Supplementary Information

π-Extended Phenothiazines with fused pentagons and hexagons

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1. General

General: All reactions were carried out using standard Schlenk techniques under argon atmosphere unless otherwise noted. Thin layer chromatography (TLC) was performed using glass plates pre-coated with silica gel impregnated with a fluorescent indicator (Energy Chemical, #BM000035). Flash column chromatography was performed on silica gel (particle size: 200-300 mesh).

Instrumentation: Nuclear magnetic resonance (NMR) spectra were recorded on Bruker AV 600 (^{1}H: 600 MHz and ^{13}C: 150 MHz) NMR spectrometers. Chemical shift values for ^{1}H are referenced to tetramethylsilane (δ 0.00 ppm) or the residual signal of chloroform-*d* (δ 7.26), benzene-d_6 (δ 7.16) or methylene chloride-d_2 (δ 5.32) and chemical shift values for ^{13}C are referenced to the carbon resonance of chloroform-*d* (δ 77.2) or benezene-d_6 (δ 128.1). Infrared (IR) spectra were recorded as KBr-pellets on a Bruker VERTEX 80V spectrometer. HRMS experiments were carried out on a ThermoFisher LTQ Orbitrap XL. Decomposition points and melting points were recorded on an OptiMelt MPA-100 apparatus. X-ray crystallography analysis was performed on XtaLAB Synergy R, DW system, HyPix or XtaLAB Synergy-ED, HyPix-ED, electron source at 200keV. Ultraviolet/visible (UV/vis) absorption spectra were recorded on a Shimadzu UV2600. Emission spectra, absolute quantum yields, as well as fluorescence lifetimes were measured on FluoroMax-4 spectrometer equipped with an integral sphere and a time-correlated single photon counting system with a NanoLED laser. Cyclic voltammograms (CV) was obtained using a glassy carbon working electrode, a platinum counter electrode, and a silver wire reference electrode tested on CHI660E station.

Materials: All the reagents were purchased from Energy Chemical or Bidepharm and used as received. The following reagents were prepared according to the literature procedures: 1,9-dibromo-3,7-di-*tert*-butyl-10*H*-phenothiazine.[1] In biological experiments, 3-(4,5-dimethyl-2-thiazolyl)-2,5-diphenyl-2-H-tetrazolium bromide (MTT), dimethyl sulfoxide (DMSO), Dulbecco's modified Eagle's medium (DMEM), fetal bovine serum (FBS), phosphate-buffered saline (PBS), penicillin/streptomycin and trypsin were purchased commercially. HeLa, HepG2, MCF-7, PC-3, A549 and HUVECs cells were purchased from National Collection of Authenticated Cell Cultures. MitoDeedRed (KGE2708), ER-Tracker Red (KGE2102-20) and Hoechst 33342 (KGA1804-10) were provided by Nanjing KeyGEN BioTECH Co., Ltd. The cells were imaged using the Olympus FV3000 confocal microscope.

2. Synthesis of Compounds

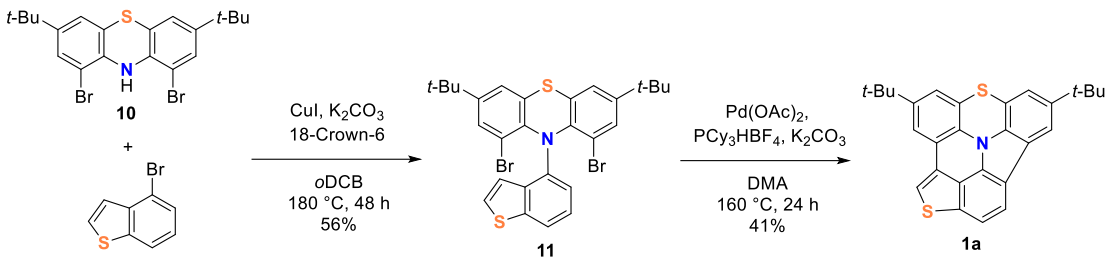
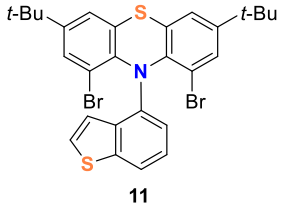


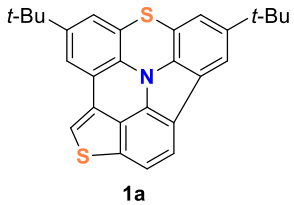
Figure S1. Synthetic route to compound **1a**.

10-(benzo[*b*]thiophen-4-yl)-1,9-dibromo-3,7-di-*tert*-butyl-10*H*-phenothiazine (11)



A 38 mL screw capped glass vial was charged with **10** (934 mg, 2.0 mmol), 4-bromobenzo[*b*]thiophene (848 mg, 4.0 mmol), potassium carbonate (414 mg, 3.0 mmol), copper(I) iodide (76 mg, 0.4 mmol) and 18-crown-6 (106 mg, 0.4 mmol). Under the protection of argon, *o*-dichlorobenzene (2 mL) was added to the vial and the mixture was bubbled with argon for 3 minutes. The vial was quickly sealed and heated at 180 ℃ for 48 hours. After cooling down to room temperature and dilution with dichloromethane (50 mL), the mixture was washed with water (30 mL × 3) and evaporated *in vacuo*. The crude product was purified by silica gel column chromatography eluted with hexane to obtain compound **11** as a pale yellow solid (672 mg, 1.12 mmol, 56%). R_f = 0.50 (hexane); mp 215 °C (dec); IR (neat) cm^{-1} 2964, 1578, 1558, 1544, 1448, 1397, 1361, 1344, 1296, 1262, 1215, 956, 875, 861, 811, 775, 740, 707; ^{1}H NMR (600 MHz, $CDCl_3$, 298 K) δ 7.93–7.68 (m, 2H), 7.61–7.43 (m, 3H), 7.15 (t, J = 8.4 Hz, 1H), 7.13–7.00 (m, 1H), 6.67 (t, J = 7.8 Hz, 1H), 5.92–5.86 (m, 1H), 1.36 (s, 18H). Due to the steric hindrance of bromine atoms, atropisomers form, with ^{1}H NMR and ^{13}C NMR spectra exhibiting multiple signal sets. HRMS (ESI) m/z : [M+H$^+$] calcd. For $C_{28}H_{28}NS_2Br_2$, 600.0030; found, 600.0021.

4,8-di-*tert*-butyl-1,6-dithia-2b^2-azacyclopenta[*fg*]naphtho[3,2,1,8-*mnoa*]aceanthrylene (1a)



A 120 mL screw capped glass vial was charged with compound **11** (401 mg, 0.67 mmol), $Pd(OAc)_2$ (29 mg, 0.13 mmol), PCy_3HBF_4 (96 mg, 0.26 mmol) and potassium carbonate (552 mg, 4 mmol). Under the protection of argon, DMA (8 mL) was added to the vial and the mixture was bubbled with argon for 3 minutes. The vial was quickly sealed and heated at 160 °C for 24 hours. After cooling down to room temperature, the reaction mixture was diluted with dichloromethane (50 mL), the mixture was washed with water (30 mL × 3) and evaporated *in vacuo*. The crude product was purified by silica gel column chromatography eluted with hexane to obtain compound **1a** as a yellow solid (120 mg, 0.27 mmol, 41%). R_f = 0.40 (hexane/dichloromethane = 50/1); mp 306 °C (dec); IR (neat) cm^{-1} 2947, 1539, 1501, 1455, 1371, 1358, 1318, 1266, 1180, 851, 802, 782, 769, 745, 707, 685, 668, 519, 508, 502; ^1H NMR (600 MHz, $CDCl_3$, 298 K) δ 7.82 (d, J = 8.4 Hz, 1H), 7.67 (d, J = 1.2 Hz, 1H), 7.54 (d, J = 8.4 Hz, 1H), 7.51 (d, J = 1.8 Hz, 1H), 7.41 (s, 1H), 7.06 (d, J = 1.8 Hz, 1H), 7.04 (d, J = 1.2 Hz, 1H), 1.42 (s, 9H), 1.37 (s, 9H);^1H NMR (600 MHz, C_6D_6, 298 K) δ 7.71 (d, J = 1.2 Hz, 1H), 7.65 (d, J = 8.4 Hz, 1H), 7.35 (d, J = 8.4 Hz, 1H), 7.34 (d, J = 1.2 Hz, 1H), 7.08 (d, J = 0.6 Hz, 1H), 7.02 (d, J = 1.8 Hz, 1H), 6.84 (s, 1H), 1.30 (s, 9H), 1.17 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$, 298 K) δ 148.0, 147.2, 134.8, 132.2, 129.9, 127.7, 127.6, 127.3, 122.9, 122.8, 122.1, 120.4, 120.3, 120.2, 116.8, 116.7, 115.6, 115.4, 114.8, 113.4, 35.5, 35.0, 32.1(3C), 31.5(3C); HRMS (ESI) m/z : [M^+] calcd. For $C_{28}H_{25}NS_2$, 439.1428; found, 439.1431.

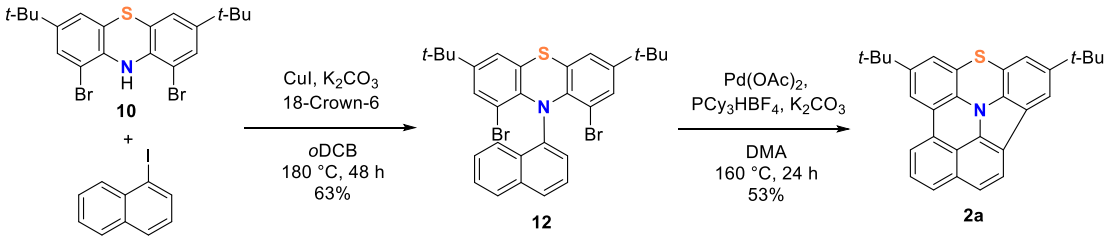
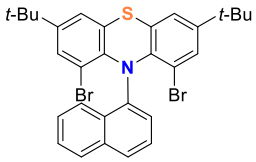


Figure S2. Synthetic route to compound **2a**.

1,9-dibromo-3,7-di-*tert*-butyl-10-(naphthalen-1-yl)-10*H*-phenothiazine (12)

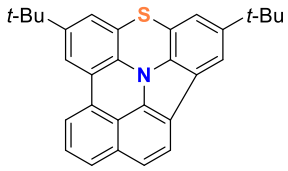


12

A 38 mL screw capped glass vial was charged with **10** (934 mg, 2.0 mmol), 1-iodonaphthalene (1.02 g, 4.0 mmol) potassium carbonate (414 mg, 3.0 mmol), copper(I) iodide (76 mg, 0.4 mmol), and 18-crown-6 (106 mg, 0.4 mmol). Under the protection of argon, *o*-dichlorobenzene (2 mL) was added to the vial and the mixture was bubbled with argon for 3 minutes. The vial was quickly sealed and heated at 180 °C for 48 hours. After cooling down to room temperature and dilution with dichloromethane (50 mL), the mixture was washed with water (30 mL × 3) and evaporated *in vacuo*. The crude product was purified by silica gel column chromatography eluted with hexane to obtain compound **12** as a pale yellow solid (750 mg, 1.26 mmol, 63%). R_f= 0.50 (hexane); mp 198 °C (dec); IR (neat) cm^{-1} 2960, 1568, 1538, 1474, 1446, 1395, 1362, 1299, 1267, 1213, 1102, 1022, 872, 784, 766, 718, 655, 635; ^1H NMR (600 MHz, CD_2Cl_2, 298 K) δ 7.96–7.94 (m, 1H), 7.73 (d, J = 8.4 Hz, 1H), 7.70–7.68 (m, 1H), 7.58–7.56 (m, 1H), 7.54–

7.53 (m, 1H), 7.40 (d, J = 7.8 Hz, 1H), 7.28 (t, J = 7.8 Hz, 1H), 7.23–7.16 (m, 2H), 7.01 (t, J = 7.8 Hz, 1H), 6.75–6.68 (m, 1H), 1.33 (d, J = 3.0 Hz, 18H). Due to the steric hindrance of bromine atoms, atropisomers form, with ^{1}H NMR and ^{13}C NMR spectra exhibiting multiple signal sets. HRMS (ESI) m/z : [M+H$^+$] calcd. For $C_{30}H_{30}NSBr_2$, 594.0466; found, 594.0461.

5,9-di-*tert*-butylnaphtho[8',1',2':7,8,1]indolizino[2,3,4,5,6-*klmn*]phenothiazine (2a)



2a

A 38 mL screw capped glass vial was charged with compound **12** (200 mg, 0.34 mmol), $Pd(OAc)_2$ (16 mg, 0.07 mmol), PCy_3HBF_4 (52 mg, 0.14 mmol) and potassium carbonate (276 mg, 2 mmol). Under the protection of argon, DMA (2 mL) was added to the vial and the mixture was bubbled with argon for 3 minutes. The vial was quickly sealed and heated at 160 °C for 24 hours. After cooling down to room temperature, the reaction mixture was diluted with dichloromethane (50 mL), the mixture was washed with water (30 mL × 3) and evaporated *in vacuo*. The crude product was purified by silica gel column chromatography eluted with hexane to obtain compound **2a** as a yellow solid (78 mg, 0.18 mmol, 53%). R_f = 0.40 (hexane/dichloromethane = 50/1); mp 303 °C (dec); IR (neat) cm^{-1} 2948, 1546, 1499, 1480, 1457, 1398, 1376, 1361, 851, 817, 789, 755, 691, 646, 600, 557, 523, 514; ^{1}H NMR (600 MHz, $CDCl_3$, 298 K) δ 8.02 (d, J = 9.0 Hz, 1H), 7.99 (d, J = 7.8 Hz, 1H), 7.90 (d, J = 7.8 Hz, 1H), 7.87 (d, J = 1.2 Hz, 1H), 7.73 (d, J = 1.2 Hz, 1H), 7.68 (t, J = 7.8 Hz, 1H), 7.58 (d, J = 9.0 Hz, 1H), 7.16 (d, J = 1.2 Hz, 1H), 7.06 (d, J = 1.2 Hz, 1H), 1.45 (s, 9H), 1.42 (s, 9H); ^{1}H NMR (600 MHz, C_6D_6, 298 K) δ 7.93 (d, J = 8.4 Hz, 1H), 7.80–7.79 (s+d overlapping, J = 8.4 Hz, 2H), 7.76 (d, J = 7.2 Hz, 1H), 7.73 (s, 1H), 7.53–7.49 (d+t overlapping, J = 8.4 Hz, 2H), 7.11–7.10 (m, 2H), 1.34 (s, 9H), 1.20 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$, 298 K) δ 147.7, 147.4, 132.0, 130.7, 127.9, 127.7, 126.9, 126.6, 124.5, 122.9, 122.0, 121.7, 121.3, 121.2, 119.8, 118.4, 118.2, 116.9, 116.1, 115.9, 114.3, 111.9, 35.6, 35.2, 32.1(3C), 31.6(3C); HRMS (ESI) m/z : [M$^+$] calcd. For $C_{30}H_{27}NS$, 433.1864; found, 433.1855.

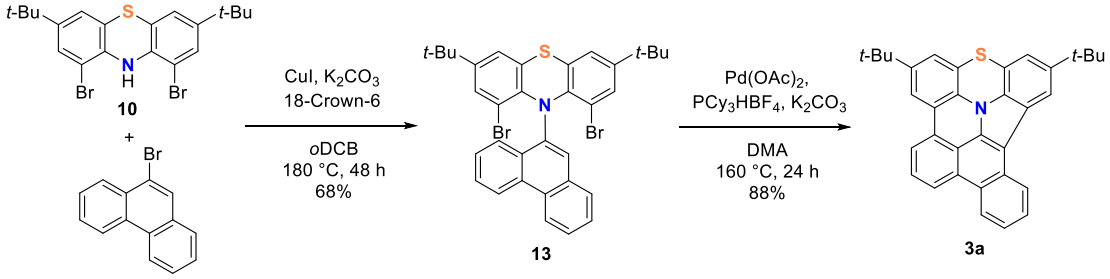
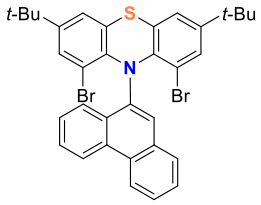


Figure S3. Synthetic route to compound **3a**.

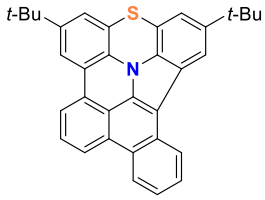
1,9-dibromo-3,7-di-*tert*-butyl-10-(phenanthren-9-yl)-10*H*-phenothiazine (13)



13

A 38 mL screw capped glass vial was charged with **10** (934 mg, 2.0 mmol), 9-bromophenanthrene (1.02 g, 4.0 mmol), potassium carbonate (414 mg, 3.0 mmol), copper(I) iodide (76 mg, 0.4 mmol) and 18-crown-6 (106 mg, 0.4 mmol). Under the protection of argon, *o*-dichlorobenzene (2 mL) was added to the vial and the mixture was bubbled with argon for 3 minutes. The vial was quickly sealed and heated at 180 ℃ for 48 hours. After cooling down to room temperature and dilution with dichloromethane (50 mL), the mixture was washed with water (30 mL × 3) and evaporated *in vacuo*. The crude product was purified by silica gel column chromatography eluted with hexane to obtain compound **13** as a pale yellow solid (877 mg, 1.36 mmol, 68%). R_f = 0.50 (hexane); mp 206 °C (dec); IR (neat) cm^{-1} 2962, 2867, 1614, 1591, 1574, 1474, 1449, 1432, 1385, 1310, 1264, 868, 781, 760, 743, 719; ^1H NMR (600 MHz, C_6D_6, 298 K) δ 8.51–8.49 (m, 1H), 8.35–8.33 (m, 1H), 8.18–8.00 (m, 1H), 7.71–7.38 (m, 6H), 7.29–7.23 (m, 4H), 1.00 (s, 18H). Due to the steric hindrance of bromine atoms, atropisomers form, with ^1H NMR and ^{13}C NMR spectra exhibiting multiple signal sets. HRMS (ESI) m/z : [M+H^+] calcd. For $C_{34}H_{32}NSBr_2$, 644.0622; found, 646.0623.

2,6-di-*tert*-butylphenanthro[1',10',9':7,8,1]indolizino[2,3,4,5,6-*klmn*]phenothiazine (3a)



3a

A 120 mL screw capped glass vial was charged with compound **13** (450 mg, 0.7 mmol), $Pd(OAc)_2$ (31 mg, 0.14 mmol), PCy_3HBF_4 (103 mg, 0.28 mmol) and potassium carbonate (579 mg, 4.2 mmol). Under the protection of argon, DMA (8 mL) was added to the vial and the mixture was bubbled with argon for 3 minutes. The vial was quickly sealed and heated at 160 ℃ for 24 hours. After cooling down to room temperature, the reaction mixture was diluted with dichloromethane (50 mL), the mixture was washed with water (30 mL × 3) and evaporated *in vacuo*. The crude product was purified by silica gel column chromatography eluted with hexane to obtain compound **3a** as a yellow solid (298 mg, 0.62 mmol, 88%). R_f = 0.40 (hexane/dichloromethane = 50/1); mp 330 °C (dec); IR (neat) cm^{-1} 2951, 1586, 1551, 1501, 1469, 1361, 1317, 1256, 1157, 854, 839, 806, 744, 732, 646, 504; ^1H NMR (600 MHz, C_6D_6, 298 K) δ 8.70 (d, J = 7.2 Hz, 1H), 8.61 (d, J = 8.4 Hz, 1H), 8.39 (d, J = 8.4 Hz, 1H), 8.11 (s, 1H), 7.89 (d, J = 7.8 Hz, 1H), 7.74 (s, 1H), 7.66 (t, J = 7.8 Hz, 1H), 7.56 (t, J = 7.8 Hz, 1H), 7.47 (t, J = 7.8 Hz, 1H), 7.12 (s, 1H), 7.11 (s, 1H), 1.39 (s, 9H), 1.23 (s, 9H); ^{13}C NMR (150 MHz, C_6D_6/CS_2, 298 K) δ 147.5, 147.4, 130.6, 130.1, 128.8, 127.6, 127.4, 127.1, 126.9, 126.4, 125.7, 124.4, 124.0, 123.2, 122.8, 122.6, 121,7, 121.4, 120.8, 119.7, 118.6, 118.1, 117.2, 114.9,

114.7, 114.6, 35.5, 35.0, 32.1(3C), 31.5(3C); HRMS (ESI) m/z : [M^+] calcd. For $C_{34}H_{29}NS$, 483.2021; found, 483.2026.

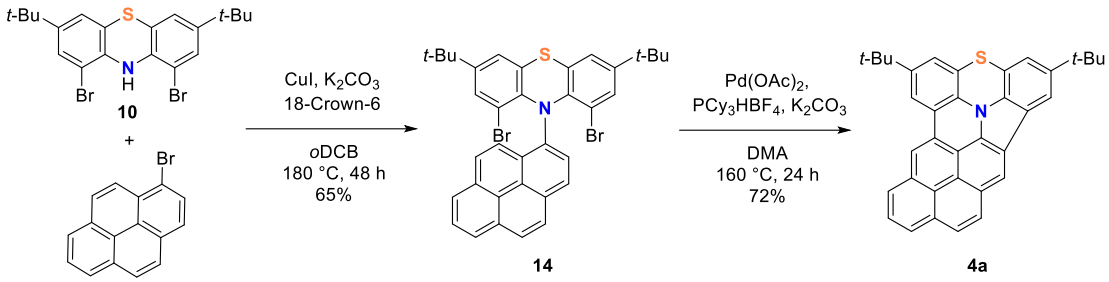
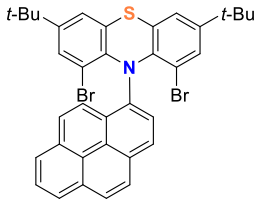


Figure S4. Synthetic route to compound **4a**.

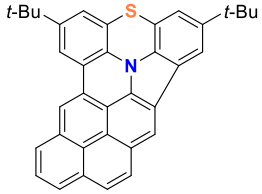
1,9-dibromo-3,7-di-*tert*-butyl-10-(pyren-1-yl)-10*H*-phenothiazine (14)



14

A 38 mL screw capped glass vial was charged with **10** (934 mg, 2.0 mmol), 1-bromopyrene (1.12 g, 4.0 mmol), potassium carbonate (414 mg, 3.0 mmol), copper(I) iodide (76 mg, 0.4 mmol) and 18-crown-6 (106 mg, 0.4 mmol). Under the protection of argon, *o*-dichlorobenzene (2 mL) was added to the vial and the mixture was bubbled with argon for 3 minutes. The vial was quickly sealed and heated at 180 ℃ for 48 hours. After cooling down to room temperature and dilution with dichloromethane (50 mL), the mixture was washed with water (30 mL × 3) and evaporated *in vacuo*. The crude product was purified by silica gel column chromatography eluted with hexane to obtain compound **14** as a pale yellow solid (870 mg, 1.30 mmol, 65%). R_f= 0.50 (hexane); mp 193 °C (dec); IR (neat) cm^{-1} 3042, 2961, 2867, 1603, 1506, 1463, 1435, 1385, 1362, 1323, 1260, 1234, 1218, 1178, 1105, 833, 708; ^{1}H NMR (600 MHz, $CDCl_3$, 298 K) δ 8.02 (d, J = 7.8 Hz, 1H), 7.98 (d, J = 8.4 Hz, 1H), 7.92–7.90 (m, 2H), 7.88–7.85 (m, 2H), 7.75–7.73 (m, 2H), 7.61–7.45 (m, 4H), 7.37–7.32 (m, 1H), 1.39 (s, 18H). Due to the steric hindrance of bromine atoms, atropisomers form, with ^{1}H NMR and ^{13}C NMR spectra exhibiting multiple signal sets. HRMS (ESI) m/z : [M^+] calcd. For $C_{36}H_{31}NSBr_2$, 667.0544; found, 667.0535.

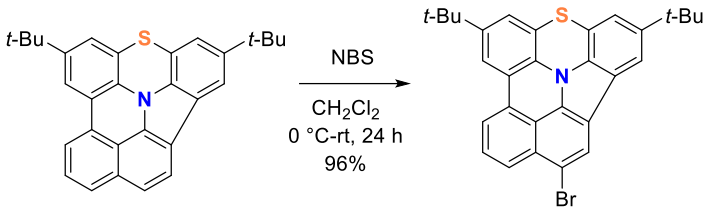
2,6-di-*tert*-butylpyreno[10',1',2':7,8,1]indolizino[2,3,4,5,6-*klmn*]phenothiazine (4a)



4a

A 120 mL screw capped glass vial was charged with compound **14** (400 mg, 0.6 mmol), $Pd(OAc)_2$ (27 mg, 0.12 mmol), PCy_3HBF_4 (88 mg, 0.24 mmol) and potassium carbonate (496

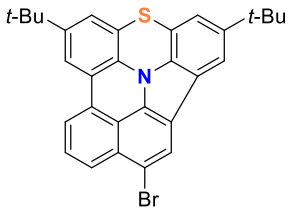
mg, 3.6 mmol). Under the protection of argon, DMA (8 mL) was added to the vial and the mixture was bubbled with argon for 3 minutes. The vial was quickly sealed and heated at 160 ℃ for 24 hours. After cooling down to room temperature, the reaction mixture was diluted with dichloromethane (50 mL), the mixture was washed with water (30 mL × 3) and evaporated *in vacuo*. The crude product was purified by silica gel column chromatography eluted with hexane to obtain compound **4a** as a yellow solid (220 mg, 0.43 mmol, 72%). R_f = 0.40 (hexane/dichloromethane = 50/1); mp 370 °C (dec); IR (neat) cm^{-1} 2947, 1518, 1497, 1391, 1372, 1302, 1253, 1256, 1160, 856, 847, 800, 738, 680, 666, 632, 530, 520, 509, 502; ^1H NMR (600 MHz, CD_2Cl_2, 298 K) δ 8.51 (s, 1H), 8.23 (s, 1H), 8.08 (d, J = 7.8 Hz, 1H), 8.01 (d, J = 9.0 Hz, 1H), 7.96–7.91 (m, 4H), 7.81 (d, J = 9.0 Hz, 1H), 7.19 (d, J = 6.0 Hz, 2H), 1.48 (s, 9H), 1.47 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3/CS_2$, 298 K) δ 147.6, 147.0, 132.8, 131.8, 129.5, 129.1, 128.4, 127.1, 126.7, 126.6, 126.1, 125.3, 125.0, 124.9, 123.5, 123.0, 122.6, 122.0, 121.9, 121.6, 121.3, 118.6, 118.0, 117.6, 116.6, 115.5, 115.3, 114.2, 35.5, 35.1, 32.1(3C), 31.6(3C); HRMS (ESI) m/z : [M^+] calcd. For $C_{36}H_{29}NS$, 507.2021; found, 507.2019.



2a 5a

Figure S5. Synthetic route to compound **5a**.

12-bromo-5,9-di-*tert*-butylnaphtho[8',1',2':7,8,1]indolizino[2,3,4,5,6-*klmn*]phenothiazine (5a)



5a

A 250 mL single neck flask was charged with compound **2a** (350 mg, 0.81 mmol) in dichloromethane (70 mL) at 0 ℃ under the argon atmosphere. N-bromosuccinimde (173 mg, 0.97 mmol) was added to the via portionwise. The reaction mixture was allowed to warm to room temperature gradually and stirred for 24 hours. The reaction was quenched by addition of saturated aqueous Na_2SO_3 solution. The resulting mixture was extracted with dichloromethane (30 mL × 3), and the combined organic layers were washed with water (50 mL), dried over anhydrous Na_2SO_4, and evaporated *in vacuo*. The crude product was purified by washing with dichloromethane (10 mL) to obtain compound **5a** as a pale yellow solid (400 mg, 0.78 mmol, 96%). R_f = 0.40 (hexane/dichloromethane = 50/1); mp 385 °C (dec); IR (neat) cm^{-1} 2955, 1548, 1502, 1477, 1372, 1357, 1318, 1280, 1250, 846, 804, 753, 688, 654, 622, 526, 519; ^1H NMR (600 MHz, C_6D_6, 298 K) δ 8.36 (d, J = 8.4 Hz, 1H), 8.25 (s, 1H), 7.75 (d, J = 7.8 Hz, 1H), 7.72

(d, J = 1.2 Hz, 1H), 7.62 (d, J = 1.2 Hz, 1H), 7.55 (t, J = 7.8 Hz, 1H), 7.11 (d, J = 1.8 Hz, 1H), 7.09 (d, J = 1.2 Hz, 1H), 1.34 (s, 9H), 1.20 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$, 298 K) δ 148.1, 147.9, 130.4, 129.6, 127.8, 127.6, 126.4, 124.9, 124.4, 123.2, 121.8, 121.3, 121.2, 120.8, 119.9, 119.8, 118.5, 117.1, 116.4, 114.3, 112.3, 111.6, 35.6, 35.2, 32.1(3C), 31.6(3C); HRMS (ESI) m/z : [M^+] calcd. For $C_{30}H_{26}NSBr$, 511.0969; found, 511.0968.

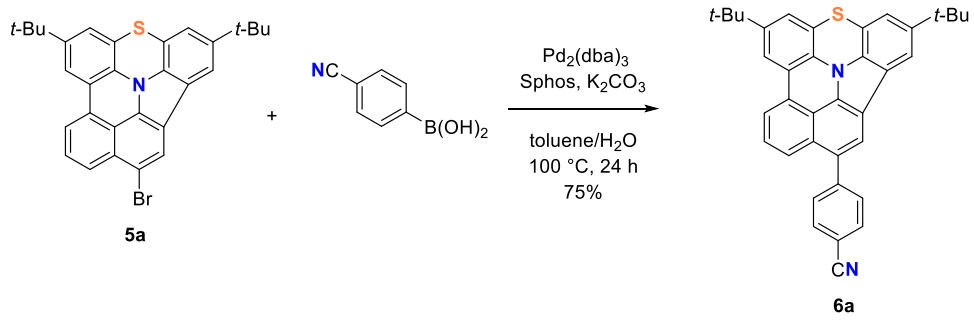
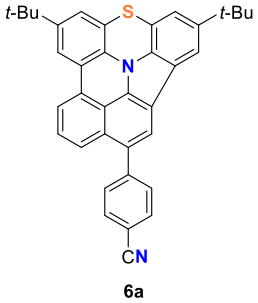


Figure S6. Synthetic route to compound **6a**.

4-(5,9-di-*tert*-butylnaphtho[8',1',2':7,8,1]indolizino[2,3,4,5,6-*klmn*]phenothiazin-12-yl)benzonitrile (6a)



A 120 mL screw capped glass vial was charged with compound **5a** (100 mg, 0.20 mmol), 4-cyanophenylboronic acid (85 mg, 0.58 mmol), $Pd_2(dba)_3$ (37 mg, 0.04 mmol), SPhos (33 mg, 0.08 mmol) and potassium carbonate (80 mg, 0.58 mmol). Under the protection of argon, toluene (10 mL) and water (1 mL) were added to the vial and the mixture was bubbled with argon for 3 minutes. The vial was quickly sealed and heated at 100 ℃ for 24 hours. After cooling down to room temperature, the reaction mixture was diluted with dichloromethane (50 mL), the mixture was washed with water (30 mL × 3) and evaporated *in vacuo*. The crude product was purified by silica gel column chromatography eluted with hexane to obtain compound **6a** as a yellow solid (78 mg, 0.15 mmol, 75%). R_f = 0.30 (hexane/dichloromethane = 20/1); mp 380 °C (dec); IR (neat) cm^{-1} 2957, 2225, 1582, 1546, 1498, 1370, 1317, 1258, 896, 851, 815, 766, 737, 694, 658, 602, 548, 503; ^{1}H NMR (600 MHz, $CDCl_3$, 298 K) δ 8.08 (d, J = 7.8 Hz, 1H), 8.02 (s, 1H), 7.92–7.90 (m, 2H), 7.83 (d, J = 6.6 Hz, 2H), 7.78 (d, J = 8.4 Hz, 2H), 7.74 (s, 1H), 7.70 (t, J = 7.8 Hz, 1H), 7.19 (d, J = 1.8 Hz, 1H), 7.09 (s, 1H), 1.43 (s, 9H), 1.42 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$, 298 K) δ 148.1, 147.9, 146.8, 132.5, 130.9, 130.7, 130.0, 129.3, 128.2, 128.0, 127.2, 126.6, 123.2, 122.8, 122.5, 121.9, 121.8, 121.2, 119.9, 119.3, 118.5, 117.1, 116.8, 116.4, 114.3, 111.8, 110.6, 33.6, 35.2, 32.1(3C), 31.6(3C); [M^+] calcd. For $C_{37}H_{30}N_2S$, 534.2130; found, 534.2126.

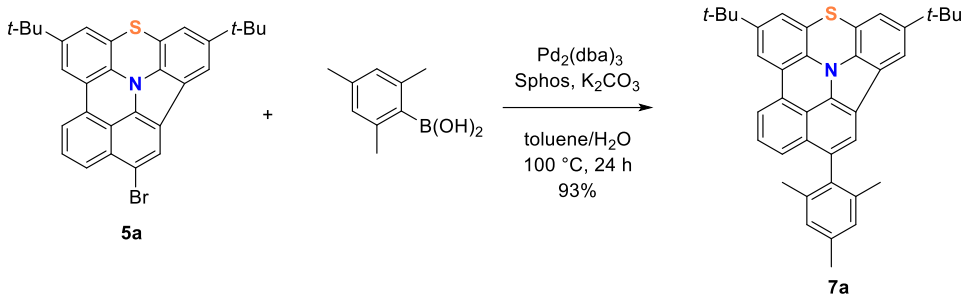
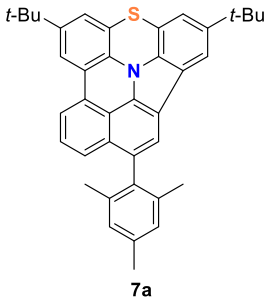


Figure S7. Synthetic route to compound **7a**.

5,9-di-*tert*-butyl-12-mesitylnaphtho[8',1',2':7,8,1]indolizino[2,3,4,5,6-*klmn*]phenothiazine (7a)



A 120 mL screw capped glass vial was charged with compound **5a** (100 mg, 0.20 mmol), 2,4,6-trimethylphenylboronic acid (95 mg, 0.58 mmol), $Pd_2(dba)_3$ (37 mg, 0.04 mmol), SPhos (33 mg, 0.08 mmol) and potassium carbonate (80 mg, 0.58 mmol). Under the protection of argon, toluene (10 mL) and water (1 mL) were added to the vial and the mixture was bubbled with argon for 3 minutes. The vial was quickly sealed and heated at 100 °C for 24 hours. After cooling down to room temperature, the reaction mixture was diluted with dichloromethane (50 mL), the mixture was washed with water (30 mL × 3) and evaporated *in vacuo*. The crude product was purified by silica gel column chromatography eluted with hexane to obtain compound **7a** as a yellow solid (100 mg, 0.18 mmol, 93%). R_f = 0.40 (hexane/dichloromethane = 50/1); mp 327 °C (dec); IR (neat) cm^{-1} 2958, 1545, 1508, 1486, 1370, 1316, 1273, 863, 852, 844, 817, 766, 739, 694, 656, 644, 536, 513, 502; ^1H NMR (600 MHz, C_6D_6, 298 K) δ 7.81 (d, J = 7.2 Hz, 1H), 7.78 (s, 2H), 7.75 (s, 1H), 7.57 (d, J = 8.4 Hz, 1H), 7.44 (t, J = 7.8 Hz, 1H), 7.14 (s, 2H), 7.08 (s, 2H), 2.37 (s, 3H), 2.11 (s, 6H), 1.35 (s, 9H), 1.20 (s, 9H); ^{13}C NMR (150 MHz, C_6D_6, 298 K) δ 147.6, 147.4, 137.9, 137.7, 136.9, 131.2, 130.4, 130.0, 128.8, 128.4, 128.3, 127.4, 127.1, 123.1, 122.8, 122.7, 122.1, 121.9, 121.7, 120.5, 118.4, 117.4, 116.5, 116.0, 114.8, 112.4, 35.5, 34.9, 32.1(3C), 31.4(3C), 21.4, 20.6(2C); [M^+] calcd. For $C_{39}H_{37}NS$, 551.2647; found, 551.2642.

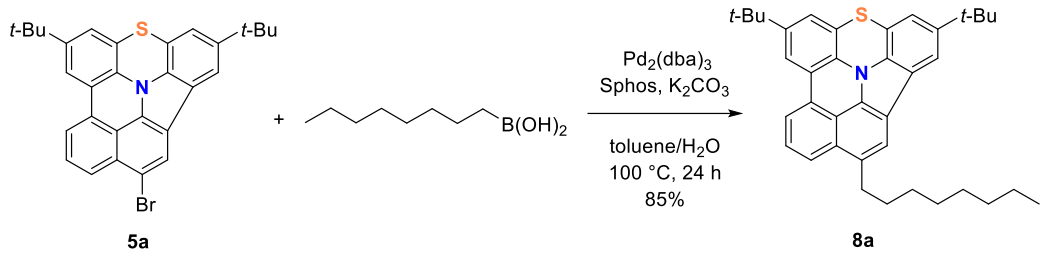
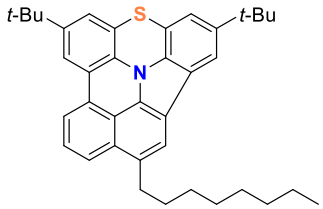


Figure S8. Synthetic route to compound **8a**.

5,9-di-*tert*-butyl-12-octylnaphtho[8',1',2':7,8,1]indolizino[2,3,4,5,6-*klmn*]phenothiazine (8a)



A 120 mL screw capped glass vial was charged with compound **5a** (100 mg, 0.20 mmol), octylboronic acid (92 mg, 0.58 mmol), $Pd_2(dba)_3$ (37 mg, 0.04 mmol), SPhos (33 mg, 0.08 mmol) and potassium carbonate (80 mg, 0.58 mmol). Under the protection of argon, toluene (10 mL) and water (1 mL) were added to the vial and the mixture was bubbled with argon for 3 minutes. The vial was quickly sealed and heated at 100 °C for 24 hours. After cooling down to room temperature, the reaction mixture was diluted with dichloromethane (50 mL), the mixture was washed with water (30 mL × 3) and evaporated *in vacuo*. The crude product was purified by silica gel column chromatography eluted with hexane to obtain compound **8a** as a yellow solid (91 mg, 0.17 mmol, 85%). R_f = 0.40 (hexane/dichloromethane = 50/1); mp 169 °C (dec); IR (neat) cm^{-1} 2921, 1546, 1504, 1461, 1359, 1319, 1272, 1120, 842, 814, 726, 692, 644, 522, 501; ^1H NMR (600 MHz, C_6D_6, 298 K) δ 8.06 (d, J = 8.4 Hz, 1H), 7.96 (s, 1H), 7.88 (d, J = 7.8 Hz, 1H), 7.85 (s, 1H), 7.81 (s, 1H), 7.63 (t, J = 8.4 Hz, 1H), 7.12 (d, J = 7.8 Hz, 2H), 3.19 (t, J = 7.8 Hz, 2H), 1.94–1.89 (m, 2H), 1.55–1.50 (m, 2H), 1.42–1.38 (m, 2H), 1.36 (s, 9H), 1.33–1.27 (m, 6H), 1.21 (s, 9H), 0.91 (t, J = 7.2 Hz, 3H); ^{13}C NMR (150 MHz, $CDCl_3$, 298 K) δ 147.5, 147.2, 130.9, 130.0, 129.5, 128.2, 127.8, 126.9, 126.3, 122.9, 121.9, 121.8, 121.5, 121.1, 120.2, 120.0, 118.4, 116.9, 116.0, 115.7, 114.2, 111.5, 35.6, 35.2, 33.9, 32.2, 32.1(3C), 31.6, 30.9(3C), 30.0, 29.8, 29.5, 22.8, 14.3; [M^+] calcd. For $C_{38}H_{43}NS$, 545.3116; found, 545.3115.

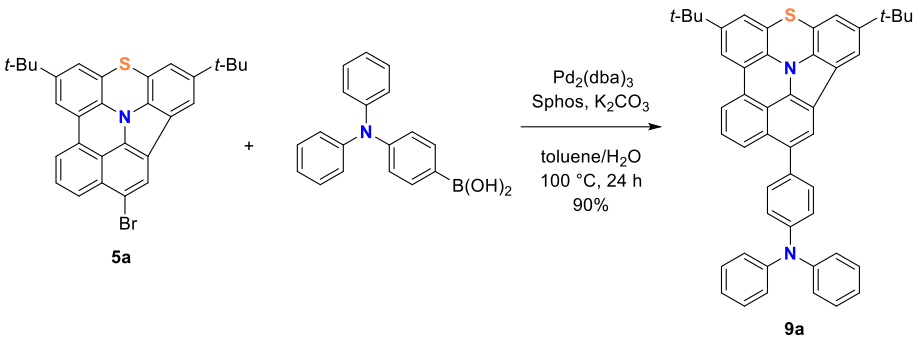
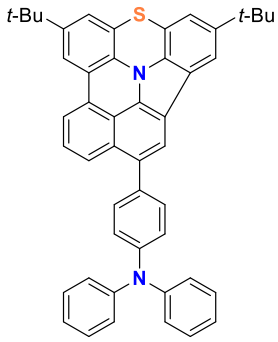


Figure S9. Synthetic route to compound **9a**.

4-(5,9-di-*tert*-butylnaphtho[8',1',2':7,8,1]indolizino[2,3,4,5,6-*klmn*]phenothiazin-12-yl)-*N*,*N*-diphenylaniline (9a)



A 120 mL screw capped glass vial was charged with compound **5a** (100 mg, 0.20 mmol), 4-(diphenylamino)phenylboronic acid (168 mg, 0.58 mmol), $Pd_2(dba)_3$ (37 mg, 0.04 mmol), SPhos (33 mg, 0.08 mmol) and potassium carbonate (80 mg, 0.58 mmol). Under the protection of argon, toluene (10 mL) and water (1 mL) were added to the vial and the mixture was bubbled with argon for 3 minutes. The vial was quickly sealed and heated at 100 °C for 24 hours. After cooling down to room temperature, the reaction mixture was diluted with dichloromethane (50 mL), the mixture was washed with water (30 mL × 3) and evaporated *in vacuo*. The crude product was purified by silica gel column chromatography eluted with hexane to obtain compound **9a** as a yellow solid (119 mg, 0.18 mmol, 90%). R_f = 0.40 (hexane/dichloromethane = 50/1); mp 302 °C (dec); IR (neat) cm^{-1} 2959, 1585, 1546, 1486, 1350, 1318, 1270, 1176, 852, 839, 813, 758, 692, 663, 625; ^1H NMR (600 MHz, C_6D_6, 298 K) δ 8.23 (d, J = 7.8 Hz, 1H), 8.00 (s, 1H), 7.85 (d, J = 7.8 Hz, 1H), 7.81 (t, J = 2.4 Hz, 2H), 7.54 (d, J = 8.4 Hz, 2H), 7.49 (t, J = 7.8 Hz, 1H), 7.33 (d, J = 7.8 Hz, 2H), 7.29 (d, J = 7.2 Hz, 5H), 7.14 (d, J = 7.8 Hz, 5H), 6.91 (t, J = 7.2 Hz, 2H), 1.36 (s, 9H), 1.22 (s, 9H); ^{13}C NMR (150 MHz, C_6D_6, 298 K) δ 148.6, 147.7, 147.5, 147.3, 136.8, 131.5, 131.2, 130.6, 129.8, 128.6, 128.5, 128.3, 128.0, 127.3, 126.8, 124.7, 123.8, 123.2, 122.9, 122.7, 122.5, 122.2, 121.7, 120.5, 118.4, 117.4, 116.6, 116.2, 114.6, 112.4, 35.5, 34.9, 32.1(3C), 31.4(3C); [M^+] calcd. For $C_{48}H_{40}N_2S$, 676.2912; found, 676.2914.

3. NMR Spectra

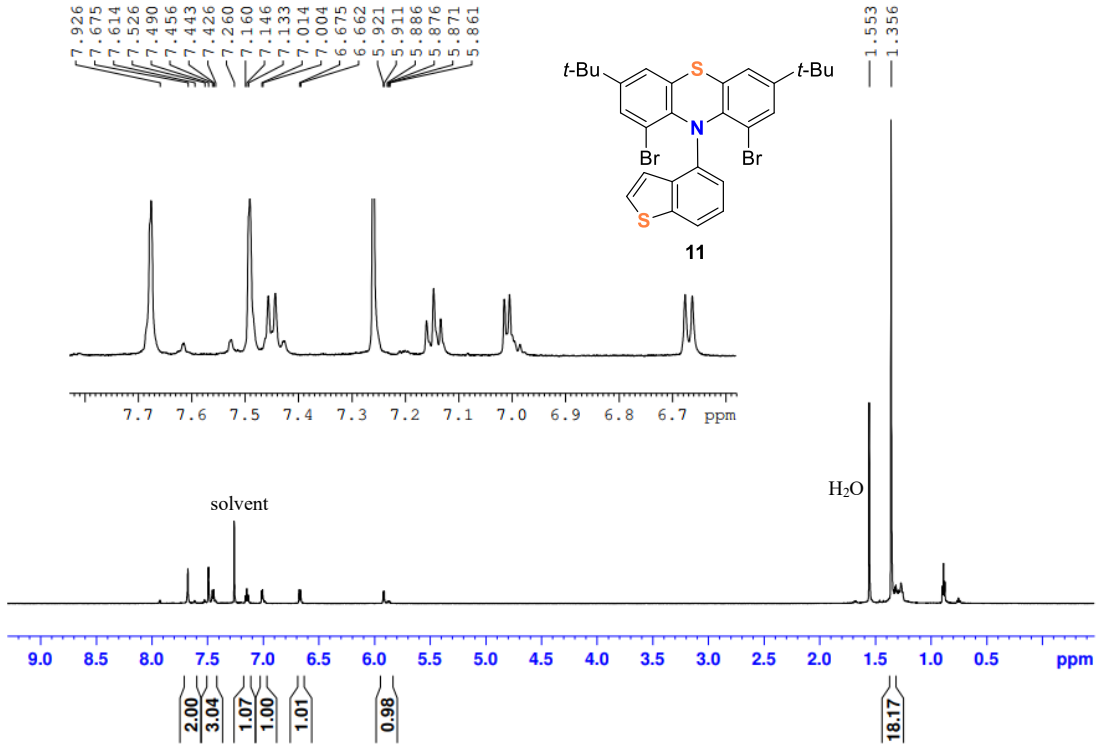


Figure S10. ^{1}H NMR spectrum of **11** (600 MHz, $CDCl_3$, 298 K).

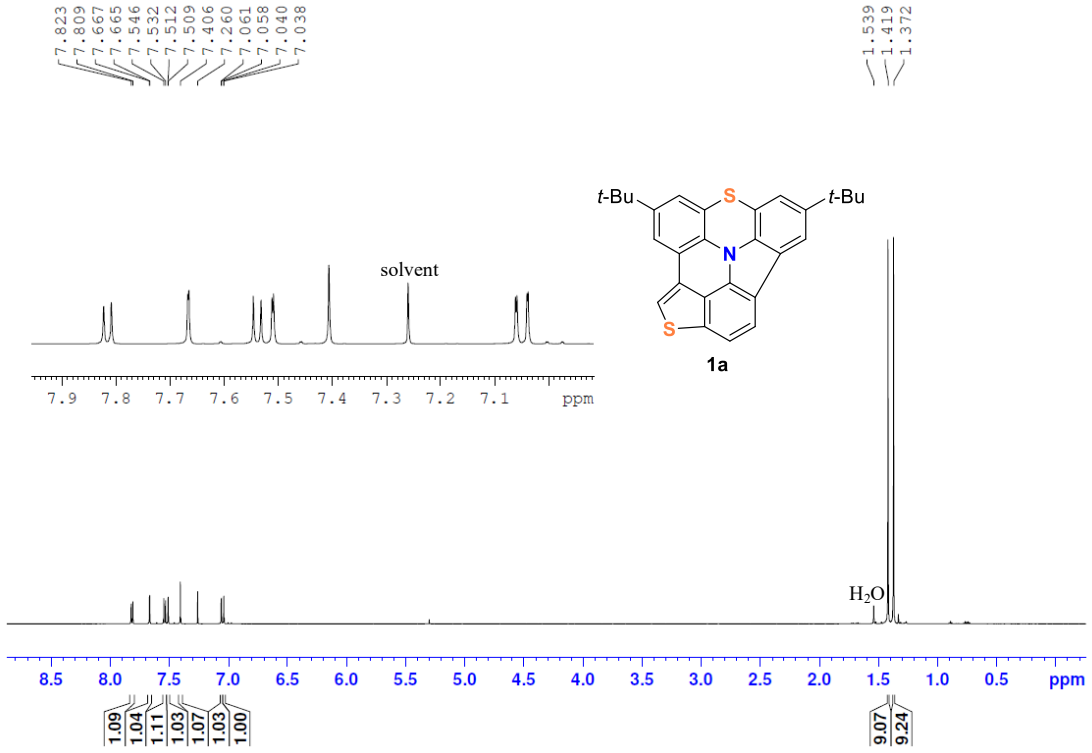


Figure S11. ^{1}H NMR spectrum of **1a** (600 MHz, $CDCl_3$, 298 K).

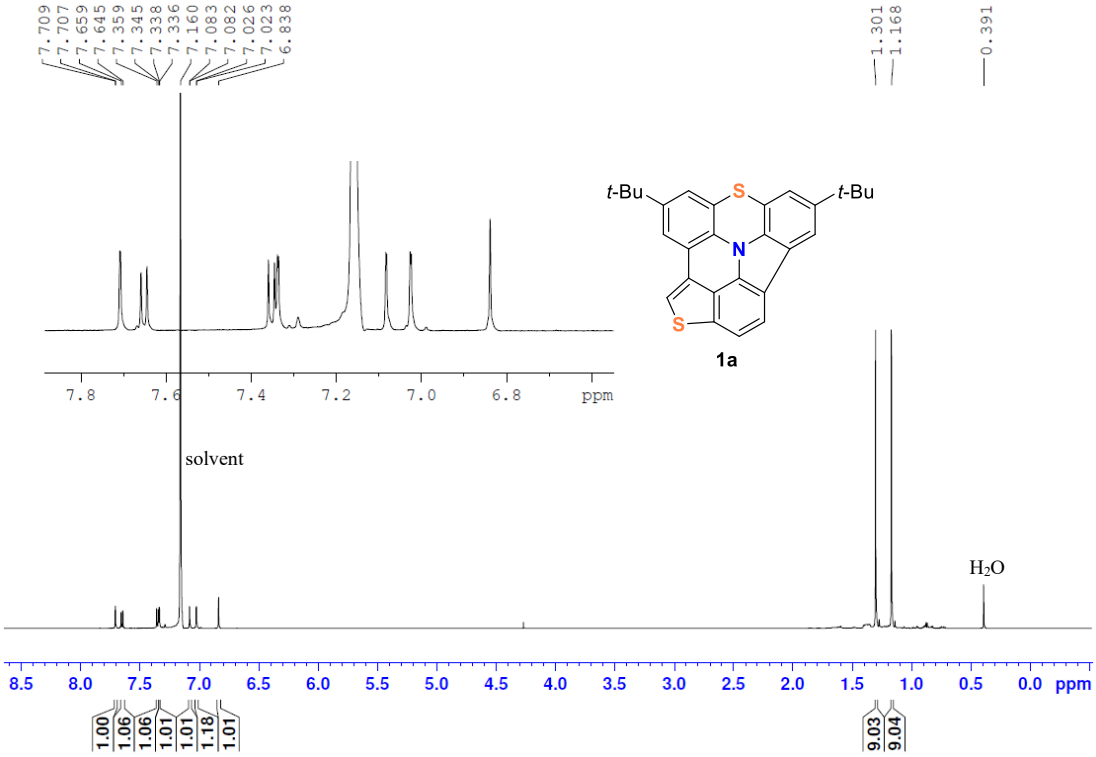


Figure S12. ^{1}H NMR spectrum of **1a** (600 MHz, C_6D_6, 298 K).

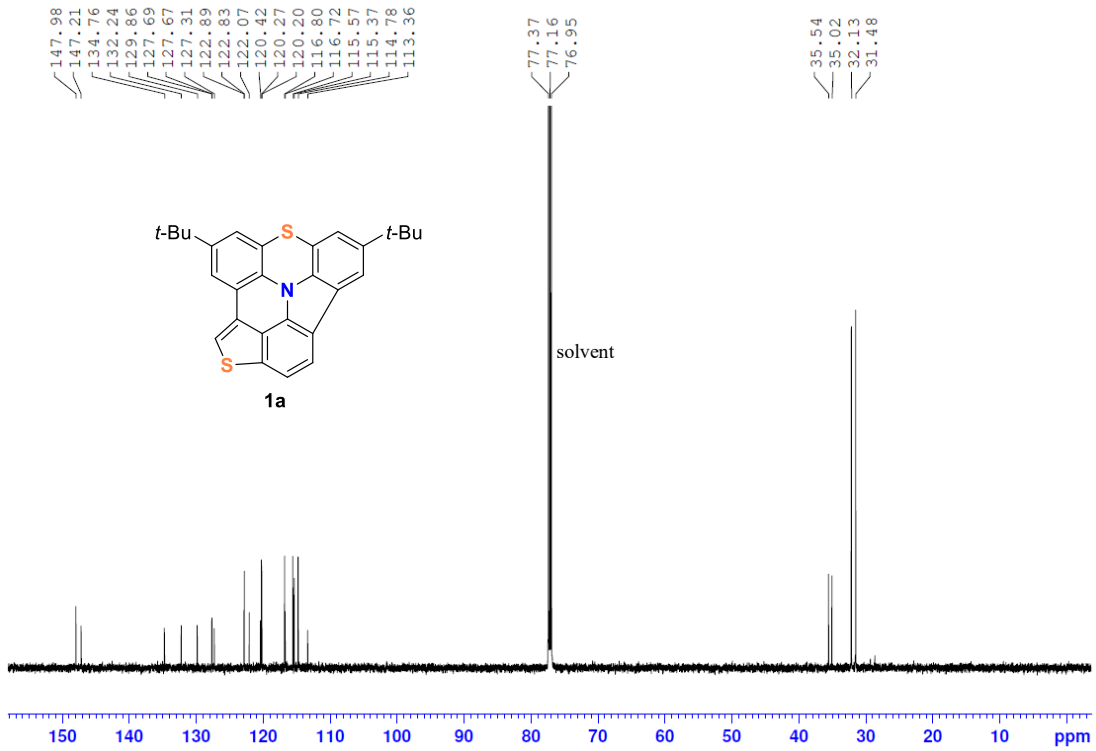


Figure S13. ^{13}C NMR spectrum of **1a** (150 MHz, $CDCl_3$, 298 K).

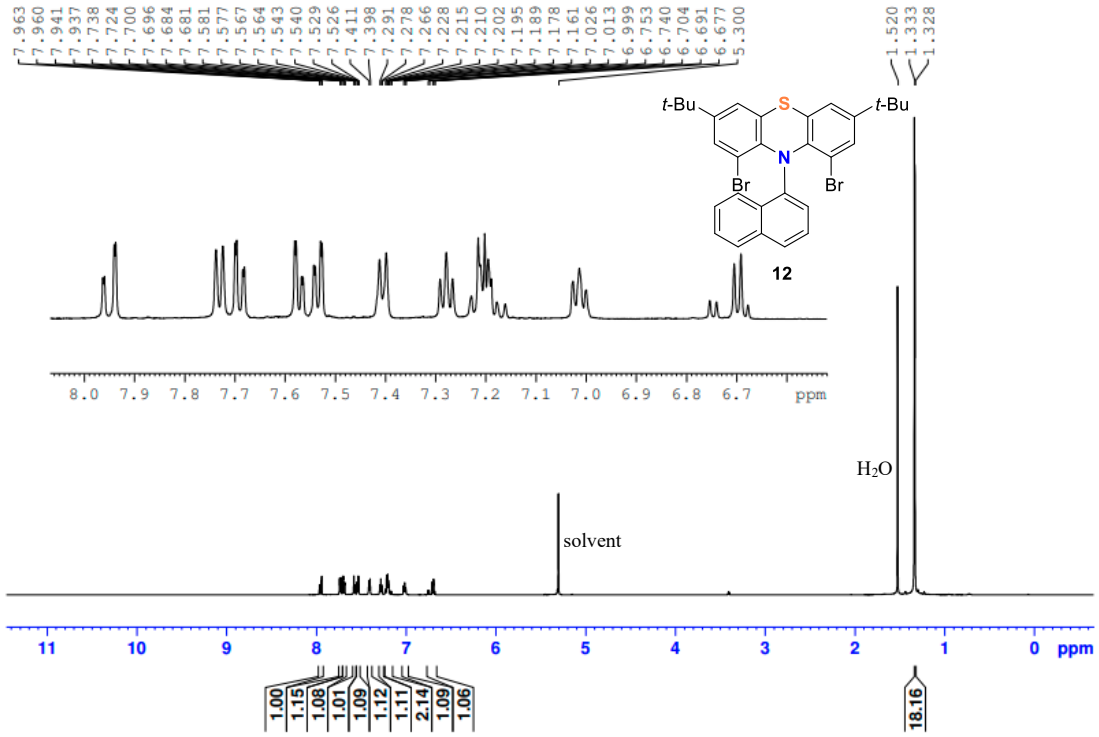


Figure S14. ^{1}H NMR spectrum of **12** (600 MHz, CD_2Cl_2, 298 K).

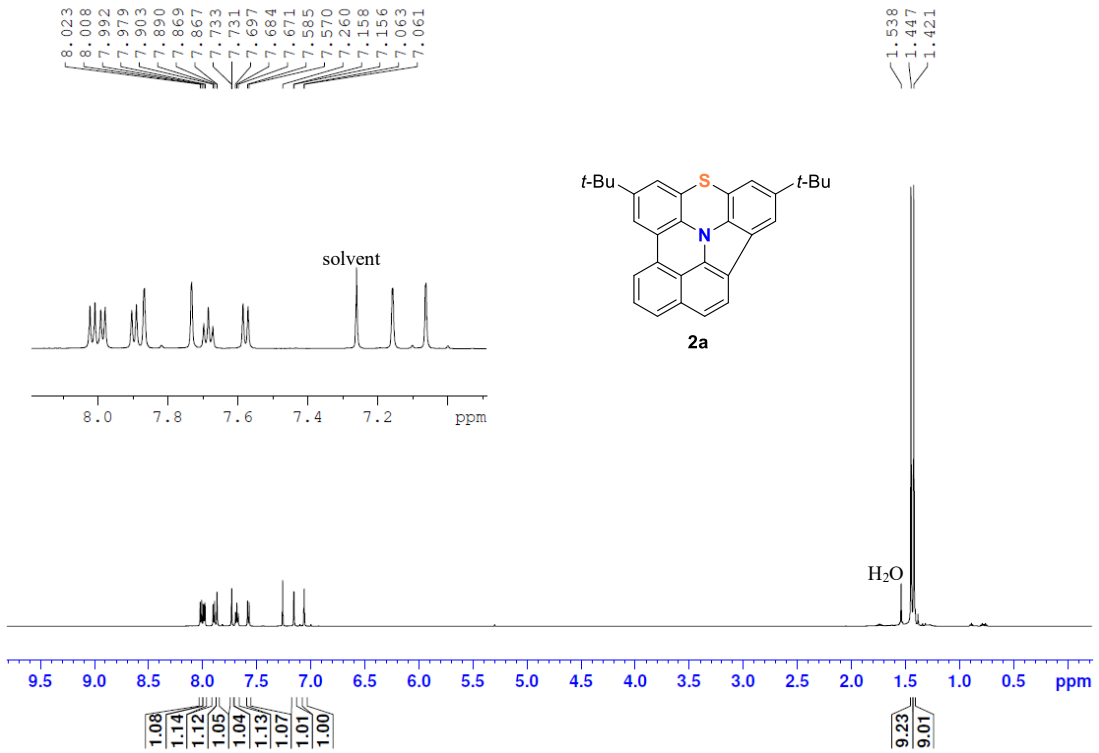


Figure S15. ^{1}H NMR spectrum of **2a** (600 MHz, $CDCl_3$, 298 K).

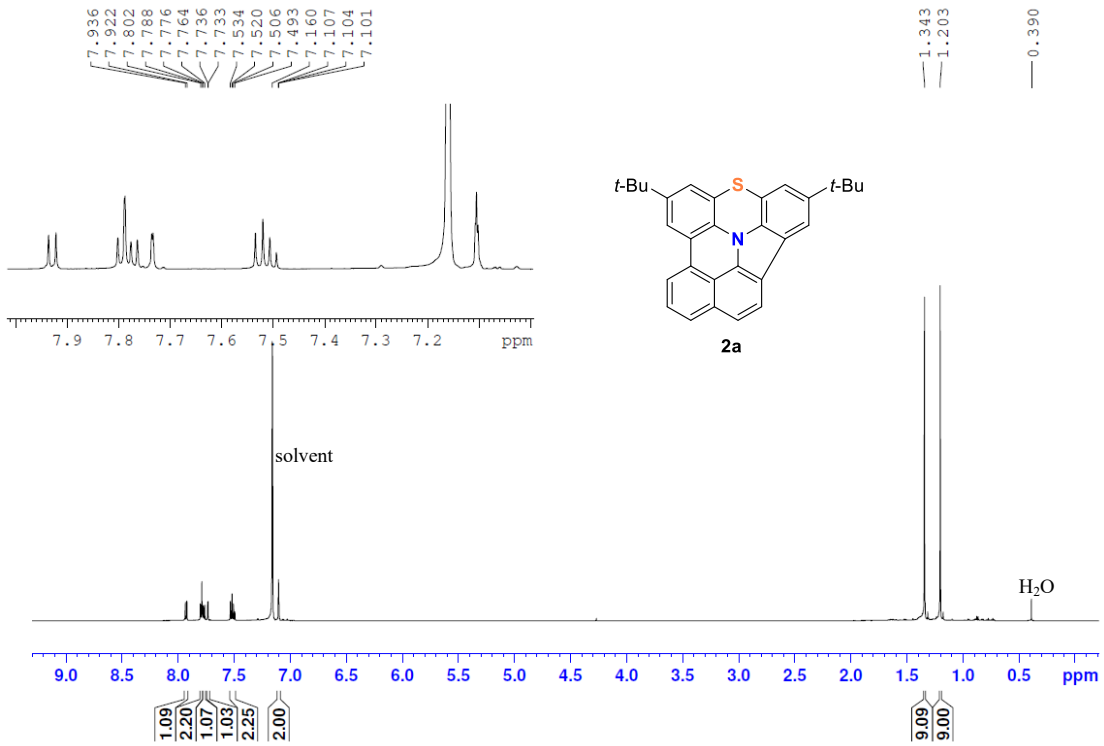


Figure S16. ^{1}H NMR spectrum of **2a** (600 MHz, C_6D_6, 298 K).

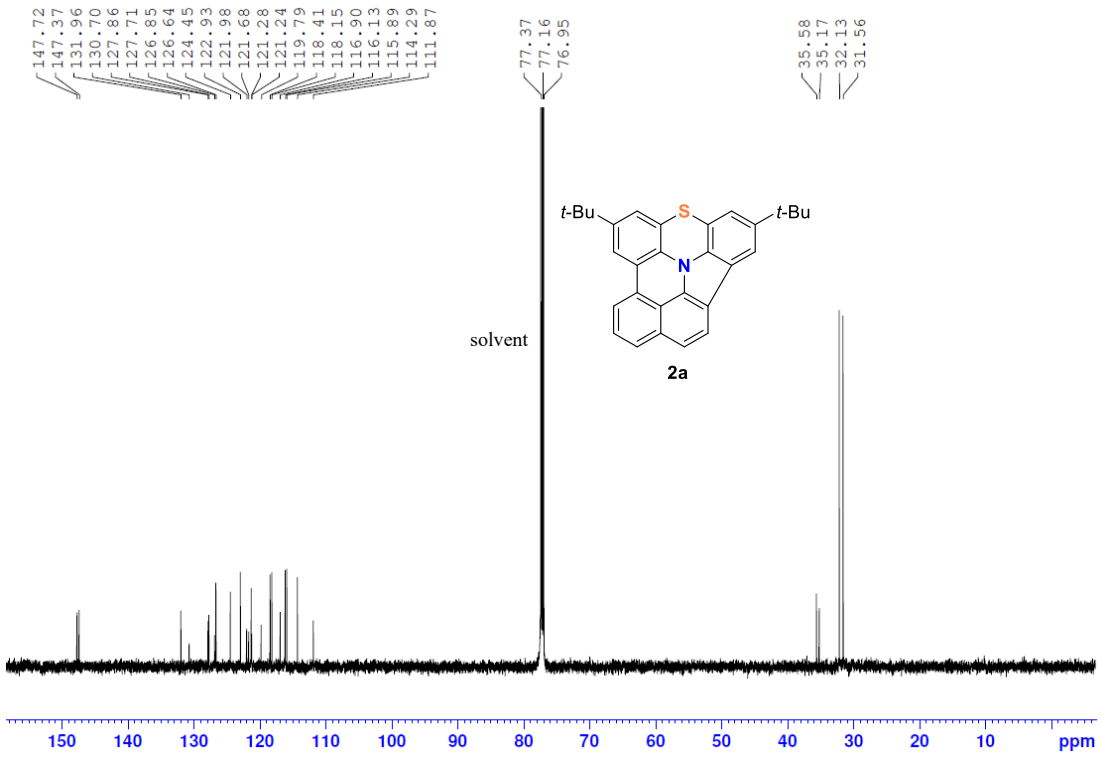


Figure S17. ^{13}C NMR spectrum of **2a** (150 MHz, $CDCl_3$, 298 K).

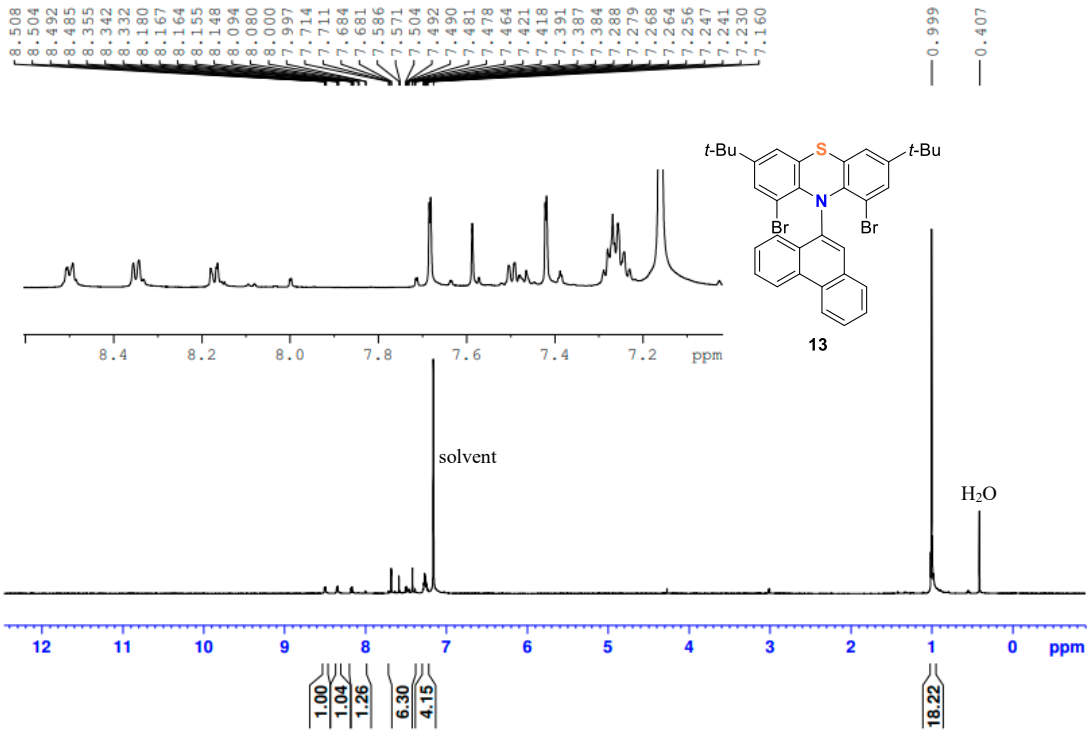


Figure S18. ^{1}H NMR spectrum of **13** (600 MHz, C_6D_6, 298 K).

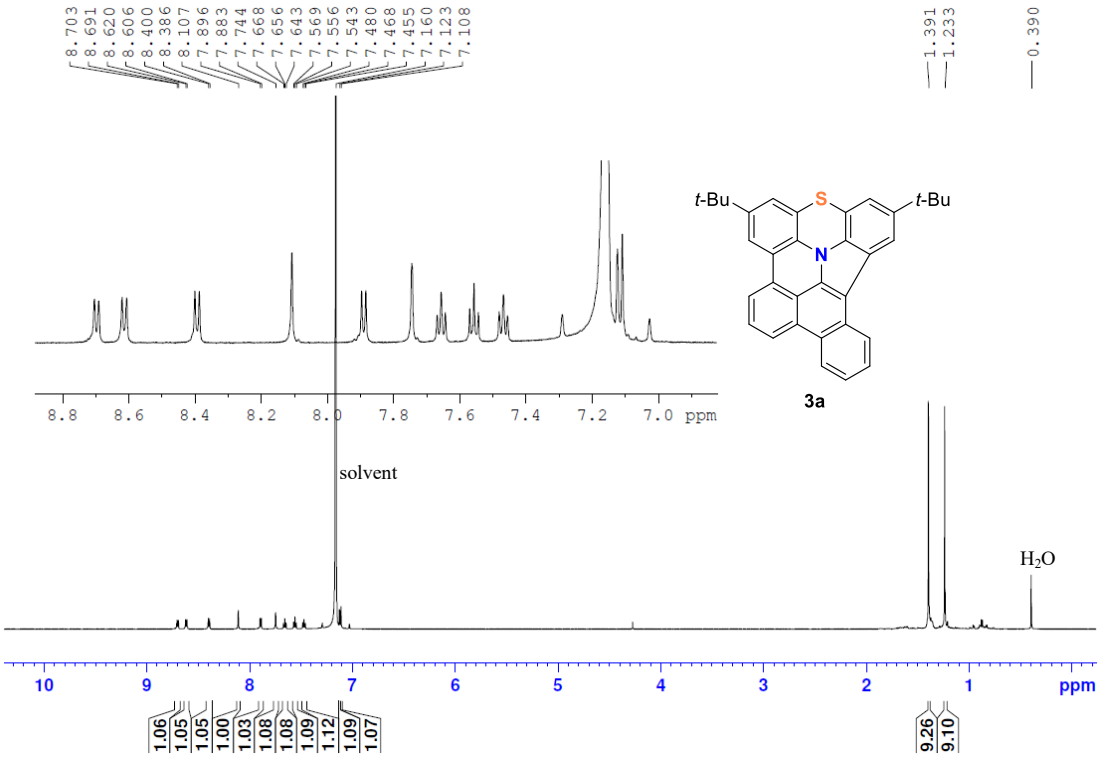


Figure S19. ^{1}H NMR spectrum of **3a** (600 MHz, C_6D_6, 298 K).

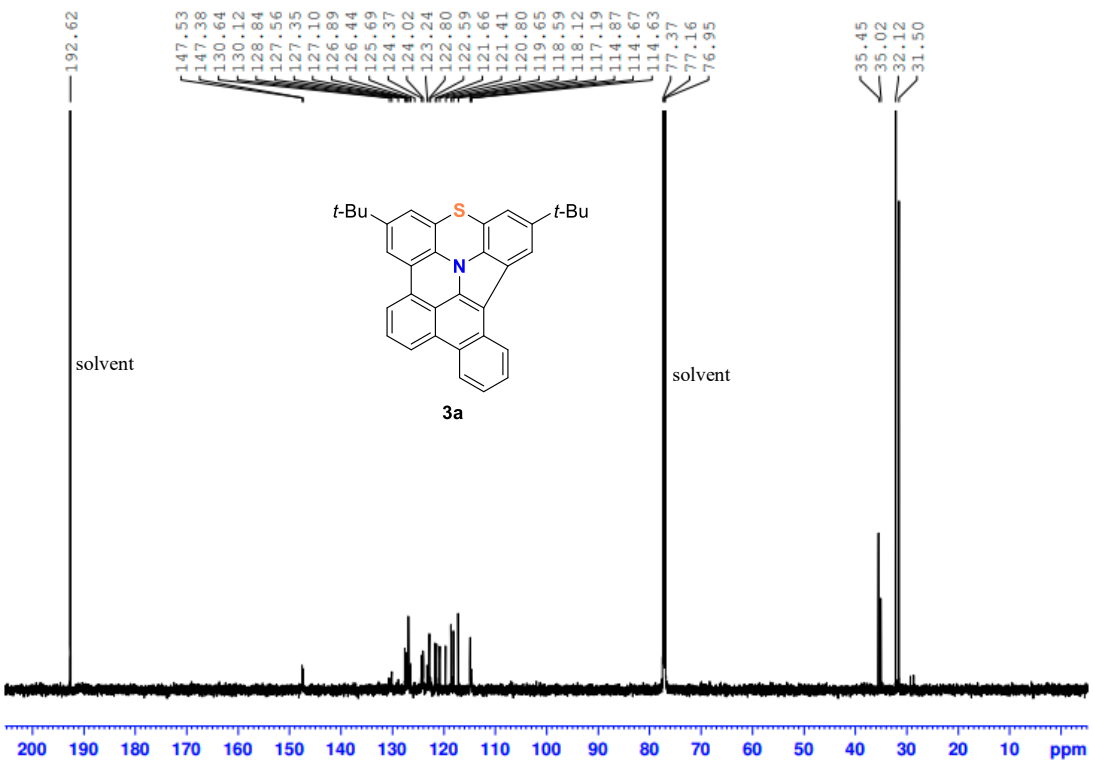


Figure S20. ^{13}C NMR spectrum of **3a** (150 MHz, C_6D_6/CS_2, 298 K).

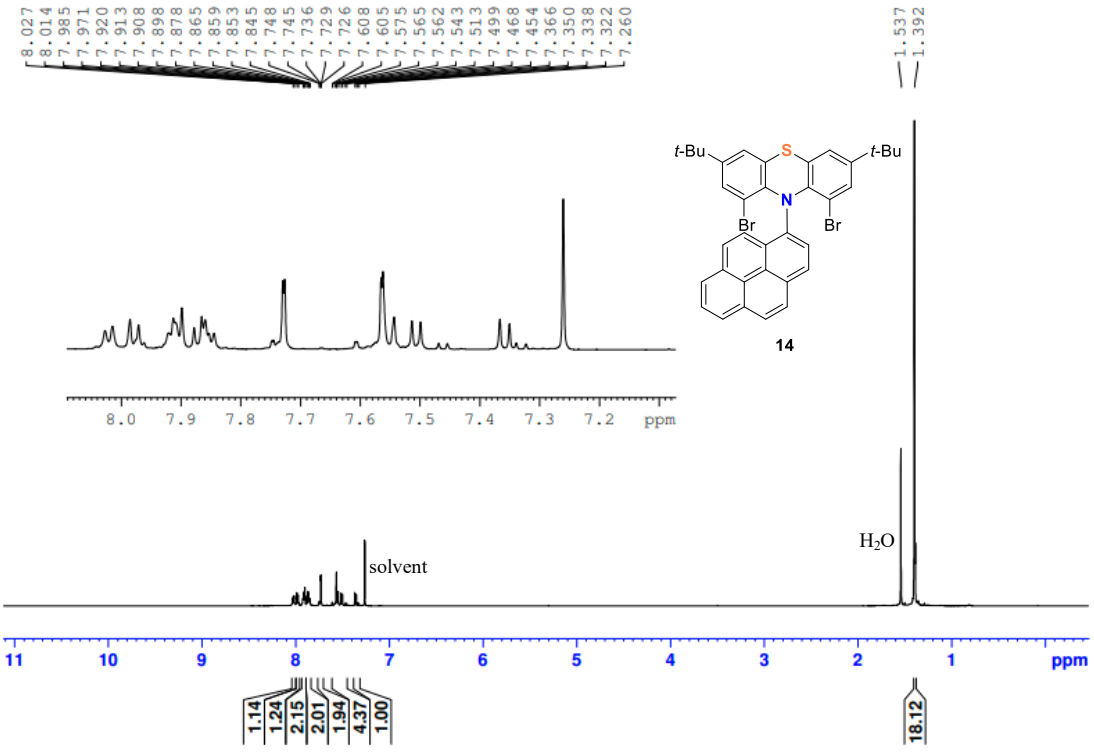


Figure S21. ^{1}H NMR spectrum of **14** (600 MHz, $CDCl_3$, 298 K).

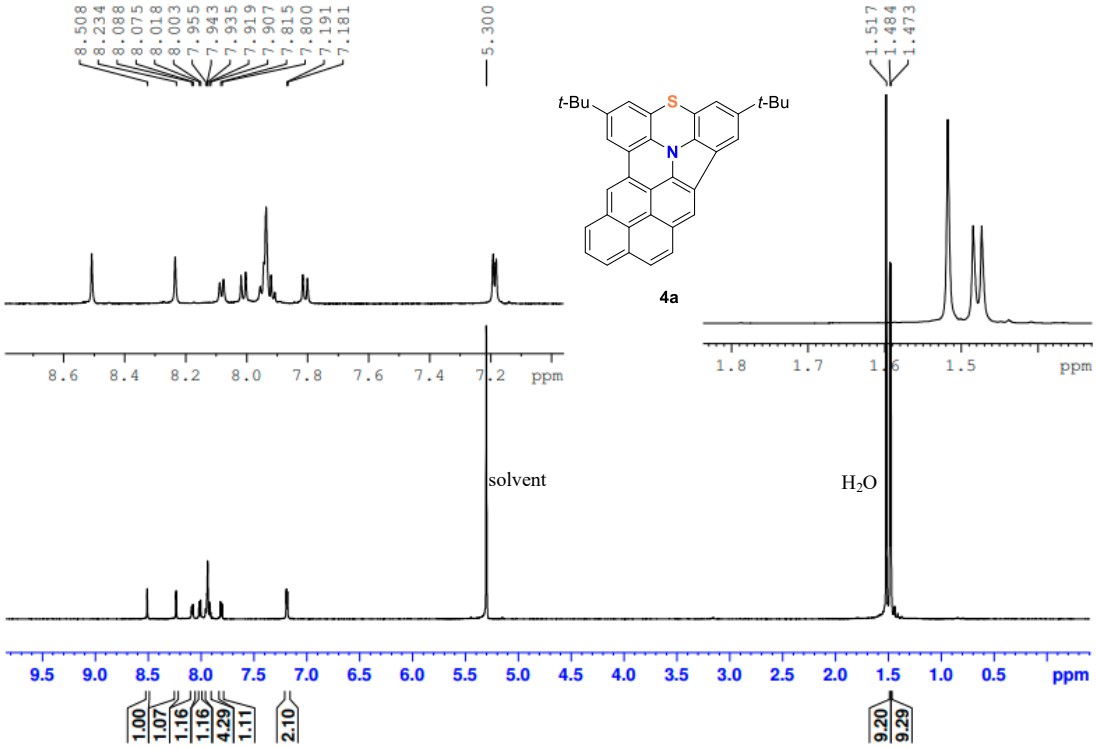


Figure S22. ^{1}H NMR spectrum of **4a** (600 MHz, CD_2Cl_2, 298 K).

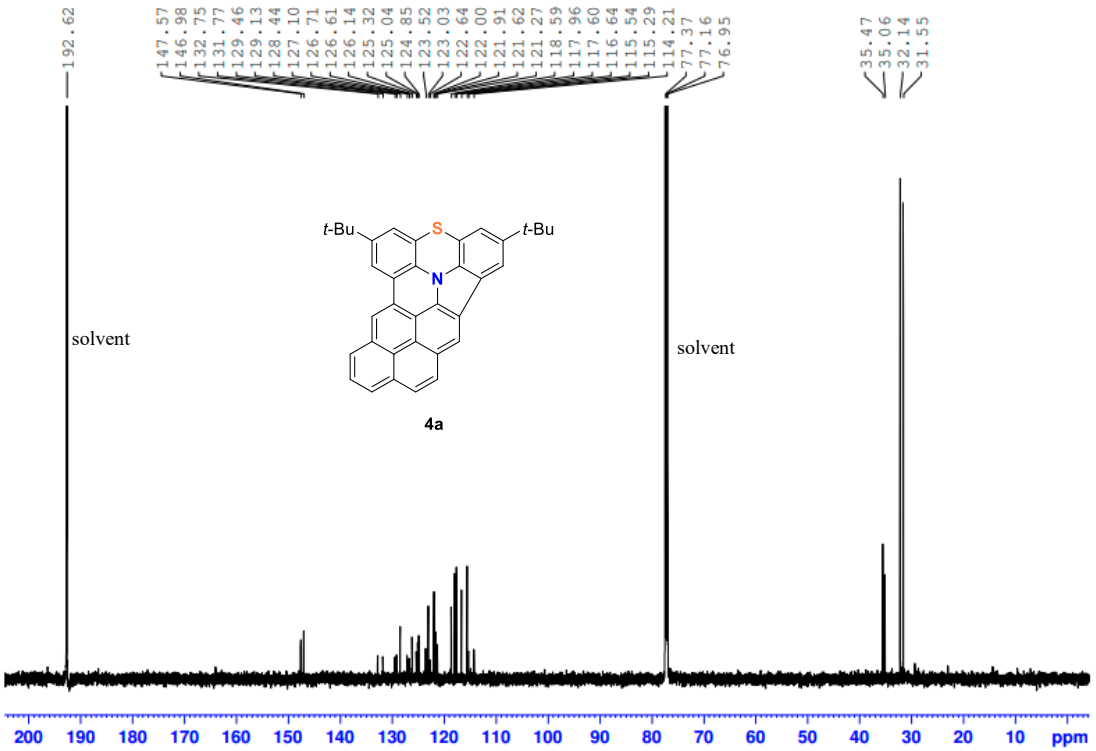


Figure S23. ^{13}C NMR spectrum of **4a** (150 MHz, $CDCl_3/CS_2$, 298 K).

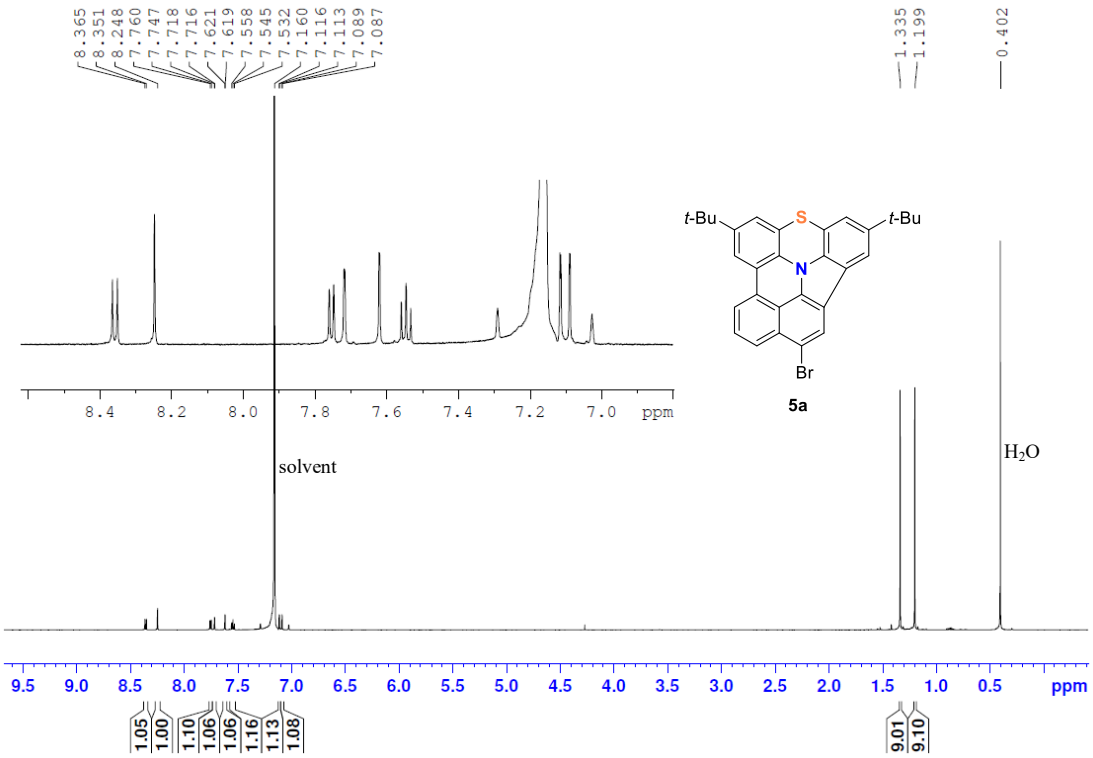


Figure S24. ^{1}H NMR spectrum of **5a** (600 MHz, C_6D_6, 298 K).

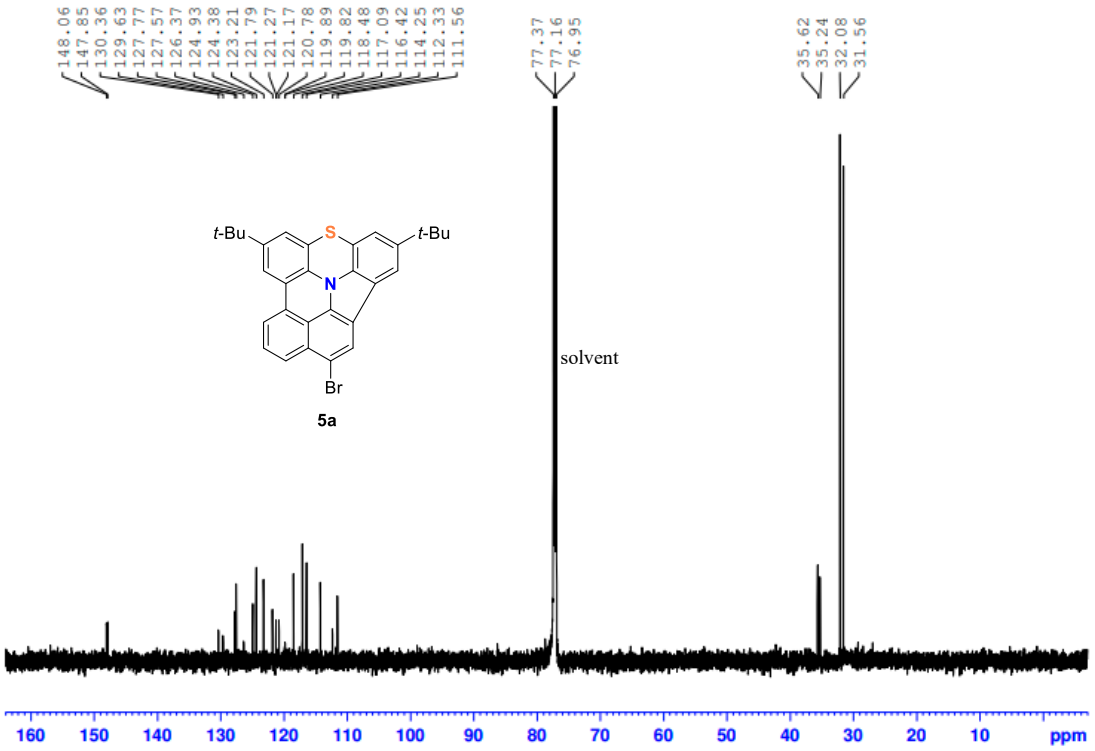


Figure S25. ^{13}C NMR spectrum of **5a** (150 MHz, $CDCl_3$, 298 K).

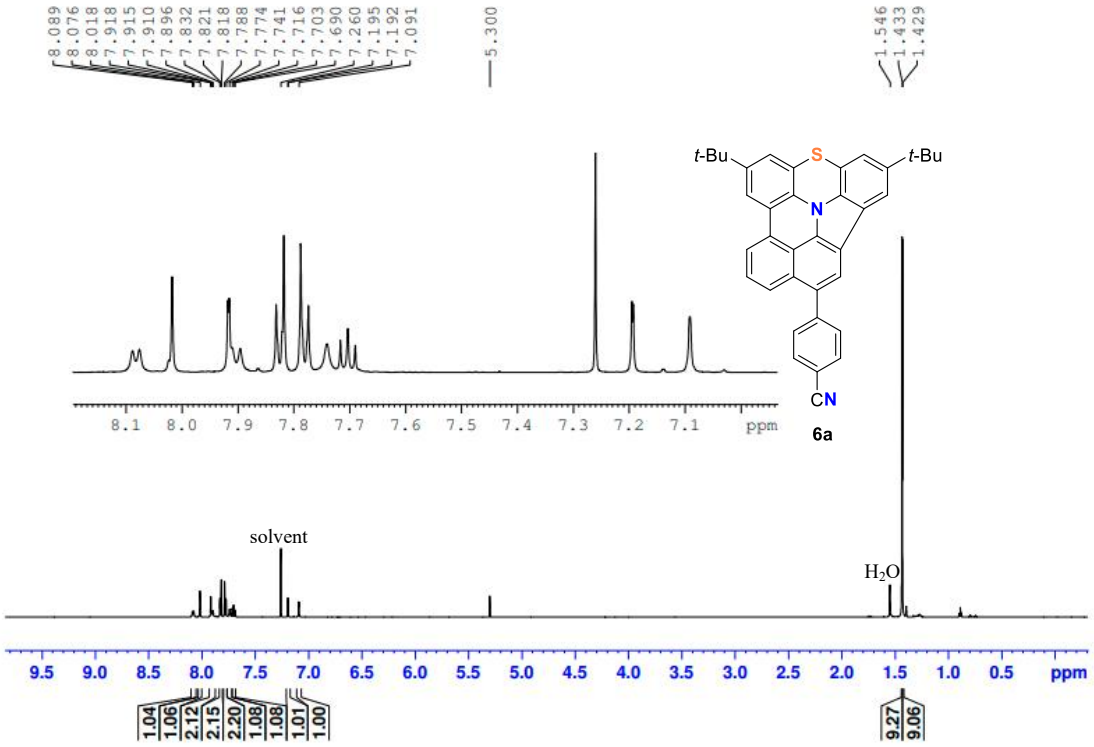


Figure S26. ^{1}H NMR spectrum of **6a** (600 MHz, $CDCl_3$, 298 K).

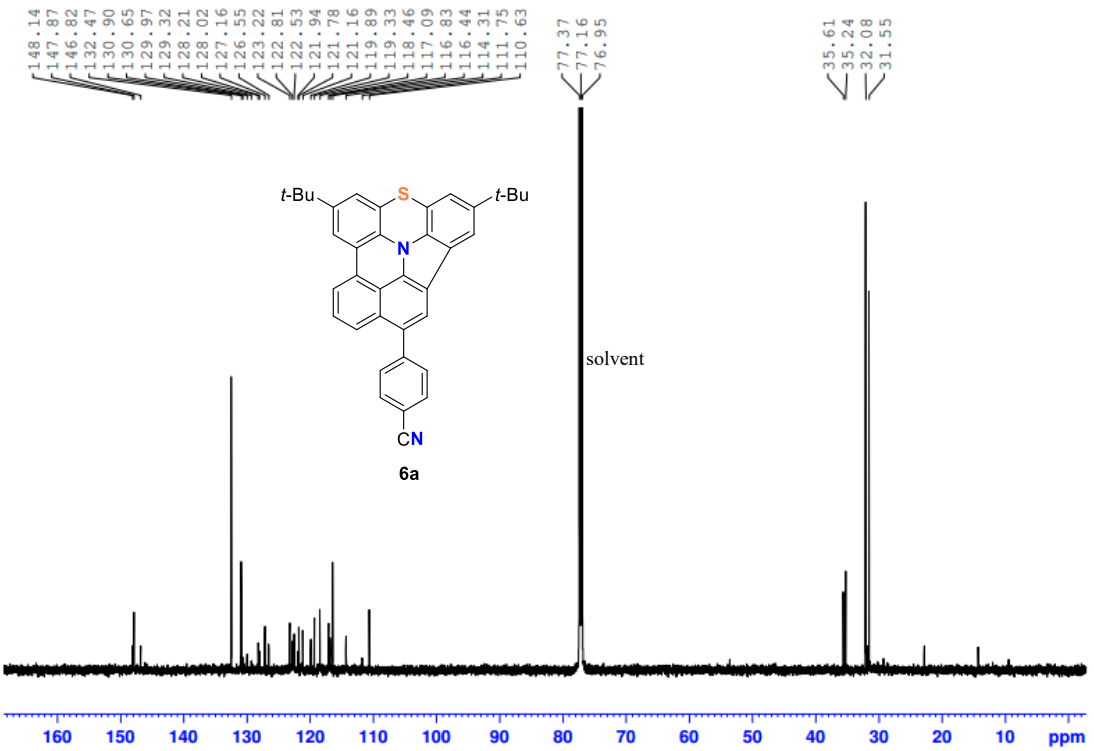


Figure S27. ^{13}C NMR spectrum of **6a** (150 MHz, $CDCl_3$, 298 K).

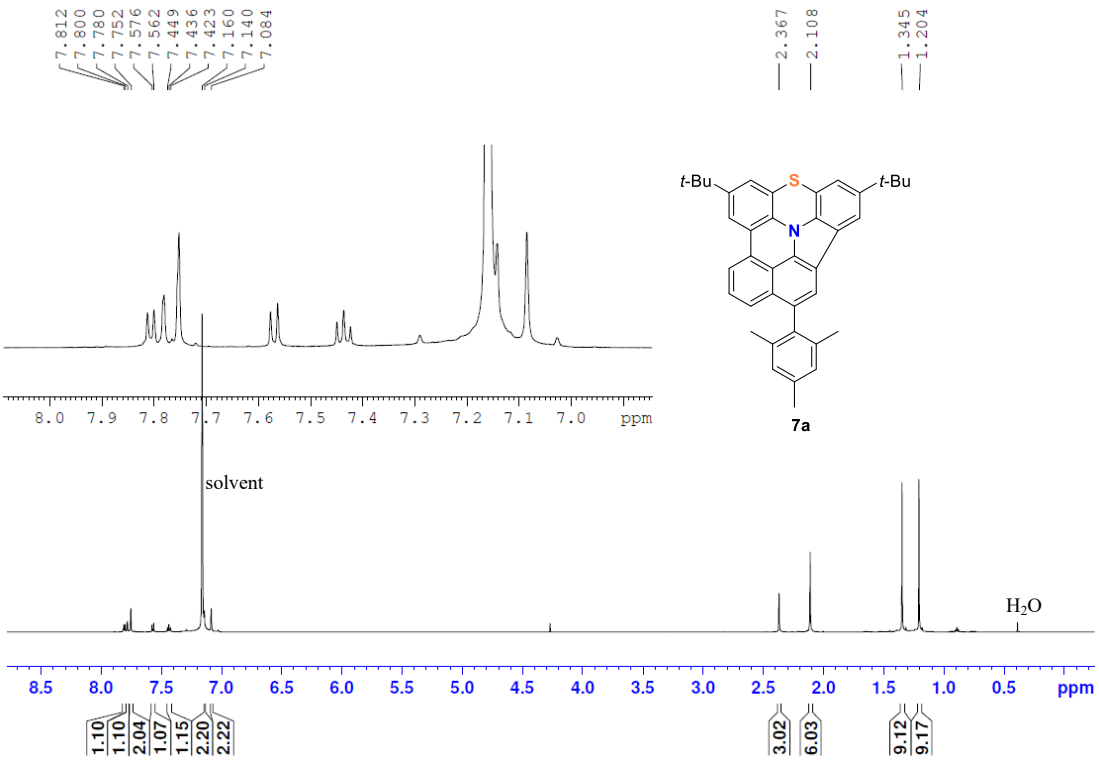


Figure S28. ^{1}H NMR spectrum of **7a** (600 MHz, C_6D_6, 298 K).

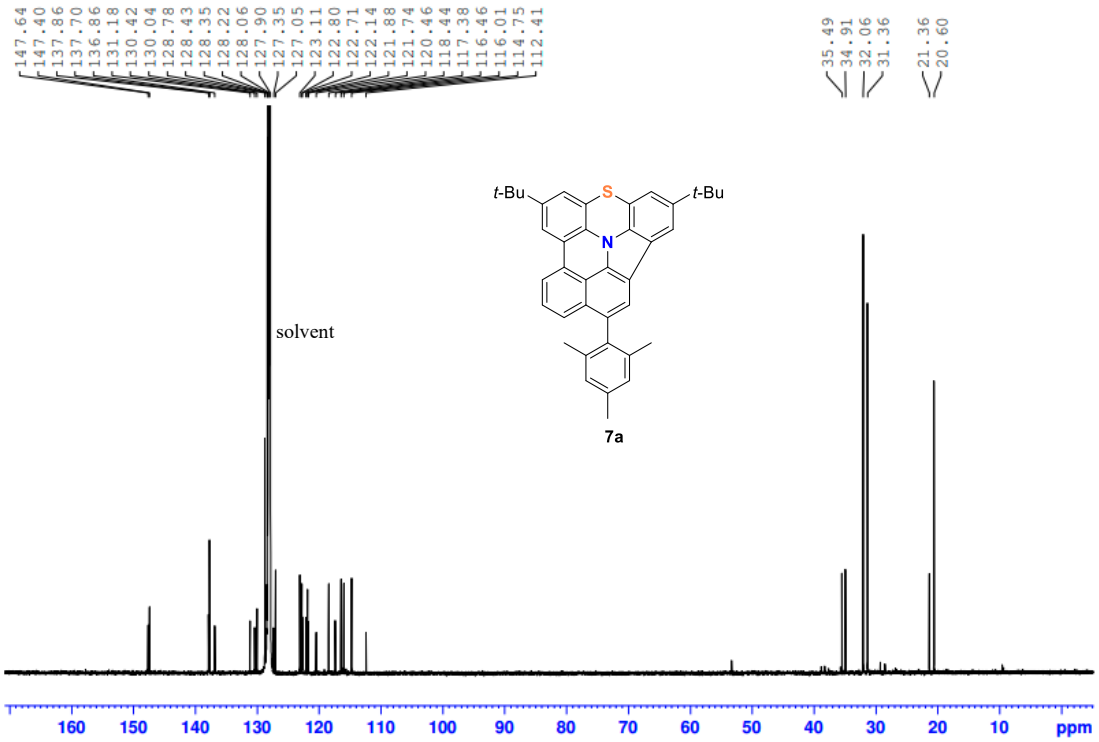


Figure S29. ^{13}C NMR spectrum of **7a** (150 MHz, C_6D_6, 298 K).

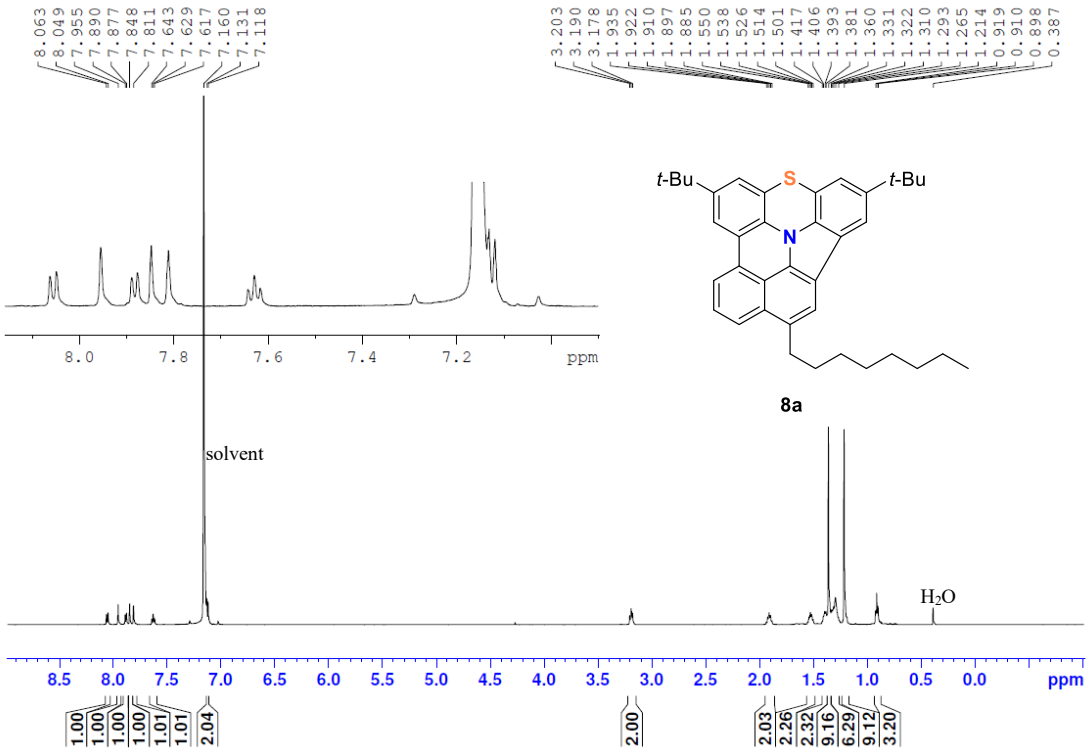


Figure S30. ^{1}H NMR spectrum of **8a** (600 MHz, C_6D_6, 298 K).

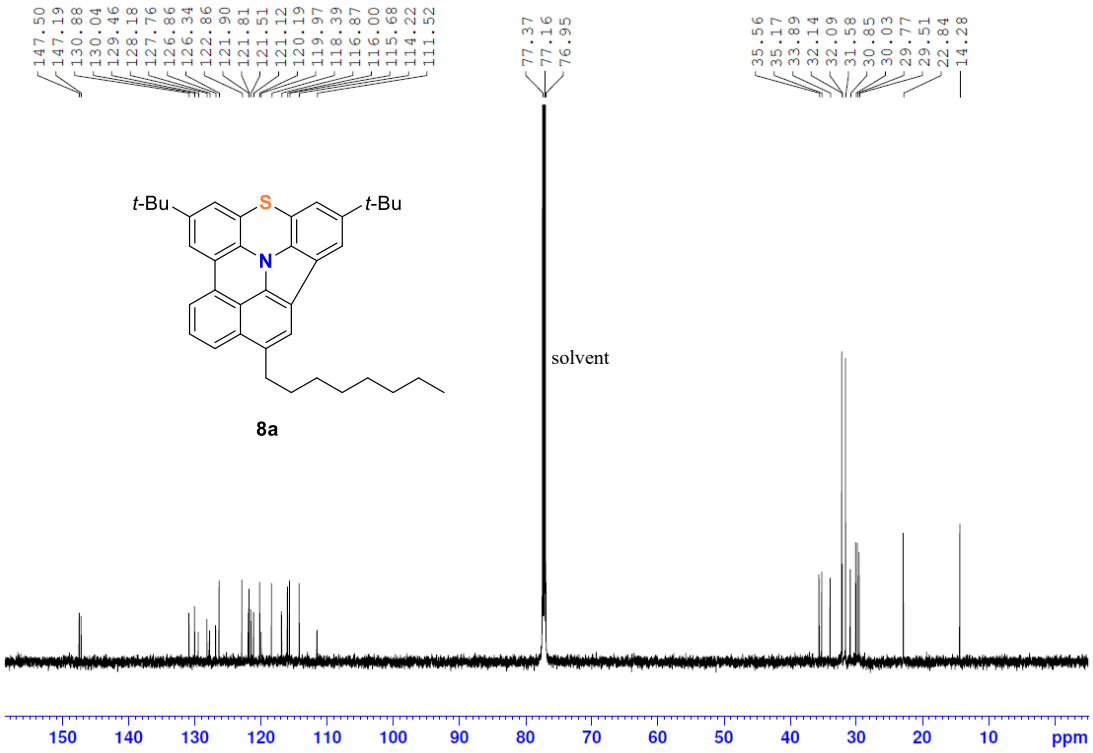


Figure S31. ^{13}C NMR spectrum of **8a** (150 MHz, C_6D_6, 298 K).

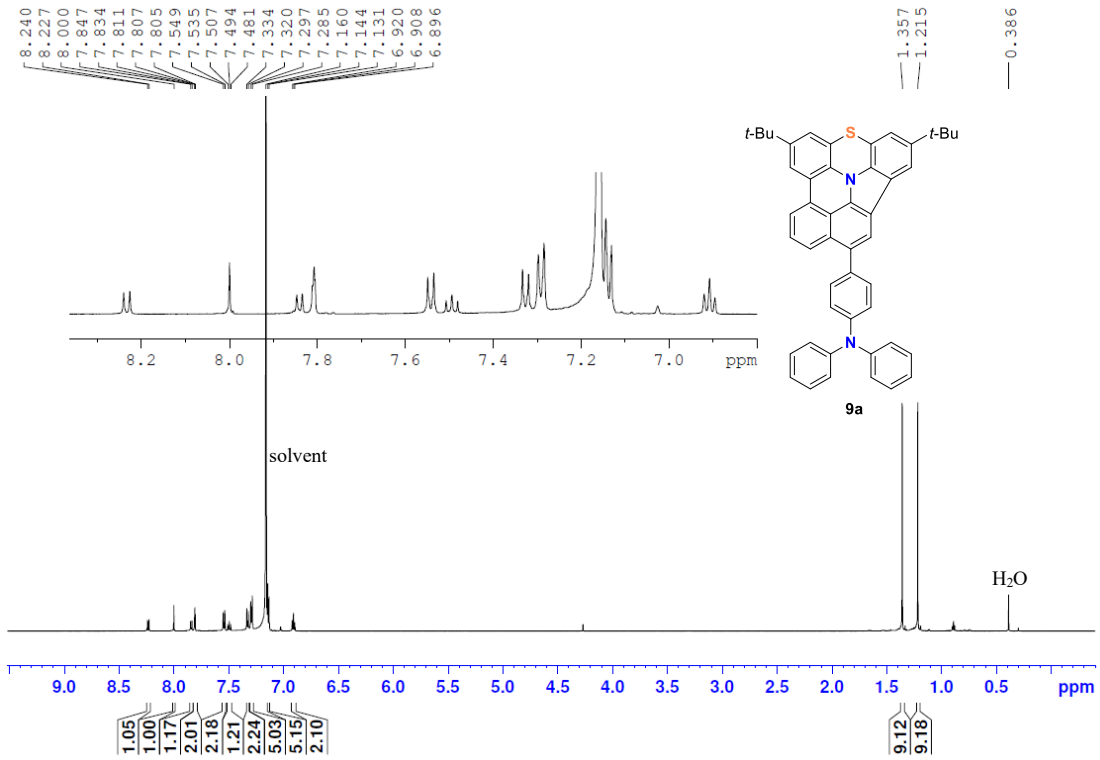


Figure S32. ^{1}H NMR spectrum of **9a** (600 MHz, C_6D_6, 298 K).

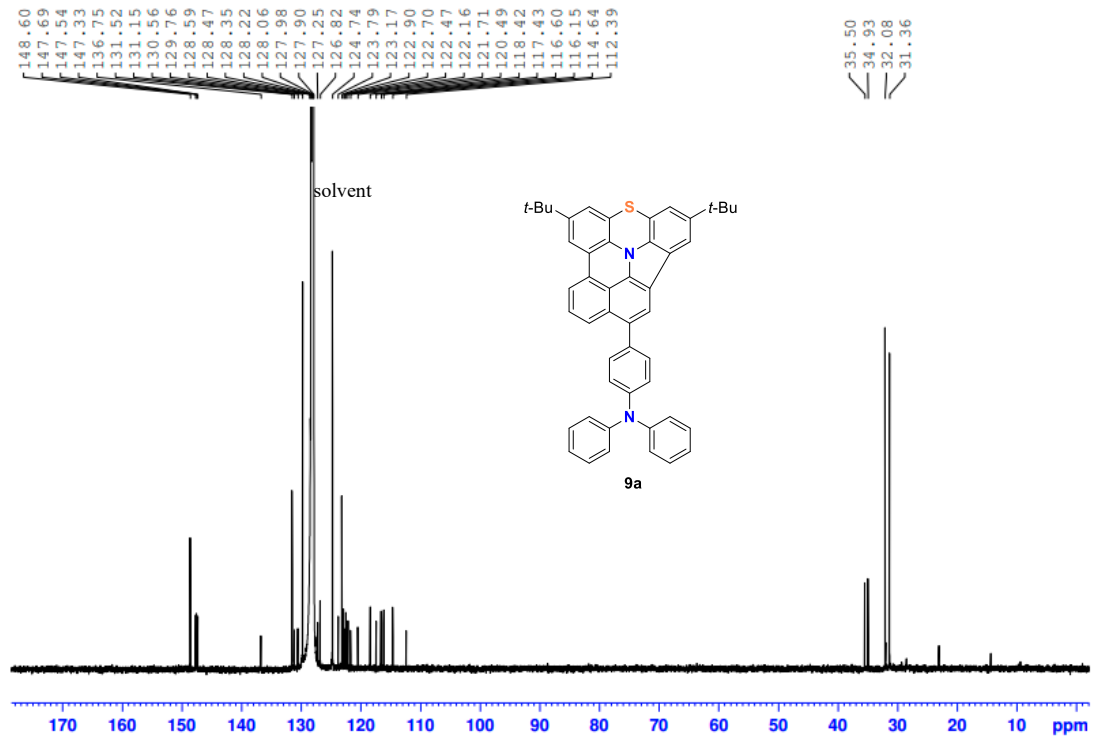


Figure S33. ^{13}C NMR spectrum of **9a** (150 MHz, C_6D_6, 298 K).

4. X-Ray Crystallographic Data

Table S1. Crystal data and structure refinement for **2a**.

compound	**2a**
CCDC number	2456726
Molecular formula	$C_{30}H_{27}NS$
Formula weight	433.58
Temperature (K)	100(10)
Wavelength (Å)	1.54184
Crystal system	orthorhombic
Space group	*Pbam*
Unit cell dimensions a (Å)	23.2388(5)
b (Å)	28.2512(5)
c (Å)	6.80870(10)
α (°)	90
β(°)	90
γ(°)	90
Volume ($Å^3$)	4470.07(14)
Z	8
Density (calculated) ($mg \cdot m^{-3}$)	1.289
Absorption coefficient (mm^{-1})	1.406
F(000)	1840
Crystal size (mm^3)	0.37×0.042×0.029
Theta range (°)	2.462 to 76.684
Reflections collected	16125
Min. and max. transmission	0.573, 1.000
Data / restraints / parameters	4789 / 1060 / 580
Goodness-of-fit on F^2	1.031
Final *R* indices [$I > 2\sigma(I)$]	$R_1 = 0.0768$
	$wR_2 = 0.2222$
R indices (all data) [$I > 2\sigma(I)$]	$R_1 = 0.0991$
	$wR_2 = 0.2452$
Largest diff. peak and hole ($e.Å^{-3}$)	0.90, -0.38

Table S2. Crystal data and structure refinement for **3a**.

compound	**3a**
CCDC number	2456729
Molecular formula	$C_{34}H_{29}NS$
Formula weight	499.70
Temperature (K)	298.00(10)
Wavelength (Å)	0.0251
Crystal system	orthorhombic
Space group	*Ibam*
Unit cell dimensions a (Å)	21.862(10)
b (Å)	38.138(13)
c (Å)	6.9916(14)
α (°)	90
β(°)	90
γ(°)	90
Volume ($Å^3$)	5829(4)
Z	8
Density (calculated) ($mg \cdot m^{-3}$)	1.139
Absorption coefficient (mm^{-1})	0.000
F(000)	890
Crystal size (mm^3)	0.000001×0×0
Theta range (°)	0.038 to 0.899
Reflections collected	11302
Min. and max. transmission	0.365, 1.000
Data / restraints / parameters	2977 / 503 / 226
Goodness-of-fit on F^2	0.977
Final *R* indices [$I > 2\sigma(I)$]	$R_1 = 0.1763$
	$wR_2 = 0.4265$
R indices (all data) [$I > 2\sigma(I)$]	$R_1 = 0.3555$
	$wR_2 = 0.5335$
Largest diff. peak and hole ($e.Å^{-3}$)	0.15, -19

Table S3. Crystal data and structure refinement for **4a**.

compound	**4a**
CCDC number	2456731
Molecular formula	$C_{36}H_{29}NS$
Formula weight	507.66
Temperature (K)	100(10)
Wavelength (Å)	1.54184
Crystal system	triclinic
Space group	P_1
Unit cell dimensions a (Å)	6.8922(3)
b (Å)	13.7416(7)
c (Å)	14.3528(6)
α (°)	74.020(4)
β(°)	80.891(4)
γ(°)	80.756(4)
Volume ($Å^3$)	1280.49(11)
Z	2
Density (calculated) ($mg \cdot m^{-3}$)	1.317
Absorption coefficient (mm^{-1})	1.312
F(000)	536
Crystal size (mm^3)	0.381×0.028×0.019
Theta range (°)	3.226 to 76.734
Reflections collected	8654
Min. and max. transmission	0.663, 1.000
Data / restraints / parameters	3654 / 0 / 350
Goodness-of-fit on F^2	1.094
Final *R* indices [$I > 2\sigma(I)$]	$R_1 = 0.0779$
	$wR_2 = 0.2142$
R indices (all data) [$I > 2\sigma(I)$]	$R_1 = 0.0877$
	$wR_2 = 0.2237$
Largest diff. peak and hole ($e.Å^{-3}$)	0.86, -0.50

Table S4. Crystal data and structure refinement for **7a**.

compound	**7a**
CCDC number	2456732
Molecular formula	$C_{39}H_{37}NS$
Formula weight	551.75
Temperature (K)	100(10)
Wavelength (Å)	1.54184
Crystal system	monoclinic
Space group	$P2_1/n$
Unit cell dimensions a (Å)	12.9992(3)
b (Å)	15.7713(4)
c (Å)	14.4358(4)
α (°)	90
β(°)	100.225(2)
γ(°)	90
Volume ($Å^3$)	2912.54(13)
Z	4
Density (calculated) ($mg \cdot m^{-3}$)	1.258
Absorption coefficient (mm^{-1})	1.191
F(000)	1176
Crystal size (mm^3)	0.16×0.14×0.12
Theta range (°)	4.188 to 73.799
Reflections collected	21728
Min. and max. transmission	0.419, 1.000
Data / restraints / parameters	5625 / 0 / 379
Goodness-of-fit on F^2	1.032
Final R indices [$I > 2\sigma(I)$]	$R_1 = 0.0859$
	$wR_2 = 0.2255$
R indices (all data) [$I > 2\sigma(I)$]	$R_1 = 0.1052$
	$wR_2 = 0.2404$
Largest diff. peak and hole ($e.Å^{-3}$)	1.41, -0.61

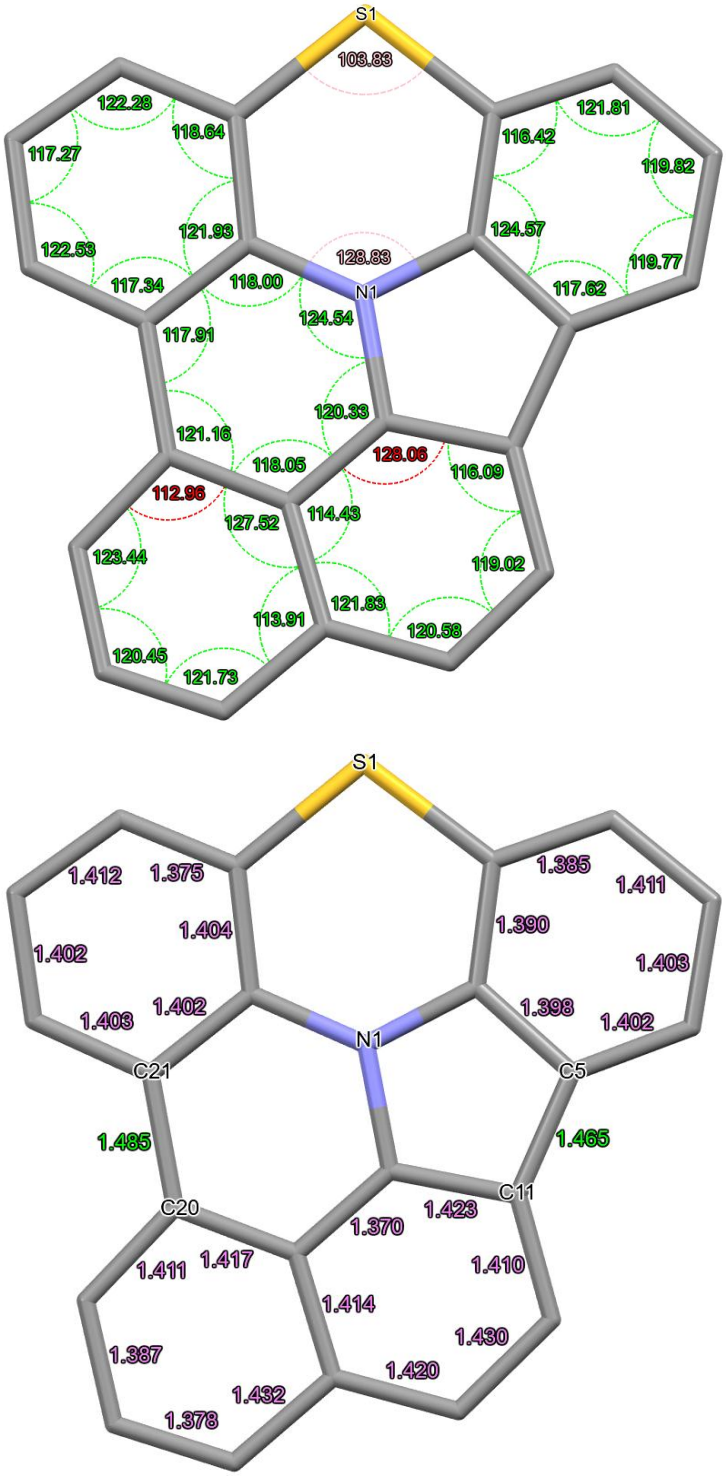


Figure S34. Selected bond angles and bond lengths of **2a** determined by X-ray diffraction analysis. The *tert*-butyl groups, and hydrogen atoms were omitted for clarity.

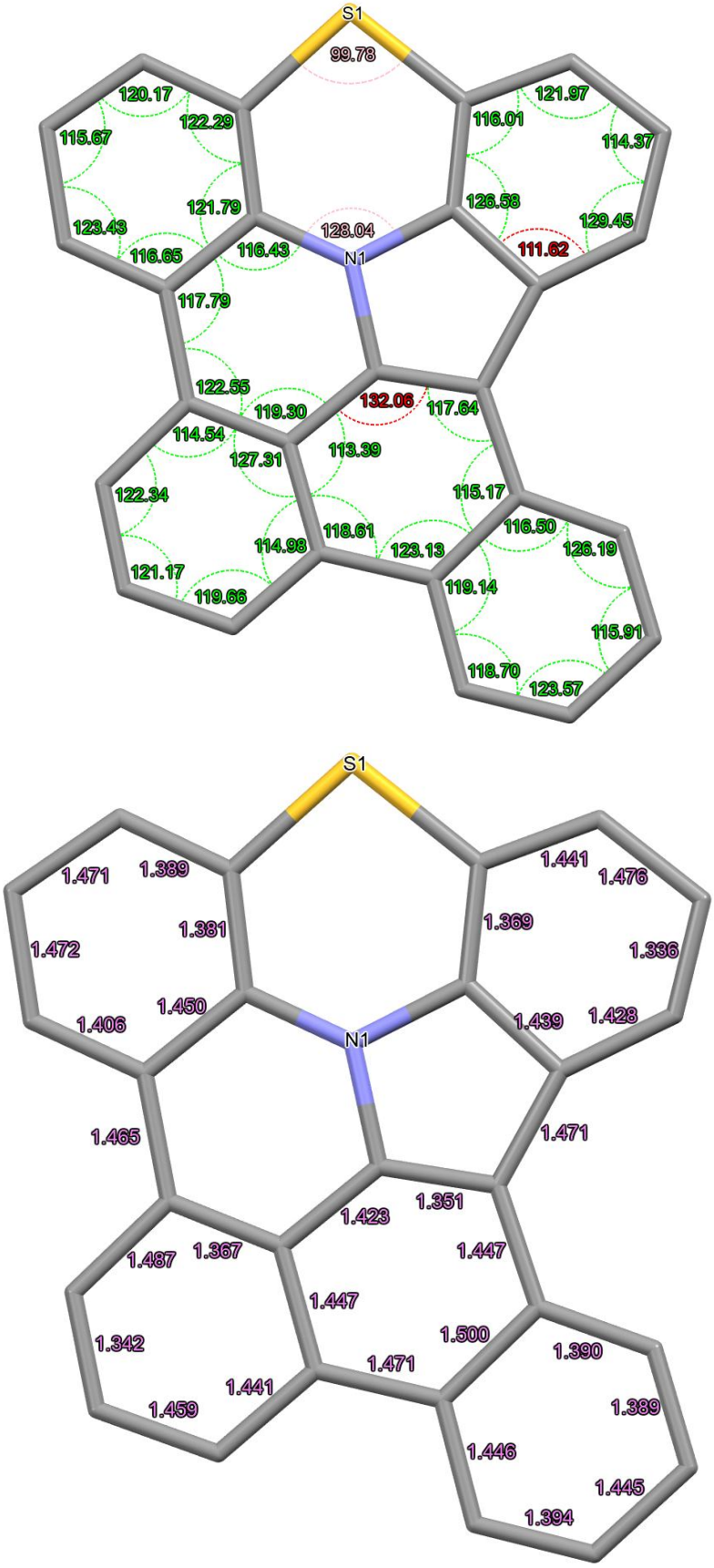


Figure S35. Selected bond angles and bond lengths of **3a** determined by X-ray diffraction analysis. The *tert*-butyl groups, and hydrogen atoms were omitted for clarity.

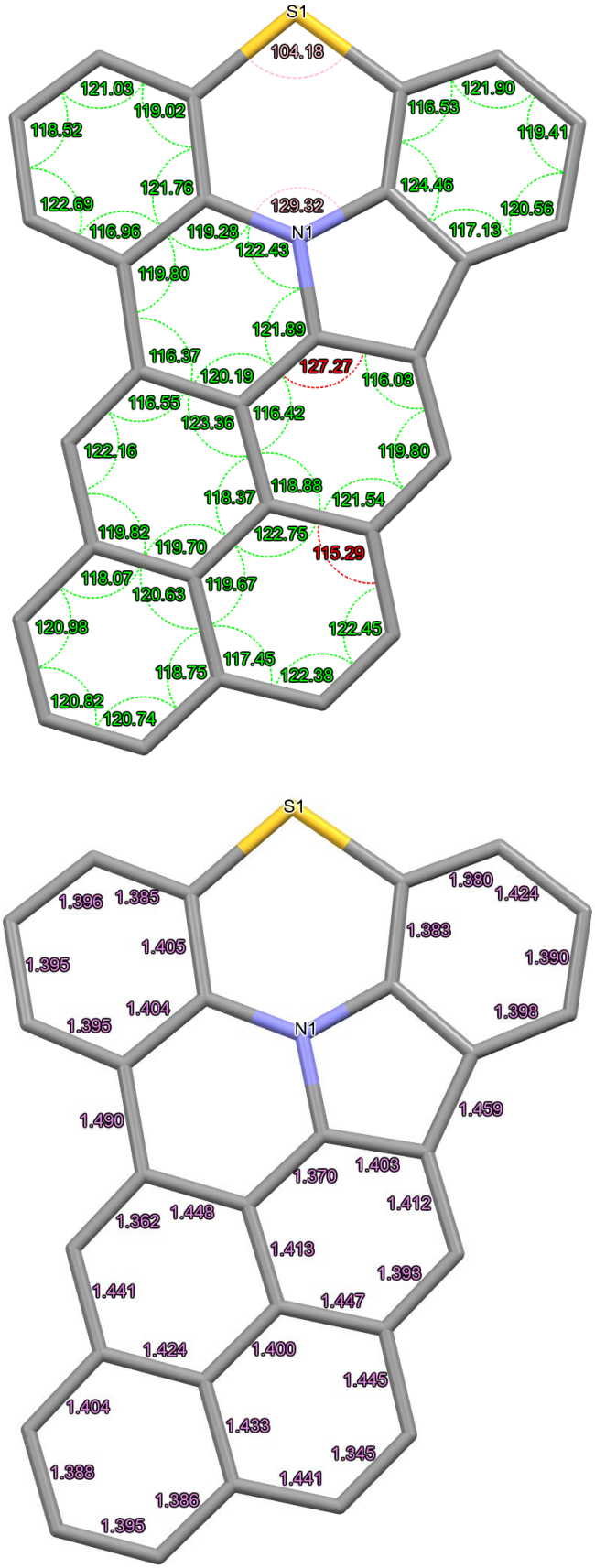


Figure S36. Selected bond angles and bond lengths of **4a** determined by X-ray diffraction analysis. The *tert*-butyl groups, and hydrogen atoms were omitted for clarity.

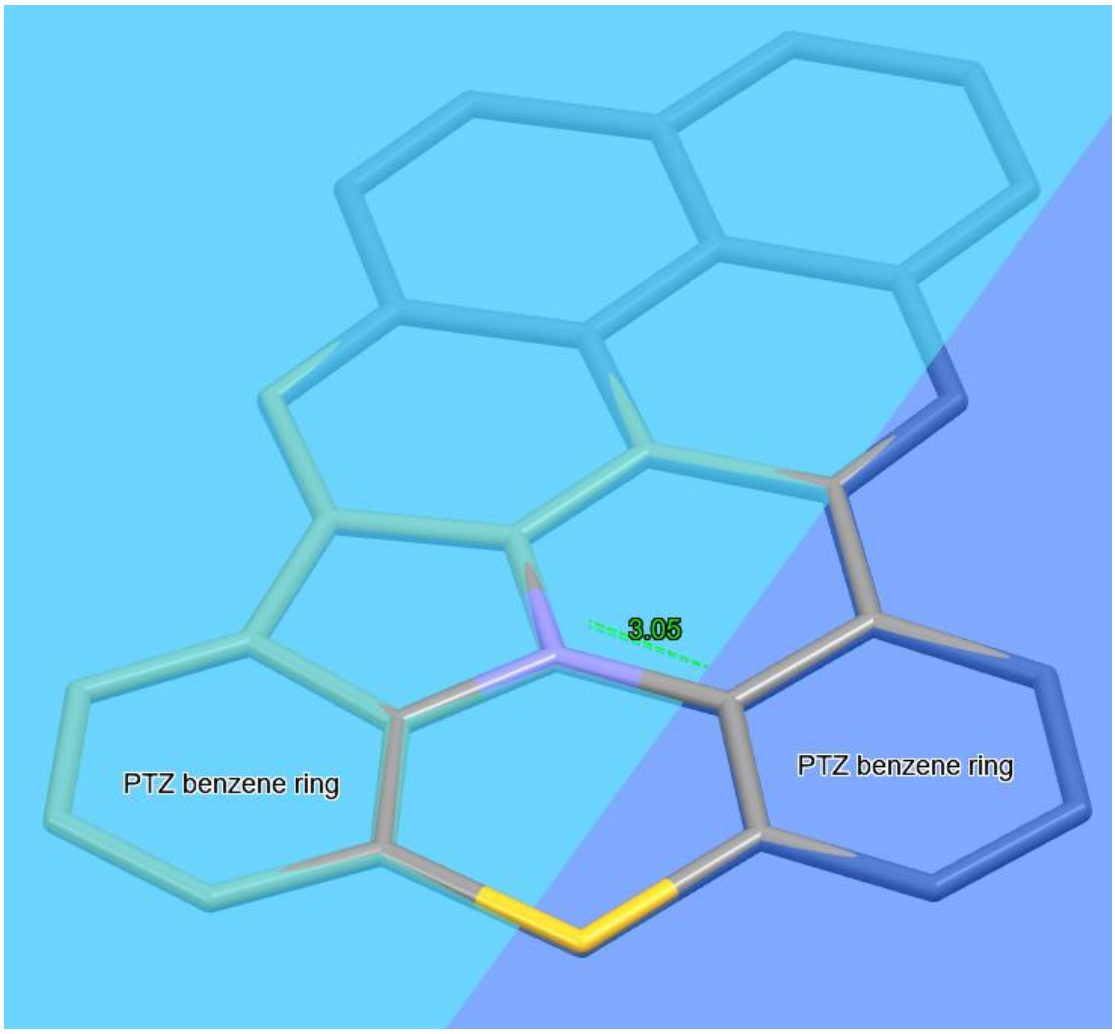


Figure S37. The dihedral angle between the phenothiazine benzene rings in **4a**. determined by X-ray diffraction analysis. The tert-butyl groups, and hydrogen atoms were omitted for clarity.

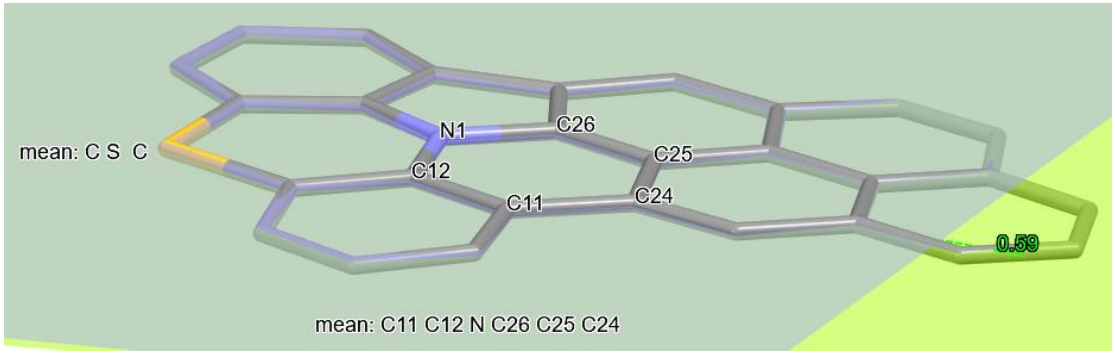


Figure S38. The dihedral angle between the C-S-C triangle plane and the C11-C12-N-C26-C25-C24 plane in **4a**. determined by X-ray diffraction analysis. The tert-butyl groups, and hydrogen atoms were omitted for clarity.

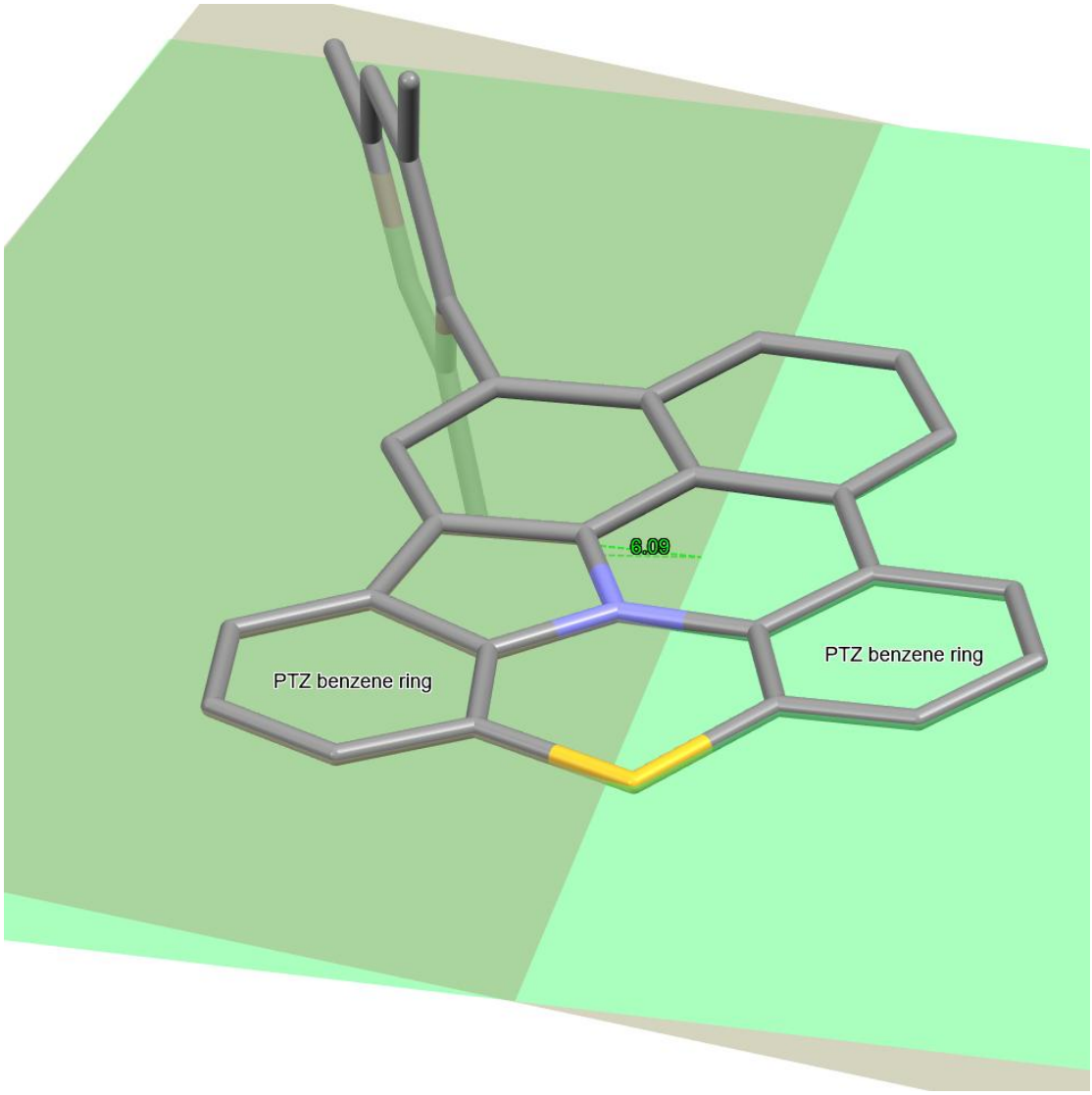


Figure S39. The dihedral angle between the phenothiazine benzene rings in **7a**. determined by X-ray diffraction analysis. The tert-butyl groups, and hydrogen atoms were omitted for clarity.

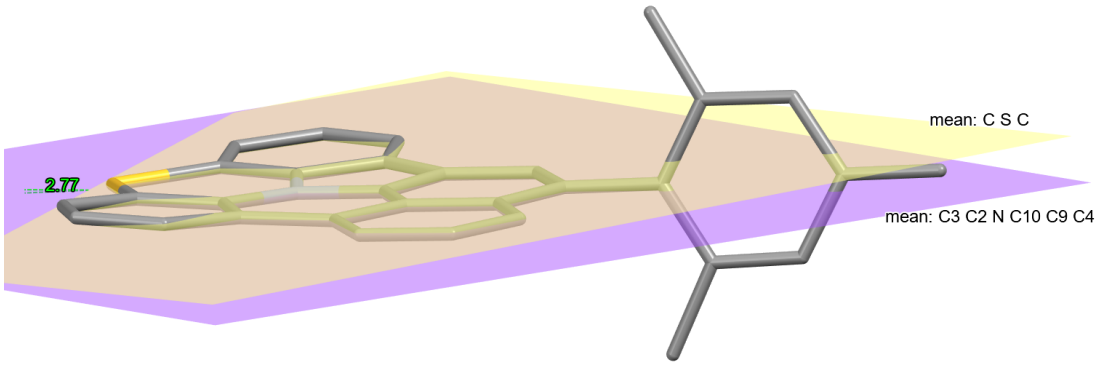


Figure S40. The dihedral angle between the C-S-C triangle plane and the C3-C2-N-C10-C9-C4 plane in **7a**. determined by X-ray diffraction analysis. The tert-butyl groups, and hydrogen atoms were omitted for clarity.

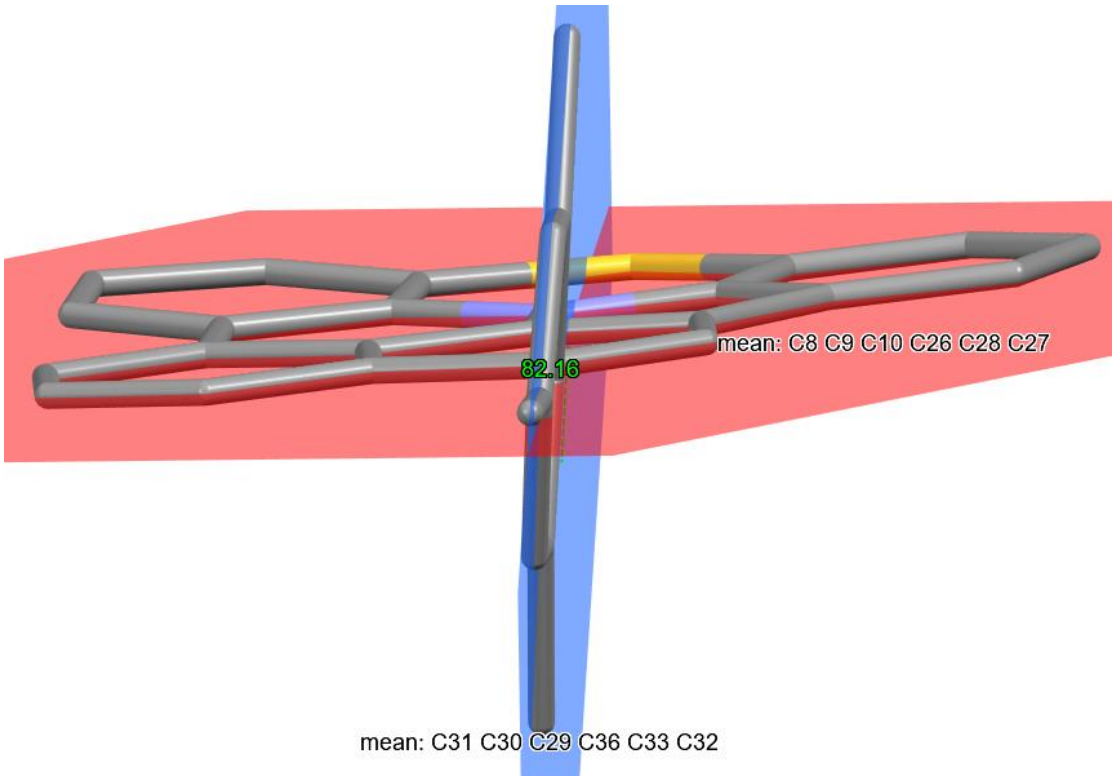


Figure S41. The dihedral angle between the mesityl group plane and the C8-C9-C10-C26-C28-C27 plane in **7a**. determined by X-ray diffraction analysis. The tert-butyl groups, and hydrogen atoms were omitted for clarity.

5. Delayed Photoluminescence Curves

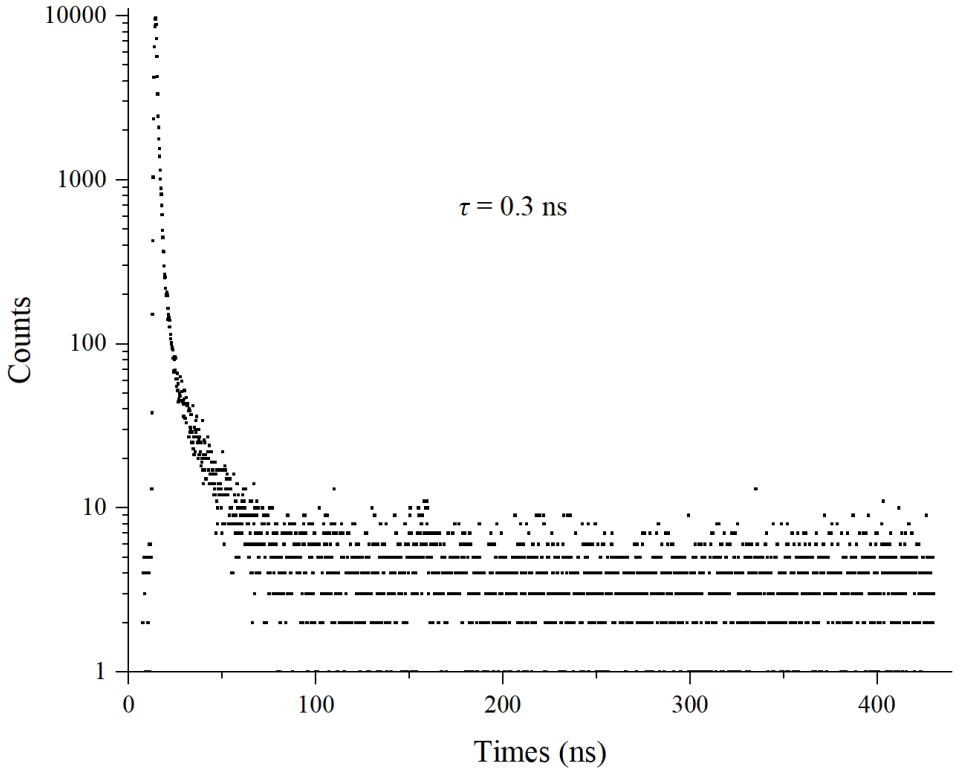


Figure S42. Fluorescence decay curve of **1a** measured in dichloromethane.

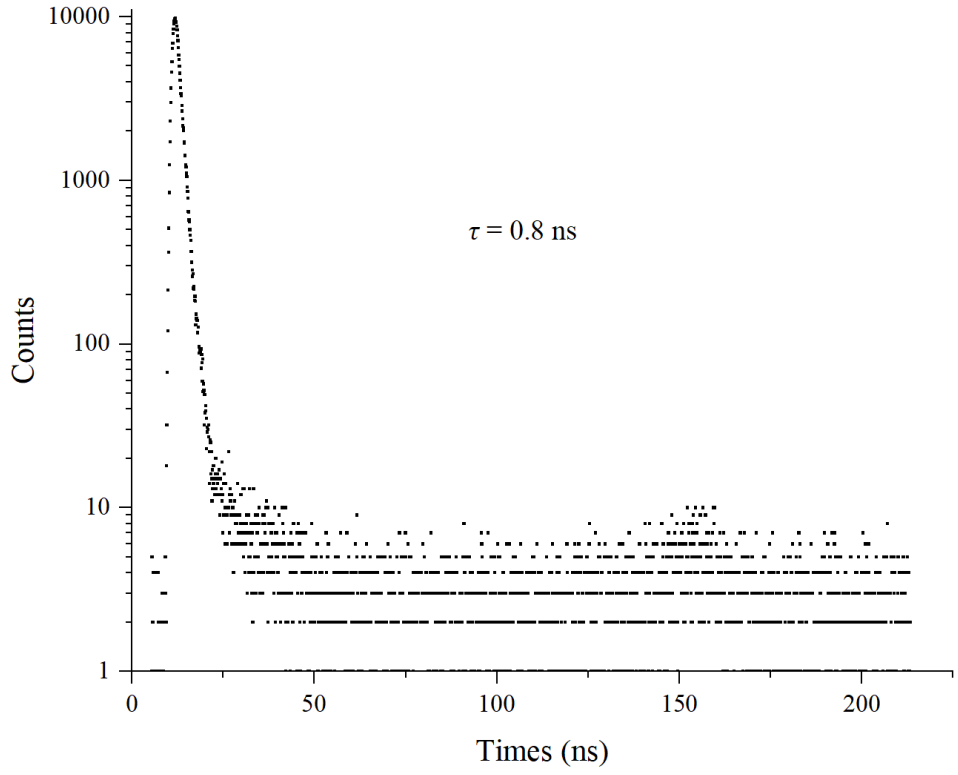


Figure S43. Fluorescence decay curve of **2a** measured in dichloromethane.

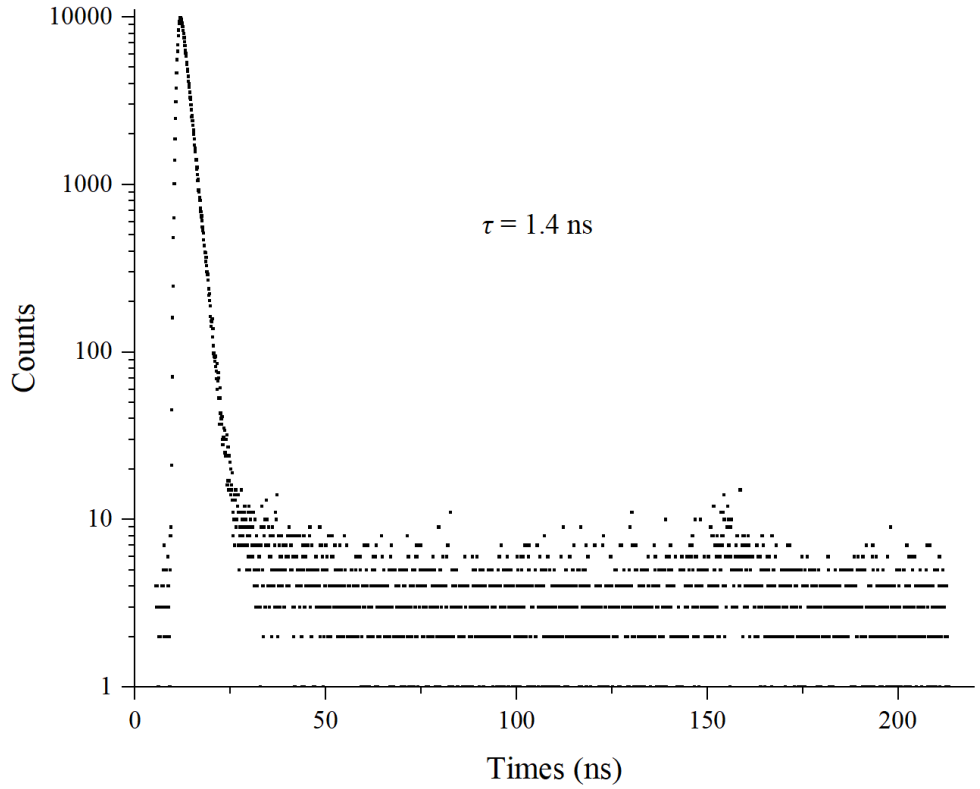


Figure S44. Fluorescence decay curve of **3a** measured in dichloromethane.

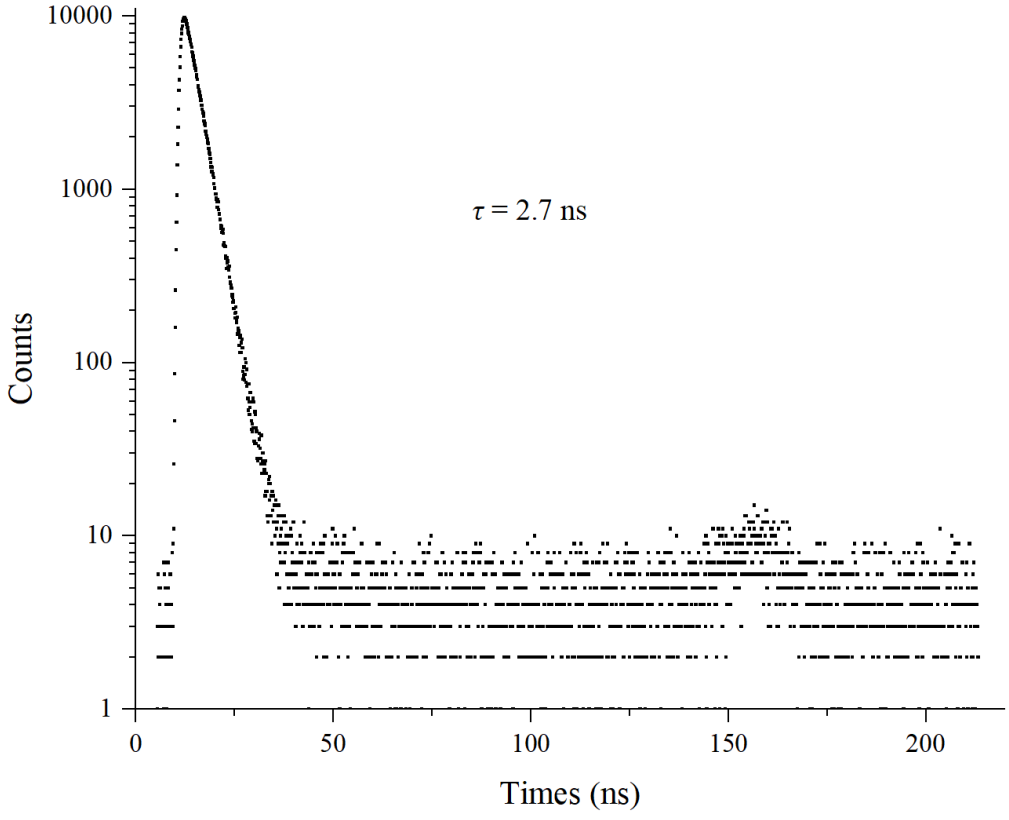


Figure S45. Fluorescence decay curve of **4a** measured in dichloromethane.

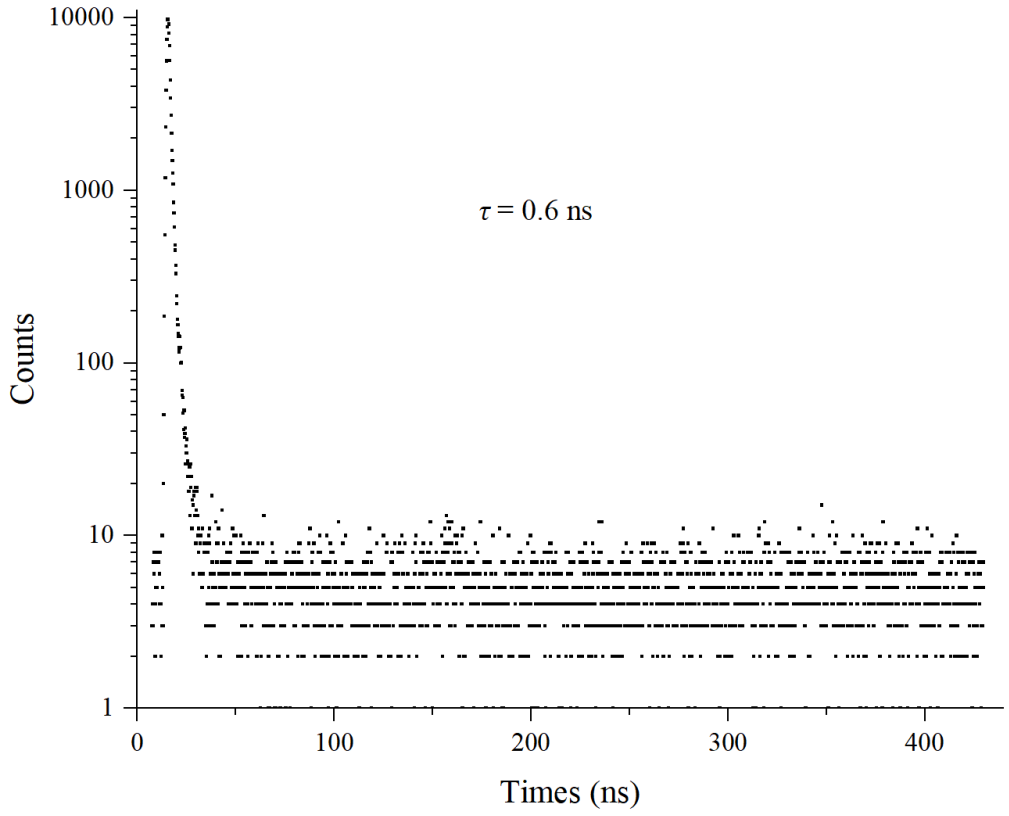


Figure S46. Fluorescence decay curve of **5a** measured in dichloromethane.

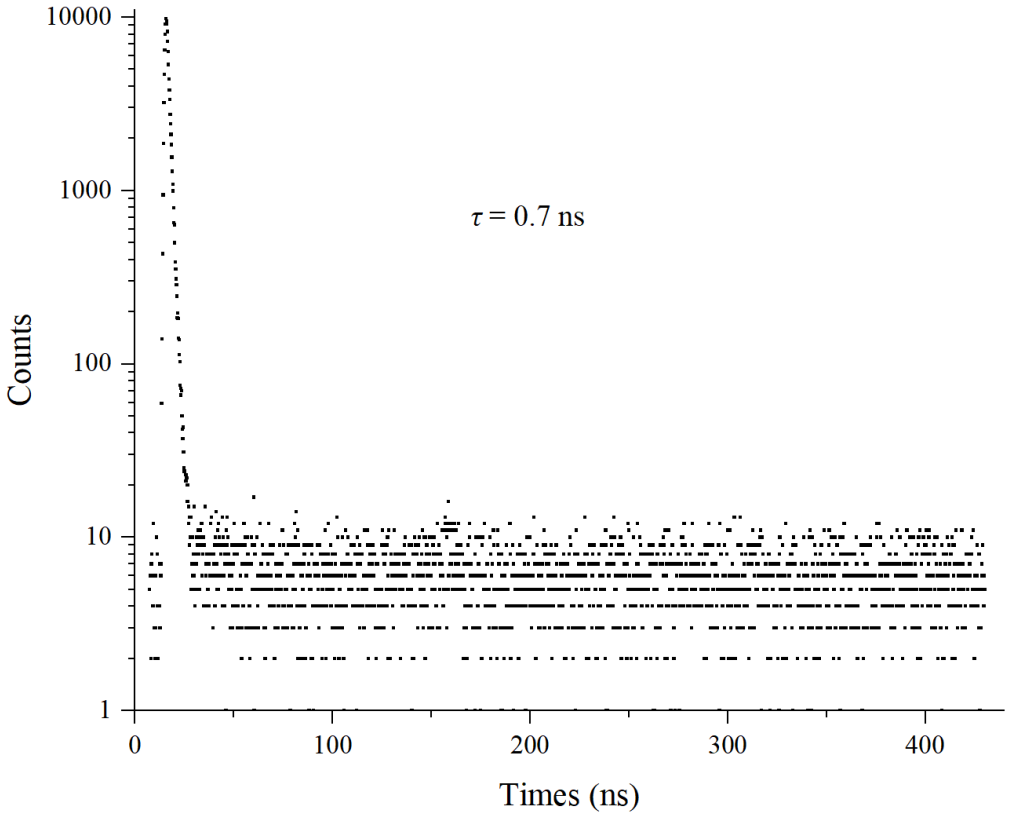


Figure S47. Fluorescence decay curve of **6a** measured in dichloromethane.

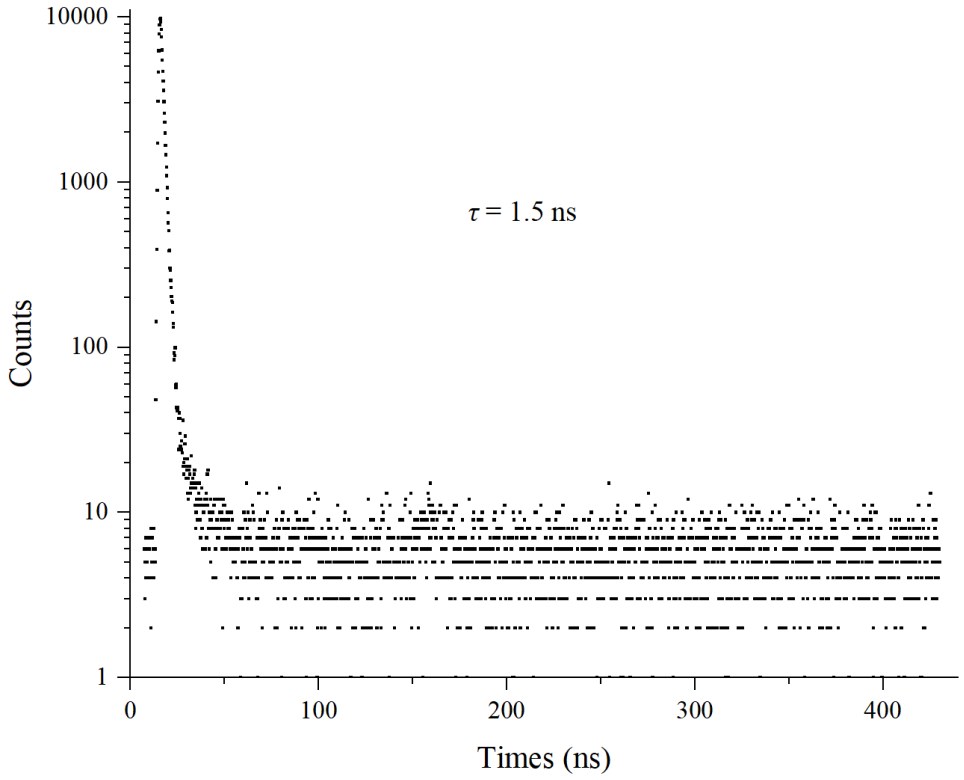


Figure S48. Fluorescence decay curve of **7a** measured in dichloromethane.

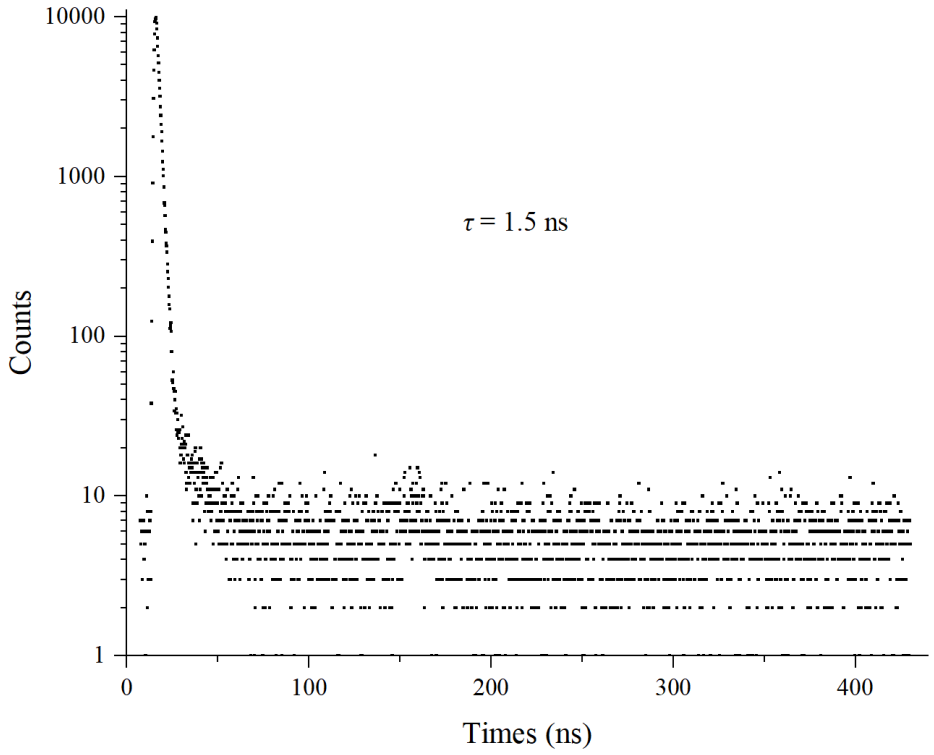


Figure S49. Fluorescence decay curve of **8a** measured in dichloromethane.

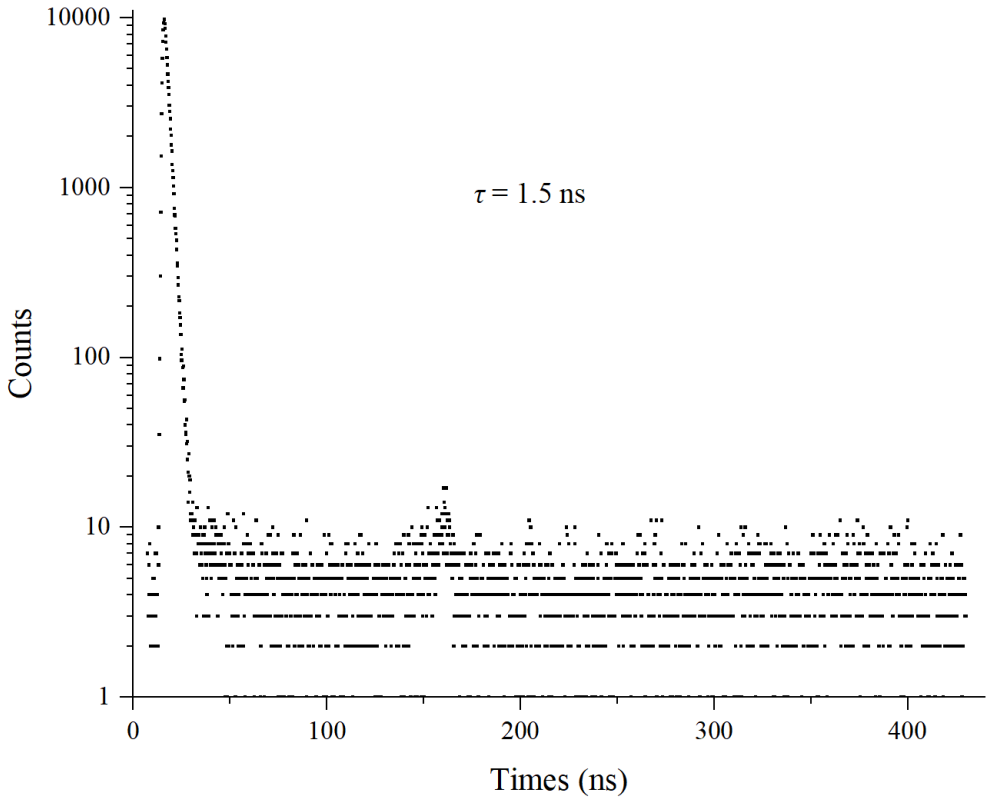


Figure S50. Fluorescence decay curve of **9a** measured in dichloromethane.

6. Electrochemical Properties

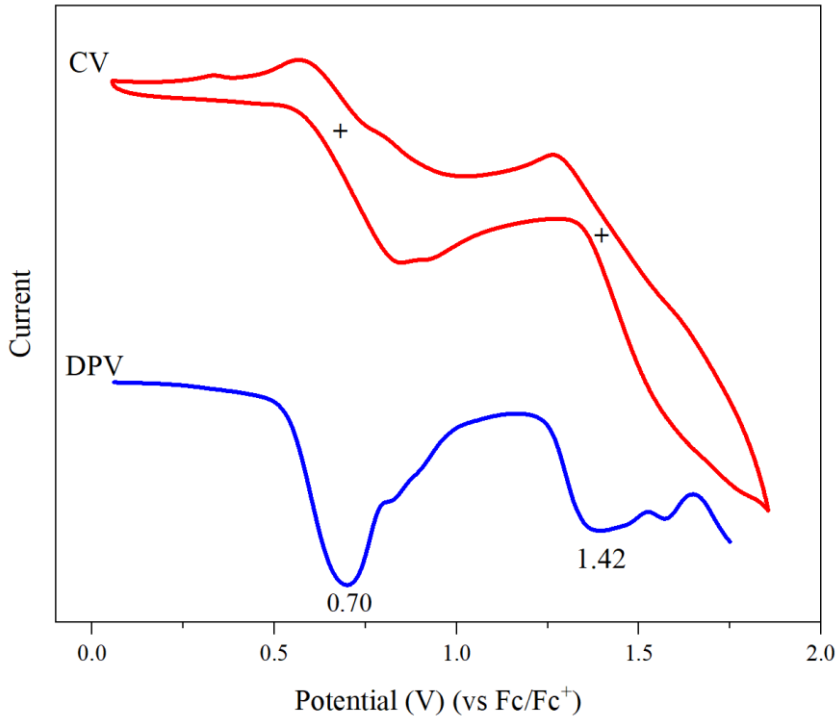


Figure S51. CV and DPV curves of **1a** measured in dichloromethane using nBu$_4$NPF$_6$ (0.1 M) as the supporting electrolyte and ferrocene as internal standard.

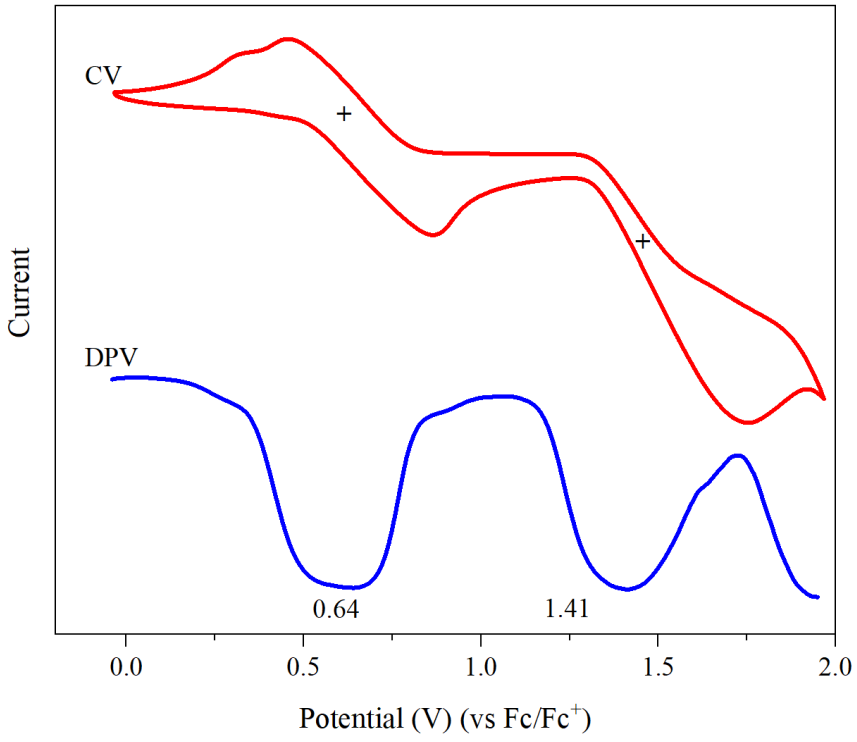


Figure S52. CV and DPV curves of **2a** measured in dichloromethane using nBu$_4$NPF$_6$ (0.1 M) as the supporting electrolyte and ferrocene as internal standard.

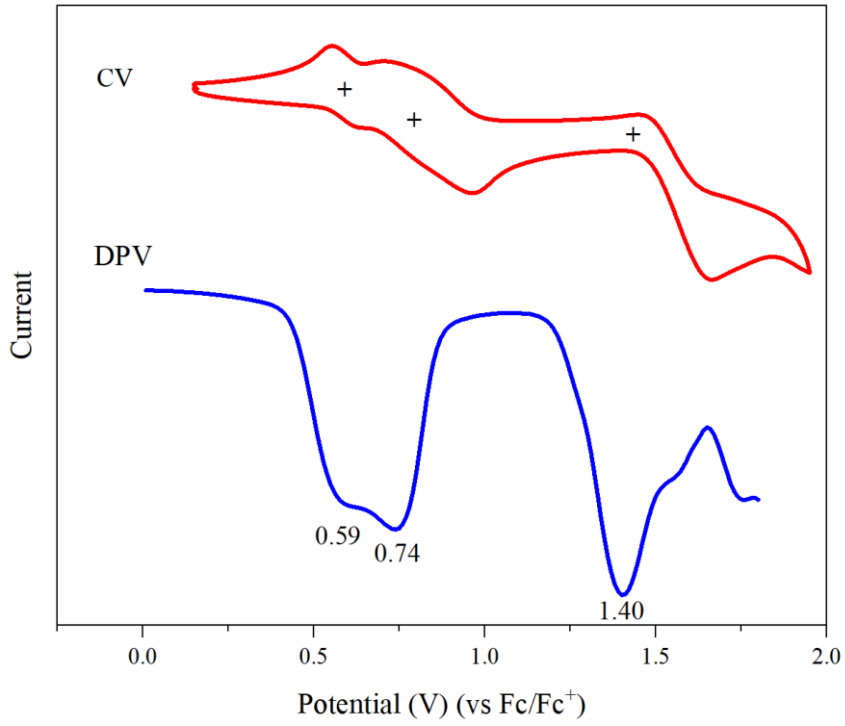


Figure S53. CV and DPV curves of **3a** measured in dichloromethane using nBu$_4$NPF$_6$ (0.1 M) as the supporting electrolyte and ferrocene as internal standard.

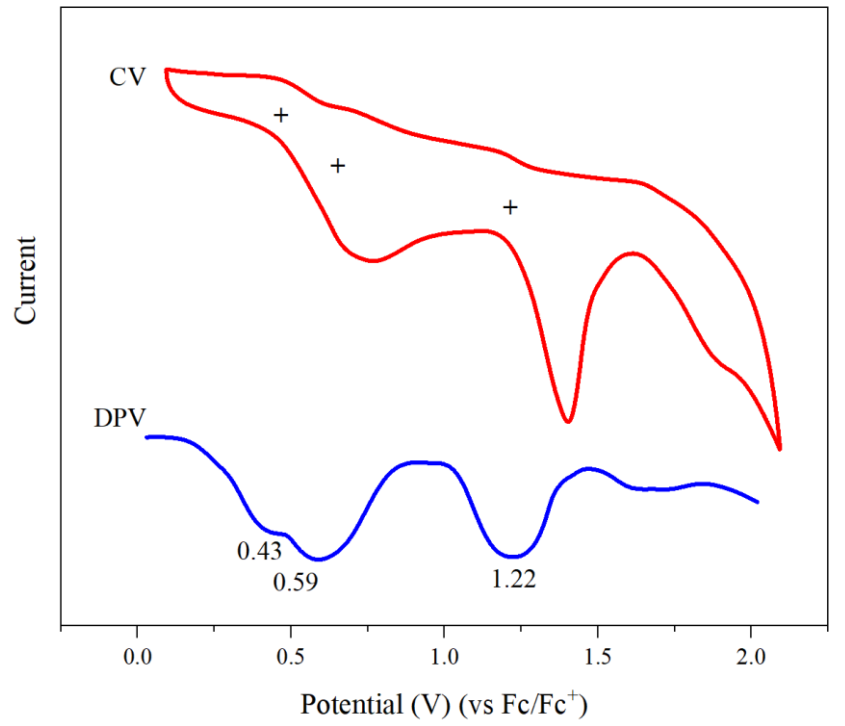


Figure S54. CV and DPV curves of **4a** measured in dichloromethane using nBu$_4$NPF$_6$ (0.1 M) as the supporting electrolyte and ferrocene as internal standard.

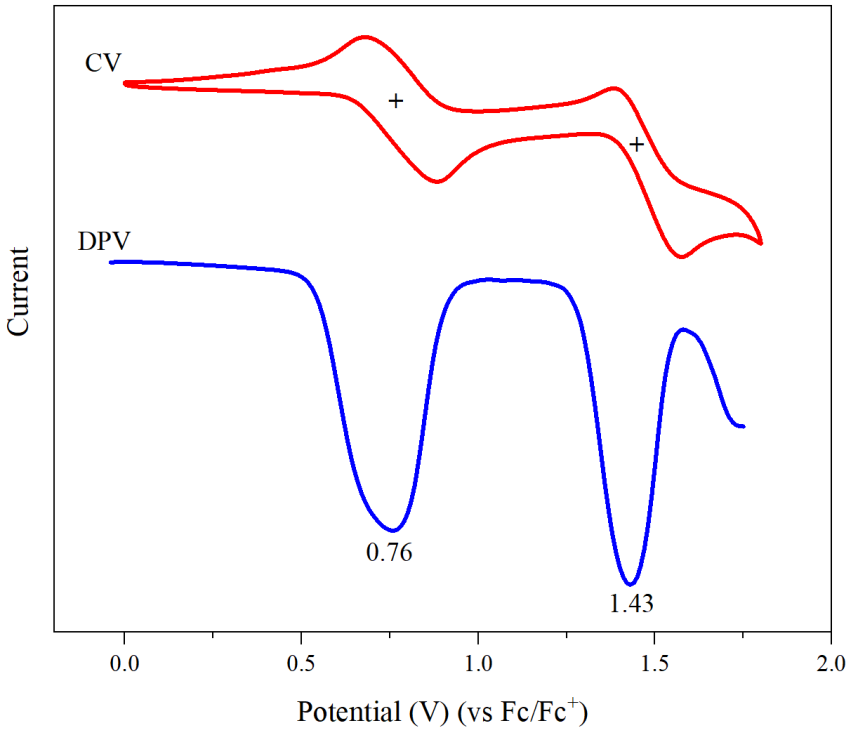


Figure S55. CV and DPV curves of **5a** measured in dichloromethane using nBu$_4$NPF$_6$ (0.1 M) as the supporting electrolyte and ferrocene as internal standard.

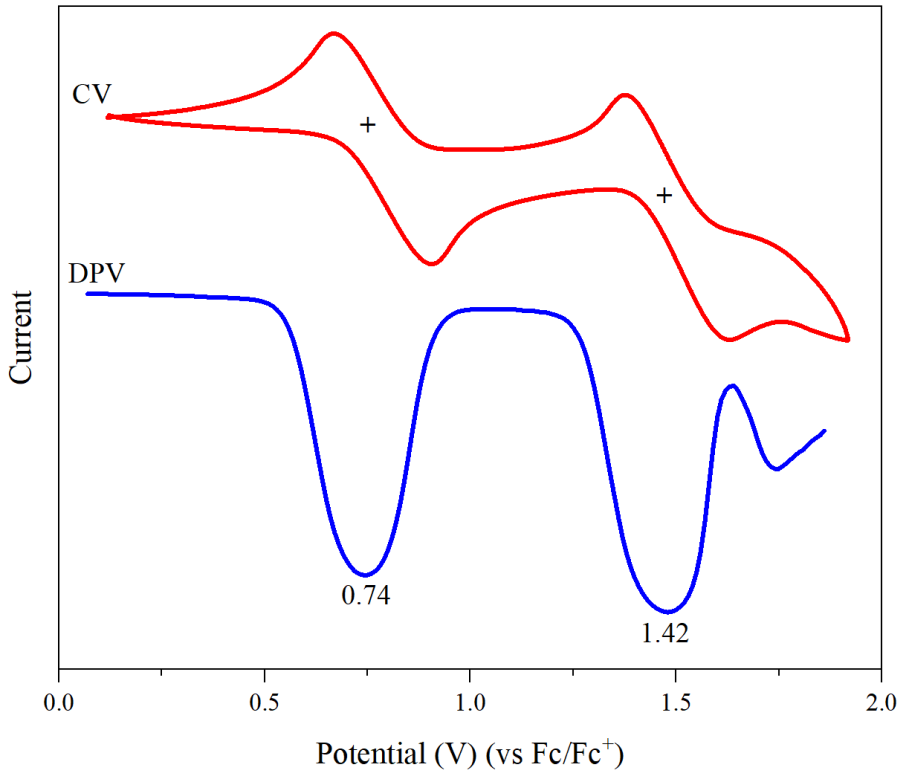


Figure S56. CV and DPV curves of **6a** measured in dichloromethane using nBu$_4$NPF$_6$ (0.1 M) as the supporting electrolyte and ferrocene as internal standard.

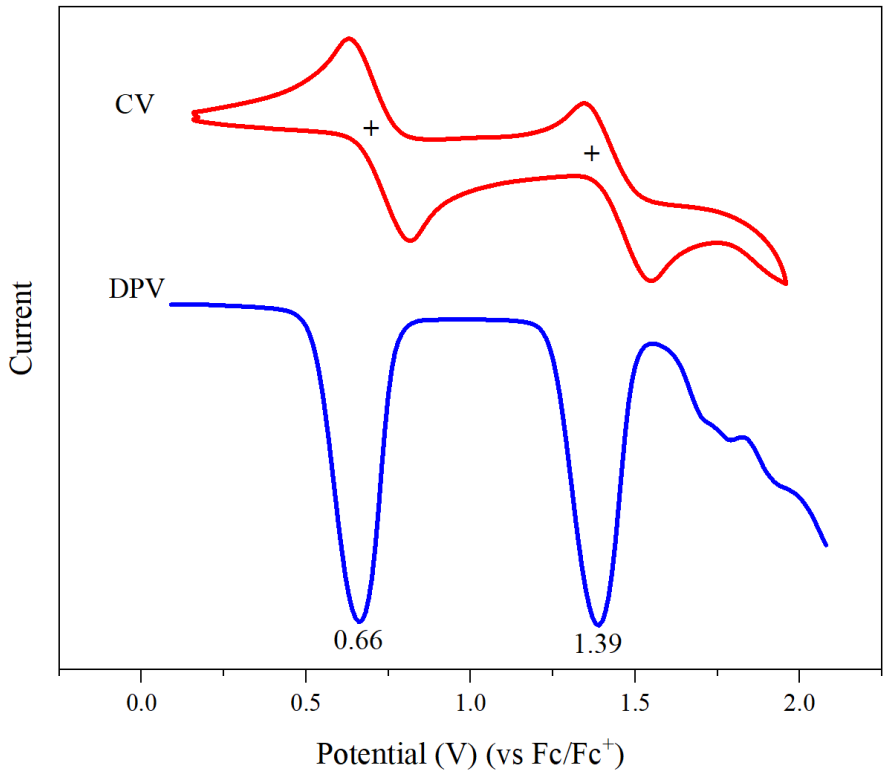


Figure S57. CV and DPV curves of **7a** measured in dichloromethane using nBu$_4$NPF$_6$ (0.1 M) as the supporting electrolyte and ferrocene as internal standard.

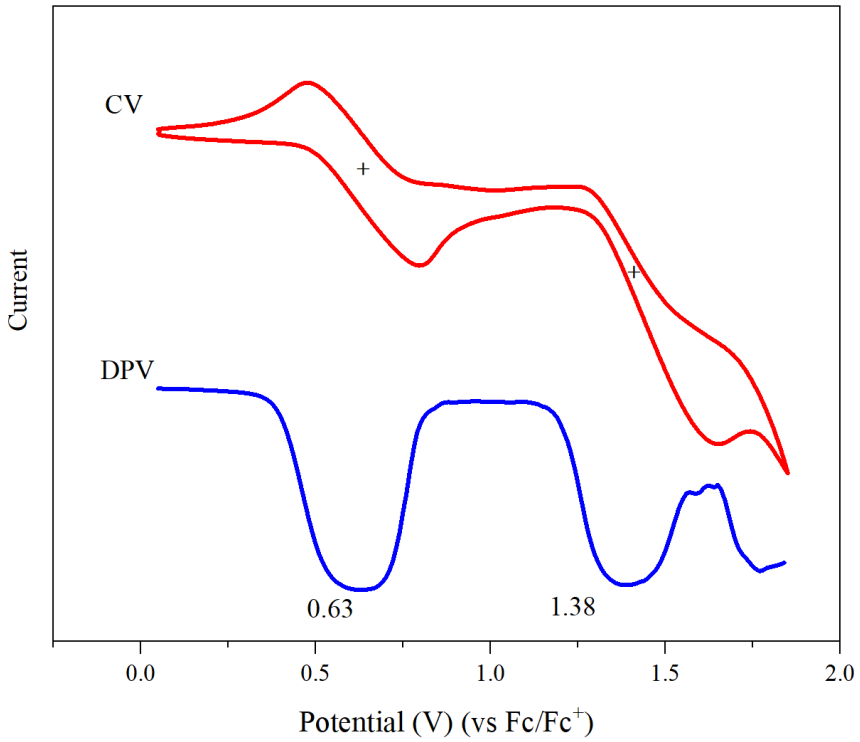


Figure S58. CV and DPV curves of **8a** measured in dichloromethane using nBu$_4$NPF$_6$ (0.1 M) as the supporting electrolyte and ferrocene as internal standard.

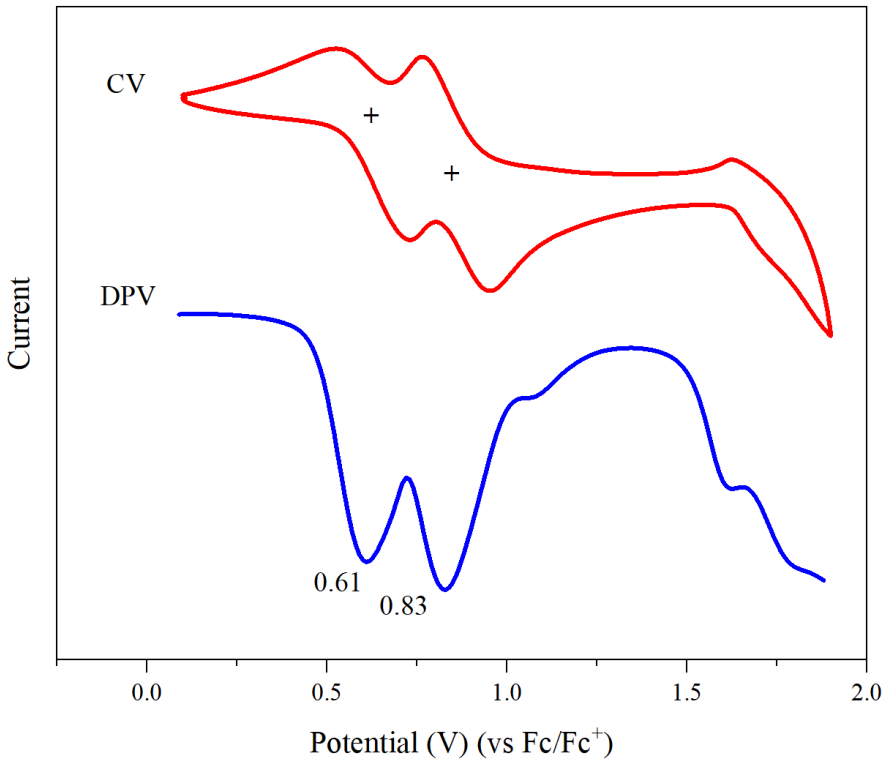


Figure S59. CV and DPV curves of **9a** measured in dichloromethane using nBu$_4$NPF$_6$ (0.1 M) as the supporting electrolyte and ferrocene as internal standard.

7. Theoretical Calculations

All the theoretical calculations were performed by using Gaussian 16 software.[2] All the calculations were based on the optimized geometries at B3LYP/6-31G(d,p) level of theory. The frontier molecular orbitals are calculated at the B3LYP/6-311+G(d,p) level of theory. The calculation of excited state properties was performed using time-depended DFT methods at B3LYP/6-311G+(d,p) level of theory in the solvent dichloromethane. The nucleus-independent chemical shift (NICS) calculation was done at GIAO-B3LYP/6-311G(d) level of theory. Bq atoms were inserted at the calculated positions and the Bq positions that are at the 1 Å away above the molecule were fixed with the assistant of Multiwfn software, as well as the generation of isotropic chemical shielding surfaces (ICSS), and related quantities.[3]

7-1. NICS Analysis

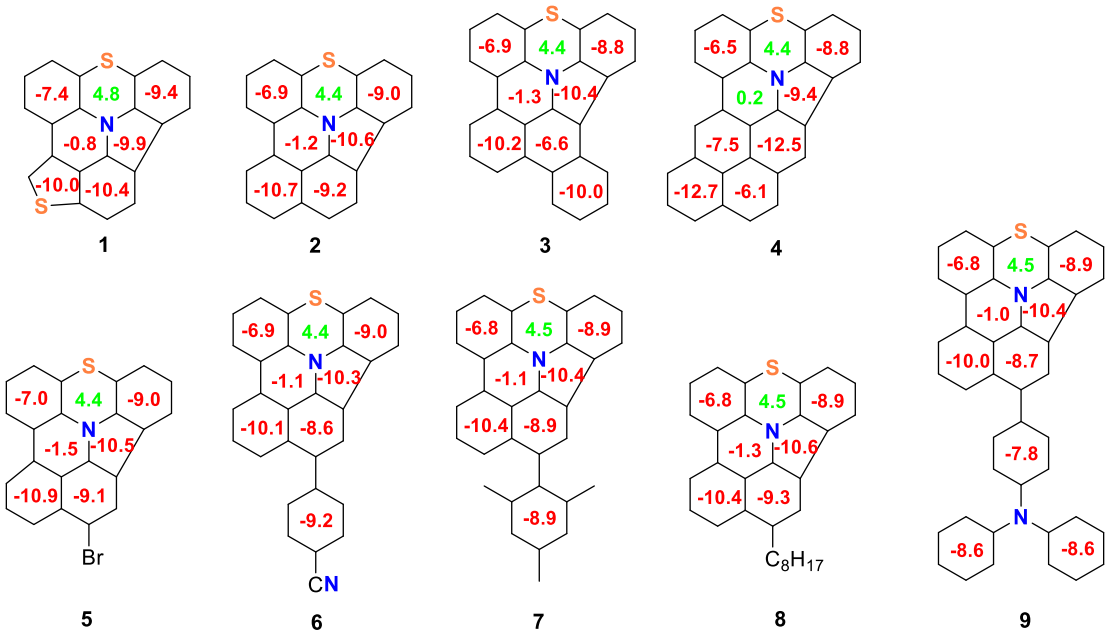


Figure S60. Calculated NICS(1)zz values of phenothiazine derivatives **1-9**.

7-2. 3D ICSS Maps

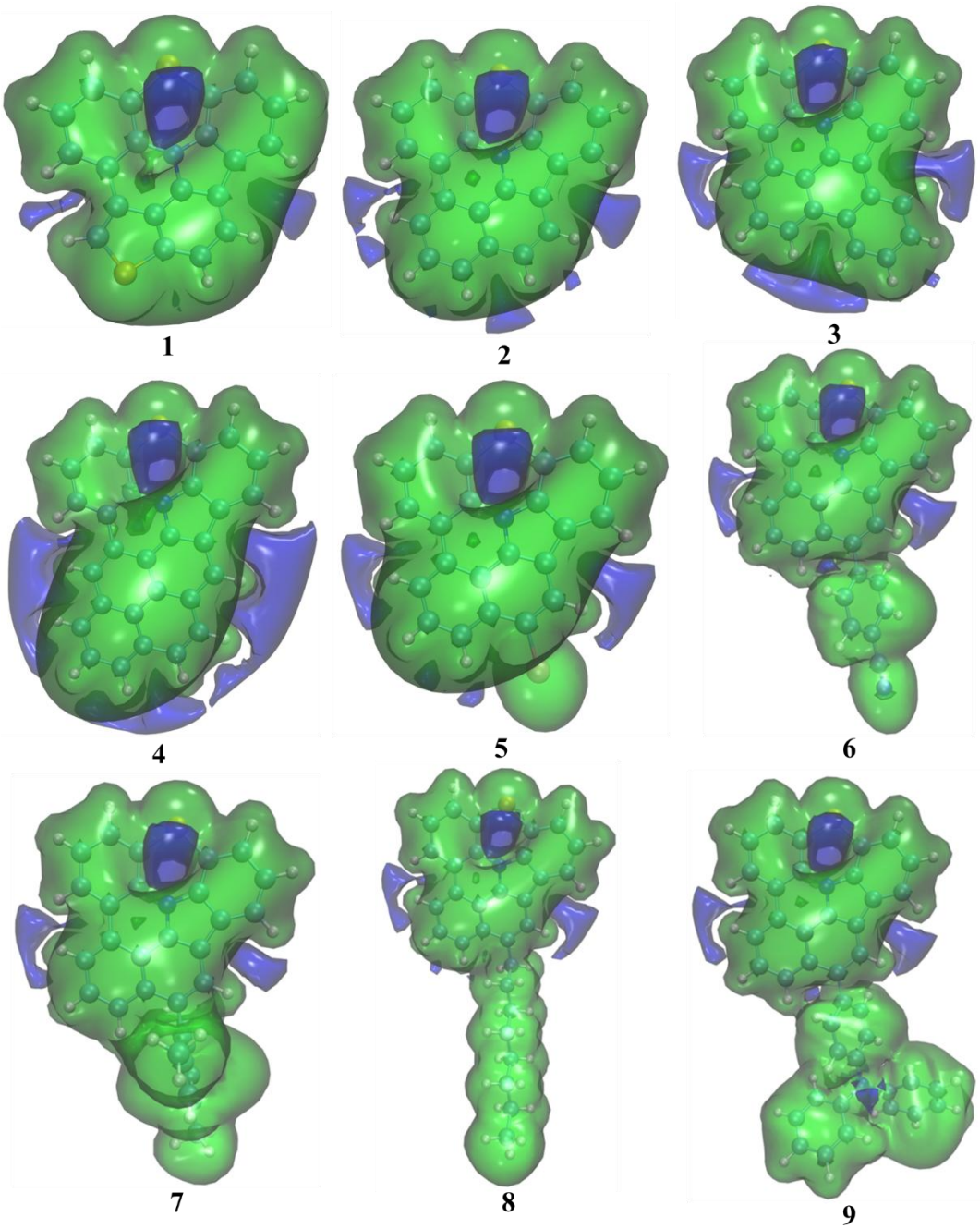


Figure S61. Calculated 3D ICSS maps of phenothiazine derivatives **1-9**. The green and blue colors in 3D ICSS maps represent magnetically shielding and deshielding regions, respectively.

7-3. TD-DFT Calculations

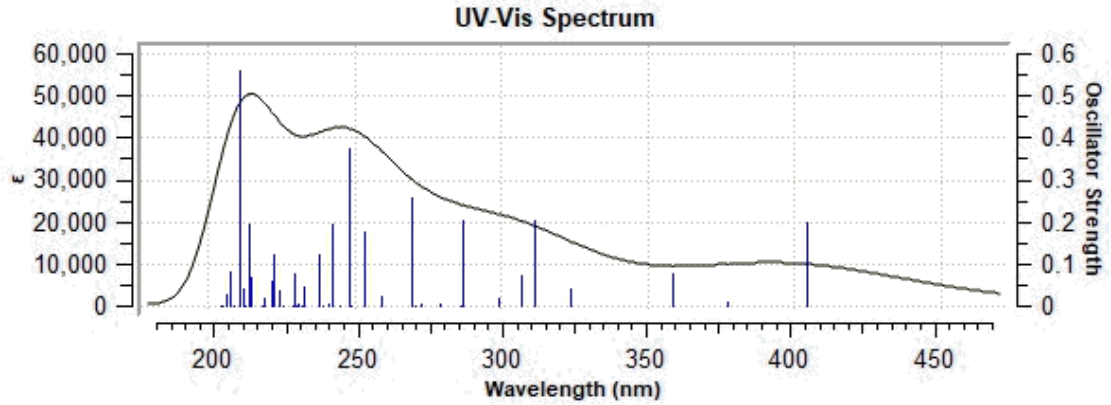


Figure S62. Simulated UV-visible absorption spectrum of **1**.

Table S5. TD-DFT calculated first ten excited states of compound **1** in dichloromethane at B3LYP/6-311G+(d,p) level and the corresponding contributions.

Excited State 1:	Singlet-A	3.0655 eV	404.45 nm	f=0.1997	<S**2>=0.000
84 -> 85	0.69117				
Excited State 2:	Singlet-A	3.2856 eV	377.36 nm	f=0.0078	<S**2>=0.000
84 -> 86	0.63675				
84 -> 87	-0.28797				
Excited State 3:	Singlet-A	3.4567 eV	358.68 nm	f=0.0759	<S**2>=0.000
84 -> 86	0.28400				
84 -> 87	0.62582				
Excited State 4:	Singlet-A	3.8292 eV	323.79 nm	f=0.0421	<S**2>=0.000
82 -> 85	0.18466				
83 -> 85	0.55222				
84 -> 88	0.38305				
Excited State 5:	Singlet-A	3.9772 eV	311.73 nm	f=0.2019	<S**2>=0.000
83 -> 85	-0.33652				
83 -> 86	0.34873				
84 -> 88	0.47728				
Excited State 6:	Singlet-A	4.0404 eV	306.86 nm	f=0.0726	<S**2>=0.000
82 -> 87	0.10703				
83 -> 85	0.18246				
83 -> 86	0.59163				
84 -> 88	-0.27705				

Excited State 7:	Singlet-A	4.1468 eV	298.99 nm	f=0.0167	<S**2>=0.000
82 -> 85	0.66117				
82 -> 86	0.10943				
83 -> 85	-0.15139				
Excited State 8:	Singlet-A	4.3213 eV	286.92 nm	f=0.2022	<S**2>=0.000
82 -> 86	0.31913				
82 -> 87	-0.14781				
83 -> 87	0.55842				
84 -> 92	0.15425				
Excited State 9:	Singlet-A	4.3346 eV	286.03 nm	f=0.0000	<S**2>=0.000
83 -> 91	-0.13057				
84 -> 89	0.63336				
84 -> 91	-0.21630				
Excited State 10:	Singlet-A	4.4388 eV	279.32 nm	f=0.0037	<S**2>=0.000
82 -> 86	0.51562				
82 -> 87	-0.18871				
83 -> 86	-0.10641				
83 -> 87	-0.37277				
84 -> 92	0.15538				

84: HOMO; 85: LUMO

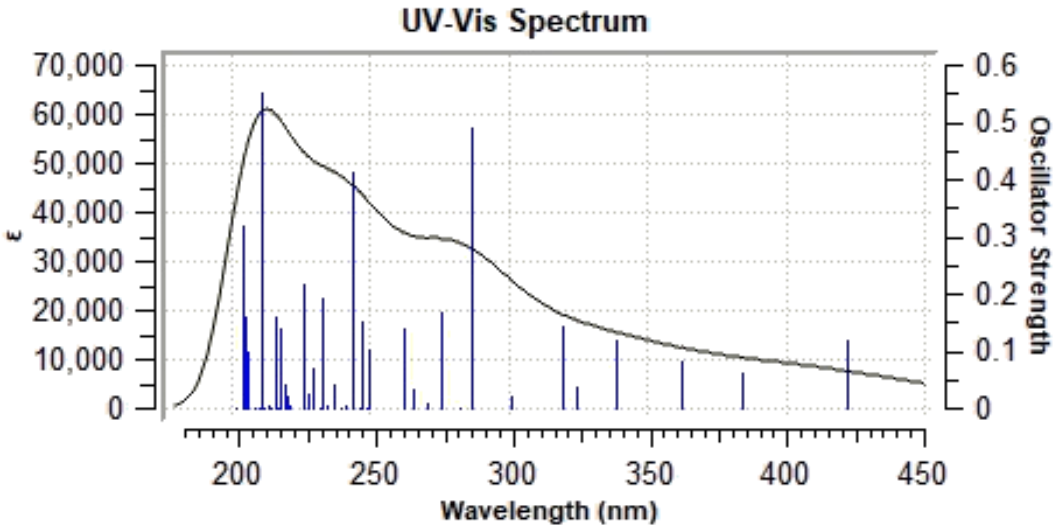


Figure S63. Simulated UV-visible absorption spectrum of **2**.

Table S6. TD-DFT calculated first ten excited states of compound **2** in dichloromethane at B3LYP/6-311G+(d,p) level and the corresponding contributions.

Excited State 1:	Singlet-A	2.9376 eV	422.06 nm	f=0.1178	<S**2>=0.000
83 -> 84	0.69379				
Excited State 2:	Singlet-A	3.2277 eV	384.13 nm	f=0.0626	<S**2>=0.000
83 -> 85	0.65042				
83 -> 86	0.24302				
Excited State 3:	Singlet-A	3.4217 eV	362.35 nm	f=0.0804	<S**2>=0.000
81 -> 84	0.11693				
82 -> 84	0.21165				
83 -> 85	-0.20843				
83 -> 86	0.61803				
Excited State 4:	Singlet-A	3.6599 eV	338.77 nm	f=0.1172	<S**2>=0.000
82 -> 84	0.61806				
82 -> 85	-0.13023				
82 -> 86	-0.13522				
83 -> 86	-0.16592				
83 -> 87	-0.20515				
Excited State 5:	Singlet-A	3.8148 eV	325.01 nm	f=0.0368	<S**2>=0.000
82 -> 85	-0.38223				
83 -> 87	0.56312				
Excited State 6:	Singlet-A	3.8740 eV	320.04 nm	f=0.1444	<S**2>=0.000
81 -> 84	0.19939				
82 -> 84	0.18058				
82 -> 85	0.52112				
83 -> 86	-0.11043				
83 -> 87	0.33481				
Excited State 7:	Singlet-A	4.1125 eV	301.48 nm	f=0.0208	<S**2>=0.000
81 -> 84	0.48950				
82 -> 84	-0.15984				
82 -> 86	-0.45466				
Excited State 8:	Singlet-A	4.3287 eV	286.42 nm	f=0.4880	<S**2>=0.000
81 -> 84	0.41029				
82 -> 85	-0.20051				
82 -> 86	0.46861				
83 -> 88	0.13828				

Excited State 9:	Singlet-A	4.3832 eV	282.86 nm	f=0.0000	<S**2>=0.000
82 -> 89	0.18463				
83 -> 89	0.66232				
Excited State 10:	Singlet-A	4.4974 eV	275.68 nm	f=0.1687	<S**2>=0.000
81 -> 85	0.55506				
81 -> 86	0.20291				
82 -> 87	0.10979				
83 -> 88	0.29315				
83 -> 91	0.17619				

83: HOMO; 84: LUMO

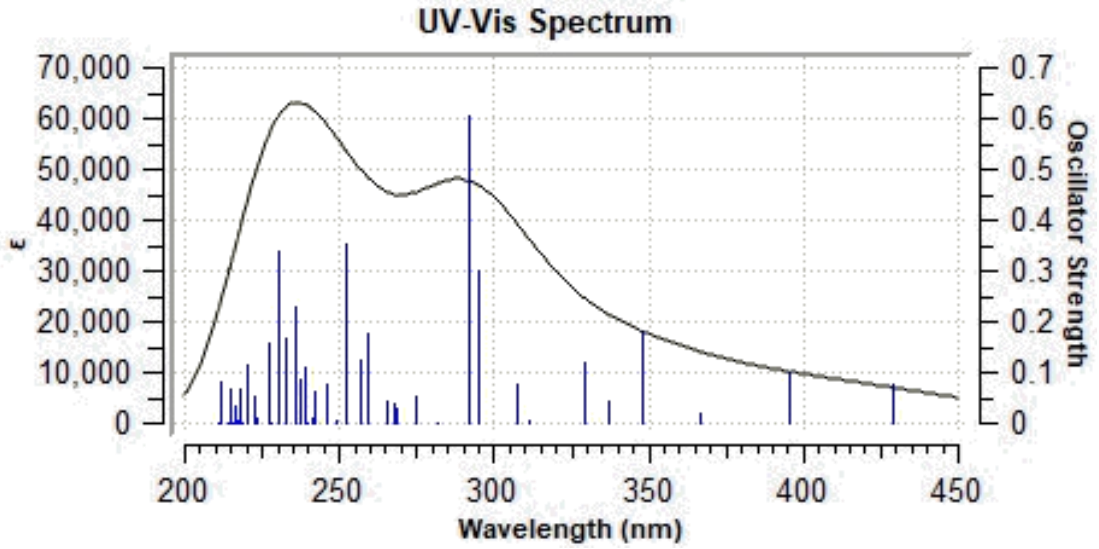


Figure S64. Simulated UV-visible absorption spectrum of **3**.

Table S7. TD-DFT calculated first ten excited states of compound **3** in dichloromethane at B3LYP/6-311G+(d,p) level and the corresponding contributions.

Excited State 1:	Singlet-A	2.8910 eV	428.87 nm	f=0.0784	<S**2>=0.000
96 -> 97	0.69766				
Excited State 2:	Singlet-A	3.1339 eV	395.62 nm	f=0.0986	<S**2>=0.000
96 -> 98	0.67996				
96 -> 99	0.10151				
Excited State 3:	Singlet-A	3.3820 eV	366.60 nm	f=0.0202	<S**2>=0.000
95 -> 97	0.24606				
96 -> 99	0.64557				

Excited State 4:	Singlet-A	3.5655 eV	347.73 nm	f=0.1824	<S**2>=0.000
95 -> 97	0.62895				
95 -> 99	-0.11483				
96 -> 98	0.12406				
96 -> 99	-0.22027				
Excited State 5:	Singlet-A	3.6774 eV	337.15 nm	f=0.0412	<S**2>=0.000
94 -> 97	0.20000				
95 -> 98	0.63267				
95 -> 99	0.11986				
96 ->100	0.12794				
96 ->101	-0.13476				
Excited State 6:	Singlet-A	3.7659 eV	329.23 nm	f=0.1181	<S**2>=0.000
94 -> 98	0.21204				
96 ->100	0.64167				
Excited State 7:	Singlet-A	3.9844 eV	311.17 nm	f=0.0055	<S**2>=0.000
94 -> 97	0.18638				
94 -> 98	-0.21818				
94 -> 99	-0.11369				
95 -> 99	0.10360				
96 ->101	0.60901				
Excited State 8:	Singlet-A	4.0321 eV	307.49 nm	f=0.0741	<S**2>=0.000
94 -> 97	0.54171				
95 -> 97	-0.12364				
95 -> 98	-0.11752				
95 -> 99	-0.38639				
Excited State 9:	Singlet-A	4.2025 eV	295.03 nm	f=0.3014	<S**2>=0.000
94 -> 97	0.30632				
95 -> 98	-0.22437				
95 -> 99	0.53105				
96 ->101	-0.14025				
96 ->102	0.12307				
Excited State 10:	Singlet-A	4.2515 eV	291.63 nm	f=0.6067	<S**2>=0.000
94 -> 98	0.60117				
95 ->100	-0.12576				
96 ->100	-0.20667				
96 ->101	0.20573				

96: HOMO; 97: LUMO

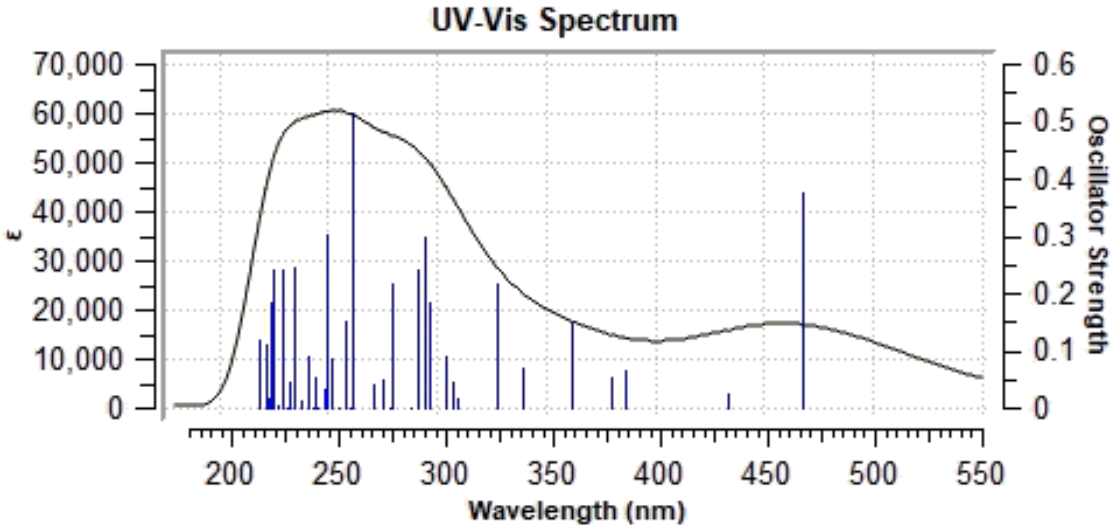


Figure S65. Simulated UV-visible absorption spectrum of **4**.

Table S8. TD-DFT calculated first ten excited states of compound **4** in dichloromethane at B3LYP/6-311G+(d,p) level and the corresponding contributions.

Excited State 1:	Singlet-A	2.6534 eV	467.26 nm	f=0.3757	<S**2>=0.000
102 ->103	0.68659				
Excited State 2:	Singlet-A	2.8584 eV	433.75 nm	f=0.0228	<S**2>=0.000
102 ->104	0.68763				
102 ->105	-0.11871				
Excited State 3:	Singlet-A	3.2064 eV	386.67 nm	f=0.0642	<S**2>=0.000
100 ->103	-0.17743				
101 ->103	-0.13734				
102 ->105	0.53814				
102 ->106	0.37528				
Excited State 4:	Singlet-A	3.2659 eV	379.64 nm	f=0.0532	<S**2>=0.000
100 ->103	0.15264				
101 ->103	0.11840				
102 ->105	-0.32902				
102 ->106	0.58146				
Excited State 5:	Singlet-A	3.4226 eV	362.25 nm	f=0.1485	<S**2>=0.000
101 ->103	0.65956				
102 ->105	0.18825				
Excited State 6:	Singlet-A	3.6502 eV	339.66 nm	f=0.0702	<S**2>=0.000
100 ->103	0.41718				
101 ->104	0.50248				

102 ->105	0.11108				
102 ->107	-0.16164				
Excited State 7:	Singlet-A	3.7872 eV	327.38 nm	f=0.2175	<S**2>=0.000
100 ->103	0.44022				
100 ->104	-0.14293				
101 ->104	-0.41417				
101 ->105	0.16206				
101 ->106	0.18244				
102 ->105	0.13802				
Excited State 8:	Singlet-A	4.0090 eV	309.26 nm	f=0.0175	<S**2>=0.000
99 ->103	0.29756				
100 ->104	0.18847				
101 ->105	0.33510				
102 ->107	0.42304				
102 ->108	-0.20491				
102 ->111	-0.11760				
Excited State 9:	Singlet-A	4.0421 eV	306.73 nm	f=0.0460	<S**2>=0.000
100 ->103	0.15397				
100 ->104	-0.33875				
100 ->105	0.10646				
101 ->105	-0.32764				
101 ->106	-0.20920				
102 ->107	0.40095				
Excited State 10:	Singlet-A	4.0809 eV	303.82 nm	f=0.0904	<S**2>=0.000
100 ->104	-0.33312				
101 ->104	0.22994				
101 ->105	0.18533				
101 ->106	0.47694				
102 ->107	0.17097				
102 ->108	0.11177				

102: HOMO; 103: LUMO

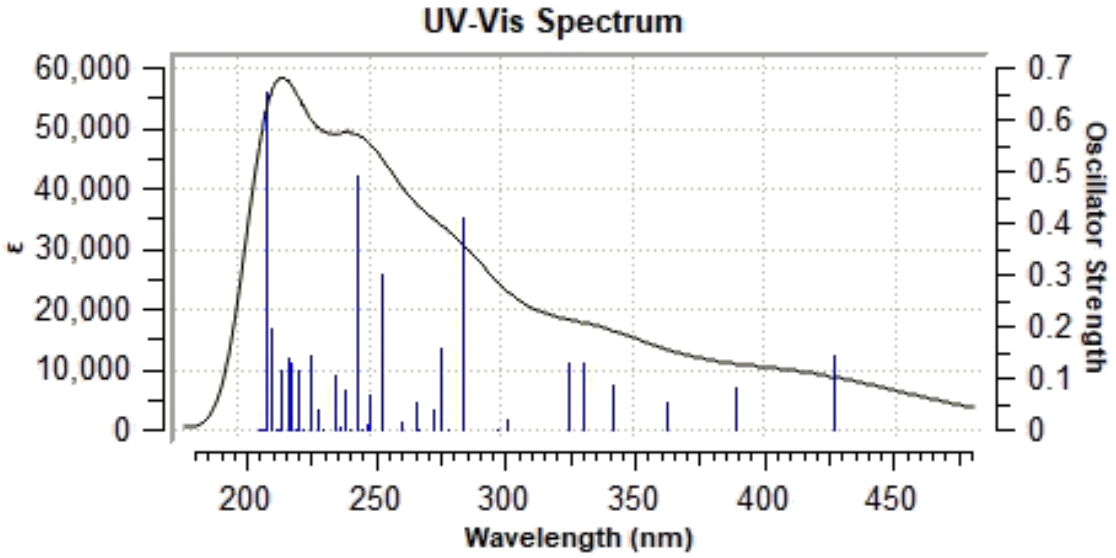


Figure S66. Simulated UV-visible absorption spectrum of **5**.

Table S9. TD-DFT calculated first ten excited states of compound **5** in dichloromethane at B3LYP/6-311G+(d,p) level and the corresponding contributions.

Excited State 1:	Singlet-A	2.9078 eV	426.39 nm	f=0.1423	<S**2>=0.000
100 ->101	0.69350				
Excited State 2:	Singlet-A	3.1859 eV	389.17 nm	f=0.0809	<S**2>=0.000
100 ->102	0.67002				
100 ->103	0.17297				
Excited State 3:	Singlet-A	3.4167 eV	362.88 nm	f=0.0512	<S**2>=0.000
99 ->101	0.21944				
100 ->102	-0.13826				
100 ->103	0.63684				
Excited State 4:	Singlet-A	3.6145 eV	343.02 nm	f=0.0844	<S**2>=0.000
99 ->101	0.60641				
99 ->103	-0.11099				
100 ->103	-0.15957				
100 ->104	-0.27334				
Excited State 5:	Singlet-A	3.7443 eV	331.12 nm	f=0.1278	<S**2>=0.000
99 ->101	0.18151				
99 ->102	-0.25279				
100 ->103	-0.11872				
100 ->104	0.59774				
Excited State 6:	Singlet-A	3.8075 eV	325.63 nm	f=0.1308	<S**2>=0.000

98 ->101	0.16738				
99 ->101	0.15523				
99 ->102	0.60951				
100 ->104	0.20145				
Excited State 7:	Singlet-A	4.1028 eV	302.20 nm	f=0.0173	<S**2>=0.000
98 ->101	0.49081				
99 ->101	-0.13473				
99 ->103	-0.46518				
Excited State 8:	Singlet-A	4.1522 eV	298.60 nm	f=0.0004	<S**2>=0.000
99 ->105	-0.14498				
100 ->105	0.68054				
Excited State 9:	Singlet-A	4.3365 eV	285.91 nm	f=0.4108	<S**2>=0.000
98 ->101	0.42385				
99 ->102	-0.18964				
99 ->103	0.45841				
100 ->106	0.16659				
Excited State 10:	Singlet-A	4.4255 eV	280.16 nm	f=0.0000	<S**2>=0.000
99 ->107	0.16560				
100 ->107	0.62852				
100 ->108	-0.19403				

100: HOMO; 101: LUMO

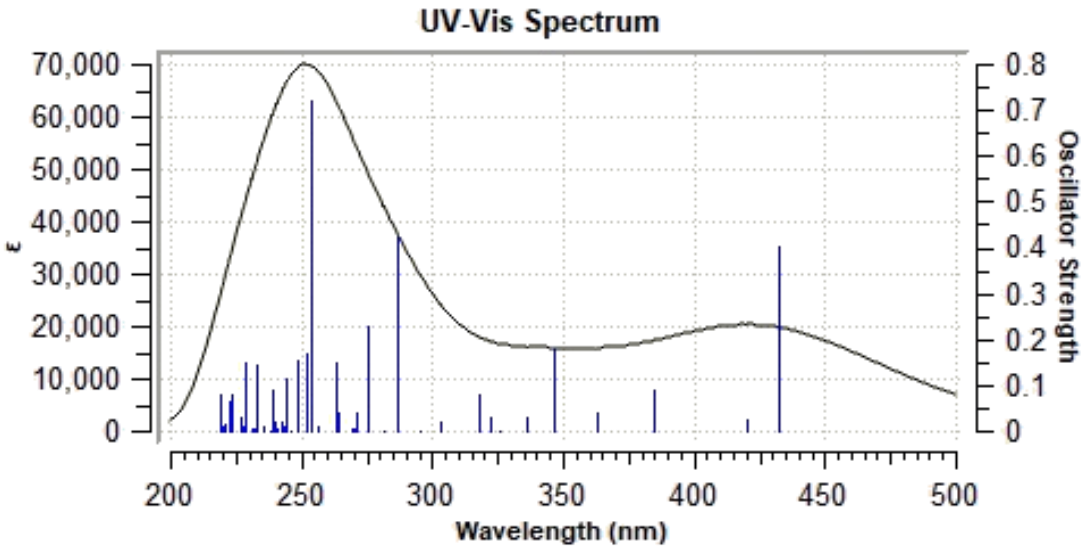


Figure S67. Simulated UV-visible absorption spectrum of **6**.

Table S10. TD-DFT calculated first ten excited states of compound **6** in dichloromethane at B3LYP/6-311G+(d,p) level and the corresponding contributions.

Excited State 1:	Singlet-A	2.8682 eV	432.28 nm	f=0.4009	<S**2>=0.000
109 ->110	0.68737				
109 ->111	-0.12573				
Excited State 2:	Singlet-A	2.9521 eV	419.99 nm	f=0.0265	<S**2>=0.000
109 ->110	0.12568				
109 ->111	0.68117				
Excited State 3:	Singlet-A	3.2251 eV	384.43 nm	f=0.0915	<S**2>=0.000
109 ->112	0.66569				
109 ->113	0.16570				
Excited State 4:	Singlet-A	3.4171 eV	362.84 nm	f=0.0391	<S**2>=0.000
108 ->110	-0.20666				
108 ->111	0.13856				
109 ->112	-0.12604				
109 ->113	0.62989				
Excited State 5:	Singlet-A	3.5794 eV	346.38 nm	f=0.1792	<S**2>=0.000
108 ->110	0.63611				
108 ->111	-0.13922				
109 ->113	0.20680				
109 ->115	-0.12286				
Excited State 6:	Singlet-A	3.6860 eV	336.36 nm	f=0.0321	<S**2>=0.000
108 ->110	0.17349				
108 ->111	0.60494				
108 ->112	-0.25225				
108 ->113	-0.14477				
Excited State 7:	Singlet-A	3.8074 eV	325.64 nm	f=0.0021	<S**2>=0.000
108 ->114	-0.10386				
109 ->114	0.69190				
Excited State 8:	Singlet-A	3.8490 eV	322.12 nm	f=0.0305	<S**2>=0.000
107 ->110	-0.21362				
107 ->111	0.13411				
108 ->111	0.21589				
108 ->112	0.59345				
Excited State 9:	Singlet-A	3.8997 eV	317.93 nm	f=0.0799	<S**2>=0.000

109 ->115	0.66987				
Excited State 10:	Singlet-A	4.0932 eV	302.90 nm	f=0.0223	<S**2>=0.000
107 ->110	0.54795				
108 ->111	0.16006				
108 ->112	0.16112				
108 ->113	0.35427				

109: HOMO; 110: LUMO

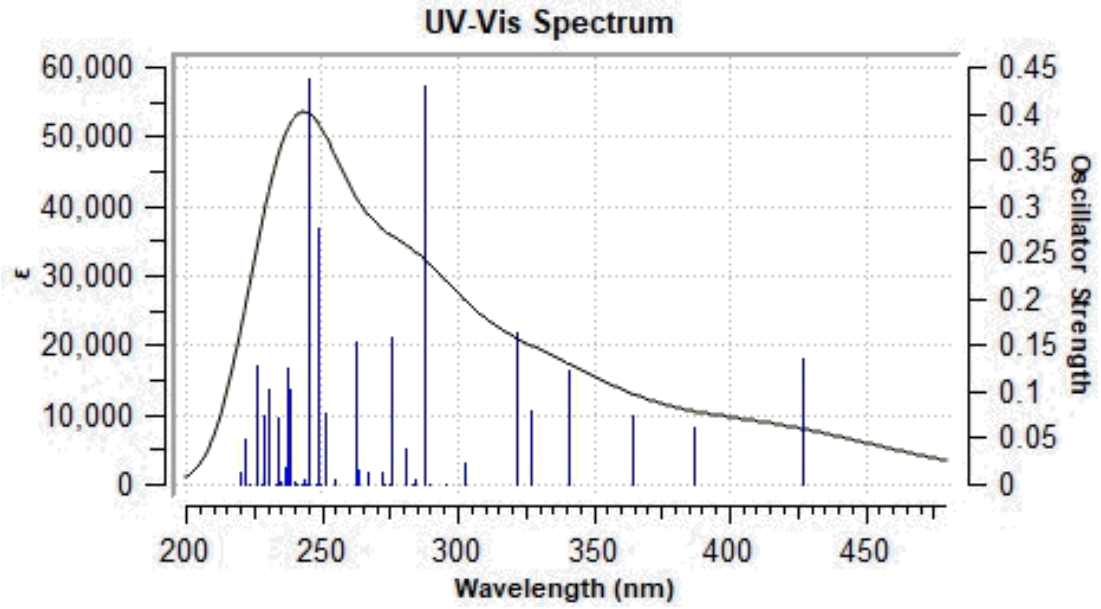


Figure S68. Simulated UV-visible absorption spectrum of **7**.

Table S11. TD-DFT calculated first ten excited states of compound **7** in dichloromethane at B3LYP/6-311G+(d,p) level and the corresponding contributions.

Excited State 1:	Singlet-A	2.9028 eV	427.11 nm	f=0.1348	<S**2>=0.000
115 ->116	0.69441				
Excited State 2:	Singlet-A	3.2014 eV	387.28 nm	f=0.0610	<S**2>=0.000
115 ->117	0.65394				
115 ->118	0.23284				
Excited State 3:	Singlet-A	3.4012 eV	364.53 nm	f=0.0741	<S**2>=0.000
113 ->116	0.11601				
114 ->116	-0.21292				
115 ->117	-0.19813				
115 ->118	0.62126				

Excited State 4:	Singlet-A	3.6414 eV	340.48 nm	f=0.1229	<S**2>=0.000
114 ->116	0.62331				
114 ->117	0.11568				
114 ->118	0.13441				
115 ->118	0.16976				
115 ->119	-0.19484				
Excited State 5:	Singlet-A	3.7930 eV	326.87 nm	f=0.0785	<S**2>=0.000
114 ->117	0.31732				
115 ->119	0.59941				
Excited State 6:	Singlet-A	3.8539 eV	321.71 nm	f=0.1637	<S**2>=0.000
113 ->116	0.18509				
114 ->116	-0.15881				
114 ->117	0.56943				
115 ->119	-0.27709				
Excited State 7:	Singlet-A	4.0988 eV	302.49 nm	f=0.0221	<S**2>=0.000
113 ->116	0.49828				
114 ->116	0.15267				
114 ->118	-0.44897				
Excited State 8:	Singlet-A	4.1966 eV	295.44 nm	f=0.0000	<S**2>=0.000
112 ->116	0.69490				
Excited State 9:	Singlet-A	4.2845 eV	289.38 nm	f=0.0000	<S**2>=0.000
115 ->120	0.68335				
Excited State 10:	Singlet-A	4.3070 eV	287.87 nm	f=0.4290	<S**2>=0.000
113 ->116	0.39753				
114 ->117	-0.19574				
114 ->118	0.46522				
115 ->121	0.12044				
115 ->123	0.15255				

115: HOMO; 116: LUMO

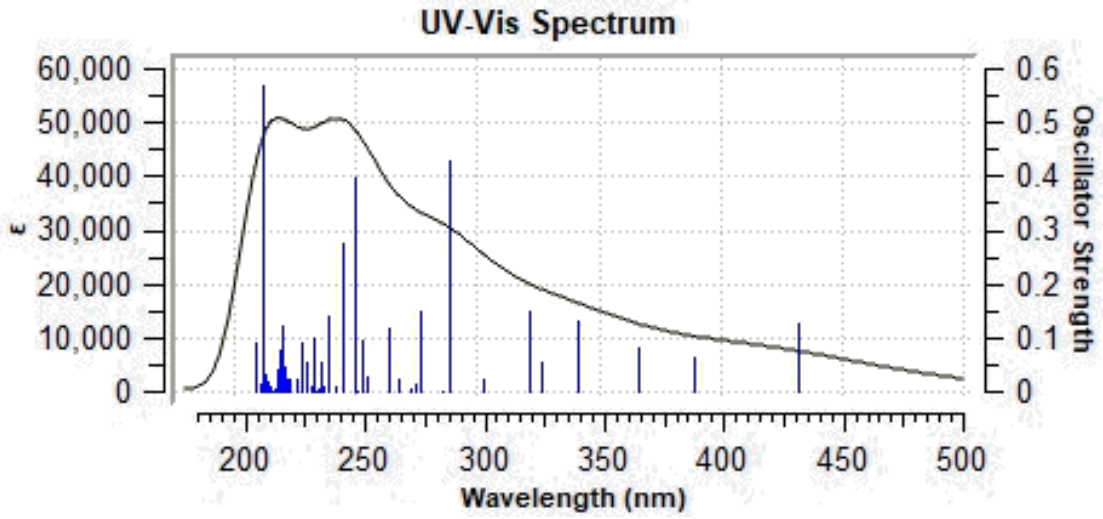


Figure S69. Simulated UV-visible absorption spectrum of **8**.

Table S12. TD-DFT calculated first ten excited states of compound **8** in dichloromethane at B3LYP/6-311G+(d,p) level and the corresponding contributions.

Excited State 1:	Singlet-A	2.8716 eV	431.76 nm	f=0.1247	<S**2>=0.000
115 ->116	0.69496				
Excited State 2:	Singlet-A	3.1868 eV	389.06 nm	f=0.0620	<S**2>=0.000
115 ->117	0.64992				
115 ->118	0.24493				
Excited State 3:	Singlet-A	3.3820 eV	366.60 nm	f=0.0826	<S**2>=0.000
113 ->116	-0.11695				
114 ->116	-0.21222				
115 ->117	-0.21124				
115 ->118	0.61747				
Excited State 4:	Singlet-A	3.6313 eV	341.43 nm	f=0.1313	<S**2>=0.000
114 ->116	0.63151				
114 ->117	0.11271				
114 ->118	0.13913				
115 ->118	0.17335				
115 ->119	0.15840				
Excited State 5:	Singlet-A	3.8001 eV	326.26 nm	f=0.0549	<S**2>=0.000
114 ->117	-0.33124				
115 ->119	0.59879				
Excited State 6:	Singlet-A	3.8563 eV	321.51 nm	f=0.1485	<S**2>=0.000
113 ->116	-0.18637				

114 ->116	-0.14338				
114 ->117	0.56210				
115 ->119	0.29851				
Excited State 7:	Singlet-A	4.0957 eV	302.72 nm	f=0.0232	<S**2>=0.000
113 ->116	0.49496				
114 ->116	-0.15212				
114 ->118	0.45363				
Excited State 8:	Singlet-A	4.2912 eV	288.92 nm	f=0.4302	<S**2>=0.000
113 ->116	-0.40424				
114 ->117	-0.19580				
114 ->118	0.46508				
115 ->120	-0.15854				
Excited State 9:	Singlet-A	4.3425 eV	285.51 nm	f=0.0001	<S**2>=0.000
114 ->121	0.17312				
115 ->120	0.15861				
115 ->121	0.63028				
115 ->122	-0.12976				
Excited State 10:	Singlet-A	4.4775 eV	276.90 nm	f=0.1510	<S**2>=0.000
113 ->117	0.46336				
113 ->118	0.15518				
115 ->120	-0.44841				
115 ->124	0.14499				

115: HOMO; 116: LUMO

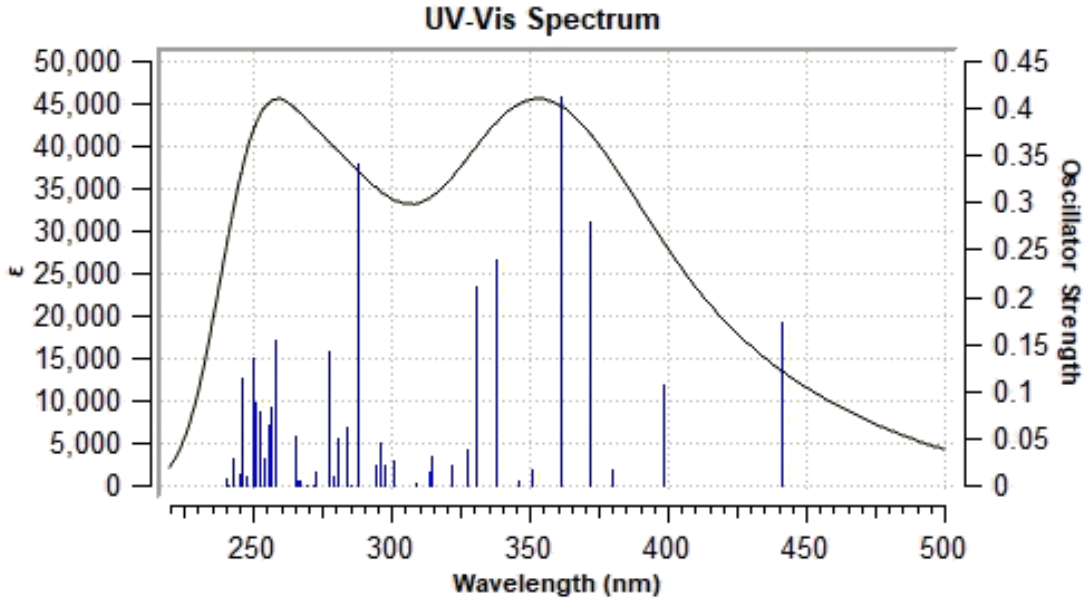


Figure S70. Simulated UV-visible absorption spectrum of **9**.

Table S13. TD-DFT calculated first ten excited states of compound **9** in dichloromethane at B3LYP/6-311G+(d,p) level and the corresponding contributions.

Excited State 1:	Singlet-A	2.8115 eV	440.98 nm	f=0.1727	<S**2>=0.000
146 -> 148	-0.10889				
147 -> 148	0.68764				
Excited State 2:	Singlet-A	3.1123 eV	398.36 nm	f=0.1065	<S**2>=0.000
146 -> 149	-0.13317				
147 -> 149	0.65064				
147 -> 150	0.16907				
Excited State 3:	Singlet-A	3.2661 eV	379.61 nm	f=0.0159	<S**2>=0.000
146 -> 148	0.65892				
147 -> 148	0.10738				
147 -> 151	-0.17253				
Excited State 4:	Singlet-A	3.3328 eV	372.01 nm	f=0.2798	<S**2>=0.000
145 -> 148	0.13234				
146 -> 151	-0.12340				
147 -> 149	-0.18061				
147 -> 150	0.62053				
Excited State 5:	Singlet-A	3.4309 eV	361.38 nm	f=0.4126	<S**2>=0.000
146 -> 148	0.16180				
146 -> 149	-0.10724				
146 -> 150	-0.12079				
147 -> 150	-0.17906				
147 -> 151	0.62204				
Excited State 6:	Singlet-A	3.5345 eV	350.78 nm	f=0.0174	<S**2>=0.000
146 -> 149	0.25521				
146 -> 152	0.28855				
147 -> 152	0.57159				
Excited State 7:	Singlet-A	3.5854 eV	345.81 nm	f=0.0045	<S**2>=0.000
145 -> 148	0.19887				
145 -> 149	-0.13958				
146 -> 149	0.57303				
146 -> 152	-0.12453				
147 -> 149	0.12325				
147 -> 152	-0.24518				
Excited State 8:	Singlet-A	3.6679 eV	338.02 nm	f=0.2393	<S**2>=0.000

145 -> 148	0.60070				
146 -> 149	-0.19770				
146 -> 150	-0.11813				
146 -> 151	0.14743				
147 -> 150	-0.11069				
147 -> 154	0.13150				
Excited State 9:	Singlet-A	3.7545 eV	330.23 nm	f=0.2097	<S**2>=0.000
146 -> 153	0.32279				
147 -> 153	0.62126				
Excited State 10:	Singlet-A	3.7921 eV	326.95 nm	f=0.0390	<S**2>=0.000
145 -> 148	0.13951				
145 -> 149	-0.16182				
146 -> 149	-0.13185				
146 -> 150	0.56690				
146 -> 151	-0.22341				
147 -> 154	-0.18103				

147: HOMO; 148: LUMO

7-4. Cartesian coordinates for theoretically optimized structures

1

C	-0.10429028	4.09351471	-0.00001223
C	1.04198496	3.30521847	-0.00000810
C	0.95596674	1.90425438	0.00000278
C	-0.35467409	1.33577140	0.00000870
C	-1.51662334	2.12586487	0.00000396
C	-1.37838984	3.51330330	-0.00000698
N	-0.49738751	-0.04821913	0.00001404
C	-1.63573727	-0.82939452	0.00000447
C	-2.93143127	-0.33906207	0.00000038
S	-3.19241931	1.43961096	0.00001486
C	-1.26993573	-2.20551858	-0.00000471
C	-2.32618526	-3.13272756	-0.00001631
C	-3.63821926	-2.65969256	-0.00002014
C	-3.95547652	-1.28384968	-0.00001242
C	2.13048733	0.99871811	0.00000198
C	0.56882519	-0.89331020	0.00001090
C	1.84817683	-0.40298626	0.00000840
C	2.90509173	-1.30635377	0.00000425
C	2.61589446	-2.69735546	0.00000464
C	1.28918421	-3.15222737	0.00001266

C	0.19994812	-2.23955410	0.00000997
C	3.48978134	1.17947948	-0.00000592
S	4.38755625	-0.34866346	-0.00000868
H	-0.01439718	5.17564683	-0.00002242
H	2.02124511	3.77483043	-0.00001419
H	-2.26250830	4.14452342	-0.00001136
H	-2.13202233	-4.20118365	-0.00002162
H	-4.45616247	-3.37455534	-0.00002847
H	-4.99542548	-0.97087839	-0.00001590
H	3.42058445	-3.42572388	-0.00000028
H	1.11212412	-4.22409261	0.00001377
H	4.05981533	2.09925165	-0.00001441

2

C	-0.10107562	4.06805195	0.00045302
C	-1.21079641	3.23279063	0.00040059
C	-1.06769192	1.83299695	0.00008389
C	0.25986554	1.32760420	-0.00003176
C	1.39168620	2.16406254	0.00001816
C	1.19722092	3.54272851	0.00022970
N	0.43673217	-0.04633581	0.00004927
C	1.61170149	-0.77069295	-0.00046466
C	2.88987657	-0.23080760	-0.00023369
S	3.09025667	1.55107890	-0.00034341
C	1.30838339	-2.15730722	-0.00021873
C	2.40006100	-3.04580762	0.00005011
C	3.68990217	-2.52198448	0.00006792
C	3.94999683	-1.13287084	-0.00004375
C	-3.56102060	1.25285682	-0.00058353
C	-4.56443653	0.26163117	-0.00055091
C	-4.26949916	-1.09379455	-0.00013270
C	-2.92300720	-1.52651453	0.00021185
C	-1.93091541	-0.50420995	0.00035682
C	-2.21544670	0.89330515	-0.00003470
C	-2.48659140	-2.89592756	0.00020304
C	-1.15193965	-3.25792489	0.00014116
C	-0.14617404	-2.25270200	0.00037680
C	-0.60495824	-0.93245741	0.00052318
H	-0.23754920	5.14536606	0.00069910
H	-2.20368741	3.66965268	0.00067735
H	2.05434770	4.21013378	0.00029669
H	2.24580935	-4.12074870	0.00019583

H	4.53695055	-3.20224266	0.00022206
H	4.97605829	-0.77707842	0.00011039
H	-3.85951596	2.29638302	-0.00112537
H	-5.60436956	0.57747615	-0.00090861
H	-5.07158379	-1.82753963	-0.00013607
H	-3.24728003	-3.67218885	0.00015499
H	-0.88125926	-4.31028301	0.00003236

3

C	-3.28846613	0.41763316	0.00007389
C	-1.93028702	0.78708263	0.00001463
N	-0.95670383	-0.19954667	-0.00008083
C	-1.12185922	-1.56909207	-0.00004384
C	-2.34011806	-2.23489969	-0.00005806
S	-3.86210996	-1.29100874	-0.00008815
C	-4.25063623	1.42435852	0.00021931
C	-3.86024915	2.76864172	0.00028784
C	-2.51718867	3.12148083	0.00020201
C	-1.50796480	2.14083906	0.00004980
C	0.15444477	-2.19230448	-0.00003083
C	0.16384252	-3.60297589	-0.00008698
C	-1.04842945	-4.28521479	-0.00010044
C	-2.29718637	-3.62535314	-0.00007370
C	0.38792929	0.06301662	-0.00004601
C	0.87153670	1.38231649	-0.00005269
C	2.28137271	1.54733185	-0.00009010
C	3.13396835	0.34787444	-0.00000477
C	2.56462878	-0.97556699	0.00002641
C	1.12904249	-1.11025937	-0.00004081
C	-0.06080161	2.45840476	-0.00005073
C	0.46749679	3.75044706	-0.00016285
C	1.85548131	3.94275577	-0.00025305
C	2.74881918	2.87625234	-0.00021455
C	4.54099423	0.45839897	0.00009094
C	5.36613295	-0.65383305	0.00019576
C	4.80473440	-1.93975575	0.00022379
C	3.42967667	-2.09129455	0.00014494
H	-5.30519428	1.16351774	0.00027968
H	-4.62129292	3.54322597	0.00040943
H	-2.24627797	4.17159508	0.00026997
H	1.09356080	-4.16157677	-0.00012402
H	-1.04178935	-5.3716383	-0.00013387

H	-3.21511879	-4.20558418	-0.00007481
H	-0.1830688	4.61879051	-0.00019652
H	2.24503564	4.9571634	-0.00036060
H	3.812113	3.08937919	-0.00030610
H	4.99920152	1.44188082	0.00010566
H	6.44512335	-0.52737823	0.00026518
H	5.44676348	-2.8165713	0.00032084
H	3.00014391	-3.08754422	0.00020185

4

C	-1.91712439	4.09943872	0.00070095
C	-0.64878572	3.53252599	0.00073448
C	-0.47439949	2.13703071	0.00032541
C	-1.65606319	1.34653151	0.00007764
C	-2.94542575	1.90996560	0.00001399
C	-3.06479137	3.29727817	0.00030045
N	-1.52598976	-0.03393969	0.00020233
C	-2.51129291	-1.00329801	-0.00049609
C	-3.87602780	-0.75867517	-0.00044724
S	-4.46641258	0.93431569	-0.00067575
C	-1.91244561	-2.28823694	-0.00026584
C	-2.77705836	-3.39525897	-0.00008451
C	-4.15289419	-3.17083440	-0.00022264
C	-4.71078143	-1.87448449	-0.00038016
C	5.73088499	-0.11144540	-0.00049741
C	4.51245160	-0.80503803	-0.00003349
C	3.29849313	-0.05453407	0.00012758
C	3.31563879	1.38015494	-0.00030762
C	4.56977311	2.02342299	-0.00079277
C	5.75033670	1.28605929	-0.00085544
C	4.41790054	-2.24341182	0.00018370
C	3.21683197	-2.88978864	0.00038062
C	1.96931907	-2.17240022	0.00048171
C	2.05409747	-0.73418217	0.00054087
C	0.87522901	0.04139987	0.00071080
C	0.85919568	1.48069235	0.00025451
C	2.08207165	2.11569705	-0.00034083
C	0.71632581	-2.82108838	0.00035250
C	-0.46441439	-2.06387076	0.00052121
C	-0.31319077	-0.66184180	0.00076751
H	-2.02455625	5.17999840	0.00103769

H	0.22208629	4.17940274	0.00116142
H	-4.0495686	3.75586824	0.00028684
H	-2.38772671	-4.40899159	0.00008395
H	-4.82826313	-4.02155916	-0.00014754
H	-5.79004912	-1.75309680	-0.00036553
H	6.66385332	-0.66962676	-0.00060956
H	4.60723225	3.11006096	-0.00112941
H	6.70451387	1.80652838	-0.00121648
H	5.34227367	-2.81607219	0.00014267
H	3.18570933	-3.97700039	0.00047776
H	2.14978774	3.19994370	-0.00096345
H	0.6861123	-3.90777617	0.00013810

5

C	-3.46501525	3.36269828	-0.00002626
C	-2.07718198	3.42082021	-0.00003500
C	-1.30074905	2.24778071	-0.00001392
C	-2.00752473	1.01595966	-0.00001171
C	-3.41235772	0.94417204	0.00001440
C	-4.13599274	2.13386385	0.00000541
N	-1.27143620	-0.15662636	0.00002377
C	-1.72012153	-1.46333406	-0.00005677
C	-3.05099278	-1.85615511	0.00001771
S	-4.33647742	-0.60652271	0.00005098
C	-0.60692708	-2.34198710	-0.00007055
C	-0.88558843	-3.72179075	-0.00005576
C	-2.21438789	-4.13465424	-0.00001214
C	-3.29712067	-3.22579354	0.00002843
C	0.18231815	2.24921819	-0.00000353
C	0.09448291	-0.18009039	0.00000825
C	0.98776636	3.38491089	-0.00001359
C	2.39034649	3.26130800	-0.00000101
C	3.03059177	2.03106358	0.00001831
C	2.27173087	0.83964775	0.00000939
C	0.85274873	0.98940412	0.00001033
C	2.78205472	-0.50802555	0.00000405
C	1.98664957	-1.63691030	-0.00002470
C	0.57528283	-1.49129170	-0.00002931
Br	4.68528887	-0.75860651	0.00001638
H	-4.04223227	4.28244152	-0.00005902
H	-1.58755064	4.38863102	-0.00004992

H	-5.22194143	2.10674517	0.00003290
H	-0.08383300	-4.45411890	-0.00006646
H	-2.43819601	-5.19765924	-0.00000536
H	-4.31542223	-3.60310935	0.00008679
H	0.55064766	4.37810948	-0.00004196
H	2.99182606	4.16627051	-0.00001292
H	4.11336140	1.97623135	0.00003265
H	2.45184662	-2.61645289	-0.00004438

6

C	-4.67646552	-3.00508879	-0.02521255
C	-3.30514233	-3.22301626	-0.05368667
C	-2.39807635	-2.14709852	-0.04084520
C	-2.95725678	-0.84353226	0.00492324
C	-4.34461528	-0.60936010	0.03256545
C	-5.20087350	-1.70705471	0.01628558
N	-2.08915105	0.23565735	0.01816048
C	-2.38466601	1.58489210	0.03949130
C	-3.66085124	2.12859272	0.06982989
S	-5.08217231	1.03695699	0.09250760
C	-1.17809838	2.33018948	0.02394620
C	-1.29497089	3.73219588	0.04307211
C	-2.56765847	4.29595685	0.07345935
C	-3.74709014	3.51802881	0.08635297
C	-0.73028166	0.10083280	-0.01159956
C	-0.92522992	-2.31879211	-0.07533083
C	-0.26099149	-3.54022749	-0.14467364
C	1.14473582	-3.57825760	-0.20019036
C	1.92334677	-2.43007039	-0.17158394
C	1.31696940	-1.15433525	-0.07553089
C	-0.11017797	-1.14653621	-0.04778787
C	2.01462612	0.12188733	-0.04663803
C	1.31394136	1.32569895	-0.02992252
C	-0.10100498	1.34809861	-0.01100037
C	3.50083968	0.18011119	-0.02351360
C	4.19547408	0.99066627	-0.93959170
C	5.58118784	1.09780003	-0.90482098
C	6.31589800	0.38474195	0.05661570
C	5.63730761	-0.42870486	0.98013041
C	4.25149753	-0.52469120	0.93631074
C	7.74481549	0.48587417	0.09623953

N	8.90519239	0.56782466	0.12870691
H	-5.35641916	-3.85161987	-0.03584570
H	-2.93113220	-4.24054743	-0.08591870
H	-6.27627681	-1.55510249	0.03619438
H	-0.41447484	4.36761121	0.03457491
H	-2.66659299	5.37761144	0.08826925
H	-4.71535937	4.00913521	0.11000556
H	-0.81127807	-4.47507793	-0.17035677
H	1.63628317	-4.54452062	-0.27526612
H	3.00207729	-2.51622953	-0.23820695
H	1.87590178	2.25488471	0.00251172
H	3.63596641	1.52979106	-1.69828590
H	6.10212558	1.72293546	-1.62311065
H	6.20132367	-0.97067218	1.73265888
H	3.73719045	-1.13669299	1.67082036

7

C	-4.67356517	-3.09964495	0.00011433
C	-3.29638976	-3.28021031	0.00008849
C	-2.41843232	-2.18043735	0.00001078
C	-3.01322758	-0.89094062	-0.00002905
C	-4.40690479	-0.69518307	-0.00004733
C	-5.23323546	-1.81566082	0.00004869
N	-2.17692640	0.21252207	-0.00005673
C	-2.50705853	1.55249352	-0.00000515
C	-3.79713265	2.06332949	-0.00003850
S	-5.18909618	0.93257163	-0.00030831
C	-1.31872067	2.32870187	0.00013464
C	-1.47408373	3.72759155	0.00025352
C	-2.76124017	4.25815117	0.00021521
C	-3.92061834	3.44982042	0.00008236
C	-0.81267251	0.11465951	0.00011971
C	-0.94067935	-2.31288191	-0.00002603
C	-0.23666319	-3.51438290	-0.00012728
C	1.17243284	-3.51192408	-0.00014371
C	1.91512714	-2.33972440	-0.00007622
C	1.26324310	-1.08314676	0.00000984
C	-0.16202146	-1.11688580	0.00004169
C	1.93139033	0.20466605	0.00006098
C	1.20544877	1.38874366	0.00015925
C	-0.21510772	1.37595687	0.00022536

C	3.43116642	0.26042937	0.00001263
C	4.13927969	0.29273646	-1.22021279
C	5.53633313	0.36138297	-1.19764894
C	6.25556344	0.39423859	-0.00005632
C	5.53640579	0.36114400	1.19756452
C	4.13934697	0.29247850	1.22019966
C	3.41160363	0.26087476	-2.54624638
C	3.41175442	0.26028092	2.54626789
C	7.76630373	0.43666812	-0.00012502
H	-5.33020632	-3.96455119	0.00018970
H	-2.89380203	-4.28743955	0.00014372
H	-6.31254170	-1.69236289	0.00007970
H	-0.61043330	4.38591891	0.00036241
H	-2.88849376	5.33706170	0.00030230
H	-4.90171355	3.91550060	0.00008213
H	-0.75757511	-4.46656755	-0.00019115
H	1.69284587	-4.46611151	-0.00021025
H	2.99973262	-2.38108382	-0.00010462
H	1.74668472	2.33138214	0.00022946
H	6.07580997	0.39113780	-2.14270224
H	6.07594539	0.39071874	2.14258571
H	2.77738873	-0.62880604	-2.63693794
H	2.75251899	1.12845501	-2.66764832
H	4.12045022	0.25653277	-3.38014514
H	4.12064664	0.25579607	3.38012673
H	2.75261636	1.12778926	2.66789112
H	2.77760640	-0.62946579	2.63679974
H	8.15314469	0.95254905	-0.88561375
H	8.15329174	0.94985698	0.88685273
H	8.19423128	-0.57506021	-0.00172299

8

C	-5.20790878	-3.11522408	0.86007528
C	-3.88357840	-3.27413538	0.47291225
C	-3.07252162	-2.16186386	0.18021503
C	-3.67723404	-0.88320897	0.30340852
C	-5.01808142	-0.70921042	0.69446789
C	-5.77941726	-1.84122326	0.97161284
N	-2.90580826	0.23085082	0.02278468
C	-3.26191827	1.56354517	0.05434837
C	-4.51234906	2.05456588	0.40156622

S	-5.80970425	0.90521263	0.86229812
C	-2.14756978	2.35600269	-0.32653865
C	-2.33830648	3.75041858	-0.34834166
C	-3.58656745	4.26113783	-0.00313457
C	-4.67256957	3.43688824	0.36958538
C	-1.59665159	0.15351345	-0.36797991
C	-1.65399586	-2.27157565	-0.24098791
C	-0.95268363	-3.46349622	-0.40219070
C	0.39369216	-3.44204758	-0.81389581
C	1.07452118	-2.26066201	-1.07111993
C	0.42535189	-1.01000138	-0.92655733
C	-0.93813116	-1.06600212	-0.50943522
C	1.02812635	0.28661823	-1.17486497
C	0.29395603	1.45346014	-1.01670222
C	-1.06300188	1.42107219	-0.59970905
C	10.84936241	0.17956540	1.78390746
C	9.86471553	0.28557933	0.61487100
C	8.39606197	0.20100402	1.05018807
C	7.40317310	0.30743197	-0.11434621
C	5.93454658	0.22262241	0.32139797
C	4.94231774	0.33293830	-0.84366414
C	3.47468536	0.24659725	-0.40647515
C	2.48504228	0.37934384	-1.58323683
H	-5.81335964	-3.98941166	1.08026854
H	-3.47063372	-4.27415859	0.39552715
H	-6.81715274	-1.73484387	1.27480321
H	-1.53118147	4.42065111	-0.62885477
H	-3.74073697	5.33645177	-0.01845013
H	-5.62608572	3.88716182	0.62937054
H	-1.42813847	-4.42142378	-0.21740951
H	0.91532585	-4.38799774	-0.93395644
H	2.11165540	-2.30537662	-1.38650139
H	0.77755880	2.40623294	-1.21974917
H	11.88823943	0.24342964	1.44035780
H	10.68908541	0.98491446	2.51142135
H	10.73241212	-0.77288883	2.31563335
H	10.07295439	-0.51194028	-0.11265939
H	10.03002669	1.23277234	0.08177740
H	8.18821966	0.99846122	1.77932467
H	8.23074821	-0.74699225	1.58385191
H	7.61215990	-0.48974068	-0.84339243
H	7.56933396	1.25565241	-0.64715901
H	5.72580595	1.01839658	1.05169753
H	5.76726111	-0.72637961	0.85219796

H	5.15190141	-0.46160097	-1.57570971
H	5.10874855	1.28283357	-1.37356607
H	3.25927387	1.03696939	0.32571950
H	3.30119058	-0.70413612	0.11550565
H	2.71885733	-0.38425343	-2.33790183
H	2.65405798	1.34593549	-2.07466549

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C	-7.17686023	-2.87098027	-0.16495042
C	-5.81475392	-3.13843902	-0.21404112
C	-4.86676157	-2.10037621	-0.14974559
C	-5.37555855	-0.78065124	-0.03039444
C	-6.75302662	-0.49649776	0.01888071
C	-7.65107137	-1.55808905	-0.05050290
N	-4.46757934	0.26224951	0.03596084
C	-4.70972098	1.61765260	0.13396953
C	-5.96327365	2.20861467	0.20191140
S	-7.42607171	1.17203603	0.17151949
C	-3.47406772	2.31489817	0.15346569
C	-3.53695865	3.71738520	0.25109672
C	-4.78628626	4.32798894	0.31990087
C	-5.99560712	3.59710062	0.29630120
C	-3.11317728	0.07736241	-0.00843570
C	-3.40121794	-2.32601858	-0.20333436
C	-2.78462504	-3.56592783	-0.34391300
C	-1.38101365	-3.65395973	-0.40937653
C	-0.55959270	-2.53928390	-0.32223129
C	-1.11614131	-1.24811992	-0.15373847
C	-2.54185683	-1.18866709	-0.11655451
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C	-1.02077706	1.21960437	0.03468205
C	-2.43577658	1.29577377	0.05861730
C	1.12308186	-0.01051946	-0.05294233
C	1.84543064	0.80948606	-0.93618663
C	3.23639921	0.85040297	-0.92277938
C	3.96389255	0.07560290	-0.00554781
C	3.25337105	-0.74058339	0.88993450
C	1.86319557	-0.78496933	0.85798283
N	5.38276796	0.11601853	0.01791279
C	6.12616362	-1.08172274	0.20474455
C	6.06305256	1.35382720	-0.14738526

C	7.20980067	1.43483533	-0.95400252
C	7.87911358	2.64777477	-1.10510271
C	7.41064196	3.80184831	-0.47357030
C	6.26541793	3.72625967	0.32207639
C	5.59984160	2.51408423	0.49417131
C	7.24743856	-1.10026966	1.05011878
C	7.97869728	-2.27390491	1.22277117
C	7.59818259	-3.45067150	0.57414488
C	6.47852560	-3.43745967	-0.26039916
C	5.75172044	-2.26427416	-0.45380558
H	-7.88858665	-3.68953866	-0.21637633
H	-5.47971201	-4.16620255	-0.30295270
H	-8.71976297	-1.36639808	-0.01523130
H	-2.63211953	4.31743221	0.27266396
H	-4.84261524	5.41029560	0.39515007
H	-6.94396149	4.12326465	0.35276667
H	-3.37049392	-4.47647852	-0.41771799
H	-0.92712512	-4.63288958	-0.53956146
H	0.51537192	-2.65918144	-0.39575251
H	-0.42263014	2.12267585	0.11694716
H	1.30434818	1.40440341	-1.66720652
H	3.76708783	1.47866472	-1.63108145
H	3.79724479	-1.33218251	1.61952117
H	1.33938306	-1.40553529	1.57968375
H	7.57041809	0.54403109	-1.45841268
H	8.76496847	2.69151842	-1.73344789
H	7.93091104	4.74705208	-0.59957870
H	5.89263050	4.61387711	0.82671402
H	4.71870213	2.45808706	1.12542419
H	7.53945862	-0.19198432	1.56757120
H	8.84355113	-2.26950275	1.88115718
H	8.16651763	-4.36532869	0.71686103
H	6.17429499	-4.34313387	-0.77878265
H	4.89126152	-2.25585571	-1.11531579

8. Biological Experiments

MTT assay *in vitro*. HeLa, HepG2, MCF-7, PC-3, A549, and HUVEC cells were maintained at 37°C in a 5% CO_2 humidified atmosphere. Cells were seeded into 96-well plates at a density of 1×10^4 cells per well and allowed to adhere for 24 h. Following incubation, the medium was aspirated and replaced with fresh medium containing serial dilutions of the test compound (EA) for 48 h. Subsequently, the compound-containing medium was removed, and cells were incubated with MTT solution (1 mg/mL in culture medium) for 4 h at 37°C. The formazan crystals were dissolved in DMSO, and absorbance was measured at 595 nm using a microplate reader. Cell viability was calculated as follows:

Cell viability (%) = Absorbance of the experimental group/ Absorbance of the blank control group× 100%.[6-8] All experiments included triplicate wells per concentration and were performed in at least three independent biological replicates.

***In vivo* experiment**. The *in vivo* experiment was performed by Nanjing KeyGEN BioTECH Co., Ltd, China. Female BALB/c nude mice (5-6 weeks old) were used. Cultured HeLa cells were harvested and resuspended in PBS at a density of 1×10^7 cells/mL. A volume of 0.1 mL (containing 1×10^6 cells) was subcutaneously inoculated into the right flank of each mouse. When the average tumor volume reached approximately 100 mm^3, tumor-bearing mice were randomly assigned into two groups (n = 5 per group): (1) Control Group: Received intravenous injections of PBS. (2) Treatment Group: Received injections of compound **3a** at a dose of 1.0 mg/kg body weight (in a volume of 100 μL per 10 g body weight). Treatments were administered once daily. Body weight and tumor volume were recorded every 3 days for a total observation period of 21 days. Tumor volume (V) was calculated using the formula: V (mm^3) = (Length × $Width^2$) / 2. At the experimental endpoint (day 21), mice were euthanized, and tumors were surgically excised and weighed. Tumor tissues and major organs (heart, kidneys, liver, lungs, spleen) were fixed, paraffin-embedded, sectioned, and stained with hematoxylin and eosin (H&E). Histopathological evaluation was performed by a certified pathologist. The tumor growth inhibition rate (TGI%) was calculated as follows: Inhibition efficiency (%) = (1 - The weight of the experimental group/The weight of the control group) ×100%.[6,8]

Confocal fluorescence images. After 24-hour drug treatment in confocal dishes, wash the HeLa cells twice with serum-free cell culture medium. Staining solutions were added the staining solutions to the cells and incubate at 37°C in a cell culture incubator for 30 minutes, with 0.5 μM of Mitochondrial probe (MitoTracker Deep Red) and 1 μM of Endoplasmic reticulum probe (ER-Tracker Red). Cells were washed three times with serum-free cell culture medium to thoroughly remove uninternalized probes. Diluted Hoechst 33342 nuclear dye was added and incubated for 15 minutes. Cells were washed three times with PBS, then 1 mL of fresh culture medium were added. Finally, stained cells were observed using a confocal laser scanning microscope at 600x magnification.

DNA binding modes. The binding mode of compound **3a** to herring sperm DNA (hsDNA) was evaluated by ethidium bromide (EB) fluorescence displacement assay. In this assay, 3 mL of DNA-EB mixture (CDNA / CEB = 5~10) was added to the sample cuvette. Successive additions of equivolume compound solutions were made to incrementally increase the compound-to-

DNA concentration ratio. Fluorescence emission spectra were recorded at 520 nm excitation wavelength.

Data analysis. Data are presented as mean ± standard deviation (SD). All analyses were performed using SPSS 17.0 (IBM, USA) software. The data obtained were managed statistically using one-way ANOVA at a 0.05% level of reliability. Origin 2022 (OriginLab Crop., USA) was used to analyze the IC_{50} Value with linear fitting. All experiments were repeated at least three independent biological replicates.

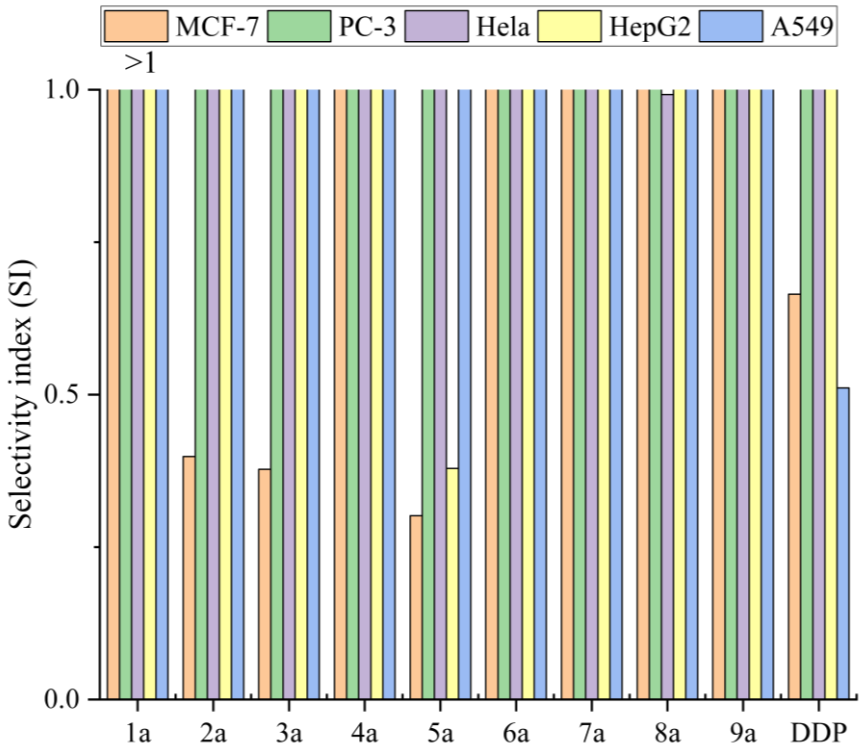

Figure S71. The selectivity index (SI) of compounds **1a-9a** and DDP. (SI = IC_{50} (HUVEC) / IC_{50} (cancer cell line)).

Animal ethics proof

Animal ethics proof of Nanjing Advanced Academy of Life and Health

COF-F009

Application Date: 03/03/2025	Acceptance Number: NAALH-W-2503002

Experiment Title	Efficacy test of the compound on human HepG2/HeLa cell transplanted tumor in nude mice			
Experiment Goal	To investigate the effect of the compound on human HepG2/HeLa cell transplanted tumor in nude mice			
Project Sources	Institute of Botany, Jiangsu Province and Chinese Academy of Sciences			
Project Leader	Fengyi Zhao	**Tel**	13701580481	
Experiment Leader	Jun Feng	**Tel**	19962096401	
Department	Research Reagents and Technical Services Department			
Animal Experimental Facility Use License No		SYXK(Su)2017-0040		
Experiment Time	20/03/2025-05/05/2025			
Animal Information	**Animal Origin**	SiPeiFu Biotechnology Co. LTD	**Fitness Certification**	□No ☑Yes
	Variety Strain	□Rat_____ ☑Mouse_BALB/C nude mice___ □Other_____	**Level**	□Clean ☑SPF □Other
Other Information	Animal Euthanasia Methods: CO_2 anesthesia			
	Audit result: Agreement Jun Feng Date: 06/03/2025			

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