Supporting Information

Stereoisomeric Engineering of Aggregation-Induced Emission Photosensitizers towards Fungal Killing

Wenping Zhu,[a] † Ying Li,[b] † Shaoxun Guo,[a] Wu-Jie Guo,[a] Tuokai Peng,[a] Hui Li,[a] Bin Liu,[a] Hui-Qing Peng,*[a][d] and Ben Zhong Tang*[c]

[a] Beijing Advanced Innovation Center for Soft Matter Science and Engineering, State Key Laboratory of Chemical Resource Engineering Beijing University of Chemical Technology, Beijing 100029, China
[b] Guangzhou Municipal and Guangdong Provincial Key Laboratory of Molecular Target & Clinical Pharmacology, the NMPA and State Key Laboratory of Respiratory Disease, School of Pharmaceutical Sciences and the Fifth Affiliated Hospital Guangzhou Medical University, Guangzhou 511436, China
[c] School of Science and Engineering, Shenzhen Institute of Aggregate Science and Technology, The Chinese University of Hong Kong Shenzhen, Guangdong 518172, China
[d] Guangdong Provincial Key Laboratory of Luminescence from Molecular Aggregates, South China University of Technology, Guangzhou 510640, China

*Corresponding Author: hqpeng@mail.buct.edu.cn (Hui-Qing Peng);
tangbenz@cuhk.edu.cn.(Ben Zhong Tang)

Materials and Instruments.

All reagents were purchased from commercial suppliers (Energy Chemical, Sigma-Aldrich, TCI) and used without further purification. ^{1}H NMR and ^{13}C NMR spectra were measured on a Bruker Advance III (400 MHz) instrument using $CDCl_3$ and D_2O and DMSO-d_6 as the solvent and tetramethylsilane as the internal reference. The mixed solvent of DMSO-d_6 and D_2O (*v*: *v*, 1:5) was used in the ^{1}H NMR titration experiment. X-Ray single-crystal diffraction data were collected on a Gemini E X-ray diffraction (Agilent, Oxford) with graphite-monochromator Mo-Kα (λ = 0.71073 Å) at 110 K. UV-Vis absorption spectra were measured by a SHIMADZU UV-2600i spectrophotometer. The photoluminescence spectra were measured by a SHIMADZU RF-600 spectro fluorophotometer. ROS assays were conducted by using a Xenon lamp (Microsolar300, Beijing Perfectlight). The quantum efficiencies were measured using an Edinburgh FS5 fluorescence spectrophotometer. Dynamic light scattering (DLS) investigations were carried out with a Malvern Zetasizer Nano ZS90 (Malvern Instruments, UK). ESR analysis was performed on a Bruker E 500 spectrometer. The lifetime of triplet states was determined on Edinburgh LP 980 spectrometer. High resolution Scanning electron microscope (HR-SEM) images were obtained using a Thermo APREOS instrument. The fluorescence images were taken by a confocal laser scanning microscope (CLSM, ZEISS-LSM900).

Syntheses of compounds

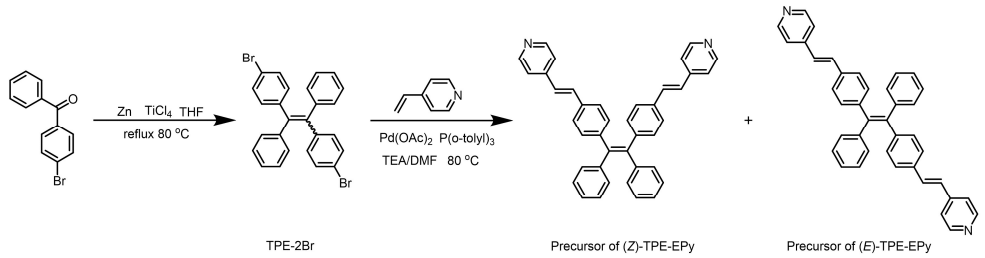
Synthesis of TPE-2Br. The synthetic procedures of 1,2-bis(4-bromophenyl)-1,2-diphenylethene (TPE-2Br) was reported in literature.[1]

Synthesis of the precursors of (*Z*)-TPE-EPy and (*E*)-TPE-EPy. Tris-o-tolylphosphine (100 mg, 20%) and Pd(II) $(OAc)_2$ (35 mg, 10%) and were introduced into a dry and degassed TEA/DMF (15 mL, v/v= 10:5) mixture, which was stirred for 15 min. The mixture was degassed again by gentle bubbling of nitrogen, and TPE-2Br (555 mg,1.0 equiv) and 4-vinylpyridine (215 μL, 1.3 equiv) were added. The system was stirred at 90 °C under nitrogen for 8 h. The resulting mixture was allowed to cool to RT, and TEA was removed in vacuo. The crude mixture was diluted with dichloromethane and washed with water and saturated $NaHCO_3$, after concentration, the residue was purified by column chromatography (Ethyl Acetate/ petroleum ether (60-90 °C) 1:50 to 2:1 with 1% TEA). (*Z*)-TPE-DPy was obtained in yield of 36%, then (*E*)-TPE-DPy was obtained in yield of 28%. (*Z*)-TPE-DPy ^{1}H NMR (400 MHz, $CDCl_3$): δ= 8.57 (d, J = 5.5 Hz, 4H), 7.51 (d, J = 5.9 Hz, 4H), 7.38 - 7.29 (m, 6H), 7.16 - 7.08 (m, 10H), 7.07 - 6.96 (m, 6H). (*E*)-TPE-DPy ^{1}H NMR (400 MHz, $CDCl_3$): δ= 8.58 (d, *J* = 6.1 Hz, 4H), 7.44 (d, *J* = 6.1 Hz, 4H), 7.35-7.28 (m, 6H), 7.21-7.15 (m, 6H), 7.13 -7.05 (m, 8H), 6.98 (d, *J* = 16.3 Hz, 2H).

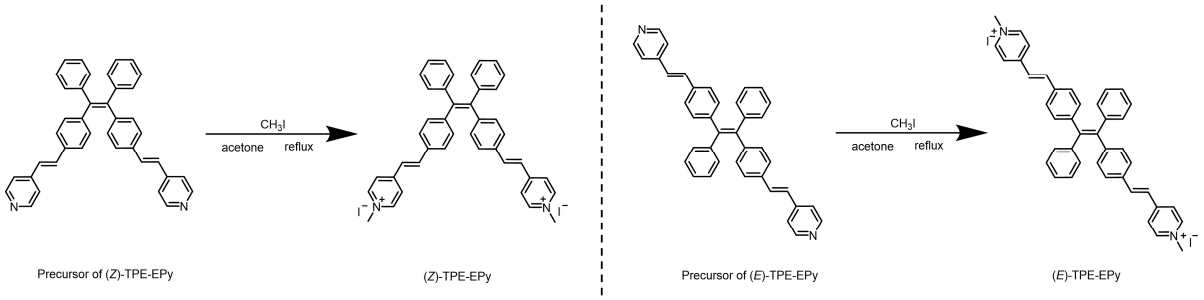
Synthesis of (*Z*)-TPE-EPy. Into a 50 mL two-necked round-bottom flask was placed (*Z*)-TPE-DPy (108 mg, 0.25 mmol). The flask was evacuated under vacuum and flushed with dry nitrogen three times. After

acetone (20 mL) was added and stirred for 10 min, a large excess of iodomethane (1mL) was injected dropwise via a hypodermic syringe. The mixture was allowed to react at 65 °C for 6 h and deep red precipitate was formed. The red precipitate was collected by filtration and washed with DCM for three times, then dried under vacuum at 40 °C to a constant weight. *(Z)*-TPE-EPy (red powder) was obtained in yield of 90%. (*Z*)-TPE-EPy ^{1}H NMR (400 MHz, DMSO-d_6) :δ=8.84 (d, *J* = 6.7 Hz, 4H), 8.17 (d, *J* = 6.7 Hz, 4H), 7.92 (d, *J* = 16.3 Hz, 2H), 7.56 (d, *J* = 8.3 Hz, 4H), 7.45 (d, *J* = 16.3 Hz, 2H), 7.24-7.15 (m, 6H), 7.13 (d, *J* = 8.2 Hz, 4H), 7.03-7.01 (m, 4H), 4.25 (s, 6H). ^{13}C NMR (101MHz, DMSO-d_6): δ=145.72, 145.54, 140.47, 131.98, 131.19, 128.47, 128.26, 127.46, 123.91, 123.78, 47.42. HRMS (MALDI-TOF): m/z ($[C_{42}H_{36}N_2]^{2+}$) = 284.1436; calcd = 284.1434.

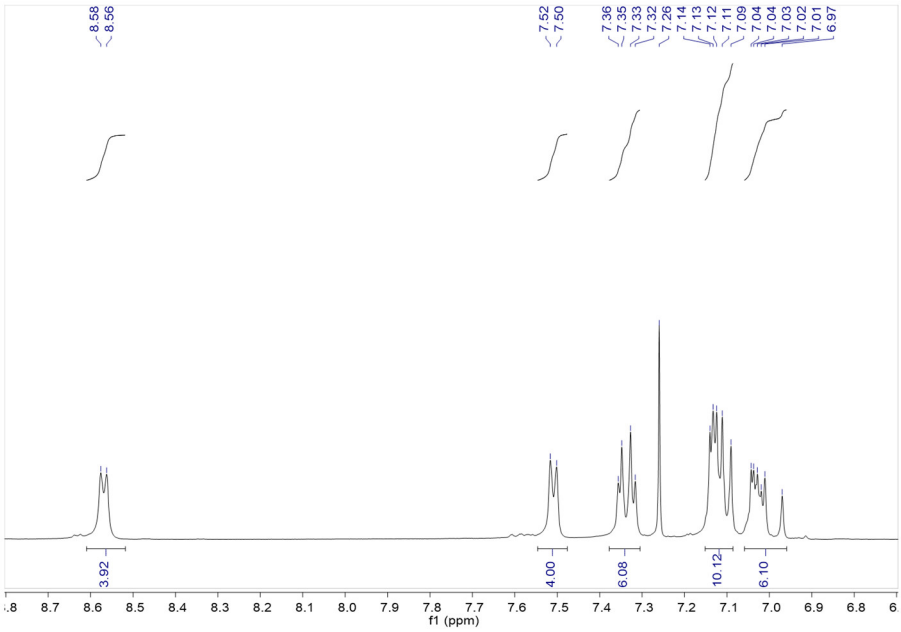
Synthesis of (*E*)-TPE-EPy. Into a 50 ml two-necked round-bottom flask was placed (*E*)-TPE-DPy (108 mg, 0.25 mmol). The flask was evacuated under vacuum and flushed with dry nitrogen three times. After acetone (20 mL) was added and stirred for 10 min, a large excess of iodomethane (1mL) was injected dropwise via a hypodermic syringe. The mixture was allowed to react at 65°C for 6 h and yellow precipitate was formed. The red precipitate was collected by filtration and washed with DCM for three times, then dried under vacuum at 40°C to a constant weight. *(E)*-TPE-EPy (yellow powder) was obtained in yield of 86%. (*E*)-TPE-EPy ^{1}H NMR (400 MHz, DMSO-d_6): δ=8.85 (d, *J* = 6.8 Hz, 4H), 8.18 (d, *J* = 6.8 Hz, 4H), 7.91 (d, *J* = 16.3 Hz, 2H), 7.54 (d, *J* = 8.3 Hz, 4H), 7.44 (d, *J* = 16.3 Hz, 2H), 7.23-7.17 (m, 6H), 7.11-7.01 (m, 8H), 4.25 (s, 6H). ^{13}C NMR (101 MHz, DMSO-d_6) δ =152.83, 145.66, 145.52, 143.05, 141.39, 140.48, 133.96, 131.89, 131.26, 128.60, 128.16, 127.60, 123.92, 123.73, 47.42. HRMS (MALDI-TOF): m/z ($[C_{42}H_{36}N_2]^{2+}$) = 284.1435; calcd = 284.1434.



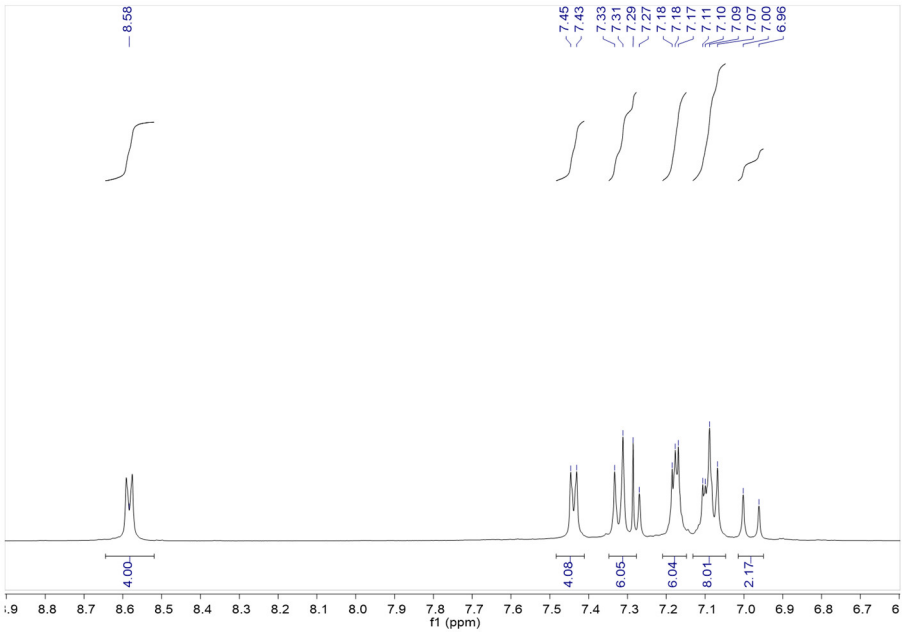
Supplementary Scheme S1. Synthetic route to the precursor of (*Z*)-TPE-EPy and (*E*)-TPE-EPy.



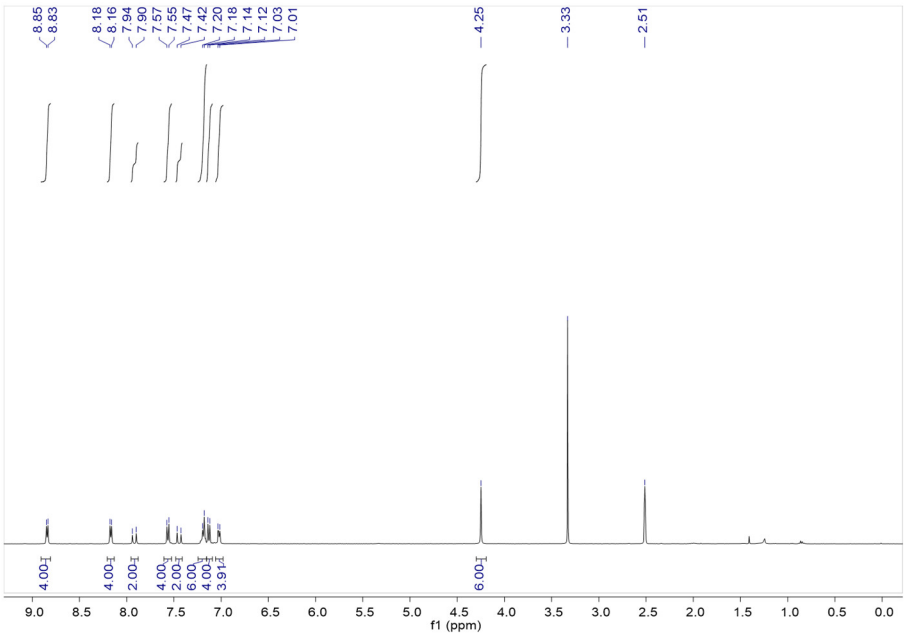
Supplementary Scheme S2. Synthetic route to (*Z*)-TPE-EPy and (*E*)-TPE-EPy.



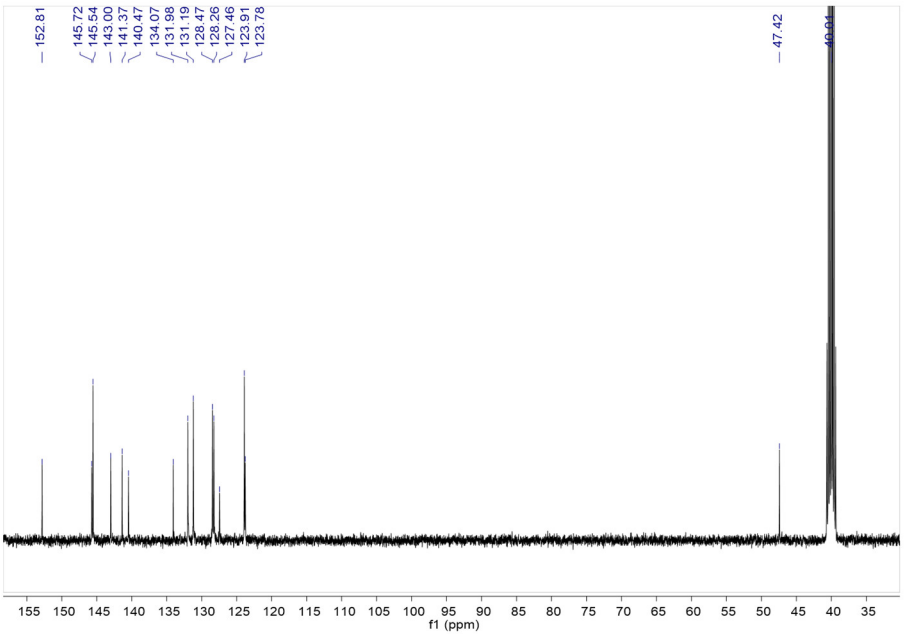
Supplementary Figure S1. ^{1}H NMR spectrum of the precursor of (*Z*)-TPE-EPy in $CDCl_3$.



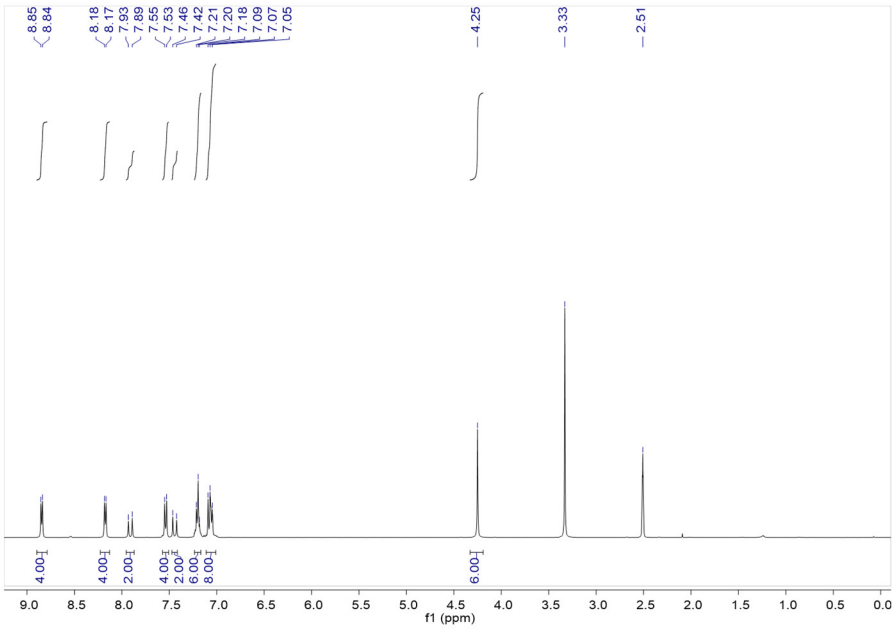
Supplementary Figure S2. ^{1}H NMR spectrum of the precursor of (*E*)-TPE-EPy in $CDCl_3$.



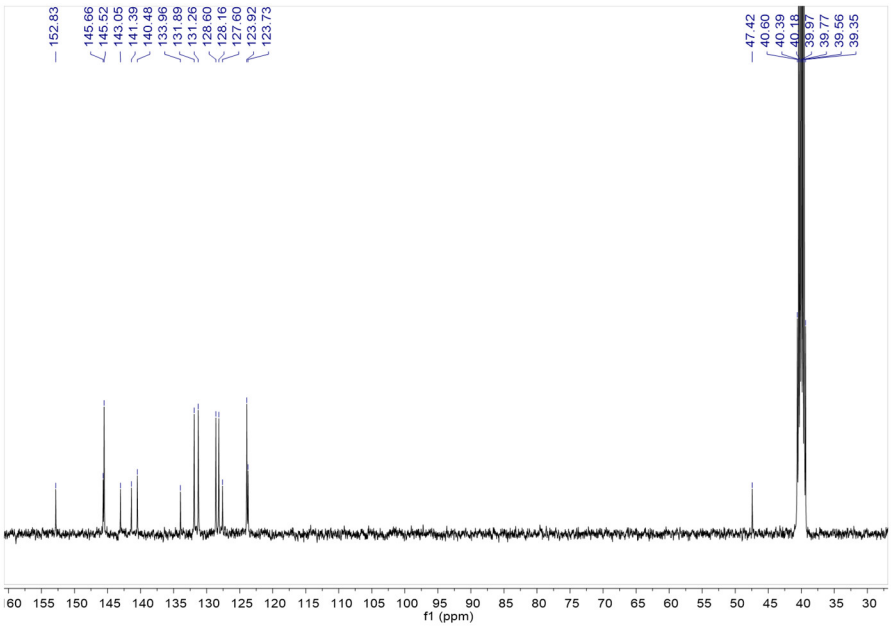
Supplementary Figure S3. ^{1}H NMR spectrum of (*Z*)-TPE-EPy in DMSO-d_6.



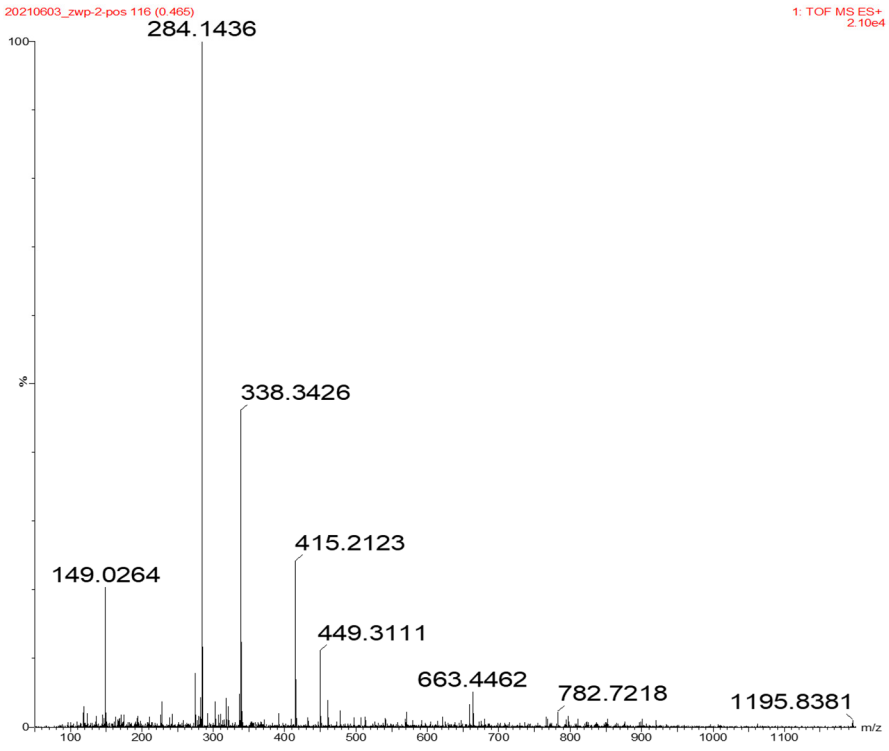
Supplementary Figure S4. ^{13}C NMR spectrum of (*Z*)-TPE-EPy in DMSO-d_6.



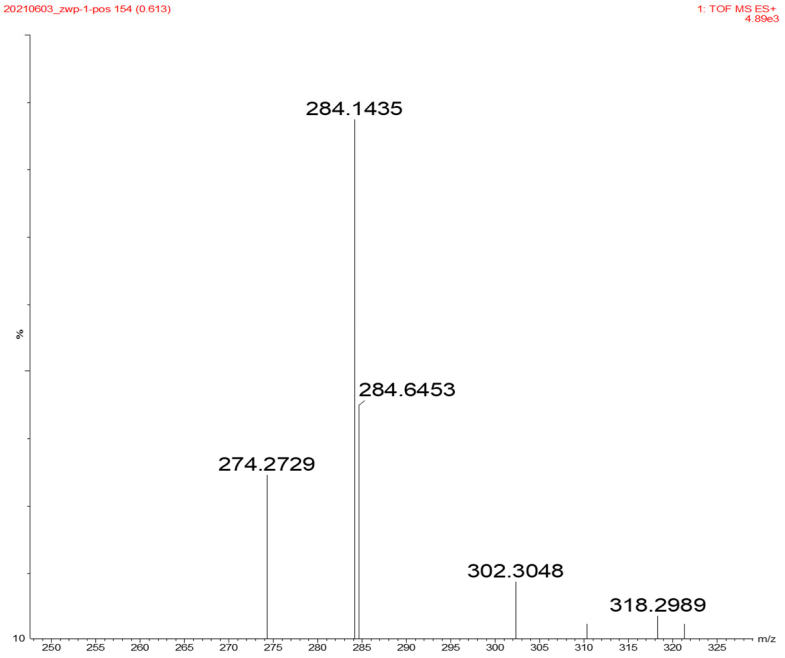
Supplementary Figure S5. ^{1}H NMR spectrum of (*E*)-TPE-EPy in DMSO-d_6.



Supplementary Figure S6. ^{13}C NMR spectrum of (*E*)-TPE-EPy in DMSO-d_6.



Supplementary Figure S7. HRMS spectra of (*Z*)-TPE-EPy.

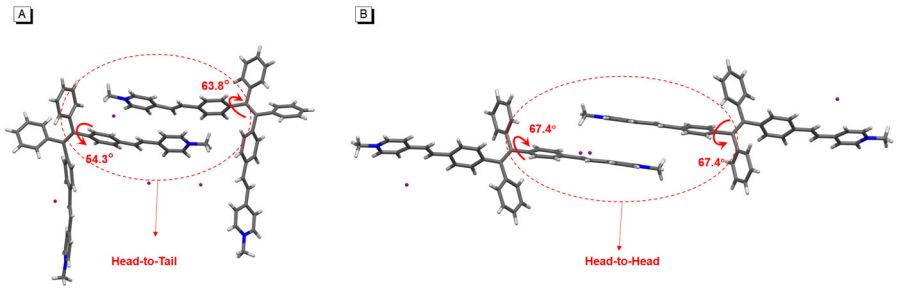


Supplementary Figure S8. HRMS spectra of (*E*)-TPE-EPy.

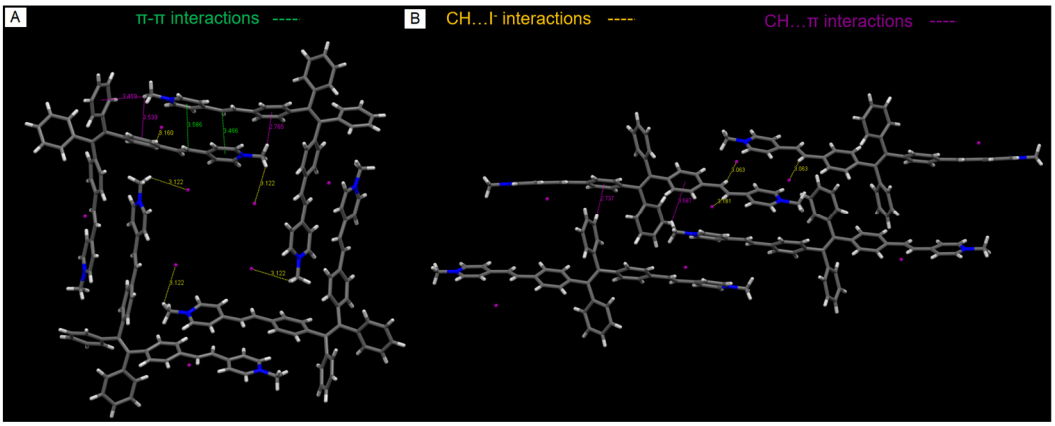
Supplementary Table S1. Crystallographic and structural refinement data of (*Z*)-TPE-EPy (CCDC 2165387) and (*E*)-TPE-EPy (CCDC 2165372). [a]

Identification code	(*Z*)-TPEEPy	(*E*)-TPE-EPy
Empirical formula	$C_{42}H_{36}I_2N_2$	$C_{42}H_{36}I_2N_2$
Formula weight	822.53	822.53
Temperature / K	170.00(14)	112.10(14)
Crystal system	Tetragonal	Monoclinic
Space group	$P4_2/n$	I_2/a
a / Å	42.1139(3)	17.058(2)
b / Å	42.1139(3)	16.4766(18)
c / Å	9.22650(10)	32.030(5)
α / °	90	90.00
β / °	90	103.272(16)
γ /°	90	90.00
Volume / $Å^3$	16363.9(3)	8762(2)
Z	16	8

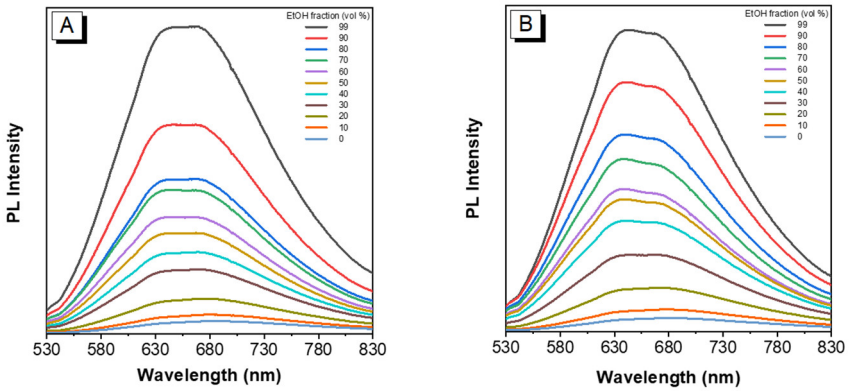
[a] Deposition Number 2165387 and 2165372 contains the supplementary crystallographic data for this paper. These data are provided free of charge by the joint Cambridge Crystallographic Data Centre and Fachinformationszentrum Karlsruhe Access Structures service www.ccdc.cam.ac.uk/structures.



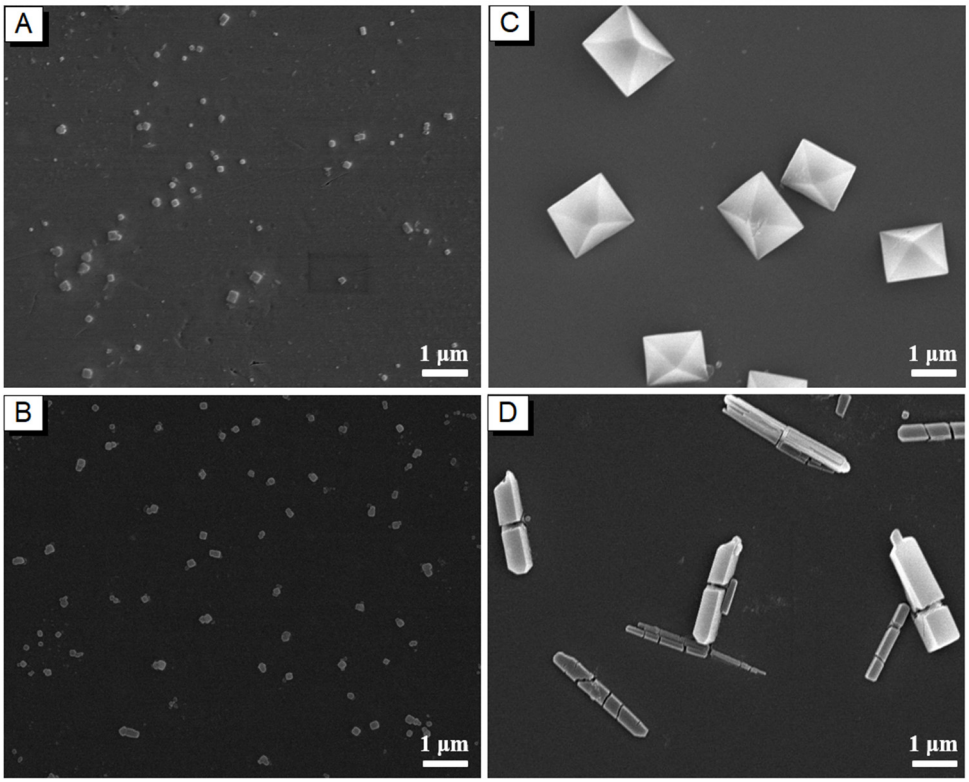
Supplementary Figure S9. Intermolecular stacking of (*Z*)-TPE-EPy and (*E*)-TPE-EPy in crystal.



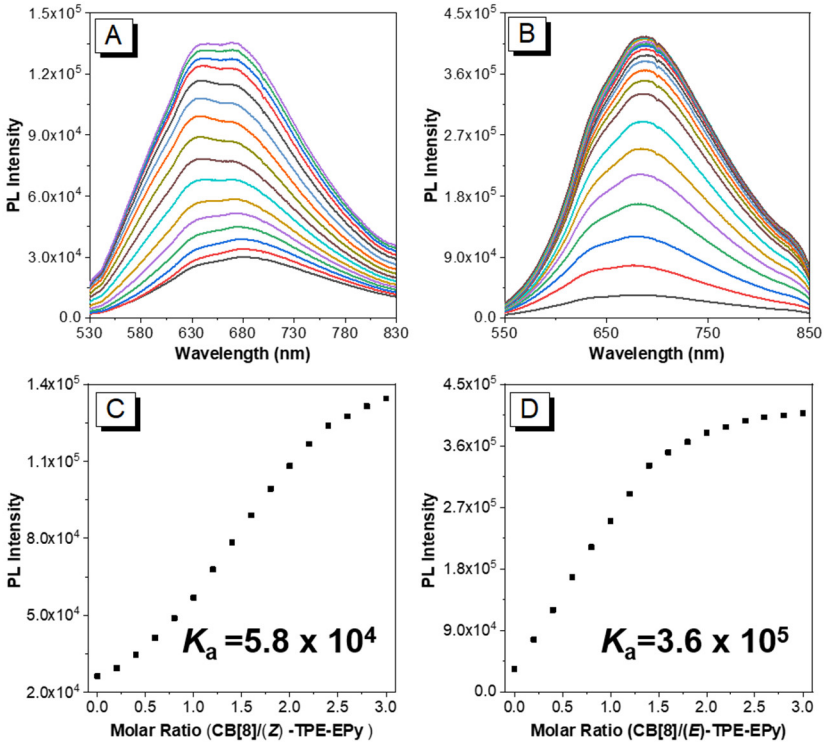
Supplementary Figure S10. Single-crystal X-ray diffraction analysis of (*Z*)-TPE-EPy and (*E*)-TPE-EPy.



Supplementary Figure S11. A) (*Z*)-TPE-EPy and B) (*E*) -TPE-EPy (10 μM) in H_2O/EtOH mixtures with different EtOH fractions (vol %).

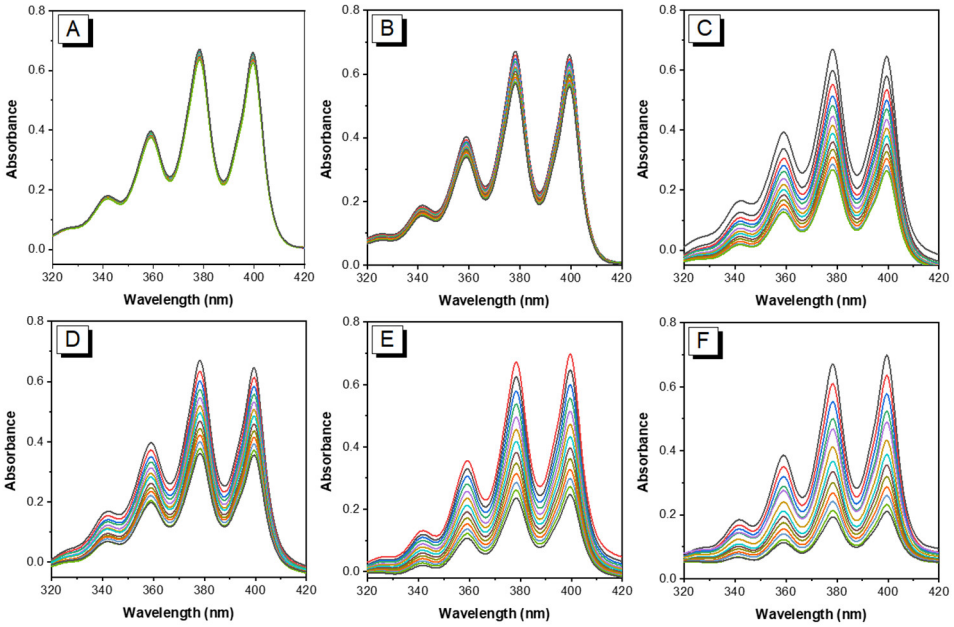


Supplementary Figure S12. SEM images of A) (*Z*)-TPE-EPy, B) (*E*)-TPE-EPy, C) (*Z*)-TPE-EPy@CB[8], D) (*E*)-TPE-EPy@CB[8]. The concentration of each sample was 10 μM and the scale bar was 1 μm.

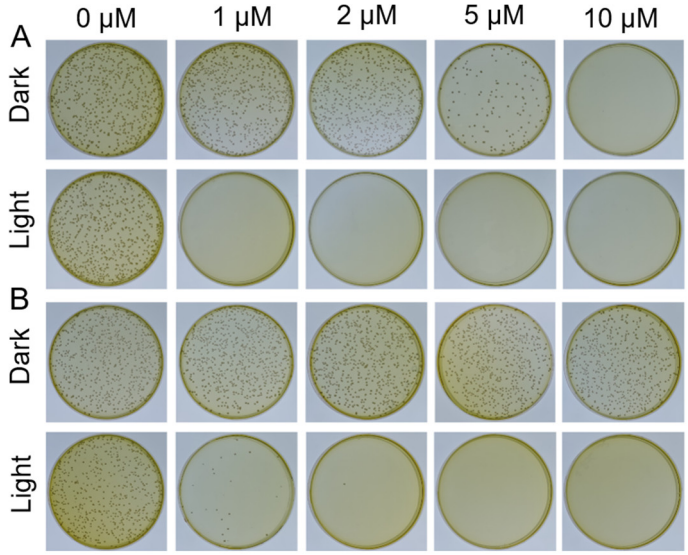


Supplementary Figure S13. A) Fluorescence titration spectra of (*Z*)-TPE-EPy (30 μM) with different amounts of CB[8] (0-150 μM) in water. B) Fluorescence titration spectra of (*E*) -TPE-EPy (30 μM) with

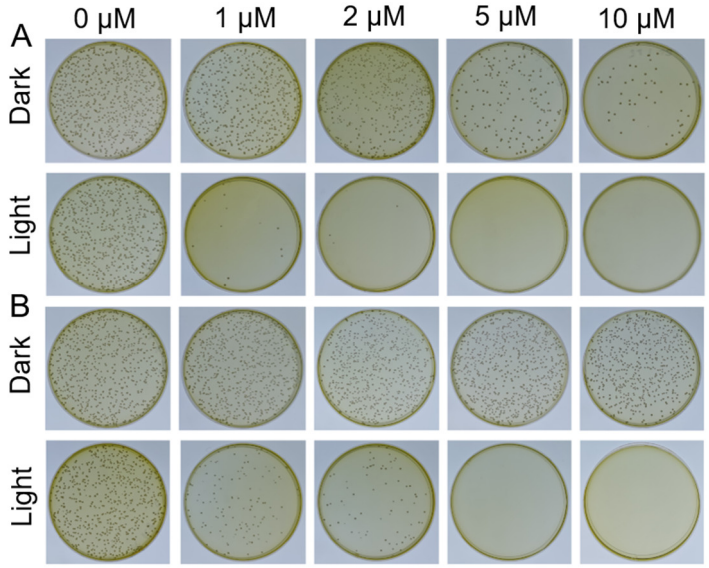
different amounts of CB[8] (0-120 μM) in water. The linear fitting curves of fluorescence intensity C) from Figure A) at 638 nm and D) from Figure B) at 686 nm.



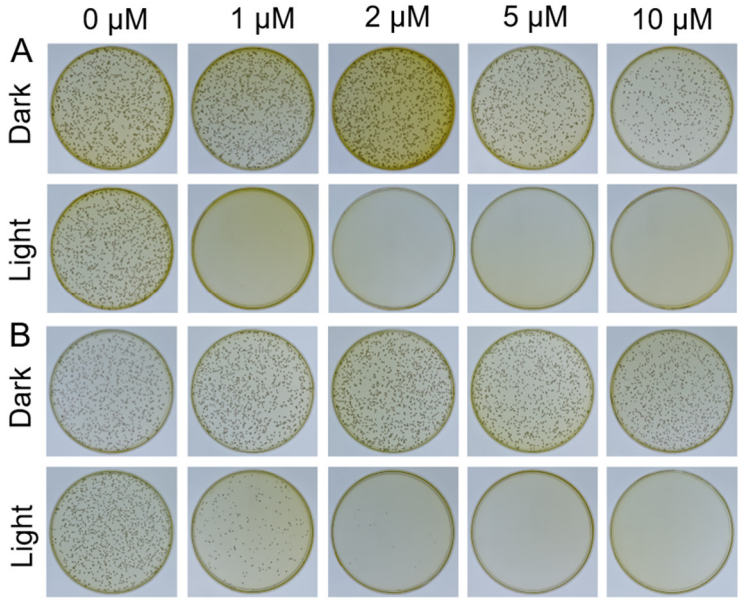
Supplementary Figure S14. A) UV-Vis spectra of ABDA in the absence of PSs under white light irradiation (26 mW·cm^{-2}) in aqueous solution. UV-Vis spectra of ABDA in the presence of B) Rose Bengal, C) (*Z*)-TPE-EPy, D) (*Z*)-TPE-EPy@CB[8], E) (*E*)-TPE-EPy, and F) (*E*)-TPE-EPy@CB[8] under white light irradiation (26 mW·cm^{-2}) in the aqueous solution. Concentrations of Rose Bengal and (*Z*)-TPE-EPy, (*E*)-TPE-EPy, (*Z*)-TPE-EPy@CB[8], (*E*)-TPE-EPy@CB[8] are 50 μM and 5 μM. Time interval for UV measurement: 10s. Time interval for UV measurement:10s.



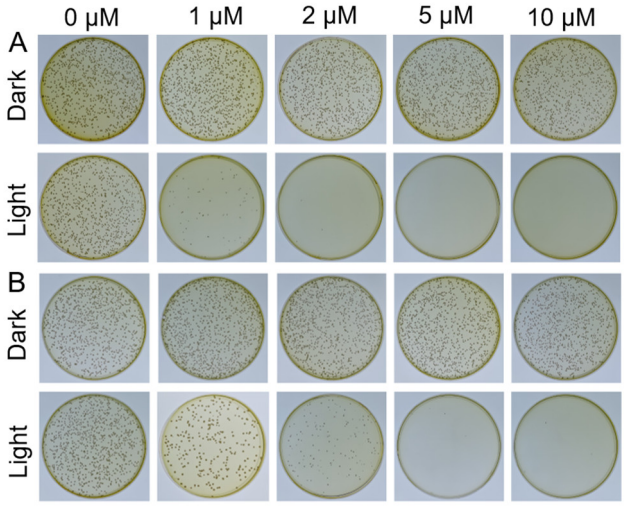
Supplementary Figure S15. Photographs of *S. cerevisiae* cultured on yeast agar plate supplemented with different concentration of A) (*Z*)-TPE-EPy, and B) (*Z*)-TPE-EPy@CB[8], in the darkness or upon white light irradiation (16 mW cm^{-2}) for 10 min (n = 3).



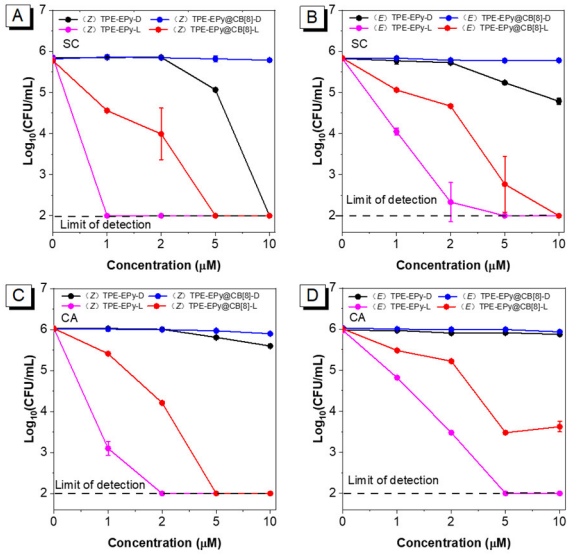
Supplementary Figure S16. Photographs of *S. cerevisiae* cultured on yeast agar plate supplemented with different concentration of A) (*E*)-TPE-EPy, and B) (*E*)-TPE-EPy@CB[8], in the darkness or upon white light irradiation (16 mW cm^{-2}) for 10 min (n = 3).



Supplementary Figure S17. Photographs of *C. albicans* cultured on yeast agar plate supplemented with different concentration of A) (*Z*)-TPE-EPy, and B) (*Z*)-TPE-EPy@CB[8], in the darkness or upon white light irradiation (16 mW cm^{-2}) for 10 min (n = 3).



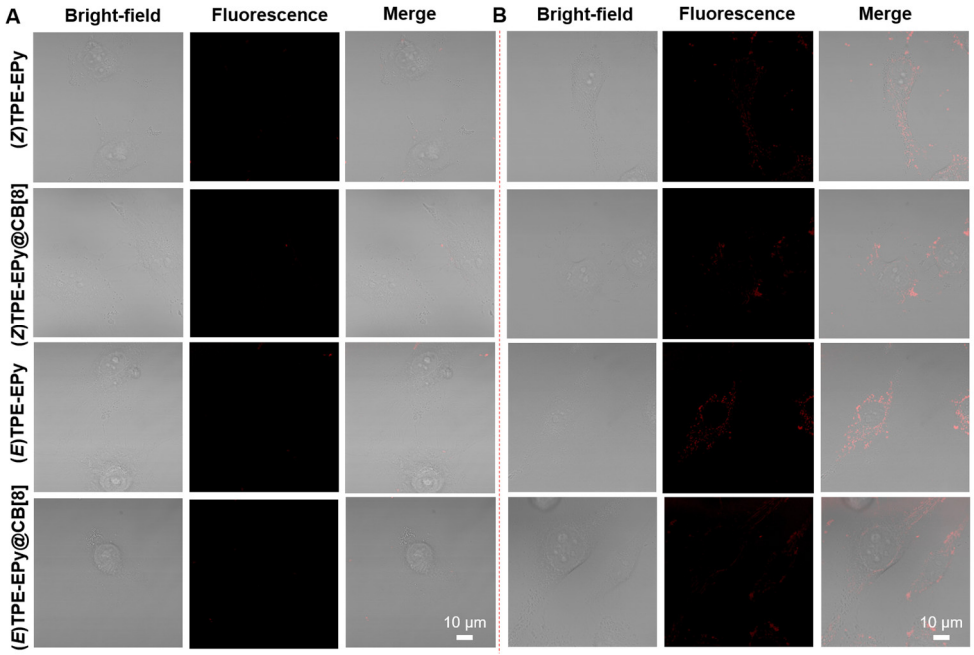
Supplementary Figure S18. Photographs of *C. albicans* cultured on agar plate supplemented with different concentration of A) (*E*)-TPE-EPy, and B) (*E*)-TPE-EPy@CB[8], in the darkness or upon white light irradiation (16 mW cm^{-2}) for 10 min (n = 3).



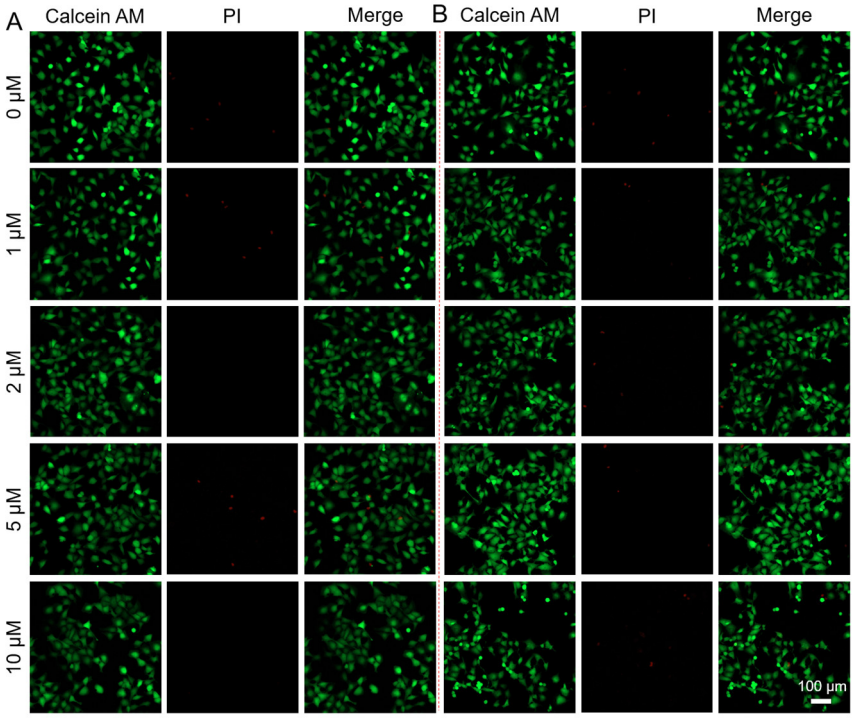
Supplementary Figure S19. Colony count of A), B) *S. cerevisiae* and C), D) *C. albicans* in darkness or unpon light irradiation (16 mW cm^{-2}) following the treatment of different concentrations of (*Z*)-TPE-EPy, (*E*)-TPE-EPy, (*Z*)-TPE-EPy@CB[8], (*E*)-TPE-EPy@CB[8] for 10 min, respectively. Dashed lines indicate limit of detection.

		(*Z*)TPE-EPy	(*Z*)TPE-EPy@CB[8]	(*E*)TPE-EPy	(*E*)TPE-EPy@CB[8]
		8.21 ± 0.36	12.2 ± 2.41	6.24 ± 0.29	9.33 ± 1.53
SC	-4.07 ± 0.39	-3.03 ± 0.09	-2.81 ± 0.19	-3.17 ± 0.04	-2.87 ± 0.16
CA	-3.19 ± 0.32	-3.01 ± 0.13	-2.99 ± 0.08	-3.09 ± 0.33	-3.02 ± 0.22

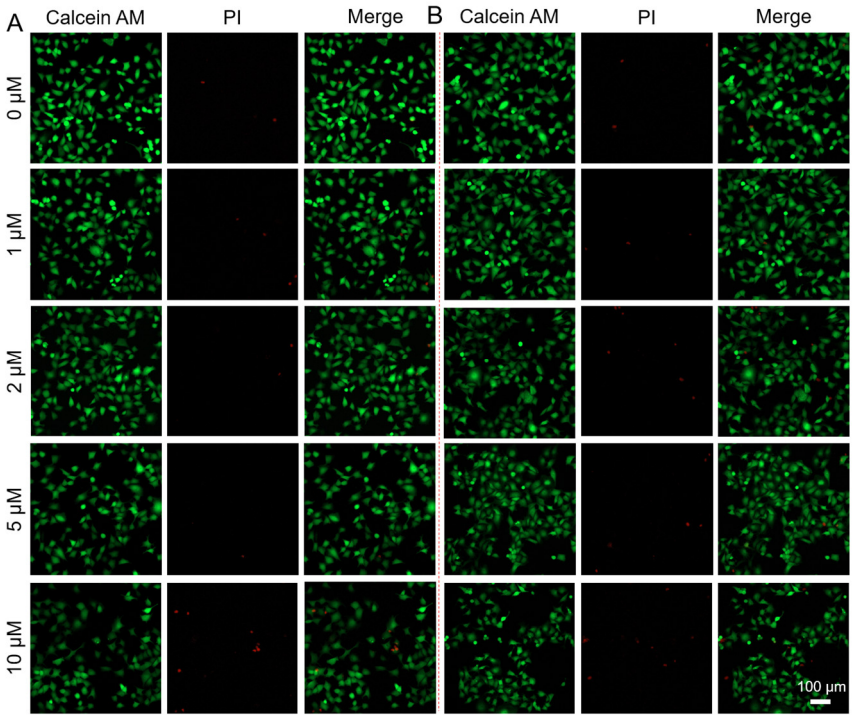
Supplementary Figure S20. Zeta potential results of *S. cerevisiae* (SC) and *C. albicans* (CA) in PBS solution pre-treated with or without (*Z*)-TPE-EPy, (*E*)-TPE-EPy, (*Z*)-TPE-EPy@CB[8], and (*E*)-TPE-EPy@CB[8].



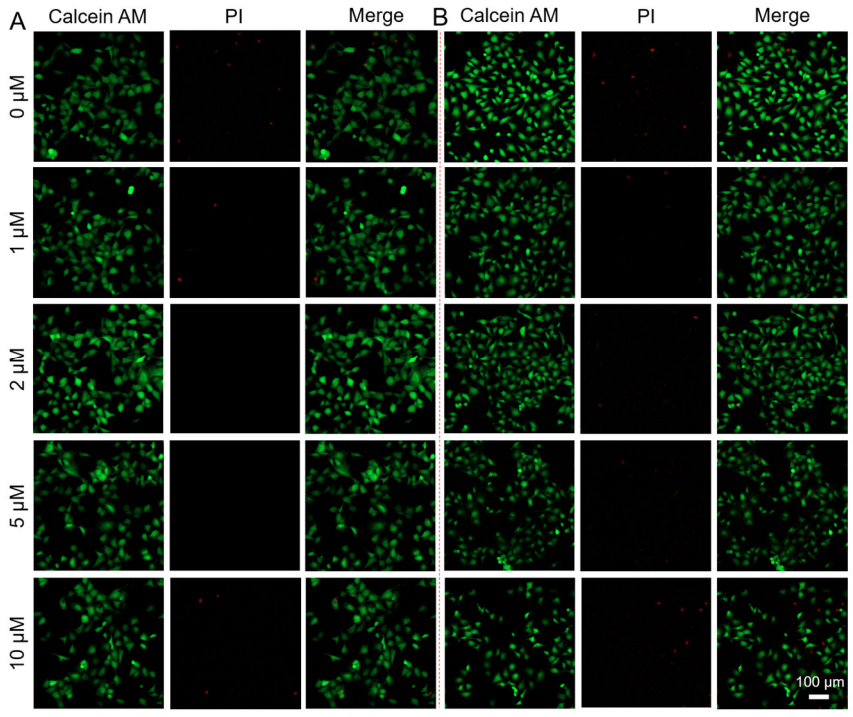
Supplementary Figure S21. Bright-field and fluorescent images of HUVECs incubated with A) 2 μM and B) 10 μM of the stereoisomers for 10 min. (*Z*)-TPE-EPy, (*E*)-TPE-EPy, (*Z*)-TPE-EPy@CB[8]: λ_{ex} = 405 nm, λ_{em} = 600-640 nm. (*E*)-TPE-EPy@CB[8]: λ_{ex} = 488 nm, λ_{em} = 600-640 nm.



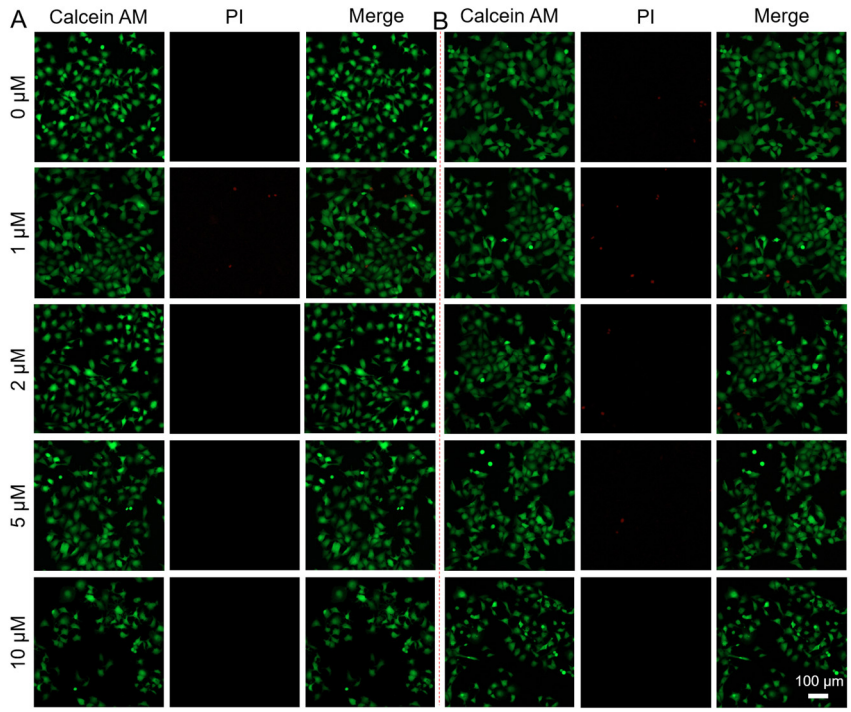
Supplementary Figure S22. Fluorescence images of calcein AM/PI stained HUVECs and cells treated by different concentrations of A) (*Z*)-TPE-EPy in darkness and B) upon light irradiation (16 mW·cm^{-2}) for 10 min. The fields of vision were randomly selected. Calcein AM: λ_{ex} = 488 nm, λ_{em}= 500-550 nm; PI: λ_{ex}= 561 nm, λ_{em}= 600-700 nm.



Supplementary Figure S23. Fluorescence images of calcein AM/PI stained HUVECs and cells treated by different concentrations of A) (*Z*)-TPE-EPy@CB[8] in darkness and B) upon light irradiation (16 mW·cm^{-2}) for 10 min. The fields of vision were randomly selected. Calcein AM: λ_{ex} = 488 nm, λ_{em} = 500-550 nm; PI: λ_{ex} = 561 nm, λ_{em} = 600-700 nm.



Supplementary Figure S24. Fluorescence images of calcein AM/PI stained HUVECs and cells treated by different concentrations of A) (*E*)-TPE-EPy in darkness and B) upon light irradiation (16 mW·cm^{-2}) for 10 min. The fields of vision were randomly selected. Calcein AM: λ_{ex} = 488 nm, λ_{em} = 500-550 nm; PI: λ_{ex} = 561 nm, λ_{em} = 600-700 nm.



Supplementary Figure S25. Fluorescence images of calcein AM/PI stained HUVECs and cells treated by different concentrations of A) (*E*)-TPE-EPy@CB[8] in darkness and B) upon light irradiation (16 $mW \cdot cm^{-2}$) for 10 min. The fields of vision were randomly selected. Calcein AM: λ_{ex} = 488 nm, λ_{em} = 500-550 nm; PI: λ_{ex} = 561 nm, λ_{em} = 600-700 nm.

Cartesian coordinates

(*Z*)-TPE-EPy S_0-geometry:

C	-0.64964600	2.91781100	-0.19400900
C	0.64958200	2.91782200	0.19390400
C	-1.47614600	1.68573900	-0.30110000
C	-1.51567800	0.73494100	0.73101700
C	-2.32161100	1.50681500	-1.40400400
C	-2.38857800	-0.33766900	0.67908500
H	-0.87385100	0.86446400	1.59637800
C	-3.17928100	0.42229800	-1.46847600
H	-2.31581600	2.24065100	-2.20361600
C	-3.25192100	-0.50559200	-0.41688000
H	-2.40414500	-1.04162500	1.50553900
H	-3.83034900	0.30845200	-2.33144100
C	1.47610600	1.68576800	0.30100700
C	2.32153800	1.50685200	1.40393800
C	1.51570400	0.73498700	-0.73112300
C	3.17923500	0.42235800	1.46842600
H	2.31569500	2.24067800	2.20355900
C	2.38863100	-0.33760000	-0.67917400
H	0.87390900	0.86450700	-1.59650800
C	3.25193700	-0.50551600	0.41682100
H	3.83027500	0.30851800	2.33141300
H	2.40424800	-1.04154400	-1.50563800
C	-1.37850400	4.17617900	-0.52654400

C	-0.84868600	5.08675900	-1.44639300
C	-2.62267100	4.44629900	0.05406500
C	-1.53943600	6.25007300	-1.76438400
H	0.11369800	4.88386800	-1.90606500
C	-3.30744700	5.61590100	-0.25517200
H	-3.04958600	3.74083900	0.76228300
C	-2.76723300	6.52041600	-1.16579700
H	-1.11687100	6.94814200	-2.48009300
H	-4.26398900	5.82204400	0.21498100
H	-3.30293100	7.43221800	-1.41025600
C	1.37838700	4.17619700	0.52652500
C	0.84847200	5.08674400	1.44634800
C	2.62259100	4.44636300	-0.05398500
C	1.53916400	6.25007100	1.76441500
H	-0.11394800	4.88382000	1.90593300
C	3.30731000	5.61597900	0.25532800
H	3.04957900	3.74092900	-0.76218500
C	2.76700000	6.52046000	1.16593000
H	1.11652100	6.94811700	2.48010200
H	4.26388300	5.82215800	-0.21474700
H	3.30265300	7.43227200	1.41044800
C	4.25762200	-1.55192600	0.49507200
H	4.76529400	-1.60772800	1.45706700
C	4.64573400	-2.38979800	-0.49348800
H	4.18449200	-2.31713700	-1.47441700
C	-4.25758300	-1.55202500	-0.49510700
H	-4.76529000	-1.60782800	-1.45708400
C	-4.64563800	-2.38991700	0.49345900
H	-4.18436300	-2.31725600	1.47437100
C	5.70660500	-3.36560300	-0.37941400
C	6.12071200	-4.07921500	-1.52496700
C	6.39443800	-3.66825700	0.81742000
C	7.14264100	-4.99164700	-1.46033800
H	5.63988700	-3.90896600	-2.48155900
C	7.40911300	-4.58908600	0.82762900
H	6.14042300	-3.18992800	1.75492700
H	7.48432300	-5.54292300	-2.32809200
H	7.95722400	-4.83575200	1.72912700
C	-5.70649100	-3.36574600	0.37941400
C	-6.12053900	-4.07938000	1.52497300
C	-6.39436300	-3.66840400	-0.81739900
C	-7.14245100	-4.99183500	1.46037400
H	-5.63968300	-3.90913000	2.48155000
C	-7.40901500	-4.58925500	-0.82757800
H	-6.14039400	-3.19005700	-1.75491000
H	-7.48408500	-5.54312600	2.32813700
H	-7.95715700	-4.83592800	-1.72905700
N	-7.78263800	-5.24527600	0.29653700
N	7.78279200	-5.24508700	-0.29647900
C	8.91500100	-6.18672100	-0.25605300
H	8.90797500	-6.71650000	0.69661700
H	8.80944200	-6.91003100	-1.06409000

H	9.85179200	-5.63731900	-0.37066000
C	-8.91482100	-6.18694300	0.25611100
H	-8.90754700	-6.71700800	-0.69640000
H	-8.80945300	-6.91000600	1.06439300
H	-9.85164800	-5.63752200	0.37032600

(*Z*)-TPE-EPy T_1-geometry:

C	-0.47724400	2.40810300	-0.57392700
C	0.47724300	2.40810300	0.57392900
C	-1.52141700	1.44558500	-0.61545600
C	-1.85202000	0.68152100	0.54479600
C	-2.26851100	1.17295300	-1.79751800
C	-2.90002000	-0.20330300	0.54922100
H	-1.28179900	0.83492800	1.45551800
C	-3.30327200	0.26870300	-1.78979800
H	-2.00023400	1.66686800	-2.72412200
C	-3.67502400	-0.42490300	-0.61542900
H	-3.12898000	-0.73417600	1.46772400
H	-3.85131400	0.08397500	-2.71020900
C	1.52141200	1.44558100	0.61546100
C	2.26852800	1.17297700	1.79751600
C	1.85199500	0.68149400	-0.54478100
C	3.30328500	0.26872300	1.78979900
H	2.00027100	1.66692000	2.72411200
C	2.89999200	-0.20333400	-0.54920400
H	1.28176000	0.83488400	-1.45549700
C	3.67501400	-0.42491100	0.61543900
H	3.85134400	0.08401600	2.71020300
H	3.12893500	-0.73422700	-1.46769900
C	-0.29979600	3.46836000	-1.56593600
C	0.99113500	3.94608800	-1.86100900
C	-1.39745900	4.09615200	-2.18531500
C	1.17844600	4.97119100	-2.77572400
H	1.85318900	3.49818200	-1.37552600
C	-1.20595800	5.13178300	-3.08931800
H	-2.40709900	3.80064100	-1.91855000
C	0.08133900	5.56599200	-3.39681000
H	2.18287900	5.31540600	-3.00042500
H	-2.06569500	5.61314300	-3.54432500
H	0.22851700	6.37587800	-4.10397700
C	0.29982000	3.46837600	1.56592500
C	-0.99109700	3.94614600	1.86099000
C	1.39750000	4.09613800	2.18530400
C	-1.17838000	4.97126400	2.77569500
H	-1.85316400	3.49826300	1.37550800
C	1.20602800	5.13178200	3.08929700
H	2.40713200	3.80058900	1.91854800
C	-0.08125600	5.56603500	3.39678000
H	-2.18280200	5.31551200	3.00039000
H	2.06577800	5.61311800	3.54430600
H	-0.22841100	6.37593200	4.10394000

C	4.81404500	-1.30070200	0.66268400
H	5.27282900	-1.38396400	1.64669200
C	5.36995300	-1.98655800	-0.37419700
H	4.93800700	-1.90075000	-1.36720600
C	-4.81405800	-1.30069100	-0.66267400
H	-5.27282600	-1.38397100	-1.64668800
C	-5.36998300	-1.98652700	0.37421100
H	-4.93805000	-1.90070400	1.36722400
C	6.53731500	-2.82052700	-0.28218300
C	7.04787500	-3.43850200	-1.44843700
C	7.25032600	-3.08351300	0.91282000
C	8.16481200	-4.22928100	-1.40121300
H	6.55924300	-3.29133300	-2.40491900
C	8.36183400	-3.88232400	0.90421900
H	6.93946900	-2.66635800	1.86225900
H	8.57584400	-4.70696000	-2.28246100
H	8.92665900	-4.09536800	1.80389800
C	-6.53734600	-2.82049300	0.28219500
C	-7.04792300	-3.43845000	1.44845100
C	-7.25034200	-3.08349600	-0.91281400
C	-8.16486100	-4.22922700	1.40122400
H	-6.55930300	-3.29126800	2.40493600
C	-8.36185200	-3.88230300	-0.90421600
H	-6.93947200	-2.66635600	-1.86225500
H	-8.57590600	-4.70689200	2.28247400
H	-8.92666700	-4.09535900	-1.80389900
N	-8.81901200	-4.45331500	0.23672300
N	8.81897700	-4.45335400	-0.23671700
C	10.04903400	-5.26102200	-0.21860400
H	10.12997600	-5.77172300	0.74095900
H	10.00093400	-6.00673400	-1.01198800
H	10.91637100	-4.61455800	-0.36953700
C	-10.04907100	-5.26098000	0.21860500
H	-10.12999100	-5.77171000	-0.74094600
H	-10.00099200	-6.00666900	1.01201200
H	-10.91640900	-4.61451000	0.36949800

(*E*)-TPE-EPy S_0-geometry:

C	-0.41512700	0.73901300	0.21591100
C	0.39146300	-0.35048500	0.19108700
C	0.11331500	2.13161700	0.28278500
C	-0.32243000	3.09544100	-0.63361600
C	1.02066600	2.50679600	1.27860300
C	0.16497000	4.39607900	-0.57631500
H	-1.04210600	2.81925300	-1.39977900
C	1.49911900	3.81092000	1.34293700
H	1.34895500	1.76989600	2.00586000
C	1.07764500	4.75680400	0.41237800
H	-0.17178000	5.13106700	-1.30082700
H	2.19720000	4.09058500	2.12597700
H	1.45086300	5.77489500	0.46291000

C	-0.12252400	-1.73943400	0.36129300
C	-0.92419200	-2.07814100	1.45610000
C	0.22281600	-2.73622800	-0.55851600
C	-1.38908100	-3.37902200	1.61541800
H	-1.18033700	-1.31533500	2.18557300
C	-0.25141100	-4.03398600	-0.40518000
H	0.86086800	-2.48802200	-1.40261800
C	-1.05922000	-4.35833900	0.68244100
H	-2.00430800	-3.62976400	2.47408300
H	0.01401300	-4.79502800	-1.13248000
H	-1.42154800	-5.37399600	0.80728200
C	-1.90061300	0.63363300	0.21132800
C	-2.65889100	1.42922100	1.07832600
C	-2.57645700	-0.20909100	-0.68539500
C	-4.04237200	1.35780000	1.07423800
H	-2.15538100	2.10608100	1.76122800
C	-3.95708300	-0.27259900	-0.69917900
H	-2.00555800	-0.81843100	-1.37742700
C	-4.71997200	0.50674300	0.18773500
H	-4.60968200	1.97468900	1.76640100
H	-4.44111300	-0.93157200	-1.41288300
C	1.86740900	-0.24536000	0.02308100
C	2.71885000	-1.00474600	0.84114100
C	2.43939600	0.55847100	-0.96979100
C	4.09250300	-0.93619700	0.69934500
H	2.28869700	-1.65163200	1.59932600
C	3.81471100	0.61988400	-1.12046100
H	1.79974900	1.14097500	-1.62362000
C	4.66958700	-0.11910900	-0.28756600
H	4.71579000	-1.52750500	1.36250900
H	4.23639500	1.24949300	-1.89967400
C	6.10416400	-0.00618500	-0.49408500
H	6.38408000	0.67102700	-1.29978400
C	7.08174400	-0.63976600	0.19309900
H	6.82103300	-1.32284000	0.99634800
C	8.49867400	-0.49227800	-0.05182900
C	9.41668900	-1.23056600	0.72598300
C	9.06242800	0.35312400	-1.03409300
C	10.76830800	-1.12058100	0.52134100
H	9.06439500	-1.90302300	1.49987800
C	10.42066500	0.42607600	-1.19782400
H	8.44440700	0.96211700	-1.68165000
H	11.49083700	-1.67674500	1.10628800
H	10.88036700	1.06609000	-1.94151800
C	-6.17281700	0.48586400	0.22652900
H	-6.60533100	1.16357000	0.96114200
C	-7.00214600	-0.26656200	-0.53203700
H	-6.58912500	-0.95329900	-1.26527000
C	-8.44541400	-0.24361100	-0.45486700
C	-9.19177100	0.58189500	0.41638500
C	-9.19851100	-1.09234200	-1.29472600
C	-10.56090200	0.53527200	0.42231800

H	-8.70933200	1.26919600	1.09976000
C	-10.56921900	-1.09991400	-1.24936100
H	-8.70100900	-1.75757900	-1.99124900
H	-11.15829900	1.15750500	1.07802400
H	-11.16724000	-1.74160300	-1.88505000
N	-11.24600100	-0.29652100	-0.39804800
N	11.26766300	-0.30273800	-0.43260800
C	-12.71879000	-0.28156000	-0.39217800
H	-13.07284800	-0.16229700	0.63203300
H	-13.07900400	0.54312800	-1.01077300
H	-13.08883000	-1.22743000	-0.78641800
C	12.72276100	-0.16017900	-0.61088000
H	13.07380600	0.71935900	-0.06707300
H	13.21989100	-1.05191000	-0.23044800
H	12.94619200	-0.05632400	-1.67288500

(*E*)-TPE-EPy T_1-geometry

C	-0.45531400	1.77062000	-0.46981100
C	0.39271900	1.46471400	0.72186000
C	0.08509100	2.70910200	-1.45049500
C	-0.19701500	2.59117800	-2.82567800
C	0.96621900	3.72826200	-1.03942200
C	0.35093400	3.47783800	-3.74217300
H	-0.81939800	1.77438600	-3.17813100
C	1.49791700	4.62177000	-1.95665900
H	1.21705600	3.82650700	0.01294100
C	1.19051400	4.50289800	-3.31144000
H	0.12952300	3.36354700	-4.79862800
H	2.15719000	5.41371600	-1.61596800
H	1.61286100	5.19889900	-4.02904700
C	-0.08231100	1.93235600	2.02106000
C	-0.88066100	3.09013900	2.10468800
C	0.17901600	1.22034100	3.20858800
C	-1.35075800	3.54357600	3.32765500
H	-1.11518500	3.64475300	1.20062500
C	-0.30742300	1.66949500	4.42835200
H	0.73458600	0.28855100	3.16479000
C	-1.06393600	2.83767100	4.49536100
H	-1.94592600	4.45002500	3.37230100
H	-0.10362600	1.10089100	5.33025200
H	-1.43836400	3.19023600	5.45100200
C	-1.74939900	1.18558400	-0.56252700
C	-2.77950500	1.73207900	-1.37882400
C	-2.09124500	0.05265900	0.23404300
C	-4.03540300	1.17371500	-1.40481600
H	-2.58773800	2.63229600	-1.95082300
C	-3.34299100	-0.50720500	0.19171800
H	-1.33588600	-0.38401900	0.87908700
C	-4.35894300	0.03762400	-0.62995000
H	-4.80437300	1.63097300	-2.02214300
H	-3.54455100	-1.37904600	0.80578100

C	1.63274700	0.79296200	0.52351400
C	2.70097200	0.86487000	1.46574900
C	1.88640000	0.08206100	-0.68261900
C	3.90999700	0.26076800	1.22671600
H	2.57591000	1.45478300	2.36627200
C	3.09402100	-0.53477900	-0.90683600
H	1.10610600	0.01633400	-1.43353200
C	4.14428100	-0.46693300	0.03622600
H	4.69845500	0.37264000	1.96392800
H	3.24735200	-1.08176700	-1.83351400
C	5.39496800	-1.10960400	-0.27014100
H	5.41878600	-1.60550500	-1.23934100
C	6.51009600	-1.14746900	0.50925900
H	6.50197100	-0.66181900	1.48071900
C	7.74860000	-1.78724900	0.15590100
C	8.83580700	-1.74774800	1.06034300
C	7.98575400	-2.47494200	-1.05889100
C	10.03180300	-2.34271200	0.75819800
H	8.73667500	-1.24259300	2.01441200
C	9.20090900	-3.05254000	-1.31071400
H	7.21946700	-2.56474900	-1.81838900
H	10.87767000	-2.32206000	1.43473200
H	9.40917800	-3.58187500	-2.23284100
C	-5.69767900	-0.48415800	-0.69926900
H	-6.34993000	0.05358900	-1.38552100
C	-6.20926000	-1.54020700	-0.00953600
H	-5.57681600	-2.08558600	0.68510700
C	-7.56311700	-2.01446300	-0.11026300
C	-8.55395300	-1.45596700	-0.95422200
C	-7.97830000	-3.11431600	0.67679600
C	-9.82252400	-1.96883200	-0.97965200
H	-8.34121200	-0.61167200	-1.59755900
C	-9.26163300	-3.58860800	0.61270100
H	-7.28173800	-3.59893200	1.35144300
H	-10.59837100	-1.56048300	-1.61629700
H	-9.59982900	-4.42912000	1.20658700
N	-10.18018800	-3.02197600	-0.20473100
N	10.21651400	-2.99272800	-0.41518300
C	-11.54174100	-3.57268200	-0.29692900
H	-12.25138100	-2.75663900	-0.43531600
H	-11.60238700	-4.26600400	-1.13867100
H	-11.78134000	-4.09505000	0.62886500
C	11.52491300	-3.58068200	-0.74405800
H	12.12302900	-2.85825900	-1.30380000
H	12.03943800	-3.85046400	0.17793600
H	11.37513600	-4.48067300	-1.34070600

References

1. Chen, X., et al. A Pyridinyl-functionalized Tetraphenylethylene Fluorogen for Specific Sensing of Trivalent Cations. *Chem. Commun.* **49**, 1503-1505 (2013).