Supplementary Information (SI)

Impact of tunable 2-(1*H*-indol-3-yl)acetonitrile based fluorophores towards optical, thermal and electroluminescence properties

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Chart 1: ^{1}H and ^{13}C NMR spectra of BIPIAN

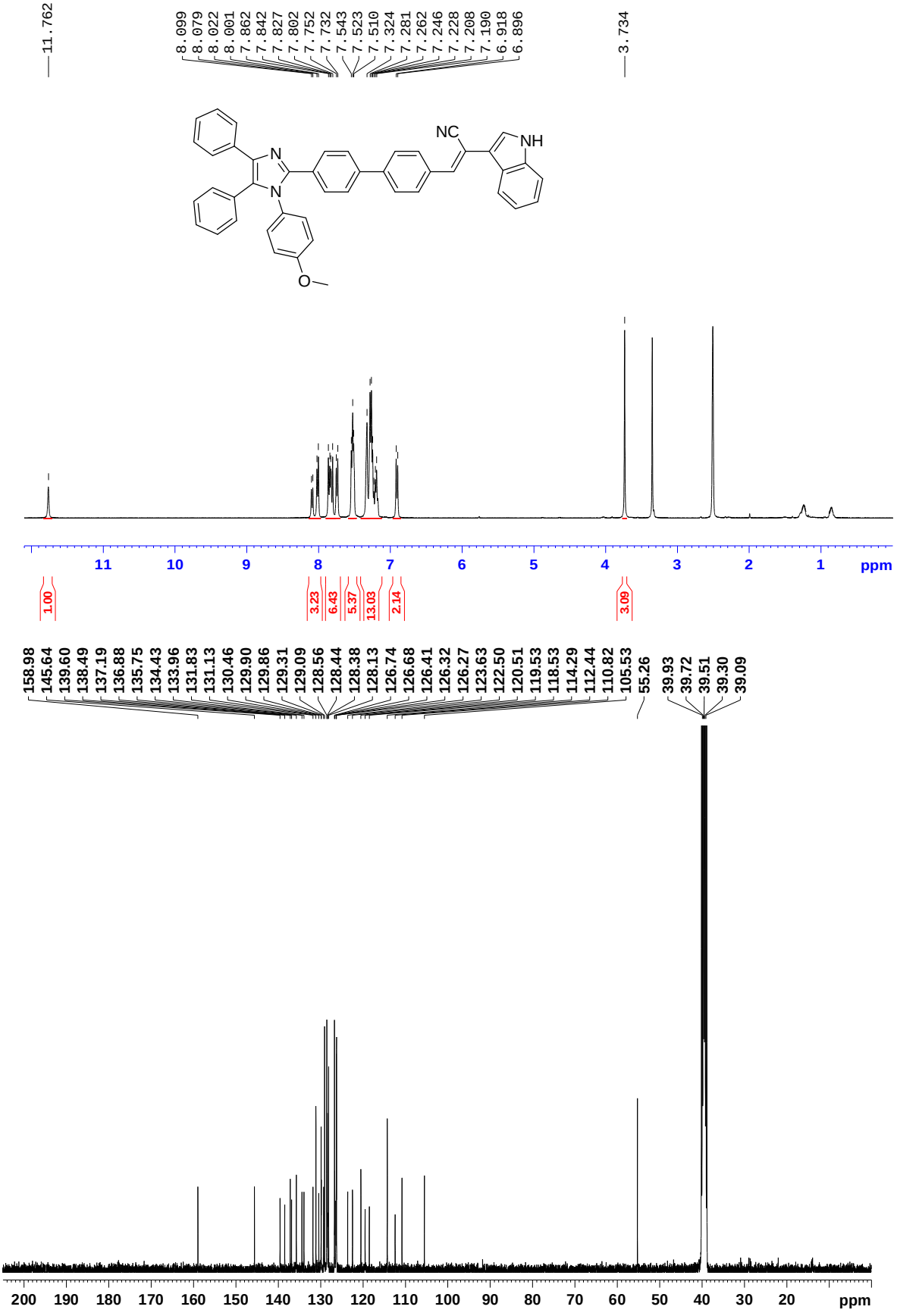


Chart 2: HRMS spectrum of BIPIAN

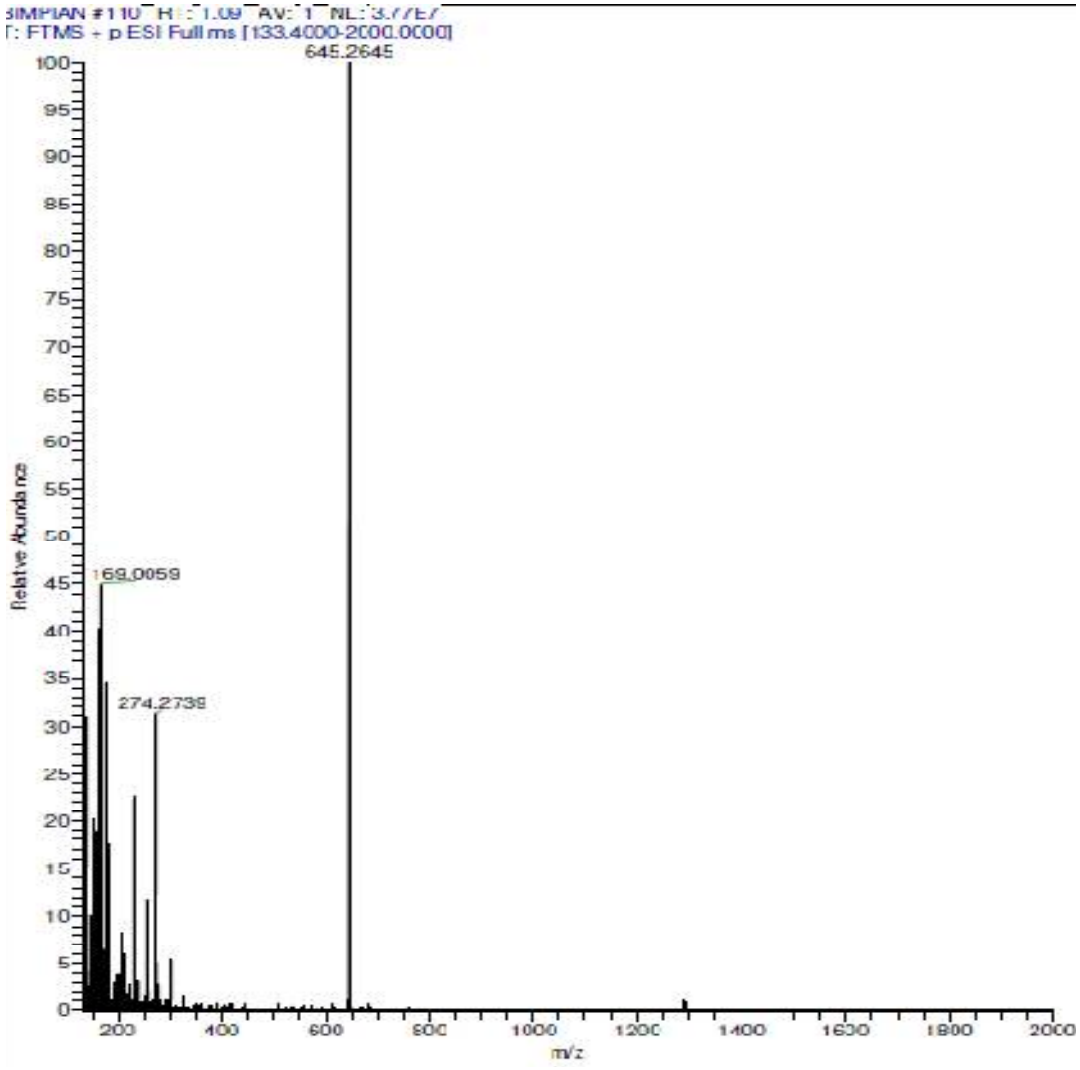


Chart 3: ^{1}H and ^{13}C NMR spectra of BITIAN

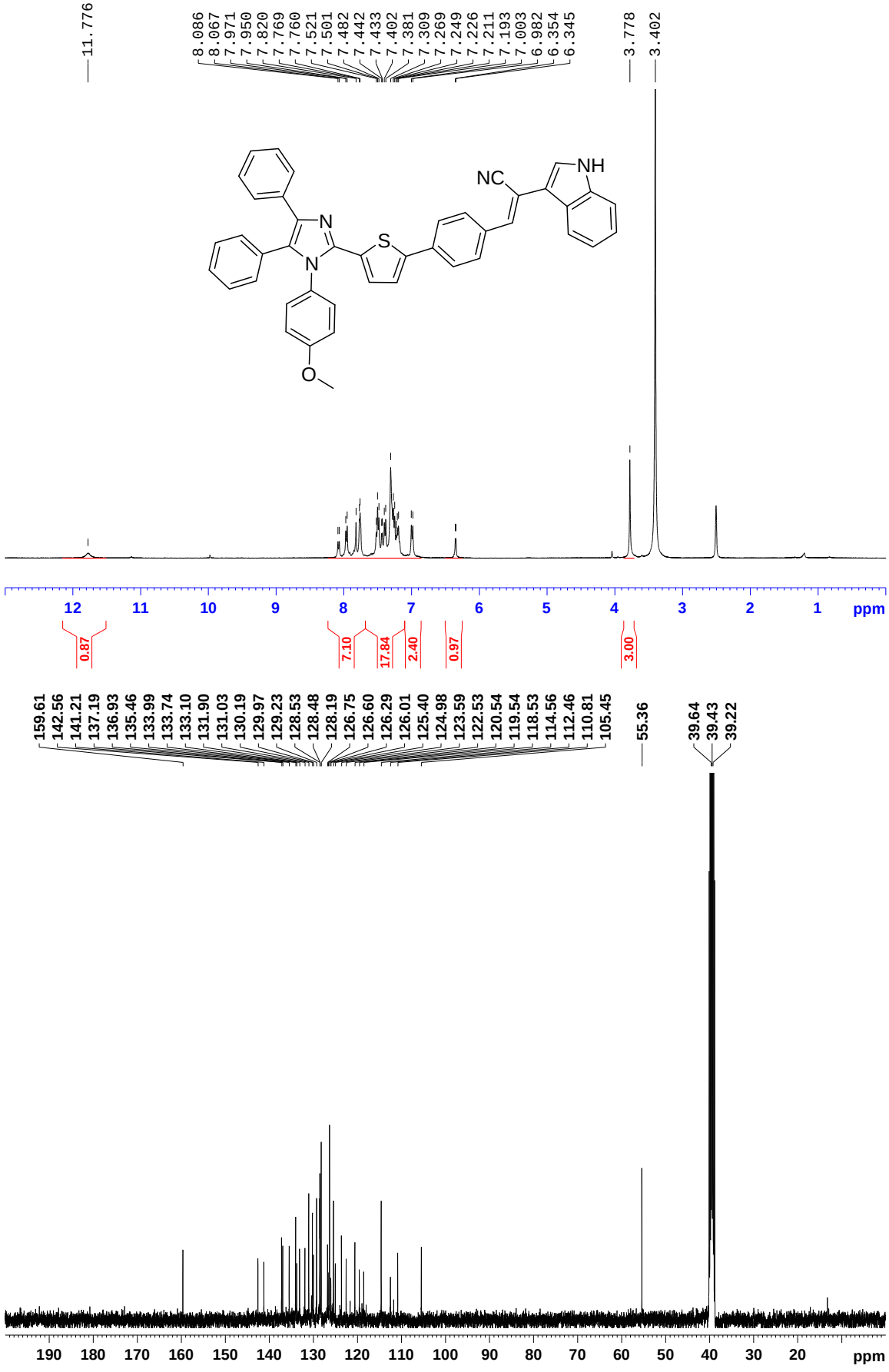
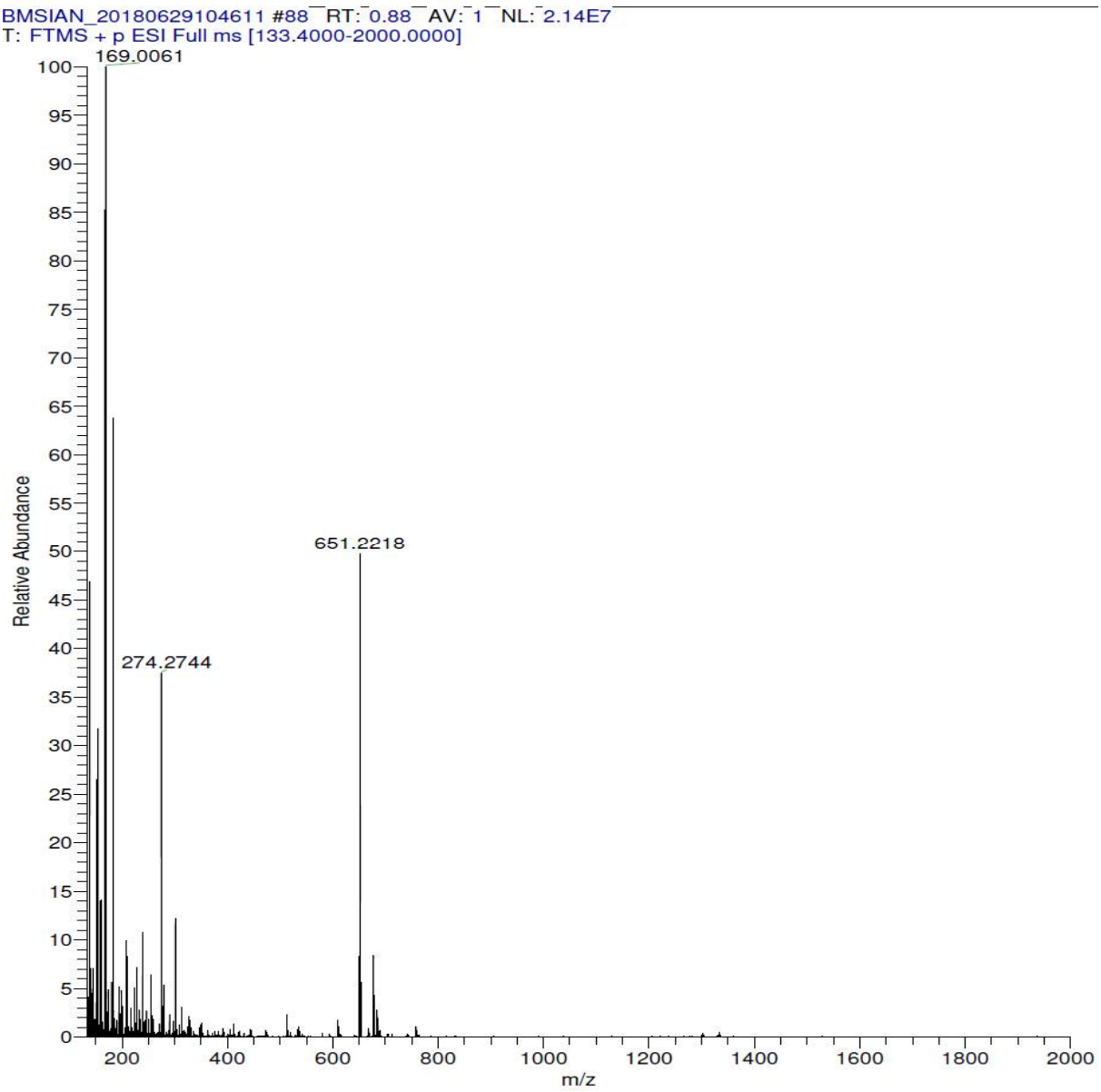


Chart 4: HRMS spectrum of BITIAN



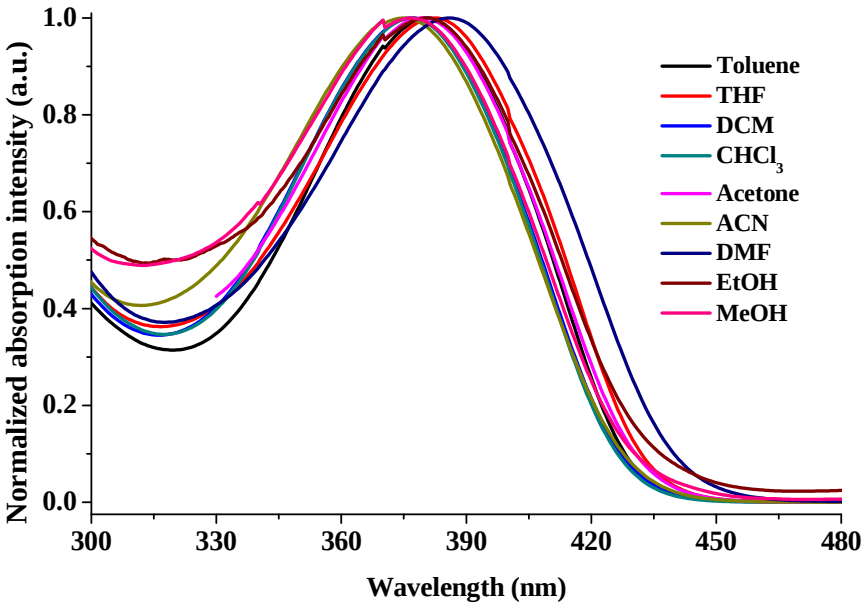


Figure S1. Absorption spectra of BIPIAN in different solvents

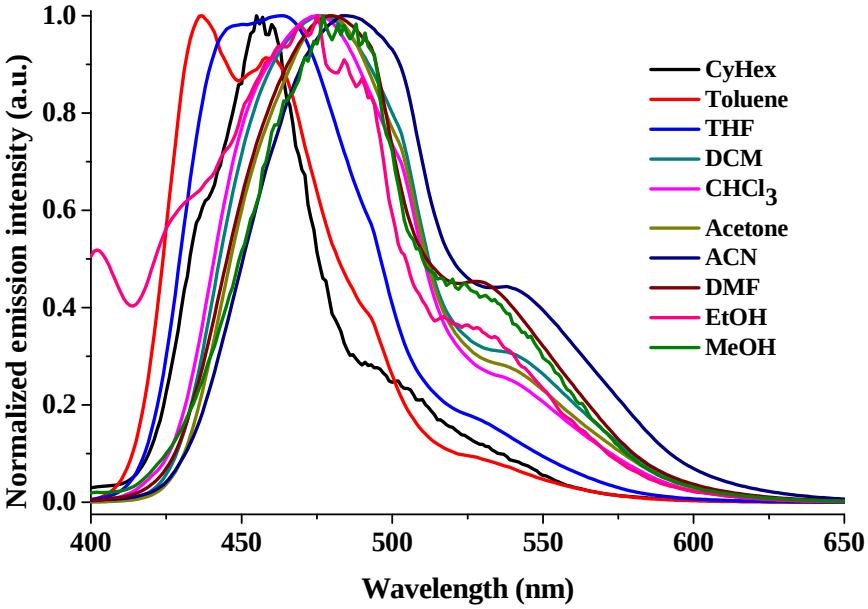


Figure S2. Emission spectra of BIPIAN in different solvents

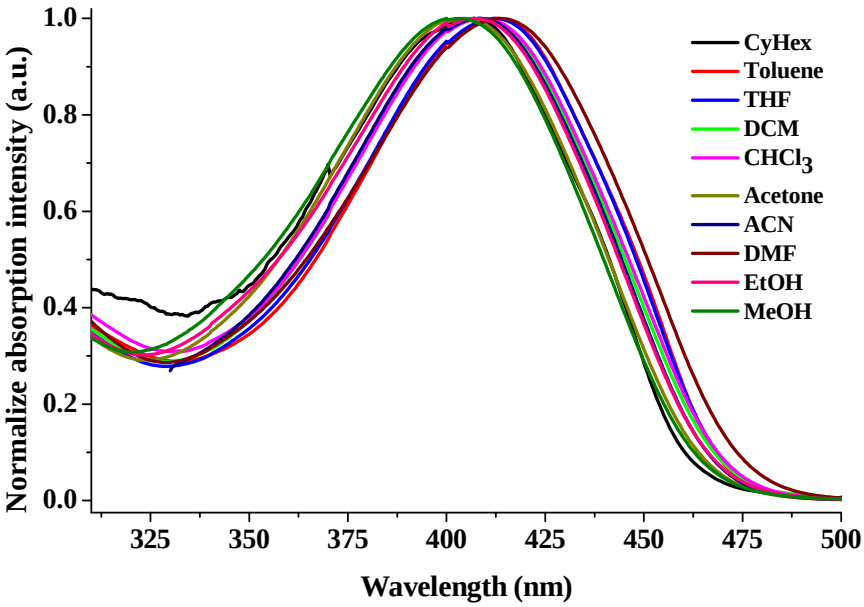


Figure S3. Absorption spectra of BITIAN in different solvents

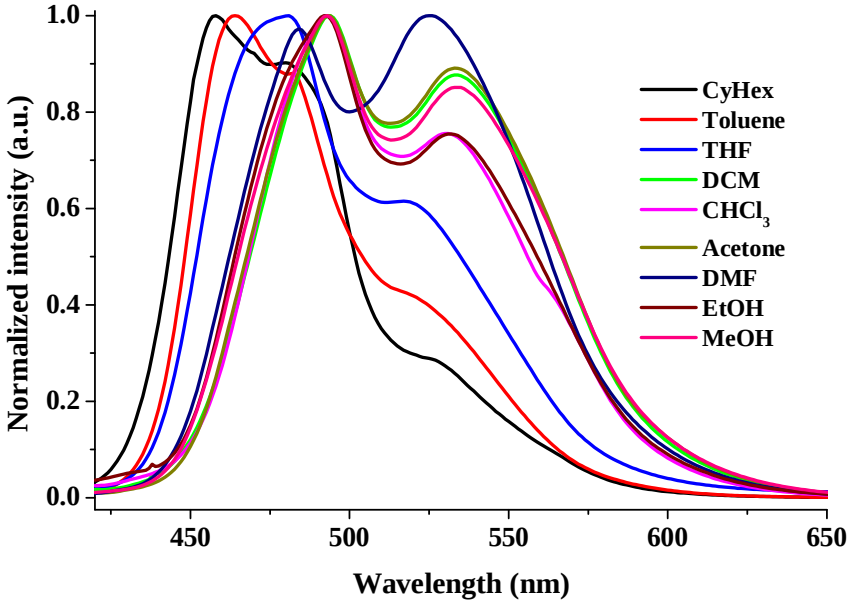


Figure S4. Emission spectra of BITIAN in different solvents

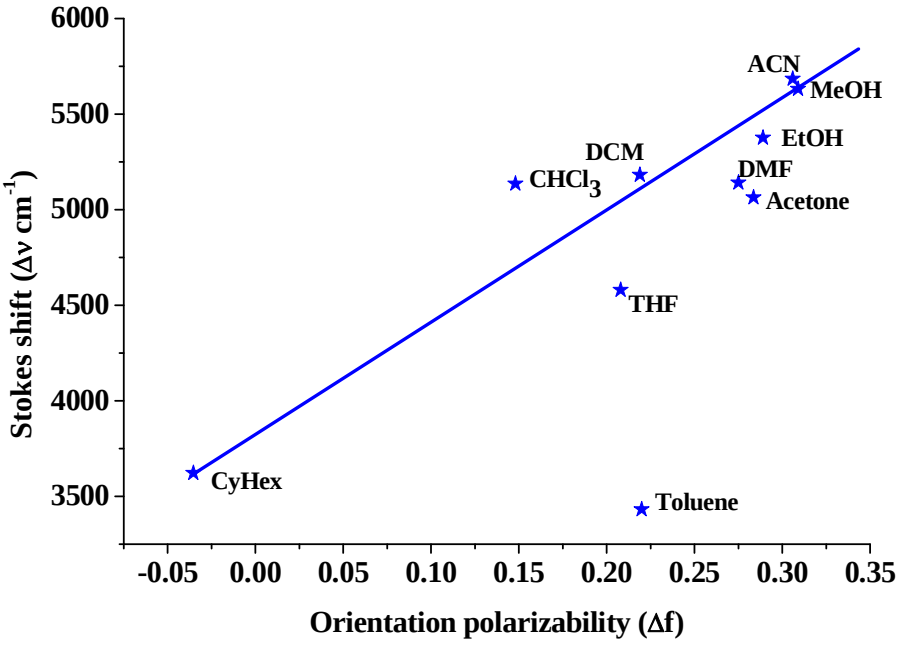


Figure S5. Lippert-mataga plot for BIPIAN

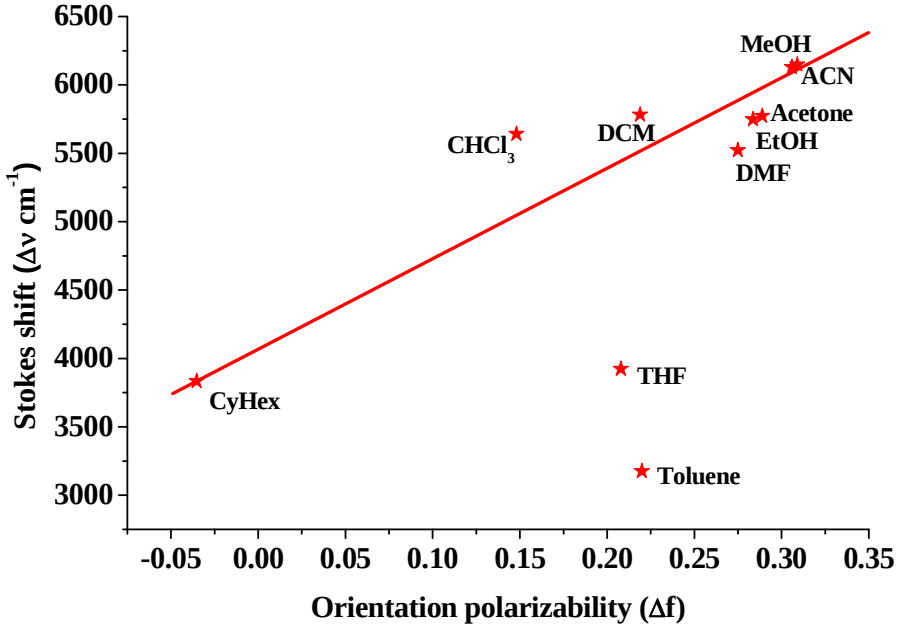


Figure S6. Lippert-mataga plot for BITIAN

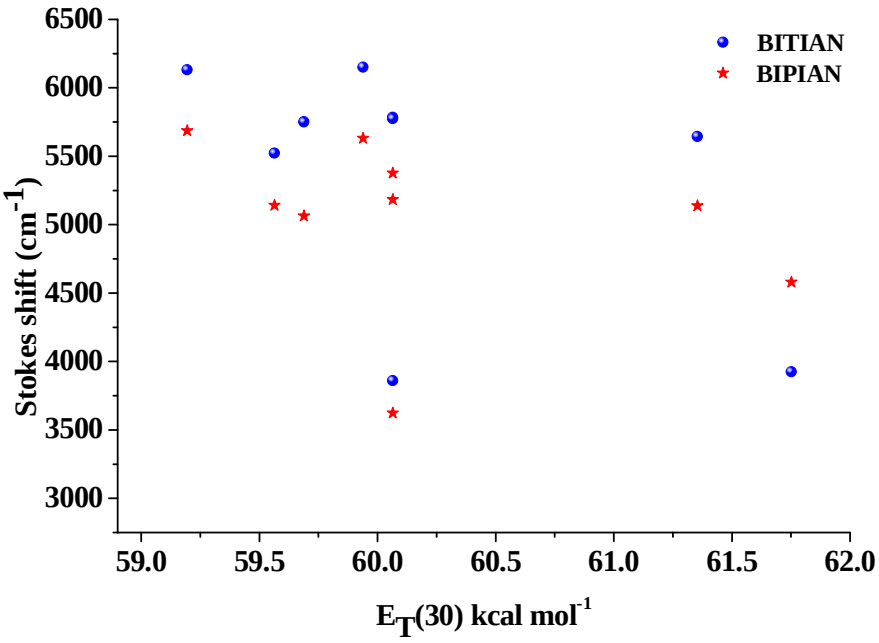


Figure S7. Representation of E_T (30) *versus* Stokes shift for BIPIAN and BITIAN

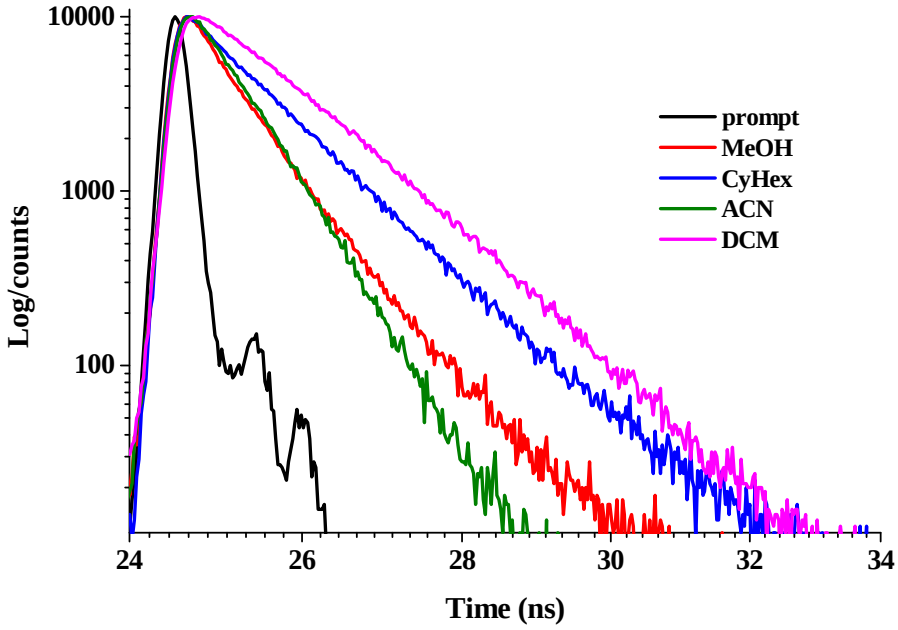


Figure S8. Fluorescence decay curves of BIPIAN in various solvents

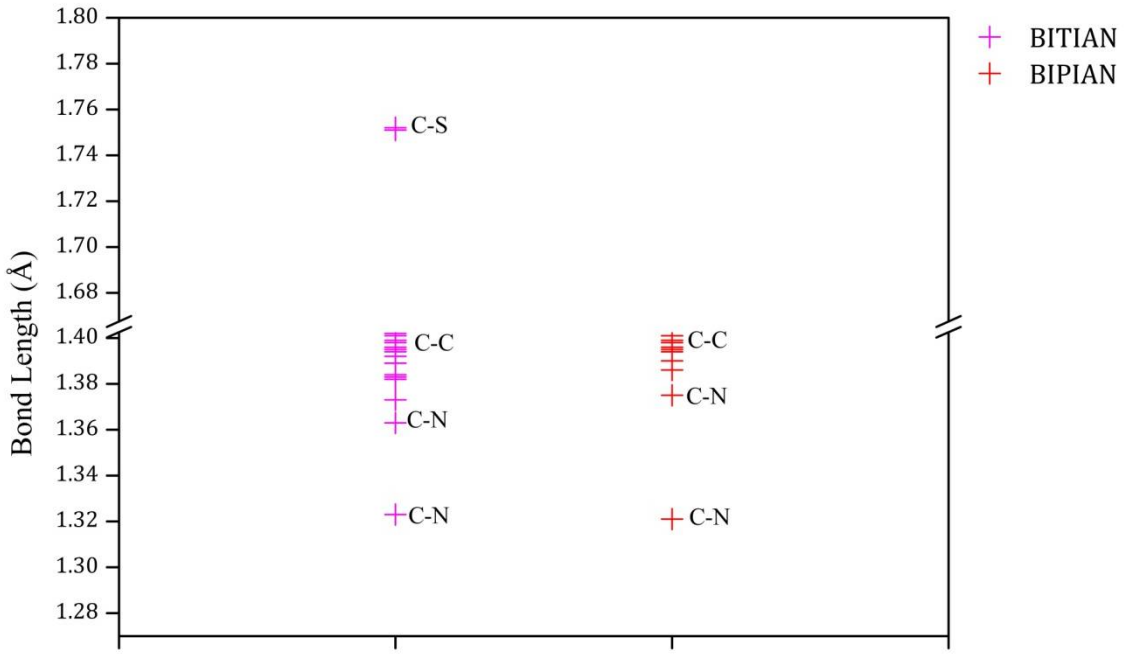
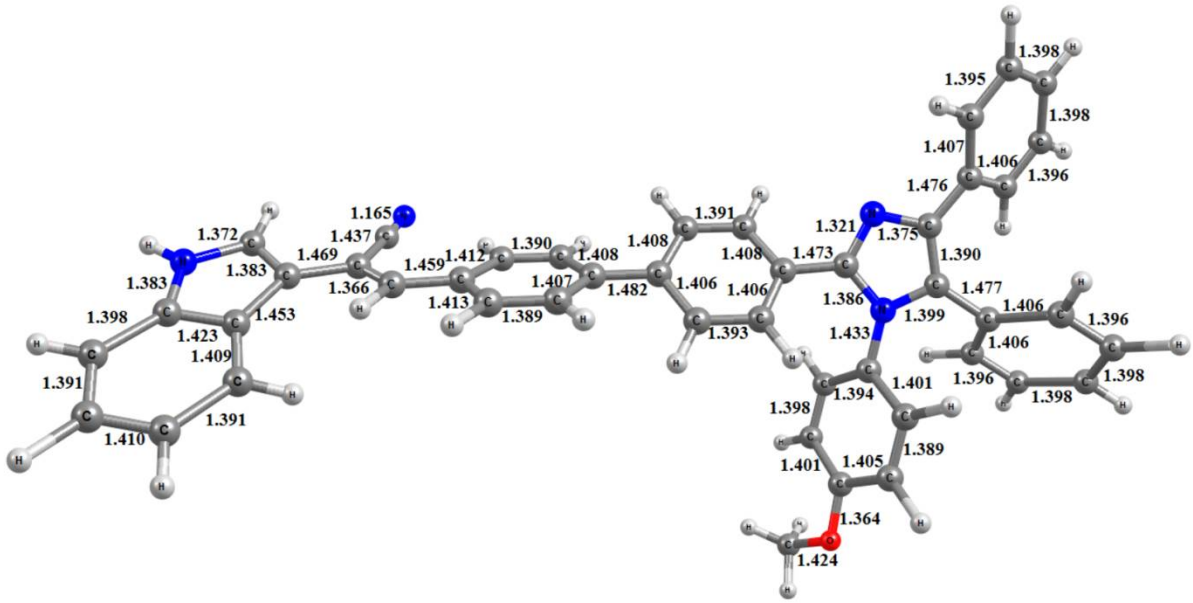


Figure S9. Illustration of π-delocalization from calculated C-C, C-S and C-N bond lengths at B3LYP/6-31G+(d,p) level

BIPIAN



BITIAN

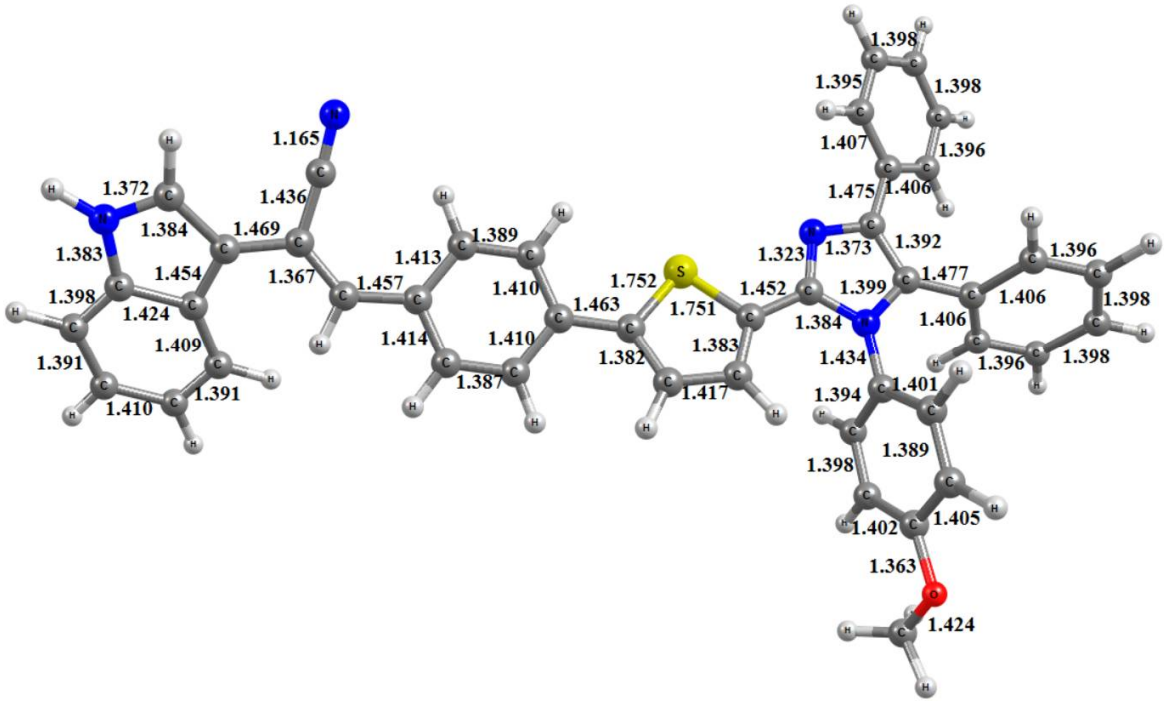


Figure S10. The optimized ground state geometries and important bond lengths of BIPIAN and BITIAN obtained using B3LYP/6-31G+(d,p) level

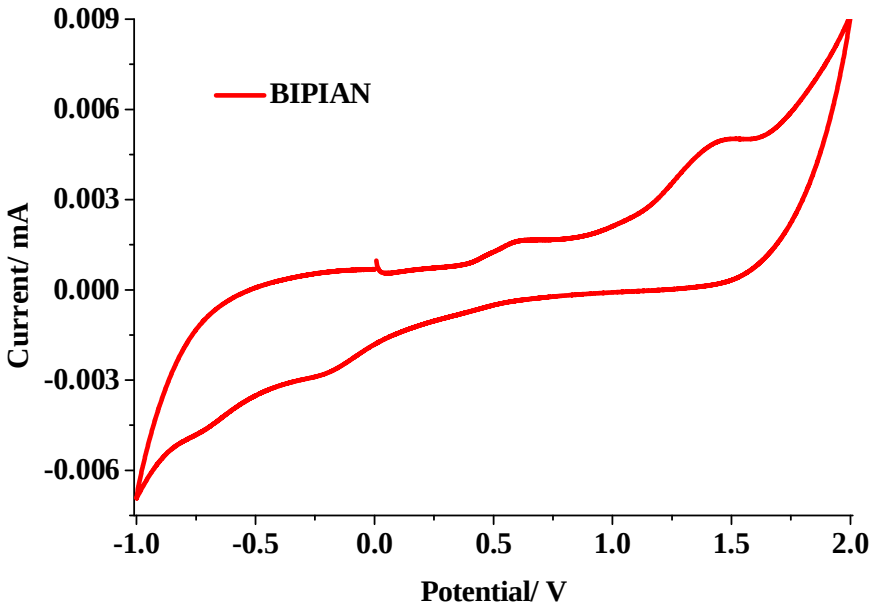


Figure S11. Cyclic voltammogram of BIPIAN

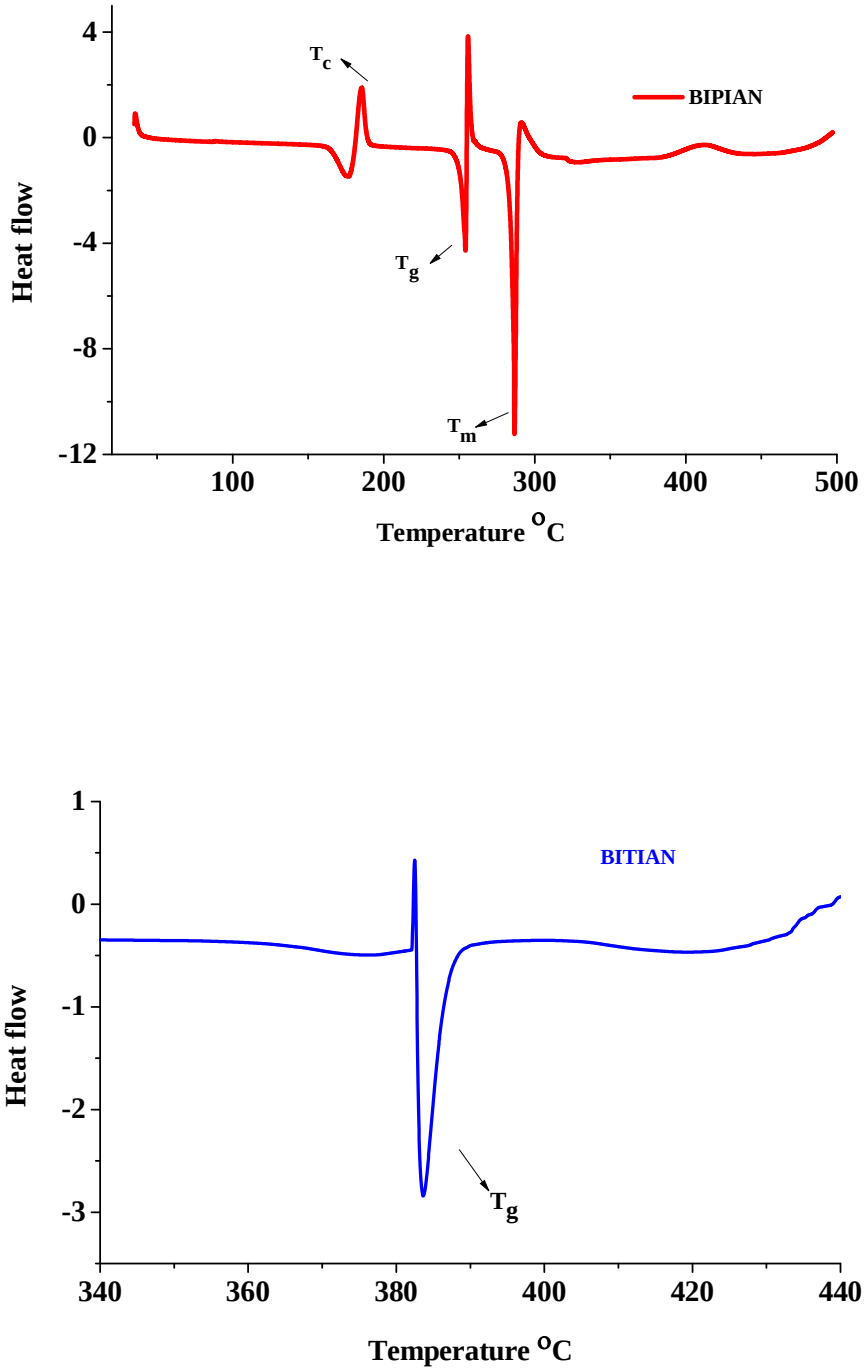
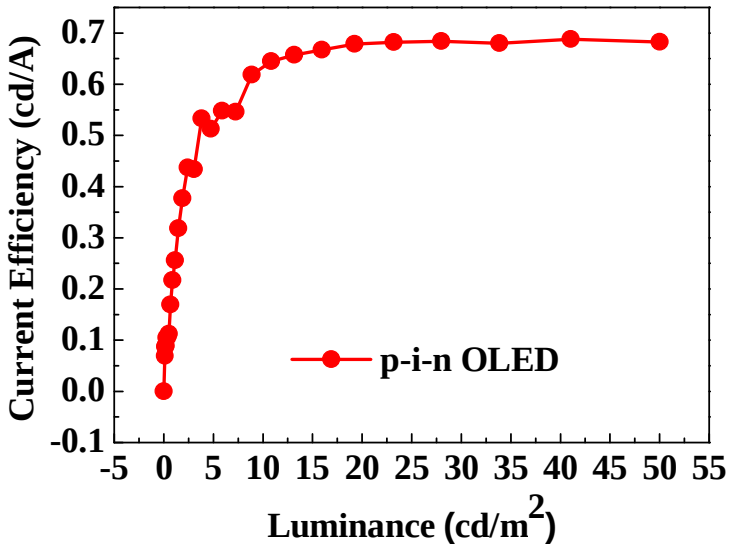
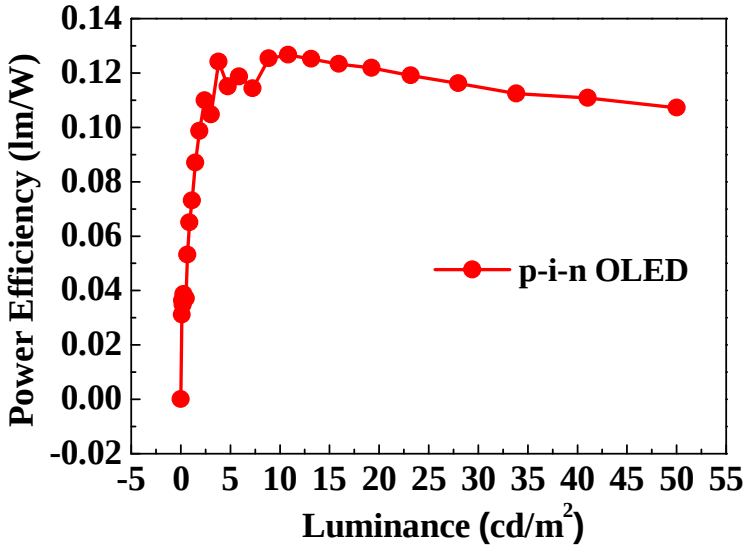


Figure S12. Differential scanning calorimetry of BIPIAN and BITIAN

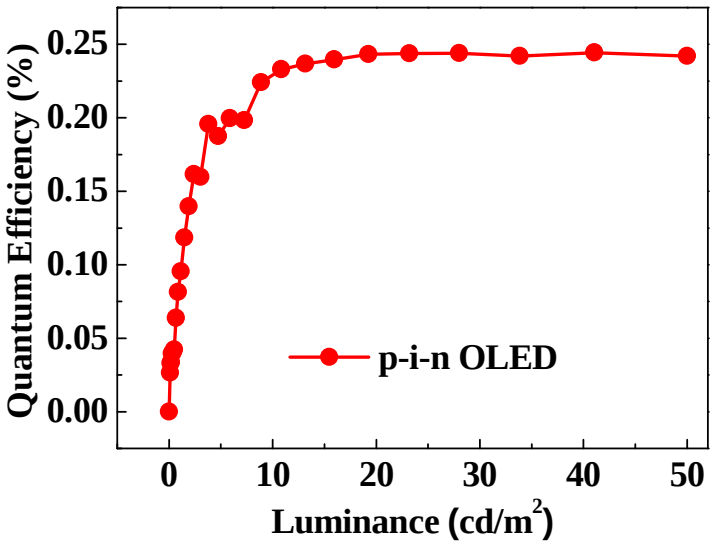
(a)


Current Efficiency (cd/A)
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
-0.1
-5 0 5 10 15 20 25 30 35 40 45 50 55
Luminance (cd/m2)
p-i-n OLED

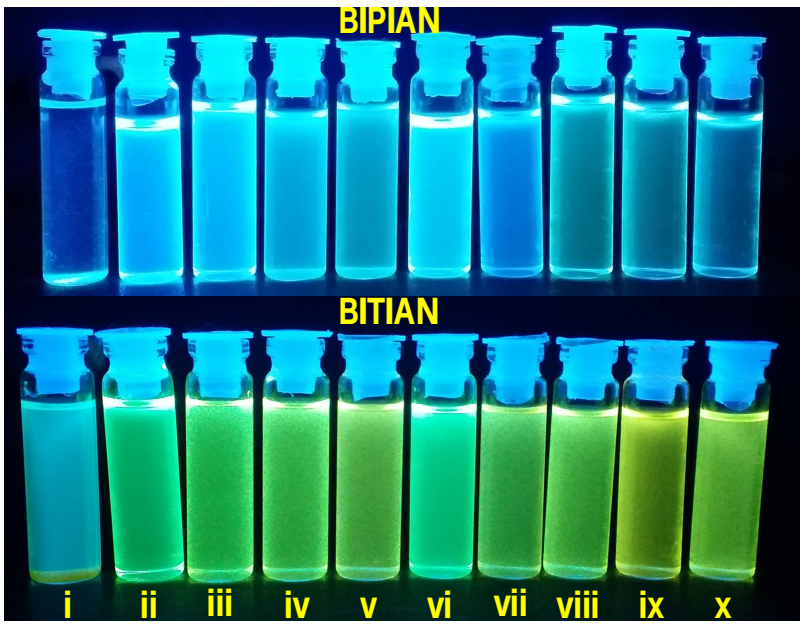
(b)


Power Efficiency (lm/W)
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
-0.02
-5 0 5 10 15 20 25 30 35 40 45 50 55
Luminance (cd/m2)
p-i-n OLED

(c)



(d)



I. Cyclohexane
II. Toluene
III. THF
IV. CHCl3
V. DCM
VI. Acetone
VII. MeCN
VIII. DMF
IX. EtOH
X. MeOH

Figure S13. (a) Current density (*J*)-luminance (*L*), **(b)** Power efficiency (η_p)-luminance and **(c)** External Quantum efficiency -luminescence characteristics of p-i-n fluorescent OLED with BITIAN as emitting material and (d) Fluorescence image of BIPIAN and BITIAN in various solvent with varying polarity under 365 nm UV light illumination

Table S1. Lifetime measurements for BIPIAN and BITIN compounds

Solvents	BIPIAN								BITIAN							
	[a]τ_1 [ns]	α_1 [%]	τ_2 [ns]	α_2 [%]	[b]<τ> ns	χ^2	[c]K_r ($10^7 s^{-1}$)	[d]K_{nr} ($10^7 s^{-1}$)	τ_1 [ns]	α_1 [%]	τ_2 [ns]	α_2 [%]	<τ> ns	χ^2	K_r ($10^7 s^{-1}$)	K_{nr} ($10^7 s^{-1}$)
CyHex	0.50	25.83	1.03	74.17	0.955	1.1	0.52	0.52	0.61	16.06	1.07	83.94	1.033	1.25	0.62	0.34
DCM	1.08	------	-----	-----	-------	1.01	----	----	0.59	20.45	1.28	79.55	1.20	1.18	0.55	0.27
ACN	0.28	14.22	0.50	85.78	0.481	1.25	0.63	1.44	0.38	11.68	1.38	88.32	1.34	1.25	0.17	0.57
MeOH	42.84	0.42	0.76	57.16	0.660	2.62	0.87	0.63	0.58	2.01	1.19	97.99	1.18	1.52	0.36	0.48

[a] Lifetime (τ), [b] average lifetime (< τ >), [c] radiative (k_r) and [d] non-radiative (k_{nr}) rate constants of BIPIAN and BITIAN in various solvents.

Table S2. Computed absorption spectra in both gas and solvent phase of BIPIAN and BITIAN along with experimental data

	States	Electron Transition	Cal. λ_{max} (nm)	Exp. λ_{max} (nm)	Oscillator Strength (f)	E (eV)	Main Contributing Configurations
BIPIAN	**Gas-phase**	$S_0 \rightarrow S_1$	357.2	-	1.722	3.47	HOMO → LUMO (61%) HOMO-1 → LUMO (30%)
	CYHEX	$S_0 \rightarrow S_1$	369.7	406	1.748	3.35	HOMO → LUMO (67%) HOMO-1 → LUMO (24%)
	TOLEUNE	$S_0 \rightarrow S_1$	371.3	380	1.742	3.34	HOMO → LUMO (69%) HOMO-1 → LUMO (23%)
	THF	$S_0 \rightarrow S_1$	372.7	382	1.679	3.33	HOMO → LUMO (77%) HOMO-1 → LUMO (15%)
	DCM	$S_0 \rightarrow S_1$	373.2	376	1.676	3.32	HOMO → LUMO (77%) HOMO-1 → LUMO (14%)
	$CHCl_3$	$S_0 \rightarrow S_1$	372.5	376	1.699	3.33	HOMO → LUMO (74%) HOMO-1 → LUMO (17%)
	ACN	$S_0 \rightarrow S_1$	372.9	374	1.647	3.32	HOMO → LUMO (80%) HOMO-1 → LUMO (11%)
	ACETONE	$S_0 \rightarrow S_1$	372.9	379	1.654	3.32	HOMO → LUMO (79%) HOMO-1 → LUMO (12%)
	DMF	$S_0 \rightarrow S_1$	374.4	385	1.656	3.31	HOMO → LUMO (80%) HOMO-1 → LUMO (11%)
	MeOH	$S_0 \rightarrow S_1$	372.6	376	1.646	3.33	HOMO → LUMO (80%) HOMO-1 → LUMO (11%)
	EtOH	$S_0 \rightarrow S_1$	373.1	379	1.653	3.32	HOMO → LUMO (80%) HOMO-1 → LUMO (12%)
BITIAN	**Gas-phase**	$S_0 \rightarrow S_1$	392.6	-	1.829	3.16	HOMO → LUMO (81%) HOMO-1 → LUMO (7%)
	CYHEX	$S_0 \rightarrow S_1$	405.2	405	1.941	3.06	HOMO → LUMO (81%) HOMO-1 → LUMO (7%)
	TOLEUNE	$S_0 \rightarrow S_1$	406.7	412	1.948	3.05	HOMO → LUMO (81%) HOMO-1 → LUMO (7%)
	THF	$S_0 \rightarrow S_1$	407.0	411	1.917	3.05	HOMO → LUMO (83%) HOMO-1 → LUMO (5%)
	DCM	$S_0 \rightarrow S_1$	407.5	408	1.919	3.04	HOMO → LUMO (83%) HOMO-1 → LUMO (5%)
	$CHCl_3$	$S_0 \rightarrow S_1$	407.2	408	1.929	3.05	HOMO → LUMO (83%) HOMO-1 → LUMO (6%)
	ACN	$S_0 \rightarrow S_1$	406.8	404	1.897	3.05	HOMO → LUMO (84%) HOMO-1 → LUMO (4%)
	ACETONE	$S_0 \rightarrow S_1$	406.9	408	1.902	3.05	HOMO → LUMO (84%) HOMO-1 → LUMO (4%)
	DMF	$S_0 \rightarrow S_1$	408.3	413	1.912	3.04	HOMO → LUMO (84%) HOMO-1 → LUMO (4%)
	MeOH	$S_0 \rightarrow S_1$	406.4	402	1.894	3.05	HOMO → LUMO (84%) HOMO-1 → LUMO (4%)
	EtOH	$S_0 \rightarrow S_1$	407.0	407	1.902	3.05	HOMO → LUMO (84%) HOMO-1 → LUMO (4%)

Table S3. Ionization potential (IP), Electron affinity (EA) and Reorganization energy (λ) of BIPIAN and BITIAN

Molecule	**IP(v)**	**IP(a)**	**HEP**	**EA(v)**	**EA(a)**	**EEP**	λ_{hole}	$\lambda_{electron}$
BIPIAN	6.33	6.19	6.06	1.07	1.25	1.43	0.27	0.36
BITIAN	6.15	6.00	5.86	1.17	1.34	1.34	0.28	0.32