Supporting Information

for

6-Aryl- and 6,7-diaryl-1,3-dimethyl-1*H*-perimidin-2(3*H*)-ones: synthesis, conformational stability, crystal structure and optical properties

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Experimental details, copies of NMR, UV-vis and fluorescence spectra, calculations of experimental and theoretical barriers of *syn/anti* isomerization

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EXPERIMENTAL SECTION

General Information: ^{1}H and ^{13}C NMR spectra were recorded on 250 and 600 MHz spectrometers. Chemical shifts are reported in ppm relative to Me_4Si. The electronic absorption spectra of the studied compounds have been recorded on an Agilent 8453 spectrophotometer equipped with a temperature-controlled cell holder at 293 K. Fluorescence emission spectra have been collected using an Eclipse Varian spectrofluorimeter. Mass spectra were performed in electrospray ionization (ESI) modes (HR-ESI MS). Melting points were determined in glass capillaries and are uncorrected. Flash column chromatography was performed on Al_2O_3 and SiO_2. Starting 1,3-Dimethyl-1H-perimidin-2(3H)-one,[1] and 6-bromo-1,3-dimethyl-1*H*-perimidin-2(3*H*)-one **5**[2] were synthesized as it was described earlier.

Crystal Structure Determination: X-ray measurements were conducted with diffractometer SyperNova, Dual, Cu at home/near, AtlasS2'. Atomic coordinates, bond lengths, bond angles and thermal parameters have been deposited at the Cambridge Crystallographic Data Centre (CCDC): CCDC 2391756 (**3a**), CCDC 2391755 (**3c**), CCDC 2391757 (**3g**), CCDC 2391758 (**3h**). These data can be obtained free of charge from Cambridge Crystallographic Data Centre.

Synthesis of 6,7-dibromo-1,3-dimethyl-1*H*-perimidin-2(3*H*)-one (7). To a solution of 1,3-dimethyl-1*H*-perimidin-2(3H)-one (1.27 g, 6 mmol) in DMF (15 mL) a solution of NBS (2.14 g, 12 mmol) in DMF (12 ml) was added over 2.5 h at room temperature. The reaction mixture was stirred for 24 h. The resulting light-yellow precipitate was filtered off, washed with water and dried in air. Recrystallization from acetonitrile gave compound **3** (1.96 g, 88%) as a colorless solid with mp 195-196 ºC (lit. 202-203 ºC [2]).

Synthesis of 6-aryl-1,3-dimethyl-1*H*-perimidin-2(3*H*)-ones 6 (Table 1).

Method A. A mixture of 6-bromo-1,3-dimethyl-1*H*-perimidin-2(3*H*)-one **5** (175 mg, 0.6 mmol), 5% Pd/C (64 mg, 0.03 mmol), PPh_3 (31 mg, 0.12 mmol), phenylboronic acid (80 mg, 0.66 mmol) and 2M K_2CO_3 (3 mL) in toluene (4 mL) was stirred at 95 °C for 24 h under argon. The reaction mixture was then diluted with water (10 mL) and extracted with CH_2Cl_2 (3 × 10 mL). The extract was dried over Na_2SO_4 and evaporated to dryness. The residue was purified by flash column chromatography on Al_2O_3 (2×20 cm), using CH_2Cl_2 as an eluent. The fraction with R_f 0.8 gave compound **6a** (130 mg, 75%).

Compounds **6a-e** were synthesized similarly using the corresponding arylboronic acid.

Method B (general procedure). A mixture of 6-bromo-1,3-dimethyl-1*H*-perimidin-2(3*H*)-one **5** (175 mg, 0.6 mmol), $Pd(PPh_3)_4$ (35 mg, 0.03 mmol), arylboronic acid (0.66 mmol), 2M K_2CO_3 (3 mL) in toluene (4 mL) was refluxed for 24-48 h under argon. The reaction mixture was then diluted with water (10 mL) and extracted with CH_2Cl_2 (3 × 10 mL). The extract was dried over Na_2SO_4 and evaporated to dryness. In cases of compounds **6b-e**, the residue was purified by flash column chromatography on Al_2O_3 (2×20 cm), using CH_2Cl_2 as an eluent. The fraction with R_f 0.8 gave compound **6**. In cases of compounds **6f,i,j**, the chromatography was carried out on silica (2×20 cm), using CH_2Cl_2 as an eluent. The fraction with R_f 02-0.4 gave compound **6**. In cases of compounds **6g,h**, the flash column chromatography on silica (2×20 cm) with CH_2Cl_2 as an eluent allowed to separate starting compound **5** (R_f 0.4). Elution was then continued using a mixture of CH_2Cl_2-EtOAc (10:1, v:v) as the eluent. The fraction with R_f 0.1 (silica, CH_2Cl_2) gave product **6**. Compounds **6d-j** were further purified by boiling in ethanol to remove soluble impurities.

1,3-Dimethyl-6-phenyl-1H-perimidin-2(3H)-one (**6a**), colorless solid with mp 200–202 ºC (EtOH). ^{1}H NMR (600 MHz, $CDCl_3$): δ = 3.45 (s, 3 H), 3.47 (s, 3 H), 6.60 (d, J = 7.2 Hz, 1 H), 6.63 (d, J = 7.9 Hz, 1 H), 7.30-7.33 (m, 2 H), 7.35-7.40 (m, 2 H), 7.42-7.48 (m, 4 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$): δ = 30.7, 30.8, 103.8, 104.3, 114.9, 117.6, 127.1, 127.8, 128.4, 128.7, 129.8, 131.8, 132.4, 137.2, 138.0, 140.5, 150.9 ppm. HRMS (ESI): *m/z* calcd. for $C_{19}H_{16}N_2O$ [M]: 288.1257, found 289.1260; [M+H$^+$]: 289.1335, found 289.1320; [M+Na$^+$]: 311.1155, found 311.1155.

1,3-Dimethyl-6-(p-tolyl)-1H-perimidin-2(3H)-one (**6b**), colorless solid with mp 212–214 ºC (EtOH). ^{1}H NMR (250 MHz, $CDCl_3$): δ = 2.45 (s, 3 H), 3.48 (s, 3 H), 3.49 (s, 3 H), 6.57–6.70 (m, 2 H), 7.25–7.43 (m, 7 H) ppm. ^{13}C NMR (62.9 MHz, $CDCl_3$): δ = 21.3, 30.8, 30.9, 103.9, 104.3, 115.0, 117.7, 127.8, 128.6, 129.2, 129.7, 131.8, 132.5, 136.8, 137.1, 137.6, 137.9, 150.9 ppm. HRMS (ESI): *m/z* calcd. for $C_{20}H_{18}N_2NaO$ [M+Na$^+$]: 325.1311, found 325.1302.

1,3-Dimethyl-6-(m-tolyl)-1H-perimidin-2(3H)-one (**6c**), colorless solid with mp 194–195 ºC (EtOH). ^{1}H NMR (250 MHz, $CDCl_3$): δ = 2.41 (s, 3 H), 3.45 (s, 3 H), 3.46 (s, 3 H), 6.55–6.68 (m, 2 H), 7.15–7.40 (m, 7 H) ppm. ^{13}C NMR (62.9 MHz, $CDCl_3$): δ = 21.6, 30.8, 30.9, 103.9, 104.3, 115.0, 117.7, 126.9, 127.8, 127.9, 128.3, 128.6, 130.5, 132.0, 132.4, 137.1, 137.9, 138.1, 140.5, 150.9 ppm. HRMS (ESI): *m/z* calcd. for $C_{20}H_{18}N_2NaO$ [M+Na$^+$]: 325.1311, found 325.1307.

6-(4-Methoxyphenyl)-1,3-dimethyl-1H-perimidin-2(3H)-one (**6d**), colorless solid with mp 211–213 ºC. ^{1}H NMR (250 MHz, $CDCl_3$): δ = 3.45 (s, 3 H), 3.46 (s, 3 H), 3.86 (s, 3 H), 6.57–6.65 (m, 2 H), 6.99 (dm, J = 8.8 Hz, 2 H), 7.27–7.40 (m, 5 H) ppm. ^{13}C NMR (62.9 MHz, $CDCl_3$): δ = 30.7, 30.8, 55.4, 103.9, 104.3, 113.9, 115.0, 117.7, 127.7, 128.6, 130.9, 131.5, 132.6, 132.9, 137.0, 138.0, 150.9, 158.8 ppm. HRMS (ESI): *m/z* calcd. for $C_{20}H_{18}N_2NaO_2$ [M+Na$^+$]: 341.1260, found 341.1252.

1,3-Dimethyl-6-(naphthalen-1-yl)-1H-perimidin-2(3H)-one (**6e**), colorless solid with mp 239–240 ºC. ^{1}H NMR (250 MHz, $CDCl_3$): δ = 3.51 (s, 3 H), 3.54 (s, 3 H), 6.62 (d, J = 7.6 Hz, 1 H), 6.73 (d, J = 7.9 Hz, 1 H), 6.83 (d, J = 8.3 Hz, 1 H), 7.20 (t, J = 8.2 Hz, 1 H), 7.31 (ddd, J = 8.5, 7.9, 1.2 Hz, 1 H), 7.37–7.53 (m, 4 H), 7.58 (m, 1 H), 7.94 (d, J = 7.9 Hz, 2 H) ppm. ^{13}C NMR (62.9 MHz, $CDCl_3$): δ = 30.8, 30.9, 103.8, 104.3, 114.7, 118.3, 125.6, 125.9, 126.0, 126.4, 127.8, 127.9(2C), 128.3, 129.6, 129.9, 132.8, 133.6, 133.7, 137.5, 137.9, 138.2, 151.0 ppm. HRMS (ESI): *m/z* calcd. for $C_{23}H_{19}N_2O$ [M+H$^+$]: 339.1492, found 339.1494.

1,3-Dimethyl-6-(naphthalen-2-yl)-1H-perimidin-2(3H)-one (**6f**), colorless solid with mp 273-274 ºC. ^{1}H NMR (600 MHz, $CDCl_3$): δ = 3.48 (s, 3 H), 3.50 (s, 3 H), 6.63 (d, J = 7.6 Hz, 1 H), 6.68 (d, J = 7.9 Hz, 1 H), 7.32 (dd, J = 8.5, 7.6 Hz, 1 H), 7.39 (dd, J = 8.6, 0.8 Hz, 1 H), 7.42 (d, J = 7.8 Hz, 1 H), 7.48–7.52 (m, 2 H), 7.57 (dd, J = 8.3, 1.7 Hz, 1 H), 7.83-7.92 (m, 4 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$): δ = 30.7, 30.8, 103.9, 104.3, 115.1, 117.7, 125.9, 126.2, 127.7, 127.8, 127.9, 128.0, 128.3, 128.4, 129.0, 131.8, 132.6, 132.7, 133.7, 137.5, 138.1, 138.2, 150.9 ppm. HRMS (ESI): *m/z* calcd. for $C_{23}H_{19}N_2O$ [M+H$^+$]: 339.1492, found 339.1494.

1,3-Dimethyl-6-(pyridin-3-yl)-1H-perimidin-2(3H)-one (**6g**), beige solid with mp 233–234 ºC. ^{1}H NMR (250 MHz, $CDCl_3$): δ = 3.46 (s, 3 H), 3.47 (s, 3 H), 6.61–6.68 (m, 2 H), 7.26–7.47 (m, 4 H), 7.78 (br d, J = 7.8 Hz, 1 H), 8.40–9.00 (m, 2 H) ppm. ^{13}C NMR (62.9 MHz, $CDCl_3$): δ = 30.8, 30.9, 103.9, 104.7, 115.0, 116.8, 127.7, 128.4, 129.3, 132.3, 137.2, 138.0, 138.1, 148.2, 150.4, 150.8 ppm. HRMS (ESI): *m/z* calcd. for $C_{18}H_{16}N_3O$ [M+H$^+$]: 290.1288, found 290.1283.

1,3-Dimethyl-6-(quinolin-3-yl)-1H-perimidin-2(3H)-one (**6h**), pale yellow solid with mp 323-325 ºC. ^{1}H NMR (250 MHz, $CDCl_3$): δ = 3.49 (s, 3 H), 3.51 (s, 3 H), 6.67 (dd, J = 6.9, 1.7 Hz, 1 H), 6.71 (d, J = 8.0 Гц, 1 H), 7.30-7.38 (m, 2 H), 7.42 (d, J = 7.9 Hz, 1 H), 7.60 (ddd, J = 8.1, 6.9, 1.2 Hz, 1 H), 7.75 (ddd, J = 8.4, 6.9, 1.5 Hz, 1 H), 7.87 (dd, J = 8.1, 1.3 Hz, 1 H), 8.18 (d, J = 8.8 Hz, 1 H), 8.23 (d, J = 2.2 Hz, 1 H), 9.01 (d, J = 2.2 Hz, 1 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$): δ = 30.8, 30.9, 104.0, 104.7, 115.0, 116.9, 126.9, 127.8, 128.0, 128.4, 129.3, 129.4, 129.7, 132.6, 133.5, 135.8, 138.1, 138.2, 147.3, 150.8, 152.0 ppm. HRMS (ESI): *m/z* calcd. for $C_{22}H_{18}N_3O$ [M+H$^+$]: 340.1444, found 340.1449.

6-(Anthracen-9-yl)-1,3-dimethyl-1H-perimidin-2(3H)-one (**6i**), pale yellow solid with mp 332-334 ºC (decomp.). ^{1}H NMR (250 MHz, $CDCl_3$): δ = 3.53 (s, 3 H), 3.60 (s, 3 H), 6.49 (d, J = 8.3 Hz, 1 H), 6.61 (d, J = 7.6 Hz, 1 H), 6.83 (d, J = 7.8 Hz, 1 H), 7.12 (t, J = 8.1 Hz, 1 H), 7.21-7.32 (m, 2 H), 7.40-7.53 (m, 5 H), 8.10 (d, J = 8.4 Hz, 2 H), 8.57 (s, 1 H) ppm. ^{13}C NMR (62.9 MHz, $CDCl_3$): δ = 30.9 (2C), 104.0, 104.4, 114.9, 118.3, 125.2, 125.6, 126.7, 126.9, 127.6, 128.1, 128.5, 130.9, 131.0, 131.6, 134.2, 134.7, 137.8, 138.0, 151.1 ppm. HRMS (ESI): *m/z* calcd. for $C_{27}H_{21}N_2O$ [M+H$^+$]: 389.1648, found 389.1649.

1,3-Dimethyl-6-(pyren-1-yl)-1H-perimidin-2(3H)-one (**6j**), beige solid with mp 331-332 ºC (decomp.). ^{1}H NMR (250 MHz, $CDCl_3$): δ = 3.51 (s, 3 H), 3.57 (s, 3 H), 6.62 (d, J = 7.6 Hz, 1 H), 6.77-6.84 (m, 2 H), 7.19 (t, J = 8.3 Hz, 1 H), 7.51 (d, J = 7.8 Hz, 1 H), 7.68 (d, J = 9.2 Hz, 1 H), 7.89 (d, J = 9.2 Hz, 1 H), 7.93-8.05 (m, 2 H), 8.08-8.15 (m, 3 H), 8.20 (d, J = 8.5 Hz, 1 H), 8.26 (d, J = 7.8 Hz, 1 H) ppm. ^{13}C NMR (62.9 MHz, $CDCl_3$): δ = 30.9 (2C), 103.9, 104.4, 118.4, 124.78, 124.86, 124.91, 125.0, 125.2, 125.6, 126.1, 127.4, 127.5, 128.0, 128.5, 129.8, 129.9, 130.1, 130.2, 130.9, 131.0, 131.4, 133.7, 135.6, 137.6, 138.0, 165.5 ppm. HRMS (ESI): *m/z* calcd. for $C_{29}H_{21}N_2O$ [M+H$^+$]: 413.1648, found 413.1650.

Synthesis of 7-aryl-6-brom-1,3-dimethyl-1*H*-perimidin-2(3*H*)-ones 8 (general procedure, Table 2). A mixture of 6,7-dibromo-1,3-dimethyl-1*H*-perimidin-2(3*H*)-one **7** (185 mg, 0.5 mmol), $Pd(PPh_3)_4$ (29 mg, 0.025 mmol), arylboronic acid (0.75–1.00 mmol), 2M K_2CO_3 (3 mL) in toluene (5 mL) was refluxed for 24-48 h under argon. The reaction mixture was then diluted with water (10 mL) and extracted with CH_2Cl_2 (3 × 10 mL). The extract was dried over Na_2SO_4 and evaporated to dryness.

In cases of compounds **8a,d** syntheses, the residue was purified by flash column chromatography on Al_2O_3 (2×20 cm), using CH_2Cl_2–hexane (1:1, v/v) as an eluent. The fraction with R_f 0.6-0.7 gave compound **8** with a small admixture of compounds **7** and **3**. Purification of compounds **8b,c,e** was carried out by column chromatography on silica (2×20 cm), using CH_2Cl_2 as an eluent. The fraction with R_f 0.2-0.4 (for **8b,c**) or 0.1 (**8e**) gave the corresponding compound **5** with a small admixture of compounds **7** and **3**. Compounds **8** were more soluble in most organic solvents. The crude product **8** was heated with 2 mL of acetonitrile (heptane or EtOH) and insoluble impurities **7** and **3** were filtered off.

From subsequent fractions with a lower R_f, the starting dibromide **7** and then the corresponding diaryl derivative **3** were isolated.

6-Bromo-1,3-dimethyl-7-phenyl-1H-perimidin-2(3H)-one (**8a**), colorless solid with mp 153-155 ºC. ^{1}H NMR (250 MHz, $CDCl_3$): δ = 3.44 (s, 3 H), 3.47 (s, 3 H), 6.47 (d, J = 8.4 Hz, 1 H), 6.69 (d, J = 8.1 Hz, 1 H), 7.20–7.45 (m, 6 H), 7.65 (d, J = 8.3 Hz, 1 H) ppm. ^{13}C NMR (62.9 MHz, $CDCl_3$): δ = 31.17, 31.20, 104.7, 105.5, 110.3, 116.7, 126.8, 127.4, 129.8, 130.3, 132.1, 132.9, 135.1, 137.5, 137.9, 142.5, 150.3 ppm. HRMS (ESI): *m/z* calcd. for $C_{19}H_{15}BrN_2O$ [M]: 366.0362 (^{79}Br), 368.0344 (^{81}Br), found 366.0369 (^{79}Br), 368.0358 (^{81}Br).

6-Bromo-1,3-dimethyl-7-(m-tolyl)-1H-perimidin-2(3H)-one (**8b**), colorless solid with mp 157-159 °C. ^{1}H NMR (250 MHz, $CDCl_3$): δ = 2.39 (s, 3 H), 3.48 (s, 3 H), 3.50 (s, 3 H), 6.50 (d, J = 8.3 Hz, 1 H), 6.65–6.80 (m, 2 H), 7.05–7.45 (m, 5 H), 7.68 (d, J = 8.3 Hz, 1 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$): δ = 21.4, 31.1, 104.6, 105.3, 110.4, 116.7, 127.2, 127.37, 127.41, 129.8, 131.1, 132.2, 132.8, 135.0, 136.8, 137.4, 137.9, 142.3, 150.3 ppm. HRMS (ESI): *m/z* calcd. for $C_{20}H_{17}BrN_2NaO$ [M+Na$^+$]: 403.0416 (^{79}Br), 405.0401 (^{81}Br), found 403.0404 (^{79}Br), 405.0385 (^{81}Br).

6-Bromo-7-(4-metoxyphenyl)-1,3-dimethyl-1H-perimidin-2(3H)-one (**8c**), colorless solid with mp 188-190 °C. ^{1}H NMR (250 MHz, $CDCl_3$): δ = 3.47 (s, 3 H), 3.50 (s, 3 H), 3.88 (s, 3 H), 6.49 (d, J = 8.4 Hz, 1 H), 6.70 (d, J = 8.1 Hz, 1 H), 6.92 (dm, J = 8.7 Hz, 2 H), 7.19 (dm, J = 8.7 Hz, 2 H), 7.37 (d, J = 8.0 Hz, 1 H), 7.68 (d, J = 8.3 Hz, 1 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$): δ = 31.1, 55.3, 104.6, 105.3, 110.3, 112.8, 116.7, 130.0, 131.2, 131.7, 132.9, 134.8, 135.0, 137.3, 137.9, 150.2, 158.8 ppm. HRMS (ESI): *m/z* calcd. for $C_{20}H_{17}BrN_2NaO_2$ [M+Na$^+$]: 419.0366 (^{79}Br), 421.0351 (^{81}Br), found 419.0359 (^{79}Br), 421.0339 (^{81}Br).

6-Bromo-1,3-dimethyl-7-(naphthalen-1-yl)-1H-perimidin-2(3H)-one (**8d**), beige solid with mp 214-216 °C (decomp.). ^{1}H NMR (250 MHz, $CDCl_3$): δ = 3.48 (s, 3 H), 3.52 (s, 3 H), 6.49 (d, J = 8.4 Hz, 1 H), 6.76 (d, J = 8.1 Hz, 1 H), 7.27–7.32 (m, 2 H), 7.35 (dd, J = 7.0, 1.2 Hz, 1 H), 7.43–7.53 (m, 3 H), 7.59 (d, J = 8.4 Hz, 1H), 7.85–7.92 (m, 2 H) ppm. ^{13}C NMR (62.9 MHz, $CDCl_3$): δ = 31.2 (2C), 104.9, 105.6, 110.2, 116.6, 125.1, 125.5, 125.8, 126.4, 127.6, 128.1 (2C), 129.6, 130.8, 133.1, 133.4, 134.6, 135.1, 137.9, 138.0, 140.2, 150.4 ppm. HRMS (ESI): *m/z* calcd. for $C_{23}H_{17}BrN_2NaO$ [M+Na$^+$]: 439.0417 (^{79}Br), 441.0399 (^{81}Br), found 439.0418 (^{79}Br), 441.0411 (^{81}Br).

6-Bromo-1,3-dimethyl-7-(quinolin-3-yl)-1H-perimidin-2(3H)-one (**8e**), yellow-orange solid with mp 255-256 °C (decomp.). ^{1}H NMR (250 MHz, $CDCl_3$): δ = 3.50 (s, 3 H), 3.53 (s, 3 H), 6.57 (d, J = 8.4 Hz, 1 H), 6.77 (d, J = 8.1 Hz, 1 H), 7.44 (d, J = 8.1 Hz, 1 H), 7.62 (ddd, J = 8.1, 6.9, 1.2 Hz, 1 H), 7.68–7.80 (m, 2 H), 7.86 (dd, J = 8.1, 1.3 Hz, 1 H), 8.09 d, J = 2.2 Hz, 1 H), 8.20 (d, J = 8.5 Hz, 1 H), 8.88 (d, J = 2.2 Hz, 1 H) ppm. ^{13}C NMR (62.9 MHz, $CDCl_3$): δ = 31.26, 31.30, 104.8, 106.0, 109.9, 116.8, 127.1, 127.68, 127.75, 128.0, 128.9, 129.5, 130.0, 134.1, 135.3, 135.5, 136.0, 138.1, 138.5, 146.3, 150.2, 151.9 ppm. HRMS (ESI): *m/z* calcd. $C_{22}H_{17}BrN_3O$ [M+H$^+$]: 418.0550 (^{79}Br), 420.0535 (^{81}Br), found 418.0556 (^{79}Br), 420.0538 (^{81}Br).

Synthesis of 6,7-diaryl-1,3-dimethyl-1*H*-perimidin-2(3*H*)-ones 3a-d,f (general procedure, Table 2). A mixture of 6,7-dibromo-1,3-dimethyl-1*H*-perimidin-2(3*H*)-one **7** (185 mg, 0.5 mmol), $Pd(PPh_3)_4$ (29 mg, 0.025 mmol), arylboronic acid (1.5 mmol), 2M K_2CO_3 (3 mL) in toluene (5 mL) was refluxed for 48 h under argon. The reaction mixture was then diluted with water (10 mL) and extracted with CH_2Cl_2 (3 × 10 mL). The extract was dried over Na_2SO_4 and evaporated to dryness.

In the case of compound **3a** synthesis, the residue was purified by flash column chromatography on Al_2O_3 (2×20 cm), using CH_2Cl_2–hexane (1:1, v/v) as an eluent. The fraction with R_f 0.8 gave a mixture of compounds **8a** and **3a**. Purification of compounds **3b-d,f** was carried out by column chromatography on silica (2×20 cm), using CH_2Cl_2 as an eluent. The fraction with R_f 0.2-0.4 (for **3b**,**d,f**) or 0.1 (for **3c**) gave the corresponding compound **3** together with compound **8**. Compounds **8** were more soluble in most organic solvents. The crude product was heated with 2-4 mL of acetonitrile (or EtOH) and insoluble compound **3** was filtered off. The corresponding compound **8** was isolated from the filtrate.

1,3-Dimethyl-6,7-diphenyl-1H-perimidin-2(3H)-one (**3a**), colorless solid with mp 237–239 ºC. ^{1}H NMR (600 MHz, $CDCl_3$): δ = 3.52 (s, 6 H), 6.75 (d, J = 8.0 Hz, 2 H), 6.85-6.95 (m, 10 H), 7.34 (d, J = 8.0 Hz, 2 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$): δ = 31.0, 104.5, 116.3, 125.5, 127.2, 127.4, 129.5, 129.8, 130.3, 132.2, 132.7, 137.5, 142.6, 150.7 ppm. HRMS (ESI): *m/z* calcd. for $C_{25}H_{20}N_2NaO$ [M+Na$^+$]: 387.1468, found 387.1470.

1,3-Dimethyl-6,7-di(m-tolyl)-1H-perimidin-2(3H)-one (**3b**), colorless solid with mp 275-277 ºC. ^{1}H NMR (600 MHz, $CDCl_3$, +55 ºC): δ = 2.06 (s, 6 H), 3.52 (s, 6 H), 6.40–7.05 (m, 10 H), 7.33 (d, J = 8.0 Hz, 2 H) ppm. ^{1}H NMR (600 MHz, $CDCl_3$, -50 ºC): δ = 1.94 (s, 3.3 H), 2.14 (s, 3 H), 3.52 (s, 6.3 H), 6.36 (s, 1 H), 6.65–6.79 (m, 6.5 H), 6.82 (t, J = 7.5 Hz, 1.1 H), 7.07 (d, J = 5.1 Hz, 2.2 H), 7.37–7.41 (m, 2.1 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$): δ = 21.0, 31.0, 104.4, 116.3, 125.8, 126.2, 126.9, 127.2, 129.9, 130.4, 132.3, 132.4, 136.2, 137.4, 142.5, 150.7 ppm. HRMS (ESI): *m/z* calcd. for $C_{27}H_{24}N_2NaO$ [M+Na]: 415.1781, found 415.1776.

6,7-Di(4-methoxyphenyl)-1,3-dimethyl-1H-perimidin-2(3H)-one (**3c**), colorless needles with mp 276-278 ºC. ^{1}H NMR (250 MHz, $CDCl_3$): δ = 3.53 (s, 6 H), 3.71 (s, 6 H), 6.47 (dm, J = 8.7 Hz, 4 H), 6.74 (d, J = 8.1 Hz, 2 H), 6.79 (dm, J = 8.7 Hz, 4 H), 7.33 (d, J = 8.1 Hz, 2 H) ppm. ^{13}C NMR (62.9 MHz, $CDCl_3$): δ = 31.1, 55.3, 104.5, 112.8 (2C), 116.3, 130.2, 130.6 (2C), 131.8, 132.3, 135.3, 137.3, 150.7, 157.5 ppm. HRMS (ESI): *m/z* calcd. for $C_{27}H_{24}N_2NaO_3$ [M+Na$^+$]: 447.1679, found 447.1672.

1,3-Dimethyl-6-(naphthalen-1-yl)-1H-perimidin-2(3H)-one (**3d**), colorless solid with mp 244-246 ºC. ^{1}H NMR (600 MHz, $CDCl_3$): δ = 3.58 (s, 6 H), 6.30 (dd, J = 8.1, 7.1 Hz, 2 H), 6.40 (dd, J = 6.9, 0.9 Hz, 2 H), 6.77 (d, J = 7.9 Hz, 2 H), 7.04 (d, J = 8.2 Hz, 2 H), 7.19 (d, J = 7.8 Hz, 2 H), 7.20–7.27 (m, 4 H), 7.31 (ddd, J = 8.0, 6.5, 1.4 Hz, 2 H), 7.53 (d, J = 8.1 Hz, 2 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$): δ = 31.1, 104.4, 115.7, 123.4, 124.9, 125.2, 126.2, 126.4, 127.0, 127.8, 130.3, 132.4, 132.59, 132.65, 132.7, 137.8, 138.9, 150.8 ppm. HRMS (ESI): *m/z* calcd. for $C_{33}H_{25}N_2O$ [M+H$^+$]: 465.1961, found 465.1964.

1,3-Dimethyl-6,7-di(naphthalen-2-yl)-1H-perimidin-2(3H)-one (**3f**), colorless solid with mp 234-236 ºC. ^{1}H NMR (600 MHz, $CDCl_3$, +30 ºC): δ = 3.56 (s, 6 H), 6.80 (d, J = 8.0 Hz, 2 H), 6.90–7.22 (m, 8 H), 7.27–7.38 (m, 4 H), 7.46 (d, J = 8.0 Hz, 2 H), 7.49–7.59 (m, 2 H) ppm. ^{1}H NMR (600 MHz, $CDCl_3$, -45 ºC): δ = 3.56 and 3.57 (two s, 6 H), 6.73 (d, J = 8.4 Hz, 1 H), 6.80–6.87 (m, 3 H), 6.96 (dd, J = 8.4, 1.7 Hz, 1 H), 6.97–7.02 (m, 1 H), 7.05 (ddd, J = 8.0, 6.8, 1.1 Hz, 1 H), 7.15–7.22 (m, 3 H), 7.25–7.36 (m, 4 H), 7.45–7.55 (m, 3 H), 7.60 (d, J = 8.0 Hz, 1 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$): δ = 31.1, 104.5, 116.3, 124.9, 125.2, 125.9, 126.3, 126.9, 127.2, 127.5, 128.0, 131.2, 132.2, 132.5, 133.7, 150.7 ppm. HRMS (ESI): *m/z* calcd. for $C_{33}H_{24}N_2NaO$ [M+Na$^+$]: 487.1781, found 487.1776.

Synthesis of 6,7-diaryl-1,3-dimethyl-1*H*-perimidin-2(3*H*)-ones 3g,h (general procedure). A mixture of 6-bromo-1,3-dimethyl-7-(naphthalen-1-yl)-1*H*-perimidin-2(3*H*)-one **8d** (210 mg, 0.5 mmol), $Pd(PPh_3)_4$ (29 mg, 0.025 mmol), arylboronic acid (0.85 mmol), 2M K_2CO_3 (3 mL) in toluene (5 mL) was refluxed for 24 h under argon. The reaction mixture was then diluted with water (10 mL) and extracted with CH_2Cl_2 (3 × 10 mL). The extract was dried over Na_2SO_4 and evaporated to dryness. The residue was purified by flash column chromatography on silica (2×20 cm), using CH_2Cl_2 as an eluent. The fraction with R_f 0.2-0.3 gave the corresponding compound **3** with a small admixture of **8d**. The crude product was heated with 2 mL EtOH and less soluble compound **6** was filtered off.

1,3-Dimethyl-6-(naphthalen-1-yl)-7-phenyl-1H-perimidin-2(3H)-one (**3g**), colorless solid with mp 227-229 °C. ^{1}H NMR (250 MHz, $CDCl_3$): δ = 3.60 (s, 3 H), 3.61 (s, 3 H), 6.27 (t, J = 7.3 Hz, 1 H), 6.38 (d, J = 7.7 Hz, 1 H), 6.57–6.67 (m, 1 H), 6.70–6.82 (m, 3 H), 6.84 (d, J = 8.0 Hz, 1 H), 7.13–7.50 (m, 8 H), 7.63 (d, J = 8.2 Hz, 1 H) ppm. ^{13}C NMR (62.9 MHz, $CDCl_3$): δ = 31.1 (2C), 104.4, 104.5, 115.9, 124.9, 125.1, 125.2, 125.4, 126.0, 126.3, 126.9, 127.9, 127.9, 128.0, 129.5, 127.9, 131.3, 132.3, 132.4, 132.8, 133.0, 133.1, 137.5, 137.9, 140.7, 141.6, 150.5 ppm. HRMS (ESI): *m/z* calcd. for $C_{29}H_{22}N_2NaO$ [M+Na^+]: 437.1624, found 437.1624.

1,3-Dimethyl-6-(naphthalen-1-yl)-7-(m-tolyl)-1H-perimidin-2(3H)-one (**3h**), colorless solid with mp 250–252 °C (MeCN). ^{1}H NMR (600 MHz, $CDCl_3$, -50 °C): δ = 1.35 (s, 4.3 H), 1.99 (s, 3 H), 3.560, 3.561, 3.57 and 3.58 (four s, 14.2 H), 6.18–6.20 (m, 2.3 H), 6.25 (t, J = 7.7 Hz, 1 H), 6.38–6.42 (m, 1.9 H), 6.45 (d, J = 7.5 Hz, 1.5 H), 6.68 (d, J = 7.6 Hz, 1.4 H), 6.73 (t, J = 7.5 Hz, 2.4 H), 6.76–6.78 (m, 2.4 H), 6.82 (d, J = 8.1 Hz, 1.4 H), 6.84 (d, J = 8.1 Hz, 1 H), 6.93 (dd, J = 7.0, 1.2 Hz, 1.4 H), 7.07–7.11 (m, 2.6 H), 7.14 (ddd, J = 8.5, 7.9, 1.2 Hz, 1 H), 7.18 (d, J = 8.0 Hz, 1 H), 7.24 (d, J = 7.9 Hz, 1.7 H), 7.29–7.47 (m, 11 H), 7.57 (d, J = 8.2 Hz, 1 H), 7.62–7.64 (m, 1.4 H), 7.70–7.72 (m, 1.4 H) ppm. ^{13}C NMR (150 MHz, $CDCl_3$): δ = 20.3, 21.1, 31.1, 104.26, 104.31, 104.5, 115.8, 116.0, 123.4, 124.4, 125.0, 125.1, 125.2, 125.25, 125.3, 125.4, 126.15, 126.25, 126.3, 126.35, 126.7, 126.9, 127.65, 127.7, 128.0, 128.2, 129.6, 129.8, 130.1, 130.8, 131.3, 131.4, 132.1, 132.4, 132.44, 132.8, 133.0, 133.1, 133.2, 133.3, 134.8, 135.8, 137.4, 137.5, 137.8, 137.9, 140.3, 141.0, 144.9, 150.7 ppm. HRMS (ESI): *m/z* calcd. for $C_{30}H_{24}N_2NaO$ [M+Na^+]: 451.1781, found 451.1783.

Copies of NMR spectra

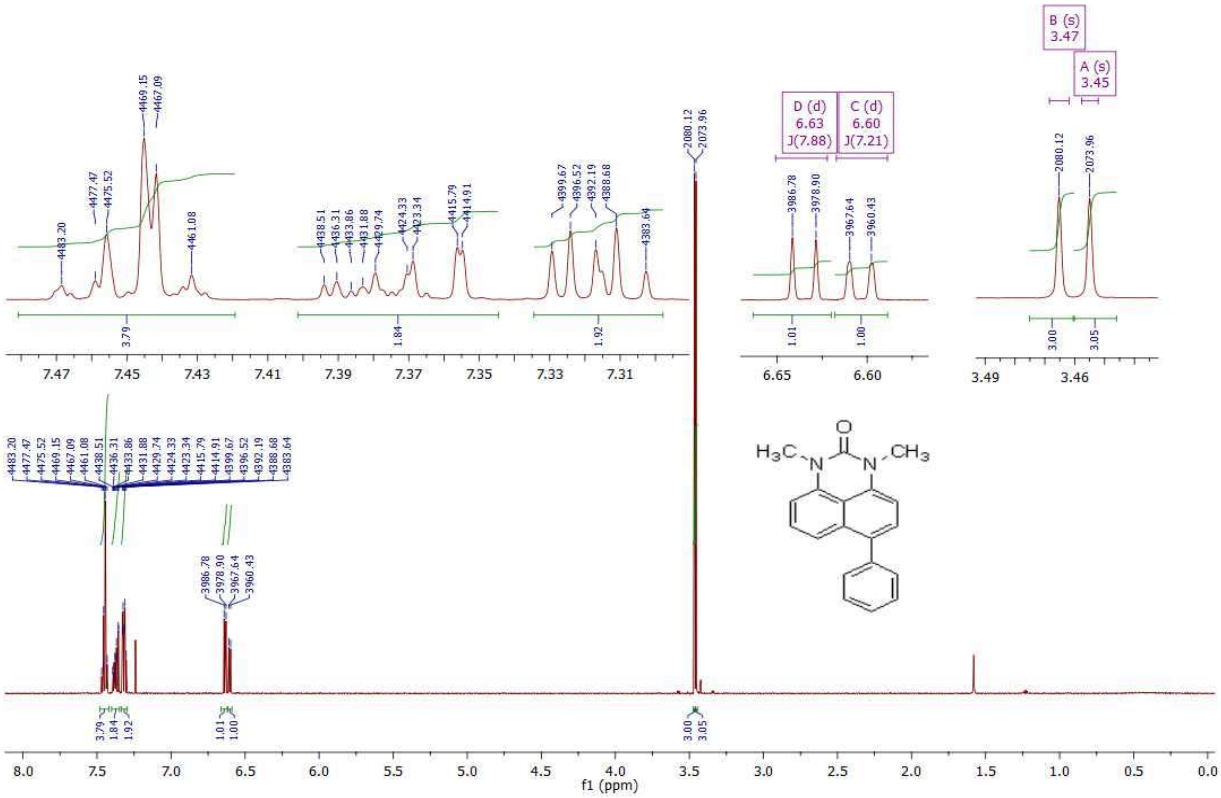


Fig. S1. ^{1}H NMR spectrum of compound **6a** (600 MHz, $CDCl_3$).

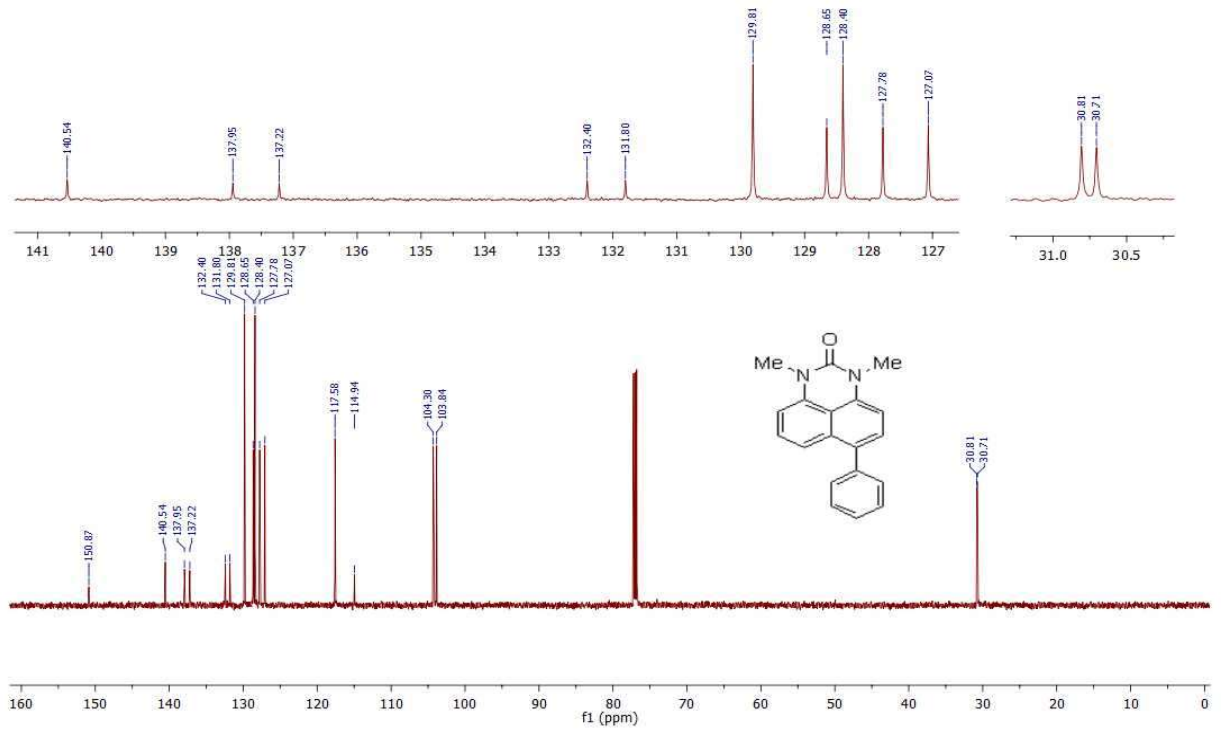


Fig. S2. $^{13}C\{^{1}H\}$ NMR spectrum of compound **6a** (150 MHz, $CDCl_3$).

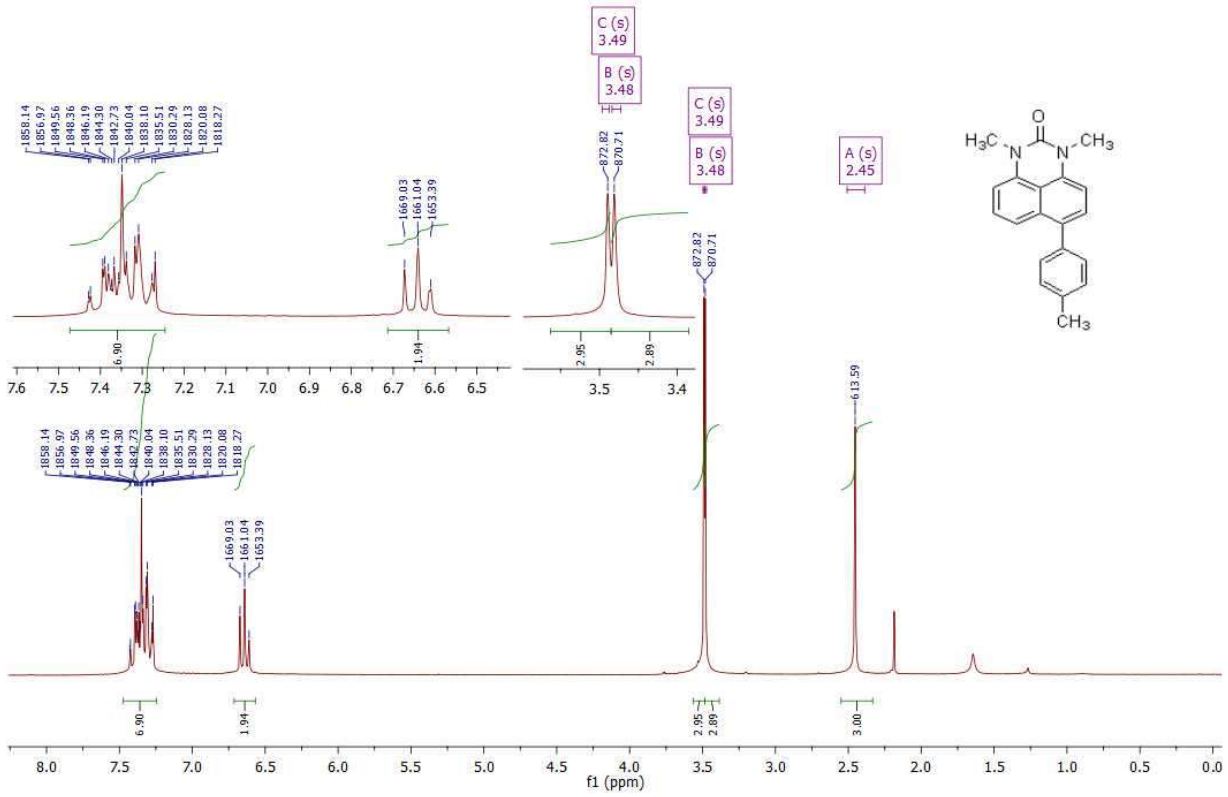


Fig. S3. ^{1}H NMR spectrum of compound **6b** (250 MHz, $CDCl_3$).

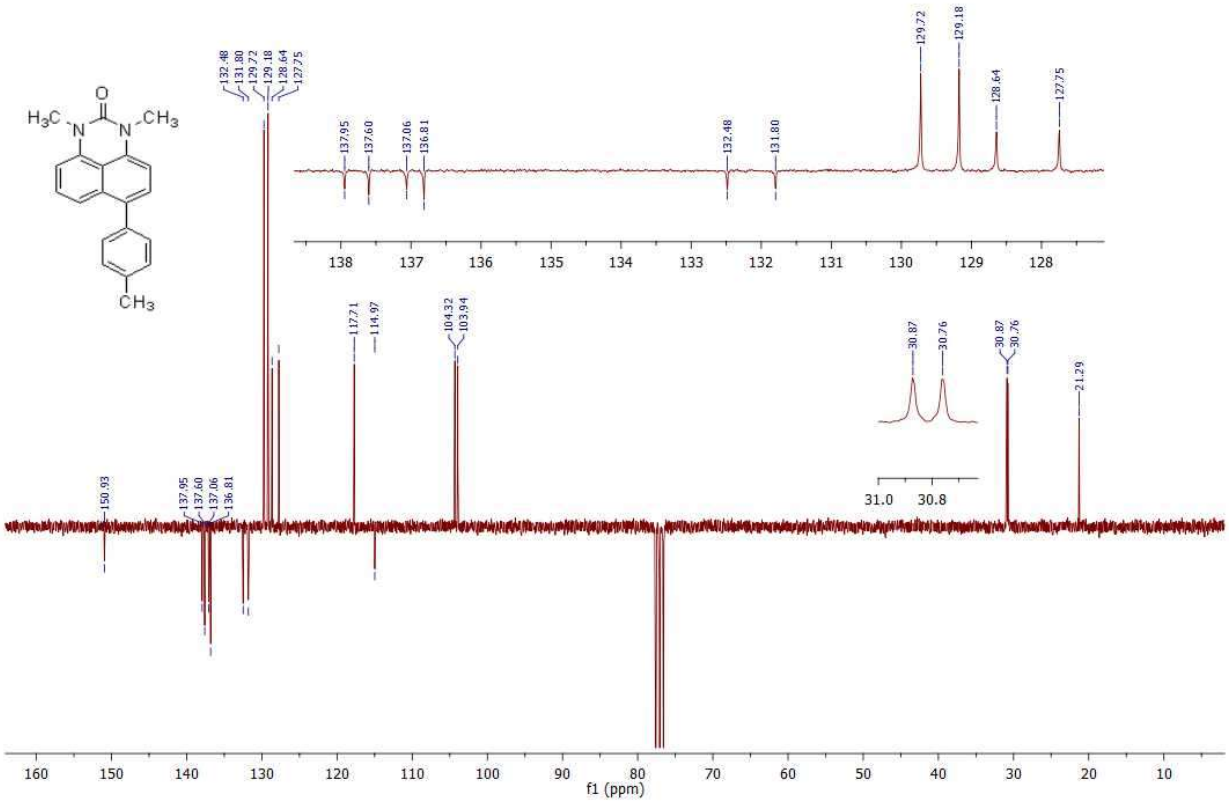


Fig. S4. $^{13}C\{^{1}H\}$ APT-NMR spectrum of **6b** (62.9 MHz, $CDCl_3$).

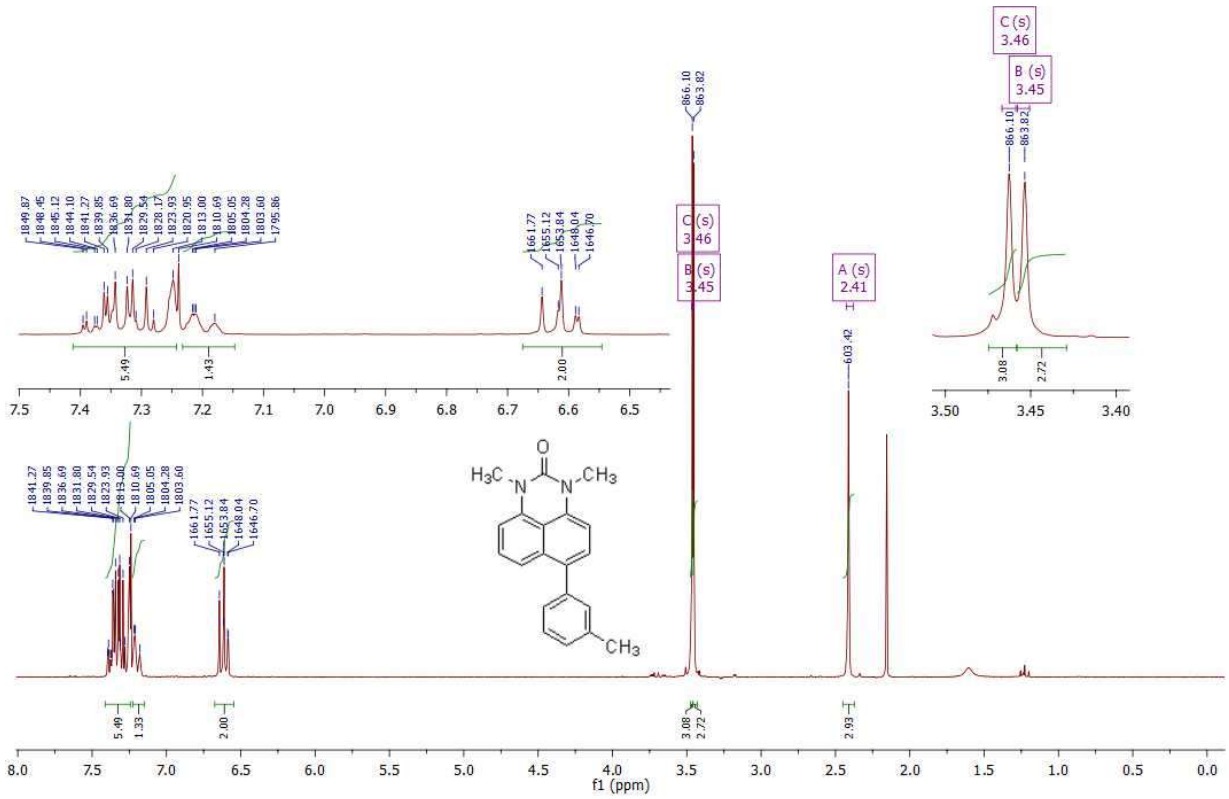


Fig. S5. ^{1}H NMR spectrum of compound **6c** (250 MHz, $CDCl_3$).

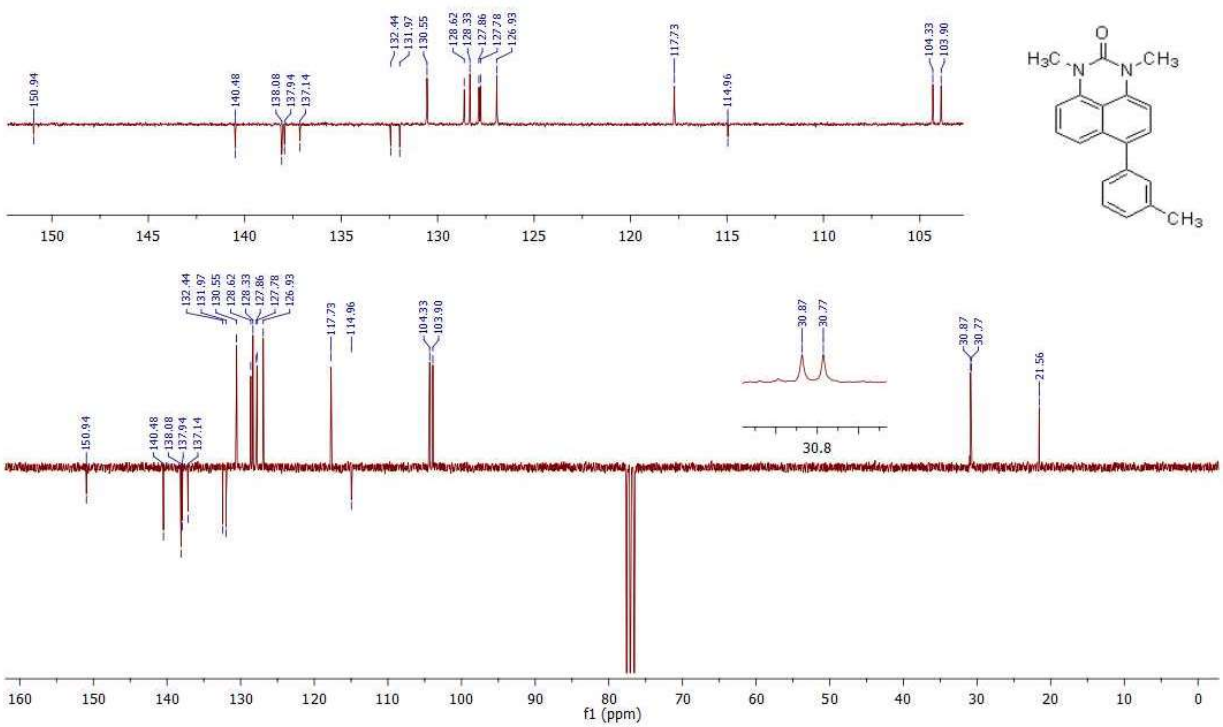


Fig. S6. $^{13}C\{^{1}H\}$ APT-NMR spectrum of compound **6c** (62.9 MHz, $CDCl_3$).

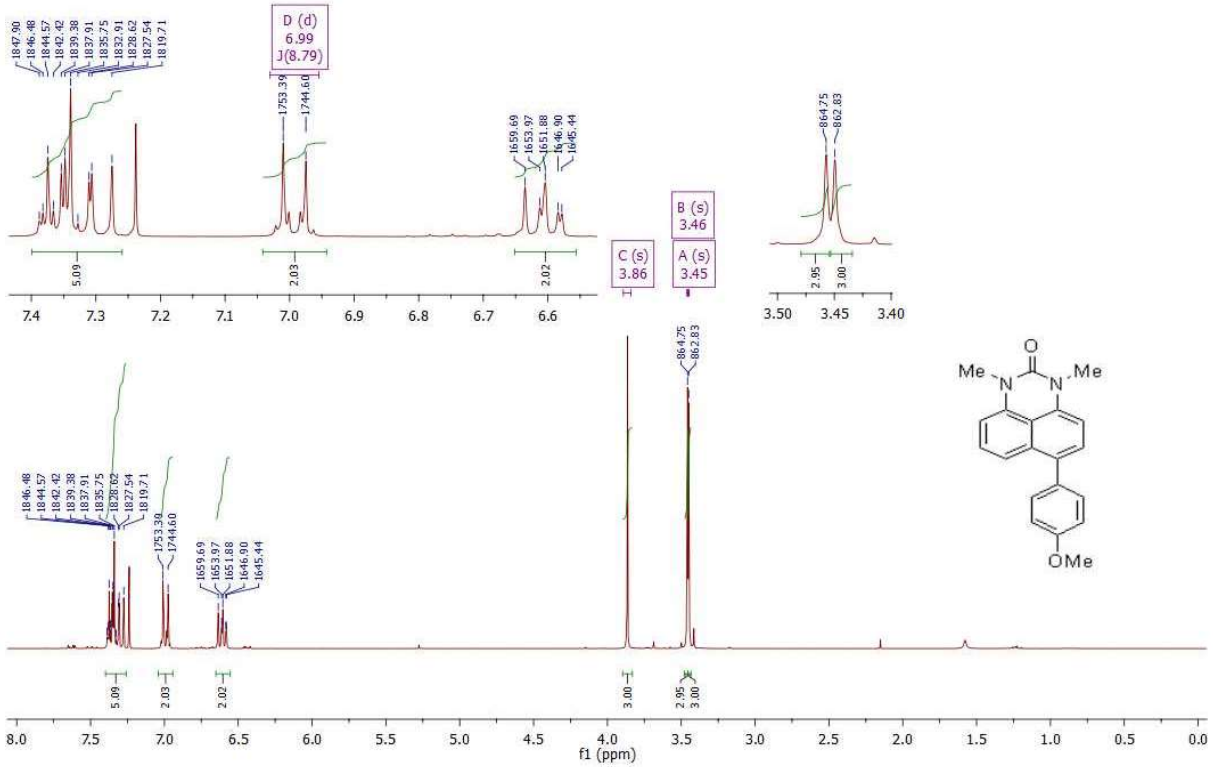


Fig. S7. ^{1}H NMR spectrum of compound **6d** (250 MHz, $CDCl_3$).

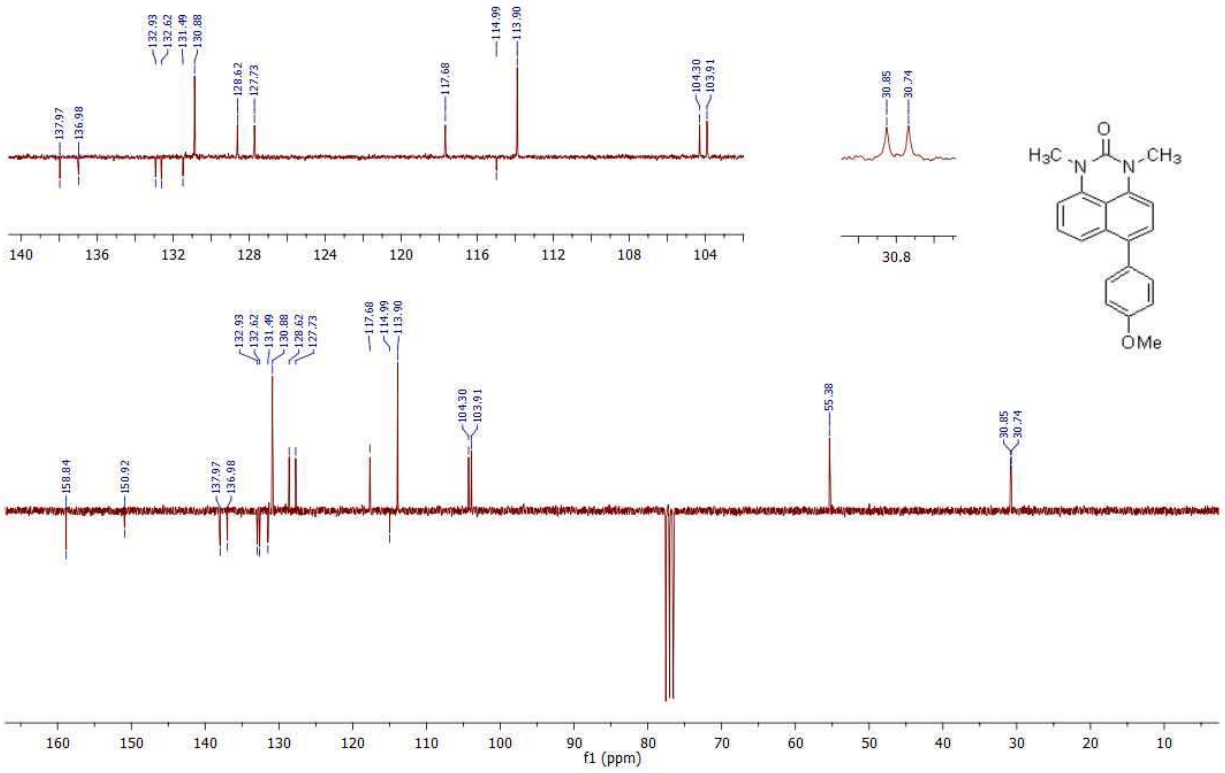


Fig. S8. $^{13}C\{^{1}H\}$ APT-NMR spectrum of compound **6d** (62.9 MHz, $CDCl_3$).

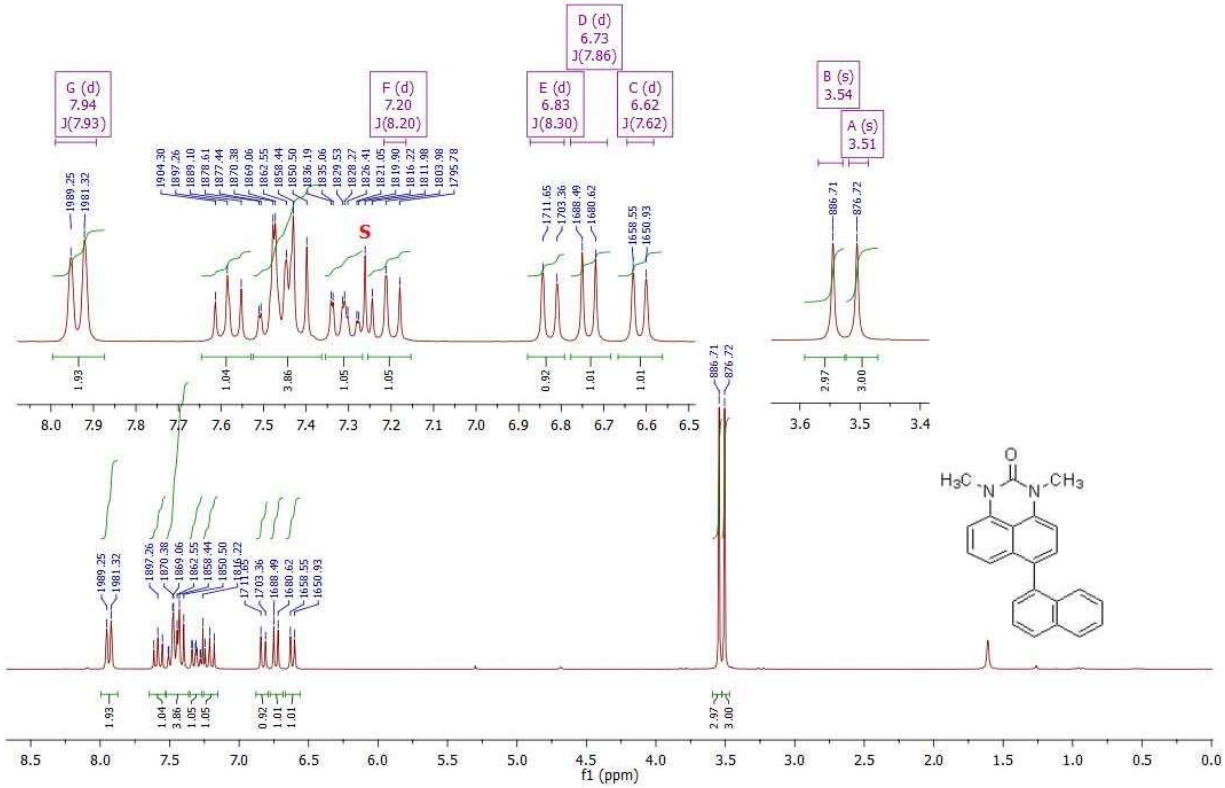


Fig. S9. ^{1}H NMR spectrum of compound **6e** (250 MHz, $CDCl_3$).

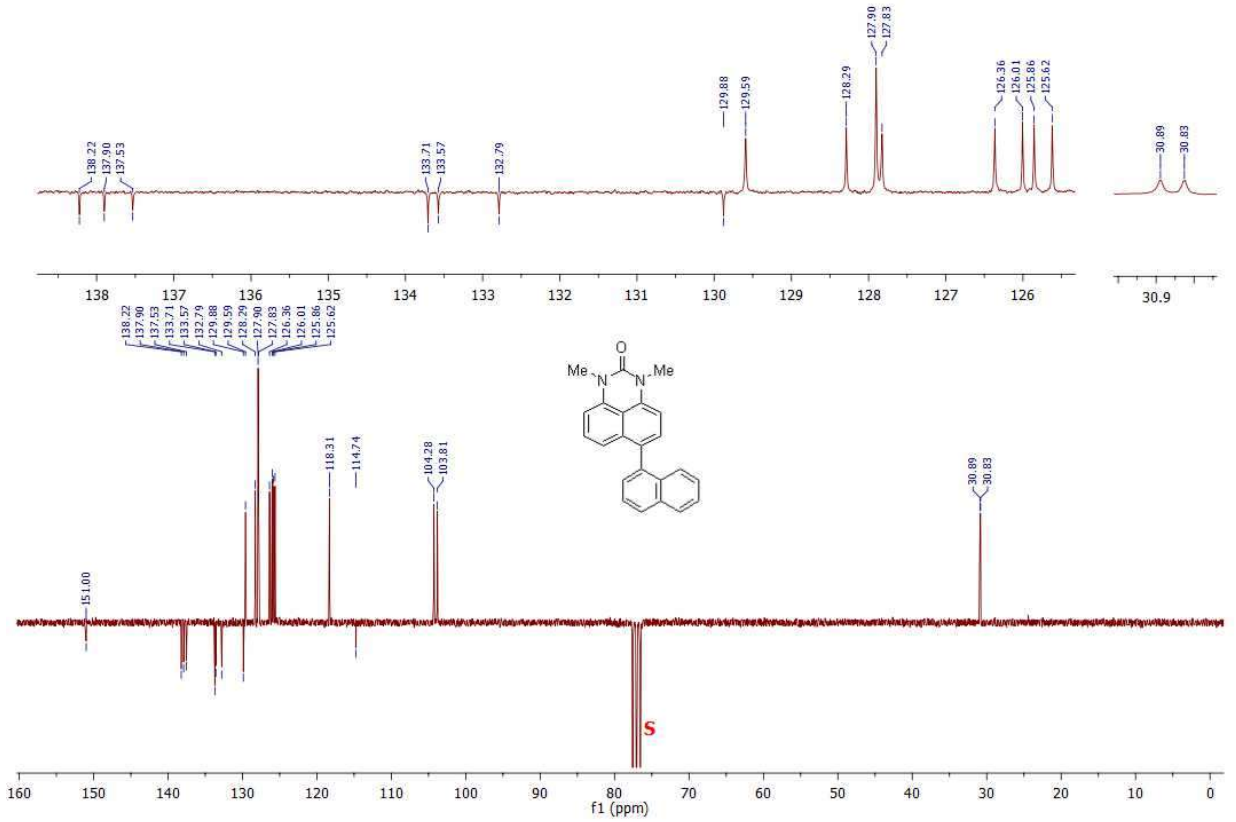


Fig. S10. $^{13}C\{^{1}H\}$ APT-NMR spectrum of compound **6e** (150 MHz, $CDCl_3$).

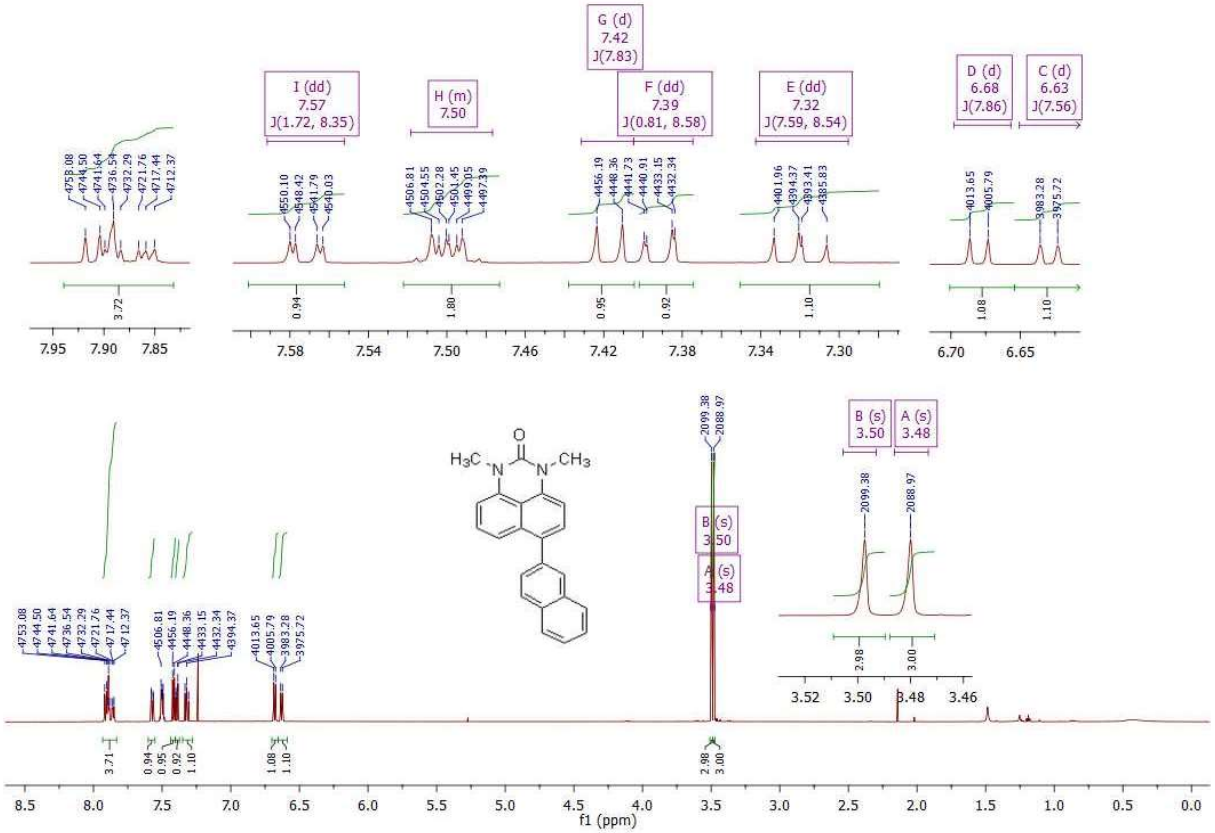


Fig. S11. ^{1}H NMR spectrum of compound **6f** (600 MHz, $CDCl_3$).

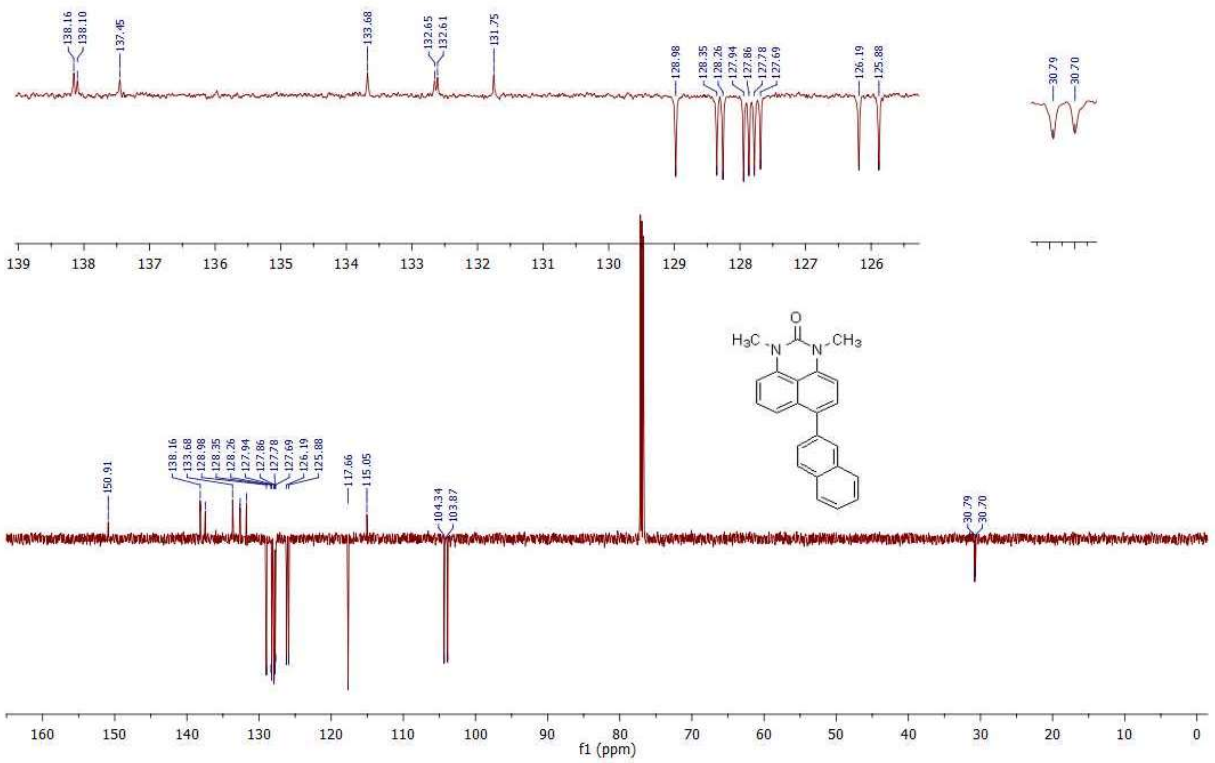


Fig. S12. $^{13}C\{^{1}H\}$ APT-NMR spectrum of compound **6f** (150 MHz, $CDCl_3$).

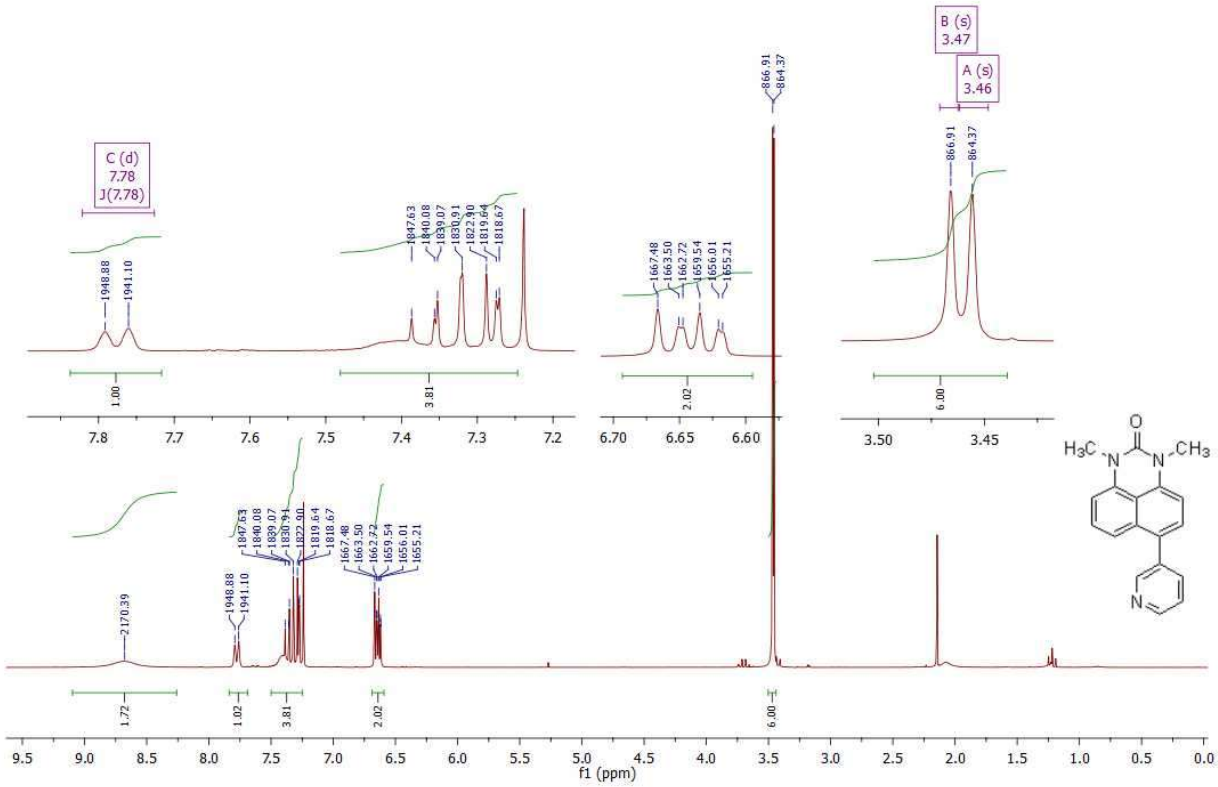


Fig. S13. ^{1}H NMR spectrum of compound **6g** (250 MHz, $CDCl_3$).

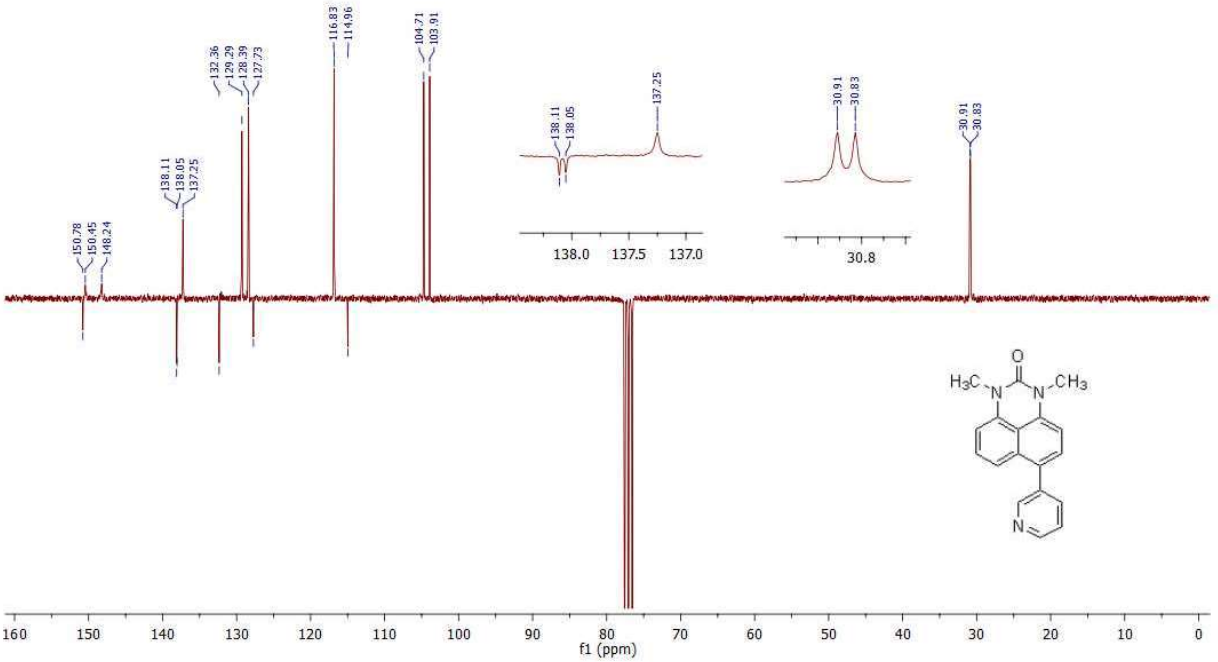


Fig. S14. $^{13}C\{^{1}H\}$ APT-NMR spectrum of compound **6g** (62.9 MHz, $CDCl_3$).

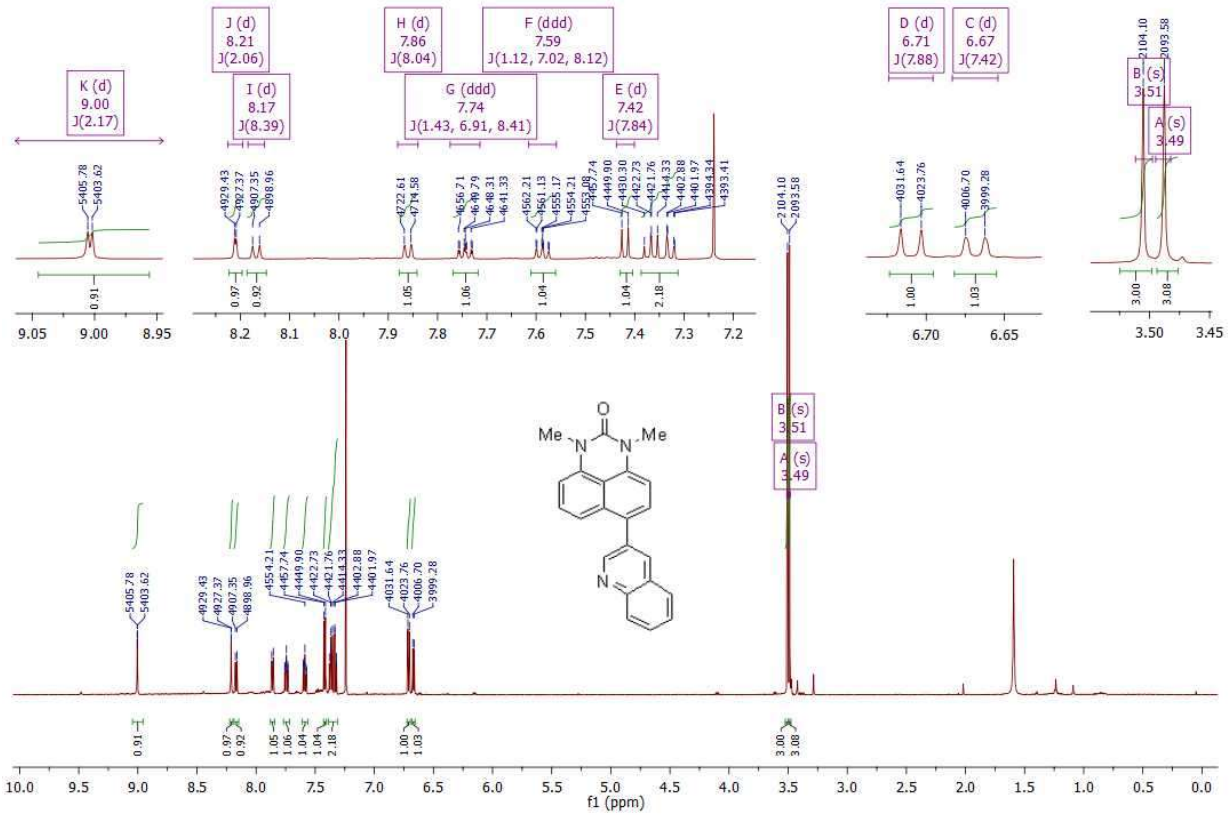


Fig. S15. ^{1}H NMR spectrum of compound **6h** (600 MHz, $CDCl_3$).

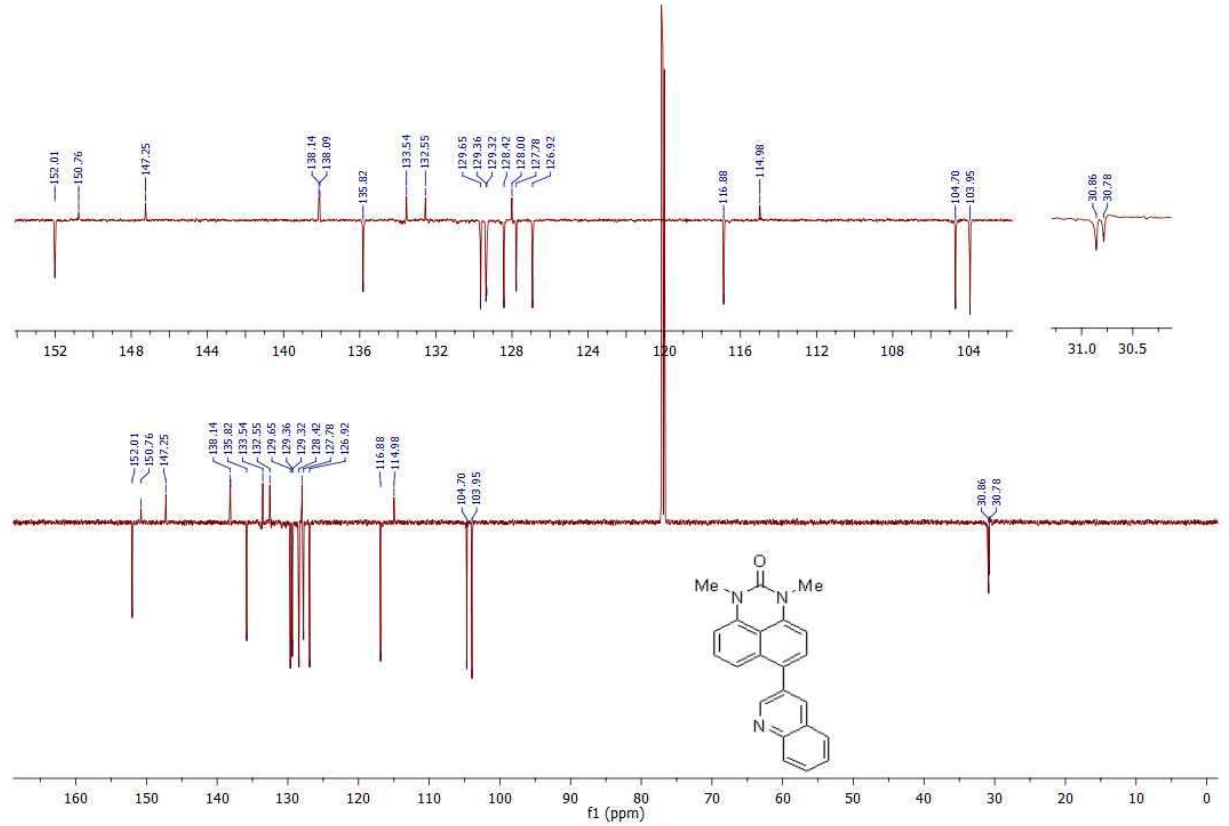


Fig. S16. $^{13}C\{^{1}H\}$ APT-NMR spectrum of compound **6h** (150 MHz, $CDCl_3$).

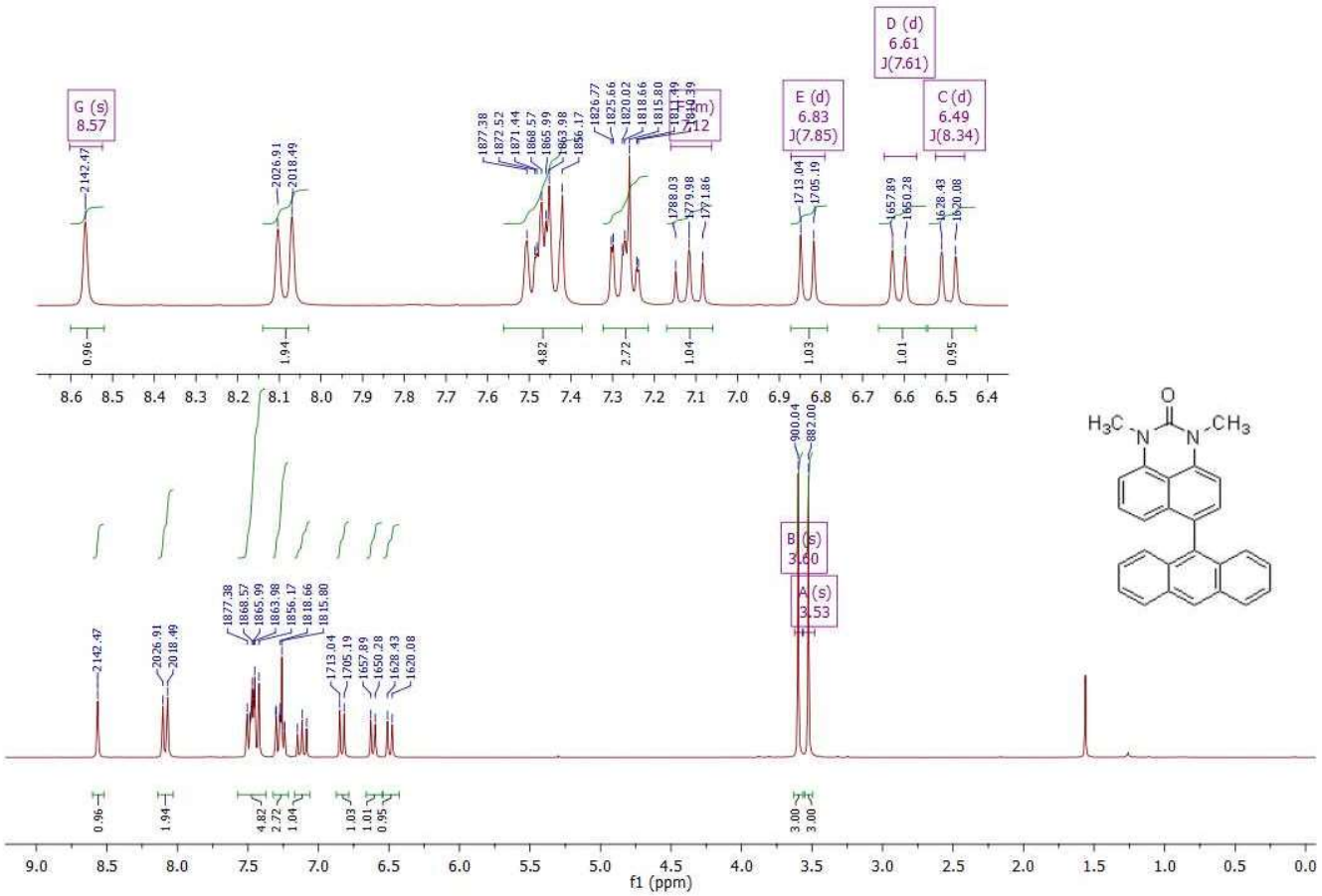


Fig. S17. ^{1}H NMR spectrum of compound **6i** (250 MHz, $CDCl_3$).

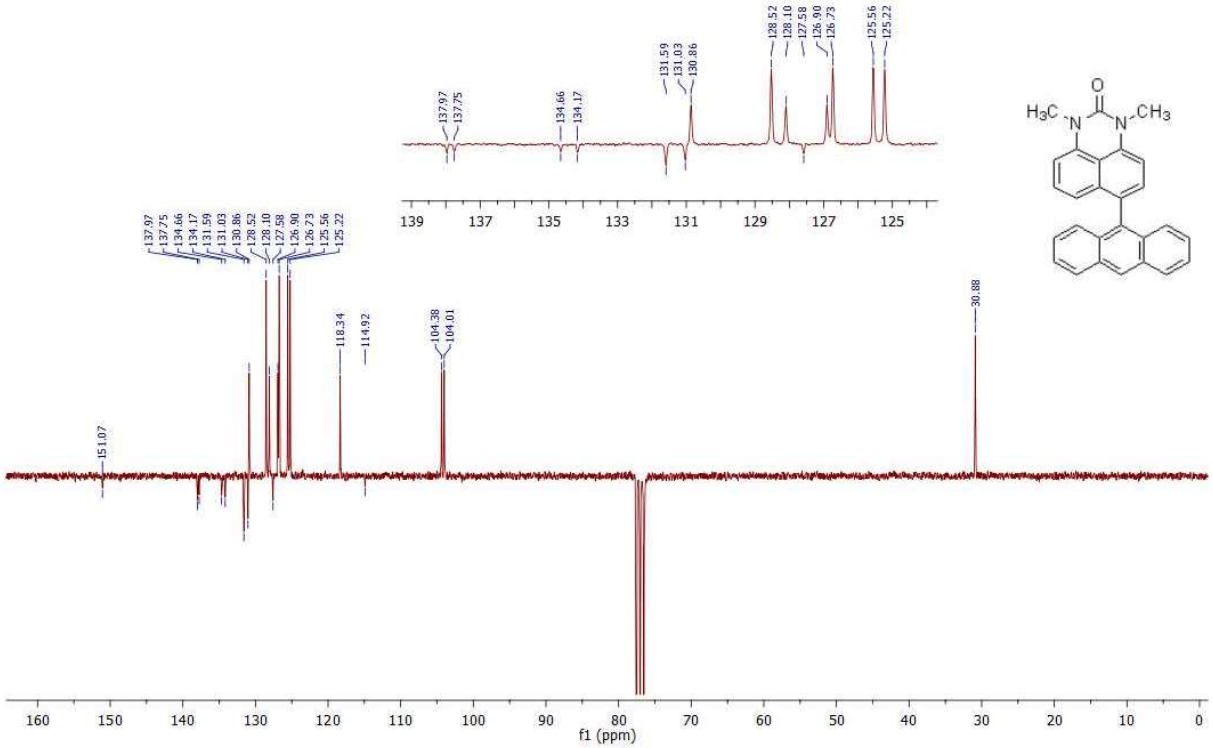


Fig. S18. $^{13}C\{^{1}H\}$ APT-NMR spectrum of compound **6i** (62.9 MHz, $CDCl_3$).

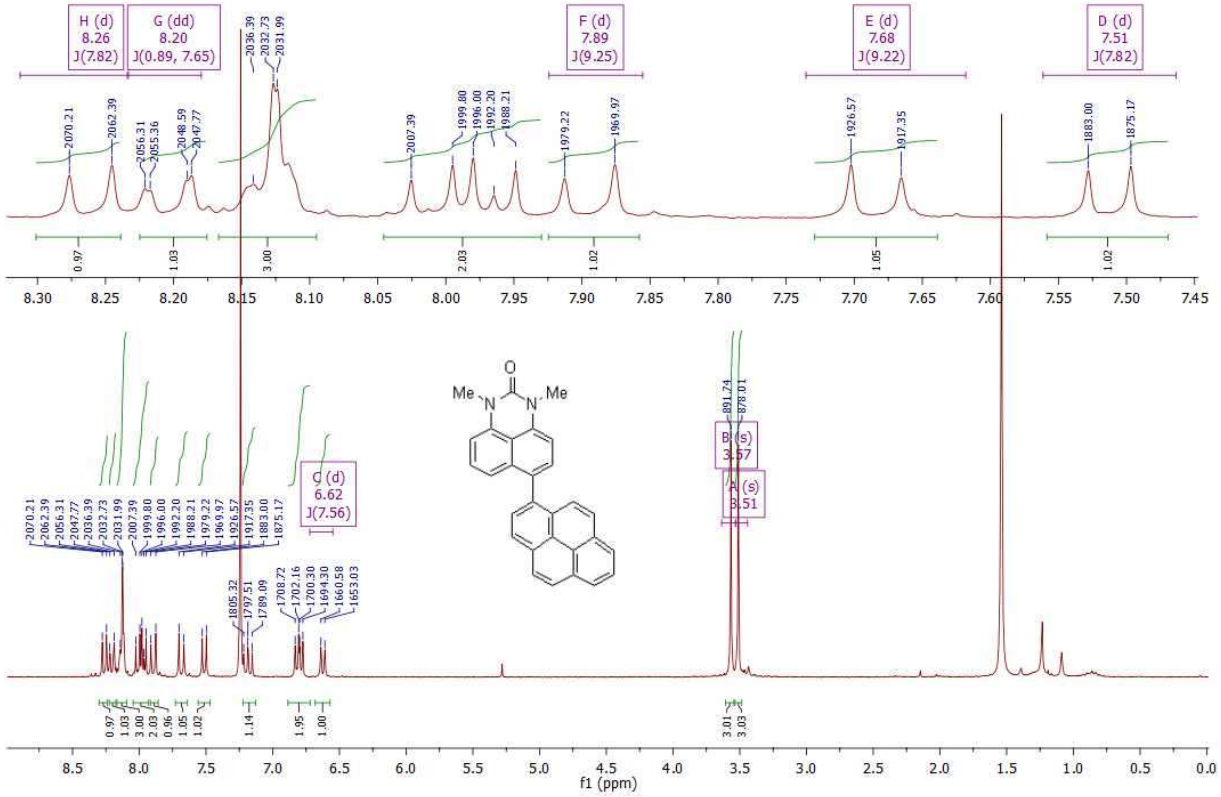


Fig. S19. ^{1}H NMR spectrum of compound **6j** (250 MHz, $CDCl_3$).

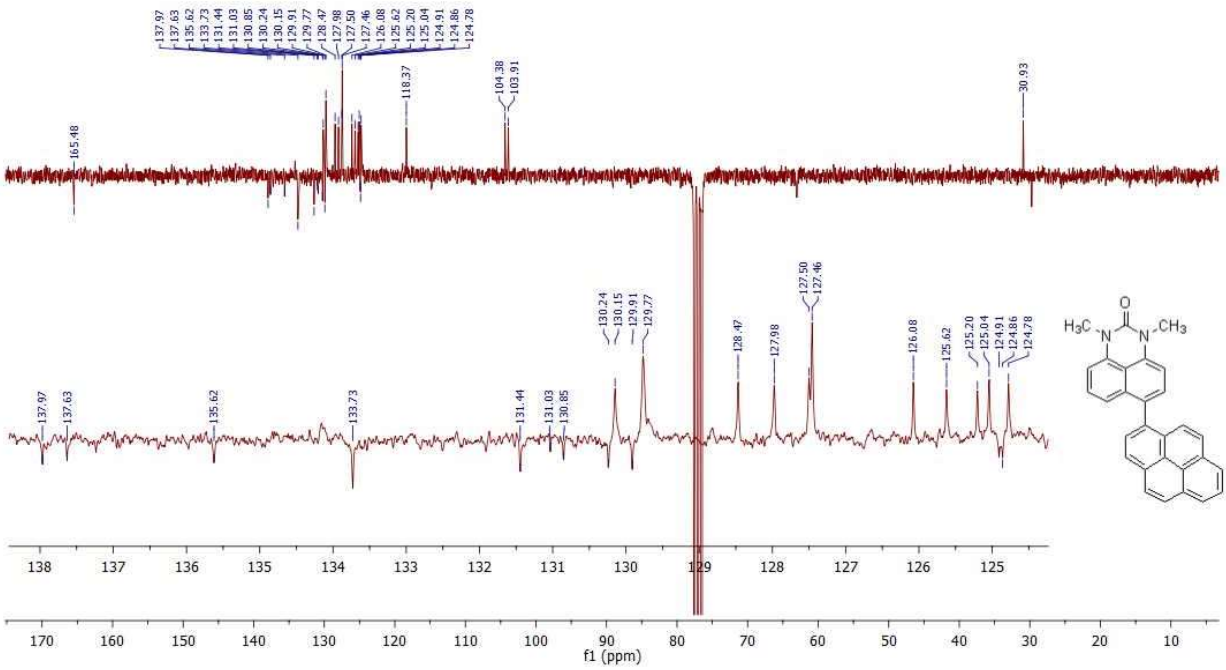


Fig. S20. $^{13}C\{^{1}H\}$ APT-NMR spectrum of compound **6j** (62.9 MHz, $CDCl_3$).

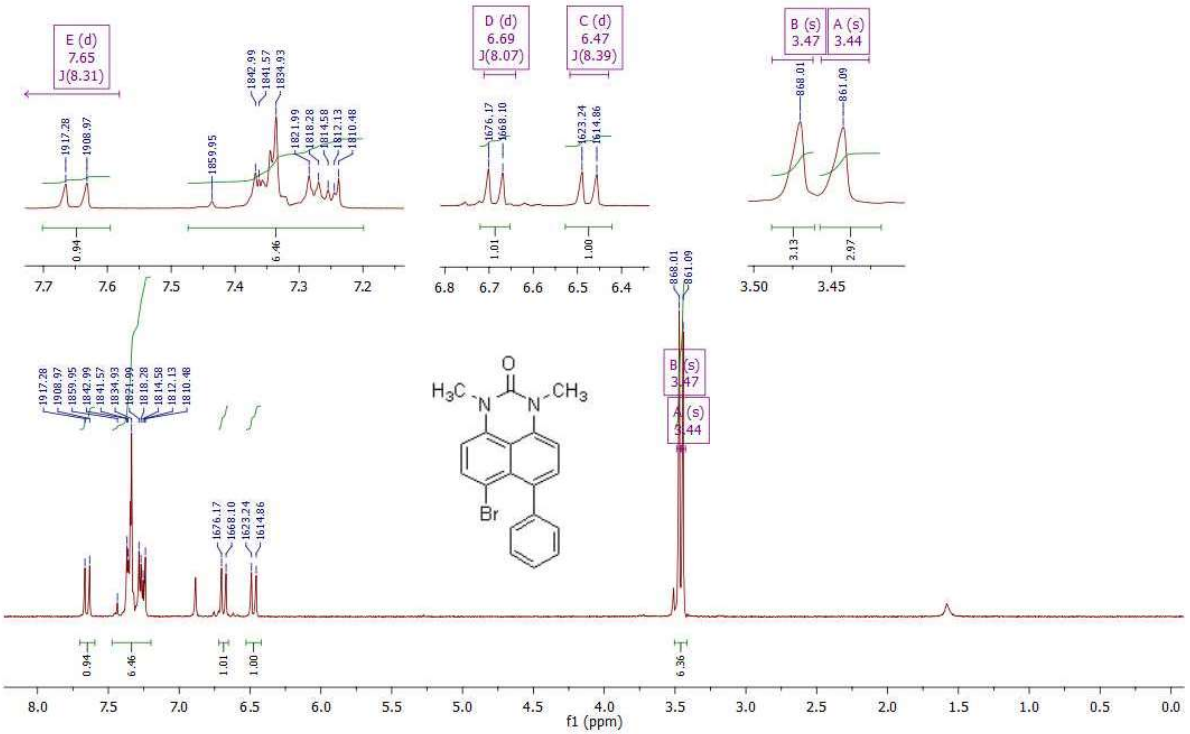


Fig. S21. ^{1}H NMR spectrum of compound **8a** (250 MHz, $CDCl_3$).

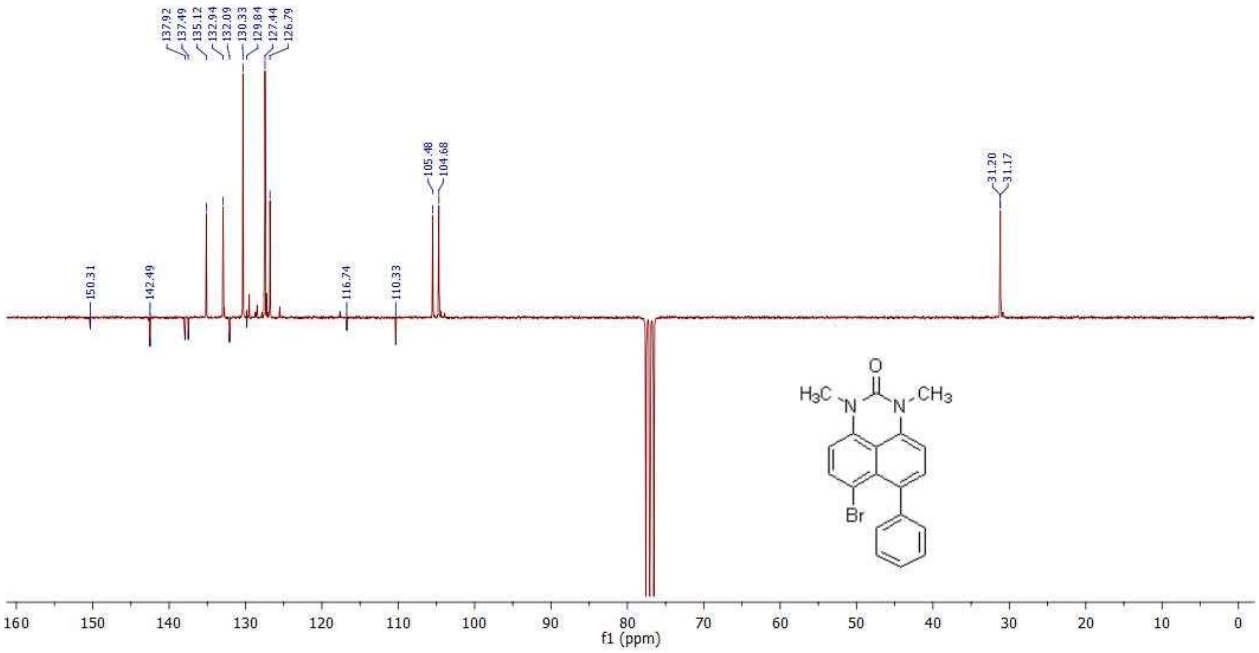


Fig. S22. $^{13}C\{^{1}H\}$ APT-NMR spectrum of compound **8a** (62.9 MHz, $CDCl_3$).

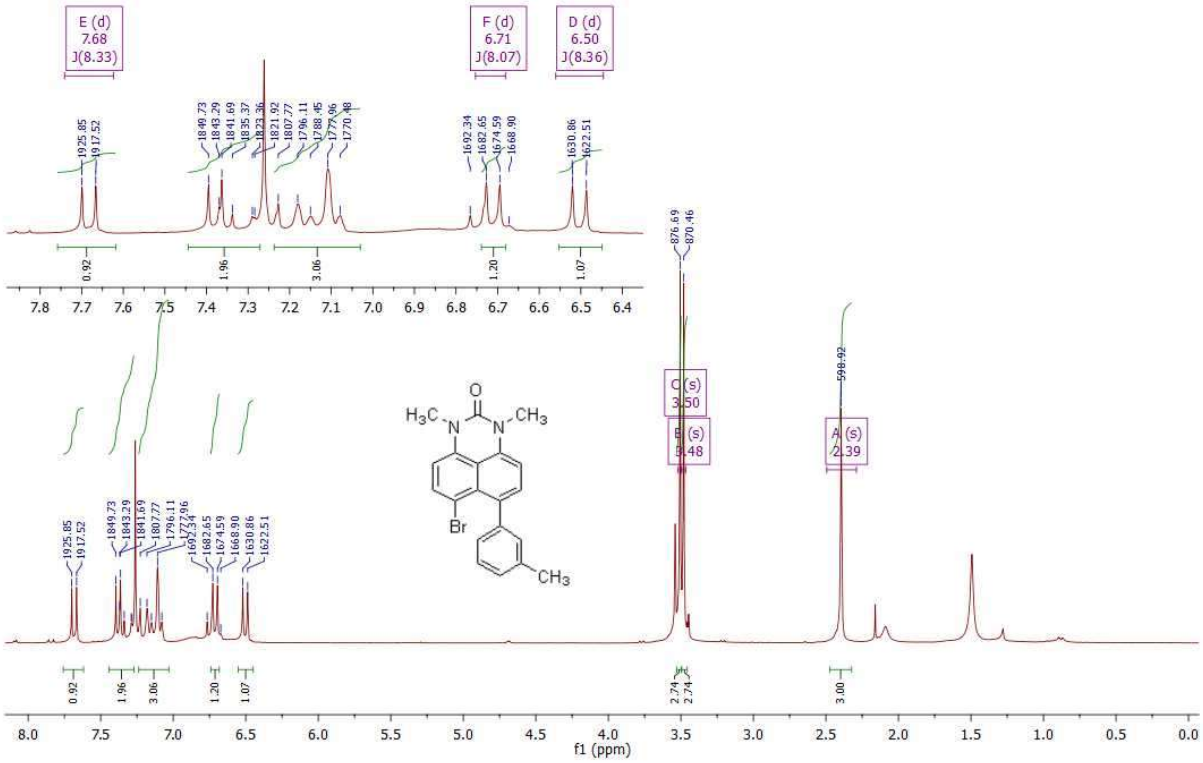


Fig. S23. ^{1}H NMR spectrum of compound **8b** (250 MHz, $CDCl_3$).

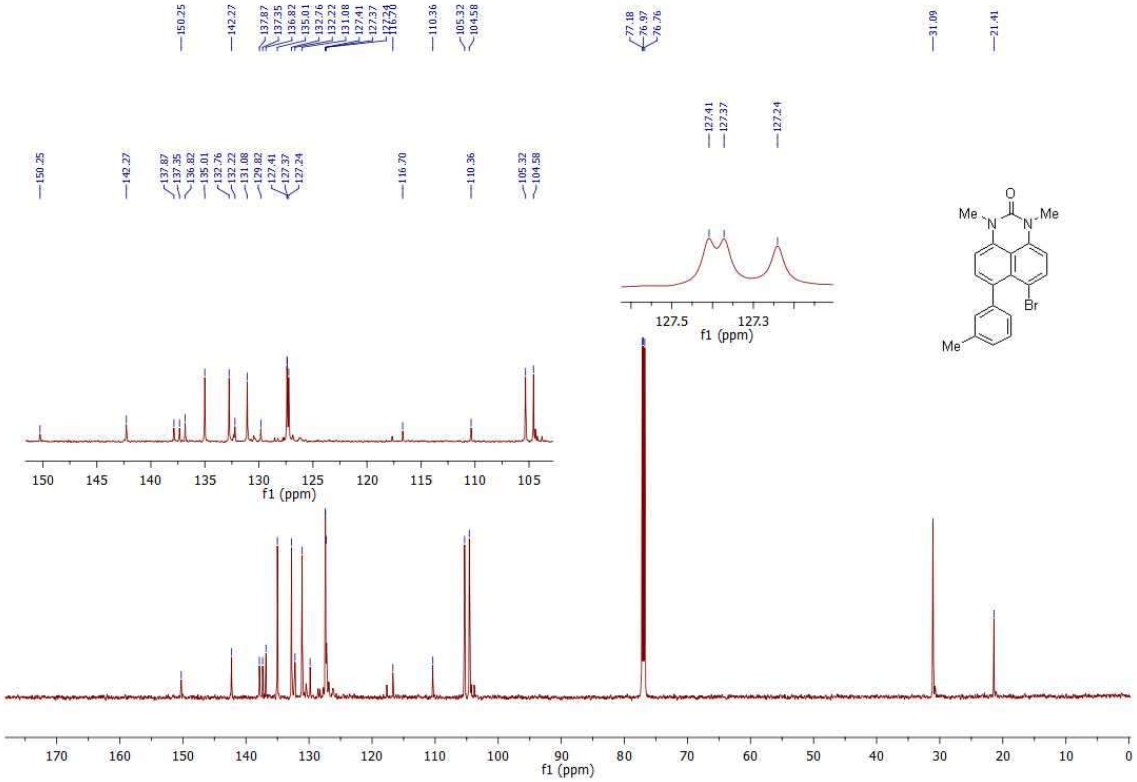


Fig. S24. $^{13}C\{^{1}H\}$ NMR spectrum of compound **8b** (150 MHz, $CDCl_3$).

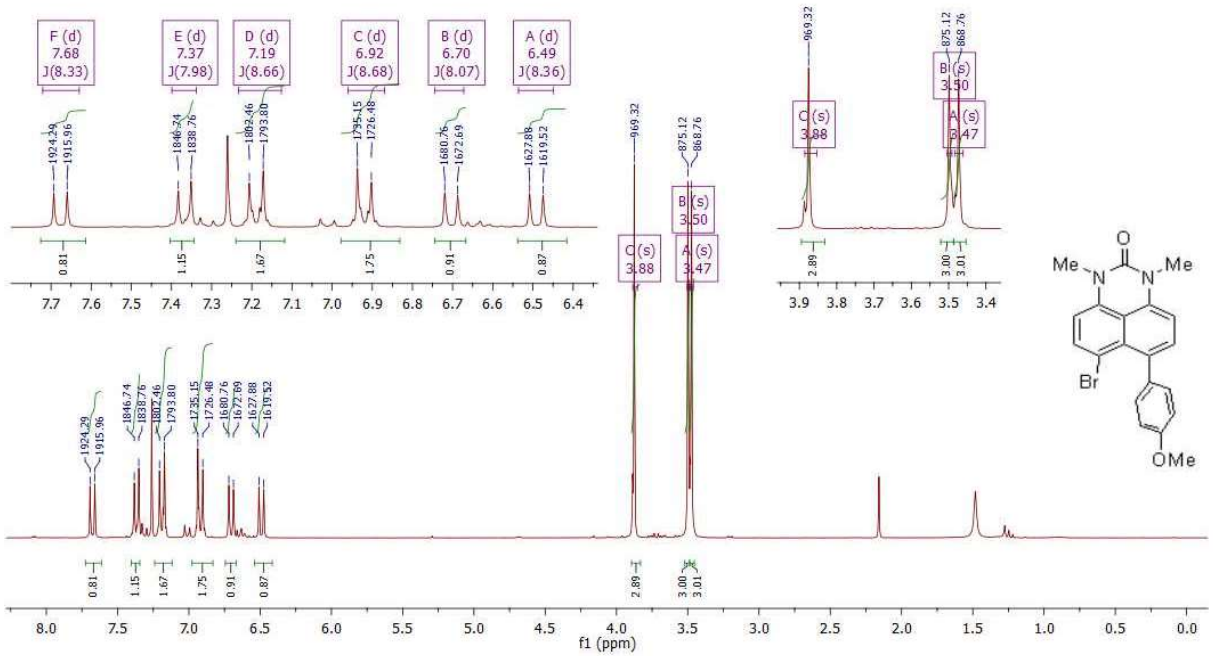


Fig. S25. ^{1}H NMR spectrum of compound **8c** (250 MHz, $CDCl_3$).

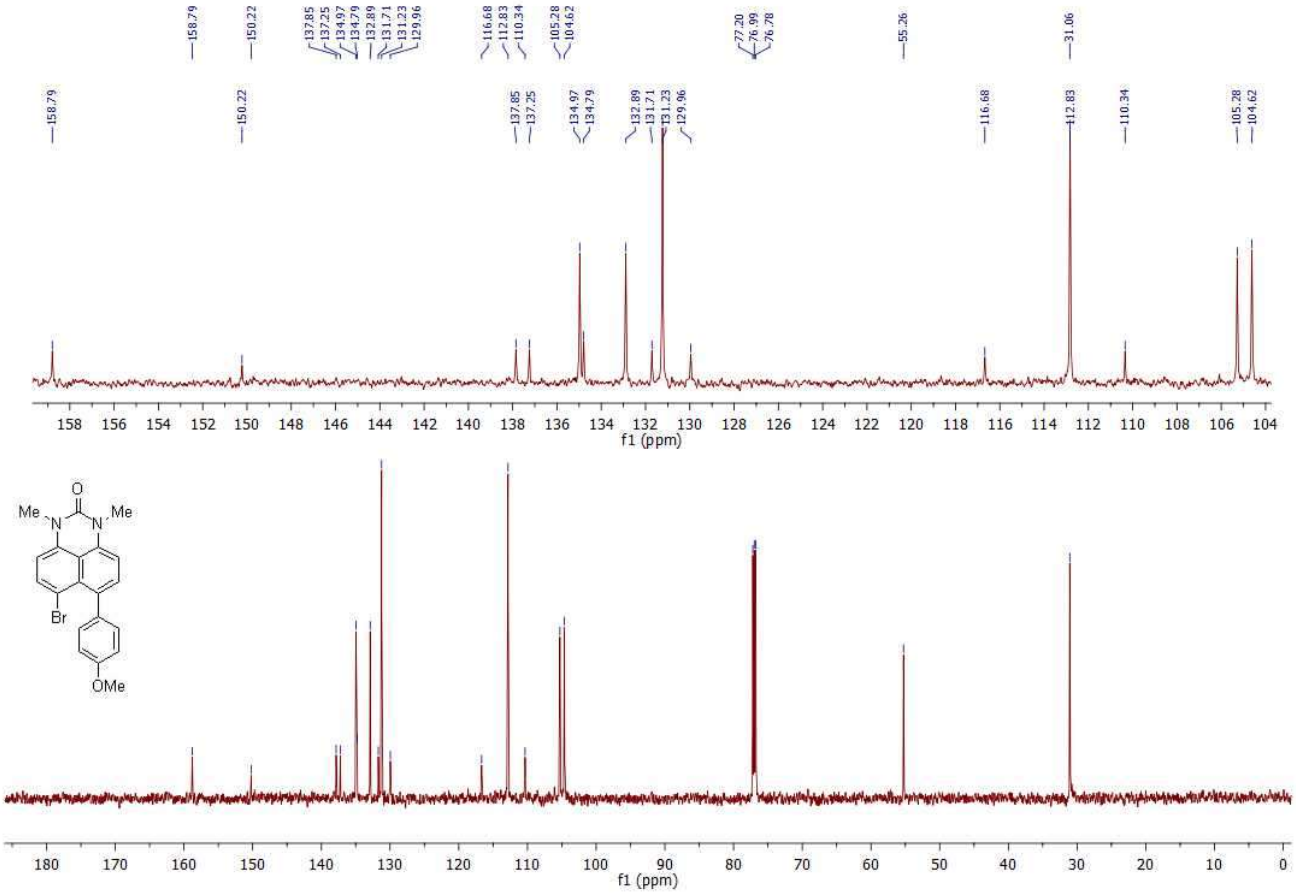


Fig. S26. $^{13}C\{^{1}H\}$ NMR spectrum of compound **8c** (150 MHz, $CDCl_3$).

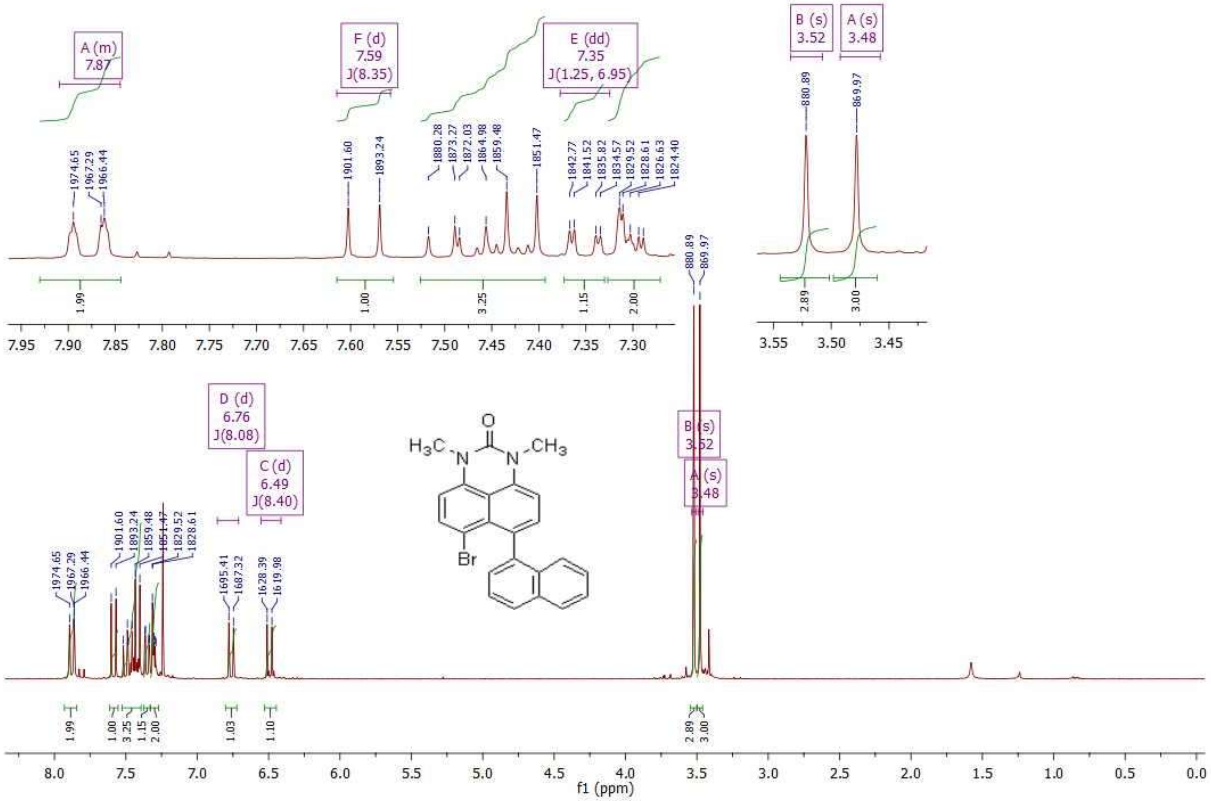


Fig. S27. ^{1}H NMR spectrum of compound **8d** (250 MHz, $CDCl_3$).

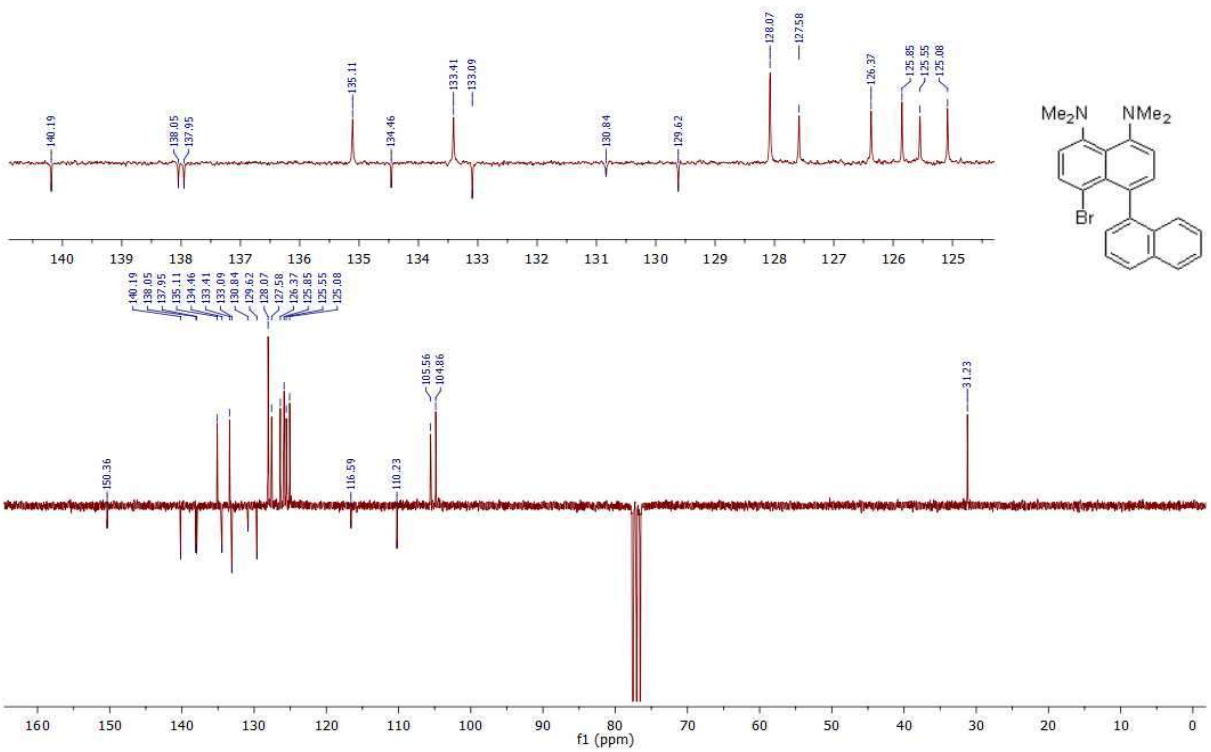


Fig. S28. $^{13}C\{^{1}H\}$ APT-NMR spectrum of compound **8d** (62.9 MHz, $CDCl_3$).

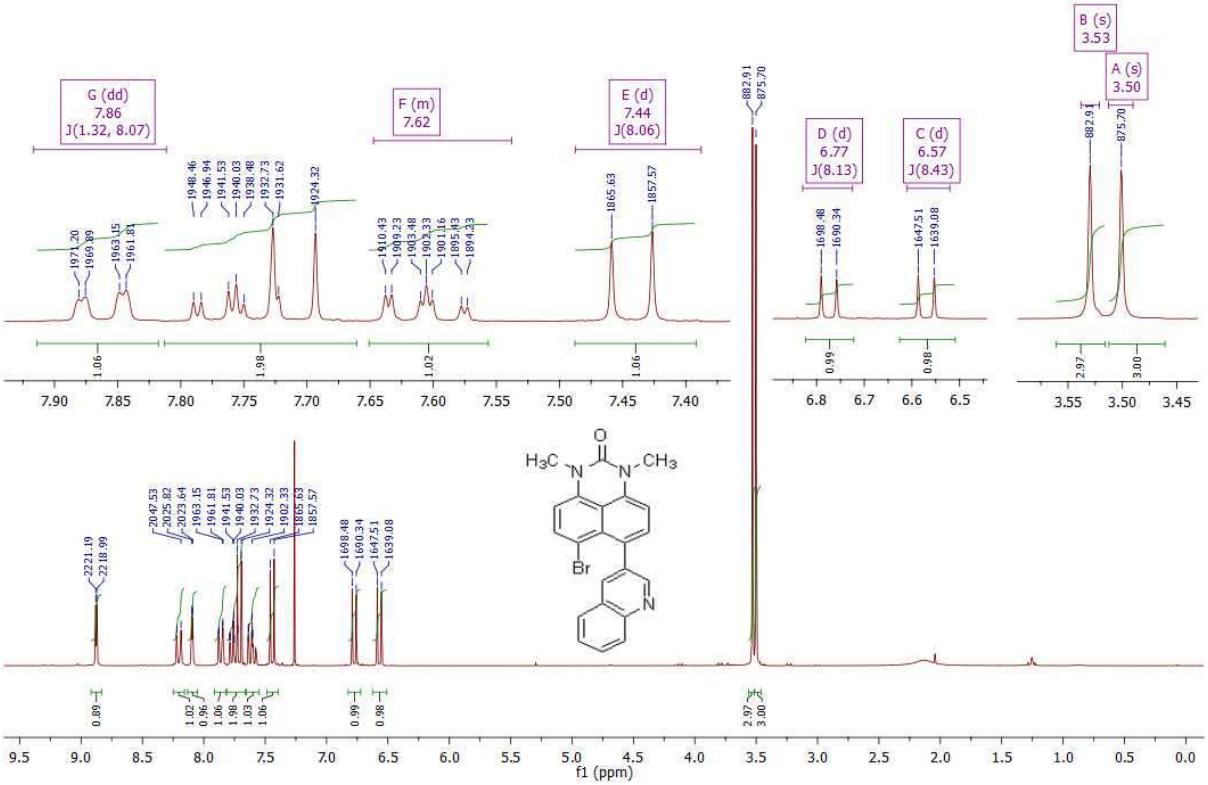


Fig. S29. ^{1}H NMR spectrum of compound **8e** (250 MHz, $CDCl_3$).

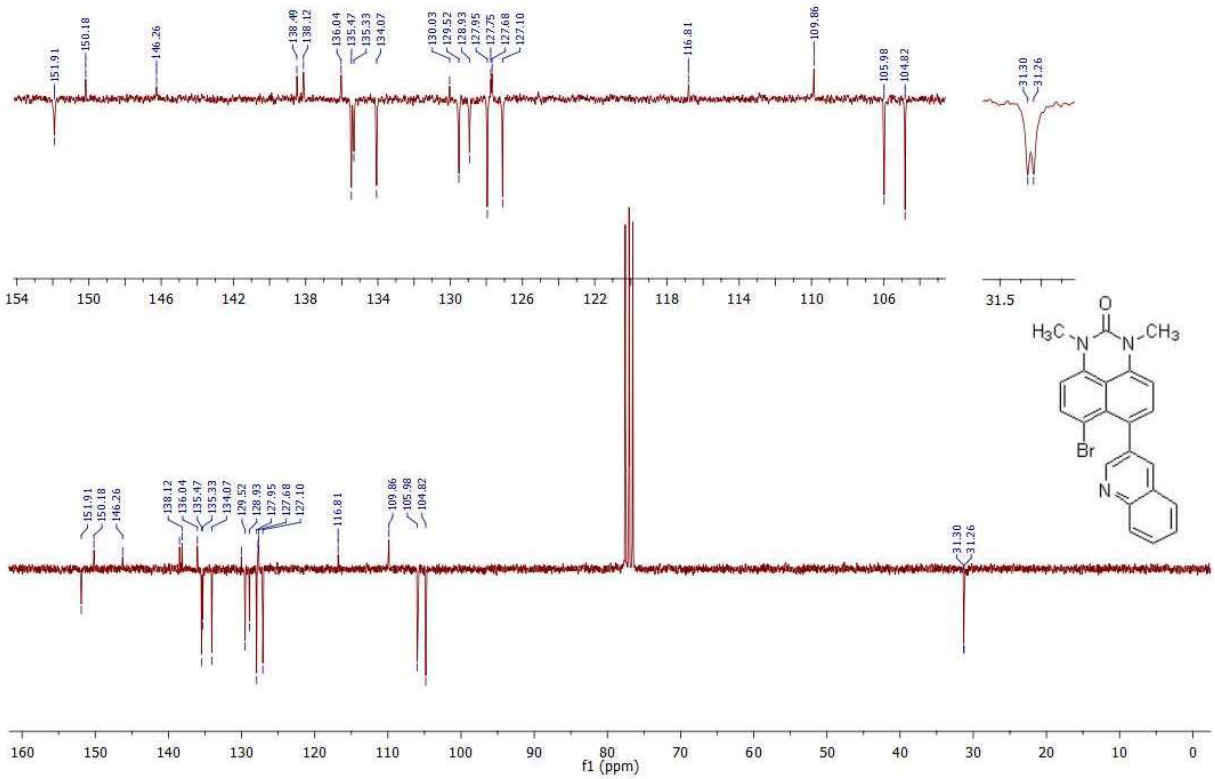


Fig. 30. $^{13}C\{^{1}H\}$ APT-NMR spectrum of compound **8e** (62.9 MHz, $CDCl_3$).

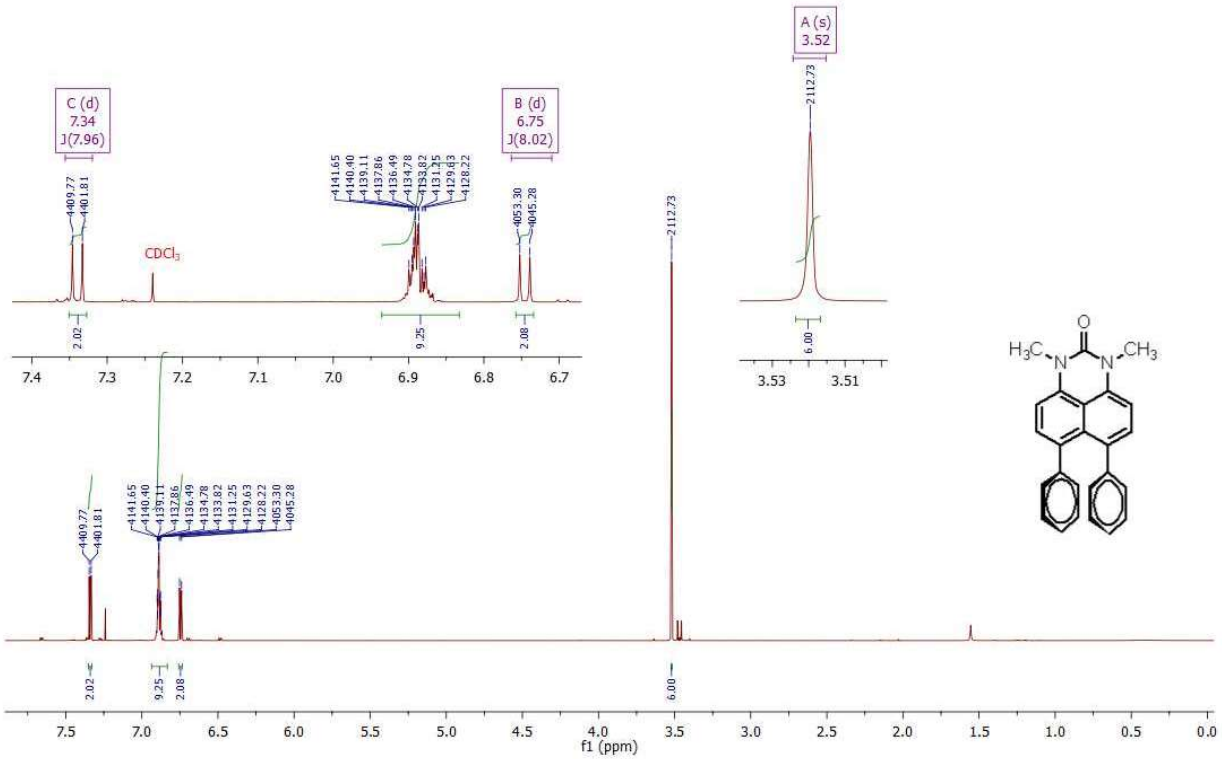


Fig. S31. ^{1}H NMR spectrum of compound **3a** (600 MHz, $CDCl_3$).

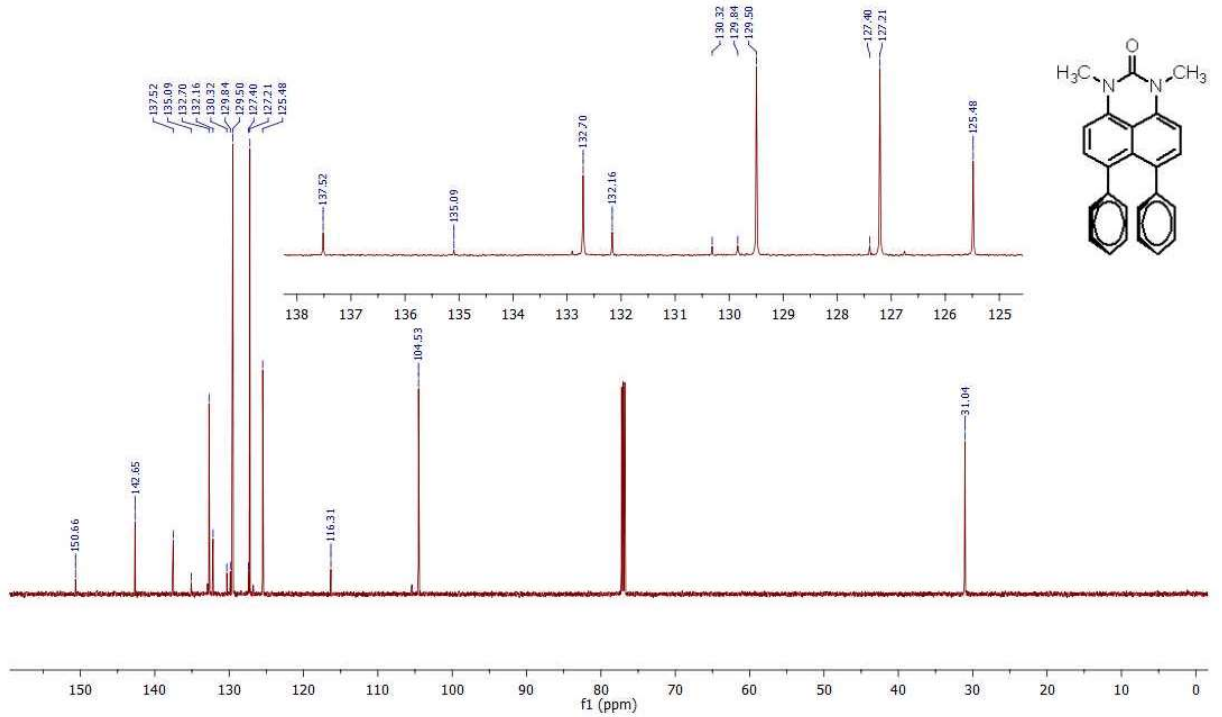


Fig. S32. $^{13}C\{^{1}H\}$ NMR spectrum of compound **3a** (150 MHz, $CDCl_3$).

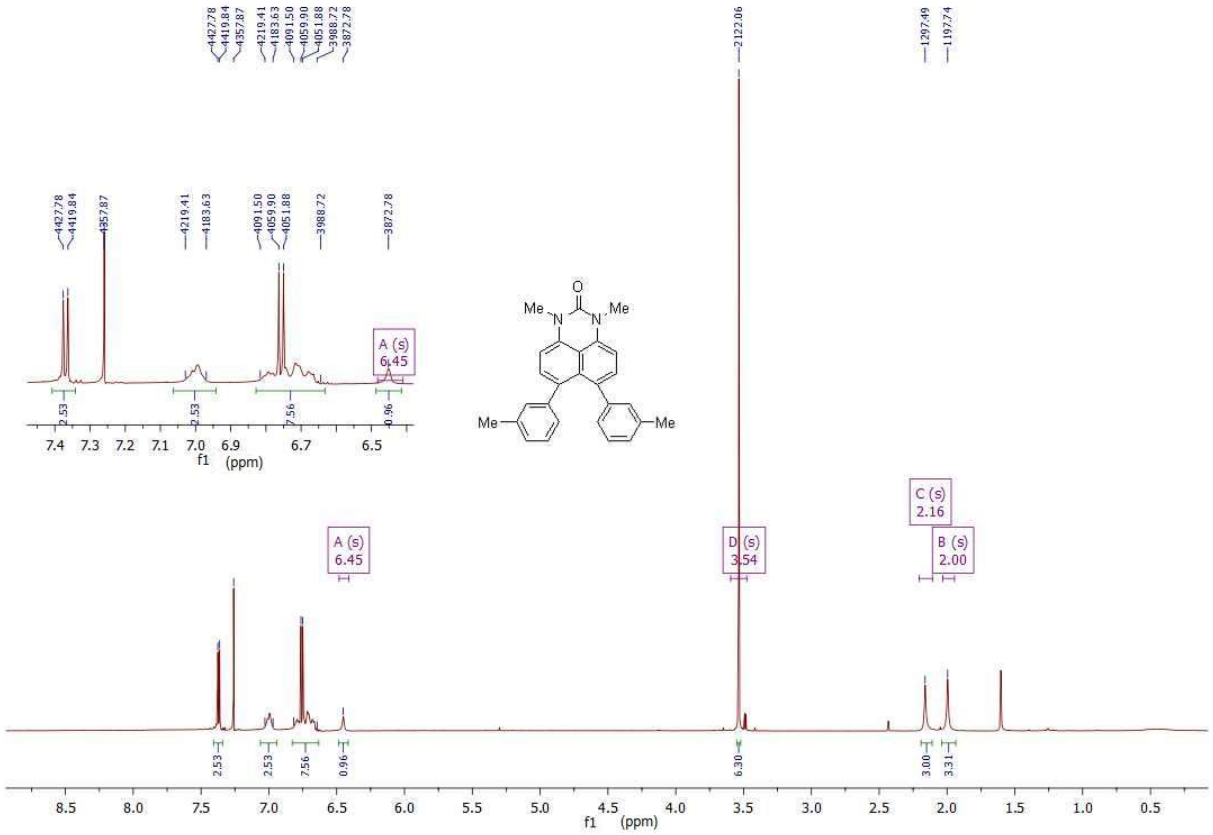


Fig. S33. ^{1}H NMR spectrum of compound **3b** (600 MHz, $CDCl_3$, +20 ºC).

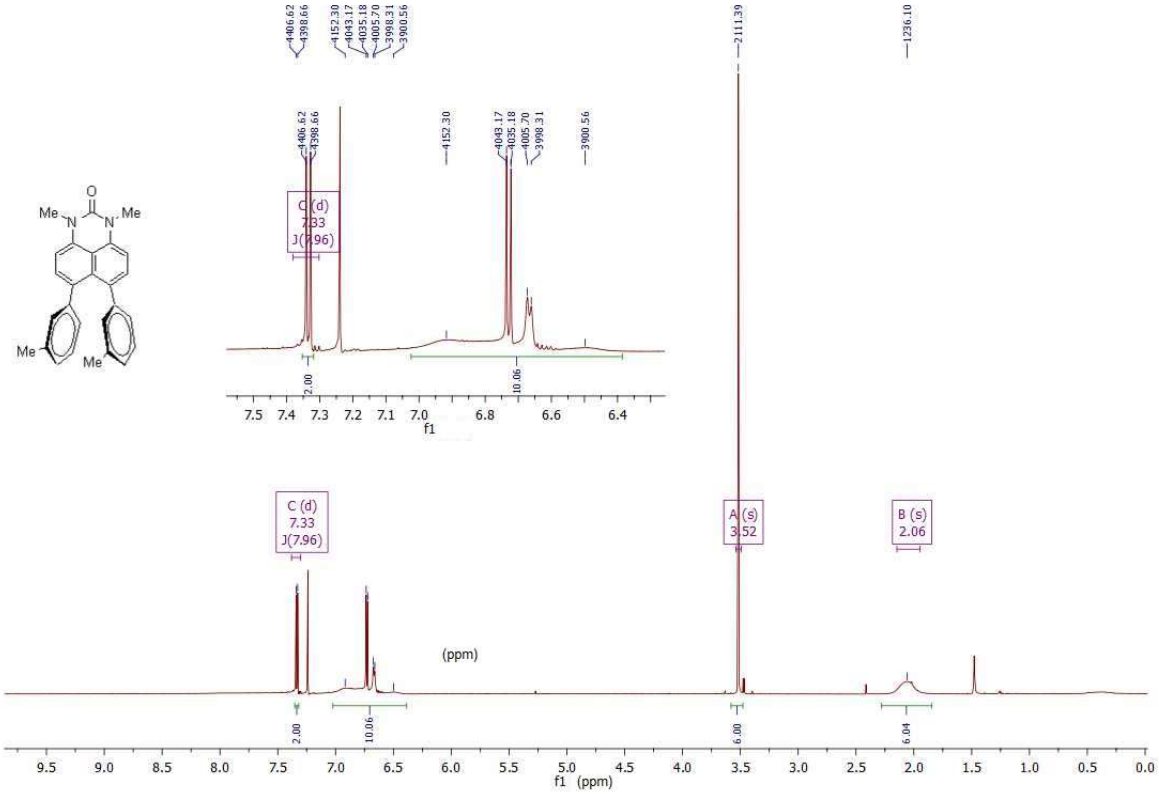


Fig. S34. ^{1}H NMR spectrum of compound **3b** (600 MHz, $CDCl_3$, +55 ºC).

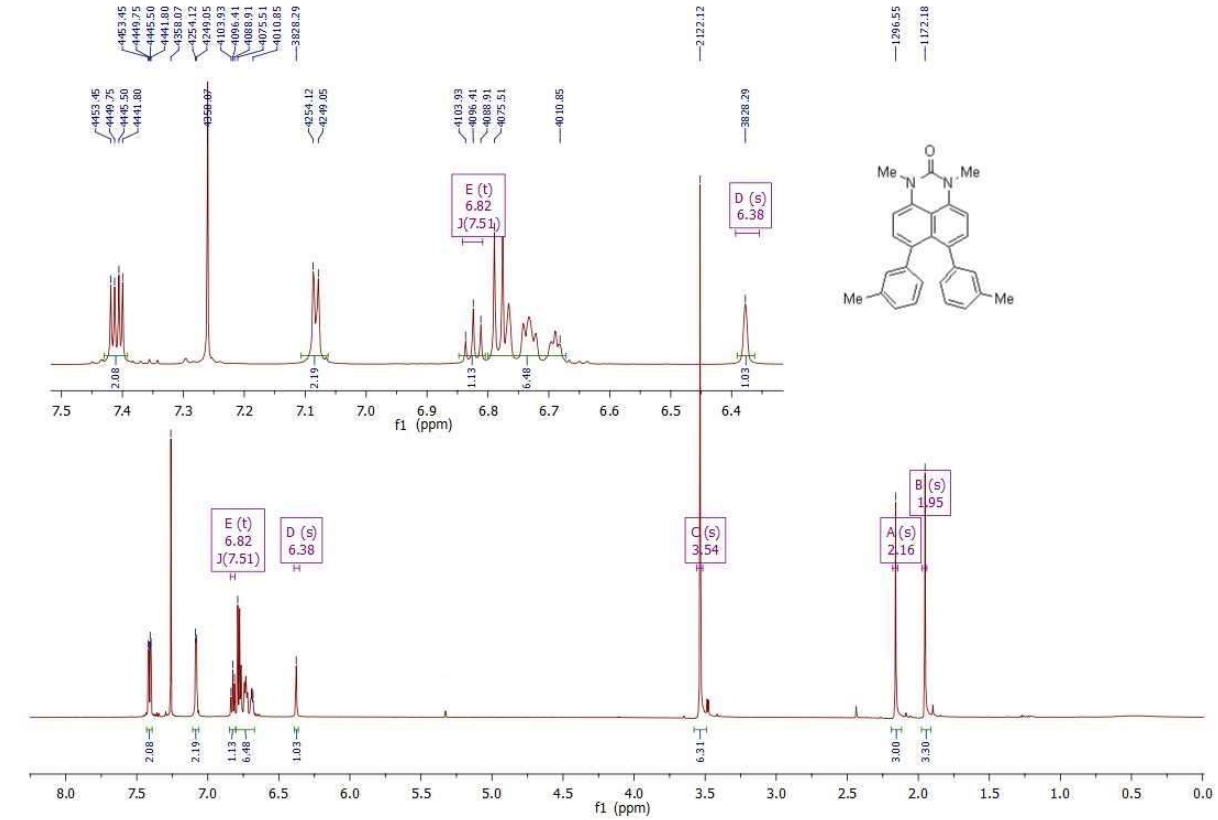


Fig. S35. ^{1}H NMR spectrum of compound **3b** (600 MHz, $CDCl_3$, –50 ºC).

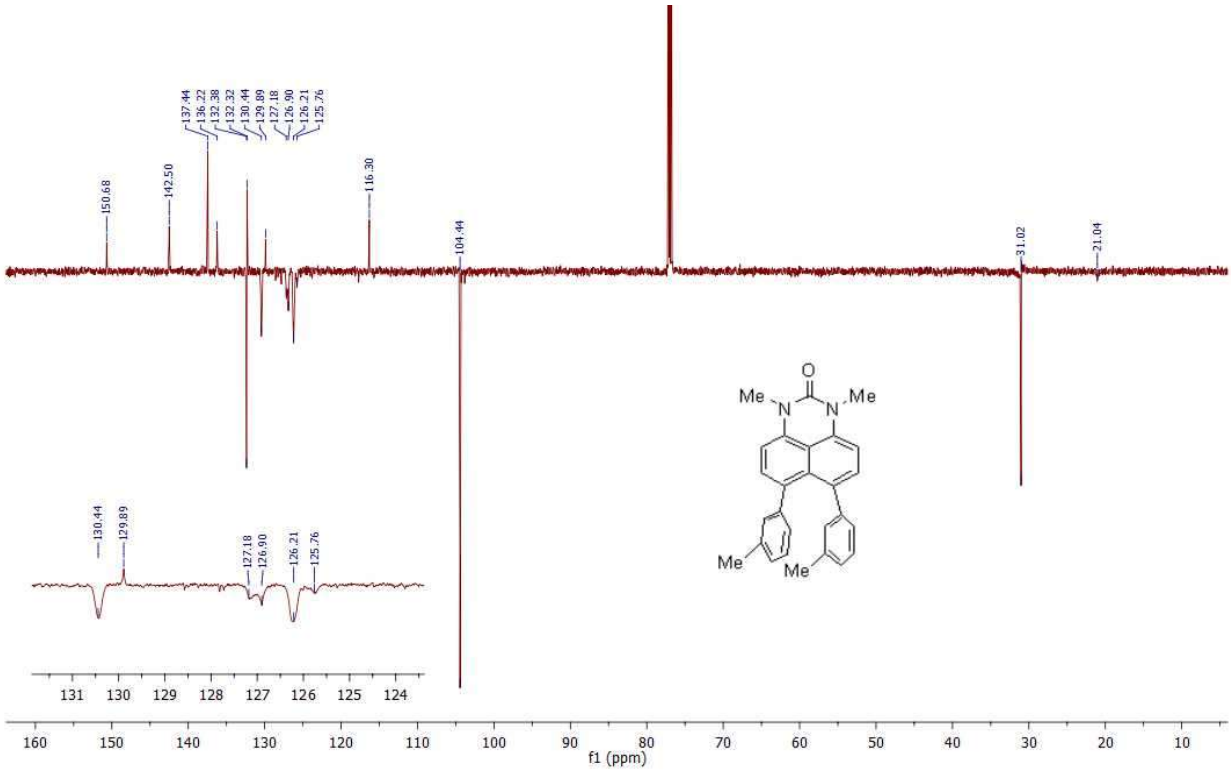


Fig. S36. $^{13}C\{^{1}H\}$ APT-NMR spectrum of compound **3b** (150 MHz, $CDCl_3$, +30 ºC).

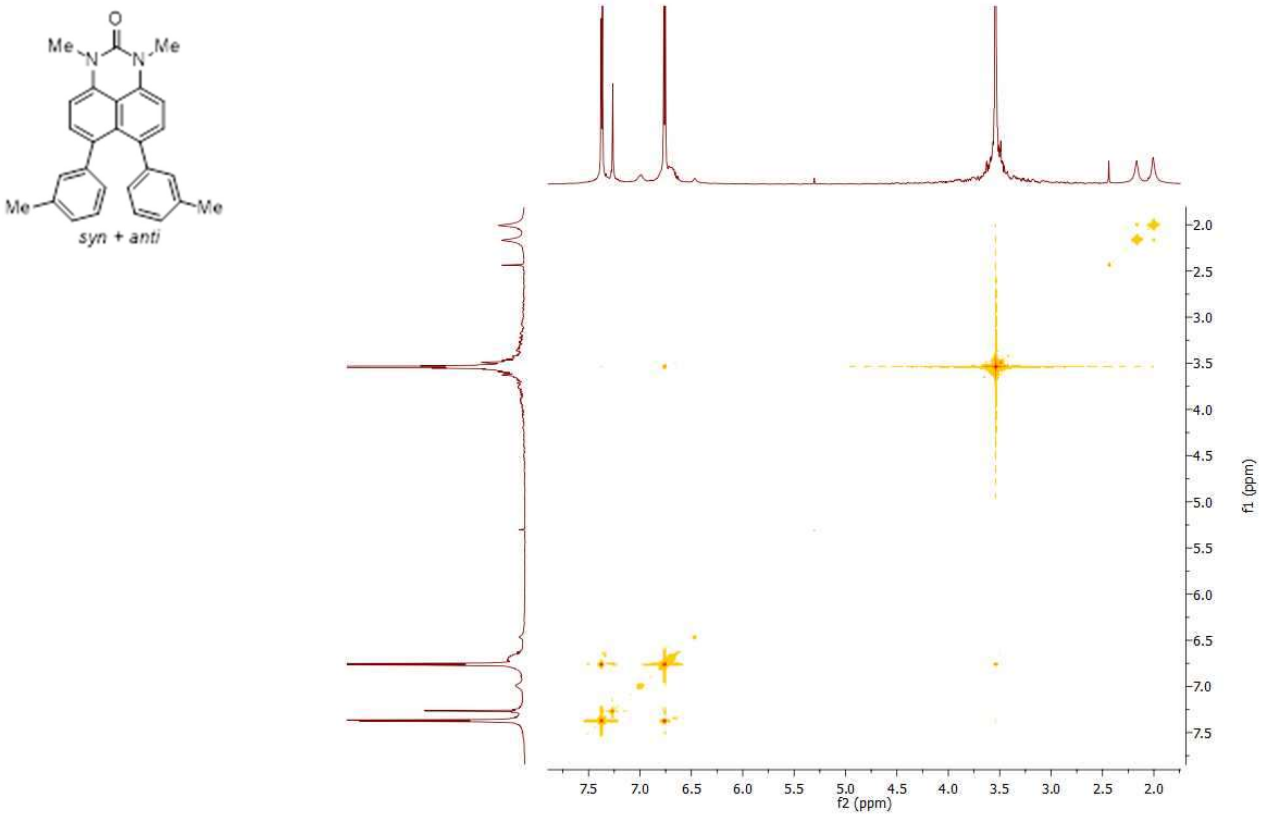


Fig. S37. ^{1}H-^{1}H COSY spectrum of compound **3b** (600 MHz, $CDCl_3$, +30 ºC).

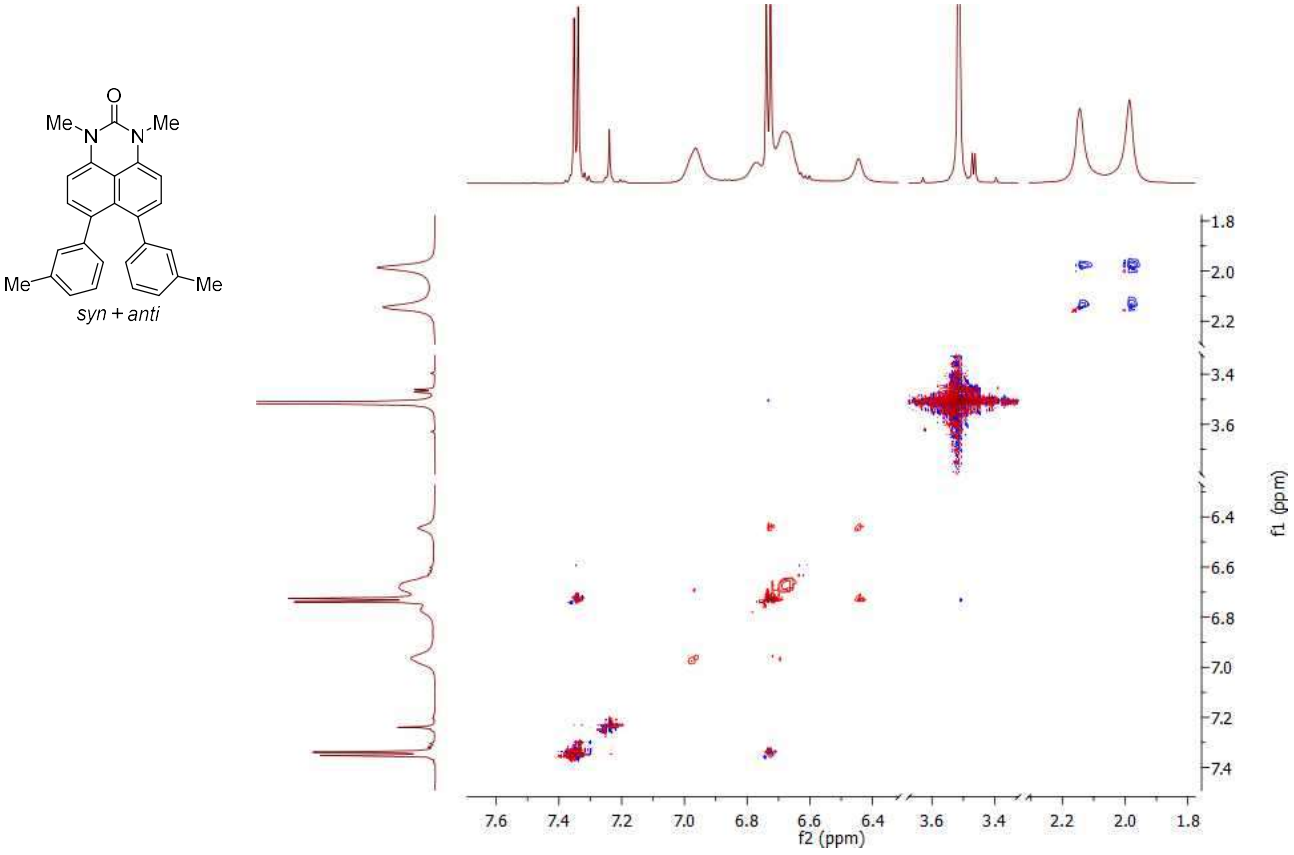


Fig. S38. 2D NOESY spectrum of compound **3b** (600 MHz, $CDCl_3$, +30 ºC).

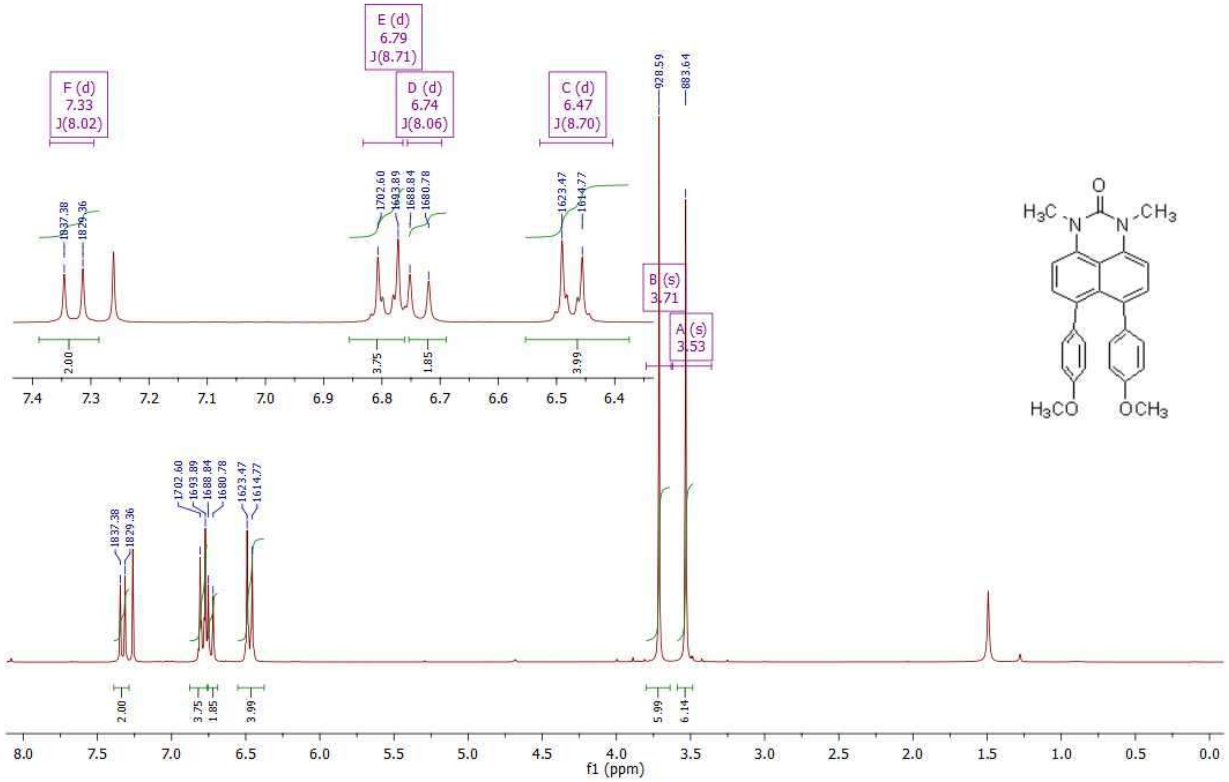


Fig. S39. ^{1}H NMR spectrum of compound **3c** (250 MHz, $CDCl_3$).

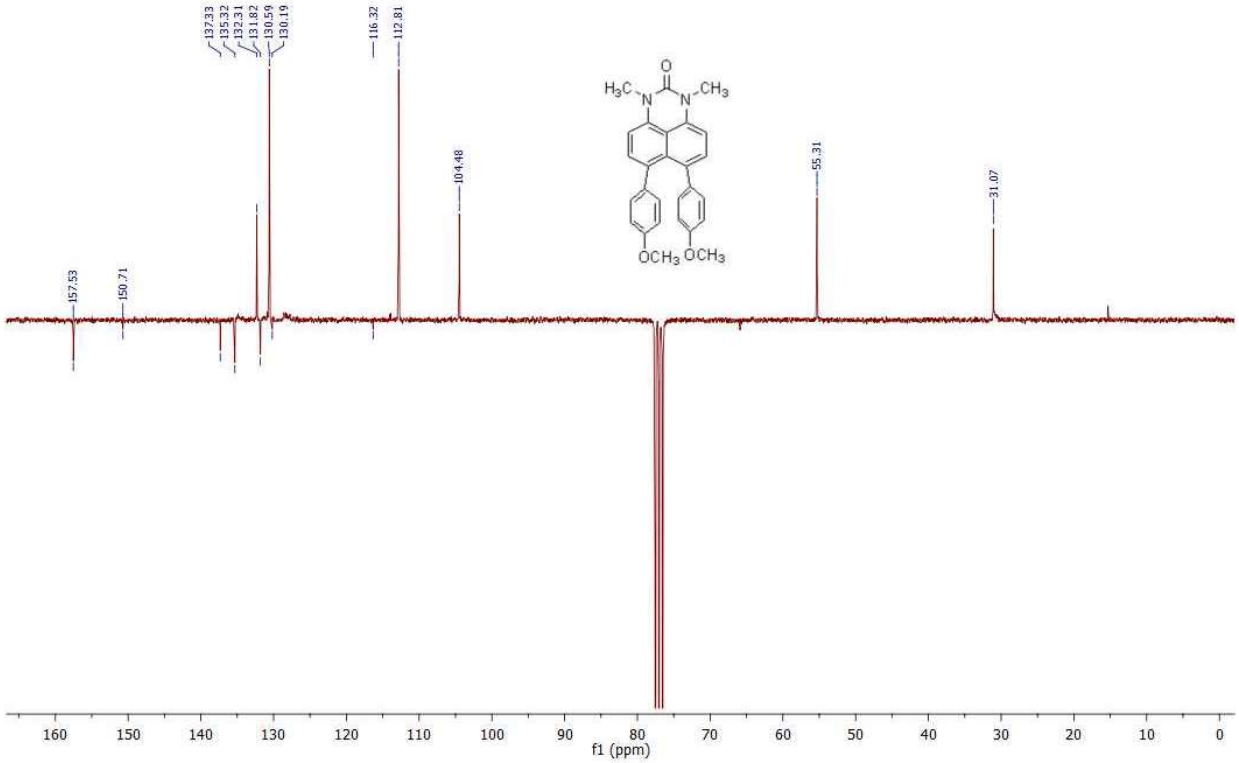


Fig. S40. $^{13}C\{^{1}H\}$ APT-NMR spectrum of compound **3c** (62.9 MHz, $CDCl_3$).

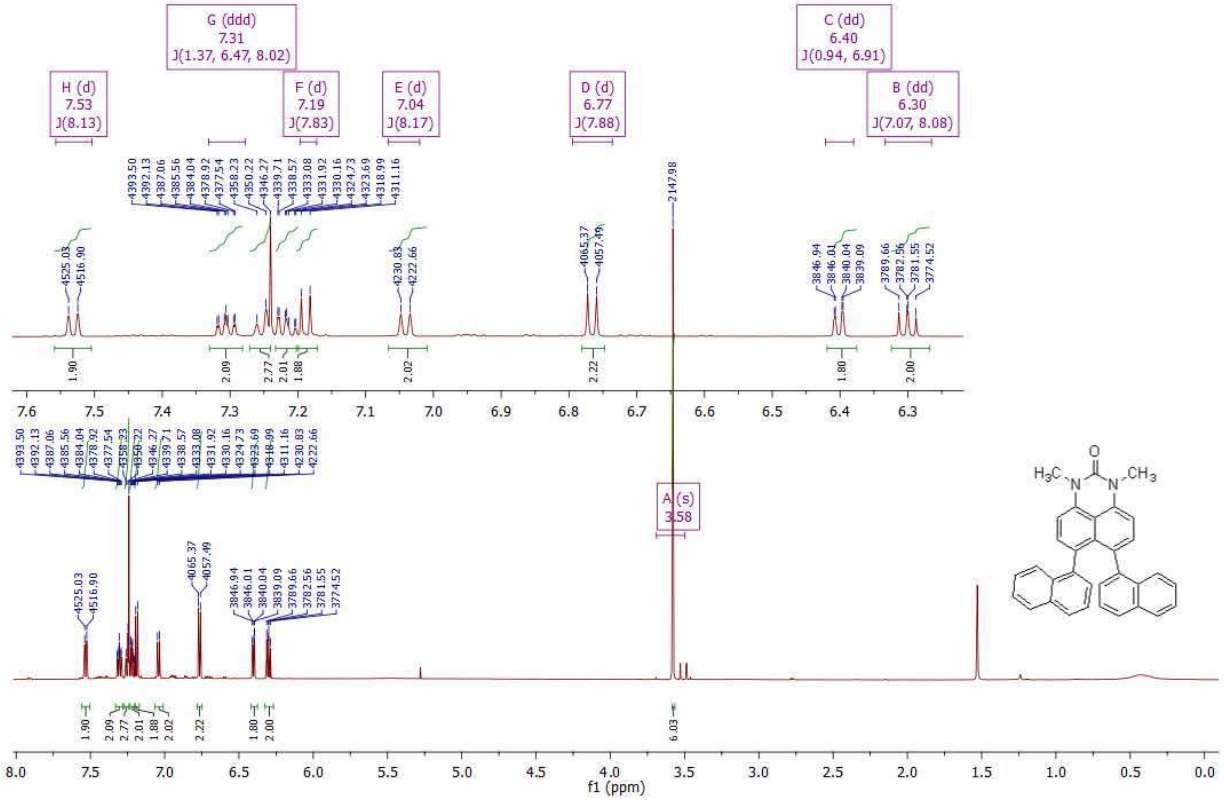


Fig. S41. ^{1}H NMR spectrum of compound **3d** (600 MHz, $CDCl_3$, +30 ºC).

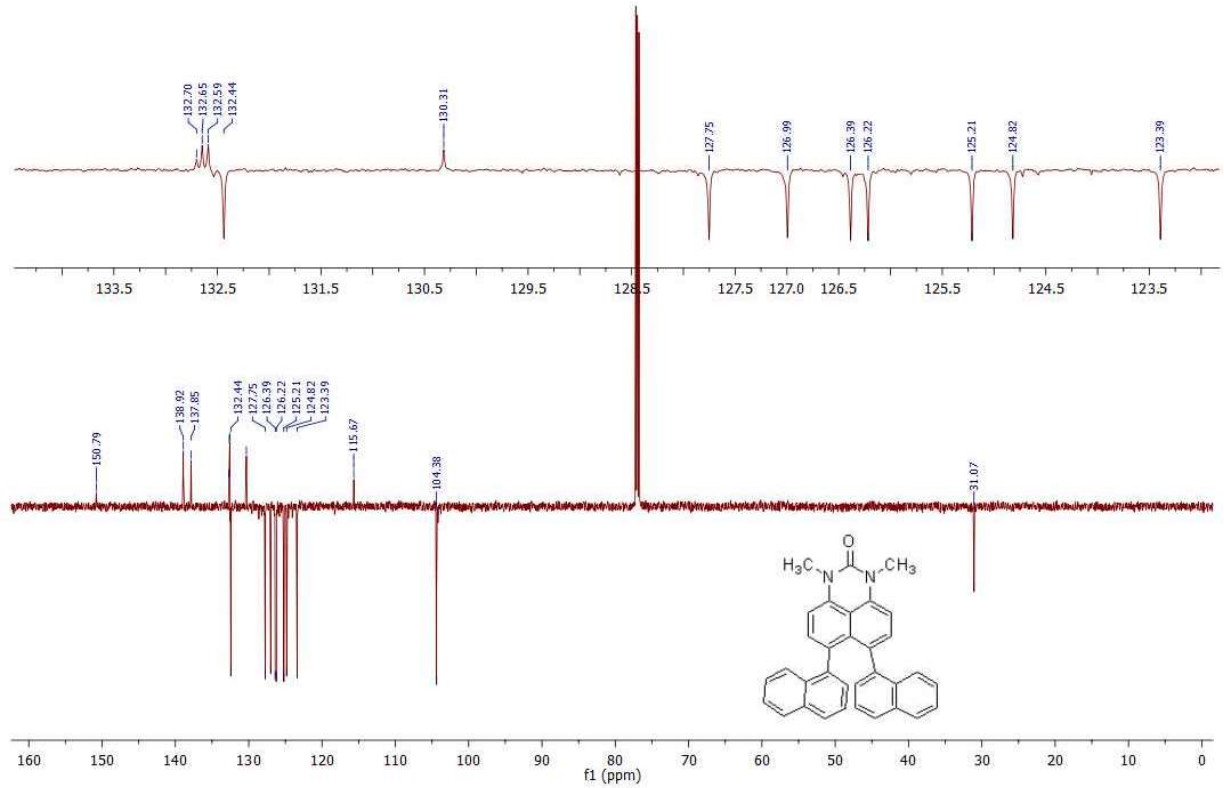


Fig. S42. $^{13}C\{^{1}H\}$ APT-NMR spectrum of compound **3d** (150 MHz, $CDCl_3$).

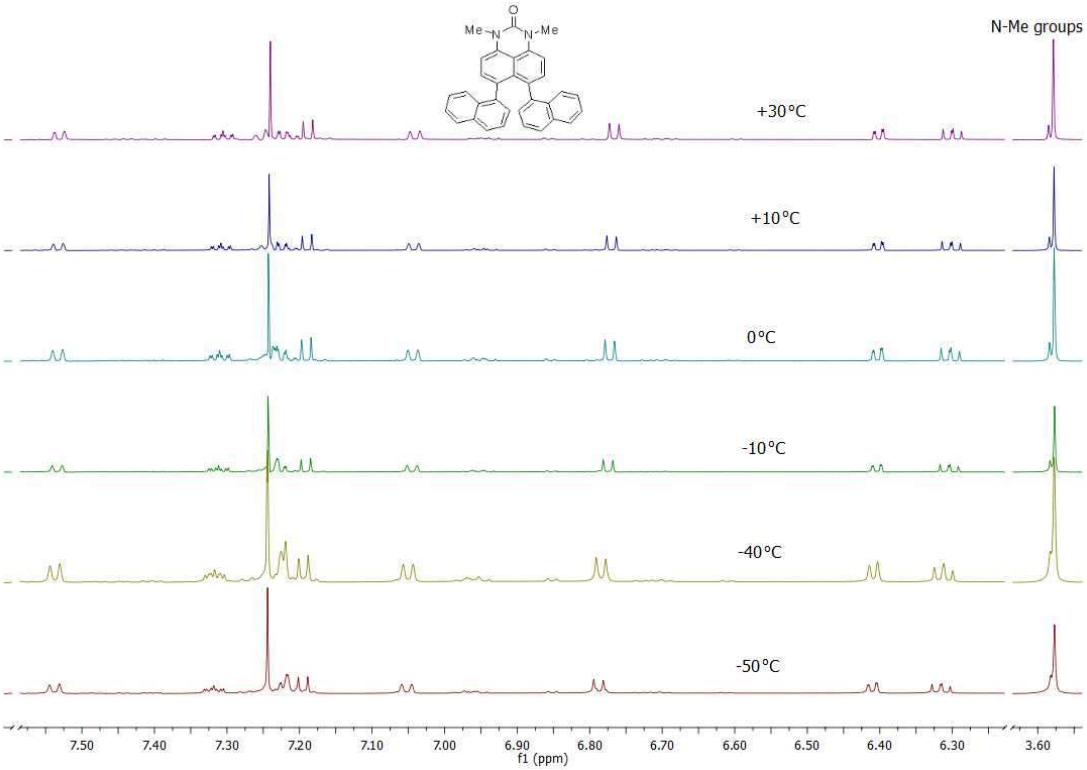


Fig. S43. Variable-temperature ^{1}H NMR spectra of **3d** ($CDCl_3$, 600MHz).

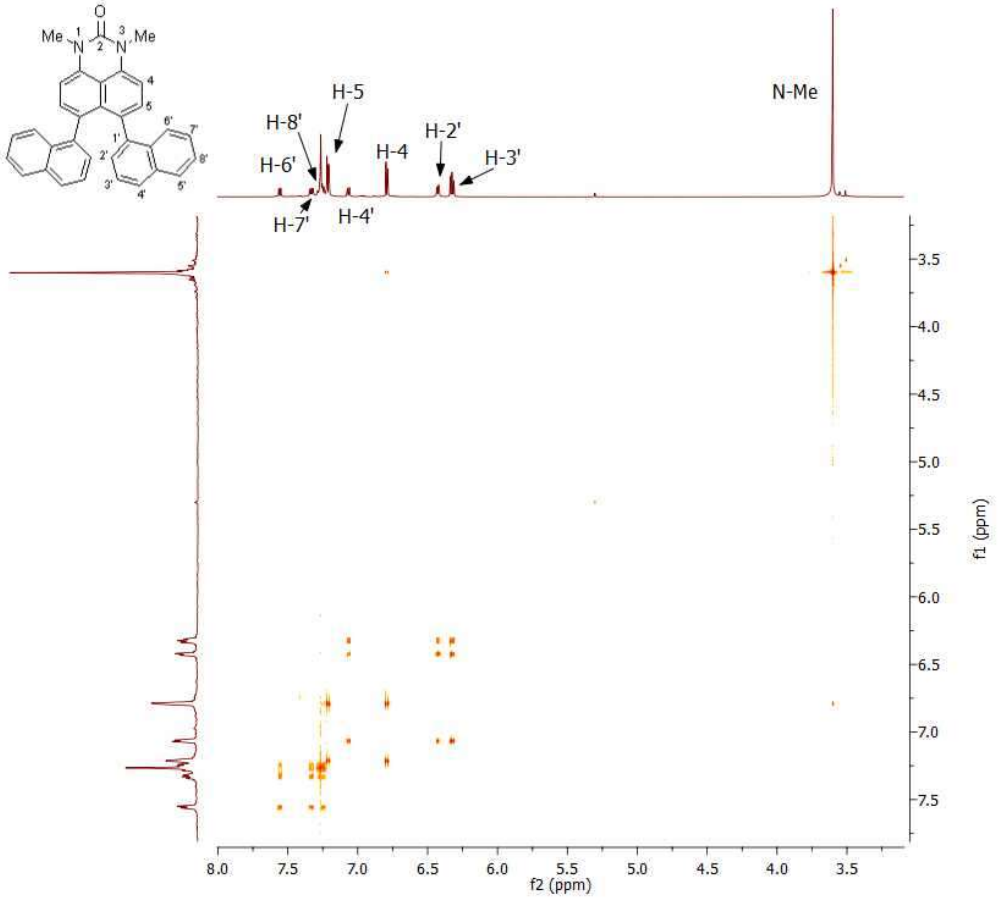


Fig. S44. ^{1}H-1H COSY spectra of **3d** ($CDCl_3$, 600MHz).

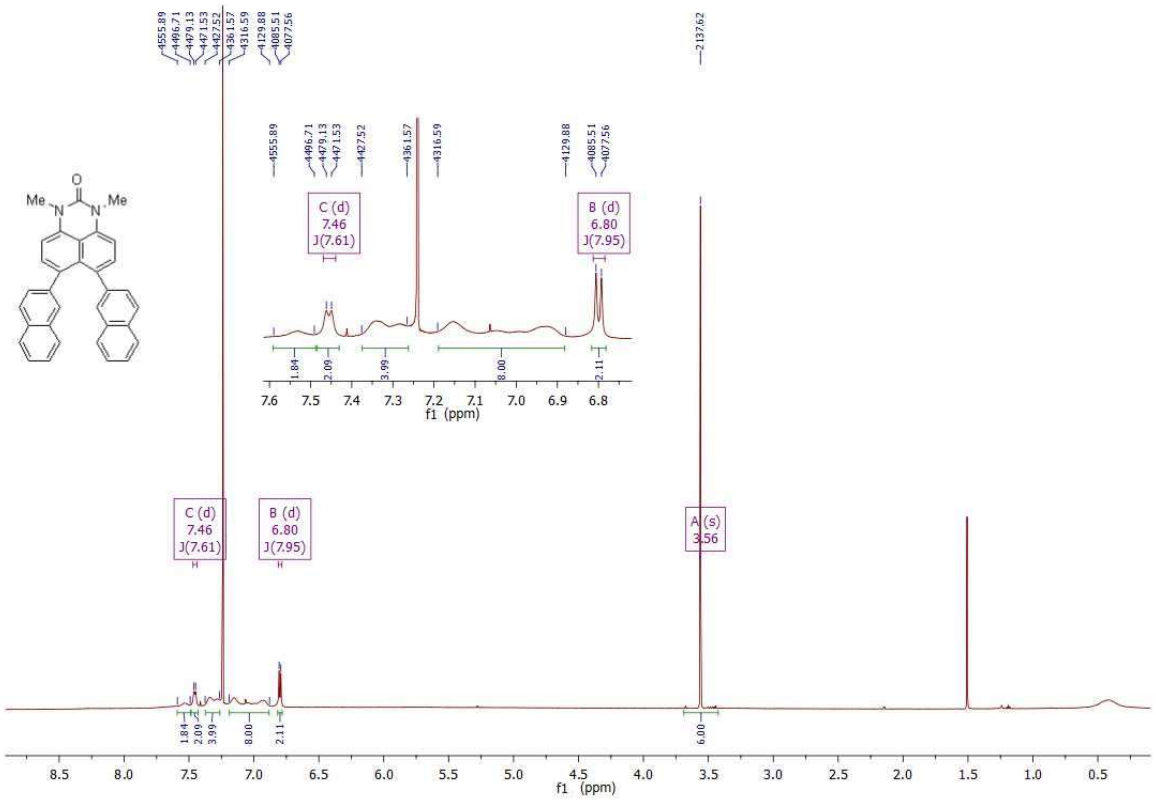


Fig. S45. ^{1}H NMR spectrum of compound **3f** (600 MHz, $CDCl_3$, +30 ºC).

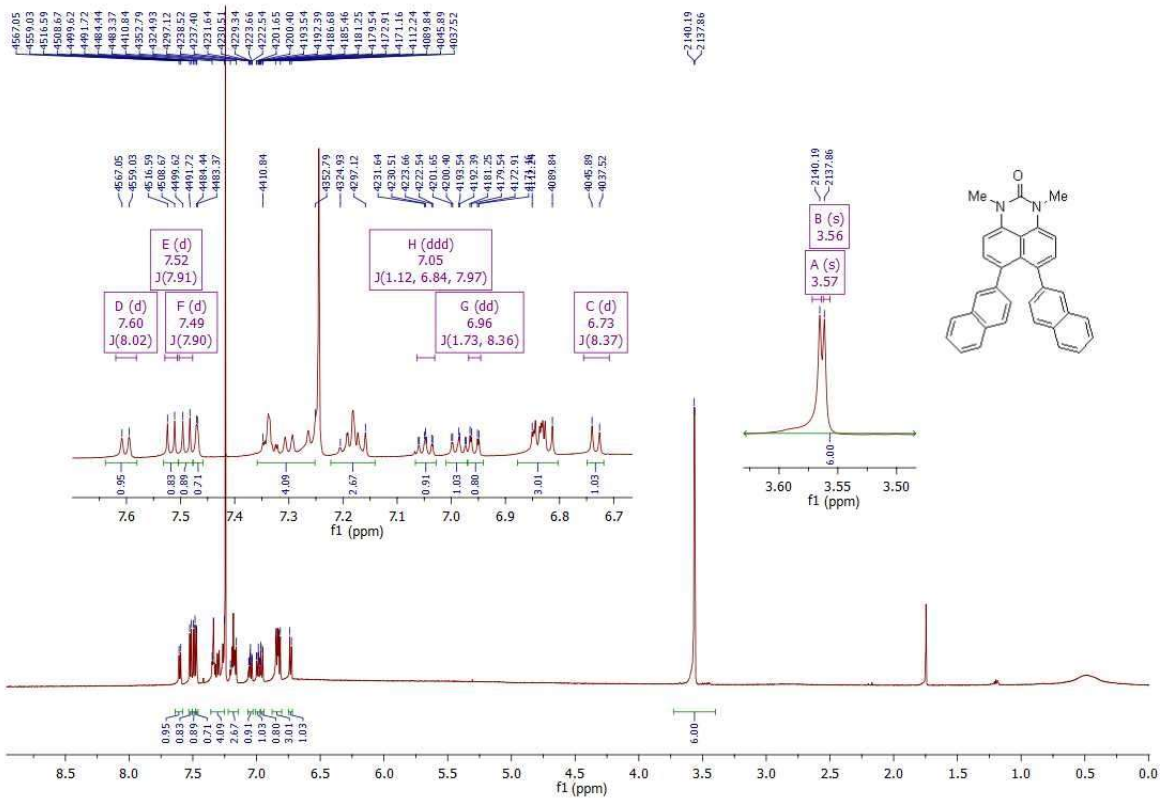


Fig. S46. ^{1}H NMR spectrum of compound **3f** (600 MHz, $CDCl_3$, -45 ºC).

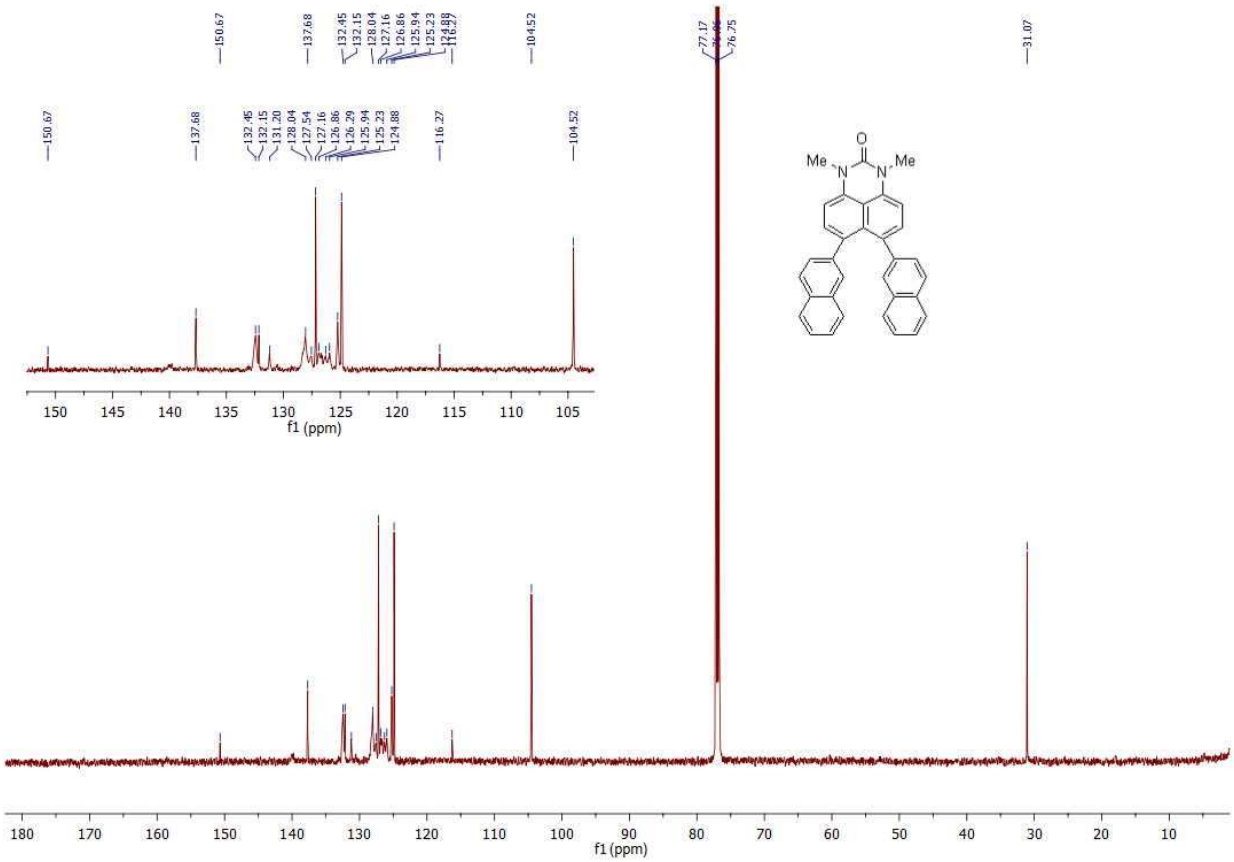


Fig. S47. $^{13}C\{^{1}H\}$ APT-NMR spectrum of compound **3f** (150 MHz, $CDCl_3$, +30 °C).

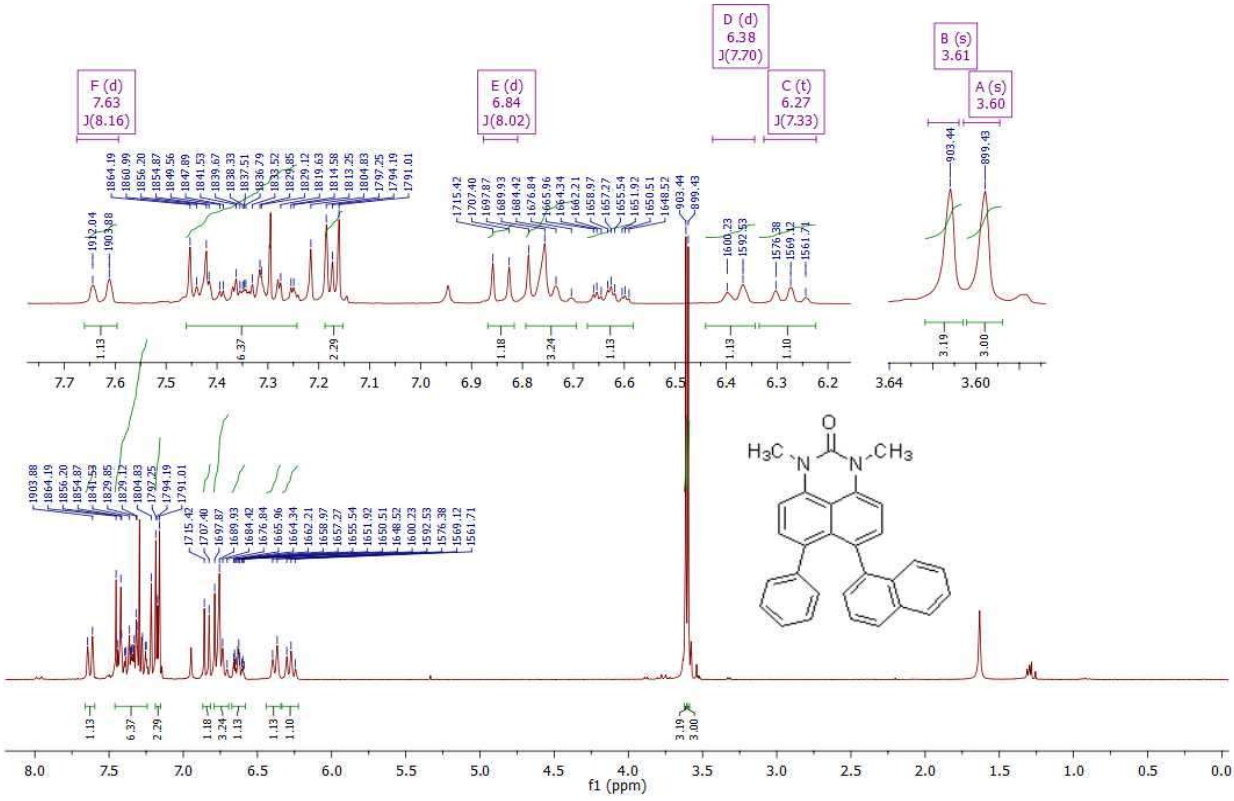


Fig. S48. ^{1}H NMR spectrum of compound **3g** (250 MHz, $CDCl_3$).

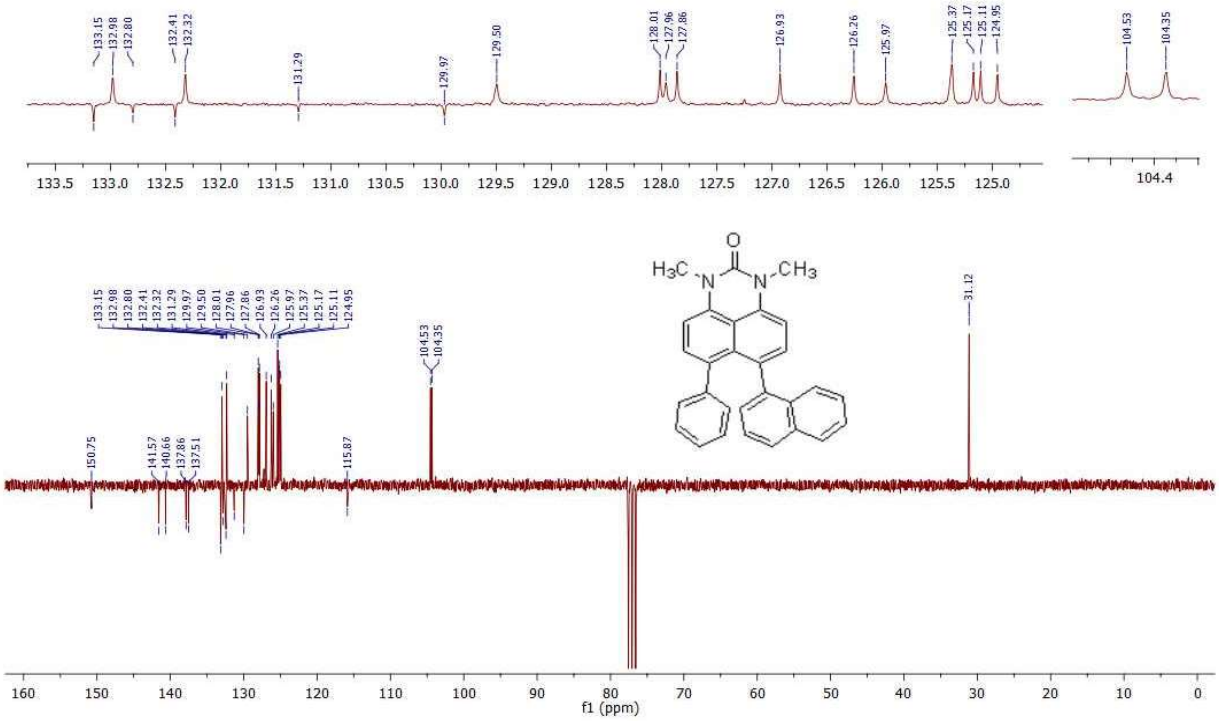


Fig. S49. $^{13}C\{^{1}H\}$ APT-NMR spectrum of compound **3g** (62.9 MHz, $CDCl_3$).

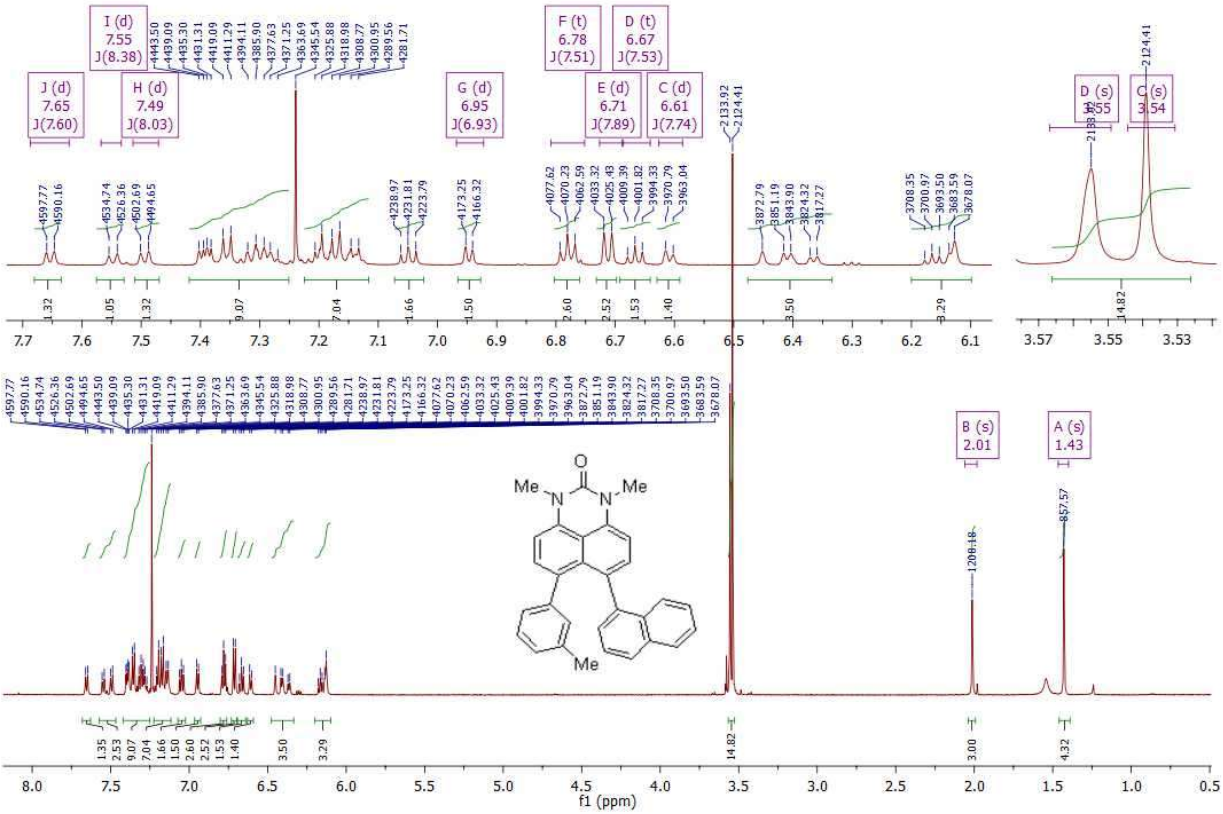


Fig. S50. ^{1}H NMR spectrum of compound **3h** (600 MHz, $CDCl_3$, +30 ^{o}C).

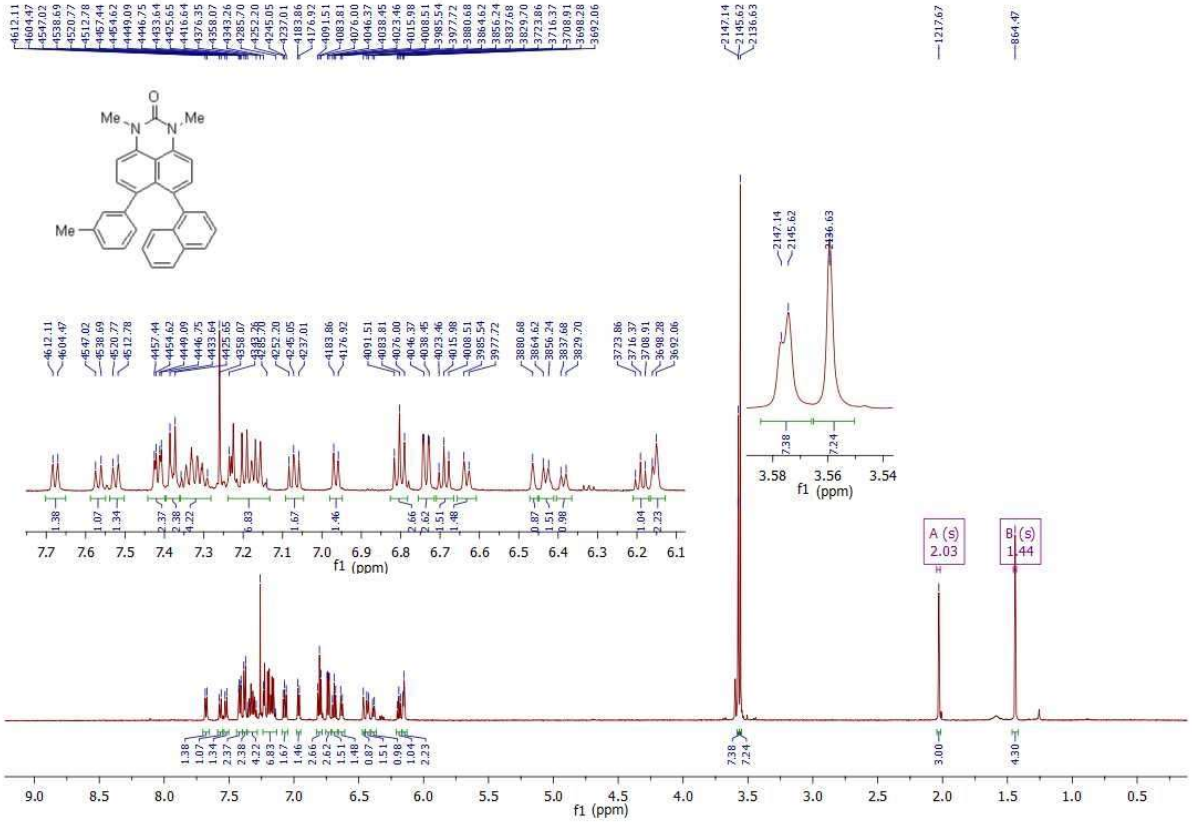


Fig. S51. ^{1}H NMR spectrum of compound **3h** (600 MHz, $CDCl_3$, +20 ºC).

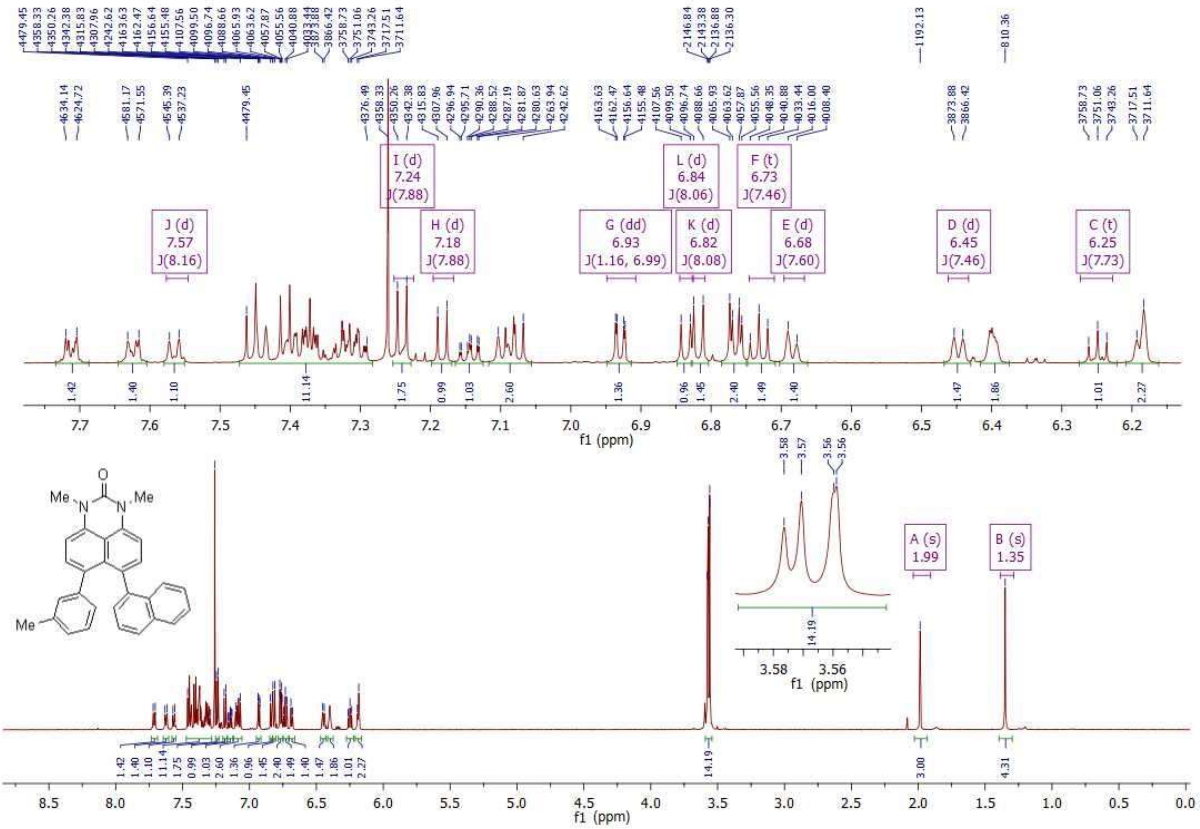


Fig. S52. ^{1}H NMR spectrum of compound **3h** (600 MHz, $CDCl_3$, –50 ºC).

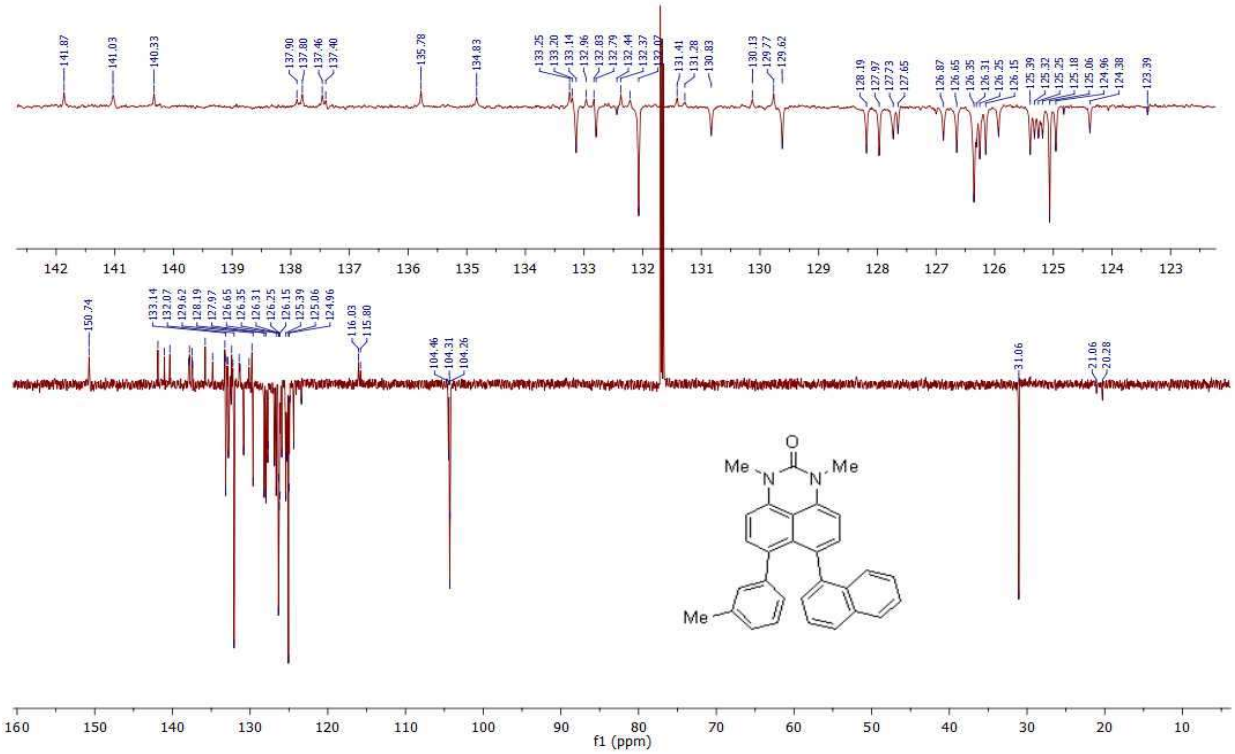


Fig. S53. ^{13}C APT-NMR spectrum of compound **3h** (150 MHz, DMSO-d_6).

UV-vis, excitation and emission spectra

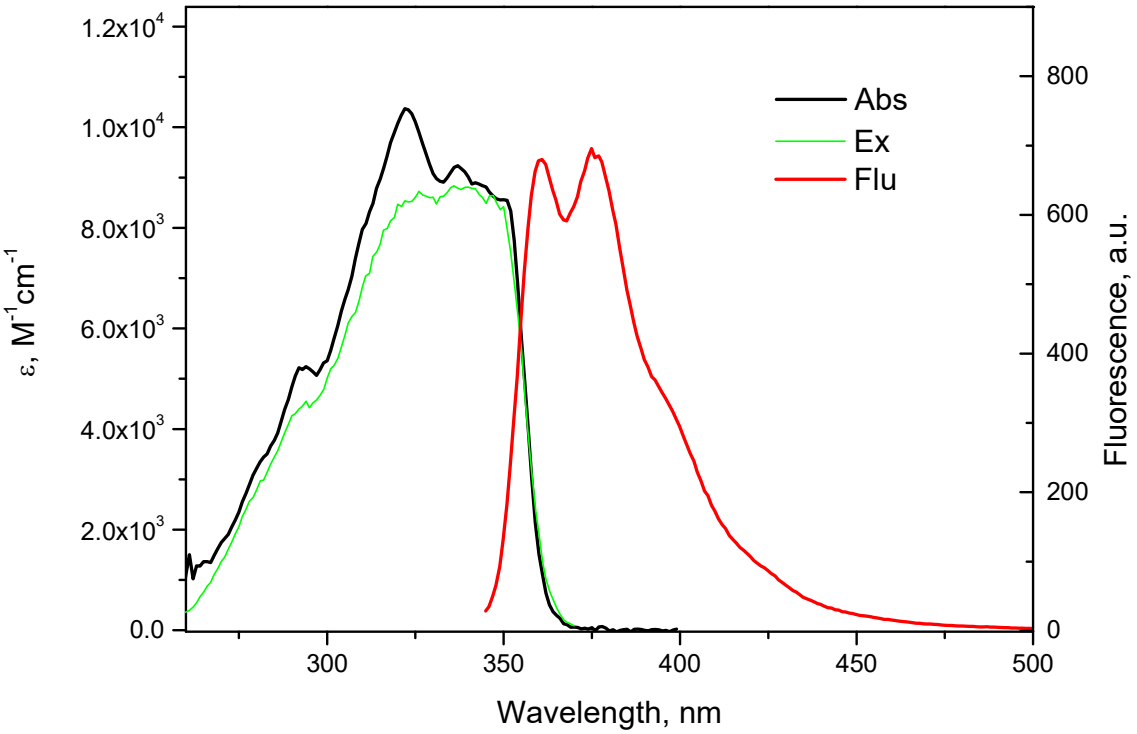


Fig. S54. Absorption, excitation and emission spectra of 1,3-dimethyl-1*H*-perimidin-2(3*H*)-one in DMSO, T = 293 K.

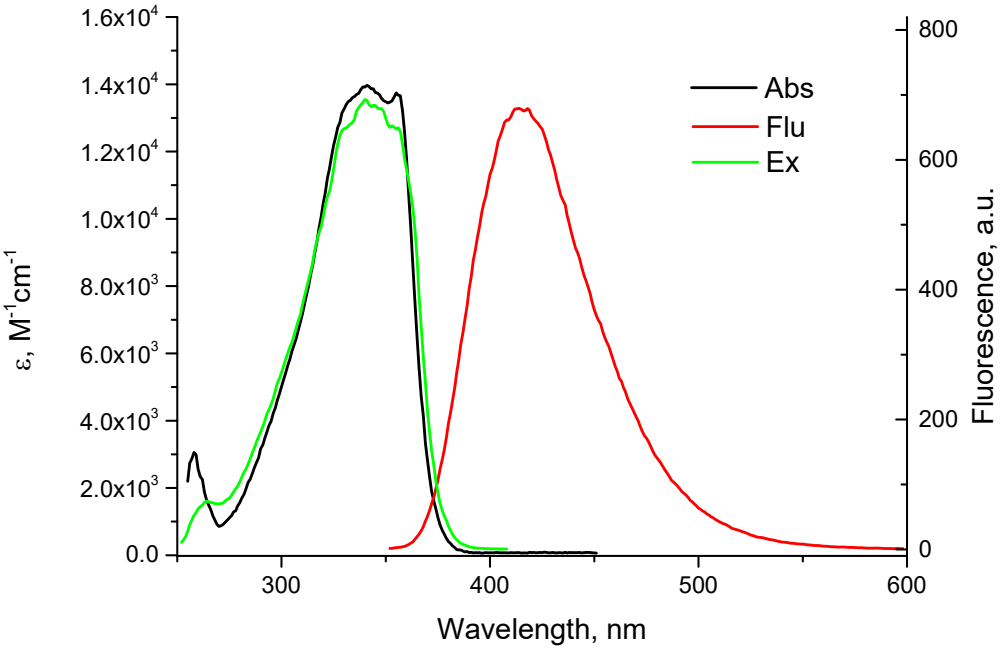


Fig. S55. Absorption, excitation and emission spectra of **6a** in DMSO, T = 293 K.

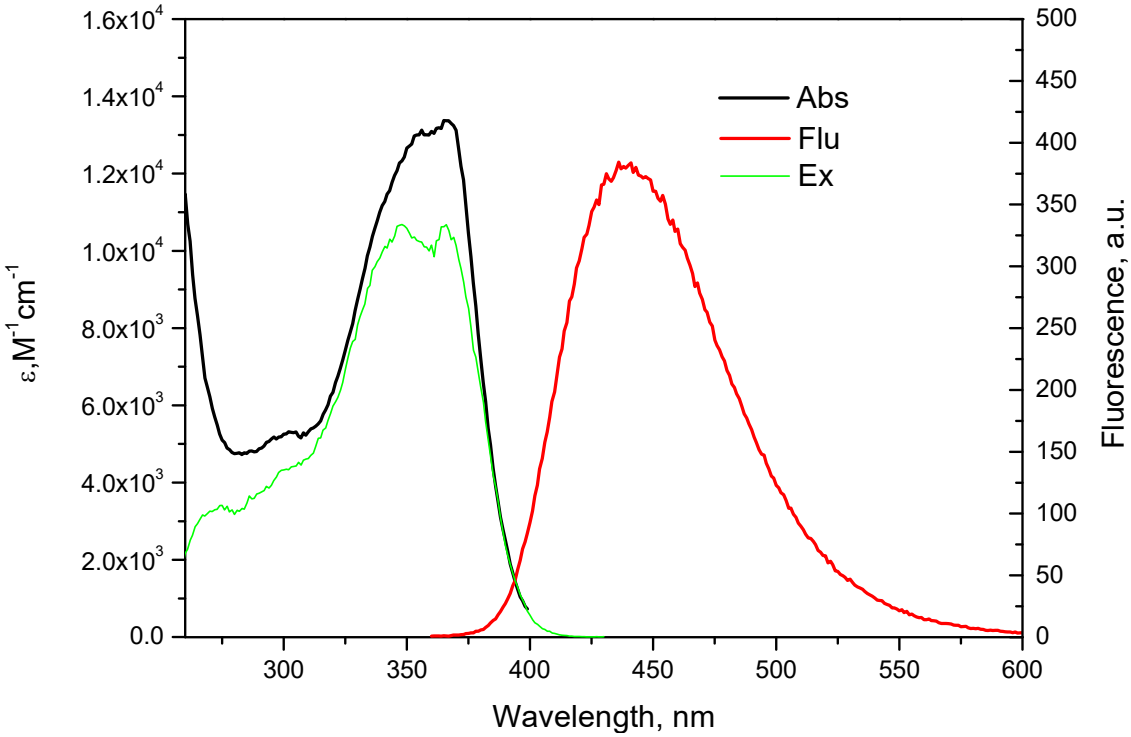


Fig. S56. Absorption, excitation and emission spectra of **6d** in DMSO, T = 293 K.

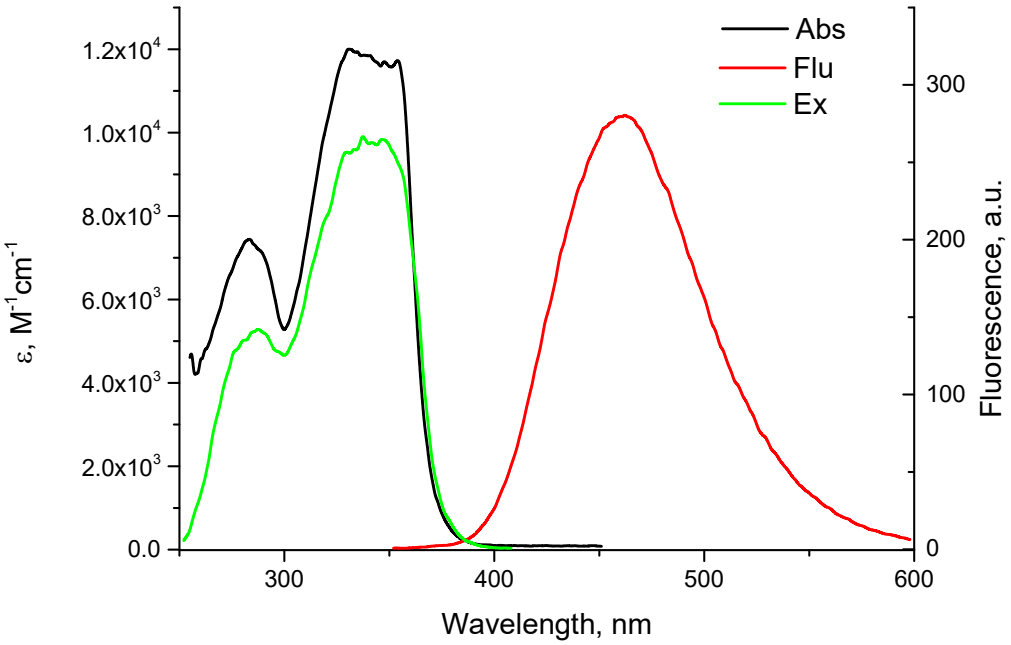


Fig. S57. Absorption, excitation and emission spectra of **6e** in DMSO, T = 293K.

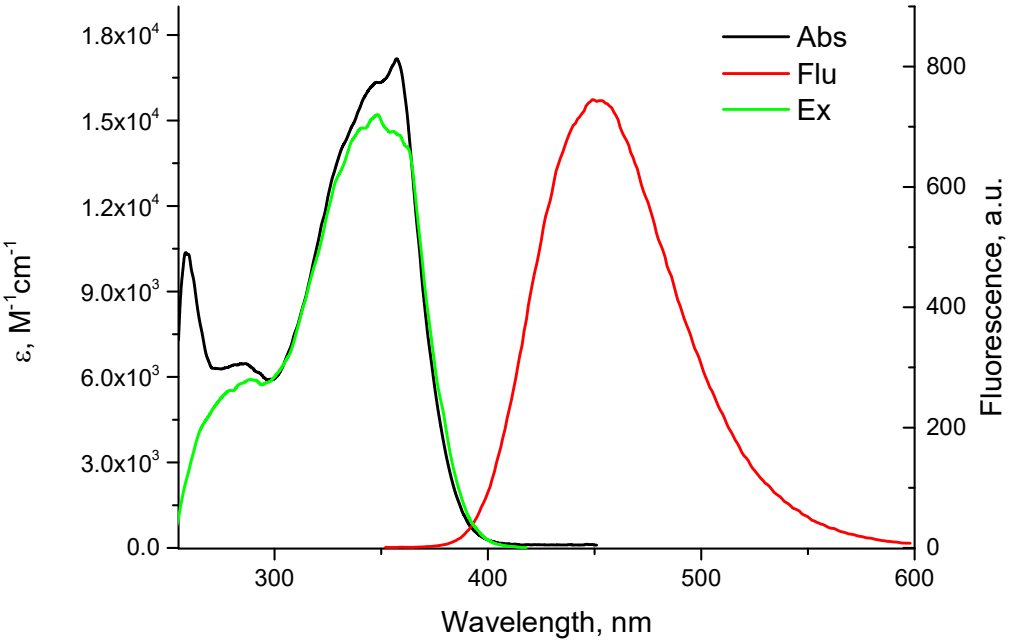


Fig. S58. Absorption, excitation and emission spectra of **6f** in DMSO, T = 293K.

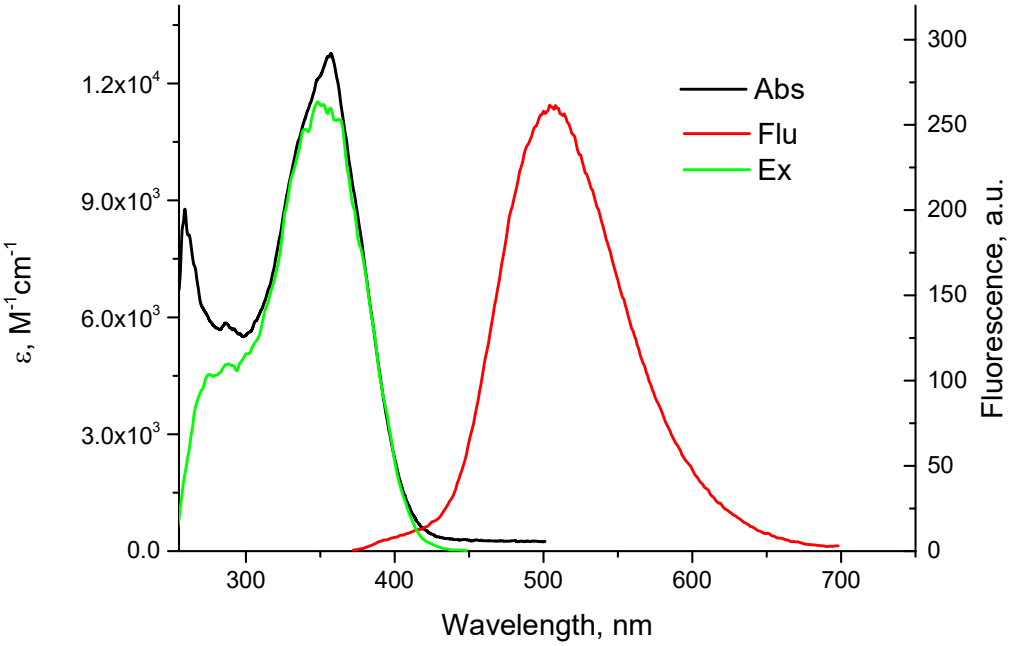


Fig. S59. Absorption, excitation and emission spectra of **6h** in DMSO, T = 293K.

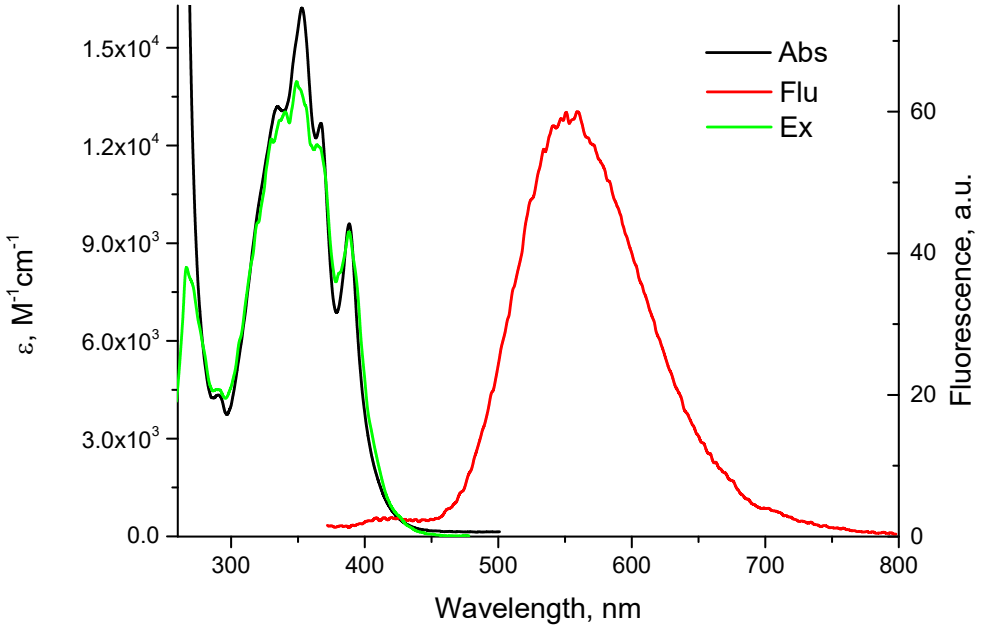


Fig. S60. Absorption, excitation and emission spectra of **6i** in DMSO, T = 293K.

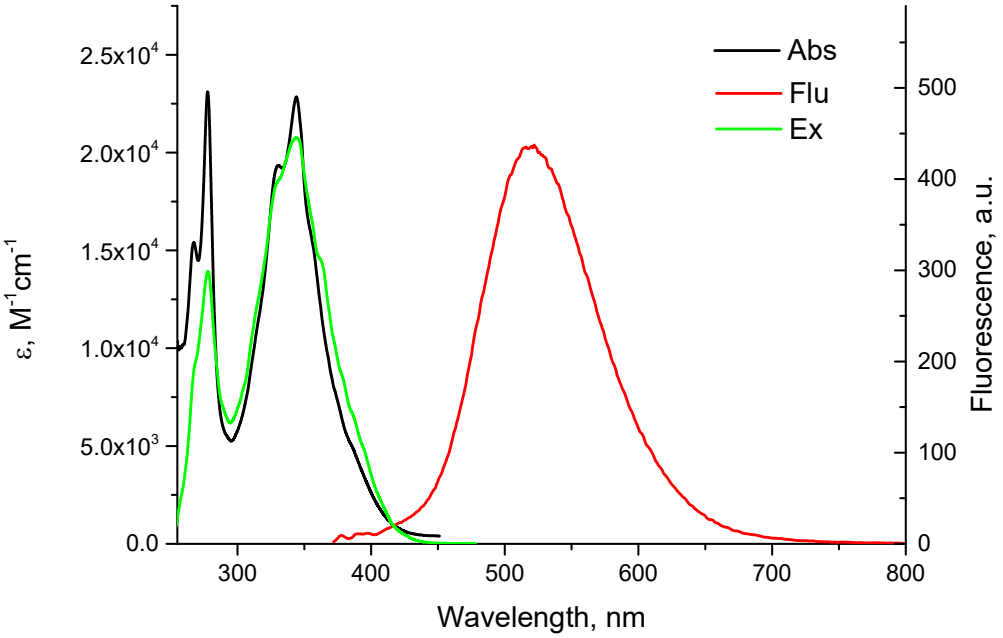


Fig. S61. Absorption, excitation and emission spectra of **6j** in DMSO, T = 293K.

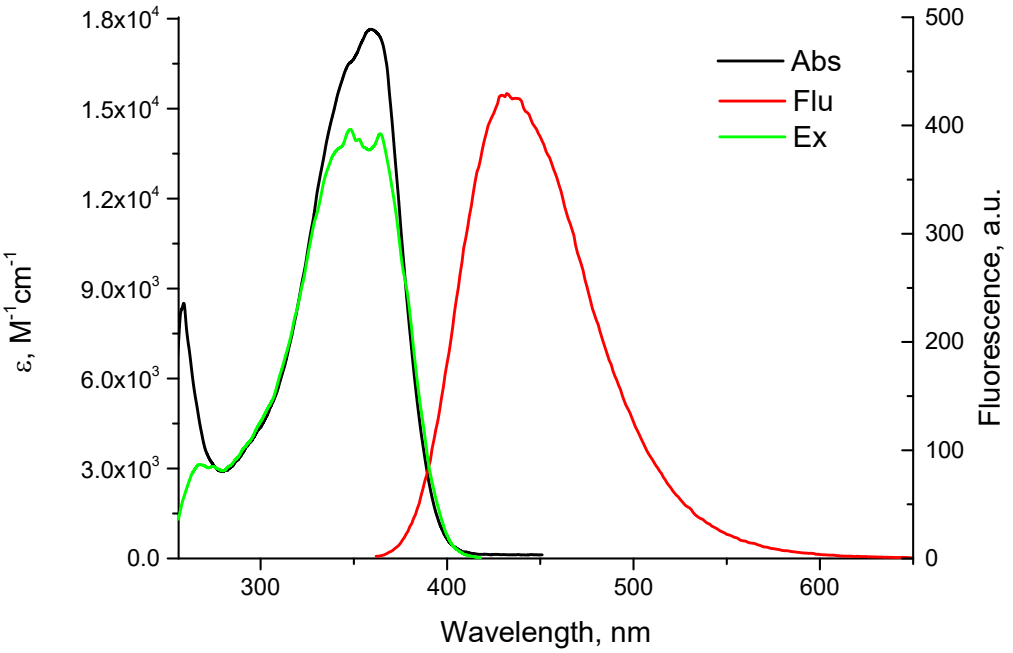


Fig. S62. Absorption, excitation and emission spectra of **3a** in DMSO, T = 293K.

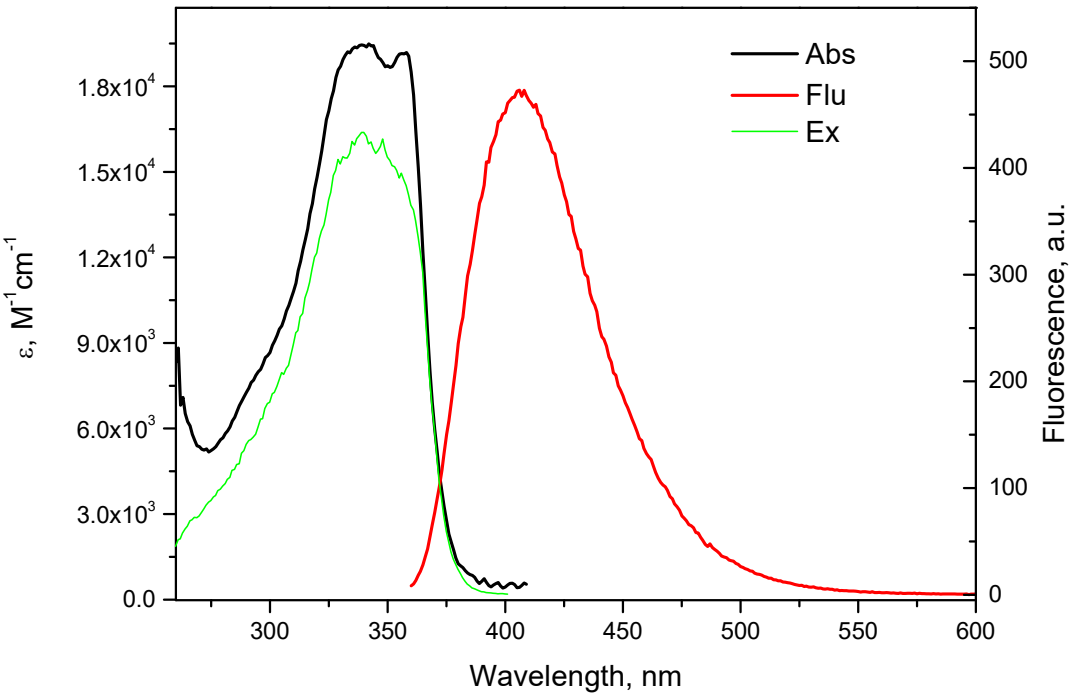
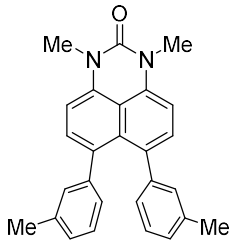


Fig. S63. Absorption, excitation and emission spectra of **3c** in DMSO, T = 293K.

Calculations of the experimental *syn/anti*-isomerization barrier of compounds 3b and 3f

The *syn/anti*-isomerization barriers of compounds **3** were determined by the dynamic NMR, coalescence method (H. Günther, *NMR Spectroscopy: An Introduction*, John Wiley and Sons, Chichester – New York – Brisbane – Toronto, 1980, 436 p.).



For compound **3b**, signals of the C-methyl groups were used for calculations, $\Delta\nu_{AB}$ - difference in chemical shifts of signals of C-Me groups of rotamers under conditions of rapid exchange, $\Delta\nu_{AB}^{*}$ - difference in chemical shifts of signals of C-Me groups of rotamers under conditions of slow exchange (-50 °C).

Calculation of the *syn/anti*-isomerization barrier using the Eyring equation, T_{coal} = 328K (see Fig.5 in the main text and Table S1):

$$\Delta G^{\neq} = 19.14T[10.32 - \log (k/T)],$$

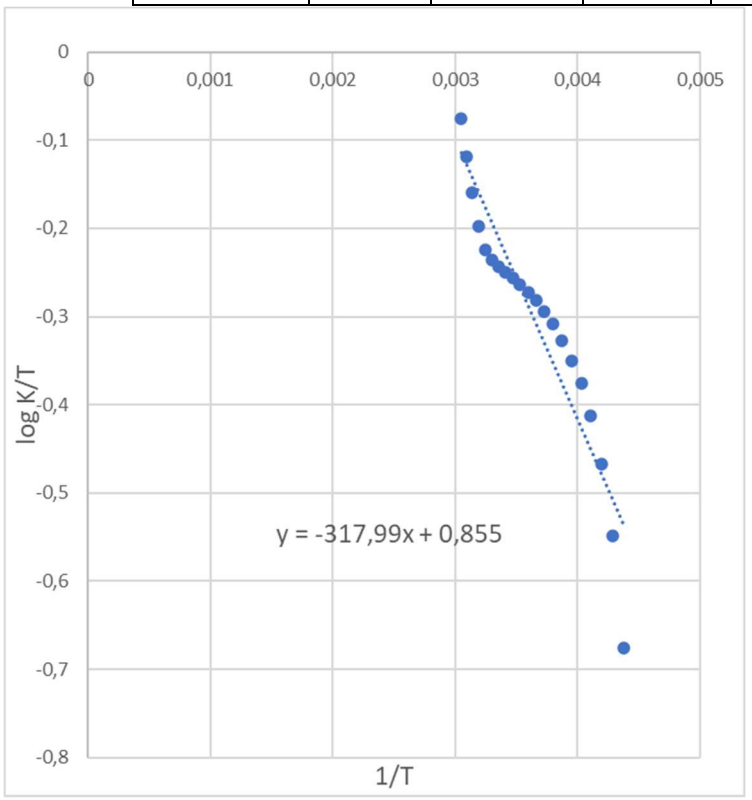
the rate constant at the coalescence point can be estimated using the formula: $k = \pi\, \Delta\nu_{AB}^{*} / \sqrt{2}$

$$\Delta G^{\neq} = 19.14 \times 328(10.32 - (-0.075)) = 65\ 259\ \text{J mol}^{-1} = 15.59\ \text{kcal mol}^{-1}$$

Table S1. Calculation of the activation parameters of *syn/anti*-isomerization of compound **3b** using the Eyring plot

T, °C	T, K	1/T	$\Delta\nu_{AB}$, Hz	$\Delta\nu_{AB}^2$	$\sqrt{(\Delta\nu_{AB}^{*2} - \Delta\nu_{AB}^2)}$	$k = \pi \sqrt{(\Delta\nu_{AB}^{*2} - \Delta\nu_{AB}^2)} / \sqrt{2}$	k/T	log k/T
-50	223.15	0,00448	124.4	15475				
-45	228.15	0,00438	122.5	15006	21.656	48.108	0.2109	-0,676
-40	233.15	0,00429	120.8	14593	29.698	65.972	0.2830	-0,548
-35	238.15	0,00420	118.9	14137	36.579	81.258	0.3412	-0,467
-30	243.15	0,00411	117.0	13689	42.261	93.880	0.3861	-0,413
-25	248.15	0,00403	115.2	13271	46.947	104.290	0.4203	-0,376
-20	253.15	0,00395	113.5	12882	50.922	113.120	0.4468	-0,350
-15	258.15	0,00387	111.7	12477	54.754	121.633	0.4712	-0,327
-10	263.15	0,00380	109.9	12078	58.284	129.474	0.4920	-0,308
-5	268.15	0,00373	108.2	11707	61.384	136.361	0.5085	-0,294
0	273.15	0,00366	106.5	11342	64.288	142.812	0.5228	-0,282
+5	278.15	0,00360	105.0	11025	66.708	148.188	0.5328	-0,273

+10	283.15	0,00353	103.2	10650	69.462	154.306	0.5450	-0,264
+15	288.15	0,00347	101.5	10302	71.923	159.773	0.5545	-0,256
+20	293.15	0,00341	99.8	9960	74.263	164.971	0.5628	-0,250
+25	298.15	0,00335	98.0	9604	76.622	170.211	0.5709	-0,243
+30	303.15	0,00330	95.9	9197	79.233	176.011	0.5806	-0,236
+35	308.15	0,00325	92.8	8612	82.843	184.031	0.5972	-0,224
+40	313.15	0,00319	86.6	7500	89.303	198.381	0.6335	-0,198
+45	318.15	0,00314	75.3	5670	99.020	219.967	0.6914	-0,160
+50	323.15	0,00309	56.7	3215	110.725	245.969	0.7612	-0,119
+55 Coalescence	328.15	0,00305	83			276.347	0.8421	-0,075

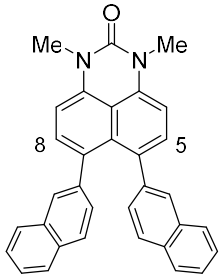


$-317.99 = -\Delta H^{\neq} / 19.14$ $\Delta H^{\neq} = 6086.32$ J mol^{-1}

$0.855 = 10.32 + \Delta S^{\neq}/19.14$ $\Delta S^{\neq} = -181.16$ J mol^{-1} K^{-1}

$\Delta G^{\neq} = \Delta H^{\neq} - T\Delta S^{\neq}$ for 328 K

$\Delta G^{\neq} = 65506$ J mol^{-1} = 15.66 kcal mol^{-1}



Calculation of the *syn/anti*-isomerization barrier of compound **3f** using the Eyring equation,

T_{coal} = 298K (see Fig.7, main text, Table S2):

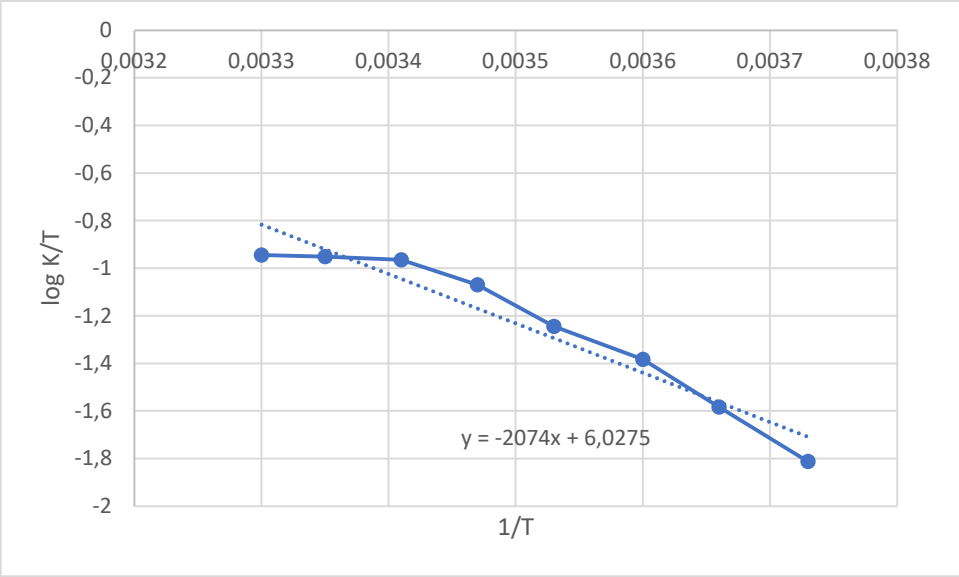
$\Delta G^{\neq} = 19.14T[10.32 - \log (k/T)] = 19.14 \times 298(10.32 - (-0.891)) = 63944$ J mol^{-1} = 15.28 kcal mol^{-1}

Table S2. Calculation of the *syn/anti*-isomerization barrier of compound **3f** using the Eyring plot

(signals of the H(5), H(8) protons at -10….+30 °C were used for calculations, $\Delta\nu_{AB}$ - difference in chemical shifts of signals of the H(5), H(8) protons of rotamers under conditions of rapid exchange, $\Delta\nu_{AB}^{*}$ - difference in chemical shifts of signals of the H(5), H(8) protons of rotamers under conditions of slow exchange (-10 °C))

T, °C	T, K	1/T	$\Delta\nu_{AB}$, Hz	$\Delta\nu_{AB}^2$	$\sqrt{(\Delta\nu_{AB}^{*2} - \Delta\nu_{AB}^2)}$	$k = \pi\sqrt{(\Delta\nu_{AB}^{*2} - \Delta\nu_{AB}^2)}/\sqrt{2}$	k/T	log k/T
-45	228,15	0,00438	17,0	289				
-40	233,15	0,00429	17,1	292,41				
-35	238,15	0,00420	17,1	292,41				
-30	243,15	0,00411	17,2	295,84				
-25	248,15	0,00403	17,2	295,84				
-20	253,15	0,00395	17,2	295,84				
-15	258,15	0,00387	17,2	295,84				
-10	263,15	0,00380	17,2	295,84				
-5	268,15	0,00373	17,1	292,41	1,85	4,12	0,0154	-1,8124
0	273,15	0,00366	16,9	285,61	3,20	7,13	0,0261	-1,5833
+5	278,15	0,00360	16,4	268,96	5,18	11,53	0,0414	-1,3830
+10	283,15	0,00353	15,6	243,36	7,24	16,12	0,0569	-1,2448
+15	288,15	0,00347	13,2	174,24	11,02	24,54	0,0852	-1,0695
+20	293,15	0,00341	9,6	92,16	14,27	31,77	0,1084	-0,9650

+25 Coalescence	298,15	0,00335	8.5	72,25	14.95	33,29	0,1117	-0,9519
+30	303,15	0,00330	7.5	56,25	15,48	34,47	0,1137	-0,9442
+35	308,15	0,00324	7.7	59,29	15,38	34,25	0,1111	-0,9543
+40	313,15	0,00319	7.8	60,84	15,33	34.14	0,1090	-0,9625
+45	318,15	0,00314	7.8	60,84	15,33	34.14	0,1073	-0,9694
+50	323,15	0,00309	7.8	60,84	15,33	34.14	0,1056	-0,9763



$-2074 = -\Delta H^{\neq} / 19.14 \qquad \Delta H^{\neq} = 39\,696{,}36 \text{ J mol}^{-1}$

$6.0275 = 10.32 + \Delta S^{\neq}/19.14 \qquad \Delta S^{\neq} = -82.158 \text{ J mol}^{-1} \text{ K}^{-1}$

$\Delta G^{\neq} = \Delta H^{\neq} - T\Delta S^{\neq}$ for 298 K $\quad \Delta G^{\neq} = 64\,179 \text{ J mol}^{-1} = 15.34 \text{ kcal mol}^{-1}$

Dynamic NMR simulation for compounds 3b and 3f

Spectral parameters were determined by iterative full line shape analysis using the gNMR simulation program: P. H. M. Budzelaar, gNMR, Version 5.0.6.0, 2006

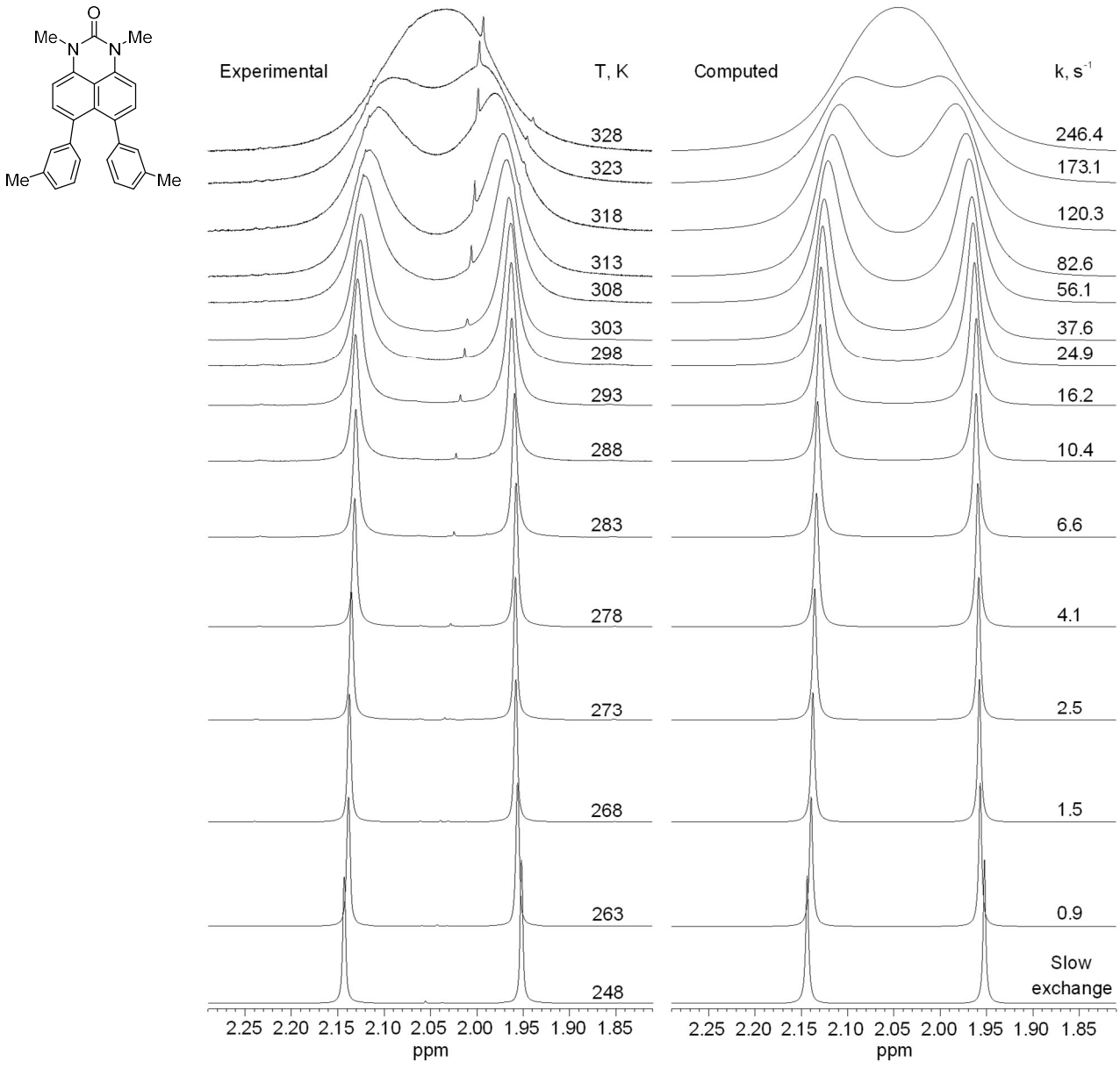


Figure S64. Experimental and calculated NMR of the methyl resonances for compound **3b**

Table S3. The data on dynamic NMR simulation for compound **3b** using the Eyring equation (signals of the C-methyl groups were used for calculations)

T, K	k, s^{-1}	$\Delta G^{\#}_{sim}$, kcal mol^{-1}
223,15	0,01	15,20
263,15	0,90	15,38
268,15	1,52	15,40
273,15	2,53	15,42
278,15	4,12	15,44
283,15	6,61	15,46
288,15	10,44	15,49
293,15	16,24	15,51
298,15	24,88	15,53
303,15	37,60	15,55
308,15	56,09	15,57
313,15	82,62	15,60
318,15	120,27	15,62
323,15	173,09	15,64
328,15	246,42	15,66

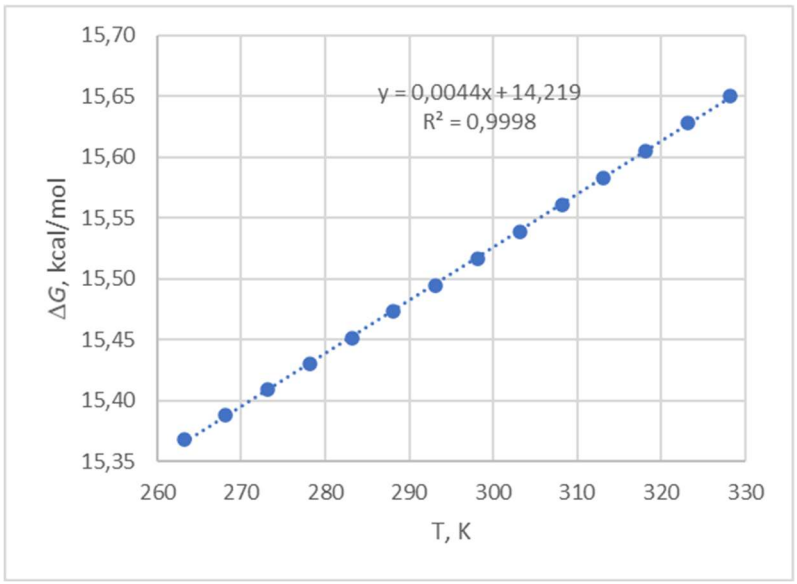
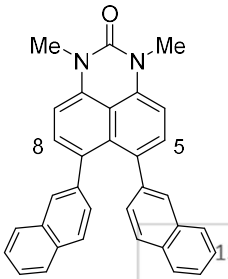
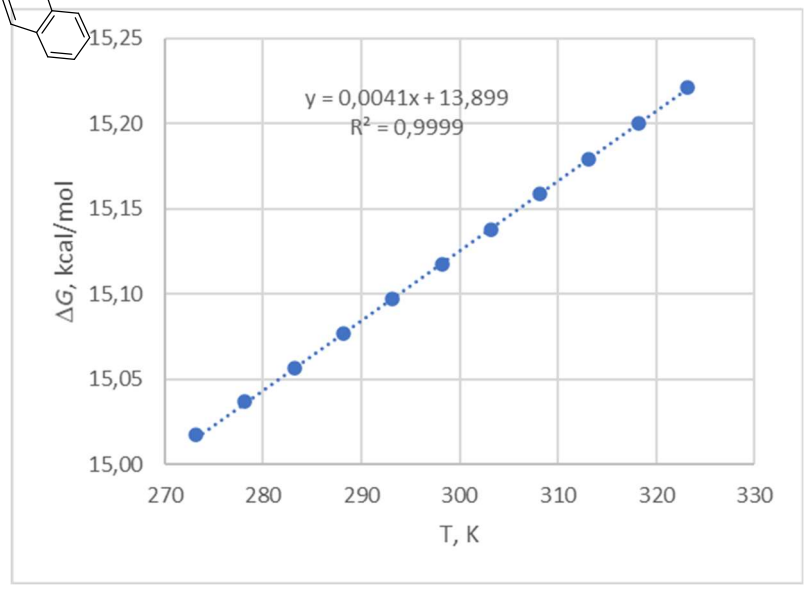


Table S4. The data on dynamic NMR simulation for compound **3f** using the Eyring equation (signals of the H(5), H(8) protons at 0….+50 ºC were used for calculations)



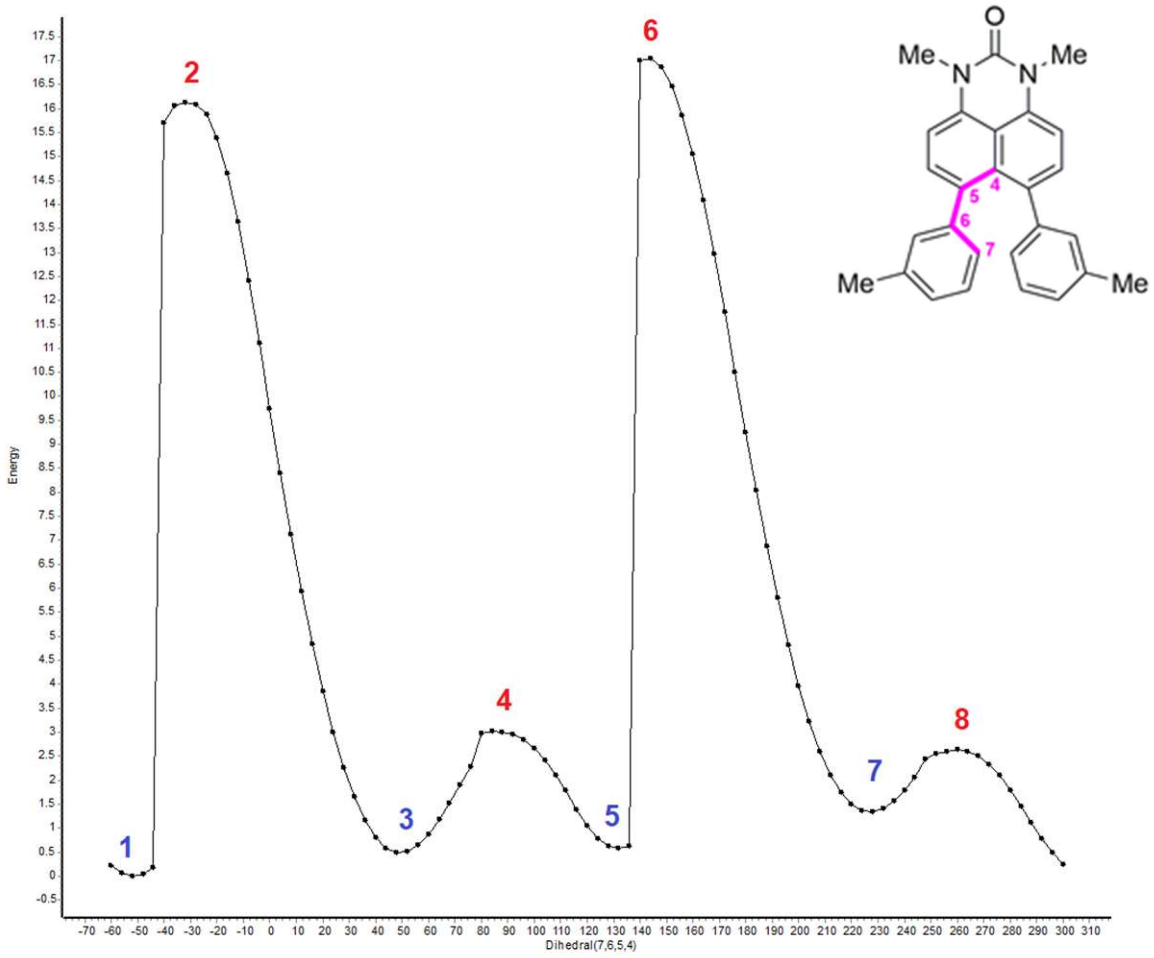


T, K	k, s^{-1}	$\Delta G^{\#}_{sim}$, kcal mol^{-1}
223,15	0,01	14,81
273,15	5,30	15,02
278,15	8,56	15,04
283,15	13,60	15,06
288,15	21,26	15,08
293,15	32,74	15,10
298,15	49,70	15,12
303,15	74,45	15,14
308,15	110,10	15,16
313,15	160,84	15,18
318,15	232,25	15,20
323,15	331,63	15,22

Quantum-chemical calculations of the *syn/anti* isomerization barriers of compounds 3

Theoretical Calculations. All calculations were performed using the PBE0 exchange-correlation functional[3] with the def2-SVP basis set[4] and D3(BJ) dispersion correction[5]. Relaxed surface scans were conducted using the ORCA 5.04 software[6], with solvent effects (chloroform) considered through the CPCM model.[7] The naphthyl-aryl torsion was changed in four-degree increments (from 300 to -60 degree). The corresponding dihedral angle was fixed and the rest of the molecule fully relaxed. These calculations were carried out for 91 points and resulted in smooth and continuous energy profiles. The structures corresponding to the maxima and minima on the energy profile are given in Tables S5–S8. The atom coordinates of the optimized structures of *syn*- and *anti*-isomers and their energies are given in Table S9.

Table S5. Dependence of the rotamer energy on dihedral angle C(7)-C(6)-C(5)-C(4) for compound **3b**



Dihedral (7,6,5,4)	Energy	Dihedral (7,6,5,4)	Energy
300	0,25487617932	120	1.04588255095
296	0,48359133065	116	1.39436733890
292	0,77687789239	112	1.79414897770
288	1,11472960336	108	2.09350306367
284	1,45781584292	104	2.41556256302
280	1,79787482418	100	2.66235757527
276	2,09760639650	96	2.83879787072
272	2,33291006451	92	2.95519873382
268	2,50398128266	88	3.00998951805
264	2,60761847641	**84**	**3.01397382180**
260	**2,63671189819**	80	2.97100952526
256	2,60254463221	76	2.28839569578
252	2,55442367965	72	1.91079344874
248	2,44248459305	68	1.53098357858
244	2,06630184395	64	1.18110268122
240	1,78576181994	60	0.87694573114
236	1,56209140127	56	0.65076129101
232	1,41216684044	52	0.50854591390
228	**1,34464718458**	**48**	**0.48914731805**
224	1,37186499189	44	0.58841386290
220	1,49941143587	40	0.81236407551
216	1,74153436127	36	1.16671574828
212	2,10833183853	32	1.65233535609
208	2,60517506358	28	2.25257050831
204	3,22696621129	24	2.99411462273
200	3,96790247305	20	3.85956235037
196	4,82257871139	16	4.84507389534
192	5,78999909169	12	5.93841368088
188	6,86418705509	8	7.12826866318
184	8,02991285197	4	8.40586383977
180	9,25698848809	0	9.74082803079
176	10,51438844923	-4	11.09803785838
172	11,76751812097	-8	12.41681480732
168	12,97770141910	-12	13.64636882365
164	14,08986649901	-16	14.65338957578
160	15,05462932264	-20	15.38475841594
156	15,86269675135	-24	15.87492333846
152	16,46905361205	-28	16.08675721042
148	16,85656719034	**-32**	**16.12578297825**
144	**17,04302254636**	-36	16.05010974950
140	17,00370659184	-40	15.70818922877
136	0,63477557551	-44	0.18302006077

132	**0,57068365662**	-48	0.03478110646
128	0,61649318798	**-52**	**0.00000000000**
124	0,78072197921	-56	0.06531492626
		-60	0.22127187216

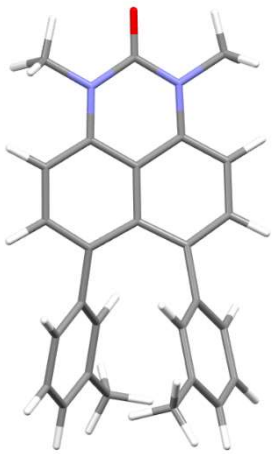
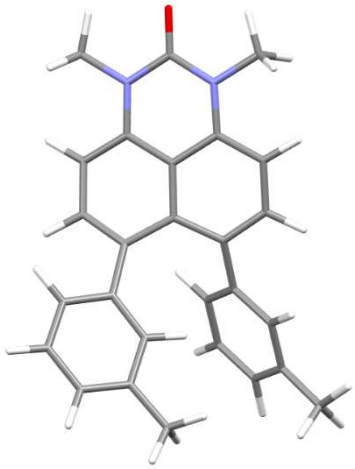
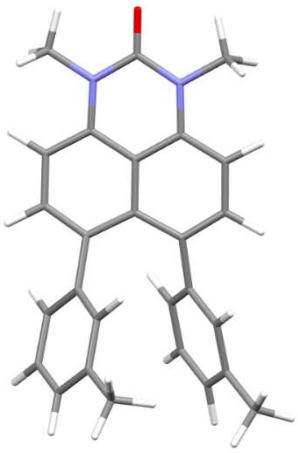
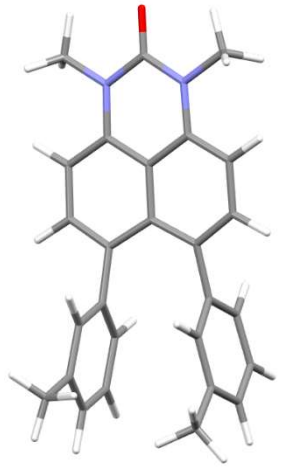
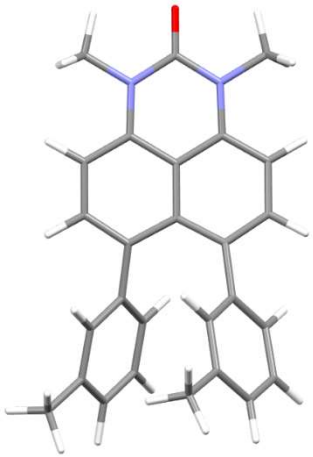
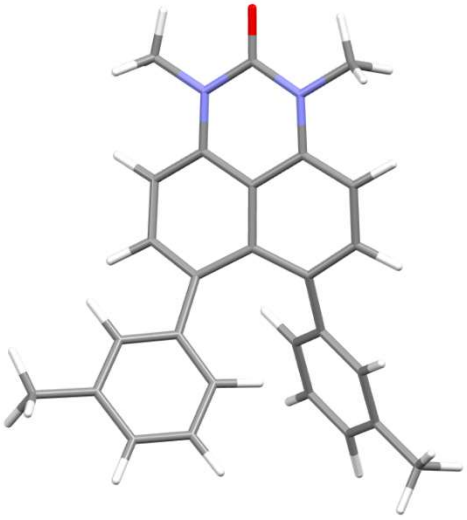
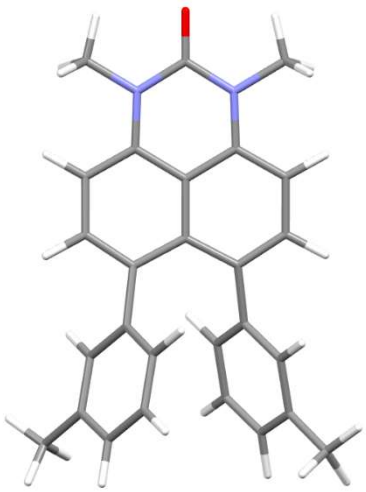
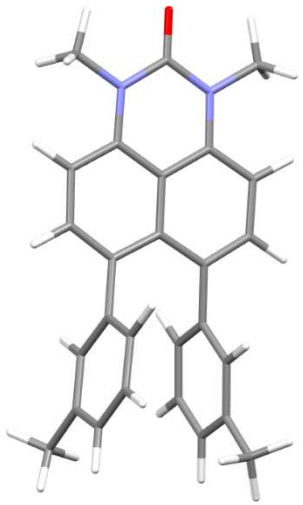
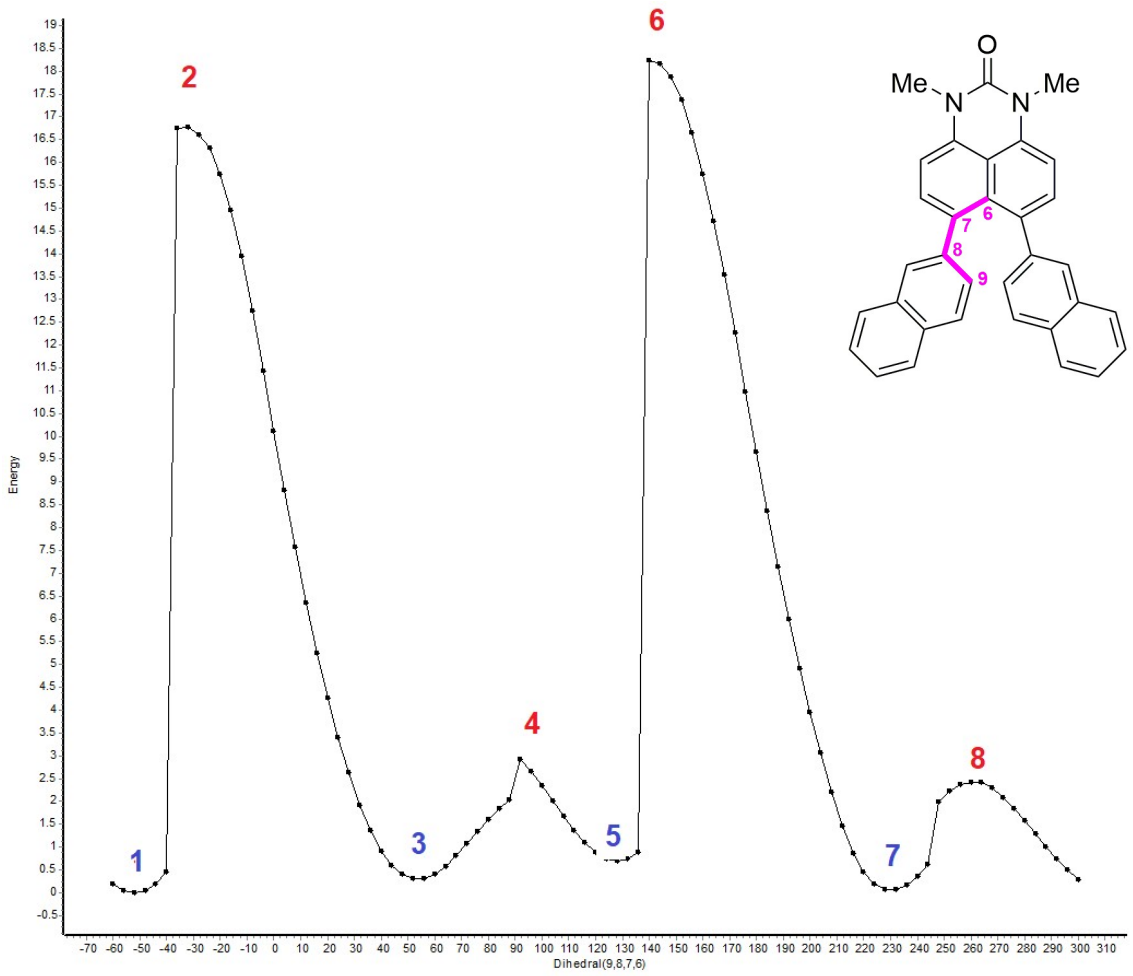
			
1 Minimum *anti*-conformer	**2**	**3** Minimum *syn*-conformer	**4**
			
5	**6**	**7**	**8**

Table S6. Dependence of the rotamer energy on dihedral angle C(9)-C(8)-C(7)-C(6) for compound **3f**



Dihedral (9,8,7,6)	Energy	Dihedral (9,8,7,6)	Energy
300	0.28703355991	116	1.09756000769
296	0.49766046949	112	1.37192767440
292	0.74498332393	108	1.68622671172
288	1.01686844949	104	2.02255057136
284	1.29454984511	100	2.35689172926
280	1.57040375664	96	2.66330840647
276	1.83905665861	**92**	**2.92212206039**
272	2.08531329208	88	2.04554230354
268	2.28717379732	84	1.83663678926
264	2.40725717596	80	1.59856360127
260	**2.42724405261**	76	1.34310318924
256	2.37338770774	72	1.07442971893
252	2.23666908108	68	0.80590182572
248	1.98375775262	64	0.57097316301
244	0.62273385206	60	0.40012209464
240	0.36270662172	**56**	**0.31176313773**
236	0.17170488918	52	0.31288116948
232	0.06447794644	48	0.40833545166
228	**0.06012707729**	44	0.60693842702
224	0.18254689536	40	0.92101843844
220	0.44932034364	36	1.35851913043
216	0.87248183043	32	1.92264035739
212	1.45803540215	28	2.64247911779
208	2.21100875186	24	3.39687600354
204	3.07483943201	20	4.26641893087
200	3.94709316472	16	5.25467625602
196	4.91645022945	12	6.35848428375
192	5.97711761393	8	7.55837541630
188	7.13189263276	4	8.81120008342
184	8.36498464920	0	10.10422494861
180	9.65005894525	-4	11.42669384732
176	10.96589311322	-8	12.73918414256
172	12.27392422115	-12	13.93769606962
168	13.53257710048	-16	14.94173855119
164	14.71285062641	-20	15.74556682009
160	15.75116127008	-24	16.30625485789
156	16.64824833731	-28	16.61449315109
152	17.36661256143	**-32**	**16.76684088458**
148	17.87517673270	-36	16.73832815676
144	18.15945456913	-40	0.46360662458
140	**18.23091365672**	-44	0.19314661524
136	0.89353897784	-48	0.04106898250

132	0.73465189891	**-52**	**0.00000000000**
128	**0.68785141582**	-56	0.05640049730
124	0.73900479610	-60	0.19345788747
120	0.88097878222		

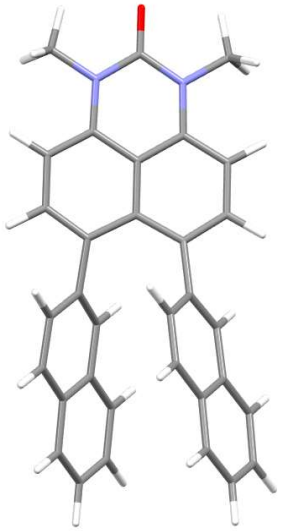
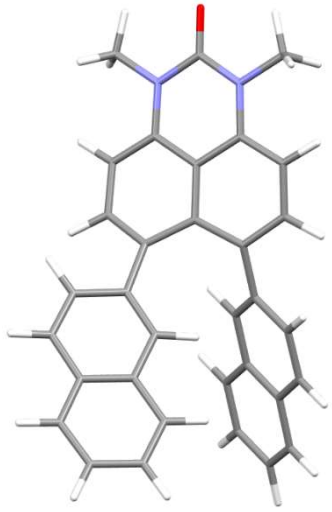
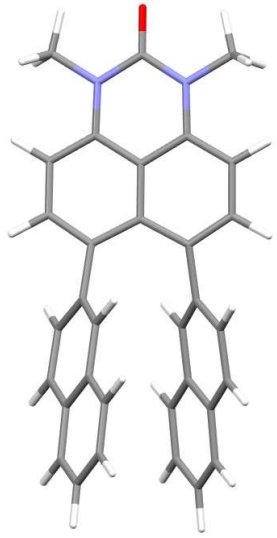
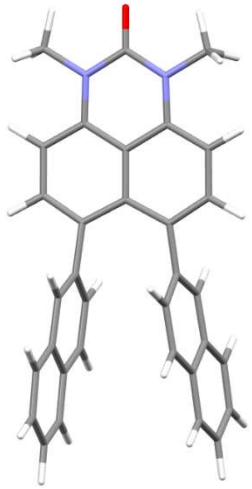
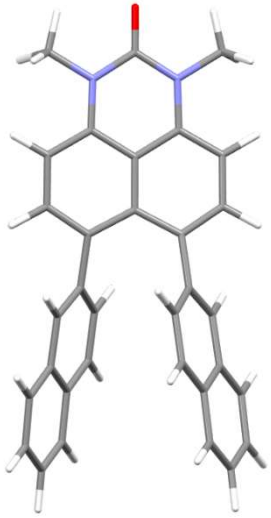
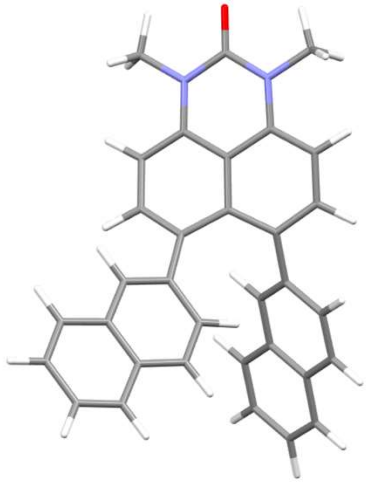
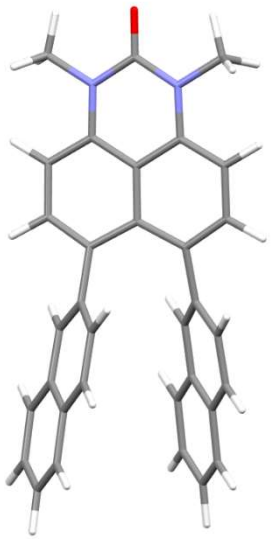
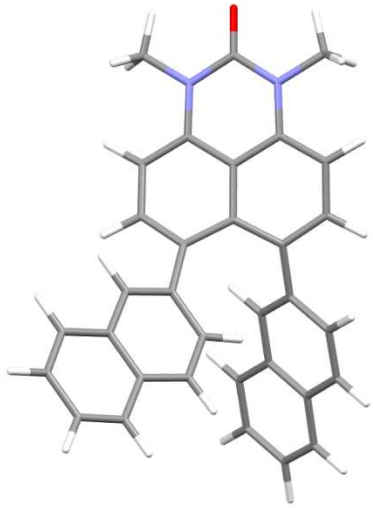
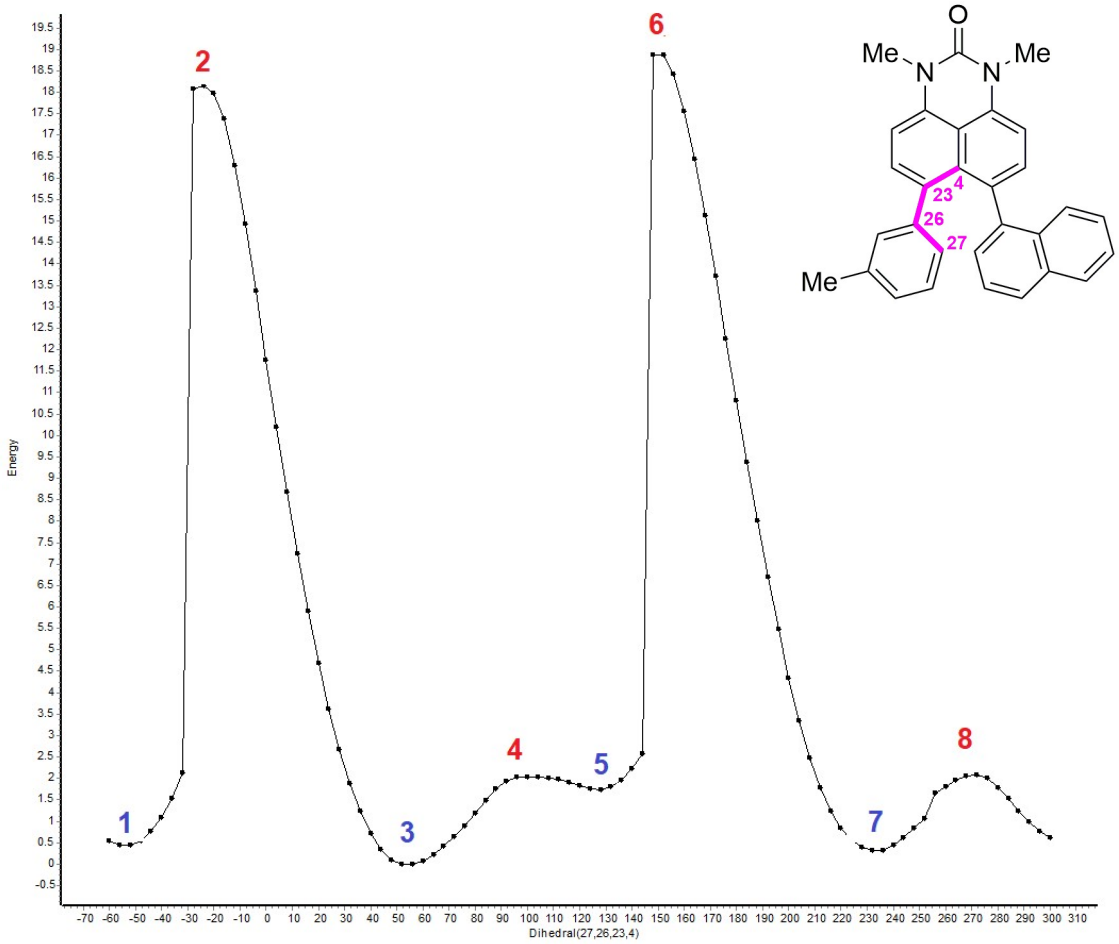
			
1 Minimum *syn*-conformer	**2**	**3** Minimum *anti*-conformer	**4**
			
5	**6**	**7**	**8**

Table S7. Dependence of the rotamer energy on dihedral angle C(28)-C(27)-C(24)-C(5) for compound **3h**



Dihedral (28,27,24,5)	Energy	Dihedral (28,27,24,5)	Energy
300	0.61032891374	116	1.91993030963
296	0.76391917052	112	1.98703488604
292	0.98134802395	108	2.01962963199
288	1.24726950183	104	2.03169267014
284	1.52849817414	**100**	**2.04124495034**
280	1.79059473756	96	2.02115606966
276	2.00462146536	92	1.93318219391
272	**2.09092006698**	88	1.75777072521
268	2.05637430920	84	1.49012477786
264	1.95308488630	80	1.19512000599
260	1.81592125381	76	0.90110762490
256	1.66491261928	72	0.63483782200
252	1.07040621095	68	0.40961006478
248	0.83120893504	64	0.21976828469
244	0.61282258001	60	0.07612097558
240	0.43418399878	**56**	**0.00000000000**
236	0.32644277251	52	0.00087605164
232	**0.30898504915**	48	0.10951512921
228	0.39140823489	44	0.34353251808
224	0.56014567187	40	0.71302923444
220	0.83250302843	36	1.22833087599
216	1.23106243491	32	1.87781535962
212	1.78492444876	28	2.67296919330
208	2.48728645397	24	3.61258302607
204	3.34078412793	20	4.68733024861
200	4.34657091080	16	5.90040462478
196	5.46711926917	12	7.23673168797
192	6.68707675765	8	8.67334768649
188	7.99640966108	4	10.18320538597
184	9.38140741714	0	11.76403572321
180	10.81131510629	-4	13.36342900068
176	12.25744398759	-8	14.91710586920
172	13.70789123118	-12	16.28516091210
168	15.12315333992	-16	17.37688253013
164	16.43258046138	-20	17.96732093684
160	17.56779034455	**-24**	**18.16118085904**
156	18.43237269267	-28	18.06558430864
152	18.86461354422	-32	2.13092852784
148	**18.86867370962**	-36	1.54830526993
144	2.58523630062	-40	1.09425048068
140	2.21854408619	-44	0.76452525125
136	1.96134990429	-48	0.55251578821

132	1.80701490035	-52	0.44544835277
128	**1.74422247268**	**-56**	**0.43982809968**
124	1.76125839112	-60	0.53795333909
120	1.84170675801		

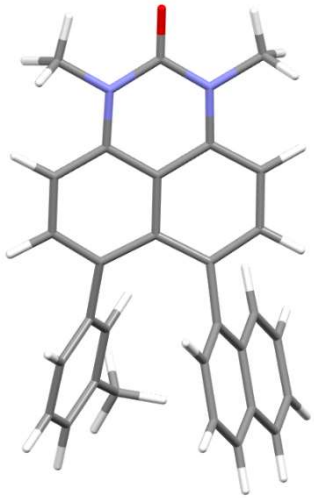
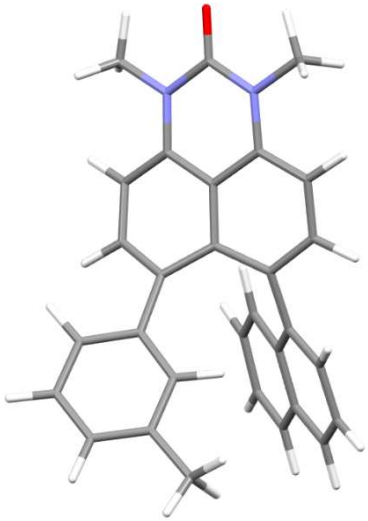
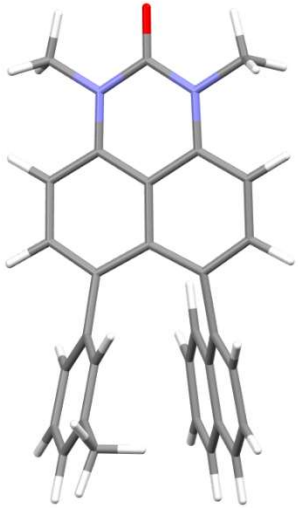
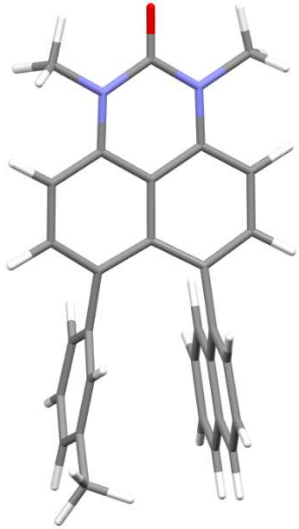
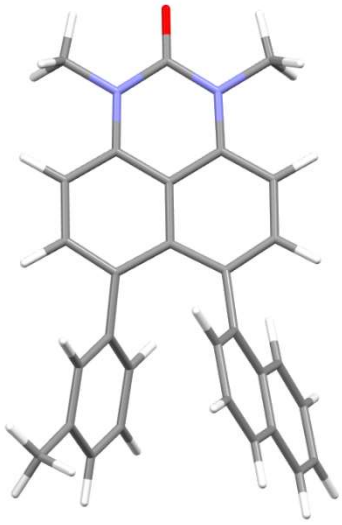
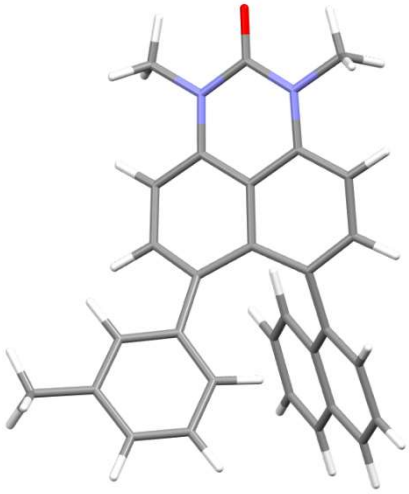
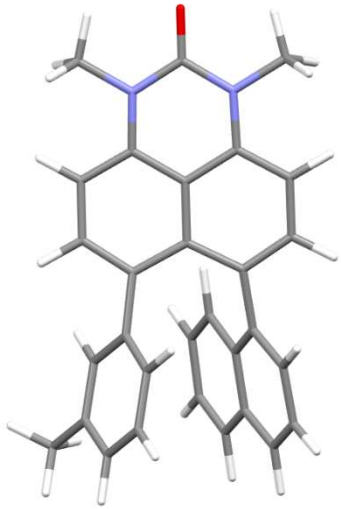
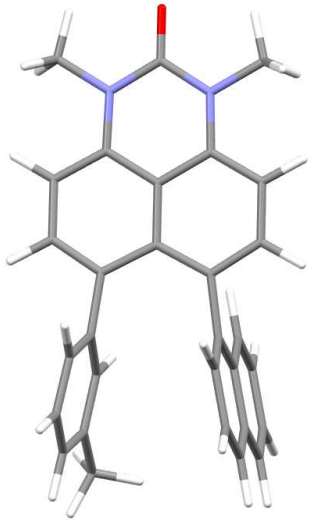
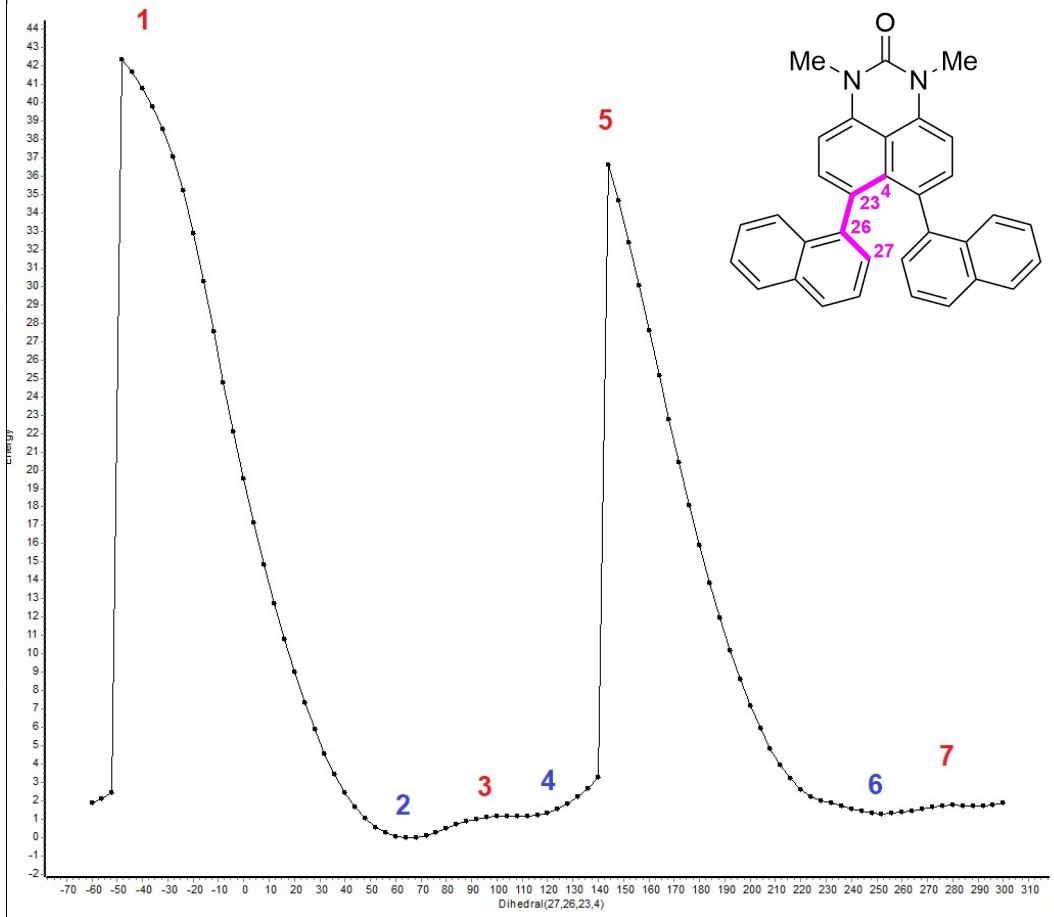
			
1	**2**	**3** Minimum *anti*-conformer	**4**
			
5	**6**	**7** Minimum *syn*-conformer	**8**

Table S8. Dependence of the rotamer energy on dihedral angle C(28)-C(27)-C(24)-C(5) for compound **3d**



Dihedral (28,27,24,5)	Energy	Dihedral (28,27,24,5)	Energy
300	1.89936564039	116	1.22646293836
296	1.77513113013	112	1.16036084415
292	1.70713665792	**108**	**1.13899405460**
288	1.69543101475	104	1.14522311430
284	1.72682706529	**100**	**1.15171558110**
280	**1.76577942941**	96	1.10917514648
276	1.71781320937	92	1.00880112200
272	1.64187236992	88	0.87990337914
268	1.54569679317	84	0.71158665401
264	1.44603677735	80	0.50188797840
260	1.36526128829	76	0.29125509184
256	1.31517360991	72	0.12585010057
252	**1.30317887070**	68	0.02490893435
248	1.33878320741	**64**	**0.00000000000**
244	1.43331163394	60	0.06880109718
240	1.56089646189	56	0.25463764405
236	1.72370633560	52	0.57322669030
232	1.91565847773	48	1.03986438657
228	1.98904412810	44	1.66654153482
224	2.23806249613	40	2.46069496015
220	2.63655333715	36	3.42600328452
216	3.20272616318	32	4.56405017077
212	3.94574845148	28	5.87310362226
208	4.86535443006	24	7.34849450148
204	5.95090596295	20	8.98514085490
200	7.19583676389	16	10.78153089488
196	8.60746517719	12	12.73773117066
192	10.19364667522	8	14.84990204589
188	11.95062405960	4	17.11479198690
184	13.86815581131	0	19.52771287858
180	15.92517993553	-4	22.08385746357
176	18.10532717527	-8	24.76472419447
172	20.39172487767	-12	27.51914756027
168	22.76484773455	-16	30.28047447231
164	25.17644166013	-20	32.90973122443
160	27.60467344548	-24	35.20863241820
156	30.03015177993	-28	37.06229922499
152	32.40173448810	-32	38.53542790173
148	34.64865288022	-36	39.77790654418
144	**36.62451981643**	-40	40.80307988164
140	3.26147820092	-44	41.66025755870
136	2.67920586137	**-48**	**42.34056444424**

	132	2.21502840765	-52	2.43447490551
	128	1.85091174319	-56	2.09162728839
	124	1.56819704865	-60	1.87032140396
	120	1.36014328947		

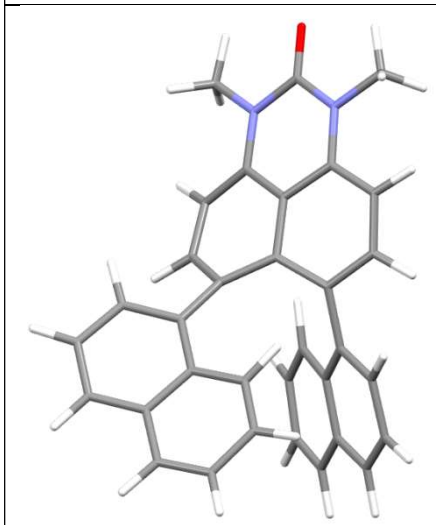
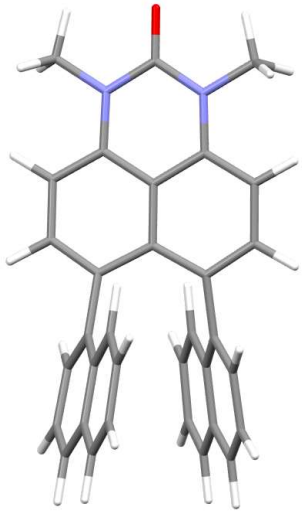
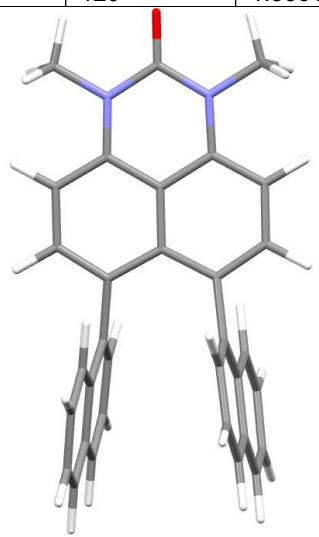
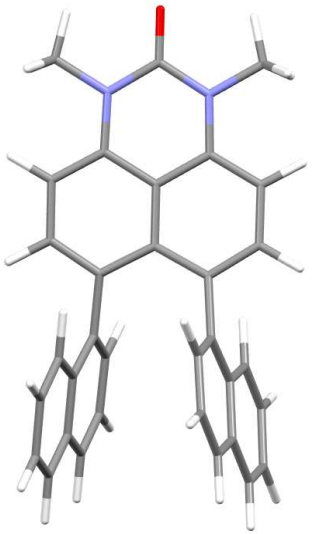
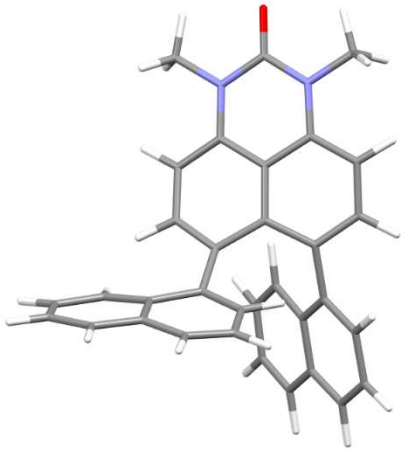
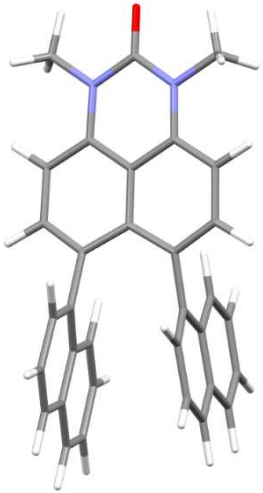
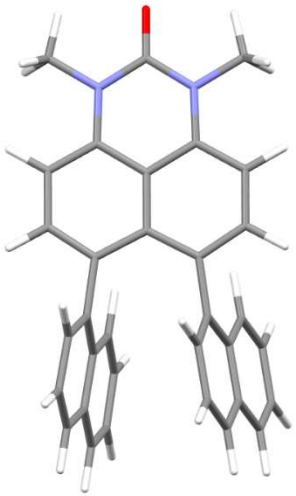
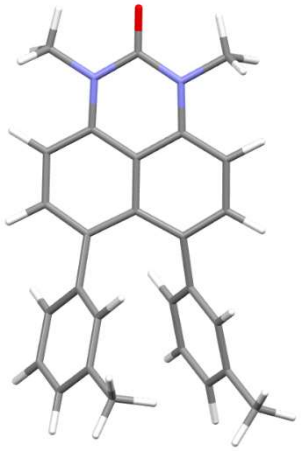
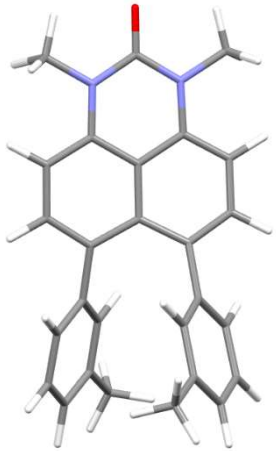
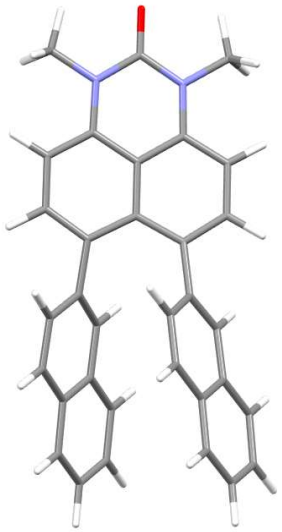
			
1	**2** Minimum *anti*-conformer	**3**	**4**
			
5	**6** Minimum *syn*-conformer	**7**	

Table S9 Optimized structures and their energies

Structure of compound	Absolute energy (a.u.) and atom coordinates	Structure of compound	Absolute energy (a.u.) and atom coordinates
Syn-**3b**		*Anti*-**3b**	
	FINAL SINGLE POINT ENERGY -1225.920236995705 C 3.001815000 -1.164566000 -1.399621000 N 3.098975000 0.274192000 -1.535502000 C 1.953765000 1.045961000 -1.364041000 C 2.047095000 2.459996000 -1.492971000 C 0.892290000 3.296878000 -1.318855000 C 1.092567000 4.720969000 -1.321560000 C 0.086324000 5.708291000 -0.861345000 C -0.572739000 5.537933000 0.361459000 C -1.497871000 6.471351000 0.838734000 C -2.227531000 6.221685000 2.125997000 C -1.744177000 7.616935000 0.072299000 C -1.077862000 7.816377000 -1.136412000 C -0.170596000 6.869888000 -1.603835000 C 2.343076000 5.213282000 -1.658764000 C 3.446836000 4.394188000 -1.926413000 C 3.318229000 3.020207000 -1.800693000 N 4.408947000 2.172528000 -1.967024000		FINAL SINGLE POINT ENERGY -1225.921016501542 C 2.984057000 -0.866105000 -2.931318000 N 3.075696000 0.477236000 -2.397394000 C 1.905752000 1.145343000 -2.048972000 C 1.991587000 2.468365000 -1.531636000 C 0.809297000 3.197930000 -1.162003000 C 0.968927000 4.574866000 -0.778231000 C -0.146730000 5.539795000 -0.616565000 C -1.090025000 5.722301000 -1.633994000 C -2.127820000 6.652114000 -1.518506000 C -3.161634000 6.771554000 -2.599463000 C -2.195923000 7.434819000 -0.358937000 C -1.248275000 7.286343000 0.652792000 C -0.230428000 6.344437000 0.528493000 C 2.250657000 5.080133000 -0.633405000 C 3.406479000 4.338736000 -0.906764000 C 3.284155000 3.047130000 -1.393115000 N 4.402547000 2.300639000 -1.751382000 C 5.717194000 2.890008000 -1.600961000 C 4.338951000 1.016030000 -2.253629000 O 5.343127000 0.392332000 -2.555046000 C -0.446181000 2.497476000 -1.204906000 C -1.709359000 2.997400000 -0.608796000 C -1.749790000 3.433243000 0.720477000 C -2.934870000 3.876856000 1.315002000 C -2.925292000 4.409317000 2.717513000 C -4.111989000 3.850792000 0.555978000 C -4.095854000 3.392915000 -0.760595000 C -2.903411000 2.970547000 -1.342802000 C -0.477738000 1.223434000 -1.747884000 C 0.664471000 0.547208000 -2.193986000 H 2.506866000 -1.540280000 -2.203839000 H 3.998170000 -1.215930000 -3.141537000 H 2.393973000 -0.872932000 -3.860417000 H -1.017729000 5.113273000 -2.539221000 H -3.722162000 7.714025000 -2.522491000

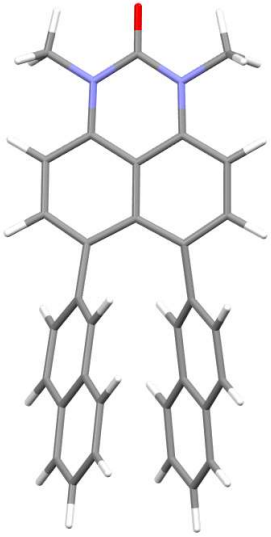
C	5.700578000	2.744615000	-2.286789000
C	4.339735000	0.799276000	-1.838838000
O	5.321011000	0.089670000	-1.986168000
C	-0.381218000	2.649754000	-1.157067000
C	-1.691847000	3.336636000	-1.266295000
C	-2.682898000	3.135038000	-0.295114000
C	-3.948993000	3.717019000	-0.398277000
C	-4.990373000	3.499333000	0.661725000
C	-4.223014000	4.515635000	-1.516639000
C	-3.255268000	4.712518000	-2.499636000
C	-1.996950000	4.127230000	-2.380435000
C	-0.412172000	1.273353000	-1.002836000
C	0.729604000	0.465298000	-1.073872000
H	2.658351000	-1.435053000	-0.389466000
H	3.994574000	-1.588329000	-1.572902000
H	2.294274000	-1.575165000	-2.136058000
H	-0.361393000	4.645883000	0.957161000
H	-2.733130000	7.128069000	2.487912000
H	-2.994418000	5.440792000	1.988253000
H	-1.545485000	5.866723000	2.913352000
H	-2.463837000	8.359228000	0.428820000
H	-2.707619000	6.715748000	-3.600196000
H	-3.886344000	5.942628000	-2.526593000
H	-2.999722000	8.168627000	-0.251623000
H	-1.309363000	7.905232000	1.551874000
H	0.496557000	6.212618000	1.333866000
H	2.365941000	6.125722000	-0.337820000
H	4.380814000	4.806277000	-0.780989000
H	6.456518000	2.155242000	-1.930667000
H	5.804970000	3.799726000	-2.214363000
H	5.904752000	3.153029000	-0.548829000
H	-0.826217000	3.435471000	1.305506000
H	-2.570312000	5.454082000	2.722744000
H	-3.928953000	4.395283000	3.165763000
H	-2.245265000	3.834154000	3.363367000
H	-5.049536000	4.191366000	1.004483000
H	-5.021272000	3.374047000	-1.342251000
H	-2.888559000	2.636565000	-2.383332000
H	-1.435176000	0.698129000	-1.781825000
H	0.563584000	-0.457904000	-2.598143000

	H -1.276904000 8.714942000 -1.726305000 H 0.328693000 7.017494000 -2.564753000 H 2.491791000 6.295716000 -1.661802000 H 4.402228000 4.853049000 -2.172339000 H 6.421046000 1.926553000 -2.369851000 H 5.655631000 3.291593000 -3.240918000 H 6.022261000 3.438382000 -1.495166000 H -2.447695000 2.526083000 0.582760000 H -5.379334000 4.457883000 1.039944000 H -5.851659000 2.938674000 0.263292000 H -4.584672000 2.934749000 1.513072000 H -5.205401000 4.986057000 -1.616872000 H -3.483590000 5.332053000 -3.370852000 H -1.241981000 4.285107000 -3.154093000 H -1.382199000 0.786967000 -0.874529000 H 0.627002000 -0.611528000 -0.956438000		
Syn-**3f**		*Anti*-**3f**	



FINAL SINGLE POINT ENERGY -1454.171925940164

O	-6.150973000	-4.546179000	2.809433000
C	-5.403013000	-3.634164000	3.119922000
N	-5.694113000	-2.318670000	2.819059000
C	-6.928937000	-2.058799000	2.107488000
C	-4.871928000	-1.248174000	3.156111000
C	-3.652162000	-1.498185000	3.845230000
C	-2.768570000	-0.421504000	4.208167000
C	-1.606705000	-0.751367000	4.992331000
C	-0.692487000	0.238624000	5.614501000
C	0.670429000	0.160330000	5.401302000
C	1.568708000	1.096974000	5.970705000
C	2.963484000	1.056919000	5.710980000
C	3.805213000	2.010907000	6.236864000
C	3.289651000	3.046729000	7.051358000
C	1.941802000	3.105165000	7.329104000
C	1.049954000	2.138061000	6.799619000
C	-0.346937000	2.169010000	7.053450000
C	-1.190292000	1.247996000	6.484771000
C	-1.333488000	-2.084770000	5.249998000
C	-2.159535000	-3.136244000	4.836085000

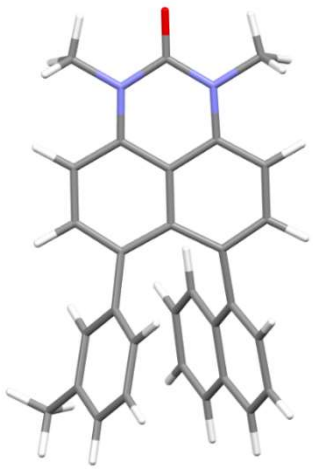


FINAL SINGLE POINT ENERGY -1454.171382037626

O	-6.266727000	-4.344530000	2.644910000
C	-5.448745000	-3.498225000	2.964906000
N	-5.820080000	-2.201999000	3.262018000
C	-7.231194000	-1.882978000	3.189371000
C	-4.919259000	-1.200651000	3.610325000
C	-3.533945000	-1.514534000	3.700160000
C	-2.568198000	-0.513405000	4.065910000
C	-1.208480000	-0.941821000	4.258158000
C	-0.135045000	-0.092109000	4.829821000
C	-0.267656000	0.500173000	6.069927000
C	0.736680000	1.349709000	6.593592000
C	0.578657000	2.020806000	7.834839000
C	1.545684000	2.883981000	8.295787000
C	2.723460000	3.107568000	7.542015000
C	2.912175000	2.459402000	6.342692000
C	1.929364000	1.568699000	5.837783000
C	2.078180000	0.896378000	4.598152000
C	1.077253000	0.092186000	4.109909000
C	-0.868428000	-2.246978000	3.945258000
C	-1.797212000	-3.200849000	3.511920000
C	-3.134834000	-2.851401000	3.419034000
N	-4.100441000	-3.783520000	3.051346000
C	-3.688313000	-5.138205000	2.746060000
C	-3.037687000	0.837860000	4.218507000
C	-2.163142000	2.025634000	4.379815000
C	-1.171491000	2.329257000	3.468060000
C	-0.323741000	3.449886000	3.645142000
C	0.735339000	3.740119000	2.744368000
C	1.574014000	4.808326000	2.965267000
C	1.387598000	5.643784000	4.093414000
C	0.361729000	5.396097000	4.976626000
C	-0.516628000	4.299347000	4.778222000
C	-1.577101000	4.005483000	5.672514000
C	-2.373899000	2.904108000	5.478384000
C	-4.399364000	1.082002000	4.152643000
C	-5.347105000	0.090742000	3.872688000
H	-7.769155000	-2.792911000	2.910540000
H	-7.414352000	-1.103675000	2.433800000
H	-7.596326000	-1.524937000	4.163987000
H	-1.183059000	0.352484000	6.648576000

	C -3.335277000 -2.849401000 4.162599000 N -4.218199000 -3.859001000 3.792001000 C -3.892406000 -5.231820000 4.120441000 C -3.115954000 0.900637000 3.758284000 C -2.235967000 2.089383000 3.865458000 C -0.942926000 2.084815000 3.379265000 C -0.093103000 3.207254000 3.528603000 C 1.260228000 3.185514000 3.098827000 C 2.079139000 4.272677000 3.298851000 C 1.579499000 5.438334000 3.928382000 C 0.269033000 5.494051000 4.345489000 C -0.597813000 4.385794000 4.160706000 C -1.949210000 4.397385000 4.591166000 C -2.740888000 3.284206000 4.449425000 C -4.333063000 1.092498000 3.124802000 C -5.220725000 0.052568000 2.830205000 H -7.422860000 -3.017188000 1.926805000 H -6.722687000 -1.564818000 1.145889000 H -7.590776000 -1.412282000 2.703570000 H 1.070766000 -0.608018000 4.734055000 H 3.356764000 0.259623000 5.074270000		H -0.336457000 1.853508000 8.409030000 H 1.406817000 3.404112000 9.246915000 H 3.482615000 3.798429000 7.916954000 H 3.819296000 2.628360000 5.756071000 H 2.993221000 1.050743000 4.020258000 H 1.189733000 -0.388489000 3.134831000 H 0.169338000 -2.560700000 4.083270000 H -1.459469000 -4.212226000 3.295658000 H -4.579564000 -5.708083000 2.470376000 H -3.211398000 -5.604912000 3.621615000 H -2.974716000 -5.144488000 1.908241000 H -1.005073000 1.678446000 2.605998000 H 0.881854000 3.087608000 1.879531000 H 2.391596000 5.015220000 2.270079000 H 2.062760000 6.486813000 4.259719000 H 0.212123000 6.036748000 5.849920000 H -1.735037000 4.656421000 6.536438000 H -3.165053000 2.669499000 6.194870000 H -4.749290000 2.109150000 4.282105000 H -6.399982000 0.360330000 3.823009000

	H 4.876333000 1.973634000 6.022928000 H 3.966320000 3.801587000 7.459476000 H 1.538509000 3.904276000 7.957100000 H -0.746291000 2.950594000 7.705135000 H -2.263095000 1.292772000 6.684759000 H -0.449047000 -2.325428000 5.844474000 H -1.884623000 -4.158647000 5.086587000 H -4.703064000 -5.867809000 3.755253000 H -3.791253000 -5.354124000 5.209518000 H -2.948004000 -5.530785000 3.640603000 H -0.545004000 1.187712000 2.899455000 H 1.645291000 2.280072000 2.622584000 H 3.122904000 4.238127000 2.977040000 H 2.240954000 6.294466000 4.082657000 H -0.121868000 6.391973000 4.831982000 H -2.345996000 5.300345000 5.063115000 H -3.768222000 3.295142000 4.822201000 H -4.594153000 2.101693000 2.797026000 H -6.151525000 0.277317000 2.313875000		
Syn-**3h**		*Anti*-**3h**	



FINAL SINGLE POINT ENERGY -1340.046099146739

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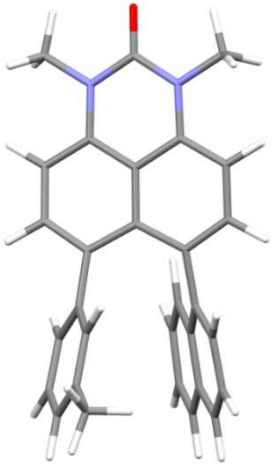
C	2.654565000	0.950254000	-0.907747000
C	2.476962000	0.628976000	0.467281000
C	1.251999000	0.944562000	1.150186000
C	1.102397000	0.472256000	2.500456000
C	-0.154130000	0.541489000	3.289504000
C	-0.156951000	1.195711000	4.508365000
C	-1.322399000	1.283199000	5.297888000
C	-2.496886000	0.717435000	4.861664000
C	-2.535414000	0.000301000	3.638080000
C	-1.345200000	-0.122222000	2.853971000
C	-1.391584000	-0.909586000	1.674121000
C	-2.562555000	-1.503699000	1.262075000
C	-3.749308000	-1.343842000	2.013625000
C	-3.730589000	-0.614302000	3.180024000
C	2.180994000	-0.140625000	3.115691000
C	3.403656000	-0.374080000	2.474137000
C	3.548317000	-0.021054000	1.142580000
N	4.722089000	-0.293123000	0.446839000



FINAL SINGLE POINT ENERGY -1340.046648311965

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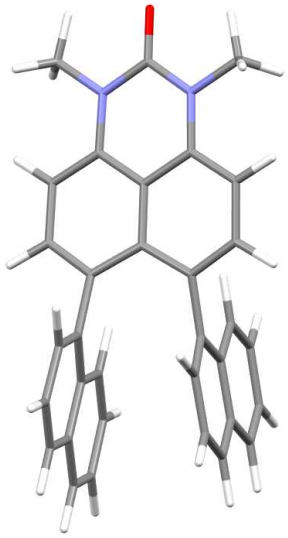
N	3.787688000	0.035105000	-1.524780000
C	2.524232000	0.333210000	-1.022797000
C	2.361473000	0.519209000	0.378628000
C	1.075820000	0.831774000	0.939979000
C	0.969230000	0.877861000	2.373711000
C	-0.306229000	0.997618000	3.125276000
C	-0.482942000	2.049318000	4.006286000
C	-1.675501000	2.203829000	4.743650000
C	-2.705663000	1.307195000	4.586813000
C	-2.556626000	0.188431000	3.727410000
C	-1.331331000	0.005169000	3.012472000
C	-1.176772000	-1.165459000	2.224858000
C	-2.193935000	-2.085790000	2.112905000
C	-3.421871000	-1.879355000	2.781975000
C	-3.593737000	-0.769243000	3.576302000
C	2.120747000	0.751551000	3.132257000
C	3.387605000	0.527887000	2.578559000
C	3.510765000	0.379520000	1.206841000
N	4.738461000	0.092114000	0.618801000
C	4.915891000	-0.089324000	-0.738801000
O	6.008970000	-0.345677000	-1.216105000
C	5.909114000	-0.031330000	1.462979000
C	-0.014833000	1.053815000	0.030510000
C	0.189005000	0.822445000	-1.319555000
C	1.426215000	0.449648000	-1.859489000
C	-1.342734000	1.594011000	0.417105000
C	-1.451118000	2.823360000	1.075095000
C	-2.693405000	3.373741000	1.409799000
C	-2.766254000	4.672345000	2.158053000
C	-3.850049000	2.672206000	1.051516000
C	-3.761322000	1.457149000	0.372489000
C	-2.517609000	0.920560000	0.053934000
H	5.001899000	-0.369888000	-3.147645000
H	3.329675000	-0.991410000	-3.304180000
H	3.654300000	0.757957000	-3.496196000
H	0.306469000	2.799449000	4.099313000
H	-1.782550000	3.054565000	5.421196000
H	-3.646301000	1.433354000	5.129374000
H	-0.233568000	-1.330471000	1.701232000

	C	4.913121000	0.013899000	-0.886065000			
	O	5.955871000	-0.245693000	-1.463436000			
	C	5.815673000	-0.941332000	1.141590000			
	C	0.257053000	1.688977000	0.427705000			
	C	0.464806000	1.941571000	-0.917975000			
	C	1.629578000	1.572061000	-1.601810000			
	C	-0.960238000	2.290743000	1.029838000			
	C	-2.220705000	2.029977000	0.479601000			
	C	-3.383536000	2.628295000	0.976807000			
	C	-4.725059000	2.282680000	0.396786000			
	C	-3.262119000	3.527527000	2.041749000			
	C	-2.011598000	3.813956000	2.589794000			
	C	-0.866279000	3.201982000	2.090227000			
	H	5.035303000	0.638204000	-3.228284000			
	H	3.283855000	0.437665000	-3.544275000			
	H	3.932005000	2.042103000	-3.087008000			
	H	0.757292000	1.691428000	4.844250000			
	H	-1.289796000	1.824019000	6.246877000			
	H	-3.413171000	0.802688000	5.451865000			
	H	-0.480817000	-1.037439000	1.086555000			
	H	-2.575997000	-2.104196000	0.349096000			
					H	-2.053310000	-2.980871000	1.501926000
					H	-4.227873000	-2.609907000	2.676767000
					H	-4.532536000	-0.610826000	4.114021000
					H	2.030220000	0.790904000	4.220374000
					H	4.247302000	0.431924000	3.238418000
					H	6.085903000	0.904186000	2.014995000
					H	5.781141000	-0.851045000	2.186444000
					H	6.767887000	-0.243405000	0.820718000
					H	-0.647222000	0.983136000	-2.004251000
					H	1.514268000	0.299813000	-2.933515000
					H	-0.538940000	3.366705000	1.336139000
					H	-3.786577000	5.081171000	2.162836000
					H	-2.092299000	5.426356000	1.723400000
					H	-2.456006000	4.528664000	3.206633000
					H	-4.830025000	3.085282000	1.307184000
					H	-4.671853000	0.919131000	0.096343000
					H	-2.448775000	-0.042335000	-0.457034000

	H -4.676144000 -1.812146000 1.673028000 H -4.638222000 -0.501332000 3.779237000 H 2.058864000 -0.493158000 4.142593000 H 4.205015000 -0.867014000 3.020391000 H 6.146506000 -0.329939000 1.994800000 H 5.507032000 -1.930470000 1.513145000 H 6.641802000 -1.059653000 0.435499000 H -0.300599000 2.498435000 -1.463727000 H 1.727041000 1.818130000 -2.657168000 H -2.298447000 1.317696000 -0.346309000 H -5.058189000 1.292228000 0.748947000 H -4.688722000 2.238630000 -0.702308000 H -5.491006000 3.015165000 0.688899000 H -4.157394000 4.009371000 2.444983000 H -1.929496000 4.525370000 3.415541000 H 0.112204000 3.433438000 2.516624000		
Syn-**3d**		*Anti*-**3d**	



FINAL SINGLE POINT ENERGY -1454.170269881807

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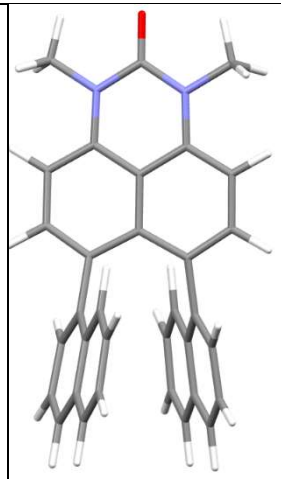
N	4.528848000	2.628302000	3.683369000
C	3.564356000	3.569766000	4.029489000
C	2.375554000	3.126263000	4.673431000
C	1.356608000	4.058795000	5.051687000
C	0.242596000	3.570132000	5.807776000
C	-0.691262000	4.476274000	6.533084000
C	-0.249874000	5.070311000	7.700930000
C	-1.081935000	5.929213000	8.448320000
C	-2.361938000	6.195697000	8.021023000
C	-2.865622000	5.593035000	6.840862000
C	-2.030169000	4.704444000	6.092795000
C	-2.556865000	4.098190000	4.922867000
C	-3.838736000	4.365950000	4.502634000
C	-4.660640000	5.253625000	5.235277000
C	-4.183575000	5.851208000	6.378645000
C	0.122097000	2.208763000	6.015896000
C	1.074309000	1.281780000	5.565107000
C	2.219890000	1.736339000	4.929975000
N	3.228166000	0.864289000	4.531320000



FINAL SINGLE POINT ENERGY -1454.172392151713

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N	3.429055000	1.455753000	3.078737000
C	2.402476000	2.389142000	3.183941000
C	2.030471000	2.866671000	4.472336000
C	0.971843000	3.824964000	4.629775000
C	0.584752000	4.179464000	5.967902000
C	-0.590832000	5.018103000	6.320869000
C	-0.401562000	6.199441000	7.014662000
C	-1.486906000	7.018501000	7.389167000
C	-2.772192000	6.651963000	7.067468000
C	-3.021506000	5.428664000	6.394971000
C	-1.924171000	4.582121000	6.040030000
C	-2.204541000	3.330280000	5.432099000
C	-3.496575000	2.952912000	5.147430000
C	-4.578182000	3.809435000	5.459826000
C	-4.342589000	5.015883000	6.076858000
C	1.321497000	3.679778000	7.028049000
C	2.400023000	2.800243000	6.870245000
C	2.740878000	2.366438000	5.599758000
N	3.768208000	1.449633000	5.400248000
C	4.138787000	0.970206000	4.159349000
O	5.042618000	0.162049000	4.025447000
C	4.498693000	0.953902000	6.548733000
C	0.375828000	4.363150000	3.437693000
C	0.756300000	3.846641000	2.211193000
C	1.739223000	2.859455000	2.062506000
C	-0.595699000	5.487196000	3.412018000
C	-0.217316000	6.797976000	3.842645000
C	1.097963000	7.106028000	4.279326000
C	1.423628000	8.369825000	4.714527000
C	0.447466000	9.393411000	4.734717000
C	-0.828404000	9.134920000	4.290530000
C	-1.191978000	7.844798000	3.821399000
C	-2.491857000	7.579500000	3.320127000
C	-2.811079000	6.330500000	2.842492000
C	-1.860750000	5.289451000	2.889495000
H	4.142644000	1.786062000	1.125443000
H	4.603339000	0.235141000	1.893612000
H	2.935646000	0.474480000	1.284888000
H	0.616958000	6.522782000	7.239027000

	C 4.392078000 1.271786000 3.908083000 O 5.253475000 0.475421000 3.573958000 C 3.069363000 -0.553412000 4.781450000 C 1.505633000 5.424735000 4.640002000 C 2.688478000 5.813844000 4.041334000 C 3.733107000 4.918364000 3.759240000 C 0.380638000 6.400940000 4.648609000 C -0.602414000 6.315329000 3.610567000 C -0.545321000 5.329613000 2.589010000 C -1.504924000 5.270501000 1.604248000 C -2.577401000 6.191081000 1.594799000 C -2.658276000 7.162303000 2.565739000 C -1.676629000 7.259394000 3.586446000 C -1.732220000 8.273829000 4.575509000 C -0.753843000 8.362026000 5.537631000 C 0.303665000 7.427367000 5.567902000 H 6.285777000 3.785513000 3.670589000 H 6.368217000 2.198436000 2.843990000 H 5.507175000 3.567978000 2.074105000 H 0.773008000 4.882341000 8.037102000 H -0.699712000 6.387873000 9.363681000		H -1.295052000 7.955968000 7.916495000 H -3.619587000 7.290450000 7.330861000 H -1.374904000 2.665227000 5.184877000 H -3.690078000 1.985725000 4.676748000 H -5.600053000 3.503661000 5.221799000 H -5.173073000 5.676815000 6.339867000 H 1.024779000 3.959937000 8.041582000 H 2.928454000 2.443748000 7.751887000 H 3.821924000 0.430281000 7.241193000 H 4.982393000 1.783985000 7.085616000 H 5.261185000 0.257759000 6.189548000 H 0.291795000 4.256287000 1.311081000 H 1.992820000 2.507308000 1.064776000 H 1.855687000 6.320137000 4.269567000 H 2.442229000 8.586059000 5.046435000 H 0.714133000 10.391616000 5.090915000 H -1.584609000 9.924747000 4.283848000 H -3.228534000 8.387266000 3.312179000 H -3.808581000 6.129466000 2.444605000 H -2.141147000 4.291014000 2.547667000

	H -3.010394000 6.871594000 8.584981000 H -1.919154000 3.422267000 4.351153000 H -4.222241000 3.898213000 3.592896000 H -5.675933000 5.462995000 4.889137000 H -4.814013000 6.535682000 6.952846000 H -0.732045000 1.841250000 6.590544000 H 0.921106000 0.222890000 5.763806000 H 2.173994000 -0.938044000 4.269703000 H 2.971199000 -0.746599000 5.860628000 H 3.955980000 -1.065722000 4.398584000 H 2.796076000 6.855437000 3.728001000 H 4.637458000 5.290453000 3.281746000 H 0.278436000 4.613193000 2.591525000 H -1.440154000 4.505682000 0.826207000 H -3.338863000 6.131198000 0.813124000 H -3.481552000 7.881875000 2.564286000 H -2.561302000 8.986133000 4.554517000 H -0.794547000 9.149291000 6.294209000 H 1.060684000 7.495771000 6.352262000		

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