# Supporting information

# Hydroxyphenyl-Benzothiazole Based Full Color Organic Emitting Materials Generated by Facile Molecular Modification

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## S1. Synthesis details of the compounds

**2-(benzo[d]thiazol-2-yl)-5-(dimethylamino)phenol (*p*MeOH)**. (1) Dissolved *p* (1.33 g, 5.496 mmol) and NaH (790 mg, 32.917 mmol ) in dried THF (100 mL) and added $CH_3I$ (2.05 mL, 32.915 mmol) under nitrogen, The mixture was slightly refluxed for 20 h. When cooled to the room temperature, the reaction mixture was added slowly water-free methanol in order to remove odd NaH. After removal of THF, the residue was extracted by dichloromethane and further purified by column chromatography (silica, dichloromethane: petroleum ether = 1 : 1) to dry to yield white powder *p*Meme. (2) Methoxyl group of *p*Meme reverted to hydroxyl group by pyridine hydrochloride (2.25 g, 19.480 mmol) in 170 ~ 185 ℃ for no more than 2 h, and the reaction mixture was cooled to the room temperature. After neutralized with excessive $NaHCO_3$ (aq) and extracted by dichloromethane, the crude product was further purified by column chromatography (silica, dichloromethane: petroleum ether = 1 : 1) and dried to yield yellow powder *p*MeOH (744.9 mg, 50 % yield). PS: the byproduct was 2-(benzo[d]thiazol-2-yl)- 5-(methylamino)phenol). ***p*Meme:** $^1$H NMR (DMSO, ppm): δ 8.22 (1 H, d, *J* = 9.00 Hz), 8.00 (1 H, d, *J* = 7.80 Hz), 7.90 (1 H, d, *J* = 7.80 Hz), 7.44 (1 H, t, *J* = 7.65 Hz), 7.31 (1 H, t, *J* = 7.50 Hz), 6.50 (1 H, dd, *J* = 9.00, 2.40 Hz), 6.39 (1 H, s), 4.03 (3 H, s), 3.05 (3 H, s). Ms *m/z*: 283.94 $[M]^+$ (calcd: 284.10). Anal. Calcd. (%) for $C_{16}H_{16}N_2OS$: C, 67.58; H, 9.85; N, 5.67; S, 11.28. Found: C, 67.71; H, 9.83; N, 5.631; S, 11.563. ***p*MeOH:** $^1$H NMR (DMSO, ppm): δ 11.77 (1 H, s), 8.04 (1 H, d, *J* = 7.80 Hz), 7.91 (1 H, d, *J* = 8.10 Hz), 7.74 (1 H, d, *J* = 8.70 Hz), 7.47 (1 H, t, *J* = 7.65 Hz), 7.35 (1 H, t, *J* = 7.50 Hz), 6.42 (1 H, dd, *J* = 9.00, 2.40Hz), 6.24 (1 H, s), 3.00 (6 H, s). Ms *m/z*: 269.93 $[M]^+$ (calcd: 270.08). Anal. Calcd. (%) for $C_{15}H_{14}N_2OS$: C, 66.64; H, 10.36; N, 5.22; S, 11.86. Found: C, 66.75; H, 10.34; N, 5.131; S, 11.933.

**4-(benzo[d]thiazol-2-yl)-3-methoxyaniline (*p*Hme)**. The product was synthesized with three steps: (1) The mixture of isobenzofuran-1,3-dione (4 g, 16.529 mmol) and *p* (2.69 g, 18.176 mmol) was added xylene (200 mL, without further purification) as

solvent and triethylamine (4 ml) as base under nitrogen, and refluxed for 9 h subsequently. After cooled to the room temperature, the reaction mixture was filtered and dried to yield light yellow solid **(*p*DoOH)**. (2) Added acetonitrile (300 mL, without further purification) into a mixture of $K_2CO_3$ (3.33 g, 24.130 mmol) and *p*DoOH under nitrogen, the mixture refluxed for 3 h. After cooled to room temperature, the mixture was added $CH_3I$ (1.5 mL, 24.084 mmol) under nitrogen and stirred at around 50 ℃ for 6 h. Filtering the reaction mixture and washing the residue with dichloromethane, filtrate was dried as the next step material (***p*Dome**) (3) Ethanol (250 mL) and methylamine (2 mL) were added into *p*Dome to revert the amino group and the mixture refluxed for 3 h. After the solvent was removed, the crude product was purified by column chromatography (silica, dichloromethane: ethyl acetate = 50 : 1) to yield white powder ***p*Hme** (3.07 g, 72 % yield).

**2-(benzo[d]thiazol-2-yl)-5-(diphenylamino)phenol** (***p*PhOH**). (1) DMF (2 mL, water-free purification with CaH) was added into the mixture of *p*Hme **(**456.7 mg, 1.784 mmol**)**, 1,10-phenanthraline (117.7 mg,0.594 mmol), CuI (56.8 mg, 0.297 mmol), $Cs_2CO_3$ (1.74 g, 5.354 mmol), iodobenzene (0.8 mL, 7.137 mmol), and the mixture was refluxed for 10 h under nitrogen. After cooled to the room temperature, the reaction mixture was filtrated and washed with dichloromethane. Filtrate was purified by column chromatography (silica, dichloromethane: petroleum ethyl = 1 : 1) to yield absinthe-green powder *p*Phme. (2) The procedure that methoxyl group of *p*Phme reverted to hydroxyl group is the similar as the one of *p*Meme with a little differences: pyridine hydrochloride was excessive (more than 10eq) and the mixture was heated in 190 ~ 200 ℃ for 2 h. And the crude product was purified by column chromatography (silica, dichloromethane: petroleum ether = 1 : 1) and dried to yield light yellow powder *p*PhOH (519.9 mg, 73 % yield). ***p*Phme:** $^1$H NMR (DMSO, ppm): δ 8.29 (1 H, d, *J* = 8.70 Hz), 8.07 (1 H, d, *J* = 7.20 Hz), 7.97 (1 H, d, *J* = 7.80 Hz), 7.48 (1 H, t, *J* = 7.65 Hz), 7.43 ~ 7.35 (5 H, m), 7.20 ~ 7.16 (6 H, m), 6.67 (1 H, s), 6.61 (1 H, dd, *J* = 8.70, 2.10 Hz), 3.83 (3 H, s). Ms *m/z*: 407.89 $[M]^+$ (calcd: 408.13). Anal. Calcd. (%) for $C_{26}H_{20}N_2OS$: C, 76.44; H, 4.93; N, 6.86; S, 7.85. Found: C, 76.60; H, 4.913; N, 6.89; S, 7.881. ***p*PhOH:** $^1$H NMR (DMSO, ppm): δ 11.46 (1 H, s),

8.07 (1 H, d, *J* = 8.10 Hz), 7.99 ~ 7.950 (2 H, m), 7.49 (1 H, t, *J* = 7.65 Hz), 7.44 ~ 7.35 (5 H, m), 7.21 ~ 7.15 (6 H, m), 6.49 (1 H, dd, *J* = 8.55, 2.25 Hz), 6.46 (1 H, s). Ms *m/z*: 393.92 $[M]^+$ (calcd: 394.11). Anal. Calcd. (%) for $C_{25}H_{18}N_2OS$: C, 76.12; H, 7.10; N, 4.60; S, 8.13. Found: C, 76.23; H, 7.05; N, 4.576; S, 8.258.

**2-(benzo[d]thiazol-2-yl)-5-iodophenol (*p*Ime)**: the mixture of *p*Hme (766 mg, 2.992 mmol) in 15 % HCl (aq, 25 mL) was added dropwise $NaNO_2$ (aq, 0.45 mol/L, 10 mL) for around 20 min at 0 ~ 5 ℃. Keeping the low temperature, the mixture was continue added droplets of KI (aq, 0.30 mol/L, 40 mL) for 30 ~ 50 min and stirred for 10 h at the room temperature. After being added excessive $Na_2S_2O_3$ powder to consume iodine, extracted with dichloromethane and dried, the crude product was further purified by column chromatography (silica, dichloromethane: petroleum ether = 1 : 1.5) to gain white powder ***p*Ime** (1.0g, 91 % yield).

**2-(benzo[d]thiazol-2-yl)-5-(9H-carbazol-9-yl)phenol (*p*CzOH):** (1) The mixture of *p*Ime (1.0 g, 2.725 mmol)**,** carbazole (910 mg, 5.450 mmol), 1,10-phenanthraline (359.7 mg, 1.817 mg), $K_2CO_3$ (3.7 g, 26.811 mmol), CuI (173.5 mg, 0.908 mmol) was dissolved into xylene (60 mL, without further purification) and refluxed for 30 h under nitrogen. The reaction mixture was filtrated and washed with dichloromethane. The filtrate was further purified by column chromatography (silica, dichloromethane: petroleum ether = 1 : 1.5) and dried to gain white powder ***p*Czme**. (2) The procedure that methoxy group of *p*Czme reverted to hydroxyl group is the same as the one of *p*Phme, and green powder was obtained ***p*CzOH** (90 % yield). ***p*Czme:** $^1$H NMR (DMSO, ppm): δ 8.7 (1 H, d, *J* = 8.70 Hz), 8.28 (2 H, d, *J* = 7.80 Hz), 8.18 (1 H, d, *J* = 7.80 Hz), 8.11 (1 H, d, *J* = 8.10 Hz), 7.65 ~ 7.55 (4 H, m), 7.51 ~ 7.44 (4 H, m), 7.34 (2 H, t, *J* = 7.35 Hz), 4.16 (3 H, s). Ms *m/z*: 405.92 $[M]^+$ (calcd: 406.11). Anal. Calcd. (%) for $C_{26}H_{18}N_2OS$: C, 76.82; H, 4.46; N, 6.89; S, 7.89. Found: C, 77.01; H, 4.437; N, 6.93; S, 8.13. ***p*CzOH:** $^1$H NMR (DMSO, ppm): δ 11.95 (1 H, s), 8.54 (1 H, d, *J* = 8.70 Hz), 8.28 (2 H, d, *J* = 7.50 Hz), 8.19 (1 H, d, *J* = 7.20 Hz), 8.11 (1 H, d, *J* = 7.80 Hz), 7.62 ~ 7.55 (3 H, m), 7.52 ~ 7.45 (3 H, m), 7.36 ~ 7.31 (4 H, m). Ms *m/z*: 391.95 $[M]^+$ (calcd: 392.10). Anal. Calcd. (%) for $C_{25}H_{16}N_2OS$: C, 76.51; H, 7.14; N, 4.11; S, 8.17. Found: C, 76.70; H, 7.11; N, 4.058; S, 8.275.

**2-(benzo[d]thiazol-2-yl)-4-(dimethylamino)phenol (*m*MeOH)**: Same procedure as *p*MeOH to give orange red powder *m*MeOH (25 % yield). ***m*Meme:** $^1$H NMR (DMSO, ppm): δ 8.12 (1 H, d, *J* = 7.80 Hz), 8.07 (1 H, d, *J* = 7.80 Hz), 7.80 (1 H, s), 7.52 (1 H, t, *J* = 7.65 Hz), 7.43 (1 H, t, *J* = 7.80 Hz), 7.20 (1 H, d, *J* = 9.30 Hz), 7.03 (1 H, dd, *J* = 4.50, 3.00 Hz), 3.98 (3 H, s), 2.934 (6 H, s). Ms *m/z*: 283.88 $[M]^+$ (calcd: 284.10). Anal. Calcd. (%) for $C_{16}H_{16}N_2OS$: C, 67.58; H, 5.67; N, 9.85; S, 11.28. Found: C, 67.77; H, 5.649; N, 9.86; S, 11.422. ***m*MeOH:** $^1$H NMR (DMSO, ppm): δ 10.79 (1 H, s), 8.12 (1 H, d, J = 8.10 Hz), 8.06 (1 H, d, J = 8.1 Hz), 7.53 (1 H, t, J = 7.65 Hz), 7.46 ~ 7.40 (2 H, m), 6.98 (2 H, s), 2.89 (6 H, s). Ms *m/z*: 269.91 $[M]^+$ (calcd: 270.08). Anal. Calcd. (%) for $C_{15}H_{14}N_2OS$: C, 66.64; H, 10.36; N, 5.22; S, 11.86. Found: C, 66.78; H, 10.39; N, 5.219; S, 11.921.

**3-(benzo[d]thiazol-2-yl)-4-methoxyaniline (*m*Hme).** Same procedure as *p*Hme to give light yellow powder *m*Hme(73% yield).

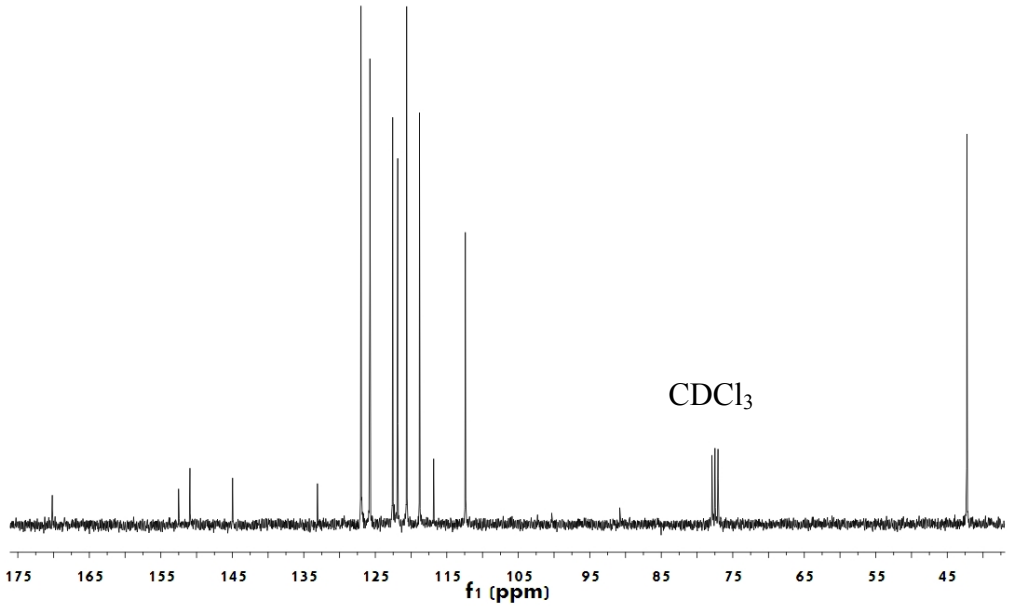
**2-(benzo[d]thiazol-2-yl)-4-(diphenylamino)phenol (*m*PhOH).** Same procedure as *p*Phme to give orange powder *m*PhOH (29 % yield). ***m*Phme:** $^1$H NMR (DMSO, ppm): δ 8.17 (1 H, s), 8.12 (1 H, d, J = 7.20 Hz), 7.99 (1 H, d, J = 7.50 Hz), 7.49 (1 H, t, J = 7.58 Hz), 7.42 (1 H, t, J = 7.50 Hz), 7.34 ~ 7.24 (6 H, m), 7.03 ~ 6.99 (6 H, m), 4.073 (3 H, s). Ms *m/z*: 408.14 $[M]^+$ (calcd: 408.13). Anal. Calcd. (%) for $C_{26}H_{20}N_2OS$: C, 76.44; H, 4.93; N, 6.86; S, 7.85. Found: C, 76.41; H, 4.806; N, 6.73; S, 8.069. ***m*PhOH:** $^1$H NMR (DMSO, ppm): δ 11.41 (1 H, s), 8.11 (1 H, d, *J* = 7.80 Hz), 8.01 ~ 7.98 (2 H, m), 7.49 (1 H, t, *J* = 7.58 Hz), 7.41 (1 H, t, *J* = 7.50 Hz), 7.31 ~ 7.25 (4 H, m), 7.18 ~ 7.08 (2 H, m), 7.02 ~ 6.96 (6 H, m). Ms *m/z*: 393.90 $[M]^+$ (calcd: 394.11). Anal. Calcd. (%) for $C_{25}H_{18}N_2OS$: C, 76.12; H, 4.60; N, 7.10; S, 8.13. Found: C, 76.24; H, 7.07; N, 4.596; S, 8.067.

**2-(benzo[d]thiazol-2-yl)-4-iodophenol (*m*Ime)**: Same procedure as *p*Ime to give white powder *m*Ime (54 % yield).

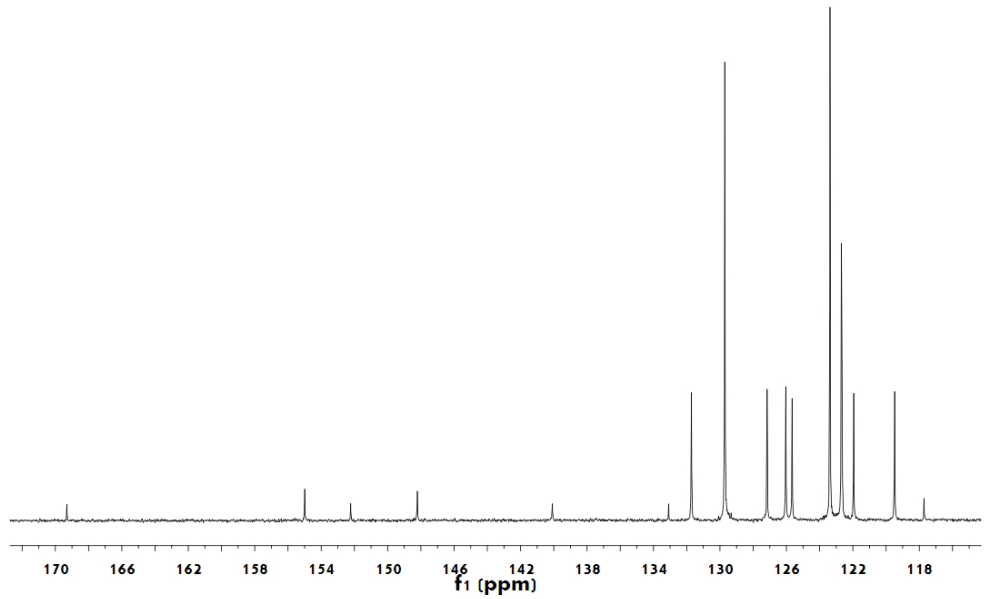
**2-(benzo[d]thiazol-2-yl)-4-(9H-carbazol-9-yl)phenol (*m*CzOH)**: Same procedure as *p*CzOH to give light yellow powder *m*CzOH (73 % yield). ***m*Czme:** $^1$H NMR (DMSO, ppm): δ 8.56 (1 H, s), 8.28 (1 H, d, *J* = 7.50 Hz), 8.17 (1 H, d, *J* = 7.80 Hz), 8.00 (1 H, d, *J* = 7.80 Hz), 7.84 (1 H, dd, *J* = 8.70, 2.70 Hz), 7.63 (1 H, d, *J* = 9.00 Hz), 7.55 ~

7.43 (4 H, m), 7.38 (2 H, d, *J* = 8.10 Hz), 7.31 (2 H, t, *J* = 7.28 Hz), 4.21 (3 H, s). Ms *m/z*: 406.14 $[M]^+$ (calcd: 406.11). Anal. Calcd. (%) for $C_{26}H_{18}N_2OS$: C, 76.82; H, 4.46; N, 6.89; S, 7.89. Found: C, 76.61; H, 4.406; N, 6.89; S, 8.095. ***m*CzOH:** $^1$H NMR (DMSO, ppm): δ 11.86 (1 H, s), 8.404 (1 H, s), 8.27 (2 H, d, *J* = 7.80 Hz), 8.16 (1 H, d, *J* = 7.50 Hz), 8.01 (1 H, d, *J* = 8.10 Hz), 7.65 (1 H, dd, *J* = 8.55, 2.40 Hz), 7.52 (1 H, t, *J* = 7.58 Hz), 7.45 (3 H, t, *J* = 7.43 Hz), 7.39 ~ 7.36 (3 H, m), 7.30 (2 H, t, *J* = 7.35 Hz). Ms *m/z*: 391.92 $[M]^+$ (calcd: 392.10). Anal. Calcd. (%) for $C_{25}H_{16}N_2OS$: C, 76.51; H, 4.11; N, 7.14; S, 8.17. Found: C, 76.74; H, 4.143; N, 7.11; S, 8.226.

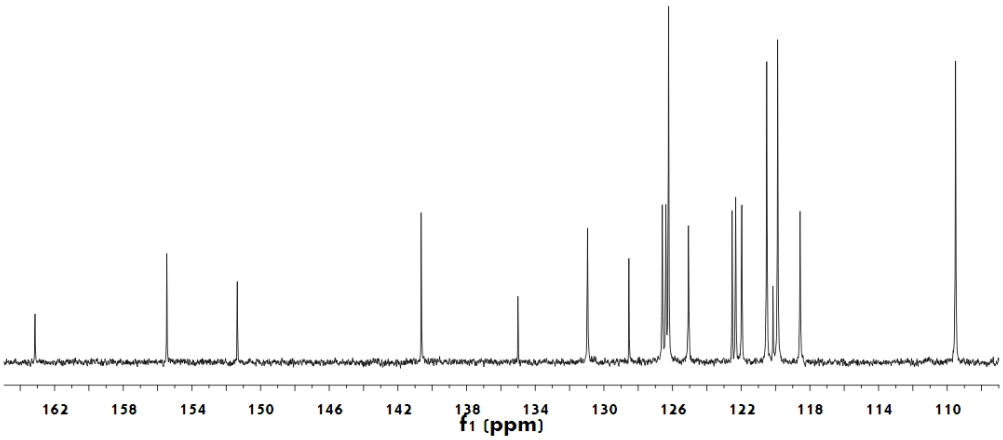
# S2. $^{13}$C NMR Spectra



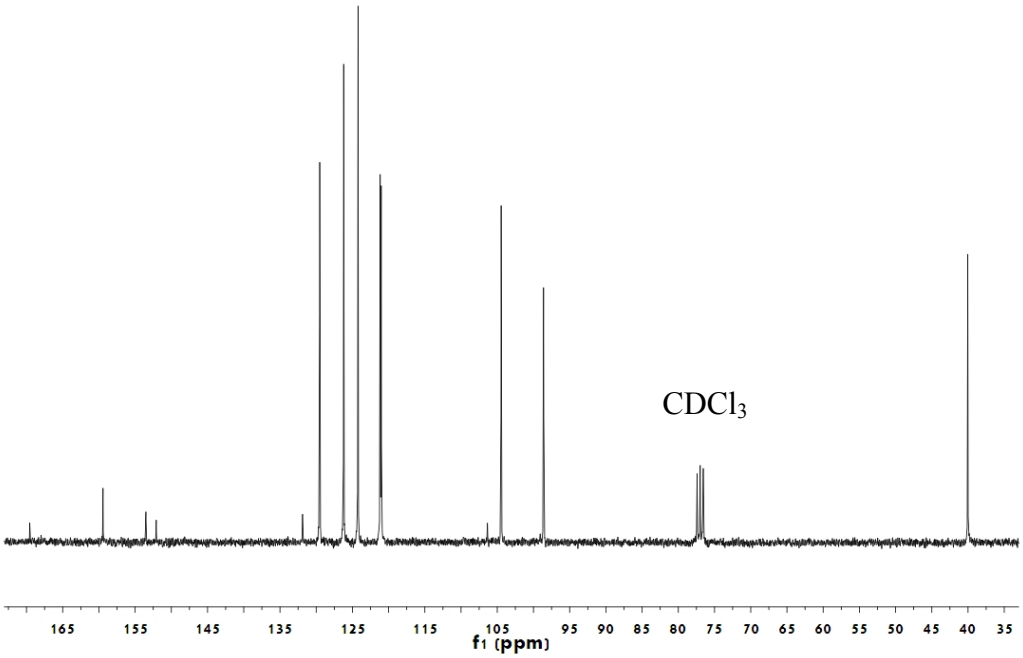

**mMeOH**: $\delta_C$ (75 MHz, DMSO) 170.18, 152.52, 150.93, 144.96, 133.09, 127.00, 125.75, 122.56, 121.86, 120.61, 118.81, 116.83, 112.40, 42.25.



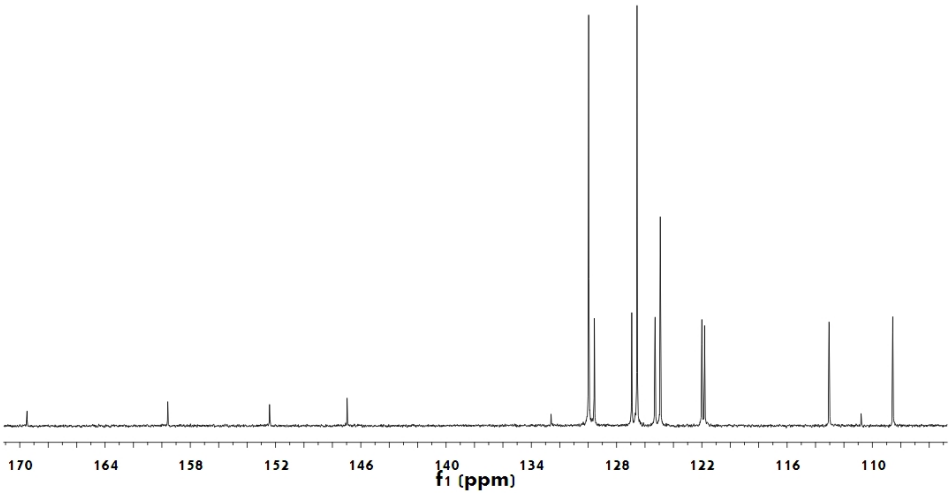

**mPhOH**: $\delta_C$ (75 MHz, $CDCl_3$) 169.31, 154.99, 152.23, 148.21, 140.08, 133.08, 131.72, 129.70, 127.16, 126.03, 125.65, 123.38, 122.69, 122.64, 121.95, 119.48, 117.72.



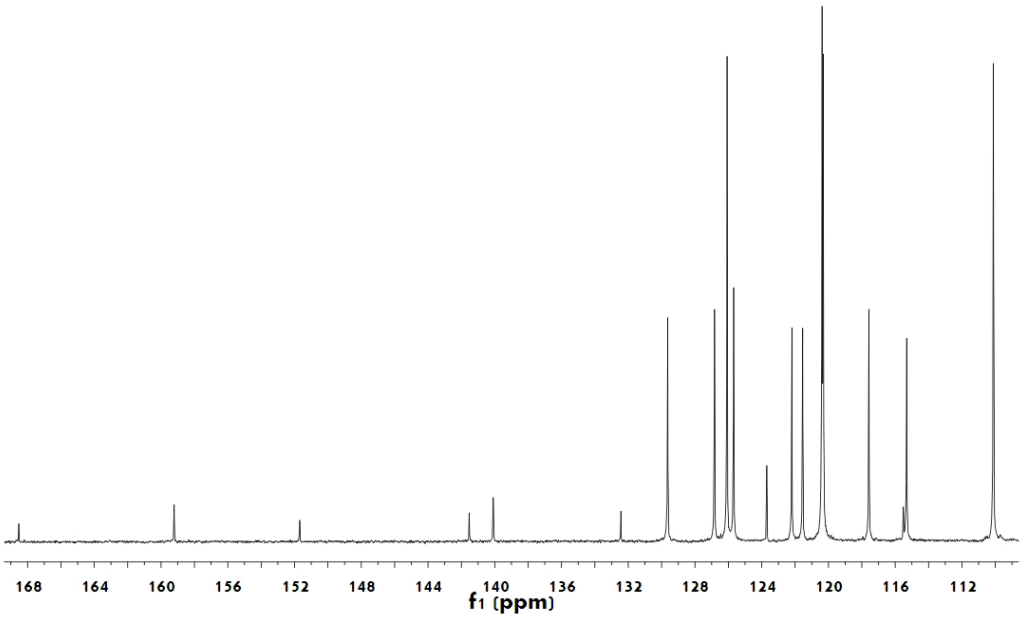

**mCzOH**: $\delta_C$ (75 MHz, DMSO) 163.14, 155.46, 151.36, 140.64, 135.00, 130.95, 128.54, 126.60, 126.39, 126.23, 125.07, 122.53, 122.32, 121.97, 120.51, 120.15, 119.87, 118.57, 109.51.




**pMeOH**: $\delta_C$ (75 MHz, $CDCl_3$) 169.55, 159.43, 153.51, 152.08, 131.88, 129.52, 126.20, 124.22, 121.16, 121.02, 106.36, 104.46, 98.61, 40.04.




**pPhOH**: $\delta_C$ (75 MHz, $CDCl_3$) 169.49, 159.58, 152.42, 146.96, 132.61, 129.97, 129.56, 126.93, 126.56, 125.29, 124.92, 122.00, 121.81, 113.05, 110.79, 108.57.




**pCzOH**: $\delta_C$ (75 MHz, $CDCl_3$) 168.53, 159.22, 151.69, 141.53, 140.09, 132.44, 129.64, 126.82, 126.08, 125.68, 123.70, 122.19, 121.55, 120.38, 120.31, 117.58, 115.51, 115.31, 110.12.

## S3. Theorietical calculation

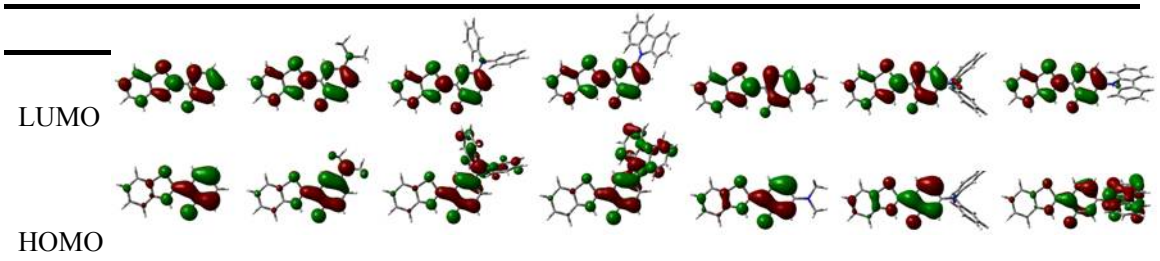



**Fig. S1** Calculated HOMO and LUMO in the lowest singlet excited ($S_1$) states for keto-BTZ and keto-BTZ derivatives by B3LYP/6-31G*. The structures of keto-BTZ and keto-BTZ derivatives in $S_1$ states were optimized at CIS/6-31G* level of theory. All calculations were performed using Gaussian 03 program package.

## S4. Crystal data and Structures

**Table S1.** Crystal data and structural refinement for ***m*MeOH**, ***m*PhOH**, ***m*CzOH, *p*PhOH and *p*CzOH**.

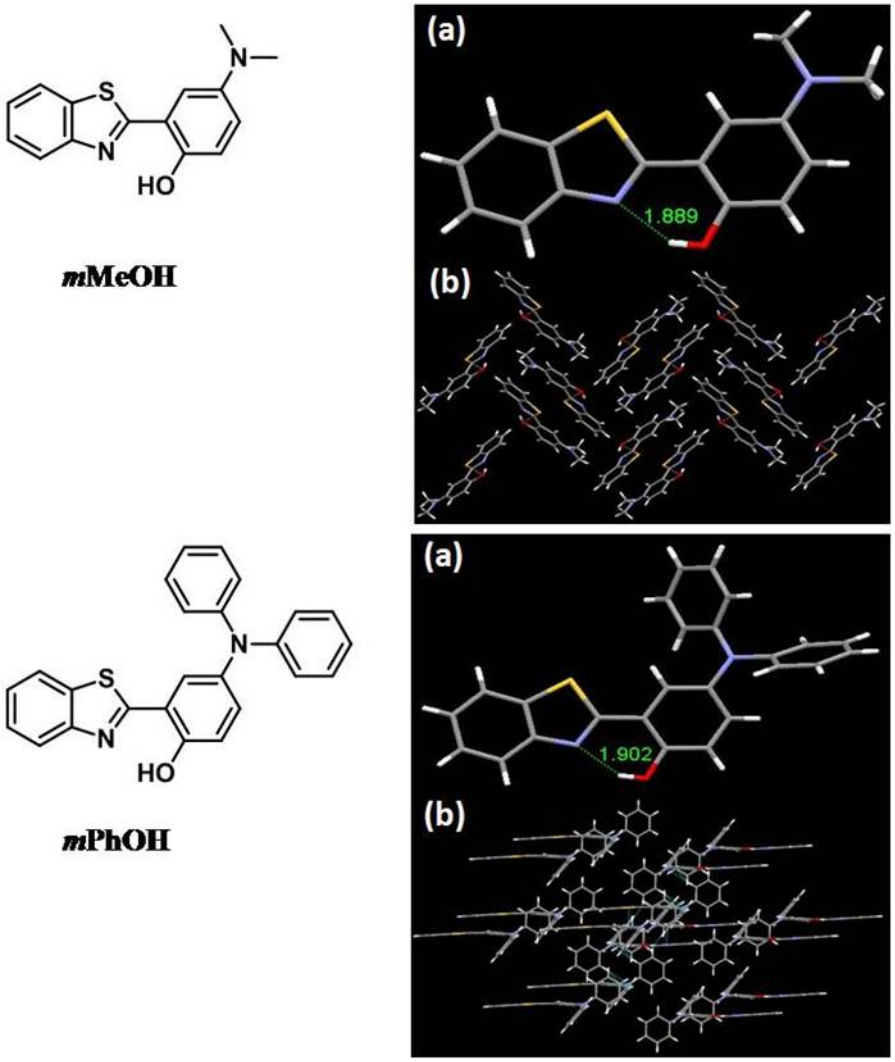
| | *m*MeOH | *m*PhOH | *m*CzOH | *p*PhOH | *p*CzOH |
|---|---|---|---|---|---|
| formula | C15H14N2OS | C25H18N2OS | C25H16N2OS | C25H18N2OS | C25H16N2OS |
| fw | 270.34 | 394.47 | 392.46 | 394.47 | 392.46 |
| crystal system | Monoclinic | Triclinic | Monoclinic | Monoclinic | Monoclinic |
| space group | P2(1)/n | P-1 | P2(1)/c | P2(1)/c | P2(1)/n |
| $a$ (Å) | 6.9711(14) | 8.8320(6) | 8.3907(4) | 20.542(4) | 9.949(2) |
| $b$ (Å) | 11.626(2) | 9.9071(7) | 30.6491(14) | 7.2295(14) | 15.759(3) |
| $c$ (Å) | 16.440(3) | 11.6033(8) | 7.7677(4) | 13.494(3) | 13.031(3) |
| $\alpha$ (deg) | 90 | 84.8300(10) | 90 | 90 | 90 |
| $\beta$ (deg) | 90.97(3) | 84.4180(10) | 105.2680(10) | 98.92(3) | 109.10(3) |
| $\gamma$ (deg) | 90 | 79.0620(10) | 90 | 90 | 90 |
| $V$ (Å$^3$) | 1332.2(5) | 989.44(12) | 1927.09(16) | 1979.8(7) | 1930.5(7) |
| $Z$ | 4 | 2 | 4 | 4 | 4 |
| $D_c$ (g cm$^{-3}$) | 1.348 | 1.324 | 1.353 | 1.323 | 1.350 |
| $\theta_{max}$ (deg) | 27.48 | 28.39 | 28.28 | 27.48 | 27.48 |
| no. of reflns meads | 12828 | 7414 | 14128 | 18151 | 18395 |
| no. of reflns used | 3040 | 4924 | 4779 | 4505 | 4382 |
| no. of parameters | 175 | 263 | 263 | 263 | 263 |
| $R_{int}$ | 0.0339 | 0.0255 | 0.0328 | 0.0599 | 0.0813 |
| final $R$ [I > 2σ(I)] | | | | | |
| R1 | 0.0601 | 0.0496 | 0.0466 | 0.0577 | 0.0408 |
| wR2 | 0.1732 | 0.1039 | 0.1225 | 0.1239 | 0.1032 |
| $R$ (all data) | | | | | |
| R1 | 0.0864 | 0.1083 | 0.0830 | 0.1105 | 0.0600 |
| wR2 | 0.1886 | 0.1258 | 0.1461 | 0.1428 | 0.1116 |
| GOF on $F^2$ | 1.103 | 0.966 | 1.059 | 1.030 | 1.040 |

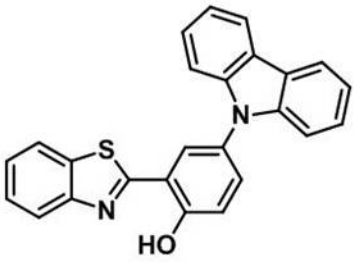
**Table S2.** Selected bond lengths (Å) and angles (deg) for ***m*MeOH**, ***m*PhOH**, ***m*CzOH, *p*PhOH and *p*CzOH**.

| | *m*MeOH | *m*PhOH | *m*CzOH | *p*PhOH | *p*CzOH |
|---|---|---|---|---|---|
| O(1)-H(1) | 0.8200 | 0.8200 | 0.8200 | 0.8200 | 0.8200 |
| O(1)-C(9) | 1.377(4) | 1.361(2) | 1.351(2) | 1.358(2) | 1.3438(18) |
| N(2)-C(12)[a] | 1.385(4) | 1.423(2) | 1.430(2) | 1.408(3) | 1.4177(19) |
| N(2)-C(14) | 1.442(4) | 1.426(2) | 1.394(2) | 1.420(3) | 1.402(2) |
| C(7)-C(8) | 1.448(4) | 1.458(3) | 1.466(3) | 1.446(3) | 1.455(2) |
| C(7)-N(1) | 1.301(3) | 1.308(2) | 1.317(2) | 1.324(3) | 1.3045(19) |
| C(7)-S(1) | 1.751(3) | 1.743(2) | 1.741(2) | 1.748(2) | 1.7459(16) |
| | | | | | |
| H(1)-O(1)-C(9) | 109.5 | 109.5 | 109.5 | 109.5 | 109.5 |
| O(1)-C(9)-C(8) | 123.1(3) | 122.41(18) | 122.61(18) | 121.5(2) | 122.56(14) |
| C(9)-C(8)-C(7) | 119.7(2) | 120.78(16) | 120.15(17) | 121.01(18) | 120.35(14) |
| C(8)-C(7)-N(1) | 123.4(3) | 122.77(18) | 122.53(18) | 122.70(19) | 123.17(14) |
| C(7)-N(1)-C(6) | 111.1(2) | 110.80(17) | 110.74(17) | 111.13(18) | 111.28(14) |
| N(1)-C(7)-S(1) | 115.0(2) | 115.28(15) | 115.16(15) | 114.60(16) | 115.19(12) |
| C(7)-S(1)-C(1) | 89.07(13) | 89.37(10) | 89.33(10) | 89.68(11) | 89.04(8) |
| C(12)-N(2)-C(14)[b] | 120.2(3) | 118.51(15) | 125.10(16) | 122.89(19) | 125.44(14) |

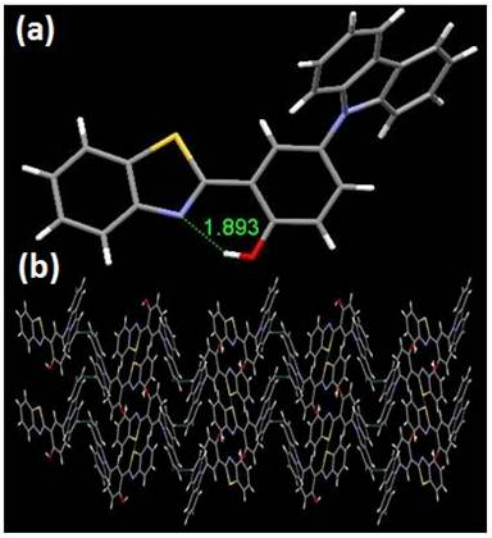
(a) N(2)-C(11) for *p*PhOH and *p*CzOH; (b) C(11)-N(2)-C(14) for *p*PhOH and *p*CzOH.

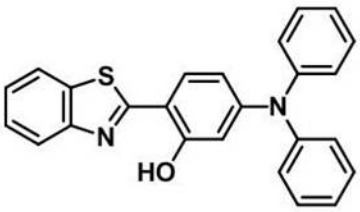
**Fig. S2.** View of the intra- or intermolecular interaction of compounds: (a) intramolecular H-bonding in the single molecule (b) stacking structure among molecules.



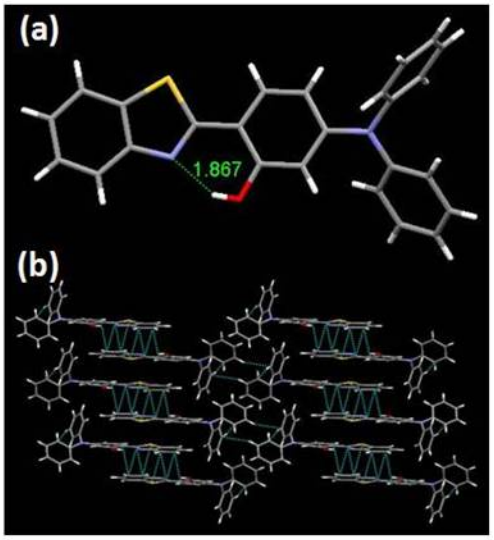


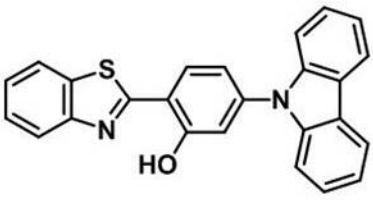

*m*CzOH



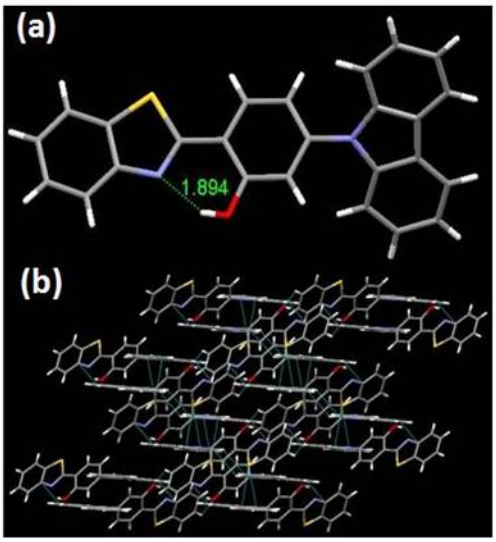




*p*PhOH




*p*CzOH



## S5. Thermal Analysis

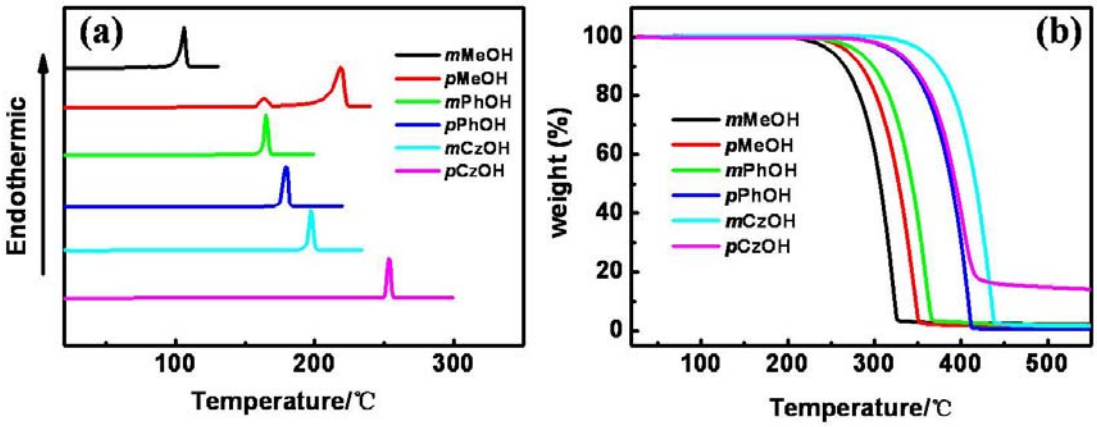



**Fig. S3.** DSC (a) and TGA (b) curves of *m*OH and *p*OH under nitrogen atmosphere at a heating rate of 10℃/min

**Table S3.**

| | *m*MeOH | *m*PhOH | *m*CzOH | *p*MeOH | *p*PhOH | *p*CzOH |
|---|---|---|---|---|---|---|
| Melting point (Tg)* (℃) | 106 | 165 | 197 | 219(164) | 179 | 253 |
| Decomposition temperature (℃, 5% weight loss) | 250 | 281 | 356 | 269 | 322 | 325 |

* Tg = glass transition temperature

The melting points of the materials studied in this manuscript were obtained from the DSC curves. For every compound, before decomposition temperature there is a strongly endothermic peak, which suggests the melting point. The DSC curves of the six compounds revealed that only *p*MeOH has glass transition (Tg) at around 164 ℃. For *p*MeOH three is an endothermic peak in its DSC curve suggesting that this compound has a Tg. The compounds *m*MeOH, *m*PhOH, *m*CzOH, *p*MeOH, *p*PhOH and *p*CzOH are crystalline in solid state.

## S6. Electroluminescent properties

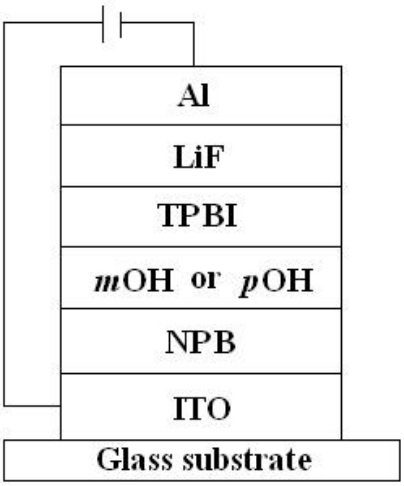



**Fig. S4.** Structure of devices for these derivatives

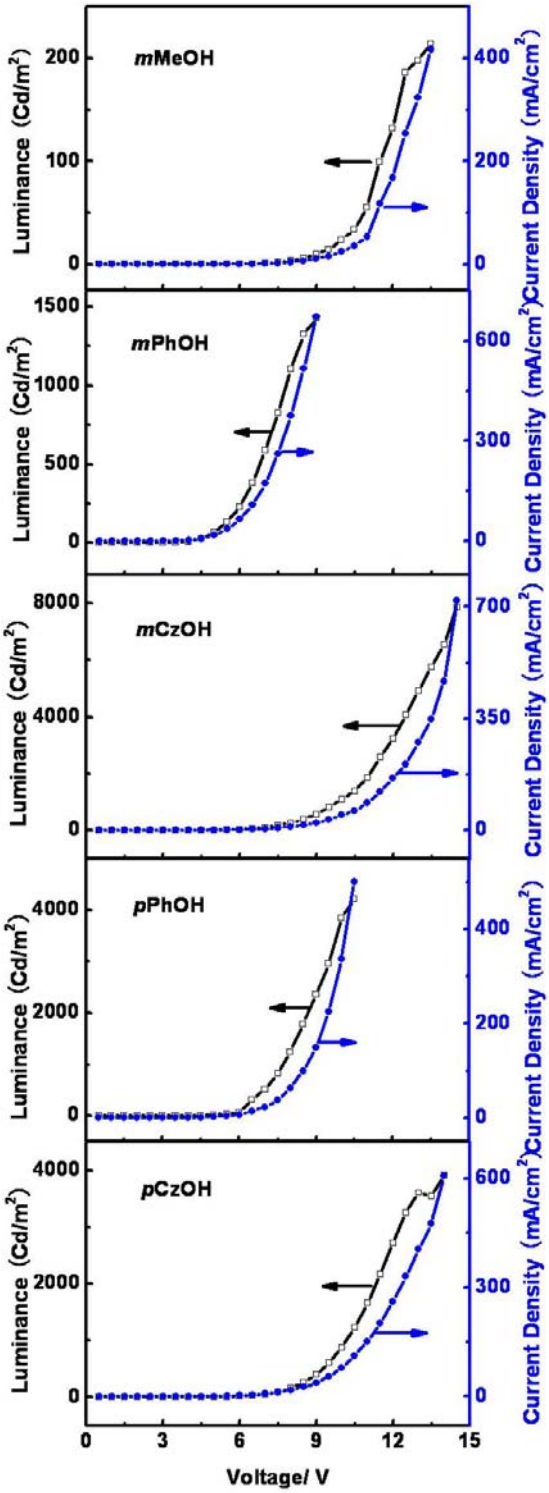



**Fig. S5.** Luminance-voltage-current (*L-V-J*) characteristics of derivatives.

**Table S4.** The cofigurations of three-layer device for these derivatives

| Device | NPB | *m*OH or *p*OH | TPBI | LiF | Al |
|---|---|---|---|---|---|
| *m*MeOH or *p*MeOH | 30 nm | 5 nm | 50 nm | 0.5 nm | 200 nm |
| *m*PhOH or *p*PhOH | 20 nm | 5 nm | 50 nm | 0.5 nm | 200 nm |
| *m*CzOH or *p*CzOH | 15 nm | 5 nm | 75 nm | 0.5 nm | 200 nm |

## S7. The fluorescence quantum yield measurement

The solid state PL quantum yields were measured and calculated by a calibrated integrating sphere based on the approach reported by L.-O. Pålsson and A. P. Monkan (L.-O. Pålsson, A. P. Monkan, *Adv. Mater.* **2002**, *14*, 757.).