Included in this dataset are three Excel spreadsheets containing, in separate tabs: the UV/Vis absorbance spectrum of the acceptor+peptide molecule and calculated epsilon (spectrum normalised to molar extinction coefficient of acceptor), the raw and normalised fluorescence emission spectra of the donor+peptide molecule, the calculated overlap (), and the raw fluorescence emission spectrum of the acceptor+peptide+donor molecule. A tab labelled values lists the values taken from literature to carry out calculations alongside values taken/calculated from the collected data.

For each pair, the Förster distance () was calculated with , where = dipole orientation factor ( taken to be 2/3), = fluorescence quantum yield of donor in absence of acceptor, = refractive index of medium, and = spectral overlap integral, calculated with , where normalized donor emission spectrum, = acceptor absorption spectrum normalized to molar extinction coefficient of acceptor. FRET efficiency (), is typically calculated from a fluorescence quenching or enhancement using Equation S1 and S2, respectively:

E**quation S1**

**Equation S2**

where is the fluorescence emission from the donor alone, and is the fluorescence emission from the donor in the presence of the acceptor. In all cases, *FD* and *FDA* were corrected for concentration and as described below, in some cases these fluorescence emission values were also corrected for background signal by subtracting the counts measured at the lowest wavelength of the emission scan.The donor-to-acceptor distance () is calculated using the FRET efficiency using:

.

In addition, there are Excel spreadsheets tabulating raw spectral data concerned with relative determination of the fluorescence quantum yield of EB (as compared to rhodamine 6G (R6G)), as well as steady state fluorescence anisotropy measurements for each of the compounds **[1]-[5]**.

In the spreadsheet titled “QYdetermination.xlsx” the UV/Vis and fluorescence emission spectra of **[3]**, unbound TPP, R6G, and **[5]**, at concentrations of 2M, 2M, 0.25M, and 20M respectively, are given in separate tabs. Quantum yield of **[3]** and **[5]** then determined by the following:

Where Q = fluorescence quantum yield, I = integrated fluorescence emission intensity, OD = optical density, n = refractive index of medium, and subscript R refers to the reference standard. Literature value of 0.98 taken for , and 0.13 for .

In the spreadsheet titled “Anisotropy.xlsx” fluorescence emission scans recorded for each sample **[1]**-**[5]** in four polarisation configurations (V = vertical polariser rotation, H = horizontal polarizer rotation, first subscript = excitation polariser, second subscript = emission polariser ): , , , and . Samples of compounds **[1]**,**[2]**, and **[4]** were 40M, 10 M for **[5]**, and 2 M for **[3]**.

Steady state anisotropy for a given emission wavelength () then determined by:

Resultant anisotropy plots recorded in separate tabs of the spreadsheet. Average anisotropy values reported were averaged across the following wavelengths:

|  |  |
| --- | --- |
| EB-pep **[5]** | 540-590 nm |
| TPP-pep **[3]** | 645-670 nm + 700-725nm |
| ZnTPP-pep **[4]** | 580-630 nm |
| EB-pep-TPP **[2]** | 540-590 nm (EB region), 645-670 nm + 700-725nm (TPP region) |
| TPP-pep-ZnTPP **[1]** | 580-630 nm (ZnTPP region),  645-670 nm + 700-725 nm (TPP region) |