Supporting Information

Mechanochromic Luminescent Property of A Polypeptide-based Dendron

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**Experimentals**

$^1$H NMR was recorded on 400 MHz (Bruker ARX400) and $^{13}$C NMR spectra were recorded on Bruker 100 MHz spectrometer at room temperature with DMSO as the solvents and tetramethylsilane (TMS) as the internal standard. ESI high resolution mass-spectra (HRMS) were acquired on a Bruker Apex IV FTMS mass spectrometer. Differential scanning calorimetry (DSC) measurements were carried out on TA Instruments DSC Q100. Polarized optical microscopy (POM) images were recorded using a Leica DLMP microscope. 1D small angle X-ray scattering (SAXS) experiments were performed with a SAXS instrument (SAXSess, Anton Paar) equipped with Kratky block-collimation system. The scattering patterns of SAXS were simultaneously recorded on an imaging plate (IP) with a pixel size of 42.3×42.3μm$^2$ which extended to high-angle range (the $q$ range covered by the IP was from 0.06 to 29 nm$^{-1}$). The scattering peak positions were calibrated with silicon powder for wide-angle region and silver behenate for small-angle region, respectively. After background subtraction, desmearing was performed according to the Lake’s method. 1D WAXD powder experiments were performed on a Philips X’Pert Pro diffractometer with a 3 kW ceramic tube as the X-ray source (Cu KR) and an X’celerator detector. The reflection peak positions were calibrated with silicon powder ($2\theta > 15^\circ$) and silver behenate ($2\theta< 10^\circ$). FT-IR spectrum was obtained using a Nicolet Magna IR-750 spectrometer in a CaF$_2$ plate. UV-vis spectra were acquired on a Varian CARY 1E UV-vis spectrophotometer. Fluorescence spectra and the calculation of quantum yield were performed on the Nanolog/ FluoroLog-3-2- Ihr320.
combined measurement system for infrared fluorescence equipped with an integrating sphere. Fluorescence decay spectra were measured on FLS 920 lifetime and steady state spectrometer ($\lambda_{ex} = 345$ nm). Geometry optimization of 1 was performed by “Forcite” modules in Material Studio Modeling 5.0 Software package. Atomic force microscopy (AFM) measurement was implemented on a SPA-400 multimode AFM and SPI3800N probe station.

1. Synthesis of 1

Gly-Asp G2-NH$_2$CF$_3$COO (280 mg, 0.28 mmol) [1], TEA (0.5 mL) and 1-pyrenecarboxylic acid (82 mg, 0.33 mmol) were mixed in chloroform (20 mL) with stirring in ice-salt bath. N,N'-dicyclohexylcarbodiimide (86 mg, 0.42 mmol) and N-Hydroxybenzotriazole (10 mg, 0.074 mmol) was added after 10 min. The reaction mixture was stirred for 2 day and concentrated under vacuum. Pure 1 (green solid) was obtained by the purification of silica gel column chromatography using CHCl$_3$/THF (5:1) as the eluent (yield 58%).
\(^1\)H NMR (400 MHz, DMSO, TMS, \(T = 298\) K): 8.67-8.64 (d, 1H, pyrene-H), 8.51-8.10 (m, 8H, pyrene-H), 7.34-7.29 (m, 20H, Ph-H), 5.08-5.02 (m, 8H, \(-CH_2\)-Ph), 4.78-4.69 (m, 3H, \(-CH_2\)-), 4.16-4.05 (m, 2H, \(-CH_2\)-), 3.83-3.70 (m, 4H, \(-CH_2\)-), 2.94-2.60 (m, 6H, \(-CH_2\)-).

\(^{13}\)C NMR (400 MHz, DMSO, TMS, \(T = 298\) K): 171.11, 170.29, 169.89, 169.81, 169.78, 169.70, 169.36, 169.28, 169.08, 168.89, 168.73, 135.77, 135.65, 131.69, 131.37, 130.69, 130.21, 128.36, 128.00, 127.96, 127.87, 127.65, 127.62, 127.18, 126.55, 125.76, 125.59, 125.32, 124.91, 124.35, 123.75, 123.63, 66.25, 65.86, 49.82, 48.50, 42.70, 41.87, 37.38, 35.72.

Element Cal. For \(C_{63}H_{58}N_6O_{14}\). C, 67.37; H, 5.20, N, 7.48. Found. C, 67.19; H, 5.47, N, 7.43. HR-ESI Cal. For \(C_{63}H_{58}N_6O_{14}\): 1122.4011. Found. [M+H]: 1123.4071
2. Fluorescence decay profile of 1 in solution, drop cast aggregates and ground solids.

Figure S1. Fluorescence life time decay profile of 1 in CH₂Cl₂ solution (black) and instrument response function (red).

Figure S2. Fluorescence life time decay profile of drop cast aggregates (black) and instrument response function (red).
**Figure S3.** Fluorescence life time decay profile of grinding solid (black) and instrument response function (red).

3. UV-vis spectra of 1 in different states.

**Figure S4.** The absorption spectra of 1 in different states.
4. The optimized geometry of 1.

Figure S5. The optimized geometry of 1 in the gas phase calculated by using Forcite in Material Studio 5.0

5. Illustration of self-assembled structure of 1 in drop cast aggregates.

Figure S6. Illustration of self-assembled structure of 1 in drop cast aggregates.
6. Illustration of self-assembled structure of 1 in grinding solid.

Figure S7. Illustration of self-assembled structure of 1 in grinding solid.

7. SAXS profiles of 1 in different states.

Figure S8. SAXS profiles of original drop cast aggregates (black lines) and grinding solid treated with CH₂Cl₂ (red line).
8. Infrared absorption of 1 in different states

![Infrared absorption graph]

**Figure S9.** Infrared absorption of 1 before (black) and after grinding (red). (normalized to the C-H stretching at 2922 cm⁻¹).

9. Thermoanalytical profiles of 1.

The heating process was kept at the rate of 10 °C/min. The thermal gravimetric analysis (TGA) profile exhibited no decomposition of 1 during the temperature range.

![DSC profiles graph]

**Figure S10.** DSC profiles of drop cast aggregates (black) and finely grinding sample (red).
10. Fluorescent spectra of 1 at different cooling rates.

![Fluorescent spectra](image)

**Figure S11.** The fluorescence of 1 under different processing conditions. a) slow cooling at 10 °C/min from isotropic state. b) fast quenching from isotropic state.

11. Visual observation and AFM images of 1 at different cooling rates.

![Visual observation and AFM images](image)

**Figure S12.** Visual observation under 365 nm UV light (up) and AFM images (down) of 1 at room temperature by a) cooling at less than 10 °C/min from isotropic state; b) fast quenching from isotropic state.
12. WAXD pattern for drop cast aggregates 1 at different cooling rates.

![WAXD pattern](image)

**Figure S13.** WAXD patterns for drop cast aggregates 1 at different cooling rates from isotropic state.

13. Photopatterned images prepared by drop cast aggregates of 1.

![Photopatterned images](image)

**Figure S14.** The drop cast aggregates of 1 with “T” shape shearing under ambient light (left) and 365 nm UV light irradiation (right).
Reference