Aggregation-Induced Emission and Organogels with Chiral and Racemic
Pyrene substituted Cyanostyrenes

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Supporting Information

Characterization data of the synthesized compounds
Absorption, Emission spectra for the synthesized compounds
Cryo-SEM, drop-cast SEM, DLS data & NMR-study
\(^1\)H&\(^{13}\)C-NMR spectra of synthesized compounds

\(^1\)H, \(^{13}\)C NMR Characterization data of the intermediate phenolic derivatives.

**Compound 7:** Yield 70% (400mg), Mp: 292-295 °C, \(^1\)H-NMR (500MHz, DMSO-d6), \(\delta\) (ppm)
10.02 (s, 1H), 8.82 (s, 1H), 8.54-8.49 (dd, 2H), 8.43-8.39 (m, 3H), 8.35-8.34 (d, 1H), 8.31-8.25 (dd, 3H), 8.17-8.14 (t, 1H), 7.83-7.81 (d, 2H), 6.98-6.96 (d, 2H)

\(^{13}\)C-NMR (125MHz, DMSO-d6): \(\delta\) (ppm), 159.35, 138.43, 132.26, 131.30, 130.85, 129.58, 129.38, 128.92, 128.87, 128.22, 127.79, 127.14, 126.70, 126.56, 126.42, 126.56, 126.70, 126.56, 126.42, 125.29, 125.10, 124.32, 124.16, 124.09, 118.65, 116.48, 115.11, HRMS (ESI-Q-TOF): C\(_{25}\)H\(_{15}\)NO [M + H]+: cal. \(m/z\)346.1226, found, \(m/z\) 346.1234 (error 2.3 ppm)

**Compound 8:** Yield 70% (450mg) Mp: 273-276 °C, \(^1\)H-NMR (500MHz, DMSO-d6), \(\delta\) (ppm)
9.55 (s, 1H), 9.33 (s, 1H), 8.72 (s, 1H), 8.53-8.51 (d, 2H), 8.48-8.46 (d, 2H), 8.41-8.38 (m, 2H), 8.34-8.32 (d, 1H), 8.30-8.24 (dd, 2H), 8.16-8.13 (t, 1H), 7.37 (s,1H),7.32-7.30 (dd, 1H), 6.94-6.93(d, 1H)

\(^{13}\)C-NMR (125MHz, DMSO-d6): \(\delta\) (ppm) 147.70, 146.30, 138.15, 132.22, 131.30, 129.55, 129.40, 128.87, 127.80, 127.14, 126.72, 126.56, 126.41, 125.56, 125.29, 124.32, 124.16, 124.04, 118.71, 118.31, 116.57, 115.33, 113.94, HRMS (ESI-Q-TOF): C\(_{25}\)H\(_{15}\)NO\(_2\) [M + H]+: cal. \(m/z\)362.1176, found, \(m/z\) 362.1187 (error 3ppm)

**Compound 9:** Yield 65% (370mg) Mp: 250-255 °C, \(^1\)H-NMR (500MHz, DMSO-d6), \(\delta\) (ppm)
9.28 (s, 1H), 8.75(s,1H), 8.64 (s, 1H), 8.52-8.50 (d, 1H), 8.46-8.39 (m, 4H), 8.35-8.33 (d, 1H), 8.31-8.25 (dd, 2H), 8.17-8.14 (t,1H), 6.94 (s, 2H)
\(^{13}\)C-NMR (125MHz, DMSO-d6): \(\delta\) (ppm) 146.99, 137.99, 135.57, 132.20, 131.30, 129.51, 129.36, 128.88, 127.79, 127.14, 126.72, 126.56, 126.40, 125.27, 124.65, 124.32, 124.16, 123.94, 118.73, 115.58, 105.85. HRMS (ESI-Q-TOF): \(C_{25}H_{15}NO_3\) [M + H]^+: cal. \(m/z\) 378.1125, found, \(m/z\) 378.1134 (error 2.4ppm)

\(^1\)H, \(^{13}\)C NMR Characterization data of the compounds

**Compound (1) MA**: Yield 65% (130mg): Yellow solid, m.p.: 105-110°C, \(\epsilon\) in CH\(_3\)CN = 14449 M\(^{-1}\)cm\(^{-1}\), \(^1\)H-NMR (500MHz, CDCl\(_3\)), \(\delta\) (ppm): 8.63-8.62 (d, 1H), 8.46 (s,1H), 8.29-8.26 (m, 4H), 8.25-8.24 (d, 2H), 8.06-8.05 (dd, 1H), 7.78-7.76 (d, 2H), 7.04-7.02 (d, 2H), 5.14-5.11 (t, 1H), 4.11-4.07 (m, 2H), 2.05-1.57 (m,16H), 1.43-1.41 (d, 3H)

\(^{13}\)C-NMR (125MHz, CDCl\(_3\)): \(\delta\) (ppm) 160.27, 138.01, 132.57, 131.40, 130.76, 129.72, 128.57,128.54, 128.37, 127.55, 127.46, 126.92, 126.29, 126.11, 125.88, 124.98, 124.77, 124.65, 122.71, 118.34, 115.13, 114.63, 109.81, 66.63, 37.16, 37.16, 36.09, 29.59, 25.74, 25.49, 19.60, 17.70, HRMS (ESI-Q-TOF): \(C_{35}H_{34}NO\) [M + H]^+: cal. \(m/z\) 484.2635, found, \(m/z\) 484.2650 (error 3ppm)

**Compound (2) MC**: Yield 65% (130mg): Yellow solid, Mp: 105-110°C, \(\epsilon\) CH\(_3\)CN = 14449 M\(^{-1}\)cm\(^{-1}\), \(^1\)H-NMR (500MHz, CDCl\(_3\)), \(\delta\) (ppm): 8.63-8.62 (d, 1H), 8.46 (s,1H), 8.29-8.23 (d, 2H), 8.19-8.17 (d, 1H) 8.15-8.09 (dd, 2H), 7.78-7.76 (d, 2H), 7.41-7.39 (dd, 1H), 7.00-6.98 (d, 1H), 5.13-5.11 (t, 1H), 4.11-4.07 (m, 2H), 2.17-1.25 (m, 23H), 1.01-0.99 (d, 6H)

\(^{13}\)C-NMR (125MHz, CDCl\(_3\)): \(\delta\) (ppm) 150.61, 149.53, 138.35, 132.60, 131.35, 130.31, 131.84, 130.78, 129.73, 128.60, 128.56, 127.48, 127.42, 126.32, 126.21, 126.13, 125.90, 125.00, 124.79, 124.73, 124.70, 124.65, 122.78, 119.45, 118.33, 114.95, 113.59, 111.68, 68.00, 67.70, 37.27, 37.23, 36.35, 36.11, 29.75, 29.73, 25.72, 25.70, 25.55, 19.65, 19.63, 17.66, HRMS (ESI-Q-TOF): \(C_{45}H_{52}NO_2\) [M + H]^+: cal. \(m/z\) 638.3993, found, \(m/z\) 638.4020 (error 4ppm)

**Compound (3) DA**: Yellow semi-solid, \(\epsilon\) (CH\(_3\)CN) = 15596 M\(^{-1}\)cm\(^{-1}\), Yield 55% (120mg), \(^1\)H-NMR (500MHz,CDC\(_3\)) \(\delta\) (ppm): 8.61-8.60 (d, 1H), 8.44 (s, 1H), 8.28-8.23(dd, 4H) 8.19-8.17 (d, 1H) 8.15-8.09 (dd, 2H), 8.13-8.09 (dd, 1H), 7.41-7.39 (dd, 1H), 7.33 (s, 1H), 7.00-6.98 (d, 1H), 5.13-5.11 (m, 2H), 4.16-4.11 (m, 2H), 2.17-1.25 (m, 23H), 1.01-0.99 (d, 6H)

\(^{13}\)C-NMR (125MHz, CDCl\(_3\)): \(\delta\) (ppm) 150.61, 149.53, 138.35, 132.60, 131.35, 131.31, 131.84, 130.78, 129.73, 128.60, 128.56, 127.48, 127.42, 126.32, 126.21, 126.13, 125.90, 125.00, 124.79, 124.73, 124.70, 124.65, 122.78, 119.45, 118.33, 114.95, 113.59, 111.68, 68.00, 67.70, 37.27, 37.23, 36.35, 36.11, 29.75, 29.73, 25.72, 25.70, 25.55, 19.65, 19.63, 17.66, HRMS (ESI-Q-TOF): \(C_{45}H_{52}NO_2\) [M + H]^+: cal. \(m/z\) 638.3993, found, \(m/z\) 638.4020 (error 4ppm)

**Compound (4) DC**: Yellow semi-solid, \(\epsilon\) in CH\(_3\)CN = 15596 M\(^{-1}\)cm\(^{-1}\), Yield 60%(120mg): \(^1\)H-NMR (500MHz,CDC\(_3\)) \(\delta\) (ppm): 8.61-8.60 (d, 1H), 8.44 (s,1H), 8.28-8.23 (dd, 4H) 8.19-8.17


(d, 1H) 8.15-8.09 (dd, 2H), 8.13-8.09 (dd, 1H), 7.41-7.39 (dd, 1H), 7.33 (s, 1H), 7.00-6.98 (d, 1H), 5.13-5.11(m, 2H), 4.16-4.11(m, 4H), 2.17-1.25 (m, 23H), 1.01-0.99(d, 6H)

$^{13}$C-NMR (125 MHz, CDCl$_3$): δ (ppm) 150.61, 149.53, 138.35, 132.60, 131.35, 131.31, 131.84, 130.78, 129.73, 128.60, 128.56, 127.48, 127.42, 126.32, 126.21, 126.13, 125.90, 125.00, 124.79, 124.73, 124.70, 124.65, 124.62, 122.78, 119.45, 118.33, 114.95, 113.59, 111.68, 68.00, 67.70, 37.27, 37.25, 36.35, 36.11, 29.75, 29.73, 25.72, 25.70, 25.55, 19.65, 19.63, 17.66, HRMS (ESI-Q-TOF): C$_{45}$H$_{52}$NO$_2$ [M + H]$^+$: cal. m/z 638.3993, found, m/z 638.4020 (error 4ppm)

**Compound (5) TA:** Yellow liquid, (ε) in CH$_3$CN= 10621 M$^{-1}$cm$^{-1}$, Yield 50% (159mg): $^1$H-NMR (500MHz, CDCl$_3$), δ (ppm): 8.60-8.59 (d, 1H), 8.4 (s,1H), 8.27-8.24 (m,4H), 8.20-8.18 (d,1H), 8.18-8.16 (dd, 2H), 8.12-8.05 (dd, 1H), 7.01(s, 2H), 5.13-5.11 (m,3H), 4.15-4.0 (m,6H), 2.04-1.22 (m,48H), 0.99-0.97 (t, 9H),

$^{13}$C-NMR (125MHz, CDCl$_3$): δ (ppm) 153.64, 139.72, 139.61, 132.75, 131.34, 131.23, 131.09, 130.77, 129.79, 129.76, 128.70, 128.31, 127.48, 126.36, 126.24, 126.22, 125.99, 135.02, 124.91, 124.78, 124.69, 124.62, 122.76, 115.24, 105.13, 71.87, 67.81, 37.39, 37.28, 37.25, 37.23, 29.62, 29.52, 29.34, 25.71, 25.69, 25.38, 19.57, 19.54, 19.51, 17.67, 17.62, HRMS (ESI-Q-TOF): C$_{55}$H$_{70}$NO$_3$ [M + H]$^+$: cal. m/z 792.5350, found, m/z 792.5375 (error 3.1ppm)

**Compound (6) TC:** Yellow liquid, (ε) in CH$_3$CN = 10621 M$^{-1}$cm$^{-1}$, Yield 50% (159mg): $^1$H-NMR (500MHz, CDCl$_3$), δ (ppm): 8.60-8.59 (d, 1H), 8.4(s,1H), 8.27-8.24 (m,4H), 8.20-8.18 (d, 1H), 8.18-8.16 (dd, 2H), 8.12-8.05 (dd, 1H), 7.01(s, 2H), 5.13-5.11(m, 3H), 4.15-4.0(m, 6H), 2.04-1.22 (m,48H) 0.99-0.97 (t, 9H)

$^{13}$C-NMR (125MHz, CDCl$_3$): δ (ppm) 153.64, 139.72, 139.61, 132.75, 131.34, 131.23, 131.09, 130.77, 129.79, 129.76, 128.70, 128.31, 127.48, 126.36, 126.24, 126.22, 125.99, 135.02, 124.91, 124.78, 124.69, 124.62, 122.76, 115.24, 105.13, 71.87, 67.81, 37.39, 37.28, 37.25, 37.23, 29.62, 29.52, 29.34, 25.71, 25.69, 25.38, 19.57, 19.54, 19.51, 17.67, 17.62, HRMS (ESI-Q-TOF): C$_{55}$H$_{70}$NO$_3$ [M + H]$^+$: cal. m/z 792.5350, found, m/z 792.5375 (error 3.1ppm)
Fig.S1 Absorption spectra of a) MA b) MC in different organic solvents and water. Concentration 20µM, ExWl 385nm

Fig.S2 Absorption spectra of a) TA b) TC in different organic solvents and water. Concentration 20µM, ExWl 385nm
Fig S3 Normalized Emission spectra of a) DA b) DC in different organic solvents and water. Concentration 20μM, ExWl 385nm

Fig.S4 Normalized Emission spectra of a) TA b) TC in different organic solvents and water. Concentration 20μM, ExWl 385nm
Fig. S5 Emission spectra of a) MA b) MC in water/binary mixture. Concentration 20μM, ExWl 380nm

Fig. S6 Emission spectra of a) TA b) TC in water/binary mixture. Concentration 20μM, ExWl 385nm

Fig. S7 Lifetime decay of a) MA & b) MC in 90% water solution at 405nm excitation
Fig.S8 Lifetime decay of a) DA & b) DC in 90% water solution at 405nm excitation.

Fig.S9 Lifetime decay of a) TA & b) TC in 90% water solution at 405nm excitation.
Fig.S10 Cryo-SEM images of MC, DC and TC.
Fig.S11 DLS data of a) MA, b) MC, c) DA, d) DC, e) TA, and f) TC.
Fig S12: Dropcast SEM images obtained for a) MA, MC b) DA, DC and c) TA and TC
Fig. S13 The emission of organogels of a) MA and b) DA and their solution state.

Fig. S14 The emission spectra of MA & MC in solid state. Ex. W1 385nm
Fig. S15  Powder XRD data of DA & DC obtained in its xerogel state. The compounds are semisolids and hence powdered measurement was not performed.

Fig. S16  $^1$H-NMR titration spectra of MA in CDCl$_3$ solution (aromatic region)
Fig. S17 $^1$H-NMR titration spectra of DA in CDCl$_3$ solution (aromatic region)

Fig. S18 $^1$H-NMR titration spectra of MA in CDCl$_3$ solution (aliphatic region)
Fig.S19 $^1$H-NMR titration spectra of DA in CDCl$_3$ solution (aliphatic region)
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Fig. S23 $^1$H and $^{13}$C NMR spectrum of MA I
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Fig. S27 $^1$H and $^{13}$C NMR spectrum of TA 5
Fig.S28 $^1$H and $^{13}$C NMR spectrum of TC 6.