

Supporting Information (SI)

The Impact of Aggregation of AIE and ACQ moiety integration material on the Excited State Dynamics

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1. Materials and methods

All solvents were dried according to standard procedures and all of them were degassed under N₂ for 30 minutes before use. ¹H and ¹³C NMR spectra were recorded on Bruker 400MHz Spectrometer (5 ¹H: 400 MHz; ¹³C: 100 MHz) at 298 K. The ¹H and ¹³C NMR chemical shifts are reported relative to the residual solvent signals (δ 0.0). Electrospray ionization (ESI) mass spectra were recorded with a Waters Synapt G2 mass spectrometer. UV-vis spectra were recorded in a quartz cell (light path 10 mm) on a Cary 50Bio UV-Visible spectrophotometer. Steady-state fluorescence spectra were recorded in a conventional quartz cell (light path 10 mm) on a Cary Eclipse fluorescence spectrophotometer. DLS 10 measurements were performed under a Malvern Zetasizer Nano-ZS light scattering apparatus (Malvern Instruments, U. K.) with a He-Ne laser (633 nm, 4 mW). For the single crystals, the data sets were treated with the SQUEEZE program to remove highly disordered solvent molecules. The crystallographic formulae include the number of solvent molecules was suggested by the SQUEEZE program. All the femtosecond transient absorption spectroscopy was acquired with a typical 15 transmission pump-probe (UV/vis pump-broadband supercontinuum probe) instrument. In this arrangement, a Ti:sapphire regenerative amplifier (Spitfire Ace, Spectra Physics, Inc.) was employed to produce laser pulses (6 mJ, 1 kHz) with a pulse width of 80 fs and center wavelength at 800 nm. The output laser was split into several laser beams, one of which was used to generate wavelength-tunable light serving as the pump laser for TAS via a downstream TOPAS instrument. The pump laser 20 was further chopped with a 500 Hz mechanical chopper. Another laser beam propagated through an optical delay line (0-8 ns) and was then focused into a CaF₂ crystal to produce white light continuum, which serves as the probe light in the fs-TA. For the measurements, both solution and film samples were excited at 500 nm and then probe with a WLC pulse ranging from 350 to 700 nm. The instrument response function (IRF) of this system was determined to be ~120 fs by measuring solvent responses 25 under the same experimental conditions. Nanosecond transient absorption (TA) spectra and kinetics were measured using TA spectrometer (Helios-EOS fire, Ultrafast System). A commercial spectrometer S12 (EOS, Ultrafast Systems) that utilized a photonic crystal fiber broadband probe source.

2. Photophysical properties of TPEIP.

Table S1. Photophysical properties of TPEIP.

solvents	$\lambda_{\text{abs}}/\text{nm}$	$\lambda_{\text{em}}/\text{nm}$	$\tau_{\text{F}}/\text{ns}$	$\Phi/\%$
DMSO	413	544	1.97	8.92
ACN	406	537	1.16	4.73
DMF	411	544	1.59	6.58
MeOH	412	568	/	/
EtOH	412	554	0.33	2.41
Acetone	407	532	1.21	5.05
THF	409	538	0.68	3.38
EA	407	530	0.73	3.85
DCM	411	545	1.71	7.25
CHCl_3	413	537	2.34	12.26
Tol	412	532	1.28	4.56

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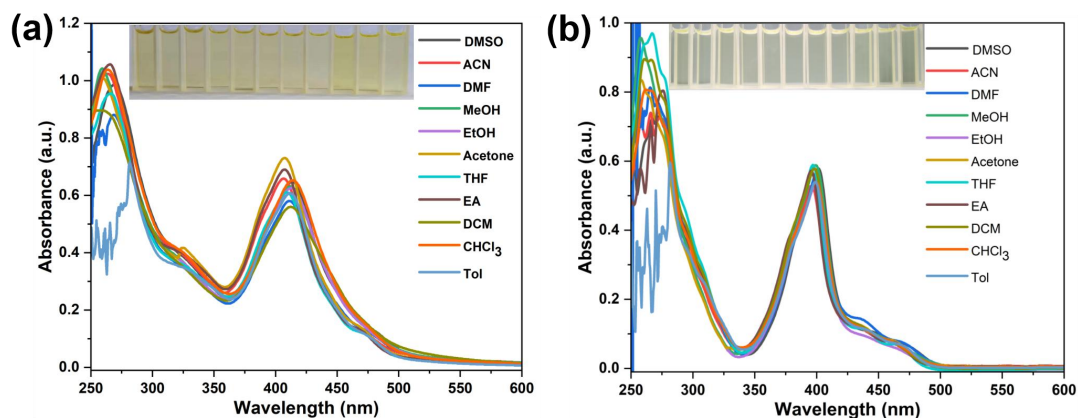


Figure S1. The UV absorption spectra of TPEIP (a) and PIP (b) (2×10^{-5} mol/L) in various solvents.

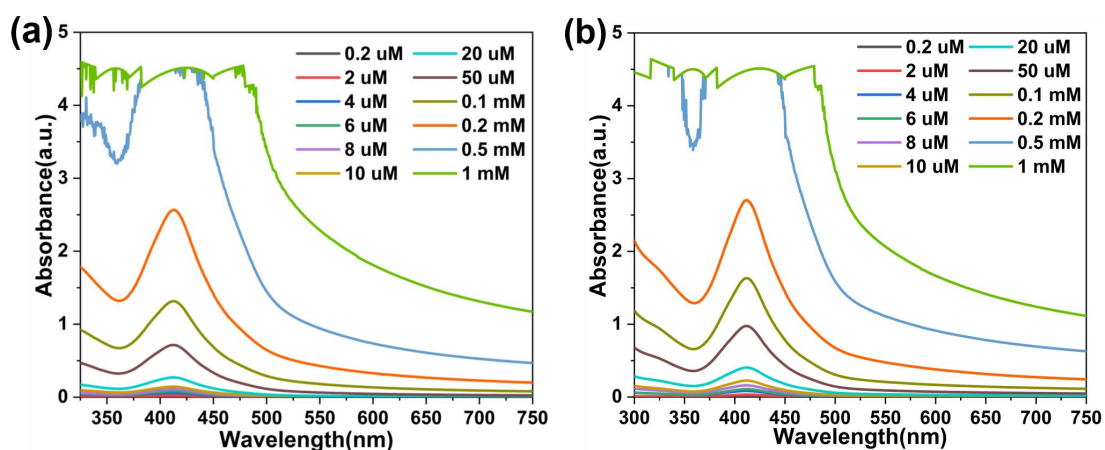


Figure S2. The UV absorption of **TPEIP** (1.0 mM, 0.5 mM, 0.2 mM, 0.1 mM, 0.05 mM, 0.02 mM, 5 8.0 μ M, 6.0 μ M, 4.0 μ M, 2.0 μ M, 0.2 μ M) in EtOH (a) and MeOH (b) solvents.

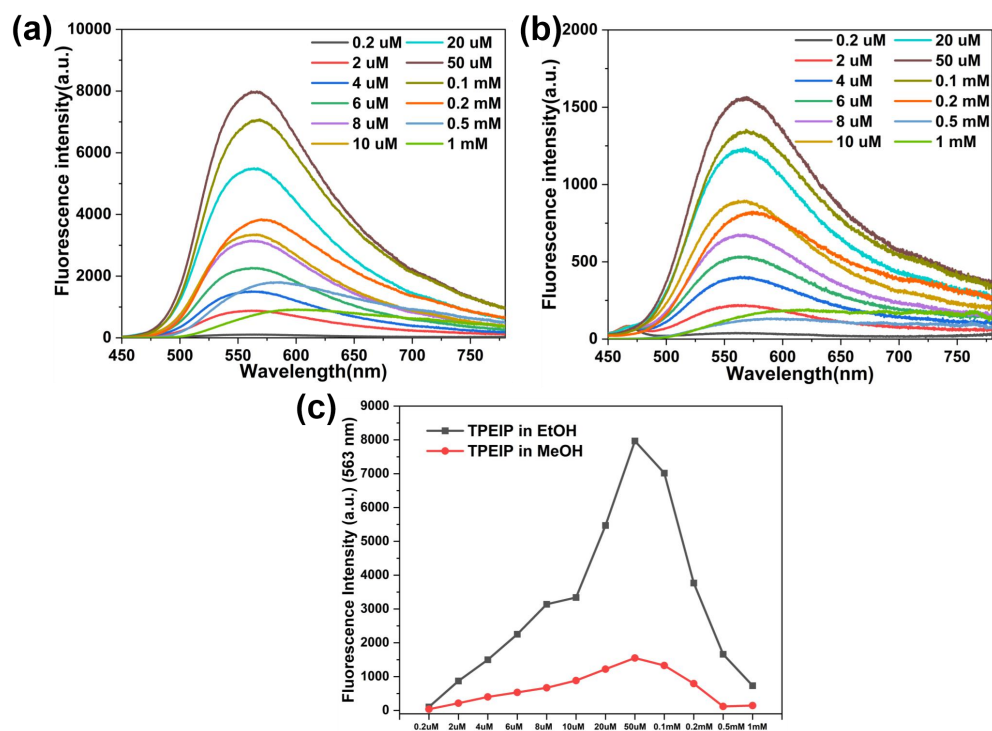


Figure S3. The fluorescence spectra of **TPEIP** (1.0 mM, 0.5 mM, 0.2 mM, 0.1 mM, 0.05 mM, 0.02 mM, 8.0 μ M, 6.0 μ M, 4.0 μ M, 2.0 μ M, 0.2 μ M) in EtOH (a) and MeOH (b) solvents, and fluorescence intensity at 563 nm (c).

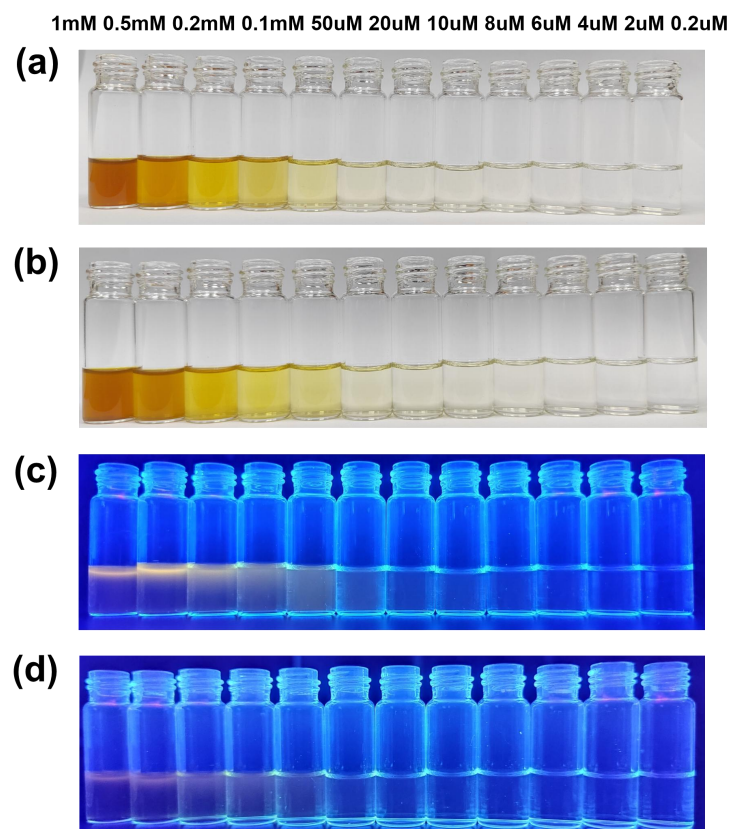


Figure S4. The solution color of **TPEIP** (1.0 mM, 0.5 mM, 0.2 mM, 0.1 mM, 0.05 mM, 0.02 mM, 8.0 μ M, 6.0 μ M, 4.0 μ M, 2.0 μ M, 0.2 μ M) in EtOH (a) or MeOH (b) in daylight, and the fluorescence emission color of **TPEIP** (1.0 mM, 0.5 mM, 0.2 mM, 0.1 mM, 0.05 mM, 0.02 mM, 8.0 μ M, 6.0 μ M, 4.0 μ M, 2.0 μ M, 0.2 μ M) in EtOH (c) or MeOH (d) under the irradiation of 365nm ultraviolet lamp.

3. Dynamic Light Scattering measurement of the TPEIP

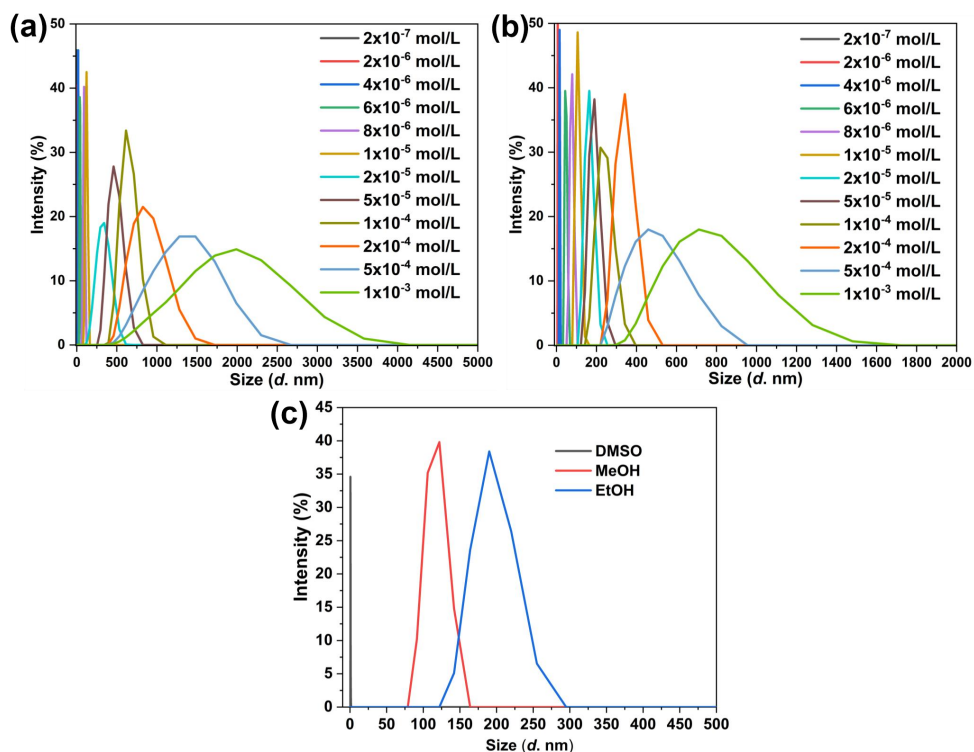


Figure S5. Dynamic Light Scattering: size distributions of TPEIP (1.0 mM, 0.5 mM, 0.2 mM, 0.1 mM, 0.05 mM, 0.02 mM, 8.0 μ M, 6.0 μ M, 4.0 μ M, 2.0 μ M, 0.2 μ M) in EtOH (a) and MeOH (b) solvents, and Dynamic Light Scattering: size distributions of TPEIP (0.02 mM) in DMSO, EtOH and 5 MeOH.

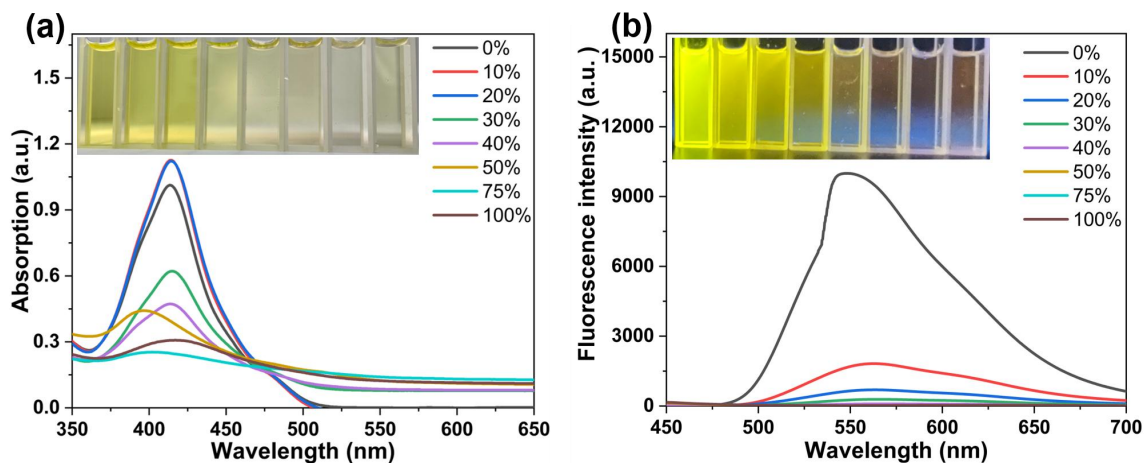


Figure S6. The UV absorption (a) and fluorescence spectra (b) of TPEIP (2×10^{-5} mol/L) in DMSO/water mixed solvents with 0%, 10%, 20%, 30%, 40%, 50%, 60%, 70%, 80%, 90%, 100% of water content.

10 4. Theoretical Simulation of Absorption of TPEIP

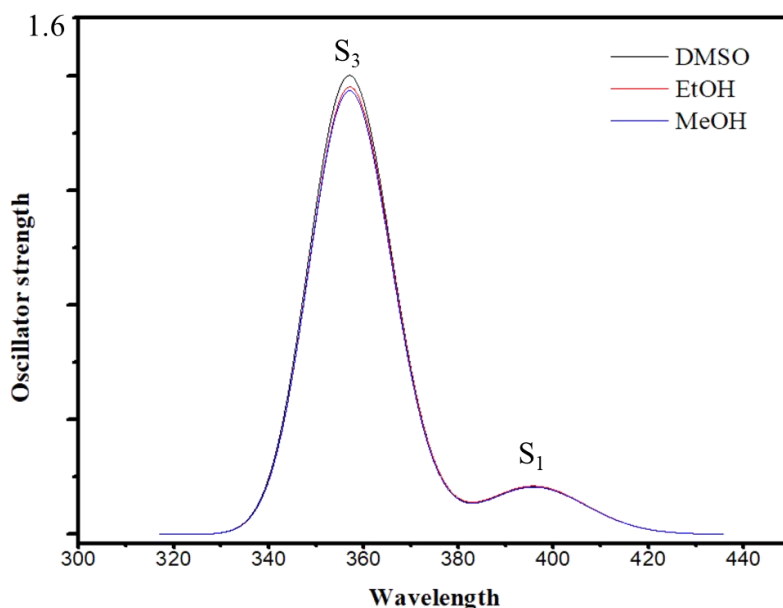


Figure S7. Absorption spectra of TPEIP-monomers calculated in DMSO, EtOH and MeOH.

Table S2. Calculated emission wavelength, oscillator strength, radiative rate (K_r) and nonradiative rate (K_{nr}) of TPEIP-monomers in MeOH and crystal state.

	Emission(nm)	f	K_r (s^{-1})	K_{nr} (s^{-1})
MeOH	478	0.4291	1.25×10^8	6.69×10^7
Solid	507	0.0008	2.07×10^5	6.59×10^7

5. Additional experimental and computational results

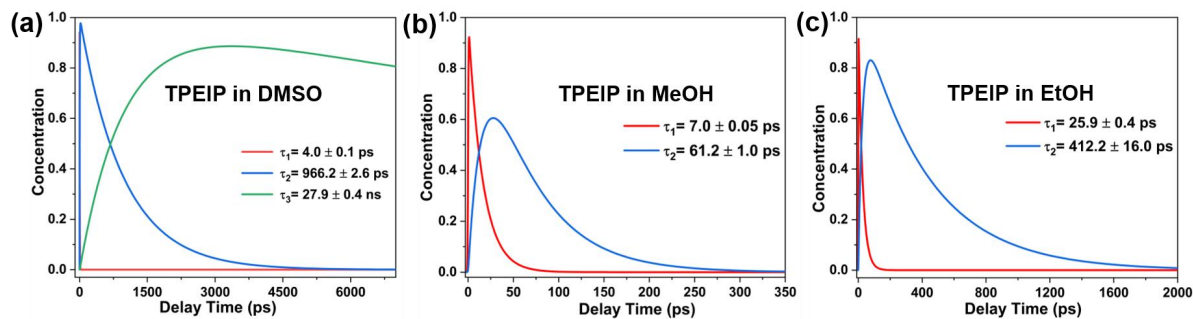


Figure S8. Concentrations of the SADS components as a function of time in different viscous solvents (a, DMSO; b, MeOH; c, EtOH).

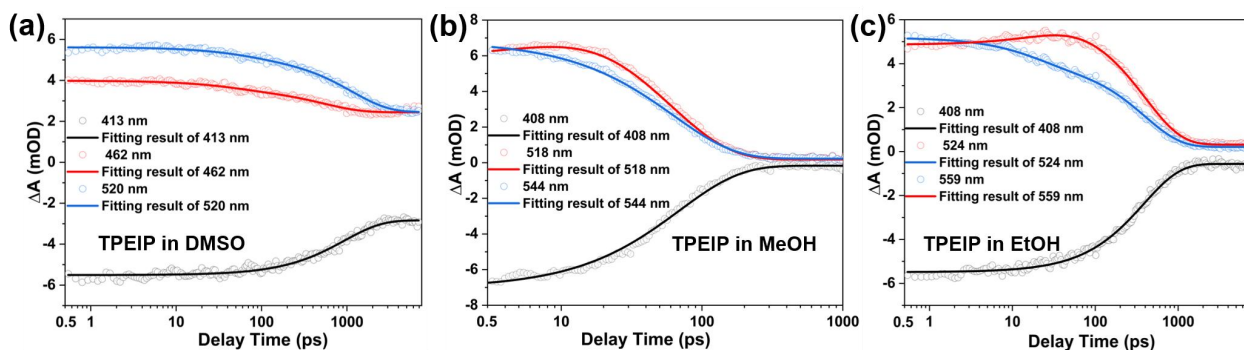


Figure S9. Kinetics of femtosecond broadband transient absorption spectra of **TPEIP** in DMSO, MeOH and EtOH solvents at selected wavelengths are plotted (circle) together with global fitting curves (line) of all collected time traces for the showing fitting quality.

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Table S3. Best fitting parameters of femtosecond TA of **TPEIP** in DMSO, MeOH and EtOH at selected wavelengths.

	Wavelength (nm)	τ_1 (ps)	τ_2 (ps)	τ_3 (ns)
TPEIP in DMSO	413 nm	3.6 (± 0.4)	984.9 (± 34.4)	/
	462 nm	52.5 (± 8.2)	857.0 (± 83.1)	202.1 (± 0.9)
	520 nm	62.0 (± 10.5)	1140.2 (± 36.3)	
TPEIP in MeOH	408 nm	66.8 (± 1.1)	/	/
	518 nm	8.8 (± 0.3)	57.1 (± 0.6)	/
	544 nm	64.0 (± 0.5)	/	/
TPEIP in EtOH	408 nm	385.6 (± 6.1)	/	/
	524 nm	25.8 (± 1.9)	399.5 (± 4.9)	/
	559 nm	18.3 (± 1.1)	394.6 (± 6.1)	/

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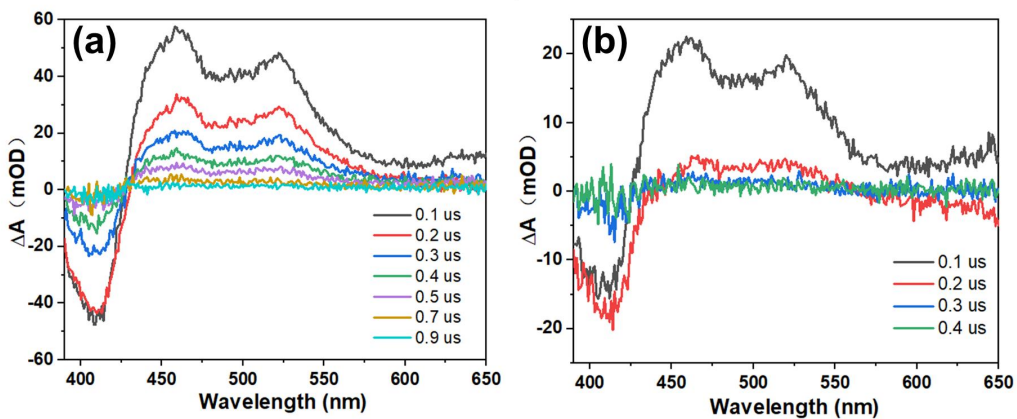


Figure S10. Nano-microsecond broadband TA spectra of **TPEIP** under deaerated (a) and aerobic (b) conditions in DMSO.

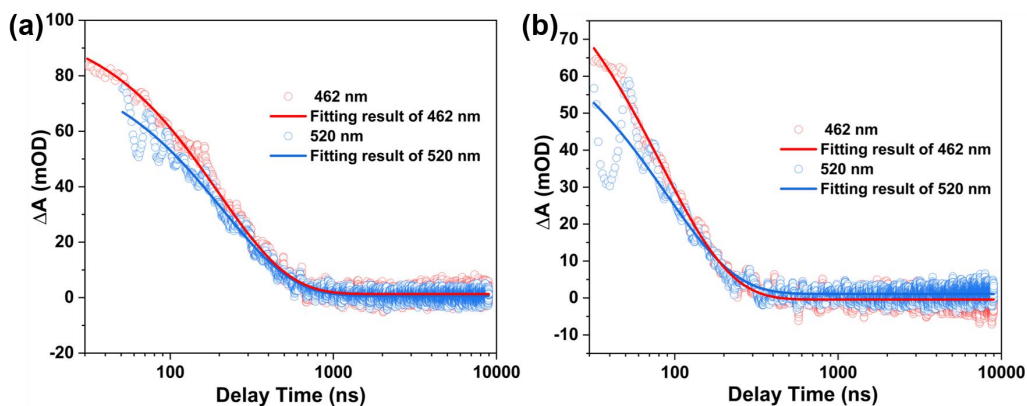


Figure S11. Kinetics of nano-microsecond broadband TA spectra of **TPEIP** under deaerated (a) and aerobic (b) conditions in DMSO solvents at selected wavelengths are plotted (circle) together with global fitting curves (line) of all collected time traces for the showing fitting quality.

Table S4. Best fitting parameters of nano-microsecond TA of **TPEIP** in DMSO.

	Wavelength (nm)	τ_1 (ns)
Deaerated conditions	462	198.1 ns (± 0.9 ns)
	520	210.0 ns (± 0.9 ns)
Aerobic conditions	462	81.9 ns (± 0.6 ns)
	520	87.7 ns (± 0.8 ns)

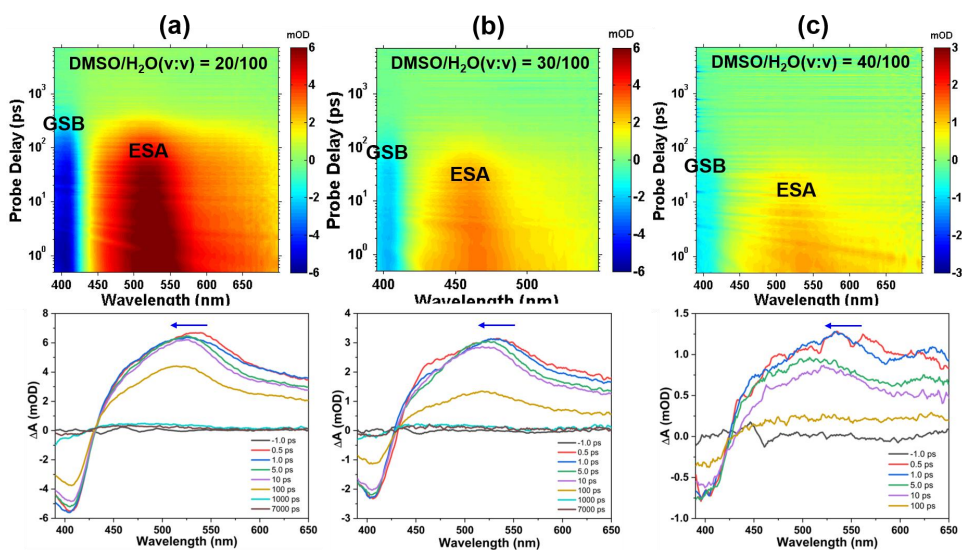


Figure S12. Differential absorption 3D map of the TAS data matrix after 380 nm excitation (upper row) and time evolution of the TA spectra (lower row) of **TPEIP** in DMSO/H₂O mixed 5 solvents with 20% (a), 30% (b), 40% (c) of H₂O content.

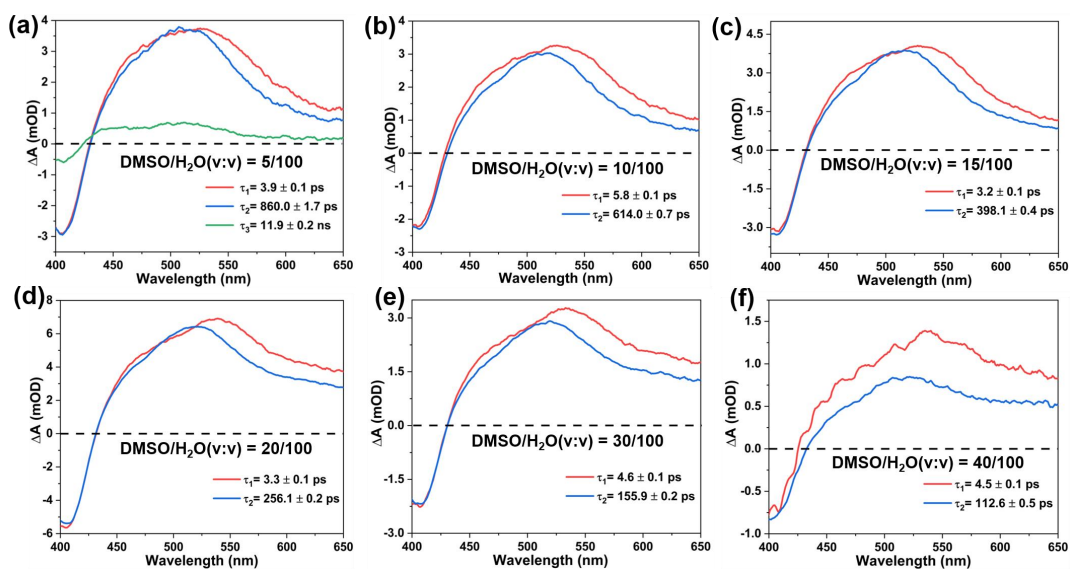
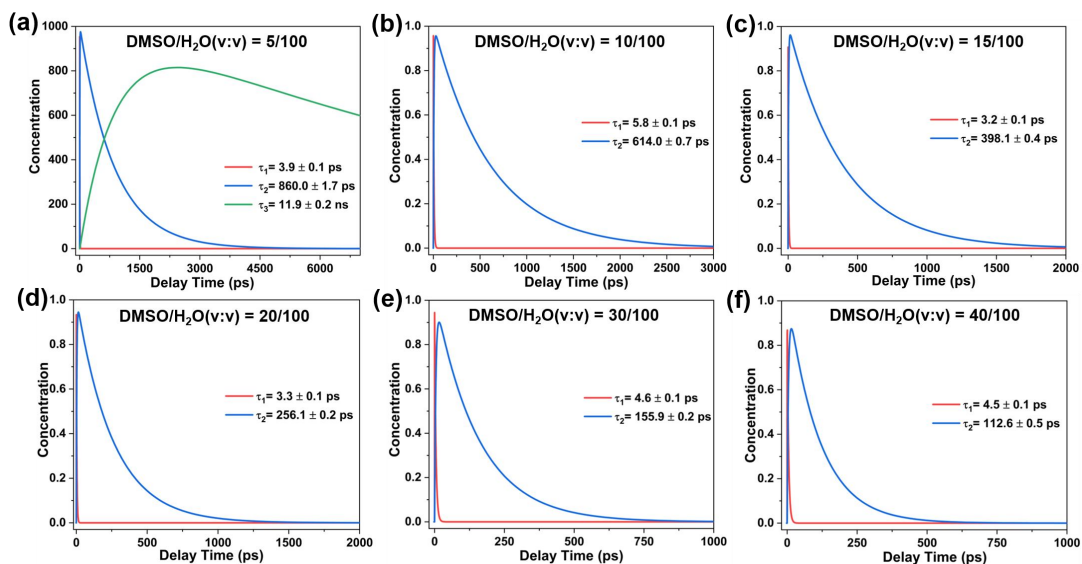


Figure S13. The species-associated difference spectra (SADS) obtained from global fitting in DMSO/H₂O mixed solvents with 5% (a), 10% (b), 15% (c), 20% (d), 30% (e), 40% (f) of H₂O content.



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Figure S14. Concentrations of the SADS components as a function of time in DMSO/H₂O mixed solvents with 5% (a), 10% (b), 15% (c), 20% (d), 30% (e), 40% (f) of H₂O content.

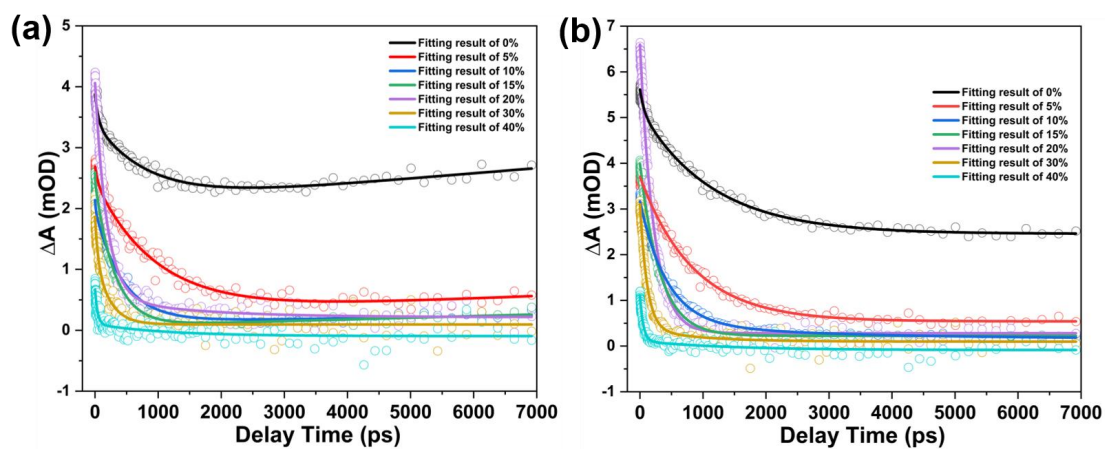


Figure S15. Best fitting parameters of femtosecond TA of **TPEIP** in DMSO/H₂O mixed solvents with 0%, 5%, 10%, 15%, 20%, 30%, 40% of H₂O content at wavelength 462 nm (a) and 520 nm (b).

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Table S5. Best fitting parameters of femtosecond TA of **TPEIP** in DMSO/H₂O mixed solvents with 10 0%, 5%, 10%, 15%, 20%, 30%, 40% of H₂O content at wavelength 462 nm.

DMSO/H ₂ O(V:V)	τ_1 (ps)	τ_2 (ps)	τ_3 (ns)
0%	52.5 (\pm 8.2)	857.0 (\pm 83.1)	202.1 (\pm 0.9)
5%	49.3 (\pm 15.5)	977.1 (\pm 71.4)	12.2 (\pm 0.5)
10%	13.0 (\pm 6.0)	636.5 (\pm 20.1)	/
15%	2.5 (\pm 1.0)	408.9 (\pm 6.3)	/
20%	/	226.1 (\pm 4.1)	/
30%	/	142.5 (\pm 6.3)	/
40%	/	102.9 (\pm 7.3)	/

Table S6. Best fitting parameters of femtosecond TA of **TPEIP** in DMSO/H₂O mixed solvents with 0%, 5%, 10%, 15%, 20%, 30%, 40% of H₂O content at wavelength 520 nm.

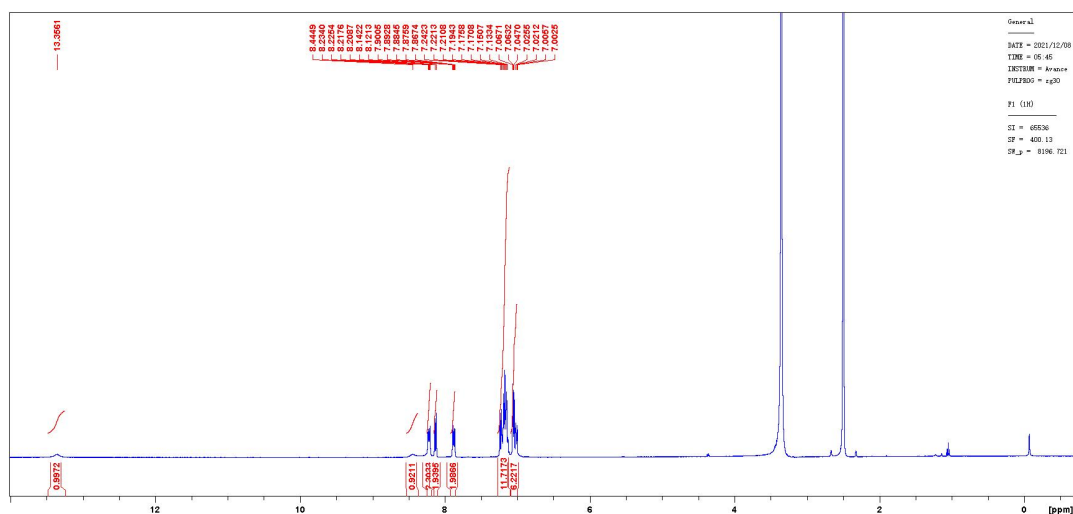
DMSO/H ₂ O(V:V)	τ_1 (ps)	τ_2 (ps)
0%	62.0 (\pm 10.5)	2140.2 (\pm 36.3)
5%	846.7 (\pm 14.0)	/
10%	472.3 (\pm 9.5)	/
15%	316.8 (\pm 3.8)	/
20%	225.5 (\pm 2.2)	/
30%	128.7 (\pm 1.9)	/
40%	67.0 (\pm 3.6)	/

5 6. Synthesis of compounds and Molecular structures characterization.

Synthesis of compounds **TPEIP** and **PIP**

A mixture of 2,3-diamino-phenazine (0.21 mg, 1.0 mmol), 4-(1,2,2-triphenylvinyl)benzaldehyde (**TPEIP**) (1.08 g, 3 mmol), 1.0 mL acetic acid (AcOH) and N,N-Dimethylformamide (DMF) were magnetically stirred and heated at 90 °C for 10 12 h. After cooling to room temperature, the yellow precipitate was filtrated, washed with hot absolute ethanol three times, then recrystallized with DMF-H₂O to get yellow powdery product **TPEIP** (0.25 g, 0.45 mmol) in 45% yield, ¹H-NMR (DMSO-*d*₆, 400 MHz) 13.36 (s 1H, NH), 8.44 (s 1H, ArH), 8.23–8.21 (m 2H, ArH), 8.13 (d *J* = 8.36 Hz, 2H, ArH), 7.90–7.89 (m 2H, ArH), 7.24-7.13 (m 12H, ArH), 7.07-7.0 (m 6H, ArH).
15 ¹³C-NMR (DMSO-*d*₆, 100 MHz) 159.25, 147.05, 142.87, 142.68, 142.02, 141.82, 140.11, 139.78, 131.57, 130.80, 130.67, 129.82, 128.97, 128.1, 127.94, 127.37, 127.02,

126.93, 126.69. ESI-MS m/z : Calcd. for $C_{39}H_{26}N_4$, 550.22; Found, 551.22. The 2-phenyl-1H-imidazo[4,5-b]phenazine (**PIP**) was synthesized by similar procedures (Scheme 1). PIP: Yield 55%, 1H NMR (DMSO- d_6 , 400 MHz) δ : 13.41 (s, 1H), 8.47 (s, 1H), 8.35 (d, $J = 3.6$ Hz, 2H), 8.20 (d, $J = 4$ Hz 3H), 7.85 (d, $J = 6.4$ Hz, 2H), 7.64 (d, $J = 6.2$ Hz, 3H); ^{13}C NMR (DMSO- d_6 , 100 MHz) δ : 159.90, 149.24, 142.12, 140.62, 132.24, 129.61, 128.18, 115.27, 106.30; ESI-MS m/z : Calcd. for $C_{19}H_{12}N_4$, 296.11, Found, 297.11.



10 **Figure S16.** 1H NMR spectrum (400 MHz, DMSO- d_6 , 298K) of **TPEIP**.

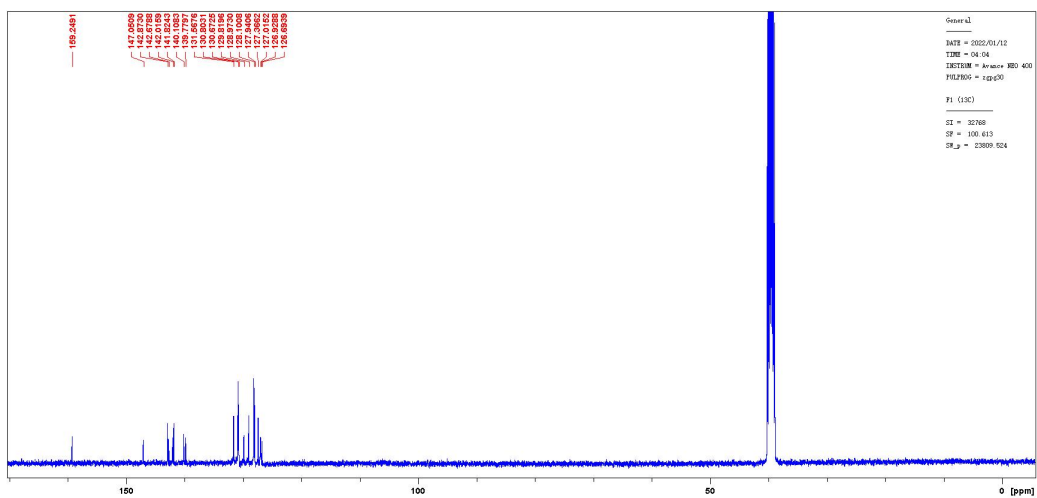


Figure S17. ^{13}C NMR spectrum (100 MHz, $\text{DMSO-}d_6$, 298K) of TPEIP.

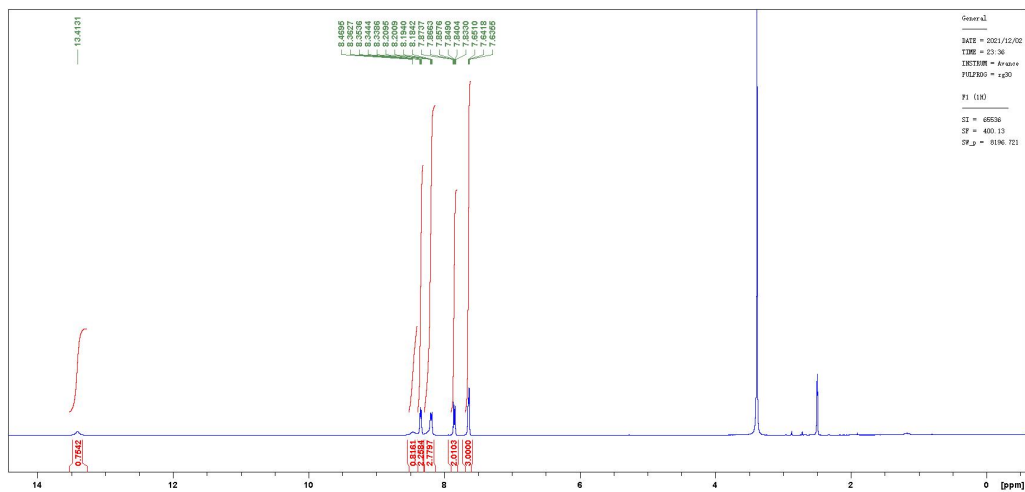


Figure S18. ^1H NMR spectrum (400 MHz, $\text{DMSO-}d_6$, 298K) of PIP.

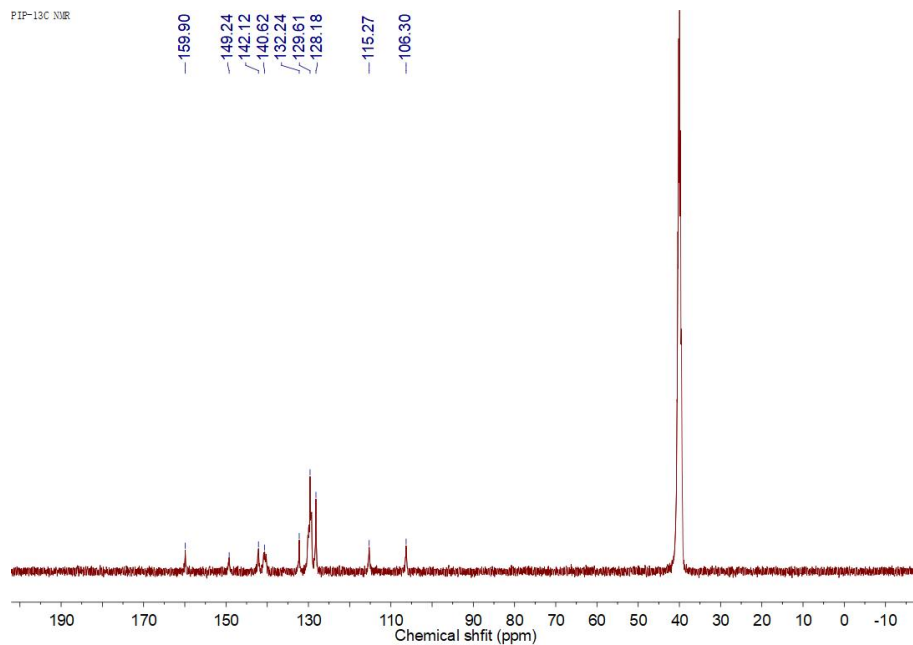


Figure S19. ¹³C NMR spectrum (400 MHz, DMSO-*d*₆, 298K) of **PIP**.

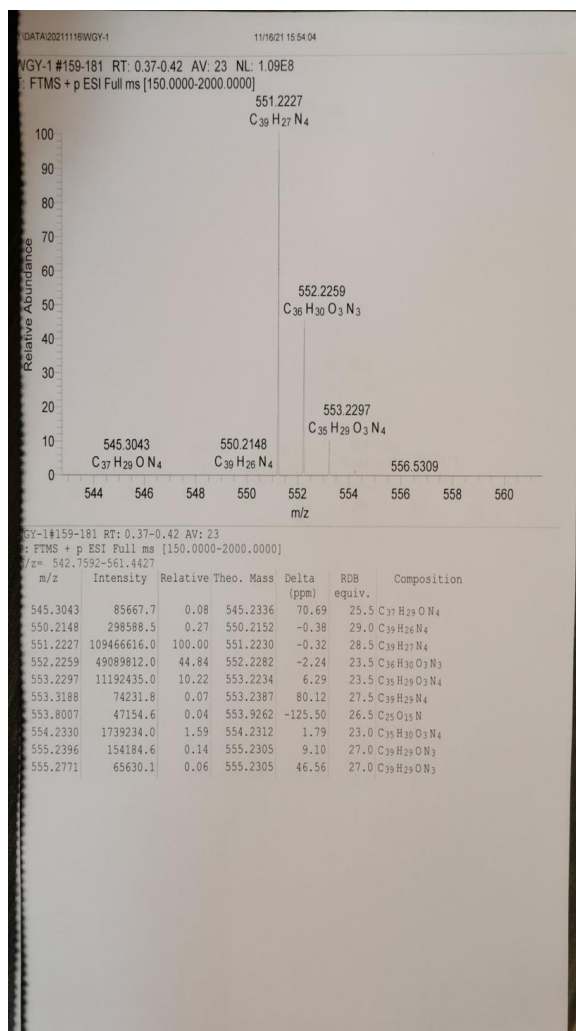


Figure S20. The ESI-MS of TPEIP.

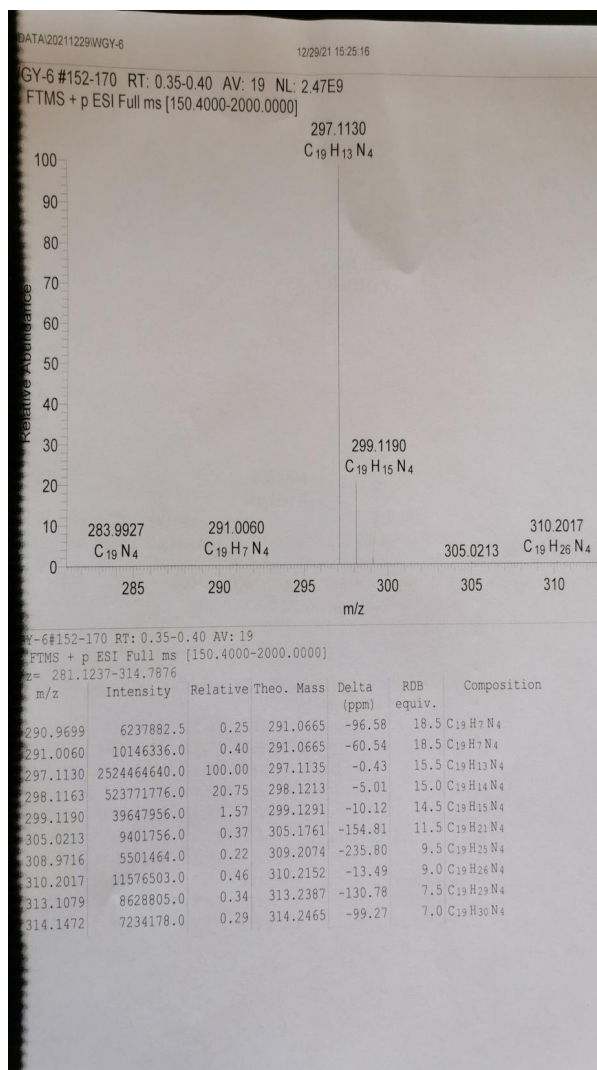


Figure S21. The ESI-MS of PIP.