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Supporting Information

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

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Figure S1: Relationship between σ^{2PA} and oscillator strength (*f*, a), CT distance (D_{CT} , b), amount of transferred charge (q_{CT} , c), change in dipole moment between the ground to the excited states (μ_{CT} , d) and normalized 2PA cross-section (σ^{2PA}/N_e , e) for series **A** and **B** series.



Figure S2: Relationship between σ^{2PA} and f (a), D_{CT} (b), q_{CT} (c), μ_{CT} (d) and σ^{2PA}/N_e (e) for series **A** and **C**. Only the molecules in the series **A** including acceptor substituents at R (C₆H₄-CF₃, C₆H₄-F and C₆F₅) are considered for the sake of consistency with the **C** series.



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

^{*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_{CT} , q_{CT} and μ_{CT} .



Table S2: Density difference plot, σ^{2PA} , λ^{1PA} and CT parameters of **B**-derivatives with **enerph** linker determined using the TD-CAM-B3LYP/6-31+G(d) level of theory.^{*a*}

^{*a*} See Table S1 for more details.



Table S3: Density difference plot, σ^{2PA} , λ^{1PA} and CT parameters of **C**-derivatives with **enen** linker and $R = C_6F_5$ determined using the TD-CAM-B3LYP/6-31+G(d) level of theory. ^{*a*}

^{*a*} See Table S1 for more details.



Figure S3: Graphical representation of D_{CT} of C-derivatives with **enen** linker, $R = C_6F_5$, $R'' = NMe_2$, and $R' = NMe_2$ or R' = 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