Supporting Information for:

# White-Light Generation on All-solution-processed OLEDs using a Benzothiazole-salophen derivative reactive to the ESIPT process

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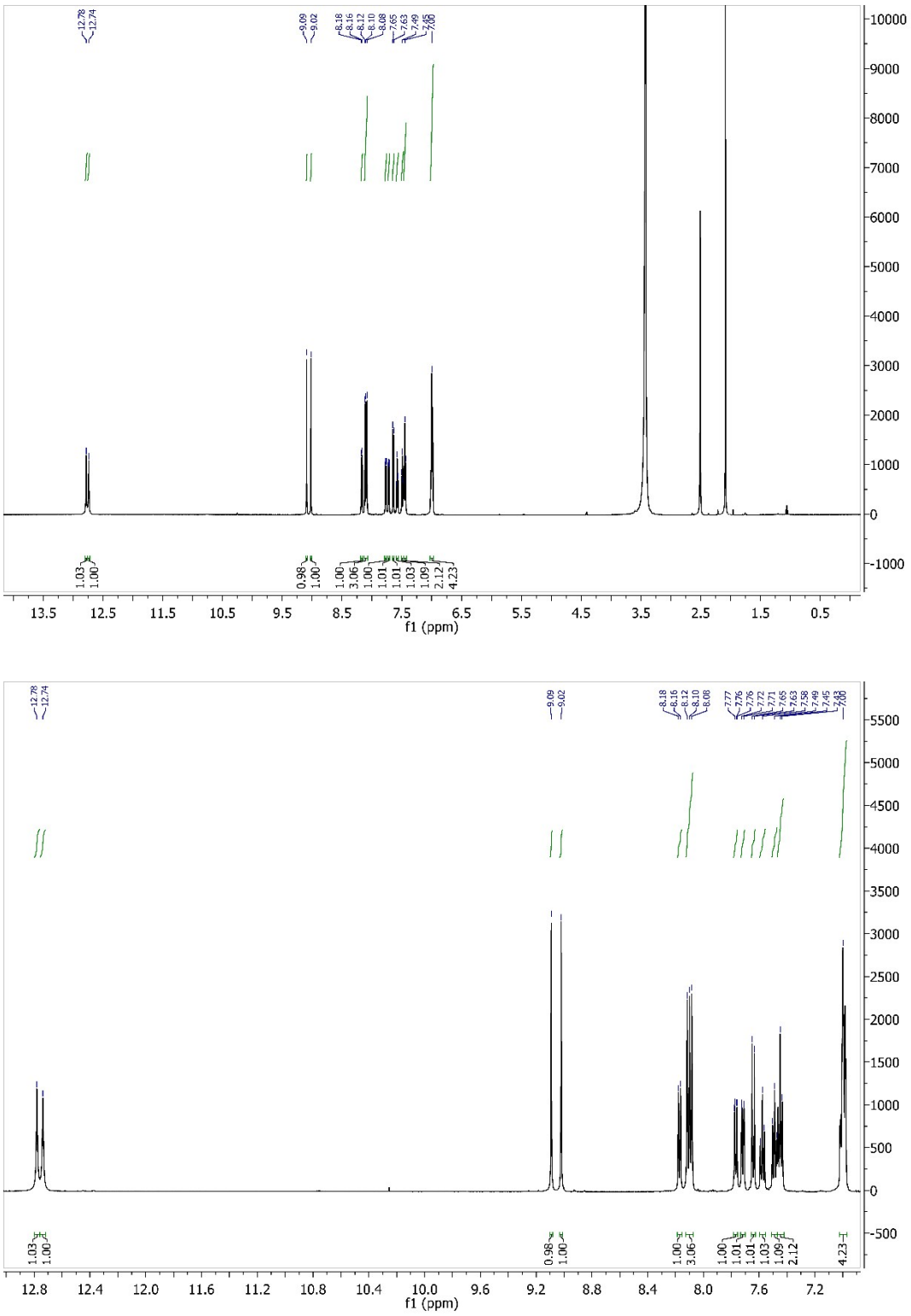


**Fig. S1** $^{1}$H NMR spectrum.

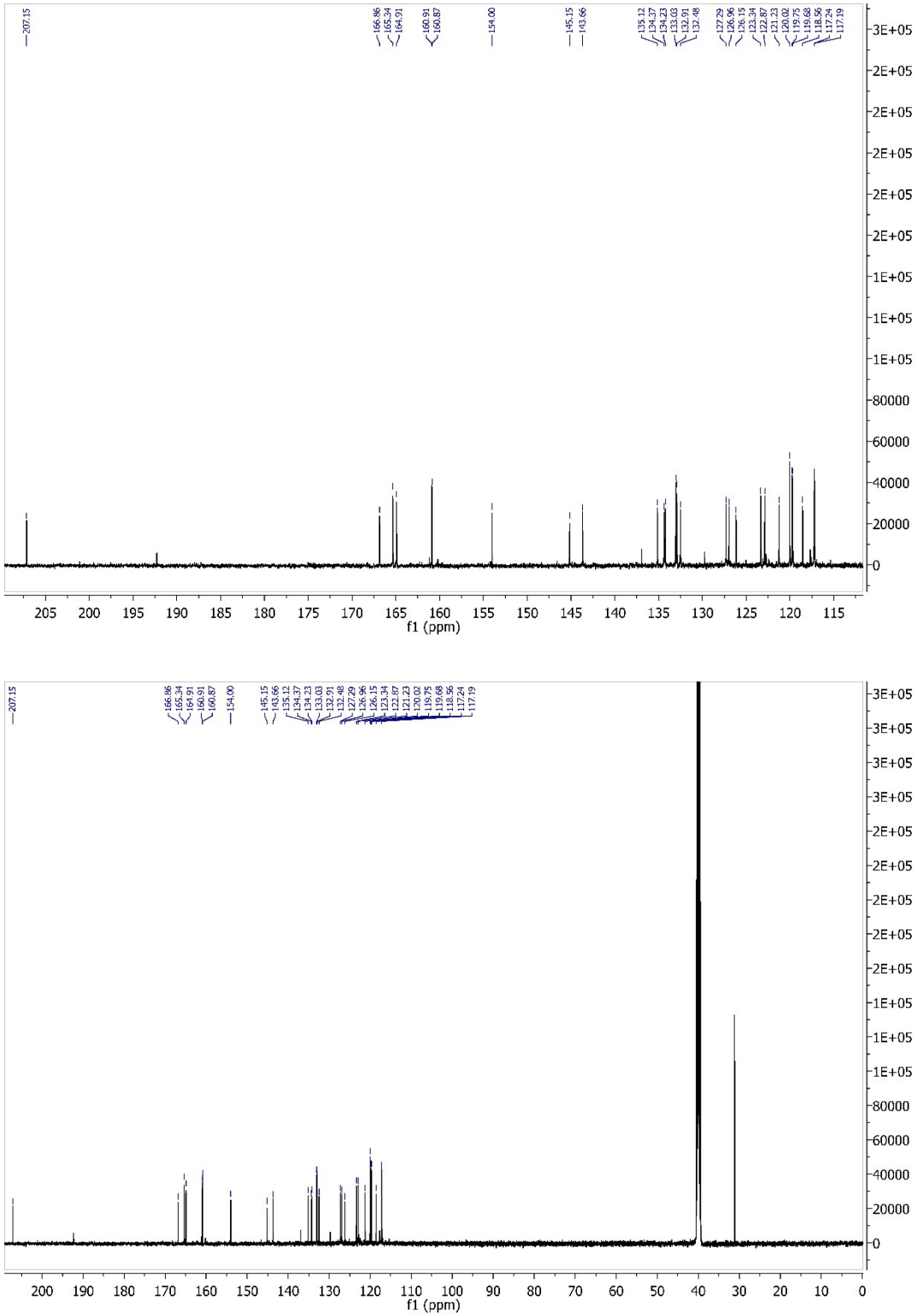


**Fig. S2** $^{13}$C NMR spectrum.

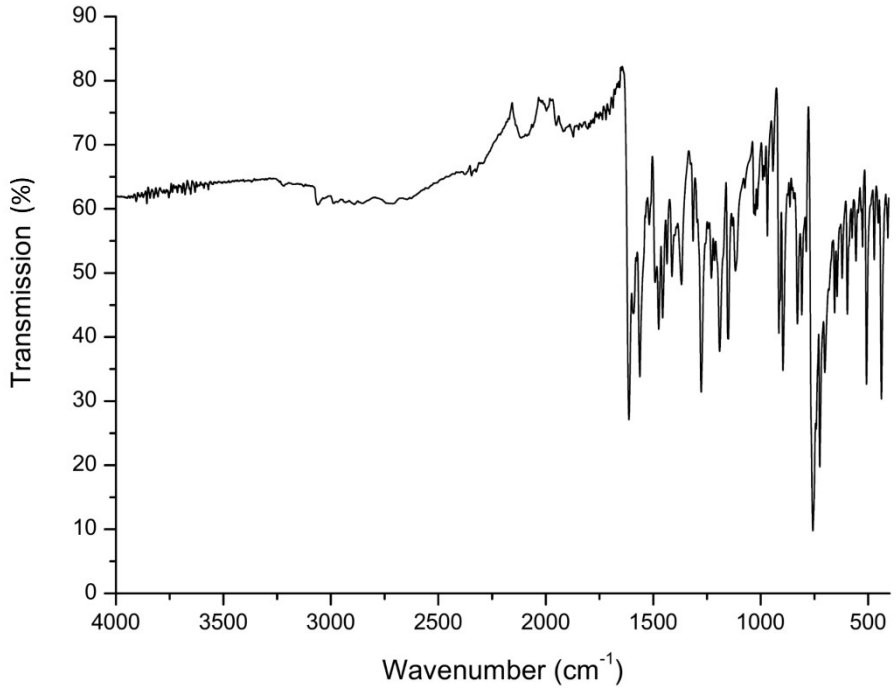


**Fig. S3** BTS FTIR spectrum.

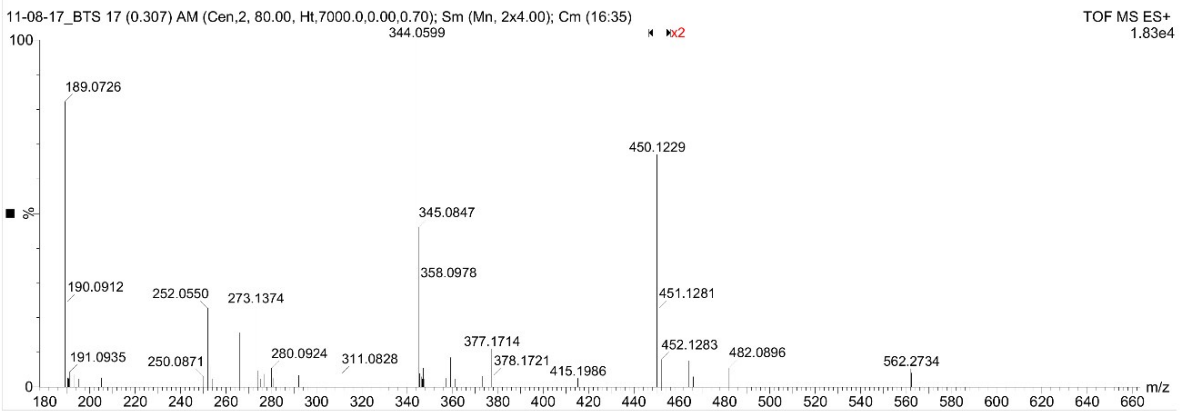


**Fig. S4** BTS mass spectrum.

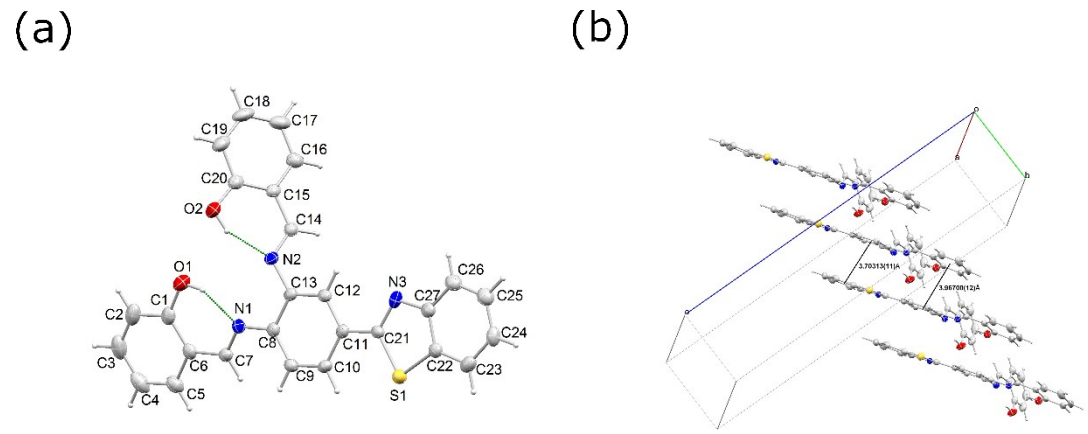


**Fig. S5** (a) Molecular structure of BTS with 50% probability displacement ellipsoids. Intramolecular hydrogen bonds are shown as dashed lines. (b) Parallel alignment of BTS molecules, with plane centroid to plane centroid distances shown as black lines.

**Table S1** Crystal data and structure refinement for BTS.

| | |
|---|---|
| Identification code | BTS |
| Empirical formula | $C_{27}H_{19}N_3O_2S$ |
| Formula weight | 449.51 |
| Temperature/K | 150(2) |
| Crystal system | monoclinic |
| Space group | $P2_1/c$ |
| a/Å | 12.7652(5) |
| b/Å | 6.1962(2) |
| c/Å | 26.7849(9) |
| α/° | 90 |
| β/° | 91.423(2) |
| γ/° | 90 |
| Volume/Å$^3$ | 2117.92(13) |
| Z | 4 |
| $\rho_{calc}$g/cm$^3$ | 1.410 |
| μ/mm$^{-1}$ | 1.612 |
| F(000) | 936.0 |
| Crystal size/mm$^3$ | 0.210 × 0.095 × 0.034 |
| Radiation | CuKα (λ = 1.54178) |
| 2Θ range for data collection/° | 9.454 to 132.824 |
| Index ranges | -12 ≤ h ≤ 14, -7 ≤ k ≤ 7, -21 ≤ l ≤ 31 |
| Reflections collected | 16160 |
| Independent reflections | 3582 [$R_{int}$ = 0.0550, $R_{sigma}$ = 0.0536] |
| Data/restraints/parameters | 3582/0/304 |
| Goodness-of-fit on $F^2$ | 1.024 |
| Final R indexes [I>=2σ (I)] | $R_1$ = 0.0425, $wR_2$ = 0.1083 |

| | |
|---|---|
| Final R indexes [all data] | $R_1 = 0.0548$, $wR_2 = 0.1154$ |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.46/-0.37 |

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

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| S1 | 1398.2(4) | -231.6(8) | 5256.5(2) | 29.50(18) |
| O1 | 2112.6(12) | 11934(3) | 3292.3(5) | 33.9(4) |
| O2 | 4620.9(13) | 10419(3) | 3768.8(6) | 39.8(4) |
| N1 | 1383.1(13) | 8690(3) | 3796.4(5) | 23.1(4) |
| N2 | 3368.5(12) | 7083(3) | 3816.2(6) | 24.0(4) |
| N3 | 3283.7(14) | 196(3) | 4901.2(6) | 27.4(4) |
| C1 | 1107.3(17) | 12567(3) | 3231.0(7) | 28.2(5) |
| C2 | 895(2) | 14506(4) | 2987.3(7) | 36.1(6) |
| C3 | -117(2) | 15180(4) | 2907.1(8) | 42.5(6) |
| C4 | -957(2) | 13928(4) | 3063.6(8) | 45.2(7) |
| C5 | -759.0(18) | 12014(4) | 3307.7(8) | 35.9(5) |
| C6 | 272.4(16) | 11303(3) | 3401.8(7) | 25.6(5) |
| C7 | 452.3(16) | 9318(3) | 3672.0(7) | 24.0(4) |
| C8 | 1561.4(15) | 6786(3) | 4071.6(7) | 22.0(4) |
| C9 | 804.8(16) | 5709(3) | 4340.5(7) | 24.8(5) |
| C10 | 1040.8(15) | 3858(3) | 4602.3(7) | 24.2(4) |
| C11 | 2059.0(15) | 3011(3) | 4605.8(7) | 22.1(4) |
| C12 | 2823.4(15) | 4067(3) | 4335.8(7) | 22.8(4) |
| C13 | 2586.0(15) | 5940(3) | 4068.7(7) | 21.4(4) |
| C14 | 3959.4(15) | 6093(3) | 3510.3(7) | 23.8(5) |
| C15 | 4847.7(15) | 7158(3) | 3290.2(7) | 24.9(5) |
| C16 | 5444.4(16) | 6061(4) | 2938.8(8) | 32.3(5) |
| C17 | 6327.9(17) | 6987(4) | 2742.4(8) | 40.4(6) |
| C18 | 6636.3(18) | 9014(4) | 2906.6(9) | 44.3(7) |
| C19 | 6073.7(18) | 10146(4) | 3251.8(9) | 39.7(6) |
| C20 | 5163.5(16) | 9250(4) | 3439.8(8) | 30.1(5) |
| C21 | 2334.4(15) | 1078(3) | 4892.6(7) | 22.2(4) |
| C22 | 2333.4(16) | -2129(3) | 5426.3(7) | 25.0(5) |
| C23 | 2232.9(18) | -3960(4) | 5726.3(7) | 32.6(5) |
| C24 | 3119.2(18) | -5252(3) | 5801.9(8) | 32.4(5) |
| C25 | 4054.8(18) | -4713(4) | 5583.2(8) | 35.4(5) |
| C26 | 4159.6(17) | -2929(4) | 5290.7(8) | 33.2(5) |
| C27 | 3284.5(16) | -1630(3) | 5206.6(7) | 26.1(5) |

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

| Atom | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{23}$ | $U_{13}$ | $U_{12}$ |
|---|---|---|---|---|---|---|

| | | | | | | |
|---|---|---|---|---|---|---|
| S1 | 26.6(3) | 27.8(3) | 34.3(3) | 4.4(2) | 4.0(2) | 1.0(2) |
| O1 | 32.1(9) | 36.3(9) | 33.4(8) | 5.8(7) | -1.2(7) | -7.8(7) |
| O2 | 33.6(9) | 28.7(9) | 57.6(10) | -3.9(8) | 9.3(8) | -9.4(7) |
| N1 | 24.1(9) | 22.0(9) | 23.1(8) | -1.1(7) | -1.7(7) | 0.2(7) |
| N2 | 20.1(9) | 24.4(9) | 27.4(8) | 2.9(7) | -0.4(7) | -2.5(7) |
| N3 | 40.6(11) | 20.1(9) | 21.3(8) | 0.5(7) | -1.0(8) | -6.5(8) |
| C1 | 39.1(13) | 25.3(11) | 20.0(9) | -4.8(8) | -2.5(9) | -2.2(10) |
| C2 | 59.9(16) | 27.2(12) | 21.1(10) | -0.2(9) | -2.3(10) | -3.9(11) |
| C3 | 73.8(19) | 30.4(13) | 23(1) | 0.1(9) | -4.6(11) | 11.2(13) |
| C4 | 51.8(16) | 49.5(16) | 33.9(12) | -1.2(11) | -7.0(11) | 24.7(13) |
| C5 | 35.8(13) | 41.3(14) | 30.3(11) | 1.4(10) | -1.7(9) | 10.7(11) |
| C6 | 30.1(12) | 25.1(11) | 21.5(9) | -3.1(8) | -1.3(8) | 3.3(9) |
| C7 | 23.7(11) | 24.7(11) | 23.6(9) | -2.2(8) | 1.6(8) | -1.8(9) |
| C8 | 24.1(11) | 21.1(10) | 20.7(9) | -3.6(8) | -1.5(8) | -1.2(8) |
| C9 | 20.2(11) | 27.5(11) | 26.7(10) | -0.1(9) | -0.1(8) | 1.6(9) |
| C10 | 21.9(11) | 26.5(11) | 24.5(9) | 0.9(8) | 2.9(8) | -4.0(9) |
| C11 | 23.5(11) | 21.1(10) | 21.6(9) | -2.9(8) | 0.2(8) | -2.4(8) |
| C12 | 17.9(10) | 25.1(11) | 25.3(10) | -1.7(8) | -0.8(8) | -1.2(8) |
| C13 | 20.4(10) | 22.1(10) | 21.5(9) | -2.2(8) | 0.0(8) | -4.1(8) |
| C14 | 21.1(10) | 24.7(11) | 25.6(10) | 2.1(8) | -2.8(8) | 0.0(9) |
| C15 | 17.9(10) | 29.0(11) | 27.6(10) | 6.2(9) | -2.4(8) | 0.6(8) |
| C16 | 25.9(12) | 38.9(13) | 32.0(11) | 6.1(10) | 0.6(9) | 4.2(10) |
| C17 | 23.7(12) | 60.1(17) | 37.9(12) | 11.0(12) | 6(1) | 5.9(11) |
| C18 | 21.6(12) | 61.1(17) | 50.3(14) | 22.2(13) | 2.1(11) | -8.0(12) |
| C19 | 26.4(13) | 39.8(14) | 52.7(14) | 13.6(11) | -2.8(11) | -8.4(10) |
| C20 | 22.3(11) | 32.4(12) | 35.4(11) | 7.8(9) | -2.6(9) | -0.6(9) |
| C21 | 19.5(10) | 22.7(11) | 24.2(9) | -3.6(8) | 0.0(8) | -0.5(8) |
| C22 | 26.0(11) | 25.1(11) | 23.9(9) | -2.2(8) | -0.7(8) | -0.7(9) |
| C23 | 35.9(13) | 33.4(13) | 28.7(10) | -1.0(9) | 3.8(9) | -8.3(10) |
| C24 | 43.8(14) | 25.0(11) | 27.8(10) | 4.4(9) | -9.7(10) | 0.4(10) |
| C25 | 32.5(13) | 39.1(14) | 34.3(11) | 0.2(10) | -7.3(10) | 3.9(10) |
| C26 | 26.6(12) | 37.9(13) | 34.7(11) | 0.5(10) | -4.8(9) | 2(1) |
| C27 | 25.7(11) | 26.3(11) | 26.2(10) | -3.6(9) | -2.0(8) | -2.2(9) |

**Table S4** Bond Lengths for BTS.

| **Atom** | **Atom** | **Length/Å** | **Atom** | **Atom** | **Length/Å** |
|---|---|---|---|---|---|
| S1 | C22 | 1.728(2) | C9 | C10 | 1.374(3) |
| S1 | C21 | 1.759(2) | C10 | C11 | 1.401(3) |
| O1 | C1 | 1.348(3) | C11 | C12 | 1.392(3) |
| O2 | C20 | 1.346(3) | C11 | C21 | 1.461(3) |
| N1 | C7 | 1.286(3) | C12 | C13 | 1.393(3) |
| N1 | C8 | 1.407(3) | C14 | C15 | 1.450(3) |
| N2 | C14 | 1.283(3) | C15 | C16 | 1.401(3) |
| N2 | C13 | 1.411(2) | C15 | C20 | 1.412(3) |

| | | | | | |
|---|---|---|---|---|---|
| N3 | C21 | 1.329(3) | C16 | C17 | 1.381(3) |
| N3 | C27 | 1.397(3) | C17 | C18 | 1.385(4) |
| C1 | C2 | 1.391(3) | C18 | C19 | 1.377(4) |
| C1 | C6 | 1.408(3) | C19 | C20 | 1.393(3) |
| C2 | C3 | 1.369(4) | C22 | C27 | 1.397(3) |
| C3 | C4 | 1.396(4) | C22 | C23 | 1.398(3) |
| C4 | C5 | 1.375(3) | C23 | C24 | 1.397(3) |
| C5 | C6 | 1.405(3) | C24 | C25 | 1.384(3) |
| C6 | C7 | 1.442(3) | C25 | C26 | 1.363(3) |
| C8 | C9 | 1.389(3) | C26 | C27 | 1.391(3) |
| C8 | C13 | 1.409(3) | | | |

**Table S5** Bond Angles for BTS.

| **Atom** | **Atom** | **Atom** | **Angle/°** | **Atom** | **Atom** | **Atom** | **Angle/°** |
|---|---|---|---|---|---|---|---|
| C22 | S1 | C21 | 89.15(10) | C8 | C13 | N2 | 118.97(17) |
| C7 | N1 | C8 | 121.73(17) | N2 | C14 | C15 | 121.33(19) |
| C14 | N2 | C13 | 120.03(17) | C16 | C15 | C20 | 118.7(2) |
| C21 | N3 | C27 | 109.30(17) | C16 | C15 | C14 | 119.73(19) |
| O1 | C1 | C2 | 118.8(2) | C20 | C15 | C14 | 121.53(19) |
| O1 | C1 | C6 | 121.64(18) | C17 | C16 | C15 | 121.1(2) |
| C2 | C1 | C6 | 119.5(2) | C16 | C17 | C18 | 119.0(2) |
| C3 | C2 | C1 | 120.6(2) | C19 | C18 | C17 | 121.8(2) |
| C2 | C3 | C4 | 120.8(2) | C18 | C19 | C20 | 119.6(2) |
| C5 | C4 | C3 | 119.3(2) | O2 | C20 | C19 | 118.0(2) |
| C4 | C5 | C6 | 121.1(2) | O2 | C20 | C15 | 122.13(19) |
| C5 | C6 | C1 | 118.7(2) | C19 | C20 | C15 | 119.8(2) |
| C5 | C6 | C7 | 119.6(2) | N3 | C21 | C11 | 123.59(18) |
| C1 | C6 | C7 | 121.66(18) | N3 | C21 | S1 | 115.64(14) |
| N1 | C7 | C6 | 121.50(19) | C11 | C21 | S1 | 120.76(15) |
| C9 | C8 | N1 | 124.66(18) | C27 | C22 | C23 | 120.98(19) |
| C9 | C8 | C13 | 118.79(18) | C27 | C22 | S1 | 109.92(15) |
| N1 | C8 | C13 | 116.55(17) | C23 | C22 | S1 | 129.09(17) |
| C10 | C9 | C8 | 121.25(19) | C24 | C23 | C22 | 117.6(2) |
| C9 | C10 | C11 | 120.49(19) | C25 | C24 | C23 | 120.3(2) |
| C12 | C11 | C10 | 118.85(18) | C26 | C25 | C24 | 122.5(2) |
| C12 | C11 | C21 | 119.72(18) | C25 | C26 | C27 | 118.2(2) |
| C10 | C11 | C21 | 121.42(18) | C26 | C27 | N3 | 123.6(2) |
| C11 | C12 | C13 | 120.80(18) | C26 | C27 | C22 | 120.5(2) |
| C12 | C13 | C8 | 119.81(18) | N3 | C27 | C22 | 115.98(18) |
| C12 | C13 | N2 | 121.13(17) | | | | |

**Table S6** Hydrogen Bonds for BTS.

| D | H | A | d(D-H)/Å | d(H-A)/Å | d(D-A)/Å | D-H-A/° |
|---|---|---|---|---|---|---|
| O1 | H1A | N1 | 0.85(3) | 1.82(3) | 2.606(2) | 152(2) |
| O2 | H2A | N2 | 0.85(3) | 1.84(3) | 2.618(2) | 151(2) |

**Table S7** Torsion Angles for BTS.

| A | B | C | D | Angle/° | A | B | C | D | Angle/° |
|---|---|---|---|---|---|---|---|---|---|
| O1 | C1 | C2 | C3 | 178.44(18) | C20 | C15 | C16 | C17 | 0.3(3) |
| C6 | C1 | C2 | C3 | -0.8(3) | C14 | C15 | C16 | C17 | -176.49(17) |
| C1 | C2 | C3 | C4 | -0.6(3) | C15 | C16 | C17 | C18 | 1.5(3) |
| C2 | C3 | C4 | C5 | 1.0(3) | C16 | C17 | C18 | C19 | -1.4(3) |
| C3 | C4 | C5 | C6 | 0.0(3) | C17 | C18 | C19 | C20 | -0.6(3) |
| C4 | C5 | C6 | C1 | -1.4(3) | C18 | C19 | C20 | O2 | -178.63(19) |
| C4 | C5 | C6 | C7 | 178.15(19) | C18 | C19 | C20 | C15 | 2.5(3) |
| O1 | C1 | C6 | C5 | -177.42(18) | C16 | C15 | C20 | O2 | 178.82(18) |
| C2 | C1 | C6 | C5 | 1.8(3) | C14 | C15 | C20 | O2 | -4.4(3) |
| O1 | C1 | C6 | C7 | 3.0(3) | C16 | C15 | C20 | C19 | -2.3(3) |
| C2 | C1 | C6 | C7 | -177.77(17) | C14 | C15 | C20 | C19 | 174.43(18) |
| C8 | N1 | C7 | C6 | 178.26(16) | C27 | N3 | C21 | C11 | -179.64(16) |
| C5 | C6 | C7 | N1 | -175.01(18) | C27 | N3 | C21 | S1 | 0.61(19) |
| C1 | C6 | C7 | N1 | 4.6(3) | C12 | C11 | C21 | N3 | -2.2(3) |
| C7 | N1 | C8 | C9 | -17.0(3) | C10 | C11 | C21 | N3 | 178.90(17) |
| C7 | N1 | C8 | C13 | 162.97(17) | C12 | C11 | C21 | S1 | 177.55(14) |
| N1 | C8 | C9 | C10 | -179.73(17) | C10 | C11 | C21 | S1 | -1.4(2) |
| C13 | C8 | C9 | C10 | 0.3(3) | C22 | S1 | C21 | N3 | -1.00(15) |
| C8 | C9 | C10 | C11 | 0.3(3) | C22 | S1 | C21 | C11 | 179.24(15) |
| C9 | C10 | C11 | C12 | -0.6(3) | C21 | S1 | C22 | C27 | 1.05(14) |
| C9 | C10 | C11 | C21 | 178.32(17) | C21 | S1 | C22 | C23 | -177.74(19) |
| C10 | C11 | C12 | C13 | 0.4(3) | C27 | C22 | C23 | C24 | 0.7(3) |
| C21 | C11 | C12 | C13 | -178.54(16) | S1 | C22 | C23 | C24 | 179.37(15) |
| C11 | C12 | C13 | C8 | 0.1(3) | C22 | C23 | C24 | C25 | -0.2(3) |
| C11 | C12 | C13 | N2 | 176.57(16) | C23 | C24 | C25 | C26 | 0.2(3) |
| C9 | C8 | C13 | C12 | -0.5(3) | C24 | C25 | C26 | C27 | -0.8(3) |
| N1 | C8 | C13 | C12 | 179.53(16) | C25 | C26 | C27 | N3 | -177.83(18) |
| C9 | C8 | C13 | N2 | -176.98(16) | C25 | C26 | C27 | C22 | 1.3(3) |
| N1 | C8 | C13 | N2 | 3.0(2) | C21 | N3 | C27 | C26 | 179.46(18) |
| C14 | N2 | C13 | C12 | 52.3(2) | C21 | N3 | C27 | C22 | 0.3(2) |
| C14 | N2 | C13 | C8 | -131.22(18) | C23 | C22 | C27 | C26 | -1.3(3) |
| C13 | N2 | C14 | C15 | -172.63(15) | S1 | C22 | C27 | C26 | 179.79(15) |
| N2 | C14 | C15 | C16 | -176.84(17) | C23 | C22 | C27 | N3 | 177.92(17) |
| N2 | C14 | C15 | C20 | 6.4(3) | S1 | C22 | C27 | N3 | -1.0(2) |

**Table S8** Hydrogen Atom Coordinates (Å×$10^4$) and Isotropic Displacement Parameters (Å$^2$×$10^3$) for BTS.

| Atom | *x* | *y* | *z* | U(eq) |
|---|---|---|---|---|
| H2 | 1457 | 15371 | 2875 | 43 |
| H3 | -249 | 16515 | 2743 | 51 |

| | | | | |
|---|---|---|---|---|
| H4 | -1657 | 14394 | 3002 | 54 |
| H5 | -1329 | 11158 | 3414 | 43 |
| H7 | -130 | 8455 | 3760 | 29 |
| H9 | 111 | 6264 | 4343 | 30 |
| H10 | 510 | 3146 | 4782 | 29 |
| H12 | 3515 | 3503 | 4334 | 27 |
| H14 | 3812 | 4633 | 3426 | 29 |
| H16 | 5238 | 4656 | 2834 | 39 |
| H17 | 6718 | 6244 | 2498 | 49 |
| H18 | 7253 | 9641 | 2778 | 53 |
| H19 | 6305 | 11528 | 3361 | 48 |
| H23 | 1585 | -4313 | 5873 | 39 |
| H24 | 3080 | -6507 | 6004 | 39 |
| H25 | 4646 | -5620 | 5639 | 43 |
| H26 | 4813 | -2583 | 5148 | 40 |
| H1A | 2091(19) | 10780(50) | 3466(9) | 39 |
| H2A | 4120(20) | 9620(40) | 3857(9) | 39 |

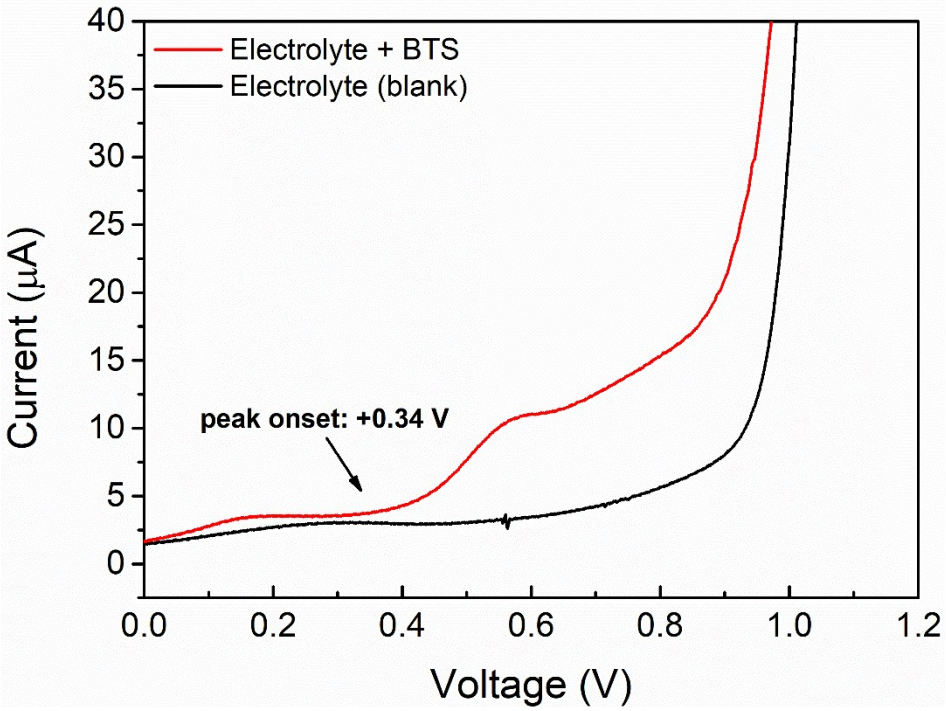


**Fig. S6** Cyclic voltammogram of 1.0 x $10^{-4}$ mol $L^{-1}$ tetrabutylammonium hexafluorophosphate solution in acetonitrile (scan rate 20 mV s-1) in the presence and absence of BTS. For clarity, only anodic sweep is shown.

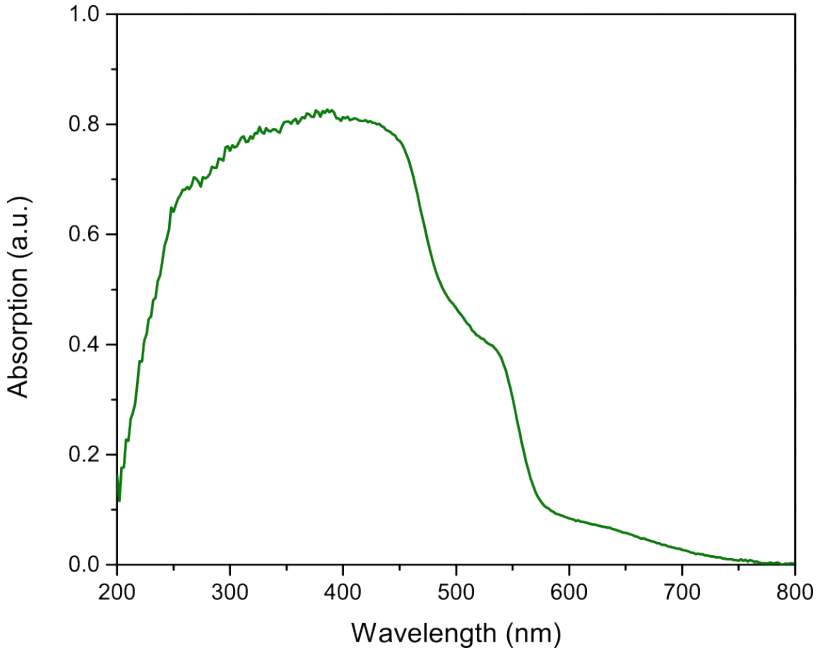


**Fig. S7** Solid-state electronic absorption spectrum of BTS on diffuse reflectance mode.

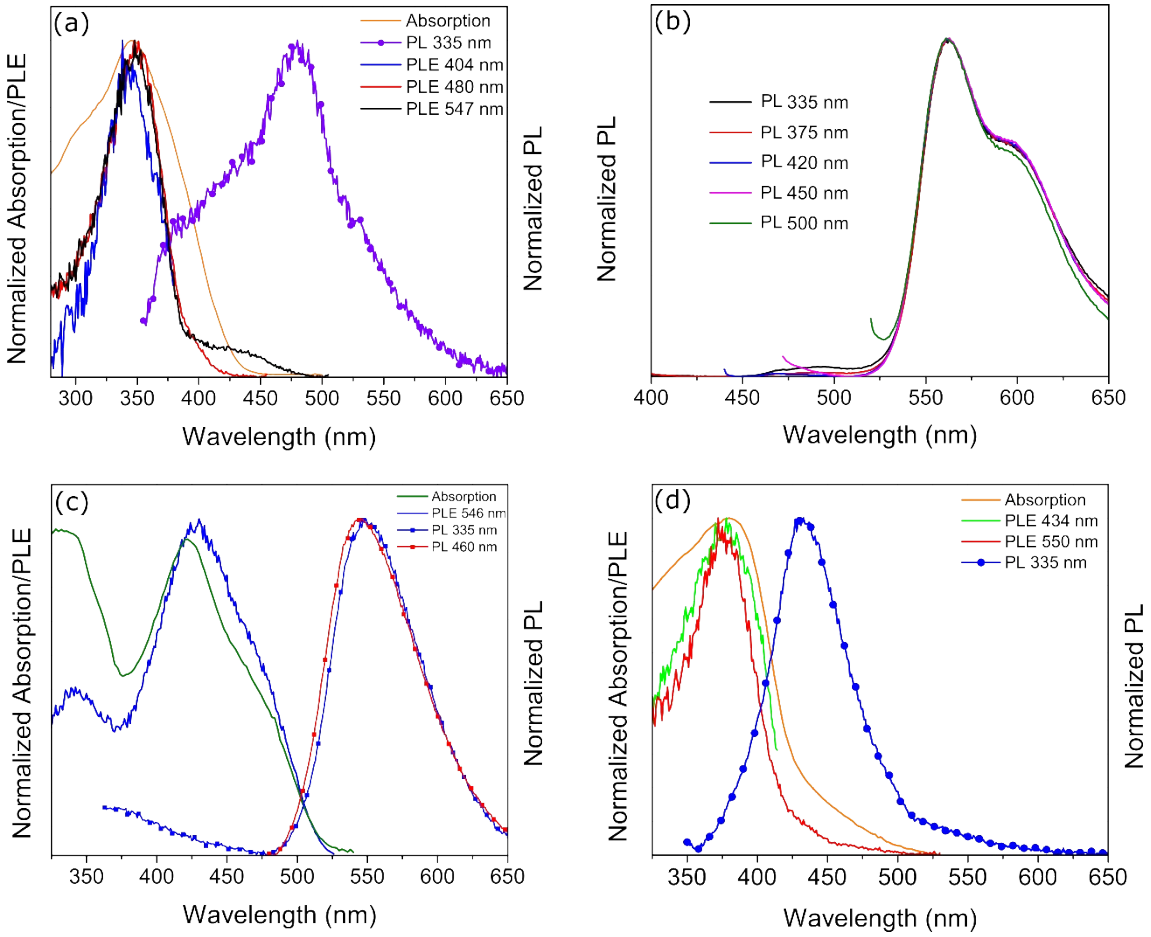

**Fig. S8** Normalized steady-state electronic absorption, PLE and PL spectra of BTS in (a) DCM. (b) BTS PL in the solid-state. Steady-state electronic absorption, PLE and PL spectra of BTS in (c) pyridine and (c) DCM with trace amounts of TFA. Concentration: 8.5 μmol $L^{-1}$.

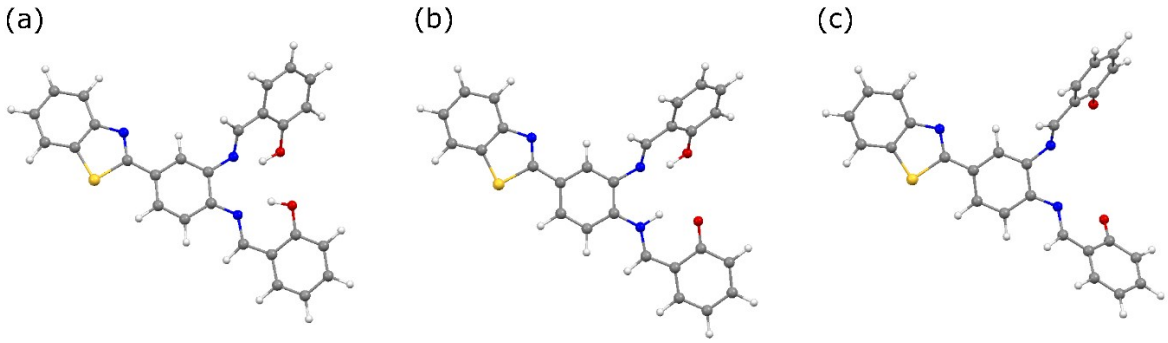


**Fig. S9** Optimized geometries for (a) neutral, (b) tautomeric and (d) deprotonated forms of BTS at the CAM-B3LYP/6-311++G(d,p) level.

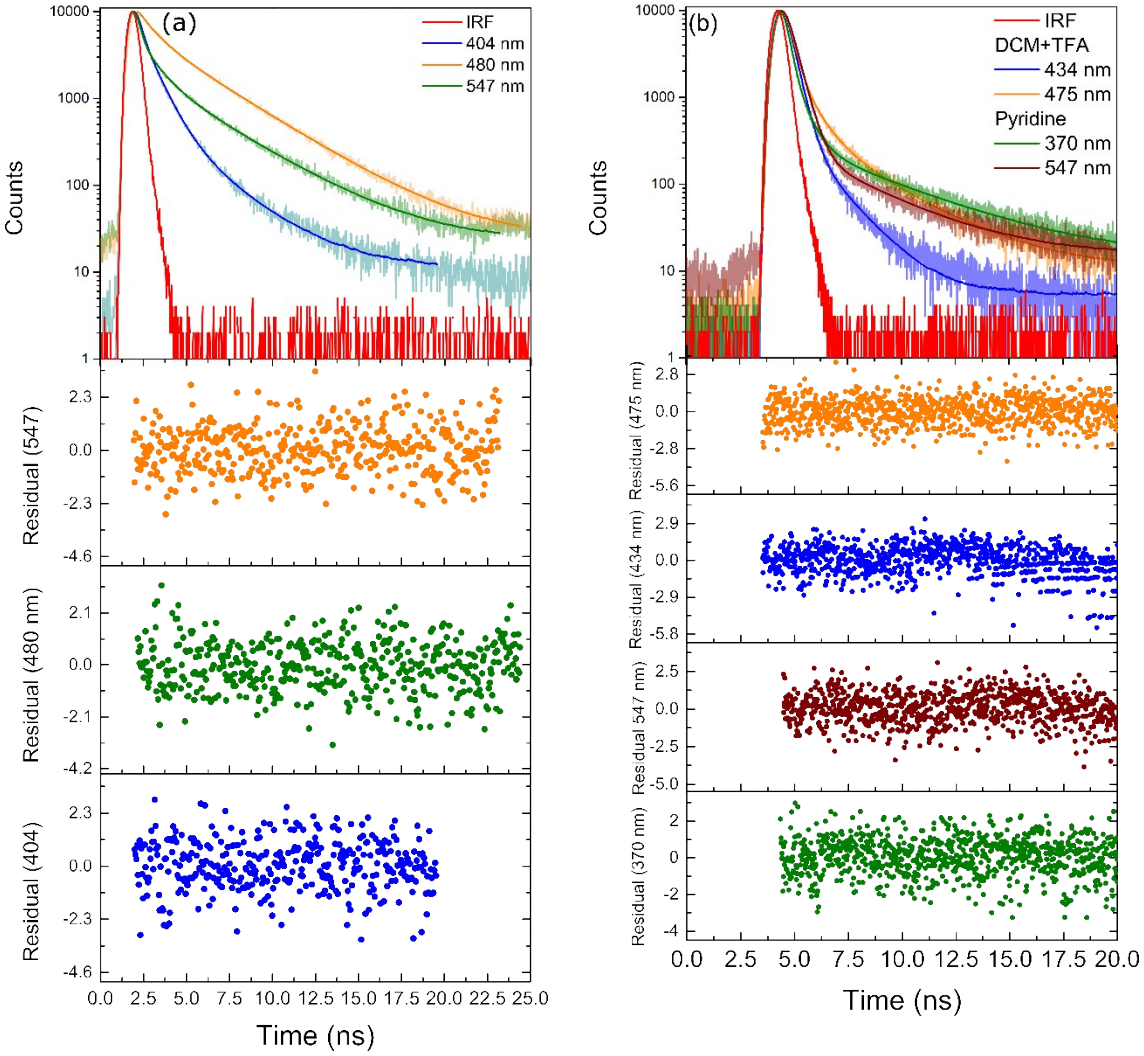

**Fig. S10** Fluorescence decays of BTS in (a) DCM, (b) DCM with trace amounts of TFA and in pyridine ($\lambda_{exc}$= 335.2 nm). Concentration: 8.5 µmol $L^{-1}$. Emission wavelengths used to record the decays along to IRF profiles are related in the figure.

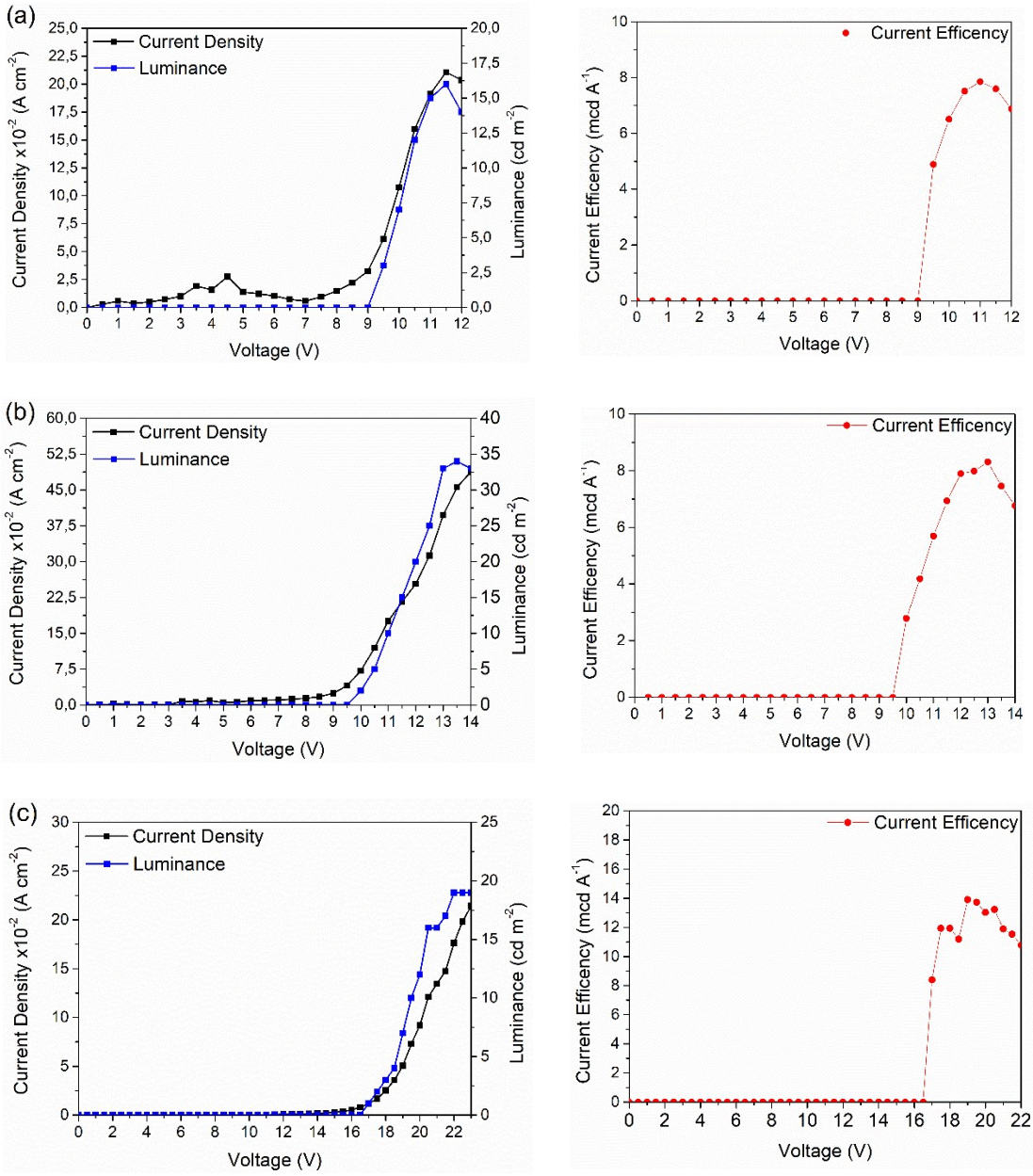

**Fig. S11** Current density *vs*. voltage, Luminance *vs*. voltage and Current efficiency *vs*. voltage curves for the diodes composed of PVK:BTS in the molar fractions of (a) 0.5%, (b) 1.0% and (c) 2.5% as active layers.

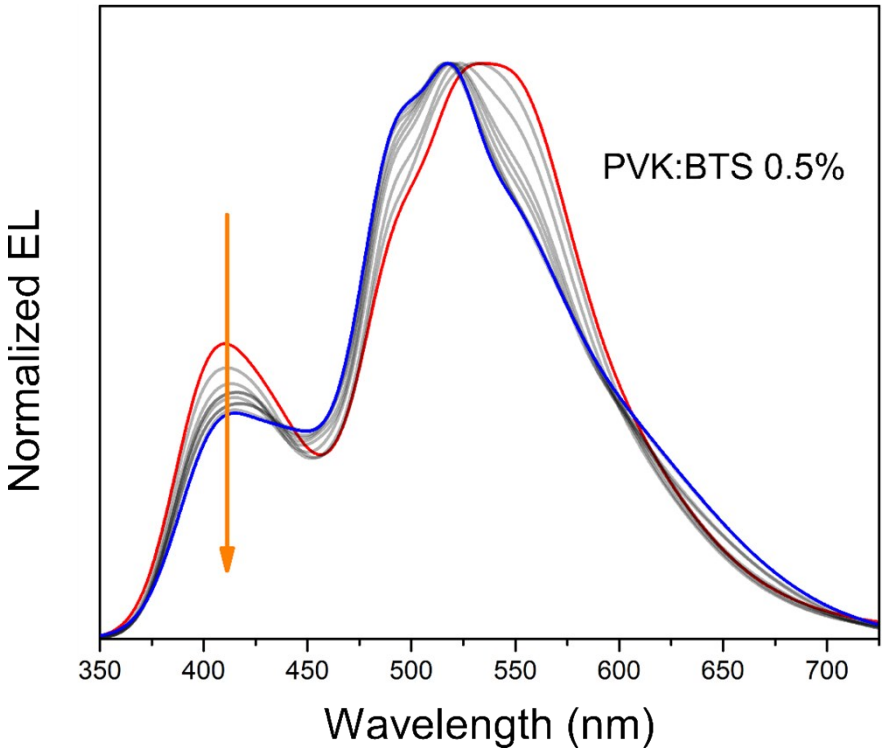


**Fig. S12** EL dependency with the applied field to the device with 0.5% mol/mol of BTS in PVK. The orange arrow indicates the increase of voltage.