

Electronic Supplementary Information

Spirocyclic rhodamine B benzoisothiazole derivative: A multi-stimuli fluorescent switch manifesting ethanol-responsiveness, photo responsiveness, and acidochromism

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For **RHBIT** ESI-MS m/z^+ calculated for $C_{35}H_{33}N_5O_4S$: 619.23, found ($[M+H]^+$) 620

MassPeaks:5

RawMode:Averaged 0.38-0.76(131-261) BasePeak:620.2500(11109778)

BG Mode:Averaged 0.01-0.36(3-125) Segment 1 - Event 1

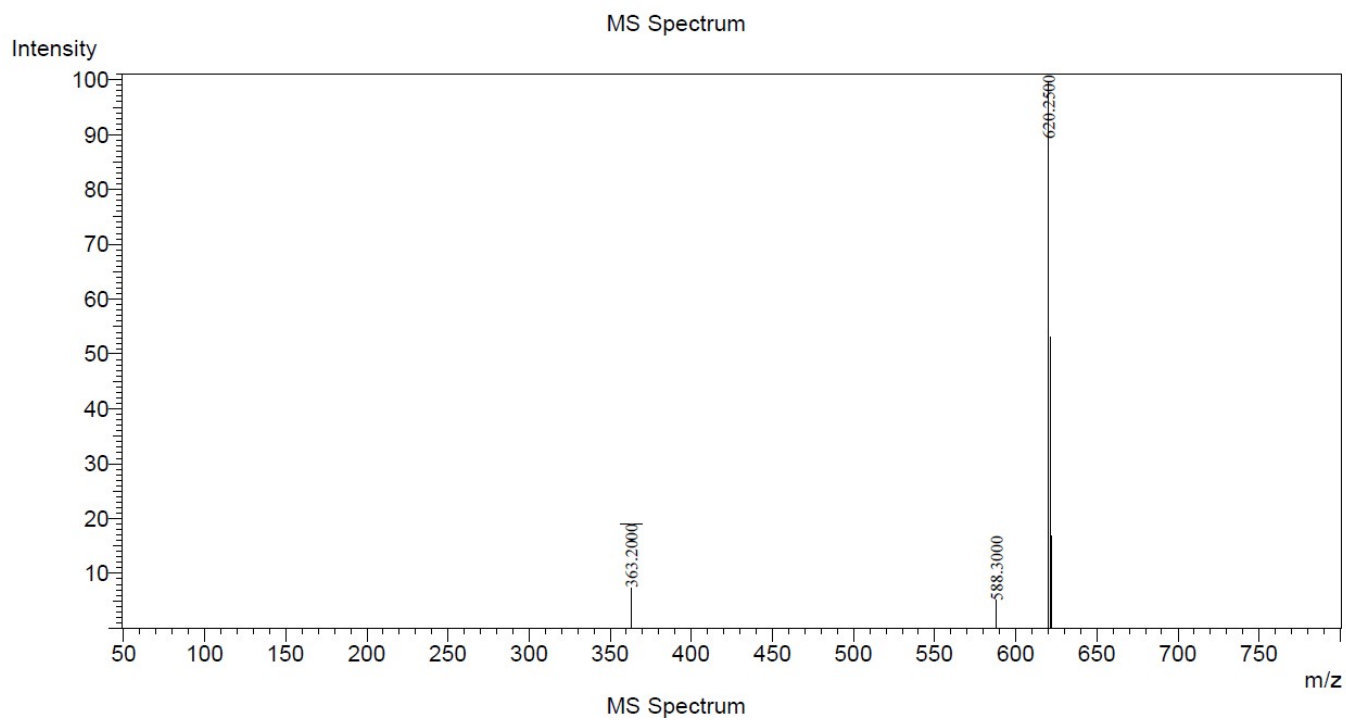


Fig. S1 Mass spectrum of **RHBIT**.

.GB-BIT #13-31 RT: 0.10-0.24 AV: 19 NL: 1.53E6
: FTMS (1,1) + p APCI corona Full ms [90.00-1800.00]

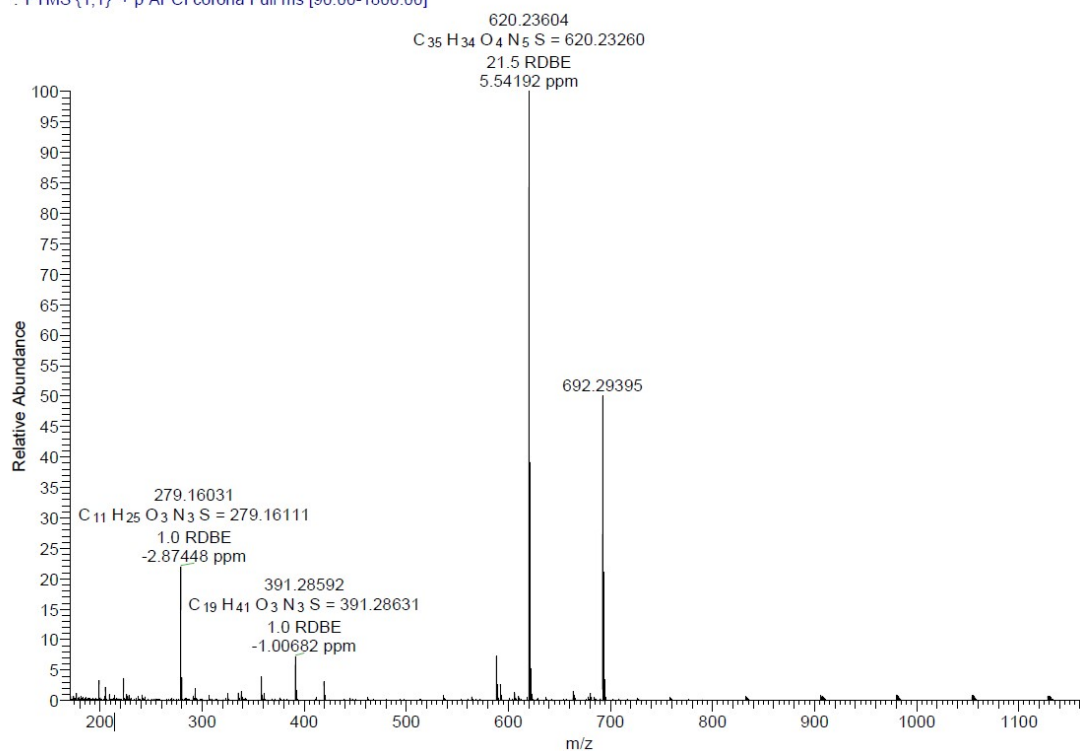


Fig. S2 HRMS spectrum for **RHBIT** HRMS (EI): calcd for C₃₅H₃₃N₅O₄S [M+H]⁺ m/z, 619.23; found m/z, 620.

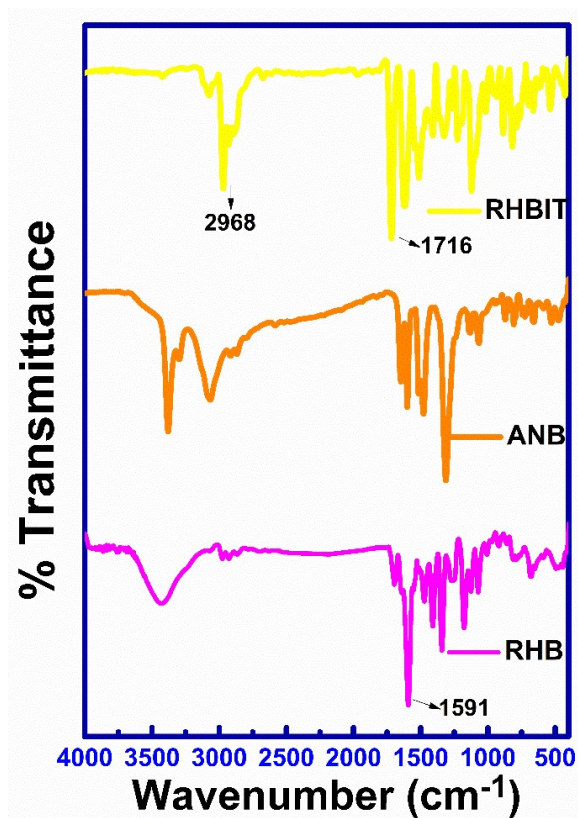


Fig. S3 Comparative FT-IR spectrum of RHB, ANB, and **RHBIT**, depicting the change in the frequency of carbonyl group on transformation from acid (1591 cm^{-1}) to cyclic amide (1716 cm^{-1}) functionality.

^1H NMR and ^{13}C NMR spectra of **RHBIT**:

^1H NMR (400 MHz, CDCl_3) δ 8.55 (d, 1H, $J = 1.9$ Hz, Ar-H), 8.03 – 8.00 (dd, 1H, Ar-H), 7.97 (dd, 1H, $J = 9.7, 2.3$ Hz, Ar-H), 7.55 – 7.47 (m, 3H, Ar-H), 7.15 (dd, 1H, $J = 6.4, 1.3$ Hz, Ar-H), 6.60 (d, 2H, $J = 8.9$ Hz, Ar-H), 6.28 (d, 2H, $J = 2.5$ Hz, Ar-H), 6.22 (dd, 2H, $J = 8.9, 2.6$ Hz, Ar-H), 3.24 (q, 8H, $J = 7.2$ Hz, $-\text{CH}_2$), 1.06 (t, 12H, $J = 7.1$ Hz, $-\text{CH}_3$).

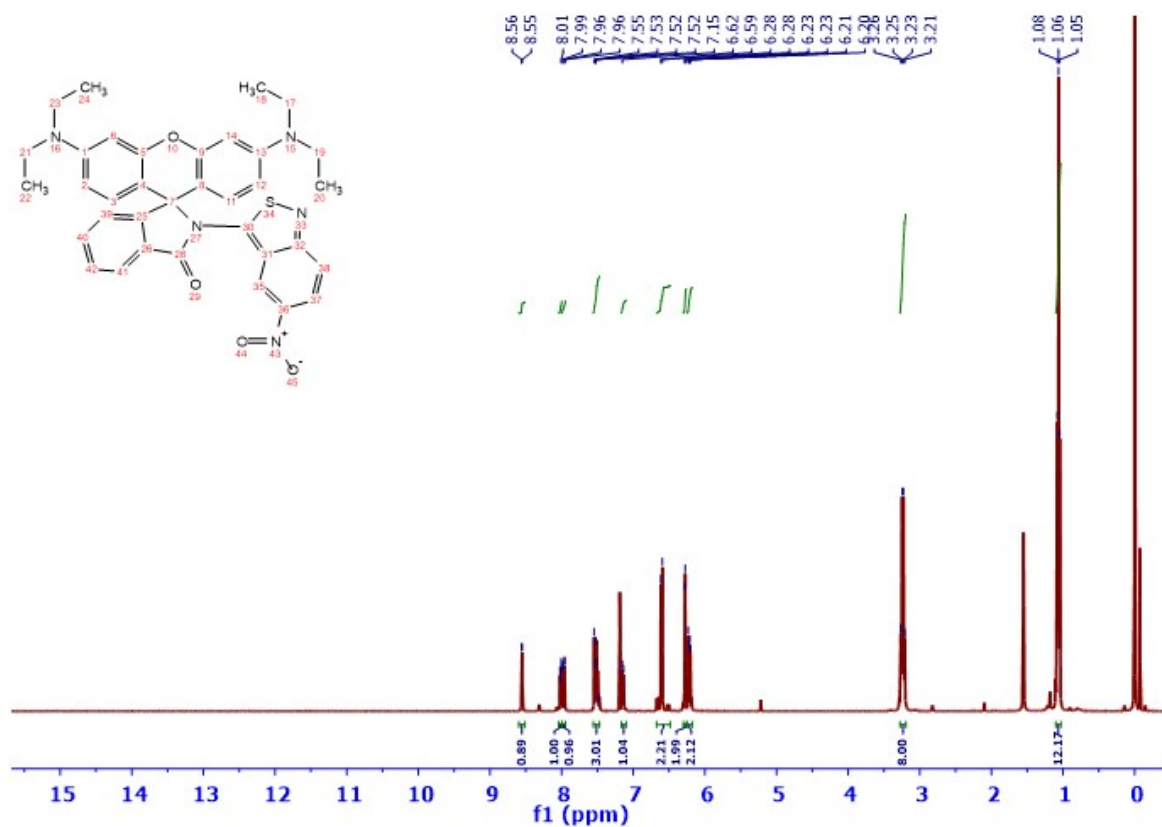


Fig. S4 ^1H NMR spectrum of **RHBIT** in CDCl_3 :

^{13}C NMR (101 MHz, CDCl_3) δ 164.6, 162.1, 158.9, 152.6, 152.4, 148.5, 142.3, 133.4, 127.8, 127.2, 123.3, 123.1, 121.5, 120.8, 120.3, 107.5, 102.6, 97.0, 68.4, 43.3, 11.4

Identification code	RHBIT
Empirical formula	C ₃₅ H ₃₃ N ₅ O ₄ S
Formula weight	619.72
Temperature/K	100
Crystal system	monoclinic
Space group	P2 ₁
a/Å, b/Å, c/Å	10.65490(10); 24.1161(3); 12.8100(2)
α/°, β/°, γ/°	90, 111.908(2), 90

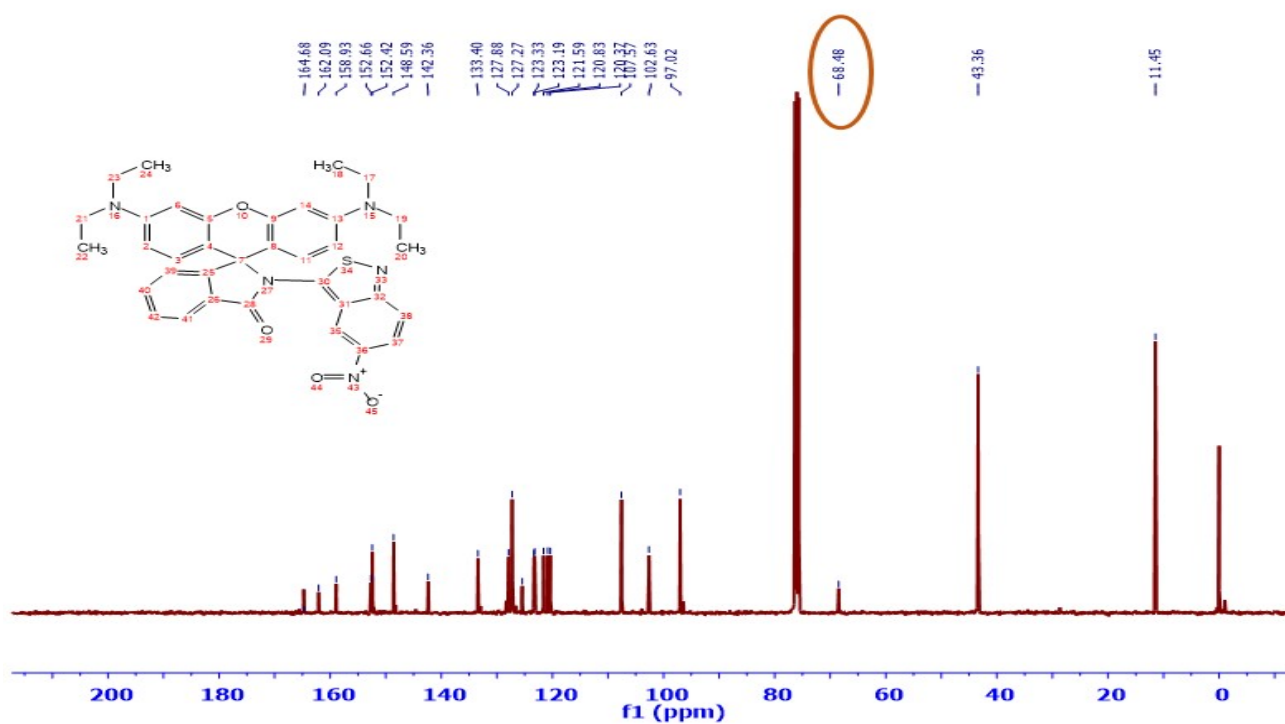


Fig. S5 ¹³C NMR spectrum of **RHBIT** in CDCl₃

Table S1 Crystal data and refinement parameters for **RHBIT**.

Volume/Å ³	3053.88(8)
Z	4
$\rho_{\text{calc}}/\text{g}/\text{cm}^3$	1.348
μ/mm^{-1}	1.339
F(000)	1304.0
Crystal size/mm ³	0.2 × 0.1 × 0.05
Radiation	Cu K α ($\lambda = 1.54184$)
2 Θ range for data collection/°	7.438 to 159.564
Index ranges	-13 ≤ h ≤ 13; -30 ≤ k ≤ 30; -15 ≤ l ≤ 10
Reflections collected	37072
Independent reflections	12789[R _{int} = 0.0451; R _{sigma} = 0.0451]
Data/restraints/parameters	12789/1/819
Goodness-of-fit on F ²	1.038
Final R indexes [I ≥ 2 σ (I)]	R ₁ = 0.0513, wR ₂ = 0.1403
Final R indexes [all data]	R ₁ = 0.0553, wR ₂ = 0.1437
CCDC	2202193

Table S2 (a) Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **RHBIT**. U_{eq} is defined as 1/3 of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	U_{eq}
S1	5912.1(10)	4955.3(4)	10689.2(8)	33.6(2)
O1	3001(3)	5254.5(10)	11468(2)	30.9(6)
O2	4620(3)	5634.7(12)	7200(2)	31.3(6)
O3	9727(3)	6817.9(16)	8731(4)	54.7(9)
O4	7625(3)	6801.7(13)	7629(3)	41.2(7)
N1	2505(3)	3312.7(13)	10934(3)	30.0(7)

N2	3018(4)	7165.2(14)	12325(3)	40.4(9)
N3	4223(3)	5508.2(13)	8850(2)	23.3(6)
N4	7547(3)	5064.0(17)	11214(3)	38.4(8)
N5	8568(4)	6642.6(14)	8470(3)	34.7(7)
C1	2895(4)	4823.1(15)	10745(3)	26.0(7)
C2	2732(4)	4309.1(15)	11157(3)	27.1(7)
C3	2644(4)	3825.4(15)	10524(3)	26.2(7)
C4	2738(4)	3890.1(15)	9458(3)	28.0(7)
C5	2868(4)	4408.4(15)	9061(3)	27.0(7)
C6	2945(3)	4894.1(15)	9682(3)	24.9(7)
C7	3026(4)	5456.9(14)	9204(3)	23.9(7)
C8	3055(4)	5905.9(15)	10039(3)	25.2(7)
C9	3035(4)	6468.5(16)	9771(3)	30.8(8)
C10	3020(4)	6884.4(16)	10501(3)	32.7(8)
C11	3042(4)	6757.4(16)	11588(3)	30.5(8)
C12	3077(4)	6192.7(15)	11864(3)	28.6(7)
C13	3063(4)	5787.9(14)	11101(3)	26.0(7)
C14	2363(4)	2813.7(16)	10261(4)	34.4(8)
C15	941(5)	2706(2)	9413(4)	44.8(10)
C16	2296(4)	3262.6(16)	11998(3)	34.5(8)
C17	891(5)	3402(2)	11937(5)	52.6(12)
C18	2966(5)	7749.4(16)	12021(4)	37.4(9)
C19	4340(5)	7978.5(19)	12152(5)	47.2(11)
C20	2956(6)	7027.1(19)	13415(4)	43.9(11)
C21	1537(6)	6861(2)	13323(5)	53.4(12)
C22	1886(4)	5544.0(14)	8078(3)	25.6(7)
C23	502(4)	5561.3(17)	7843(4)	35.3(9)
C24	-355(5)	5630.1(19)	6731(4)	44.2(11)
C25	138(5)	5674(2)	5869(4)	45.4(11)
C26	1508(4)	5658.9(17)	6102(3)	34.7(8)
C27	2366(4)	5598.1(15)	7222(3)	28.4(7)
C28	3851(4)	5580.9(14)	7694(3)	25.8(7)
C29	5537(4)	5411.5(15)	9592(3)	25.5(7)
C30	6756(4)	5653.5(16)	9630(3)	27.4(7)
C31	7002(4)	6063.3(15)	8935(3)	27.8(7)
C32	8310(4)	6228.8(16)	9198(4)	30.9(8)
C33	9420(4)	6024.0(19)	10125(4)	36.4(9)
C34	9215(4)	5630(2)	10803(4)	38.7(9)
C35	7867(4)	5431.8(18)	10571(4)	32.8(8)
S2	3036.7(9)	5087.2(4)	3940.2(8)	33.2(2)
O5	6271(3)	4698.3(11)	3228(2)	32.4(6)
O6	4330(3)	4409.0(12)	7396(2)	32.5(6)
O7	1405(4)	3111.4(14)	6805(3)	46.3(8)
O8	-708(4)	3113.4(17)	5708(4)	65.5(12)
N6	5708(4)	2796.2(15)	2261(3)	35.4(7)
N7	7044(5)	6625.9(15)	3781(3)	46.3(10)
N8	4750(3)	4516.3(12)	5754(2)	23.2(6)

N9	1402(4)	4968.3(16)	3413(3)	36.4(7)
N10	457(4)	3288.5(15)	5991(4)	41.8(9)
C36	5996(4)	4183.1(16)	3540(3)	27.0(7)
C37	5963(4)	3765.9(16)	2786(3)	29.7(8)
C38	5754(4)	3211.8(16)	3006(3)	30.9(8)
C40	5605(4)	3528.9(16)	4755(4)	33.2(8)
C41	5815(4)	4081.3(15)	4541(3)	25.8(7)
C42	5925(4)	4536.1(15)	5378(3)	25.9(7)
C43	6069(3)	5097.7(15)	4900(3)	25.4(7)
C44	6072(4)	5591.7(16)	5468(3)	29.0(7)

Table S2 (b) Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **RHBIT**. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{ij} tensor

C45	6335(4)	6097.7(16)	5095(3)	29.6(8)
C46	6657(4)	6136.4(16)	4120(3)	31.9(8)
C47	6595(4)	5642.2(17)	3522(3)	32.8(8)
C48	6298(4)	5143.7(16)	3904(3)	27.7(7)
C49	5725(6)	2217.1(19)	2586(4)	49.3(12)
C50	7076(8)	2026(2)	3411(5)	73(2)
C51	5967(4)	2929.0(19)	1242(4)	36.8(9)
C52	7447(5)	3031(3)	1423(5)	55.3(14)
C53	7186(5)	7132.4(17)	4427(4)	44.1(10)
C54	8547(6)	7179(2)	5378(5)	55.0(13)
C55	7728(6)	6617(2)	2916(4)	51.7(12)
C56	6726(6)	6673(3)	1765(5)	60.0(13)
C57	7065(4)	4428.6(15)	6503(3)	28.7(8)
C58	8431(4)	4361.4(18)	6711(4)	36.3(9)
C59	9293(5)	4267(2)	7816(5)	48.8(12)
C60	8828(5)	4245(2)	8685(4)	46.7(11)
C61	7446(5)	4311.0(18)	8482(4)	39.0(9)
C62	6595(4)	4395.5(15)	7360(3)	30.7(8)
C63	5109(4)	4442.7(15)	6901(3)	27.5(7)
C64	3426(4)	4611.2(16)	5000(3)	26.0(7)
C65	2232(4)	4348.3(15)	4945(3)	27.0(7)
C66	2007(4)	3915.5(16)	5598(3)	29.9(8)
C67	709(4)	3735.2(17)	5315(4)	33.3(8)
C68	-419(4)	3958.6(19)	4410(4)	38.0(9)
C69	-224(4)	4375.2(19)	3778(4)	36.3(9)
C70	1108(4)	4579.8(17)	4015(3)	31.8(8)
C39	5576(5)	3103.7(17)	4029(4)	35.8(9)

Table S3 (a) Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **RHBIT**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^*2U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
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Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
S1	29.6(4)	41.0(5)	29.9(4)	11.0(4)	10.8(4)	1.5(4)
O1	51.9(16)	18.7(12)	28.2(13)	1.4(9)	22.1(12)	-1.8(11)
O2	38.6(15)	33.2(14)	26.6(13)	0.8(10)	17.5(12)	-2.7(11)
O3	38.6(18)	52(2)	80(3)	4.3(18)	29.0(18)	-11.3(15)
O4	45.8(17)	37.6(16)	43.5(17)	3.4(13)	20.5(14)	-6.0(13)
N1	34.9(16)	22.5(14)	35.9(17)	2.5(12)	16.9(14)	-1.8(12)
N2	68(3)	21.8(15)	35.1(18)	-3.6(13)	23.9(18)	-0.5(15)
N3	22.6(14)	27.8(15)	21.6(14)	0.3(11)	10.6(11)	-0.9(11)
N4	30.2(16)	50(2)	33.0(17)	8.9(16)	10.1(14)	4.6(15)
N5	35.7(17)	29.6(16)	47(2)	-5.5(14)	25.4(16)	-5.9(13)
C1	25.8(17)	23.7(17)	30.3(18)	-1.1(13)	12.6(14)	-1.2(13)
C2	29.9(17)	23.7(17)	30.4(18)	1.0(13)	14.3(14)	-2.6(13)
C3	23.8(16)	22.5(16)	32.8(19)	2.0(14)	11.2(14)	1.6(12)
C4	29.2(18)	24.7(17)	34(2)	0.0(14)	16.7(15)	-1.2(14)
C5	26.9(17)	25.9(17)	30.3(18)	-2.3(14)	13.2(14)	-0.3(13)
C6	21.0(15)	25.5(17)	29.2(17)	1.8(14)	10.5(13)	-1.5(12)
C7	23.8(16)	23.8(16)	26.6(17)	1.8(13)	12.4(14)	-0.3(12)
C8	27.8(17)	22.9(16)	25.9(17)	0.6(13)	11.3(14)	-1.9(13)
C9	41(2)	23.1(17)	31.0(19)	-0.1(14)	15.8(16)	-1.1(14)
C10	44(2)	25.2(18)	31.1(19)	1.9(14)	15.9(16)	-0.1(15)
C11	36.3(19)	23.9(17)	32.9(19)	-2.8(14)	14.7(16)	-1.6(14)
C12	37(2)	23.3(17)	28.5(18)	0.2(14)	15.8(15)	-2.5(14)
C13	29.1(17)	21.9(17)	29.2(18)	2.4(13)	13.3(15)	-0.4(13)
C14	38(2)	23.1(17)	44(2)	2.3(16)	17.7(18)	-0.6(15)

Table S3 (b) Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **RHBIT**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^2U_{11}+2hka^*b^*U_{12}+\dots]$.

Atom	U ₁₁	U ₂₂	U ₃₃	U ₂₃	U ₁₃	U ₁₂
C15	42(2)	41(2)	47(3)	-1.8(19)	12(2)	-8.0(19)
C16	46(2)	25.6(17)	37(2)	6.2(15)	20.7(18)	-1.2(15)
C17	50(3)	55(3)	66(3)	-6(2)	37(3)	-13(2)
C18	49(2)	23.2(18)	41(2)	-2.1(16)	18.0(18)	4.6(16)
C19	45(2)	32(2)	60(3)	-11.4(19)	15(2)	-2.2(18)
C20	68(3)	34(2)	31(2)	-8.1(16)	21(2)	1(2)
C21	66(3)	53(3)	48(3)	-8(2)	29(2)	7(2)
C22	26.2(17)	20.2(15)	28.2(18)	-0.2(13)	7.8(14)	-0.1(12)
C23	28.6(19)	31.5(19)	45(2)	-0.4(16)	12.8(17)	0.0(15)
C24	30(2)	37(2)	55(3)	4.8(19)	3.0(19)	1.1(17)
C25	43(2)	36(2)	40(2)	2.0(18)	-4.0(19)	-1.3(18)
C26	40(2)	29.8(19)	26.7(19)	2.3(15)	4.2(16)	-0.5(16)
C27	31.7(18)	24.3(17)	28.0(18)	1.2(13)	9.8(15)	-0.8(14)
C28	36.2(19)	21.0(16)	21.0(16)	1.9(12)	11.6(14)	-0.5(13)

C29	24.2(17)	26.0(17)	28.5(17)	0.7(13)	12.1(14)	0.8(13)
C30	24.6(17)	30.2(18)	30.0(18)	-3.8(15)	13.2(14)	0.8(14)
C31	28.9(17)	24.3(17)	32.9(19)	-4.2(14)	14.5(15)	-2.6(13)
C32	31.6(19)	28.9(18)	38(2)	-3.9(15)	19.2(16)	-2.2(14)
C33	26.2(18)	43(2)	42(2)	-5.4(18)	15.5(17)	-1.6(16)
C34	27.0(19)	52(3)	35(2)	1.6(18)	8.6(16)	0.8(17)
C35	27.6(19)	41(2)	32(2)	-0.5(16)	12.9(15)	0.8(16)
S2	30.5(4)	38.6(5)	30.7(4)	10.7(4)	11.5(4)	1.1(4)
O5	47.9(16)	24.1(13)	32.4(14)	-1.9(10)	23.4(12)	-5.4(11)
O6	43.1(15)	31.7(14)	31.3(14)	3.7(11)	23.8(12)	1.7(11)
O7	57(2)	36.0(16)	52(2)	6.6(14)	28.3(17)	-3.1(14)
O8	42.8(19)	53(2)	105(3)	17(2)	33(2)	-13.0(16)
N6	38.0(18)	28.8(16)	37.7(18)	-8.2(14)	12.1(15)	0.5(13)
N7	77(3)	26.1(17)	42(2)	-1.7(14)	30(2)	-13.2(17)
N8	25.4(14)	26.3(14)	20.6(14)	1.5(11)	11.6(11)	-0.5(11)
N9	31.9(16)	44.0(19)	33.3(17)	6.7(15)	12.1(13)	2.8(15)
N10	44(2)	30.8(17)	59(2)	-0.8(16)	28.9(19)	-2.8(15)
C36	25.8(16)	26.3(17)	31.6(19)	1.0(14)	13.7(14)	-0.9(13)
C37	30.0(18)	28.9(18)	31.8(19)	-1.5(15)	13.1(15)	0.3(14)
C38	30.3(18)	28.5(18)	33(2)	-4.1(15)	10.7(15)	1.4(14)
C40	43(2)	26.4(18)	32(2)	1.1(15)	15.9(17)	-0.7(15)
C41	25.8(16)	24.4(17)	29.0(18)	-1.1(13)	12.2(14)	0.8(13)
C42	24.4(16)	26.1(17)	29.4(18)	-0.3(14)	12.7(14)	-2.2(13)
C43	23.6(16)	25.0(17)	29.0(17)	0.7(14)	11.4(13)	0.6(13)
C44	31.4(18)	26.6(18)	32.6(19)	0.5(14)	16.2(15)	-0.7(14)
C45	33.6(19)	23.8(17)	32.3(19)	-0.8(14)	13.3(16)	0.0(14)
C46	38(2)	25.9(17)	31.6(19)	4.5(14)	13.4(16)	-3.4(15)

Table S3 (c) Anisotropic Displacement Parameters ($\text{\AA}^2 \times 10^3$) for **RHBIT**. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\dots]$.

C47	42(2)	29.5(19)	31.3(19)	-2.0(15)	19.0(17)	-4.8(16)
C48	33.1(17)	25.3(16)	26.9(17)	-2.6(13)	13.9(14)	-1.2(14)
C49	65(3)	30(2)	46(3)	-10.6(18)	13(2)	-3(2)
C50	98(5)	40(3)	61(3)	-9(2)	5(3)	24(3)
C51	34(2)	40(2)	39(2)	-13.6(17)	16.9(17)	-2.7(16)
C52	44(3)	59(3)	68(3)	-27(3)	26(2)	-9(2)
C53	64(3)	23.6(19)	50(3)	0.9(17)	28(2)	-4.6(18)
C54	74(4)	46(3)	48(3)	-8(2)	27(3)	-17(2)
C55	61(3)	35(2)	55(3)	4(2)	17(2)	-11(2)
C56	71(4)	50(3)	64(3)	3(3)	30(3)	0(3)
C57	28.7(18)	23.1(17)	30.9(19)	-0.5(14)	7.1(15)	-2.3(14)
C58	28.4(19)	35(2)	43(2)	0.9(17)	10.0(17)	0.2(15)
C59	32(2)	43(3)	55(3)	9(2)	-3(2)	1.2(18)

C60	43(2)	39(2)	41(2)	6.8(18)	-4(2)	-3.0(19)
C61	46(2)	32(2)	29(2)	0.6(15)	2.3(18)	-0.7(17)
C62	36(2)	23.5(17)	29.9(19)	0.4(14)	9.3(16)	0.8(14)
C63	34.3(19)	22.0(16)	25.7(17)	0.7(13)	10.7(14)	0.0(13)
C64	27.0(17)	27.3(17)	26.3(17)	0.9(13)	12.9(14)	0.1(14)
C65	26.9(17)	26.8(17)	28.3(18)	-0.4(14)	11.6(14)	1.4(13)
C66	31.0(19)	26.7(18)	35(2)	0.0(14)	15.3(16)	1.2(14)
C67	32.0(19)	29.5(19)	43(2)	-3.1(16)	19.7(17)	-3.7(15)
C68	29.5(19)	40(2)	49(3)	-4.1(18)	19.2(18)	-2.2(16)
C69	25.2(18)	43(2)	40(2)	3.0(17)	11.7(16)	5.2(16)
C70	30.9(19)	33.4(19)	31.3(19)	0.1(15)	11.8(15)	3.1(15)
C39	46(2)	24.2(17)	36(2)	-0.3(15)	14.3(18)	-2.4(16)

Table S4 (a) Bond Lengths for RHBIT

Atom	Atom	Length/Å	Atom	Atom	Length/Å
S1	N4	1.637(4)	S2	N9	1.641(4)
S1	C29	1.711(4)	S2	C64	1.707(4)
O1	C1	1.370(4)	O5	C36	1.370(4)
O1	C13	1.380(4)	O5	C48	1.373(4)
O2	C28	1.214(5)	O6	C63	1.221(5)
O3	N5	1.227(5)	O7	N10	1.226(5)
O4	N5	1.229(5)	O8	N10	1.230(5)
N1	C3	1.373(5)	N6	C38	1.372(5)
N1	C14	1.455(5)	N6	C49	1.455(6)
N1	C16	1.466(5)	N6	C51	1.467(6)
N2	C11	1.370(5)	N7	C46	1.373(5)
N2	C18	1.457(5)	N7	C53	1.451(6)

Table S4 (b) Bond Lengths for RHBIT

N2	C20	1.460(6)	N7	C55	1.536(7)
N3	C7	1.510(4)	N8	C42	1.501(4)
N3	C28	1.395(5)	N8	C63	1.384(5)
N3	C29	1.387(5)	N8	C64	1.400(5)
N4	C35	1.338(6)	N9	C70	1.323(5)
N5	C32	1.460(5)	N10	C67	1.469(6)
C1	C2	1.383(5)	C36	C37	1.386(5)
C1	C6	1.392(5)	C36	C41	1.387(5)
C2	C3	1.403(5)	C37	C38	1.400(6)
C3	C4	1.415(5)	C38	C39	1.418(6)
C4	C5	1.376(5)	C40	C41	1.395(5)

C5	C6	1.401 (5)	C40	C39	1.376 (6)
C6	C7	1.505 (5)	C41	C42	1.508 (5)
C7	C8	1.513 (5)	C42	C43	1.517 (5)
C7	C22	1.515 (5)	C42	C57	1.521 (5)
C8	C9	1.397 (5)	C43	C44	1.395 (5)
C8	C13	1.388 (5)	C43	C48	1.390 (5)
C9	C10	1.376 (5)	C44	C45	1.377 (5)
C10	C11	1.417 (6)	C45	C46	1.417 (6)
C11	C12	1.404 (5)	C46	C47	1.405 (5)
C12	C13	1.377 (5)	C47	C48	1.379 (5)
C14	C15	1.521 (6)	C49	C50	1.506 (8)
C16	C17	1.507 (6)	C51	C52	1.525 (6)
C18	C19	1.514 (7)	C53	C54	1.511 (8)
C20	C21	1.526 (8)	C55	C56	1.469 (8)
C22	C23	1.392 (5)	C57	C58	1.388 (6)
C22	C27	1.378 (5)	C57	C62	1.369 (6)
C23	C24	1.386 (7)	C58	C59	1.389 (7)
C24	C25	1.392 (8)	C59	C60	1.378 (8)
C25	C26	1.377 (7)	C60	C61	1.405 (7)
C26	C27	1.391 (5)	C61	C62	1.399 (6)
C27	C28	1.468 (5)	C62	C63	1.473 (6)
C29	C30	1.408 (5)	C64	C65	1.399 (5)
C30	C31	1.418 (5)	C65	C66	1.413 (5)
C30	C35	1.440 (6)	C65	C70	1.449 (5)
C31	C32	1.366 (5)	C66	C67	1.364 (6)
C32	C33	1.416 (6)	C67	C68	1.427 (6)
C33	C34	1.358 (7)	C68	C69	1.354 (6)
C34	C35	1.436 (6)	C69	C70	1.424 (6)

Table S5 (a) Bond Angles for RHBIT

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N4	S1	C29	96.95(18)	N9	S2	C64	96.61(18)
C1	O1	C13	118.7(3)	C36	O5	C48	118.8(3)
C3	N1	C14	121.4(3)	C38	N6	C49	120.6(4)
C3	N1	C16	120.4(3)	C38	N6	C51	119.3(4)
C14	N1	C16	117.7(3)	C49	N6	C51	118.5(4)
C11	N2	C18	121.2(4)	C46	N7	C53	121.5(4)
C11	N2	C20	120.9(3)	C46	N7	C55	119.6(4)
C18	N2	C20	117.7(3)	C53	N7	C55	116.5(4)
C28	N3	C7	113.1(3)	C63	N8	C42	114.3(3)
C29	N3	C7	122.0(3)	C63	N8	C64	124.2(3)
C29	N3	C28	124.3(3)	C64	N8	C42	121.3(3)
C35	N4	S1	109.3(3)	C70	N9	S2	109.3(3)
O3	N5	O4	122.8(4)	O7	N10	O8	123.5(4)
O3	N5	C32	118.1(4)	O7	N10	C67	118.9(4)
O4	N5	C32	119.1(3)	O8	N10	C67	117.7(4)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	C1	C2	114.4(3)	O5	C36	C37	114.1(3)
O1	C1	C6	123.0(3)	O5	C36	C41	123.3(3)
C2	C1	C6	122.6(3)	C37	C36	C41	122.6(3)
C1	C2	C3	121.0(3)	C36	C37	C38	121.2(4)
N1	C3	C2	121.4(3)	N6	C38	C37	121.7(4)
N1	C3	C4	121.7(3)	N6	C38	C39	121.8(4)
C2	C3	C4	116.9(3)	C37	C38	C39	116.6(4)
C5	C4	C3	120.7(3)	C39	C40	C41	122.9(4)
C4	C5	C6	122.8(4)	C36	C41	C40	116.0(3)
C1	C6	C5	115.9(3)	C36	C41	C42	121.9(3)
C1	C6	C7	122.5(3)	C40	C41	C42	122.0(3)
C5	C6	C7	121.5(3)	N8	C42	C41	110.7(3)
N3	C7	C8	110.9(3)	N8	C42	C43	112.4(3)
N3	C7	C22	99.7(3)	N8	C42	C57	99.1(3)
C6	C7	N3	112.3(3)	C41	C42	C43	110.8(3)
C6	C7	C8	110.3(3)	C41	C42	C57	111.9(3)
C6	C7	C22	111.4(3)	C43	C42	C57	111.6(3)
C8	C7	C22	111.8(3)	C44	C43	C42	122.2(3)
C9	C8	C7	121.8(3)	C48	C43	C42	121.4(3)
C13	C8	C7	122.5(3)	C48	C43	C44	116.3(3)
C13	C8	C9	115.7(3)	C45	C44	C43	122.5(4)
C10	C9	C8	123.0(4)	C44	C45	C46	120.8(4)
C9	C10	C11	120.7(4)	N7	C46	C45	122.4(4)
N2	C11	C10	121.6(4)	N7	C46	C47	121.0(4)
N2	C11	C12	121.9(4)	C47	C46	C45	116.6(3)
C12	C11	C10	116.5(3)	C48	C47	C46	121.1(4)
C13	C12	C11	121.2(4)	O5	C48	C43	123.2(3)
O1	C13	C8	122.8(3)	O5	C48	C47	114.3(3)
C12	C13	O1	114.1(3)	C47	C48	C43	122.5(3)

Table S5 (b) Bond Angles for RHBIT

C12	C13	C8	123.0(3)	N6	C49	C50	113.7(5)
N1	C14	C15	114.9(4)	N6	C51	C52	115.3(4)
N1	C16	C17	115.2(4)	N7	C53	C54	112.8(4)
N2	C18	C19	112.6(4)	C56	C55	N7	111.1(5)
N2	C20	C21	112.5(4)	C58	C57	C42	127.7(4)
C23	C22	C7	128.2(4)	C62	C57	C42	111.6(3)
C27	C22	C7	111.6(3)	C62	C57	C58	120.7(4)
C27	C22	C23	120.3(4)	C57	C58	C59	117.5(4)
C24	C23	C22	117.6(4)	C60	C59	C58	122.0(5)
C23	C24	C25	121.7(4)	C59	C60	C61	120.9(4)
C26	C25	C24	120.6(4)	C62	C61	C60	116.1(4)
C25	C26	C27	117.5(4)	C57	C62	C61	122.8(4)
C22	C27	C26	122.2(4)	C57	C62	C63	109.6(3)
C22	C27	C28	109.4(3)	C61	C62	C63	127.6(4)
C26	C27	C28	128.3(4)	O6	C63	N8	126.0(4)
O2	C28	N3	125.9(4)	O6	C63	C62	128.7(3)
O2	C28	C27	128.0(3)	N8	C63	C62	105.3(3)

N3	C28	C27	106.1(3)	N8	C64	S2	122.8(3)
N3	C29	S1	122.5(3)	C65	C64	S2	108.6(3)
N3	C29	C30	129.5(3)	C65	C64	N8	128.6(3)
C30	C29	S1	108.0(3)	C64	C65	C66	131.0(4)
C29	C30	C31	130.6(4)	C64	C65	C70	108.9(3)
C29	C30	C35	109.5(3)	C66	C65	C70	120.0(3)
C31	C30	C35	119.8(3)	C67	C66	C65	117.2(4)
C32	C31	C30	117.4(4)	C66	C67	N10	117.9(4)
C31	C32	N5	117.4(4)	C66	C67	C68	123.9(4)
C31	C32	C33	124.1(4)	C68	C67	N10	118.2(4)
C33	C32	N5	118.5(4)	C69	C68	C67	119.7(4)
C34	C33	C32	119.8(4)	C68	C69	C70	119.5(4)
C33	C34	C35	119.2(4)	N9	C70	C65	116.7(4)
N4	C35	C30	116.2(4)	N9	C70	C69	123.7(4)
N4	C35	C34	124.0(4)	C69	C70	C65	119.6(4)
C34	C35	C30	119.7(4)	C40	C39	C38	120.7(4)

Table S6 (a) Torsion Angles for RHBIT

A	B	C	D	Angle/°	A	B	C	D	Angle/°
S1	N4	C35	C30	1.9(5)	S2	N9	C70	C65	-1.1(5)
S1	N4	C35	C34	178.6(4)	S2	N9	C70	C69	-179.5(3)
S1	C29	C30	C31	-178.3(3)	S2	C64	C65	C66	177.7(4)
S1	C29	C30	C35	-0.1(4)	S2	C64	C65	C70	-0.4(4)
O1	C1	C2	C3	-178.3(3)	O5	C36	C37	C38	177.2(3)
O1	C1	C6	C5	177.9(3)	O5	C36	C41	C40	-177.0(4)
O1	C1	C6	C7	-4.3(5)	O5	C36	C41	C42	-0.6(6)
O3	N5	C32	C31	176.0(4)	O7	N10	C67	C66	2.9(6)
O3	N5	C32	C33	-4.0(6)	O7	N10	C67	C68	-176.5(4)
O4	N5	C32	C31	-3.8(5)	O8	N10	C67	C66	-177.4(4)
O4	N5	C32	C33	176.2(4)	O8	N10	C67	C68	3.2(6)
N1	C3	C4	C5	179.5(3)	N6	C38	C39	C40	-179.0(4)
N2	C11	C12	C13	178.1(4)	N7	C46	C47	C48	175.5(4)
N3	C7	C8	C9	59.5(4)	N8	C42	C43	C44	50.0(4)
N3	C7	C8	C13	-122.5(4)	N8	C42	C43	C48	-134.4(3)
N3	C7	C22	C23	-177.9(4)	N8	C42	C57	C58	175.6(4)
N3	C7	C22	C27	3.5(4)	N8	C42	C57	C62	-3.7(4)
N3	C29	C30	C31	0.3(7)	N8	C64	C65	C66	-1.2(7)
N3	C29	C30	C35	178.5(4)	N8	C64	C65	C70	-179.3(4)
N4	S1	C29	N3	-177.7(3)	N9	S2	C64	N8	178.8(3)
N4	S1	C29	C30	1.0(3)	N9	S2	C64	C65	-0.1(3)
N5	C32	C33	C34	-178.6(4)	N10	C67	C68	C69	179.2(4)
C1	O1	C13	C8	-1.6(5)	C36	O5	C48	C43	0.6(5)
C1	O1	C13	C12	175.9(3)	C36	O5	C48	C47	179.5(3)
C1	C2	C3	N1	178.9(3)	C36	C37	C38	N6	179.4(4)
C1	C2	C3	C4	0.4(5)	C36	C37	C38	C39	0.1(6)
C1	C6	C7	N3	124.7(4)	C36	C41	C42	N8	132.4(3)
C1	C6	C7	C8	0.5(5)	C36	C41	C42	C43	7.1(5)

C1	C6	C7	C22	-124.3(4)	C36	C41	C42	C57	-118.2(4)
C2	C1	C6	C5	-2.1(5)	C37	C36	C41	C40	0.4(6)
C2	C1	C6	C7	175.7(3)	C37	C36	C41	C42	176.8(3)
C2	C3	C4	C5	-1.9(5)	C37	C38	C39	C40	0.3(6)
C3	N1	C14	C15	-81.3(5)	C38	N6	C49	C50	-71.9(6)
C3	N1	C16	C17	76.0(5)	C38	N6	C51	C52	75.3(5)
C3	C4	C5	C6	1.5(6)	C40	C41	C42	N8	-51.4(5)
C4	C5	C6	C1	0.5(5)	C40	C41	C42	C43	-176.7(4)
C4	C5	C6	C7	-177.3(3)	C40	C41	C42	C57	58.1(5)
C5	C6	C7	N3	-57.6(4)	C41	C36	C37	C38	-0.5(6)
C5	C6	C7	C8	178.2(3)	C41	C40	C39	C38	-0.4(7)
C5	C6	C7	C22	53.4(4)	C41	C42	C43	C44	174.4(3)
C6	C1	C2	C3	1.7(6)	C41	C42	C43	C48	-10.0(5)

Table S6 (b) Torsion Angles for RHBIT

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C6	C7	C8	C9	-175.5(3)	C41	C42	C57	C58	58.9(5)
C6	C7	C8	C13	2.5(5)	C41	C42	C57	C62	-120.4(3)
C6	C7	C22	C23	63.4(5)	C42	N8	C63	O6	-179.3(3)
C6	C7	C22	C27	-115.2(3)	C42	N8	C63	C62	-1.3(4)
C7	N3	C28	O2	179.7(3)	C42	N8	C64	S2	-36.8(5)
C7	N3	C28	C27	1.6(4)	C42	N8	C64	C65	141.9(4)
C7	N3	C29	S1	29.9(5)	C42	C43	C44	C45	173.5(4)
C7	N3	C29	C30	-148.6(4)	C42	C43	C48	O5	6.8(5)
C7	C8	C9	C10	178.0(4)	C42	C43	C48	C47	-171.9(4)
C7	C8	C13	O1	-2.1(5)	C42	C57	C58	C59	179.9(4)
C7	C8	C13	C12	-179.4(4)	C42	C57	C62	C61	-178.6(4)
C7	C22	C23	C24	-178.1(4)	C42	C57	C62	C63	3.3(4)
C7	C22	C27	C26	177.3(3)	C43	C42	C57	C58	-65.8(5)
C7	C22	C27	C28	-2.8(4)	C43	C42	C57	C62	114.8(4)
C8	C7	C22	C23	-60.6(5)	C43	C44	C45	C46	-1.8(6)
C8	C7	C22	C27	120.7(3)	C44	C43	C48	O5	-177.3(3)
C8	C9	C10	C11	0.8(7)	C44	C43	C48	C47	3.9(6)
C9	C8	C13	O1	176.0(4)	C44	C45	C46	N7	-173.9(4)
C9	C8	C13	C12	-1.3(5)	C44	C45	C46	C47	4.4(6)
C9	C10	C11	N2	-179.5(4)	C45	C46	C47	C48	-2.9(6)
C9	C10	C11	C12	-0.2(6)	C46	N7	C53	C54	84.0(6)
C10	C11	C12	C13	-1.2(6)	C46	N7	C55	C56	92.0(5)
C11	N2	C18	C19	-80.7(5)	C46	C47	C48	O5	179.8(4)
C11	N2	C20	C21	-78.0(6)	C46	C47	C48	C43	-1.3(6)
C11	C12	C13	O1	-175.5(3)	C48	O5	C36	C37	178.6(3)
C11	C12	C13	C8	2.0(6)	C48	O5	C36	C41	-3.8(5)
C13	O1	C1	C2	-175.1(3)	C48	C43	C44	C45	-2.3(6)
C13	O1	C1	C6	4.8(5)	C49	N6	C38	C37	169.3(4)
C13	C8	C9	C10	-0.1(6)	C49	N6	C38	C39	-11.5(6)
C14	N1	C3	C2	177.6(3)	C49	N6	C51	C52	-90.4(5)
C14	N1	C3	C4	-3.9(5)	C51	N6	C38	C37	3.8(6)

C14	N1	C16	C17	-95.3(4)	C51	N6	C38	C39	-176.9(4)
C16	N1	C3	C2	6.7(5)	C51	N6	C49	C50	93.7(5)
C16	N1	C3	C4	-174.8(4)	C53	N7	C46	C45	1.9(7)
C16	N1	C14	C15	89.8(5)	C53	N7	C46	C47	-176.4(4)
C18	N2	C11	C10	0.0(7)	C53	N7	C55	C56	-105.0(5)
C18	N2	C11	C12	-179.3(4)	C55	N7	C46	C45	164.1(4)
C18	N2	C20	C21	98.3(5)	C55	N7	C46	C47	-14.2(7)
C20	N2	C11	C10	176.1(4)	C55	N7	C53	C54	-78.7(5)
C20	N2	C11	C12	-3.2(7)	C57	C42	C43	C44	-60.3(4)
C20	N2	C18	C19	103.1(5)	C57	C42	C43	C48	115.4(4)
C22	C7	C8	C9	-50.9(5)	C57	C58	C59	C60	-0.6(7)
C22	C7	C8	C13	127.1(4)	C57	C62	C63	O6	176.7(4)
C22	C23	C24	C25	0.8(7)	C57	C62	C63	N8	-1.3(4)
C22	C27	C28	O2	-177.3(4)	C58	C57	C62	C61	2.0(6)
C22	C27	C28	N3	0.7(4)	C58	C57	C62	C63	-176.1(4)
C23	C22	C27	C26	-1.4(6)	C58	C59	C60	C61	0.8(7)
C23	C22	C27	C28	178.5(3)	C59	C60	C61	C62	0.3(7)
C23	C24	C25	C26	-1.1(7)	C60	C61	C62	C57	-1.7(6)
C24	C25	C26	C27	0.1(7)	C60	C61	C62	C63	176.0(4)

Table S6 (c) Torsion Angles for RHBIT

A	B	C	D	Angle/°	A	B	C	D	Angle/°
C25	C26	C27	C22	1.1(6)	C61	C62	C63	O6	-1.3(7)
C25	C26	C27	C28	-178.8(4)	C61	C62	C63	N8	-179.3(4)
C26	C27	C28	O2	2.6(7)	C62	C57	C58	C59	-0.8(6)
C26	C27	C28	N3	-179.4(4)	C63	N8	C42	C41	120.6(3)
C27	C22	C23	C24	0.4(6)	C63	N8	C42	C43	-115.0(3)
C28	N3	C7	C6	115.0(3)	C63	N8	C42	C57	3.0(4)
C28	N3	C7	C8	-121.0(3)	C63	N8	C64	S2	137.8(3)
C28	N3	C7	C22	-3.1(4)	C63	N8	C64	C65	-43.5(6)
C28	N3	C29	S1	-140.5(3)	C64	S2	N9	C70	0.7(3)
C28	N3	C29	C30	41.1(6)	C64	N8	C42	C41	-64.3(4)
C29	S1	N4	C35	-1.7(3)	C64	N8	C42	C43	60.1(4)
C29	N3	C7	C6	-56.3(4)	C64	N8	C42	C57	178.1(3)
C29	N3	C7	C8	67.6(4)	C64	N8	C63	O6	5.8(6)
C29	N3	C7	C22	-174.4(3)	C64	N8	C63	C62	-176.2(3)
C29	N3	C28	O2	-9.2(6)	C64	C65	C66	C67	-178.2(4)
C29	N3	C28	C27	172.8(3)	C64	C65	C70	N9	1.0(5)
C29	C30	C31	C32	178.4(4)	C64	C65	C70	C69	179.4(4)
C29	C30	C35	N4	-1.2(5)	C65	C66	C67	N10	-179.5(3)
C29	C30	C35	C34	-178.0(4)	C65	C66	C67	C68	-0.2(6)
C30	C31	C32	N5	178.8(3)	C66	C65	C70	N9	-177.3(4)
C30	C31	C32	C33	-1.2(6)	C66	C65	C70	C69	1.1(6)
C31	C30	C35	N4	177.3(4)	C66	C67	C68	C69	-0.1(7)
C31	C30	C35	C34	0.4(6)	C67	C68	C69	C70	0.9(7)
C31	C32	C33	C34	1.3(7)	C68	C69	C70	N9	176.9(4)
C32	C33	C34	C35	-0.5(7)	C68	C69	C70	C65	-1.4(6)
C33	C34	C35	N4	-176.9(4)	C70	C65	C66	C67	-0.3(6)

C33	C34	C35	C30	-0.3(7)	C39	C40	C41	C36	0.1(6)
C35	C30	C31	C32	0.3(5)	C39	C40	C41	C42	-176.4(4)

Table S7 (a) Hydrogen Atom Coordinates ($\text{\AA}\times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2\times 10^3$) for RHBIT

Atom	x	y	z	U(eq)
H2	2679	4283	11879	33
H4	2712	3572	9012	34
H5	2906	4438	8334	32
H9	3031	6568	9053	37
H10	2994	7261	10275	39
H12	3111	6088	12588	34
H14A	2650	2491	10774	41
H14B	2985	2841	9850	41
H15A	656	3015	8881	67

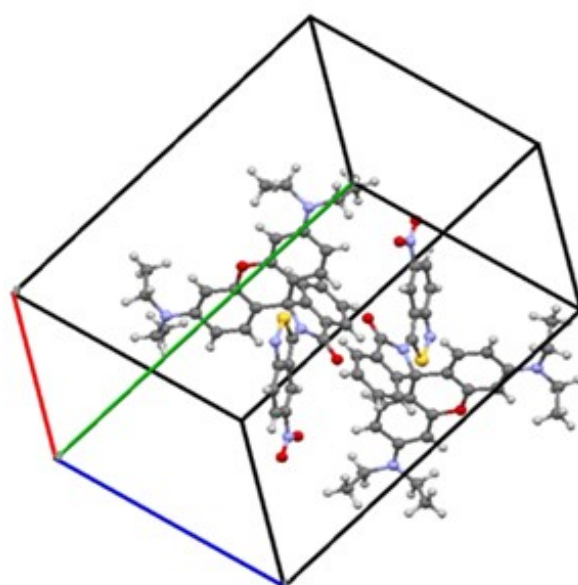
Table S7 (b) Hydrogen Atom Coordinates ($\text{\AA}\times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2\times 10^3$) for RHBIT

Atom	x	y	z	Ueq
H15B	316	2670	9810	67
H15C	935	2362	9004	67
H16A	2947	3509	12559	41
H16B	2507	2877	12274	41
H17A	238	3150	11409	79
H17B	673	3785	11677	79
H17C	850	3362	12684	79
H18A	2601	7965	12502	45
H18B	2339	7796	11230	45
H19A	4748	7742	11741	71
H19B	4925	7985	12951	71
H19C	4235	8356	11847	71
H20A	3257	7351	13921	53
H20B	3588	6718	13755	53
H21A	1219	6550	12797	80
H21B	923	7176	13047	80
H21C	1559	6749	14065	80
H23	156	5527	8425	42

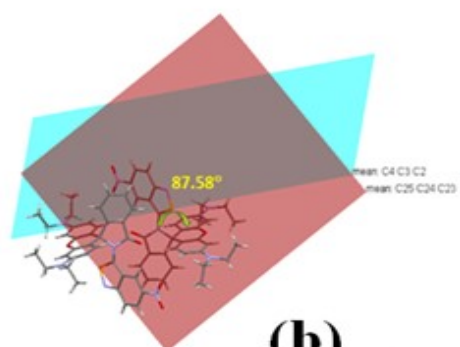
H24	-1303	5648	6552	53
H25	-477	5714	5113	54
H26	1855	5689	5520	42
H31	6285	6217	8312	33
H33	10305	6162	10273	44
H34	9954	5488	11424	46
H37	6085	3857	2109	36
H40	5477	3442	5432	40
H44	5886	5578	6138	35
H45	6301	6425	5496	36
H47	6762	5652	2844	39
H49A	5468	1984	1902	59
H49B	5035	2161	2922	59
H50A	7699	1972	3018	110
H50B	6963	1675	3752	110
H50C	7445	2306	4000	110
H51A	5440	3264	893	44
H51B	5626	2620	701	44
H52A	7511	3154	716	83
H52B	7961	2687	1673	83
H52C	7818	3318	1998	83
H53A	6466	7145	4740	53
H53B	7059	7455	3919	53
H54A	9265	7157	5076	82

Table S7 (c) Hydrogen Atom Coordinates ($\text{\AA}\times 10^4$) and Isotropic Displacement Parameters ($\text{\AA}^2\times 10^3$) for RHBIT

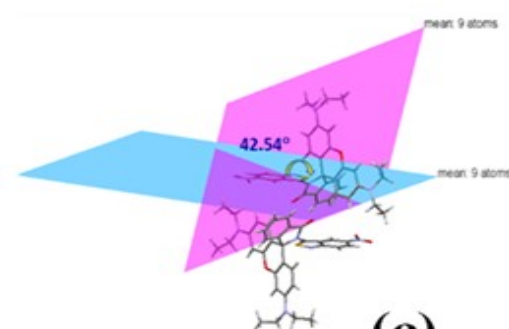
Atom	x	y	z	U_{eq}
H54B	8652	6876	5913	82
H54C	8606	7535	5763	82
H55A	8390	6924	3076	62
H55B	8226	6263	2984	62
H56A	7191	6682	1234	90
H56B	6216	7018	1703	90
H56C	6103	6357	1591	90
H58	8764	4379	6119	44
H59	10231	4217	7978	59
H60	9450	4185	9432	56
H61	7110	4299	9072	47
H66	2730	3757	6209	36
H68	-1301	3815	4252	46
H69	-971	4530	3181	44
H39	5434	2734	4217	43



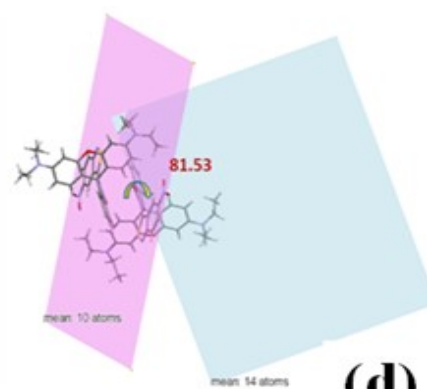
(a)



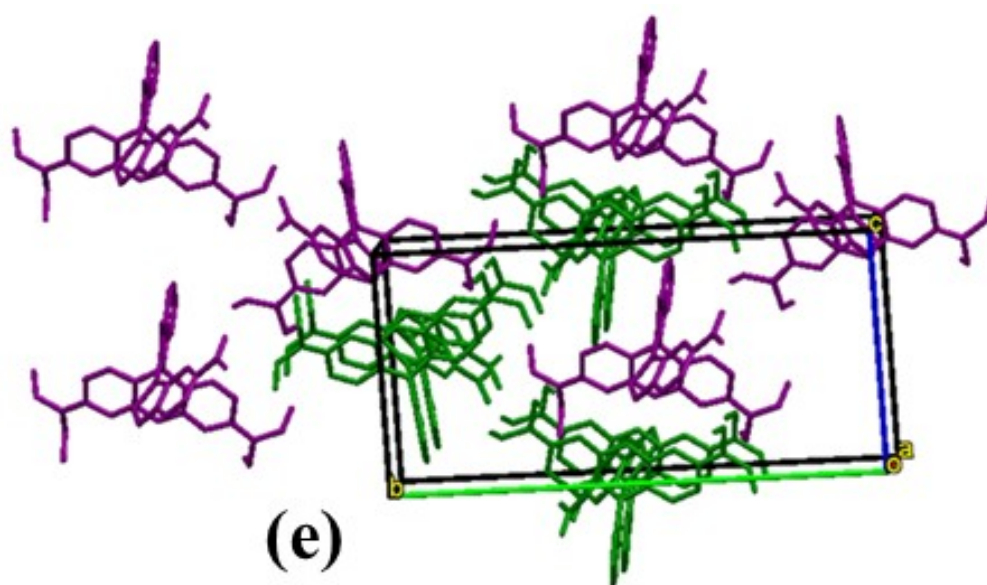
(b)



(c)



(d)



(e)

Fig. S6. (a) Asymmetric unit comprising two units of **RHBIT** arranged antiparallel to each other (b) angle between the xanthene ring and spiro lactam unit (c) angle between the spiro lactam ring and the ANB moiety (d) angle between the xanthene ring and ANB moiety (e) parallel arrangement of two units along the axis *oa*.

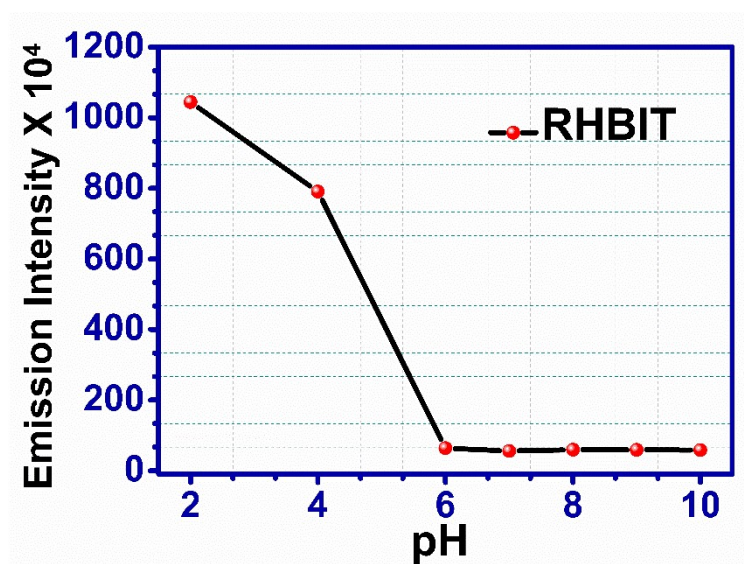


Fig. S7 Shows the variation in fluorescence emission ($\lambda_{\text{max}} \sim 575$ nm) intensity of **RHBIT** when excited at 520 nm at different pH conditions, emerging in the increased emission intensity at pH <6 (under acidic conditions); and cyclic form of **RHBIT** was relatively stable within pH 6-10.

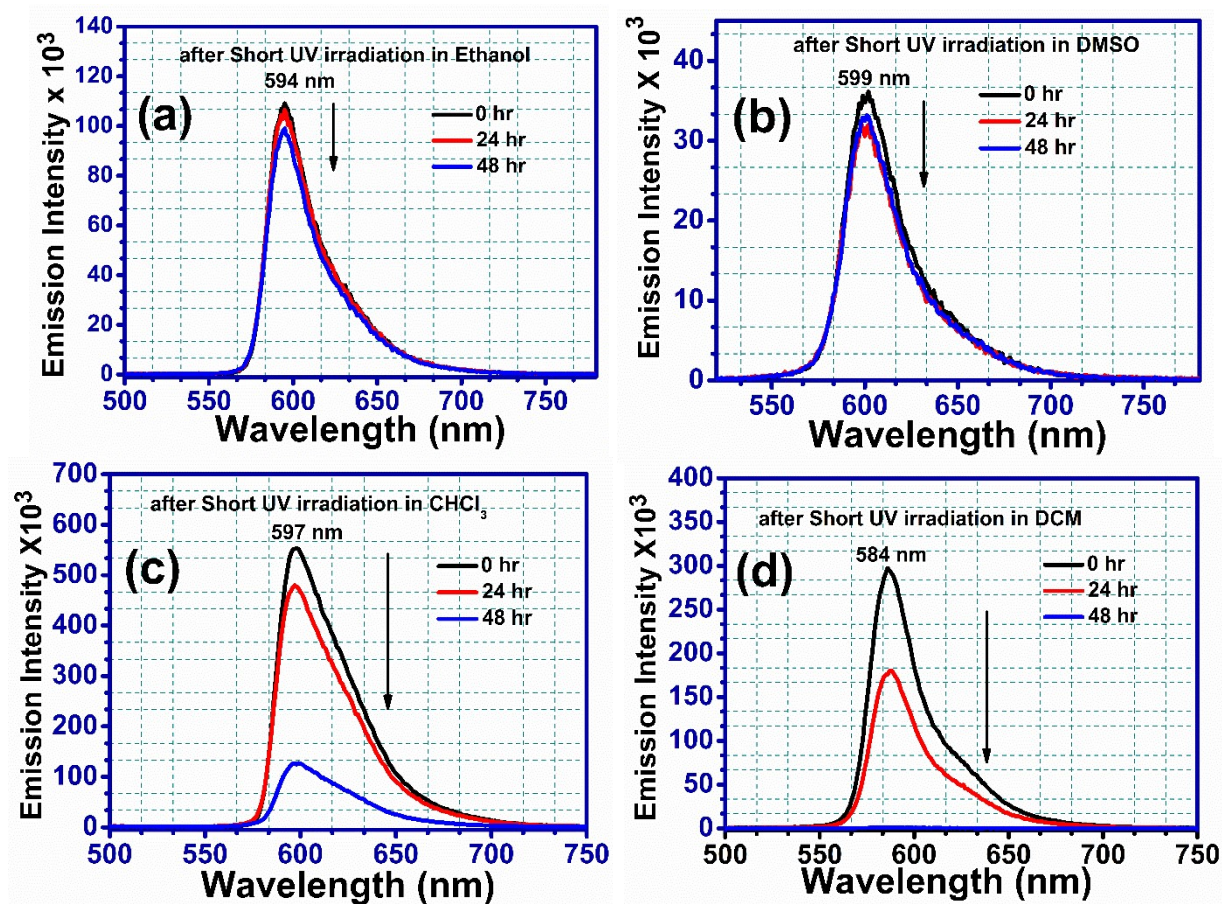


Fig. S8 Change in the emission intensity of **RHBIT** in (a) EtOH, (b) DMSO, (c) CHCl_3 , and (d) DCM after exposure to short UV light at different intervals of time; observed minimal decrease in intensity for ethanol and DMSO but a drastic decrease in case of CHCl_3 , and DCM solvents predicting that **RHBIT** is reverted back to closed form after 48 hours of UV irradiation.

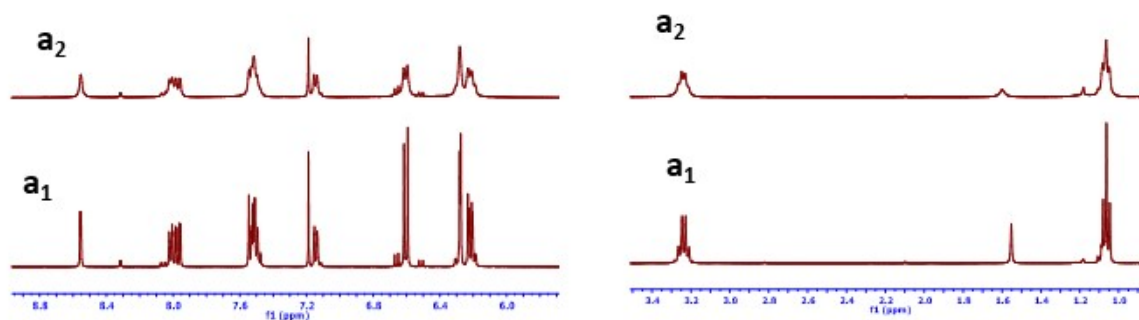


Fig. S9 ^1H NMR spectra of **RHBIT** before and after UV light (254 nm) irradiation over 10 min at RT in CDCl_3 . **a**₁ and **a**₂ represents proton spectra of **RHBIT** before and after UV exposure respectively.

The response of the signals becomes broadened after UV irradiation and no new characteristic signal is found in the downfield region.

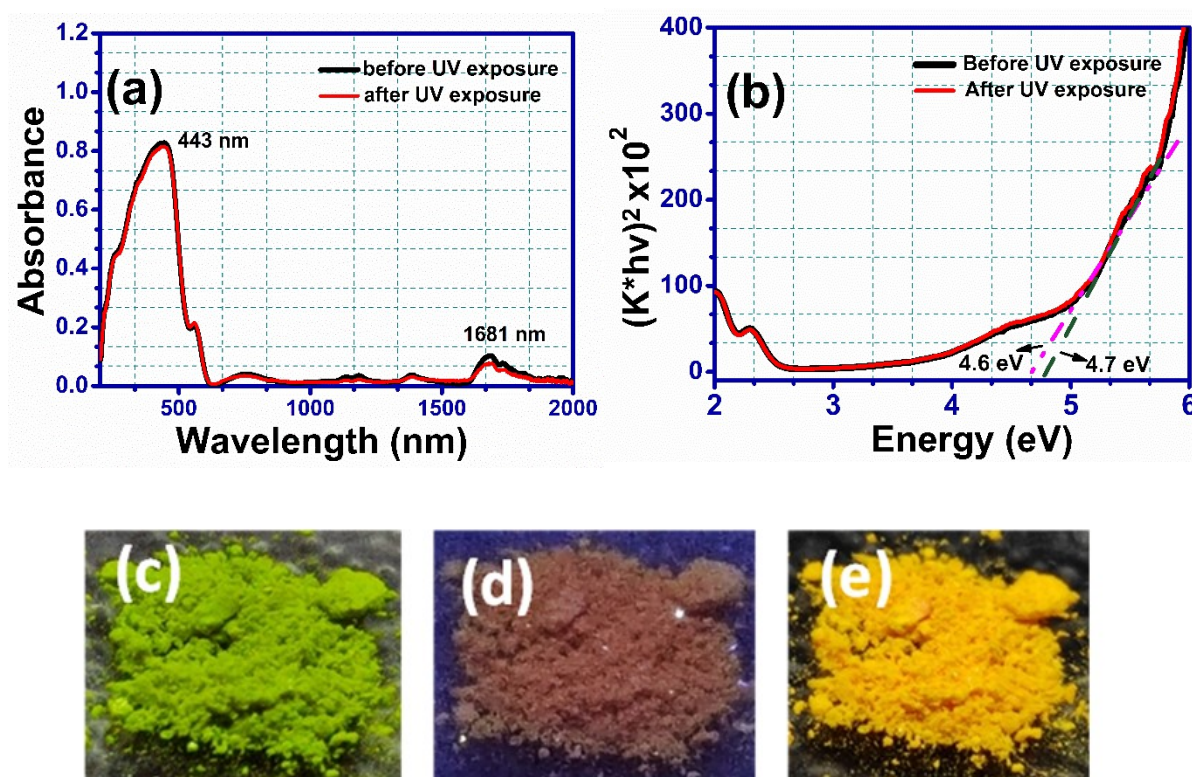


Fig. S10 (a) absorption, (b) optical bandgap spectra of **RHBIT** in solid state before and after exposure to UV light with λ_{max} absorption at ~ 443 nm and a faint absorption at 1681 nm indicating weak charge-transfer interaction. The optical bandgap of **RHBIT** obtained as ~ 4.7 eV (before UV), ~ 4.6 eV (after UV) through the Kubelka-Munk plot from the diffuse reflectance spectrum. (c), (d) & (e) displays the solid sample images under short UV, long UV and visible light.

Lifetime and Quantum yield calculation:

The average fluorescent lifetime, radiative (k_r) and non-radiative (k_{nr}) decay values of **RHBIT** in different solvents were calculated by using the following equations (S1&S2), where τ , α_i , τ_i , are the average lifetime, individual component contribution, and lifetime of individual components respectively.¹ The exponential fitting of the decay profiles was determined by judging the chi-square (χ^2) values varied between 0.8-1.2.

$$\tau = \frac{\sum \alpha_i \tau_i^2}{\sum \alpha_i \tau_i} \quad (\text{S1})$$

$$k_r = \frac{\phi_f}{\langle \tau \rangle}, \quad k_{nr} = \frac{(1 - \phi_f)}{\langle \tau \rangle} \quad (\text{S2})$$

The relative quantum yield was measured with respect to quinine sulphate ($\Phi_f = 0.54$) in 0.1M H_2SO_4 and rhodamine B ($\Phi_f = 0.97$)^{2,3} in ethanol as reference by using the formula (S3), where, error limit = $\pm 5\%$; Φ_f = quantum yield of the probe, Φ_{Ref} = quantum yield of quinine sulphate / rhodamine b, A_{Sample} = Area under the curve of emission spectra of sample in different solvents before and after exposure to UV irradiation, A_{Ref} = Area under the curve of emission spectra of quinine sulphate / rhodamine b, Abs_{Sample} = Absorbance of the sample in different solvents, Abs_{Ref} = Absorbance of the standard reference quinine sulphate / rhodamine b, η = refractive index of the sample and reference in corresponding solvent.⁴

$$\Phi_f = \Phi_{Ref} \times (A_{Sample}/A_{Ref}) \times (Abs_{Ref}/Abs_{Sample}) \times (\eta_{Sample}^2/\eta_{Ref}^2) \quad (S3)$$

Table S8 Lifetime decay, quantum yield, radiative and non-radiative decay values of probe **RHBIT** before (B) and after exposure (A) to UV irradiation.

RHBIT in different solvents	τ_1 (ns)		τ_2 (ns)		α_1 (%)		α_2 (%)		Average lifetime < τ > (ns)		Φ_f		k_r (s^{-1}) $\times 10^9$		K_{nr} (s^{-1}) $\times 10^9$	
	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A
MeOH	0.15	0.23	0.96	0.95	0.48	0.37	0.52	0.63	0.85	0.86	0.01	0.02	0.01	0.02	1.16	1.14
EtOH	0.32	0.31	1.41	1.37	0.56	0.59	0.44	0.41	1.16	1.11	0.30	0.33	0.25	0.29	0.60	0.60
n-PrOH	0.35	0.47	0.95	0.99	0.47	0.52	0.53	0.48	0.80	0.82	0.05	0.08	0.06	0.09	1.18	1.12
n-BuOH	0.39	0.51	0.93	0.98	0.52	0.61	0.48	0.39	0.76	0.77	0.006	0.01	0.007	0.01	1.30	1.28
DMF	0.27	0.30	0.93	0.94	0.45	0.45	0.55	0.55	0.80	0.80	0.003	0.004	0.003	0.005	1.24	1.24
DMSO	0.45	0.39	0.96	1.40	0.53	0.59	0.47	0.41	0.78	1.11	0.004	0.23	0.004	0.20	1.27	0.69
ACN	0.15	0.13	0.90	0.90	0.37	0.37	0.63	0.63	0.83	0.84	0.002	0.003	0.003	0.003	1.20	1.18
1,4-Dioxane	0.28	0.28	0.89	0.90	0.48	0.48	0.52	0.52	0.75	0.76	0.07	0.08	0.08	0.09	1.24	1.21
EtOAc	0.16	0.15	0.90	0.91	0.44	0.44	0.56	0.56	0.81	0.82	0.01	0.01	0.01	0.01	1.22	1.20
THF	0.19	0.20	0.98	1.01	0.45	0.45	0.55	0.55	0.87	0.89	0.05	0.02	0.06	0.01	1.08	1.10
CHCl ₃	0.14	0.26	1.36	2.6	0.45	0.40	0.55	0.60	1.26	2.47	0.02	0.66	0.01	0.26	0.78	0.13
DCM	0.14	0.19	1.35	3.5	0.37	0.35	0.63	0.65	1.28	3.41	0.004	0.99	0.003	0.29	0.77	0.002

References:

1. Lakowicz, J. R. (Ed.), *Principles of fluorescence spectroscopy*, Boston, MA: springer US, 2006.
2. Z. Yang, M. She, B. Yin, J. Cui, Y. Zhang, W. Sun, J. Li and Z. shi, *J. Org. Chem.*, 2012, **77**, 1143-1147.
3. H. Battula, S. Muduli, S. Priyanka Bandi, S. Kapoor, S. Mishra, H. Aggarwal, V. Vamsi Krishna Venuganti and S. Jayanty, *J. Photochem. Photobiol. A Chem.*, 2022, **426**, 113748-113766.
4. J.N. Demas and G.A. Crosby, *J. Phys. Chem.*, 1971, **75**, 991-1024.

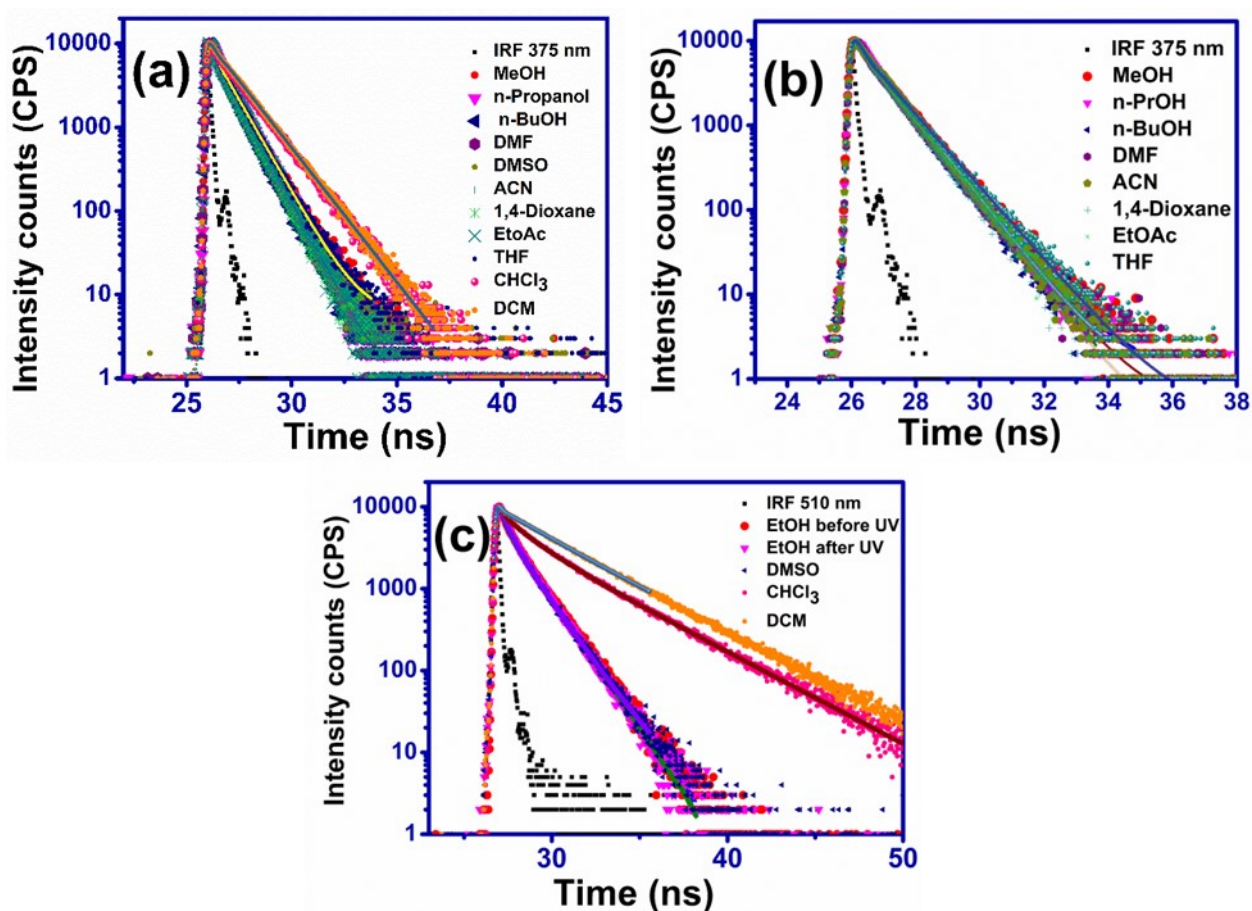


Fig. S11 Time-resolved fluorescence decay curves of **RHBIT** (Intensity vs time in nanoseconds) in different solvents **(a)** before UV irradiation (IRF 375 nm), **(b)** after UV irradiation (IRF 375 nm) **(c)** after UV irradiation in ethanol (before and after), DMSO, CHCl₃ and DCM (IRF 510 nm). The average fluorescence lifetime after UV irradiation at 254 nm shows longer values in DMSO, CHCl₃, and DCM confirming the ring-open mechanism of **RHBIT**.

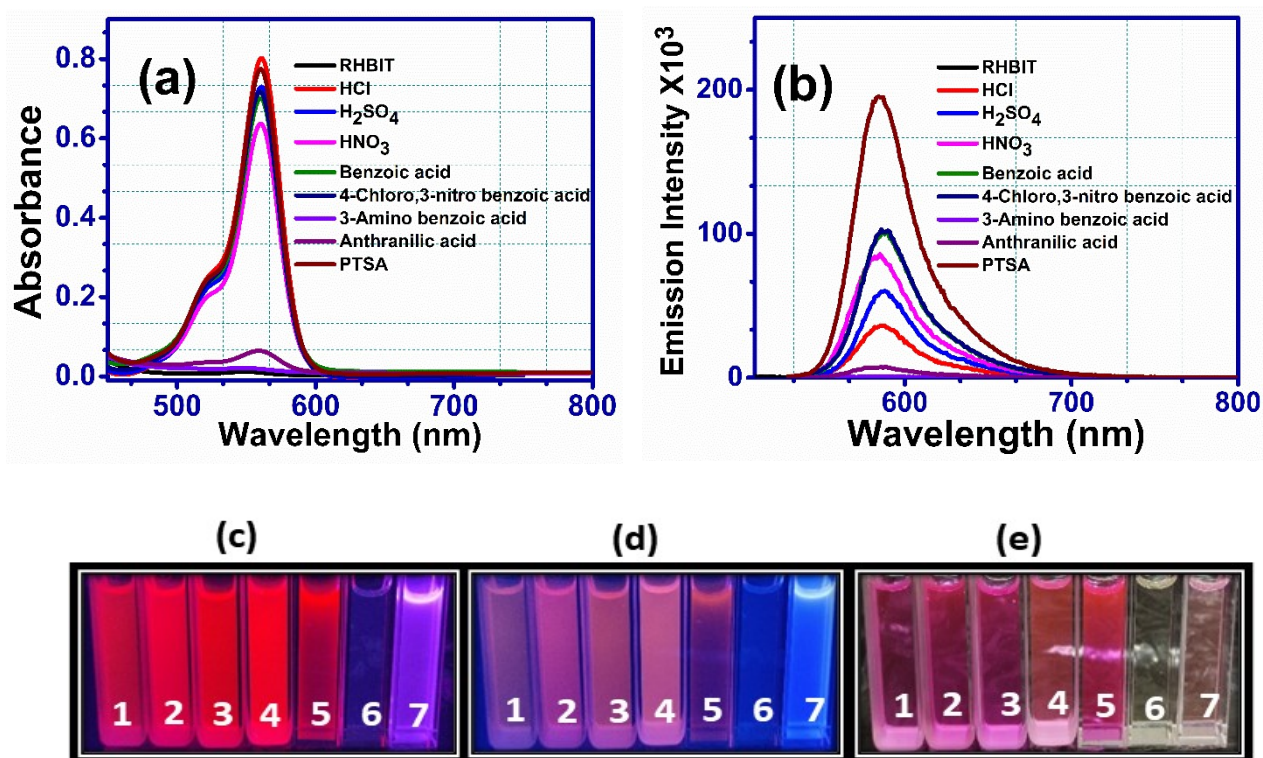


Fig. S12 (a) absorption and (b) emission spectra of **RHBIT** with different acids excited at 520 nm ($\lambda_{\text{abs}} \sim 560$ nm, $\lambda_{\text{em}} \sim 584$ nm) exhibiting a 150-fold increase in emission intensity after the addition of PTSA to **RHBIT** and photographic images of **RHBIT** sensing different acids **1**, HCl; **2**, H₂SO₄; **3**, HNO₃; **4**, Benzoic acid; **5**, 4-chloro,3-nitro Benzoic acid; **6**, 3-amino Benzoic acid; **7**, Anthranilic acid under (c) 254 nm short UV, (d) 365 nm long UV, (e) visible light.

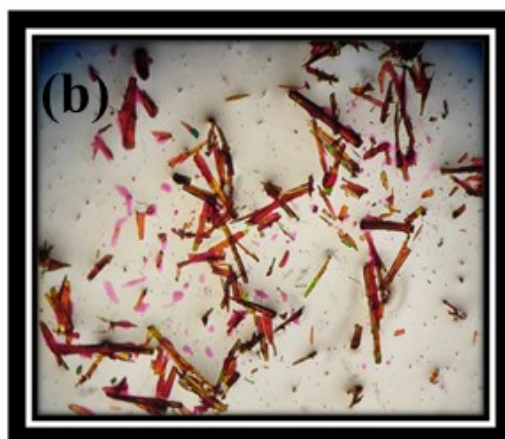
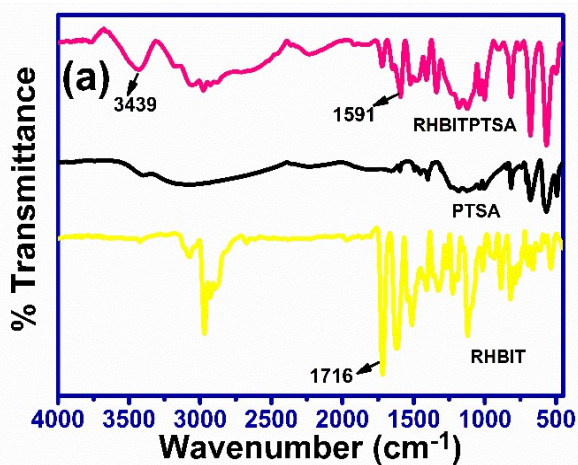


Fig. S13 (a) FT-IR spectra of **RHBIT** (yellow), PTSA (black), and RHBIT-PTSA (pink) showing marked significant changes of the -C=O group (converting from cyclic lactam to open chain amide) due to proton transfer from PTSA, (b) crystals of RHBIT-PTSA with brown-pink color on their surface (cyclic form) and supernatant solution was pink in color.

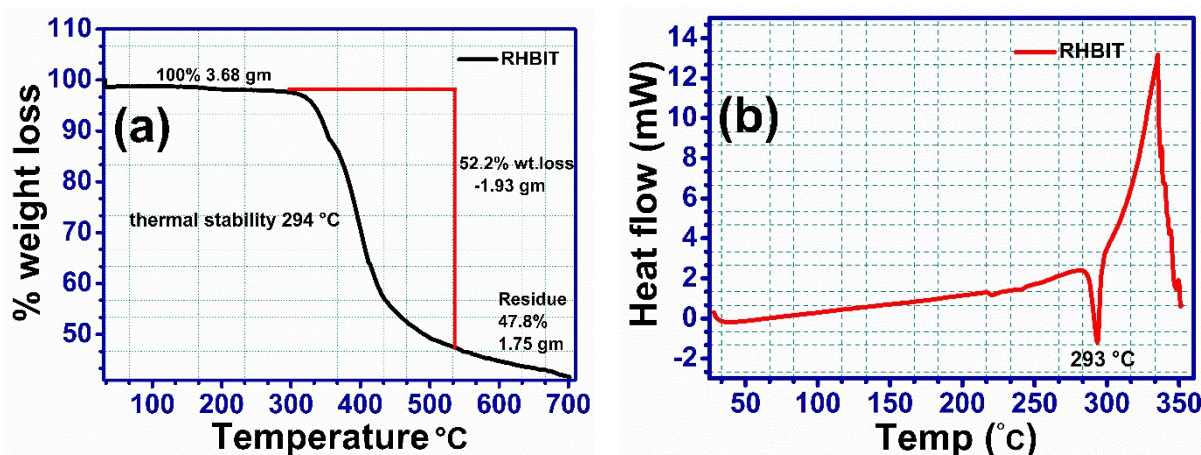


Fig. S14 Thermogram obtained from (a) TGA and (b) DSC analysis for **RHBIT**, showcasing the thermal stability of **RHBIT** at 293 °C.

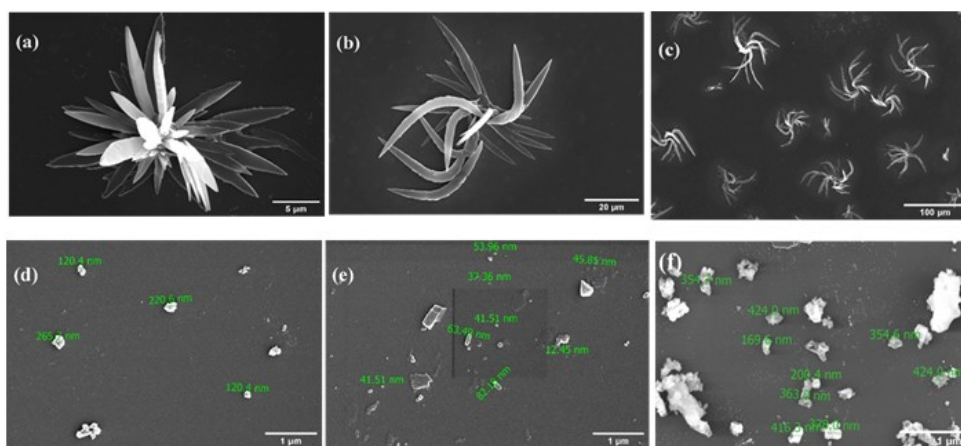


Fig. S15 SEM images of drop cast films of **RHBIT** in various solvents (a), (b), (c) in acetonitrile at 5, 20, 100 μm magnification present bent petal-like structures; (d) *i*-propanol (e) *n*-butanol, (f) DMF at 1 μm magnification intimates aggregates.