Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Electrochemical phenothiazination of naphthylamines and its application in photocatalysis

Song Chen,[a] Ya-Nan Li,[a] Shao-Hua Xiang,*[a,b] Shaoyu Li*[a,b] and Bin Tan*[a]

[a] *Shenzhen Grubbs Institute, Department of Chemistry, Southern University of Science and Technology, Shenzhen 518055, China.*

[b] *Academy for Advanced Interdisciplinary Studies, Southern University of Science and Technology, Shenzhen 518055, China.*

Email: tanb@sustech.edu.cn; lisy@sustech.edu.cn;xiangsh@sustech.edu.cn

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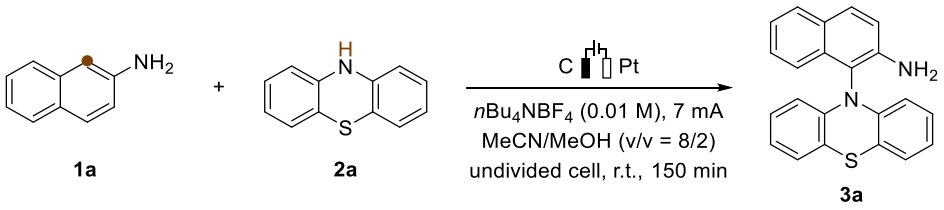
1. General information

Chemicals were purchased from commercial suppliers and used without further purification unless otherwise stated. The instrument for electrolysis is DC power supply (HY3005MT) (made in China). The anodic electrode was graphite rod (ϕ 6 mm, hard) and cathodic electrode was platinum plate (10 mm×10 mm×1.0 mm). These electrodes are commercially available from GaossUnion, China. Cyclic voltammograms were obtained on a CHI-602E electrochemical workstation. UV-Vis absorption spectroscopy was measured on Shimadzu UV-VIS-NIR spectrophotometer (UV-3600). EPR measurements were performed on a Bruker ELEXSYS-II E500 system. Analytical thin layer chromatography (TLC) was performed on precoated silica gel 60 GF254 plates. Flash column chromatography was performed using Tsingtao silica gel (60, particle size 0.040-0.063 mm). Visualization on TLC was achieved by use of UV light (254 nm). ^{1}H and ^{13}C NMR spectra were recorded on Bruker 400 MHz spectrometer in $CDCl_3$ or DMSO-d_6 with tetramethylsilane (TMS) as internal standard. The chemical shifts are expressed in ppm and coupling constants are given in Hz. Data for ^{1}H NMR are recorded as follows: chemical shift (δ, ppm), multiplicity (s = singlet; d = doublet; t = triplet; q = quartet; m = multiplet; br = broad), coupling constant (Hz), integration. Data for ^{1}H NMR, ^{13}C NMR, and ^{19}F are reported in terms of chemical shift (δ, ppm). High resolution mass spectroscopy (HRMS) analyses were performed at a Q-Exactive (Thermo Scientific) Inc mass instrument (HESI).

2. Optimization of the reaction conditions

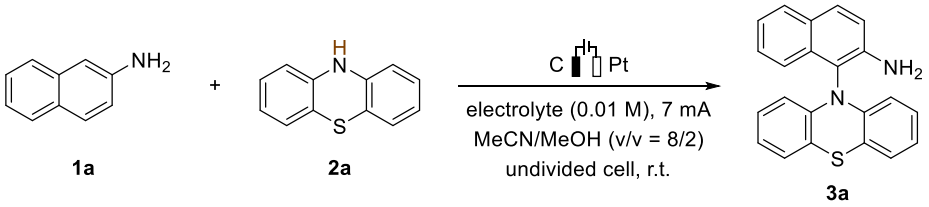
Table S1 Reaction condition development and optimization[a]



Entry	Variation from above conditions	Yield (%)
1	none	73
2	*n*Bu_4NPF_6	74
3	*n*Bu_4NI	65
4	*n*Bu_4NCl	73
5	Me_3PhNI	72
6	*n*Bu_4NOTf	77
7	*n*Bu_4NOTf, MeCN/MeOH (5/5)	79
8	*n*Bu_4NOTf, MeCN/MeOH (2/8)	51
9	*n*Bu_4NOTf, MeCN/MeOH (7/3)	88 (87)[b]
10	*n*Bu_4NOTf, MeCN	54
11	*n*Bu_4NOTf, MeOH	38
12	4 mA	80
13	9 mA	83
14	platinum plate anode	67
15	graphite rod cathode	76
16	platinum plate anode, graphite rod cathode	58
17	under Ar	85
18	without electric current	n.r.

[a] Reaction conditions: graphite rod anode (ϕ 6 mm), platinum plate cathode (10 mm × 10 mm × 1 mm), constant current = 7.0 mA, **1a** (0.24 mmol), **2a** (0.20 mmol), *n*Bu_4NOTf (0.10 mmol), MeCN/MeOH (10 mL, 7/3), room temperature, air, 150 min. Yields were determined by ^1H NMR using 1,3,5-trimethoxybenzene as internal standard. n.r. = no reaction. [b] Isolated yield was provided in the parentheses.

Table S2. Electrolyte Screening[a]

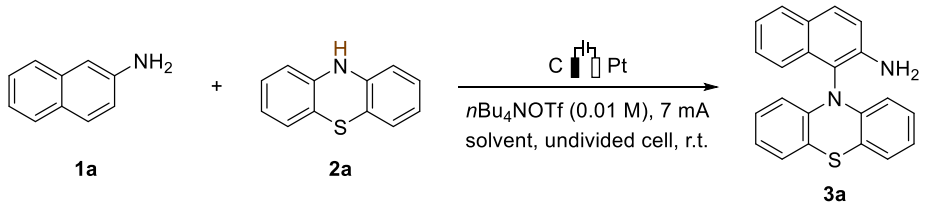


1a **2a** **3a**

Entry	Electrolyte	Yield (%)
1	nBu$_4$NBF$_4$	73
2	nBu$_4$NPF$_6$	74
3	nBu$_4$NI	65
4	nBu$_4$NCl	73
5	nBu$_4$NBr	37
6	**nBu$_4$NOTf**	**77**
7	Me$_3$PhNI	72
8	NH$_4$BF$_4$	76
9	NH$_4$PF$_6$	53
10	KI	62

[a]Reaction conditions: **1a** (0.24 mmol), **2a** (0.20 mmol) in 10 mL solvent. Yield was determined by ^{1}H NMR using 1,3,5-trimethoxybenzene as internal standard.

Table S3. Solvent Screening[a]

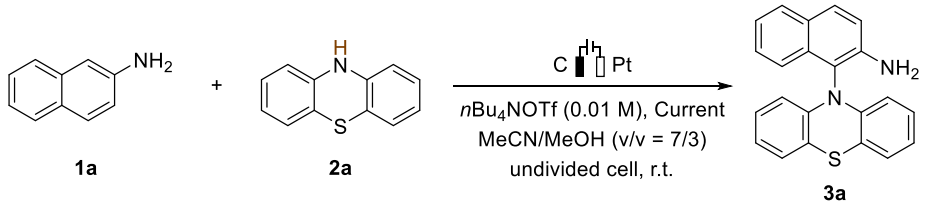


1a **2a** **3a**

Entry	Solvent	Yield (%)
1	MeCN/MeOH (5/5)	79
2	MeCN/MeOH (2/8)	51
3	**MeCN/MeOH (7/3)**	**88**
4	MeCN	54
5	MeOH	38
6	DMF	64
7	DMSO	18
8	THF	trace
9	EtOAc	trace
10	DCM	NR

[a]Reaction conditions: **1a** (0.24 mmol), **2a** (0.20 mmol) in 10 mL solvent. Yield was determined by ^{1}H NMR using 1,3,5-trimethoxybenzene as internal standard.

Table S4. Current Screening[a]

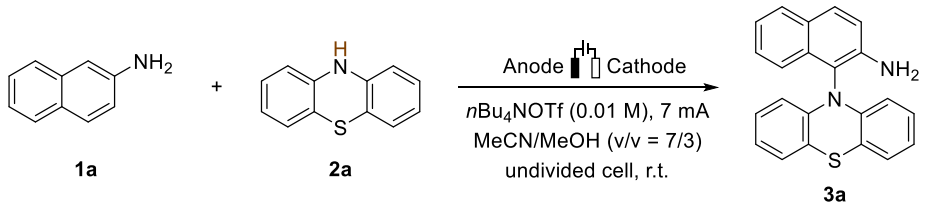


1a 2a 3a

Entry	Current (mA)	Yield (%)
1	2	79
2	4	80
3	5	82
4	6	85
5	**7**	**88**
6	9	83

[a]Reaction conditions: **1a** (0.24 mmol), **2a** (0.20 mmol) in 10 mL solvent. Yield was determined by ^{1}H NMR using 1,3,5-trimethoxybenzene as internal standard.

Table S5. Electrode Screening[a]

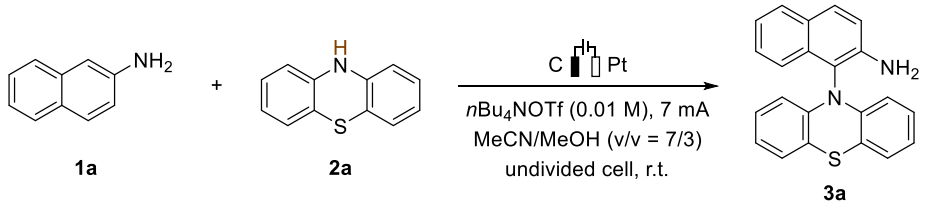


1a 2a 3a

Entry	Anode/Cathode	Yield (%)
1	**C/Pt**	**88**
2	Pt/C	58
3	Pt/Pt	67
4	C/C	76

[a]Reaction conditions: **1a** (0.24 mmol), **2a** (0.20 mmol) in 10 mL solvent. Yield was determined by ^{1}H NMR using 1,3,5-trimethoxybenzene as internal standard.

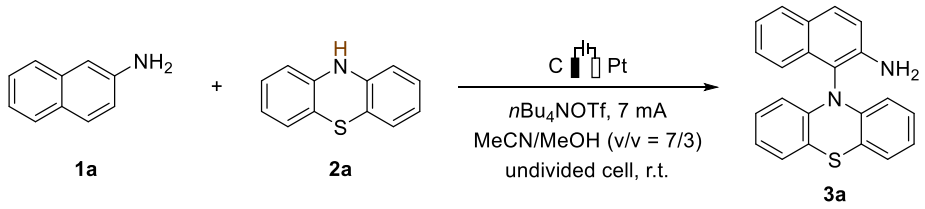
Table S6. Material Ratio Screening[a]



Entry	**1a** (equiv)	Yield (%)
1	**1.2**	**88**
2	1.1	83
3	1.0	78
4	1.5	87

[a]Reaction conditions: **1a** (1.0-1.5 equiv), **2a** (0.2 mmol) in 10 mL solvent. Yield was determined by ^{1}H NMR using 1,3,5-trimethoxybenzene as internal standard.

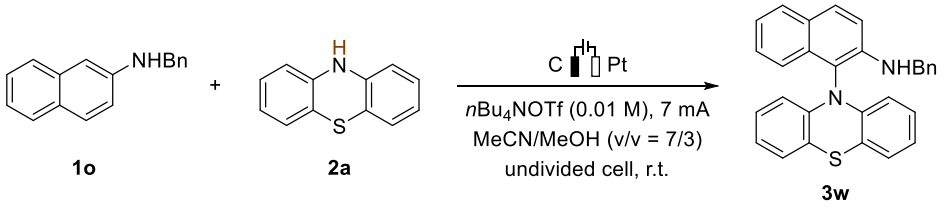
Table S7. Equivalent screening of electrolyte[a]



Entry	nBu$_4$NOTf (equiv)	Yield (%)
1	**0.5**	**88**
2	0.25	54
3	0.75	76

[a]Reaction conditions: **1a** (0.24 mmol), **2a** (0.20 mmol) in 10 mL solvent. Yield was determined by ^{1}H NMR using 1,3,5-trimethoxybenzene as internal standard.

Table S8. Equivalent screening of **1o**[a]



Entry	**1o** (equiv)	Yield (%)
1	**1.0**	**96**
2	1.2	96

[a]Reaction conditions: **2a** (0.20 mmol), **1o** (1.0 or 1.2 equiv) in 10 mL solvent. Yield was determined by ^{1}H NMR using 1,3,5-trimethoxybenzene as internal standard.

3. Procedure for electrochemical cross-coupling of phenothiazines with anilines

In an undivided two-necked bottle (10 mL) equipped with a stir bar, naphthylamine (0.24 mmol) or *N*-substituted naphthylamine (0.2 mmol), phenothiazine (0.20 mmol, 40.0 mg), *n*Bu_4NOTf (0.10 mmol, 39.1 mg) and MeCN/MeOH (7.0 mL/3.0 mL) were combined and added. The bottle was equipped graphite rod (ϕ 6 mm, about 12 mm immersion depth in solution) as the anode and platinum plate (10 mm×10 mm×0.1 mm) as the cathode. The reaction mixture was stirred and electrolyzed at a constant current of 7 mA under room temperature until complete consumption of phenothiazine (monitored by TLC). The pure product was obtained by flash column chromatography on silica gel (petroleum: dichloromethane = 5:1 to 3:1).

4. Procedure for the gram-scale synthesis

In an undivided two-necked bottle (100 mL) equipped with a stir bar, *N*-benzylnaphthalen-2-amine (5.0 mmol, 1.17 g), phenothiazine (5.0 mmol, 1.00 g), *n*Bu_4NOTf (0.50 mmol, 0.20 g) and MeCN/MeOH (72.0 mL/18.0 mL) were combined and added. The bottle was equipped graphite rod (ϕ 6 mm, about 42 mm immersion depth in solution) as the anode and platinum plate (15 mm×15 mm×0.1 mm) as the cathode. The reaction mixture was stirred and electrolyzed at a constant current of 70 mA under room temperature until complete consumption of phenothiazine (monitored by TLC). The pure product was obtained by flash column chromatography on silica gel (petroleum: dichloromethane = 10:1 to 5:1).

5. Procedure for cyclic voltammetry (CV)

Cyclic voltammetry was performed in a three-electrode cell. The working electrode was a steady glassy carbon disk electrode (ϕ 3 mm) while the counter electrode was a platinum wire, the reference was an Ag/AgCl electrode. MeCN/MeOH (7.0 mL/3.0 mL) containing 0.1 M nBu$_4$NOTf were poured into the electrochemical cell in cyclic voltammetry experiments. The CV of all substrates was measured at the concentration of 0.01 M. The scan rate was 0.10 Vs^{-1}, the test ranging depends on the practical testing of the substrate.

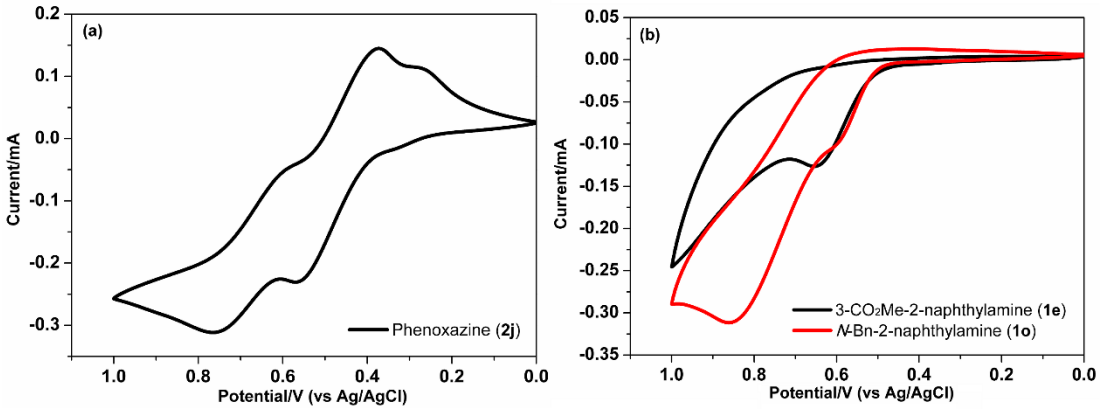


Figure S1. Cyclic voltammetry of **2j** (a), **1e** (b, black line) and **1o** (b, red line).

6. Procedure for UV-Vis absorption spectroscopy (UV-Vis)

Compound (0.1 mmol) was dissolved in DCM (10 mL), and 0.5 ml of solution was taken and diluted to 10 ml to obtain solution (0.05 mM). The solution was used to test UV-Vis absorption spectroscopy.

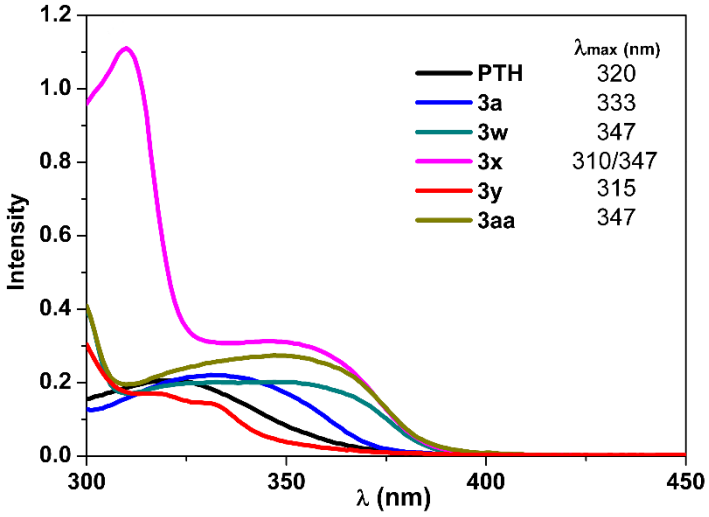


Figure S2. UV-vis absorption spectroscopy of PTH and representative products.

7. Procedure for the Electron Paramagnetic Resonance (EPR) experiment

In an undivided two-necked bottle (10 mL) equipped with a stir bar, substrates (0.2 mmol), *n*Bu_4NOTf (0.1 mmol, 39.1 mg) and MeCN/MeOH (7 mL/3 mL) or MeCN/HFIP (5 mL/5 mL) were combined and added. The bottle was equipped graphite rod (ϕ 6 mm, about 12 mm immersion depth in solution) as the anode and platinum plate (10 mm×10 mm×0.1 mm) as the cathode. The reaction mixture was stirred and electrolyzed at a constant current of 7 mA under room temperature for 15 min. Then the samples were taken out by a capillary (borosilicate glass, 0.5×100 mm), and analyzed by EPR at room temperature.

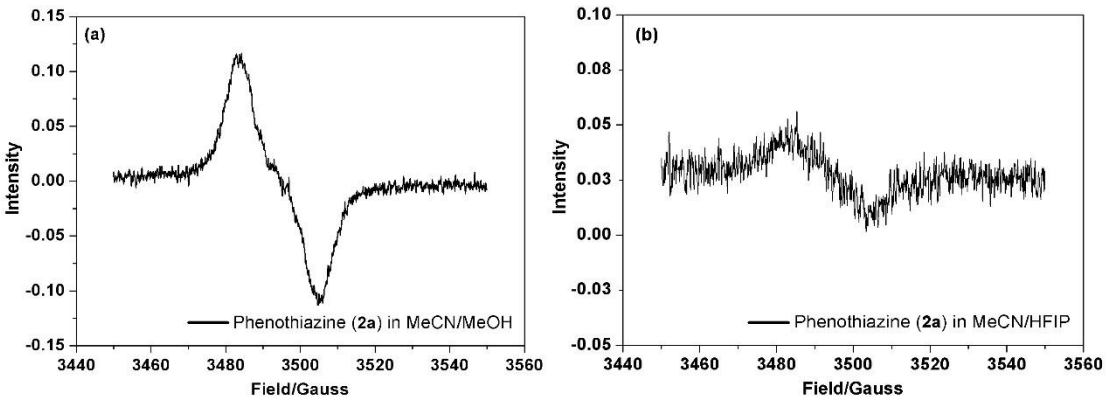


Figure S3. EPR spectrum of **2a** obtained by electrolysis in MeCN/MeOH (a) and MeCN/HFIP (b).

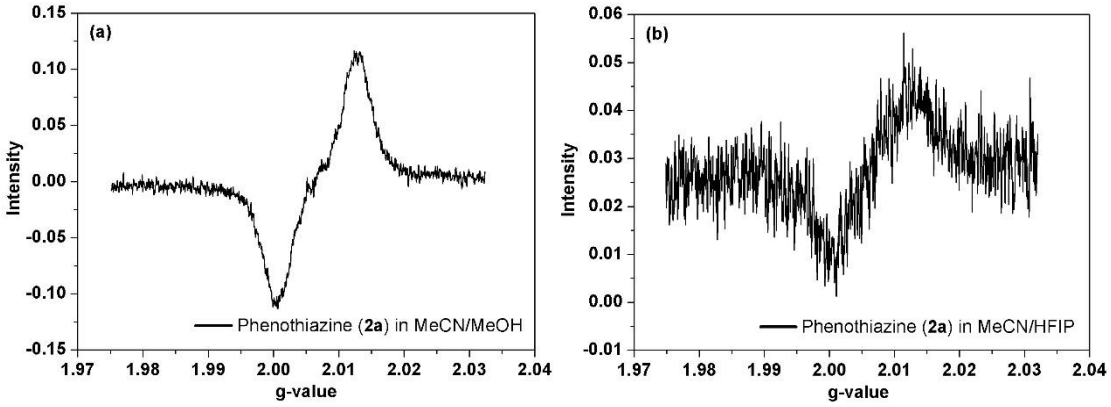


Figure S4. The g-value of **2a** obtained by electrolysis in MeCN/MeOH (a) and MeCN/HFIP (b).

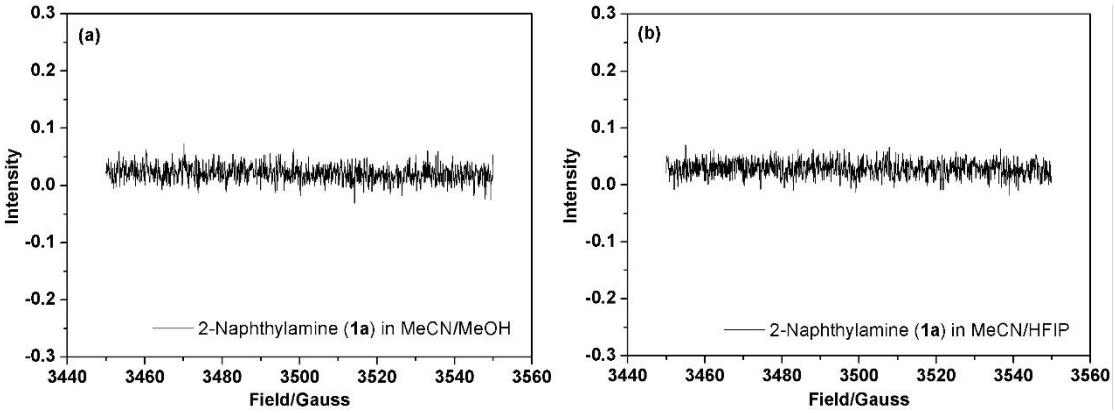


Figure S5. EPR spectrum of **1a** obtained by electrolysis in MeCN/MeOH (a) and MeCN/HFIP (b).

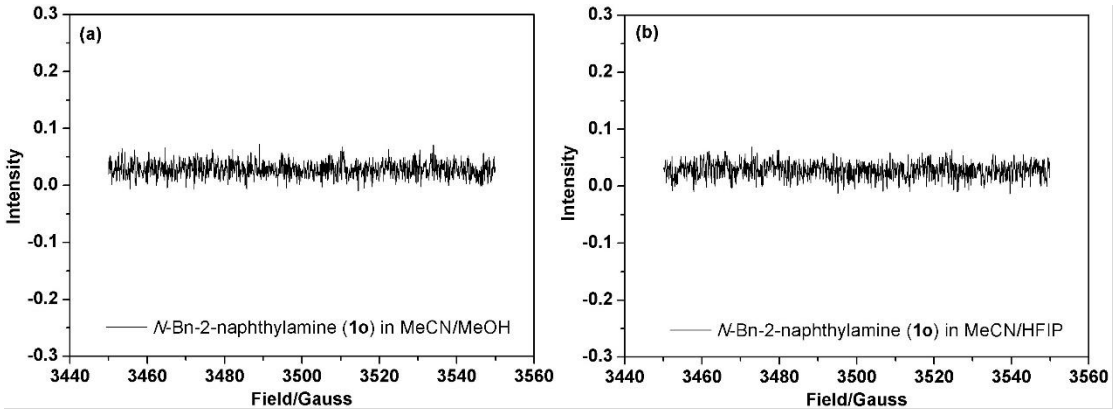


Figure S6. EPR spectrum of **1o** obtained by electrolysis in MeCN/MeOH (a) and MeCN/HFIP (b).

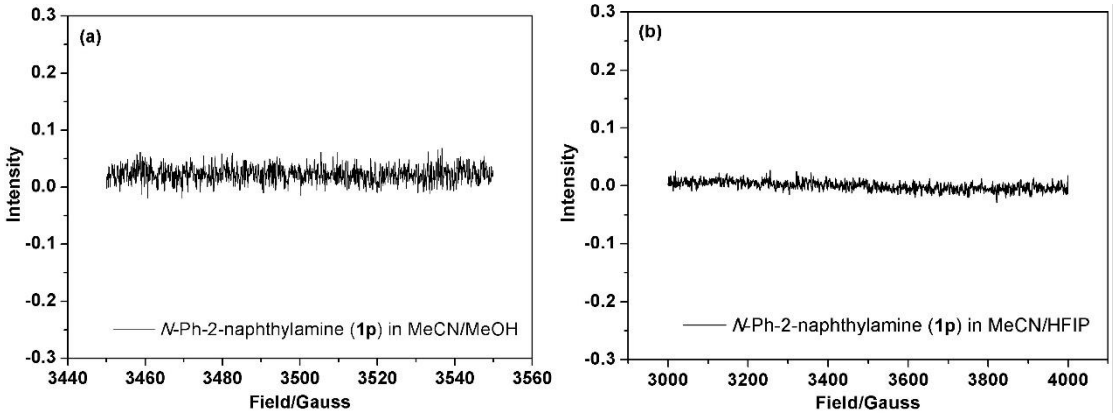


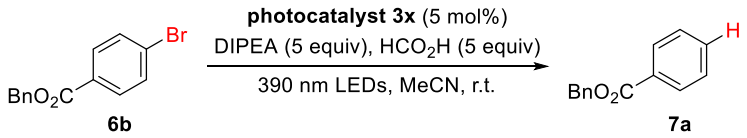
Figure S7. EPR spectrum of **1p** obtained by electrolysis in MeCN/MeOH (a) and MeCN/HFIP (b).

8. Photochemical application

8.1. Procedure for the radical dehalogenation reaction

A 10 mL tube equipped with a magnetic stir bar and charged with substrate (0.2 mmol), catalyst (5 mol%), the atmosphere was exchanged by applying vacuum and backfilling with Ar (this process was conducted a total of three times). Under Ar atmosphere, the tube was charged with formic acid (38 μL, 1 mmol), DIPEA (164 μL, 1 mmol) and acetonitrile (2 mL) via syringe. The tube was then stirred vigorously in front of 390 nm LEDs under room temperature until complete consumption of substrate (monitored by TLC). The acetonitrile was removed in vacuo before redissolving in ethyl acetate and washing with 2 M HCl. The aqueous layer was extracted again with ethyl acetate, and the organic layers were combined and washed with saturated $NaHCO_3$, brine, and dried over $MgSO_4$. The pure product was obtained by flash column chromatography on silica gel.

Table S9. Exclusion of Background Reactions for Radical Dehalogenation Reaction of **6b**[a]



6b **7a**

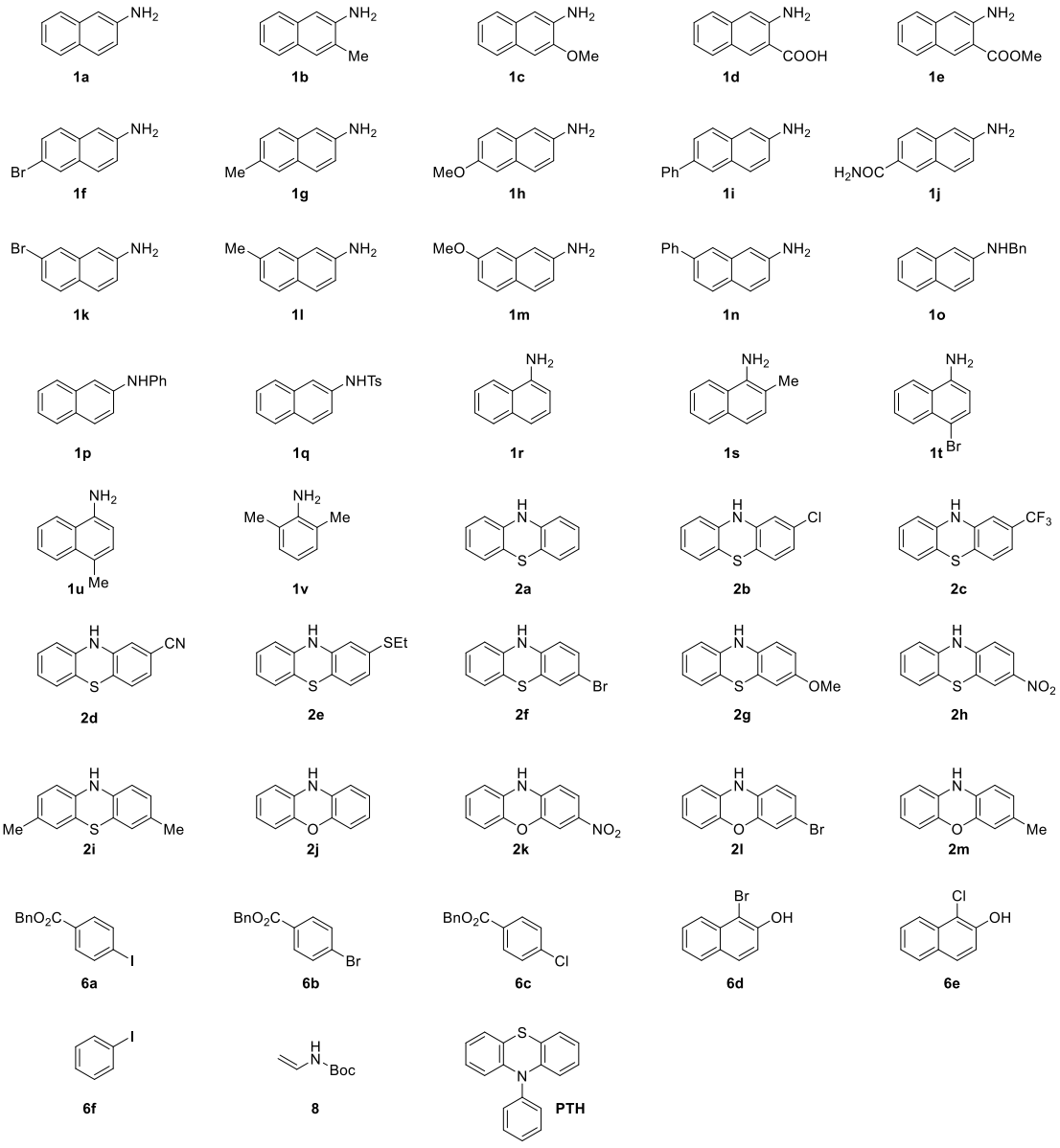
Entry	Variation from the above conditions	Yield (%)
1	No light	No reaction
2	No **3x**	< 5

[a]Yield was determined by ^1H NMR using 1,3,5-trimethoxybenzene as internal standard.

8.2. Procedure for the regioselective arylethylamine synthesis.

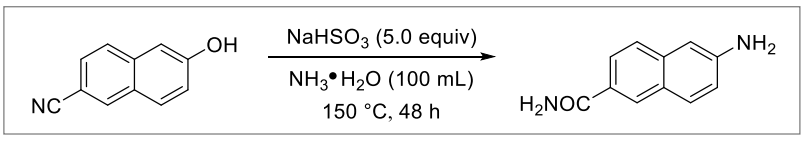
A 25 mL tube equipped with a magnetic stir bar and charged with alkene (2.5 equiv), sodium formate (3 equiv) and **3w** (10.8 mg, 5 mol%) or **3x** (10.4 mg, 5 mol%), the atmosphere was exchanged by applying vacuum and backfilling with Ar (this process was conducted a total of three times). Under Ar atmosphere, the tube was charged with Iodobenzene (0.5 mmol), cyclohexanethiol (5 mol%) and 20:1 DMSO:H_2O (0.1 M) via syringe. The resulting mixture was stirred vigorously for 24 hours under irradiation with a 450 nm LEDs with cooling from compressed air. The reaction was quenched with ethyl acetate (30 mL) and water (30 mL). The aqueous layer was extracted with ethyl acetate (3 x 10 mL), and the organic phases were combined and washed with water (3 x 10 mL), brine, and dried over $MgSO_4$. The pure product was obtained by flash column chromatography on silica gel.

9. Synthetic procedures and characterization of substrates



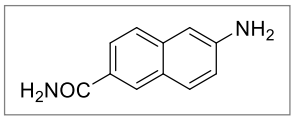
Substrate **1a**, **1d**, **1p**, **1r**, **1s**, **1t**, **1v**, **2a**, **2b**, **2c**, **2d**, **2e**, **2j**, **6d**, **6e** and **6f** were purchased, and **1b**,[1] **1c**,[2] **1e**,[3] **1f**,[4] **1g**,[4] **1h**,[4] **1i**,[4] **1k**,[4] **1l**,[4] **1m**,[4] **1n**,[4] **1o**,[5] **1q**,[6] **1u**,[7] **2f**,[8] **2g**,[9] **2h**,[9] **2k**,[10] **2l**,[8] **2m**,[10] **6a**,[11] **6b**,[11] **6c**,[11] **8**[12] and **PTH**[13] were prepared according to procedure of the reported literature.

Synthesis of 6-amino-2-naphthamide (**1j**)[4]



6-Hydroxy-2-naphthonitrile (50 mmol), $NaHSO_3$ (5.0 eq) and 25% ammonium hydroxide

(100 mL) were added to an autoclave, and reacted at 150 °C for 48 hours. The reaction mixture was cooled to room temperature, and then the mixture was diluted with ethyl acetate and washed with saturated brine. The organic layer was dried over $MgSO_4$ and concentrated in vacuo. The crude product was purified by silica gel column chromatography to afford the product.



6-amino-2-naphthamide (1j)

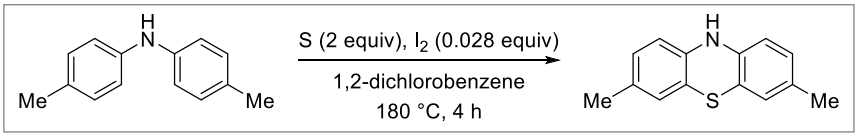
13% yield (petroleum ether/EA = 2/1)

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.24 – 8.22 (m, 1H), 7.91 (s, 1H), 7.75 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.66 (d, *J* = 8.8 Hz, 1H), 7.50 (d, *J* = 8.6 Hz, 1H), 7.19 (s, 1H), 6.98 (dd, *J* = 8.7, 2.2 Hz, 1H), 6.83 (d, *J* = 2.2 Hz, 1H), 5.65 (s, 2H).

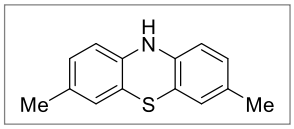
^{13}C NMR (100 MHz, DMSO-d_6) δ 168.81, 148.86, 137.03, 130.35, 128.43, 126.82, 125.48, 125.10, 125.01, 119.33, 105.74.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{11}H_{11}N_2O^+$, 187.0866, found: 187.0867.

Synthesis of 3,7-dimethyl-10*H*-phenothiazine (**2i**)[14]



To a 50 mL two-neck round-bottomed flask equipped with a stirrer bar was added di-*p*-tolylamine (4.93 g, 25 mmol, 1 equiv), sulfur (1.60 g, 50 mmol, 2 equiv) and I_2 (178 mg, 0.7 mmol, 0.028 equiv). Under a flow of argon was added 1,2-dichlorobenzene (15 mL). The reaction mixture was then deoxygenated by bubbling with argon for 30 minutes, and was then heated to 180 °C for 4 hours. After cooling the reaction mixture to room temperature, the reaction was quenched by adding ethyl acetate, and then extracted with saturated NaCl (3×15 mL), the aqueous phase was combined and extracted with ethyl acetate (3×10 mL). The solvent was removed under reduced pressure and the product was obtained with 44% yield by recrystallization using petroleum ether and ethyl acetate.

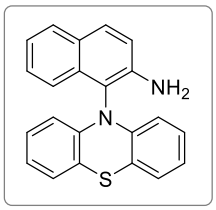


3,7-dimethyl-10*H*-phenothiazine (2i)

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.31 (s, 1H), 6.78 – 6.75 (m, 2H), 6.72 – 6.70 (m, 2H), 6.56 (d, *J* = 8.0 Hz, 2H), 2.11 (s, 6H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 140.31, 130.76, 128.33, 126.90, 116.62, 114.60, 20.40.

10. Characterization of products

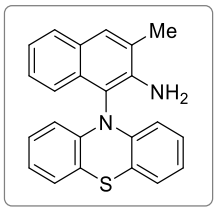


1-(10*H*-phenothiazin-10-yl)naphthalen-2-amine (3a)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.81 – 7.78 (m, 2H), 7.69 (d, *J* = 8.4 Hz, 1H), 7.36 – 7.32 (m, 1H), 7.26 (d, *J* = 8.9 Hz, 1H), 7.20 – 7.16 (m, 1H), 7.02 – 6.98 (m, 2H), 6.80 - 6.74 (m, 4H), 6.03 – 5.97 (m, 2H), 5.63 (s, 2H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 145.20, 141.89, 132.18, 130.04, 128.94, 128.05, 127.93, 127.82, 126.72, 122.88, 122.13, 120.63, 119.54, 119.37, 115.75, 114.22.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{22}H_{17}N_2S^+$, 341.1107, found: 341.1104.

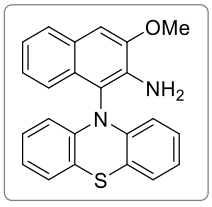


3-methyl-1-(10*H*-phenothiazin-10-yl)naphthalen-2-amine (3b)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.75 (d, *J* = 8.0 Hz, 1H), 7.71 (s, 1H), 7.62 (d, *J* = 8.4 Hz, 1H), 7.31 – 7.27 (m, 1H), 7.20 – 7.16 (m, 1H), 7.03 – 6.98 (m, 2H), 6.78 – 6.74 (m, 4H), 5.98 – 5.94 (m, 2H), 5.30 (s, 2H), 2.39 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 144.16, 141.94, 130.65, 129.34, 128.22, 127.92, 127.78, 126.90, 126.76, 122.99, 122.37, 120.77, 119.64, 115.82, 114.98, 18.94.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{23}H_{19}N_2S^+$, 355.1263, found: 355.1258.



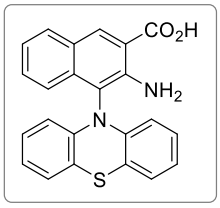
3-methoxy-1-(10*H*-phenothiazin-10-yl)naphthalen-2-amine (3c)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.80 – 7.77 (m, 1H), 7.63 – 7.61 (m, 1H), 7.39 (s, 1H), 7.25 – 7.18 (m, 2H), 7.02 – 6.98 (m, 2H), 6.79 – 6.74 (m, 4H), 6.00 – 5.96 (m, 2H), 5.33 (s,

2H), 4.01 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 148.65, 141.74, 137.66, 127.92, 127.73, 127.61, 127.12, 126.74, 125.33, 122.97, 122.90, 120.56, 119.54, 115.70, 114.79, 106.31, 56.25.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{23}H_{19}N_2OS^+$, 371.1213, found: 371.1209.

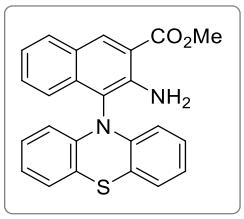


3-amino-4-(10*H*-phenothiazin-10-yl)-2-naphthoic acid (3d)

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.70 (s, 1H), 7.98 (d, *J* = 8.1 Hz, 1H), 7.68 (d, *J* = 8.5 Hz, 1H), 7.48 (t, *J* = 7.8 Hz, 1H), 7.24 (t, *J* = 7.7 Hz, 1H), 7.03 – 7.00 (m, 2H), 6.80 – 6.77 (m, 5H), 5.99 – 5.95 (m, 2H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 169.67, 145.40, 141.42, 134.86, 134.40, 130.89, 130.68, 128.05, 126.79, 125.86, 123.12, 122.90, 120.68, 119.54, 116.43, 115.97, 115.64.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{23}H_{17}N_2O_2S^+$, 385.1005, found: 385.1001.

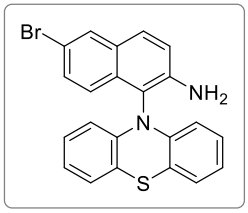


methyl 3-amino-4-(10*H*-phenothiazin-10-yl)-2-naphthoate (3e)

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.72 (s, 1H), 8.00 (d, *J* = 8.2 Hz, 1H), 7.70 (d, *J* = 8.4 Hz, 1H), 7.51 – 7.47 (m, 1H), 7.27 – 7.23 (m, 1H), 7.04 – 6.99 (m, 2H), 6.80 – 6.76 (m, 4H), 6.52 (s, 2H), 5.95 – 5.95 (m, 2H), 3.95 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 167.93, 145.02, 141.36, 134.59, 134.54, 130.96, 128.04, 126.81, 125.89, 123.16, 123.12, 120.76, 119.60, 116.76, 115.63, 115.15, 52.79.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{24}H_{19}N_2O_2S^+$, 399.1162, found: 399.1158.

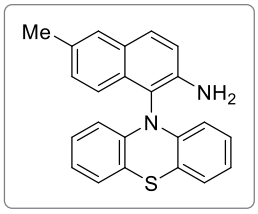


6-bromo-1-(10*H*-phenothiazin-10-yl)naphthalen-2-amine (3f)

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.05 (d, *J* = 2.1 Hz, 1H), 7.80 (d, *J* = 8.9 Hz, 1H), 7.59 (d, *J* = 8.9 Hz, 1H), 7.46 (dd, *J* = 8.9, 2.1 Hz, 1H), 7.31 (d, *J* = 8.9 Hz, 1H), 7.02 – 6.97 (m, 2H), 6.81 – 6.74 (m, 4H), 6.00 – 5.95 (m, 2H), 5.79 (s, 2H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 145.77, 141.68, 131.02, 130.71, 130.62, 129.33, 129.23, 127.98, 126.78, 123.00, 122.96, 120.67, 119.55, 115.62, 114.66, 114.00.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{22}H_{16}BrN_2S^+$, 419.0212, found: 419.0209.

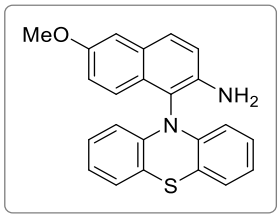


6-methyl-1-(10*H*-phenothiazin-10-yl)naphthalen-2-amine (3g)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.71 (d, *J* = 8.8 Hz, 1H), 7.58 – 7.54 (m, 2H), 7.23 (d, *J* = 8.8 Hz, 1H), 7.18 (dd, *J* = 8.6, 1.8 Hz, 1H), 7.01 – 6.97 (m, 2H), 6.80 – 6.73 (m, 4H), 6.00 – 5.95 (m, 2H), 5.48 (s, 2H), 2.35 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 144.26, 141.93, 131.10, 130.35, 129.83, 129.38, 128.30, 128.02, 127.90, 126.71, 122.86, 120.81, 119.47, 119.44, 115.73, 114.40, 21.24.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{23}H_{19}N_2S^+$, 355.1263, found: 355.1259.



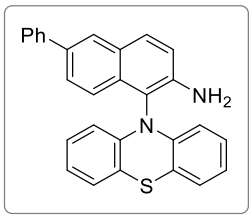
6-methoxy-1-(10*H*-phenothiazin-10-yl)naphthalen-2-amine (3h)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.73 (d, *J* = 8.9 Hz, 1H), 7.59 (d, *J* = 9.1 Hz, 1H), 7.28 (d, *J* = 2.0 Hz, 1H), 7.24 (d, *J* = 8.8 Hz, 1H), 7.05 (dd, *J* = 9.1, 2.1 Hz, 1H), 7.00 – 6.97 (m, 2H),

6.81 – 6.74 (m, 4H), 6.00 – 5.98 (m, 2H), 5.34 (s, 2H), 3.80 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 155.14, 143.22, 141.92, 129.02, 128.90, 127.93, 127.25, 126.72, 122.89, 122.37, 120.02, 119.73, 119.44, 115.75, 114.93, 108.21, 55.61.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{23}H_{19}N_2OS^+$, 371.1213, found: 371.1209.

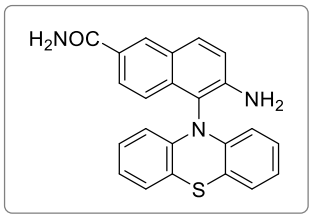


1-(10*H*-phenothiazin-10-yl)-6-phenylnaphthalen-2-amine (3i)

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.11 (d, *J* = 1.9 Hz, 1H), 7.90 (d, *J* = 8.9 Hz, 1H), 7.77 (d, *J* = 8.7 Hz, 1H), 7.72 – 7.68 (m, 3H), 7.46 – 7.43 (m, 2H), 7.34 – 7.30 (m, 2H), 7.03 – 6.98 (m, 2H), 6.82 – 6.75 (m, 4H), 6.08 – 6.03 (m, 2H), 5.72 (s, 2H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 145.40, 141.88, 140.69, 133.95, 131.53, 130.54, 129.39, 128.38, 127.98, 127.40, 127.01, 126.96, 126.75, 126.62, 122.92, 121.45, 119.86, 119.52, 115.76, 114.12.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{28}H_{21}N_2S^+$, 417.1420, found: 417.1417.

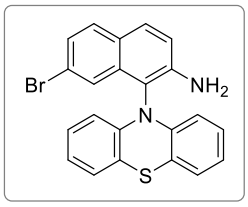


6-amino-5-(10*H*-phenothiazin-10-yl)-2-naphthamide (3j)

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.38 (d, *J* = 1.8 Hz, 1H), 7.93 (s, 1H), 7.88 (d, *J* = 8.9 Hz, 1H), 7.81 (dd, *J* = 8.8, 1.8 Hz, 1H), 7.65 (d, *J* = 8.8 Hz, 1H), 7.32 (d, *J* = 8.9 Hz, 1H), 7.28 (s, 1H), 7.03 – 6.98 (m, 2H), 6.82 – 6.75 (m, 4H), 6.01 – 5.97 (m, 2H), 5.92 (s, 2H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 168.52, 146.75, 141.79, 133.86, 131.23, 129.24, 127.97, 127.87, 126.89, 126.77, 126.43, 122.97, 120.34, 119.99, 119.57, 115.67, 114.00.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{23}H_{18}N_3OS^+$, 384.1165, found: 384.1162.

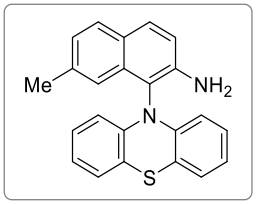


7-bromo-1-(10*H*-phenothiazin-10-yl)naphthalen-2-amine (3k)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.86 (d, *J* = 2.0 Hz, 1H), 7.82 (d, *J* = 8.9 Hz, 1H), 7.76 (d, *J* = 8.6 Hz, 1H), 7.32 – 7.27 (m, 2H), 7.04 – 7.02 (m, 2H), 6.85 – 6.77 (m, 4H), 6.06 – 6.04 (m, 2H), 5.89 (s, 2H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 146.53, 141.74, 133.75, 131.28, 130.19, 128.07, 126.91, 126.42, 124.85, 123.14, 122.14, 121.76, 119.91, 119.85, 115.71, 113.18.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{22}H_{16}BrN_2S^+$, 419.0212, found: 419.0206.

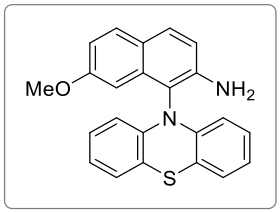


7-methyl-1-(10*H*-phenothiazin-10-yl)naphthalen-2-amine (3l)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.74 (d, *J* = 8.8 Hz, 1H), 7.69 (d, *J* = 8.2 Hz, 1H), 7.48 (s, 1H), 7.20 – 7.17 (m, 1H), 7.03 – 6.98 (m, 3H), 6.81 – 6.74 (m, 4H), 6.04 – 6.00 (m, 2H), 5.55 (s, 2H), 2.28 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 145.09, 141.96, 136.99, 132.49, 129.80, 128.94, 127.95, 126.78, 126.30, 124.27, 122.89, 119.65, 119.61, 118.34, 115.75, 114.01, 22.36.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{23}H_{19}N_2S^+$, 355.1263, found: 355.1259.

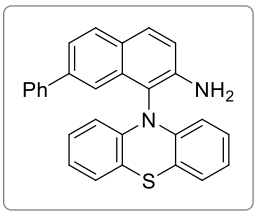


7-methoxy-1-(10*H*-phenothiazin-10-yl)naphthalen-2-amine (3m)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.71 (d, *J* = 8.1 Hz, 2H), 7.18 (s, 1H), 7.10 (d, *J* = 8.8 Hz, 1H), 7.02 (d, *J* = 6.6 Hz, 2H), 6.88 – 6.76 (m, 5H), 6.15 (d, *J* = 7.9 Hz, 2H), 5.63 (s, 2H), 3.66 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 159.16, 145.96, 142.19, 133.74, 130.64, 129.73, 127.97, 126.78, 123.22, 123.01, 120.21, 116.56, 116.12, 114.69, 113.01, 100.82, 55.36.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{23}H_{19}N_2OS^+$, 371.1213, found: 371.1209.

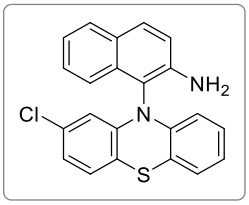


1-(10*H*-phenothiazin-10-yl)-7-phenylnaphthalen-2-amine (3n)

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.00 (s, 1H), 7.90 (d, *J* = 8.4 Hz, 1H), 7.84 (d, *J* = 8.8 Hz, 1H), 7.55 – 7.50 (m, 3H), 7.43 (t, *J* = 7.5 Hz, 2H), 7.34 – 7.28 (m, 2H), 7.04 (dd, *J* = 7.4, 1.8 Hz, 2H), 6.86 – 6.77 (m, 4H), 6.15 (dd, *J* = 7.8, 1.6 Hz, 2H), 5.73 (s, 2H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 145.87, 142.29, 140.87, 139.32, 132.59, 129.77, 129.52, 128.02, 128.00, 127.28, 127.11, 126.87, 123.07, 121.28, 120.05, 119.52, 118.04, 116.09, 115.16.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{28}H_{21}N_2S^+$, 417.1420, found: 417.1414.

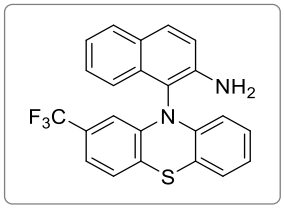


1-(2-chloro-10*H*-phenothiazin-10-yl)naphthalen-2-amine (3o)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.81 (t, *J* = 8.3 Hz, 2H), 7.73 (d, *J* = 8.4 Hz, 1H), 7.39 – 7.35 (m, 1H), 7.27 (d, *J* = 8.9 Hz, 1H), 7.21 – 7.17 (m, 1H), 7.03 – 6.99 (m, 2H), 6.82 – 6.77 (m, 3H), 6.04 – 5.99 (m, 1H), 5.93 (d, *J* = 2.2 Hz, 1H), 5.80 (s, 2H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 145.32, 143.32, 141.10, 132.27, 131.76, 130.44, 129.02, 128.14, 128.11, 127.98, 127.92, 126.81, 123.43, 122.29, 120.16, 119.33, 119.29, 118.80, 116.07, 115.03, 113.37.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{22}H_{16}ClN_2S^+$, 375.0717, found: 375.0712.



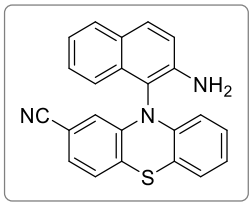
1-(2-(trifluoromethyl)-10*H*-phenothiazin-10-yl)naphthalen-2-amine (3p)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.84 – 7.76 (m, 3H), 7.38 – 7.34 (m, 1H), 7.29 (d, *J* = 8.9 Hz, 1H), 7.20 – 7.16 (m, 2H), 7.07 – 7.05 (m, 1H), 7.03 – 6.99 (m, 1H), 6.82 – 6.77 (m, 2H), 6.18 (d, *J* = 1.9 Hz, 1H), 6.04 – 5.99 (m, 1H), 5.86 (s, 2H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 145.44, 142.58, 141.08, 131.69, 130.56, 129.04, 128.49 (q, *J* = 31.4 Hz), 128.38, 128.12, 127.99, 127.39, 126.84, 125.48 (q, *J* = 1.3 Hz), 124.31 (q, *J* = 270.3 Hz), 123.55, 122.29, 120.05, 119.27, 119.19 (q, *J* = 4 Hz), 118.71, 116.09, 113.04, 111.15 (q, *J* = 4 Hz).

^{19}F NMR (376 MHz, DMSO-d$_6$) δ -61.77.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{23}H_{16}F_3N_2S^+$, 409.0981, found: 409.0978.

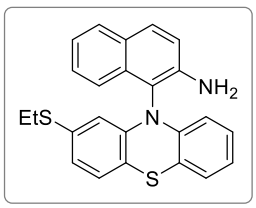


10-(2-aminonaphthalen-1-yl)-10*H*-phenothiazine-2-carbonitrile (3q)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.85 – 7.80 (m, 2H), 7.76 (d, *J* = 8.4 Hz, 1H), 7.40 – 7.36 (m, 1H), 7.29 (d, *J* = 8.9 Hz, 1H), 7.22 – 7.18 (m, 1H), 7.16 (d, *J* = 1.0 Hz, 2H), 7.01 – 6.97 (m, 1H), 6.83 – 6.76 (m, 2H), 6.06 (s, 1H), 6.01 – 5.96 (m, 1H), 5.88 (s, 2H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 145.42, 142.54, 140.71, 131.51, 130.62, 129.08, 128.53, 128.20, 128.04, 127.59, 127.50, 126.86, 126.27, 123.62, 122.32, 119.94, 119.38, 119.17, 118.39, 117.00, 116.09, 112.63, 110.06.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{23}H_{16}N_3S^+$, 366.1059, found: 366.1056.

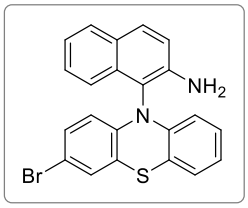


1-(2-(ethylthio)-10*H*-phenothiazin-10-yl)naphthalen-2-amine (3r)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.82 – 7.79 (m, 2H), 7.70 – 7.67 (m, 1H), 7.37 – 7.33 (m, 1H), 7.26 (d, *J* = 8.9 Hz, 1H), 7.21 – 7.17 (m, 1H), 7.02 – 6.98 (m, 1H), 6.95 (d, *J* = 8.0 Hz, 1H), 6.82 – 6.75 (m, 2H), 6.73 (dd, *J* = 8.0, 1.9 Hz, 1H), 6.04 – 5.98 (m, 1H), 5.92 (d, *J* = 1.9 Hz, 1H), 5.69 (s, 2H), 2.63 – 2.54 (m, 2H), 0.96 (t, *J* = 7.3 Hz, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 145.27, 142.24, 141.60, 135.50, 131.99, 130.21, 128.96, 127.97, 127.91, 127.10, 126.76, 123.05, 122.28, 122.18, 120.45, 119.55, 119.28, 116.93, 115.93, 115.15, 113.83, 26.68, 14.49.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{24}H_{21}N_2S_2^+$, 401.1141, found: 401.1137.

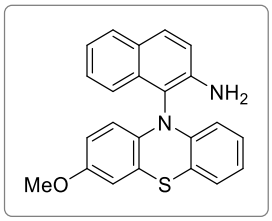


1-(3-bromo-10*H*-phenothiazin-10-yl)naphthalen-2-amine (3s)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.81 – 7.78 (m, 2H), 7.69 (d, *J* = 8.8 Hz, 1H), 7.37 – 7.32 (m, 1H), 7.26 (d, *J* = 8.9 Hz, 1H), 7.19 – 7.16 (m, 2H), 7.01 – 6.97 (m, 1H), 6.95 (dd, *J* = 8.8, 2.3 Hz, 1H), 6.81 – 6.74 (m, 2H), 6.03 – 5.96 (m, 1H), 5.89 (d, *J* = 8.8 Hz, 1H), 5.71 (s, 2H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 145.16, 141.39, 141.37, 131.90, 130.42, 130.25, 128.98, 128.41, 128.18, 128.04, 127.96, 126.79, 123.15, 122.20, 122.18, 120.34, 119.38, 118.83, 117.23, 115.84, 113.80, 113.52.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{22}H_{16}BrN_2S^+$, 419.0212, found: 419.0208.



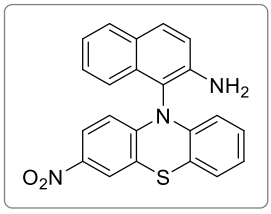
1-(3-methoxy-10*H*-phenothiazin-10-yl)naphthalen-2-amine (3t)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.79 (d, *J* = 8.3 Hz, 2H), 7.67 (d, *J* = 8.3 Hz, 1H), 7.36 – 7.32 (m, 1H), 7.26 (d, *J* = 8.9 Hz, 1H), 7.20 – 7.16 (m, 1H), 6.99 (dd, *J* = 7.3, 1.8 Hz, 1H),

6.80 – 6.71 (m, 2H), 6.65 (d, *J* = 2.8 Hz, 1H), 6.40 (dd, *J* = 9.0, 2.9 Hz, 1H), 5.98 (dd, *J* = 7.9, 1.6 Hz, 1H), 5.94 (d, *J* = 9.0 Hz, 1H), 5.58 (s, 2H), 3.62 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 155.39, 145.21, 142.28, 135.29, 132.34, 129.92, 128.92, 128.08, 127.95, 127.73, 126.67, 122.32, 122.10, 120.85, 120.76, 119.36, 118.80, 116.61, 115.41, 114.66, 113.11, 112.17, 55.81.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{23}H_{19}N_2OS^+$, 371.1213, found: 371.1208.

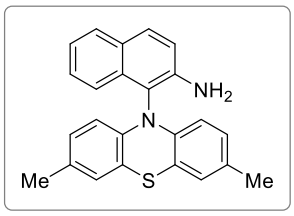


1-(3-nitro-10*H*-phenothiazin-10-yl)naphthalen-2-amine (3u)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.85 – 7.80 (m, 3H), 7.70 – 7.66 (m, 2H), 7.41 – 7.36 (m, 1H), 7.25 (d, *J* = 8.9 Hz, 1H), 7.22 – 7.18 (m, 1H), 7.04 (dd, *J* = 7.2, 1.9 Hz, 1H), 6.88 – 6.80 (m, 2H), 6.02 – 5.97 (m, 2H), 5.92 (s, 2H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 147.98, 144.99, 142.01, 139.70, 131.28, 130.69, 129.05, 128.45, 128.29, 127.92, 126.86, 124.78, 124.62, 122.31, 121.71, 120.41, 119.69, 119.36, 118.75, 116.61, 114.73, 112.26.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{22}H_{16}N_3O_2S^+$, 386.0958, found: 386.0954.

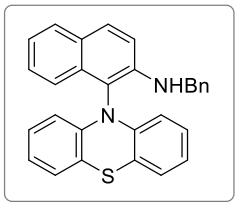


1-(3,7-dimethyl-10*H*-phenothiazin-10-yl)naphthalen-2-amine (3v)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.78 (d, *J* = 8.7 Hz, 2H), 7.63 (d, *J* = 8.3 Hz, 1H), 7.34 – 7.30 (m, 1H), 7.26 (d, *J* = 8.9 Hz, 1H), 7.19 – 7.15 (m, 1H), 6.81 (d, *J* = 2.0 Hz, 2H), 6.58 – 6.55 (m, 2H), 5.86 (d, *J* = 8.3 Hz, 2H), 5.52 (s, 2H), 2.08 (s, 6H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 145.07, 139.56, 132.32, 131.61, 129.87, 128.92, 128.25, 128.10, 127.66, 126.98, 122.09, 120.84, 119.38, 119.11, 115.44, 114.61, 20.18.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{24}H_{21}N_2S^+$, 369.1420, found: 369.1415.

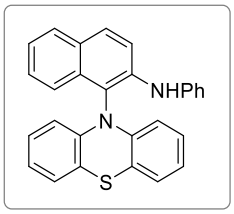


***N*-benzyl-1-(10*H*-phenothiazin-10-yl)naphthalen-2-amine (3w)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 (d, *J* = 8.6 Hz, 2H), 7.74 (d, *J* = 8.4 Hz, 1H), 7.41 – 7.37 (m, 1H), 7.29 – 7.18 (m, 7H), 7.07 – 7.04 (m, 2H), 6.85 – 6.76 (m, 4H), 6.16 – 6.14 (m, 2H), 5.39 (br, 1H), 4.54 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 143.26, 142.13, 139.28, 132.68, 129.99, 128.61, 128.59, 127.82, 127.64, 127.41, 127.11, 126.82, 126.63, 122.89, 122.45, 121.97, 120.47, 116.62, 115.93, 114.75, 47.30.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{29}H_{23}N_2S^+$, 431.1576, found: 431.1571.

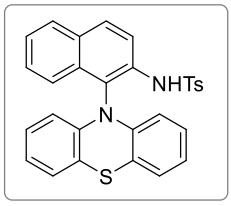


1-(10*H*-phenothiazin-10-yl)-*N*-phenylnaphthalen-2-amine (3x)

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.01 (s, 1H), 7.94 – 7.87 (m, 3H), 7.62 (d, *J* = 9.0 Hz, 1H), 7.42 (t, *J* = 7.5 Hz, 1H), 7.32 – 7.27 (m, 3H), 7.22 (d, *J* = 7.9 Hz, 2H), 7.01 – 6.96 (m, 3H), 6.76 – 6.71 (m, 4H), 6.07 – 6.02 (m, 2H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 142.44, 142.02, 141.93, 131.78, 130.01, 129.88, 129.57, 129.05, 128.19, 127.88, 126.63, 123.79, 122.89, 122.75, 121.64, 121.33, 119.48, 119.41, 118.18, 115.71.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{28}H_{21}N_2S^+$, 417.1420, found: 417.1417.



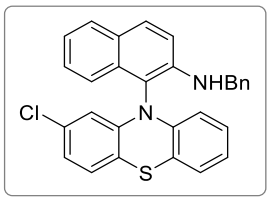
***N*-(1-(10*H*-phenothiazin-10-yl)naphthalen-2-yl)-4-methylbenzenesulfonamide (3y)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.22 (d, *J* = 9.1 Hz, 1H), 7.96 (d, *J* = 9.1 Hz, 1H), 7.92 (d, *J* =

8.1 Hz, 1H), 7.63 (s, 1H), 7.58 (d, *J* = 8.3 Hz, 1H), 7.47 – 7.37 (m, 4H), 7.10 (dd, *J* = 7.6, 1.5 Hz, 2H), 6.86 – 6.82 (m, 4H), 6.59 – 6.55 (m, 2H), 5.71 (d, *J* = 8.2 Hz, 2H), 2.21 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 143.65, 142.54, 135.64, 133.93, 132.04, 131.57, 130.14, 129.50, 128.92, 127.84, 127.31, 126.94, 126.74, 125.67, 124.56, 124.18, 123.38, 121.37, 119.89, 116.22, 21.48.

HRMS-ESI (m/z) $[M-H]^-$ calcd for $C_{29}H_{21}N_2O_2S_2^-$, 493.1050, found: 493.1042.

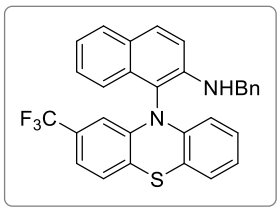


***N*-benzyl-1-(2-chloro-10*H*-phenothiazin-10-yl)naphthalen-2-amine (3z)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 – 7.79 (m, 2H), 7.74 – 7.71 (m, 1H), 7.43 – 7.39 (m, 1H), 7.29 – 7.27 (m, 1H), 7.26 – 7.16 (m, 6H), 7.02 (dd, *J* = 7.5, 1.7 Hz, 1H), 6.93 (d, *J* = 8.1 Hz, 1H), 6.85 – 6.75 (m, 3H), 6.12 – 6.10 (m, 2H), 5.21 (br, 1H), 4.55 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 143.21, 143.11, 141.33, 139.10, 133.28, 132.19, 130.40, 128.70, 128.66, 127.90, 127.61, 127.25, 127.22, 126.80, 126.65, 123.35, 122.73, 122.64, 121.46, 120.08, 118.87, 116.14, 115.84, 115.81, 114.59, 47.27.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{29}H_{22}ClN_2S^+$, 465.1187, found: 465.1185.



***N*-benzyl-1-(2-(trifluoromethyl)-10*H*-phenothiazin-10-yl)naphthalen-2-amine (3aa)**

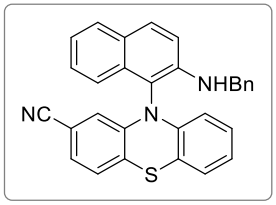
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.83 – 7.79 (m, 2H), 7.75 (d, *J* = 8.5 Hz, 1H), 7.42 – 7.38 (m, 1H), 7.29 – 7.16 (m, 7H), 7.09 (d, *J* = 8.0 Hz, 1H), 7.05 – 7.00 (m, 2H), 6.86 – 6.82 (m, 1H), 6.80 – 6.76 (m, 1H), 6.32 (s, 1H), 6.12 – 6.10 (m, 1H), 5.16 (br, 1H), 4.55 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 143.26, 142.51, 141.28, 139.06, 132.05, 130.63, 129.79 (q, *J* = 32.4 Hz), 128.75, 128.71, 127.98, 127.97, 127.93, 127.27, 126.85, 126.73, 126.71, 125.31, 123.83 (q, *J* = 270.5 Hz), 123.56, 122.74, 121.28, 119.51 (q, *J* = 3.9 Hz), 119.44,

116.18, 115.48, 114.52, 112.02 (q, *J* = 3.9 Hz), 47.25.

^{19}F NMR (376 MHz, $CDCl_3$) δ -62.90.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{30}H_{22}F_3N_2S^+$, 499.1450, found: 499.1445.

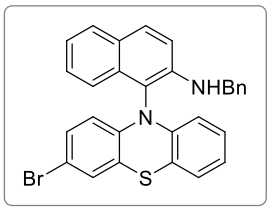


10-(2-(benzylamino)naphthalen-1-yl)-10*H*-phenothiazine-2-carbonitrile (3ab)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84 – 7.80 (m, 2H), 7.65 (d, *J* = 8.4 Hz, 1H), 7.41 – 7.37 (m, 1H), 7.30 – 7.25 (m, 2H), 7.24 – 7.17 (m, 5H), 7.02 – 7.01 (m, 2H), 6.96 (dd, *J* = 7.5, 1.7 Hz, 1H), 6.85 – 6.81 (m, 1H), 6.79 – 6.75 (m, 1H), 6.20 – 6.19 (m, 1H), 6.07 (dd, *J* = 8.1, 1.4 Hz, 1H), 5.12 (br, 1H), 4.54 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 143.01, 142.58, 140.70, 138.94, 131.72, 130.78, 128.92, 128.76, 128.12, 128.10, 127.56, 127.37, 126.91, 126.79, 126.67, 126.30, 123.73, 122.86, 121.00, 118.82, 118.74, 117.88, 116.22, 114.95, 114.65, 110.76, 47.31.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{30}H_{22}N_3S^+$, 456.1529, found: 456.1523.

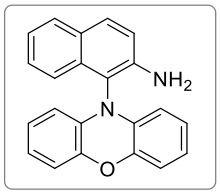


***N*-benzyl-1-(3-bromo-10*H*-phenothiazin-10-yl)naphthalen-2-amine (3ac)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.81 – 7.78 (m, 2H), 7.66 – 7.63 (m, 1H), 7.40 – 7.36 (m, 1H), 7.28 – 7.27 (m, 1H), 7.25 – 7.20 (m, 3H), 7.19 – 7.16 (m, 3H), 7.14 (d, *J* = 2.3 Hz, 1H), 7.02 (dd, *J* = 7.5, 1.7 Hz, 1H), 6.85 – 6.81 (m, 2H), 6.80 – 6.75 (m, 1H), 6.11 (dd, *J* = 8.1, 1.4 Hz, 1H), 5.94 (d, *J* = 8.8 Hz, 1H), 5.29 (br, 1H), 4.53 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 143.15, 141.68, 141.37, 139.13, 132.31, 130.22, 129.98, 128.72, 128.68, 128.63, 127.82, 127.78, 127.67, 127.20, 126.79, 126.67, 123.18, 122.67, 122.57, 121.64, 119.62, 117.10, 116.04, 115.99, 114.78, 114.77, 47.31.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{29}H_{22}BrN_2S^+$, 509.0682, found: 509.0680.

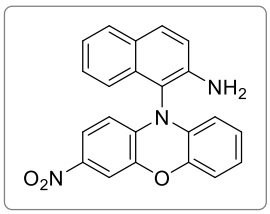


1-(10*H*-phenoxazin-10-yl)naphthalen-2-amine (4a)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.79 – 7.76 (m, 2H), 7.51 (d, *J* = 8.3 Hz, 1H), 7.32 – 7.28 (m, 1H), 7.22 (d, *J* = 8.9 Hz, 1H), 7.17 – 7.13 (m, 1H), 6.71 (dd, *J* = 7.8, 1.5 Hz, 2H), 6.62 – 6.58 (m, 2H), 6.53 – 6.49 (m, 2H), 5.78 (s, 2H), 5.65 (dd, *J* = 7.9, 1.5 Hz, 2H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 145.51, 144.41, 132.76, 131.92, 130.16, 129.11, 128.20, 127.64, 124.13, 121.85, 121.49, 120.49, 119.53, 115.59, 112.96, 109.79.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{22}H_{17}N_2O^+$, 325.1335, found: 325.1332.

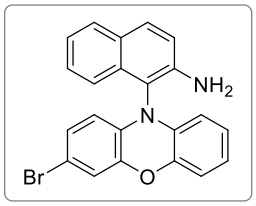


1-(3-nitro-10*H*-phenoxazin-10-yl)naphthalen-2-amine (4b)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.83 – 7.80 (m, 2H), 7.55 – 7.51 (m, 2H), 7.44 (d, *J* = 2.5 Hz, 1H), 7.36 – 7.32 (m, 1H), 7.23 – 7.17 (m, 2H), 6.80 (dd, *J* = 7.9, 1.6 Hz, 1H), 6.76 – 6.72 (m, 1H), 6.62 – 6.58 (m, 1H), 6.08 (s, 2H), 5.75 – 5.72 (m, 2H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 145.06, 144.43, 144.24, 140.77, 140.15, 130.88, 130.73, 129.21, 128.16, 127.90, 124.70, 123.63, 122.11, 121.94, 119.82, 119.59, 115.90, 114.01, 111.95, 110.23, 107.95.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{22}H_{16}N_3O_3^+$, 370.1186, found: 370.1187.



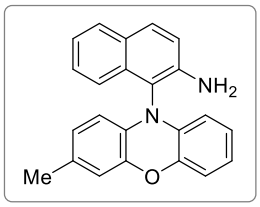
1-(3-bromo-10*H*-phenoxazin-10-yl)naphthalen-2-amine (4c)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.79 – 7.77 (m, 2H), 7.52 (d, *J* = 8.3 Hz, 1H), 7.32 – 7.28 (m, 1H), 7.23 (d, *J* = 8.9 Hz, 1H), 7.18 – 7.14 (m, 1H), 6.90 (d, *J* = 2.2 Hz, 1H), 6.73 – 6.69

(m, 2H), 6.64 – 6.59 (m, 1H), 6.55 – 6.51 (m, 1H), 5.89 (s, 2H), 5.67 (dd, *J* = 8.0, 1.6 Hz, 1H), 5.57 (d, J = 8.5 Hz, 1H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 145.48, 145.42, 144.12, 132.50, 132.28, 131.76, 130.38, 129.16, 128.13, 127.80, 126.63, 124.51, 121.93, 121.75, 120.28, 119.58, 118.16, 115.72, 114.28, 113.10, 111.68, 109.08.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{22}H_{16}BrN_2O^+$, 403.0441, found: 403.0441.

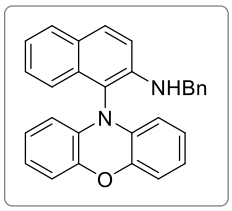


1-(3-methyl-10*H*-phenoxazin-10-yl)naphthalen-2-amine (4d)

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.79 – 7.76 (m, 2H), 7.51 (d, *J* = 8.3 Hz, 1H), 7.30 – 7.23 (m, 2H), 7.16 – 7.13 (m, 1H), 6.72 – 6.70 (m, 1H), 6.60 – 6.56 (m, 2H), 6.52 – 6.48 (m, 1H), 6.33 (dd, *J* = 8.0, 1.9 Hz, 1H), 5.74 (s, 2H), 5.67 – 5.64 (m, 1H), 5.57 (d, *J* = 8.0 Hz, 1H), 2.08 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 145.51, 144.30, 144.12, 132.94, 132.00, 130.70, 130.20, 130.07, 129.09, 128.24, 127.55, 124.14, 124.08, 121.84, 121.17, 120.60, 119.53, 116.32, 115.61, 112.83, 112.80, 110.11, 20.48.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{23}H_{19}N_2O^+$, 339.1492, found: 339.1488.

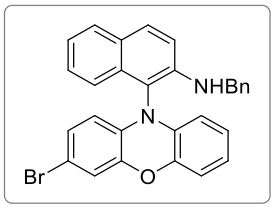


***N*-benzyl-1-(10*H*-phenoxazin-10-yl)naphthalen-2-amine (4e)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 – 7.75 (m, 3H), 7.36 - 7.32 (m, 1H), 7.29 – 7.21 (m, 6H), 7.13 (d, *J* = 9.0 Hz, 1H), 6.76 (dd, *J* = 7.9, 1.5 Hz, 2H), 6.69 – 6.65 (m, 2H), 6.57 – 6.53 (m, 2H), 5.84 (dd, *J* = 7.9, 1.5 Hz, 2H), 5.19 (br, 1H), 4.53 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 144.42, 143.83, 139.25, 132.26, 131.76, 130.20, 128.61, 128.57, 128.25, 127.57, 127.16, 126.87, 123.81, 122.43, 121.71, 121.37, 115.63, 114.47, 113.23, 112.73, 47.24.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{29}H_{23}N_2O^+$, 415.1805, found: 415.1801.

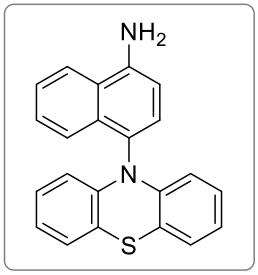


***N*-benzyl-1-(3-bromo-10*H*-phenoxazin-10-yl)naphthalen-2-amine (4f)**

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 – 7.76 (m, 2H), 7.73 – 7.70 (m, 1H), 7.38 – 7.34 (m, 1H), 7.29 – 7.22 (m, 6H), 7.14 (d, *J* = 9.0 Hz, 1H), 6.90 (d, *J* = 2.2 Hz, 1H), 6.78 – 6.75 (m, 1H), 6.71 – 6.67 (m, 1H), 6.66 – 6.62 (m, 1H), 6.59 – 6.55 (m, 1H), 5.86 – 5.84 (m, 1H), 5.68 (d, *J* = 8.5 Hz, 1H), 5.15 (br, 1H), 4.53 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 145.12, 144.01, 143.76, 139.13, 131.76, 131.69, 131.46, 130.47, 128.68, 128.26, 127.75, 127.28, 126.87, 126.43, 124.23, 122.58, 122.04, 121.09, 118.79, 115.82, 114.49, 114.31, 113.37, 112.96, 112.16, 47.24.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{29}H_{22}BrN_2O^+$, 493.0910, found: 493.0907.

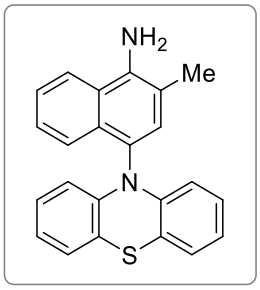


4-(10*H*-phenothiazin-10-yl)naphthalen-1-amine (5a)

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.25 – 8.21 (m, 1H), 7.77 – 7.73 (m, 1H), 7.44 – 7.38 (m, 2H), 7.35 (d, *J* = 8.0 Hz, 1H), 7.03 – 6.98 (m, 2H), 6.85 (d, *J* = 8.0 Hz, 1H), 6.78 – 6.73 (m, 4H), 6.16 (s, 2H), 6.06 – 6.02 (m, 2H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 146.23, 144.31, 131.55, 130.73, 127.67, 127.40, 126.79, 124.81, 124.35, 124.02, 123.88, 123.03, 122.74, 118.94, 115.99, 107.74.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{22}H_{17}N_2S^+$, 341.1107, found: 341.1105.

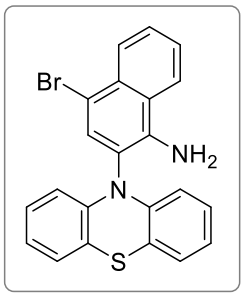


2-methyl-4-(10*H*-phenothiazin-10-yl)naphthalen-1-amine (5b)

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.31 (d, *J* = 8.4 Hz, 1H), 7.72 – 7.69 (m, 1H), 7.42 – 7.38 (m, 1H), 7.35 – 7.31 (m, 2H), 7.01 – 6.96 (m, 2H), 6.75 – 6.70 (m, 4H), 6.02 – 5.98 (m, 2H), 5.84 (s, 2H), 2.33 (s, 3H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 144.27, 142.85, 132.85, 130.17, 127.63, 126.73, 126.35, 124.85, 124.06, 123.77, 123.63, 122.98, 122.67, 118.86, 116.03, 115.09, 18.33.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{23}H_{19}N_2S^+$, 355.1263, found: 355.1261.

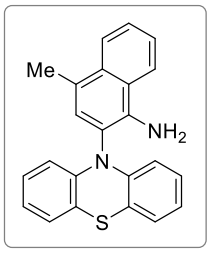


4-bromo-2-(10*H*-phenothiazin-10-yl)naphthalen-1-amine (5c)

^{1}H NMR (400 MHz, DMSO-d_6) δ 8.37 (d, *J* = 8.4 Hz, 1H), 8.11 – 8.08 (m, 1H), 7.74 – 7.69 (m, 1H), 7.61 – 7.56 (m, 2H), 7.01 (dd, *J* = 7.5, 1.7 Hz, 2H), 6.89 – 6.85 (m, 2H), 6.82 – 6.78 (m, 2H), 6.17 (dd, *J* = 8.1, 1.4 Hz, 2H), 6.07 (s, 2H).

^{13}C NMR (100 MHz, DMSO-d_6) δ 143.43, 142.42, 132.79, 132.02, 128.81, 127.91, 127.04, 126.81, 125.95, 124.95, 124.42, 123.08, 119.74, 118.18, 115.99, 107.35.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{22}H_{16}BrN_2S^+$, 419.0212, found: 419.0208.

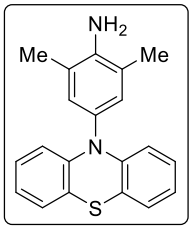


4-methyl-2-(10*H*-phenothiazin-10-yl)naphthalen-1-amine (5d)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (d, *J* = 8.4 Hz, 1H), 7.87 (d, *J* = 8.3 Hz, 1H), 7.60 – 7.56 (m, 1H), 7.51 – 7.47 (m, 1H), 7.18 (s, 1H), 7.01 – 6.97 (m, 2H), 6.81 – 6.75 (m, 4H), 6.31 – 6.26 (m, 2H), 4.38 (s, 2H), 2.62 (s, 3H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 143.09, 138.83, 133.09, 129.24, 127.31, 126.74, 126.62, 125.99, 125.20, 125.09, 125.06, 122.77, 122.25, 120.22, 119.47, 115.71, 19.02.

HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{23}H_{19}N_2S^+$, 355.1263, found: 355.1262.

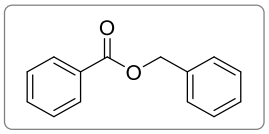


2,6-dimethyl-4-(10*H*-phenothiazin-10-yl)aniline (5e)

^{1}H NMR (400 MHz, DMSO-d_6) δ 6.97 – 6.95 (m, 2H), 6.88 – 6.83 (m, 4H), 6.78 – 6.74 (m, 2H), 6.22 – 6.20 (m, 2H), 4.86 (s, 2H), 2.16 (s, 6H).

^{13}C NMR (101 MHz, DMSO-d_6) δ 144.92, 144.88, 129.74, 127.96, 127.56, 126.71, 123.16, 122.49, 118.78, 116.08, 18.32.

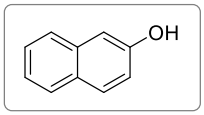
HRMS-ESI (m/z) $[M+H]^+$ calcd for $C_{20}H_{19}N_2S^+$, 319.1263, found: 319.1261.



Benzyl benzoate (7a)

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.12 – 8.09 (m, 2H), 7.59 – 7.55 (m, 1H), 7.49 – 7.34 (m, 7H), 5.39 (s, 2H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 166.47, 136.11, 133.07, 130.19, 129.75, 128.64, 128.42, 128.28, 128.21, 66.73.

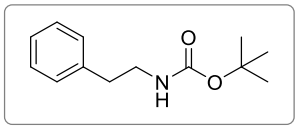


2-naphthol (7b)

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.80 (t, *J* = 8.8 Hz, 2H), 7.71 (d, *J* = 8.2 Hz, 1H), 7.49 – 7.45

(m, 1H), 7.39 – 7.35 (m, 1H), 7.19 – 7.13 (m, 2H), 5.36 (s, 1H).

^{13}C NMR (100 MHz, $CDCl_3$) δ 153.34, 134.63, 129.91, 128.99, 127.82, 126.58, 126.43, 123.68, 117.79, 109.58.

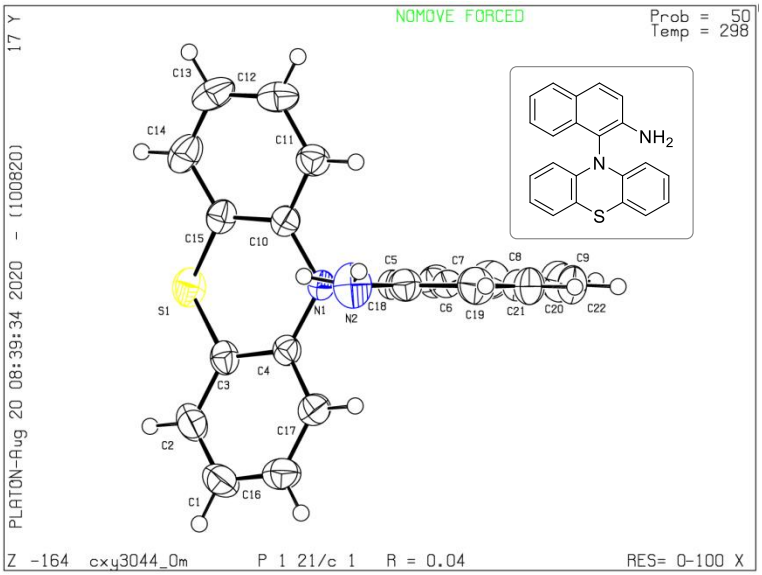


***tert*-Butyl phenethylcarbamate (9)**

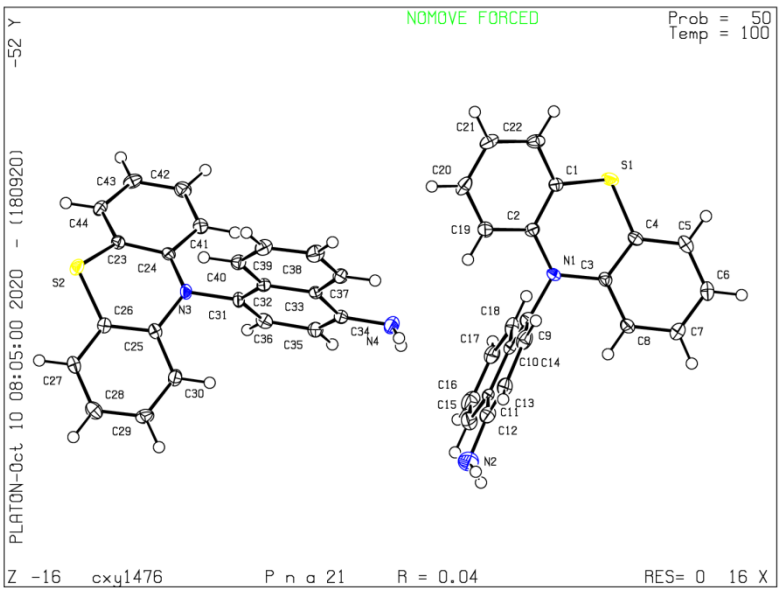
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.33 – 7.29 (m, 2H), 7.24 – 7.18 (m, 3H), 4.58 (s, 1H), 3.41 – 3.36 (m, 2H), 2.80 (t, *J* = 7.1 Hz, 2H), 1.44 (s, 9H).

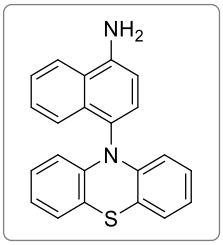
^{13}C NMR (100 MHz, $CDCl_3$) δ 155.89, 139.04, 128.82, 128.58, 126.40, 79.20, 41.80, 36.23, 28.43.

11. X-ray crystal structural parameters



Identification code	**3a** (CCDC: 2077101)
Empirical formula	$C_{22}H_{16}N_2S$
Formula weight	340.43
Temperature/K	298
Crystal system	monoclinic
Space group	$P2_{1/c}$
a/Å	12.1982(16)
b/Å	8.3863(11)
c/Å	17.209(2)
α/°	90
β/°	107.749(5)
γ/°	90
Volume/Å^3	1676.7(4)
Z	4
ρ_{calc}g/cm^3	1.349
μ/mm^{-1}	1.743
F(000)	712.0
Crystal size/mm^3	0.23 × 0.22 × 0.16
Radiation	CuKα (λ = 1.54178)
2Θ range for data collection/°	7.61 to 145.41
Index ranges	$-15 \leqslant h \leqslant 12$, $-10 \leqslant k \leqslant 10$, $-20 \leqslant l \leqslant 21$
Reflections collected	41395
Independent reflections	3290 [R_{int} = 0.0396, R_{sigma} = 0.0255]
Data/restraints/parameters	3290/0/228
Goodness-of-fit on F^2	1.065
Final R indexes [I>=2σ (I)]	R_1 = 0.0353, wR_2 = 0.0973
Final R indexes [all data]	R_1 = 0.0359, wR_2 = 0.0978
Largest diff. peak/hole / e Å^{-3}	0.24/-0.24





Identification code	**5a** (CCDC: 2077102)
Empirical formula	$C_{22}H_{16}N_2S$
Formula weight	340.43
Temperature/K	100
Crystal system	orthorhombic
Space group	$Pna2_1$
a/Å	13.9618(5)
b/Å	8.6489(3)
c/Å	26.7485(10)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	3230.0(2)
Z	8
ρ_{calc}g/cm^3	1.400
μ/mm^{-1}	0.207
F(000)	1424.0
Crystal size/mm^3	0.4 × 0.33 × 0.26
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.95 to 55.07
Index ranges	$-18 \leqslant h \leqslant 18, -11 \leqslant k \leqslant 11, -34 \leqslant l \leqslant 34$
Reflections collected	44238
Independent reflections	7433 [R_{int} = 0.0386, R_{sigma} = 0.0282]
Data/restraints/parameters	7433/1/453
Goodness-of-fit on F^2	1.036
Final R indexes [I>=2σ (I)]	R_1 = 0.0424, wR_2 = 0.1069
Final R indexes [all data]	R_1 = 0.0479, wR_2 = 0.1111
Largest diff. peak/hole / e Å^{-3}	0.83/-0.26
Flack parameter	0.48(9)

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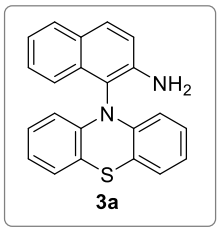
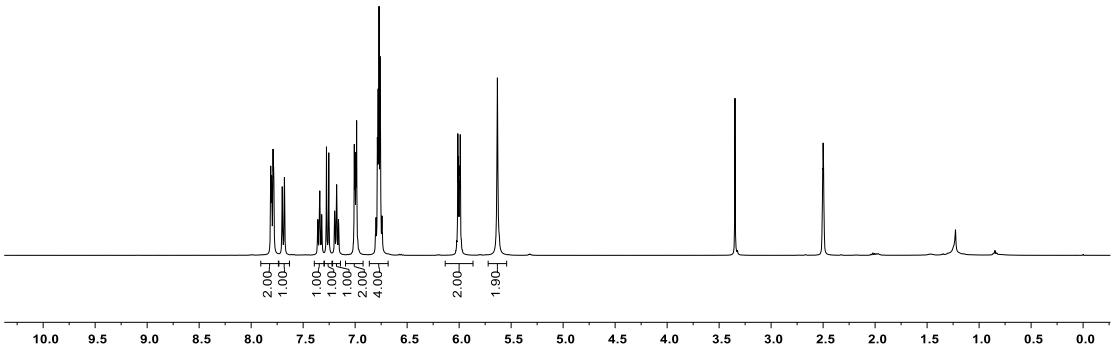
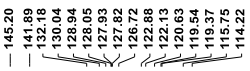
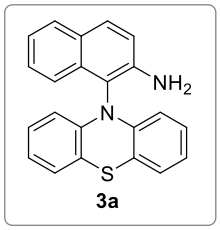
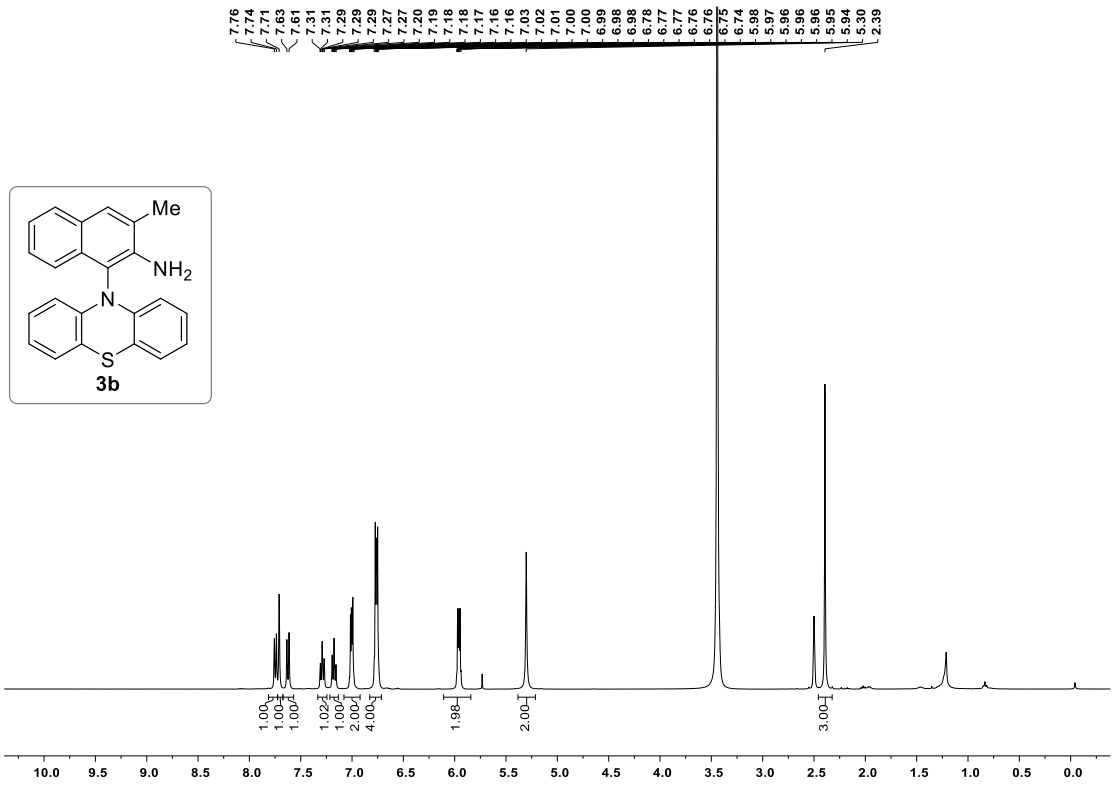
Copies of NMR spectra







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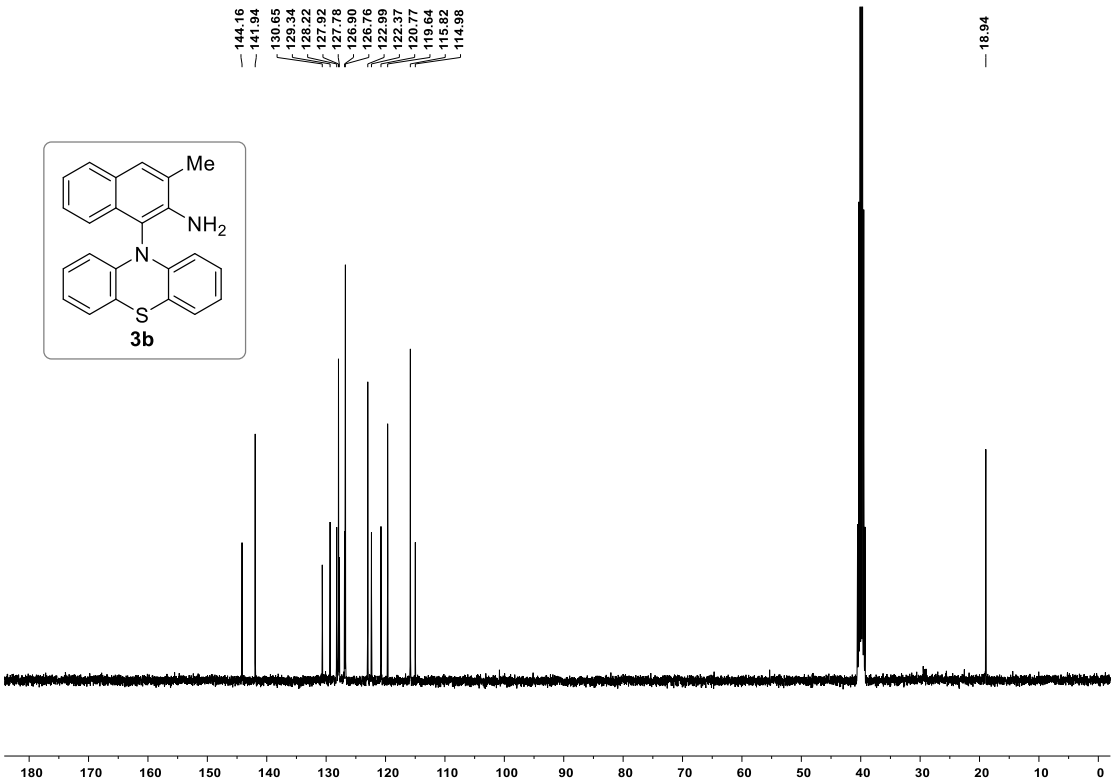
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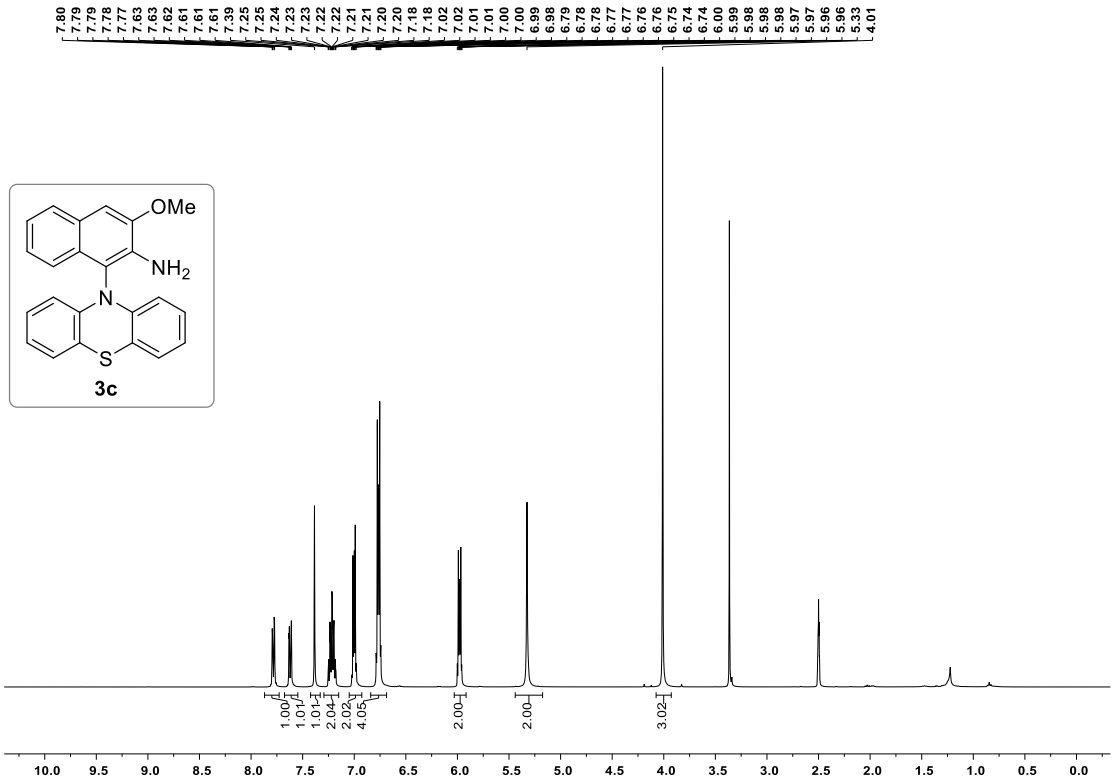
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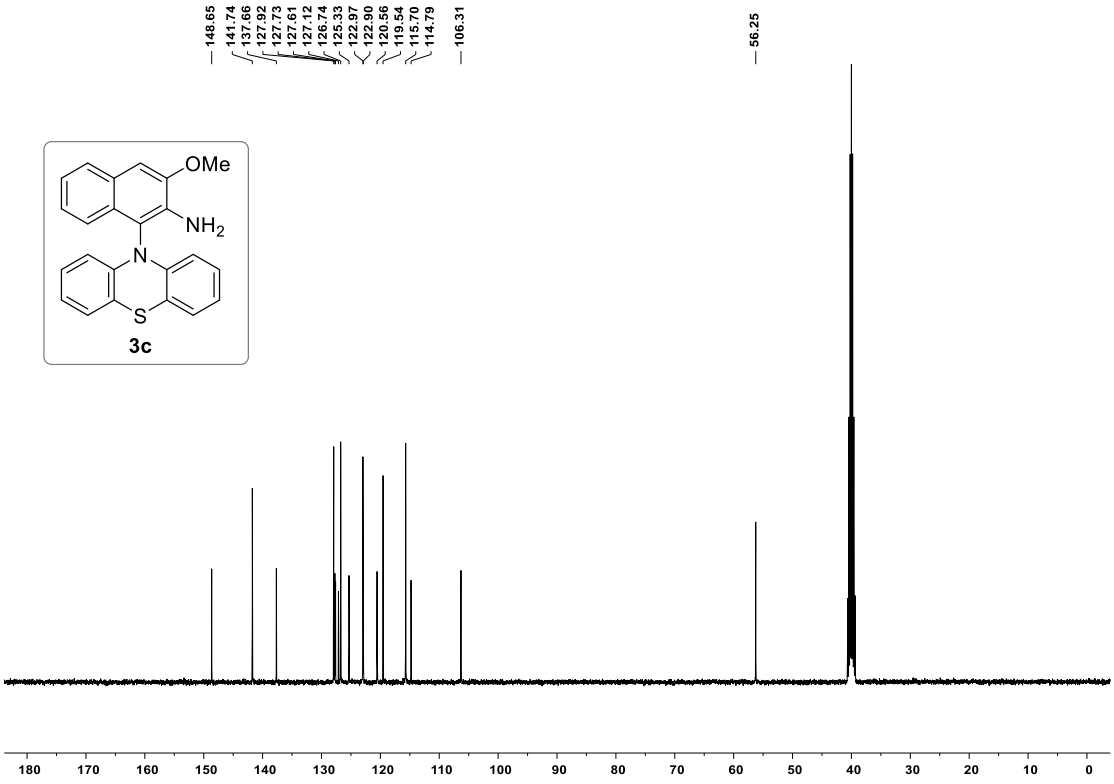
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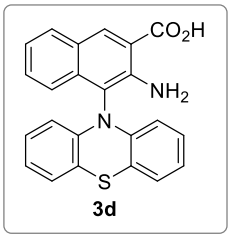
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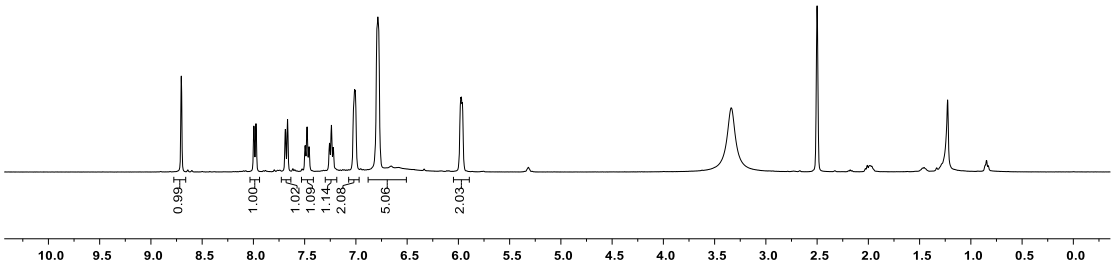
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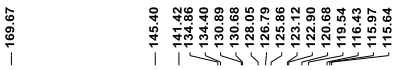
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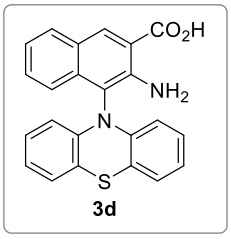
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NH2
N
S

3d

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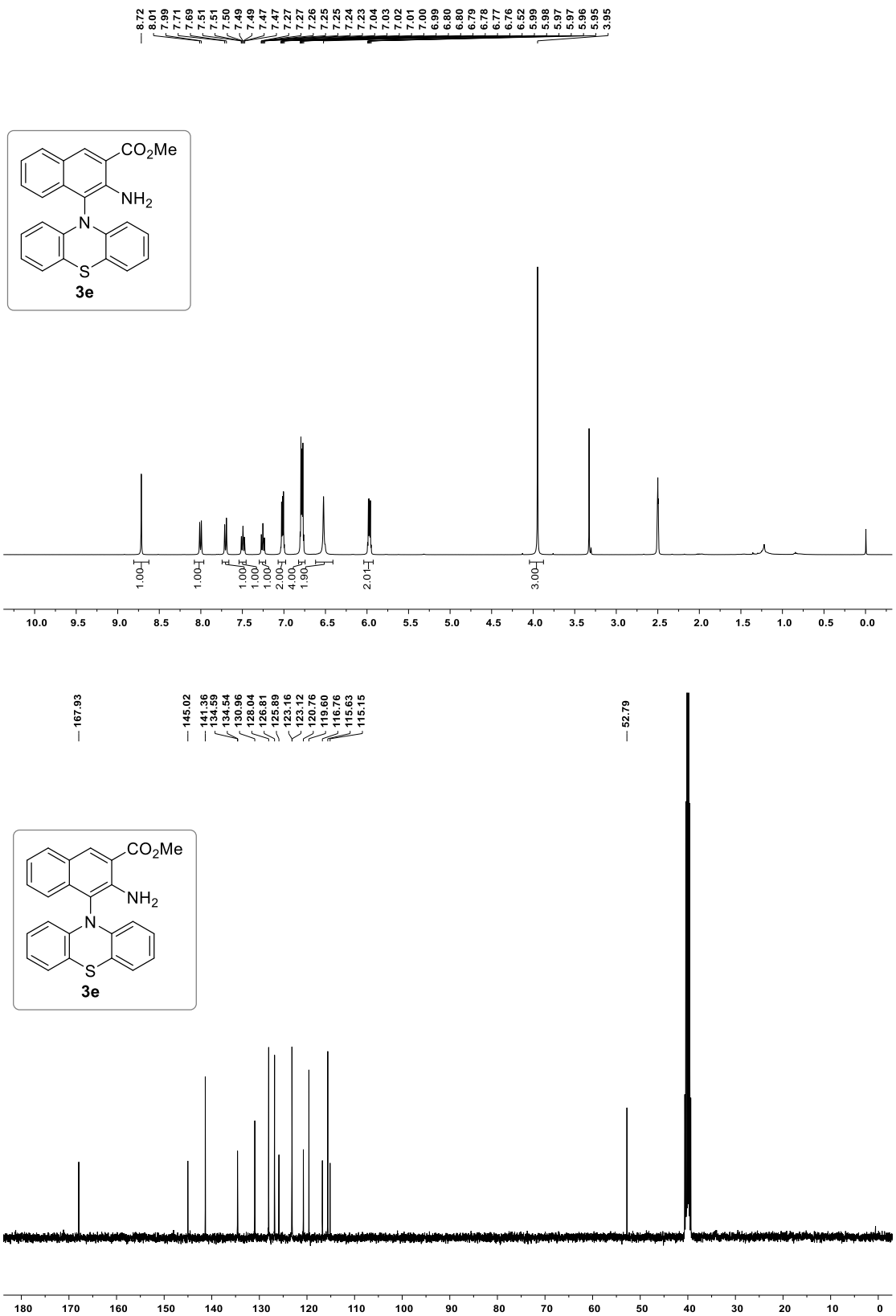
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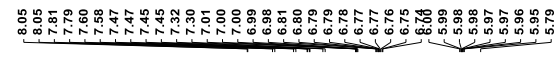
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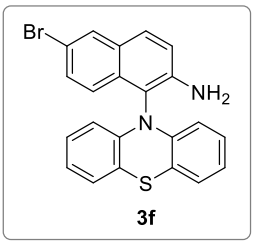
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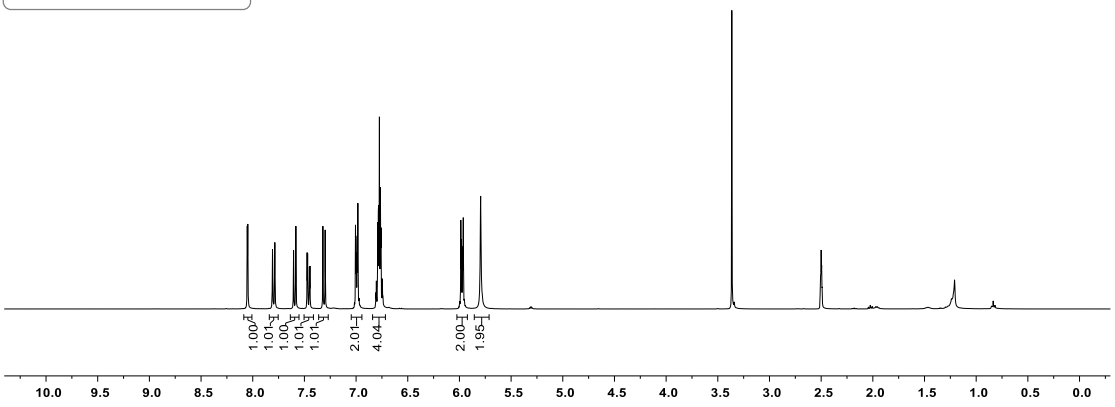
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7.5
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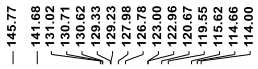
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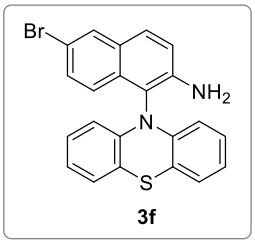
Br
NH2
N
S

3f

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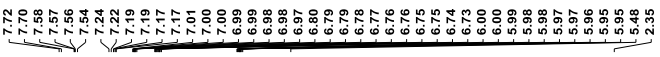
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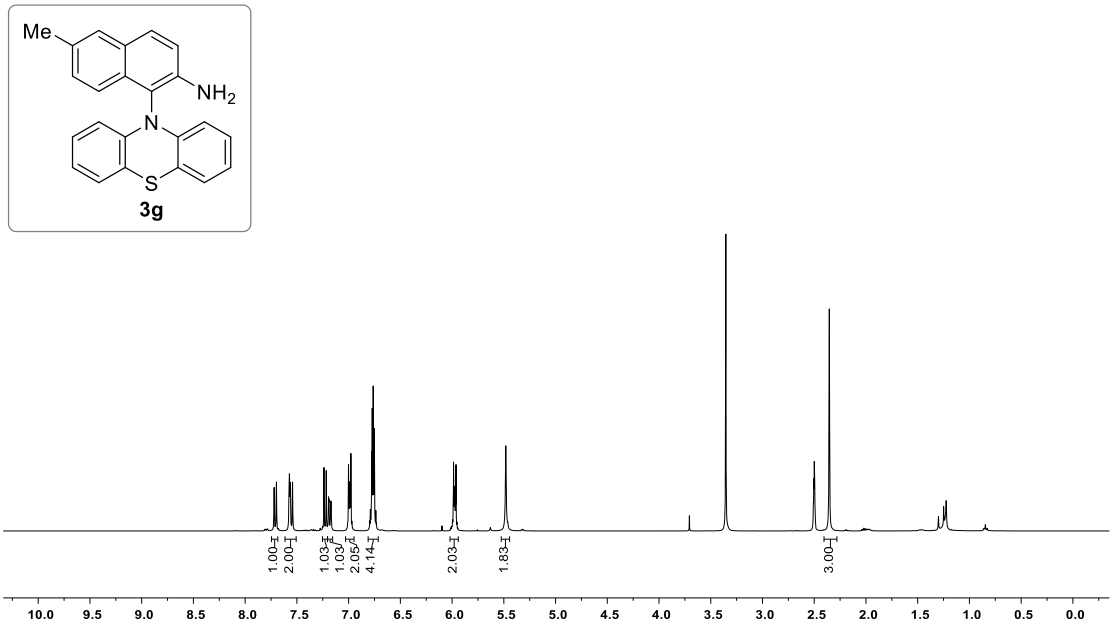
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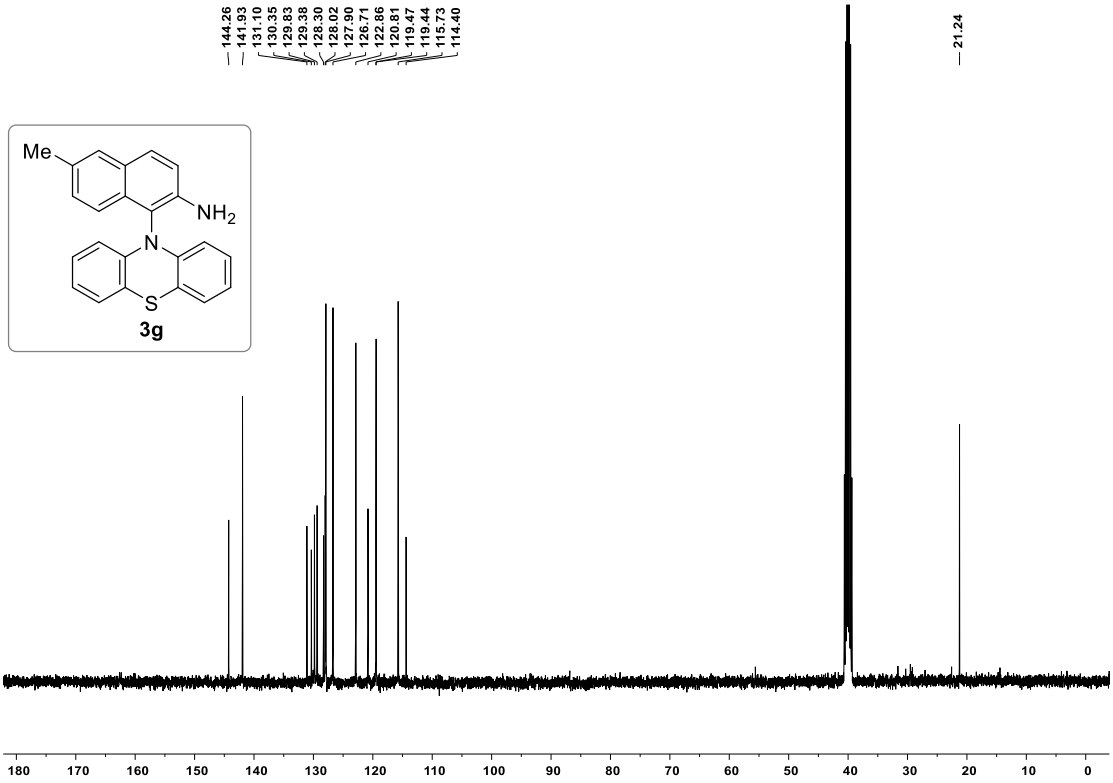
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S
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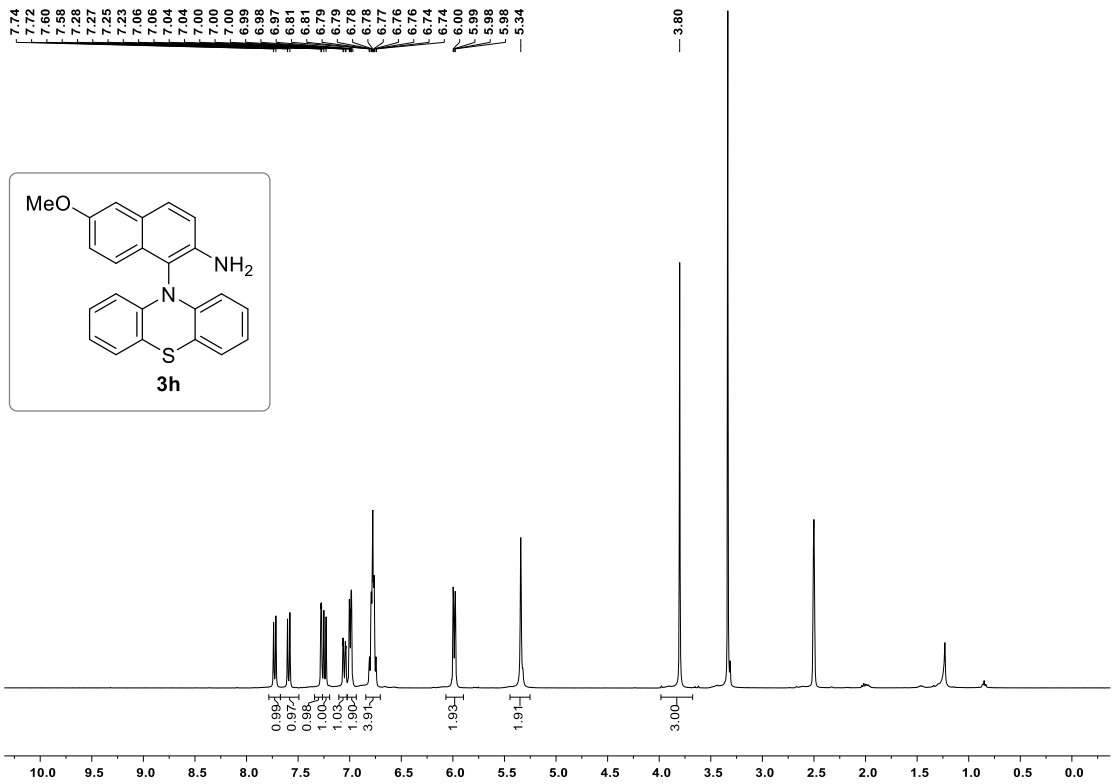
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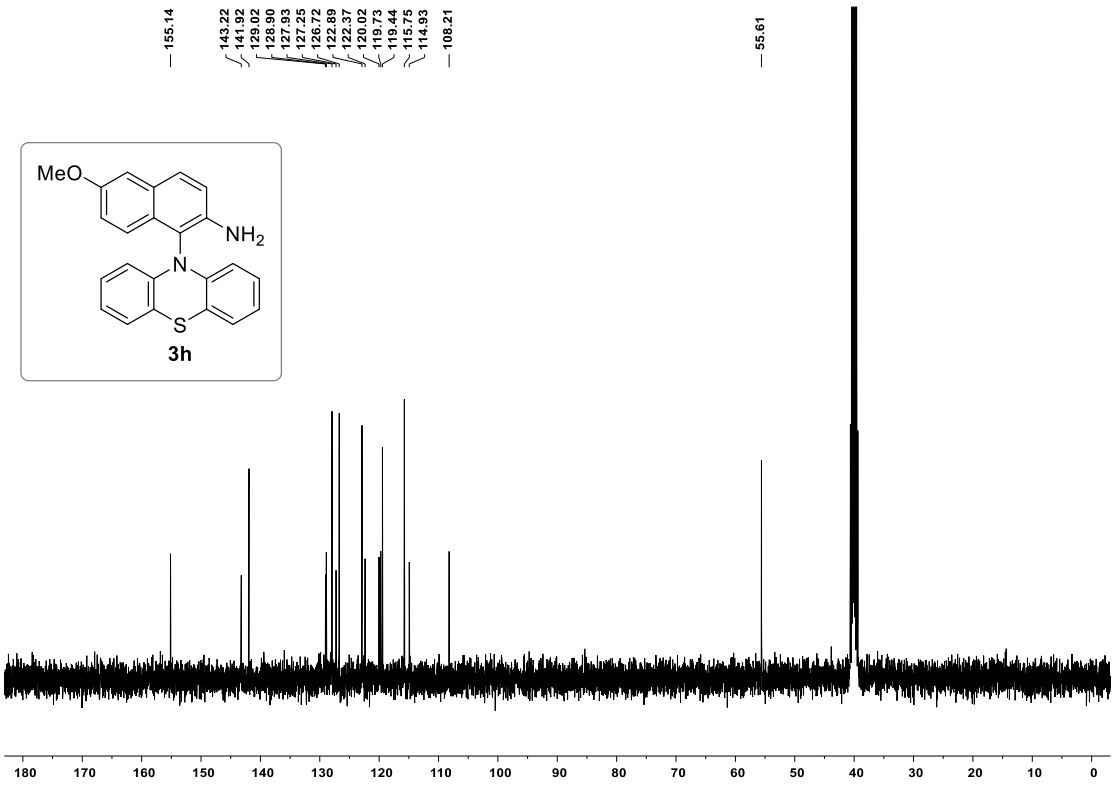
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S
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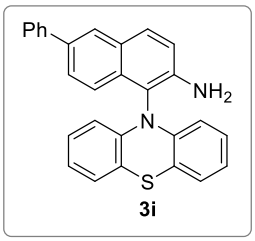
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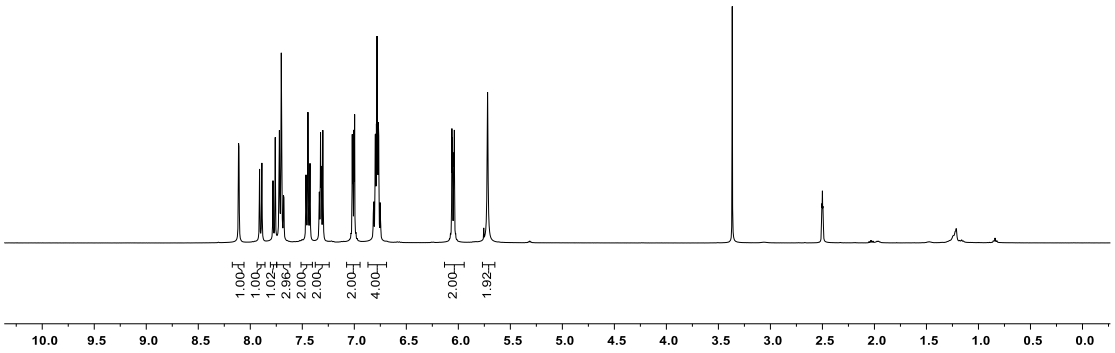
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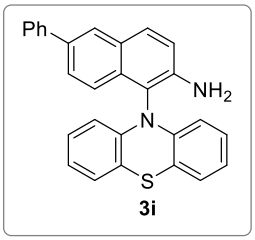
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S

3i

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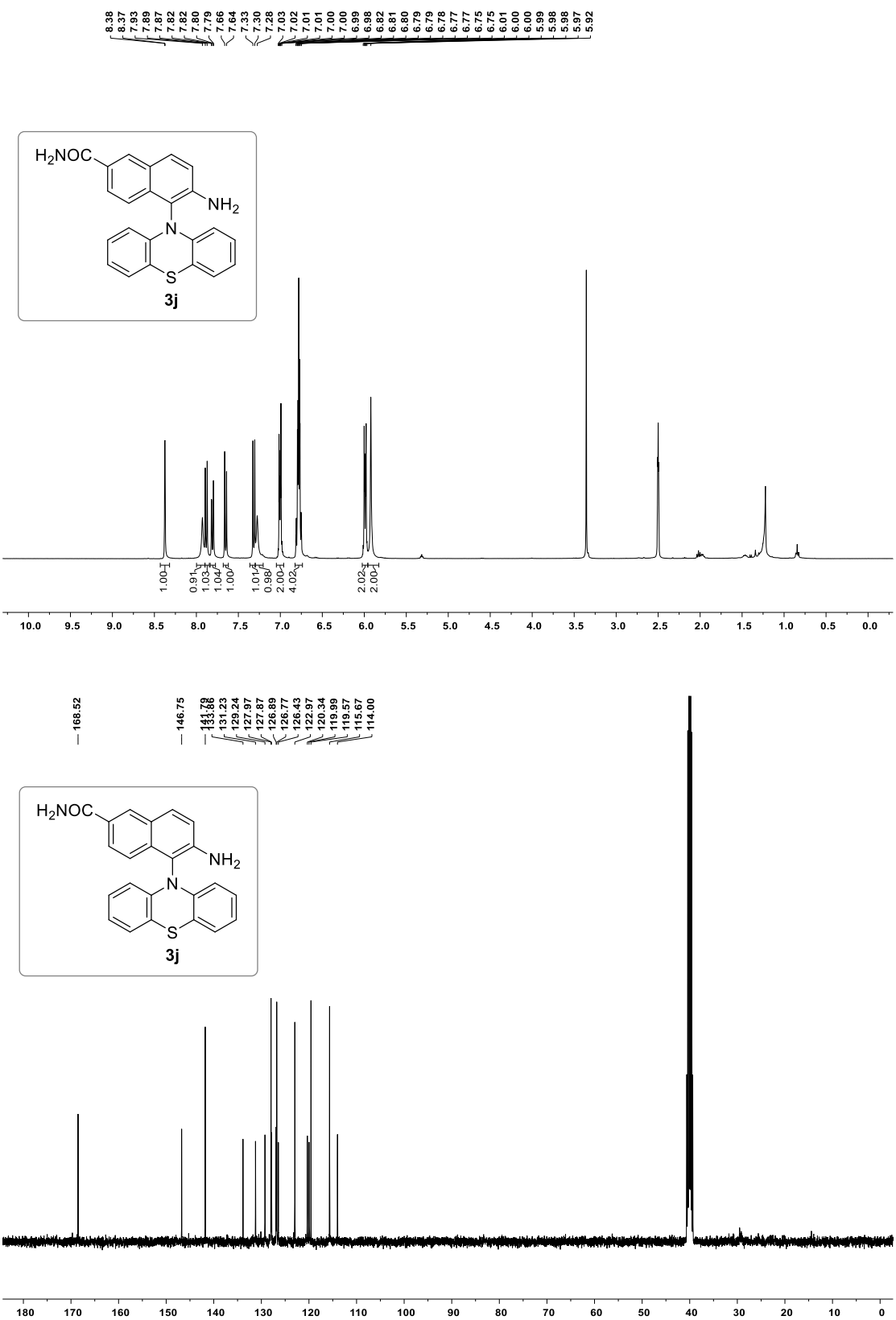
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5.98
5.97
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NH2
N
S
3j
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1.03
1.04
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3j
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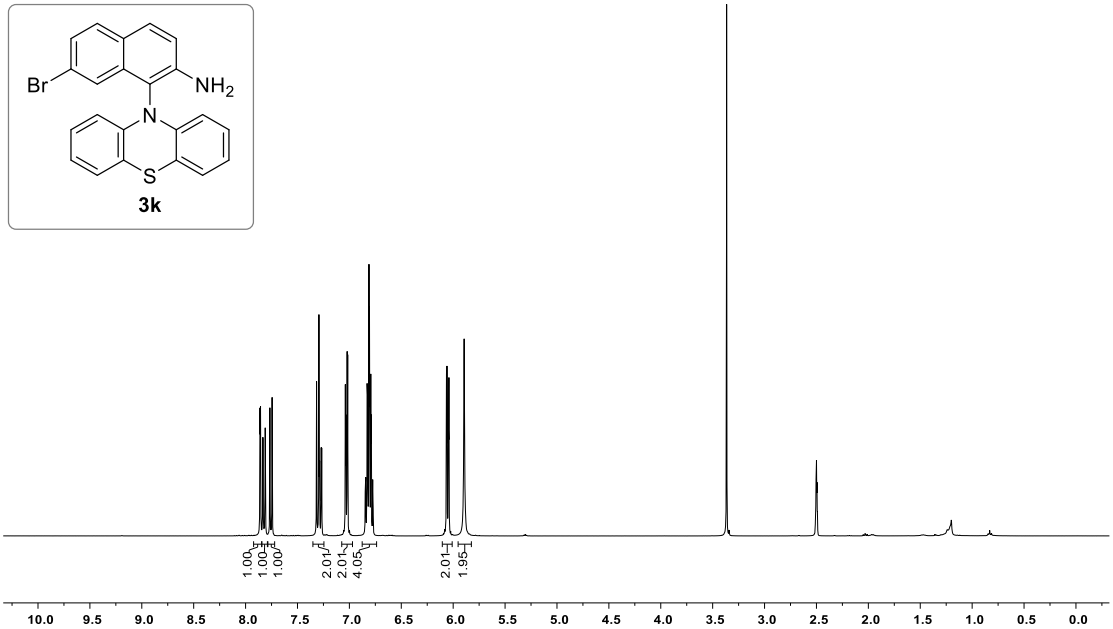
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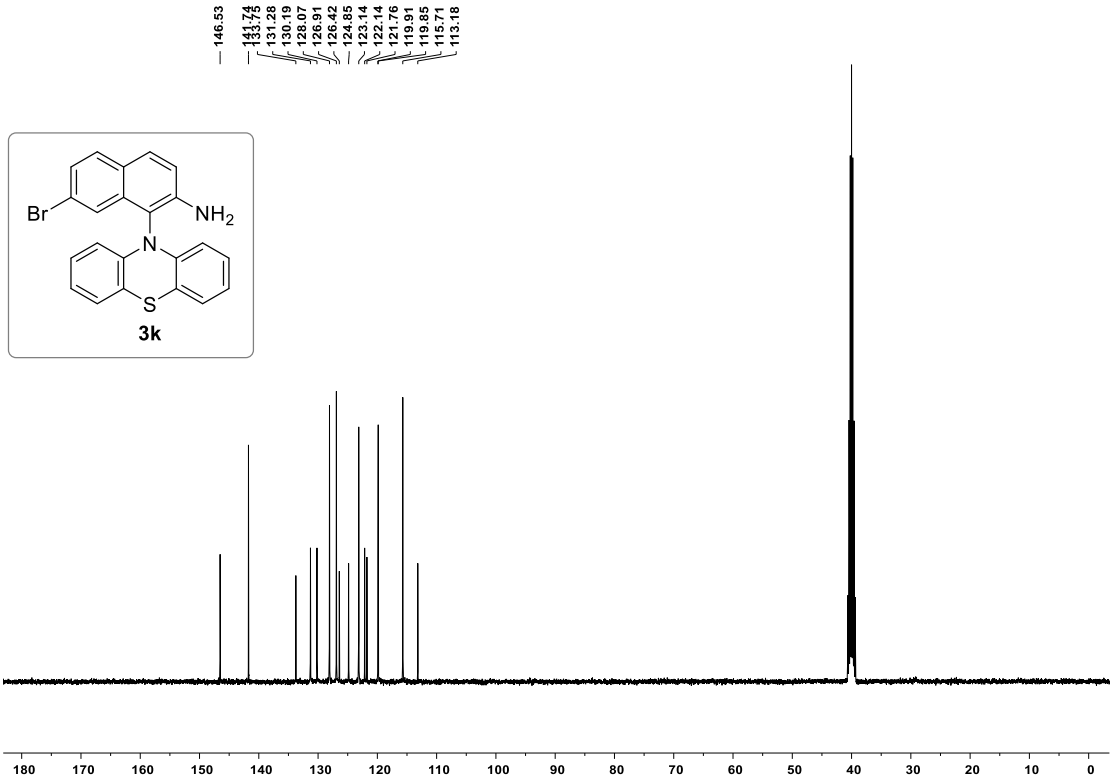
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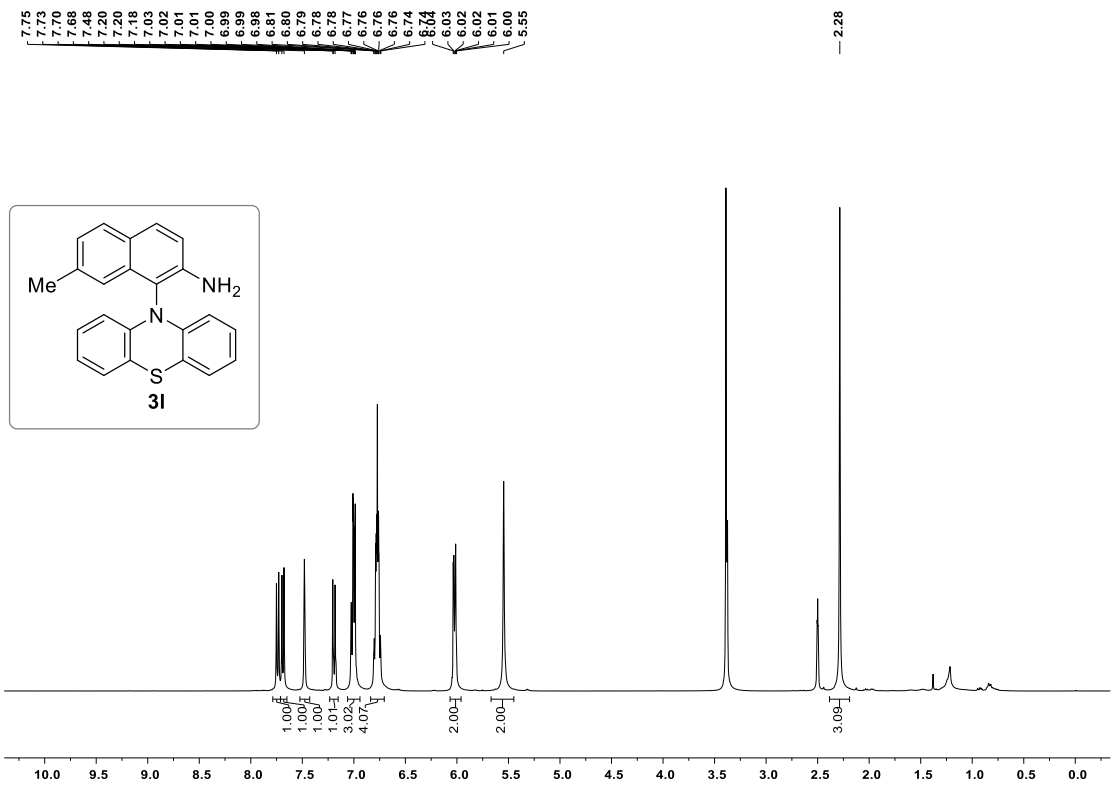
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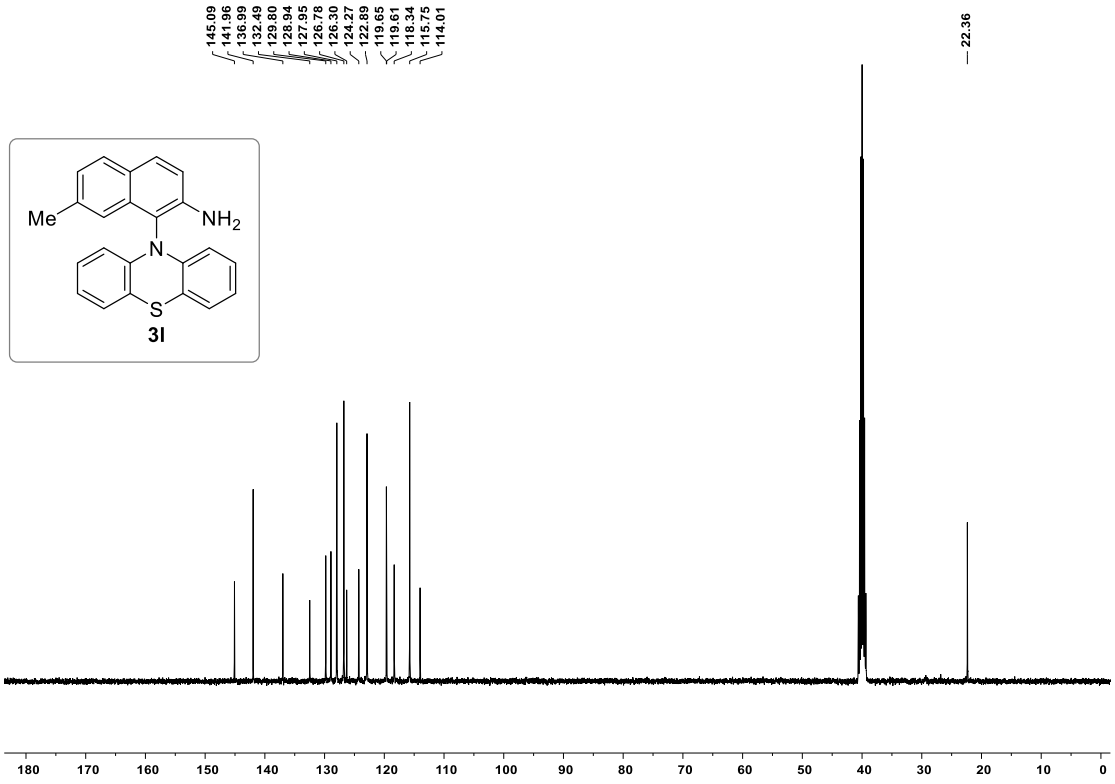
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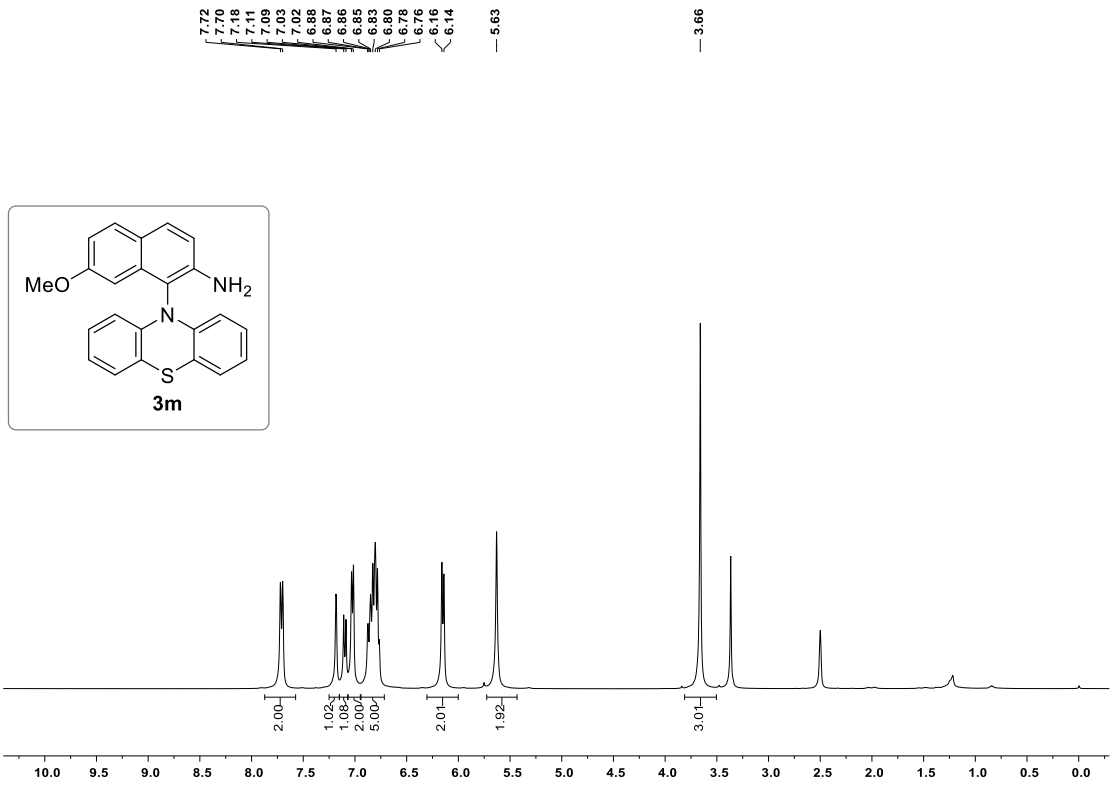
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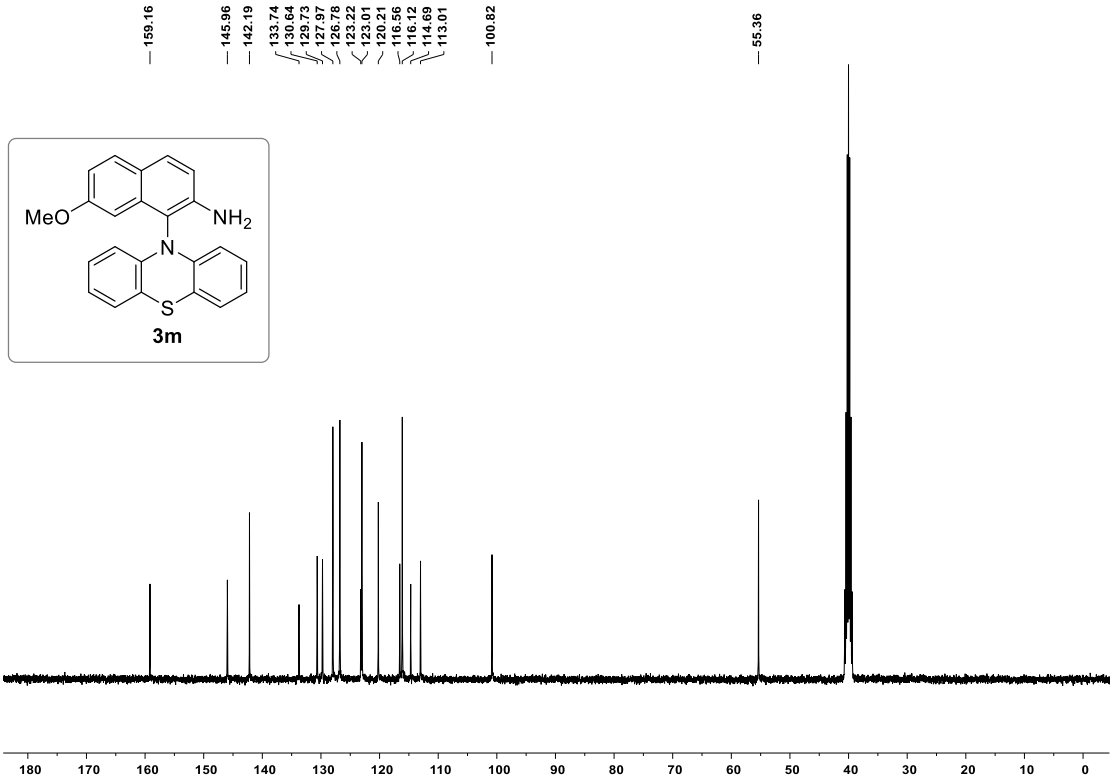
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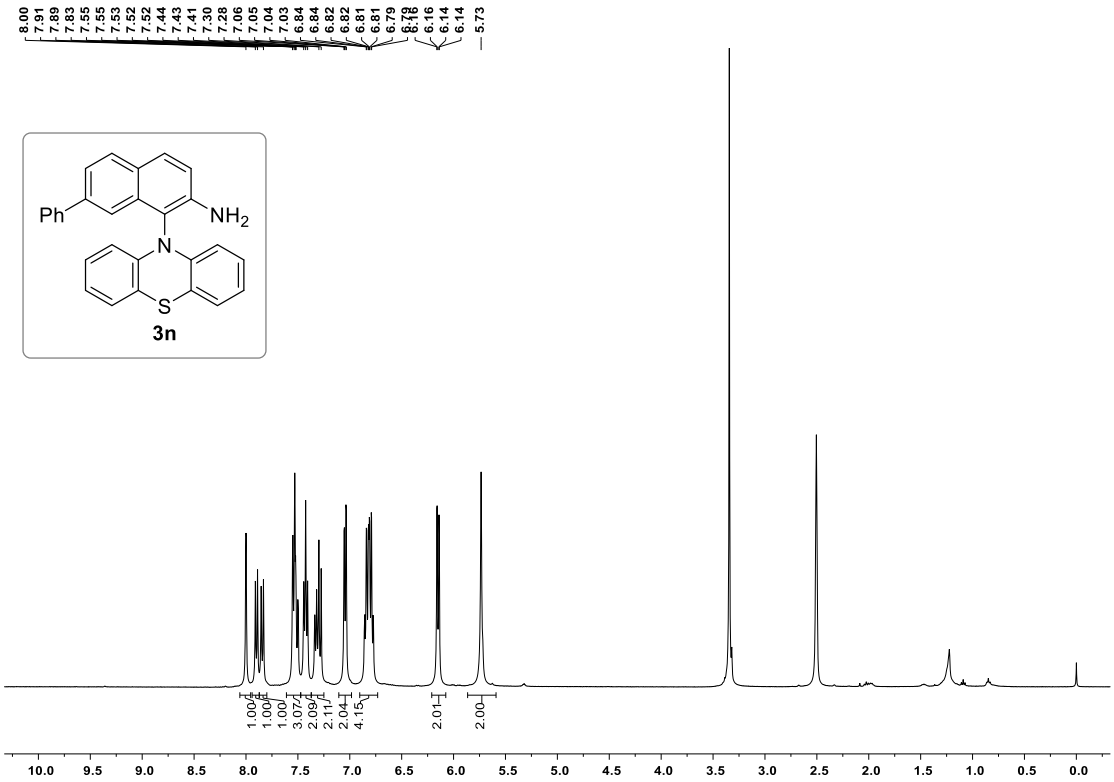
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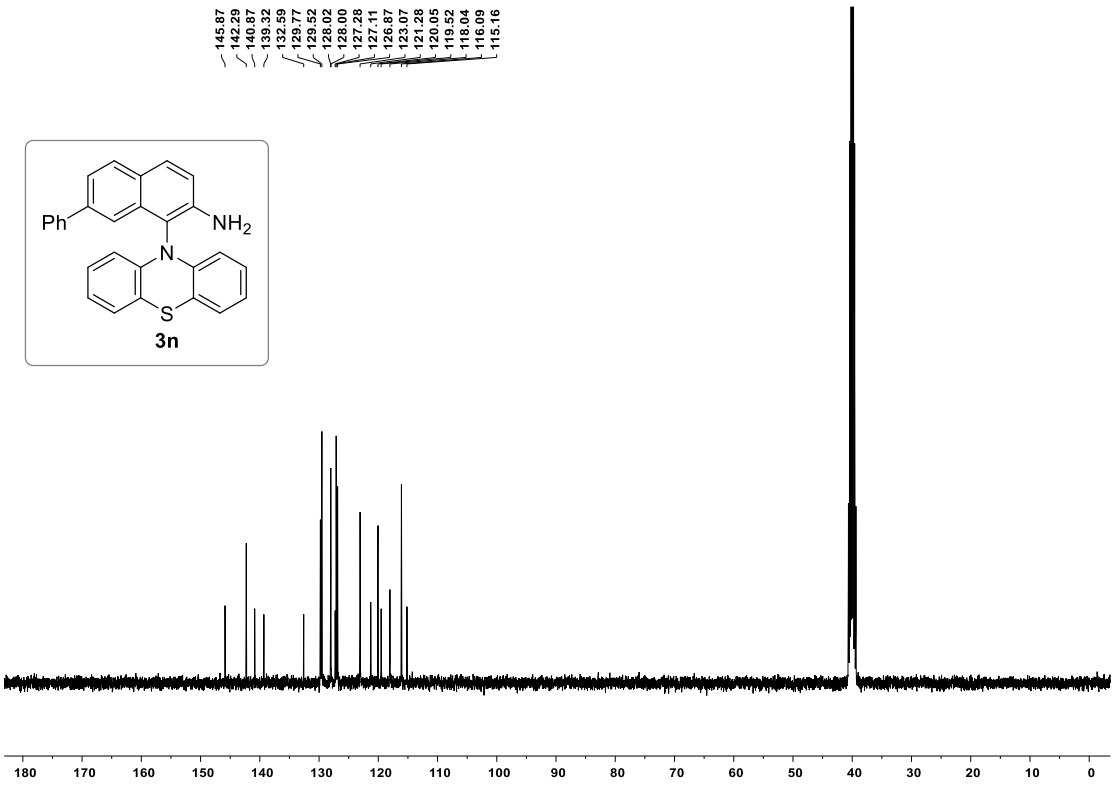
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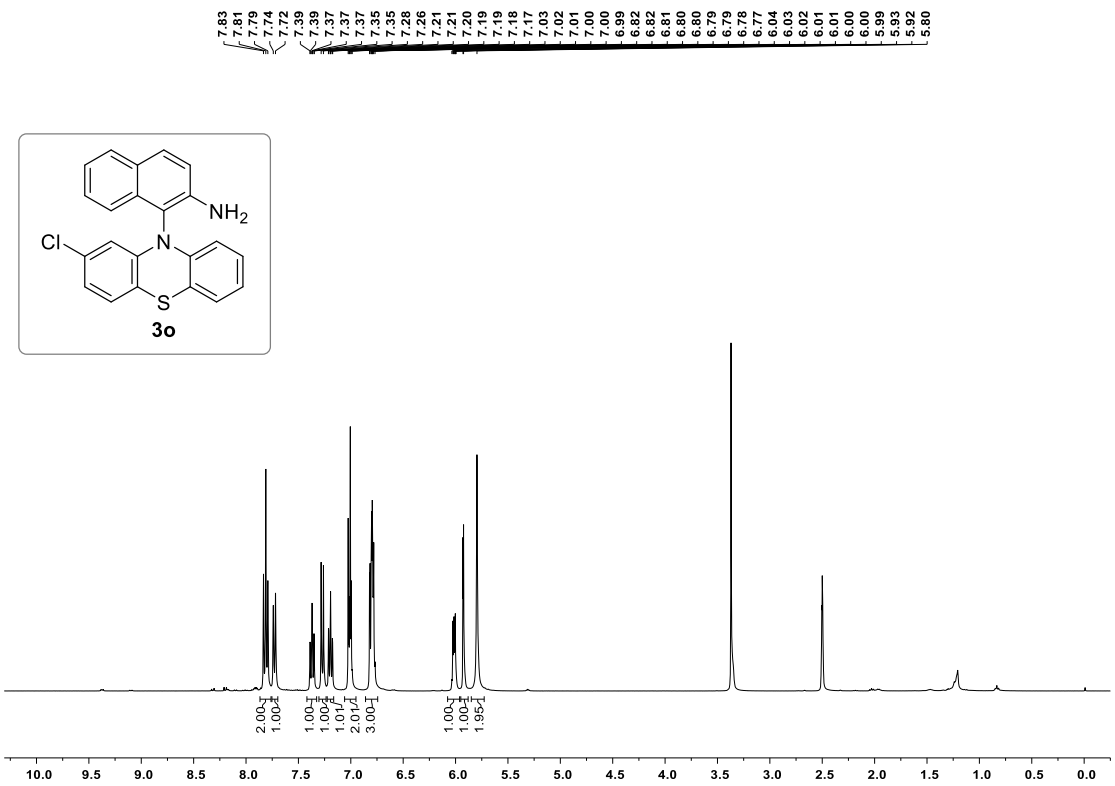
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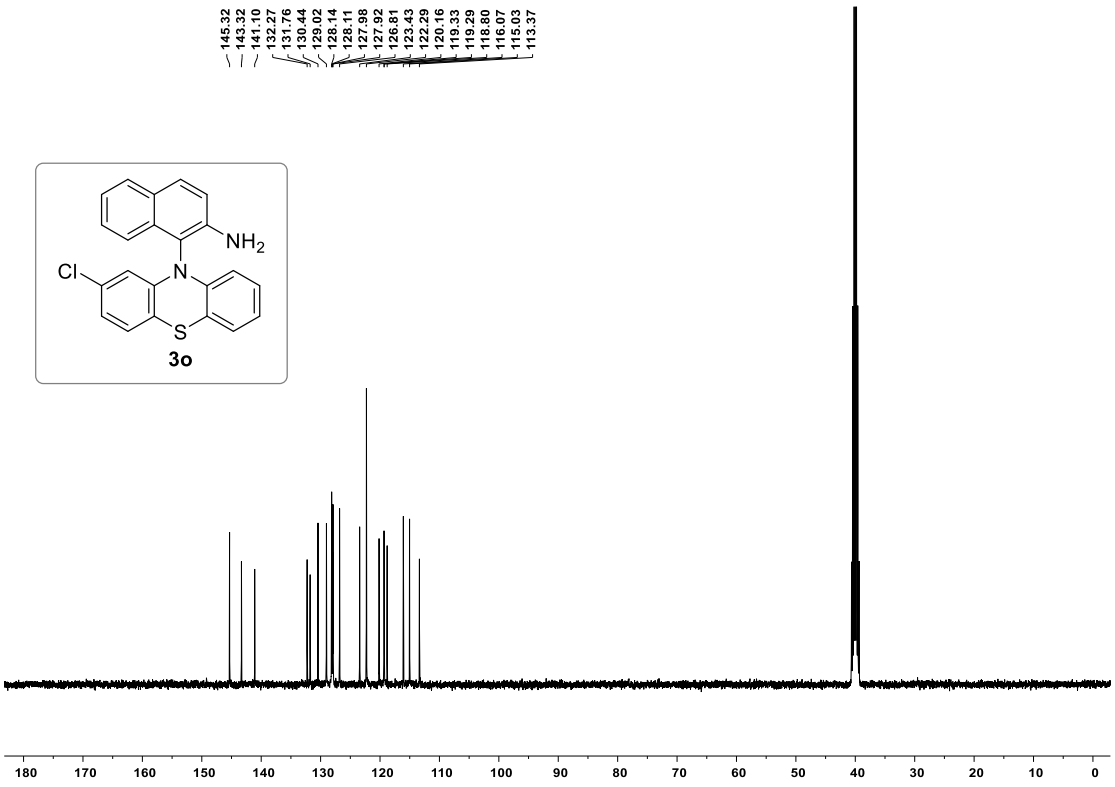
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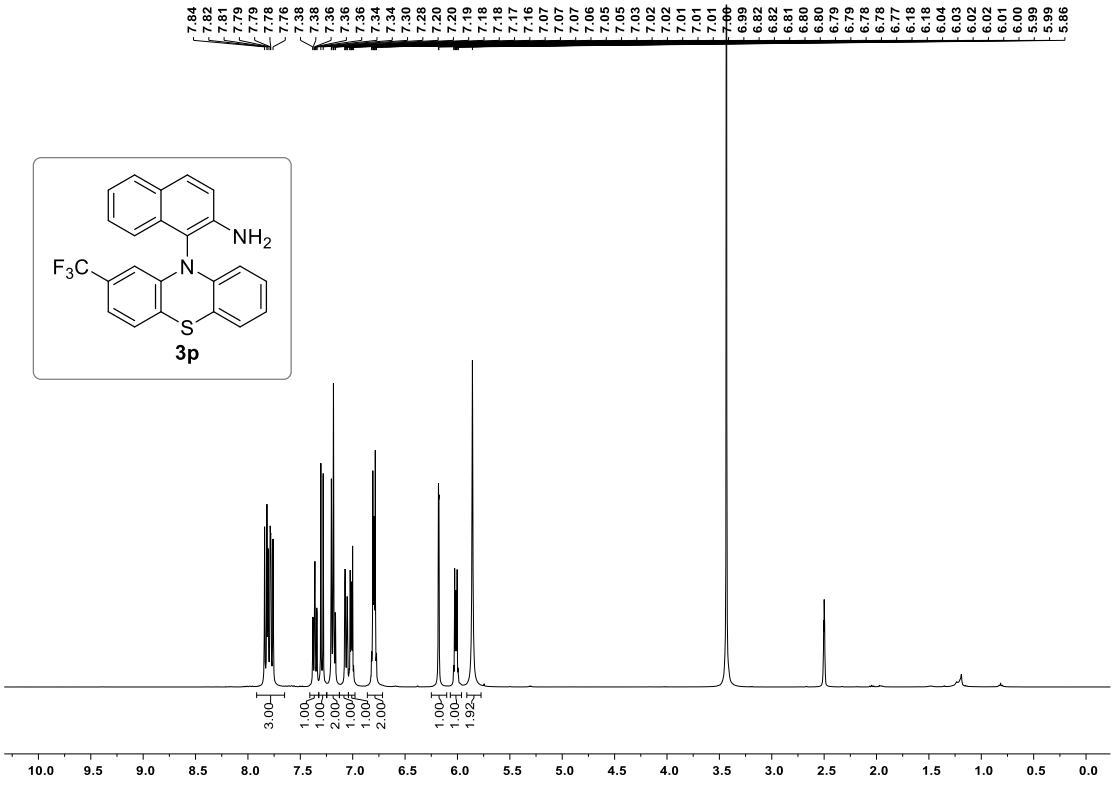
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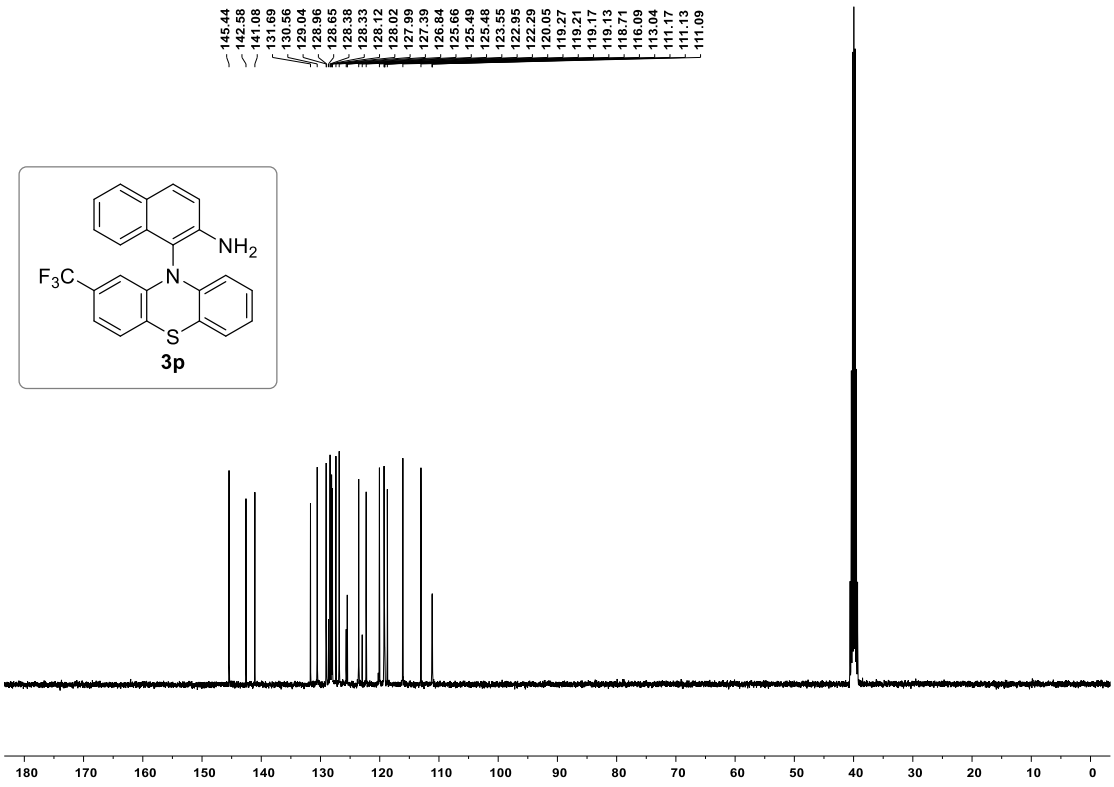
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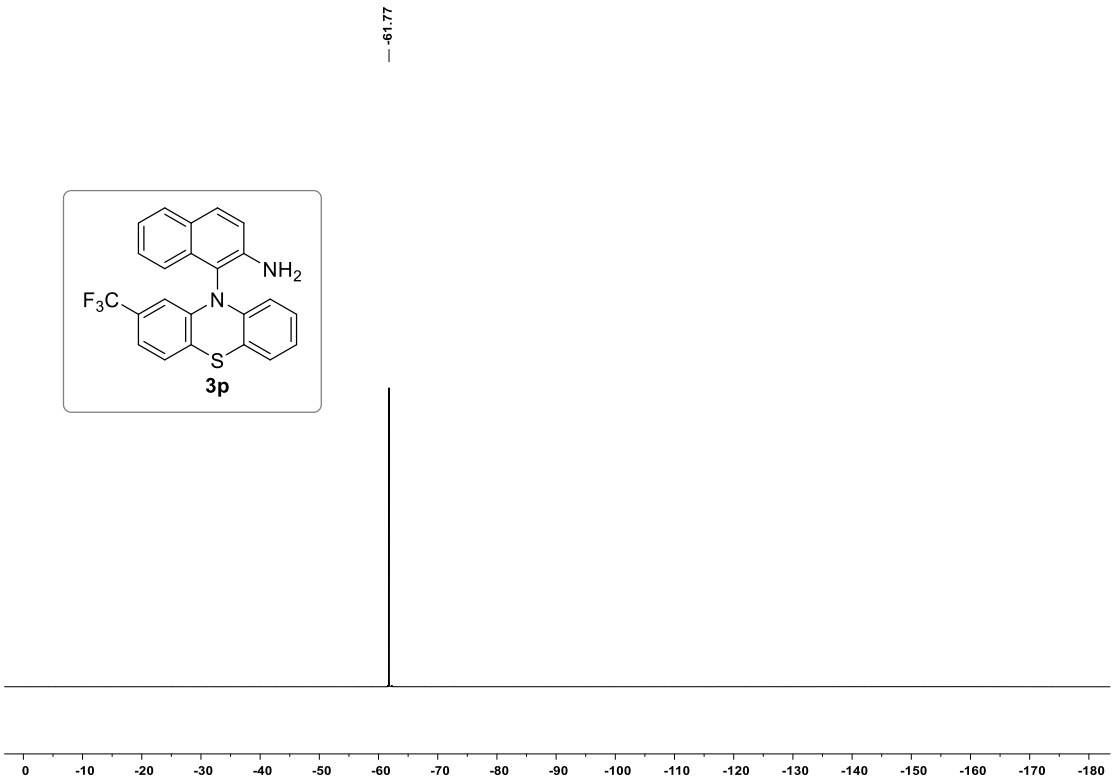
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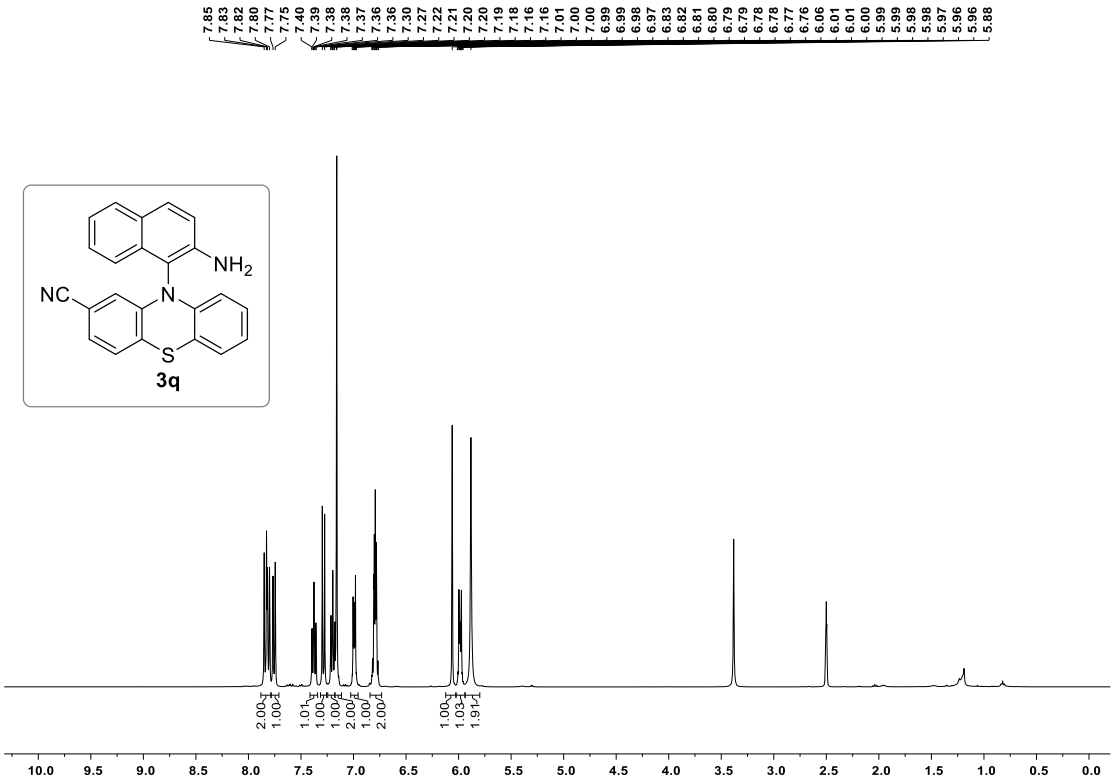
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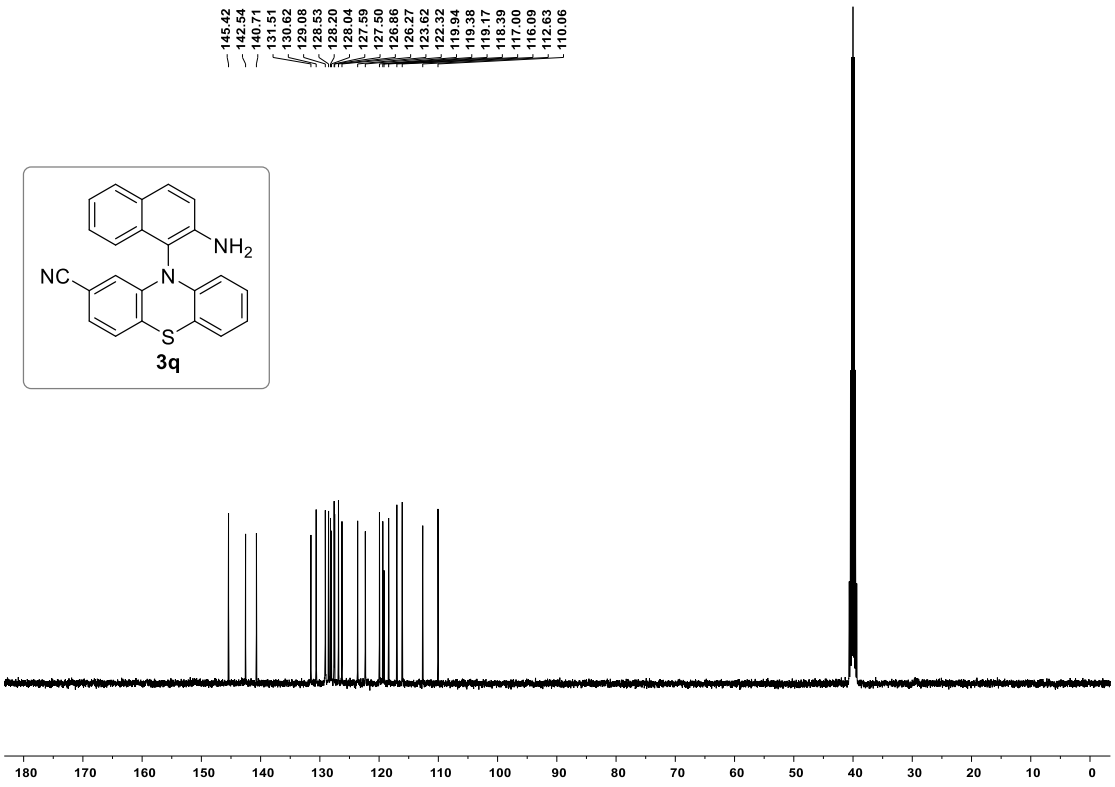
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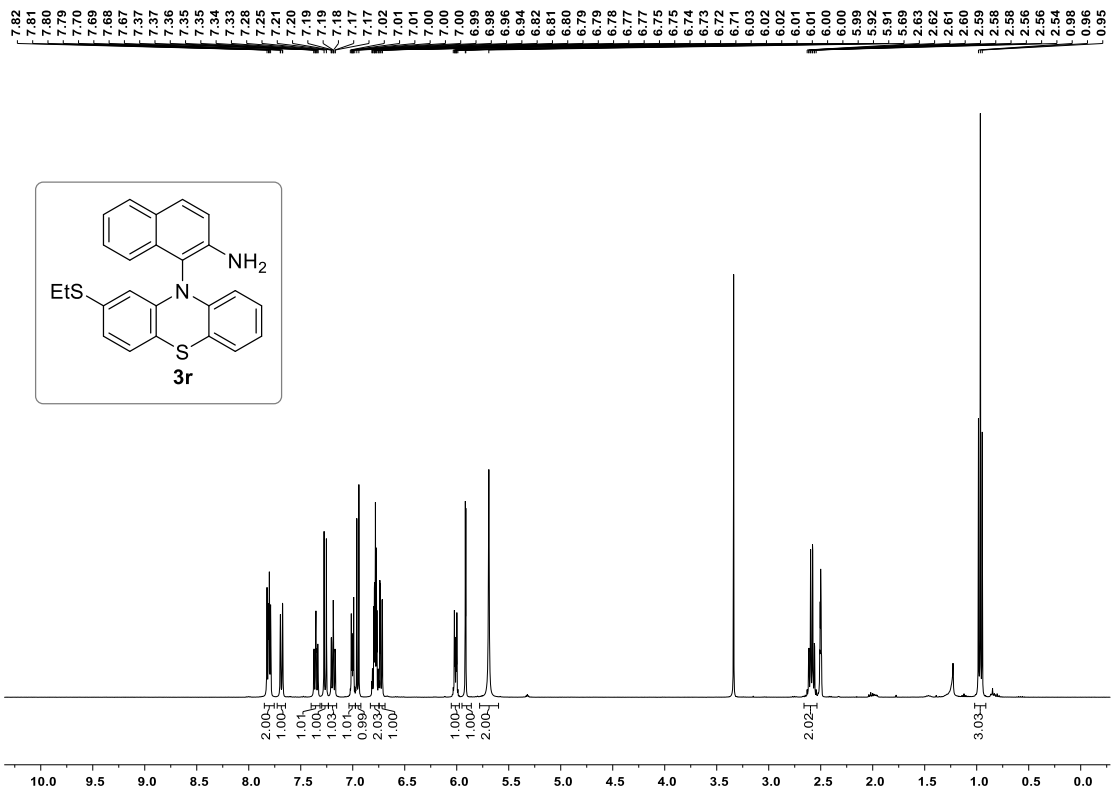
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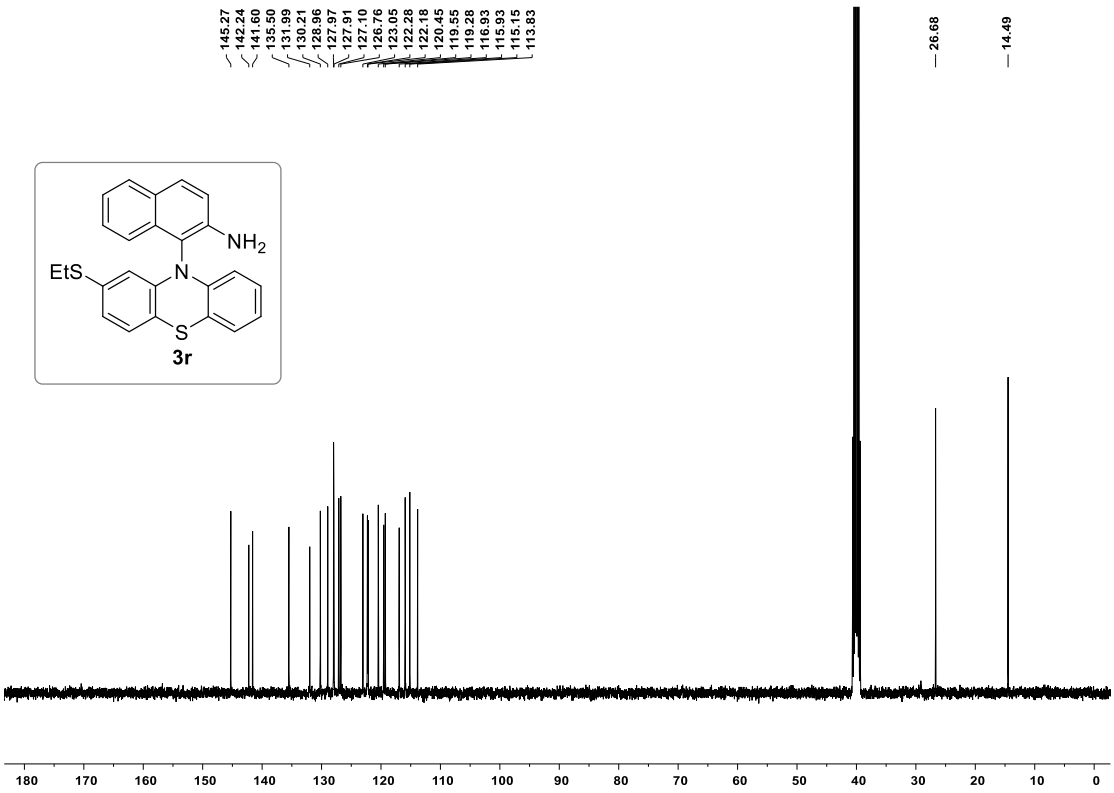
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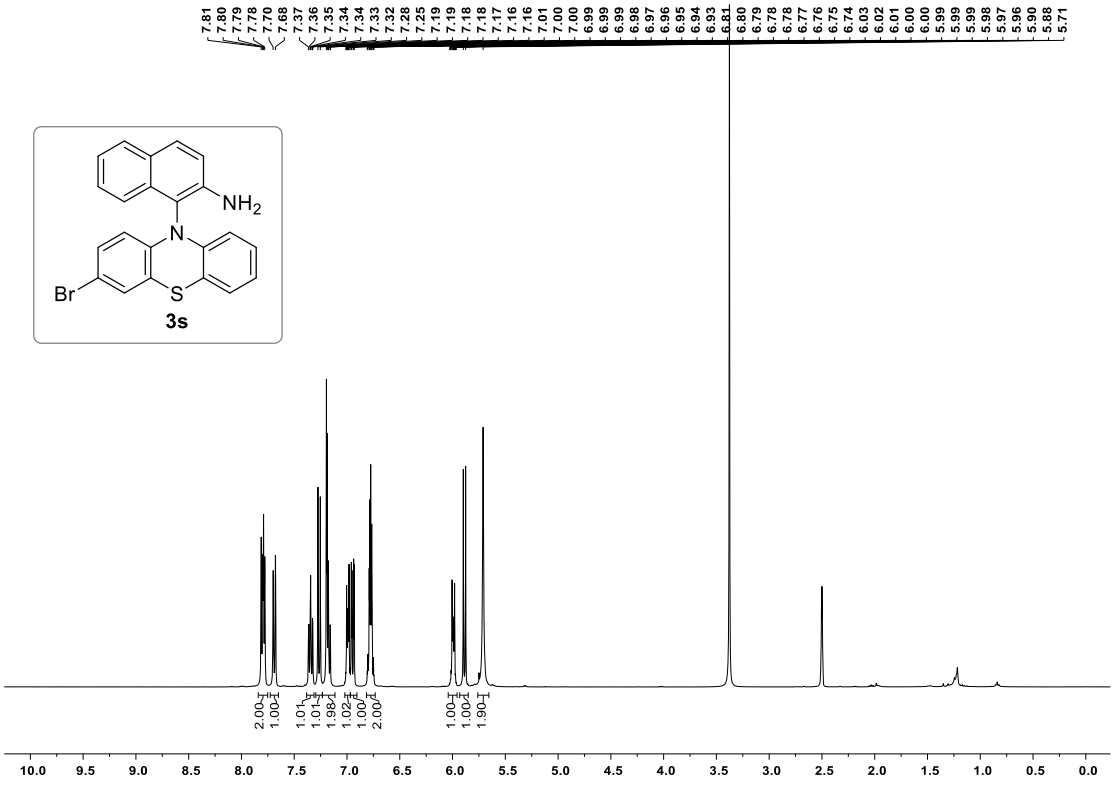
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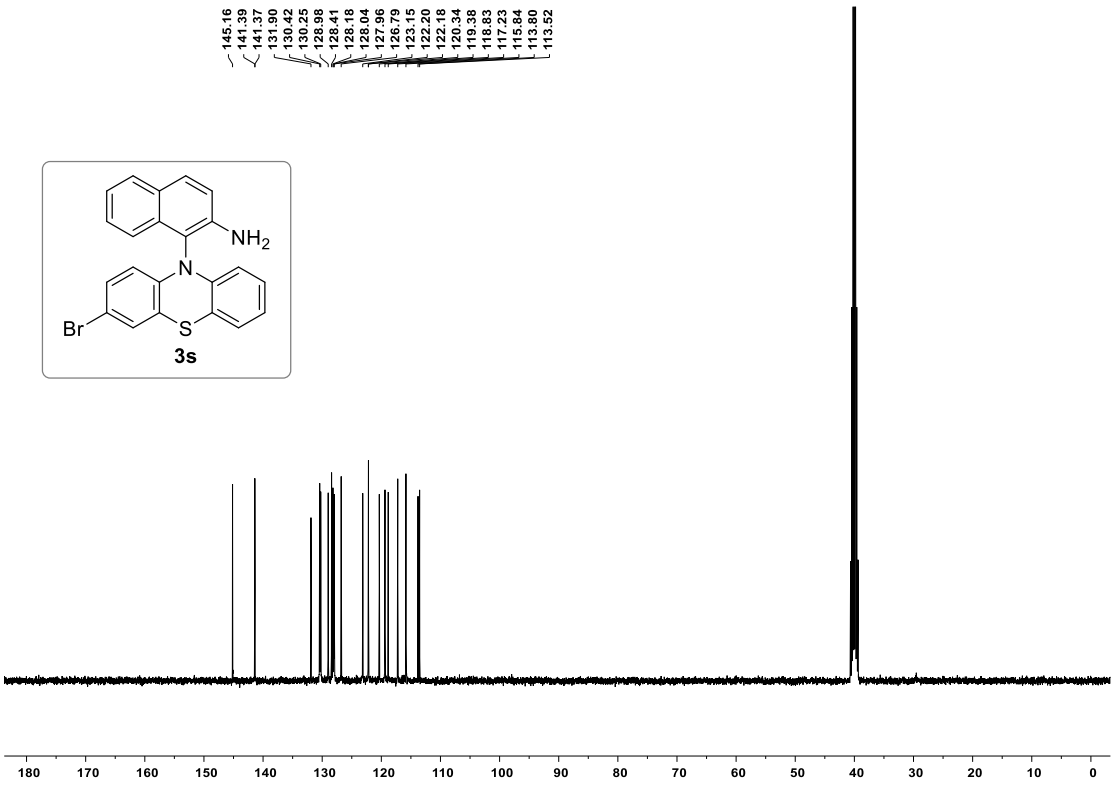
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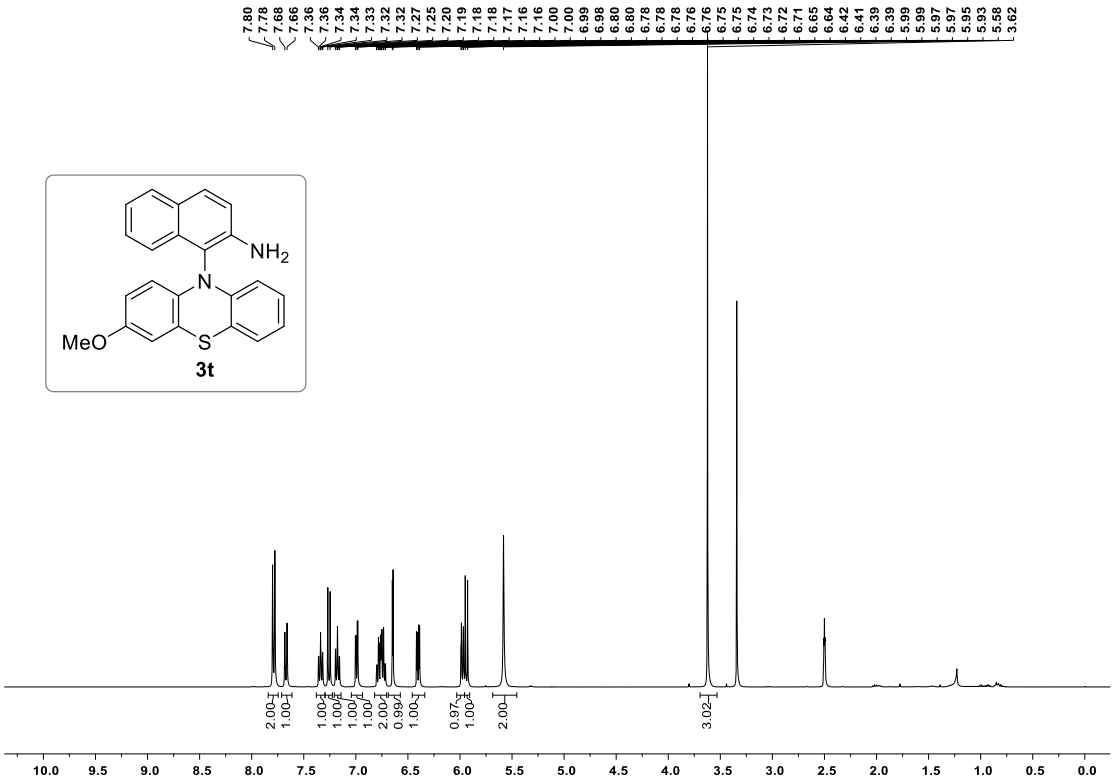
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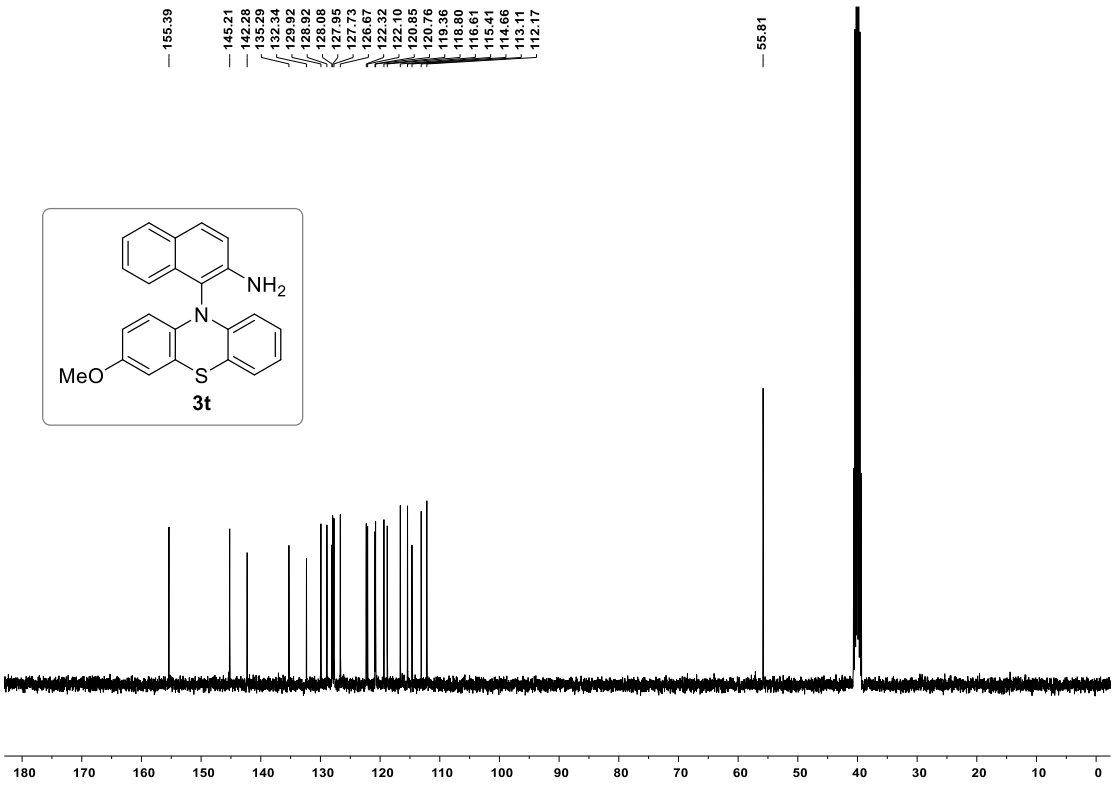
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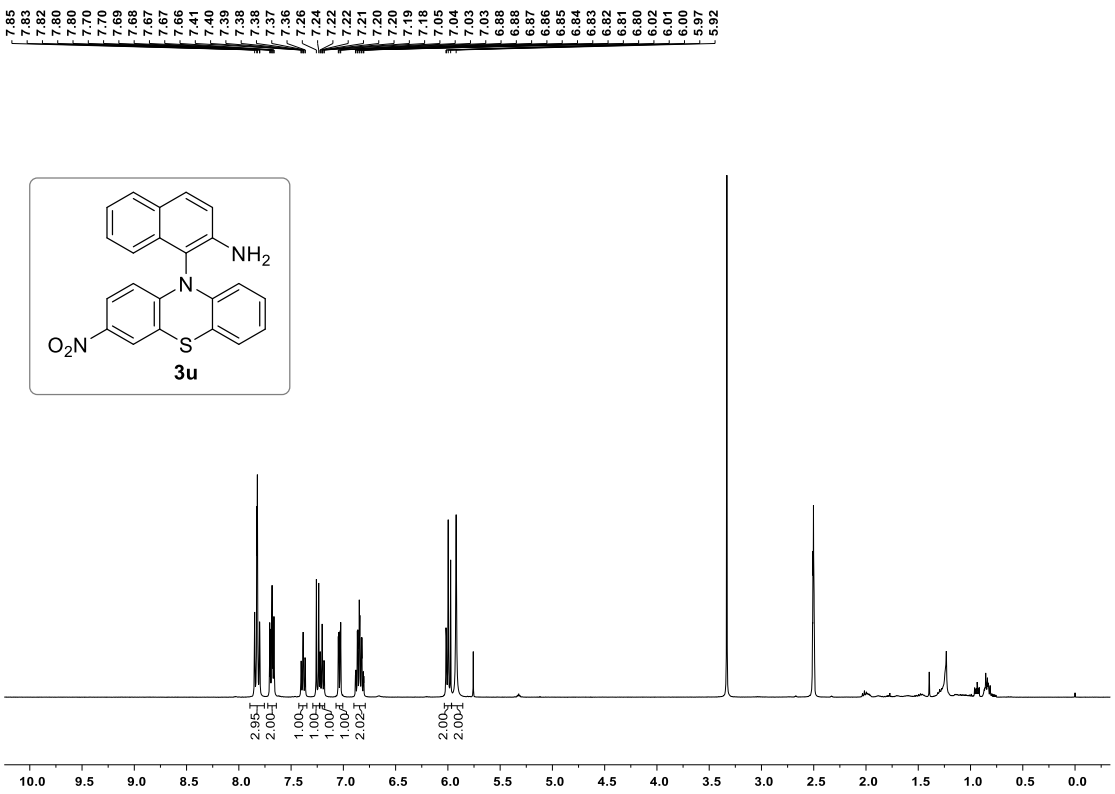
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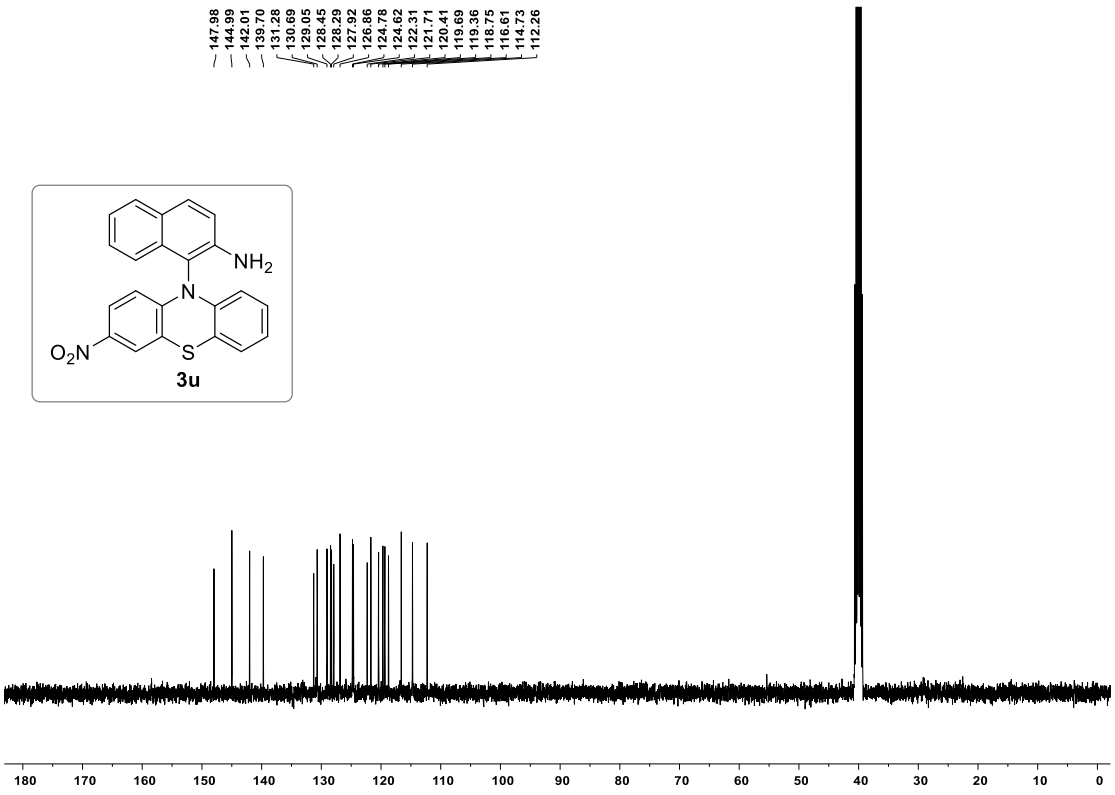
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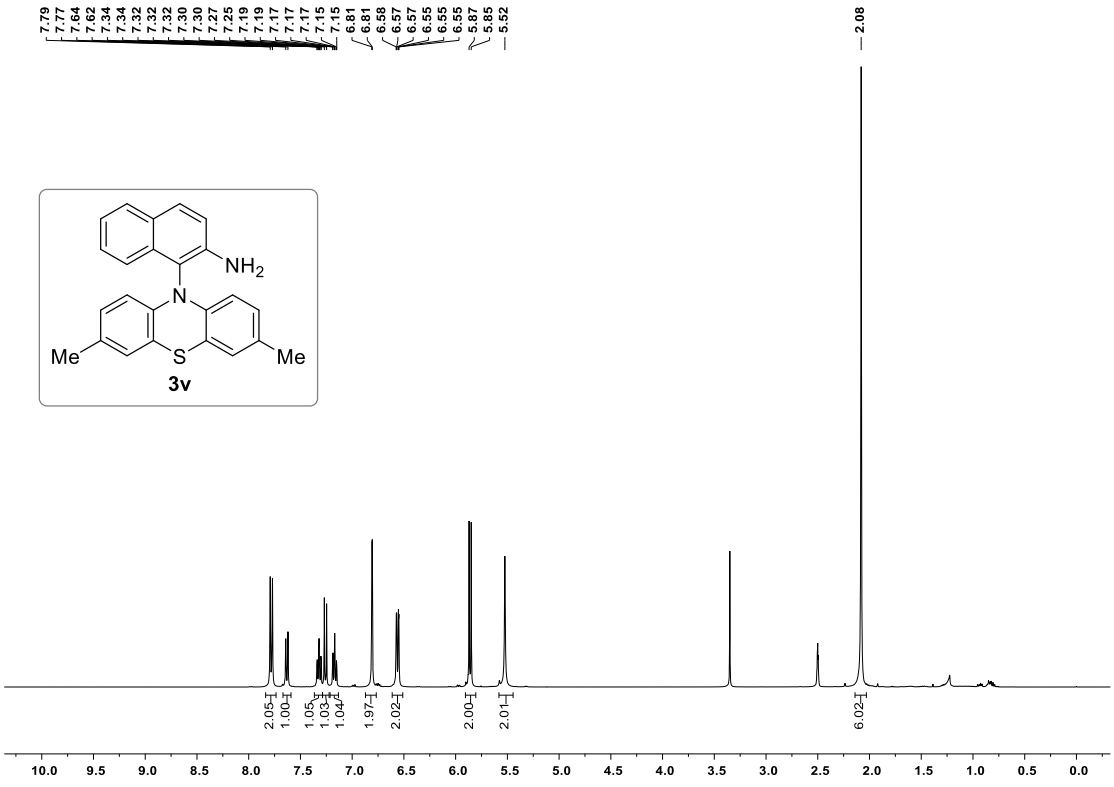
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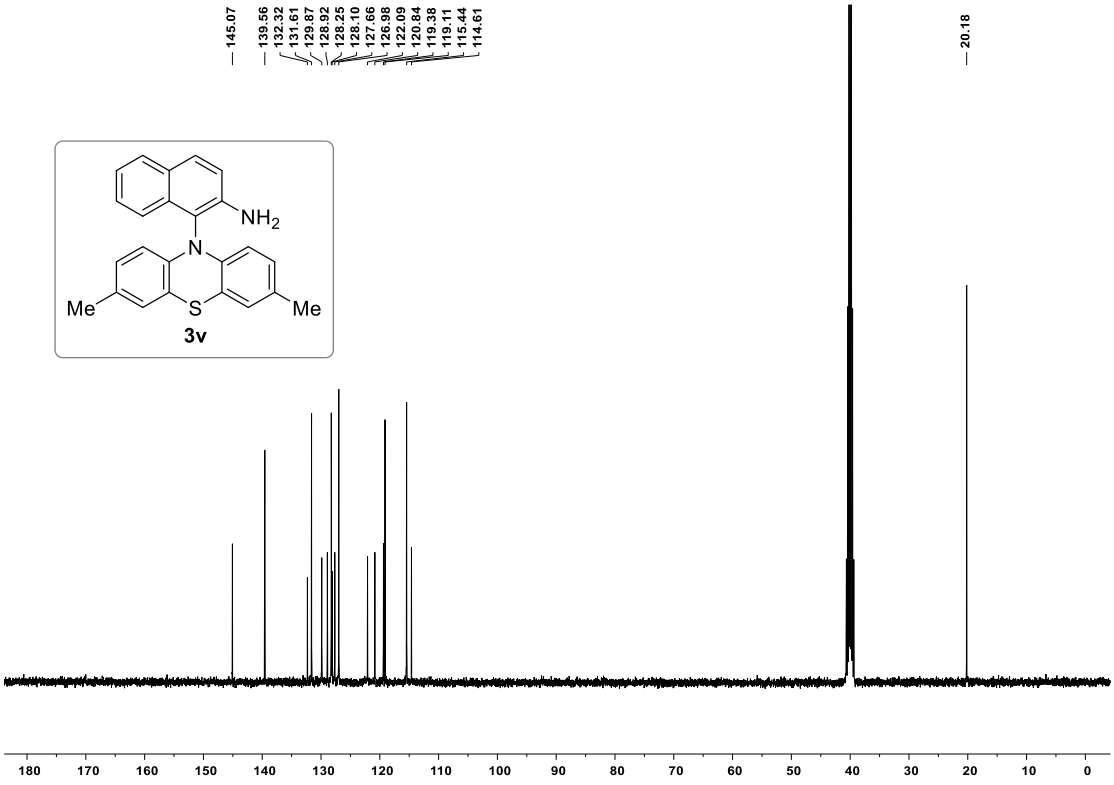
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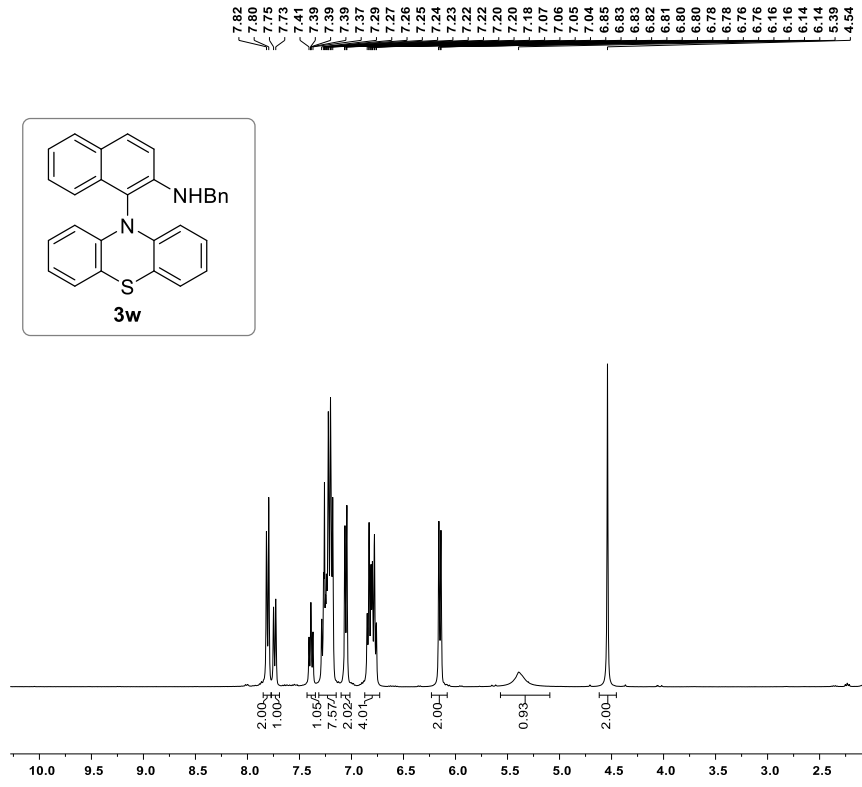
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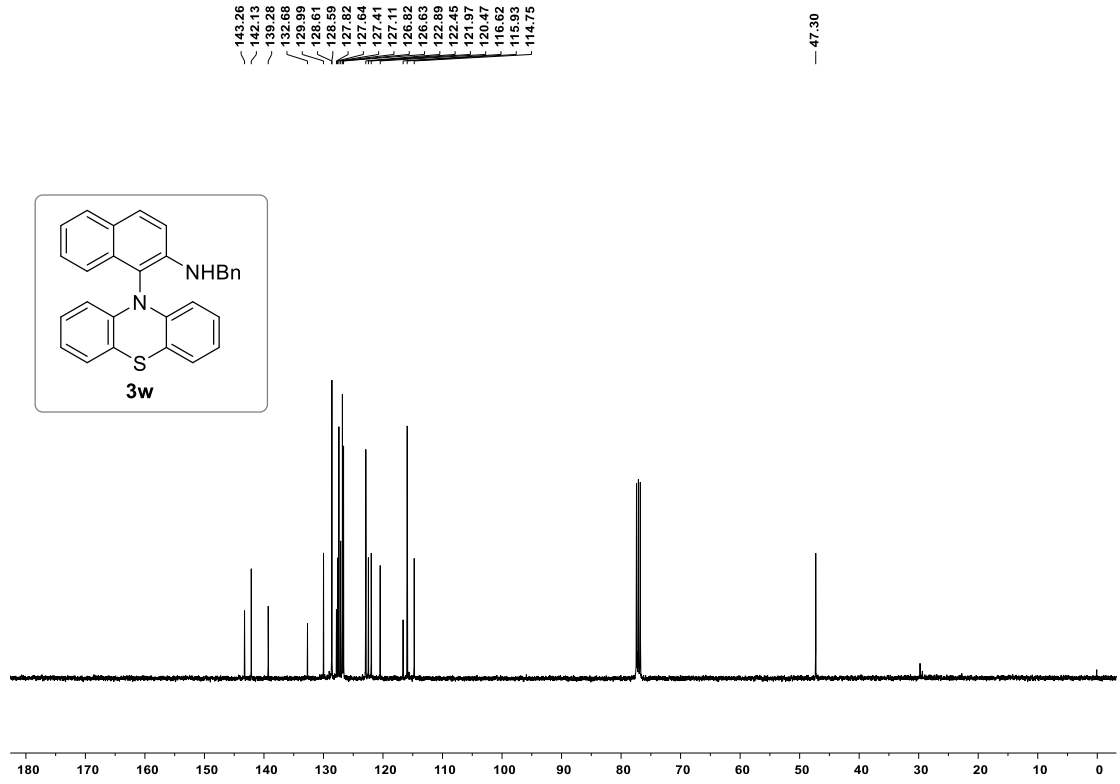
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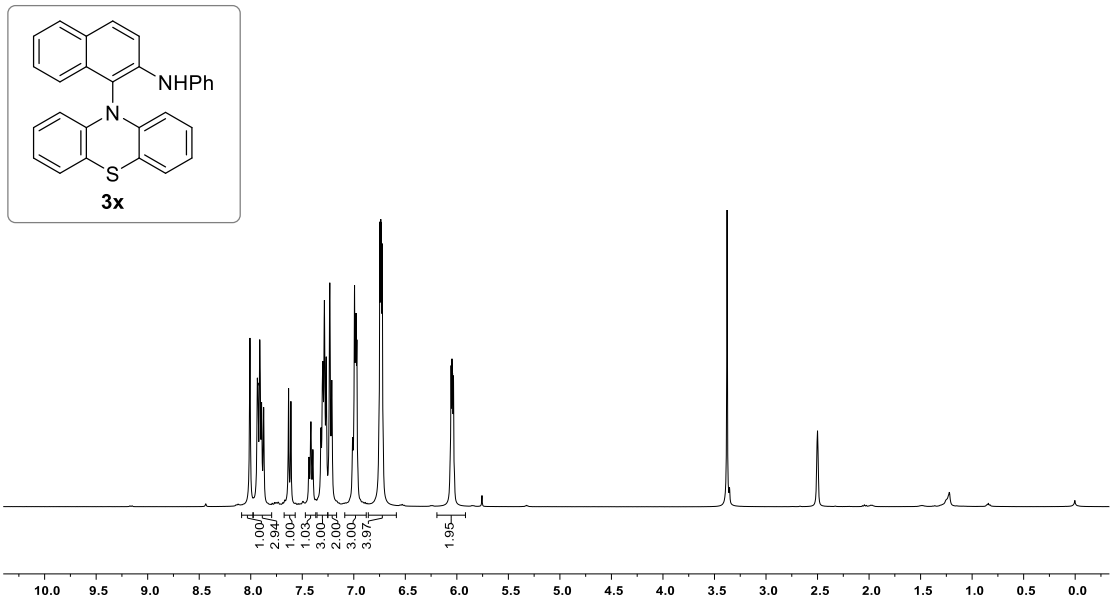
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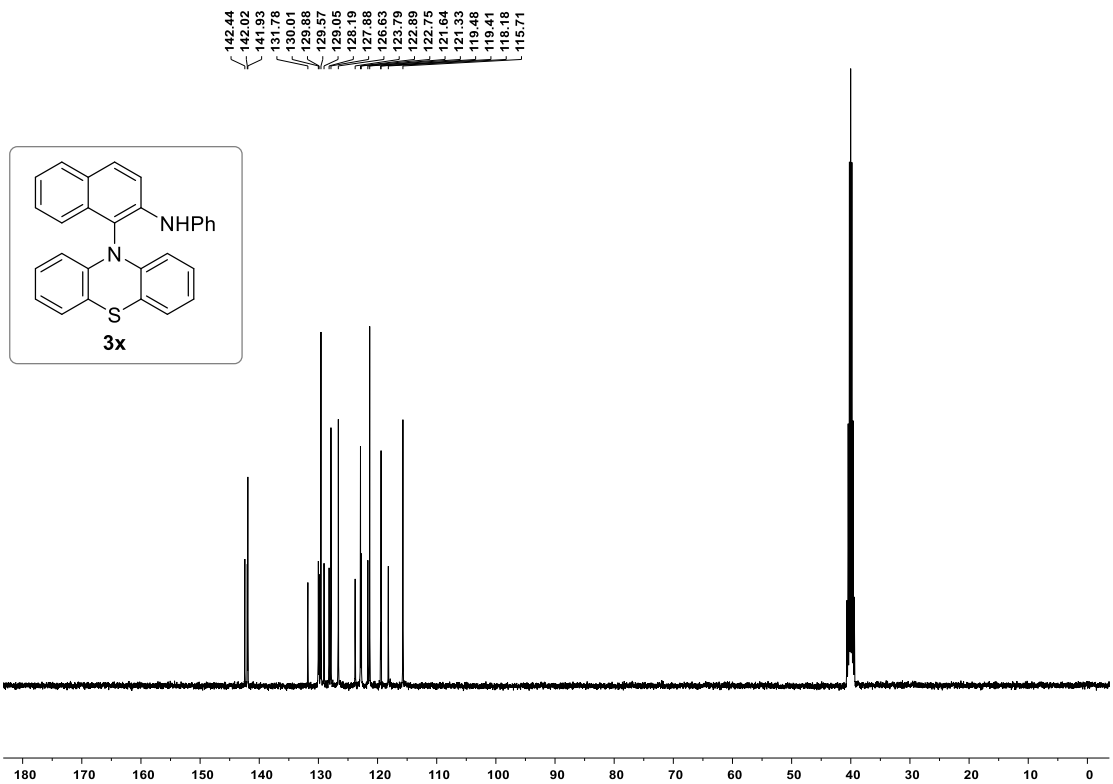
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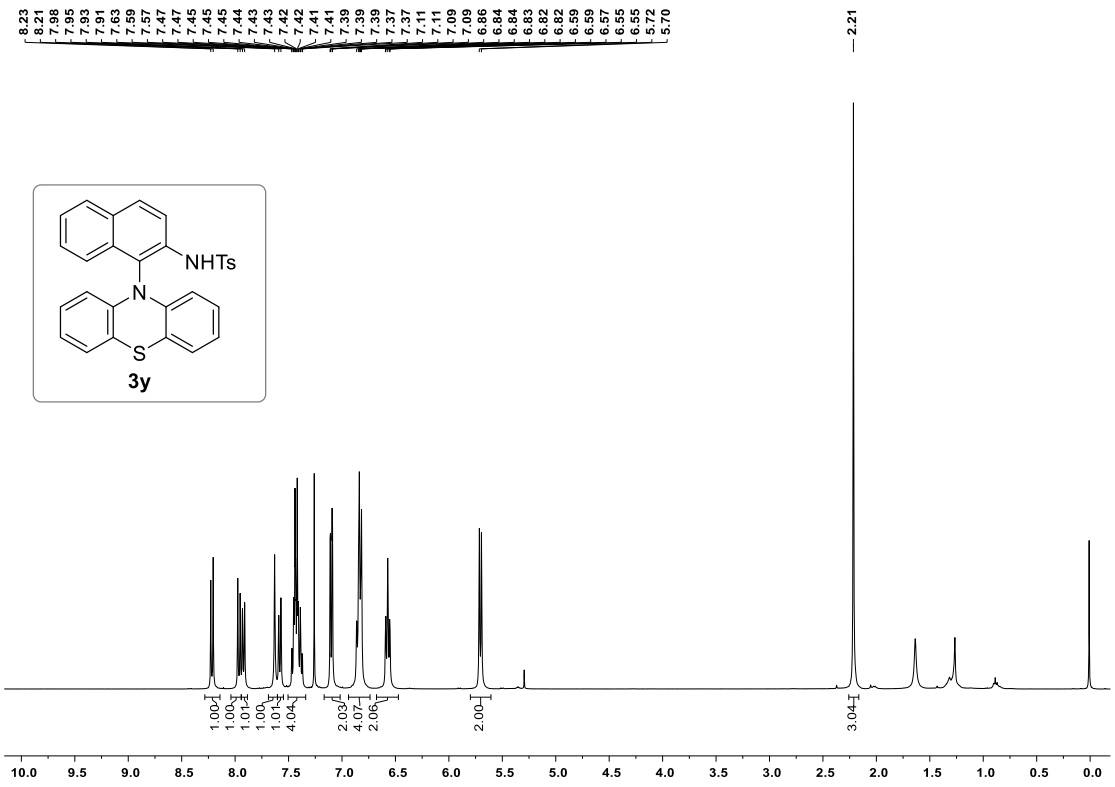
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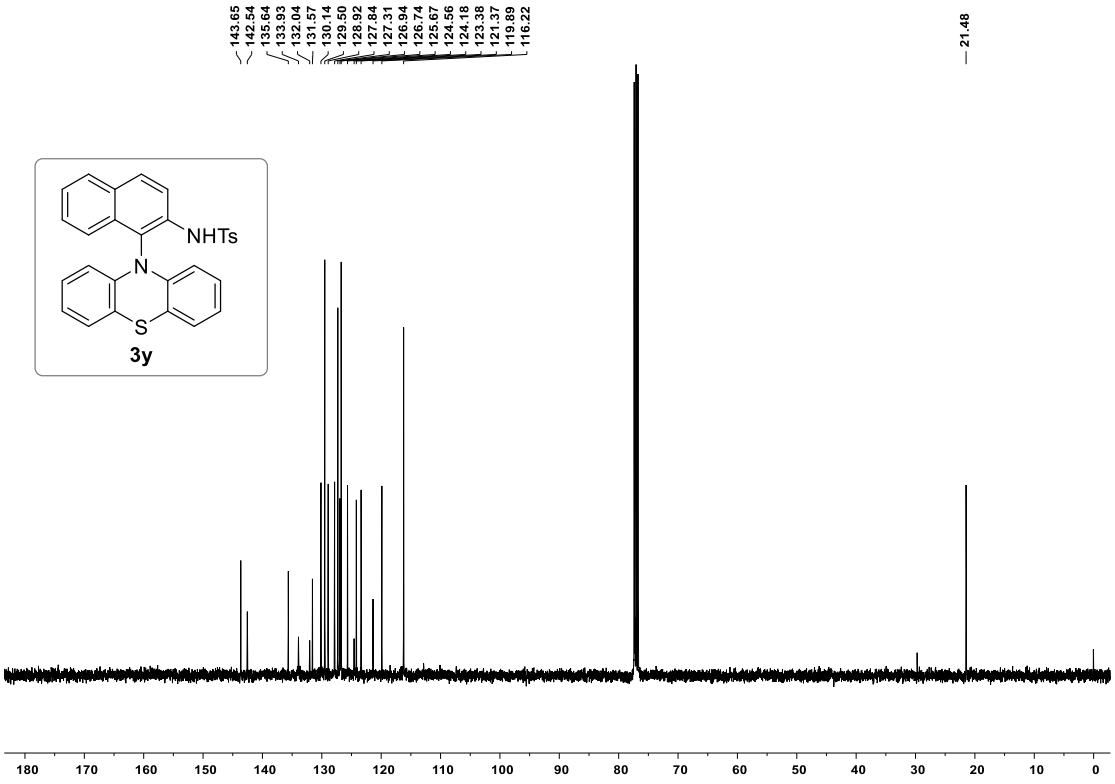
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N
S
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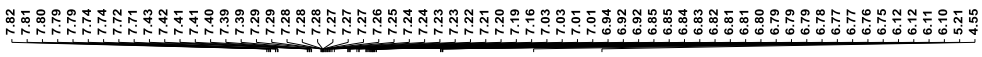
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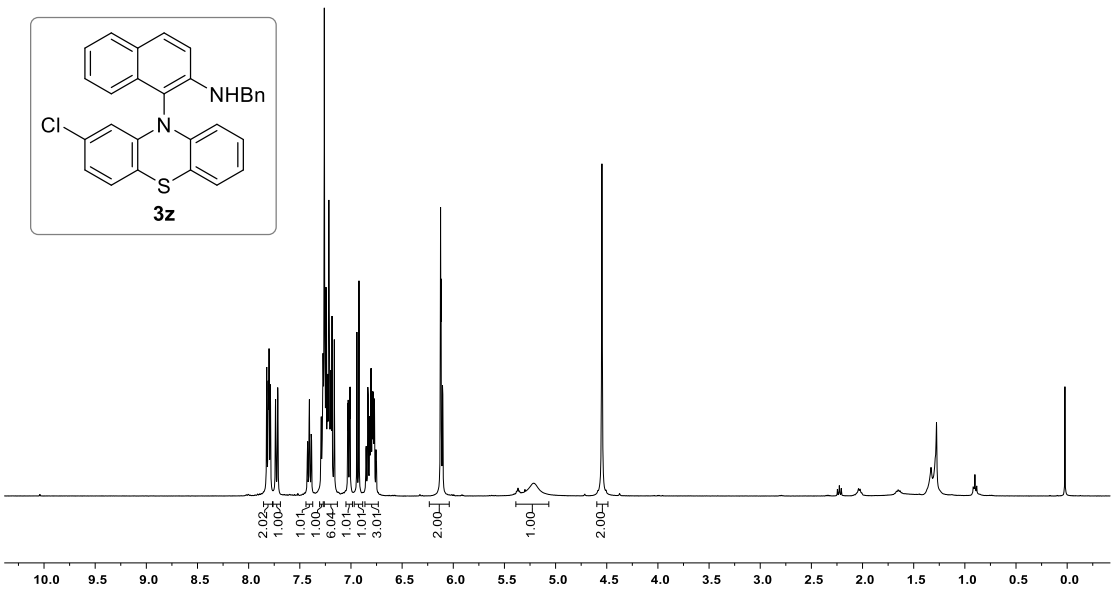
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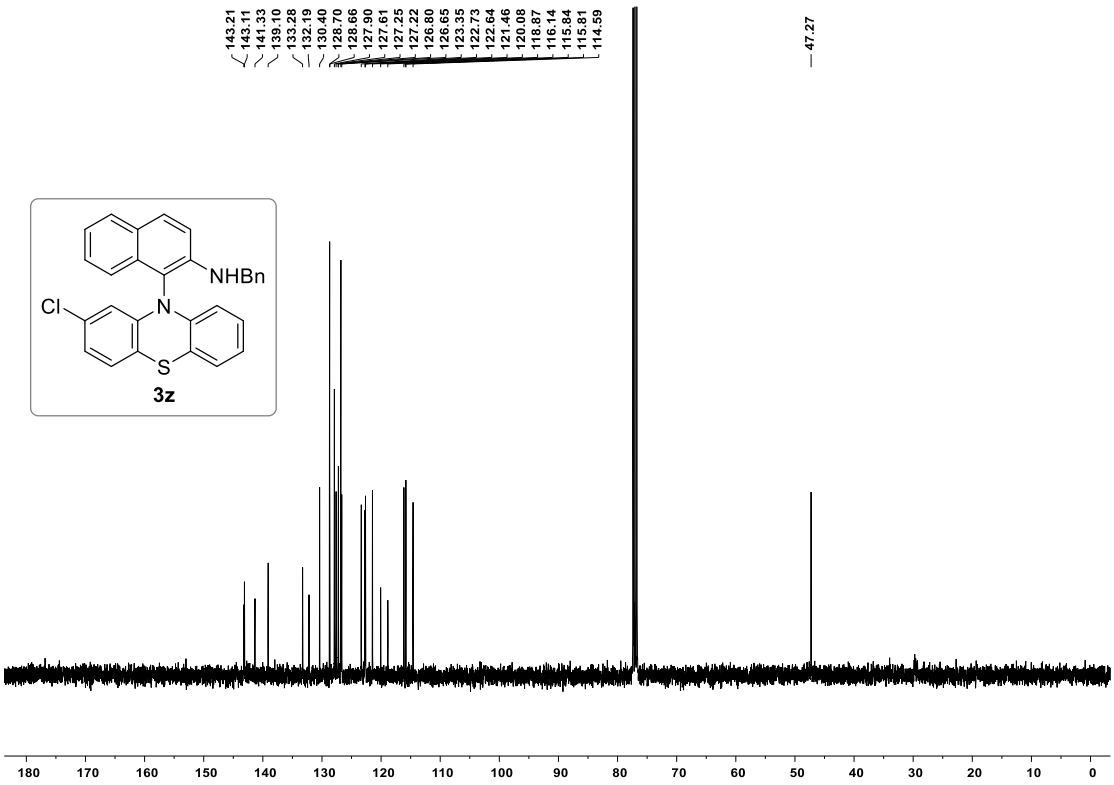
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Cl
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S
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30
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10
0


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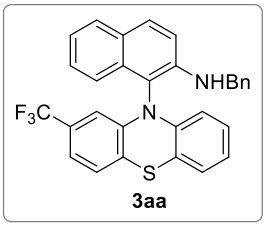
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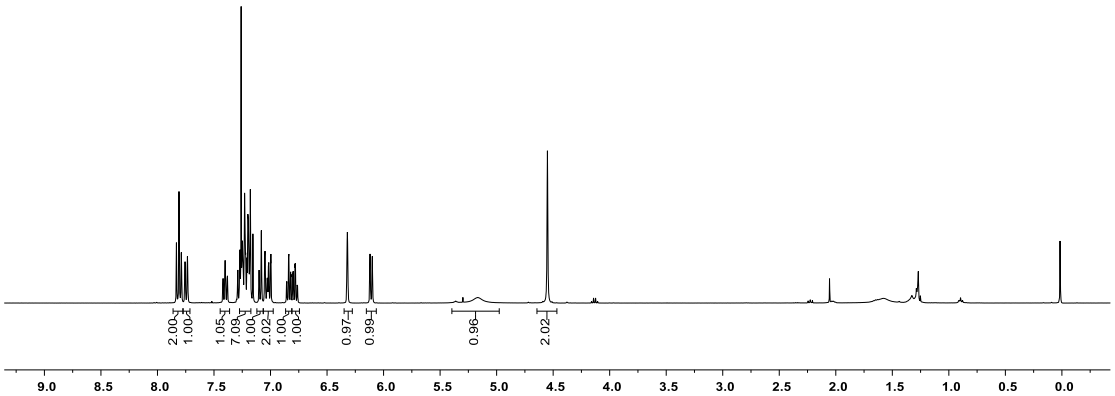
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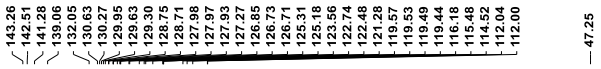
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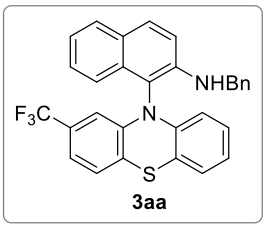
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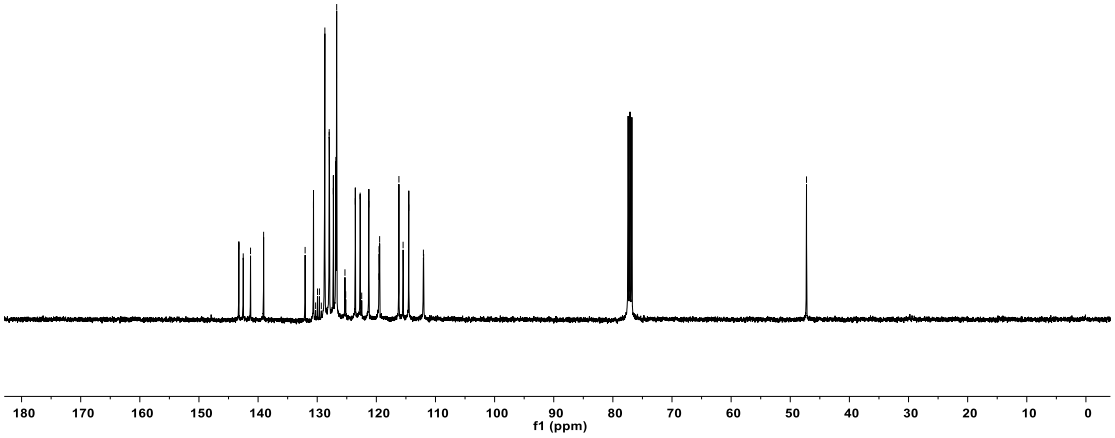
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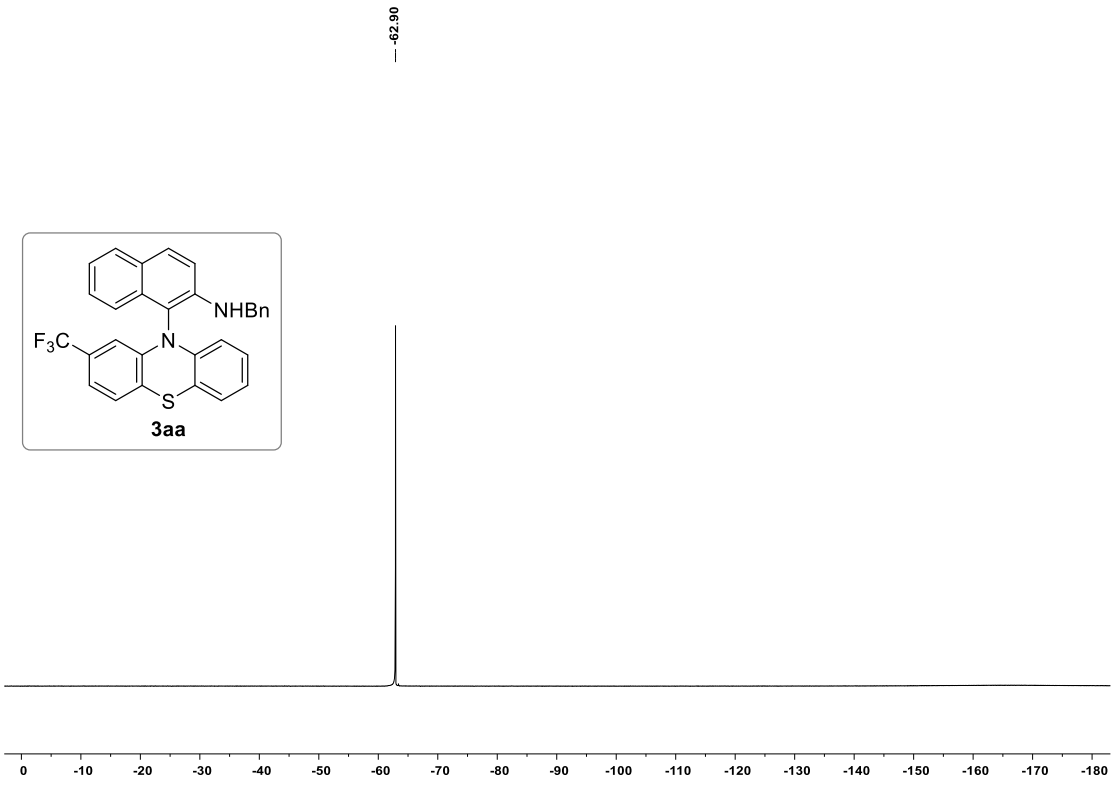
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-150
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-170
-180


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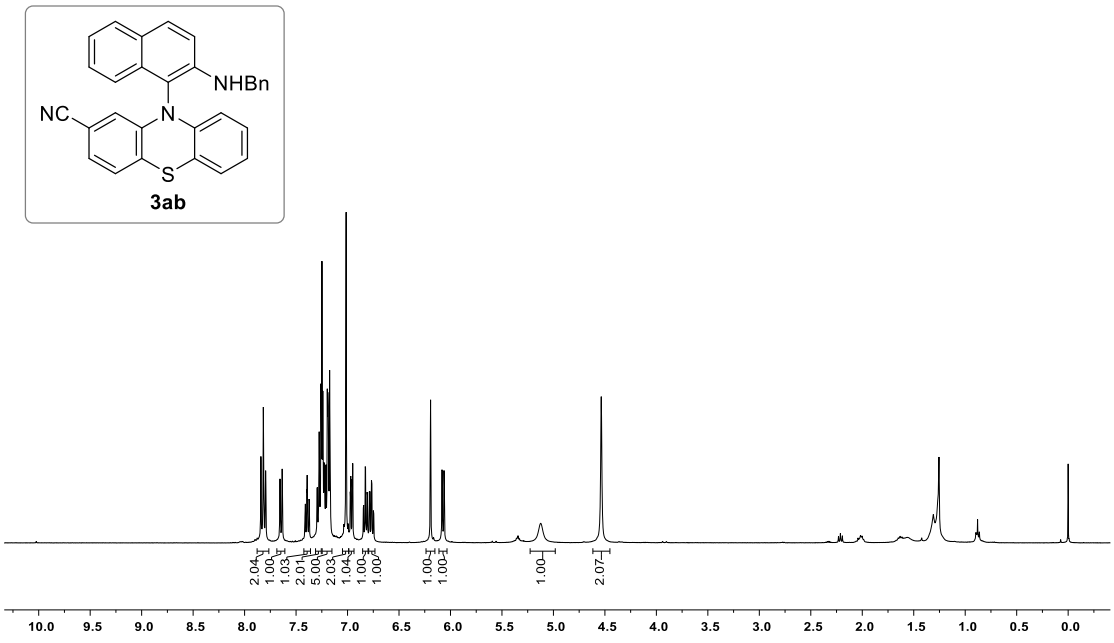
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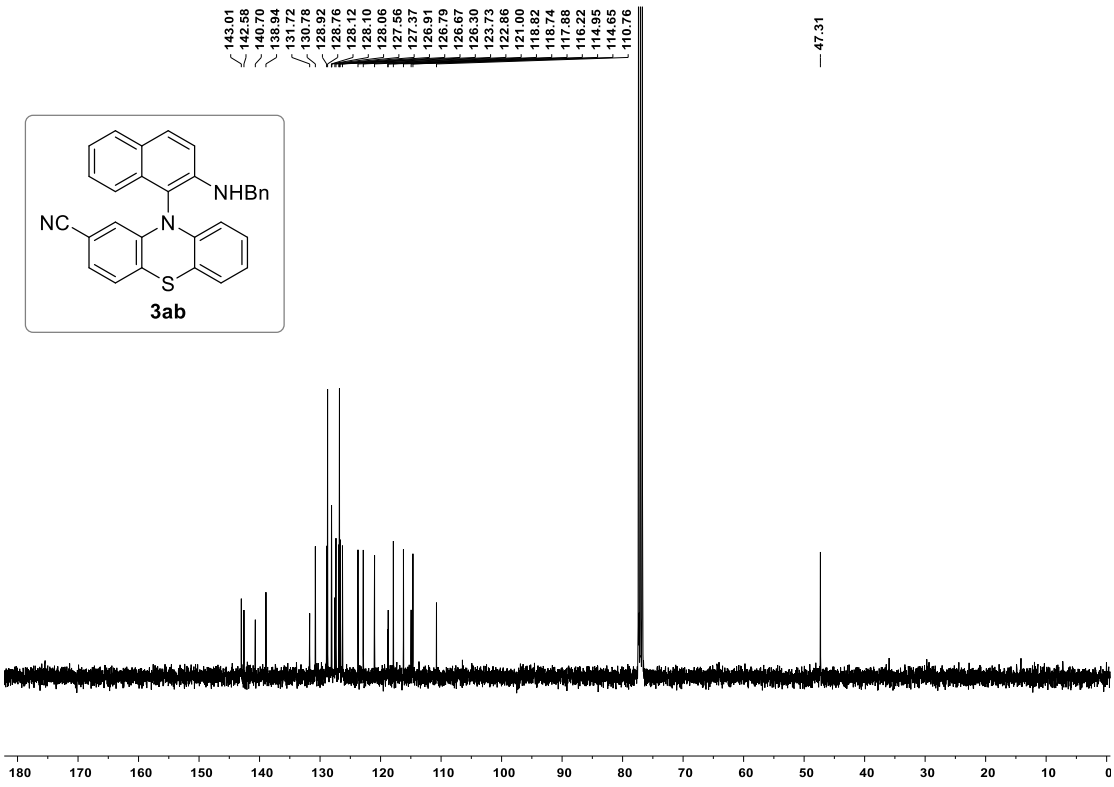
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S
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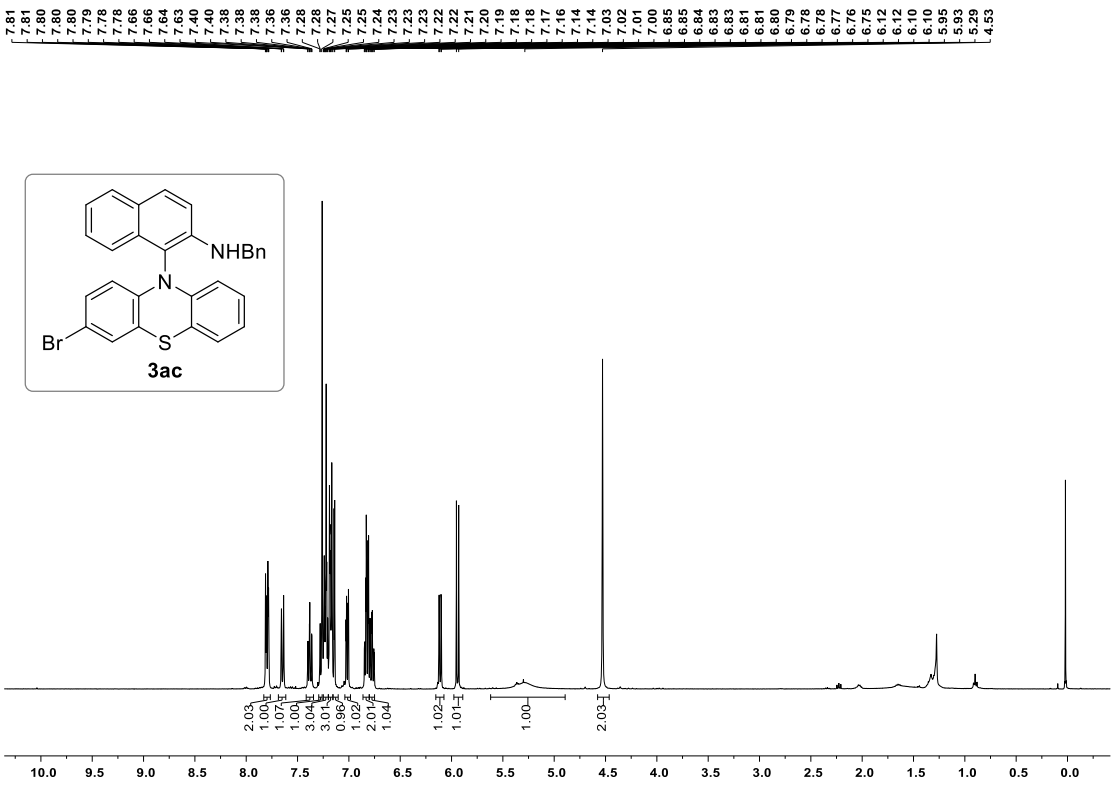
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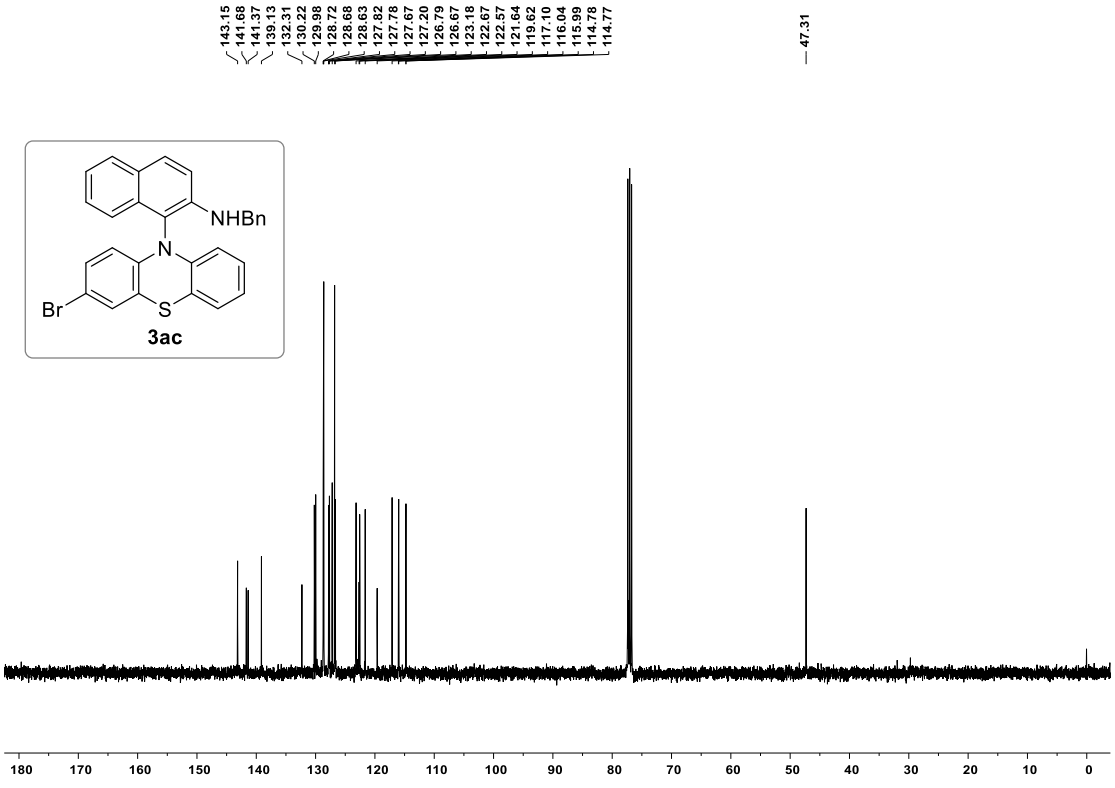
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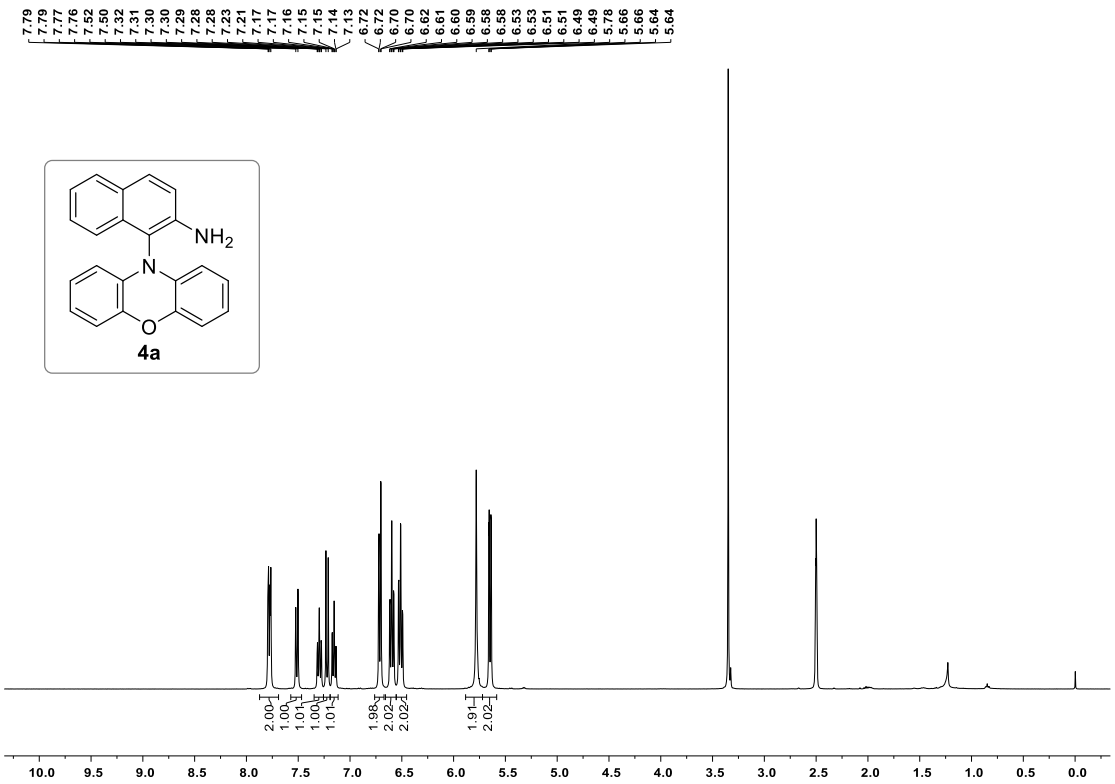
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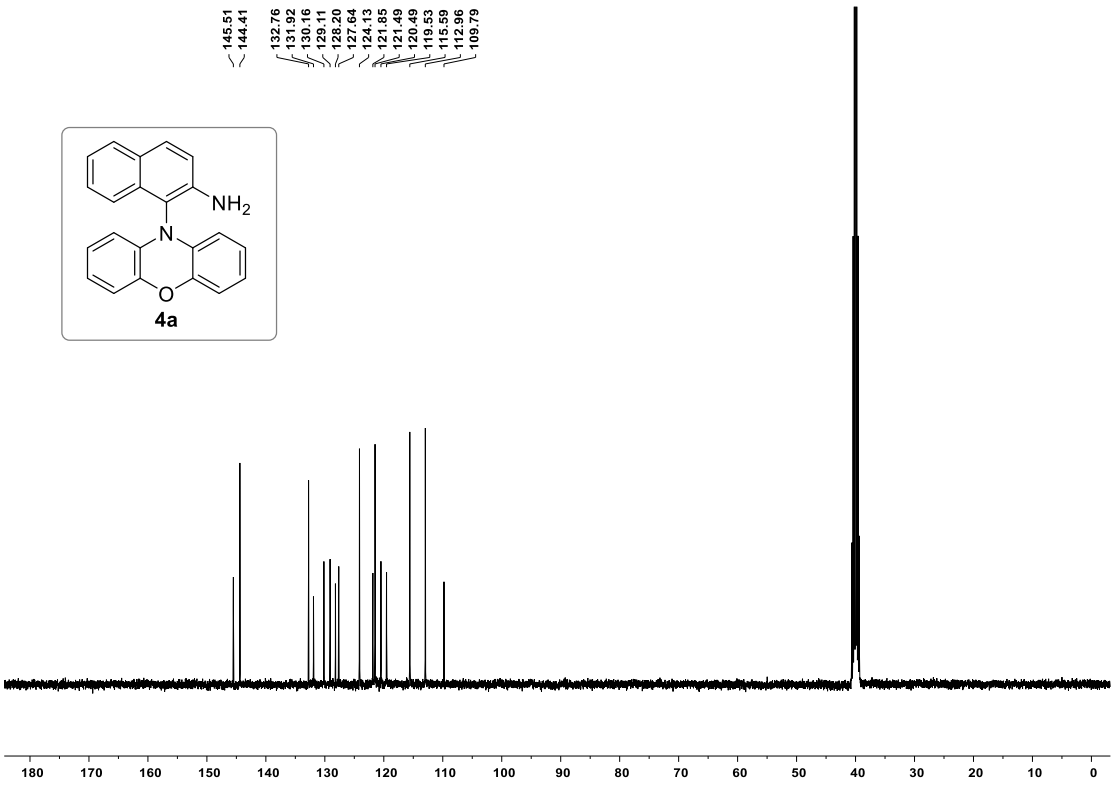
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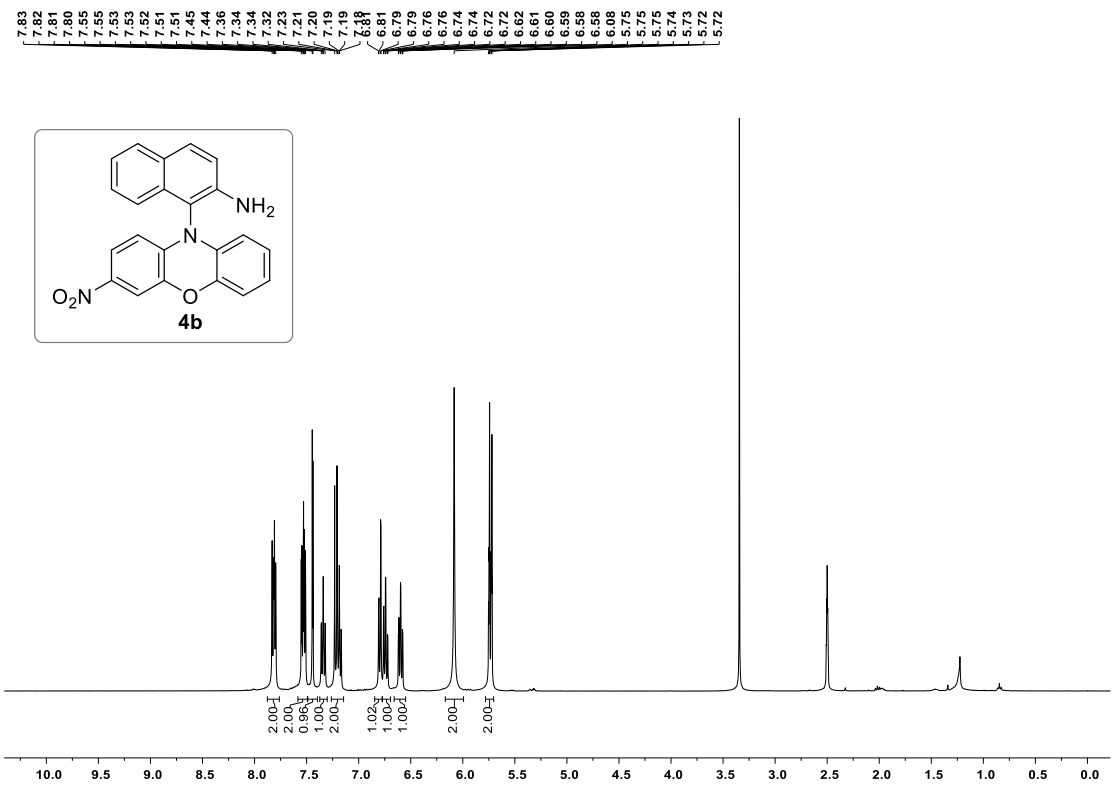
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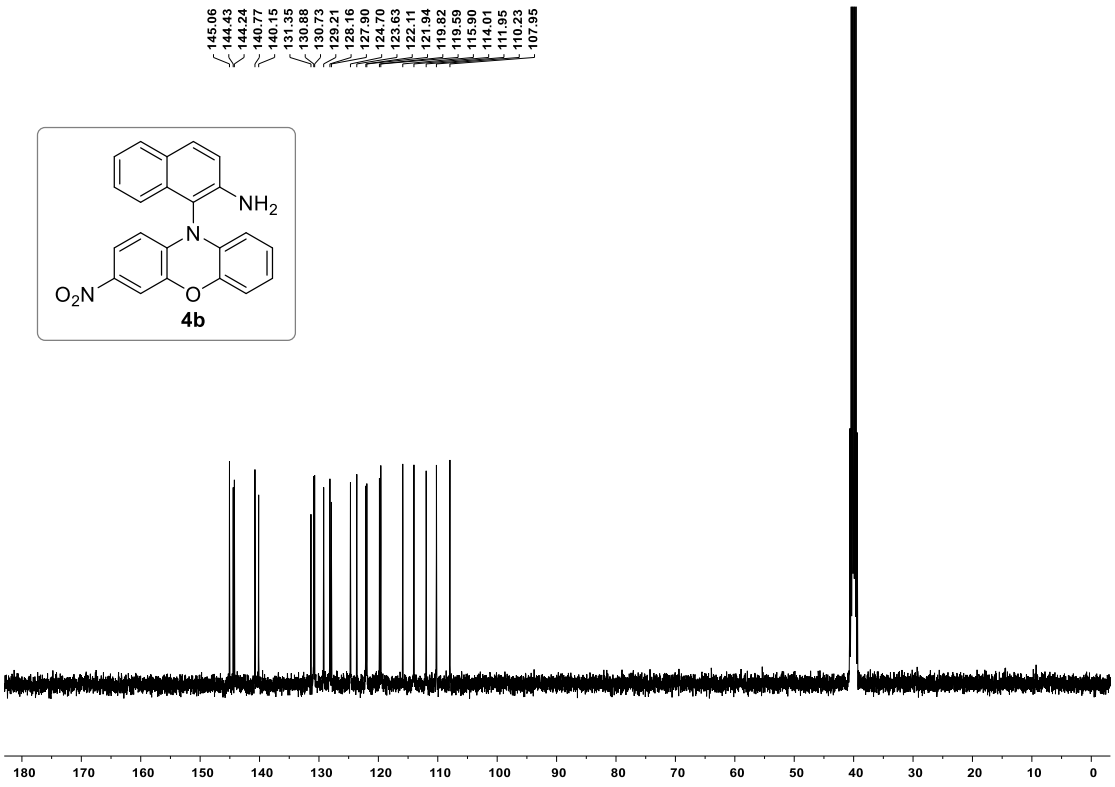
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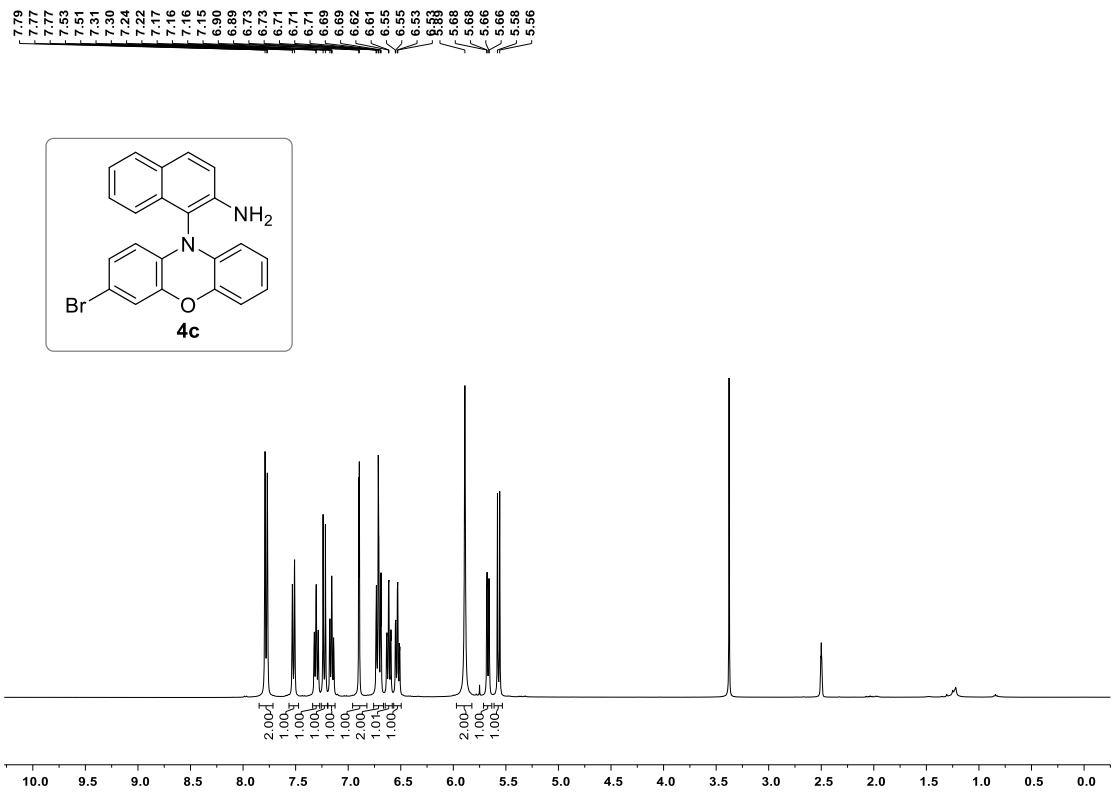
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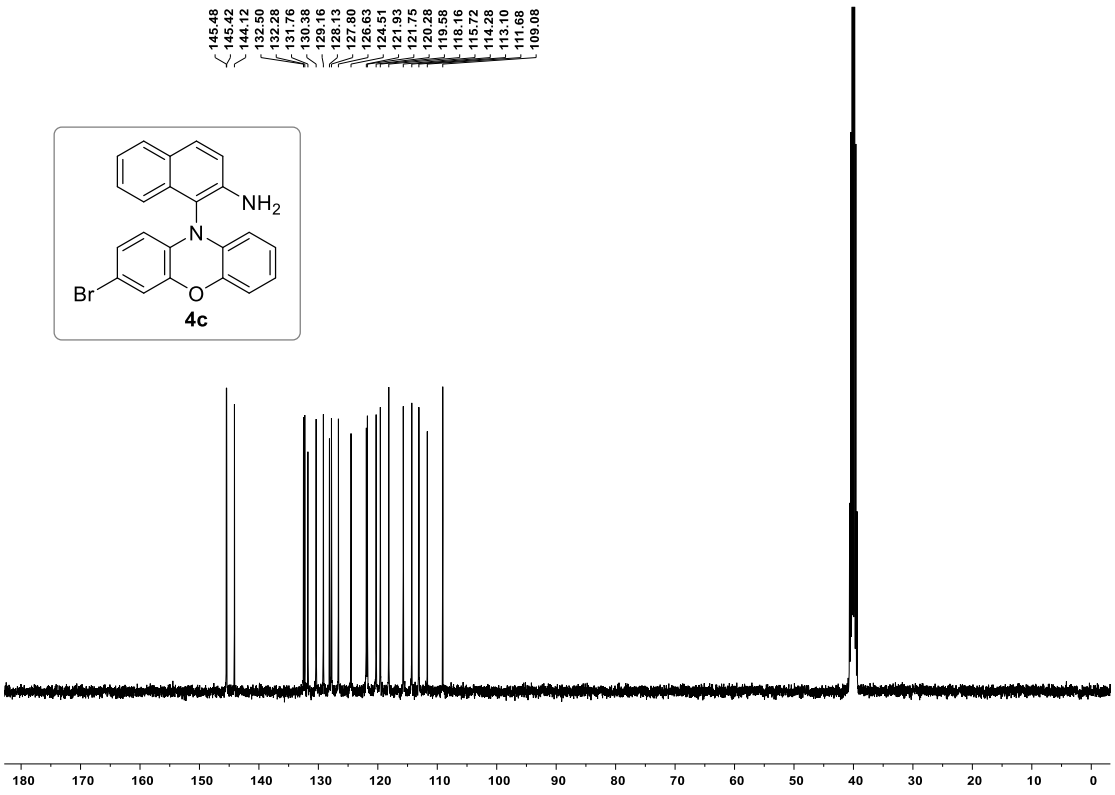
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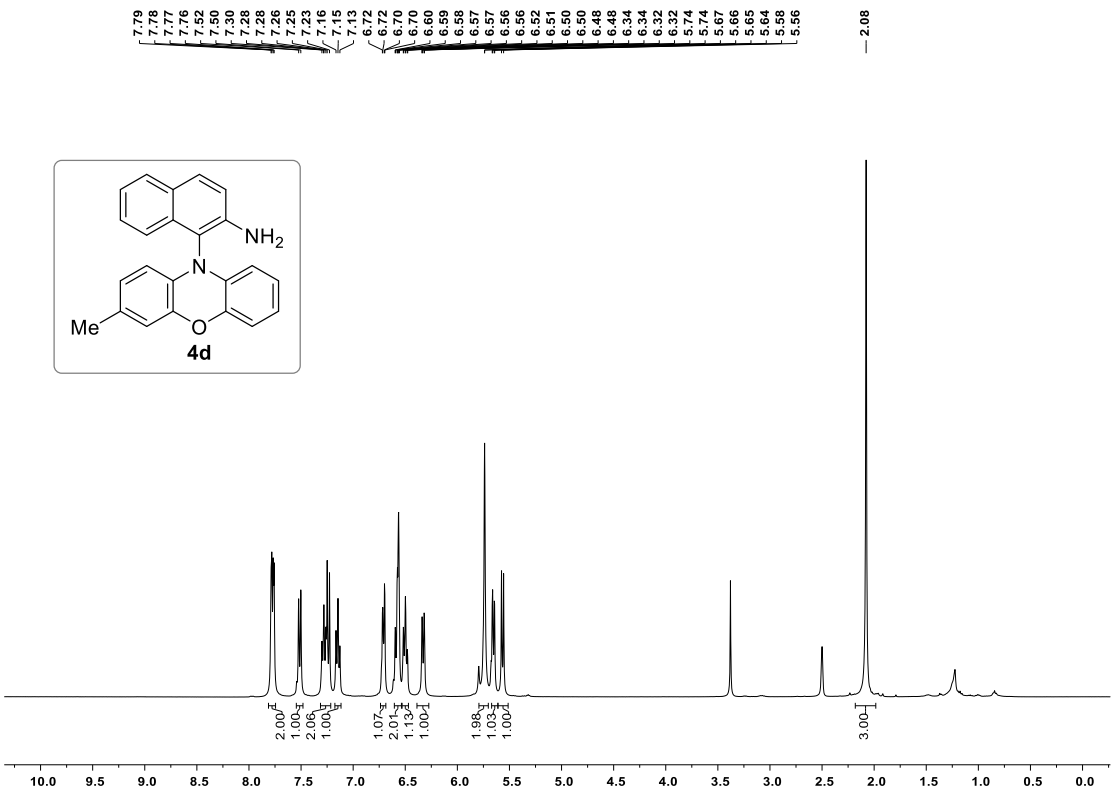
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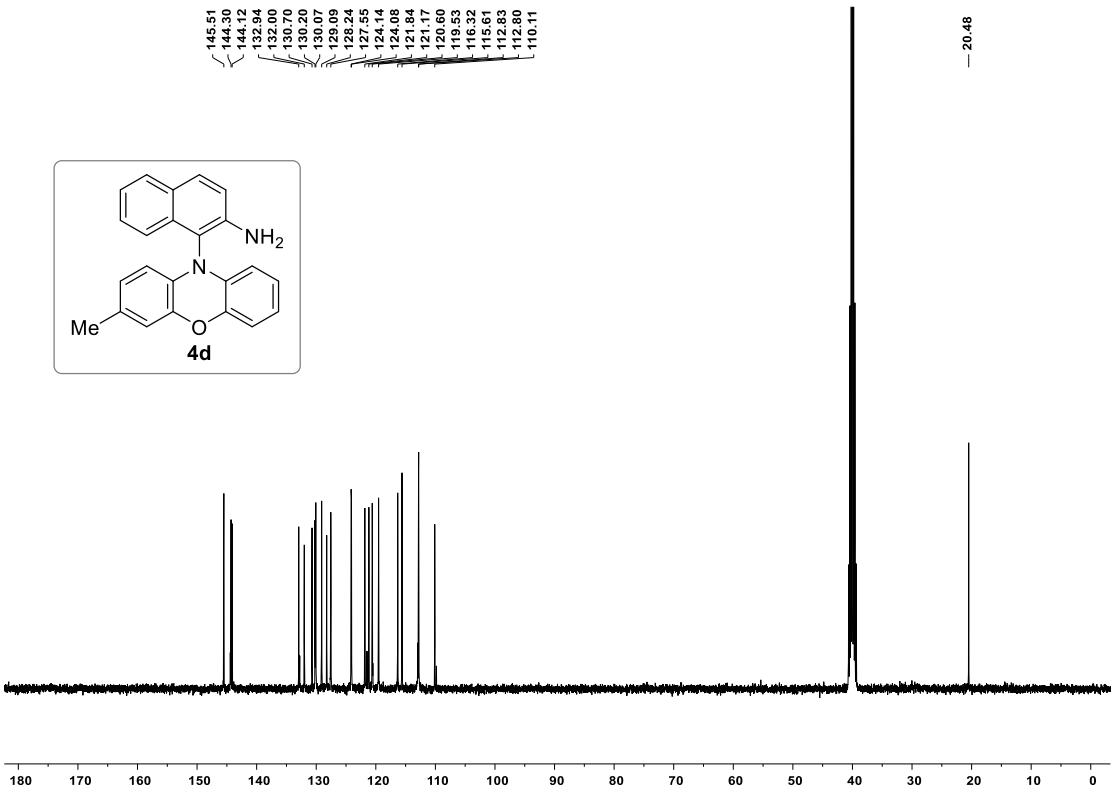
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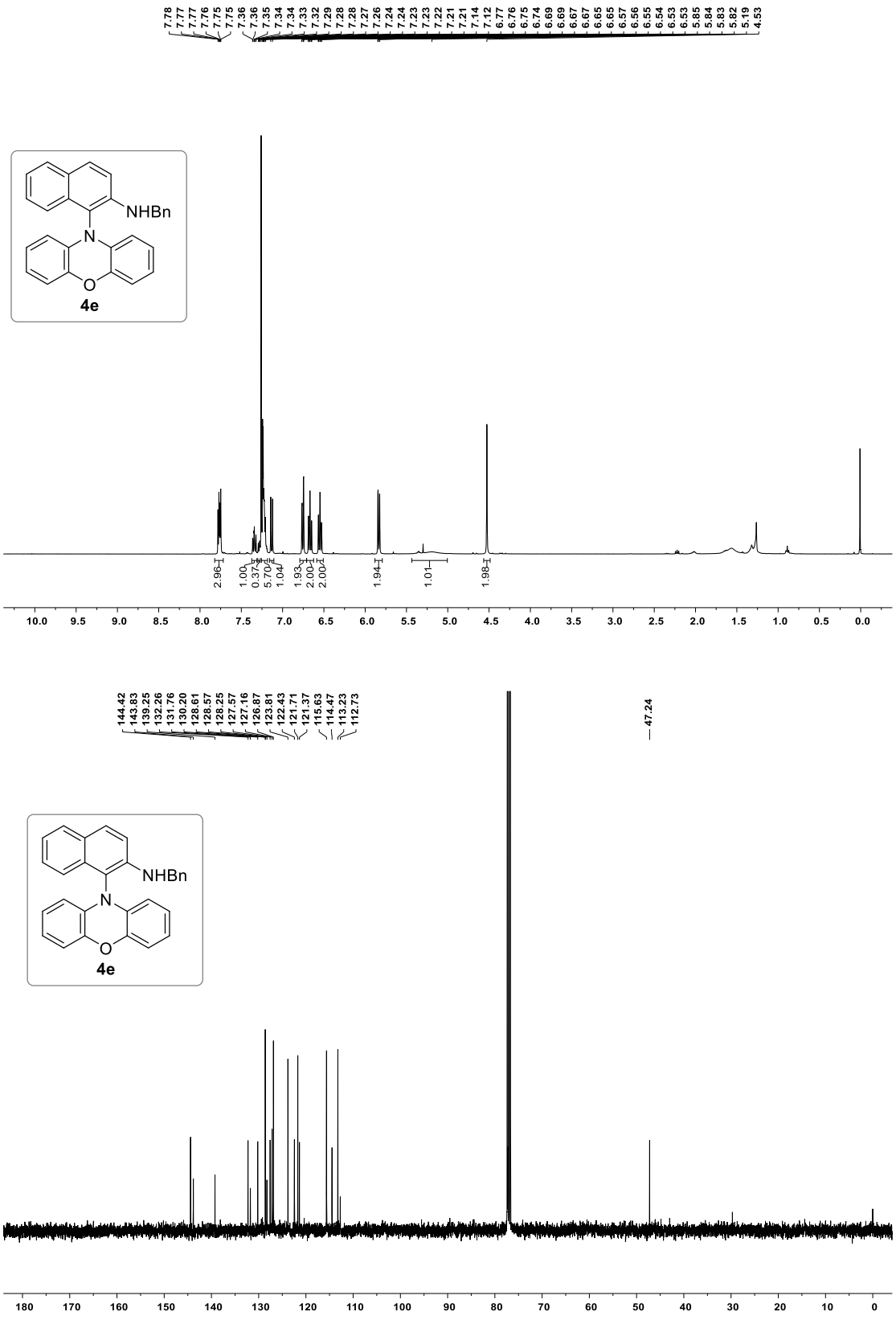
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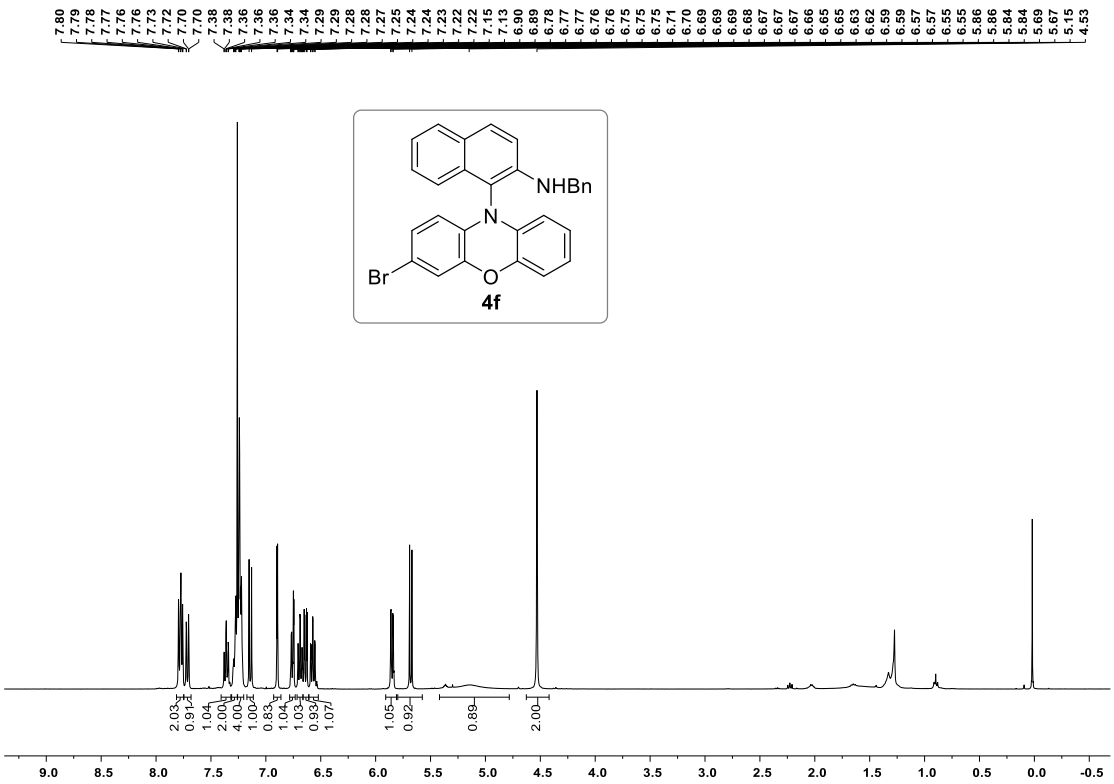
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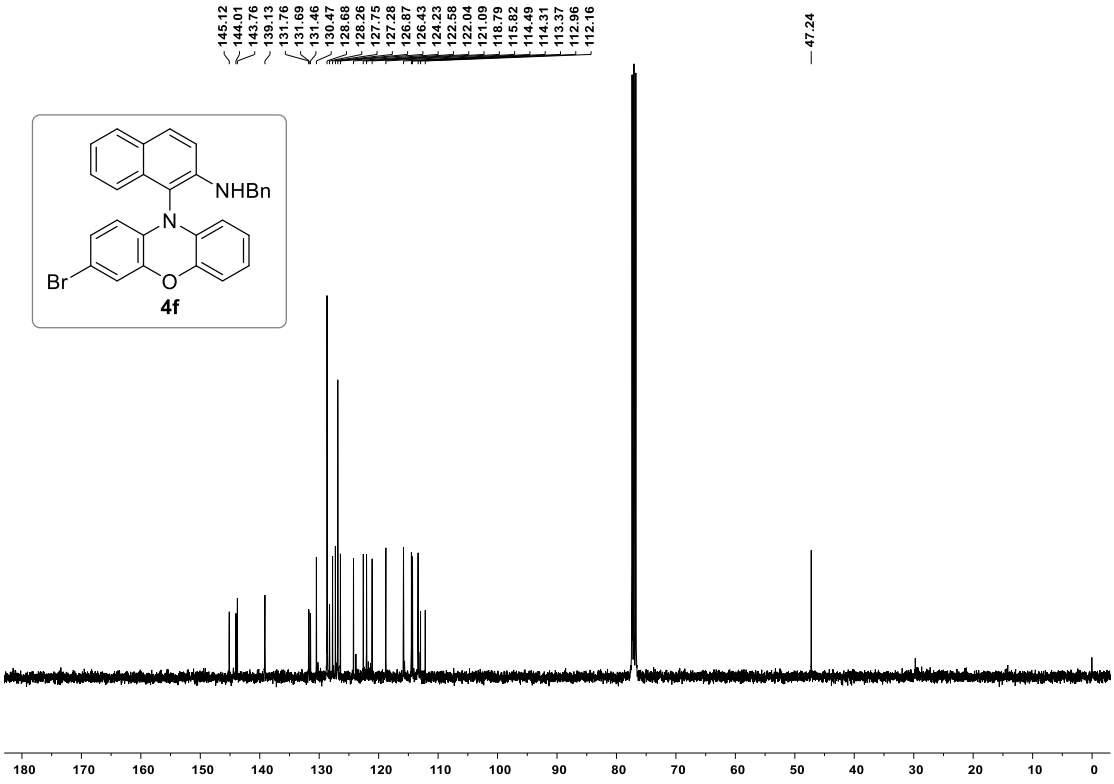
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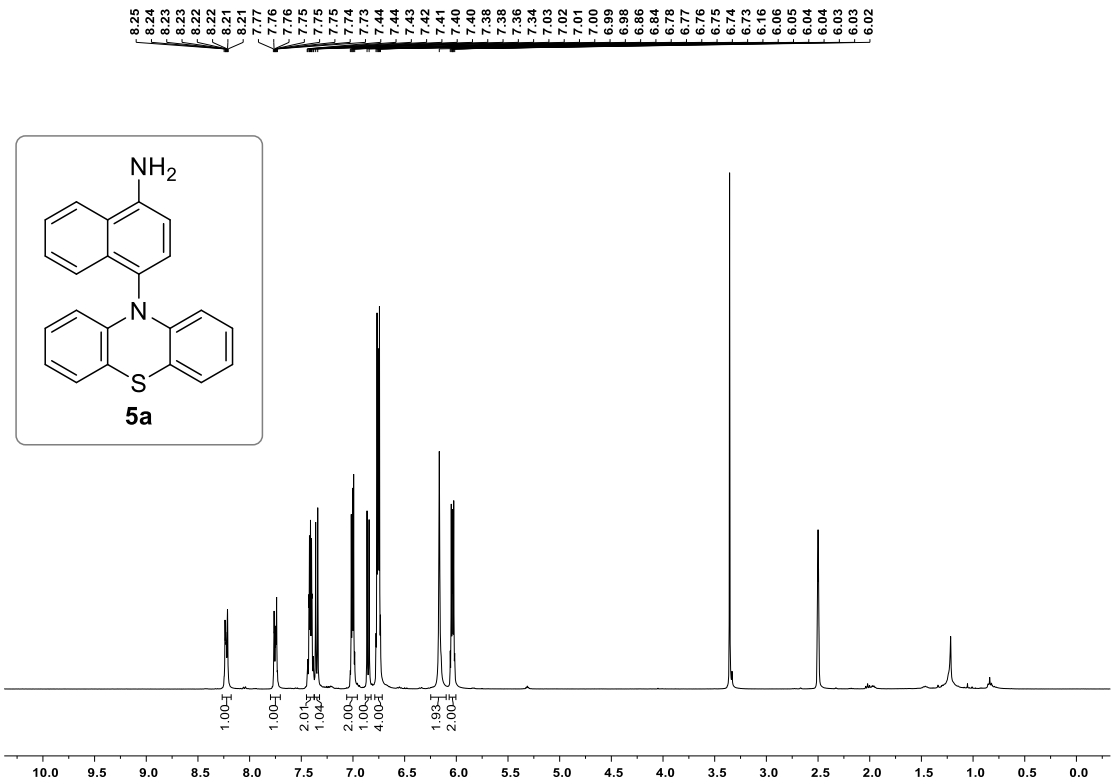
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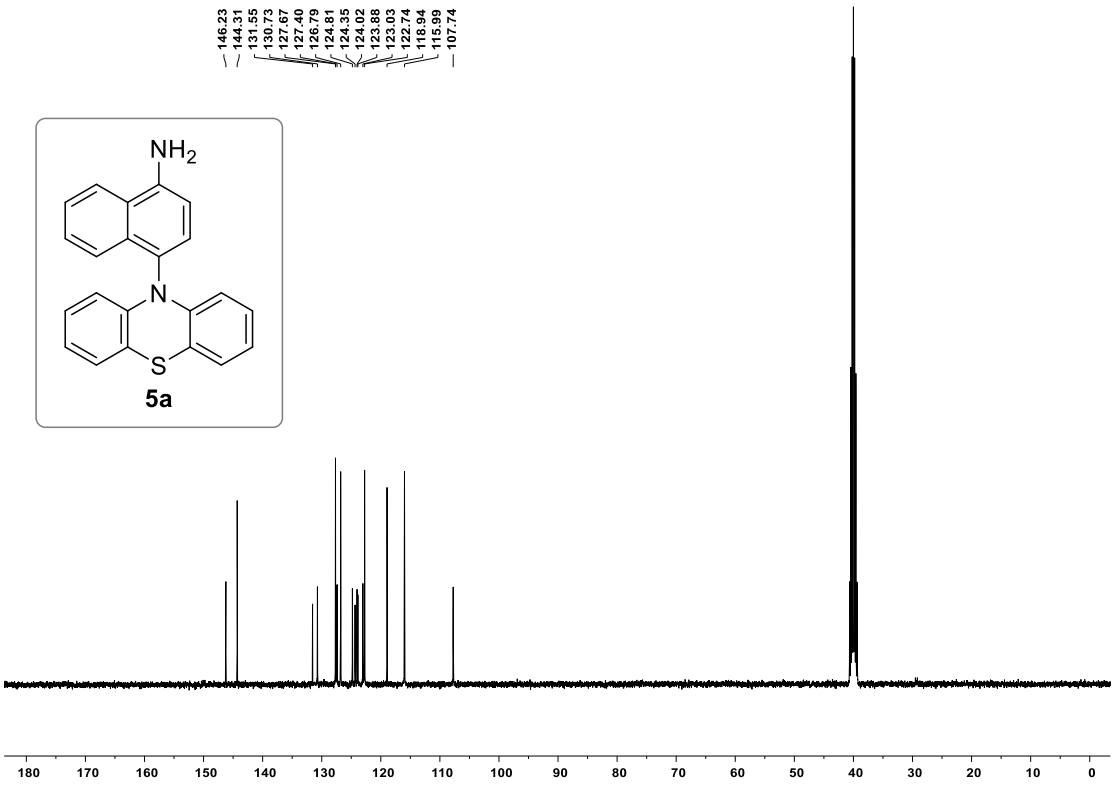
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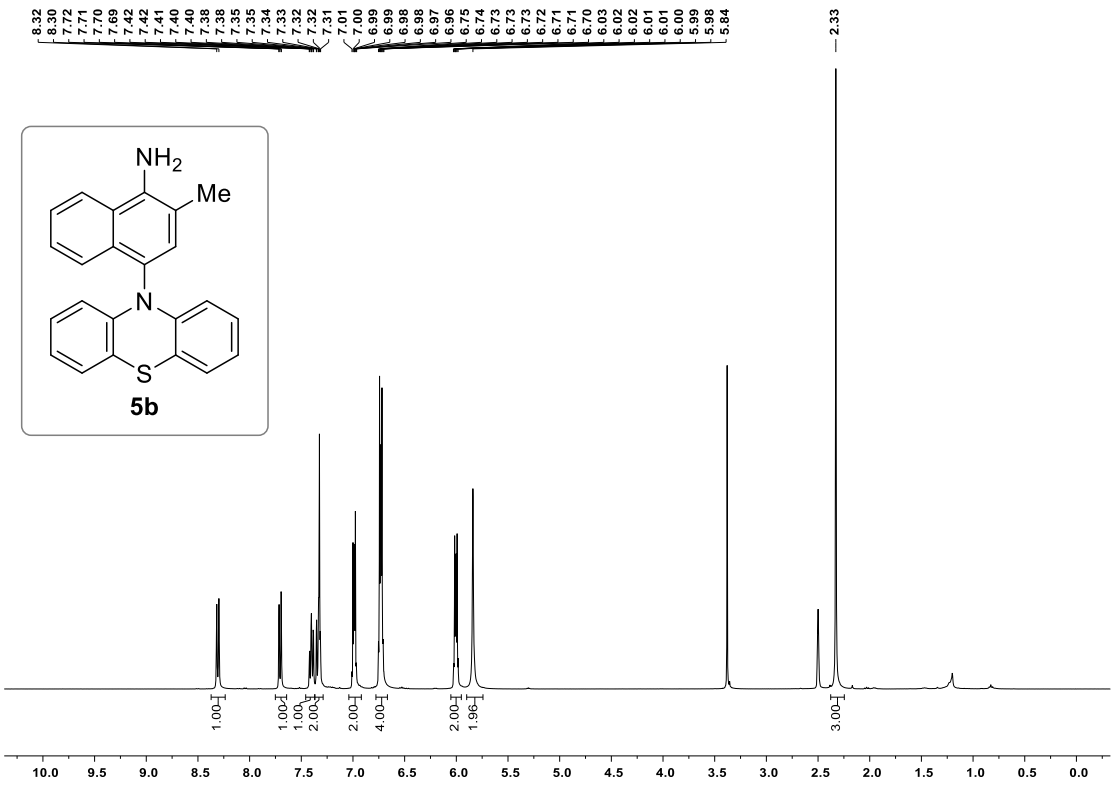
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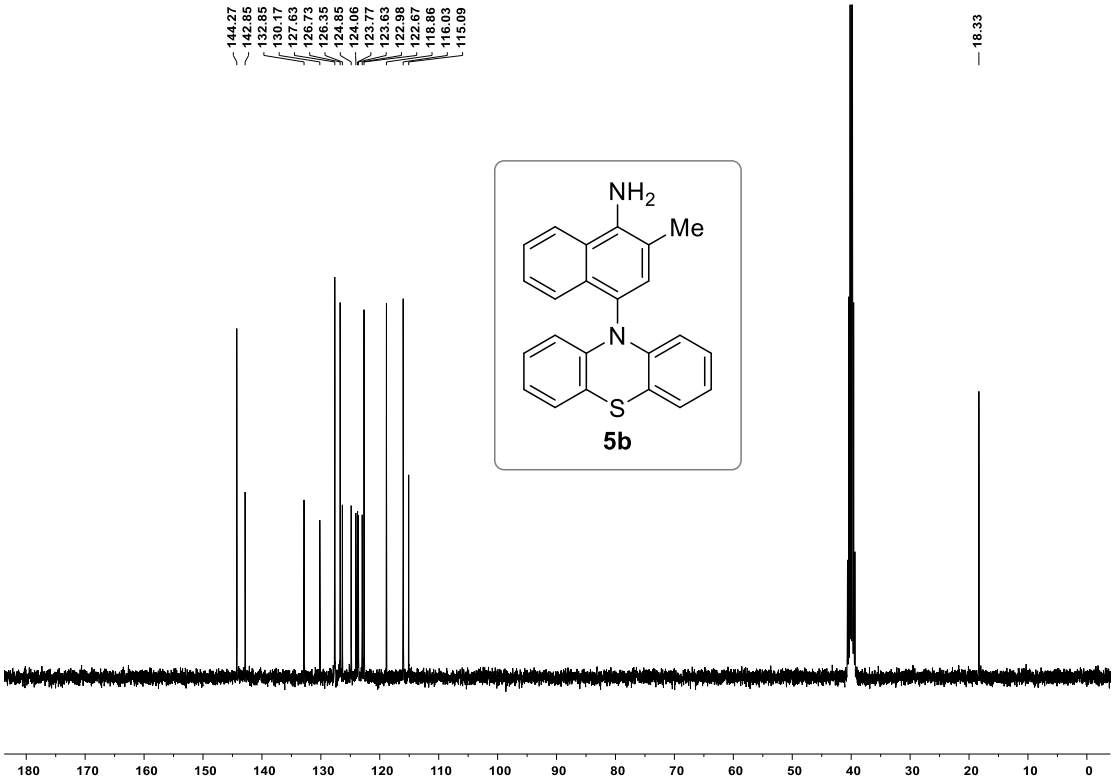
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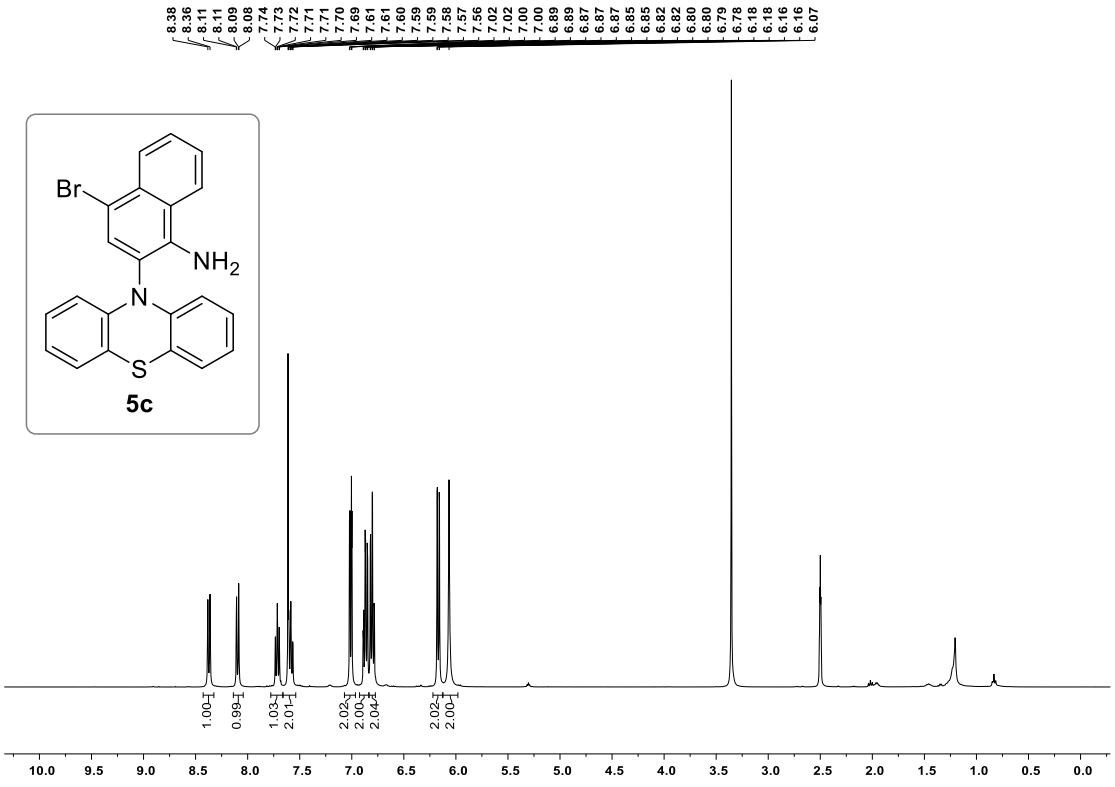
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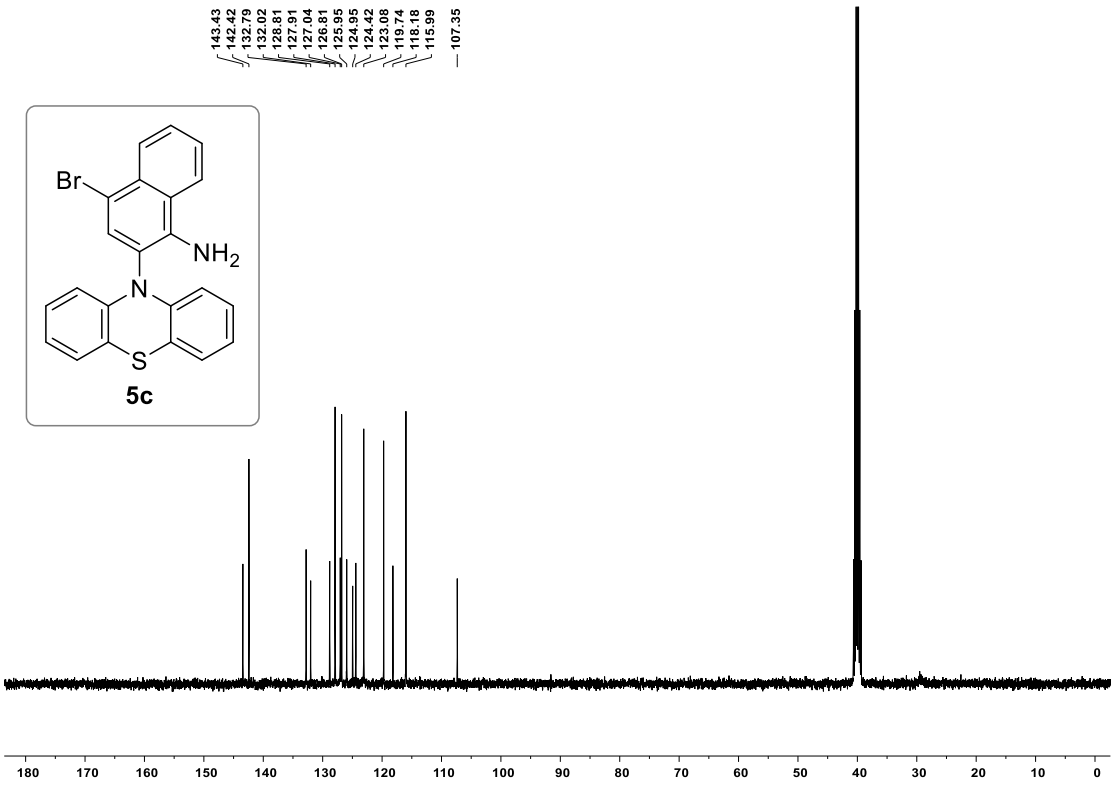
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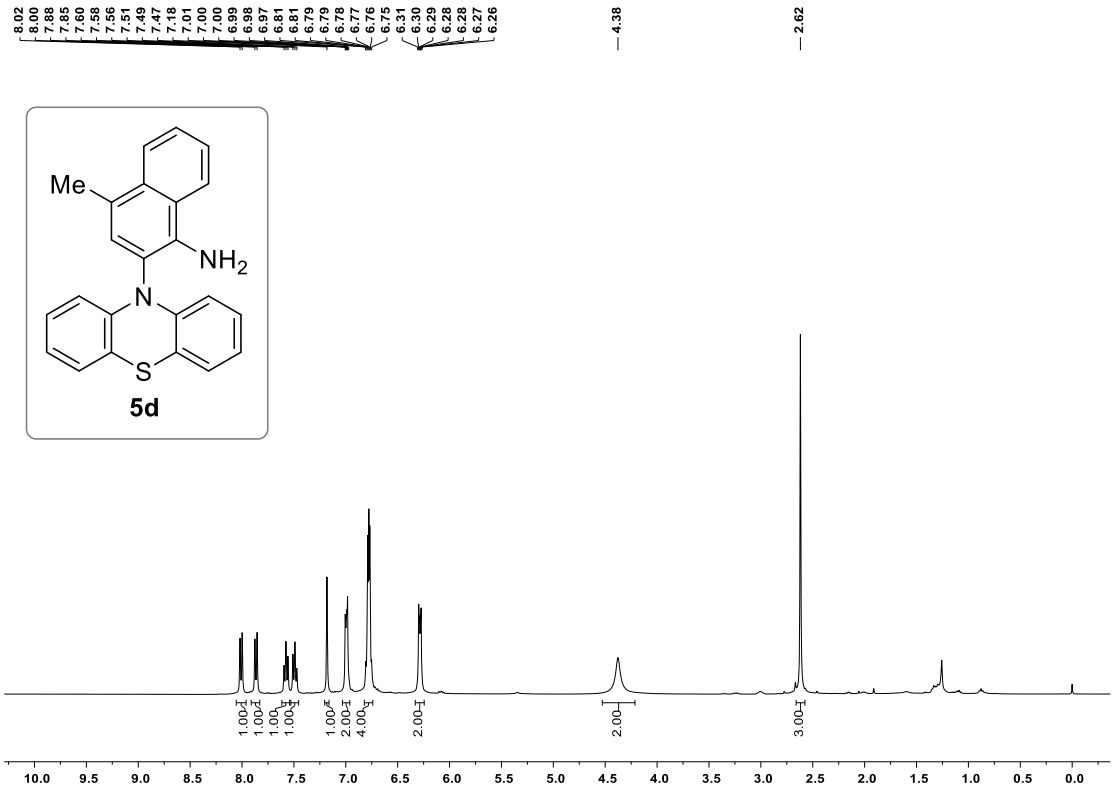
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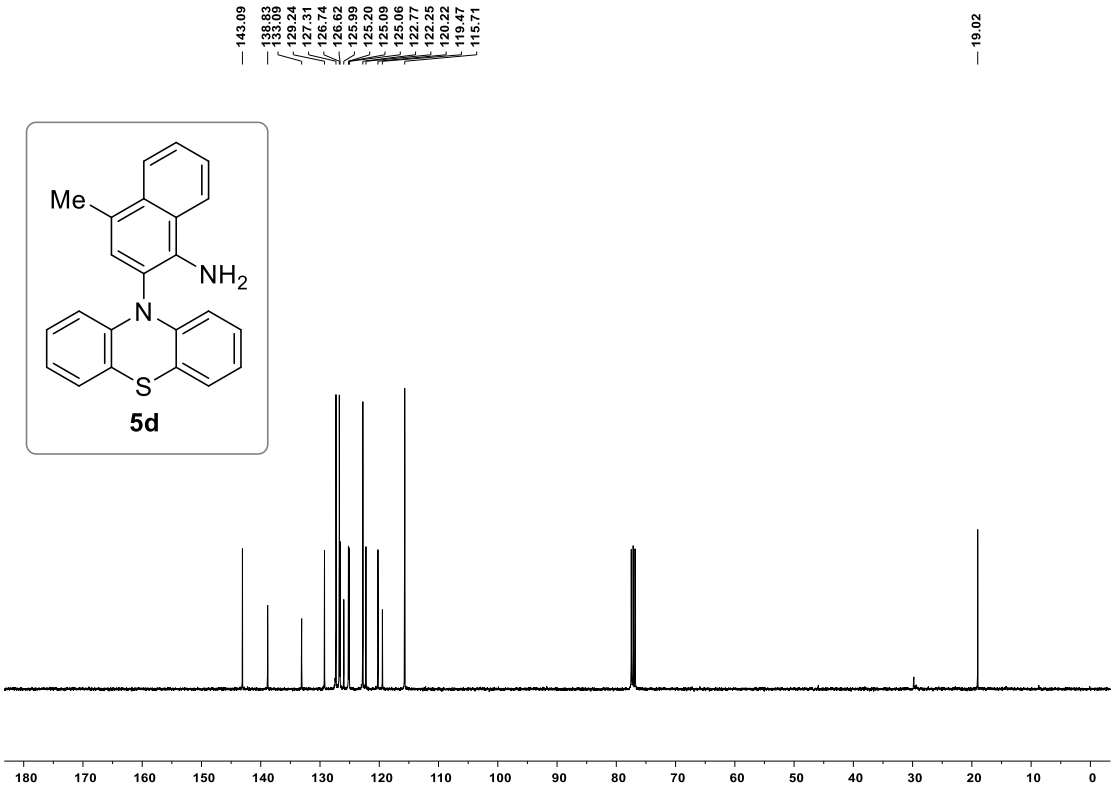
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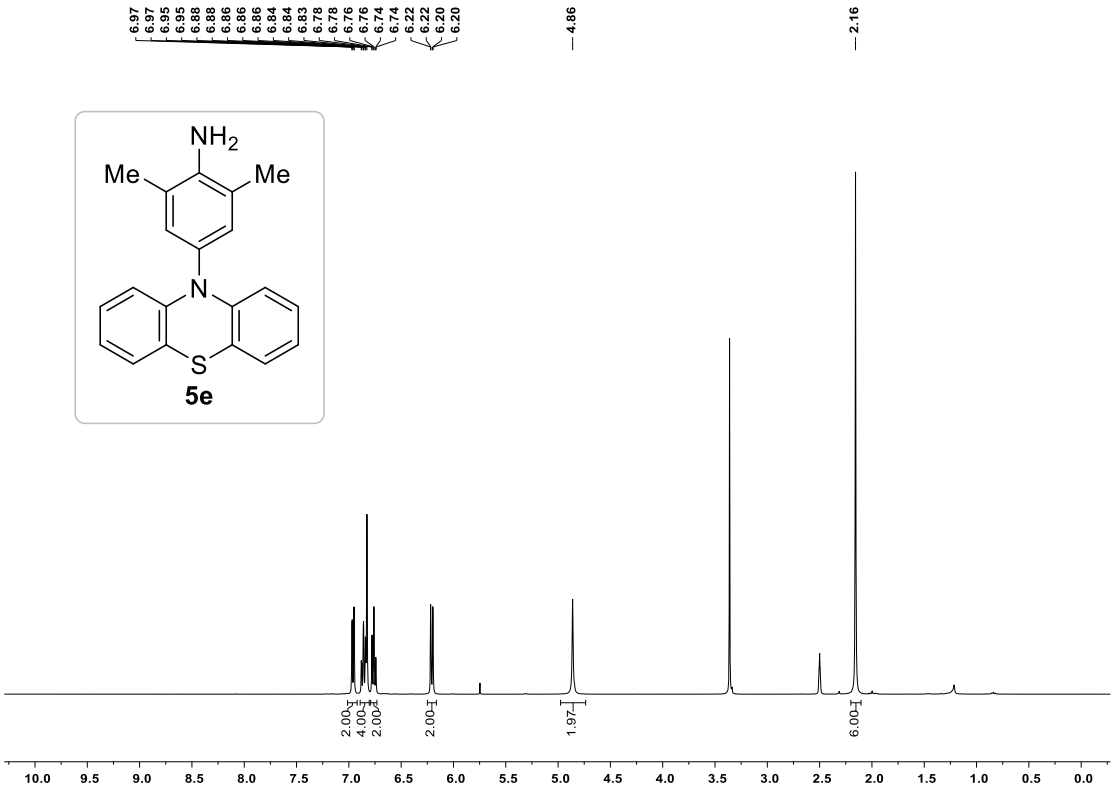
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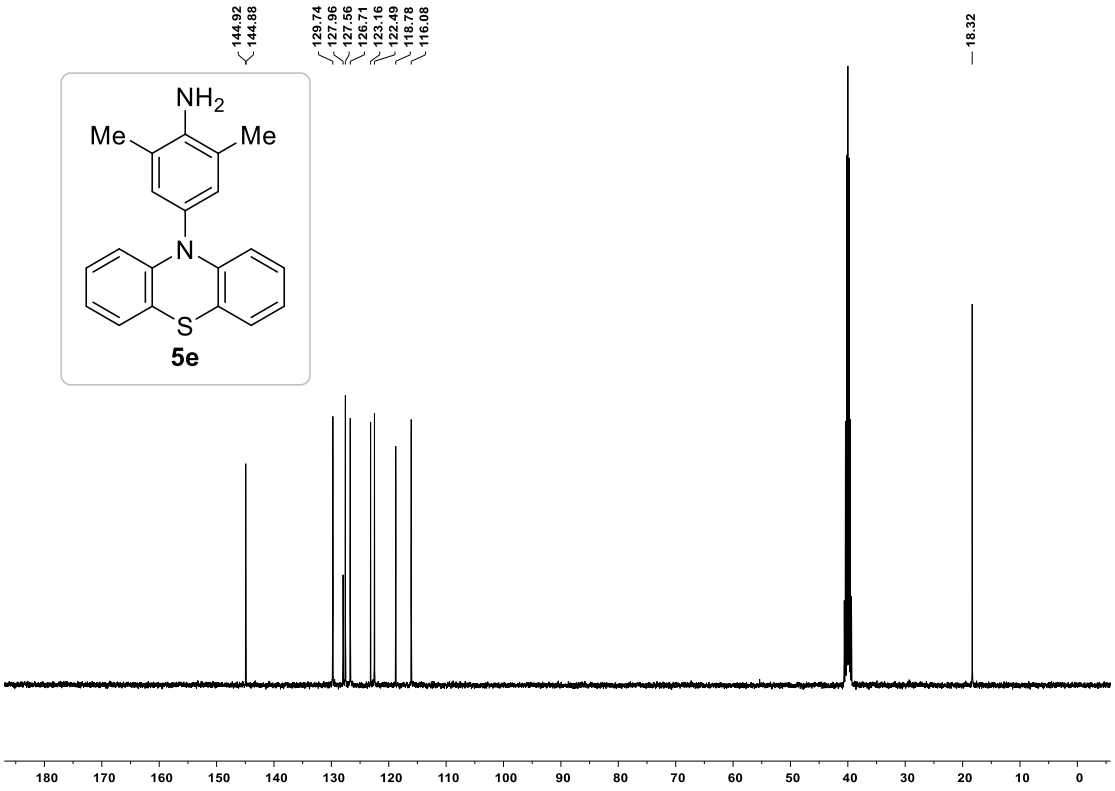
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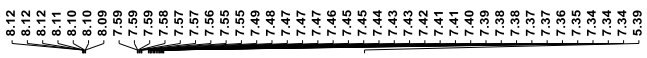
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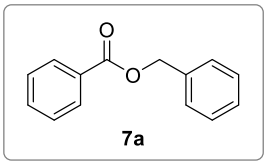
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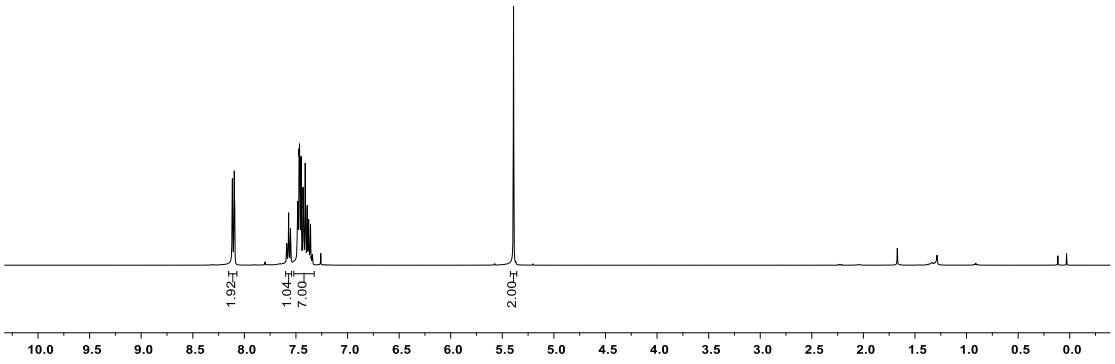
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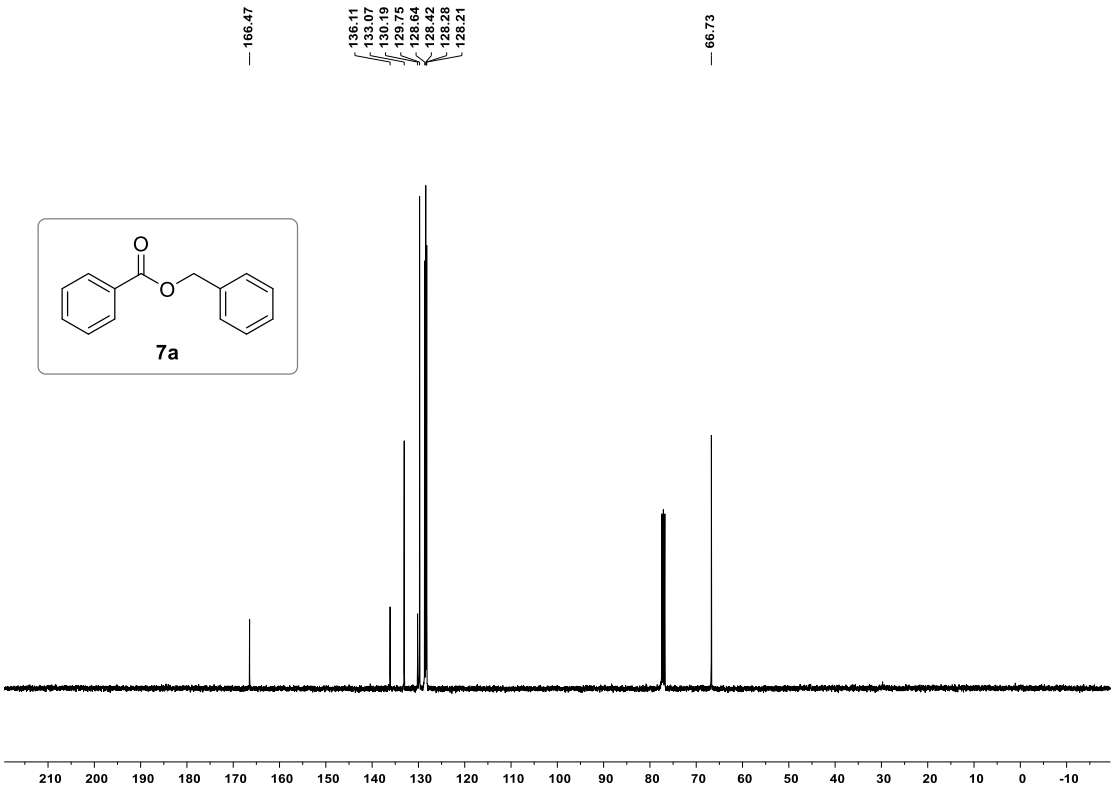
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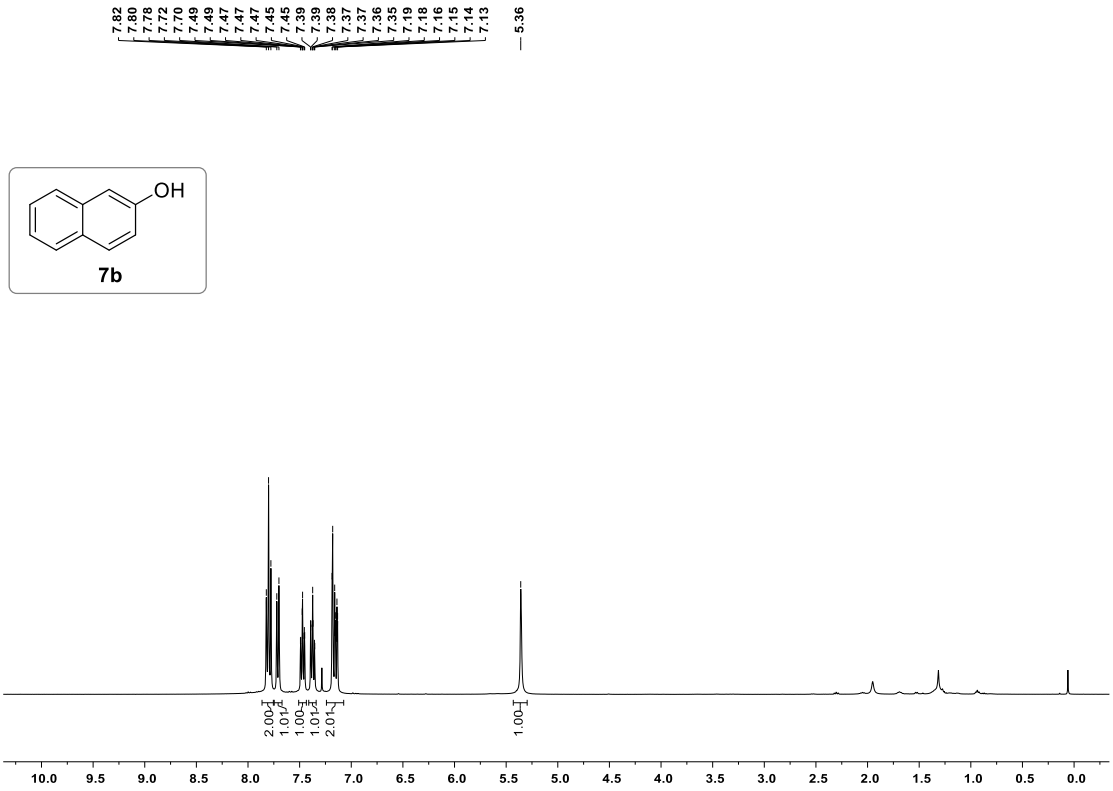
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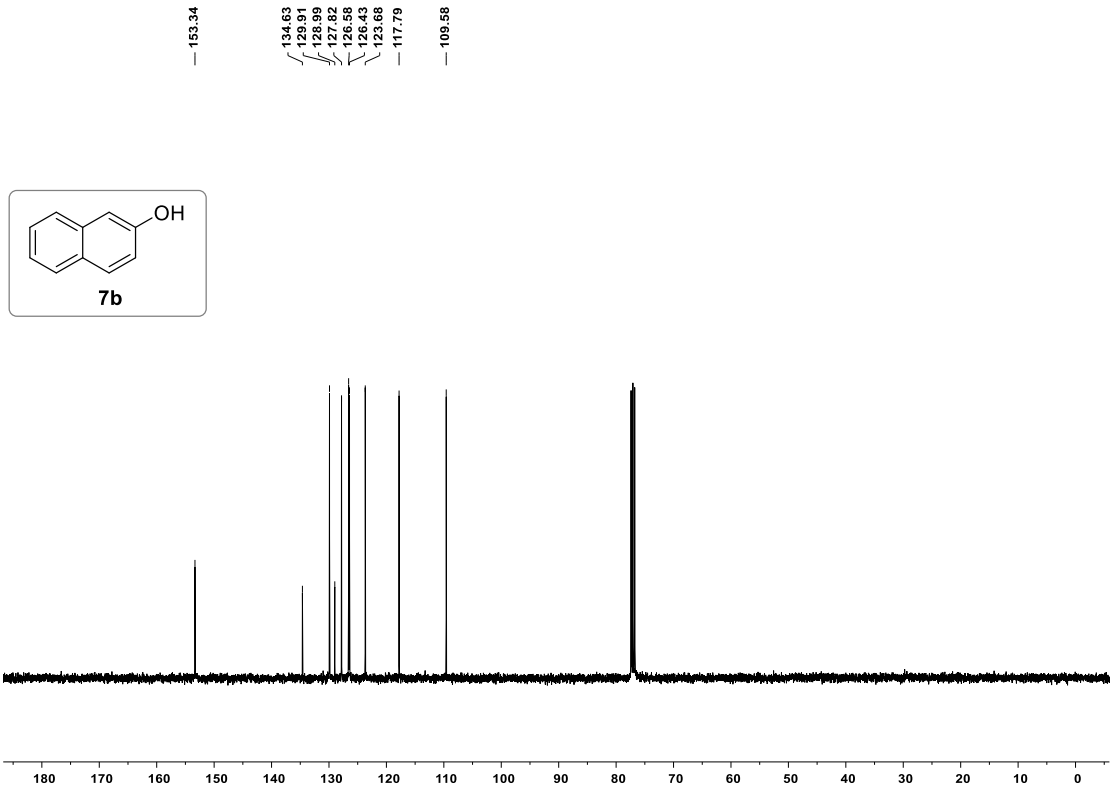
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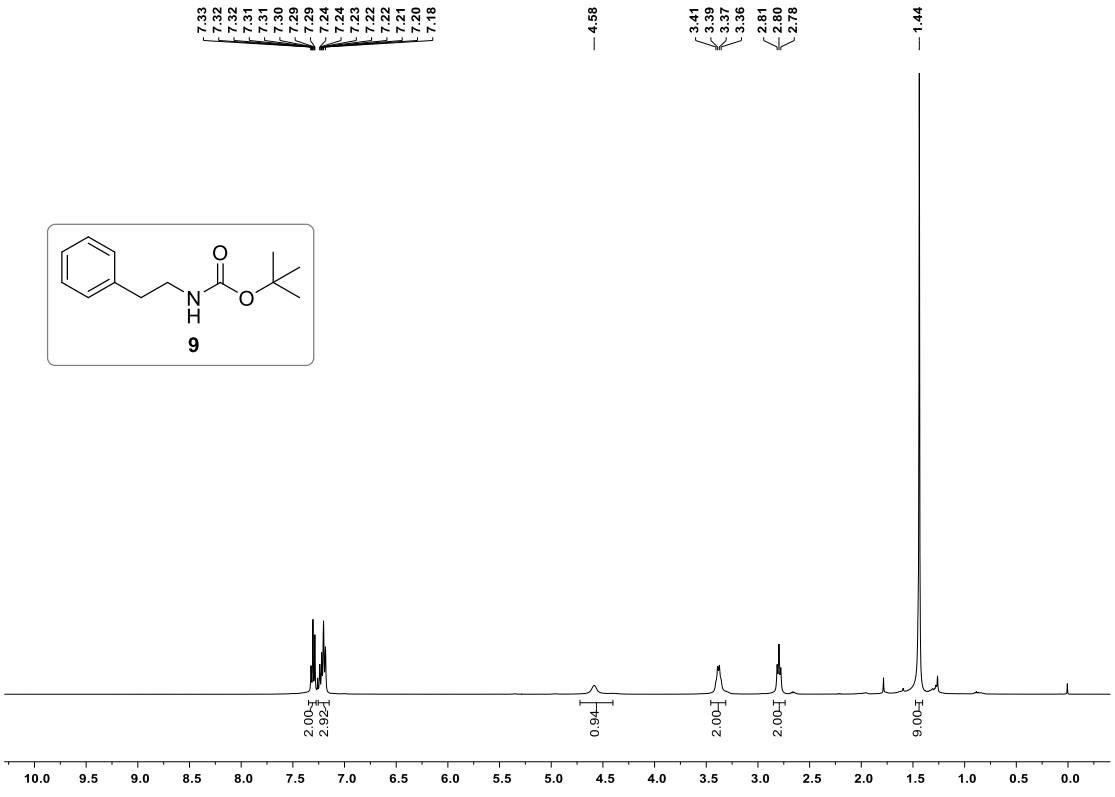
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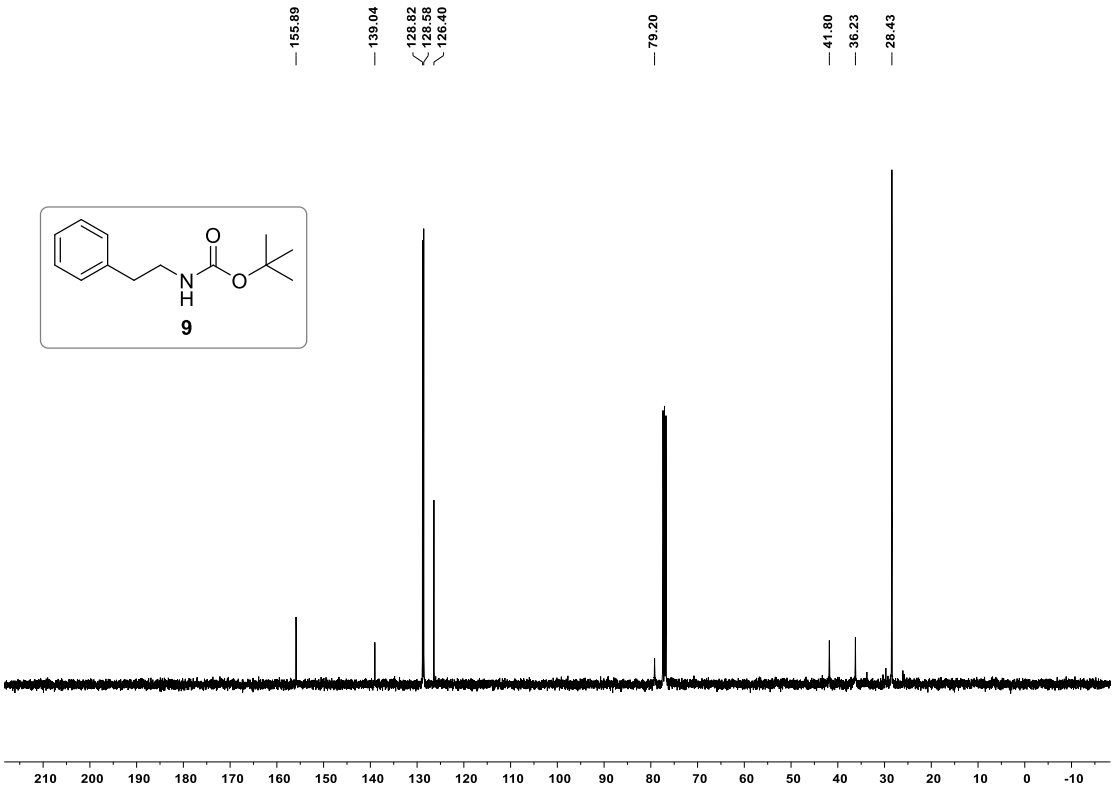
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