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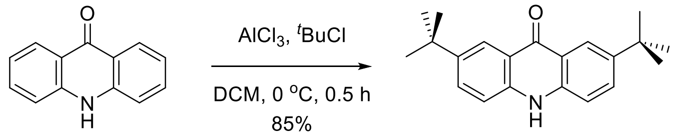
1. General remarks

All reagents and solvents were commercially available and were used without further purification unless otherwise noted. For thin layer chromatography Silica gel 60 F254 plates from Merck were used and examined under UV-light irradiation (254 nm and 365 nm). Flash column chromatography was performed on silica gel (particle size: 200-300 mesh). Melting points were measured with a MPA100 OptiMelt. IR-Spectra were recorded as KBr-pellets on a Bruker VERTEX 80V spectrometer. NMR spectra were taken on Bruker AVANCE III HD (600 MHz) and Bruker AVANCE NEO (400 MHz). Chemical shifts (δ) are reported in parts per million (ppm) relative to traces of $CHCl_3$ in the corresponding deuterated solvent. HRMS experiments were carried out on a ThermoFisher LTQ Orbitrap XL. 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. The chiral resolutions of aza[7]helicenes were performed on a Shimadzu LC-20AD equipped with a chiral column (Chiralpak IE-3). Circular Dichromism spectra were recorded on a Bio-Logic MOS-500. Crystal structure analysis was accomplished with a SuperNova, Dual, Cu at zero, AtlasS2 diffractometer. Cyclic voltammagrams were obtained using a glassy carbon working electrode, a platinum counter electrode, and a Ag reference electrode tested on CHI660E station. The mean-plane-deviation (MPD) values are average deviations of the core atoms from their mean-planes. The mean planes are defined by core carbon and nitrogen atoms (33 atoms for **2**, 34 atoms for **3** and 38 atoms for **4**). Acridone was synthesized according to the reported method. [S1]

2. Experimental section



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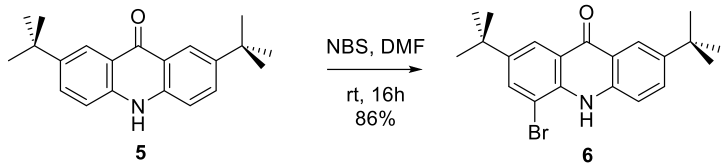
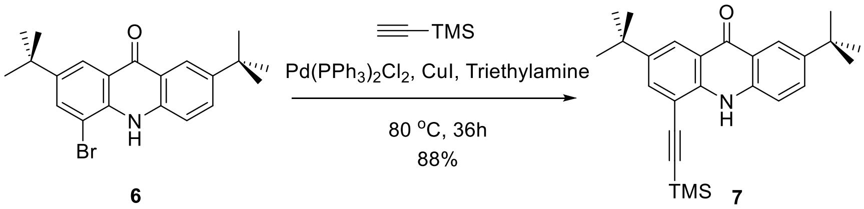
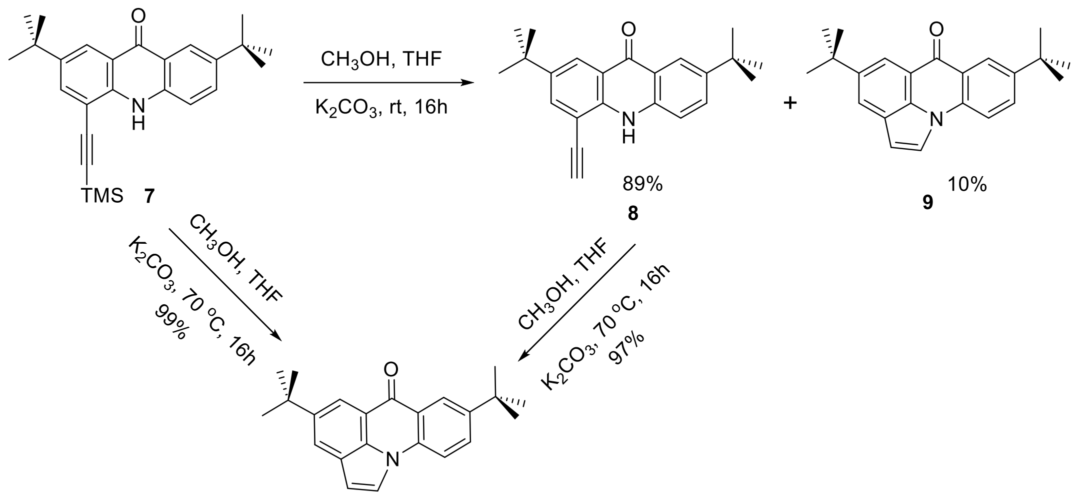
2,7-di-*tert*-butylacridone (5). The synthesis of acridone was carried out by a modified method.[S2] A 250 mL two-necked flask was charged with the powder of acridone (2.93 g, 15 mmol) and anhydrous dichloromethane (75 mL) under the protection of argon. The flask was cooled in an ice-bath and aluminum trichloride (4.00 g, 30 mmol) was added to the flask. ^{t}BuCl (7.25 mL) was added dropwise to the suspension and the mixture was stirred at 0 ºC for 0.5 h. The reaction mixture was quenched with water and diluted with dichloromethane (500 mL), then washed with water and dried over Na_2SO_4. The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane) to give the product **5** as yellow solid (3.92 g, 85%). ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 8.86 (br s, 1H), 8.49 (d, J = 2.3 Hz, 2H), 7.72 (dd, J = 8.7, 2.3 Hz, 2H), 7.36 (d, J = 8.7 Hz, 2H), 1.38 (s, 18H). Analytical data are in agreement with those published before.[S2]



4-bromo-2,7-di-*tert*-butylacridone (6). Acridone **5** (922 mg, 3 mmol), *N*-bromosuccinimide (588 mg, 3.3 mmol) and DMF (15 mL) were stirred at room temperature for 16 h. The reaction mixture was quenched with water and diluted with dichloromethane (200 mL), then washed with water (5×200 mL) and dried over Na_2SO_4. The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane) to give compound **6** as yellow solid (1.01 g, 86%). m.p. 206-209 ºC. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 8.46 (d, J = 2.1 Hz, 1H), 8.45 (d, J = 2.3 Hz, 1H), 8.40 (br s, 1H), 7.94 (d, J = 2.1 Hz, 1H), 7.77 (dd, J = 8.7, 2.3 Hz, 1H), 7.36 (d, J = 8.6 Hz, 1H), 1.41 (s, 9H), 1.40 (s, 9H). ^{13}CNMR (150 MHz, $CDCl_3$) δ (ppm) = 178.2, 145.5, 145.5, 138.1, 135.8, 134.4, 132.2, 123.1, 123.0, 122.3, 120.7, 116.7, 110.4, 35.0, 34.9, 31.5, 31.5. IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 3409, 3278, 2962, 2863, 1627, 1587, 1508, 1363, 1261, 1153, 894, 835, 647. HRMS(ESI) (*m/z*) : $[M+K]^+$ calcd. for $C_{21}H_{24}NOBrK$, 424.0673; found, 424.0694.



2,7-di-*tert*-butyl-4-trimethylsilylethynylacridone (7). A 120 mL screw capped glass vial was charged with **6** (733 mg, 2 mmol), CuI (4 mg, 0.02 mmol) and $Pd(PPh_3)_2Cl_2$ (30 mg, 0.04 mmol). Anhydrous triethylamine (10 mL) was added to the vial and the mixture was bubbled with argon for 3 minutes, followed by adding trimethylsilylacetylene (393 mg, 4 mmol). The vial was quickly sealed and heated at 80 ºC for 36 hours. After cooling down to room temperature, the reaction mixture was diluted with dichloromethane (250 mL) and washed with water (200 mL) and dried over Na_2SO_4. The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane) to give the product **7** as light yellow solid (710 mg, 88%). m.p. 240-242 ºC. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 8.52 (br s, 1H), 8.46 (d, J = 2.3 Hz, 1H), 8.45 (d, J = 2.2 Hz, 1H), 7.86 (d, J = 2.3 Hz, 1H), 7.75 (dd, J = 8.6, 2.3 Hz, 1H), 7.27-7.25 (m, 1H), 1.41 (s, 9H), 1.40 (s, 9H), 0.39 (s, 9H).^{13}CNMR (150 MHz, $CDCl_3$) δ (ppm) = 178.52, 145.22, 143.94, 138.82, 137.92, 134.36, 131.94, 124.36, 123.00, 121.14, 120.79, 116.52, 110.08, 103.02, 99.86, 34.88, 34.83, 31.54, 31.49, 0.22. IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 3401, 3264, 3181, 2962, 2871, 2154, 1627, 1581, 1504, 1459, 1315, 1261, 1172, 842, 761, 651. HRMS(ESI) (*m/z*) : $[M+H]^+$ calcd. for $C_{23}H_{33}NOSi$, 404.2404; found, 404.2424.

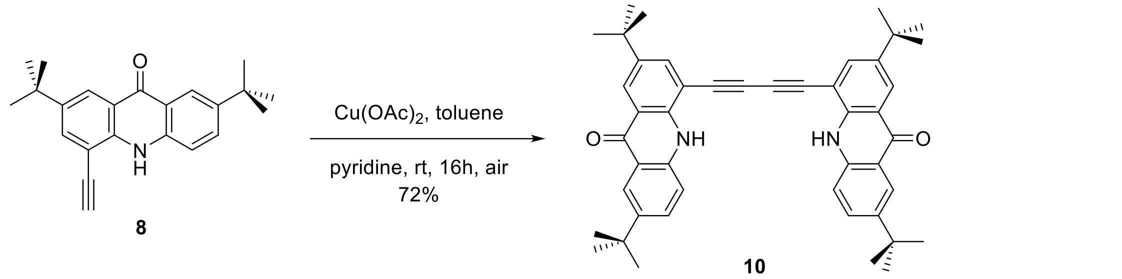


2,7-di-*tert*-butyl-4-ethynylacridone (8) and quinolone-fused indole (9). Compound **7** (2.26 g, 5.6 mmol), K_2CO_3 (3.10 g, 22.4 mmol), methanol (20 mL) and tetrahydrofuran (20 mL) was stirred at room temperature for 16 h. The reaction mixture was quenched with water and diluted with dichloromethane (200 mL), then washed with water (3×200 mL) and dried over Na_2SO_4. The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane) to give compound **8** (1.66 g, 89%) and **9** (181 mg, 10%) as yellow solids. Compound **8**: m.p. 130-132 ºC. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 8.60 (br s, 1H), 8.50 (d, J = 2.3 Hz, 1H), 8.45 (d, J = 2.2 Hz, 1H), 7.90 (d, J = 2.3 Hz, 1H), 7.74 (dd, J = 8.7, 2.3 Hz, 1H), 7.34 (d, J = 8.6 Hz, 1H), 3.66 (s, 1H), 1.40 (s, 9H), 1.39 (s, 9H). ^{13}CNMR (150 MHz, $CDCl_3$) δ (ppm) = 178.4, 145.3, 143.9, 139.1, 138.1, 135.0, 132.0, 124.7, 122.9, 121.1, 120.9, 116.6, 108.9, 85.0, 79.0, 34.9, 34.8, 31.5, 31.4. IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 3409, 3295, 2962, 2900, 2863, 1627, 1581, 1513, 1448, 1365, 1261, 1176, 896, 825, 603. HRMS(ESI) (*m/z*) : [M+K]$^+$ calcd. for $C_{23}H_{25}NOK$, 370.1568; found, 370.1585.

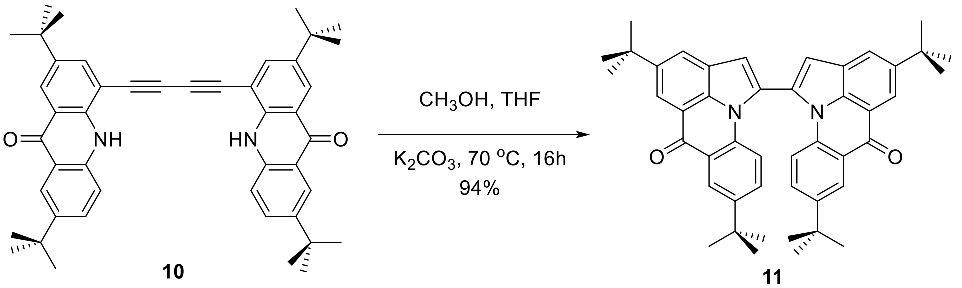
Compound **9**: m.p. 186-188 ºC. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 8.56 (d, J = 2.3 Hz, 1H), 8.39 (d, J = 1.5 Hz, 1H), 8.10 (d, J = 1.6 Hz, 1H), 7.88 (d, J = 3.4 Hz, 1H), 7.81 (dd, J = 8.6, 2.3 Hz, 1H), 7.70 (d, J = 8.6 Hz, 1H), 6.90 (d, J = 3.4 Hz, 1H), 1.49 (s, 9H), 1.44 (s, 9H). ^{13}CNMR (150 MHz, $CDCl_3$) δ (ppm) = 179.9, 146.9, 146.9, 135.8, 133.1, 131.6, 128.9, 125.0, 124.8, 124.6, 122.7, 119.7, 119.0, 114.1, 108.1, 35.5, 35.0, 32.2, 31.5. IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 2954, 2903, 2865, 1647, 1628, 1605, 1566, 1517, 1498, 1360, 1327, 1284, 1246, 1218, 1168, 1103, 886, 810, 719. HRMS(ESI) (*m/z*) : [M+H]$^+$ calcd. for $C_{23}H_{26}$, 332.2009; found, 332.2007.

Synthesis of **9** from **7**: The mixture of **7**, K_2CO_3 (83 mg, 0.6 mmol), methanol (0.6 mL), tetrahydrofuran (0.6 mL) was stirred at 70 ºC for 16 h. After cooling down to room temperature, the reaction mixture was diluted with dichloromethane (100 mL) and washed with water (100 mL). The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane) to give product **9** as yellow solid (50 mg, 99%).

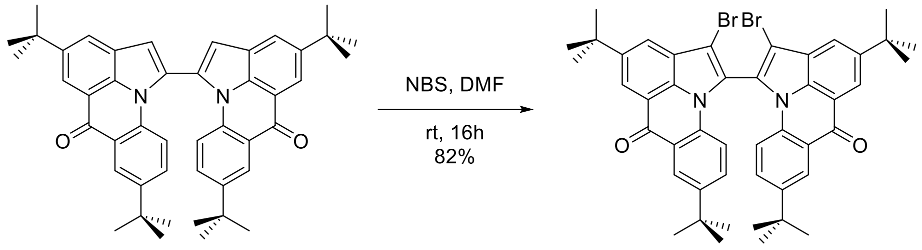
Synthesis of **9** from **8**: The mixture of **8** (33 mg, 0.1 mmol), K_2CO_3 (55 mg, 0.4 mmol), methanol (0.4 mL) and tetrahydrofuran (0.4 mL) was stirred at 70 ºC for 16 h. After cooling down to room temperature, the reaction mixture was diluted with dichloromethane (100 mL) and washed with water (100 mL). The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane) to give product **9** as yellow solid (32 mg, 97%).



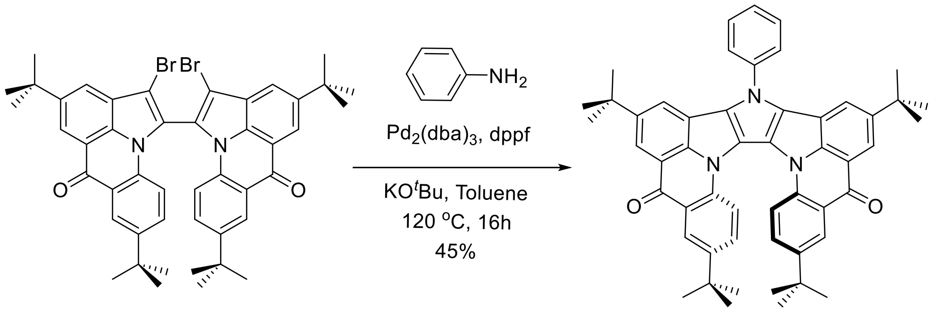
4,4'-(buta-1,3-diyne-1,4-diyl)bis(2,7-di-*tert*-butylacridone) (10). The mixture of **8** (994 mg, 3 mmol) and $Cu(OAc)_2$ (5.45 g, 30 mmol) in toluene (120 mL) and pyridine (12 mL) was stirred in air at room temperature for 16 h. The reaction mixture was washed with water (5x200 mL) and dried over Na_2SO_4. The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane / ethyl acetate 100:1) to give the product **10** as yellow solid (720 mg, 72%). m.p. 390 ºC (dec.). ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 9.04 (br s, 2H), 8.61 (d, J = 2.3 Hz, 2H), 8.50 (d, J = 2.2 Hz, 2H), 7.86 (d, J = 2.3 Hz, 2H), 7.72 (dd, J = 8.7, 2.3 Hz, 2H), 7.46 (d, J = 8.7 Hz, 2H), 1.43 (s, 18H), 1.39 (s, 18H).^{13}CNMR(150 MHz, $CDCl_3$) δ (ppm) = 178.4, 145.6, 144.2, 139.9, 138.2, 136.0, 132.2, 126.0, 123.0, 121.3, 121.1, 116.8, 108.3, 80.7, 79.1, 34.9, 34.9, 31.5, 31.5. IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 3417, 3251, 3151, 2954, 2861, 1583, 1509, 1446, 1317, 1266, 1172, 914, 831, 748. HRMS(ESI) (*m/z*) : [M+H]$^+$ calcd. for $C_{46}H_{49}N_2O_2$, 661.3789; found, 661.3774.



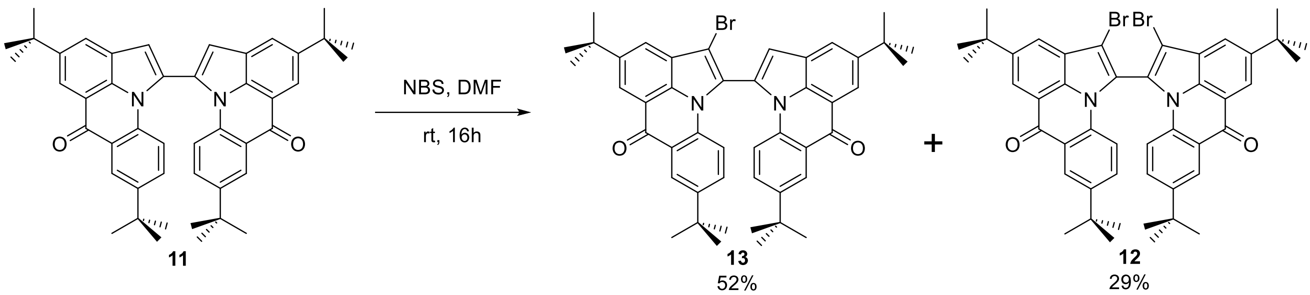
4,4',8,8'-tetra-*tert*-butyl-[1,1'-bipyrrolo[3,2,1-de]acridone-6,6'-dione (11). A 120 mL screw capped glass vial was charged with **10** (660 mg, 1 mmol), K_2CO_3 (550 mg, 4 mmol), methanol (4 mL) and tetrahydrofuran (4 mL). The vial was sealed and heated in an oil-bath at 70 ºC for 16 hours. After cooling down to room temperature, the reaction mixture was diluted with dichloromethane (250 mL), then washed with water (3x200 mL) and dried over Na_2SO_4. The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane / petroleum ether 1:1) to give the dimer **11** as yellow solid (624 mg, 94%).m.p. 355-358 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) = 8.56 (d, J = 1.7 Hz, 2H), 8.54 (d, J = 2.5 Hz, 2H), 8.20 (d, J = 1.7 Hz, 2H), 7.27 - 7.24 (m, 2H), 7.15 (s, 2H), 6.84 (d, J = 8.9 Hz, 2H), 1.56 (s, 18H), 1.26 (s, 18H). ^{13}CNMR (100 MHz, $CDCl_3$) δ (ppm) = 179.7, 147.7, 147.2, 136.5, 134.4, 132.1, 129.9, 127.6, 125.2, 124.9, 121.2, 119.7, 114.5, 113.5, 35.6, 34.8, 32.2, 31.3. IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 3116, 2956, 2913, 2873, 1656, 1606, 1565, 1481, 1359, 1311, 1276, 1249, 1199, 1147, 894, 825, 601. HRMS(ESI) (*m/z*) : [M+H]$^+$ calcd. for $C_{46}H_{49}N_2O_2$, 661.3788; found, 661.3789.



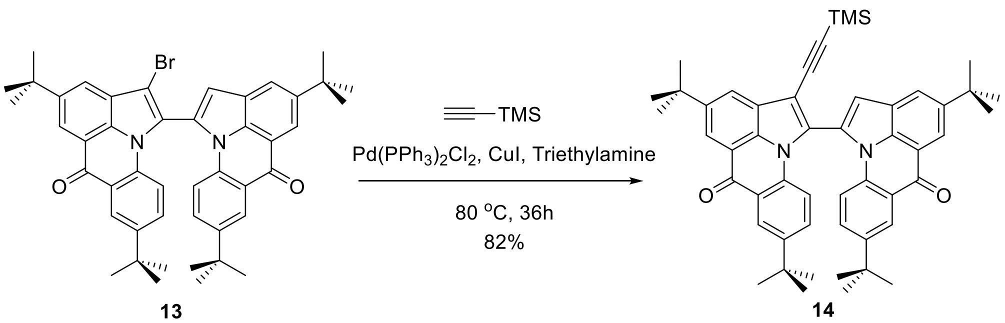
2,2'-dibromo-4,4',8,8'-tetra-*tert*-butyl-[1,1'-bipyrrolo[3,2,1-de]acridone-6,6'-dione (12). The mixture of **11** (390 mg, 0.59 mmol), *N*-bromosuccinimide (221 mg, 1.24 mmol) and DMF (6 mL) was stirred at room temperature for 16 h. The reaction mixture was quenched with water and diluted with dichloromethane (100 mL), then washed with water (3×100 mL) and dried over Na_2SO_4. The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane) to give the product **12** as yellow solid (396 mg, 82%). m.p. 327-329 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) = 8.63 (d, J = 1.6 Hz, 2H), 8.55 (d, J = 2.4 Hz, 2H), 8.16 (d, J = 1.6 Hz, 2H), 7.33 (dd, J = 8.9, 2.4 Hz, 2H), 6.88 (d, J = 8.9 Hz, 2H), 1.59 (s, 18H), 1.28 (s, 18H). ^{13}CNMR (100 MHz, $CDCl_3$) δ (ppm) = 179.0, 148.4, 147.8, 136.3, 133.5, 132.6, 127.0, 125.7, 125.5, 125.2, 123.6, 123.0, 119.9, 113.8, 105.8, 35.8, 34.9, 32.1, 31.3. IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 3060, 2960, 2910, 2865, 1662, 1608, 1562, 1486, 1367, 1257, 1193, 1110, 1027, 892, 815, 661. HRMS(ESI) (*m/z*) : $[M+H]^+$ calcd. for $C_{46}H_{47}N_2O_2Br_2$, 819.1978; found, 819.1971.



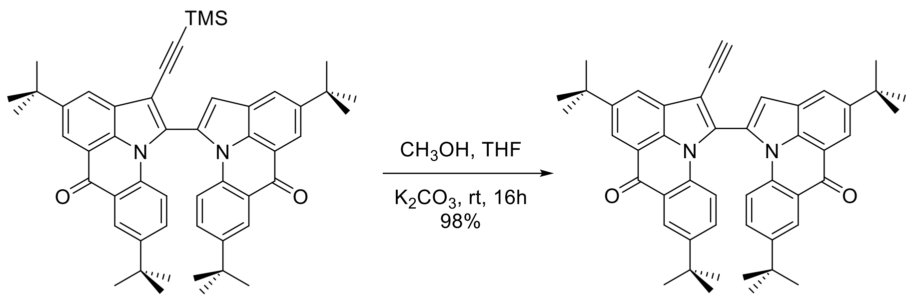
triaza[7]helicene (2). A 8 mL screw capped glass vial was charged with **12** (163 mg, 0.2 mmol), aniline (20 mg, 0.21 mmol) and KO^{t}Bu (54 mg, 0.48 mmol). Anhydrous toluene (0.3 mL) was added to the vial and the mixture was bubbled with argon for 3 minutes, followed by adding $Pd_2(dba)_3$ (9 mg, 0.01 mmol) and dppf (11 mg, 0.02 mmol). The vial was quickly sealed and heated at 120 ºC for 16 hours. After cooling down to room temperature, the reaction mixture was diluted with dichloromethane (150 mL), washed with water (100 mL) and dried over Na_2SO_4. The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane) to give the product **2** as light yellow solid (67 mg, 45%). m.p. > 400 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) = 8.54 (d, J = 2.2 Hz, 2H), 8.36 (s, 2H), 8.01 (d, J = 7.9 Hz, 2H), 7.98 (d, J = 1.7 Hz, 2H), 7.92 (d, J = 8.6 Hz, 2H), 7.77 (t, J = 7.8 Hz, 2H), 7.62 (t, J = 7.5 Hz, 1H), 7.42 (dd, J = 8.6, 2.3 Hz, 2H), 1.45 (s, 18H), 1.40 (s, 18H). ^{13}CNMR (100 MHz, $CDCl_3$) δ (ppm) = 180.0, 146.9, 146.7, 139.1, 138.2, 136.8, 130.3, 130.1, 129.1, 128.3, 124.7, 124.0, 124.0, 120.4, 119.8, 119.4, 119.3, 118.2, 117.8, 35.5, 34.9, 32.0, 31.5. IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 3058, 2958, 2900, 2865, 1650, 1606, 1498, 1369, 1320, 1286, 1257, 1209, 1170, 921, 825, 750. HRMS(ESI) (*m/z*) : $[M+Na]^+$ calcd. for $C_{52}H_{51}N_3O_2Na$, 772.3873; found, 772.3852.



2-bromo-4,4’,8,8’-tetra-*tert*-butyl-[1,1’-bipyrrolo[3,2,1-de]acridone-6,6’-dione (13). The mixture of **11** (661 mg, 1 mmol), *N*-bromosuccinimide (196 mg, 1.1 mmol) and DMF (10 mL) was stirred at room temperature for 16 h. The reaction mixture was dichloromethane (100 mL), washed with water (3×50 mL) and dried over Na_2SO_4. The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane) to give compound **13** (382 mg, 52%) and **12** (240 mg, 29%) as yellow solids. m.p. 245-249 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 8.60 (s, 1H), 8.58 (s, 1H), 8.56 (d, J = 2.4 Hz, 1H), 8.53 (d, J = 2.5 Hz, 1H), 8.24 (d, J = 1.7 Hz, 1H), 8.13 (d, J = 1.7 Hz, 1H), 7.31 (dd, J = 8.9, 2.5 Hz, 1H), 7.27 (dd, J = 9.0, 2.4 Hz, 1H), 7.20 (s, 1H), 6.90 (d, J = 8.9 Hz, 1H), 6.83 (d, J = 8.9 Hz, 1H), 1.58 (s, 9H), 1.57 (s, 9H), 1.28 (s, 9H), 1.27 (s, 9H). ^{13}CNMR (150 MHz, $CDCl_3$) δ (ppm) = 179.9, 179.1, 148.4, 147.7, 147.6, 147.3, 136.5, 136.3, 134.4, 133.2, 132.4, 132.3, 127.7, 127.6, 127.5, 127.0, 125.4, 125.3, 125.3, 125.2, 125.1, 123.5, 122.6, 121.6, 119.8, 119.7, 114.5, 114.4, 114.0, 104.7, 35.8, 35.7, 34.8, 34.8, 32.2, 32.1, 31.3, 31.3. IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 2962, 2869, 1657, 1608, 1563, 1490, 1474, 1364, 1313, 1275, 1256, 1199, 1150, 1110, 1061, 814. HRMS(ESI) (*m/z*) : [M+H]$^+$ calcd. for $C_{46}H_{48}N_2O_2Br$, 739.2894; found, 739.2887.

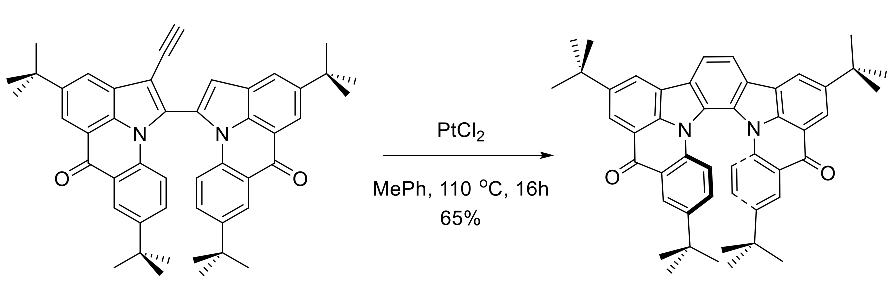


4,4’,8,8’-tetra-*tert*-butyl-2-(trimethylsilylethynyl)-[1,1’-bipyrrolo[3,2,1-de]acridone-6,6’-dione (14). A 38 mL screw capped glass vial was charged with **13** (400 mg, 0.54 mmol), CuI (1.9 mg, 0.01 mmol) and $Pd(PPh_3)_2Cl_2$ (15 mg, 0.02 mmol). Anhydrous triethylamine (5 mL) was added to the vial and the mixture was bubbled with argon for 3 minutes, followed by adding trimethylsilylacetylene (158 mg, 1.1 mmol). The vial was quickly sealed and heated in an oil-bath at 80 ºC for 36 hours. After cooling down to room temperature, the reaction mixture was diluted with dichloromethane (150 mL), washed with water (200 mL) and dried over Na_2SO_4. The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane) to give the product **14** as yellow solid (335 mg, 82%). m.p. 328-330 °C. ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 8.57 (d, J = 1.7 Hz, 1H), 8.55 (d, J = 1.8 Hz, 1H), 8.54 (d, J = 2.4 Hz, 1H), 8.52 (d, J = 2.5 Hz, 1H), 8.23 (d, J = 1.7 Hz, 1H), 8.23 (d, J = 1.7 Hz, 1H), 7.30 (dd, J = 8.9, 2.5 Hz, 1H), 7.27-7.25 (m, 1H), 7.22 (s, 1H), 6.93 (d, J = 3.1 Hz, 1H), 6.91 (d, J = 3.2 Hz, 1H), 1.57 (s, 9H), 1.57 (s, 9H), 1.28 (s, 9H), 1.26 (s, 9H), 0.03 (s, 9H). ^{13}CNMR (150 MHz, $CDCl_3$) δ (ppm) = 179.8, 179.4, 148.4, 147.8, 147.6, 147.2, 136.6, 136.0, 134.5, 133.3, 132.6, 132.2, 132.1, 128.1, 128.0, 127.8, 125.4, 125.3, 125.2, 125.1, 124.9, 124.0, 122.0, 121.3, 119.7, 119.7, 114.8, 114.5, 114.1, 109.2, 103.3, 96.0, 35.7, 35.6, 34.8, 34.8, 32.2, 32.1, 31.3, 31.3, 0.1. IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 2962, 2904, 2869, 2151, 1657, 1608, 1563, 1490, 1474, 1364, 1313, 1275, 1256, 1199, 1150, 1110, 1061, 813, 793, 738. HRMS(ESI) (*m/z*) : $[M+H]^+$ calcd. for $C_{51}H_{57}N_2O_2Si$, 757.4184; found, 757.4179.



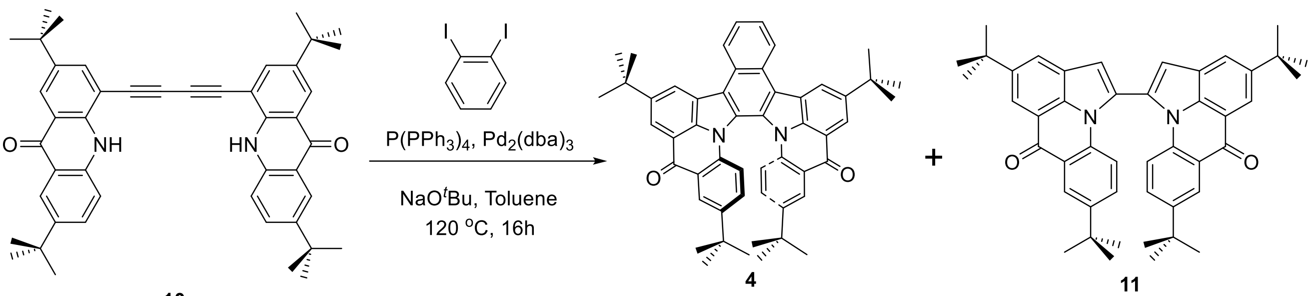
14 15

4,4',8,8'-tetra-*tert*-butyl-2-ethynyl-[1,1'-bipyrrolo[3,2,1-de]acridone-6,6'-dione (15). A 8 mL screw capped glass vial was charged with **14** (190 mg, 0.25 mmol), K_2CO_3 (70 mg, 0.5 mmol), methanol (2 mL) and tetrahydrofuran (2 mL). The mixture was stirred at room temperature for 16 h. The reaction mixture was diluted with dichloromethane (50 mL), washed with water (3×100 mL) and dried over Na_2SO_4. The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane) to give the product **15** as yellow solid (168 mg, 98%). m.p. 323°C (dec.). ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 8.57 (s, 1H), 8.57 (s, 1H), 8.54 (d, J = 2.4 Hz, 1H), 8.52 (d, J = 2.4 Hz, 1H), 8.28 (d, J = 1.7 Hz, 1H), 8.23 (d, J = 1.7 Hz, 1H), 7.29 (dd, J = 8.9, 2.5 Hz, 1H), 7.26-7.24 (m, 1H), 7.24 (s, 1H), 6.84 (d, J = 8.9 Hz, 1H), 6.79 (d, J = 9.0 Hz, 1H), 3.27 (s, 1H), 1.58 (s, 9H), 1.56 (s, 9H), 1.27 (s, 9H), 1.26 (s, 9H). ^{13}CNMR (150 MHz, $CDCl_3$) δ (ppm) = 179.7, 179.4, 148.5, 147.9, 147.7, 147.3, 136.5, 136.0, 134.5, 133.2, 132.9, 132.3, 132.2, 128.1, 127.7, 127.7, 125.4, 125.4, 125.3, 125.2, 125.1, 124.0, 122.2, 121.5, 119.8, 119.8, 114.6, 114.1, 114.1, 107.9, 84.7, 75.1, 35.8, 35.6, 34.8, 34.8, 32.2, 32.1, 31.3, 31.3. IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 3117, 3048, 2961, 2868, 1656, 1607, 1490, 1472, 1364, 1313, 1275, 1256, 1199, 1150, 1110, 1061, 813, 793, 738. HRMS(ESI) (*m/z*) : $[M+H]^+$ calcd. for $C_{48}H_{49}N_2O_2$, 685.3789; found, 685.3779.



15 3

diaza[7]helicene (3). A 8 mL screw capped glass vial was charged with **15** (116 mg, 0.17 mmol) and $PtCl_2$ (2.27 mg, 5% mmol). Anhydrous toluene (5 mL) was added to the vial and the mixture was bubbled with argon for 3 minutes. The vial was quickly sealed and heated in a heating mantle at 110 ºC for 16 hours. After cooling down to room temperature, the reaction mixture was diluted with dichloromethane (50 mL), washed with water (100 mL) and dried over Na_2SO_4. The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane / petroleum ether 1:1) to give the product **3** as yellow solid (76 mg, 65%). m.p. > 400 ºC (dec.). ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 8.53 (s, 2H), 8.52 (s, 2H), 8.46 (d, J = 2.3 Hz, 2H), 8.26 (s, 2H), 7.54 (d, J = 8.7 Hz, 2H), 7.02 (dd, J = 8.7, 2.3 Hz, 2H), 1.58 (s, 18H), 1.24 (s, 18H). ^{13}CNMR (150 MHz, $CDCl_3$) δ (ppm) = 180.4, 147.8, 147.0, 138.5, 138.4, 129.6, 128.5, 126.7, 125.2, 124.6, 124.3, 122.6, 121.7, 119.9, 118.6, 116.8, 35.7, 34.7, 32.2, 31.4. IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 2959, 2867, 1657, 1609, 1486, 1462, 1418, 1394, 1363, 1344, 1310, 1279, 1247, 1192, 1160, 1133, 828, 811, 699. HRMS(ESI) (*m/z*) : $[M+H]^+$ calcd. for $C_{48}H_{49}N_2O_2$, 685.3789; found, 685.3787.



10 4 57% 11 23%

diaza[7]helicene (4). A 8 mL screw capped glass vial was charged with **10** (264 mg, 0.4 mmol), 1,2-diiodobenzene (158 mg, 0.48 mmol) and NaO^{t}Bu (85 mg, 0.88 mmol). Anhydrous toluene (1 mL) was added to the vial and the mixture was bubbled with argon for 3 minutes, followed by adding $Pd_2(dba)_3$ (8 mg, 0.0087 mmol) and $Pd(PPh_3)_4$ (24 mg, 0.02 mmol). The vial was quickly sealed and heated at 120 ºC for 16 hours. After cooling down to room temperature, the reaction mixture was diluted with dichloromethane (150 mL), washed with water (100 mL) and dried over Na_2SO_4. The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane) to give the product **4** (167 mg, 57%) and **11** (61 mg, 23%) as yellow solids. m.p. 300-302 ºC. ^{1}H NMR (400 MHz, $CDCl_3$) δ (ppm) = 9.07 - 9.05 (m, 2H), 9.04 (br s, 2H), 8.61 (d, J = 1.5 Hz, 2H), 8.45 (d, J = 2.3 Hz, 2H), 7.90 - 7.88 (m, 2H), 7.52 (d, J = 8.8 Hz, 2H), 7.03 (dd, J = 8.8, 2.3 Hz, 2H), 1.67 (s, 18H), 1.23 (s, 18H). ^{13}CNMR (100 MHz, $CDCl_3$) δ (ppm) = 180.5, 148.1, 147.4, 137.8, 137.8, 129.8, 127.7, 126.6, 126.1, 125.6, 124.9, 124.8, 124.6, 124.4, 122.8, 121.3, 120.1, 118.2, 35.9, 34.7, 32.3, 31.4. IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 3091, 2962, 2904, 2873, 1660, 1602, 1536, 1481, 1367, 1268, 1209, 1070, 831, 744. HRMS(ESI) (*m/z*) : $[M+H]^+$ calcd. for $C_{52}H_{51}N_2O_2$, 735.3945; found, 735.3952.

3. NMR Spectra

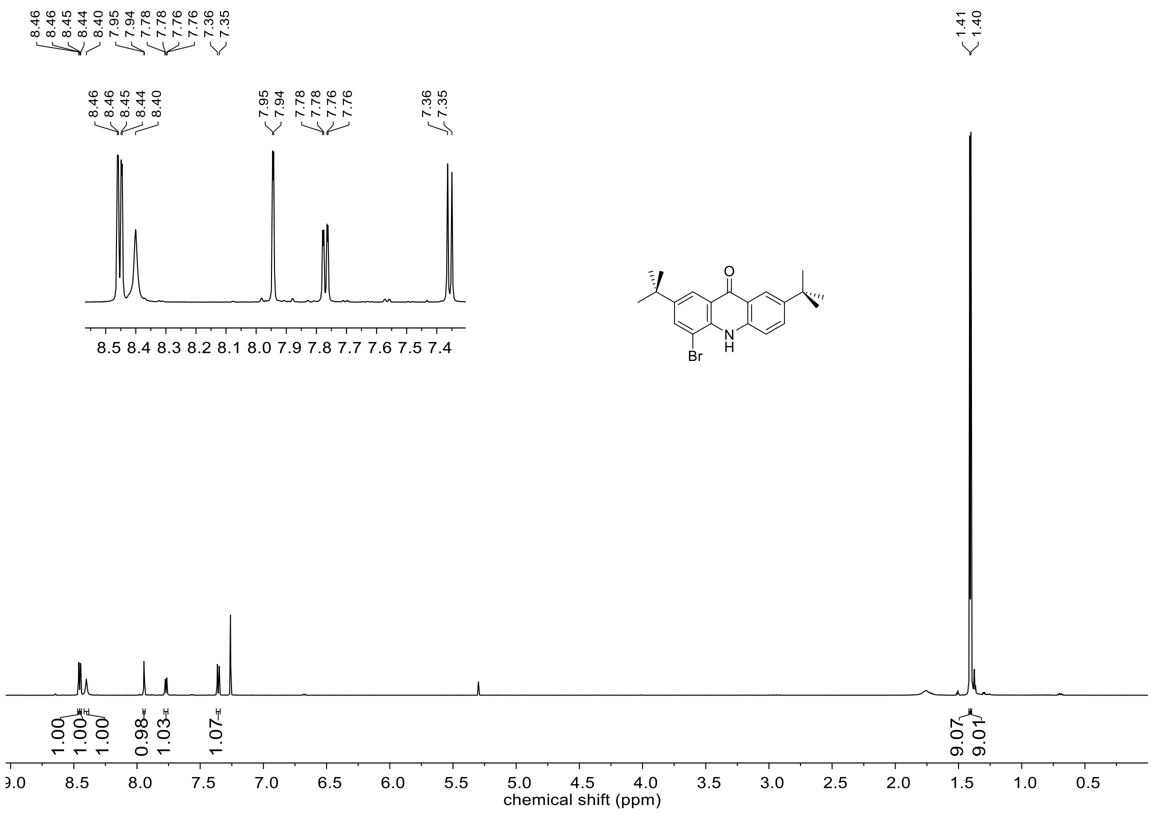


Figure S1. [1]H NMR spectrum ($CDCl_3$, 600 MHz) of **6**

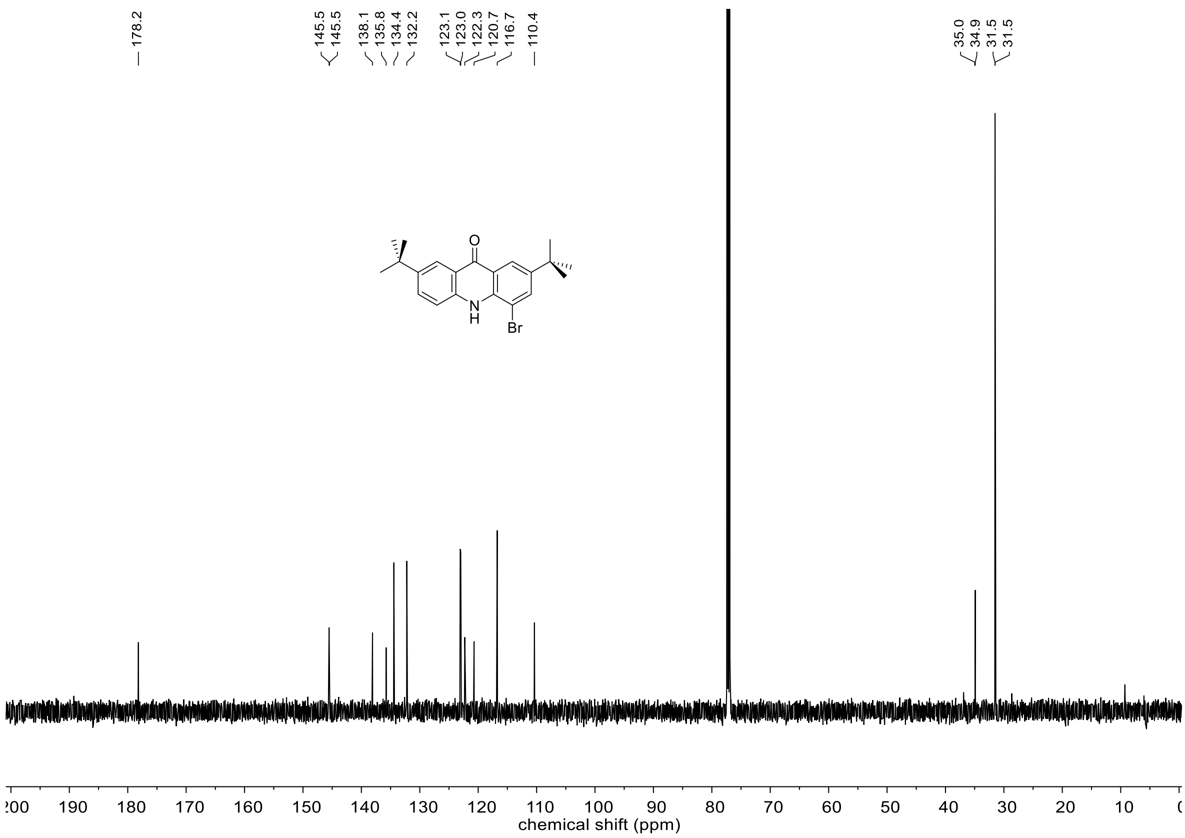


Figure S2. [13]C NMR spectrum ($CDCl_3$, 150 MHz) of **6**

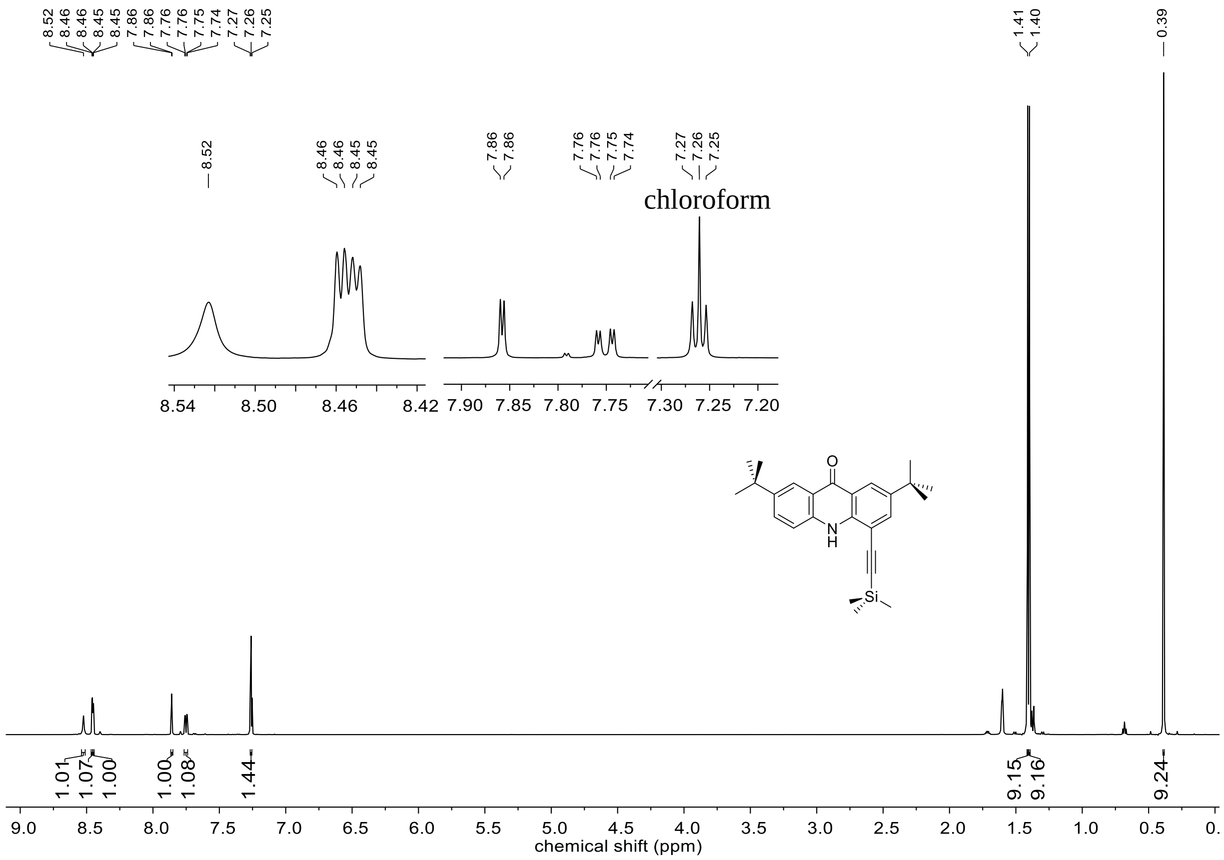


Figure S3. ^{1}H NMR spectrum ($CDCl_3$, 600 MHz) of **7**

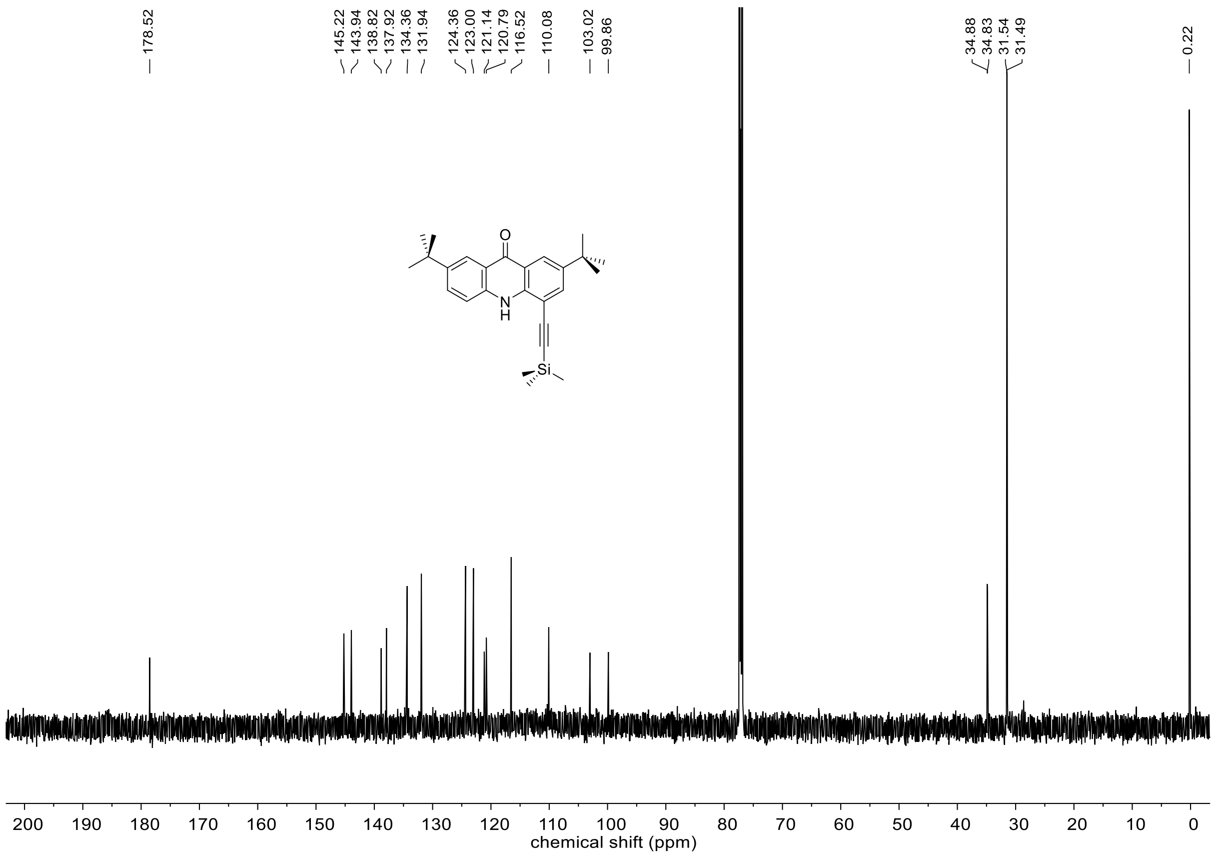


Figure S4. ^{13}C NMR spectrum ($CDCl_3$, 150 MHz) of **7**

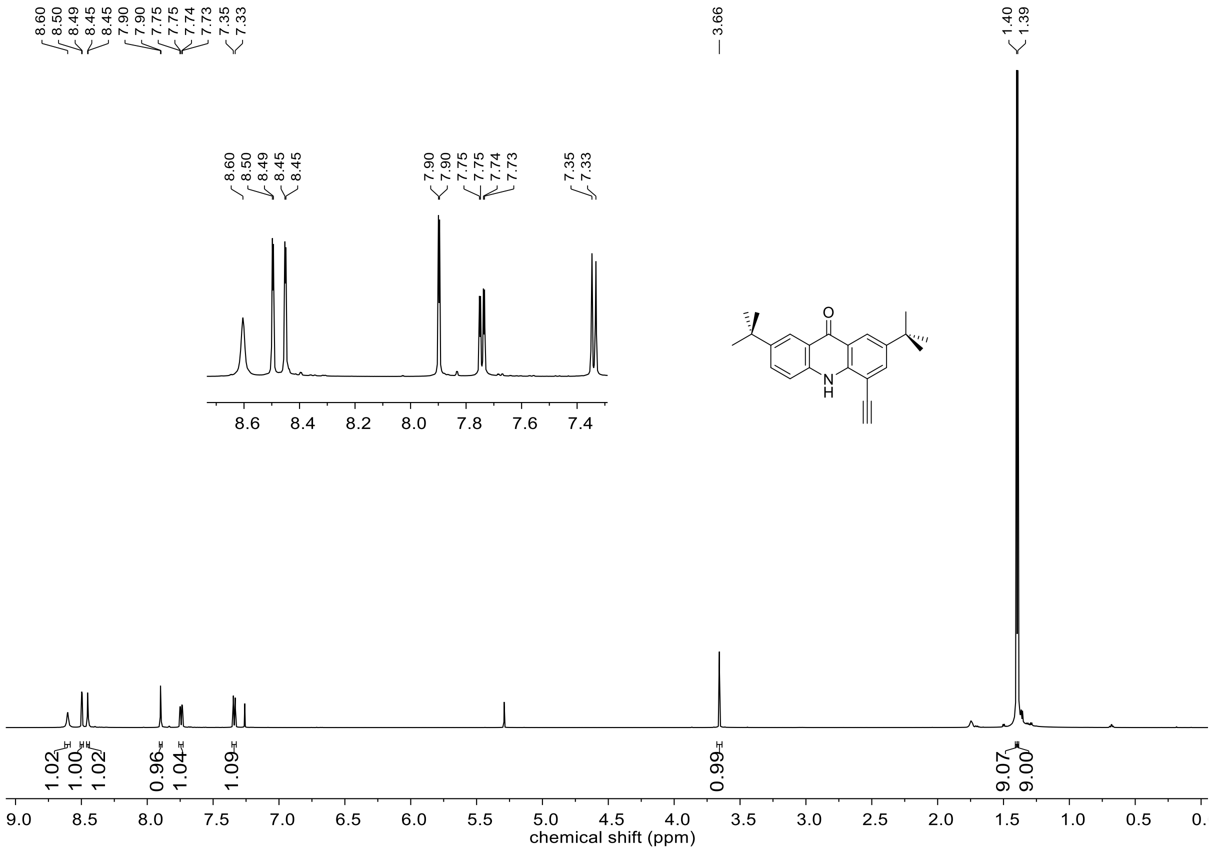


Figure S5. [1]H NMR spectrum ($CDCl_3$, 600 MHz) of **8**

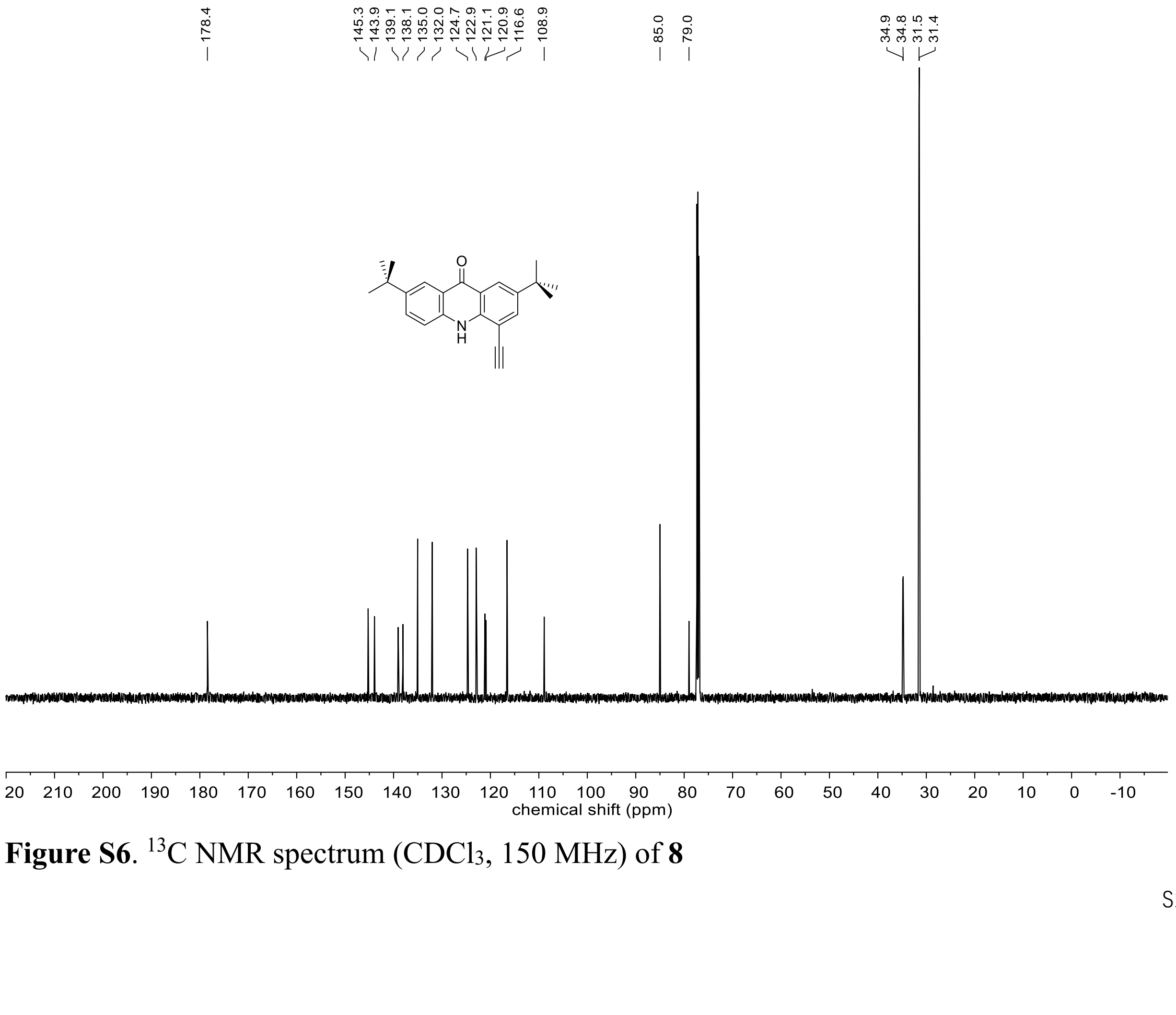


Figure S6. [13]C NMR spectrum ($CDCl_3$, 150 MHz) of **8**

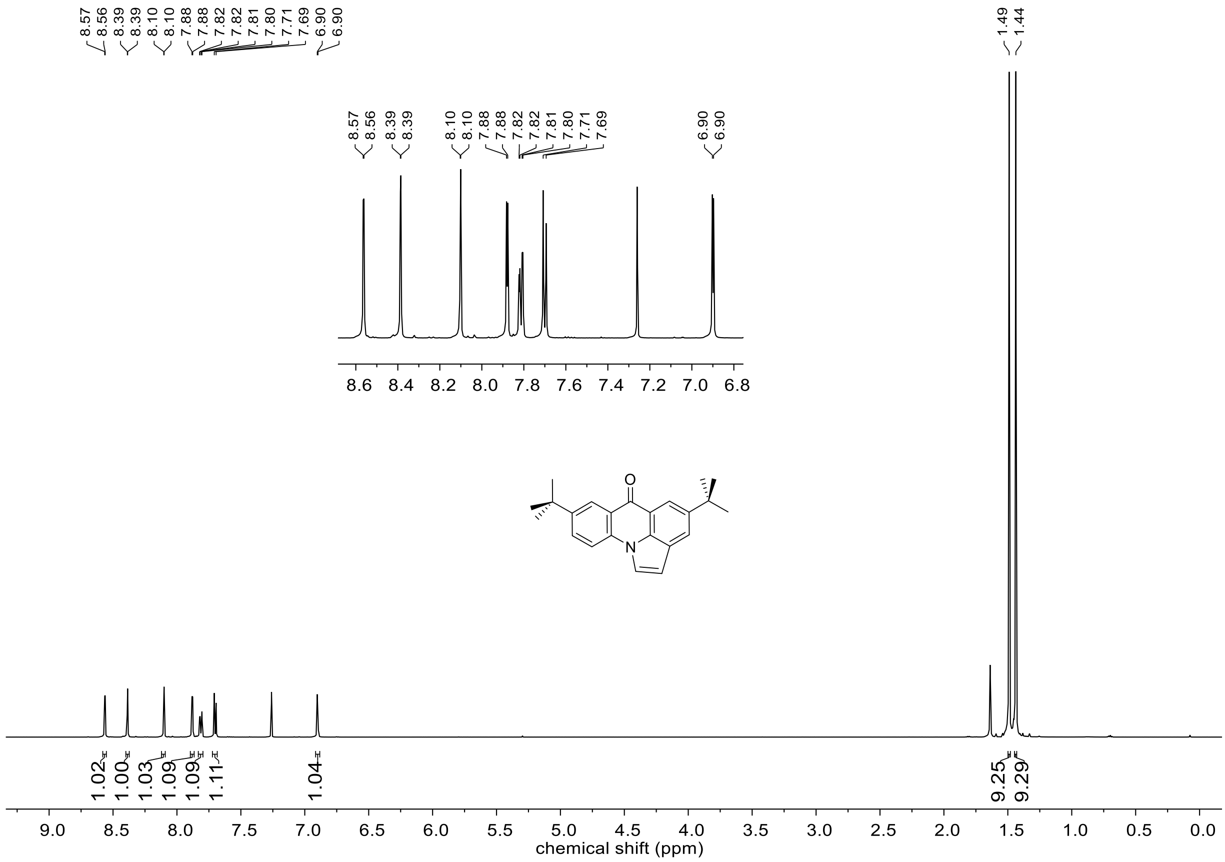


Figure S7. ${}^{1}H$ NMR spectrum ($CDCl_3$, 600 MHz) of **9**

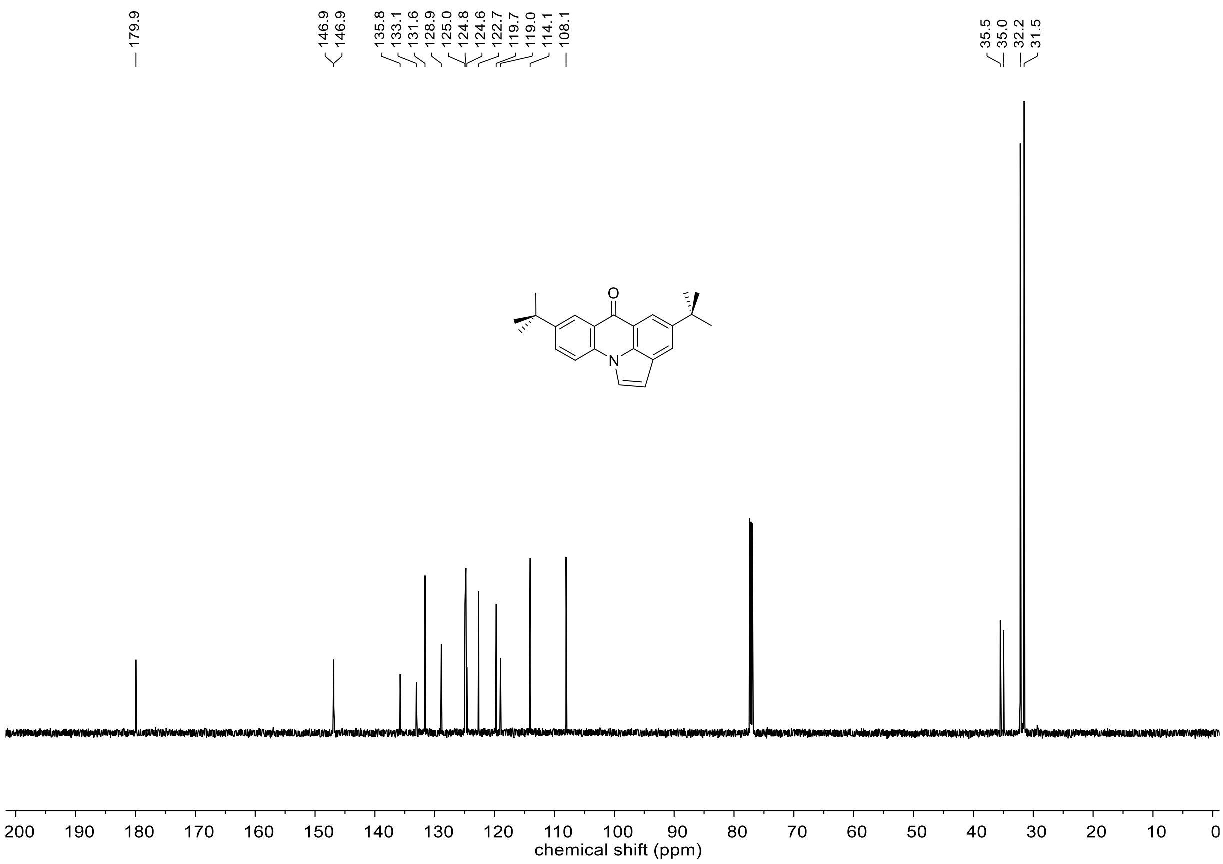


Figure S8. ${}^{13}C$ NMR spectrum ($CDCl_3$, 150 MHz) of **9**

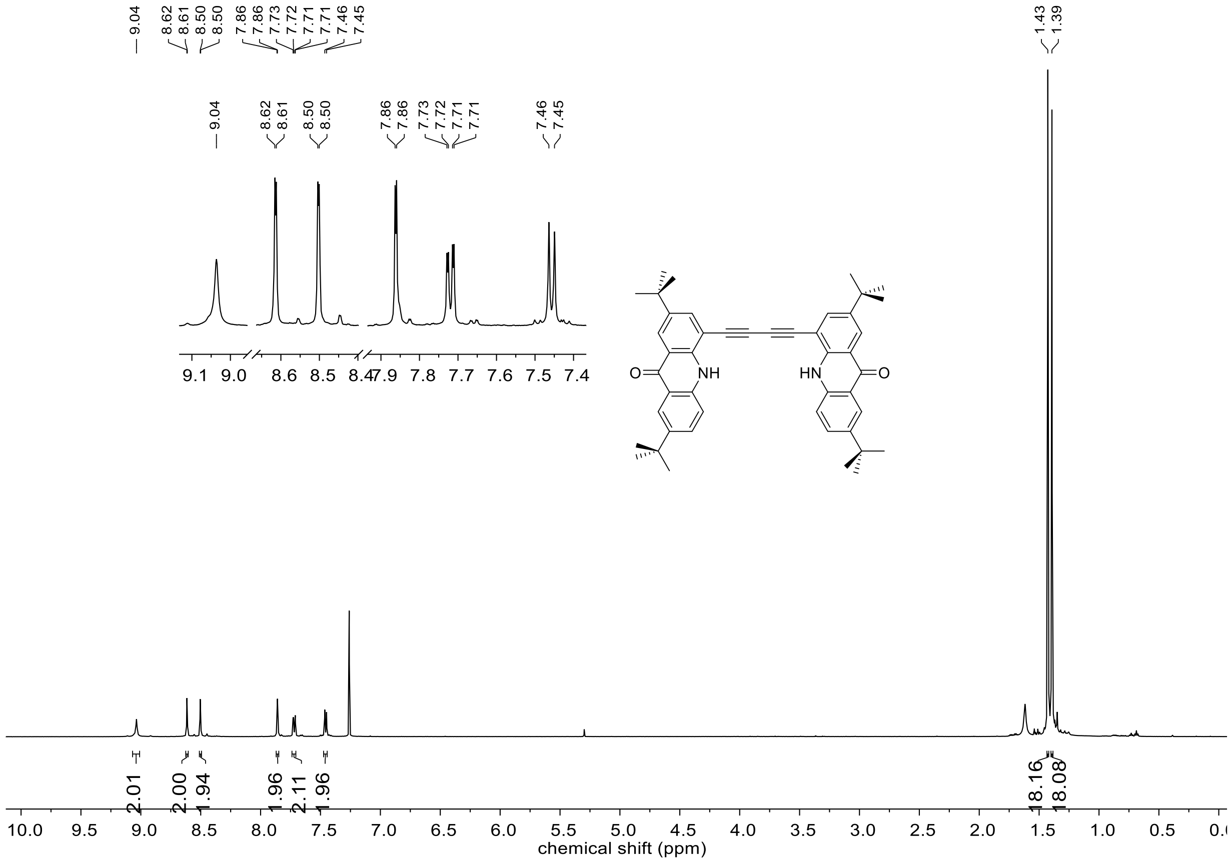


Figure S9. ^{1}H NMR spectrum ($CDCl_3$, 600 MHz) of **10**

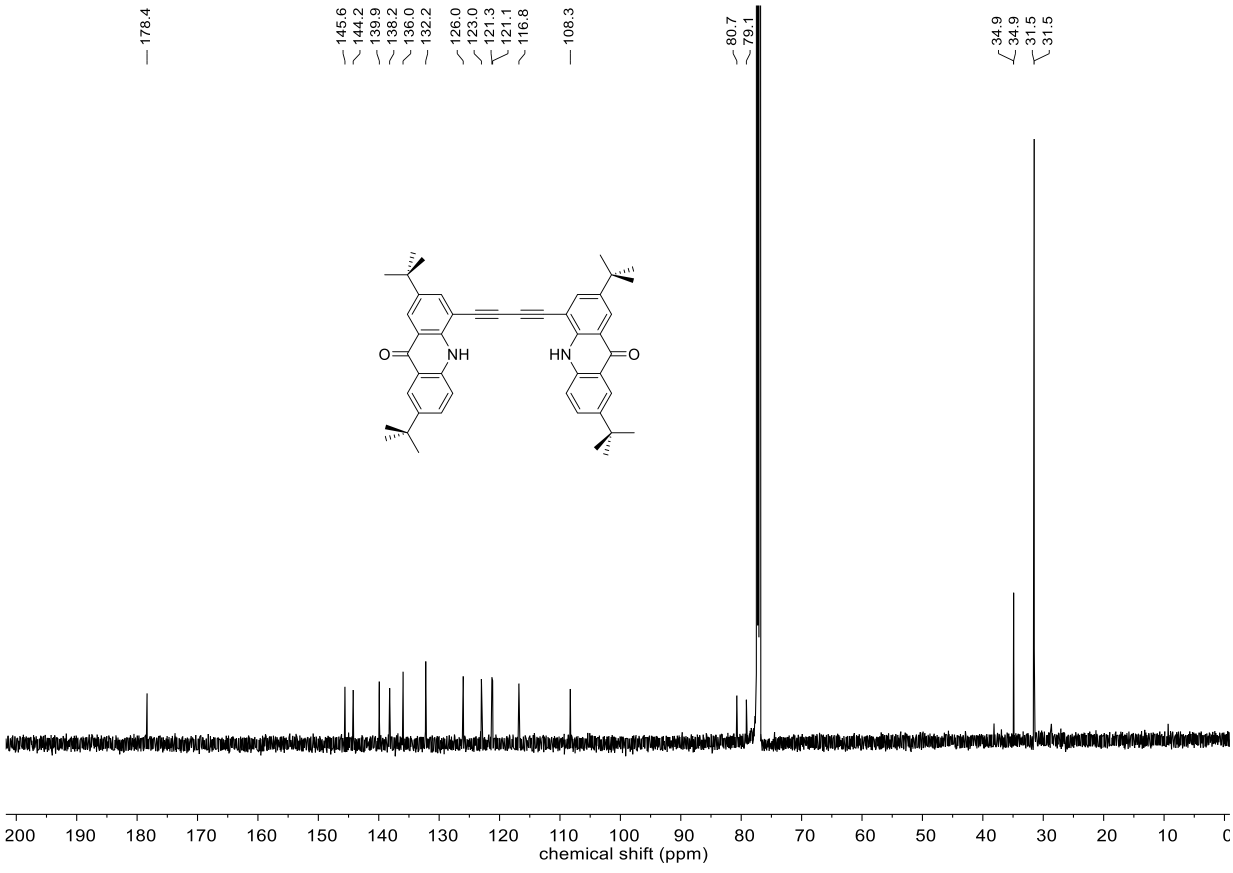


Figure S10. ^{13}C NMR spectrum ($CDCl_3$, 150 MHz) of **10**

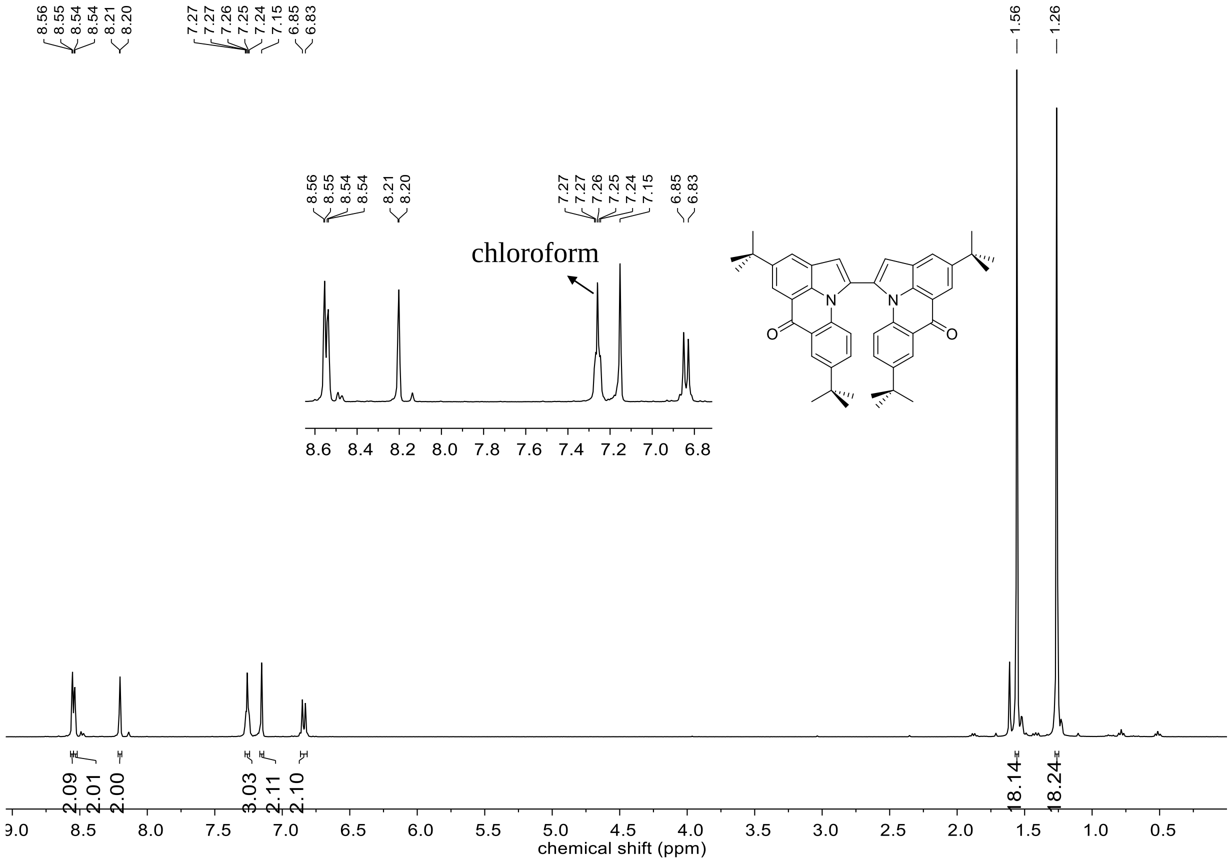


Figure S11. [1]H NMR spectrum ($CDCl_3$, 400 MHz) of **11**

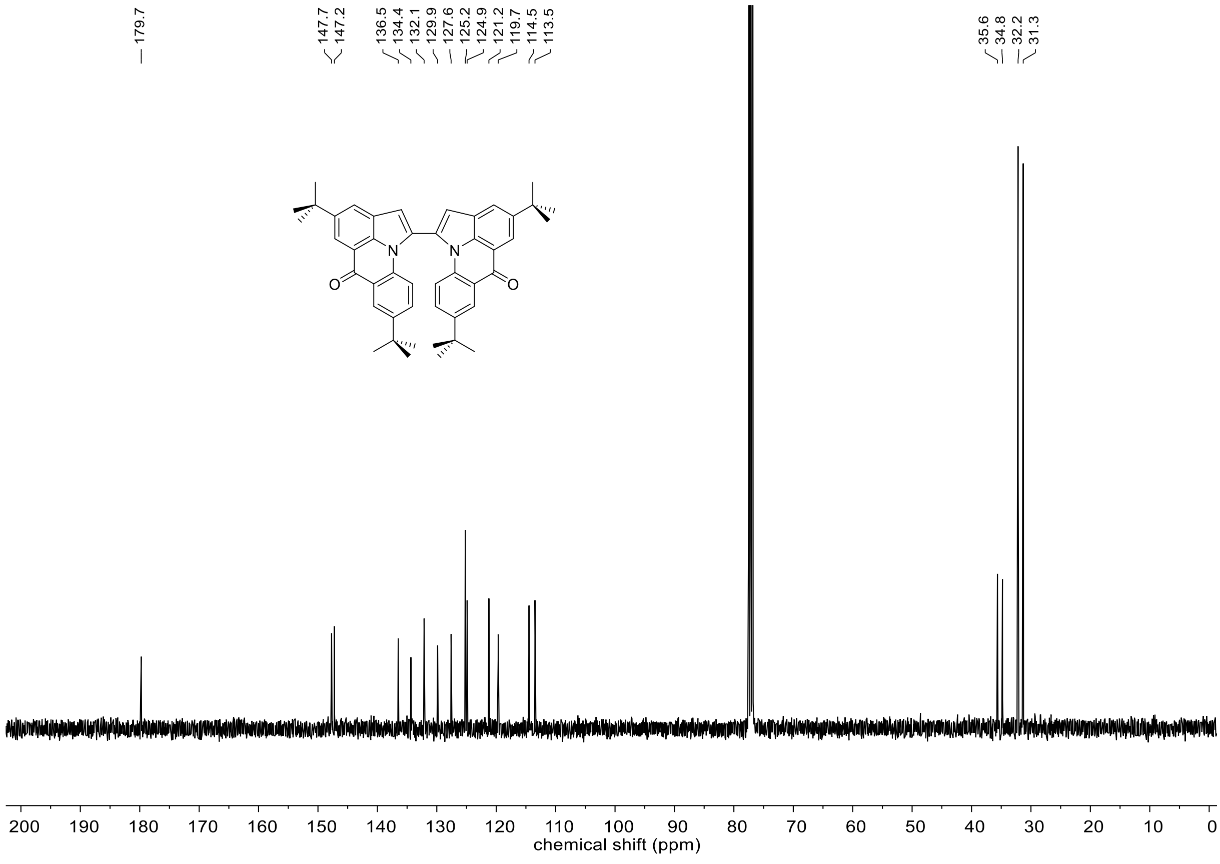


Figure S12. [13]C NMR spectrum ($CDCl_3$, 100 MHz) of **11**

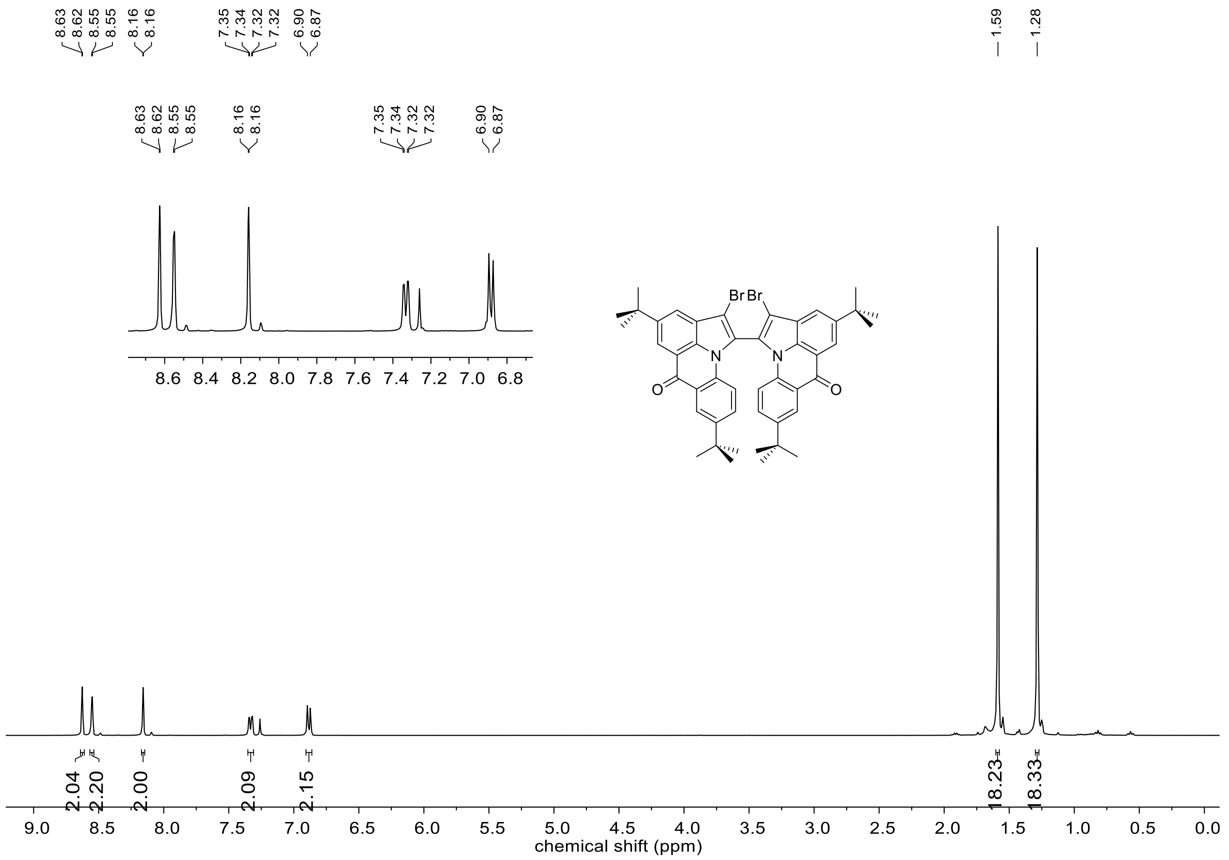


Figure S13. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **12**

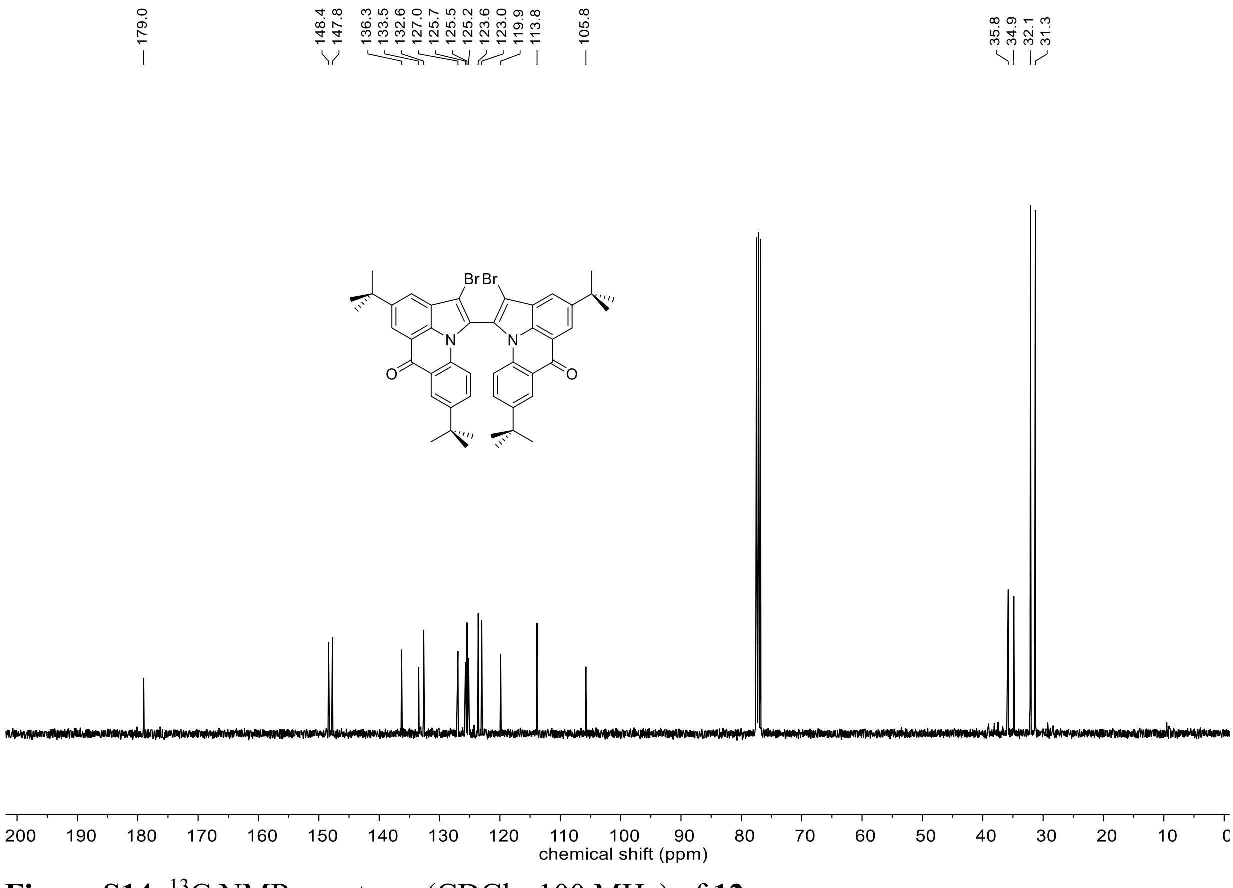


Figure S14. ^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of **12**

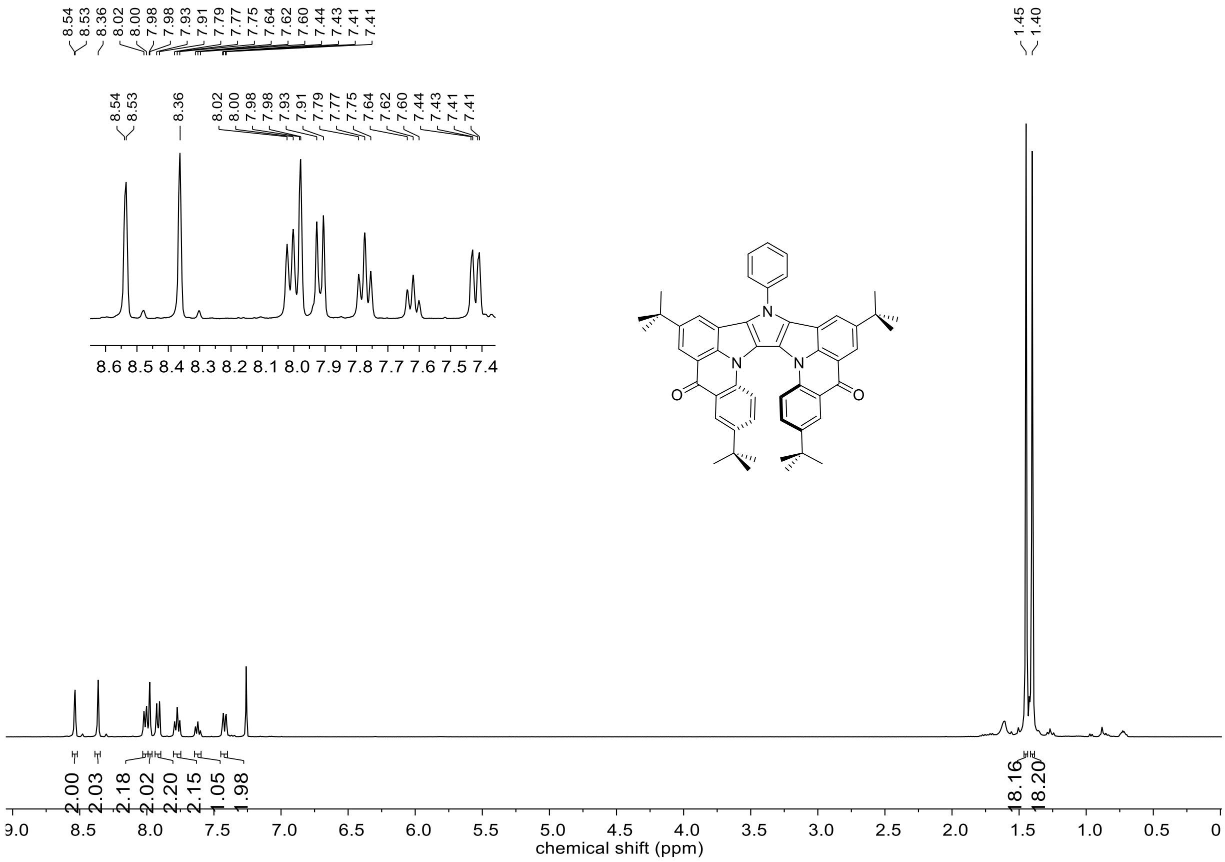


Figure S15. [1]H NMR spectrum ($CDCl_3$, 400 MHz) of **2**

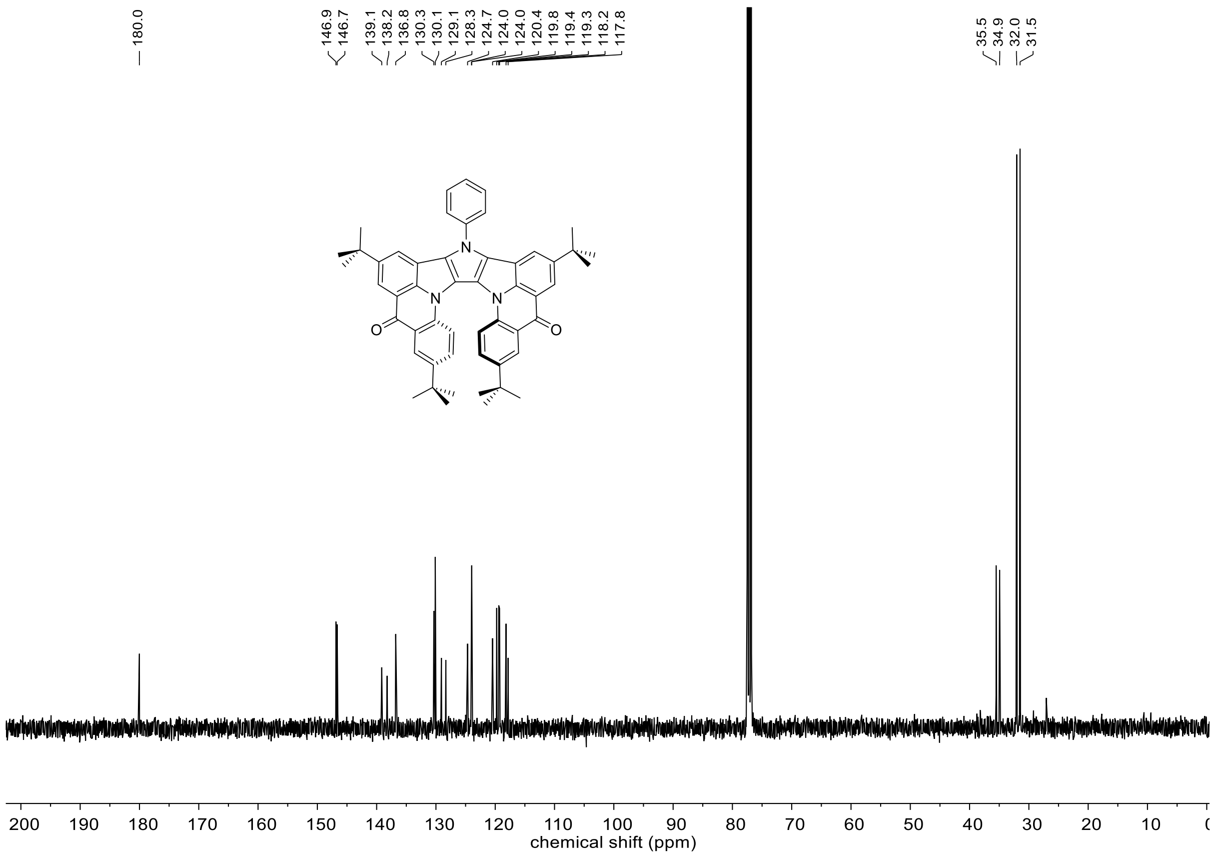


Figure S16. [13]C NMR spectrum ($CDCl_3$, 100 MHz) of **2**.

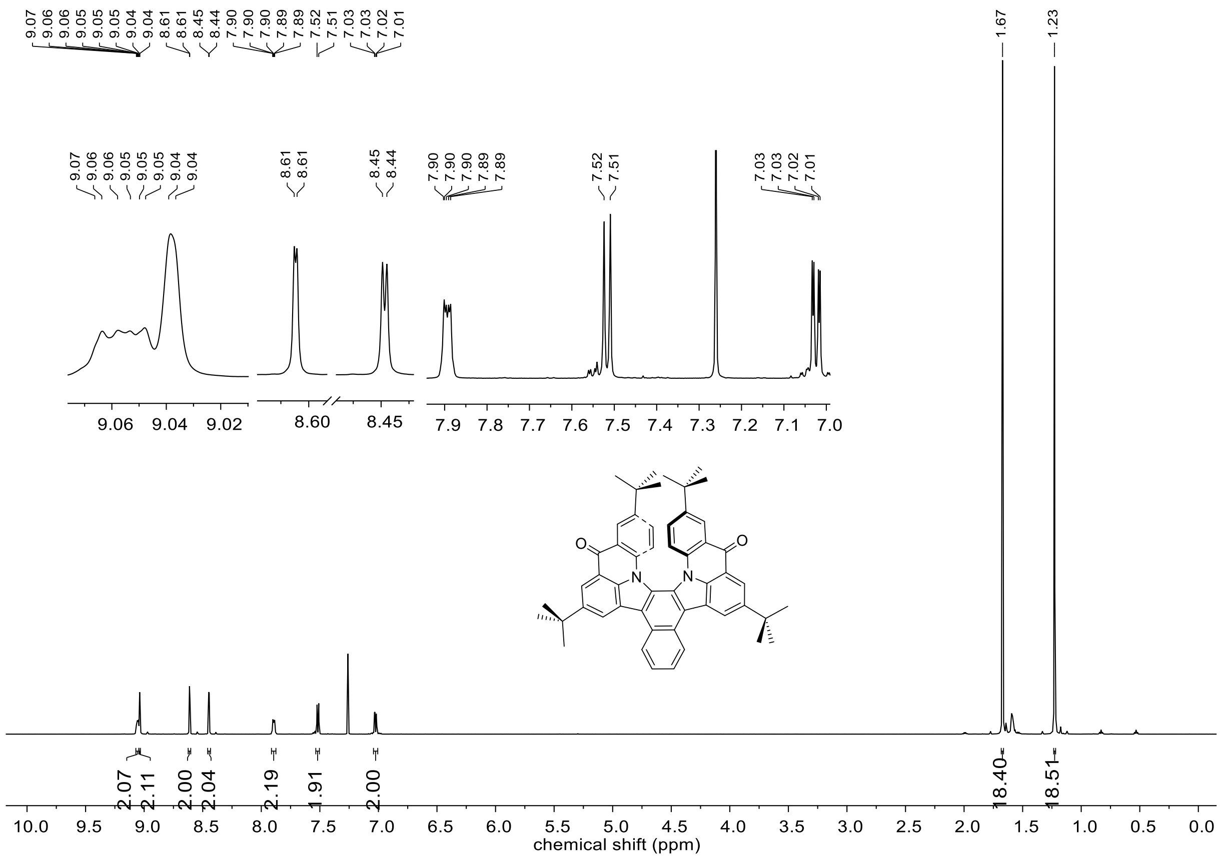


Figure S17. [1]H NMR spectrum ($CDCl_3$, 400 MHz) of **4**

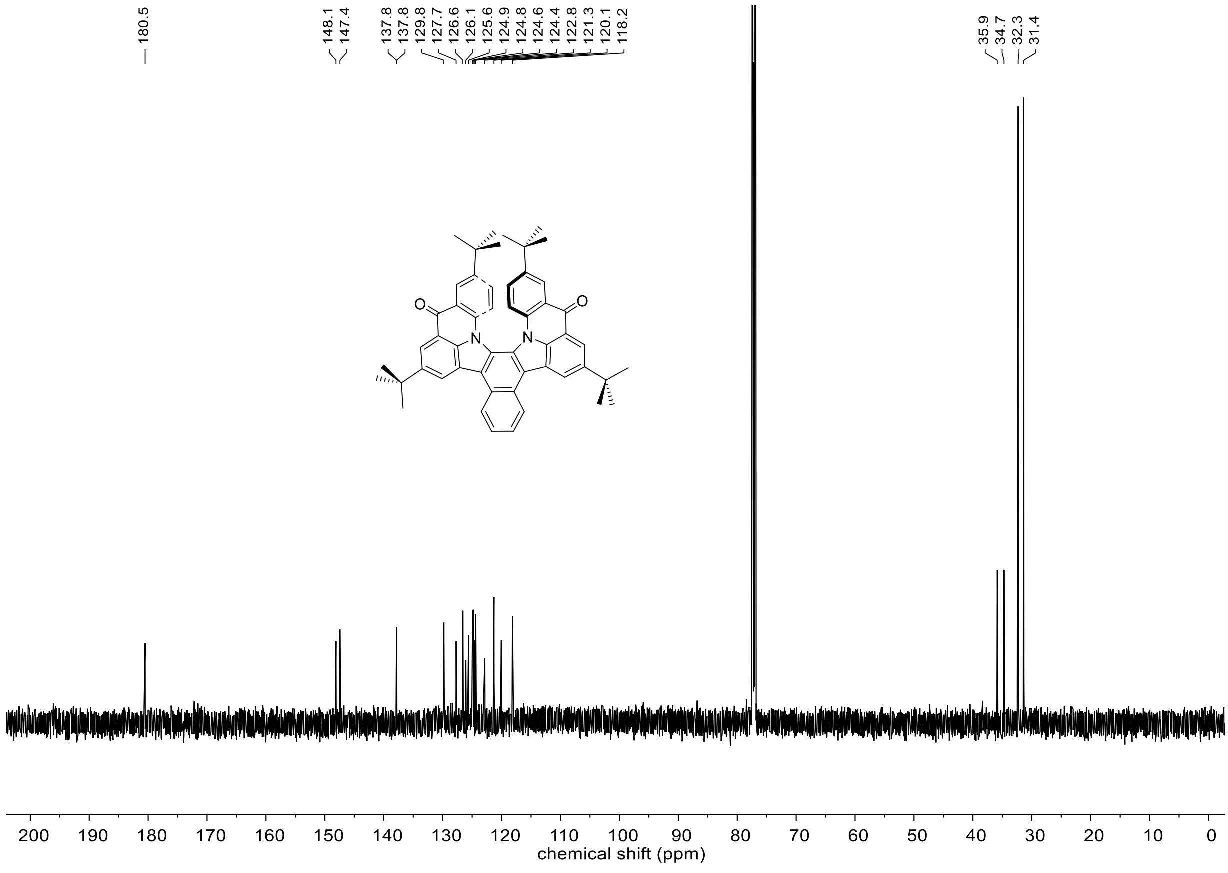


Figure S18. [13]C NMR spectrum ($CDCl_3$, 100 MHz) of **4**

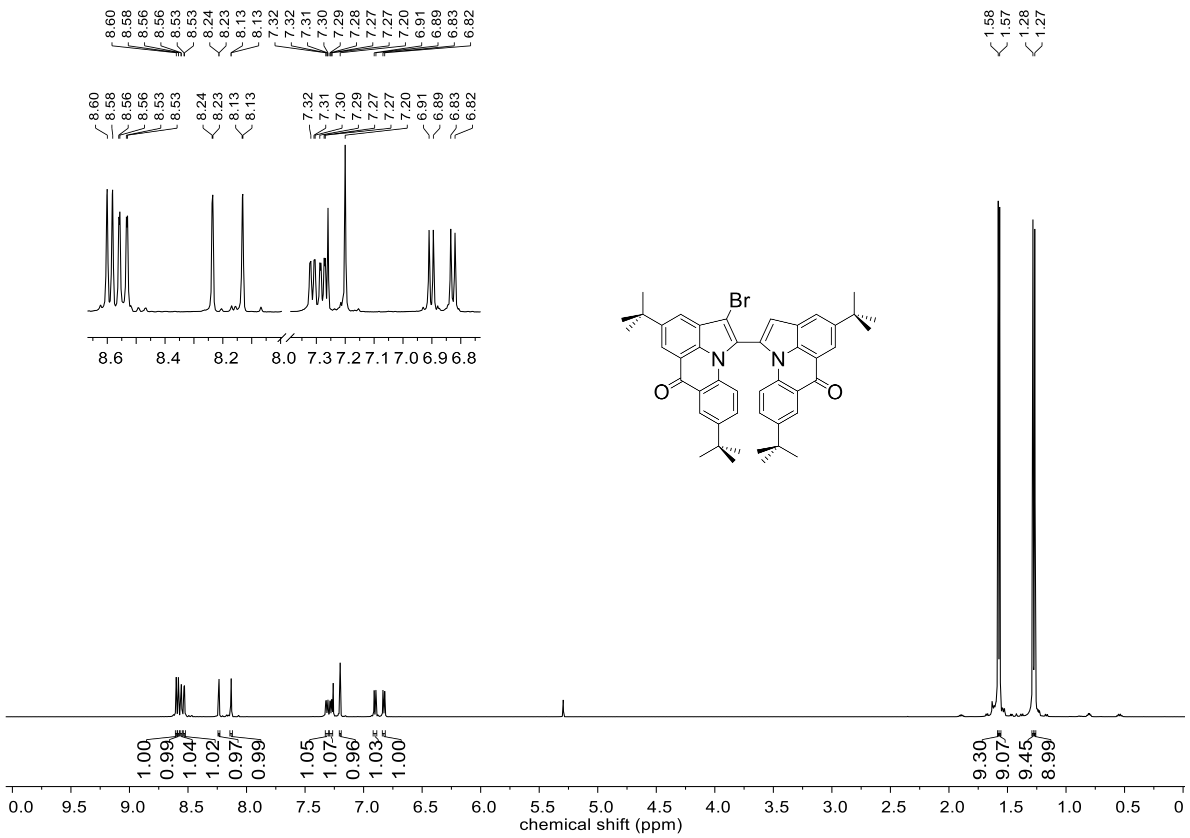


Figure S19. ^{1}H NMR spectrum ($CDCl_3$, 600 MHz) of **13**

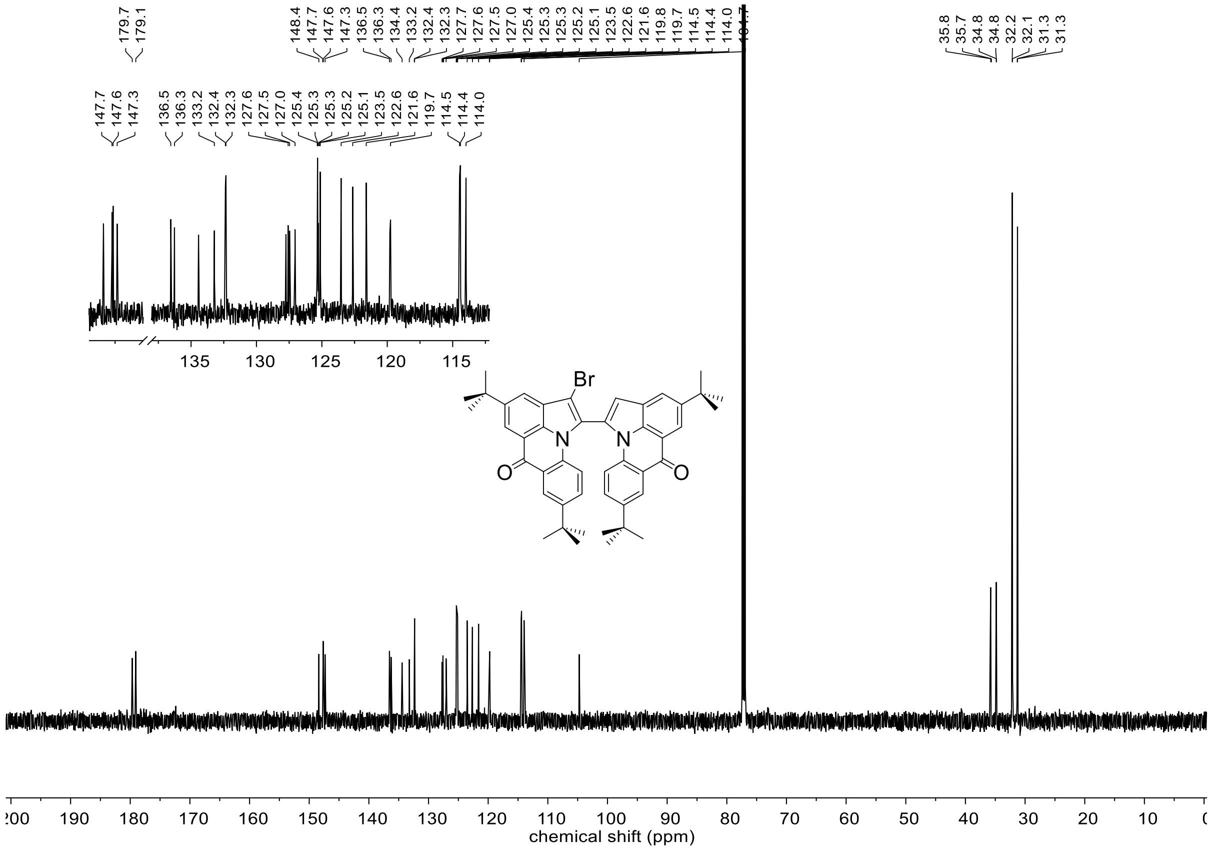


Figure S20. ^{13}C NMR spectrum ($CDCl_3$, 150 MHz) of **13**

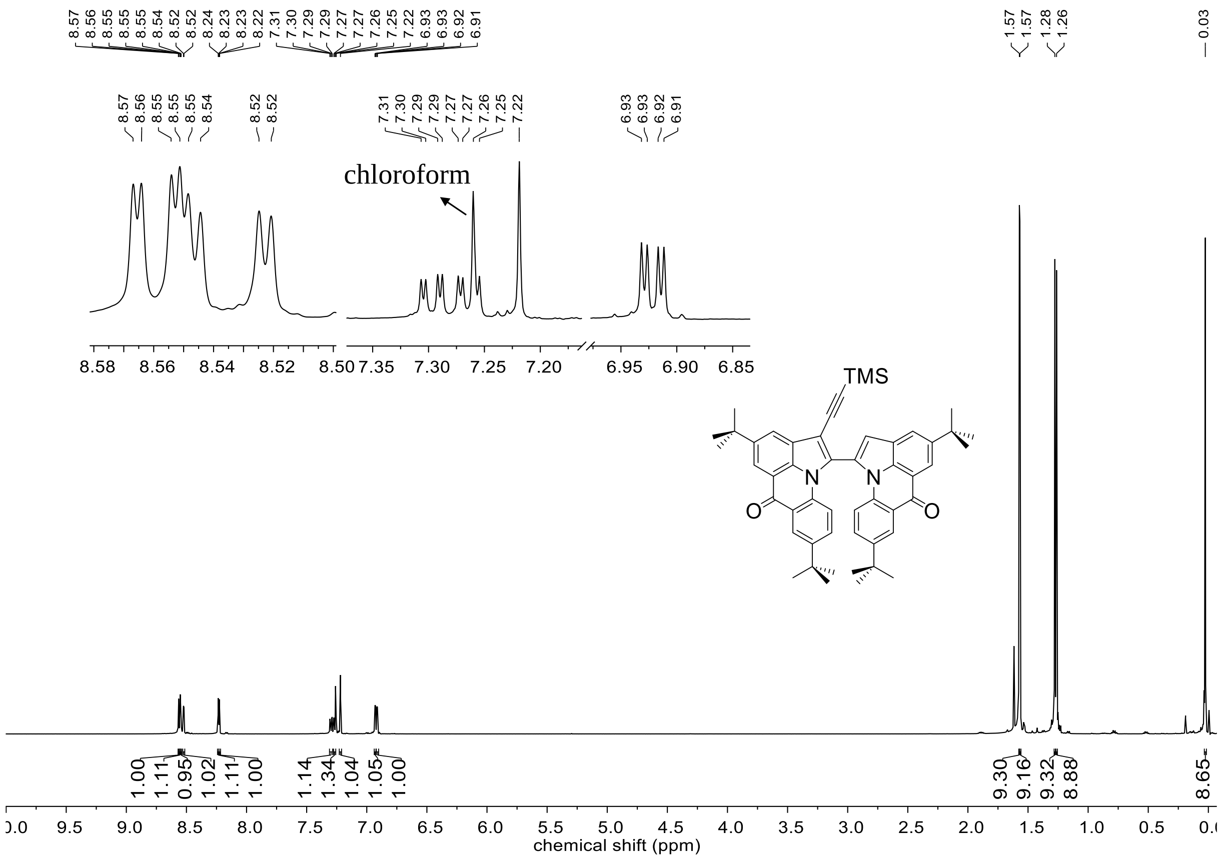


Figure S21. ^{1}H NMR spectrum ($CDCl_3$, 600 MHz) of **14**

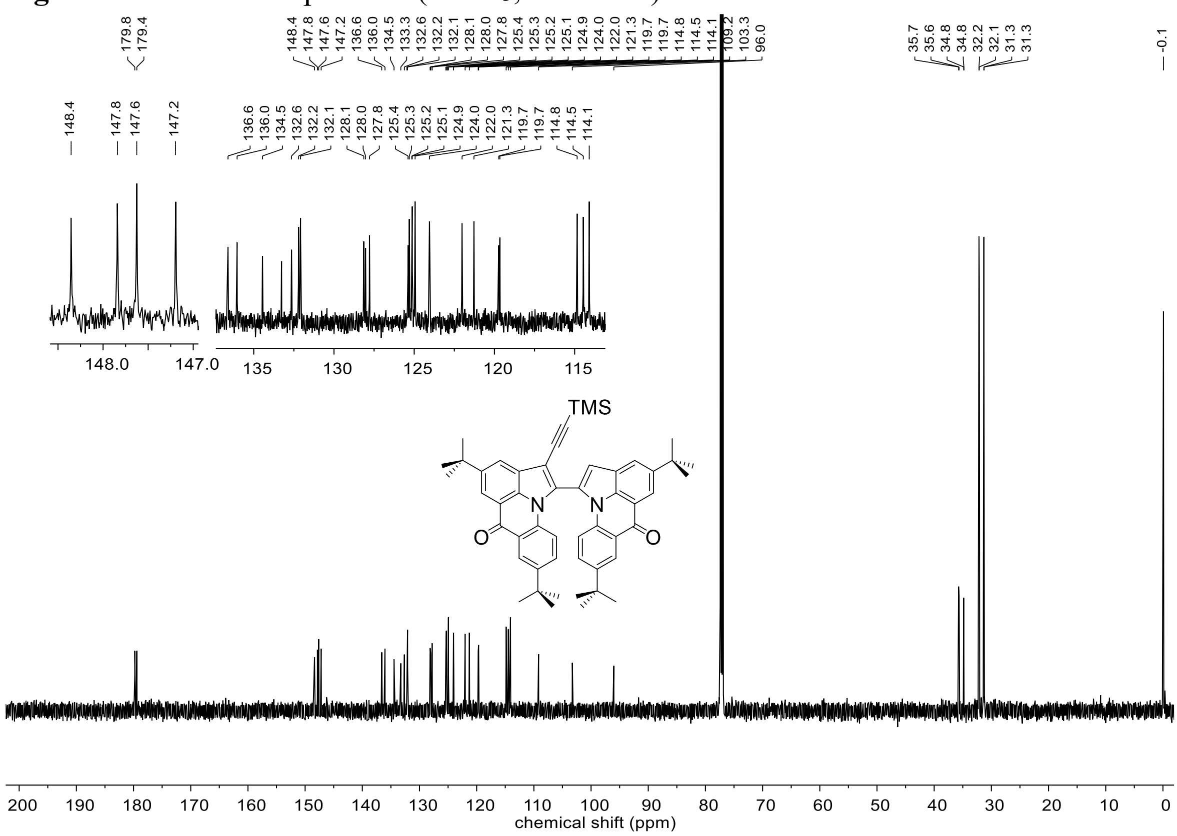


Figure S22. ^{13}C NMR spectrum ($CDCl_3$, 150 MHz) of **14**

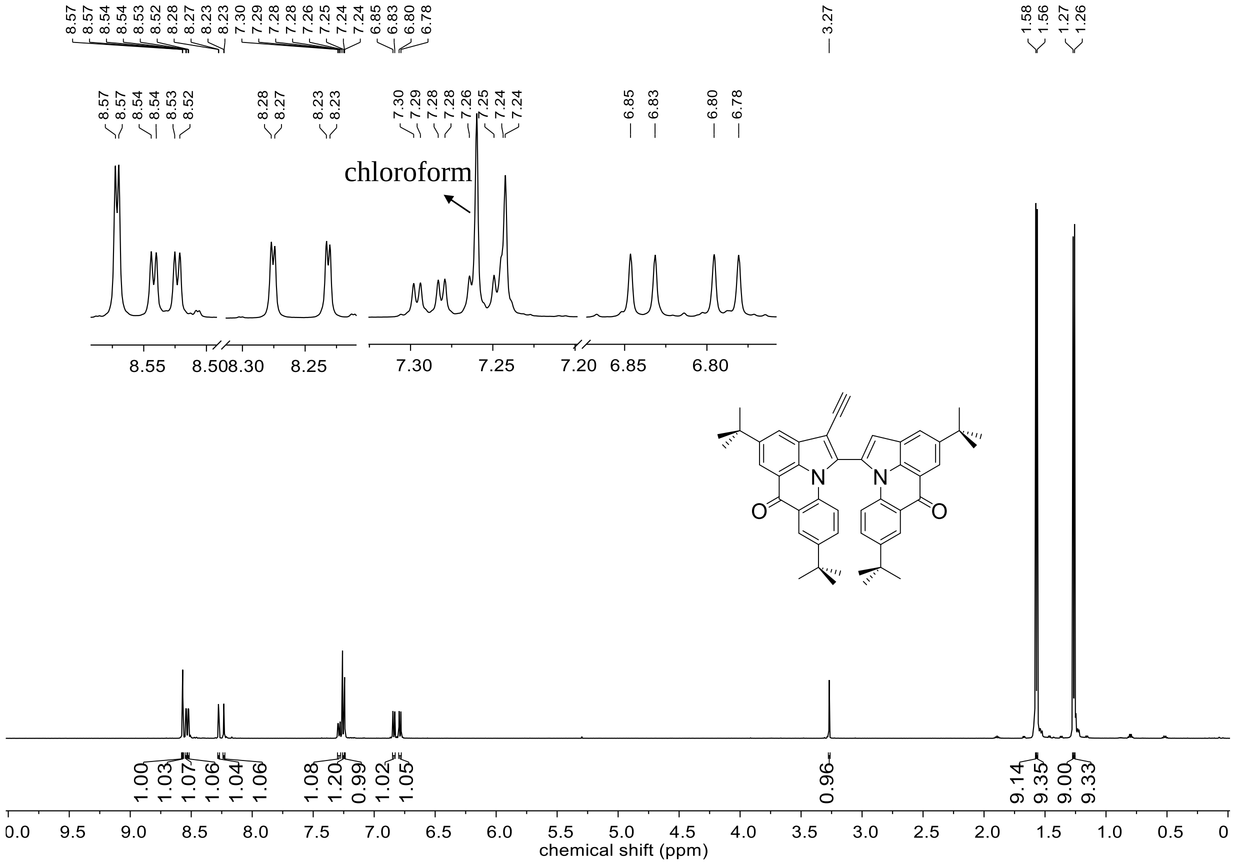


Figure S23. ^{1}H NMR spectrum ($CDCl_3$, 600 MHz) of 1**5**

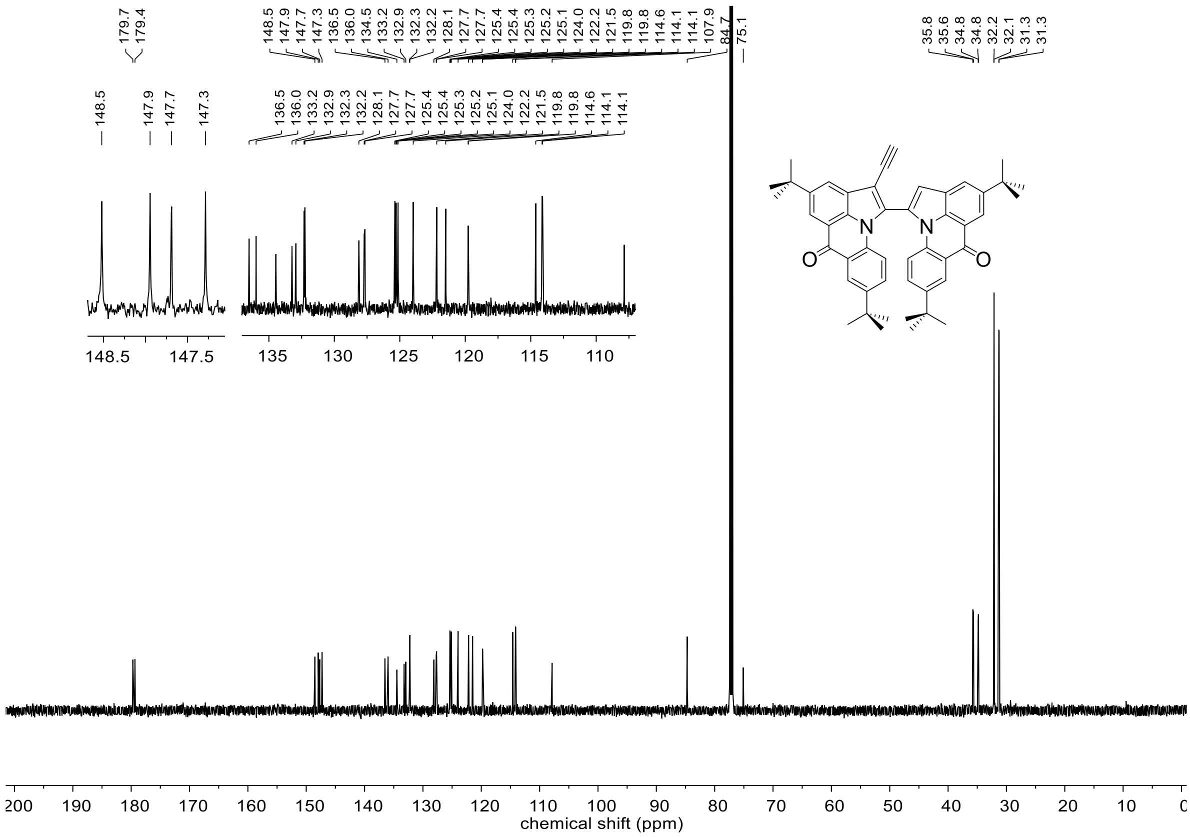


Figure S24. ^{13}C NMR spectrum ($CDCl_3$, 150 MHz) of **15**

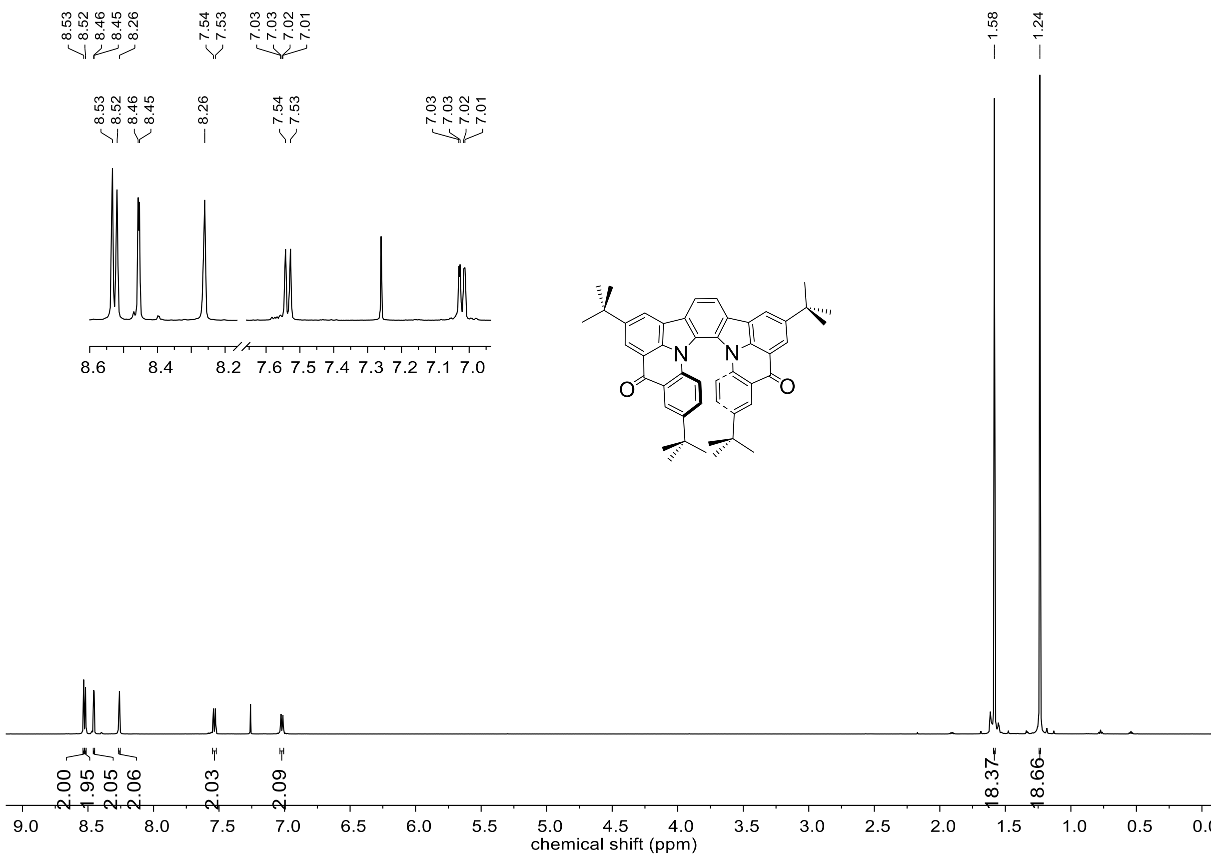


Figure S25. ^{1}H NMR spectrum ($CDCl_3$, 600 MHz) of **3**

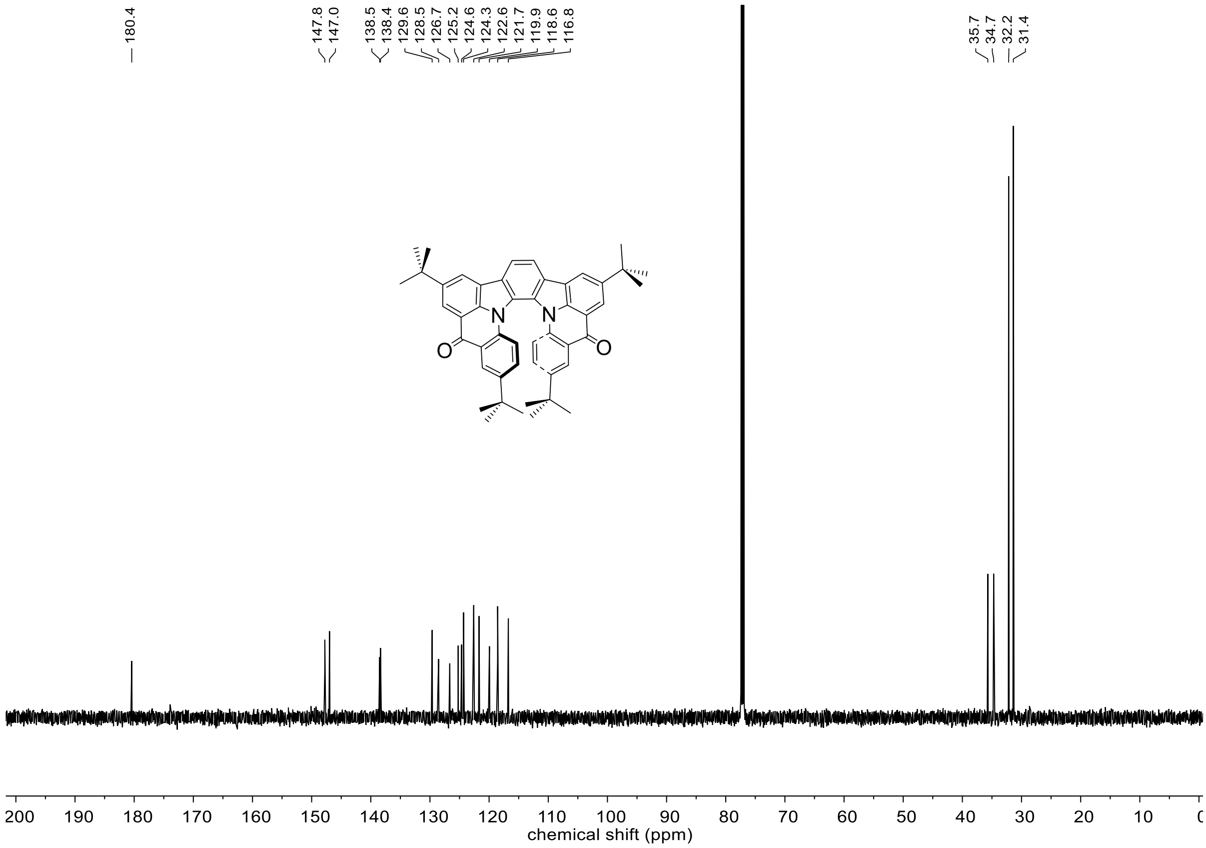


Figure S26. ^{13}C NMR spectrum ($CDCl_3$, 150 MHz) of **3**

4. Fluorescence spectra

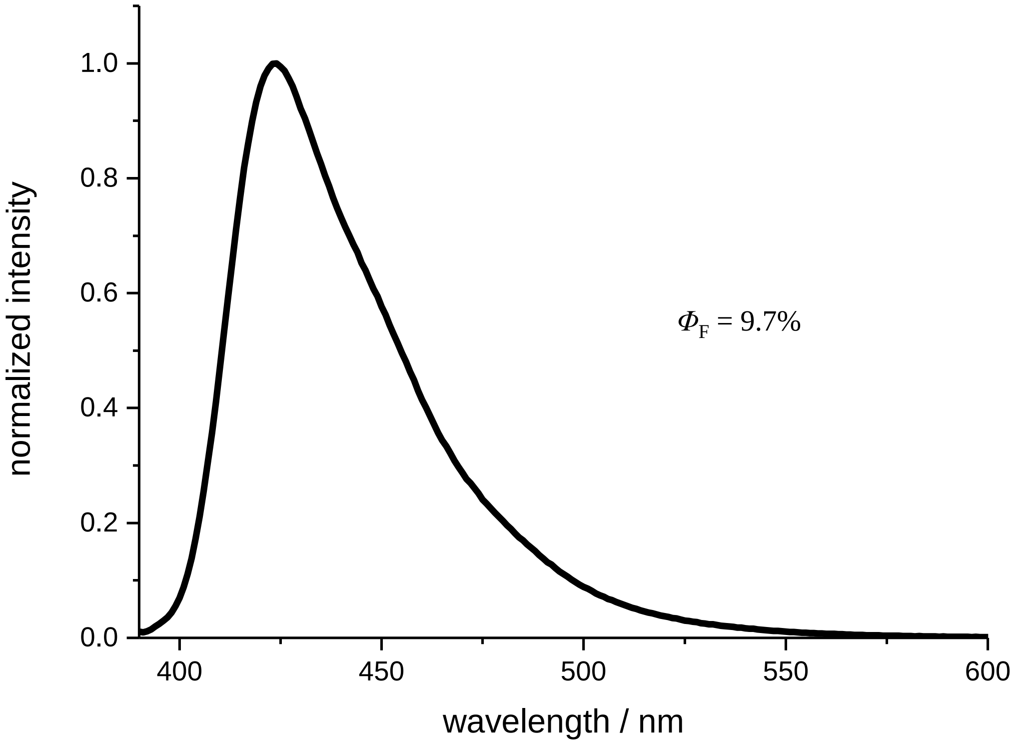


Figure S27. Normalized emission spectra of **9** in dichloromethane (concentration: 5 μM).

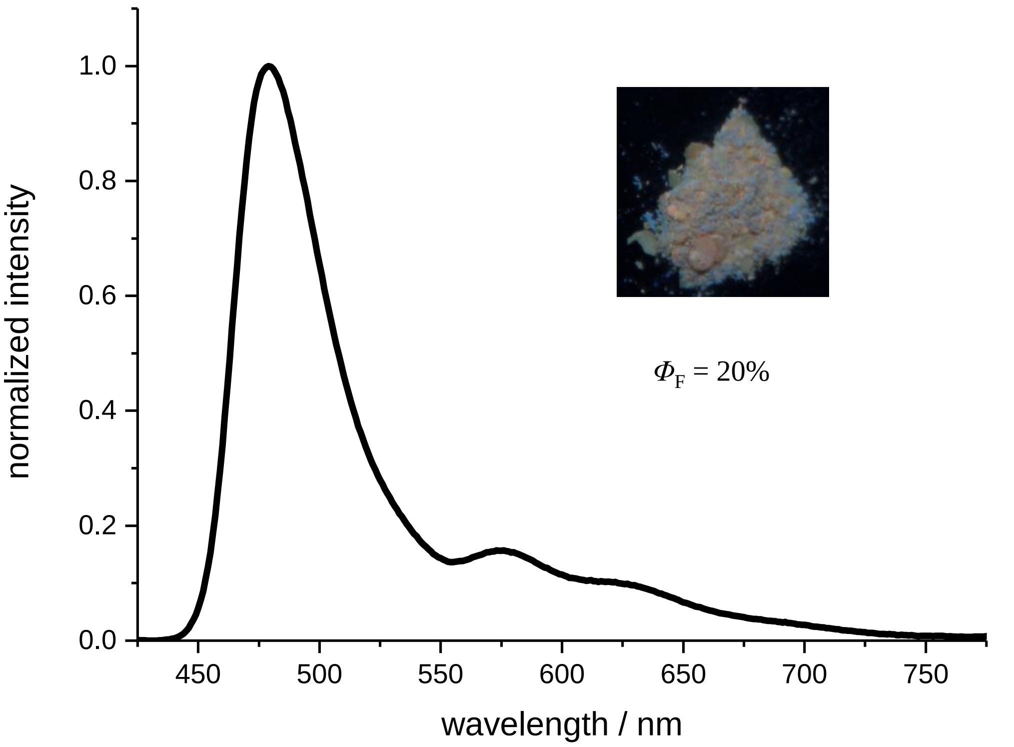


Figure S28. Normalized emission spectra of **9** in solid state.

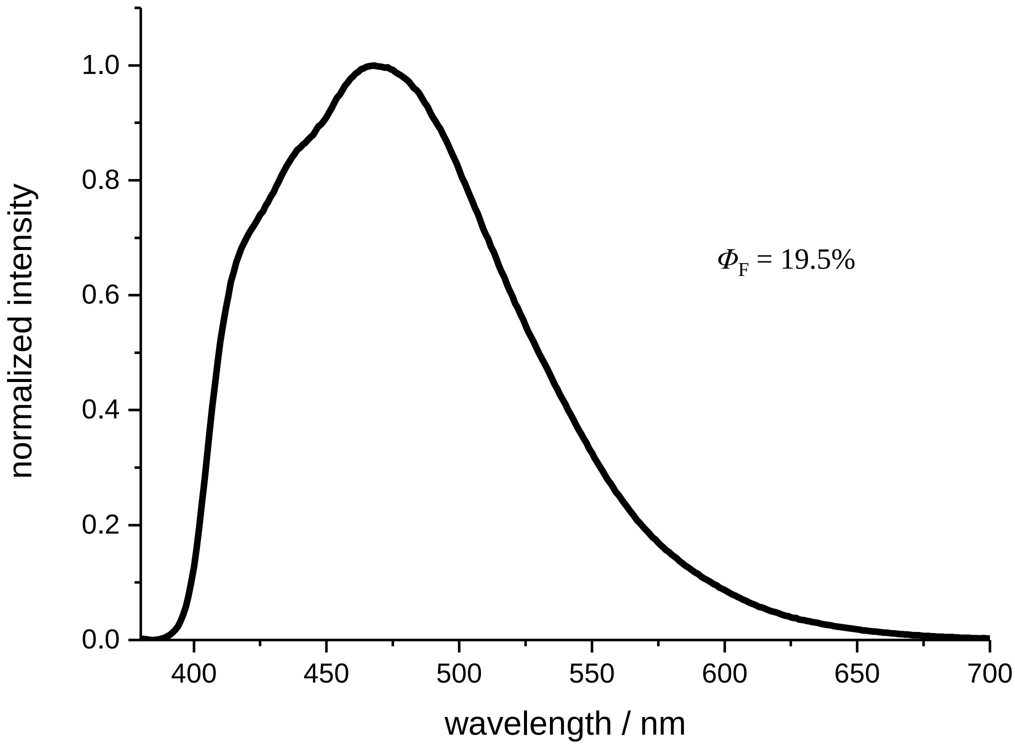


Figure S29. Normalized emission spectra of **11** in dichloromethane (concentration: 5 μM).

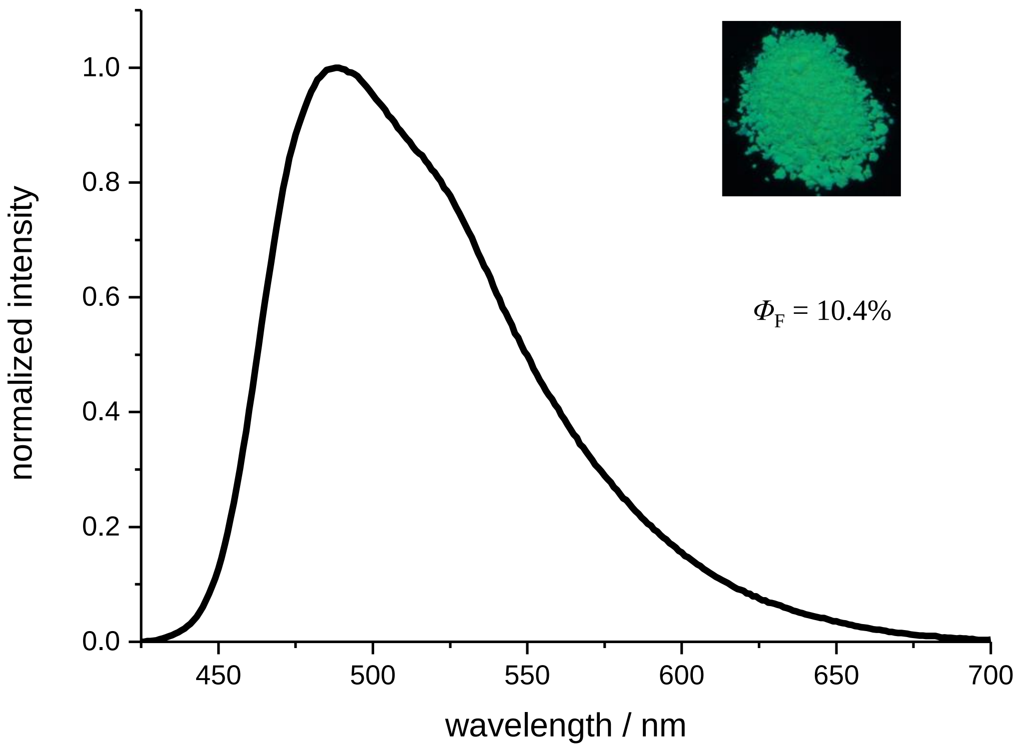


Figure S30. Normalized emission spectra of **11** in solid state.

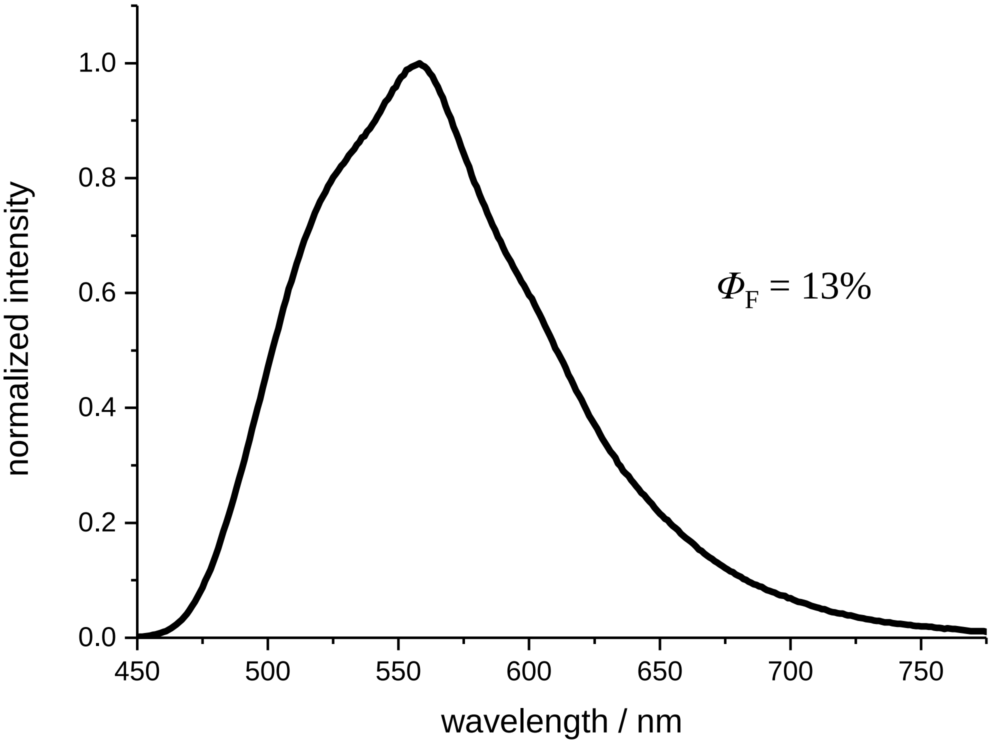


Figure S31. Normalized emission spectra of **2** in dichloromethane (concentration: 5 μM).

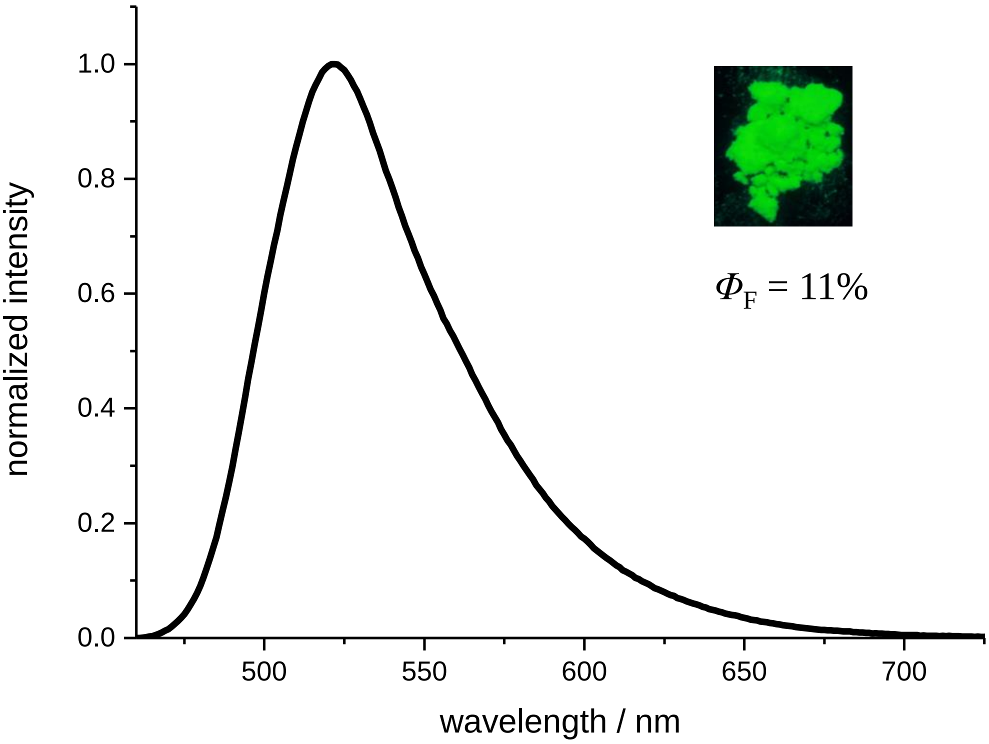


Figure S32. Normalized emission spectra of **2** in solid state.

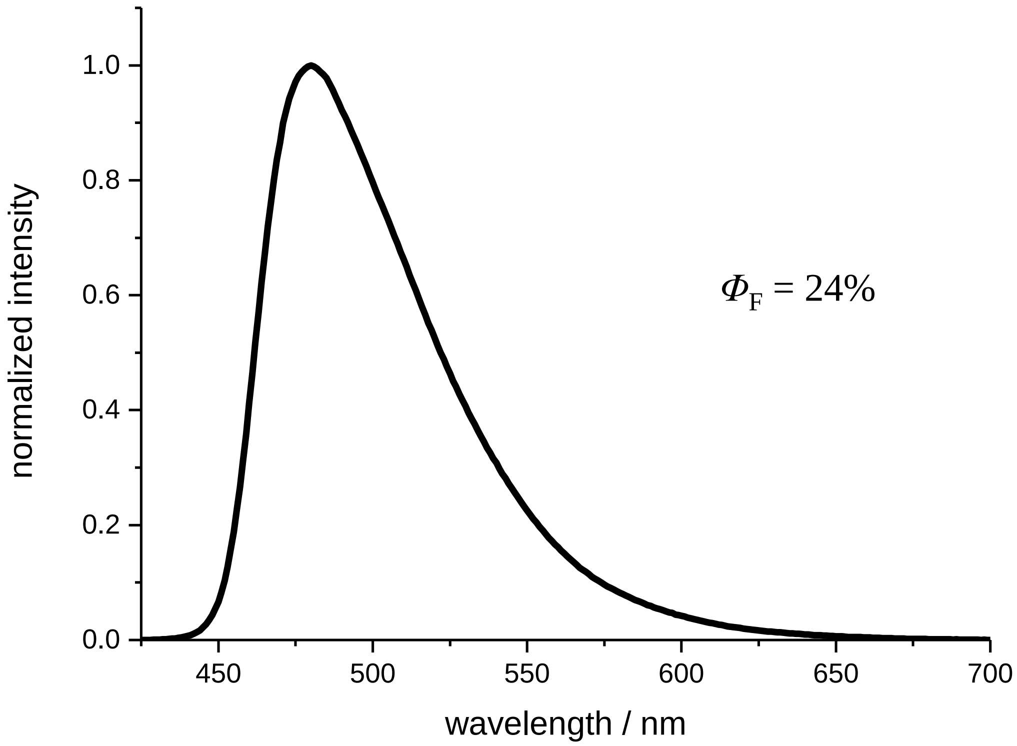


Figure S33. Normalized emission spectra of **3** in dichloromethane (concentration: 5 μM).

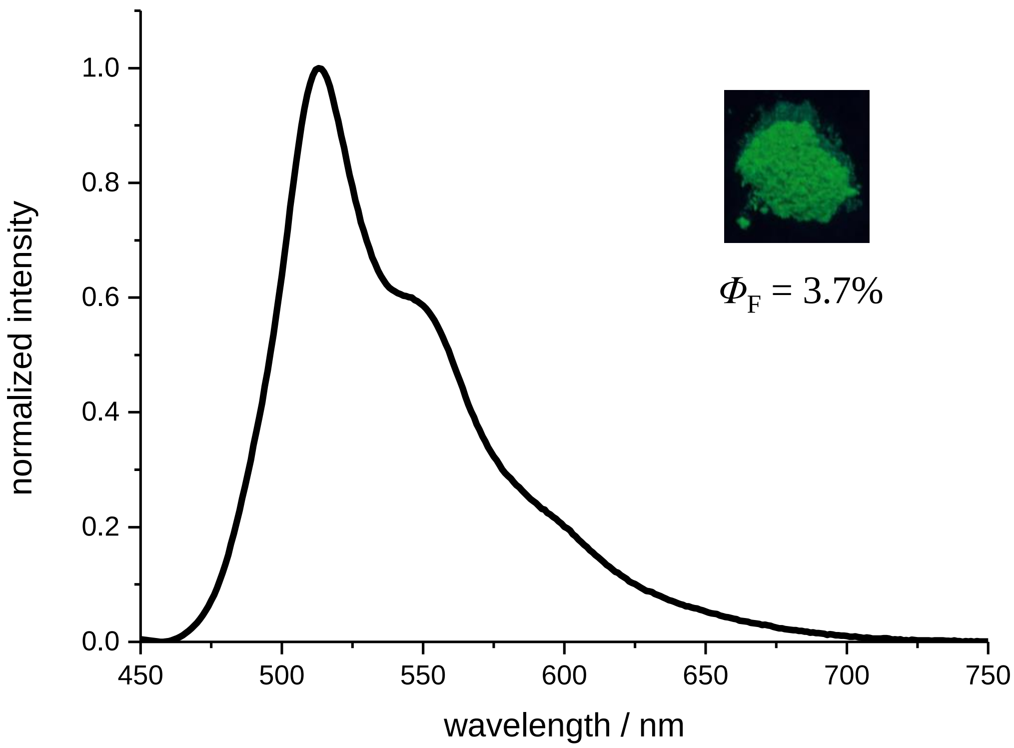


Figure S34. Normalized emission spectra of **3** in solid state.

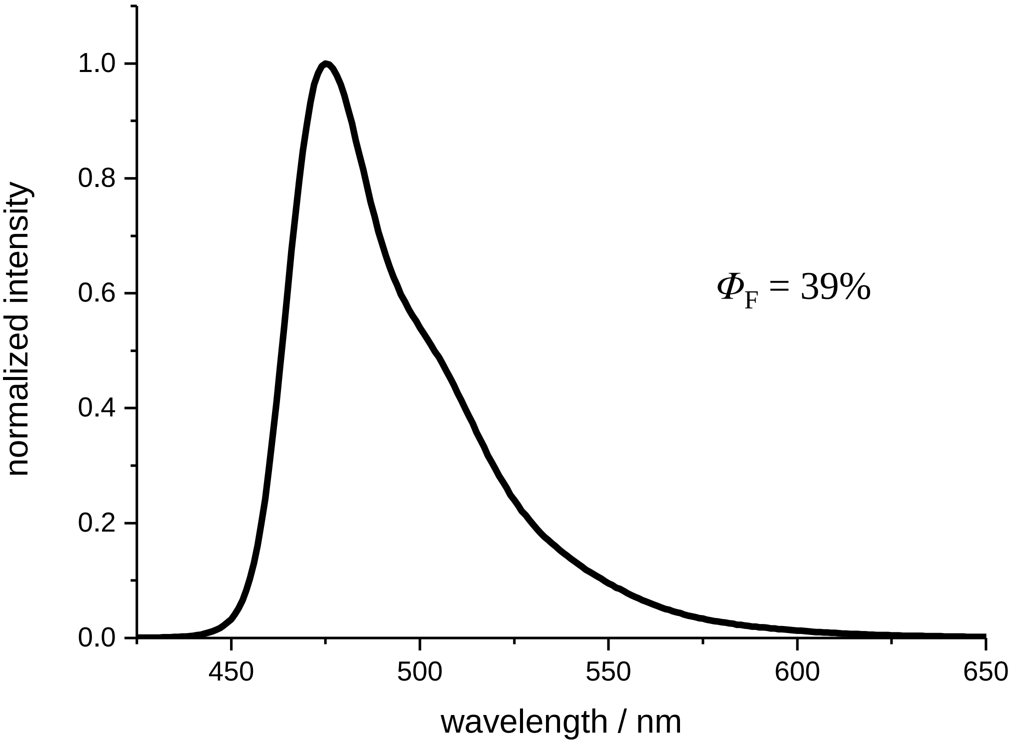


Figure S35. Normalized emission spectra of **4** in dichloromethane (concentration: 5 μM).

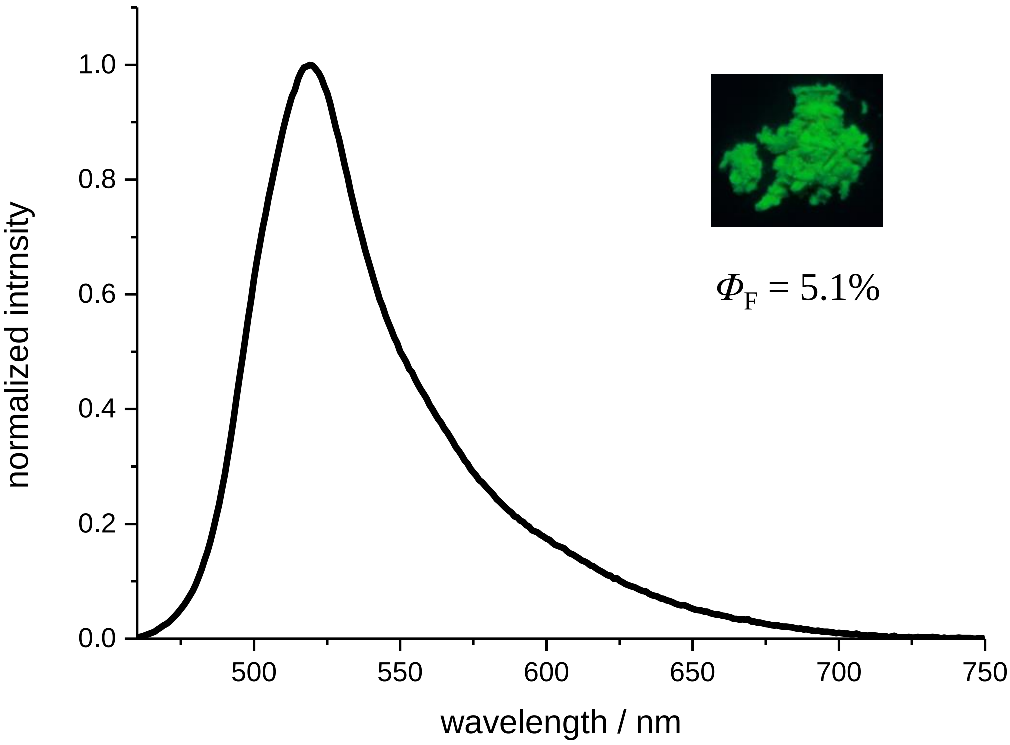
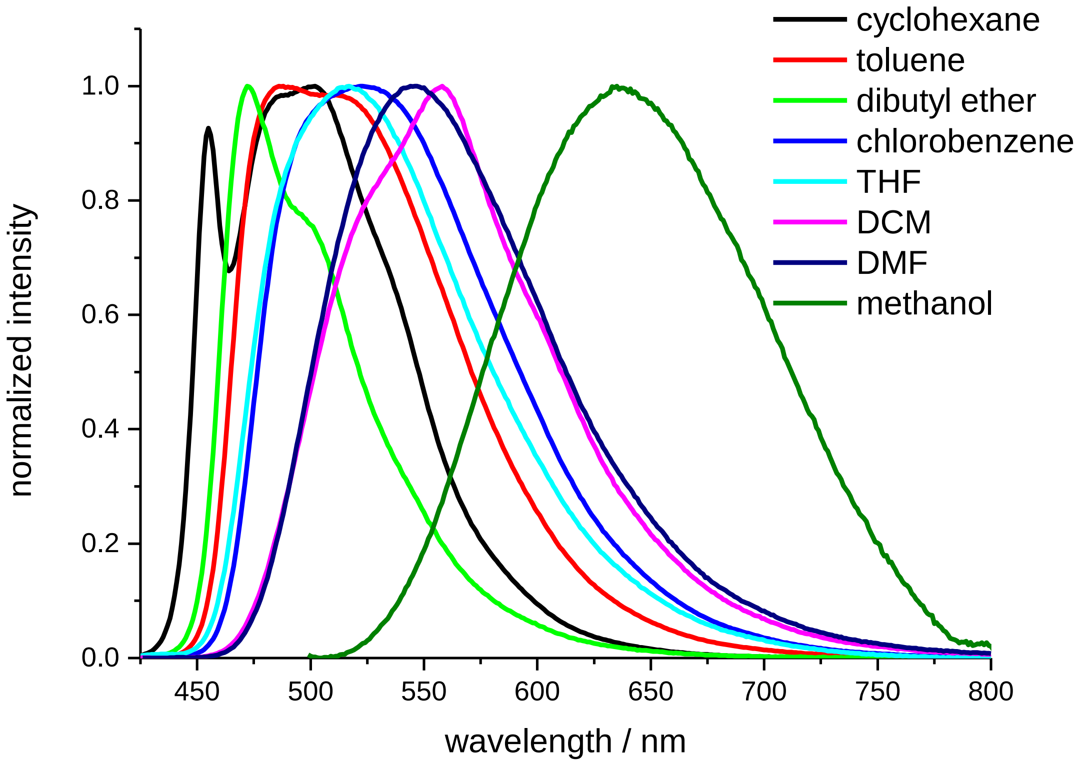


Figure S36 Normalized emission spectra of **4** in solid state.



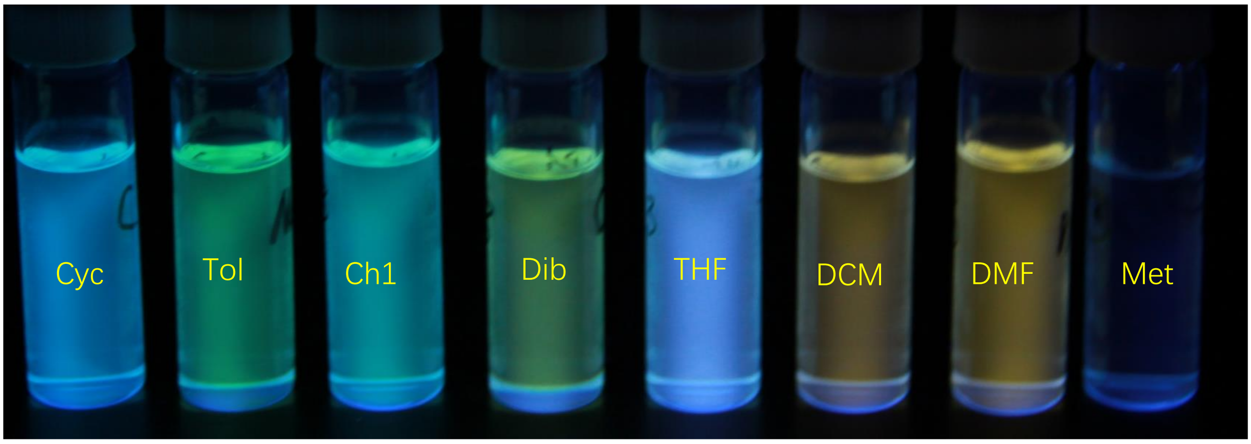
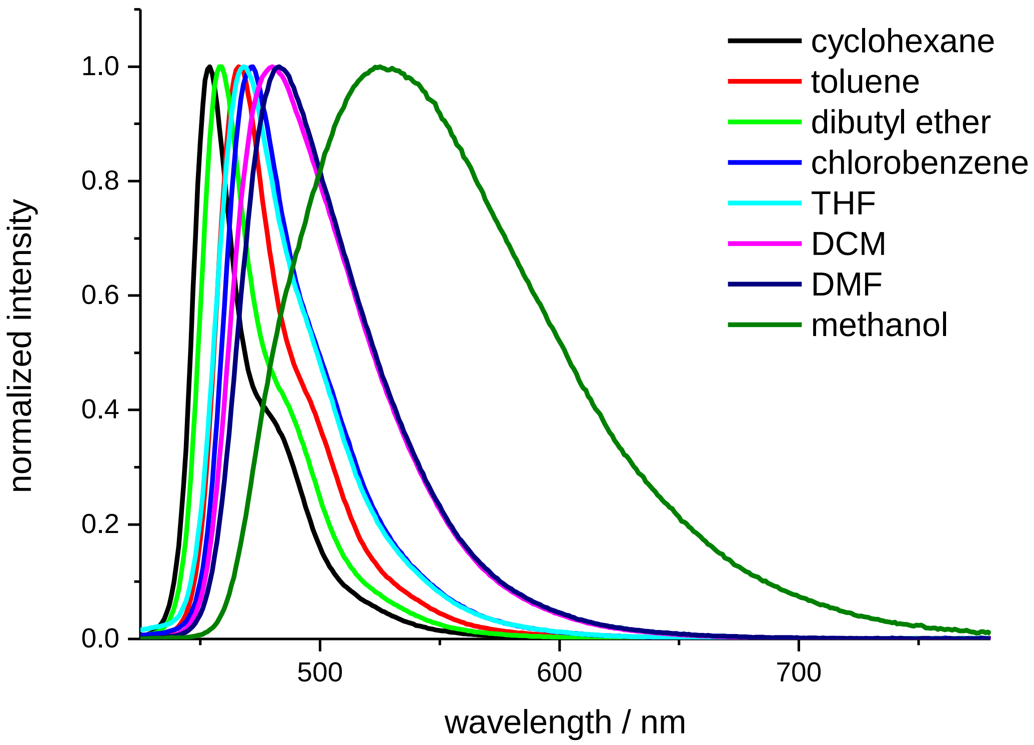


Figure S37. Normalized emission spectra of **2** in different solvents at room temperature, concentration: 5 μM and the photographs of **2** in different solvents under 365 nm UV light.



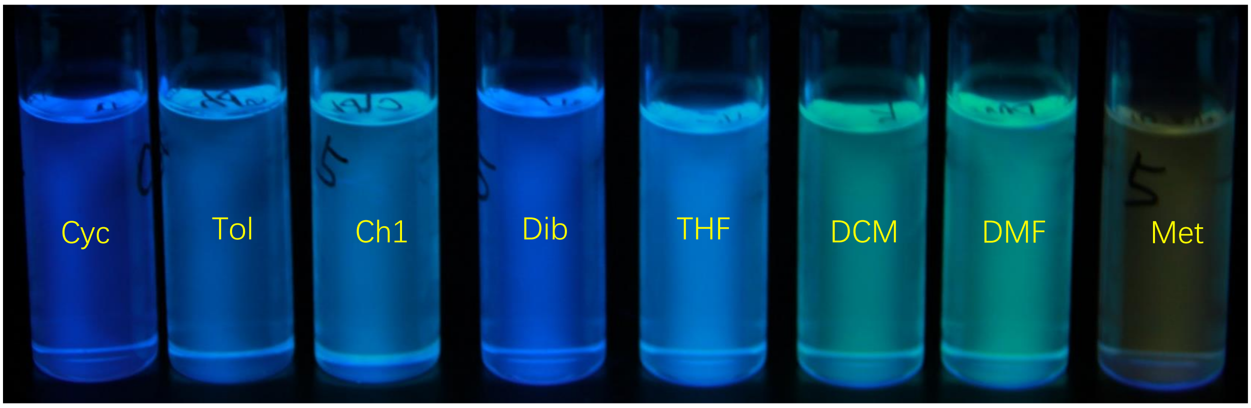
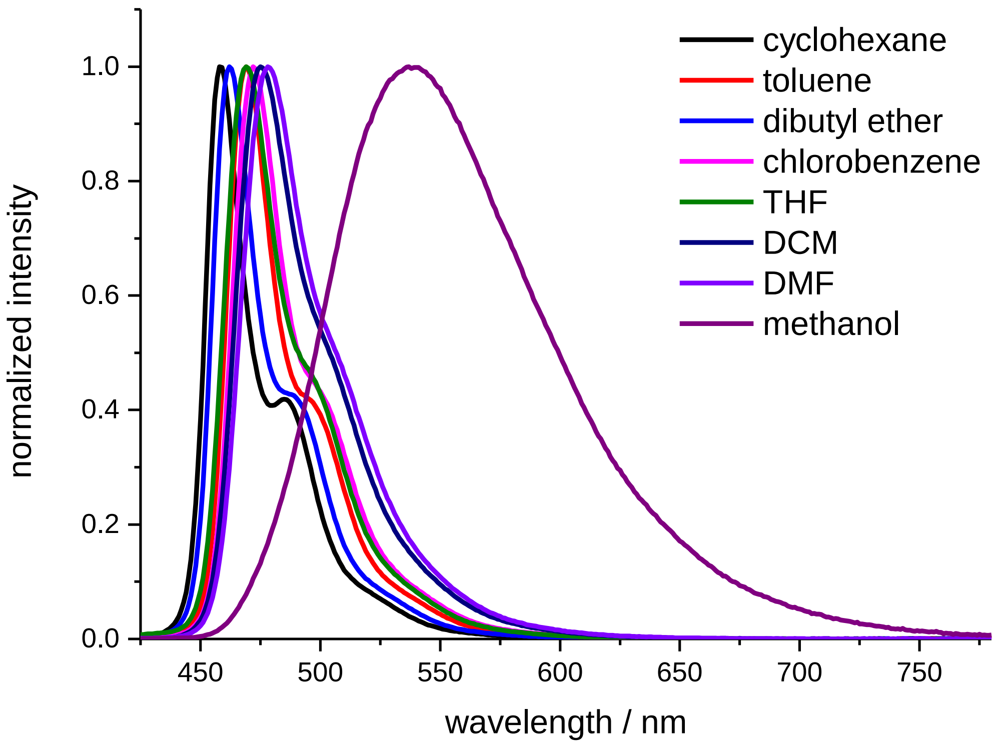


Figure S38. Normalized emission spectra of **3** in different solvents at room temperature, concentration: 5 µM and the photographs of **3** in different solvents under 365 nm UV light.



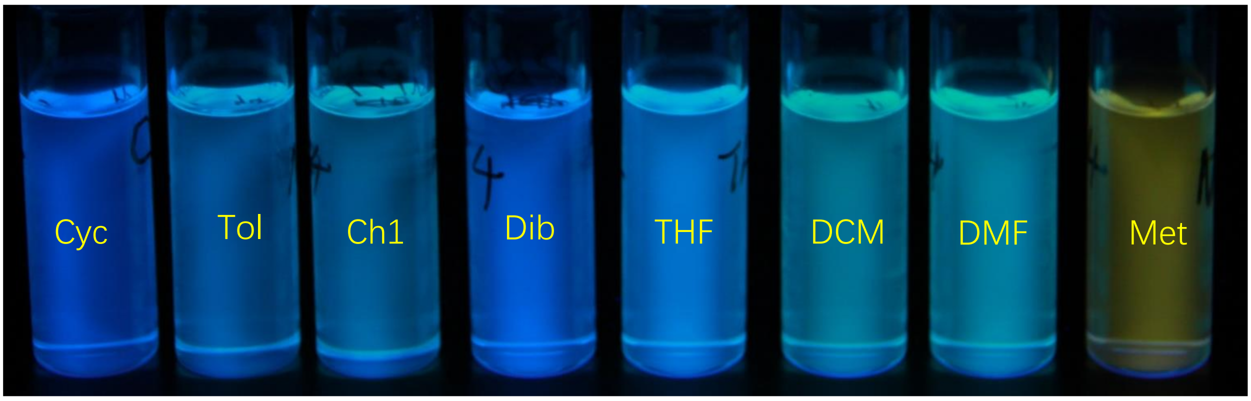


Figure S39. Normalized emission spectra of **4** in different solvents at room temperature, concentration: 5 μM and the photographs of **4** in different solvents under 365 nm UV light.

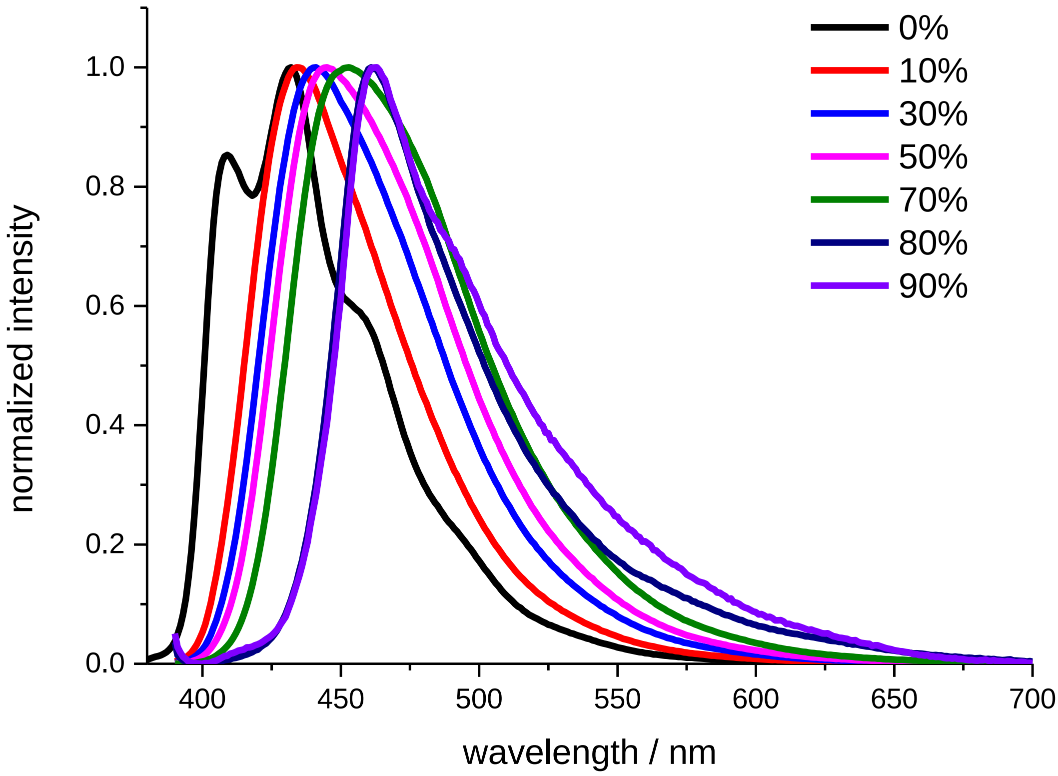


Figure S40. Fluorescence emission spectra of **9** in the mixture of water/THF with different water contents. Solutions concentration: 10 μM.

5. Fluorescence decay curves

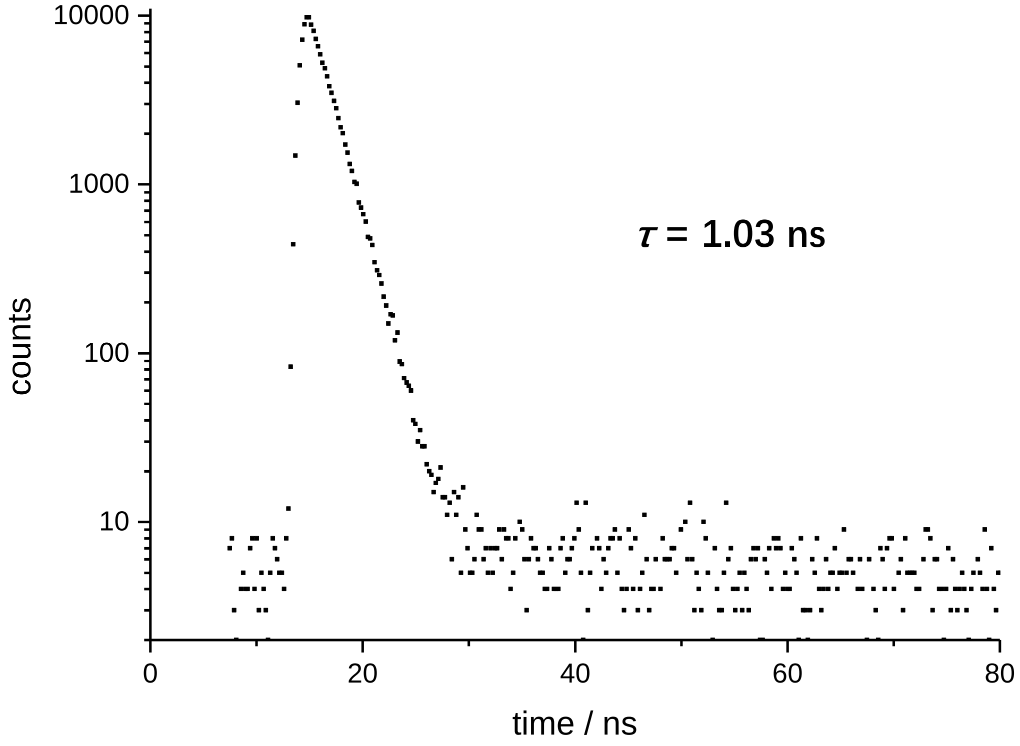


Figure S41. Fluorescence decay curve of **9** in dichloromethane at room temperature (concentration: 5 μM).

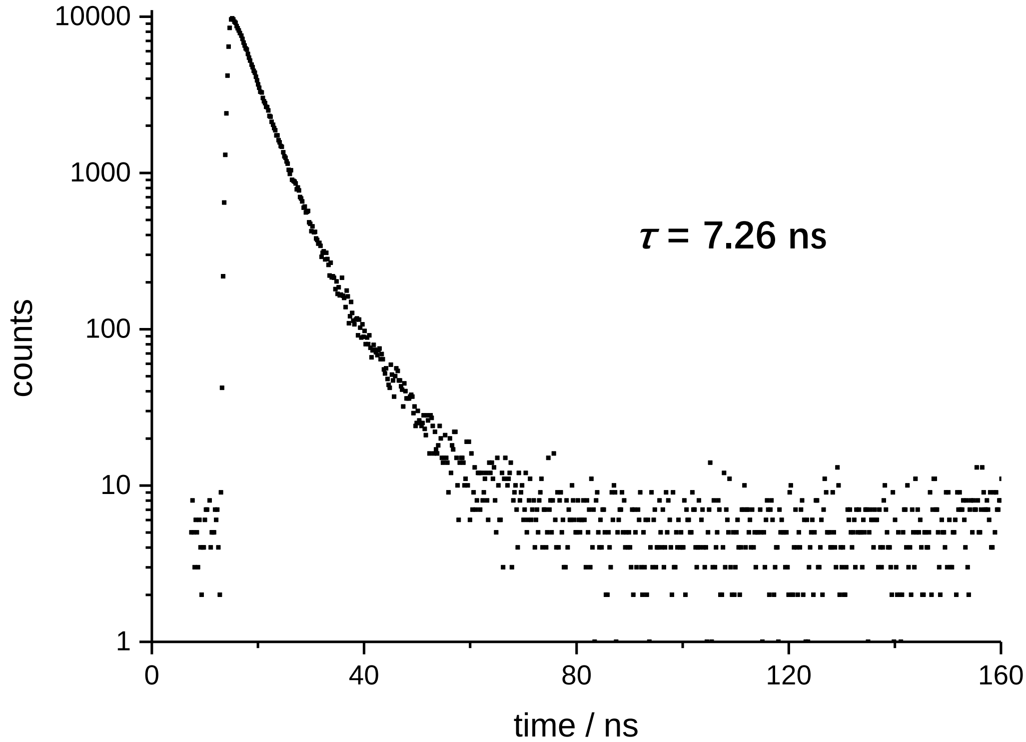


Figure S42. Fluorescence decay curve of **9** in solid state at room temperature .

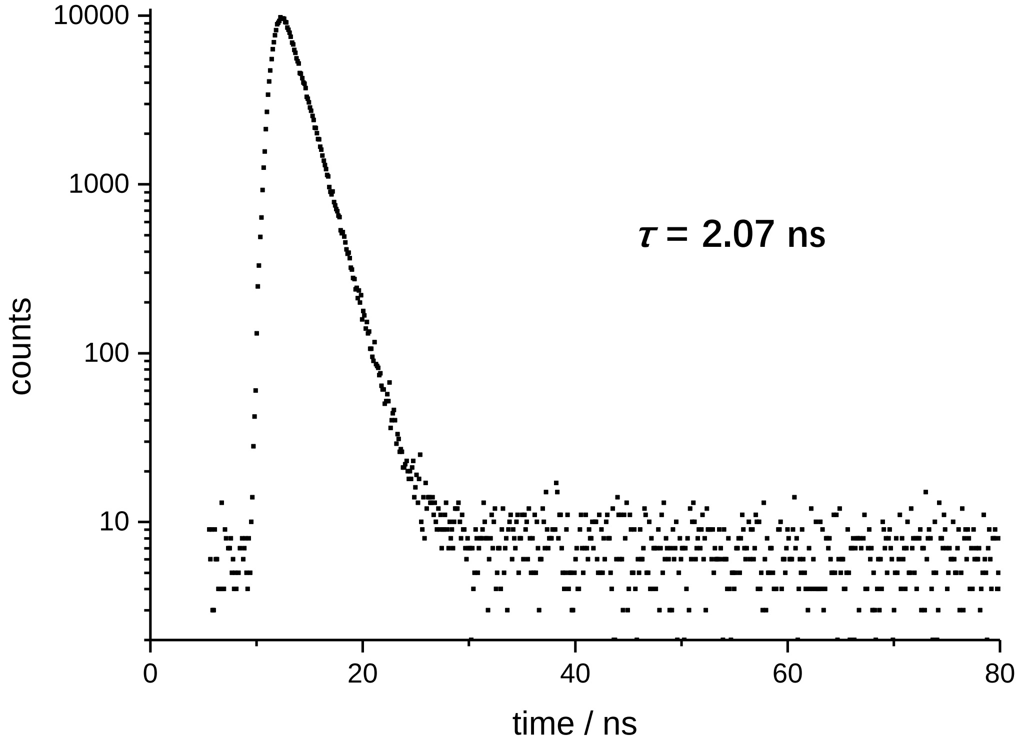


Figure S43. Fluorescence decay curve of **11** in dichloromethane at room temperature (concentration: 5 μM).

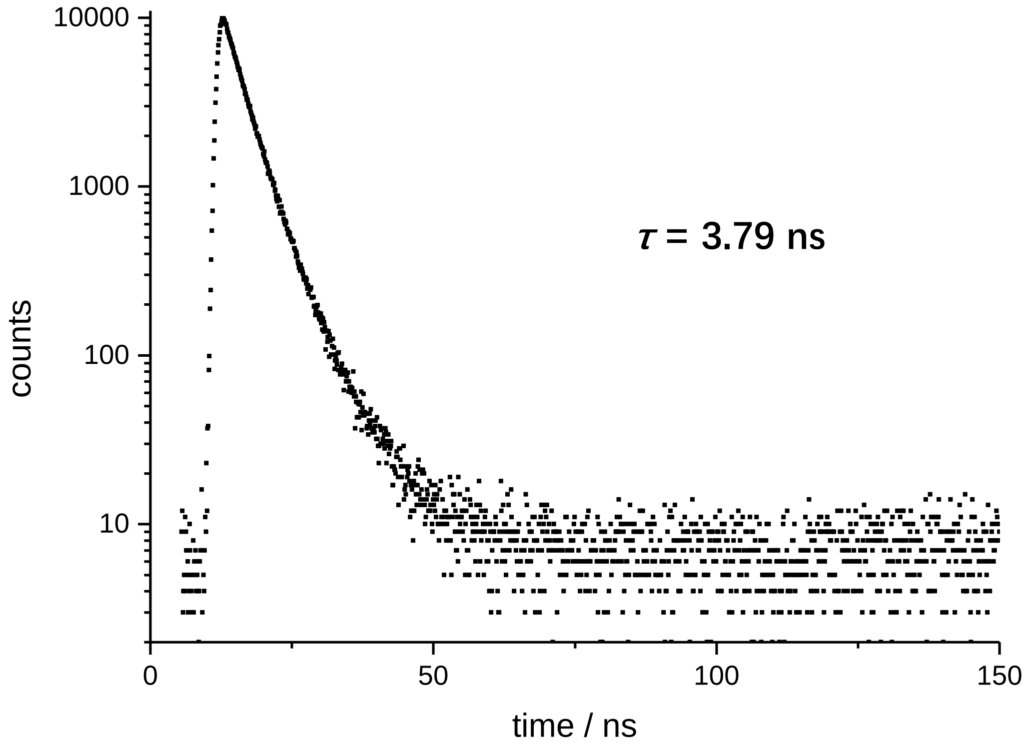


Figure S44. Fluorescence decay curve of **11** in solid state at room temperature.

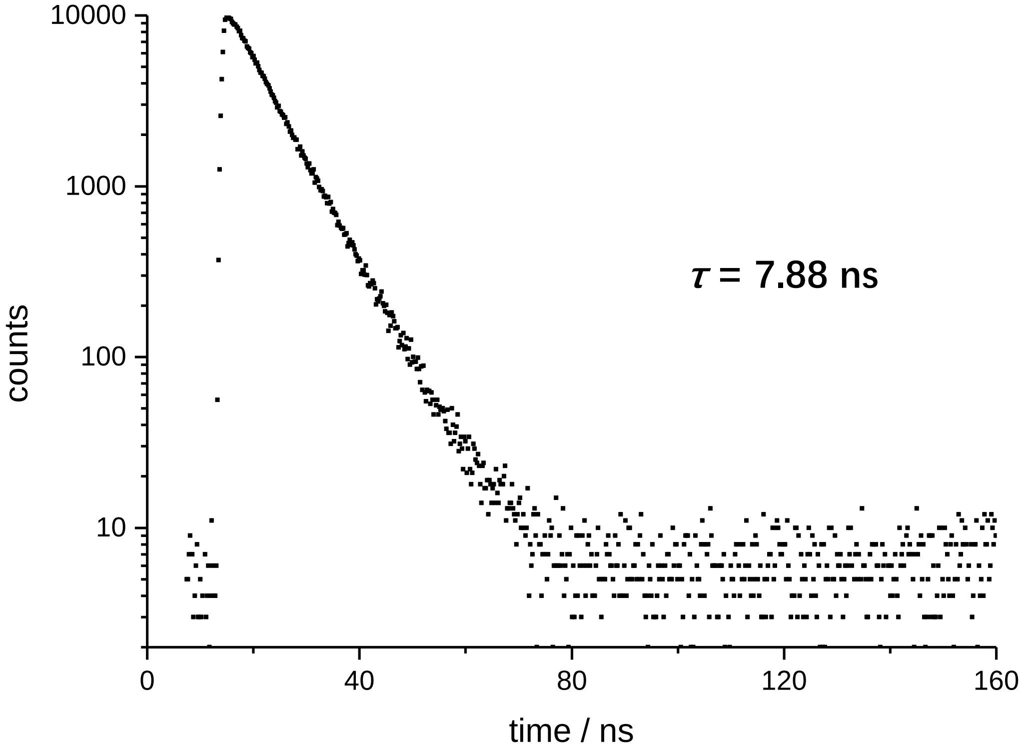


Figure S45. Fluorescence decay curve of **2** in dichloromethane at room temperature (concentration: 5 μM).

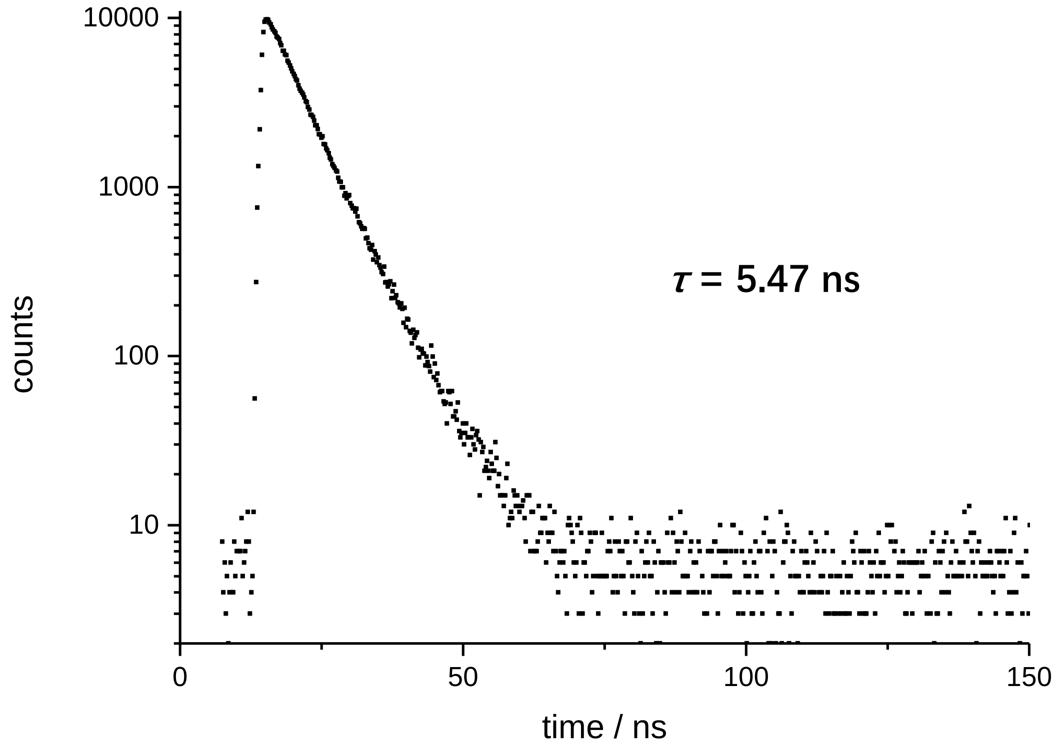


Figure S46. Fluorescence decay curve of **2** in solid state at room temperature.

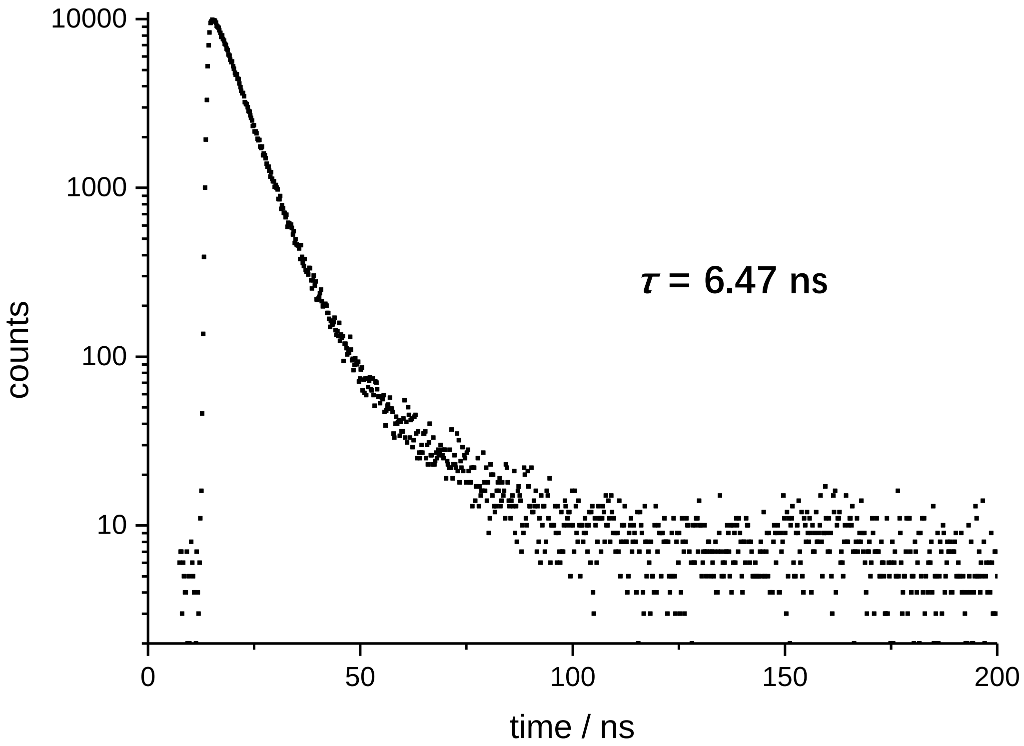


Figure S47. Fluorescence decay curve of **3** in dichloromethane at room temperature (concentration: 5 μM).

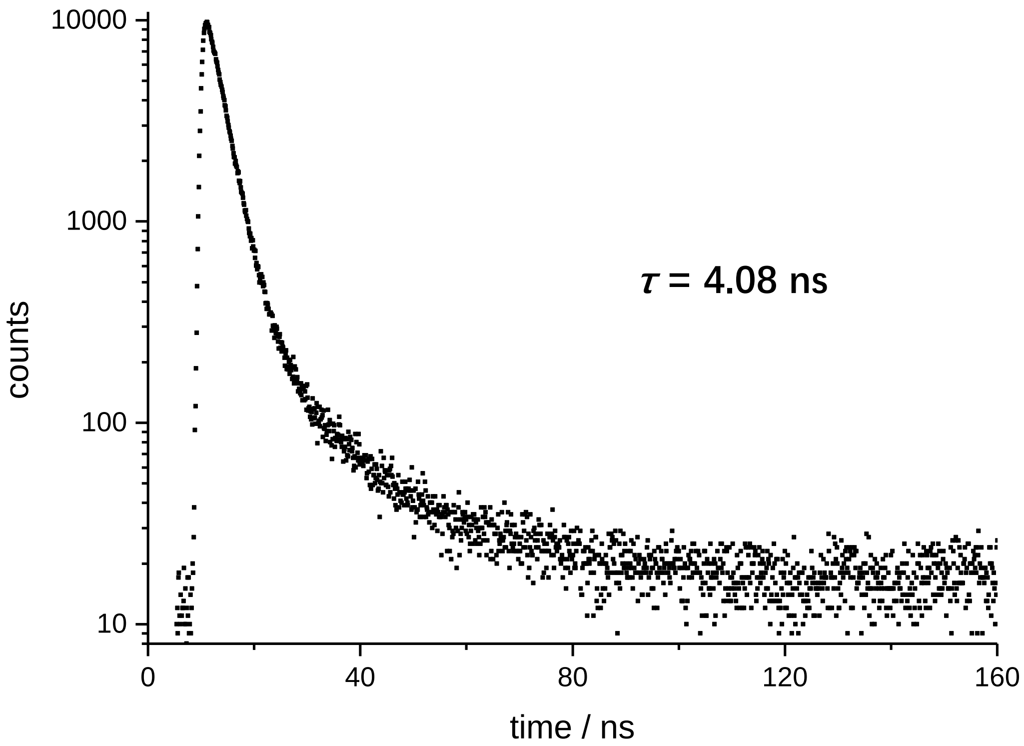


Figure S48. Fluorescence decay curve of **3** in solid state at room temperature.

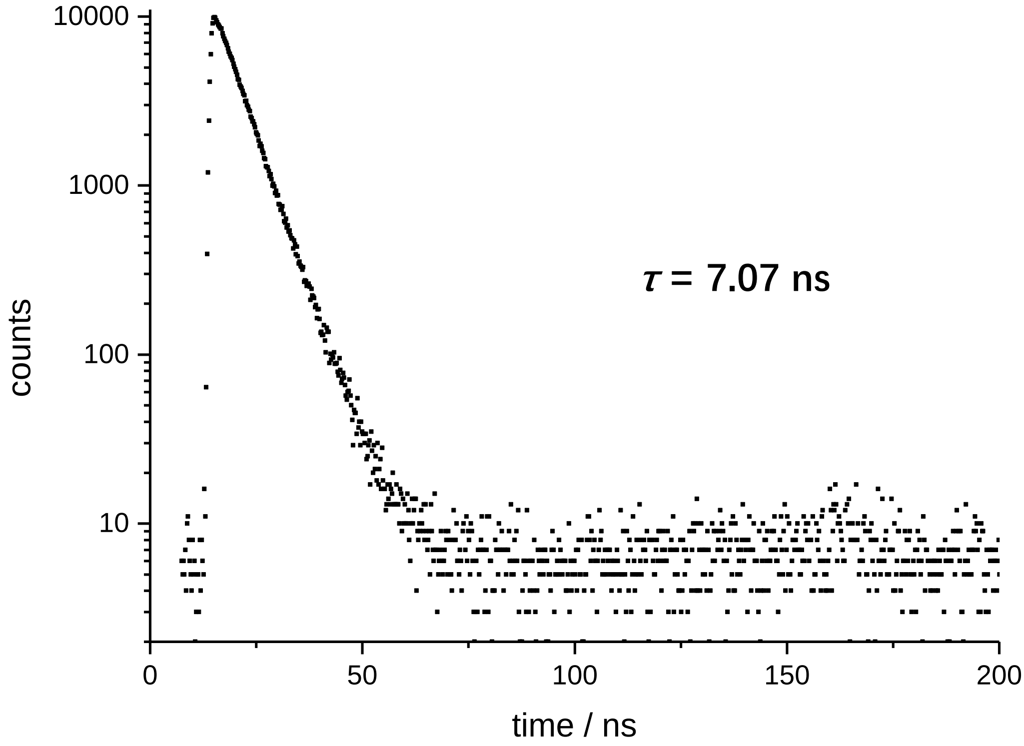


Figure S49. Fluorescence decay curve of **4** in dichloromethane at room temperature (concentration: 5 μM).

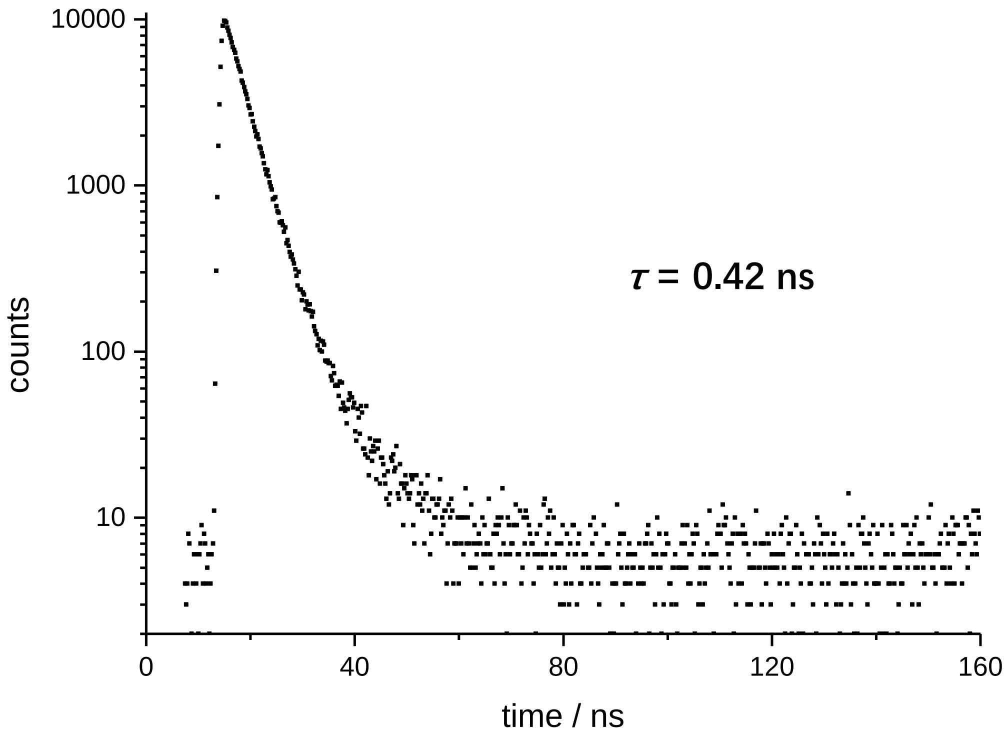


Figure S50. Fluorescence decay curve of **4** in solid state at room temperature.

6. UV/vis absorption spectra

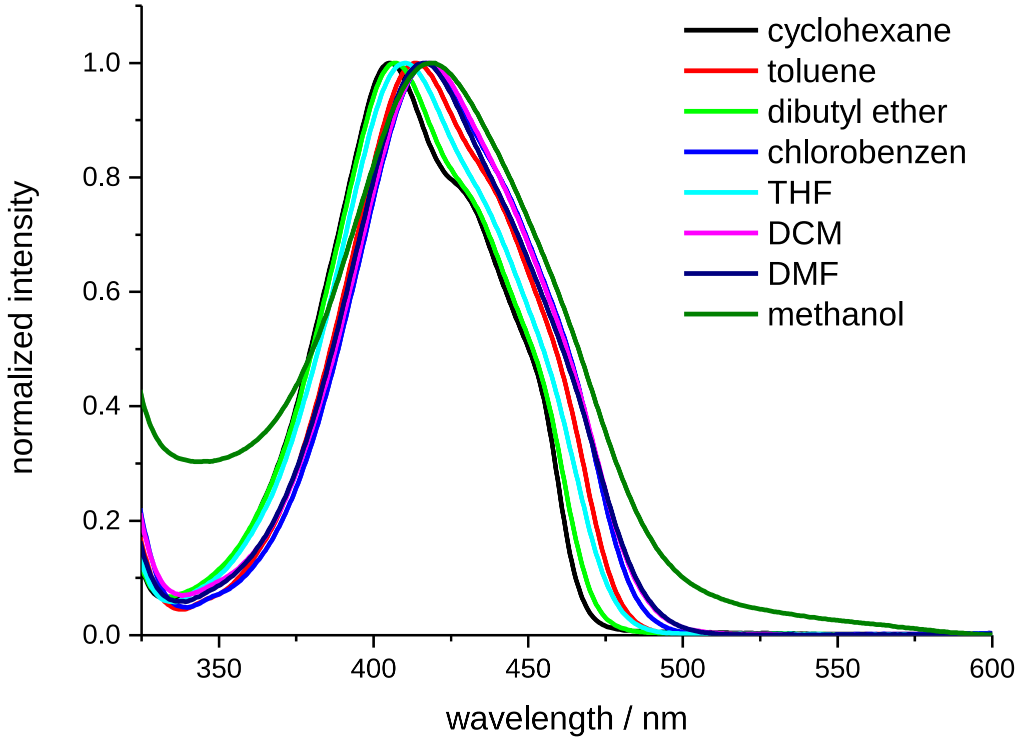


Figure S51. Normalized absorption spectra of **2** in different solvents at room temperature. Solutions concentration: 5 μM.

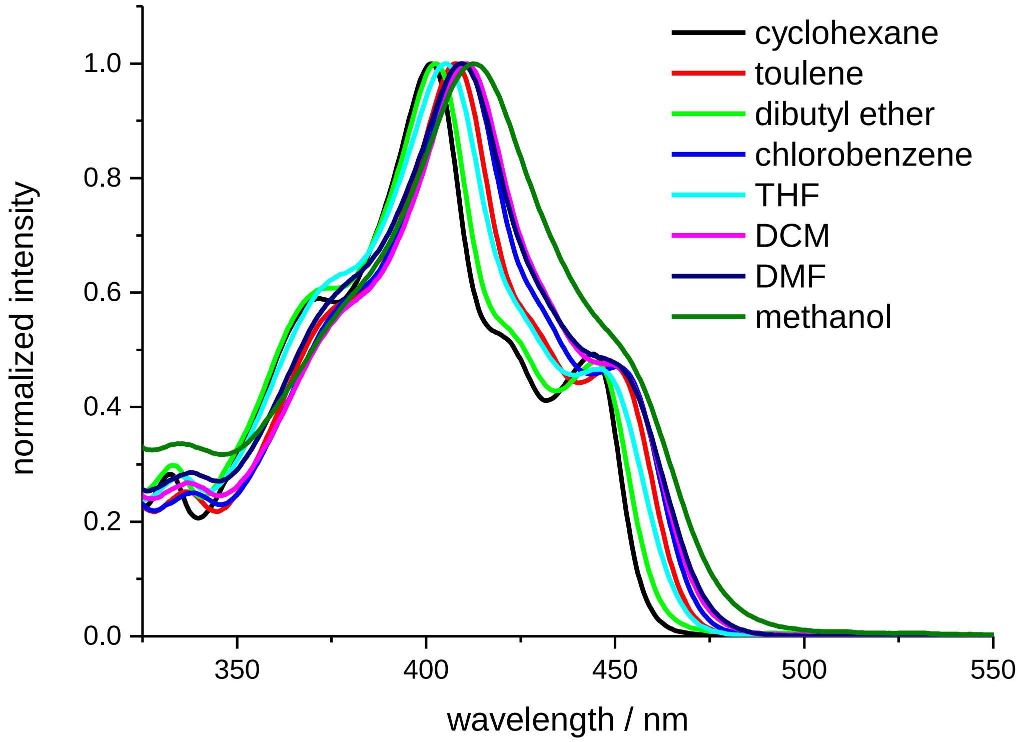


Figure S52. Normalized absorption spectra of **3** in different solvents at room temperature. Solutions concentration: 5 μM.

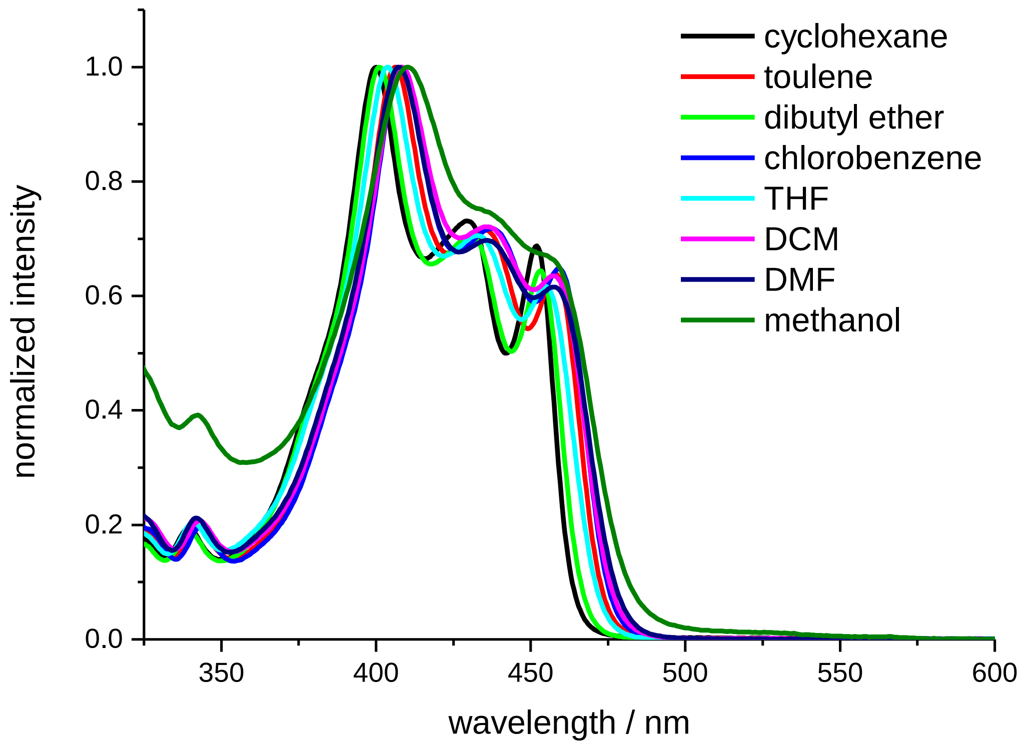


Figure S53. Normalized absorption spectra of **4** in different solvents at room temperature. Solutions concentration: 5 μM.

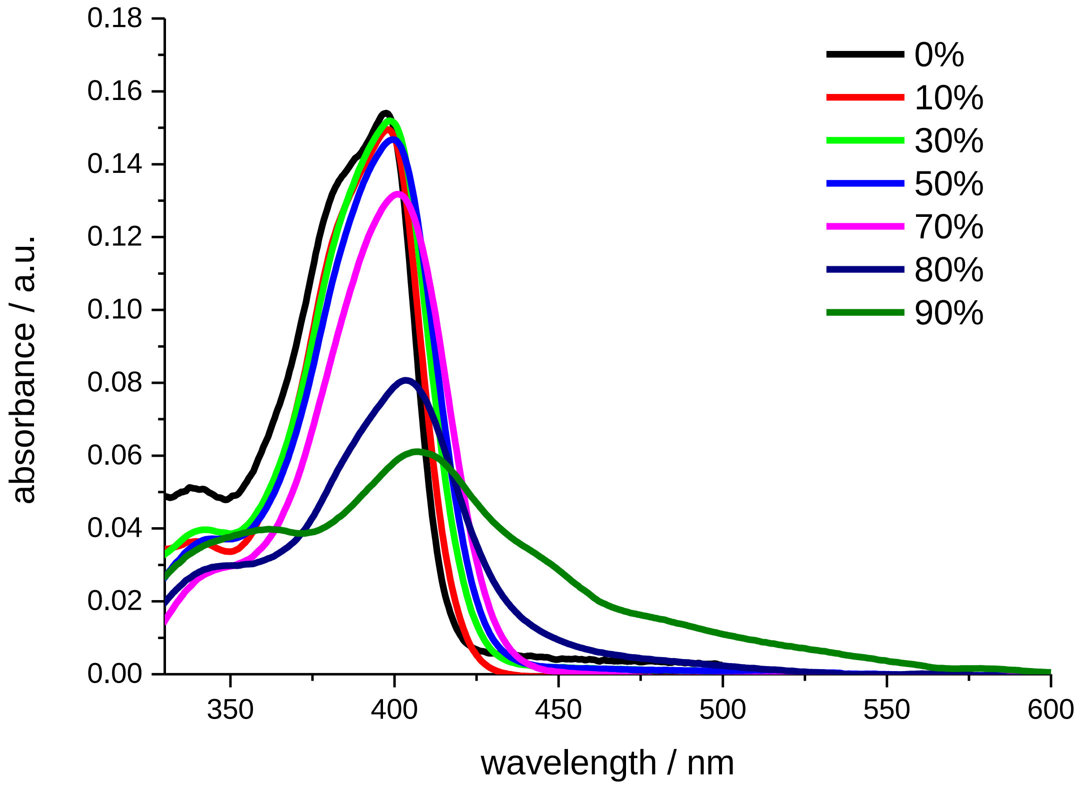


Figure S54. UV/vis absorption spectra of **9** in the mixture of water/THF with different water contenes. Solutions concentration: 10 μM.

7. Lippert−Mataga plots

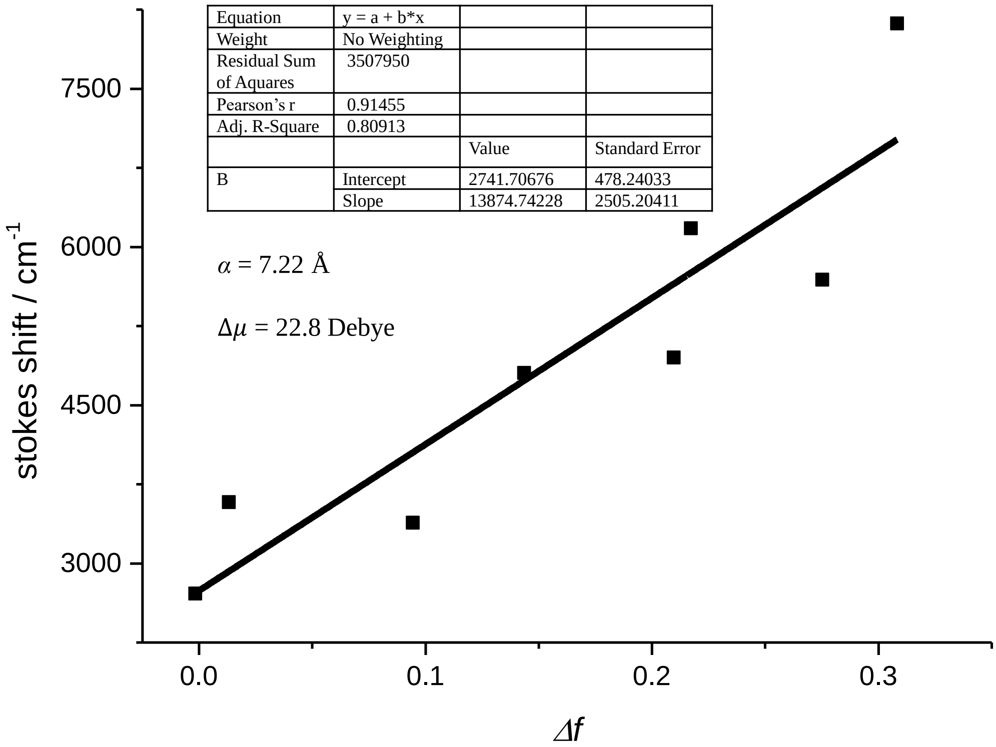


Figure S55. Lippert−Mataga plots, Onsager cavity radius and the calculated difference of dipole moments of **2**.

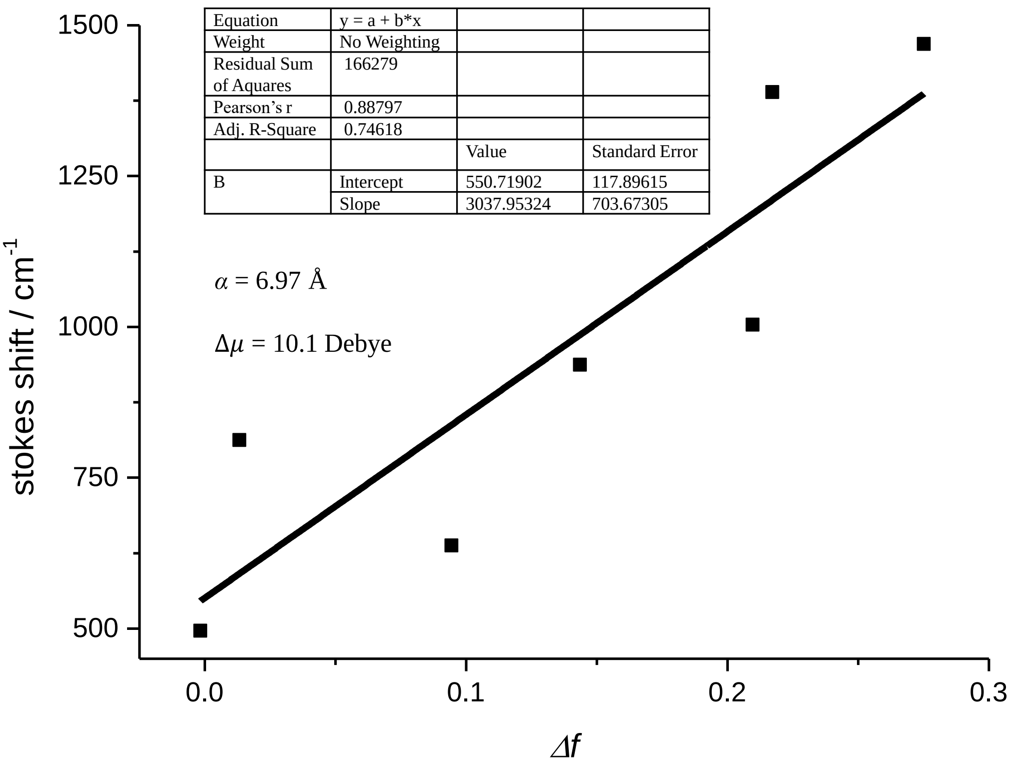


Figure S56. Lippert−Mataga plots, Onsager cavity radius and the calculated difference of dipole moments of **3**.

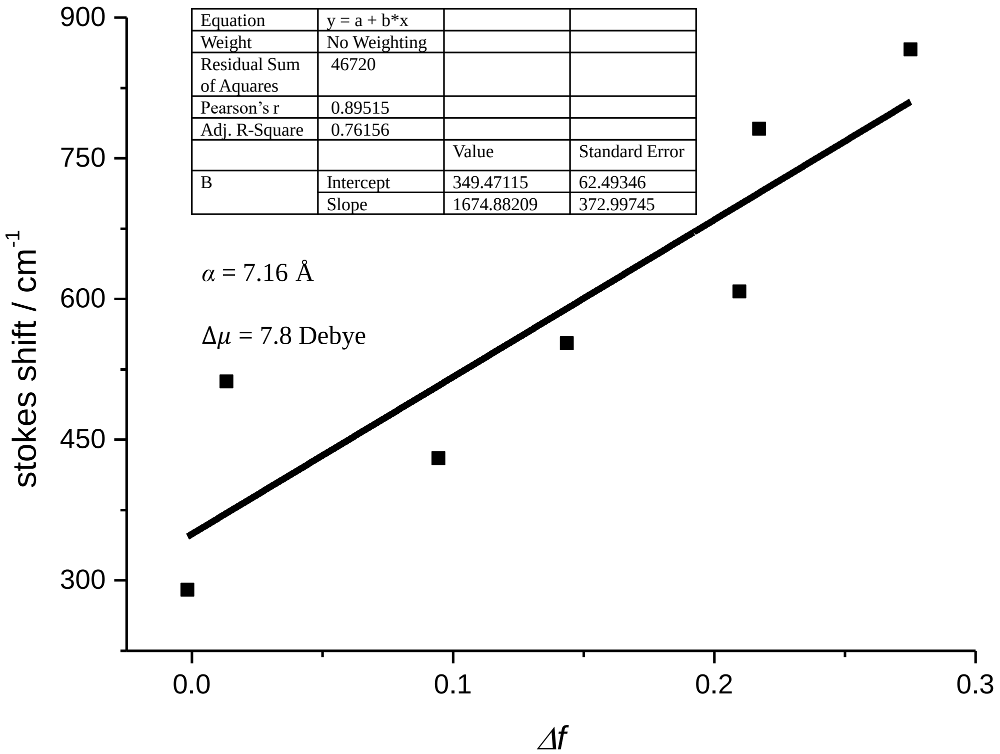


Figure S57. Lippert−Mataga plots, Onsager cavity radius and the calculated difference of dipole moments of **4**.

8. CV curves

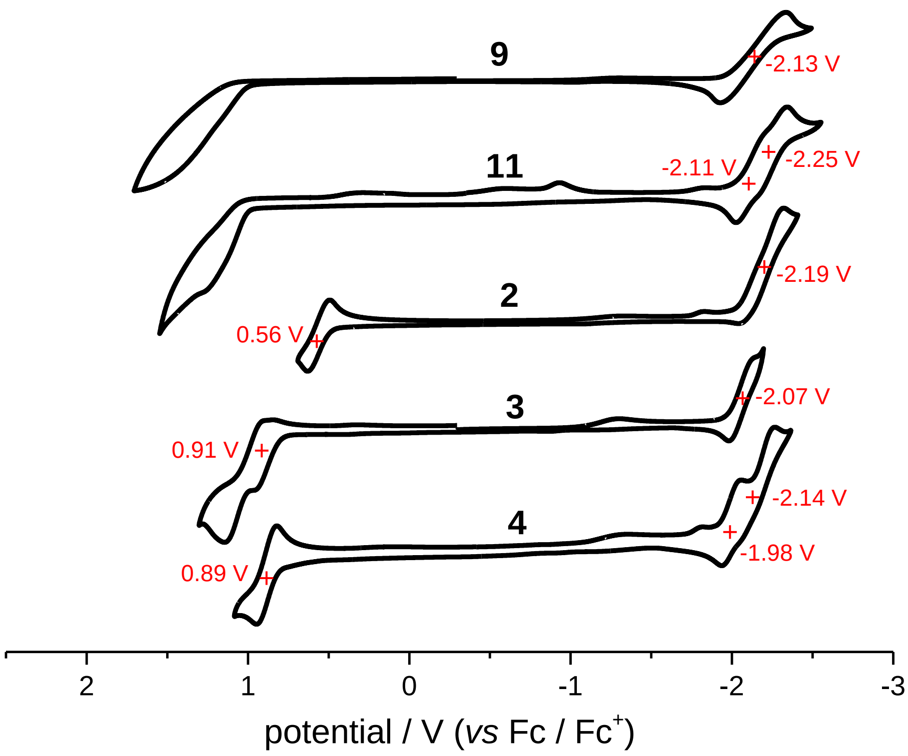


Figure S58. CV curves of key intermediates **9**, **11** and aza[7]helcenes **2**, **3**, and **4.**

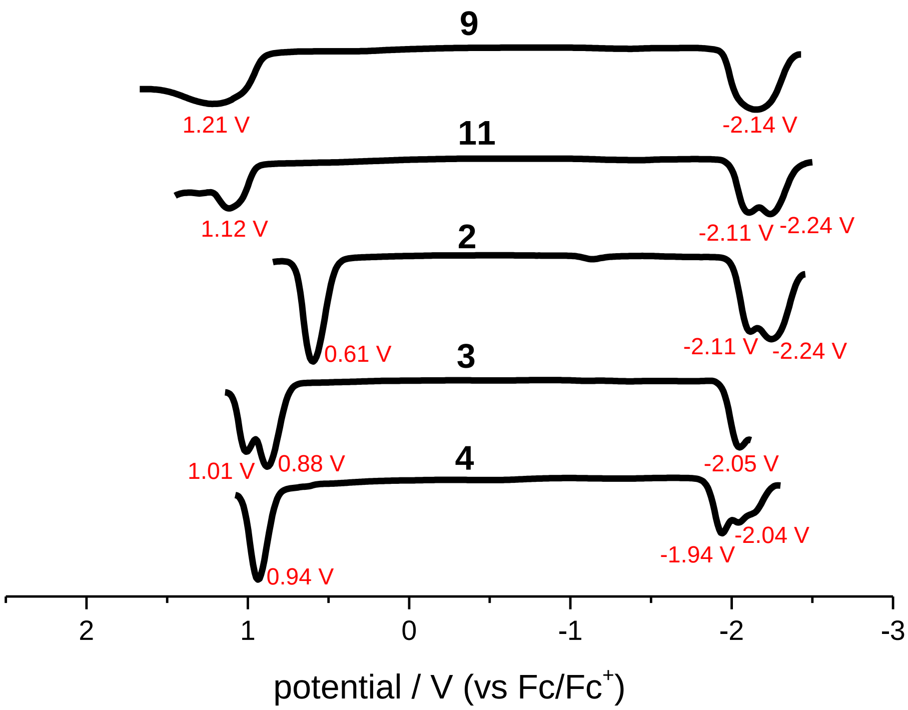
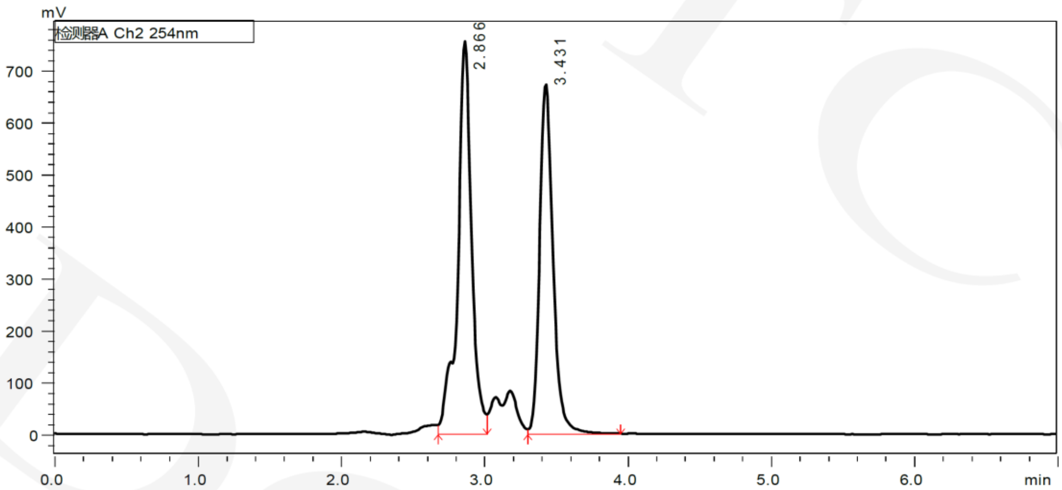


Figure S59. DPV curves of key intermediates **9**, **11** and aza[7]helcenes **2**, **3**, and **4.**

9. Chiral resolution and CD spectra

Column	:	CHIRALPAK IE-3(IE30CE-UL006)
Column size	:	0.46 cm I.D. × 15 cm L
Injection	:	4 ul
Mobile phase	:	Hexane/EtOAc=50/50(V/V)
Flow rate	:	1.0 ml/min
Wave length	:	UV 254 nm
Temperature	:	35 ºC
HPLC equipment	:	Shimadzu LC-20AD CP-HPLC-08
Sample name	:	Raw Material

<Chromatogram>



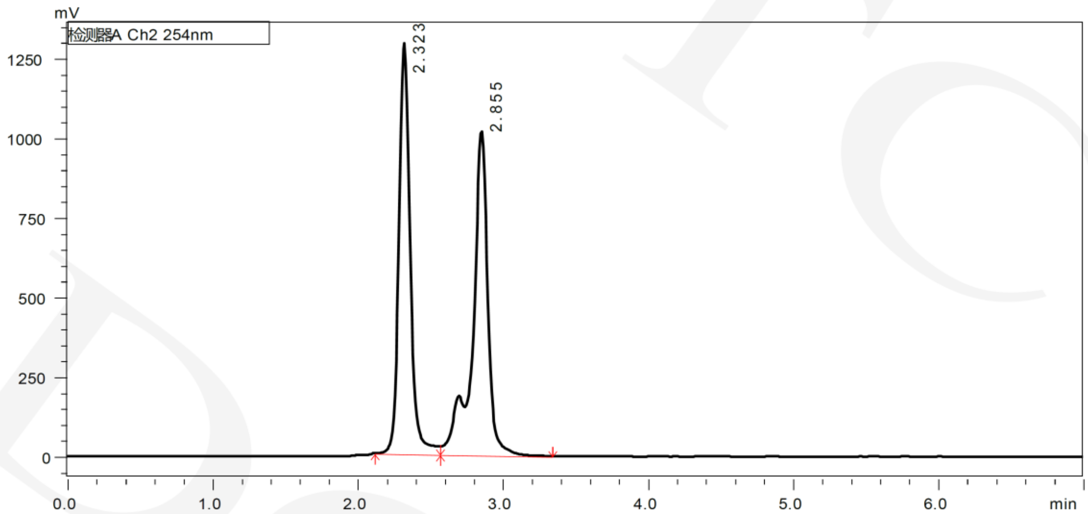
<Peak Table>

Peak#	Ret. Time	Area	Area%	T.Plate#	Tailing F.	Resolution
1	2.866	5069019	53.829	4514	0.967	--
2	3.431	4347856	46.171	5971	1.242	3.243

Figure S60. Chiral chromatography report of aza[7]helicene **3**.

Column	:	CHIRALPAK IE-3(IE30CE-UL006)
Column size	:	0.46 cm I.D. × 15 cm L
Injection	:	4 ul
Mobile phase	:	EtOAc/MeOH=90/10(V/V)
Flow rate	:	1.0 ml/min
Wave length	:	UV 254 nm
Temperature	:	35 °C
HPLC equipment	:	Shimadzu LC-20AD CP-HPLC-08
Sample name	:	Raw Material

<Chromatogram>



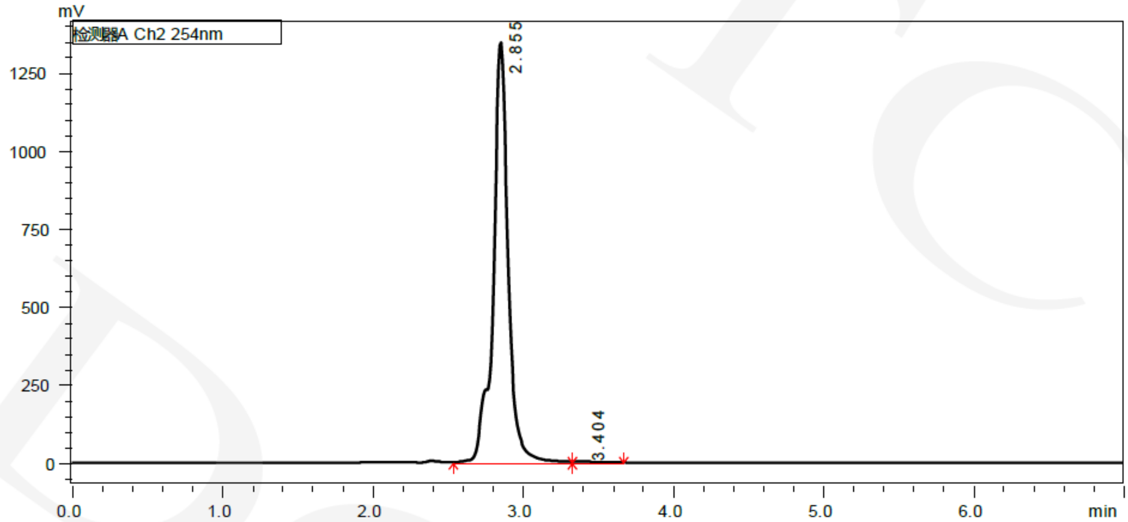
<Peak Table>

Peak#	Ret. Time	Area	Area%	T.Plate#	Tailing F.	Resolution
1	2.323	6984060	48.682	3788	1.152	--
2	2.855	7362231	51.318	4579	0.749	3.331

Figure S61. Chiral chromatography report of aza[7]helicene **4**.

Column	:	CHIRALPAK IE-3(IE30CE-UL006)
Column size	:	0.46 cm I.D. × 15 cm L
Injection	:	4 ul
Mobile phase	:	Hexane/EtOAc=50/50(V/V)
Flow rate	:	1.0 ml/min
Wave length	:	UV 254 nm
Temperature	:	35 °C
HPLC equipment	:	Shimadzu LC-20AD CP-HPLC-08
Sample name	:	Peak 1

<Chromatogram>



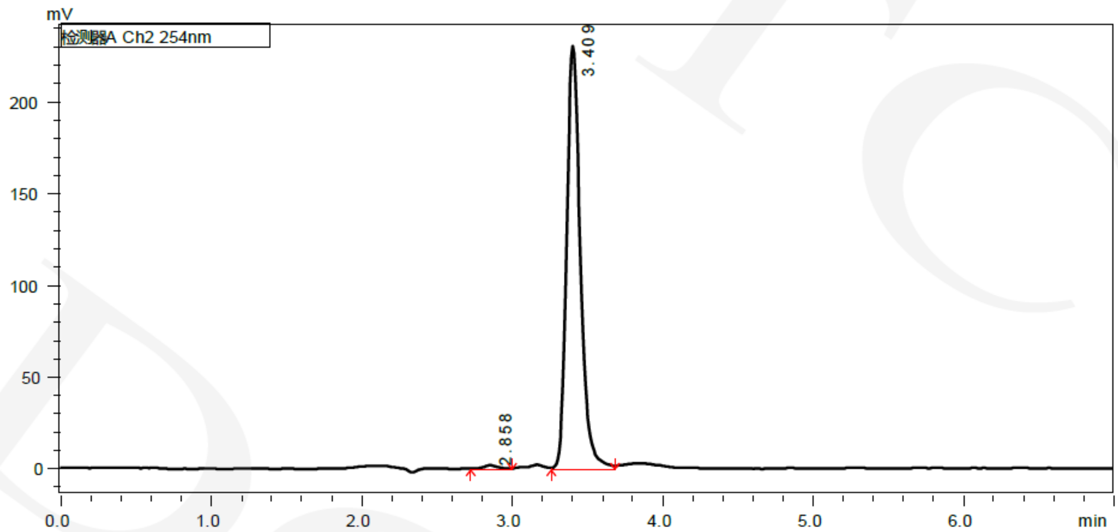
<Peak Table>

Peak#	Ret. Time	Area	Area%	T.Plate#	Tailing F.	Resolution
1	2.855	9269877	99.735	4356	0.951	--
2	3.404	24663	0.265	4040	--	2.835

Figure S62. Chiral chromatography report of the first peak of aza[7]helicene **3**.

Column	:	CHIRALPAK IE-3(IE30CE-UL006)
Column size	:	0.46 cm I.D. × 15 cm L
Injection	:	4 ul
Mobile phase	:	Hexane/EtOAc=50/50(V/V)
Flow rate	:	1.0 ml/min
Wave length	:	UV 254 nm
Temperature	:	35 °C
HPLC equipment	:	Shimadzu LC-20AD CP-HPLC-08
Sample name	:	Peak 2

<Chromatogram>



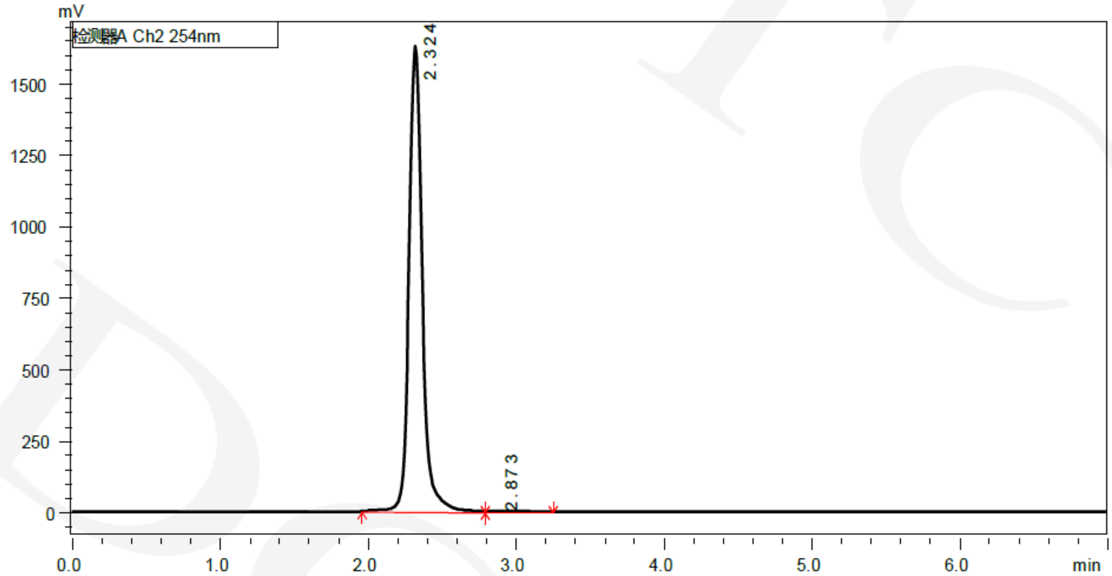
<Peak Table>

Peak#	Ret. Time	Area	Area%	T.Plate#	Tailing F.	Resolution
1	2.858	8595	0.586	5412	1.126	--
2	3.409	1458897	99.414	6010	1.237	3.326

Figure S63. Chiral chromatography report of the second peak of aza[7]helicene **3**.

Column	:	CHIRALPAK IE-3(IE30CE-UL006)	
Column size	:	0.46 cm I.D. × 15 cm L	
Injection	:	4 ul	
Mobile phase	:	EtOAc/MeOH=90/10(V/V)	
Flow rate	:	1.0 ml/min	
Wave length	:	UV 254 nm	
Temperature	:	35 °C	
HPLC equipment	:	Shimadzu LC-20AD	CP-HPLC-08
Sample name	:	Peak 1	

<Chromatogram>



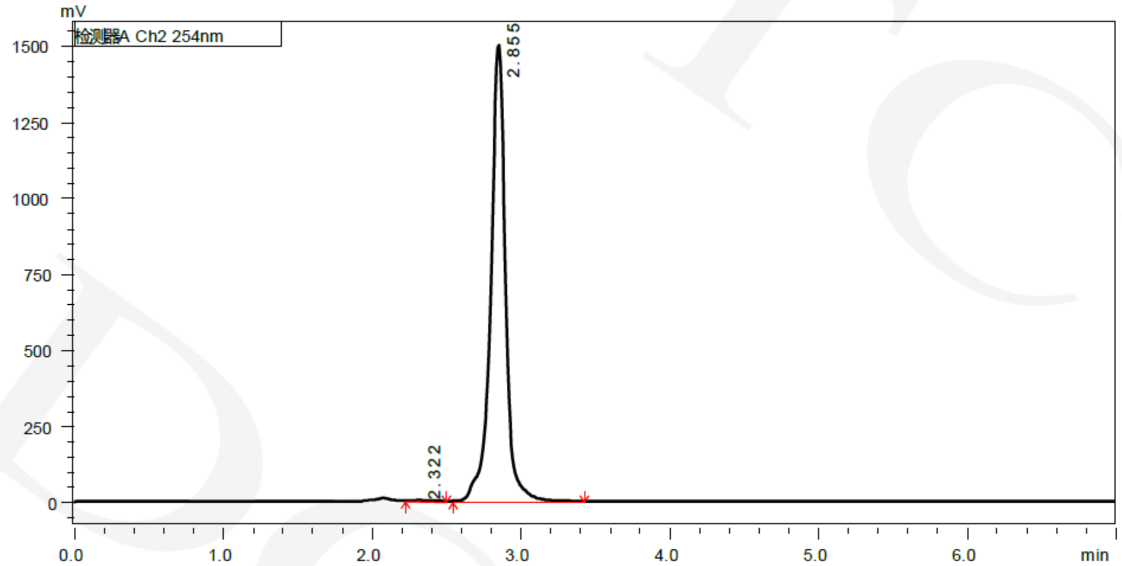
<Peak Table>

Peak#	Ret. Time	Area	Area%	T.Plate#	Tailing F.	Resolution
1	2.324	1015925	99.730	3112	1.173	
2	2.873	27550	0.270	1405		2.316

Figure S64. Chiral chromatography report of the first peak of aza[7]helicene **4**.

Column	:	CHIRALPAK IE-3(IE30CE-UL006)
Column size	:	0.46 cm I.D. × 15 cm L
Injection	:	4 ul
Mobile phase	:	EtOAc/MeOH=90/10(V/V)
Flow rate	:	1.0 ml/min
Wave length	:	UV 254 nm
Temperature	:	35 °C
HPLC equipment	:	Shimadzu LC-20AD CP-HPLC-08
Sample name	:	Peak 2

<Chromatogram>



<Peak Table>

Peak#	Ret. Time	Area	Area%	T.Plate#	Tailing F.	Resolution
1	2.322	15234	0.148	4150	1.750	--
2	2.855	10288555	99.852	4134	0.890	3.313

Figure S65. Chiral chromatography report of the second peak of aza[7]helicene **4**.

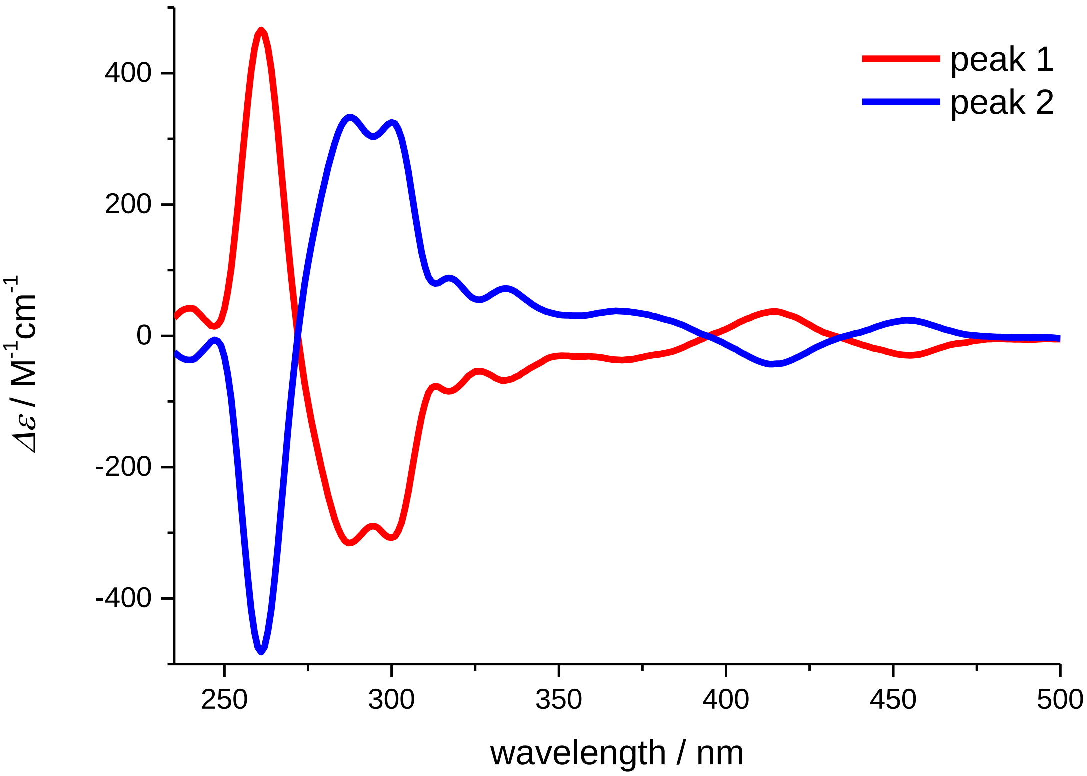


Figure S66. CD spectra of the enantiomers of aza[7]helicene **3** in dichloromethane.

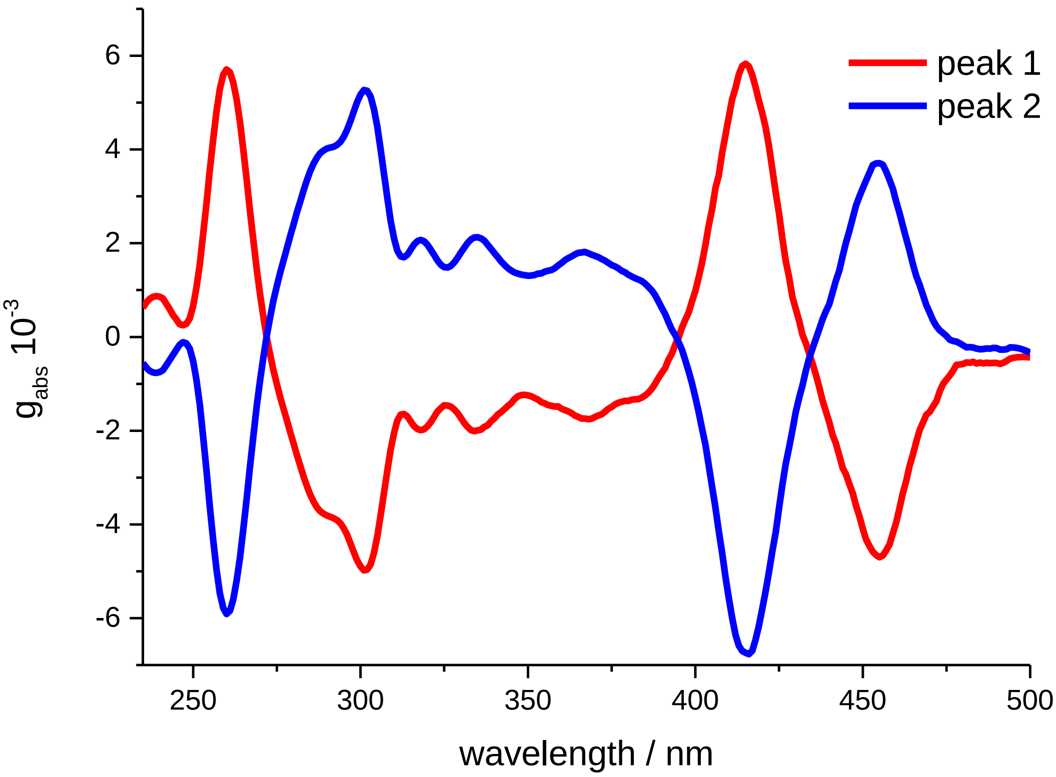


Figure S67. Asymmetric factors of the enantiomers of aza[7]helicene **3** in dichloromethane.

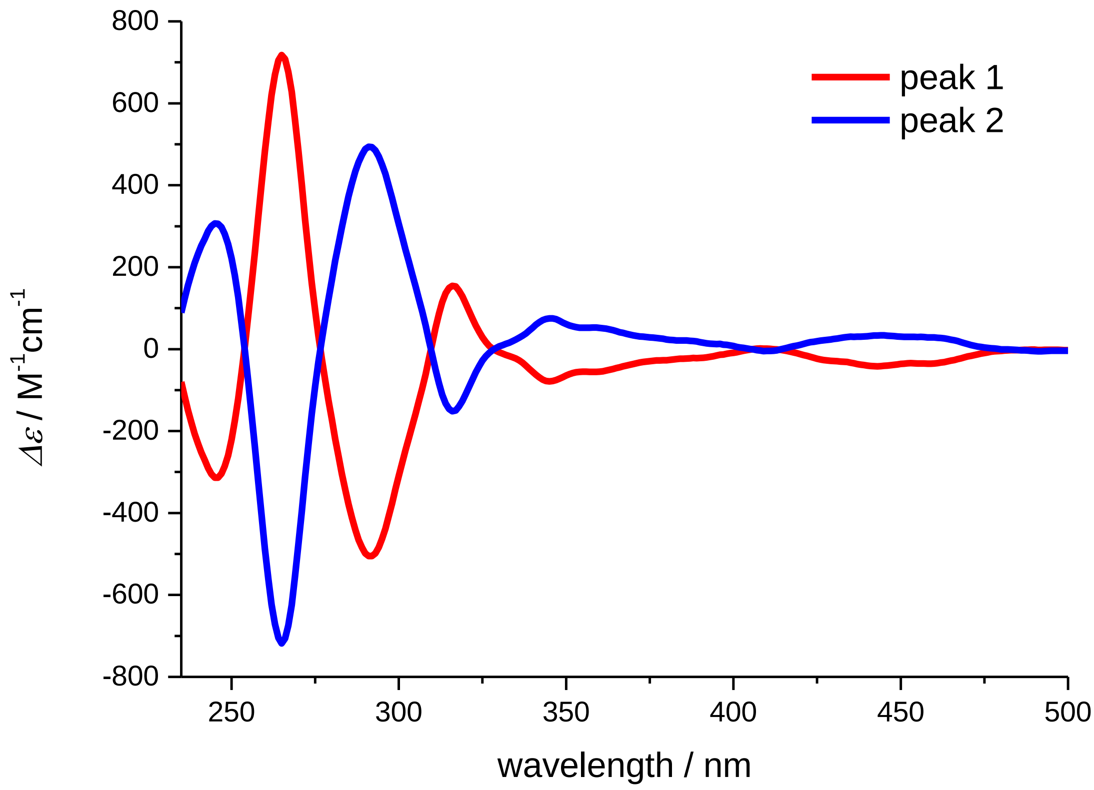


Figure S68. CD spectra of the enantiomers of aza[7]helicene **4** in dichloromethane.

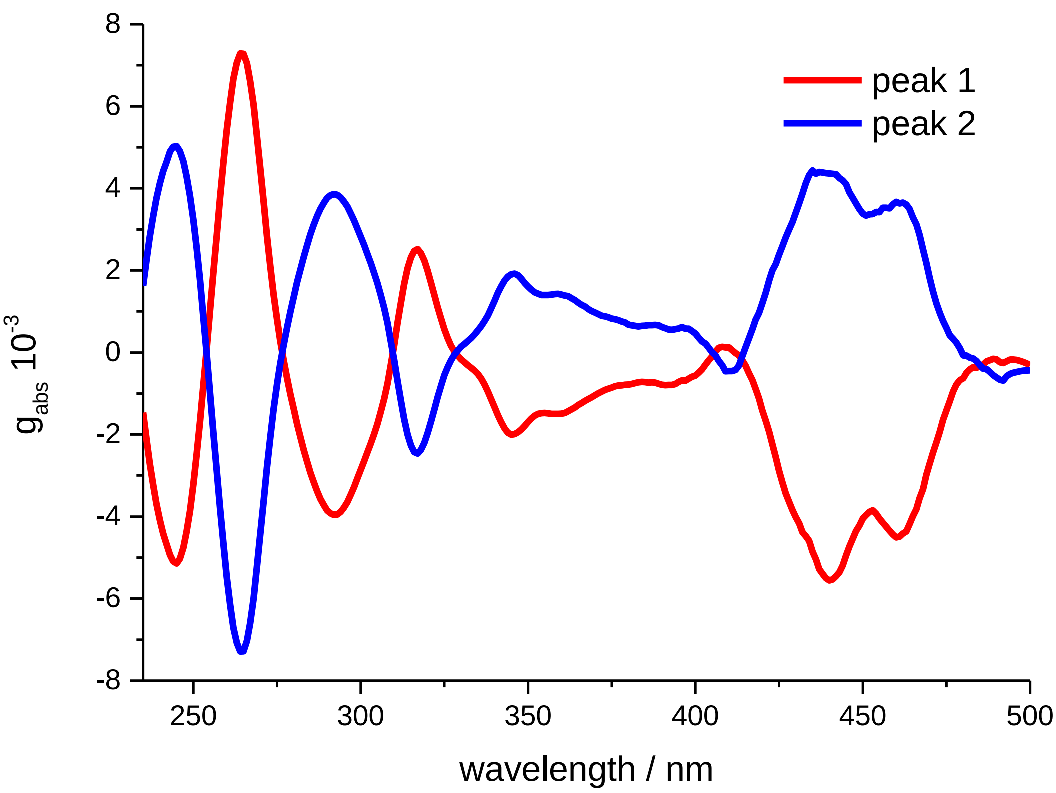


Figure S69. Asymmetric factors of the enantiomers of aza[7]helicene **4** in dichloromethane.

10. Thermal racemization

The thermal racemizations of *P*-**3** and *P*-**4** were performed in 1,2-dichlorobenzene at 180 ºC. The ratio of *P*/*M* isomers were monitored by measuring the optical rotation values. The transformation of *P*-isomer to *M*-isomer follows a reversible first order reaction.[S3] The rate constant k can obtained by fitting the experimental data (α, mole ratio of *P*-**3** or **4** at time t) using the following equation:

$\ln(2\alpha - 1) = -2kt$

The racemization barriers ($\Delta G^{\ddagger}$) of **3** and **4** were calculated from the following equation:

$\Delta G^{\ddagger}(\mathrm{T}) = -RT\ln(kh/k_BT)$

Here R is the gas constant (8.31441 J·K^{-1}), h is the Planck constant (6.626176 × 10^{-34} J·s), k_B is the Boltzmann constant (1.380662 × 10^{-23} J·K^{-1}) and T is temperature (K).

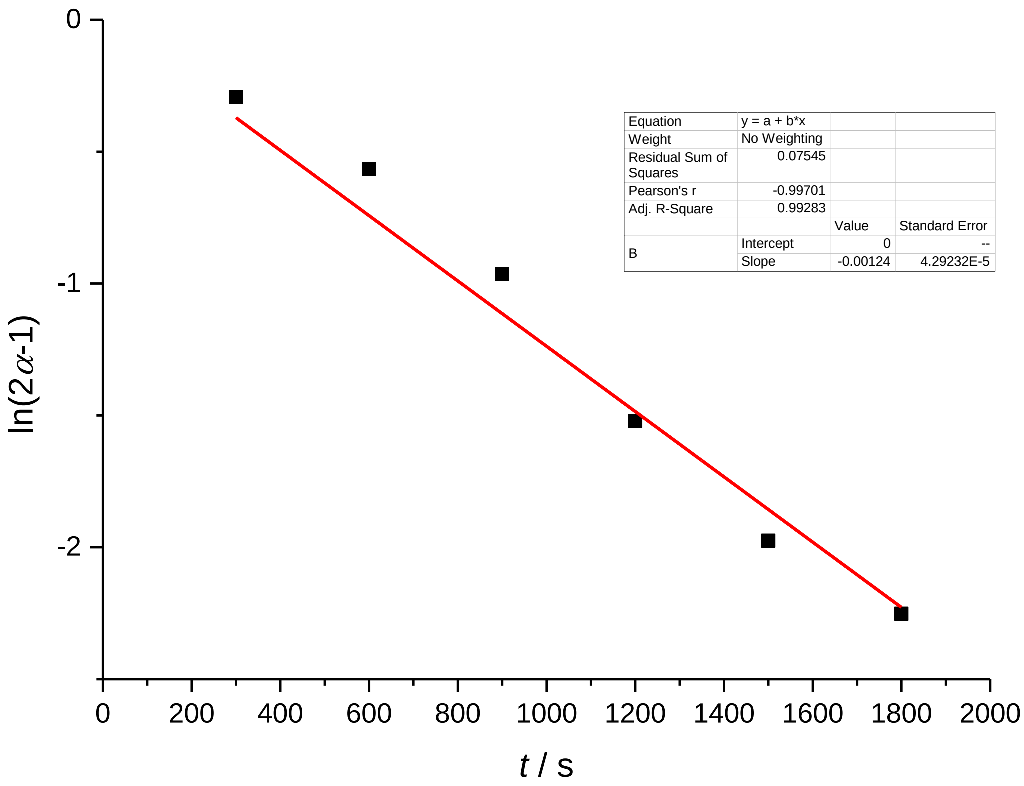


Figure S70. Fitting plot of thermal racemization of *P*-**3** in 1,2-dichlorobenzene at 180 ºC.

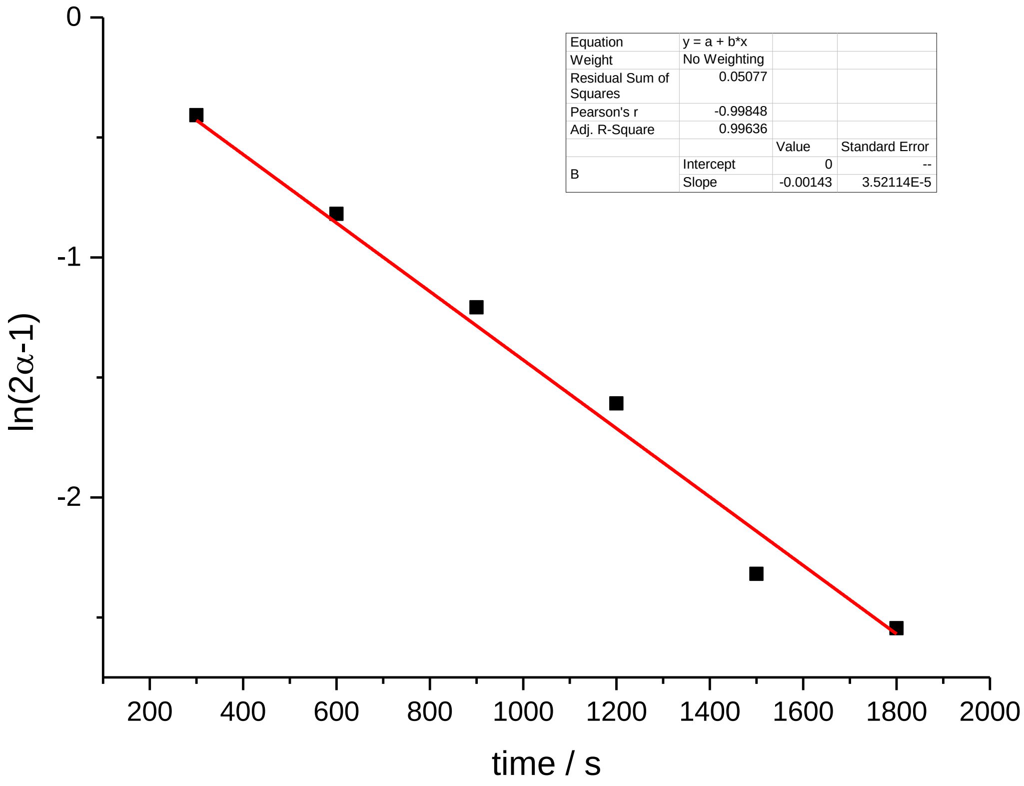


Figure S71. Fitting plot of thermal racemization of *P*-**4** in 1,2-dichlorobenzene at 180 ºC.

11. X-ray crystallographic structure determination

Table S1. Crystal data and structure refinement for **11**

Empirical formula	$C_{46}H_{48}N_2O_2$
Formula weight	660.86
Temperature/K	150.00(10)
Crystal system	monoclinic
Space group	C2/c
a/Å	15.8874(7)
b/Å	24.6931(11)
c/Å	40.961(2)
α/°	90
β/°	94.789(5)
γ/°	90
Volume/Å^3	16013.4(13)
Z	16
ρ_{calc}g/cm^3	1.096
μ/mm^{-1}	0.512
F(000)	5664.0
Crystal size/mm^3	0.12 × 0.11 × 0.1
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	4.33 to 133.2
Index ranges	$-18 \leq h \leq 17$, $-29 \leq k \leq 28$, $-48 \leq l \leq 40$
Reflections collected	29054
Independent reflections	13990 [R_{int} = 0.0426, R_{sigma} = 0.0582]
Data/restraints/parameters	13990/91/956
Goodness-of-fit on F^2	1.037
Final R indexes [I>=2σ (I)]	R_1 = 0.0999, wR_2 = 0.2848
Final R indexes [all data]	R_1 = 0.1389, wR_2 = 0.3233
Largest diff. peak/hole / e Å^{-3}	0.59/-0.64

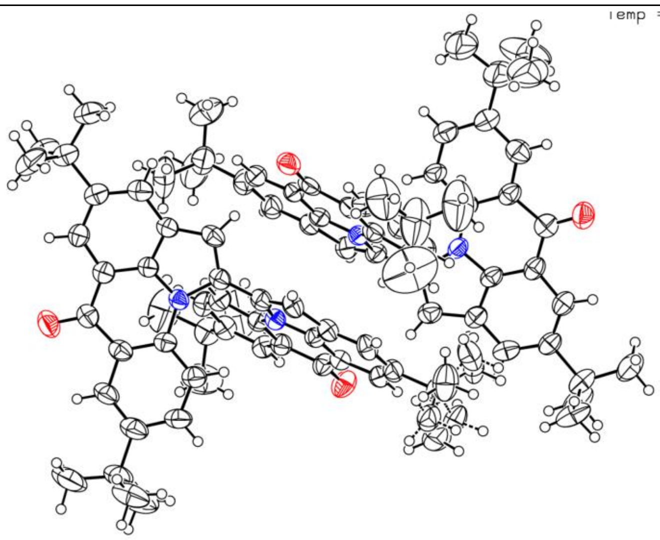


Figure S72. Crystal structure of **11** with an ellipsoid contour at the 50% probability level.

Table S2. Crystal data and structure refinement for **2**

Empirical formula	$C_{52}H_{51}N_3O_2$
Formula weight	749.95
Temperature/K	99.9(4)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	17.0401(3)
b/Å	16.9978(3)
c/Å	33.2623(6)
α/°	90
β/°	90.342(2)
γ/°	90
Volume/Å^3	9634.1(3)
Z	8
ρ_{calc}g/cm^3	1.034
μ/mm^{-1}	0.485
F(000)	3200.0
Crystal size/mm^3	0.13 × 0.12 × 0.11
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.314 to 147.532
Index ranges	$-21 \leq h \leq 20$, $-20 \leq k \leq 17$, $-41 \leq l \leq 40$
Reflections collected	44345
Independent reflections	18865 [R_{int} = 0.0369, R_{sigma} = 0.0413]
Data/restraints/parameters	18865/14/1051
Goodness-of-fit on F^2	1.063
Final R indexes [I>=2σ (I)]	R_1 = 0.0649, wR_2 = 0.1769
Final R indexes [all data]	R_1 = 0.0751, wR_2 = 0.1863
Largest diff. peak/hole / e Å^{-3}	0.55/-0.53

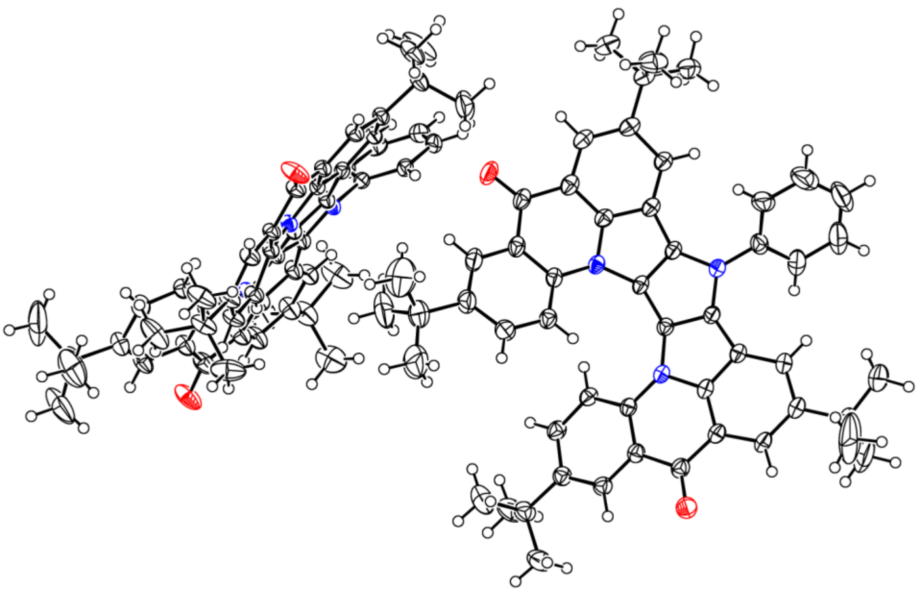


Figure S73. Crystal structure of **2** with an ellipsoid contour at the 50% probability level.

Table S3. Crystal data and structure refinement for **3**

Empirical formula	$C_{48}H_{48}N_2O_2$
Formula weight	684.88
Temperature/K	150.00(10)
Crystal system	triclinic
Space group	P-1
a/Å	10.9969(6)
b/Å	11.4966(4)
c/Å	15.0565(5)
α/°	92.345(3)
β/°	97.135(4)
γ/°	93.016(4)
Volume/Å^3	1884.03(14)
Z	2
ρ_{calc}g/cm^3	1.207
μ/mm^{-1}	0.563
F(000)	732.0
Crystal size/mm^3	0.13 × 0.11 × 0.09
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.922 to 147.778
Index ranges	$-13 \leq h \leq 13$, $-14 \leq k \leq 14$, $-18 \leq l \leq 12$
Reflections collected	12954
Independent reflections	7325 [R_{int} = 0.0534, R_{sigma} = 0.0673]
Data/restraints/parameters	7325/0/512
Goodness-of-fit on F^2	1.144
Final R indexes [I>=2σ (I)]	R_1 = 0.0762, wR_2 = 0.1882
Final R indexes [all data]	R_1 = 0.1105, wR_2 = 0.1972
Largest diff. peak/hole / e Å^{-3}	0.32/-0.32

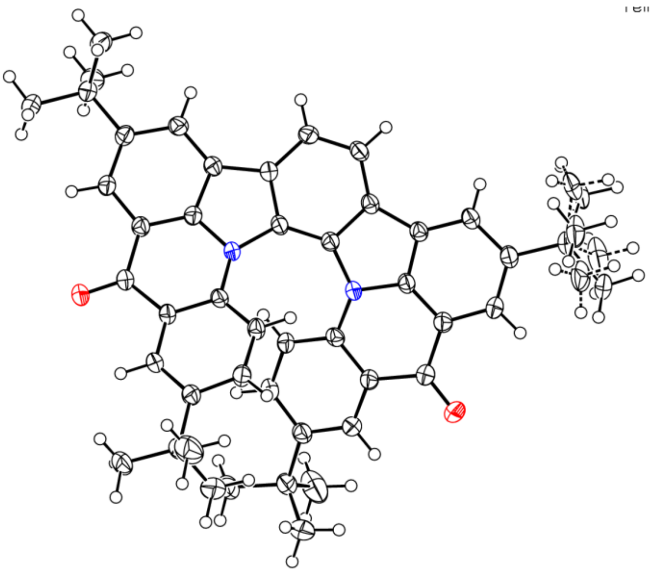


Figure S74. Crystal structure of **3** with an ellipsoid contour at the 50% probability level.

Table S4. Crystal data and structure refinement for **4**

Empirical formula	$C_{52}H_{50}N_2O_2$
Formula weight	734.94
Temperature/K	100.0(3)
Crystal system	monoclinic
Space group	$P2_1/n$
a/Å	15.8931(6)
b/Å	10.9347(4)
c/Å	24.8340(8)
α/°	90
β/°	92.737(3)
γ/°	90
Volume/Å^3	4310.9(3)
Z	4
ρ_{calc}g/cm^3	1.132
μ/mm^{-1}	0.525
F(000)	1568.0
Crystal size/mm^3	0.14 × 0.1 × 0.08
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.466 to 147.622
Index ranges	$-18 \leq h \leq 19$, $-13 \leq k \leq 7$, $-30 \leq l \leq 30$
Reflections collected	15244
Independent reflections	8393 [R_{int} = 0.0621, R_{sigma} = 0.0751]
Data/restraints/parameters	8393/0/560
Goodness-of-fit on F^2	1.050
Final R indexes [I>=2σ (I)]	R_1 = 0.0795, wR_2 = 0.2015
Final R indexes [all data]	R_1 = 0.1038, wR_2 = 0.2187
Largest diff. peak/hole / e Å^{-3}	0.75/-0.46

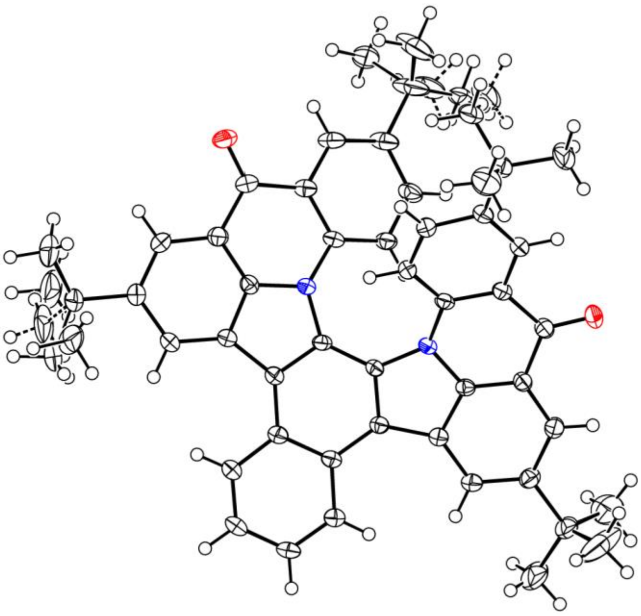


Figure S75. Crystal structure of **4** with an ellipsoid contour at the 50% probability level.

12. Theoretical calculations

All the theoretical calculations were carried out using a *Gaussian 16* software. [S4] 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 calculations of excited state properties and ECD spectra were performed using time-depended DFT methods at B3LYP/6-311G+(d,p) level of theory in the solvent dichloromethane.

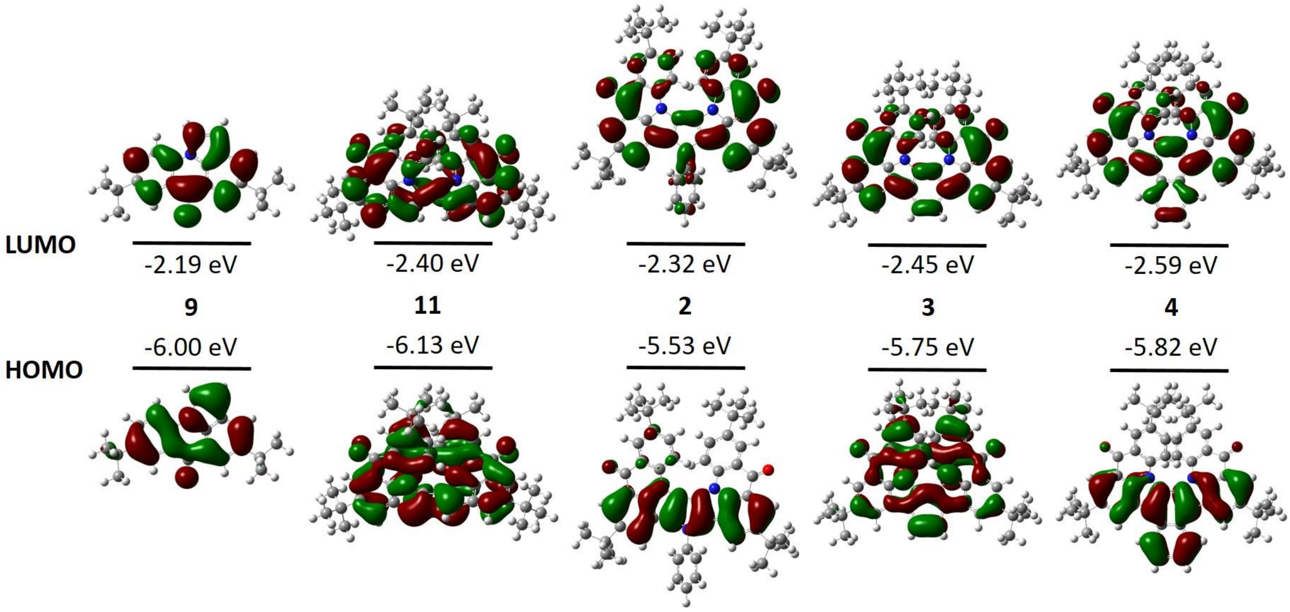


Figure S76. Calculated frontier molecular orbitals and energy levels.

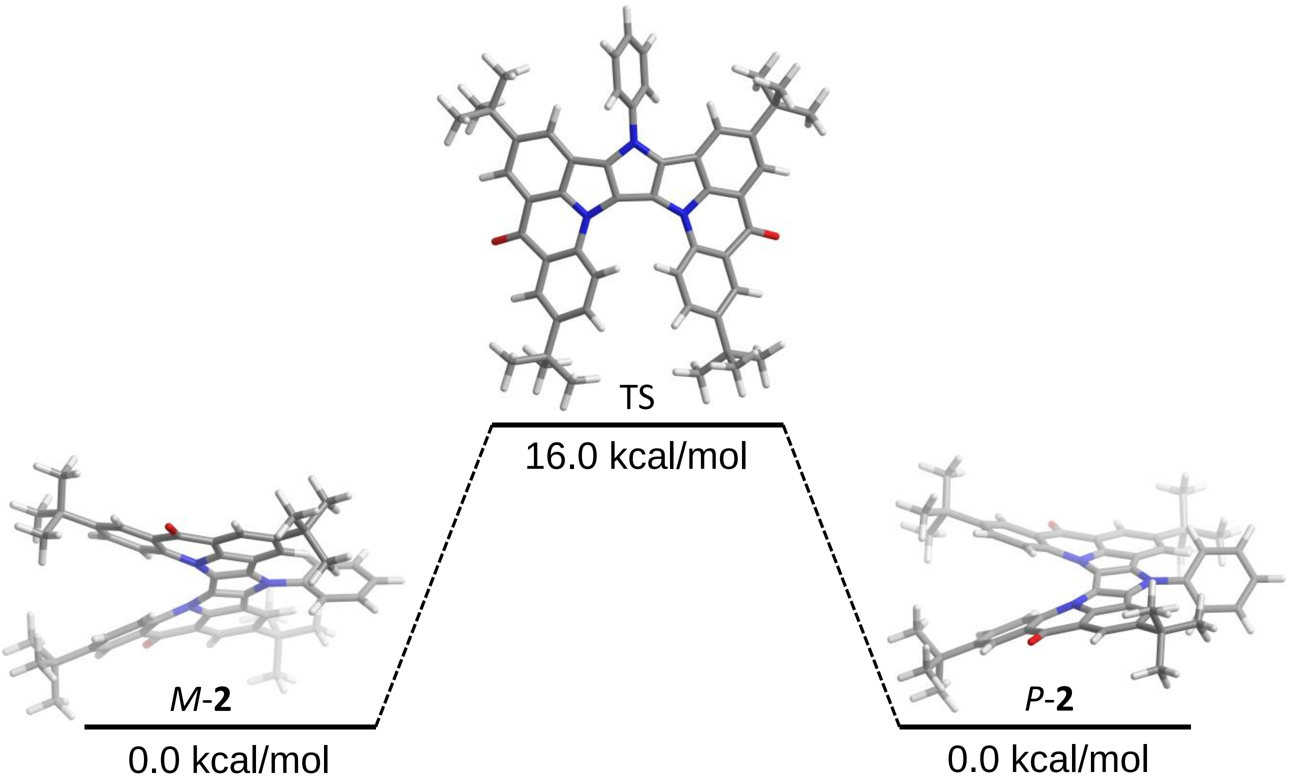


Figure S77. Energy diagram of racemization process of triaza[7]helicene **2**.

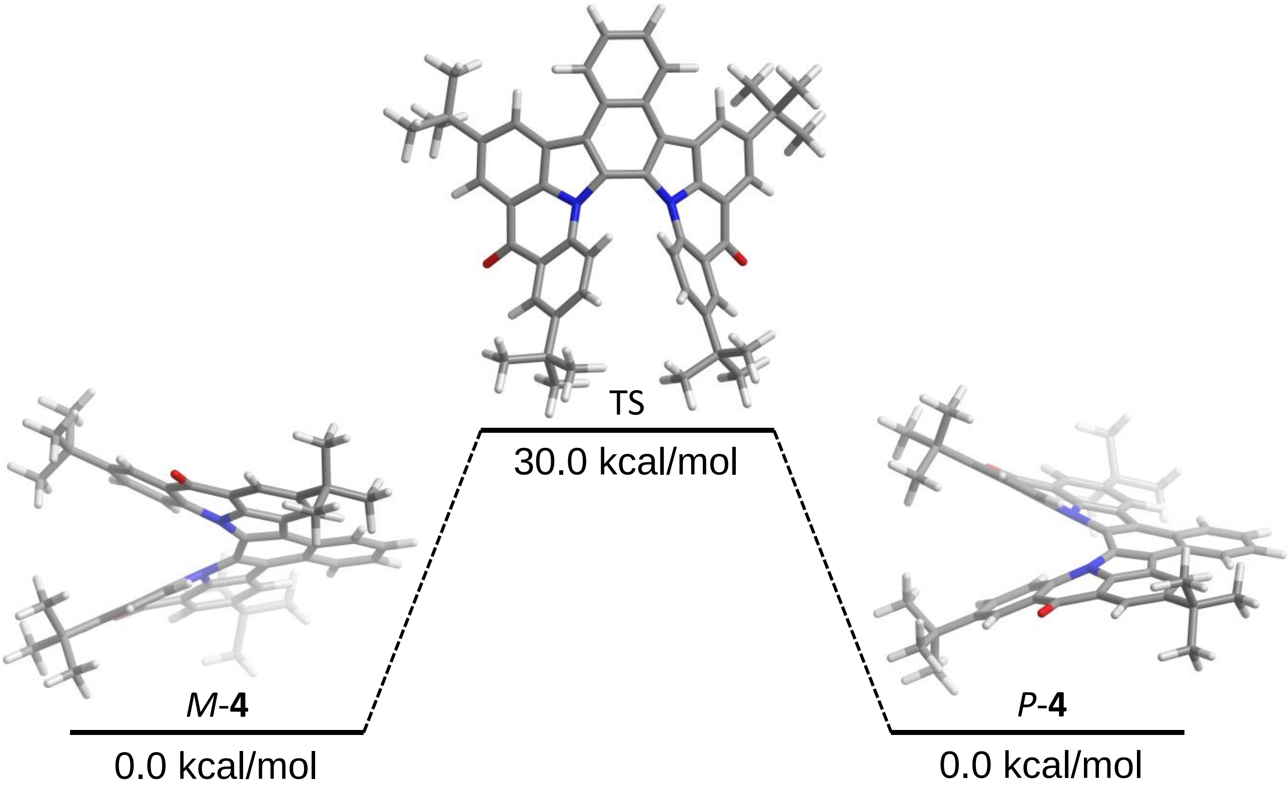


Figure S78. Energy diagram of racemization process of triaza[7]helicene **4**.

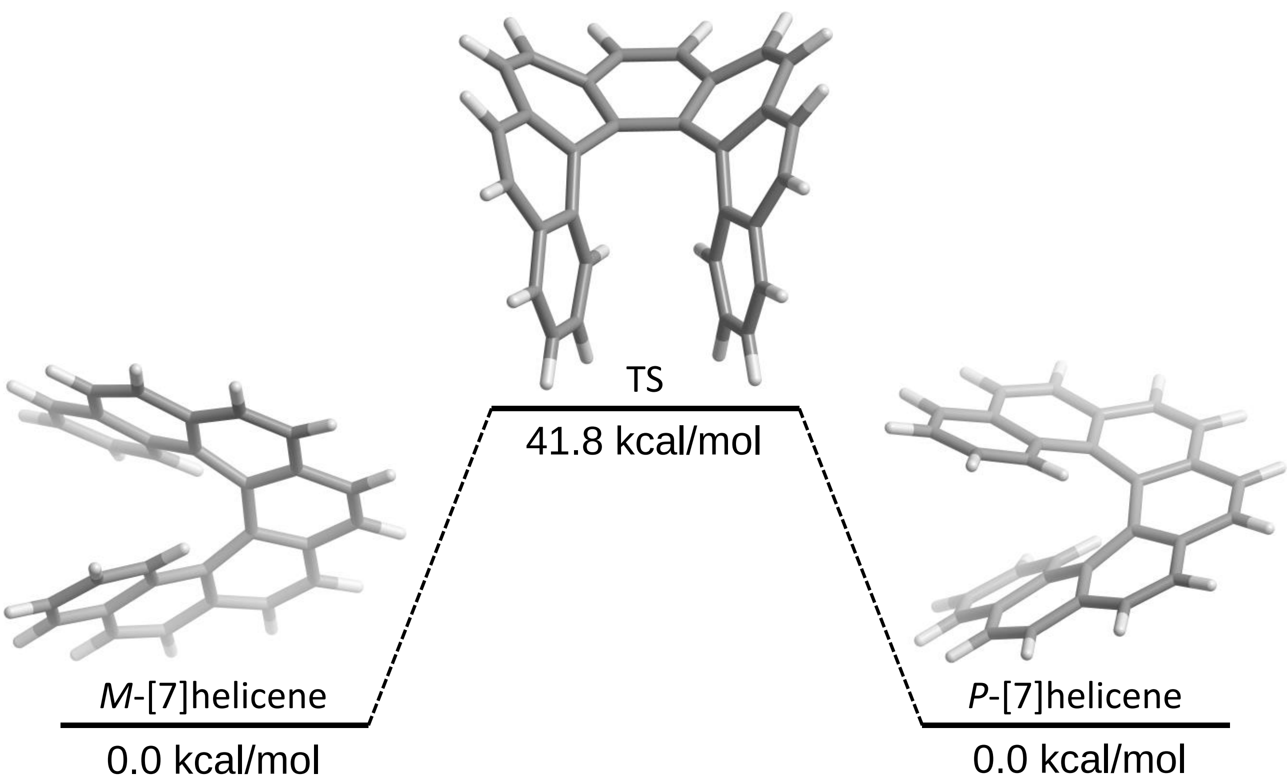


Figure S79. Energy diagram of racemization process of carbo[7]helicene.

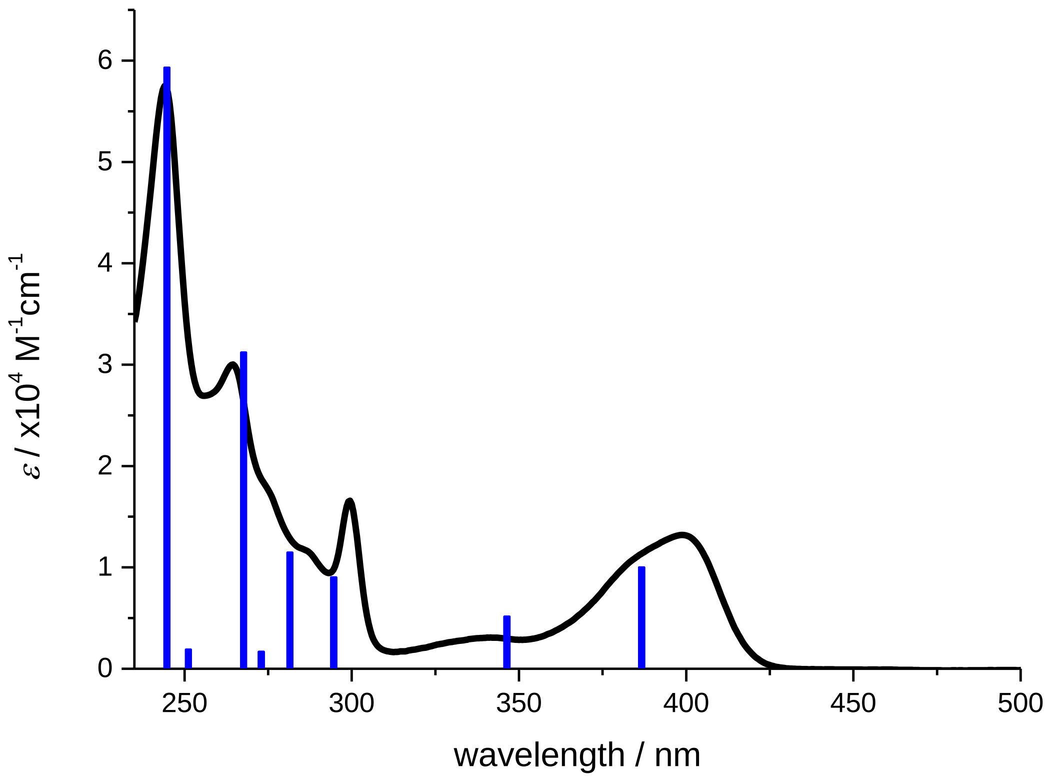


Figure S80. UV/Vis absorption spectrum of compound **9** and TD-DFT calculated oscillator strength (blue column) in dichloromethane solvent at B3LYP/6-311G+(d,p) level.

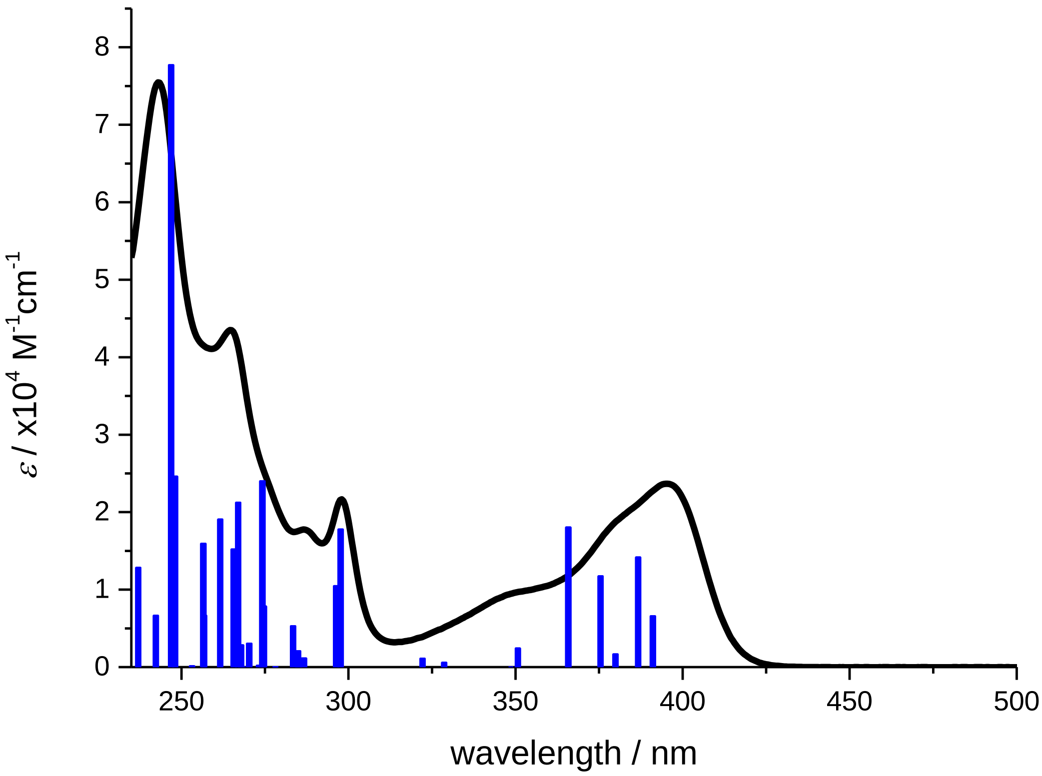


Figure S81. UV/Vis absorption spectrum of compound **11** and TD-DFT calculated oscillator strength (blue column) in dichloromethane solvent at B3LYP/6-311G+(d,p) level.

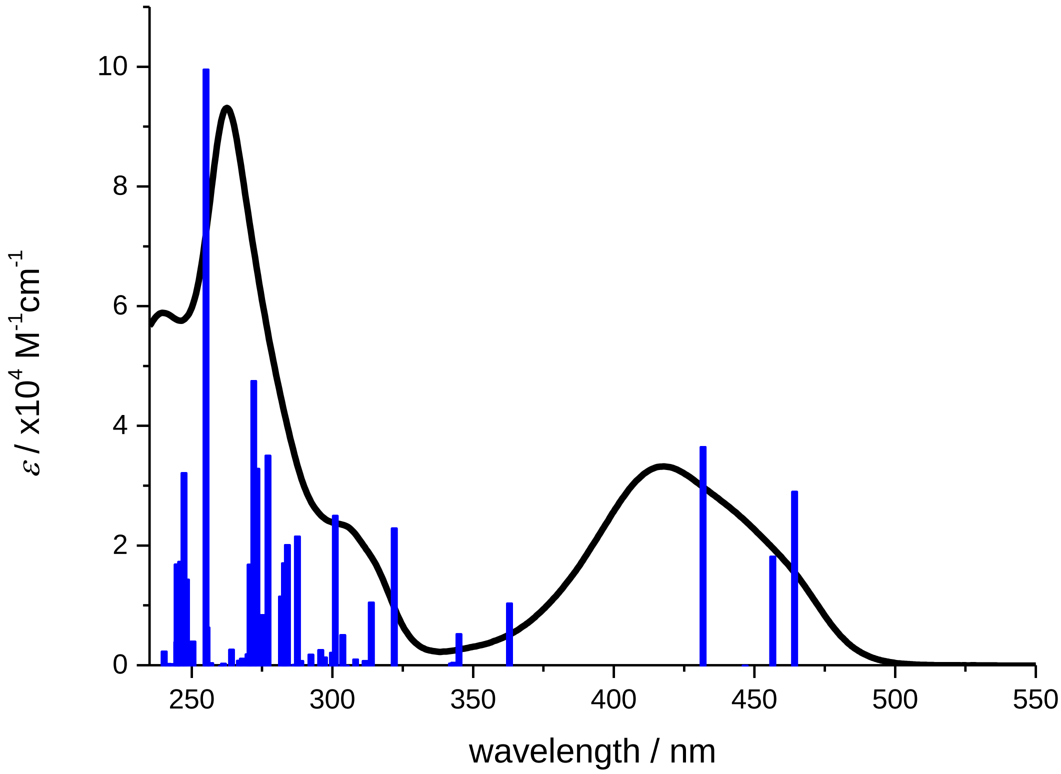


Figure S82. UV/Vis absorption spectrum of compound **2** and TD-DFT calculated oscillator strength (blue column) in dichloromethane solvent at B3LYP/6-311G+(d,p) level.

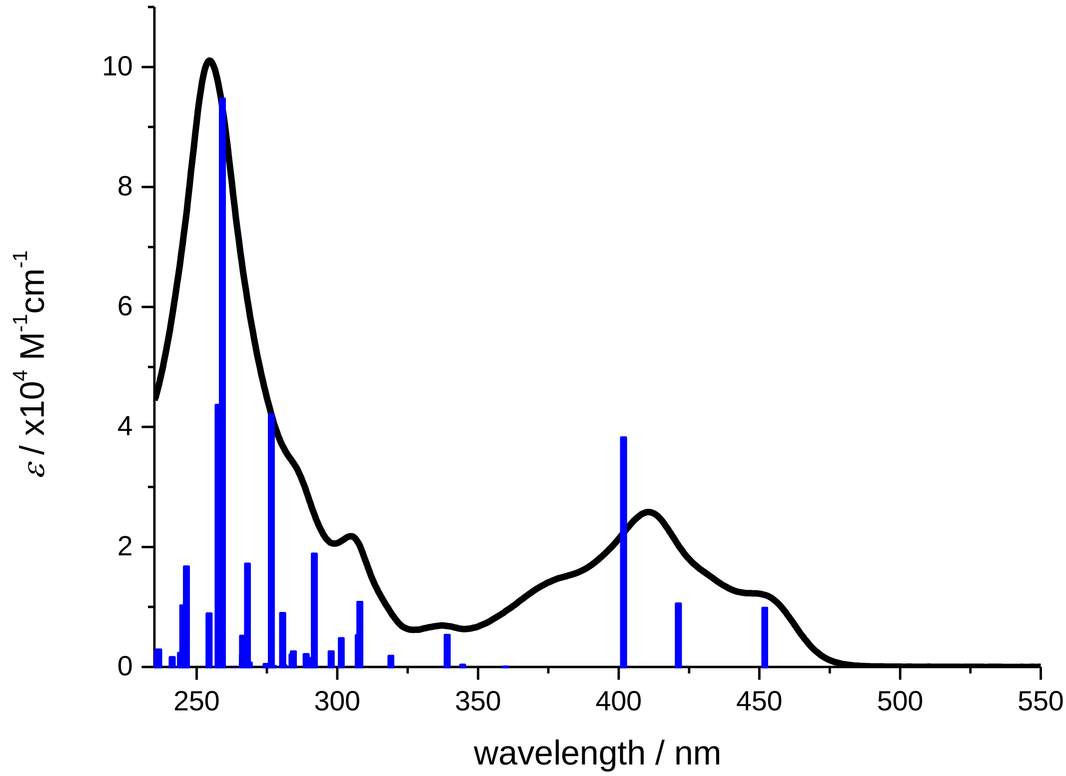


Figure S83. UV/Vis absorption spectrum of compound **3** and TD-DFT calculated oscillator strength (blue column) in dichloromethane solvent at B3LYP/6-311G+(d,p) level.

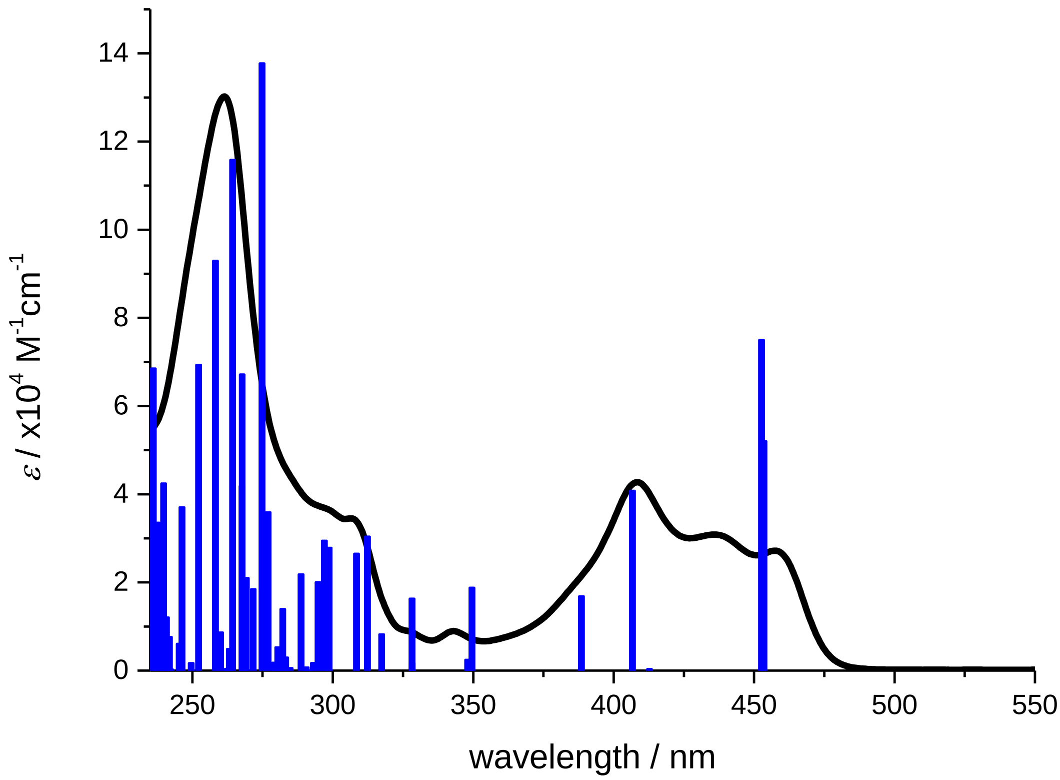


Figure S84. UV/Vis absorption spectrum of compound **4** and TD-DFT calculated oscillator strength (blue column) in dichloromethane solvent at B3LYP/6-311G+(d,p) level.

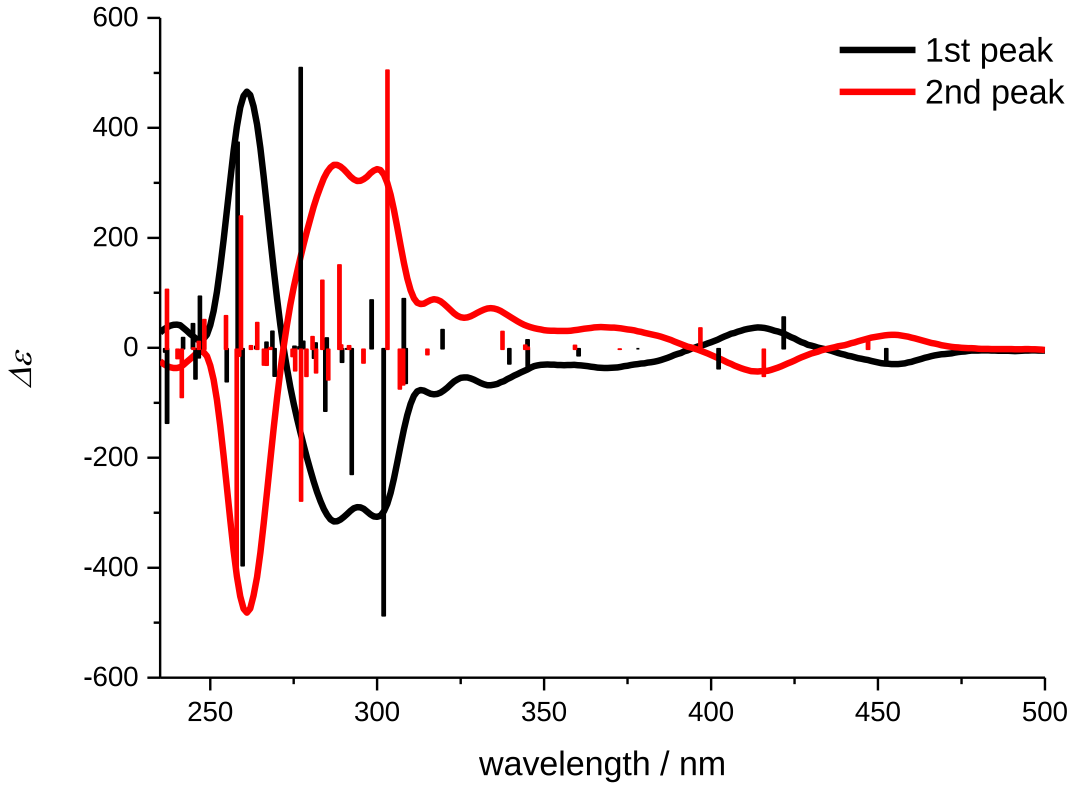


Figure S85. CD spectra (solid line) of compound **3** and TD-DFT calculated rotational strength (bar) in dichloromethane solvent at B3LYP/6-311G+(d,p) level.

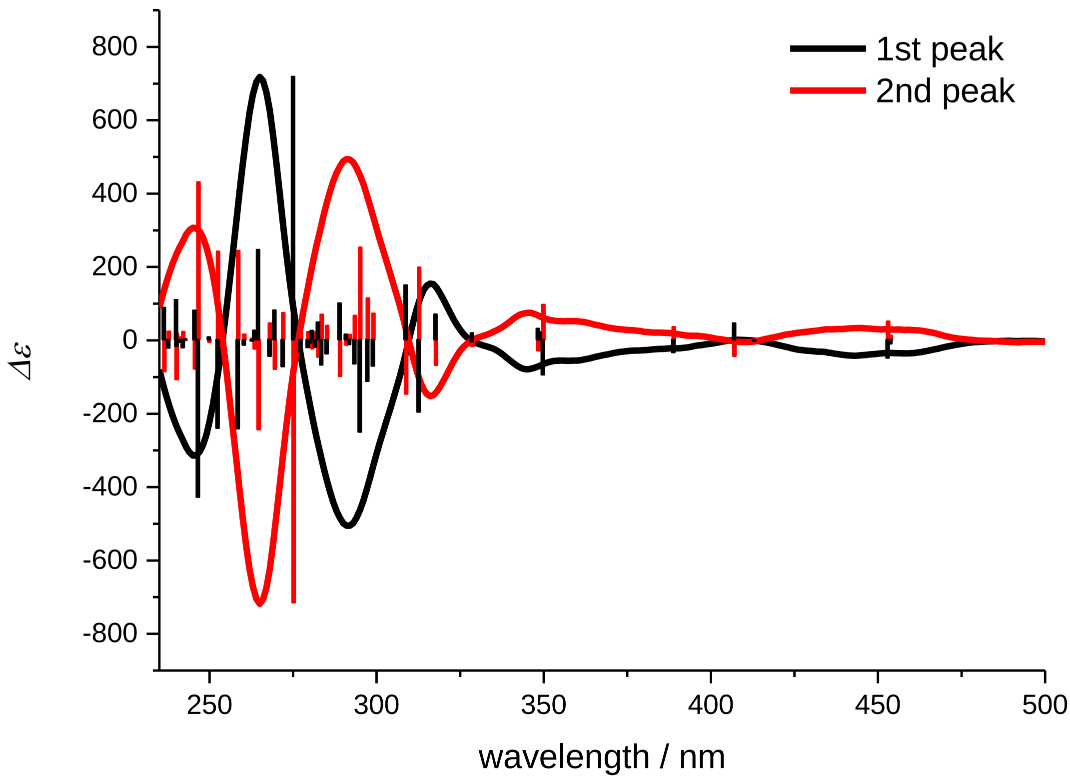


Figure S86. CD spectra (solid line) of compound **4** and TD-DFT calculated rotational strength (bar) in dichloromethane solvent at B3LYP/6-311G+(d,p) level.

Table S5. TD-DFT calculated first-ten electron transitions of **9** in dichloromethane at B3LYP / 6-311+G(d,p) level

Excited State	1:	Singlet-A	3.2065 eV	386.67 nm	f=0.1297	<S**2>=0.000
89 -> 90		0.69286				
Excited State	2:	Singlet-A	3.5791 eV	346.41 nm	f=0.0665	<S**2>=0.000
88 -> 90		0.69149				
Excited State	3:	Singlet-A	3.5900 eV	345.36 nm	f=0.0000	<S**2>=0.000
86 -> 90		0.69815				
Excited State	4:	Singlet-A	4.2081 eV	294.63 nm	f=0.1169	<S**2>=0.000
87 -> 90		0.63732				
88 -> 92		0.10543				
89 -> 91		0.23915				
Excited State	5:	Singlet-A	4.4037 eV	281.55 nm	f=0.1487	<S**2>=0.000
85 -> 90		-0.40393				
87 -> 90		-0.20324				
88 -> 92		-0.13609				
89 -> 91		0.50107				
Excited State	6:	Singlet-A	4.5416 eV	273.00 nm	f=0.0214	<S**2>=0.000
85 -> 90		-0.36796				

89 -> 91	-0.30250				
89 -> 92	0.50632				
Excited State 7:	Singlet-A	4.6315 eV	267.70 nm	f=0.4057	<S**2>=0.000
85 -> 90	0.41269				
87 -> 91	-0.11998				
88 -> 91	0.12495				
88 -> 92	-0.10241				
89 -> 91	0.26303				
89 -> 92	0.44613				
Excited State 8:	Singlet-A	4.9357 eV	251.20 nm	f=0.0242	<S**2>=0.000
88 -> 91	0.66934				
88 -> 92	0.16910				
89 -> 92	-0.10005				
Excited State 9:	Singlet-A	5.0653 eV	244.77 nm	f=0.7713	<S**2>=0.000
87 -> 90	-0.16020				
88 -> 91	-0.13239				
88 -> 92	0.62404				
89 -> 91	0.12527				
89 -> 95	-0.14690				
Excited State 10:	Singlet-A	5.3611 eV	231.27 nm	f=0.0549	<S**2>=0.000
84 -> 90	0.66523				

HOMO: 89, LUMO: 90

Table S6. TD-DFT calculated first-ten electron transitions of **11** in dichloromethane at B3LYP / 6-311+G(d,p) level

Excited State 1:	Singlet-A	3.1673 eV	391.45 nm	f=0.0646	<S**2>=0.000
177 -> 178	0.69206				
Excited State 2:	Singlet-A	3.2034 eV	387.04 nm	f=0.1393	<S**2>=0.000
176 -> 178	0.65116				
177 -> 179	-0.24562				
Excited State 3:	Singlet-A	3.2605 eV	380.26 nm	f=0.0164	<S**2>=0.000
176 -> 178	0.25591				
177 -> 179	0.65080				
Excited State 4:	Singlet-A	3.2991 eV	375.81 nm	f=0.1153	<S**2>=0.000
175 -> 178	0.19371				
176 -> 179	0.66906				
Excited State 5:	Singlet-A	3.3862 eV	366.14 nm	f=0.1773	<S**2>=0.000
175 -> 178	0.66366				
176 -> 179	-0.18675				
Excited State 6:	Singlet-A	3.5317 eV	351.06 nm	f=0.0239	<S**2>=0.000
175 -> 179	0.68577				
Excited State 7:	Singlet-A	3.5527 eV	348.98 nm	f=0.0001	<S**2>=0.000
170 -> 179	-0.46129				
171 -> 178	0.50428				

172 -> 179	-0.10580				
Excited State 8:	Singlet-A	3.5530 eV	348.96 nm	f=0.0000	<S**2>=0.000
170 -> 178	0.49504				
171 -> 179	-0.46587				
172 -> 178	0.11031				
Excited State 9:	Singlet-A	3.7685 eV	329.00 nm	f=0.0058	<S**2>=0.000
174 -> 178	0.68751				
Excited State 10:	Singlet-A	3.8442 eV	322.52 nm	f=0.0111	<S**2>=0.000
174 -> 179	0.68798				
175 -> 178	0.10602				

HOMO: 177, LUMO: 178

Table S7. TD-DFT calculated first-ten electron transitions of **2** in dichloromethane at B3LYP / 6-311+G(d,p) level

Excited State 1:	Singlet-A	2.6705 eV	464.27 nm	f=0.2077	<S**2>=0.000
199 -> 202	-0.11701				
200 -> 201	0.69012				
Excited State 2:	Singlet-A	2.7159 eV	456.52 nm	f=0.1306	<S**2>=0.000
199 -> 201	0.66478				
200 -> 202	-0.22133				
Excited State 3:	Singlet-A	2.7754 eV	446.72 nm	f=0.0011	<S**2>=0.000
199 -> 201	0.22046				
200 -> 202	0.66761				
Excited State 4:	Singlet-A	2.8716 eV	431.76 nm	f=0.2609	<S**2>=0.000
199 -> 202	0.69039				
200 -> 201	0.11364				
Excited State 5:	Singlet-A	3.4159 eV	362.96 nm	f=0.0749	<S**2>=0.000
198 -> 201	0.69616				
Excited State 6:	Singlet-A	3.5938 eV	345.00 nm	f=0.0385	<S**2>=0.000
198 -> 202	0.67702				
Excited State 7:	Singlet-A	3.6140 eV	343.06 nm	f=0.0044	<S**2>=0.000
192 -> 201	-0.15177				
192 -> 202	0.14197				
193 -> 201	0.38125				
193 -> 202	-0.29079				
194 -> 201	0.24461				
194 -> 202	-0.23798				
195 -> 201	0.19435				
195 -> 202	-0.13057				
198 -> 202	-0.12745				
Excited State 8:	Singlet-A	3.6218 eV	342.33 nm	f=0.0035	<S**2>=0.000
192 -> 201	-0.11262				
192 -> 202	-0.11593				

193 -> 201	-0.20634				
193 -> 202	-0.25587				
194 -> 201	0.34116				
194 -> 202	0.35473				
195 -> 201	-0.16573				
195 -> 202	-0.18697				
197 -> 201	-0.11394				
197 -> 202	-0.11282				
Excited State 9:	Singlet-A	3.8500 eV	322.04 nm	f=0.1642	<S**2>=0.000
200 -> 203	0.68010				
200 -> 206	-0.12217				
Excited State 10:	Singlet-A	3.9502 eV	313.87 nm	f=0.0761	<S**2>=0.000
199 -> 203	0.68395				

HOMO: 200, LUMO: 201

Table S8. TD-DFT calculated first-ten electron transitions of **3** in dichloromethane at B3LYP / 6-311+G(d,p) level

Excited State 1:	Singlet-A	2.7422 eV	452.14 nm	f=0.1025	<S**2>=0.000
183 -> 184	0.70127				
Excited State 2:	Singlet-A	2.9419 eV	421.44 nm	f=0.1098	<S**2>=0.000
183 -> 185	0.70149				
Excited State 3:	Singlet-A	3.0845 eV	401.96 nm	f=0.3910	<S**2>=0.000
182 -> 184	0.69449				
Excited State 4:	Singlet-A	3.2820 eV	377.77 nm	f=0.0000	<S**2>=0.000
182 -> 185	0.70068				
Excited State 5:	Singlet-A	3.4439 eV	360.01 nm	f=0.0027	<S**2>=0.000
181 -> 184	0.69369				
Excited State 6:	Singlet-A	3.5960 eV	344.78 nm	f=0.0061	<S**2>=0.000
175 -> 184	0.11834				
176 -> 185	0.39672				
177 -> 184	0.44297				
178 -> 184	-0.21680				
179 -> 185	0.22605				
181 -> 185	0.10318				
Excited State 7:	Singlet-A	3.5966 eV	344.73 nm	f=0.0010	<S**2>=0.000
175 -> 185	0.10787				
176 -> 184	0.43630				
177 -> 185	0.40512				
178 -> 185	-0.18630				
179 -> 184	0.27195				
Excited State 8:	Singlet-A	3.6543 eV	339.28 nm	f=0.0567	<S**2>=0.000
181 -> 185	0.68810				
Excited State 9:	Singlet-A	3.8830 eV	319.30 nm	f=0.0210	<S**2>=0.000
178 -> 184	0.12019				

182 -> 187	-0.14535				
183 -> 186	0.66129				
Excited State 10:	Singlet-A	4.0219 eV	308.27 nm	f=0.1125	<S**2>=0.000
179 -> 184	-0.13905				
182 -> 186	0.12322				
183 -> 187	0.66106				

HOMO: 183, LUMO: 184

Table S9. TD-DFT calculated first-ten electron transitions of **4** in dichloromethane at B3LYP / 6-311+G(d,p) level

Excited State 1:	Singlet-A	2.7326 eV	453.72 nm	f=0.2013	<S**2>=0.000
195 -> 197	0.69942				
Excited State 2:	Singlet-A	2.7379 eV	452.85 nm	f=0.2902	<S**2>=0.000
196 -> 197	0.69878				
Excited State 3:	Singlet-A	3.0023 eV	412.97 nm	f=0.0014	<S**2>=0.000
196 -> 198	0.70294				
Excited State 4:	Singlet-A	3.0467 eV	406.94 nm	f=0.1578	<S**2>=0.000
194 -> 197	0.13955				
195 -> 198	0.68673				
Excited State 5:	Singlet-A	3.1892 eV	388.77 nm	f=0.0654	<S**2>=0.000
194 -> 197	0.68590				
195 -> 198	-0.14366				
Excited State 6:	Singlet-A	3.5449 eV	349.76 nm	f=0.0728	<S**2>=0.000
189 -> 198	0.18834				
190 -> 197	-0.21555				
191 -> 197	0.11264				
194 -> 198	0.61229				
Excited State 7:	Singlet-A	3.5548 eV	348.78 nm	f=0.0017	<S**2>=0.000
187 -> 198	-0.10826				
189 -> 197	0.46342				
189 -> 199	-0.12152				
190 -> 198	-0.38906				
191 -> 198	0.14153				
192 -> 197	0.25079				
Excited State 8:	Singlet-A	3.5602 eV	348.25 nm	f=0.0096	<S**2>=0.000
187 -> 197	0.11323				
189 -> 198	-0.34132				
190 -> 197	0.42363				
190 -> 199	-0.11221				
191 -> 197	-0.14270				
192 -> 198	-0.16401				
194 -> 198	0.33258				
Excited State 9:	Singlet-A	3.7739 eV	328.53 nm	f=0.0067	<S**2>=0.000
191 -> 197	-0.13644				

195 -> 199	0.62237					
196 -> 200	0.26180					
Excited State 10:	Singlet-A	3.7751 eV	328.43 nm	f=0.0632	<S**2>=0.000	
195 -> 200	-0.10627					
196 -> 199	0.68237					

HOMO: 196, LUMO: 197

Cartesian coordinates for theoretically optimized structures

9 opt B3LYP/6-31G(d,p) Imaginary Frequency 0 HF = -1021.5626969 hartree

C	0.43549000	3.12887700	-0.00002600
C	1.80248300	3.18551000	0.00001400
C	2.29561000	1.82617900	0.00001500
C	1.15062200	1.00961600	-0.00001000
N	0.02216200	1.79133900	-0.00003300
C	-1.24343000	1.19538400	-0.00003600
C	-2.42514800	1.94865600	-0.00002500
C	-1.32014600	-0.21794600	-0.00004700
C	-3.65449900	1.30675300	-0.00002000
H	-2.38370600	3.03254400	-0.00001500
C	-2.58466500	-0.82805800	-0.00004100
C	-3.77109000	-0.09916500	-0.00002300
H	-4.54971700	1.92123800	-0.00001400
H	-2.58062400	-1.91125800	-0.00006000
C	-0.10863700	-1.10005400	-0.00005700
O	-0.19594800	-2.32675700	-0.00007900
C	3.54485400	1.19109600	0.00001000
H	4.44575900	1.79329900	0.00002400
C	3.63200500	-0.21372200	-0.00001900
C	2.44476100	-0.97785000	-0.00003200
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C	1.18083300	-0.38225900	-0.00002800
C	-5.16259300	-0.75561300	0.00002500
C	-5.94044000	-0.31346300	1.26230500
H	-6.93714600	-0.76832400	1.27388300
H	-5.41629100	-0.62096100	2.17289400
H	-6.07185000	0.77220900	1.30273400
C	-5.07667000	-2.29312900	-0.00019300
H	-6.08555300	-2.71792000	-0.00015700
H	-4.55800900	-2.67209700	-0.88642900
H	-4.55785700	-2.67237600	0.88583300
C	-5.94075600	-0.31316500	-1.26194500
H	-6.07213200	0.77252000	-1.30215000

H	-5.41688000	-0.62051900	-2.17274100
H	-6.93748900	-0.76797000	-1.27333500
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C	5.09254800	-1.83736000	1.26242700
H	5.03110800	-1.23235400	2.17296700
H	4.29350900	-2.58293800	1.30302900
H	6.04863100	-2.37270900	1.27388500
C	5.09240500	-1.83786500	-1.26203300
H	5.03093400	-1.23322100	-2.17281300
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H	4.29333500	-2.58342800	-1.30230400
C	6.18472100	0.02181000	-0.00026900
H	6.19106400	0.66301500	-0.88795000
H	6.19137200	0.66321800	0.88726200
H	7.11938800	-0.54784200	-0.00035100
H	-0.28593200	3.93098100	-0.00003400
H	2.38975400	4.09271500	0.00001900

11 opt B3LYP/6-31G(d,p) Imaginary Frequency 0 HF = -2041.9245919 hartree

C	-0.73044000	-1.77475200	-0.05492500
C	-1.48434700	-2.68060200	-0.76244900
C	-2.87171700	-2.33876900	-0.60513900
C	-2.88758200	-1.20530900	0.22690000
N	-1.60485200	-0.85373700	0.58107000
C	-1.40581200	0.22212000	1.46988000
C	-0.14166600	0.59249200	1.95159000
C	-2.54081900	0.95298800	1.90383800
C	-0.01317800	1.66836100	2.81820400
H	0.73970000	0.03746300	1.66468800
C	-2.36539700	2.03658100	2.77940200
C	-1.11718400	2.42738600	3.25385500
H	0.98468900	1.91906200	3.16504900
H	-3.27320400	2.55178600	3.06865100
C	-3.93944800	0.61955600	1.49358500
O	-4.90901600	1.27480400	1.87181800
C	-4.09738400	-2.84013600	-1.06664300
H	-4.10290200	-3.71351200	-1.70806200
C	-5.30345900	-2.21839300	-0.70242100
C	-5.25992700	-1.08333000	0.13634200
H	-6.17152600	-0.57804400	0.43701800
C	-4.05866300	-0.55806200	0.61644100
C	-0.91147300	3.61476000	4.20943800
C	-0.25697600	3.11465600	5.51915200
H	-0.09868300	3.95146500	6.20839800

H	-0.89459800	2.37869900	6.01951500
H	0.71551900	2.64681700	5.33815200
C	-2.24012500	4.30641400	4.56640200
H	-2.04809000	5.14434600	5.24405600
H	-2.74232500	4.70614700	3.67976600
H	-2.93193600	3.62458400	5.07104600
C	0.01489500	4.65736900	3.53959100
H	0.99456600	4.23634200	3.29405800
H	-0.42773400	5.03632500	2.61280800
H	0.17801000	5.50779200	4.21084800
C	-6.67310700	-2.73467700	-1.18831800
C	-7.54103700	-3.11837100	0.03369100
H	-7.06446800	-3.91153100	0.61902100
H	-7.70772600	-2.26669700	0.69923000
H	-8.52140400	-3.48092700	-0.29496800
C	-7.38557700	-1.62225700	-1.99380500
H	-6.79723600	-1.33640500	-2.87190900
H	-8.36486700	-1.97109600	-2.34004400
H	-7.54675700	-0.72293000	-1.39269800
C	-6.54620500	-3.97446100	-2.09349600
H	-5.96591800	-3.76314700	-2.99781900
H	-6.07674000	-4.81531500	-1.57221500
H	-7.54159000	-4.30023100	-2.41126000
H	-1.06734500	-3.48386300	-1.35296400
C	0.73044200	-1.77475100	0.05494400
C	1.48435000	-2.68059400	0.76247500
N	1.60485300	-0.85374000	-0.58105900
C	2.87172000	-2.33876200	0.60516000
H	1.06735000	-3.48385200	1.35299600
C	2.88758300	-1.20530700	-0.22688600
C	1.40581200	0.22210900	-1.46987800
C	4.09738700	-2.84012500	1.06666700
C	4.05866300	-0.55806300	-0.61643400
C	0.14166500	0.59247400	-1.95159200
C	2.54081700	0.95297400	-1.90384300
H	4.10290800	-3.71349600	1.70809300
C	5.30346300	-2.21838400	0.70243800
C	3.93944700	0.61954800	-1.49358700
C	5.25992900	-1.08332600	-0.13633300
C	0.01317500	1.66833500	-2.81821600
H	-0.73970000	0.03744700	-1.66468500
C	2.36539400	2.03655800	-2.77941800
C	6.67311100	-2.73466300	1.18833700
O	4.90901400	1.27478800	-1.87183300

H	6.17152600	-0.57804300	-0.43701400
C	1.11718000	2.42735700	-3.25387500
H	-0.98469200	1.91903100	-3.16506500
H	3.27320000	2.55176200	-3.06867200
C	7.54103800	-3.11837300	-0.03366900
C	7.38558500	-1.62223400	1.99380900
C	6.54621100	-3.97443600	2.09353100
C	0.91146800	3.61472200	-4.20946900
H	7.06446500	-3.91153900	-0.61898900
H	7.70772600	-2.26670700	-0.69921800
H	8.52140500	-3.48092800	0.29499100
H	6.79724600	-1.33637200	2.87191200
H	8.36487600	-1.97106900	2.34004900
H	7.54676300	-0.72291400	1.39269100
H	5.96592900	-3.76311000	2.99785500
H	6.07674000	-4.81529500	1.57226300
H	7.54159600	-4.30020600	2.41129300
C	0.25697200	3.11460400	-5.51917900
C	2.24011900	4.30637400	-4.56644000
C	-0.01490100	4.65733600	-3.53963300
H	0.09867800	3.95140600	-6.20843300
H	0.89459500	2.37864300	-6.01953500
H	-0.71552300	2.64676500	-5.33817400
H	2.04808300	5.14430000	-5.24410200
H	2.74231900	4.70611600	-3.67980800
H	2.93193100	3.62454000	-5.07107800
H	-0.99457200	4.23631000	-3.29409600
H	0.42772700	5.03630200	-2.61285300
H	-0.17801700	5.50775200	-4.21089800

2 opt B3LYP/6-31G(d,p) Imaginary Frequency 0 HF = -2327.108323 hartree

C	-1.56488600	-1.55445500	-0.08582600
C	-0.83604600	-0.35530600	-0.00429200
C	0.53564800	-0.71989600	0.01100800
C	0.57313900	-2.12333500	0.09488200
N	-0.70920900	-2.64059400	0.00523700
C	1.93270600	-2.55822500	0.26653800
C	2.67663900	-1.35348500	0.22874900
C	-2.96123200	-1.25766700	-0.26010500
C	-3.00908600	0.16051500	-0.22617500
N	-1.75166300	0.71950800	-0.03607300
N	1.86390500	-0.24284600	0.03996600
C	2.45750100	0.94449100	-0.41615300

C	1.73019300	1.95848300	-1.04548600
C	3.86224800	1.09202800	-0.27908900
C	2.36431900	3.12784200	-1.45346200
H	0.67149400	1.83213800	-1.23176500
C	4.46161800	2.28787800	-0.69183500
C	3.74216400	3.33652200	-1.26846000
H	1.75728900	3.88558600	-1.93474000
H	5.53691300	2.34576600	-0.55715200
C	-1.67690900	2.04544600	0.41733100
C	-0.54306700	2.56524000	1.04814500
C	-2.82252800	2.87076500	0.27610900
C	-0.51366000	3.89566700	1.45410900
H	0.31244800	1.92978700	1.23764700
C	-2.74952000	4.20712300	0.68653000
C	-1.60564100	4.76075000	1.26506600
H	0.38819700	4.25269100	1.93729500
H	-3.65370400	4.79117300	0.54837300
C	4.74541000	-0.01798400	0.18624000
O	5.95238500	0.12997600	0.36821900
C	-4.13954400	2.34486900	-0.19111400
O	-5.11288200	3.07334300	-0.37654400
C	-1.07591000	-4.01631100	0.00107300
C	-0.66181100	-4.85145400	1.04400100
C	-1.84947700	-4.52770300	-1.04629500
C	-1.01613300	-6.20044300	1.02998400
H	-0.07996900	-4.43797400	1.86102900
C	-2.21468100	-5.87382800	-1.04103200
H	-2.14642800	-3.87432200	-1.85992200
C	-1.79619400	-6.71416500	-0.00764300
H	-0.69398400	-6.84640800	1.84101000
H	-2.81417000	-6.26851100	-1.85572800
H	-2.07610200	-7.76292800	-0.01101500
C	2.63121700	-3.76110100	0.43102600
H	2.08139600	-4.69283500	0.44690700
C	4.03261300	-3.76370900	0.56574500
C	4.72538900	-2.54058400	0.50933100
H	5.80581300	-2.50350200	0.59691400
C	4.06448400	-1.32114300	0.32355000
C	-4.16307100	-1.94917800	-0.42320400
H	-4.15586300	-3.03310000	-0.43530900
C	-5.38510700	-1.25446400	-0.56373300
C	-5.38029900	0.14653800	-0.51222400
H	-6.29379900	0.72020900	-0.60350200
C	-4.19543700	0.87616300	-0.32486900

C	4.46213700	4.62821600	-1.69562900
C	5.53364200	4.29300200	-2.75996900
H	6.06147700	5.20228000	-3.06872500
H	6.27821900	3.58873000	-2.37811500
H	5.07658300	3.84709000	-3.64938100
C	5.14791500	5.26261100	-0.46259500
H	5.67597200	6.17876300	-0.74975300
H	4.41190000	5.52191600	0.30561000
H	5.87767500	4.58487100	-0.01055700
C	3.49299400	5.66456300	-2.29482400
H	3.00359100	5.29188900	-3.20075000
H	2.71553300	5.95699000	-1.58102600
H	4.04483100	6.56908900	-2.56933800
C	4.83133400	-5.06849300	0.76309700
C	5.83414200	-5.23978500	-0.40259500
H	5.31162100	-5.30039800	-1.36286500
H	6.53952200	-4.40601300	-0.45862700
H	6.41521800	-6.15975500	-0.27304000
C	5.60734900	-4.99747500	2.09970300
H	4.92121500	-4.88558200	2.94570600
H	6.18820700	-5.91406800	2.25218400
H	6.30373700	-4.15458100	2.12180300
C	3.92571300	-6.31390100	0.80123800
H	3.20595300	-6.27086800	1.62553900
H	3.37004600	-6.44534500	-0.13309700
H	4.53874700	-7.20885100	0.94726200
C	-1.58998000	6.24030600	1.68939400
C	-0.23739600	6.65857600	2.29583600
H	-0.00340600	6.09312100	3.20391900
H	0.58677600	6.52484000	1.58708800
H	-0.26819000	7.71814000	2.56864600
C	-1.86212100	7.12903300	0.45273300
H	-2.82946800	6.90250100	-0.00459300
H	-1.86668300	8.18713700	0.73747300
H	-1.08992800	6.98647500	-0.31050400
C	-2.69255300	6.48503600	2.74664900
H	-3.68655300	6.24363200	2.35952100
H	-2.52315600	5.87290700	3.63850600
H	-2.69996000	7.53712800	3.05290000
C	-6.68300200	-2.06508700	-0.75703500
C	-6.90392200	-2.98679200	0.46588800
H	-7.82211000	-3.57168800	0.34108700
H	-6.07818500	-3.69154900	0.60259000
H	-6.99765100	-2.40005700	1.38535900

C	-6.56714200	-2.92902200	-2.03535900
H	-6.41502200	-2.30135500	-2.91940700
H	-5.73224500	-3.63410100	-1.97804600
H	-7.48287000	-3.51162300	-2.18592400
C	-7.92001000	-1.15914600	-0.90360000
H	-8.08146800	-0.54210600	-0.01412600
H	-7.83867100	-0.49467900	-1.76962400
H	-8.81293400	-1.77681400	-1.04317500

2 transition state opt B3LYP/6-31G(d,p) Imaginary Frequency 1 HF = -2327.084404 hartree

C	1.78043300	-1.06953800	-0.68455800
C	0.42230600	-0.70016900	-0.56839300
C	0.42394500	0.74815600	-0.50796300
C	1.77932900	1.13333200	-0.59081700
N	2.59929100	0.03646600	-0.72128900
C	1.94178000	2.52265600	-0.28333100
C	0.62750200	2.95132900	0.00649500
C	1.97011700	-2.44923800	-0.35041800
C	0.66963300	-2.89985700	-0.05086400
N	-0.28756000	-1.90580400	-0.24006100
N	-0.30969600	1.94221600	-0.19717300
C	-1.65658300	2.34294100	-0.22627100
C	-2.63853200	1.64196300	-0.92786800
C	-2.02928200	3.56801500	0.38393800
C	-3.96601300	2.04106900	-0.89518300
H	-2.33307400	0.82732500	-1.55962900
C	-3.38385300	3.93614000	0.41788600
C	-4.38747900	3.17883300	-0.17946400
H	-4.68731800	1.46072400	-1.46281800
H	-3.59593300	4.87578900	0.91373300
C	-1.62986500	-2.32691400	-0.24306500
C	-2.64019400	-1.64106000	-0.91241300
C	-1.96998600	-3.56181300	0.37499200
C	-3.96555100	-2.05835600	-0.84678700
H	-2.36957800	-0.81534900	-1.54485000
C	-3.31368600	-3.94802000	0.43819000
C	-4.34867700	-3.20307800	-0.13010200
H	-4.70504000	-1.48005200	-1.38867000
H	-3.50361100	-4.89479200	0.93370800
C	-1.02893900	4.56750300	0.84616300
O	-1.34179700	5.61171400	1.41643800
C	-0.94525300	-4.54584000	0.81833800
O	-1.23186000	-5.59518100	1.39239500

C	4.02545600	0.01289600	-0.73824700
C	4.75111500	0.54781500	0.33107300
C	4.68977100	-0.56897000	-1.82247000
C	6.14532500	0.51044500	0.30372300
H	4.22293000	0.97770800	1.17517800
C	6.08390600	-0.61703800	-1.83283500
H	4.11091200	-0.97107600	-2.64753700
C	6.81398700	-0.07346800	-0.77418800
H	6.70809100	0.92460900	1.13472600
H	6.59851400	-1.06942000	-2.67497300
H	7.89896400	-0.10619300	-0.78807100
C	2.98894100	3.43758400	-0.15740800
H	3.99802400	3.12954700	-0.40516300
C	2.74756400	4.75117900	0.29787800
C	1.43593400	5.11764700	0.62775300
H	1.20128600	6.10158500	1.01366800
C	0.35769300	4.23124300	0.48161000
C	3.04845500	-3.32894500	-0.19816500
H	4.04666700	-2.98747700	-0.43807300
C	2.83904800	-4.63659400	0.27529500
C	1.52984700	-5.03403700	0.59824900
H	1.32523000	-6.02123300	0.99839800
C	0.43034200	-4.18367600	0.43805900
C	-5.87647700	3.55982800	-0.13286000
C	-6.39719700	3.80510900	-1.56888600
H	-7.45935400	4.07318000	-1.54776300
H	-5.85012200	4.62262300	-2.04927300
H	-6.29363500	2.91702600	-2.19995500
C	-6.12005100	4.83557100	0.69447800
H	-7.19130400	5.05944000	0.71960100
H	-5.78039100	4.72000200	1.72858100
H	-5.61133500	5.70404900	0.26439800
C	-6.67706000	2.40317500	0.51138500
H	-6.57120500	1.47112500	-0.05270000
H	-6.33750300	2.21416800	1.53477300
H	-7.74377400	2.65092800	0.54694200
C	3.93412800	5.72734800	0.42600500
C	4.58574100	5.92794000	-0.96288400
H	4.95844200	4.98713800	-1.37921400
H	3.86715800	6.34660500	-1.67480800
H	5.43362000	6.61829800	-0.89027700
C	3.49895300	7.10649200	0.95586900
H	3.05299800	7.03830500	1.95315400
H	4.37100700	7.76427200	1.02783700

H	2.77535500	7.58863000	0.29109100
C	4.98270900	5.14610000	1.40405900
H	4.54944000	4.99672400	2.39840400
H	5.37364200	4.18349300	1.06029400
H	5.83192100	5.83138400	1.50338000
C	-5.80788600	-3.67403800	-0.00525400
C	-6.79156200	-2.70612200	-0.68916500
H	-6.73657000	-1.69968300	-0.26041900
H	-6.61046700	-2.63142500	-1.76671300
H	-7.81645300	-3.06592700	-0.55445000
C	-5.96063700	-5.06683600	-0.66099400
H	-5.31316200	-5.81082200	-0.18835000
H	-6.99442300	-5.41889500	-0.57113400
H	-5.70585500	-5.02943300	-1.72523700
C	-6.18398700	-3.76974400	1.49220200
H	-5.53752000	-4.47081200	2.02772600
H	-6.09707900	-2.79424500	1.98171000
H	-7.21767300	-4.11566900	1.60399700
C	3.99847900	-5.63473300	0.46699500
C	4.08177600	-6.04682300	1.95593800
H	4.89630500	-6.76401600	2.10772100
H	4.27202500	-5.17677900	2.59283900
H	3.15626700	-6.51640300	2.30074700
C	5.35926300	-5.04092400	0.05688400
H	5.37617600	-4.74889700	-0.99846200
H	5.62235600	-4.16501300	0.65896500
H	6.14520100	-5.78851000	0.20384800
C	3.74183200	-6.89143900	-0.39809700
H	2.80523100	-7.38710100	-0.12775800
H	3.68743900	-6.63150800	-1.46041800
H	4.55282200	-7.61658800	-0.26675300

3 opt B3LYP/6-31G(d,p) Imaginary Frequency 0 HF = -2118.154953 hartree

C	-1.37757100	-2.89325900	-0.12678100
C	-0.70143400	-1.64425600	0.03173400
C	0.70144200	-1.64425400	-0.03170200
C	1.37758900	-2.89324900	0.12681300
C	2.79309400	-2.59545000	0.26362100
C	2.91441600	-1.21118200	0.08605300
C	-2.79307800	-2.59547400	-0.26357100
C	-2.91441400	-1.21121600	-0.08597300
N	-1.67830000	-0.62272900	0.14546700
N	1.67829600	-0.62270700	-0.14538900
C	1.66703500	0.63395000	-0.78562200

C	0.56351200	1.11775100	-1.49385700
C	2.85324300	1.41282200	-0.75181500
C	0.60502600	2.37678000	-2.08450900
H	-0.32606500	0.51094700	-1.59713300
C	2.84978700	2.68082800	-1.34557400
C	1.73797600	3.20462500	-2.00745500
H	-0.27622600	2.70775400	-2.62124000
H	3.78260800	3.23181300	-1.28234900
C	-1.66704500	0.63394300	0.78566600
C	-0.56352100	1.11776800	1.49388400
C	-2.85325800	1.41280600	0.75184500
C	-0.60503900	2.37681300	2.08450300
H	0.32606200	0.51097300	1.59716600
C	-2.84980600	2.68082800	1.34557300
C	-1.73799500	3.20464800	2.00743500
H	0.27621600	2.70780800	2.62121700
H	-3.78263100	3.23180500	1.28233900
C	4.14691400	0.89603100	-0.21190500
O	5.15058500	1.59826400	-0.11046900
C	-4.14692500	0.89599900	0.21194200
O	-5.15059500	1.59822800	0.11047800
C	3.95112400	-3.34137600	0.49883000
H	3.87340600	-4.41391300	0.63190300
C	5.20783600	-2.70864500	0.56261600
C	5.27580900	-1.31787200	0.35508200
H	6.22640200	-0.79571200	0.37812800
C	4.13714100	-0.54709700	0.09542700
C	-3.95109800	-3.34140400	-0.49883800
H	-3.87335900	-4.41393400	-0.63194800
C	-5.20781100	-2.70868400	-0.56262400
C	-5.27580100	-1.31791400	-0.35504900
H	-6.22640000	-0.79576500	-0.37811600
C	-4.13714500	-0.54713400	-0.09536700
C	1.79827500	4.60933600	-2.63353300
C	2.91864600	4.65123500	-3.69959300
H	2.97926700	5.64875000	-4.14894700
H	3.89729300	4.41942400	-3.26974400
H	2.72519700	3.92959900	-4.49998100
C	2.10603900	5.64676700	-1.52808600
H	2.16290400	6.65390000	-1.95583300
H	1.32310500	5.64707200	-0.76224800
H	3.05875300	5.44058500	-1.03191100
C	0.47185300	5.00342400	-3.30984100
H	0.21615400	4.32861300	-4.13348100

H	-0.36234400	5.00988300	-2.60045500
H	0.55704400	6.01164600	-3.72726900
C	6.50783600	-3.49051000	0.84023000
C	7.47726000	-3.31929500	-0.35335200
H	7.03482700	-3.70783000	-1.27646100
H	7.73447400	-2.26987700	-0.52242900
H	8.40931800	-3.86454000	-0.16750700
C	7.17303000	-2.93934300	2.12382400
H	6.51192700	-3.05583000	2.98881600
H	8.10350400	-3.47917200	2.33211200
H	7.41800400	-1.87744000	2.03169800
C	6.25613700	-4.99692900	1.04023500
H	5.59592400	-5.19195500	1.89189400
H	5.81667300	-5.46024600	0.15056200
H	7.20548000	-5.50423500	1.23831300
C	-1.79830300	4.60936900	2.63348900
C	-0.47186500	5.00349700	3.30974200
H	-0.21612300	4.32871000	4.13338900
H	0.36230600	5.00995400	2.60032500
H	-0.55706000	6.01172700	3.72715000
C	-2.10613000	5.64678100	1.52804300
H	-3.05885500	5.44057700	1.03190100
H	-2.16300300	6.65391600	1.95578400
H	-1.32322100	5.64709900	0.76217800
C	-2.91863800	4.65125200	3.69959100
H	-3.89729300	4.41941300	3.26977300
H	-2.72514300	3.92962700	4.49997600
H	-2.97926800	5.64877000	4.14893900
C	-6.50780700	-3.49054300	-0.84027900
C	-7.47728400	-3.31923100	0.35325400
H	-8.40933000	-3.86449400	0.16741000
H	-7.03487900	-3.70768800	1.27640800
H	-7.73449800	-2.26979600	0.52222800
C	-6.25613400	-4.99698600	-1.04018400
H	-5.59594400	-5.19208500	-1.89184300
H	-5.81665700	-5.46024600	-0.15048800
H	-7.20548700	-5.50429400	-1.23820900
C	-7.17292800	-2.93943000	-2.12392100
H	-7.41785500	-1.87750600	-2.03189000
H	-6.51181400	-3.05601600	-2.98889200
H	-8.10342700	-3.47922000	-2.33219900
C	-0.68685800	-4.11173700	-0.09885100
H	-1.23197100	-5.04539100	-0.19307400
C	0.68688600	-4.11173300	0.09889700

H	1.23200400	-5.04538300	0.19312600

3 transition state opt B3LYP/6-31G(d,p) Imaginary Frequency 1 HF = -2118.105102 hartree

C	-1.33058800	-2.56251500	-1.25903500
C	-0.69192300	-1.31459700	-0.94323800
C	0.73866300	-1.30642800	-0.93624900
C	1.39477100	-2.54789800	-1.23731100
C	2.73269000	-2.50307100	-0.68175000
C	2.85200400	-1.24795800	-0.08231300
C	-2.67686400	-2.53394900	-0.72580100
C	-2.81712700	-1.28695700	-0.12061600
N	-1.70449600	-0.48086400	-0.35284300
N	1.73510800	-0.45577500	-0.34045600
C	2.00997500	0.93257700	-0.29887800
C	1.51356500	1.84011400	-1.23571600
C	3.00071000	1.39393500	0.60582100
C	1.84719100	3.18763000	-1.16838600
H	0.93519400	1.46713600	-2.06666200
C	3.28828200	2.76440800	0.67538900
C	2.70638100	3.69917400	-0.17851100
H	1.44771500	3.84924900	-1.93113100
H	4.04630500	3.04534100	1.39666400
C	-1.99226600	0.90539900	-0.29472300
C	-1.49317600	1.83066600	-1.20666100
C	-2.99916400	1.34492400	0.60821600
C	-1.83870800	3.17903200	-1.12544900
H	-0.89675800	1.47815600	-2.03289700
C	-3.29869300	2.70758400	0.69067900
C	-2.71615600	3.66459900	-0.14530000
H	-1.42873600	3.85083900	-1.87057800
H	-4.07074000	2.97610100	1.40455300
C	3.95245600	0.46532400	1.28623200
O	4.74279100	0.82611100	2.15374100
C	-3.95090800	0.39748500	1.26271700
O	-4.75319900	0.73664300	2.12740100
C	3.77252900	-3.41942200	-0.53020800
H	3.69937100	-4.39579300	-0.99938600
C	4.90861600	-3.09611200	0.24260200
C	4.96639900	-1.83455700	0.85504300
H	5.80473000	-1.54705900	1.47715900
C	3.94741700	-0.88449400	0.69281700
C	-3.70926600	-3.46902800	-0.59704800
H	-3.61250500	-4.43695000	-1.07445400
C	-4.85435400	-3.16488300	0.16078000

C	-4.93175600	-1.90550900	0.78681500
H	-5.78411200	-1.63966700	1.40305100
C	-3.92690900	-0.94360100	0.64864000
C	3.03766500	5.20049700	-0.12885300
C	3.72791300	5.62153100	-1.44805900
H	3.96570700	6.69093800	-1.42902200
H	4.66118700	5.06861700	-1.59497200
H	3.09063200	5.43956000	-2.31897000
C	3.97698200	5.54639500	1.04168500
H	4.16084000	6.62533400	1.05918400
H	3.54269700	5.26698500	2.00685200
H	4.94734400	5.04900900	0.94813600
C	1.73164500	6.00965300	0.04409500
H	1.03947100	5.84190100	-0.78651300
H	1.21814800	5.73297300	0.97059900
H	1.94926400	7.08269600	0.08251000
C	6.03298200	-4.13964300	0.39892400
C	6.60182800	-4.49631000	-0.99492700
H	5.83582700	-4.91397400	-1.65535300
H	7.01907300	-3.61106700	-1.48567200
H	7.40017800	-5.24087300	-0.90131100
C	7.19206700	-3.62145200	1.27094200
H	6.86290600	-3.38083900	2.28673800
H	7.96558900	-4.39203100	1.34878800
H	7.65757900	-2.72834200	0.84207400
C	5.46514200	-5.41640400	1.06320900
H	5.05942900	-5.19386400	2.05530000
H	4.66429100	-5.86603900	0.46844800
H	6.25367300	-6.16828000	1.17911900
C	-3.10543500	5.14727500	-0.01241000
C	-2.41885400	6.02752700	-1.07277400
H	-1.32795900	5.98399000	-0.99467500
H	-2.70350200	5.73817400	-2.09004100
H	-2.71622000	7.07162400	-0.93353800
C	-4.63598700	5.30253400	-0.17800400
H	-5.18903500	4.74072200	0.57964700
H	-4.92161000	6.35606900	-0.08373300
H	-4.96211000	4.94918200	-1.16168400
C	-2.68945700	5.65245700	1.38926100
H	-3.17534400	5.07924900	2.18427400
H	-1.60701800	5.56902900	1.53118600
H	-2.96926100	6.70443000	1.51477900
C	-6.01280100	-4.16622800	0.34119700
C	-6.18459500	-4.48967200	1.84436500

H	-7.01022200	-5.19525600	1.98972700
H	-5.27540400	-4.94136800	2.25429200
H	-6.40574400	-3.59395100	2.43160100
C	-5.76758100	-5.48899700	-0.40890300
H	-5.66276700	-5.33388100	-1.48793500
H	-4.87222800	-6.00500000	-0.04652900
H	-6.61755500	-6.16115400	-0.25511800
C	-7.32013300	-3.54132100	-0.20117400
H	-7.57629100	-2.61552300	0.32174700
H	-7.23073900	-3.30907200	-1.26747900
H	-8.15635200	-4.23786800	-0.07405200
C	-0.64698600	-3.68501000	-1.74003400
H	-1.19984700	-4.58272600	-1.99716800
C	0.73121200	-3.67830400	-1.72713600
H	1.29751700	-4.57069900	-1.97337400

4 opt B3LYP/6-31G(d,p) Imaginary Frequency 0 HF = -2271.797866 hartree

C	-1.40423000	-2.52548400	-0.12048200
C	-0.70700700	-1.30824900	0.04956400
C	0.70686000	-1.30830000	-0.04955800
C	1.40399000	-2.52559000	0.12046000
C	2.81829800	-2.18773800	0.22439900
C	2.89624100	-0.80256600	0.00000900
C	-2.81851100	-2.18752400	-0.22440100
C	-2.89635500	-0.80235700	0.00002500
N	-1.64096300	-0.26132300	0.22091700
N	1.64089000	-0.26143600	-0.22088300
C	1.56731300	0.98100700	-0.88677100
C	0.42721600	1.40852400	-1.57969500
C	2.72195000	1.79988900	-0.90400100
C	0.41680700	2.64561000	-2.20749600
H	-0.44369400	0.77070400	-1.64398500
C	2.66680400	3.05191600	-1.53767700
C	1.52699500	3.51366400	-2.18917700
H	-0.48637500	2.93581600	-2.73540400
H	3.58244300	3.62999300	-1.50934400
C	-1.56727700	0.98112000	0.88679500
C	-0.42709000	1.40856200	1.57964200
C	-2.72183800	1.80008600	0.90405300
C	-0.41654900	2.64564800	2.20741200
H	0.44376200	0.77065400	1.64387100
C	-2.66655300	3.05213700	1.53769100
C	-1.52668100	3.51380000	2.18911600

H	0.48667300	2.93582700	2.73526300
H	-3.58214800	3.63028400	1.50940000
C	4.04089900	1.34471300	-0.37493800
O	5.02061300	2.08436100	-0.30997400
C	-4.04084700	1.34500200	0.37506600
O	-5.02052400	2.08471000	0.31020000
C	4.01999100	-2.86392800	0.48510800
H	4.01038400	-3.92574500	0.68320100
C	5.24877000	-2.17878300	0.51150900
C	5.26316000	-0.79716000	0.24673300
H	6.19099300	-0.23533500	0.24142200
C	4.09068700	-0.08865100	-0.02724500
C	-4.02026700	-2.86362600	-0.48508600
H	-4.01073900	-3.92543500	-0.68322600
C	-5.24899300	-2.17839500	-0.51142100
C	-5.26327700	-0.79676700	-0.24663600
H	-6.19107800	-0.23488800	-0.24128900
C	-4.09075100	-0.08835000	0.02733300
C	1.45257400	4.87936400	-2.89272100
C	2.76848900	5.66860100	-2.76345200
H	2.66857500	6.63543300	-3.26690400
H	3.02454400	5.86478500	-1.71740300
H	3.60814200	5.14043300	-3.22622100
C	0.31778900	5.71995800	-2.26104200
H	0.24285600	6.69322600	-2.75858900
H	-0.65470800	5.22629500	-2.34879800
H	0.50873700	5.89619200	-1.19743200
C	1.15769500	4.66992400	-4.39711500
H	1.94831700	4.08075100	-4.87282100
H	0.20875300	4.15009500	-4.56000200
H	1.09808700	5.63595700	-4.91053500
C	6.58006700	-2.89683000	0.81428800
C	7.53585000	-2.73696200	-0.39191100
H	7.10537600	-3.18228500	-1.29479300
H	7.74889300	-1.68609500	-0.60702900
H	8.49042200	-3.23514600	-0.18911400
C	7.22828500	-2.26515100	2.06918700
H	6.57688700	-2.37232300	2.94271300
H	8.18136200	-2.75690900	2.29366400
H	7.42858500	-1.19891600	1.93104100
C	6.39291200	-4.40265300	1.07931800
H	5.74883600	-4.58950600	1.94512000
H	5.96693900	-4.92116400	0.21379000
H	7.36431400	-4.86098100	1.28936300

C	-1.45208000	4.87949000	2.89267400
C	-1.15752500	4.66998300	4.39709600
H	-1.94835400	4.08096900	4.87266700
H	-0.20872800	4.14994000	4.56015200
H	-1.09780200	5.63598900	4.91055300
C	-0.31699700	5.71984100	2.26117500
H	-0.50777800	5.89613900	1.19755000
H	-0.24194400	6.69306600	2.75878400
H	0.65538100	5.22597000	2.34905700
C	-2.76777300	5.66904800	2.76311900
H	-3.02352800	5.86530000	1.71701000
H	-3.60768500	5.14110500	3.22568700
H	-2.66774700	6.63584800	3.26661100
C	-6.58032400	-2.89635400	-0.81426800
C	-7.53646900	-2.73584300	0.39157800
H	-8.49104200	-3.23397800	0.18866900
H	-7.10634500	-3.18086200	1.29477300
H	-7.74944900	-1.68486500	0.60620600
C	-6.39329600	-4.40232200	-1.07854400
H	-5.74902000	-4.58966900	-1.94409400
H	-5.96760000	-4.92045000	-0.21265400
H	-7.36470000	-4.86063000	-1.28862800
C	-7.22806300	-2.26512500	-2.06962700
H	-7.42819100	-1.19878700	-1.93201000
H	-6.57643600	-2.37279000	-2.94292700
H	-8.18116300	-2.75680400	-2.29418800
C	-0.71161200	-3.77883500	-0.10228500
C	0.71128100	-3.77888900	0.10223100
C	1.37952100	-5.02489700	0.20231200
H	2.45210900	-5.04298100	0.34053900
C	-1.37994200	-5.02479200	-0.20239500
H	-2.45253200	-5.04279600	-0.34061400
C	-0.69705300	-6.21853600	-0.10183400
H	-1.23589600	-7.15821700	-0.17650800
C	0.69654700	-6.21858900	0.10171700
H	1.23532200	-7.15831100	0.17636400

4 transition state opt B3LYP/6-31G(d,p) Imaginary Frequency 1 HF = -2271.750008 hartree

C	-1.05668100	-2.38293800	-1.10362900
C	-0.57590300	-1.06922200	-0.86782500
C	0.86104700	-0.87948500	-0.85865800
C	1.66898300	-2.02321200	-1.08015100
C	2.93784800	-1.81635600	-0.40964100

C	2.87020300	-0.52760600	0.13448000
C	-2.34525900	-2.51565200	-0.45453100
C	-2.62004100	-1.26016300	0.09510800
N	-1.63735900	-0.33792300	-0.24300700
N	1.68828900	0.10681700	-0.22828600
C	1.78596500	1.51962200	-0.26210800
C	1.22957900	2.30043300	-1.27631500
C	2.65974300	2.15107400	0.65817200
C	1.39856400	3.68002800	-1.28340100
H	0.73329800	1.81197500	-2.10138400
C	2.78098200	3.54765000	0.64856400
C	2.14224500	4.35042500	-0.29472300
H	0.96087000	4.24146700	-2.10335200
H	3.45778200	3.96248700	1.38580200
C	-2.09557500	1.00338300	-0.26508000
C	-1.74981100	1.91375100	-1.25939900
C	-3.11265400	1.37705000	0.65387800
C	-2.26590100	3.20920700	-1.25526500
H	-1.13438800	1.58302200	-2.08197500
C	-3.58596700	2.69178000	0.65471100
C	-3.16578100	3.64901300	-0.27379300
H	-1.97141800	3.87213800	-2.06049600
H	-4.35765800	2.91355100	1.38483500
C	3.66387400	1.38358700	1.45502400
O	4.34787200	1.88847100	2.34059700
C	-3.89463300	0.36565200	1.42762600
O	-4.69315500	0.66402700	2.31040300
C	4.05333400	-2.60011900	-0.09437600
H	4.12478500	-3.61254300	-0.47285800
C	5.07253100	-2.10635500	0.74634900
C	4.95184500	-0.80740700	1.26438200
H	5.70024800	-0.38991100	1.92613400
C	3.85381300	0.00749300	0.95825600
C	-3.22455400	-3.57037500	-0.16193400
H	-3.02059600	-4.55887900	-0.54910100
C	-4.34339600	-3.36464900	0.66326400
C	-4.56793200	-2.07919200	1.19381100
H	-5.40933900	-1.88287400	1.84970800
C	-3.71941900	-1.00633700	0.91222600
C	2.29853700	5.88027800	-0.33656100
C	3.01154700	6.28966200	-1.64742000
H	3.12686500	7.37825900	-1.69433400
H	4.00759600	5.83964300	-1.70787400
H	2.44923000	5.97757500	-2.53294400

C	3.12488100	6.40939600	0.85061400
H	3.18441000	7.50121000	0.79957900
H	2.67088400	6.14524500	1.81100100
H	4.14899000	6.02361800	0.84045900
C	0.90276800	6.54319300	-0.28702700
H	0.28116500	6.24196100	-1.13560800
H	0.37218500	6.27240100	0.63154100
H	0.99710200	7.63426100	-0.31658500
C	6.27288200	-3.01575400	1.08011800
C	6.99795600	-3.41494800	-0.22699500
H	6.33930000	-3.95851300	-0.91116300
H	7.37050200	-2.53061600	-0.75408300
H	7.85273600	-4.06361100	-0.00549300
C	7.29378100	-2.31887600	1.99922800
H	6.85302200	-2.03959500	2.96139100
H	8.12727900	-2.99843000	2.20331200
H	7.70845600	-1.41656500	1.53852600
C	5.77114900	-4.29090900	1.79857100
H	5.25871400	-4.03764600	2.73216600
H	5.07303100	-4.86255000	1.17965800
H	6.61400800	-4.94782900	2.04075100
C	-3.74529700	5.07378500	-0.23010600
C	-3.20533200	5.95821400	-1.36896100
H	-2.11656000	6.06150900	-1.32364700
H	-3.47345100	5.56371100	-2.35487100
H	-3.63391400	6.96225300	-1.29036100
C	-5.28615000	5.01292700	-0.35802500
H	-5.74139100	4.43753600	0.45272700
H	-5.70874000	6.02328100	-0.32594200
H	-5.58337400	4.55050900	-1.30494600
C	-3.37068300	5.72951400	1.11986400
H	-3.75850300	5.15720500	1.96759300
H	-2.28406100	5.80006500	1.23380200
H	-3.78584100	6.74172100	1.18059100
C	-5.32129200	-4.50302000	1.01842300
C	-5.33618100	-4.70917600	2.55175800
H	-6.03306300	-5.51072400	2.82104000
H	-4.34251700	-4.98503700	2.91941500
H	-5.64873800	-3.80512200	3.08190300
C	-4.93326600	-5.83997300	0.35925100
H	-4.92939000	-5.77095400	-0.73376300
H	-3.94743700	-6.18706500	0.68596800
H	-5.66001000	-6.60993700	0.63658300
C	-6.74281800	-4.12545200	0.53817600

H	-7.09856500	-3.20224800	1.00431800
H	-6.76471900	-3.98182200	-0.54711900
H	-7.45332700	-4.92062800	0.79008600
C	-0.24735400	-3.41300300	-1.67930200
C	1.16470500	-3.22742100	-1.66498400
C	-0.77736900	-4.60307500	-2.22995500
C	1.99540800	-4.23886300	-2.20114700
C	0.05638000	-5.57667000	-2.74721800
C	1.45219300	-5.39340600	-2.73258500
H	-1.85231900	-4.72634000	-2.29397600
H	3.06675700	-4.07962500	-2.24323400
H	2.10254700	-6.15023000	-3.16063700
H	-0.36763700	-6.47453800	-3.18652600

Carbo[7]helicene opt B3LYP/6-31G(d,p) Imaginary Frequency 0 HF = -1154.105822 hartree

C	-1.68543500	3.43866500	-0.85855700
C	-0.47320000	2.90719700	-0.32878000
C	-0.44175700	1.59263800	0.21142200
C	-1.58481400	0.72872500	-0.03510700
C	-2.82413100	1.36244200	-0.35153400
C	-2.84299600	2.72168100	-0.78024500
C	0.70138000	1.24247300	1.04496500
C	-1.58487100	-0.72860300	0.03510800
C	-0.44188300	-1.59260600	-0.21142400
C	0.70128100	-1.24252800	-1.04496500
C	-0.47342900	-2.90716400	0.32877500
C	-1.68570500	-3.43853600	0.85855300
C	-2.84321000	-2.72146100	0.78024400
C	-2.82423800	-1.36222300	0.35153500
C	-4.04916400	-0.64409500	0.22316100
C	-4.04911300	0.64441100	-0.22315700
H	-4.97990900	1.16611800	-0.42747500
H	-4.98000100	-1.16572900	0.42747900
H	-1.68191800	4.45174700	-1.25109500
H	-3.79331300	3.15977800	-1.07244100
H	-1.68226800	-4.45161900	1.25108900
H	-3.79356000	-3.15948300	1.07244100
C	0.70164700	3.72393800	-0.31310000
C	1.84644900	3.30181800	0.28950100
C	1.86038100	2.08177200	1.03345500
H	0.65619700	4.69470000	-0.79944900
H	2.74222600	3.91675000	0.27707100
C	1.86021600	-2.08191800	-1.03345700

C	0.70135300	-3.72399700	0.31309200
H	0.65582600	-4.69475700	0.79943900
C	1.84618800	-3.30196600	-0.28950700
H	2.74191600	-3.91696900	-0.27707900
C	0.69213500	0.16754100	1.96982500
H	-0.20496500	-0.42404300	2.08699800
C	2.98610200	1.74150600	1.82254600
H	3.86275100	2.38235700	1.77510700
C	1.78947000	-0.12331600	2.75614100
C	2.96351600	0.64907100	2.66244500
H	1.73901700	-0.94927500	3.45938300
H	3.82902600	0.40502900	3.27127300
C	0.69212300	-0.16759100	-1.96981900
H	-0.20493100	0.42406500	-2.08699000
C	2.98596600	-1.74173700	-1.82254600
C	2.96346600	-0.64929700	-2.66244000
H	3.82899600	-0.40532000	-3.27126600
C	1.78948100	0.12318400	-2.75613300
H	1.73909300	0.94915000	-3.45937100
H	3.86256300	-2.38265700	-1.77510900

Carbo[7]helicene transition state opt B3LYP/6-31G(d,p) Imaginary Frequency 1 HF = -1154.039185 hartree

C	-2.77434500	1.37772700	-0.72889100
C	-1.52001400	0.74020200	-0.45957000
C	-1.52058800	-0.73912900	-0.45958300
C	-2.77531900	-1.37576700	-0.72901600
C	-0.99634200	-2.65878900	1.00030200
C	-0.99422200	2.65951300	1.00012500
C	0.90015600	-1.71037300	-0.15485600
C	1.39528800	-1.42507100	-1.44796900
C	1.78571800	-2.37442500	0.75486100
C	2.71291000	-1.66438500	-1.78734400
H	0.69706200	-1.08043100	-2.20106600
C	3.15411100	-2.51037200	0.42324700
C	3.61688100	-2.15885800	-0.82901800
H	3.05166200	-1.46889800	-2.80032500
H	3.82006200	-2.97460300	1.14604000
C	0.90157900	1.70963200	-0.15498800
C	1.39665500	1.42305300	-1.44782600
C	1.78755800	2.37369100	0.75435900
C	2.71439500	1.66145300	-1.78736600
H	0.69830800	1.07813900	-2.20065400
C	3.15599100	2.50886800	0.42257600

C	3.61858500	2.15631400	-0.82945000
H	3.05310200	1.46482800	-2.80013900
H	3.82216100	2.97327000	1.14505700
C	1.23932300	-3.05694900	1.88586800
C	1.24173100	3.05679300	1.88519000
C	-0.10381300	-3.27931100	1.93480800
C	-0.10129500	3.27974600	1.93437300
C	-3.82363700	0.68122100	-1.39469700
H	-4.68397500	1.24279700	-1.74779300
C	-3.82409100	-0.67845300	-1.39480800
H	-4.68473600	-1.23938400	-1.74817700
H	4.65961400	-2.31246300	-1.09068700
H	1.91122600	-3.51350700	2.60722800
H	4.66134200	2.30944200	-1.09130300
H	1.91399300	3.51323900	2.60628500
C	-0.51855300	-1.63330900	0.14113000
C	-0.51718500	1.63362700	0.14098800
H	-0.53107400	-3.94775000	2.67763000
H	-0.52817700	3.94850300	2.67713200
C	-2.32552900	-3.14994100	0.84709800
H	-2.64907300	-3.99350700	1.45010700
C	-3.11780400	-2.62817700	-0.13109200
H	-4.09116000	-3.05535000	-0.35405800
C	-3.11595000	2.63031500	-0.13087100
H	-4.08902400	3.05820500	-0.35369300
C	-2.32308600	3.15152000	0.84711300
H	-2.64595300	3.99526200	1.45025800

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