Supporting Information

Efficient Long-Wavelength-Excited Triplet–Triplet Annihilation Upconversion with Phenyl-Diketopyrrolopyrroles as the Annihilators

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Chemicals and Characterization

Chemcials: Naphthalene, metal sodium (Na), thiophenol, triphenylphosphine (PPh_3), *N*-chlorinated succinimide (NCS), 3-chloroperbenzoic acid (m-CPBA), 1,8-diazabicyclo[5.4.0]undec-7-ene (DBU), potassium t-butoxide (t-BuOK), ethyl isocyanoacetate, potassium hydroxide (KOH), $Pd(PPh_3)_4$, 4-chlorobenzaldehyde, 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ), boron trifluoride etherate, platinum(II) chloride ($PtCl_2$), benzonitrile, 2-methylbenzonitrile, 1-naphthalenecarbonitrile, 2-naphthalenecarbonitrile, 2-thiophenecarbonitrile, 3-thiophenecarbonitrile, methyl methacrylate (MMA), ethyl a-bromophenylacetate (EBP), ethylene glycol dimethacrylate (DEGMA), trimethylolpropane ethoxylate triacrylate, dichloromethane (DCM), tetrahydrofuran (THF), toluene, ethyl acetate (EtOAc), acetonitrile (MeCN), ethanol (EtOH) and polydimethylsiloxane were purchased from Aladdin. All the above-mentioned chemicals were used as received without further purification.

Characterization: ^{1}H NMR spectra were recorded with a Bruker 400 MHz spectrometer ($CDCl_3$ as solvent, TMS as standard, $\delta = 0.00$ ppm). UV-vis absorption spectra were recorded using a Shimadzu UV-3600 spectrophotometer with a 1-cm quartz cell. Steady-state and time-resolved spectra of fluorescence and phosphorescence were recorded with an FLS-1000 (Edinburgh Instruments, UK) spectrofluorometer equipped with double excitation and emission monochromators. A 405 nm laser diode with a pulse repetition rate of 1 MHz was used as the light source. Triplet fusion upconversion spectra were measured on an Edinburgh instrument, the FLS-1000 fluorescence spectrometer, with a 690 nm diode laser as the excitation source (Changchun New Industries Optoelectronics Technology Co., Ltd., China).

Synthesis details

The synthesis processes followed the literature methods (An-1−An-6,[1] PtTNP[2]).

An-3: Under an argon (Ar) atmosphere, sodium (1.15 g, 50.0 mmol), $FeCl_3$ (0.05 g), and dry tert-amyl alcohol (30 mL) were mixed. The mixture was heated to 100 °C until the sodium disappeared completely. Then benzonitrile (2.06 g, 20 mmol) was added. A solution of diisopropyl succinate (1.61 g, 8.0 mmol) in dry tert-amyl alcohol (5 mL) was added dropwise over 30 min at 100 ^{o}C. After the solution was allowed to stand for 12 h at 110 °C, acetic acid (15 mL) was added. 30 minutes later, the precipitate was filtered and washed with deionized water and methanol. The red precipitate went directly to the next reaction step due to its poor solubility. Under Ar, the dry red precipitate (500 mg) was dissolved in 10 mL dry DMF, and then t-BuOK (8.0 mmol, 900 mg) was added to the solution in the ice bath. After stirring for 30 minutes, butyl bromide (6.0 mmol, 822 mg) was added dropwise, and the resultant mixture was then heated to 110 ^{o}C. After a 6-h reaction, water (50 mL) was added to the solution, and the product was extracted with CH_2Cl_2 (3×100 mL). The organic phase was dried over Na_2SO_4, and the solvent was evaporated under reduced pressure. The obtained crude products were then purified by column chromatography (silica gel, CH_2Cl_2/hexane = 2/1 v/v). The deep yellow band was collected to give a red solid (yield: 26%).^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.82-7.80 (m, 4H), 7.56-7.52 (m, 6H), 3.77-3.74 (m, 4H), 1.61-1.55 (m, 4H), 1.30-1.23 (m, 4H), 0.86-0.83 ppm (m, 6H). The characterization data were consistent with the literature.[1]

The synthesis steps of An-1, An-2, An-4, An-5, and An-6 are similar to those of An-3.

An-1: ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.40-7.34 (m, 5H), 7.31-7.28 (m, 3H), 3.55-3.45 (m, 4H), 2.47-2.44 (d, J = 12.0 Hz, 6H), 1.43-1.29 (m, 4H), 1.17-1.08 (m, 4H), 0.75-0.71 ppm (q, 6H). ^{13}C NMR (100 MHz, CDCl3): δ =161.8, 147.7, 137.9, 137.7, 130.1, 130.3, 128.6, 128.5, 128. 2, 125.8, 110.3, 40.1, 31.3, 19.6, 13.5 ppm.

An-2: ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.05-8.03 (d, J = 8.0Hz, 2H), 7.97-7.94 (m, 4H), 7.80-7.76 (m, 2H), 7.65-7.57 (m, 6H), 3.72-3.60 (m, 2H), 3.37-3.22 (m, 2H), 1.32-1.22 (m, 4H), 1.04-1.00 (m, 4H), 0.63-0.58 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 162.0, 161.9, 147.6, 147.4, 133.7, 131.3, 131.2, 130.5, 130.4, 128.8, 128.7, 128.1, 127.9, 127.37, 126.7, 126.6, 126.2, 126.1, 125.3, 125.2, 111.1, 111.0, 41.6, 31.4, 19.7, 13.4 ppm.

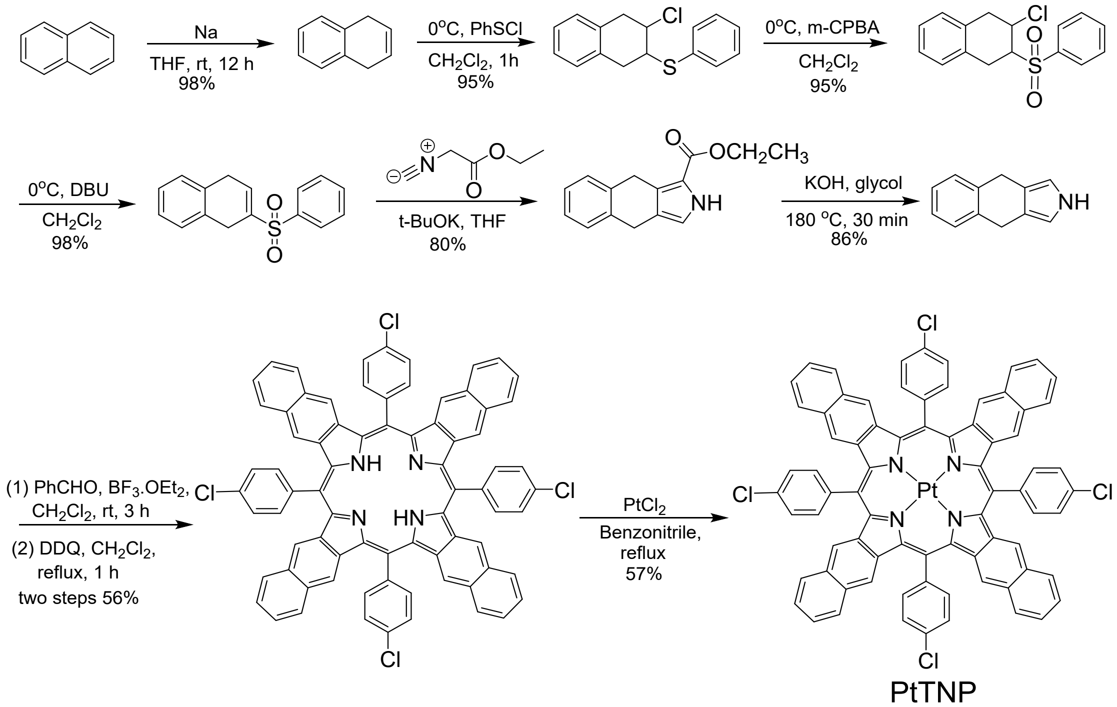
An-4: ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.34 (s, 2H), 7.94-7.83 (m, 8H), 7.60-7.52 (m, 4H), 3.88-3.86 (m, 4H), 1.27-0.92 (m, 20H), 0.70-0.66 (m, 12H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 162.9, 148.7, 134.3, 132.9, 129.2, 129.0, 128.6, 127.9, 127.8, 126.8, 126.0, 125.1, 110.1, 45.2, 38.6, 30.6, 28.3, 23.8, 22.9, 13.9, 10.5 ppm.

An-5: ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.55-8.54 (d, 2H, J = 4.0Hz), 7.93-7.92 (d, 2H, J = 4.0Hz), 7.49-7.47 (m, 2H), 3.97-3.93 (m, 4H), 1.75-1.68 (m, 4H), 1.47-1.38 (m, 4H), 0.98-0.94 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ =162.1, 141.6, 130.4, 129.7, 127.5, 126.5, 108.3, 41.9, 31.8, 20.2, 13.8 ppm.

An-6: ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.93-8.92(d, 2H, J = 4.0Hz), 7.64-7.63 (d, 2H, J = 4.0Hz), 7.30-7.27 (m, 2H), 4.11-4.07 (m, 4H), 1.79-1.71 (m, 4H), 1.50-1.42 (m, 4H), 0.99-0.95 (m, 6H). ^{13}C NMR (100 MHz, $CDCl_3$): δ =161.4, 140.6, 135.3, 130.7, 129.8, 128.6, 107.7, 42.0, 32.0, 20.2, 13.8 ppm.

Meso-tetraphenyl-tetranaphthoporphyrin platinum, **PtTNP,** was synthesized according to references.[2]

Scheme S1. The preparation process of PtTNP.



PtTNP: ^{1}H NMR (400 MHz, $CDCl_3$), δ = 8.40-8.30 (broad, 20H), 7.95-7.90 ppm (broad, 20H). MALDI-TOF: $C_{76}H_{40}Cl_4N_4Pt$, calculation: 1346.0680, found: 1346.1628.

The measurement and analysis of photophysical properties

Measurement of the absolute fluorescence quantum yield (Φ_f) for annihilators (An-1−An-6). The absolute fluorescence quantum yields of AN-1−AN-6 (two concentrations of 10 μM and 1 mM) in toluene were measured with integrating sphere in FLS 1000 instrument using equation 1 listed below.

$$\Phi_f = \frac{I_{em}}{I_{abs}} \quad (1)$$

where I_{abs} represents an absorbed photon and I_{em} represents an emitted photon.

Measurement of the absolute phosphorescence quantum yield for PtTNP. The absolute phosphorescence quantum yield of PtTNP in Ar-saturated toluene was measured with an integrating sphere using equation 1. The concentration of PtTNP is 1.0 μM, and the excitation wavelength is 690 nm.

Measurement of the phosphorescence lifetime for PtTNP. Phosphorescence decays of PtTNP were measured in Ar-saturated toluene. Decays were measured using an Edinburgh Instruments FLS1000 spectrometer outfitted with a 690 nm nano-pulsed diode laser setup. The instrument response function (IRF) was collected by using a scatterer with fresh milk. Samples were prepared in a glovebox using 1 cm^2 special optical cuvettes with a screw cap and septum (Yixing Jingke optical instrument co., ltd., China). The concentration of PtTNP is 1.0 μM and the excitation wavelength is 690 nm. The decays were monitored at the phosphorescence maximum of PtTNP (900 nm). A mono-exponential tail fitting of the decay was performed with the Fluoracle program (Edinburgh Instruments, UK).

TTA-UC characterization in Ar-saturated toluene. Samples of the photosensitizers PdTPBP or PtTNP, in conjunction with the annihilator (An-1–An-6), were excited with an optical fiber coupling at 635 nm (PdTPBP) or 690 nm (PtTNP) as the excitation light source (Changchun New Industries Optoelectronics Technology Co., Ltd., China), respectively. The laser power was calibrated before testing with an optical power meter (Model: TS15, Changchun New Industries Optoelectronics Technology Co., Ltd. China). The upconversion spectra were measured using the FLS1000 as the sample chamber and detector. The photosensitizer concentrations are 10 μM for PdTPBP and 5 μM for PtTNP in Ar-saturated toluene, respectively. The dependence of upconversion emission intensity on excitation power density was measured by altering the laser power (and thus power density) via a neutral density filter.

Measurement of the reversible triplet energy transfer between PtTNP and annihilators. First, the phosphorescence lifetime of PtTNP without annihilator was determined. In the presence of 100 μM annihilator, the phosphorescence lifetime of PtTNP at 875 nm was monitored via the FLS 1000 instrument with 690 nm pulsed laser excitation. The decay traces of the phosphorescent lifetime of PtTNP were fitted to further confirm the quenching types of the triplet state of PtTNP such as intermolecular triplet energy equilibrium (An-3−An-5) and exothermic triplet energy transfer (exo-TET) processes (DPP-6).

Stern-Volmer quenching experiment for PtTNP phosphorescence lifetime. The mixture of PtTNP (5 μM) and the annihilator was prepared in a glove box, in which the concentration was changing from 0 μM, 20 μM, 40 μM, 60 μM, 80 μM and 100 μM. The phosphorescence lifetime of PtTNP at 875 nm upon different concentrations was monitored and the k_{sv} was calculated according to equation 2,[3] where τ_o and τ_t stand for the phosphorescence lifetime of PtTNP in the absence and presence of DPP annihilator, respectively. Q is the concentration of the annihilator. The triplet energy transfer constants (k_{TET}) were calculated by equation 3.[4] The τ_p is the phosphorescence lifetime of PtTNP in Ar, 14.2 μs.

$$\frac{\tau_0}{\tau_t} = 1 + k_{sv} Q \qquad (2)$$

$$k_{sv} = k_{TET} \times \tau_p \qquad (3)$$

The phosphorescence intensity quenching of PtTNP with the addition of annihilators was also measured on an FLS1000 spectrometer equipped with a NIR-1700 detector (HAMAMATSU) to further confirm the quenching of the triplet state of PtTNP in the presence of annihilators.

Calculation of reversible triplet energy transfer rates from PtTNP to annihilators

The reversible triplet energy transfer rate (k_{RTET}) is calculated based on the method established in the literature using Equation 4.[5]

$$k_{RTET} = k_{TET} \exp\left(-\frac{\Delta E_T}{k_B T}\right) \qquad (4)$$

k_{TET} is the forward triplet energy transfer rate, ΔE_T is the triplet state energy gap between the photosensitizer and annihilator, k_B is the Boltzmann constant, and T is the temperature.

Calculation of the T_1 state of An-1–An-6 according to a reported protocol[5]. The rate of triplet energy transfer follows the Boltzmann distribution and can be written as:

$$k_{TET} = \frac{k_{diff}}{1 + exp(-\frac{\Delta E_T}{k_B T})} \qquad (5)$$

where k_{diff} is the diffusion constant (approximately 1×10^{10} M^{-1} s^{-1} in toluene[5]), and ΔE_T is the triplet energy gap between the sensitizer and the annihilator at temperature T (298 K). k_B is the Boltzmann constant. Thus, by using the k_{TET} values obtained from the above-mentioned Stern-Volmer quenching experiment, we can calculate ΔE_T via equation 5 and then the T_1 state of An-1−An-6.

Measurement of the TTA-UC quantum yield (Φ_{UC}) under 690 nm light illumination. The Φ_{UC} was calculated by using methylene blue (MB) with a fluorescence quantum yield ($\Phi_{f,\mathrm{ref}}$, in methanol) of 3% as the reference for PdTPBP/An-1 and PdTPBP/An-2.[6] The reference of ZnPc ($\Phi_{f,\mathrm{ref}}$ = 17% in DMF) was used to test the TTA-UC yield for PtTNP coupling with An-2−An-6.[4] We have uniformized the sensitivity of the fluorometer at different wavelengths. The upconversion yield was calculated with the following equation 6:[7]

$$\Phi_{UC} = \Phi_{f,ref} \times \left(\frac{A_{std}}{A_{unk}}\right) \times \left(\frac{I_{unk}}{I_{std}}\right) \times \left(\frac{\eta_{std}}{\eta_{unk}}\right)^2 \quad \text{.................................... (6)}$$

where A_{std}, I_{std}, and η_{std} represent the absorbance, the integrated photoluminescence intensity, and the refractive index of the solvent for reference. The other set with the subscript of *unk* are the respective data for the tested sample. The refractive index of toluene and methanol is 1.4967, 1.3290 respectively.

Unless otherwise noted, the upconversion quantum yield (Φ_{UC}) in this work is defined using the conventional 50% maximum for TTA-UC. Accordingly, Φ_{UC} can be written as equation 7:

$$\Phi_{UC} = \frac{1}{2} f \times \Phi_{ISC} \times \Phi_{TET} \times \Phi_{TTA} \times \Phi_f \quad \text{.................................... (7)}$$

where Φ_{ISC}, Φ_{TET}, Φ_{TTA}, Φ_f, and f represent the intersystem crossing efficiency of the sensitizer, triplet energy transfer efficiency, triplet-triplet annihilation quantum yield, fluorescence quantum yield of the annihilator, and the spin statistical factor, respectively. The maxima of Φ_{UC} to be 50%. The concentration of methylene blue and ZnPc was kept low (absorbance of 0.05 at excitation wavelength) to reduce the inner filter effect. The power-dependent TTA-UC yield was also measured according to the reported method.[5]

Following the reported method, the corrected upconversion quantum yield (Φ_{UCg}) was obtained by dividing the measured upconversion quantum yield (Φ_{UC}) by the fluorescence quantum yield (Φ_f) of the corresponding annihilator following equation 8:

$$\Phi_{UCg} = \frac{\Phi_{UC}}{\Phi_f} \quad \text{... (8)}$$

Here, Φ_{UC} is the experimentally measured upconversion quantum yield, and Φ_f is the fluorescence quantum yield of the annihilator. Thus, Φ_{UCg} reflects the upconversion performance after removing the influence of annihilator fluorescence efficiency. All Φ_{UC} values in this work are reported using the conventional 50% maximum for TTA-UC.

Triplet-triplet energy transfer (TET) quantum yield (Φ_{TET}) measurements. The triplet-triplet energy transfer efficiency (Φ_{TET}) from PtTNP to the annihilator was calculated using the following equation 9.[8] τ_0 represents the phosphorescence lifetime of PtTNP, whereas τ_t represents the PtTNP phosphorescence lifetime in response to the addition of the annihilator.

$$\Phi_{TET} = 1 - \frac{\tau}{\tau_0} = 1 - \frac{I}{I_0} \quad (9)$$

Analysis of threshold power intensity (I_{th}) [5]. The threshold power intensity (I_{th}) of TTA-UC was determined by equation 10:

$$I_{th} = \frac{2 \times (k_A^T)^2}{k_{TTA}\alpha(\lambda)\Phi_{TET}} \quad (10)$$

where k_A^T is the spontaneous decay rate of the annihilator triplet state, k_{TTA} is the second-order decay rate of TTA and $\alpha(\lambda)$ is the absorption coefficient of the sensitizer at the excitation wavelength. Thus, for systems with the same sensitizer and similar Φ_{TET}, the value of I_{th} provides a reliable evaluation for analyzing the triplet state of annihilators. Moreover, k_A^T [An] = k_{TTA}[An]^2 at I_{th}, thus I_{th} marks the transition between these regimes and is a useful parameter to compare different upconversion systems. Triplet state equilibrium between PtTNP and the annihilator (An-3−An-5) minimizes the loss of excited state energy during the TET process to maintain a high T_1 state for the annihilator so that the non-radiative transition of the annihilator is suppressed to give a small I_{th}. However, the triplet state (1.16 eV) is too low for An-6, leading to a rapid non-radiative transition from the triplet state to the ground state, so that a high concentration of triplet annihilator can only be obtained under high power excitation intensity to make k_A^T [An] = k_{TTA}[An]^2.

Measurement of power-dependent upconversion emission[5]**.** The upconversion fluorescence lifetime was measured on an FLS1000 spectrometer from Edinburgh Instruments equipped with a nanosecond pulsed diode laser (635 nm, 690 nm) set-up. The instrument response function (IRF) was collected by using a scatterer with fresh milk. The concentrations of PdTPBP and PtTNP are 10 μM and 5 μM, respectively. The concentration of An-1−An-6 is 500 μM in argon-saturated toluene.

Determination of triplet excited state lifetimes and TTA efficiency (β) of annihilators[5]. The TTA efficiency (β) measurements were performed under pulsed excitation generated by modulating a continuous-wave laser with a pulse-width controller. Using time-resolved emission measurements, the triplet lifetimes of the annihilators (An-1−An-6) were determined. For data fitting, equation 11 was utilized to account for the first- and second-order decays:

$$I(t) \propto \left([^3A^*]_0 \frac{1-\beta}{\exp\left(\frac{t}{\tau_T}\right)-\beta}\right)^n \quad \text{(11)}$$

where I(t) is the emission intensity, $[^3A^*]_0$ is the initial concentration of the annihilator triplet, β is a dimensionless parameter between 0 and 1 indicating the fraction of the initial decay dominated by the second-order channels (β = 1 implies that all initial decay is of the second order), t is time, τ_T is the annihilator triplet lifetime, and n is a dimensionless parameter describing the emission power versus triplet concentration. The analytical expression for β is given by equation 12:

$$\beta = \frac{2k_{TTA}[^3A^*]_0}{k_T + 2k_{TTA}[^3A^*]_0} \quad \text{(12)}$$

where k_{TTA} and k_T ($k_T = 1/\tau_T$) are the second-order TTA decay and first-order intrinsic triplet decay rate constants, respectively. In the case of annihilators, the UC emission resulting from second-order TTA events is measured. In this situation, n = 2.

The initial decay through the second-order channel is partially determined by the excitation intensity, as this governs the initial concentration of excited triplets. Consequently, emission measurements are performed at a variety of intensities at the 690 nm excitation pump, and the kinetics are then fitted globally with equation 1 using a shared τ_T, while β is fitted individually to each trajectory.

Electrochemical measurements of An-1−An-6[9]. Cyclic voltammetry experiments were carried out with an electrochem luminescence analyzer instrument (LanLiKe (Tianjin) Chemcial&Electronic High-Tech Co. Ltd.) using a single-chamber electrolyzer containing a glassy carbon working electrode, a platinum wire counter electrode, and a silver-silver nitrate electrode reference electrode. The sample (1 mM) dissolve in CH_2Cl_2 with 0.1 M tetrabutylammonium hexafluorophosphate (n-Bu_4NPF_6, TCI, electrochemical grade) as a supporting electrolyte. The scan rate is 100 mV/s. The ferrocenium/ferrocene couple (Fc^+/Fc, 0.42 V vs. SCE) was used as the internal standard. The sample was degassed with N_2 for 15 minutes before measurement and then kept under N_2 gas flow during the measurement.

Calculation of the standard oxidation/reduction potential for the DPPs[9]. If the DPP presented reversible redox behavior, the standard oxidation (E_{ox}) / reduction (E_{red}) potentials were obtained from CV as the half sum of anodic (E_{pa}) and cathodic (E_{pc}) peak potentials. If the DPP sample exhibited irreversible redox behavior, E_{ox} and E_{red} were taken from the peak potentials.

Gibbs free energy (ΔG_{ET}) calculation[10]. The electron transfer Gibbs free energy (ΔG_{ET}) from the An-3 excited state to the initiator EBP was calculated with the listing equation 13 from Rehm-Weller analysis.[10]

$$\Delta G_{ET} = E_{OX} - E_{red} - E^* \quad (13)$$

E_{ox} is the oxidation potential of electron donor (An-3), whereas E_{red} is the reduction potential of an electron acceptor, EBP (–0.74 V vs. SCE).[11] E^* represents the energy of the excited state, which for An-3 is 1.30 (T_1) and 2.43 (S_1) eV, respectively.

Blue light-driven polymerization. The crosslinker of ethylene glycol dimethacrylate (DEGMA, 400 μL), the monomer of methyl methacrylate (MMA, 3.6 mL), the initiator of ethyl α-bromophenylacetate (EBP, 50 μL) and 500 μM An-3 were mixed in a dry 25 mL single-mouth flask. The mixture was degassed for 15 minutes to remove the oxygen and then irradiated with blue light (445 nm, 50 mW/cm^2). After one hour, the formation of a solid hydrogel was observed, which confirmed that An-3 is capable of catalyzing the atom transfer radical polymerization (ATRP) reaction under blue light illumination.

Long-wavelength-light-driven polymerization via TTA-UC. In a dry 25 mL single-mouth flask, the crosslinker ethylene glycol dimethacrylate (DEGMA, 400 μL), the monomer methyl methacrylate (MMA, 3.6 mL), the initiator ethyl α-bromophenylacetate (EBP, 50 μL), and the TTA-UC pair of PtTNP (10 μM) and An-3 (500 μM) were mixed. The mixture was degassed for 15 minutes to remove the oxygen and then irradiated by 690 nm light (50 mW/cm^2). After one hour, a free-standing hydrogel was detected, which verified the successful photopolymerization via TTA-UC.

Highly spatial-confined photopolymerization via TTA-UC. In a 2 mL cuvette coupled with a silicone gasket, the crosslinker ethylene glycol dimethacrylate (DEGMA, 1 mL), the monomer trimethylolpropane ethoxylate triacrylate (1.0 mL), the initiator ethyl α-bromophenylacetate (EBP, 20 μL), and the TTA-UC pair of PtTNP (5 μM) and An-3 (500 μM) were mixed. The mixture was degassed for 15 minutes to remove the oxygen before being exposed to long-wavelength-light (721 nm, 5.7 W/cm^2) through 40× objective focusing. After 10 min, a tiny polymer droplet (~1.0 mm) was observed at the focus point, which verified the successful operation of highly spatially confined photopolymerization. Moreover, for the reference group without EBP, we just observed TTA-UC emission and no polymer formation.

Supplementary Tables

Table S1. Comparison between representative long-wavelength-excited TTA-UC systems and this work.

Sensitizer/annihilator	Φ_{UC} (%)	Reference
PtTNP/perylene derivative	1.0	*Nature* **565**, 343-346 (2019).
PtTNP/anthracene derivative	–	*Adv. Funct. Mater.* **31**, 2010907, (2021).
PtTNP/perylene derivative	7.1	*J. Am. Chem. Soc.* **142**, 18460-18470 (2020).
PdPc/rubrene	3.3± 0.2	*Chem. Commun.* **49**, 7406-7408 (2013).
PtTNP/tetracene derivative	2	*Angew. Chem. Int. Ed.* **46**, 7693-7696 (2007).
PdPc/tetracene derivative	2.5	*J. Am. Chem. Soc.* **142**, 19917-19925 (2020).
PdPc/Furan-DPP	1.6	*J. Am. Chem. Soc.* **141**, 3777-3781 (2019).
Ru complexes/PDI	3.0± 0.25	*J. Am. Chem. Soc.* **132**, 14203-14211 (2010).
$Os(bptpy)_2{}^{2+}$/ perylene derivative	1.4	*J. Mater. Chem. C* **5**, 5063-5067 (2017)
$Os(tpy)_2{}^{2+}$/anthracene derivative	5.5	*Chem. Commun.* **56**, 7017-7020 (2020)
$Os(peptpy)_2{}^{2+}$/ perylene derivative	3	*Angew. Chem. Int. Ed.* **58**, 17827-17833 (2019)
$PtAg_{24}$/perylene	1.1	*Angew. Chem. Int. Ed.* **60**, 2822-2827 (2021)
$PtAg_{24}$/anthracene derivative	1.2	*Angew. Chem. Int. Ed.* **60**, 2822-2827 (2021)
BNS/perylene	1.5	*Angew. Chem. Int. Ed.* **62,** e202303093 (2023).
BNS/anthracene derivative	2.9	*Angew. Chem. Int. Ed.* **62,** e202303093 (2023).
PdTPBP/An-1	**13.2**	**This work**
PdTPBP/An-2	**4.1**	**This work**
PtTNP/An-3	**8.6**	**This work**
PtTNP/An-4	**4.3**	**This work**
PtTNP/An-5	**4.8**	**This work**

Upconversion quantum yield (Φ_{UC}, 50%)

Table S2. Photophysical properties of annihilators. [a]

	λ_{abs} [b]	ε [c]	λ_{em} [d]	Φ_f [e]	Φ_f [f]	τ_f (ns) [g]	S-S [h]	S_1 [i]
An-1	439	0.17	484	1.0	0.95	5.79	45	2.66
An-2	445	0.15	546	0.63	0.61	4.15	101	2.51
An-3	473	0.16	533	1.0	0.94	6.17	60	2.43
An-4	486	0.22	559	1.0	0.90	4.87	73	2.34
An-5	510	0.22	530	0.95	0.72	5.70	20	2.38
An-6	552	0.33	567	1.0	0.64	5.67	15	2.21

[a] In toluene (10 μM). [b] Maximum absorbing wavelength (nm). [c] Molar absorption coefficient (10^5 M^{-1} cm^{-1}). [d] Maximum fluorescence wavelength (nm). [e] Absolute fluorescence quantum yield at 10 μM. [f] Absolute fluorescence quantum yield at 1.0 mM. [g] Fluorescence lifetime at 10 μM. [h] Stokes-shift (nm). [i] S_1 is obtained by calculating the crossing point of the absorption and fluorescence emission spectra (eV).

Table S3. The phosphorescence lifetime of PtTNP with different An-1 concentration [a]

An-1(μM)	τ_p (μs)	(%)
0	14.56	100
20	14.52	100
40	14.38	100
60	14.30	100
80	14.48	100
100	14.17	100

[a] in argon saturated toluene, PtTNP 5 μM, λ_{ex} = 690 nm.

Table S4. The phosphorescence lifetime of PtTNP with different An-2 concentration [a]

An-2 (μM)	τ_p^1 (μs)	(%)	τ_p^2 (μs)	(%)
0	14.65	100		
20	14.83	100		
40	14.67	98.41	213.5	1.59
60	14.25	97.09	91.4	2.91
80	14.33	96.08	74.84	3.92
100	13.21	90.04	76.83	9.96

[a] in argon saturated toluene, PtTNP 5 μM, λ_{ex} = 690 nm.

Table S5. The phosphorescence lifetime of PtTNP with different An-3 concentration [a]

An-3 (μM)	τ_p^1 (μs)	(%)	τ_p^2 (μs)	(%)
0	14.55	100		
20	10.05	94.39	102.9	5.61
40	7.80	77.43	107.5	22.57
60	6.33	70.83	109.3	29.17
80	5.25	66.8	111.7	33.2
100	4.67	63.16	115.5	36.84

[a] in argon saturated toluene, PtTNP 5 μM, λ_{ex} = 690 nm.

Table S6. The phosphorescence lifetime of PtTNP with different An-4 concentration [a]

An-4 (μM)	τ_p^1 (μs)	(%)	τ_p^2 (μs)	(%)
0	14.49	100		
20	11.63	97.94	63.44	2.04
40	9.69	98.06	49.92	1.94
60	8.44	96.25	55.10	3.75
80	7.39	95.07	77.66	4.93
100	6.41	95.11	74.32	4.89

[a] in argon saturated toluene, PtTNP 5 μM, λ_{ex} = 690 nm.

Table S7. The phosphorescence lifetime of PtTNP with different An-5 concentration [a]

An-5 (μM)	τ_p^1 (μs)	(%)	τ_p^2 (μs)	(%)
0	14.40	100	-	-
20	9.67	97.03	78.99	2.93
40	7.34	93.54	85.16	6.64
60	5.47	94.14	83.41	5.86
80	4.64	94.09	80.0	5.91
100	3.77	94.07	86.51	5.93

[a] in argon saturated toluene, PtTNP 5 μM, λ_{ex} = 690 nm.

Table S8. The phosphorescence lifetime of PtTNP with different An-6 concentration [a]

An-6 (μM)	τ_p (μs)	(%)
0	14.50	100
20	8.61	100
40	6.07	100
60	4.76	100
80	3.97	100
100	3.43	100

[a] in argon saturated toluene, PtTNP 5 μM, λ_{ex} = 690 nm.

Table S9. Density functional theory (DFT) calculation for annihilators. The electronic excitation energies (eV) and corresponding oscillator strengths (*f*), main conFigureurations, and CI coefficients of the low-lying electronic excited states of compound An-1−An-6 are listed.[a]

		Electronic transition[b]	Energy[c]	*f* [d]	CI[e]	Composition[f]
An-1	Singlet	$S_0 \to S_1$	2.8221 eV /439.33 nm	0.4254	0.70440	H→L
		$S_0 \to S_2$	3.3997 eV / 364.69 nm	0.0002	0.69092	H-1→L
	Triplet	$S_0 \to T_1$	1.3807 eV / 897.97 nm	0.0000[g]	0.71198	H→L
		$S_0 \to T_2$	3.0223 eV / 410.23 nm	0.0000[g]	0.57813	H-1→L
An-2	Singlet	$S_0 \to S_1$	2.5770 eV / 481.11 nm	0.4764	0.69913	H→L
		$S_0 \to S_2$	3.1900 eV / 388.67 nm	0.0002	0.63080	H-1→L
	Triplet	$S_0 \to T_1$	1.3138 eV / 943.67 nm	0.0000[g]	0.69552	H→L
		$S_0 \to T_2$	2.4730 eV / 501.35 nm	0.0000[g]	0.44971	H-1→L
An-3	Singlet	$S_0 \to S_1$	2.5511 eV / 486.01 nm	0.5119	0.70808	H→L
		$S_0 \to S_2$	3.2990 eV / 375.82 nm	0.0000	0.69945	H-1→L
	Triplet	$S_0 \to T_1$	1.2188 eV / 1017.25 nm	0.0000[g]	0.71448	H→L
		$S_0 \to T_2$	2.8631 eV / 433.04 nm	0.0000[g]	0.47389	H→L+1
An-4	Singlet	$S_0 \to S_1$	2.3655 eV / 524.13 nm	0.6841	0.70756	H→L
		$S_0 \to S_2$	3.1088 eV / 398.81 nm	0.0023	0.63367	H-1→L
	Triplet	$S_0 \to T_1$	1.1659 eV / 1063.39 nm	0.0000[g]	0.70566	H→L
		$S_0 \to T_2$	2.4180 eV / 512.75 nm	0.0000[g]	0.42709	H-1→L
An-5	Singlet	$S_0 \to S_1$	2.5216 eV / 491.70 nm	0.5870	0.70943	H→L
		$S_0 \to S_2$	3.2831 eV / 377.64 nm	0.0000	0.66004	H-1→L
	Triplet	$S_0 \to T_1$	1.1381 eV / 1089.43 nm	0.0000[g]	0.71846	H→L
		$S_0 \to T_2$	2.7762 eV / 446.59 nm	0.0000[g]	0.49990	H→L+1
An-6	Singlet	$S_0 \to S_1$	2.3357 eV / 530.83 nm	0.5958	0.71019	H→L
		$S_0 \to S_2$	3.2564 eV / 380.74 nm	0.0000	0.68643	H-1→L
	Triplet	$S_0 \to T_1$	1.0579 eV / 1171.95 nm	0.0000[g]	0.71803	H→L
		$S_0 \to T_2$	2.5438 eV / 487.39 nm	0.0000[g]	0.59037	H→L+1

[a] The electronic transitions were calculated by TD-DFT//B3LYP/6-31G(d), based on the DFT//B3LYP/6-31G(d)-optimized ground state and excited state geometries. [b] Based on the DFT//B3LYP/6-31G(d)-optimized ground state geometries. [c] Only the selected low-lying excited states are presented. [d] Oscillator strengths. [e] CI coefficients are in absolute values. [f] TD-DFT//B3LYP/6-31G(d)-optimized excited state geometries. [g] No spin−orbital coupling effect was considered; thus, the *f* values are zero.

Table S10. A summary of the energy levels for singlet/triplet excited states of An-1−An-6.

	An-1	An-2	An-3	An-4	An-5	An-6
S_1 (eV)	2.66	2.51	2.43	2.34	2.38	2.21
T_1 (eV)	1.53	1.48	1.41	1.40	1.40	1.16
$2T_1>S_1$ [a]	Yes	Yes	Yes	Yes	Yes	Yes

[a] According to the energetic requirements of TTA-UC ($^3[Sen]^* > {}^3[An]^*$; $2 \times {}^3[An]^* > {}^1[An]^*$).

Table S11. TTA-UC related parameters. Sensitizer/annihilator = 5/500 μM in Ar-saturated toluene.

TTA pair	Φ_{TET} [a]	Φ_f [b]	Φ_{UC} [c]	Φ_{UCg} [d]	$f\times\Phi_{TTA}$	Φ_{TTA} (β) [e]	f [f]
PdTPBP/An-1	97.2	72.6	13.2	18.2	0.37	0.90	0.42
PdTPBP/An-2	98.4	41.8	4.1	9.8	0.20	0.82	0.24
PtTNP/An-3	80.1	76.0	8.6	11.3	0.28	0.67	0.42
PtTNP/An-4	85.6	60.6	4.3	7.1	0.17	0.56	0.30
PtTNP/An-5	93.2	55.6	4.8	8.6	0.19	0.70	0.26
PtTNP/An-6	94.3	48.1	1.5	3.1	0.07	0.27	0.25

[a] Triplet energy transfer efficiency (%); [b] Fluorescence quantum yield (%). [c] Upconversion quantum yield (%).[d] Reabsorption-corrected internal upconversion quantum yield (%) [e] TTA efficiency (β), excitation intensity of 1.3 W/cm^2.[f] The spin statistical factor (*f*).

Table S12. Redox potentials of An-1−An-6. [a]

	An-1	An-2	An-3	An-4	An-5	An-6
E_{ox} (V)	0.91	0.91, 1.17	0.87, 1.19	0.83, 1.20	0.82, 1.09	0.82, 1.09
E_{red} (V)	–	–	–	-1.62	–	–

[a] Cyclic voltammetry in N_2 saturated DCM with 0.10 M Bu_4NPF_6 as supporting electrolyte. The counter electrode is Pt electrode, the working electrode is glassy carbon electrode, and the Ag/$AgNO_3$ couple is the reference electrode.

Table S13. Gibbs free energies for electron transfer from the excited states of An-3 to the initiator of EBP. [a]

	E_{ox} (V)	S_1 (eV)	T_1 (eV)
An-3	+0.84	2.46	1.30
ΔG_{ET} (V)	-	-0.88[a]	+0.28[a]

[a] $E_{(EBP/EBP^{\bullet -})}$ = –0.74 V vs SCE.[17]

Table S14. Photopolymerization under various conditions.[a]

Entry	Condition	Gel formation
1	PtTNP/An-3 + *hv* (690 nm)	YES
2	PtTNP/An-3	NO
3	An-3 + *hv* (690 nm)	NO
4	PtTNP + *hv* (690 nm)	NO
5	An-3 + *hv* (445 nm)	YES

[a] 3.6 mL MMA, 0.4 mL ethylene glycol dimethacrylate, EBP (50 μL), An-3 (500 μM), PtTNP (10.0 μM).

Supplementary Figures

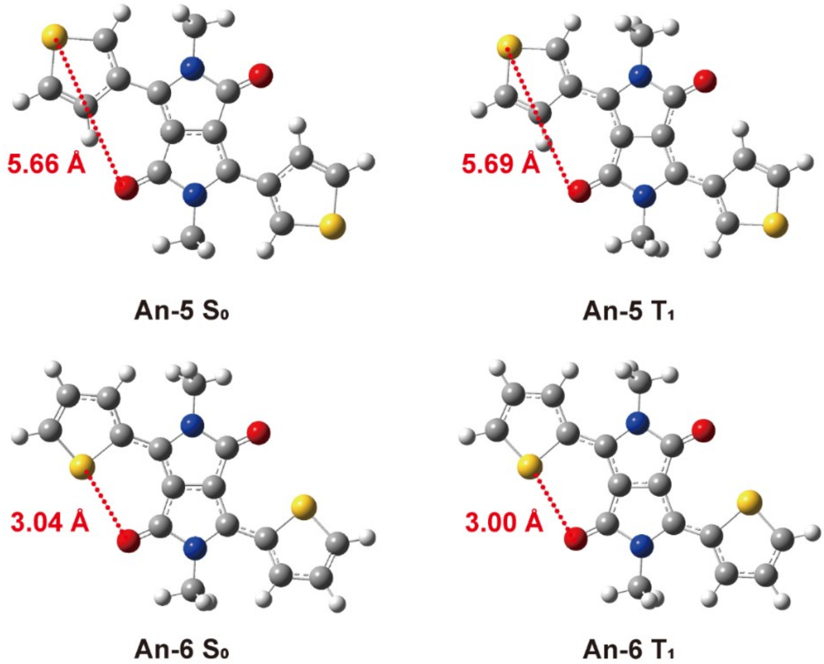


Figure S1. Optimized geometric conformations of S_o and T_1 for An-5 and An-6 in toluene. Gaussian 16 was used for calculation at the DFT-B3LYP/6-31G(d) level in toluene.

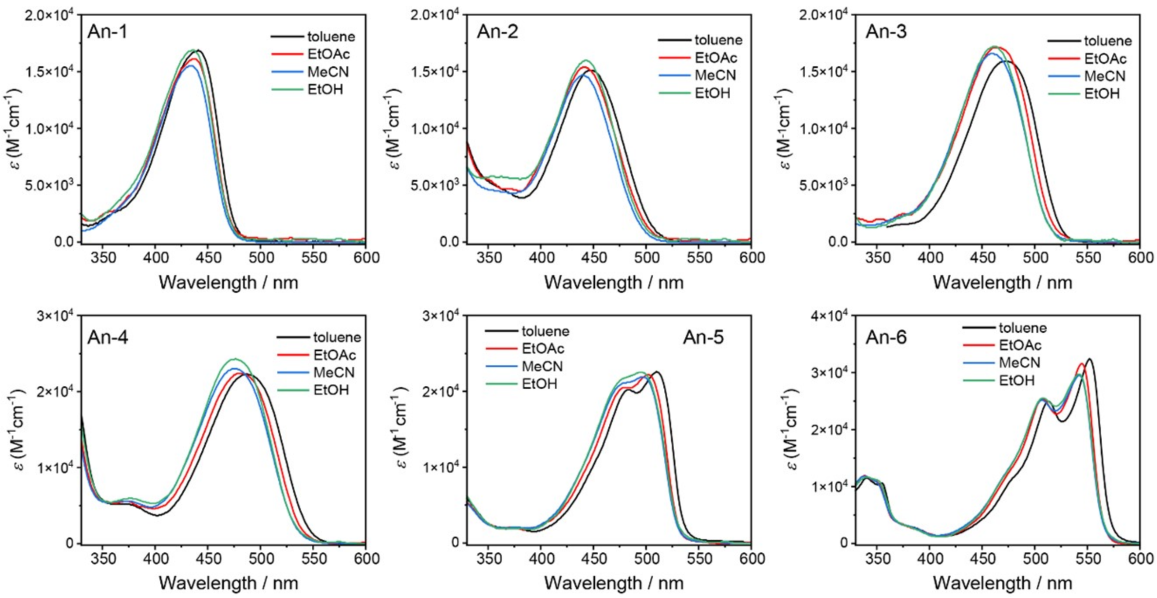


Figure S2. UV-vis absorption spectra of An-1–An-6 in different solvents (toluene, EtOAc, MeCN, and EtOH), 10 μM.

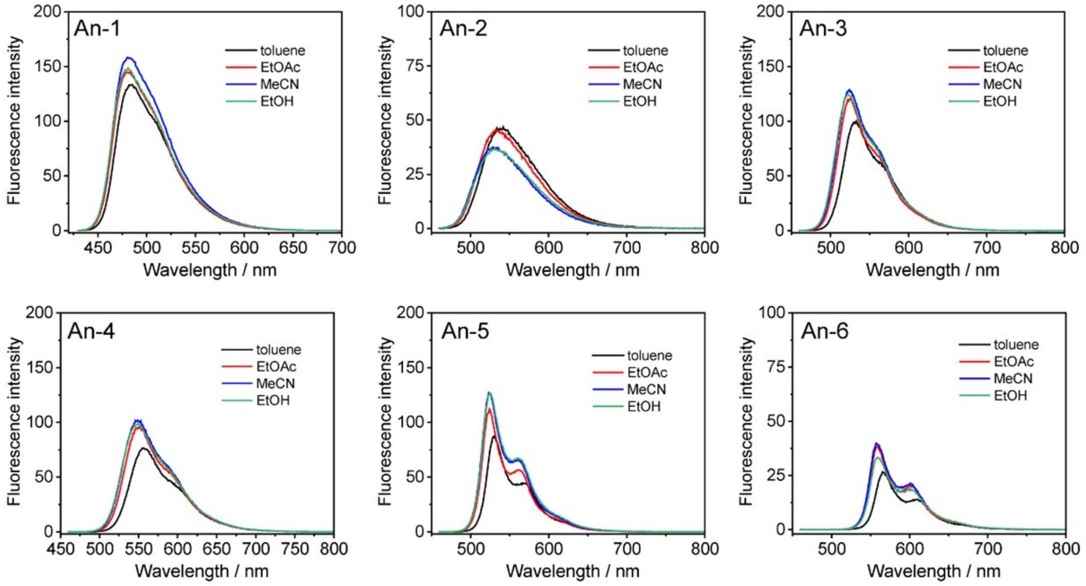


Figure S3. Fluorescence emission spectra of An-1−An-6 in different solvents (toluene, EtOAc, MeCN, and EtOH), 10 μM. An-1 (λ_{ex} = 420 nm), An-2−An-6 (λ_{ex} = 460 nm).

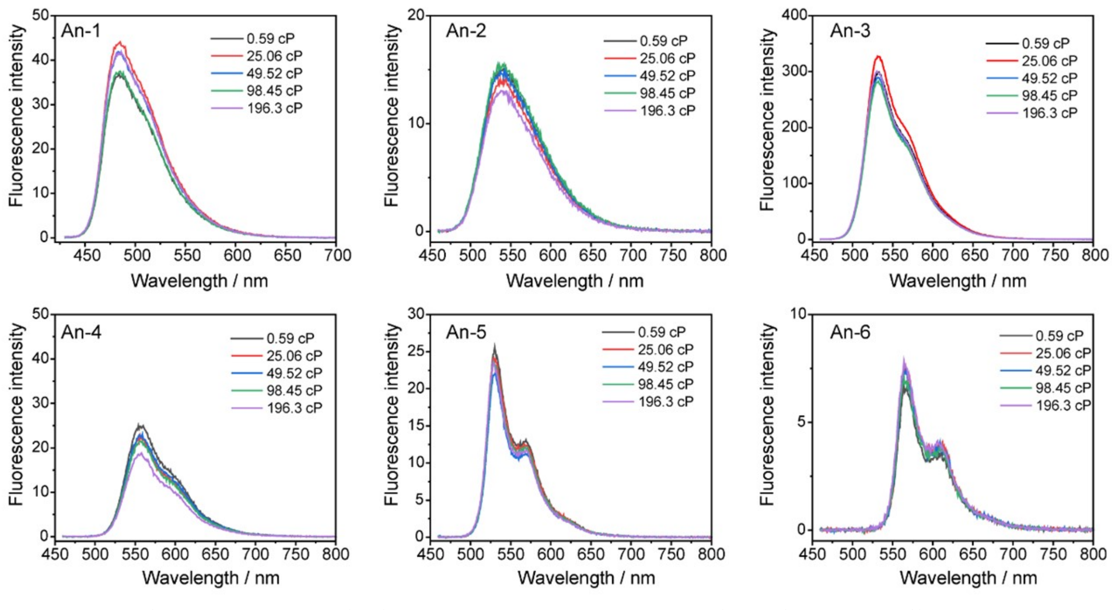


Figure S4. Fluorescence emission spectra of An-1−An-6 in solvents of different viscosity (different proportions of toluene and PDMS), 10 μM, An-1 (λ_{ex} = 420 nm), An-2−An-6 (λ_{ex} = 460 nm).

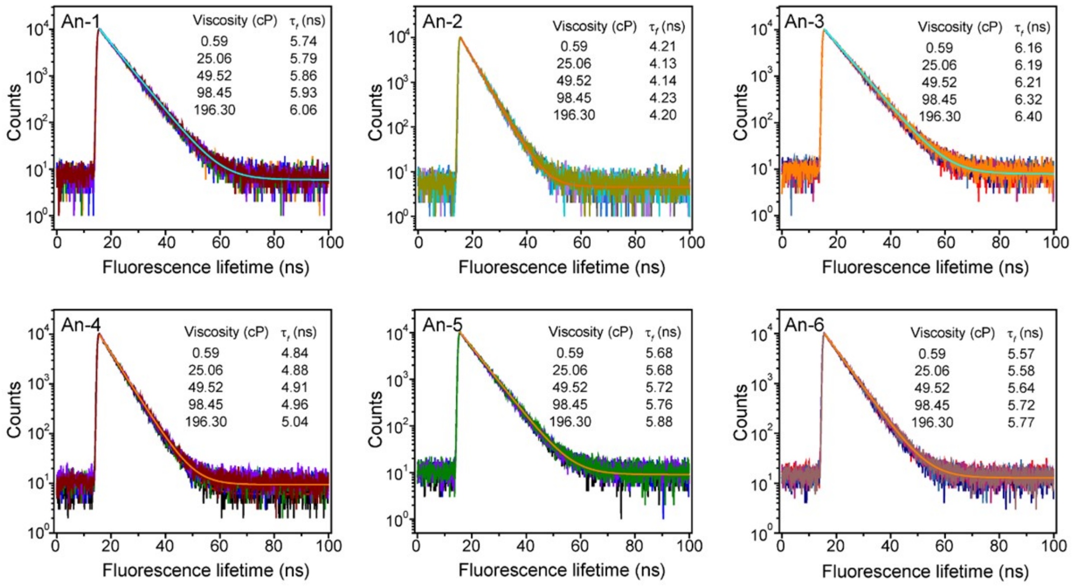


Figure S5. Fluorescence lifetime decay traces of An-1−An-6 in solvents of different viscosity (different proportions of toluene and PDMS), 10 μM, 405 nm picosecond pulsed laser.

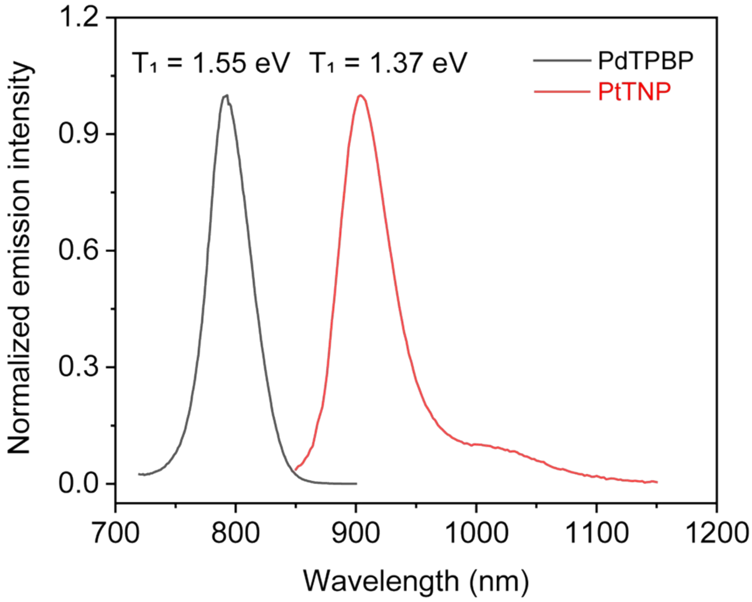


Figure S6. Normalized phosphorescence emission spectra of PtTNP and PdTPBP in argon-saturated toluene. PdTPBP (λ_{ex} = 635 nm), PtTNP (λ_{ex} = 690 nm).

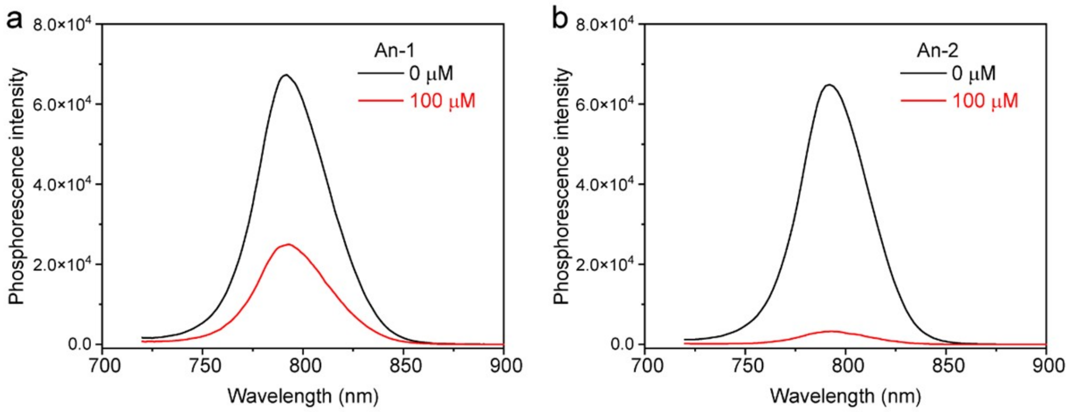


Figure S7. Phosphorescence spectra of PdTPBP (10 μM) with or without (a) An-1 and (b) An-2, λ_{ex} = 635 nm, in argon-saturated toluene.

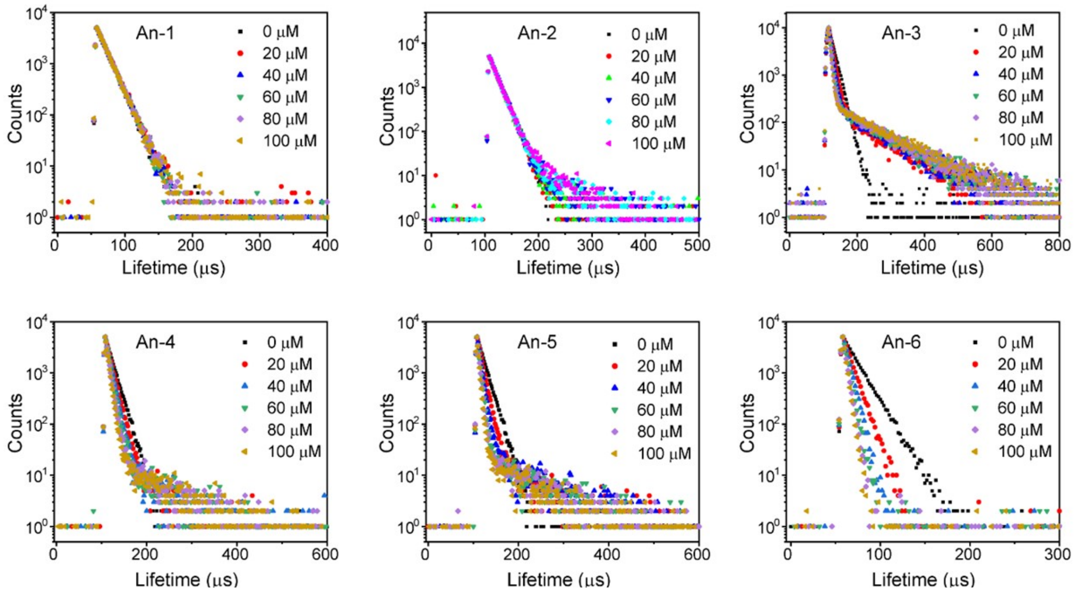


Figure S8. Phosphorescence lifetime decay traces of PtTNP (5 μM) at different concentrations of annihilators (An-1–An-6). λ_{ex} = 690 nm pulsed laser, in argon-saturated toluene.

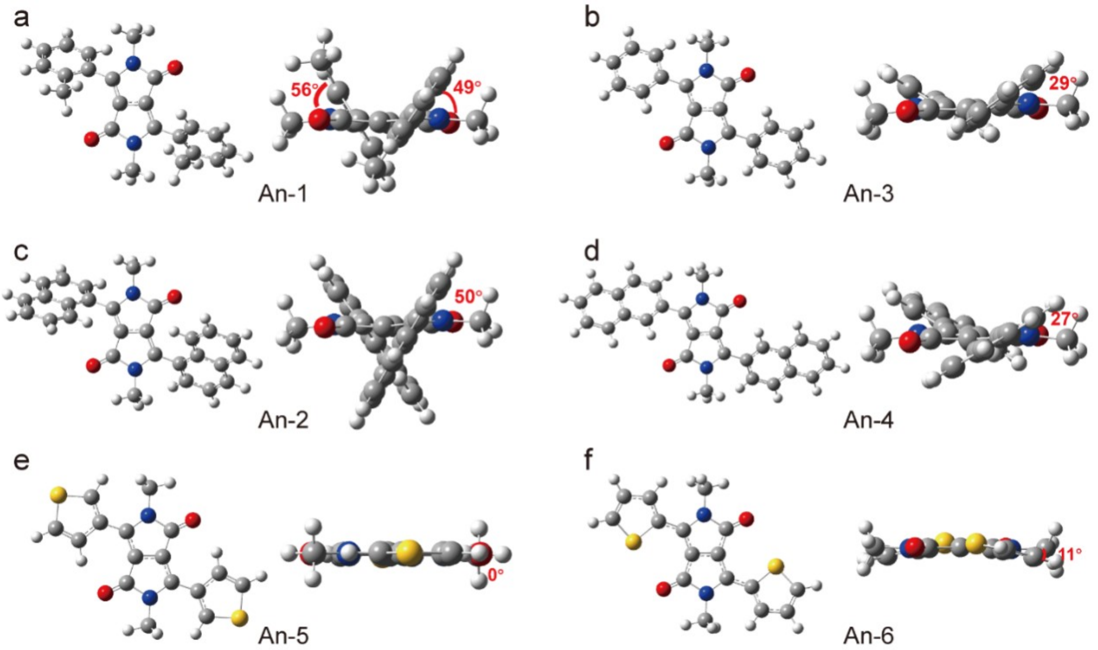


Figure S9. The calculated dihedral angle and ground state configuration of An-1−An-6. Gaussian 16 was used for calculation at the DFT-B3LYP/6-31G(d) level in toluene.

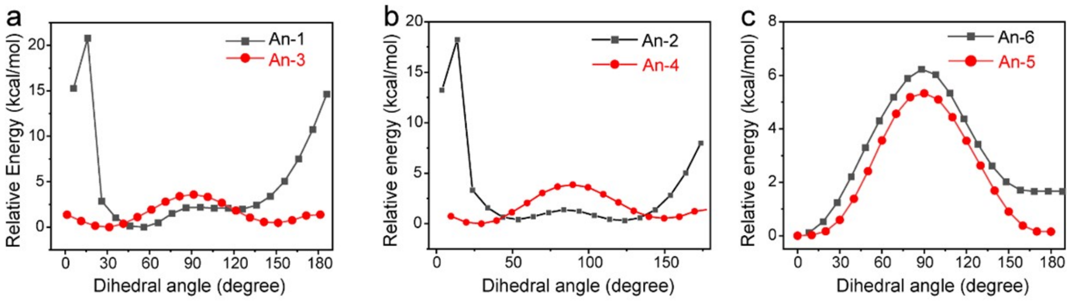


Figure S10. The ground state potential energy curves of An-1−An-6 as a function of the dihedral angle between the cores and substituents (step: 10°). (a) An-1 and An-3; (b) An-2 and An-4, and (c) An-5 and An-6. All the calculations were performed at the B3LYP/6-31G (d) level in toluene with Gaussian 16.

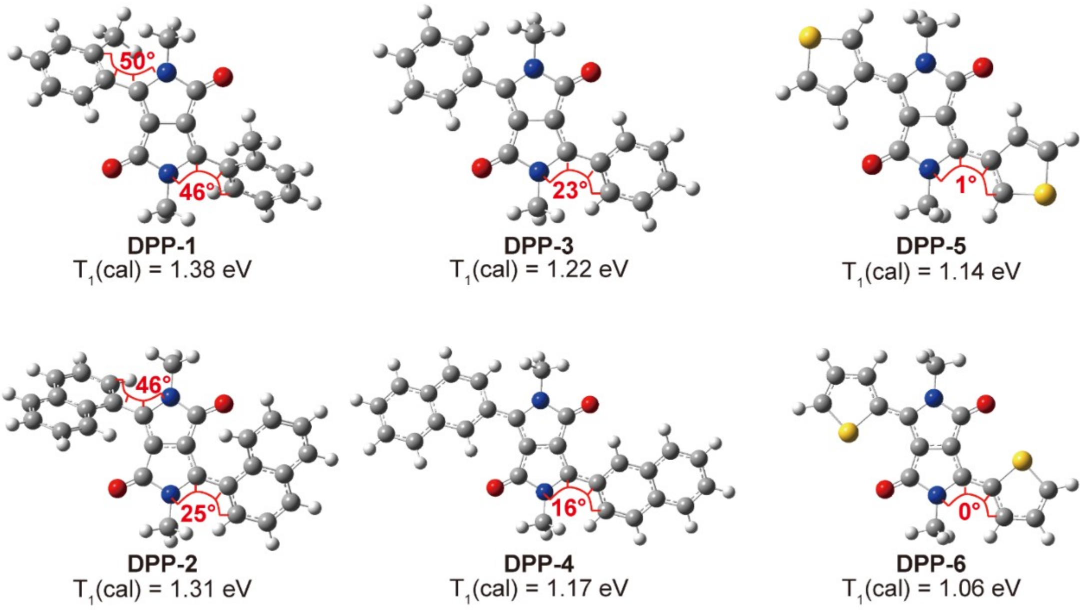


Figure S11. The optimized T_1 state configuration of An-1−An-6. Gaussian 16 was used for calculation at the DFT-B3LYP/6-31G(d) level in toluene.

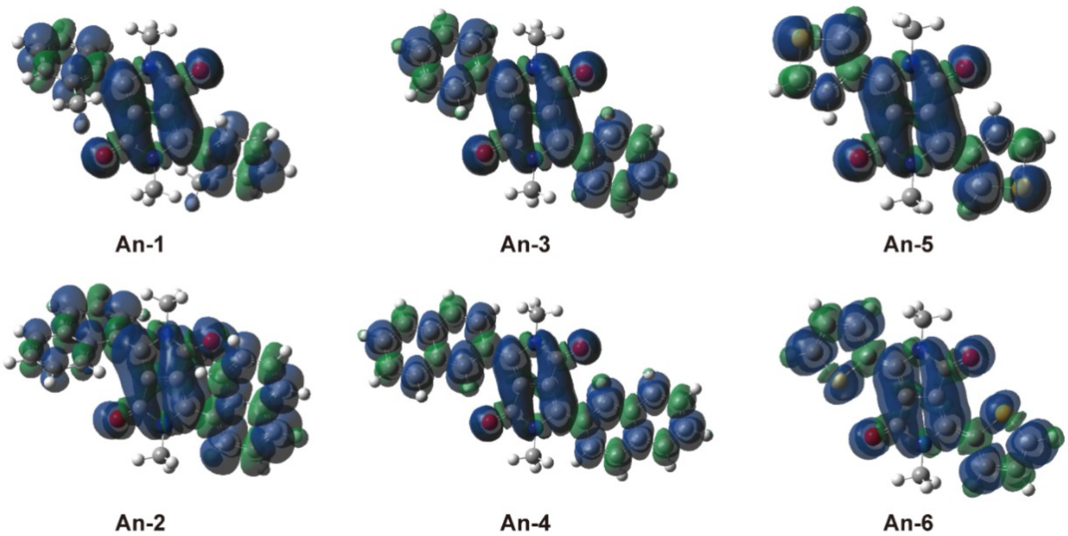


Figure S12. Triplet spin density surfaces of the triplet states of An-1–An-6 in toluene at the optimized triplet state geometries (isovalue = 0.002). Calculated with Gaussian 16 based on the DFT-B3LYP/6-31G(d) level.

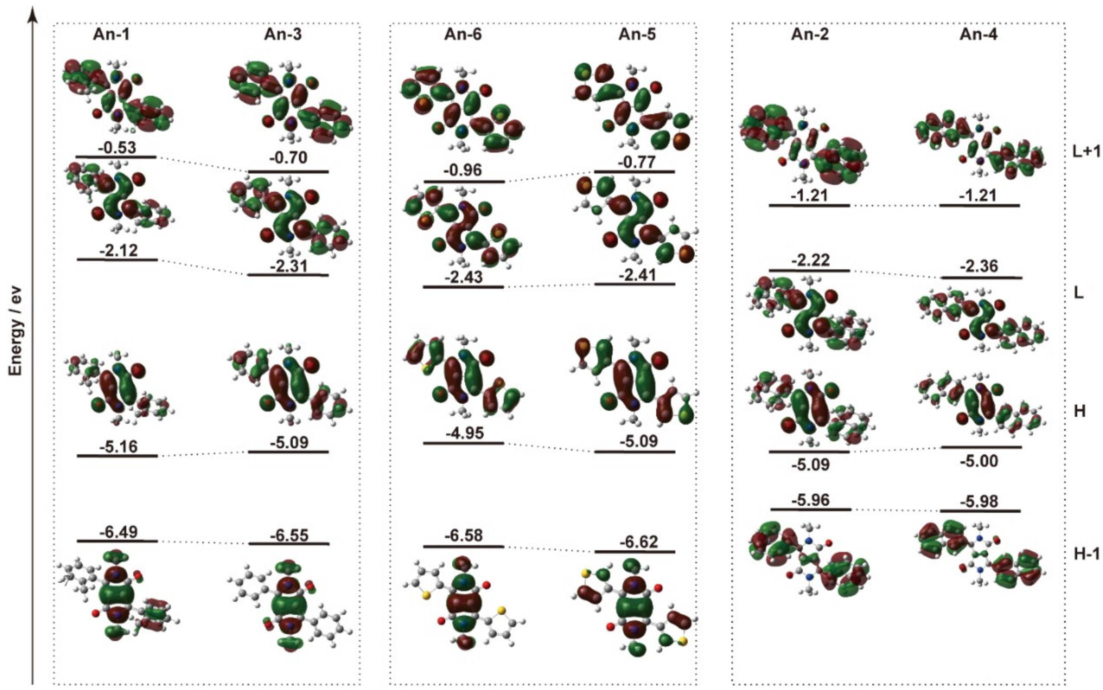


Figure S13. Electron density maps of the frontier molecular orbitals of An-1−An-6. Based on ground state optimized geometry by the DFT calculations at the B3LYP/6-31G(d) with Gaussian 16.

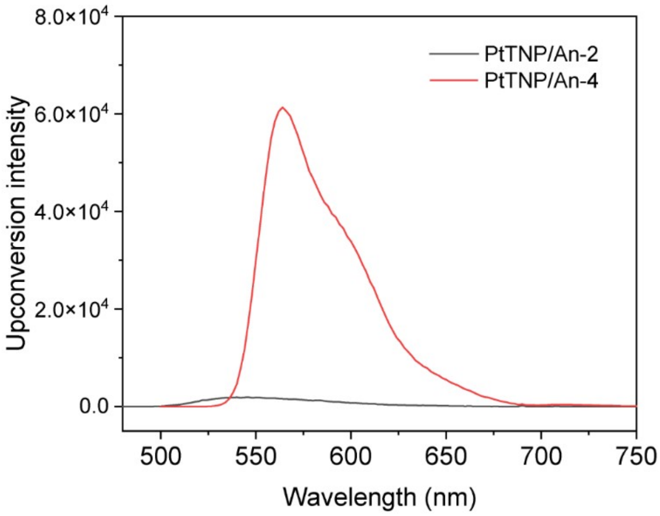


Figure S14. TTA-UC spectra of PtTNP/An-2 and PtTNP/An-4, in toluene, λ_{ex} = 690 nm.

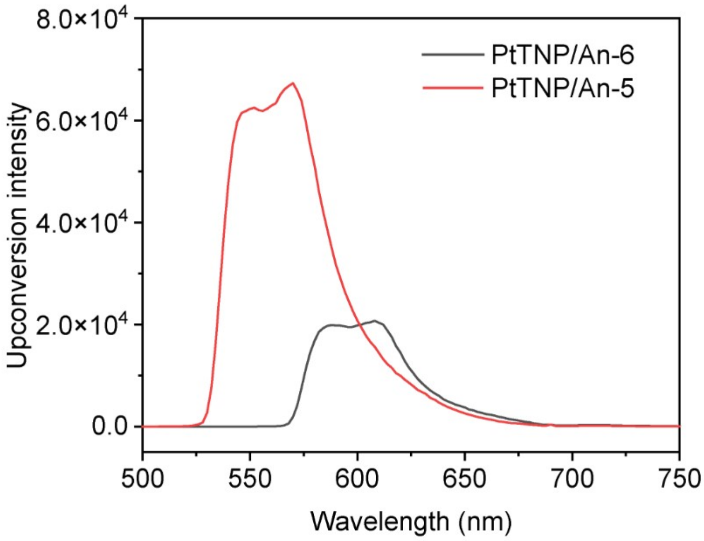


Figure S15. TTA-UC spectra of PtTNP/An-5 and PtTNP/An-6, in toluene, λ_{ex} = 690 nm.

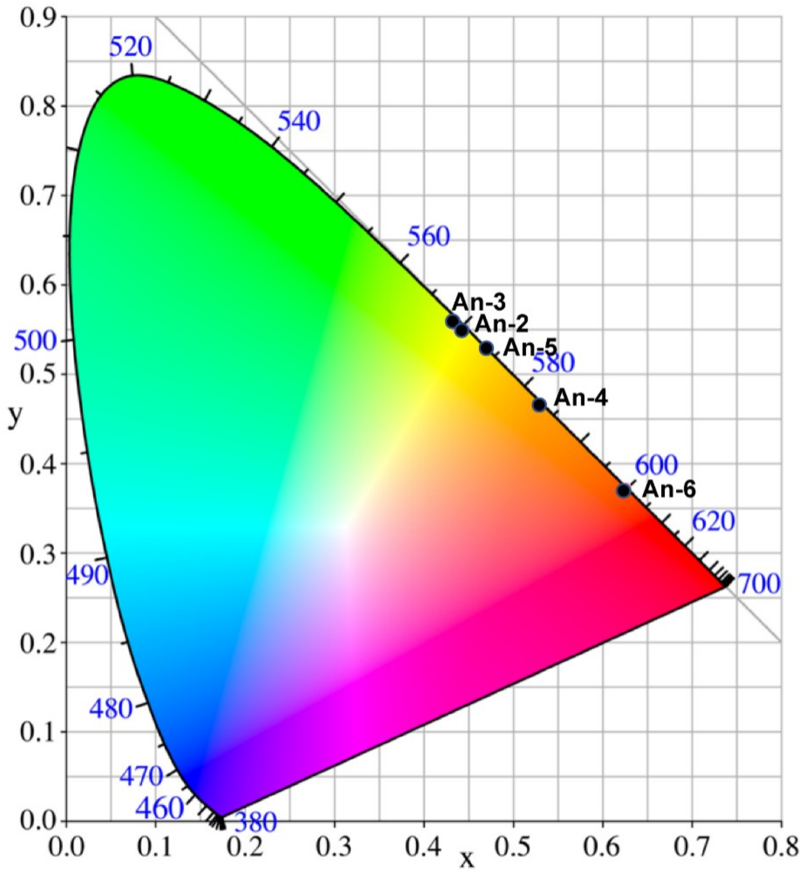


Figure S16. CIE diagram representing the adjustable upconversion emission colors for An-2−An-6 in coupling with PtTNP.

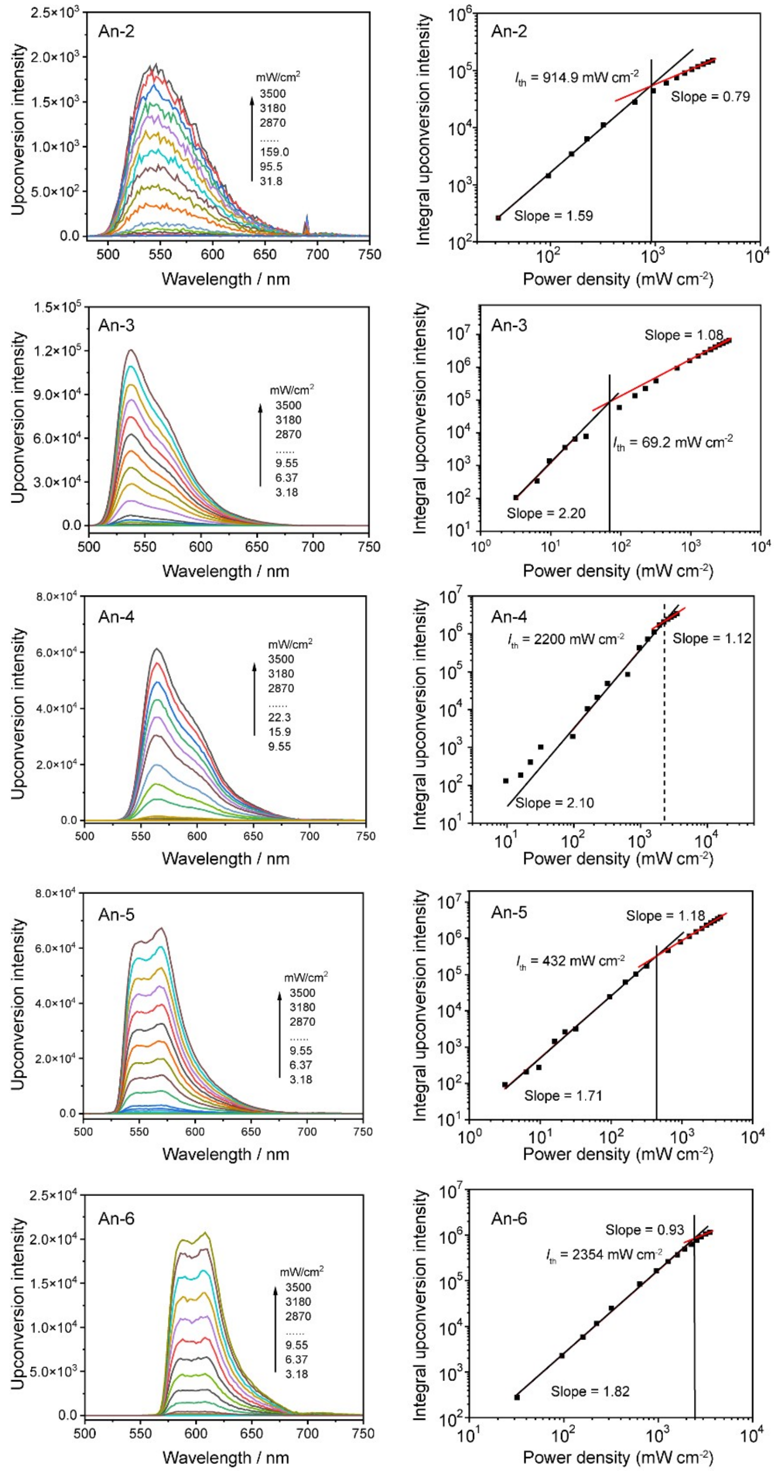


Figure S17. Upconversion emission spectra of the TTA-UC system under argon with various excitation intensities (λ_{ex} = 690 nm), PtTNP (5 μM), annihilator (500 μM) in toluene.

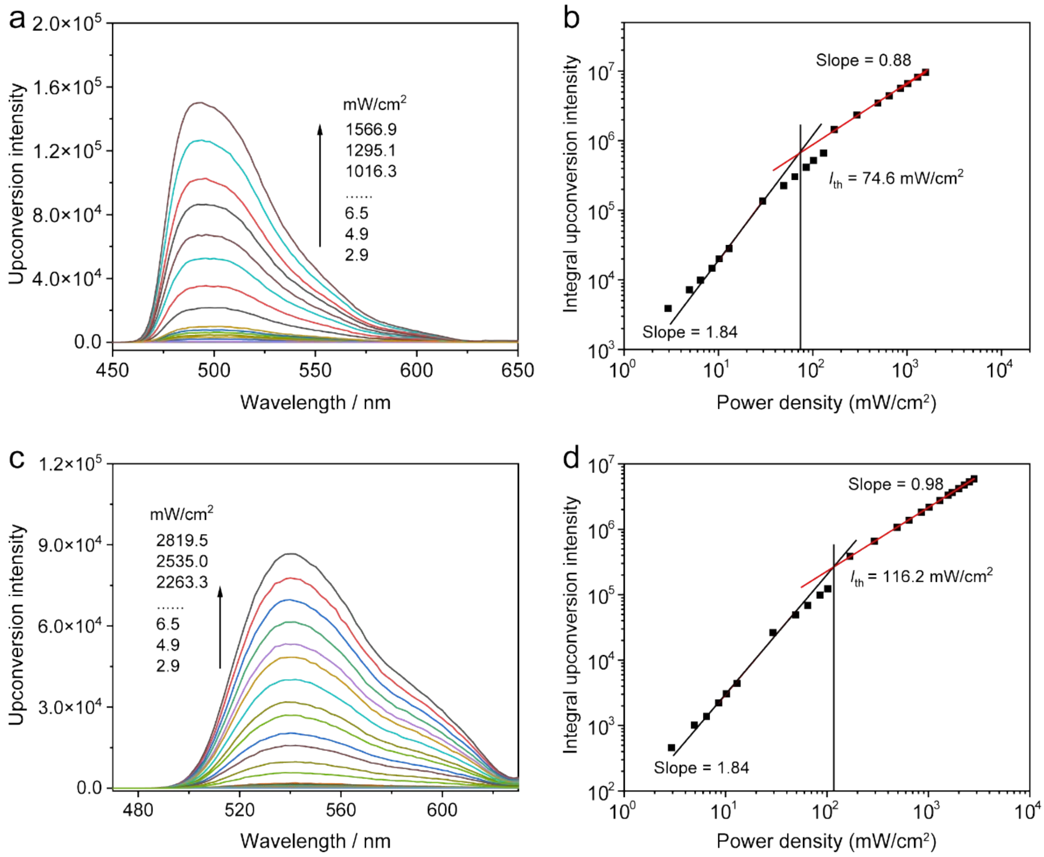


Figure S18. (a) Upconversion emission spectra of the TTA-UC system of PdTPBP (10 μM) and An-1 (500 μM) under argon with various excitation intensities (λ_{ex} = 635 nm); (b) Dependence of the TTA-UC intensity of PdTPBP/An-1 on the incident power density. (c) Upconversion emission spectra of the TTA-UC system of PdTPBP (10 μM) and An-2 (500 μM) under argon with various excitation intensities (λ_{ex} = 635 nm); (b) Dependence of the TTA-UC intensity of PdTPBP/An-2 on the incident power density.

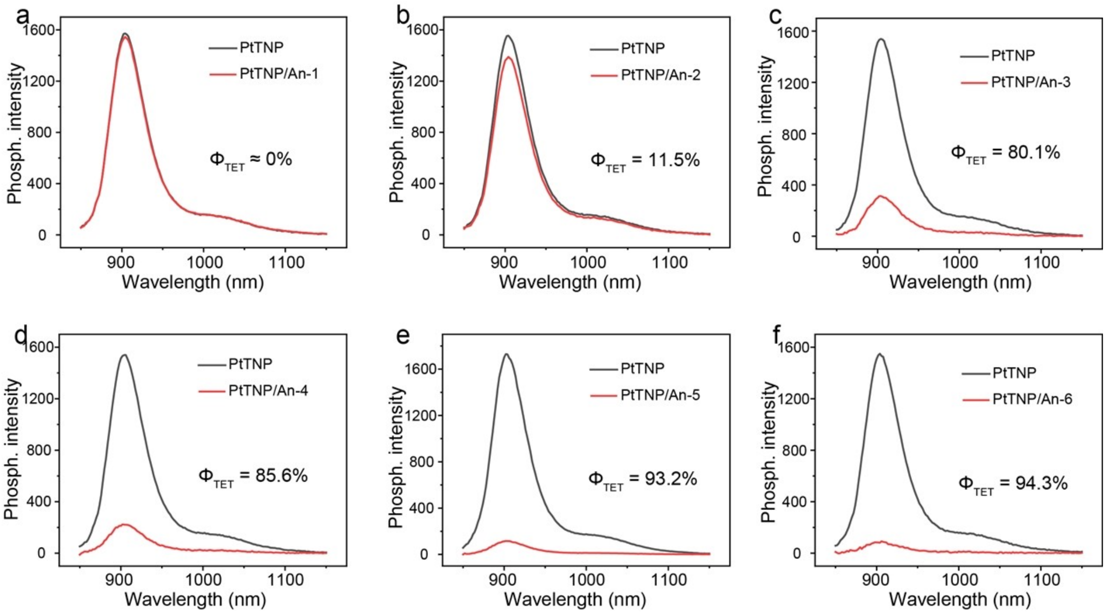


Figure S19. Phosphorescence spectra of PtTNP (5 μM) with or without 500 μM (**a**) PdTPBP/An-1 and (**b**) PdTPBP/An-2, (**c**) PtTNP/An-3, (**d**) PtTNP/An-4, (**e**) PtTNP/An-5 and (**f**) PtTNP/An-6, λ_{ex} = 690 nm, in argon-saturated toluene.

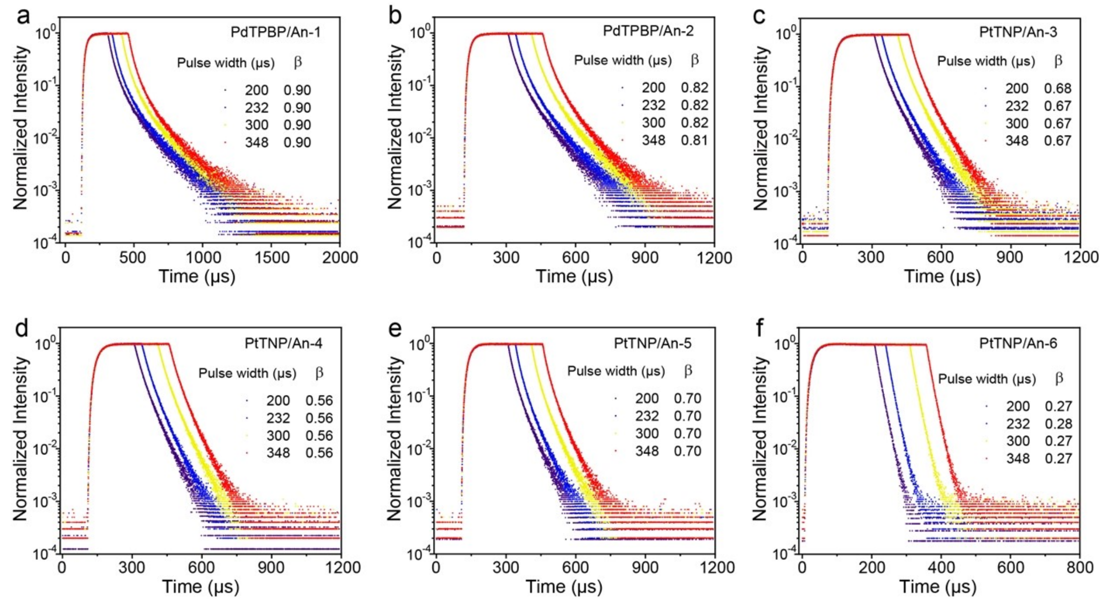


Figure S20. Normalized upconversion emission intensity at excitation intensity of 12.9 W/cm² for 5/500 μM (**a**) PdTPBP/An-1 and (**b**) PdTPBP/An-2, (**c**) PtTNP/An-3, (**d**) PtTNP/An-4, (**e**) PtTNP/An-5 and (**f**) PtTNP/An-6 in Ar-saturated toluene. The fitted values of β at various pulse widths are listed on the right top corner. This demonstrates that the 200μs pulse width is sufficient to ensure the stable excitation of the TTA-UC pairs, thereby enabling an accurate calculation of β.

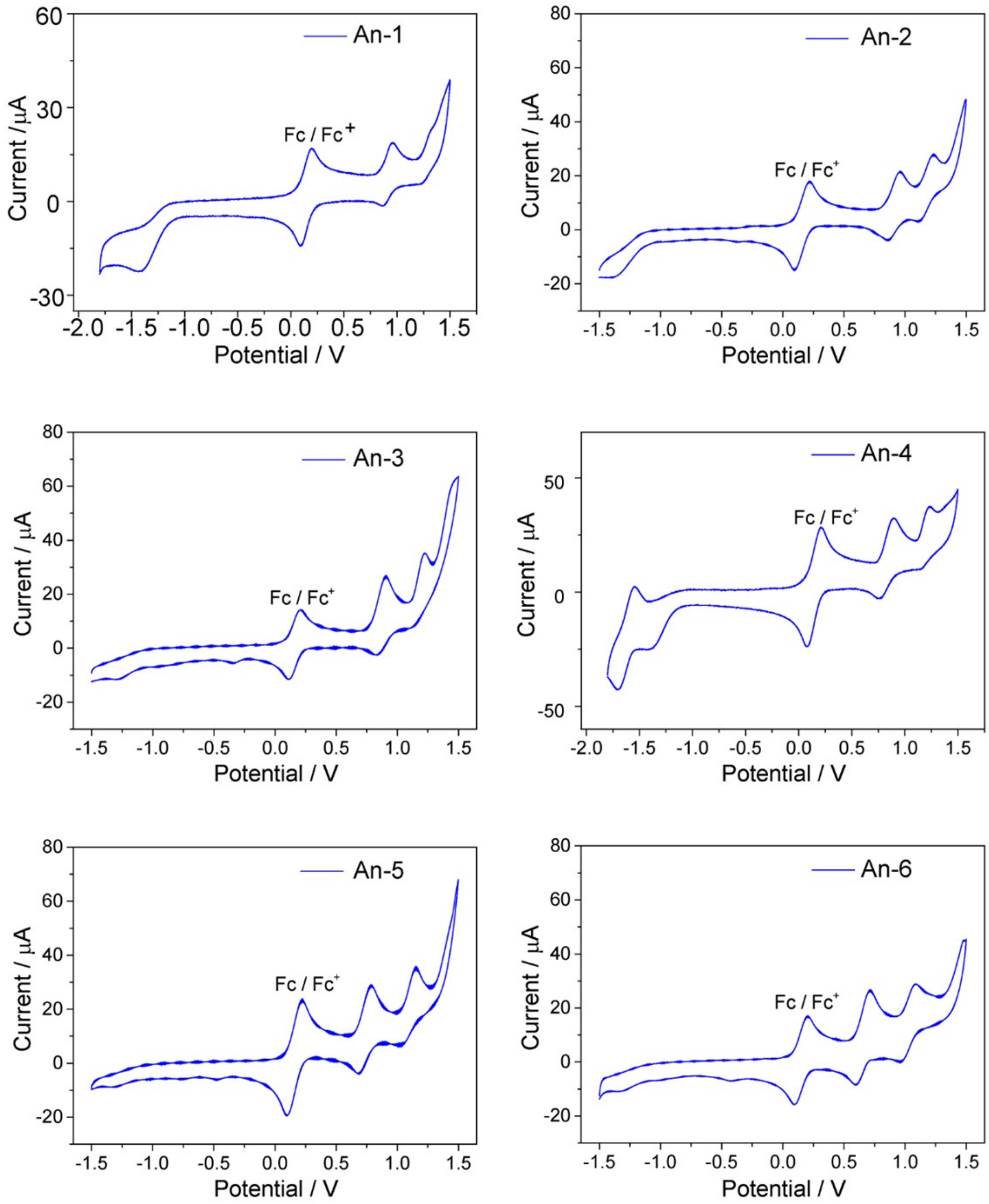


Figure S21. Cyclic voltammograms of An-1−An-6. Ferrocene (Fc) was used as an internal reference. Condition: in deaerated DCM containing 0.10 M Bu_4NPF_6 as the supporting electrolyte and $Ag/AgNO_3$ as a reference electrode. Scan rates: 100 mV/s. c = 1.0 × 10^{-3} M, 25 °C.

Figure S22. Photograph of the flask after blue light (445 nm)-driven polymerization.

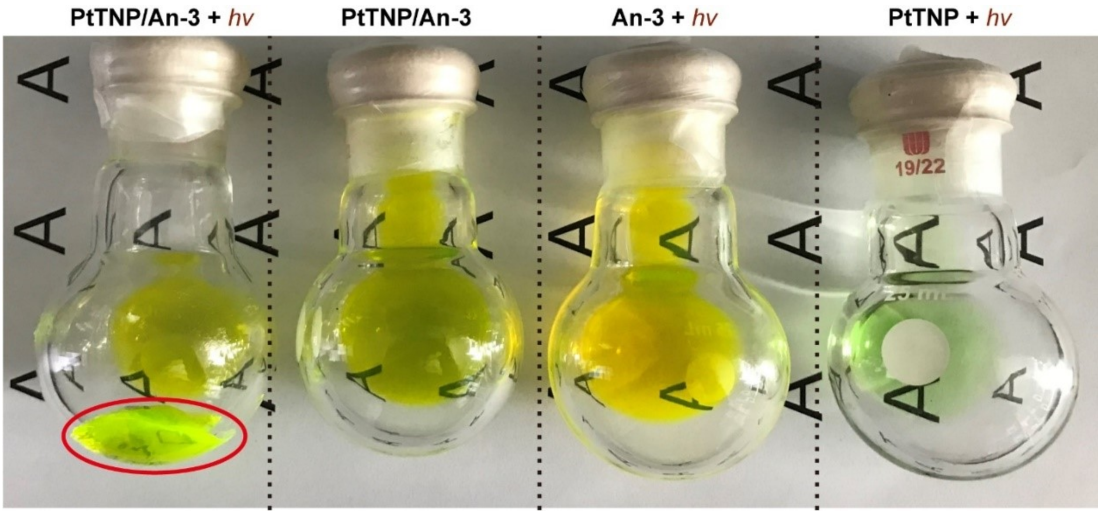


Figure S23. The photographs show the reaction mixture under different conditions, including PtTNP/An-3 + *hv*, PtTNP/An-3, An-3 + *hv*, and PtTNP + *hv*. PtTNP (10 μM), An-3 (500 μM), λ_{ex} = 690 nm. The red circle highlights the formed gel.

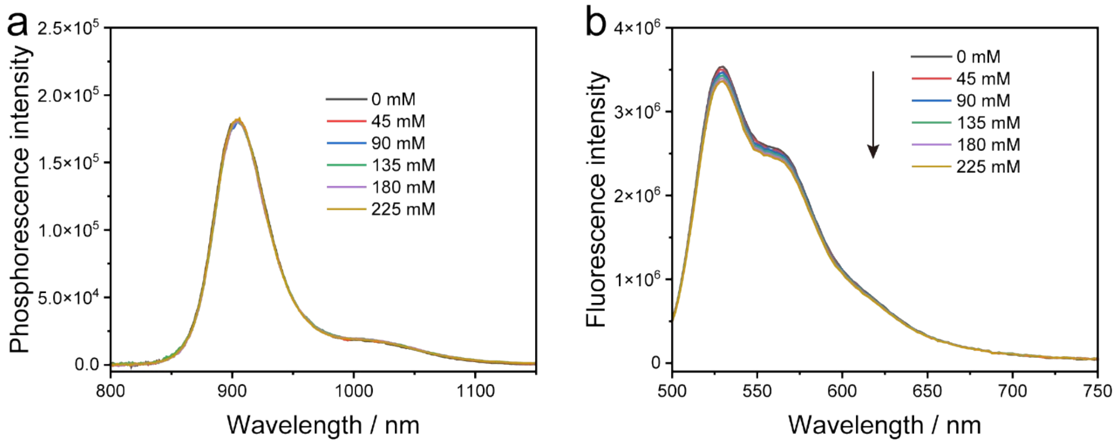


Figure S24. (a) Phosphorescence intensity change of PtTNP via titration of the initiator EBP. λ_{ex} = 690 nm. (b) Fluorescence intensity change of An-3 via titration of the initiator EBP. λ_{ex} = 470 nm in the Ar-saturated MMA/ ethylene glycol dimethacrylate (9/1, v/v), c (PtTNP) = 10 μM, c(An-3) = 500 μM.

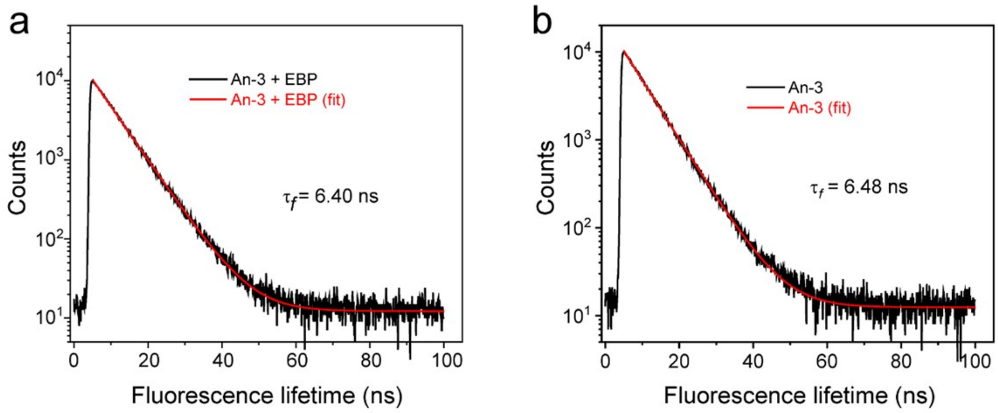


Figure S25. Fluorescence decay traces of An-3 (500 μM) in Ar-saturated MMA/ethylene glycol dimethacrylate (9/1, v/v) with (a) and without (b) initiator EBP (50 μL). λ_{ex} = 405 nm.

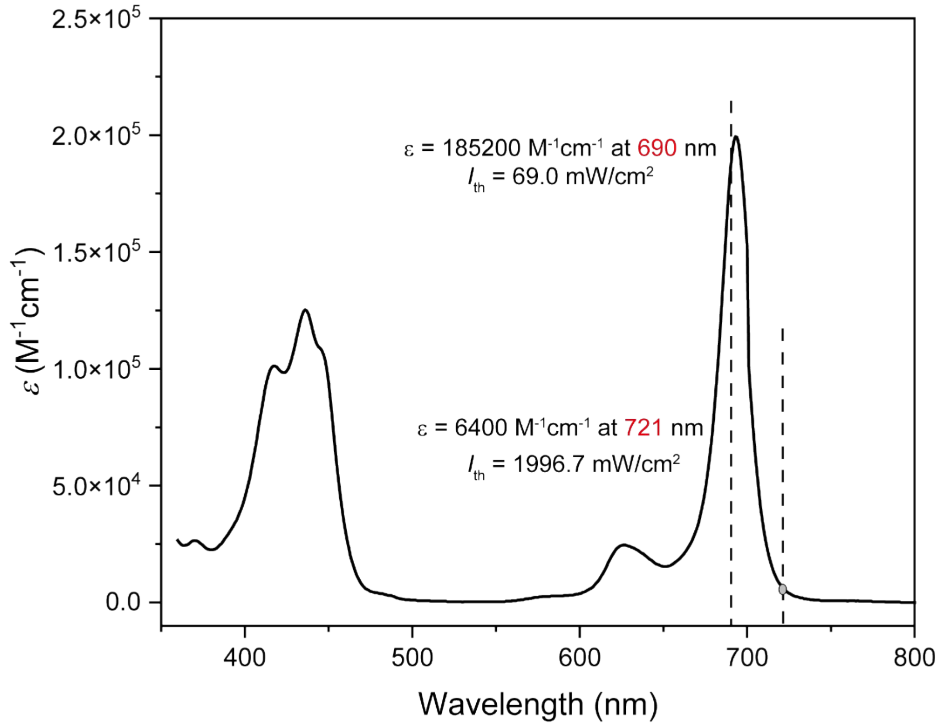


Figure S26. UV-vis absorption spectra of PtTNP and its I_{th} values at 690 nm and 721 nm.

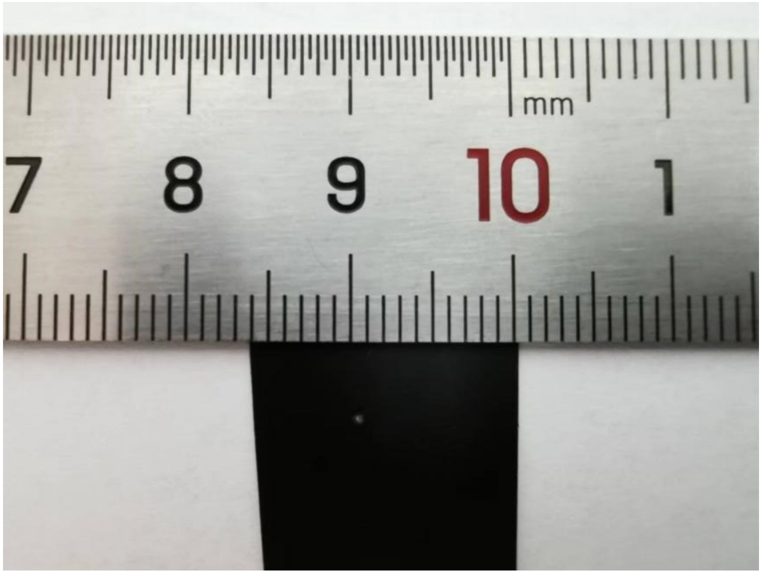


Figure S27. The spot size of 721 nm light after 40× objective focus.

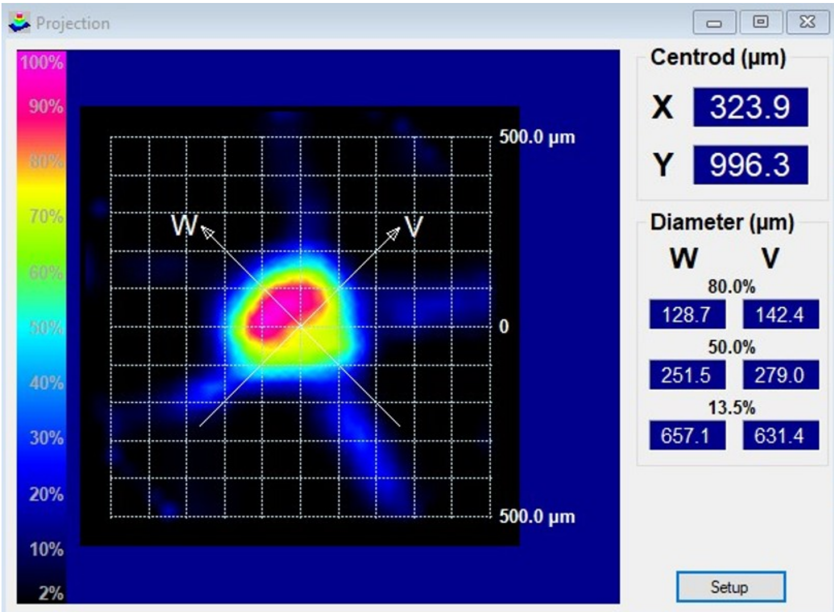


Figure S28. Beam profiler image of the focused 721 nm laser.

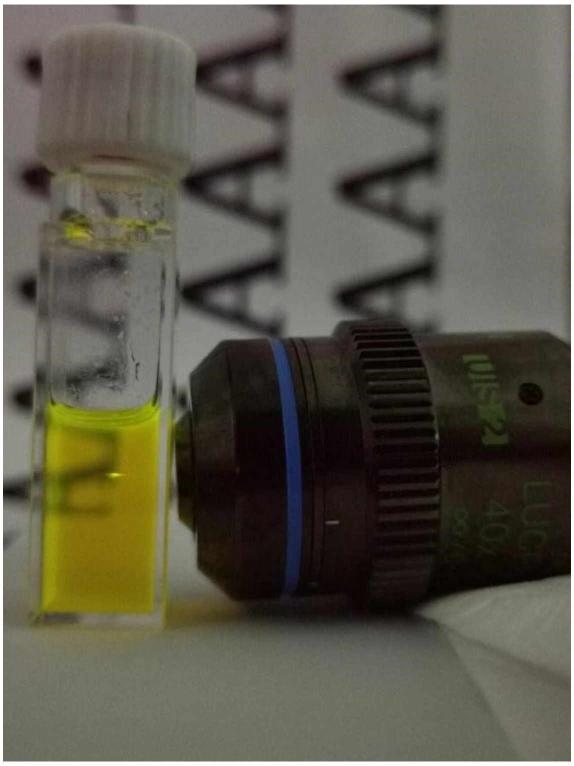


Figure S29. TTA-UC photographed in Ar-saturated ethylene glycol dimethacrylate/trimethylolpropane ethoxylate triacrylate (1/1, v/v). c (PtTNP) = 5 μM, c (An-3) = 0.5 mM, λ_{ex} = 721 nm.

[1]H NMR and Mass spectral data of the synthesized compounds

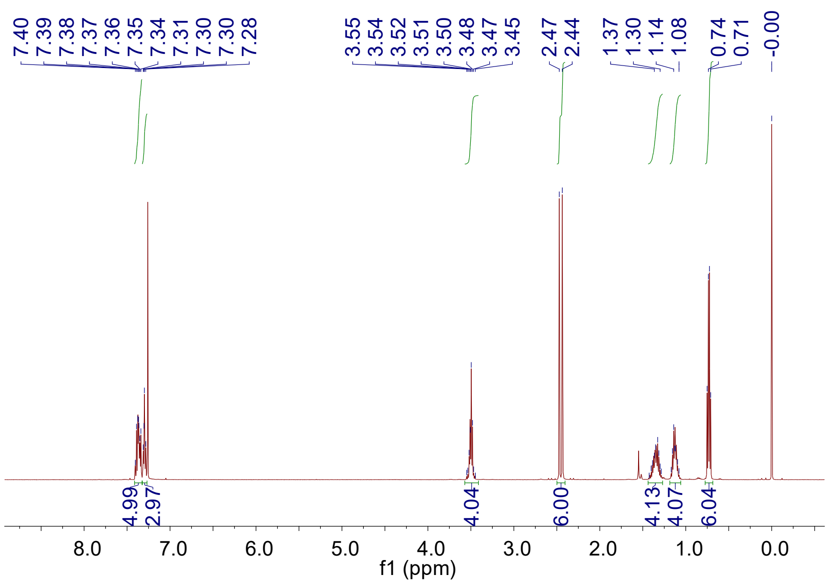


Figure S30. ^{1}H NMR of An-1 (400 MHz, $CDCl_3$).

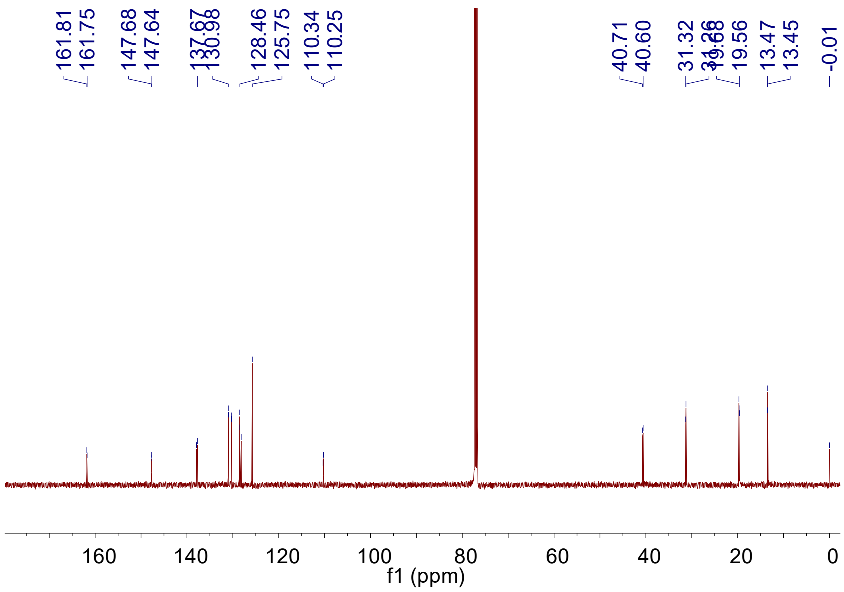


Figure S31. ^{13}C NMR of An-1 (100 MHz, $CDCl_3$).

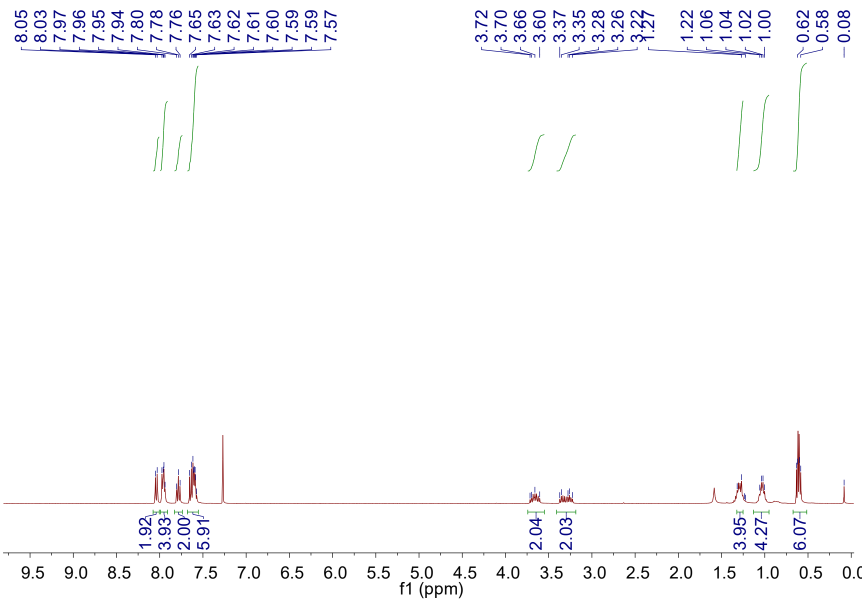


Figure S32. ^{1}H NMR of An-2 (400 MHz, $CDCl_3$).

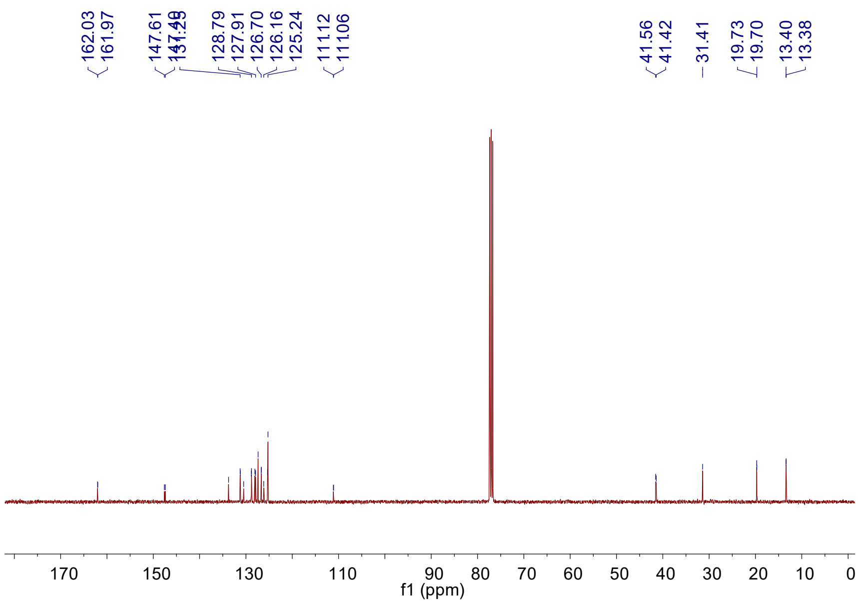


Figure S33. ^{13}C NMR of An-2 (100 MHz, $CDCl_3$).

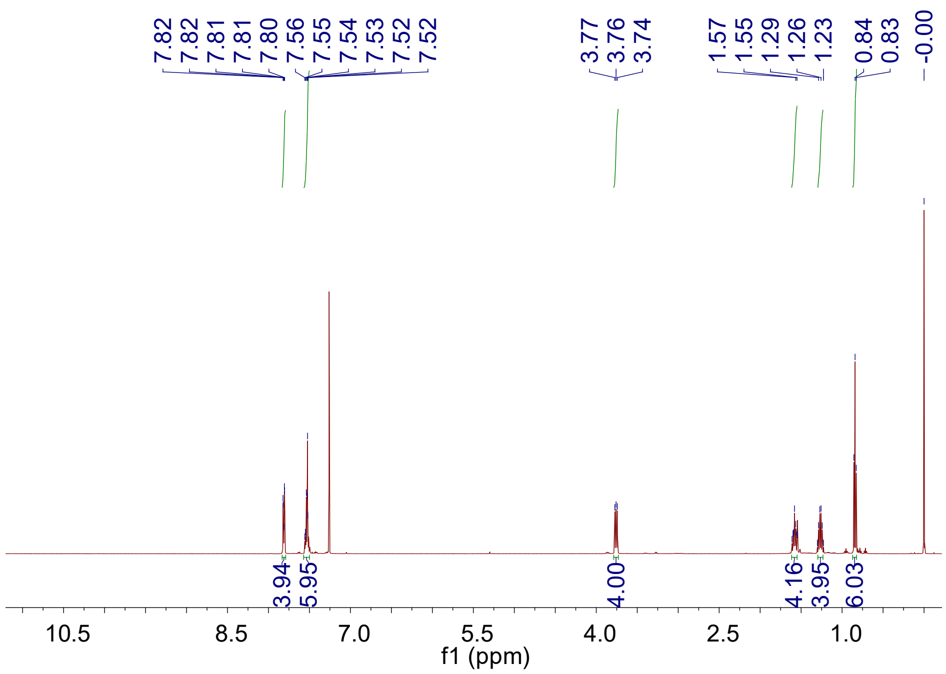


Figure S34.^{1}H NMR of An-3 (400 MHz, $CDCl_3$).

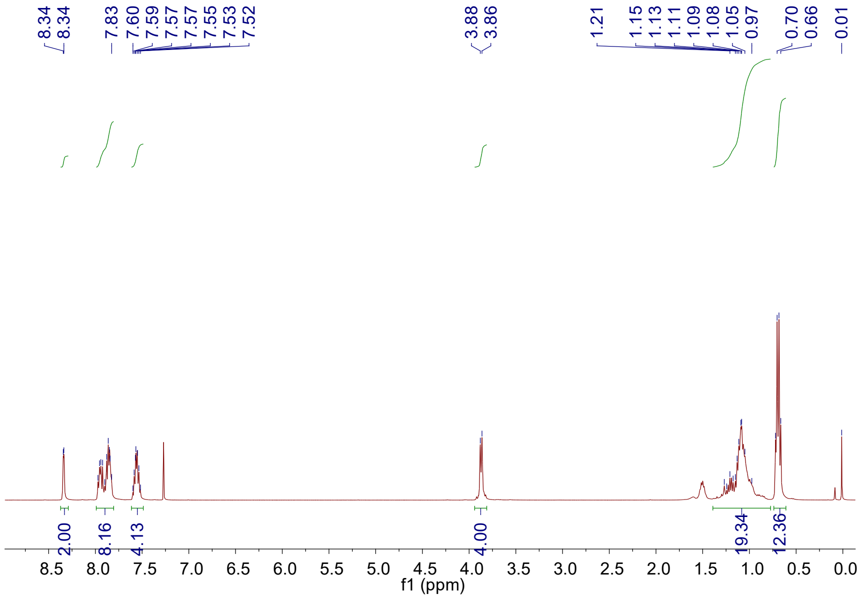


Figure S35.[1]H NMR of An-4 (400 MHz, $CDCl_3$).

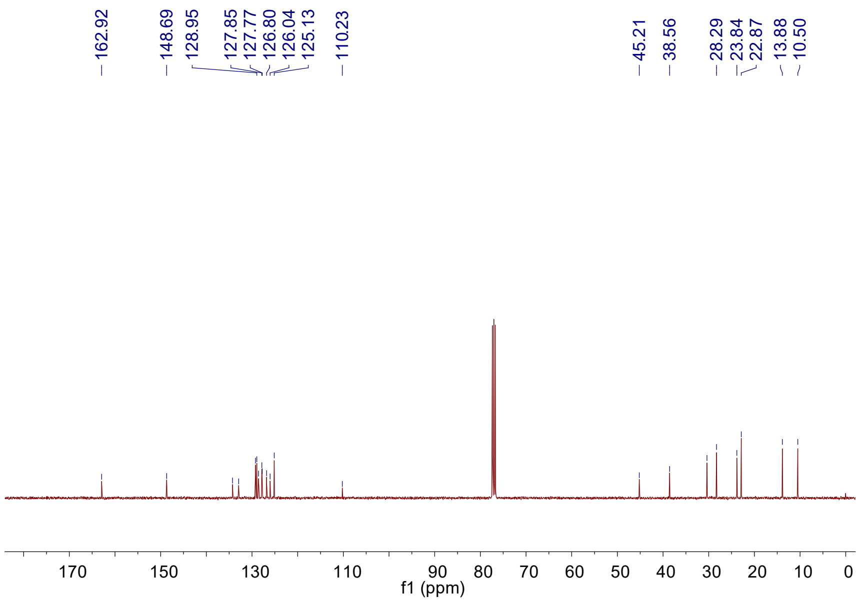


Figure S36.[13]C NMR of An-4 (100 MHz, $CDCl_3$).

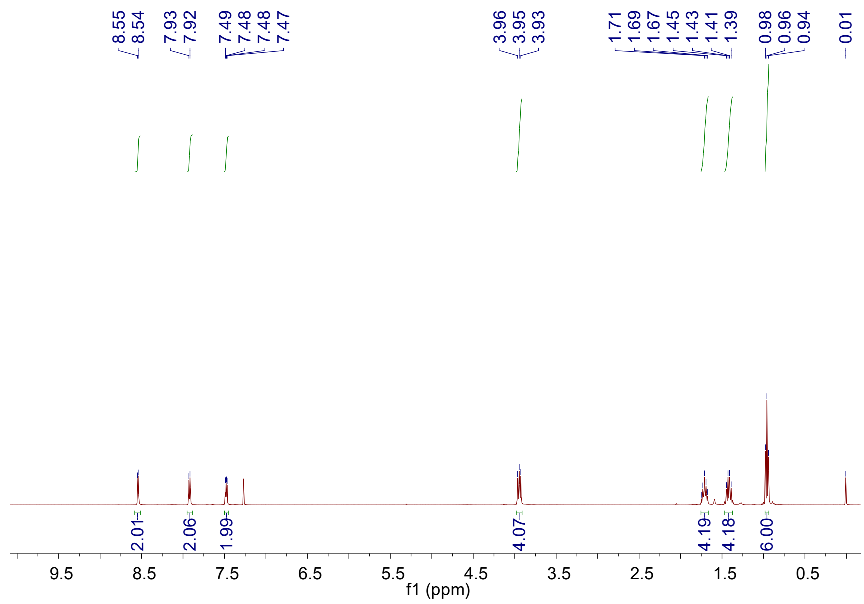


Figure S37.[1]H NMR of An-5 (400 MHz, $CDCl_3$).

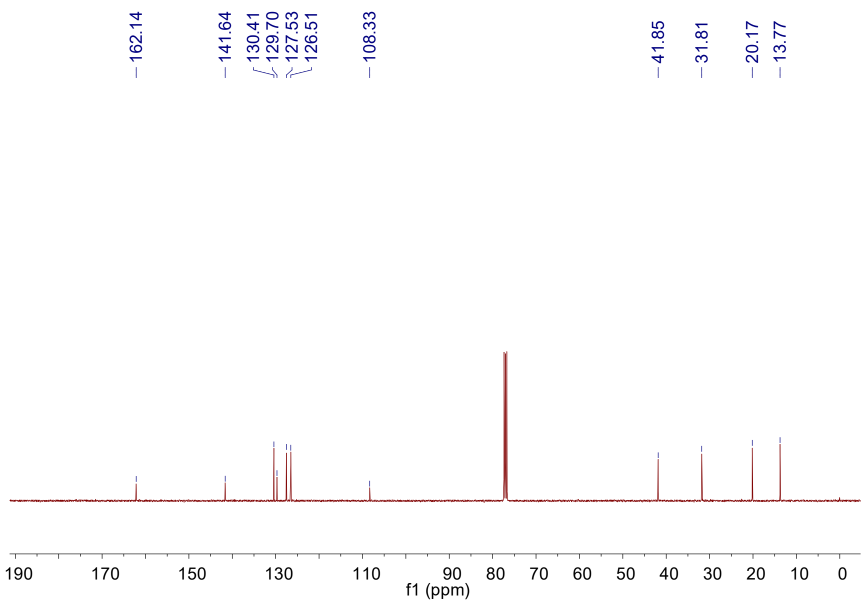


Figure S38.[13]C NMR of An-5 (100 MHz, $CDCl_3$).

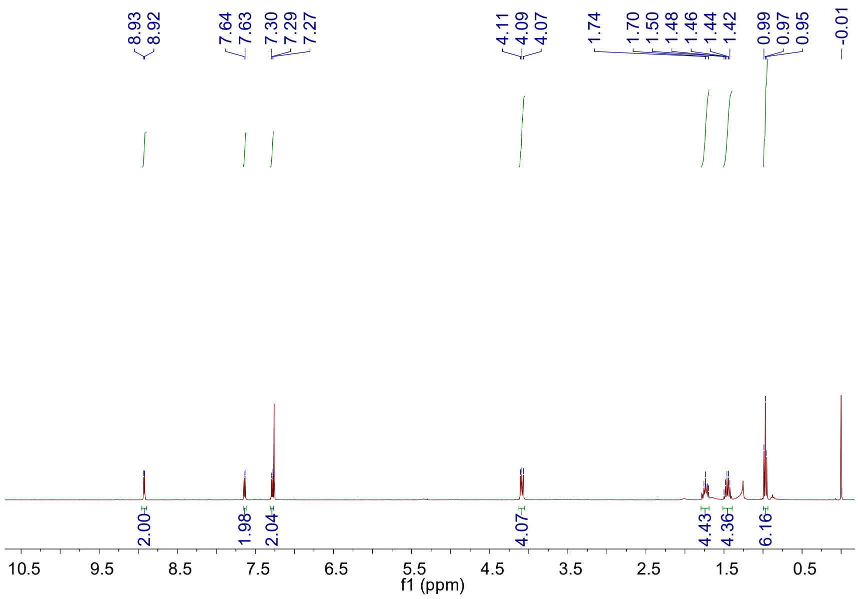


Figure S39.[1]H NMR of An-6 (400 MHz, $CDCl_3$).

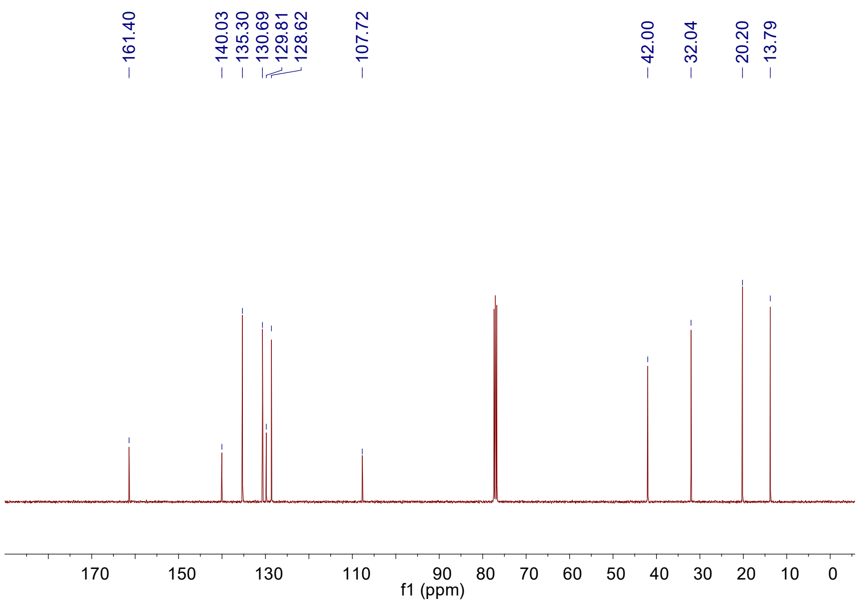


Figure S40.[13]C NMR of An-6 (100 MHz, $CDCl_3$).

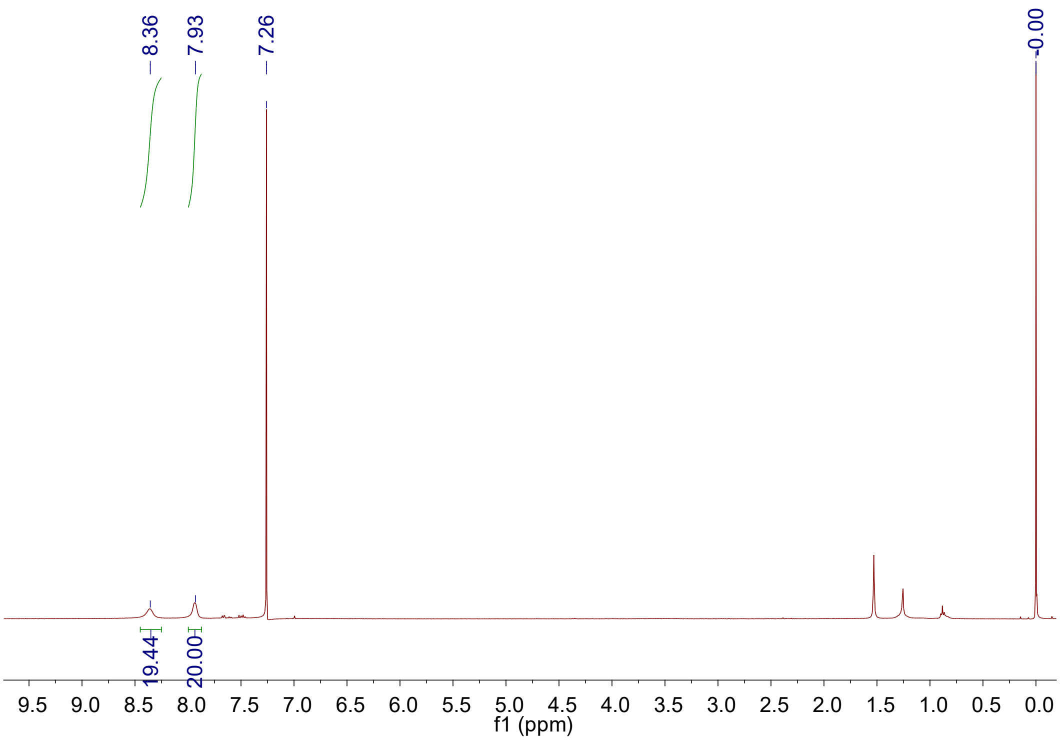


Figure S41.[1]H NMR of PtTNP (400 MHz, $CDCl_3$).

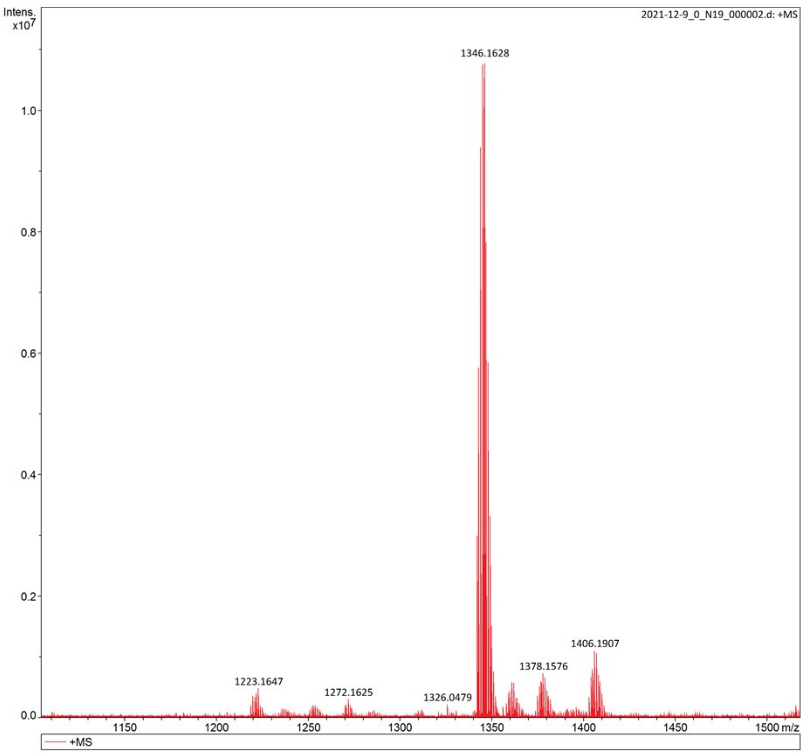


Figure S42. MALDI-TOF of PtTNP.

Detailed DFT calculation data

Theoretical calculations. The ground state geometries of An-1–An-6 were optimized by density functional theory (DFT) using the B3LYP functional with the 6-31G(d) basis set. The long alkyl chains were simplified as methyl groups in the computation. The energies of the singlet and triplet excited states were calculated by the TD-DFT method based on the optimized ground state geometries. All these calculations were performed with Gaussian 16.

An-1 S_0
C -0.61966000 -0.31175100 0.18703200
C 0.57943200 0.47158000 0.22438000
C 0.21572500 1.87566300 0.14203400
N -1.21708100 1.84121400 0.03159100
C -1.70395800 0.53586900 0.04927000
C -0.23759300 -1.71227200 0.12804700
N 1.19413400 -1.67496500 0.11606700
C 1.67237100 -0.36817300 0.15887000
C 3.10191300 -0.00643200 0.13028000
C -3.13171500 0.23263000 -0.14952500
O -0.86772400 -2.76554900 0.12806600
O 0.85803800 2.91670500 0.18050300
C -3.79388600 0.82740000 -1.24138400
C -5.13026200 0.55367200 -1.51042900
C -5.83238400 -0.31507700 -0.67374100
C -5.18878800 -0.89882000 0.41567300
C -3.83978700 -0.64991200 0.70350400
C 3.98124400 -0.42244600 -0.89834400
C 5.31697500 -0.00345700 -0.83197400
C 5.78378100 0.80549000 0.20226400
C 4.90510900 1.23601400 1.19735900
C 3.57362000 0.83656500 1.15354300
C 1.95361200 -2.90442900 0.27234900
C -1.98732500 3.07357900 0.08183400
C 3.53304900 -1.25146700 -2.08082200
C -3.20434800 -1.31337400 1.89933200
H -3.23891000 1.48566200 -1.90310800
H -5.61653400 1.01108600 -2.36745000
H -6.87873600 -0.53653400 -0.86678900
H -5.74362500 -1.56821400 1.06843800
H 5.99840100 -0.30865800 -1.62289100
H 6.82635300 1.11178000 0.22095400

H 5.25178900 1.88146900 1.99933000
H 2.88095900 1.16902800 1.91990900
H 2.97588200 -2.66713800 0.56827300
H 1.48540400 -3.51886600 1.04657000
H 1.96887100 -3.48104500 -0.65799300
H -1.35435900 3.83415300 0.54387600
H -2.26887100 3.42297400 -0.91751600
H -2.89173600 2.93420600 0.67813500
H 2.46744900 -1.13085800 -2.29472500
H 4.08820100 -0.96112400 -2.97906800
H 3.72036900 -2.32133200 -1.92316700
H -3.97192500 -1.73287300 2.55766400
H -2.54282600 -2.12908900 1.58331200
H -2.60079800 -0.61274100 2.48676400

An-1 S_1
C -0.61325600 -0.31735300 0.21692200
C 0.55319500 0.45194900 0.22394300
C 0.18493500 1.85328900 0.10912500
N -1.24085200 1.83256300 0.01660300
C -1.75532100 0.54389300 0.07099600
C -0.21688700 -1.71353200 0.12133800
N 1.22225300 -1.67845600 0.09225600
C 1.71422400 -0.39024300 0.13176200
C 3.09470700 0.02417500 0.08688300
C -3.15482700 0.23995900 -0.13608300
O -0.83616300 -2.77469500 0.10003400
O 0.84499400 2.89039000 0.12459200
C -3.86261600 0.93424300 -1.15464300
C -5.19408900 0.66253100 -1.43005200
C -5.87189200 -0.30762700 -0.68533600
C -5.19786600 -0.98371800 0.33495100
C -3.85661400 -0.73849500 0.63672200
C 4.10448500 -0.57307900 -0.73614500
C 5.41061500 -0.08653200 -0.63823200
C 5.75375900 0.97295600 0.20344800
C 4.75477500 1.60648800 0.95260900
C 3.45009500 1.14892900 0.88619400
C 1.95283300 -2.91487400 0.33295000
C -1.98307700 3.08274300 0.08781500
C 3.81070900 -1.61407700 -1.79258800
C -3.22120700 -1.45275900 1.80245300
H -3.33019200 1.65313100 -1.76913600
H -5.69864700 1.19375900 -2.23280700

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H -5.73515200 -1.71750700 0.93140100
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H 2.67722700 1.64059000 1.46557600
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H -3.98460500 -1.95859600 2.40266800
H -2.50338000 -2.20711000 1.46363300
H -2.68419100 -0.75697300 2.45864100

An-1 T_1

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C 1.76280900 0.50667600 -0.05592800
C 0.24402500 -1.71663000 -0.10941500
N -1.19762900 -1.64807500 -0.14642200
C -1.72427400 -0.34327000 -0.12652900
C -3.14158900 0.02092000 -0.10724400
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O -0.84108600 2.93225300 -0.13908500
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An-2 S_0

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C -3.60163500 1.39165600 -1.63454400
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An-2 S_1
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C 3.56329700 -1.74006000 -1.40795400
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C 4.31537500 1.58768400 2.10565500
C 5.67777100 1.64257800 1.75090600
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H -0.40078400 3.94626700 0.24670100
H -1.28684600 3.83281000 -1.28176600
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H 6.35819200 2.28546300 2.30292400
H 7.19867400 0.87893400 0.44355300
H -7.19879500 -0.87853200 0.44356300
H -6.35848800 -2.28508800 2.30298500
H -3.94845900 -2.18130300 2.93829300
H -2.40041700 -0.73356400 1.71147100

An-2 T_1

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N 2.14853300 -0.03831900 0.64520500
C 1.32880400 -0.03449400 -0.49300400
C -1.32792900 -0.14286900 -0.44519300
N -2.10971300 -0.20890100 0.71524000
C -1.31152700 -0.15614600 1.87284800
C -1.86251900 -0.36010700 3.21701700
C 1.74367100 -0.22684400 -1.85417500
O -1.82953100 -0.15247000 -1.62327800
O 1.91103400 0.02799800 2.96785500
C 2.93123000 -0.93565400 -2.18750100
C 3.23795300 -1.27769600 -3.50108300
C 2.38524300 -0.94750400 -4.54921000
C 1.20964100 -0.20119100 -4.28286800
C 0.89622000 0.19985000 -2.94296100
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C -2.05509700 0.20718000 5.62173200
C -2.93293500 -0.89605200 5.78920500
C -3.27195500 -1.68760600 4.71570200
C -2.73685000 -1.41979100 3.43965000
C -3.56247600 -0.19598700 0.63836900
C 3.58704500 0.15848500 0.70533600
C -0.67698000 1.63837800 4.18844700
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C -0.89205200 2.13365400 6.55290100
C -1.71577900 1.04445800 6.71949100
C 0.34366700 0.19014400 -5.33808000
C -0.76936300 1.01051400 -5.12304400
C -1.03311200 1.48174200 -3.84828700
C -0.22497100 1.07570900 -2.75884200
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H 4.14584200 -1.84080400 -3.70131600
H 2.61372400 -1.23680700 -5.57059500
H -3.33263000 -1.10219600 6.77917900
H -3.93973000 -2.53499700 4.84606900
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H 3.91897500 0.80469000 -0.11084100

H -0.27740800 1.88530100 3.21279000
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H -0.64184600 2.76628000 7.40051600
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H 0.57165000 -0.15430700 -6.34342500
H -1.39926900 1.29655200 -5.95992100
H -1.86092400 2.15687300 -3.66052600
H -0.30647500 1.62231700 -1.83138400

An-3 S_0
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C 0.60539600 0.37887900 0.19475200
C 0.25659200 1.78688700 0.14583000
N -1.17575200 1.78326500 0.07354500
C -1.68493600 0.48500900 0.08917800
C -0.25657900 -1.78689000 0.14549700
N 1.17578900 -1.78323600 0.07349400
C 1.68494500 -0.48499000 0.08940300
C 3.10510000 -0.14902100 -0.03270900
C -3.10511200 0.14904100 -0.03284500
O -0.91539400 -2.82071400 0.19856400
O 0.91544800 2.82068200 0.19910100
C -4.01678400 0.95488600 -0.74387500
C -5.35364800 0.58114300 -0.85767900
C -5.80908400 -0.59842100 -0.26526800
C -4.91152800 -1.41394500 0.42836600
C -3.57296400 -1.05047100 0.54150300
C 4.01664800 -0.95490600 -0.74385700
C 5.35349900 -0.58118500 -0.85787300
C 5.80904100 0.59838100 -0.26553900
C 4.91160800 1.41391600 0.42824200
C 3.57305200 1.05046800 0.54158700
C 1.90026900 -3.03808100 0.20524300
C -1.90021900 3.03816100 0.20474000
H -3.67775800 1.85686200 -1.23953200
H -6.03950400 1.21135700 -1.41722900
H -6.85364500 -0.88496400 -0.35231100
H -5.25396000 -2.34018100 0.88144400
H -2.87728700 -1.70114600 1.05830800
H 3.67751300 -1.85689100 -1.23943000
H 6.03926100 -1.21141800 -1.41751600
H 6.85359100 0.88491500 -0.35274900
H 5.25413000 2.34014400 0.88126800
H 2.87745700 1.70115400 1.05849700

H 2.78481500 -2.90654900 0.83166600
H 1.22259800 -3.75493400 0.67337600
H 2.20140400 -3.44206300 -0.76773000
H -1.22253200 3.75518400 0.67259100
H -2.20130700 3.44174900 -0.76841000
H -2.78477900 2.90693500 0.83121100

An-3 S_1
C -0.59023100 -0.37099100 0.09003800
C 0.59032200 0.37100500 0.09007100
C 0.23378900 1.77847300 0.04163300
N -1.19872000 1.78566400 0.00753200
C -1.73184000 0.50780800 0.02399700
C -0.23387600 -1.77843700 0.04140700
N 1.19870500 -1.78573800 0.00734900
C 1.73194500 -0.50797000 0.02391000
C 3.12352000 -0.15601500 -0.02756600
C -3.12342100 0.15585800 -0.02748900
O -0.89734300 -2.81445600 0.05496900
O 0.89716800 2.81456900 0.05548900
C -4.14637400 1.02606800 -0.50240400
C -5.47444200 0.62406100 -0.51920400
C -5.84484200 -0.64949700 -0.07002200
C -4.85230000 -1.52886700 0.37895100
C -3.51971400 -1.14471700 0.39972000
C 4.14679500 -1.02646200 -0.50139000
C 5.47480300 -0.62424300 -0.51809900
C 5.84488600 0.64975000 -0.06990200
C 4.85204000 1.52935400 0.37794200
C 3.51950900 1.14503000 0.39855400
C 1.88994000 -3.06174200 0.10631500
C -1.89016900 3.06151700 0.10696700
H -3.89680000 2.00028100 -0.90091400
H -6.23030900 1.30752800 -0.89769600
H -6.88757100 -0.95417100 -0.08158600
H -5.12140700 -2.52634500 0.71668200
H -2.76534700 -1.84854600 0.73198600
H 3.89763600 -2.00110300 -0.89907300
H 6.23089200 -1.30795200 -0.89571000
H 6.88757400 0.95456300 -0.08139200
H 5.12084400 2.52718900 0.71486800
H 2.76492800 1.84910000 0.72986100
H 2.71572600 -2.99630100 0.81823200
H 1.15920000 -3.79335500 0.45469400

H 2.26771200 -3.39291800 -0.86682300
H -1.15979000 3.79303500 0.45630300
H -2.26743400 3.39329300 -0.86615600
H -2.71638700 2.99543300 0.81832700

An-3 T_1

C -0.62729000 -0.40026300 0.07187600
C 0.62732600 0.40026800 0.07189800
C 0.26069600 1.78663900 0.09071200
N -1.18107600 1.75859600 0.09110800
C -1.73912100 0.46563400 0.04501700
C -0.26070900 -1.78663800 0.09060400
N 1.18106000 -1.75862900 0.09104100
C 1.73914900 -0.46567200 0.04504000
C 3.14826100 -0.14262100 -0.04885800
C -3.14823100 0.14257700 -0.04886000
O -0.89832500 -2.83932100 0.13626700
O 0.89824000 2.83936200 0.13646700
C -4.12246100 1.02982000 -0.57040600
C -5.46212100 0.66103700 -0.63768000
C -5.87864800 -0.59919300 -0.19991100
C -4.92561700 -1.49763300 0.29173600
C -3.58520100 -1.14111800 0.36743800
C 4.12261300 -1.02996900 -0.57000000
C 5.46225600 -0.66111000 -0.63728500
C 5.87867500 0.59928600 -0.19991000
C 4.92553300 1.49782000 0.29136000
C 3.58513700 1.14124600 0.36705300
C 1.87953600 -3.01208700 0.28622500
C -1.87962400 3.01199100 0.28646600
H -3.83124300 1.99642600 -0.96192600
H -6.18481200 1.36168900 -1.04808200
H -6.92638300 -0.88133400 -0.25394000
H -5.22981800 -2.48768800 0.62138600
H -2.85884000 -1.85921400 0.73158000
H 3.83155000 -1.99674400 -0.96120200
H 6.18501800 -1.36187200 -1.04737600
H 6.92639600 0.88147400 -0.25394200
H 5.22963200 2.48800500 0.62071600
H 2.85871500 1.85942500 0.73091200
H 2.75527900 -2.86011600 0.92014300
H 1.17674300 -3.70458900 0.75411000
H 2.19570500 -3.44830800 -0.66974300
H -1.17700600 3.70437600 0.75478700

H -2.19552100 3.44848500 -0.66946600
H -2.75558200 2.85978100 0.92003200

An-4 S_0
C 0.66944800 0.24697700 0.08675200
C -0.66947500 -0.24679600 0.08666000
C -0.61519000 -1.69541000 0.04252200
N 0.78669600 -1.98643200 -0.02643600
C 1.55215100 -0.81951200 -0.01462200
C 0.61515200 1.69559400 0.04277500
N -0.78672500 1.98662200 -0.02624200
C -1.55217200 0.81969200 -0.01465000
C -3.00916300 0.78074600 -0.13654400
C 3.00912300 -0.78064400 -0.13652300
O 1.47222900 2.57274400 0.10312600
O -1.47225300 -2.57257500 0.10272500
C 3.74752400 -1.79478400 -0.82303300
C 5.11331900 -1.71720800 -0.93763100
C 5.84059600 -0.63213000 -0.37724400
C 5.10968700 0.40233600 0.29357100
C 3.70161100 0.30308600 0.39424000
C -3.74764000 1.79470800 -0.82322900
C -5.11342300 1.71699100 -0.93785700
C -5.84061600 0.63192800 -0.37732600
C -5.10963000 -0.40234300 0.29370800
C -3.70156400 -0.30294000 0.39440800
C -1.23302600 3.36231700 0.13722400
C 1.23295100 -3.36212200 0.13730600
C -7.25297600 0.52859100 -0.46928200
C -7.91461000 -0.54930900 0.07772800
C -7.19351300 -1.57441100 0.73967100
C -5.82308700 -1.50306500 0.84541700
C 7.25297500 -0.52896400 -0.46914600
C 7.91469600 0.54896000 0.07770800
C 7.19367300 1.57425900 0.73943100
C 5.82323600 1.50308400 0.84511600
H 3.22443900 -2.61811900 -1.29359600
H 5.65689100 -2.49151500 -1.47362700
H 3.15782800 1.10463700 0.88238100
H -3.22459200 2.61804100 -1.29382200
H -5.65705000 2.49117100 -1.47397900
H -3.15773500 -1.10435400 0.88271900
H -2.12005900 3.40710200 0.77262200
H -0.41636100 3.91099800 0.61106900

H -1.44912000 3.84175900 -0.82416400
H 0.41650700 -3.91059100 0.61177800
H 1.44849000 -3.84191900 -0.82403600
H 2.12033500 -3.40671800 0.77221100
H -7.80474400 1.31408300 -0.98013800
H -8.99648000 -0.61849100 0.00193900
H -7.72918300 -2.41933000 1.16362800
H -5.26415700 -2.28733800 1.34956800
H 7.80468000 -1.31460500 -0.97983900
H 8.99657800 0.61801100 0.00196700
H 7.72941600 2.41919500 1.16326500
H 5.26436400 2.28750800 1.34909800

An-4 S_1
C 0.65844800 0.23070400 0.05942000
C -0.65844100 -0.23074200 0.05966700
C -0.62359200 -1.68411800 0.03274200
N 0.76810000 -2.01010400 0.00684000
C 1.57297200 -0.88026300 -0.00164300
C 0.62355100 1.68408200 0.03228100
N -0.76813900 2.01006000 0.00708300
C -1.57296600 0.88019300 -0.00106800
C -3.00253300 0.84938500 -0.09174200
C 3.00253400 -0.84944400 -0.09207900
O 1.49974700 2.54811200 0.06462800
O -1.49978100 -2.54811100 0.06563000
C 3.79769400 -1.96489700 -0.53644500
C 5.16177900 -1.88350000 -0.60706400
C 5.86228600 -0.69330600 -0.24938200
C 5.08649400 0.44195700 0.16819600
C 3.68538800 0.34130300 0.23804500
C -3.79754900 1.96481500 -0.53636300
C -5.16162700 1.88346200 -0.60723100
C -5.86222100 0.69332800 -0.24953500
C -5.08653900 -0.44192800 0.16828700
C -3.68544200 -0.34131400 0.23837800
C -1.15537400 3.40174100 0.18697100
C 1.15540300 -3.40181000 0.18632800
C -7.26862700 0.58493900 -0.30984300
C -7.90195600 -0.59867100 0.02688500
C -7.14363400 -1.72209800 0.43543600
C -5.77008900 -1.64863400 0.50565900
C 7.26869400 -0.58489100 -0.30947700
C 7.90193100 0.59878300 0.02722000

C 7.14350300 1.72222100 0.43552800
C 5.76994600 1.64872400 0.50554300
H 3.31880300 -2.87628500 -0.86692600
H 5.73412900 -2.73789900 -0.96101300
H 3.11977700 1.21603400 0.54165900
H -3.31848500 2.87614400 -0.86674300
H -5.73387900 2.73784600 -0.96137500
H -3.11988400 -1.21601300 0.54220300
H -1.98076200 3.47951800 0.89777700
H -0.28202200 3.92651200 0.57783600
H -1.43806800 3.87283500 -0.76051100
H 0.28204000 -3.92671300 0.57696500
H 1.43827100 -3.87253200 -0.76128500
H 1.98073200 -3.47974300 0.89719300
H -7.84955300 1.44769200 -0.62801900
H -8.98509500 -0.66953200 -0.02368700
H -7.65234900 -2.64722400 0.69333600
H -5.18354200 -2.50965900 0.81618100
H 7.84969600 -1.44766200 -0.62746500
H 8.98507400 0.66968300 -0.02319900
H 7.65214300 2.64739600 0.69340200
H 5.18332800 2.50977300 0.81586400

An-4 T_1
C 0.67233800 0.23650200 0.10135600
C -0.67235700 -0.23647700 0.10140800
C -0.63713500 -1.68106800 0.07501800
N 0.75440600 -2.01284000 0.03624000
C 1.56257100 -0.87078700 0.03100900
C 0.63712000 1.68109100 0.07490100
N -0.75442000 2.01286700 0.03637700
C -1.56259500 0.87082900 0.03121100
C -2.98990100 0.84911400 -0.07566600
C 2.98986300 -0.84909900 -0.07577700
O 1.51403900 2.54874100 0.12511100
O -1.51403800 -2.54872100 0.12546300
C 3.77246900 -1.96706100 -0.51101400
C 5.13944000 -1.89285100 -0.60629700
C 5.85575200 -0.70004400 -0.27669100
C 5.09389400 0.44435400 0.13632600
C 3.69095200 0.35338600 0.22999600
C -3.77250500 1.96708300 -0.51090800
C -5.13946600 1.89284400 -0.60626000
C -5.85575300 0.70001500 -0.27671200

C -5.09389600 -0.44436900 0.13632200
C -3.69095200 -0.35336700 0.23004100
C -1.14472400 3.39494600 0.25933600
C 1.14478600 -3.39488100 0.25928200
C -7.25645100 0.60470800 -0.36179400
C -7.91119000 -0.58526800 -0.05050600
C -7.17099100 -1.71153300 0.35098300
C -5.78912100 -1.64716900 0.44393800
C 7.25644000 -0.60477500 -0.36171000
C 7.91121200 0.58520300 -0.05039700
C 7.17102800 1.71147000 0.35104200
C 5.78913800 1.64713600 0.44395200
H 3.28774200 -2.88440700 -0.81476300
H 5.70037800 -2.75639500 -0.95561300
H 3.13220500 1.23512900 0.52357800
H -3.28777300 2.88445300 -0.81455400
H -5.70041100 2.75639000 -0.95555800
H -3.13219800 -1.23510200 0.52365000
H -1.95412500 3.45457400 0.99171300
H -0.26561500 3.91492300 0.64452300
H -1.45178400 3.89458900 -0.66662600
H 0.26562900 -3.91493100 0.64425600
H 1.45211400 -3.89448200 -0.66661300
H 1.95404500 -3.45442300 0.99183600
H -7.82659000 1.47565800 -0.67660000
H -8.99364800 -0.64318500 -0.12047300
H -7.68586400 -2.63838000 0.58899500
H -5.21579300 -2.51774800 0.75140400
H 7.82657900 -1.47573100 -0.67649700
H 8.99367500 0.64307700 -0.12032600
H 7.68589900 2.63831900 0.58905100
H 5.21582200 2.51773600 0.75137800

An-5 S_0

C 0.59552500 0.39340200 0.00006600
C -0.59552600 -0.39344800 0.00008000
C -0.20805300 -1.78876300 -0.00027100
N 1.22338000 -1.75292500 -0.00043000
C 1.70733800 -0.44720800 -0.00022000
C 0.20806700 1.78872300 -0.00013100
N -1.22337000 1.75288500 -0.00021800
C -1.70733700 0.44718200 -0.00009200
C -3.11279300 0.07306300 0.00004900
C 3.11278700 -0.07304300 -0.00005800

O 0.83801800 2.84532900 -0.00019500
O -0.83800600 -2.84537500 -0.00039800
C -1.96418900 3.00079200 -0.00022800
C 1.96421100 -3.00082800 -0.00059900
C 4.21410600 -0.91472500 -0.00037900
S 5.70236500 -0.04567000 0.00012300
C 4.86721900 1.47997000 0.00085900
C 3.51820700 1.31514400 0.00068500
C -3.51823500 -1.31512100 0.00135700
C -4.86724700 -1.47993100 0.00138200
S -5.70237200 0.04572000 -0.00021200
C -4.21409900 0.91476300 -0.00089100
H -2.58567300 3.09694900 0.89572400
H -1.22085500 3.79961000 0.00040500
H -2.58467900 3.09756300 -0.89682500
H 1.22089900 -3.79966300 -0.00066100
H 2.58517100 -3.09718700 -0.89690400
H 2.58525300 -3.09738200 0.89563100
H 4.25311800 -1.99142800 -0.00099300
H 5.42705600 2.40609100 0.00139700
H 2.80670700 2.13397900 0.00097700
H -2.80672400 -2.13395300 0.00211000
H -5.42709400 -2.40604500 0.00226700
H -4.25312700 1.99146400 -0.00205500

An-5 S_1
C 0.58027200 0.38793000 0.00021900
C -0.58025400 -0.38790700 0.00007100
C -0.18620100 -1.78467100 0.00008000
N 1.24344500 -1.75364600 0.00021500
C 1.74467900 -0.46396900 0.00025100
C 0.18622600 1.78467300 0.00032800
N -1.24346500 1.75364400 0.00015900
C -1.74469700 0.46400600 0.00001800
C -3.12313200 0.08579700 -0.00008700
C 3.12312300 -0.08580000 0.00003200
O 0.82327000 2.84029700 0.00052000
O -0.82327800 -2.84027800 0.00003300
C -1.98206000 3.00266400 0.00021700
C 1.98206600 -3.00265300 0.00039100
C 4.25144800 -0.91701000 -0.00023900
S 5.72495900 -0.02359100 -0.00048500
C 4.86401300 1.49337500 -0.00018700
C 3.52003900 1.31126300 0.00005800

C -3.52002400 -1.31126400 0.00021700
C -4.86399700 -1.49339300 0.00009500
S -5.72496200 0.02356700 -0.00042400
C -4.25147100 0.91699800 -0.00046800
H -2.60553300 3.09094100 0.89554300
H -1.24279200 3.80475100 0.00057700
H -2.60502400 3.09131700 -0.89543400
H 1.24281800 -3.80475900 0.00078600
H 2.60506600 -3.09138000 -0.89523000
H 2.60550300 -3.09084200 0.89574800
H 4.30613500 -1.99310100 -0.00036800
H 5.41145300 2.42709500 -0.00023500
H 2.79966700 2.12319700 0.00026300
H -2.79964000 -2.12318400 0.00045700
H -5.41143600 -2.42711400 0.00026400
H -4.30614500 1.99308700 -0.00086300

An-5 T_1
C 0.61809400 0.41124400 0.00549500
C -0.61808100 -0.41122300 0.00571500
C -0.22433200 -1.79099700 0.00433000
N 1.21318400 -1.74194800 0.00334300
C 1.74665300 -0.44005000 0.00290800
C 0.22436200 1.79098900 0.00366000
N -1.21318600 1.74192700 0.00339800
C -1.74663300 0.44000700 0.00341800
C -3.13916300 0.08383000 0.00009400
C 3.13915600 -0.08385000 -0.00015700
O 0.85037300 2.85354900 0.00334500
O -0.85035300 -2.85353500 0.00470300
C -1.94830100 2.98685800 0.00612300
C 1.94826900 -2.98691200 0.00582700
C 4.25263100 -0.92798900 -0.02448200
S 5.74557300 -0.05394100 -0.01862600
C 4.90017900 1.47023800 0.01667700
C 3.55323200 1.30564700 0.02297000
C -3.55324600 -1.30564400 0.02226700
C -4.90020200 -1.47023500 0.01575000
S -5.74556700 0.05397300 -0.01861400
C -4.25261000 0.92802300 -0.02377100
H -2.59240500 3.05693500 0.88948000
H -1.21185600 3.79099100 0.02862100
H -2.55979600 3.08101400 -0.89848900
H 1.21176600 -3.79098300 0.02882600

H 2.55916100 -3.08120000 -0.89918500
H 2.59287700 -3.05690600 0.88880600
H 4.29501200 -2.00428400 -0.04923800
H 5.45618400 2.39874500 0.03086300
H 2.84551100 2.12747300 0.04147100
H -2.84556800 -2.12751000 0.04033800
H -5.45622900 -2.39873900 0.02922700
H -4.29495600 2.00435200 -0.04740300

An-6 S_0
C 0.61865400 -0.35111200 0.05662400
C -0.61866400 0.35096200 0.05659300
C -0.33442500 1.76804500 0.03325400
N 1.09796800 1.83432800 -0.00197600
C 1.67048800 0.56091000 0.00308400
C 0.33438300 -1.76819600 0.03329900
N -1.09802800 -1.83446600 -0.00183400
C -1.67051600 -0.56103600 0.00314300
C -3.09052000 -0.31019900 -0.05466100
C 3.09049900 0.31021400 -0.05469500
O 1.04663000 -2.76764200 0.05891000
O -1.04668500 2.76747700 0.05900800
C -1.75066100 -3.12943000 0.05569100
C 1.75062400 3.12927800 0.05556400
C 4.14159400 1.17746100 -0.32486700
C 5.41417900 0.55711400 -0.30029000
C 5.34153700 -0.78078600 -0.00986800
S 3.71891400 -1.31790800 0.22162200
C -4.14167600 -1.17729500 -0.32503500
C -5.41420800 -0.55683600 -0.30043400
C -5.34144800 0.78103100 -0.00989500
S -3.71879100 1.31798200 0.22175200
H -2.49688200 -3.15914900 0.85447500
H -2.22028600 -3.39083900 -0.89910500
H -0.96812600 -3.86075700 0.26591600
H 0.96816600 3.86059300 0.26609900
H 2.49705600 3.15883300 0.85414800
H 2.22001100 3.39078300 -0.89932900
H 4.01235100 2.22470000 -0.55598600
H 6.34273400 1.08326300 -0.49302900
H 6.15616300 -1.48998500 0.07029700
H -4.01252100 -2.22451300 -0.55626900
H -6.34280600 -1.08287700 -0.49326100
H -6.15601500 1.49029000 0.07034500

An-6 S_1

C 0.60426600 -0.34619500 -0.00088900
C -0.60429700 0.34627000 -0.00093200
C -0.31322800 1.76625700 -0.01010800
N 1.11754100 1.83735100 -0.01257600
C 1.70727800 0.58061100 -0.00750800
C 0.31319400 -1.76620900 -0.01005800
N -1.11750200 -1.83734300 -0.01264800
C -1.70731100 -0.58060800 -0.00762300
C -3.10006000 -0.32114400 -0.00687600
C 3.10005800 0.32106800 -0.00687800
O 1.02729000 -2.76616800 -0.01439400
O -1.02725100 2.76626400 -0.01451500
C -1.75855600 -3.13888000 -0.01117400
C 1.75857200 3.13888600 -0.01095900
C 4.19784500 1.20176700 -0.04310000
C 5.44686900 0.55470300 -0.02559300
C 5.34457100 -0.81720000 0.02526600
S 3.70241800 -1.35618800 0.05030000
C -4.19788800 -1.20182400 -0.04296400
C -5.44688200 -0.55473200 -0.02543500
C -5.34456100 0.81718300 0.02530200
S -3.70240300 1.35615700 0.05019500
H -2.39154000 -3.26585500 0.87258800
H -2.35329300 -3.28903300 -0.91802400
H -0.95718900 -3.87899000 0.01343300
H 0.95718500 3.87896500 0.01399700
H 2.39177200 3.26564400 0.87268400
H 2.35308600 3.28930400 -0.91791700
H 4.10536700 2.27632600 -0.08555900
H 6.39437900 1.08274700 -0.05071500
H 6.14684900 -1.54441100 0.04614700
H -4.10540300 -2.27639100 -0.08528600
H -6.39441100 -1.08274800 -0.05043400
H -6.14684100 1.54439100 0.04618500

An-6 T_1

C 0.61354000 -0.35516900 -0.00014500
C -0.61352100 0.35517700 -0.00017400
C -0.32789700 1.76099500 -0.00007700
N 1.11627600 1.84552900 -0.00011400
C 1.70311300 0.58304200 -0.00012600
C 0.32790300 -1.76099200 -0.00013700

N -1.11627000 -1.84550700 -0.00008800
C -1.70310200 -0.58302100 -0.00012100
C -3.08543300 -0.31719800 -0.00005500
C 3.08544500 0.31721600 -0.00010900
O 1.03744000 -2.76725200 -0.00007900
O -1.03745700 2.76724900 -0.00003200
C -1.75242400 -3.14570000 -0.00035800
C 1.75242800 3.14571200 0.00015500
C 4.19477900 1.20862600 -0.00085800
C 5.43415800 0.56838200 -0.00060900
C 5.33286700 -0.81470500 0.00032600
S 3.68991700 -1.36588600 0.00085800
C -4.19474400 -1.20863400 -0.00036300
C -5.43414100 -0.56842500 -0.00021300
C -5.33288300 0.81466700 0.00024700
S -3.68994900 1.36589100 0.00047500
H -2.36595800 -3.29460300 0.89514800
H -2.36558900 -3.29444200 -0.89614200
H -0.94719000 -3.88256900 -0.00025000
H 0.94719000 3.88257700 0.00084500
H 2.36620300 3.29412100 0.89556900
H 2.36535800 3.29498600 -0.89570800
H 4.09525000 2.28328100 -0.00164600
H 6.38251800 1.09499400 -0.00112800
H 6.13951600 -1.53706800 0.00066700
H -4.09516900 -2.28328400 -0.00066400
H -6.38249400 -1.09505000 -0.00045500
H -6.13955600 1.53700200 0.00044900

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