

## Supplementary Information

### Solution-processable naphthalene and phenyl substituted carbazole core based hole transporting materials for efficient organic light-emitting diodes

Sudhir Kumar<sup>a,b</sup>, Chih-Chia An<sup>a</sup>, Snehasis Sahoo,<sup>a</sup> R. Griniene<sup>c</sup>, D. Volyniuk<sup>c</sup>, Juozas V. Grazulevicius<sup>c</sup>, Saulius Grigalevicius<sup>c,\*</sup>, Jwo-Huei Jou<sup>a,\*</sup>

<sup>a</sup>Department of Materials Science and Engineering, National Tsing-Hua University, No.101, Kung-Fu Rd. Hsin-Chu 30013 Taiwan, R.O.C.

<sup>b</sup>Present address: Institute for Chemical and Bioengineering, ETH Zürich, Vladimir Prelog Web 1, 8093 Zürich, Switzerland.

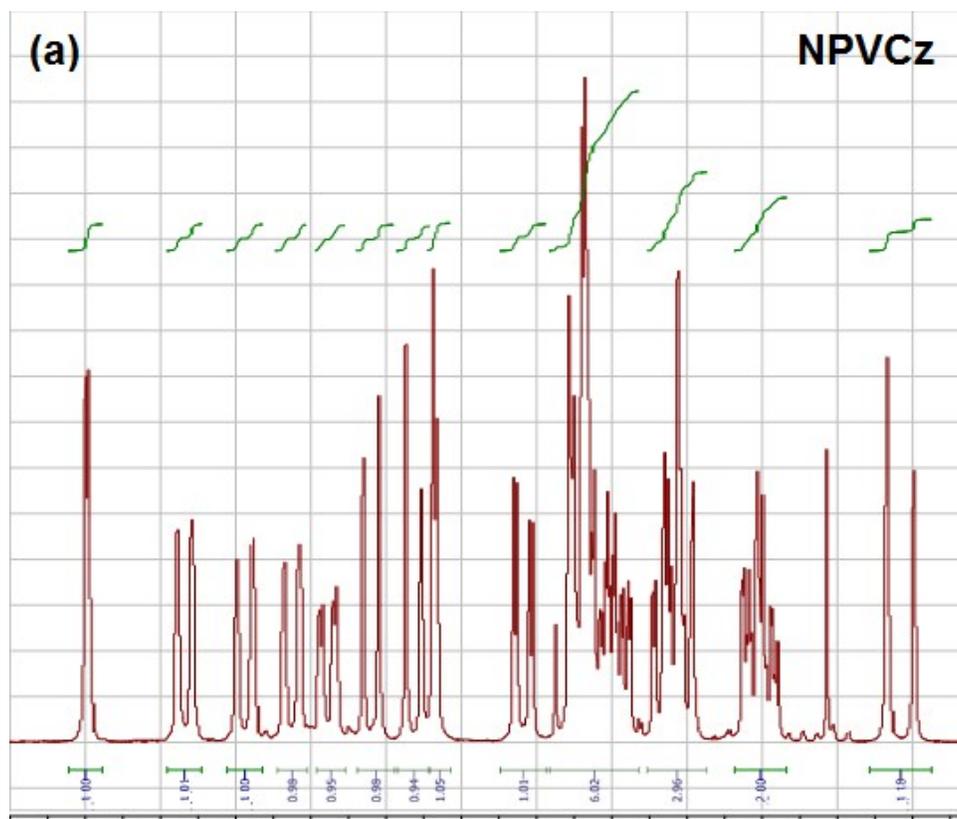
<sup>c</sup>Department of Polymer Chemistry and Technology, Kaunas University of Technology, Radvilenu plentas 19, LT50254, Kaunas, Lithuania.

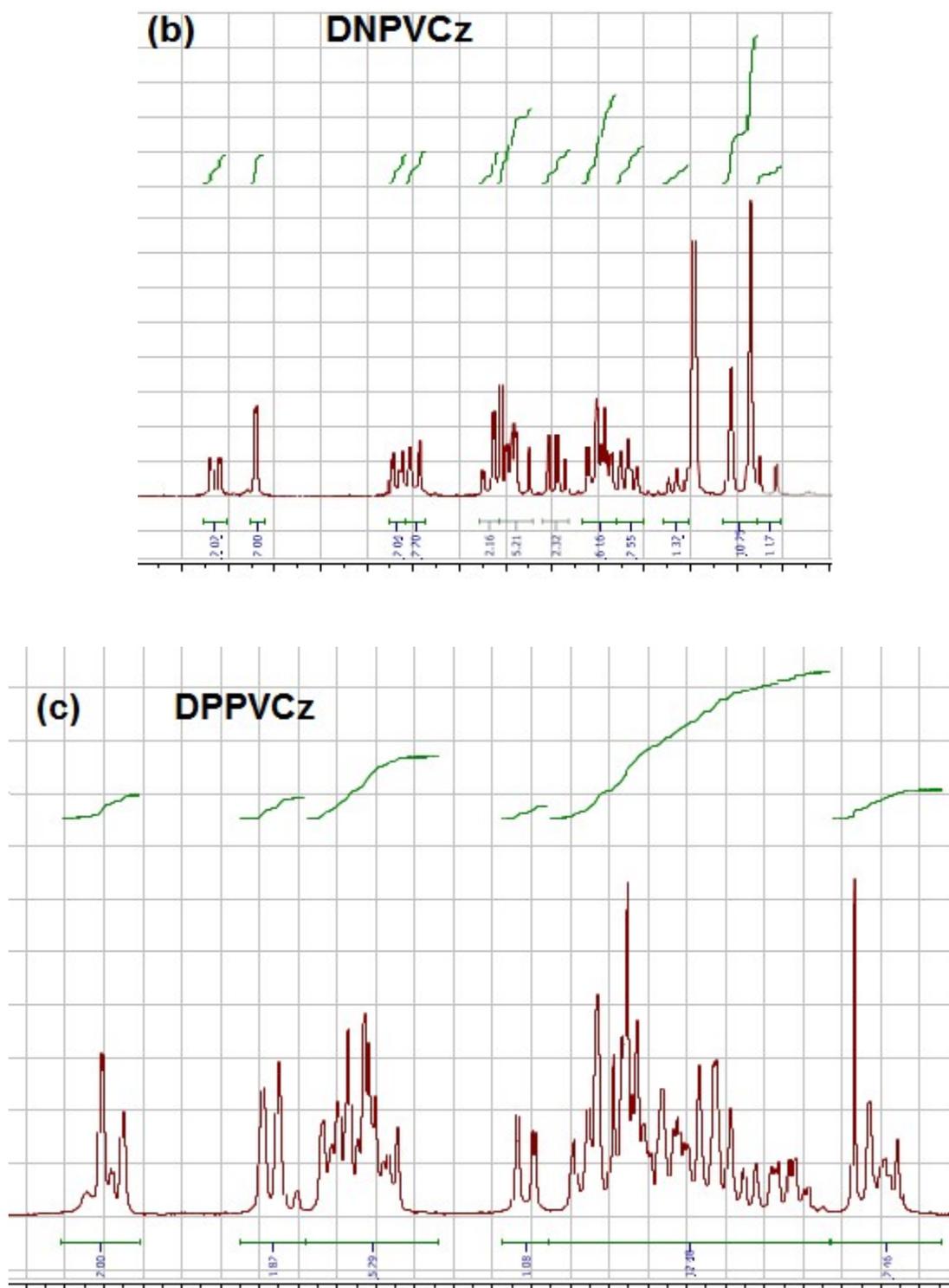
### Contents

<b>Figure S1.</b> H <sup>1</sup> NMR spectra of HTMs, (a) NPVCz, (b) DNPVCz, and (c) DPPVCz.....	3
<b>Figure S2.</b> IR spectra of HTMs, (a) NPVCz, (b) DNPVCz, and (c) DPPVCz.....	5
<b>Figure S3.</b> Mass-spectrum of NPVCz compound.....	6
<b>Figure S4.</b> Mass-spectrum of DNPVCz compound.....	7
<b>Figure S5.</b> Mass-spectrum of DPPVCz compound.....	8
<b>Figure S6.</b> PL spectra of NPVCz, DPPVCz and DNPVCz, in THF solution at 77 K.....	9
<b>Figure S7.</b> TGA plots of NPVCz, DNPVCz, and DPPVCz.....	9
<b>Figure S8.</b> DSC curves of (a) NPVCz, (b) DNPVCz, and (c) DPPVCz.....	11
<b>Figure S9.</b> Double-logarithmic representation of transient photocurrents curves of the newly synthesized HTMs, (a) NPVCz, (b) DNPVCz, and (c) DPPVCz, and inset show the TOF transient curves.....	12
<b>Figure S10.</b> Effect of the HTMs, NPB, NPVCz, DNPVCz, and DPPVCz, on the EL spectra of the fluorescent green OLED devices.....	13

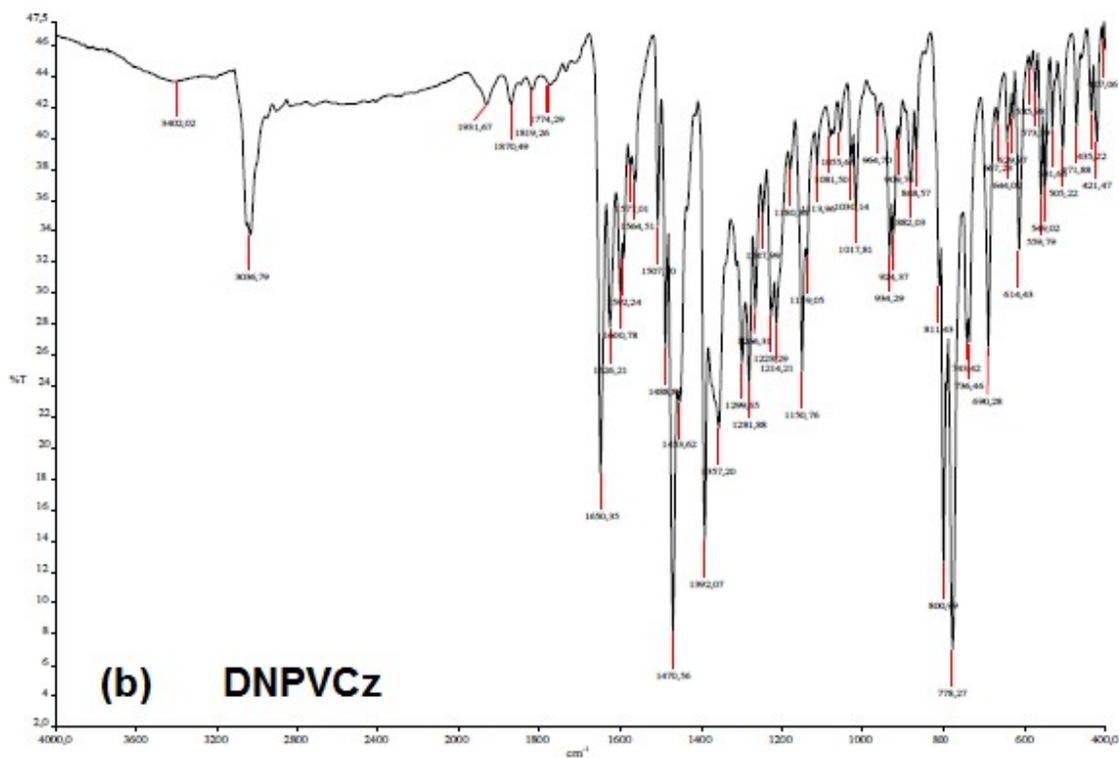
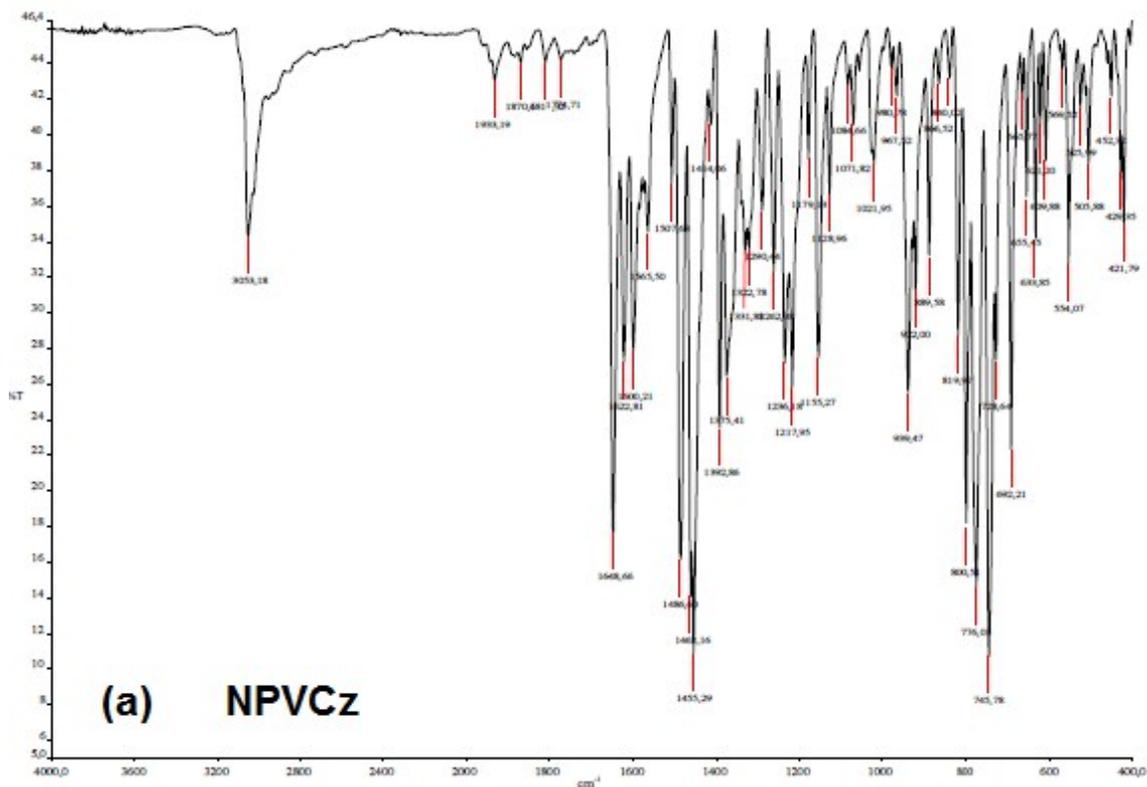
**Figure S11.** Effects of typical HTM, NPB, on (a) current density and luminance, (b) current efficiency- luminance-power efficiency, and (c) EL spectra of phosphorescent OLED devices. .14

**Figure S12.** Normalized luminance as a function of operational lifetime of solution-processed HTLs, NPVCz, DNPVCz, DPPVCz, and conventional NPB, based phosphorescent OLEDs. ....15





**Figure S1.** <sup>1</sup>H NMR spectra of HTMs, (a) NPVCz, (b) DNPVCz, and (c) DPPVCz.



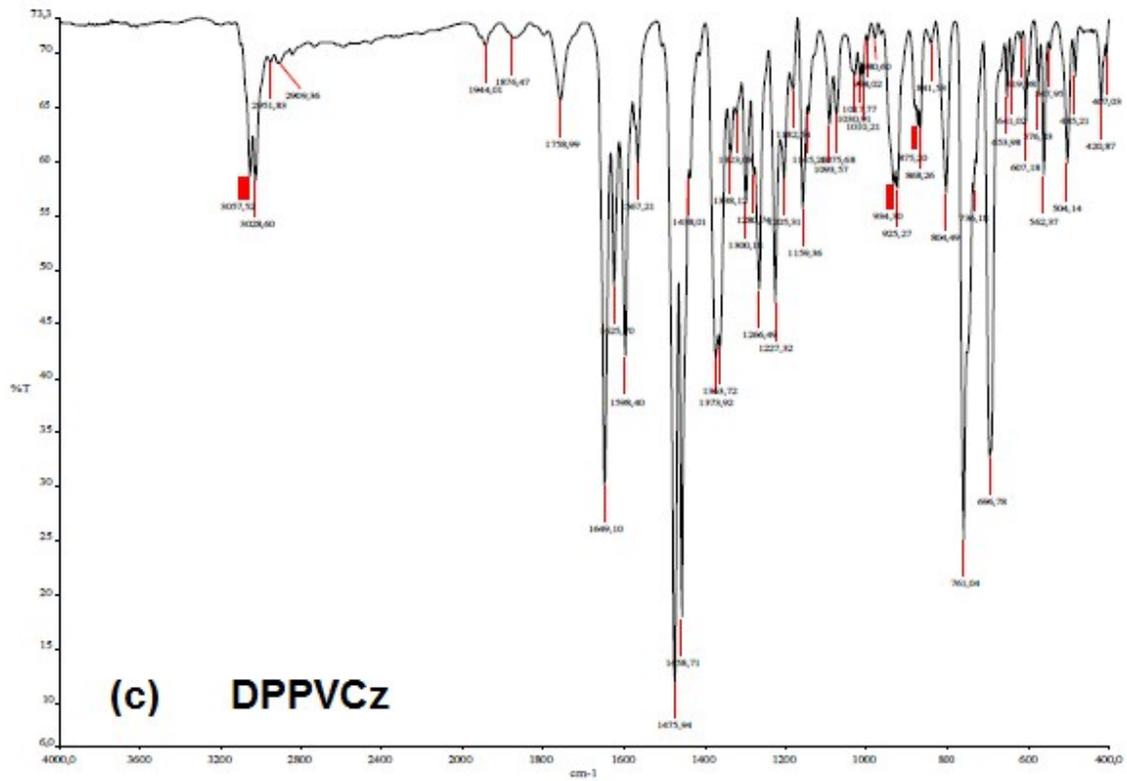


Figure S2. IR spectra of HTMs, (a) NPVCz, (b) DNPVCz, and (c) DPPVCz.

# MS-Flowinjection

## Analysis Info

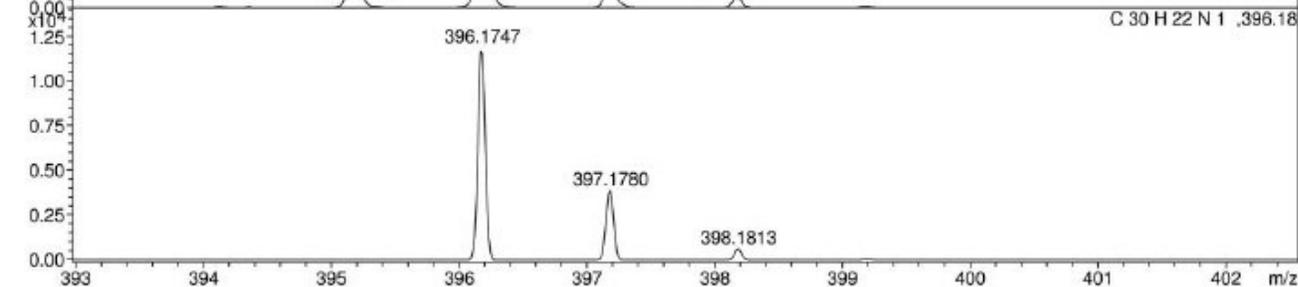
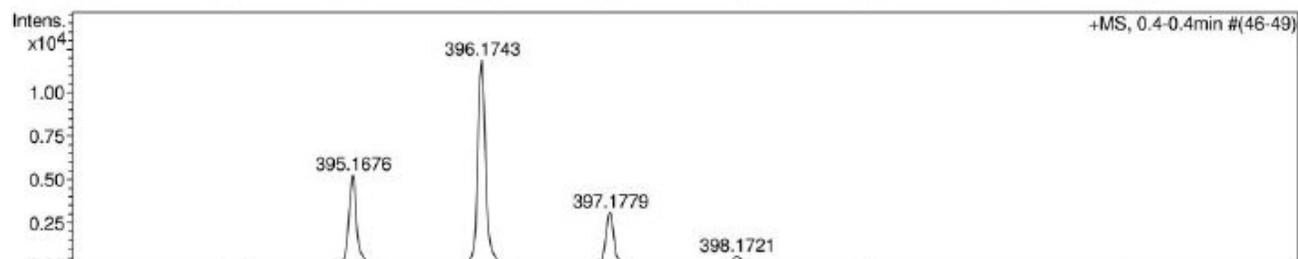
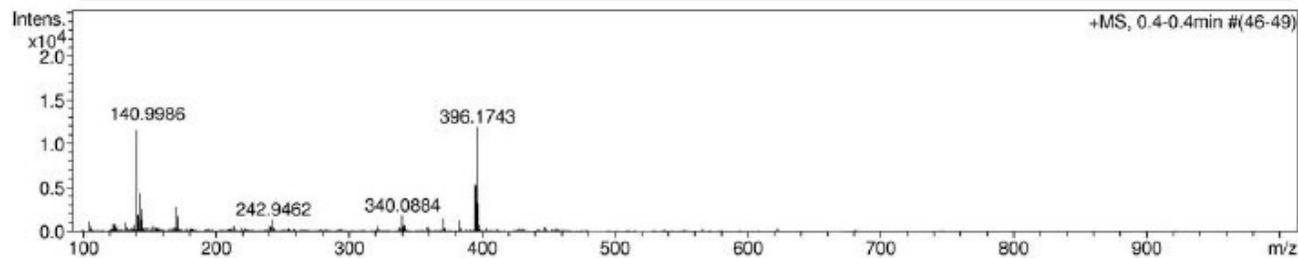
Analysis Name D:\Data\141112\mcrq13 APCI\_000002.d  
 Method APCI\_1min\_50\_bis\_1000\_posb\_Standardneu.m  
 Sample Name mcrq13 APCI  
 Comment APCI: Flowinjection.

Acquisition Date 12.11.2014 10:44:45

Operator ip  
 Instrument / Ser# micrOTOF 168

## Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	100 m/z	Set Capillary	4000 V	Set Dry Gas	5.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



## Generate Molecular Formula Parameter

Formula, min.	C30H22N				
Formula, max.					
Measured m/z	396.174	Tolerance	4 mDa	Charge	1
Check Valence	no	Minimum	0	Maximum	0
Nitrogen Rule	no	Electron Configuration both			
Filter H/C Ratio	no	Minimum	0	Maximum	3
Estimate Carbon	yes				

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdb	N Rule	e <sup>-</sup>
C 30 H 22 N 1	0.038	396.1747	1.01	2.15	0.40	20.50	ok	even

**Figure S3.** Mass-spectrum of NPVCz compound.

## MS-Flowinjection

### Analysis Info

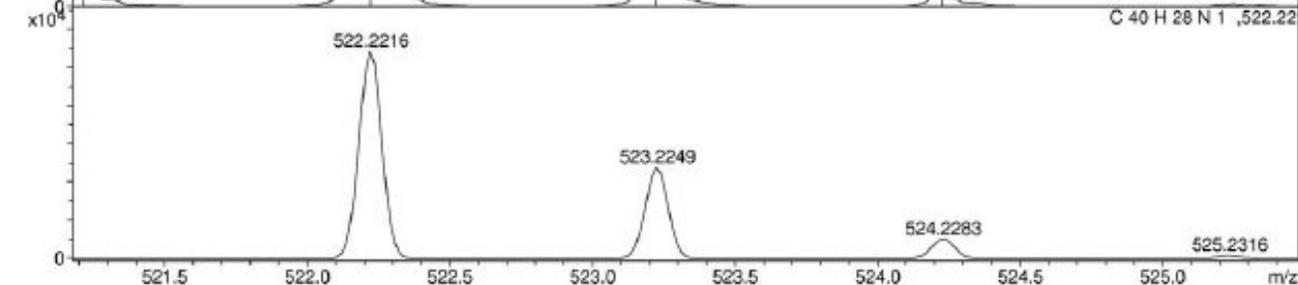
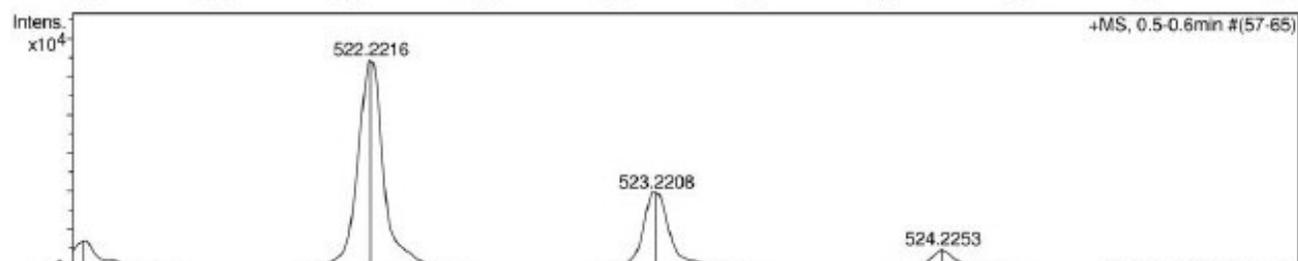
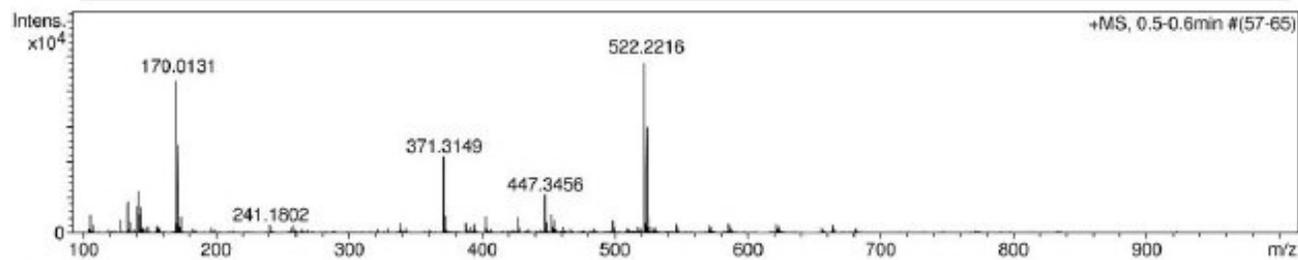
Analysis Name D:\Data\141112\mrcg32 APCI\_000001.d  
 Method APCI\_1min\_50\_bis\_1000\_posb\_Standardneu.m  
 Sample Name mrcg32 APCI  
 Comment APCI: Flowinjection.

Acquisition Date 12.11.2014 11:27:04

Operator ip  
 Instrument / Ser# micrOTOF 168

### Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	100 m/z	Set Capillary	4000 V	Set Dry Gas	5.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



### Generate Molecular Formula Parameter

Formula, min.	C40H28N				
Formula, max.					
Measured m/z	522.222	Tolerance	4 mDa	Charge	1
Check Valence	no	Minimum	0	Maximum	0
Nitrogen Rule	no	Electron Configuration	both		
Filter H/C Ratio	no	Minimum	0	Maximum	3
Estimate Carbon	yes				

Sum Formula	Sigma	m/z	Err (ppm)	Mean Err (ppm)	Err (mDa)	rdb	N Rule	e <sup>-</sup>
C 40 H 28 N 1	0.040	522.2216	-0.04	2.36	-0.02	27.50	ok	even

**Figure S4.** Mass-spectrum of DNPVCz compound.

# MS-Flowinjection

## Analysis Info

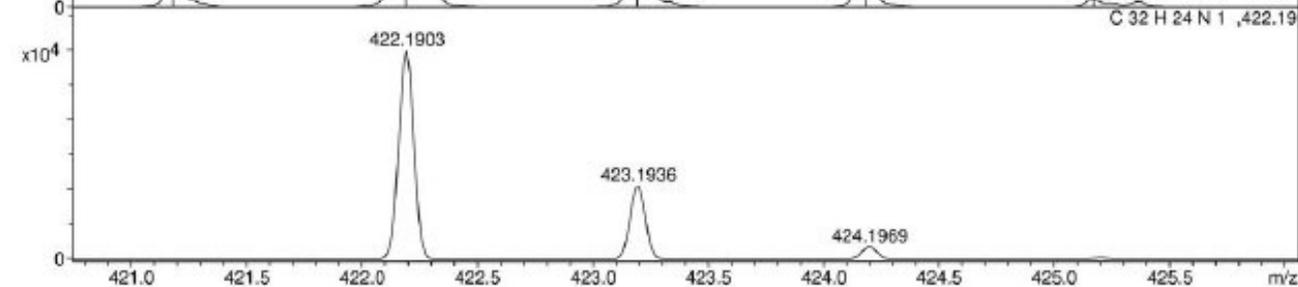
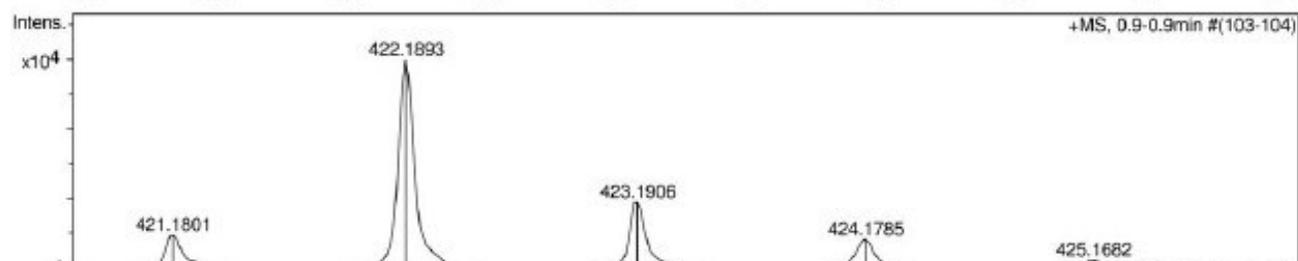
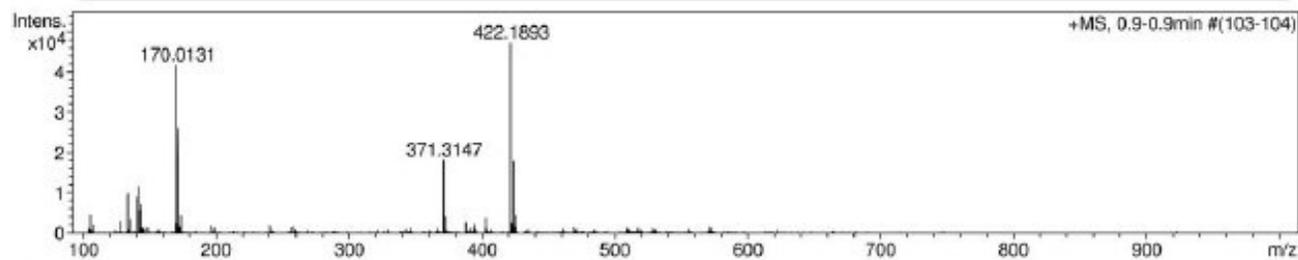
Analysis Name D:\Data\141112\mrcg31 APCI\_000001.d  
 Method APCI\_1min\_50\_bis\_1000\_posb\_Standardneu.m  
 Sample Name mrcg31 APCI  
 Comment APCI: Flowinjection.

Acquisition Date 12.11.2014 10:51:51

Operator ip  
 Instrument / Ser# micrOTOF 168

## Acquisition Parameter

Source Type	APCI	Ion Polarity	Positive	Set Nebulizer	3.0 Bar
Focus	Not active			Set Dry Heater	200 °C
Scan Begin	100 m/z	Set Capillary	4000 V	Set Dry Gas	5.0 l/min
Scan End	1000 m/z	Set End Plate Offset	-500 V	Set Divert Valve	Source



## Generate Molecular Formula Parameter

Formula, min.	C32H24N				
Formula, max.					
Measured m/z	422.189	Tolerance	4 mDa	Charge	1
Check Valence	no	Minimum	0	Maximum	0
Nitrogen Rule	no	Electron Configuration	both		
Filter H/C Ratio	no	Minimum	0	Maximum	3
Estimate Carbon	yes				

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	Err [mDa]	rdB	N Rule	e <sup>-</sup>
C 32 H 24 N 1	0.049	422.1903	2.35	6.46	0.99	21.50	ok	even

**Figure S5.** Mass-spectrum of DPPVCz compound.

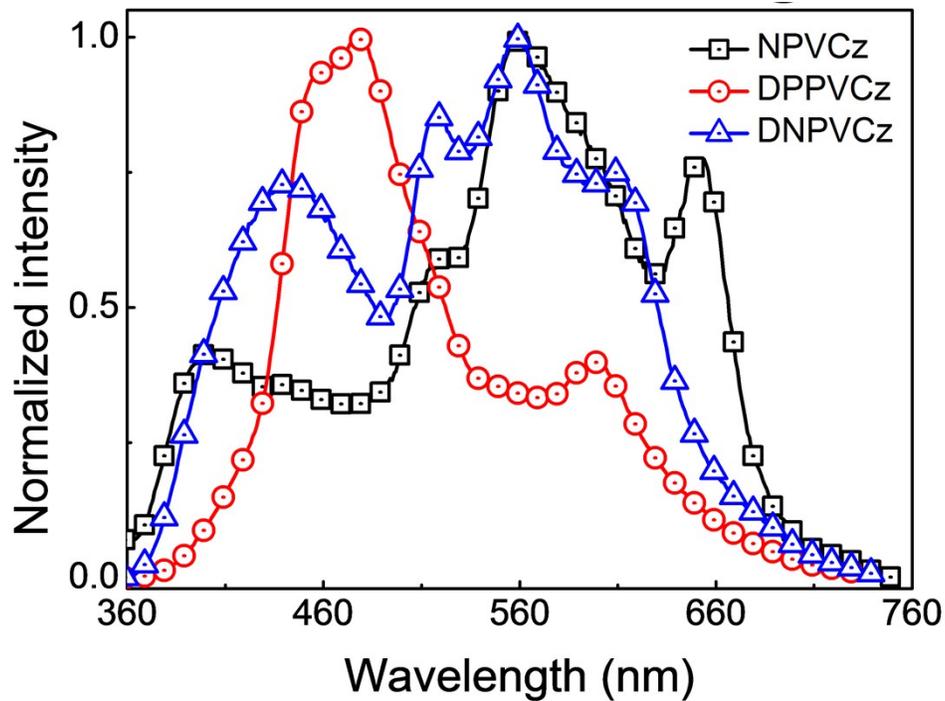


Figure S6. PL spectra of NPVCz, DPPVCz and DNPVCz, in THF solution at 77 K.

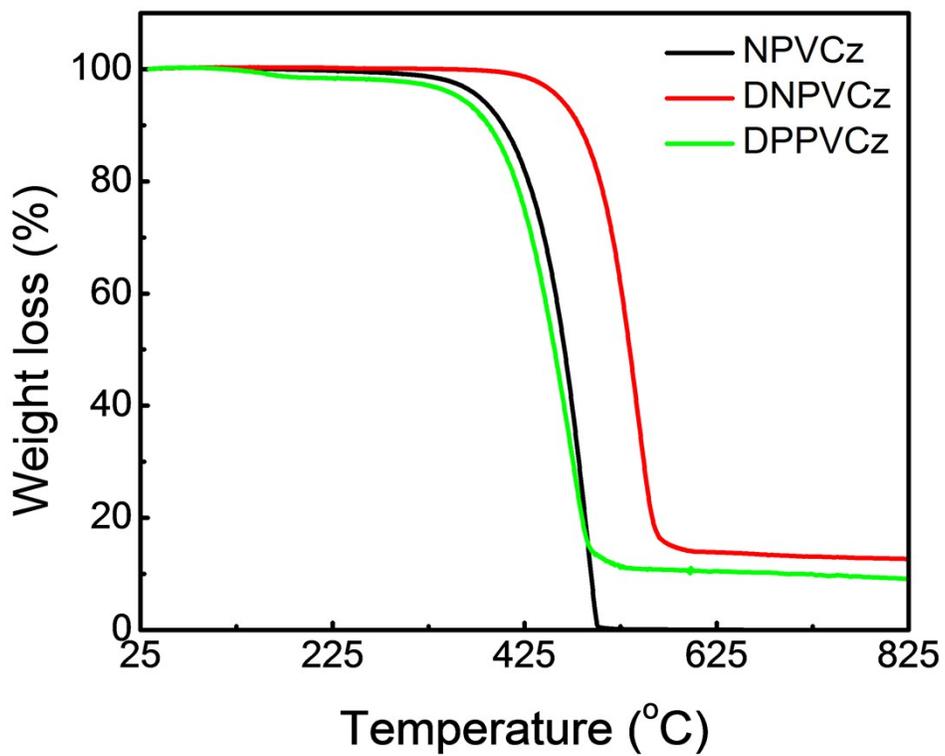
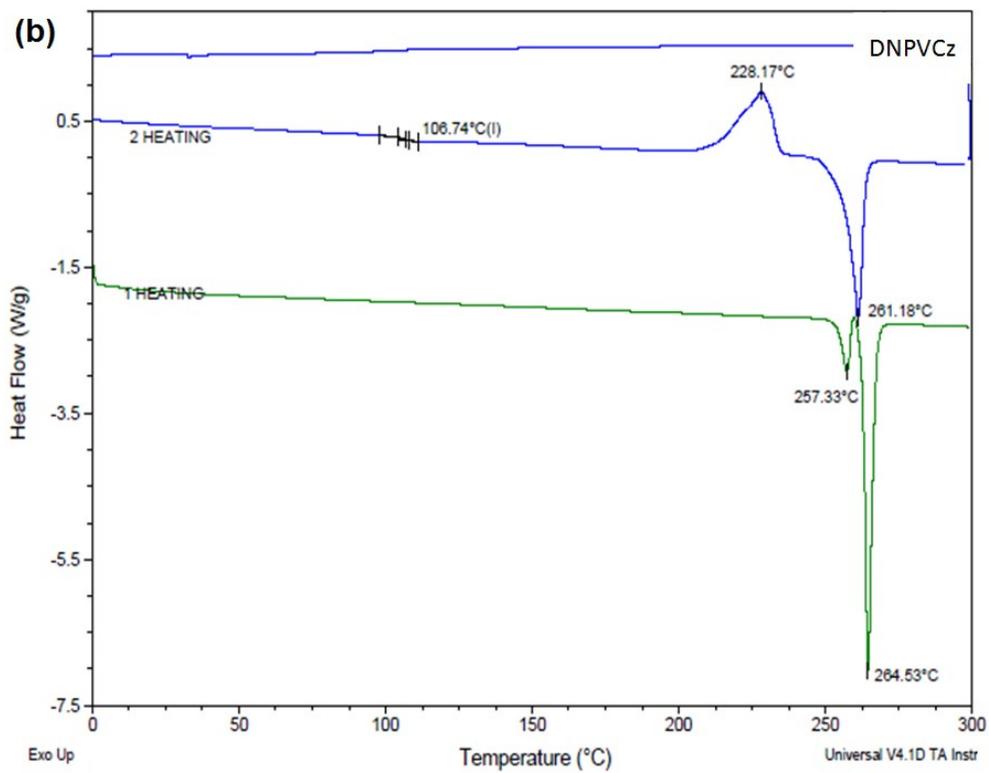
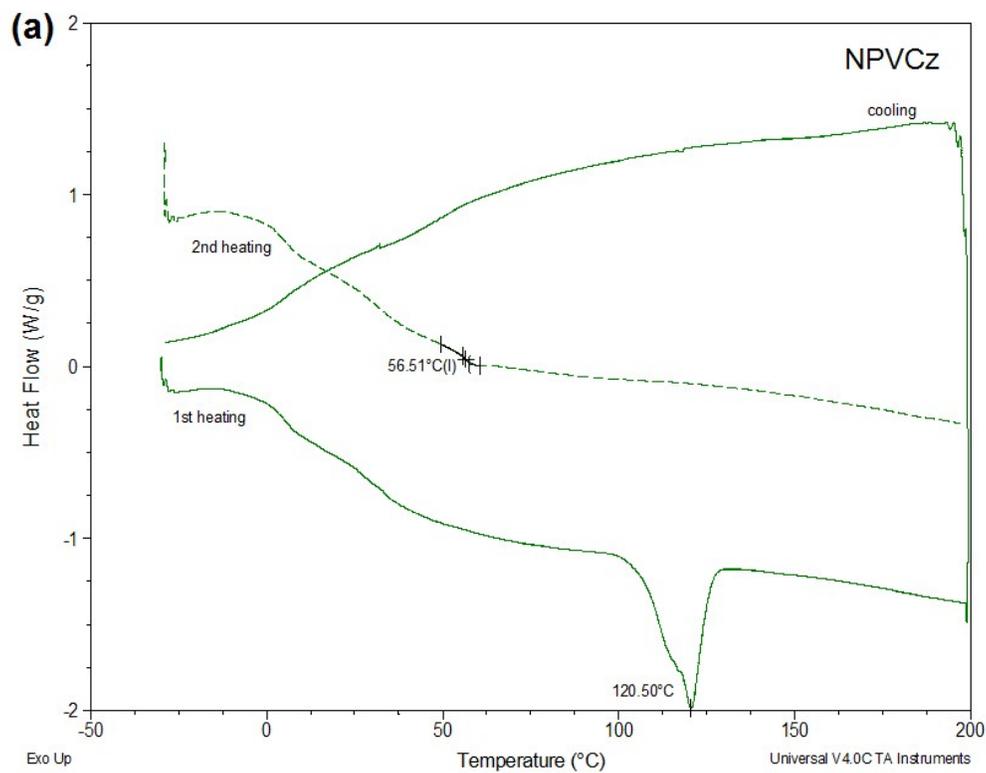


Figure S7. TGA plots of NPVCz, DNPVCz, and DPPVCz.



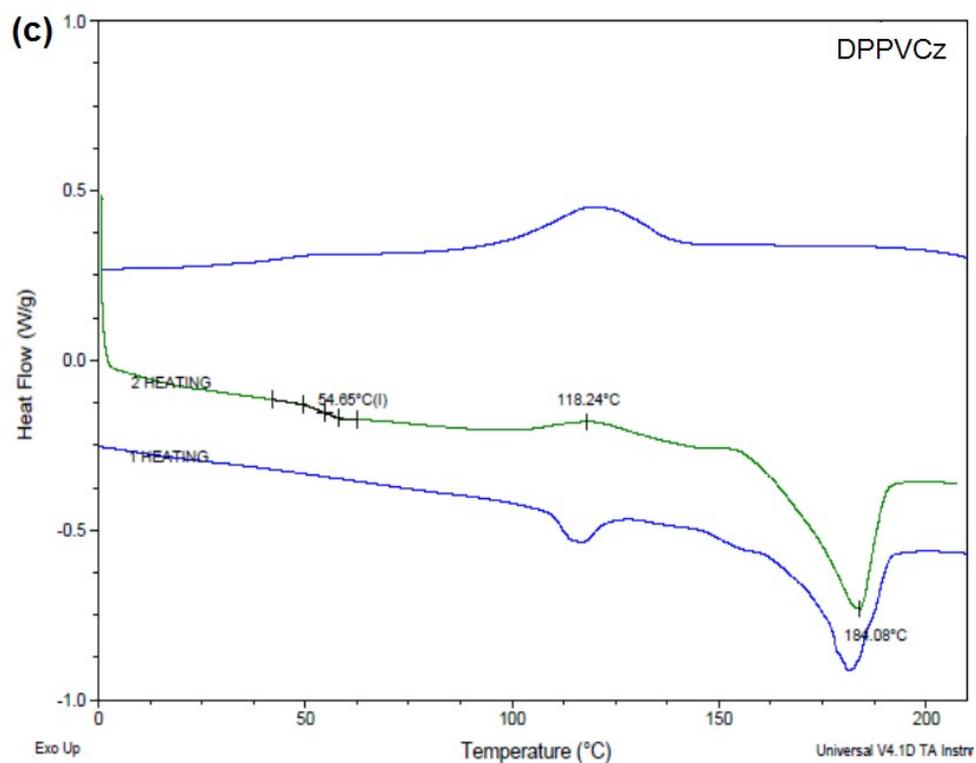
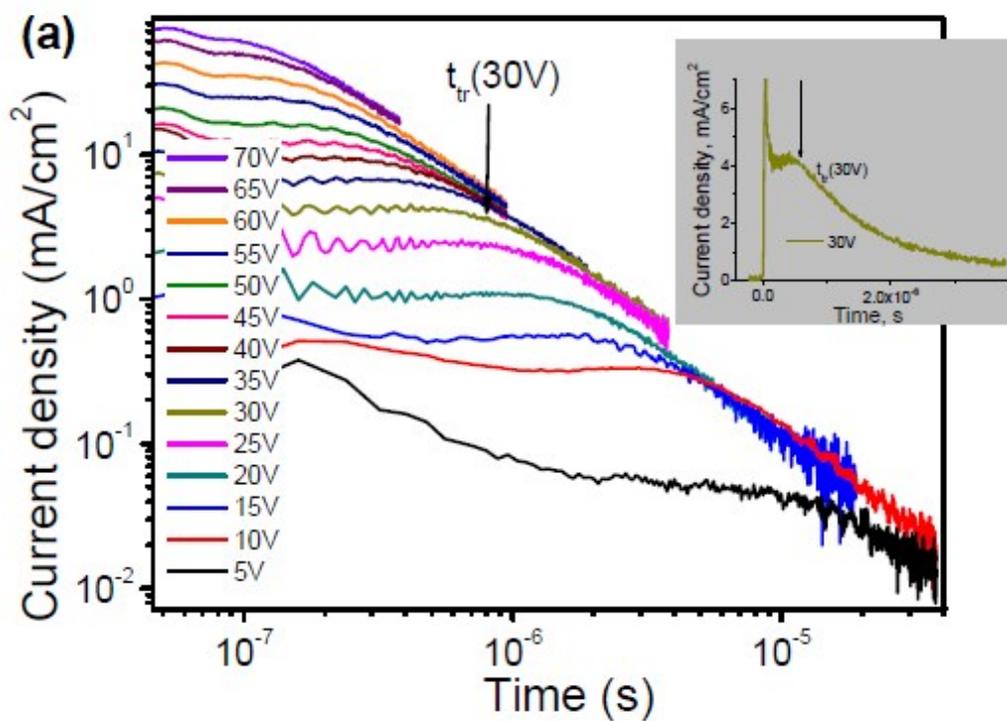
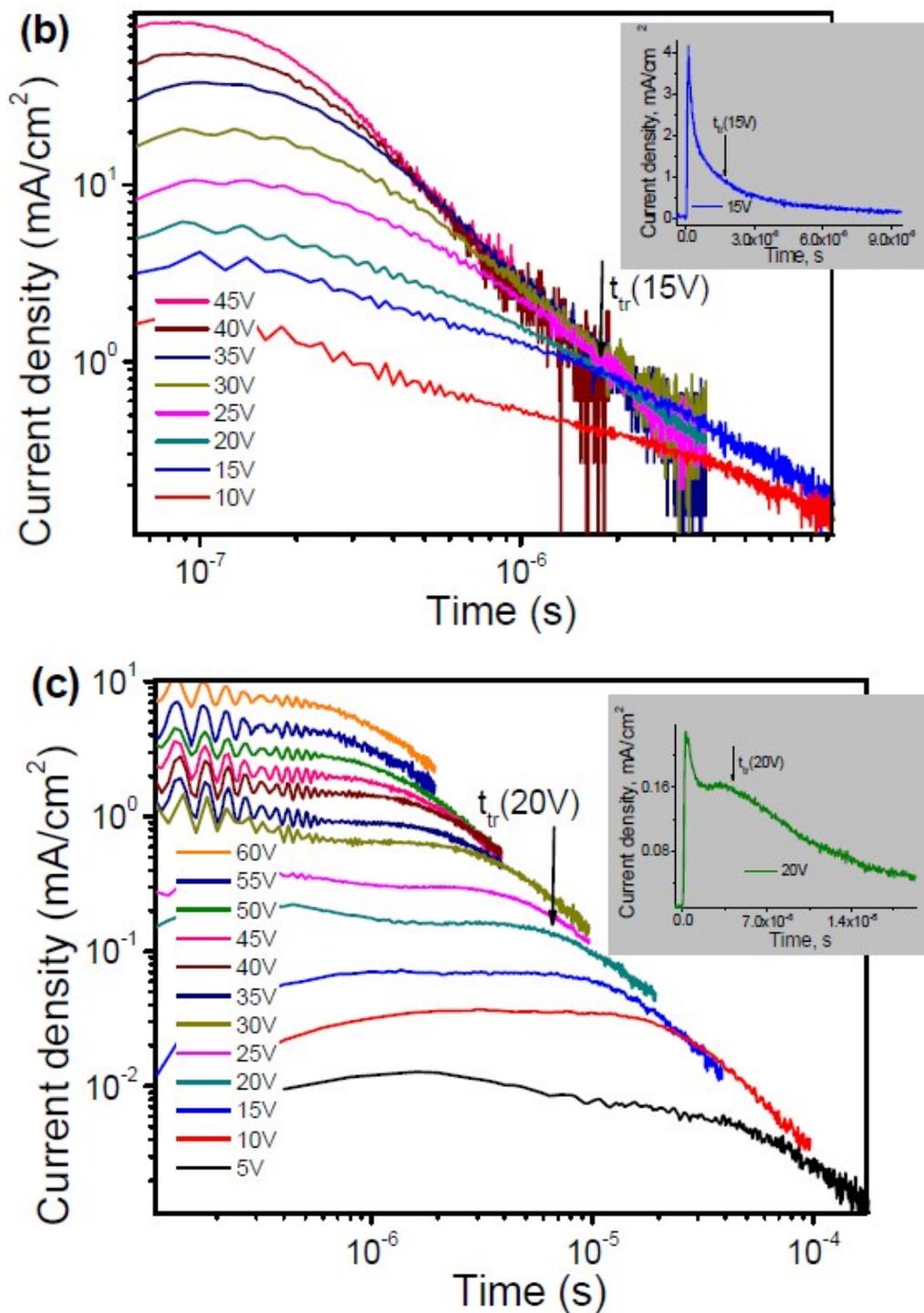
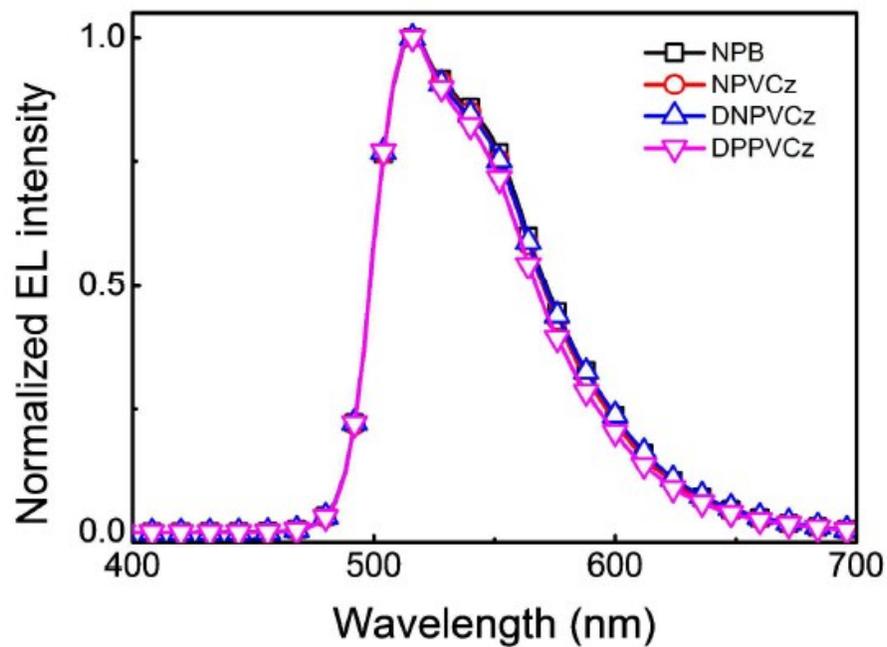


Figure S8. DSC curves of (a) NPVCz, (b) DNPVCz, and (c) DPPVCz.

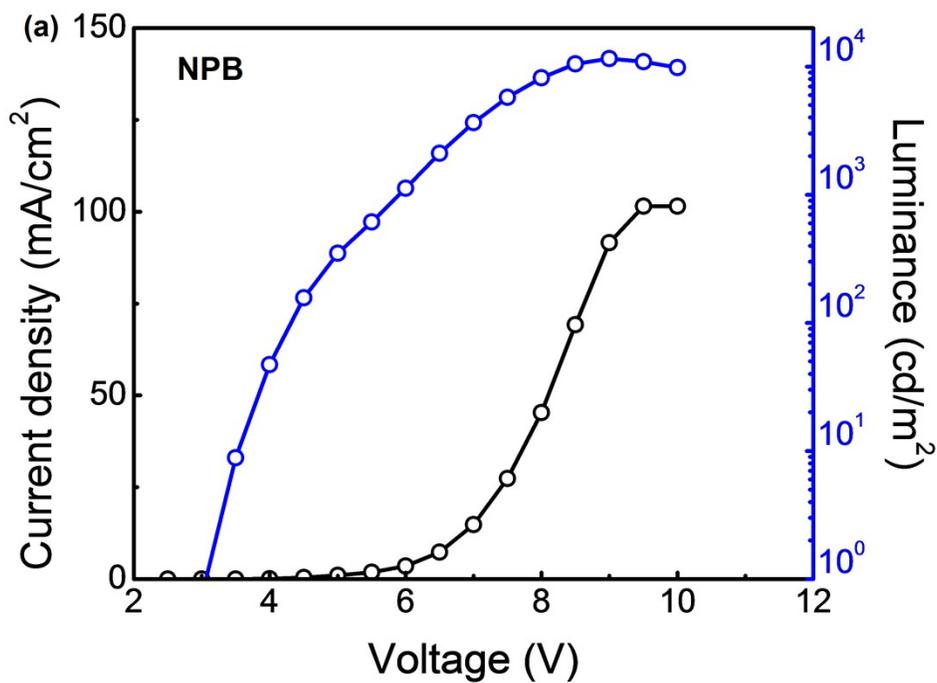


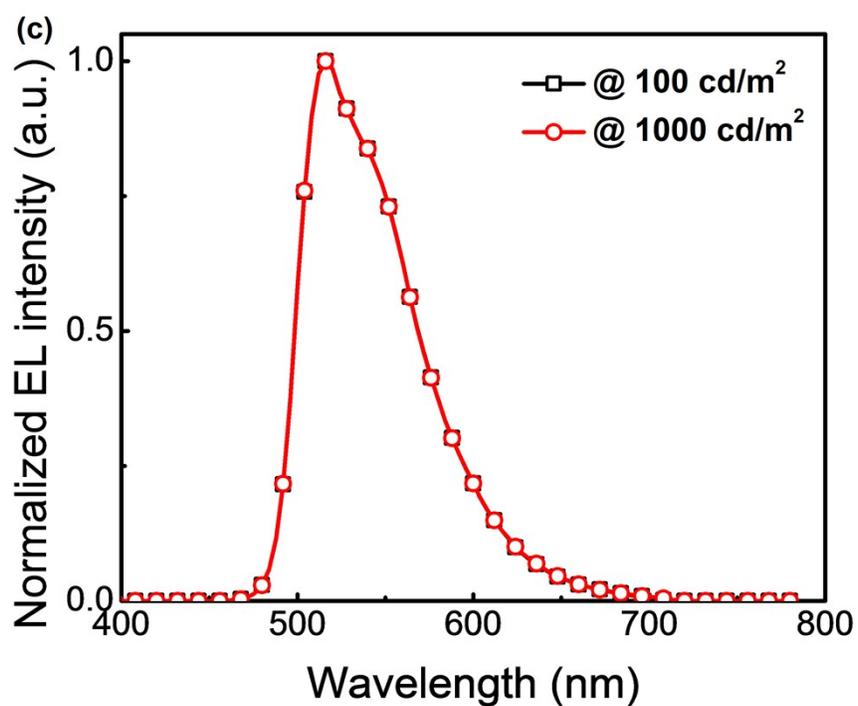
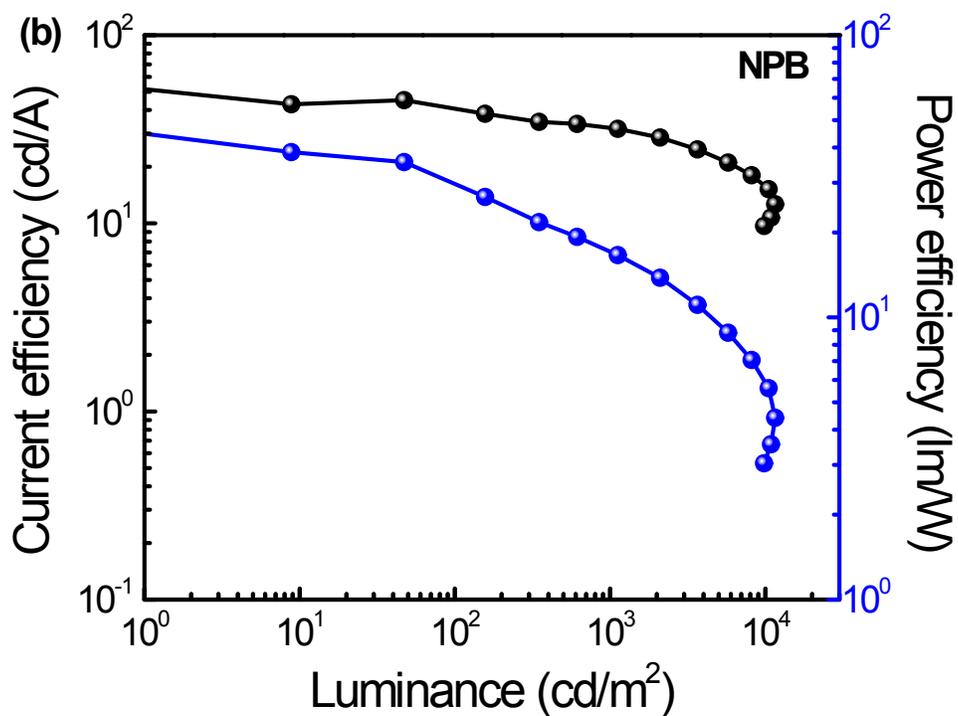


**Figure S9.** Double-logarithmic representation of transient photocurrents curves of the newly synthesized HTMs, (a) NPVCz, (b) DNPVCz, and (c) DPPVCz, and inset show the TOF transient curves.

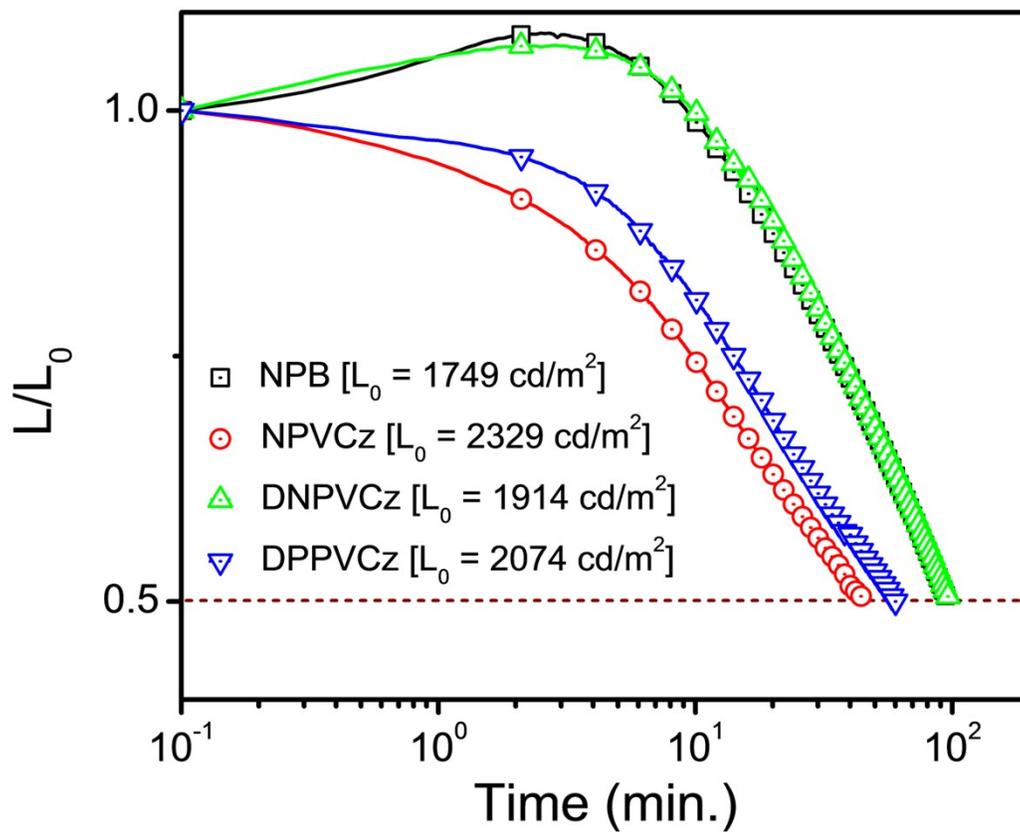


**Figure S10.** Effect of the HTMs, NPB, NPVCz, DNPVCz, and DPPVCz, on the EL spectra of fluorescent green OLED devices.





**Figure S11.** Effects of typical HTM, NPB, on (a) current density and luminance, (b) current efficiency- luminance-power efficiency, and (c) EL spectra of phosphorescent OLED devices.



**Figure S12.** Normalized luminance as a function of operational lifetime of solution-processed HTLs, NPVCz, DNPVCz, DPPVCz, and conventional NPB, based phosphorescent OLEDs.