Supporting Information

for

A dual-functional AIE luminogen for sensitive nitro explosive detection and efficient photolabeling

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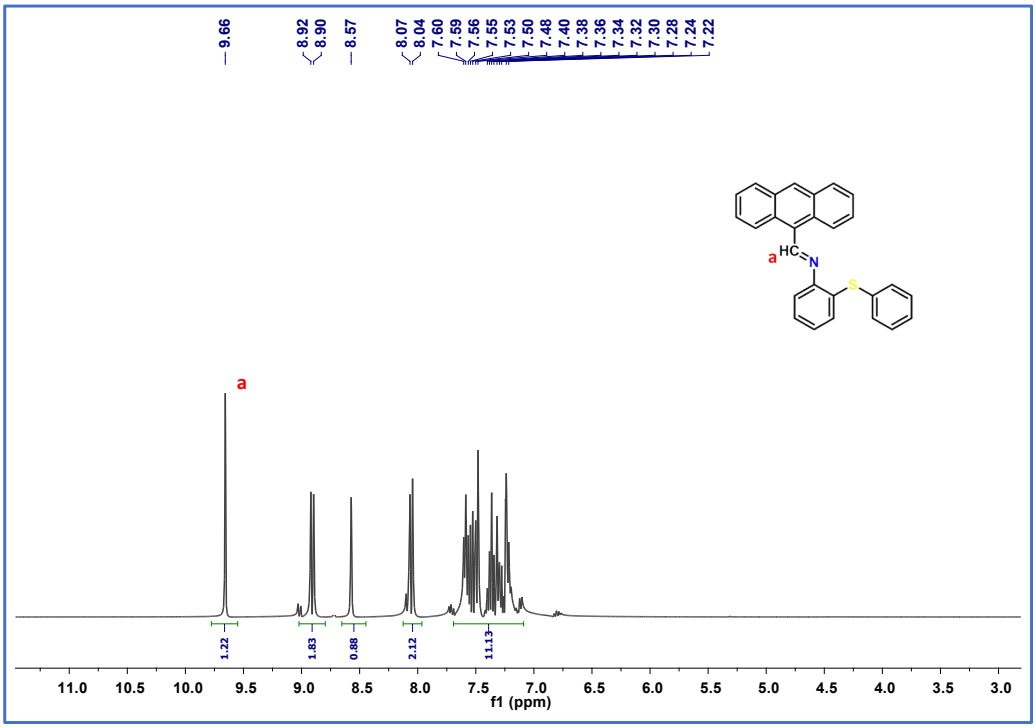

Fig. S1 ^{1}H NMR spectrum of **AnTPh** in $CDCl_3$ at room temperature.

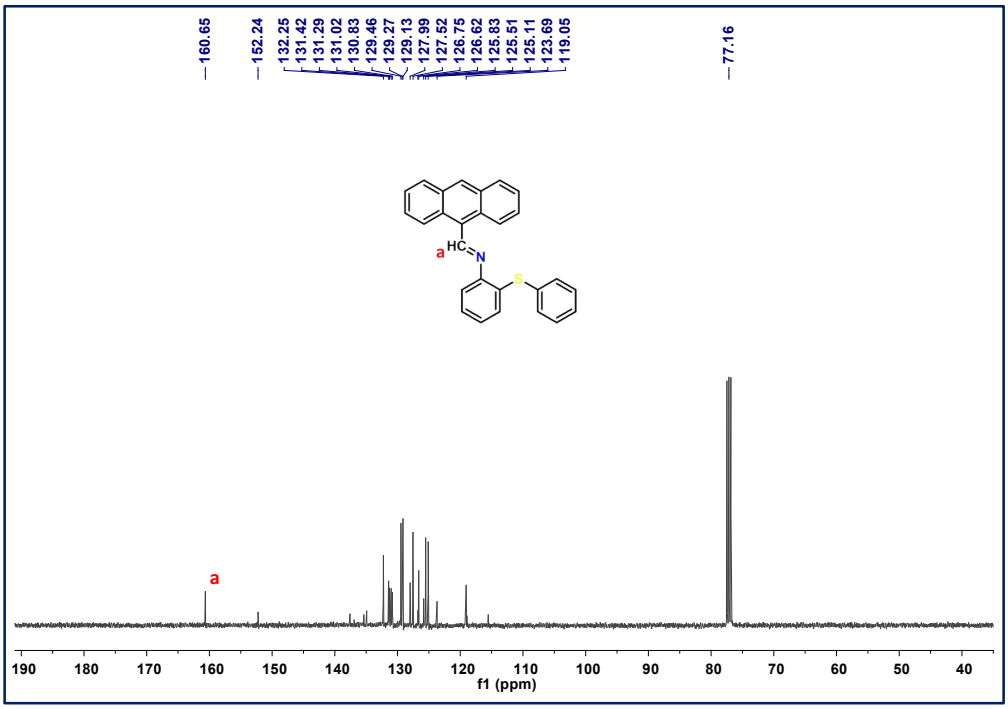

Fig. S2 ^{13}C NMR spectrum of **AnTPh** in $CDCl_3$ at room temperature.

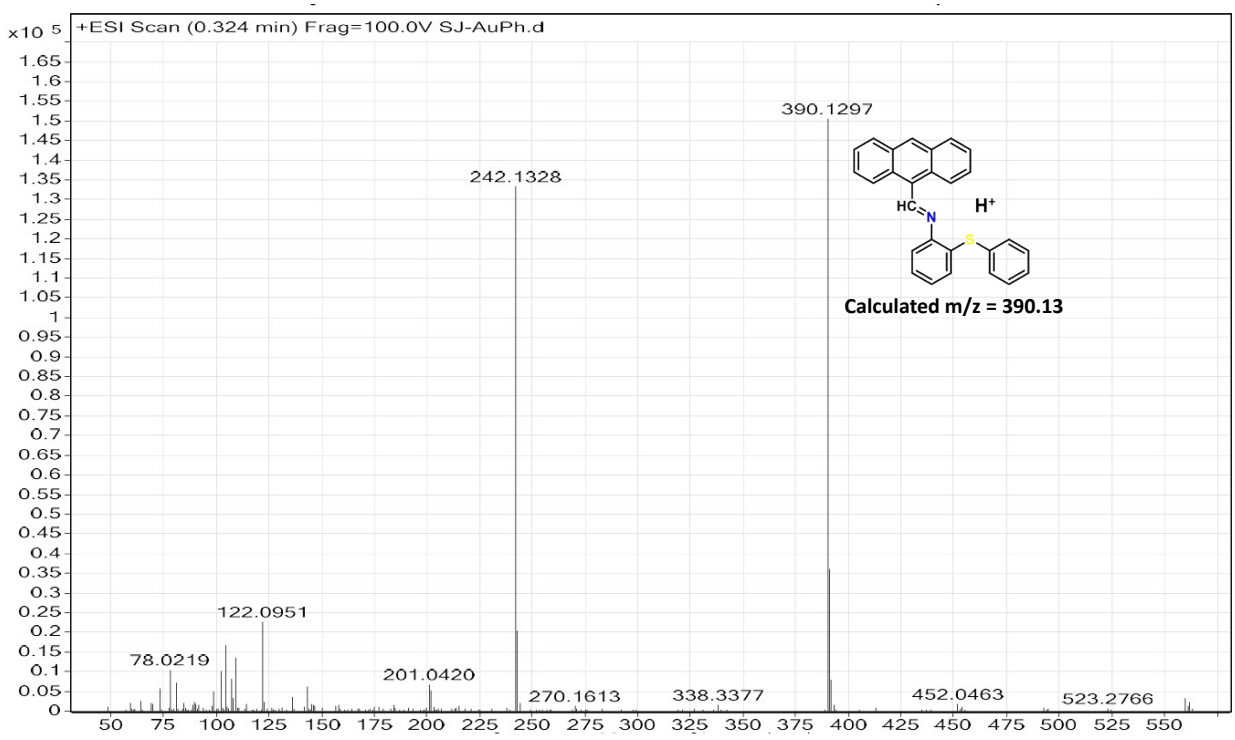

Fig. S3 Mass spectrum of **AnTPh** in CH_3CN solution.

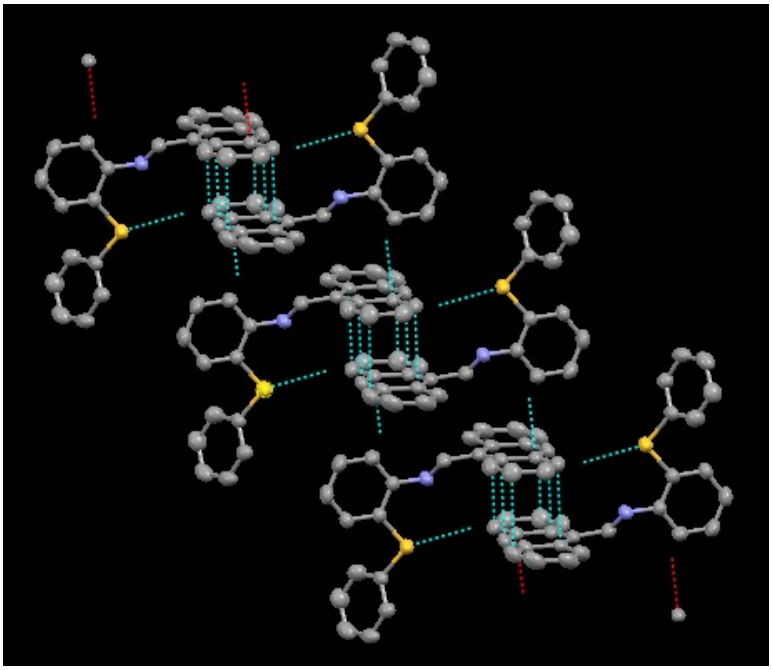

Fig. S4 Crystal packing highlighting the non-covalent interactions existing between neighbouring **AnTPh** molecules.

Table S1. Selected bond lengths [Å] and angles [°] in the single crystal of **AnTPh**.

Bond Length (Å)		**Bond Angle (°)**	
N(1)-C(15)	1.251(2)	C(21)-S(1)-C(22)	104.78(8)
N(1)-C(16)	1.417(2)	C(15)-N(1)-C(16)	119.11(15)
S(1)- C(22)	1.7702(18)	N(1)-C(15)-C(10)	123.65(17)
S(1)- C(21)	1.7635(17)	C(21)-C(16)-N(1)	117.87(14)

Table S2. Crystallographic data for **AnTPh**.

	AnTPh
Formula	$C_{27}H_{19}NS$
Formula weight ($gmol^{-1}$)	389.49
Space group	P-1
Temperature/K	293(2)
λ (Å) Mo Kα	0.71073
Crystal system	Triclinic
a (Å)	8.9312(5)
b (Å)	10.4343(7)
c (Å)	12.5929(7)
α(˚)	73.098(5)
β (˚)	70.992(5)
γ (˚)	65.822(6)
V ($Å^3$)	995.24(12)
Z	2
ρ_{calc}(gcm^{-3})	1.300
Crystal size (mm)	0.02 × 0.02 × 0.02
F(000)	408.0
Index ranges	$-10 \leq h \leq 11$ $-13 \leq k \leq 13$ $-15 \leq l \leq 15$
Restraints/para./reflns.	0/262/4120

GOF on F^2	1.106
$R1^a$ [$I > 2\sigma(I)$]	0.0486
$R1$[all data]	0.0674
$wR2^b$ [$I > 2\sigma(I)$]	0.1290
$wR2$ [all data]	0.1411

$^a R1 = \Sigma||Fo|-|Fc||/\Sigma|Fo|$; $^b wR2 = |\Sigma w(|Fo|^2 - |Fc|^2)|/\Sigma|w(Fo)^2|^{1/2}$

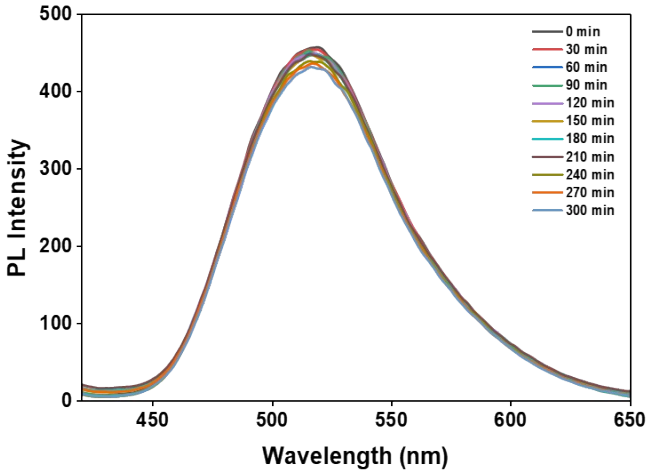

Fig. S5 Photostability experiment of **AnTPh** aggregates upon light irradiation at different time intervals.

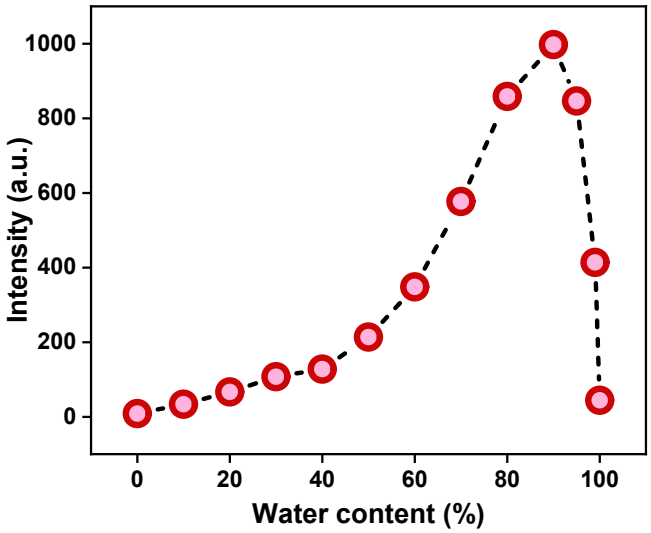

Fig. S6 Variation in emission intensity of **AnTPh** with increasing water content.

Table S3. UV-Vis spectroscopic data for **AnTPh**.

Wavelength (nm)	**Absorbance (A)**	**Molar Absorptivity (ε) (M^{-1} cm^{-1})**
233	0.33	6.60×10^4
261	0.59	1.18×10^5
307	0.037	7.40×10^3
370	0.044	8.80×10^3
400	0.045	9.00×10^3

Table S4. Emission lifetime of **AnTPh** at varying water fractions (f_w).

f_w **(%)**	τ_1 **(ps)**	τ_2 **(ps)**	τ_{av} **(ps)**	χ^2
0	24.56	3678.56	165.66	1.044
10	69.33	4172.39	225.44	1.093
20	121.59	4183.14	252.78	1.092
30	180.76	4173.03	296.03	1.052
40	256.65	3749.86	346.21	1.175
50	360.11	3134.51	425.93	1.131
60	513.99	1493.72	582.74	1.117
70	932.51	-	932.51	1.166
80	1405.58	-	1405.58	1.054
90	1696.35	-	1696.35	1.028

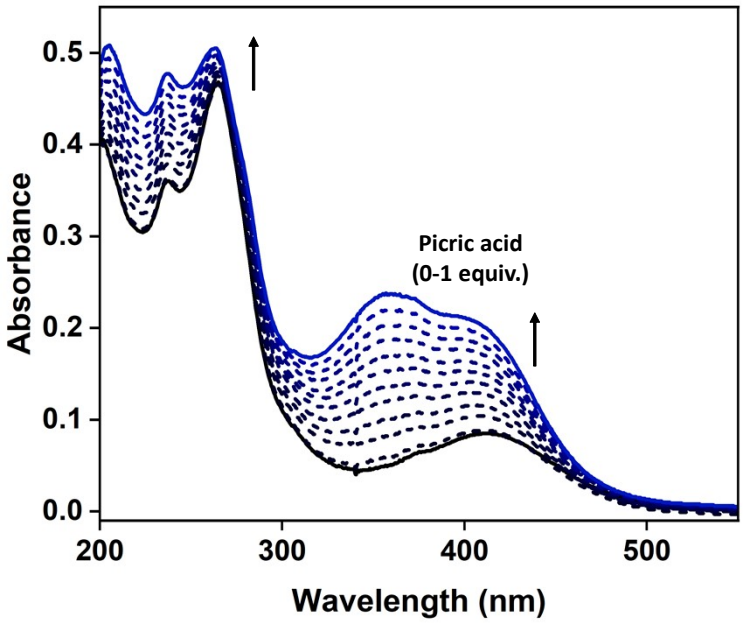

Fig. S7 Absorption spectra of **AnTPh** aggregates with variable concentrations of picric acid (0-1.0 equiv).

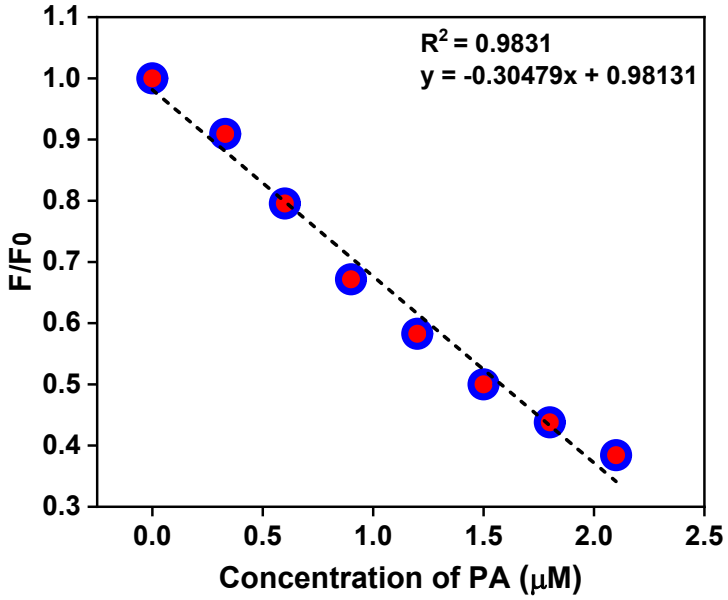

Fig. S8 Calibration plot to determine LoD for PA.

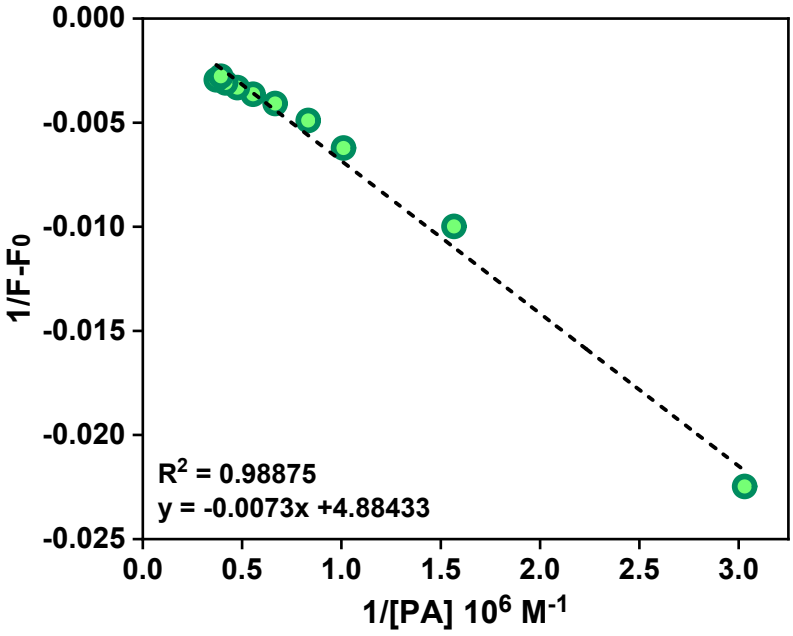

Fig. S9 Determination of binding constant of **AnTPh** with PA using the Benesi-Hildebrand plot.

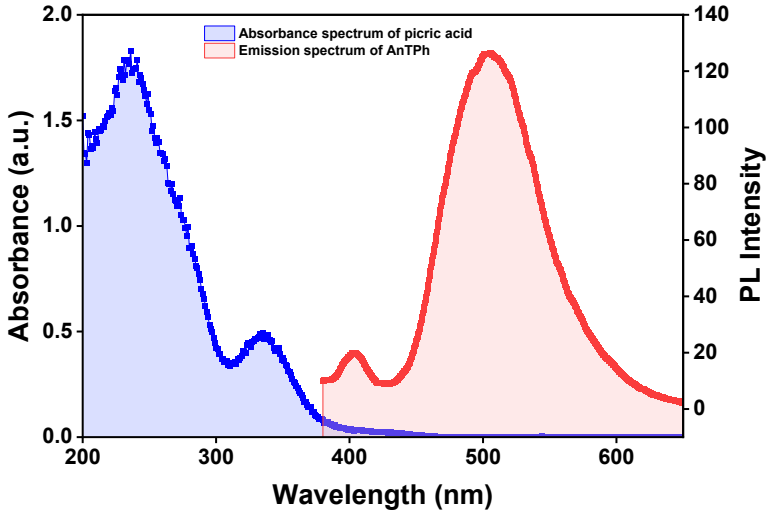

Fig. S10 Absorption spectrum of PA and emission spectrum of **AnTPh**.

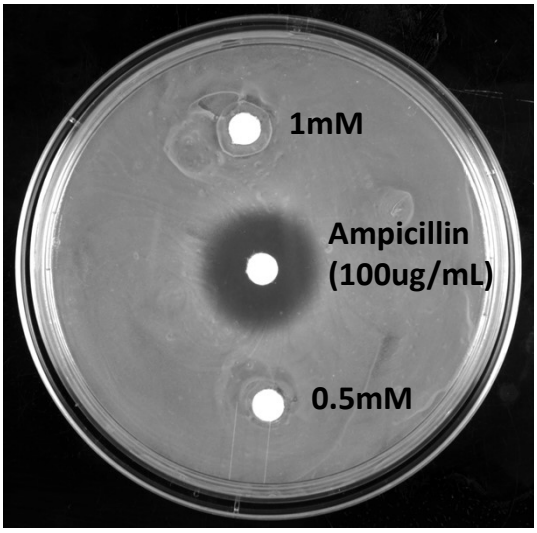

Fig. S11 *in-vitro* antimicrobial activity of **AnTPh** by disc diffusion method in *S. aureus*.