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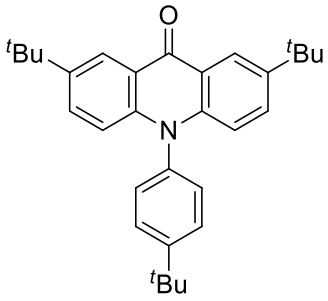
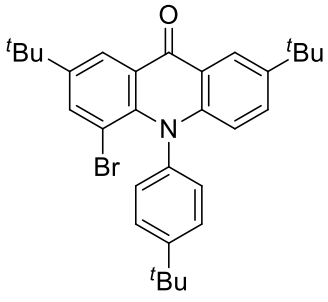
1. General Remarks

All reagents and solvents were commercially available and were used without further purification unless otherwise noted. IR-Spectra were recorded as KBr-pellets on a Bruker VERTEX 80V spectrometer. NMR spectra were taken on Bruker AVANCE NEO (400MHz). 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. Crystal structure analysis was accomplished with a XtaLAB AFC12 (RINC): Kappa single diffractometer. 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. Electrochemical data were obtained in dichloromethane solution of tetrabutylammonium hexafluorophosphate (0.1 M) and ferrocene was used as an internal standard. Cyclic voltammagram (CV) and differential pulse voltammagrams (DPV) were obtained using a glassy carbon working electrode, a platinum counter electrode, and a Ag reference electrode tested on CHI660E station. Compound **4** was synthesized according to the previously reported method.[S1]

2. Experimental part

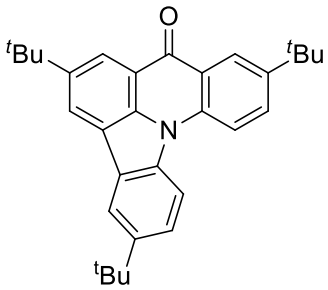


A 120 mL screw capped glass vial was charged with 2,7-di-*tert*-butylacridone **4** (1.95 g, 10 mmol), 4-*tert*-butyl-bromobenzen (2.34 g, 11 mmol), CuI (210 mg, 1.1 mmol), K_2CO_3 (2.28 g, 16.5 mmol) and 2,2,6,6-tetramethylheptane-3,5-dione (405 mg, 2.2 mmol). Under the protection of argon, dry DMAc (30 mL) was added to the vial. After bubbling with argon for three minutes, the vial was quickly sealed. The vial was heated in an oil bath at 160 °C for 36 hours. After cooling down to room temperature, the mixture was diluted with dichloromethane (200 mL) and washed with water (3×200 mL). The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane) to give product **5** (2.78 g, 6.32 mmol, 63%) as light-yellow solid. m.p. 260°C; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm)= 8.59 (d, J = 2.5 Hz, 2H), 7.69-7.66 (m, 2H), 7.58 (dd, J = 9.0, 2.5 Hz, 2H), 7.27-7.24 (m, 2H), 6.76 (d, J = 9.0 Hz, 2H), 1.39 (s, 18H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) = 180.17, 148.41, 147.05, 146.65, 139.10, 136.35, 136.14, 131.10, 130.42, 129.08, 125.83, 124.27, 124.17, 122.25, 121.85, 121.73, 119.63, 117.00, 106.68, 35.55, 34.97, 34.88, 32.09, 31.76, 31.54; IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 3433, 3035, 2960, 2903, 2868, 1644, 1608, 1553, 1509, 1488, 1395, 1363, 1328, 1300, 1259, 1204, 1169, 1148, 1110, 1019, 925, 874, 838, 818, 796, 588, 543, 492; HRMS(ESI) (*m/z*): $[M+H]^+$ calculated for $C_{31}H_{38}NO$, 440.2953; found, 440.2957.

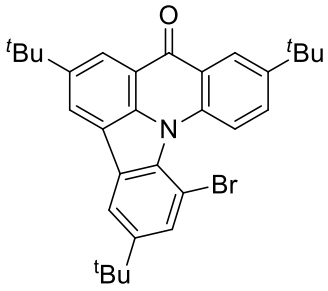


A 100 mL flask was charged with compound **5** (2.58 g, 5.88 mmol), dichloromethane (60 mL) and liquid bromine (4.69 g, 29.35 mmol). The mixture was stirred at room temperature for 1 hour and potassium carbonate (813 mg, 5.88 mmol) was added. The mixture was then stirred for another 15 hours and the reaction was quenched by adding the aqueous sodium sulfite solution. Additional dichloromethane (200 mL) was added to the reaction mixture, which was further washed with water (3×200 mL). The solvent was removed by rotary evaporation and the crude product was purified by silica gel column chromatography (light petroleum/dichloromethane 2:3) to give product **6** (2.22 g, 4.29 mmol, 73%) as yellow solid. m.p. 222°C; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 8.65

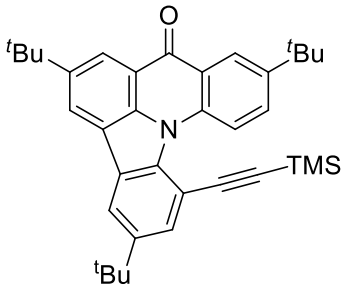
(d, *J* = 2.6 Hz, 1H), 8.51 (d, *J* = 2.5 Hz, 1H), 7.91 (d, *J* = 2.5 Hz, 1H), 7.58 (dd, *J* = 9.1, 2.5 Hz, 1H), 7.53 (d, *J* = 8.4 Hz, 2H), 7.27 (d, *J* = 8.4 Hz, 2H), 7.05 (d, *J* = 9.1 Hz, 1H), 1.41 (s, 9H), 1.39 (s, 9H), 1.37 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) = 178.12, 152.68, 145.82, 145.25, 142.87, 139.54, 138.76, 138.08, 131.08, 126.45, 125.11, 123.71, 122.67, 121.12, 109.57, 34.99, 34.58, 34.52, 31.59, 31.37, 31.29; IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 3437, 2960, 2905, 2869, 1643, 1614, 1598, 1508, 1489, 1465, 1396, 1364, 1317, 1271, 1202, 1153, 1113, 1021, 927, 883, 842, 819, 793, 762, 702, 625, 591, 454; HRMS(ESI) (*m/z*): $[M+H]^+$ calculated for $C_{31}H_{37}BrNO$, 518.2059; found, 518.2059.



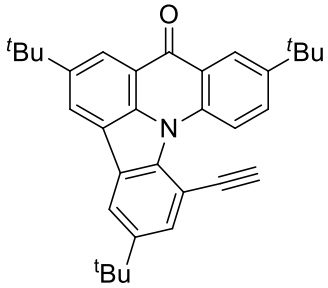
A 120 mL screw capped glass vial was charged with compound **6** (2.07 g, 4 mmol), $Pd(OAc)_2$ (54 mg, 0.24 mmol) and K_2CO_3 (1.11 g, 8 mmol). Under the protection of argon, dry DMF (20 mL) and PCy_3HBF_4 (177 mg, 0.48 mmol) were added to the vial. After bubbling with argon for three minutes, the vial was quickly sealed. The vial was heated in an oil bath at 130 °C for 36 hours. After cooling down to room temperature, the mixture was diluted with dichloromethane (200 mL) and washed with water (3×200 mL). The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane/light petroleum ether 1:1) to give product **7** (1.66 g, 3.81 mmol, 95%) as cyan solid. m.p. 261°C; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 8.70 (d, *J* = 2.4 Hz, 1H), 8.52 (s, 1H), 8.45 (s, 1H), 8.36 (dd, *J* = 9.4, 3.1 Hz, 1H), 8.21 (s, 1H), 8.20-8.16 (m, 1H), 7.93 (dd, *J* = 8.8, 2.3 Hz, 1H), 7.66 (d, *J* = 8.7 Hz, 1H), 1.56 (s, 9H), 1.51 (s, 9H), 1.48 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) = 179.18, 146.60, 146.23, 146.14, 137.76, 137.63, 137.40, 131.70, 126.63, 125.36, 125.25, 125.13, 124.83, 122.67, 121.16, 119.17, 118.06, 115.37, 113.50, 35.56, 34.98, 34.89, 32.15, 31.89, 31.53; IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 3435, 2961, 2904, 2868, 1654, 1612, 1556, 1492, 1417, 1393, 1363, 1310, 1291, 1266, 1203, 1151, 876, 805, 623, 593; HRMS(ESI) (*m/z*): $[M+H]^+$ calculated for $C_{31}H_{36}NO$, 438.2797; found,438.2797.



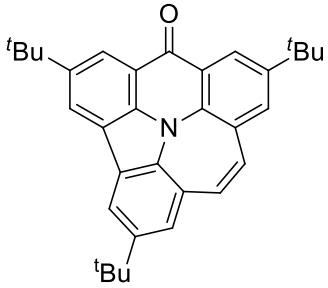
A 100 mL flask was charged with compound **7** (144 mg, 0.33 mmol), dichloromethane (6 mL) and liquid bromine (210 mg, 1.32 mmol). The mixture was stirred at room temperature for 1 hour and potassium carbonate (92 mg, 0.66 mmol) was added. The mixture was then stirred for another 15 hours and the reaction was quenched by adding the aqueous sodium sulfite solution. Additional dichloromethane (100 mL) was added to the reaction mixture, which was further washed with water (3×100 mL). The solvent was removed by rotary evaporation and the crude product was purified by silica gel column chromatography (light petroleum/dichloromethane 2:3) to give product **8** (145 mg, 0.28 mmol, 85%) as yellow solid. m.p. 266°C; ^{1}H NMR (600 MHz, $CDCl_3$) δ (ppm) = 8.54 (d, *J* = 2.4 Hz, 1H), 8.44 (d, *J* = 1.7 Hz, 1H), 8.36 (d, *J* = 1.8 Hz, 1H), 8.19 (d, *J* = 8.7 Hz, 1H), 8.14 (d, *J* = 1.8 Hz, 1H), 7.80 (d, *J* = 1.8 Hz, 1H), 7.78 (dd, *J* = 8.8, 2.5 Hz, 1H), 1.53 (s, 9H), 1.50 (s, 9H), 1.45 (s, 9H); ^{13}C NMR (150 MHz, $CDCl_3$) δ (ppm) = 78.39, 152.72, 144.19, 141.30, 136.41, 131.20, 129.46, 127.80, 122.77, 121.31, 116.75, 35.02, 34.56, 31.50, 31.43; IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 3434, 2960, 2903, 2867, 1653, 1611, 1542, 1487, 1461, 1392, 1364, 1343, 1301, 1281, 1253, 1202, 1171, 1137, 1097, 1080, 882, 867, 827, 794, 633, 598, 493; HRMS(ESI) (*m/z*): $[M+Na]^+$ calculated for $C_{31}H_{34}BrNONa$, 538.1721; found, 538.1722.



A 120 mL screw capped glass vial was charged with compound **8** (717 mg, 1.39 mmol), CuI (3 mg, 0.016 mmol) and $PdCl_2(PPh_3)_2$ (20 mg, 0.028 mmol). Under the protection of argon, dry triethylamine (7 mL) and trimethylsilylacetylene (273 mg, 2.78 mmol) were added to the vial. After bubbling with argon for three minutes, the vial was quickly sealed. The vial was heated in an oil bath at 85 ºC for 16 hours. After cooling down to room temperature, the mixture was diluted with dichloromethane (200 mL) and washed with water (3×200 mL). The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane/light petroleum ether 1:1) to give product **9** (738 mg, 1.38 mmol, 99%) as yellow solid. m.p. 315℃; ^{1}H NMR (600 MHz, CD_2Cl_2) δ (ppm) = 8.62 (d, J = 2.5 Hz, 1H), 8.48-8.44 (m, 2H), 8.41 (s, 1H), 8.38 (d, J = 8.8 Hz, 1H), 8.22 (s, 1H), 7.99 (dd, J = 8.8, 2.5 Hz, 1H), 1.69 (s, 9H), 1.55 (s, 9H), 1.48 (s, 9H), 0.34 (s, 9H); ^{13}C NMR (150 MHz, CD_2Cl_2) δ (ppm) = 178.85, 147.55, 147.25, 146.80, 138.18, 137.68, 137.42, 132.14, 126.86, 125.17, 125.10, 125.08, 123.23, 121.62, 121.30, 120.78, 119.55, 118.89, 115.90, 107.63, 101.51, 36.32, 35.75, 35.07, 32.11, 31.51, 30.35; IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 3433, 2958, 2905, 2870, 2145, 1659, 1615, 1565, 1492, 1414, 1363, 1307, 1268, 1251, 1158, 1050, 908, 880, 860, 841, 799, 758, 676, 640, 591, 527; HRMS(ESI) (*m/z*): $[M+Na]^+$ calculated for $C_{36}H_{43}NOSiNa$, 556.3012; found, 556.3003.

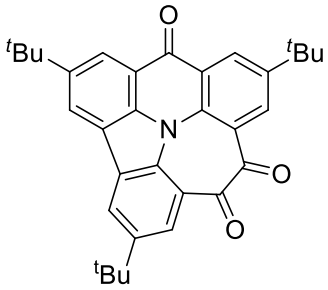


A 100 mL flask was charged with compound **9** (738 mg, 1.38 mmol), K_2CO_3 (573 mg, 4.15 mmol), methanol (7 mL) and THF (7 mL). The mixture was stirred at room temperature for 16 hours. The reaction mixture was diluted with dichloromethane (150 mL) and washed with water (3×150 mL). The solvent was removed by rotary evaporation and the crude product was purified by silica gel column chromatography (light petroleum/dichloromethane 1:1) to give product **10** (635 mg, 1.37 mmol, 99%) as yellow solid. m.p.=155℃; ^{1}H NMR (600 MHz, DMSO-d_6) δ (ppm) = 8.91 (s, 1H), 8.80 (d, J = 8.8 Hz, 1H), 8.68 (s, 1H), 8.38 (d, J = 2.4 Hz, 1H), 8.25 (s, 1H), 7.96 (d, J = 8.9 Hz, 1H), 7.79 (s, 1H), 4.91 (s, 1H), 1.50 (s, 9H), 1.47 (s, 9H), 1.41 (s, 9H). ^{13}C NMR (150 MHz，CD_2Cl_2) δ (ppm) = 179.63, 147.22, 147.05, 146.83, 138.70, 137.52, 136.92, 132.66, 129.62, 128.51, 125.64, 124.76, 124.22, 122.68, 121.47, 121.36, 119.75, 119.68, 108.15, 87.23, 83.26, 35.73, 35.06, 35.04, 32.13, 31.72, 31.57. IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 3435, 3306, 2960, 2904, 2868, 1655, 1611, 1554, 1488, 1461, 1387, 1364, 1308, 1283, 1253, 1198, 1098, 1049, 873, 822, 794, 639, 599, 521, 491. HRMS(ESI) (*m/z*): $[M+H]^+$ calculated for $C_{33}H_{36}NO$, 462.2797; found, 462.2797.



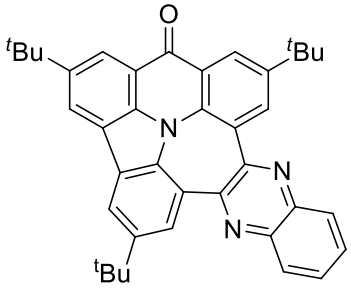
A 120 mL screw capped glass vial was charged with compound **10** (526 mg, 1.14 mmol), $PtCl_2$ (15 mg, 0.057 mmol) and toluene (6 mL). The vial was sealed and heated in an oil bath at 100 ºC for 36 hours. After cooling down to room temperature, the mixture was diluted with dichloromethane (150 mL) and washed with water (3×150 mL). The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane/light petroleum ether 1:1) to give product **11** (328 mg, 0.71 mmol, 62%) as orange solid. m.p. 250℃; ^{1}H NMR (600 MHz, CD_2Cl_2) δ (ppm) = 8.30 (d, J = 1.8 Hz, 1H), 8.26 (d, J = 1.8 Hz, 1H), 8.10 (d, J = 2.5 Hz, 1H), 7.61 (d, J = 1.9 Hz, 1H), 7.05 (d, J = 2.5 Hz, 1H), 6.77 (d, J = 1.9 Hz, 1H), 5.88-5.77 (m, 2H), 1.51 (s, 9H), 1.37 (s, 9H), 1.35 (s, 9H). ^{13}C NMR (150 MHz，CD_2Cl_2) δ (ppm) = 178.04, 147.95, 147.45, 146.90, 140.58, 139.80, 136.31, 136.08, 132.62, 129.93, 128.48, 126.82, 126.21, 126.20, 126.07, 125.24, 125.10, 122.89, 120.71, 118.68, 117.96, 35.64, 34.75, 34.56, 32.07, 31.45, 31.04. IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 3435, 2958, 2904, 2867, 1653, 1596, 1559, 1477, 1446,

1391, 1361, 1298, 1272, 1255, 1233, 1202, 1176, 1015, 954, 895, 866, 795, 752, 714, 633, 575. HRMS(ESI) (*m/z*): $[M+Na]^+$ calculated for $C_{33}H_{35}NONa$, 484.2616; found, 484.2609.

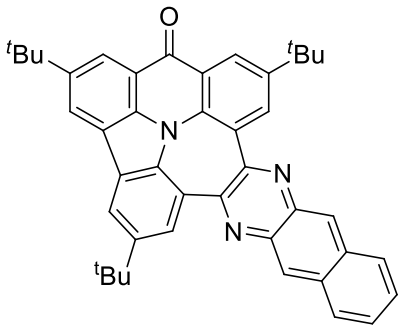


Method A: A 38 mL screw capped glass vial was charged with compound **11** (160 mg, 0.35 mmol), SeO_2 (77 mg, 0.69 mmol) and *o*-dichlorobenzene (1 mL). The vial was sealed and heated in an oil bath at 120 °C for 2 days. After cooling down to room temperature, the mixture was diluted with dichloromethane (100 mL) and washed with water (3×100 mL). The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane/light petroleum ether 1:1) to give product **12** (34 mg, 0.069 mmol, 20%) as orange solid.

Method B: A 38 mL screw capped glass vial was charged with compound **11** (133 mg, 0.29 mmol), benzeneseleninic acid anhydride (114 mg, 0.32 mmol) and toluene (3 mL). The vial was sealed and heated in an oil bath at 140 °C for 36 hours. After cooling down to room temperature, the mixture was diluted with dichloromethane (150 mL) and washed with water (3×150 mL). The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane/light petroleum ether 1:1) to give product **12** (134 mg, 0.27 mmol, 94%) as orange solid. m.p. 315°C; ^{1}H NMR (600 MHz, DMSO-d_6) δ (ppm) = 9.04 (dd, J = 5.9, 1.9 Hz, 2H), 8.86 (d, J = 2.6 Hz, 1H), 8.48 (d, J = 2.6 Hz, 1H), 8.29 (d, J = 1.8 Hz, 1H), 8.20 (d, J = 2.0 Hz, 1H), 1.53 (s, 9H), 1.51 (s, 9H), 1.47 (s, 9H). ^{13}C NMR (150 MHz, C_6D_6) δ (ppm) = 190.74, 187.93, 177.59, 148.47, 148.40, 147.96, 138.09, 135.41, 135.38, 133.43, 132.61, 127.58, 126.27, 125.86, 125.50, 124.90, 124.13, 122.67, 122.24, 120.03, 119.67, 35.42, 35.07, 34.90, 31.82, 31.48, 31.04. IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 3433, 2961, 2870, 1657, 1616, 1591, 1554, 1481, 1409, 1364, 1306, 1273, 1258, 1230, 1200, 1163, 1100, 1018, 911, 889, 847, 824, 793, 757, 634, 572, 414. HRMS(ESI) (*m/z*): $[M+Na]^+$ calculated for $C_{33}H_{33}NO_3Na$, 514.2358; found, 514.2363.



A 120 mL screw capped glass vial was charged with compound **12** (325 mg, 0.66 mmol), benzene-1,2-diamine (93 mg, 0.86 mmol), chloroform (13 mL) and acetic acid (7 mL). The vial was sealed and heated in an oil bath at 80 °C for 40 hours. After cooling down to room temperature, the mixture was diluted with dichloromethane (200 mL) and washed with water (3×200 mL). The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane/light petroleum ether 3:2) to give product **13** (283 mg, 0.5 mmol, 76%) as yellow solid. m.p. 190°C; ^{1}H NMR (600 MHz, DMSO-d_6) δ (ppm) = 8.98 (d, J = 2.6 Hz, 1H), 8.84 (d, J = 1.9 Hz, 1H), 8.78 (d, J = 1.8 Hz, 1H), 8.44 (dd, J = 13.4, 2.3 Hz, 2H), 8.17 (d, J = 1.8 Hz, 1H), 7.97 (t, J = 8.6 Hz, 2H), 7.80-7.72 (m, 2H), 1.50 (s, 9H), 1.48 (s, 9H), 1.42 (s, 9H). ^{13}C NMR (150 MHz, CD_2Cl_2) δ (ppm) = 178.30, 149.88, 148.70, 147.92, 147.85, 147.71, 142.41, 141.53, 138.86, 138.48, 137.86, 137.62, 130.77, 130.33, 129.60, 129.22, 128.58, 127.47, 126.67, 126.63, 125.88, 125.23, 123.06, 122.92, 120.93, 120.89, 119.24, 35.72, 35.38, 35.20, 32.08, 31.76, 31.35. IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 3436, 2959, 2904, 2868, 1657, 1598, 1559, 1479, 1405, 1364, 1329, 1275, 1239, 1200, 1168, 1120, 1103, 906, 878, 793, 757, 578. HRMS(ESI) (*m/z*): $[M+Na]^+$ calculated for $C_{39}H_{37}N_3ONa$, 586.2834; found, 586.2823.



A 38 mL screw capped glass vial was charged with compound **12** (34 mg, 0.069 mmol), naphthalene-2,3-diamine (15 mg, 0.09 mmol), chloroform (2 mL) and acetic acid (1 mL). The vial was sealed and heated in an oil bath at 80 °C for 40 hours. After cooling down to room temperature, the mixture was diluted with dichloromethane (50 mL) and washed with water (3×50 mL). The solvent was removed by rotatory evaporation and the crude product was purified by silica gel column chromatography (dichloromethane/light petroleum ether 3:1) to give product **14** (36 mg, 0.058 mmol, 84%) as orange solid. m.p. > 400°C (dec.); ^{1}H NMR (600 MHz, CD_2Cl_2) δ (ppm) = 9.20 (dd, *J* = 5.2, 2.3 Hz, 2H), 8.74 (d, *J* = 2.6 Hz, 1H), 8.62 (d, *J* = 5.8 Hz, 2H), 8.49 (d, *J* = 1.8 Hz, 1H), 8.44 (d, *J* = 1.8 Hz, 1H), 8.25 (d, *J* = 2.0 Hz, 1H), 8.08 (dt, *J* = 5.4, 3.3 Hz, 2H), 7.58-7.52 (m, 2H), 1.59 (s, 9H), 1.57 (s, 9H), 1.55 (s, 9H). ^{13}C NMR (150 MHz, CD_2Cl_2 + CS_2) δ (ppm) = 177.68, 150.51, 149.10, 147.74, 147.72, 139.23, 138.62, 138.31, 138.25, 138.08, 137.82, 135.19, 134.89, 129.49, 129.08, 129.06, 128.24, 127.73, 127.39, 127.30, 127.29, 126.65, 126.14, 125.39, 123.08, 122.78, 121.42, 121.27, 119.59, 35.70, 35.45, 35.28, 32.36, 32.10, 31.67. IR (KBr) $\tilde{\nu}$ (cm^{-1}) = 3434, 2958, 2867, 1657, 1637, 1597, 1558, 1481, 1405, 1364, 1333, 1307, 1265, 1201, 1166, 1102, 875, 793, 740, 583, 513, 485. HRMS(ESI) (*m/z*): $[M+H]^+$ calculated for $C_{43}H_{39}N_3O$, 614.3171; found, 614.3165.

Chemical oxidation of **11**: The solution of $AgSbF_6$ (15 mg, 0.044 mmol) in dry dichloromethane (10 mL) was added to the solution of compound **11** (20 mg, 0.043) in dry dichloromethane (10 mL) under the protection of Argon. The solution was stirred at room temperature for 1 hour and the color was changed from dark blue to blackish green. The solution was filtered through a syringe and the solvent was removed under reduced pressure. The residue was further washed with hexane (5 mL) to afford $\mathbf{11}^{\bullet+}$ quantitatively as a dark brown solid. Elemental anal. calculated for $C_{33}H_{35}F_6NOSb$: C 56.83 H 5.06 N 2.01, found: C 56.92 H 4.95 N 2.07.

3. NMR spectra

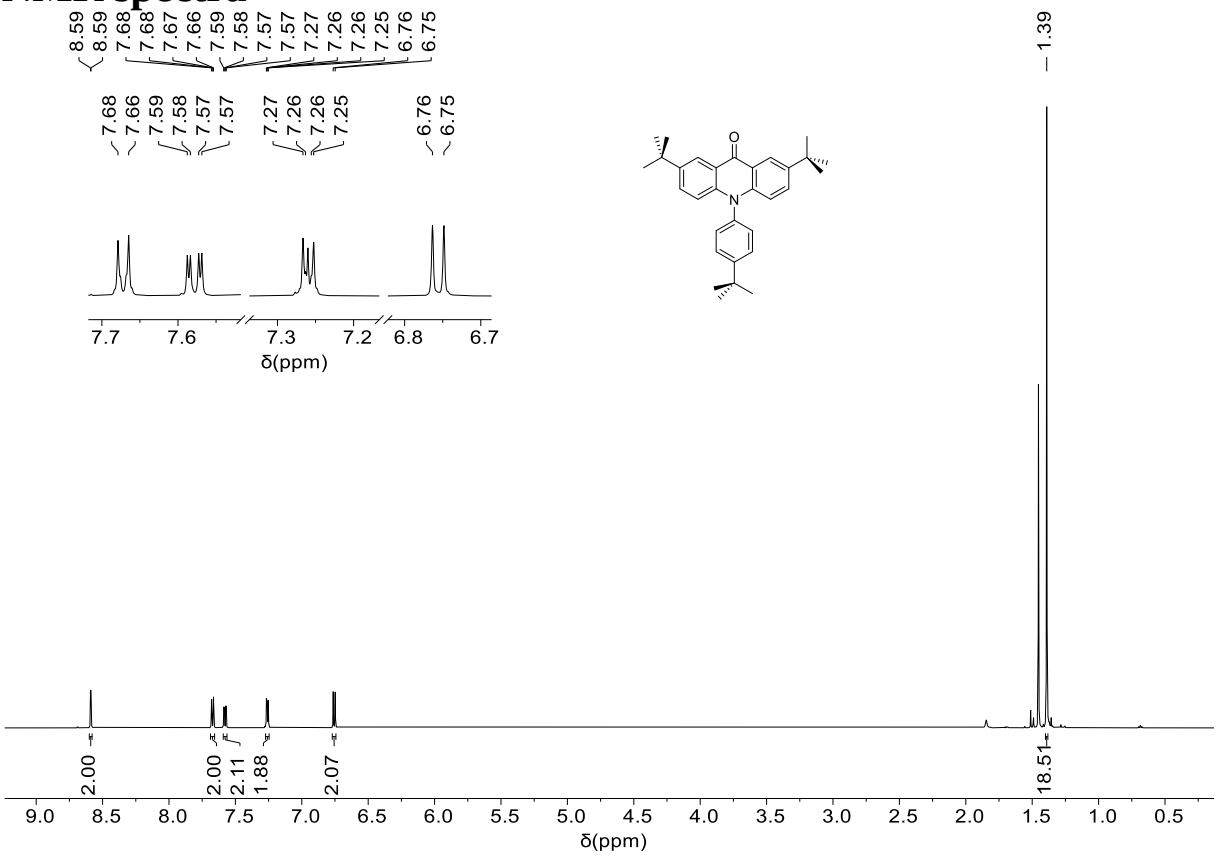


Figure S1. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of compound **5**.

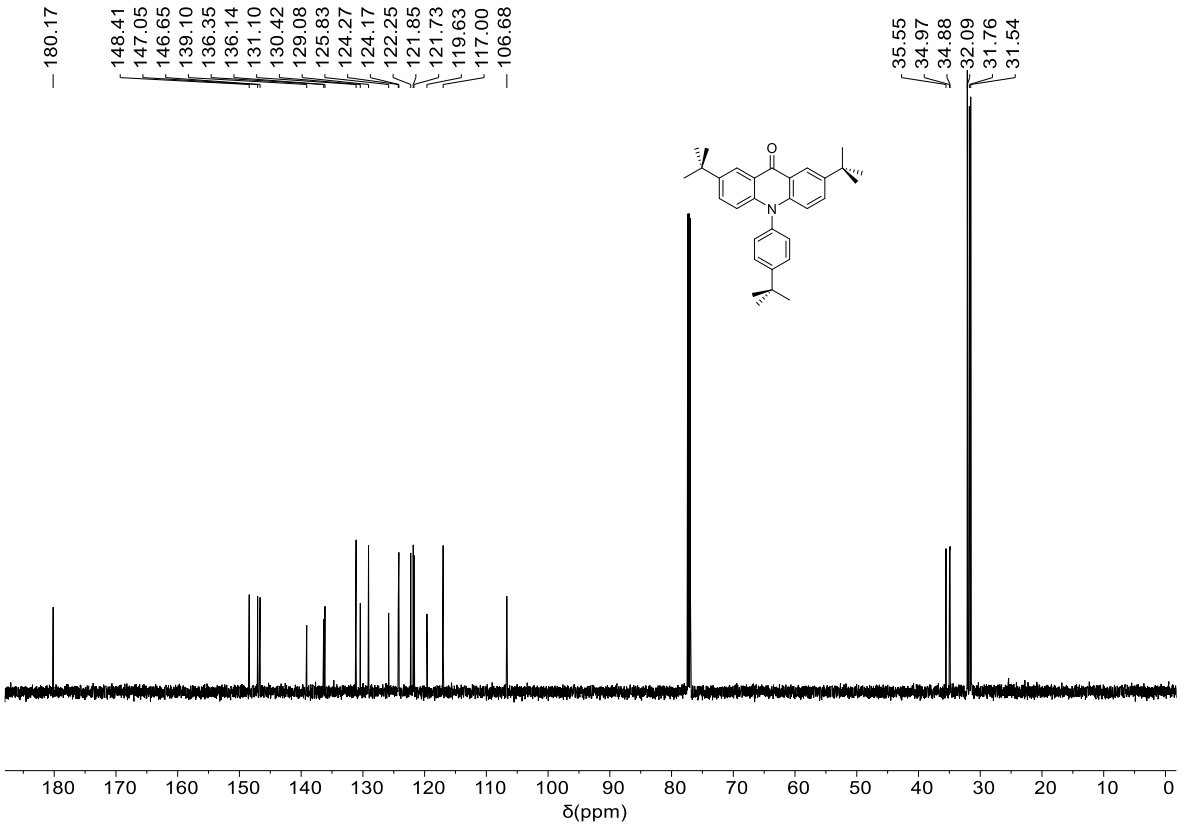


Figure S2. ^{13}C NMR spectrum (150 MHz, $CDCl_3$) of compound **5**.

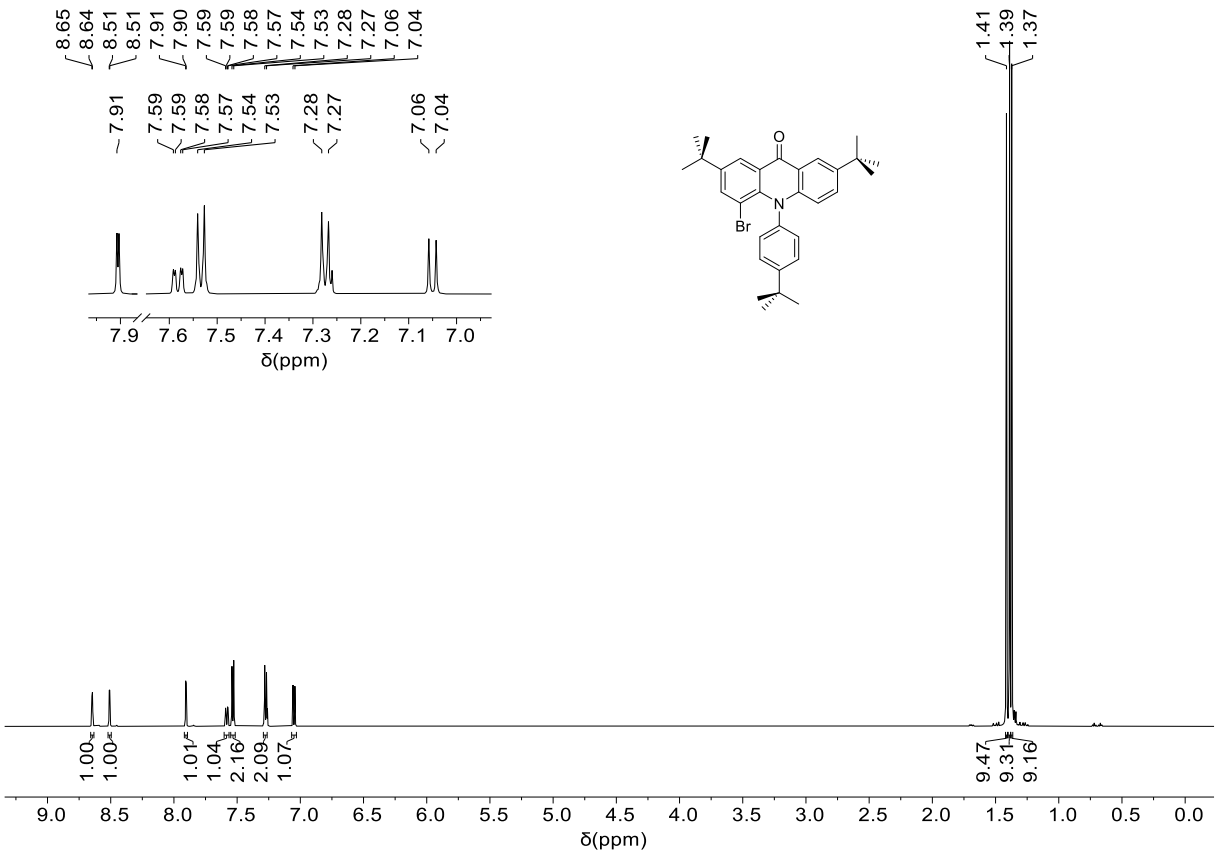


Figure S3. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of compound **6**.

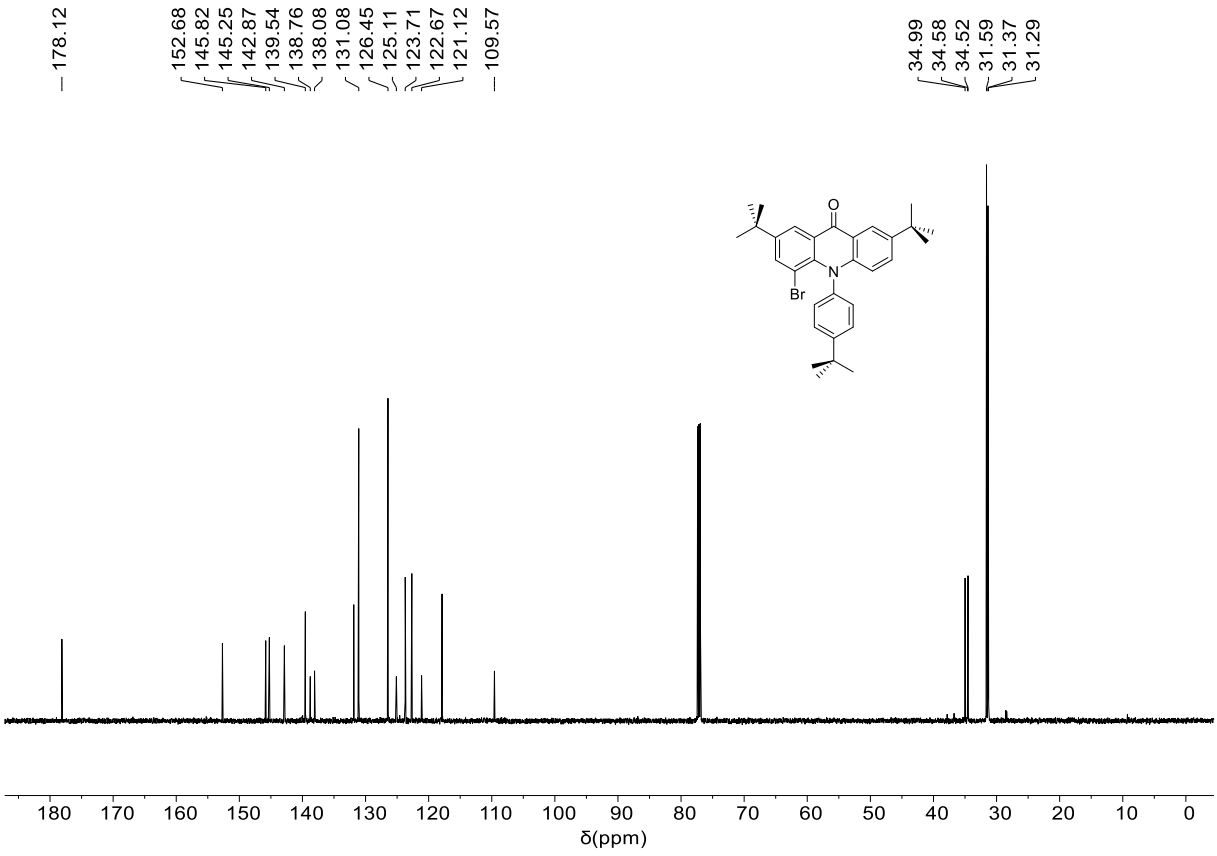


Figure S4. ^{13}C NMR spectrum (150 MHz, $CDCl_3$) of compound **6**.

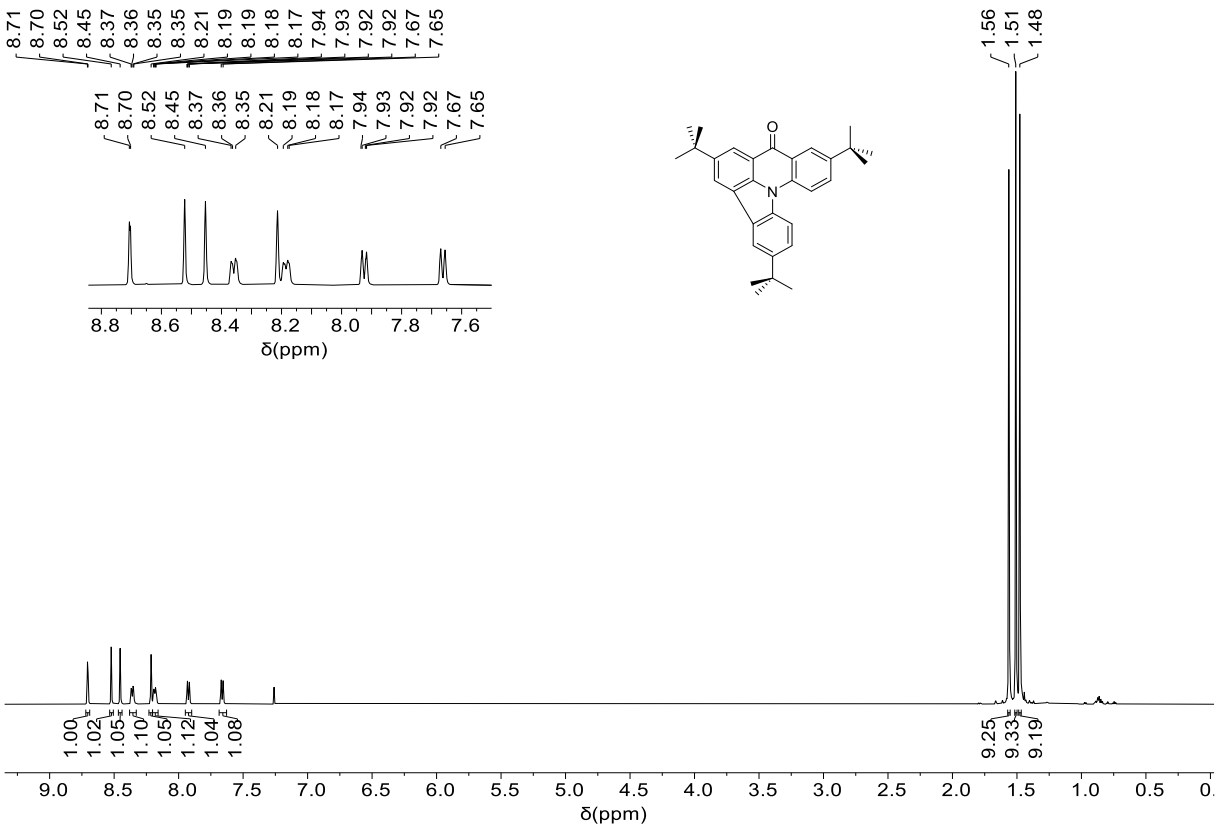


Figure S5. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of compound **7**.

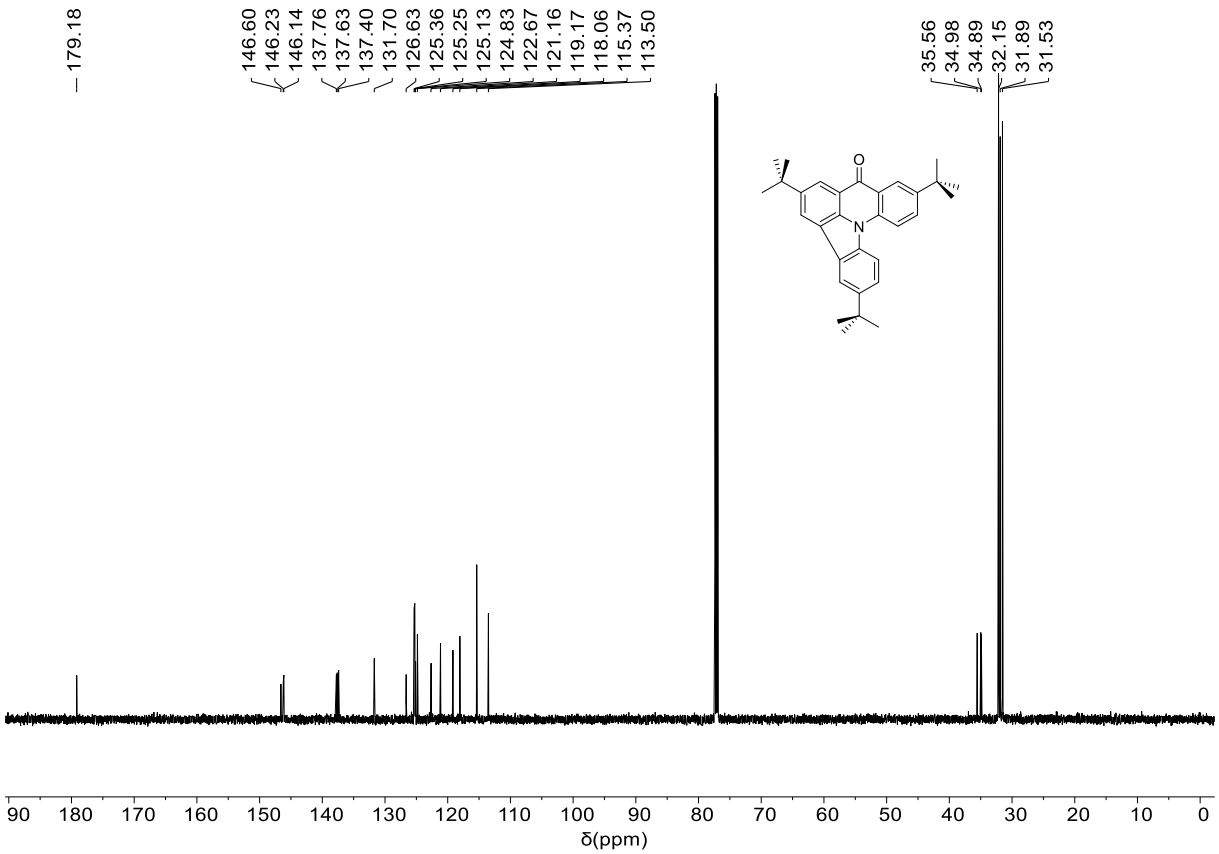


Figure S6. ^{13}C NMR spectrum (150 MHz, $CDCl_3$) of compound **7**.

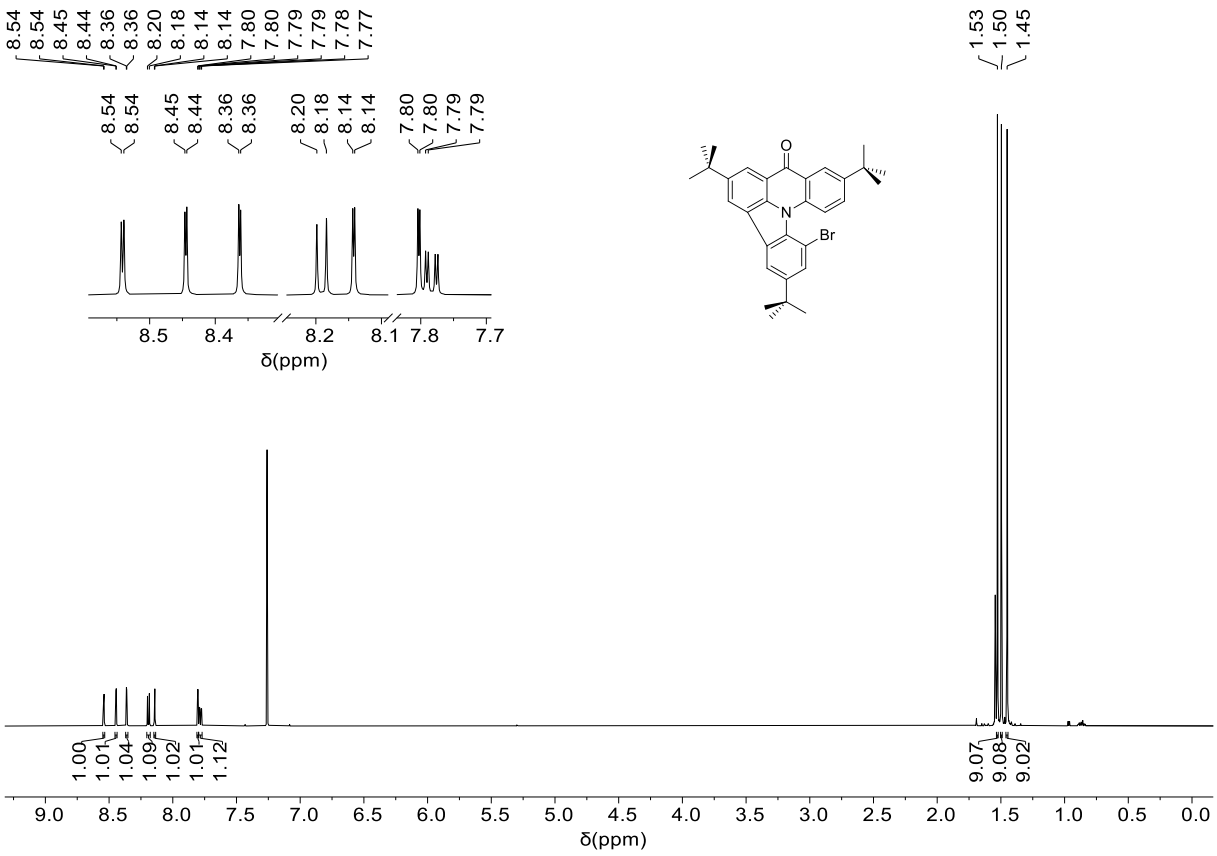


Figure S7. ^{1}H NMR spectrum (600 MHz, $CDCl_3$) of compound **8**.

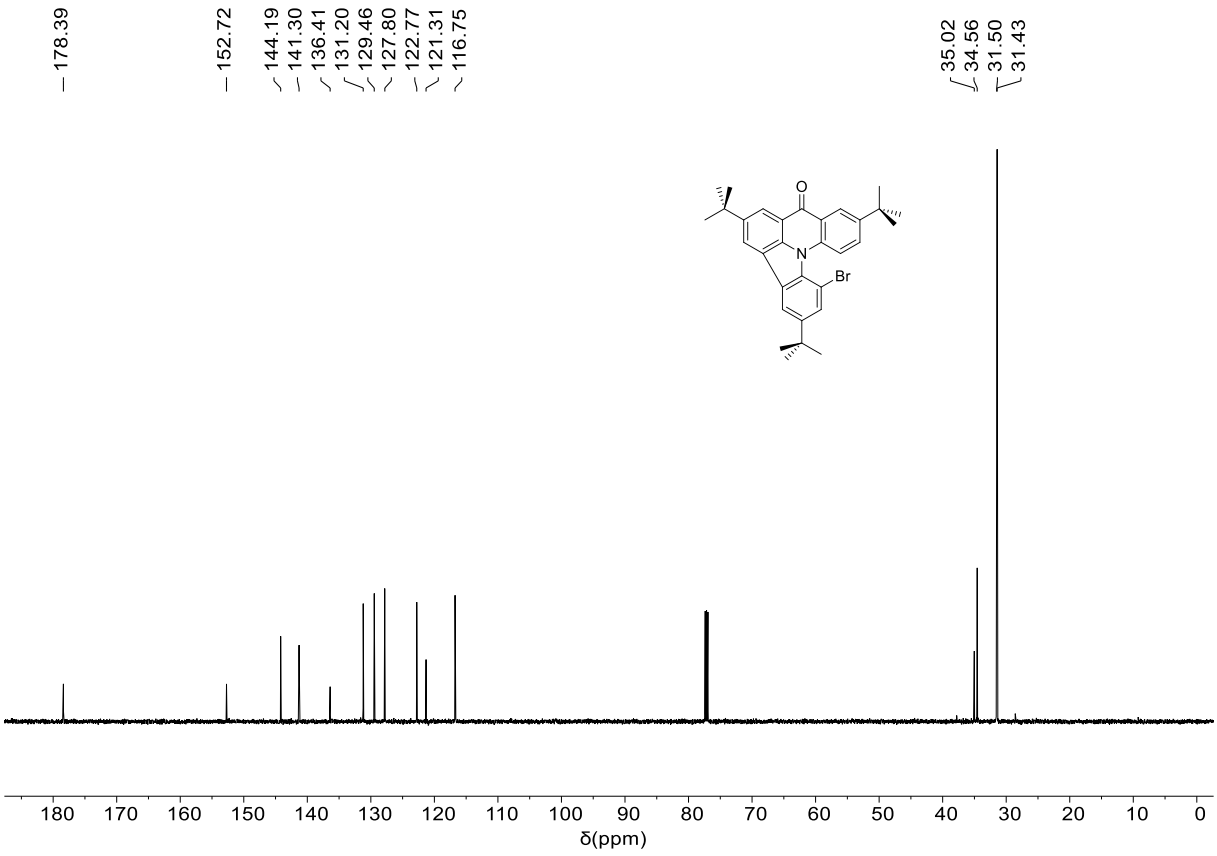


Figure S8. ^{13}C NMR spectrum (150 MHz, $CDCl_3$) of compound **8**.

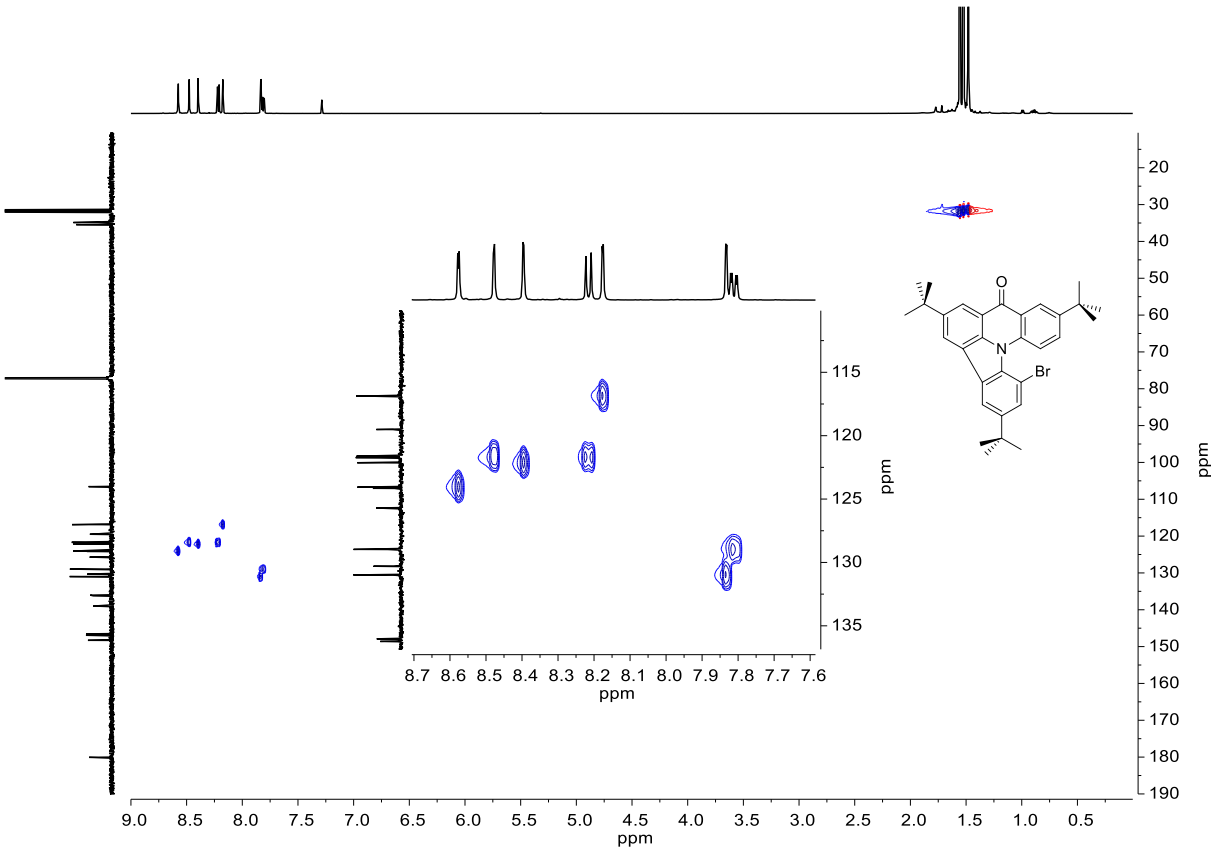


Figure S9. HSQC NMR spectrum of compound **8**.

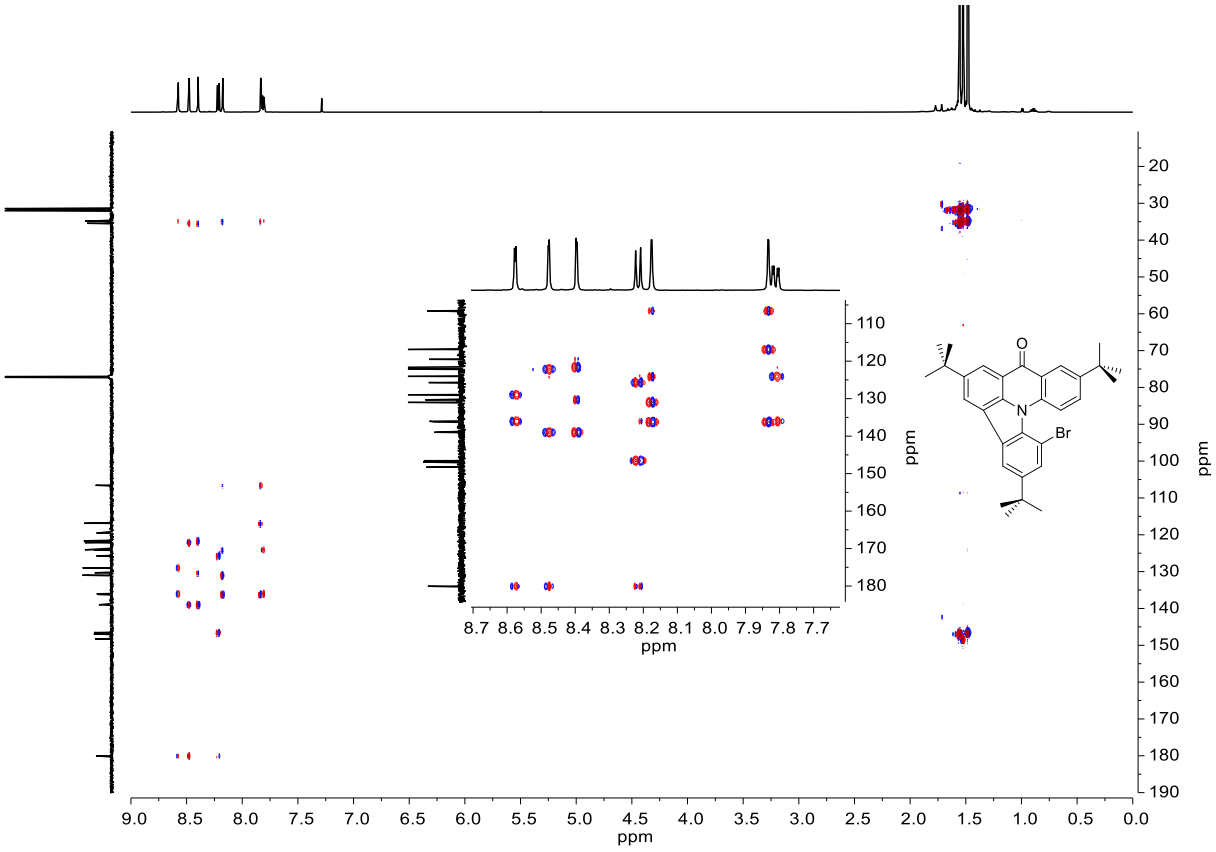


Figure S10. HMBC NMR spectrum of compound **8**.

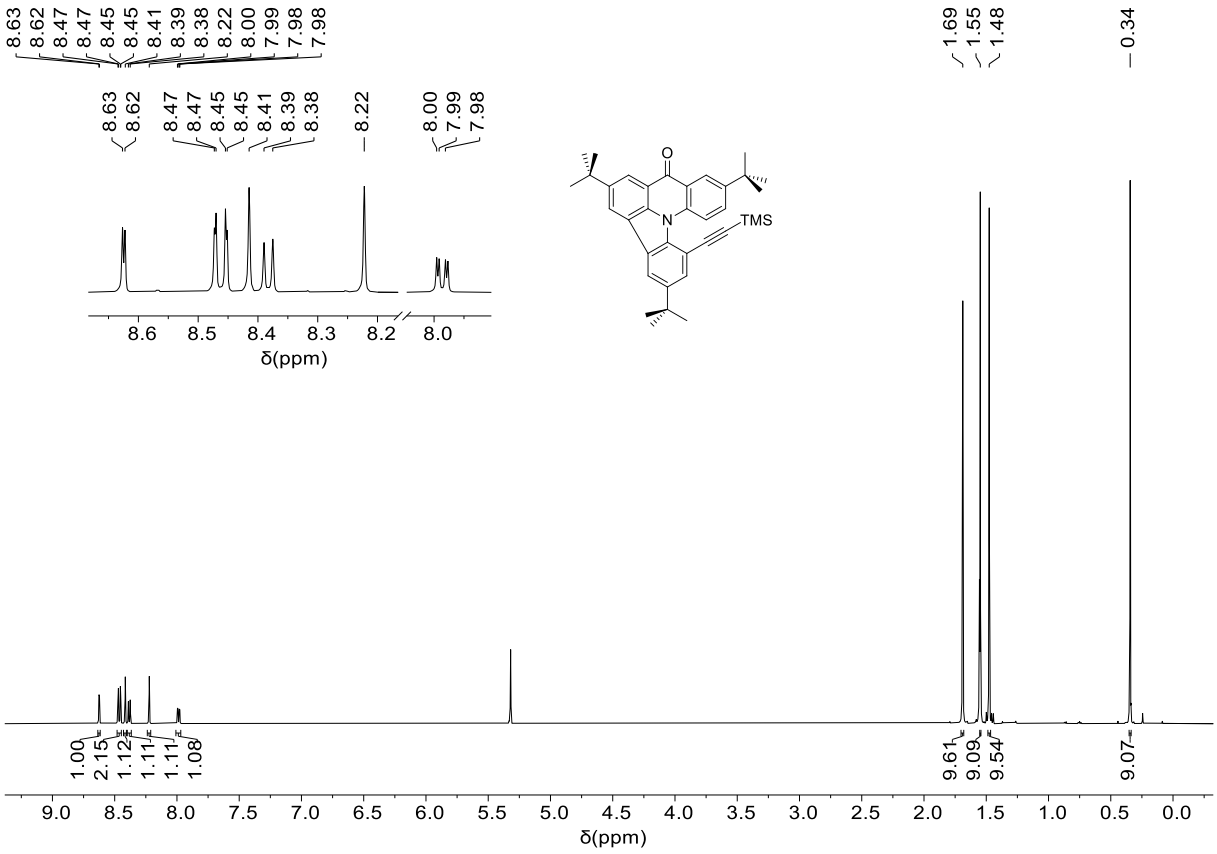


Figure S11. ^{1}H NMR spectrum (600 MHz, CD_2Cl_2) of compound **9**.

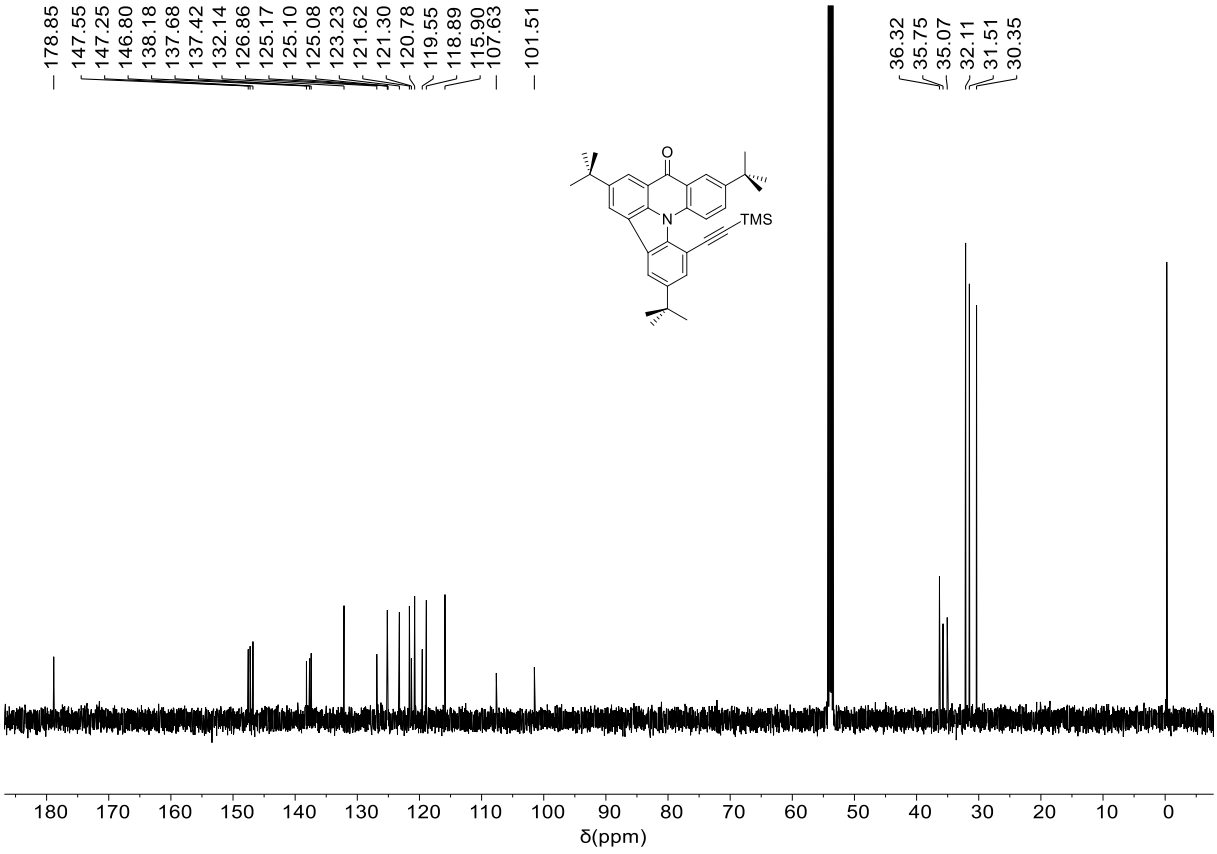


Figure S12. ^{13}C NMR spectrum (150 MHz, CD_2Cl_2) of compound **9**.

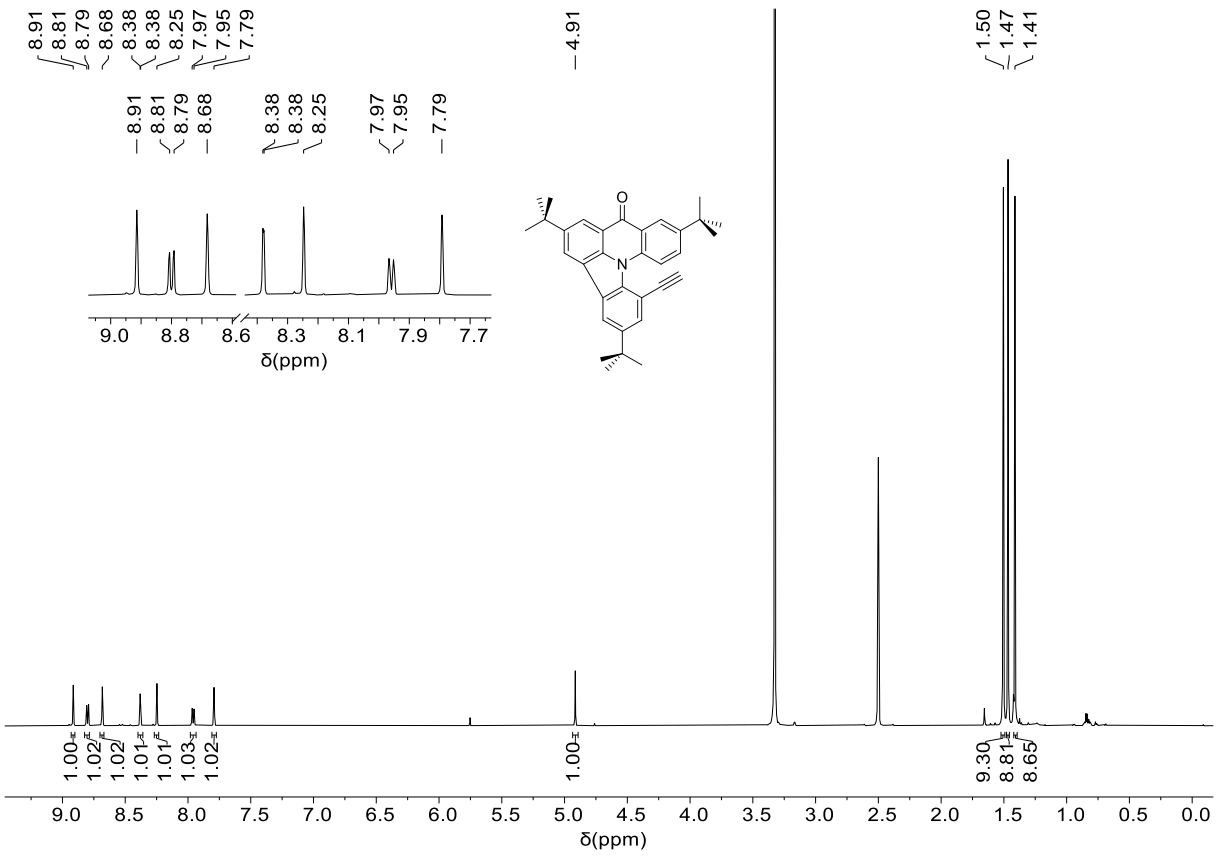


Figure S13. ^{1}H NMR spectrum (600 MHz, DMSO-d_6) of compound **10**.

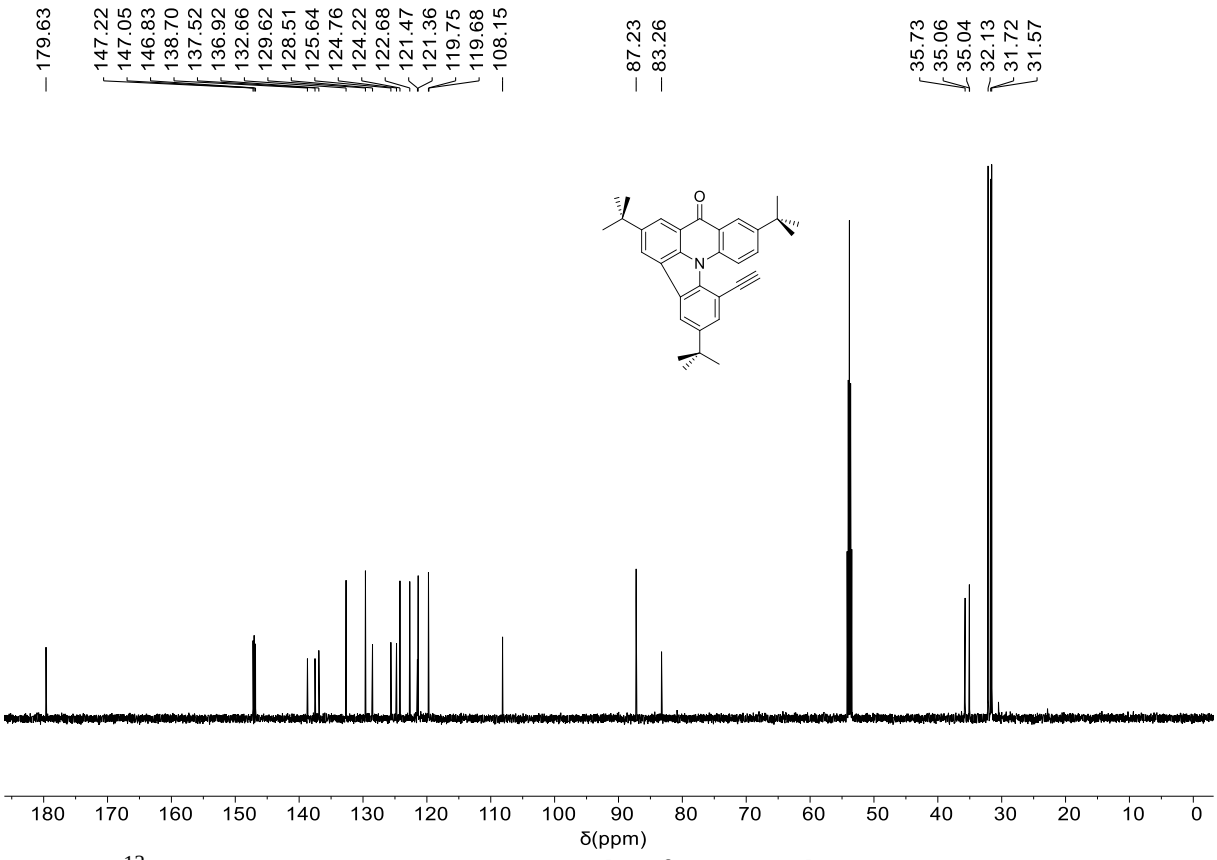


Figure S14. ^{13}C NMR spectrum (150 MHz, CD_2Cl_2) of compound **10**.

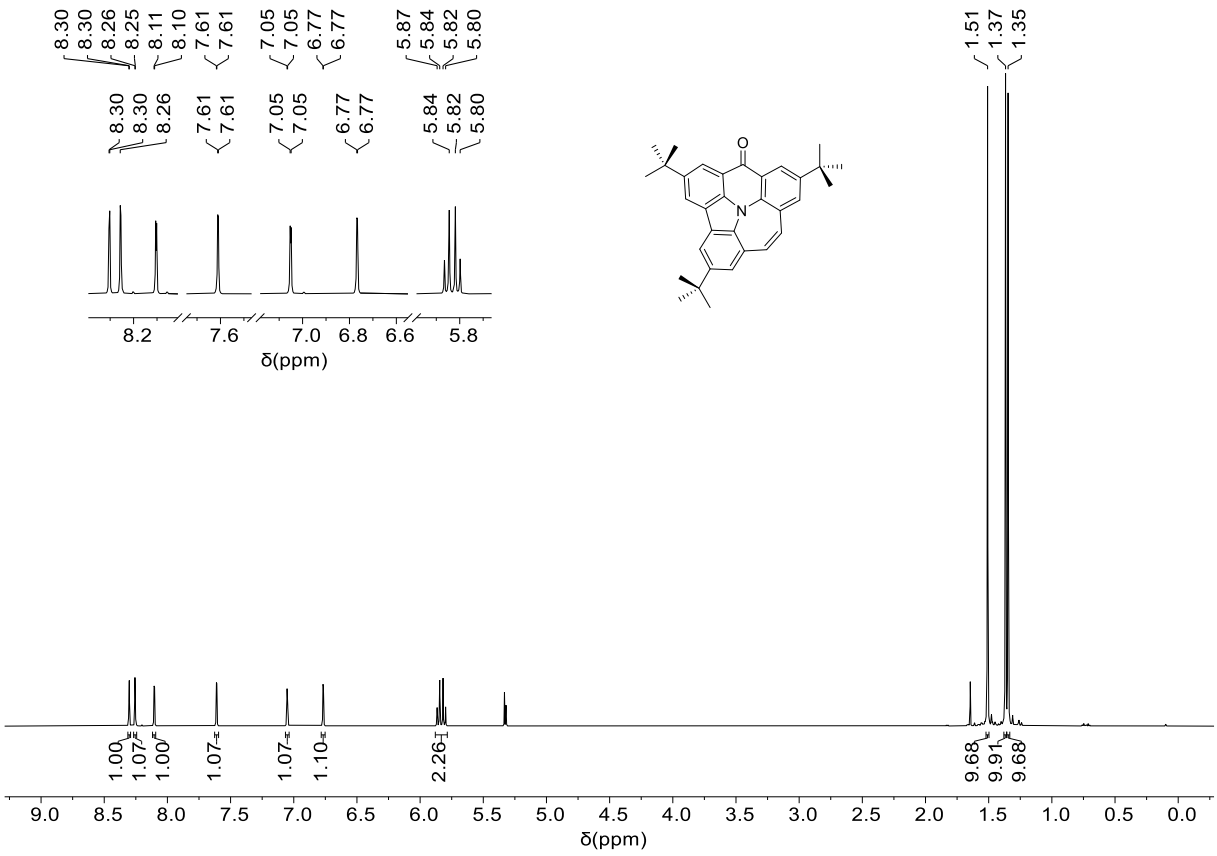


Figure S15. ^{1}H NMR spectrum (600 MHz, CD_2Cl_2) of compound **11**.

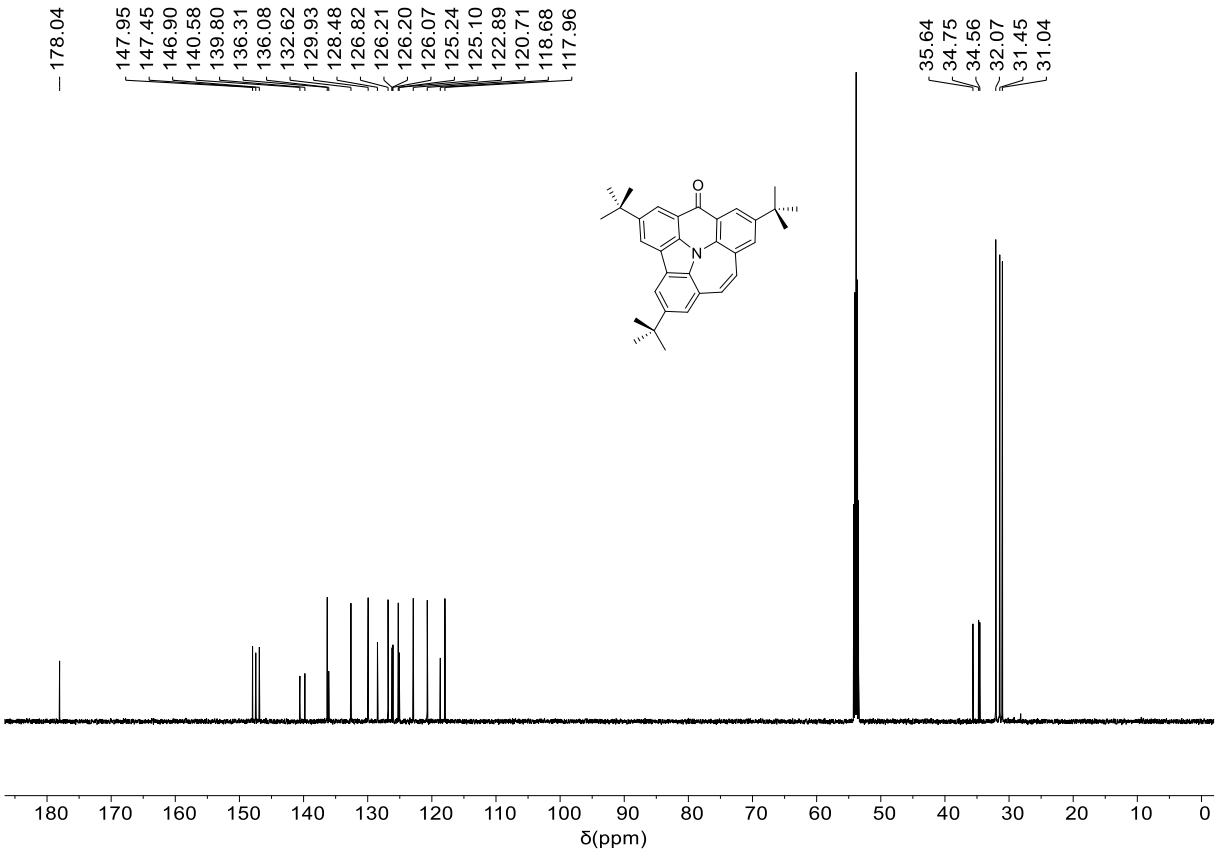


Figure S16. ^{13}C NMR spectrum (150 MHz, CD_2Cl_2) of compound **11**.

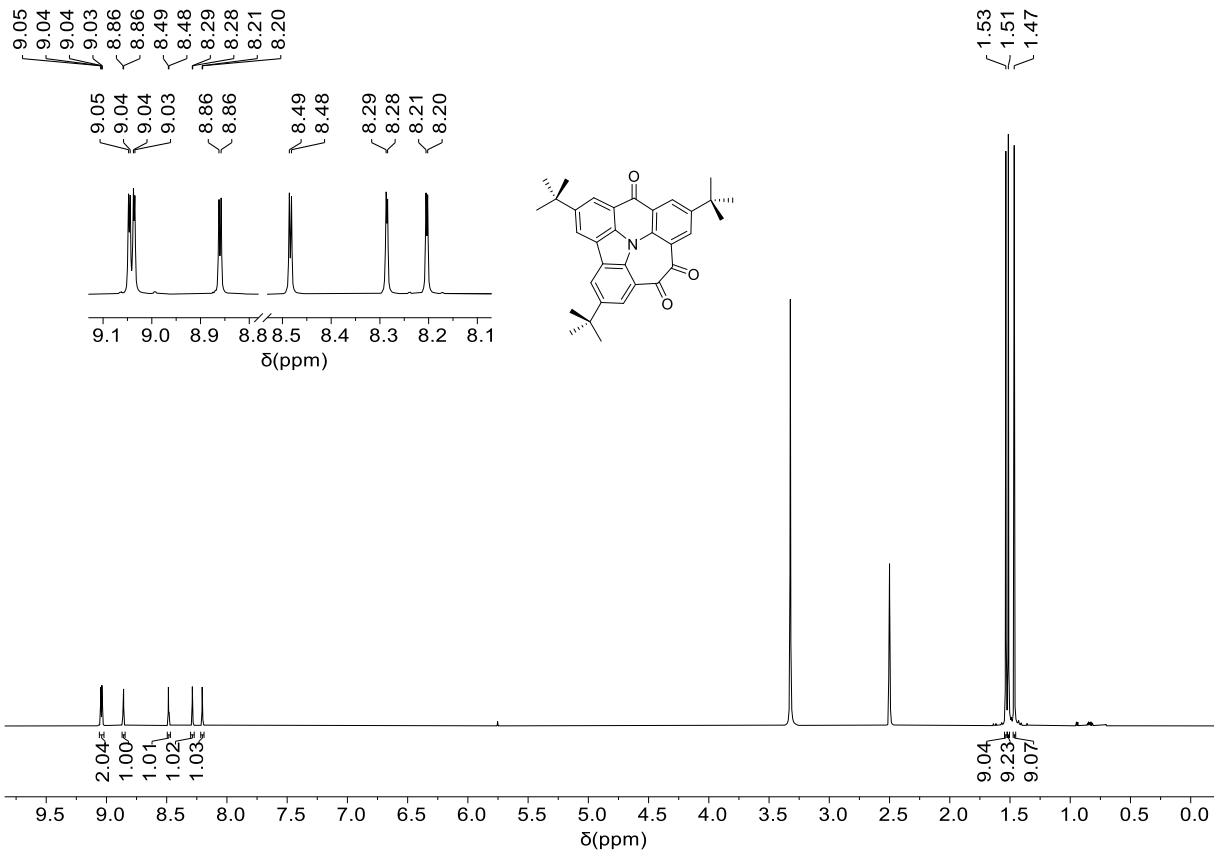


Figure S17. ^{1}H NMR spectrum (600 MHz, DMSO-d_6) of compound **12**.

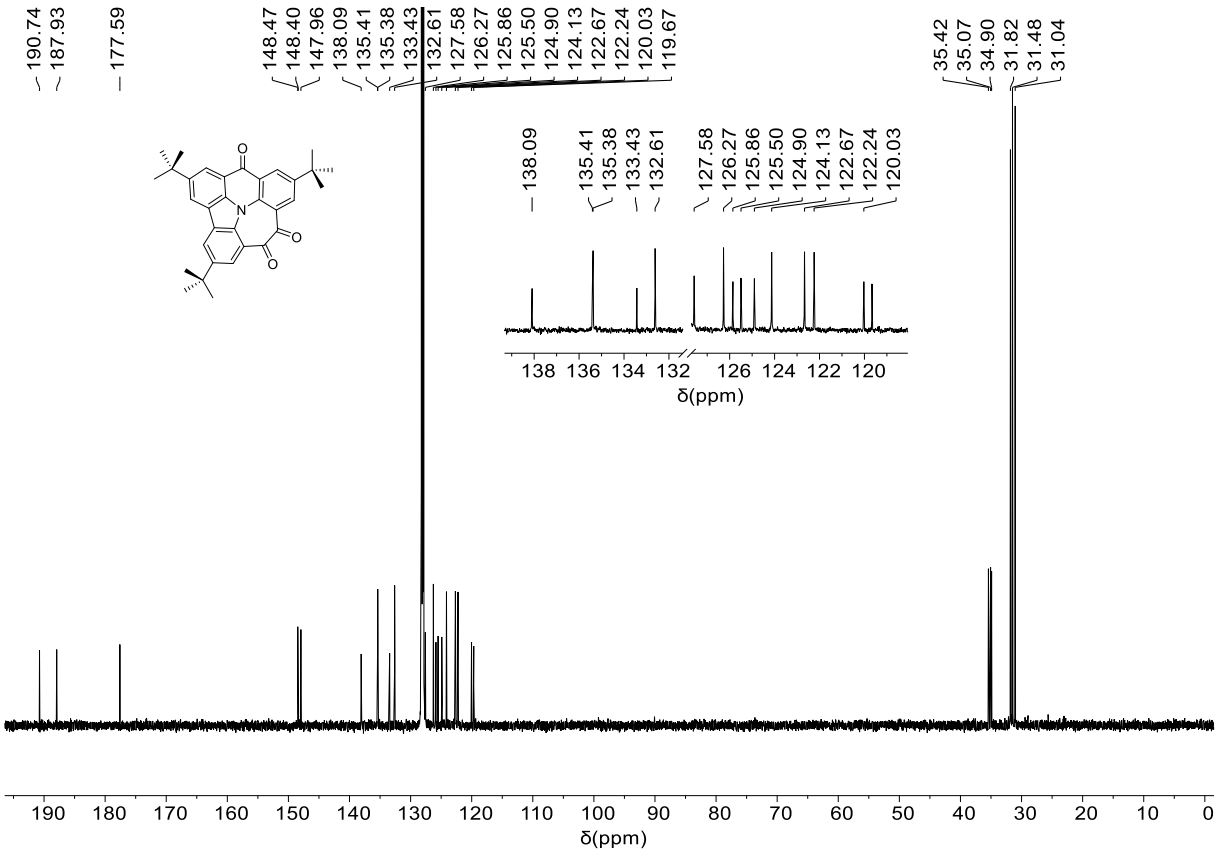


Figure S18. ^{13}C NMR spectrum (150 MHz, C_6D_6) of compound **12**.

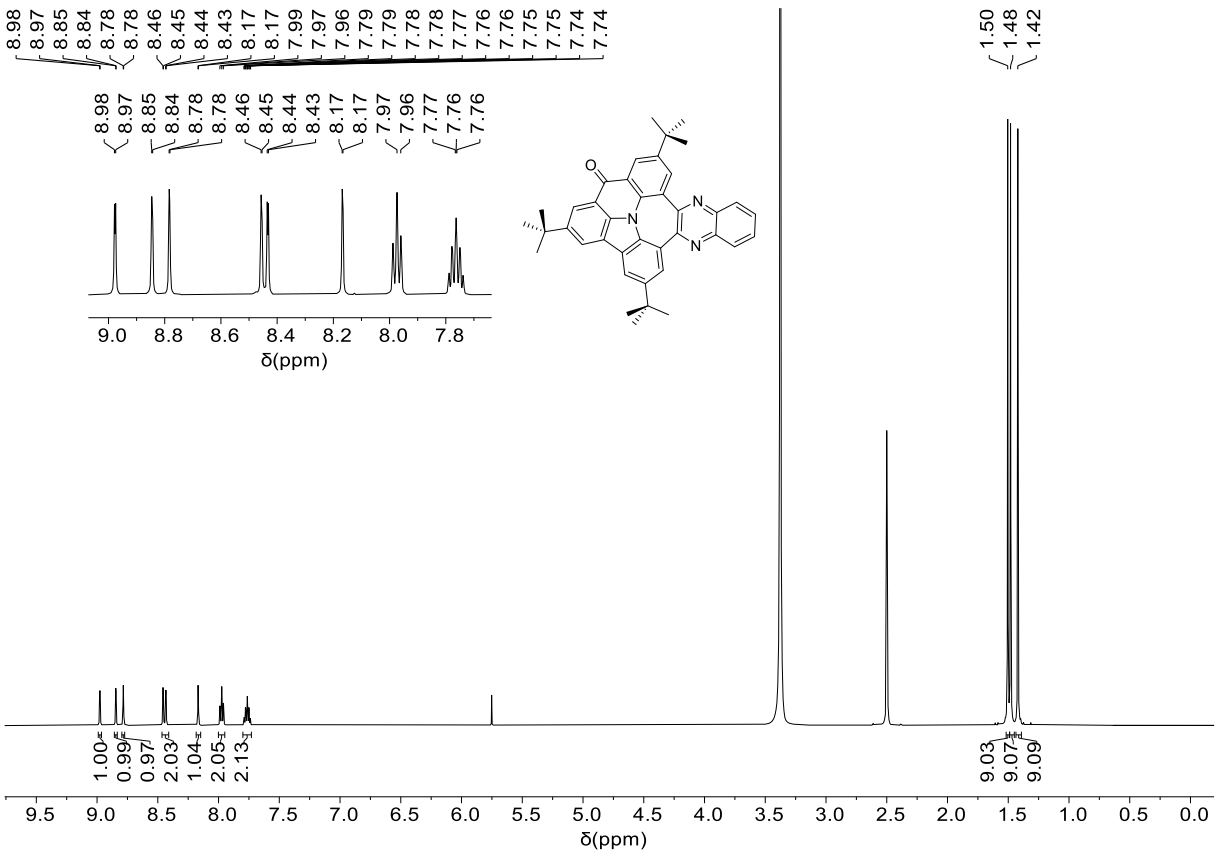


Figure S19. ^{1}H NMR spectrum (600 MHz, DMSO-d_6) of compound **13**.

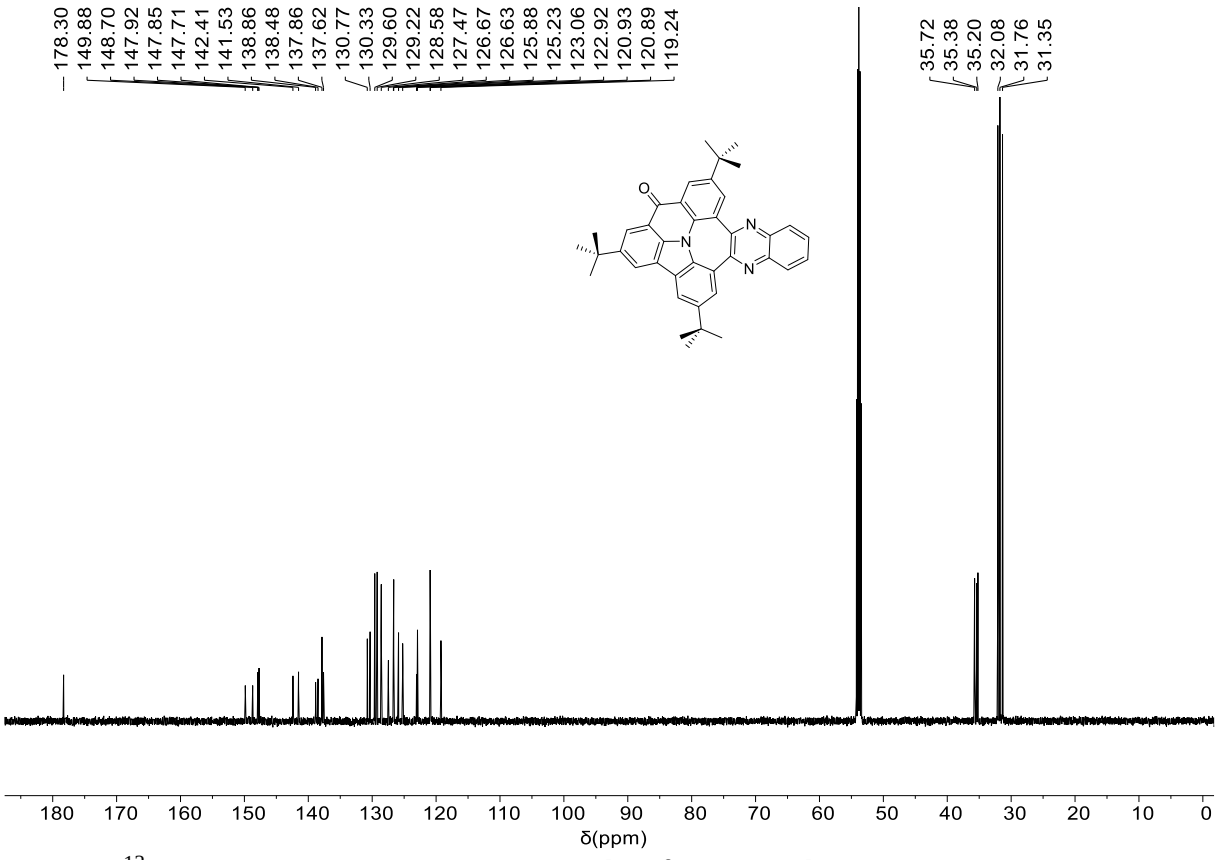


Figure S20. ^{13}C NMR spectrum (150 MHz, CD_2Cl_2) of compound **13**.

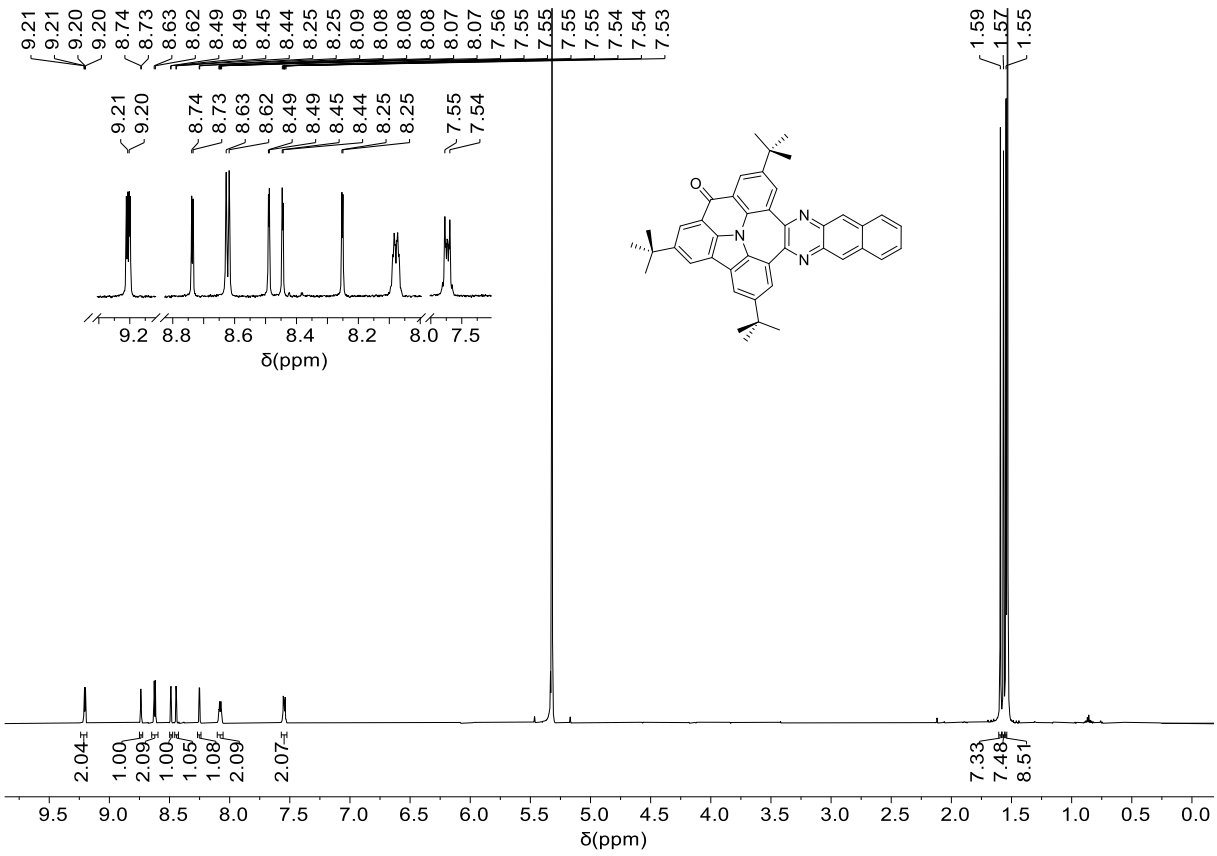


Figure S21. ^{1}H NMR spectrum (600 MHz, CD_2Cl_2) of compound **14**.

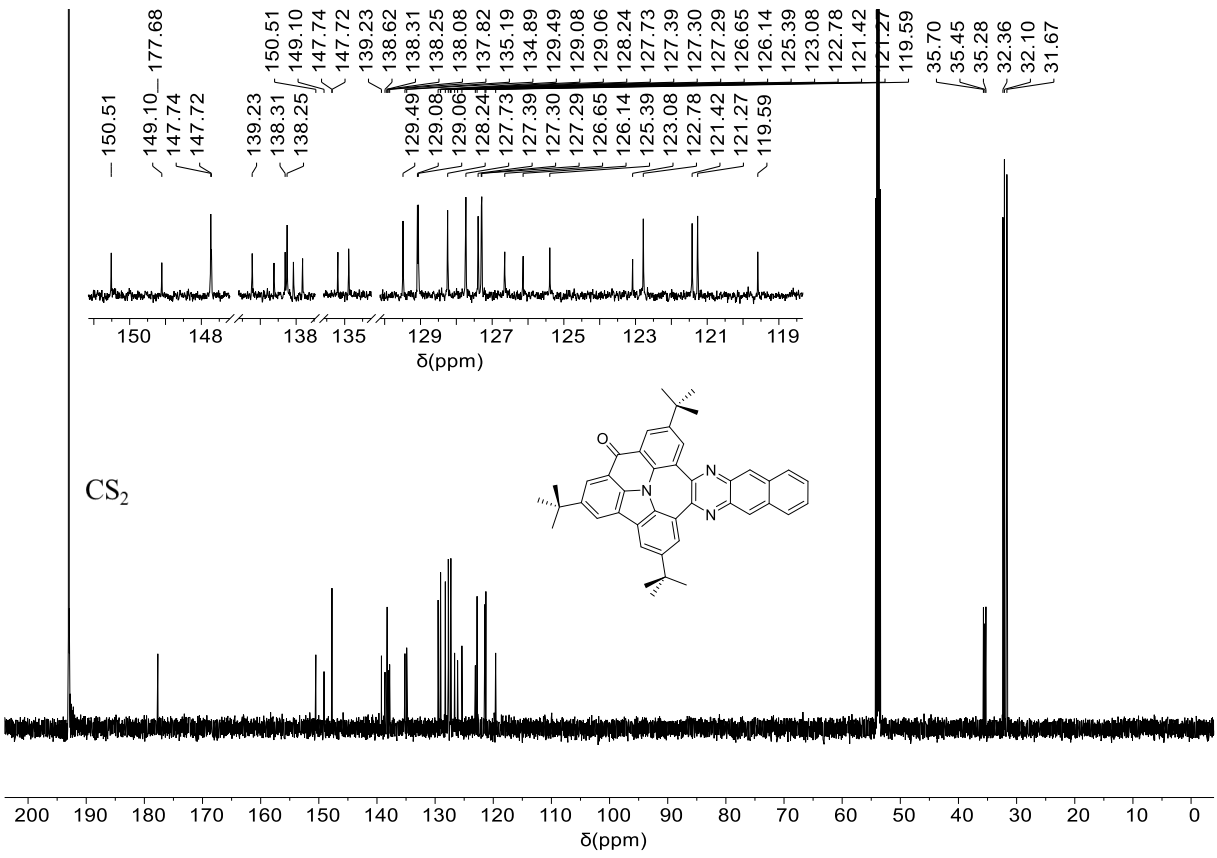


Figure S22. ^{13}C NMR spectrum (150 MHz, CD_2Cl_2+CS_2) of compound **14**.

4. X-ray crystallographic structure determination

Table S1. Crystal data and structure refinement for compound **12**.

Empirical formula	$C_{33}H_{33}NO_3$
Formula weight	491.60
Temperature/K	156(50)
Crystal system	triclinic
Space group	P-1
a/Å	8.5381(13)
b/Å	11.5788(12)
c/Å	13.9638(13)
α/°	104.306(9)
β/°	101.301(11)
γ/°	96.055(10)
Volume/Å^3	1294.4(3)
Z	2
ρ_{calc}g/cm^3	1.261
μ/mm^{-1}	0.629
F(000)	524.0
Crystal size/mm^3	0.15 × 0.1 × 0.08
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.714 to 133.196
Index ranges	$-9 \leq h \leq 10$, $-13 \leq k \leq 12$, $-16 \leq l \leq 15$
Reflections collected	11854
Independent reflections	4527 [R_{int} = 0.1236, R_{sigma} = 0.2148]
Data/restraints/parameters	4527/39/374
Goodness-of-fit on F^2	0.937
Final R indexes [I>=2σ (I)]	R_1 = 0.0863, wR_2 = 0.1918
Final R indexes [all data]	R_1 = 0.1681, wR_2 = 0.2444
Largest diff. peak/hole / e Å^{-3}	0.28/-0.28

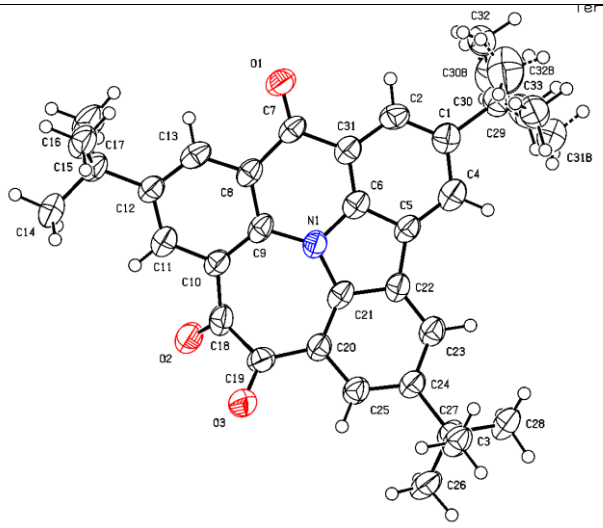


Figure S23. Crystal structure of **12** with an ellipsoid contour at the 50% probability level.

Table S2. Crystal data and structure refinement for compound **13**.

Empirical formula	$C_{39}H_{37}N_3O$
Formula weight	563.71
Temperature/K	101(2)
Crystal system	monoclinic
Space group	I2/a
a/Å	16.4721(5)
b/Å	27.0374(10)
c/Å	43.8324(19)
α/°	90
β/°	90.02(2)
γ/°	90
Volume/Å^3	19521.3(13)
Z	16
ρ_{calc}g/cm^3	0.767
μ/mm^{-1}	0.357
F(000)	4800.0
Crystal size/mm^3	0.15 × 0.13 × 0.1
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.876 to 133.18
Index ranges	$-18 \leq h \leq 19$, $-31 \leq k \leq 32$, $-52 \leq l \leq 45$
Reflections collected	60687
Independent reflections	17067 [R_{int} = 0.0656, R_{sigma} = 0.0607]
Data/restraints/parameters	17067/46/818
Goodness-of-fit on F^2	1.525
Final R indexes [I>=2σ (I)]	R_1 = 0.1336, wR_2 = 0.3892
Final R indexes [all data]	R_1 = 0.1659, wR_2 = 0.4164
Largest diff. peak/hole / e Å^{-3}	0.55/-0.61

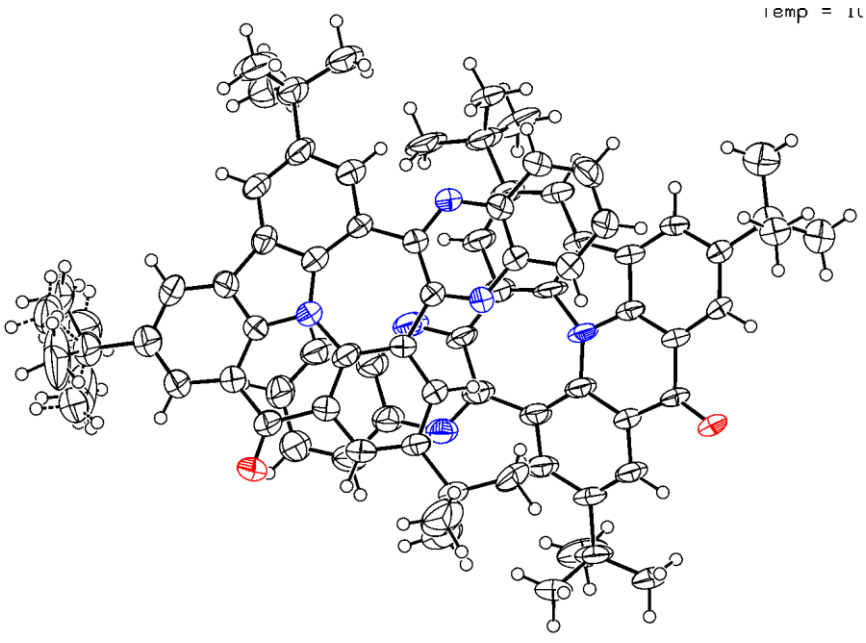


Figure S24. Crystal structure of **13** with an ellipsoid contour at the 50% probability level.

5. Delayed photoluminescence curves

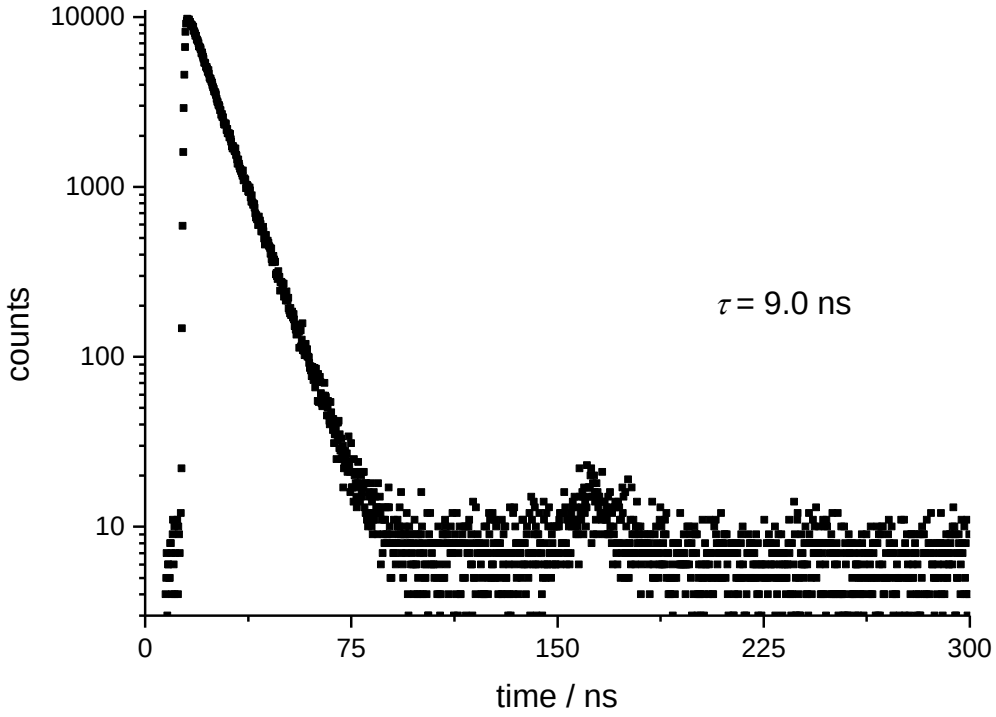


Figure S25. Fluorescence decay curve of **5** in dichloromethane at room temperature.

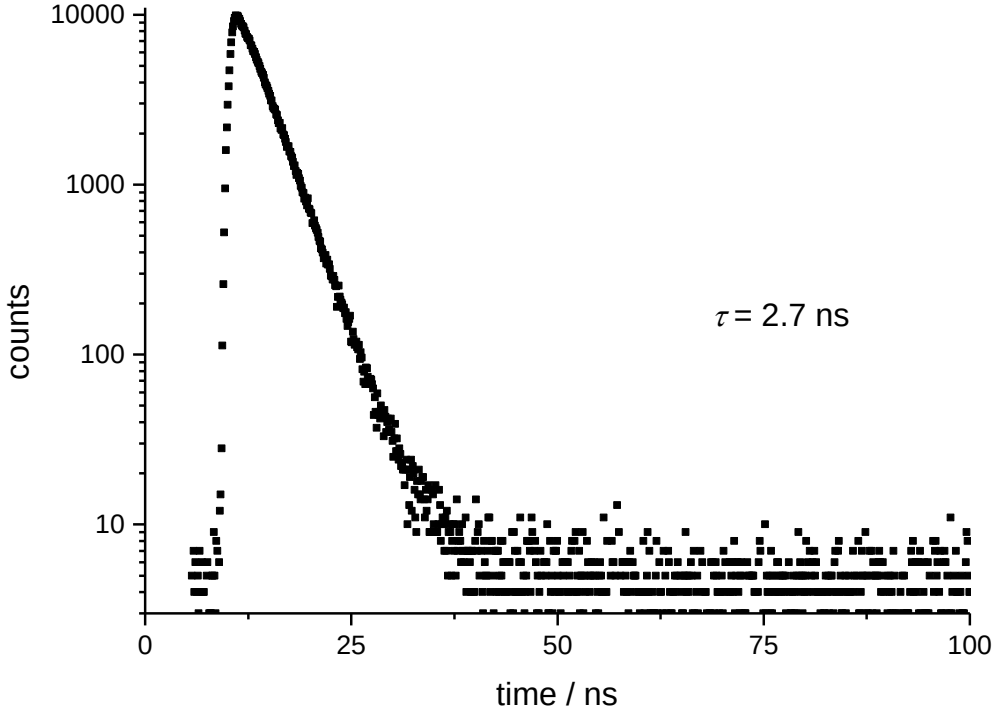


Figure S26. Fluorescence decay curve of **7** in dichloromethane at room temperature.

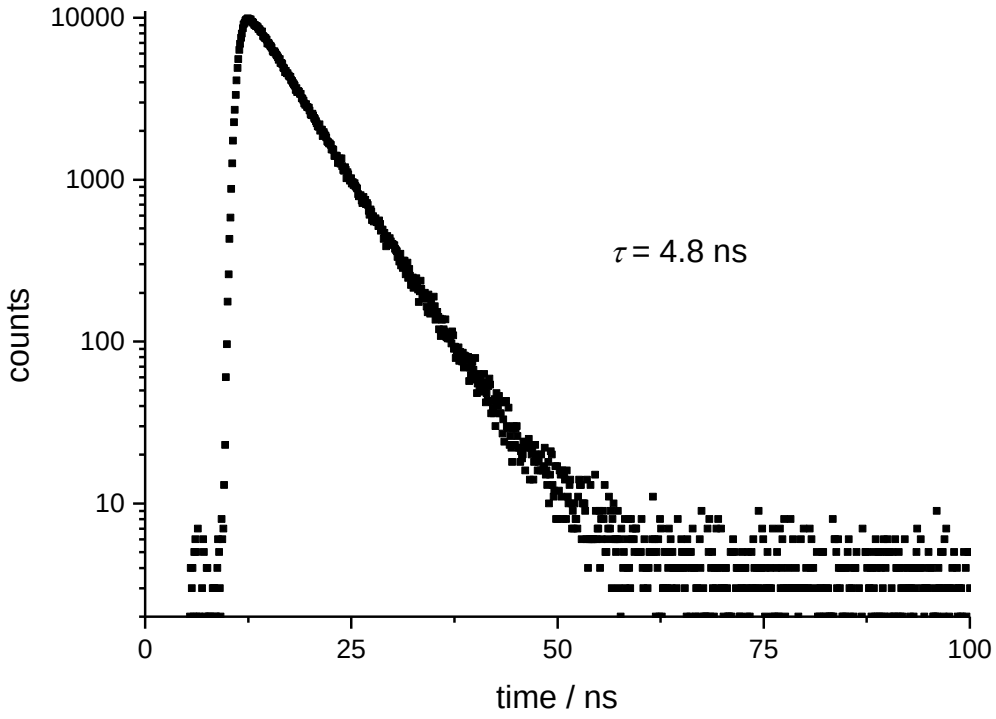


Figure S27. Fluorescence decay curve of **11** in dichloromethane at room temperature.

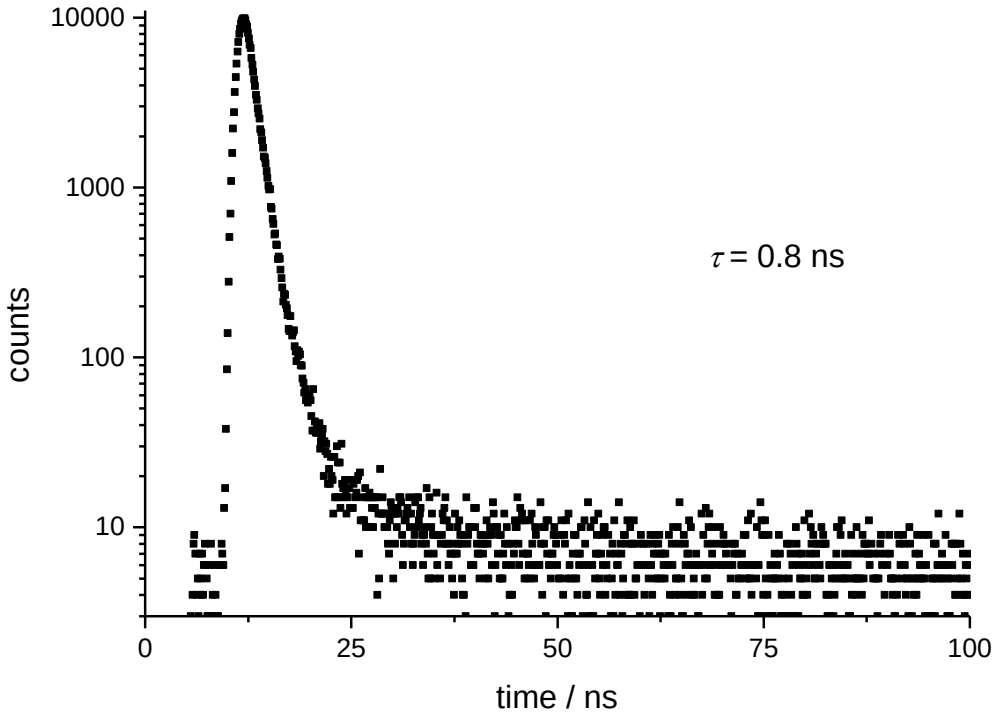


Figure S28. Fluorescence decay curve of **12** in dichloromethane at room temperature.

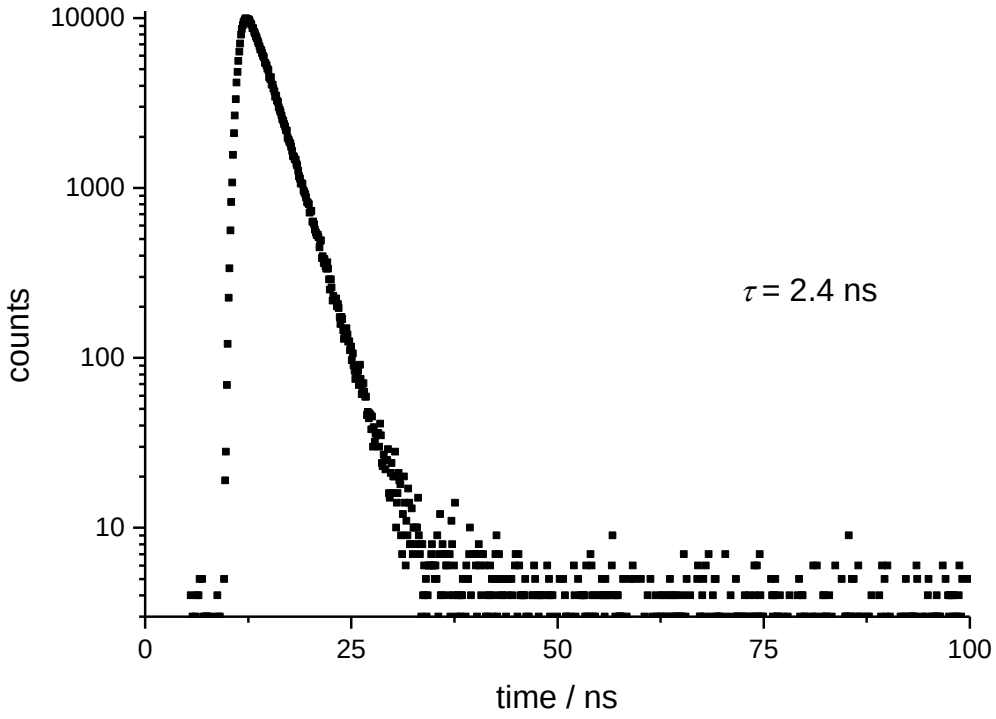


Figure S29. Fluorescence decay curve of **13** in dichloromethane at room temperature.

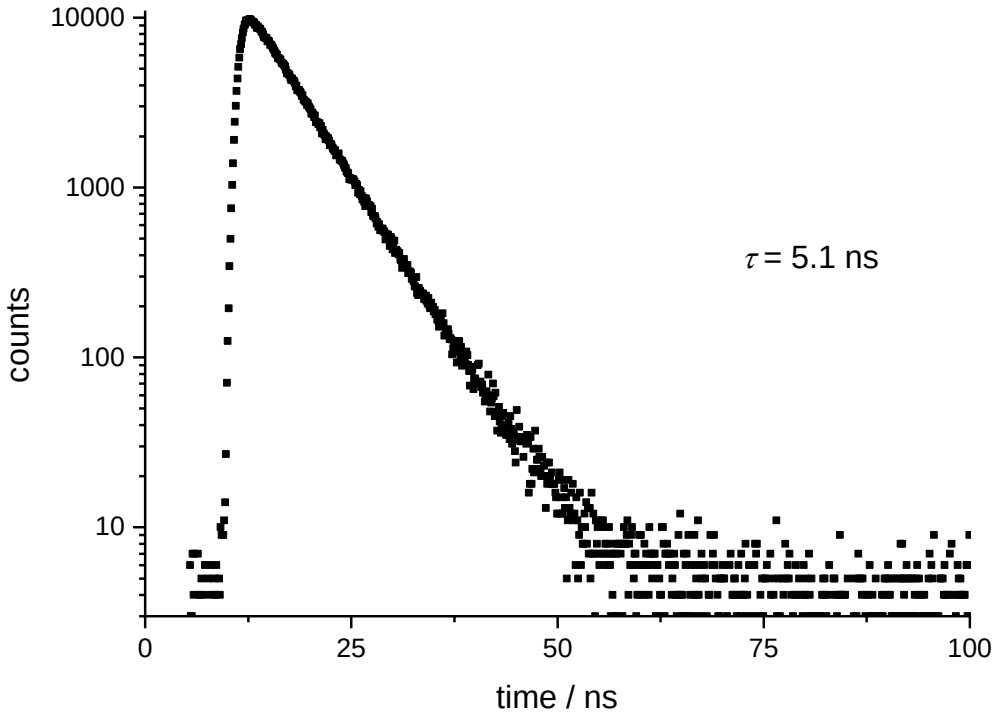


Figure S30. Fluorescence decay curve of **14** in dichloromethane at room temperature.

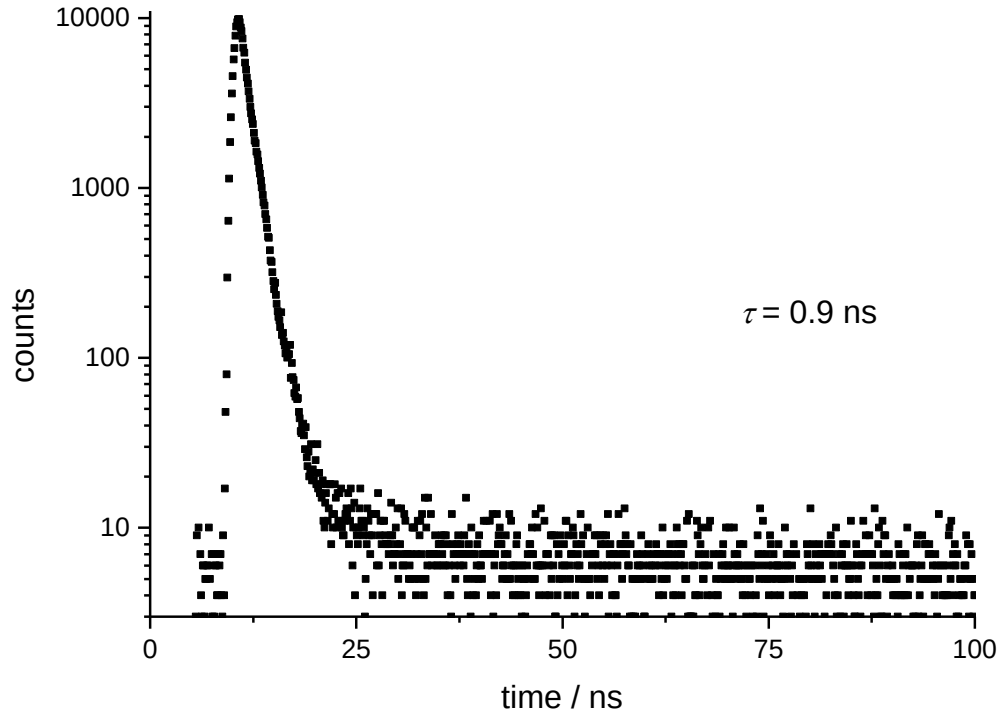


Figure S31. Fluorescence decay curve of *tert*-butylated **1** in dichloromethane at room temperature.

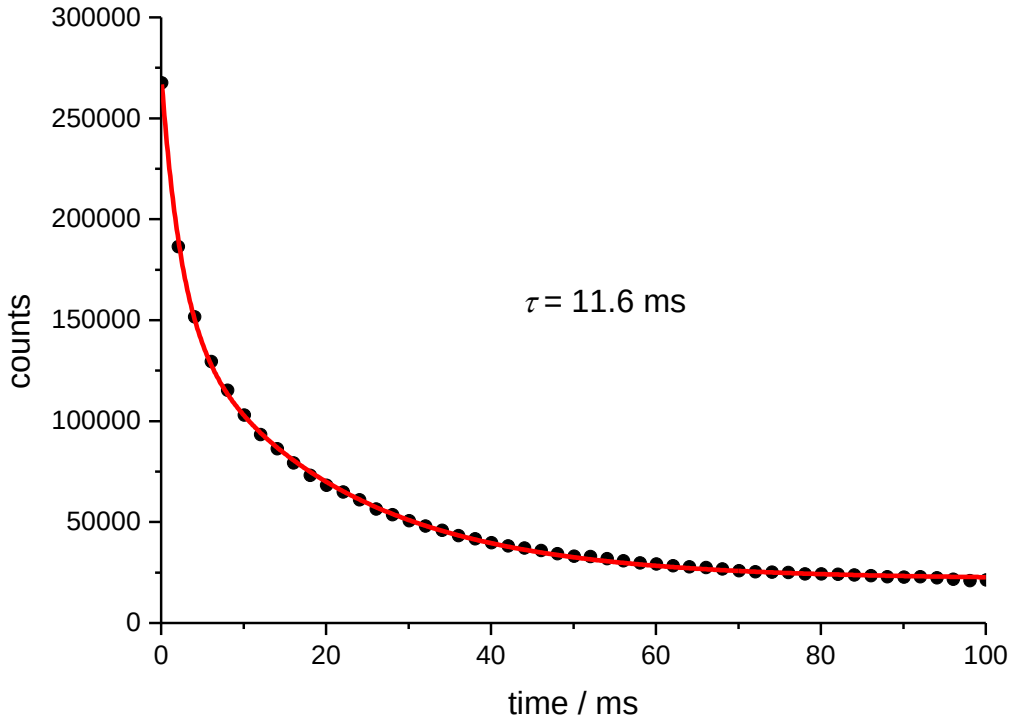


Figure S32. Phosphorescence decay curve of **12** in crystalline state at room temperature, 0.1 ms delayed.

6. Electrochemical property

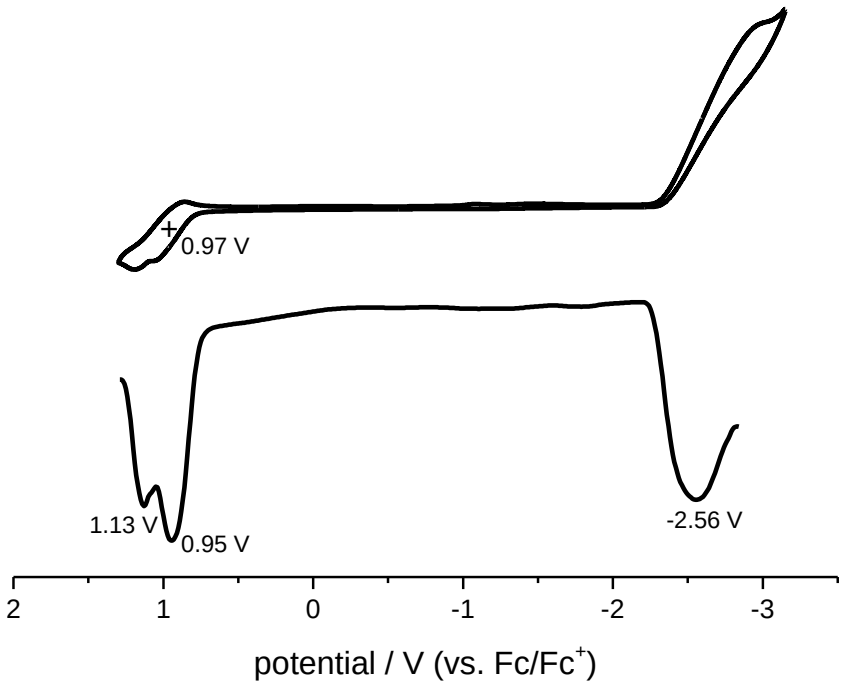


Figure S33. CV and DPV curves of **5** measured in dichloromethane using nBu$_4$NPF$_6$ (0.1 M) as the supporting electrolyte and ferrocene as internal standard.

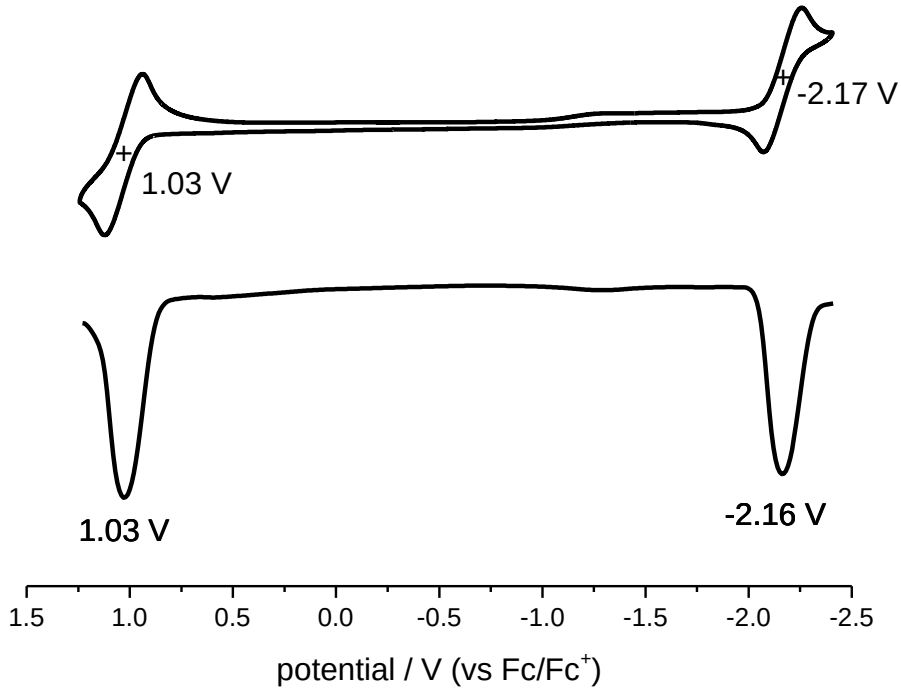


Figure S34. CV and DPV curves of **7** measured in dichloromethane using nBu$_4$NPF$_6$ (0.1 M) as the supporting electrolyte and ferrocene as internal standard.

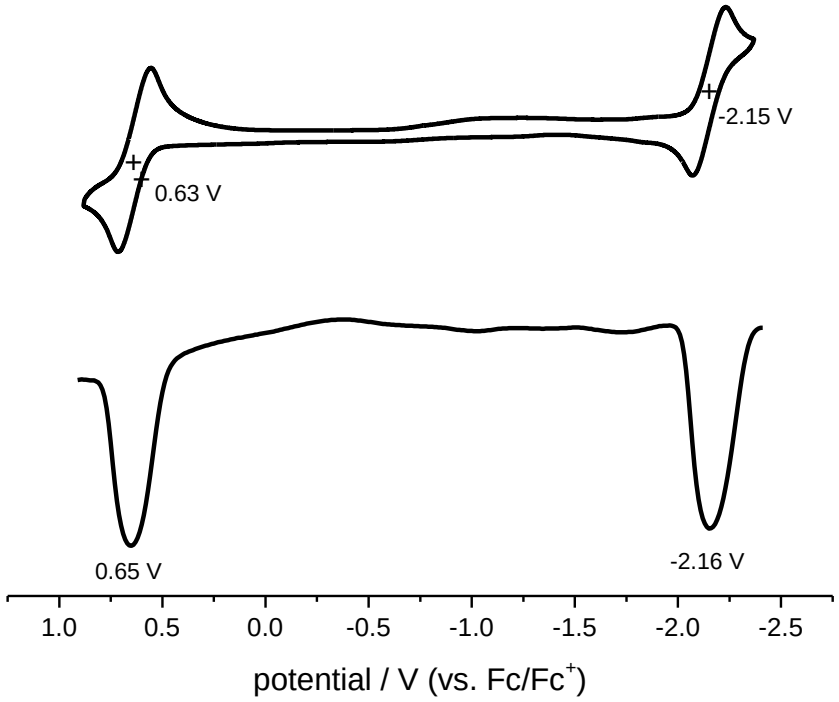


Figure S35. CV and DPV curves of **11** measured in dichloromethane using *n*Bu_4NPF_6 (0.1 M) as the supporting electrolyte and ferrocene as internal standard.

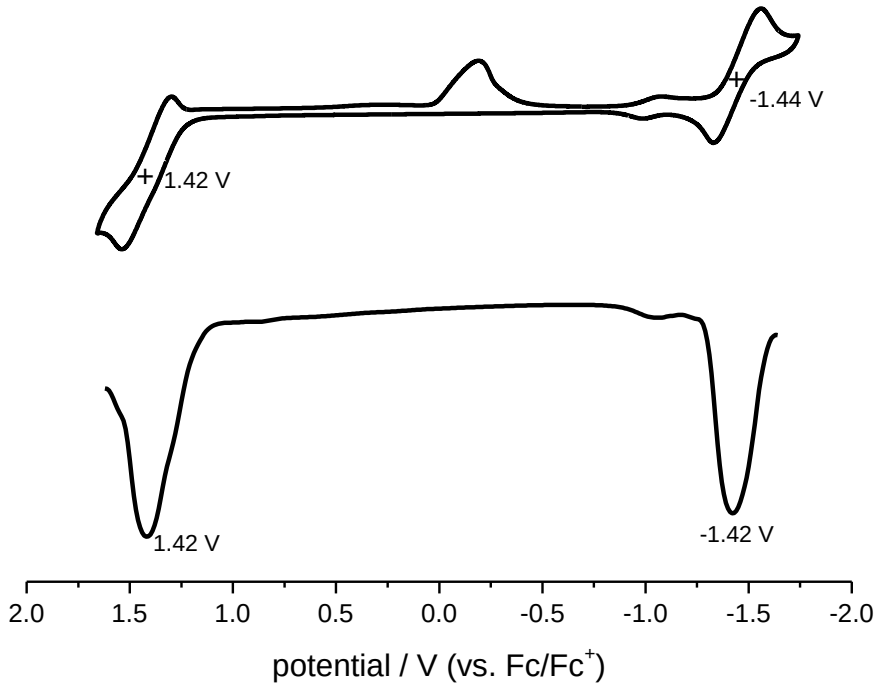


Figure S36. CV and DPV curves of **12** measured in dichloromethane using *n*Bu_4NPF_6 (0.1 M) as the supporting electrolyte and ferrocene as internal standard.

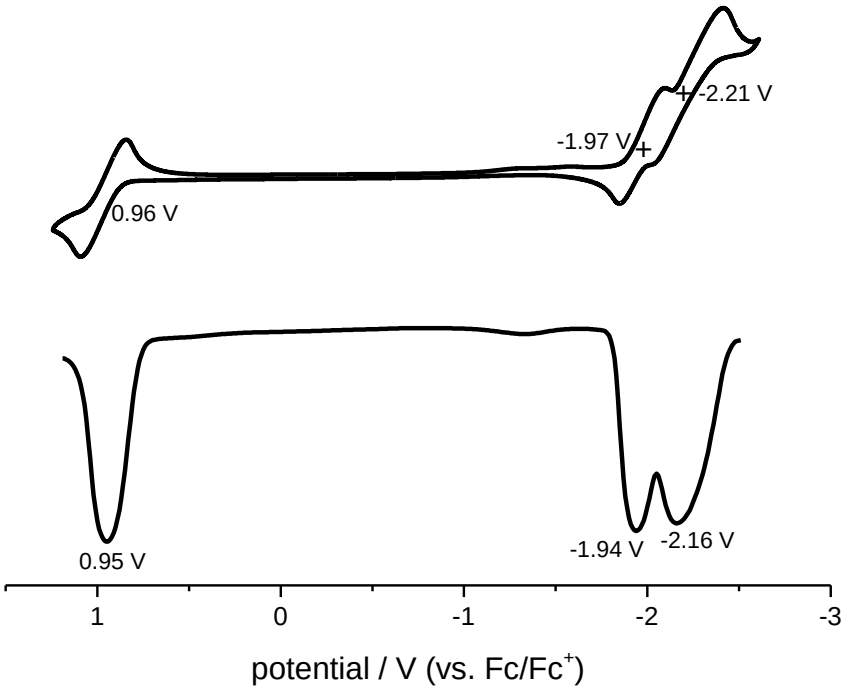


Figure S37. CV and DPV curves of **13** measured in dichloromethane using *n*Bu_4NPF_6 (0.1 M) as the supporting electrolyte and ferrocene as internal standard.

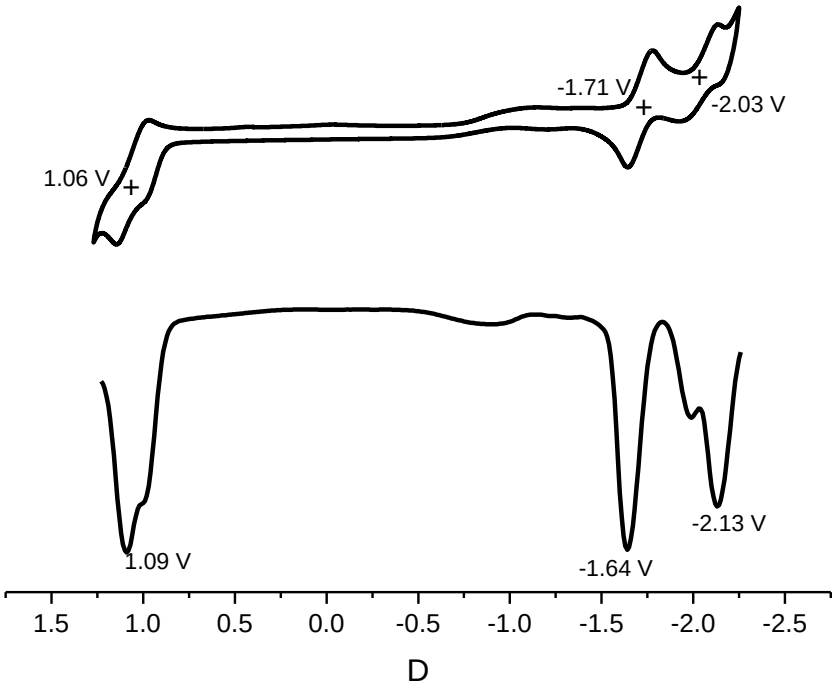


Figure S38. CV and DPV curves of **14** measured in dichloromethane using *n*Bu_4NPF_6 (0.1 M) as the supporting electrolyte and ferrocene as internal standard.

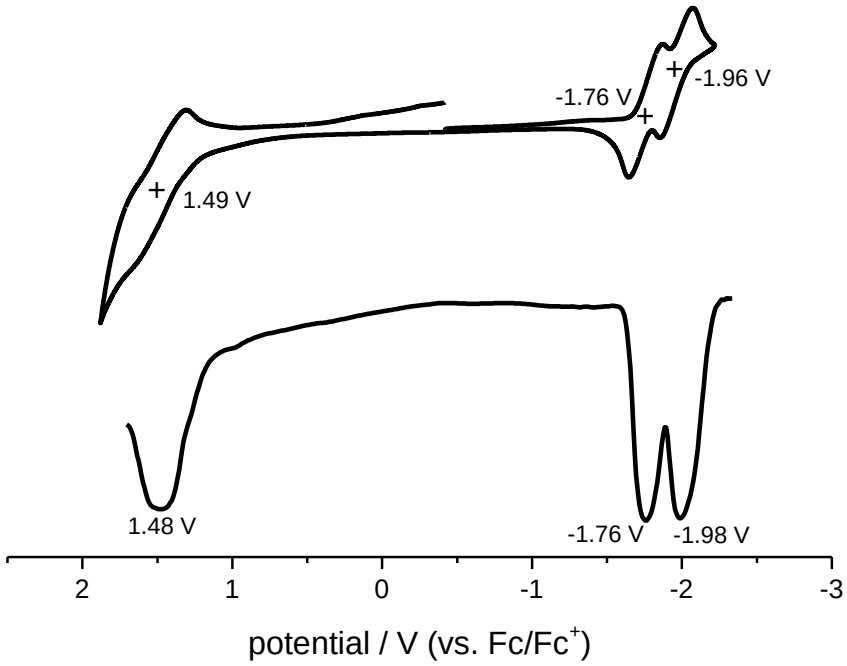


Figure S39. CV and DPV curves of *tert*-butylated **1** measured in dichloromethane using *n*Bu$_4$NPF$_6$ (0.1 M) as the supporting electrolyte and ferrocene as internal standard.

7. EPR spectra

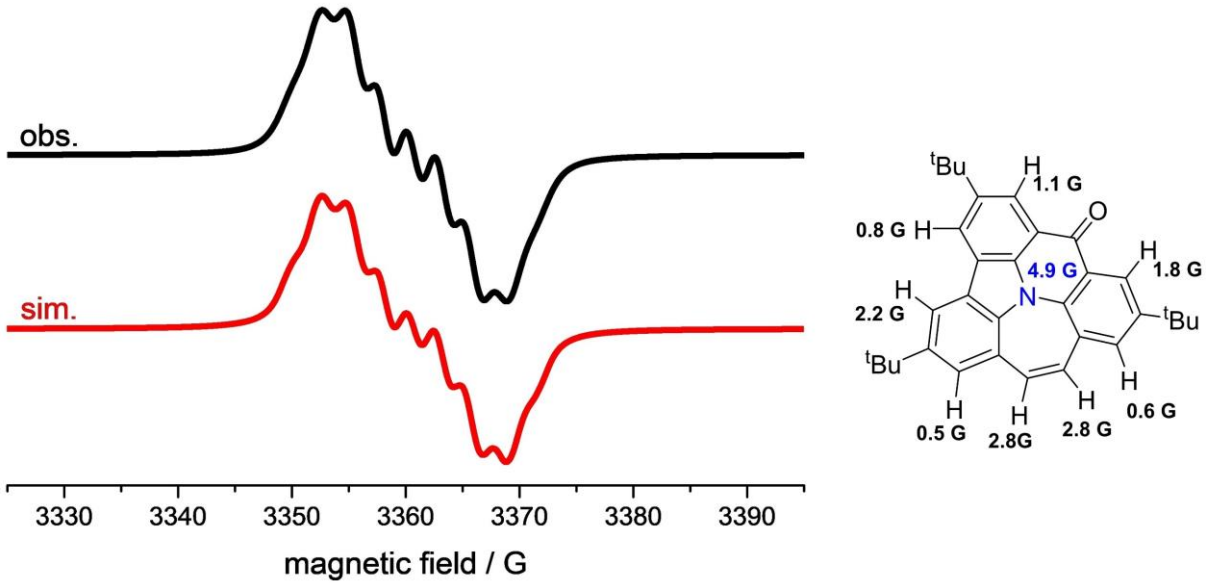


Figure S40. Experimental and simulated EPR spectra, and simulated hyperfine coupling constants of **11**$^{\bullet+}$.

8. The theoretical calculations

All the theoretical calculations were carried out using a *Gaussian 16* software.[S2] All the calculations were based on the optimized geometries at B3LYP/6-31G(d,p) level of theory. The frontier molecular orbitals are calculated at the B3LYP/6-311+G(d,p) level of theory. The calculation of excited state properties was performed using time-depended DFT methods at B3LYP/6-311G+(d,p) level of theory in the solvent dichloromethane. The nucleus-independent chemical shift (NICS) calculation was done at GIAO-B3LYP/6-311G(d) level of theory. Bq atoms were inserted at the calculated positions and the Bq positions that are at the 1 Å away above the molecule were fixed with the assistant of Multiwfn software, as well as the generation of isotropic chemical shielding surfaces (ICSS), and related quantities. [S3]

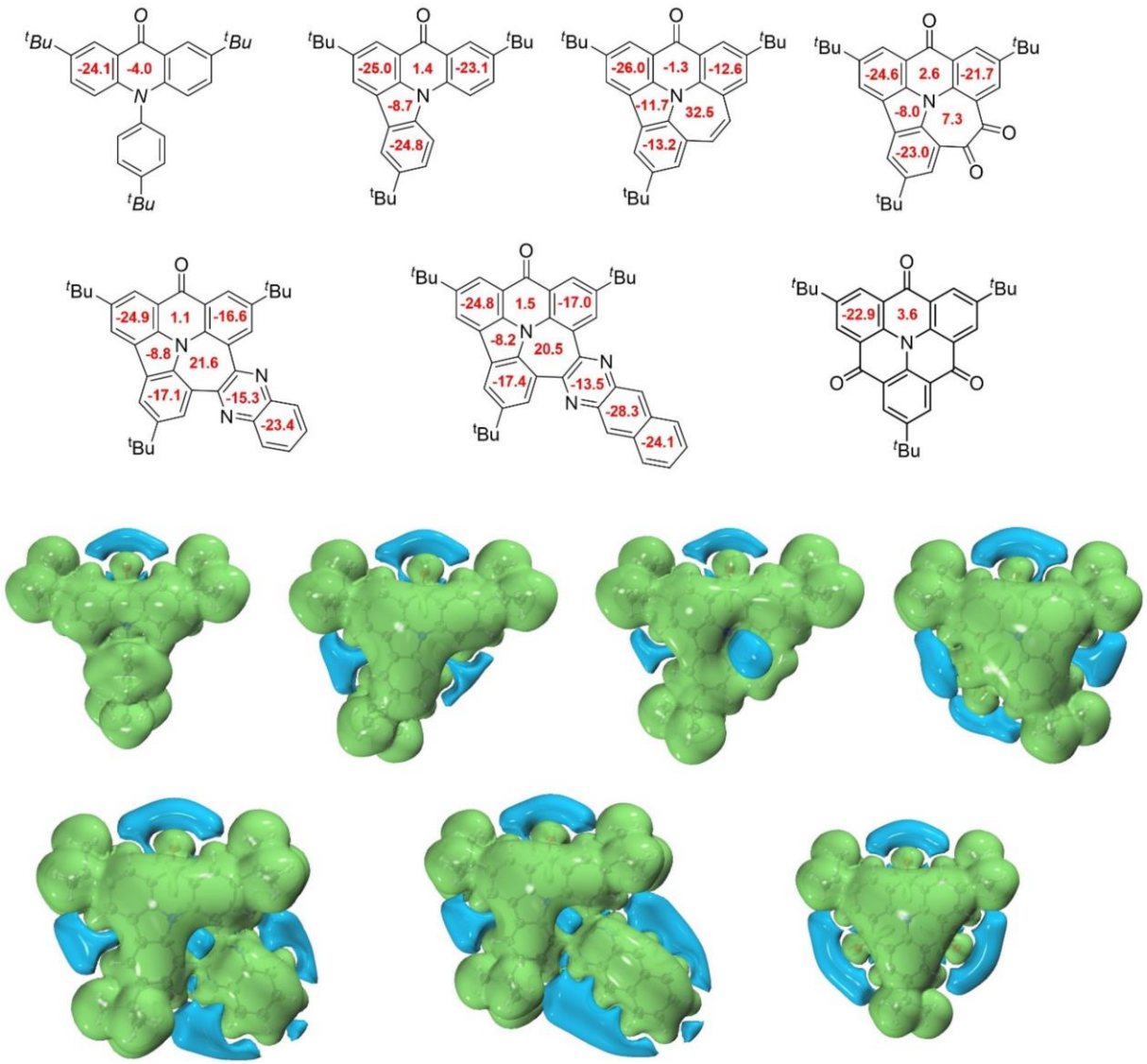


Figure S41. Calculated NICS(1)$_{zz}$ values and 3D ICSS maps of related compounds. The green and blue colors in 3D ICSS maps represent magnetically shielding and deshielding regions, respectively.

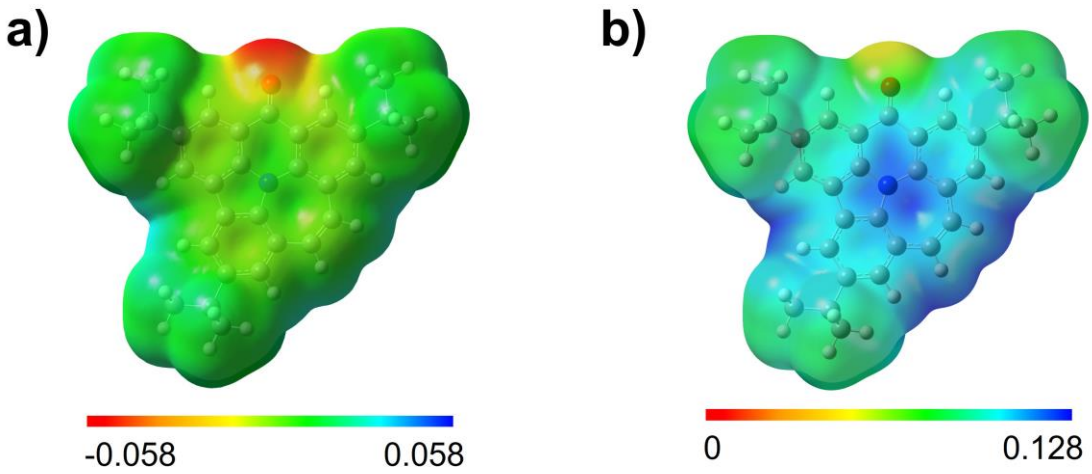


Figure S42. (a) Calculated electrostatic potential maps of (a) **11** (left) and (b) **11**$^{\bullet+}$ (right).

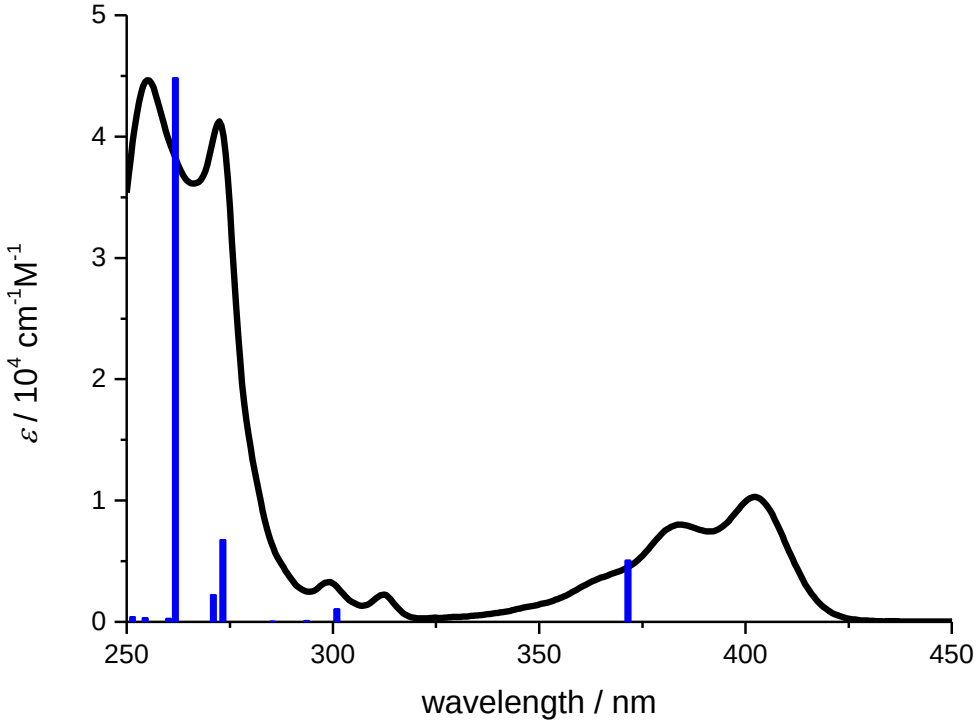


Figure S43. UV/Vis absorption spectrum of compound **5** and TD-DFT calculated oscillator strength (blue column) in dichloromethane at B3LYP/6-311+G(d,p) level.

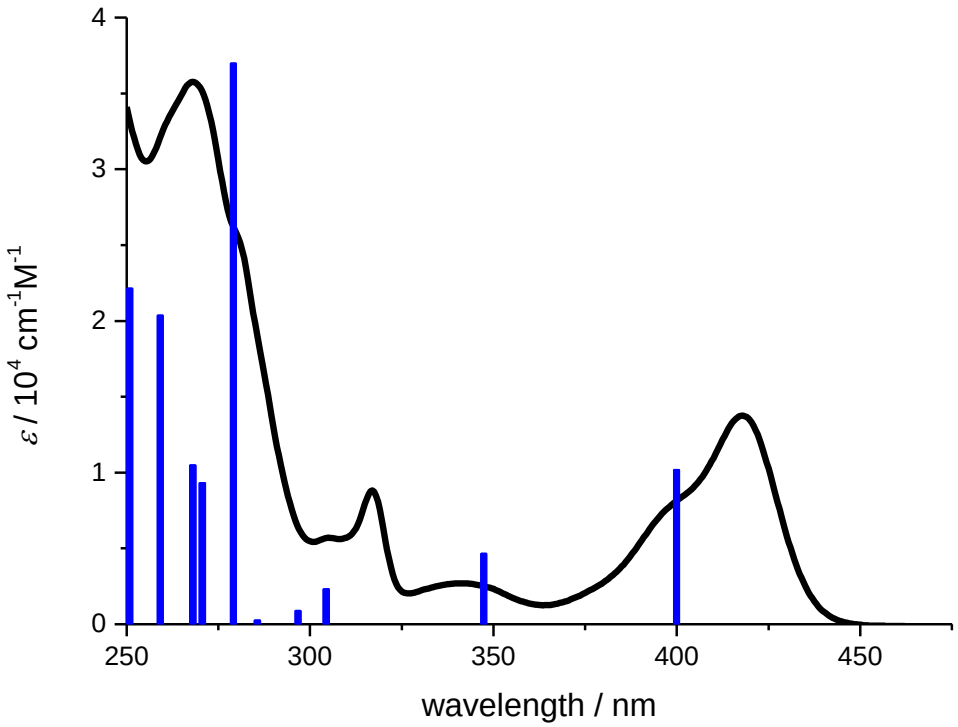


Figure S44. UV/Vis absorption spectrum of compound **7** and TD-DFT calculated oscillator strength (blue column) in dichloromethane at B3LYP/6-311+G(d,p) level.

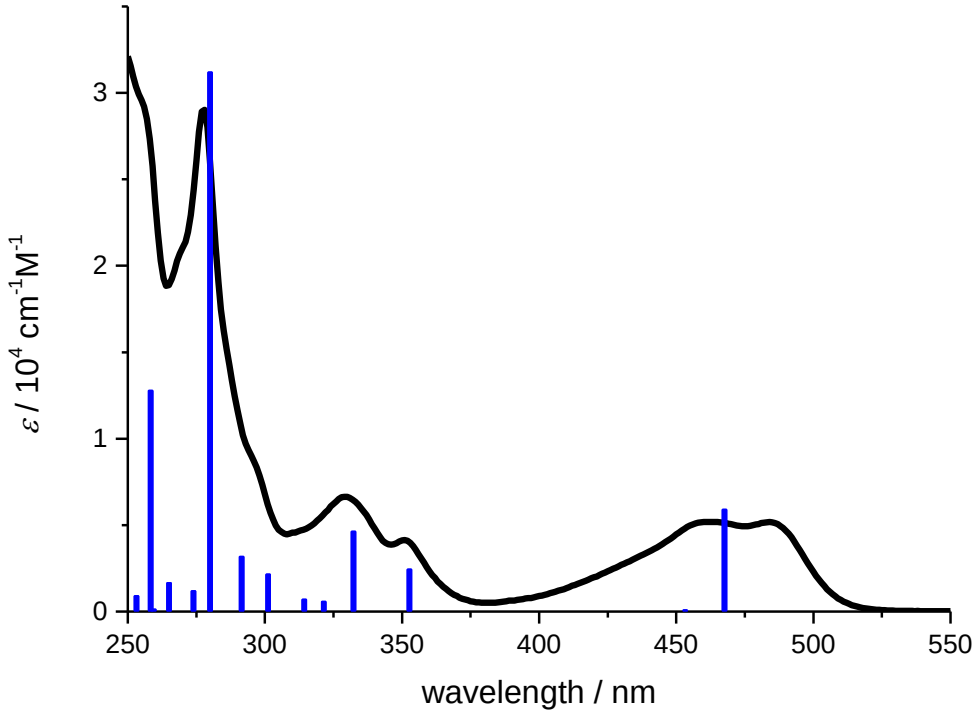


Figure S45. UV/Vis absorption spectrum of compound **11** and TD-DFT calculated oscillator strength (blue column) in dichloromethane at B3LYP/6-311+G(d,p) level.

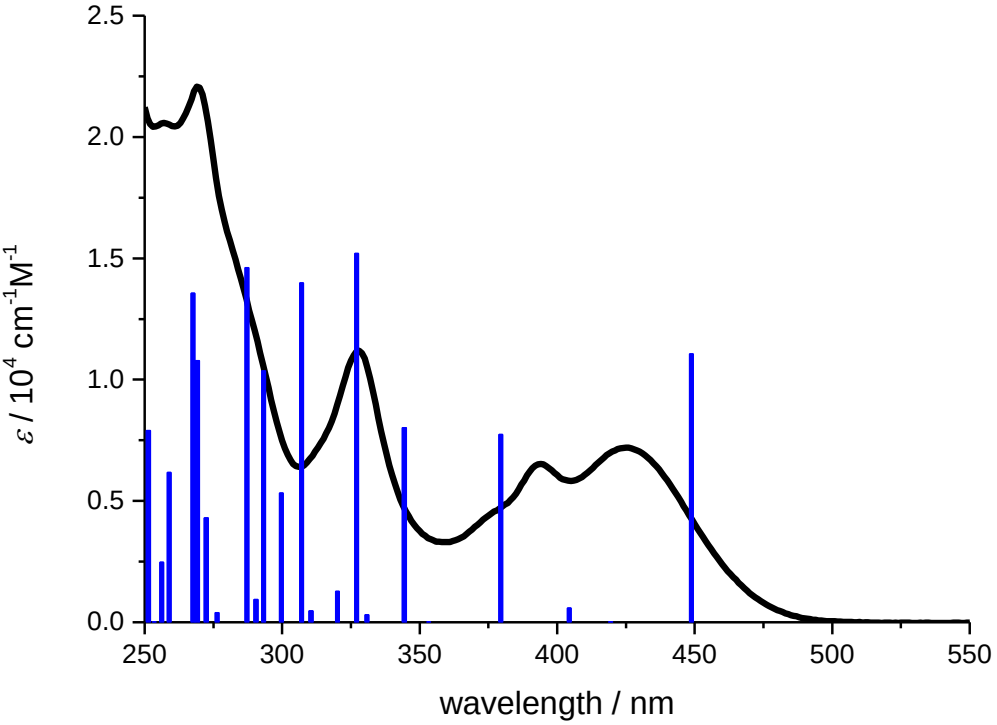


Figure S46. UV/Vis absorption spectrum of compound **12** and TD-DFT calculated oscillator strength (blue column) in dichloromethane at B3LYP/6-311+G(d,p) level.

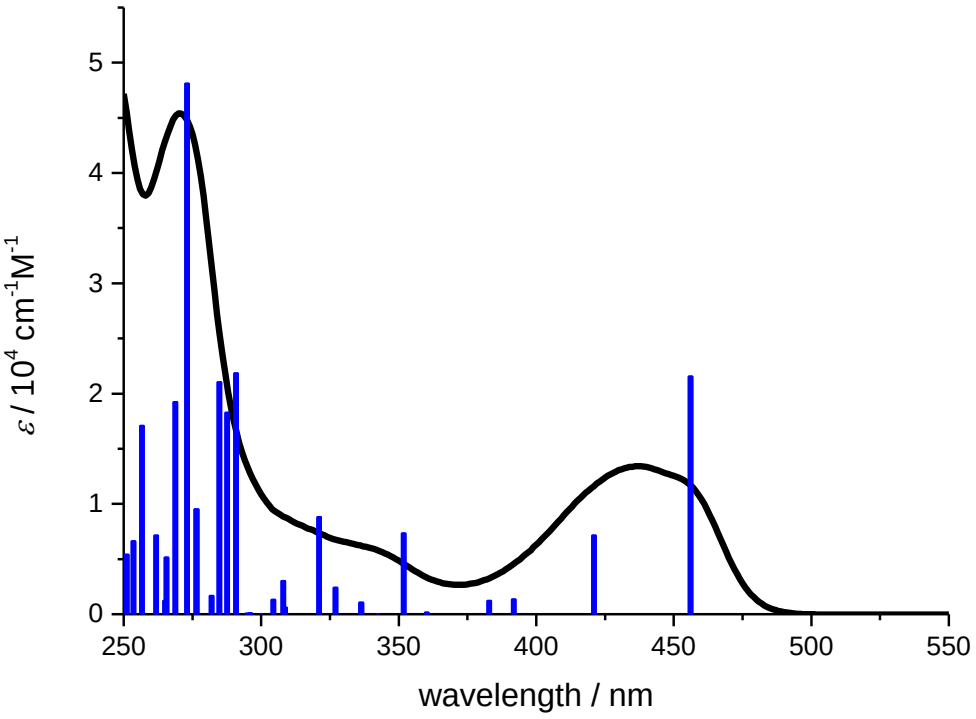


Figure S47. UV/Vis absorption spectrum of compound **13** and TD-DFT calculated oscillator strength (blue column) in dichloromethane at B3LYP/6-311+G(d,p) level.

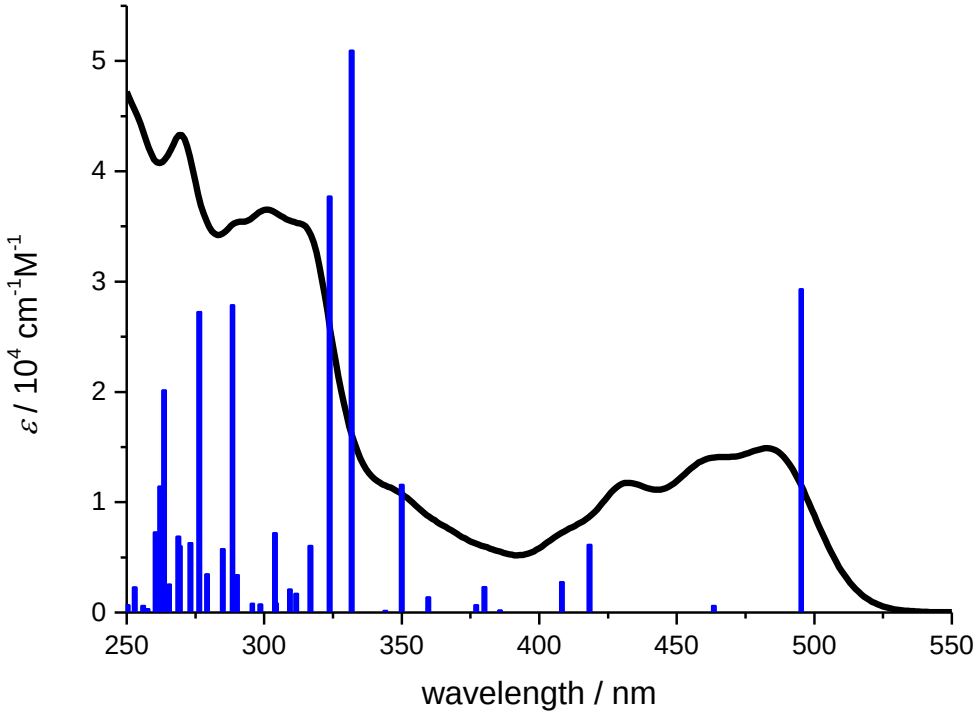


Figure S48. UV/Vis absorption spectrum of compound **14** and TD-DFT calculated oscillator strength (blue column) in dichloromethane at B3LYP/6-311+G(d,p) level.

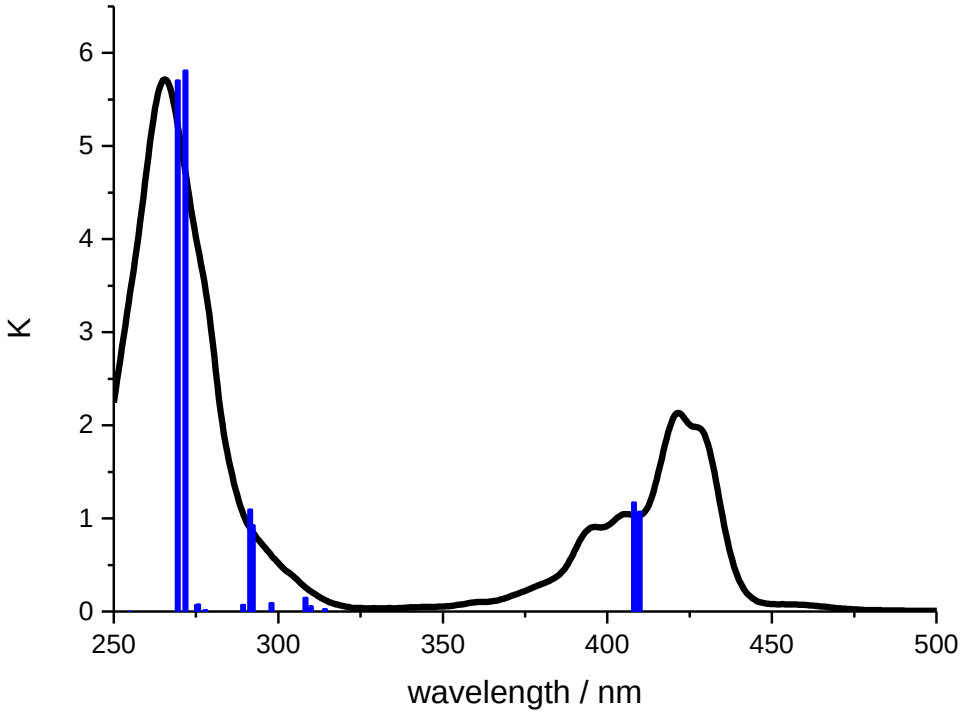


Figure S49. UV/Vis absorption spectrum of *tert*-butylated **1** and TD-DFT calculated oscillator strength (blue column) in dichloromethane at B3LYP/6-311+G(d,p) level.

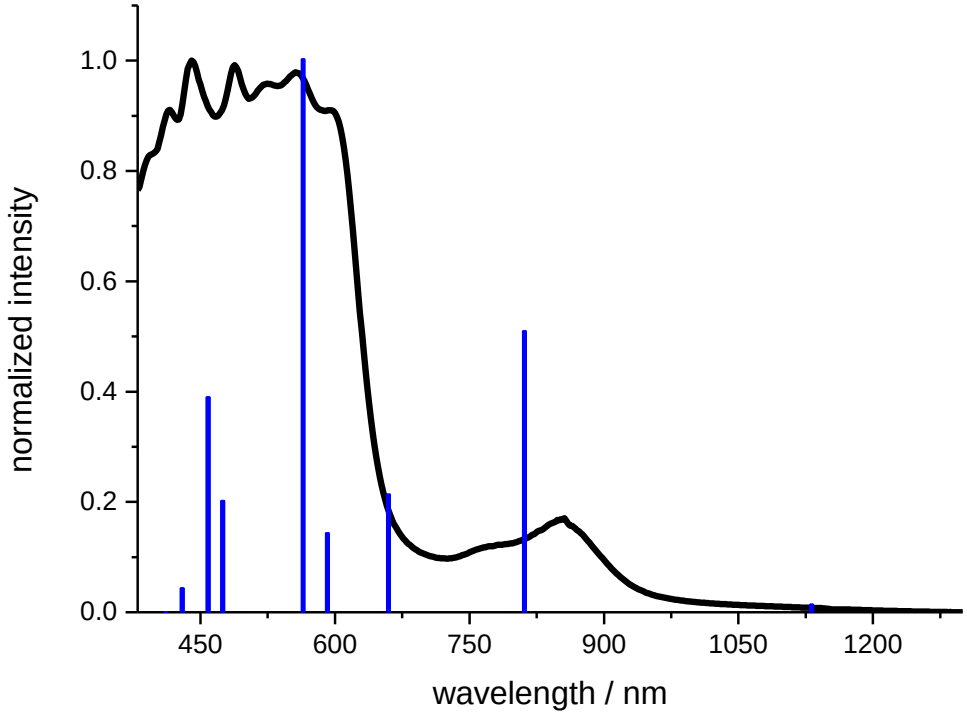


Figure S50. UV/Vis absorption spectrum of compound **11**$^{\bullet+}$ and TD-DFT calculated oscillator strength (blue column) in dichloromethane at UB3LYP/6-311+G(d,p) level.

Table S3. TD-DFT calculated first ten excited states of compound **5** in dichloromethane at B3LYP/6-311G+(d,p) level and the corresponding contributions.

Excited State	1:	3.3351 eV	371.75 nm	f=0.1415
119 ->120		97.1%		
Excited State	2:	3.7388 eV	331.61 nm	f=0.0000
116 ->120		2.3%		
118 ->120		95.1%		
Excited State	3:	4.1167 eV	301.17 nm	f=0.0293
117 ->120		15.4%		
119 ->121		81.1%		
Excited State	4:	4.2182 eV	293.92 nm	f=0.0022
117 ->120		4.7%		
119 ->122		93.3%		
Excited State	5:	4.3408 eV	285.63 nm	f=0.0012
117 ->120		23.9%		
119 ->121		9.4%		
119 ->122		3.5%		
119 ->123		62.3%		
Excited State	6:	4.5318 eV	273.58 nm	f=0.1894

115 ->120	26.3%
116 ->120	26.1%
117 ->120	28.2%
119 ->123	12.7%
Excited State 7:	4.5709 eV 271.25 nm f=0.0619
115 ->120	20.0%
116 ->120	68.6%
117 ->120	4.8%
119 ->123	2.9%
Excited State 8:	4.7319 eV 262.02 nm f=1.2539
115 ->120	49.2%
116 ->120	2.1%
117 ->120	19.4%
119 ->121	5.5%
119 ->123	19.3%
Excited State 9:	4.7615 eV 260.39 nm f=0.0071
114 ->120	96.3%
Excited State 10:	4.8668 eV 254.76 nm f=0.0093
114 ->123	3.3%
119 ->124	93.3%

119: HOMO, 120: LUMO

Table S4. TD-DFT calculated first ten excited states of compound **7** in dichloromethane at B3LYP/6-311G+(d,p) level and the corresponding contributions.

Excited State 1:	3.0978 eV 400.23 nm f=0.1781
118 ->119	97.5%
Excited State 2:	3.5663 eV 347.66 nm f=0.0814
117 ->119	96.2%
Excited State 3:	3.6292 eV 341.63 nm f=0.0000
115 ->119	96.2%
Excited State 4:	4.0690 eV 304.70 nm f=0.0404
118 ->120	92.6%
Excited State 5:	4.1742 eV 297.03 nm f=0.0155
116 ->119	61.7%
117 ->120	3.6%
118 ->121	30.4%
Excited State 6:	4.3365 eV 285.91 nm f=0.0045
114 ->119	88.8%

117 ->120	4.0%		
118 ->121	2.2%		
Excited State 7:	4.4373 eV	279.41 nm	f=0.6467
113 ->119	10.1%		
116 ->119	20.7%		
117 ->120	7.2%		
118 ->121	52.2%		
Excited State 8:	4.5763 eV	270.93 nm	f=0.1629
113 ->119	7.7%		
116 ->119	5.4%		
117 ->120	37.1%		
118 ->121	6.4%		
118 ->122	39.3%		
Excited State 9:	4.6212 eV	268.30 nm	f=0.1832
113 ->119	70.0%		
114 ->119	2.5%		
117 ->120	3.6%		
117 ->121	4.4%		
118 ->121	5.8%		
118 ->122	9.0%		
Excited State 10:	4.7786 eV	259.46 nm	f=0.3563
113 ->119	4.5%		
116 ->119	5.7%		
117 ->120	26.3%		
117 ->121	21.4%		
118 ->122	31.4%		
118 ->126	2.3%		

118: HOMO, 119: LUMO

Table S5. TD-DFT calculated first ten excited states of compound **11** in dichloromethane at B3LYP/6-311G+(d,p) level and the corresponding contributions.

Excited State 1:	2.6492 eV	468.01 nm	f=0.1672
124 ->125	96.9%		
Excited State 2:	2.7335 eV	453.58 nm	f=0.0009
124 ->126	99.3%		
Excited State 3:	3.5116 eV	353.07 nm	f=0.0682
122 ->125	3.1%		
123 ->125	92.0%		

Excited State	4:	3.6353 eV	341.06 nm	f=0.0000
120 ->125	85.4%			
120 ->126	6.2%			
121 ->125	4.3%			
Excited State	5:	3.7265 eV	332.71 nm	f=0.1310
123 ->126	79.9%			
124 ->127	9.2%			
124 ->128	4.6%			
Excited State	6:	3.8531 eV	321.78 nm	f=0.0151
121 ->125	2.9%			
122 ->126	4.4%			
123 ->126	6.9%			
124 ->127	72.8%			
124 ->128	6.6%			
Excited State	7:	3.9389 eV	314.77 nm	f=0.0190
122 ->125	85.8%			
123 ->125	2.5%			
124 ->127	2.4%			
124 ->128	4.9%			
Excited State	8:	4.1118 eV	301.53 nm	f=0.0604
121 ->125	34.0%			
122 ->125	2.1%			
122 ->126	3.7%			
123 ->126	3.4%			
124 ->127	2.8%			
124 ->128	47.0%			
Excited State	9:	4.2474 eV	291.91 nm	f=0.0894
119 ->125	3.1%			
121 ->125	7.1%			
122 ->125	2.8%			
122 ->126	63.9%			
123 ->127	2.3%			
124 ->127	4.0%			
124 ->128	12.5%			
Excited State	10:	4.4218 eV	280.39 nm	f=0.8895
119 ->125	5.5%			
121 ->125	39.0%			
122 ->125	2.0%			

122 ->126	15.4%
123 ->126	2.4%
123 ->127	6.0%
124 ->127	3.8%
124 ->128	17.5%

124: HOMO, 125: LUMO

Table S6. TD-DFT calculated first ten excited states of compound **12** in dichloromethane at B3LYP/6-311G+(d,p) level and the corresponding contributions.

Excited State 1:	2.7601 eV 449.20 nm f=0.1314
131 ->132	97.9%
Excited State 2:	2.9534 eV 419.80 nm f=0.0002
126 ->132	2.2%
127 ->132	8.3%
129 ->132	80.0%
130 ->132	3.2%
Excited State 3:	3.0631 eV 404.77 nm f=0.0070
129 ->132	2.6%
130 ->132	92.8%
131 ->133	2.6%
Excited State 4:	3.2639 eV 379.87 nm f=0.0919
130 ->132	2.4%
131 ->133	94.0%
Excited State 5:	3.5055 eV 353.69 nm f=0.0001
127 ->132	41.6%
127 ->133	30.1%
128 ->132	2.4%
128 ->133	2.5%
129 ->132	4.8%
129 ->133	14.2%
Excited State 6:	3.5959 eV 344.80 nm f=0.0952
128 ->133	2.6%
130 ->133	91.7%
131 ->134	2.3%
Excited State 7:	3.7431 eV 331.23 nm f=0.0036
123 ->132	3.1%
125 ->132	3.7%
126 ->132	6.4%

127 ->132	3.0%
128 ->132	69.0%
131 ->134	7.7%
Excited State 8:	3.7866 eV 327.43 nm f=0.1805
126 ->132	10.4%
128 ->132	4.0%
131 ->134	78.4%
Excited State 9:	3.8688 eV 320.47 nm f=0.0151
123 ->132	16.5%
124 ->132	6.1%
125 ->132	26.9%
126 ->132	6.8%
127 ->133	8.4%
128 ->132	18.6%
129 ->134	10.4%
Excited State 10:	3.9883 eV 310.87 nm f=0.0055
125 ->132	2.3%
126 ->132	2.3%
127 ->132	43.4%
127 ->133	16.5%
129 ->132	3.3%
129 ->133	26.2%

131: HOMO, 132: LUMO

Table S7. TD-DFT calculated first ten excited states of compound **13** in dichloromethane at B3LYP/6-311G+(d,p) level and the corresponding contributions.

Excited State 1:	2.7185 eV 456.07 nm f=0.2940
150 -> 151	98.3%
Excited State 2:	2.9454 eV 420.94 nm f=0.0974
150 -> 152	96.0%
Excited State 3:	3.1648 eV 391.76 nm f=0.0185
149 -> 151	6.5%
150 -> 153	91.0%
Excited State 4:	3.2377 eV 382.94 nm f=0.0166
149 -> 151	88.6%
150 -> 153	6.2%
Excited State 5:	3.4420 eV 360.21 nm f=0.0024
144 -> 151	28.7%

145 -> 151	2.7%
146 -> 151	45.2%
147 -> 151	12.3%
149 -> 151	3.2%
149 -> 152	3.1%
Excited State 6:	3.5247 eV 351.76 nm f=0.1002
149 -> 152	90.3%
Excited State 7:	3.6199 eV 342.50 nm f=0.0002
144 -> 151	5.4%
144 -> 152	10.3%
145 -> 151	15.4%
145 -> 152	53.5%
145 -> 153	3.0%
146 -> 152	6.6%
Excited State 8:	3.6860 eV 336.36 nm f=0.0143
148 -> 151	90.5%
Excited State 9:	3.7914 eV 327.02 nm f=0.0331
144 -> 151	4.6%
146 -> 151	3.5%
147 -> 151	44.2%
148 -> 151	3.1%
148 -> 153	2.8%
149 -> 153	34.7%
Excited State 10:	3.8619 eV 321.05 nm f=0.1203
144 -> 151	3.1%
147 -> 151	26.5
148 -> 152	5.1%
148 -> 153	2.8%
149 -> 153	55.2%

150: HOMO, 151: LUMO

Table S8. TD-DFT calculated first ten excited states of compound **14** in dichloromethane at B3LYP/6-311G+(d,p) level and the corresponding contributions.

Excited State 1:	2.5014 eV 495.66 nm f=0.3989
163 -> 164	97.8%
Excited State 2:	2.6728 eV 463.87 nm f=0.0076
162 -> 164	97.8%
Excited State 3:	Singlet-A 2.9612 eV 418.69 nm f=0.0828

161 -> 164	9.6%
163 -> 165	87.0%
Excited State 4:	3.0348 eV 408.54 nm f=0.0369
161 -> 164	85.7%
163 -> 165	8.4%
Excited State 5:	3.2109 eV 386.14 nm f=0.0019
157 -> 164	22.1%
158 -> 164	7.7%
159 -> 164	53.2%
160 -> 164	10.3%
161 -> 164	2.2%
Excited State 6:	3.2589 eV 380.44 nm f=0.0305
162 -> 165	12.9%
163 -> 166	82.2%
Excited State 7:	3.2842 eV 377.52 nm f=0.0083
160 -> 164	3.5%
162 -> 165	76.7%
163 -> 166	13.2%
Excited State 8:	3.4432 eV 360.09 nm f=0.0181
159 -> 164	4.5%
160 -> 164	43.7%
161 -> 165	2.5%
162 -> 165	5.7%
162 -> 166	37.6%
Excited State 9:	3.5390 eV 350.33 nm f=0.1570
160 -> 164	2.6%
161 -> 165	89.8%
Excited State 10:	3.6000 eV 344.40 nm f=0.0012
157 -> 164	10.6%
157 -> 165	24.9%
158 -> 164	11.9%
158 -> 165	38.8%
159 -> 165	5.9%

163: HOMO, 164: LUMO

Table S9. TD-DFT calculated first ten excited states of *tert*-butylated **1** in dichloromethane at B3LYP/6-311G+(d,p) level and the corresponding contributions.

Excited State 1:	3.0232 eV 410.11 nm f=0.1403

131 ->132 95.2%

131 ->133 2.4%

Excited State 2: 3.0358 eV 408.41 nm f=0.1532

131 ->132 2.4%

131 ->133 95.1%

Excited State 3: 3.3923 eV 365.49 nm f=0.0000

126 ->132 7.5%

126 ->133 3.7%

127 ->132 4.7%

127 ->133 6.6%

127 ->136 2.9%

130 ->132 2.5%

130 ->133 71.2%

Excited State 4: 3.4003 eV 364.63 nm f=0.0000

126 ->132 5.9%

126 ->133 8.8%

126 ->136 2.8%

127 ->132 10.0%

127 ->133 4.9%

130 ->132 64.4%

130 ->133 2.3%

Excited State 5: 3.5789 eV 346.43 nm f=0.0000

126 ->132 45.0%

127 ->133 45.7%

130 ->136 5.0%

Excited State 6: 3.9421 eV 314.52 nm f=0.0037

128 ->132 27.5%

129 ->133 66.7%

Excited State 7: 3.9965 eV 310.24 nm f=0.0075

128 ->132 14.3%

128 ->133 29.5%

129 ->132 49.8%

129 ->133 2.2%

Excited State 8: 4.0175 eV 308.61 nm f=0.0192

125 ->133	4.4%	
128 ->132	52.1%	
128 ->133	3.0%	
129 ->132	11.7%	
129 ->133	24.8%	
Excited State 9:	4.0628 eV	305.17 nm f=0.0000
126 ->132	10.8%	
126 ->133	19.3%	
127 ->132	27.2%	
127 ->133	10.2%	
130 ->132	30.8%	
Excited State 10:	4.0848 eV	303.53 nm f=0.0000
126 ->132	24.4%	
126 ->133	8.7%	
127 ->132	14.8%	
127 ->133	26.9%	
130 ->133	23.6%	

131: HOMO, 132: LUMO

Table S10. TD-DFT calculated first ten excited states of **11**$^{\bullet+}$ in dichloromethane at B3LYP/6-311G+(d,p) level and the corresponding contributions.

Excited State 1:	2.024-A	1.0963 eV 1130.91 nm f=0.0022 <S**2>=0.774
122B ->124B	1.1%	
123B ->124B	97.6%	
Excited State 2:	2.029-A	1.5297 eV 810.49 nm f=0.0787 <S**2>=0.779
121B ->124B	3.1%	
122B ->124B	93.6%	
123B ->124B	1.0%	
Excited State 3:	2.029-A	1.8818 eV 658.85 nm f=0.0330 <S**2>=0.779
121B ->124B	93.9%	
122B ->124B	3.2%	
Excited State 4:	2.090-A	1.9132 eV 648.06 nm f=0.0000 <S**2>=0.842
120B ->124B	96.2%	
120B ->126B	2.3%	
Excited State 5:	2.094-A	2.0991 eV 590.66 nm f=0.0222 <S**2>=0.846
122A ->125A	2.0%	

124A ->125A	57.5%				
124A ->126A	1.4%				
119B ->124B	35.3%				
Excited State 6:	2.112-A	2.1996 eV	563.66 nm	f=0.1549	<S**2>=0.865
124A ->125A	23.7%				
124A ->126A	9.7%				
119B ->124B	56.8%				
122B ->125B	1.7%				
123B ->125B	2.9%				
Excited State 7:	2.429-A	2.6156 eV	474.01 nm	f=0.0312	<S**2>=1.224
122A ->126A	1.3%				
123A ->125A	3.6%				
123A ->126A	6.1%				
124A ->125A	2.6%				
124A ->126A	8.8%				
118B ->124B	63.1%				
123B ->126B	5.7%				
Excited State 8:	2.098-A	2.7083 eV	457.79 nm	f=0.0602	<S**2>=0.850
124A ->125A	6.0%				
124A ->126A	68.9%				
118B ->124B	15.9%				
119B ->124B	2.6%				
122B ->126B	1.4%				
123B ->125B	1.4%				
Excited State 9:	3.198-A	2.8907 eV	428.91 nm	f=0.0068	<S**2>=2.306
120A ->126A	1.4%				
123A ->125A	18.5%				
123A ->126A	13.6%				
123A ->127A	2.9%				
124A ->125A	1.1%				
124A ->126A	4.0%				
118B ->124B	14.3%				
121B ->126B	1.2%				
123B ->125B	16.6%				

123B ->126B	12.6%	
123B ->127B	2.2%	
Excited State 10:	3.423-A	3.0203 eV 410.50 nm f=0.0001 <S**2>=2.679
120A ->125A	1.4%	
122A ->125A	1.5%	
123A ->125A	28.9%	
123A ->126A	21.8%	
124A ->125A	1.3%	
119B ->125B	1.1%	
123B ->125B	16.5%	
123B ->126B	18.3%	

124A: HOMO (α), 125A: LUMO (α), 123B: HOMO (β), 124B: LUMO (β)

Cartesian coordinates for theoretically optimized structures

5 opt B3LYP/6-31G(d,p) HF = -1333.674290 Hartree imaginary frequency 0

C	-0.54677800	-3.64133300	0.00744800
C	0.15421700	-2.44836500	0.01149300
C	-0.53487500	-1.21686000	0.00822100
C	-1.94568400	-1.24456100	0.00070000
C	-2.62368200	-2.47750600	-0.00304100
C	-1.95908600	-3.69605900	0.00014900
C	-1.94564600	1.24461700	0.00074100
C	-0.53483800	1.21687300	0.00826900
C	0.15429200	2.44835700	0.01161000
H	1.23694300	2.46381500	0.01753000
C	-0.54666700	3.64134600	0.00760800
C	-1.95897300	3.69611500	0.00029000
C	-2.62360600	2.47758300	-0.00295600
H	0.02666400	-4.56389600	0.01015000
H	-3.70488700	-2.41153100	-0.00863200
H	0.02680400	4.56389100	0.01036300
H	-3.70481300	2.41164100	-0.00855700
C	-2.73508100	0.00004000	-0.00338600
O	-3.96953500	0.00005900	-0.00967700
C	1.59365100	-0.00002600	0.01834600
C	2.30250300	0.00005000	-1.18578200
C	2.29267600	-0.00012200	1.22384200
C	3.69442600	0.00003100	-1.17259900
C	3.68928700	-0.00014300	1.22470400
H	1.74213900	-0.00018000	2.15947400
C	4.42304900	-0.00006600	0.03027000
H	4.21990900	0.00009200	-2.12249800
H	4.20091600	-0.00021900	2.17970100
N	0.15354600	-0.00000400	0.01236600
C	-2.67921500	-5.05471300	-0.00383800
C	-2.28077100	-5.85383700	1.25967500
C	-4.21086000	-4.89606500	-0.01153000
C	-2.26799200	-5.85317200	-1.26366800

H	-1.20226200	-6.03384000	1.30607800
H	-2.56922100	-5.31656200	2.16892200
H	-2.78033000	-6.82918900	1.26805800
H	-4.55948500	-4.35852700	-0.89898300
H	-4.68422700	-5.88330300	-0.01420900
H	-4.56842700	-4.35905100	0.87267800
H	-2.76731400	-6.82858300	-1.27756200
H	-2.54734900	-5.31548600	-2.17550900
H	-1.18904500	-6.03300200	-1.29929800
C	-2.67906000	5.05479100	-0.00364600
C	-2.26778100	5.85330500	-1.26342300
C	-4.21071000	4.89619100	-0.01138600
C	-2.28062400	5.85383600	1.25992100
H	-1.18882800	6.03310300	-1.29901700
H	-2.54713400	5.31567700	-2.17529900
H	-2.76707200	6.82873200	-1.27727600
H	-4.56831800	4.35914900	0.87278800
H	-4.68404600	5.88344300	-0.01403500
H	-4.55932700	4.35870200	-0.89887200
H	-2.78015400	6.82920200	1.26834400
H	-2.56911200	5.31652000	2.16913200
H	-1.20211100	6.03380400	1.30635900
C	5.96224800	-0.00008400	-0.00531200
C	6.45809500	-1.26255000	-0.74996700
C	6.45812800	1.26247700	-0.74978400
C	6.58012100	-0.00019500	1.40557300
H	6.12657200	-2.17361800	-0.24135500
H	6.08935800	-1.30129700	-1.77909900
H	7.55285700	-1.27455700	-0.78855200
H	6.12663200	2.17348000	-0.24103700
H	7.55289100	1.27445900	-0.78836900
H	6.08939000	1.30138400	-1.77890900
H	7.67184800	-0.00020400	1.32830600
H	6.29122500	0.88713000	1.97824900

H	6.29120200	-0.88759500	1.97812000
H	1.75812700	0.00012300	-2.12498500
H	1.23686700	-2.46385700	0.01739300

7 opt B3LYP/6-31G(d,p) HF = -1332.481996 Hartree imaginary frequency 0

C	-2.29785700	1.98406100	0.00024600
C	-1.62218200	0.76858100	0.00013800
C	-0.21600200	0.77971700	-0.00003900
C	0.52406400	1.95625600	-0.00016400
C	-0.18749100	3.16743200	-0.00007900
C	-1.58776800	3.20709800	0.00014000
C	2.52107000	0.46468200	-0.00025900
C	1.68873800	-0.68583700	0.00001600
C	2.30630400	-1.94791200	0.00050200
H	1.71792400	-2.85175600	0.00101600
C	3.68854300	-2.05756500	0.00052800
C	4.53875100	-0.93417700	0.00009800
C	3.91690800	0.30932300	-0.00024500
H	-3.38370200	1.99105200	0.00039600
H	0.40439700	4.07415200	-0.00019500
H	4.11443700	-3.05658800	0.00092200
H	4.48398600	1.23227700	-0.00048400
C	1.99056100	1.85911100	-0.00041300
O	2.72847800	2.84462600	-0.00074000
C	-0.80646400	-1.40187600	-0.00015400
C	-2.00480400	-0.63371800	0.00009000
C	-0.88788900	-2.79292500	-0.00056500
C	-3.24826800	-1.26007100	0.00011600
C	-2.15091500	-3.39224600	-0.00053700
H	-0.01800100	-3.43289300	-0.00104200
C	-3.34893900	-2.65833600	-0.00015700
H	-4.14395700	-0.64602500	0.00031900
H	-2.18401900	-4.47503900	-0.00085400
N	0.29699900	-0.50819800	-0.00011100
C	-2.37602100	4.53188600	0.00025400

C	-3.26777400	4.60187100	1.26272800
C	-1.44879700	5.76176000	0.00008900
C	-3.26819100	4.60184900	-1.26192600
H	-3.98503700	3.77648000	1.30407300
H	-2.66079800	4.56251600	2.17299300
H	-3.83827300	5.53730800	1.27474500
H	-0.80735300	5.78887100	-0.88646700
H	-2.05126200	6.67575800	0.00017700
H	-0.80706400	5.78889100	0.88643700
H	-3.83869000	5.53728900	-1.27377300
H	-2.66151600	4.56247400	-2.17239100
H	-3.98547200	3.77646200	-1.30301900
C	6.06563500	-1.11705300	0.00009300
C	6.48946900	-1.90576100	-1.26170700
C	6.80855500	0.23172000	-0.00037400
C	6.48959300	-1.90495200	1.26235700
H	6.02326700	-2.89509700	-1.30135800
H	6.20884900	-1.36714400	-2.17257000
H	7.57552500	-2.05050600	-1.27331700
H	6.56948900	0.82854600	0.88547800
H	7.88921400	0.05681600	-0.00037900
H	6.56938900	0.82798700	-0.88657500
H	7.57565200	-2.04967300	1.27395900
H	6.20904900	-1.36575800	2.17290200
H	6.02341300	-2.89427000	1.30268300
C	-4.73678300	-3.32699700	-0.00008100
C	-5.51836900	-2.89141800	1.26212000
C	-5.51884300	-2.89078800	-1.26177000
C	-4.64687600	-4.86479400	-0.00048800
H	-4.99164200	-3.19422000	2.17289600
H	-5.65601400	-1.80681000	1.30208700
H	-6.51205600	-3.35318800	1.27416700
H	-4.99245400	-3.19312300	-2.17289600
H	-6.51252800	-3.35256800	-1.27367700

H	-5.65652800	-1.80616400	-1.30114100
H	-5.65460500	-5.29226200	-0.00041400
H	-4.12926100	-5.24324900	-0.88803900
H	-4.12894000	-5.24370200	0.88668300

11 opt B3LYP/6-31G(d,p) HF = -1408.692864 Hartree imaginary frequency 0

C	-2.40591800	2.12827500	-0.00000800
C	-1.70660600	0.92614800	-0.00003500
C	-0.29935700	0.96664900	-0.00006200
C	0.41495100	2.15801900	-0.00004400
C	-0.31961200	3.35500100	-0.00001800
C	-1.72061900	3.36556400	-0.00000500
C	2.43436100	0.69085700	-0.00001200
C	1.63340700	-0.47706500	-0.00004700
C	2.27504600	-1.74896200	-0.00005600
C	3.67394200	-1.77115800	-0.00000600
C	4.49321700	-0.62839000	0.00004700
C	3.83868200	0.59165000	0.00003500
H	-3.49168500	2.11375300	0.00001400
H	0.25343400	4.27368600	-0.00000600
H	4.14252400	-2.75096400	-0.00001400
H	4.37006900	1.53503800	0.00006100
C	1.87820300	2.07946900	-0.00002800
O	2.60528100	3.07336300	-0.00000200
C	-0.85350600	-1.21507300	-0.00005700
C	-2.05920300	-0.48263500	-0.00003000
C	-0.86492300	-2.61749800	-0.00007700
C	-3.29765000	-1.14070000	-0.00001000
C	-2.12373100	-3.23266200	-0.00005200
C	-3.34917500	-2.53342800	-0.00001700
H	-4.20465400	-0.54809600	0.00000900
H	-2.13668200	-4.31863500	-0.00006400
N	0.23694500	-0.30730900	-0.00008300
C	-2.53592500	4.67386600	0.00002300
C	-3.42916500	4.72546700	1.26235700

C	-1.63427800	5.92263100	0.00000800
C	-3.42922700	4.72548400	-1.26226600
H	-4.12942200	3.88559400	1.30349400
H	-2.82168600	4.69848000	2.17273600
H	-4.01868500	5.64903500	1.27432000
H	-0.99342300	5.96306000	-0.88647500
H	-2.25549000	6.82398100	0.00002100
H	-0.99339100	5.96305900	0.88646800
H	-4.01874800	5.64905200	-1.27418600
H	-2.82179300	4.69851200	-2.17267600
H	-4.12948600	3.88561200	-1.30338200
C	6.02411500	-0.77254100	0.00008900
C	6.46916200	-1.54846300	-1.26225700
C	6.72881500	0.59658400	0.00021700
C	6.46909300	-1.54865300	1.26234000
H	6.03100400	-2.55046500	-1.30301800
H	6.17384700	-1.01711000	-2.17271300
H	7.55879600	-1.66271600	-1.27366100
H	6.47258000	1.18593400	0.88624800
H	7.81395400	0.45232200	0.00026500
H	6.47267800	1.18605200	-0.88576500
H	7.55872700	-1.66290100	1.27378600
H	6.17372700	-1.01744100	2.17286200
H	6.03094500	-2.55066700	1.30292800
C	1.62705100	-3.06701200	-0.00012800
H	2.34721100	-3.88185900	-0.00018200
C	0.33508700	-3.44328000	-0.00013300
H	0.14332300	-4.51384800	-0.00019000
C	-4.67217500	-3.32165200	0.00002000
C	-5.90134800	-2.39350900	0.00000800
C	-4.74290100	-4.21350600	-1.26232500
C	-4.74285900	-4.21342900	1.26242200
H	-5.92803300	-1.75269000	0.88746900
H	-5.92804000	-1.75272500	-0.88747800

H	-6.81652800	-2.99397500	0.00002500
H	-3.91716000	-4.92991100	-1.30323800
H	-5.67839300	-4.78398000	-1.27387700
H	-4.70336500	-3.60681000	-2.17280600
H	-5.67834500	-4.78391100	1.27403900
H	-3.91710700	-4.92982000	1.30335300
H	-4.70330100	-3.60667500	2.17286500

12 opt B3LYP/6-31G(d,p) HF = -1557.925811 Hartree imaginary frequency 0

C	2.61984300	2.19105900	0.09570100
C	1.84100900	1.03822700	0.08211600
C	0.44481800	1.17287300	0.02568200
C	-0.18860300	2.40412500	-0.04551300
C	0.62214100	3.55080000	-0.03420500
C	2.01898900	3.46986100	0.04288000
C	-2.29908200	1.06918900	-0.10806000
C	-1.57459600	-0.15140000	0.00599000
C	-2.31005600	-1.35385300	0.16159200
C	-3.71204000	-1.29498800	0.14720900
C	-4.44306100	-0.11662100	-0.02706000
C	-3.69841200	1.05515300	-0.13881000
H	3.70100800	2.10496700	0.14224900
H	0.11330000	4.50453400	-0.09383800
H	-4.22217100	-2.24068600	0.29010300
H	-4.16861400	2.02539100	-0.24423300
C	-1.65203500	2.41783200	-0.15783900
O	-2.30624100	3.45272000	-0.27030600
C	0.83747600	-1.04693700	0.02933200
C	2.09762200	-0.39225800	0.07790500
C	0.78085800	-2.44166800	-0.08565600
C	3.28138500	-1.12607500	0.06269000
C	1.99993800	-3.14119700	-0.12083200
C	3.25446500	-2.52541100	-0.03258600
H	4.22434500	-0.59422600	0.11248100
H	1.91944900	-4.21772400	-0.22131300

N	-0.17822700	-0.07218100	0.02037000
C	2.91767700	4.72206600	0.06229800
C	3.87357500	4.69023100	-1.15398200
C	2.10089600	6.02617900	-0.00344400
C	3.74794500	4.73848900	1.36783300
H	4.52033800	3.80762000	-1.14510800
H	3.31197900	4.68376600	-2.09364400
H	4.52074900	5.57411300	-1.15122800
H	1.41941100	6.12441700	0.84749000
H	2.77934400	6.88476200	0.01644400
H	1.51139300	6.09316300	-0.92329800
H	4.39541100	5.62175400	1.39485800
H	3.09589600	4.76871300	2.24665900
H	4.38889300	3.85614500	1.45761000
C	-5.97998600	-0.15335400	-0.06358000
C	-6.51133000	-0.72803300	1.27097300
C	-6.58330700	1.24891200	-0.26538500
C	-6.44069900	-1.05724300	-1.23142300
H	-6.14553400	-1.74259800	1.45439600
H	-6.20559100	-0.10352400	2.11656000
H	-7.60595800	-0.76711400	1.25617400
H	-6.25767900	1.70172900	-1.20745600
H	-7.67505200	1.17783100	-0.29292500
H	-6.31792100	1.92946000	0.54998300
H	-7.53463100	-1.10074200	-1.26717800
H	-6.08521700	-0.67030000	-2.19195300
H	-6.07143400	-2.08157800	-1.12485400
C	4.53151400	-3.38598600	-0.05587000
C	5.80951800	-2.53264500	0.04797200
C	4.50748300	-4.36978800	1.13791200
C	4.58857200	-4.18558500	-1.37911300
H	5.90446100	-1.83396700	-0.79001600
H	5.84418300	-1.95955200	0.98059400
H	6.68820400	-3.18463100	0.03122800

H	3.64089300	-5.03586400	1.09914100
H	5.40762000	-4.99413000	1.13269400
H	4.47352100	-3.83117000	2.09054700
H	5.48945500	-4.80827500	-1.40663300
H	3.72459500	-4.84611200	-1.49444400
H	4.61370100	-3.51372100	-2.24320800
C	-1.77775100	-2.72890000	0.41107500
O	-2.44380500	-3.54437000	1.02694500
C	-0.45512400	-3.24583100	-0.18467400
O	-0.45602900	-4.37466700	-0.64629400

13 opt B3LYP/6-31G(d,p) HF = -1748.062872 Hartree imaginary frequency 0

C	4.16643400	0.32578500	-0.20990500
C	2.78359100	0.45758700	-0.13798700
C	1.99096300	-0.69860200	-0.21961900
C	2.53696900	-1.97109100	-0.30228500
C	3.93540300	-2.07597900	-0.37787600
C	4.76525300	-0.94775200	-0.34712300
C	0.18410400	-2.74792600	-0.01623600
C	-0.30689300	-1.41123600	-0.02842900
C	-1.70729800	-1.19710600	0.06937800
C	-2.51076900	-2.31809600	0.32906400
C	-2.04471800	-3.63523200	0.41693900
C	-0.68777600	-3.82303400	0.19772500
H	4.79079800	1.21213100	-0.15099700
H	4.34231900	-3.07706600	-0.44461500
H	-3.56984700	-2.12407800	0.42839800
H	-0.22877700	-4.80391300	0.19529800
C	1.62008400	-3.11083400	-0.22186500
O	1.99653000	-4.28111800	-0.28361600
C	0.54314200	1.01189800	0.03483300
C	1.85485400	1.55612600	0.05154700
C	-0.57337800	1.84830800	0.16170400
C	2.06935900	2.91799900	0.25424500
C	-0.30411100	3.21061500	0.38850600

C	0.98013000	3.77093100	0.45054800
H	3.08607900	3.29276400	0.26697400
H	-1.17165300	3.84856400	0.48956500
N	0.64104000	-0.38588800	-0.13906700
C	6.30067900	-1.04970500	-0.43632600
C	6.93492500	-0.45750000	0.84465100
C	6.78047100	-2.50625000	-0.57929100
C	6.79716600	-0.25618900	-1.66830900
H	6.67224300	0.59560700	0.98347600
H	6.60444100	-1.00426000	1.73364500
H	8.02749400	-0.52170300	0.79286200
H	6.38359000	-2.97927200	-1.48310100
H	7.87278700	-2.52787900	-0.64707400
H	6.49118100	-3.11781600	0.28118100
H	7.88865500	-0.31464900	-1.74431400
H	6.37036400	-0.66011500	-2.59199100
H	6.52550900	0.80220600	-1.61022300
C	-3.02603100	-4.78199100	0.71246700
C	-4.09720700	-4.84469700	-0.40208200
C	-2.31230500	-6.14493400	0.77727800
C	-3.71611100	-4.52791600	2.07323100
H	-4.66264900	-3.91113100	-0.47777500
H	-3.63655000	-5.03582900	-1.37667700
H	-4.81000800	-5.65178100	-0.19901900
H	-1.54944600	-6.16799500	1.56210500
H	-3.04029500	-6.93184400	0.99892700
H	-1.83080300	-6.39870900	-0.17243100
H	-4.42551000	-5.33275000	2.29575100
H	-2.98155400	-4.48940800	2.88422800
H	-4.27107900	-3.58499400	2.07910200
C	1.13593100	5.28148400	0.70841000
C	2.61375100	5.71361300	0.75087700
C	0.43347700	6.07387300	-0.41950900
C	0.48896000	5.64067500	2.06682500

H	3.16521700	5.20338800	1.54762600
H	3.12349200	5.51945900	-0.19870700
H	2.67777000	6.78922500	0.94317700
H	-0.63330800	5.83996500	-0.47758500
H	0.53058800	7.15138300	-0.24517200
H	0.87847600	5.84602800	-1.39360500
H	0.58593300	6.71443500	2.26275900
H	-0.57611500	5.39296700	2.08773300
H	0.97370900	5.10075000	2.88680100
C	-1.98813000	1.44203800	-0.03920300
C	-2.46833400	0.07763800	-0.17095700
C	-4.13680700	2.23389400	-0.43510300
C	-5.04644500	3.31553200	-0.54749500
C	-4.59037000	0.90585300	-0.65648600
C	-6.35835100	3.06661800	-0.88699500
H	-4.67814500	4.32043600	-0.36872400
C	-5.94225300	0.67506800	-1.01530000
C	-6.80705600	1.74197900	-1.12638300
H	-7.06008700	3.89021100	-0.97824400
H	-6.26289600	-0.34722800	-1.18723900
H	-7.84482900	1.57282700	-1.39728200
N	-2.83334800	2.45545400	-0.14954700
N	-3.73299800	-0.13094500	-0.50663100

14 opt B3LYP/6-31G(d,p) HF = -1901.704441 Hartree imaginary frequency 0

C	-4.68073300	-1.18816600	-0.32924800
C	-3.31016100	-0.99798000	-0.18726800
C	-2.80050200	0.30849900	-0.25100700
C	-3.61839600	1.42073600	-0.38415100
C	-4.99780100	1.20110900	-0.53007500
C	-5.54751700	-0.08734900	-0.51926700
C	-1.52335800	2.71947900	-0.00374600
C	-0.73886000	1.53063100	0.03235500
C	0.66726800	1.64538500	0.19483900
C	1.17890700	2.92436000	0.46853500

C	0.42004100	4.09897600	0.51011500
C	-0.93249500	3.96743900	0.22757000
H	-5.08746000	-2.19389100	-0.28482900
H	-5.61906000	2.08152500	-0.63543500
H	2.24821000	2.97901400	0.61952800
H	-1.60349400	4.81651200	0.18632400
C	-2.99241800	2.74128400	-0.28142300
O	-3.62380900	3.79304200	-0.38191000
C	-1.01324400	-1.02154900	0.10386700
C	-2.16548300	-1.85254900	0.06679900
C	0.25672600	-1.57975900	0.30167200
C	-2.07436800	-3.22499500	0.28481000
C	0.29256400	-2.96700200	0.54071500
C	-0.83046600	-3.80522600	0.55061600
H	-2.97826000	-3.82204200	0.25546500
H	1.27654100	-3.38811100	0.69659900
N	-1.42010700	0.31462300	-0.09916900
C	-7.05868900	-0.34154900	-0.68521200
C	-7.60637400	-1.04995500	0.57653700
C	-7.85072300	0.96438700	-0.88380700
C	-7.29554800	-1.24081500	-1.92180900
H	-7.11687000	-2.01286000	0.75134900
H	-7.45666600	-0.43237600	1.46796600
H	-8.68036300	-1.23926600	0.47068600
H	-7.52485500	1.50690100	-1.77691600
H	-8.91377500	0.73387400	-1.00626700
H	-7.75558400	1.63460000	-0.02365000
H	-8.36600700	-1.43512700	-2.05167800
H	-6.92490100	-0.75951100	-2.83256400
H	-6.79263600	-2.20802600	-1.82726700
C	1.09638500	5.44354900	0.82668700
C	2.17377800	5.74301700	-0.24244300
C	0.08572700	6.60534800	0.83659300
C	1.76381700	5.36626200	2.21986900

H	2.94102200	4.96387900	-0.27778500
H	1.72606600	5.81598700	-1.23883800
H	2.67239800	6.69388900	-0.02351100
H	-0.69714200	6.45745700	1.58739800
H	0.60197700	7.54065800	1.07532200
H	-0.39720500	6.73430200	-0.13724700
H	2.25743700	6.31505800	2.45782800
H	1.02189600	5.16505900	2.99951100
H	2.52057100	4.57745000	2.26622800
C	-0.65129100	-5.30945300	0.82978800
C	-1.99222900	-6.06707400	0.81069500
C	0.26906600	-5.92913500	-0.24836600
C	-0.00881400	-5.50066500	2.22387900
H	-2.68493900	-5.68957300	1.57025300
H	-2.48411400	-6.00253300	-0.16559500
H	-1.81946700	-7.12724900	1.02095400
H	1.25614800	-5.45834500	-0.25995500
H	0.41088600	-6.99905200	-0.05860500
H	-0.16618200	-5.81607800	-1.24665400
H	0.13180200	-6.56660200	2.43541400
H	0.96928200	-5.01580200	2.29050200
H	-0.64462500	-5.07959000	3.00956800
C	1.55186500	-0.86708400	0.16401600
C	1.71269700	0.58157300	0.01190900
C	3.84661300	-1.14529300	-0.10414900
C	4.96603600	-1.97993800	-0.13385300
C	3.99190000	0.25557500	-0.35829600
C	6.23529000	-1.45996700	-0.42786100
H	4.83272300	-3.03894100	0.06530600
C	5.24810200	0.78335000	-0.66380500
C	7.40050800	-2.28601900	-0.47014200
C	6.37889600	-0.04585500	-0.70562700
H	5.33286700	1.84813700	-0.85874000
C	8.62933200	-1.75692000	-0.76639500

H	7.29081900	-3.34676800	-0.26202700
C	7.67913200	0.46241600	-1.00996400
C	8.77048900	-0.36571500	-1.03977400
H	9.50567400	-2.39752600	-0.79469000
H	7.78434800	1.52361500	-1.21808200
H	9.75237900	0.03514300	-1.27281100
N	2.90203800	1.06955300	-0.27681700
N	2.60621500	-1.65536400	0.12986700

tert-butylated **1** opt B3LYP/6-31G(d,p) HF = -1557.972702 Hartree imaginary frequency 0

C	-0.25631400	3.70949600	-0.00000600
C	-0.63524500	2.36045300	-0.00000600
C	0.34664000	1.34793500	-0.00000200
C	1.70360500	1.74312600	0.00000100
C	2.03629700	3.09972900	-0.00000100
C	1.07738200	4.11924200	-0.00000400
C	2.35614700	-0.65628700	0.00000600
C	0.98572900	-1.00225700	0.00000300
C	0.65082300	-2.37219300	0.00000400
C	1.66035000	-3.34401900	0.00000700
C	3.01801800	-3.02255200	0.00001000
C	3.32948000	-1.65798000	0.00000900
H	-1.07346700	4.42061800	-0.00001000
H	3.09888700	3.31962400	0.00000200
H	1.31522700	-4.37084200	0.00000800
H	4.35734600	-1.31030600	0.00001100
C	2.79456400	0.75127100	0.00000900
O	3.98171300	1.07431500	-0.00000400
C	-1.36728500	-0.38111700	-0.00000400
C	-2.38749000	0.59682700	-0.00000800
C	-1.75257500	-1.73777900	-0.00000300
C	-3.72859400	0.20668200	-0.00000900
C	-3.11032800	-2.08409000	-0.00000600
C	-4.13182400	-1.13363600	-0.00000900
H	-4.45042400	1.01685700	-0.00001200

H	-3.31769800	-3.14732300	-0.00000500
N	-0.01134300	-0.01151700	-0.00000100
C	1.50929400	5.59487500	-0.00000400
C	0.30118500	6.54966600	-0.00001800
C	2.35767500	5.87785100	1.26231700
C	2.35770100	5.87784700	-1.26230800
H	-0.32658800	6.41441900	-0.88670100
H	-0.32660200	6.41442800	0.88665500
H	0.65273300	7.58606600	-0.00002100
H	3.25412900	5.25192100	1.29996800
H	2.68188300	6.92411100	1.27318900
H	1.78000100	5.69240000	2.17366900
H	2.68190800	6.92410700	-1.27317700
H	3.25415700	5.25191800	-1.29993900
H	1.78004600	5.69239200	-2.17367100
C	4.13728600	-4.07669400	0.00001500
C	5.01228600	-3.89141500	-1.26229900
C	5.01228200	-3.89140700	1.26233100
C	3.57855700	-5.51157200	0.00001900
H	4.42023200	-4.02385300	-2.17367100
H	5.46876600	-2.89788400	-1.30008200
H	5.82140100	-4.62973900	-1.27317400
H	4.42022400	-4.02383700	2.17370100
H	5.82139600	-4.62973300	1.27321400
H	5.46876300	-2.89787700	1.30010800
H	4.40627900	-6.22751600	0.00002300
H	2.96863500	-5.71259400	0.88667700
H	2.96863800	-5.71260000	-0.88664100
C	-5.62583900	-1.49700500	-0.00000900
C	-6.29492500	-0.90351300	-1.26231800
C	-5.84923200	-3.02052800	-0.00002700
C	-6.29491400	-0.90354300	1.26232000
H	-6.20048700	0.18575700	-1.30023600
H	-5.84583000	-1.31147800	-2.17366200

H	-7.36325800	-1.14528400	-1.27302800
H	-5.41833300	-3.49669900	0.88662900
H	-6.92263300	-3.23390800	-0.00003100
H	-5.41833000	-3.49667800	-0.88669400
H	-7.36324700	-1.14531000	1.27303400
H	-5.84581200	-1.31153300	2.17365100
H	-6.20047000	0.18572500	1.30026400
C	-0.75317100	-2.82092100	0.00000200
O	-1.06714300	-4.01090200	-0.00000300
C	-2.07312800	2.03740600	-0.00001400
O	-2.94640600	2.90432200	0.00000600

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