

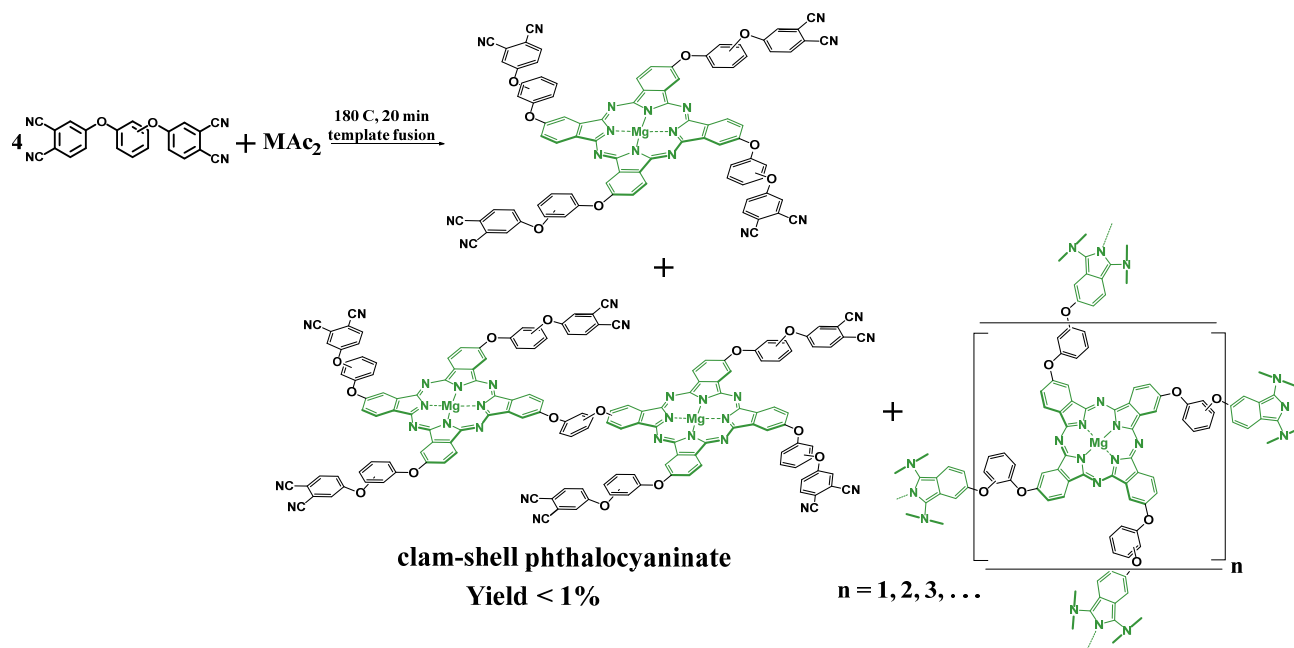
Electronic Supplementary Materials

Enhanced Visible Light Absorption and Photophysical Features of Novel Isomeric Magnesium Phthalocyaninates with Cyanophenoxy Substitution

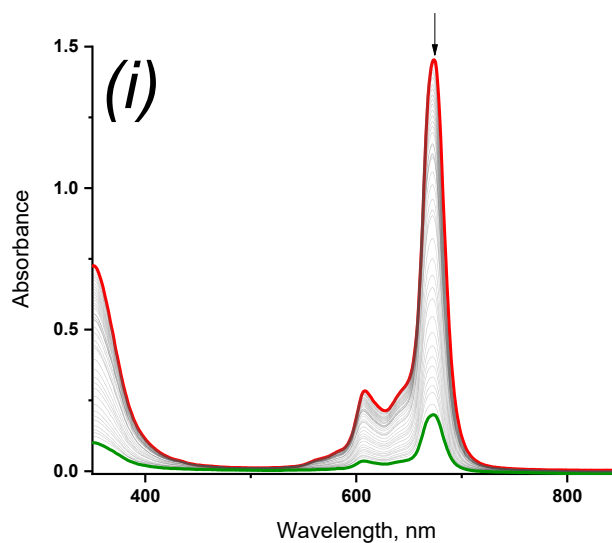
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Scheme S1. The main reaction products of template tetramerization of substituted phthalonitriles 2 and 3.



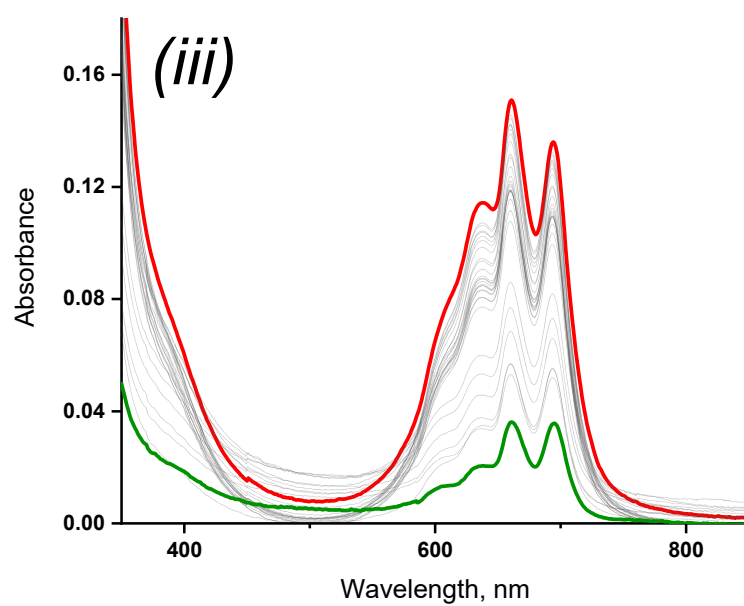
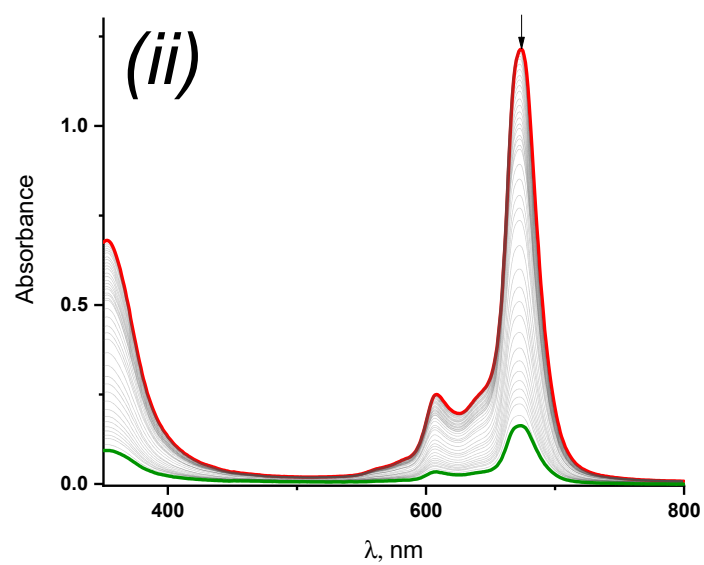
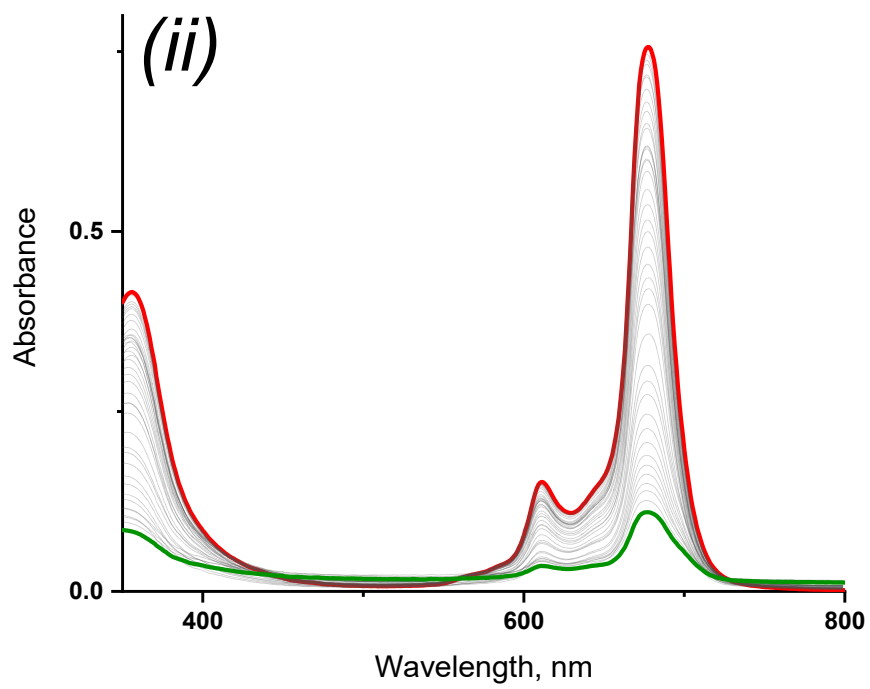
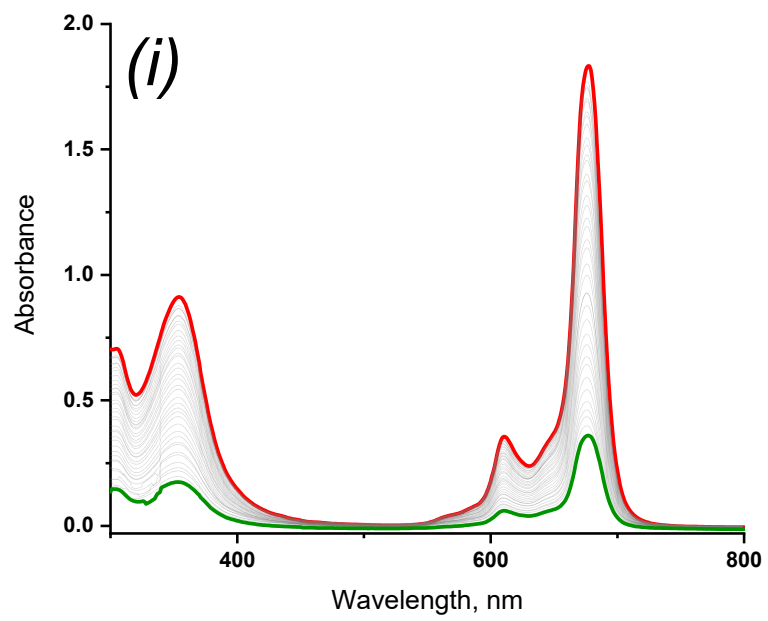


Figure S1. Changes in UV-vis spectra of compounds 4(i), 5(ii) and 7(iii) solutions in acetone upon dilution
(note: spectrum for compound 6 is presented in the manuscript)



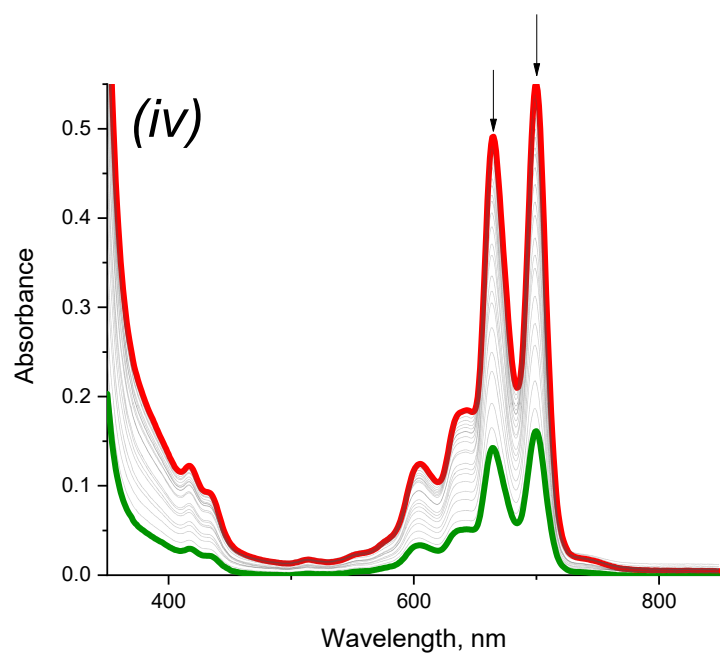
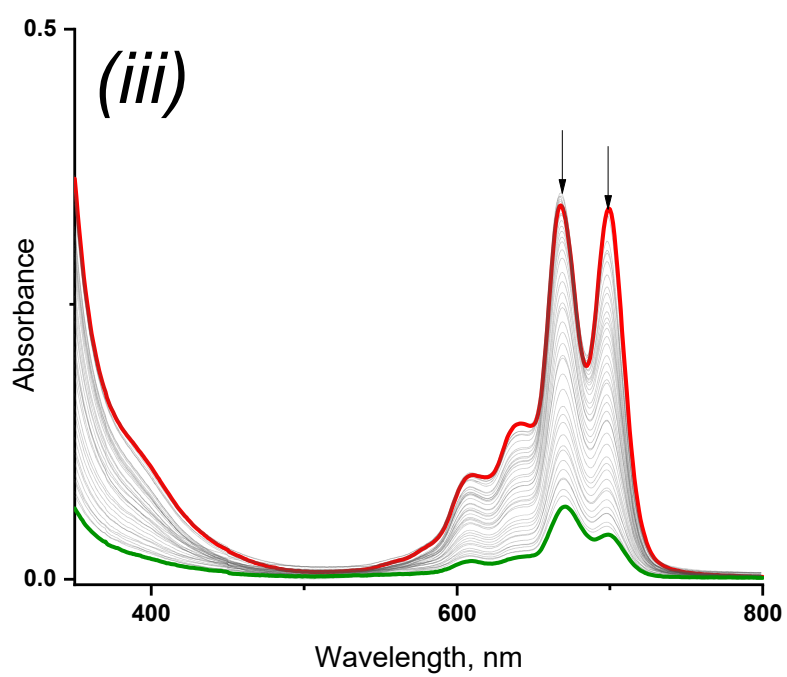
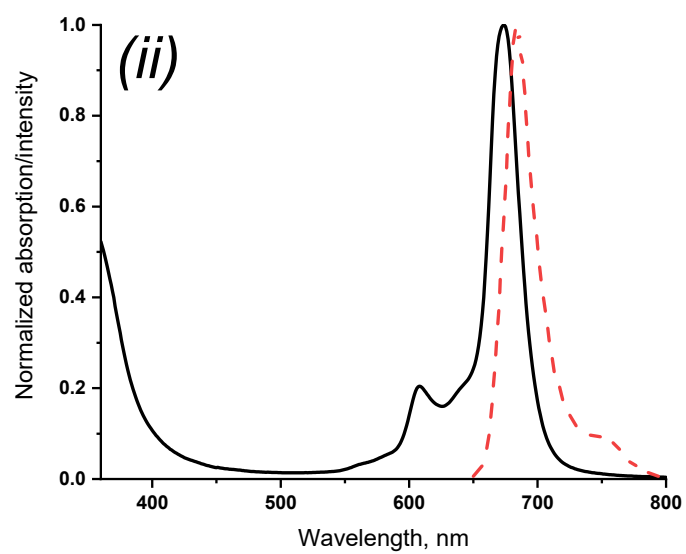
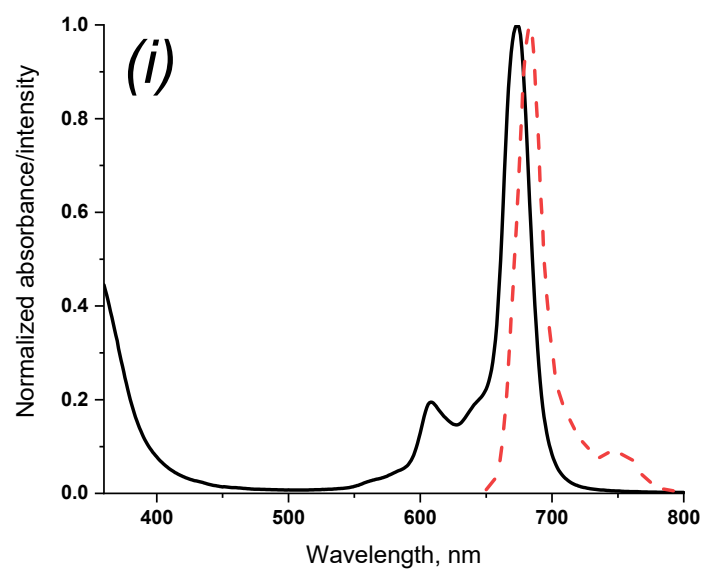


Figure S2. Changes in UV-vis spectra of compounds 4(i), 5(ii), 6(iii) and 7(iv) solutions in DMF upon dilution



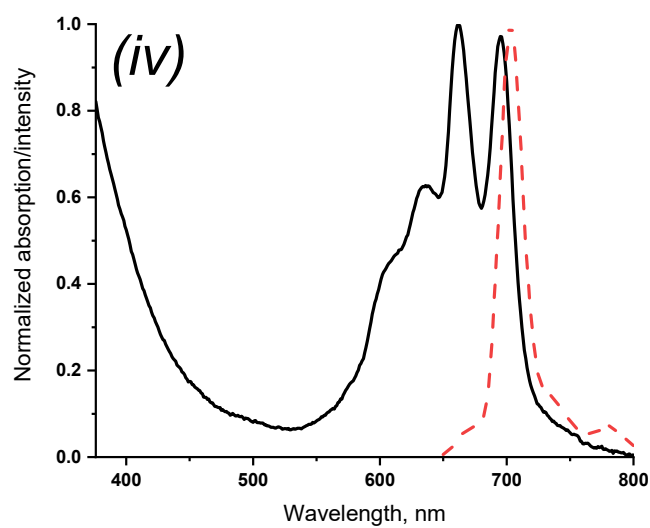
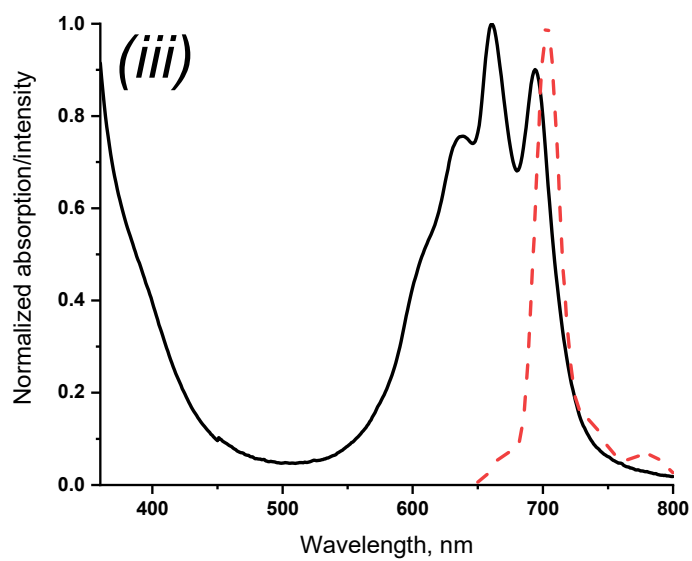
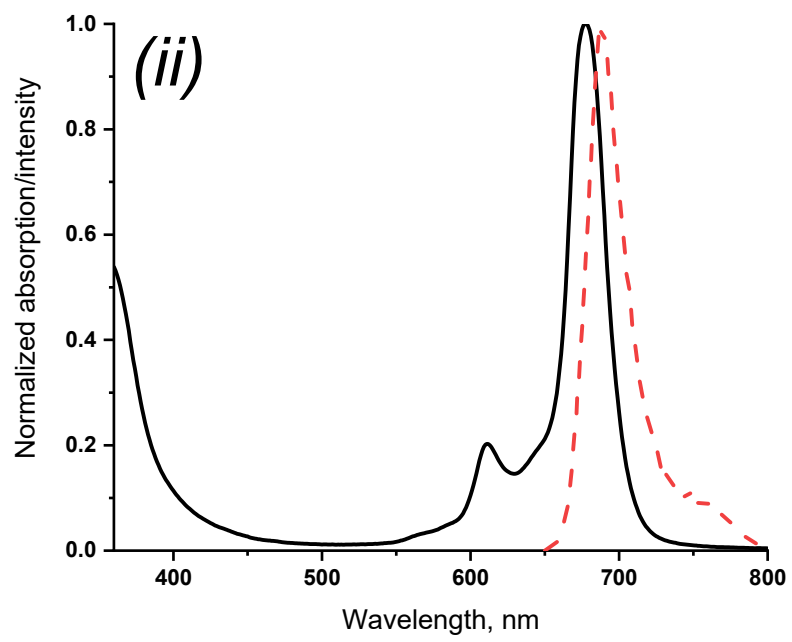
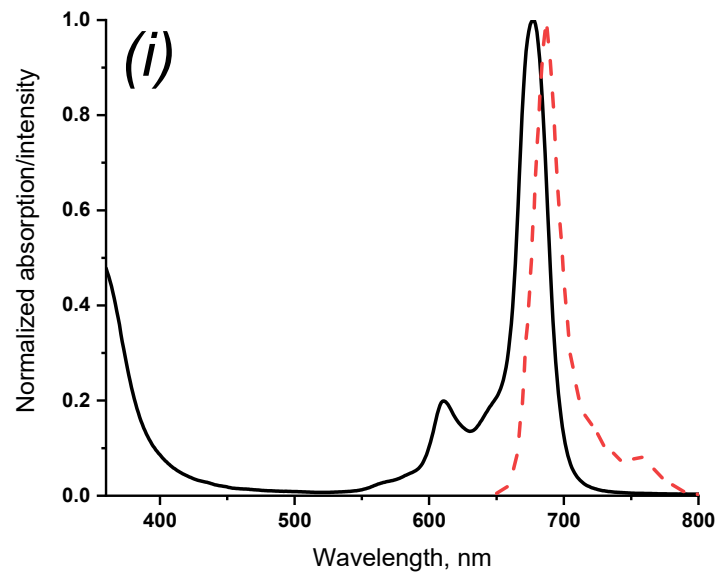


Figure S3. Normalized UV-Vis absorption spectra (black) and fluorescence spectra (dashed red) for compounds 4(i), 5(ii), 6(iii) and 7(iv) solutions in acetone, sample concentration $\sim 10 \mu\text{M}$. For fluorescence measurements, excitation was performed at the absorption maximum of the vibrational satellite (about 610 nm).



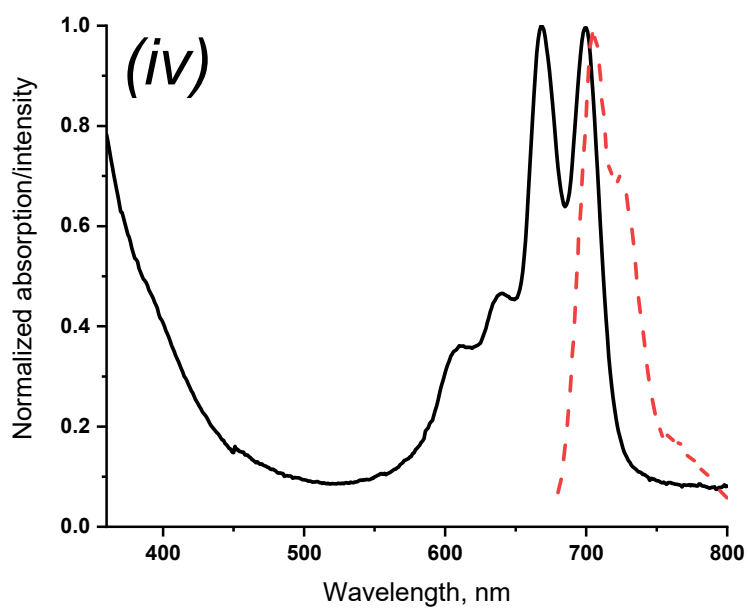
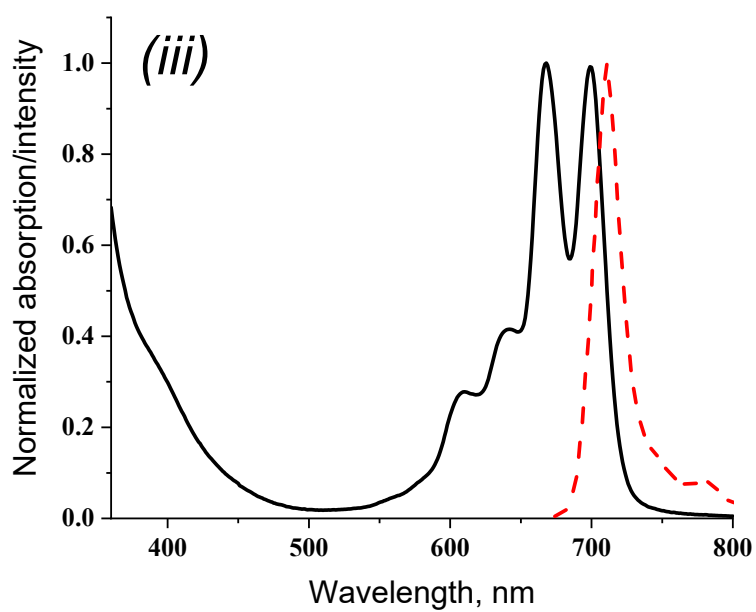
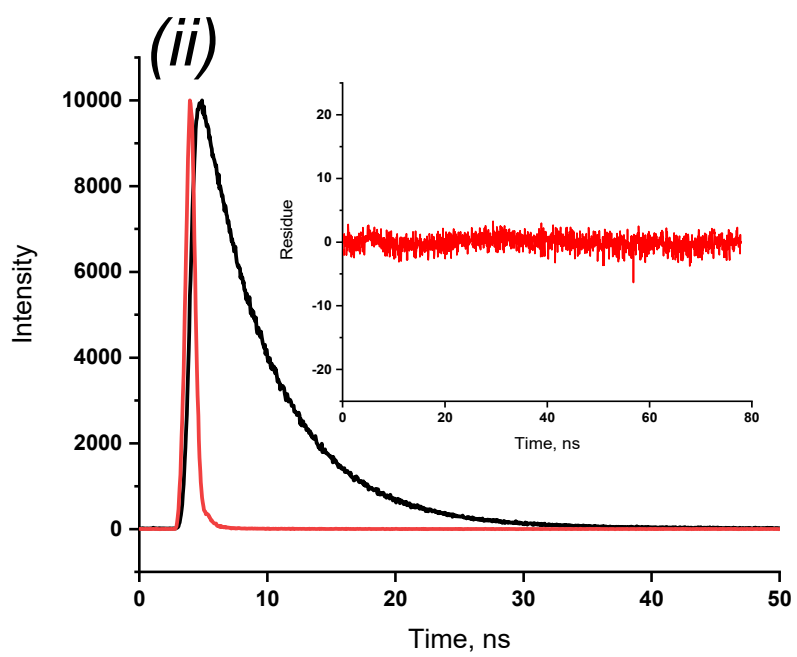
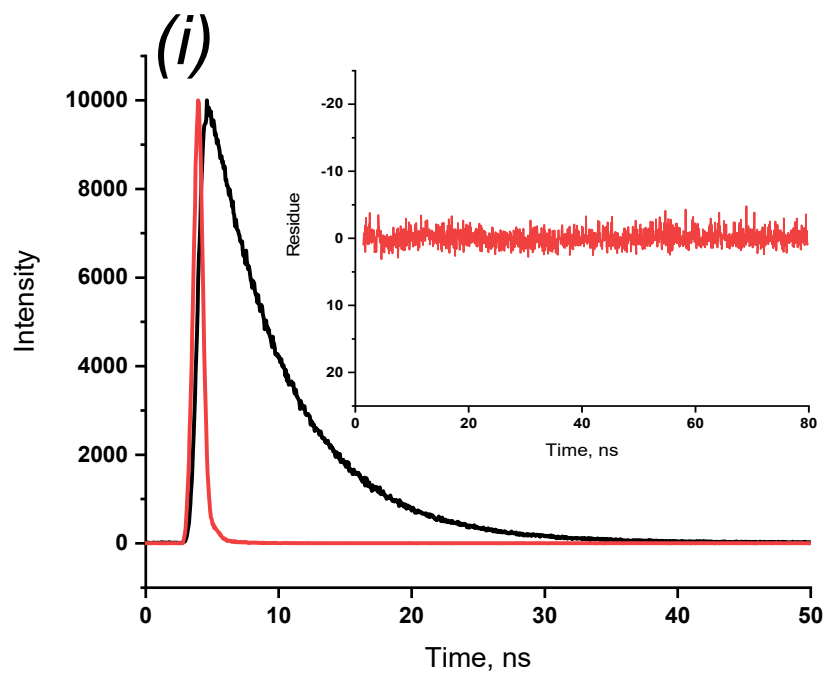


Figure S4. Normalized UV-Vis absorption spectra (*black*) and fluorescence spectra (*dashed red*) for compounds 4(*i*), 5(*ii*), 6(*iii*) and 7(*iv*) solutions in DMF, sample concentration $\sim 10 \mu\text{M}$. For fluorescence measurements, excitation was performed at the absorption maximum of the vibrational satellite (about 610 nm).



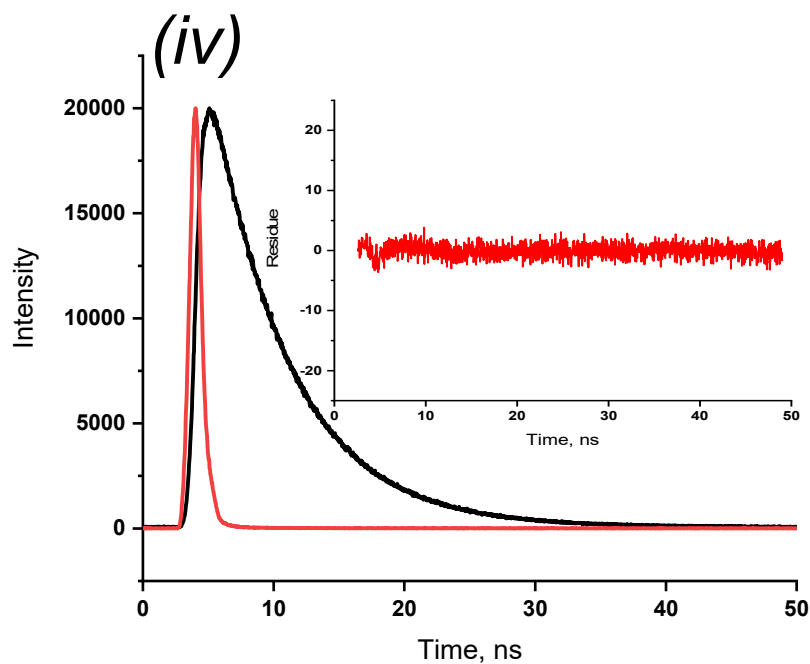
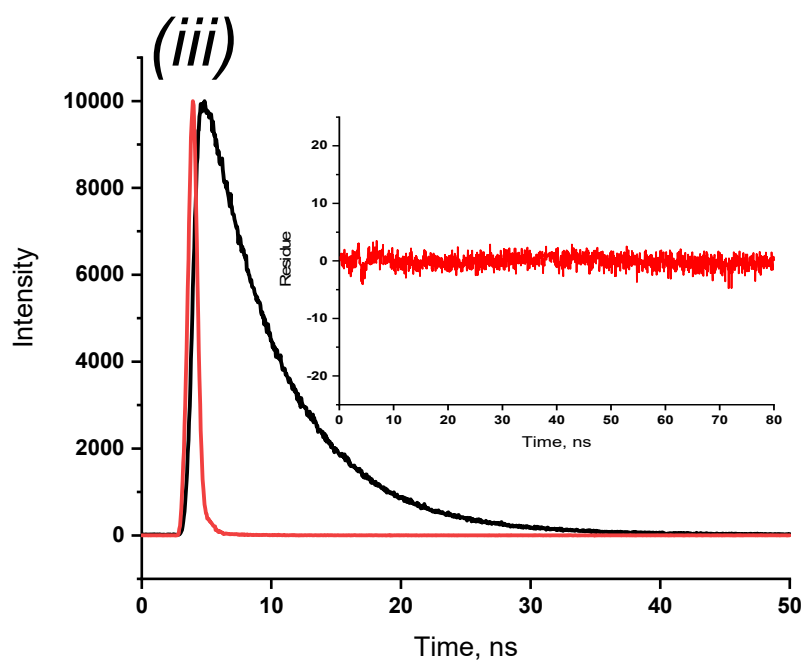
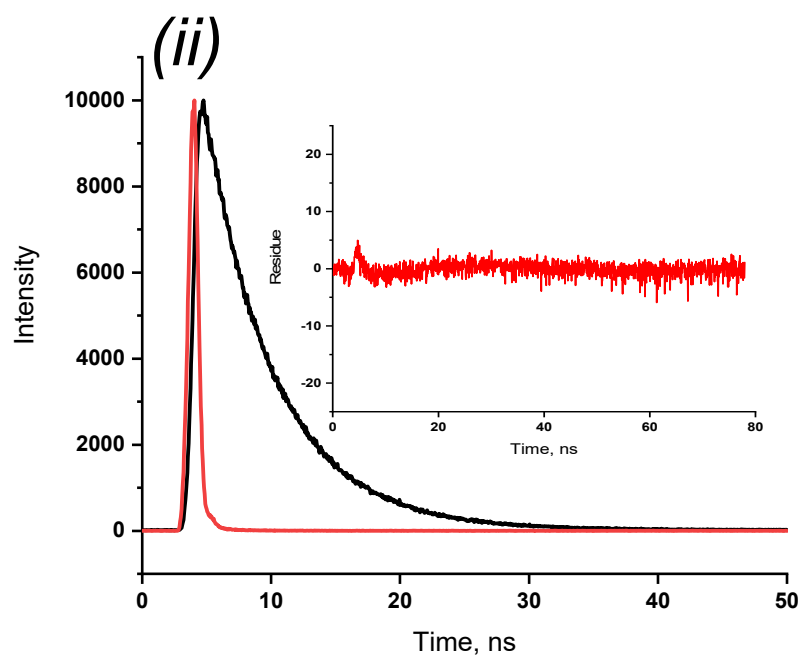
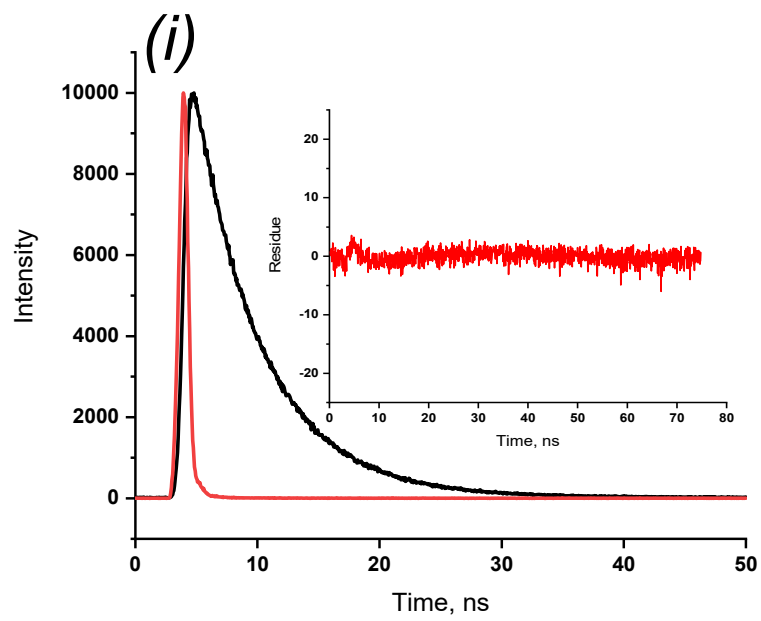


Figure S5. Fluorescence decays with excitation at the absorption maximum of the vibrational satellite for compounds **4(i)**, **5(ii)**, **6(iii)** and **7(iv)**

solutions in acetone, sample concentration $\sim 10 \mu\text{M}$. Data fitting to monoexponential function using deconvolution method, the chi squared value

is between 1.00 and 1.15.



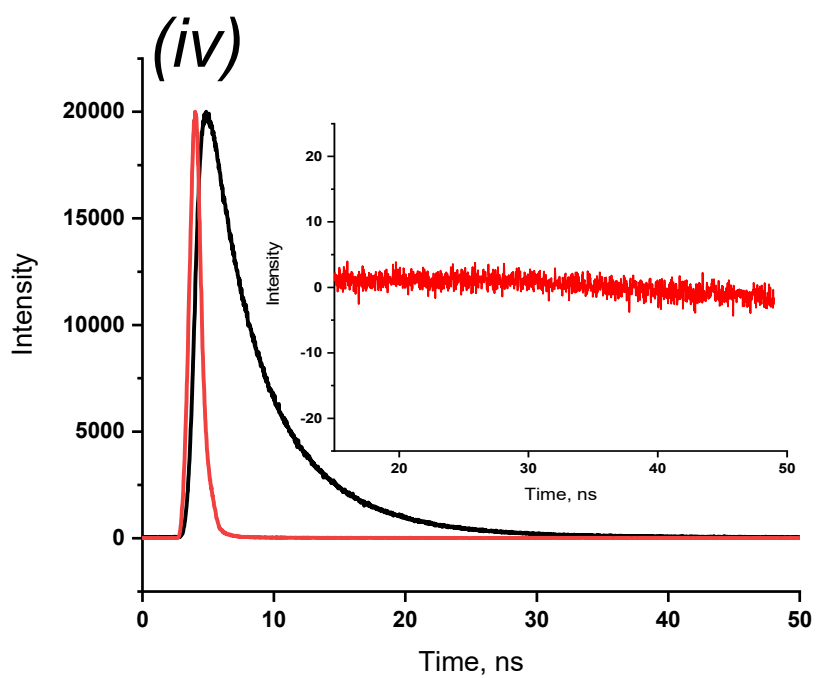
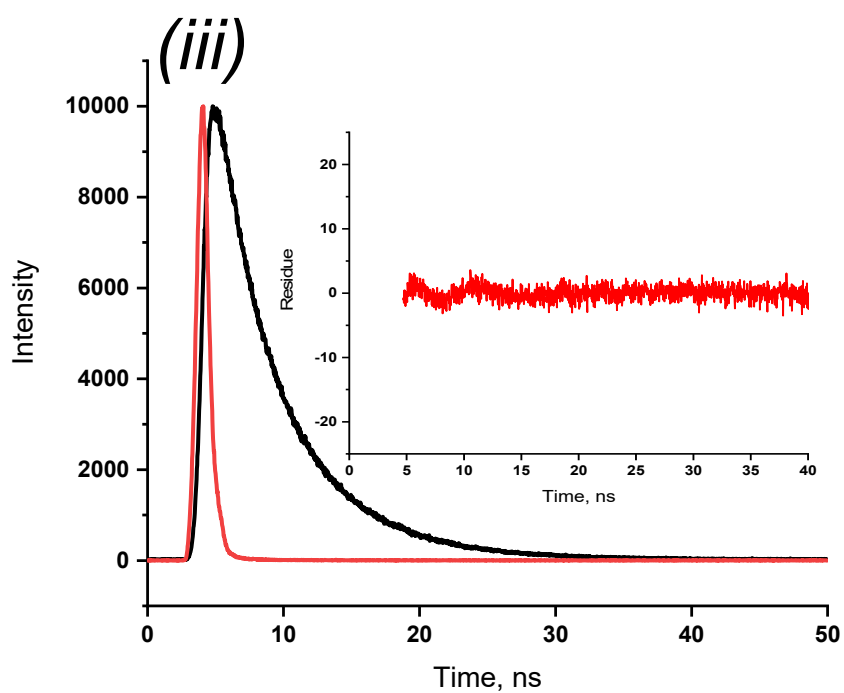
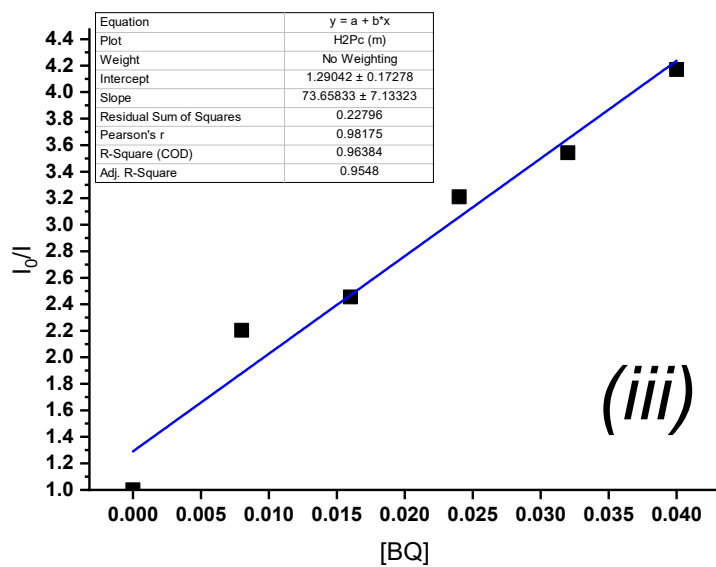
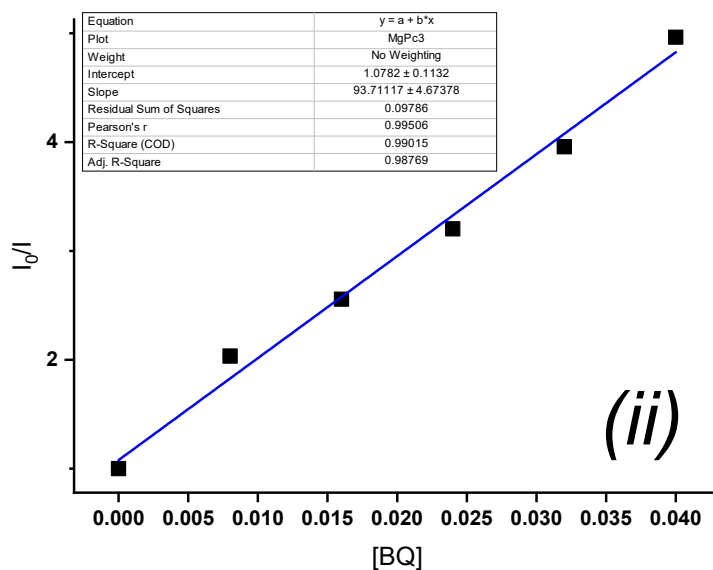
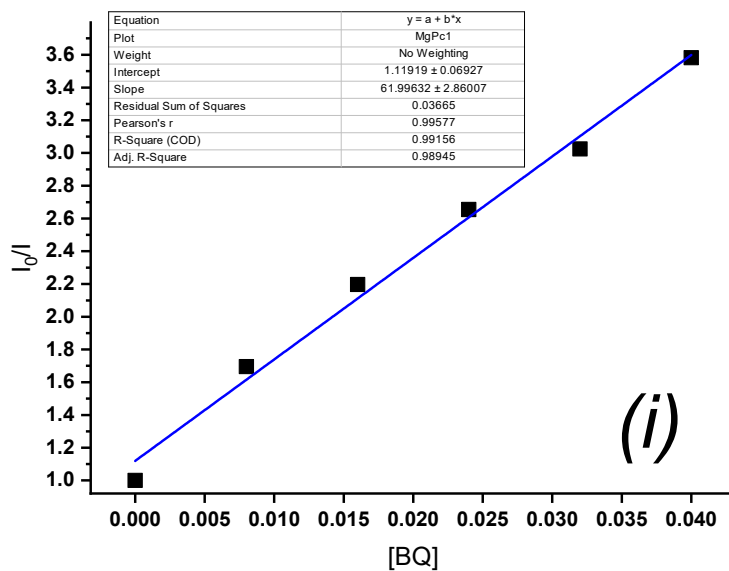


Figure S6. Fluorescence decays with excitation at the absorption maximum of the vibrational satellite for compounds **4(i)**, **5(ii)**, **6(iii)** and **7(iv)**

solutions in DMF, sample concentration $\sim 10 \mu\text{M}$. Data fitting to monoexponential function using deconvolution method, the chi squared value is

between 1.00 and 1.15.



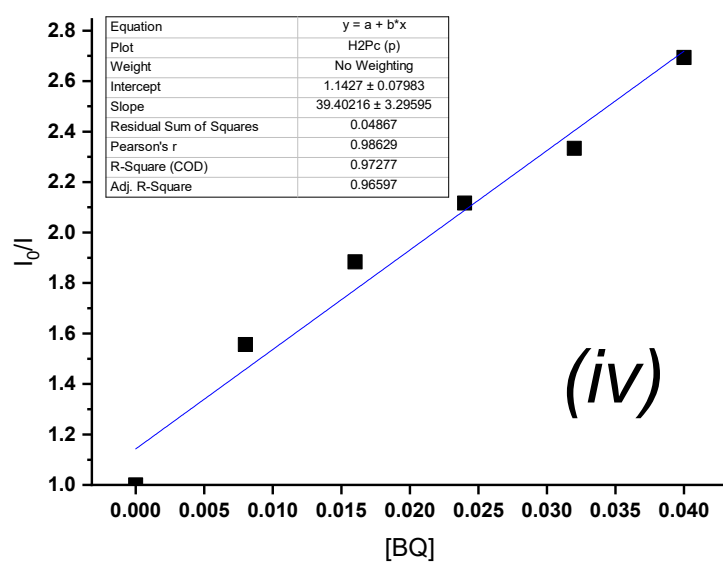
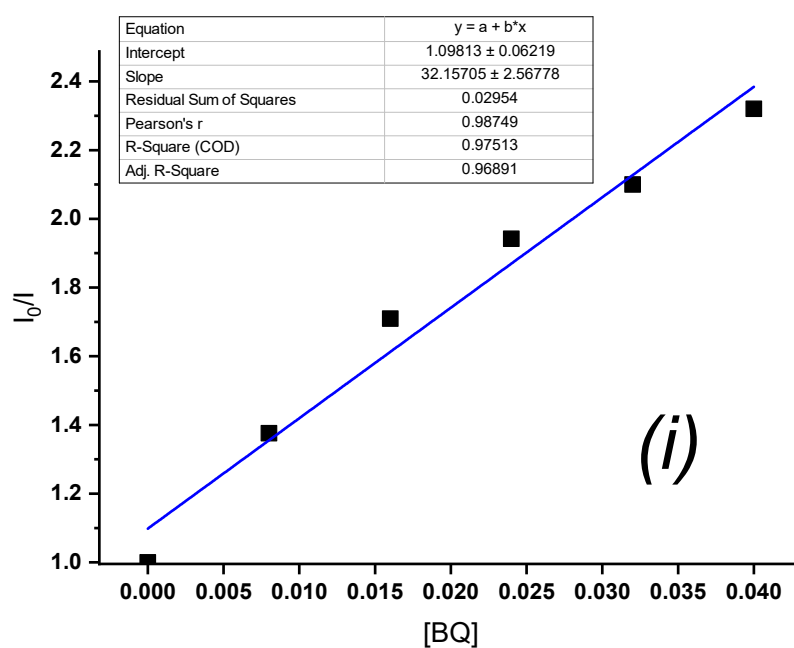
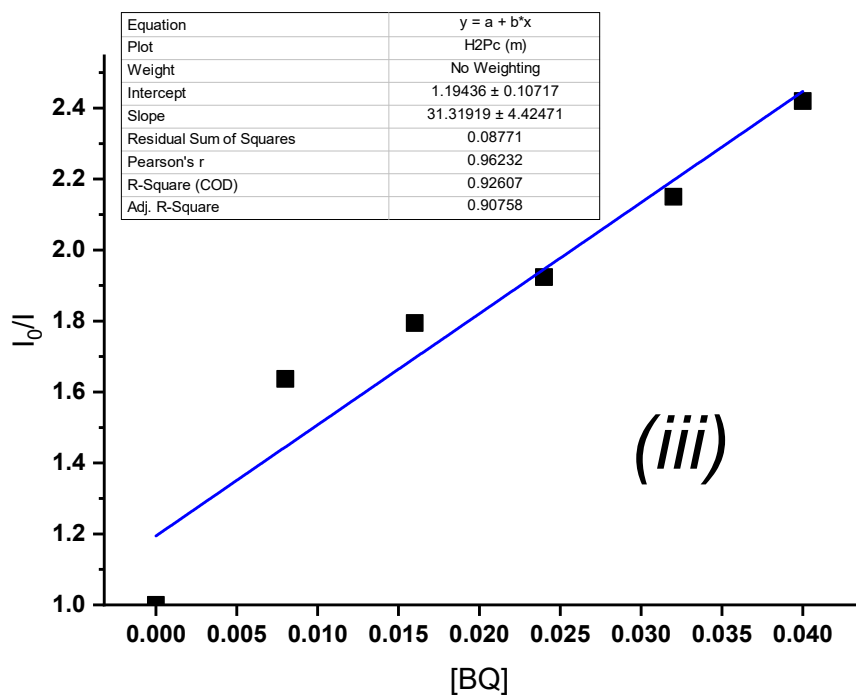
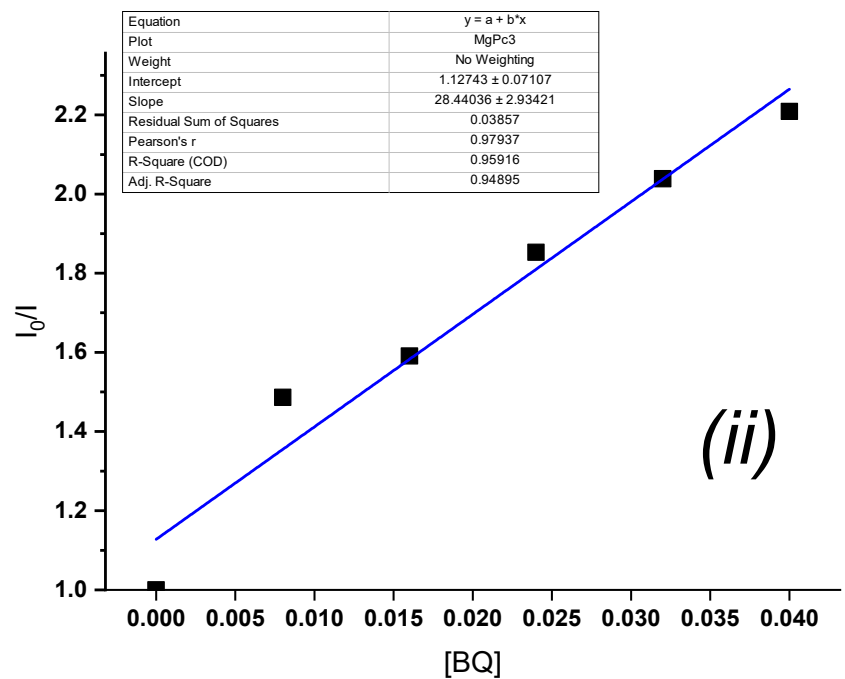


Figure S7. Stern–Volmer plots for benzoquinone (BQ) quenching of **4-7** in acetone. [BQ] = 0, 0.008, 0.016, 0.024, 0.032, 0.040 mol/L.





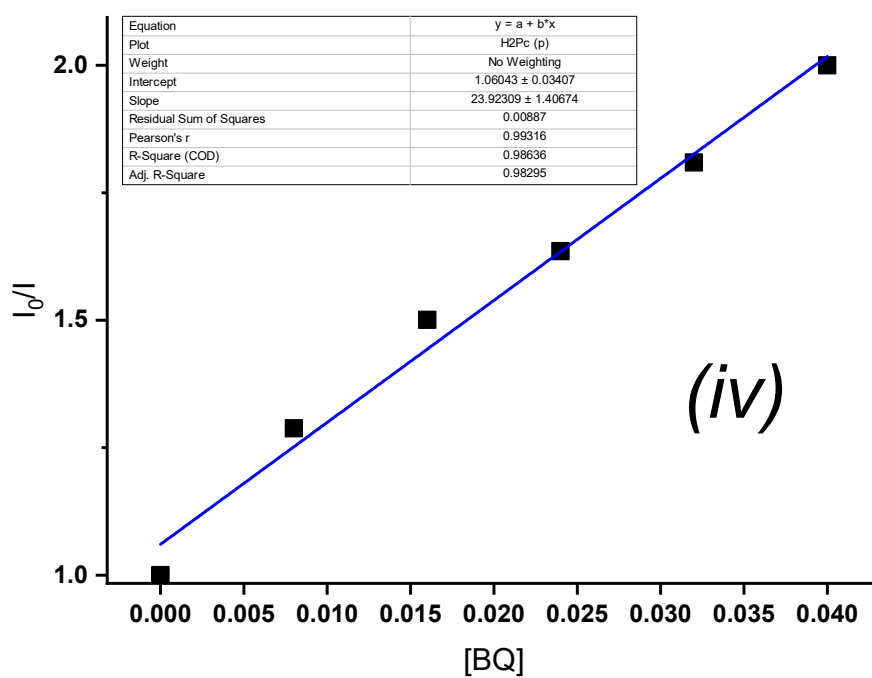
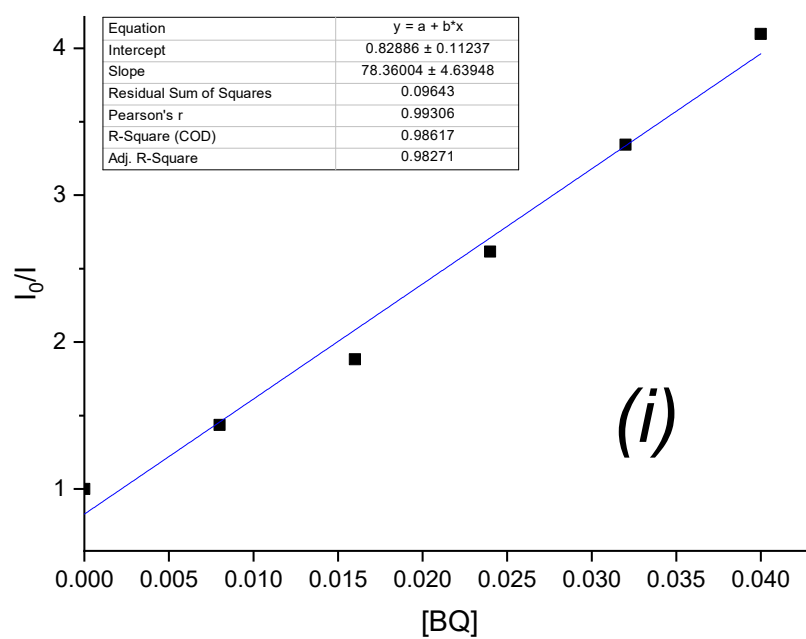
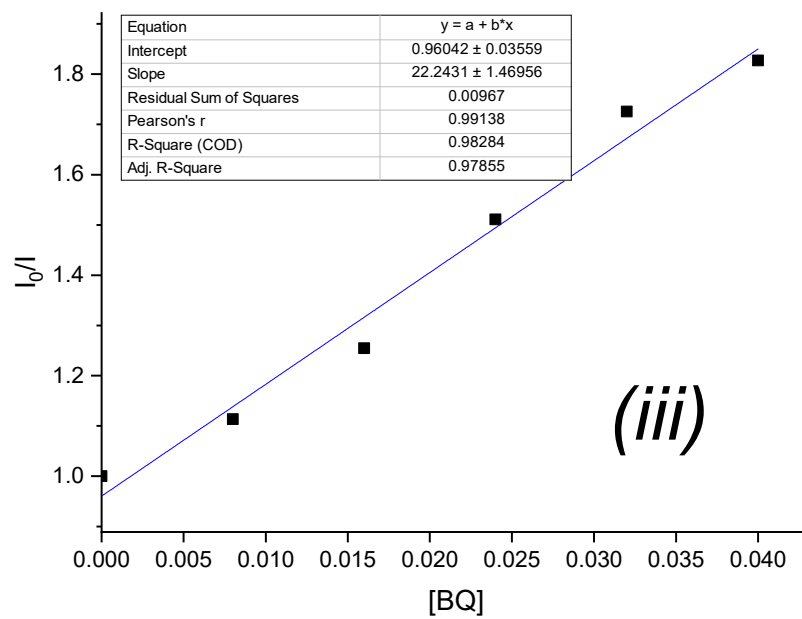
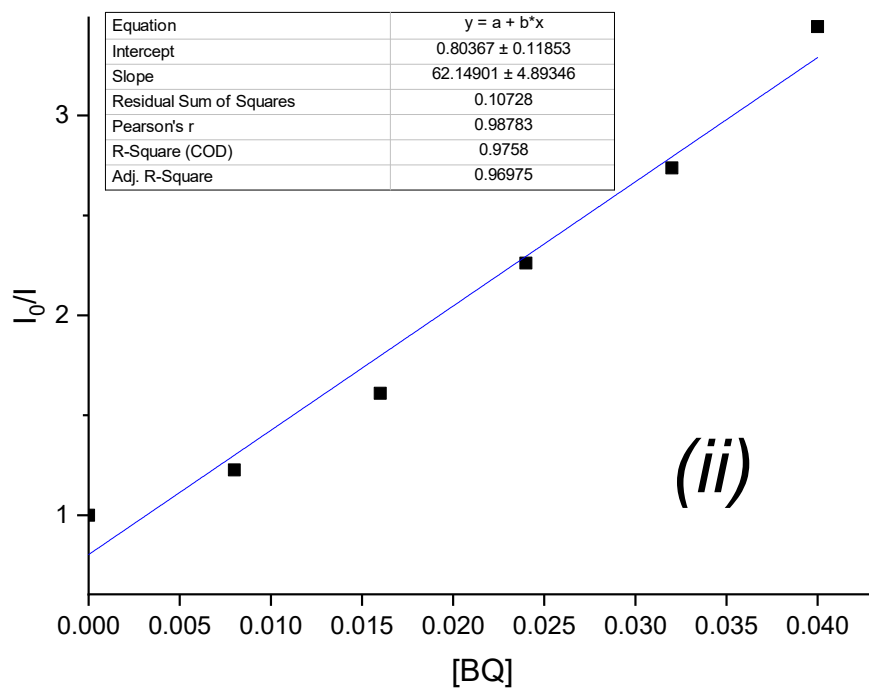


Figure S8. Stern–Volmer plots for benzoquinone (BQ) quenching of **4-7** in DMF. [BQ] = 0, 0.008, 0.016, 0.024, 0.032, 0.040 mol/L.





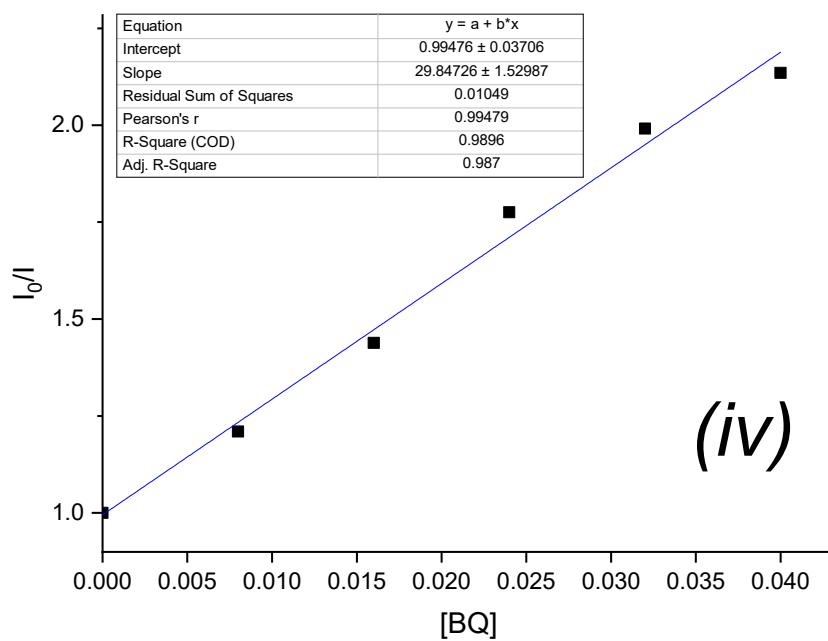


Figure S9. Stern–Volmer plots for benzoquinone (BQ) quenching of **4(i)**, **5(ii)**, **6(iii)**, **7(iv)** in CHCl_3 . $[\text{BQ}] = 0, 0.008, 0.016, 0.024, 0.032, 0.040 \text{ mol/L}$

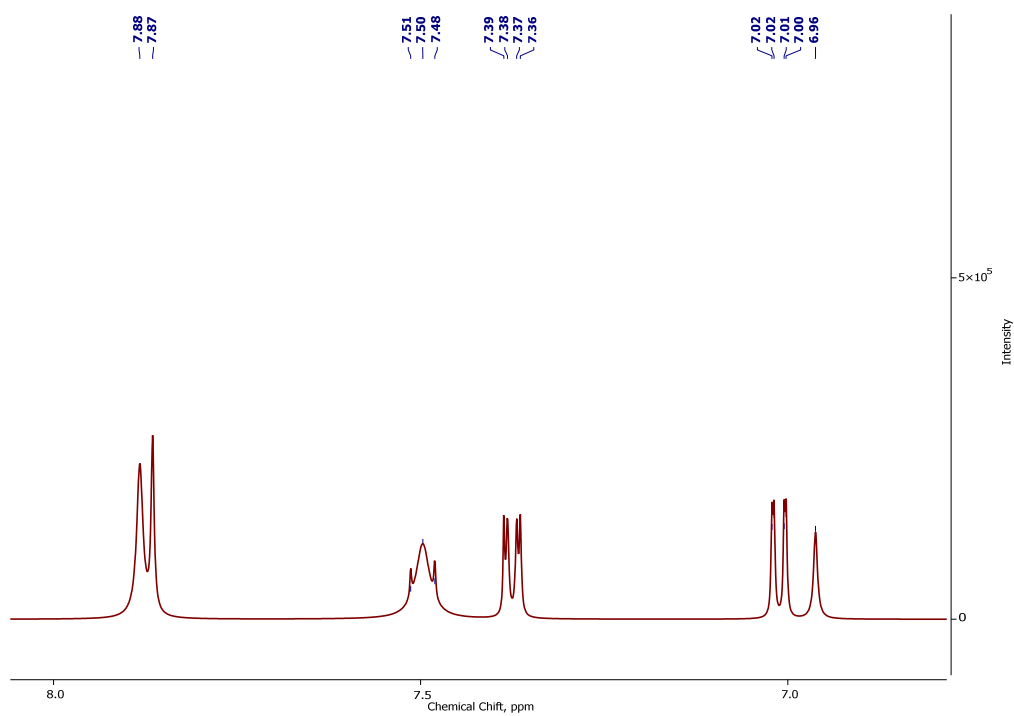


Figure S10. ^1H NMR spectrum of **4** in DMSO-d_6 .

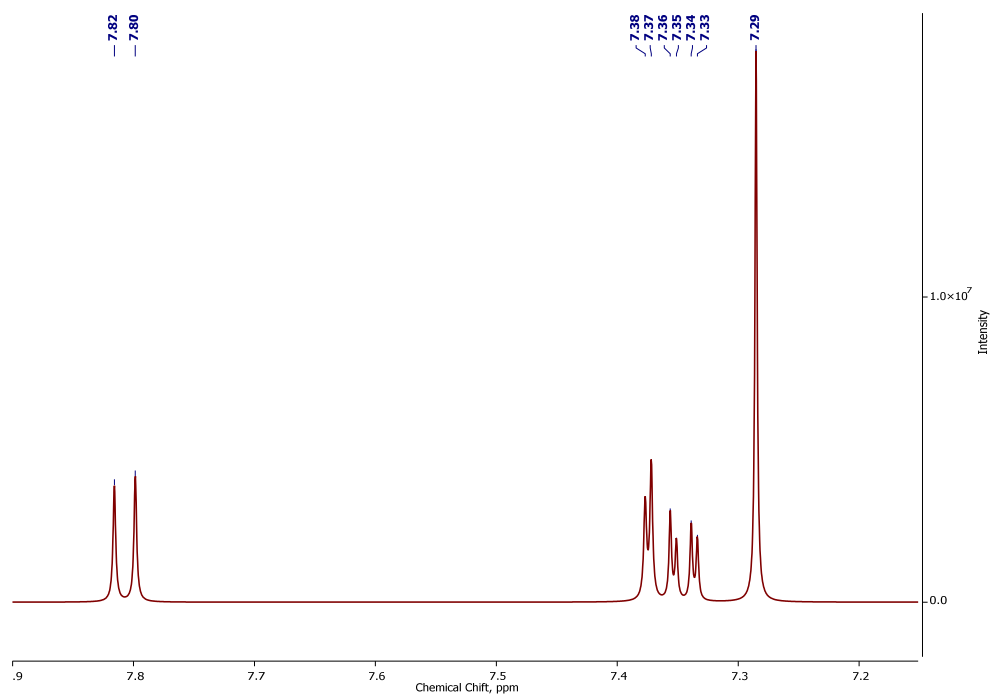


Figure S11. ¹H NMR spectrum of **5** in DMSO-d₆.

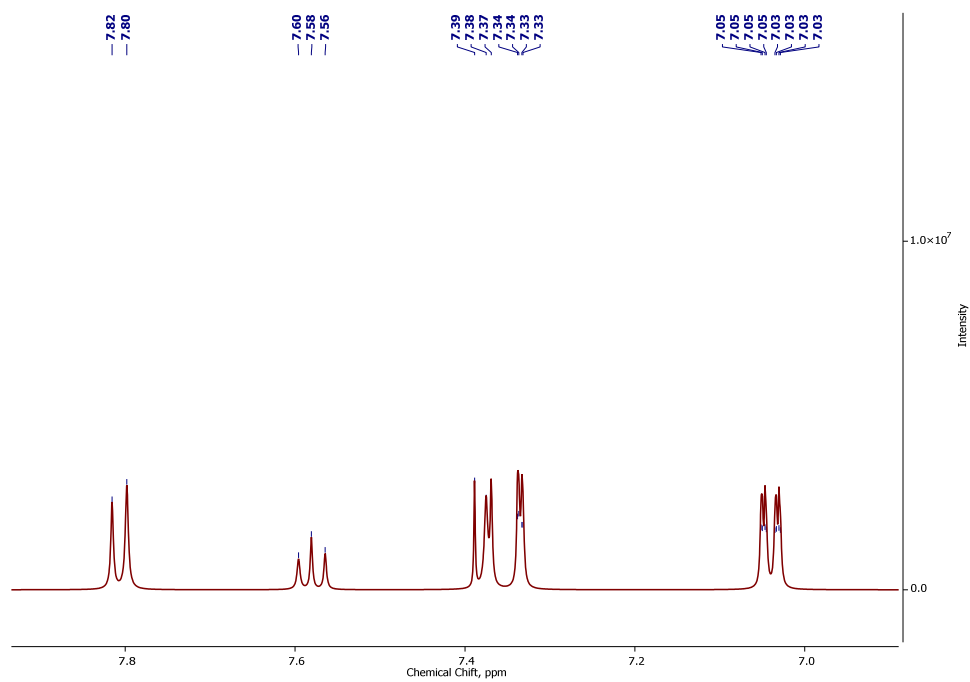


Figure S12. ¹H NMR spectrum of **6** in DMSO-d₆.

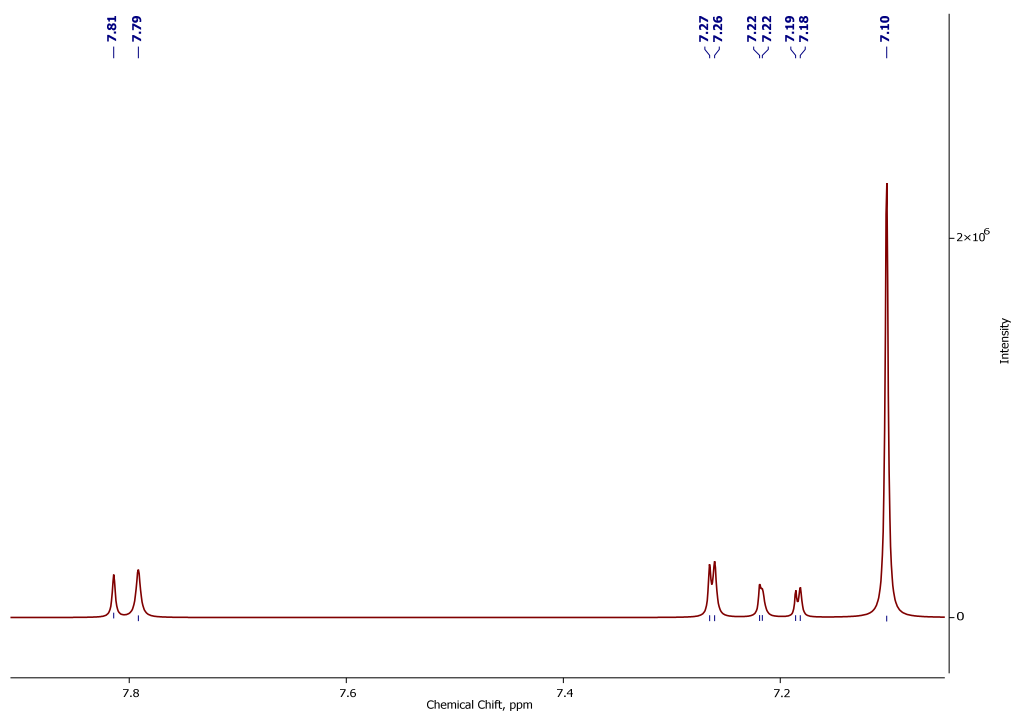


Figure S13. ¹H NMR spectrum of 7 in DMSO-d₆.

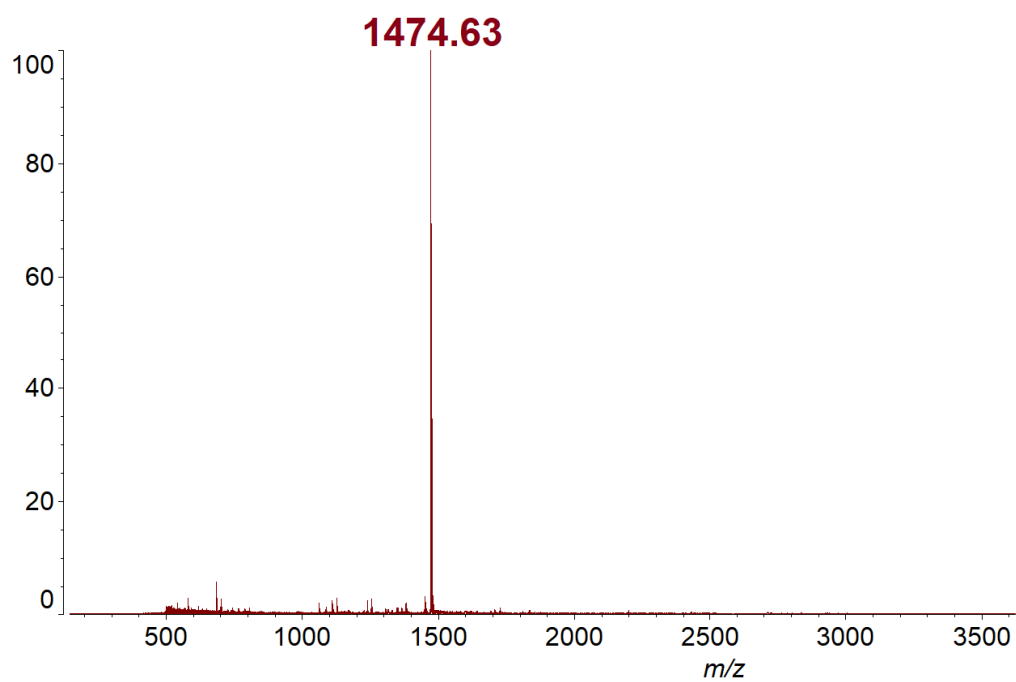


Figure S14. HR MALDI-TOF mass spectrum of 4.

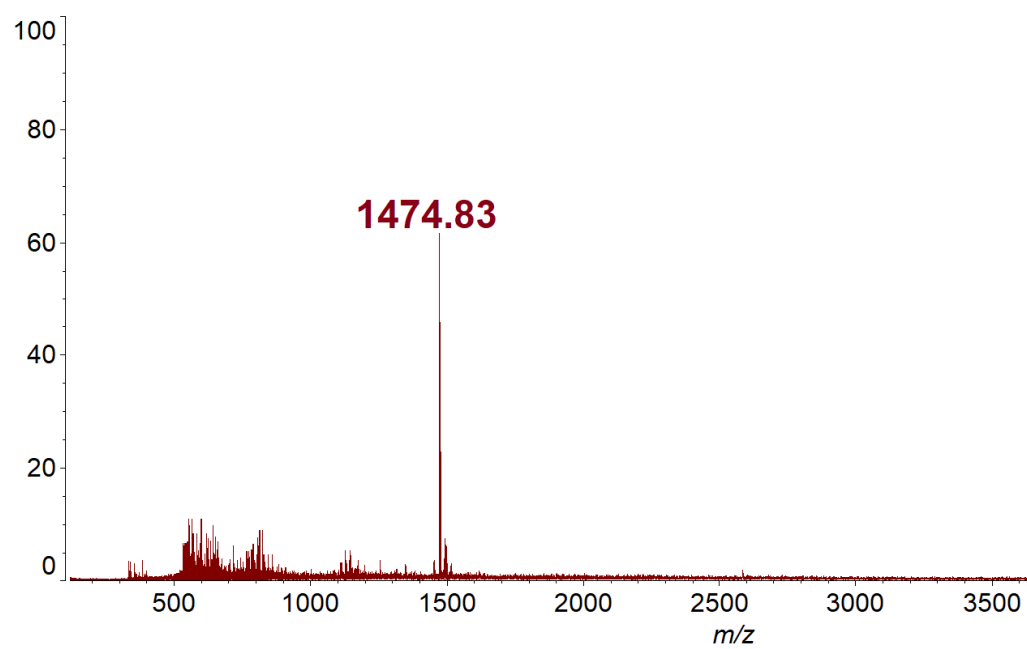


Figure S15. HR MALDI-TOF mass spectrum of 5.

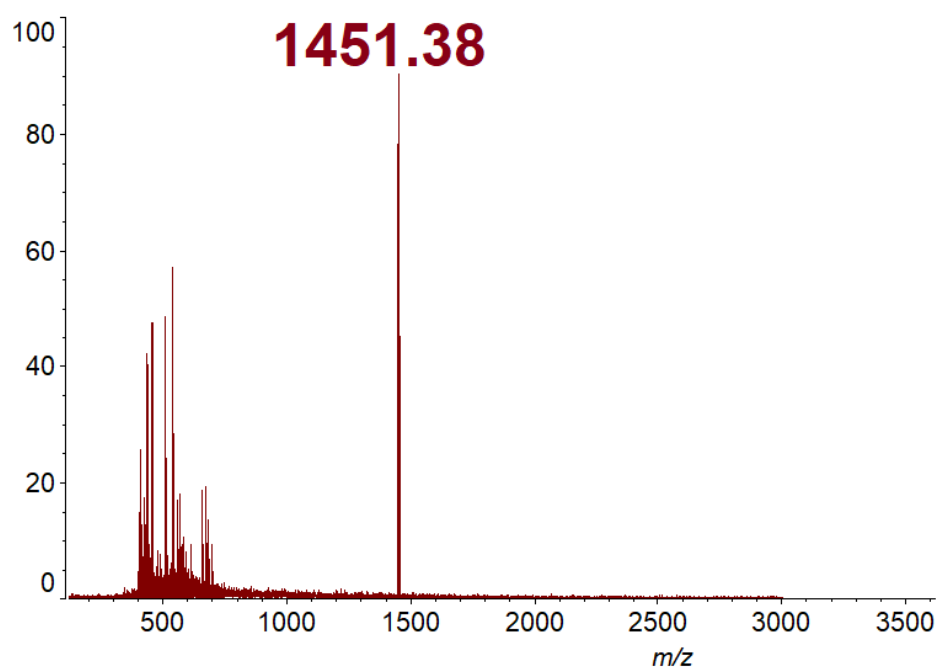


Figure S16. HR MALDI-TOF mass spectrum of 6.

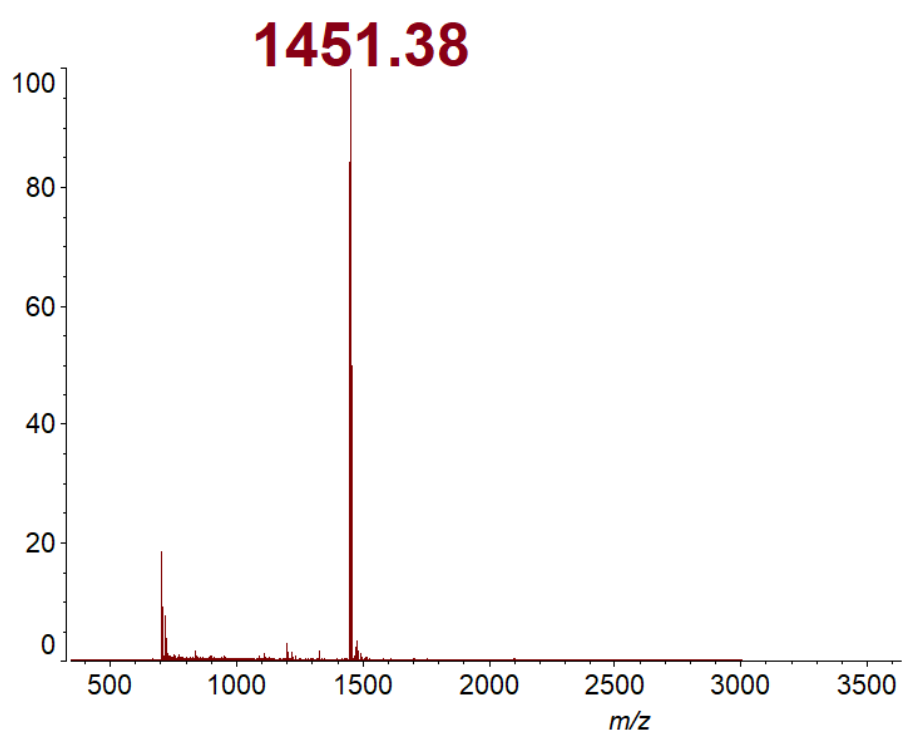


Figure S17. HR MALDI-TOF mass spectrum of 7.

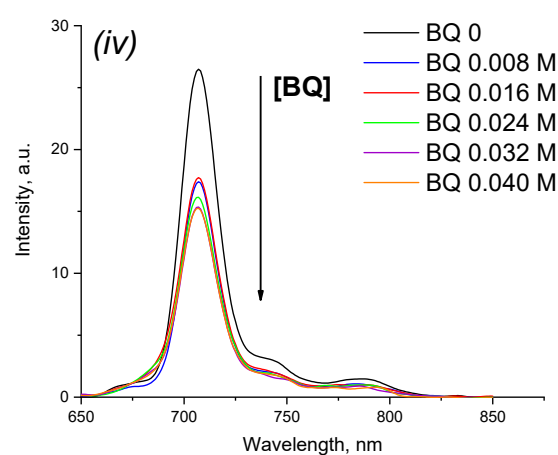
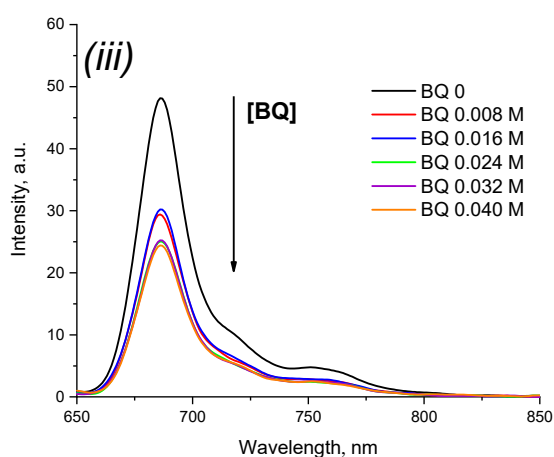
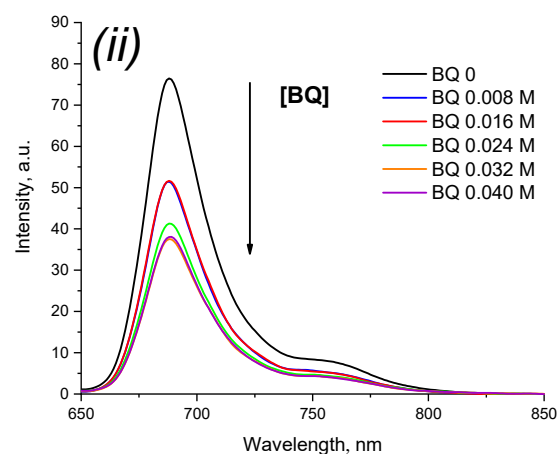
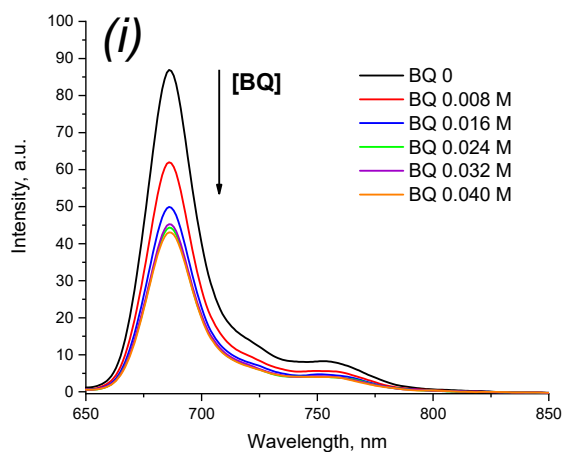
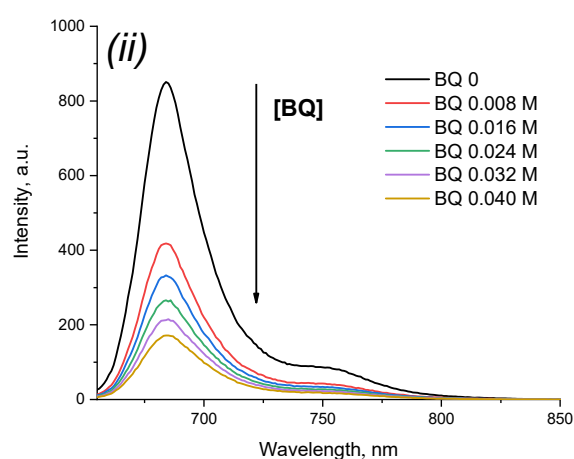
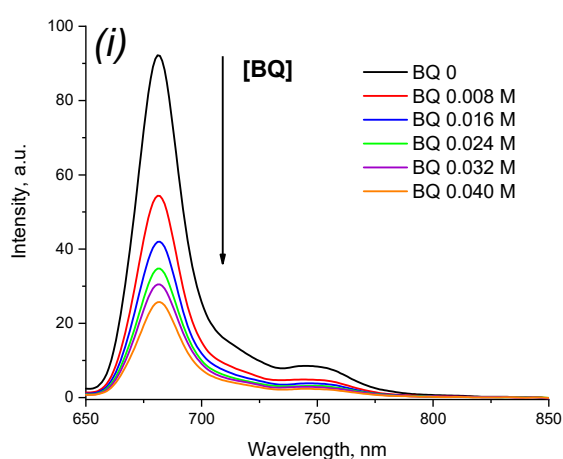


Figure S18. Fluorescence emission spectra changes of 4(i), 5(ii), 6(iii) and 7(iv) upon addition of different concentrations of BQ in DMF. [BQ] = 0, 0.008, 0.016, 0.024, 0.032, 0.040 mol/L.



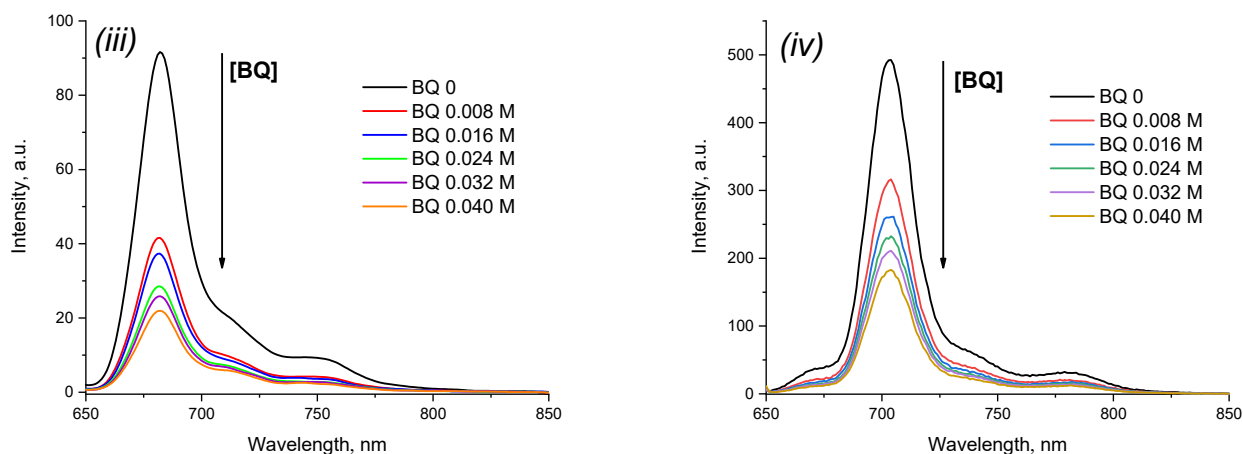


Figure S19. Fluorescence emission spectra changes of **4(i)**, **5(ii)**, **6(iii)** and **7(iv)** upon addition of different concentrations of BQ in acetone. [BQ] = 0, 0.008, 0.016, 0.024, 0.032, 0.040 mol/L.

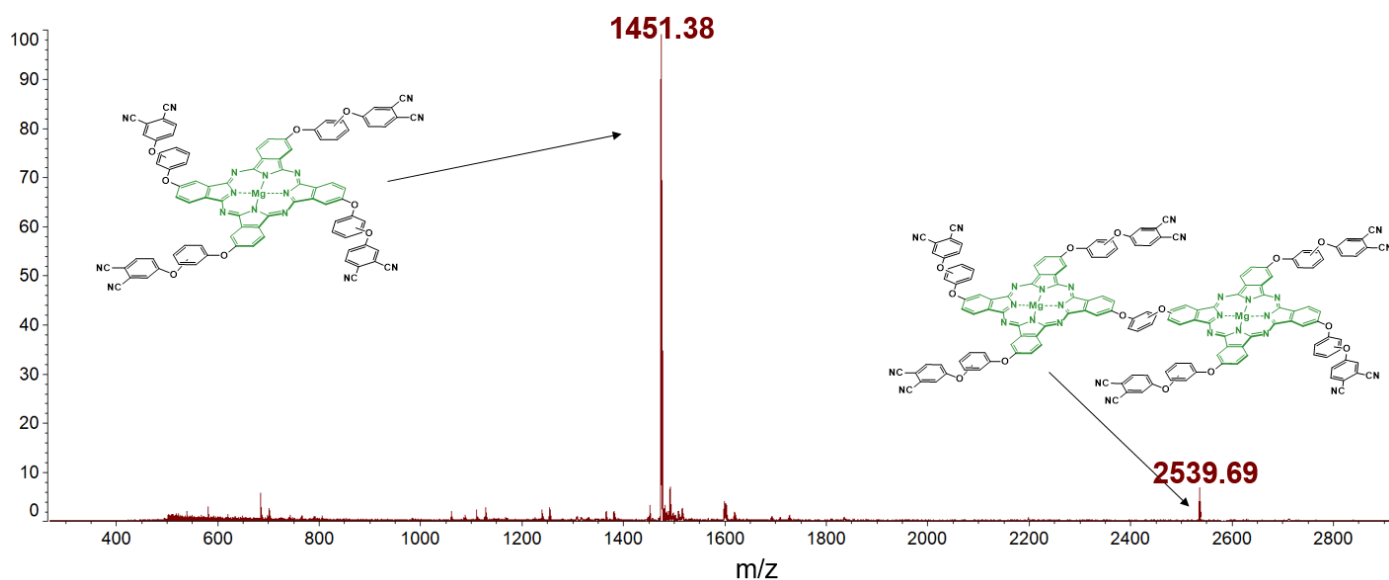
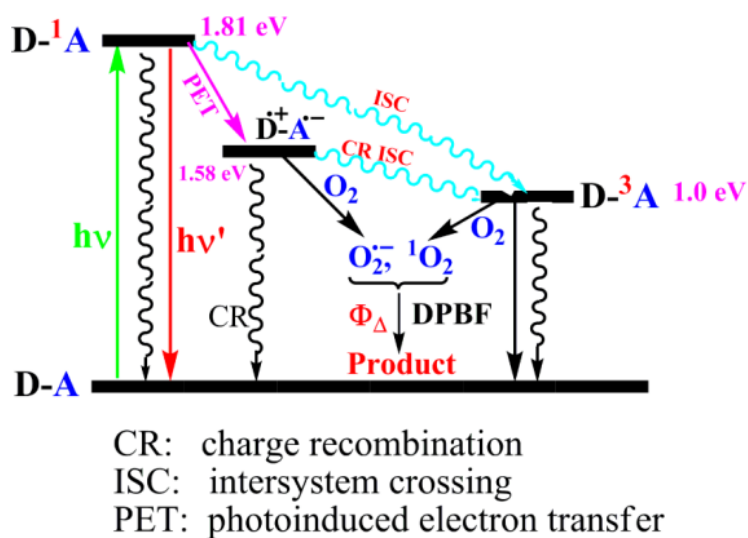


Figure S20. MALDI-TOF mass spectrum of reaction mixture of **4** after the template fusion.



Scheme S2. Photophysical and photochemical processes involved in the photooxidation in the presence of phthalocyanine [36].

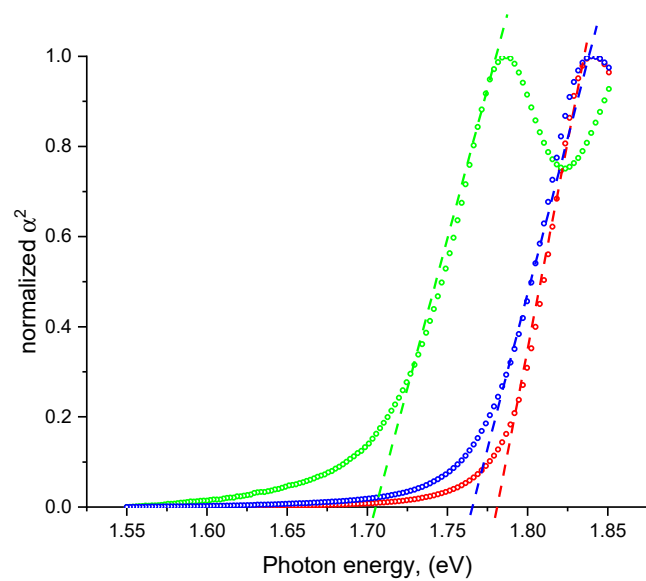


Figure S21. Plot of α^2 versus photon energy of samples **4** (green line), **5** (blue line) and **6** and **7** (red line). The extrapolating light dashed line intersects the value of optical band gap at the photon energy axis.

Table S1. The values of the optical band gap energies (E_g) for phthalocyanines **4-7**

Sample	E_g (eV)
4	1.705
5	1.766
6	1.781
7	1.781