

Supporting Information

Benzotriquinoxaline-based discotic liquid crystals stabilizing room temperature columnar self-assembly with high charge carrier mobility

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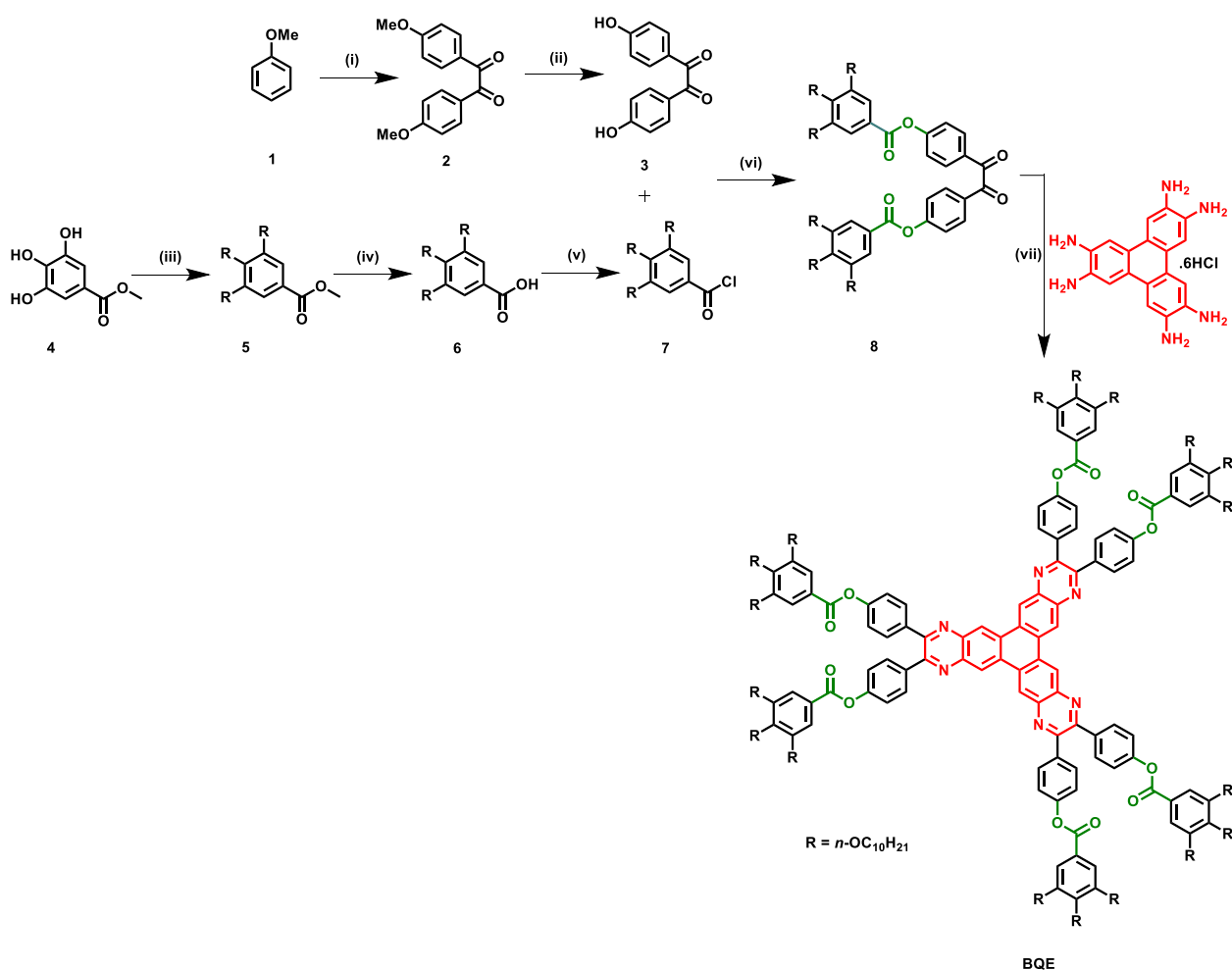
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1. Materials and methods

Commercially available chemicals were utilized as received, and solvents were dried following standard procedures. Column chromatography was conducted using either silica gel (60-120 mesh or 100-200 mesh) or neutral aluminum oxide as the stationary phase. Thin-layer chromatography was performed using aluminum sheets pre-coated with silica gel as the stationary phase. IR spectra were recorded at room temperature on a PerkinElmer Universal ATR Two FT-IR spectrometer, with spectral positions reported in wavenumbers (cm^{-1}). NMR spectra were acquired using a Bruker 600 MHz NMR spectrometer (Make: Bruker, Model: AVANCE III HD). The chemical shifts in the ^1H NMR spectra were referenced to TMS as the internal standard and are reported in ppm while the coupling constants are given in Hz. Mass spectra were obtained using a MALDI-TOF mass spectrometer (Matrix Assisted Laser Desorption Ionization- Time Of Flight, Make: BRUKER Model: AUTOFLEX SPEED) with α -Cyano-4-hydroxycinnamic acid used as the matrix. The birefringence and fluidity properties of the final compounds were investigated using a polarizing optical microscope (Nikon Eclipse LV100POL) equipped with a programmable hot stage (Mettler Toledo FP90). Clean glass slides and cover slips were used for the polarizing optical microscopy studies. Transition temperatures and corresponding enthalpy changes were determined using a differential scanning calorimeter (Mettler Toledo DSC1) under a nitrogen atmosphere. The transition temperatures determined from calorimetric measurements during the heating and cooling cycles at a rate of $5\text{ }^\circ\text{C}/\text{min}$ are recorded. Variable temperature XRD studies were performed on samples contained in Lindemann capillaries. Data were collected using a high-resolution X-ray powder diffractometer (PANalytical X'Pert PRO) equipped with a fast PIXCEL detector. Sample temperature was regulated with a Mettler hot stage/programmer (FP82HT/FP90). Thermogravimetric analysis (TGA) was performed on a Mettler Toledo thermogravimetric analyzer (model TG/SDTA 851e) under a nitrogen atmosphere, with a heating rate of $10\text{ }^\circ\text{C}/\text{min}$. UV-Vis spectra were recorded with a Perkin-Elmer Lambda 365+ UV/VIS/NIR spectrometer, while fluorescence emission measurements in solution state were recorded using a Horiba Fluoromax-4 fluorescence. Cyclic voltammetry studies were conducted using a Metrohm Autolab PGSTAT204 electrochemical workstation, operated with NOVA software. The determination of hole and electron mobilities has been carried out by using space charge limited current (SCLC) technique.

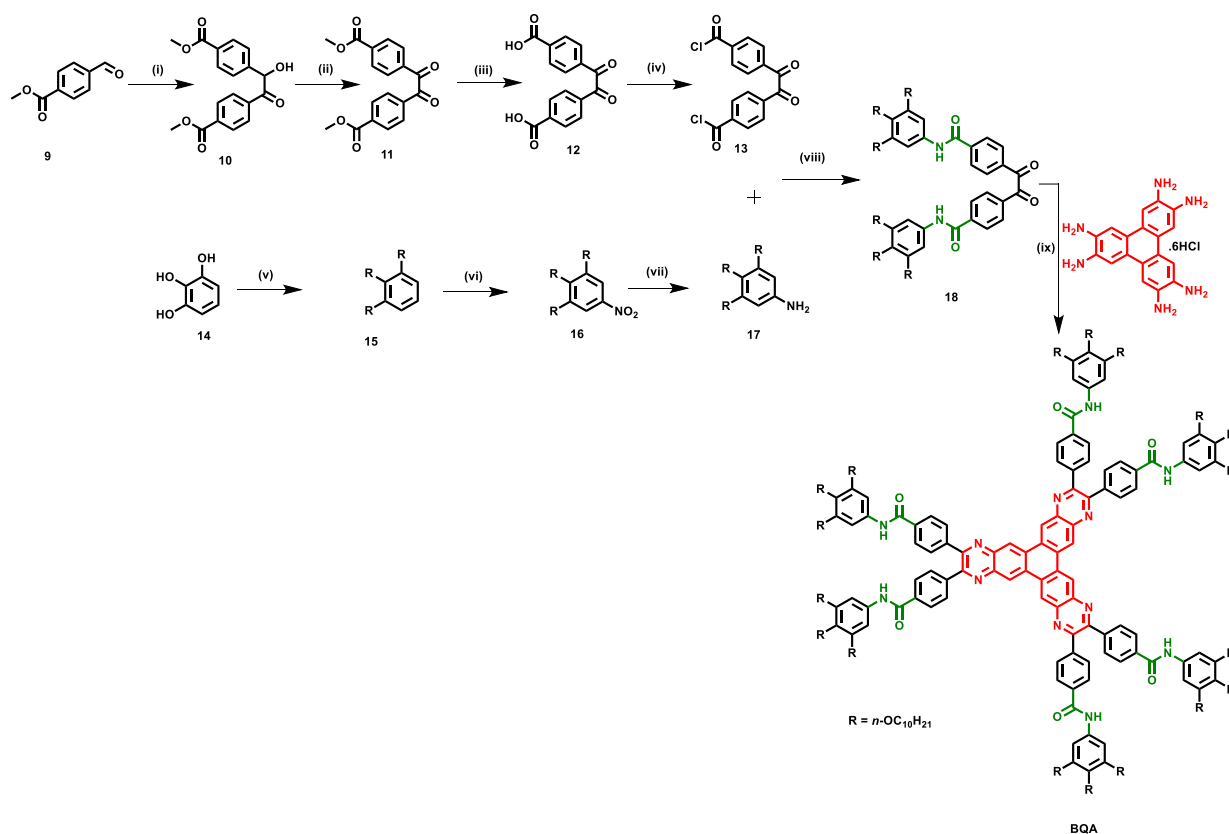
2. Experimental Section

Scheme S1. Synthesis of BQE^a



^a**Reagents and conditions:** (i) Oxalyl chloride, anhydrous AlCl₃, dry DCM, 0 °C (30 min), RT (24 h), 60%; (ii) 47% HBr, glacial acetic acid, reflux, 16 h, 82% (iii) *n*-C₁₀H₂₁Br, K₂CO₃, DMF, 80 °C, 17 h, 85%; (iv) NaOH, EtOH, reflux, 17 h, 86%; (v) SOCl₂, reflux, 2 h, quantitative yield; (vi) TEA, dry DCM, rt, 12 h, 66%; (vii) methanol: acetic acid (1:3), 130 °C, triethylamine, 12 h, 78%.

Scheme S1. Synthesis of BQA^a



^a**Reagents and conditions:** (i) Vit B₁, MeOH:H₂O (3:1), 3M NaOH, 0 °C, 10 mins, 85 °C, 4 hours, 85% (ii) HBr, DMSO, 60 °C, 90%; (iii) H₂SO₄/H₂O, AcOH, reflux, overnight, 90% (iv) SOCl₂, reflux, 2 h, quantitative yield (v) C₁₀H₂₁Br, K₂CO₃, DMF, 90 °C, 24 hours, 80%; (vi) HNO₃, CH₂Cl₂-HAc (50:50), 0 °C to RT, 86%; (vii) 10% Pd-C, NH₂-NH₂·H₂O, CH₃CH₂OH, overnight, reflux, quantitative yield; (viii) dry DCM, TEA, rt, overnight, 58%; (ix) methanol: acetic acid (1:3), 130 °C, triethylamine, 12 h, 48%.

Synthesis of 1,2-bis(methoxyphenyl)ethane-1,2-dione (**2**)^{1,2}

A dried 250 mL two-necked round-bottom flask was charged with anisole (27.74 mmol, 1.0 equiv.) dissolved in dry dichloromethane (40 mL) under a nitrogen atmosphere. The solution was cooled to 0 °C using an ice bath. Oxalyl chloride (16.65 mmol, 0.6 equiv.) was slowly injected via syringe. After stirring at 0 °C for 10 min, anhyd. AlCl₃ (13.87 mmol, 0.5 equiv.) was added. After stirring the reaction mixture at 0 °C for 30 minutes, it was allowed to warm to room temperature and stirred overnight. The resulting mixture was then poured into 100 mL of 1M HCl. The organic layer was extracted twice with dichloromethane. The combined organic extracts were washed with brine, dried over anhyd. Na₂SO₄, and concentrated. The crude residue was purified by column chromatography on silica gel, eluting with a 1:1 mixture of DCM and hexane, to afford the pure yellow solid product **2**.

2: R_f = 0.37 (50% DCM-hexanes); yellow solid; yield: 60%; IR ν_{max} in cm⁻¹: 1652, 1594, 1568, 1504, 1420, 1311, 1259, 1218, 1152, 1112, 1011, 873, 830, 786, 745, 638, 601, 505; ¹H NMR (600 MHz, CDCl₃, 299 K): 7.95-7.94 (d, *J* = 8.4 Hz, 4H, H_{Ar}), 6.98-6.96 (d, *J* = 9 Hz, 4H, H_{Ar}),

3.89 (s, 6H, 2× OCH₃); ¹³C NMR (150 MHz, CDCl₃, 298.1K): 193.49, 164.85, 132.38, 126.31, 114.29, 55.64.

Synthesis of 1,2-bis(4-hydroxyphenyl)ethane-1,2-dione (**3**)^{2,3}

Compound **2** (3.00 g, 18.10 mmol), 47% hydrobromic acid (35 mL), and glacial acetic acid (35 mL) were taken in a 250 mL round-bottom flask and refluxed for 16 hours. After completion, the reaction mixture was cooled to room temperature and extracted using EtOAc. The extract was neutralized with 50 mL of 1M NaOH solution. The organic layer was dried over anhyd. Na₂SO₄ and concentrated. The resulting crude product was recrystallized from water, yielding a yellowish solid.

3: R_f = 0.50 (20% Acetone-DCM); yellow solid; yield: 82%; IR ν_{max} in cm⁻¹: 3393, 1643, 1597, 1564, 1509, 1332, 1289, 1216, 1162, 875, 846, 808, 753, 703, 638, 597, 511, 449; ¹H NMR (600 MHz, DMSO-d₆, 299 K): 11.03 (br s, 2H, 2 × OH), 7.75-7.73 (d, J = 8.4 Hz, 4H, H_{Ar}), 6.94-6.92 (d, J = 8.4 Hz, 4H, H_{Ar}); ¹³C NMR (150 MHz, DMSO-d₆, 298.1K): 194.23, 164.35, 132.75, 124.63, 116.60.

Synthesis of methyl 3,4,5-tris(decyloxy)benzoate (**5**)^{4,5}

A mixture of methyl 3,4,5-trihydroxybenzoate, (**4**) (16.29 mmol, 1 equiv.) and anhydrous K₂CO₃ (107.52 mmol, 6.6 equiv.) was taken in dry DMF (35 mL) and stirred for 1 hour at 60 °C. After that, n-bromodecane (53.76 mmol, 3.3 equiv.) was added, and the mixture was heated at 80 °C for 24 hours under a nitrogen atmosphere. After completion, the reaction mixture was poured into ice-cold water and extracted with CH₂Cl₂. The combined organic layers were washed successively with water and brine, dried over anhydrous Na₂SO₄, and concentrated. The crude product was purified by column chromatography on silica gel (100-200 mesh). Elution with hexanes, followed by 5-10% ethyl acetate in hexanes, afforded the desired product **5**.

5: R_f = 0.60 (10% EtOAc-hexanes); white solid; yield: 85%; IR ν_{max} in cm⁻¹: 2922, 2853, 1721, 1586, 1499, 1462, 1431, 1381, 1333, 1214, 1111, 1014, 863, 763, 722; ¹H NMR (600 MHz, CDCl₃, 299 K): 7.25 (s, 2H, H_{Ar}), 4.03-4.00 (m, 6H, 3× OCH₂), 3.89 (s, 3H, 1× OCH₃), 1.83-1.79 (m, 4H, 2 × CH₂), 1.77-1.72 (m, 2H, 1 × CH₂), 1.50-1.45 (m, 6H, 3 × CH₂), 1.35-1.27 (m, 36H, 20 × CH₂), 0.89-0.87 (t, 9H, 3 × CH₃); ¹³C NMR (150 MHz, CDCl₃, 298.1K): 166.96, 152.82, 142.35, 124.66, 107.98, 73.50, 69.17, 52.11, 31.96, 31.93, 30.34, 29.75, 29.69, 29.65, 29.61, 29.58, 29.41, 29.37, 29.32, 26.10, 26.07, 22.71, 14.12.

Synthesis of 3,4,5-tris(decyloxy)benzoic acid (**6**)⁶

The compound methyl 3,4,5-tris(decyloxy)benzoate (**5**) (4.96 mmol, 1 equiv.) was dissolved in 50 mL of ethanol. To this solution, a minimum amount of water containing NaOH (9.92 mmol, 2 equiv.) was added. The reaction mixture was then heated, and any frothing observed during heating was suppressed by addition of water. The mixture was refluxed for 17 hours. After completion, excess solvent was removed by evaporation, and the residue was added to ice water. The mixture was acidified with HCl and extracted with EtOAc. The combined organic extracts were dried over anhydrous Na₂SO₄ and concentrated under reduced pressure. The crude product obtained was recrystallized from ethanol to yield a white solid.

6: $R_f = 0.31$ (50% EtOAc-hexanes); white solid; yield: 86%; IR ν_{\max} in cm^{-1} : 2918, 2850, 1684, 1586, 1504, 1465, 1429, 1387, 1330, 1275, 1229, 1117, 929, 864, 765, 724, 682, 542, 433; ^1H NMR (600 MHz, CDCl_3 , 299 K): 7.32 (s, 2H, H_{Ar}), 4.05-4.01 (m, 6H, $3 \times \text{OCH}_2$), 1.84-1.80 (m, 4H, $2 \times \text{CH}_2$), 1.77-1.73 (m, 2H, $1 \times \text{CH}_2$), 1.50-1.45 (m, 6H, $3 \times \text{CH}_2$), 1.36-1.28 (m, 36H, $18 \times \text{CH}_2$), 0.89-0.87 (t, 9H, $3 \times \text{CH}_3$); ^{13}C NMR (151 MHz, CDCl_3) δ 171.04, 152.85, 143.11, 123.55, 108.55, 77.23, 77.02, 76.80, 73.57, 69.20, 31.95, 31.92, 30.34, 29.73, 29.68, 29.64, 29.59, 29.57, 29.40, 29.36, 29.28, 26.08, 26.05, 22.70, 14.12.

Synthesis of oxalylbis(4,1-phenylene) bis(3,4,5-tris(decyloxy)benzoate) (**8**)⁷

3,4,5-tris(decyloxy)benzoic acid (**6**) (2.03 mmol, 2.5 equiv.) in thionyl chloride (SOCl_2) (10 mL) was refluxed for 2 hours under N_2 atmosphere to obtain the corresponding acyl chloride. Excess SOCl_2 was distilled off, and the crude acyl chloride was used directly in the next step. To the acyl chloride, a mixture of 1,2-bis(4-hydroxyphenyl)ethane-1,2-dione (Compound **3**, 0.81 mmol, 1 equiv.) in dry dichloromethane (30 mL) and triethylamine (4.06 mmol, 5 equiv.) was added. The reaction was stirred for 12 hours at room temperature. The solvent and residual triethylamine were evaporated under reduced pressure. The resulting solid was redissolved in dichloromethane, washed sequentially with brine and water, dried over anhydrous Na_2SO_4 , and concentrated. The crude product was purified by column chromatography using a 20:1 mixture of hexane and EtOAc as the eluent, to afford the white solid product **8**.

8: $R_f = 0.68$ (10% EtOAc-hexanes); white solid; mp: 73-74 °C; yield: 66%; IR ν_{\max} in cm^{-1} : 2918, 2851, 1745, 1671, 1592, 1502, 1469, 1434, 1384, 1337, 1214, 1188, 1158, 1127, 1087, 1017, 943, 887, 865, 788, 743, 676, 620, 510; ^1H NMR (600 MHz, CDCl_3 , 299 K): 8.10-8.08 (d, $J = 8.4$ Hz, 4H, H_{Ar}), 7.40 (s, 4H, H_{Ar}), 7.39-7.38 (d, $J = 8.4$ Hz, 4H, H_{Ar}), 4.08-4.04 (m, 12H, $6 \times \text{OCH}_2$), 1.86-1.81 (m, 8H, $4 \times \text{CH}_2$), 1.79-1.74 (m, 4H, $2 \times \text{CH}_2$), 1.51-1.46 (m, 12H, $6 \times \text{CH}_2$), 1.36-1.28 (m, 72H, $36 \times \text{CH}_2$), 0.89-0.87 (m, 18H, $6 \times \text{CH}_3$); ^{13}C NMR (151 MHz, CDCl_3) δ 192.90, 164.27, 156.32, 153.05, 143.45, 131.74, 130.43, 123.06, 122.66, 108.71, 73.64, 69.34, 31.95, 31.92, 30.35, 29.74, 29.68, 29.64, 29.59, 29.57, 29.40, 29.36, 29.30, 26.09, 26.05, 22.71, 22.69, 14.12; MALDI-TOF exact mass calculated for $\text{C}_{88}\text{H}_{138}\text{O}_{12}$ (M): 1387.0188, found: 1387.133.

Synthesis of benzo[1,2-g:3,4-g':5,6-g'']triquinoxaline-2,3,8,9,14,15-hexaylhexas(4,1-dyl) hexakis(3,4,5-tris(decyloxy)benzoate)⁸(**BQE**)

Compound **8** (0.36 mmol, 3.0 equiv.) and triphenylene-2,3,6,7,10,11-hexamine hexahydrochloride (0.12 mmol, 1.0 equiv.) were transferred into a 100 mL two-necked RB flask with 8 mL methanol and 24 mL acetic acid (1:3) under a nitrogen atmosphere, which was heated to 100 °C. After the addition of 1.0 mL of trimethylamine, the oil bath was maintained at 130 °C to ensure continuous reflux of the reaction mixture for 12 hours. Later, the reaction mixture was concentrated. The crude product was purified by column chromatography on neutral alumina with 5-10% ethyl acetate-hexane to yield a yellow solid product (**BQE**).

BQE: $R_f = 0.52$ (10% EtOAc-Hexane); Gummy yellow solid, yield: 78%; IR ν_{\max} in cm^{-1} : 2921, 2852, 1733, 1586, 1499, 1466, 1429, 1387, 1334, 1192, 1166, 1115, 1054, 1015, 959, 860, 780, 749, 721, 572, 546; ^1H NMR (600 MHz, CDCl_3 , 299 K): 9.58 (s, 6H, H_{Ar}), 7.81-7.80 (d, $J = 8.4$ Hz, 12H, H_{Ar}), 7.44 (s, 12H, H_{Ar}), 7.33-7.31 (d, $J = 8.4$ Hz, 12H, H_{Ar}), 4.09-4.06 (m, 36H, $18 \times$

OCH₂), 1.87-1.83 (m, 24H, 12 × CH₂), 1.81-1.76 (m, 12H, 6 × CH₂), 1.53-1.48 (m, 36H, 24 × CH₂), 1.40-1.37 (m, 36H, 24 × CH₂), 1.35-1.28 (m, 180H, 90 × CH₂), 0.91-0.87 (m, 54H, 18 × CH₃); ¹³C NMR (151 MHz, CDCl₃) δ 164.78, 153.74, 153.07, 152.13, 143.33, 140.78, 136.39, 132.22, 131.32, 125.13, 123.74, 121.98, 108.79, 73.65, 69.41, 31.97, 31.94, 30.41, 29.76, 29.70, 29.66, 29.61, 29.44, 29.42, 29.39, 29.36, 26.15, 26.10, 22.72, 22.70, 14.10; MALDI-TOF exact mass calculated for C₂₈₂H₄₂₀N₆O₃₀ (M): 4371.152, found: 4371.153; Elemental analysis (C₂₈₂H₄₂₀N₆O₃₀): calculated [%] N 1.92, C 77.43, H 9.68, O 10.97; found [%] N 1.89, C 76.71, H 10.23, O 9.93.

Synthesis of dimethyl 4,4'-(1-hydroxy-2-oxoethane-1,2-diyl)dibenzoate) (**10**)⁹

Vitamin B1 (0.91 mmol, 0.05 equiv.), MeOH (6 mL) and H₂O (2 mL) were added to a 50 mL round-bottomed flask, and the mixture was cooled down in ice water. Subsequently, 2 M NaOH solution was introduced to adjust the pH to 9 over a period of time, followed by methyl 4-formylbenzoate (18.27 mmol, 1 equiv.). Then, the contents were gradually heated to 85 °C and kept for 4 h. After cooling down to room temperature, the resultant precipitate was filtered, washed with cold MeOH and water, and dried in an 80 °C oven to obtain **10** as an off-white solid in 85 % yield. The product obtained was used for the next step without further purification.

Synthesis of dimethyl 4,4'-oxalyldibenzoate) (**11**)⁹

A mixture of **10** (9.14 mmol, 1 equiv.), DMSO (7.5 mL) and 40% aqueous HBr (1.5 mL) were placed in a 150 mL round-bottomed flask. And the mixture was stirred at 60 °C for 12 h. After completion of the reaction, the mixture was poured into ice-cold water. The yellow precipitate was collected by filtration, washed with water, and dried. The crude product was recrystallized from MeOH to afford **11** as a yellow solid in 90% yield.

11: R_f = 0.54 (50% DCM-Hexane); Pale yellow solid, yield: 90%; IR ν_{max} in cm⁻¹: 1718, 1665, 1570, 1501, 1434, 1406, 1283, 1201, 1103, 1013, 948, 889, 860, 780, 731, 711, 675, 533; ¹H NMR (600 MHz, CDCl₃, 299 K): 8.18-8.16 (d, J = 7.8 Hz, 4H, H_{Ar}), 8.05-8.04 (d, J = 7.8 Hz, 4H, H_{Ar}), 3.96 (s, 6H, 2 × O-CH₃); ¹³C NMR (151 MHz, CDCl₃) δ 192.85, 165.80, 135.74, 135.53, 130.15, 129.86, 52.66.

Synthesis of 4,4'-oxalyldibenzoic acid (**12**)¹⁰

Dimethyl 4,4'-oxalyldibenzoate (**11**) (15.32 mmol, 1 equiv.) was mixed in acetic acid (350 ml) and a 4:1 H₂SO₄/H₂O solution (175 ml). The reaction mixture was heated to reflux and stirred for 10 hours. Then 250 mL of water was added, and the mixture was cooled on ice. After cooling, the product was filtered, washed with water (3 × 20 ml), and dried at 70 °C in a vacuum to obtain **12** as a pale yellow solid with 90% yield.

12: R_f = 0.00 (50% DCM-Hexane); Pale yellow solid, yield: 90%; IR ν_{max} in cm⁻¹: ¹H NMR (600 MHz, DMSO-d₆, 299 K): 13.53 (bs, 2H, 2 × COOH), 8.15-8.14 (d, J = 7.8 Hz, 4H, H_{Ar}), 8.09-8.07 (d, J = 7.2 Hz, 4H, H_{Ar}); ¹³C NMR (151 MHz, DMSO) δ 193.81, 166.76, 136.89, 135.48, 130.54, 130.51.

Synthesis of 1,2,3-tris(decyloxy)benzene (**15**)^{4,11}

A mixture of pyrogallol (23.79 mmol, 1 equiv.) and anhydrous K₂CO₃ (157.00 mmol, 6.6 equiv.) was taken in dry DMF (35 mL) and stirred for 1 hour at 60 °C. After that, n-bromodecane (78.50 mmol, 3.3 equiv.) was added, and the mixture was heated at 80 °C for 24 hours under a nitrogen atmosphere. After completion, the reaction mixture was poured into ice-cold water and extracted with CH₂Cl₂. The combined organic layers were washed successively with water and brine, dried over anhydrous Na₂SO₄, and concentrated. The crude product was purified by column chromatography on silica gel (100-200 mesh). Elution with hexanes, followed by 5-10% ethyl acetate in hexanes, afforded the desired product.

15: R_f = 0.60 (10% EtOAc-Hexane); white waxy solid, yield: 80%; IR ν_{\max} in cm⁻¹: ¹H NMR (500 MHz, CDCl₃, 299 K): 6.92-6.89 (t, J₁ = 8.5 Hz, J₂ = 8 Hz, 1H, H_{Ar}), 6.55-6.54 (d, J = 8 Hz, 2H, H_{Ar}), 3.98-3.95 (m, 6H, 3 × OCH₂), 1.83-1.73 (m, 6H, 3 × CH₂), 1.49-1.45 (m, 6H, 3 × CH₂), 1.28 (m, 36H, 18 × CH₂), 0.90-0.88 (t, 9H, 3 × CH₃); ¹³C NMR (126 MHz, CDCl₃) δ 153.45, 138.52, 123.11, 106.86, 73.39, 69.13, 31.96, 31.93, 30.37, 29.77, 29.70, 29.67, 29.64, 29.61, 29.47, 29.45, 29.42, 29.37, 26.17, 26.13, 22.70, 14.10.

Synthesis of 1,2,3-tris(decyloxy)-5-nitrobenzene (**16**)^{11,12}

An appropriate mixture of compound 1,2,3-tris(decyloxy)benzene (**15**) (7.31 mmol, 1 equiv.) and NaNO₂ (1.02 mmol, 0.14 equiv.) was dissolved in CH₂Cl₂ and stirred at 0 °C for 30 mins. To this well-stirred suspension, 70% HNO₃ (0.98 mL, 21.93 mmol, 3 equiv., 10% solution in dichloromethane) was added dropwise. This mixture was stirred at room temperature for 1 hour. Then it was poured into water, and the aqueous layer was extracted with CH₂Cl₂. The organic layer was washed with H₂O, brine, and dried over Na₂SO₄, then it was evaporated to dryness. The crude product was purified by column chromatography on silica gel (60-120 mesh) using hexane and CH₂Cl₂ as eluent to obtain a slightly yellowish solid (hexane: CH₂Cl₂ = 20: 1).

16: R_f = 0.45 (10% EtOAc-Hexane); Pale yellow solid, yield: 86%; IR ν_{\max} in cm⁻¹: ¹H NMR (600 MHz, CDCl₃, 299 K): 7.47 (s, 2H, H_{Ar}), 4.07-4.02 (m, 6H, 3 × OCH₂), 1.86-1.80 (m, 6H, 3 × CH₂), 1.77-1.71 (m, 6H, 3 × CH₂), 1.51-1.45 (m, 6H, 3 × CH₂), 1.36-1.27 (m, 30H, 15 × CH₂), 0.89-0.87 (t, 9H, 3 × CH₃); ¹³C NMR (150 MHz, CDCl₃) δ 152.71, 143.87, 143.16, 102.19, 73.83, 69.48, 31.93, 31.90, 30.30, 29.70, 29.65, 29.59, 29.56, 29.50, 29.38, 29.33, 29.11, 26.01, 25.98, 22.68, 14.09.

Synthesis of 3,4,5-tris(decyloxy)aniline (**17**)^{11,12}

To a suspension of nitro compound **16** (5.07 mmol, 1 equiv.) and 10% Pd-C (10% weight of the nitro compound) in absolute ethanol, hydrazine monohydrate (25.34 mmol, 5 equiv.) was added and refluxed under N₂ atmosphere for 24 hours. The reaction mixture was cooled to room temperature, and CH₂Cl₂ was added and filtered through a celite bed. The filtrate was extracted with CH₂Cl₂ (3 × 50 mL). The combined extracts were washed with water, brine, and dried over anhydrous Na₂SO₄, and the solvent was concentrated via rotary evaporation, and cooled methanol was added to get a precipitate, then filtered to get the product. The product **17** was used directly in the next step without further purification.

Synthesis of 4,4'-oxalyldibenzamide (18)^{7,13}

4,4'-oxalyldibenzoic acid (**13**) (3.35 mmol, 0.5 equiv.) in thionyl chloride (SOCl₂) (10 mL) was refluxed for 2 hours under N₂ atmosphere to obtain the corresponding acyl chloride. Excess SOCl₂ was distilled off, and the crude acyl chloride was used directly in the next step. To the acyl chloride, a mixture of 3,4,5-tris(decyloxy)aniline (Compound **17**, 1.68 mmol, 1 equiv.) in dry dichloromethane (30 mL) and triethylamine (8.38 mmol, 5 equiv.) was added. The reaction was stirred for 12 hours at room temperature. The solvent and residual triethylamine were evaporated under reduced pressure. The resulting solid was redissolved in dichloromethane, washed sequentially with brine and water, dried over anhydrous Na₂SO₄, and concentrated. The crude product was purified by column chromatography using a 10:1 mixture of hexane and EtOAc as the eluent, to afford the brown sticky product **18**.

18: R_f = 0.30 (15% EtOAc-Hexane); Brown sticky solid, yield: 58%; IR ν_{max} in cm⁻¹: 3372, 2957, 2921, 2851, 1667, 1604, 1537, 1505, 1467, 1425, 1385, 1305, 1230, 1211, 1385, 1305, 1230, 1211, 1112, 1018, 833, 844, 703, 619, 583; ¹H NMR (600 MHz, CDCl₃, 299 K): 8.04-8.03 (d, J = 8.4 Hz, 4H, H_{Ar}), 7.97-7.96 (d, J = 7.8 Hz, 4H, H_{Ar}), 6.92 (s, 4H, H_{Ar}), 3.96-3.92 (m, 12H, 6 × OCH₂), 1.81-1.76 (m, 8H, 4 × CH₂), 1.75-1.71 (m, 4H, 2 × CH₂), 1.49-1.41 (m, 12H, 6 × CH₂), 1.33-1.25 (m, 72H, 36 × CH₂), 0.89-0.86 (m, 18H, 6 × CH₃); ¹³C NMR (151 MHz, CDCl₃) δ 192.74, 164.22, 153.28, 140.78, 135.44, 134.75, 133.03, 130.29, 127.69, 99.36, 73.59, 69.19, 31.95, 31.92, 30.31, 29.76, 29.69, 29.66, 29.64, 29.61, 29.43, 29.41, 29.36, 26.14, 26.11, 22.70, 22.69, 14.11; MALDI-TOF exact mass calculated for C₈₈H₁₄₀N₂O₁₀ (M): 1385.051, found: 1385.689

Synthesis of 4,4',4'',4''',4''''- (benzo[1,2-g:3,4-g':5,6-g'']triquinoxaline-2,3,8,9,14,15-hexayl)hexakis(N-(3,4,5-tris(decyloxy)phenyl)benzamide) (BQA)⁸

Compound **18** (0.36 mmol, 3.0 equiv.) and triphenylene-2,3,6,7,10,11-hexamine hexahydrochloride (0.12 mmol, 1.0 equiv.) were transferred into a 50 mL two-necked RB flask with 8 mL methanol and 24 mL acetic acid (1:3) under a nitrogen atmosphere, which was heated to 100 °C. After the addition of 1.0 mL of trimethylamine, the oil bath was maintained at 130 °C to ensure continuous reflux of the reaction mixture for 12 hours. Later, the reaction mixture was concentrated. The crude product was purified by column chromatography on neutral alumina with 10-20% ethyl acetate-hexane to yield a brown solid product (**BQA**).

BQA: R_f = 0.25 (100% Chloroform); Brown solid, yield: 48%; IR ν_{max} in cm⁻¹: 3281, 2921, 2852, 1649, 1602, 1535, 1504, 1467, 1424, 1382, 1340, 1229, 1112, 1054, 1017, 973, 879, 854, 813, 720, 674, 618; ¹H NMR (600 MHz, CDCl₃, 299 K): 8.77 (s, 6H, H_{Ar}), 8.51 (s, 6H, NH), 7.95-7.76 (d, J = 118.2 Hz, 24H, H_{Ar}), 7.01 (s, 12H, H_{Ar}), 3.93 (m, 12H, 6 × OCH₂), 3.81 (m, 24H, 12 × OCH₂), 1.75-1.74 (m, 36H, 18 × CH₂), 1.50 (m, 12H, 6 × CH₂), 1.42 (m, 24H, 12 × CH₂), 1.28-1.25 (m, 216H, 108 × CH₂), 0.91-0.84 (m, 54H, 18 × CH₃); ¹³C NMR (151 MHz, CDCl₃) δ 165.30, 153.23, 141.65, 140.25, 135.88, 135.31, 133.23, 131.39, 130.45, 127.49, 125.02, 124.54, 99.51, 73.54, 68.95, 37.11, 32.00, 31.98, 30.51, 29.87, 29.79, 29.75, 29.72, 29.63, 29.51, 29.48, 29.44, 26.28, 26.23, 22.74, 22.72, 14.14; MALDI-TOF exact mass calculated for C₂₈₂H₄₂₀N₁₂O₂₄ (M): 4365.2483; found: 4365.027; Elemental analysis (C₂₈₂H₄₂₆N₁₂O₂₄): calculated [%] N 3.85, C 77.53, H 9.83, O 8.79; found [%] N 3.68, C 75.77, H 10.22, O 8.43.

3. NMR spectra

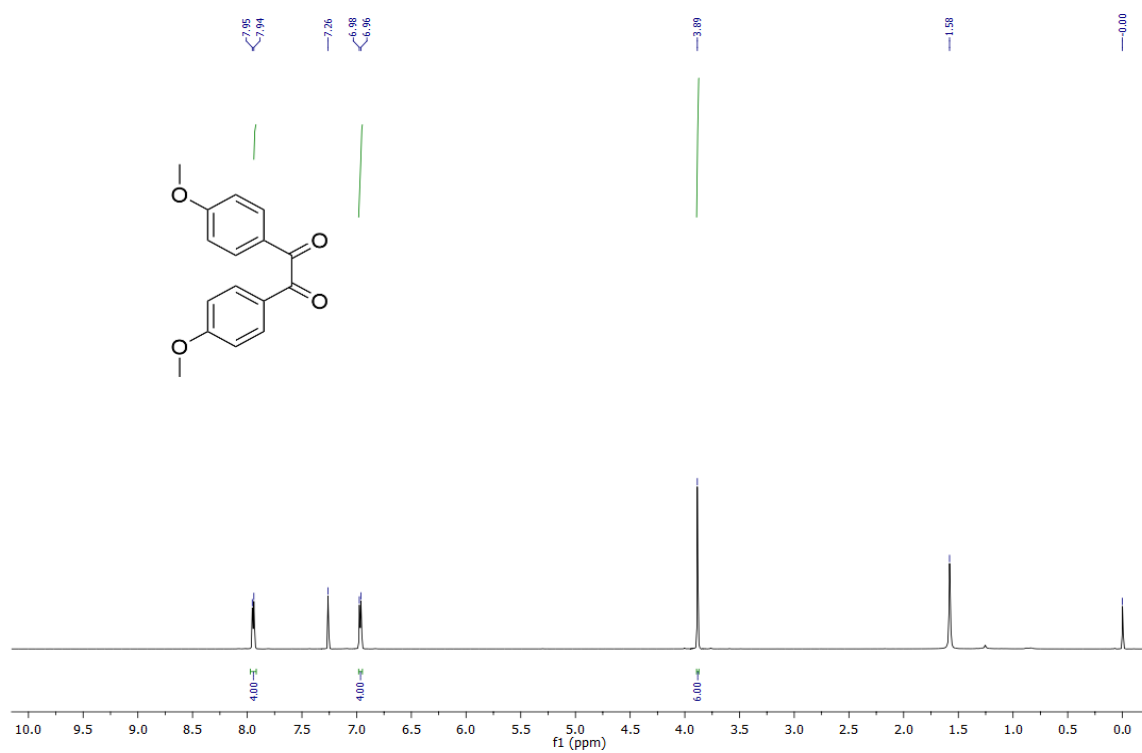


Figure S1. ¹H NMR (600 MHz) spectrum of **2** in CDCl₃.

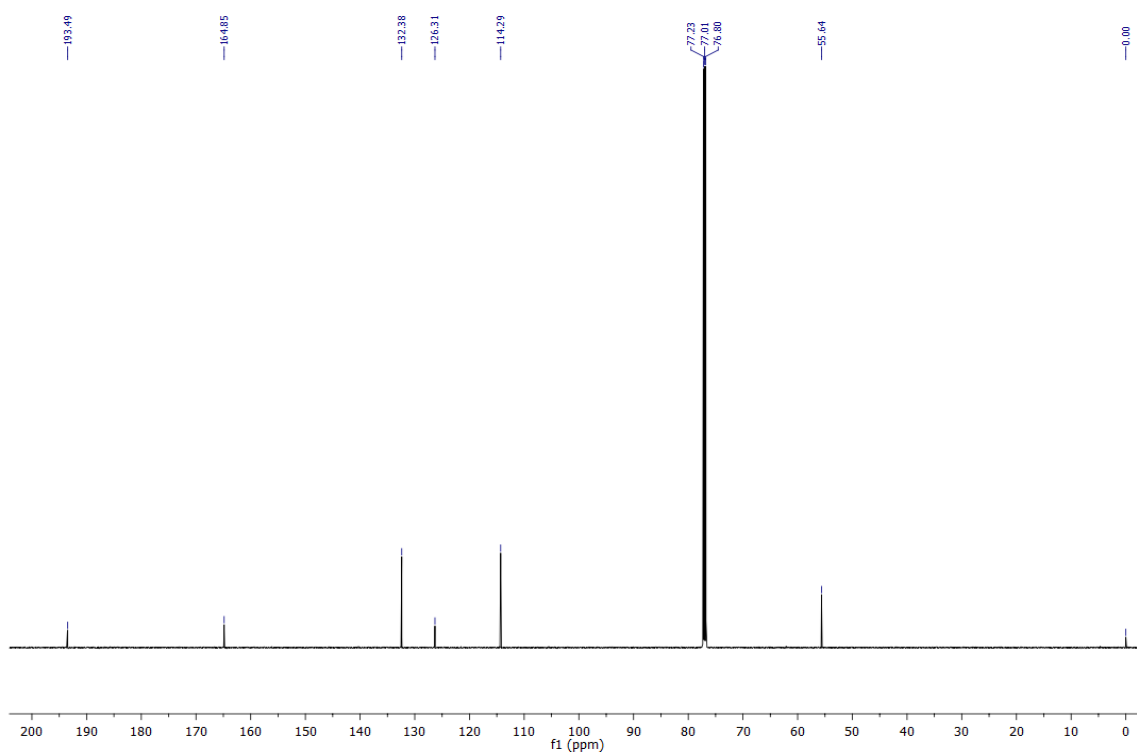


Figure S2. ¹³C NMR (150 MHz) spectrum of **2** in CDCl₃.

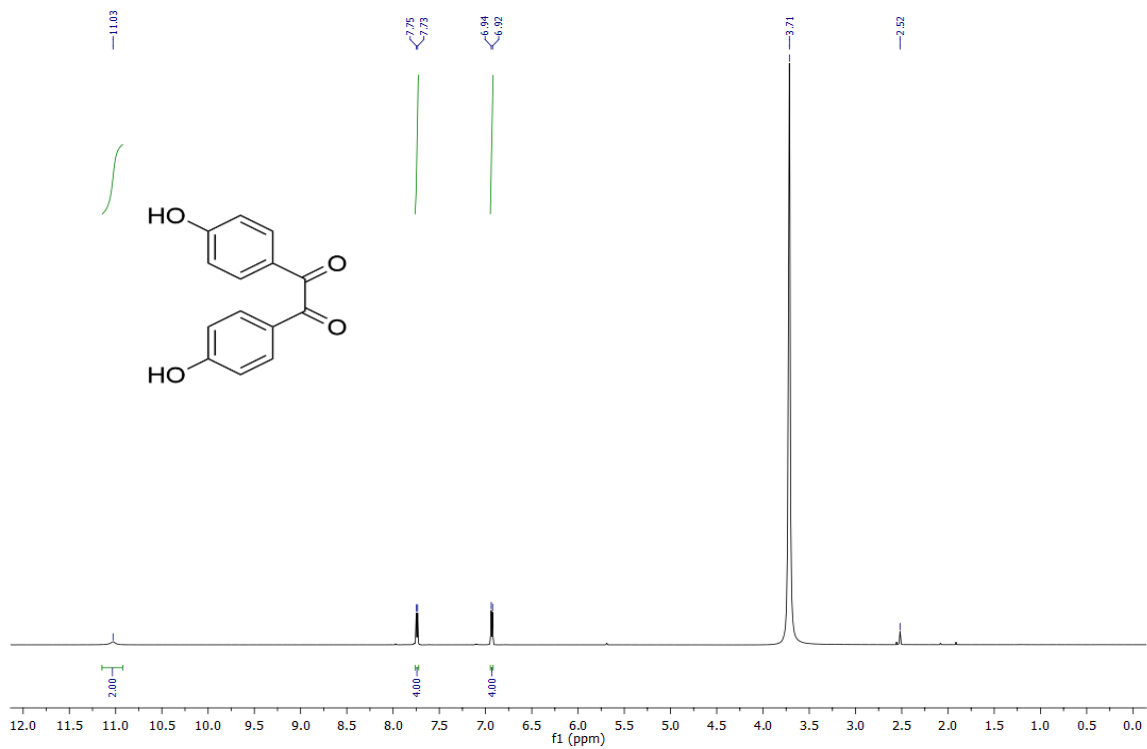


Figure S3. ^1H NMR (600 MHz) spectrum of **3** in CDCl_3 .

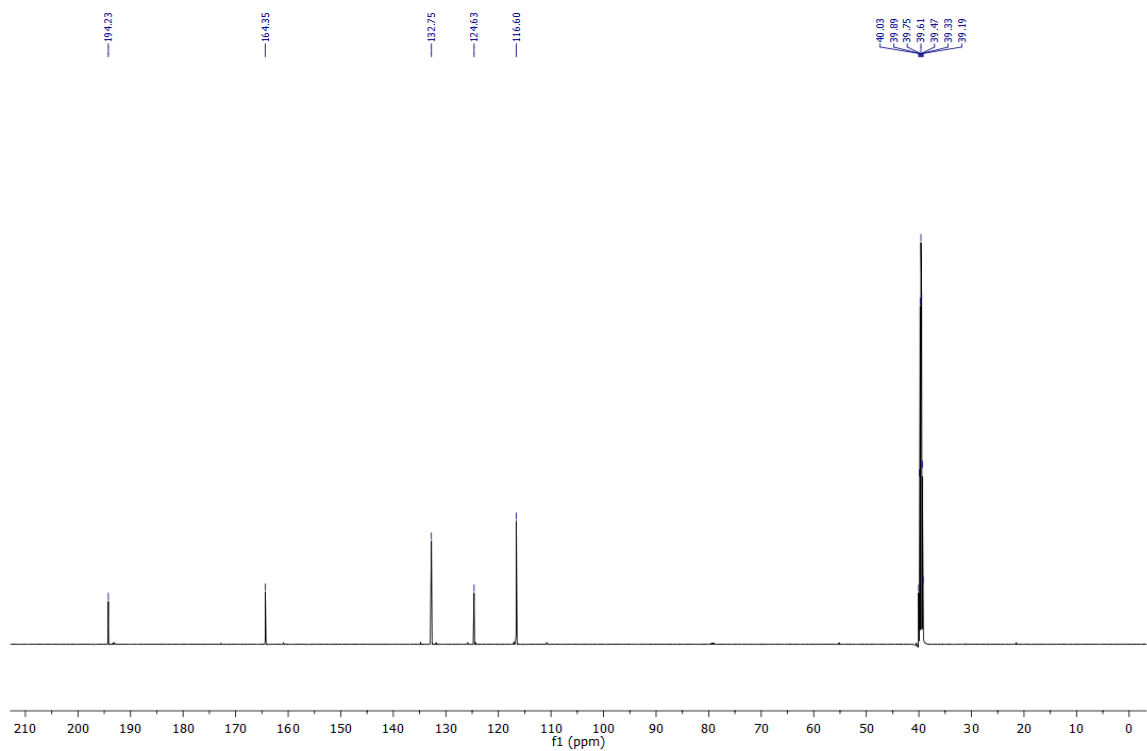


Figure S4. ^{13}C NMR (150 MHz) spectrum of **3** in CDCl_3 .

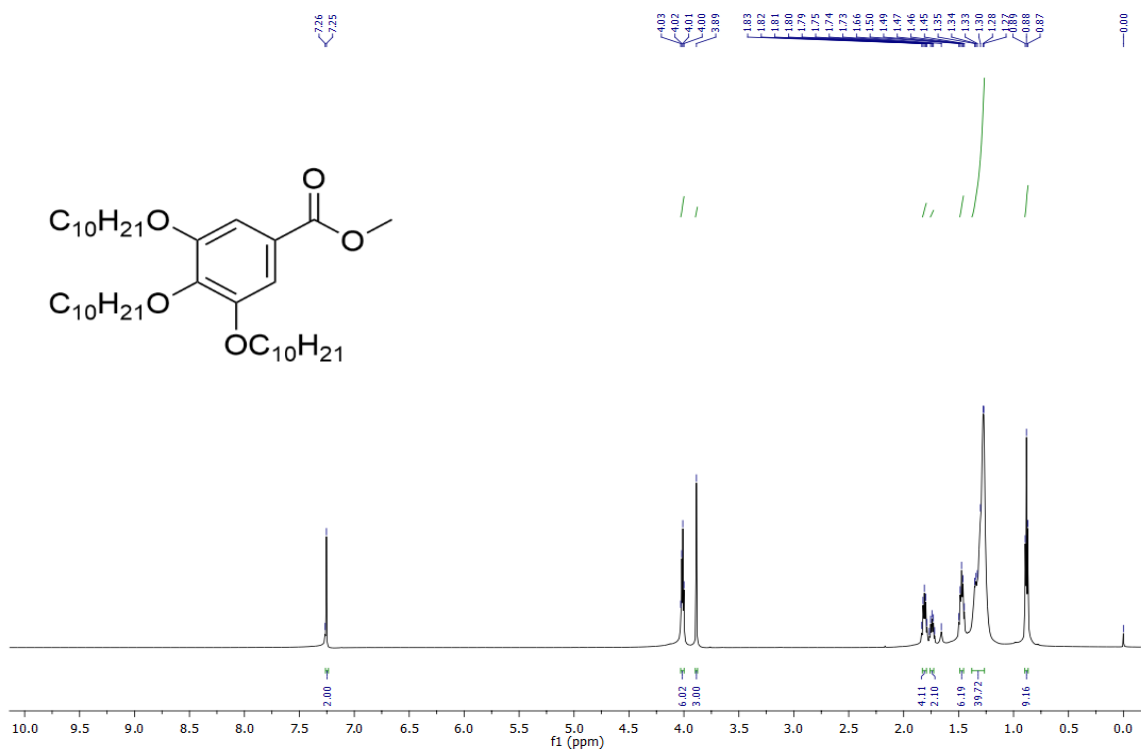
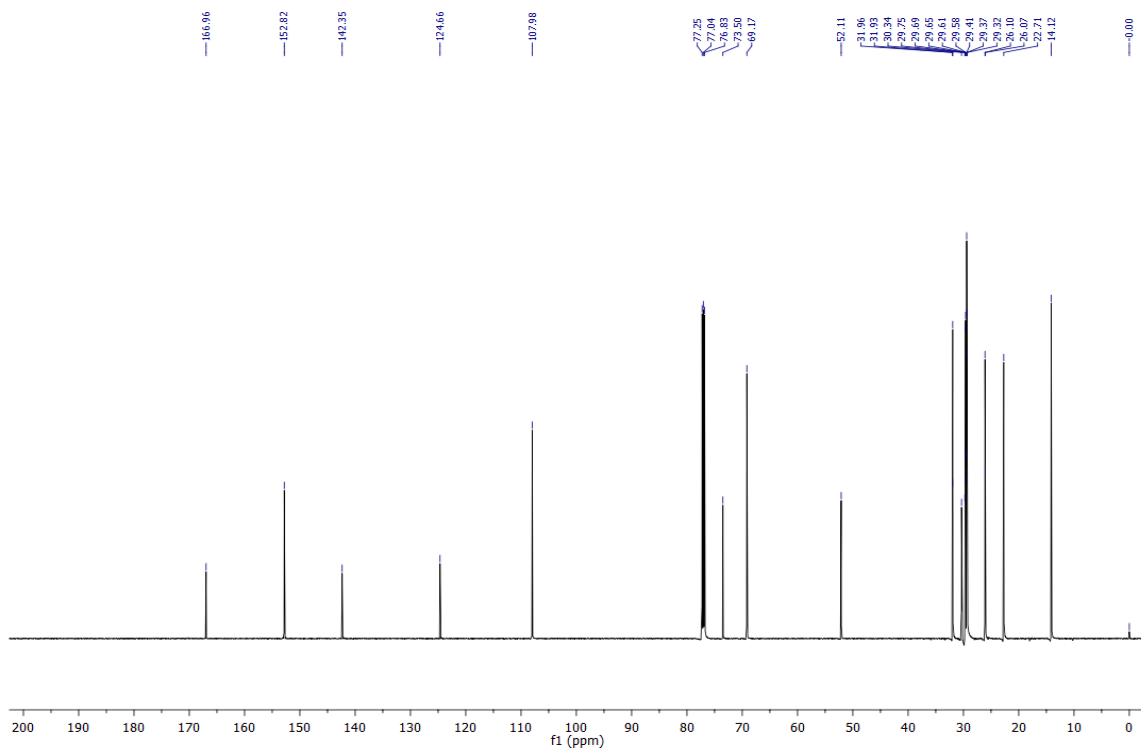


Figure S5. ¹H NMR (600 MHz) spectrum of **5** in CDCl₃.



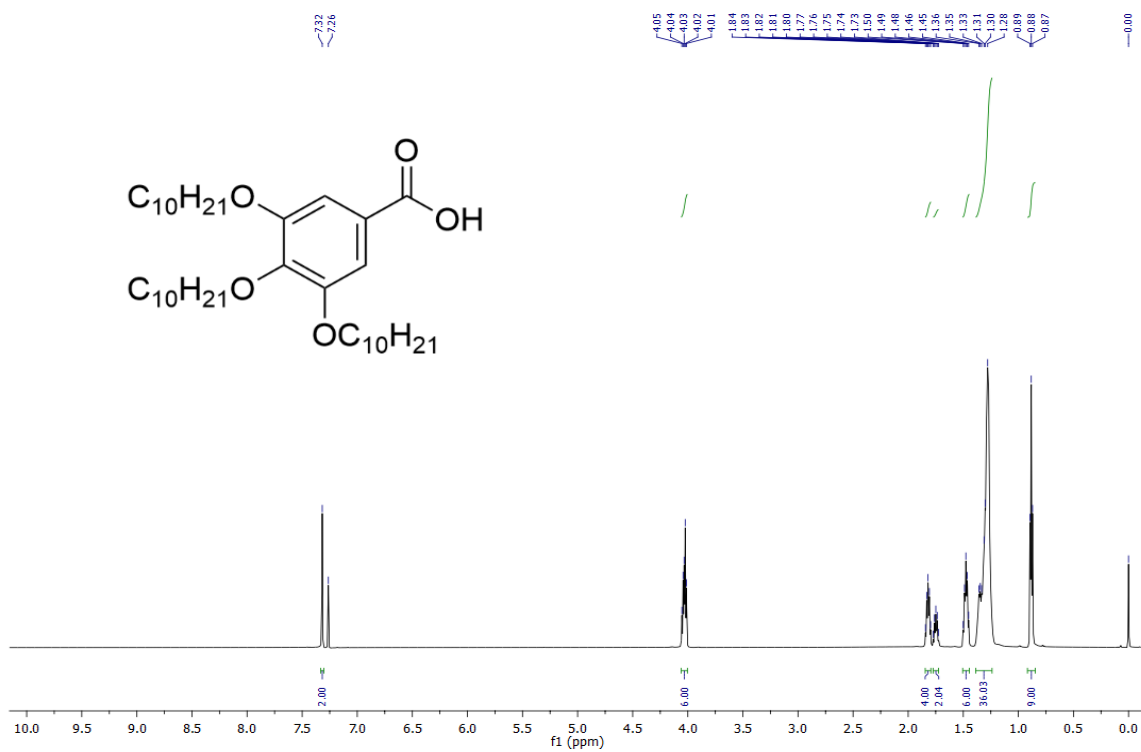


Figure S7. ¹H NMR (600 MHz) spectrum of **6** in CDCl₃.

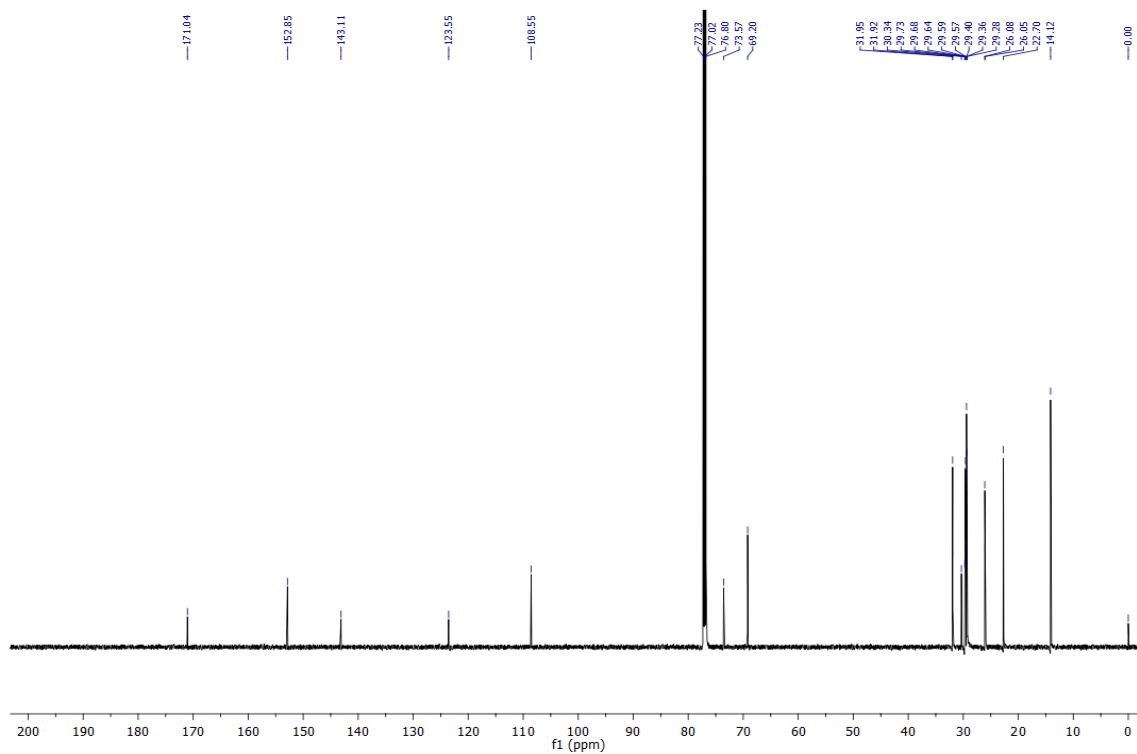


Figure S8. ¹³C NMR (150 MHz) spectrum of **6** in CDCl₃.

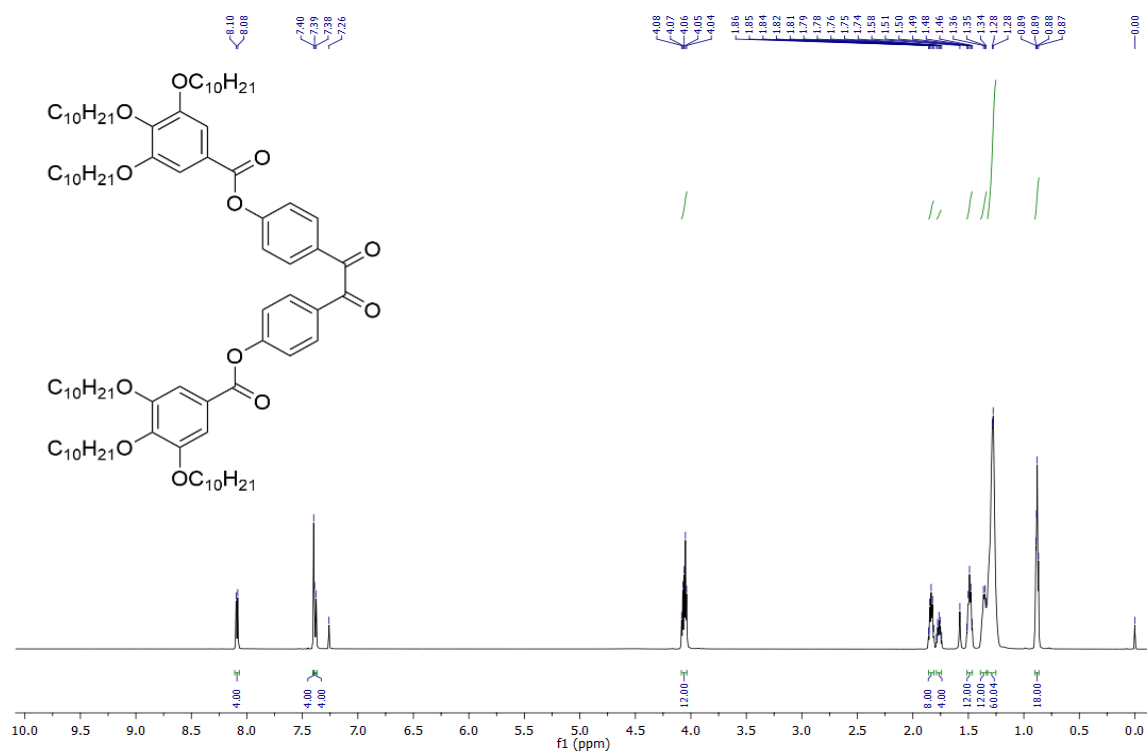


Figure S9. ^1H NMR (600 MHz) spectrum of **8** in CDCl_3 .

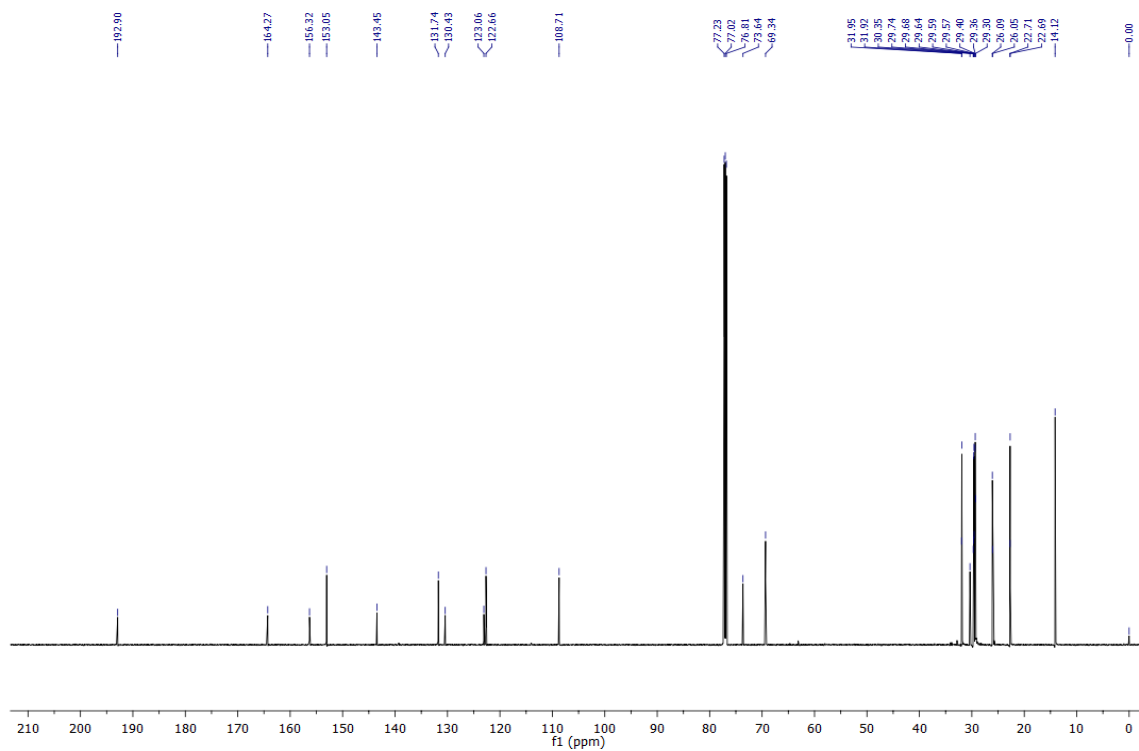


Figure S10. ^{13}C NMR (150 MHz) spectrum of **8** in CDCl_3 .



Figure S13. ¹H NMR (600 MHz) spectrum of **11** in CDCl₃.

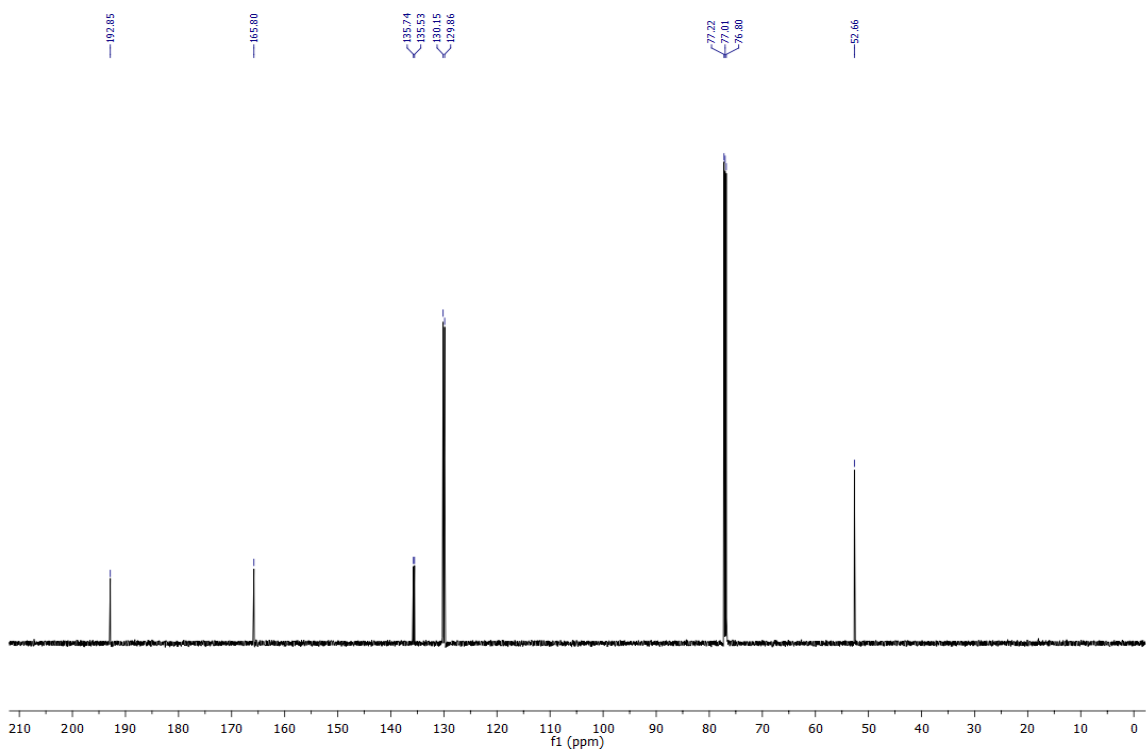


Figure S14. ¹³C NMR (150 MHz) spectrum of **11** in CDCl₃.

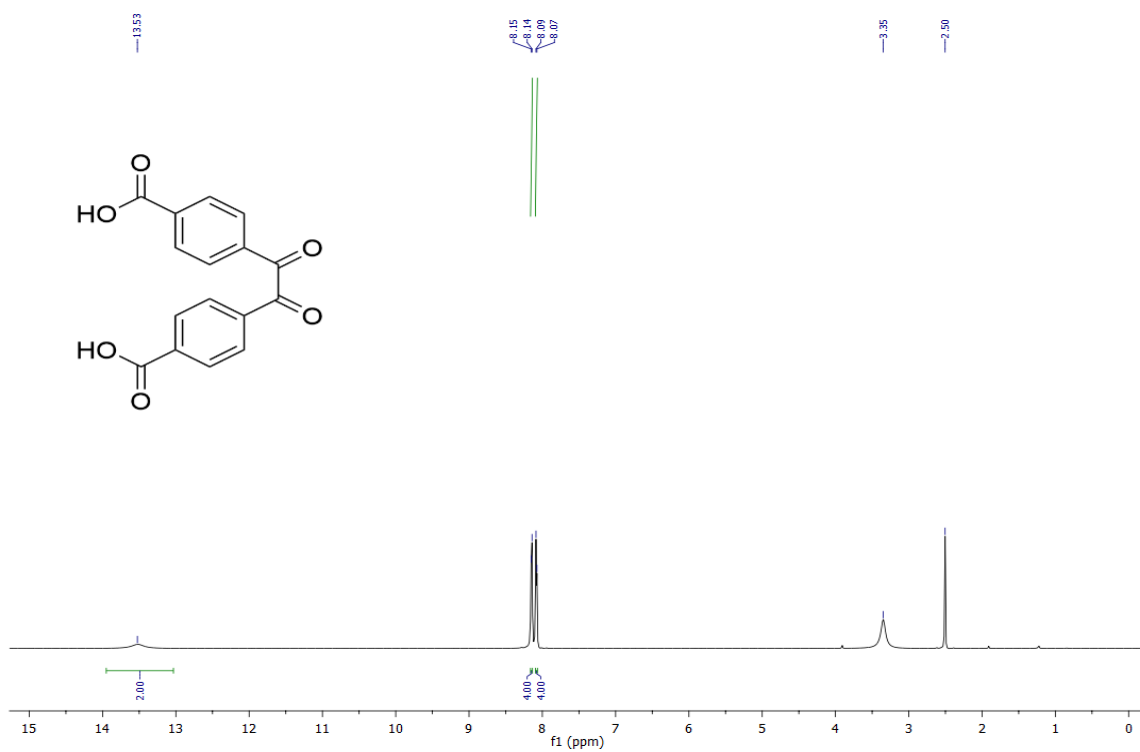


Figure S15. ¹H NMR (600 MHz) spectrum of **12** in DMSO-d₆.

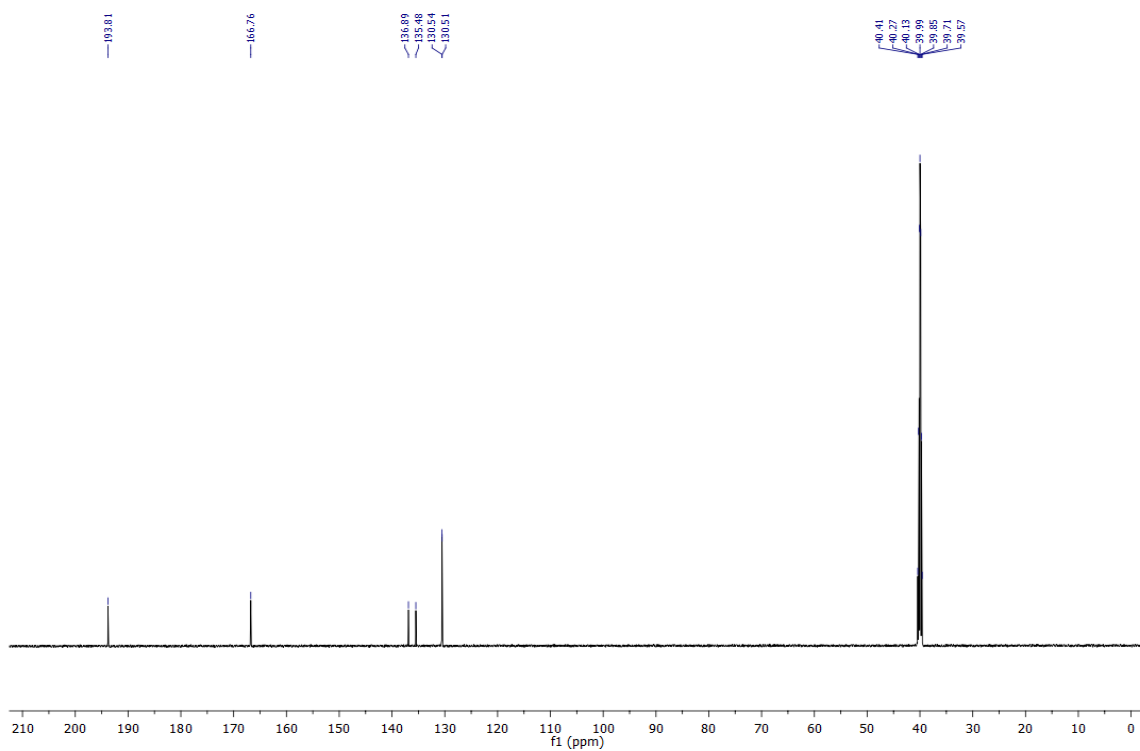


Figure S16. ¹³C NMR (150 MHz) spectrum of **12** in DMSO-d₆.

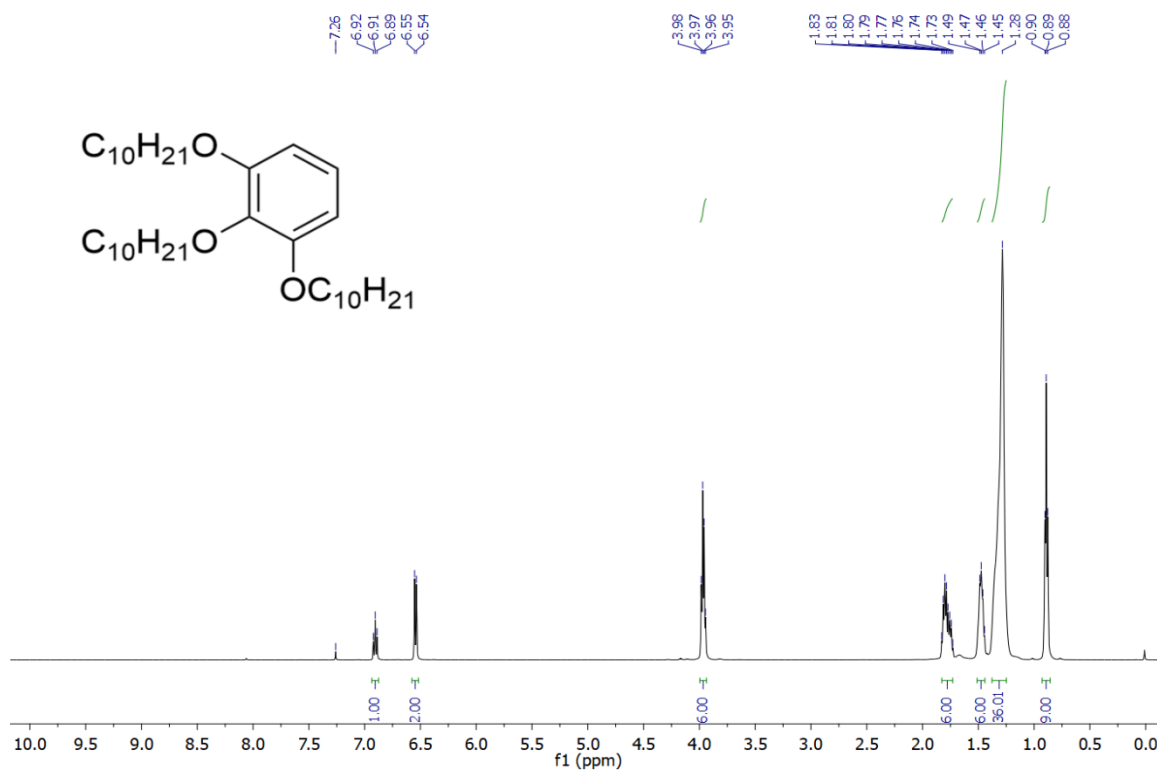


Figure S17. ¹H NMR (500 MHz) spectrum of **15** in CDCl₃.

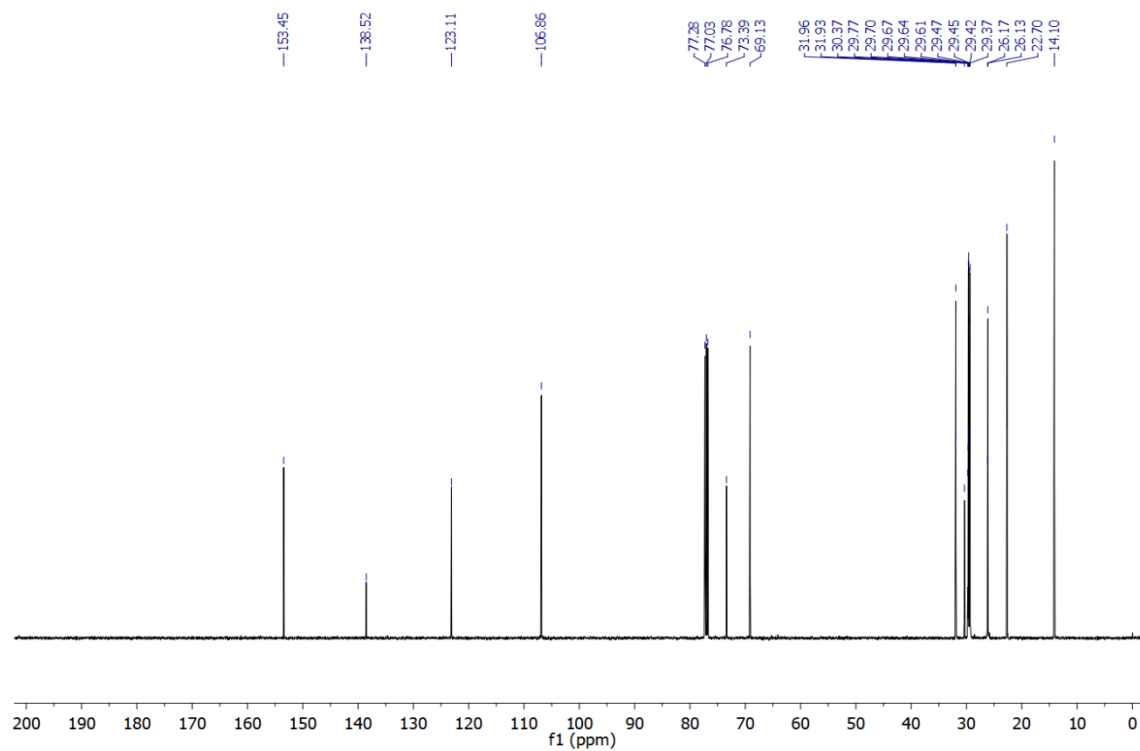


Figure S18. ¹³C NMR (100 MHz) spectrum of **15** in CDCl₃.

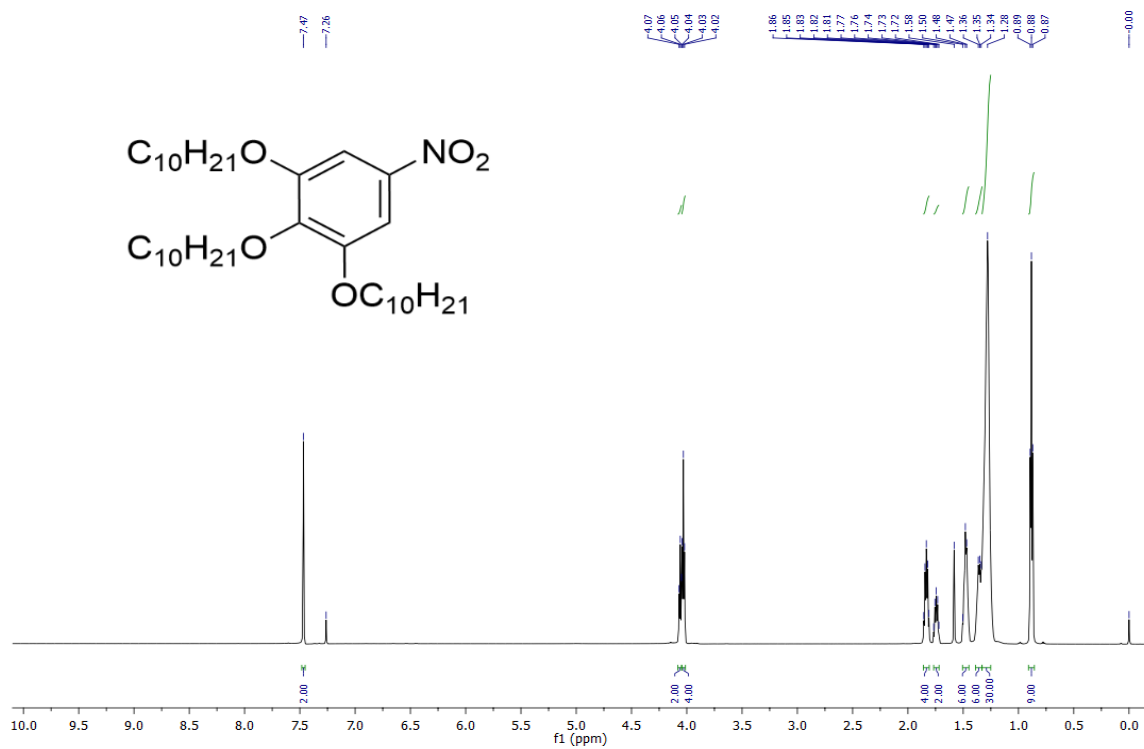


Figure S19. ¹H NMR (600 MHz) spectrum of **16** in CDCl₃.

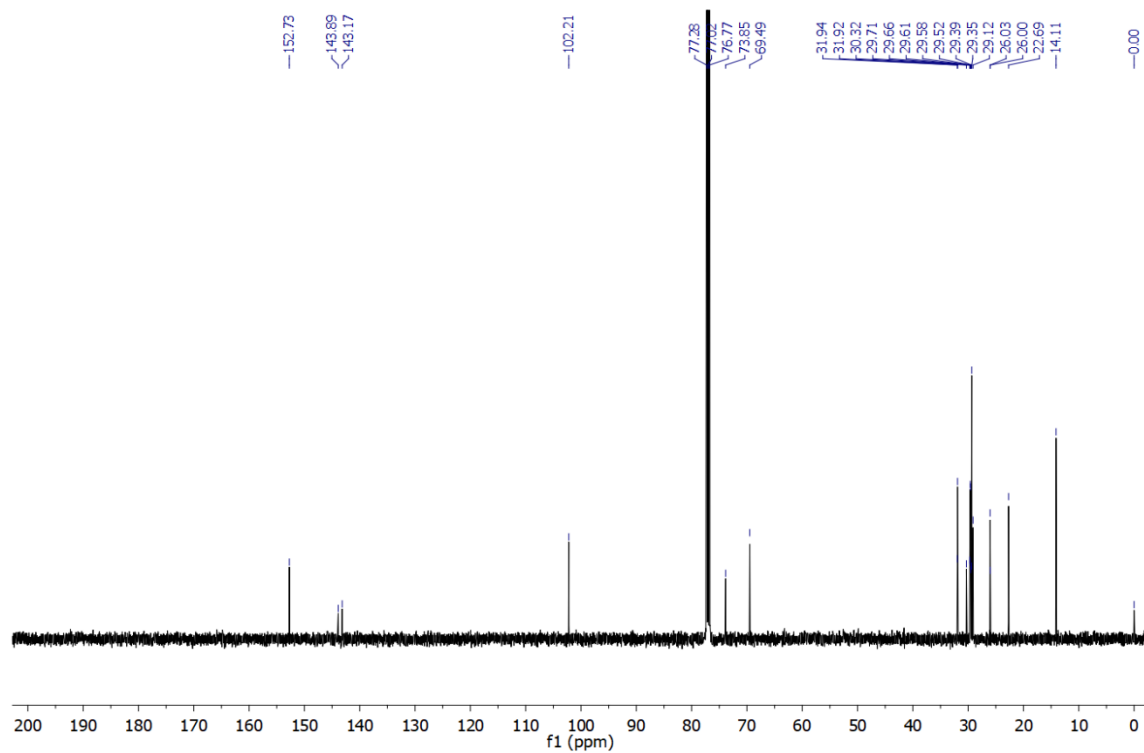


Figure S20. ¹³C NMR (150 MHz) spectrum of **16** in CDCl₃.

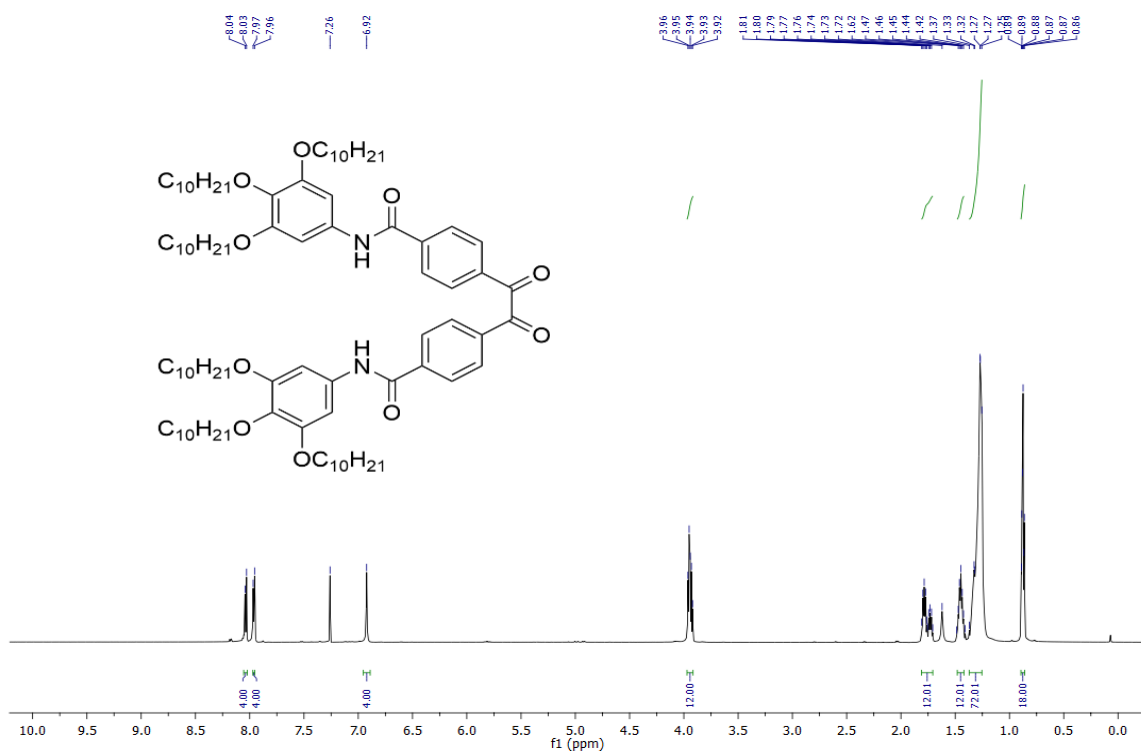


Figure S21. ¹H NMR (600 MHz) spectrum of **18** in CDCl₃.

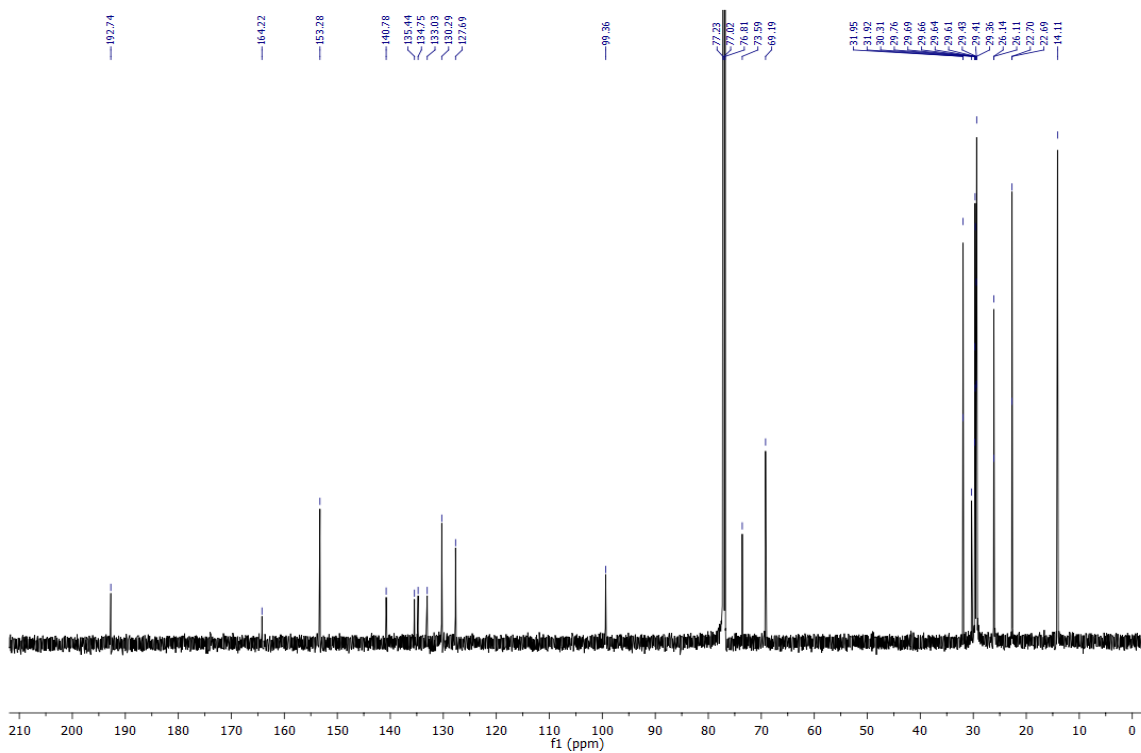


Figure S22. ¹³C NMR (150 MHz) spectrum of **18** in CDCl₃.

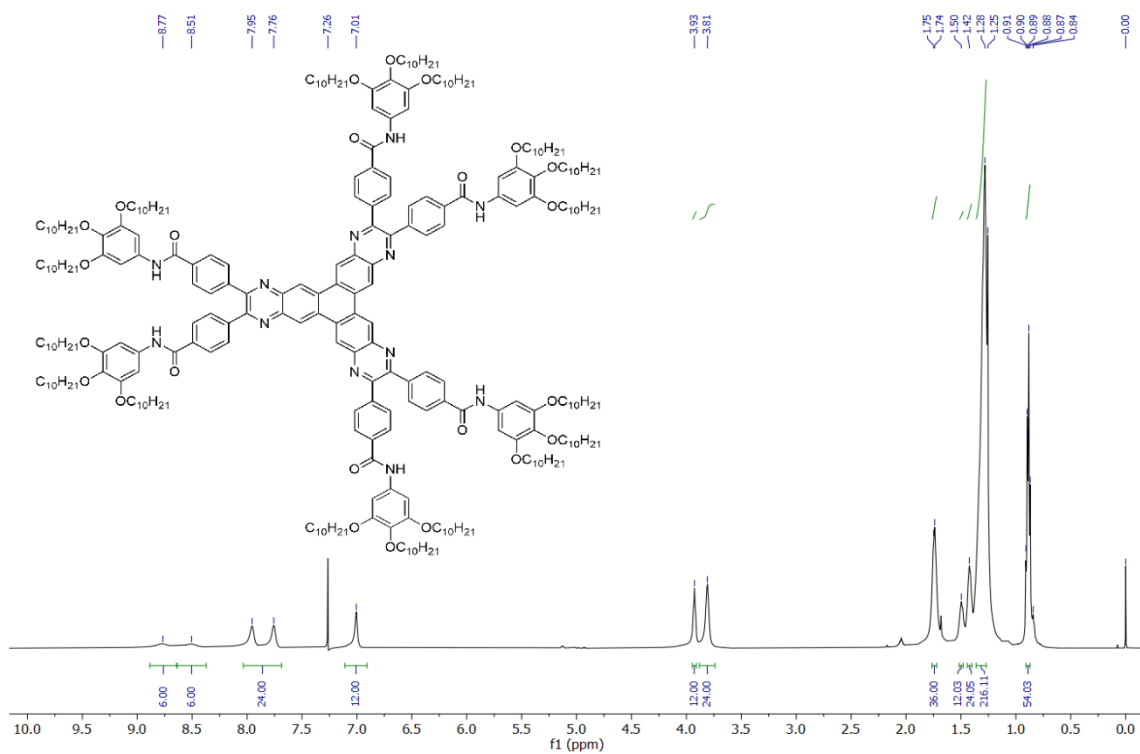


Figure S23. ¹H NMR (600 MHz) spectrum of BQA in CDCl₃.

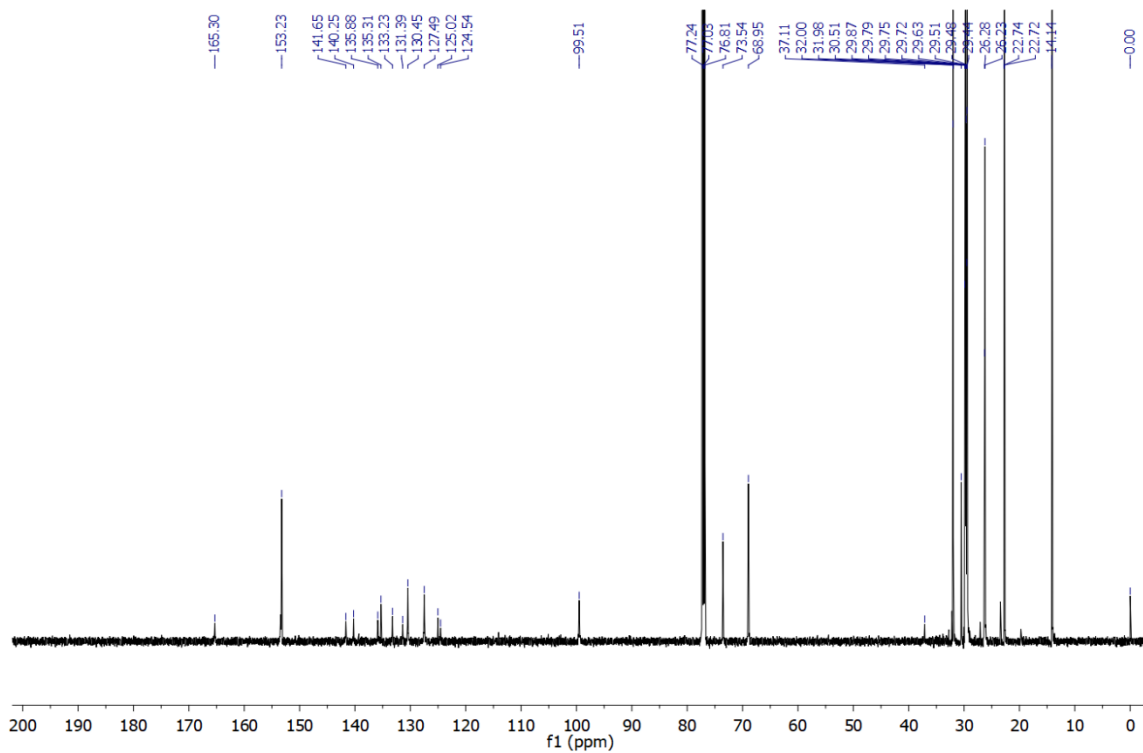


Figure S24. ¹³C NMR (150 MHz) spectrum of BQA in CDCl₃.

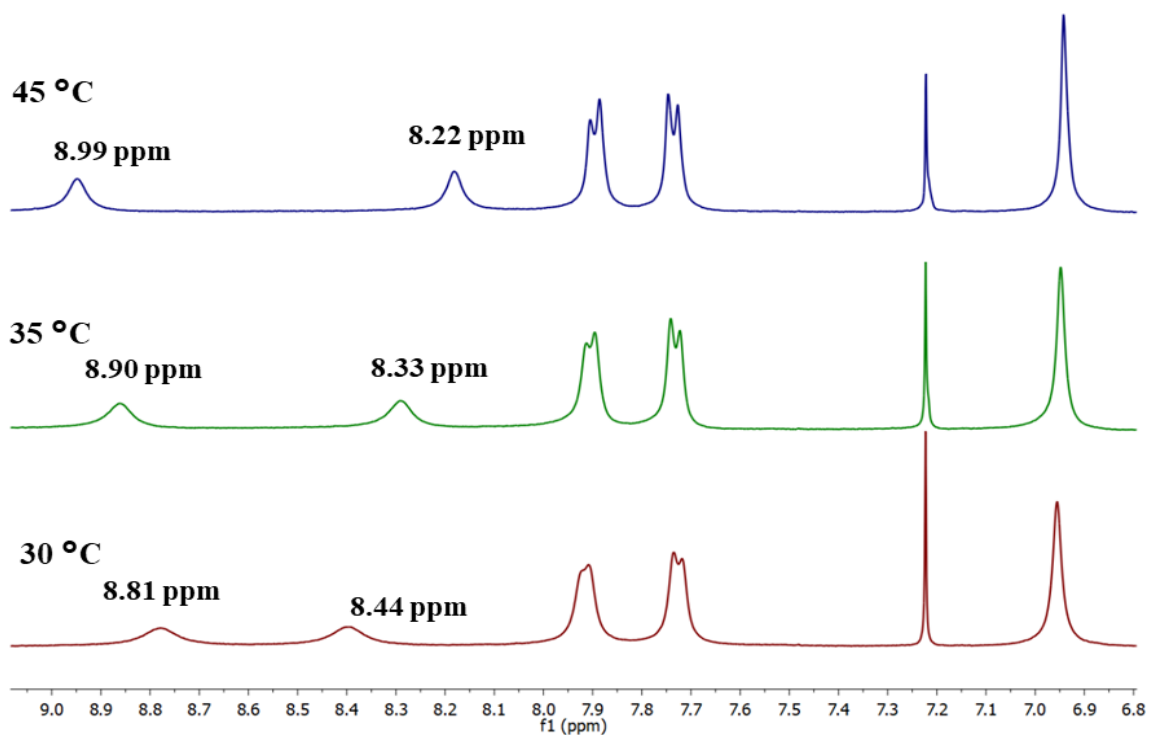


Figure S25. Stacked ^1H NMR (400 MHz) spectra of **BQA** in CDCl_3 at 30 °C, 35 °C and 45 °C.

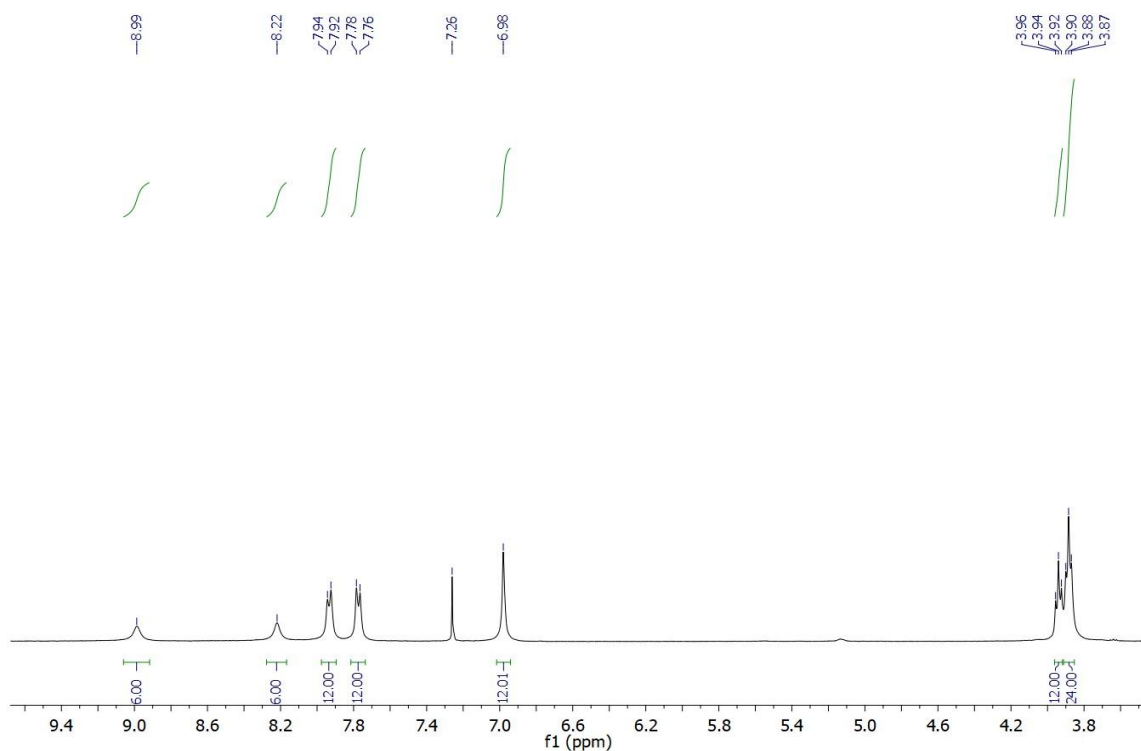


Figure S26. Integrated ^1H NMR (400 MHz) spectrum in the aromatic region of **BQA** in CDCl_3 at 45 °C.

4. MALDI-TOF Mass Spectra

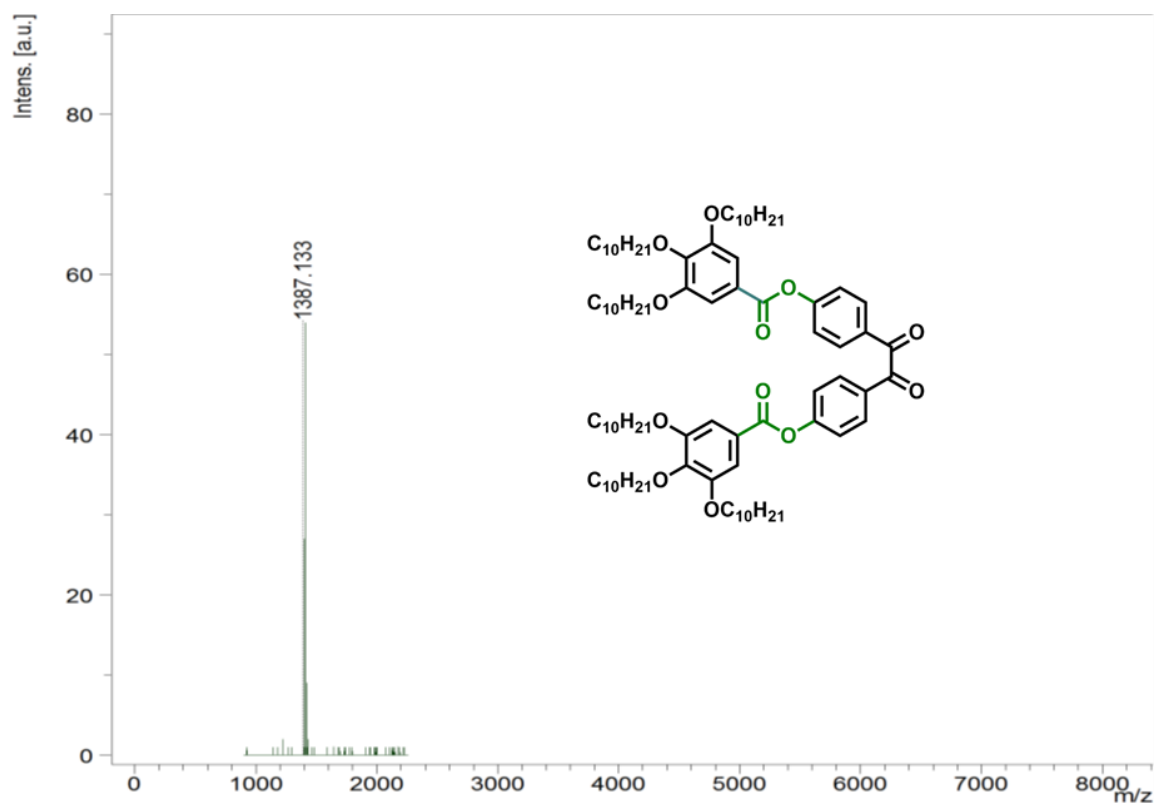


Figure S27. MALDI-TOF mass spectrum of compound **8**.

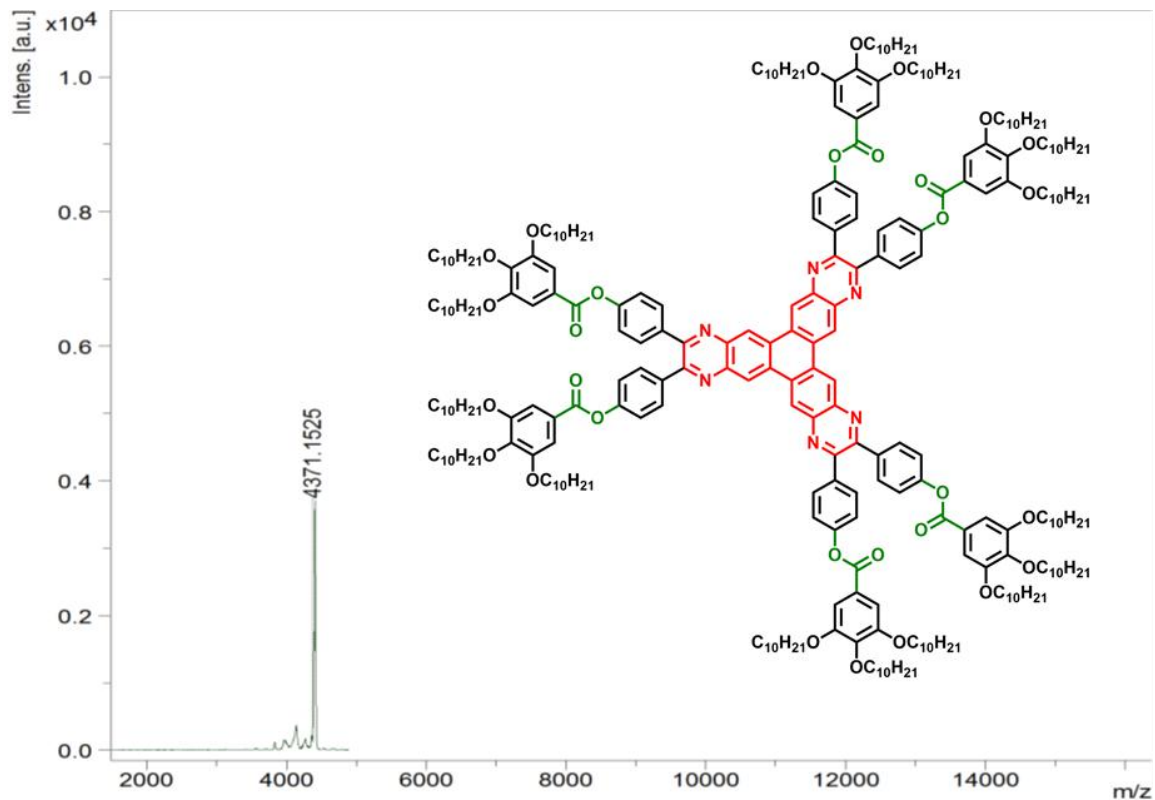


Figure S28. MALDI-TOF mass spectrum of compound **BQE**.

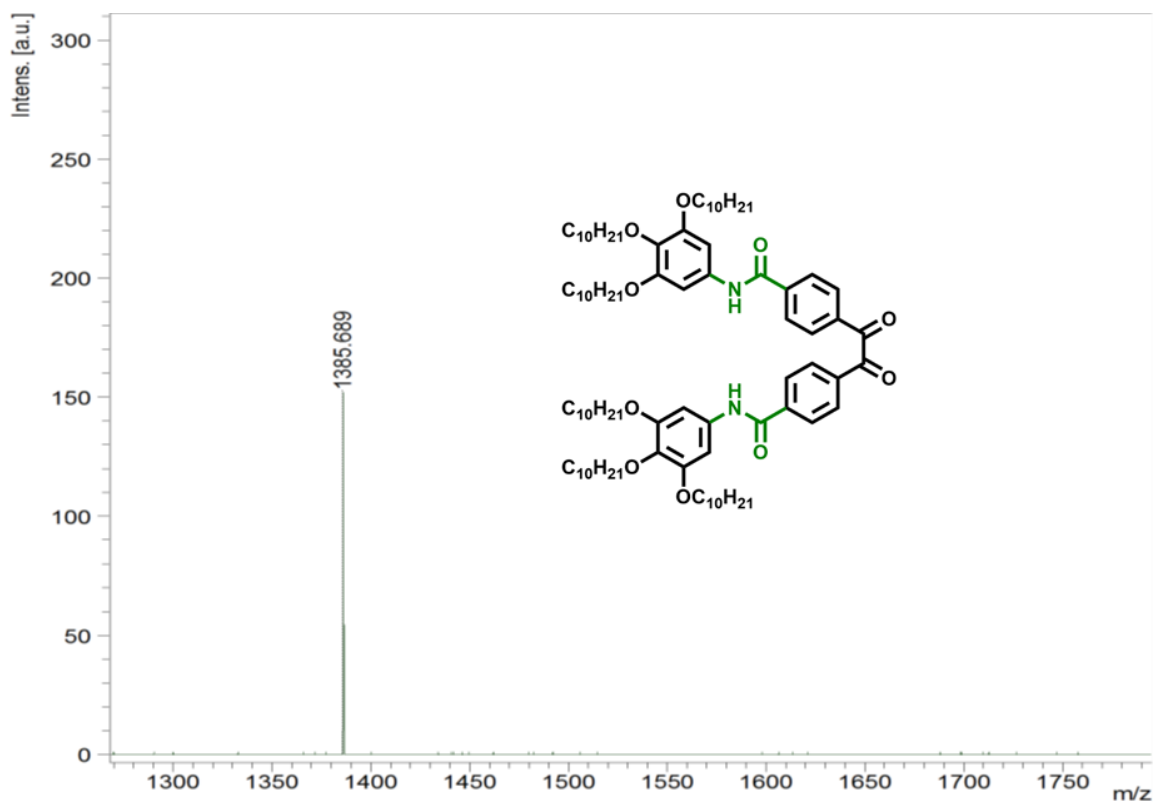


Figure S29. MALDI-TOF mass spectrum of compound 18.

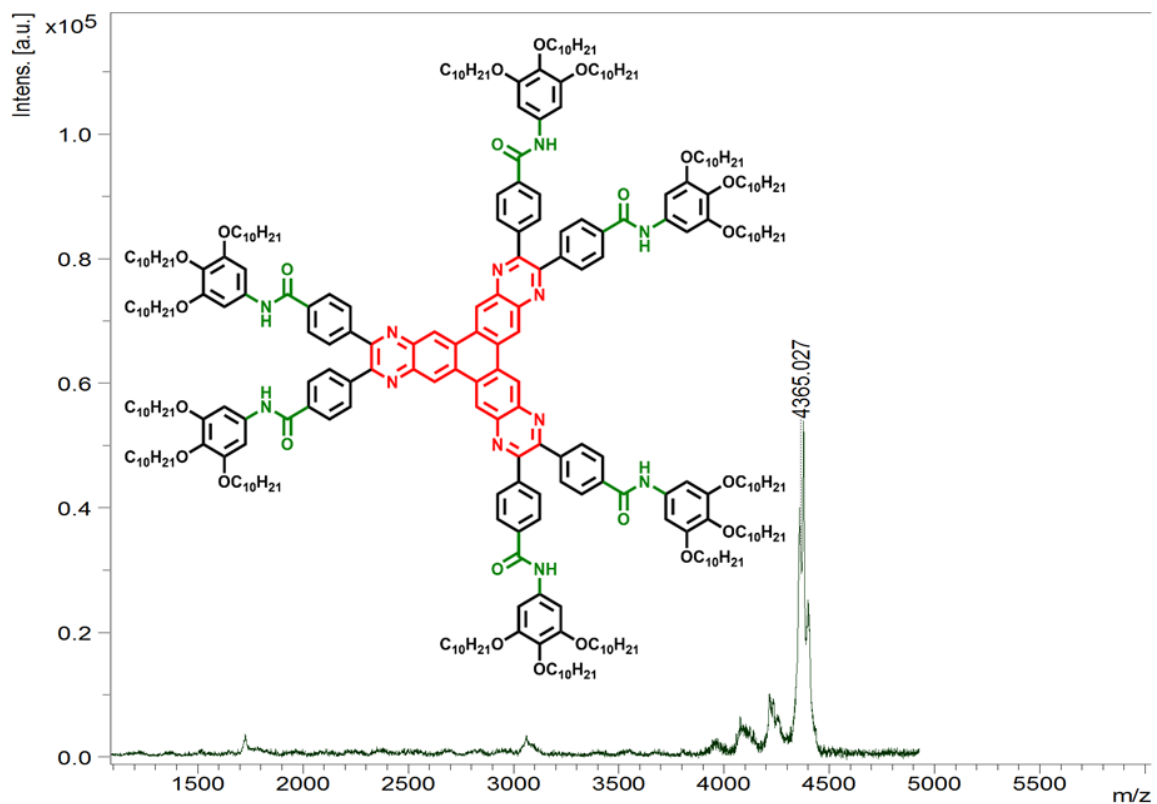


Figure S30. MALDI-TOF mass spectrum of compound BQA.

5. IR Spectra

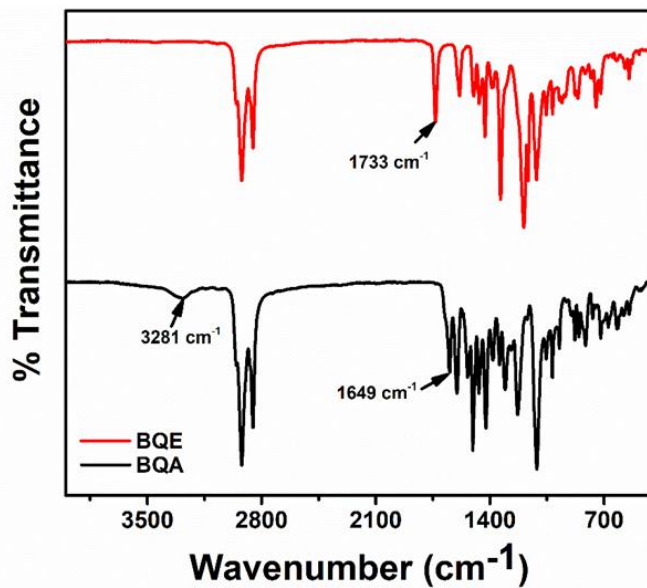


Figure S31. Stacked IR spectra of compound BQE and BQA.

6. Thermogravimetric Analysis

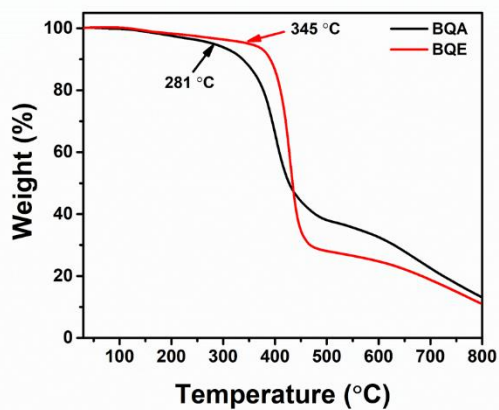


Figure S32. TGA plots (heating rate of 10 °C min⁻¹, nitrogen atmosphere) showing the temperatures at which 5 wt% decomposition occurs

7. Polarized Optical Microscopy

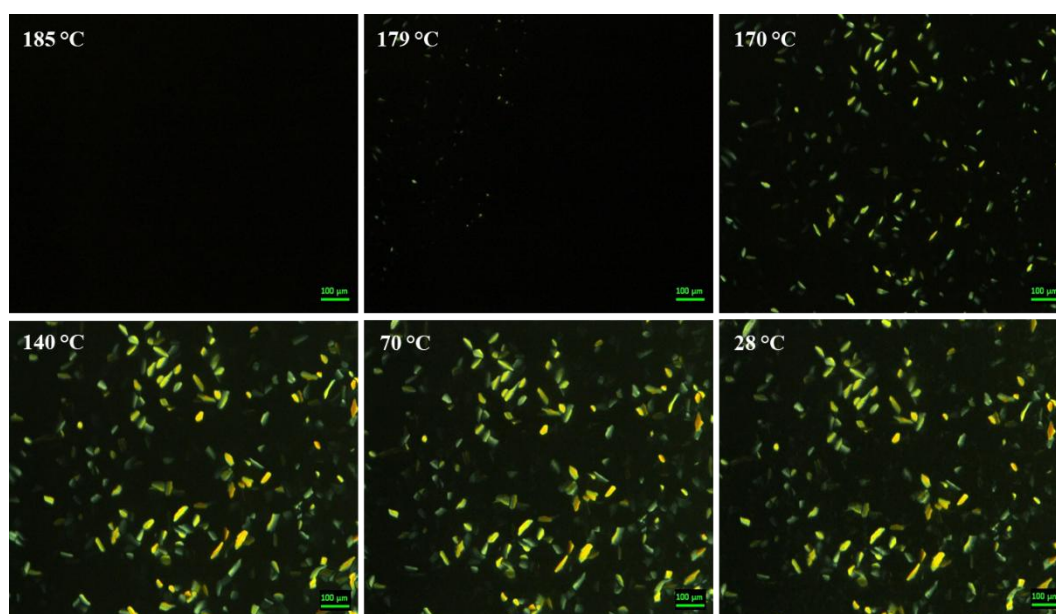


Figure S33. POM images of compound **BQE** on cooling the isotropic melt at a rate of $5\text{ }^{\circ}\text{C min}^{-1}$.

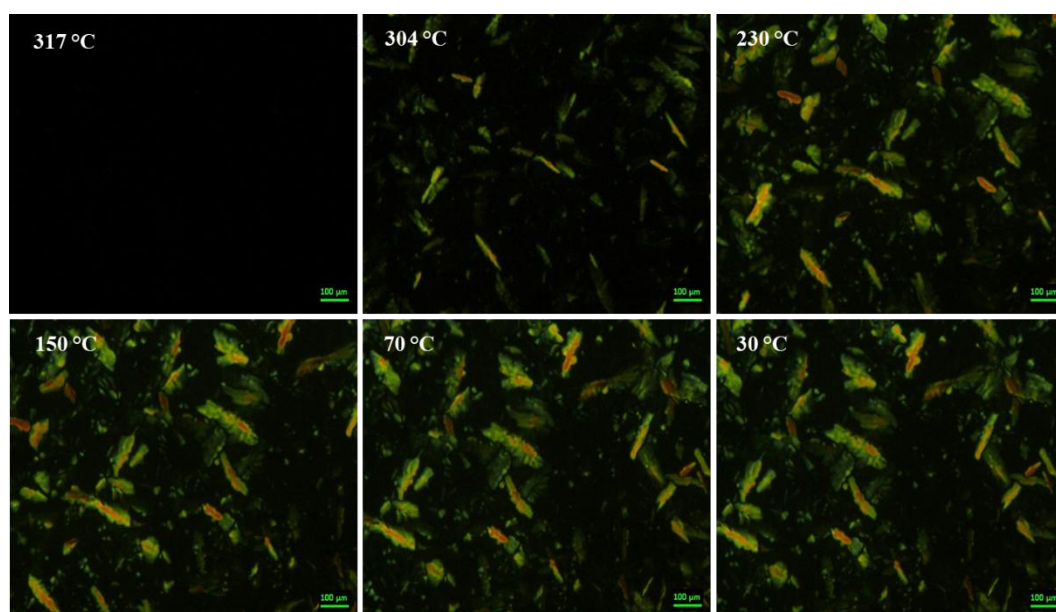


Figure S34. POM images of compound **BQA** on cooling the isotropic melt at a rate of $5\text{ }^{\circ}\text{C min}^{-1}$.

8. Differential scanning calorimetry

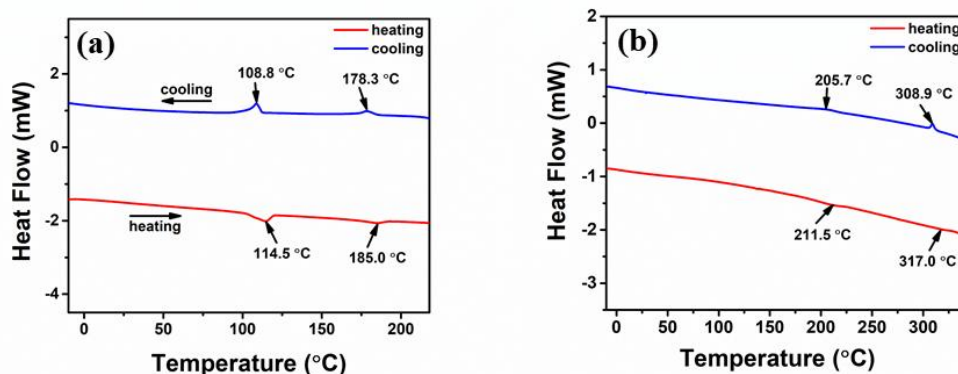


Figure S35. DSC thermograms obtained for **BQE** (a) and **BQA** (b) for the first cooling (blue trace) and second heating (red trace) taken at 5 °C/min.

Table S2. Phase-Transition Temperatures^a (°C) and Corresponding Enthalpies (kJ/mol) of compounds and decomposition temperatures obtained for **BQE** and **BQA**.

| Compounds | Phase Sequence (kJ/mol) ^a | | T ₅ ^b (°C) |
|------------|--|--|----------------------------------|
| | Second heating | First Cooling | |
| BQE | Col _{r1} 114.5 (13.99) Col _{r2} 185.0 (3.79) I | I 178.3 (4.86) Col _{r2} 108.8 (12.64) Col _{r1} | 345 |
| BQA | Col _h 317.0 (0.76) I | I 308.9 (3.43) Col _h | 281 |

^aPeak temperatures in the DSC thermograms obtained during the second heating and first cooling cycles at 5 °C/min. Col_h = Columnar hexagonal phase; Col_r = Columnar rectangular phase; I = Isotropic phase.
^bTemperature at which 5 wt% decomposition was observed in TGA.

9. X-ray diffraction studies

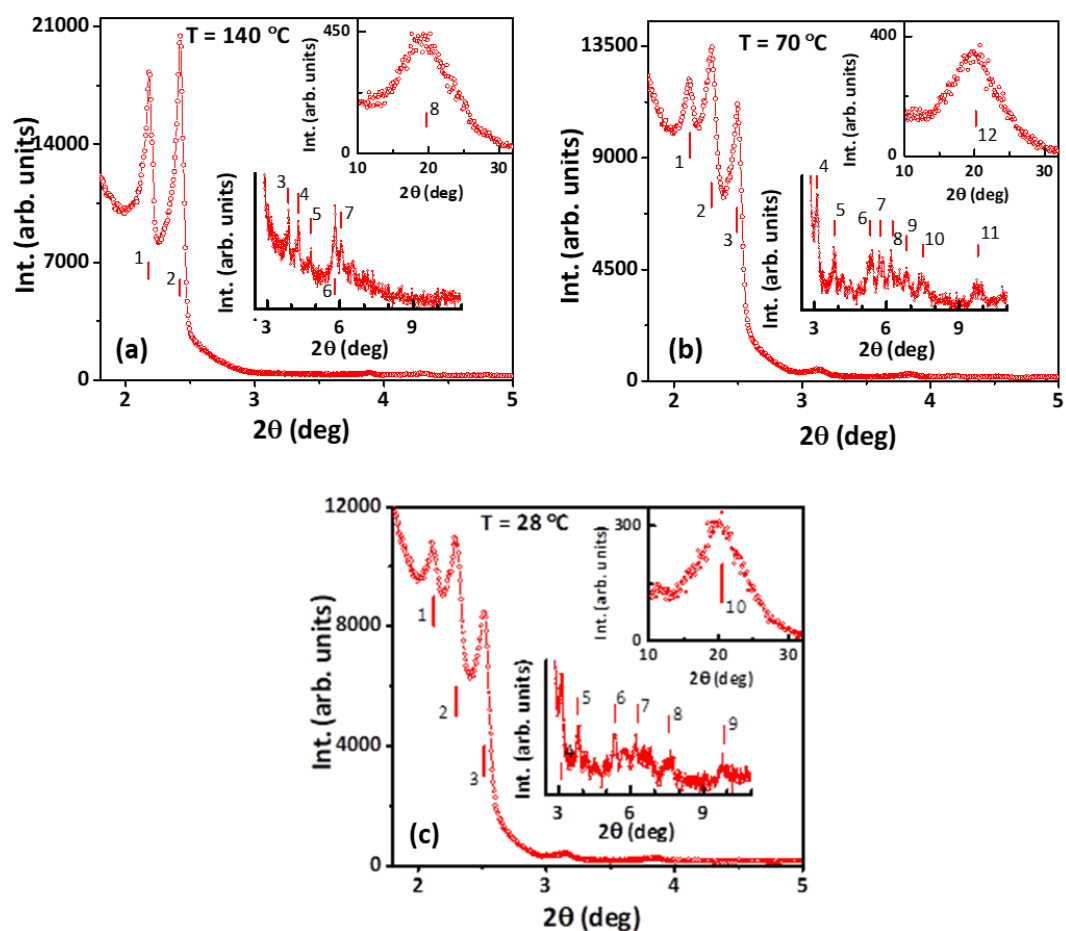


Figure S36. Plot of the intensity against 2θ obtained from the powder XRD pattern of the Col_r phases for compound **BQE** at $140\text{ }^{\circ}\text{C}$ (a), $70\text{ }^{\circ}\text{C}$ (b) and $28\text{ }^{\circ}\text{C}$ (c).

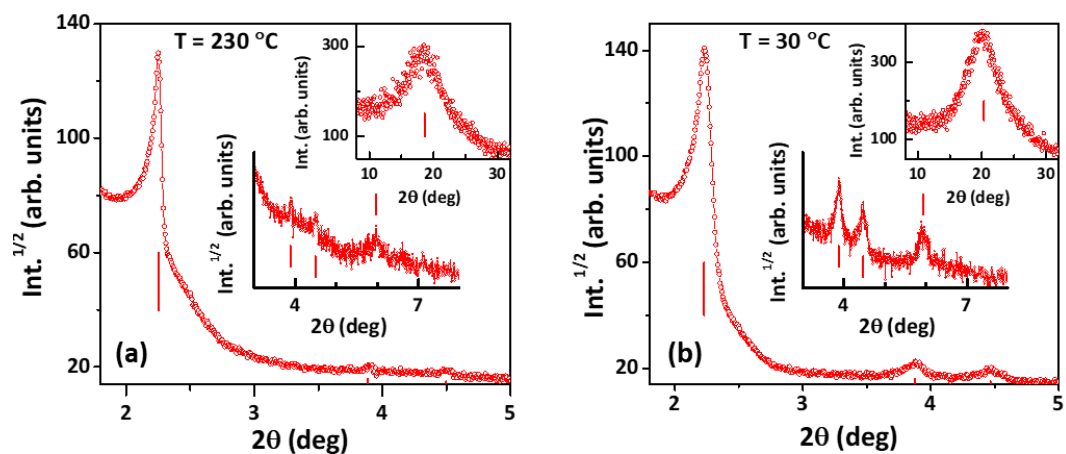


Figure S37. Plot of the intensity against 2θ obtained from the powder XRD pattern of the Col_h phases for compound **BQA** at $230\text{ }^{\circ}\text{C}$ (a) and $30\text{ }^{\circ}\text{C}$ (b).

Calculation procedure for parameters from XRD:

The number of molecules per unit cell, Z is calculated using the formula below.

$$Z = \frac{\rho N_A V_{\text{unit cell}}}{M} \text{----- S(1)}$$

ρ = density of the liquid crystal phase (usually taken as 1 for organic molecules)

N_A = Avogadro's constant

$V_{\text{unit cell}}$ = Volume of the unit cell

M = Molecular weight

The volumes were estimated by using the following equations.

$$V = S \times h_c \text{----- S(2)}$$

S = Lattice area; h_c = thickness of a columnar slice

The lattice area is calculated using the following equations

$$S = a^2 \times \sin 60^\circ; 'a' \text{ is hexagonal lattice parameter}$$

$$S = a \times b; 'a' \text{ and 'b' are rectangular lattice parameters}$$

Table S3. Results of (*hkl*) Indexation of XRD Profiles of **BQE** and **BQA** at a Given Temperature (*T*) of the Mesophase^a

| Compound (<i>D</i> /Å) | Phase (<i>T</i> /°C) | <i>d</i> _{obs} (Å) | <i>d</i> _{cal} (Å) | Miller index hk | lattice spacing (Å), lattice area <i>S</i> (Å ²), molecular volume <i>V</i> (Å ³) |
|--|-------------------------------|------------------------------|-----------------------------|--------------------|---|
| BQE (41.56 Å) MW: 4374.47 | Col _{r2} (140 °C) | 40.6 | 40.6 | 10 | <i>a</i> = 40.6 |
| | | 36.5 | 36.5 | 01 | <i>b</i> = 36.5 |
| | | 22.8 | 20.3 | 20 | <i>c</i> = 4.5 |
| | | 20.6 | 20.3 | 20 | <i>S</i> = 1481.9 |
| | | 18.5 | 18.3 | 02 | <i>V</i> = 6668.7 |
| | | 15.3 | 16.6 | 12 | <i>Z</i> ≈ 1 |
| | | 14.6 | 13.6 | 22 | |
| | | 4.5 (<i>h_c</i>) | | | |
| | Col _{r1} (70 °C) | 41.6 | 41.6 | 10 | <i>a</i> = 41.6 |
| | | 38.6 | 38.6 | 01 | <i>b</i> = 38.6 |
| | | 35.4 | 38.6 | 01 | <i>c</i> = 4.4 |
| | | 28.3 | 28.3 | 11 | <i>S</i> = 1604.1 |
| | | 23.1 | 20.8 | 20 | <i>V</i> = 7058.2 |
| | | 15.4 | 14.1 | 22 | <i>Z</i> ≈ 1 |
| | | 14.2 | 14.1 | 22 | |
| | | 12.9 | 12.9 | 03 | |
| | | 11.8 | 11.3 | 32 | |
| | | 9.0 | 9.2 | 42 | |
| | 4.4 (<i>h_c</i>) | | | | |
| | Col _{r1} (28 °C) | 41.7 | 41.7 | 10 | <i>a</i> = 41.7 |
| | | 38.5 | 38.5 | 01 | <i>b</i> = 38.5 |
| | | 35.1 | 38.5 | 01 | <i>c</i> = 4.3 |
| | | 28.1 | 28.3 | 11 | <i>S</i> = 1602.7 |
| | | 23.1 | 20.8 | 20 | <i>V</i> = 6923.6 |
| 16.5 | | 17.5 | 12 | <i>Z</i> ≈ 1 | |
| 14.1 | | 14.1 | 22 | | |
| 11.6 | | | 32 | | |
| 9.0 | | 9.2 | 42 | | |
| 4.3 (<i>h_c</i>) | | | | | |
| BQA (56.75 Å) MW: 4368.57 | Col _h (230 °C) | 39.2 | 39.2 | 10 | <i>a</i> = 45.3 |
| | | 22.7 | 22.6 | 11 | <i>c</i> = 4.8 |
| | | 19.7 | 19.6 | 20 | <i>S</i> = 1773.9 |
| | | 14.8 | 14.8 | 21 | <i>V</i> = 8451.8 |
| | | 4.8 (<i>h_c</i>) | | | <i>Z</i> ≈ 1 |
| | Col _h (30 °C) | 39.6 | 39.6 | 10 | <i>a</i> = 45.8 |
| | | 22.8 | 22.9 | 11 | <i>c</i> = 4.4 |
| | | 19.8 | 19.8 | 20 | <i>S</i> = 1814.5 |
| | | 14.9 | 15.0 | 21 | <i>V</i> = 7946.3 |
| | | 4.4 (<i>h_c</i>) | | | <i>Z</i> ≈ 1 |

^aThe diameter (D) of the disk (estimated from Chem 3D Pro 8.0 molecular model software from Cambridge Soft). d_{obs} : spacing observed; d_{cal} : spacing calculated (deduced from the lattice parameters; a for the Col_h phase). The spacing marked h_c corresponds to diffuse reflection in the wide-angle region. Z indicates the number of molecules per columnar slice of thickness h_c , estimated from the lattice area S and the volume V .

10. Photophysical studies

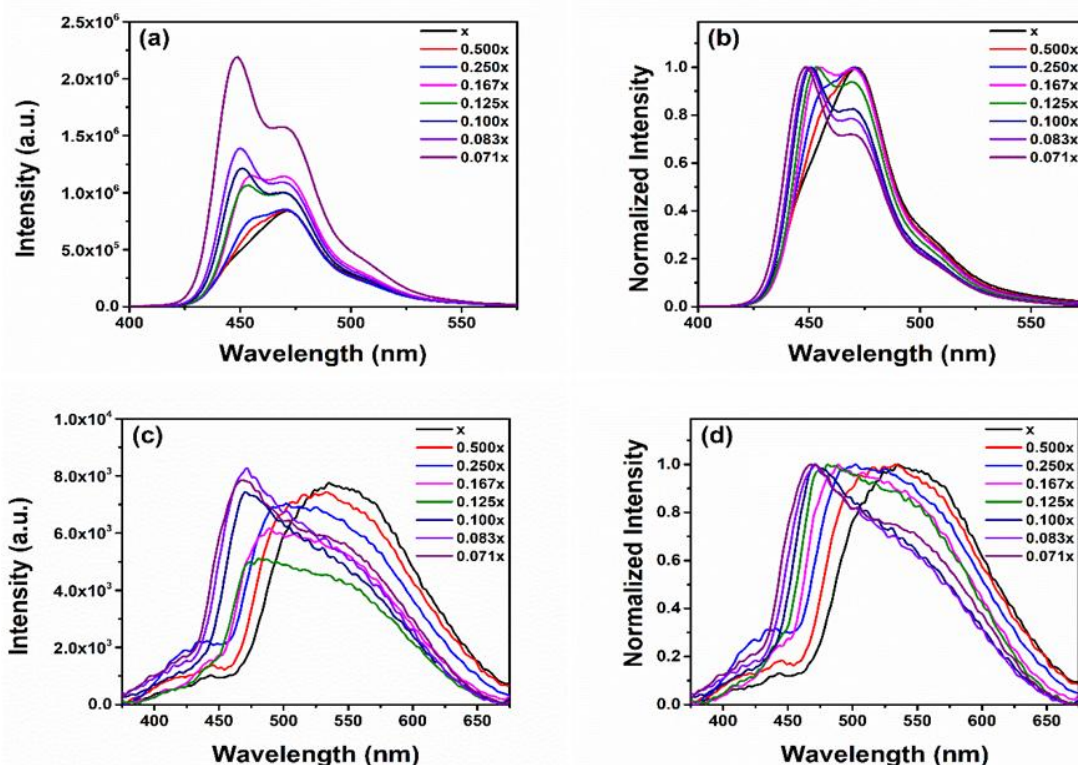


Figure S38. Concentration dependent emission spectra (a) and normalized emission spectra (b) of **BQE**; concentration dependent emission spectra (c) and normalized emission spectra (d) of **BQA** in on dilution from 2000 micromolar chloroform solutions [$x = 2000 \mu\text{M}$].

Table S4. Photophysical properties of compounds in chloroform solution^a and thin film^b states

| Entry | Solution state | | | | | | Solid State | | | |
|------------|--------------------|----------------------------|----------------------------------|----------------------------|--|----------------------------------|--------------------|----------------------------|----------------------------------|-----------------------------|
| | Absorption (nm) | Emission ^c (nm) | Stokes Shift (cm ⁻¹) | Absolute Quantum Yield (%) | Molar Extinction Coefficient (L mol ⁻¹ cm ⁻¹) | $\Delta E_{\text{g,opt}}^d$ (eV) | Absorption (nm) | Emission ^e (nm) | Stokes Shift (cm ⁻¹) | Absolute Quantum Yield* (%) |
| BQE | 290, 347, 408, 440 | 445, 469 | 12011 | 55.12 | 162906, 152767, 83901, 110323 | 2.77 | 279, 344, 414, 440 | 485 | 15229 | 2.05 |
| BQA | 295, 348, 408, 432 | 468 | 7368 | 0.38 | 123277, 185650, 98319, 120282 | 2.77 | 303, 339, 415, 440 | 573 | 12042 | 0.37 |

^aMicromolar solution in CHCl₃. ^bPrepared by drop casting of millimolar solution in toluene. ^cExcitation wavelength $\lambda_{\text{ex}} = 290$ and 348 nm for **BQE** and **BQA**. ^dCalculated from the red edge of the absorption band. ^eExcited at the respective absorption maxima of the thin film; 279 and 339 nm for **BQE** and **BQA**. *solid sample (not thin film)

11. Electrochemical properties

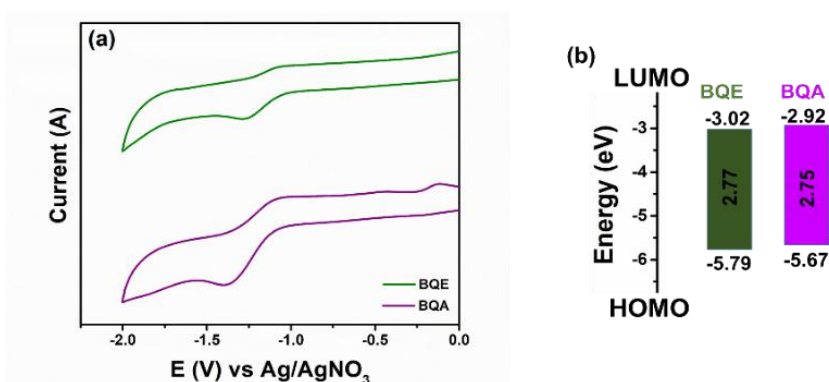


Figure S39. Cyclic voltammograms of **BQE** and **BQA** (a); Compared energy band level diagram showing HOMO and LUMO energy levels of **BQE** and **BQA** (b).

Table S5. Electrochemical^{a,b} data and data obtained from DFT^h calculations for the derivatives.

| Entry | Electrochemical data | | | | Data from DFT calculations | | |
|------------|------------------------------|---------------------------|---------------------------|-----------------------------------|----------------------------|---------------------------|-------------------------------|
| | $E_{\text{red,onset}}^{[c]}$ | $E_{\text{LUMO}}^{[d,e]}$ | $E_{\text{HOMO}}^{[d,f]}$ | $\Delta E_{\text{g,opt}}^{[d,g]}$ | $E_{\text{LUMO}}^{[d,h]}$ | $E_{\text{HOMO}}^{[d,h]}$ | $\Delta E_{\text{g}}^{[d,h]}$ |
| BQE | -1.26 | -3.04 | -5.81 | 2.77 | -2.56 | -5.81 | 3.25 |
| BQA | -1.35 | -2.95 | -5.70 | 2.75 | -2.89 | -5.55 | 2.67 |

^[a]0.5 mM dichloromethane solutions; ^[b]experimental conditions: Ag/AgNO₃ as reference electrode, glassy carbon working electrode, platinum wire counter electrode, TBAP (0.1M) as a supporting electrolyte, room temperature; ^[c]in volts (V); ^[d]in eV; ^[e]estimated from the formula by using $E_{\text{LUMO}} = -(4.8 - E_{1/2, \text{Fc}/\text{Fc}^+} + E_{\text{red,onset}})$ eV; ^[f]estimated from the formula $E_{\text{HOMO}} = (E_{\text{LUMO}} - E_{\text{g,opt}})$ eV; ^[g]calculated from the red edge of the absorption band of each compound. $E_{1/2, \text{Fc}/\text{Fc}^+} = 0.50$ V. ^[h]Obtained from DFT calculations by employing the combination of Becke3-Lee-Yang-Parr (B3LYP) hybrid functional and 6-31G(d,p) basis set using the Gaussian 09 package.

12. DFT studies

DFT calculations were performed using the B3LYP hybrid functional, which combines Becke's three-parameter exchange with the Lee-Yang-Parr correlation functional, and the 6-31G(d,p) basis set, and executed with Gaussian 09.¹⁴

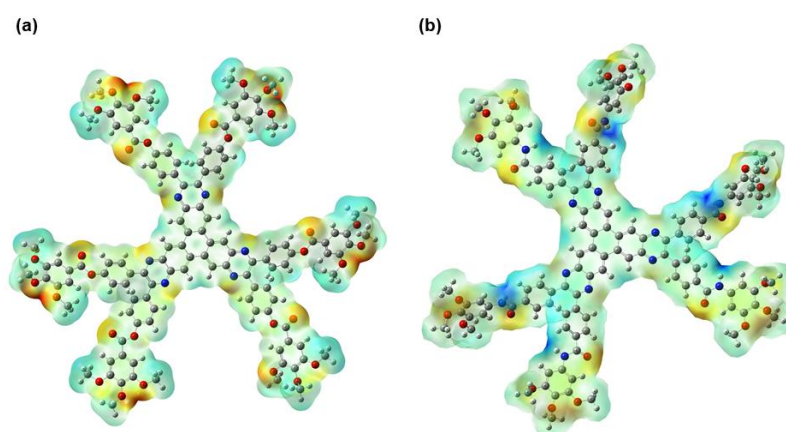


Figure S40. 3D molecular electrostatic potential contour map of optimized structure of **BQE** (a) and **BQA** (b) (In the mapped electrostatic potential surface, the red and blue colors refer to the electron-rich and electron-poor regions, respectively, whereas the green color signifies the zero electrostatic potential; chain length is limited to methoxy for clarity).

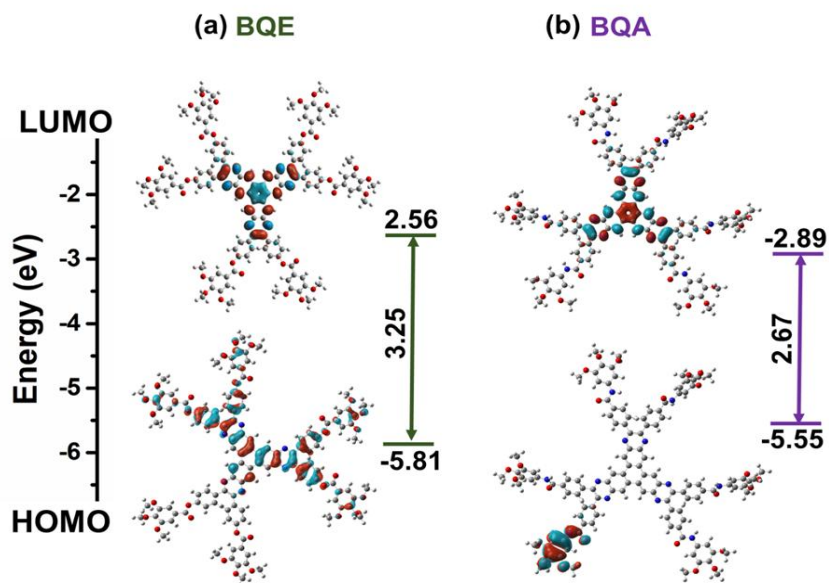


Figure S41. Frontier molecular orbitals of **BQE** (a) and **BQA** (b). DFT calculations at the B3LYP/6-31G(d,p) level. (Chain length is limited to methoxy for clarity).

DFT calculations for BQE (Chain length limited to methyl)

| Center No. | Atomic No. | Atomic Type | Coordinates (Angstroms) | | |
|------------|------------|-------------|-------------------------|-----------|-----------|
| | | | X | Y | Z |
| 1 | 6 | 0 | -13.423324 | 8.652049 | -2.117622 |
| 2 | 6 | 0 | -12.550388 | 9.653687 | -2.592310 |
| 3 | 6 | 0 | -11.168216 | 9.501003 | -2.483228 |
| 4 | 6 | 0 | -10.642806 | 8.334075 | -1.906424 |
| 5 | 6 | 0 | -11.494422 | 7.322626 | -1.435933 |
| 6 | 6 | 0 | -12.878452 | 7.484780 | -1.539150 |
| 7 | 8 | 0 | -14.794009 | 8.720680 | -2.272245 |
| 8 | 8 | 0 | -13.800161 | 6.553569 | -1.092495 |
| 9 | 8 | 0 | -13.161419 | 10.761933 | -3.166950 |
| 10 | 6 | 0 | -15.517770 | 9.841489 | -1.656555 |
| 11 | 6 | 0 | -13.310086 | 5.305306 | -0.535413 |
| 12 | 6 | 0 | -12.320582 | 11.791161 | -3.757275 |
| 13 | 6 | 0 | -9.174223 | 8.227374 | -1.823492 |
| 14 | 8 | 0 | -8.376818 | 9.084231 | -2.228310 |
| 15 | 8 | 0 | -8.777182 | 7.034304 | -1.227348 |
| 16 | 6 | 0 | -7.447124 | 6.616101 | -0.999754 |
| 17 | 6 | 0 | -6.300181 | 7.231981 | -1.514574 |
| 18 | 6 | 0 | -5.050706 | 6.684340 | -1.207374 |
| 19 | 6 | 0 | -4.925546 | 5.536439 | -0.404435 |
| 20 | 6 | 0 | -6.101006 | 4.925715 | 0.077261 |
| 21 | 6 | 0 | -7.351225 | 5.465063 | -0.208019 |
| 22 | 6 | 0 | -3.614189 | 4.894158 | -0.133690 |
| 23 | 6 | 0 | -2.365399 | 5.618395 | 0.070035 |
| 24 | 7 | 0 | -1.203337 | 4.961686 | 0.078736 |
| 25 | 6 | 0 | -1.204162 | 3.592055 | -0.008555 |
| 26 | 6 | 0 | -2.434124 | 2.879262 | -0.045934 |

| | | | | | |
|----|---|---|-----------|-----------|-----------|
| 27 | 7 | 0 | -3.622629 | 3.559317 | -0.137027 |
| 28 | 6 | 0 | -2.274087 | 7.076170 | 0.337333 |
| 29 | 6 | 0 | -1.171597 | 7.798950 | -0.152198 |
| 30 | 6 | 0 | -1.004065 | 9.159752 | 0.117845 |
| 31 | 6 | 0 | -1.956825 | 9.804099 | 0.916992 |
| 32 | 6 | 0 | -3.050878 | 9.102693 | 1.437809 |
| 33 | 6 | 0 | -3.209527 | 7.750590 | 1.147769 |
| 34 | 8 | 0 | -1.938154 | 11.167074 | 1.287443 |
| 35 | 6 | 0 | -0.983663 | 12.110675 | 0.922821 |
| 36 | 6 | 0 | -1.284436 | 13.438635 | 1.490522 |
| 37 | 8 | 0 | -0.005900 | 11.851117 | 0.208219 |
| 38 | 6 | 0 | -0.388628 | 14.478257 | 1.195568 |
| 39 | 6 | 0 | -0.625459 | 15.756199 | 1.701868 |
| 40 | 6 | 0 | -1.749331 | 16.009283 | 2.516208 |
| 41 | 6 | 0 | -2.639709 | 14.952118 | 2.804550 |
| 42 | 6 | 0 | -2.412484 | 13.672182 | 2.291951 |
| 43 | 8 | 0 | -2.068100 | 17.271941 | 2.977166 |
| 44 | 6 | 0 | -1.109208 | 17.964931 | 3.848545 |
| 45 | 8 | 0 | 0.192221 | 16.851032 | 1.447238 |
| 46 | 6 | 0 | 1.320306 | 16.680622 | 0.545673 |
| 47 | 8 | 0 | -3.713060 | 15.279428 | 3.615426 |
| 48 | 6 | 0 | -4.696030 | 14.252485 | 3.911467 |
| 49 | 6 | 0 | 0.005810 | 2.876749 | -0.007278 |
| 50 | 6 | 0 | 0.031361 | 1.482592 | -0.018696 |
| 51 | 6 | 0 | -1.219107 | 0.758274 | -0.020812 |
| 52 | 6 | 0 | -2.415565 | 1.473966 | -0.039512 |
| 53 | 6 | 0 | 1.310948 | 0.745960 | -0.017302 |
| 54 | 6 | 0 | 1.312586 | -0.698991 | 0.003339 |
| 55 | 6 | 0 | 0.035047 | -1.439029 | -0.003008 |
| 56 | 6 | 0 | -1.217311 | -0.718135 | -0.010334 |
| 57 | 6 | 0 | 0.013317 | -2.833233 | -0.012783 |
| 58 | 6 | 0 | -1.194516 | -3.551950 | -0.018999 |
| 59 | 6 | 0 | -2.426739 | -2.842540 | 0.008351 |
| 60 | 6 | 0 | -2.411921 | -1.437172 | 0.000299 |
| 61 | 7 | 0 | -1.189073 | -4.921778 | -0.103663 |
| 62 | 7 | 0 | -3.614012 | -3.525785 | 0.092087 |
| 63 | 6 | 0 | 2.529312 | 1.423779 | -0.041181 |
| 64 | 6 | 0 | 3.755485 | 0.736709 | -0.030817 |
| 65 | 6 | 0 | 3.756784 | -0.684039 | 0.031303 |
| 66 | 6 | 0 | 2.532291 | -1.373899 | 0.034362 |
| 67 | 7 | 0 | 4.939414 | 1.423500 | -0.130933 |
| 68 | 7 | 0 | 4.941674 | -1.368168 | 0.137502 |
| 69 | 6 | 0 | 14.794143 | 6.427464 | -2.627122 |
| 70 | 6 | 0 | 13.969630 | 7.317586 | -1.907360 |
| 71 | 6 | 0 | 12.731247 | 6.901120 | -1.419024 |
| 72 | 6 | 0 | 12.308349 | 5.580599 | -1.637536 |
| 73 | 6 | 0 | 13.117460 | 4.677943 | -2.344567 |
| 74 | 6 | 0 | 14.353305 | 5.103015 | -2.839282 |
| 75 | 8 | 0 | 16.059843 | 6.769518 | -3.062500 |
| 76 | 8 | 0 | 15.215785 | 4.294608 | -3.559692 |
| 77 | 8 | 0 | 14.481301 | 8.596891 | -1.723624 |
| 78 | 6 | 0 | 16.198847 | 7.880252 | -4.014300 |

| | | | | | |
|-----|---|---|-----------|------------|-----------|
| 79 | 6 | 0 | 14.849424 | 2.905382 | -3.771004 |
| 80 | 6 | 0 | 13.721847 | 9.539461 | -0.917942 |
| 81 | 6 | 0 | 10.992256 | 5.197262 | -1.092462 |
| 82 | 8 | 0 | 10.244206 | 5.949430 | -0.453158 |
| 83 | 8 | 0 | 10.680928 | 3.873199 | -1.382980 |
| 84 | 6 | 0 | 9.506622 | 3.184279 | -1.006781 |
| 85 | 6 | 0 | 8.468913 | 3.703266 | -0.222279 |
| 86 | 6 | 0 | 7.375804 | 2.881459 | 0.064834 |
| 87 | 6 | 0 | 7.305692 | 1.553862 | -0.393682 |
| 88 | 6 | 0 | 8.360388 | 1.064976 | -1.190795 |
| 89 | 6 | 0 | 9.450711 | 1.874134 | -1.497204 |
| 90 | 6 | 0 | 6.090937 | 0.748797 | -0.109282 |
| 91 | 6 | 0 | 6.091600 | -0.690477 | 0.123647 |
| 92 | 6 | 0 | 7.304942 | -1.495480 | 0.415502 |
| 93 | 6 | 0 | 8.358332 | -1.008371 | 1.210179 |
| 94 | 6 | 0 | 9.458754 | -1.806315 | 1.537868 |
| 95 | 6 | 0 | 9.503822 | -3.118592 | 1.052870 |
| 96 | 6 | 0 | 8.462673 | -3.632411 | 0.270401 |
| 97 | 6 | 0 | 7.368691 | -2.829172 | -0.035870 |
| 98 | 8 | 0 | 10.530331 | -4.053393 | 1.314479 |
| 99 | 6 | 0 | 11.785314 | -3.764856 | 1.843076 |
| 100 | 6 | 0 | 12.606100 | -4.980459 | 1.995619 |
| 101 | 8 | 0 | 12.149770 | -2.619847 | 2.142584 |
| 102 | 6 | 0 | 13.904719 | -4.816695 | 2.502788 |
| 103 | 6 | 0 | 14.726831 | -5.931848 | 2.664639 |
| 104 | 6 | 0 | 14.259956 | -7.222065 | 2.336087 |
| 105 | 6 | 0 | 12.949832 | -7.369715 | 1.830405 |
| 106 | 6 | 0 | 12.126182 | -6.254614 | 1.655286 |
| 107 | 8 | 0 | 15.059518 | -8.346060 | 2.406037 |
| 108 | 6 | 0 | 15.623328 | -8.729713 | 3.707704 |
| 109 | 8 | 0 | 16.032094 | -5.866408 | 3.137596 |
| 110 | 6 | 0 | 16.604426 | -4.559723 | 3.419897 |
| 111 | 8 | 0 | 12.563868 | -8.667382 | 1.541750 |
| 112 | 6 | 0 | 11.242272 | -8.889103 | 0.982282 |
| 113 | 6 | 0 | -1.697087 | -15.979278 | -2.509496 |
| 114 | 6 | 0 | -0.561236 | -15.714065 | -1.715871 |
| 115 | 6 | 0 | -0.324217 | -14.431643 | -1.221101 |
| 116 | 6 | 0 | -1.231877 | -13.399621 | -1.506524 |
| 117 | 6 | 0 | -2.371885 | -13.645301 | -2.287201 |
| 118 | 6 | 0 | -2.599279 | -14.929615 | -2.788636 |
| 119 | 8 | 0 | -2.015584 | -17.246499 | -2.957502 |
| 120 | 8 | 0 | -3.683935 | -15.268691 | -3.579186 |
| 121 | 8 | 0 | 0.267698 | -16.802142 | -1.468766 |
| 122 | 6 | 0 | -1.066964 | -17.939883 | -3.839825 |
| 123 | 6 | 0 | -4.678495 | -14.249983 | -3.865005 |
| 124 | 6 | 0 | 1.408857 | -16.619816 | -0.586299 |
| 125 | 6 | 0 | -0.930622 | -12.066402 | -0.951652 |
| 126 | 8 | 0 | 0.058626 | -11.795450 | -0.257121 |
| 127 | 8 | 0 | -1.899200 | -11.132266 | -1.302749 |
| 128 | 6 | 0 | -1.922645 | -9.767724 | -0.937890 |
| 129 | 6 | 0 | -0.977560 | -9.119169 | -0.133097 |
| 130 | 6 | 0 | -1.151141 | -7.758425 | 0.133448 |

| | | | | | |
|-----|---|---|------------|------------|-----------|
| 131 | 6 | 0 | -2.252243 | -7.039737 | -0.365092 |
| 132 | 6 | 0 | -3.180111 | -7.718461 | -1.180587 |
| 133 | 6 | 0 | -3.015304 | -9.070604 | -1.467239 |
| 134 | 6 | 0 | -2.349406 | -5.581561 | -0.101562 |
| 135 | 6 | 0 | -3.601624 | -4.860584 | 0.091652 |
| 136 | 6 | 0 | -4.912416 | -5.506927 | 0.355023 |
| 137 | 6 | 0 | -5.038183 | -6.649986 | 1.164574 |
| 138 | 6 | 0 | -6.287348 | -7.201637 | 1.466211 |
| 139 | 6 | 0 | -7.432734 | -6.594050 | 0.938098 |
| 140 | 6 | 0 | -7.336828 | -5.448307 | 0.138633 |
| 141 | 6 | 0 | -6.086933 | -4.904964 | -0.140120 |
| 142 | 8 | 0 | -8.762547 | -7.027626 | 1.137581 |
| 143 | 6 | 0 | -9.171290 | -8.130736 | 1.873799 |
| 144 | 6 | 0 | -10.640265 | -8.275063 | 1.870977 |
| 145 | 8 | 0 | -8.388382 | -8.893619 | 2.456994 |
| 146 | 6 | 0 | -11.483729 | -7.393330 | 1.185197 |
| 147 | 6 | 0 | -12.867642 | -7.581289 | 1.229728 |
| 148 | 6 | 0 | -13.421757 | -8.647733 | 1.962301 |
| 149 | 6 | 0 | -12.557127 | -9.551385 | 2.623884 |
| 150 | 6 | 0 | -11.178257 | -9.360927 | 2.586496 |
| 151 | 8 | 0 | -14.800061 | -8.806589 | 1.947912 |
| 152 | 6 | 0 | -15.516145 | -8.842017 | 3.233054 |
| 153 | 8 | 0 | -13.663789 | -6.632098 | 0.593317 |
| 154 | 6 | 0 | -14.582284 | -7.096004 | -0.456248 |
| 155 | 8 | 0 | -13.175973 | -10.602379 | 3.291102 |
| 156 | 6 | 0 | -12.340389 | -11.595240 | 3.948915 |
| 157 | 1 | 0 | -10.479141 | 10.253734 | -2.840966 |
| 158 | 1 | 0 | -11.064245 | 6.437152 | -0.993069 |
| 159 | 1 | 0 | -16.569139 | 9.626197 | -1.844880 |
| 160 | 1 | 0 | -15.330098 | 9.864547 | -0.577494 |
| 161 | 1 | 0 | -15.227399 | 10.787314 | -2.115032 |
| 162 | 1 | 0 | -14.206435 | 4.739254 | -0.285777 |
| 163 | 1 | 0 | -12.712372 | 4.750442 | -1.267840 |
| 164 | 1 | 0 | -12.716097 | 5.477474 | 0.370137 |
| 165 | 1 | 0 | -13.015935 | 12.520175 | -4.170988 |
| 166 | 1 | 0 | -11.686667 | 12.268317 | -3.001410 |
| 167 | 1 | 0 | -11.695219 | 11.377452 | -4.555890 |
| 168 | 1 | 0 | -6.379558 | 8.113348 | -2.130931 |
| 169 | 1 | 0 | -4.165893 | 7.157995 | -1.615410 |
| 170 | 1 | 0 | -6.016414 | 4.021541 | 0.667720 |
| 171 | 1 | 0 | -8.259417 | 5.008440 | 0.166892 |
| 172 | 1 | 0 | -0.432195 | 7.278080 | -0.748738 |
| 173 | 1 | 0 | -0.160104 | 9.703584 | -0.275712 |
| 174 | 1 | 0 | -3.760079 | 9.627467 | 2.066381 |
| 175 | 1 | 0 | -4.055376 | 7.216626 | 1.563474 |
| 176 | 1 | 0 | 0.465057 | 14.259682 | 0.568819 |
| 177 | 1 | 0 | -3.082717 | 12.853875 | 2.507172 |
| 178 | 1 | 0 | -1.617183 | 18.883507 | 4.140843 |
| 179 | 1 | 0 | -0.898241 | 17.357823 | 4.735682 |
| 180 | 1 | 0 | -0.187545 | 18.186477 | 3.309345 |
| 181 | 1 | 0 | 1.775955 | 17.667301 | 0.474659 |
| 182 | 1 | 0 | 2.045173 | 15.963534 | 0.947218 |

| | | | | | |
|-----|---|---|-----------|------------|-----------|
| 183 | 1 | 0 | 0.985985 | 16.352214 | -0.444503 |
| 184 | 1 | 0 | -5.440481 | 14.748520 | 4.532750 |
| 185 | 1 | 0 | -5.167112 | 13.877012 | 2.995633 |
| 186 | 1 | 0 | -4.248364 | 13.417892 | 4.464190 |
| 187 | 1 | 0 | 0.910212 | 3.468694 | 0.022422 |
| 188 | 1 | 0 | -3.378981 | 0.983761 | -0.066498 |
| 189 | 1 | 0 | 0.919529 | -3.422711 | -0.034967 |
| 190 | 1 | 0 | -3.376844 | -0.949607 | 0.019924 |
| 191 | 1 | 0 | 2.586957 | 2.502608 | -0.086516 |
| 192 | 1 | 0 | 2.591984 | -2.452603 | 0.079992 |
| 193 | 1 | 0 | 12.082279 | 7.564121 | -0.863476 |
| 194 | 1 | 0 | 12.766139 | 3.669536 | -2.502293 |
| 195 | 1 | 0 | 17.259551 | 7.898432 | -4.262963 |
| 196 | 1 | 0 | 15.608694 | 7.681127 | -4.915501 |
| 197 | 1 | 0 | 15.891972 | 8.821487 | -3.556841 |
| 198 | 1 | 0 | 15.681314 | 2.478481 | -4.329513 |
| 199 | 1 | 0 | 14.730954 | 2.375984 | -2.818487 |
| 200 | 1 | 0 | 13.926624 | 2.819970 | -4.357152 |
| 201 | 1 | 0 | 14.332871 | 10.440525 | -0.887360 |
| 202 | 1 | 0 | 12.751708 | 9.762537 | -1.376166 |
| 203 | 1 | 0 | 13.571094 | 9.156601 | 0.097332 |
| 204 | 1 | 0 | 8.512627 | 4.716384 | 0.144634 |
| 205 | 1 | 0 | 6.552577 | 3.273060 | 0.650341 |
| 206 | 1 | 0 | 8.324473 | 0.055969 | -1.583180 |
| 207 | 1 | 0 | 10.262339 | 1.509573 | -2.115094 |
| 208 | 1 | 0 | 8.322202 | 0.003762 | 1.594868 |
| 209 | 1 | 0 | 10.260702 | -1.416370 | 2.144519 |
| 210 | 1 | 0 | 8.525279 | -4.655339 | -0.081132 |
| 211 | 1 | 0 | 6.545914 | -3.223686 | -0.619562 |
| 212 | 1 | 0 | 14.239417 | -3.818138 | 2.748286 |
| 213 | 1 | 0 | 11.121167 | -6.352916 | 1.273791 |
| 214 | 1 | 0 | 16.130604 | -9.675457 | 3.519449 |
| 215 | 1 | 0 | 16.327416 | -7.975653 | 4.060990 |
| 216 | 1 | 0 | 14.820257 | -8.877002 | 4.438064 |
| 217 | 1 | 0 | 17.627184 | -4.762044 | 3.734805 |
| 218 | 1 | 0 | 16.608133 | -3.930146 | 2.523409 |
| 219 | 1 | 0 | 16.060100 | -4.053016 | 4.224752 |
| 220 | 1 | 0 | 11.180820 | -9.965461 | 0.827822 |
| 221 | 1 | 0 | 10.455652 | -8.568181 | 1.675480 |
| 222 | 1 | 0 | 11.123493 | -8.369323 | 0.024444 |
| 223 | 1 | 0 | 0.538530 | -14.203986 | -0.610192 |
| 224 | 1 | 0 | -3.051223 | -12.832741 | -2.495541 |
| 225 | 1 | 0 | -1.574645 | -18.862917 | -4.118194 |
| 226 | 1 | 0 | -0.873581 | -17.337244 | -4.733976 |
| 227 | 1 | 0 | -0.135618 | -18.153129 | -3.314119 |
| 228 | 1 | 0 | -5.429755 | -14.754617 | -4.470947 |
| 229 | 1 | 0 | -5.136907 | -13.872152 | -2.943732 |
| 230 | 1 | 0 | -4.245528 | -13.415840 | -4.429968 |
| 231 | 1 | 0 | 1.871603 | -17.603303 | -0.516976 |
| 232 | 1 | 0 | 2.122911 | -15.900731 | -1.003397 |
| 233 | 1 | 0 | 1.088317 | -16.287736 | 0.407214 |
| 234 | 1 | 0 | -0.134062 | -9.659583 | 0.266120 |

| | | | | | |
|-----|---|---|------------|------------|-----------|
| 235 | 1 | 0 | -0.417677 | -7.234145 | 0.734331 |
| 236 | 1 | 0 | -4.024725 | -7.187758 | -1.602908 |
| 237 | 1 | 0 | -3.718523 | -9.598545 | -2.099893 |
| 238 | 1 | 0 | -4.154212 | -7.116238 | 1.582984 |
| 239 | 1 | 0 | -6.369091 | -8.073594 | 2.095465 |
| 240 | 1 | 0 | -8.244754 | -4.999638 | -0.246256 |
| 241 | 1 | 0 | -6.002225 | -4.004330 | -0.735952 |
| 242 | 1 | 0 | -11.087847 | -6.554850 | 0.630603 |
| 243 | 1 | 0 | -10.495343 | -10.031514 | 3.090251 |
| 244 | 1 | 0 | -16.571184 | -8.857410 | 2.961082 |
| 245 | 1 | 0 | -15.246036 | -9.735507 | 3.795334 |
| 246 | 1 | 0 | -15.291717 | -7.940190 | 3.812209 |
| 247 | 1 | 0 | -15.079561 | -6.193204 | -0.810710 |
| 248 | 1 | 0 | -14.017284 | -7.555709 | -1.275467 |
| 249 | 1 | 0 | -15.305676 | -7.803978 | -0.050613 |
| 250 | 1 | 0 | -13.038480 | -12.319083 | 4.366970 |
| 251 | 1 | 0 | -11.677573 | -12.088629 | 3.229793 |
| 252 | 1 | 0 | -11.745363 | -11.144196 | 4.750848 |

DFT calculations for BQA (Chain length limited to methyl)

| Center No. | Atomic No. | Atomic Type | Coordinates (Angstroms) | | |
|---------------|---------------|----------------|-------------------------|-----------|-----------|
| | | | X | Y | Z |
| 1 | 6 | 0 | 1.359645 | 3.112237 | 0.175628 |
| 2 | 6 | 0 | -0.012324 | 3.483442 | 0.147045 |
| 3 | 6 | 0 | -0.990482 | 2.480526 | 0.032474 |
| 4 | 6 | 0 | -0.653337 | 1.135600 | -0.077154 |
| 5 | 6 | 0 | 0.738976 | 0.762231 | -0.079335 |
| 6 | 6 | 0 | 1.703941 | 1.754940 | 0.054448 |
| 7 | 7 | 0 | 2.327296 | 4.049884 | 0.367924 |
| 8 | 6 | 0 | 1.963487 | 5.314824 | 0.477706 |
| 9 | 6 | 0 | 0.570756 | 5.706464 | 0.306837 |
| 10 | 7 | 0 | -0.376851 | 4.793954 | 0.190165 |
| 11 | 6 | 0 | 3.055934 | 6.262307 | 0.833601 |
| 12 | 6 | 0 | 0.111348 | 7.118576 | 0.198787 |
| 13 | 6 | 0 | -1.114425 | 7.490019 | 0.776158 |
| 14 | 6 | 0 | -1.597738 | 8.785304 | 0.643467 |
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| 16 | 6 | 0 | 0.331003 | 9.370114 | -0.683280 |
| 17 | 6 | 0 | 0.820134 | 8.074075 | -0.545319 |
| 18 | 6 | 0 | 2.878323 | 7.281855 | 1.783781 |
| 19 | 6 | 0 | 3.940085 | 8.099969 | 2.150636 |
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| 57 | 6 | 0 | 8.650694 | -4.639226 | -1.485591 |
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| 62 | 6 | 0 | 4.207082 | -9.246350 | -0.101114 |
| 63 | 6 | 0 | 5.032589 | -8.320589 | 0.552517 |
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| 90 | 6 | 0 | 3.699899 | -15.922789 | 0.428255 |
| 91 | 8 | 0 | 7.748180 | -16.284816 | 1.101484 |
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| 95 | 6 | 0 | -1.695739 | 0.096108 | -0.180725 |
| 96 | 6 | 0 | -1.322042 | -1.294100 | -0.257390 |
| 97 | 6 | 0 | 0.103687 | -1.674534 | -0.280599 |
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| 99 | 6 | 0 | 0.488472 | -3.007456 | -0.379724 |
| 100 | 6 | 0 | 1.841084 | -3.387606 | -0.421931 |
| 101 | 6 | 0 | 2.844469 | -2.381180 | -0.387658 |
| 102 | 6 | 0 | 2.459091 | -1.034309 | -0.274398 |
| 103 | 6 | 0 | -3.044806 | 0.433970 | -0.200796 |
| 104 | 6 | 0 | -4.052653 | -0.542653 | -0.278122 |
| 105 | 6 | 0 | -3.684968 | -1.915285 | -0.315928 |
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| 118 | 6 | 0 | -7.504308 | -5.940555 | -0.596218 |
| 119 | 6 | 0 | -8.640696 | -5.812151 | 0.213927 |
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| 122 | 6 | 0 | -8.532319 | -1.292370 | -1.564884 |
| 123 | 6 | 0 | -9.797490 | -0.779292 | -1.824211 |
| 124 | 6 | 0 | -10.246975 | 0.379505 | -1.177569 |
| 125 | 6 | 0 | -9.376984 | 1.041971 | -0.298962 |
| 126 | 6 | 0 | -8.102301 | 0.541149 | -0.054087 |
| 127 | 6 | 0 | -9.521436 | -7.023640 | 0.361848 |
| 128 | 6 | 0 | -11.634857 | 0.856497 | -1.512659 |
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| 131 | 6 | 0 | -11.888977 | -7.652951 | 0.938661 |

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| 135 | 6 | 0 | -13.139381 | -7.098137 | 1.228090 |
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| 138 | 6 | 0 | -12.822305 | -9.868395 | 1.156582 |
| 139 | 6 | 0 | -11.721334 | -9.045207 | 0.906957 |
| 140 | 6 | 0 | -13.843802 | 3.024025 | 0.552681 |
| 141 | 6 | 0 | -15.085852 | 3.658885 | 0.609536 |
| 142 | 6 | 0 | -15.979387 | 3.569954 | -0.465434 |
| 143 | 6 | 0 | -15.599749 | 2.831701 | -1.605722 |
| 144 | 6 | 0 | -14.362698 | 2.185084 | -1.668083 |
| 145 | 8 | 0 | -15.169250 | -10.135882 | 1.700707 |
| 146 | 6 | 0 | -15.769197 | -10.725724 | 0.542669 |
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| 149 | 8 | 0 | -15.456208 | -7.335445 | 1.676341 |
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| 152 | 6 | 0 | -16.203265 | 2.071368 | -3.788654 |
| 153 | 8 | 0 | -17.188935 | 4.223699 | -0.417266 |
| 154 | 6 | 0 | -18.309955 | 3.378110 | -0.139086 |
| 155 | 8 | 0 | -15.416740 | 4.316770 | 1.768642 |
| 156 | 6 | 0 | -15.611101 | 5.731219 | 1.651243 |
| 157 | 1 | 0 | -2.019087 | 2.816675 | 0.027273 |
| 158 | 1 | 0 | 2.760942 | 1.525744 | 0.090971 |
| 159 | 1 | 0 | -1.681599 | 6.745243 | 1.323380 |
| 160 | 1 | 0 | -2.544220 | 9.077259 | 1.084775 |
| 161 | 1 | 0 | 0.879334 | 10.069192 | -1.308425 |
| 162 | 1 | 0 | 1.745640 | 7.799475 | -1.039241 |
| 163 | 1 | 0 | 1.909965 | 7.423914 | 2.250789 |
| 164 | 1 | 0 | 3.816236 | 8.871459 | 2.902389 |
| 165 | 1 | 0 | 6.368536 | 6.715435 | 0.205109 |
| 166 | 1 | 0 | 4.486012 | 5.259541 | -0.417056 |
| 167 | 1 | 0 | 7.216104 | 8.592856 | 0.228791 |
| 168 | 1 | 0 | 0.406062 | 11.873837 | -0.378522 |
| 169 | 1 | 0 | 9.165561 | 9.269226 | -0.741735 |
| 170 | 1 | 0 | 8.106886 | 10.519928 | 3.240362 |
| 171 | 1 | 0 | 1.326536 | 13.925034 | -0.768964 |
| 172 | 1 | 0 | -2.937086 | 13.421083 | -0.437643 |
| 173 | 1 | 0 | 13.952658 | 12.115320 | 2.122385 |
| 174 | 1 | 0 | 12.813006 | 11.325461 | 3.245664 |
| 175 | 1 | 0 | 13.383036 | 10.456364 | 1.785432 |
| 176 | 1 | 0 | 12.335881 | 11.467175 | -2.355894 |
| 177 | 1 | 0 | 10.725601 | 12.115592 | -1.943707 |
| 178 | 1 | 0 | 12.124864 | 12.455298 | -0.880168 |
| 179 | 1 | 0 | 10.008067 | 12.688919 | 5.409830 |
| 180 | 1 | 0 | 8.537695 | 12.471273 | 4.421716 |
| 181 | 1 | 0 | 9.366404 | 11.049180 | 5.113775 |
| 182 | 1 | 0 | -1.600690 | 19.432133 | -0.246921 |
| 183 | 1 | 0 | -2.476847 | 18.075518 | 0.512288 |

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| 187 | 1 | 0 | 0.663130 | 17.874307 | -2.463995 |
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| 189 | 1 | 0 | -4.715554 | 14.560655 | -1.415100 |
| 190 | 1 | 0 | -4.629438 | 14.783709 | 0.354232 |
| 191 | 1 | 0 | 5.579807 | -5.827002 | -2.345478 |
| 192 | 1 | 0 | 7.985272 | -6.125659 | -2.873452 |
| 193 | 1 | 0 | 8.977069 | -3.005332 | -0.095384 |
| 194 | 1 | 0 | 6.589306 | -2.686756 | 0.403620 |
| 195 | 1 | 0 | 2.079782 | -7.042130 | -1.595517 |
| 196 | 1 | 0 | 2.482098 | -9.494248 | -1.344180 |
| 197 | 1 | 0 | 5.825258 | -8.655590 | 1.215552 |
| 198 | 1 | 0 | 5.457322 | -6.255123 | 0.936959 |
| 199 | 1 | 0 | 10.645337 | -4.216194 | -0.036077 |
| 200 | 1 | 0 | 6.360799 | -10.453010 | 0.294927 |
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| 212 | 1 | 0 | 15.311763 | -5.567543 | 2.378249 |
| 213 | 1 | 0 | 16.751890 | -5.154401 | 1.398516 |
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| 215 | 1 | 0 | 3.215038 | -15.329464 | 1.212476 |
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| 218 | 1 | 0 | 6.968042 | -17.272909 | -0.567825 |
| 219 | 1 | 0 | 8.601666 | -16.568660 | -0.786378 |
| 220 | 1 | 0 | 10.934744 | -14.502097 | 2.288034 |
| 221 | 1 | 0 | 9.507943 | -13.868406 | 3.151750 |
| 222 | 1 | 0 | 9.488343 | -15.533568 | 2.495100 |
| 223 | 1 | 0 | -0.234040 | -3.812033 | -0.420752 |
| 224 | 1 | 0 | 3.261305 | -0.308115 | -0.259120 |
| 225 | 1 | 0 | -3.379158 | 1.462776 | -0.171098 |
| 226 | 1 | 0 | -2.097526 | -3.317020 | -0.351639 |
| 227 | 1 | 0 | -5.755690 | -4.974564 | -1.396331 |
| 228 | 1 | 0 | -7.317081 | -6.896805 | -1.071982 |
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| 232 | 1 | 0 | -10.459465 | -1.259978 | -2.535811 |
| 233 | 1 | 0 | -9.666370 | 1.978399 | 0.170004 |
| 234 | 1 | 0 | -7.421172 | 1.071557 | 0.601937 |
| 235 | 1 | 0 | -11.091367 | -5.780277 | 0.708902 |

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|-----|---|---|------------|------------|-----------|
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| 239 | 1 | 0 | -13.180693 | 3.116313 | 1.407478 |
| 240 | 1 | 0 | -14.064449 | 1.605991 | -2.527022 |
| 241 | 1 | 0 | -16.613375 | -11.317596 | 0.902791 |
| 242 | 1 | 0 | -16.133154 | -9.953891 | -0.146040 |
| 243 | 1 | 0 | -15.061442 | -11.380424 | 0.024133 |
| 244 | 1 | 0 | -11.697040 | -12.921822 | 0.917399 |
| 245 | 1 | 0 | -11.134369 | -11.582314 | -0.120698 |
| 246 | 1 | 0 | -10.765341 | -11.574516 | 1.626115 |
| 247 | 1 | 0 | -16.984337 | -6.996937 | 2.962858 |
| 248 | 1 | 0 | -16.236577 | -8.611669 | 3.142612 |
| 249 | 1 | 0 | -15.394985 | -7.156357 | 3.757680 |
| 250 | 1 | 0 | -17.066573 | 2.179913 | -4.446474 |
| 251 | 1 | 0 | -15.315834 | 2.485444 | -4.281692 |
| 252 | 1 | 0 | -16.033519 | 1.007789 | -3.582067 |
| 253 | 1 | 0 | -19.185459 | 4.030160 | -0.109159 |
| 254 | 1 | 0 | -18.441657 | 2.628943 | -0.926341 |
| 255 | 1 | 0 | -18.193553 | 2.880119 | 0.830952 |
| 256 | 1 | 0 | -15.842240 | 6.087262 | 2.657280 |
| 257 | 1 | 0 | -14.694406 | 6.220592 | 1.297823 |
| 258 | 1 | 0 | -16.436551 | 5.965389 | 0.974824 |

13. Charge carrier mobility study

The determination of hole and electron mobilities has been carried out by using space charge limited current (SCLC) technique. The hole-only and electron-only SCLC devices consisting of BQE and BQA compounds were prepared by spin-coating. The architecture of the hole-only and electron-only SCLC devices was ITO/PEDOT:PSS/BQE (or BQA)/Au and ITO/ZnO/BQE (or BQA)/LiF/Ag, respectively (see Fig. S39).¹⁵⁻¹⁷ The active layer thickness for the BQE compound was kept around 5 μm , while for the BQA compound this thickness was around 0.5 μm due to its higher viscosity. The BQE and BQA compounds were spin-coated at two steps: First 700 rpm for 5 sec followed by a second step of 4000 rpm for 30 sec. During SCLC measurements, the devices were held on the Linkam LTS 350 hotplate connected with the Linkam TMS 94 to maintain the temperature with an accuracy of ± 0.1 $^{\circ}\text{C}$. The current density-voltage (J/V) curves were recorded using Keysight B2902A Precision Source/Measure Unit (SMU). Assuming the negligible trap contribution, the Mott–Gurney equation, shown below, was used to extract the hole and electron mobility:

$$J = \frac{9}{8} \varepsilon_0 \varepsilon \mu_{(h,e)} \frac{V^2}{d^3} \quad (1)$$

Where, J is the current density, ε_0 is the permittivity of free space, ε is the dielectric constant of the BQE/BQA compounds, $\mu_{(h,e)}$ is the hole or electron mobility, V is the voltage drop across the device, and d is the thickness of the active materials (i.e., BQE/BQA).

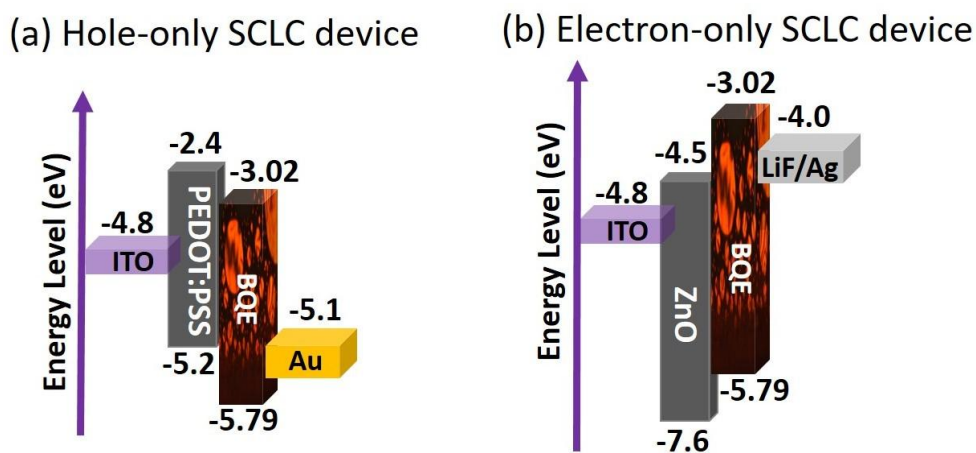


Figure S42. Energy level diagram of (a) hole-only, and (b) electron-only SCLC devices.

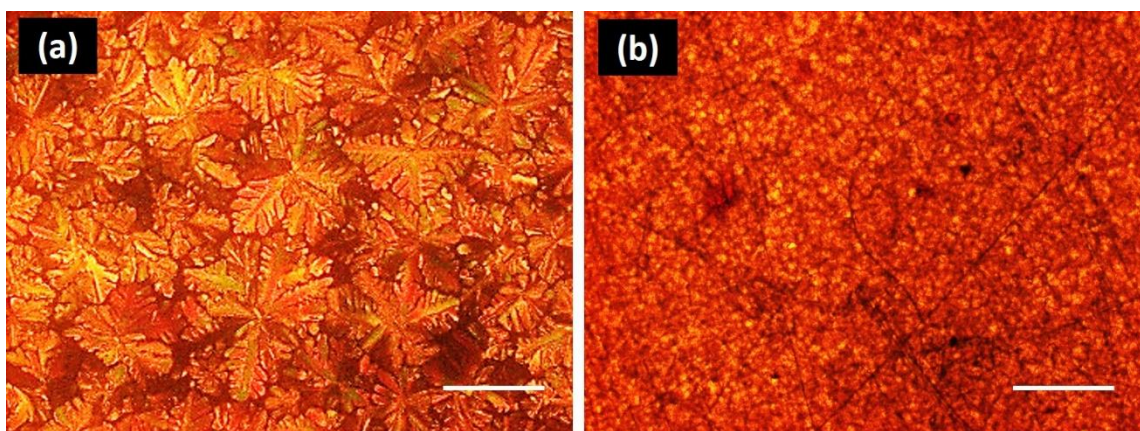


Figure S43. Polarised optical microscopic images of the molecular ordering of the (a) BQE, and (b) BQA compounds in the SCLC devices. The images were recorded in the reflection mode at 10X-optical/crossed polarisers.

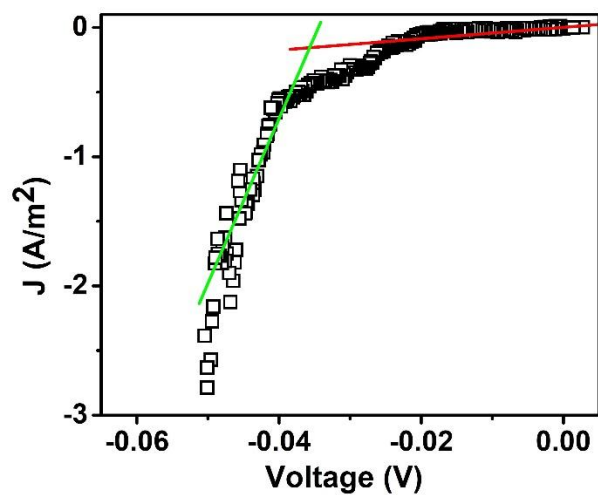


Figure S44. Current density-voltage (J-V) curve of the **BQA** compound in the electron-only SCLC device at 30 °C. The thickness and surface area of the **BQA** compound was around 0.5 μ m and 25 mm², respectively; and relative permittivity of **BQA** was 3.0.

14. References

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