

SUPPORTING INFORMATION

Synthesis and spectroscopic properties of carotenoid bis-phenylhydrazone astaxanthin: Extending conjugation to a C=N group

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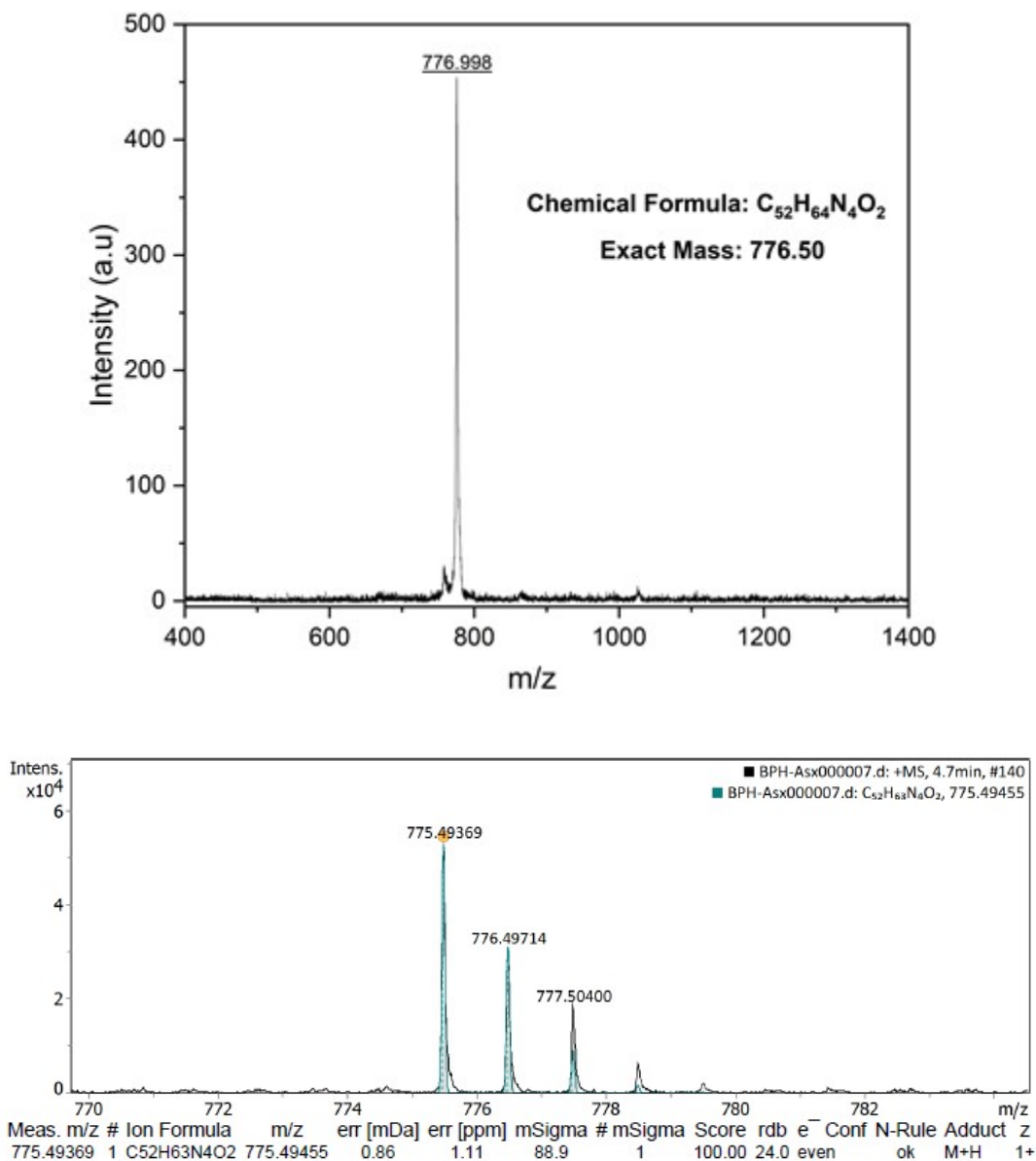


Figure S1: Top: Positive ion and linear mode MALDI TOF-MS spectrum of **BPH-Asx**. Bottom: ESI-MS Spectrum of **BPH-Asx** demonstrating difference between experimental and calculated mass of 1.1 ppm.

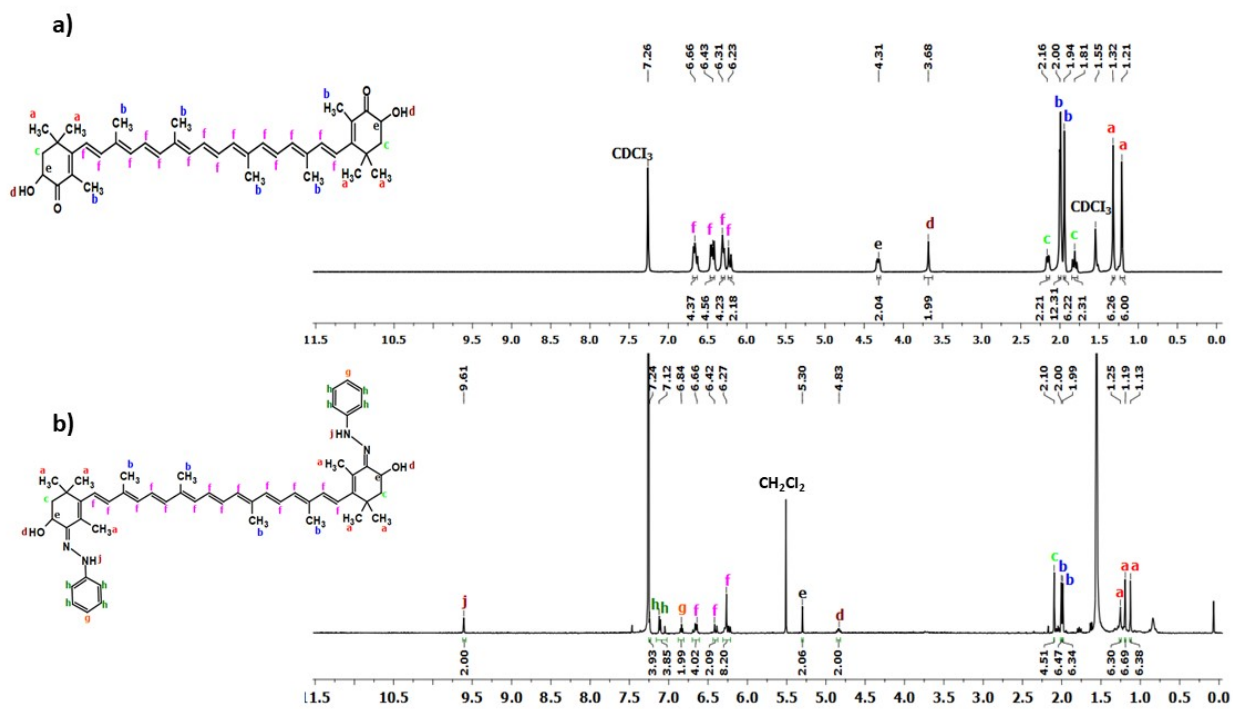


Figure S2: ^1H NMR Spectrum of a) **Asx** b) **BPH-Asx** in CDCl_3 .

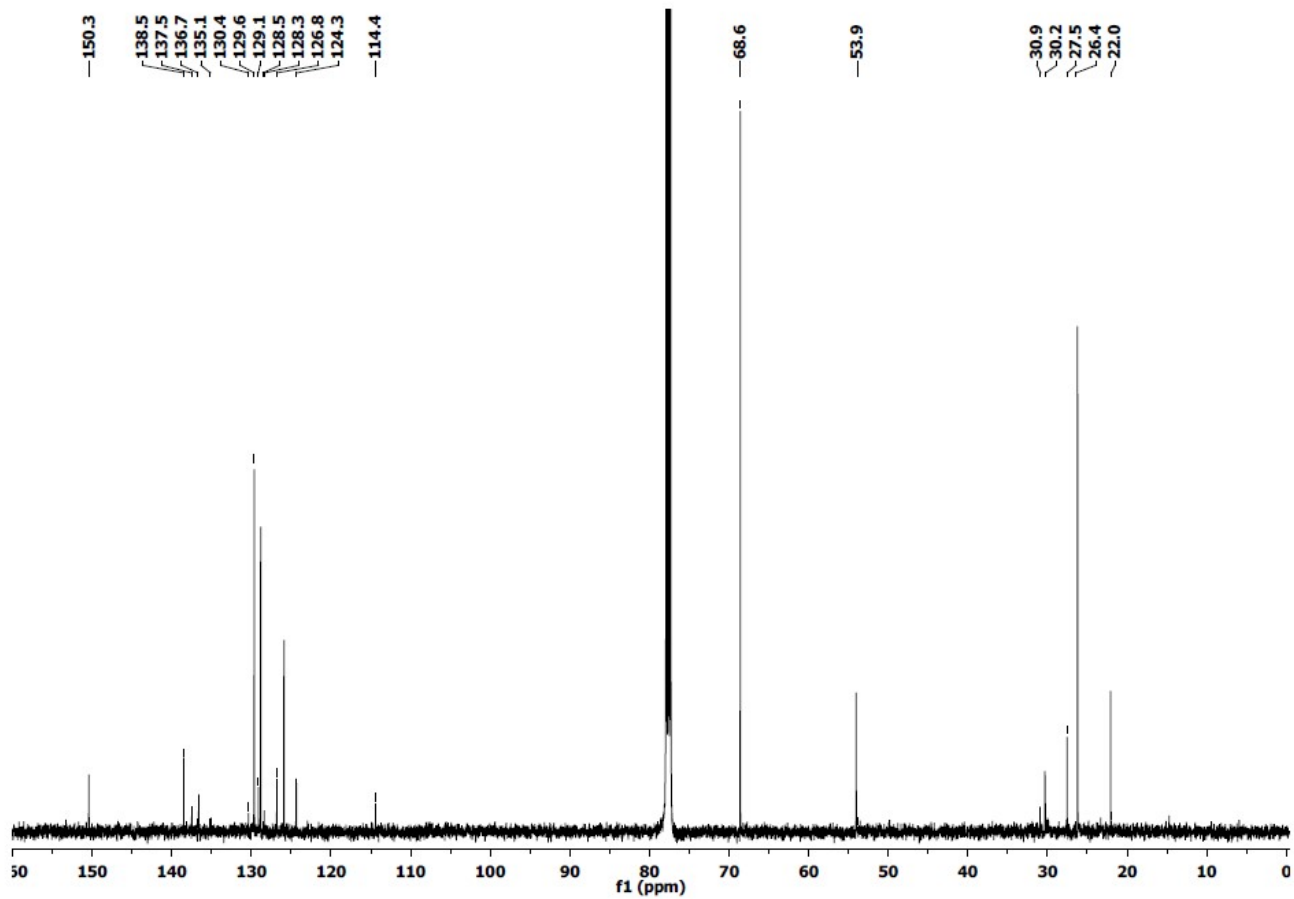


Figure S3: ^{13}C NMR Spectrum of BPH-Asx in CDCl_3 .

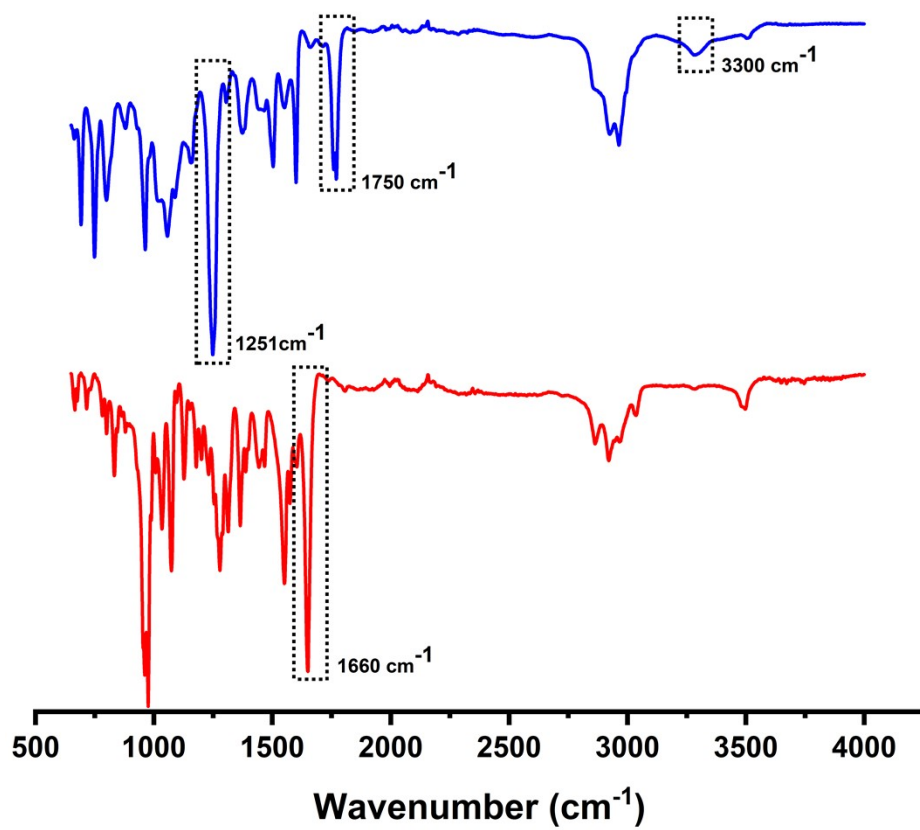


Figure S4: FT-IR Spectrum of **Asx** (red) and **BPH-Asx** (blue).

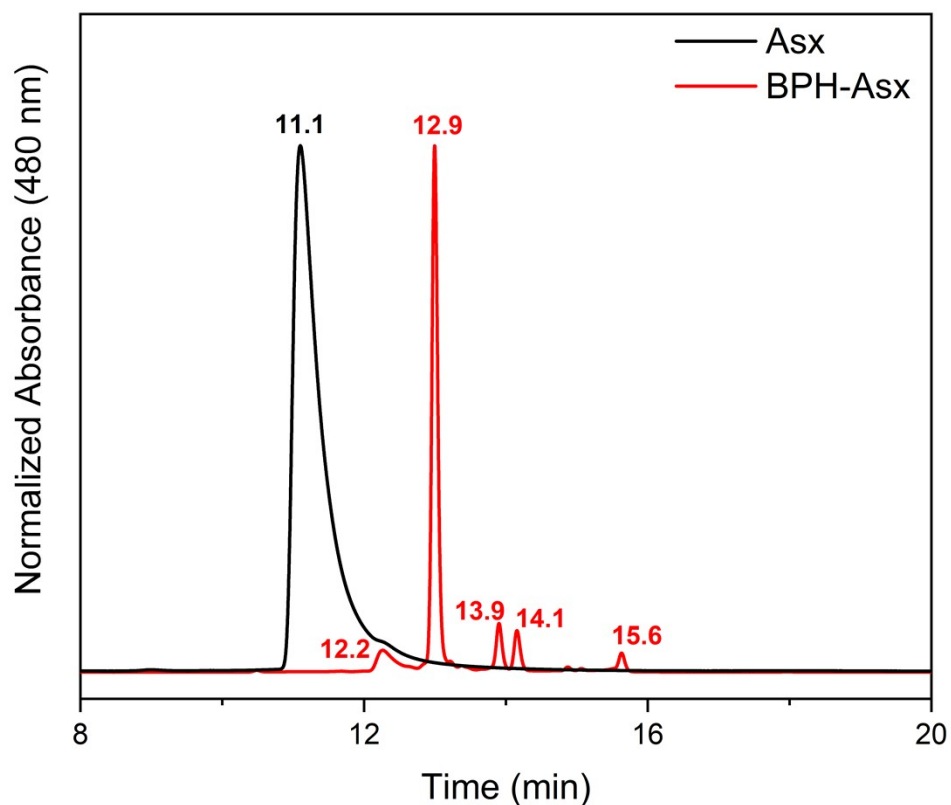


Figure S5: Normalized HPLC chromatograms of **Asx** (black) and **BPH-Asx** (red). Elution times of identified peaks are shown in the graph. The black chromatogram of **Asx** shows a single peak at 11.1 assigned to *all-trans* astaxanthin. For **BPH-Asx**, several peaks were identified at 12.2 minutes (%3), at 12.9 minutes (%81), at 13.9 minutes (%6), at 14.1 minutes (%6) and at 15.6 minutes (%4).

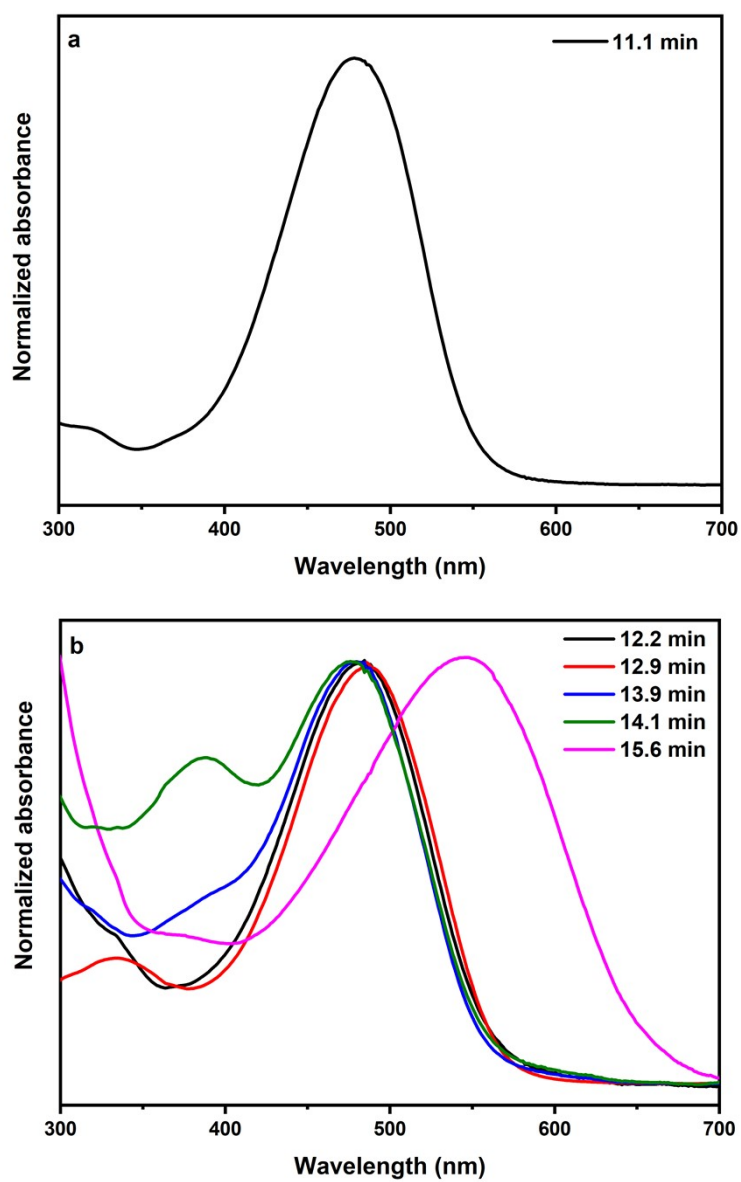


Figure S6: Normalized absorption spectra of peaks from HPLC analysis of a) **Asx** and b) **BPH-Asx**. Spectra were extracted directly from HPLC.

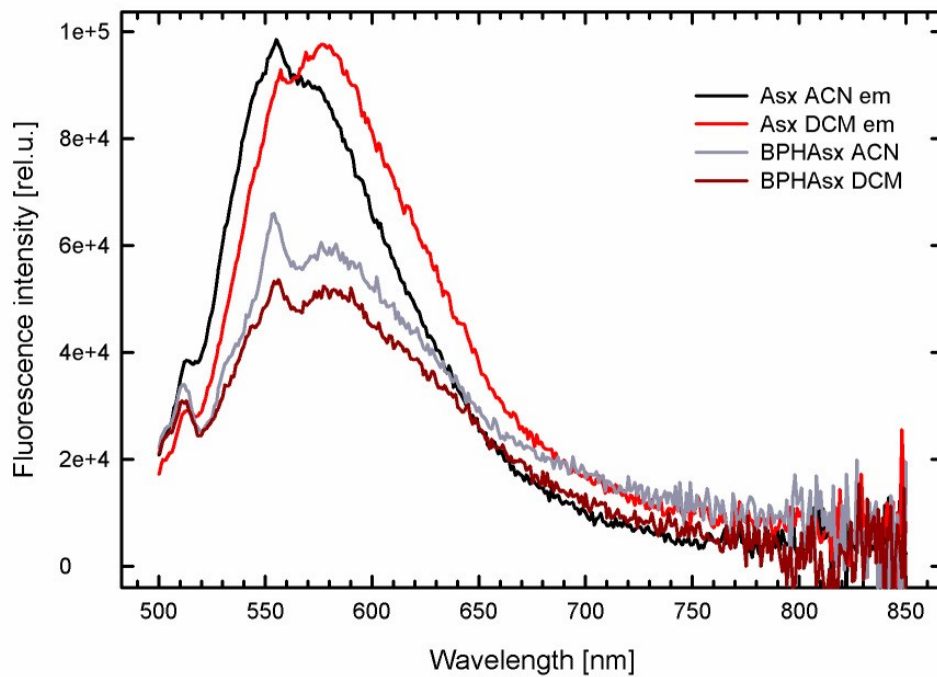


Figure S7. Fluorescence spectra of **Asx** And **BPH-Asx** in DCM and ACN. The sharp peaks are due to Raman bands. The spectra were measured with 5 nm bandpass and were corrected for instrument response. All spectra were excited at 475 nm, absorbance of the samples at this wavelength was 0.4-0.8 (3 mm path length), and the data are normalized to equal absorption at 475 nm.

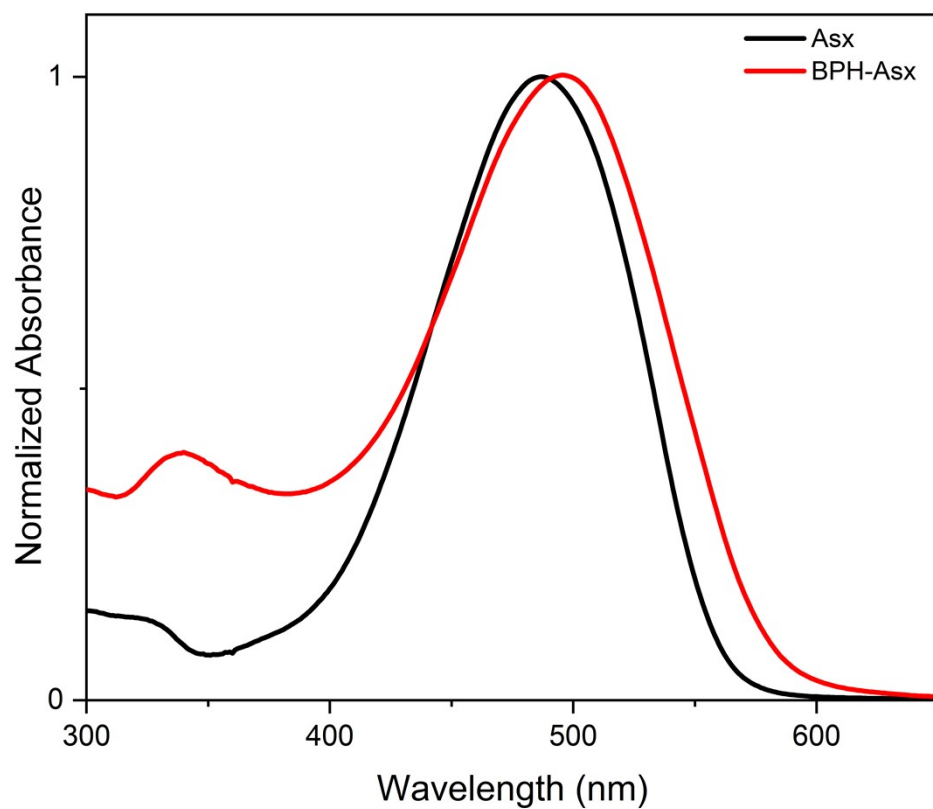


Figure S8. Steady state absorption spectra of astaxanthin (**Asx**) and **BPH-Asx** in benzene.

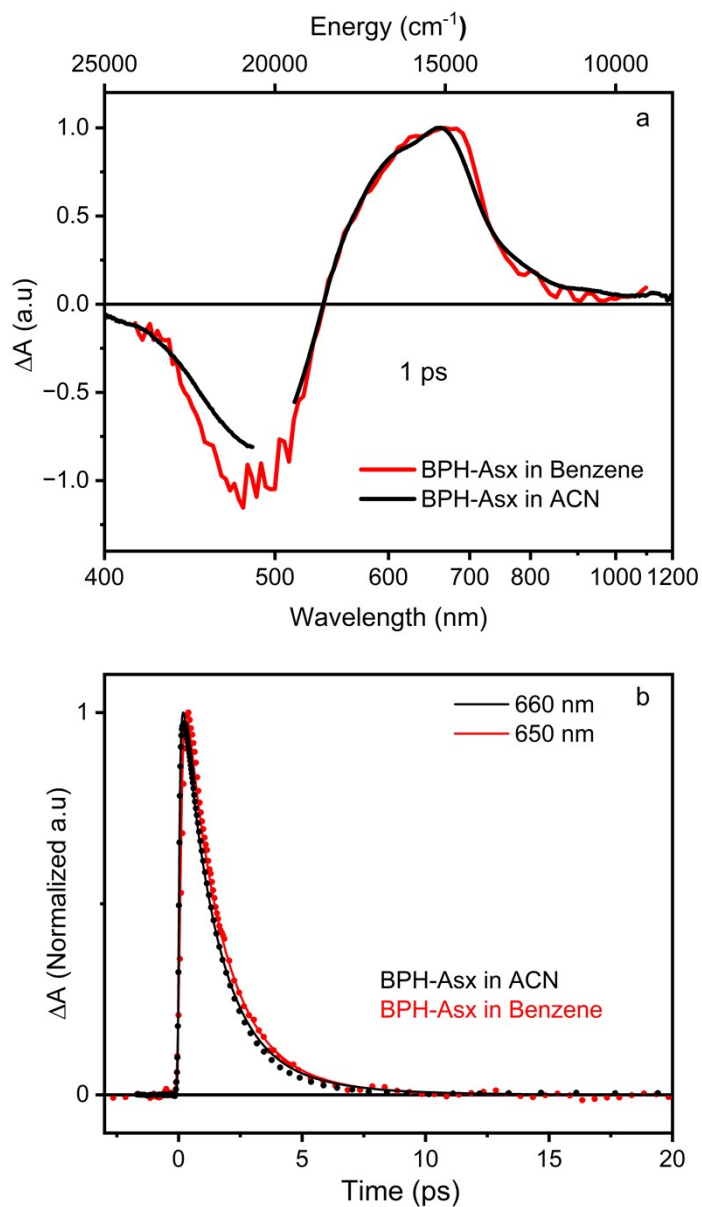


Figure S9: Normalized transient absorption spectra of a) **BPH-Asx** in ACN (black), and **BPH-Asx** in benzene (blue). The spectra were measured at 1 ps after excitation 500 nm for all compounds/solvents. Normalized kinetics b) measured at the S_1 - S_n maximum of same compounds in polar and non-polar solvents. Kinetics are also normalized to maximum; the lines represent fits obtained from global fitting analysis.

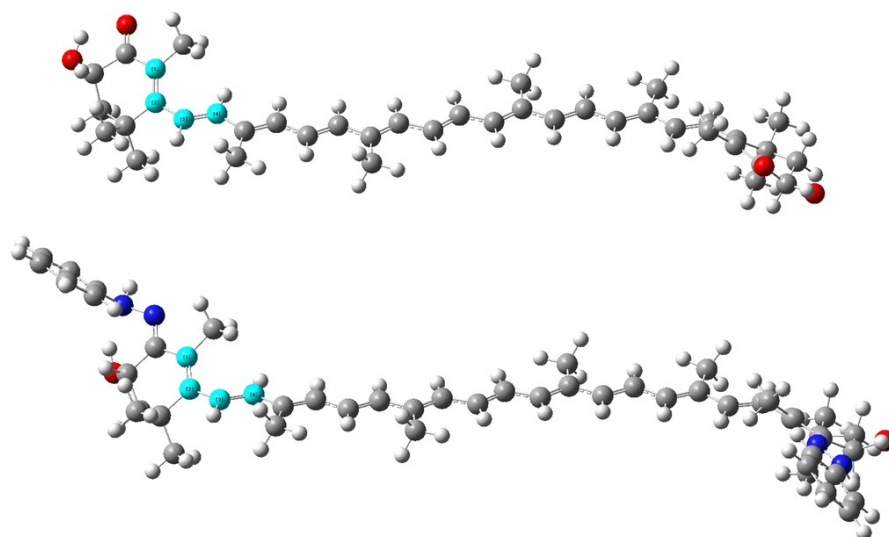


Figure S10. Relaxed ground state structures of **Asx** (top) and **BPH-Asx** (bottom). The atoms forming the dihedral angle are shown in cyan.