Shedding light on predicting and controlling emission chromaticity in multicomponent photoluminescent systems

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Supporting Information

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Experimental Section

Materials: All commercially available reagents were used as received and without further purification. Perylene (analytical standard) (SKU: 45798-100MG), Coumarin 6 (C6) (98%) (SKU: 442631-1G), and *N,N'*-Bis(3-pentyl)perylene-3,4,9,10-bis(dicarboximide) (PDI) (98% HPLC grade) (SKU: 776289-1G) were purchased from Millipore Sigma. Rhodamine 6G (R6G) (SKU: CAAAJ62315-14, Lot No. X19B036) and Nile Blue A (SKU: A17174, Lot No. 10212146) were purchased from VWR/ Alfa Aesar. HPLC-grade chloroform (stabilized with 0.75 % ethanol) was purchased from Fisher Scientific.

NMR spectra (^{1}H and ^{13}C): Spectra were recorded on a Varian Unity 400 MHz spectrometer (^{1}H: 399.945 MHz, ^{13}C: 100.577 MHz). Samples were prepared in deuterated chloroform and spectra were referenced relative to the residual non-deuterated solvent peaks at 7.26 ppm (^{1}H) and 77.16 ppm (^{13}C).

Fluorescence spectroscopy and mixing studies: Emission and excitation spectra and mixing studies were recorded in HPLC-grade chloroform (10^{-6} M) at room temperature using Edinburgh Instruments FS5 Fluorescence Spectrometer.

Absolute photoluminescent (PL) quantum yields (φ): Acquired via direct measurement at 298 K using an Edinburgh Instruments FS5 Spectrofluorimeter equipped with an SC-30 Integrating Sphere. Measurements were performed in a 1-cm quartz cuvette at room temperature. Excitation wavelengths (λ_{ex}) for each emitter were chosen such that the entire emission spectrum could be collected. All spectra were recorded in HPLC-grade chloroform at a concentration of 10^{-5} to 10^{-6} M. Resulting data was processed using the Fluoracle® software package.

Methods

General procedure for mixing experiments & prediction of expected CIE (x,y)

Stock solutions of each PL component were prepared in chloroform at c = 1.2 x 10^{-6} M. A total molecular concentration of c = 1.2 x 10^{-6} M was maintained throughout the mixing experiments and mole fractions (χ) were reported.[1] First, the excitation spectrum for each PL component's stock solution was recorded using each component's respective emission maxima (λ_{max}^{em}). Scan parameters including excitation/ emission bandwidths and number of scans were held constant to produce excitation spectra where the excitation intensities at common wavelengths ($I_{ex,i}(\lambda_{ex})$) were comparable.

The emission spectra and CIE coordinates of the stock solutions of components 1 and 2 were acquired, which corresponded to χ_1:χ_2 = 1:0 and 0:1, respectively. The measured CIE values for component 1 (χ_1:χ_2 = 1:0) and component 2 (χ_1:χ_2 = 0:1) were used as provided from Fluoracle® (5 decimal points) when calculating the expected CIE coordinates (Eq. S1 and Eq. S2) of the subsequent mixtures. Using the stock solutions of component 1 and 2, mixtures with varied mole fractions (χ_1:χ_2 = 0.75:0.25, 0.50:0.50, and 0.25:0.75) were prepared and analyzed.

$$x_{mix} = \frac{\phi_1 \cdot \chi_1 \cdot I_{ex,1}}{\phi_1 \cdot \chi_1 \cdot I_{ex,1} + \phi_2 \cdot \chi_2 \cdot I_{ex,2}} x_1 + \frac{\phi_2 \cdot \chi_2 \cdot I_{ex,2}}{\phi_1 \cdot \chi_1 \cdot I_{ex,1} + \phi_2 \cdot \chi_2 \cdot I_{ex,2}} x_2 \qquad \text{(Eq. S1)}$$

$$y_{mix} = \frac{\phi_1 \cdot \chi_1 \cdot I_{ex,1}}{\phi_1 \cdot \chi_1 \cdot I_{ex,1} + \phi_2 \cdot \chi_2 \cdot I_{ex,2}} y_1 + \frac{\phi_2 \cdot \chi_2 \cdot I_{ex,2}}{\phi_1 \cdot \chi_1 \cdot I_{ex,1} + \phi_2 \cdot \chi_2 \cdot I_{ex,2}} y_2 \qquad \text{(Eq. S2)}$$

Further Considerations

1. For accurate prediction, care was taken to ensure that the emitters' emission profiles were not sensitive to changes within the concentration range (0.3 – 1.2 x 10^{-6} M) that was explored during the mixing experiments. For example, self-absorption is observed in the case of perylene between $10^{-4} - 10^{-5}$ M, where within this concentration range, the intensity of the emission band centered around 443 nm dramatically changes.

2. A properly functioning monochromator is required for accurate results. Since excitation intensities at only one common wavelength are compared, an error in the expected emission ratio can occur if a large distribution of wavelengths is used to excite a mixture of emitters. To combat this, the excitation bandwidth was set between 1 – 2 nm (depending on the emission intensity) and held constant throughout a given mixing experiment.

3. For comparative excitation spectra, the power of the light source must be relatively constant for each set of measurements. Prior to acquiring the excitation spectra, the xenon lamp was given a 15-minute period to warm-up.

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[1] Concentrations were controlled and mole fractions were reported for simplicity and with an aim of reducing the possibility of ET. However, since the excitation intensity of an emitter in solution is proportional to its concentration, only the relative proportions of each PL solution being mixed need to be known. Consequently, one could similarly use volume fraction if the excitation intensities of the PL solutions being mixed are used to predict the resulting emission chromaticity.
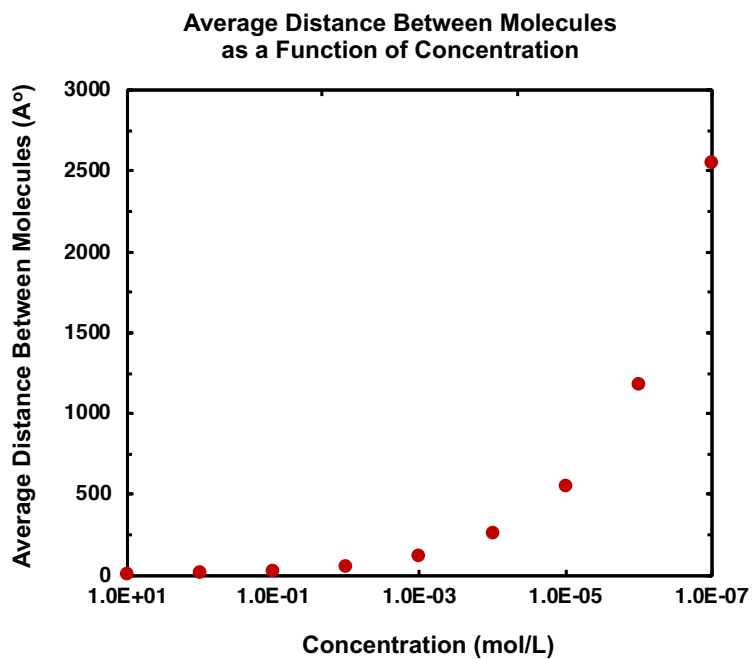
Figure S1. Average distance ($\bar{A}^o$) between molecules as a function of concentration (mol/L)

Average distance ($\bar{A}^o$) between molecules $= \dfrac{1}{\sqrt[3]{\dfrac{c \cdot N_A}{1 \times 10^{27}}}}$

where, $\quad N_A = 6.02214 \times 10^{23}$ and $c =$ concentration (mol/L)
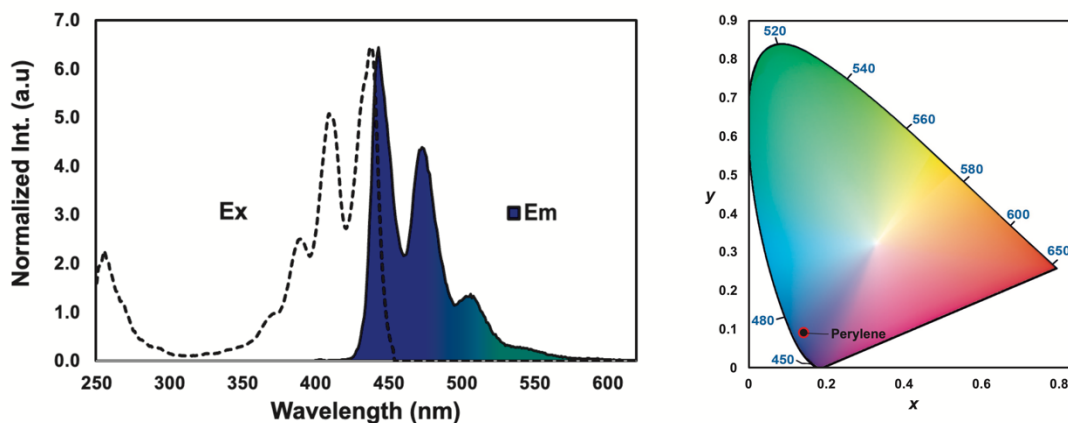
Photophysical Characterization

Perylene

Figure S2. Perylene's excitation and emission profile in chloroform at 10^{-6} M (left) and the corresponding CIE 1931 coordinates (~0.14,0.09) obtained from perylenes emission profile using Fluoracle® (right).
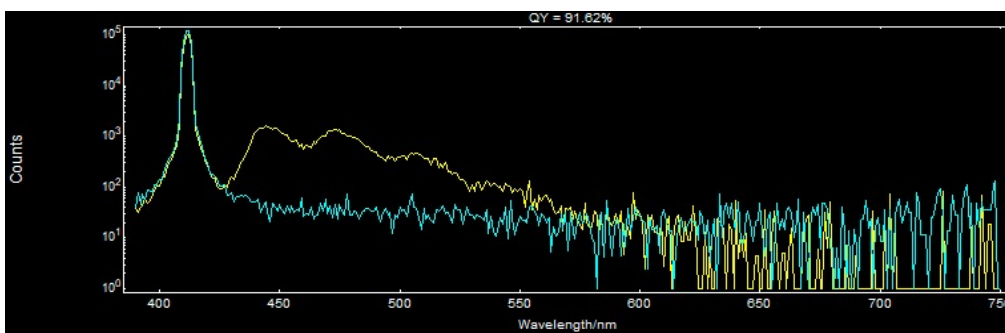

Figure S3. Perylene PLQY result (0.92) in chloroform at 10^{-6} M (λ_{ex} = 410 nm). An overlay showing the excitation scattering measured in chloroform (teal) + the excitation and emission scattering measured of perylene (yellow).

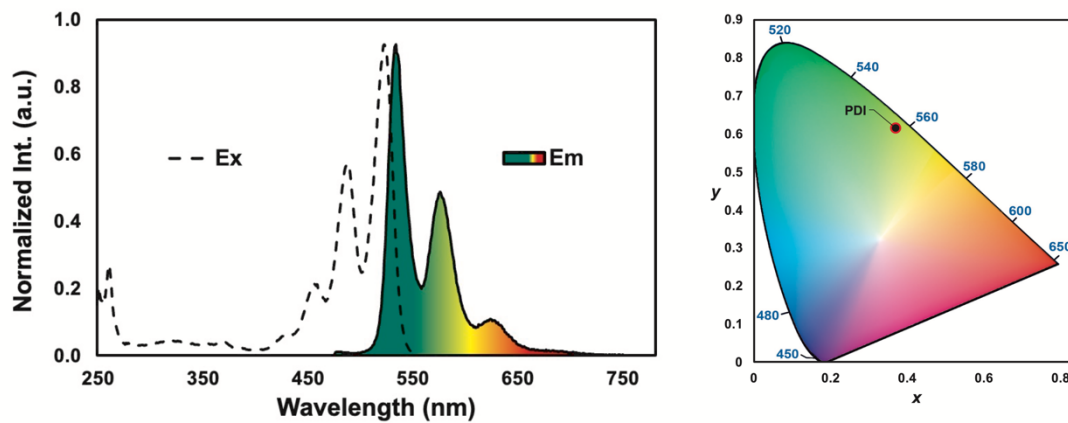**N,N'-bis(3-pentyl)perylene-3,4,9,10-bis(dicarboximide) (PDI)**

Figure S4. PDI's excitation and emission profile in chloroform at 10^{-6} M (left) and the corresponding CIE 1931 coordinates (~0.37,0.61) obtained from perylenes emission profile using Fluoracle® (right).
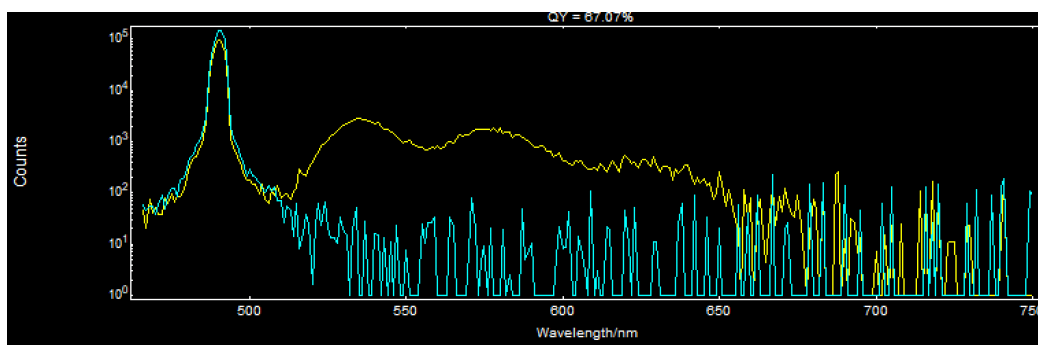

Figure S5. PDI absolute PLQY result (0.67) in chloroform at 10^{-6} M (λ_{ex} = 488 nm). An overlay showing the excitation scattering measured in chloroform (teal) + the excitation and emission scattering measured of PDI (yellow).
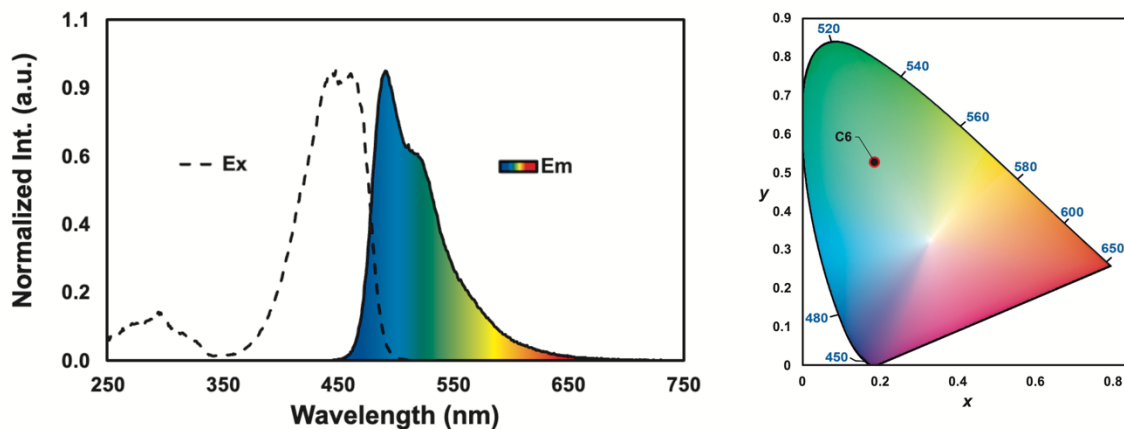
Coumarin 6 (C6)

Figure S6. C6's excitation and emission profile in chloroform at 10^{-6} M (left) and the corresponding CIE 1931 coordinates (~0.19,0.53) obtained from perylenes emission profile using Fluoracle® (right).
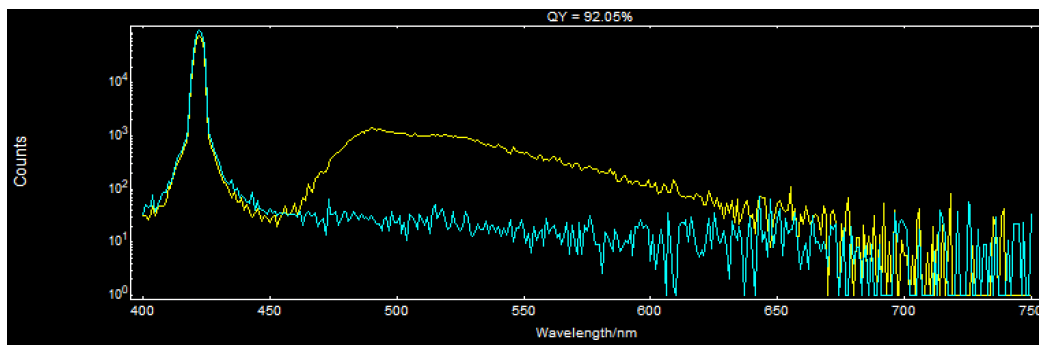

Figure S7. C6 PLQY result (0.92) in chloroform at 10^{-6} M (λ_{ex} = 420 nm). An overlay showing the excitation scattering measured in chloroform (teal) + the excitation and emission scattering measured of C6 (yellow).

Rhodamine 6G (R6G)
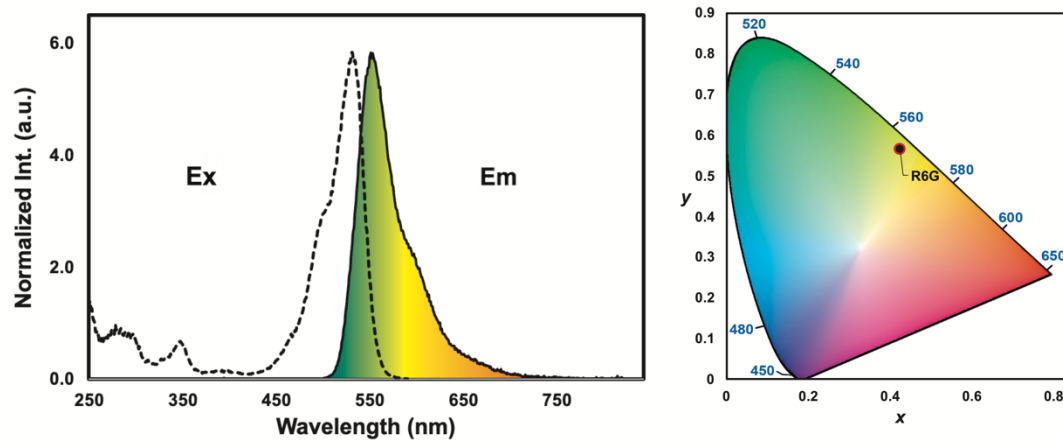
Figure S8. R6G's excitation and emission profile in chloroform at 10^{-6} M (left) and the corresponding CIE 1931 coordinates (~0.42, 0.57) obtained from R6G's emission profile using Fluoracle® (right).
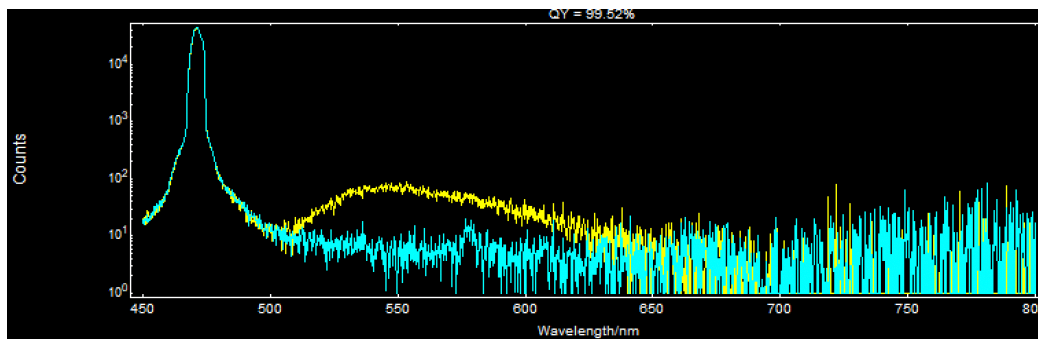
Figure S9. R6G PLQY result (~1) in chloroform at 10^{-5} M (λ_{ex} = 470 nm). An overlay showing the excitation scattering measured in chloroform (teal) + the excitation and emission scattering measured of R6G (yellow).

Nile Red (NR)
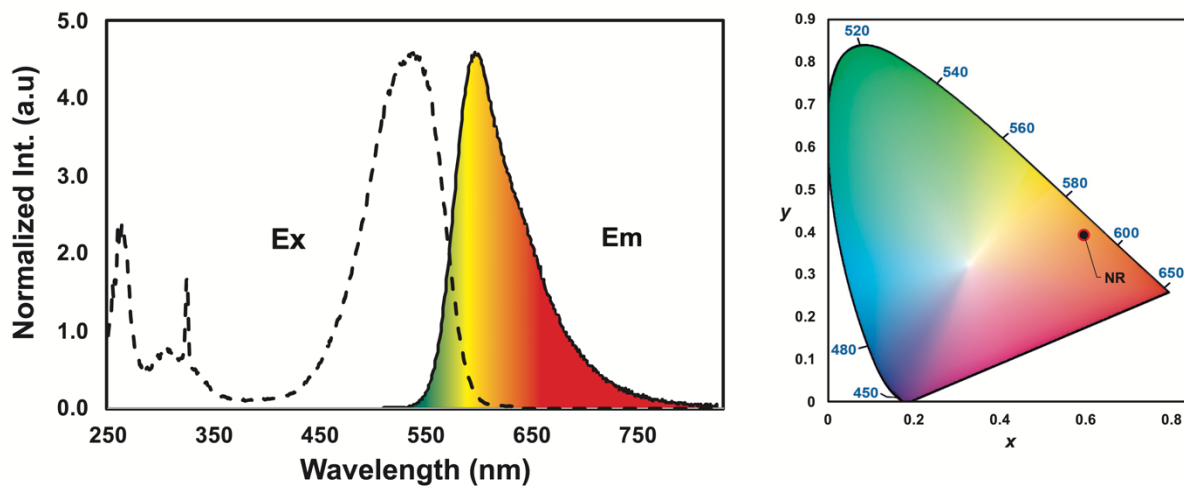
Figure S10. NR's excitation and emission profile in chloroform at 10^{-6} M (left) and the corresponding CIE 1931 coordinates (~0.60, 0.39) obtained from NR's emission profile using Fluoracle® (right).
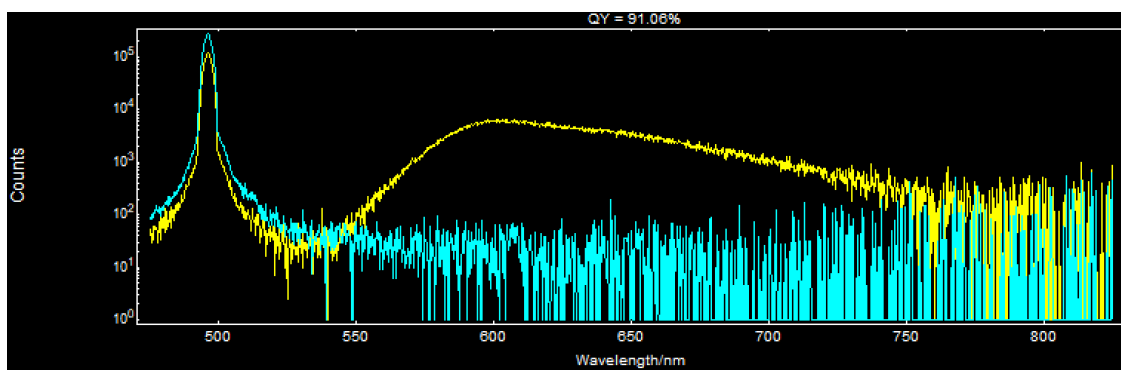
Figure S11. NR PLQY result (0.91) in chloroform at 10^{-6} M (λ_{ex} = 495 nm). An overlay showing the excitation scattering measured in chloroform (teal) + the excitation and emission scattering measured of NR (yellow).

Perylene and C6 Mixing Experiment(s)

Perylene
CIE = 0.14, 0.09
PLQY = 0.92
@ 10^{-6} in chloroform

Coumarin 6 (C6)
CIE = 0.19, 0.53
PLQY = 0.92
@ 10^{-6} in chloroform
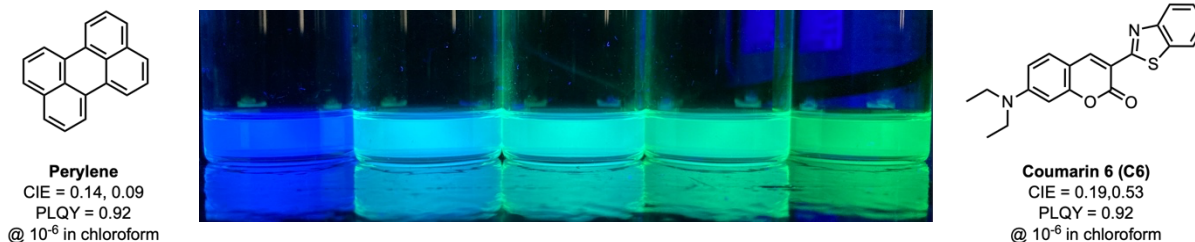
Figure S12. (From left to right) Perylene (1.2×10^{-6} M), perylene: C6 (0.9×10^{-6} M: 0.3×10^{-6} M), perylene: C6 (0.6×10^{-6} M: 0.6×10^{-6} M), perylene: C6 (0.3×10^{-6} M: 0.9×10^{-6} M), and C6 (1.2×10^{-6} M) irradiated with a long wave UV-lamp at 365 nm.

Figure S13. a) Perylene-C6 emission scans (λ_{ex} 333 nm) with differing mole fractions ($\chi_{perylene}$: χ_{C6}) and (b) the corresponding CIE diagram showing the measured (●) and predicted (○) CIE coordinates. R^2 value (0.9995) was obtained from measured data.

Table S1. Tabulated results obtained from Perylene-C6 PLCT mixing studies (λ_{ex} 333 nm). [a]

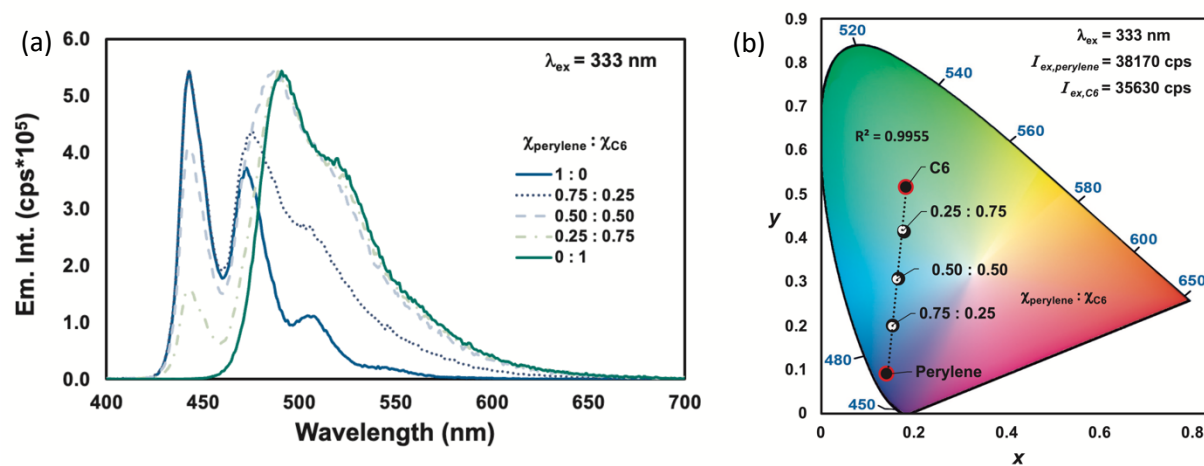| Mole Fractions (χ) Perylene to C6	λ_{ex} = 333 nm		
	Measured CIE (x,y)	Expected [b] CIE (x,y)	Absolute [c] Error
1 to 0	0.14330, 0.08953	-	-
0.75 to 0.25	0.15, 0.20 (0.15444, 0.20076)	0.15, 0.20	< 0.01 (0.004)
0.50 to 0.50	0.17, 0.31 (0.16563, 0.30603)	0.17, 0.30	< 0.01 (0.003)
0.25 to 0.75	0.18, 0.41 (0.17719, 0.41441)	0.18, 0.41	<0.01 (0.0001)
0 to 1	0.18413, 0.51508	-	-

[a] Reported solution data was measured in chloroform at a tot. molecular conc. of 1.2 x 10^-6 M. Total molecular concentration was held constant while the mole fractions (χ) each component was varied. [b] **Expected CIE (x,y) were calculated based on the measured properties of perylene ($CIE_{perylene}$ = 0.14330, 0.08953; $I_{ex,perylene}$ = 38170 cps at λ_{ex} 333 nm; $\phi_{perylene}$ = 0.92; and χ_i given in the table) and C6 (CIE_{C6} = 0.18413, 0.51508; $I_{ex,C6}$ = 35630 cps at λ_{ex} 333 nm; ϕ_{C6} = 0.92; and χ_i given in the table) using Eq. 1.** [c] Absolute error was calculated based on the distance (d) between expected and measured CIE coordinates using $d = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$.

Expected CIE (x,y) sample calculation for $\chi_{perylene}$: χ_{C6} = 0.5:0.5 @ λ_{ex} = 333 nm using Eq. S1 and Eq. S2:

$$x_{mix} = \frac{0.92 \cdot 0.5 \cdot 38170}{0.92 \cdot 0.5 \cdot 38170 + 0.92 \cdot 0.5 \cdot 35630} \cdot 0.14330 + \frac{0.92 \cdot 0.5 \cdot 35630}{0.92 \cdot 0.5 \cdot 38170 + 0.92 \cdot 0.5 \cdot 35630} \cdot 0.18413 = 0.17$$

$$y_{mix} = \frac{0.92 \cdot 0.5 \cdot 38170}{0.92 \cdot 0.5 \cdot 38170 + 0.92 \cdot 0.5 \cdot 35630} \cdot 0.08953 + \frac{0.92 \cdot 0.5 \cdot 35630}{0.92 \cdot 0.5 \cdot 38170 + 0.92 \cdot 0.5 \cdot 35630} \cdot 0.51508 = 0.30$$

(a)

(b)

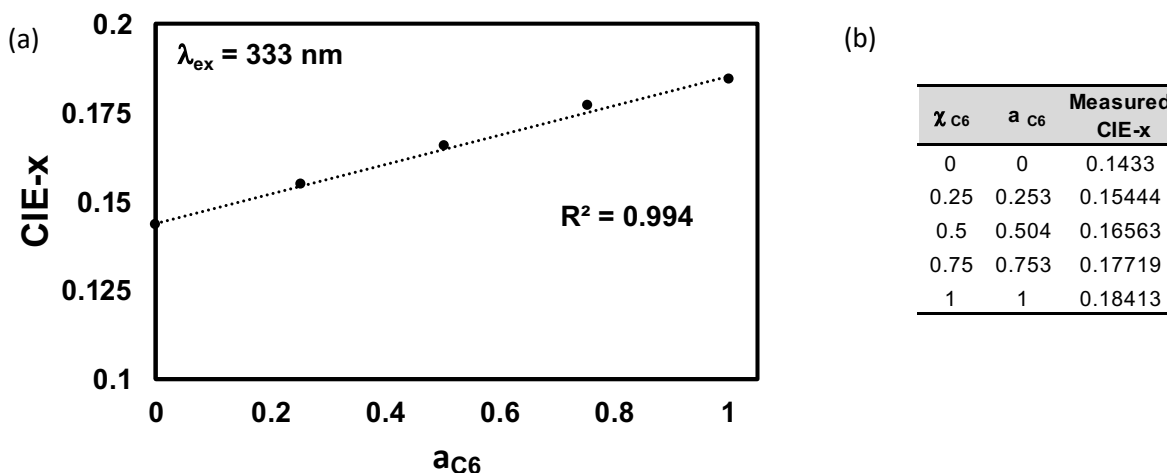| χ_{C6}	a_{C6}	Measured CIE-x
0	0	0.1433
0.25	0.253	0.15444
0.5	0.504	0.16563
0.75	0.753	0.17719
1	1	0.18413

Figure S14. a) Scatter plot showing the linear dependence (R^2 = 0.9940) of the measured CIE-x on the *relative brightness* of C6 ($a_{C6} = \frac{\phi_{C6} \cdot I_{ex,C6} \cdot \chi_{C6}}{\sum \phi_i \cdot I_{ex,i} \cdot \chi_i}$) when excited at 333 nm and b) the corresponding tabulated data.
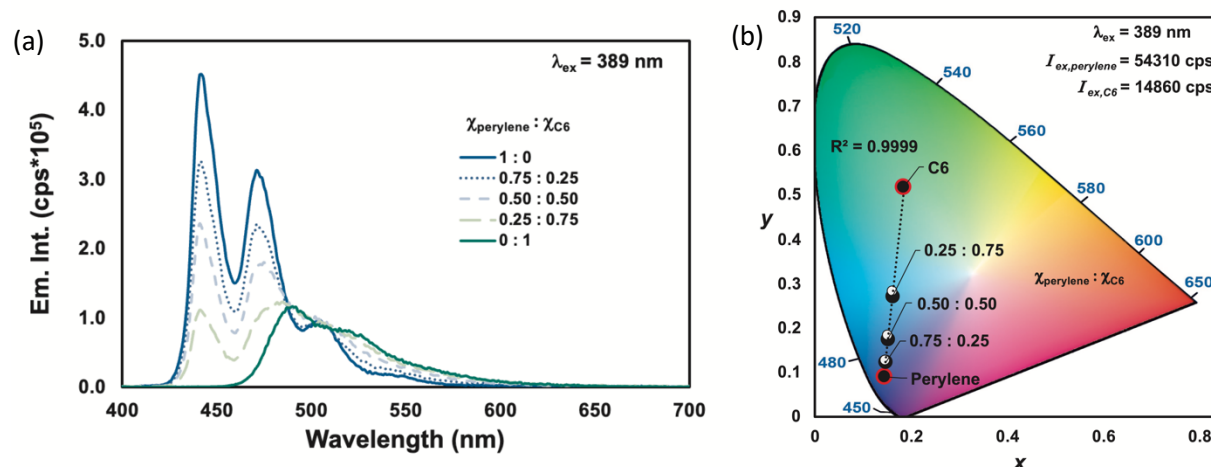
Figure S15. a) Perylene-C6 emission scans (λ_{ex} 389nm) with differing mole fractions ($\chi_{perylene}$: χ_{C6}) and (b) the corresponding CIE diagram showing the measured (●) and predicted (○) CIE coordinates. R^2 value (0.9999) was obtained from measured data.

Table S2. Tabulated results obtained from Perylene-C6 PLCT mixing studies (λ_{ex} 389 nm). [a]

Mole Fractions (χ) Perylene to C6	λ_{ex} = 389 nm		
	Measured CIE (x,y)	Expected [b] CIE (x,y)	Absolute [c] Error
1 to 0	0.14330, 0.08953	-	-
0.75 to 0.25	0.15, 0.12 (0.14622, 0.12270)	0.15, 0.13	< 0.01 (0.002)
0.50 to 0.50	0.15, 0.18 (0.15155, 0.17521)	0.15, 0.18	< 0.01 (0.006)
0.25 to 0.75	0.16, 0.27 (0.16102, 0.27159)	0.16, 0.28	0.01 (0.0010)
0 to 1	0.18413,0.51508	-	-

[a] Reported solution data was measured in chloroform at a tot. molecular conc. of 1.2 x 10^{-6} M. Total molecular concentration was held constant while the mole fractions (χ) each component was varied. [b] **Expected CIE (x,y) were calculated based on the measured properties of perylene ($CIE_{perylene}$ = 0.14330, 0.08953; $I_{ex,perylene}$ = 54310 cps at λ_{ex} 389 nm; $\phi_{perylene}$ = 0.92; and χ_i given in the table) and C6 (CIE_{C6} = 0.18413, 0.51508; $I_{ex,C6}$ = 14860 cps at λ_{ex} 389 nm; ϕ_{C6} = 0.92; and χ_i given in the table) using Eq. 1.** [c] Absolute error was calculated based on the distance (d) between expected and measured CIE coordinates using $d = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$.

Expected CIE (x,y) sample calculation for $\chi_{perylene}$: χ_{C6} = 0.5:0.5 @ λ_{ex} = 389 nm using Eq. S1 and Eq. S2:

$$x_{mix} = \frac{0.92 \cdot 0.5 \cdot 54310}{0.92 \cdot 0.5 \cdot 54310 + 0.92 \cdot 0.5 \cdot 14680} \cdot 0.14330 + \frac{0.92 \cdot 0.5 \cdot 14680}{0.92 \cdot 0.5 \cdot 54310 + 0.92 \cdot 0.5 \cdot 14680} \cdot 0.18413 = 0.15$$

$$y_{mix} = \frac{0.92 \cdot 0.5 \cdot 54310}{0.92 \cdot 0.5 \cdot 54310 + 0.92 \cdot 0.5 \cdot 14680} \cdot 0.08953 + \frac{0.92 \cdot 0.5 \cdot 14680}{0.92 \cdot 0.5 \cdot 54310 + 0.92 \cdot 0.5 \cdot 14680} \cdot 0.51508 = 0.18$$

(a)

λ_{ex} = 389 nm

CIE-x

R² = 0.9996

a $_{C6}$

(b)

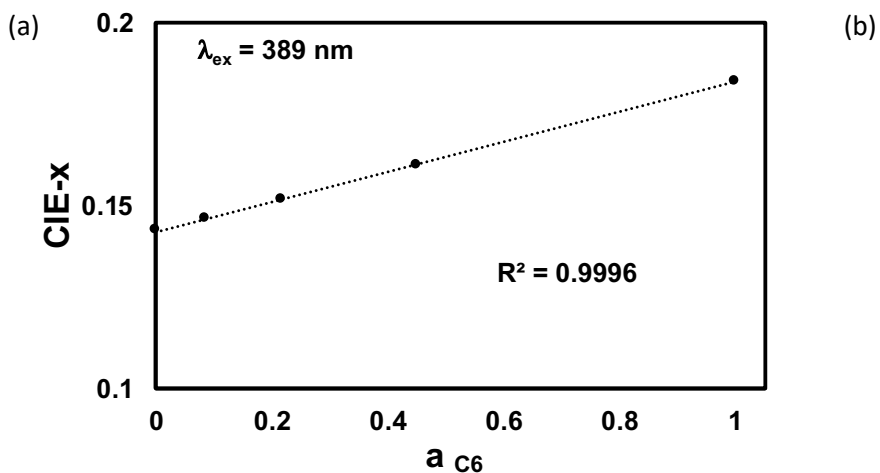| χ C6	a C6	Measured CIE-x
0	0	0.1433
0.25	0.084	0.14622
0.5	0.215	0.15155
0.75	0.451	0.16102
1	1	0.18413

Figure S16. a) Scatter plot showing the linear dependence (R² = 0.9996) of the measured CIE-x on the *relative brightness* of C6 ($a_{C6} = \frac{\phi_{C6} \cdot I_{ex,C6} \cdot \chi_{C6}}{\sum \phi_i \cdot I_{ex,i} \cdot \chi_i}$) when excited at 389 nm and b) the corresponding tabulated data.

Perylene and PDI Mixing Experiment

Perylene
CIE = 0.14, 0.09
PLQY = 0.92
@ 10^{-6} in chloroform

Perylene Diimide (PDI)
CIE = 0.37,0.61
PLQY = 0.67
@ 10^{-6} in chloroform

Figure S17. (From left to right) Perylene (1.2 x 10^{-6} M), perylene: PDI (0.9 x 10^{-6} M: 0.3 x 10^{-6} M; 0.75:0.25), perylene: PDI (0.6 x 10^{-6} M: 0.6 x 10^{-6} M; 0.50:0.50), perylene: PDI (0.3 x 10^{-6} M: 0.9 x 10^{-6} M; 0.25, 0.75), and PDI (1.2 x 10^{-6} M) irradiated with a long wave UV-lamp at 365 nm.
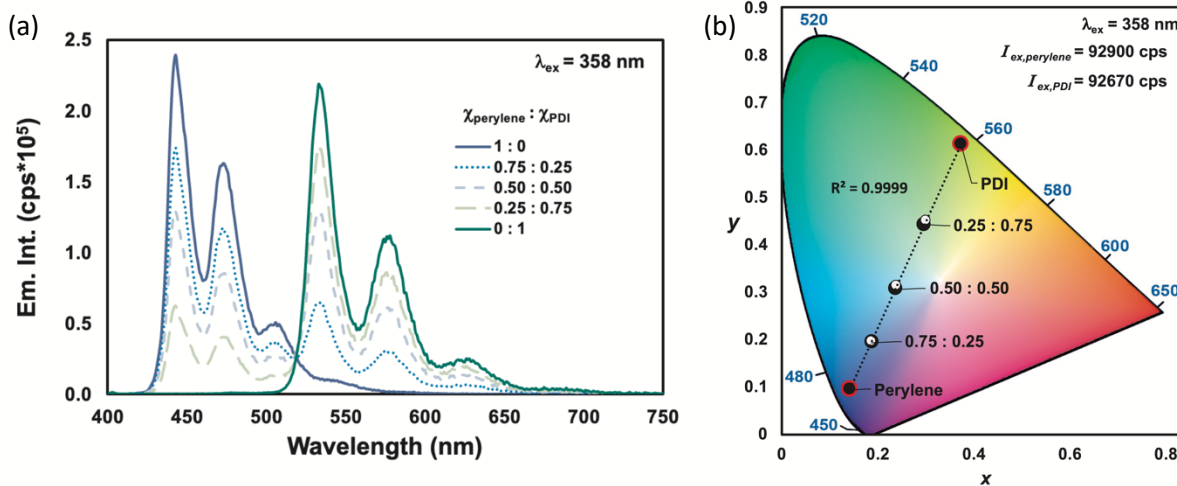

Figure S18. a) Perylene-PDI emission scans (λ_{ex} 358 nm) with differing mole fractions ($\chi_{perylene}$: χ_{PDI}) and (b) the corresponding CIE diagram showing the measured (●) and predicted (○) CIE coordinates. R^2 value (0.9999) was obtained from measured data.

**Table S3**. Tabulated results obtained from Perylene-PDI PLCT mixing studies (λ_{ex} 358 nm). [a]

Mole Fractions (χ) Perylene to PDI	λ_{ex} = 358 nm		
	Measured CIE (x,y)	Expected [b] CIE (x,y)	Absolute [c] Error
1 to 0	0.14304, 0.09429	-	-
0.75 to 0.25	0.19, 0.19 (0.18733, 0.19493)	0.19, 0.19	< 0.01 (0.0007)
0.50 to 0.50	0.24, 0.31 (0.23703, 0.30730)	0.24, 0.31	< 0.01 (0.005)
0.25 to 0.75	0.30, 0.44 (0.29707, 0.44223)	0.30, 0.45	< 0.01 (0.007)
0 to 1	0.37369, 0.61057	-	-

[a] Reported solution data was measured in chloroform at a tot. molecular conc. of 1.2 x 10^{-6} M. Total molecular concentration was held constant while the mole fractions (χ) each component was varied. [b] **Expected CIE (x,y) were calculated based on the measured properties of perylene ($CIE_{perylene}$ = 0.14304, 0.09429; $I_{ex,perylene}$ = 92900 cps at λ_{ex} 358 nm; $\phi_{perylene}$ = 0.92; and χ_i given in the table) and PDI (CIE_{PDI} = 0.37369, 0.61057; $I_{ex,PDI}$ = 92670 cps at λ_{ex} 358 nm; ϕ_{PDI} = 0.67; and χ_i given in the table) using Eq. 1.** [c] Absolute error was calculated based on the distance (d) between expected and measured CIE coordinates using $d = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$.

Expected CIE (x,y) sample calculation for $\chi_{perylene}$: χ_{PDI} = 0.5 : 0.5 @ λ_{ex} = 358 nm using Eq. S1 and Eq. S2:

$$x_{mix} = \frac{0.92 \cdot 0.5 \cdot 92900}{0.92 \cdot 0.5 \cdot 92900 + 0.67 \cdot 0.5 \cdot 92670} \cdot 0.14304 + \frac{0.67 \cdot 0.5 \cdot 92670}{0.92 \cdot 0.5 \cdot 92900 + 0.67 \cdot 0.5 \cdot 14680} \cdot 0.37369 = 0.24$$

$$y_{mix} = \frac{0.92 \cdot 0.5 \cdot 92900}{0.92 \cdot 0.5 \cdot 92900 + 0.67 \cdot 0.5 \cdot 92670} \cdot 0.09429 + \frac{0.67 \cdot 0.5 \cdot 92670}{0.92 \cdot 0.5 \cdot 92900 + 0.67 \cdot 0.5 \cdot 92670} \cdot 0.61057 = 0.31$$

(a)

(b)
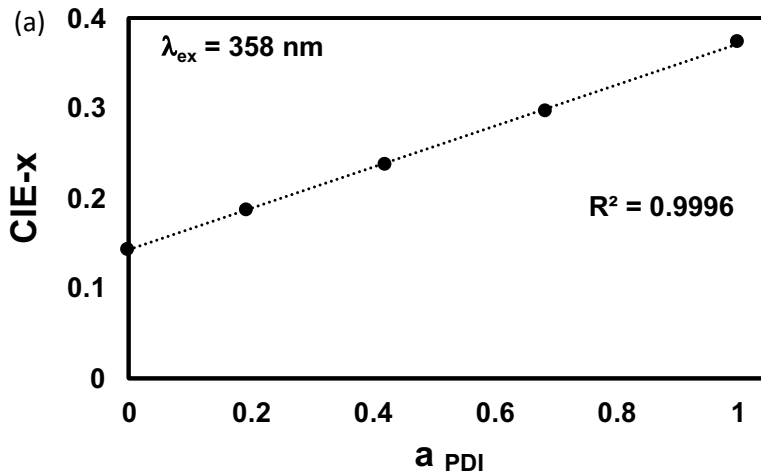
χ PDI	a PDI	Measured CIE-x
0	0	0.14304
0.25	0.195	0.18733
0.5	0.421	0.23703
0.75	0.685	0.29707
1	1	0.37369

Figure S19. a) Scatter plot showing the linear dependence (R^2 = 0.9996) of the measured CIE-x on the *relative brightness* of PDI ($a_{PDI} = \frac{\phi_{PDI} \cdot I_{ex,PDI} \cdot \chi_{PDI}}{\sum \phi_i \cdot I_{ex,i} \cdot \chi_i}$) when excited at 358 nm and b) the corresponding tabulated data.

C6 and PDI Mixing Experiment

Coumarin 6 (C6)
CIE = 0.19,0.53
PLQY = 0.92
@ 10^{-6} in chloroform

Perylene Diimide (PDI)
CIE = 0.37,0.61
PLQY = 0.67
@ 10^{-6} in chloroform

Figure S20. (From left to right) C6 (1.2×10^{-6} M), C6: PDI (0.9×10^{-6} M: 0.3×10^{-6} M), C6: PDI (0.6×10^{-6} M: 0.6×10^{-6} M), C6: PDI (0.3×10^{-6} M: 0.9×10^{-6} M), and PDI (1.2×10^{-6} M) irradiated with a long wave UV-lamp at 365 nm.
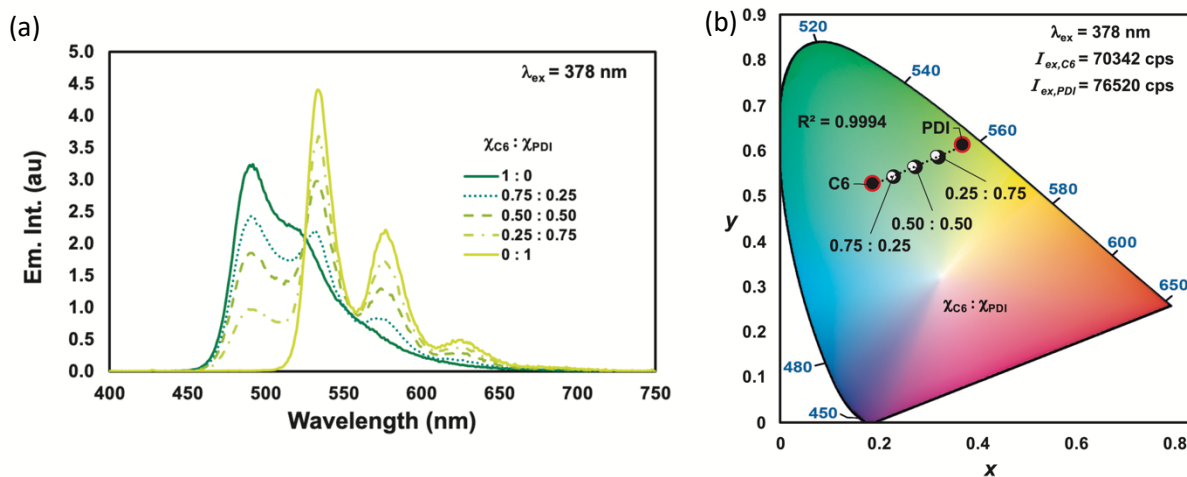

Figure S21. a) C6-PDI emission scans (λ_{ex} 378 nm) with differing mole fractions (χ_{C6}: χ_{PDI}) and (b) the corresponding CIE diagram showing the measured (●) and predicted (○) CIE coordinates. R^2 value (0.9994) was obtained from measured data.

Table S4. Tabulated results obtained from C6-PDI PLCT mixing studies (λ_{ex} 378 nm). [a]

Mole Fractions (χ) C6 to PDI	λ_{ex} = 378 nm		
	Measured CIE (x,y)	Expected [b] CIE (x,y)	Absolute [c] Error
1 to 0	0.18737, 0.52564	-	-
0.75 to 0.25	0.23, 0.54 (0.22880, 0.54495)	0.22, 0.54	< 0.01 (0.003)
0.50 to 0.50	0.27, 0.56 (0.27291, 0.56474)	0.26, 0.56	< 0.01 (0.005)
0.25 to 0.75	0.32, 0.59 (0.31983, 0.58756)	0.31, 0.59	< 0.01 (0.004)
0 to 1	0.37043, 0.61324	-	-

[a] Reported solution data was measured in chloroform at a tot. molecular conc. of 1.2 x 10^{-6} M. Total molecular concentration was held constant while the mole fractions (χ) each component was varied. [b] **Expected CIE (x,y) were calculated based on the measured properties of C6 (CIE_{C6} = 0.18737, 0.52564; $I_{ex,C6}$ = 70342 cps at λ_{ex} 378 nm; ϕ_{C6} = 0.92; and χ_i given in the table) and PDI (CIE_{PDI} = 0.37043, 0.61324; $I_{ex,PDI}$ = 76520 cps at λ_{ex} 358 nm; ϕ_{PDI} = 0.67; and χ_i given in the table) using Eq. 1.** [c] Absolute error was calculated based on the distance (d) between expected and measured CIE coordinates using $d = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$.

Predicted CIE (x,y) sample calculation for χ_{C6}: χ_{PDI} = 0.5:0.5 @ λ_{ex} = 378 nm using Eq. S1 and Eq. S2:

$$x_{mix} = \frac{0.92 \cdot 0.5 \cdot 70342}{0.92 \cdot 0.5 \cdot 70342 + 0.67 \cdot 0.5 \cdot 76520} \cdot 0.18737 + \frac{0.67 \cdot 0.5 \cdot 76520}{0.92 \cdot 0.5 \cdot 70342 + 0.67 \cdot 0.5 \cdot 76520} \cdot 0.37043 = 0.26$$

$$y_{mix} = \frac{0.92 \cdot 0.5 \cdot 70342}{0.92 \cdot 0.5 \cdot 70342 + 0.67 \cdot 0.5 \cdot 76520} \cdot 0.52564 + \frac{0.67 \cdot 0.5 \cdot 76520}{0.92 \cdot 0.5 \cdot 70342 + 0.67 \cdot 0.5 \cdot 76520} \cdot 0.51324 = 0.56$$

(a) λ_{ex} = 378 nm, R² = 0.9991

(b)
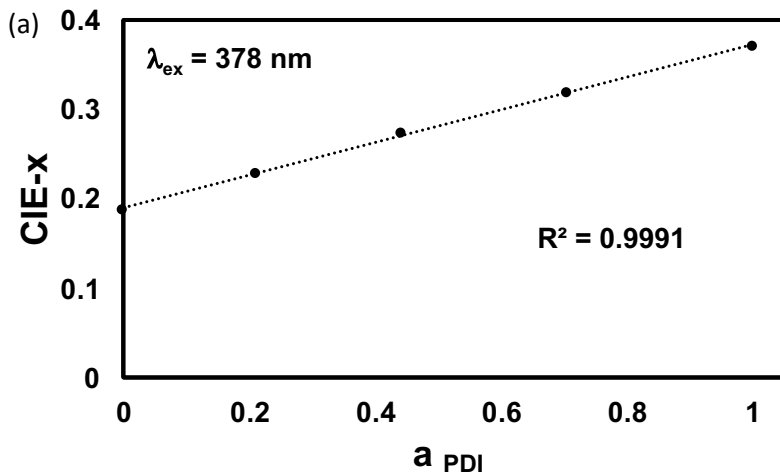
χ_{PDI}	a_{PDI}	Measured CIE-x
0	0	0.18737
0.25	0.209	0.2288
0.5	0.442	0.27291
0.75	0.704	0.31983
1	1	0.37043

Figure S22. Scatter plot showing the linear dependence (R^2 = 0.9991) of the measured CIE-x on the *relative brightness* of PDI ($a_{PDI} = \frac{\phi_{PDI} \cdot I_{ex,PDI} \cdot \chi_{PDI}}{\sum \phi_i \cdot I_{ex,i} \cdot \chi_i}$) when excited at 378 nm and b) the corresponding tabulated data.
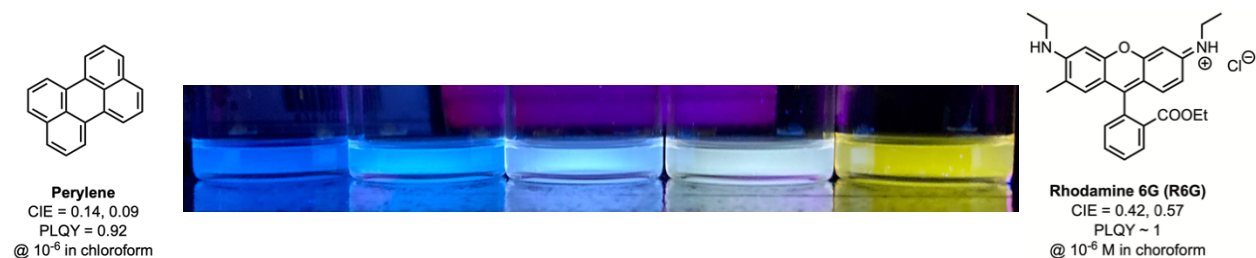
Perylene and Rhodamine 6G (R6G) Mixing Experiments

Perylene
CIE = 0.14, 0.09
PLQY = 0.92
@ 10^{-6} in chloroform

Rhodamine 6G (R6G)
CIE = 0.42, 0.57
PLQY ~ 1
@ 10^{-6} M in choroform

Figure S23. (From left to right) Perylene (1.2 x 10^{-6} M), Perylene: R6G (0.9 x 10^{-6} M: 0.3 x 10^{-6} M), Perylene: R6G (0.6 x 10^{-6} M: 0.6 x 10^{-6} M), Perylene: R6G (0.3 x 10^{-6} M: 0.9 x 10^{-6} M), and R6G (1.2 x 10^{-6} M) irradiated with a long wave UV-lamp at 365 nm.
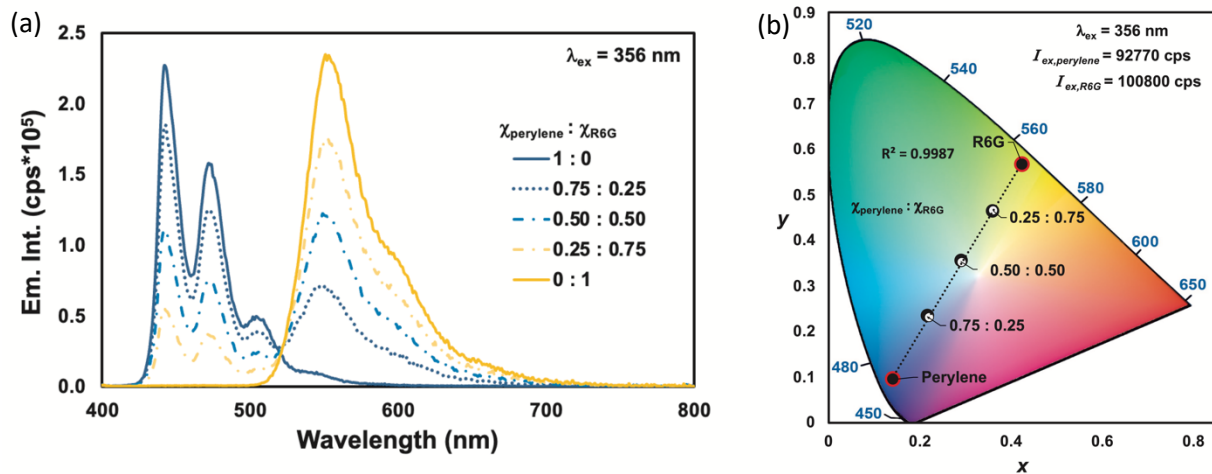

Figure S24. a) Perylene-R6G emission scans (λ_{ex} 356 nm) with differing mole fractions ($\chi_{perylene}$: χ_{R6G}) and (b) the corresponding CIE diagram showing the measured (●) and predicted (○) CIE coordinates. R^2 value (0.9987) was obtained from measured data.

**Table S5**. Tabulated results obtained from Perylene-R6G PLCT mixing studies (λ_{ex} 356 nm). [a]

Mole Fractions (χ) Perylene to R6G	λ_{ex} = 356 nm		
	Measured CIE (x,y)	Expected [b] CIE (x,y)	Absolute [c] Error
1 to 0	0.14303, 0.09447	-	-
0.75 to 0.25	0.22, 0.23 (0.21705, 0.23256)	0.22, 0.23	< 0.01 (0.007)
0.50 to 0.50	0.29, 0.35 (0.29076, 0.35416)	0.30, 0.35	< 0.01 (0.007)
0.25 to 0.75	0.36, 0.46 (0.36036, 0.46472)	0.36, 0.46	<0.01 (0.0004)
0 to 1	0.42455, 0.56565	-	-

[a] Reported solution data was measured in chloroform at a tot. molecular conc. of 1.2 x 10^{-6} M. Total molecular concentration was held constant while the mole fractions (χ) each component was varied. [b] **Expected CIE (x,y) were calculated based on the measured properties of perylene ($CIE_{perylene}$ = 0.14303, 0.09447; $I_{ex,perylene}$ = 92770 cps at λ_{ex} 356 nm; $\phi_{perylene}$ = 0.92; and χ_i given in the table) and R6G (CIE_{R6G} = 0.42455, 0.56565; $I_{ex,R6G}$ = 100800 cps at λ_{ex} 356 nm; ϕ_{R6G} = 1; and χ_i given in the table) using Eq. 1.** [c] Absolute error was calculated based on the distance (d) between expected and measured CIE coordinates using $d = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$.

Predicted CIE (x,y) sample calculation for $\chi_{perylene}$: χ_{R6G} = 0.5:0.5 @ λ_{ex} = 356 nm using Eq. S1 and Eq. S2:

$$x_{mix} = \frac{0.92 \cdot 0.5 \cdot 92770}{0.92 \cdot 0.5 \cdot 92770 + 1 \cdot 0.5 \cdot 100800} \cdot 0.14303 + \frac{1 \cdot 0.5 \cdot 100800}{0.92 \cdot 0.5 \cdot 92770 + 1 \cdot 0.5 \cdot 100800} \cdot 0.42455 = 0.30$$

$$y_{mix} = \frac{0.92 \cdot 0.5 \cdot 92770}{0.92 \cdot 0.5 \cdot 92770 + 1 \cdot 0.5 \cdot 100800} \cdot 0.09447 + \frac{1 \cdot 0.5 \cdot 100800}{0.92 \cdot 0.5 \cdot 92770 + 1 \cdot 0.5 \cdot 100800} \cdot 0.56565 = 0.35$$

(a)

(b)
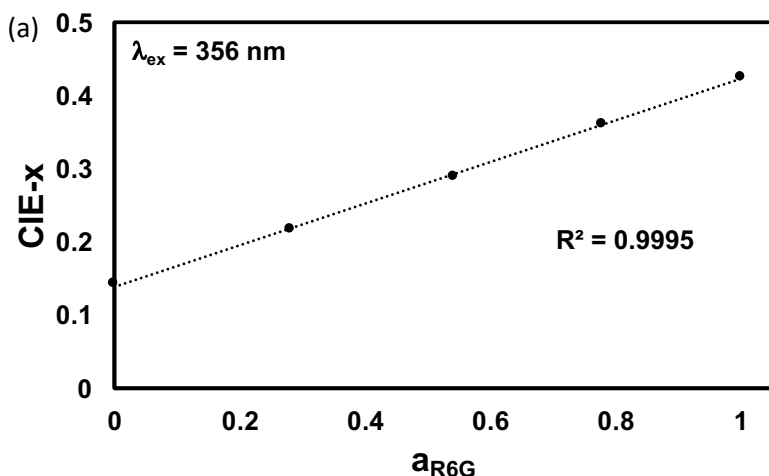
χ R6G	a R6G	Measured CIE-x
0	0	0.14303
0.25	0.282	0.21705
0.5	0.542	0.29076
0.75	0.78	0.36036
1	1	0.42455

Figure S25. a) Scatter plot showing the linear dependence (R^2 = 0.9995) of the measured CIE-x on the *relative brightness* of R6G ($a_{R6G} = \frac{\phi_{R6G} \cdot I_{ex,R6G} \cdot \chi_{R6G}}{\sum \phi_i \cdot I_{ex,i} \cdot \chi_i}$) and b) the corresponding tabulated data.
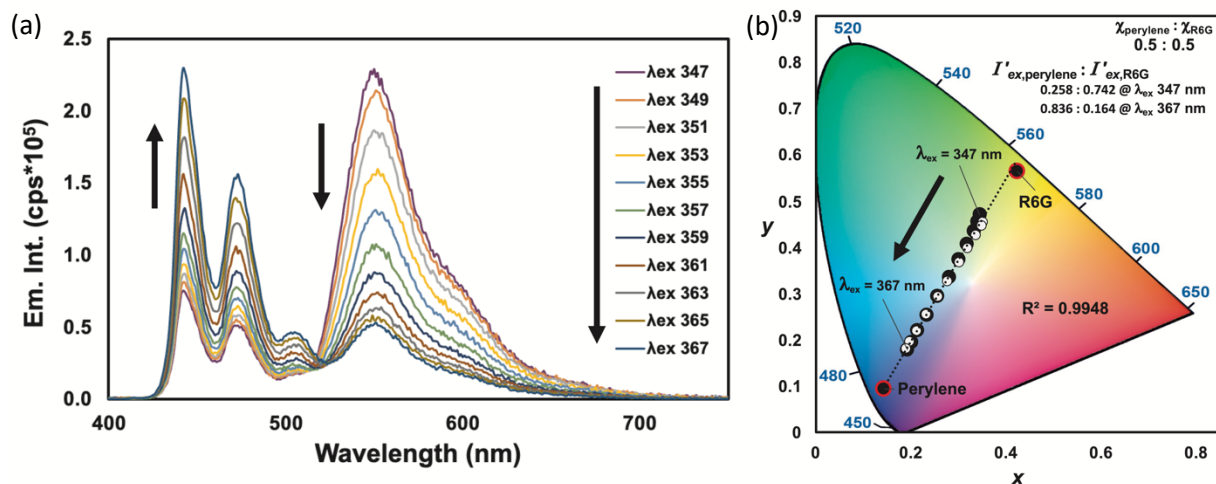
Figure S26. a) Perylene-R6G ($\chi_{perylene}$: χ_{R6G} = 0.5: 0.5) emission spectra obtained using different excitation wavelengths (λ_{ex} 347-367 nm; 2 nm intervals) and (b) the corresponding CIE diagram showing the measured (●) and predicted (○) CIE coordinates. R^2 value (0.9948) was obtained from measured data. Relative excitation intensities of perylene ($I'_{ex,perylene}$) and R6G ($I'_{ex,R6G}$) were calculated using $\frac{I_{ex,perylene}}{I_{ex,perylene}+I_{ex,R6G}}$ & $\frac{I_{ex,R6G}}{I_{ex,perylene}+I_{ex,R6G}}$, respectively, using the intensities shown in Table S6.

Table S6. Tabulated results obtained from Perylene-R6G excitation-dependant PLCT studies.

λ_{ex} (nm)	$I_{ex, perylene}$	$I_{ex, R6G}$	Measured CIE (x,y)	Expected [b] CIE (x,y)	Absolute [c] Error
347	64860	186700	0.35, 0.47 (0.346, 0.471)	0.36, 0.45 (0.356, 0.452)	0.02 (0.022)
349	66970	179400	0.34, 0.46 (0.342, 0.457)	0.35, 0.45 (0.353, 0.445)	0.02 (0.016)
351	74170	160200	0.33, 0.44 (0.334, 0.436)	0.34, 0.42 (0.340, 0.425)	0.01 (0.013)
353	82370	134400	0.32, 0.41 (0.320, 0.408)	0.32, 0.40 (0.323, 0.396)	0.01 (0.013)
355	90390	112500	0.30, 0.37 (0.303, 0.375)	0.30, 0.37 (0.305, 0.366)	0.01 (0.010)
357	102400	89870	0.28, 0.34 (0.281, 0.335)	0.28, 0.32 (0.280, 0.325)	0.01 (0.011)
359	111300	74420	0.26, 0.29 (0.258, 0.294)	0.26, 0.29 (0.260, 0.291)	< 0.01 (0.004)
361	129100	59460	0.24, 0.25 (0.235, 0.254)	0.24, 0.25 (0.237, 0.252)	< 0.01 (0.003)
363	158300	51800	0.22, 0.22 (0.216, 0.220)	0.22, 0.22 (0.217, 0.218)	< 0.01 (0.002)
365	181600	44160	0.20, 0.20 (0.202, 0.196)	0.20, 0.19 (0.202, 0.193)	< 0.01 (0.003)
367	197400	38850	0.19, 0.18 (0.193, 0.180)	0.19, 0.18 (0.193, 0.178)	< 0.01 (0.002)

[a] Reported solution data was measured in chloroform at a tot. molecular conc. of 1.2 x 10⁻⁶ M. [b] **Expected CIE (x,y) were calculated based on the measured properties of perylene ($CIE_{perylene}$ = 0.14303, 0.09447; $I_{ex,perylene}$ reported in Table S6; $\phi_{perylene}$ = 0.92; and $\chi_{perylene}$ = 0.5) and R6G (CIE_{R6G} = 0.42455, 0.56565; $I_{ex,R6G}$ reported in Table S6; ϕ_{R6G} = 1; and χ_{R6G} = 0.5) using Eq. 1**. [c] Absolute error was calculated based on the distance (d) between expected and measured CIE coordinates using $d = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$.

Predicted CIE (x,y) sample calculation for $\chi_{perylene} : \chi_{R6G} = 0.5{:}0.5$ @ $\lambda_{ex} = 347$ nm using Eq. S3 and Eq. S4:

$$x_{mix} = \frac{0.92 \cdot 0.5 \cdot 64860}{0.92 \cdot 0.5 \cdot 64860 + 1 \cdot 0.5 \cdot 186700} \cdot 0.14303 + \frac{1 \cdot 0.5 \cdot 186700}{0.92 \cdot 0.5 \cdot 64860 + 1 \cdot 0.5 \cdot 186700} \cdot 0.42455 = 0.36$$

$$y_{mix} = \frac{0.92 \cdot 0.5 \cdot 64860}{0.92 \cdot 0.5 \cdot 64860 + 1 \cdot 0.5 \cdot 186700} \cdot 0.09447 + \frac{1 \cdot 0.5 \cdot 186700}{0.92 \cdot 0.5 \cdot 64860 + 1 \cdot 0.5 \cdot 186700} \cdot 0.56565 = 0.45$$

Predicted CIE (x,y) sample calculation for $\chi_{perylene} : \chi_{R6G} = 0.5{:}0.5$ @ $\lambda_{ex} = 367$ nm using Eq. S1 and Eq. S2:

$$x_{mix} = \frac{0.92 \cdot 0.5 \cdot 197400}{0.92 \cdot 0.5 \cdot 197400 + 1 \cdot 0.5 \cdot 38850} \cdot 0.14303 + \frac{1 \cdot 0.5 \cdot 38850}{0.92 \cdot 0.5 \cdot 197400 + 1 \cdot 0.5 \cdot 38850} \cdot 0.42455 = 0.19$$

$$y_{mix} = \frac{0.92 \cdot 0.5 \cdot 197400}{0.92 \cdot 0.5 \cdot 197400 + 1 \cdot 0.5 \cdot 38850} \cdot 0.09447 + \frac{1 \cdot 0.5 \cdot 38850}{0.92 \cdot 0.5 \cdot 197400 + 1 \cdot 0.5 \cdot 38850} \cdot 0.56565 = 0.18$$

(a)

R² = 0.9975

(b)
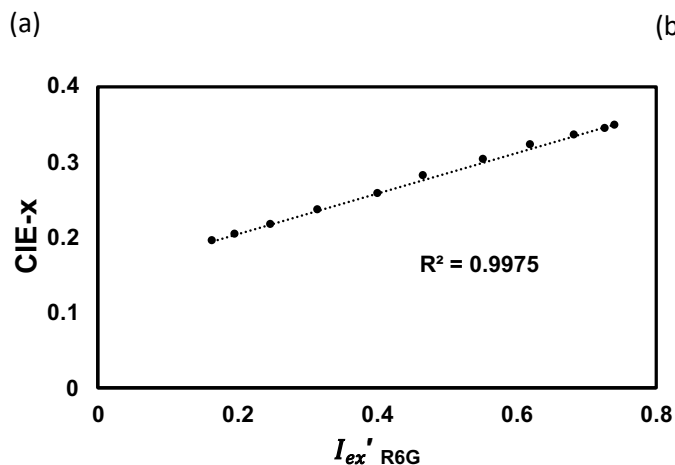
λ_{ex} (nm)	I_{ex}' R6G	CIE-x
367	0.164	0.19335
365	0.196	0.20245
363	0.247	0.21582
361	0.315	0.23511
359	0.401	0.25754
357	0.467	0.28113
355	0.554	0.30269
353	0.62	0.32023
351	0.684	0.33371
349	0.728	0.34185
347	0.742	0.34619

Figure S27. a) Scatter plot showing the linear dependence (R^2 = 0.9975) of CIE-x on the relative excitation intensity of R6G ($I'_{ex, R6G}$). Obtained from exciting a mixture of perylene-R6G with equivalent mole fractions between the range of 347 to 367 nm. b) Tabulated data showing the relative excitation intensity of R6G ($I'_{ex,R6G} = \frac{I_{ex,R6G}}{I_{ex,perylene} + I_{ex,R6G}}$) at various excitation wavelengths and the measured CIE-x coordinates.

Perylene and Nile Red (NR) Mixing Experiment

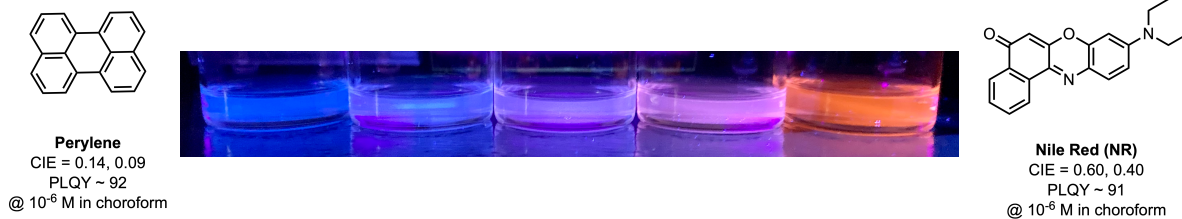**Perylene**
CIE = 0.14, 0.09
PLQY ~ 92
@ 10^{-6} M in choroform

Nile Red (NR)
CIE = 0.60, 0.40
PLQY ~ 91
@ 10^{-6} M in choroform

Figure S28. (From left to right) Perylene (1.2 x 10^{-6} M), Perylene: NR (0.9 x 10^{-6} M: 0.3 x 10^{-6} M), Perylene: NR (0.6 x 10^{-6} M: 0.6 x 10^{-6} M), Perylene: NR (0.3 x 10^{-6} M: 0.9 x 10^{-6} M), and NR (1.2 x 10^{-6} M) irradiated with a long wave UV-lamp at 365 nm.
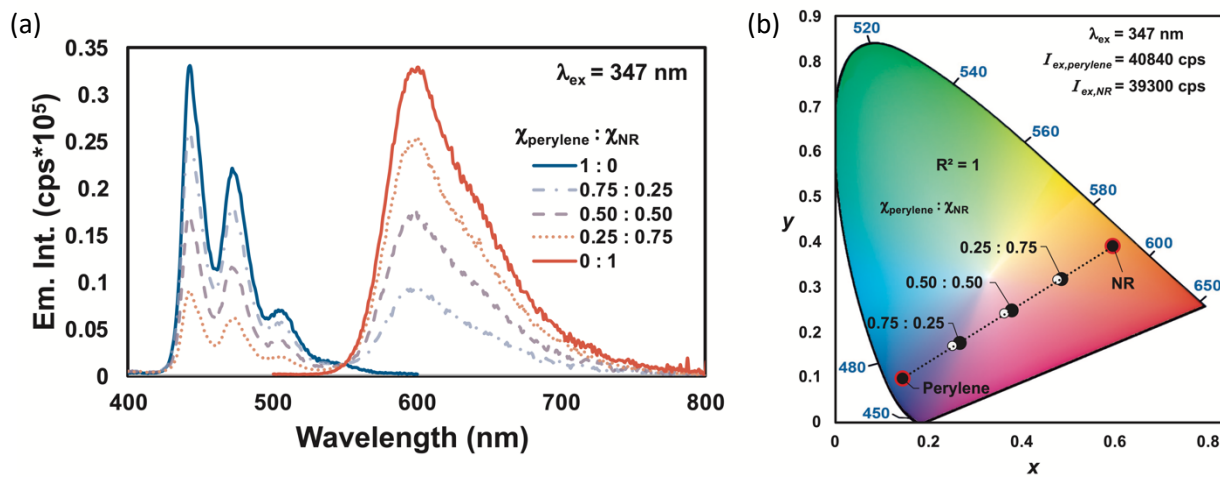

Figure S29. a) Perylene-NR emission scans (λ_{ex} 347 nm) with differing mole fractions ($\chi_{perylene}$: χ_{NR}) and (b) the corresponding CIE diagram showing the measured (●) and predicted (○) CIE coordinates. R^2 value (1) was obtained from measured data.

**Table S7**. Tabulated results obtained from Perylene-NR PLCT mixing studies (λ_{ex} = 347 nm). [a]

Mole Fractions (χ) Perylene to NR	λ_{ex} = 347 nm		
	Measured CIE (x,y)	Expected [b] CIE (x,y)	Absolute [c] Error
1 to 0	0.14513, 0.09638	-	-
0.75 to 0.25	0.27, 0.18 (0.26826, 0.17569)	0.25, 0.17	0.02 (0.016)
0.50 to 0.50	0.38, 0.25 (0.38069, 0.24836)	0.37, 0.24	0.02 (0.017)
0.25 to 0.75	0.49, 0.32 (0.48703, 0.31753)	0.48, 0.31	< 0.01 (0.008)
0 to 1	0.59787, 0.39000	-	-

[a] Reported solution data was measured in chloroform at a tot. molecular conc. of 1.2 x 10⁻⁶ M. Total molecular concentration was held constant while the mole fractions (χ) each component was varied. [b] **Expected CIE (x,y) were calculated based on the measured properties of perylene ($CIE_{perylene}$ = 0.14513, 0.09638; $I_{ex,perylene}$ = 40840 cps at λ_{ex} 347 nm; $\phi_{perylene}$ = 0.92; and χ_i given in the table) and NR (CIE_{NR} = 0.59787, 0.39000; $I_{ex,NR}$ = 39300 cps at λ_{ex} 347 nm; ϕ_{NR} = 0.91; and χ_i given in the table) using Eq. 1.** [c] Absolute error was calculated based on the distance (d) between expected and measured CIE coordinates using $d = \sqrt{(x_2 - x_1)^2 + (y_2 - y_1)^2}$.

Predicted CIE (x,y) sample calculation for $\chi_{perylene} : \chi_{NR} = 0.5:0.5$ using Eq. S1 and Eq. S2:

$$x_{mix} = \frac{0.92 \cdot 0.5 \cdot 40840}{0.92 \cdot 0.5 \cdot 40840 + 0.91 \cdot 0.5 \cdot 39300} \cdot 0.14513 + \frac{0.91 \cdot 0.5 \cdot 39300}{0.92 \cdot 0.5 \cdot 40840 + 0.91 \cdot 0.5 \cdot 39300} \cdot 0.59787 = 0.37$$

$$y_{mix} = \frac{0.92 \cdot 0.5 \cdot 40840}{0.92 \cdot 0.5 \cdot 40840 + 0.91 \cdot 0.5 \cdot 39300} \cdot 0.09638 + \frac{0.91 \cdot 0.5 \cdot 39300}{0.92 \cdot 0.5 \cdot 40840 + 0.91 \cdot 0.5 \cdot 39300} \cdot 0.39000 = 0.24$$
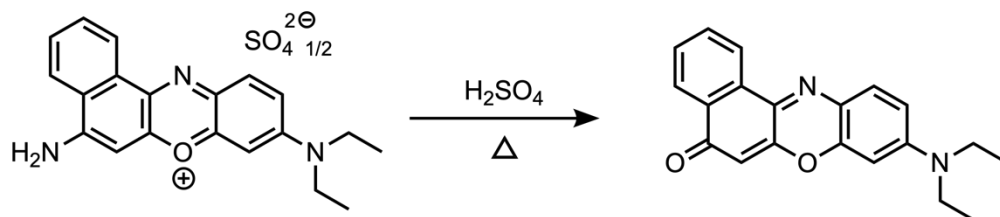
(a)

(b)
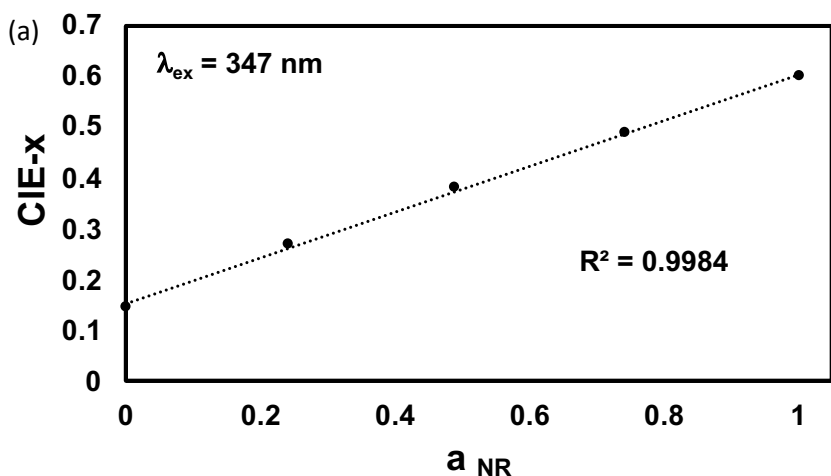
χ_{NR}	a_{NR}	Measured CIE-x
0	0	0.14513
0.25	0.241	0.26826
0.5	0.488	0.38069
0.75	0.741	0.48703
1	1	0.59787

Figure S30. a) Scatter plot showing the linear dependence (R^2 = 0.9984) of the measured CIE-x on the *relative brightness* of NR ($a_{NR} = \frac{\phi_{NR} \cdot I_{ex,NR} \cdot \chi_{NR}}{\sum \phi_i \cdot I_{ex,i} \cdot \chi_i}$) when excited at 347 nm and b) the corresponding tabulated data.

Synthesis of Nile Red[1]

Nile red: Nile blue sulfate (2.006 g, 2.737 mmol) was added to a 250 mL two-neck flask fitted with a condenser and magnetic stir bar. The flask was charged with 0.5 M H_2SO_4 (125 mL), stirring was initiated, and the temperature was ramped to achieve reflux. After 4 hr, the mixture was transferred to a separatory funnel, extracted with DCM (200 mL), and washed with H_2O (3 x 50 mL) and brine (1 x 50 mL). The organic phase was dried over $MgSO_4$, filtered, and dry-loaded onto celite for column chromatography (2:8 v/v EtOAc: Hexanes). A purple solid (0.248 g, 0.779 mmol; 14 % yield) was isolated (R_f = 0.54; 4:6 v/v EtOAc: Hexanes). ^{1}H NMR (CDCl$_3$, 400 MHz) δ 8.66 (dd, 1H), 8.31 (dd, 1H), 7.72 (m, 1H), 7.65 (m, 1H), 7.62 (d, *J* = 9.2 Hz, 1H), 6.68 (dd, *J* = 9.2, 2.8 Hz, 1H), 6.49 (d, *J* = 2.8 Hz, 1H), 6.39 (s, 1H), 3.48 (q, *J* = 7.1 Hz, 4H), 1.27 (t, *J* = 7.1 Hz, 6H); ^{13}C NMR (CDCl$_3$, 101 MHz) δ 183.9, 152.3, 150.9, 147.0, 140.2, 132.2, 131.9, 131.5, 131.3, 130.1, 125.9, 125.1, 123.9, 109.8, 105.9, 96.5, 45.2, 12.8. Both, ^{1}H and ^{13}C spectra were in agreement with previously reported literature spectra.[2]
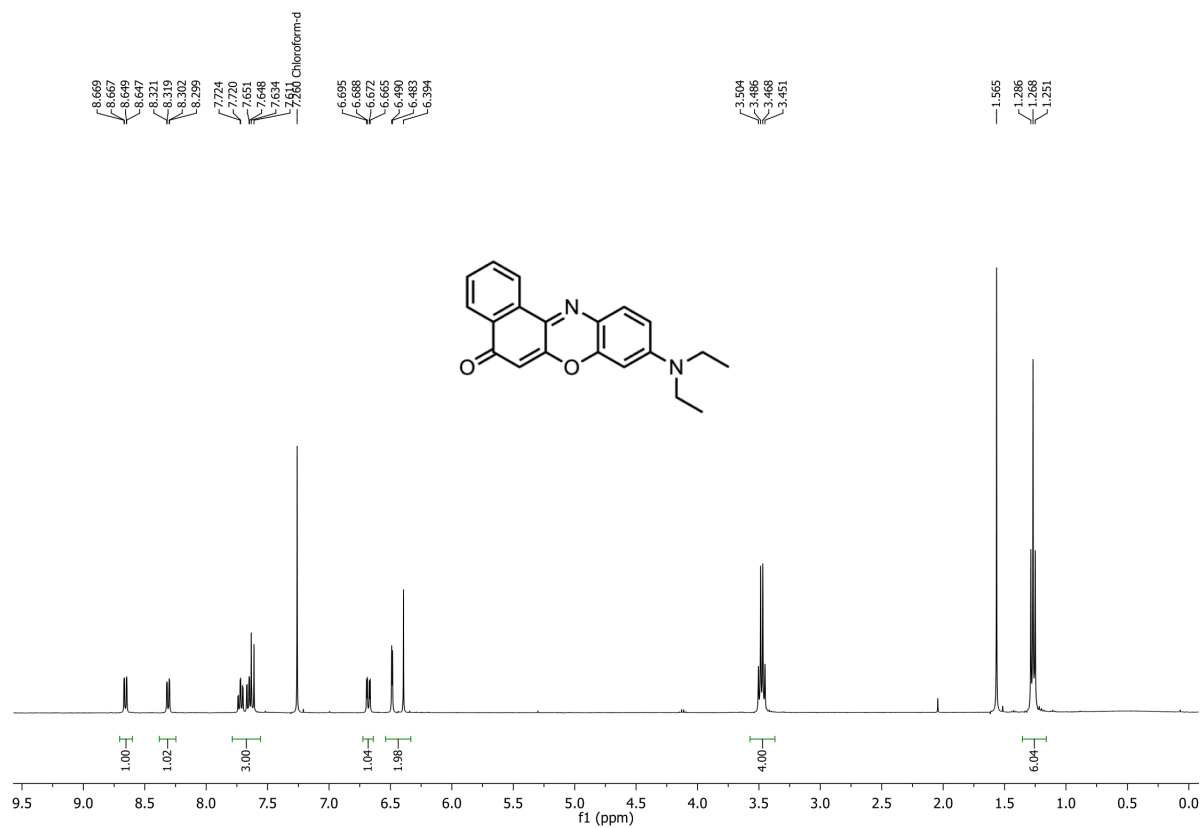
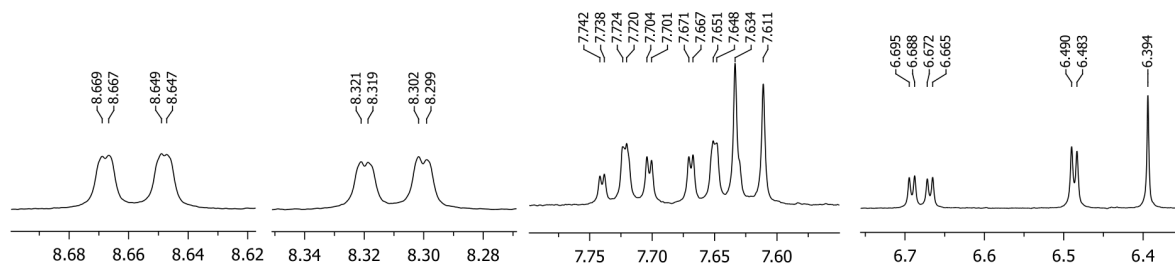**Figure S31**. ^{1}H NMR (CDCl$_3$, 400 MHz) spectrum of Nile Red.

Figure S32. ^{1}H NMR (CDCl$_3$, 400 MHz) spectrum of Nile Red.
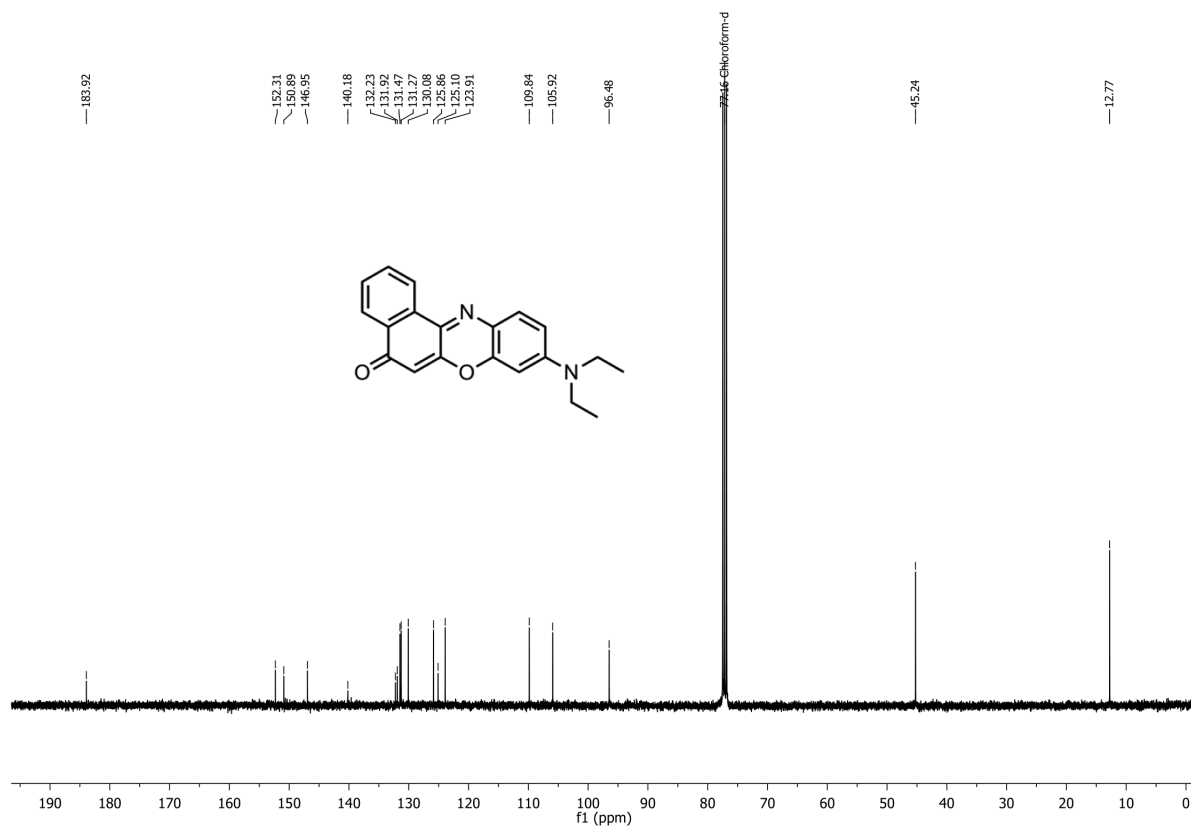
Figure S33. ^{13}C NMR (CDCl$_3$, 101 MHz) spectrum of Nile Red.
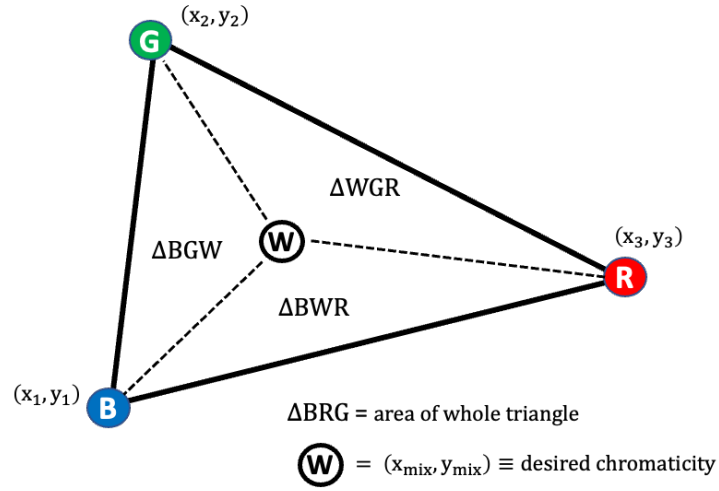
Three-component PLCT

Figure S34. Representation of the *emission* color gamut available by mixing blue (B), green (G), and red (R) PL emitters.

$$W = a_1 B + a_2 G + a_3 R \qquad \text{(Eq. S3)}$$

$$(x_{mix}, y_{mix}) = a_1(x_1, y_1) + a_2(x_2, y_2) + a_3(x_3, y_3) \qquad \text{(Eq. S4)}$$

$$a_1 = \frac{\Delta WGR}{\Delta BRG} = \frac{\left\| \overrightarrow{WG} \times \overrightarrow{WR} \right\|}{\left\| \overrightarrow{BR} \times \overrightarrow{BG} \right\|} = \frac{(x_2 - x_{mix})(y_3 - y_{mix}) - (x_3 - x_{mix})(y_2 - y_{mix})}{(x_2 - x_1)(y_3 - y_1) - (x_3 - x_1)(y_2 - y_1)} \qquad \text{(Eq. S5)}$$

$$a_2 = \frac{\Delta BWR}{\Delta BRG} = \frac{\left\| \overrightarrow{BW} \times \overrightarrow{BR} \right\|}{\left\| \overrightarrow{BR} \times \overrightarrow{BG} \right\|} = \frac{(x_{mix} - x_1)(y_3 - y_1) - (x_3 - x_1)(y_{mix} - y_1)}{(x_2 - x_1)(y_3 - y_1) - (x_3 - x_1)(y_2 - y_1)} \qquad \text{(Eq. S6)}$$

$$a_3 = \frac{\Delta BGW}{\Delta BRG} = \frac{\left\| \overrightarrow{BG} \times \overrightarrow{BW} \right\|}{\left\| \overrightarrow{BR} \times \overrightarrow{BG} \right\|} = \frac{(x_2 - x_1)(y_{mix} - y_1) - (x_{mix} - x_1)(y_2 - y_1)}{(x_2 - x_1)(y_3 - y_1) - (x_3 - x_1)(y_2 - y_1)} \qquad \text{(Eq. S7)}$$

$$a_1 = c_B \cdot \phi_B \cdot I_{ex,B} \qquad \text{(Eq. S8)}$$

$$a_2 = c_G \cdot \phi_G \cdot I_{ex,G} \qquad \text{(Eq. S9)}$$

$$a_3 = c_R \cdot \phi_R \cdot I_{ex,R} \qquad \text{(Eq. S10)}$$

Determining the composition of emitters required to achieve WLE (0.33,0.33) using $\lambda_{ex} = 274 \, nm$

1. Based on the CIE coordinates of perylene (0.14354, 0.09327), C6 (0.18737, 0.52564), and NR (0.60351, 0.39447), the *normalized* contributions of each emitter were calculated using Eq S5–S6, respectively.

$$a_{perylene} = 0.34$$
$$a_{C6} = 0.28$$
$$a_{NR} = 0.38$$

2. An arbitrary concentration of perylene was chosen ($c_{perylene}$ = 4 x 10^{-7} M) and $a_{perylene}$ was calculated using Eq. S7.

$$a_{perylene} = \phi_{perylene} \cdot c_{perylene} \cdot I_{ex,perylene}$$
$$a_{perylene} = 0.92 \cdot (4 \times 10^{-7}M) \cdot 99590 \, cps = 0.03664912$$

3. Since $a_{C6} = \frac{0.28}{0.34} a_{perylene}$, Eq. S8 can be rewritten as:

$$a_{C6} = \frac{0.28}{0.34}(0.03664912) = \phi_{C6} \cdot c_{C6} \cdot I_{ex,C6}$$

4. Plugging in $\phi_{C6} = 0.92$ and $I_{ex,C6} = 130500 \, cps$ into Eq. S8 and rearranging to solve for c_{C6}:

$$c_{C6} = \frac{\frac{0.28}{0.34}(0.03664912)}{0.92 \cdot 130500} = 2.51 \times 10^{-7}M$$

5. Similarly, since $a_{NR} = \frac{0.38}{0.34} a_{perylene}$, Eq. S9 can be rewritten as:

$$a_{NR} = \frac{0.38}{0.34}(0.03664912) = \phi_{NR} \cdot c_{NR} \cdot I_{ex,NR}$$

6. Plugging in $\phi_{NR} = 0.91$ and $I_{ex,NR} = 137900 \, cps$ into Eq. S9 and rearranging to solve for c_{NR}:

$$c_{NR} = \frac{\frac{0.38}{0.34}(0.03664912)}{0.91 \cdot 137900} = 3.26 \times 10^{-7}M$$

7. Therefore, with an $\lambda_{ex} = 274 \, nm$, the χ_i of each component required to achieve WLE:

$$\chi_{perylene} = \frac{c_{perylene}}{\sum c_i} = 0.409 \approx 0.41$$

$$\chi_{C6} = \frac{c_{C6}}{\sum c_i} = 0.257 \approx 0.26$$

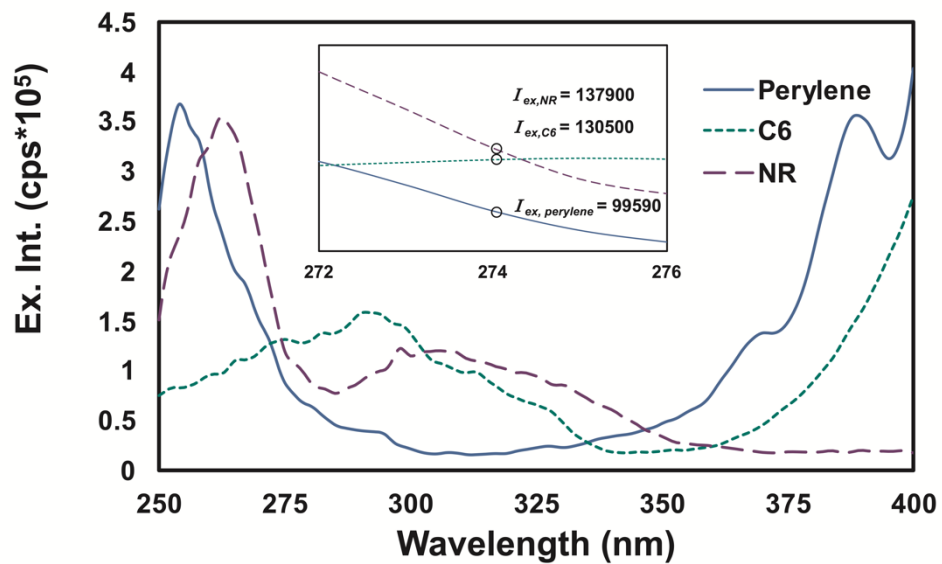$$\chi_{NR} = \frac{c_{NR}}{\sum c_i} = 0.334 \approx 0.33$$

Figure S35. Overlaid excitation scans of perylene (λ_{em} = 443 nm), C6 (λ_{em} = 491 nm), and NR (λ_{em} = 597) in chloroform (c = 1.2 x 10^{-6} M). Excitation intensities at 274 nm for each emitter ($I_{ex,perylene}$ = 99590 cps, $I_{ex,C6}$ = 130500 cps, $I_{ex,NR}$ = 137900 cps) are highlighted in the inset.

References

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