

Supplementary Information

New 9-Aminoacridine Derivative: Synthesis, Study and Potential Application as pH Indicator in Organic Solvents

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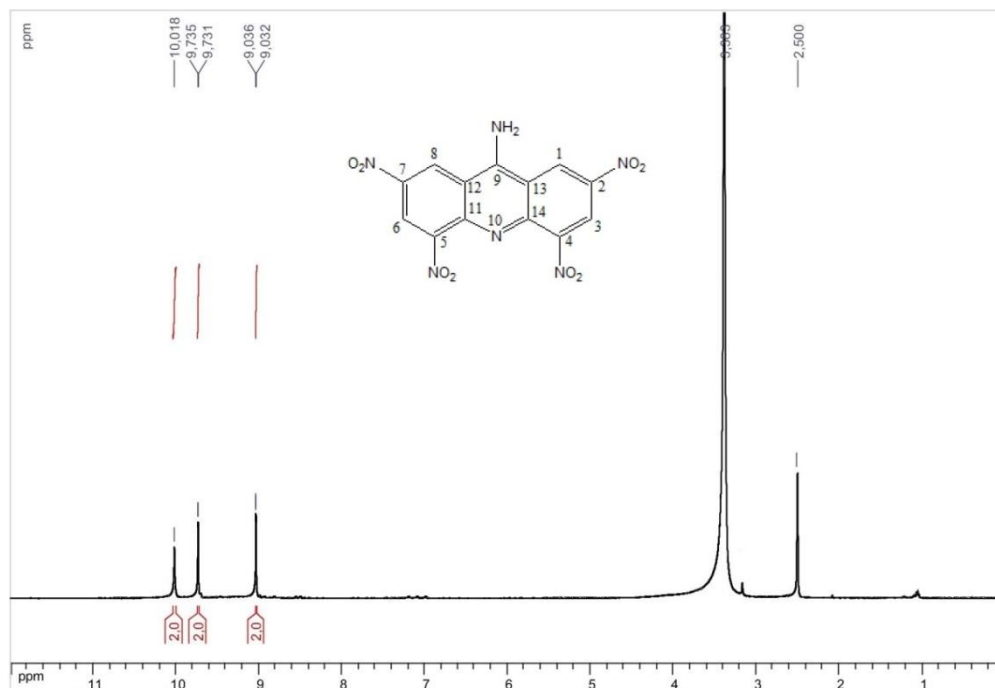


Figure S1. ¹H NMR spectrum of TNA (500 MHz, DMSO-*d*₆).

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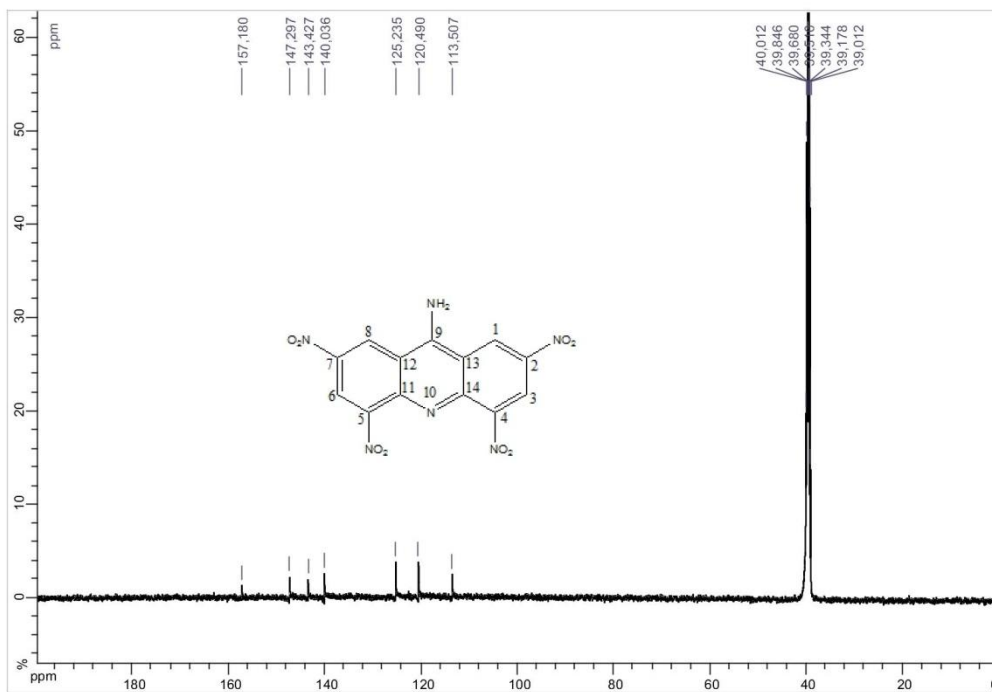


Figure S2. ¹³C NMR spectrum of TNA (125 MHz, DMSO-*d*₆).

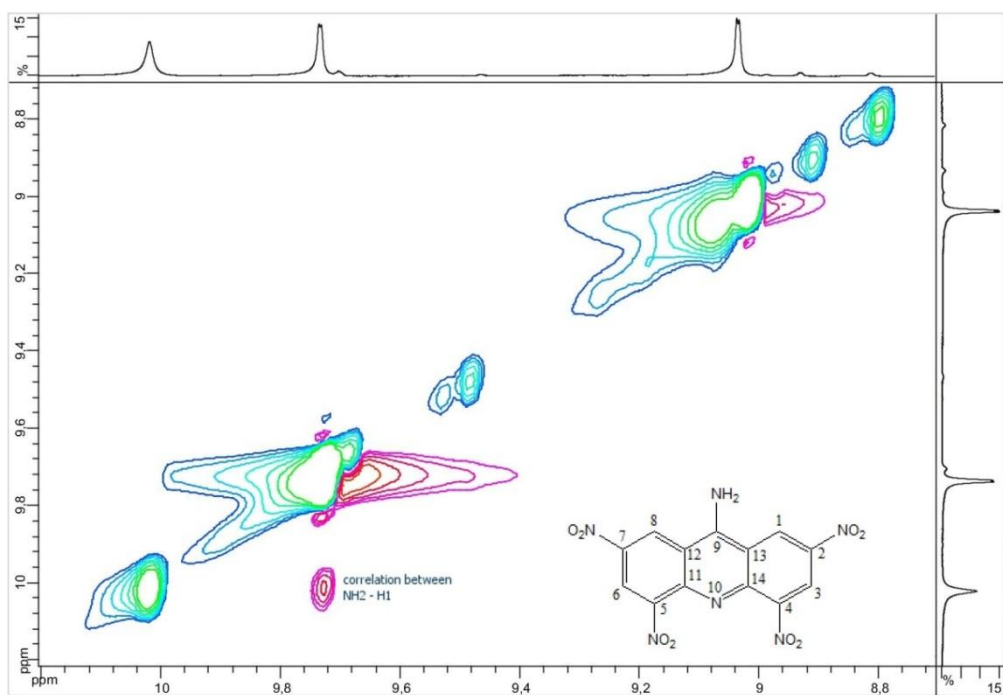


Figure S3. NOESY contour map of TNA (region between 8.70-10.20 ppm).

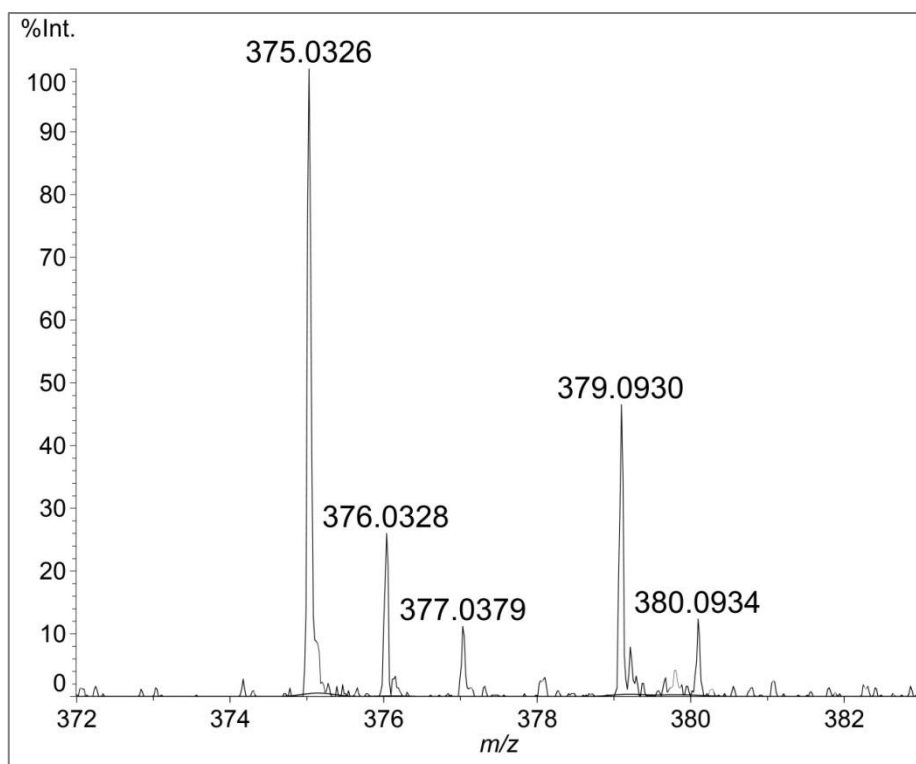


Figure S4. Mass spectrum (MALDI-TOF) of TNA (region between 372-383 m/z).

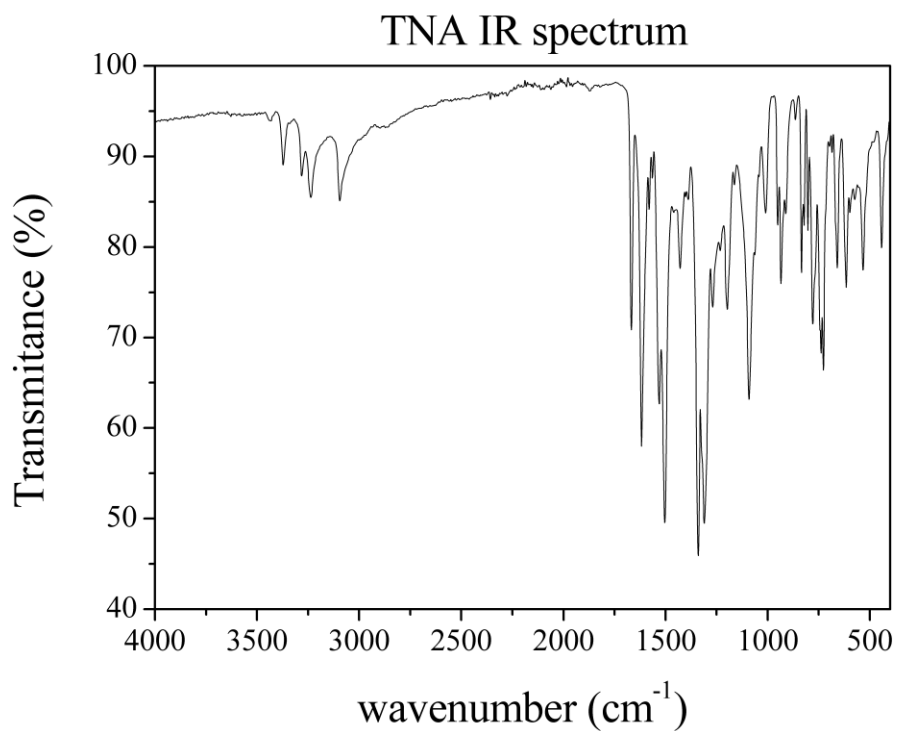


Figure S5. Infrared spectrum of neutral TNA.

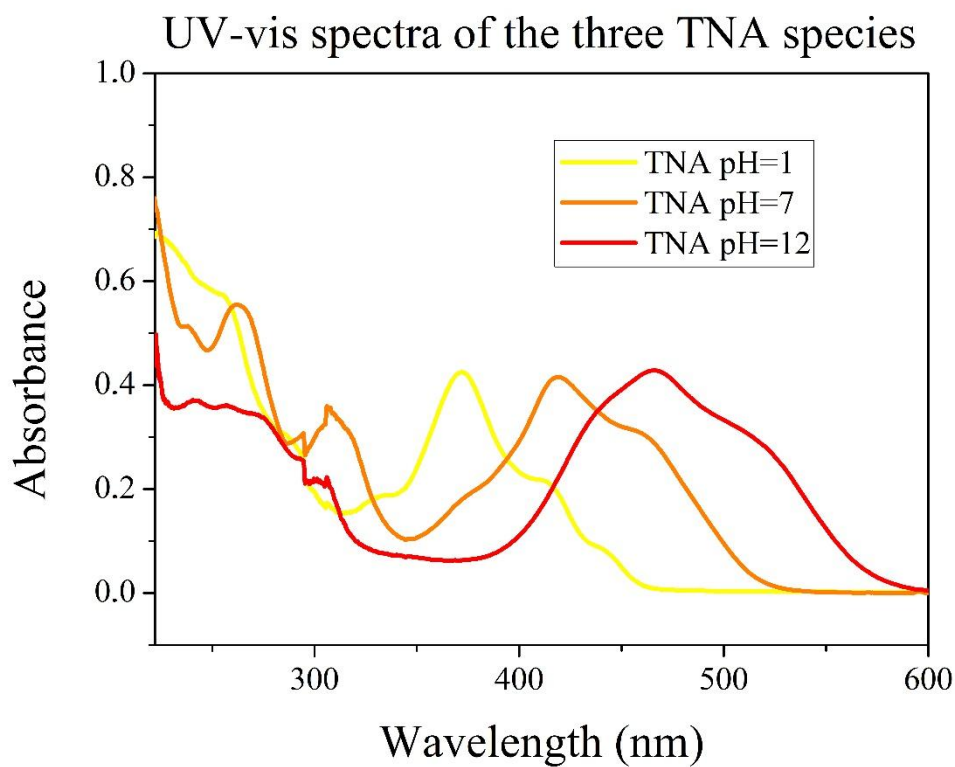


Figure S6. UV-Vis spectra of the three TNA species, mediums acid, neutral and basic in ethanol.

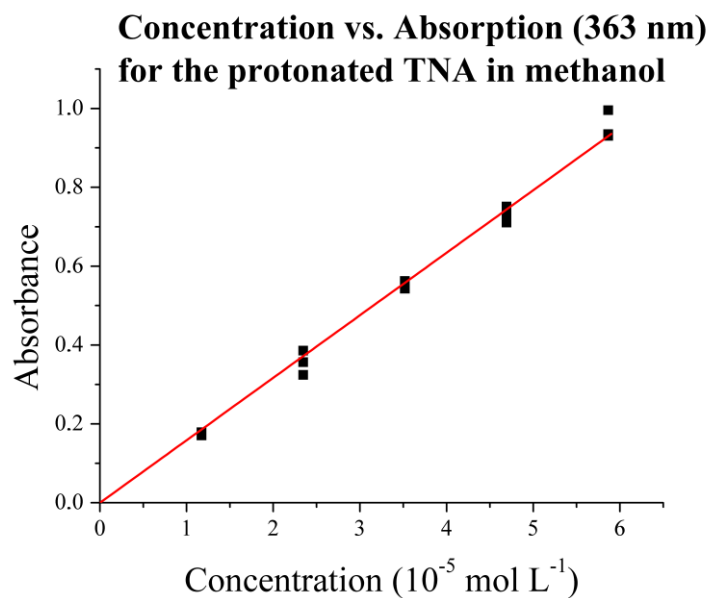


Figure S7. Linear regression curve for the protonated TNA in methanol.

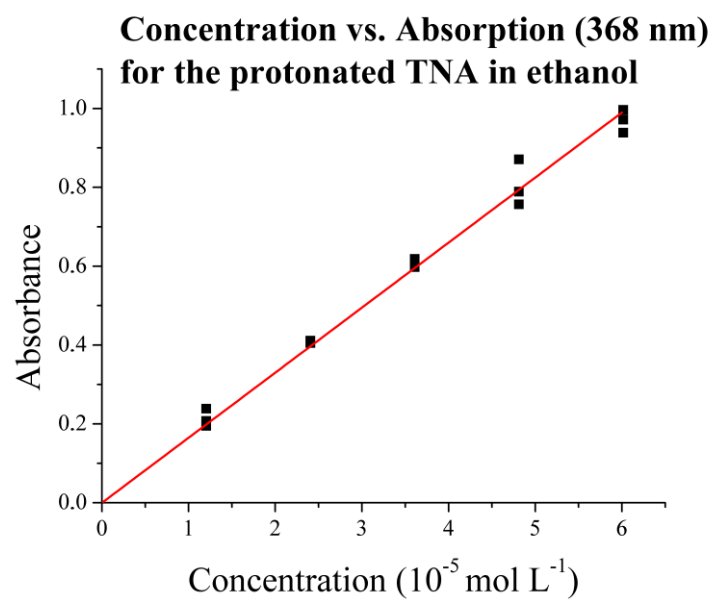


Figure S8. Linear regression curve for the protonated TNA in ethanol.

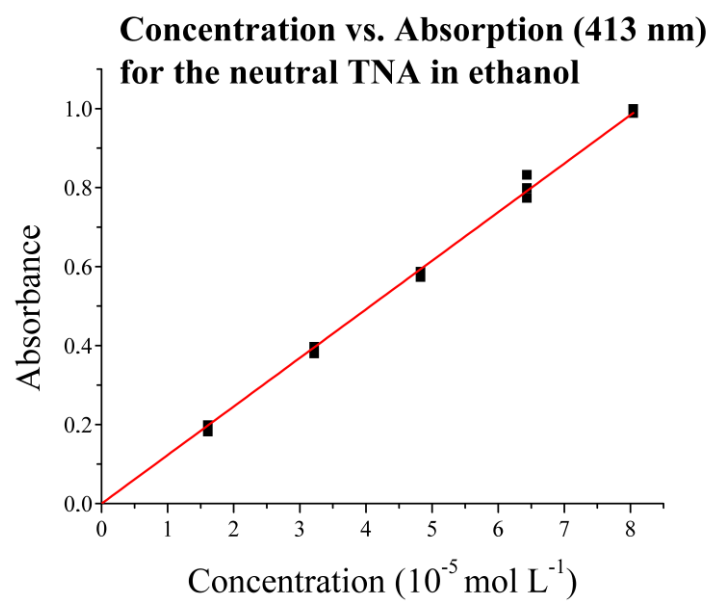


Figure S9. Linear regression curve for the neutral TNA in ethanol.

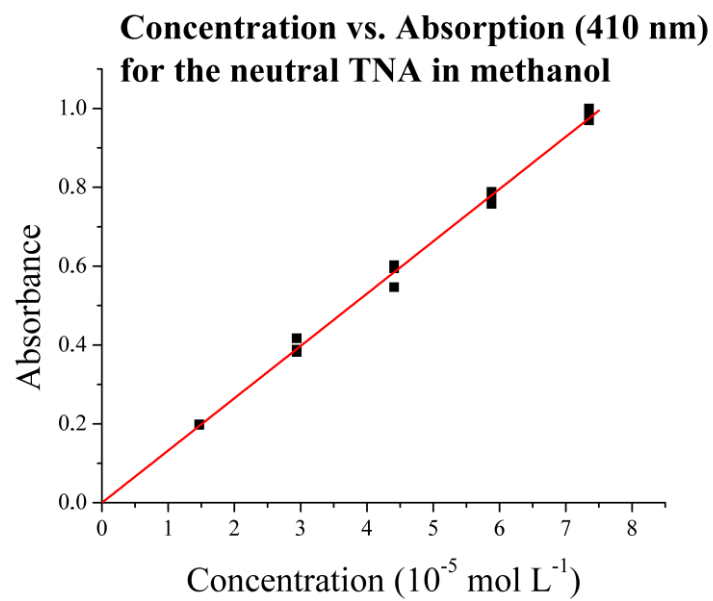


Figure S10. Linear regression curve for the neutral TNA in methanol.

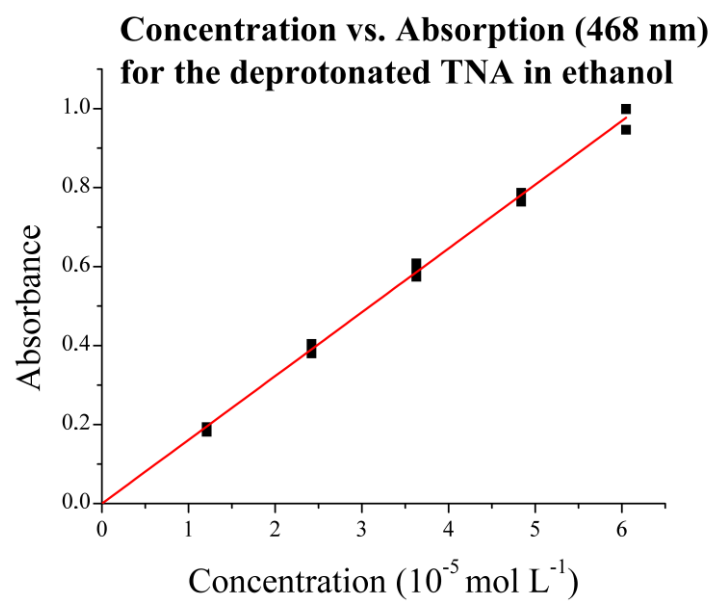


Figure S11. Linear regression curve for the deprotonated TNA in ethanol.

Table S1. Experimental and theoretical electronic transitions data in the visible region for TNA in methanol

	MO _t ^a	$\lambda_{\text{Exp}} / \lambda_{\text{max}}^{\text{b}} / \text{nm}$	$\lambda_{\text{Calc}} / \text{nm}$	OS ^c	$\Delta E^{\text{d}} / \text{eV}$
Protonated TNA	HOMO → LUMO	400-450 / 400	405	0.1183	3.06
Neutral TNA	HOMO → LUMO	400-510 / 416	460	0.0488	2.69
	HOMO → LUMO + 1		437	0.4602	2.83
Deprotonated TNA	HOMO → LUMO	400-565 / 500	526	0.5854	2.36
	HOMO → LUMO + 1		515	0.0657	2.41
	HOMO → LUMO + 3		481	0.0566	2.58
	HOMO → LUMO + 2		440	0.0112	2.82

^aMolecular orbitals in transition; ^bexperimental range of spectral band / maximum wavelength in visible spectrum; ^coscillator strength; ^dgap between molecular orbitals involved in transition.

Table S2. Solubility of the neutral TNA in polar protic, polar aprotic, and non-polar solvents

Solvent type	Solvent	Solubility coefficient / (mg mL ⁻¹)
Polar protic	methanol	0.24
	ethanol	0.18
	water	^a
Polar aprotic	methylene chloride	0.30
	tetrahydrofuran	0.80
	acetone	3.36
	dimethylformamide	14.60
	acetonitrile	1.20
	dimethyl sulfoxide	13.10
Non-Polar	hexane	^a
	toluene	0.28
	diethyl ether	^a

^aInsoluble or soluble in concentrations lower than 0.1 mg mL⁻¹.