Electronic Supplementary Information

Acridone and quinacridone derivatives with carbazole or phenoxazine substituents: synthesis, electrochemistry, photophysics and application as TADF electroluminophores

Irena Kulszewicz-Bajer,[a*] Matas Guzauskas,[b] Małgorzata Makowska-Janusik,[c] Małgorzata Zagórska,[a] Malek Mahmoudi,[b] Juozas V. Grazulevicius,[b] Adam Proń,[a*] Dmytro Volyniuk,[b*]

[a] Faculty of Chemistry, Warsaw University of Technology, Noakowskiego 3, 00-664 Warsaw, Poland. E-mails: *ikulsz@ch.pw.edu.pl*

[b] Department of Polymer Chemistry and Technology, Kaunas University of Technology, Barsausko 59, LT-51423, Kaunas, Lithuania. E-mails: *dmytro.volyniuk@ktu.lt*,

[c] Faculty of Science and Technology, Jan Dlugosz University, Al. Armii Krajowej 13/15, 42-200 Częstochowa, Poland.

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1. Synthesis

Characterization techniques

^{1}H and ^{13}C NMR spectra were recorded on a Varian Mercury (500 and 125 MHz) spectrometer and referenced with respect to TMS and solvents. IR spectra were monitored on Bio-RAD FTS-165 spectrometer using KBr pellets. Mass spectra were measured by EI method on an AMD 604 mass spectrometer. All synthesized compounds studied were subject to C, H, N elemental combustion analysis.

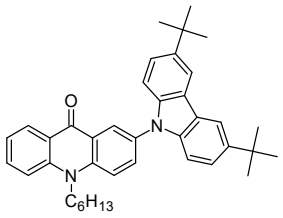
Reagents

Carbazole, CuI, *trans*-1,2-cyclohexanediamine, Pd_2dba_3, $Pd(PPh_3)_4$, 2-isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolane, potassium phosphate, K_3PO_4, anhydrous dioxane, were purchased from Aldrich. Acridone was purchased from Acros Organics. Quinacridone and phenoxazine were purchased from TCI.

All glassware was oven dried, assembled hot, and cooled under a dry argon stream before use. All reactions were performed under dry argon.

N-hexyl-2-bromoacridone

It was prepared according to the procedure described in [1].



1

2-(3,6-tert-butylcarbazole)-N-hexylacridone, 1

CuI (19 mg, 0.1 mmol) and *trans*-1,2-cyclohexanediamine (114 µl, 1.0 mmol) were mixed in 1 ml of dry dioxane and stirred under an argon atmosphere for 0.5 h. Then 2-bromo-N-hexylacridone (0.358 g, 1.0 mmol), 3,6-di-*tert*-butylcarbazole (0.307 g, 1.1 mmol), K_3PO_4 (0.425 g, 2 mmol) and 4 ml of dry dioxane were added to the reaction flask. The mixture was stirred and heated at 110 ºC for 24 h. Then the mixture was cooled to room temperature and passed through short column with silica gel extracted with $CHCl_3$. After evaporation of the

solvent the crude product was purified by chromatography on silica gel eluting with CH_2Cl_2 with 2.5% $_v$ of THF. The product was crystallized from CH_2Cl_2 to give 0.54 g (0.97 mmol, 97% yield) of light yellow crystals.

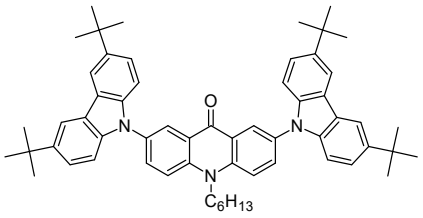
^{1}H NMR (500 MHz, $CDCl_3$) δ, 8.79 (d, J=3.5 Hz, 1H), 8.63 (dd, J=10, 2 Hz, 1H), 8.16 (dd, J=2, 0.5 Hz, 2H), 7.92 (dd, J=11.5, 3.5 Hz, 1H), 7.79 (td, J=10, 2 Hz, 1H), 7.70 (d, J=11.5 Hz, 1H), 7.57 (d, J=11.5 Hz, 1H), 7.46 (dd, J=10, 2.5 Hz, 2H), 7.37 (dd, J=10, 0.5 Hz, 2H), 7.35 (td, J=11.5, 2 Hz, 1H), 4.44 (t, J=10.5 Hz, 2H), 2.06-2.02 (m, 2H), 1.64-1.59 (m, 2H), 1.44 (s, 18H), 1.42-1.38 (m, 4H), 0.97 (t, J=9 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 177.57,143.14, 141.89, 140.53, 139.47, 134.31, 132.55, 131.90, 128.30, 125.48, 123.84, 123.55, 123.53, 122.56, 121.75, 116.48, 116.40, 114.79, 109,20, 46.74, 34.89, 32.17, 31.69, 27.44, 26.80, 22.84, 14.18.

IR (cm^{-1}): 3054, 2956, 2930, 2864, 1641, 1603, 1491, 1474, 1362, 1295, 1262, 1176, 808, 754, 652.

Anal. calcd. for $C_{39}H_{44}N_2O_1$: C, 84.11; H, 7.96; N, 5.05; O, 2.88.

Found: C, 84.72; H, 8.05; N, 4.97.



2

2,7-bis(3,6-tert-butylcarbazole)-N-hexylacridone, 2

CuI (19 mg, 0.1 mmol) and *trans*-1,2-cyclohexanediamine (114 µl, 1.0 mmol) were mixed in 1 ml of dry dioxane and stirred under an argon atmosphere for 0.5 h. Then 2,7-dibromo-N-hexylacridone (0.437 g, 1.0 mmol), 3,6-di-*tert*-butylcarbazole (0.614 g, 2.2 mmol), K_3PO_4 (0.85 g, 4 mmol) and 4 ml of dry dioxane were added to the reaction flask. The mixture was stirred and heated at 110 ºC for 24 h. Then the mixture was cooled to room temperature and passed through short column with silica gel extracted with $CHCl_3$. After evaporation of the solvent the crude product was purified by chromatography on silica gel eluting with CH_2Cl_2 with 2.5% $_v$ of THF. The product was crystallized from CH_2Cl_2 to give 0.53 g (0.636 mmol, 64% yield) of yellow crystals.

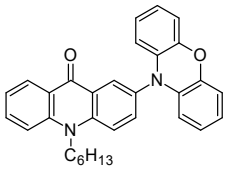
^{1}H NMR (500 MHz, $CDCl_3$) δ, 8.82 (d, J=3 Hz, 2H), 8.17 (dd, J=2.5, 0.5 Hz, 4H), 7.97 (dd, J=11.5, 3 Hz, 2H), 7.77 (d, J=11.5 Hz, 2H), 7.48 (dd, J=11, 2.5 Hz, 4H), 7.41 (dd, J=11, 0.5 Hz, 4H), 4.53 (t, J=10.5 Hz, 2H), 2.15-2.11 (m, 2H), 1.70-1.63 (m, 2H), 1.56-1.52 (m, 4H), 1.48 (s, 36H), 0.98 (t, J=4.5 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ, 177.04, 143.22, 140.42, 139.39, 132.76, 132.26, 125.46, 123.88, 123.58, 123.48, 116.61, 116.44, 109.20, 47.05, 34.91, 32.16, 31.70, 27.56, 27.05, 22.87, 14.21.

IR (cm^{-1}): 3047, 2957, 2864, 1646, 1612, 1493, 1362, 1294, 1262, 1233, 1176, 807, 740, 653.

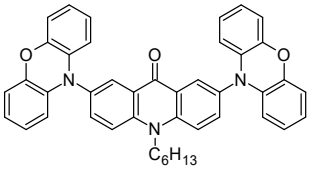
Anal. calcd. for $C_{59}H_{67}N_3O_1$: C, 84.95; H, 8.09; N, 5.04, O, 1.92.

Found: C, 85.03; H, 8.13; N, 4.88.



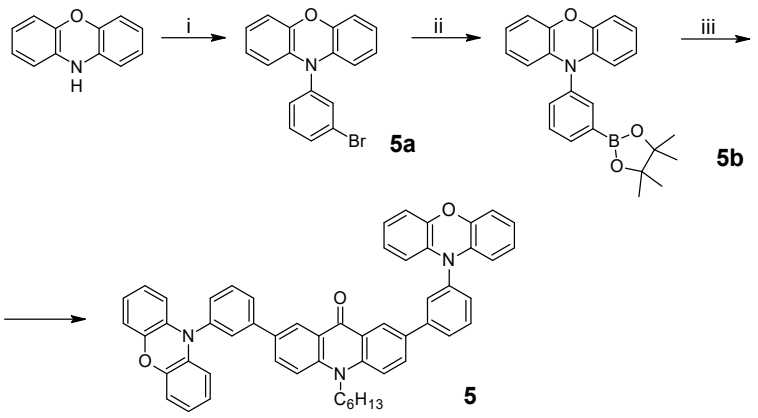
2-Phenoxazine-N-hexylacridone, 3

The compound **3** was prepared according to the procedure described in [1].

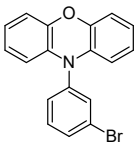


2,7-bis-phenoxazine-N-hexylacridone, 4

The compound **4** was prepared according to the procedure described in [1].



Scheme S1. Synthesis of compound **5** (i) 1-bromo-3-iodobenzene, Pd_2dba_3, Xantphos, *t*-BuONa, toluene, 80 °C, ii), n-BuLi, 2-isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolane, THF, -78 °C, iii) $Pd(PPh_3)_4$, 2M K_2CO_3, toluene, dioxane.



Compound 5a

Pd_2dba_3 (54.9 mg, 0.06 mmol) and Xantphos (138.9 mg, 0.24 mmol) were mixed in 1 ml of dry toluene and stirred under an argon atmosphere for 0.5 h. Then 1-bromo-3-iodobenzene (1.7 g, 6 mmol), phenoxazine (1 g, 5.46 mmol), *t*-BuONa (0.75 g, 7.8 mmol) and 9 ml of dry toluene were added to the reaction flask. The mixture was stirred and heated at 80 ºC for 20 h. Then the mixture was cooled to room temperature, water was added and the mixture was extracted with diethyl ether. The combined organic layers were dried over Na_2SO_4. After evaporation of the solvent the crude product was purified by chromatography on silica gel eluting with CH_2Cl_2/hexanes, 2:1. The product was obtained as a white powder, 1.75 g (5.18 mmol) with a yield of 95%.

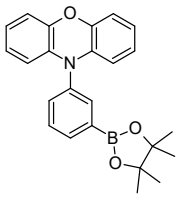
^{1}H NMR (500 MHz, $CDCl_3$) δ, 7.62 (dq, J=8.1, 1.9, 1.0 Hz, 1H), 7.54 (t, J=1.9 Hz, 1H), 7.48 (t, J=8.1 Hz, 1H), 7.31 (dq, J=8.1, 1.9, 1.0 Hz, 1H), 6.71-6.66 (m, 4H), 6.62 (td, J=8.0, 1.5 Hz, 2H), 5.92 (dd, J=8.0, 1.5 Hz, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ, 143.99, 140.59, 134.26, 132.41, 131.96, 129.92, 129.18, 128.37, 123.43, 121.86, 115.74, 113.42.

IR (cm^{-1}): 3057, 3029, 2914, 1586, 1487, 1460, 1336, 1273, 1258, 731, 696.

Anal. calcd. for $C_{18}H_{12}Br_1N_1O_1$: C, 63.93; H, 3.58; N, 4.14; Br, 23.63; O, 4.73.

Found: C, 66.51; H, 3.79; N, 4.22.

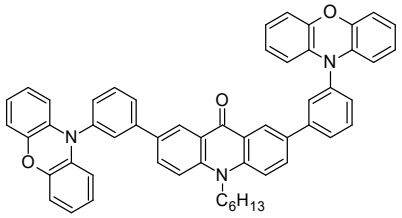


Compound 5b

Compound **5a**, 1.69 g (5 mmol) was dissolved in 15 ml of anhydrous THF and cooled to -78 °C. A solution of n-BuLi, 2.4 ml (6 mmol) was added dropwise. The solution was stirred at -78 °C for 1 h. Then 2-isopropoxy-4,4,5,5-tetramethyl-1,3,2-dioxaborolane, 1.21 g (6.5 mmol) was added dropwise. The mixture was stirred at -78 °C for 0.5 h and then at room temperature overnight. 50 ml of NH4Cl solution was added and the product was extracted with ethyl acetate. The organic phase was dried over Na_2SO_4. The product was crystallized from diethyl ether/MeOH mixture to give the titled compound as a white powder, 1.5 g (3.9 mmol) with a yield of 78%.

^{1}H NMR (500 MHz, $CDCl_3$) δ, 7.89 (dt, J=7.4, 1.2 Hz, 1H), 7.77 (s, 1H), 7.58 (t, J=7.4 Hz, 1H), 7.42 (dd, J=7.4, 1.2 Hz, 1H), 6.73-6.50 (m, 6H), 5.87 (d, J=6.7 Hz, 2H), 1.34 (s, 12H).

^{13}C NMR (125 MHz, $CDCl_3$) δ, 144.07, 137.29, 134.84, 134.05, 130.59, 129.91, 129.18, 128.13, 123.31, 121.29, 115.44, 113.54, 84.25, 25.05.



2,7-bis[3-(phenoxazine)phenyl)-N-hexylacridone, 5

2,7-dibromo-N-hexylacridone (0.13 g, 0.3 mmol), compound **5b**, 0.25 g (0.66 mmol), $Pd(PPh_3)_4$ (34.6 mg, 0.03 mmol) were mixed in 1.5 ml of dry dioxane and 3 ml of dry toluene. The solution of 2M K_2CO_3 (1.5 ml) was added and the mixture was stirred and heated at 100

ºC for 20 h. Then the mixture was cooled to room temperature, washed with 50 ml of water and extracted with $CHCl_3$. The combined organic layers were dried over Na_2SO_4. After evaporation of the solvent the crude product was purified by chromatography on silica gel eluting with $CHCl_3$/hexanes, 2:1. The product was crystallized from CH_2Cl_2/diethyl ether mixture to give the product as a yellow powder, 0.16 g (0.2 mmol) with a yield of 67%.

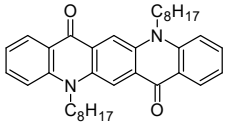
^{1}H NMR (500 MHz, $CDCl_3$) δ, 8.85 (d, J=2.4 Hz, 2H), 7.99 (dd, J=9.0, 2.5 Hz, 2H), 7.86 (ddd, J=7.8, 1.8, 1.0 Hz, 2H), 7.73-7.67 (m, 4H), 7.58 (d, J=9.0 Hz, 2H), 7.34 (ddd, J=7.8, 1.8, 1.0 Hz, 2H), 6.7 (dd, J=7.8, 1.6 Hz, 4H), 6.65-6.59 (m 8H), 6.02 (dd, J=7.8, 1.6 Hz, 4H), 4.42 (t, J=7.6 Hz, 2H), 1.96-1.84 (m, 2H), 1.63-1.54 (m, 2H), 1.47-1.36 (m, 4H), 0.94 (t, J=7.2 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ, 177.94, 144.09, 142.91, 141.31, 139.82, 134.49, 132.89, 132.65, 131.78, 129.75, 129.13, 127.05, 125.98, 123.45, 122.87, 121.50, 115.69, 115.59, 113.48, 46.51, 31.65, 27.42, 26.73, 22.76, 14.15.

IR (cm^{-1}): 3059, 2951, 2926, 2854, 1644, 1614, 1486, 1334, 1272, 793, 740.

Anal. calcd. for $C_{55}H_{43}N_3O_3$: C, 83.20; H, 5.46; N, 5.29; O, 6.05.

Found: C, 81.38; H, 5.61; N, 5.37.

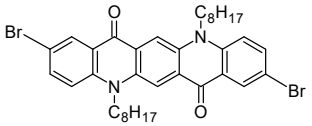


N,N'-dioctylquinacridone, QA-C8

This compound was prepared according to the procedure described in [2].

^{1}H NMR (500 MHz, $CDCl_3$) δ, 8.77 (s, 2H), 8.58 (dd, J=1.5, 8 Hz, 2H), 7.76 (td, J=1.5, 8 Hz, 2H), 7.52 (d, J=8 Hz, 2H), 7.28 (d, J=8 Hz, 2H), 4.51 (t, J=8 Hz, 4H), 2.04-1.98 (m, 4H), 1.65-1.59 (m, 4H), 1.50-1.45 (m, 4H), 1.38-1.30 (m, 12H), 0.90 (t, J=7 Hz, 6H). **IR** (cm^{-1}): 3073, 2976, 2926, 2858, 1636, 1590, 1492, 1473, 1388, 1262, 1204, 753.

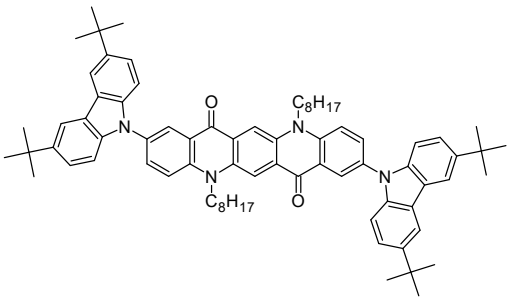
Anal. Calcd. for $C_{36}H_{44}N_2O_2$: C, 80.56; H, 8.26; N, 5.22; O, 5.96. Found: C, 80.82; H, 8.13; N, 5.05. **M/z**=536.2.



2,9-dibromo-N,N'-dioctylquinacridone

N,N-dioctylquinacridone (1.34 g, 2.5 mmol) and sodium acetate (1.07 g) were dissolved in 20 ml of acetic acid and heated at 130 °C under an argon atmosphere. Bromine (0.31 g, 6 mmol) was dissolved in 15 ml of acetic acid and added drop wise during 2 h to the solution of quinacridone. Then, the reaction mixture was heated for additional 0.5 h. After cooling to room temperature the mixture was purred into 300 ml of water and extracted with chloroform. The organic phase was washed with basic solution of Na_2SO_3, then with water and dried over Na_2SO_4. The crude product was purified by chromatography on silica gel eluting with $CHCl_3$ to give 0.97 g (1.4 mmol, 56% yield) of N-hexyl-2-bromoacridone.

^{1}H NMR (500 MHz, $CDCl_3$) δ, 8.57 (s, 2H), 8.52 (d, J=2.5 Hz, 2H), 7.75 (dd, J=9.0, 2.5 Hz, 2H), 7.31 (d, J=9.0 Hz, 2H), 4.42 (t, J=8.0 Hz, 4H), 1.94-1.91 (m, 4H), 1.60-1.55 (m, 4H), 1.46-1.42 9M, 4H), 1.38-1.30 (m, 12H), 0.90 (t, J=7.0 Hz, 6H).



2,9-bis(3,6-*tert*-butylcarbazole)- N,N'-dioctylquinacridone, 6

CuI (9.3 mg, 0.049 mmol) and *trans*-1,2-cyclohexanediamine (55.8 µl, 0.49 mmol) were mixed in 1 ml of dry dioxane and stirred under an argon atmosphere for 0.5 h. Then 2,9-dibromo-N,N'-dioctylquinacridone (0.17 g, 0.245 mmol), 3,6-di-*tert*-butylcarbazole (0.15 g, 0.539 mmol), K_3PO_4 (0.21 g, 0.98 mmol) and 4 ml of dry dioxane were added to the reaction flask. The mixture was stirred and heated at 110 ºC for 24 h. Then the mixture was cooled to room temperature and passed through short column with silica gel extracted with $CHCl_3$. After evaporation of the solvent the crude product was purified by chromatography on silica gel eluting with $CHCl_3$. The product was crystallized from $CHCl_3$ to give 0.15 g (0.137 mmol, 61.4% yield) of red crystals.

^{1}H NMR (500 MHz, $CDCl_3$) δ, 8.89 (s, 1H), 8.82 (d, J=3.5 Hz, 1H), 8.18 (dd, J=2.5, 0.5 Hz, 2H), 7.98 (dd, J=11.5, 3.5, 1H), 7.76 (d, J=11.5 Hz, 1H), 7.47 (dd, J=11.5, 2.5 Hz, 2H), 7.42 (dd, J=11.5, 0.5 Hz, 2H), 4.63 (t, J=9.5 Hz, 2H), 2.13-2.08 (m, 2H), 1.58-1.49 (m, 2H), 1.48 (s, 36H), 1.47-1.38 (m, 8H), 0.90 (t, J=8.8 Hz, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ, 177.84, 143.26, 141.06, 139.40, 136.06, 133.42, 131.66, 126.50, 125.45, 123.89, 123.89, 123.59, 122.15, 116.62, 116.49, 114.01, 109.18, 47.05, 34.92, 32.17, 31.95, 29.58, 29.49, 27.46, 27.23, 22.81, 14.27.

IR (cm^{-1}): 3050, 2955, 2927, 2856, 1638, 1616, 1511, 1489, 1472, 1457, 1323, 1294, 1262, 1155, 806, 740, 654.

Anal. calcd. for $C_{76}H_{90}N_4O_2$: C, 83.63; H, 8.31; N, 5.13; O, 2.93.

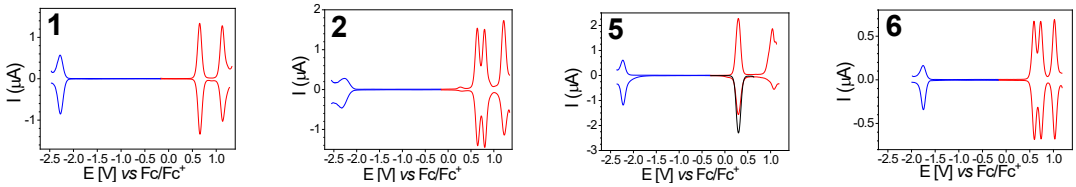
Found: C, 83.22; H, 8.47; N, 5.04.

2. Cyclic voltammetry (CV) and Differential Pulse Volatmmetry (DPV)

Cyclic voltammograms (scan rate 50 mV/s) and differential pulse voltammograms (modulation time: 50 ms, modulation amplitude: 10 mV, step potential: 5 mV) were registered using an Autolab potentiostat (EcoChemie, the Netherlands). The studied compounds were dissolved at concentration of 10^{-3} M in 0.1 M Bu_4NPF_6/dichloromethane (compounds **1** and **6**) and in 0.1 M Bu_4NBF_4/dichloromethane (compounds **2** and **5**) electrolyte. The measurements were performed in an inert atmosphere, using a platinum disk working electrode of the surface area of 2 mm^2, a platinum wire counter electrode and an Ag/0.1 M Ag^+/acetonitrile reference electrode, whose potential was verified using the ferrocene couple at the end of each set of experiment.

Notably, CV and DPV curves should not be directly compared because their measurement principles are totally different (Figure 1a, S1). Some advantages of DPV with respect to CV come from reduced contribution from background currents (from interfacial capacitance and/or competing for faradaic processes). The cases in which CV peaks of essentially irreversible nature are transformed in DPV into a pair of peaks of apparent partial reversibility are common. For example in an electroreduction process, contrary to the standard CV procedure, the DPV technique (especially upon its backward pulse) allows for retaining a fraction of previously

electrosorbed species, which then could become electrooxidized in the forward anodic sweep. This is one of the reasons of differences in reversibility as detected by CV and DPV. The additional reason arises from the fact CV slopes are characterized by varying tangents, in DPV appear as peaks. Thus, a totally irreversible process as probed by CV in DPV may resemble a partly reversible one by the presence of two peaks. Since these peaks strongly differ in their surface area, the studied redox process has to be considered as irreversible.



(a) (b) (c) (d)

Figure S1. Differential pulse voltammograms registered for **1**, **2**, **5** and **6**. Electrolyte: 0.1M Bu_4NBF_4/CH_2Cl_2, scan rate: 50 mV/s (CV). Modulation time: 50 ms, modulation amplitude: 10 mV, step potential: 5 mV (DPV).

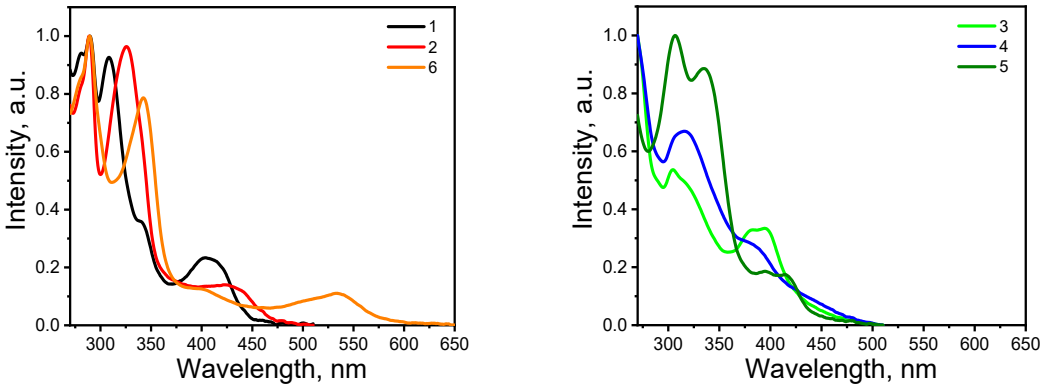
3. Ultraviolet Photoelectron Spectroscopy

A home-made setup consisting of the deep UV deuterium light source ASBN-D130-CM, monochromator CM110 1/8 m and electrometer Keithley 6517B was used for recording photoelectron emission spectra of the studied samples in air. The samples were vacuum-deposited onto fluorine-doped tin oxide (FTO) coated glass slides. The thermo-vacuum depositions were carried out in a glove box (MB EcoVap4G) using Kurt J. Lesker vacuum equipment.

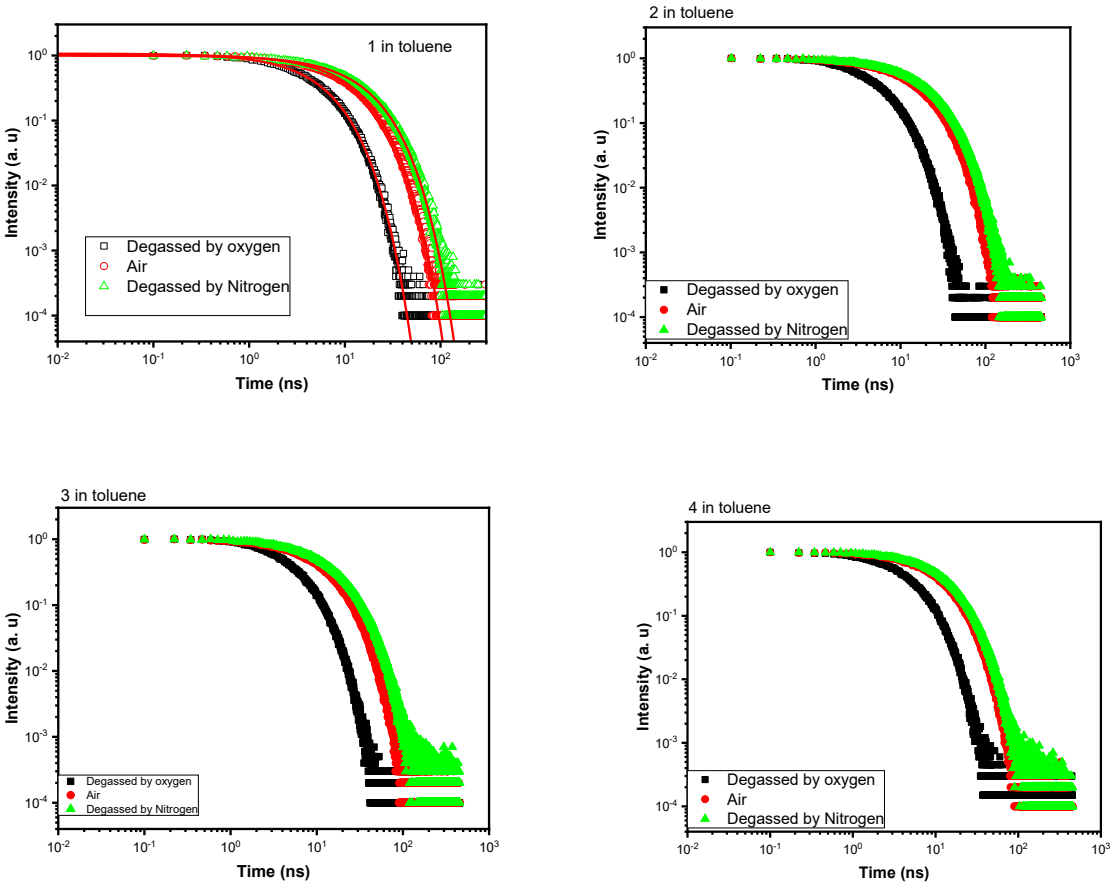
4. Optical measurements

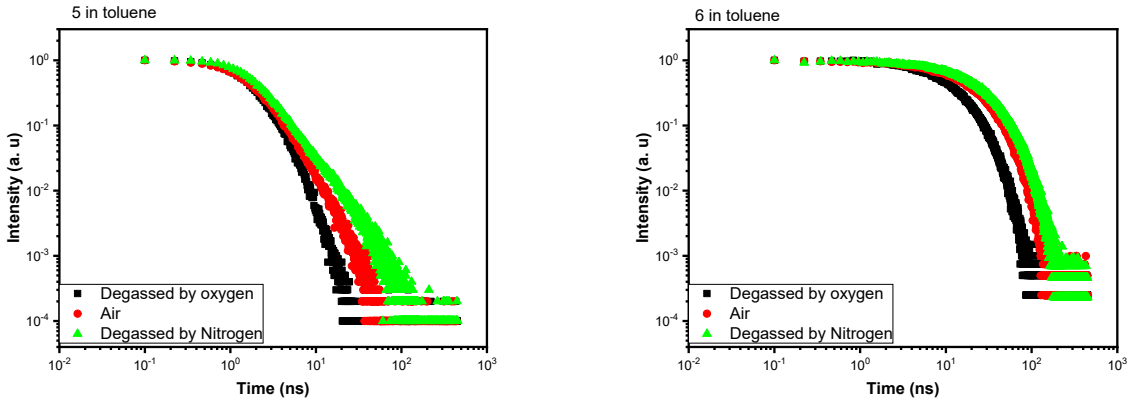
Edinburgh Instruments FLS980 and Avantes spectrometers were used for studying photophysical properties of the synthesized compounds. Photoluminescence (PL) spectra were recorded selecting excitation wavelength of 330 nm. The PicoQuant LDH-D-C-375 laser (wavelength 374 nm) as the excitation source was used for recording PL decay curves at

maxima of PL spectra if other is not noted. The after excitation delay time of 1 ms was selected to record phosphorescence spectra at 77 K.



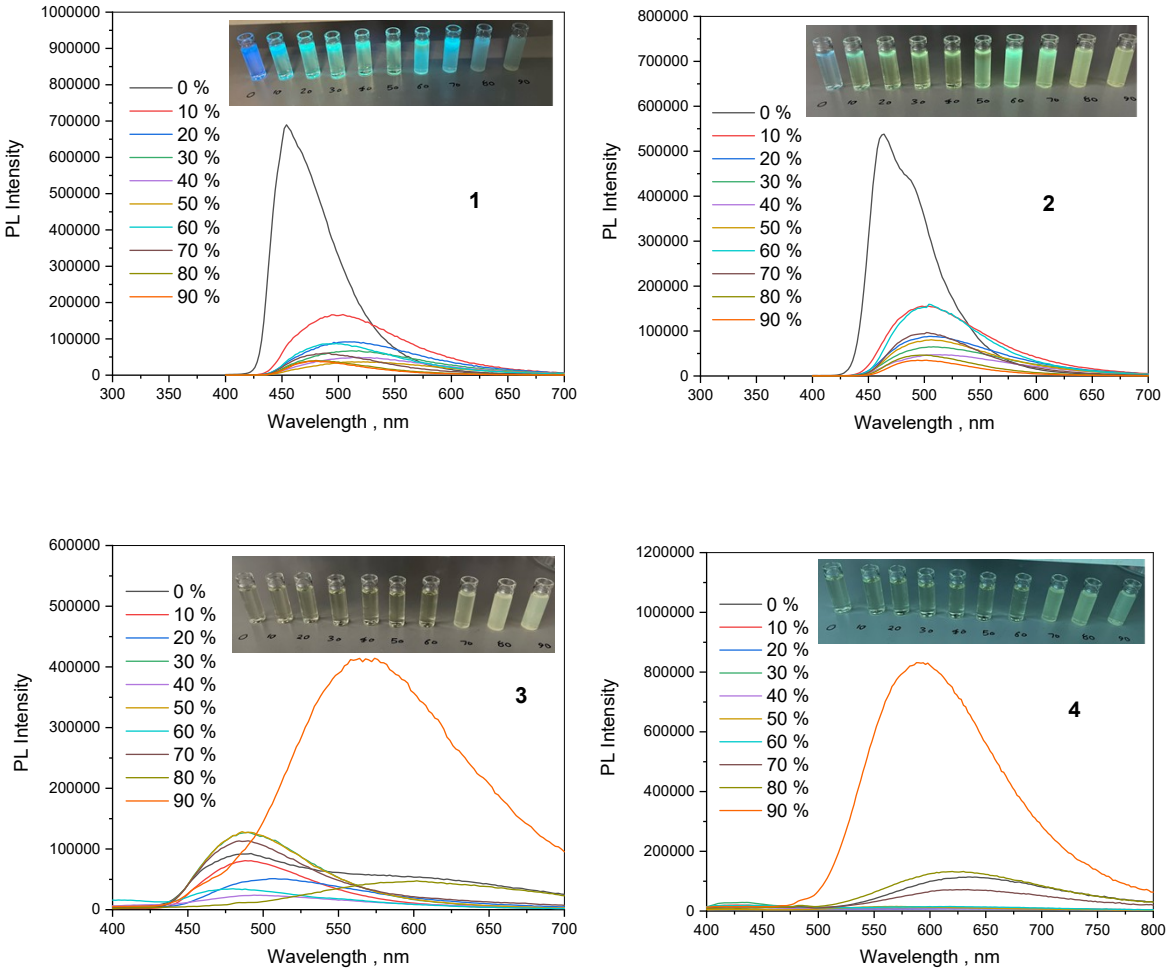
(a)





(b)

Figure S2. Abpsortion spectra of non-doped films (a) and PL decays (b) of toluene solutions of compounds **1-6**.



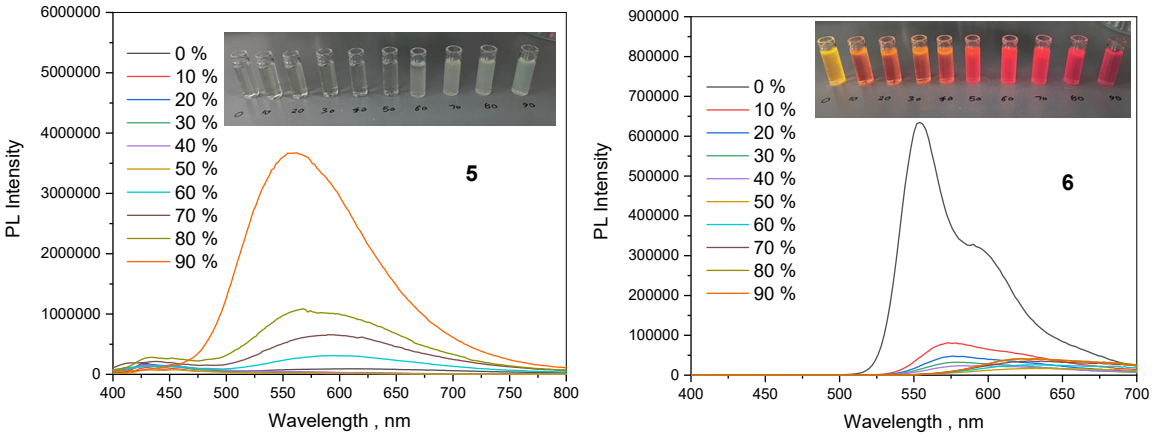
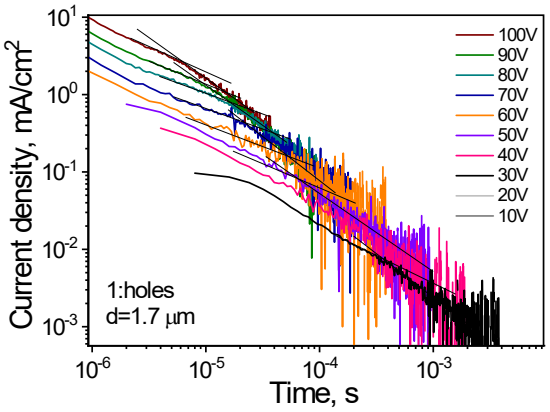


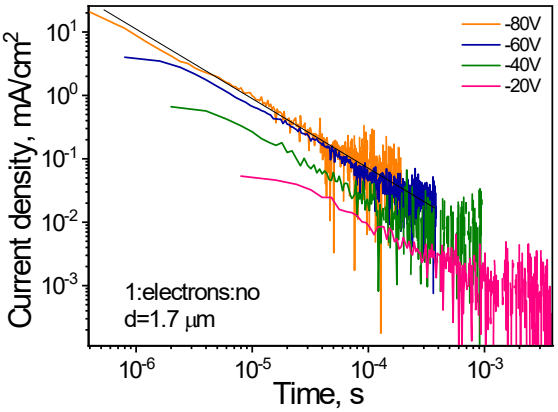
Figure S3**.** PL spectra of the dispersions of compounds **1-6** in THF/water mixtures with various water fractions (a). Inset shows photographs of the dispersions under UV excitation.

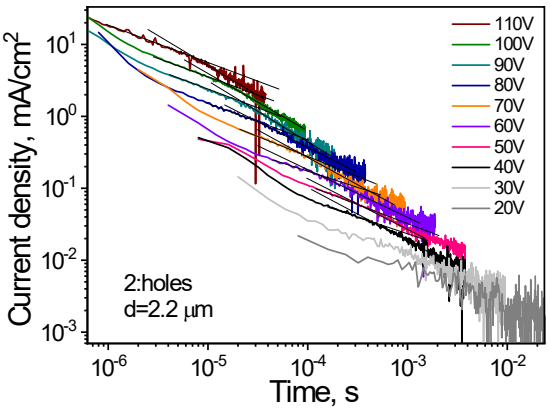
5. Charge carriers mobility determination

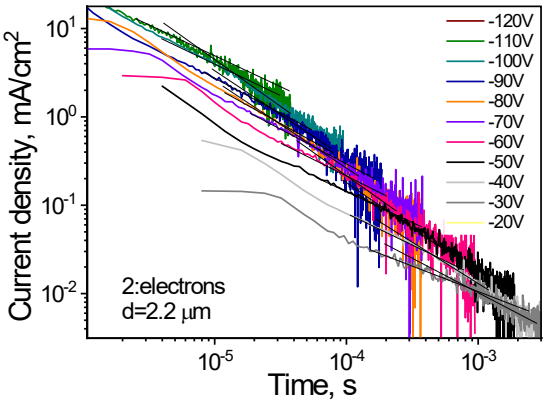
The time of flight (TOF) technique was used for hole and electron mobility measurements. TOF setup consisted of a Nd:YAG laser EKSPLA NL300 (third-harmonic of 355 nm and pulse duration of 3-6 ns), electrometer Keithley 6517B and oscilloscope Tektronix TDS 3032C. The formula $\mu=d^2/U\cdot t_{tr}$ was used for calculation of the drift mobility. In the formula, d is the layer thickness, U is the applied voltage at the moment of laser excitation, t_{tr} is the transit time which was obtained from the TOF transients built in log-log scales.

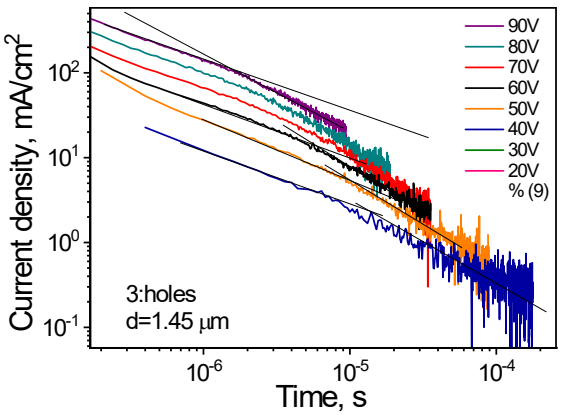
Measurements were determined in air and at room temperature. The thickness of the vacuum evaporated layers varied from 1.45 to 2.4 μm.

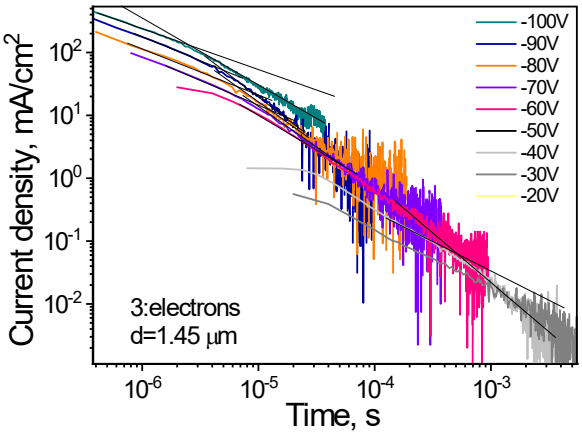

Current density, mA/cm2
Time, s
100V
90V
80V
70V
60V
50V
40V
30V
20V
10V
1:holes
d=1.7 μm

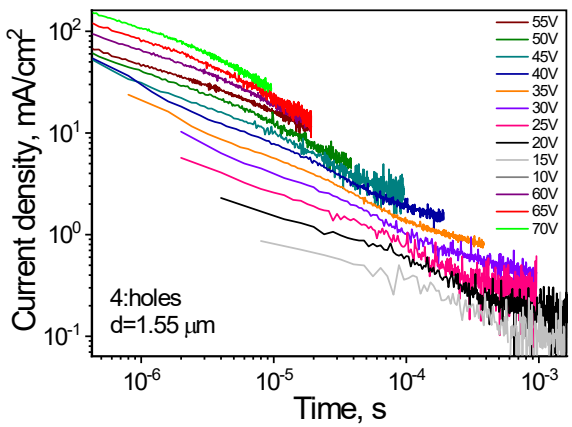

Current density, mA/cm2
Time, s
-80V
-60V
-40V
-20V
1:electrons:no
d=1.7 μm

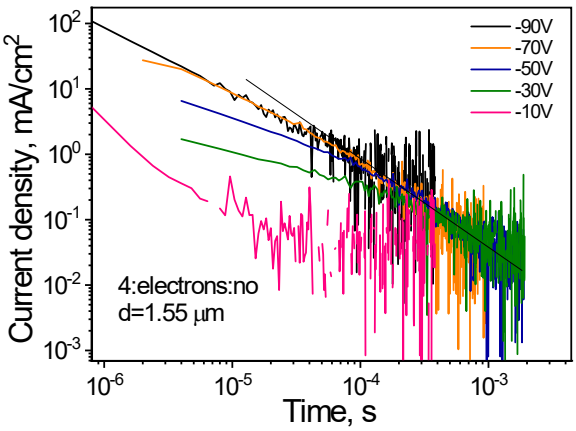

Current density, mA/cm2
Time, s
110V
100V
90V
80V
70V
60V
50V
40V
30V
20V
2:holes
d=2.2 μm


Current density, mA/cm2
Time, s
-120V
-110V
-100V
-90V
-80V
-70V
-60V
-50V
-40V
-30V
-20V
2:electrons
d=2.2 μm


Current density, mA/cm2
Time, s
90V
80V
70V
60V
50V
40V
30V
20V
% (9)
3:holes
d=1.45 μm


Current density, mA/cm2
Time, s
-100V
-90V
-80V
-70V
-60V
-50V
-40V
-30V
-20V
3:electrons
d=1.45 μm


Current density, mA/cm2
Time, s
55V
50V
45V
40V
35V
30V
25V
20V
15V
10V
60V
65V
70V
4:holes
d=1.55 μm


Current density, mA/cm2
Time, s
-90V
-70V
-50V
-30V
-10V
4:electrons:no
d=1.55 μm

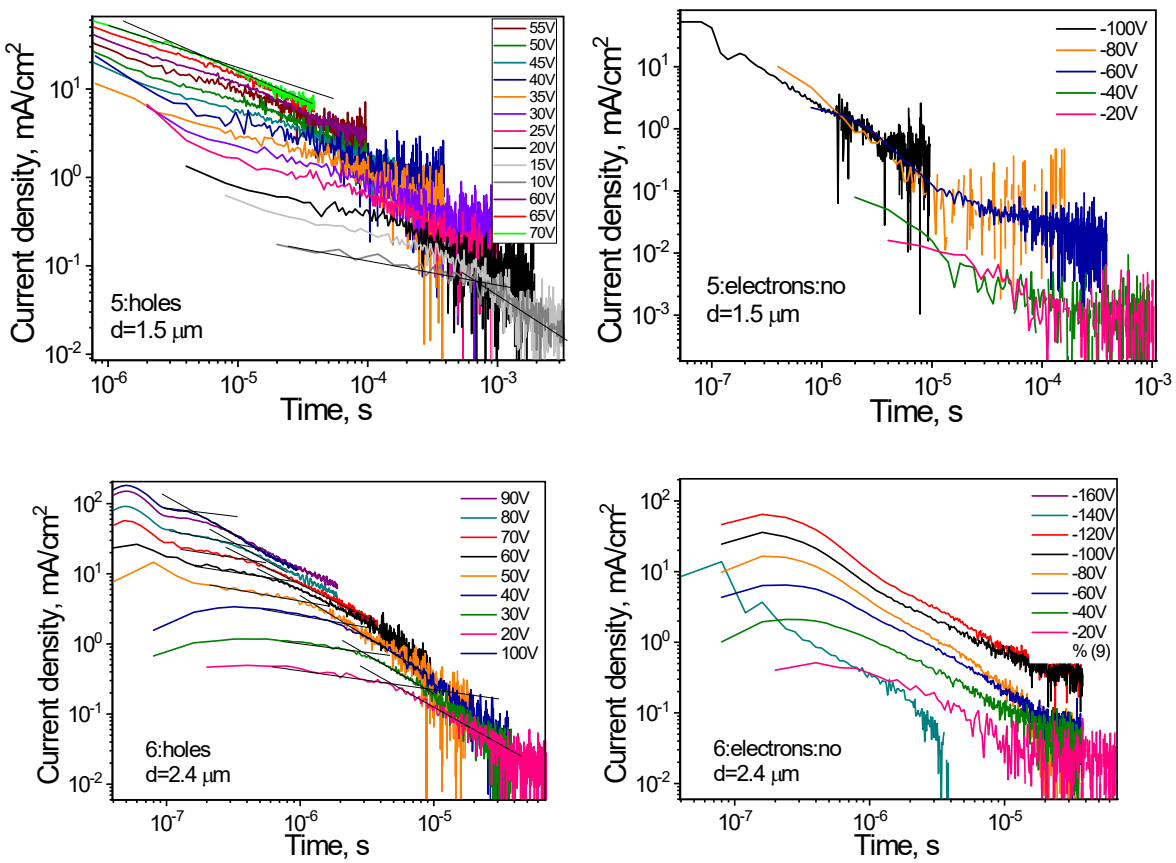


Figure S4. TOF signals for holes and electrons in the vacuum-deposited layers **1-6**.

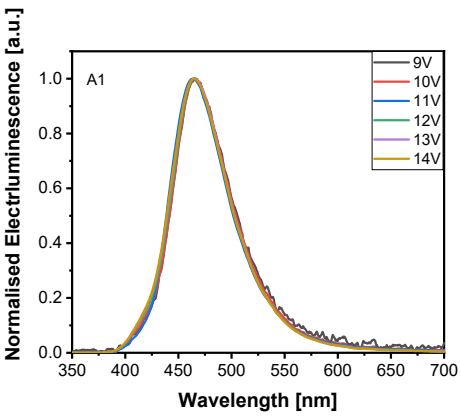
6. Electroluminescent investigations.

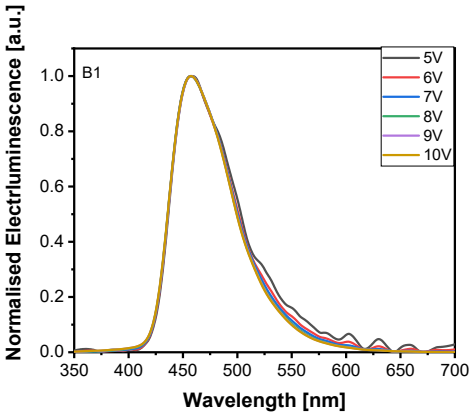
Device fabrication and characterization

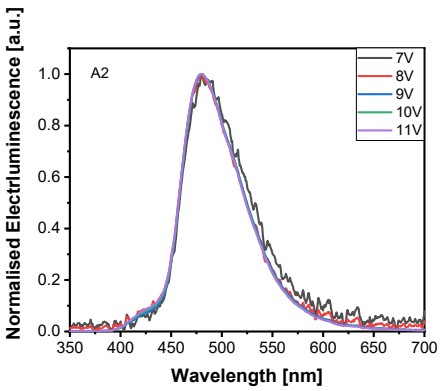
Purchased from Sigma Aldrich or Lumtec companies compounds and materials for test OLEDs fabrication *i.e.* molybdenum oxide (MoO_3), N,N′-di(1-naphthyl)-N,N′-diphenyl-(1,1′-biphenyl)-4,4′-diamine (NPB), 1,3-bis(9-carbazolyl)benzene (mCP), diphenyl-4-triphenylsilyl-phenylphosphineoxide (TSPO1) and 2,2',2''-(1,3,5-benzinetriyl)-tris(1-phenyl-1-H-benzimidazole) (TPBi), lithium fluoride (LiF) were used as received.

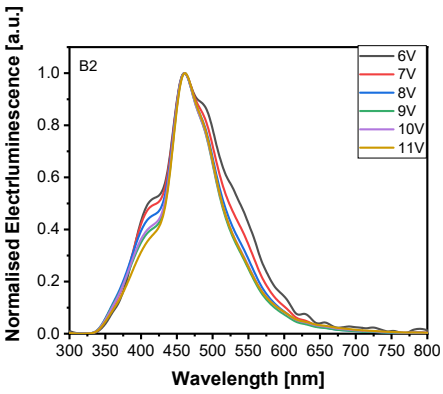
OLEDs with acridone or quonacridone derivatives as emitters were fabricated by vacuum deposition (at vacuum of ca. 2×10^{-6} mBar). For all devices, layers were deposited at the same time except the light-emitting layers. Pre-cleaned and pre-patterned indium tin oxide (ITO)

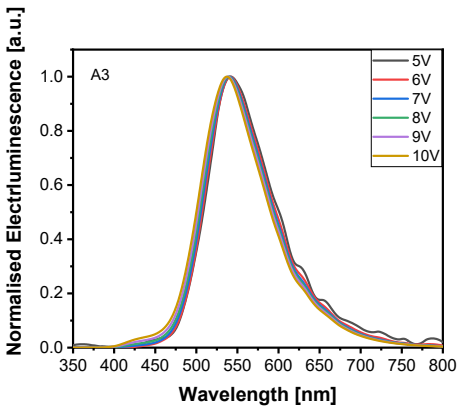
coated glass substrates with a sheet resistance of 15 Ω/sq were used for device fabrications. A certificated photodiode PH100-Si-HA-D0 together with the PC-Based Power and Energy Monitor 11S-LINK (from STANDA) and Keithley 2400C source meter were used for collecting current density-voltage and brightness-voltage characteristics. An Avantes AvaSpec-2048XL spectrometer was used for recording electroluminescence (EL) spectra. The characteristics of brightness and current density as a function of voltage together with EL spectra were used for calculating of device efficiencies.

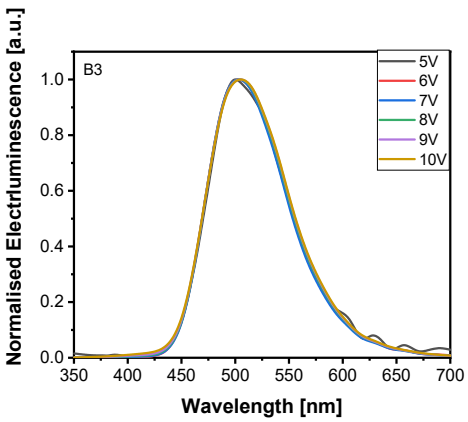












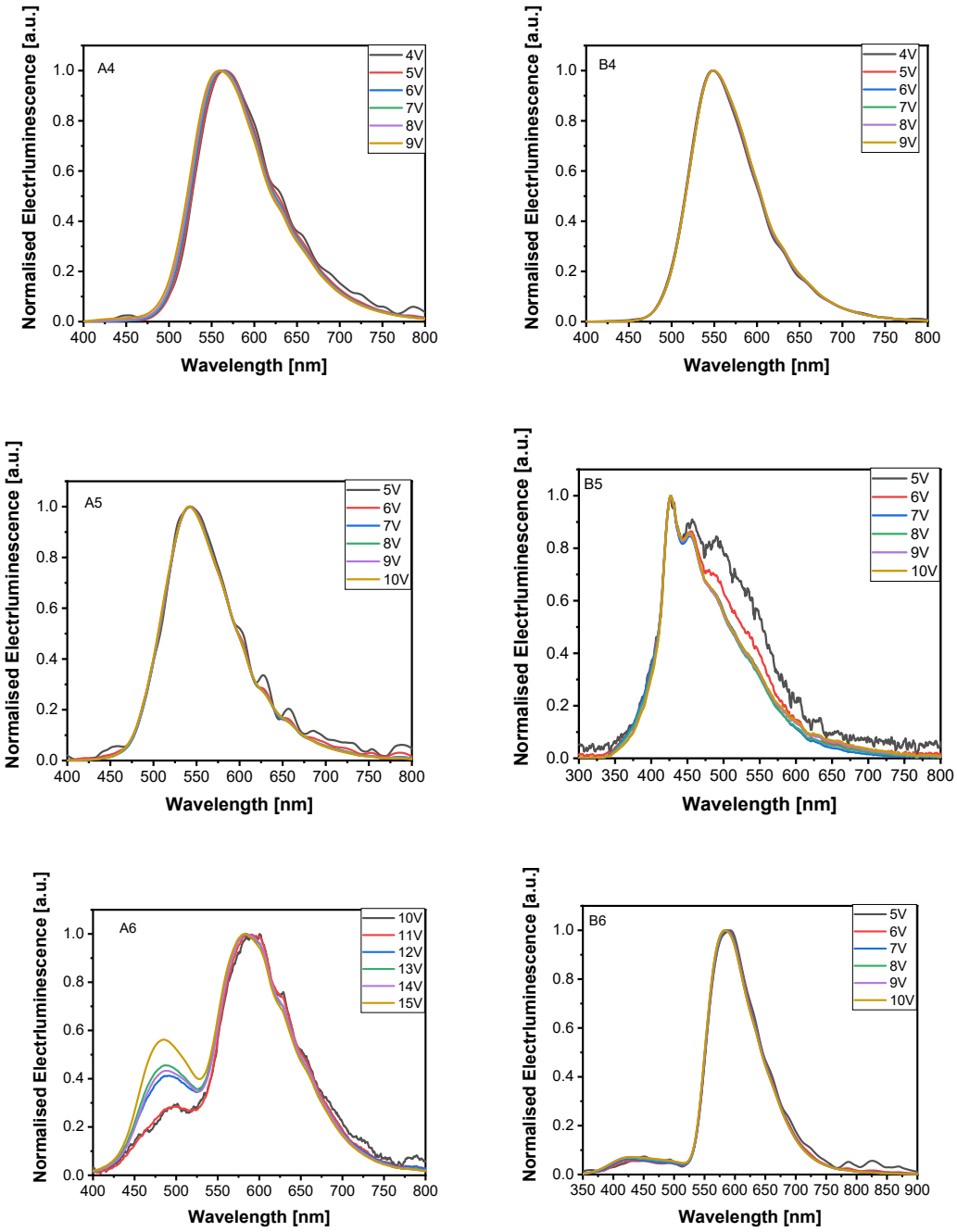


Figure S5. EL spectra at different voltages for the non-doped A1-A6 (left) and doped B1-B6 (right) devices.

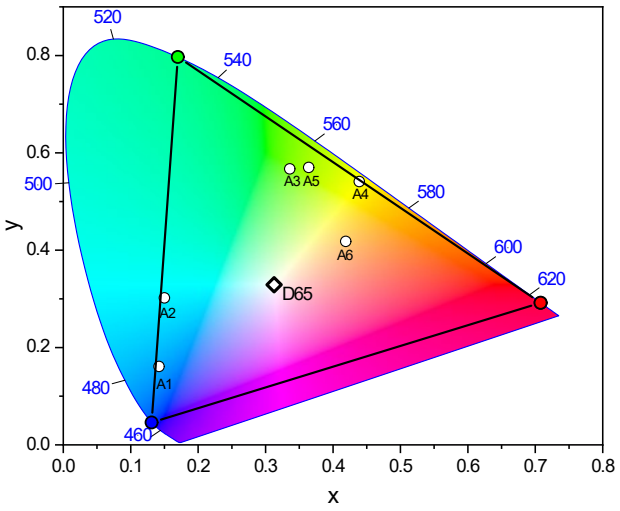
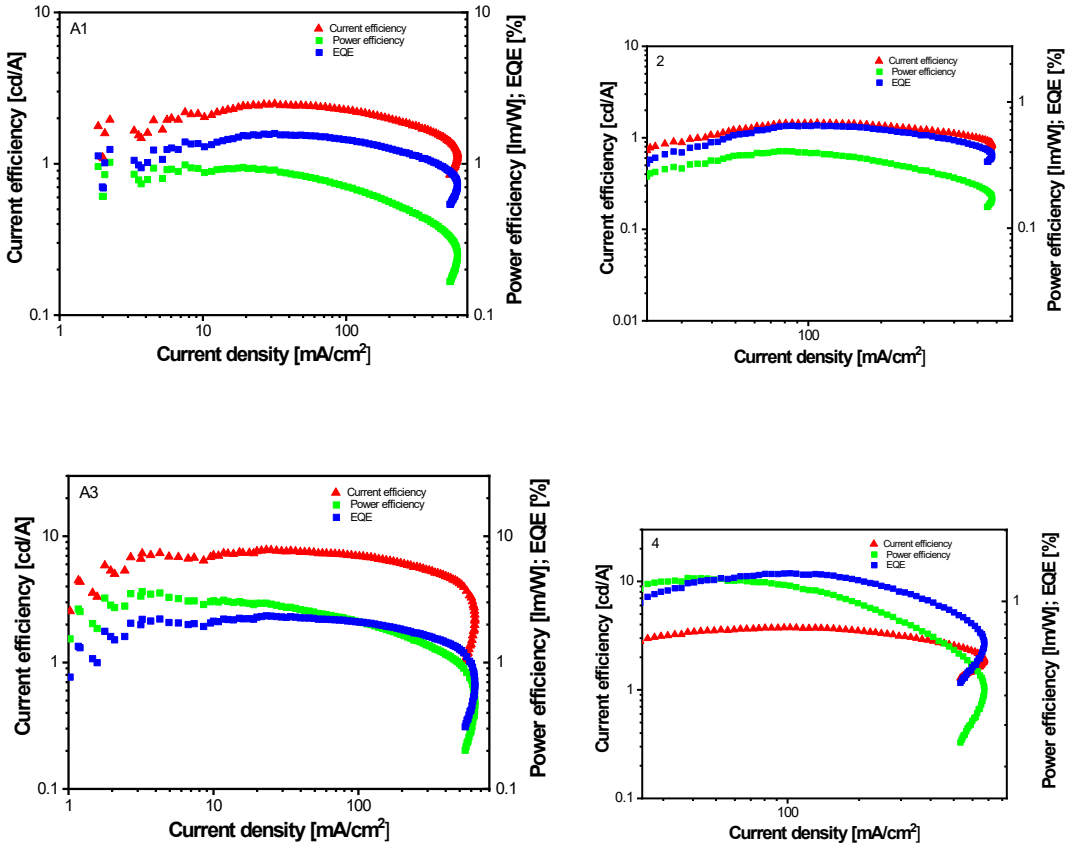
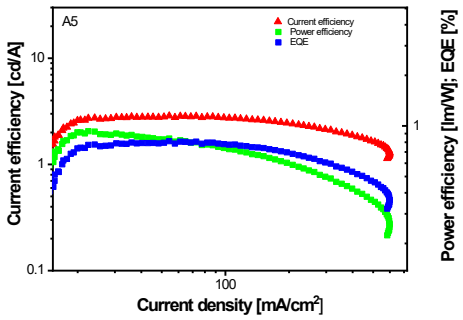


Figure S6. CIE colour diagram for non-doped devices.





a)

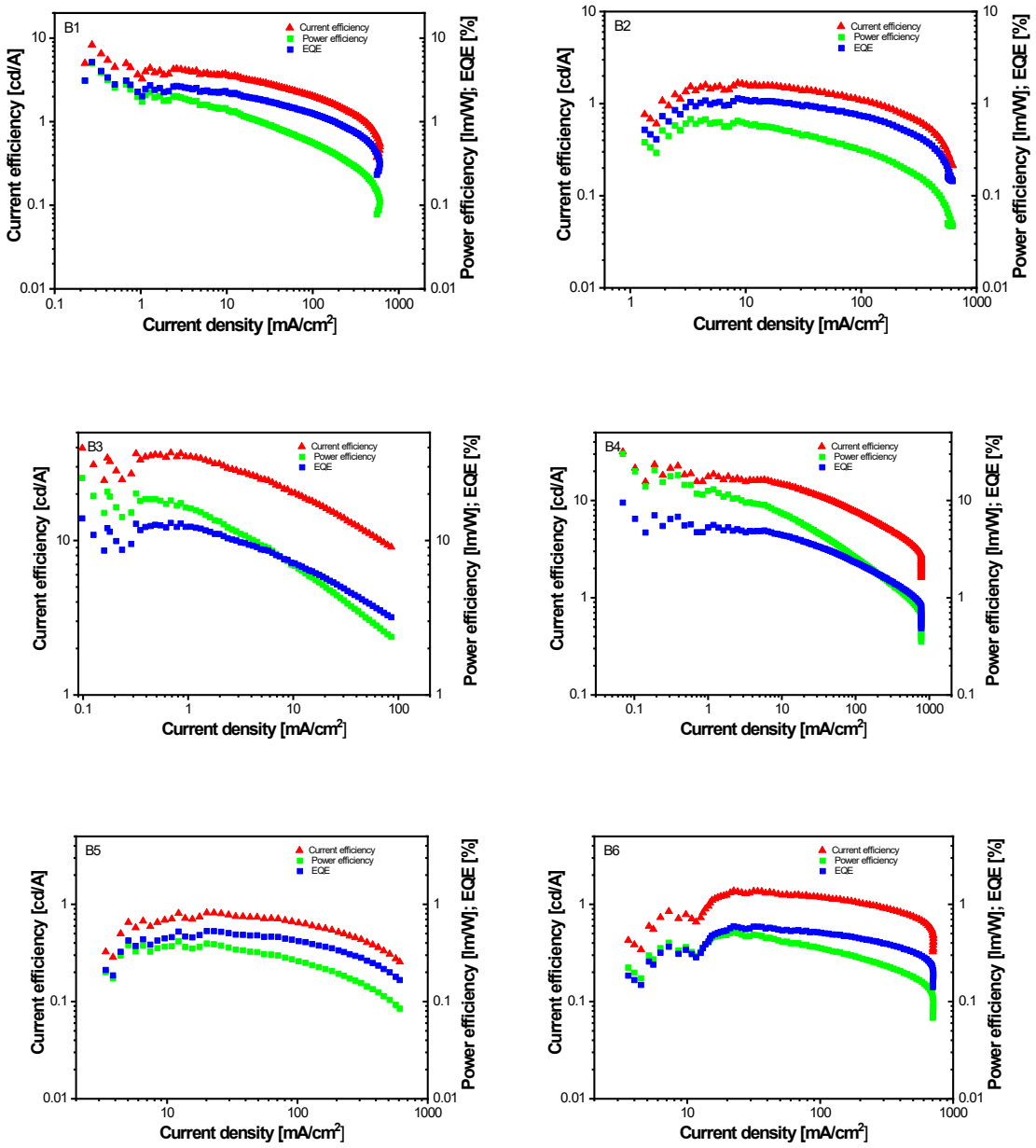


Figure S7. Device efficiencies as function of current density.

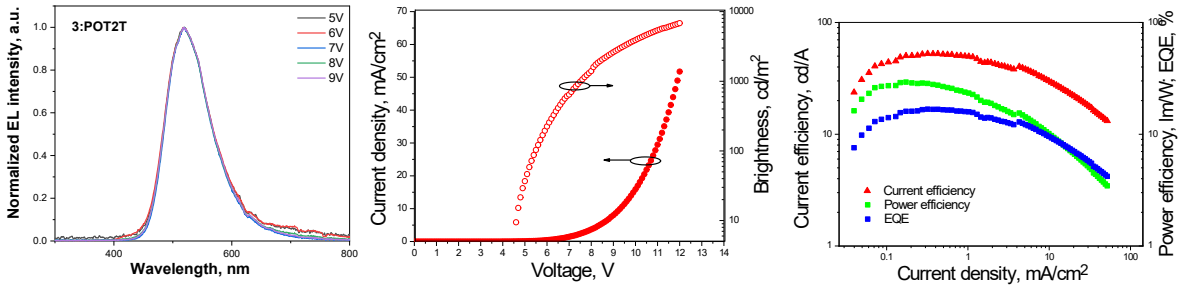


Figure S8. EL spectra recorded at different voltages (a), current density and brightness as the function of applied voltages (b), current efficiency, and EQE versus current density plots (c) of device C3 with structure ITO / MoO3 (0.3 nm) / TCTA (40 nm) / 3:POT2T(20 wt%) (24 nm) / TSPO1 (4 nm)/ TPBi (40 nm) /LiF (0.3 nm)/ Al (120 nm).

Table S1. Output electroluminescent parameters of OLEDs with non-doped (**A1**-**A6**) EMLs.

Device name*	EML	λ_{EL}**, nm	V_{ON}, V	L_{MAX}, cd/m²	CE_{MAX}, cd/A	PE_{MAX}, lm/W	EQE_{MAX}, %	CIE 1931, x; y
A1	**1**	464	5.7	7475	2.56	0.9	1.6	0.142; 0.161
A2	**2**	481	7.9	5135	1.53	0.4	0.7	0.150; 0.302
A3	**3**	540	5.1	21200	8.02	3.6	2.3	0.336; 0.567
A4	**4**	563	6.1	13200	3.8	1.26	1.32	0.439; 0.541
A5	**5**	542	6.3	8460	2.77	0.91	0.76	0.364; 0.570
A6	**6**	484,585	11.4	443	0.4	0.06	0.12	0.419; 0.418

*Device structure is ITO / MoO_3 / NPB / mCP / **EML** / TSPO1 / TPBi / LiF / Al

**Collected parameters are: EL maximum (λ_{EL}); turn-on voltage (V_{ON}); maximum brightness (L_{MAX}); maximum current (CE_{MAX}); power (PE_{MAX}) and external quantum (EQE_{MAX}) efficiencies; colour coordinates (CIE 1931).

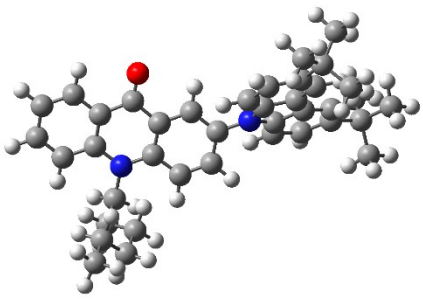
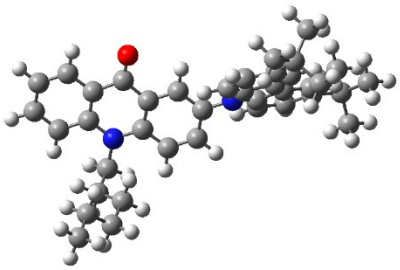
7. Methodology of quantum chemical calculations

Before starting calculations that are more detailed, geometries of the studied molecules (**1-6**) were optimized using the hybrid Density Functional Theory (DFT) method with B3LYP [3,4]functional. The chosen method was augmented by the Grimme empirical dispersion correction with the Becke-Johnson damping (GD3BJ)[5] with the goal to account for intramolecular dispersion forces acting between conjugated molecular moieties. Electron parameters were defined by 6-311++G(d,p) basis set. Calculations were performed for isolated molecules in vacuum as well as in solvent using Gaussian 16 program package.[6] The minimum of the potential energy surface was calculated at restricted Hartree-Fock (RHF) level in C_1 symmetry. The Berny algorithm based on eigenvalue-following method augmented by Hessian techniques was used to reach the geometries of **1-6** molecules corresponding to the minimum of their total energy. The obtained equilibrium structures were checked by the normal mode analysis and no imaginary frequencies were found. The RMS force criterion was chosen as

3ß10^{-4} Hartrees/Bohr. The SCF convergence criterion was equal to 10^{-8} Hartrees in convergence on RMS density matrix and 10^{-6} Hartrees in convergence in energy change. Solvation effect was calculated applying of the polarizable continuum model (PCM) using the integral equation formalism variant.[7]

To predict electron and optical properties of the **1-6** molecules the quantum chemical calculations were performed using the structure with optimized geometry. Computations were performed in Gaussian 16 for the molecules in vacuum and in dichloromethane. Calculations were carried out by applying the DFT/B3LYP-GD3BJ/6-311++G(d,p) method at the ground-state molecular geometries. The optical properties were determined using the time dependent DFT (TDDFT) formalism. It is considered to be the most prominent method to calculate the excited state of medium-size and large molecules. The SCF convergence criterion was chosen as 10^{-12} Hartrees in convergence on RMS density matrix and 10^{-8} Hartrees in convergence in energy change. Vertical and adiabatic ionization potentials and electron affinities were evaluated from the differences of the total energies of the neutral molecules and respective ion-radicals.

Geometry of the 1-6 molecules was relaxed in vacuum and in dichloromethane applying DFT/B3LYP-GD3BJ/6-311++G(d,p) method as it is described in original text. The atom structures are presented in Fig. S6. Next, the coordinates of the atoms of all studied molecules are presented.

Molecule	**Geometry in vacuum**	**Geometry in dichloromethane**
1		

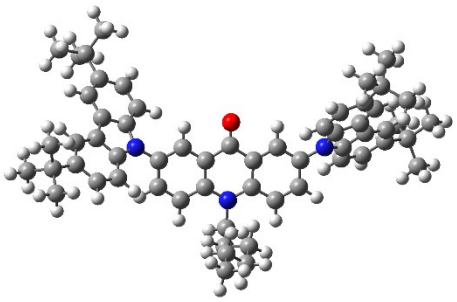
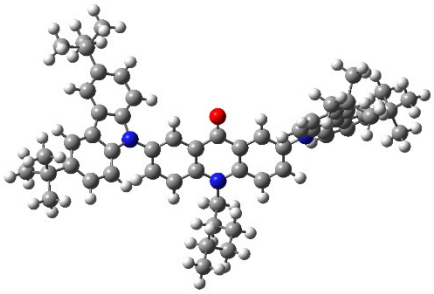
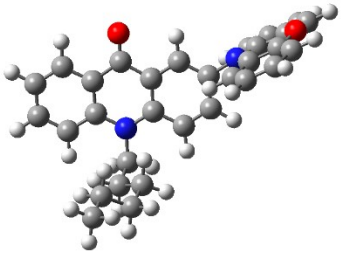
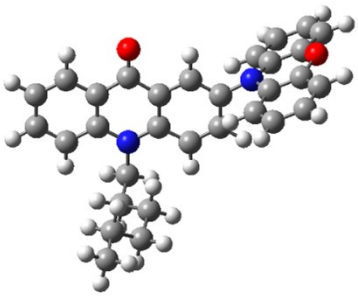
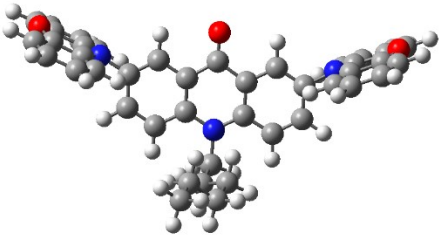
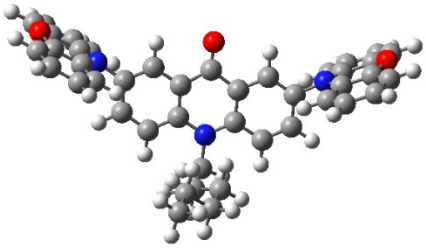
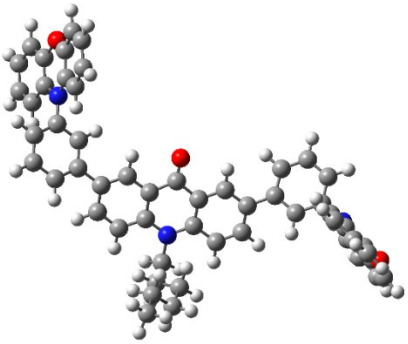
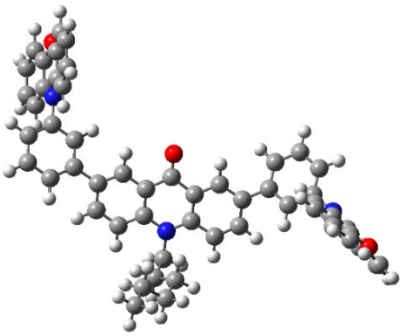
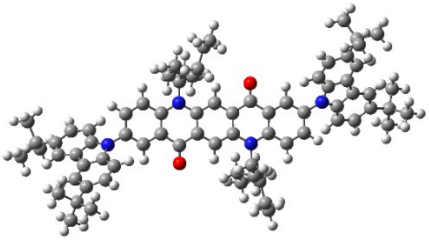
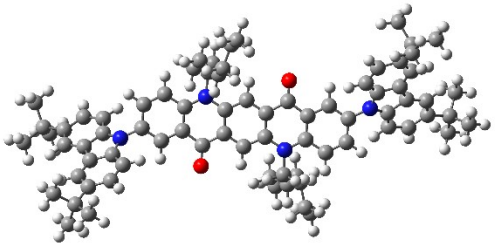
2		
3		
4		
5		
6		

Figure S9. Geometry of the 1-6 molecule equilibrated in vacuum and in dichloromethane

Coordinates of molecule **1** relaxed in vacuum

Symbol	X	Y	Z
C	3.5025210	-3.3167050	-0.0465430
C	4.7642840	-2.6987300	0.0906210
C	4.8132540	-1.3064840	0.1279810
C	3.6380550	-0.5549920	0.0421380
C	2.3912030	-1.2084260	-0.0791110
C	2.3164330	-2.5989720	-0.1354770
H	3.4447780	-4.3975300	-0.0909310
H	5.7588190	-0.7892290	0.2189500
H	1.3699270	-3.1102860	-0.2559970
C	3.3690520	0.8688140	0.0283470
C	1.9670440	1.0209830	-0.1015720
C	4.1799720	1.9975620	0.1260180
C	3.6216740	3.2785130	0.1009660
C	2.2241290	3.3907500	-0.0182190
C	1.3848300	2.2827750	-0.1189940
H	5.2516680	1.8696400	0.2241780
H	1.7650590	4.3692600	-0.0374150
H	0.3145060	2.4124000	-0.2119080
C	6.0215840	-3.5739140	0.1847040
C	6.1484790	-4.4328940	-1.0915130
C	7.3028460	-2.7375350	0.3267230
C	5.9133650	-4.4984080	1.4160720
C	4.5405200	4.5051300	0.2027720
C	5.5336000	4.5004850	-0.9789120
C	3.7590210	5.8278490	0.1642250
C	5.3252060	4.4506360	1.5308200
H	6.2259740	-3.7976730	-1.9776290
H	5.2853990	-5.0885340	-1.2248100
H	7.0425440	-5.0617760	-1.0400950
H	7.2867680	-2.1237490	1.2311290
H	7.4539130	-2.0802720	-0.5335070
H	8.1683290	-3.4019080	0.3920610
H	6.8033020	-5.1299200	1.4980070
H	5.0421790	-5.1539110	1.3530050
H	5.8243360	-3.9102360	2.3331910
H	4.9993800	4.5364360	-1.9318210
H	6.1556470	3.6028450	-0.9783850
H	6.1968500	5.3692090	-0.9235280
H	4.4563530	6.6662500	0.2394920
H	3.0549500	5.9065880	0.9966680
H	3.2026580	5.9423300	-0.7695590
H	5.9422460	3.5520780	1.5977400
H	4.6411700	4.4509860	2.3834790
H	5.9856020	5.3187280	1.6195900
C	-0.6158500	-1.3669970	0.6908360
C	-0.0070970	-0.5134190	-0.2426070
C	-0.7969270	0.0735620	-1.2117990
C	-2.1762910	-0.1666110	-1.2688030

C	-2.7917290	-1.0472070	-0.3499100
C	-1.9683750	-1.6359000	0.6363400
H	-0.0151110	-1.8093600	1.4757240
H	-0.3762530	0.7347900	-1.9580370
H	-2.3806380	-2.2805780	1.3951100
C	-2.9540540	0.5198810	-2.3109040
C	-4.3890860	0.2125810	-2.3204600
C	-4.9538030	-0.6838120	-1.3840290
N	-4.1596980	-1.3064620	-0.4217260
O	-2.4375630	1.2977090	-3.1096320
C	-5.2001450	0.8270330	-3.2870980
C	-6.5552530	0.5757480	-3.3512350
C	-7.1186730	-0.3113450	-2.4259920
C	-6.3437560	-0.9284380	-1.4604370
H	-4.7110510	1.5026110	-3.9776480
H	-7.1733250	1.0542200	-4.1006280
H	-8.1815840	-0.5225770	-2.4557910
H	-6.8301980	-1.5935200	-0.7648460
C	-4.7970320	-2.2426590	0.5164940
C	-5.5159930	-1.5549510	1.6831080
C	-4.5975830	-0.7706520	2.6247690
C	-5.3507040	-0.0205040	3.7305280
C	-6.2059150	1.1486500	3.2303280
C	-6.8764910	1.9188620	4.3693830
H	-4.0408720	-2.9320600	0.8818840
H	-5.4961840	-2.8574330	-0.0513470
H	-6.0454590	-2.3297850	2.2507300
H	-6.2815930	-0.8885210	1.2802000
H	-3.8817470	-1.4600160	3.0859240
H	-4.0052090	-0.0531510	2.0473560
H	-5.9843080	-0.7242490	4.2859150
H	-4.6209140	0.3645550	4.4518060
H	-6.9753160	0.7845860	2.5415700
H	-5.5729840	1.8288240	2.6480360
H	-7.5361840	1.2669710	4.9505450
H	-6.1319440	2.3322430	5.0565720
H	-7.4780630	2.7492430	3.9908400
N	1.3787250	-0.2480730	-0.1648640

Coordinates of molecule **1** relaxed in dichloromethane

Symbol	X	Y	Z
C	3.5171810	-3.3100780	0.0580330
C	4.7785540	-2.6820300	0.1625490
C	4.8222190	-1.2885680	0.1557720
C	3.6411920	-0.5454710	0.0572680
C	2.3958280	-1.2083270	-0.0325110
C	2.3262340	-2.6009160	-0.0421820
H	3.4633050	-4.3918960	0.0515630
H	5.7660780	-0.7644670	0.2225070
H	1.3806050	-3.1205530	-0.1294880

C	3.3636220	0.8764430	0.0057260
C	1.9582860	1.0156940	-0.1145060
C	4.1689000	2.0132670	0.0646980
C	3.6011600	3.2900220	0.0098190
C	2.2007990	3.3900120	-0.0996250
C	1.3674780	2.2736600	-0.1618990
H	5.2421090	1.8947270	0.1568630
H	1.7349520	4.3647660	-0.1398870
H	0.2950460	2.3933050	-0.2457250
C	6.0408270	-3.5486370	0.2715230
C	6.1625740	-4.4400460	-0.9830140
C	7.3187880	-2.7027930	0.3841950
C	5.9439350	-4.4427700	1.5262500
C	4.5122710	4.5253800	0.0720900
C	5.4989370	4.4947020	-1.1147890
C	3.7212340	5.8411880	0.0027120
C	5.3061860	4.5115450	1.3959410
H	6.2362970	-3.8273930	-1.8855630
H	5.3003520	-5.1011390	-1.0936910
H	7.0586720	-5.0644720	-0.9183380
H	7.3046160	-2.0651570	1.2720180
H	7.4623320	-2.0676630	-0.4937870
H	8.1864740	-3.3627350	0.4622280
H	6.8382480	-5.0665180	1.6165680
H	5.0763410	-5.1047360	1.4841740
H	5.8596570	-3.8322030	2.4293710
H	4.9591230	4.5051120	-2.0655240
H	6.1266830	3.6012110	-1.0934310
H	6.1563930	5.3687860	-1.0841510
H	4.4146250	6.6847300	0.0499780
H	3.0224240	5.9382750	0.8376600
H	3.1574540	5.9261790	-0.9298510
H	5.9291830	3.6187400	1.4827740
H	4.6276170	4.5342220	2.2529880
H	5.9614520	5.3858410	1.4542560
C	-0.6175820	-1.3341230	0.7768670
C	-0.0088250	-0.5330280	-0.2039520
C	-0.7926470	-0.0087710	-1.2102180
C	-2.1733700	-0.2571840	-1.2621790
C	-2.7896630	-1.0824860	-0.2904380
C	-1.9672580	-1.6096190	0.7331580
H	-0.0202080	-1.7303720	1.5883150
H	-0.3631370	0.6084410	-1.9877850
H	-2.3794620	-2.2127850	1.5245260
C	-2.9484510	0.3523330	-2.3452120
C	-4.3780240	0.0467960	-2.3385280
C	-4.9430200	-0.7903400	-1.3458230
N	-4.1521930	-1.3491290	-0.3474140
O	-2.4269190	1.0779080	-3.2017520
C	-5.1944380	0.5975560	-3.3427120

C	-6.5479040	0.3408670	-3.3888520
C	-7.1097130	-0.4891120	-2.4075320
C	-6.3337290	-1.0426790	-1.4070800
H	-4.7150350	1.2300260	-4.0787500
H	-7.1681260	0.7701760	-4.1656380
H	-8.1719060	-0.7037390	-2.4233810
H	-6.8177930	-1.6653580	-0.6723790
C	-4.7947620	-2.2152560	0.6605230
C	-5.5083320	-1.4379410	1.7714050
C	-4.5881890	-0.5732290	2.6378920
C	-5.3374000	0.2420390	3.6993210
C	-6.2257550	1.3538760	3.1310170
C	-6.8904150	2.1938310	4.2235660
H	-4.0418490	-2.8788330	1.0738670
H	-5.4946510	-2.8664440	0.1385150
H	-6.0228650	-2.1708370	2.4031460
H	-6.2856840	-0.8142700	1.3249600
H	-3.8542990	-1.2161970	3.1351070
H	-4.0186630	0.1126770	2.0012940
H	-5.9468940	-0.4317840	4.3151470
H	-4.6031400	0.6939090	4.3761350
H	-7.0003530	0.9239680	2.4877490
H	-5.6174480	2.0009990	2.4876860
H	-7.5247070	1.5730230	4.8642180
H	-6.1408410	2.6710010	4.8626190
H	-7.5167640	2.9819340	3.7970020
N	1.3777320	-0.2566710	-0.1365140

Coordinates of molecule **2** relaxed in vacuum

Symbol	X	Y	Z
C	-7.4370170	-0.5545260	-2.8390010
C	-8.5119400	-0.9868980	-2.0326620
C	-8.3141530	-1.0532900	-0.6547260
C	-7.0849600	-0.6890220	-0.0983880
C	-6.0362710	-0.2466610	-0.9353880
C	-6.2029300	-0.1867980	-2.3177190
H	-7.5667370	-0.5087210	-3.9134820
H	-9.1048600	-1.3913640	0.0013100
H	-5.3984020	0.1238340	-2.9720100
C	-6.5750150	-0.6734680	1.2579870
C	-5.2345110	-0.2223450	1.1881970
C	-7.1351280	-0.9848310	2.4951100
C	-6.3870020	-0.8517770	3.6680650
C	-5.0621230	-0.3902670	3.5610630
C	-4.4714200	-0.0712910	2.3397580
H	-8.1615190	-1.3302400	2.5370120
H	-4.4615240	-0.2752060	4.4524410
H	-3.4480700	0.2784080	2.3006460
C	-9.8408750	-1.3707510	-2.6976000
C	-9.6056140	-2.5314950	-3.6875820

C	-10.8941150	-1.8222650	-1.6738320
C	-10.4042920	-0.1528030	-3.4604220
C	-7.0277930	-1.2094070	5.0174110
C	-7.4525100	-2.6933140	5.0050240
C	-6.0663170	-0.9977550	6.1974950
C	-8.2705780	-0.3232460	5.2468840
H	-9.2049940	-3.4059090	-3.1683490
H	-8.8984700	-2.2559660	-4.4727850
H	-10.5457120	-2.8182250	-4.1686590
H	-11.1265960	-1.0304540	-0.9569500
H	-10.5659090	-2.7047350	-1.1185400
H	-11.8204300	-2.0826710	-2.1922850
H	-11.3534550	-0.4095380	-3.9406820
H	-9.7175070	0.1892720	-4.2375750
H	-10.5801770	0.6823730	-2.7774140
H	-6.5872440	-3.3409250	4.8418650
H	-8.1768770	-2.8979560	4.2137640
H	-7.9114860	-2.9668780	5.9600540
H	-6.5691990	-1.2649980	7.1304960
H	-5.7486830	0.0449910	6.2791270
H	-5.1746000	-1.6237680	6.1106990
H	-9.0174650	-0.4654350	4.4629310
H	-7.9938430	0.7342210	5.2575550
H	-8.7398660	-0.5653420	6.2053720
C	-3.6599150	1.6957020	-1.4300120
C	-3.6845840	0.5478550	-0.6216770
C	-2.4843520	-0.0456770	-0.2835550
C	-1.2631510	0.4802160	-0.7271200
C	-1.2321550	1.6187370	-1.5653330
C	-2.4698790	2.2140240	-1.8981290
H	-4.5910060	2.1903800	-1.6768240
H	-2.4488890	-0.9351320	0.3317540
H	-2.5154270	3.1102000	-2.4949360
C	-0.0280670	-0.1913390	-0.3001970
C	1.2128890	0.4097260	-0.8057520
C	1.1871040	1.5410400	-1.6516790
N	-0.0194540	2.1262590	-2.0292900
O	-0.0327560	-1.1796960	0.4292930
C	2.4322070	-0.1619690	-0.4184620
C	3.6350480	0.3413090	-0.8750090
C	3.6159940	1.4524990	-1.7331090
C	2.4271220	2.0487370	-2.1024140
H	2.3944620	-1.0100840	0.2526330
H	4.5510000	1.8441860	-2.1136410
H	2.4743810	2.9073400	-2.7530220
C	0.0163770	3.2995350	-2.9158980
C	0.3426550	4.6100540	-2.1899120
C	-0.6936070	5.0338020	-1.1450400
C	-0.2952790	6.2921050	-0.3636270
C	0.9003820	6.0992760	0.5755130

C	1.2160610	7.3525770	1.3940000
H	-0.9375480	3.3707070	-3.4306870
H	0.7509370	3.1039260	-3.6979440
H	0.4401790	5.3955290	-2.9489460
H	1.3216500	4.5152560	-1.7154120
H	-1.6540340	5.2106500	-1.6414960
H	-0.8591790	4.2138620	-0.4383640
H	-0.0796120	7.1078640	-1.0658100
H	-1.1553270	6.6223020	0.2298630
H	1.7878050	5.8130500	0.0013430
H	0.6909120	5.2611990	1.2508540
H	1.4560810	8.1983450	0.7421490
H	0.3615460	7.6442310	2.0121540
H	2.0687320	7.1917980	2.0586510
N	-4.9143990	0.0371820	-0.1503130
C	5.0429460	-3.9182130	-1.1821610
C	6.3655790	-4.1521060	-0.7470720
C	7.0986290	-3.0708580	-0.2628250
C	6.5256480	-1.7969570	-0.2089820
C	5.1958620	-1.6035240	-0.6435670
C	4.4443110	-2.6657950	-1.1412820
H	4.4575710	-4.7454390	-1.5645250
H	8.1180980	-3.2005080	0.0745670
H	3.4267870	-2.5297040	-1.4836100
C	7.0228590	-0.5032980	0.2142860
C	5.9711950	0.4251010	0.0171690
N	4.8641650	-0.2499140	-0.5066890
C	8.2344080	-0.0699540	0.7478000
C	8.4214420	1.2714770	1.0942770
C	7.3503560	2.1623590	0.8989710
C	6.1250120	1.7612700	0.3686210
H	9.0314400	-0.7890440	0.8964780
H	7.4631560	3.2027870	1.1702520
H	5.3196410	2.4746240	0.2487510
C	6.9391910	-5.5735160	-0.8236250
C	6.9194940	-6.0586440	-2.2888540
C	8.3880030	-5.6437510	-0.3164840
C	6.0808570	-6.5206460	0.0417620
C	9.7699720	1.7197540	1.6771280
C	10.8920410	1.4245190	0.6591710
C	9.7998100	3.2224620	1.9977530
C	10.0475370	0.9454600	2.9833110
H	7.5225550	-5.4015300	-2.9209130
H	5.9060280	-6.0758080	-2.6950200
H	7.3262650	-7.0720200	-2.3599070
H	8.4649620	-5.3387810	0.7304060
H	9.0551320	-5.0127540	-0.9096680
H	8.7520360	-6.6717580	-0.3897030
H	6.4770130	-7.5398070	-0.0013790
H	5.0436830	-6.5495870	-0.2984900

H	6.0812600	-6.1959380	1.0854650
H	10.7166790	1.9631690	-0.2757590
H	10.9530110	0.3596870	0.4247620
H	11.8617620	1.7365980	1.0588790
H	10.7784410	3.4897130	2.4046820
H	9.0467150	3.4927440	2.7424720
H	9.6351290	3.8303710	1.1042720
H	10.0884680	-0.1322270	2.8118210
H	9.2629050	1.1371680	3.7197640
H	11.0054590	1.2537100	3.4132780

Coordinates of molecule **2** relaxed in dichloromethane

Symbol	X	Y	Z
C	-7.4315590	-0.7557480	-2.7970350
C	-8.5015820	-1.1474250	-1.9616720
C	-8.3033270	-1.1187810	-0.5819950
C	-7.0770950	-0.7026270	-0.0531900
C	-6.0333840	-0.3046670	-0.9194720
C	-6.2014810	-0.3379190	-2.3032660
H	-7.5623110	-0.7811430	-3.8720220
H	-9.0898990	-1.4207240	0.0963070
H	-5.4040570	-0.0550120	-2.9784360
C	-6.5669830	-0.5870740	1.2988130
C	-5.2318340	-0.1233850	1.1950990
C	-7.1226160	-0.8207870	2.5561610
C	-6.3742600	-0.5983390	3.7162840
C	-5.0549650	-0.1267780	3.5752680
C	-4.4695780	0.1163750	2.3331810
H	-8.1445270	-1.1751180	2.6232890
H	-4.4553870	0.0584190	4.4555680
H	-3.4517690	0.4786510	2.2680920
C	-9.8255700	-1.5926830	-2.5979140
C	-9.5758910	-2.8221480	-3.4975180
C	-10.8770270	-1.9753250	-1.5446670
C	-10.3982020	-0.4417690	-3.4527900
C	-7.0091370	-0.8701740	5.0885260
C	-7.4264610	-2.3539170	5.1751570
C	-6.0453980	-0.5759810	6.2489380
C	-8.2571170	0.0216540	5.2621720
H	-9.1737860	-3.6531340	-2.9117620
H	-8.8668030	-2.5993590	-4.2976110
H	-10.5120620	-3.1496070	-3.9594900
H	-11.1168520	-1.1343940	-0.8886920
H	-10.5431550	-2.8114440	-0.9247570
H	-11.7993570	-2.2805270	-2.0452800
H	-11.3432190	-0.7459540	-3.9126220
H	-9.7133150	-0.1538020	-4.2532480
H	-10.5863300	0.4407120	-2.8352570
H	-6.5576390	-3.0066070	5.0547900
H	-8.1528630	-2.6137180	4.4020840

H	-7.8808980	-2.5637240	6.1481110
H	-6.5446830	-0.7869840	7.1980230
H	-5.7353980	0.4721530	6.2625040
H	-5.1490540	-1.1995590	6.1989750
H	-9.0038330	-0.1762620	4.4901440
H	-7.9861530	1.0794790	5.2066200
H	-8.7223280	-0.1623980	6.2352490
C	-3.6610300	1.6312360	-1.5333050
C	-3.6852540	0.5263250	-0.6650220
C	-2.4893920	-0.0583940	-0.3051900
C	-1.2648450	0.4351160	-0.7826880
C	-1.2342930	1.5338500	-1.6758350
C	-2.4723820	2.1178400	-2.0329900
H	-4.5895630	2.1181080	-1.8035570
H	-2.4627310	-0.9138650	0.3561910
H	-2.5177340	2.9791770	-2.6781110
C	-0.0336860	-0.2190490	-0.3374140
C	1.2030700	0.3518450	-0.8710850
C	1.1759910	1.4451640	-1.7687890
N	-0.0265380	2.0145340	-2.1677690
O	-0.0382290	-1.1824920	0.4385800
C	2.4273610	-0.1996930	-0.4620270
C	3.6254190	0.2867580	-0.9423790
C	3.6045660	1.3571600	-1.8529330
C	2.4154100	1.9315030	-2.2483460
H	2.4003630	-1.0173970	0.2456320
H	4.5369920	1.7351490	-2.2528530
H	2.4596920	2.7566860	-2.9401160
C	0.0096790	3.1617500	-3.0966370
C	0.3466080	4.4905820	-2.4123440
C	-0.6710820	4.9416660	-1.3606710
C	-0.2645860	6.2283660	-0.6314260
C	0.9522640	6.0744740	0.2874130
C	1.2771820	7.3571100	1.0556510
H	-0.9459530	3.2201630	-3.6073520
H	0.7370330	2.9349210	-3.8752350
H	0.4244460	5.2511640	-3.1973070
H	1.3359150	4.4148810	-1.9562190
H	-1.6421900	5.0955530	-1.8427020
H	-0.8143410	4.1466520	-0.6207380
H	-0.0681940	7.0193760	-1.3665230
H	-1.1137990	6.5735600	-0.0306520
H	1.8284990	5.7742170	-0.2963810
H	0.7617580	5.2591530	0.9956560
H	1.4973690	8.1805650	0.3689380
H	0.4333450	7.6644580	1.6812450
H	2.1453530	7.2243730	1.7068310
N	-4.9158490	0.0471800	-0.1570970
C	5.0923110	-3.9644030	-1.1011580
C	6.4034500	-4.1722530	-0.6170740

C	7.1114890	-3.0695840	-0.1418370
C	6.5250200	-1.7994810	-0.1444170
C	5.2070670	-1.6316660	-0.6269310
C	4.4811220	-2.7165480	-1.1162510
H	4.5272870	-4.8078870	-1.4786560
H	8.1207050	-3.1791530	0.2316530
H	3.4742590	-2.5999510	-1.4958650
C	6.9960210	-0.4880170	0.2556050
C	5.9409010	0.4222430	-0.0032130
N	4.8585400	-0.2798140	-0.5411660
C	8.1874730	-0.0249900	0.8124110
C	8.3490550	1.3295480	1.1210740
C	7.2749450	2.2024840	0.8627210
C	6.0702270	1.7716780	0.3077020
H	8.9870760	-0.7299190	1.0075080
H	7.3692870	3.2528300	1.1008280
H	5.2648940	2.4736580	0.1331610
C	6.9933020	-5.5892130	-0.6339370
C	7.0297360	-6.1145720	-2.0851080
C	8.4236800	-5.6298600	-0.0738900
C	6.1133250	-6.5222330	0.2253650
C	9.6738990	1.8126600	1.7304960
C	10.8306580	1.4961720	0.7585030
C	9.6774880	3.3254000	2.0016030
C	9.9185420	1.0841070	3.0693730
H	7.6503840	-5.4697900	-2.7132420
H	6.0311030	-6.1544310	-2.5252870
H	7.4488790	-7.1248740	-2.1113950
H	8.4605340	-5.2944410	0.9658530
H	9.1056500	-5.0087790	-0.6605780
H	8.7981430	-6.6561320	-0.1056420
H	6.5220450	-7.5371460	0.2220690
H	5.0895780	-6.5716150	-0.1515890
H	6.0754630	-6.1714580	1.2602110
H	10.6810430	2.0044410	-0.1979590
H	10.9097140	0.4247730	0.5621300
H	11.7828080	1.8322420	1.1799220
H	10.6402230	3.6152710	2.4301710
H	8.8979370	3.6115850	2.7123960
H	9.5352320	3.9016680	1.0836600
H	9.9751830	0.0018530	2.9345200
H	9.1110800	1.2942550	3.7759290
H	10.8602200	1.4172920	3.5158660

Coordinates of molecule **3** relaxed in vacuum

Symbol	X	Y	Z
C	-2.7979900	3.3589240	1.6559860
C	-4.1578530	3.6296470	1.7412510
C	-5.0764550	2.6763890	1.2975680
C	-4.6320270	1.4703810	0.7845110

C	-3.2615120	1.1847020	0.6856100
C	-2.3515900	2.1467430	1.1278470
H	-2.0721720	4.0856400	2.0002920
H	-4.5101310	4.5684810	2.1498470
H	-6.1443120	2.8487940	1.3507460
H	-1.2920740	1.9382600	1.0685470
C	-5.1788260	-0.5289680	-0.3528100
C	-3.8212720	-0.8617280	-0.4785200
N	-2.8591120	-0.0598360	0.1645600
C	-6.1616520	-1.2915430	-0.9591390
C	-5.8127430	-2.4220590	-1.7004690
C	-4.4734650	-2.7681420	-1.8285580
C	-3.4831400	-1.9915370	-1.2254790
H	-7.1945700	-0.9913890	-0.8332190
H	-6.5854070	-3.0207180	-2.1663640
H	-4.1861080	-3.6449500	-2.3960380
H	-2.4421500	-2.2679140	-1.3234820
O	-5.5889830	0.5491700	0.4068250
C	-0.8867640	0.2192370	-1.2689460
C	-1.4732590	-0.2868350	-0.1005980
C	-0.6906000	-0.9916950	0.7861080
C	0.6722600	-1.2109920	0.5345190
C	1.2716260	-0.7104140	-0.6449420
C	0.4515210	0.0188000	-1.5380340
H	-1.4968620	0.7834490	-1.9643390
H	-1.1063900	-1.3925880	1.7017290
H	0.8548230	0.4533580	-2.4376900
C	1.4491560	-1.9610330	1.5323670
C	2.8708160	-2.1362050	1.2099510
C	3.4198320	-1.6215910	0.0136410
N	2.6225310	-0.9301460	-0.9006740
O	0.9441310	-2.4029370	2.5607290
C	3.6825160	-2.8357430	2.1158760
C	5.0244470	-3.0388200	1.8667100
C	5.5725270	-2.5306350	0.6831900
C	4.7956250	-1.8350620	-0.2262680
H	3.2052180	-3.2078480	3.0137470
H	5.6437910	-3.5793670	2.5714900
H	6.6248360	-2.6760480	0.4671030
H	5.2707760	-1.4548690	-1.1164170
C	3.2449040	-0.4336400	-2.1381750
C	4.0187540	0.8774380	-1.9566750
C	3.1553740	2.0782170	-1.5588300
C	3.9651630	3.3539610	-1.2955150
C	4.8492450	3.2934720	-0.0452310
C	5.5774830	4.6110810	0.2266870
H	2.4715860	-0.3243430	-2.8933210
H	3.9047160	-1.2161110	-2.5139790
H	4.5320440	1.0938480	-2.9013520
H	4.7990240	0.7243920	-1.2081440

H	2.4263560	2.2760220	-2.3522940
H	2.5757360	1.8334180	-0.6625450
H	4.5868010	3.5815470	-2.1711850
H	3.2697370	4.1945090	-1.1909870
H	5.5864390	2.4898410	-0.1437180
H	4.2267100	3.0314440	0.8185910
H	6.2279850	4.8814300	-0.6109240
H	4.8670820	5.4308340	0.3708440
H	6.1987970	4.5467790	1.1236130

Coordinates of molecule **3** relaxed in dichloromethane

Symbol	X	Y	Z
C	-2.7882880	3.3854720	1.6032770
C	-4.1488960	3.6462410	1.7177050
C	-5.0698440	2.6801710	1.3042550
C	-4.6252140	1.4729200	0.7935790
C	-3.2549160	1.1966490	0.6651290
C	-2.3430770	2.1715440	1.0763700
H	-2.0606650	4.1221960	1.9214670
H	-4.5000800	4.5863500	2.1242640
H	-6.1373140	2.8472200	1.3814390
H	-1.2831830	1.9742160	0.9916160
C	-5.1794060	-0.5365250	-0.3273700
C	-3.8210300	-0.8561300	-0.4798390
N	-2.8550880	-0.0485090	0.1470240
C	-6.1685100	-1.3037360	-0.9180660
C	-5.8242890	-2.4294020	-1.6709470
C	-4.4838100	-2.7633380	-1.8257620
C	-3.4879280	-1.9804130	-1.2386630
H	-7.2024600	-1.0150610	-0.7733030
H	-6.6008790	-3.0320060	-2.1250350
H	-4.1995260	-3.6343220	-2.4036850
H	-2.4468810	-2.2465120	-1.3612110
O	-5.5821570	0.5345170	0.4503770
C	-0.8787970	0.2145590	-1.2906060
C	-1.4686890	-0.2816410	-0.1178170
C	-0.6933870	-0.9832930	0.7749570
C	0.6711860	-1.2111150	0.5296830
C	1.2747460	-0.7182800	-0.6536260
C	0.4575750	0.0068410	-1.5549140
H	-1.4830880	0.7756640	-1.9932730
H	-1.1195180	-1.3733310	1.6899400
H	0.8627660	0.4297500	-2.4586240
C	1.4431950	-1.9549780	1.5271690
C	2.8594470	-2.1368020	1.2114960
C	3.4122570	-1.6278180	0.0118320
N	2.6214150	-0.9405190	-0.9054660
O	0.9312080	-2.3938110	2.5644640
C	3.6731430	-2.8349250	2.1212790
C	5.0137030	-3.0400570	1.8738690

C	5.5638660	-2.5366660	0.6863200
C	4.7892370	-1.8452260	-0.2259520
H	3.2026170	-3.2056760	3.0227610
H	5.6325550	-3.5779540	2.5809890
H	6.6158750	-2.6842380	0.4718200
H	5.2650080	-1.4713050	-1.1178700
C	3.2526750	-0.4365090	-2.1416360
C	4.0211300	0.8743620	-1.9455940
C	3.1547770	2.0679710	-1.5330180
C	3.9614090	3.3463780	-1.2727180
C	4.8606280	3.2840990	-0.0334530
C	5.5866910	4.6038470	0.2350080
H	2.4844660	-0.3270150	-2.9004510
H	3.9147370	-1.2165140	-2.5149980
H	4.5273960	1.0998570	-2.8909480
H	4.8066980	0.7167550	-1.2035700
H	2.4177820	2.2655920	-2.3184810
H	2.5868680	1.8181390	-0.6301560
H	4.5721310	3.5792840	-2.1544430
H	3.2631520	4.1830610	-1.1553400
H	5.5997410	2.4841750	-0.1452190
H	4.2488350	3.0166710	0.8365390
H	6.2259550	4.8787250	-0.6099300
H	4.8738060	5.4198000	0.3898230
H	6.2190070	4.5388250	1.1245510

Coordinates of molecule **4** relaxed in vacuum

Symbol	X	Y	Z
C	-5.7127290	2.2830840	2.4507530
C	-7.0014970	1.9932800	2.8806340
C	-7.5968150	0.7885750	2.5018810
C	-6.9026500	-0.1100830	1.7107940
C	-5.6025160	0.1708910	1.2635020
C	-5.0185660	1.3805130	1.6438350
H	-5.2346670	3.2112140	2.7396280
H	-7.5450430	2.6896390	3.5067650
H	-8.5981390	0.5253650	2.8195180
H	-4.0133130	1.6083620	1.3164670
C	-6.9754980	-2.0824310	0.4092800
C	-5.6770860	-1.8488190	-0.0689100
N	-4.9336460	-0.7802010	0.4686580
C	-7.7411990	-3.1259940	-0.0804820
C	-7.2212820	-3.9772230	-1.0573380
C	-5.9349530	-3.7627190	-1.5359760
C	-5.1684410	-2.7032330	-1.0485950
H	-8.7379320	-3.2630460	0.3202150
H	-7.8206540	-4.7975670	-1.4317520
H	-5.5148190	-4.4171000	-2.2900420
H	-4.1653540	-2.5439680	-1.4202680
O	-7.5261530	-1.3044760	1.4086500

C	-3.6627740	0.3429780	-1.3048920
C	-3.6873850	-0.4272900	-0.1339120
C	-2.4944880	-0.8235260	0.4277690
C	-1.2673680	-0.4725590	-0.1554140
C	-1.2327780	0.2970530	-1.3414450
C	-2.4689720	0.7020300	-1.8964340
H	-4.5991940	0.6659090	-1.7440250
H	-2.4733250	-1.4128500	1.3355880
H	-2.5103620	1.3166940	-2.7804000
C	-0.0335800	-0.9156950	0.5093340
C	1.2108290	-0.4948930	-0.1486370
C	1.1903680	0.2629330	-1.3409010
N	-0.0154140	0.6418510	-1.9272430
O	-0.0421430	-1.5823070	1.5393240
C	2.4315800	-0.8674070	0.4337420
C	3.6307590	-0.5061240	-0.1391890
C	3.6200370	0.2398550	-1.3260920
C	2.4321890	0.6197660	-1.9175530
H	2.4017480	-1.4465600	1.3478510
H	4.5624190	0.5243500	-1.7788530
H	2.4796660	1.2025500	-2.8233190
C	0.0262740	1.4416020	-3.1627710
C	0.3043090	2.9297600	-2.9210350
C	-0.7654810	3.6518840	-2.0965270
C	-0.4082680	5.1083200	-1.7740950
C	0.7609160	5.2683240	-0.7961280
C	1.0377580	6.7303820	-0.4411790
H	-0.9114650	1.3049050	-3.6929660
H	0.7884260	1.0106670	-3.8126740
H	0.4006290	3.4130160	-3.9005230
H	1.2740240	3.0322150	-2.4294340
H	-1.7165570	3.6277070	-2.6394530
H	-0.9329300	3.1120000	-1.1585330
H	-0.1825760	5.6460420	-2.7039870
H	-1.2902420	5.5986930	-1.3469170
H	1.6685490	4.8238630	-1.2177510
H	0.5402510	4.7029040	0.1172280
H	1.2882050	7.3114620	-1.3340830
H	0.1618320	7.1958020	0.0208500
H	1.8718120	6.8205860	0.2593670
C	5.7147820	2.2038690	2.3967400
C	6.9985420	1.8956570	2.8288190
C	7.5693610	0.6736710	2.4681550
C	6.8558910	-0.2237370	1.6929740
C	5.5604320	0.0754230	1.2440540
C	5.0012060	1.3023390	1.6057470
H	5.2556530	3.1457190	2.6715650
H	7.5570390	2.5911390	3.4426510
H	8.5661180	0.3960610	2.7878830
H	4.0000100	1.5448950	1.2765330

C	6.8878700	-2.2164000	0.4212950
C	5.5930180	-1.9652660	-0.0576900
N	4.8711280	-0.8751770	0.4660460
C	7.6325830	-3.2813310	-0.0546470
C	7.0943910	-4.1367900	-1.0178050
C	5.8111160	-3.9052170	-1.4966950
C	5.0658720	-2.8244120	-1.0233490
H	8.6274630	-3.4313610	0.3460010
H	7.6772850	-4.9737230	-1.3813600
H	5.3768490	-4.5626720	-2.2400000
H	4.0649030	-2.6520340	-1.3948960
O	7.4551300	-1.4347710	1.4084290

Coordinates of molecule **4** relaxed in dichloromethane

Symbol	X	Y	Z
C	-5.7087150	2.2976310	2.4256330
C	-6.9826780	1.9916200	2.8900810
C	-7.5684070	0.7737870	2.5350050
C	-6.8779670	-0.1197030	1.7344740
C	-5.5935440	0.1768310	1.2521390
C	-5.0197960	1.3994640	1.6082450
H	-5.2388250	3.2362210	2.6933430
H	-7.5222760	2.6847090	3.5232140
H	-8.5578860	0.5003730	2.8807050
H	-4.0282040	1.6430310	1.2519130
C	-6.9562830	-2.0971580	0.4364200
C	-5.6733670	-1.8438960	-0.0738550
N	-4.9312210	-0.7693010	0.4486780
C	-7.7234830	-3.1469670	-0.0380530
C	-7.2187460	-3.9880020	-1.0331450
C	-5.9471500	-3.7547570	-1.5439780
C	-5.1804920	-2.6876530	-1.0717210
H	-8.7083710	-3.3004450	0.3859210
H	-7.8183770	-4.8131820	-1.3963450
H	-5.5393270	-4.3990110	-2.3133940
H	-4.1910140	-2.5129740	-1.4717450
O	-7.4864760	-1.3312120	1.4591990
C	-3.6599790	0.3478670	-1.3335770
C	-3.6846920	-0.4183950	-0.1582600
C	-2.4953020	-0.8144380	0.4065010
C	-1.2646560	-0.4665160	-0.1751620
C	-1.2296380	0.3010520	-1.3651600
C	-2.4664690	0.7030200	-1.9242780
H	-4.5940430	0.6703070	-1.7776120
H	-2.4830670	-1.4004590	1.3160480
H	-2.5074360	1.3099580	-2.8129300
C	-0.0346950	-0.9037100	0.4875140
C	1.2059100	-0.4896160	-0.1688700
C	1.1851620	0.2671080	-1.3643030
N	-0.0164810	0.6458130	-1.9495760

O	-0.0433190	-1.5698390	1.5283880
C	2.4302880	-0.8598530	0.4114870
C	3.6259020	-0.4982650	-0.1642800
C	3.6150020	0.2458950	-1.3540720
C	2.4272970	0.6227120	-1.9439430
H	2.4096310	-1.4364950	1.3268330
H	4.5550160	0.5309570	-1.8109420
H	2.4734480	1.2009570	-2.8520760
C	0.0254530	1.4634980	-3.1794800
C	0.3051000	2.9459940	-2.9129420
C	-0.7563680	3.6518270	-2.0640170
C	-0.4016710	5.1065490	-1.7312090
C	0.7810910	5.2616630	-0.7690120
C	1.0575570	6.7216040	-0.4043210
H	-0.9117960	1.3344870	-3.7101220
H	0.7851330	1.0388790	-3.8343310
H	0.3862000	3.4425120	-3.8862290
H	1.2818280	3.0433120	-2.4343010
H	-1.7143800	3.6286410	-2.5937690
H	-0.9058700	3.1028110	-1.1278830
H	-0.1910060	5.6536790	-2.6589870
H	-1.2795300	5.5879350	-1.2853110
H	1.6834960	4.8248270	-1.2089690
H	0.5751710	4.6870850	0.1421430
H	1.2928580	7.3108620	-1.2962030
H	0.1857250	7.1787870	0.0739900
H	1.9014360	6.8086630	0.2853320
C	5.7090170	2.2091570	2.3799390
C	6.9772400	1.8834600	2.8466990
C	7.5377960	0.6496290	2.5065250
C	6.8282240	-0.2400490	1.7185730
C	5.5491400	0.0759660	1.2344950
C	5.0007820	1.3145340	1.5752730
H	5.2585810	3.1604340	2.6360380
H	7.5317160	2.5736320	3.4700870
H	8.5221990	0.3609090	2.8542700
H	4.0138150	1.5735930	1.2170340
C	6.8642430	-2.2354770	0.4462040
C	5.5855490	-1.9633150	-0.0649850
N	4.8664860	-0.8669510	0.4443560
C	7.6089140	-3.3070870	-0.0152490
C	7.0850260	-4.1512730	-0.9976850
C	5.8171320	-3.8995420	-1.5089360
C	5.0732440	-2.8108170	-1.0497940
H	8.5914230	-3.4746920	0.4088940
H	7.6670330	-4.9933100	-1.3507210
H	5.3945280	-4.5460150	-2.2684470
H	4.0863890	-2.6219920	-1.4498850
O	7.4121010	-1.4667220	1.4575020

Coordinates of molecule **5** relaxed in vacuum

Symbol	X	Y	Z
C	-3.4060610	0.7348330	-1.5087200
C	-3.0512280	-0.5303540	-1.0028070
C	-1.7265440	-0.7129360	-0.6371620
C	-0.7708340	0.3029130	-0.7615920
C	-1.1347860	1.5700790	-1.2729640
C	-2.4862370	1.7551410	-1.6391530
H	-4.4270610	0.9181890	-1.8222560
H	-1.3810700	-1.6482450	-0.2150850
H	-2.8365760	2.6996710	-2.0220280
C	0.6054690	0.0159600	-0.3330010
C	1.5487280	1.1326690	-0.4812950
C	1.1317300	2.3782870	-1.0016550
N	-0.1871280	2.5844060	-1.3987810
O	0.9425070	-1.0768780	0.1155440
C	2.8790180	0.9373220	-0.0917250
C	3.8332420	1.9385380	-0.1953820
C	3.4099940	3.1761750	-0.7161080
C	2.1045480	3.3977220	-1.1070160
H	3.1238910	-0.0352280	0.3167120
H	4.1286010	3.9784020	-0.8363170
H	1.8514180	4.3703360	-1.4982270
C	-0.5621230	3.9044470	-1.9293980
C	-0.8023810	4.9580800	-0.8418830
C	-1.9804700	4.6530530	0.0876980
C	-2.1553370	5.6802380	1.2130840
C	-1.0338650	5.6704360	2.2575480
C	-1.2879920	6.6498750	3.4049150
H	-1.4432850	3.7871830	-2.5535290
H	0.2289930	4.2278130	-2.6065820
H	-0.9699410	5.9196860	-1.3418540
H	0.1101140	5.0701290	-0.2522840
H	-2.9022970	4.6104400	-0.5025800
H	-1.8523570	3.6591500	0.5290750
H	-2.2431890	6.6860000	0.7820040
H	-3.1065350	5.4838990	1.7206560
H	-0.0765580	5.9127940	1.7842470
H	-0.9281700	4.6546340	2.6567220
H	-1.3709750	7.6765780	3.0349690
H	-2.2194580	6.4108330	3.9269940
H	-0.4785670	6.6247310	4.1390360
C	7.1950600	-2.7241230	3.4513000
C	7.8904800	-3.9092320	3.2475140
C	8.5471470	-4.1199050	2.0334130
C	8.4956190	-3.1570670	1.0410030
C	7.8015500	-1.9528230	1.2338970
C	7.1543420	-1.7490190	2.4537520
H	6.6775880	-2.5463750	4.3861440
H	7.9256510	-4.6689590	4.0182300

H	9.0972200	-5.0316320	1.8358210
H	6.6110840	-0.8282350	2.6170440
C	9.3163580	-2.4044230	-1.0460500
C	8.6406580	-1.1823370	-0.9027730
N	7.7713520	-1.0101430	0.1893410
C	10.1751750	-2.6265860	-2.1081130
C	10.3715890	-1.6333160	-3.0696860
C	9.7039830	-0.4214790	-2.9456370
C	8.8471850	-0.1945410	-1.8675240
H	10.6742990	-3.5855770	-2.1720340
H	11.0386400	-1.8143490	-3.9031960
H	9.8428280	0.3584870	-3.6844710
H	8.3290630	0.7502980	-1.7756900
O	9.1248880	-3.4422690	-0.1555080
C	7.1685470	0.2677680	0.4158950
C	7.8987220	1.2886780	1.0231940
C	7.2957790	2.5258320	1.2282930
C	5.9778180	2.7387750	0.8332730
C	5.2352450	1.7193930	0.2222540
C	5.8542860	0.4783840	0.0180570
H	8.9221550	1.1045220	1.3259540
H	7.8499770	3.3241390	1.7079360
H	5.5119380	3.6980100	1.0251770
H	5.3232500	-0.3297520	-0.4691850
C	-9.1029340	-0.9027520	-3.2787450
C	-10.3549060	-0.4564240	-2.8743190
C	-10.7023450	-0.5185570	-1.5233260
C	-9.8070390	-1.0293940	-0.6000060
C	-8.5352330	-1.4757390	-0.9915360
C	-8.1958310	-1.4043030	-2.3440380
H	-8.8198330	-0.8660530	-4.3237690
H	-11.0617440	-0.0651910	-3.5953020
H	-11.6699840	-0.1846910	-1.1696520
H	-7.2232870	-1.7527090	-2.6640730
C	-9.2570990	-1.3126870	1.6796610
C	-7.9717280	-1.7633130	1.3425740
N	-7.6669730	-1.9949660	-0.0128260
C	-9.6120920	-1.0800290	2.9966880
C	-8.6895260	-1.3078440	4.0197240
C	-7.4142100	-1.7582730	3.7020450
C	-7.0539910	-1.9794680	2.3720180
H	-10.6159400	-0.7305590	3.2041360
H	-8.9732160	-1.1334880	5.0500670
H	-6.6871070	-1.9404430	4.4840320
H	-6.0595070	-2.3287780	2.1300040
O	-10.2257230	-1.1197970	0.7130660
C	-6.3219370	-2.3246480	-0.3782760
C	-5.3756610	-1.3124220	-0.5093910
C	-4.0540420	-1.6082230	-0.8614100
C	-3.7089700	-2.9518590	-1.0725130

C	-4.6550160	-3.9614630	-0.9349190
C	-5.9699390	-3.6537080	-0.5885920
H	-5.6775250	-0.2914530	-0.3100260
H	-2.6963630	-3.2020690	-1.3646640
H	-4.3700040	-4.9924830	-1.1078190
H	-6.7217930	-4.4252860	-0.4797940

Coordinates of molecule **5** relaxed in dichloromethane

Symbol	X	Y	Z
C	-3.3956240	0.7344610	-1.5130740
C	-3.0422710	-0.5288890	-0.9955700
C	-1.7184470	-0.7123380	-0.6323660
C	-0.7571550	0.3008340	-0.7668780
C	-1.1212730	1.5656840	-1.2902000
C	-2.4744280	1.7495360	-1.6564590
H	-4.4165610	0.9202350	-1.8242630
H	-1.3814200	-1.6478190	-0.2053640
H	-2.8231060	2.6893580	-2.0508420
C	0.6151940	0.0213780	-0.3392520
C	1.5577500	1.1294310	-0.5015210
C	1.1390340	2.3717850	-1.0336880
N	-0.1769710	2.5759550	-1.4277660
O	0.9545410	-1.0741730	0.1254980
C	2.8928120	0.9411590	-0.1146910
C	3.8441710	1.9415700	-0.2323840
C	3.4171760	3.1759650	-0.7641120
C	2.1119310	3.3914460	-1.1527780
H	3.1472740	-0.0243350	0.3029970
H	4.1317950	3.9800030	-0.8925680
H	1.8566080	4.3592640	-1.5528350
C	-0.5565970	3.8998070	-1.9598580
C	-0.7879440	4.9516370	-0.8701610
C	-1.9438150	4.6354430	0.0831380
C	-2.1215810	5.6768610	1.1949240
C	-0.9802390	5.7122420	2.2169650
C	-1.2368620	6.7048280	3.3526930
H	-1.4410410	3.7815770	-2.5772290
H	0.2292630	4.2201100	-2.6427830
H	-0.9790150	5.9060090	-1.3736670
H	0.1343840	5.0814530	-0.2999220
H	-2.8736890	4.5652200	-0.4907810
H	-1.7867560	3.6522050	0.5398970
H	-2.2404210	6.6721700	0.7477220
H	-3.0577410	5.4663270	1.7246920
H	-0.0392200	5.9704380	1.7204180
H	-0.8424470	4.7061920	2.6311870
H	-1.3523120	7.7222530	2.9658040
H	-2.1525750	6.4514610	3.8959940
H	-0.4129040	6.7125250	4.0713260
C	7.2545930	-2.6228080	3.5290380

C	7.9307380	-3.8231880	3.3443620
C	8.5548080	-4.0776790	2.1202060
C	8.4904210	-3.1426100	1.1018440
C	7.8173430	-1.9226960	1.2746870
C	7.2015550	-1.6762770	2.5039720
H	6.7630550	-2.4101400	4.4706310
H	7.9766000	-4.5603650	4.1361100
H	9.0878480	-5.0031460	1.9391350
H	6.6743260	-0.7440110	2.6538520
C	9.2591310	-2.4641310	-1.0344380
C	8.6020610	-1.2297940	-0.9064660
N	7.7758650	-1.0095920	0.2077930
C	10.0794310	-2.7320030	-2.1165640
C	10.2551620	-1.7716880	-3.1164450
C	9.6055490	-0.5475780	-3.0083610
C	8.7881200	-0.2755500	-1.9095160
H	10.5666200	-3.6980740	-2.1689290
H	10.8919360	-1.9877160	-3.9651280
H	9.7285510	0.2074510	-3.7753680
H	8.2859900	0.6789950	-1.8306510
O	9.0848240	-3.4724120	-0.1033770
C	7.1784230	0.2780650	0.4036940
C	7.9177010	1.3117520	0.9766640
C	7.3194200	2.5566200	1.1507130
C	5.9993300	2.7630740	0.7583340
C	5.2487280	1.7289100	0.1815460
C	5.8622330	0.4802960	0.0080480
H	8.9429860	1.1349680	1.2775800
H	7.8796220	3.3668010	1.6020320
H	5.5413400	3.7308570	0.9227350
H	5.3258830	-0.3392520	-0.4535190
C	-9.1231700	-0.9885490	-3.2754860
C	-10.3853120	-0.5590570	-2.8816170
C	-10.7310480	-0.5954950	-1.5281770
C	-9.8237100	-1.0646640	-0.5941920
C	-8.5422190	-1.4938920	-0.9743560
C	-8.2048870	-1.4477000	-2.3291190
H	-8.8398550	-0.9696580	-4.3208990
H	-11.1004280	-0.1998450	-3.6110070
H	-11.7063510	-0.2725530	-1.1848780
H	-7.2242910	-1.7795440	-2.6418740
C	-9.2664470	-1.2869240	1.6944450
C	-7.9727410	-1.7198740	1.3636060
N	-7.6626440	-1.9678600	0.0146560
C	-9.6265860	-1.0351990	3.0068790
C	-8.6996360	-1.2269300	4.0348090
C	-7.4160660	-1.6613030	3.7243770
C	-7.0517080	-1.9009540	2.3979830
H	-10.6361320	-0.6998190	3.2111060
H	-8.9866000	-1.0373590	5.0615260

H	-6.6854470	-1.8157970	4.5090760
H	-6.0508130	-2.2364010	2.1630910
O	-10.2405410	-1.1334110	0.7234070
C	-6.3167470	-2.3059000	-0.3457820
C	-5.3704740	-1.2963520	-0.4951970
C	-4.0485690	-1.6023000	-0.8398570
C	-3.7067290	-2.9505110	-1.0281930
C	-4.6548320	-3.9564360	-0.8737680
C	-5.9690360	-3.6398900	-0.5319610
H	-5.6709640	-0.2709410	-0.3183870
H	-2.6953280	-3.2100500	-1.3160710
H	-4.3722560	-4.9906670	-1.0295840
H	-6.7207280	-4.4096670	-0.4099850

Coordinates of molecule **6** relaxed in vacuum

Symbol	X	Y	Z
C	-5.8692820	1.2560080	-1.6652990
C	-6.2025930	0.3219960	-0.6699990
C	-5.1812810	-0.2848730	0.0321420
C	-3.8370260	0.0184420	-0.2304180
C	-3.4924710	0.9361540	-1.2534530
C	-4.5541630	1.5508210	-1.9572130
H	-6.6616740	1.7636250	-2.2012500
H	-5.3861210	-1.0134940	0.8055520
H	-4.3618010	2.2935570	-2.7140580
C	-2.8117110	-0.6439660	0.5815500
C	-1.4242340	-0.2732870	0.2564450
C	-1.1375680	0.6350830	-0.7922200
N	-2.1620560	1.2180110	-1.5378140
O	-3.0830020	-1.4449970	1.4741360
C	-0.4048430	-0.8555560	1.0022880
C	0.9414870	-0.5771750	0.7607890
C	1.2289360	0.3227180	-0.2969440
C	0.2087770	0.9063510	-1.0427020
H	-0.7353010	-1.5474330	1.7598610
H	0.5371640	1.5815200	-1.8170310
C	-1.7897560	2.1473740	-2.6169900
C	-1.4215850	3.5496700	-2.1203250
C	-2.5577850	4.2935970	-1.4132830
C	-2.1280820	5.6460170	-0.8307560
C	-1.1461460	5.5315720	0.3418180
C	-0.8386940	6.8658540	1.0319540
H	-2.6075710	2.1901240	-3.3309840
H	-0.9517150	1.7061320	-3.1580330
H	-1.0842330	4.1301720	-2.9869250
H	-0.5622270	3.4718580	-1.4517740
H	-3.3808100	4.4525070	-2.1190810
H	-2.9595020	3.6705650	-0.6069040
H	-1.6930160	6.2589490	-1.6279730
H	-3.0214810	6.1803090	-0.4868220

H	-0.2042680	5.0854160	0.0032240
H	-1.5650220	4.8366140	1.0796550
H	-1.7749480	7.3150990	1.3879840
H	-0.2361080	6.6701470	1.9268100
C	2.6167260	0.6728980	-0.6456870
C	3.6454090	-0.0014380	0.1511240
C	3.2995630	-0.8870540	1.1996860
N	1.9716660	-1.1514450	1.5068280
O	2.8851000	1.4700580	-1.5425110
C	4.9910720	0.2463040	-0.1564370
C	6.0099430	-0.3381260	0.5691040
C	5.6735860	-1.2016120	1.6252910
C	4.3571000	-1.4826380	1.9264980
H	5.1999690	0.9107120	-0.9846550
H	6.4639230	-1.6509980	2.2135380
H	4.1570910	-2.1638430	2.7381030
C	1.6618770	-2.0634280	2.6199070
C	1.7764280	-3.5468190	2.2510650
C	0.7922630	-4.0122490	1.1735610
C	0.9812730	-5.4799000	0.7704130
C	2.2967840	-5.7583750	0.0329760
C	2.4128680	-7.1824480	-0.5234960
H	0.6631230	-1.8327480	2.9801700
H	2.3325470	-1.8211280	3.4451820
H	1.6169790	-4.1284040	3.1669580
H	2.7991150	-3.7532310	1.9271810
H	-0.2319240	-3.8677460	1.5323850
H	0.8986740	-3.3828820	0.2835370
H	0.9083040	-6.1106210	1.6634820
H	0.1484210	-5.7734770	0.1210860
H	3.1488910	-5.5694640	0.6963450
H	2.3903370	-5.0439540	-0.7938070
H	1.5715030	-7.3761560	-1.2013000
H	3.3190700	-7.2503930	-1.1371050
C	-0.0960250	7.8773400	0.1529040
C	0.2705500	9.1579170	0.9055480
H	-0.7082830	8.1339140	-0.7178400
H	0.8141890	7.4081030	-0.2402370
H	0.7986410	9.8653450	0.2606670
H	-0.6244170	9.6591400	1.2873540
H	0.9167790	8.9399610	1.7614870
C	2.4611370	-8.2788200	0.5455510
C	2.6639850	-9.6745650	-0.0473270
H	3.2733150	-8.0564200	1.2489390
H	1.5368860	-8.2672270	1.1323100
H	1.8515460	-9.9309150	-0.7343520
H	3.6012660	-9.7311620	-0.6095670
H	2.6952220	-10.4411110	0.7315560
C	8.2130660	3.5656610	0.2120930
C	9.5940190	3.4593860	-0.0619240

C	10.1395800	2.1851690	-0.2027960
C	9.3293270	1.0526740	-0.0803840
C	7.9494290	1.1988720	0.1834930
C	7.3807190	2.4612080	0.3387660
H	7.7707970	4.5475360	0.3286930
H	11.1939770	2.0544520	-0.4055810
H	6.3264270	2.5860020	0.5487000
C	9.5954450	-0.3699260	-0.1538870
C	8.3620400	-1.0299730	0.0695390
N	7.3662020	-0.0703560	0.2762180
C	10.7434670	-1.1190330	-0.4016170
C	10.6894120	-2.5155890	-0.4356960
C	9.4448300	-3.1365670	-0.2244890
C	8.2772180	-2.4168180	0.0245140
H	11.6815950	-0.6041510	-0.5728870
H	9.3719740	-4.2146950	-0.2578960
H	7.3355340	-2.9315260	0.1666110
C	10.4325990	4.7380540	-0.1924600
C	10.3586810	5.5395660	1.1246200
C	11.9105530	4.4366270	-0.4858460
C	9.8795870	5.5989590	-1.3481970
C	11.9729220	-3.3145760	-0.7066540
C	13.0144590	-2.9976810	0.3875250
C	11.7296670	-4.8320480	-0.7086740
C	12.5427520	-2.9188330	-2.0855030
H	10.7465270	4.9483470	1.9582580
H	9.3329350	5.8257550	1.3662180
H	10.9527660	6.4552700	1.0470330
H	12.0333020	3.8931340	-1.4263000
H	12.3700980	3.8501400	0.3140670
H	12.4656680	5.3744060	-0.5701560
H	10.4676140	6.5155930	-1.4555840
H	8.8401120	5.8858510	-1.1761340
H	9.9230860	5.0504340	-2.2926610
H	12.6321920	-3.2699020	1.3748090
H	13.2662250	-1.9352640	0.4081120
H	13.9373070	-3.5583030	0.2098220
H	12.6711170	-5.3525270	-0.9023760
H	11.0216930	-5.1278200	-1.4872030
H	11.3494430	-5.1824170	0.2544470
H	12.7840250	-1.8547920	-2.1313920
H	11.8201280	-3.1322620	-2.8773610
H	13.4584170	-3.4801570	-2.2951780
C	-9.5515010	-0.9580670	-3.3805280
C	-10.8116790	-1.1015240	-2.7606620
C	-10.9018530	-0.8589120	-1.3912680
C	-9.7709530	-0.4752780	-0.6652000
C	-8.5287890	-0.3283700	-1.3221850
C	-8.4084570	-0.5796370	-2.6876460
H	-9.4586980	-1.1540560	-4.4418280

H	-11.8442040	-0.9683590	-0.8717370
H	-7.4567910	-0.4957210	-3.1968210
C	-9.5421950	-0.1827390	0.7355740
C	-8.1673220	0.1290620	0.8710620
N	-7.5578900	0.0399520	-0.3860930
C	-10.3712940	-0.1475270	1.8547570
C	-9.8589620	0.1959870	3.1088970
C	-8.4905170	0.5096910	3.2033080
C	-7.6338100	0.4833920	2.1043500
H	-11.4218540	-0.3877590	1.7401100
H	-8.0684470	0.7823660	4.1604480
H	-6.5863450	0.7302200	2.2189750
C	-12.0202520	-1.5222800	-3.6079170
C	-11.7454750	-2.8989710	-4.2497260
C	-13.3055270	-1.6326430	-2.7729200
C	-12.2581510	-0.4771630	-4.7187100
C	-10.7954380	0.2213640	4.3261790
C	-11.4084460	-1.1803490	4.5308250
C	-10.0650920	0.6161460	5.6194920
C	-11.9259040	1.2437250	4.0828060
H	-12.6003330	-3.2141130	-4.8558150
H	-10.8668200	-2.8746690	-4.8977050
H	-11.5727140	-3.6555710	-3.4800180
H	-14.1361750	-1.9314380	-3.4174400
H	-13.2118550	-2.3832780	-1.9838480
H	-13.5708860	-0.6780430	-2.3111140
H	-13.1181270	-0.7622870	-5.3323740
H	-12.4564670	0.5069410	-4.2860990
H	-11.3923740	-0.3847210	-5.3778810
H	-12.0789440	-1.1809970	5.3957000
H	-11.9846950	-1.4989920	3.6596000
H	-10.6249250	-1.9227510	4.7031550
H	-10.7728010	0.6176330	6.4525380
H	-9.2661490	-0.0883970	5.8644500
H	-9.6323930	1.6175820	5.5507180
H	-12.6037270	1.2747020	4.9413870
H	-11.5146970	2.2455070	3.9336890
H	-12.5153840	0.9895200	3.1993590

Coordinates of molecule **6** relaxed in dichloromethane

Symbol	X	Y	Z
C	-5.8657980	1.1958020	-1.7215490
C	-6.2031880	0.3045650	-0.6875390
C	-5.1885770	-0.2759140	0.0422320
C	-3.8400890	0.0123620	-0.2265720
C	-3.4913800	0.8911500	-1.2841650
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H	-5.4048820	-0.9698290	0.8433600
H	-4.3553190	2.1832960	-2.8084030

C	-2.8202480	-0.6189290	0.6077950
C	-1.4329480	-0.2693380	0.2728880
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O	-3.0979470	-1.3887780	1.5343360
C	-0.4132540	-0.8283450	1.0373290
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C	1.2238240	0.3055120	-0.2997900
C	0.2033470	0.8650340	-1.0644910
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H	0.5244440	1.5133010	-1.8633740
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C	11.6993180	-4.8409870	-0.6221560
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H	10.7689860	4.9940560	1.8656120
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H	12.3662180	3.8617880	0.2195620
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H	10.4426960	6.4979330	-1.5686350
H	8.8177590	5.8763650	-1.2568490
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H	12.6362800	-3.2387450	1.4143400
H	13.2577670	-1.9236090	0.4095870
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C	-8.5195250	-0.4130970	-1.3087600
C	-8.3858380	-0.7504810	-2.6549820
H	-9.4154790	-1.4551930	-4.3732750
H	-11.8295210	-1.0762840	-0.8350290
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C	-9.5495050	-0.1430790	0.7285820
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C	-7.6593970	0.6503920	2.0566720
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H	-6.6170030	0.9238400	2.1579990
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C	-11.6746230	-3.2268220	-4.0758830
C	-13.2662810	-1.8891010	-2.6972740
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H	-11.9653040	-1.3094430	3.7403930
H	-10.6022730	-1.6109490	4.8251150
H	-10.8329290	1.0553840	6.3641700
H	-9.3037480	0.3447120	5.8426150
H	-9.7110660	2.0098970	5.3911250
H	-12.6702210	1.5337960	4.8046730
H	-11.6069500	2.4568380	3.7278940
H	-12.5681880	1.1170090	3.0901770

Table S1. Dihedral angles between planar donor and planar acceptor parts of molecules 1-6 as obtained by geometry optimization using DFT/B3LYP-GD3BJ/6-311++G(d,p) method.

Molecule		1	2	3	4	5*	6
in vacuum	ϕ_1[°]	53.02	53.00	79.65	79.65	48.67	51.88
	ϕ_2[°]		52.81		79.99	57.46	52.42
in DCM**	ϕ_1[°]	54.71	53.78	79.93	80.32	49.61	53.62
	ϕ_2[°]		54.11		80.76	57.81	54.61

* in the case molecule 5 the indicated angles correspond to torsion of the planar acceptor and donor moieties with respect to the plane of 1,3-phenylene linker** dichloromethane, DCM

The optical properties of the molecules **1-6** were determined using the time dependent DFT (TDDFT) formalism. It is considered to be the most prominent method to calculate the excited state of medium-size and large molecules. Obtained parameters are presented in Table S2. The electron excited singlet states with the highest strength of the oscillator are written in bold.

Table S2. Wavelengths (λ), oscillator strengths (f) and dominant configurations of the five lowest excited singlet states and the first triplet state of the (**1-6**) molecules calculated by the DFT/B3LYP-GD3BJ/6-311++G(d,p) method

Excited state	λ [nm]	f	Dominant configurations
		1	
S1	438.51	0.0212	HOMO → LUMO (97%)
S2	370.18	0.0003	HOMO-1 → LUMO (99%)
S3	348.92	0.0012	HOMO-4 → LUMO (95%)
S4	340.51	0.0658	HOMO-2 → LUMO (82%) HOMO → LUMO+1 (9%)
S5	**328.17**	**0.2947**	**HOMO-2 → LUMO (87%)** **HOMO → LUMO+1 (8%)**
T1	**501.07**		HOMO → LUMO (97%)
		2	
S1	458.49	0.0141	HOMO → LUMO (97%)

S2	441.17	0.0349	HOMO-1 → LUMO (99%)
S3	380.20	0.0003	HOMO-3 → LUMO (55%) HOMO-2 → LUMO (44%)
S4	379.94	0.0002	HOMO-2 → LUMO (55%) HOMO-3 → LUMO (44%)
S5	349.50	0.0017	HOMO-7 → LUMO (95%)
S6	**345.35**	**0.6397**	**HOMO → LUMO+1 (96%)**
T1	**534.37**		**HOMO → LUMO (81%)**
3			
S1	527.06	f=0.0001	HOMO → LUMO (99%)
S2	380.32	f=0.0007	HOMO → LUMO+1 (99%)
S3	349.82	f=0.0000	HOMO-3 → LUMO+1 (96%)
S4	**345.04**	**f=0.1034**	**HOMO-1 → LUMO (91%)**
S5	339.70	f=0.0011	HOMO → LUMO+2 (86%) HOMO → LUMO+4 (8%)
T1	**532.51**		**HOMO → LUMO (89%)**
4			
S1	554.69	f=0.0000	HOMO → LUMO (94%) HOMO-1 → LUMO (4%)
S2	552.31	f=0.0002	HOMO-1 → LUMO (94%) HOMO → LUMO (4%)
S3	398.03	f=0.0012	HOMO → LUMO+1 (90%) HOMO-1 → LUMO+1 (7%)
S4	396.96	f=0.0001	HOMO → LUMO+1 (90%) HOMO-1 → LUMO+1 (7%)
S5	351.23	f=0.0002	HOMO-5 → LUMO (91%) HOMO-3 → LUMO (2%)
S8	**345.07**	**f=0.0931**	**HOMO-2 → LUMO (91%)** **HOMO-11 → LUMO+1 (3%)**
T1	**559.95**		**HOMO → LUMO (85%)**
5			
S1	500.58	f=0.0000	HOMO → LUMO (99%)
S2	476.98	f=0.0003	HOMO-1 → LUMO (99%)
S3	434.16	f=0.0011	HOMO → LUMO+1 (88%) HOMO → LUMO+2 (10%)
S4	417.05	f=0.0028	HOMO-1 → LUMO+1 (87%) HOMO-1 → LUMO+2 (12%)
S5	375.98	f=0.0008	HOMO → LUMO+4 (76%) HOMO → LUMO+3 (17%) HOMO → LUMO+5 (3%) HOMO → LUMO+2 (2%)
S6	**368.55**	**f=0.0497**	**HOMO-2 → LUMO (92%)**
T1	**501.19**		**HOMO → LUMO (89%)**
6			
S1	542.01	f=0.0449	HOMO → LUMO (96%)
S2	521.17	f=0.0002	HOMO-1 → LUMO (98%)
S3	434.62	f=0.0637	HOMO-2 → LUMO (82%) HOMO-4 → LUMO (10%)
S4	432.36	f=0.0016	HOMO-3 → LUMO (95%) HOMO-4 → LUMO (3%)
S5	430.54	f=0.0450	HOMO-4 → LUMO (84%) HOMO-2 → LUMO (9%) HOMO-3 → LUMO (2%)
S10	**348.64**	**f=0.9656**	**HOMO → LUMO+2 (86%)** **HOMO-5 → LUMO (5%)** **HOMO-1 → LUMO+6 (3%)**
T1	**676.48**		HOMO → LUMO (86%)

8. NMR spectra

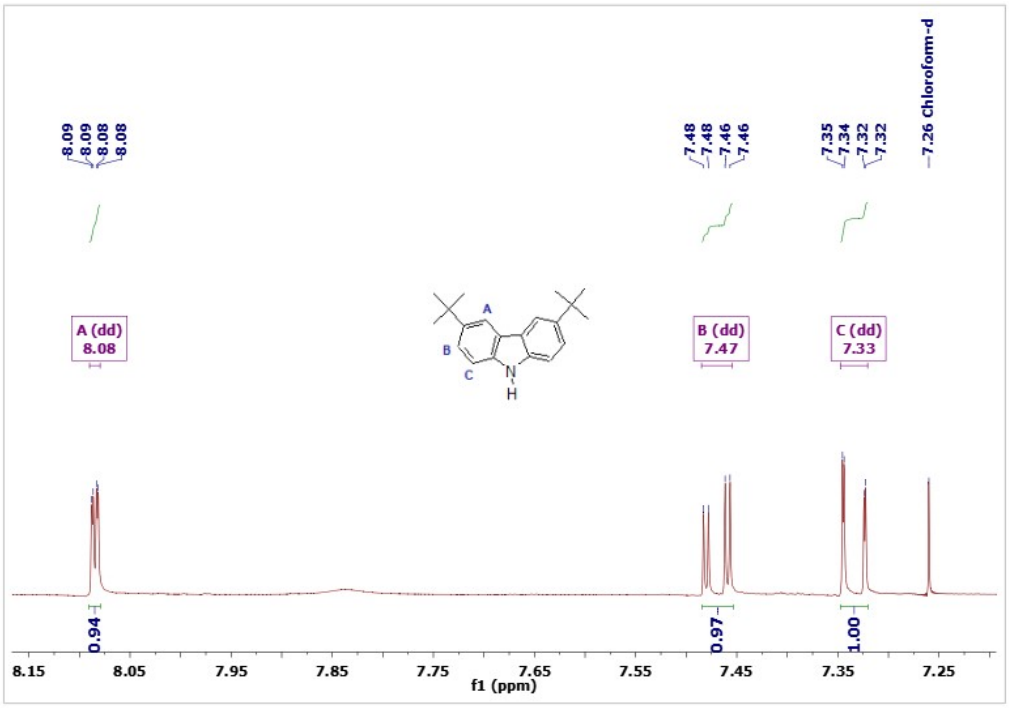

Figure S10. ^{1}H NMR spectrum of 3,6-di-(*tert*-butyl) carbazole in $CDCl_3$ (aromatic part).

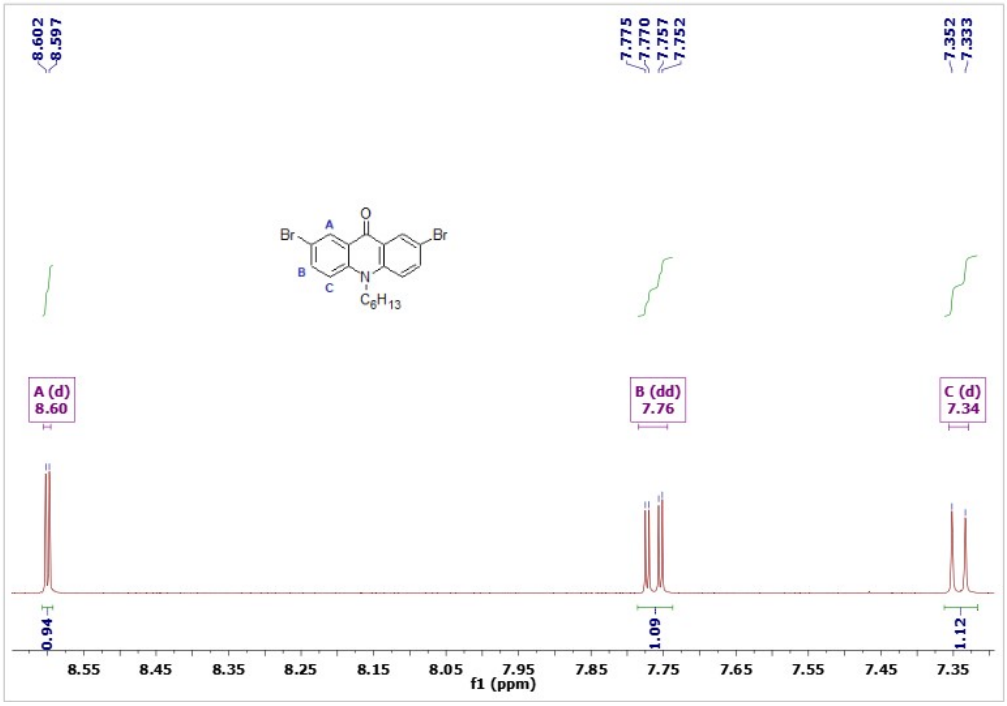

Figure S11. ^{1}H NMR spectrum of 2,7-dibromo-N-hexylacridone in $CDCl_3$ (aromatic part).

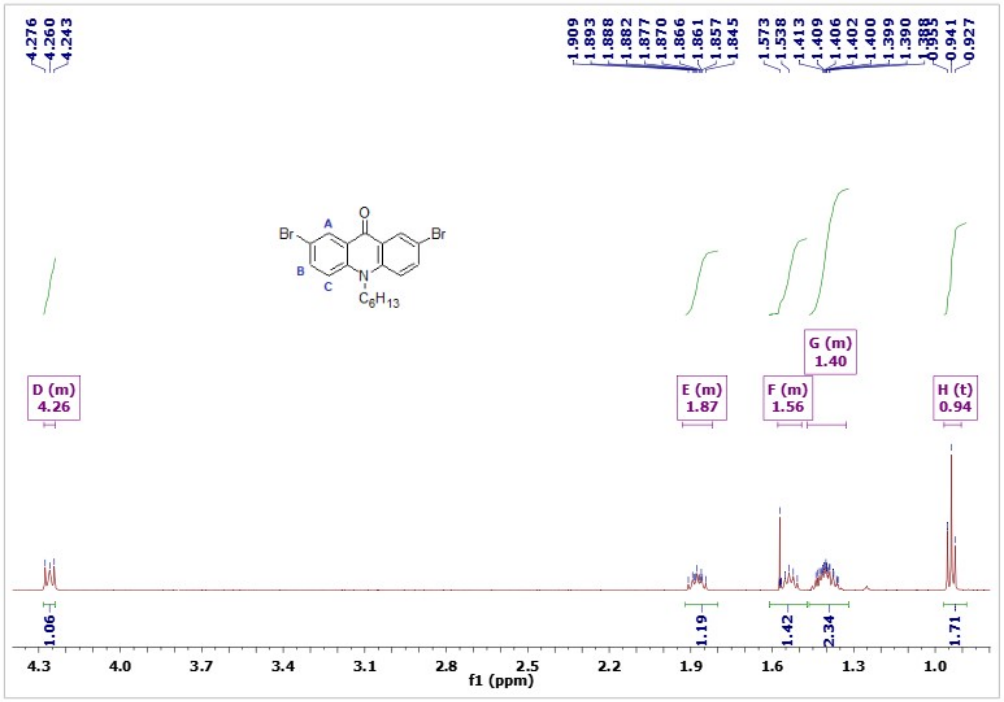

Figure S12. ^{1}H NMR spectrum of 2,7-dibromo-N-hexylacridone in $CDCl_3$ (aliphatic part).

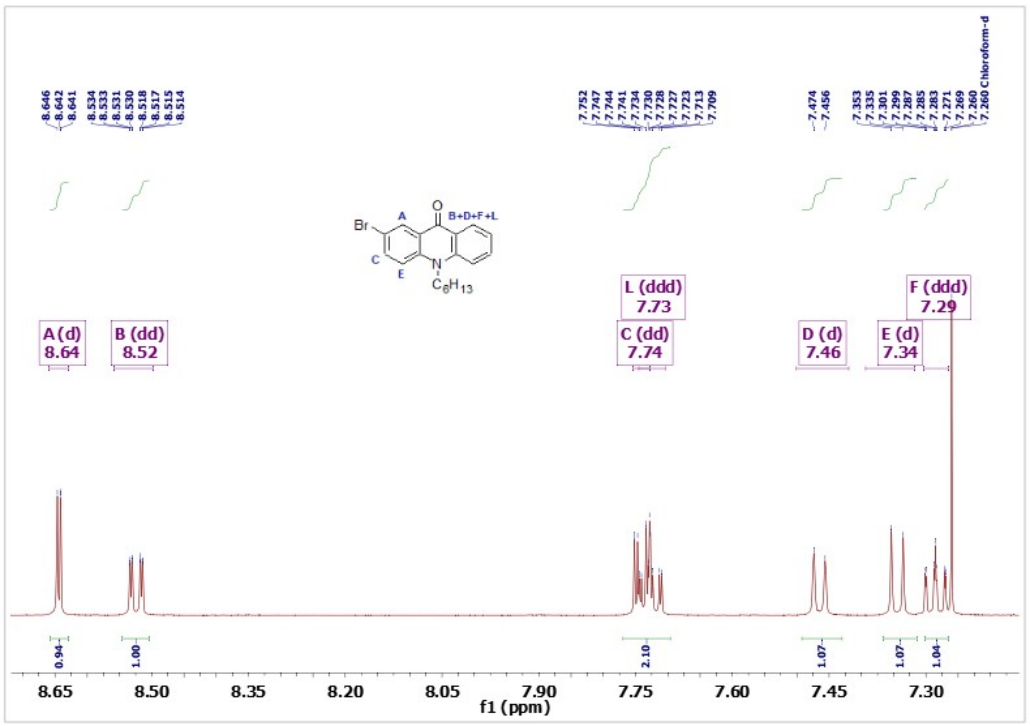

Figure S13. ^{1}H NMR spectrum of 2-bromo-N-hexylacridone in $CDCl_3$ (aromatic part).

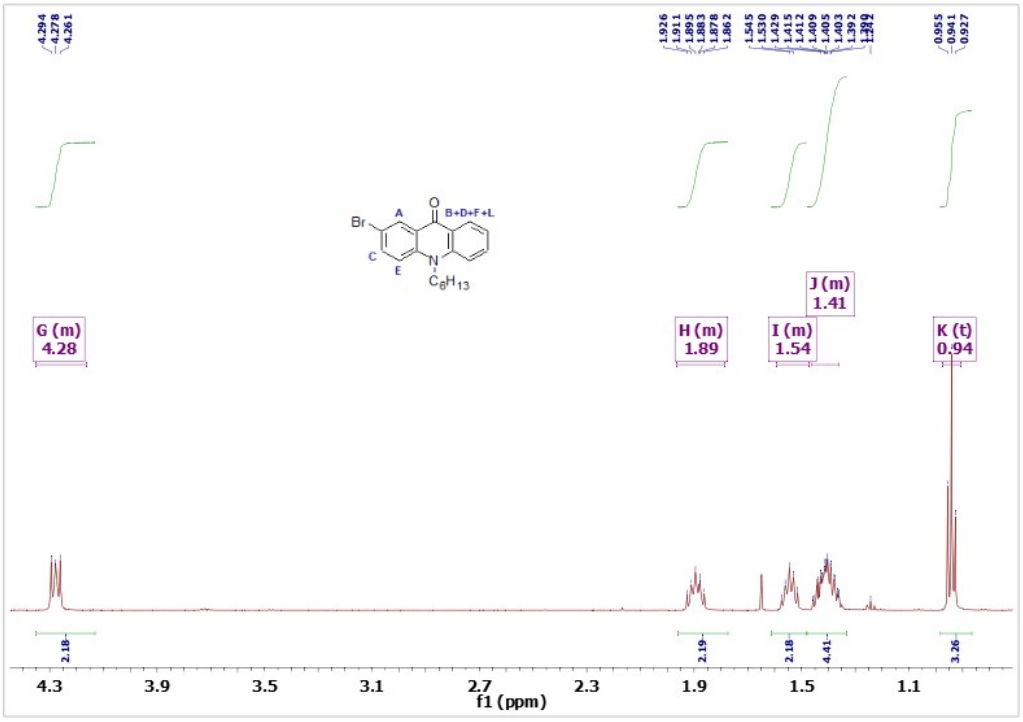

Figure S14. ^{1}H NMR spectrum of 2-bromo-N-hexylacridone in $CDCl_3$ (aliphatic part).

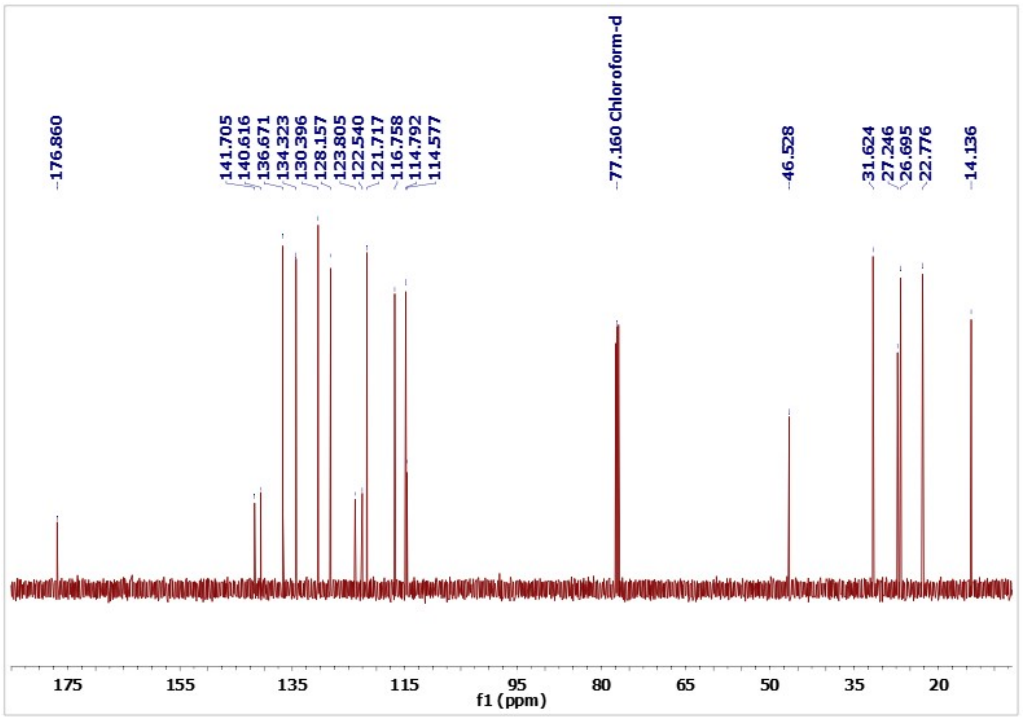

Figure S15. ^{13}C NMR spectrum of 2-bromo-N-hexylacridone in $CDCl_3$.

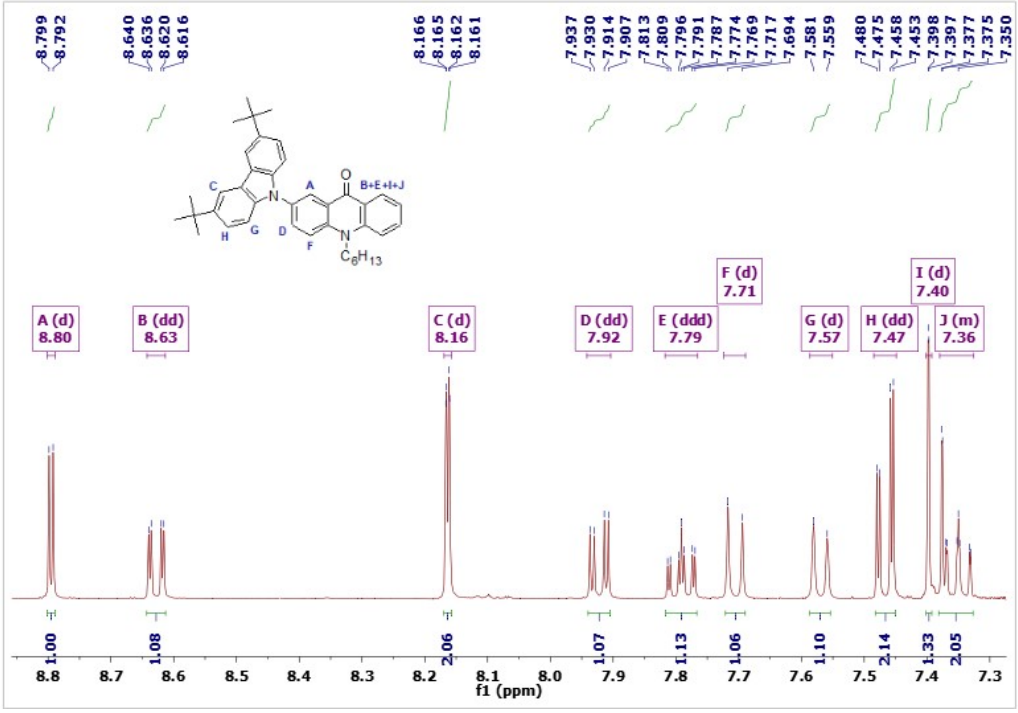

Figure S16. ^{1}H NMR spectrum of the compound **1** in $CDCl_3$ (aromatic part).

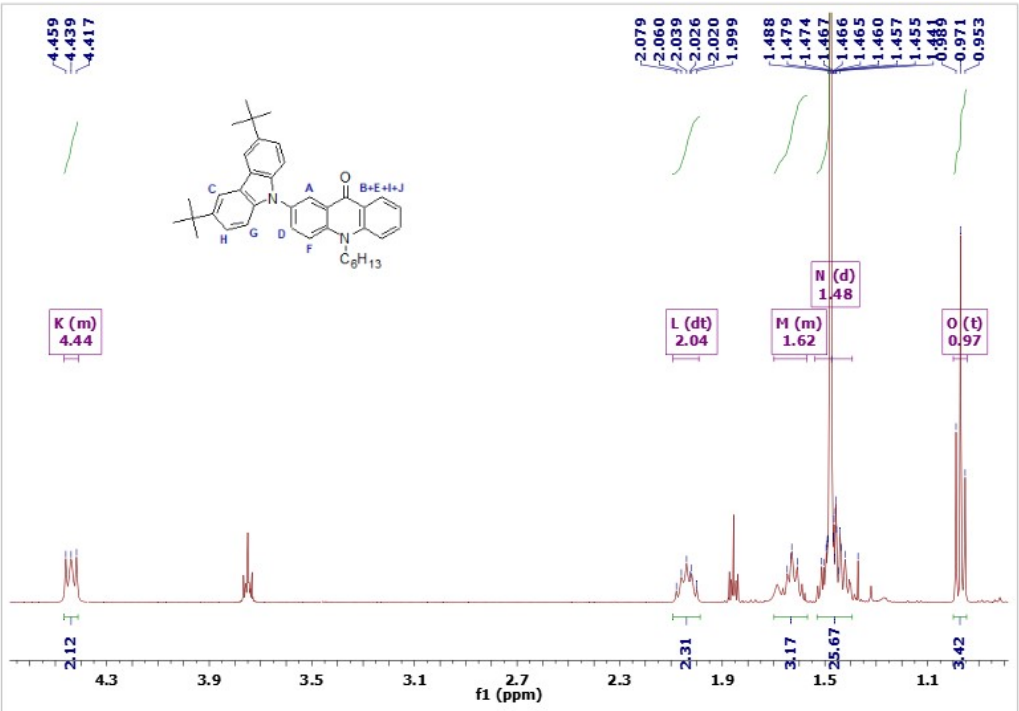

Figure S17. ^{1}H NMR spectrum of the compound **1** in $CDCl_3$ (aliphatic part).

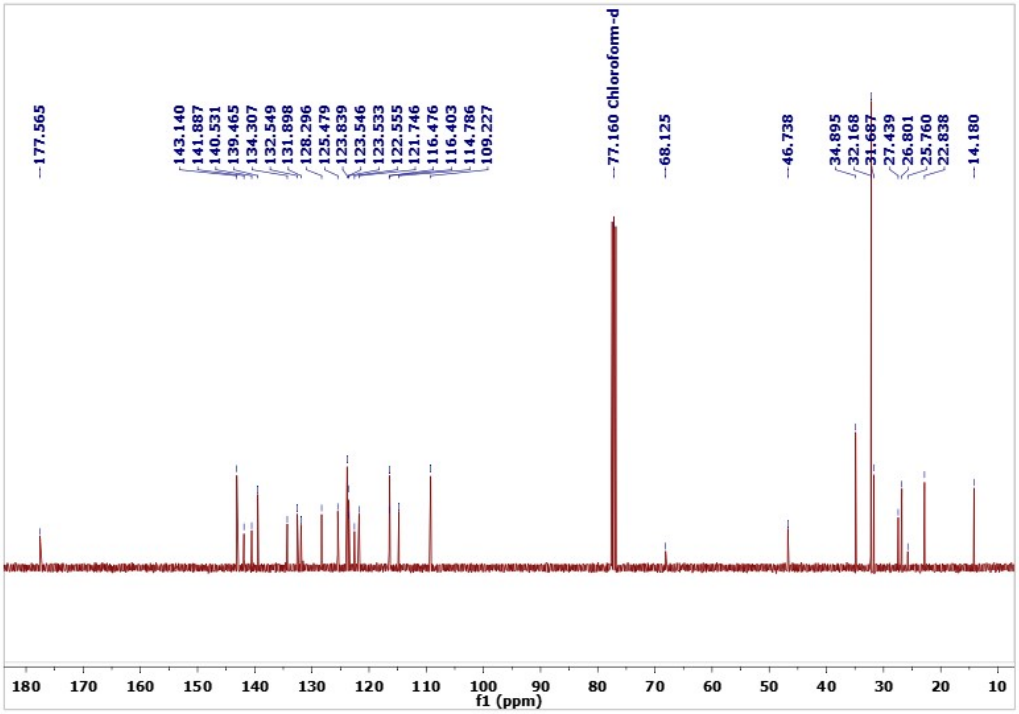

Figure S18. ^{13}C NMR spectrum of the compound **1** in $CDCl_3$.

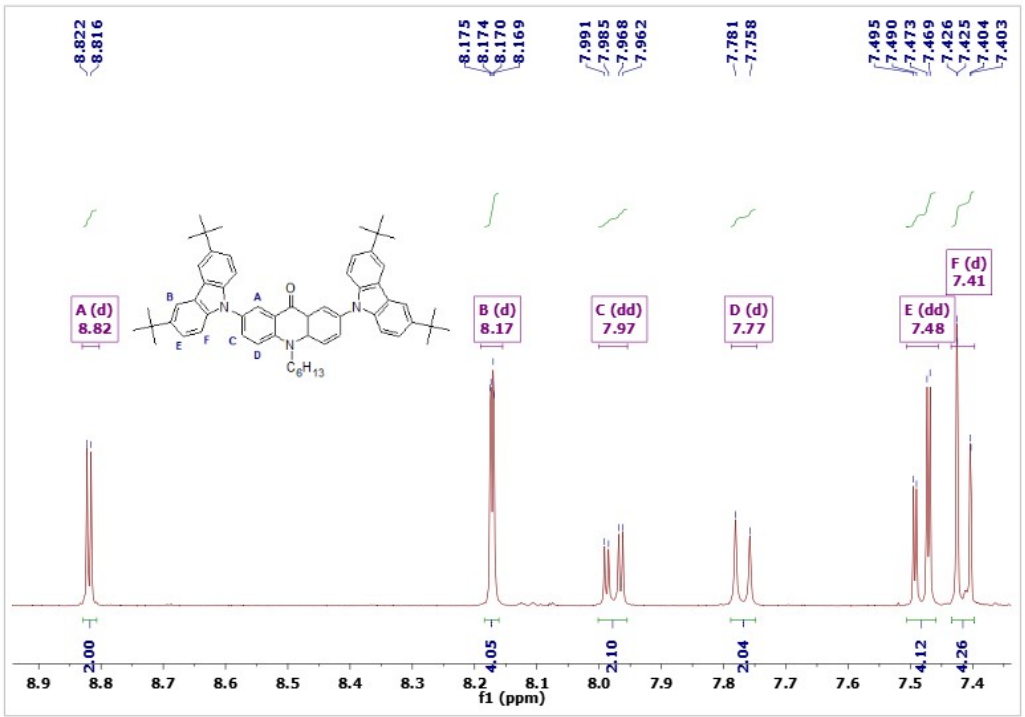

Figure S19. ^{1}H NMR spectrum of the compound **2** in $CDCl_3$ (aromatic part).

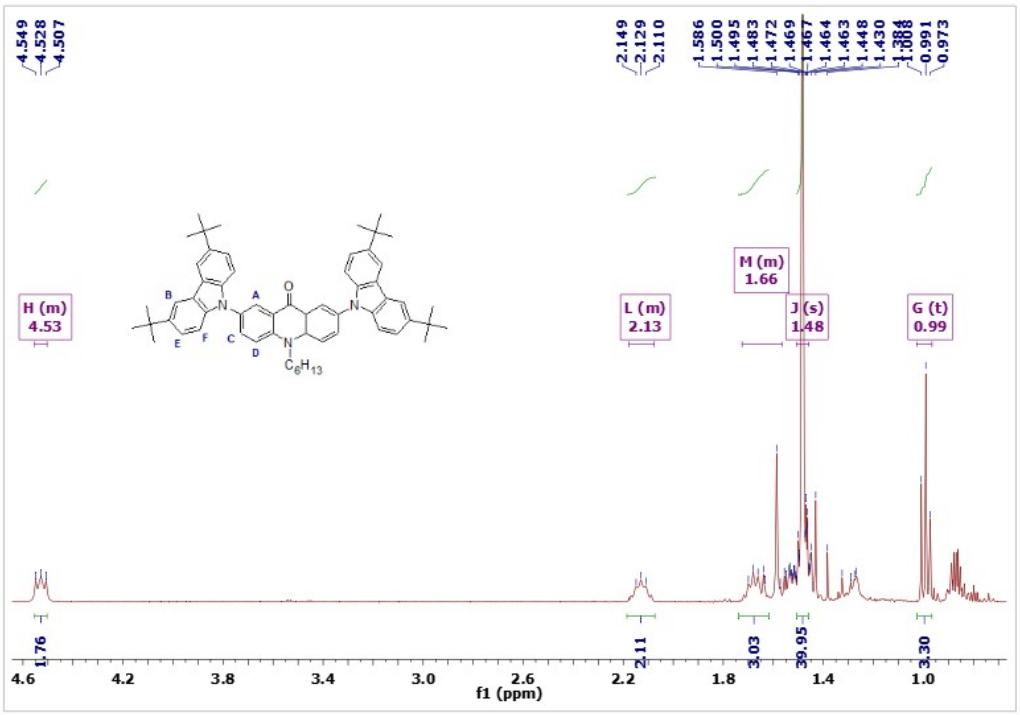

Figure S20. ^{1}H NMR spectrum of the compound **2** in $CDCl_3$ (aliphatic part).

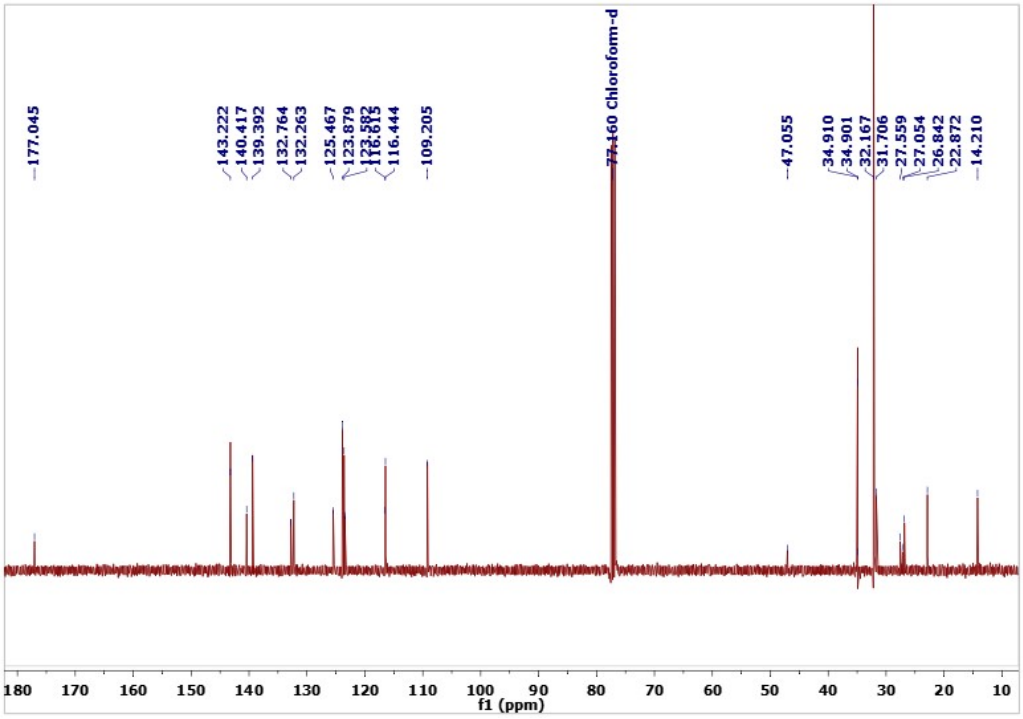

Figure S21. ^{13}C NMR spectrum of the compound **2** in $CDCl_3$.

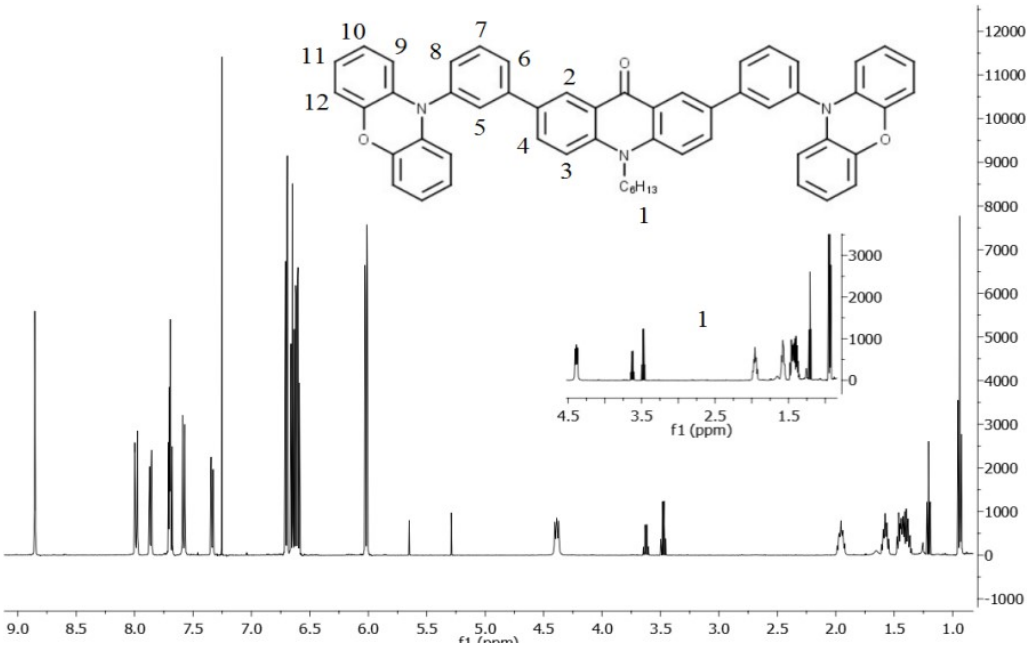

Figure S22. ^{1}H NMR spectrum of the compound **5** in $CDCl_3$.

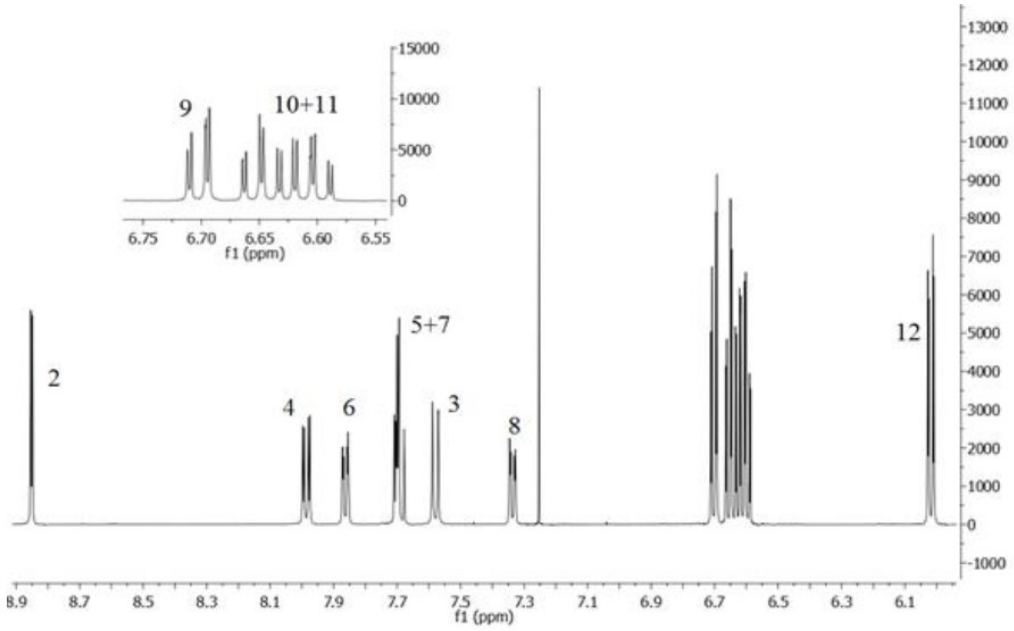

Figure S23. ^{1}H NMR spectrum of the compound **5** in $CDCl_3$ (aromatic part).

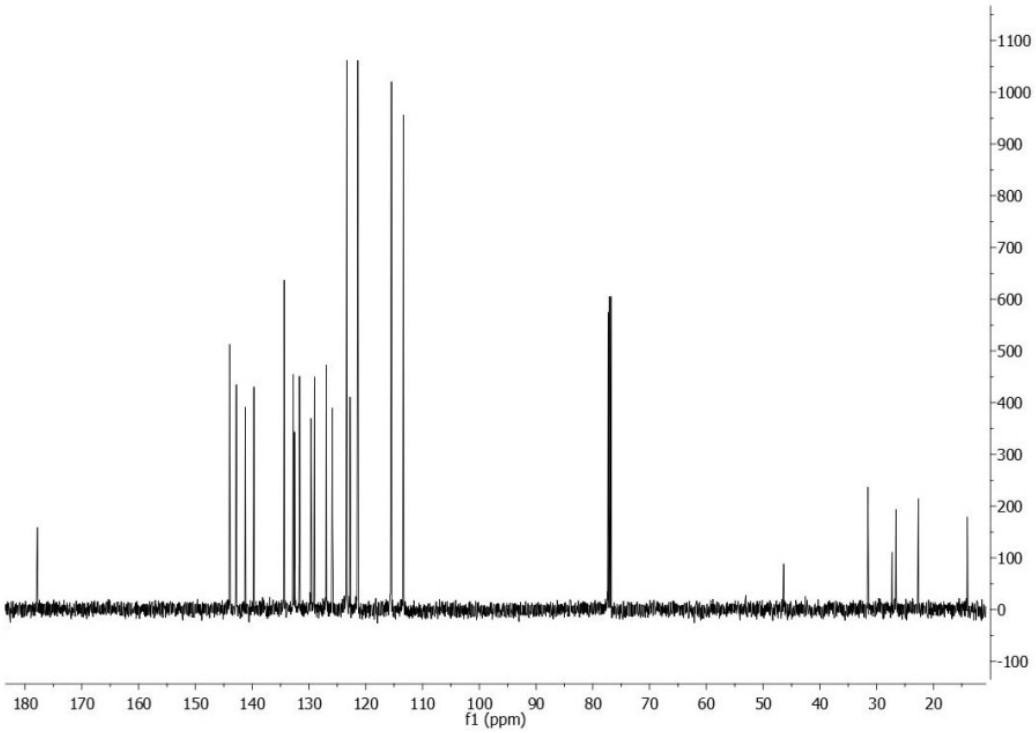

Figure S24. ^{13}C NMR spectrum of the compound **5** in $CDCl_3$.

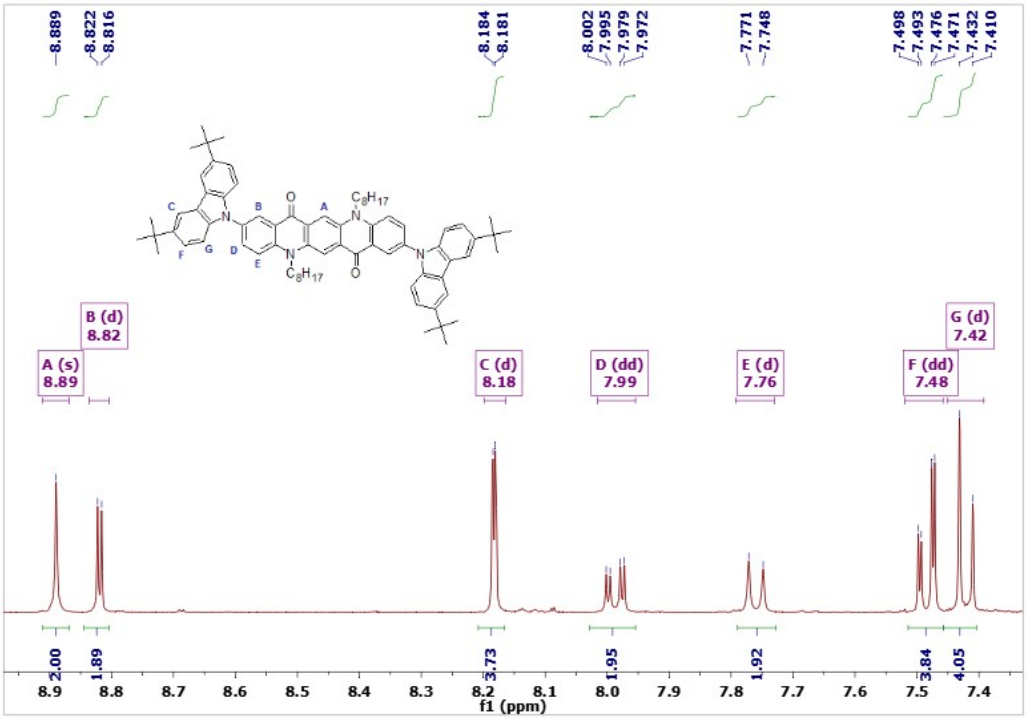

Figure S25. ^{1}H NMR spectrum of the compound **6** in $CDCl_3$ (aromatic part).

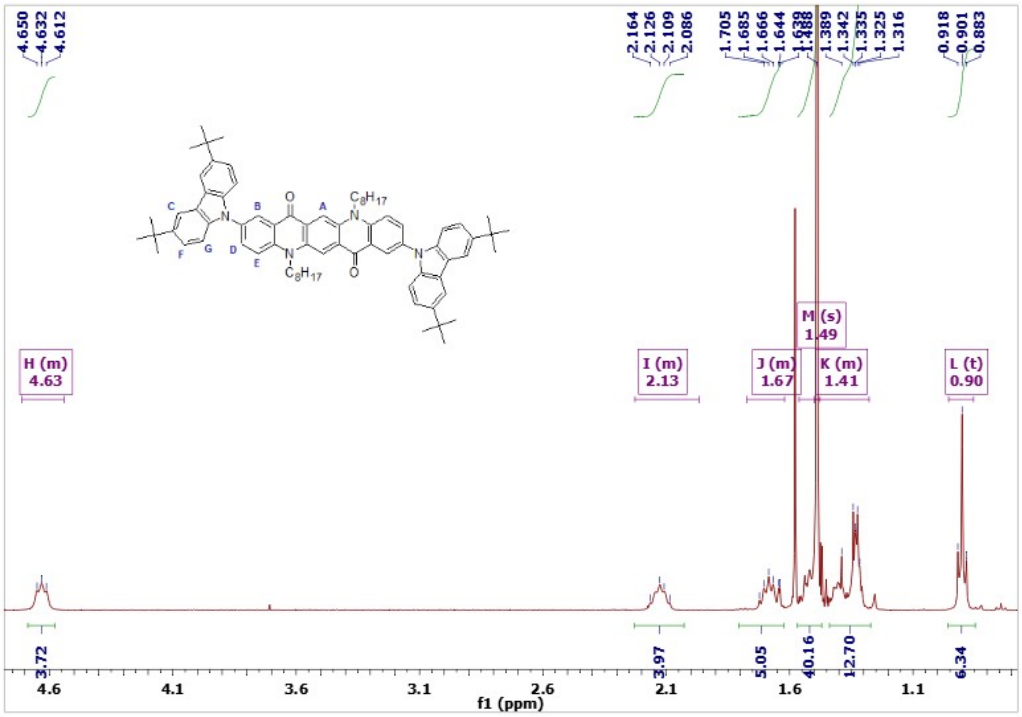

Figure S26. ^{1}H NMR spectrum of the compound **6** in $CDCl_3$ (aliphatic part).

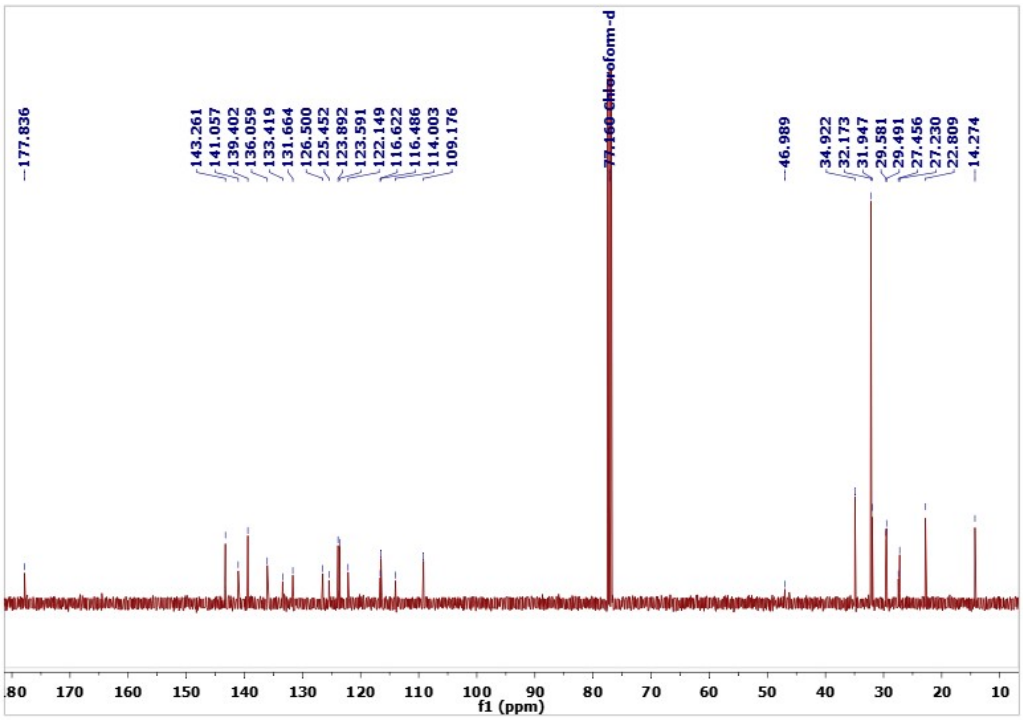

Figure S27. ^{13}C NMR spectrum of the compound **6** in $CDCl_3$.

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