

## Supporting Information

# **Molecular Design Featuring Carbazole-decorated 15H-diindolo[2,3-b:1',2',3'-lm]carbazole for Improved Efficiency and Lifetime of Thermally Activated Delayed Fluorescence Emitters**

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<b>Figure S1</b>	DSC analysis of the compounds	S2
<b>Figure S2</b>	Cyclic voltammetry measurements of the compounds	S3
<b>Table S1</b>	Excited singlet (S <sub>1</sub> ) and triplet (T <sub>1</sub> ) energies of the adjacent layers of EML	S3
<b>Table S2</b>	Lifetime comparison table of the green TADF emitters	S3
<b>Figure S3</b>	<sup>1</sup> H NMR spectra of <b>1</b> recorded in CDCl <sub>3</sub>	S4
<b>Figure S4</b>	<sup>1</sup> H NMR spectra of <b>CzDICz</b> recorded in CDCl <sub>3</sub>	S5
<b>Figure S5</b>	<sup>1</sup> H NMR spectra of <b>CzDICzTrz</b> recorded in CDCl <sub>3</sub>	S5
<b>Figure S6</b>	<sup>13</sup> C NMR spectra of <b>CzDICzTrz</b> recorded in CDCl <sub>3</sub>	S6
	References	S6

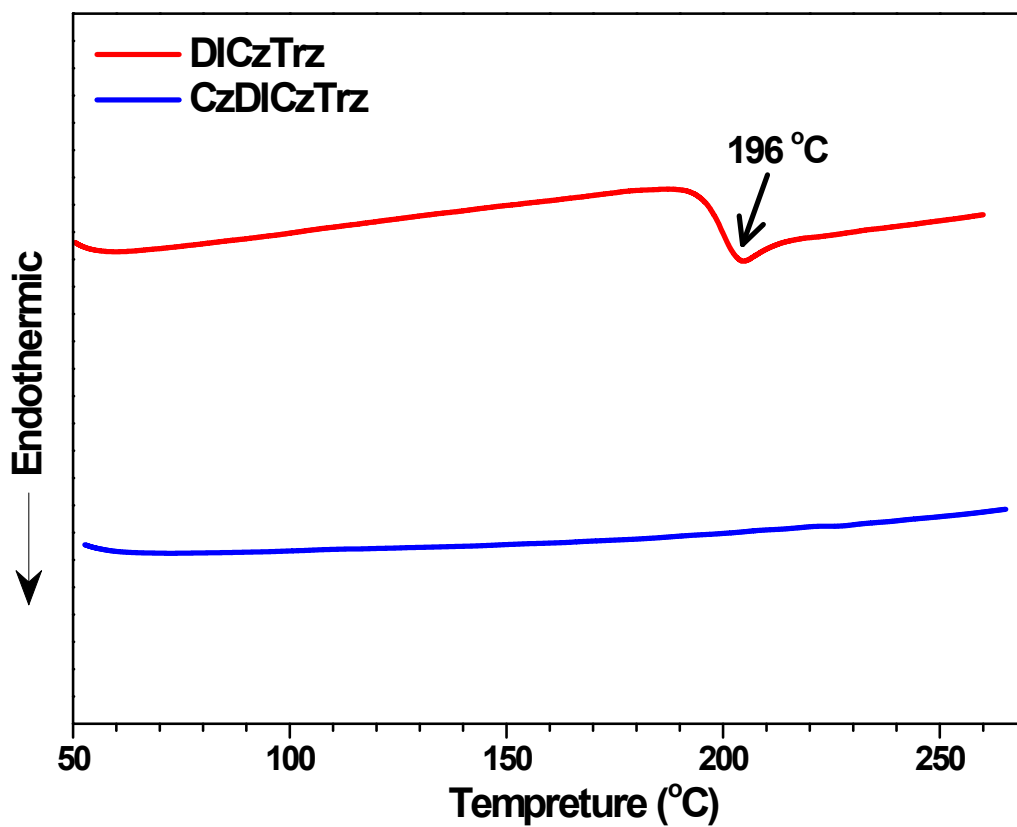
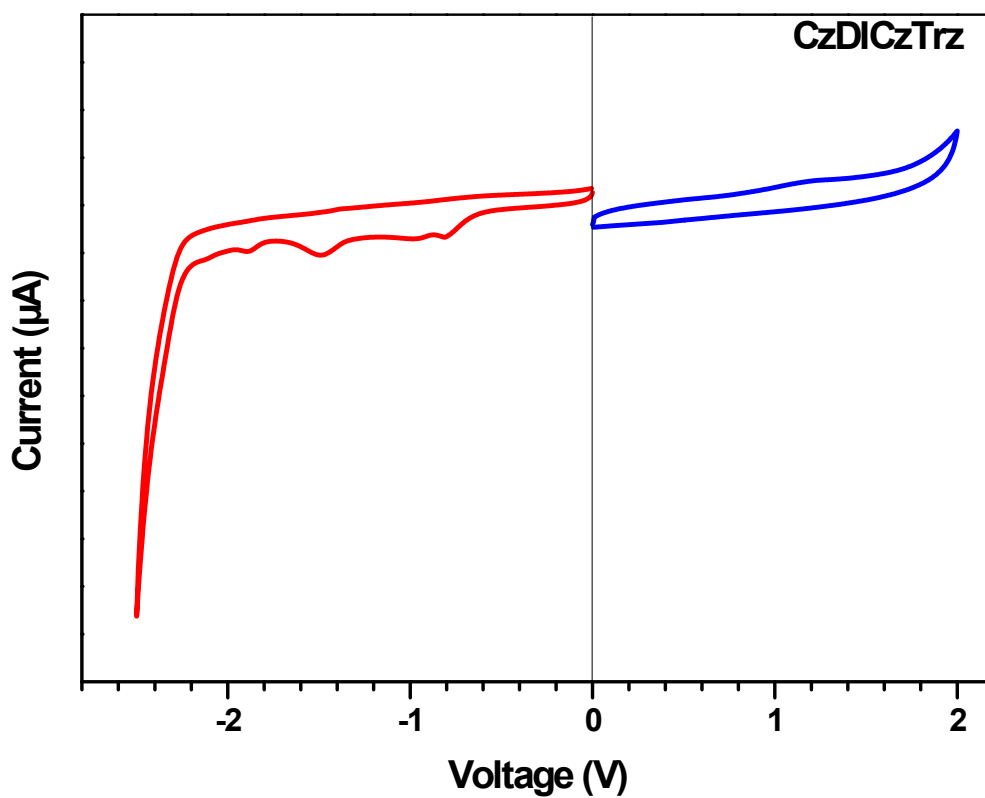
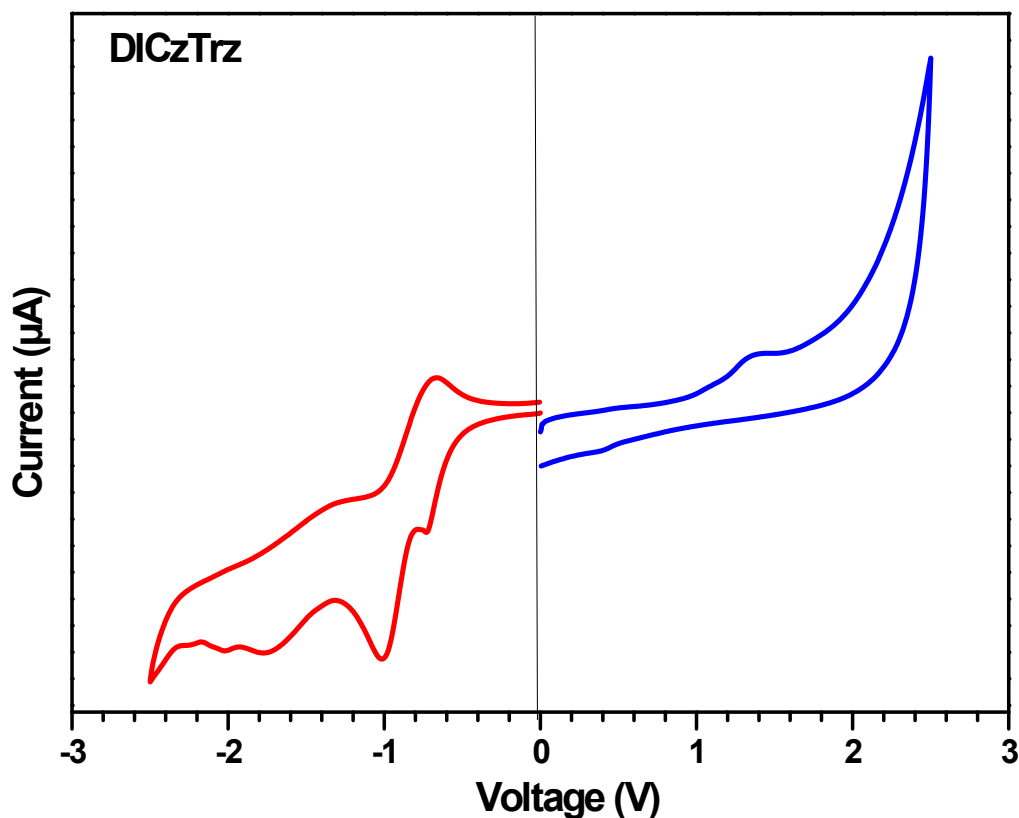


Figure S1. DSC analysis of the compounds





**Figure S2.** Cyclic voltammety measurements of the compounds

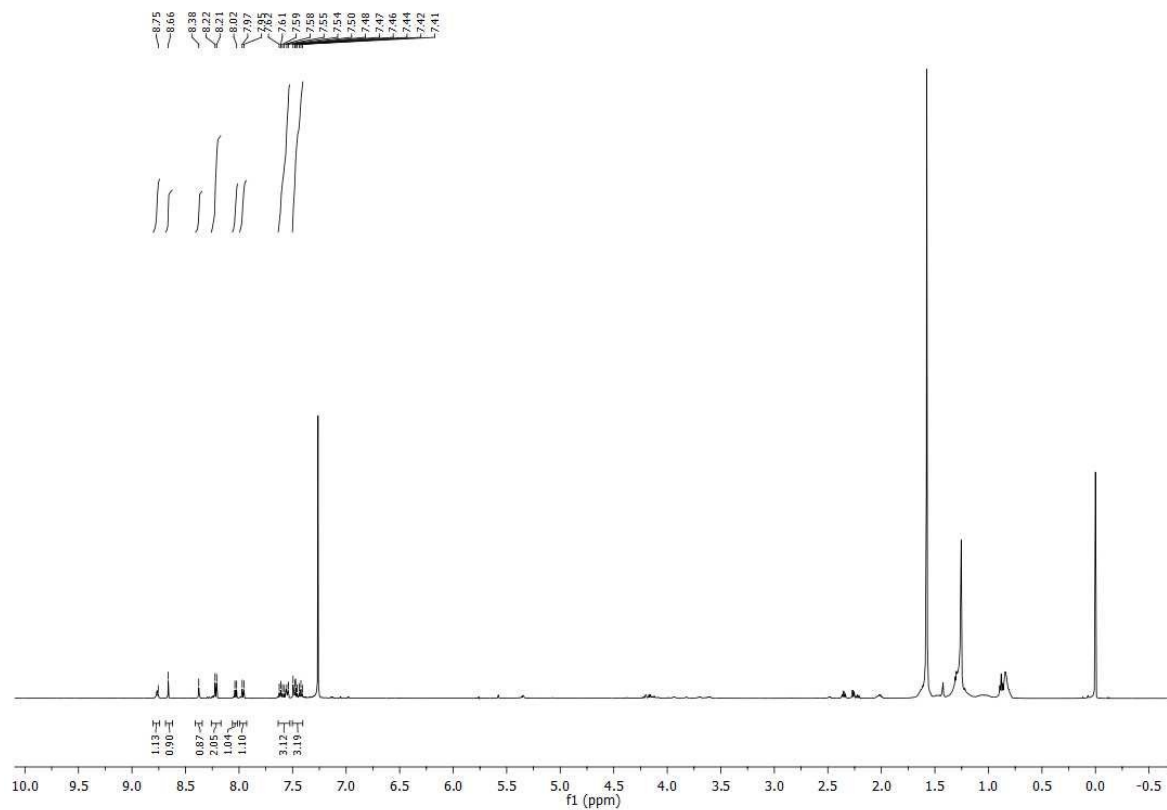
**Table S1.** Excited singlet (S<sub>1</sub>) and triplet (T<sub>1</sub>) energies of the adjacent layers of EML and host

Compound	S <sub>1</sub> (eV)	T <sub>1</sub> (eV)
PCZAC	3.35	2.99
DBFTrz	3.44	2.94
CzTrz	2.96	2.82

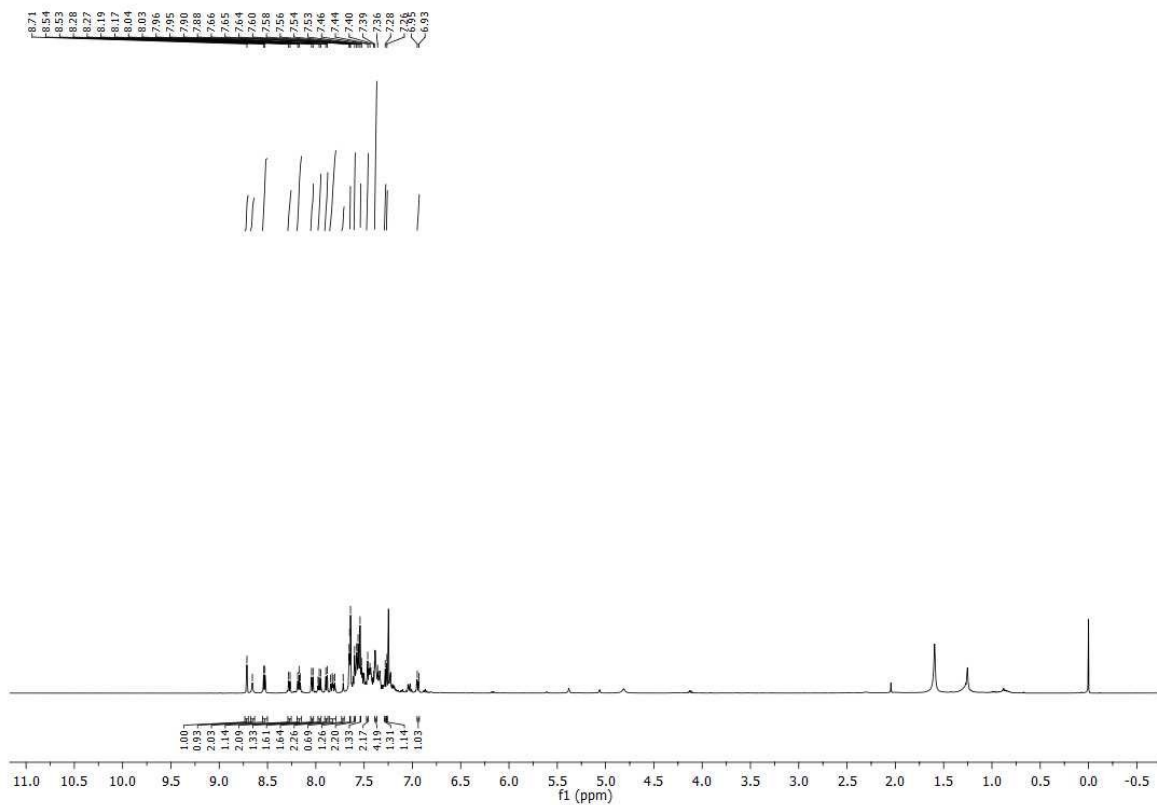
**Table S2.** Lifetime comparison table of the green TADF emitters

TADF dopant	Lifetime	Ref
CzDICzTrz	LT80 ~ 440 h @ 1000 cd/m <sup>2</sup>	<b>This work</b>
4CzIPN	LT80 ~ 250 h @ 1000 cd/m <sup>2</sup>	1
4CzIPN	LT80 ~ 1100 h @ 1000 cd/m <sup>2</sup>	2
4CzIPN	LT70 ~ 500 h @ 2000 cd/m <sup>2</sup>	3
4CzIPN-Me	LT50 ~ 1470 h @ 1000 cd/m <sup>2</sup>	4
OSTFCN	LT50 ~ 180 h @ 500 cd/m <sup>2</sup>	5

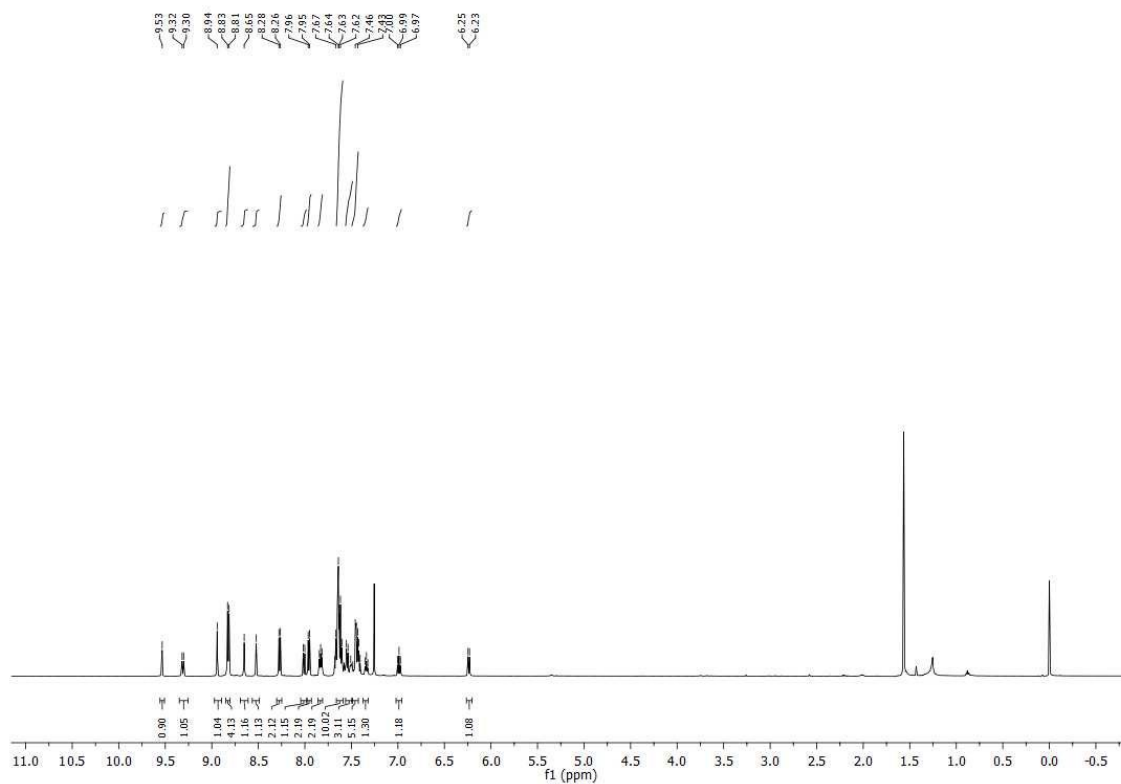
PXZ-Trz	LT50 ~ 100 h @ 2791 cd/m <sup>2</sup>	6
TXO-PhCz	LT50 ~ 80 h @ 1000 cd/m <sup>2</sup>	7
TCzTrzDBF	LT85 ~ 224 h @ 3000 cd/m <sup>2</sup>	8
BCzTrzDBF	LT85 ~ 133 h @ 3000 cd/m <sup>2</sup>	8



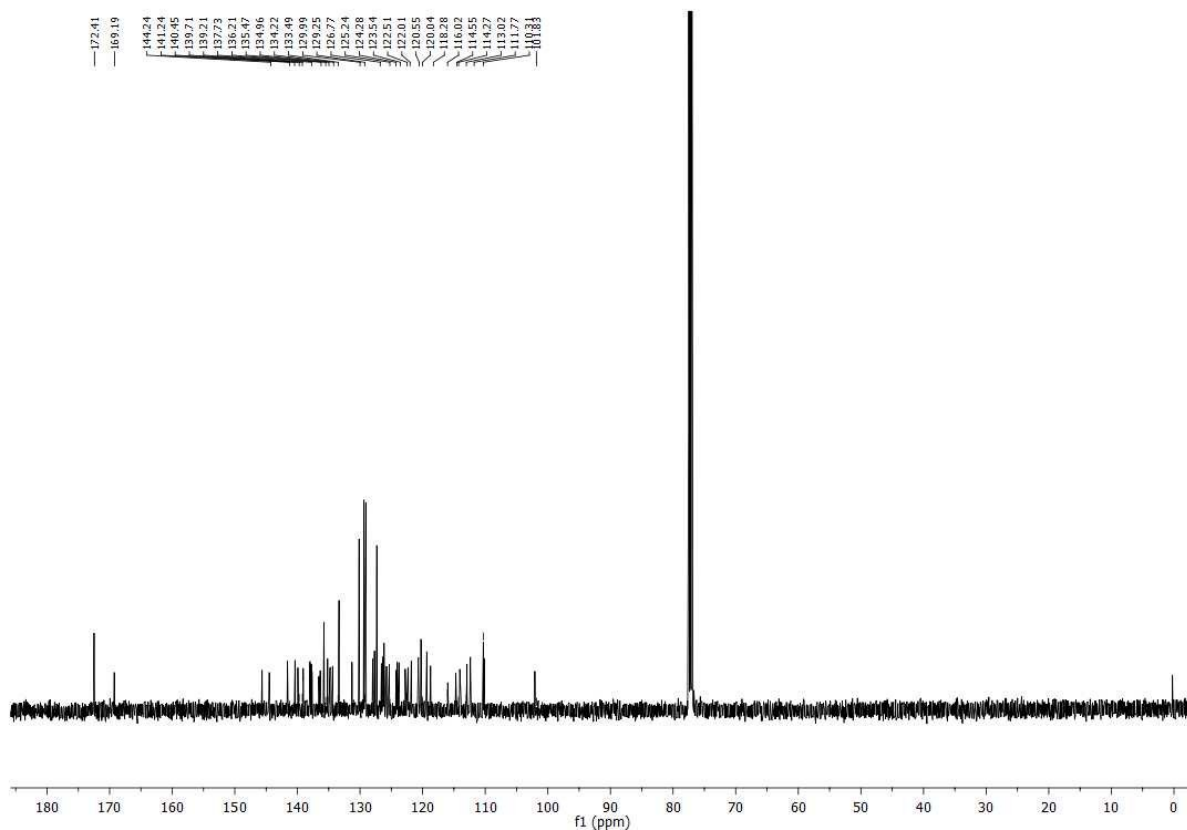
**Figure S3.** <sup>1</sup>H NMR spectra of **1** recorded in CDCl<sub>3</sub>



**Figure 4.**  $^1\text{H}$  NMR spectra of **CzDICzTrz** recorded in  $\text{CDCl}_3$



**Figure S5.**  $^1\text{H}$  NMR spectra of **CzDICzTrz** recorded in  $\text{CDCl}_3$



**Figure S6.**  $^{13}\text{C}$  NMR spectra of **CzDICzTrz** recorded in  $\text{CDCl}_3$

### References

1. Y. Im, W. Song and J. Y. Lee, *J. Mater. Chem. C*, **2015**, *3*, 8061.
2. W. Song, T. Kim, Y. Lee and J. Y. Lee, *J. Mater. Chem. C*, **2017**, *5*, 3948.
3. L. S. Cui, Y. M. Xie, Y. K. Wang, C. Zhong, Y. L. Deng, X. Y. Liu, Z. Q. Jiang and L. S. Liao, *Adv. Mater.* **2015**, *27*, 4213.
4. T. Furukawa, H. Nakanotani, M. Inoue and C. Adachi, *Sci. Rep.* **2015**, *5*, 8.
5. Y. K. Wang, S. F. Wu, Y. Yuan, S. H. Li, M. K. Fung, L. S. Liao and Z. Q. Jiang, *Org. Lett.* **2017**, *19*, 3155.
6. H. Nakanotani, T. Higuchi, T. Furukawa, K. Masui, K. Morimoto, M. Numata, H. Tanaka, Y. Sagara, T. Yasuda and C. Adachi, *Nat. Commun.* **2014**, *5*, 7.

7. X. P. Lv, H. Wang, L. Q. Meng, X. F. Wei, Y. Z. Chen, X. B. Kong, J. J. Liu, J. X. Tang, P. F. Wang and Y. Wang, *Chin. Phys. Lett.* **2016**, *33*, 4.
8. J. G. Yu, S. H. Han, H. L. Lee, W. P. Hong and J. Y. Lee, *J. Mater. Chem. C*, **2019**, *7*, 2919.