Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Tailoring Nonlinear Absorption of Fluorescent Dyes by Substitution at a Boron Center†

ELECTRONIC SUPPLEMENTARY INFORMATION

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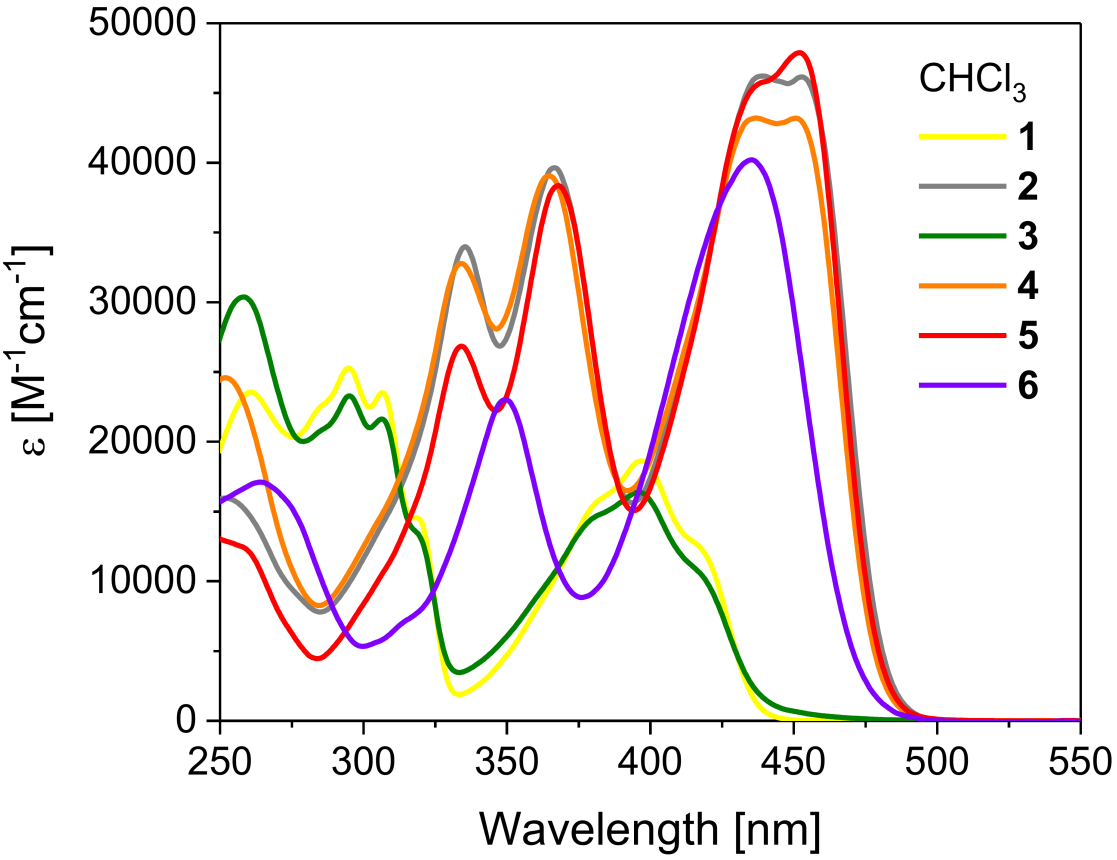


Figure S1: The absorption spectra for **1**-**6** in chloroform.

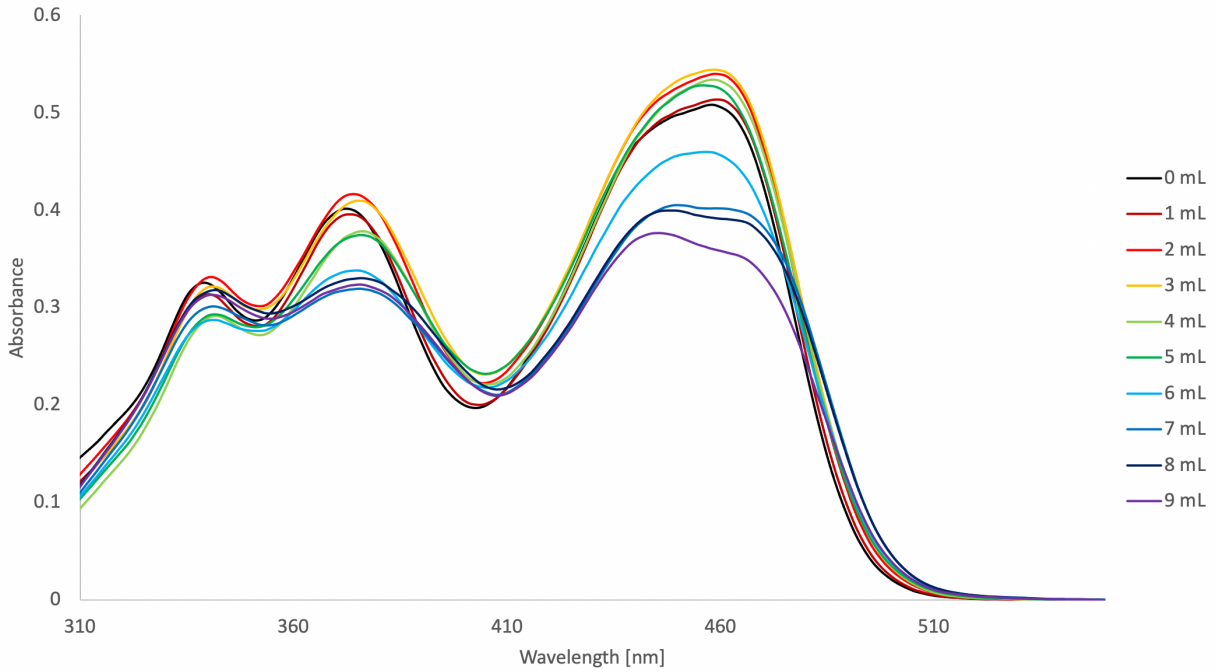


Figure S2: The absorption spectra for **2** in DMSO/water mixture (total volume is 10 ml, the amount of water is given in the legend).

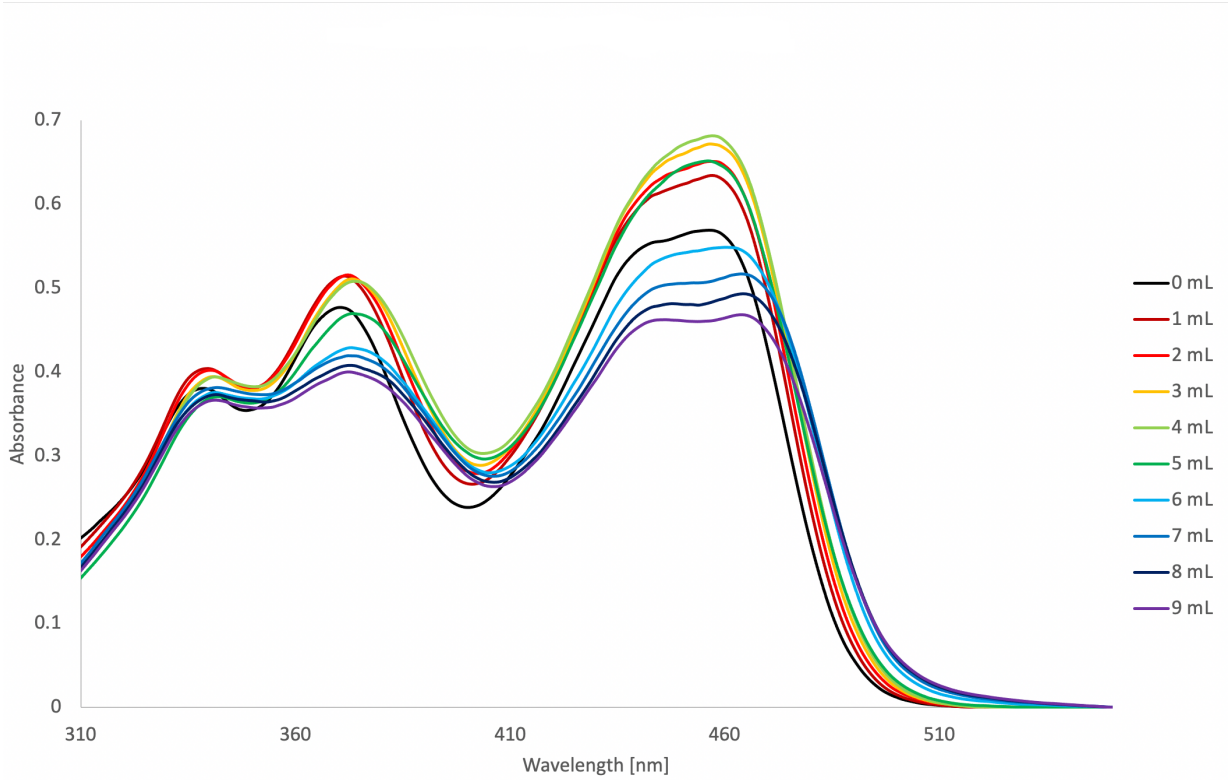


Figure S3: The absorption spectra for **4** in DMSO/water mixture (total volume is 10 ml, the amount of water is given in the legend).

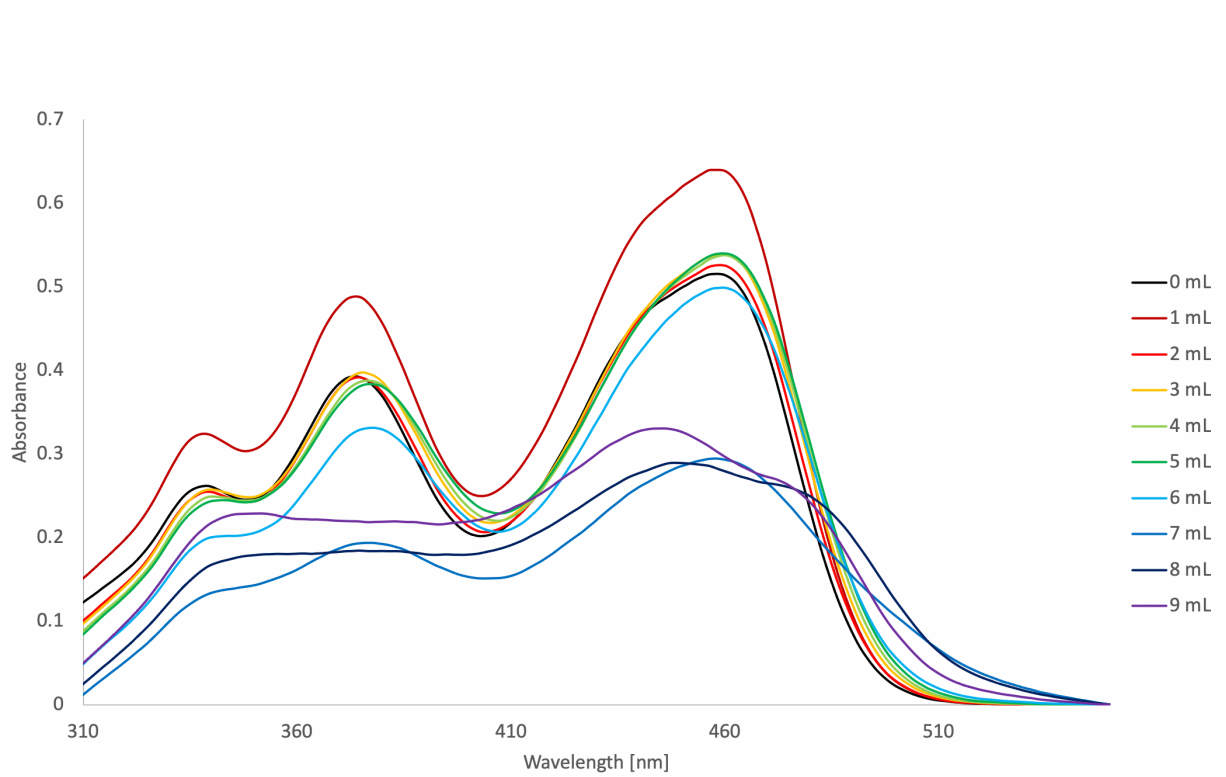


Figure S4: The absorption spectra for **5** in DMSO/water mixture (total volume is 10 ml, the amount of water is given in the legend).

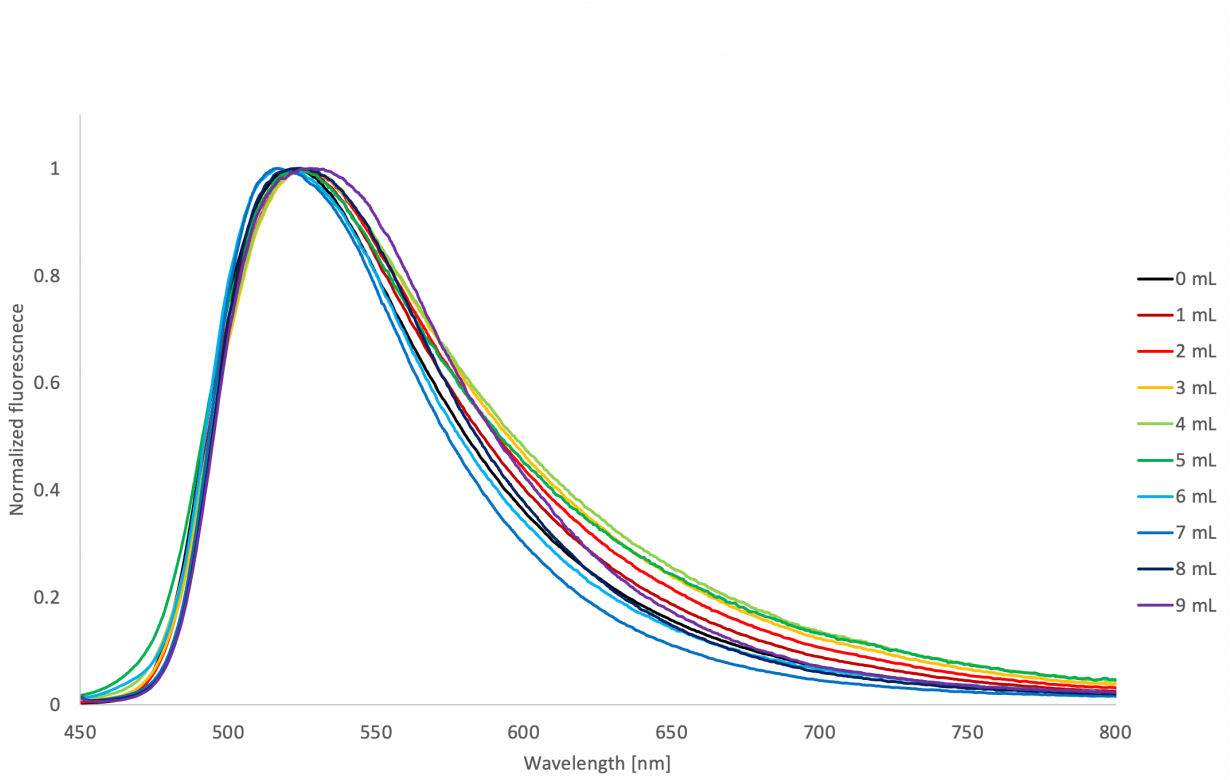


Figure S5: The fluorescence spectra for **2** in DMSO/water mixture (total volume is 10 ml, the amount of water is given in the legend).

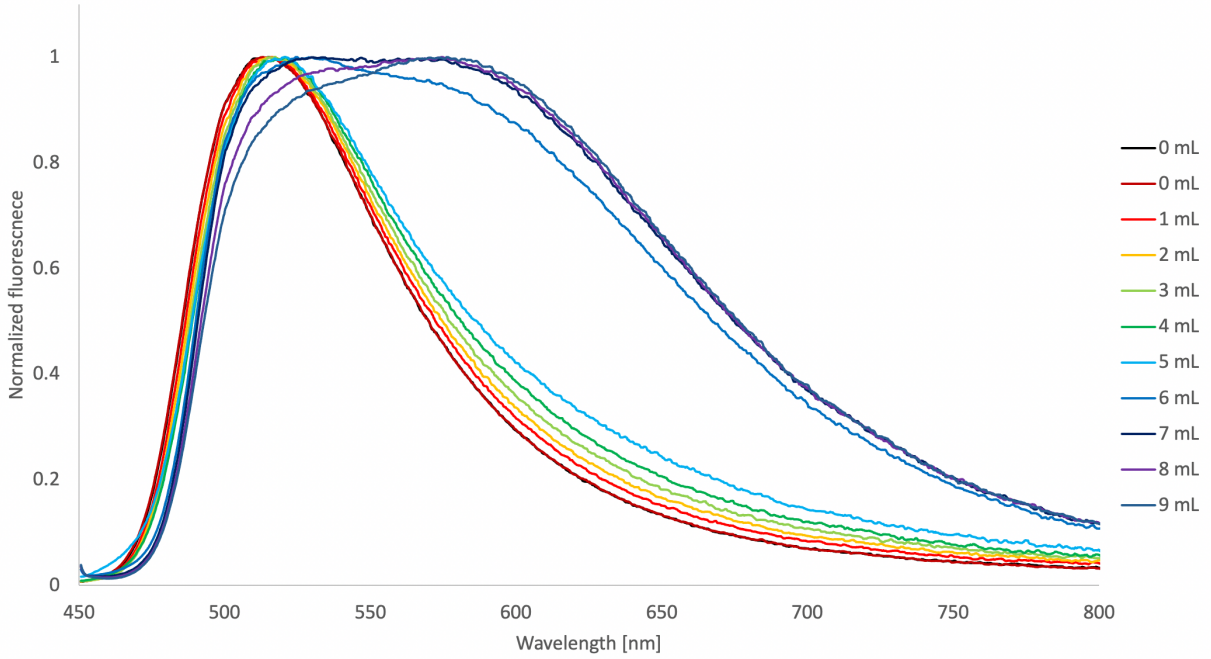


Figure S6: The fluorescence spectra for **4** in DMSO/water mixture (total volume is 10 ml, the amount of water is given in the legend).

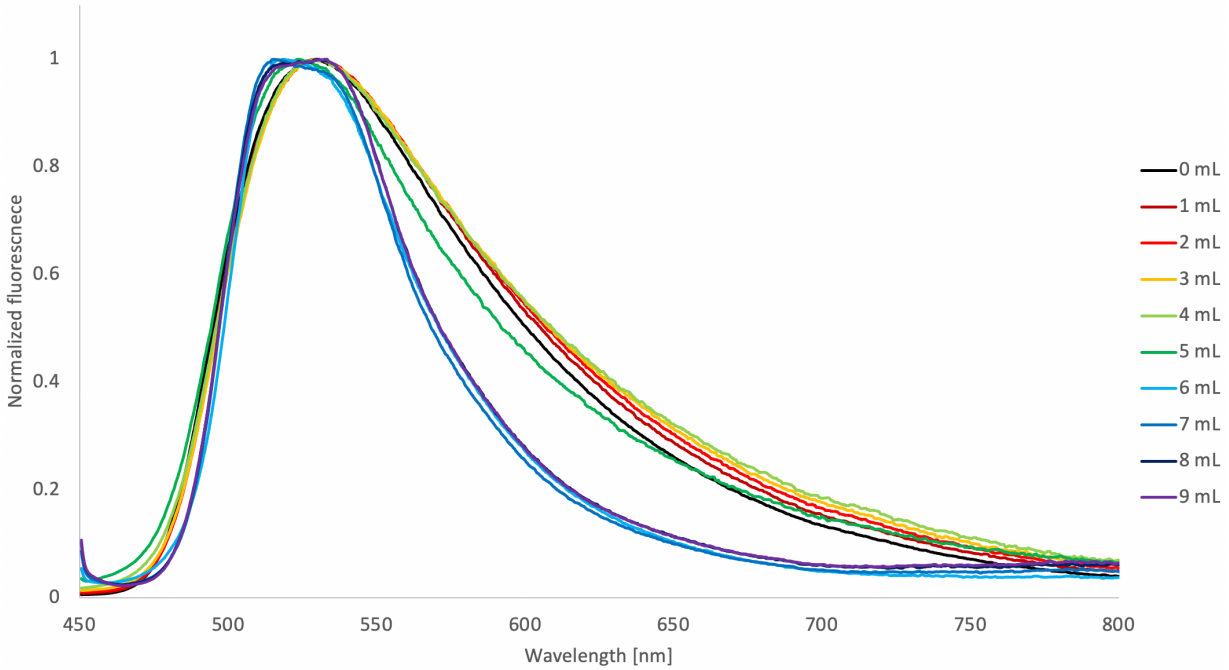


Figure S7: The fluorescence spectra for **5** in DMSO/water mixture (total volume is 10 ml, the amount of water is given in the legend).

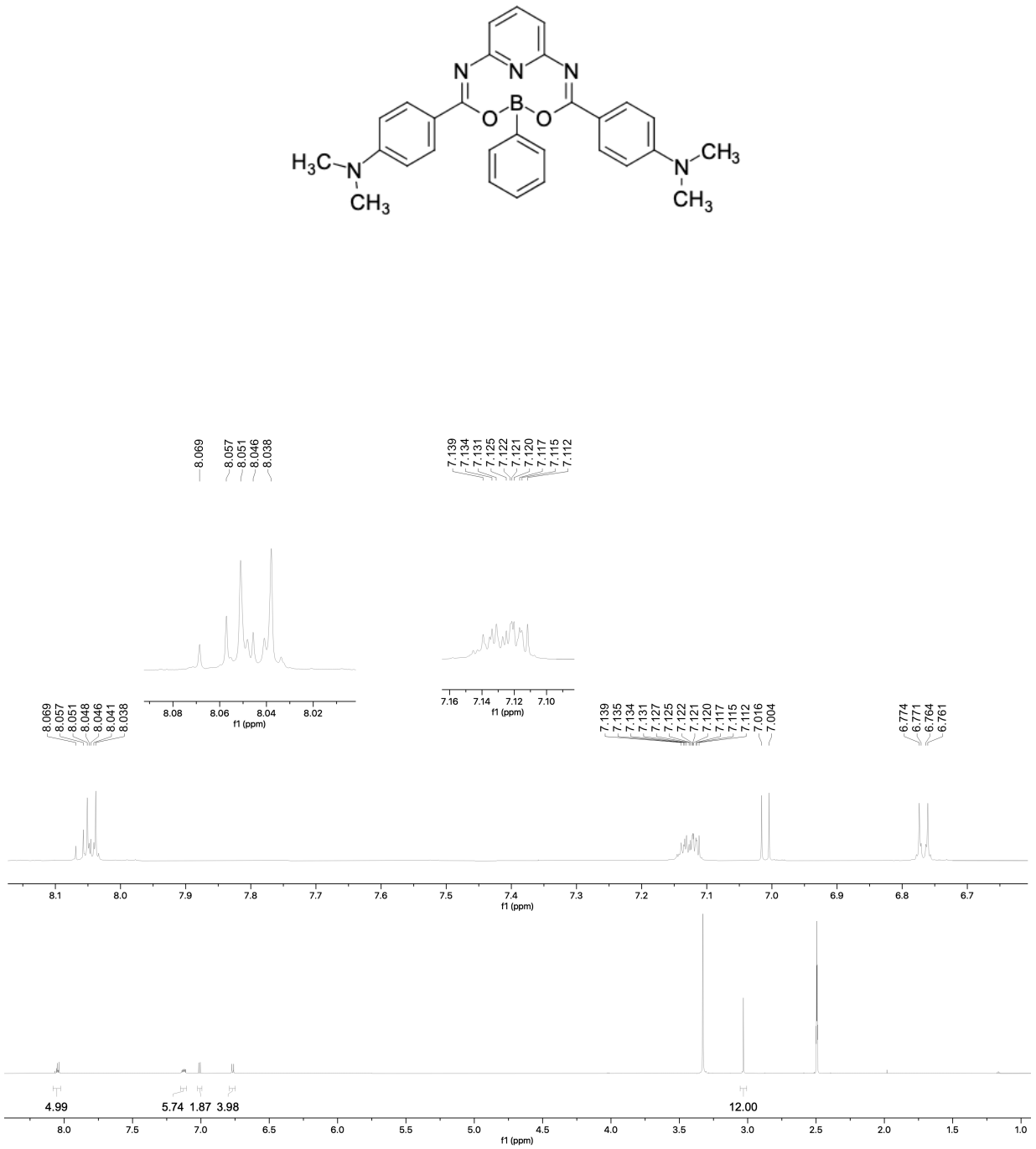


Figure S8: The ^{1}H NMR spectrum of 4-[(2Z,7Z)-7-[4-(dimethylamino)phenyl]-5-phenyl-4,6-dioxa-2,8,13-triaza-5-borabicyclo[7.3.1]trideca-1(13),2,7,9,11-pentaen-3-yl]-N,N-dimethylaniline.

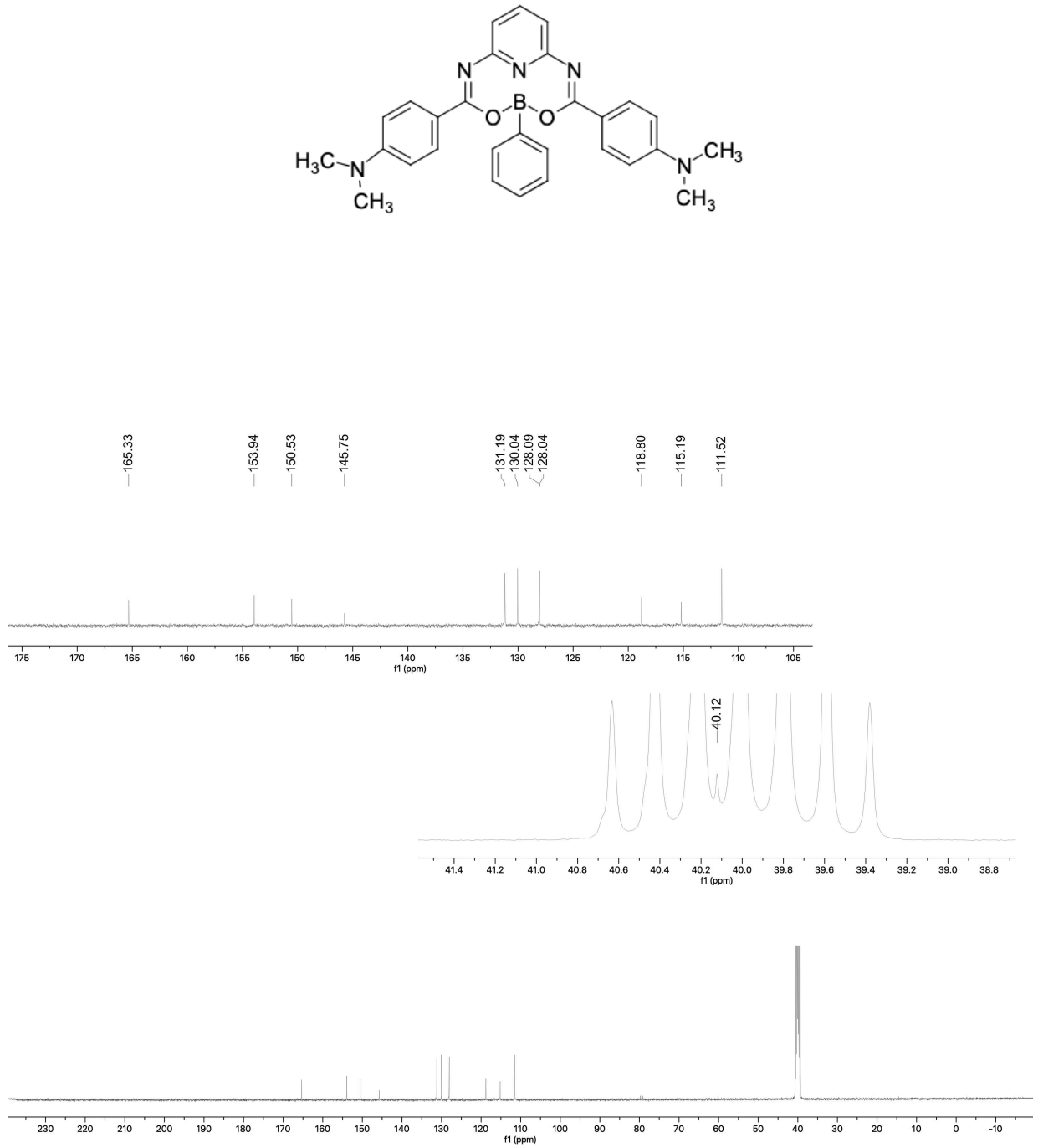


Figure S9: The ^{13}C NMR spectrum of 4-[(2Z,7Z)-7-[4-(dimethylamino)phenyl]-5-phenyl-4,6-dioxa-2,8,13-triaza-5-borabicyclo[7.3.1]trideca-1(13),2,7,9,11-pentaen-3-yl]-N,N-dimethylaniline.

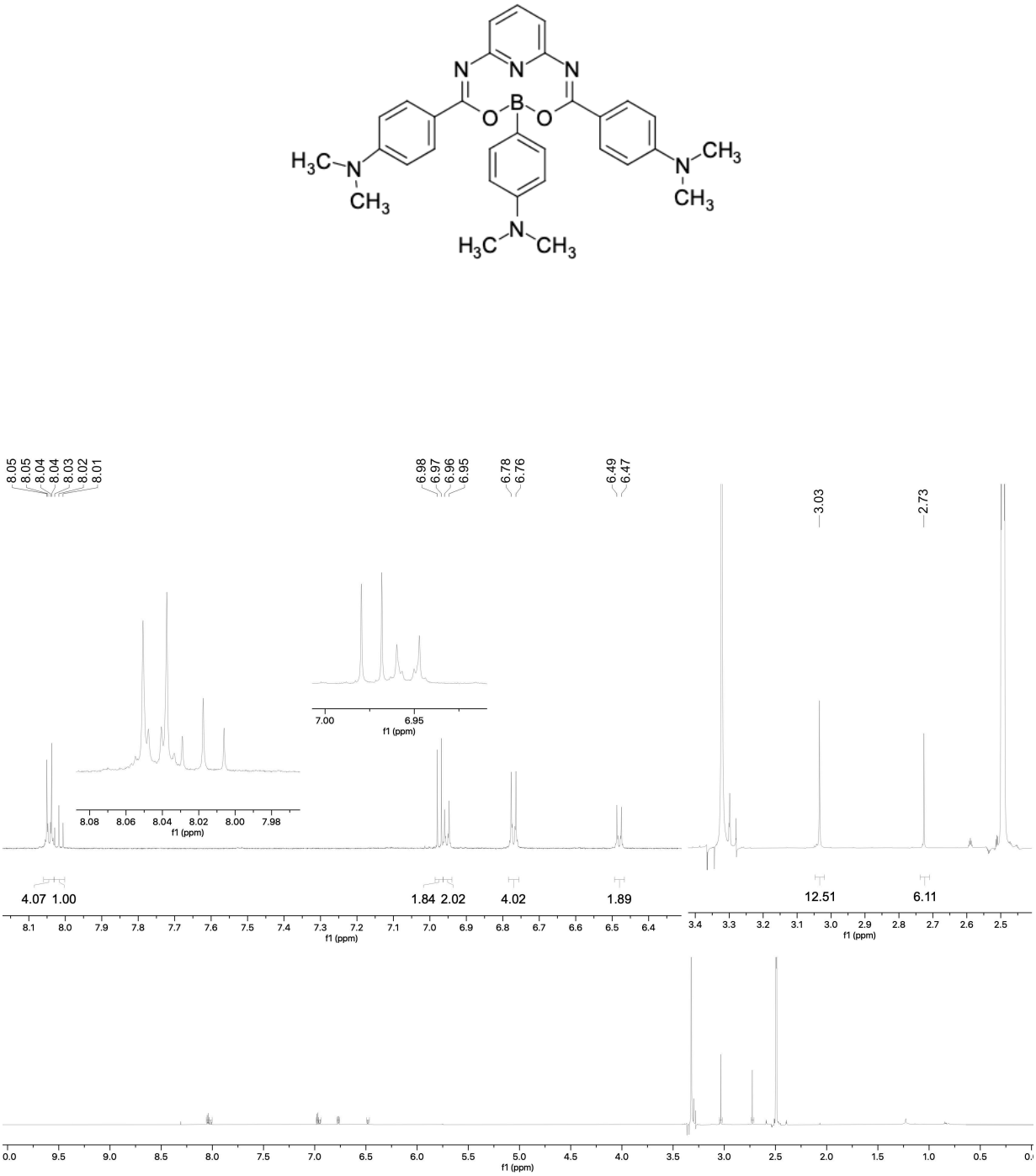
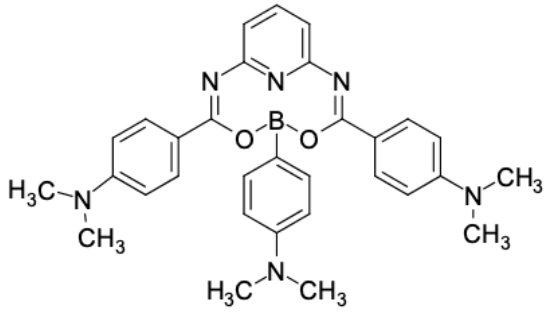


Figure S10: The ^{1}H NMR spectrum of 4-[(2Z,7Z)-3,7-bis[4-(dimethylamino)phenyl]-4,6-dioxa-2,8,13-triaza-5-borabicyclo[7.3.1]trideca-1(13),2,7,9,11-pentaen-5-yl]-N,N-dimethylaniline.



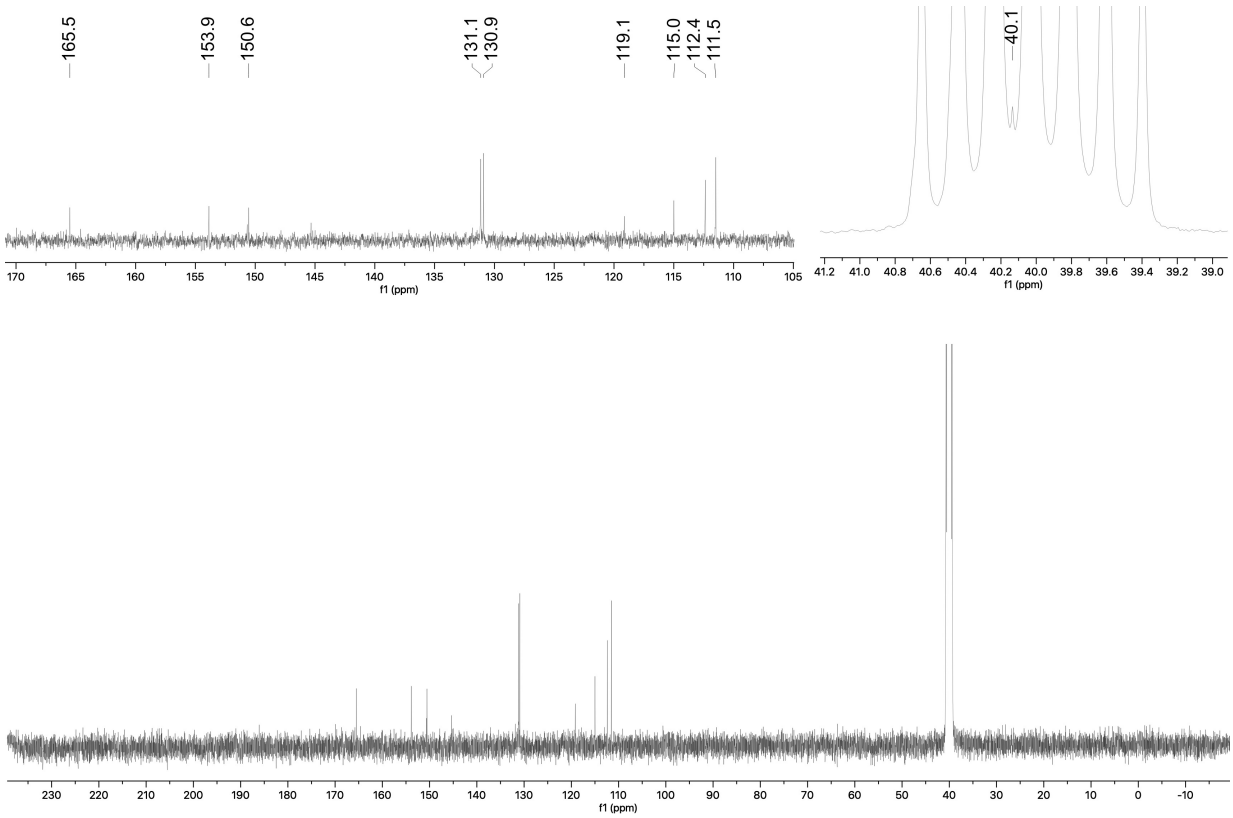


Figure S11: The ^{13}C NMR spectrum of 4-[(2Z,7Z)-3,7-bis[4-(dimethylamino)phenyl]-4,6-dioxa-2,8,13-triaza-5-borabicyclo[7.3.1]trideca-1(13),2,7,9,11-pentaen-5-yl]-N,N-dimethylaniline.

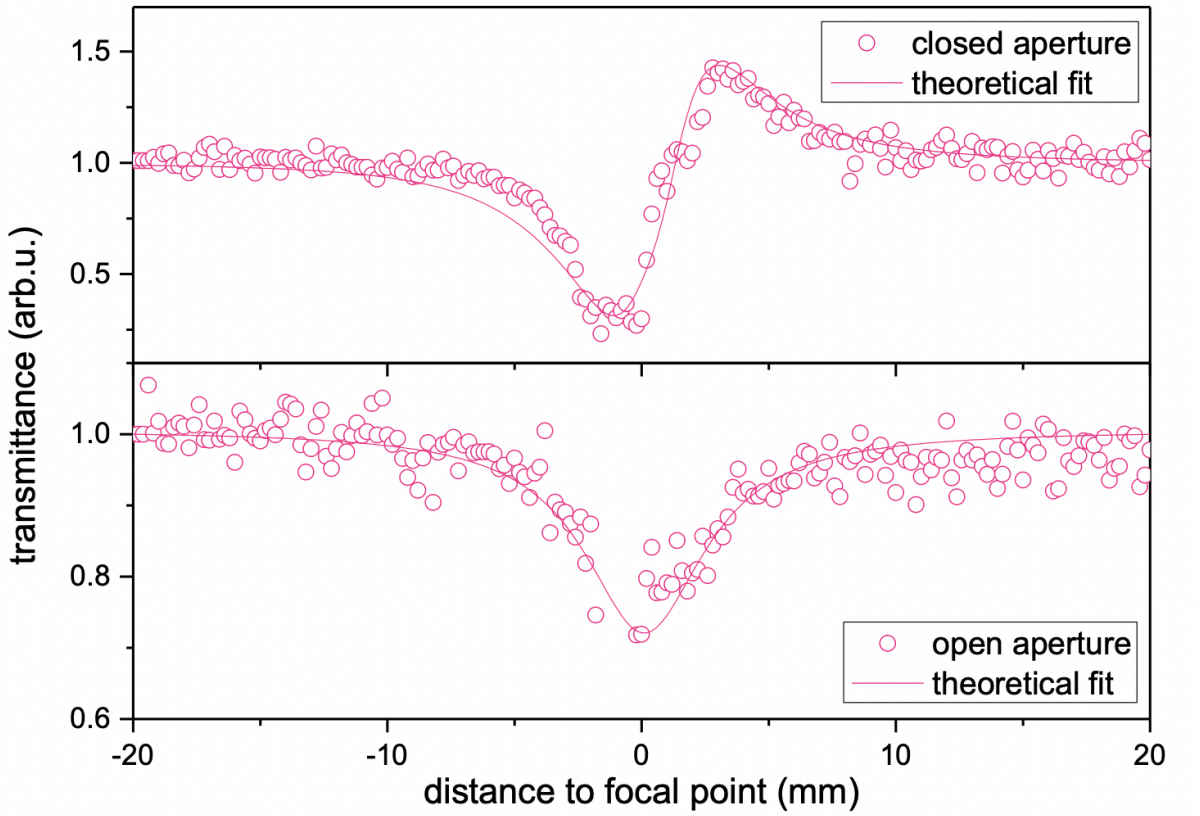


Figure S12: Representative relation between transmittance through **2** and distance to focal point (z-scan measurements) upon excitation at 725 nm.

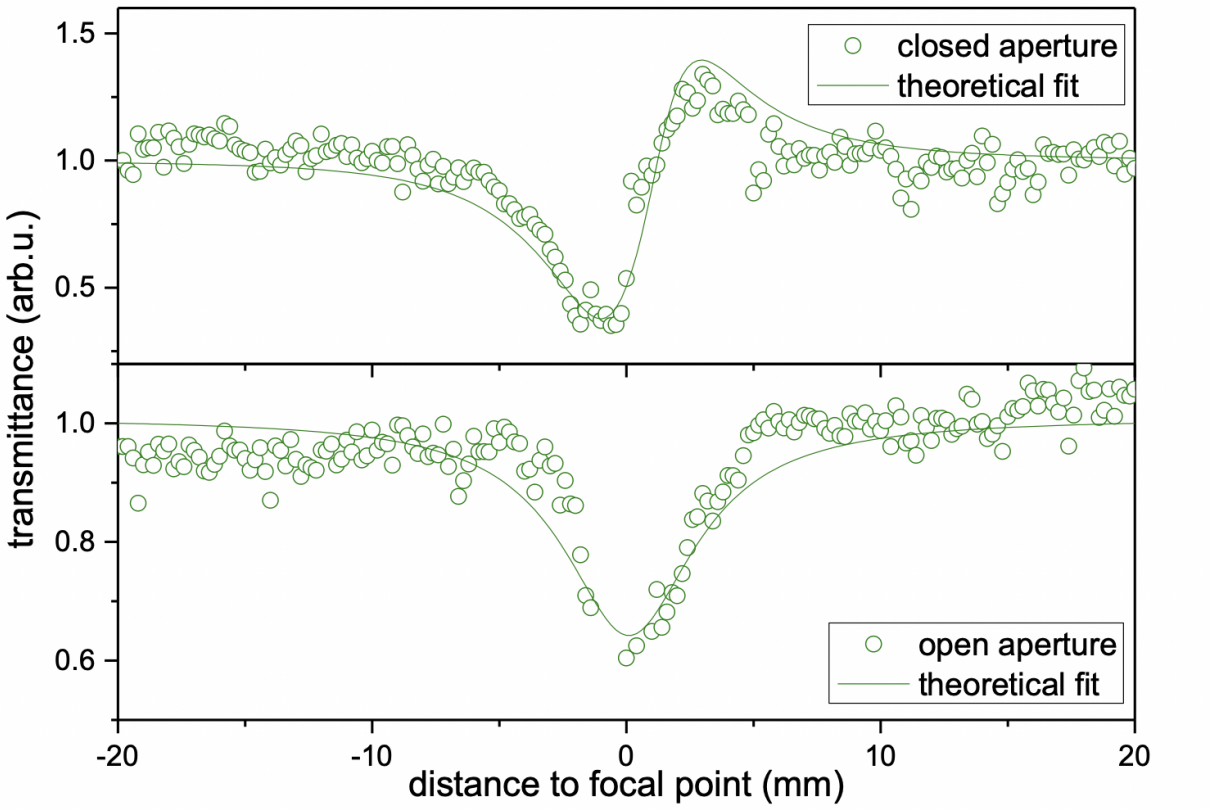


Figure S13: Representative relation between transmittance through **4** and distance to focal point (z-scan measurements) upon excitation at 725 nm.

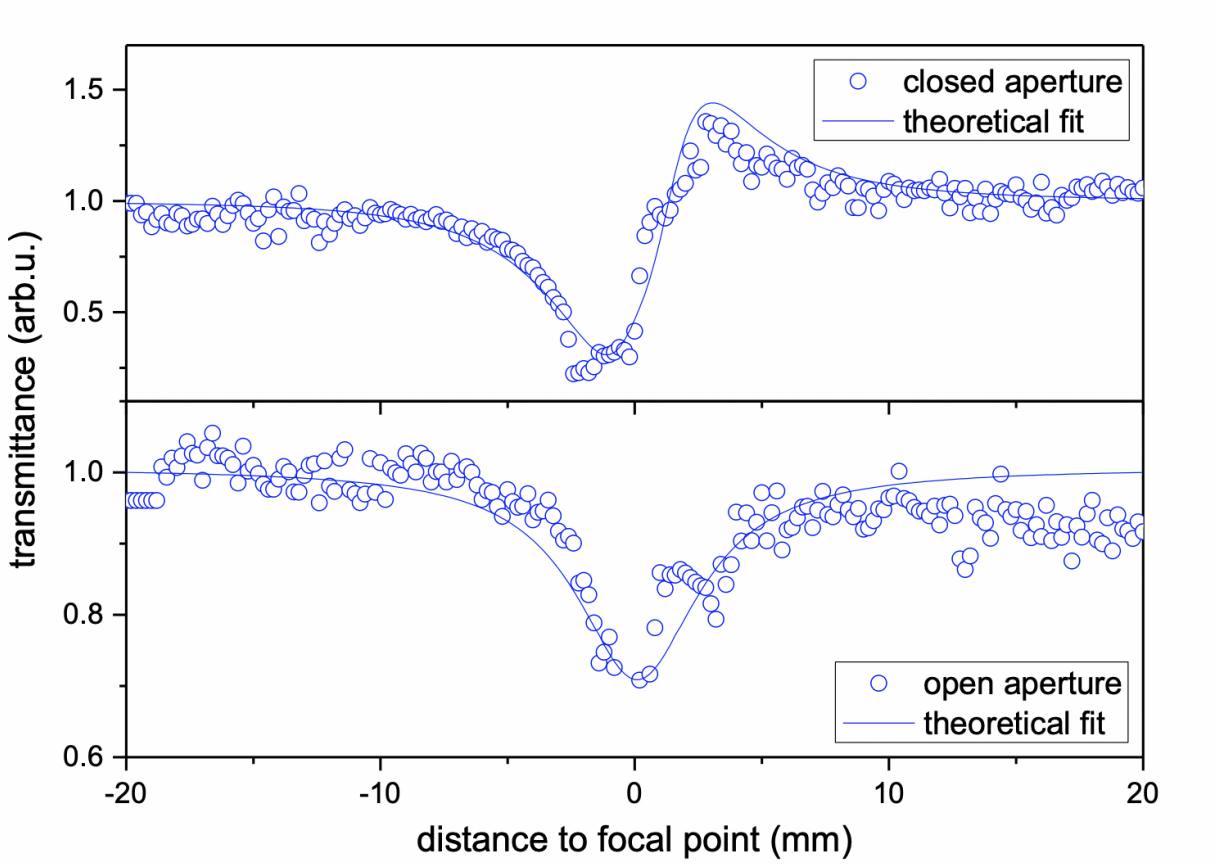


Figure S14: Representative relation between transmittance through **5** and distance to focal point (z-scan measurements) upon excitation at 725 nm.

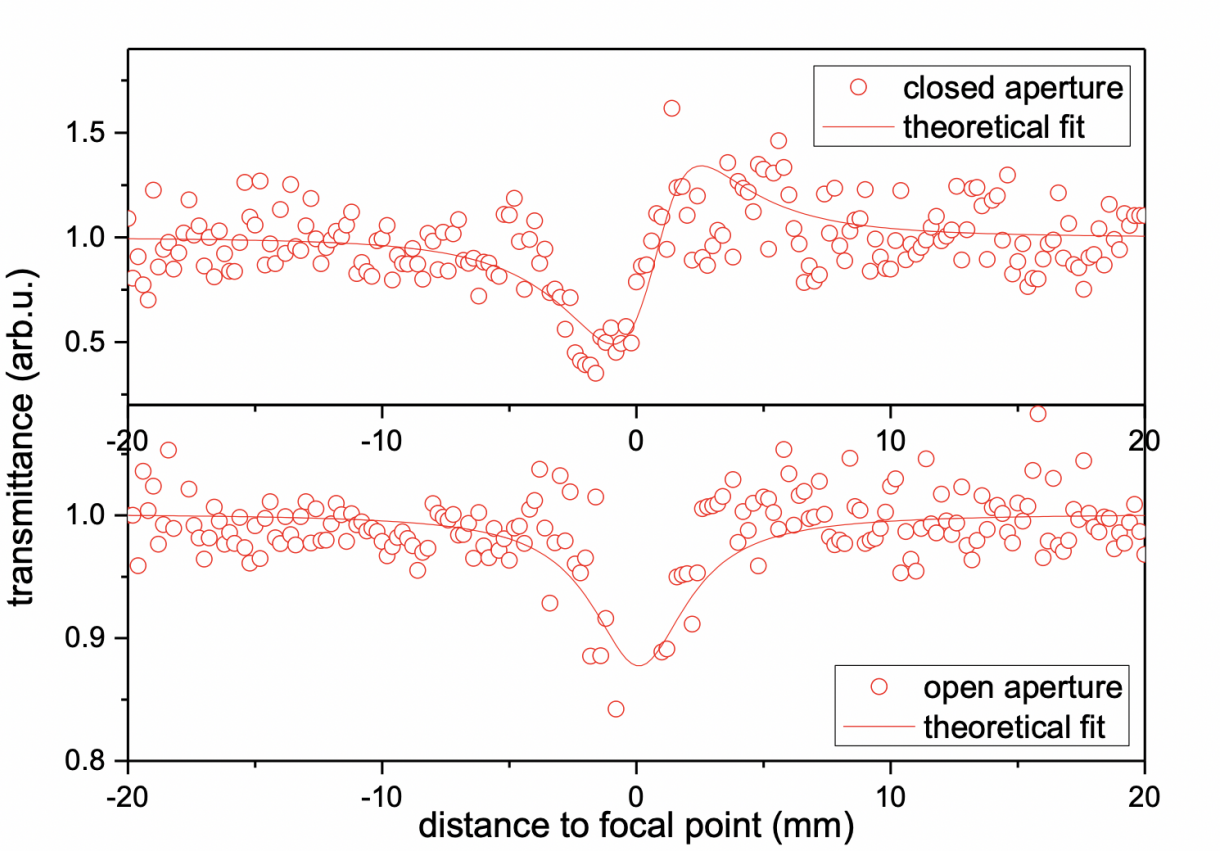


Figure S15: Representative relation between transmittance through **6** and distance to focal point (z-scan measurements) upon excitation at 800 nm.

Table S1: Summary of electronic-structure calculations at the CC2/cc-pVDZ level of theory: one-photon excitation wavelengths (λ, nm), oscillator strengths (f) and two-photon transition strengths (δ^{2PA}, au).

compound	$S_0 \rightarrow S_1$			$S_0 \rightarrow S_2$			$S_0 \rightarrow S_3$		
	λ	f	$\delta^{2PA}/10^3$	λ	f	$\delta^{2PA}/10^3$	λ	f	$\delta^{2PA}/10^3$
1	357	0.36	0.0	277	0.48	0.2	271	0.01	0.1
2	391	0.96	7.7	330	0.67	84.7	306	0.47	24.9
3	373	0.11	0.4	344	0.27	0.2	313	0.09	3.9
4	389	0.89	6.6	343	0.19	13.6	327	0.59	67.1
5	385	1.08	8.7	327	0.74	84.9	302	0.39	23.6
6	376	0.88	26.2	315	0.41	25.8	288	0.07	30.4