Supporting Information:

**Fig. S1:** pH titration curve for CBS-NH$_2$.
Fig. S2: pH titration curve for CBS-KKF-NH₂.

\[ pK_a (\text{NaOH}) = 6.27 \quad \text{and} \quad pK_a (\text{HCl}) = 6.57 \]
Fig. S3: UV Raman spectra of CBS-NH$_2$ (1 mM in water) in the range pH 2 to pH 10.
Fig. S4: NMR titration results for CBS-NH$_2$. The inset shows an enlarged view of the region 6.7 ppm – 7.1 ppm together with the structure of CBS-NH$_2$ including information on proton assignment and proton exchange.
Fig. S5: Electronic absorption spectra of CBS-NH$_2$ from pH 2 -10.