Supporting Information

Interrogating the nature of aggregates formed in a model azine based ESIPT coupled AIE active probe: stark differences in photodynamics in the solid state and aggregates in water

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1. ^{1}H NMR Spectrum of BNHMP in $CDCl_3$.

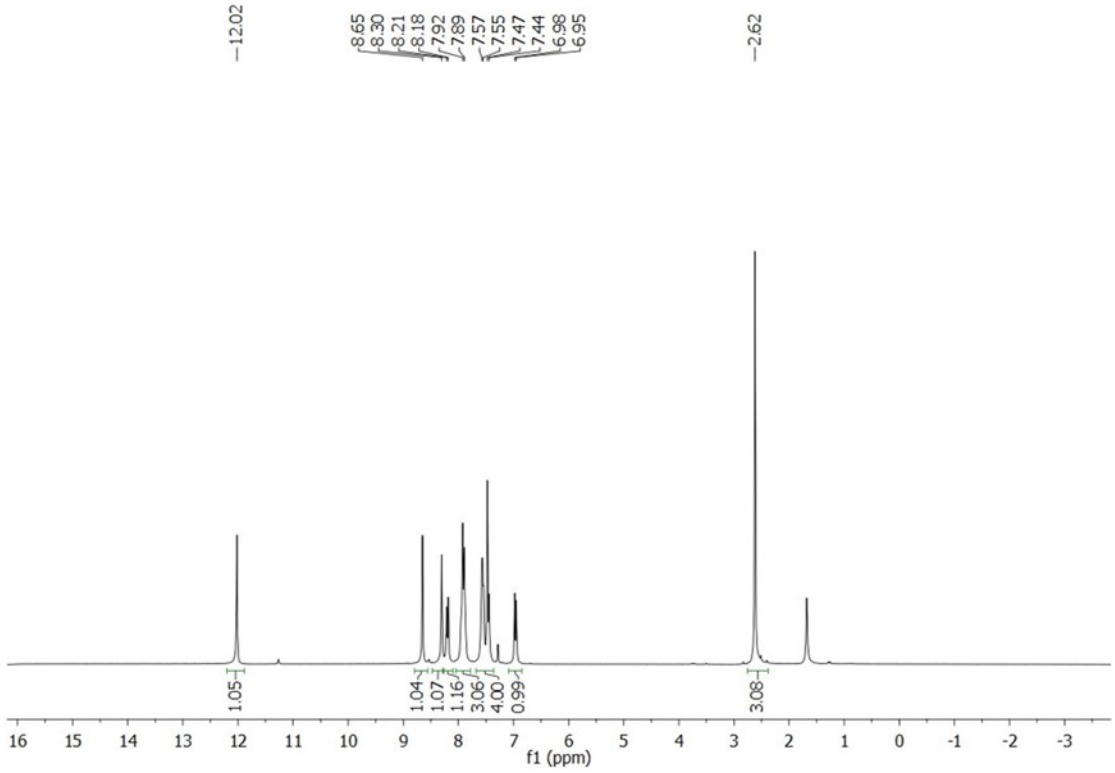

Figure S1. ^{1}H NMR Spectrum of **BNHMP** in $CDCl_3$.

2. ^{13}C NMR Spectrum of BNHMP in $CDCl_3$.

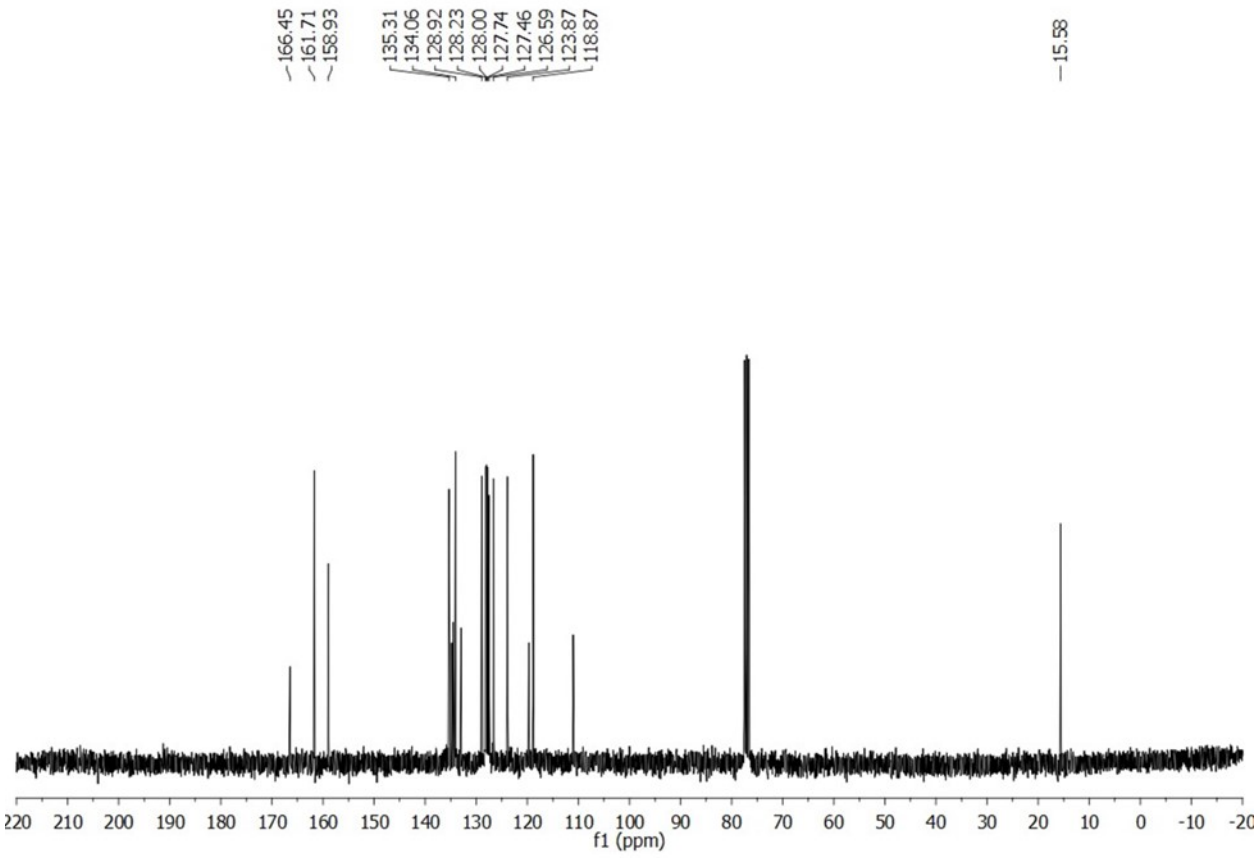

Figure S2. ^{13}C NMR Spectrum of **BNHMP** in $CDCl_3$.

3. ESI-MS of BNHMP in acetonitrile.

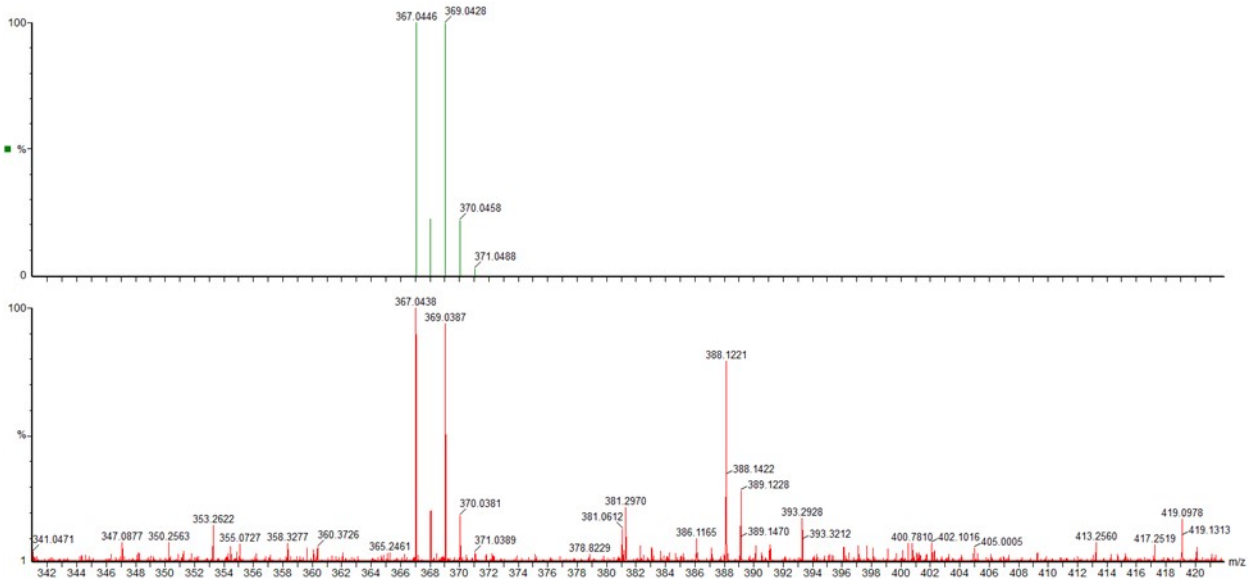

Figure S3. (Top) Experimentally obtained mass spectrum. (bottom) Simulated mass spectrum from isotopic modelling.

4. FTIR Spectrum of BNHMP.

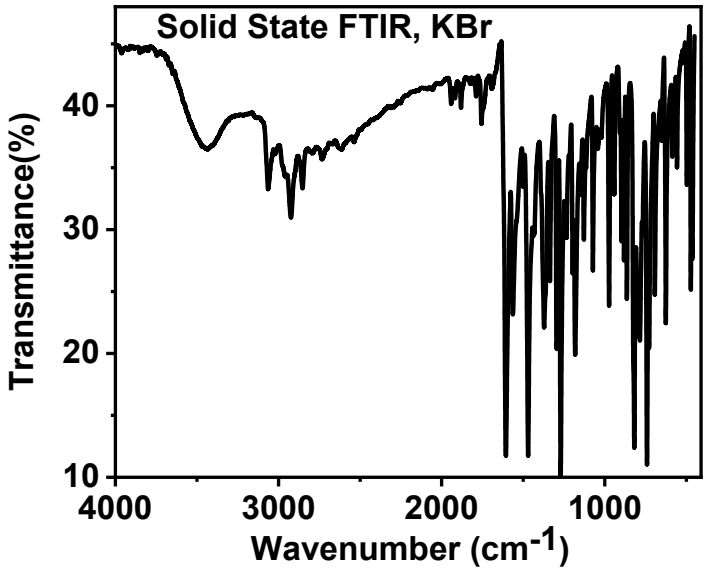

Figure S4. Solid state FTIR in **BNHMP**.

5. ORTEP diagram of BNHMP

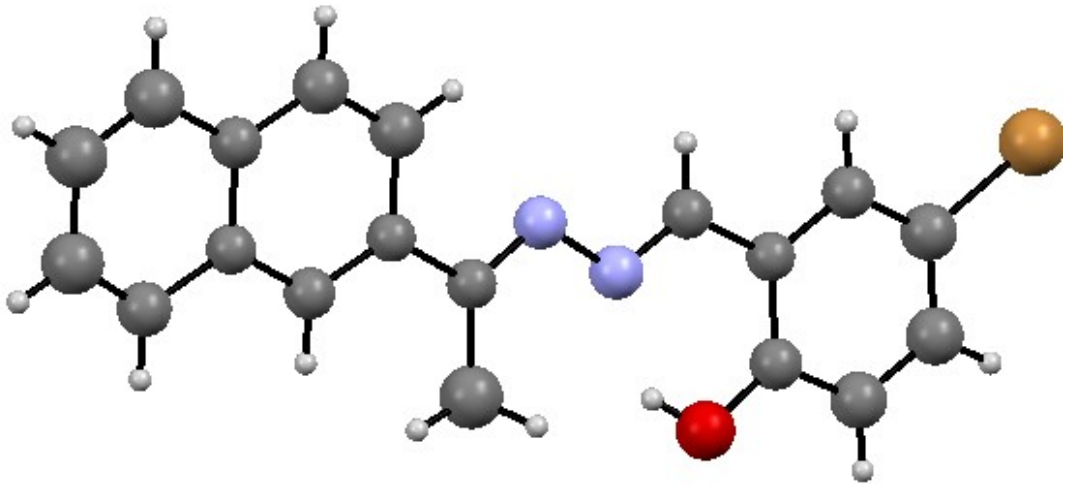

Figure S5. ORTEP diagram of **BNHMP**.

6. Table for important crystallographic parameters of BNHMP.

Parameters	**BNHMP**
Formula	C19 H15 Br N2 O
Formula Weight	367.23
Crystal System	monoclinic
Space group	P 21/n
a [Å]	6.2672(6)
b [Å]	14.7584(12)
c [Å]	17.2093(13)
α [º]	90
β [º]	94.681(4)
γ[º]	90
V [Å^3]	1586.4(2)
h, k, l (max.)	6,14,16
Z	4
D(calc) [g/cm^{-3}]	1.538
F(000)	744.0
Temperature (K)	296
θ Min-Max [º]	3.55, 19.980
No. of unique data	1255
R(int)	0.068

Observed data [I > 2.0 σ(I)]	675
R1, wR2	0.0268, 0.0712
GOF on F^2	1.068

7. Non-planarity of OH proton

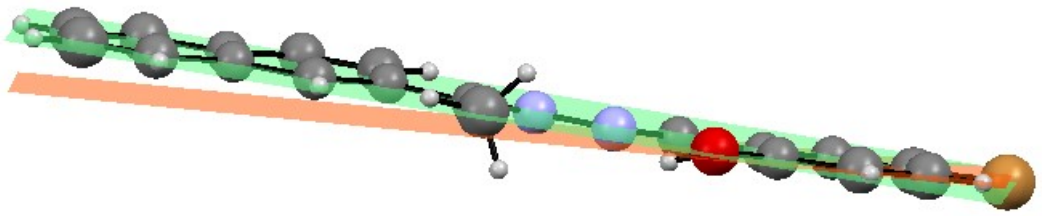

Figure S6. Non-planarity of the -OH group (contained in red plane) and the rest of **BNHMP** (contained in green plane).

8. Full scale emission spectra of BNHMP in various solvents and the corresponding CIE diagrams.

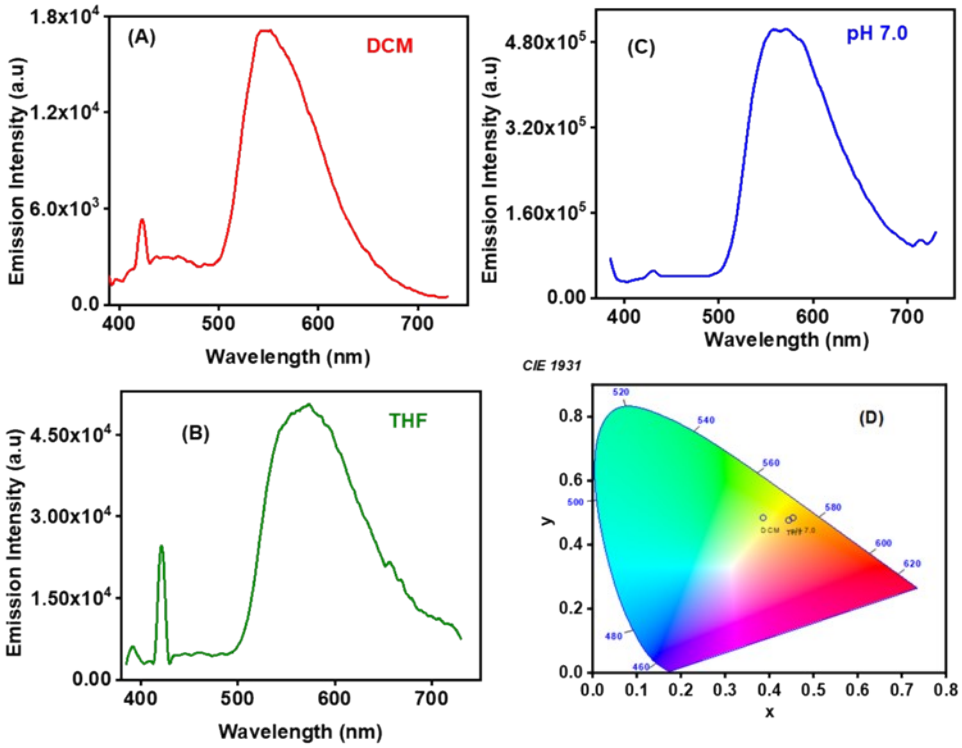

Figure S7: Full scale emission spectrum of **BNHMP** in (A) DCM, (B) THF, (C) water at pH 7.0 and (D) CIE diagram of **BNHMP** in DCM, THF and water.

9. Time-resolved emission decays of BNHMP in various solvents at all observation wavelengths.

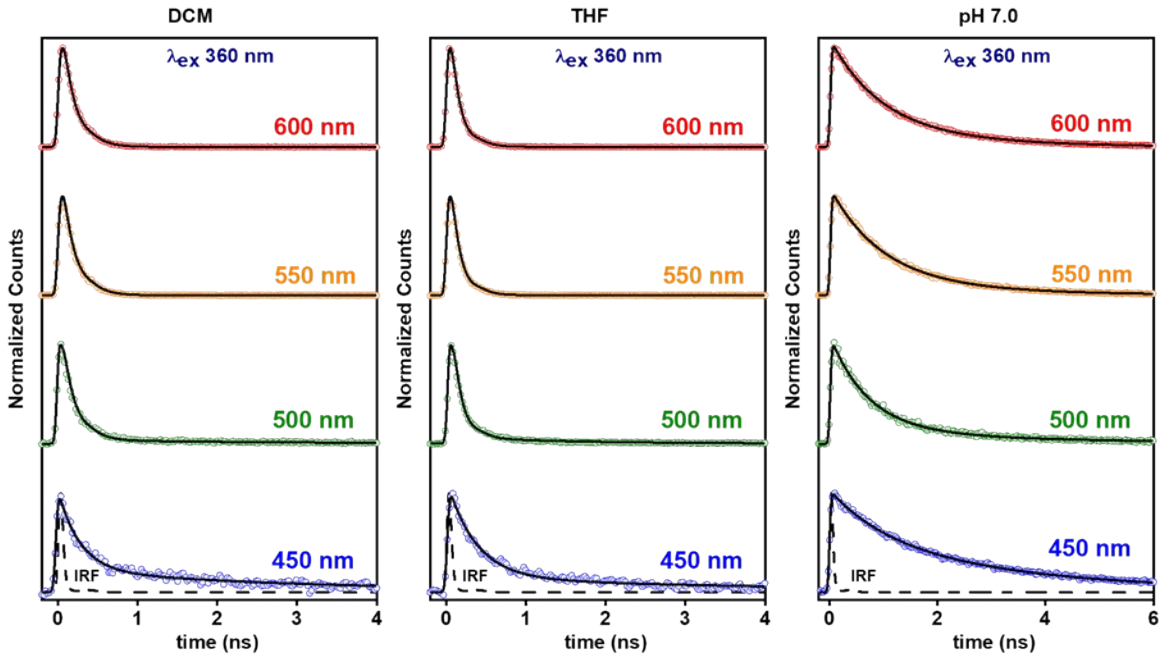

Figure S8. Lifetime emission decays of **BNHMP** in various solvents (10 μM). The excitation and monitoring wavelengths are provided in the insets. The black lines denote the best multiexponential fit of the emission decays.

10. Excited State lifetime parameters of BNHMP in DCM, THF and water.

Table S2. Excited state lifetime parameters of **BNHMP** in DCM upon normalization to 100. α_is denotes the amplitudes. The error in estimation of the lifetimes is around 10%.

λ_{mon}	τ_1 (ns)	α_1	τ_2 (ns)	α_2
450 nm		84		16
500 nm	**0.15**	97	**3.0**	03
550 nm		100		-
600 nm		100		-

Table S3. Excited state lifetime parameters of **BNHMP** in THF upon normalization to 100. α_is denotes the amplitudes. The error in estimation of the lifetimes is around 10%.

λ_{mon}	τ_1(ns)	α_1	τ_2(ns)	α_2
450 nm		82		18
500 nm	**0.10**	96	**1.5**	04
550 nm		99		01
600 nm		100		-

Table S4. Excited state lifetime parameters of **BNHMP** in water upon normalization to 100. α_is denotes the amplitudes. The error in estimation of the lifetimes is around 10%.

λ_{mon}	τ_1(ns)	α_1	τ_2(ns)	α_2
450 nm		45		55
500 nm	**0.90**	79	**3.2**	21
550 nm		86		14
600 nm		55		45

11. Steady state emission spectra of BNHMP in ethanol, PEG-400 and water.

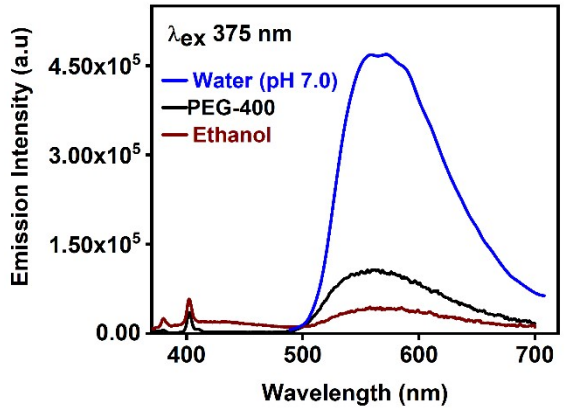

Figure S9. Steady state emission spectra of **BNHMP** (10 μM) in ethanol, PEG-400 and water. The excitation wavelength was 375 nm.

12. Full range solid state emission spectrum upon excitation at 300 nm.

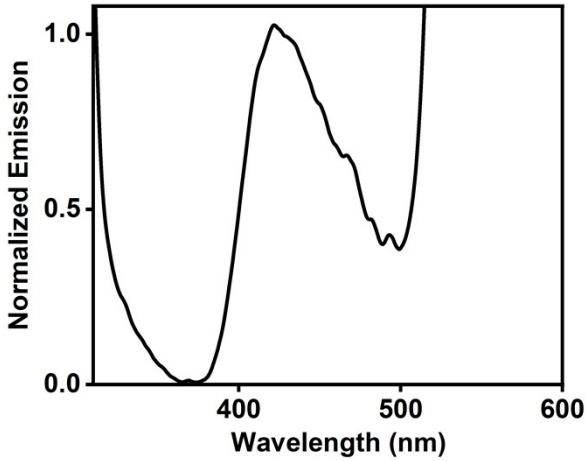

Figure S10: Full range solid state emission spectrum upon excitation at 300 nm.

13. Full scale emission spectra of BNHMP in solid-state at various wavelengths.

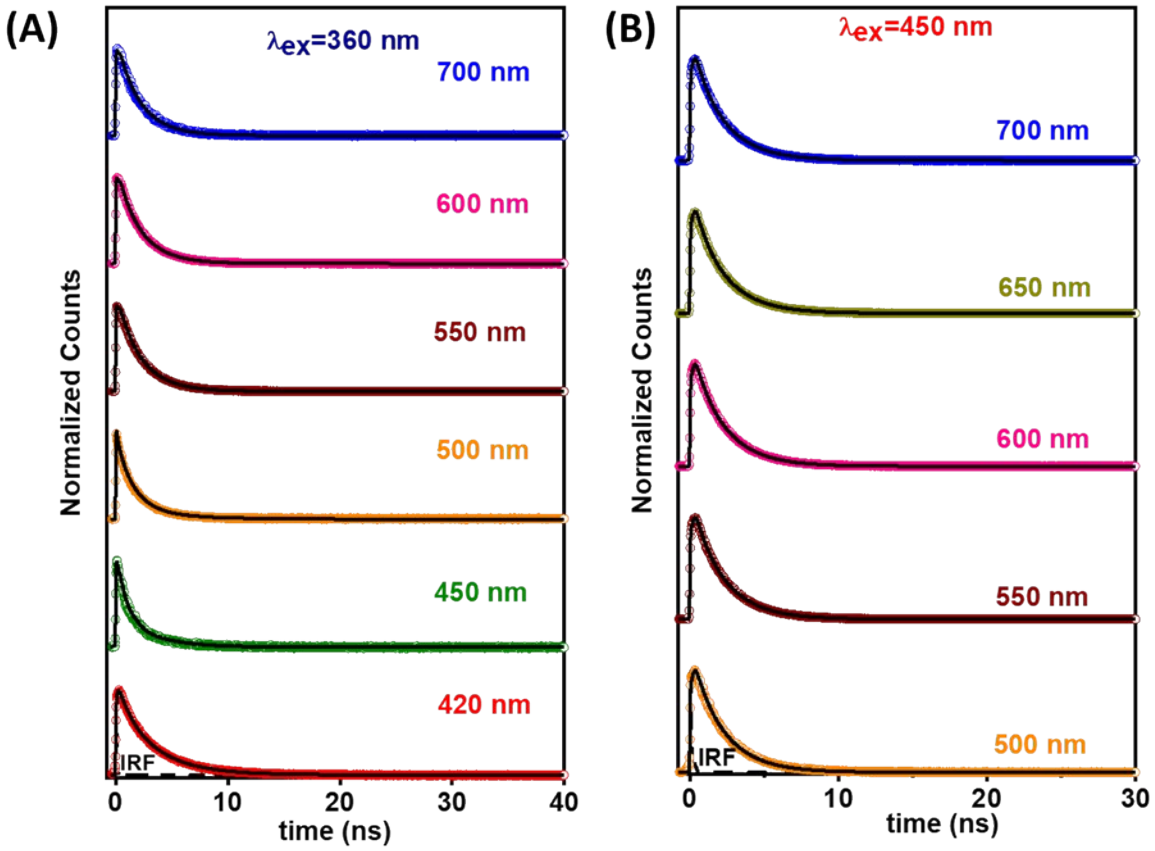

Figure S11. Full scale emission spectra of **BNHMP** in solid-state at various wavelengths upon excitation at (A) 360 nm and (B) 450 nm. The black lines denote the best multiexponential fit of the emission decays.