Electronic Supplementary Material (ESI) for Analytical Methods.

An electrostatically regulated organic self-assembly for rapid and sensitive detection of heparin in serum

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1. Instruments

NMR spectra was recorded on a Bruker Avance III spectrometer at 500 MHz for ^{1}H-NMR and 125 MHz for ^{13}C-NMR (Bruker, Germany). UV-visible spectra was measured on a TU-1901 spectrometer (Persee, China). Fluorescence spectroscopic studies were performed on a Hitachi F-7000 spectrometer (Hitachi, Japan), with 5 nm bandwidth for both excitation and emission and 700 V photomultiplier voltage. Zeta Potential and Dynamic Light Scattering (DLS) Size were measured on a Zetasizer Nano ZS90 instrument (Malvern, UK). The absolute fluorescence quantum yield was measured on a PL FS5 spectrometer (Edinburgh, UK). Conductivity was measured on a DDS-307A conductivity meter (Leici, China).

2. Preparation of stock solution

A stock solution of Tris-HCl (100 mM) was prepared by dissolving Tris-HCl solid in ultrapure water, and then adjusted to pH 7.0 with NaOH. The stock solutions of Hep (0.5 mg/mL), PRTM (0.5 mg/mL), ions (10 mM), thiols(10 mM), CA(10 mM), Glu(10 mM), BSA(10 mg/mL), ATP(10 mg/mL), Dex(10 mg/mL), HA(10 mg/mL) and ChS (10 mM) were prepared in ultrapure water and stored at 4 °C. A stock solution of PYPN (1 mM) was obtained by dissolving PYPN powder in DMSO and stored at room temperature. The test solution for conductivity was prepared by dispersing an appropriate amount of PYPN solid in ultrapure water (containing 2% DMSO) with ultrasound assistance. The ultrapure water was prepared from Milli-Q water system (18.25MΩ cm, 25 °C).

3. Calculation of detection limit

The detection limits of PYPN for Hep and PRTM were calculated according to the equation recommended by IUPAC. Detection Limit = 3σ/S, where σ is the standard deviation of the fluorescence intensity ratio of PYNN or PYNN-Hep complex in 11 parallel assays, S is the slope of the plot of fluorescence intensity ratio versus the concentration of Hep or PRTM. The detection limits of PYNN for Hep and PRTM in Tris-HCl (10 mM, pH=7.0) were calculated as 0.69 μg/mL and 2.47 μg/mL, respectively.

4. Linear relationship between the fluorescence intensity ratio F_{610}/F_{470} and Hep concentration in Tris-HCl

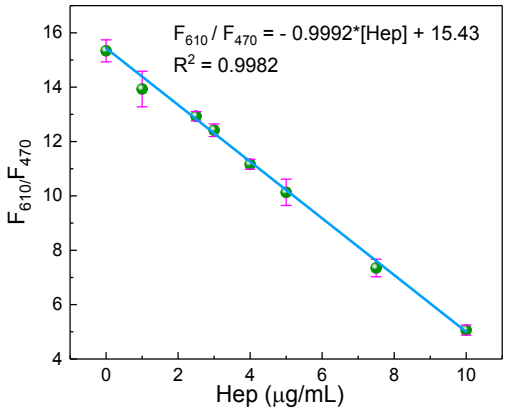

Fig. S1. The linear relationship between the fluorescence intensity ratio F_{610}/F_{470} of PYPN (20 μM) and Hep concentration (0-10 μg/mL) in Tris-HCl (10 mM, pH=7.0) solution.

5. Linear relationship between the fluorescence intensity ratio F_{610}/F_{470} and PRTM concentration

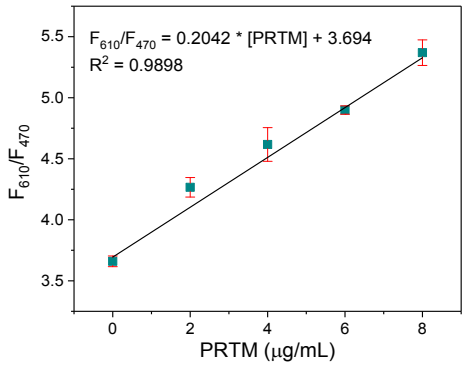

Fig. S2. The linear relationship between the fluorescence intensity ratio F_{610}/F_{470} of PYPN (20 μM) -Hep (20 μg/ml) complex and PRTM concentration (0~8 μg/mL) in Tris-HCl (10 mM, pH=7.0) solution.

6. Reponse rate of PYPN to Hep

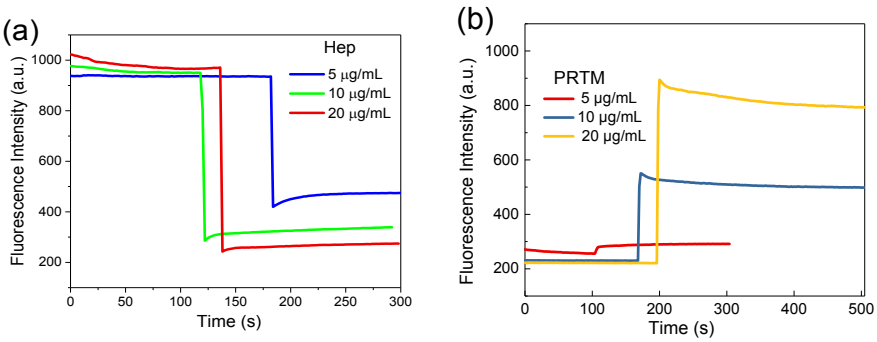

Fig. S3. The fluorescence intensity of PYPN (20 μM) at 610 nm changes with time after (a) adding Hep (5, 10 and 20 μg/mL) and (b) PRTM (5, 10 and 20 μg/mL) in sequence. The fluorescence was measured at room temperature. λ_{ex} = 405 nm.

7. The effect of acidity

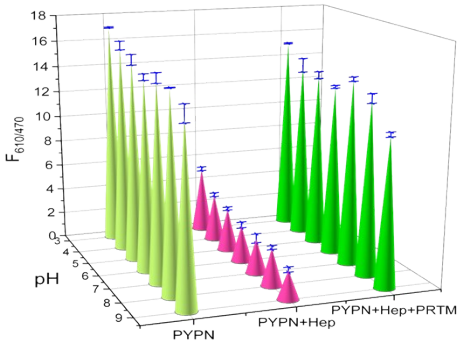

Fig. S4. The fluorescence intensity ratios F_{610}/F_{470} of PYPN (20 μM), PYPN (20 μM) -Hep (20 μg/mL) complex and PYPN (20 μM) - Hep (20 μg/mL) - PRTM (20 μg/mL) mixture in buffer solutions of different pH (3-10). The fluorescence was measured at room temperature. λ_{ex} = 405 nm.

8. Structure characterization

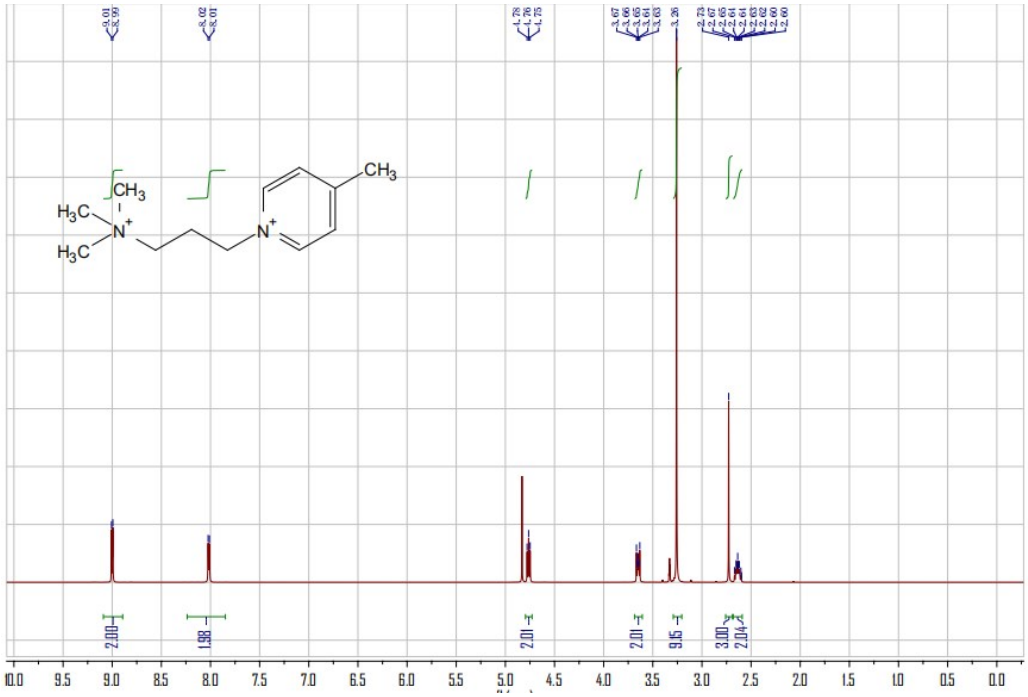

Fig. S5. ^{1}H NMR spectra of compound 1

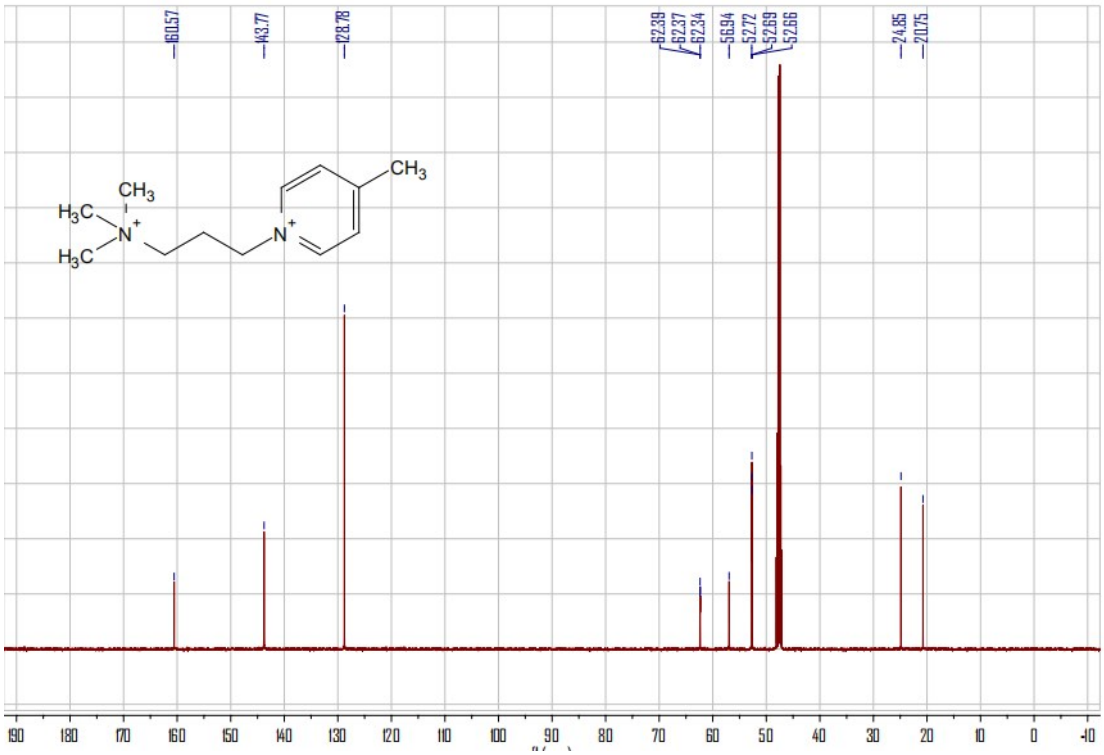

Fig. S6. ^{13}C NMR spectra of compound 1

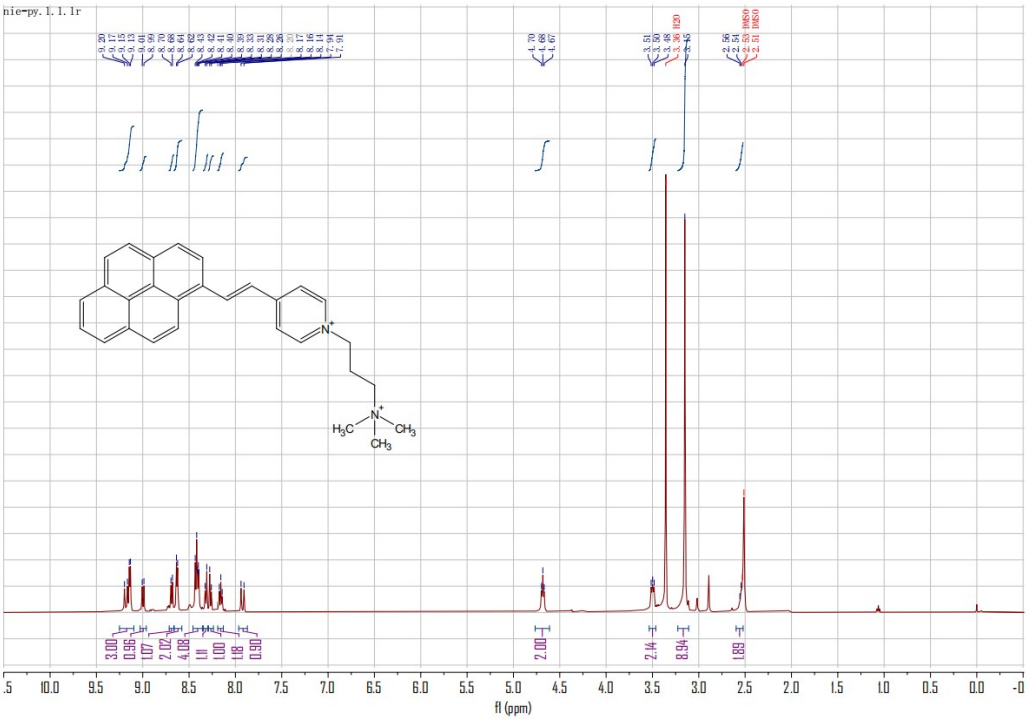

Fig. S7. ^{1}H NMR spectra of PYPN

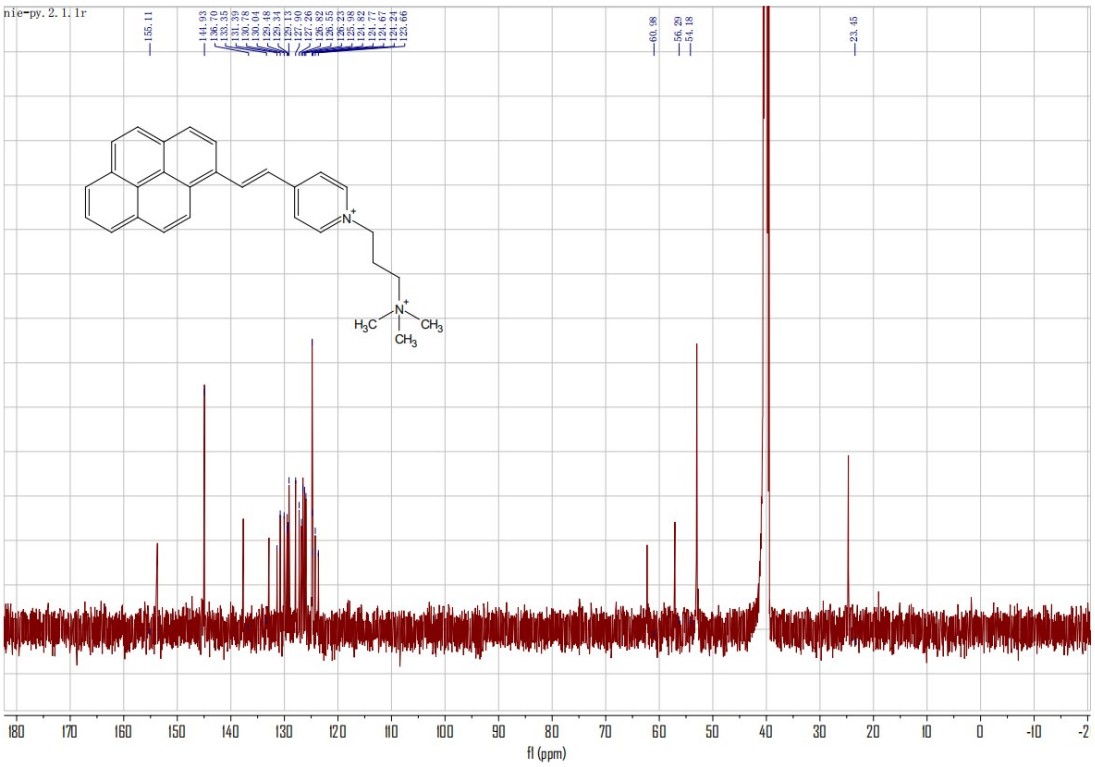

Fig. S8. ^{13}C NMR spectra of PYPN

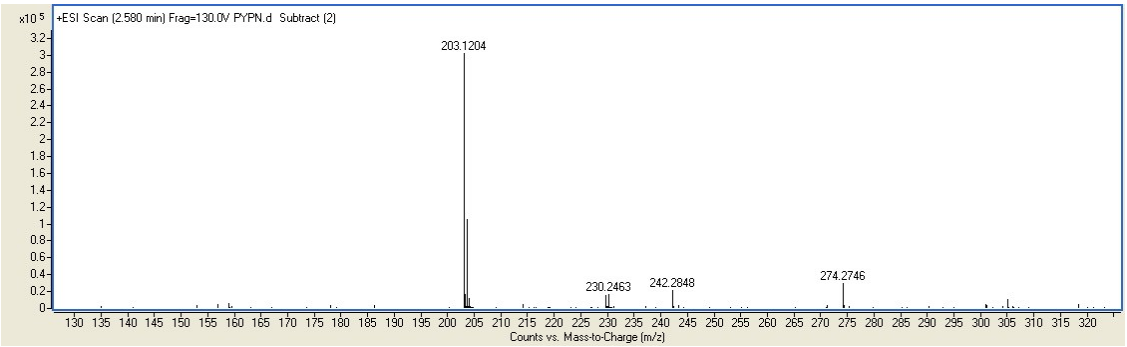

Fig. S9. EMI-MS spectra of PYPN