SUPPORTING INFORMATION

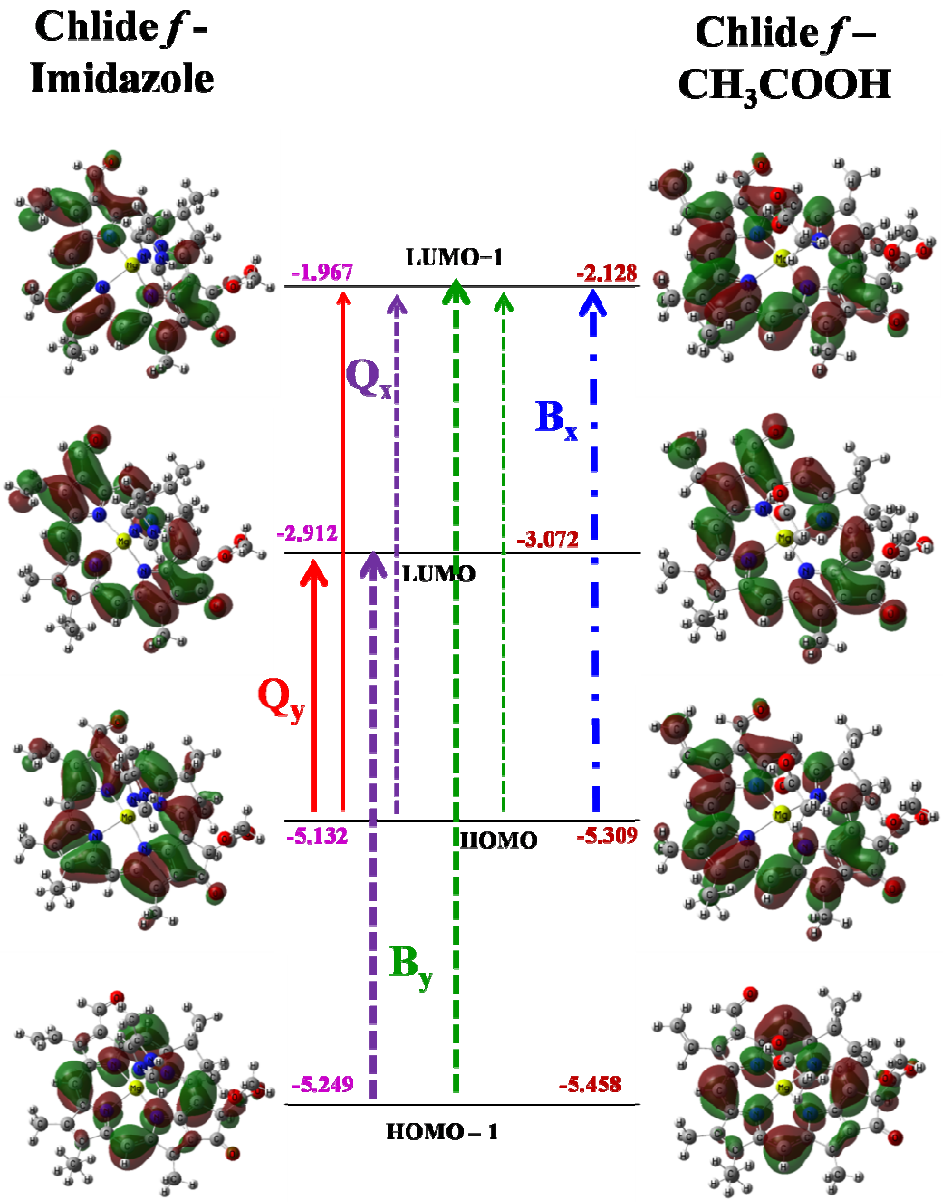

Figure S1. Orbital excitation plots of Chlide *f* -Imidazole and Chlide *f*-CH_3COOH. Corresponding MO pictures and MO energies (eV) are shown. The strength of the excitation line reflects its contribution for that absorbance band. Note that this plot clearly shows that the axial ligations do not have much contribution to absorption spectra. Isocontour values used for molecular orbital plots is = 0.02 e Bohr^{-3}

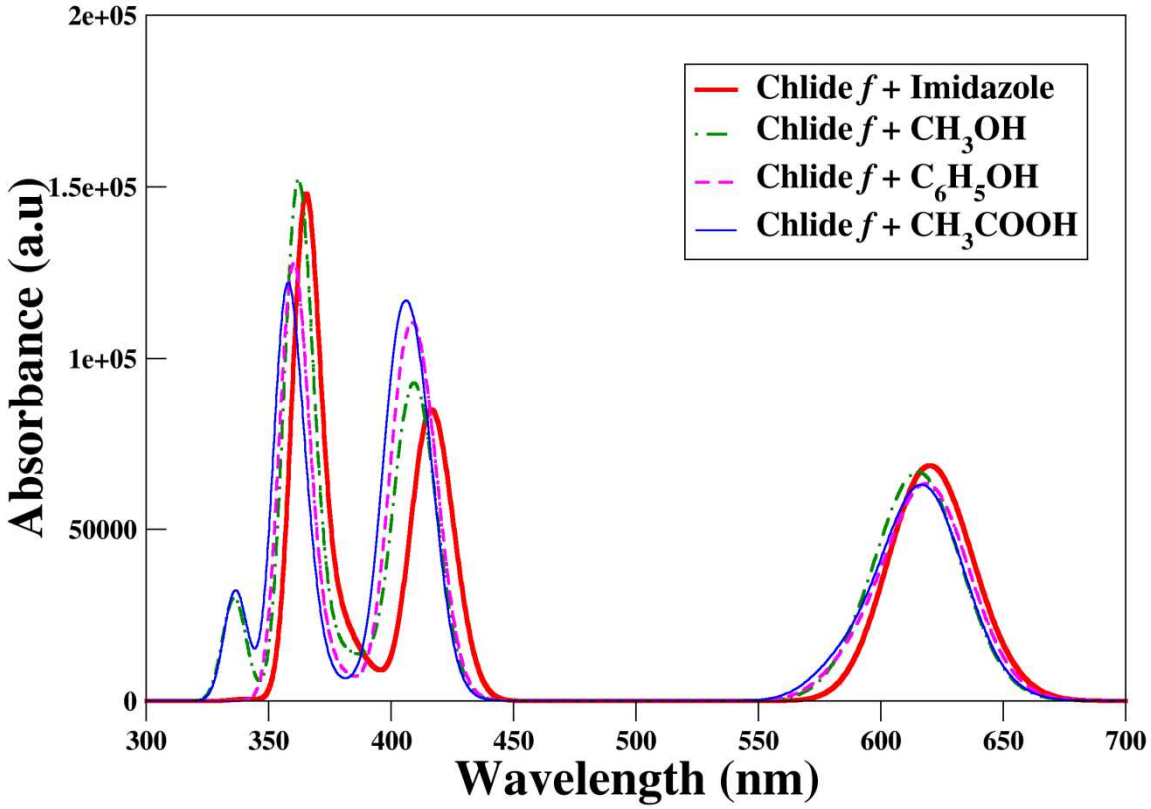

Figure S2. Absorption spectra of axial ligated Chlide *f*- (a) Imidazole, (b) CH_3OH, (c) C_6H_5OH and (d) CH_3COOH molecules. FWHM = 1000 cm^{-1}

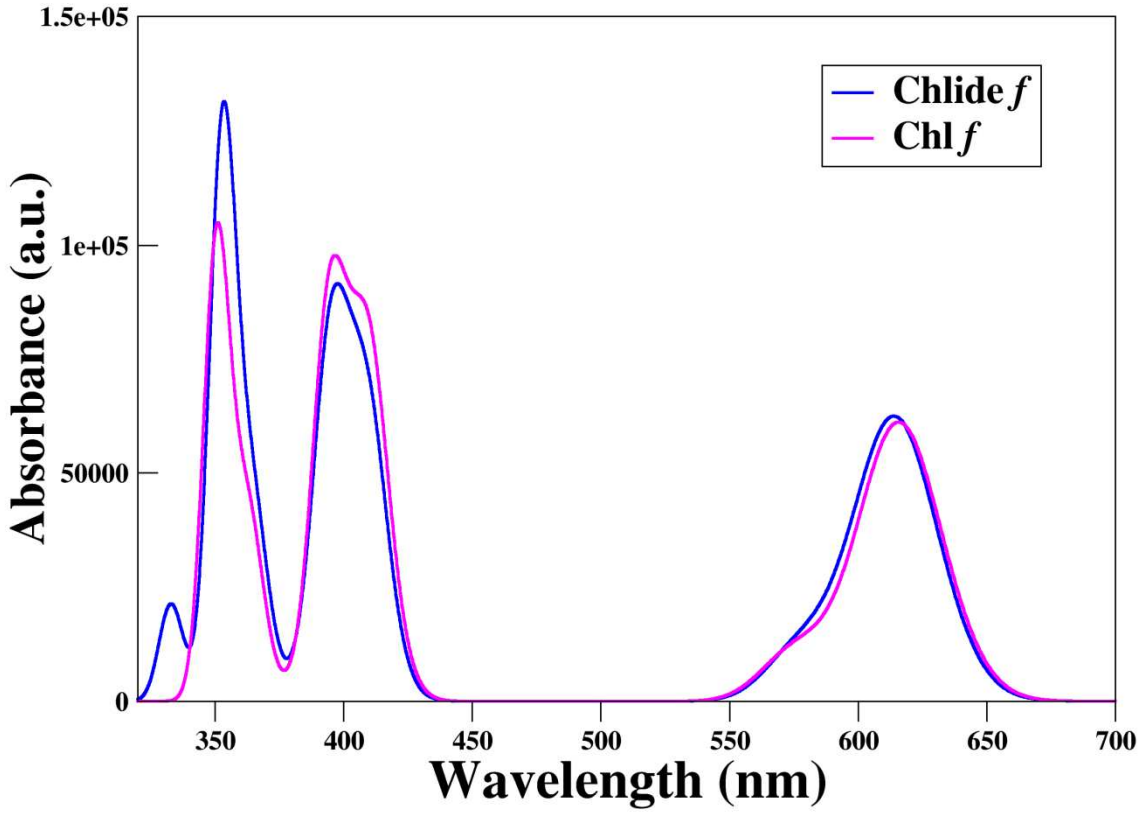

Figure S3. Absorption spectra of chl *f* and Chlide *f* molecules. FWHM = 1000 cm^{-1}

In order to see whether the consideration of the substituent at c17 of ring II will change the absorption spectrum of Chlide *f*, we performed calculations on chl *f* (i.e. with the substituent at the 17th carbon of ring II) with the same level of theory used for Chlide *f*. As expected, there is no much change in the position of the bands after the addition of c17 substituent to Chlide *f*. Line width in figure S3 is 1000 cm^{-1}.

The changes in the position of bands can be seen in the Figure S3, S4 and in Table S1. As can be noted from the Table S1and from figure S4, all the bands in chl *f* are red/blue shifted within 1-2 nm.

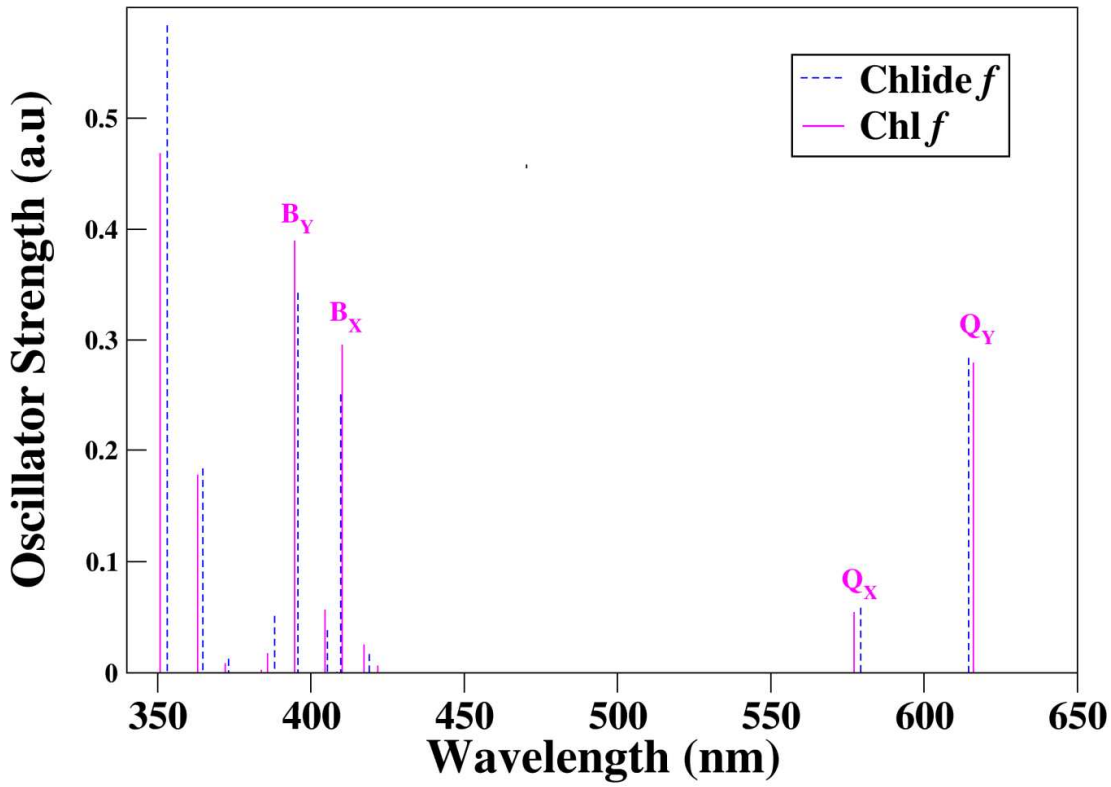

Figure S4. TDDFT computed electronic transitions of chl *f* and Chlide *f* molecules. Bands are assigned.

Molecules	Nature	Excitation Wavelength (nm)	Major molecular orbital contributions
Chl *f*	Q_y	616	H to L (0.72)
	Q_x	577	H-1 to L (0.72) and H to L + 1 (0.20)
	B_y	395	H–1 to L+1 (0.62)
	B_x	351	H to L+1 (0.50)
Chlide *f*	Q_y	615	H to L (0.72)
	Q_x	579	H-1 to L (0.73) and H to L + 1 (0.19)
	B_y	396	H–1 to L+1 (0.61)
	B_x	409	H to L+1 (0.51)

Table S1: Q and B bands of Chl *f* and Chlide *f*. Here 'H' stands for HOMO and 'L' stands for LUMO.