Luminous Nematic Threads: Single-Component Liquid Crystal Self-Assembles into Fluorescent Fibers

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General synthetic procedure

Synthesis of 4-cyano-4′-(n-bromoalkane-1-yloky) biphenyl (2a-g)

The reaction was conducted by stirring Dibromoalkanes (1), 4-cyano-4′-hydroxybiphenyl (2), potassium carbonate, and potassium iodide (in catalytic quantities) under reflux for 10 hours in 2-butanone. Afterwards, the reaction mixture was filtered, and the residue was washed with DCM. The solvent was removed using a rotary evaporator. To isolate the pure 4-cyano-4′-(n-bromoakane-1-yloxy)biphenyl from the crude product, column chromatography with silica gel and a 5% EtOAc-hexane mixture was used.

2a: 4-Cyano-4'-(4-bromobuta-1-yloxy)biphenyl: Colourless solid; R_f = 0.82 (5% EtOAc: hexanes); yield: 90 %; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.73 (d, *J* = 12.0 Hz, 2H, Ar-H), 7.67 (d, *J* = 8.0 Hz, 2H, Ar-H), 7.56 (d, *J* = 8.0 Hz, 2H, Ar-H), 7.04 (d, *J* = 12.0 Hz, 2H, Ar-H), 4.06 (t, *J* = 4.0 Hz, 2H), 3.49 (t, *J* = 8.0 Hz, 2H,), 2.10 – 1.65 (m, 4H);

2b: 4-Cyano-4'-(5-bromopenta-1-yloxy)biphenyl: Colourless solid; R_f = 0.80 (5% EtOAc: hexanes); yield: 92.3 %; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.88-7.82 (dd, *J* = 8.0 Hz, 16.0 Hz, 4H, Ar-H), 7.71-7.69 (d, *J* = 8.0 Hz, 2H, Ar-H), 7.06-7.04 (d, *J* = 8 Hz, 2H, Ar-H), 4.07 (t, *J* = 4.0 Hz, 2H), 3.70 (t, *J* = 8.0 Hz, 2H), 1.9– 1.65 (m, 6H);

2c: 4-Cyano-4'-(6-bromohexa-1-yloxy)biphenyl: Colourless solid; R_f = 0.8 (5% EtOAc: hexanes); yield: 92 %; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.88-7.82 (dd, *J* = 8.0 Hz, 16.0 Hz, 4H, Ar-H), 7.71-7.69 (d, *J* = 8 Hz, 2H, Ar-H), 7.06-7.03 (d, *J* = 12 Hz, 2H, Ar-H), 4.03-4.0 (t, *J* = 4 Hz, 2H), 3.55-3.53 (t, *J* = 8.0 Hz, 2H), 1.84 – 1.45 (m, 8H);

2d: 4-Cyano-4'-(7-bromohepta-1-yloxy)biphenyl: Colourless solid; R_f = 0.83 (5% EtOAc: hexanes); yield: 90.7 %; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.71 (d, *J* = 12.0 Hz, 2H, Ar-H), 7.67 (d, *J* = 8.0 Hz, 2H, Ar-H), 7.57 (d, *J* = 8.0 Hz, 2H, Ar-H), 7.03 (d, *J* = 12.0 Hz, 2H, Ar-H), 4.05 (t, *J* = 4.0 Hz, 2H), 3.46 (t, *J* = 8.0 Hz, 2H), 1.95 – 1.42 (m, 10H);

2e: 4-Cyano-4'-(8-bromoocta-1-yloxy)biphenyl: Colourless solid; R_f = 0.8 (5% EtOAc: hexanes); yield: 90.9 %; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.73 (d, *J* = 12.0 Hz, 2H, Ar-H), 7.67 (d, *J* = 8.0 Hz, 2H, Ar-H), 7.56 (d, *J* = 8.0 Hz, 2H, Ar-H), 7.03 (d, *J* = 12.0 Hz, 2H, Ar-H), 4.05 (t, *J* = 4.0 Hz, 2H), 3.48 (t, *J* = 8.0 Hz, 2H), 1.94 – 1.42 (m, 12H);

2f: 4-Cyano-4'-(9-bromonona-1 yloxy)biphenyl: Colourless solid; R_f = 0.82 (5% EtOAc: hexanes); yield: 89 %; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.74 (d, *J* = 12.0 Hz, 2H, Ar-H), 7.69 (d, *J* = 8.0 Hz, 2H, Ar-H), 7.58 (d, *J* = 8.0 Hz, 2H, Ar-H), 7.05 (d, *J* = 12.0 Hz, 2H, Ar-H), 4.06 (t, *J* = 4.0 Hz, 2H), 3.45 (t, *J* = 8.0 Hz, 2H), 1.93 – 1.29 (m, 14H);

2g: 4-Cyano-4'-(10-bromodec-1-yloxy)biphenyl: Colourless solid; R_f = 0.83 (5% EtOAc: hexanes); yield: 93 %; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.73 (d, *J* = 12.0 Hz, 2H, Ar-H), 7.69 (d, *J* = 8.0 Hz, 2H, Ar-H), 7.57 (d, *J* = 8.0 Hz, 2H, Ar-H), 7.02 (d, *J* = 12.0 Hz, 2H, Ar-H), 4.07 (t, *J* = 4.0 Hz, 2H), 3.46 (t, *J* = 8.0 Hz, 2H), 1.93 – 1.29 (m, 16H);

Synthesis of di-tert-butyl (1,4-phenylenebis(methylene))dicarbamate (4)

Boc anhydride was added to a solution of 1,4-phenylenedimethanamine in double-distilled water. The reaction mixture was stirred at 50 °C for 12 hours, yielding a white precipitate. After completion, the mixture was quenched with water and extracted with dichloromethane (DCM). The organic layer was washed with brine, and the solvent was removed using a rotary evaporator. To obtain the pure product, the resulting compound was washed with hexane and filtered to obtain the pure product.

4: Di-tert-butyl (1,4-phenylenebis(methylene))dicarbamate: Colourless solid; R_f = 0.75 (10% DCM;Methanol); quantitative yield; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.25 (d, J = 8.0 Hz, 4H, Ar-H), 4.8 (brs ,2H), 4.3 (d, J= 8 Hz, 4H,) 1.55 (s,19H).

Synthesis of di-tert-butyl(1,4-phenylenebis(methylene))bis((((4'-cyano-[1,1'-biphenyl]-4-yl)oxy)methyl)carbamate) (TACDn)

Potassium tertiary butoxide was added to a stirred solution of di-tert-butyl (1,4-phenylenebis(methylene))dicarbamate in DMF at 0 °C, and the mixture was stirred at RT for 1 hour. 4-cyano-4′-(n-bromoalkane-1-yloky) biphenyl is added to the stirred solution at 0 °C, and the mixture is stirred at RT overnight, then quenched with aqueous NH_4Cl, extracted with ethyl acetate, and washed with brine. Removal of the solvent followed by column chromatography (hexane/EtOAc 15% EH) afforded the pure compound.

TACD1: Di-tert-butyl (1,4-phenylenebis(methylene))bis((4-((4'-cyano-[1,1'-biphenyl]-4-yl)oxy)butyl)carbamate): Colourless solid; R_f = 0.5 (15% EtOAc: hexanes); yield: 59%; ν_{max} in cm^{-1}(KBr) 2928 (ν_{CH}), 2221 (ν_{CN}), 1683 ($\nu_{C=O}$), 1602 ($\nu_{C=C}$), 1242 (ν_{C-O}); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69-7.67 (d, *J* = 8 Hz, 4H, Ar-H), 7.64-7.62 (d, *J* = 8 Hz, 4H, Ar-H), 7.52-7.50 (d, *J* = 8 Hz, 4H, Ar-H), 7.21 (s, 4H, Ar-H), 6.96-6.94 (d, *J* = 8 Hz, 4H, Ar-H), 4.41 (s,4H), 3.99-3.96 (d, *J* = 12 Hz, 4H), 3.22-3.19 (d, *J* = 12 Hz, 4H), 1.77-1.67 (m, 8H), 1.44 (s,18H); Elemental analysis calcd (%): C,74.79; H,7.1; N,6.3; found, C,74.65; H,7.23; N,6.45.

TACD2: Di-tert-butyl (1,4-phenylenebis(methylene))bis((5-((4'-cyano-[1,1'-biphenyl]-4-yl)oxy)pentyl)carbamate): Colourless solid; R_f = 0.52 (15% EtOAc: hexanes); yield: 60%; ν_{max} in cm^{-1}(KBr) 2926 (ν_{CH}), 2224 (ν_{CN}), 1682 ($\nu_{C=O}$), 1602 ($\nu_{C=C}$), 1244 (ν_{C-O}); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70-7.68 (d, *J* = 8 Hz, 4H, Ar-H), 7.65-7.63 (d, *J* = 8 Hz, 4H, Ar-H), 7.53-7.51 (d, *J* = 8 Hz, 4H, Ar-H), 7.22 (s, 4H, Ar-H), 6.98-6.96 (d, *J* = 8 Hz, 4H, Ar-H), 4.41 (s,4H), 3.99-3.96 (t, *J* = 12 Hz, 4H), 3.23-3.2 (t, *J* = 12 Hz, 4H), 1.83-1.76 (m, 4H), 1.46 (s,18H), 1.29-1.2 (m,8H); Elemental analysis calcd (%): C, 75.15; H, 7.24; N, 6.49; found, C,75.01; H,7.11; N,6.38.

TACD3: Di-tert-butyl (1,4-phenylenebis(methylene))bis((6-((4'-cyano-[1,1'-biphenyl]-4-yl)oxy)hexyl)carbamate): Gummy mass; R_f = 0.53 (15% EtOAc: hexanes); yield: 60%; ν_{max} in cm^{-1}(KBr) 2928 (ν_{CH}), 2224 (ν_{CN}), 1683 ($\nu_{C=O}$), 1602 ($\nu_{C=C}$), 1244 (ν_{C-O}); ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69-7.67 (d, *J* = 8 Hz, 4H, Ar-H), 7.64-7.62 (d, *J* = 8 Hz, 4H, Ar-H), 7.53-7.51 (d, *J* = 8 Hz, 4H, Ar-H), 7.27 (s, 4H, Ar-H), 6.99-6.97 (d, *J* = 8 Hz, 4H, Ar-H), 4.01-3.98 (t, *J* = 12 Hz, 4H), 3.77 (s,4H), 2.66-2.63 (t, *J* = 12 Hz, 4H), 1.84-1.77 (m, 4H), 1.59-1.54 (m,4H), 1.53 (s,18H), 1.49-1.41

(m,8H); Elemental analysis calcd (%): C, 75.48; H, 7.47; N, 6.29; found, C,75.52; H,7.83; N,6.52.

TACD4: Di-tert-butyl (1,4-phenylenebis(methylene))bis((7-((4'-cyano-[1,1'-biphenyl]-4-yl)oxy)heptyl)carbamate): Colourless solid; R_f = 0.53 (15% EtOAc: hexanes); yield: 60%; v_{max} in cm^{-1}(KBr) 2927 (v_{CH}), 2225 (v_{CN}), 1681 ($v_{C=O}$), 1602 ($v_{C=C}$), 1246 (v_{C-O}); ^1H NMR (400 MHz, $CDCl_3$) δ 7.69-7.67 (d, *J* = 8 Hz, 4H, Ar-H), 7.64-7.62 (d, *J* = 12 Hz, 4H, Ar-H), 7.52-7.50 (d, *J* = 8 Hz, 4H, Ar-H), 7.25 (s, 4H, Ar-H), 6.95-6.93 (d, *J* = 8 Hz, 4H, Ar-H), 4.42 (s, 4H), 3.98-3.95 (d, *J* = 12 Hz, 4H), 3.20-3.18 (d, *J* = 12 Hz, 4H), 1.78-1.69 (m, 8H), 1.39 (s,30H); Elemental analysis calcd (%): C, 75.79; H, 7.68; N, 6.10; found, C, 75.46; H,7.51; N,6.22.

TACD5: Di-tert-butyl (1,4-phenylenebis(methylene))bis((8-((4'-cyano-[1,1'-biphenyl]-4-yl)oxy)octyl)carbamate): Colourless solid; R_f = 0.53 (15% EtOAc: hexanes); yield: 61%; v_{max} in cm^{-1}(KBr) 2928 (v_{CH}), 2224 (v_{CN}), 1681 ($v_{C=O}$), 1603 ($v_{C=C}$), 1245 (v_{C-O}); ^1H NMR (400 MHz, $CDCl_3$) δ 7.70-7.68 (d, *J* = 8 Hz, 4H, Ar-H), 7.64-7.62 (d, *J* = 8 Hz, 4H, Ar-H), 7.53-7.51 (d, *J* = 8 Hz, 4H, Ar-H), 7.23 (s, 4H, Ar-H), 6.98-6.96 (d, *J* = 8 Hz, 4H, Ar-H), 4.0-3.97 (t, *J* = 12 Hz, 4H), 3.62 (s,4H), 2.63-2.6 (t, *J* = 12 Hz, 4H), 1.8-1.69 (m, 4H), 1.55-1.49 (m,4H), 1.43 (s,18H), 1.39-1.32 (m,16H); Elemental analysis calcd (%): C, 76.08; H, 7.87; N, 5.91; found, C,75.89; H, 7.62; N,5.6.

TACD6: Di-tert-butyl (1,4-phenylenebis(methylene))bis((9-((4'-cyano-[1,1'-biphenyl]-4-yl)oxy)nonyl)carbamate): Colourless solid; R_f = 0.54 (15% EtOAc: hexanes); yield: 60%; v_{max} in cm^{-1}(KBr) 2928 (v_{CH}), 2223 (v_{CN}), 1681 ($v_{C=O}$), 1603 ($v_{C=C}$), 1244 (v_{C-O}); ^1H NMR (400 MHz, $CDCl_3$) δ 7.70-7.68 (d, *J* = 8 Hz, 4H, Ar-H), 7.65-7.63 (d, *J* = 8 Hz, 4H, Ar-H), 7.53-7.51 (d, *J* = 8 Hz, 4H, Ar-H), 7.24 (s, 4H, Ar-H), 7.0-6.98 (d, *J* = 8 Hz, 4H, Ar-H), 4.81 (s,4H), 4.01-3.98 (t, *J* = 12 Hz, 4H), 3.17-3.14 (d, *J* = 12 Hz, 4H), 1.83-1.76 (m, 4H), 1.46 (s,18H), 1.34-1.25 (m, 28H); Elemental analysis calcd (%): C, 76.35; H, 8.06; N, 5.74; found, C,75.69; H, 7.93; N,6.0.

TACD7: Di-tert-butyl (1,4-phenylenebis(methylene))bis((10-((4'-cyano-[1,1'-biphenyl]-4-yl)oxy)decyl)carbamate): Gummy mass; R_f = 0.54 (15% EtOAc: hexanes); yield: 60%; v_{max} in cm^{-1}(KBr) 2925 (v_{CH}), 2224 (v_{CN}), 1683 ($v_{C=O}$), 1603 ($v_{C=C}$), 1245 (v_{C-O}); ^1H NMR (400 MHz, $CDCl_3$) δ 7.68-7.66 (d, *J* = 8 Hz, 4H, Ar-H), 7.63-7.61 (d, *J* = 8 Hz, 4H, Ar-H), 7.52-7.50 (d, *J* = 8 Hz, 4H, Ar-H), 7.25 (s, 4H, Ar-H), 6.99-6.97 (d, *J* = 8 Hz, 4H, Ar-H), 4.28 (s,4H), 4.0-3.97 (t, *J* = 12 Hz,

4H), 3.17-3.14 (t, J = 12, 4H), 1.82-1.75 (m, 4H), 1.44 (s,18H), 1.4-1.24 (m, 28H); Elemental analysis calcd (%): C, 76.61; H, 8.24; N, 5.58; found, C,75.82; H, 8.45; N,5.83.

Synthesis of 4',4'''-((((1,4-phenylenebis(methylene))bis(azanediyl))bis(methylene))bis(oxy))bis(([1,1'-biphenyl]-4'-carbonitrile)) (SACDn)

Deprotection of di-tert-butyl(1,4-phenylenebis(methylene))bis((((4'-cyano-[1,1'-biphenyl]-4-yl)oxy)methyl)carbamate) is performed using 4M HCl in Dioxane with DCM as a solvent at RT. The reaction mixture was stirred for 4h during which a white precipitate is formed. The crude reaction mass is concentrated, and basified the residue with the aqueous sodium carbonate solution. The product was extracted with DCM and the organic layer was washed with brine. After concentrating the organic layer we recrystallize the compound to obtained pure product.

SACD1:4',4'''-((((1,4-phenylenebis(methylene))bis(azanediyl))bis(butane-4,1-diyl))bis(oxy))bis(([1,1'-biphenyl]-4'-carbonitrile)): Colourless solid; R_f = 0.5 (10% Methanol: DCM); yield: 62%; v_{max} in cm^{-1}(KBr) 3385 (v_{N-H}), 2930 (v_{CH}), 2224 (v_{CN}), 1602 ($v_{C=C}$), 1246 (v_{C-O}); ^1H NMR (400 MHz, $CDCl_3$) δ 7.70-7.68 (d, J = 8 Hz, 4H, Ar-H), 7.65-7.63 (d, J = 8 Hz, 4H, Ar-H), 7.53-7.51 (d, J = 8 Hz, 4H, Ar-H), 7.29 (s, 4H, Ar-H), 6.99-6.97 (d, J = 8 Hz, 4H, Ar-H), 4.04-4.01 (t, J = 12 Hz, 4H), 3.86 (s,2H), 3.80 (s, 4H), 2.73-2.70 (t, J = 12 Hz, 4H), 1.90-1.83 (m, 4H), 1.74-1.67 (m,4H); Elemental analysis calcd (%): C, 79.46; H, 6.67; N, 8.83; found, C,79.62; H, 6.51; N, 8.62.

SACD2:4',4'''-((((1,4-phenylenebis(methylene))bis(azanediyl))bis(pentane-5,1-diyl))bis(oxy))bis(([1,1'-biphenyl]-4'-carbonitrile)): Colourless solid; R_f = 0.5 (10% Methanol: DCM); yield: 62%; v_{max} in cm^{-1}(KBr) 3384 (v_{N-H}), 2930 (v_{CH}), 2223 (v_{CN}), 1603 ($v_{C=C}$), 1246 (v_{C-O}); ^1H NMR (400 MHz, $CDCl_3$) δ 7.70-7.68 (d, J = 8 Hz, 4H, Ar-H), 7.65-7.63 (d, J = 8 Hz, 4H, Ar-H), 7.53-7.51 (d, J = 8 Hz, 4H, Ar-H), 7.28 (s, 4H, Ar-H), 6.99-6.97 (d, J = 8 Hz, 4H, Ar-H), 4.02-3.99 (t, J = 12 Hz, 4H), 3.86 (s,2H), 3.79 (s, 4H), 2.69-2.66 (t, J = 12 Hz, 4H), 1.53-1.45 (m, 4H), 1.33-1.21 (m,4H); Elemental analysis calcd (%): C, 79.73; H, 6.99; N, 8.45; found,C, 79.64; H, 7.05; N, 8.22;

SACD3:4',4'''-((((1,4-phenylenebis(methylene))bis(azanediyl))bis(hexane-6,1-diyl))bis(oxy))bis(([1,1'-biphenyl]-4'-carbonitrile)): Colourless solid; R_f = 0.5 (10% Methanol:

DCM); yield: 62%; ν_{max} in cm^{-1}(KBr) 3386 (ν_{N-H}), 2935 (ν_{CH}), 2226 (ν_{CN}), 1603 ($\nu_{C=C}$), 1243 (ν_{C-O}); ^1H NMR (400 MHz, $CDCl_3$) δ 7.68-7.66 (d, *J* = 8 Hz, 4H, Ar-H), 7.63-7.61 (d, *J* = 8 Hz, 4H, Ar-H), 7.52-7.50 (d, *J* = 8 Hz, 4H, Ar-H), 7.25 (s, 4H, Ar-H), 6.98-6.96 (d, *J* = 8 Hz, 4H, Ar-H), 4.0-3.97 (t, *J* = 12 Hz, 4H), 3.86 (s,2H), 3.76 (s, 4H), 2.65-2.62 (t, *J* = 12 Hz, 4H), 1.83-1.76 (m, 4H), 1.52-1.39 (m,12H); Elemental analysis calcd (%): C, 79.97; H, 7.29; N, 8.11; found C , 80.1; H, 7.44; N, 8.08;

SACD4:4',4'''-((((1,4-phenylenebis(methylene))bis(azanediyl))bis(heptane-7,1-diyl))bis(oxy))bis(([1,1'-biphenyl]-4'-carbonitrile)): Colourless solid; R_f = 0.51 (10% Methanol: DCM); yield: 58%; ν_{max} in cm^{-1}(KBr) 3384 (ν_{N-H}), 2934 (ν_{CH}), 2226 (ν_{CN}), 1604 ($\nu_{C=C}$), 1243 (ν_{C-O}); ^1H NMR (400 MHz, $CDCl_3$) δ 7.69-7.67 (d, *J* = 8 Hz, 4H, Ar-H), 7.65-7.63 (d, *J* = 8 Hz, 4H, Ar-H), 7.52-7.50 (d, *J* = 8 Hz, 4H, Ar-H), 7.23 (s, 4H, Ar-H), 6.98-6.96 (d, *J* = 8 Hz, 4H, Ar-H), 4.0-3.98 (t, *J* = 12 Hz, 4H), 3.79 (s,2H), 3.69 (s,4H), 2.75-2.72 (t, *J* = 12 Hz, 4H), 1.83-1.74 (m, 4H), 1.6-1.51 (m, 4H), 1.32-1.2 (m,12H); Elemental analysis calcd (%): C, 80.19; H, 7.57; N, 7.79; found, C, 80.05; H, 7.51; N, 7.62.

SACD5:4',4'''-((((1,4-phenylenebis(methylene))bis(azanediyl))bis(octane-8,1-diyl))bis(oxy))bis(([1,1'-biphenyl]-4'-carbonitrile)): Colourless solid; R_f = 0.51 (10% Methanol: DCM); yield: 59%; ν_{max} in cm^{-1}(KBr) 3385 (ν_{N-H}), 2934 (ν_{CH}), 2224 (ν_{CN}), 1604 ($\nu_{C=C}$), 1243 (ν_{C-O}); ^1H NMR (400 MHz, $CDCl_3$) δ 7.68-7.66 (d, *J* = 8 Hz, 4H, Ar-H), 7.63-7.61 (d, *J* = 8 Hz, 4H, Ar-H), 7.51-7.49 (d, *J* = 8 Hz, 4H, Ar-H), 7.24 (s, 4H, Ar-H), 6.98-6.96 (d, *J* = 8 Hz, 4H, Ar-H), 4.05-4.02 (t, *J* = 12 Hz, 4H), 3.84 (s,2H), 3.72 (s, 4H), 2.63-2.6 (t, *J* = 12 Hz, 4H), 1.89-1.81 (m, 4H), 1.7-1.59 (m,20H); Elemental analysis calcd (%): C, 80.39; H, 7.83; N, 7.50; found, C, 80.64; H. 7.65; N, 7.49.

SACD6:4',4'''-((((1,4-phenylenebis(methylene))bis(azanediyl))bis(nonane-9,1-diyl))bis(oxy))bis(([1,1'-biphenyl]-4'-carbonitrile)): Colourless solid; R_f = 0.51 (10% Methanol: DCM); yield: 60%; ν_{max} in cm^{-1}(KBr) 3384 (ν_{N-H}), 2919 (ν_{CH}), 2234 (ν_{CN}), 1603 ($\nu_{C=C}$), 1251 (ν_{C-O}); ^1H NMR (400 MHz, $CDCl_3$) δ 7.75-7.73 (d, *J* = 8 Hz, 4H, Ar-H), 7.68-7.63 (d, *J* = 8 Hz, 4H, Ar-H), 7.63-7.61 (d, *J* = 8 Hz, 4H, Ar-H), 7.26 (s, 4H, Ar-H), 6.98-6.96 (d, *J* = 8 Hz, 4H, Ar-H), 4.0-3.97 (t, *J* = 12 Hz, 4H), 3.83 (s,2H), 3.76 (s, 4H), 2.62-2.59 (t, *J* = 12 Hz, 4H), 1.82-1.75 (m, 4H), 1.51-1.42 (m,24H); ^{13}C NMR (100MHz, $CDCl_3$): 159.85, 145.37, 132.48, 128.78, 128.45, 128.28, 127.25, 127.15, 119.18, 115.13, 110.12, 77.42, 77.10, 76.78, 68.24, 30.13, 29.57, 29.39,

29.28, 28.99, 27.42, 26.09; Elemental analysis calcd (%): C, 80.58; H, 8.06; N, 7.23; found, C, 80.49; H, 8.26; N, 7.25.

SACD7:4',4'''-((((1,4-phenylenebis(methylene))bis(azanediyl))bis(decane-10,1-diyl))bis(oxy))bis(([1,1'-biphenyl]-4'-carbonitrile)): Colourless solid; R_f = 0.51 (10% Methanol: DCM); yield: 60%; ν_{max} in cm^{-1} (KBr) 3385 (ν_{N-H}), 2934 (ν_{CH}), 2226 (ν_{CN}), 1603 ($\nu_{C=C}$), 1244 (ν_{C-O}); ^1H NMR (400 MHz, $CDCl_3$) δ 7.70-7.68 (d, *J* = 8 Hz, 4H, Ar-H), 7.65-7.63 (d, *J* = 8 Hz, 4H, Ar-H), 7.53-7.51 (d, *J* = 8 Hz, 4H, Ar-H), 7.27 (s, 4H, Ar-H), 7.0-6.98 (d, *J* = 8 Hz, 4H, Ar-H), 4.02-3.99 (t, *J* = 12 Hz, 4H), 3.85 (s,2H), 3.77 (s, 4H), 2.63-2.60 (t, *J* = 12 Hz, 4H), 1.84-1.77 (m, 4H), 1.52-1.43 (m,8H), 1.37-1.25 (m, 20H); Elemental analysis calcd (%): C, 80.76; H, 8.28; N, 6.98; found, C , 81.01; H, 8.32; N, 6.88.

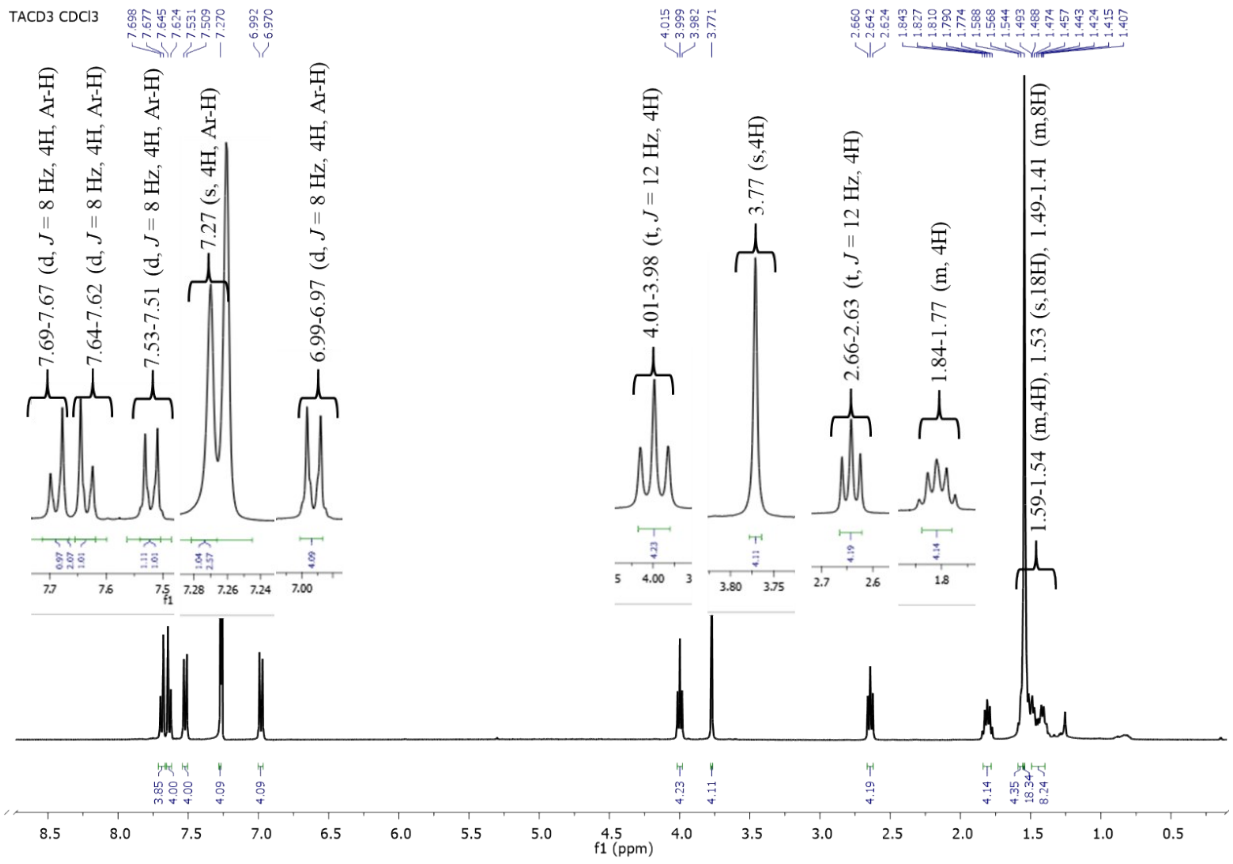


Figure S1: ^1H NMR spectra of **TACD3** in $CDCl_3$

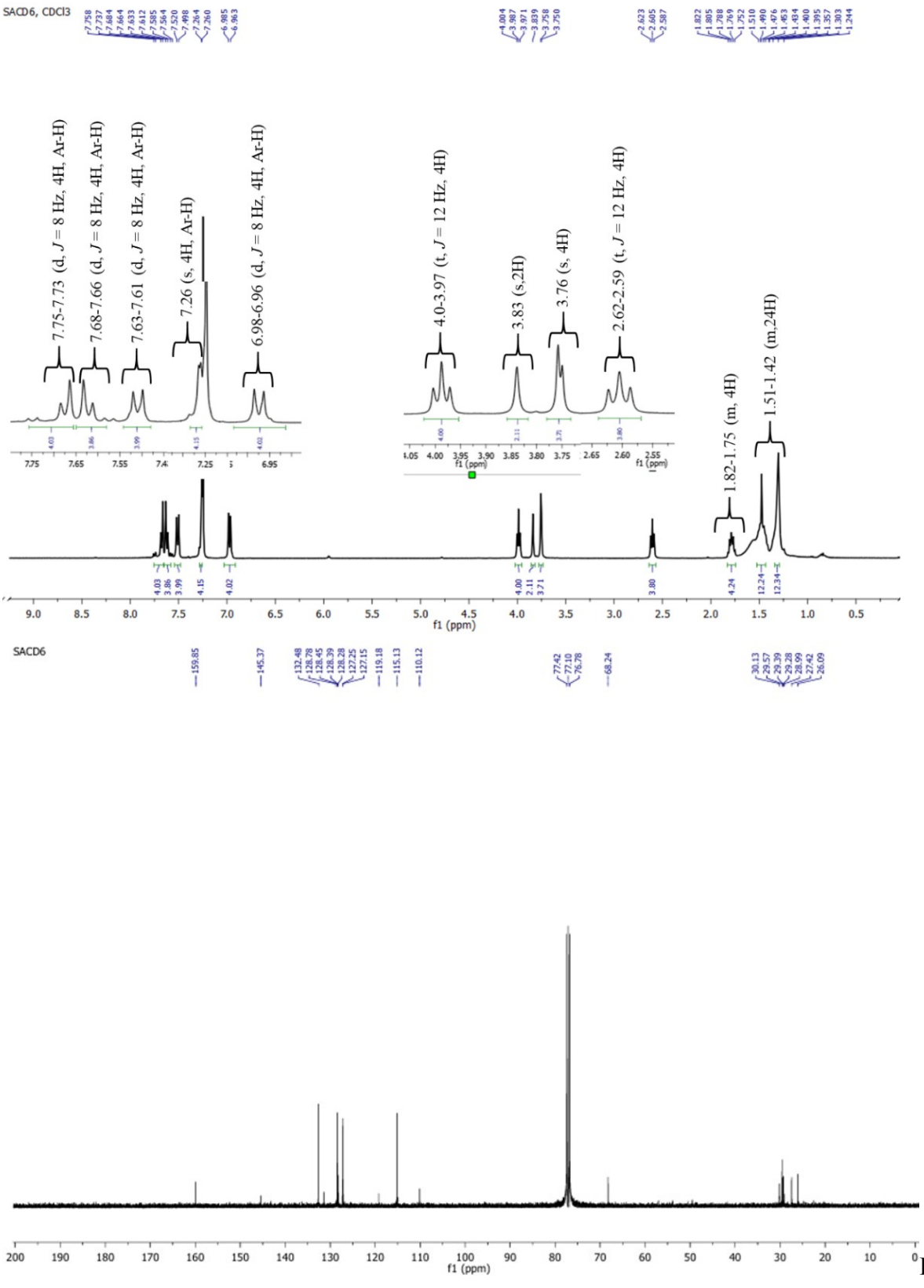
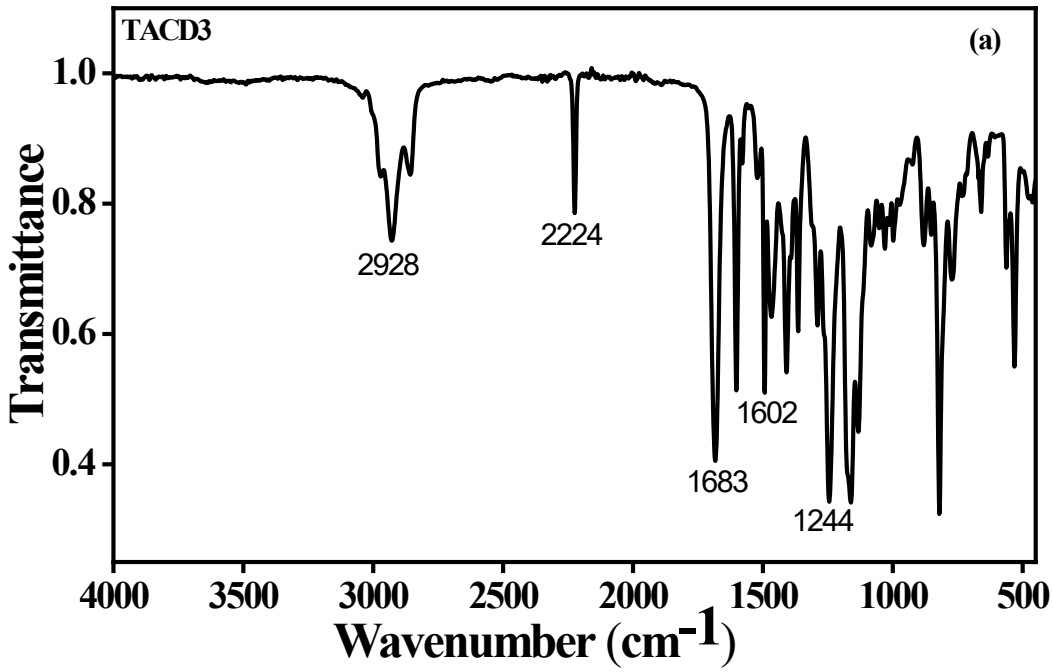
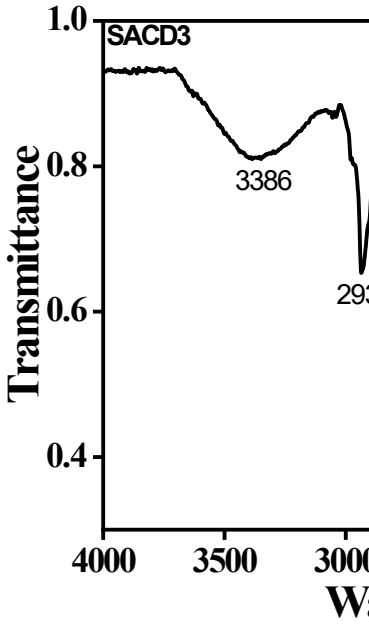


Figure S2: ^{1}H NMR and ^{13}C NMR spectra of **SACD6** in $CDCl_3$





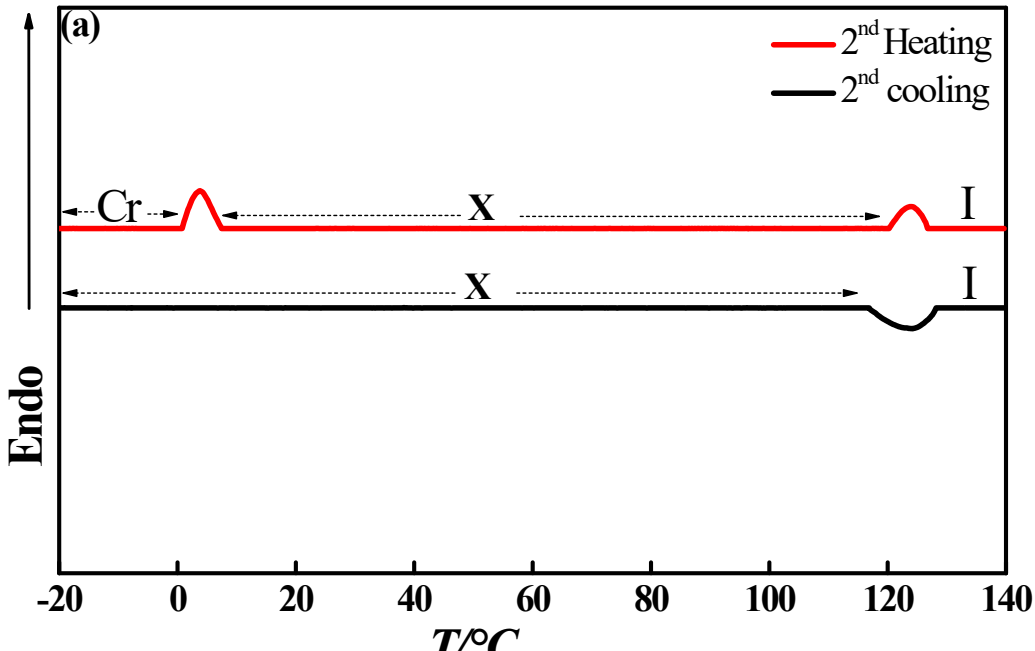


Figure S3:
IR spectra of
(a) **TACD3;**
(b) **SACD3.**

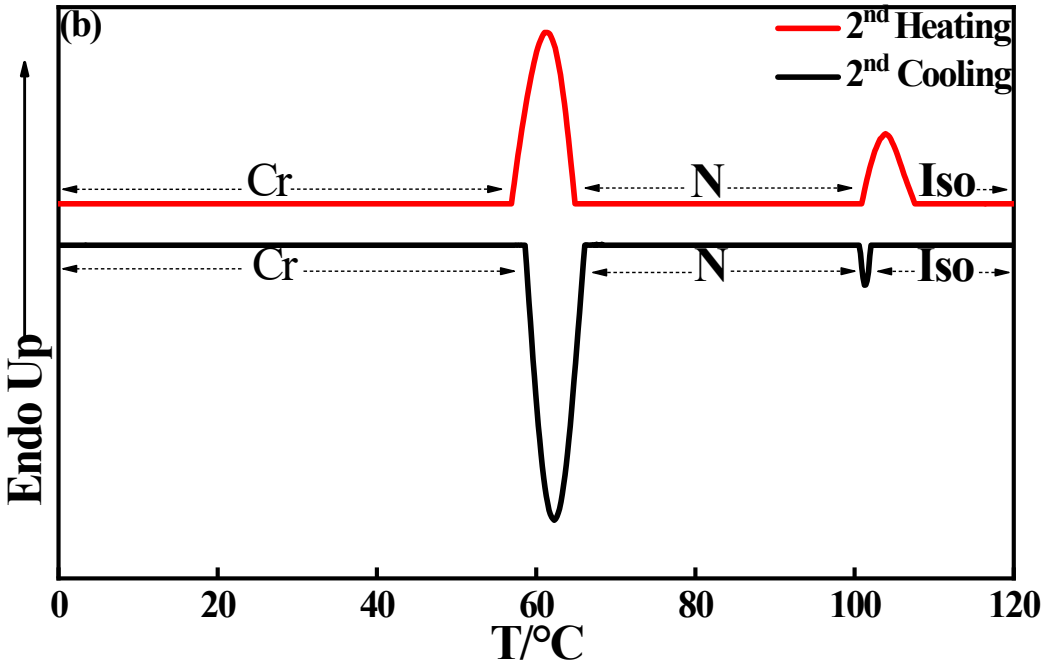
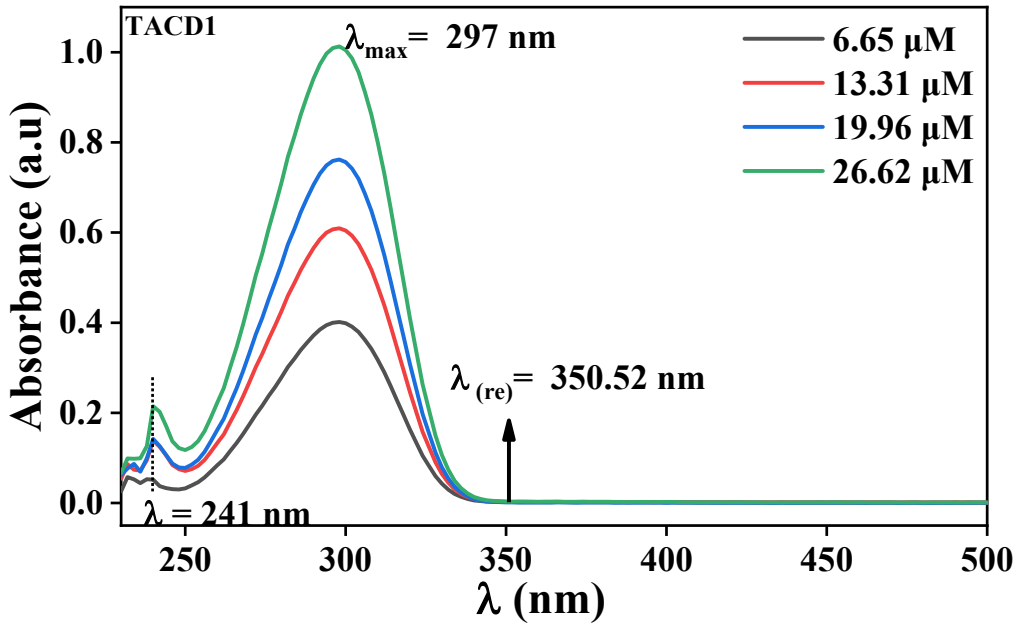
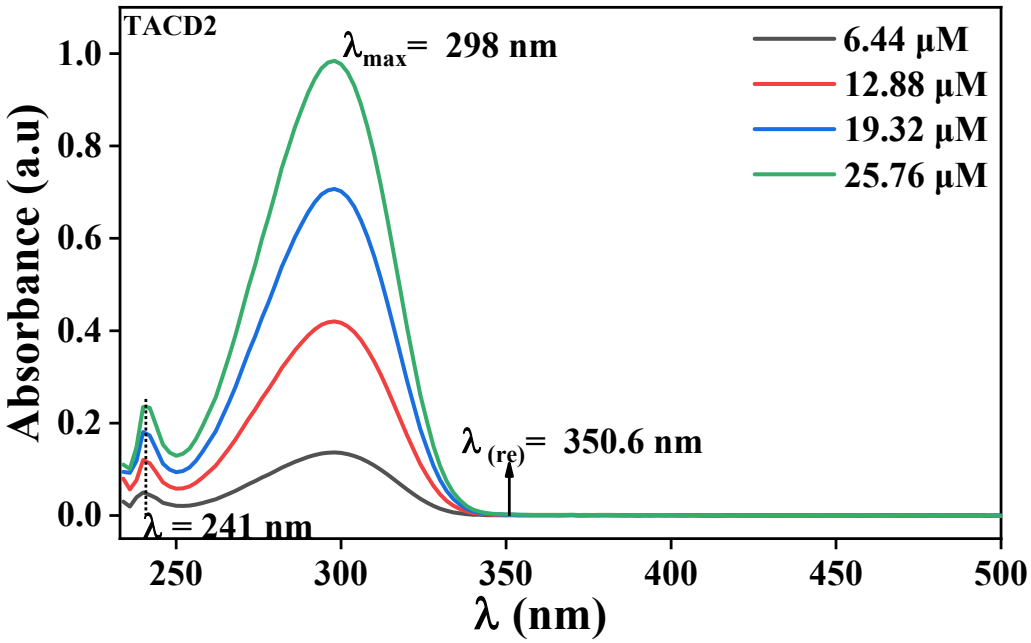
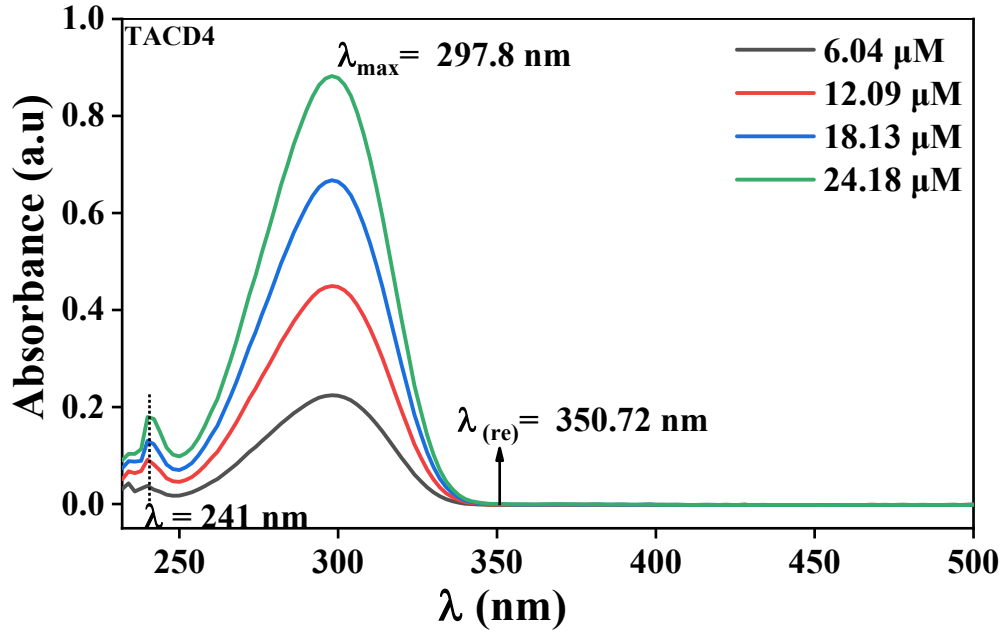


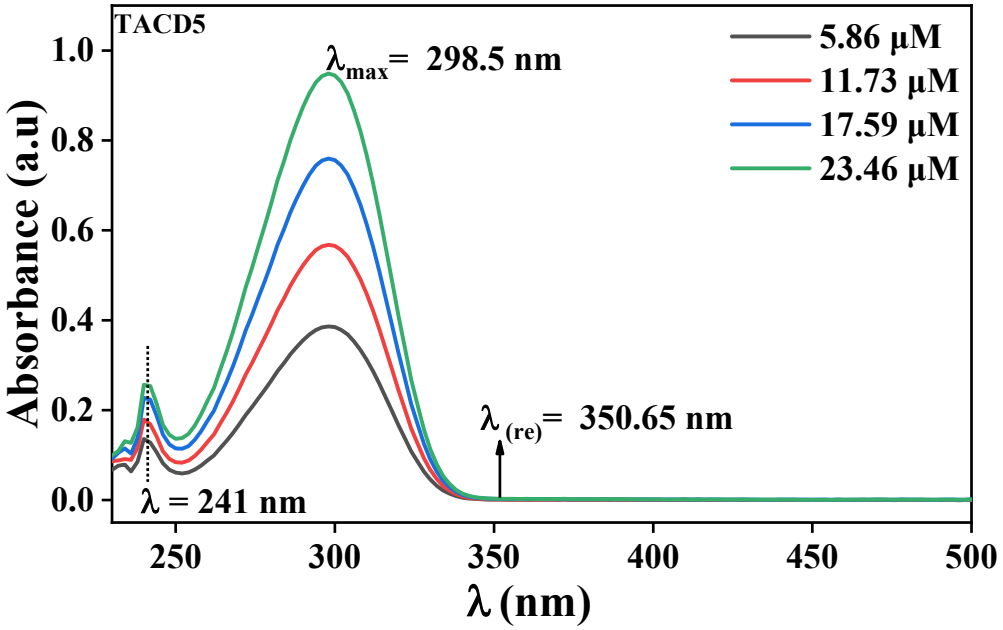
Figure S4. DSC in both 2nd heating and cooling cycles for the dimers (a) **TACD7,** X phase (grainy texture) and (b) **SACD6,** N phase.

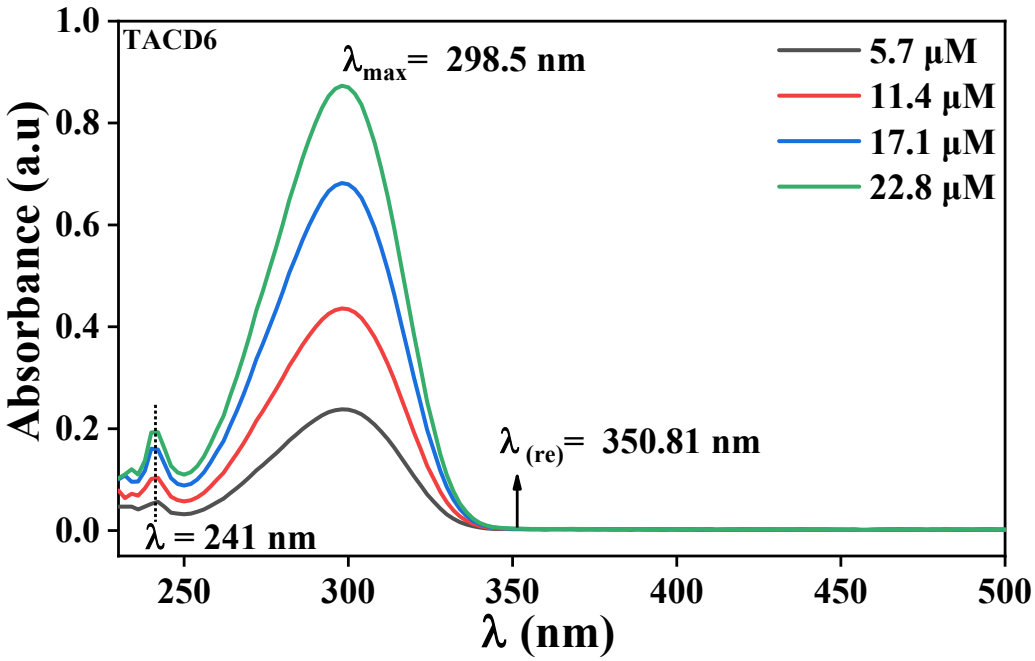
Aggregational studies:

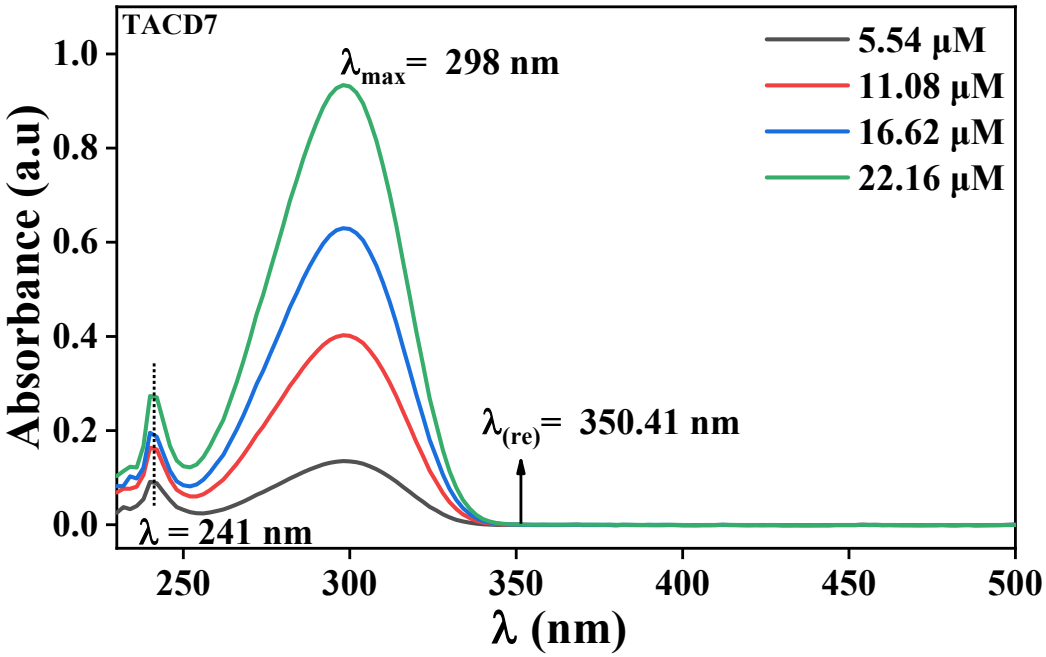


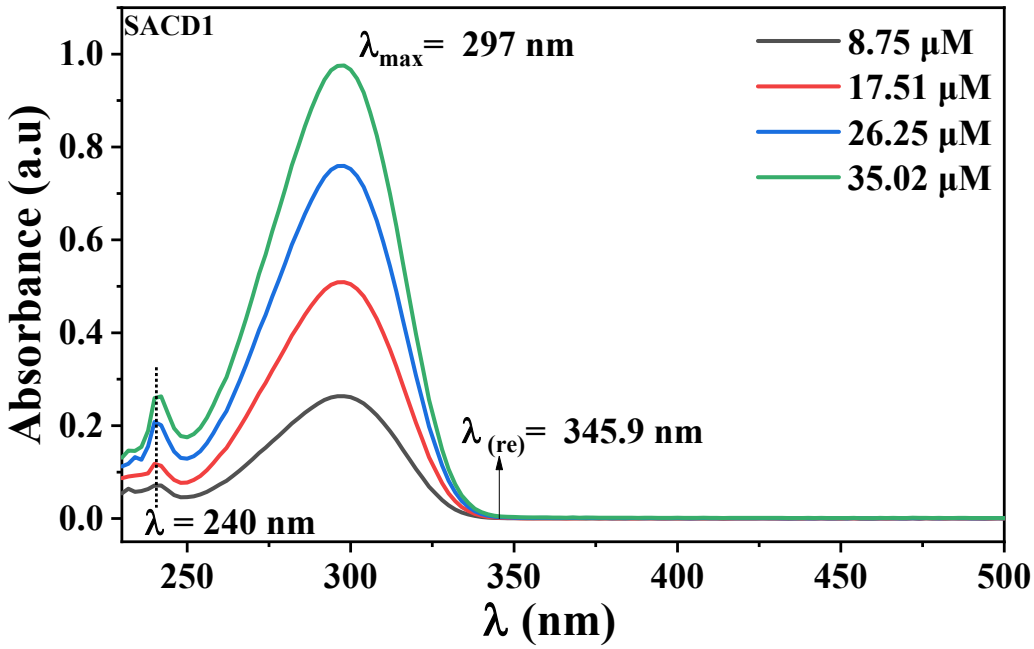


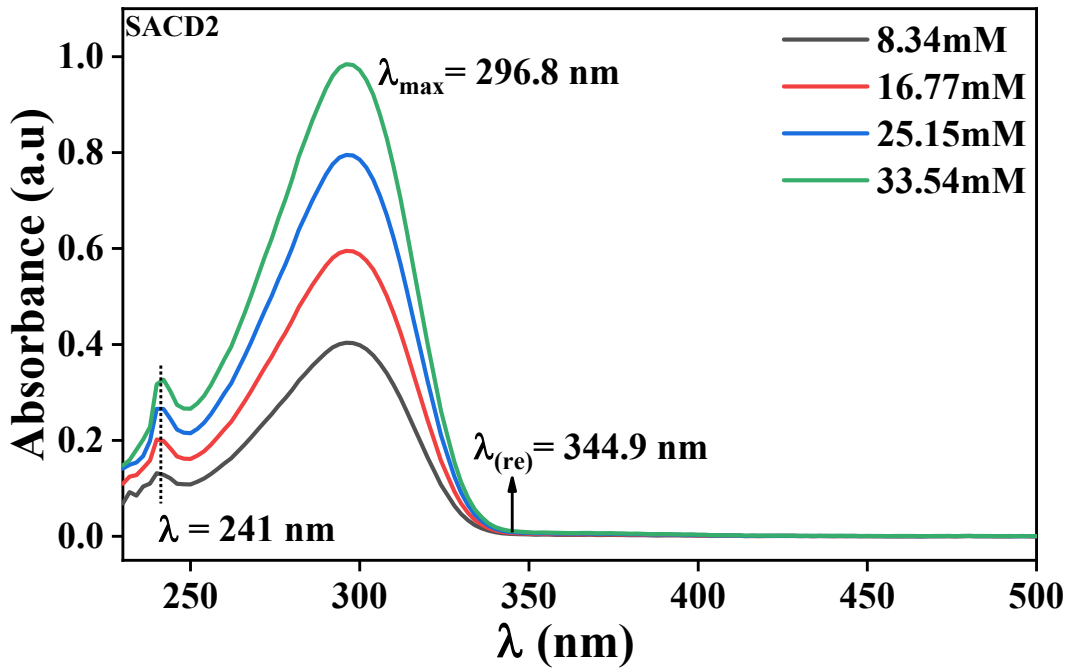

TACD4
λmax= 297.8 nm
6.04 µM
12.09 µM
18.13 µM
24.18 µM
λ (re)= 350.72 nm
λ = 241 nm
Absorbance (a.u)
λ (nm)

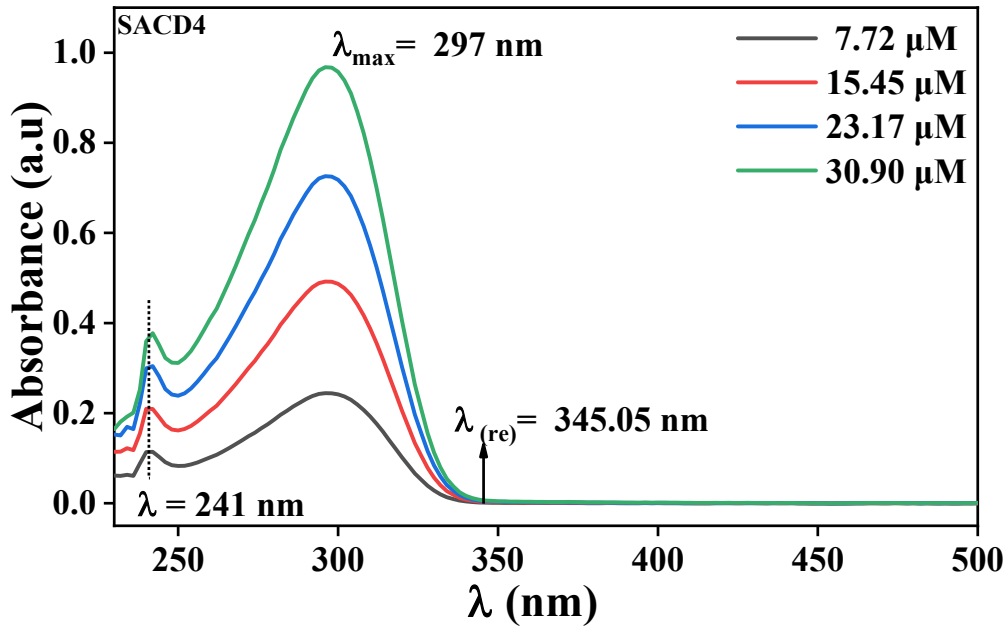

TACD5
λmax= 298.5 nm
5.86 µM
11.73 µM
17.59 µM
23.46 µM
λ (re)= 350.65 nm
λ = 241 nm
Absorbance (a.u)
λ (nm)

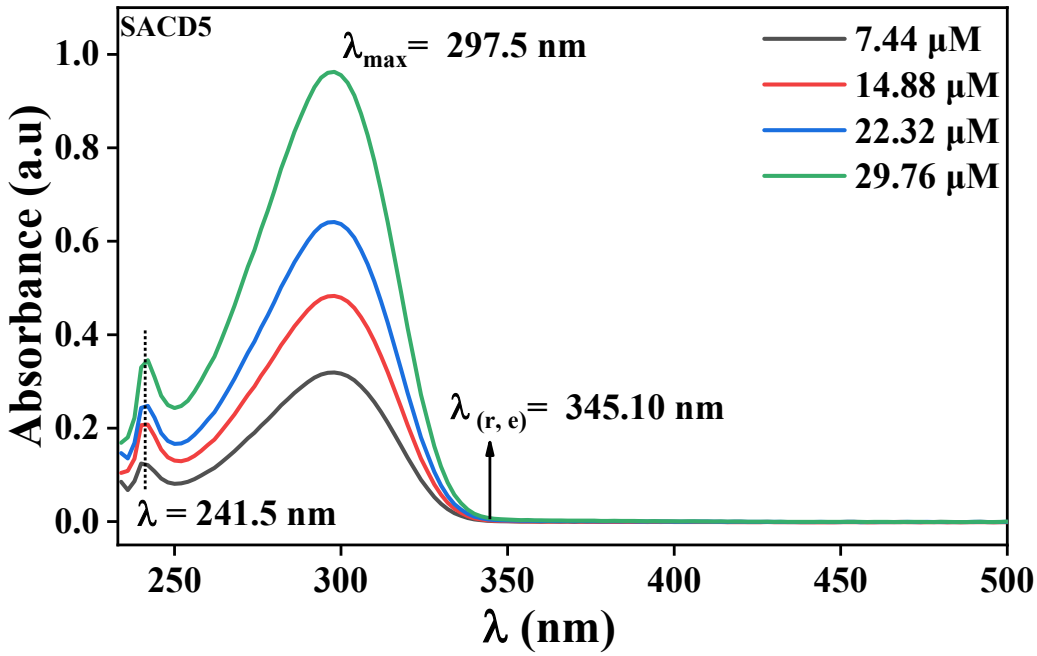

TACD6
λmax= 298.5 nm
5.7 µM
11.4 µM
17.1 µM
22.8 µM
λ (re)= 350.81 nm
λ = 241 nm
Absorbance (a.u)
λ (nm)
1.0
0.8
0.6
0.4
0.2
0.0
250
300
350
400
450
500


TACD7
λmax= 298 nm
5.54 µM
11.08 µM
16.62 µM
22.16 µM
λ(re)= 350.41 nm
λ = 241 nm
Absorbance (a.u)
λ (nm)
1.0
0.8
0.6
0.4
0.2
0.0
250
300
350
400
450
500


SACD1
λmax= 297 nm
8.75 µM
17.51 µM
26.25 µM
35.02 µM
λ (re)= 345.9 nm
λ = 240 nm
Absorbance (a.u)
λ (nm)


SACD2
λmax= 296.8 nm
8.34mM
16.77mM
25.15mM
33.54mM
λ(re)= 344.9 nm
λ = 241 nm
Absorbance (a.u)
λ (nm)


SACD4
λmax= 297 nm
7.72 µM
15.45 µM
23.17 µM
30.90 µM
λ (re)= 345.05 nm
λ = 241 nm
Absorbance (a.u)
λ (nm)


SACD5
λmax= 297.5 nm
7.44 µM
14.88 µM
22.32 µM
29.76 µM
λ (r, e)= 345.10 nm
λ = 241.5 nm
Absorbance (a.u)
λ (nm)

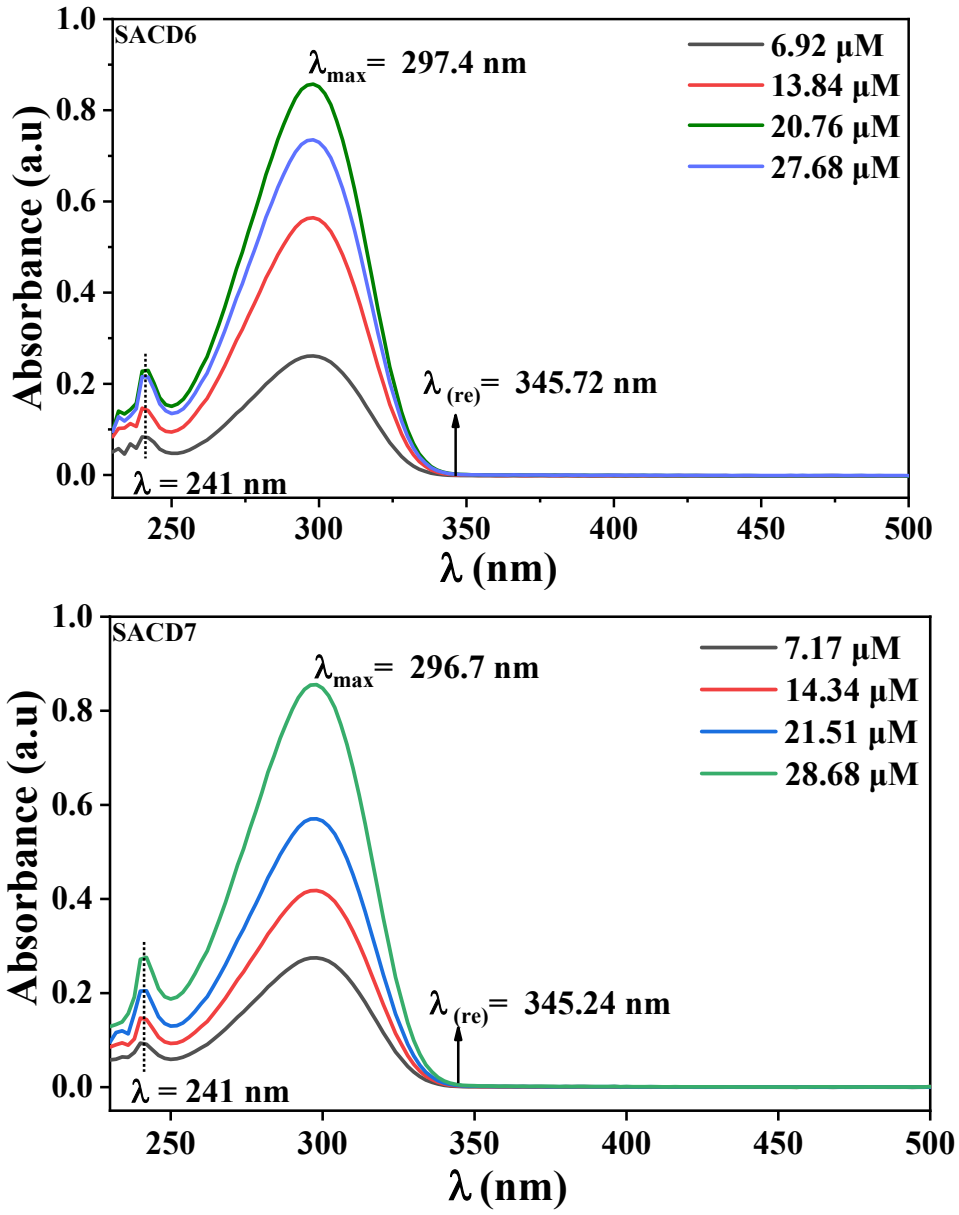
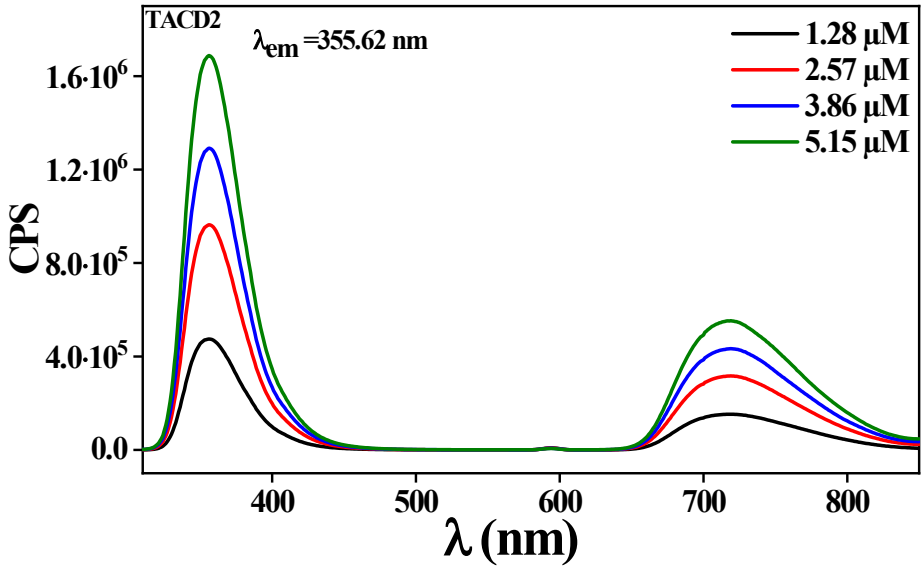
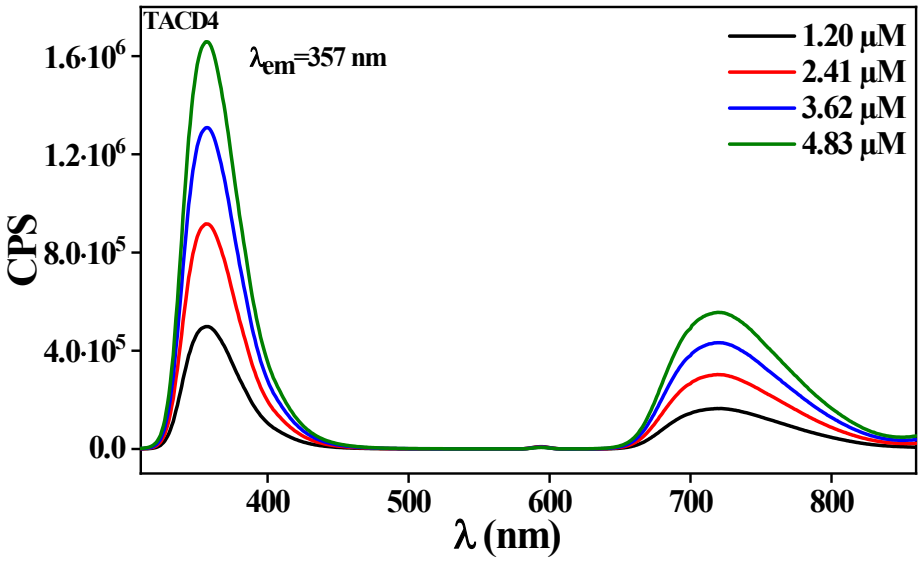
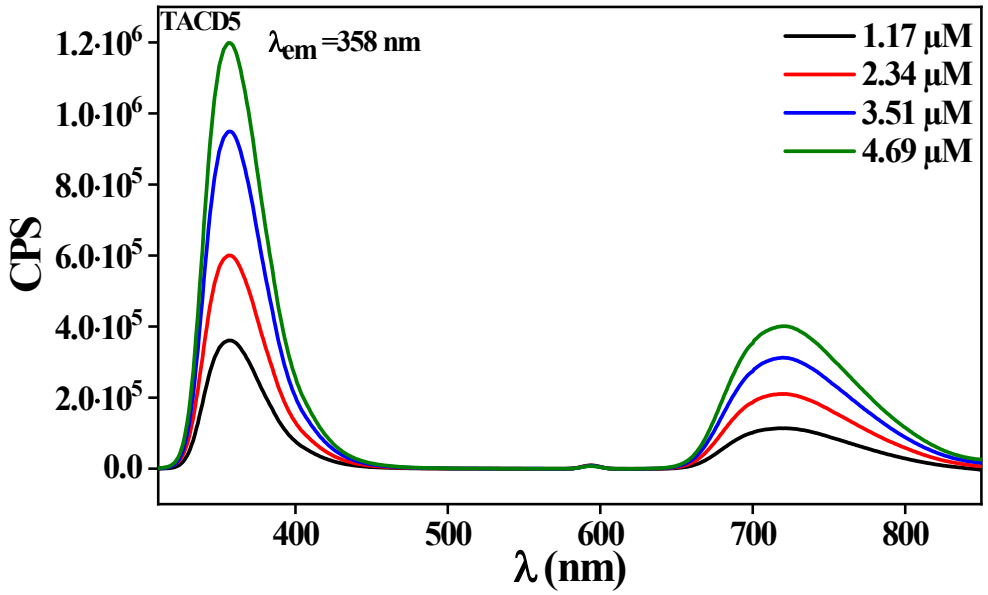


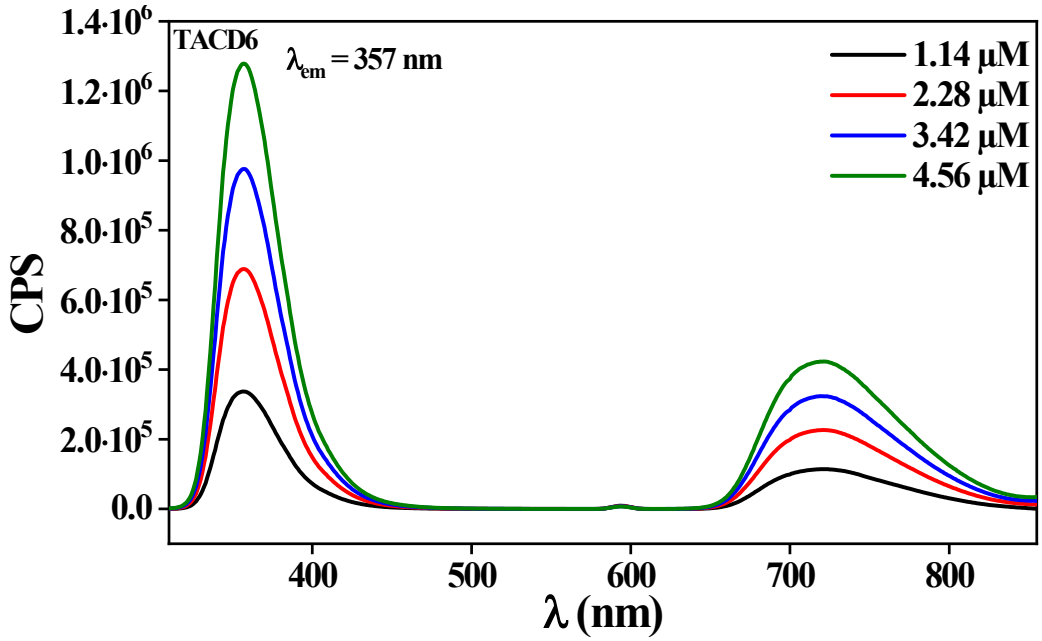
Figure S5. UV-Visible absorption spectra of **SACD (1-2, 4-7)** at room temperature in $CHCl_3$.

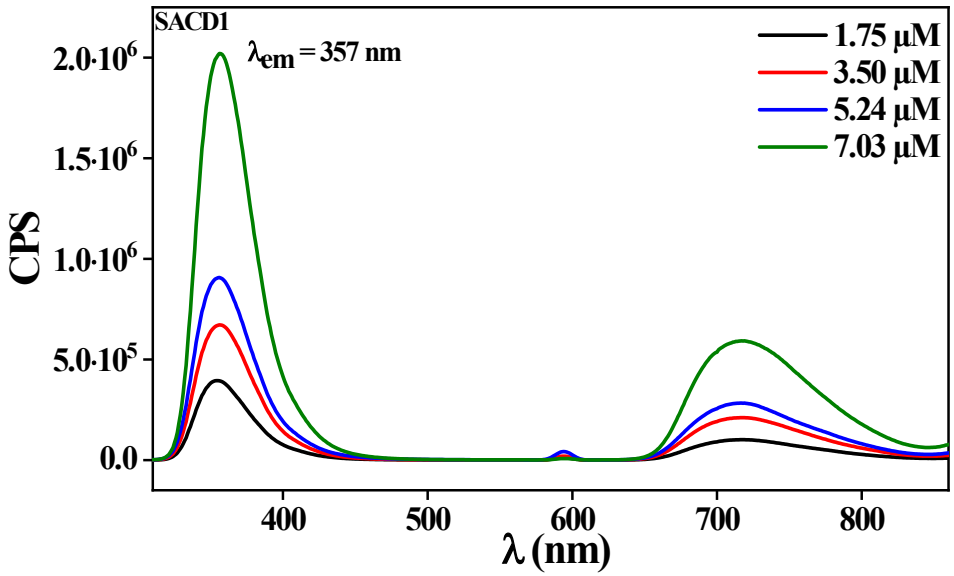
Emission studies:

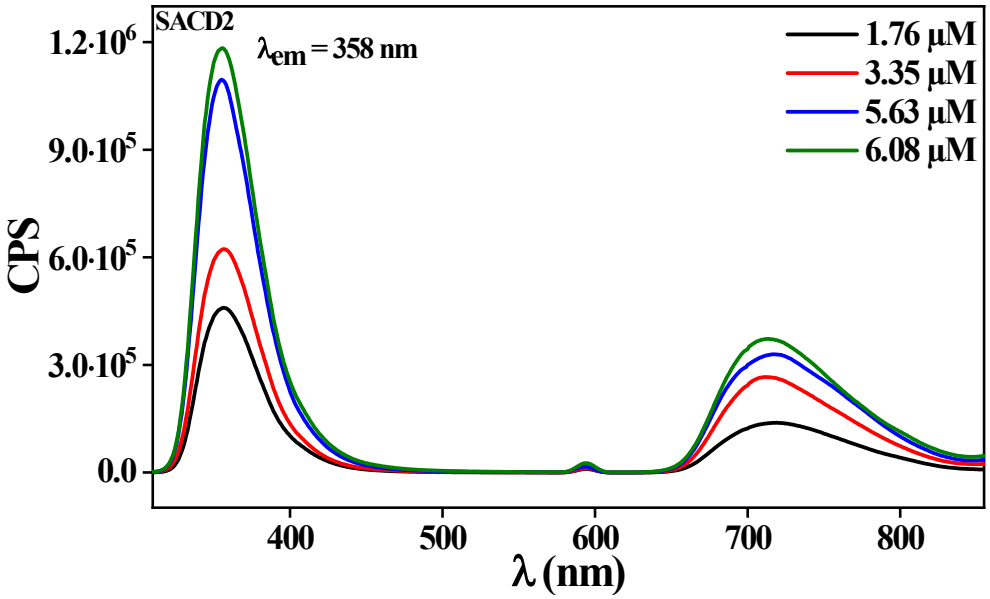


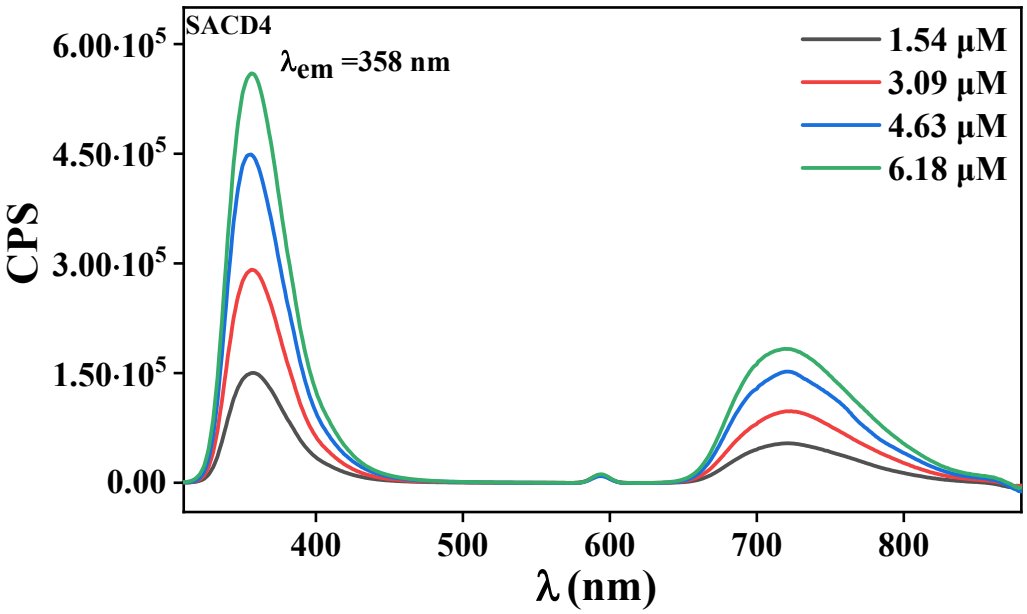


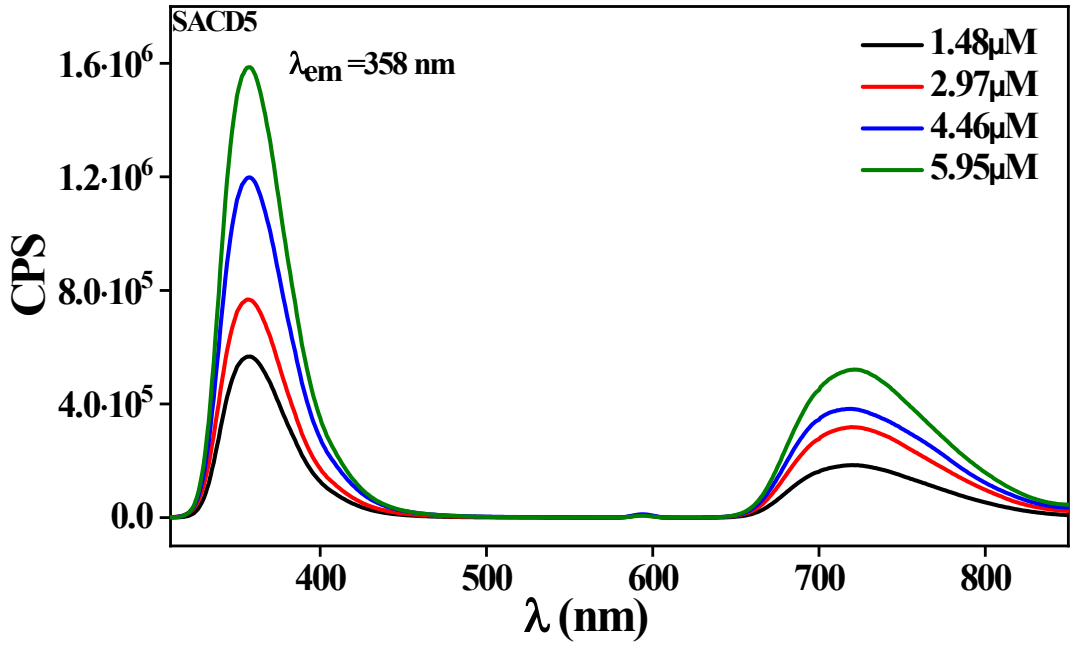

TACD5
λem =358 nm
1.17 µM
2.34 µM
3.51 µM
4.69 µM
CPS
1.2·10^6
1.0·10^6
8.0·10^5
6.0·10^5
4.0·10^5
2.0·10^5
0.0
400
500
600
700
800
λ (nm)


TACD6
λem = 357 nm
1.14 µM
2.28 µM
3.42 µM
4.56 µM
CPS
1.4·10^6
1.2·10^6
1.0·10^6
8.0·10^5
6.0·10^5
4.0·10^5
2.0·10^5
0.0
400
500
600
700
800
λ (nm)


SACD1
λem = 357 nm
1.75 µM
3.50 µM
5.24 µM
7.03 µM
CPS
2.0·10^6
1.5·10^6
1.0·10^6
5.0·10^5
0.0
400
500
600
700
800
λ (nm)


SACD2
λem = 358 nm
1.76 µM
3.35 µM
5.63 µM
6.08 µM
CPS
1.2·10^6
9.0·10^5
6.0·10^5
3.0·10^5
0.0
400
500
600
700
800
λ (nm)


SACD4
λem =358 nm
1.54 μM
3.09 μM
4.63 μM
6.18 μM
CPS
6.00·10^5
4.50·10^5
3.00·10^5
1.50·10^5
0.00
400
500
600
700
800
λ (nm)


SACD5
λem =358 nm
1.48μM
2.97μM
4.46μM
5.95μM
CPS
1.6·10^6
1.2·10^6
8.0·10^5
4.0·10^5
0.0
400
500
600
700
800
λ (nm)

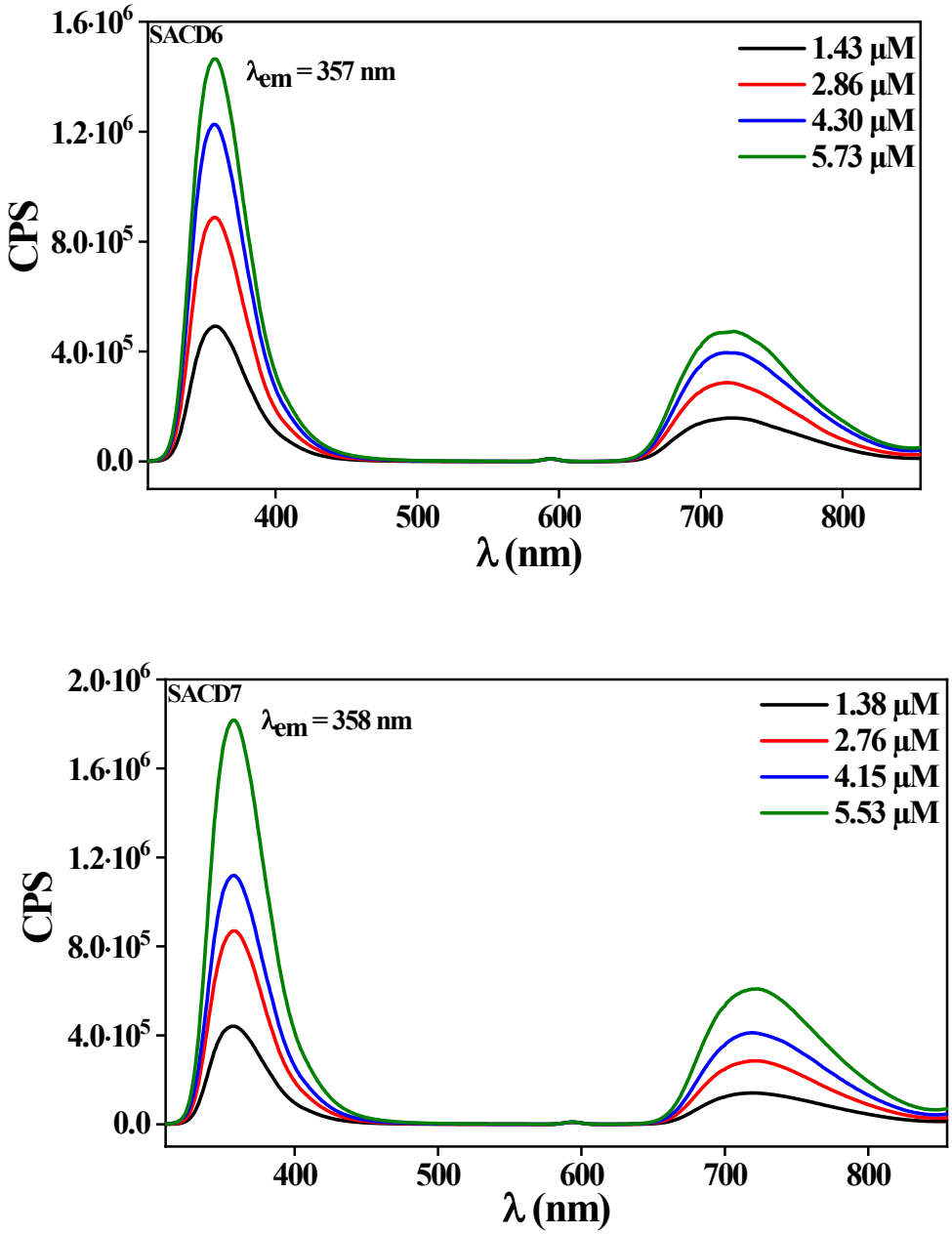


Figure S6. Emission spectra of **SACD (1-2, 4-7)** at room temperature in $CHCl_3$.