Supporting information for

Self-Assembled Carbazole Amphiphiles for Postharvest Monitoring of Pest Infestation through Uric Acid Detection

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Experimental Section

General: All chemicals (reagents, solvents, and chemicals) were bought from best-known local chemical suppliers, such as Spectrochem, Avra, Alfa Acer, etc and used without further purification. FTIR spectra were recorded on a Perkin-Elmer FTIR Spectrum BX system and were reported in wave numbers ($cm^{-1)}$. On the other hand, ^{1}H NMR and ^{13}C NMR spectra were recorded with a Bruker Advance DRX 400 spectrometer operating at 400 and 100 MHz for ^{1}H and ^{13}C NMR spectroscopy, respectively. Chemical shifts were reported in ppm downfield from the internal standard, tetramethylsilane (TMS). Mass spectra were recorded on a Micromass Q-TOF Micro TM spectrometer.

Spectroscopic studies: The UV-Vis spectroscopic studies were recorded on a Shimadzu model 2100 spectrometer, whereas the fluorescence spectra were recorded on a Cary Eclipse Spectrofluorometer. The slit-width for the experiment was kept at 5 nm. Sensing was carried out by adding requisite amounts of Uric acid and other analytes to compounds **1** and **2** (1×10^{-5} M) in water.

Detection limit determination: The method used to calculate the detection limit is known as the blank variability method. In this method, the calibration curve was prepared by recording absorption spectra of **1** in an aqueous medium with different amounts of UA. From the equation obtained from the calibration plot, the added UA concentrations were calculated. Then another calibration curve was drawn between the C_{real} (added UA) vs. $C_{calc.}$ (Calculated amount of UA). This afforded a value of the slope (b). The absorbance of **1** in water without added UA was taken as a blank reading. A total of 10 replicates of the blank were measured. The standard deviation from the blank readings was calculated by fitting the absorbance reading into the equation obtained from the first calibration curve (titration spectra). Using this standard deviation value, we calculated the decision limit by the following equation.

$L_C = t_C \times s \times (1 + 1/N)1/2$……..……... (1)

where N = the number of blank replicates taken; the value of tc for 10 blank readings is 1.833; and s = the standard deviation. The detection limit (L_D) was calculated as the double of the decision limit obtained,

$L_D = 2\ L_c$ ……. (2)

In the concentration term, the detection limit appeared as,

$x_D = 2 \times C = 2\ L_C / b$ ……... (3)

where b = slope of the calibration curve (C_{real} vs. $C_{calc.}$).

^{1}H NMR Studies. ^{1}H NMR studies of **1** and **2** (5 mM) were performed in DMSO-d_6 and $CDCl_3$ medium. The spectra were recorded using identical parameters.

Scanning Electron Microscopy: A solution of **1** and **2** (concentration 10 μM) in an aqueous medium was drop-cast over a silicon wafer attached to the brass stubs and air-dried for 48 h. The samples were then coated with gold vapor and analyzed on a Quanta 200 SEM operated at 15 kV.

Synthesis of Compounds 1 and 2

Compounds **1** and **2** were synthesized according to previously reported methods (*J. Med. Chem.*, 2014, *57*, 6973-6988) with no major modifications. The structures and purities of both compounds were verified by ^{1}H NMR and HRMS, which were consistent with the reported data.

Additional Spectra

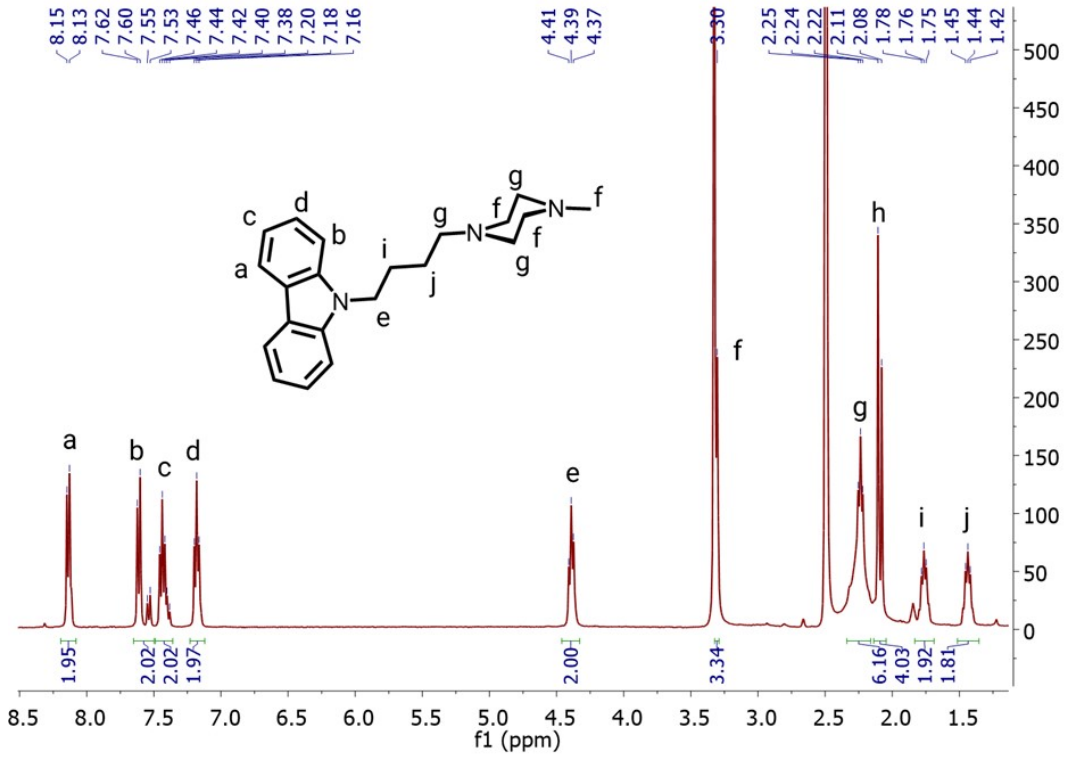

Figure S1. partial ^{1}H-NMR spectrum of 1 in DMSO-d_6 medium.

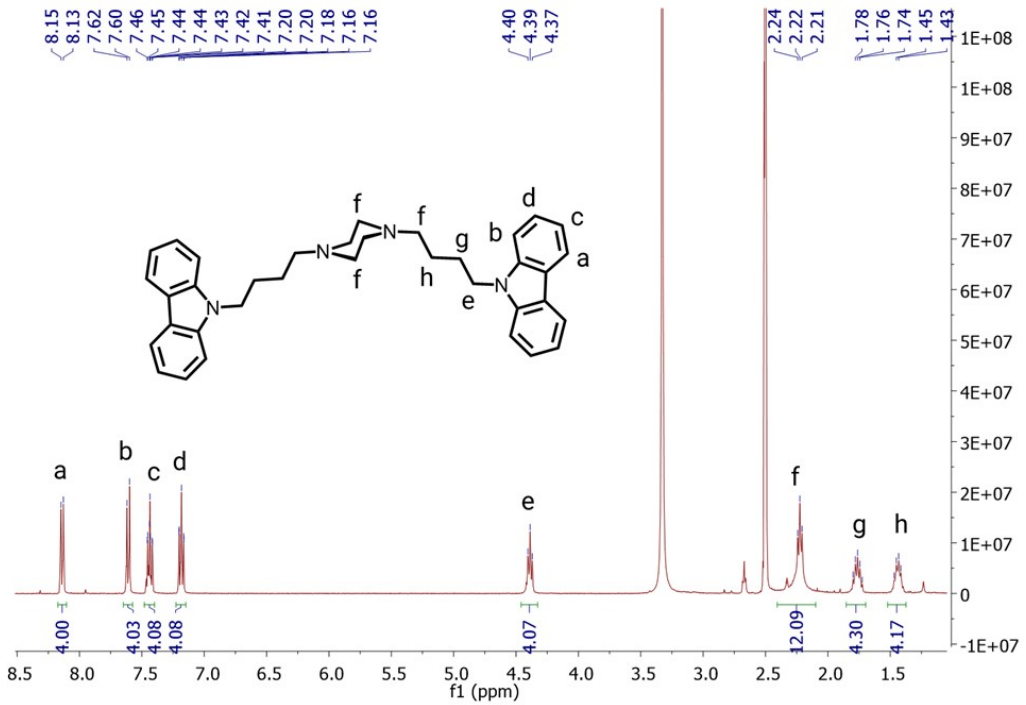

Figure S2. ^{1}H-NMR spectrum of 2 in DMSO-d_6 medium.

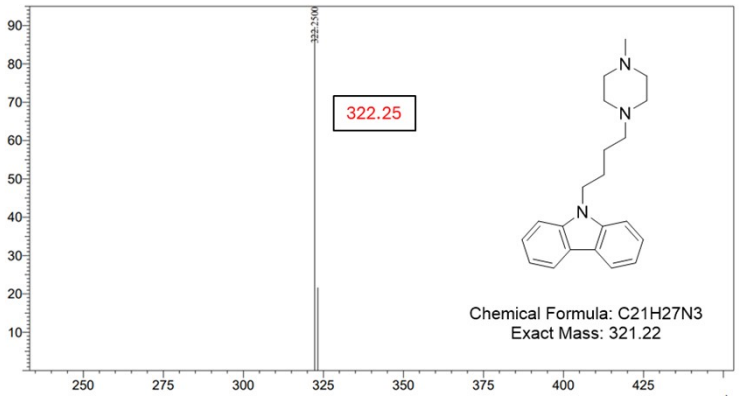

Figure S3. LCMS of compound 1.

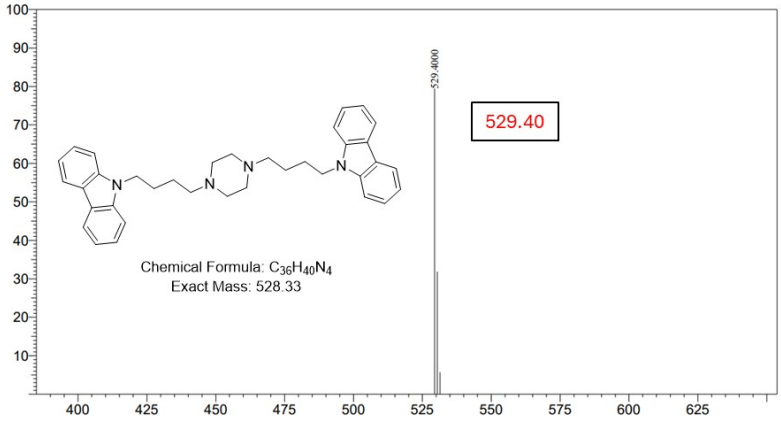

Figure S4. LCMS of compound 2.

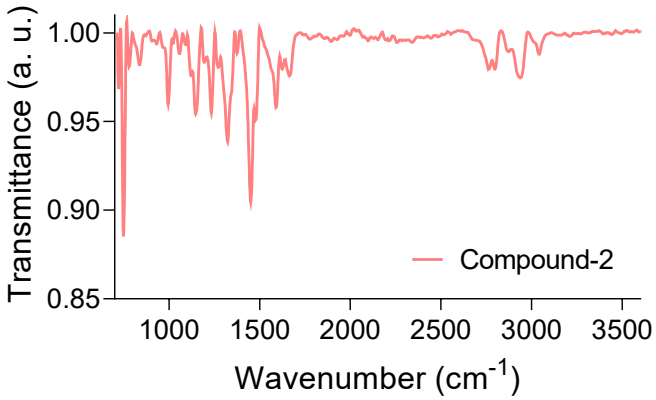

Figure S5. FTIR of compound 2.

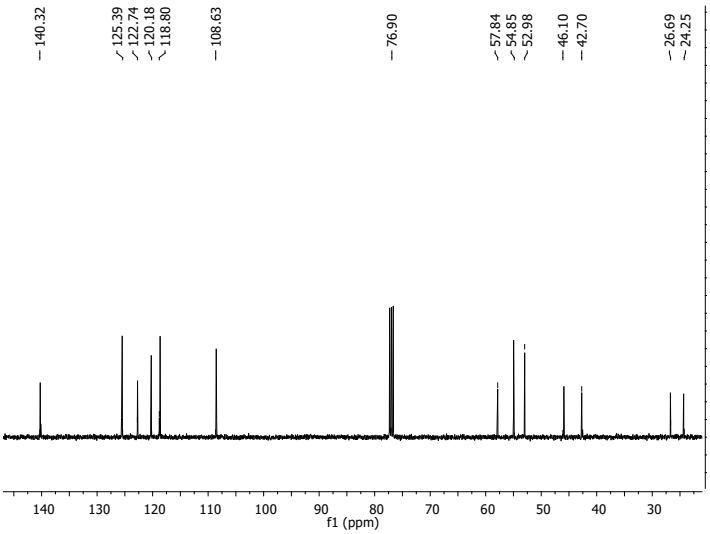

Figure S6. ^{13}C NMR of compound 1.

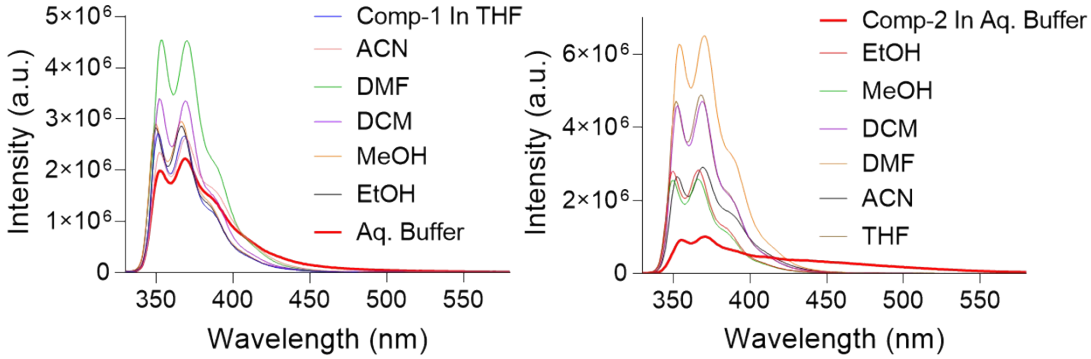

Figure S7. fluorescence spectra of 1 and 2 (10 μM, λex = 340 nm) in buffered medium (pH 7.0) and different organic solvents.

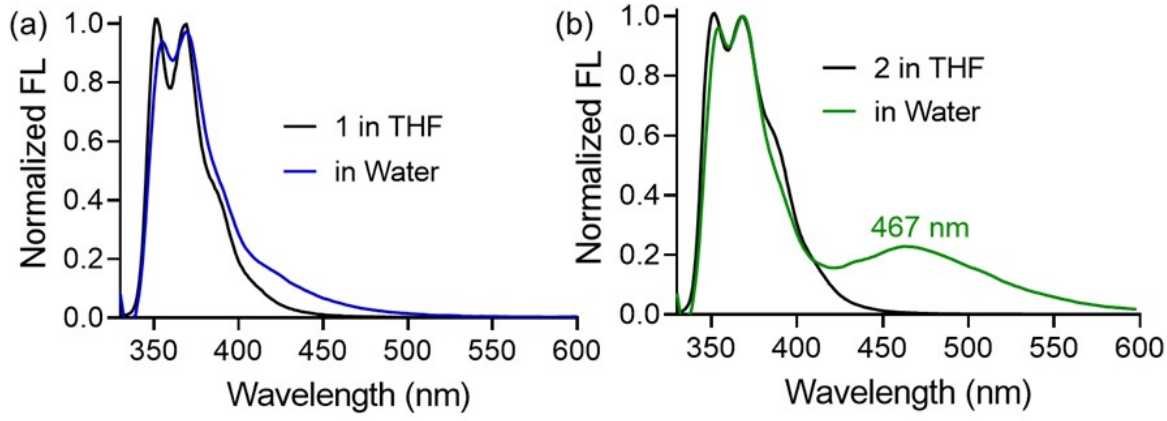

Figure S8. (a) Normalized fluorescence spectra of 1 (10 μM, λex = 340 nm) in THF and buffered medium (pH 7.0). (b) Normalized fluorescence spectra of 2 (10 μM, λex = 340 nm) in THF and buffered medium (pH 7.0).

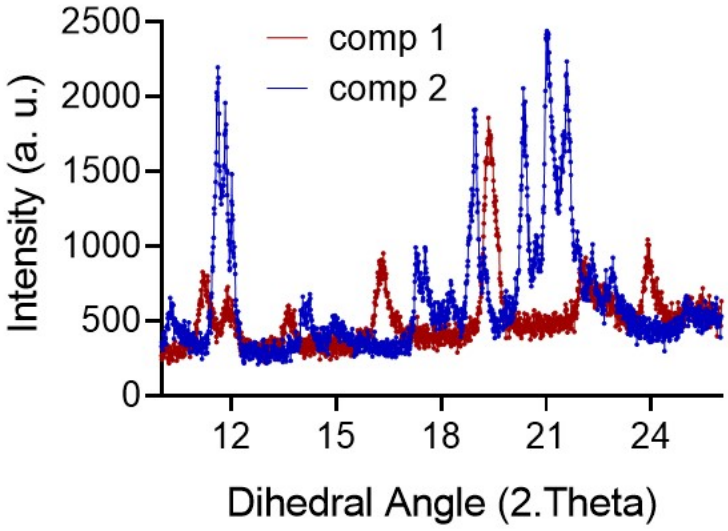

Figure S9. p-XRD of Compounds 1 and 2

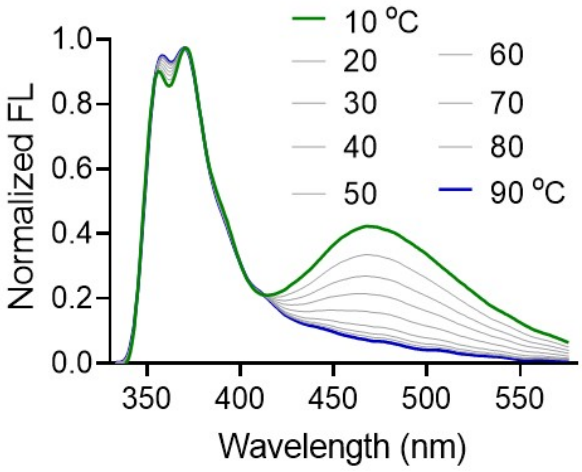

Figure S10. Normalized fluorescence spectra of 2 (10 μM, λex = 340 nm) at different temperatures in buffered medium (pH 7.0).

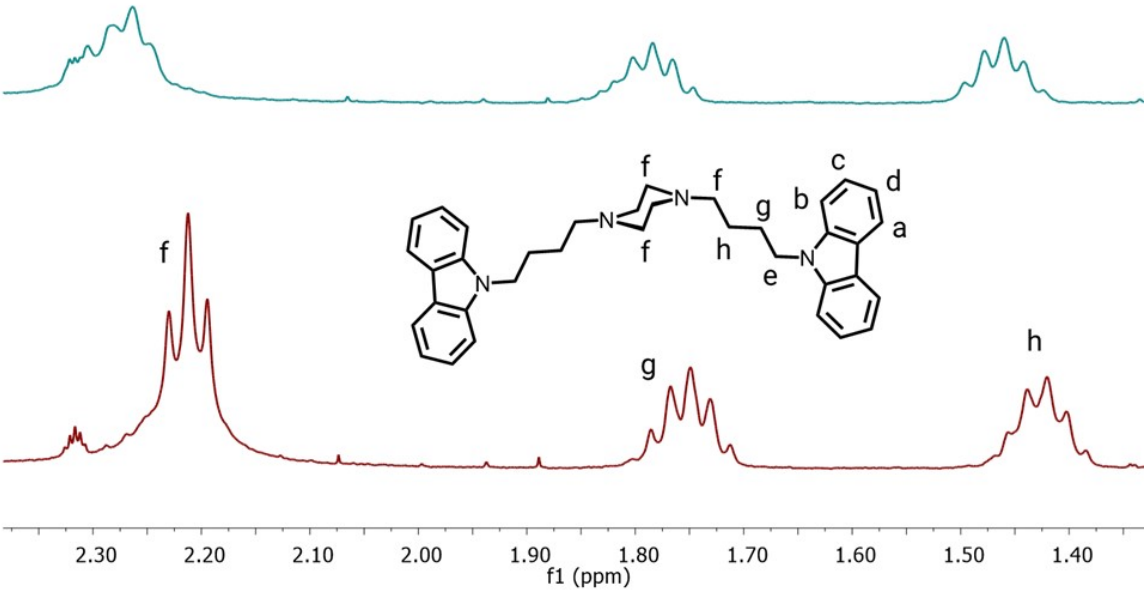

Figure S11. Partial ^{1}H-NMR spectra of 1 (5 mM, bottom) in DMSO-d_6 medium with and without UA (1 equiv, top)

	Dihedral Angle	Total Energy	HOMO	LUMO	Energy Gap (Ev)	H-bond Length (A^0)	Dipole Moment
Comp-1	55.37 (1,4 N)	-980.495	-0.187	-0.022	4.48	NA	1.58
Adduct	44.37 (1,4 N)	-1618.367	-0.198	-0.038	4.35	N1- 1.97 N4- 1.81	8.23

Table S1: DFT-calculated structural and electronic parameters of Comp-1 and Comp-1-UA complex.