# ChemPhotoChem 

## Supporting Information

## In Silico Screening of Two-Photon Absorption Properties of a Large Set of Bis-Difluoroborate Dyes

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Figure S 1 : Relationship between $\sigma^{2 \mathrm{PA}}$ and oscillator strength $\left(f\right.$, a), CT distance $\left(D_{\mathrm{CT}}, \mathrm{b}\right)$, amount of transferred charge ( $q_{\mathrm{CT}}, \mathrm{c}$ ), change in dipole moment between the ground to the excited states $\left(\mu_{\mathrm{CT}}, \mathrm{d}\right)$ and normalized 2PA cross-section $\left(\sigma^{2 \mathrm{PA}} / N_{e}\right.$, e) for series $\mathbf{A}$ and $\mathbf{B}$ series.


Figure S2: Relationship between $\sigma^{2 \mathrm{PA}}$ and $f$ (a), $D_{\mathrm{CT}}$ (b), $q_{\mathrm{CT}}$ (c), $\mu_{\mathrm{CT}}$ (d) and $\sigma^{2 \mathrm{PA}} / N_{e}$ (e) for series $\mathbf{A}$ and $\mathbf{C}$. Only the molecules in the series $\mathbf{A}$ including acceptor substituents at $\mathrm{R}\left(\mathrm{C}_{6} \mathrm{H}_{4}-\mathrm{CF}_{3}, \mathrm{C}_{6} \mathrm{H}_{4}-\mathrm{F}\right.$ and $\left.\mathrm{C}_{6} \mathrm{~F}_{5}\right)$ are considered for the sake of consistency with the $\mathbf{C}$ series.

Table S1: Density difference plot $^{a}, \sigma^{2 \mathrm{PA}}, \lambda^{1 \mathrm{PA}}$ and CT parameters ${ }^{b}$ of A-derivatives with enenph linker determined using the TD-CAM-B3LYP/6-31+G(d) level of theory.


[^0]Table S2: Density difference plot, $\sigma^{2 \mathrm{PA}}, \lambda^{1 \mathrm{PA}}$ and CT parameters of B-derivatives with enenph linker determined using the TD-CAM-B3LYP/6-31+G(d) level of theory. ${ }^{a}$


[^1]Table S3: Density difference plot, $\sigma^{2 \mathrm{PA}}, \lambda^{1 \mathrm{PA}}$ and CT parameters of $\mathbf{C}$-derivatives with enen linker and $\mathrm{R}=\mathrm{C}_{6} \mathrm{~F}_{5}$ determined using the TD-CAM-B3LYP/6-31+G(d) level of theory. ${ }^{a}$


[^2]
(a)

(b)

Figure S3: Graphical representation of $D_{\mathrm{CT}}$ of $\mathbf{C}$-derivatives with enen linker, $\mathrm{R}=\mathrm{C}_{6} \mathrm{~F}_{5}, \mathrm{R} \mathrm{R}^{\prime \prime}=\mathrm{NMe}_{2}$, and $\mathrm{R}^{\prime}=\mathrm{NMe}_{2}$ or $\mathrm{R}^{\prime}=$ OMe determined using the TD-CAM-B3LYP/6-31+G(d) level of theory.


Figure S4: Variable conjugation paths from R and R' substituents towards accepting core in A and B

## Geometries

XYZ coordinates (naming system [Core]-[linker]-[R]-[R']-[R"]-opt.xyz) can be dowloaded using the following link: https://doi.org/10.5281/zenodo. 6684597


[^0]:    ${ }^{a}$ The red (blue) regions corresponds to density increase (decrease) upon absorption and are drawn with a contour threshold of 0.0004 au. ${ }^{b} D_{\mathrm{CT}}$, $q_{\mathrm{CT}}$ and $\mu_{\mathrm{CT}}$.

[^1]:    ${ }^{a}$ See Table S1 for more details.

[^2]:    ${ }^{a}$ See Table S1 for more details.

