Supplementary Information

Exploiting Heterocycle Aromaticity to Fabricate New Hot Exciton Materials

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1. Materials and Methods.

All solvents and reagents required for experiments and testing are commercially available reagents, as indicated in special circumstances. Solvents were purified by resteaming according to standard methods. ^{1}H NMR and ^{13}C NMR were measured at Bruker DRX 600 spectrometer (600 MHz) with chloroform-d as the deuterated solvent and tetramethylsilane as the reference. Mass spectra were recorded using a VJ-ZAB-3F mass spectrometer. Elemental analyses were performed using a Vario EL III elemental analyzer. Thermal weight analysis was characterized using a Netzsch TG 209 F3 instrument. Differential scanning calorimetry was performed on a NETZSCH DSC 200 PC unit at a heating rate of 10 ℃ min^{-1} under nitrogen gas atmosphere. Cyclic voltammetry adopted CHI600E electrochemical workstation for analysis with calomal, glass carbon and platinum wire electrodes as reference, working and auxiliary electrodes, respectively, standardized for the redox couple ferricinium/ferrocene. HOMO was obtained by ionization energy determination. The LUMO levels (eV) of the three compounds were calculated according to the HOMO and E_g. The E_g were picked up by the intersection of the absorption-emission spectra. Transient electroluminescence (TrEL) decay was tested by an Agilent 8114A pulse generator, and the TrEL signal was detected using a lens coupled with the optical fifiber connected to a Hamamatsu photomultiplier (H10721-20). MEL measurements were carried out under constant voltages applied by Keithley 2450 source meter, and the EL signal was detected using a Keithley 2000 multimeter through a silicon-based photodiode.

2. Aromaticity and Quantum Chemical Calculation.

2.1 Aromaticity Analysis and Energy Diagram of Heterocycles.

All DFT calculations were performed by using the Gaussian 16 software package.[1] The ground state/excited state geometries and corresponding excitation energies were optimized and calculated at M06-2X/6-311G(d) with the polarizable continuum model solvation model (dichloromethane).[2-4] Tamm–Dancoff approximation (TDA) was applied in TDDFT calculations in consideration of the instability of triplet states.[5] Natural transition orbitals (NTOs) were conducted by utilizing Multiwfn.[6] The spin–

orbit coupling (SOC) calculations were conducted by using the PySOC software.[6-8] In aromaticity analysis, nuclear-independent chemical shift (NICS)[9-11] and electron density of delocalized bond (EDDB)[12] calculations were also performed at the M06-2X/6-311G(d) level. Anisotropy of the induced current density (ACID) plots were performed with ACID 2.0 program.

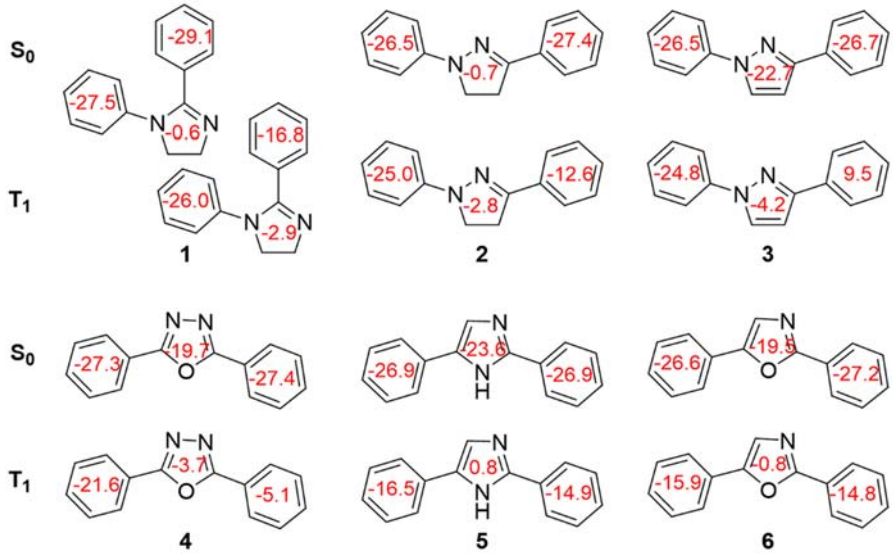


Figure S1. The NICS(1)$_{zz}$ values (ppm) of compound **1**, **2**, **3**, **4**, **5** and **6** in S_0 and T_1 states. Distinctively negative NICS(1)$_{zz}$ values suggest aromaticity whereas the close to zero values indicate nonaromaticity.

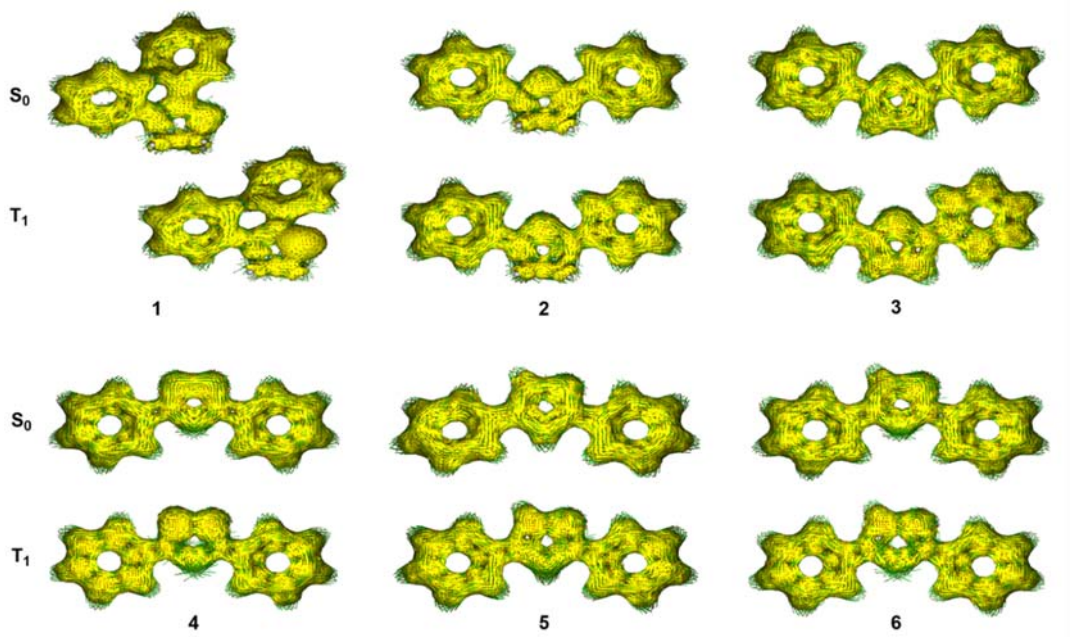


Figure S2. ACID results of compound **1**, **2**, **3**, **4**, **5** and **6** in S_0 and T_1 states. Isovalue for ACID is 0.035 a.u.

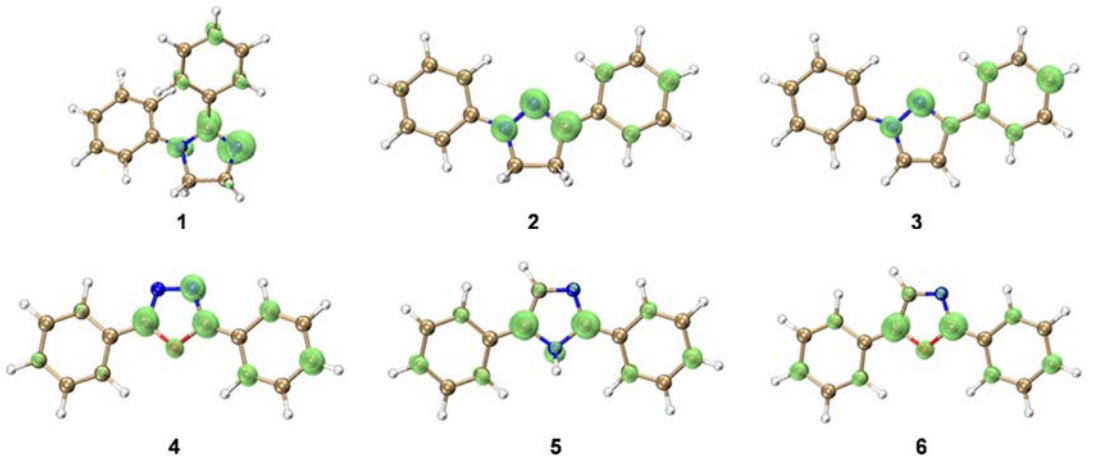


Figure S3. Spin density distributions (isovalue: 0.015 a.u.) of compound **1**, **2**, **3**, **4**, **5** and **6** in T_1 states.

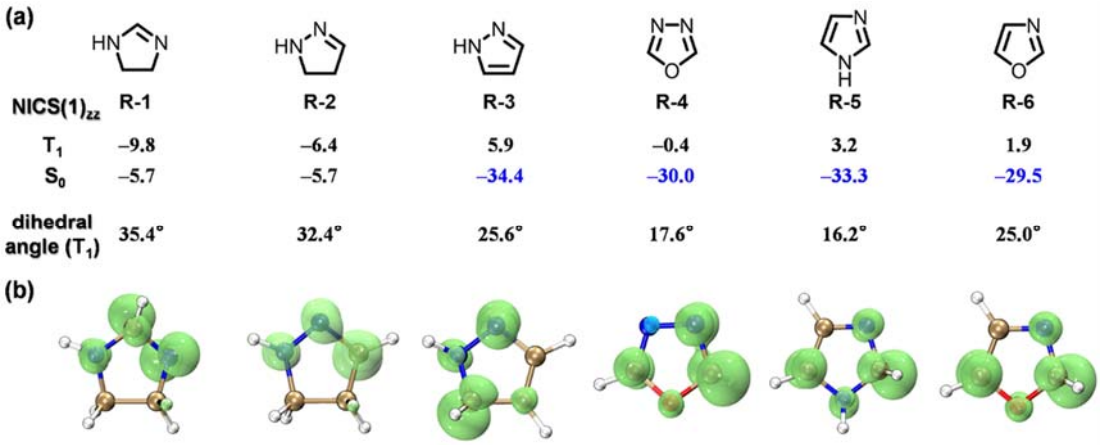


Figure S4. (a) The NICS(1)$_{zz}$ values (ppm) in the S_0 and T_1 states, and the dihedral angle in the T_1 state for individual heterocycles. (b) The spin density (isovalue: 0.015 a.u.) for individual heterocycles in the T_1 state.

Table S1. Vertical excitation energies of compound **1** at S_1-geometry at the level of TDA-M06-2X/6-311G(d)

	Excitation energy (eV)		Excitation energy (eV)
S_1	3.40	T_1	1.61
S_2	4.68	T_2	3.40
S_3	4.82	T_3	3.69
S_4	5.00	T_4	4.20
S_5	5.04	T_5	4.28
S_6	5.51	T_6	4.30
S_7	5.59	T_7	4.79
S_8	5.76	T_8	4.90
S_9	6.37	T_9	4.92
S_{10}	6.45	T_{10}	5.05

Table S2. Vertical excitation energies of compound **2** at S_1-geometry at the level of TDA-M06-2X/6-311G(d).

	Excitation energy (eV)		Excitation energy (eV)
S_1	3.39	T_1	1.64
S_2	3.99	T_2	3.93
S_3	4.75	T_3	4.01
S_4	5.43	T_4	4.16
S_5	5.58	T_5	4.33
S_6	5.62	T_6	4.59
S_7	5.77	T_7	4.70
S_8	5.95	T_8	4.89
S_9	5.98	T_9	4.98
S_{10}	6.13	T_{10}	5.06

Table S3. Vertical excitation energies of compound **3** at S_1-geometry at the level of TDA-M06-2X/6-311G(d).

	Excitation energy (eV)		Excitation energy (eV)
S_1	4.16	T_1	2.65
S_2	5.01	T_2	3.90
S_3	5.10	T_3	4.32
S_4	5.44	T_4	4.48
S_5	5.71	T_5	4.56
S_6	5.94	T_6	4.75
S_7	6.11	T_7	4.91
S_8	6.25	T_8	5.11
S_9	6.34	T_9	5.14
S_{10}	6.63	T_{10}	5.16

Table S4. Vertical excitation energies of compound **4** at S_1-geometry at the level of TDA- M06-2X/6-311G(d).

	Excitation energy (eV)		Excitation energy (eV)
S_1	3.81	T_1	2.32
S_2	4.96	T_2	3.49
S_3	4.97	T_3	4.26
S_4	4.98	T_4	4.36
S_5	5.23	T_5	4.43
S_6	5.72	T_6	4.62
S_7	5.72	T_7	4.75
S_8	6.08	T_8	4.85
S_9	6.11	T_9	4.88
S_{10}	6.70	T_{10}	4.89

Table S5. Vertical excitation energies of compound **5** at S_1-geometry at the level of TDA- M06-2X/6-311G(d)

	Excitation energy (eV)		Excitation energy (eV)
S_1	3.65	T_1	2.08
S_2	4.72	T_2	3.53
S_3	4.85	T_3	4.23
S_4	5.02	T_4	4.30
S_5	5.74	T_5	4.63
S_6	5.81	T_6	4.66
S_7	5.86	T_7	4.72
S_8	5.91	T_8	4.78
S_9	6.01	T_9	5.02
S_{10}	6.55	T_{10}	5.05

Table S6. Vertical excitation energies of compound **6** at S_1-geometry at the level of TDA- M06-2X/6-311G(d).

	Excitation energy (eV)		Excitation energy (eV)
S_1	3.59	T_1	2.06
S_2	4.81	T_2	3.54
S_3	4.89	T_3	4.32
S_4	5.06	T_4	4.33
S_5	5.71	T_5	4.63
S_6	5.74	T_6	4.64
S_7	5.87	T_7	4.69
S_8	5.90	T_8	4.82
S_9	6.63	T_9	5.05
S_{10}	6.69	T_{10}	5.06

2.2 Aromaticity Analysis and Energy Diagram of TNP System.

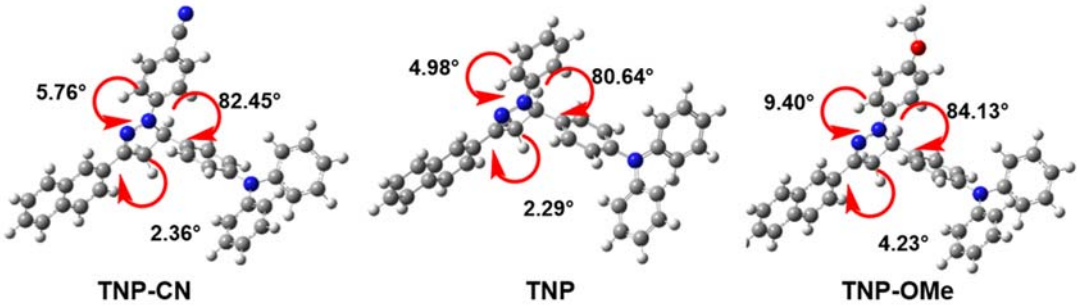


Figure S5. Optimized geometry of **TNP-CN**, **TNP** and **TNP-OMe** species.

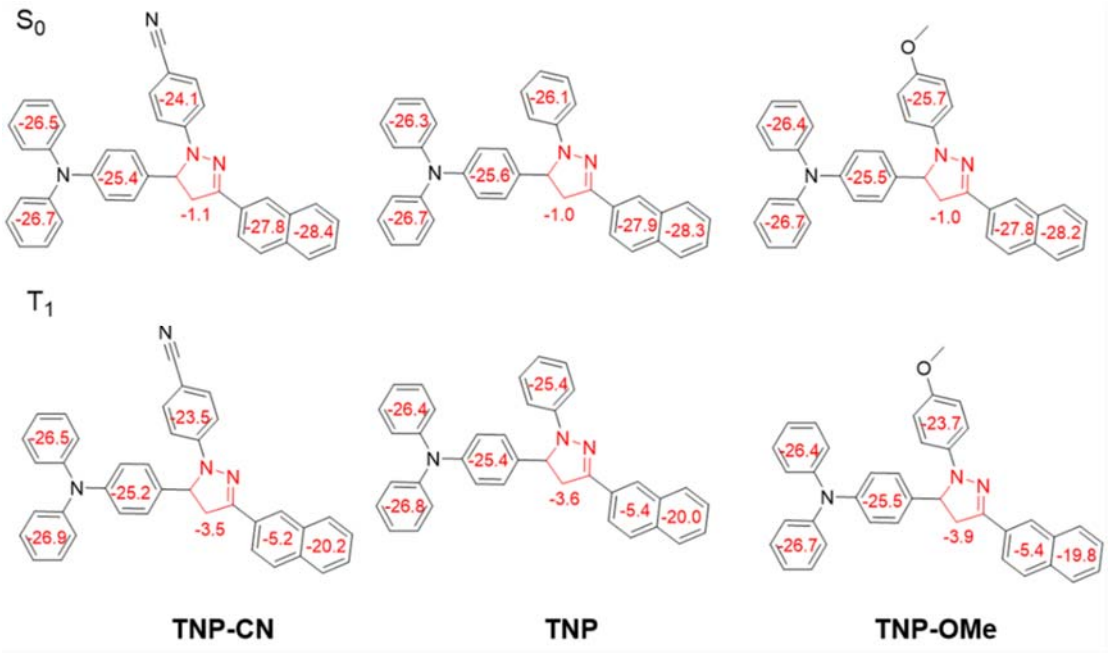


Figure S6. The NICS(1)$_{zz}$ values (ppm) of **TNP-CN, TNP, TNP-OMe** in the S_0 and T_1 states. Distinctively negative NICS(1)$_{zz}$ values suggest aromaticity whereas the close to zero values indicate nonaromaticity.

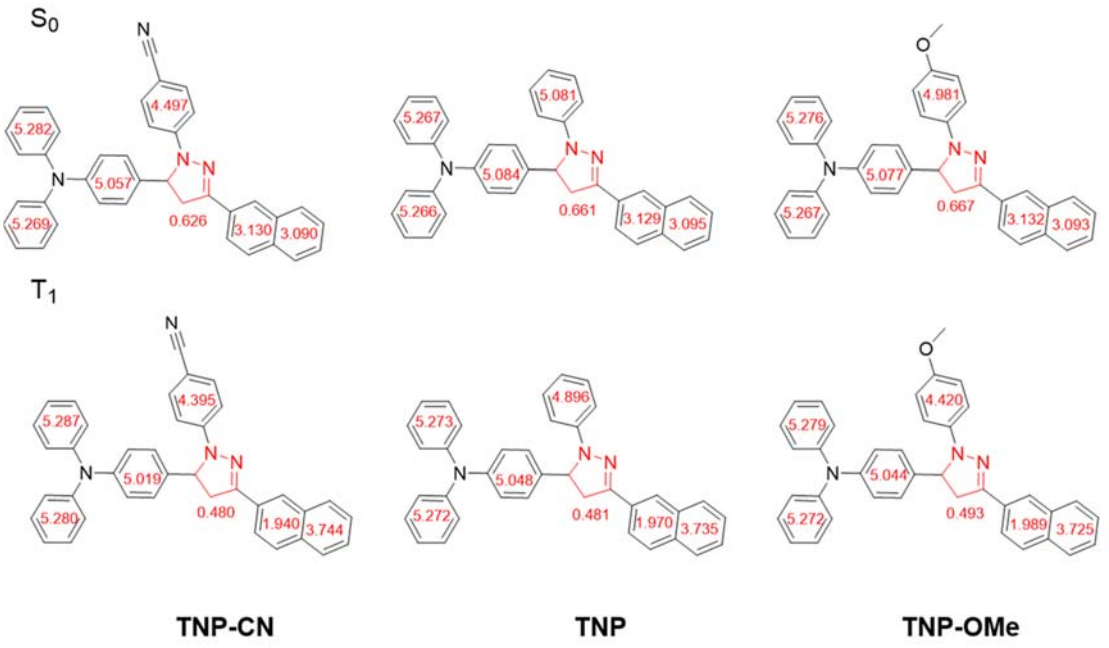


Figure S7. The EDDB values (ppm) of **TNP-CN, TNP, TNOMe** in the singlet (S_0) and triplet (T_1) states. The EDDB values of the pyrazoline core are particularly small (0.661 and 0.481 e) indicating its nonaromaticity in both the S_0 and T_1 states. The EDDB values of the individual benzene ring are around 5.000 e (5.081 and 4.896 e) whereas these of the naphthalene ring ranged from 3.095 to 3.375 e suggesting the slightly less aromaticity of the latter in both the S_0 and T_1 states. A similar difference appears in the left ring of the naphthalene, which is aromatic in the S_0 state given the EDDB value of 3.129 e, but nonaromatic in the T_1 state with a relatively small EDDB value of 1.970.

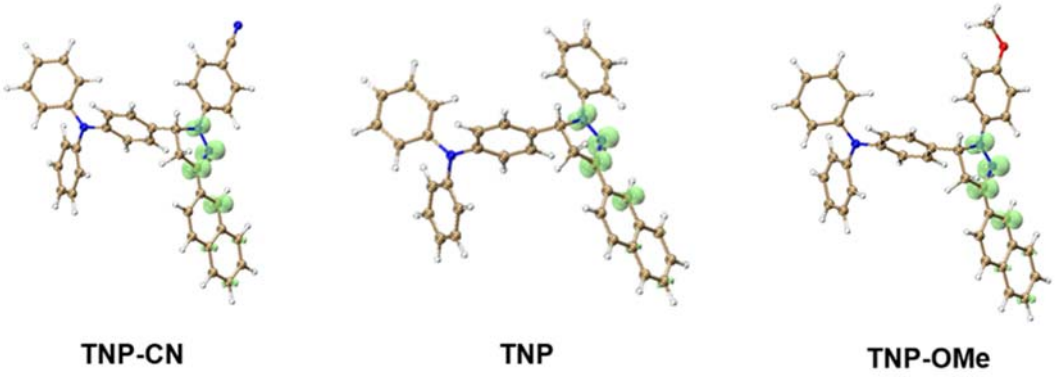


Figure S8. Spin density distributions (isovalue: 0.015 a.u.) of **TNP-CN**, **TNP** and **TNP-OMe** species in the T_1 state.

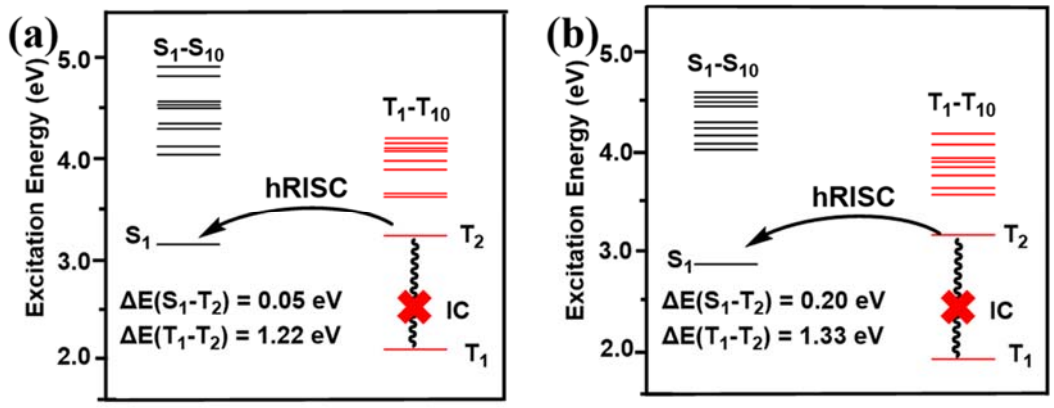


Figure S9. Energy diagram of the first ten singlet and triplet excited states for (a) **TNP-CN** and (b) **TNP-OMe** from TDA-M06-2X calculations.

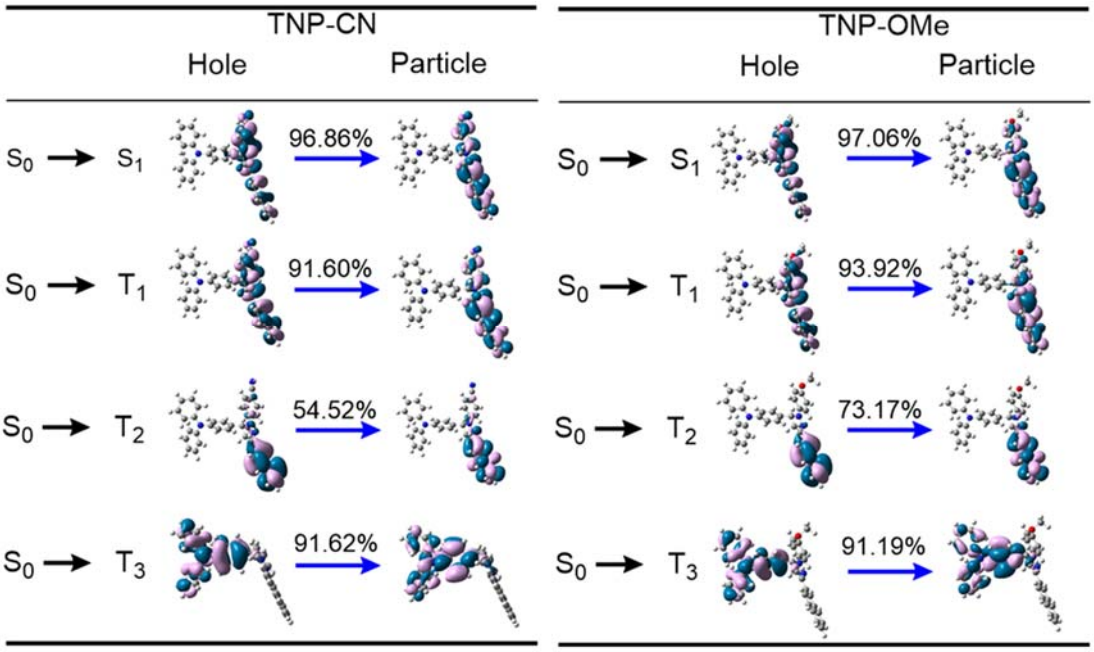


Figure S10. NTOs of **TNP-CN** and **TNP-OMe** at S_1, T_1, T_2 and T_3 states, respectively.

Table S7. Vertical excitation energies of **TNP-CN** at S_1-geometry at the level of TDA- M06-2X/6-311G(d)

	Excitation energy (eV)		Excitation energy (eV)
S_1	3.14	T_1	1.97
S_2	3.99	T_2	3.19
S_3	4.08	T_3	3.52
S_4	4.34	T_4	3.57
S_5	4.40	T_5	3.77
S_6	4.52	T_6	3.88
S_7	4.53	T_7	3.96
S_8	4.56	T_8	3.97
S_9	4.78	T_9	4.05
S_{10}	4.86	T_{10}	4.16

Table S8. Vertical excitation energies of **TNP** at S_1-geometry at the level of TDA-M06-2X/6-311G(d).

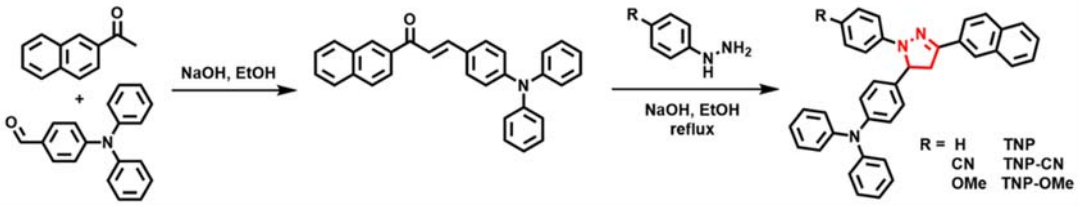
	Excitation energy (eV)		Excitation energy (eV)
S_1	3.11	T_1	1.90
S_2	4.06	T_2	3.22
S_3	4.12	T_3	3.59
S_4	4.34	T_4	3.75
S_5	4.45	T_5	3.88
S_6	4.49	T_6	3.91
S_7	4.51	T_7	3.94
S_8	4.58	T_8	4.00
S_9	4.70	T_9	4.19
S_{10}	4.80	T_{10}	4.21

Table S9. Vertical excitation energies of **TNP-OMe** at S_1-geometry at the level of TDA- M06-2X/6-311G(d).

	Excitation energy (eV)		Excitation energy (eV)
S_1	2.98	T_1	1.85
S_2	4.01	T_2	3.18
S_3	4.16	T_3	3.52
S_4	4.25	T_4	3.60
S_5	4.34	T_5	3.75
S_6	4.47	T_6	3.82
S_7	4.48	T_7	3.88
S_8	4.49	T_8	3.90
S_9	4.51	T_9	4.14
S_{10}	4.55	T_{10}	4.26

3. Molecular Synthesis.

The intermediate and desired compounds were synthesized according to the literature with some minor modifications (**Scheme S1**).[13]



Scheme S1. Molecular synthesis route of TNP derivatives.

Synthesis of Intermediate. 4-(*N*,*N*-diphenylamino)benzaldehyde (1.5 g, 5.5 mmol) and acetophenone (1.12 g, 6.6 mmol) in 20 mL absolute ethanol, 15% aqueous sodium hydroxide (4 mL) was added. The reaction mixture was stirred at room temperature for 4-8 h. Once the reaction completed, the solution was concentrated and filtered, and the filter residue was washed with water and absolute ethanol. After recrystallization, pure intermediate chalcone was obtained as an orange-yellow solid (yield 75 %).

Synthesis of TNP-CN. Intermediate chalcone (1.5 g, 3.5 mmol) and 4-cyanophenylhydrazine (0.56 g, 4.2 mmol) was added to 20 mL absolute ethnol in the presence of NaOH (0.75 g). The mixture was refluxed under the nitrogen-protected atmosphere for 24 h. The reaction solution was concentrated and ice water was added. Then the crude product was obtained by filtration and drying. After column chromatography (PE/DCM, v:v = 4:1) and recrystallization, the desired product was obtained as a light white solid (yield 62%). ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.14 (dd, *J* = 9.0, 1.2 Hz, 1H), 7.87–7.79 (m, 4H), 7.52–7.49 (m, 2H), 7.48–7.47 (d, *J* = 9.0 Hz, 2H), 7.26–7.23 (m, 4H), 7.15–7.13 (d, *J* = 9.0 Hz, 2H), 7.12–7.10 (d, *J* = 8.4 Hz, 2H), 7.07–7.05 (d, *J* = 7.8 Hz, 4H), 7.03–7.01 (t, *J* = 6.6 Hz, 4H), 5.35 (dd, *J* = 12.0, 5.4 Hz, 1H), 4.00 (dd, *J* = 17.4, 12.6 Hz, 1H), 3.38 (dd, *J* = 17.4, 6.0 Hz, 1H). ^{13}C NMR (101 MHz, CD_2Cl_2) δ 149.71, 147.24, 147.11, 146.59, 134.42, 133.36, 132.83, 129.29, 128.98, 128.87, 127.91, 127.79, 127.39, 127.06, 126.45, 126.15, 125.62, 124.61, 124.09, 123.36, 122.73, 121.97, 112.58, 100.00, 62.77, 43.15. HRMS (MALDI-TOF)

calculated for $C_{38}H_{28}N_4$: 540.231, found: m/z 540.211. Anal. calcd for $C_{38}H_{28}N_4$: C, 84.42; H, 5.22; N, 10.36; Found C, 83.10; H, 5.40; N, 11.18.

Synthesis of TNP. TNP was prepared by the same procedure using the reactant phenylhydrazine (0.5 mL, 4.2 mmol). Yellow powder (yield 62%).^{1}H NMR (400 MHz, C_4D_8O) δ 8.07 (dd, *J* = 8.8, 1.6 Hz, 1H), 7.87–7.65 (m, 4H), 7.38–7.26 (m, 2H), 7.16–7.05 (m, 6H), 7.03 (d, *J* = 4.4 Hz, 4H), 6.97–6.78 (m, 8H), 6.64–6.54 (m, 1H), 5.27 (dd, *J* = 12.0, 6.8 Hz, 1H), 3.89 (dd, *J* = 16.8, 12.4 Hz, 1H), 3.18 (dd, *J* = 16.8, 6.8 Hz, 1H). ^{13}C NMR (101 MHz, CD_2Cl_2) δ 147.26, 146.84, 146.60, 144.42, 136.13, 133.00, 132.96, 130.16, 128.82, 128.49, 127.71, 127.63, 127.34, 126.38, 126.10, 125.95, 124.65, 123.95, 123.52, 122.96, 122.53, 118.61, 112.91, 63.62, 43.02. HRMS (MALDI-TOF) calculated for $C_{37}H_{29}N_3$: 515.236, found: m/z 515.198. Anal. calcd for $C_{37}H_{29}N_3$: C, 85.43; H, 5.64; N, 8.13; Found C, 86.18; H, 5.67; N, 8.15.

Synthesis of TNP-OMe. TNP-OMe was prepared by the same procedure using the reactant 4-methoxyphenylhydrazine (0.58 g, 4.2 mmol). Light white powder (yield 62%). ^{1}H NMR (400 MHz, C_4D_8O) δ 8.04 (dd, *J* = 8.4, 1.6 Hz, 1H), 7.80–7.62 (m, 4H), 7.39–7.26 (m, 2H), 7.20–6.81 (m, 16H), 6.67–6.61 (m, 2H), 5.18 (dd, *J* = 12.0, 7.6 Hz, 1H), 3.86 (dd, *J* = 16.8, 12.0 Hz, 1H), 3.56 (s, 3H), 3.14 (dd, *J* = 16.8, 7.6 Hz, 1H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 147.41, 146.61, 145.98, 132.50, 132.45, 128.44, 128.36, 128.22, 127.49, 126.72, 126.46, 125.90, 125.35, 124.47, 124.21, 123.36, 123.15, 122.97, 122.80, 121.88, 120.60, 113.33, 103.07, 64.31, 54.51, 42.60. HRMS (MALDI-TOF) calculated for $C_{38}H_{31}N_3O$: 545.247, found: m/z 545.244. Anal. calcd for $C_{38}H_{31}N_3O$: C, 83.64; H, 5.73; N, 7.70; O, 2.93; Found C, 83.29; H, 5.48; N, 7.69; O, 3.54.

4. Triplet Sensitization Experiments.

Triplet sensitization experiments were performed using nanosecond flash photolysis (ns-TA) technique and thioxanthone (TX) as the sensitizer to describe the triplet excited state energy diagram of the studied TNP derivatives. The T_1 species of TNP molecule populated from triplet sensitization could be excited to the higher triplet levels (T_n), and then the excited state absorption (ESA) signal of $T_1 \rightarrow T_n$ transitions

could be captured and identified in the ns-TA spectra. As shown in **Figure S11**, the triplet excited state absorption (ESA) of the sensitizer TX (^{3}TX*) appears around 626 nm with a lifetime of 5.4 μs. In mixture solution (**Figure S12**), after photo-excitation, the ^{3}TX* signal appears around 626 nm at the initial 0.5 μs. Then it decays rapidly (τ_{decay} = 1.5 μs) and transforms into multi-peaks ESA bands of TNP triplets (^{3}TNP*) at 3 μs. In combination with theoretical calculations, the ESA peaks of ^{3}TNP* around 914, 710, 652, 594 and 518 nm are assigned to T_1-T_2 (1.32 eV), T_1-T_3 (1.69 eV), T_1-T_4 (1.85 eV), T_1-$T_{7\text{-}8}$ (~2.0 eV) and T_1-$T_{9\text{-}10}$ (~2.3 eV) transitions, respectively. These results indicate that the triplet state of TNP has been successfully sensitized by TX, and the theoretical calculations prove to be very plausible.

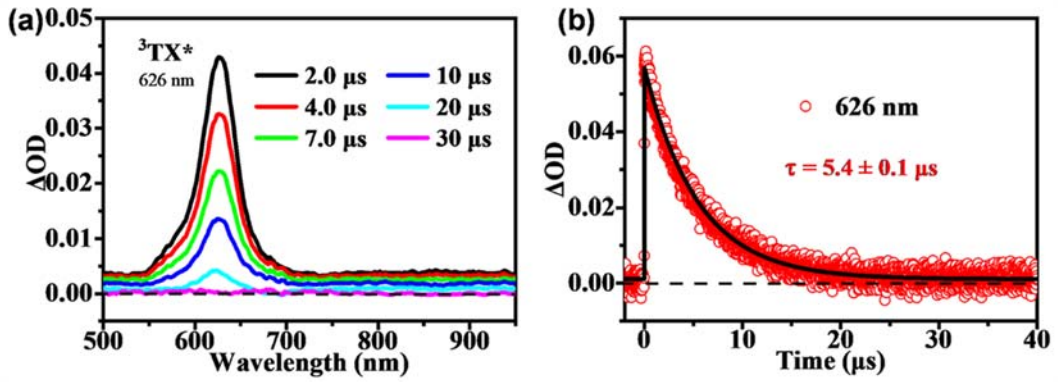


Figure S11. (a) Selected spectral slices and (b) kinetic decay curves from ns-TA measurements for sensitizer TX in dilute acetonitrile (355 nm excitation).

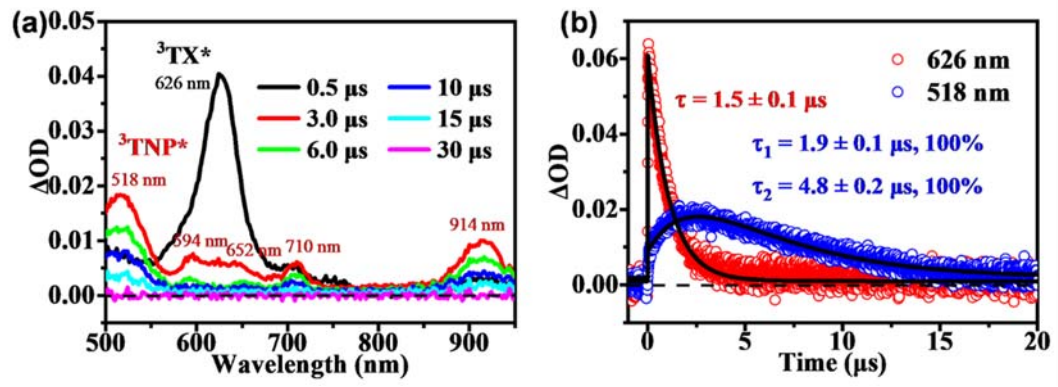


Figure S12. (a) Selected spectral slices and (b) kinetic decay curves from ns-TA measurements for a mixture of TX and TNP in dilute acetonitrile (355 nm excitation).

5. Photophysical Measurements in Dilute Solution.

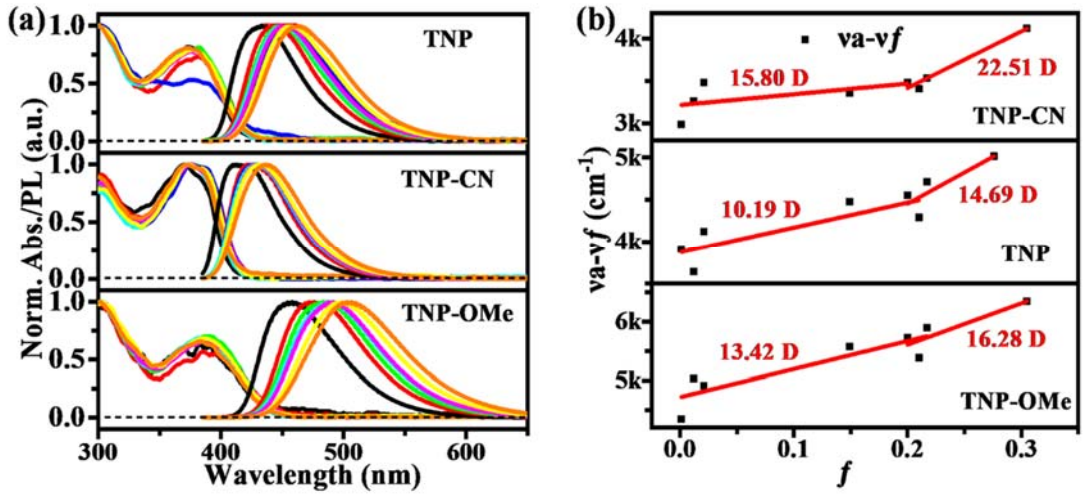


Figure S13. (a) Absorption and fluorescence spectra in different solvents. (b) The solvatochromic Lippert–Mataga models of **TNP-CN**, **TNP** and **TNOMe**.

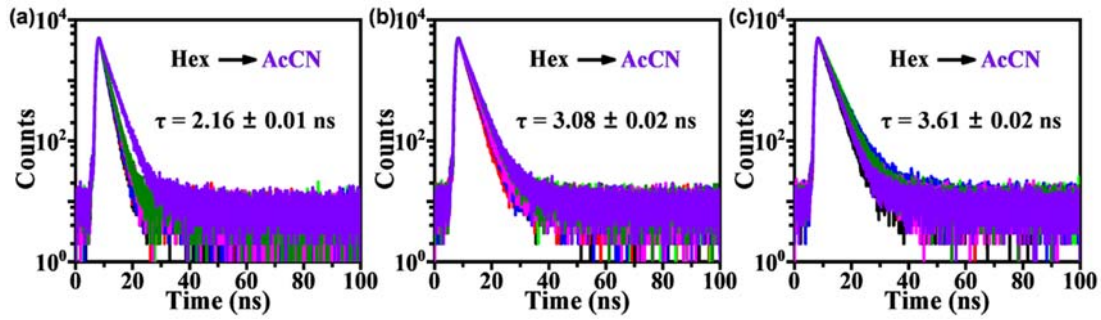


Figure S14. Transient PL decay curves of **TNP-CN** (a), **TNP** (b) and **TNP-OMe** (c) in different solvents.

6. Electrochemical and Thermal Properties.

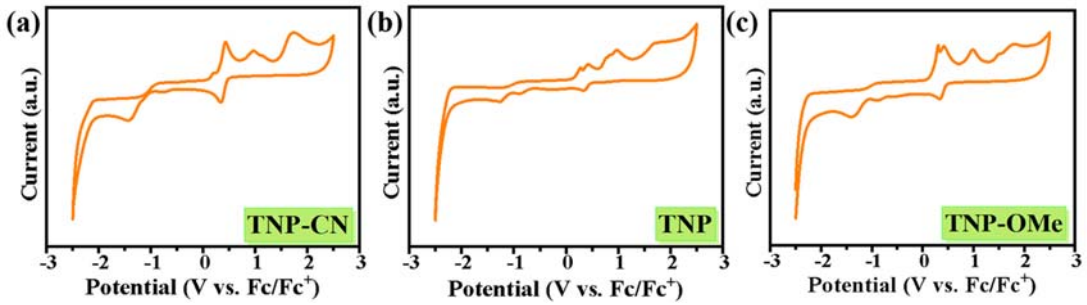


Figure S15. CV curve of **TNP-CN**, **TNP** and **TNP-OMe**.

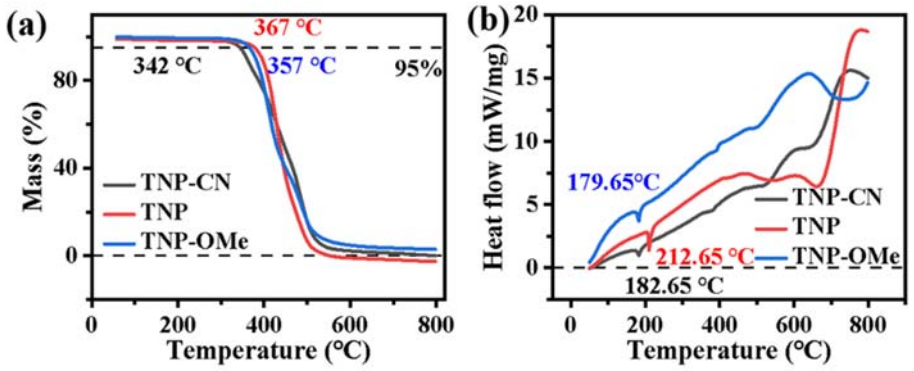


Figure S16. (a) TGA and (b) DSC curves of **TNP-CN**, **TNP** and **TNP-OMe**.

7. Single Crystal Diffraction Analysis.

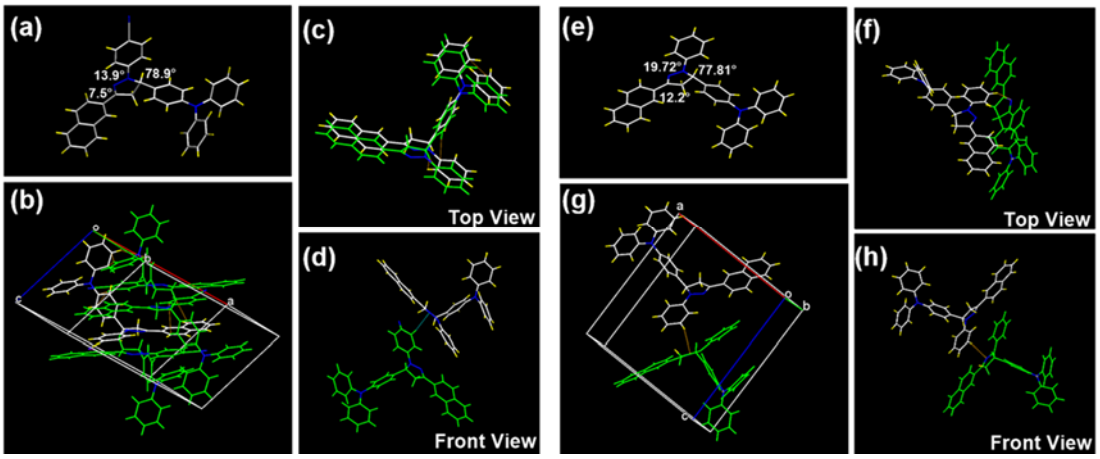


Figure S17. (a, e) Crystal structure, (b, g) packing pattern and different view (c, d, f, h) of **TNP-CN** and **TNP** in crystals. The needle-like single crystals of TNP derivatives were cultivated from petroleum ether/dichloromethane mixture solution by slow volatilization and then were analyzed by X-ray crystallography (CCDC: 2250241 and 2250242).

8. Photophysical Measurements in Solid State.

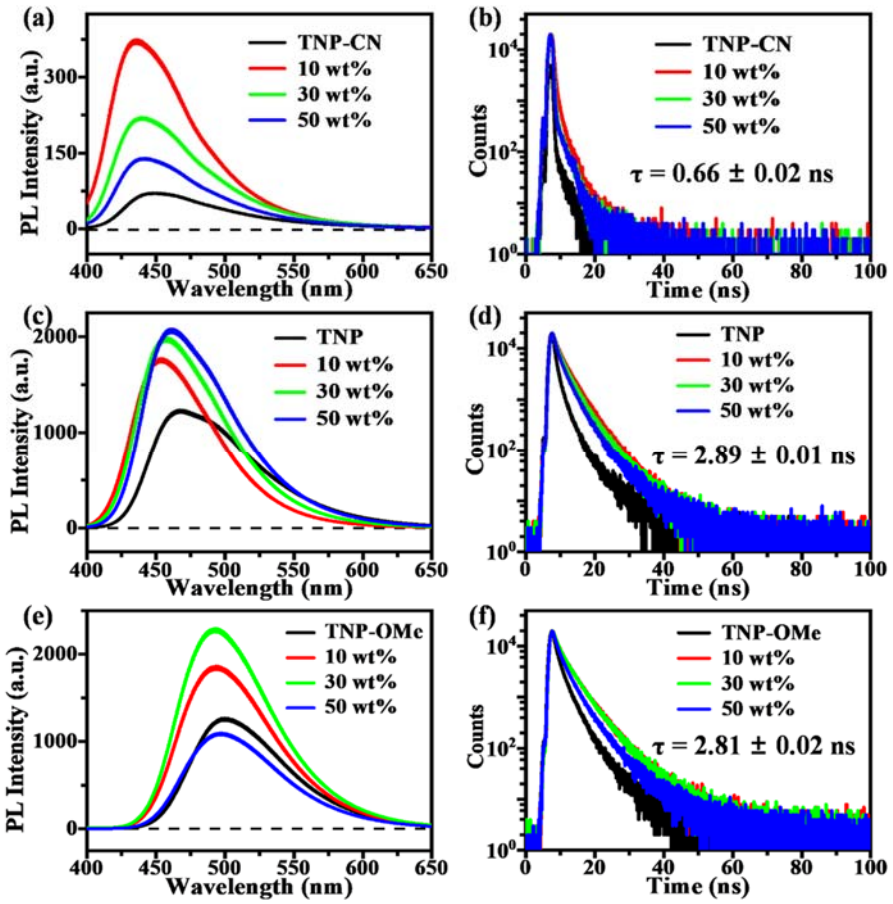


Figure S18. PL spectra and transient PL decay curves of neat and doped PMMA films of (a,b) **TNP-CN**, (c,d) **TNP** and (e,f) **TNP-OMe**.

9. Estimation of Basic Photophysical Data.

The quantum efficiencies and rate constants were determined using the following equations according to Adachi's method (Equations 1-7, 8 and 9-10).[14-16]

$$\Phi_{prompt} = \Phi_{PL} R_{prompt} \quad \text{(Eq. 1)}$$

$$\Phi_{delayed} = \Phi_{PL} R_{delayed} \quad \text{(Eq. 2)}$$

$$k_F = \Phi_{prompt}/\tau_{prompt} \quad \text{(Eq. 3)}$$

$$\Phi_{PL} = k_F/(k_F + k_{IC}) \quad \text{(Eq. 4)}$$

$$\Phi_{prompt} = k_F/(k_F + k_{IC} + k_{ISC}) \quad \text{(Eq. 5)}$$

$$\Phi_{IC} = k_{IC}/(k_F + k_{IC} + k_{ISC}) \quad \text{(Eq. 6)}$$

$$\Phi_{ISC} = k_{ISC}/(k_F + k_{IC} + k_{ISC}) = 1 - \Phi_{prompt} - \Phi_{IC} \quad \text{(Eq. 7)}$$

$$\Phi_{RISC} = \Phi_{delayed}/\Phi_{ISC} \quad \text{(Eq. 8)}$$

$$k_{RISC} = (k_p k_d \Phi_{delayed})/(k_{ISC}\Phi_{prompt}) \quad \text{(Eq. 9)}$$

$$k_p = 1/\tau_{prompt};\ k_d = 1/\tau_{delayed} \quad \text{(Eq. 10)}$$

where τ_{prompt} and $\tau_{delayed}$ represent the prompt and delayed fluorescence lifetimes, respectively, and $R_{prompt}/R_{delayed}$ mean the ratio of prompt versus delayed components.

10. Device Characterization.

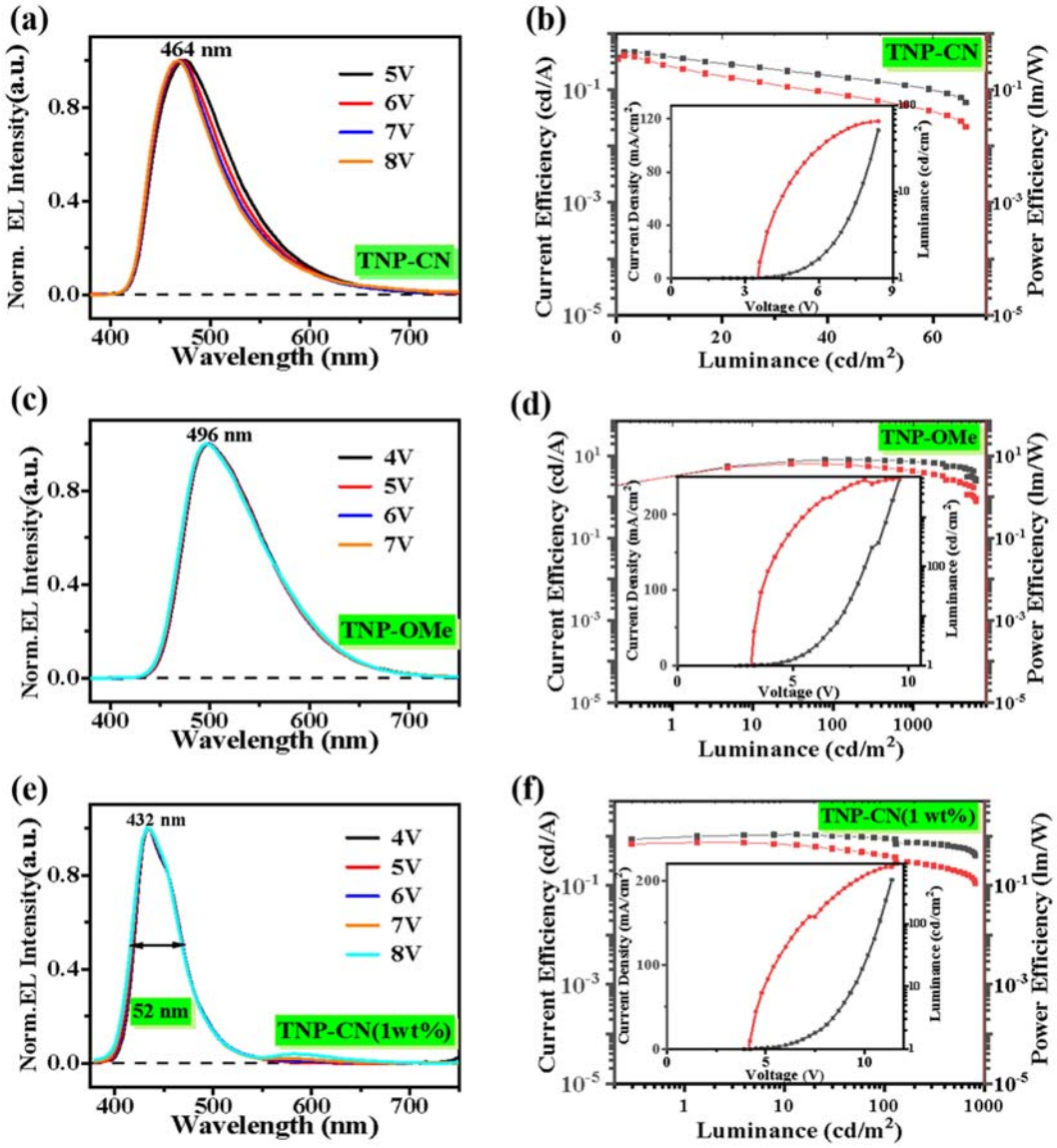


Figure S19. EL spectra, and current density-voltage-luminance (*J-V-L*) (insert: power efficiency-luminance-current efficiency) curves of (a,b) **TNP-CN**, (c,d) **TNP-OMe** and (e,f) **mCP:TNP-CN (**1 wt%).

Table S10. Device performance of **TNP-CN**, **TNP** and **TNP-OMe**.

EML		λ_{EL} (nm)	CIE(x,y)	L_{max} (cd/m^2)	EQE_{max} (%)
TNP	Non-doped	468	(0.15,0.20)	2724	4.78
	mCP:(10 wt%)	452	(0.15,0.11)	2778	5.03
	mCP:(20 wt%)	452	(0.15,0.13)	2553	3.98
	mCP:(30 wt%)	456	(0.15,0.14)	2782	3.87
	mCP:(40 wt%)	456	(0.15,0.15)	2746	3.96
	mCP:(50 wt%)	460	(0.15,0.19)	2783	3.90
TNP-CN	Non-doped	464	(0.18,0.24)	358	0.66
	mCP:(1 wt%)	432	(0.15,0.05)	812	2.03
	mCP:(2 wt%)	436	(0.15,0.06)	708	1.86
	mCP:(5 wt%)	436	(0.15,0.07)	445	1.81
	mCP:(8 wt%)	440	(0.15,0.08)	424	1.86
	mCP:(10 wt%)	440	(0.15,0.07)	401	1.88
TNP-OMe	Non-doped	496	(0.26,0.48)	6051	2.86
	mCP:(20 wt%)	480	(0.20,0.36)	4026	3.80
	mCP:(30 wt%)	484	(0.22,0.41)	3924	3.79
	mCP:(40 wt%)	488	(0.21,0.40)	4069	3.83
	mCP:(50 wt%)	488	(0.23,0.43)	4474	3.9

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12. Appendix.

NMR Data.

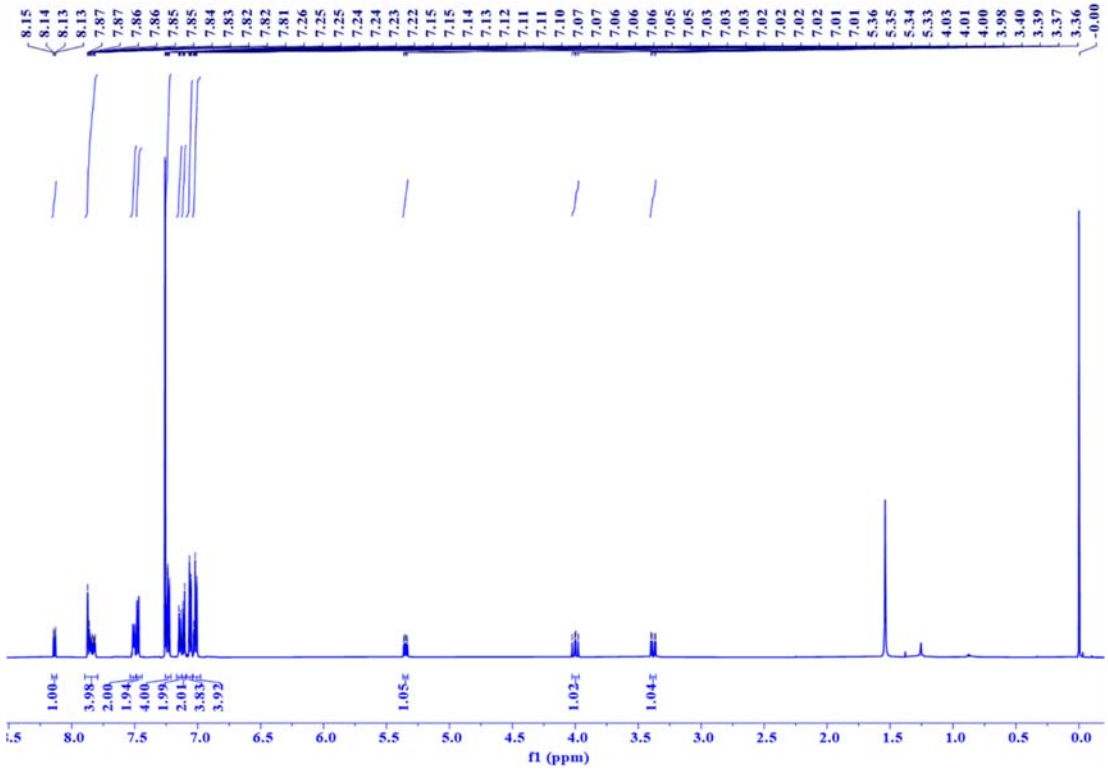

Figure S20. ^{1}H NMR of **TNP-CN** molecule ($CDCl_3$, 298 K).

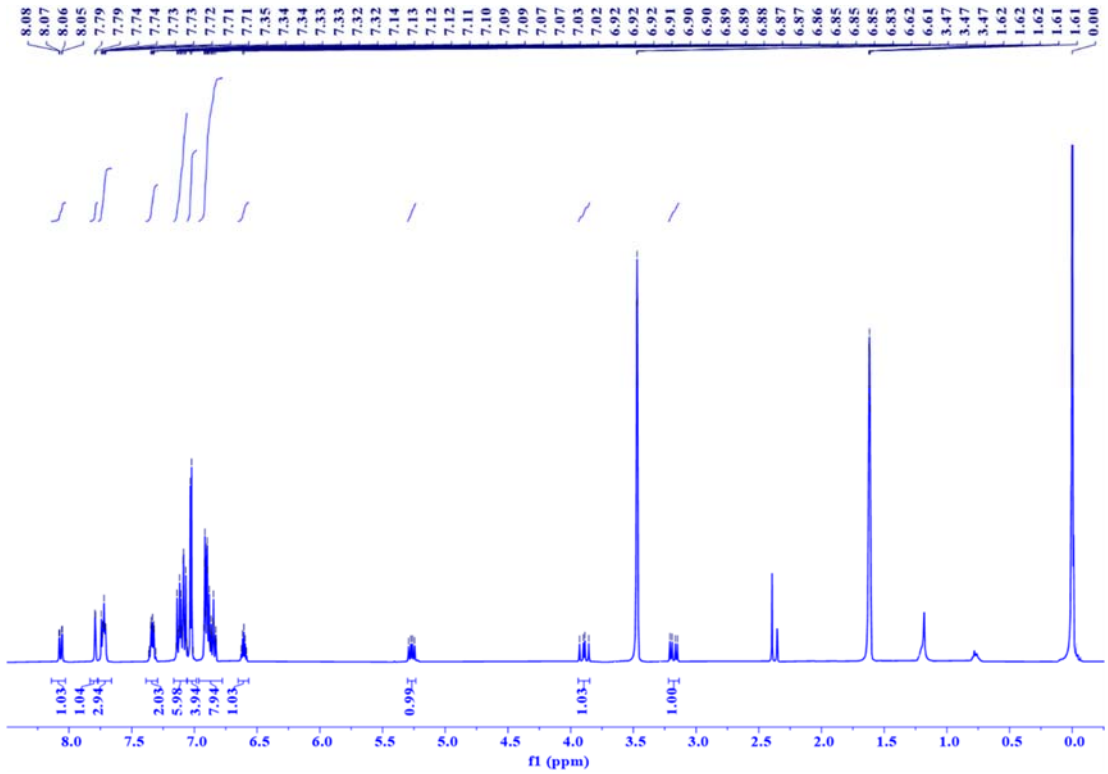

Figure S21. ^{1}H NMR of **TNP** molecule (C_4D_8O, 298 K).

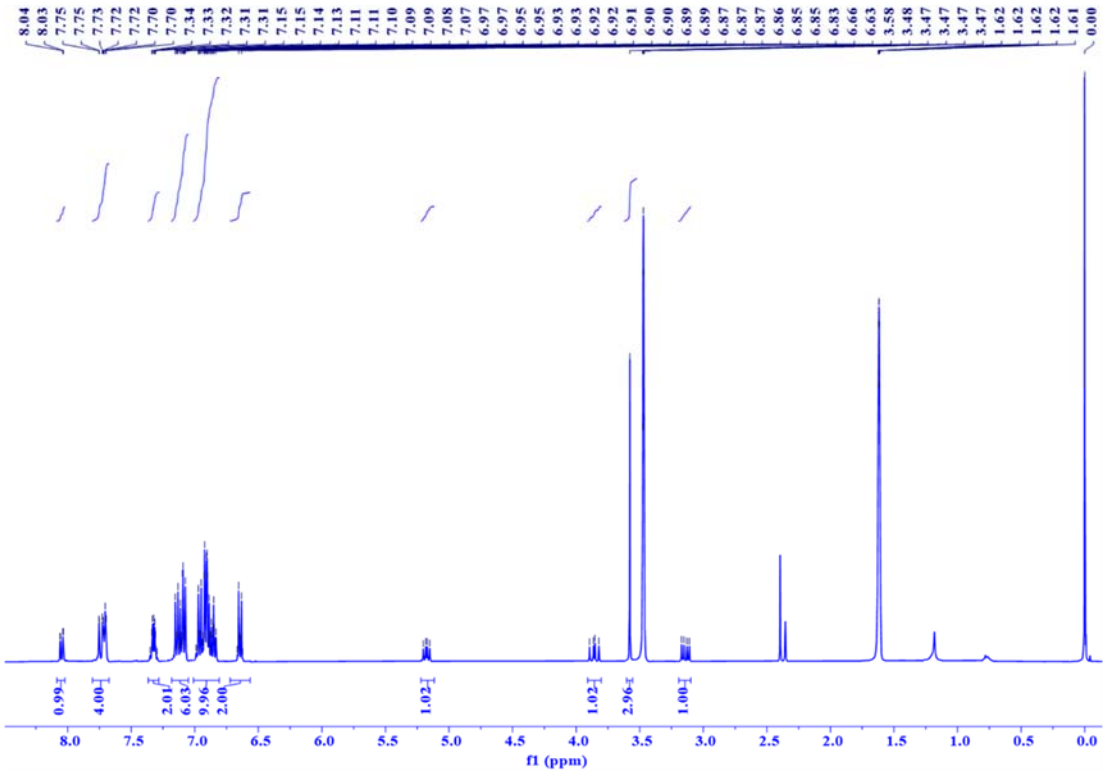

Figure S22. ^{1}H NMR of **TNP-OMe** molecule (C_4D_8O, 298 K).

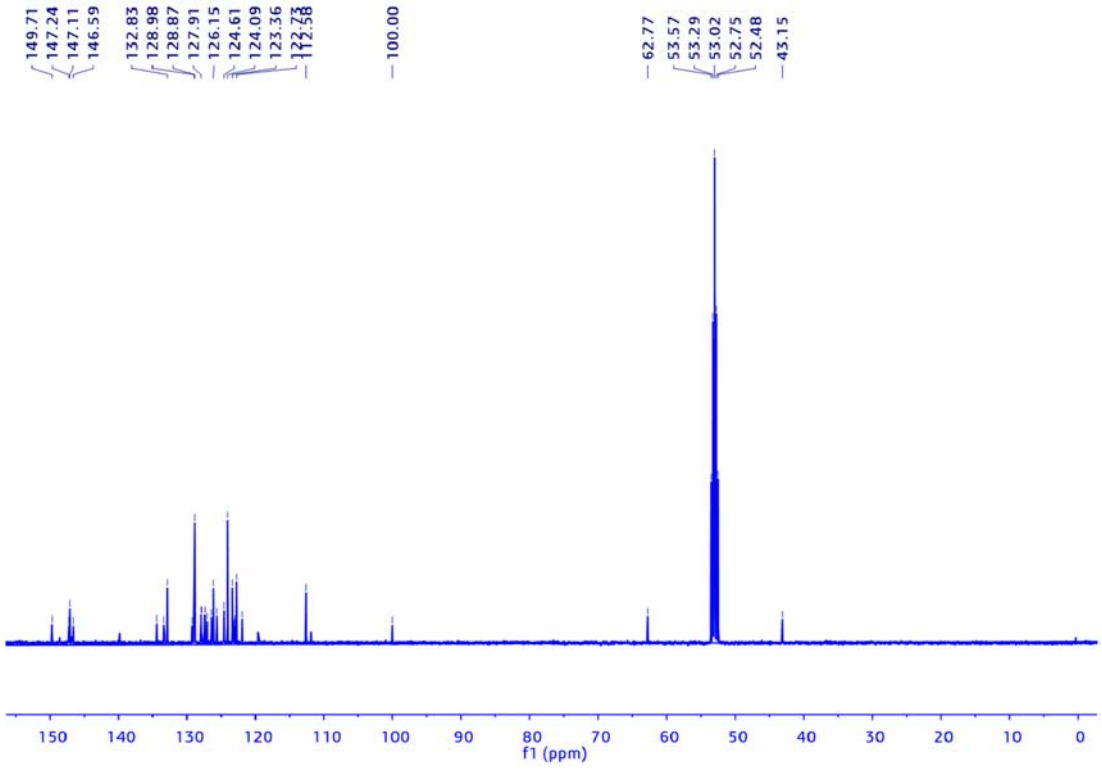

Figure S23. ^{13}C NMR of **TNP-CN** molecule (CD_2Cl_2, 298 K).

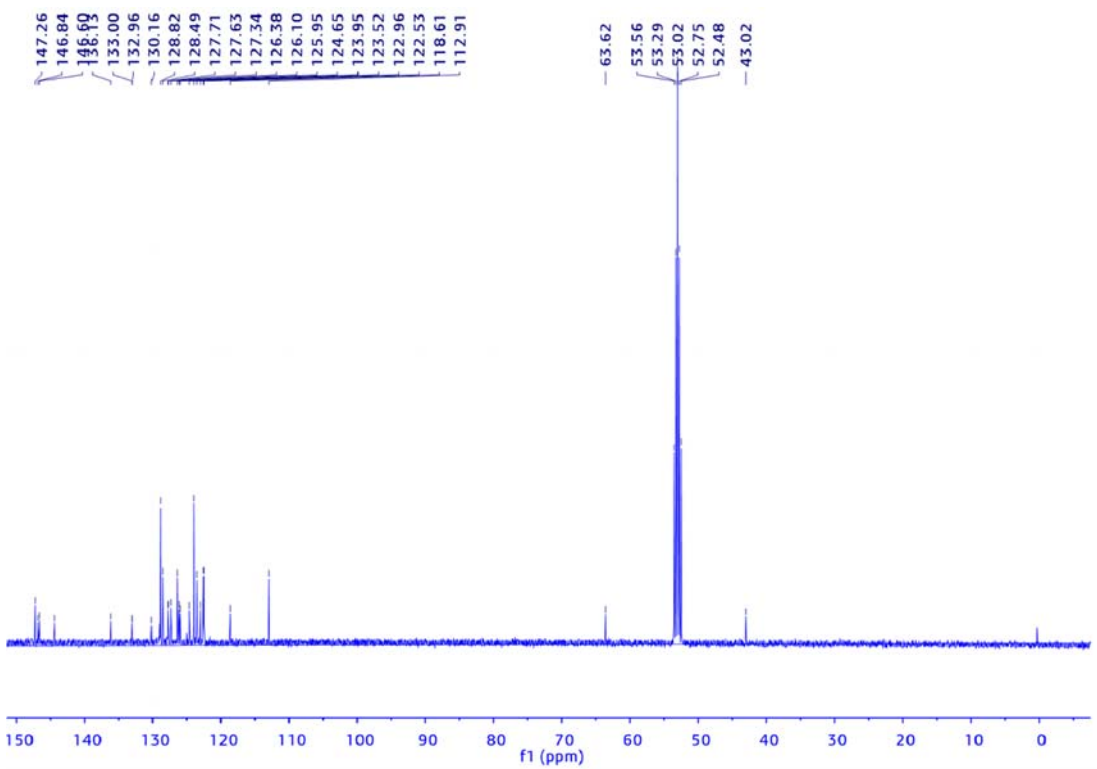

Figure S24. ^{13}C NMR of **TNP** molecule (CD_2Cl_2, 298 K).

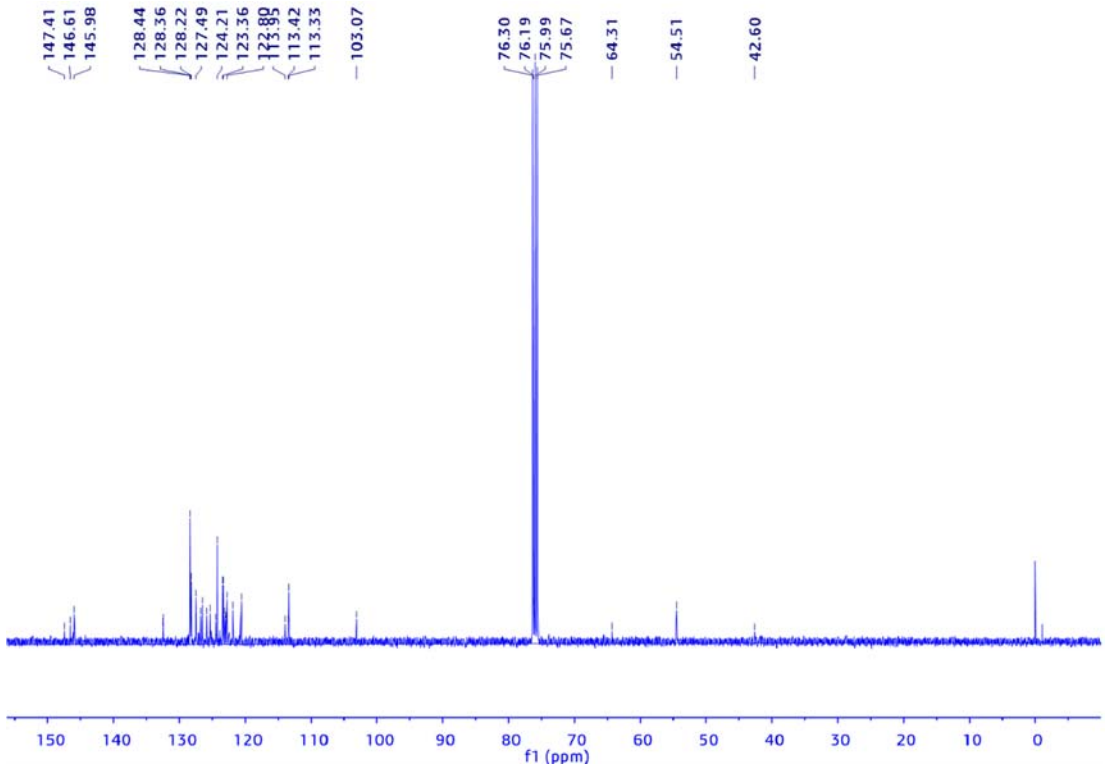

Figure S25. ^{13}C NMR of **TNP-OMe** molecule ($CDCl_3$, 298 K).

Cartesian coordinates.

TNP (S_0)

C	0.37792300	1.15371200	-1.11659900
N	-1.59881300	2.47271500	-0.39872300
C	-0.87625600	1.89435600	-1.54066600
C	-1.95327900	0.95291000	-2.11942500
C	-2.91411000	0.84881200	-0.95449100
N	-2.68330300	1.72413600	-0.04501300
C	-1.07970500	3.42100300	0.47280600
C	1.46001700	1.05758100	-1.98903600
C	2.59407400	0.33333100	-1.64632300
C	2.67495000	-0.29988300	-0.40307400
C	1.59550000	-0.19512300	0.48020900
C	0.46018600	0.51731900	0.12157200
C	-1.75395500	3.75931600	1.65618000
C	-1.23259100	4.73156800	2.49782100
C	-0.04149400	5.38587700	2.19104600
C	0.62568500	5.04807700	1.01834500
C	0.12166300	4.07607500	0.16272600
C	-4.03198800	-0.09648800	-0.87255300
C	-4.30963000	-0.94941100	-1.97634900
C	-5.35026400	-1.83692700	-1.93193500
C	-6.17700300	-1.93185400	-0.78371200
C	-5.90529000	-1.08254800	0.32555000
C	-4.82504400	-0.17437500	0.25285600
C	-7.26201600	-2.84374300	-0.70613400
C	-8.03961100	-2.90859500	0.41917300
C	-7.77018000	-2.06343500	1.52527700
C	-6.73069200	-1.17448400	1.48011100
N	3.83187700	-1.02801800	-0.04044600
C	3.70715300	-2.24564600	0.67215500
C	5.11482200	-0.53668100	-0.38469800
C	4.60016300	-2.55854900	1.70142000
C	4.47785800	-3.75787200	2.39216900
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C	2.56333300	-4.33843700	1.06243100
C	2.68866100	-3.14940000	0.35477800
C	6.11326000	-1.41208300	-0.82240300
C	7.37323200	-0.92721700	-1.15056800
C	7.65204600	0.43398800	-1.06478700
C	6.65601500	1.30736900	-0.63686300
C	5.39843100	0.82917900	-0.29013600
H	-0.61733400	2.68050200	-2.25237300
H	-2.45942600	1.39272400	-2.98396200

H	-1.53498900	-0.00714900	-2.42234700
H	1.41626900	1.54815400	-2.95700000
H	3.42557100	0.26232300	-2.33826200
H	1.65370200	-0.67171100	1.45215200
H	-0.36068100	0.59923600	0.82741800
H	-2.68065000	3.25759300	1.89893000
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H	0.35838600	6.14324000	2.85443500
H	1.55587000	5.54229000	0.76037300
H	0.66638300	3.82578600	-0.73931100
H	-3.69327000	-0.89197500	-2.86665600
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H	-8.86642900	-3.60770900	0.46993100
H	-8.39417400	-2.12600300	2.40942100
H	-6.52103900	-0.52604000	2.32463400
H	5.38802700	-1.85828700	1.95507400
H	5.17814700	-3.98615000	3.18776700
H	3.36129400	-5.58409100	2.62713400
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H	5.89604400	-2.47135300	-0.90148300
H	8.13727700	-1.61870200	-1.48756900
H	8.63383700	0.80960600	-1.32768000
H	6.86075300	2.36915700	-0.55823100
H	4.62918100	1.51069000	0.05544400

TNP (S_1)

C	0.36308500	1.10820300	-1.14254100
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C	-0.88756700	1.84239900	-1.57459400
C	-1.97673800	0.92422400	-2.15018200
C	-2.91867800	0.79249900	-0.98336600
N	-2.67530100	1.70929000	-0.02544400
C	-1.14905300	3.47957800	0.32139900
C	1.55081100	1.25620400	-1.85458600
C	2.68954500	0.54656400	-1.49696900
C	2.66789300	-0.31473500	-0.39566400
C	1.47807400	-0.44971600	0.33203200
C	0.34086000	0.24738700	-0.04272800
C	-1.88727100	3.91223700	1.45161100
C	-1.45049000	5.00947500	2.17010700
C	-0.28960800	5.69299800	1.80388800

C	0.44491600	5.25830700	0.69509600
C	0.03552800	4.16573700	-0.04284600
C	-3.95381700	-0.14790600	-0.85301100
C	-4.20979100	-1.11583200	-1.88236400
C	-5.21164900	-2.02574400	-1.76104200
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C	-4.78605900	-0.16211500	0.30105800
C	-7.09833900	-2.98368200	-0.45890400
C	-7.90389000	-2.99192200	0.66768500
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N	3.82328600	-1.03011900	-0.01772600
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C	5.10495800	-0.43870200	-0.15005100
C	4.49929100	-2.76100100	1.56557600
C	4.39584700	-4.05850400	2.05162700
C	3.49703900	-4.95688700	1.48315800
C	2.70654300	-4.54610400	0.41349600
C	2.81622700	-3.25585900	-0.09016000
C	6.18194700	-1.19112700	-0.62679700
C	7.43990900	-0.61294700	-0.74436500
C	7.63849900	0.72258300	-0.40571100
C	6.56441300	1.47434700	0.06286000
C	5.30707300	0.89941200	0.19994400
H	-0.63338500	2.65294200	-2.25849200
H	-2.47054900	1.39507000	-3.00620000
H	-1.56422500	-0.02936200	-2.48025200
H	1.58809500	1.92128100	-2.71210600
H	3.60190400	0.66126400	-2.07051700
H	1.45220100	-1.10219200	1.19695200
H	-0.56621000	0.13805600	0.54475900
H	-2.78391400	3.37763600	1.72935900
H	-2.02144200	5.33810600	3.03093400
H	0.04417800	6.54957700	2.37670400
H	1.35177400	5.77821300	0.40919400
H	0.62886700	3.83547500	-0.88540800
H	-3.59307100	-1.11607000	-2.77514000
H	-5.38969500	-2.75031000	-2.54942700
H	-4.61171300	0.56714100	1.08434000
H	-7.26590500	-3.70514200	-1.25327000
H	-8.70359600	-3.71721400	0.76276400
H	-8.31159500	-2.05855600	2.57533500
H	-6.50040100	-0.40312400	2.38049000

H	5.19139300	-2.05914700	2.01721900
H	5.01358100	-4.36341800	2.88876300
H	3.41356300	-5.96581300	1.86939100
H	2.00709600	-5.23727200	-0.04298900
H	2.20847400	-2.94270900	-0.93170600
H	6.02706400	-2.22855200	-0.90127500
H	8.26632500	-1.20882400	-1.11496600
H	8.61936000	1.17227900	-0.50457800
H	6.70665700	2.51334100	0.33793800
H	4.47530400	1.48321700	0.57817800

TNP (T_1)

C	0.33141100	1.24897200	-1.14800200
N	-1.61068400	2.58658000	-0.42112700
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C	-1.97229600	1.18267100	-2.23471100
C	-2.89879800	0.94067900	-1.07977700
N	-2.71176300	1.91332400	-0.07236000
C	-1.13803400	3.63128400	0.36882700
C	1.50483400	1.28708900	-1.89769500
C	2.60374200	0.51637600	-1.54257300
C	2.55494500	-0.30027100	-0.40898600
C	1.38083900	-0.33024800	0.35213100
C	0.28204900	0.43006300	-0.01906300
C	-1.89033900	4.06468900	1.47148500
C	-1.42750900	5.11720100	2.24584800
C	-0.22179400	5.74815500	1.94527500
C	0.52478200	5.31059800	0.85447200
C	0.08032500	4.25836400	0.06664200
C	-3.83118500	-0.06361100	-0.93110900
C	-4.04272400	-1.05545900	-1.96578700
C	-4.95431600	-2.04248100	-1.81520400
C	-5.75868800	-2.15222800	-0.62370300
C	-5.57826200	-1.18313400	0.41023700
C	-4.62951200	-0.15640100	0.24716700
C	-6.70557100	-3.17292400	-0.45704300
C	-7.46780700	-3.25585800	0.69449000
C	-7.29695500	-2.30427700	1.71800700
C	-6.37622500	-1.29154700	1.58132000
N	3.67391000	-1.07585300	-0.03325600
C	3.49051400	-2.37743800	0.49632500
C	4.98211200	-0.54898500	-0.17198500
C	4.27230700	-2.82193000	1.56651500
C	4.09511500	-4.10230400	2.07624500

C	3.12873700	-4.94945100	1.54120600
C	2.34443900	-4.50446800	0.48065800
C	2.52689000	-3.23221300	-0.04686600
C	6.02425300	-1.35958700	-0.63112900
C	7.30814600	-0.84309300	-0.75511700
C	7.56837700	0.48792100	-0.44105800
C	6.52930400	1.29774300	0.00902900
C	5.24596900	0.78488000	0.15246900
H	-0.57756200	2.87146600	-2.22968600
H	-2.47329000	1.74556900	-3.02982600
H	-1.56195300	0.27082900	-2.66704900
H	1.56164800	1.91713700	-2.78034200
H	3.50711300	0.54914500	-2.14064700
H	1.33614900	-0.94993000	1.24027600
H	-0.61429700	0.40293200	0.59386300
H	-2.82525100	3.57157700	1.69694700
H	-2.01589300	5.44799100	3.09398800
H	0.13351100	6.56894700	2.55656000
H	1.46759900	5.78791100	0.61396700
H	0.68671500	3.92304500	-0.76468300
H	-3.45987200	-0.99665000	-2.87857000
H	-5.09800200	-2.77722000	-2.60138400
H	-4.49858900	0.58045300	1.03018000
H	-6.83404200	-3.90375800	-1.24969200
H	-8.19552100	-4.05054900	0.81018100
H	-7.89628100	-2.37165300	2.61915200
H	-6.24511000	-0.55814500	2.37066600
H	5.01718700	-2.16009900	1.99379900
H	4.70900600	-4.43324200	2.90633400
H	2.98823200	-5.94465100	1.94603900
H	1.59190700	-5.15532300	0.05004100
H	1.92258200	-2.89356800	-0.88094200
H	5.82175700	-2.39365400	-0.88658300
H	8.10673400	-1.48380700	-1.11172900
H	8.56953300	0.88914600	-0.54497600
H	6.71918400	2.33415100	0.26447900
H	4.44161000	1.41417600	0.51673600

TNP-CN (S_0)

C	0.35900600	0.53285600	-1.35739300
N	-1.59445200	1.95281300	-0.80383100
C	-0.91067200	1.18868300	-1.86107200
C	-2.00729500	0.17233600	-2.24705200
C	-2.99252400	0.33283200	-1.11058600

N	-2.73079500	1.33698800	-0.35766400
C	-1.08276500	3.04382900	-0.14841000
C	1.44359700	0.35390700	-2.21303400
C	2.59674000	-0.28682200	-1.78052800
C	2.69562400	-0.74845400	-0.46445800
C	1.60992800	-0.56311100	0.39915200
C	0.45584600	0.06310800	-0.04786500
C	-1.76357200	3.61448100	0.94544200
C	-1.24499200	4.72134100	1.58448500
C	-0.03871600	5.29247900	1.15743200
C	0.63934300	4.72868100	0.07157300
C	0.13035000	3.61884600	-0.57457300
C	-4.16141400	-0.52572300	-0.89096400
C	-4.46014200	-1.55913700	-1.82074800
C	-5.55090800	-2.36596800	-1.64192900
C	-6.40823100	-2.19416100	-0.52524800
C	-6.11365200	-1.16314200	0.41051100
C	-4.98194600	-0.34355000	0.20176000
C	-7.54629900	-3.01522900	-0.31169000
C	-8.35158000	-2.82035400	0.77859900
C	-8.05902100	-1.79369900	1.71167800
C	-6.96875700	-0.98646500	1.53287100
N	3.87673000	-1.37758100	-0.01350500
C	3.80794100	-2.45944000	0.89839200
C	5.14097500	-0.90049800	-0.44332900
C	4.72719400	-2.55846800	1.94696000
C	4.66462900	-3.62721300	2.83247800
C	3.67873300	-4.60072800	2.69814900
C	2.75797700	-4.49853100	1.65902600
C	2.82373700	-3.44261900	0.75844000
C	6.15571900	-1.80068500	-0.77958700
C	7.39785100	-1.33151500	-1.18884900
C	7.64025900	0.03603800	-1.28471800
C	6.62736300	0.93302300	-0.95710200
C	5.38772000	0.47239500	-0.53054800
H	-0.67805300	1.85061300	-2.69769000
H	-2.48426700	0.42305800	-3.19825200
H	-1.61209600	-0.84109700	-2.32368700
H	1.38827700	0.71348600	-3.23626200
H	3.43062000	-0.42305500	-2.45947200
H	1.67901500	-0.90557800	1.42517700
H	-0.36903900	0.21146500	0.64278900
H	-2.69523200	3.17733400	1.27511300
H	-1.77562400	5.15276400	2.42498200

H	1.57323800	5.16306600	-0.26464400
H	0.67744400	3.19445700	-1.40611700
H	-3.82026700	-1.70739500	-2.68357600
H	-5.77250900	-3.15069200	-2.35766100
H	-4.75673200	0.44109600	0.91636900
H	-7.76701100	-3.79999800	-1.02802900
H	-9.21887600	-3.45168600	0.93400200
H	-8.70611000	-1.65190300	2.56960700
H	-6.74094900	-0.19936500	2.24418800
H	5.48898400	-1.79576400	2.06229400
H	5.38491300	-3.69046900	3.64031700
H	3.62874800	-5.42935100	3.39452200
H	1.98855000	-5.25269500	1.53792200
H	2.11304200	-3.37377800	-0.05751400
H	5.96503600	-2.86614300	-0.71527700
H	8.17609600	-2.04122100	-1.44579600
H	8.60808000	0.39869200	-1.61019600
H	6.80501700	2.00069600	-1.01968700
H	4.60473400	1.17311200	-0.26269800
C	0.49440300	6.43924800	1.82461700
N	0.92427400	7.36333900	2.36185600

TNP-CN (S_1)

C	0.34934000	0.57456400	-1.37547300
N	-1.58315300	1.97401900	-0.77836100
C	-0.90254200	1.25353800	-1.88509100
C	-2.00842800	0.28157100	-2.32572400
C	-2.95722800	0.33614900	-1.15909600
N	-2.68124000	1.36572000	-0.33029000
C	-1.10757000	3.10939800	-0.18810900
C	1.53407600	0.63875300	-2.10442800
C	2.67580600	-0.01813200	-1.66612600
C	2.65940100	-0.74143200	-0.46940200
C	1.46989100	-0.79718000	0.26937100
C	0.33031100	-0.15252800	-0.18348100
C	-1.82917900	3.68734700	0.89139100
C	-1.36553500	4.83869100	1.48175200
C	-0.17940100	5.44653000	1.03139100
C	0.54158600	4.86879800	-0.03379500
C	0.09243100	3.71785100	-0.63562400
C	-4.03060800	-0.53057700	-0.90714000
C	-4.33720500	-1.61482000	-1.79986300
C	-5.37924200	-2.45119100	-1.55585000
C	-6.21535000	-2.28591600	-0.40103100

C	-5.92571900	-1.20612900	0.50038100
C	-4.85302400	-0.35299100	0.23872600
C	-7.29718200	-3.13776400	-0.13318500
C	-8.08935400	-2.95556500	0.98664700
C	-7.81293000	-1.89705900	1.87929000
C	-6.76382200	-1.04451500	1.64772500
N	3.82106400	-1.39350800	-0.00972500
C	3.72528100	-2.63854100	0.66196300
C	5.09468600	-0.79936900	-0.20323300
C	4.52154200	-2.89798700	1.78081800
C	4.43540100	-4.12380900	2.42926000
C	3.54636300	-5.09817700	1.98434800
C	2.74793800	-4.83728700	0.87420600
C	2.84033100	-3.62094100	0.20904000
C	6.18424400	-1.58253200	-0.59259600
C	7.43393400	-1.00094200	-0.76813000
C	7.61037300	0.36631300	-0.57463000
C	6.52326200	1.14789800	-0.19330400
C	5.27407200	0.57146700	0.00107800
H	-0.65554700	1.97212500	-2.66681400
H	-2.49214700	0.62921300	-3.24393800
H	-1.61218500	-0.71727300	-2.51033900
H	1.56771400	1.19576100	-3.03586000
H	3.58736200	0.03170000	-2.25003300
H	1.44682900	-1.34325100	1.20509500
H	-0.57579300	-0.19681000	0.41419900
H	-2.73808500	3.21339100	1.23173800
H	-1.91577300	5.28271100	2.30256200
H	1.45785400	5.33362000	-0.37623400
H	0.66912500	3.28234600	-1.44021100
H	-3.72687300	-1.76150300	-2.68470200
H	-5.59753400	-3.26495700	-2.24003500
H	-4.63889200	0.46442500	0.91808800
H	-7.50670900	-3.95009900	-0.82254700
H	-8.92133100	-3.62259700	1.18020900
H	-8.43763800	-1.75932700	2.75500200
H	-6.55261100	-0.23101900	2.33455300
H	5.20639400	-2.13623900	2.13609700
H	5.05939600	-4.31179600	3.29564400
H	3.47675800	-6.05041900	2.49662800
H	2.05621300	-5.58969900	0.51267600
H	2.22739400	-3.42589900	-0.66386400
H	6.04554900	-2.64586300	-0.75310200
H	8.27125700	-1.62008900	-1.06952900

H	8.58487500	0.81777800	-0.71824200
H	6.64894200	2.21242000	-0.03104500
H	4.43165600	1.17925200	0.31219600
C	0.29436500	6.63878600	1.65144300
N	0.67931800	7.60498000	2.15133500

TNP-CN (T_1)

C	0.32146500	0.79153100	-1.38620300
N	-1.61917600	2.21142500	-0.83066100
C	-0.88203800	1.53687500	-1.92148000
C	-1.97623900	0.61016400	-2.47673200
C	-2.91080100	0.50462900	-1.30893700
N	-2.72818300	1.59526600	-0.42300000
C	-1.15268800	3.33189200	-0.16463200
C	1.49084700	0.71507100	-2.13937600
C	2.58075100	-0.01918400	-1.69283800
C	2.53009100	-0.68144200	-0.46145500
C	1.35979500	-0.59345300	0.30239100
C	0.26887900	0.12661300	-0.16051900
C	-1.91954100	3.88839800	0.87500600
C	-1.46920900	5.01359600	1.53451000
C	-0.24922100	5.60085600	1.17595700
C	0.51753500	5.04378600	0.14627600
C	0.07511900	3.91711800	-0.51989400
C	-3.84440200	-0.46898700	-1.03810300
C	-4.05334100	-1.58630300	-1.93783800
C	-4.96466700	-2.54511900	-1.66213000
C	-5.77116100	-2.50134800	-0.46713000
C	-5.59494100	-1.40692400	0.43345500
C	-4.64744000	-0.40841400	0.14106100
C	-6.71591700	-3.49367600	-0.17201500
C	-7.47995800	-3.42811300	0.97978300
C	-7.31363700	-2.35226100	1.87198100
C	-6.39455900	-1.36359600	1.60713400
N	3.63955400	-1.41615000	0.00448600
C	3.44958100	-2.60453100	0.75450500
C	4.95778500	-0.96590300	-0.26375700
C	4.25493200	-2.87064500	1.86526200
C	4.07714100	-4.04139900	2.59207800
C	3.08727300	-4.95223400	2.23398100
C	2.28024700	-4.68424500	1.13172600
C	2.46297600	-3.52446300	0.38871500
C	5.94731100	-1.87666800	-0.64300400
C	7.24180600	-1.43738400	-0.89201200

C	7.56268700	-0.08717000	-0.78294500
C	6.57537300	0.82143800	-0.41161500
C	5.28262300	0.38799300	-0.14401600
H	-0.57392300	2.28236900	-2.65584100
H	-2.46960000	1.08122500	-3.33382300
H	-1.56696100	-0.34624100	-2.79955300
H	1.55108200	1.22420800	-3.09657200
H	3.47863600	-0.07762600	-2.29679100
H	1.31062300	-1.08945500	1.26460000
H	-0.62373200	0.18828700	0.45546000
H	-2.85954200	3.42762600	1.14135200
H	-2.06038800	5.44495100	2.33297400
H	1.46400200	5.49396500	-0.12623000
H	0.69108000	3.49043800	-1.29999700
H	-3.46800000	-1.64491600	-2.84885000
H	-5.10740100	-3.37514100	-2.34701900
H	-4.52083500	0.42496300	0.82116900
H	-6.84185600	-4.32109200	-0.86354800
H	-8.20609000	-4.20292200	1.19611300
H	-7.91476700	-2.30416500	2.77303600
H	-6.26585500	-0.53418100	2.29520400
H	5.01876700	-2.15699000	2.15301200
H	4.70937400	-4.23495000	3.45125100
H	2.94651000	-5.86096000	2.80711000
H	1.50995800	-5.38809400	0.83745800
H	1.84142600	-3.32478400	-0.47699200
H	5.69571700	-2.92712100	-0.73770200
H	8.00006800	-2.15491300	-1.18445300
H	8.57158400	0.25339000	-0.98360000
H	6.81412300	1.87453400	-0.31493800
H	4.51841200	1.09513000	0.15886600
C	0.21499200	6.76764400	1.86388400
N	0.58793300	7.70626100	2.41658300

TNP-OMe (S_0)

C	0.35365000	0.53582400	-1.41106200
N	-1.60369100	1.98213900	-0.91436900
C	-0.88875000	1.22091800	-1.94864900
C	-1.98201100	0.21901800	-2.37656800
C	-2.93129800	0.29869400	-1.20015300
N	-2.68620600	1.30165800	-0.43821400
C	-1.05817000	3.03147800	-0.18137900
C	1.42450500	0.26961000	-2.26217600
C	2.55028200	-0.40376100	-1.80808200

C	2.63686600	-0.81058100	-0.47324900
C	1.56765900	-0.53659500	0.38621200
C	0.43935100	0.12126600	-0.08248500
C	-1.71338300	3.53449500	0.95243900
C	-1.17139700	4.60019700	1.65559200
C	0.02810400	5.17874500	1.25159600
C	0.67995400	4.68729100	0.12768200
C	0.14981000	3.61804700	-0.58389600
C	-4.05657300	-0.61049400	-0.96131800
C	-4.37158900	-1.60835100	-1.92442800
C	-5.42574900	-2.45972900	-1.73216800
C	-6.22878100	-2.37248300	-0.56647300
C	-5.91668300	-1.37961400	0.40450700
C	-4.82405700	-0.51236000	0.18005700
C	-7.32867300	-3.24029400	-0.33760500
C	-8.08130700	-3.12729300	0.80078300
C	-7.77046800	-2.13990700	1.76972500
C	-6.71628600	-1.28902400	1.57718200
N	3.79123600	-1.47503700	-0.00034800
C	3.67551300	-2.51597700	0.95304900
C	5.07358900	-1.07213000	-0.44971700
C	4.59160000	-2.61600400	2.00446000
C	4.48210200	-3.64495400	2.93159200
C	3.45219300	-4.57654200	2.83640600
C	2.53451900	-4.47282800	1.79468700
C	2.64649300	-3.45728900	0.85311600
C	6.04996700	-2.02868700	-0.74219700
C	7.31022100	-1.63197200	-1.17203900
C	7.60984500	-0.28192000	-1.33252600
C	6.63551100	0.67093800	-1.04877300
C	5.37800500	0.28361100	-0.60210700
H	-0.61618400	1.88139500	-2.77378700
H	-2.49209000	0.53784200	-3.29068400
H	-1.57835100	-0.77994300	-2.54214900
H	1.37797100	0.58548600	-3.30033500
H	3.37256900	-0.60810500	-2.48424200
H	1.62853900	-0.83557600	1.42634800
H	-0.37235300	0.33793300	0.60515200
H	-2.64309300	3.08345300	1.27110100
H	-1.67237400	4.98496500	2.53759700
H	1.61790900	5.13769500	-0.17840100
H	0.68374600	3.23927400	-1.44667000
H	-3.77365000	-1.69134200	-2.82536800
H	-5.65969900	-3.21520500	-2.47514900

H	-4.58560500	0.24258300	0.92187700
H	-7.56311400	-3.99492300	-1.08152300
H	-8.91975200	-3.79382100	0.96732900
H	-8.37485700	-2.06304000	2.66629300
H	-6.47521500	-0.53170100	2.31608500
H	5.38768400	-1.88500100	2.08947900
H	5.20047000	-3.70915100	3.74109400
H	3.36550600	-5.37375200	3.56512000
H	1.73062700	-5.19464200	1.70409900
H	1.93713800	-3.38732100	0.03612200
H	5.81507900	-3.08104800	-0.62812900
H	8.05761800	-2.38519800	-1.39453600
H	8.59164300	0.02411400	-1.67393500
H	6.85748500	1.72611800	-1.16182300
H	4.62537600	1.02853600	-0.36895800
O	0.57687600	6.21740200	1.97093900
C	0.09688500	7.49265900	1.56399000
H	-0.98671100	7.56192600	1.69872100
H	0.58982400	8.23245900	2.19196200
H	0.34079000	7.68143100	0.51415400

TNP-OMe (S_1)

C	0.32828500	0.50183200	-1.37508700
N	-1.54596400	1.97840900	-0.77534300
C	-0.89646600	1.23603500	-1.87557800
C	-2.04046200	0.30839500	-2.31595100
C	-2.96651300	0.37060800	-1.12917000
N	-2.66144600	1.37768600	-0.29316800
C	-1.04732700	3.09783200	-0.19144500
C	1.52577700	0.55398800	-2.08430600
C	2.64383400	-0.14512800	-1.64823000
C	2.58954900	-0.89867500	-0.47267000
C	1.38967000	-0.94101700	0.24908400
C	0.27389300	-0.25397900	-0.20106000
C	-1.74291400	3.70069300	0.89290800
C	-1.25158200	4.84547100	1.47015400
C	-0.06034700	5.43368700	1.01224700
C	0.63983300	4.83859800	-0.04970800
C	0.15815300	3.68773100	-0.64012400
C	-4.04707200	-0.49535400	-0.87401700
C	-4.37285900	-1.56334400	-1.77551200
C	-5.41992200	-2.39721100	-1.53490600
C	-6.24531000	-2.24251900	-0.37068100
C	-5.93570800	-1.17736300	0.54262400

C	-4.85600600	-0.32903700	0.28191700
C	-7.33267300	-3.08916900	-0.10549500
C	-8.11596000	-2.91962300	1.02336500
C	-7.81989100	-1.87666100	1.92665500
C	-6.76440100	-1.02896100	1.69835800
N	3.72710500	-1.59825000	-0.01392900
C	3.58347100	-2.88012600	0.57291600
C	5.01415500	-1.01832600	-0.13667300
C	4.34292200	-3.23414800	1.69181800
C	4.20589400	-4.49555300	2.25780400
C	3.30162600	-5.41327200	1.73043000
C	2.53912600	-5.05823300	0.62126900
C	2.68229800	-3.80533400	0.03812500
C	6.10911400	-1.80183200	-0.51213500
C	7.37151600	-1.23167700	-0.62052000
C	7.55819800	0.12562400	-0.37393800
C	6.46662100	0.90808200	-0.00748300
C	5.20390800	0.34283300	0.11997500
H	-0.61832400	1.94060300	-2.66080300
H	-2.52557700	0.69215000	-3.21910200
H	-1.68018300	-0.69858200	-2.52866700
H	1.58698100	1.13431700	-3.00011400
H	3.56570800	-0.10510000	-2.21692400
H	1.34031200	-1.51236700	1.16886000
H	-0.64154600	-0.28542800	0.38270900
H	-2.65748100	3.24701100	1.24579200
H	-1.77145000	5.31872300	2.29473400
H	1.56445200	5.26403300	-0.41609000
H	0.72480600	3.23823800	-1.44474900
H	-3.77394200	-1.70389600	-2.66963000
H	-5.64936900	-3.19928600	-2.22959000
H	-4.62903600	0.47620900	0.97173500
H	-7.55322600	-3.88913800	-0.80646200
H	-8.95187500	-3.58248200	1.21446900
H	-8.43455900	-1.74486900	2.81091000
H	-6.54165700	-0.22813600	2.39678800
H	5.03905300	-2.51719900	2.11237400
H	4.80168000	-4.75614000	3.12530200
H	3.19216700	-6.39357000	2.17885300
H	1.83528000	-5.76477900	0.19611800
H	2.09617500	-3.53694800	-0.83366400
H	5.96461400	-2.85696600	-0.71536600
H	8.21157400	-1.85203200	-0.91182900
H	8.54299400	0.56825200	-0.46525200

H	6.59880000	1.96492400	0.19526700
H	4.35815500	0.95188800	0.41910300
O	0.33025500	6.55146300	1.65143800
C	1.52779000	7.18471200	1.22685100
H	1.45204900	7.50234400	0.18411500
H	1.64662300	8.05487300	1.86579400
H	2.38558800	6.51926500	1.35002600

TNP-OMe (T_1)

C	0.30623800	0.62443900	-1.39406300
N	-1.56654800	2.12345900	-0.81951400
C	-0.88356600	1.40506100	-1.91119400
C	-2.02206100	0.51006200	-2.42734500
C	-2.95335800	0.48400500	-1.24995300
N	-2.69380000	1.55348200	-0.37329700
C	-1.02612300	3.22422000	-0.16463800
C	1.46365600	0.51535700	-2.16123100
C	2.54247700	-0.23998200	-1.72179900
C	2.49156200	-0.88971600	-0.48463700
C	1.33282200	-0.77232000	0.29197000
C	0.25280900	-0.03085700	-0.16319500
C	-1.73253900	3.82339700	0.89460900
C	-1.20806800	4.92262000	1.53924600
C	0.02979700	5.45656200	1.15724000
C	0.73608800	4.86329600	0.10996500
C	0.21182900	3.75422300	-0.54338100
C	-3.96140700	-0.42136200	-0.98594100
C	-4.25297600	-1.51392900	-1.89020600
C	-5.24373000	-2.39689500	-1.62833100
C	-6.05533600	-2.29075600	-0.44171800
C	-5.79355000	-1.21886400	0.46617100
C	-4.76281100	-0.30270100	0.18698100
C	-7.08562500	-3.19965800	-0.15997300
C	-7.85291400	-3.07481900	0.98439400
C	-7.60166300	-2.02117200	1.88411800
C	-6.59825200	-1.11463900	1.63341400
N	3.59470800	-1.64060700	-0.02382900
C	3.39087200	-2.83324000	0.71393500
C	4.91523300	-1.19037900	-0.27649300
C	4.19819600	-3.12608300	1.81693800
C	4.00503800	-4.30183400	2.53150900
C	2.99764400	-5.19180700	2.16994600
C	2.18793000	-4.89681600	1.07661500
C	2.38545800	-3.73191000	0.34556300

C	5.90928400	-2.09927700	-0.64937700
C	7.20589800	-1.65873800	-0.88434700
C	7.52562000	-0.30880000	-0.76790100
C	6.53412500	0.59805000	-0.40368900
C	5.23891200	0.16346900	-0.15019700
H	-0.56220200	2.12577900	-2.66504400
H	-2.50099100	0.97094800	-3.29795200
H	-1.65945200	-0.47497700	-2.72001800
H	1.52363400	1.01769300	-3.12213800
H	3.43288600	-0.32288200	-2.33420800
H	1.28542000	-1.26078900	1.25829900
H	-0.63114600	0.05949400	0.46169600
H	-2.68776100	3.41208200	1.18888900
H	-1.74258100	5.39447900	2.35526600
H	1.69715300	5.24592400	-0.20653000
H	0.78864800	3.30277400	-1.34026400
H	-3.66627100	-1.61797700	-2.79673800
H	-5.44706100	-3.20953800	-2.31893400
H	-4.57123500	0.51242500	0.87423400
H	-7.27502800	-4.00988100	-0.85771200
H	-8.64564700	-3.78480300	1.18941800
H	-8.20467200	-1.92553500	2.78034000
H	-6.40558100	-0.30278000	2.32767000
H	4.97573000	-2.42911300	2.10867300
H	4.63929700	-4.51551900	3.38443700
H	2.84513100	-6.10458000	2.73354800
H	1.40328300	-5.58353200	0.77974100
H	1.76117700	-3.51175000	-0.51316000
H	5.65935800	-3.14950900	-0.75040500
H	7.96703200	-2.37519600	-1.17200000
H	8.53631300	0.03268600	-0.95767500
H	6.77129800	1.65104600	-0.30168300
H	4.47156400	0.86971800	0.14669300
O	0.45329900	6.53412600	1.85807000
C	1.70632100	7.09720600	1.50930600
H	1.70301000	7.45375700	0.47596300
H	1.85517200	7.93698100	2.18245400
H	2.51363400	6.37275900	1.64519400