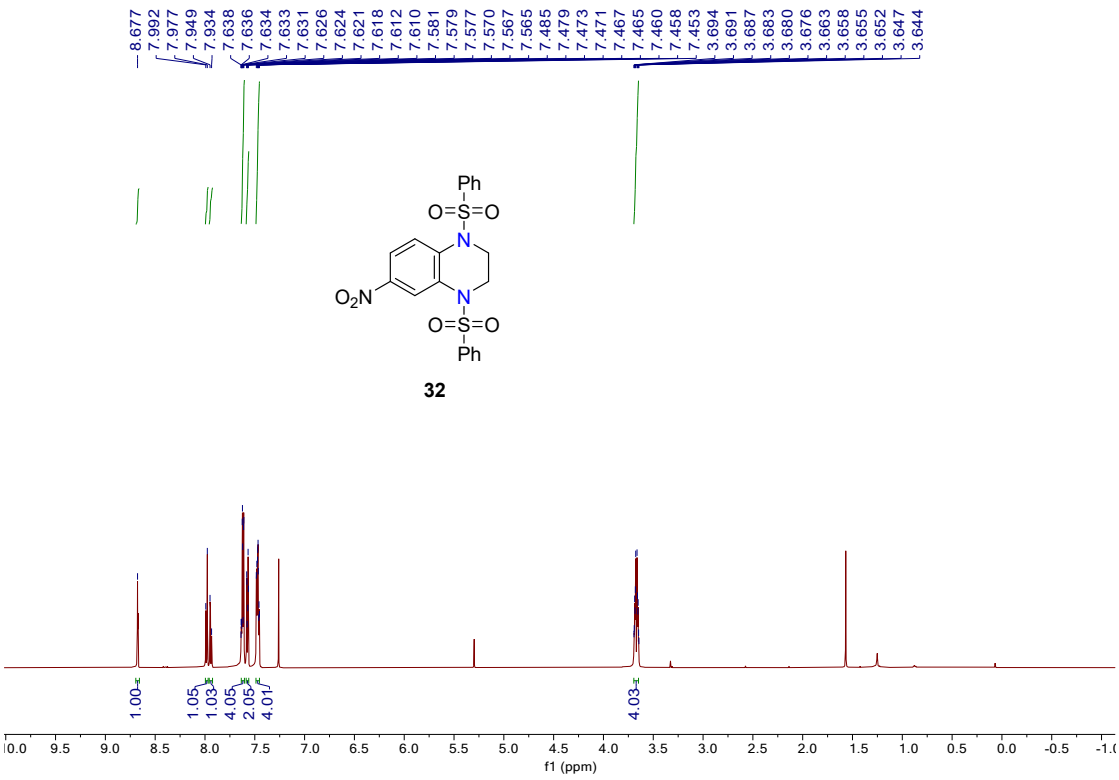
8.011
7.996
7.905
7.890
4.019
4.011
4.007
4.002
3.908
3.902
3.899
3.896
3.890
3.329
3.317
3.305
3.292
3.290
3.278
3.266
3.253
1.500
1.488
1.476
1.429
1.416
1.404
nPr
O=S=O
N
O2N
N
O=S=O
nPr
1.00
1.03
1.04
2.06
2.03
4.02
3.03
3.03
f1 (ppm)

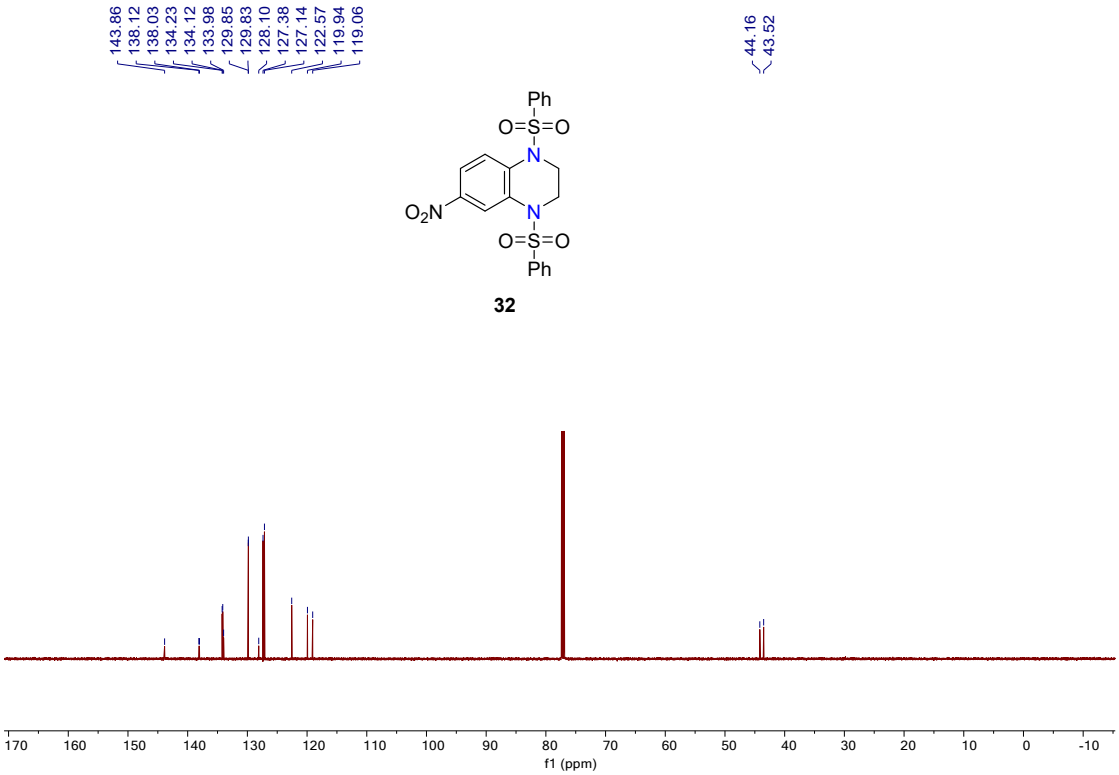
31


143.56
135.53
128.59
121.24
120.50
119.03
48.20
47.21
46.63
45.24
8.21
8.02
nPr
O=S=O
N
O2N
N
O=S=O
nPr
f1 (ppm)

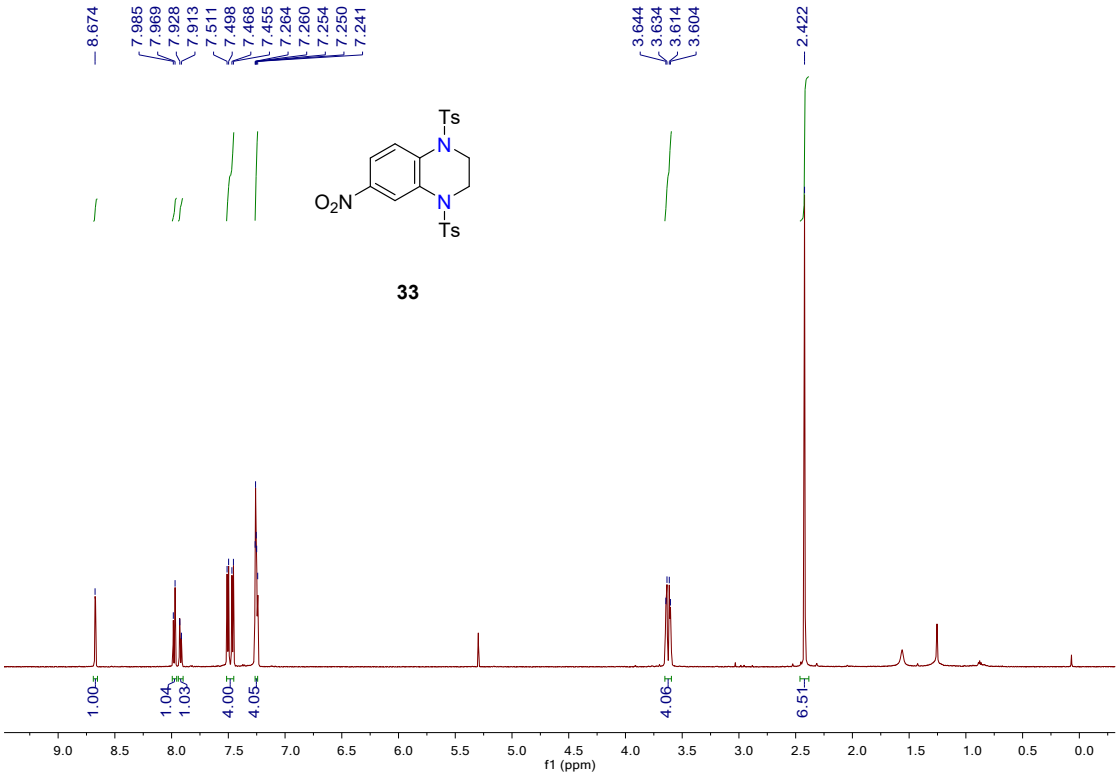
31


8.677
7.992
7.977
7.949
7.934
7.638
7.636
7.634
7.633
7.631
7.626
7.624
7.621
7.618
7.612
7.610
7.581
7.579
7.577
7.570
7.567
7.565
7.485
7.479
7.473
7.471
7.467
7.465
7.460
7.458
7.453
3.694
3.691
3.687
3.683
3.680
3.676
3.663
3.658
3.655
3.652
3.647
3.644
Ph
O=S=O
N
O2N
N
O=S=O
Ph
1.00
1.05
1.03
4.05
2.05
4.01
4.03
f1 (ppm)

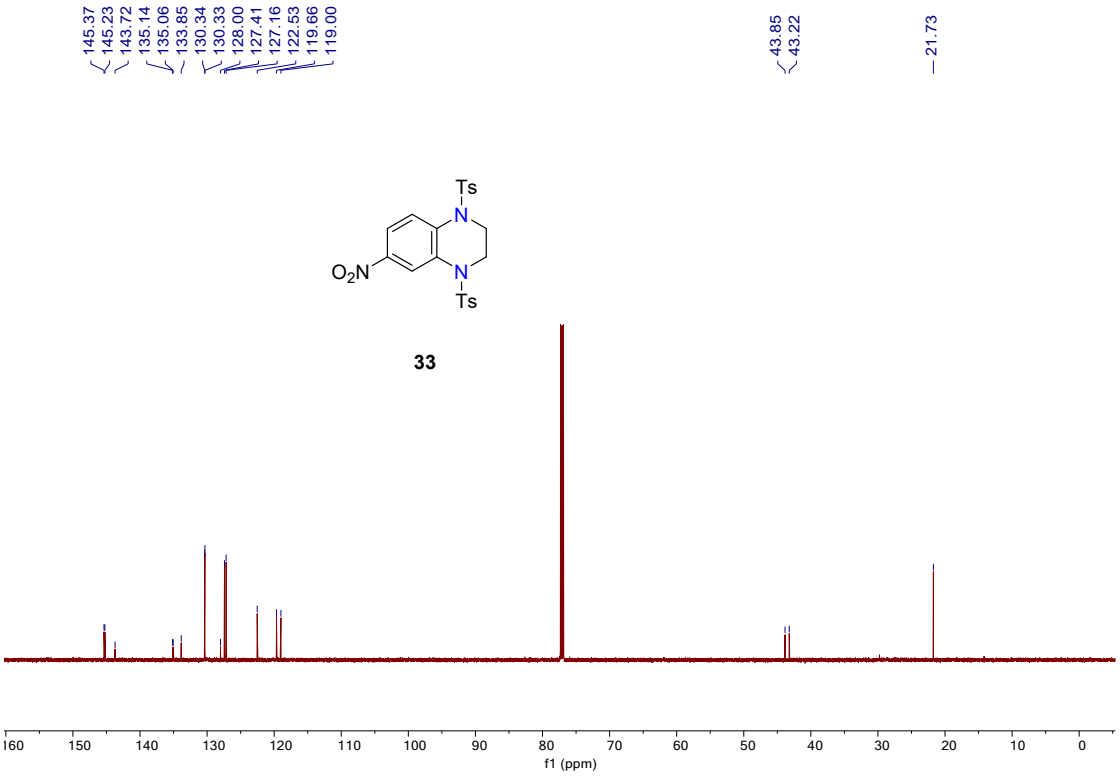
32


143.86
138.12
138.03
134.23
134.12
133.98
129.85
129.83
128.10
127.38
127.14
122.57
119.94
119.06
44.16
43.52
Ph
O=S=O
N
O2N
N
O=S=O
Ph
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

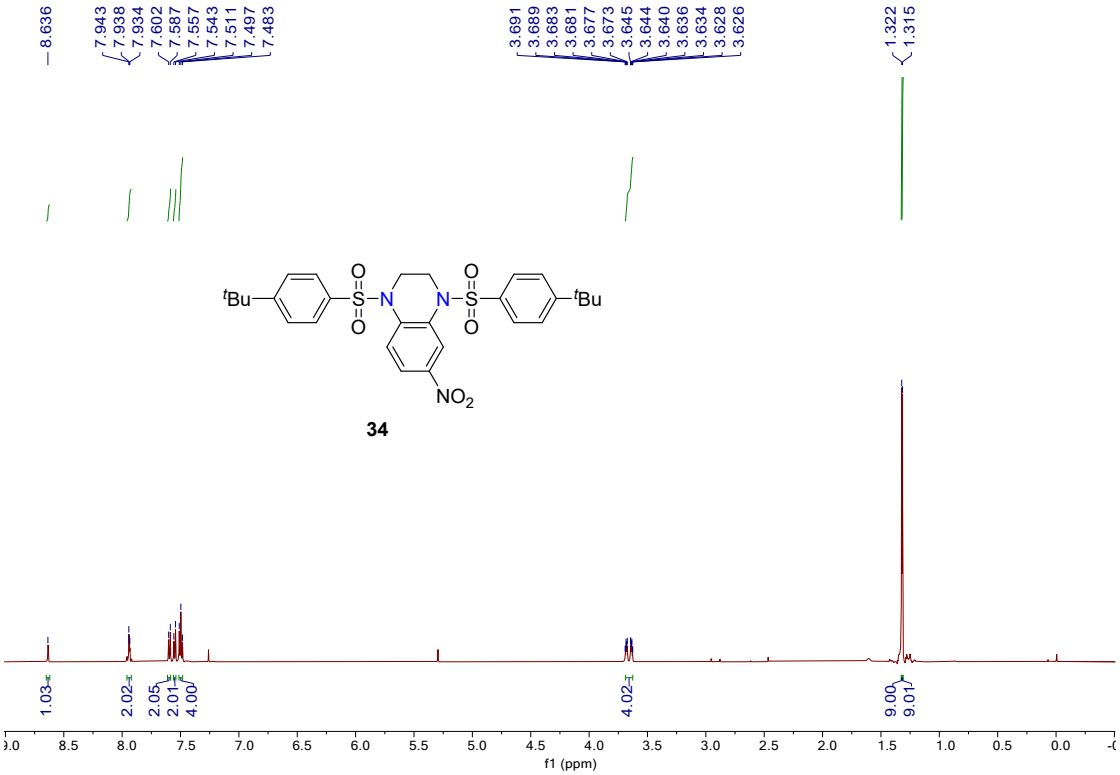
32


8.674
7.985
7.969
7.928
7.913
7.511
7.498
7.468
7.455
7.264
7.260
7.254
7.250
7.241
3.644
3.634
3.614
3.604
2.422
Ts
N
O2N
N
Ts
1.00
1.04
1.03
4.00
4.05
4.06
6.51
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)

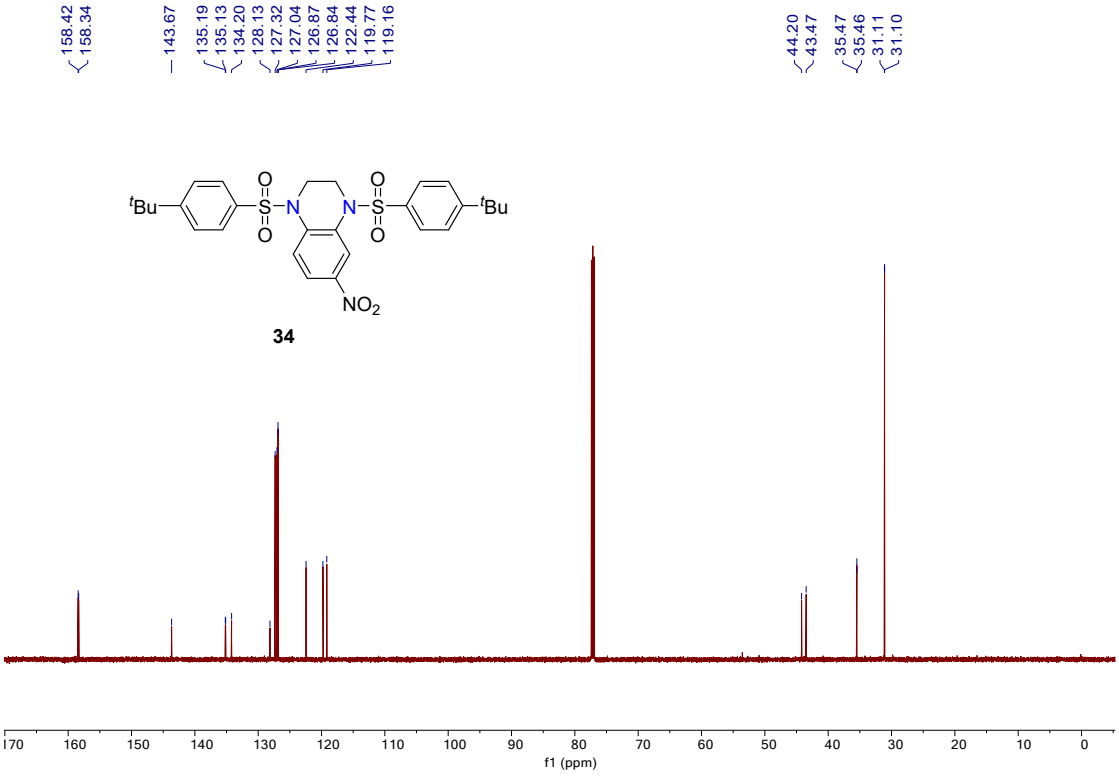
33

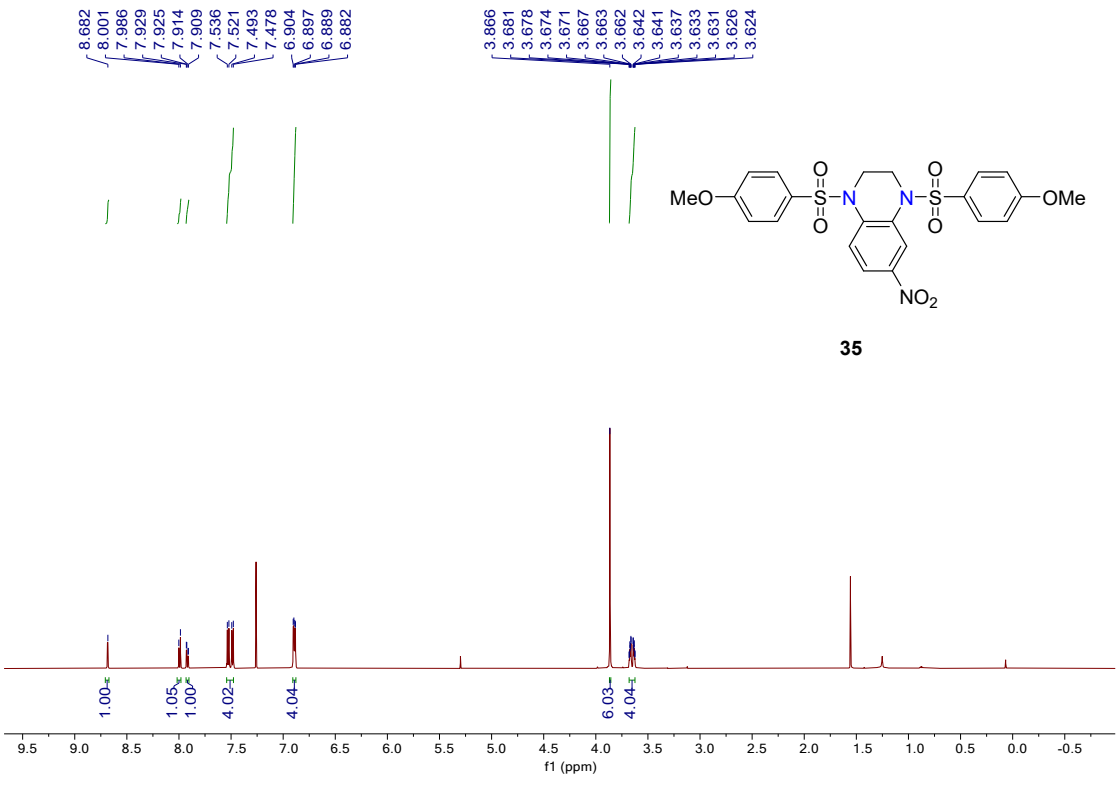

145.37
145.23
143.72
135.14
135.06
133.85
130.34
130.33
128.00
127.41
127.16
122.53
119.66
119.00
43.85
43.22
21.73
Ts
N
O2N
N
Ts
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

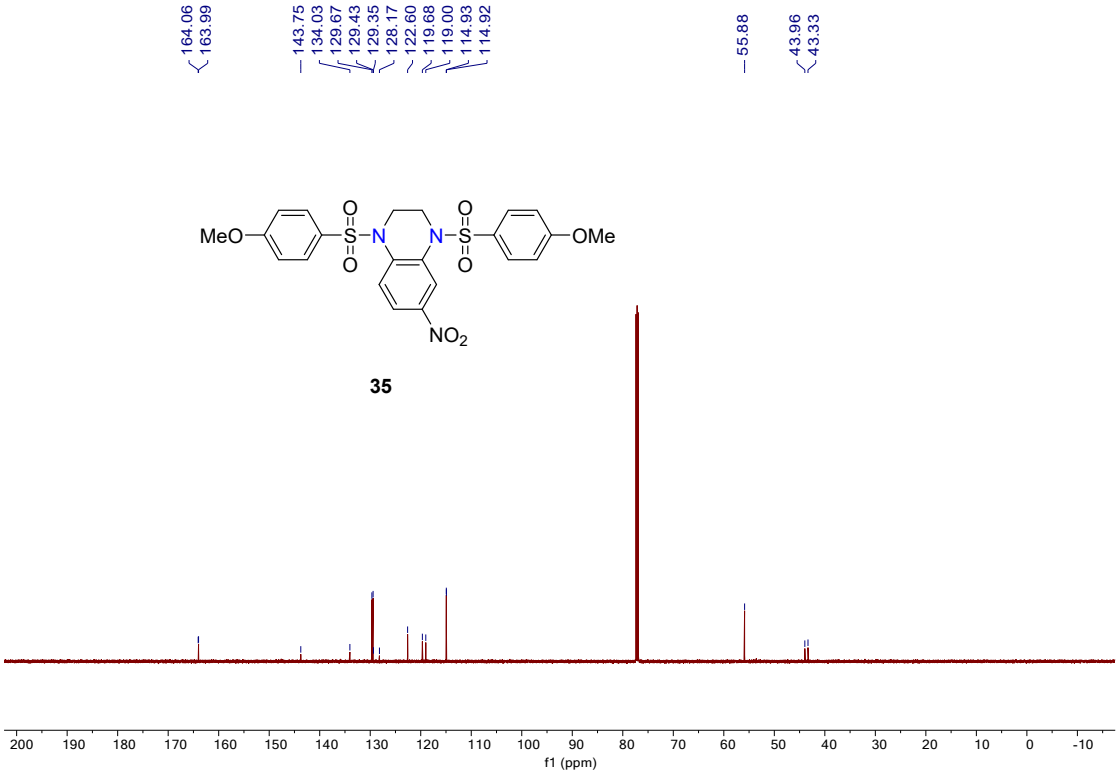
33

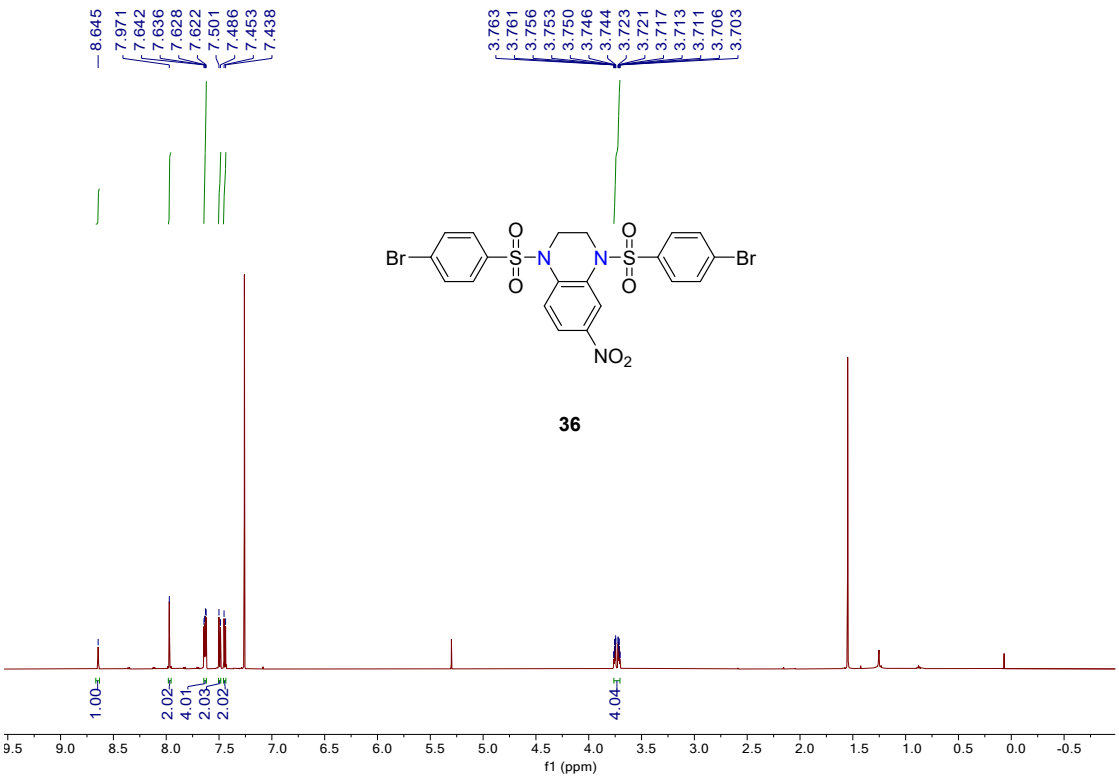

8.636
7.943
7.938
7.934
7.602
7.587
7.557
7.543
7.511
7.497
7.483
3.691
3.689
3.683
3.681
3.677
3.673
3.645
3.644
3.640
3.636
3.634
3.628
3.626
1.322
1.315
tBu
O
S
O
N
N
O
S
O
tBu
NO2
1.03
2.02
2.05
2.01
4.00
4.02
9.00
9.01
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

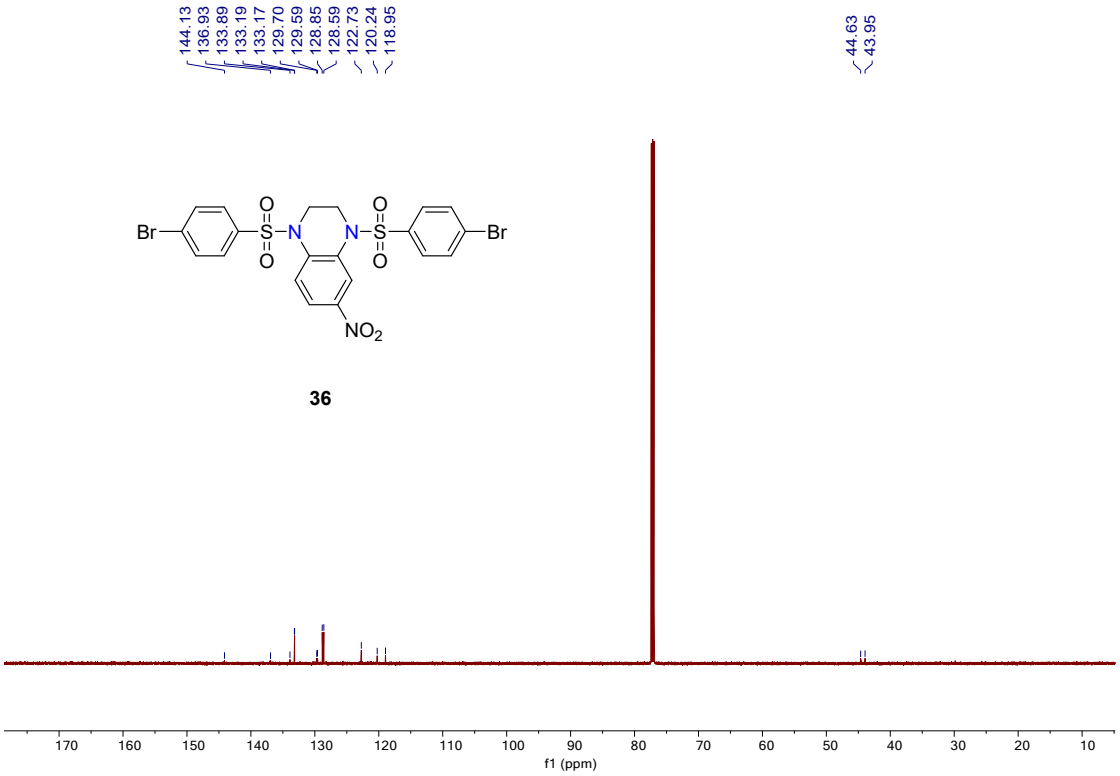
34


158.42
158.34
143.67
135.19
135.13
134.20
128.13
127.32
127.04
126.87
126.84
122.44
119.77
119.16
44.20
43.47
35.47
35.46
31.11
31.10
tBu
tBu
NO2
34
f1 (ppm)

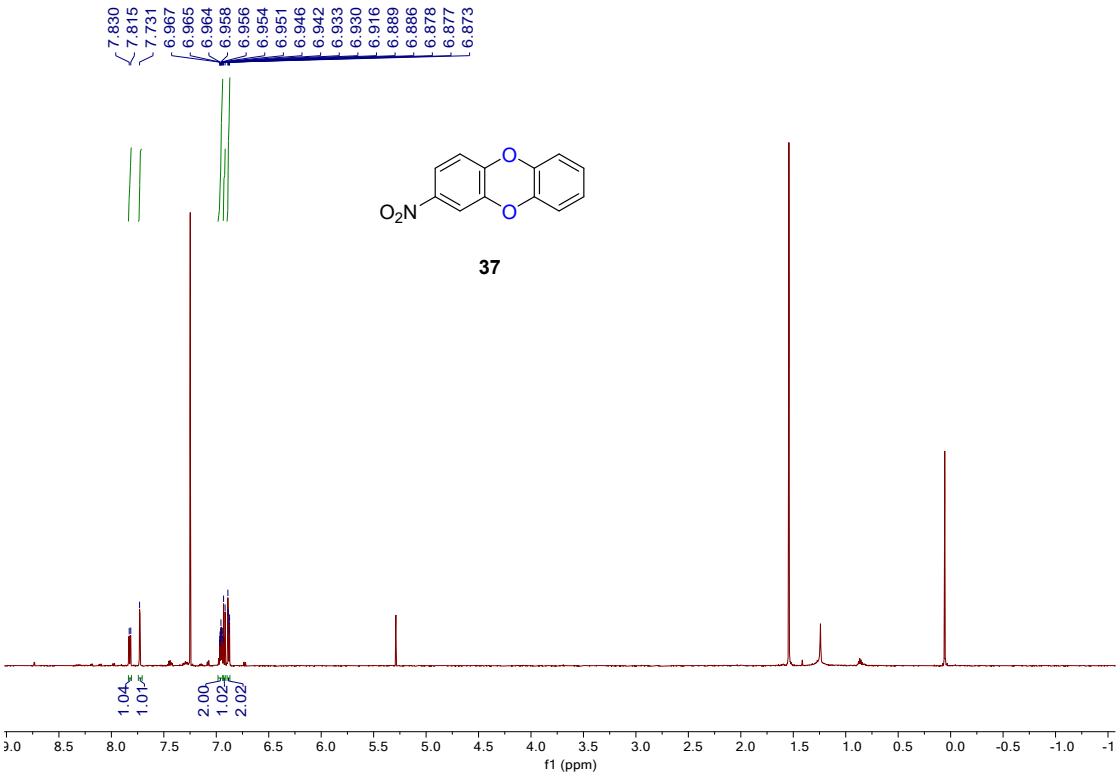

8.682
8.001
7.986
7.929
7.925
7.914
7.909
7.536
7.521
7.493
7.478
6.904
6.897
6.889
6.882
3.866
3.681
3.678
3.674
3.671
3.667
3.663
3.662
3.642
3.641
3.637
3.633
3.631
3.626
3.624
MeO
OMe
NO2
35
1.00
1.05
1.00
4.02
4.04
6.03
4.04
f1 (ppm)


164.06
163.99
143.75
134.03
129.67
129.43
129.35
128.17
122.60
119.68
119.00
114.93
114.92
55.88
43.96
43.33
MeO
OMe
NO2
35
200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)

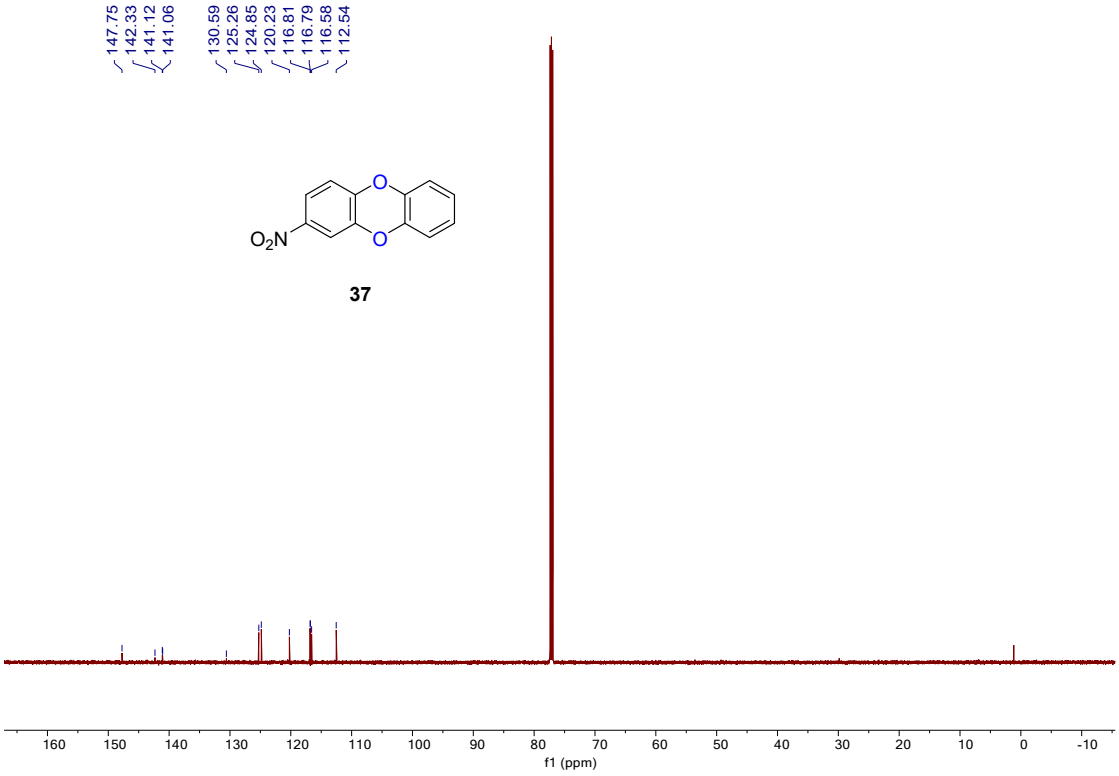

8.645
7.971
7.642
7.636
7.628
7.622
7.501
7.486
7.453
7.438
3.763
3.761
3.756
3.753
3.750
3.746
3.744
3.723
3.721
3.717
3.713
3.711
3.706
3.703
Br
Br
NO2
36
1.00
2.02
4.01
2.03
2.02
4.04
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5
f1 (ppm)


144.13
136.93
133.89
133.19
133.17
129.70
129.59
128.85
128.59
122.73
120.24
118.95
44.63
43.95
Br
Br
NO2
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

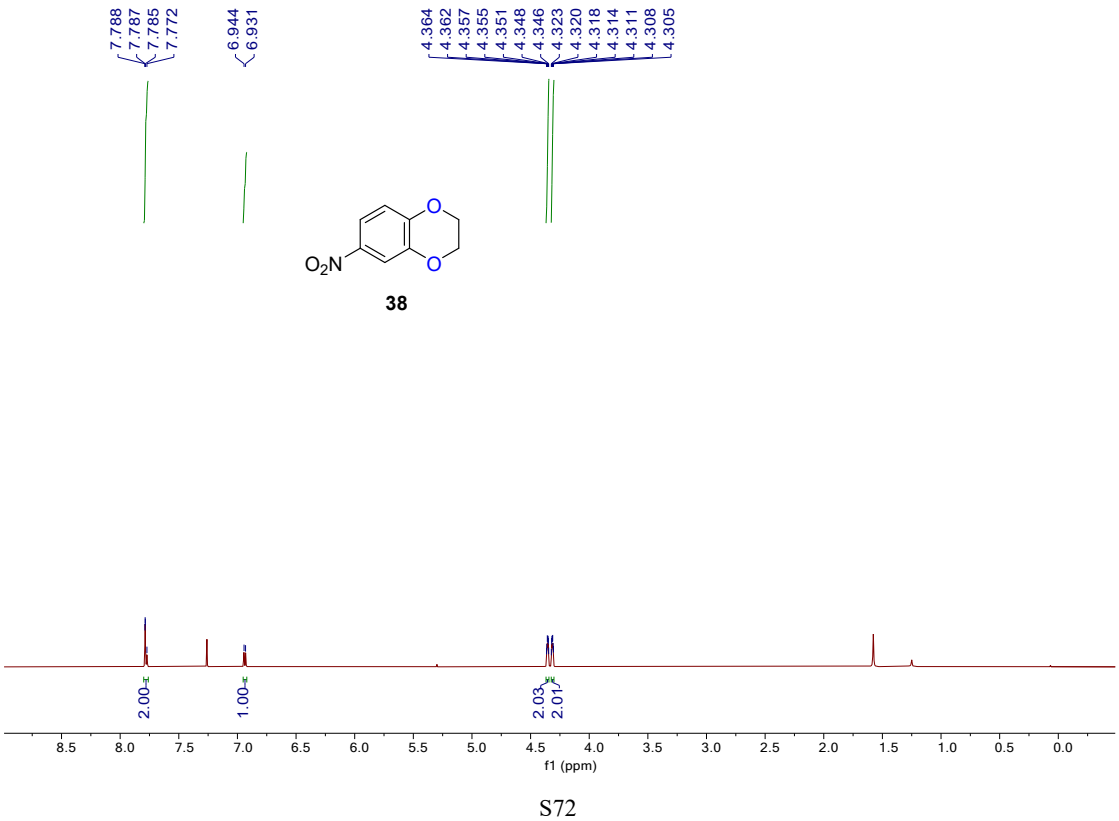
36


7.830
7.815
7.731
6.967
6.965
6.964
6.958
6.956
6.954
6.951
6.946
6.942
6.933
6.930
6.916
6.889
6.886
6.878
6.877
6.873
O2N
1.04
1.01
2.00
1.02
2.02
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
-0.5
-1.0
-1
f1 (ppm)

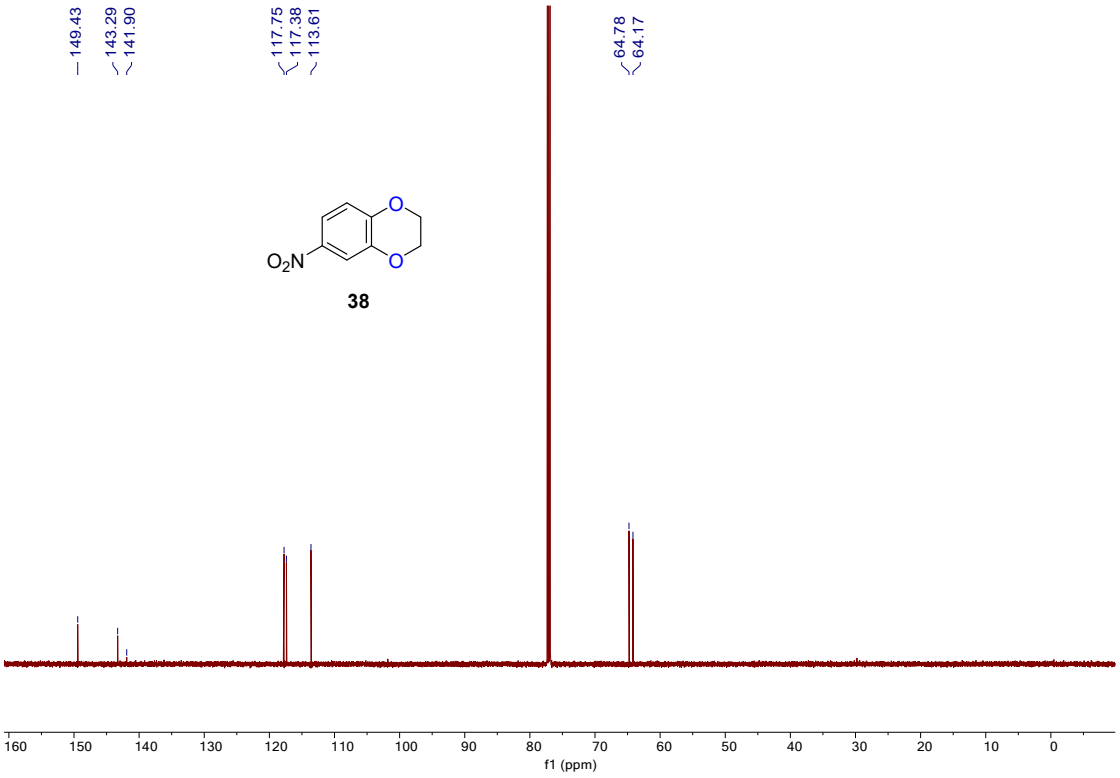
37


147.75
142.33
141.12
141.06
130.59
125.26
124.85
120.23
116.81
116.79
116.58
112.54
O
O
O2N
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

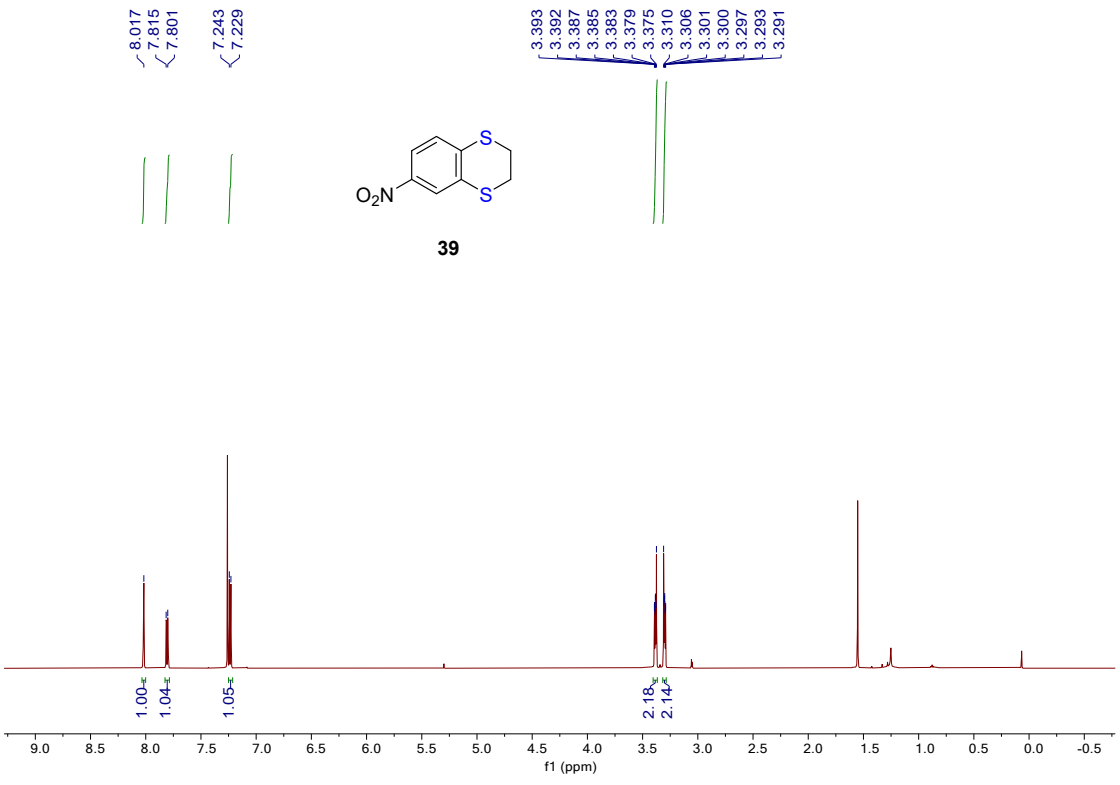
37


7.788
7.787
7.785
7.772
6.944
6.931
4.364
4.362
4.357
4.355
4.351
4.348
4.346
4.323
4.320
4.318
4.314
4.311
4.308
4.305
O
O
O2N
2.00
1.00
2.03
2.01
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)

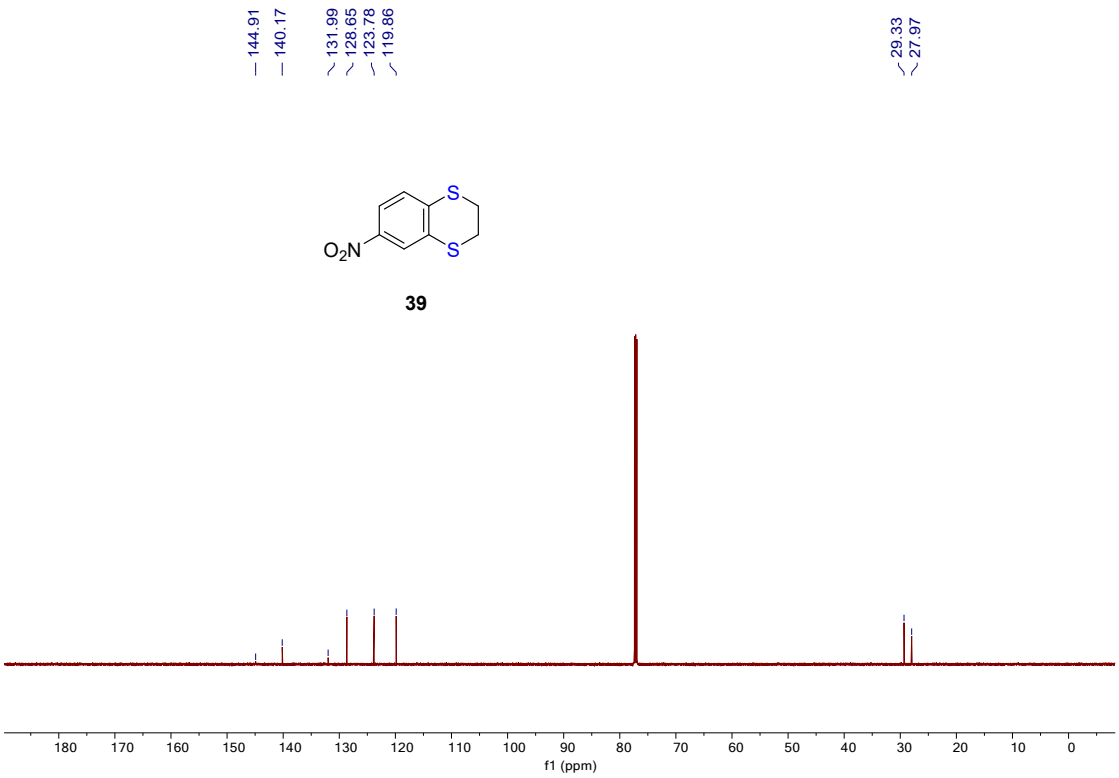
38

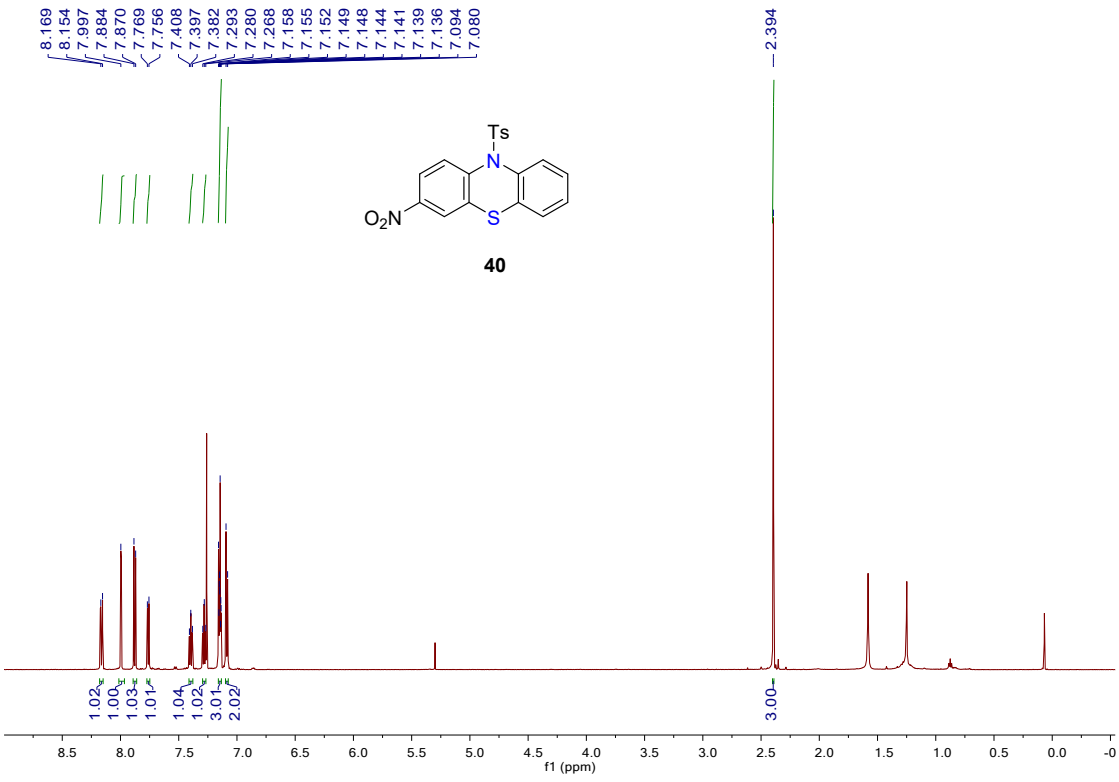

149.43
143.29
141.90
117.75
117.38
113.61
64.78
64.17
O2N
O
O
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

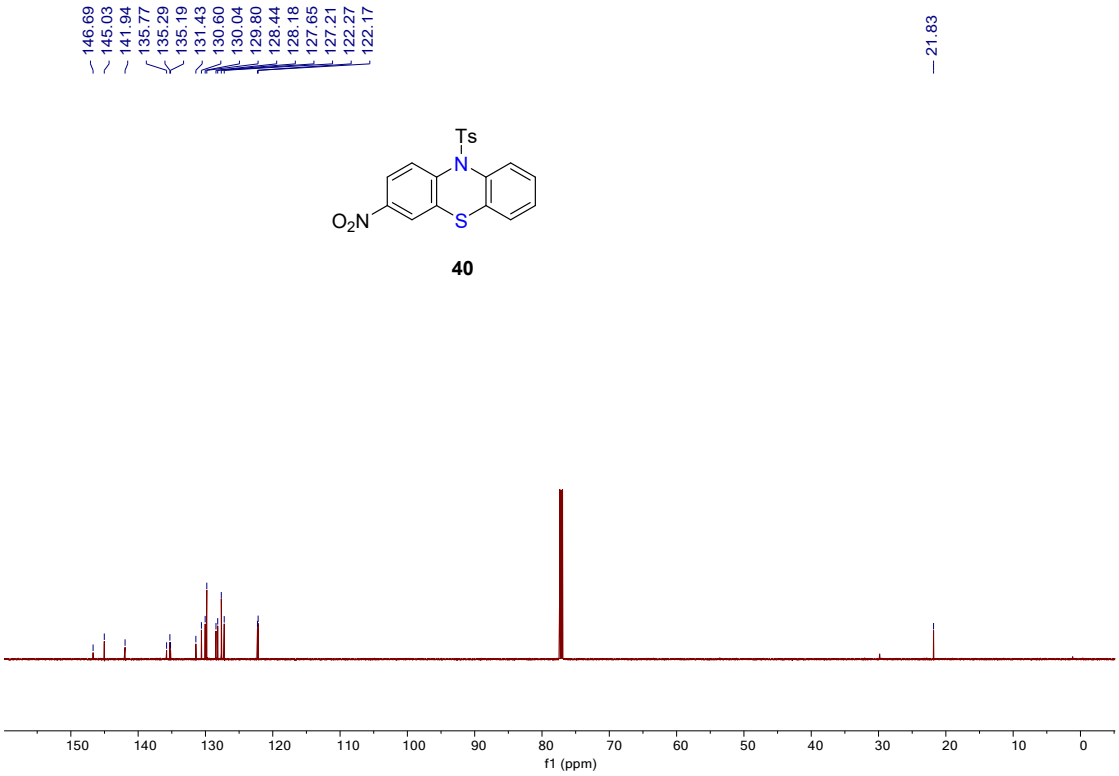
38


8.017
7.815
7.801
7.243
7.229
3.393
3.392
3.387
3.385
3.383
3.379
3.375
3.310
3.306
3.301
3.300
3.297
3.293
3.291
O2N
S
S
1.00
1.04
1.05
2.18
2.14
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)

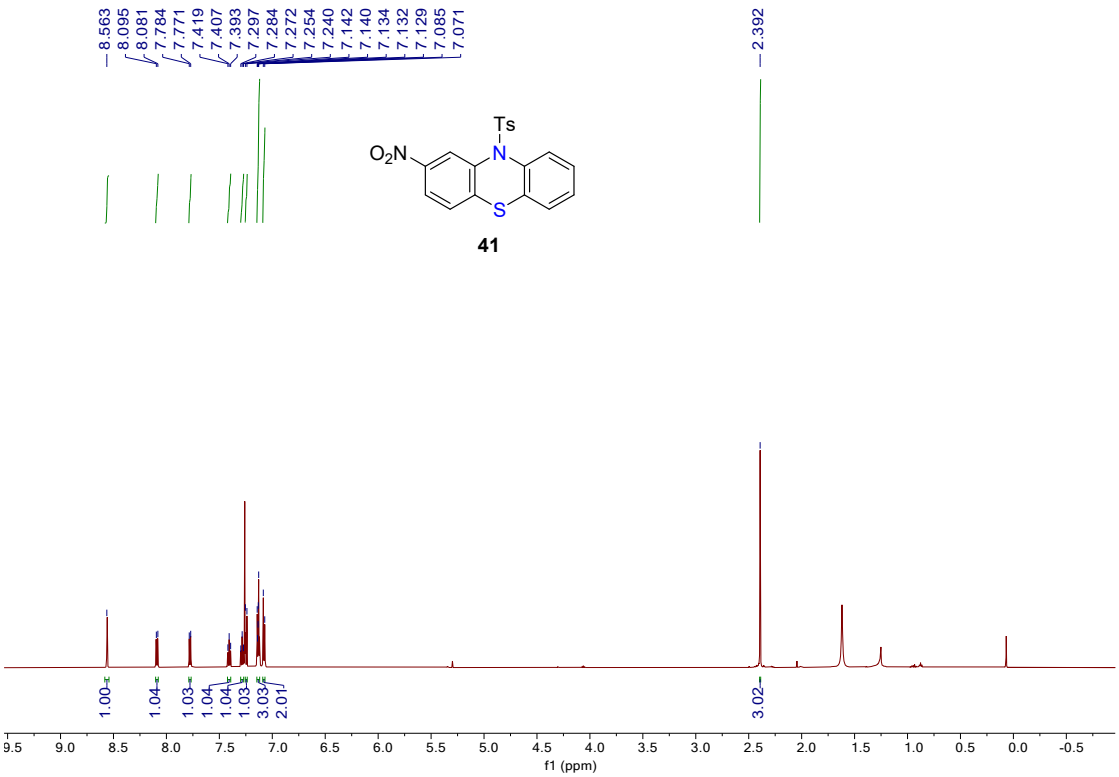
39


144.91
140.17
131.99
128.65
123.78
119.86
29.33
27.97
S
S
O2N
39
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

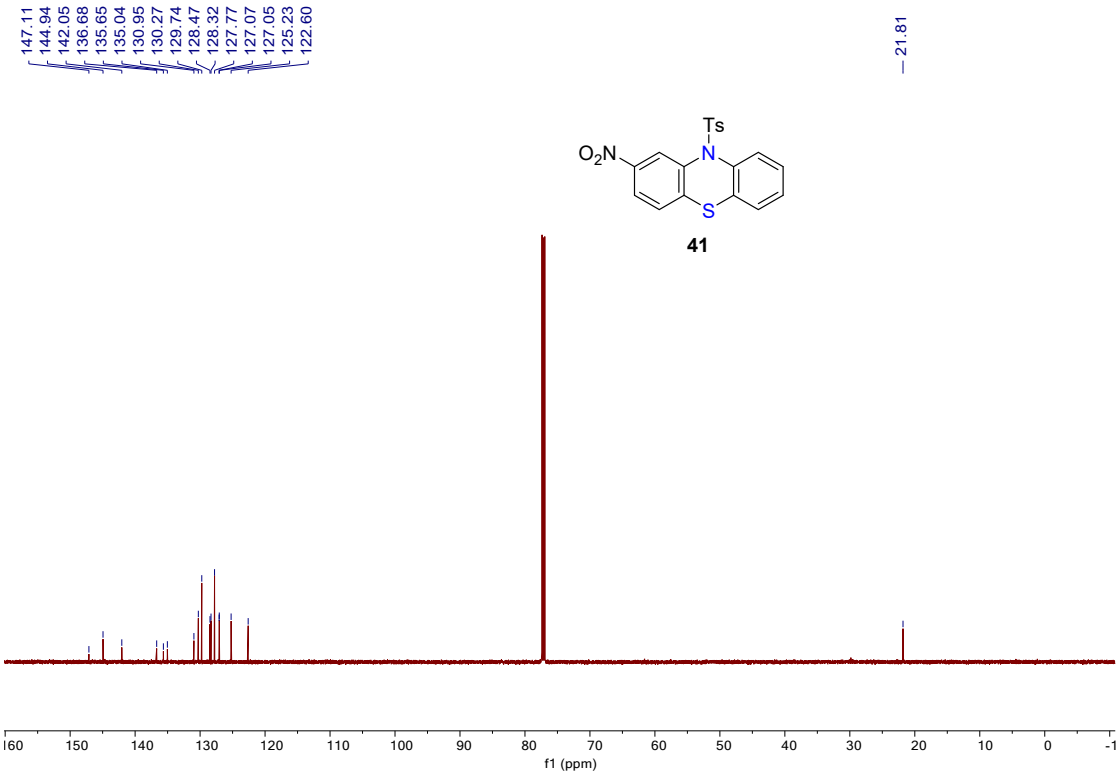

8.169
8.154
7.997
7.884
7.870
7.769
7.756
7.408
7.397
7.382
7.293
7.280
7.268
7.158
7.155
7.152
7.149
7.148
7.144
7.141
7.139
7.136
7.094
7.080
2.394
Ts
N
S
O2N
40
1.02
1.00
1.03
1.01
1.04
1.02
3.01
2.02
3.00
8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0
f1 (ppm)

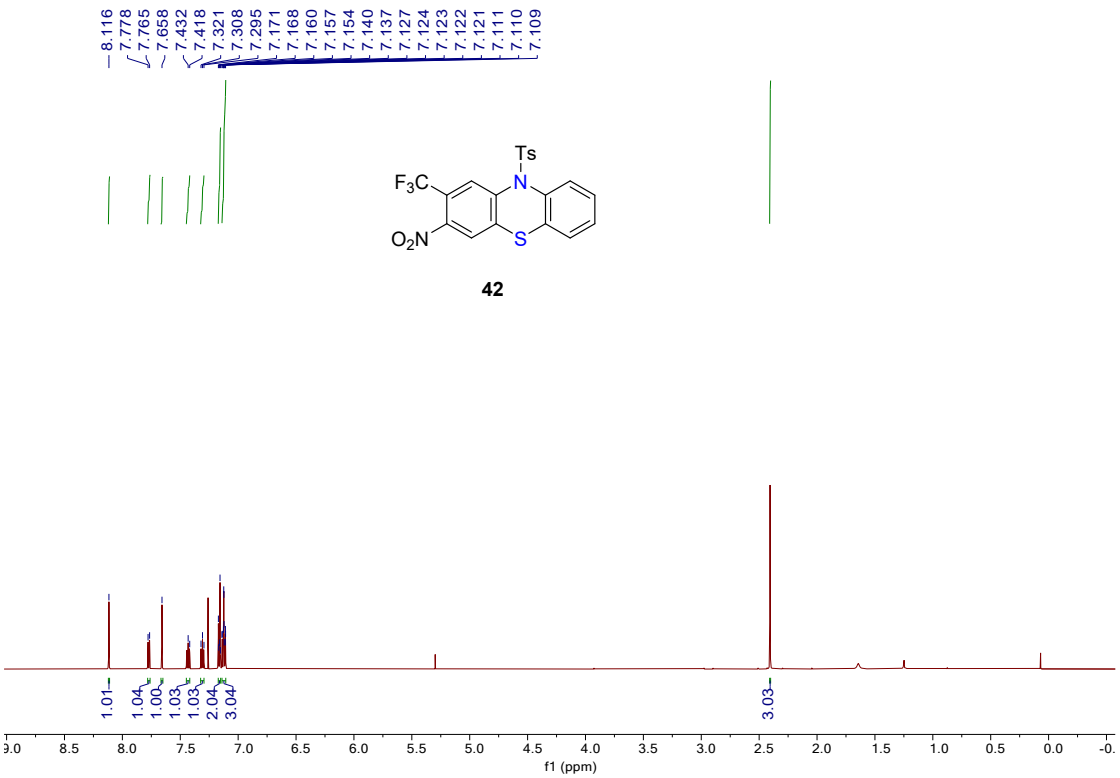

146.69
145.03
141.94
135.77
135.29
135.19
131.43
130.60
130.04
129.80
128.44
128.18
127.65
127.21
122.27
122.17
21.83
Ts
N
S
O2N
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

40


8.563
8.095
8.081
7.784
7.771
7.419
7.407
7.393
7.297
7.284
7.272
7.254
7.240
7.142
7.140
7.134
7.132
7.129
7.085
7.071
2.392
Ts
N
S
O2N
1.00
1.04
1.03
1.04
1.04
1.03
3.03
2.01
3.02
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)

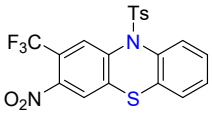
41


147.11
144.94
142.05
136.68
135.65
135.04
130.95
130.27
129.74
128.47
128.32
127.77
127.07
127.05
125.23
122.60
21.81
Ts
O2N
N
S
41
f1 (ppm)

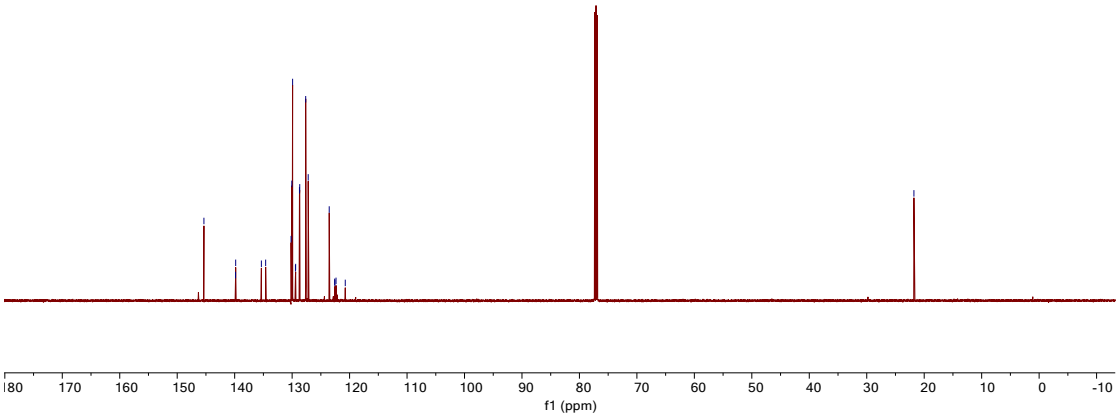

8.116
7.778
7.765
7.658
7.432
7.418
7.321
7.308
7.295
7.171
7.168
7.160
7.157
7.154
7.140
7.137
7.127
7.124
7.123
7.122
7.121
7.111
7.110
7.109
Ts
F3C
O2N
N
S
42
1.01
1.04
1.00
1.03
1.03
2.04
3.04
3.03
f1 (ppm)


145.35
139.85
139.82
135.35
134.61
130.18
130.05
129.92
129.42
129.39
128.72
128.68
127.64
127.20
123.54
122.59
122.56
122.36
120.75

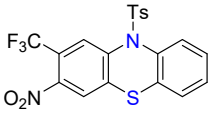

21.79


Ts
F3C
N
O2N
S

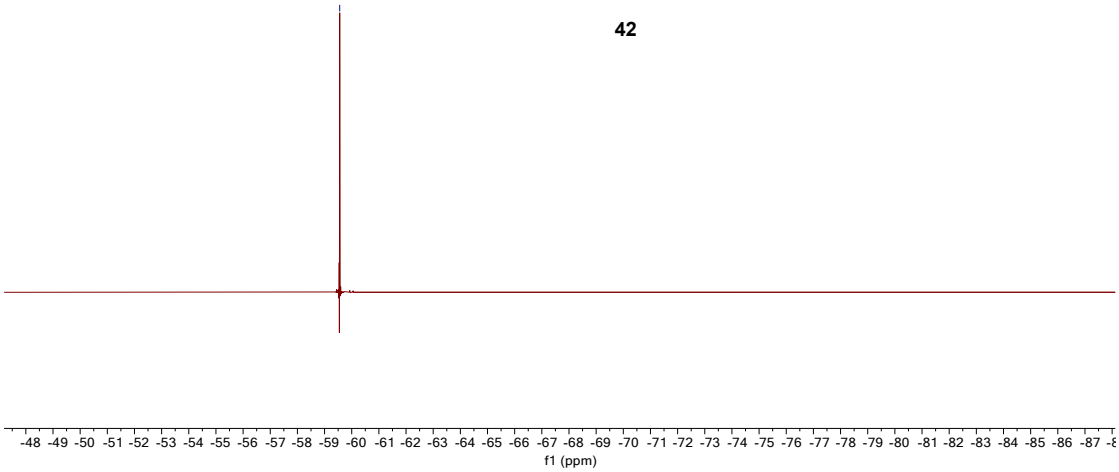
42

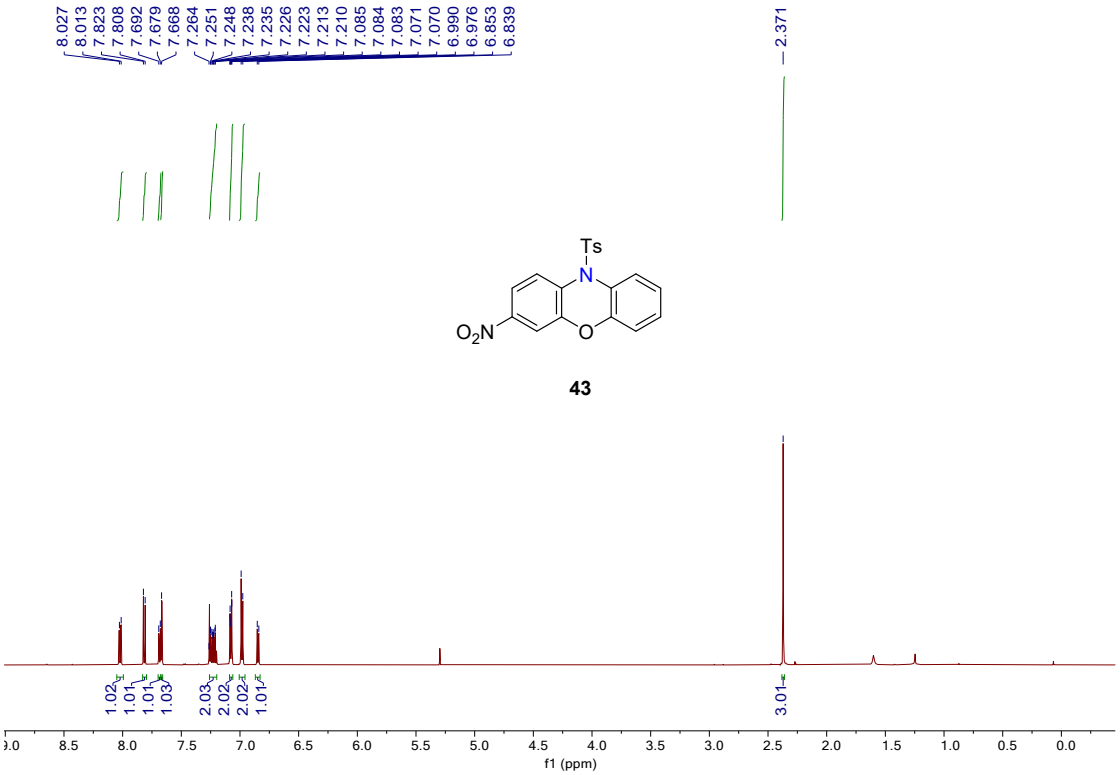

180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)


-59.557

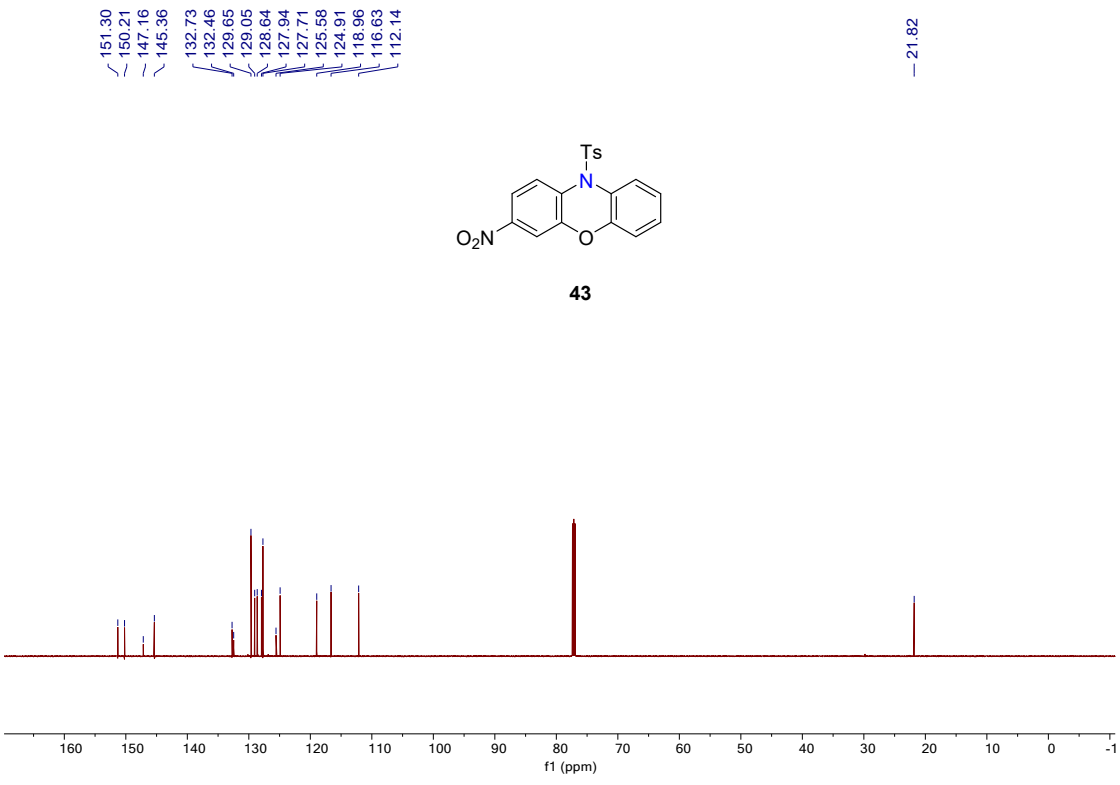

Ts
F3C
N
O2N
S

42

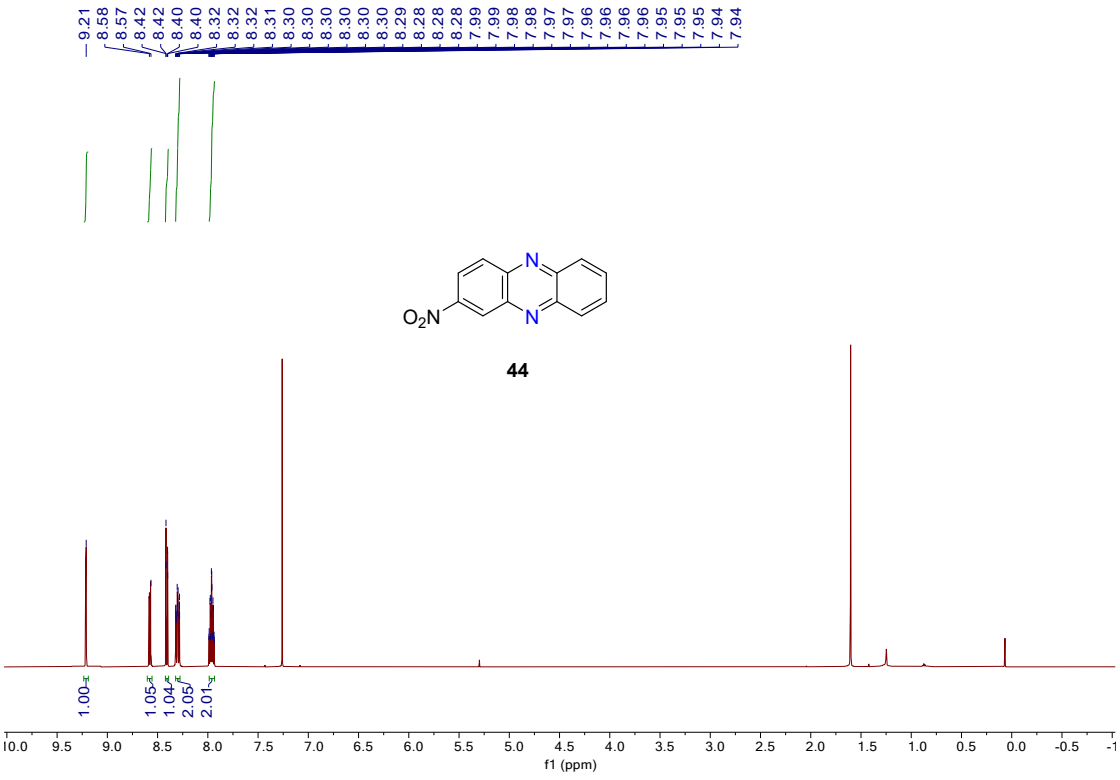

-48 -49 -50 -51 -52 -53 -54 -55 -56 -57 -58 -59 -60 -61 -62 -63 -64 -65 -66 -67 -68 -69 -70 -71 -72 -73 -74 -75 -76 -77 -78 -79 -80 -81 -82 -83 -84 -85 -86 -87
f1 (ppm)


8.027
8.013
7.823
7.808
7.692
7.679
7.668
7.264
7.251
7.248
7.238
7.235
7.226
7.223
7.213
7.210
7.085
7.084
7.083
7.071
7.070
6.990
6.976
6.853
6.839
2.371
Ts
N
O2N
O
1.02
1.01
1.01
1.03
2.03
2.02
2.02
1.01
3.01
f1 (ppm)

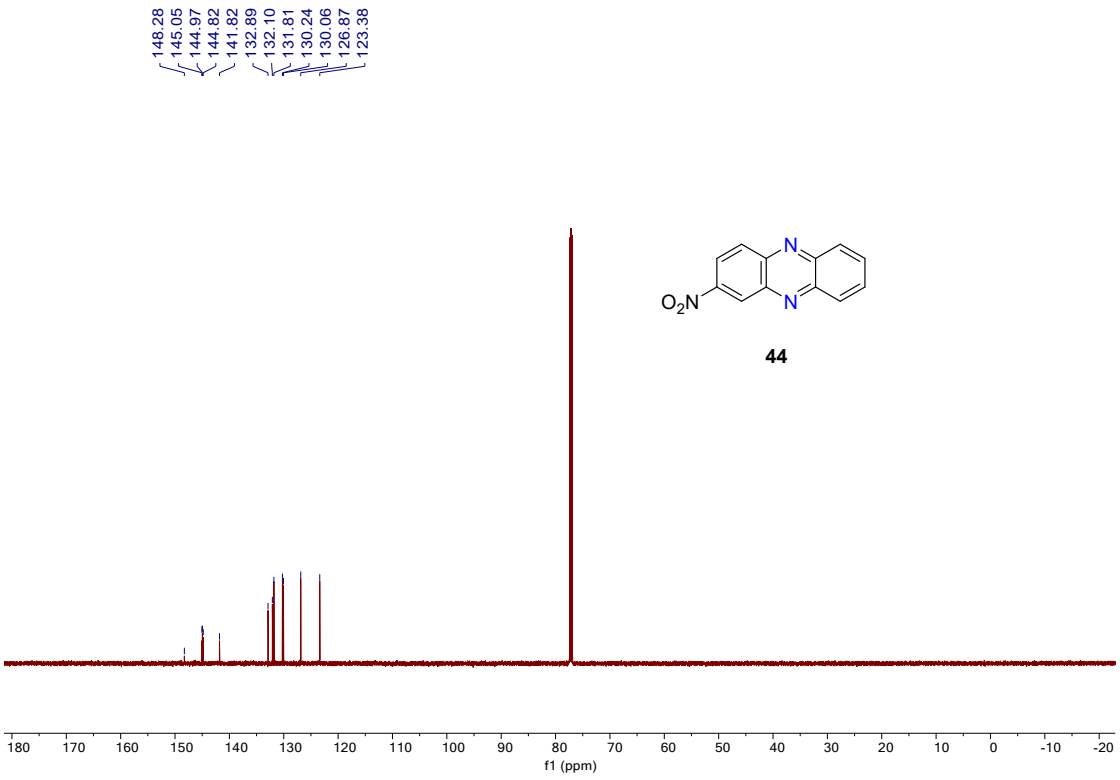
43


151.30
150.21
147.16
145.36
132.73
132.46
129.65
129.05
128.64
127.94
127.71
125.58
124.91
118.96
116.63
112.14
21.82
Ts
N
O2N
O
f1 (ppm)

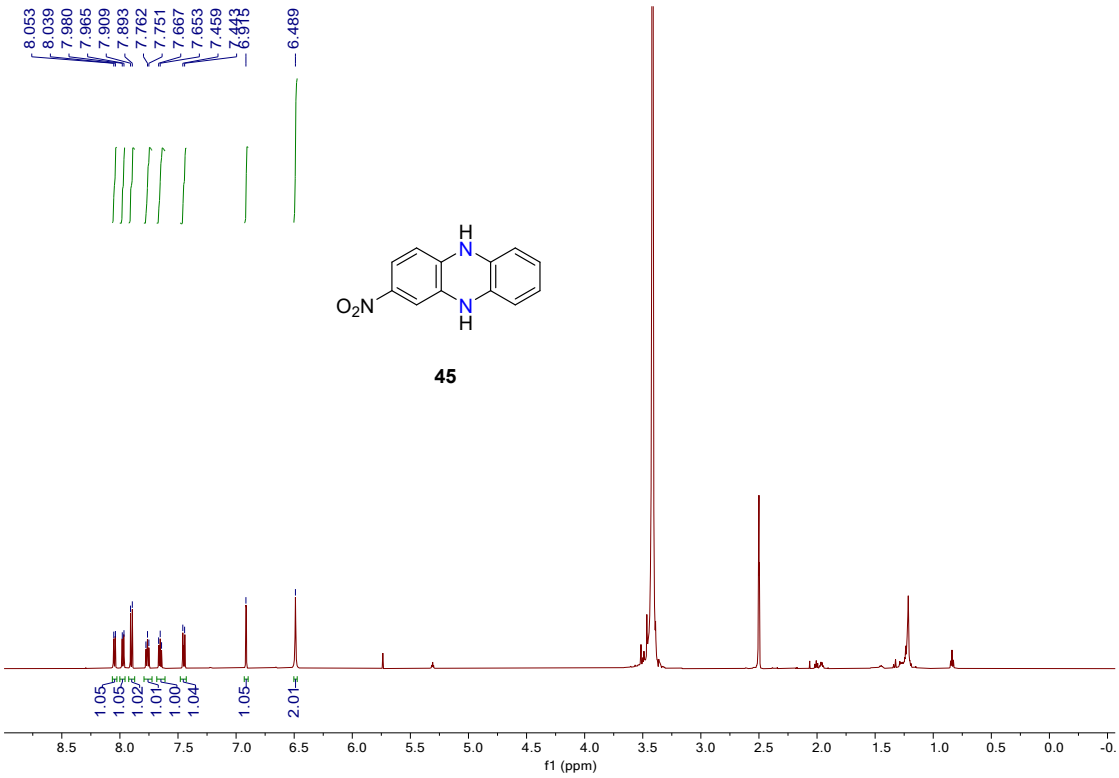
43

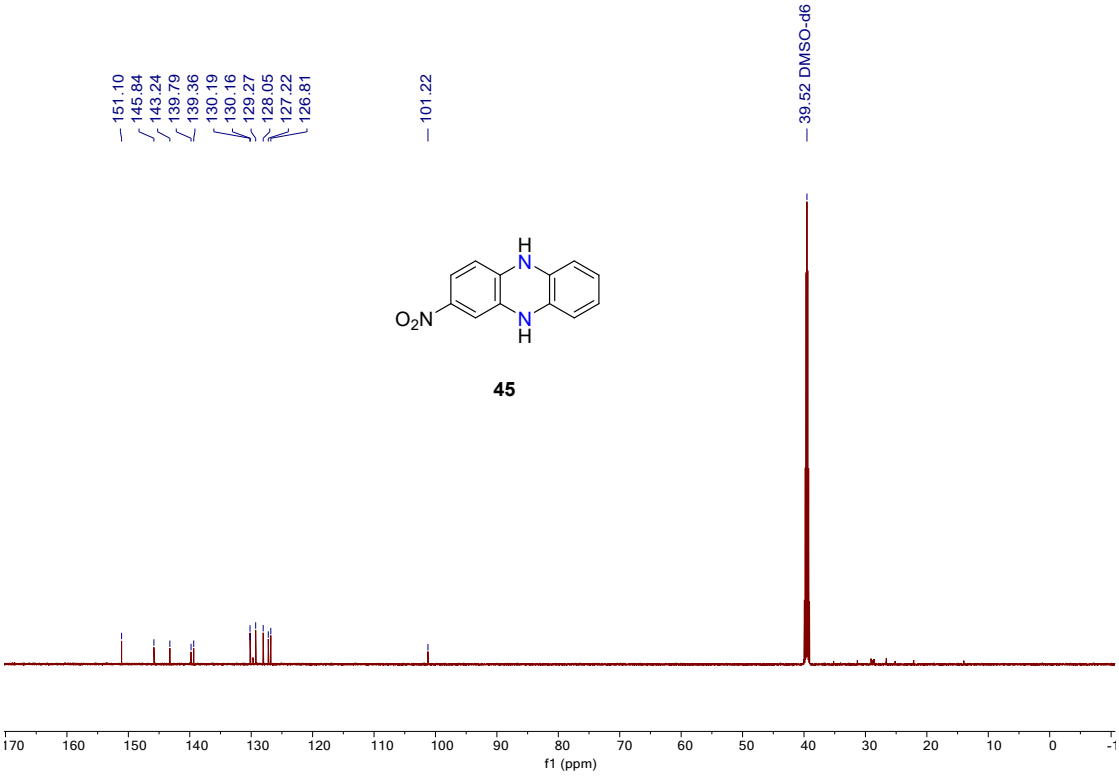

9.21
8.58
8.57
8.42
8.42
8.40
8.40
8.32
8.32
8.31
8.30
8.30
8.30
8.30
8.30
8.29
8.28
8.28
8.28
7.99
7.99
7.98
7.98
7.97
7.97
7.96
7.96
7.96
7.96
7.95
7.95
7.95
7.94
7.94
N
N
O2N
1.00
1.05
1.04
2.05
2.01
f1 (ppm)

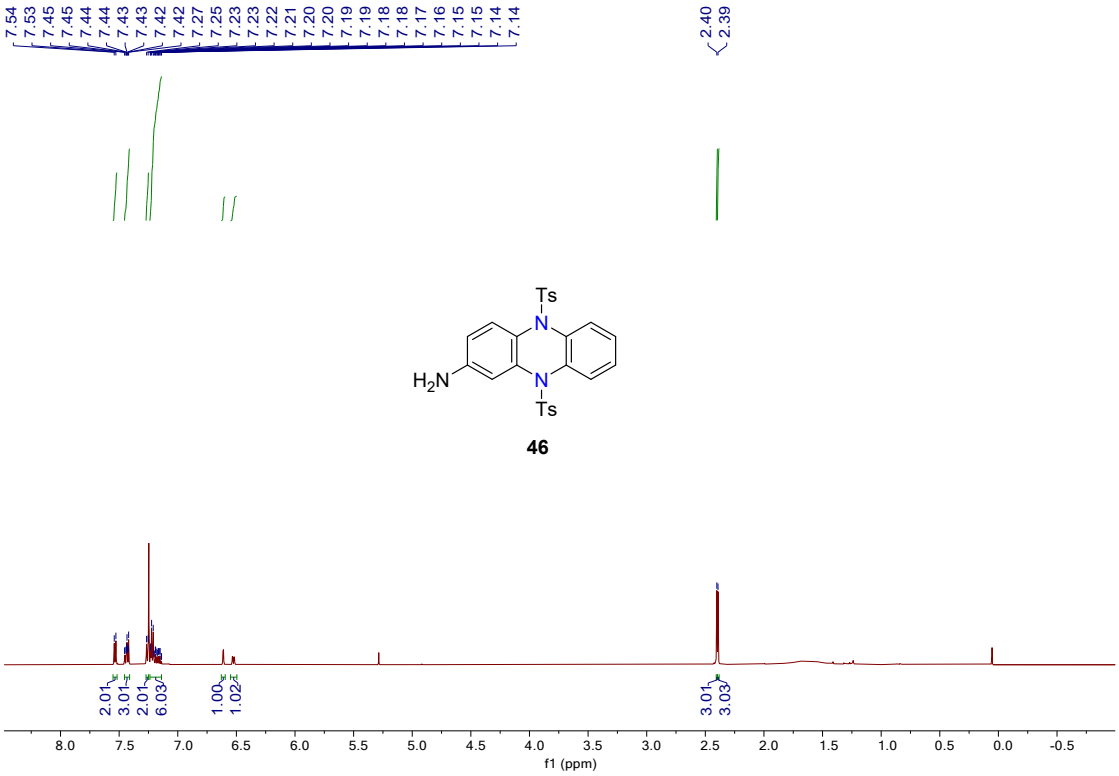
44


148.28
145.05
144.97
144.82
141.82
132.89
132.10
131.81
130.24
130.06
126.87
123.38
N
N
O2N
f1 (ppm)

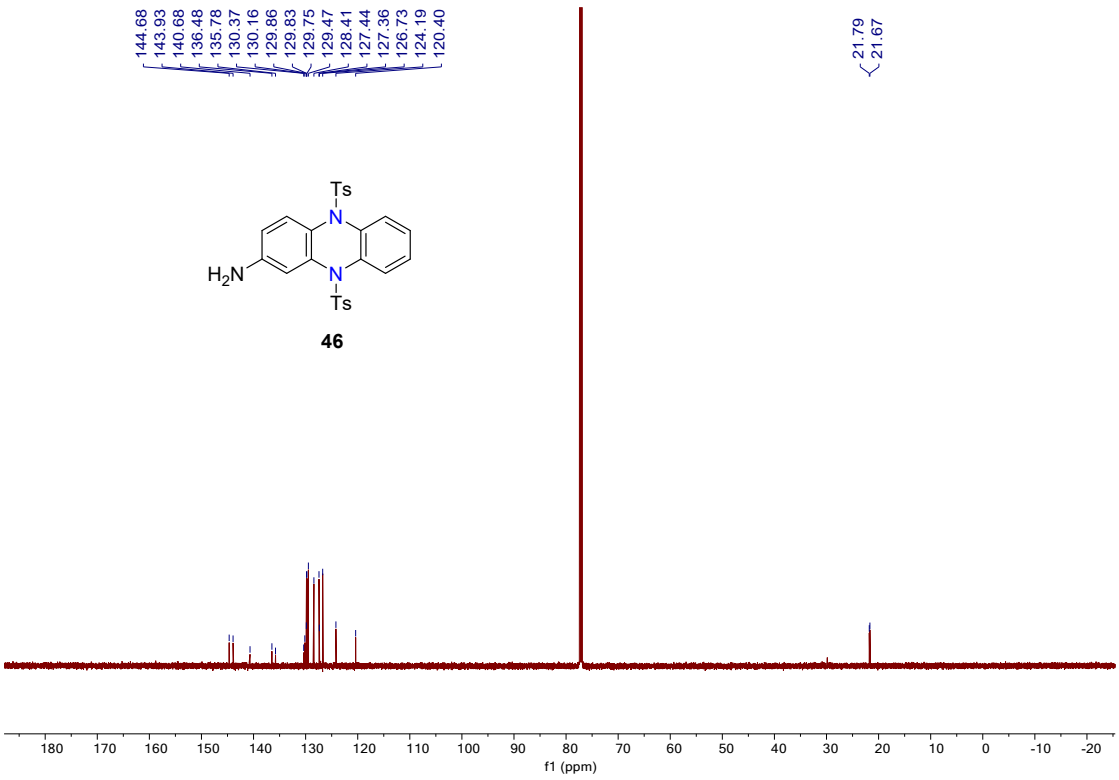
44


8.053
8.039
7.980
7.965
7.909
7.893
7.762
7.751
7.667
7.653
7.459
7.443
6.915
6.489
H
N
O2N
N
H
45
1.05
1.05
1.02
1.01
1.00
1.04
1.05
2.01
f1 (ppm)

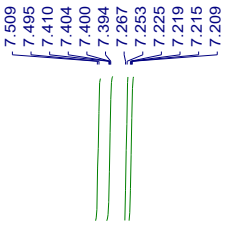

151.10
145.84
143.24
139.79
139.36
130.19
130.16
129.27
128.05
127.22
126.81
101.22
39.52 DMSO-d6
H
N
O2N
N
H
45
f1 (ppm)

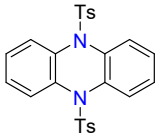

7.54
7.53
7.45
7.45
7.44
7.44
7.43
7.43
7.42
7.42
7.27
7.25
7.23
7.23
7.22
7.21
7.20
7.20
7.19
7.19
7.18
7.18
7.17
7.16
7.15
7.15
7.14
7.14
2.40
2.39
Ts
N
H2N
N
Ts
2.01
3.01
2.01
6.03
1.00
1.02
3.01
3.03
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f1 (ppm)

46

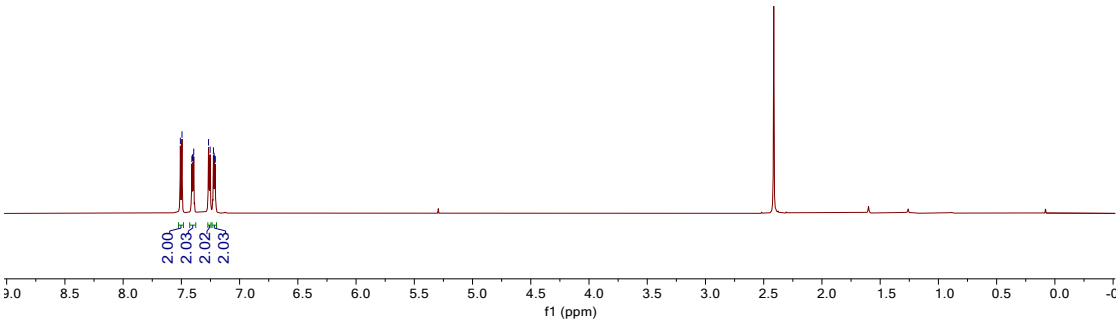

144.68
143.93
140.68
136.48
135.78
130.37
130.16
129.86
129.83
129.75
129.47
128.41
127.44
127.36
126.73
124.19
120.40
21.79
21.67
Ts
N
H2N
N
Ts
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
-20
f1 (ppm)

46

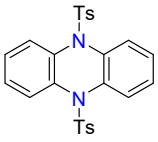

7.509
7.495
7.410
7.404
7.400
7.394
7.267
7.253
7.225
7.219
7.215
7.209


Ts
N
N
Ts

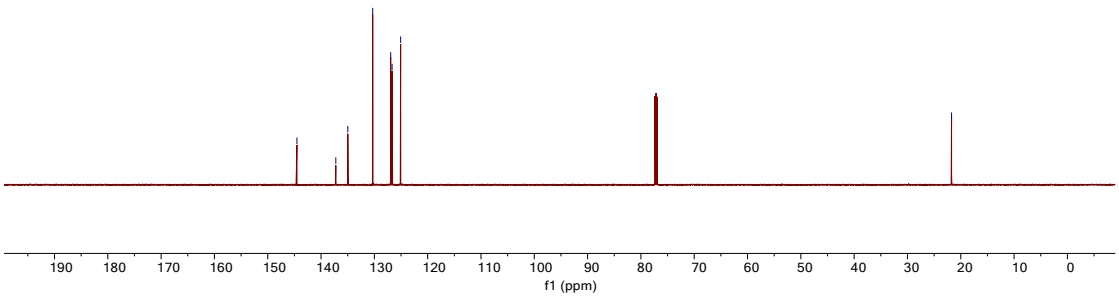
47

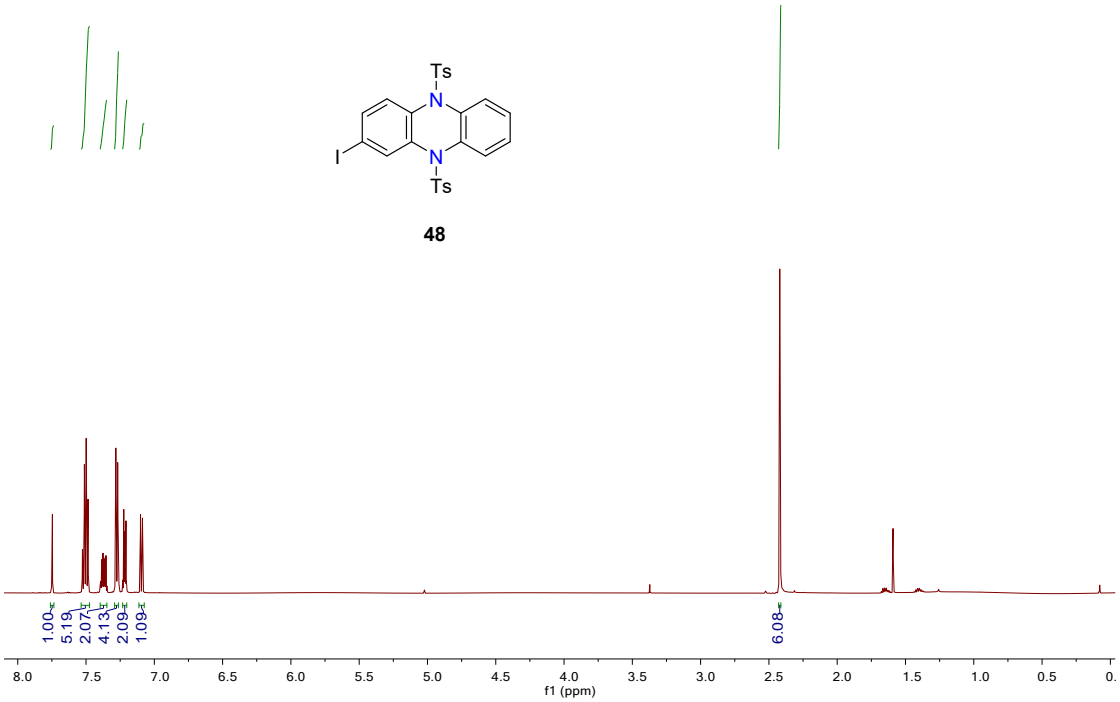

2.00
2.03
2.02
2.03
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)


144.52
137.23
134.98
130.31
126.94
126.68
125.07
21.73

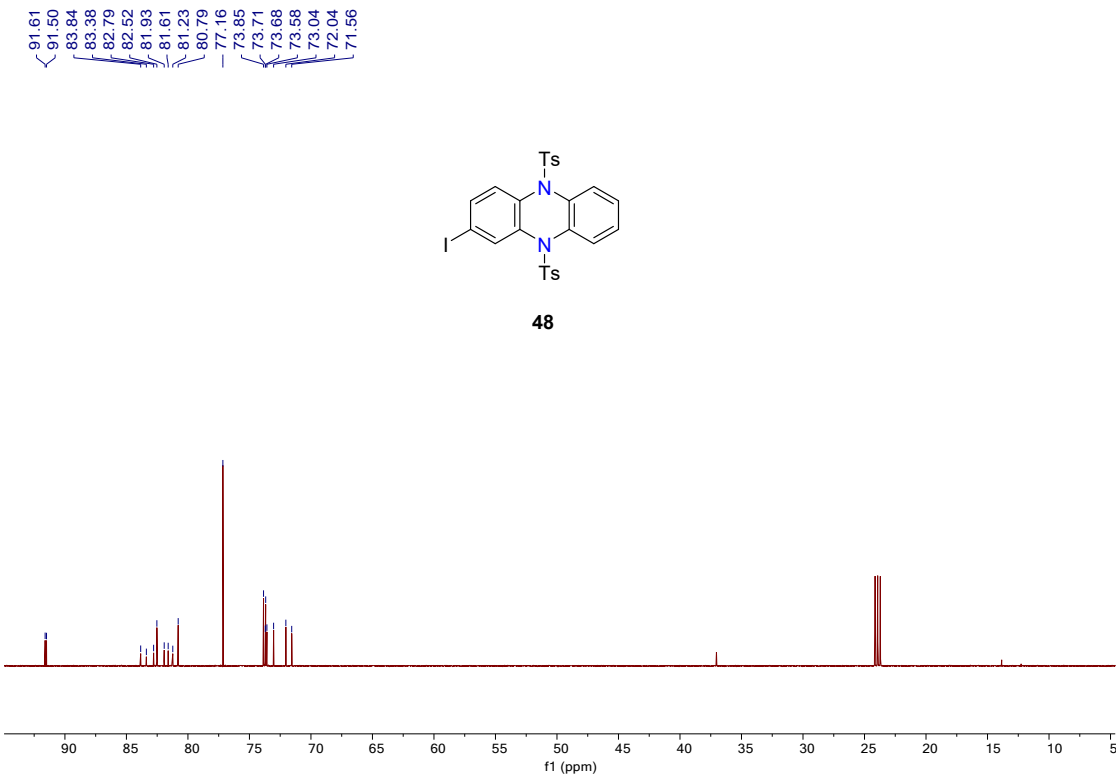

Ts
N
N
Ts

47


190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

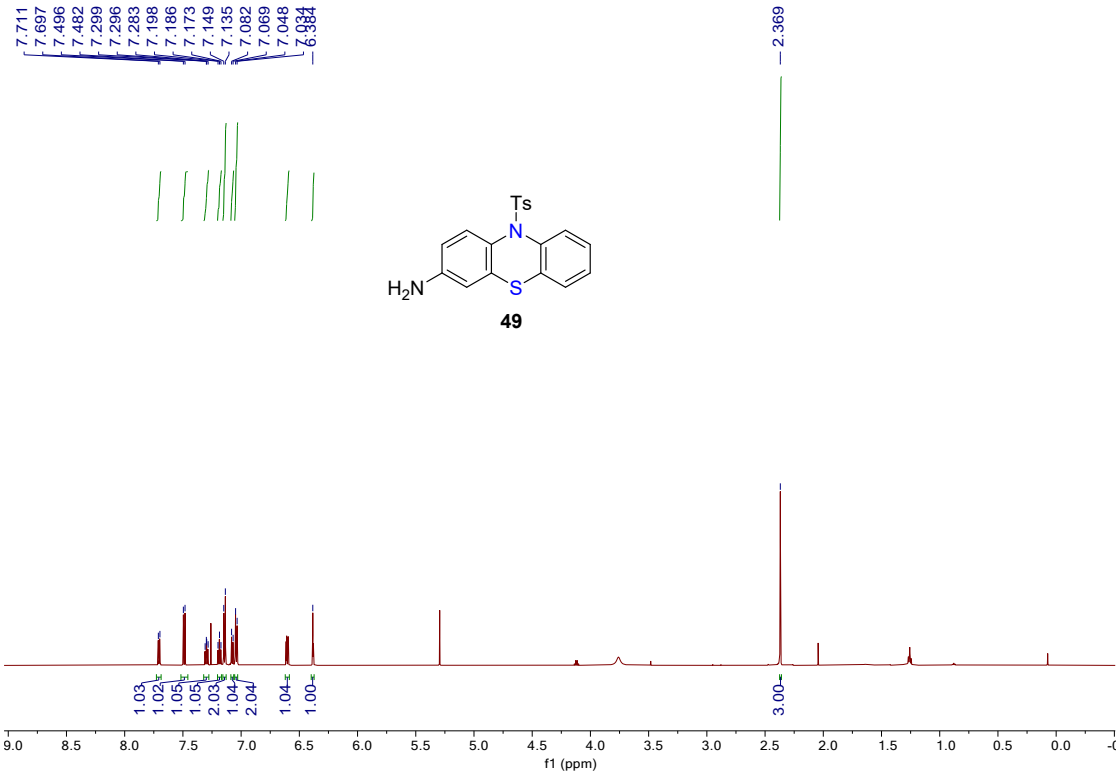


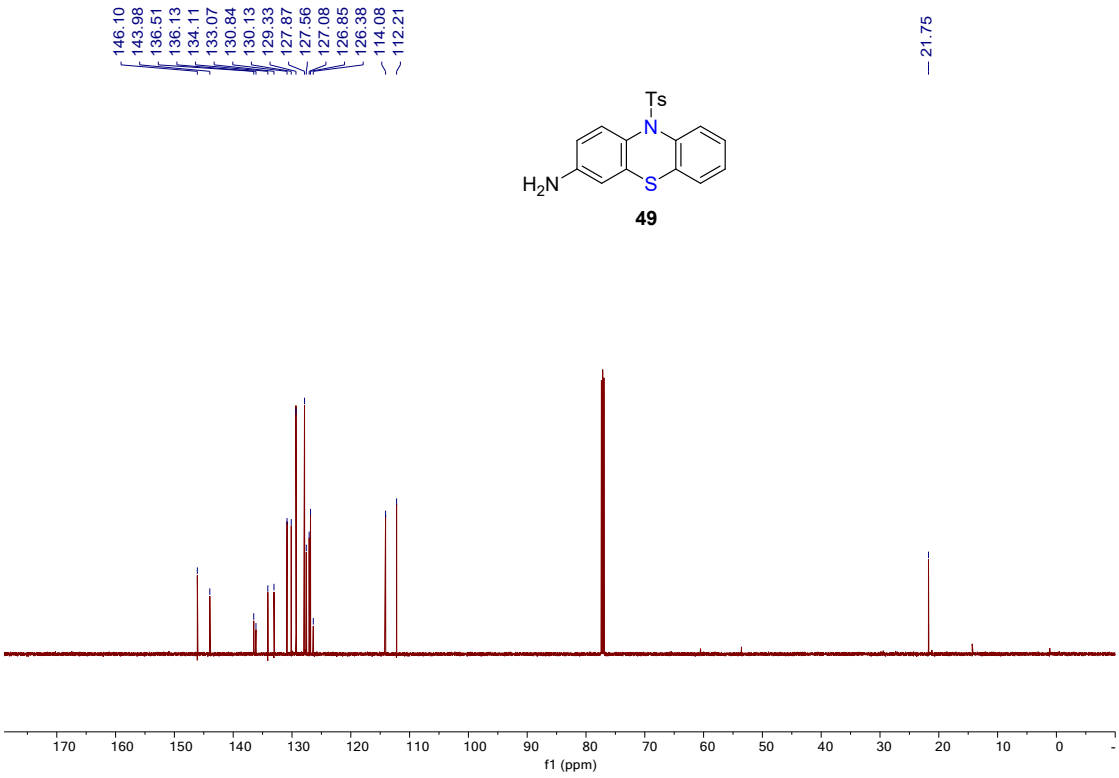
48

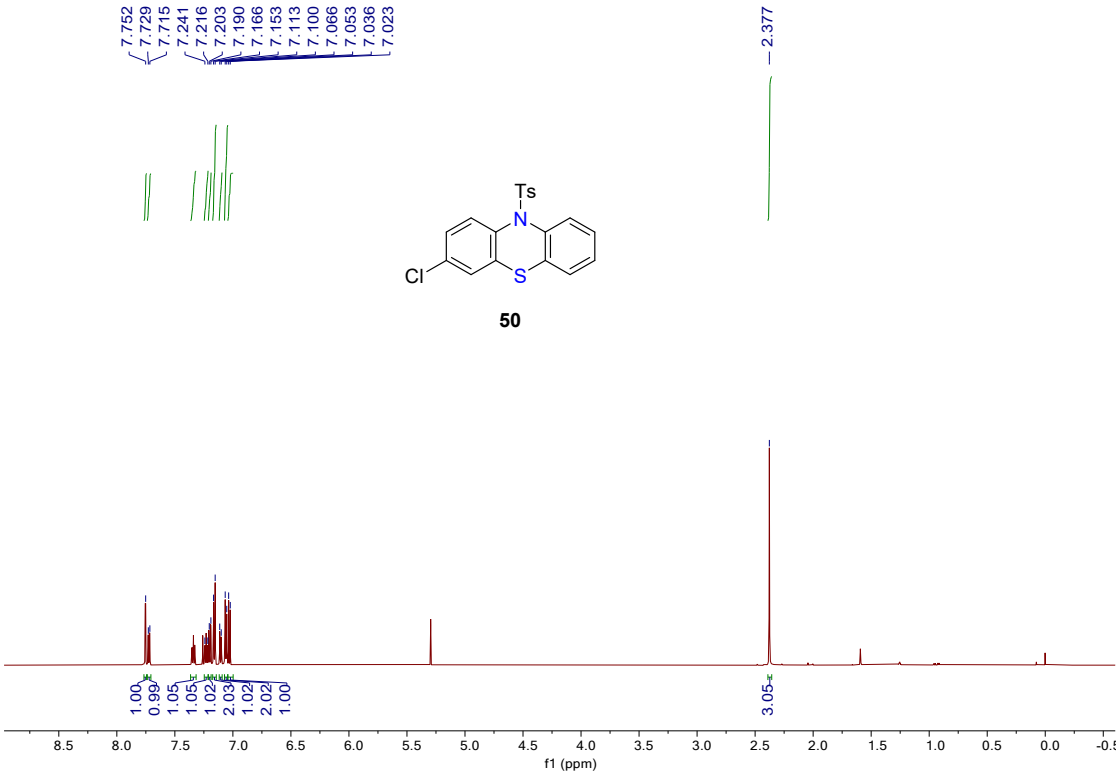


Ts
N
I
N
Ts

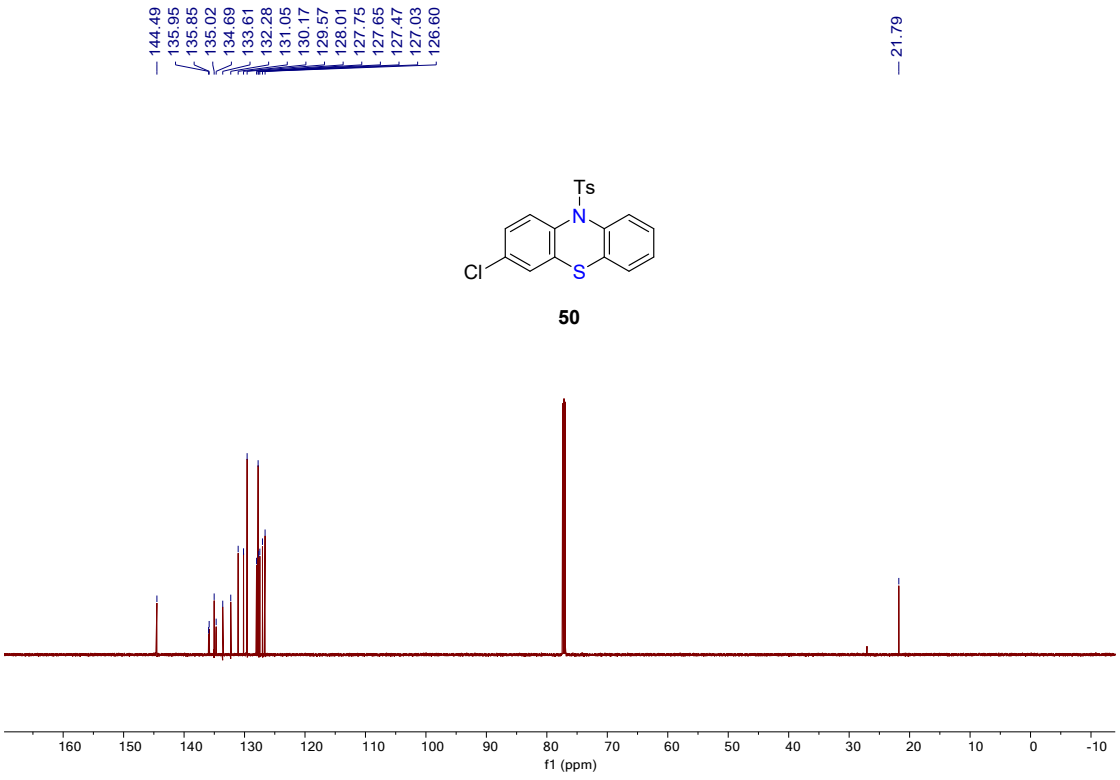
48


7.711
7.697
7.496
7.482
7.299
7.296
7.283
7.198
7.186
7.173
7.149
7.135
7.082
7.069
7.048
6.384
2.369
Ts
N
S
H2N
49
1.03
1.02
1.05
1.05
2.03
1.04
2.04
1.04
1.00
3.00
f1 (ppm)

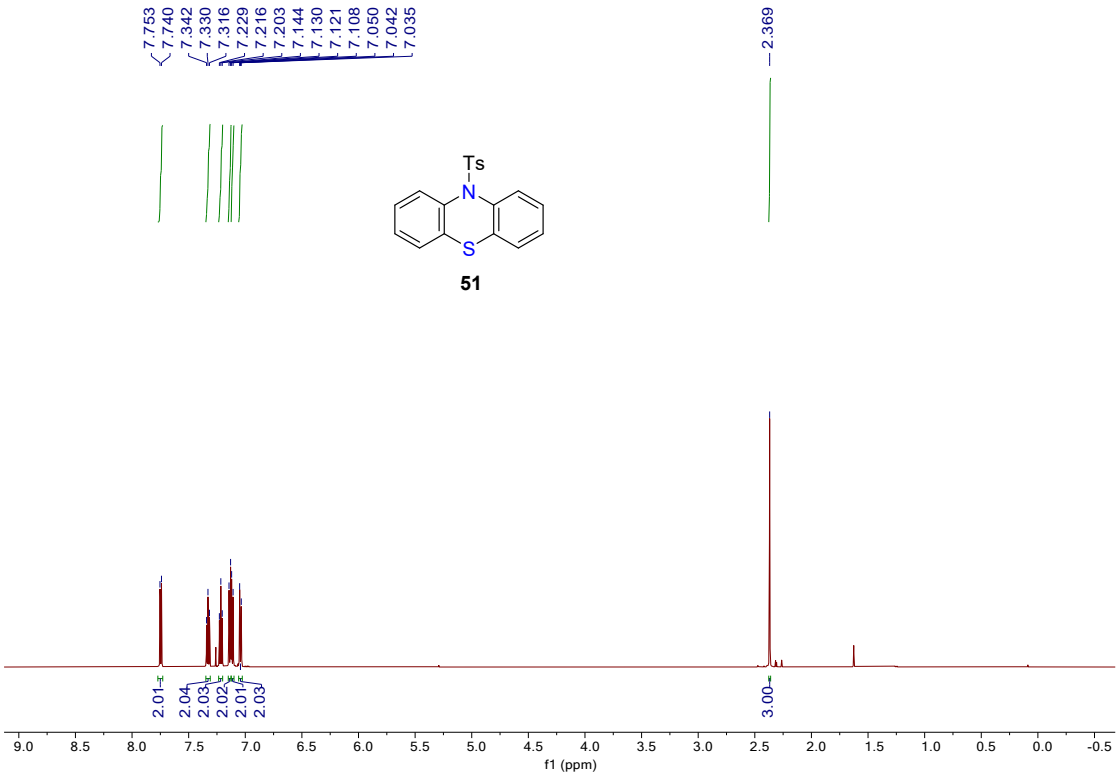

146.10
143.98
136.51
136.13
134.11
133.07
130.84
130.13
129.33
127.87
127.56
127.08
126.85
126.38
114.08
112.21
21.75
Ts
N
S
H2N
49
f1 (ppm)

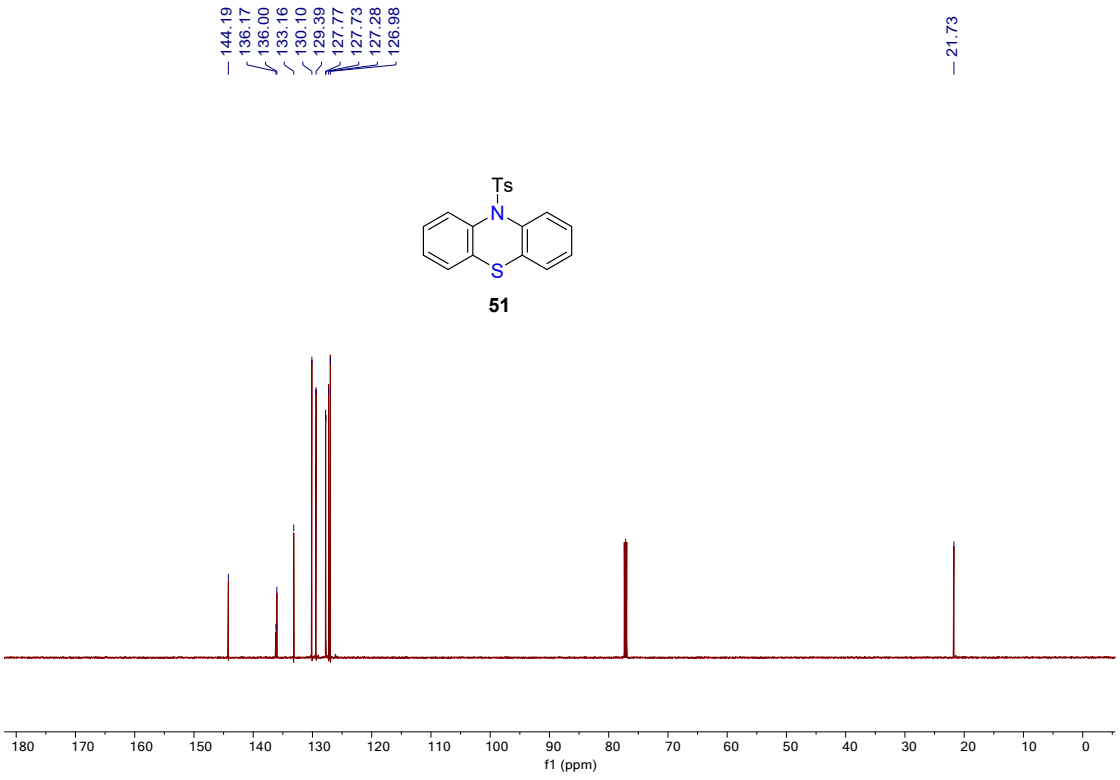

7.752
7.729
7.715
7.241
7.216
7.203
7.190
7.166
7.153
7.113
7.100
7.066
7.053
7.036
7.023
2.377
Ts
N
Cl
S
1.00
0.99
1.05
1.05
1.02
2.03
1.02
2.02
1.00
3.05
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)

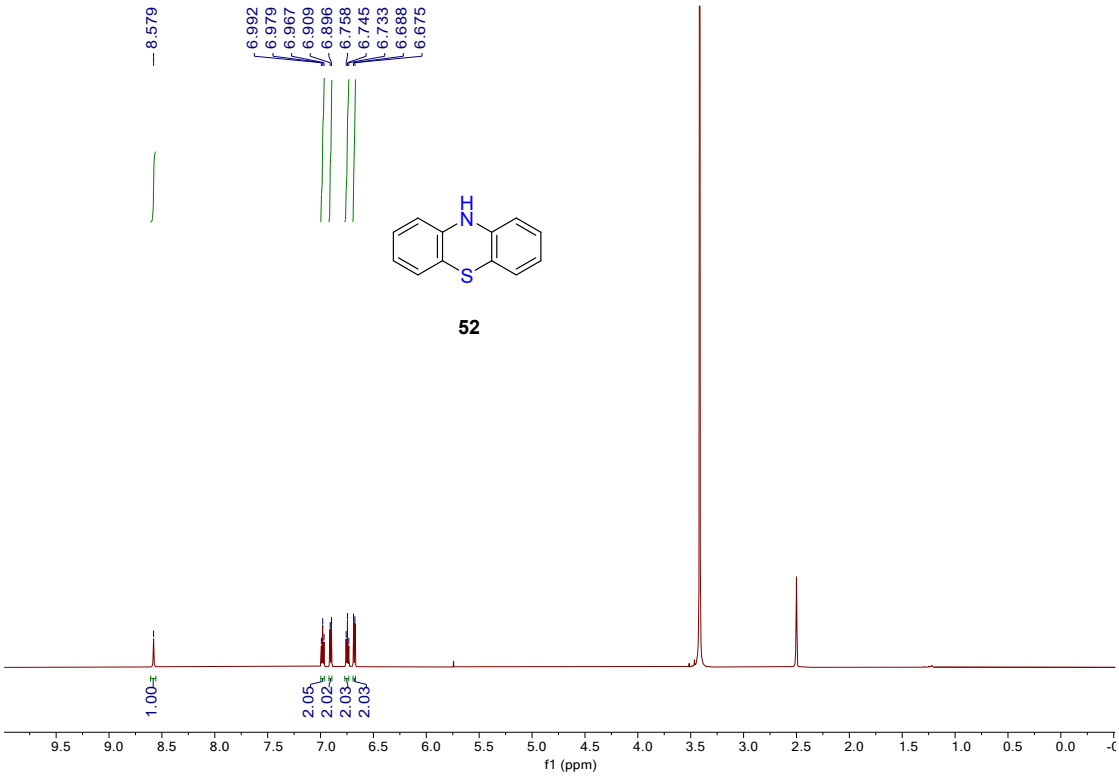
50


144.49
135.95
135.85
135.02
134.69
133.61
132.28
131.05
130.17
129.57
128.01
127.75
127.65
127.47
127.03
126.60
21.79
Ts
N
Cl
S
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

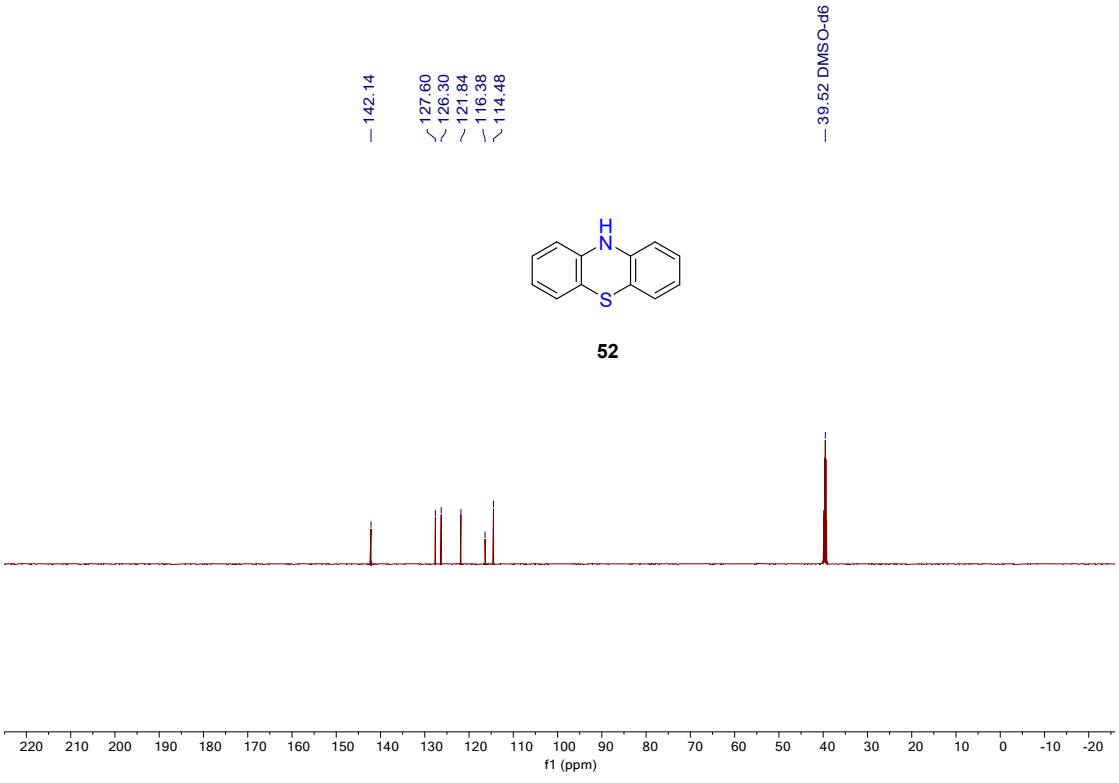
50


7.753
7.740
7.342
7.330
7.316
7.229
7.216
7.203
7.144
7.130
7.121
7.108
7.050
7.042
7.035
2.369
Ts
N
S
51
2.01
2.04
2.03
2.02
2.01
2.03
3.00
f1 (ppm)

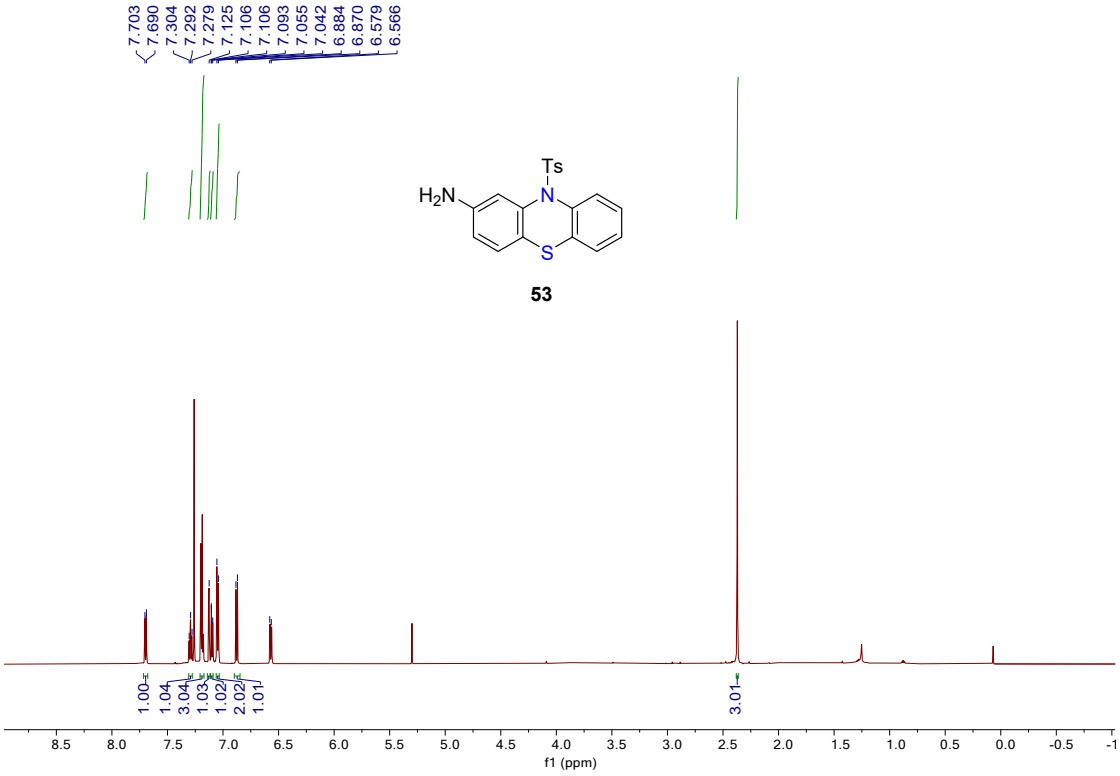

144.19
136.17
136.00
133.16
130.10
129.39
127.77
127.73
127.28
126.98
21.73
Ts
N
S
51
f1 (ppm)


8.579
6.992
6.979
6.967
6.909
6.896
6.758
6.745
6.733
6.688
6.675
H
N
S
1.00
2.05
2.02
2.03
2.03
f1 (ppm)

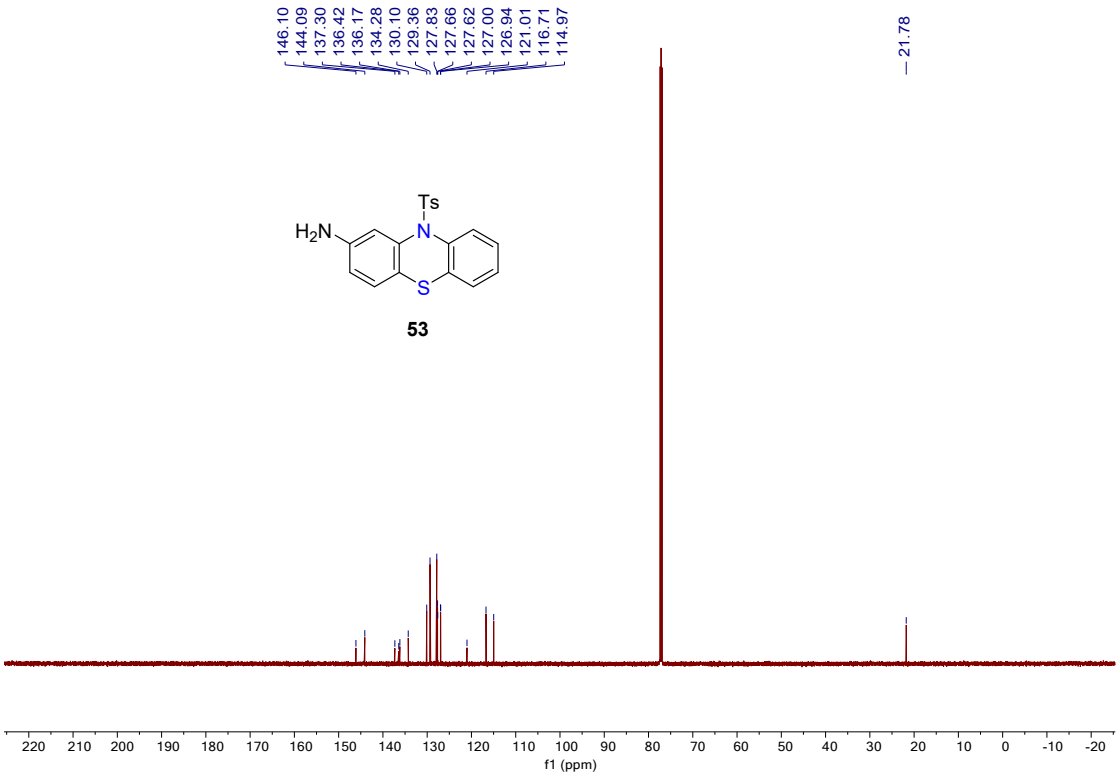
52


142.14
127.60
126.30
121.84
116.38
114.48
39.52 DMSO-d6
H
N
S
f1 (ppm)

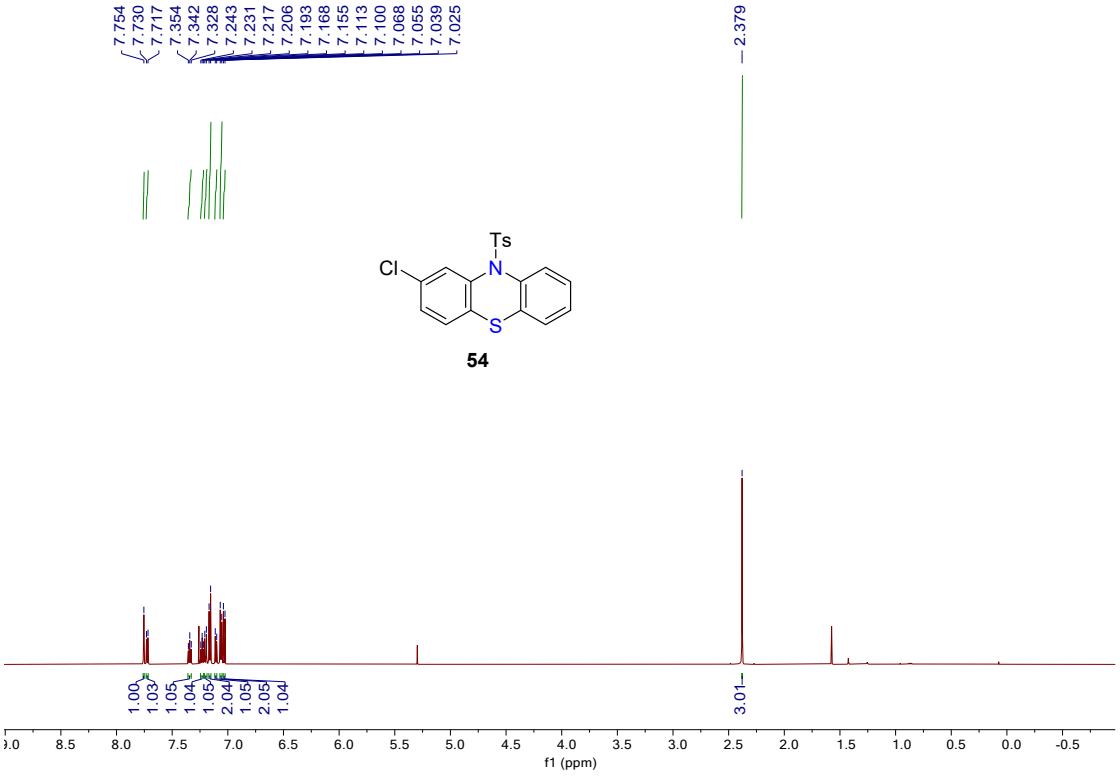
52

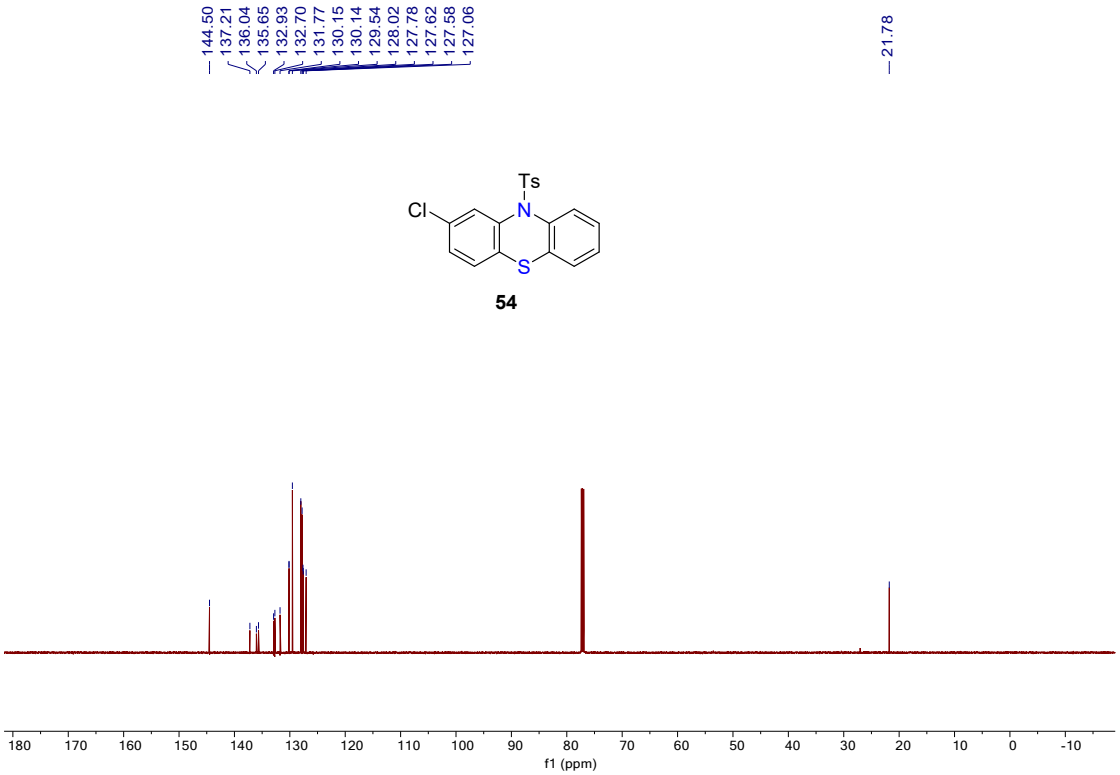

7.703
7.690
7.304
7.292
7.279
7.125
7.106
7.106
7.093
7.055
7.042
6.884
6.870
6.579
6.566
Ts
N
H_2N
S
1.00
1.04
3.04
1.03
1.02
2.02
1.01
3.01
f1 (ppm)

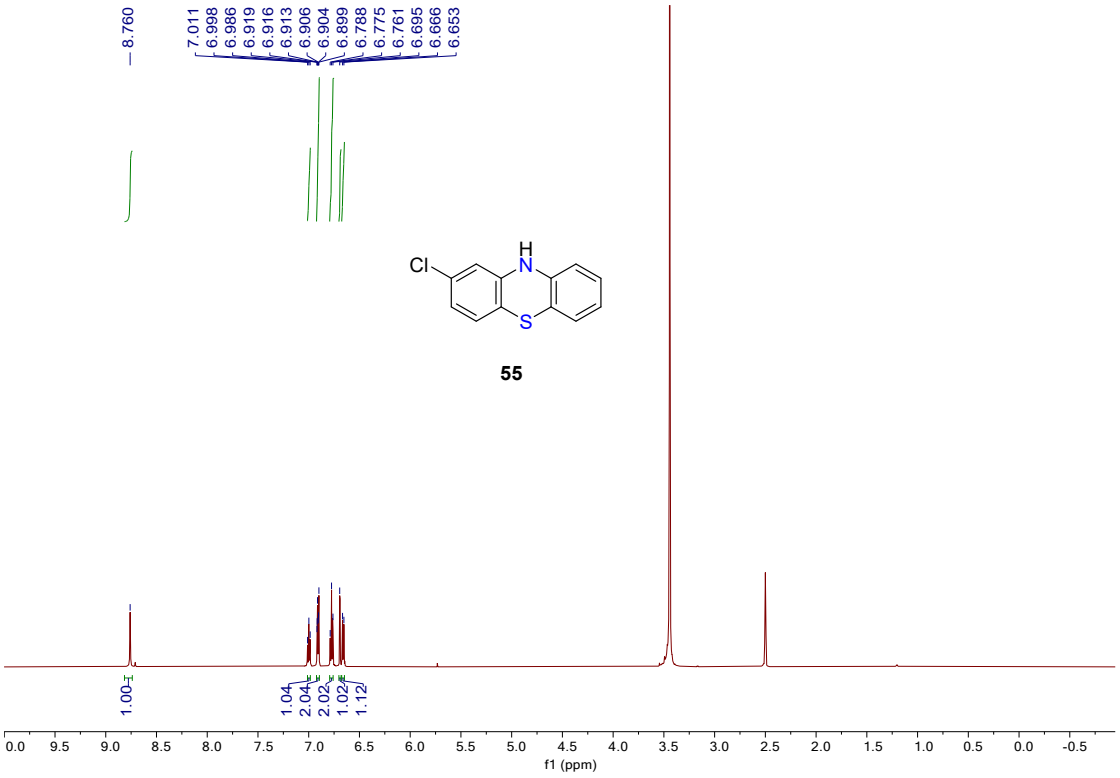
53

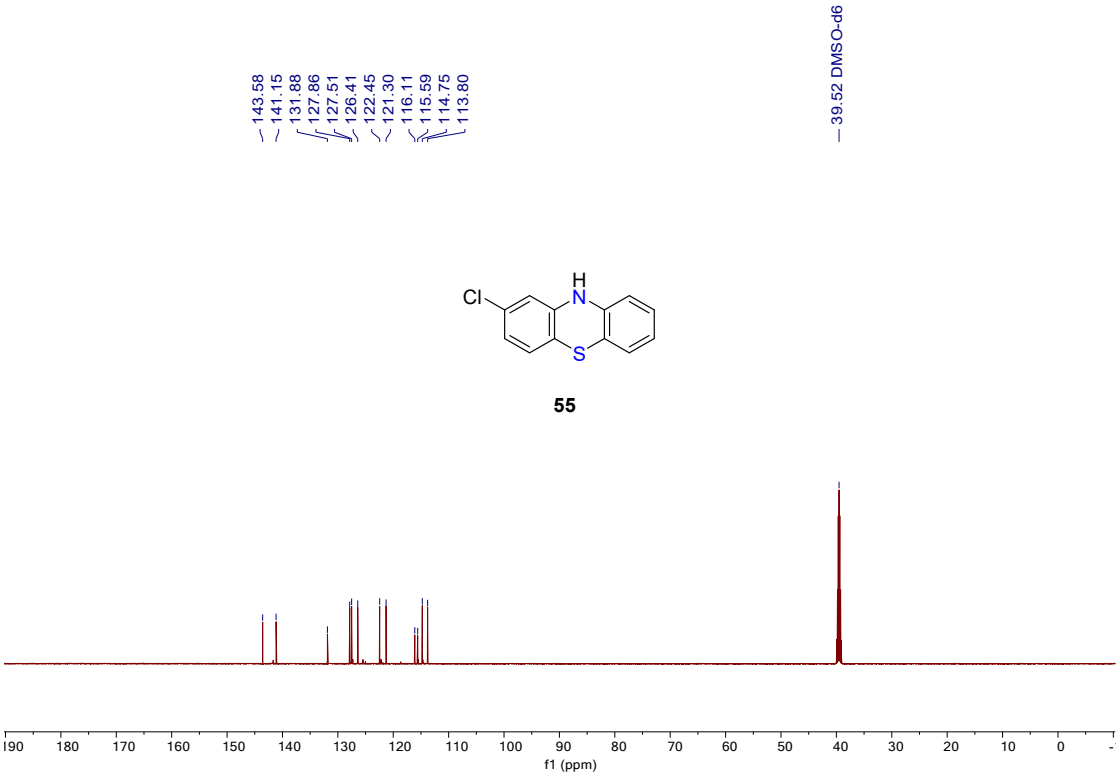

146.10
144.09
137.30
136.42
136.17
134.28
130.10
129.36
127.83
127.66
127.62
127.00
126.94
121.01
116.71
114.97
21.78
Ts
N
H_2N
S
f1 (ppm)

53


7.754
7.730
7.717
7.354
7.342
7.328
7.243
7.231
7.217
7.206
7.193
7.168
7.155
7.113
7.100
7.068
7.055
7.039
7.025
2.379
Ts
Cl
N
S
54
1.00
1.03
1.05
1.04
1.05
2.04
1.05
2.05
1.04
3.01
f1 (ppm)


144.50
137.21
136.04
135.65
132.93
132.70
131.77
130.15
130.14
129.54
128.02
127.78
127.62
127.58
127.06
21.78
Ts
Cl
N
S
54
f1 (ppm)


8.760
7.011
6.998
6.986
6.919
6.916
6.913
6.906
6.904
6.899
6.788
6.775
6.761
6.695
6.666
6.653
Cl
H
N
S
55
1.00
1.04
2.04
2.02
1.02
1.12
f1 (ppm)


143.58
141.15
131.88
127.86
127.51
126.41
122.45
121.30
116.11
115.59
114.75
113.80
39.52 DMSO-d6
Cl
H
N
S
55
f1 (ppm)