Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

Supporting Information

A multi-input/multi-output molecular system based on lanthanide(III) complexes

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1. Experimental Section

1.1. Reagents and Materials

All reagents used in this study were purchased from commercial supplies and used as received unless otherwise stated. Diethylenetriaminepentaacetic acid (DTPA) dianhydride was purchased from Acros Organics. Stock solution of TbL3 (2 mM) was obtained by dissolving the compound in DMSO and filtered using a 0.22 μM filter (organic system). Milli-Q water was used to prepare aqueous solutions.

1.2. Methods

^{1}H and ^{13}C NMR spectra were recorded on a Bruker DRX-400 spectrometer. Electrospray ionization mass spectra (ESI-MS) were acquired on an LCQ Fleet electrospray mass spectrometer. UV-Vis spectra were measured on a Shimadzu UV-3600 UV-VIS-NIR spectrophotometer. Time-resolved luminescence and steady-state fluorescence spectra were recorded on a PerkinElmer FL6500 fluorescence spectrometer. Atomic force microscopy (AFM) images were obtained with a Nanosurf Flexion 300+ atomic force microscope. Light irradiation at different wavelengths was performed with LEDs light source (CEL-LEDS35). Elemental analyses were obtained using an Elementar varioEL cube elemental analyzer.

1.3. Synthesis of TbL3

*Synthesis of 4-((4-aminophenyl)diazenyl)-N,N-dimethylaniline (**DAA**).* 4'-Nitro-4-dimethylaminoazobenzene (2.702 g, 10 mmol) was dissolved in dioxane (10 mL), subsequently 2.5 ml aqueous solution of $Na_2S{\cdot}9H_2O$ (7.925 g, 33 mmol) was added dropwise under stirring in nitrogen. The reaction mixture was stirred at 80 ℃ for 3 h. The precipitate was collected by filtration, washed with water, and dried under vacuum. The crude product was purified using silica gel column chromatography (petroleum ether : ethyl acetate = 8 : 1) to afford **DAA** as a brown solid (2.065 g, yield: 86%). ^{1}H NMR ($CDCl_3$, 400 MHz, δ, ppm): δ 7.83 (d, J = 8.8 Hz, 2H, Ph), δ 7.74 (d, J = 8.4Hz, 2H, Ph), δ 6.75 (dd, J = 9.2, 8.8 Hz, 4H, Ph), δ 3.06 (s, 6H, $-CH_3$). ^{13}C NMR (DMSO-d_6, 100 MHz, δ, ppm): 151.25, 151.13, 143.19, 142.98, 123.92, 123.41, 113.45, 111.68, 39.89. ESI-MS found (calcd) for $C_{14}H_{16}N_4$

(*m/z*): 241.25 (241.15) $[M+H]^+$. Elemental analysis found (calcd) for $C_{14}H_{16}N_4$ (%): C, 69.91 (69.97); H, 6.64 (6.71); N, 23.29 (23.31).

*Synthesis of 2,2'-((((carboxymethyl)azanediyl)bis(ethane-2,1-diyl))bis((2-((4-((4-(dimethylamino)phenyl)diazenyl)phenyl)amino)-2-oxoethyl)azanediyl))diacetic acid (**L3-3H**).* It was synthesized according to the literature.[1] **DAA** (0.96 g, 4 mmol) in DMF (3 mL) was added dropwise to DTPA dianhydride (DTPAA) (1.8 g, 5 mmol) in DMF (8 ml) and triethylamine (1 mL) under stirring in nitrogen at 0 ℃. The ice bath was removed after 2 h and the reaction mixture was stirred at room temperature for 48 h. The reaction was quenched by H_2O (20 mL) and the solvent was evaporated to 1 mL. Acetone (50 mL) was added to the residue and the resulting precipitate was filtered, washed with anhydrous chloroform and ether, and dried under vacuum to give **L3-3H** as a yellow power (1.7 g, yield: 71%). ^{1}H NMR (DMSO-d_6, 400 MHz, δ, ppm): δ 10.52 (s, 2H, -NH), δ 7.86-7.68 (br, 12H, Ph), δ 6.77 (d, J = 8.8Hz, 4H, Ph), δ 3.56-3.44 (br, 10H, -CH_2-), δ 3.02 (s, 12H, -CH_3), δ 2.99-2.97 (br, 8H, -CH_2-). ^{13}C NMR (DMSO-d_6, 100 MHz, δ, ppm): 173.28, 169.65, 152.07, 148.08, 142.60, 140.15, 124.38, 122.50, 119.57, 111.48, 58.45, 55.62, 52.30, 50.76, 45.16, 39.79. ESI-MS found (calcd) for $C_{42}H_{51}N_{11}O_8$ (*m/z*): 838.50 (838.39) $[M + H]^+$. Elemental analysis found (calcd) for $C_{42}H_{51}N_{11}O_8$ (%): C, 60.51 (60.20); H, 6.06 (6.14); N, 18.24 (18.39).

*Synthesis of Tb(L3)(H_2O) (**TbL3**) and Eu(L3)(H_2O) (**EuL3**).* A solution of $Tb(NO_3)_3{\cdot}6H_2O$ (0.0344 g, 0.1 mmol) or $Eu(NO_3)_3{\cdot}6H_2O$ (0.0446 g, 0.1 mmol) in water (5 mL) was slowly added to the aqueous solution (10 mL) of the **L3-3H** (0.838 g, 0.1 mmol). The pH of the mixture was maintained at 6 by adding aliquots of NaOH (5 M). The mixture was stirred at 45 ℃ overnight and the solvent was evaporated. The residue was dissolved in distilled water (2 mL). The product was deposited by addition of aqueous solution into 50 mL of acetone and was collected by centrifugation. Then, the obtained yellow solid was dried in vacuum. **TbL3** (0.0728 g, yield: 72%): ESI-MS found (calcd) for $C_{42}H_{50}N_{11}O_9Tb$ (*m/z*): 1016.58 (1016.29) [M –

H_2O + Na]$^+$. Elemental analysis found (calcd) for $C_{42}H_{50}N_{11}O_9Tb$ (%): C, 48.25 (49.86); H, 4.80 (4.98); N, 14.57 (15.23). **EuL3** (0.0623 g, yield: 62%): ESI-MS found (calcd) for $C_{42}H_{50}N_{11}O_9Eu$ (*m/z*): 1010.25 (1010.28) [M – H_2O + Na]$^+$. Elemental analysis found (calcd) for $C_{42}H_{50}N_{11}O_9Eu$ (%): C, 49.01 (50.20); H, 4.87 (5.02); N, 16.13 (15.33).

1.4. Photoisomerization of TbL3

A DMSO solution of TbL3 (40 μM) in a 1 cm path length quartz cuvette was irradiated at 455 nm (54 mW cm^{-2}), 520 nm (71 mW cm^{-2}), or 620 nm (86 mW cm^{-2}), respectively, until its photostationary state was reached (no further changes in absorbance were observed). The thermal isomerization process was monitored by measuring the change in absorption intensity at 428 nm as a function of time at 25 °C.

1.5. Kinetic model

We consider the isomerization from *Z,Z* to *E,E* which includes two cascade reactions i.e., *Z,Z* → *E,Z* and *E,Z* → *E,E* reactions characterized by reaction rate constants k_1 and k_2, respectively. For convenience, the concentrations of *Z,Z*, *E,Z*, and *E,E* are represented by c_A, c_B, and c_C, respectively. Hence, the thermal isomerization can be described as $A \xrightarrow{k_1} B \xrightarrow{k_2} C$. According to the integrated rat law of consecutive reactions consisting of two first order reactions, equations 1–3 can be obtained, where $c_{A,0}$ is the initial concentration of *Z,Z*.

$$c_A = c_{A,0}e^{-k_1 t} \tag{1}$$

$$c_B = \frac{k_1 c_{A,0}}{k_2 - k_1}(e^{-k_1 t} - e^{-k_2 t}) \tag{2}$$

$$c_C = c_{A,0}\left(1 - \frac{k_2 e^{-k_1 t} - k_1 e^{-k_2 t}}{k_2 - k_1}\right) \tag{3}$$

From a mass and absorbance balance, equation 4 is obtained, where ε_A, ε_B, and ε_C are, respectively, the molar extinction coefficients of *Z,Z*, *E,Z*, and *E,E* and can be approximately assigned to that of PSS-455, PSS-520, and initial state, respectively. A_t is the absorbance of TbL3 at 428 nm at different time.

$$A_t = \varepsilon_A c_A + \varepsilon_B c_B + \varepsilon_C c_C \tag{4}$$

By substituting equations 1–3 and the molar extinction coefficients of three states into equation 4, equation 5 is obtained, which was used to measure the rate constants k_1 and k_2.

$$A_t = 1.3744 + \left(\frac{0.4408k_1 - 0.6632k_2}{k_2 - k_1} \right) e^{-k_1 t} + \frac{0.2224k_1}{k_2 - k_1} e^{-k_2 t} \quad (5)$$

1.6. Atomic force microscopy (AFM)

The DMSO/H_2O solutions of TbL3 (40 μM) with different water fraction (0%, 30%, 60%, 98%) were initially prepared. Aliquots of samples were then deposited onto freshly cleaved mica and incubated at 25 ℃ for 10 min. Filter paper was used to absorb excess liquid and the samples were allowed to dry in air before AFM imaging. AFM measurements were performed with Flexion 300+ AFM (Nanosurf, Switzerland) in tapping mode in air.

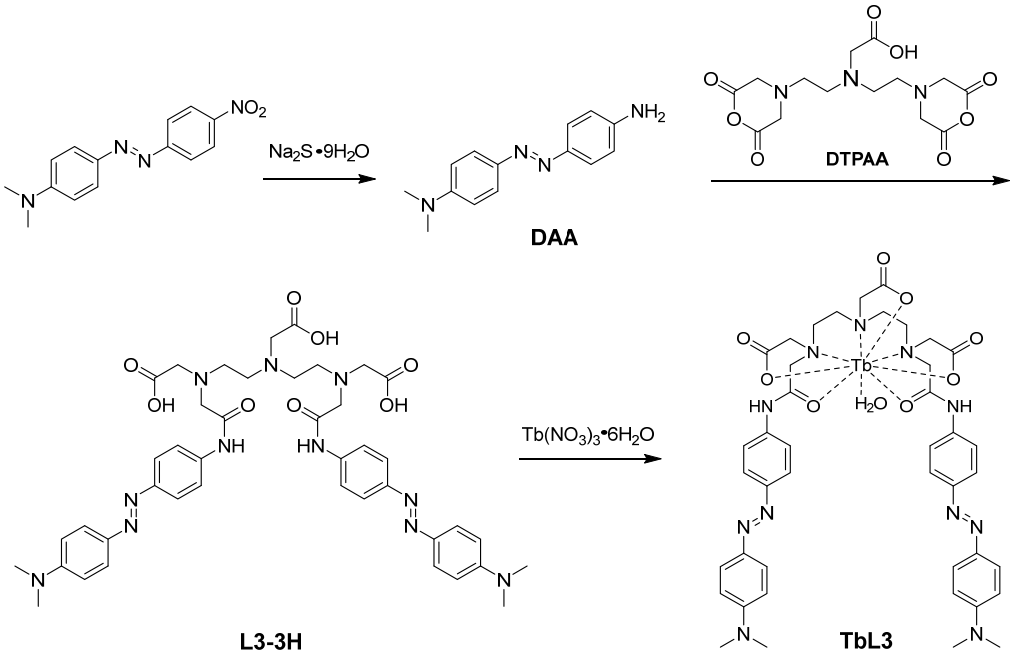
1.7. Time-resolved luminescence measurement

TbL3 (40 μM) was mixed with different concentrations of $Na_2S_2O_4$ (0, 1, 2, 3, 4, 5, and 6 mM) in DMSO/H_2O (f_w = 98%) for 5min. The time-resolved luminescence spectra (λ_{ex} = 256 nm) were measured at 25 ℃ with the following settings: delay time = 50 μs; gate time = 2 ms; cycle time = 20 ms.

1.8. Computational details

Geometry optimizations without symmetry restriction were performed by using Gaussian 16 A.03 program[2]. The calculations were carried out for all molecules using the B3LYP[3] functional with 6-31G(d)[4,5] basis set for metal free and SDD[6] basis set for terbium as well as dispersion correction by Grimme with Becke-Johnson damping D3(BJ)[7], which is termed as B3LYP+D3(BJ)/6-31G(d)/SDD. Time-dependent density functional theory (TD-DFT[8,9]) were further conducted at the the PBE0[10]+D3(BJ)/6-31G(d)/SDD level with solvent effect (i.e., DMSO) considered by using the (SMD[11]) model, for the PBE0 exchange–correlation functional is reliable in the previous studies[12-16]. Noncovalent interaction analysis was prepared using VMD and Multiwfn[17-19] at the at the B3LYP+(D3BJ)/6-31G(d)/SDD level. The structures were illustrated by CYLview[20].

2. Supplementary Schemes, Figures, and Tables



Scheme S1. Synthetic route of TbL3.

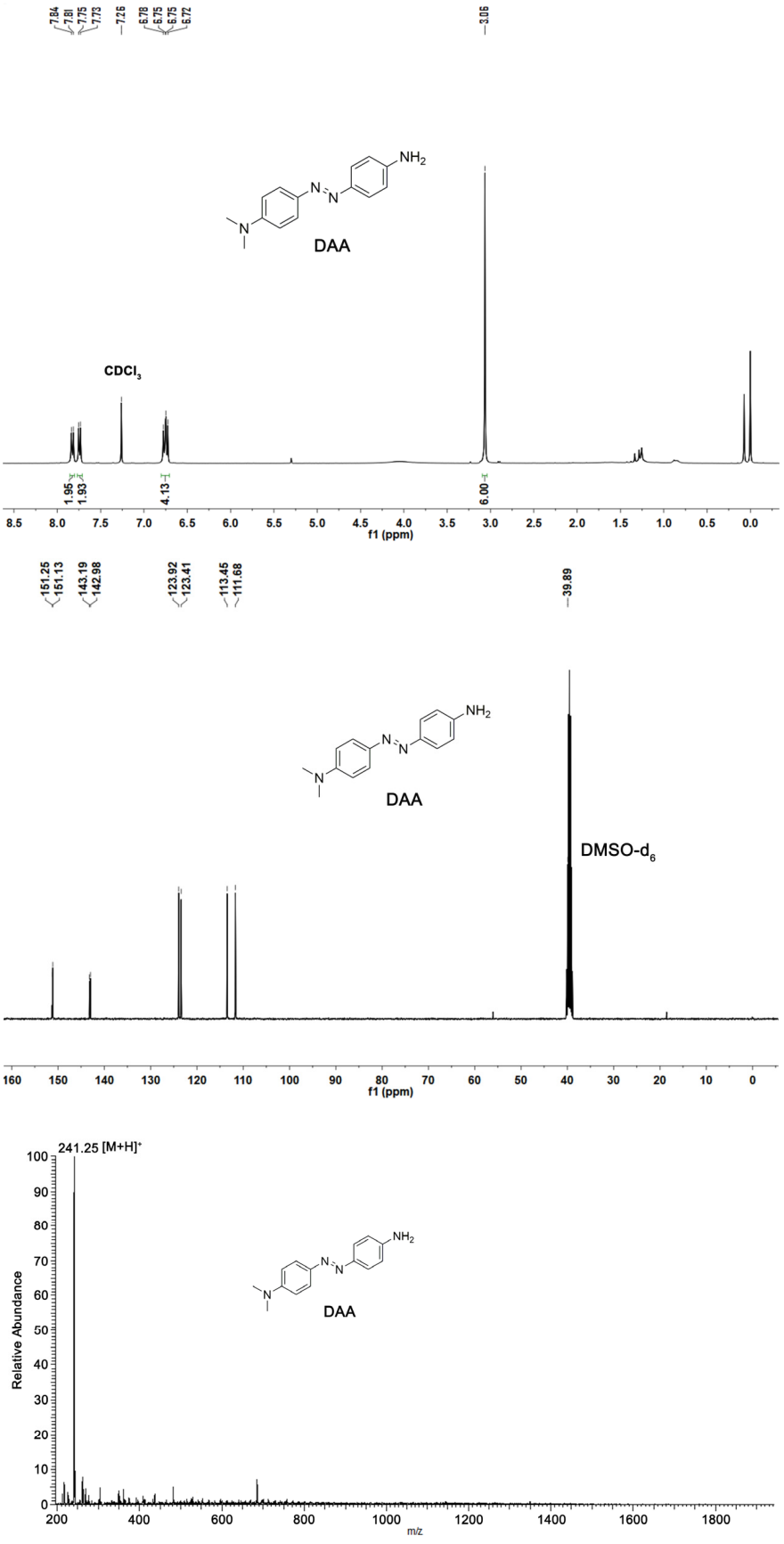


Fig. S1. ^{1}H NMR ($CDCl_3$), ^{13}C NMR (DMSO-d_6) and ESI-MS spectra for DAA.

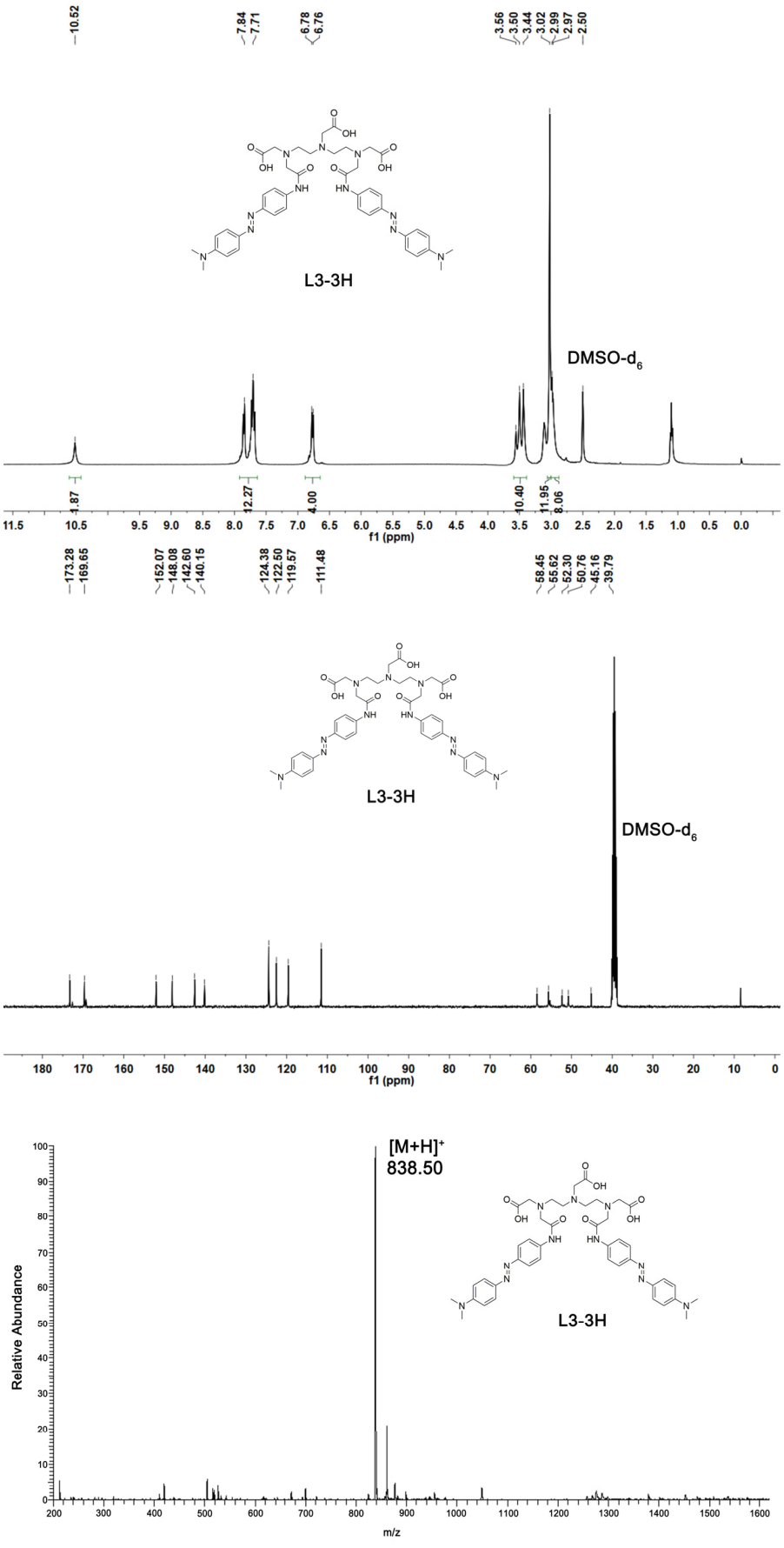


Fig. S2. ^{1}H NMR (DMSO-d_6), ^{13}C NMR (DMSO-d_6) and ESI-MS spectra for L3-3H.

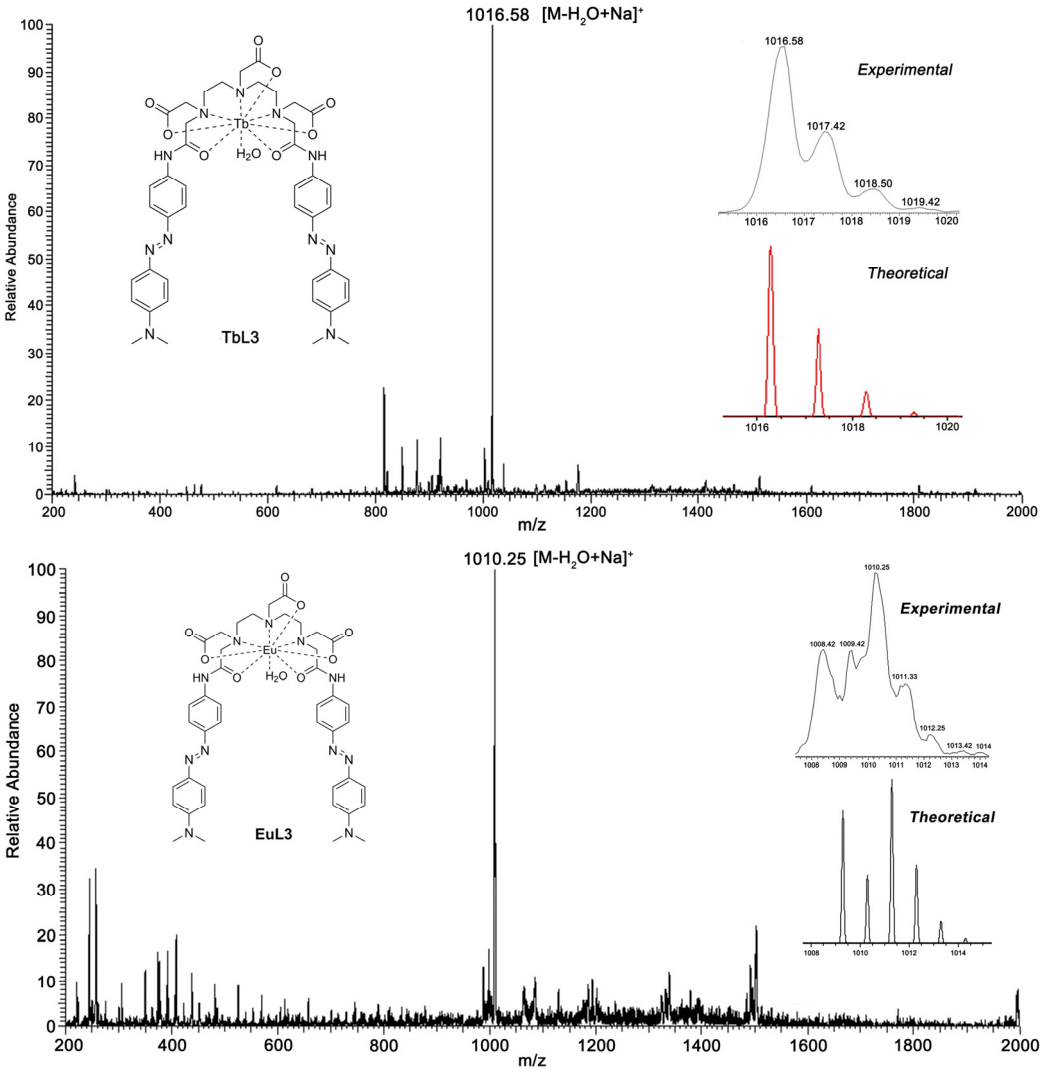


Fig. S3. ESI-MS spectra for TbL3 and EuL3.

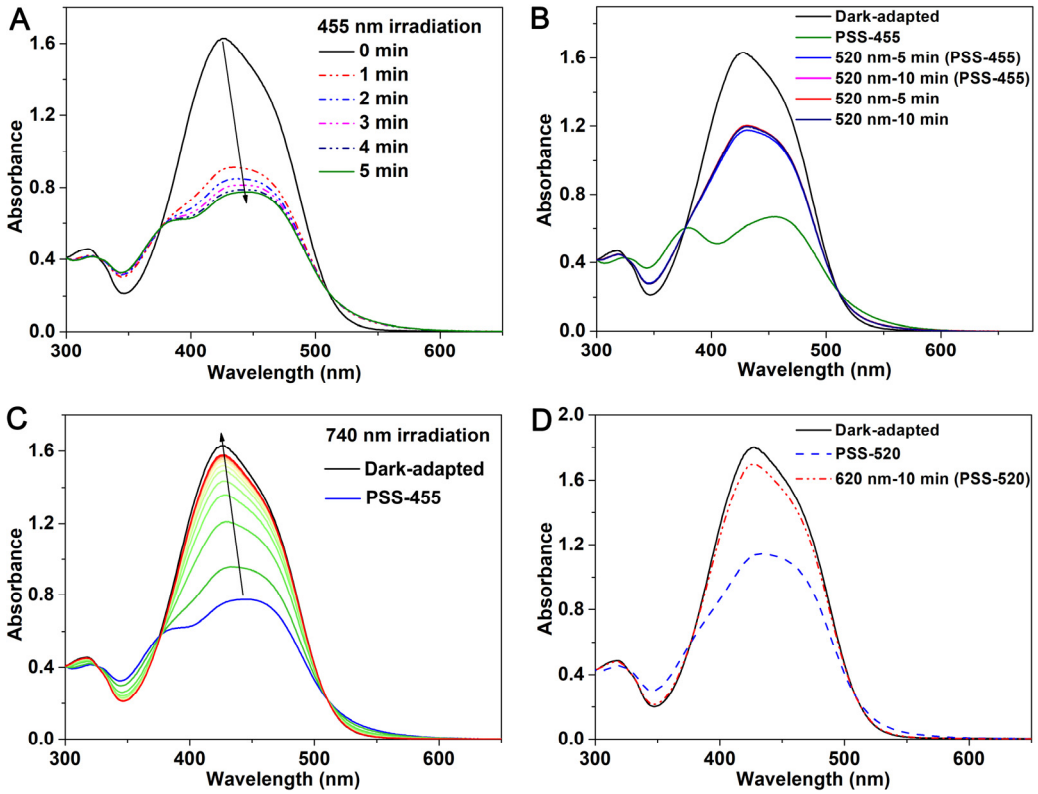


Fig. S4. (A) Changes in the absorption spectra of TbL3 upon irradiation at 455 nm. (B) Absorption spectra of TbL3 upon irradiation at 520 nm before and after irradiation at 455 nm. (C) Changes in the absorption spectra of TbL3 upon irradiation at 740 nm for 15 min after irradiation at 455 nm. The irradiation time interval is 1 min. (D) Absorption spectra of TbL3 upon irradiation at 620 nm after irradiation at 520 nm. All spectra were measured in DMSO; [TbL3] = 40 μM.

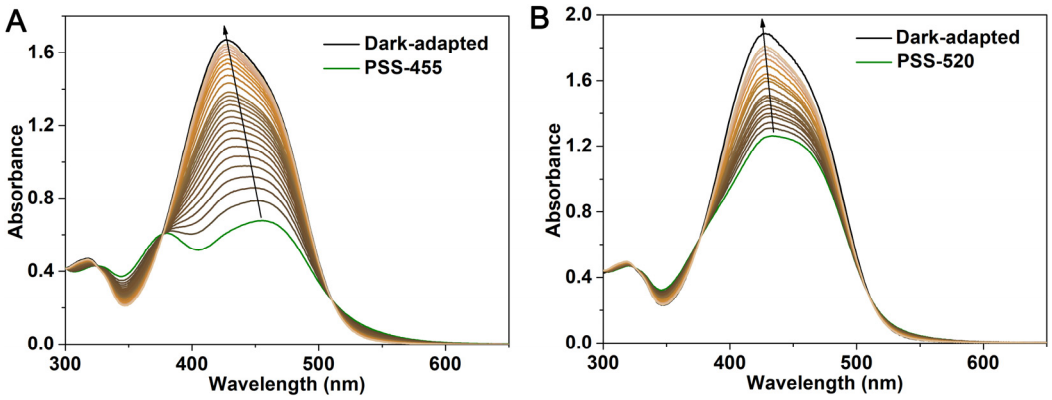


Fig. S5. Time-dependent absorption spectra variation of PSS-455 (A) and PSS-520 (B) under dark at room temperature for 65 and 80 min, respectively. All spectra were measured in DMSO; [TbL3] = 40 μM.

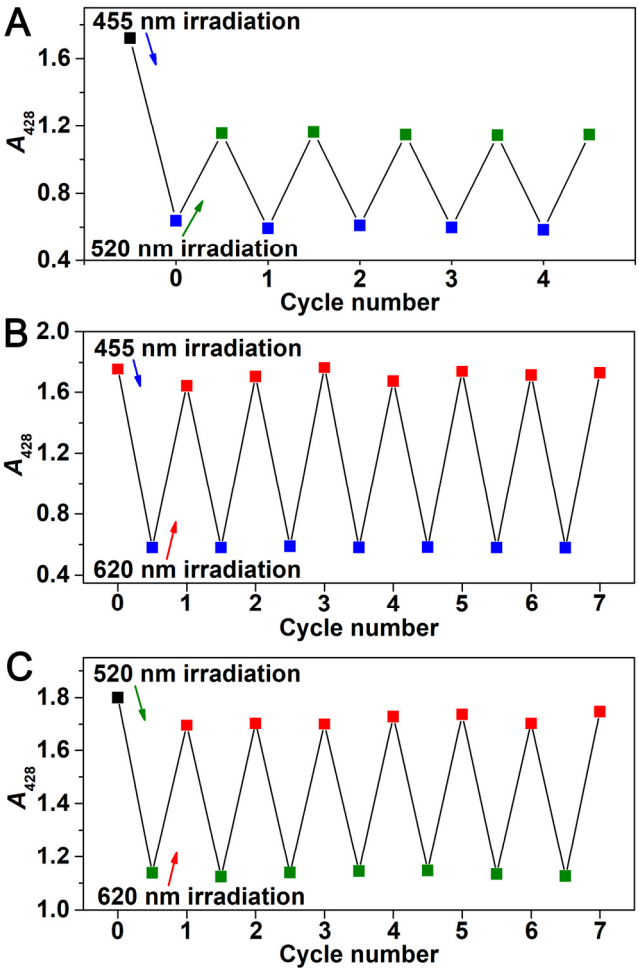


Fig. S6. Reversible changes of absorbance at 428 nm of TbL3 (40 μM) in PSS subjected to irradiation at 455 nm, 520 nm, and 620 nm.

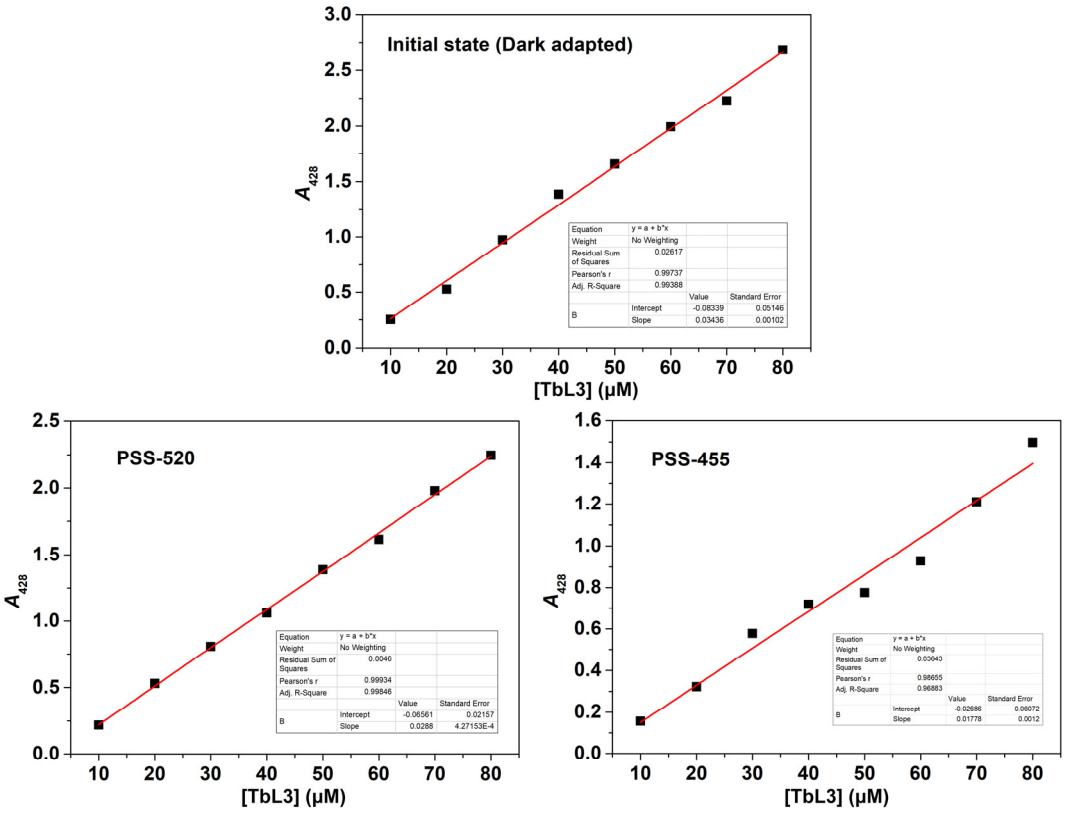


Fig. S7. Graph of the ratio between absorbance and concentration of TbL3 at different PSS, including initial state, PSS-520, and PSS-455.

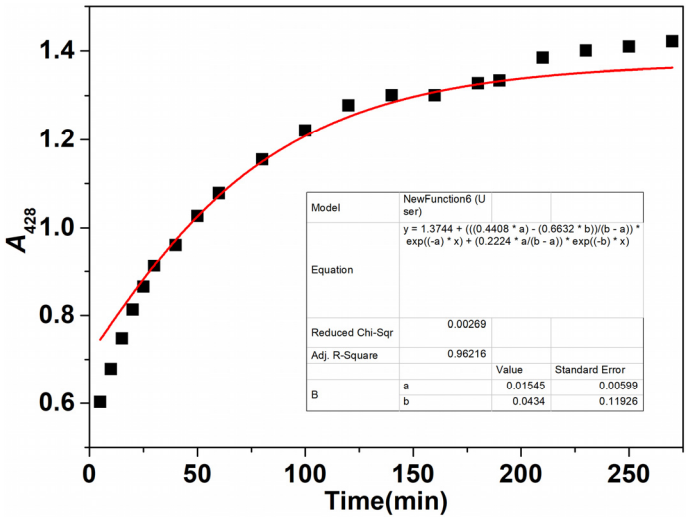


Fig. S8. Time-dependent absorption changes at 428 nm upon thermal back isomerization at room temperature of a solution of TbL3 at PSS-455. The experimental data are fitted with a kinetics model comprising two consecutive first order elementary reactions (equation 5).

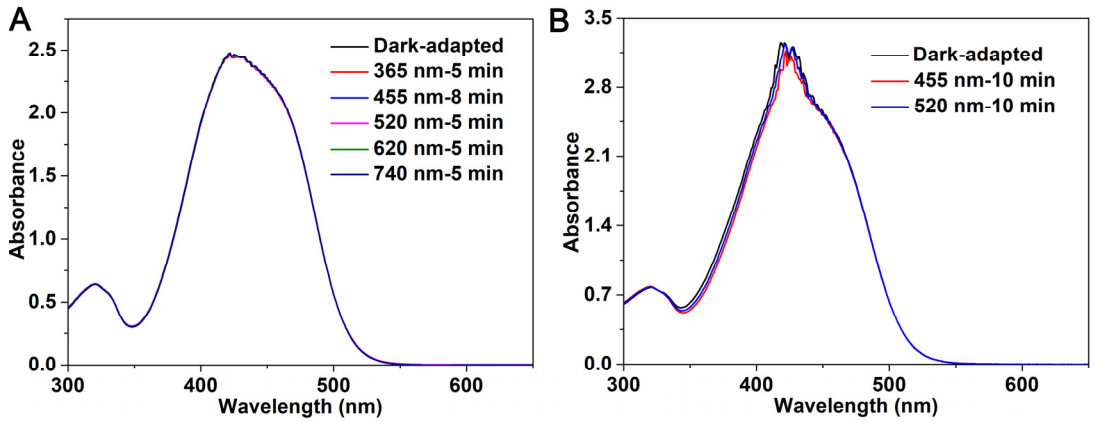


Fig. S9. Absorption spectra of L3-3H (40 μM) in the absence (A) and presence (B) of Zn^{2+} (40 μM) in DMSO upon irradiation at different wavelengths.

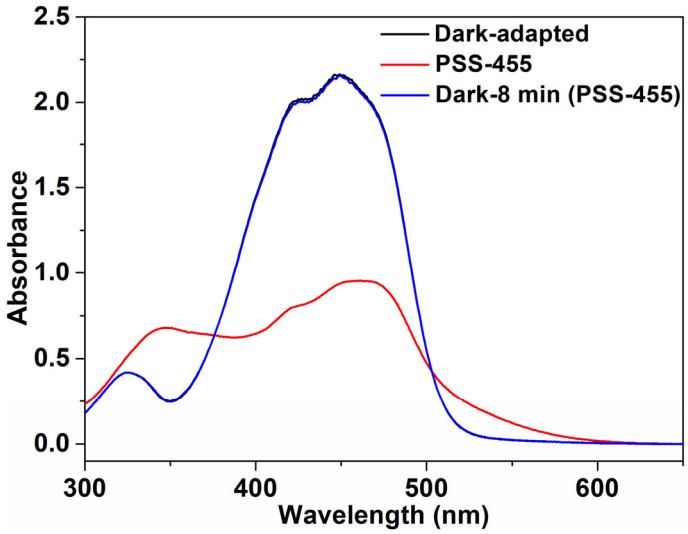


Fig. S10. Absorption spectra of DAA (40 μM) with or without irradiation at 455 nm in DMSO, followed by dark treatment.

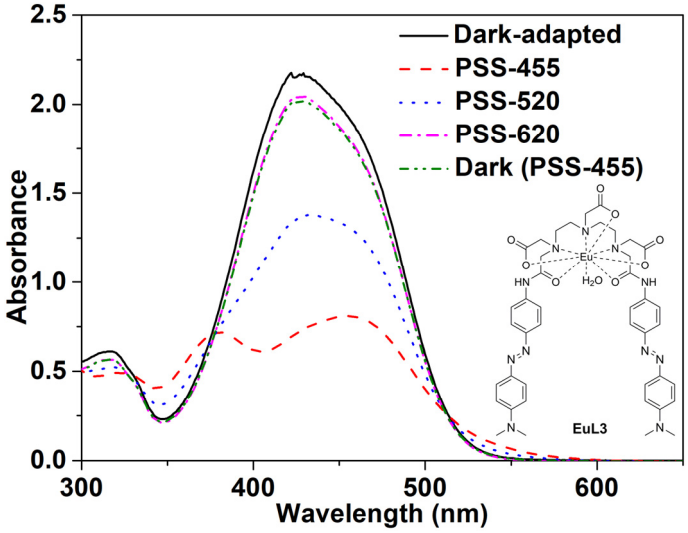


Fig. S11. Absorption spectra of EuL3 (40 μM) in different states, i.e., initial state, PSS-455, PSS-520, PSS-620, and dark-treatment from PSS-455 in DMSO at room temperature.

Table S1. Electronic energies (ΔE) of the isomers with different electronic ground states at the B3LYP+(D3BJ)/6-31G(d)/SDD level.

ΔE	Singlet	Triplet	Quintet	Septet
E,E-TbL3	504.0	112.6	70.6	0.0
E,Z-TbL3	504.1	111.4	15.8	0.0
Z,Z-TbL3	504.1	112.6	14.4	0.0

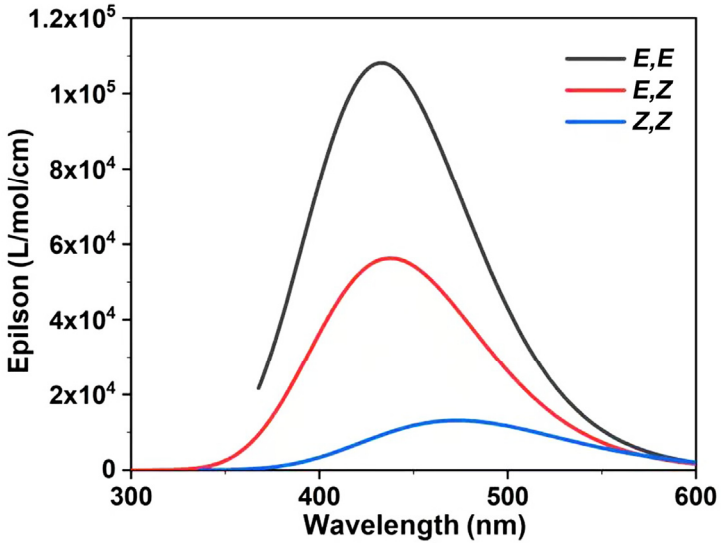


Fig. S12. Simulative UV-Vis spectra of the three isomers (*E*,*E*, *E*,*Z*, and *Z*,*Z*) of TbL3 at the PBE0+(D3BJ)/6-31G(d)/SDD (SMD, solvent=DMSO) level by time-dependent density functional theory calculations.

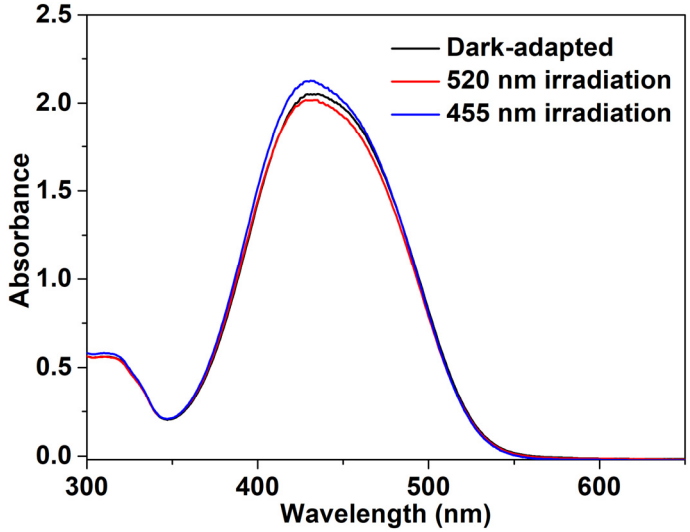


Fig. S13. Absorption spectra of TbL3 (40 μM) in DMSO/H_2O solution with 45% water content upon irradiation at 455 and 520 nm.

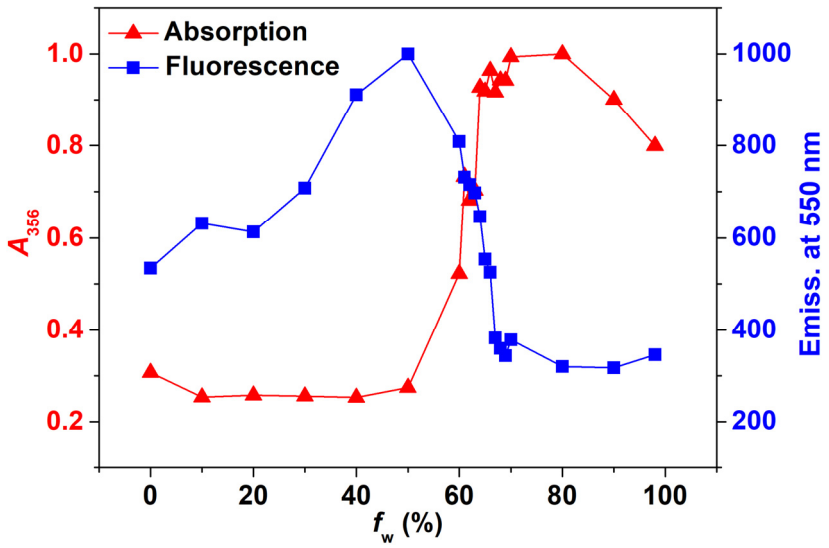


Fig. S14. The f_w-dependent changes of absorbance at 356 nm and steady-state fluorescence intensity at 550 nm of TbL3 (40 μM, λ_{ex} = 455 nm) in DMSO/H_2O mixed solvents.

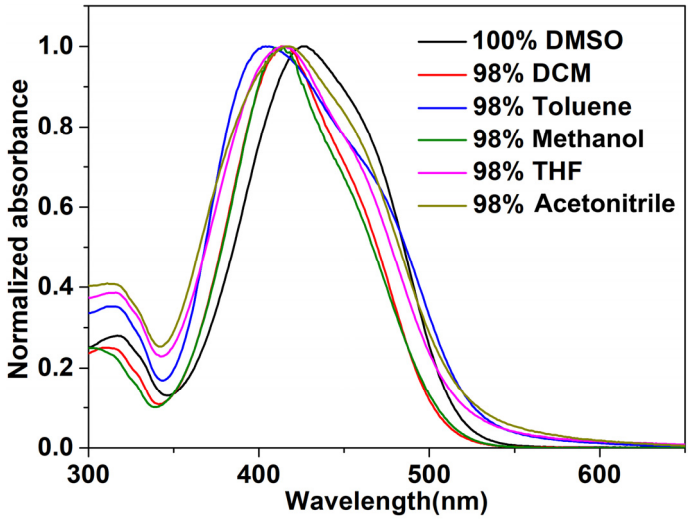


Fig. S15. Normalized absorption spectra of TbL3 (40 μM) in DMSO with or without other polar solvents (98%), including dichloromethane (DCM), toluene, methanol, tetrahydrofuran (THF), and acetonitrile.

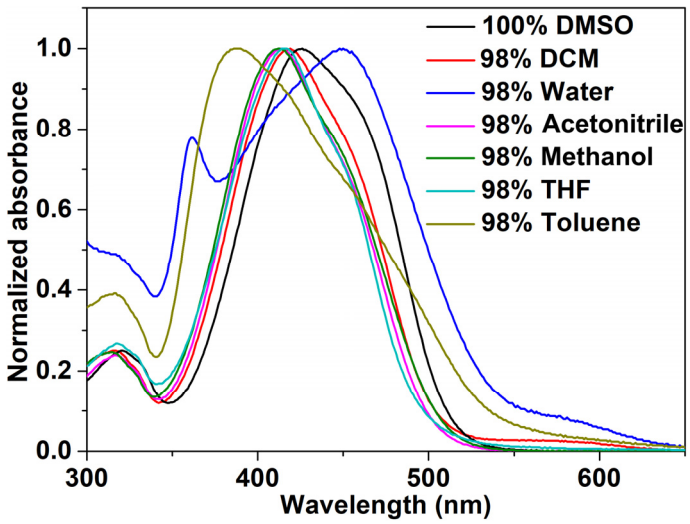
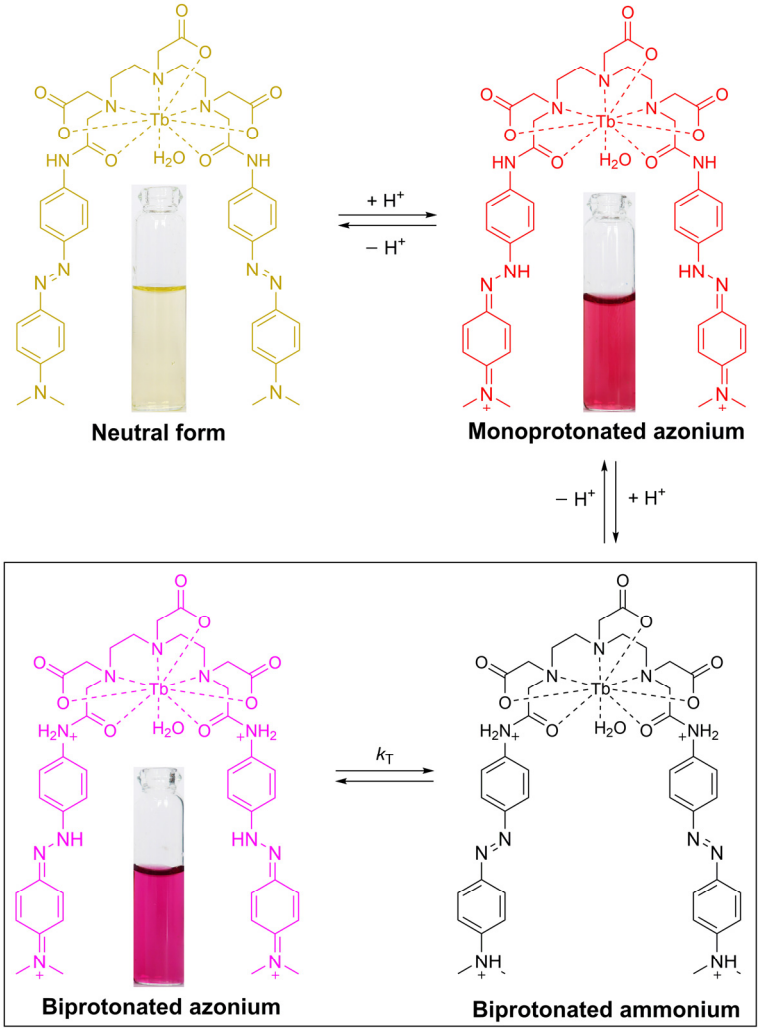


Fig. S16. Normalized absorption spectra of L3-3H (40 μM) in DMSO with or without other polar solvents (98%), including water, DCM, toluene, methanol, THF, and acetonitrile.



Scheme S2. The proposed protonation process of TbL3.

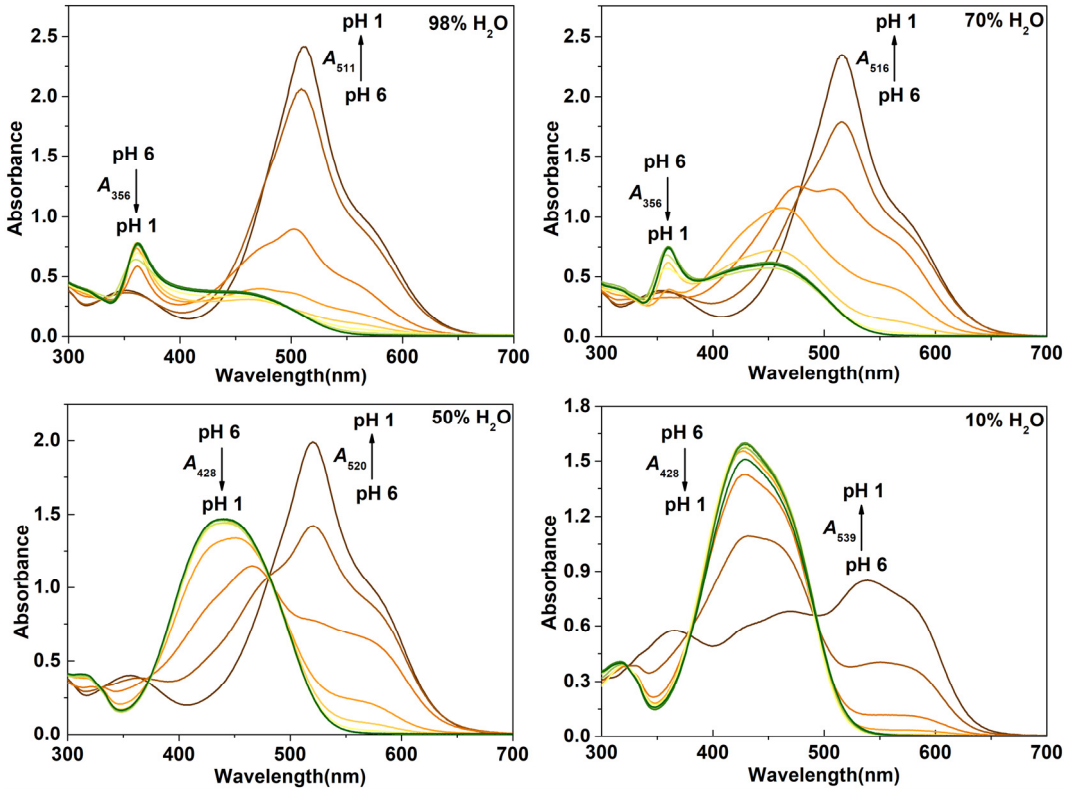


Fig. S17. pH-dependent changes of absorption spectra of TbL3 (40 μM) in DMSO/H_2O with different f_w (98%, 70%, 50%, and 10%) upon addition of 6 M HCl.

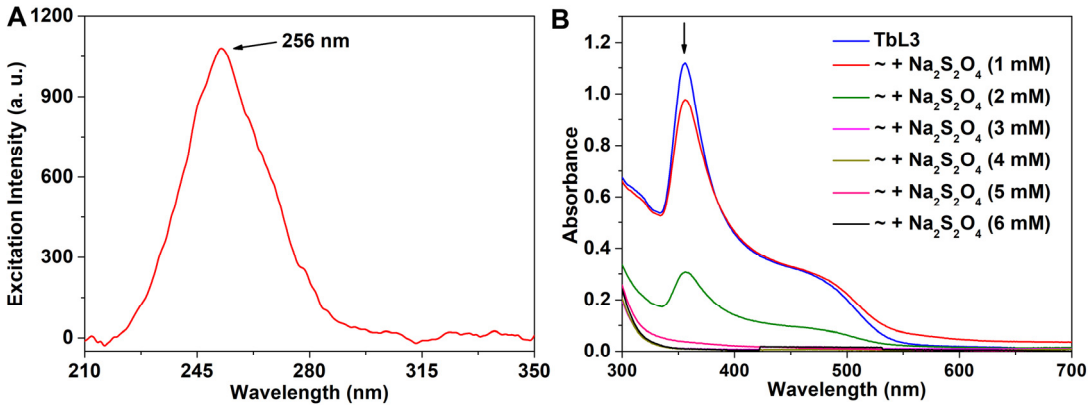


Fig. S18. Excitation (A) and Absorption (B) spectra of TbL3 (40 μM) in the presence of different concentrations of $Na_2S_2O_4$ in DMSO/H_2O (f_w = 98%).

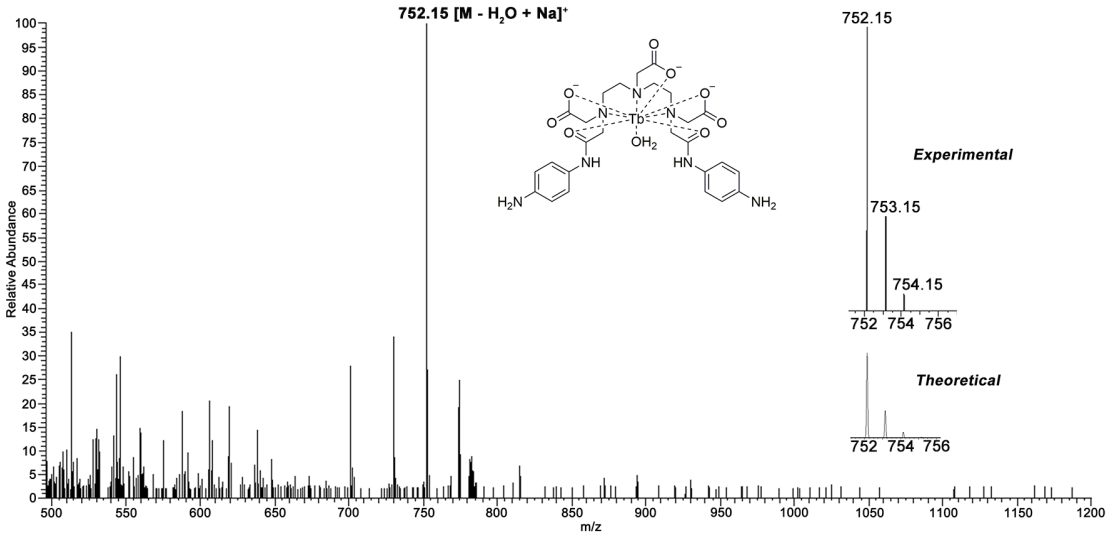


Fig. S19. The ESI-MS spectra of TbL3 in the presence of $Na_2S_2O_4$.

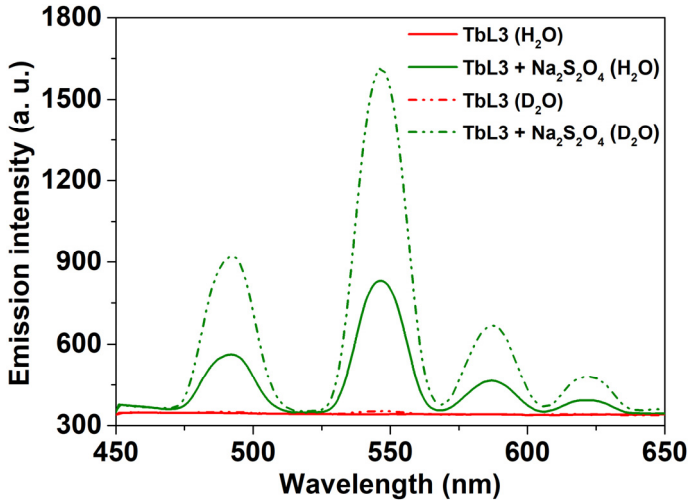


Fig. S20. The time-resolved luminescence spectra of TbL3 (40 μM, λ_{ex} = 256 nm) in the presence or absence of $Na_2S_2O_4$ (5 mM) determined in H_2O and D_2O (2% DMSO).

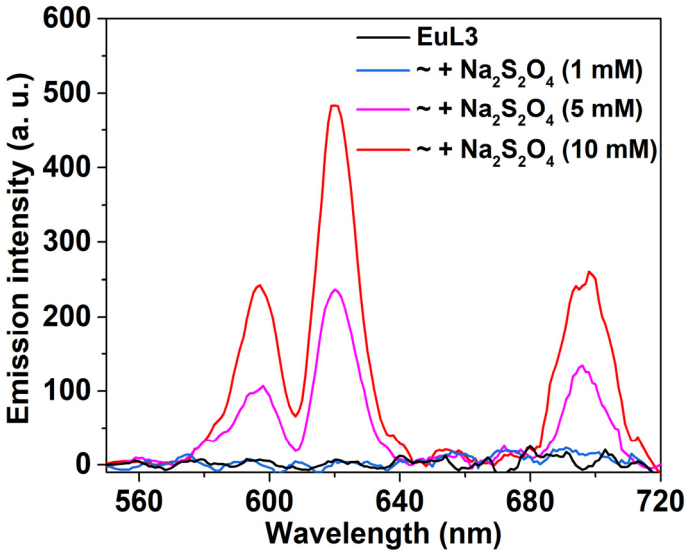


Fig. S21. The time-resolved luminescence spectra of EuL3 (40 μM, λ_{ex} = 256 nm) in the presence of different concentrations of $Na_2S_2O_4$ in DMSO/H_2O (f_w = 98%).

3. Appendix

Table S2. Coordinates and energies (a.u.) of the optimized structure at the B3LYP+(D3BJ)/6-31G(d)/SDD level by the Gaussian 16 software.

E,E

E = -3658.52736500

N	0.722005	-2.175062	2.325473
C	1.751286	-3.226067	2.515451
C	-0.497457	-2.582222	3.059647
C	-1.707943	-1.694396	2.786600
C	2.943322	-3.109392	1.565446
N	-2.041675	-1.605095	1.351352
N	2.566882	-3.130113	0.135901
C	1.254412	-0.854600	2.733638
C	2.110001	-0.218358	1.611729
O	3.170905	0.342575	1.890208
O	1.601548	-0.354245	0.435256
C	-2.763089	-0.365638	1.018308
C	-2.817487	-2.779333	0.873339
C	3.514132	-2.385073	-0.693449
C	2.316561	-4.500985	-0.347797
C	0.980137	-5.050341	0.202967
O	0.021241	-4.167530	0.195438

O	0.905997	-6.205364	0.593815
C	-2.257090	0.239334	-0.289918
C	2.785794	-1.641562	-1.807681
O	-1.051799	0.174214	-0.576870
O	1.592167	-1.900254	-2.086366
N	3.463804	-0.728396	-2.516442
N	-3.119252	0.929674	-1.059912
Tb	0.117672	-1.980023	-0.234901
C	-2.944318	-2.751511	-0.670127
O	-4.028270	-3.005989	-1.188423
O	-1.846396	-2.426345	-1.271044
H	1.270292	-4.196640	2.400913
H	2.143355	-3.179512	3.545107
H	-0.318709	-2.599368	4.147763
H	-0.717511	-3.606321	2.747385
H	-1.512036	-0.682347	3.149996
H	-2.557584	-2.078971	3.372811
H	3.634132	-3.935845	1.796048
H	3.478538	-2.181872	1.770464
H	0.417550	-0.173561	2.911220
H	1.836395	-0.924667	3.662189
H	-3.846462	-0.516641	1.006228
H	-2.553272	0.395894	1.777829
H	-2.273388	-3.690120	1.140768
H	-3.815200	-2.803713	1.331864
H	4.038813	-1.654571	-0.080881
H	4.284651	-3.027664	-1.148913
H	3.135831	-5.182434	-0.079074
H	2.236455	-4.466042	-1.439380
C	-4.540483	1.055019	-0.904766
C	-5.373912	-0.052135	-1.088258
C	-6.748727	0.109308	-0.933685
C	-7.298008	1.360877	-0.624265
C	-6.449026	2.469873	-0.460631
C	-5.076918	2.312406	-0.595402
N	-8.706088	1.401120	-0.499382
N	-9.171519	2.546758	-0.225317
C	-10.563175	2.612027	-0.096407

C	-11.102724	3.870952	0.207340
C	-12.467377	4.054236	0.357238
C	-13.360373	2.964804	0.206809
C	-12.806412	1.692095	-0.102174
C	-11.443934	1.523532	-0.248895
N	-14.717975	3.129282	0.354104
C	-15.615018	2.000816	0.177142
C	-15.261997	4.442207	0.650466
H	-4.955266	-1.023448	-1.339802
H	-7.422404	-0.731590	-1.061334
H	-6.887483	3.431506	-0.221702
H	-4.407062	3.156692	-0.457233
H	-10.417705	4.705459	0.322159
H	-12.843063	5.042346	0.590604
H	-13.455544	0.834299	-0.227465
H	-11.028514	0.550423	-0.485103
H	-15.401430	1.197509	0.894860
H	-16.641837	2.331873	0.337320
H	-15.546461	1.579944	-0.835392
H	-15.024748	5.168844	-0.138969
H	-16.347370	4.371037	0.730807
H	-14.875459	4.834718	1.600769
C	4.746193	-0.171226	-2.188803
C	5.797190	-0.306083	-3.097600
C	7.035221	0.255088	-2.799213
C	7.231721	0.937792	-1.590947
C	6.164064	1.065989	-0.684494
C	4.920010	0.526944	-0.983920
N	8.532260	1.455456	-1.387655
N	8.684735	2.049824	-0.279546
C	9.960574	2.573725	-0.049271
C	10.149853	3.232508	1.175184
C	11.371709	3.789965	1.512876
C	12.470521	3.708765	0.622333
C	12.271407	3.039432	-0.616556
C	11.047798	2.487934	-0.940541
N	13.690158	4.257930	0.942342
C	14.804705	4.154214	0.017113

C	13.872310	4.928293	2.217343
H	5.641689	-0.851219	-4.023838
H	7.872963	0.169283	-3.483439
H	6.325095	1.598852	0.244874
H	4.097022	0.633444	-0.279936
H	9.306950	3.293786	1.856648
H	11.476247	4.289046	2.467792
H	13.086940	2.955340	-1.324231
H	10.902886	1.978792	-1.886666
H	15.072270	3.107562	-0.182489
H	14.580842	4.637525	-0.943456
H	15.675277	4.649246	0.449134
H	13.195247	5.786726	2.323576
H	13.695002	4.248930	3.062406
H	14.897111	5.295087	2.286577
H	2.915900	-0.283769	-3.247164
H	-2.684806	1.356237	-1.872593

E,Z

E = -3658.5088948

N	1.634307	-1.346359	1.823363
C	2.893044	-2.127593	1.787957
C	0.570121	-2.202353	2.394843
C	-0.826628	-1.596944	2.293098
C	3.997120	-1.486047	0.946481
N	-1.203504	-1.256701	0.906542
N	3.604320	-1.222342	-0.453102
C	1.840732	-0.077621	2.559334
C	2.483346	0.999848	1.653170
O	3.412083	1.688576	2.078844
O	1.954677	1.060476	0.477668
C	-2.220715	-0.193065	0.848076
C	-1.673164	-2.441246	0.140687
C	4.291949	-0.060310	-1.015228
C	3.713289	-2.432672	-1.287385
C	2.591134	-3.438212	-0.939489
O	1.432558	-2.868104	-0.765120
O	2.843291	-4.629843	-0.842261

C	-1.924486	0.802056	-0.272620
C	3.372363	0.695448	-1.970966
O	-0.750724	1.111593	-0.531508
O	2.295866	0.197239	-2.370179
N	3.762448	1.915215	-2.374121
N	-2.956456	1.405490	-0.890405
Tb	0.936203	-0.692684	-0.637290
C	-1.834037	-2.088567	-1.358752
O	-2.829017	-2.476200	-1.964320
O	-0.862698	-1.372420	-1.824265
H	2.664113	-3.124590	1.414362
H	3.285968	-2.247108	2.811603
H	0.772375	-2.433118	3.453985
H	0.602004	-3.145134	1.842542
H	-0.875988	-0.682168	2.889198
H	-1.543392	-2.302726	2.741736
H	4.867079	-2.159553	0.981709
H	4.301509	-0.545770	1.406502
H	0.868818	0.315015	2.870050
H	2.449288	-0.230509	3.460453
H	-3.232440	-0.602357	0.773866
H	-2.180433	0.401598	1.767550
H	-0.914653	-3.226738	0.212214
H	-2.623321	-2.817144	0.543109
H	4.564236	0.625696	-0.213409
H	5.225340	-0.320867	-1.538132
H	4.694129	-2.916775	-1.173630
H	3.589085	-2.138101	-2.334383
C	-4.357788	1.128247	-0.746721
C	-4.891832	-0.077776	-1.209494
C	-6.256572	-0.310398	-1.056425
C	-7.091278	0.651737	-0.471947
C	-6.542949	1.867918	-0.027245
C	-5.181172	2.099137	-0.160682
N	-8.458788	0.304219	-0.376847
N	-9.186234	1.197377	0.150218
C	-10.543867	0.878521	0.256346
C	-11.369383	1.852932	0.837560

C	-12.729941	1.646632	0.993089
C	-13.327380	0.435075	0.565820
C	-12.484704	-0.547353	-0.023554
C	-11.129787	-0.328529	-0.172567
N	-14.676289	0.213458	0.714723
C	-15.269301	-1.028771	0.250973
C	-15.519905	1.238841	1.302101
H	-4.250940	-0.823559	-1.673029
H	-6.701512	-1.239308	-1.397574
H	-7.200238	2.602636	0.422408
H	-4.740773	3.028056	0.191120
H	-10.910835	2.781222	1.164396
H	-13.331860	2.424525	1.445300
H	-12.903212	-1.485930	-0.365282
H	-10.493440	-1.081677	-0.623269
H	-14.836358	-1.899239	0.761666
H	-16.339760	-1.013497	0.459360
H	-15.134367	-1.166291	-0.830616
H	-15.502278	2.166737	0.713790
H	-16.549008	0.879486	1.338087
H	-15.207734	1.480259	2.327116
C	4.792842	2.653999	-1.692844
C	6.105553	2.619346	-2.165902
C	7.123849	3.173220	-1.398293
C	6.819553	3.765157	-0.164584
C	5.491915	3.887717	0.253657
C	4.476986	3.301780	-0.495637
N	7.865469	4.308000	0.647219
N	8.754146	3.565241	1.132575
C	8.706503	2.142826	1.051987
C	7.561749	1.340923	1.216467
C	7.655958	-0.040402	1.165917
C	8.893045	-0.689218	0.927221
C	10.043455	0.126254	0.803964
C	9.945907	1.505711	0.901156
N	8.972376	-2.063337	0.840394
C	10.237731	-2.692436	0.506880
C	7.755873	-2.853682	0.809538

H	6.325752	2.121335	-3.105253
H	8.157479	3.109403	-1.720622
H	5.270720	4.352962	1.208107
H	3.463766	3.261458	-0.113543
H	6.594903	1.786632	1.416112
H	6.757277	-0.622330	1.323248
H	11.017486	-0.319343	0.646275
H	10.835842	2.123513	0.828749
H	10.611664	-2.380234	-0.479837
H	11.006299	-2.454380	1.252486
H	10.107132	-3.775363	0.496517
H	7.181211	-2.741977	1.738084
H	7.100719	-2.574474	-0.029883
H	8.012835	-3.908193	0.702787
H	3.077546	2.409651	-2.938352
H	-2.670858	2.099559	-1.574483

Z,Z

E = -3658.4882742

N	-1.582291	-1.750555	-1.852095
C	-2.746541	-2.511976	-1.341753
C	-0.633114	-2.704440	-2.468762
C	0.704436	-2.077845	-2.850753
C	-3.655707	-1.701545	-0.417125
N	1.378614	-1.426849	-1.708310
N	-2.957725	-1.126681	0.751471
C	-2.035653	-0.678539	-2.768321
C	-2.494808	0.572683	-1.982300
O	-3.541559	1.144735	-2.290878
O	-1.692235	0.896997	-1.025050
C	2.294960	-0.357597	-2.140398
C	2.109622	-2.404271	-0.859279
C	-3.556465	0.132018	1.195021
C	-2.798874	-2.117686	1.831322
C	-1.735981	-3.174716	1.450467
O	-0.686632	-2.658161	0.875532
O	-1.934892	-4.357045	1.685221
C	2.250694	0.834817	-1.186612

C	-2.480915	1.079869	1.719137
O	1.169867	1.188295	-0.689867
O	-1.316033	0.682139	1.946317
N	-2.829641	2.358650	1.933478
N	3.375838	1.545245	-0.982952
Tb	-0.356105	-0.566910	0.166562
C	2.590255	-1.743775	0.456533
O	3.724562	-1.977418	0.865825
O	1.706409	-0.972036	0.997789
H	-2.375406	-3.397555	-0.827980
H	-3.362677	-2.861494	-2.187164
H	-1.067055	-3.171962	-3.368205
H	-0.470861	-3.497104	-1.733558
H	0.549898	-1.323131	-3.625913
H	1.339098	-2.859179	-3.297113
H	-4.468325	-2.367970	-0.090216
H	-4.114320	-0.890540	-0.982988
H	-1.195264	-0.364425	-3.392960
H	-2.838242	-1.029007	-3.430535
H	3.313268	-0.729140	-2.288272
H	1.954364	0.044264	-3.101098
H	1.420597	-3.209111	-0.584986
H	2.964458	-2.830854	-1.400892
H	-4.041297	0.623236	0.351264
H	-4.329003	-0.004750	1.967722
H	-3.750282	-2.616037	2.067209
H	-2.448092	-1.594582	2.726680
C	4.705450	1.251880	-1.436844
C	5.393189	0.134419	-0.947379
C	6.686280	-0.119565	-1.391078
C	7.308204	0.747089	-2.304019
C	6.602644	1.848129	-2.805410
C	5.309088	2.107935	-2.361610
N	8.574135	0.443034	-2.890843
N	9.604143	0.182313	-2.221357
C	9.707435	0.361069	-0.818791
C	10.607910	-0.498760	-0.171150
C	10.825544	-0.424076	1.194222

C	10.190178	0.574411	1.972465
C	9.341273	1.489324	1.297853
C	9.097808	1.376796	-0.059562
N	10.402918	0.668715	3.328437
C	9.664974	1.643020	4.113021
C	11.229284	-0.317662	4.001432
H	4.922605	-0.527844	-0.224313
H	7.225188	-0.982705	-1.016112
H	7.079314	2.488030	-3.541093
H	4.756672	2.962171	-2.742441
H	11.116553	-1.249308	-0.768207
H	11.501299	-1.132102	1.656731
H	8.866390	2.294746	1.843812
H	8.446735	2.098975	-0.536316
H	8.578715	1.495473	4.033772
H	9.946492	1.544288	5.162102
H	9.894134	2.669581	3.797943
H	12.254506	-0.315022	3.609270
H	11.276494	-0.079526	5.064755
H	10.825549	-1.334710	3.894638
C	-4.020960	2.933108	1.365253
C	-5.195654	2.993106	2.116742
C	-6.382864	3.372187	1.500402
C	-6.384094	3.697554	0.136797
C	-5.187258	3.734018	-0.583390
C	-4.006228	3.318471	0.022304
N	-7.605274	4.062434	-0.512916
N	-8.544915	3.237618	-0.629745
C	-8.421104	1.861840	-0.279156
C	-9.575507	1.273043	0.255593
C	-9.596294	-0.057291	0.644322
C	-8.465633	-0.885050	0.444474
C	-7.331725	-0.302587	-0.174767
C	-7.304376	1.039204	-0.519032
N	-8.471741	-2.212974	0.816911
C	-7.245932	-2.985948	0.745733
C	-9.613771	-2.755884	1.530568
H	-5.180780	2.701326	3.162463

H	-7.316934	3.373930	2.051639
H	-5.203041	3.992419	-1.636593
H	-3.099324	3.203402	-0.559383
H	-10.454477	1.896141	0.389872
H	-10.497844	-0.457879	1.090267
H	-6.463095	-0.907667	-0.399190
H	-6.418465	1.429889	-1.004807
H	-6.879688	-3.062574	-0.286142
H	-6.442951	-2.548371	1.358685
H	-7.435467	-3.997439	1.106900
H	-9.784302	-2.249059	2.492311
H	-10.530130	-2.669831	0.933839
H	-9.442164	-3.814996	1.727387
H	3.238620	2.355968	-0.387161
H	-2.057538	2.963852	2.197161

***E,E*-monomer**

E = -3734.96013

N	-0.114268	-1.723209	2.490709
C	1.118806	-2.477961	2.799728
C	-1.324526	-2.519875	2.768967
C	-2.598300	-1.808736	2.303893
C	2.376308	-1.687655	2.423698
N	-2.571986	-1.479334	0.859687
N	2.451319	-1.446649	0.964258
C	-0.103605	-0.431983	3.218140
C	0.413474	0.694627	2.305207
O	1.194240	1.535822	2.751808
O	-0.035249	0.605619	1.099694
C	-3.113878	-0.134001	0.599383
C	-3.298291	-2.494082	0.067173
C	3.095091	-0.159955	0.637312
C	3.161155	-2.551544	0.284603
C	2.749739	-2.634680	-1.198935
O	1.461427	-2.674560	-1.351181
O	3.603135	-2.657591	-2.079242
C	-2.747579	0.353163	-0.799486
C	2.740485	0.282094	-0.777059

O	-1.589636	0.219831	-1.226887
O	1.588876	0.135935	-1.221605
N	3.676342	0.919366	-1.507773
N	-3.676968	1.009354	-1.521223
Tb	-0.034302	-1.304091	-0.195929
C	-2.802656	-2.514079	-1.395023
O	-3.610050	-2.477477	-2.318011
O	-1.511034	-2.578961	-1.480560
H	1.075429	-3.422115	2.250756
H	1.167328	-2.715671	3.876255
H	-1.421706	-2.736915	3.846960
H	-1.212581	-3.471039	2.243393
H	-2.744632	-0.885497	2.867924
H	-3.462991	-2.443479	2.540099
H	3.261160	-2.239295	2.772488
H	2.384912	-0.725219	2.937085
H	-1.117313	-0.166231	3.522887
H	0.493339	-0.494009	4.135132
H	-4.194957	-0.083932	0.774179
H	-2.607288	0.568499	1.268618
H	-3.081179	-3.475662	0.502006
H	-4.383711	-2.332980	0.112254
H	2.690534	0.622342	1.290548
H	4.180378	-0.202919	0.781662
H	2.866389	-3.491014	0.764435
H	4.249221	-2.442973	0.385655
O	-0.126726	-4.021261	0.285019
H	0.656944	-3.953980	-0.307259
H	-0.843833	-3.913966	-0.379898
C	-5.097109	0.982763	-1.303233
C	-5.815384	-0.185903	-1.574274
C	-7.190923	-0.194120	-1.357473
C	-7.851498	0.949891	-0.887845
C	-7.116912	2.121068	-0.630936
C	-5.743879	2.133601	-0.837519
N	-9.248672	0.821202	-0.707985
N	-9.815812	1.869604	-0.279344
C	-11.198701	1.770881	-0.095684

C	-11.847075	2.919428	0.383190
C	-13.214483	2.938108	0.601322
C	-13.999984	1.787467	0.343666
C	-13.336134	0.627347	-0.142309
C	-11.972078	0.622491	-0.355001
N	-15.358655	1.789234	0.554986
C	-16.144945	0.601469	0.270893
C	-16.016336	2.989138	1.040767
H	-5.290834	-1.065331	-1.942509
H	-7.782065	-1.082984	-1.553007
H	-7.642575	2.996635	-0.268930
H	-5.158996	3.026336	-0.636195
H	-11.244562	3.801034	0.579438
H	-13.675999	3.844993	0.970692
H	-13.901332	-0.272061	-0.353244
H	-11.472718	-0.265082	-0.726711
H	-15.821255	-0.253957	0.878931
H	-17.191904	0.802339	0.501219
H	-16.078185	0.312411	-0.786809
H	-15.889325	3.831477	0.346873
H	-17.084343	2.795033	1.146386
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C	5.093854	0.900851	-1.280629
C	5.806402	-0.289758	-1.456191
C	7.181113	-0.288795	-1.235657
C	7.847666	0.886046	-0.859937
C	7.119346	2.077721	-0.698163
C	5.746415	2.080998	-0.905460
N	9.244012	0.764441	-0.668676
N	9.819659	1.843054	-0.338698
C	11.202276	1.749156	-0.144492
C	11.861061	2.931708	0.223840
C	13.228776	2.958359	0.440947
C	14.003276	1.781189	0.296144
C	13.329134	0.586900	-0.079416
C	11.964920	0.574532	-0.292674
N	15.362089	1.789842	0.511196
C	16.139433	0.577291	0.325785

C	16.032918	3.028183	0.863406
H	5.278702	-1.192744	-1.756234
H	7.767446	-1.193769	-1.358168
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H	11.266697	3.833525	0.334409
H	13.698613	3.892188	0.722344
H	13.886049	-0.333578	-0.204053
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H	15.804711	-0.223802	0.998121
H	16.076247	0.204466	-0.705971
H	17.186769	0.786752	0.546908
H	15.644913	3.443627	1.803106
H	17.098210	2.834346	0.994566
H	15.917851	3.791588	0.081224
H	3.340486	1.221272	-2.417837
H	-3.336576	1.319920	-2.427027

***E,E*-dimer**

E = -7317.1996575

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C	-0.400596	-4.345440	-1.884453
C	3.938950	-2.641591	-3.502044
N	-0.920686	-2.964057	-2.018296
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C	2.006005	-2.364093	-0.319364
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O	2.186403	-1.323122	-1.054987
C	-1.522080	-2.537018	-0.740969
C	-1.899487	-2.890499	-3.134138
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C	1.626832	-2.639378	-5.671153
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O	1.530980	-3.540452	-6.494252

C	-1.597872	-1.021541	-0.610446
C	3.354750	0.699122	-3.056766
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O	2.106293	0.819808	-3.177549
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O	-3.441999	-1.106807	-3.581104
O	-1.251668	-0.647702	-3.655300
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H	1.150485	-5.649476	-2.571200
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H	4.845973	-2.922375	-4.063303
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H	-15.958977	-0.374084	3.947178
H	-3.478314	0.551010	-2.922999
H	1.641250	-0.444388	1.142936

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