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Supporting Information

Supramolecular Assembly of Dipeptide Functionalized Benzo[ghi]perylene Monoimide Directs White Light Emission via Donor-Acceptor Interactions

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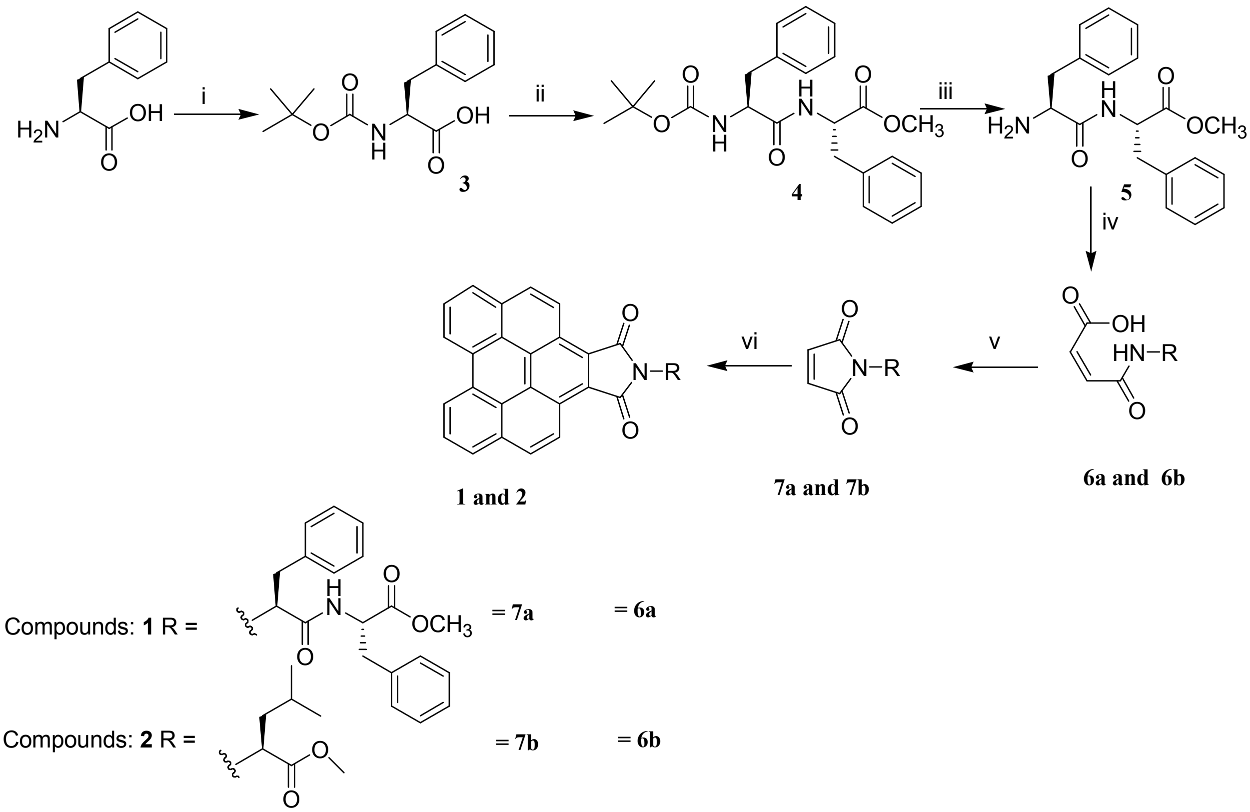
1. Synthetic Scheme



Scheme S1. Synthesis of *N*-dipeptide functionalized benzo[*ghi*]perylene-1,2-dicarboxylic monoimide. (i) Boc-anhydride, 1,4 dioxane, Na_2CO_3; (ii) phenylalanine methyl ester, HOBt/DIPC, DMF; (iii) TFA; (iv) maleic anhydride, EtOAc; (v) $ZnCl_2$/HMDS, benzene, 80 °C; (vi) perylene, *p*-chloranil, 240 °C, 3h.

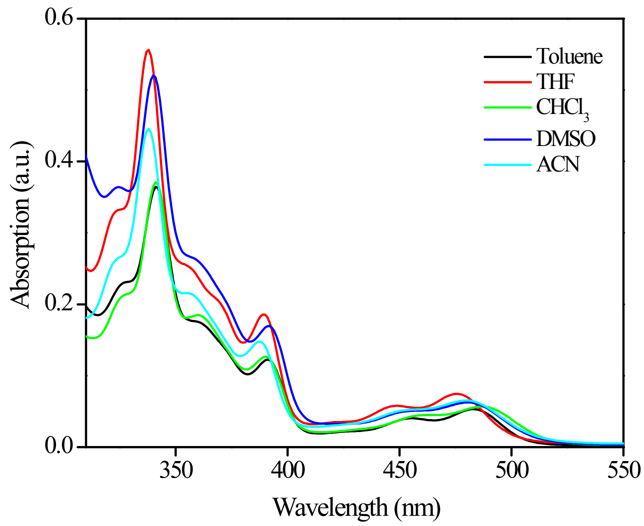


Figure S1. UV-Visible spectra of BPI-FF-OMe in different solvents listed from Table 1.

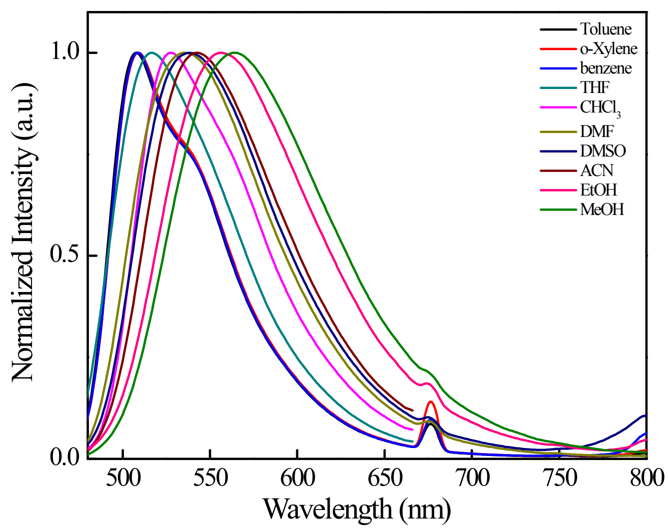


Figure S2: Normalized fluorescence spectra of BPI-FF-OMe in various nonpolar to polar solvents listed in Table 1.

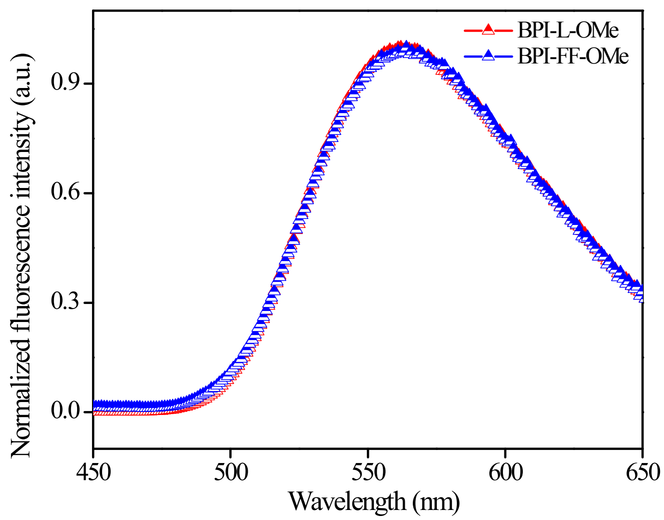


Figure S3: Normalized fluorescence spectra of BPI-FF-OMe and BPI-L-OMe in methanol.

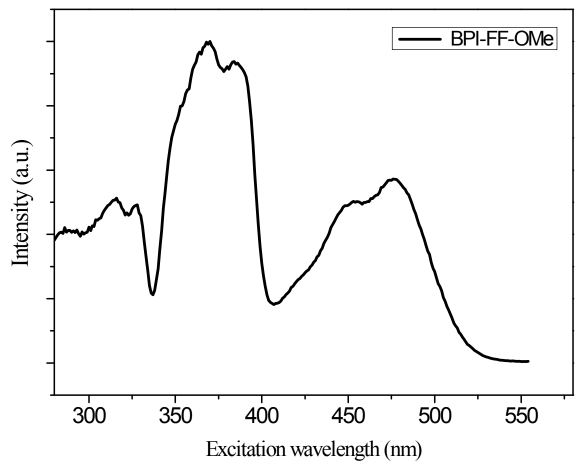


Figure S4. Fluorescence excitation spectra of donor BPI-FF-OMe in methanol (emission wavelength 564 nm).

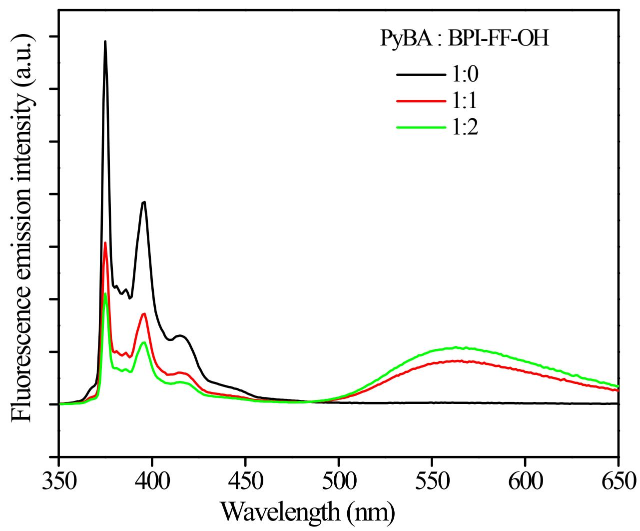


Figure S5: Fluorescence spectra of BPI-FF-OMe with equimolar mixture of PyBA cover various emission wavelength for white light emission.

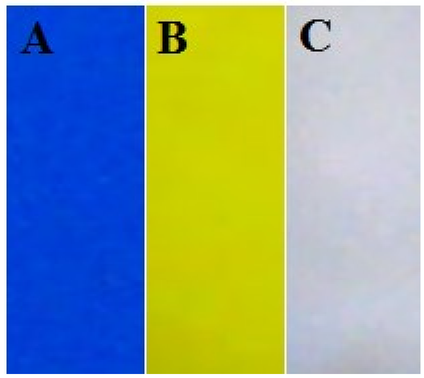


Figure S6. Optical images show solid state (thin film) blue, yellow and white emission when solution of PyBA, BPI-FF-OMe and mixture (10:1) of PyBA and BPI-FF-OMe coated over silica plate and subsequent illumination under UV lamp at 365 nm.

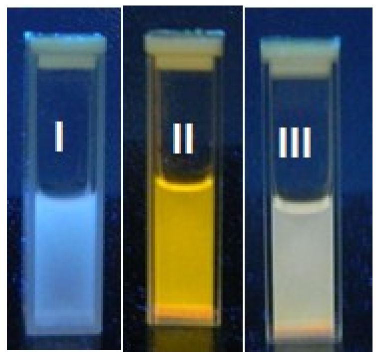


Figure S7. Optical images show blue, yellow and white emission of solution of PyBA, BPI-L-OMe and mixture (10:1) of PyBA and BPI-L-OMe upon illumination under UV lamp at 365 nm.

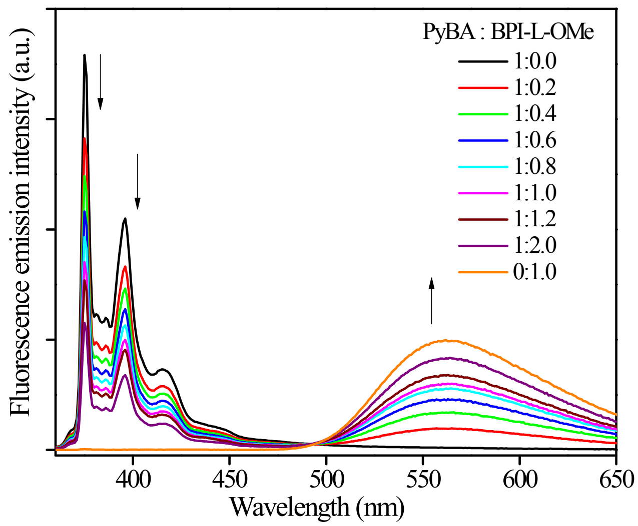


Figure S8. A) Fluorescence spectra of (1×10^{-6} mol L^{-1}) of PyBA, BPI-L-OMe and mixture of different equivalents of PyBA and BPI-L-OMe in methanol.

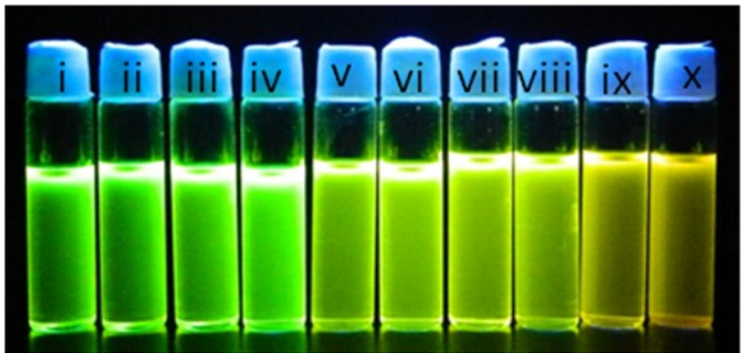
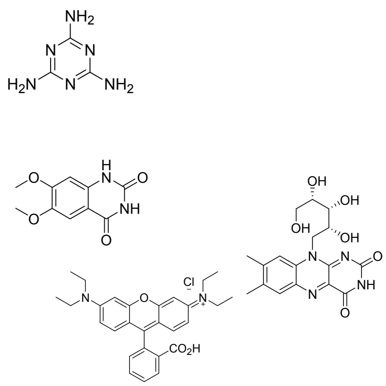
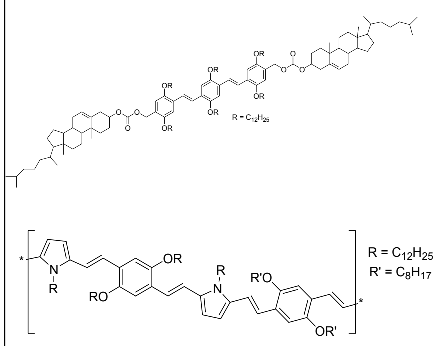
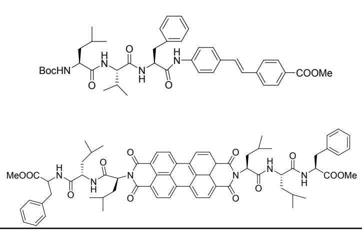
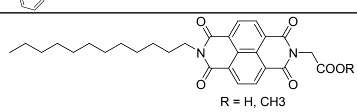
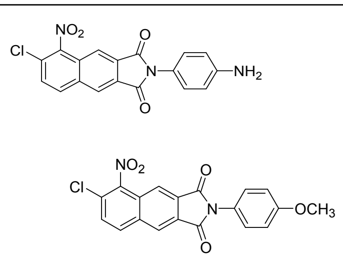
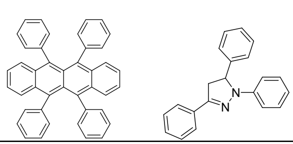
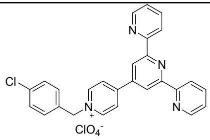
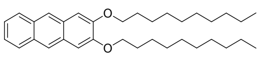
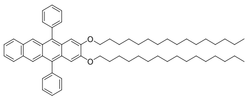
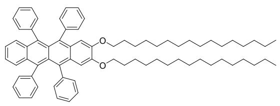
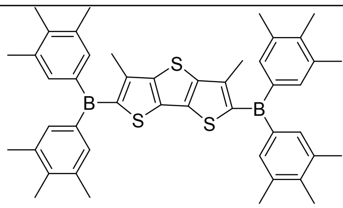
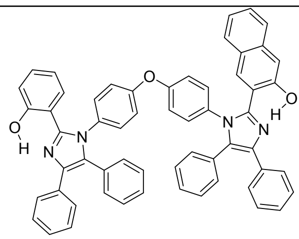
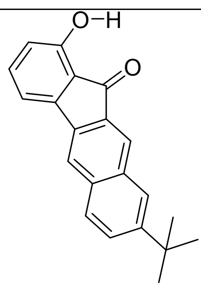
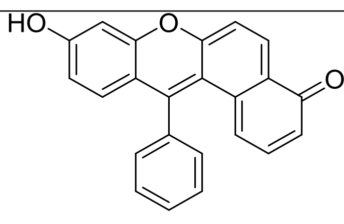
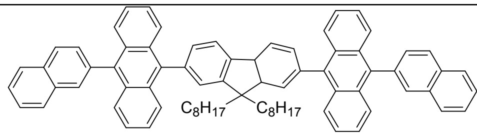
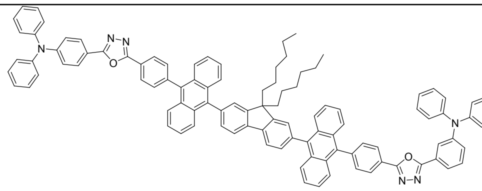
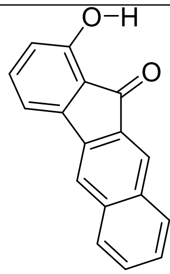
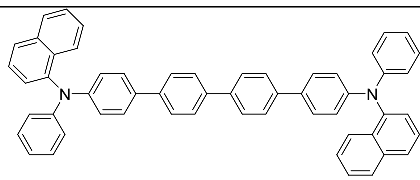
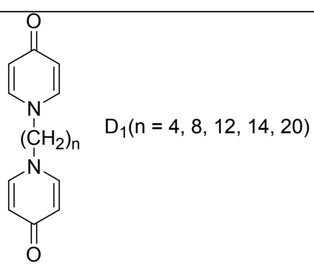
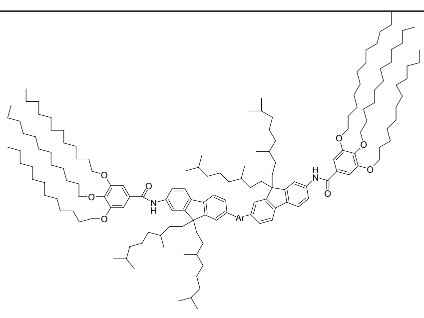


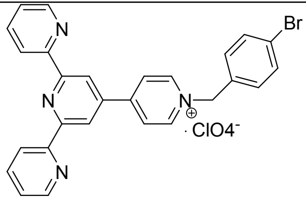
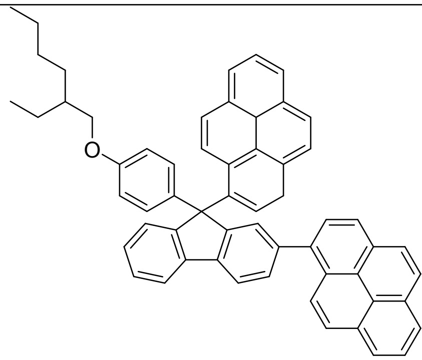
Figure S9. Optical images of BPI-FF-OMe in different solvents listed in Table 1 upon illumination under UV lamp at 365 nm.

Table S1: Reports on the white light emitting materials.

	Molecular structure	Purpose	Reference
1		White light emission	*ACS Appl. Mater. Interfaces* 2013, **5**, 5478−5485
2		White light emission	*Adv.Mater.* 2009, **21**, 2059–2063.
3		White light emission	*Chem. Commun.*, 2013, **49**, 6909-6911.
4		White light emission	*Chem. Eur. J.* 2012, **18**, 1290-1294.
5		White light emission	*Chem. Commun.,* 2010, **46**, 8002–8004.
6		White light emission	*Adv. Mater.* 2008, **20**, 79-83

7		White light emission	*Chem. Commun.*, 2014, **50**, 15878-15881
8	  	White light emission	*J. Phys. Chem. C* 2012, **116**, 21706-21716
9		White light emission	*Adv. Mater.*, 2005, **17**, 34-39
10		White light emission	*J. Am. Chem. Soc.*2009, **131**, 14043-14049.
11		White light emission	*International Journal of Photoenergy*, 2014
12		White light emission	*J. Am. Chem. Soc.*2006, **128**, 14081-14092,

13		White light emission	*J. Mater. Chem.*, 2011, **21**, 12969-12976.
14		White light emission	*J. Phys. Chem. C* 2011, **115**, 17965-17972
15		White light emission	*J. Am. Chem. Soc.* 2011, **133**, 17738-17745
16		White light emission	*Adv. Mater.* 2007, **19**, 3672-3676
17		White light emission	*Angew. chem.* 2014, **126**, 4660-4665.
18		White light emission	*Chem. Eur. J.* 2009, **15**, 9737- 9746.

19		White light emission	*J. Mater. Chem. C*, 2015, **3**, 4563-4569.
20		White light emission	*J. Phys. Chem. C* 2009, **113**, 4641-4647
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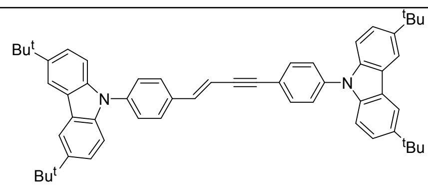
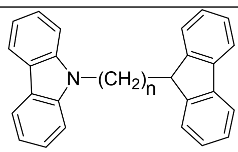
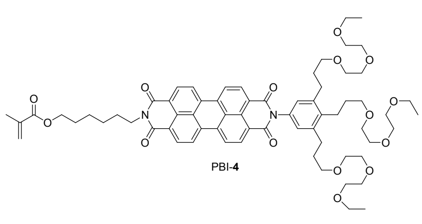
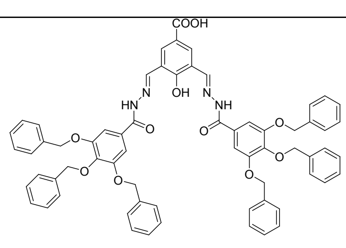
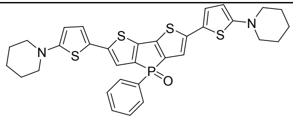
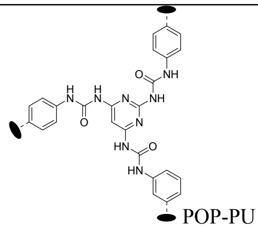
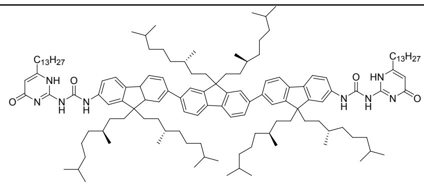
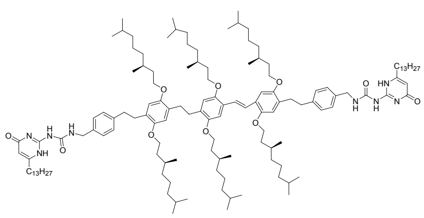
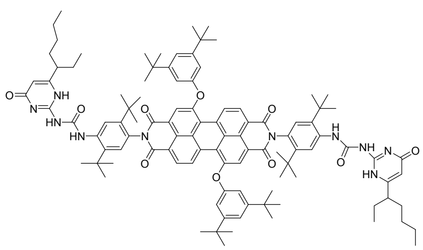
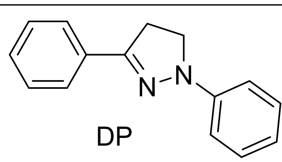
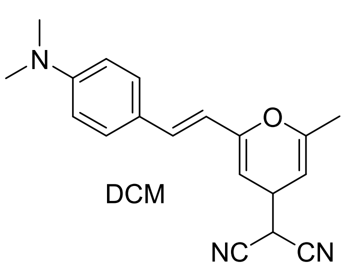
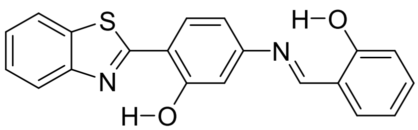
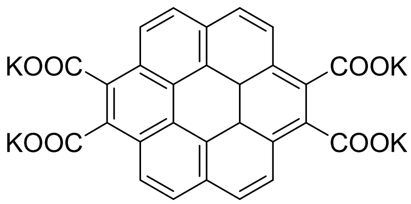
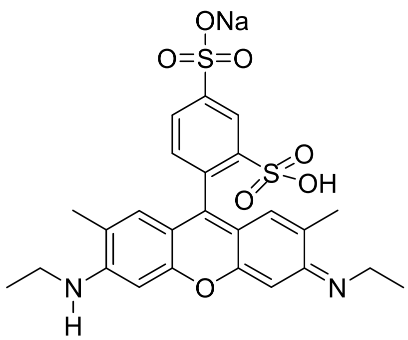
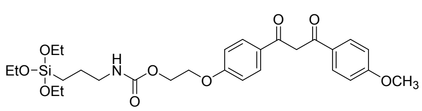
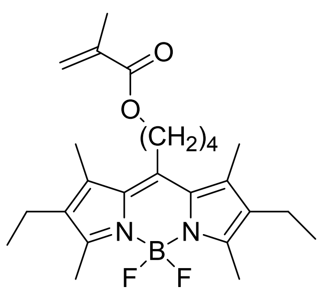
23		White light emission	*J. Am. Chem. Soc.*2006, **128**, 5592-5593
24	 n = 2, 3, 6: BCz **1**, **2**, **3** 	White light emission	*Chem. Commun.*, 2013, **49**, 8178-8180.
25		White light emission	*Chem. Commun.,* 2015, **51**, 2130-2133

26		White light emission	*Chem. Commun.*, 2013, **49**, 4899-4901
27		White light emission	*ACS Appl. Mater. Interfaces* 2014, **6**, 22569−22576
28	  	White light emission	*J. Am. Chem. Soc.* 2009,**131**, 833-843.
29	 	White light emission	*J. Am. Chem. Soc.*2010, **132**, 1742–1743

30		White light emission	*Phys. Chem. A* 2009, **113**, 5888–5895
31	 	White light emission	*Adv. Mater.* 2013, **25**, 1713–1718
32	 	White light emission	*J. Mater. Chem. C,* 2013, **1**, 4437–4444

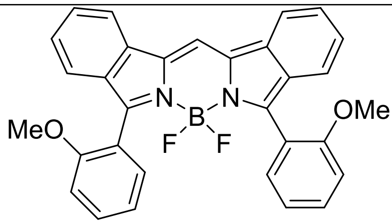
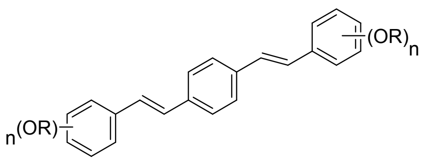
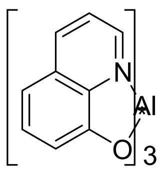
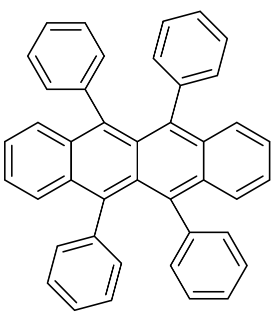
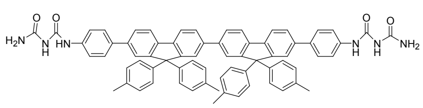
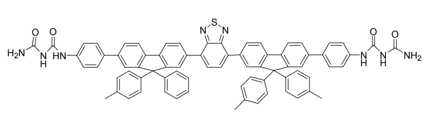
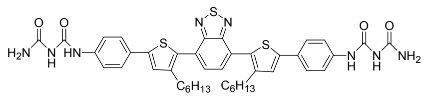
			
33	  	White light emission	*Angew. Chem. Int. Ed.* 2012, **51**, 3391 –3395
34	  	White light emission	*Angew. Chem. Int. Ed.* 2011, **50** , 7032 –7036

Table S2. DLS characterization of BPI-FF-OH nanospheres in toluene and methanol

#	Solvent	d_h/nm[a]	PD1[b]	ξ/mV[c]
1	Methanol	613	0.30	-17.97
2	Toluene	857	0.47	-25.89

[a]d_h is the hydrodynamic diameter. [b]PDI is the polydispersity index. [c]ξ is the zeta potential.

The Lippert-Mataga Equation

Equation 3 is a simplified from equation 2.

$$\bar{\nu}_{abs} - \bar{\nu}_{em} = \frac{2}{hc}\left(\frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{n^2 - 1}{2n^2 + 1}\right)\frac{(\mu_e - \mu_g)^2}{\rho^3} + C \quad (2)$$

$$\Delta\bar{\nu} = \frac{2\Delta f}{4\pi\varepsilon_0 hc\rho^3}(\mu_e - \mu_g)^2 + C \quad (3)$$

$\Delta\bar{\nu} = \bar{\nu}_{abs} - \bar{\nu}_{em}$ is the solvatochromic shift or Stokes shift (in cm^{-1}) between the absorbance and emission maxima $[\bar{\nu}_{abs} = 1/\lambda_{abs}(max), \bar{\nu}_{em} = 1/\lambda_{em}(max)]$. $\Delta f = [(\varepsilon - 1/2\varepsilon + 1) - (n^2 - 1/2n^2 + 1)]$ is solvent polarizability parameter, which is described by solvent's dielectric constants(ε) and refractive indices(n). ρ represents radius of solvated cavity of dipole. μ_e and μ_g are the dipole moments of a dye both in excited and ground states respectively. The Lippert - Mataga expression of Stokes shift strongly depends on the change of dipole moment of a dye upon excitation $(\Delta\mu_{ge} = \mu_e - \mu_g)$ and the size of the cavity radius (ρ). ε_0 denotes dielectric constant of vacuum. h and c are Plank's constant and velocity of light respectively. C is a constant.

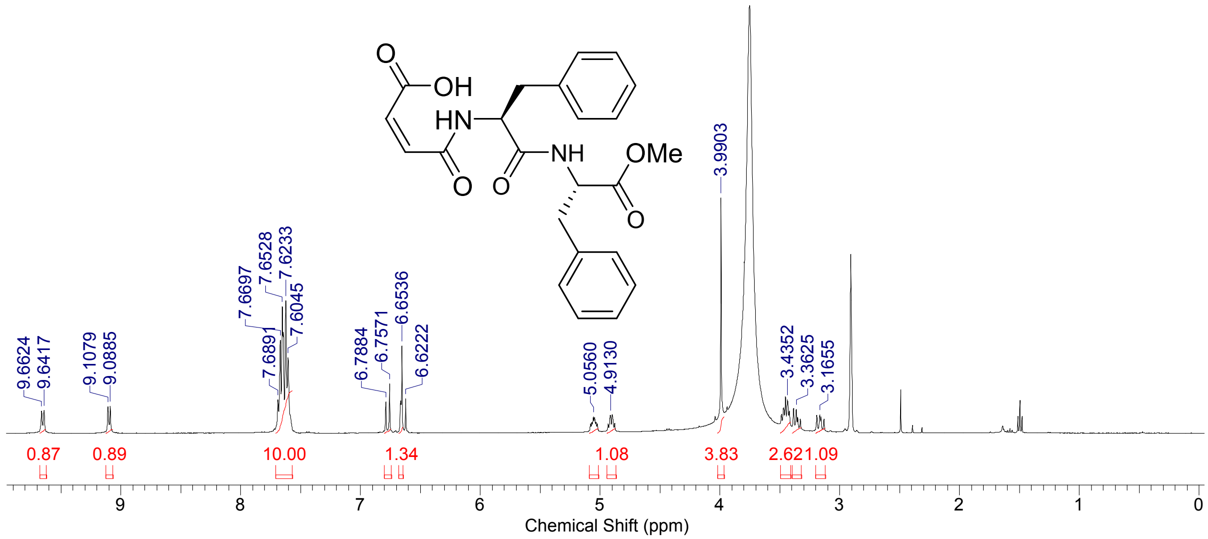


Figure S10: ^{1}H NMR spectrum (400 MHz, DMSO-d$_6$) for *N*-maleyl-L-Phe(1)-L-Phe(2)-OMe **5.**

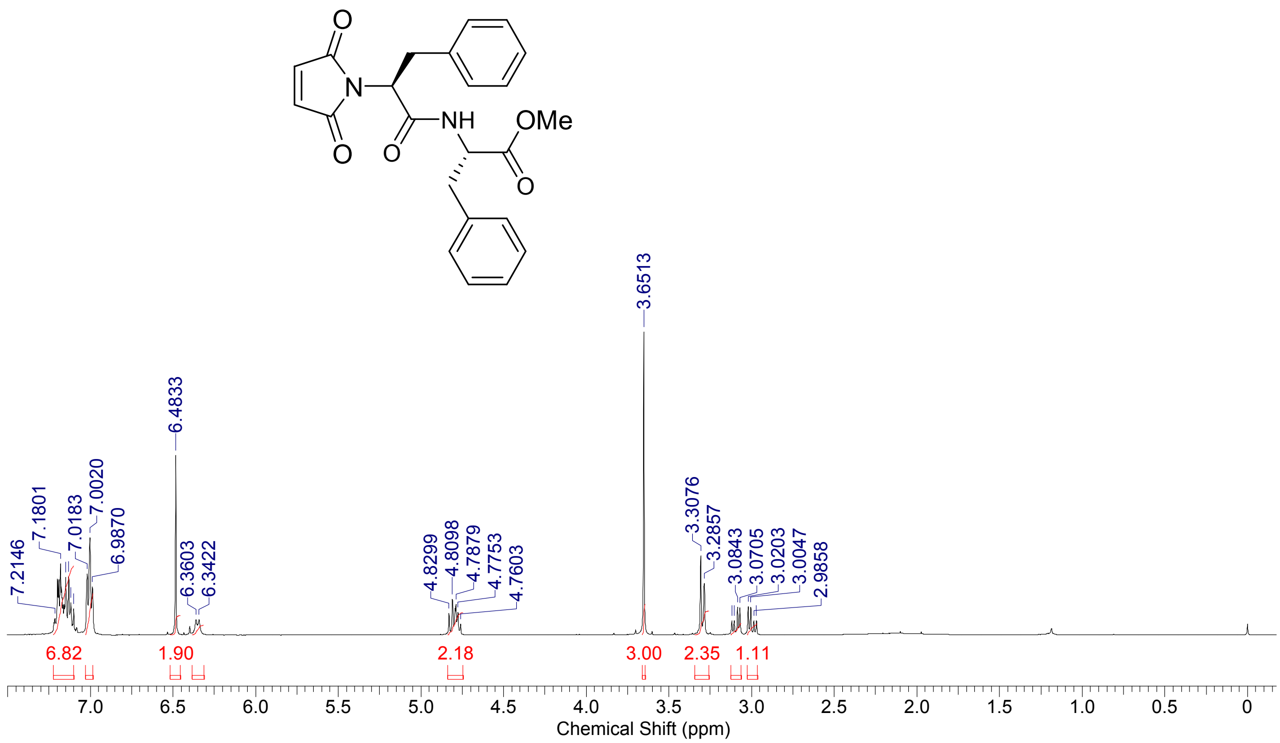


Figure S11: ^{1}H NMR spectrum (400 MHz, $CDCl_3$) for *N*-maleoyl-L-Phe(1)-L-Phe(2)-OMe **6.**

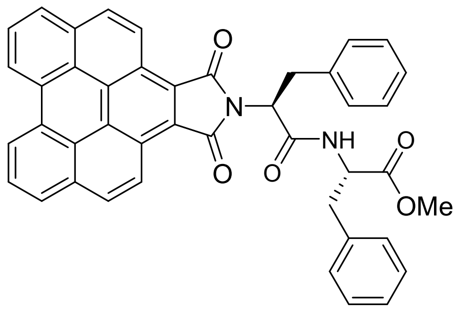
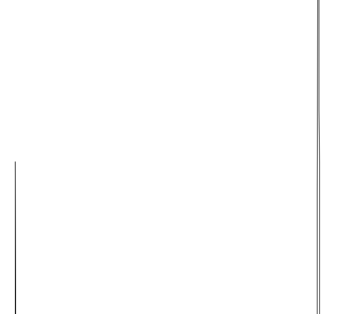


Figure S12: ^{1}H NMR spectrum (400 MHz, $CDCl_3$) for benzo[ghi]perylene-1,2-dicarboxylic(L-Phe-L-Phe-OMe)imide **1.**



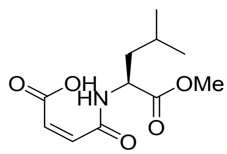
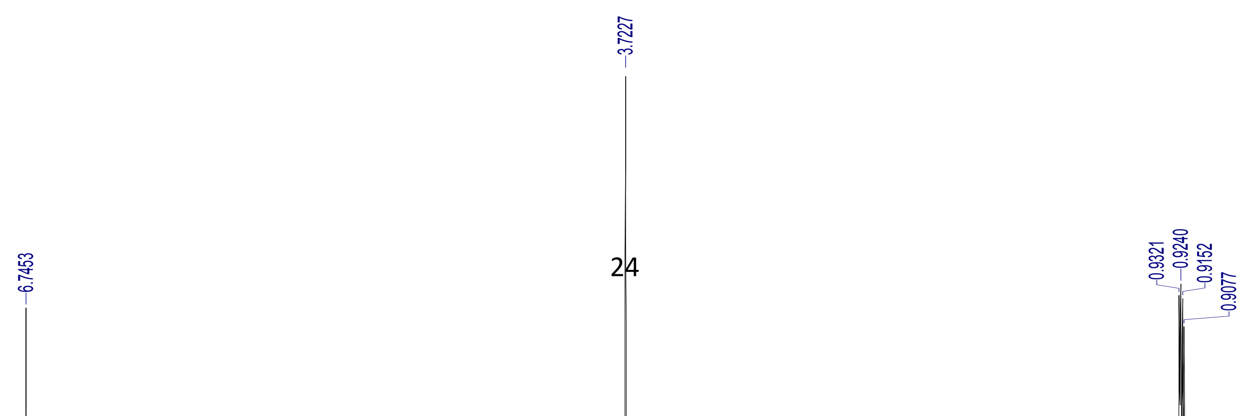


Figure S13: ^{1}H NMR spectrum (400 MHz, DMSO-d$_6$) for maleyl-Leu-OMe .



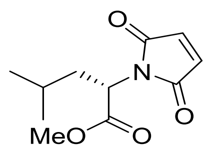


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Figure S14: ^{1}H NMR spectrum (400 MHz, $CDCl_3$) for maleoyl-L-Leu-OMe.

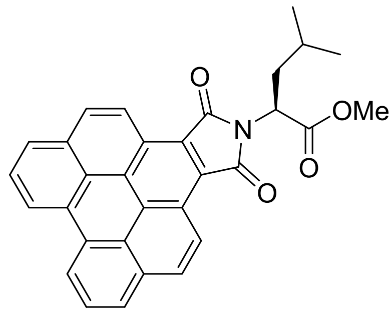

Figure S15: ^{1}H NMR spectrum (400 MHz, $CDCl_3$) for benzo[ghi]perylene-1,2-dicarboxylic(L-Leu-OMe)imide.

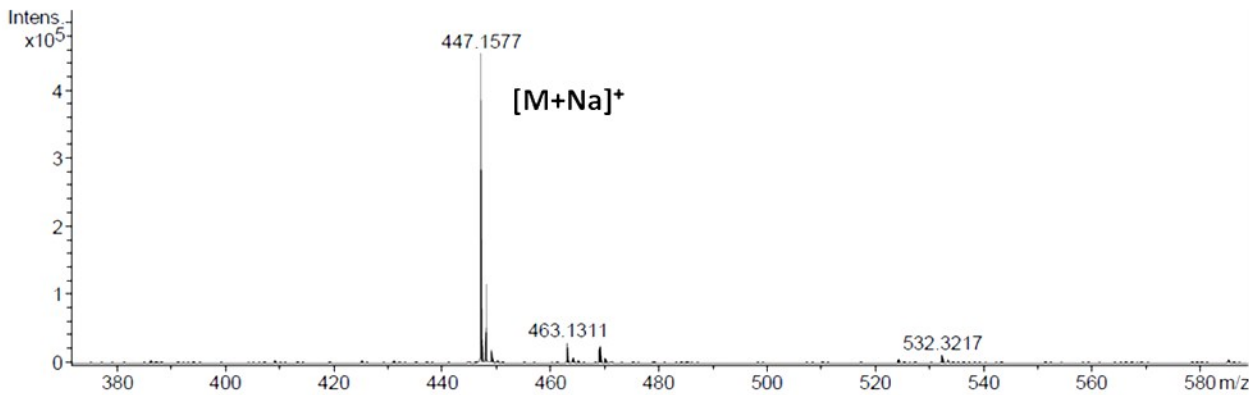

Figure S17: Mass spectra of *N*-maleyl-L-Phe(1)-L-Phe(2)-OMe **5**. The peak m/z $(M + Na)^+$ = 447.1577 corresponds to the synthesis of *N*-maleyl-L-Phe(1)-L-Phe(2)-OMe.

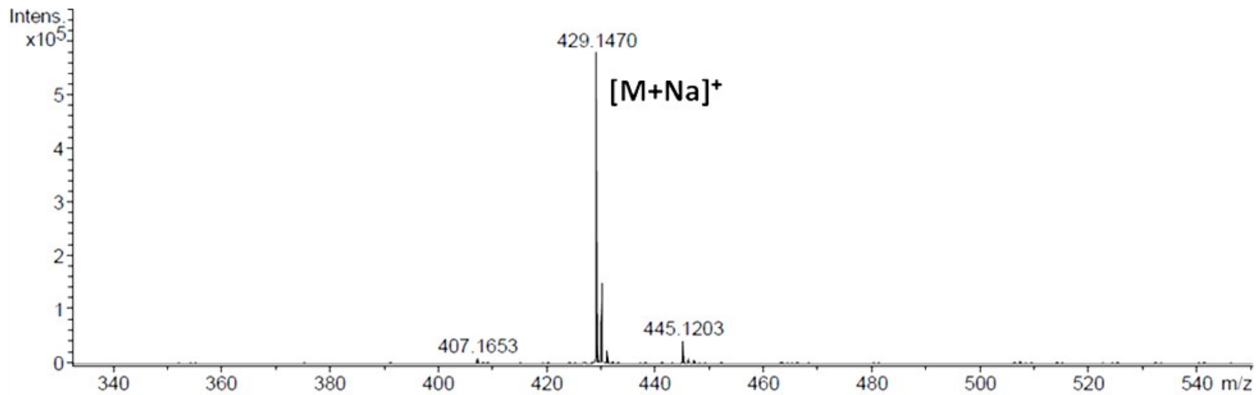

Figure S18: Mass spectra of *N*-maleoyl-L-Phe(1)-L-Phe(2)-OMe **6**. The peak m/z $(M + Na)^+ =$ 429.1470 corresponds to the synthesis of *N*-maleoyl-L-Phe(1)-L-Phe(2)-OMe.

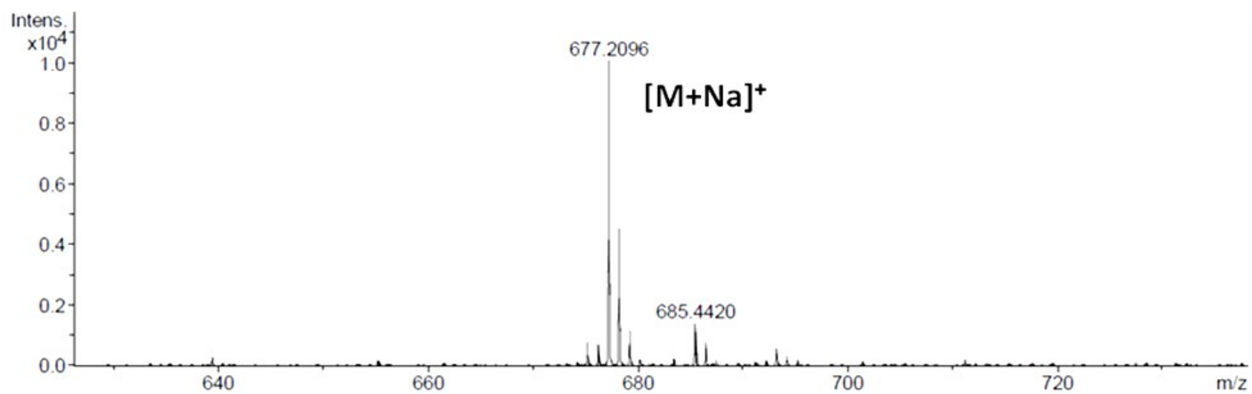

Figure S19: Mass spectra of benzo[ghi]perylene-1,2-dicarboxylic(L-Phe-L-Phe-OMe)imide **1**. The peak m/z (M + Na)$^+$ = 677.2096 corresponds to the synthesis of benzo[ghi]perylene-1,2-dicarboxylic(L-Phe-L-Phe-OMe)imide.