

Supporting Information

The Design, Synthesis and Application of Nitrogen Heteropolycyclic Compounds with Anti-UV Properties

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1. NMR spectra

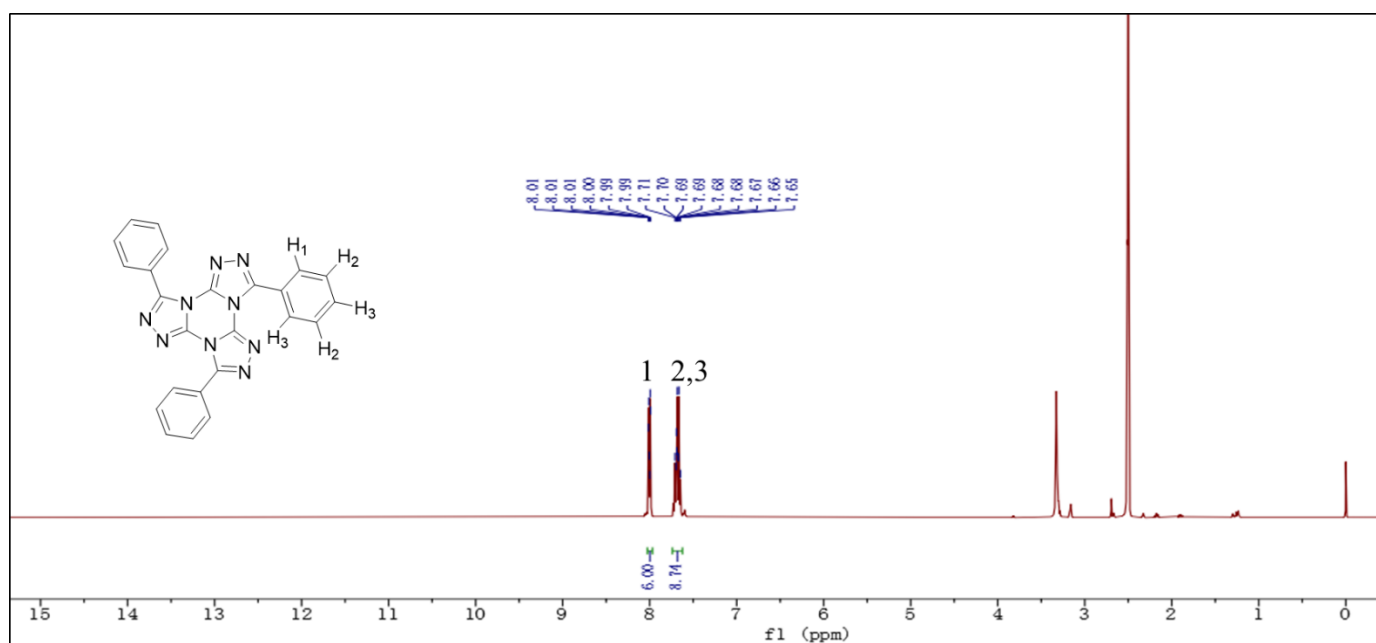


Figure S1. ^1H NMR spectrum (400 MHz) in $\text{DMSO-}d_6$ for compound TTTB.

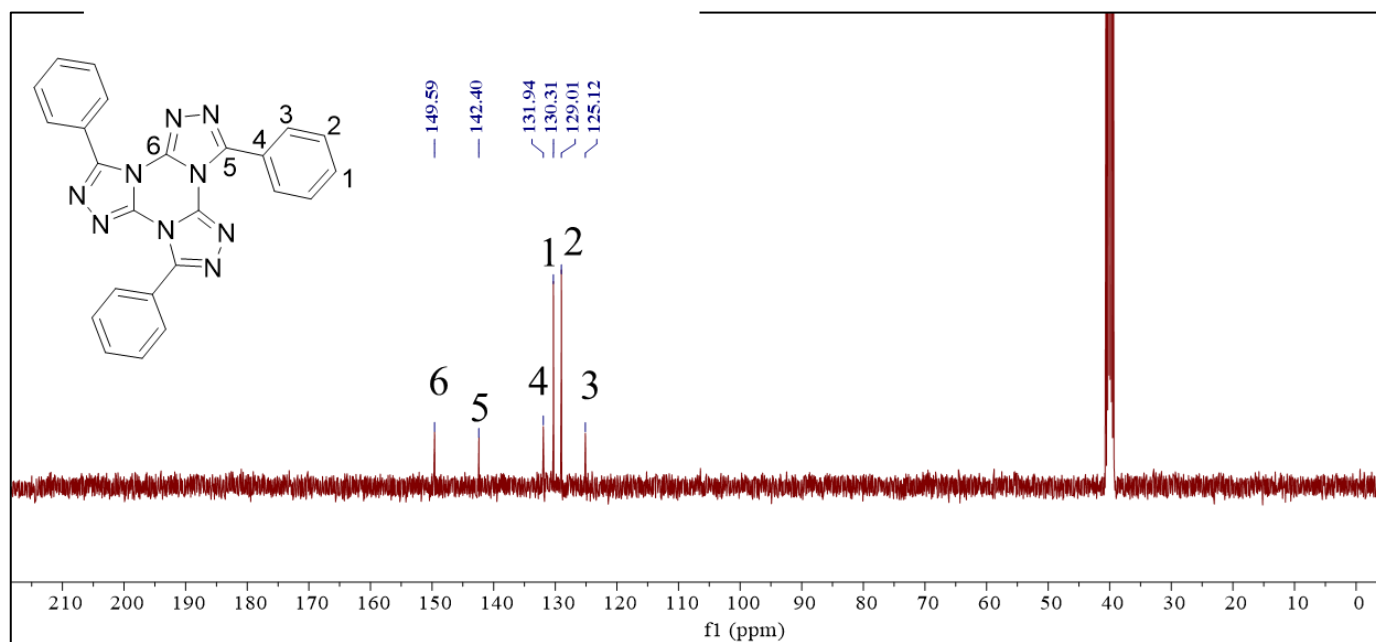


Figure S2. ^{13}C NMR spectrum (100 MHz) in $\text{DMSO-}d_6$ for compound TTTB.

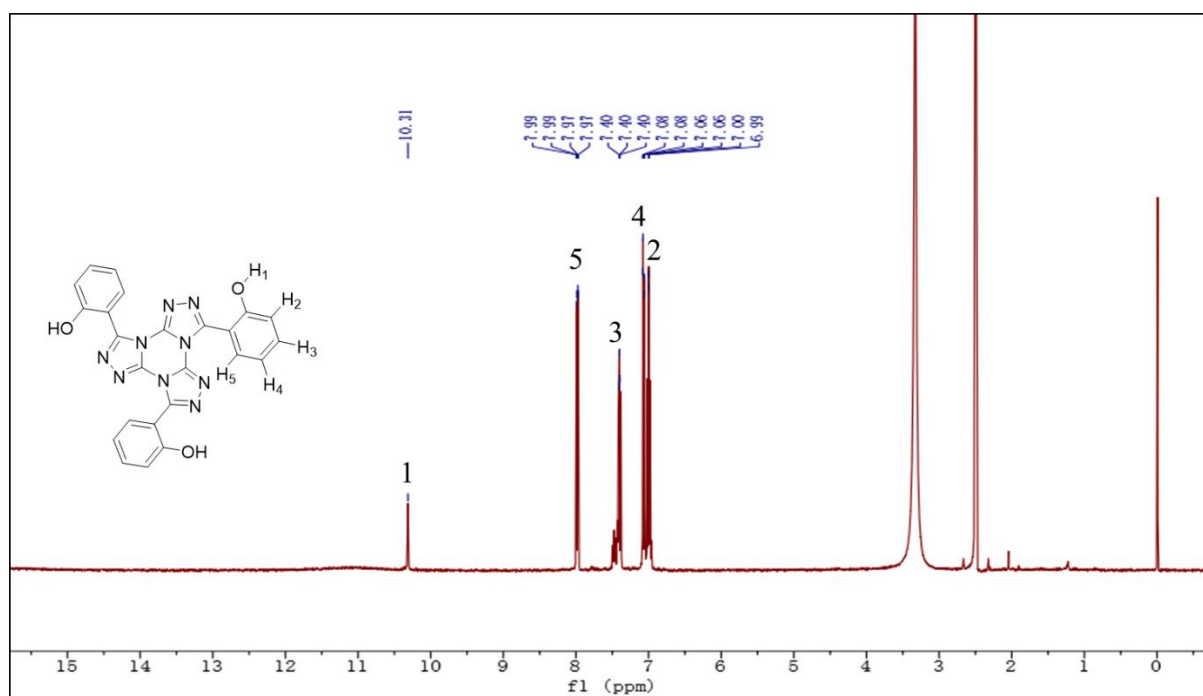


Figure S3. ¹H NMR spectrum (400 MHz) in CDCl₃ for compound TTTL.

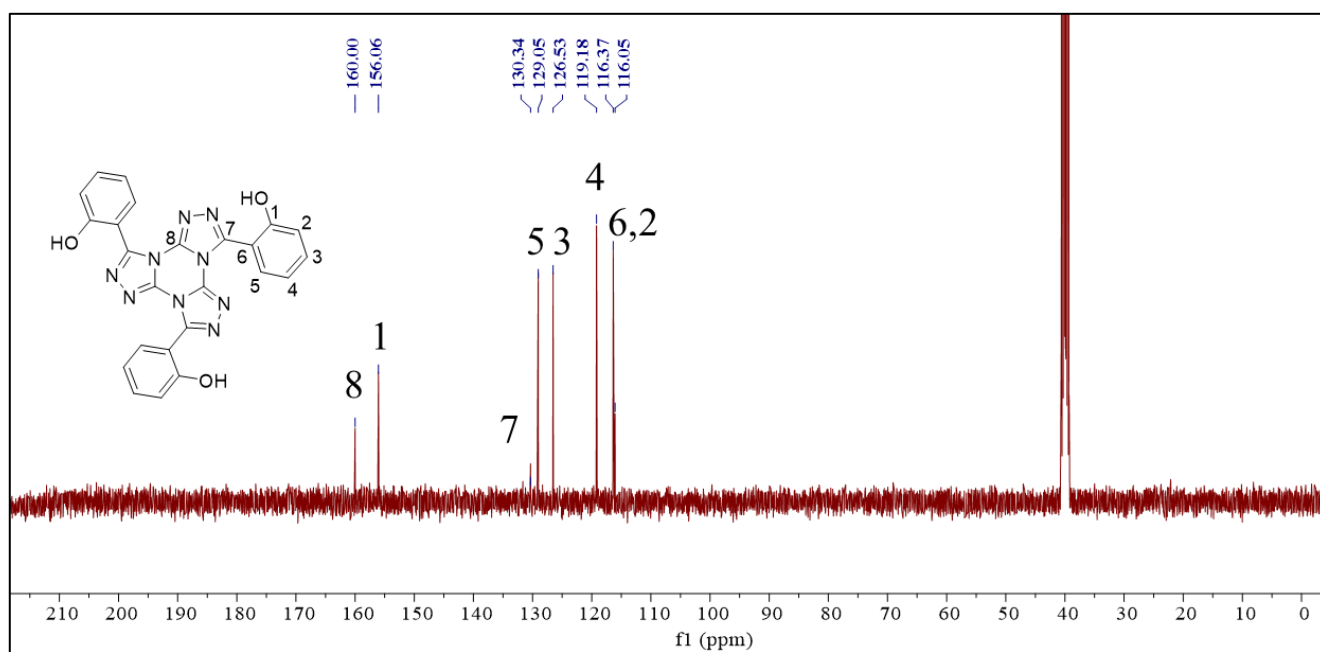


Figure S4. ¹³C NMR spectrum (100 MHz) in CDCl₃ for compound TTTL.

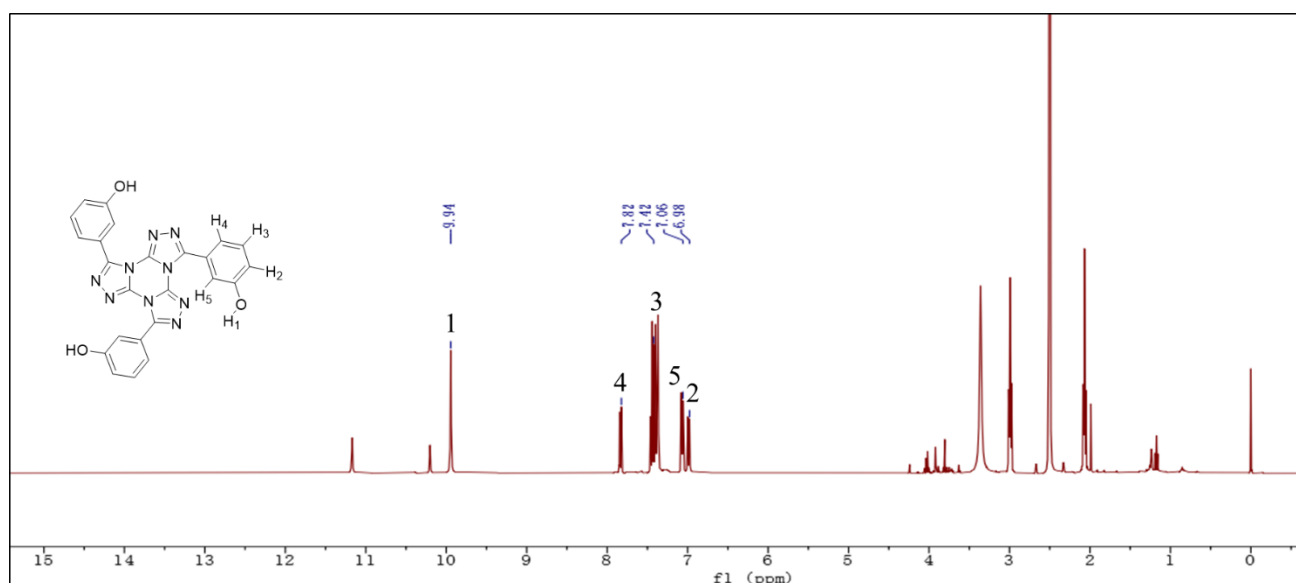


Figure S5. ¹H NMR spectrum (400 MHz) in CDCl₃ for compound TTTJ.

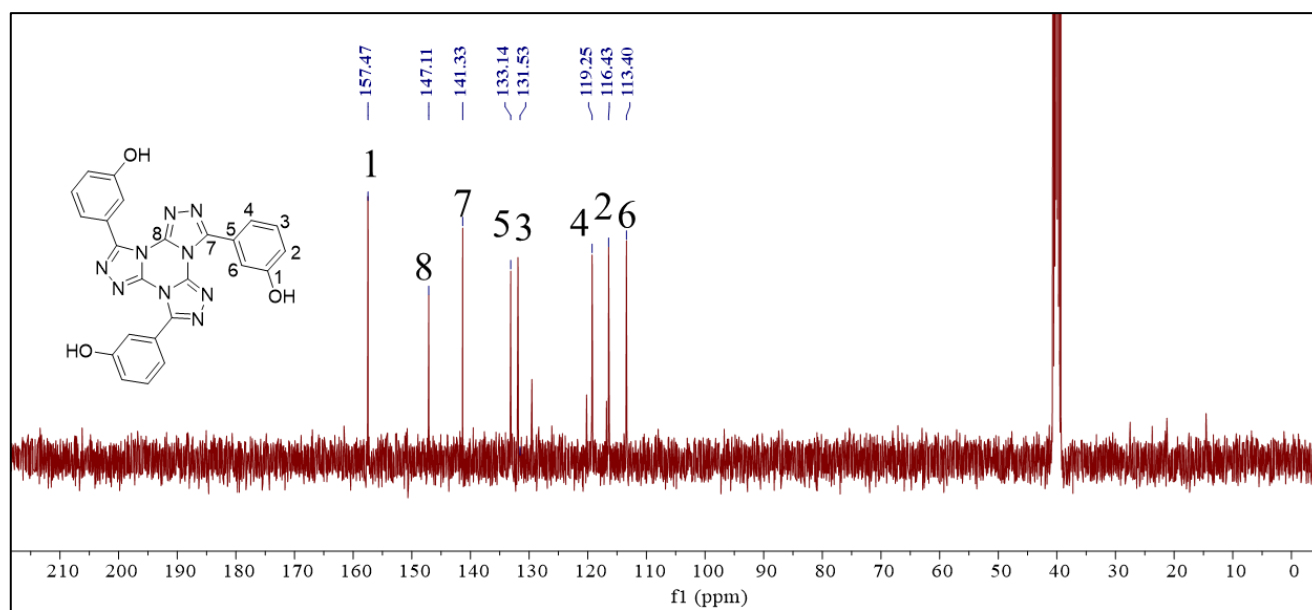


Figure S6. ¹³C NMR spectrum (100 MHz) in CDCl₃ for compound TTTJ.

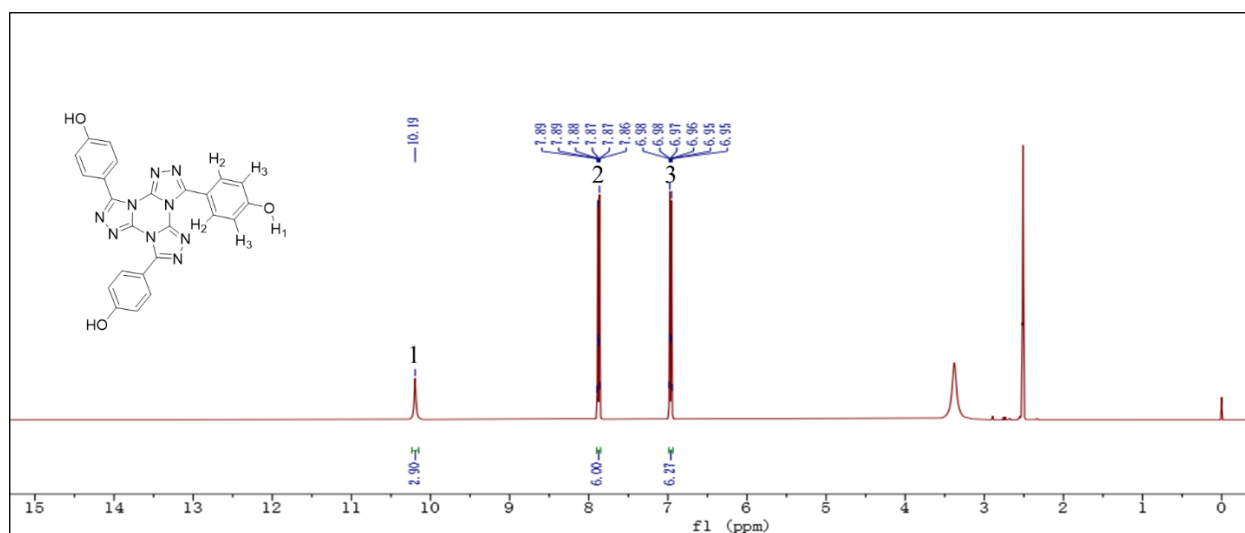


Figure S7. ¹H NMR spectrum (400 MHz) in CDCl₃ for compound TTTD.

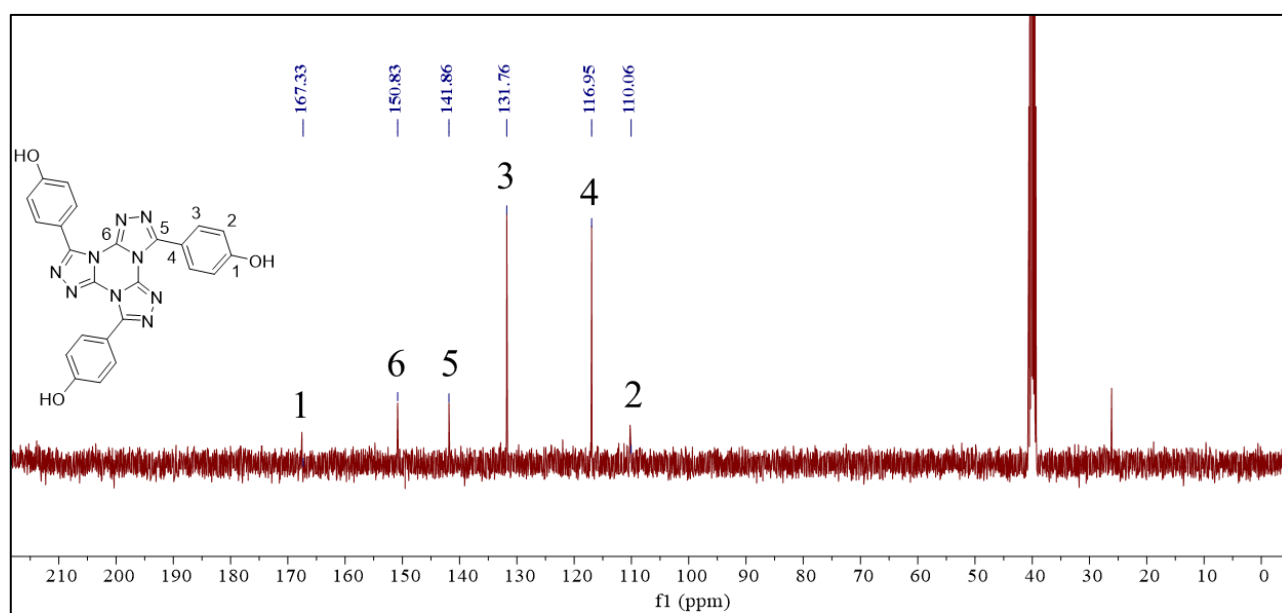


Figure S8. ¹³C NMR spectrum (100 MHz) in CDCl₃ for compound TTTD.

2. Mass spectra

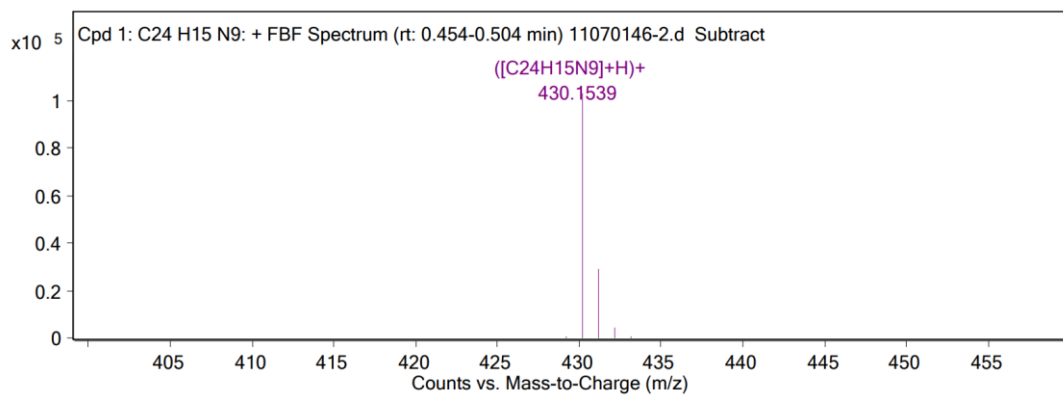


Figure S9. Mass spectrum of compound TTTB.

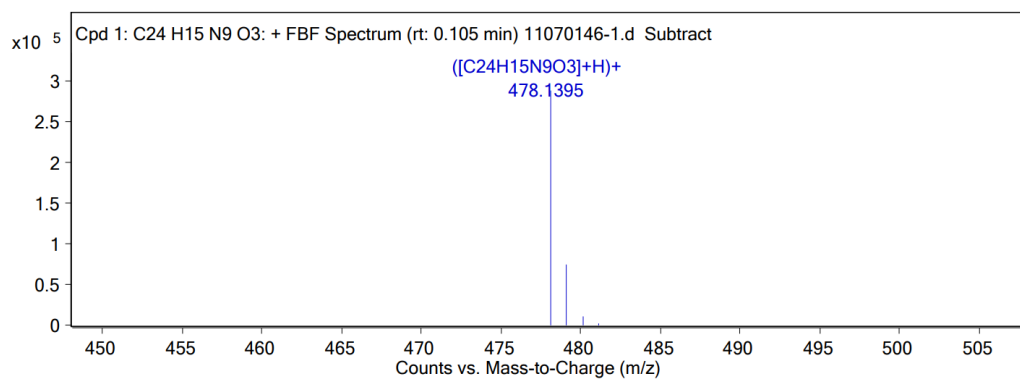


Figure S10. Mass spectrum of compound TTTL.

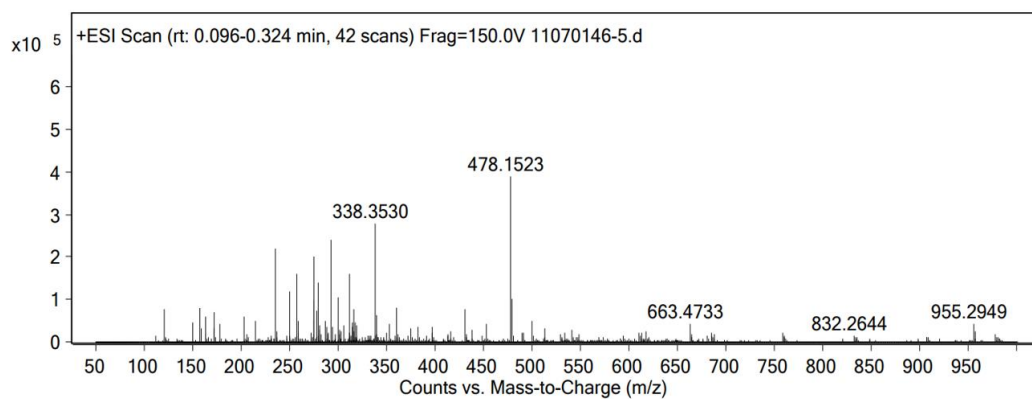


Figure S11. Mass spectrum of compound TTTJ.

7144458 #3-304 RT: 0.02-0.85 AV: 123 NL: 4.44E7
T: FTMS - p ESI Full ms [100.0000-1000.0000]

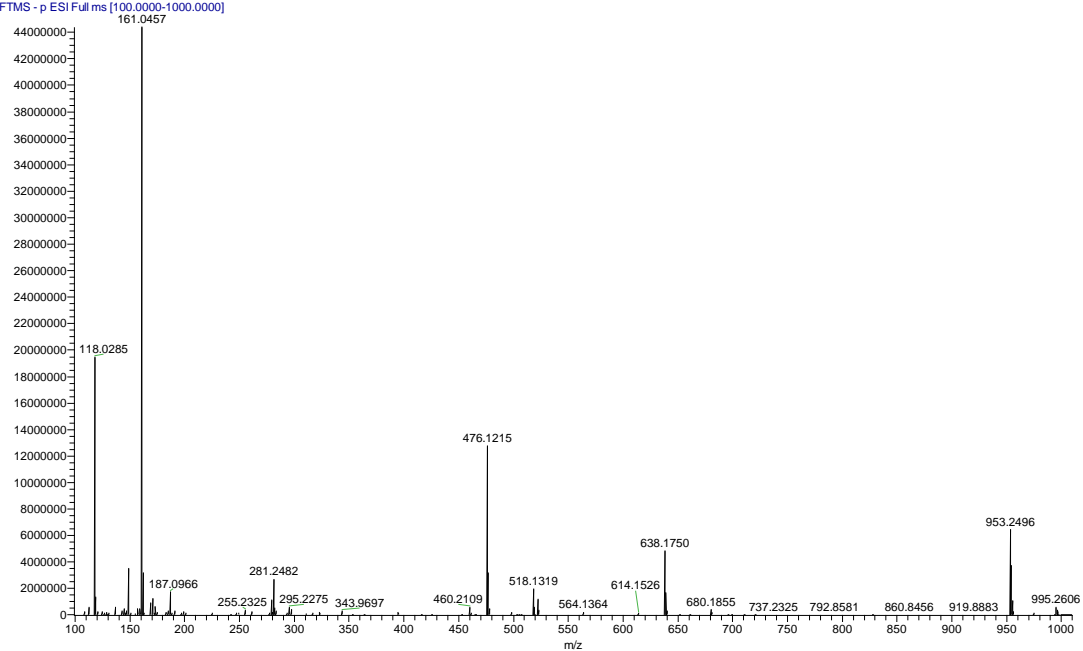


Figure S12. Mass spectrum of compound TTTD.

3. Ultraviolet absorption spectrum

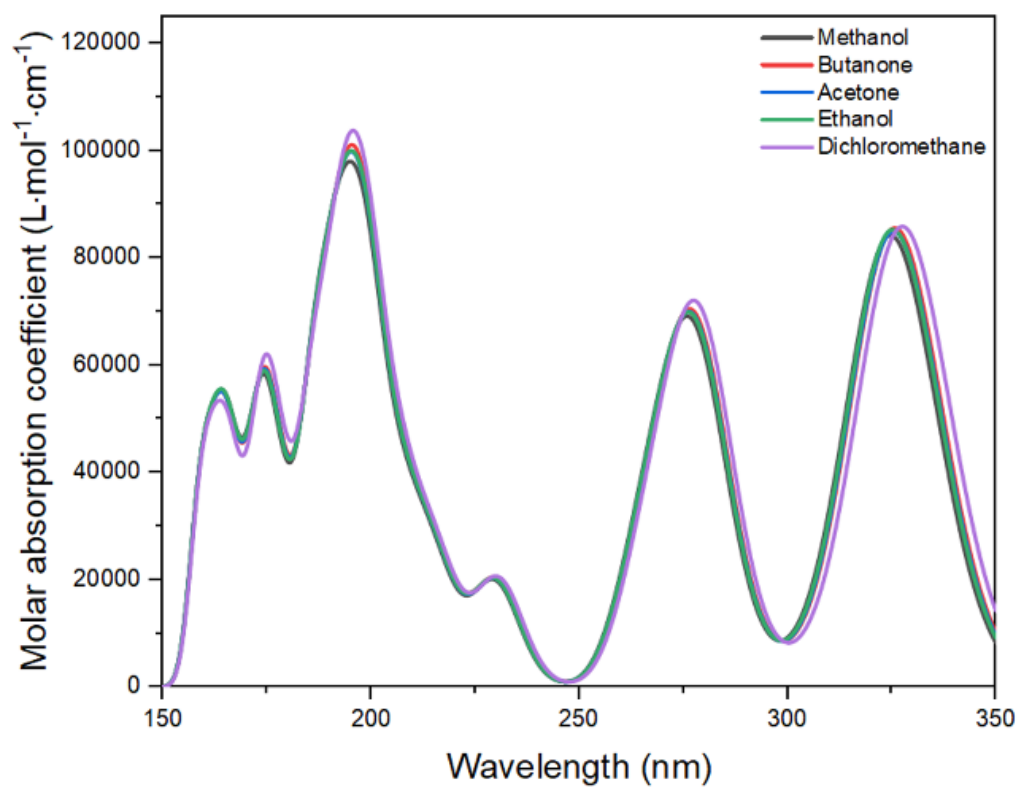


Figure S13. UV-visible absorption spectra of TTTL in different organic solvents were simulated.

4. Single crystal X diffraction pattern

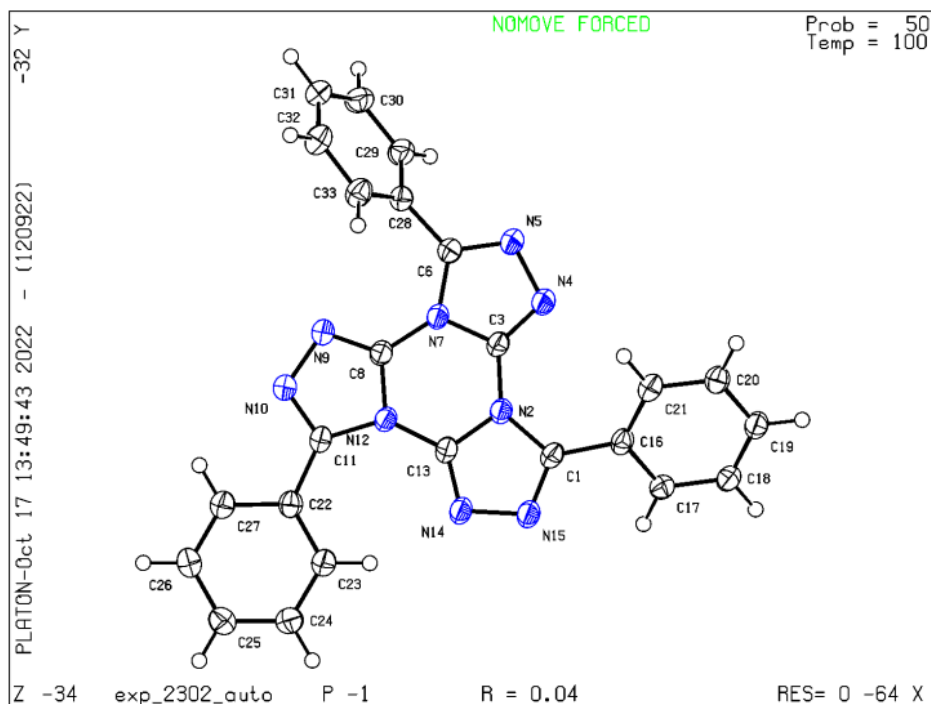


Figure S14. Infrared spectrum of compound TTTB.

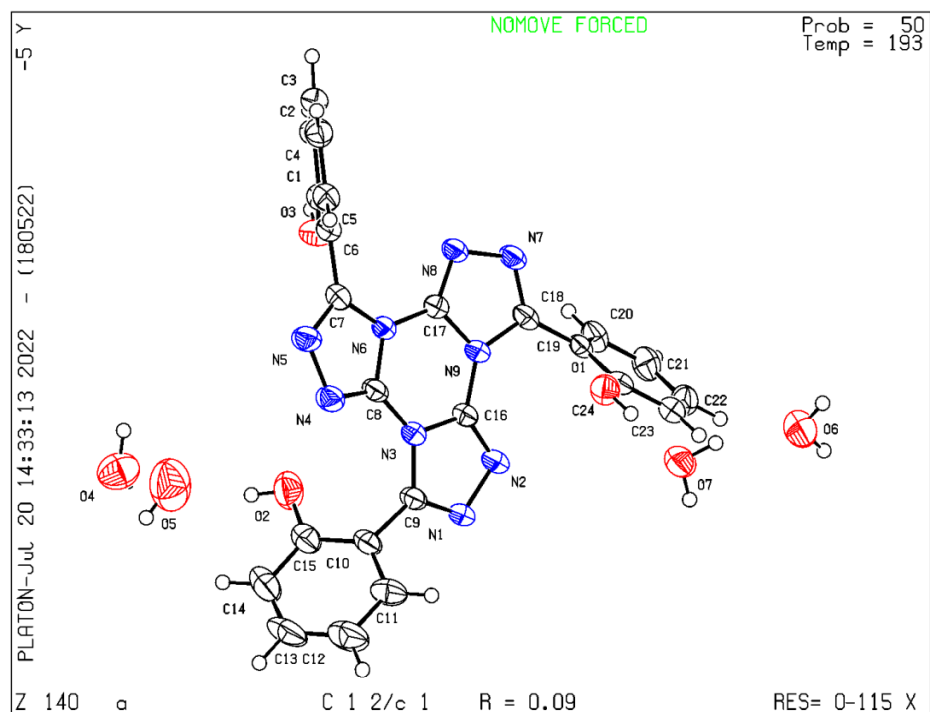


Figure S15. Infrared spectrum of compound TTTL.

Table S1. Bond Lengths for TTTB.

Chemical bond	Length / Å	Chemical bond	Length / Å
N2-C3	1.3899	C16-C1	1.4736
N2-C13	1.3857	C11-C22	1.4767
N2-C1	1.3955	C6-C28	1.4704
N12-C11	1.413	C20-C21	1.3882
N12-C8	1.3775	C20-C19	1.385
N12-C13	1.4022	C22-C23	1.393
N7-C3	1.3706	C22-C27	1.407
N7-C6	1.3905	C17-C18	1.3873
N7-C8	1.3895	C23-C24	1.391
N15-N14	1.3977	C28-C33	1.3936
N15-C1	1.307	C28-C29	1.389
N14-C13	1.2925	C26-C27	1.382
N5-N4	1.4007	C26-C25	1.388
N5-C6	1.3081	C19-C18	1.382
N4-C3	1.2925	C25-C24	1.387
N9-N10	1.3885	C33-C32	1.383
N9-C8	1.2893	C29-C30	1.384
N10-C11	1.3075	C32-C31	1.384
C16-C17	1.3981	C30-C31	1.388
C16-C21	1.393		

Table S2. Bond Lengths for TTTL.

Chemical bond	Length / Å	Chemical bond	Length / Å
O1-C24	1.351	C7-C6	1.46
O3-C1	1.363	C6-C1	1.393
N6-C17	1.394	C6-C5	1.386
N6-C7	1.392	C19-C18	1.472
N6-C8	1.375	C19-C24	1.396
N9-C17	1.37	C19-C20	1.392
N9-C16	1.389	C9-C10	1.468
N9-C18	1.385	C1-C2	1.392
N3-C16	1.369	C24-C23	1.393
N3-C9	1.386	C3-C2	1.376
N3-C8	1.387	C3-C4	1.393
N7-N8	1.408	C10-C15	1.376
N7-C18	1.309	C10-C11	1.4
O2-C15	1.348	C23-C22	1.388
N1-N2	1.396	C20-C21	1.379
N1-C9	1.307	C5-C4	1.382
N8-C17	1.287	C21-C22	1.37
N2-C16	1.291	C15-C14	1.399
N4-N5	1.401	C11-C12	1.369
N4-C8	1.292	C14-C13	1.364
N5-C7	1.311	C13-C12	1.371

Table S3. Crystal data and structure refinement for TTTB.

Empirical formula	C ₂₄ H ₁₅ N ₉
Formula weight	429.45
Temperature/K	100.01
Crystal system	triclinic
Space group	<i>P</i> -1
a /Å	6.08034 (15)
b /Å	12.5701 (4)
c /Å	13.7523 (4)
α /°	110.383 (3)
β /°	92.436 (2)
γ /°	102.329 (2)
V /Å ³	954.69 (5)
Z	2
ρ / (g·cm ⁻³)	1.494
μ /mm ⁻¹	0.780
Crystal size / mm ³	0.2 × 0.15 × 0.08
2 θ range for data collection /°	6.914 to 153.578

Table S4. Crystal data and structure refinement for TTTL.

Empirical formula	C ₂₄ H ₂₃ N ₉ O ₇
Formula weight	549.51
Temperature/K	193.00
Crystal system	monoclinic
Space group	C2/c
a / Å	40.322 (4)
b / Å	7.0682 (7)
c / Å	17.4724 (18)
α / °	90
β / °	100.180 (3)
γ / °	90
V / Å ³	4901.3 (9)
Z	8
ρ /(g·cm ⁻³)	1.489
μ / mm ⁻¹	0.113
Crystal size / mm ³	0.13 × 0.12 × 0.1
2 θ range for data collection / °	4.738 to 55.074

5. Degradation of the film during aging

Table S5. Classification of degradation grade of films in UV aging tester.

Empirical formula	0h	48h	96h	144h
PVC	0	0	1	2
PVC/TTTL	0	0	0	0
PVC/TTTJ	0	0	0	0
PVC/TTTD	0	0	0	1
PVC/TTTB	0	0	0	1
PVC/UV-0	0	0	0	1
PVC/UV-327	0	0	0	0

Notes: Grade 0: Grade 1: Cracks or holes < 2 cm; Grade 2: Cracks or holes > 2 cm; Grade 3: Large area fracture; Grade 4: Break into pieces