Electronic Supplementary Information

Effect on the conformation of monosubstituted pillar[5]arene:

Solvent, temperature, concentration, and length of linker

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Characterization

Figure S1. $^1$H NMR of M1.

Figure S2. $^1$H NMR of P1.
Figure S3. MS of P1.

Figure S4. HRMS of P1.
Figure S5. $^1$H NMR of PI1.

Figure S6. $^{13}$C NMR of PI1.
Figure S7. HRMS of PI1.

Figure S8. $^1$H NMR of M2.
Figure S9. \textsuperscript{1}H NMR of P2.

Figure S10. \textsuperscript{13}C NMR of P2.
Figure S11. MS of P2.

Figure S12. HRMS of P2.
Figure S13. $^1$H NMR of PI2.

Figure S14. $^{13}$C NMR of PI2.
Figure S15. HRMS of PI2.

Figure S16. $^1$H NMR of M3.
Figure S17. $^1$H NMR of P3.

Figure S18. $^{13}$C NMR of P3.
Figure S19. MS of P3.

Figure S20. HRMS of P3.
Figure S21. $^1$H NMR of PI3.

Figure S22. $^{13}$C NMR of PI3.
Figure S23. HRMS of PI3.

Figure S24. $^1$H NMR of M4.
Figure S25. $^1$H NMR of P4.

Figure S26. $^{13}$C NMR of P4.
Figure S27. MS of P4.

Figure S28. HRMS of P4.
Figure S29. $^1$H NMR of PI4.

Figure S30. $^{13}$C NMR of PI4.
Figure S31. HRMS of PI4.
Linker length

![Fluorescence emission spectra of the monosubstituted pillar[5]arene PLn (20 µM) in DMSO at 25°C.](image1)

**Fig. S32** Fluorescence emission spectra of the monosubstituted pillar[5]arene PLn (20 µM) in DMSO at 25°C.

![Fluorescence emission spectra of the monosubstituted pillar[5]arene PLn (20 µM) in chloroform at 25°C.](image2)

**Fig. S33** Fluorescence emission spectra of the monosubstituted pillar[5]arene PLn (20 µM) in chloroform at 25°C.
Solvent

Fig. S34 Fluorescence emission spectra of PI1 (20 μM) in various solvents.

Fig. S35 Fluorescence emission spectra of PI2 (20 μM) in various solvents.
Fig. S36 Fluorescence emission spectra of PI3 (20 μM) in various solvents.

Fig. S37 Fluorescence emission spectra of PI4 (20 μM) in various solvents.
Stoke shift and quantum yield

Table S1. Stoke shifts of PI\textsubscript{n} and DASP.

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The fluorescence quantum yield (\(\phi\)) is determined with the following equation-1,

\[ \phi_F = \frac{\phi_R (n_S^2 \times F \times A_R)}{(n_R^2 \times F_R \times A)} \quad (\text{equation-1}) \]

Where \(\phi_R\) is the fluorescence quantum yield of the reference compound (luciferin in ethanol), \(F\) and \(F_R\) are the integrated values of the fluorescence spectra for the sample and reference, \(A\) and \(A_R\) are the absorbance at the excitation wavelength, and \(n\) and \(n_R\) are the refractive indexes of the solvents.
NOESY

Fig. S38 NOESY spectrum of PI1 (50 mM, in DMSO)

Fig. S39 NOESY spectrum of PI2 (50 mM, in DMSO)
Fig. S40 NOESY spectrum of PI3 (50 mM, in DMSO)

Fig. S41 NOESY spectrum of PI4 (50 mM, in DMSO)
Fig. S42 NOESY spectrum of PI1 (50 mM, in CDCl₃)

Fig. S43 NOESY spectrum of PI2 (50 mM, in CDCl₃)
Fig. S44 NOESY spectrum of PI3 (50 mM, in CDCl$_3$)

Fig. S45 NOESY spectrum of PI4 (50 mM, in CDCl$_3$)
**Temperature**

Fig. S46 Partial $^1$H NMR spectra of PI1 at various temperature in CDCl$_3$.

Fig. S47 Partial $^1$H NMR spectra of PI3 at various temperature in CDCl$_3$. 
Fig. S48 Partial $^1$H NMR spectra of PI2 at various temperature in DMSO.

Fig. S49 Partial $^1$H NMR spectra of PI2 at various temperature in CDCl3.
**Temperature**

Fig. S50 Fluorescence emission spectra of \textbf{PI1} (20 $\mu$M) at various temperature in chloroform.

Fig. S51 Fluorescence emission spectra of \textbf{PI2} (20 $\mu$M) at various temperature in chloroform.
Fig. S52 Fluorescence emission spectra of PI3 (20 μM) at various temperature in chloroform.

Fig. S53 Fluorescence emission spectra of PI4 (20 μM) at various temperature in chloroform.
Concentration

Fig. S54 PI1 in DMSO at various concentration.

Fig. S55 PI2 in DMSO at various concentration.
Fig. S56 PI3 in DMSO at various concentration.

Fig. S57 PI4 in DMSO at various concentration.

Fig. S58 PI1 in CDCl3 at various concentration.
Fig. S59 PI2 in CDCl3 at various concentration.

Fig. S60 PI3 in CDCl3 at various concentration.
Fig. S61 2D Dosy of PI1 in CDCl3.

Fig. S62 2D Dosy of PI2 in CDCl3.
Fig. S63 2D Dossy of PI3 in CDCl₃.

Fig. S64 2D Dossy of PI4 in DMSO.