

## *Supporting Information*

### **Aggregates of hydrazono-sulfonamide adduct as picric acid sensor**

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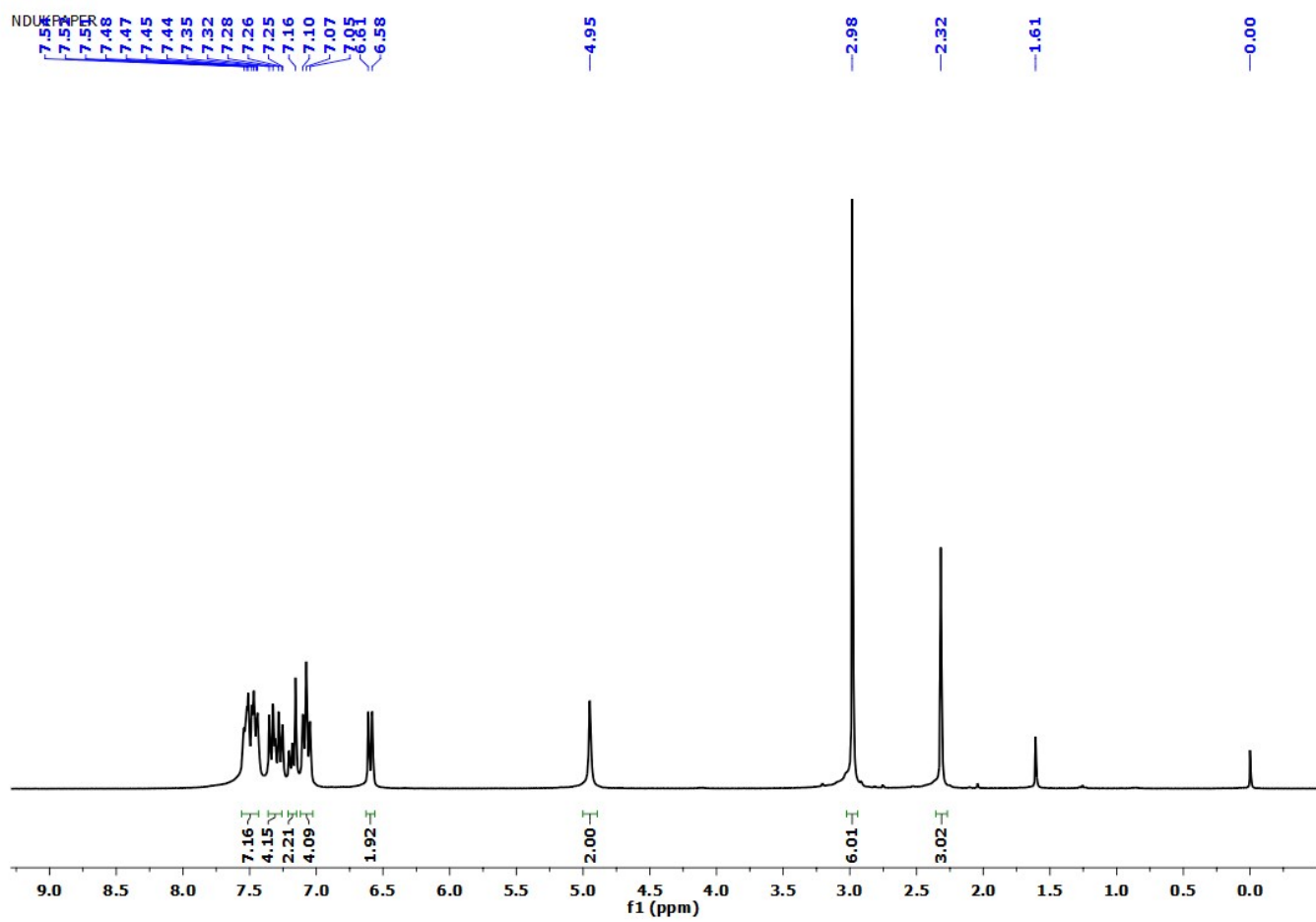
## General Methods

Unless stated otherwise, all solvents and chemicals were obtained from commercial sources and used without further purification. Analytical thin layer chromatography (TLC) was performed on precoated silica gel-G plates (Merck) using a mixture of petroleum ether (60-80 °C) and ethyl acetate (7:3) as the eluent. The  $^1\text{H}$  and  $^{13}\text{C}$  NMR spectra were recorded on a Bruker (Avance) 300 MHz instrument using TMS as an internal standard and  $\text{CDCl}_3$  as solvent. Chemical shifts are expressed in parts per million (ppm) and the coupling constants ( $J$  values) are expressed in hertz (Hz). The following abbreviations are used to indicate spin multiplicities: s (singlet), m (multiplet). Elemental analyses were carried out with Perkin-Elmer 2400 series II analyzer. Melting points were determined using open capillaries and were uncorrected. Absorption measurements were carried out in Agilent single beam UV-Diode Array spectrophotometer. Fluorescence spectra were recorded in Agilent Cary Eclipse Fluorescence spectrophotometer. The slit width was 5 nm for both excitation and emission. HPLC grade solvents were used for photophysical measurements. The stock solution of **AVM** was prepared in tetrahydrofuran (THF) for AIEE studies.

The crystal structure of compound **AVM** has been deposited at the Cambridge Crystallographic Data Centre and allocated the deposition number **CCDC 1404294**

**Caution!** The nitroaromatic compounds used in this study, specially TNT and picric acid, are very powerful explosives. They must be handled with care and also in very small quantities.

***NMR and Mass spectra for AVM***



**Figure S1.** <sup>1</sup>H NMR (CDCl<sub>3</sub>, 300 MHz) spectrum of AVM

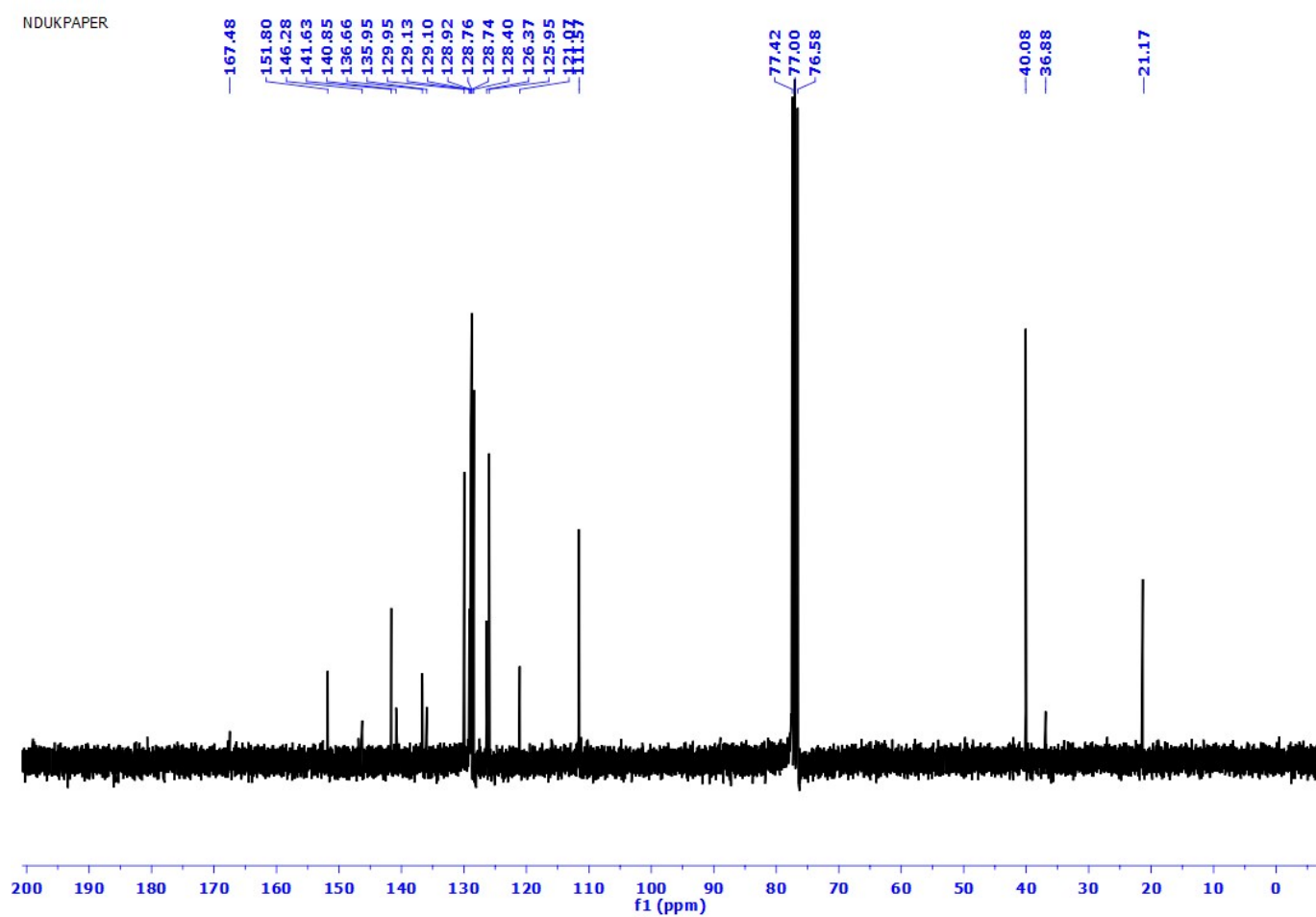


Figure S2.  $^{13}\text{C}$  NMR ( $\text{CDCl}_3$ , 75 MHz) spectrum of AVM

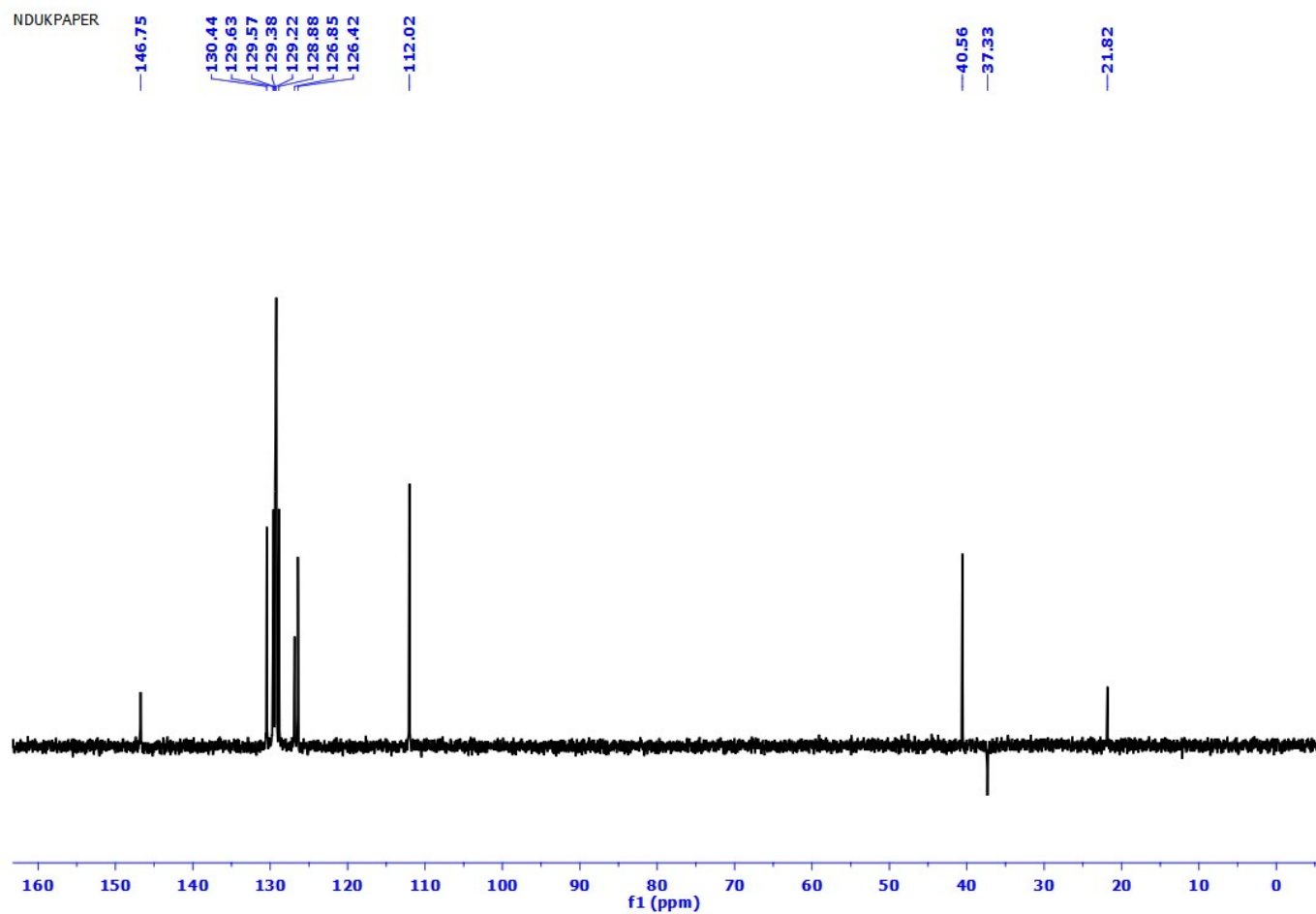
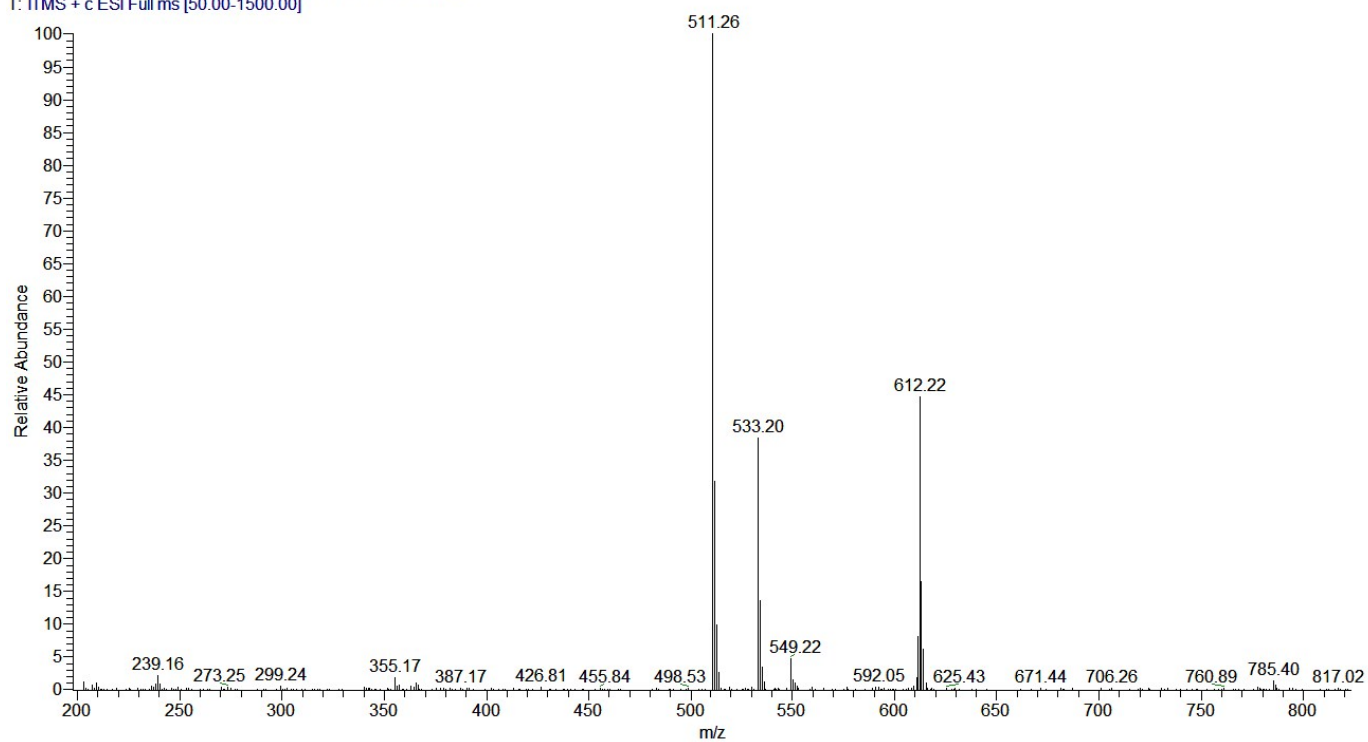
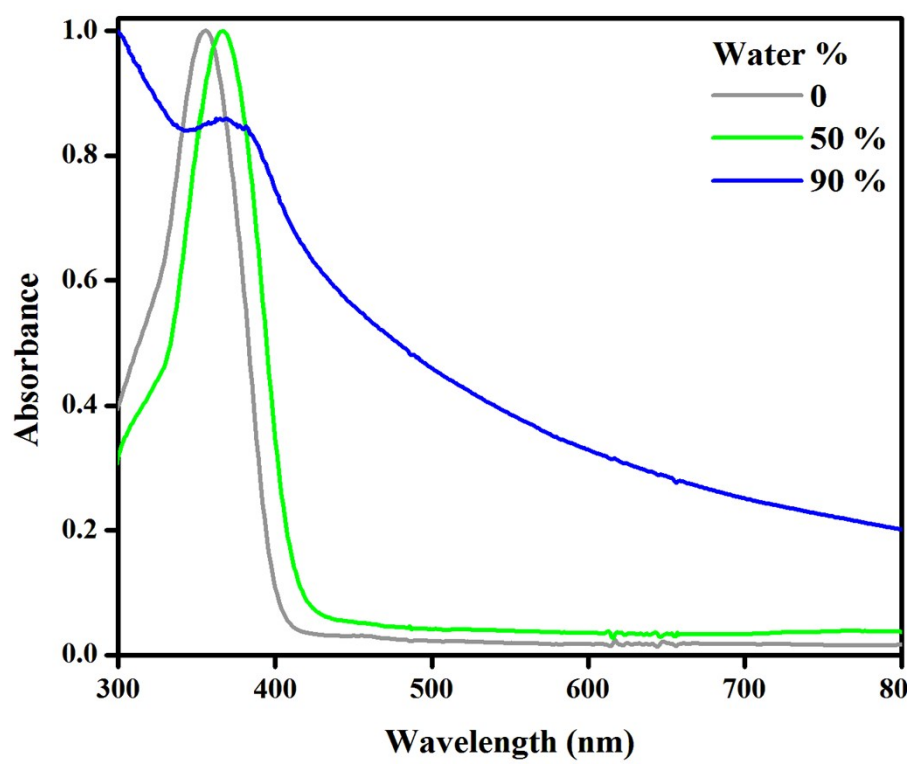


Figure S3. DEPT-135 spectrum of AVM

NDUK\_150518153207 (1) #57 RT: 0.84 AV: 1 NL: 1.11E4  
T: ITMS + c ESI Full ms [50.00-1500.00]

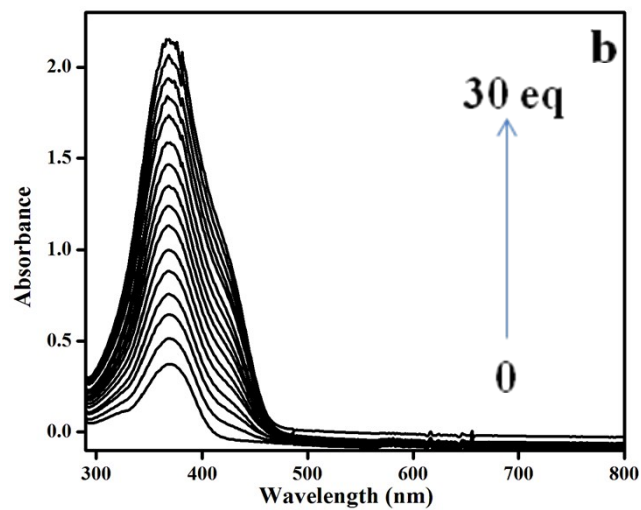
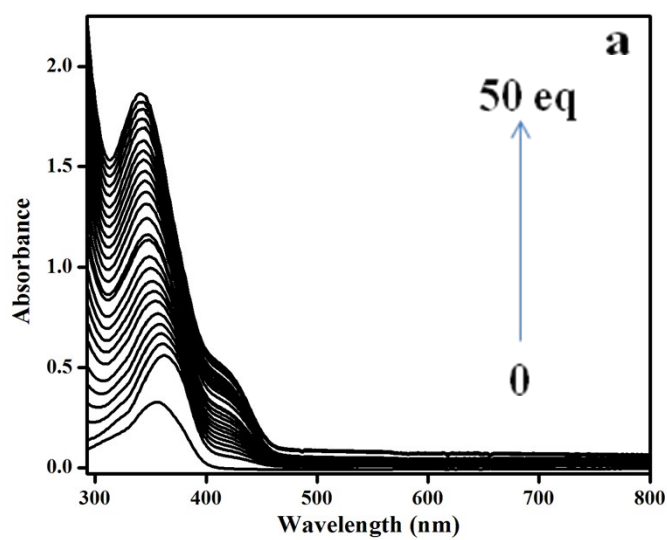


**Figure S4.** Mass spectrum of AVM

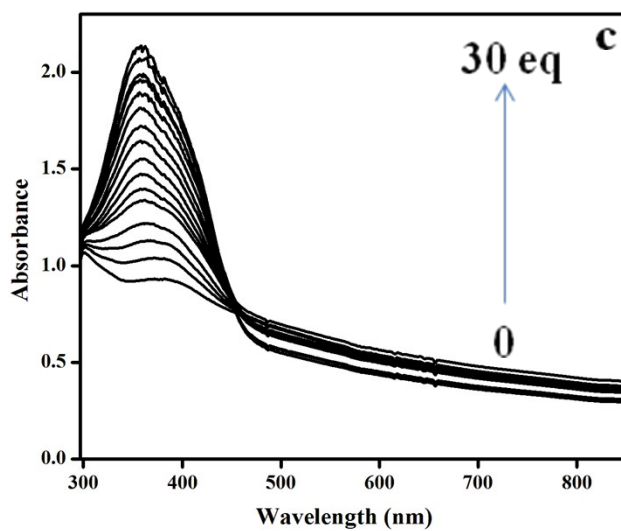


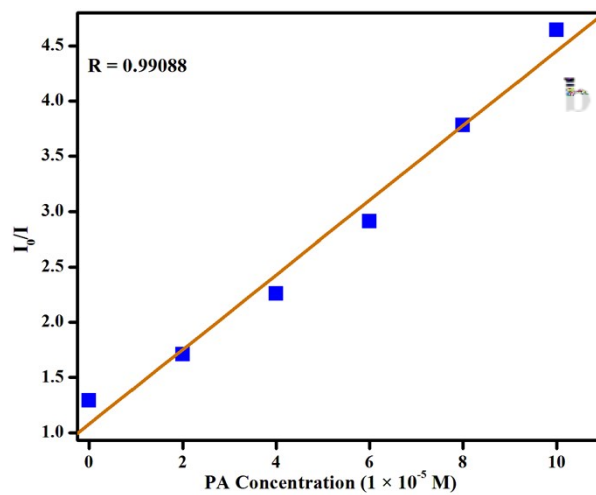
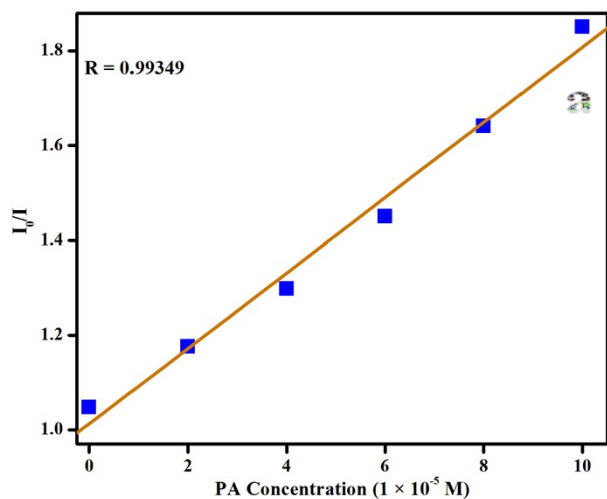
**Figure S5.** UV-vis spectrum of AVM ( $1 \times 10^{-5}$  M) in THF and THF–water mixtures



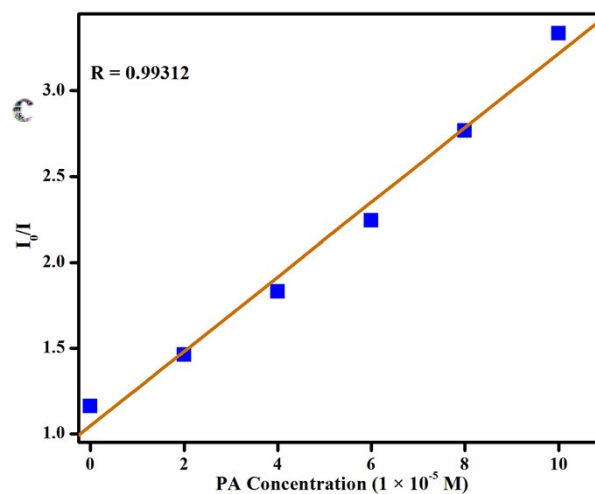


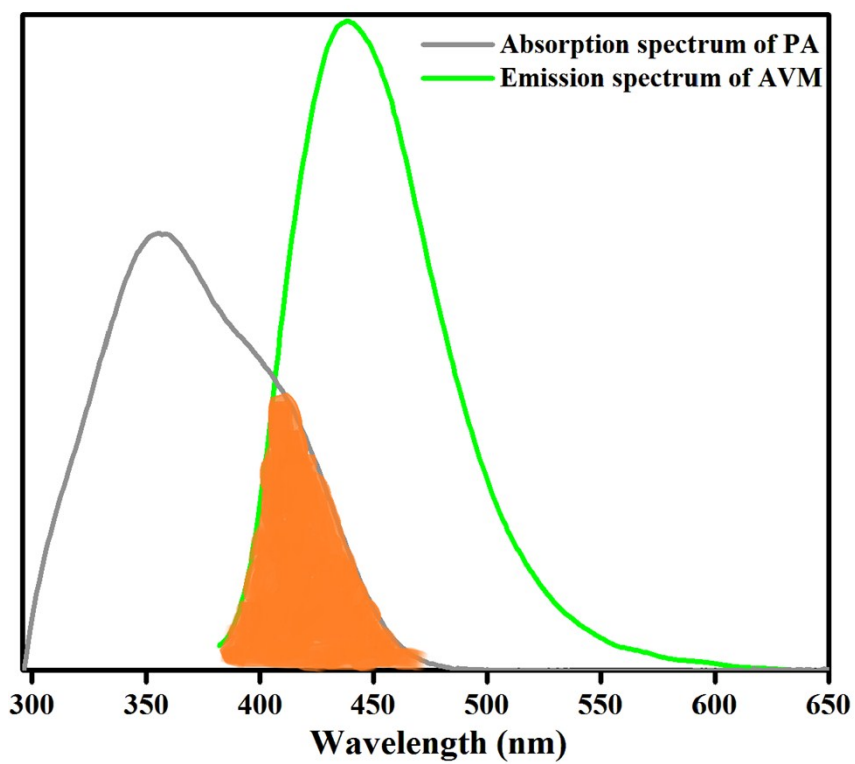
**Figure S6.** UV-vis spectral changes of AVM ( $1 \times 10^{-5}$  M) containing different concentration of PA in THF (a) and THF-water mixtures 50% (b) & 90% (c)



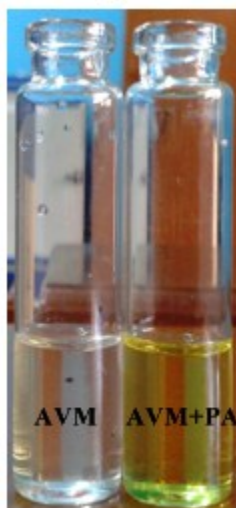


**Figure S7.** Stern-Volmer plot obtained at lower concentration of PA in THF (a) and THF–water mixtures 50% (b) & 90% (c)





**Figure S8.** Spectral overlap between absorption spectra of PA and emission spectrum of AVM



**Figure S9.** Visual color change upon mixing of PA with AVM

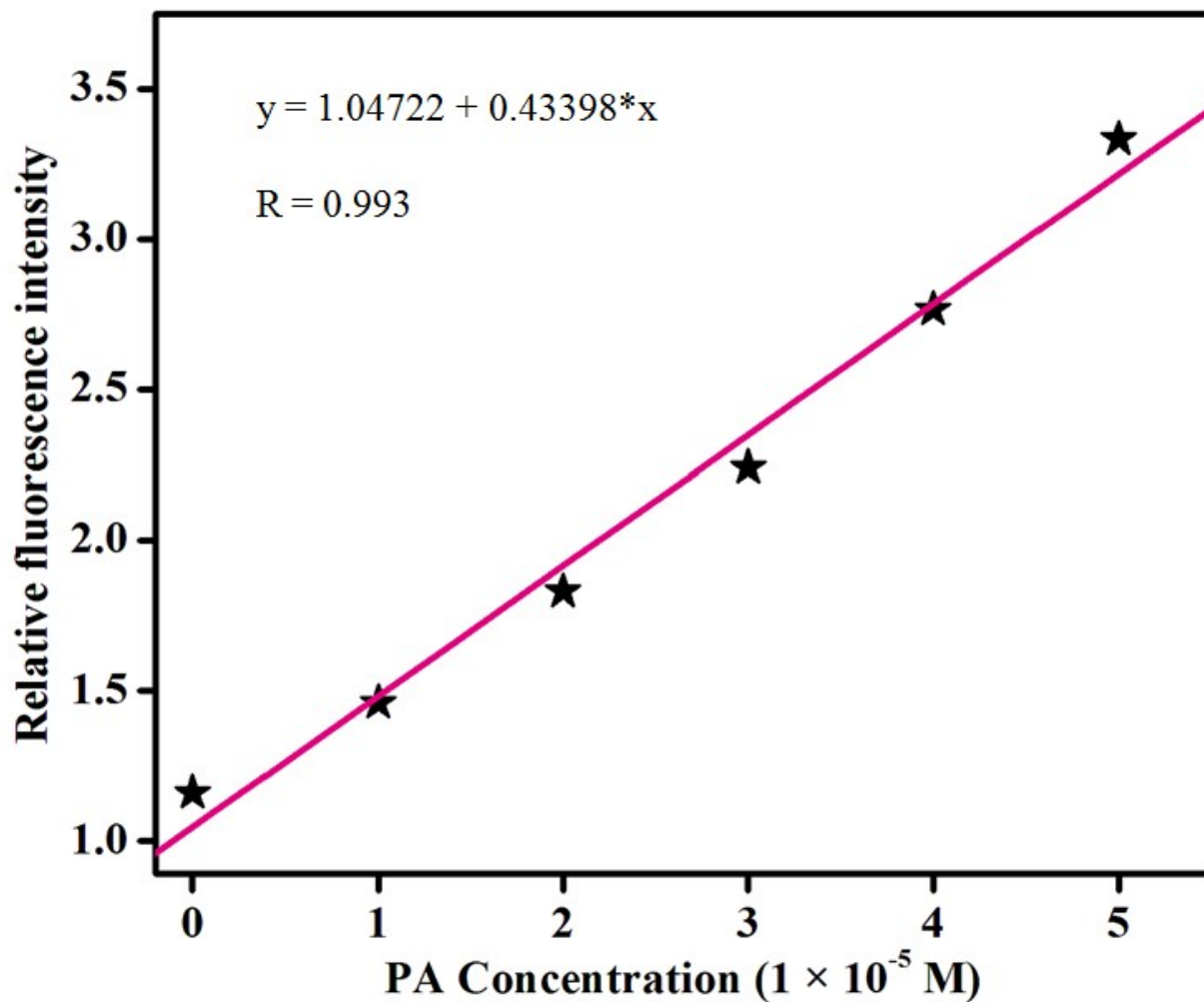
**Table S1. Optimized coordinates (Å) of AVM**

C	4.4305060	-0.9747070	0.5725640
C	5.1603040	-2.1873930	0.4641650
C	4.4450850	-3.3445430	0.0748660
C	3.0834110	-3.2810990	-0.1888180
C	2.3640480	-2.0810940	-0.0803420
C	3.0730700	-0.9283540	0.3071400
N	6.5153340	-2.2337070	0.7274460
C	7.2352850	-3.4892610	0.6140200
C	7.2240360	-1.0296360	1.1245040
C	0.9344240	-2.0633040	-0.3692870
N	0.2533530	-0.9777620	-0.2531390
N	-1.1027690	-0.9792530	-0.5318390
C	-1.7425480	0.2481610	-0.4637120
C	-1.7610920	-2.1891810	-0.9560470
C	-3.2528440	0.2333480	-0.6844920
N	-1.0026200	1.2851400	-0.2084780
S	-1.6117160	2.8316510	-0.0650990
C	-4.0632910	-0.2809790	0.5015200
C	-0.0826310	3.7513990	-0.2305490
O	-2.4807810	3.2167920	-1.1957270
O	-2.1111120	3.0272820	1.3087350

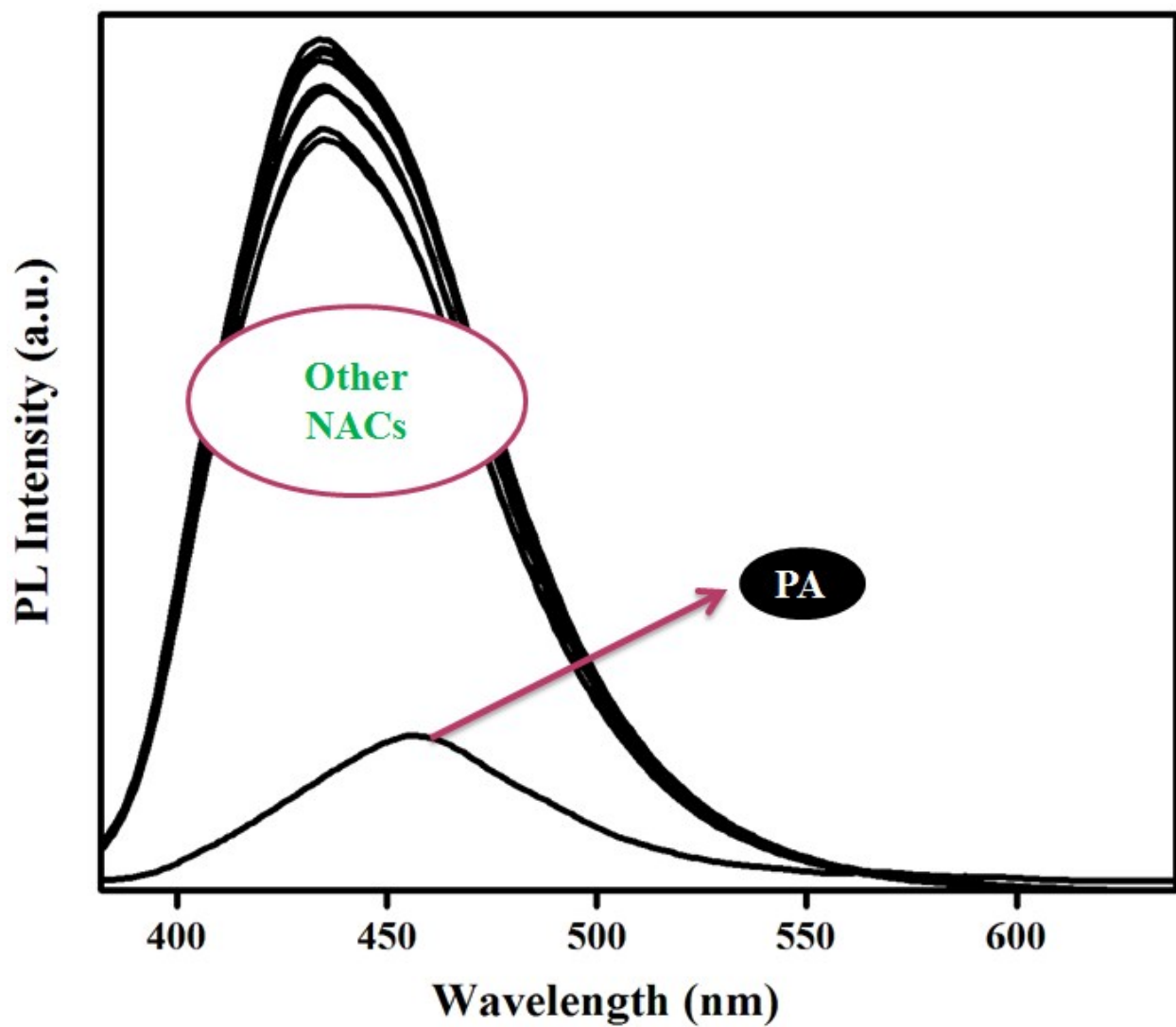
C	0.1143940	4.5527310	-1.3508330
C	1.2924340	5.2953810	-1.4569880
C	2.2709680	5.2475760	-0.4587140
C	2.0416360	4.4341210	0.6637550
C	0.8732070	3.6907110	0.7872170
C	-5.0682740	-1.2343340	0.2939210
C	-5.8571370	-1.6856610	1.3529830
C	-5.6450210	-1.1928000	2.6410280
C	-4.6467470	-0.2407100	2.8564780
C	-3.8625350	0.2174830	1.7966130
C	3.5442450	6.0525760	-0.5722730
C	-1.8595940	-2.4826920	-2.3204410
C	-2.4449890	-3.6810930	-2.7306070
C	-2.9105490	-4.5930450	-1.7803580
C	-2.7919520	-4.3055830	-0.4190350
C	-2.2164760	-3.1041930	-0.0032000
H	4.9343820	-0.0615630	0.8665720
H	4.9528160	-4.2965370	-0.0231280
H	2.5636370	-4.1896300	-0.4869590
H	2.5336940	0.0098690	0.3930960
H	6.8427260	-4.2505360	1.3034020
H	7.1857080	-3.8988620	-0.4050680
H	8.2858620	-3.3246860	0.8587250
H	7.1666480	-0.2481820	0.3536550

H	6.8290960	-0.6104920	2.0609220
H	8.2770330	-1.2689360	1.2818070
H	0.4932000	-3.0138630	-0.6829670
H	-3.5548650	1.2535300	-0.9327930
H	-3.4784550	-0.3798300	-1.5614170
H	-0.6483150	4.5923060	-2.1208280
H	1.4494150	5.9237650	-2.3303410
H	2.7886410	4.3897310	1.4533040
H	0.6974400	3.0710250	1.6602260
H	-5.2340810	-1.6285650	-0.7060170
H	-6.6341550	-2.4235980	1.1698020
H	-6.2559200	-1.5433270	3.4689160
H	-4.4803040	0.1577390	3.8539520
H	-3.1121000	0.9825060	1.9726690
H	3.5750170	6.6246950	-1.5045870
H	3.6424930	6.7617760	0.2590450
H	4.4291960	5.4045290	-0.5472710
H	-1.4803930	-1.7698680	-3.0472300
H	-2.5317200	-3.9035960	-3.7904040
H	-3.3631510	-5.5273040	-2.1010100
H	-3.1545130	-5.0121240	0.3220350
H	-2.1277690	-2.8628750	1.0509960

**Energy** = -1928.79628458 A.U.



**Figure S10.** Calibration plot for detection limit (LOD). The LOD was derived by using the formula  $3\sigma/\text{slope}$ , where  $\sigma$  is the standard deviation of the blank (5 samples) and slope was obtained from linear calibration curve.



**Figure S10.** Fluorescence changes of nanoaggregates of AVM (90% water fraction) in the presence of other NACs