

Supporting Information

for

Rational Design and In-Situ FTIR Analyses of Colorimetrically Reversible Polydiacetylene Supramolecules

by

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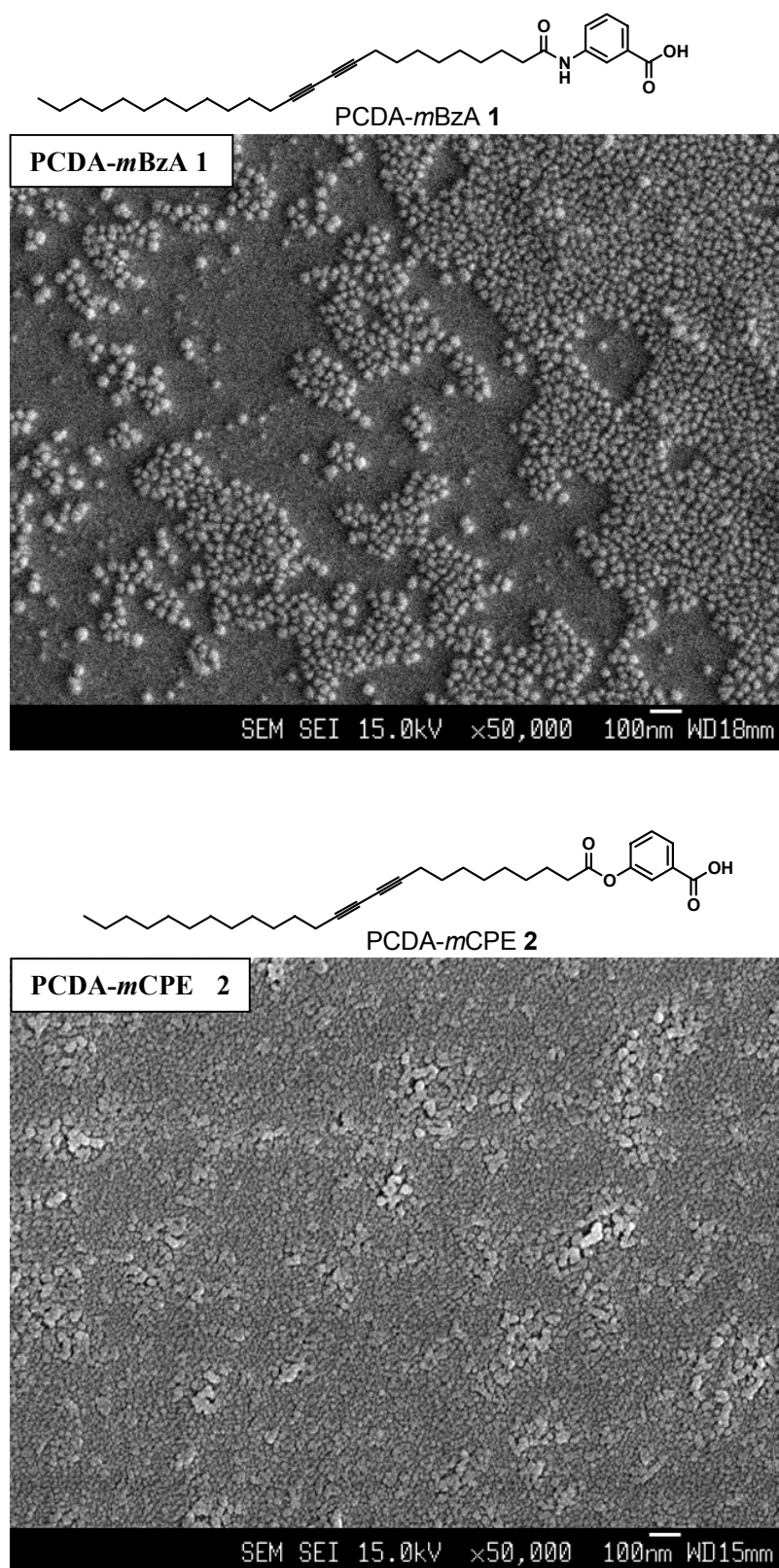


Figure S1. SEM images of polydiacetylene vesicles prepared with PCDA-*m*BzA 1 and PCDA-*m*CPE 2.

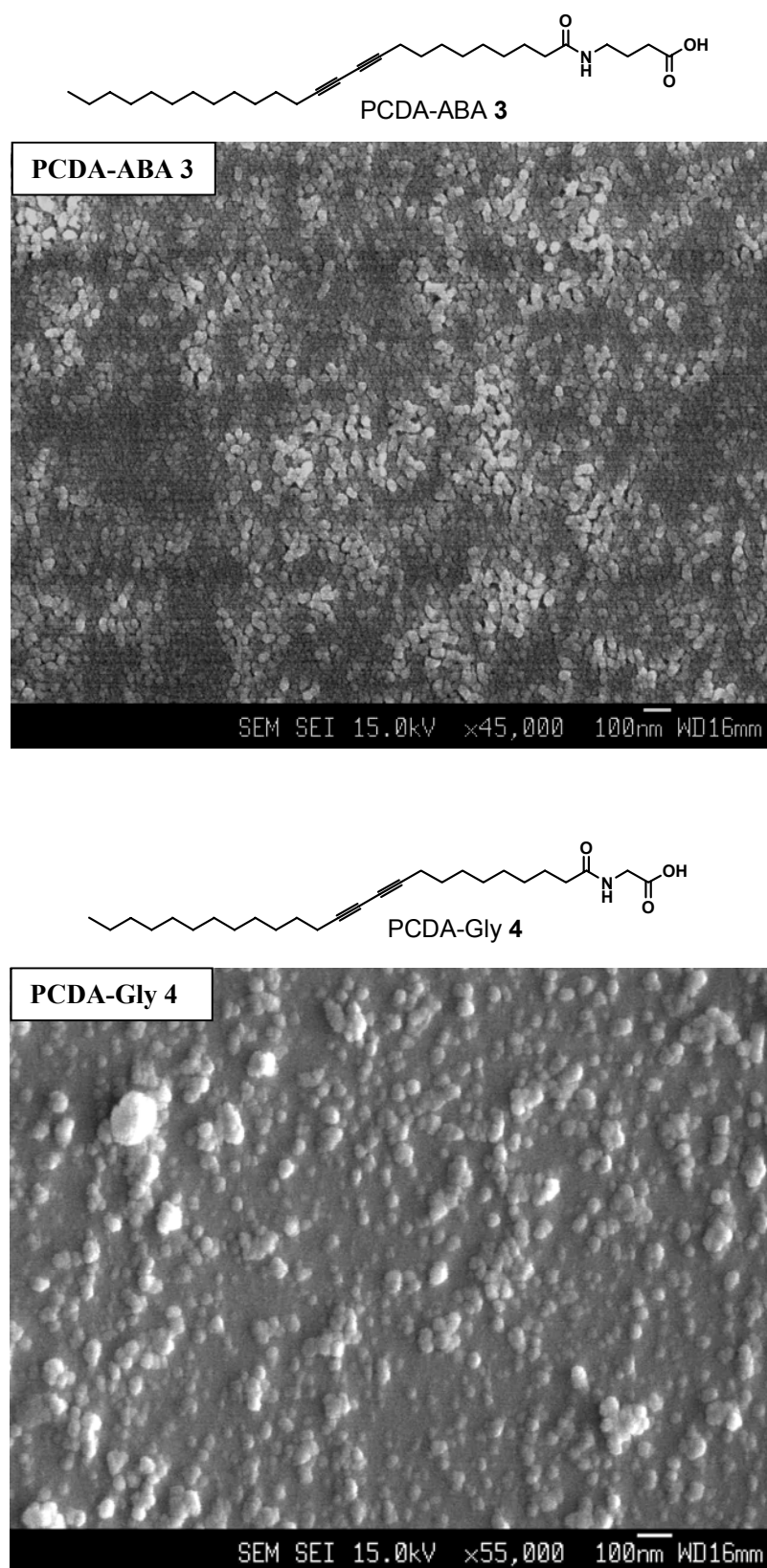


Figure S2. SEM images of polydiacetylene vesicles prepared with PCDA-ABA **3** and PCDA-Gly **4**.

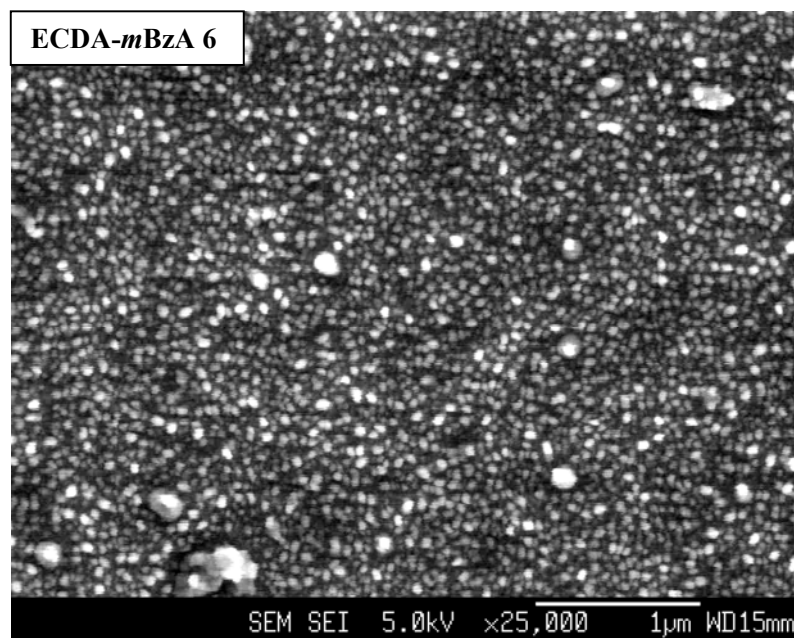
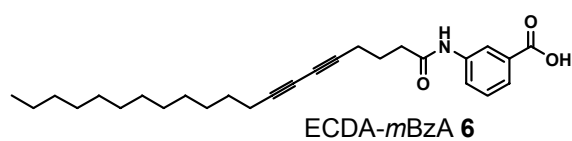
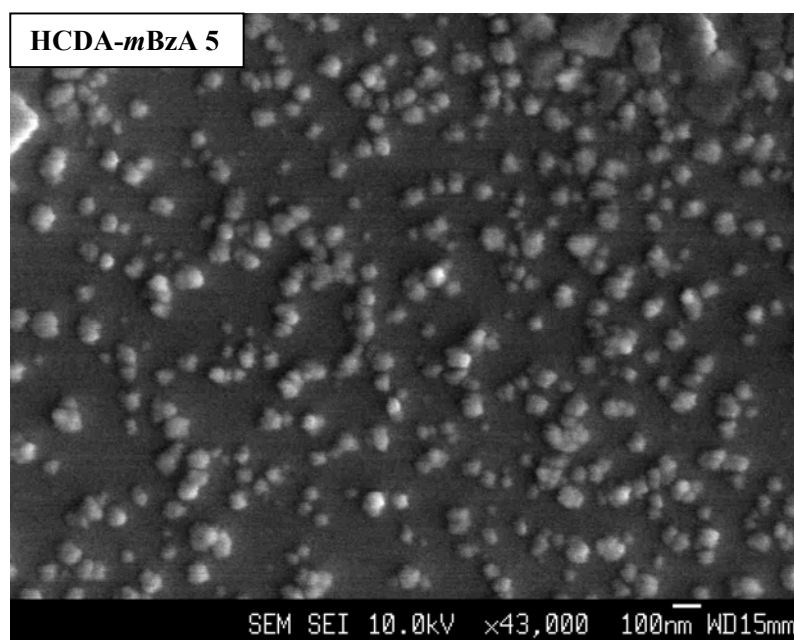
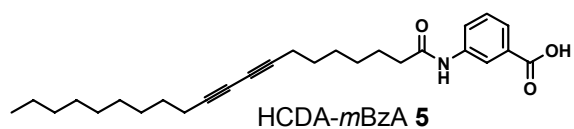


Figure S3. SEM images of polydiacetylene vesicles prepared with HCDA-*m*BzA **5** and ECDA-*m*BzA **6**.

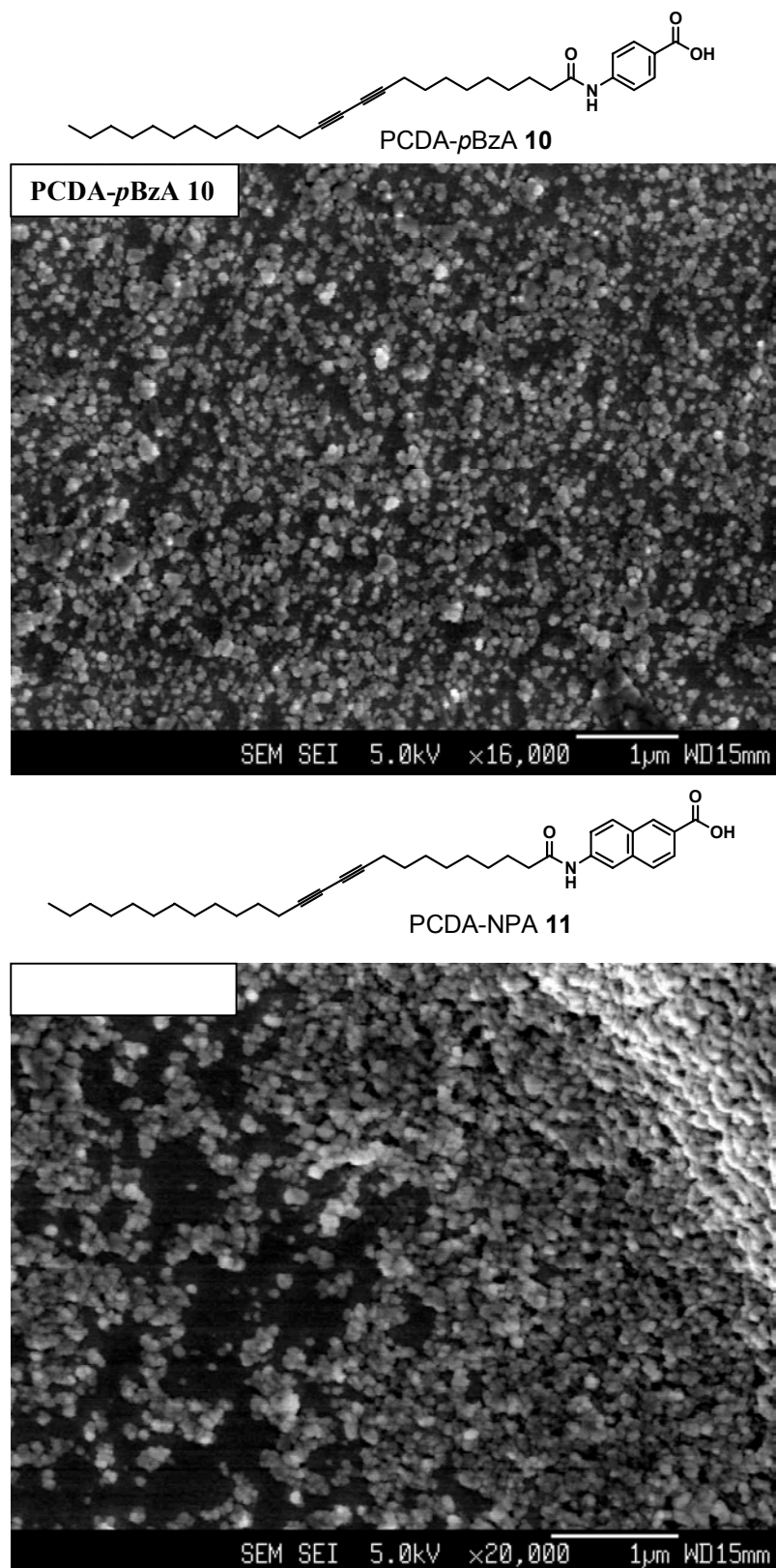


Figure S4. SEM images of polydiacetylene vesicles prepared with PCDA-*p*BzA **10** and PCDA-NPA **11**.

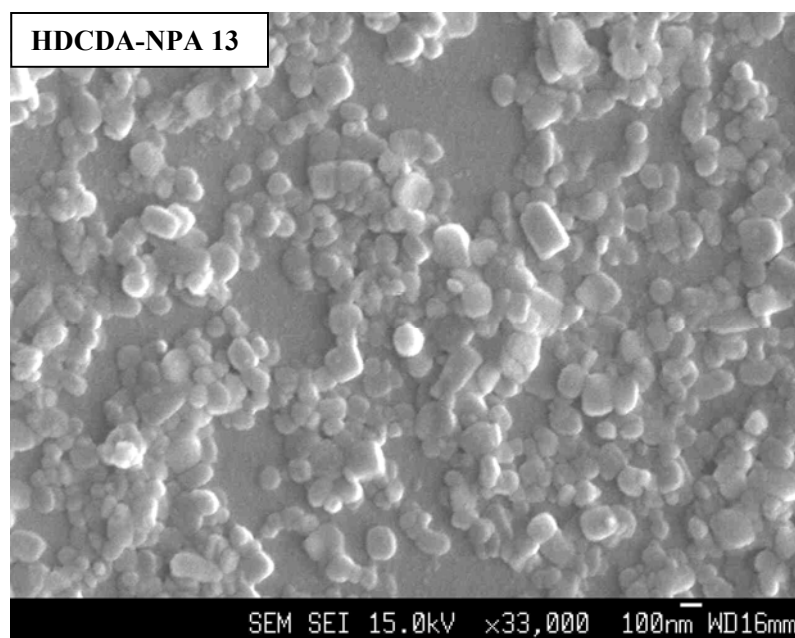
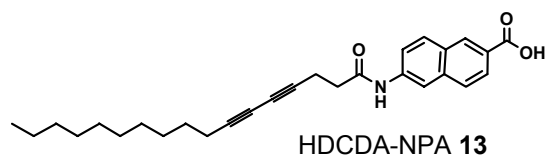
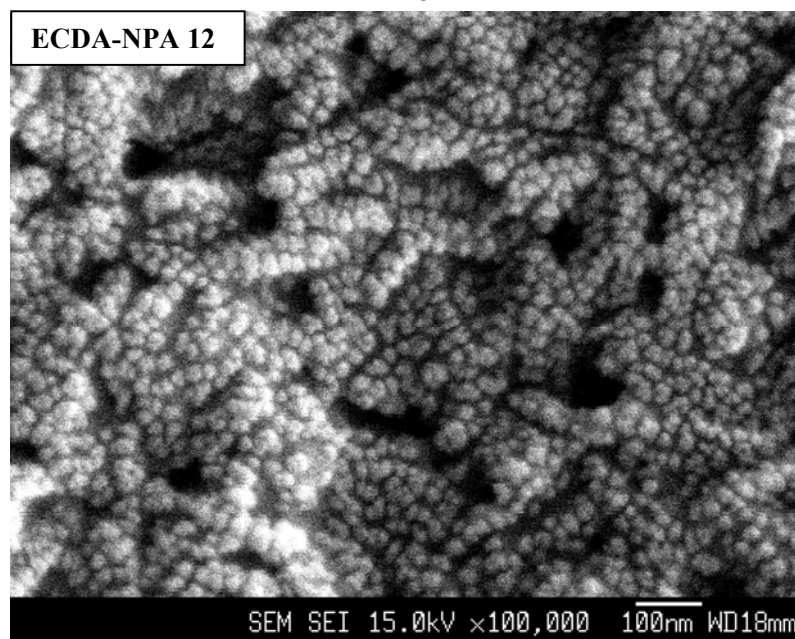
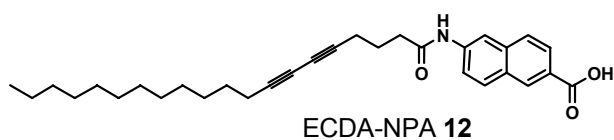


Figure S5. SEM images of polydiacetylene vesicles prepared with PCDA-NPA 11 and HDCDA-NPA 13.

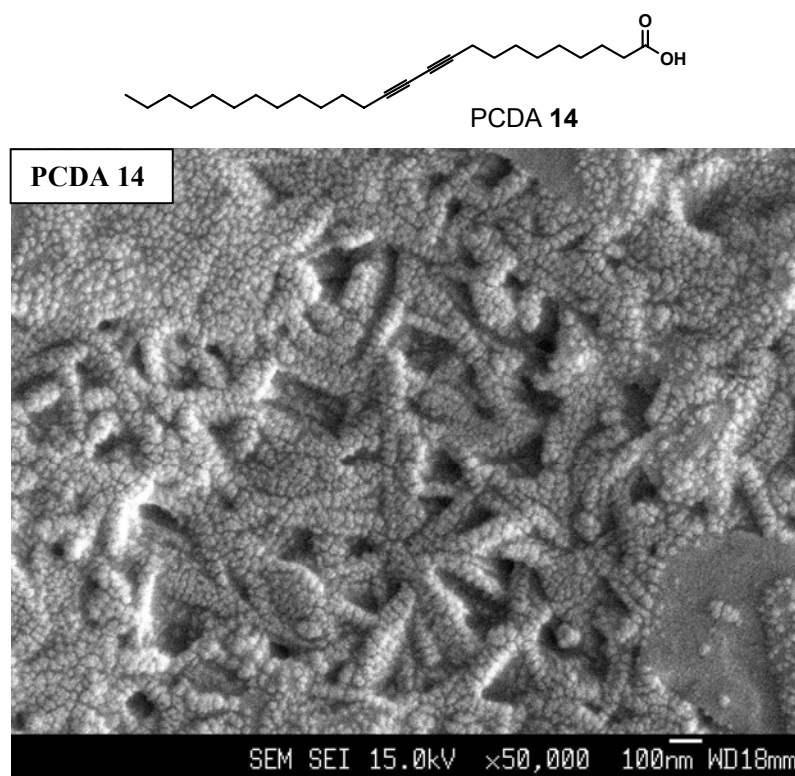
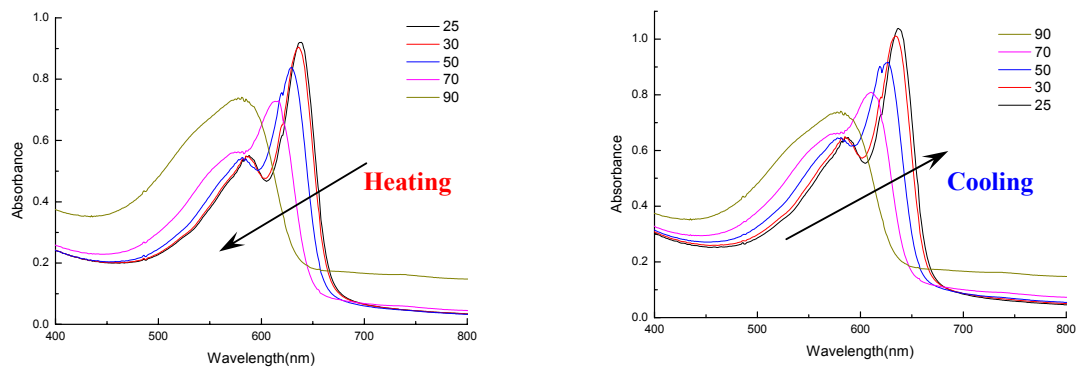
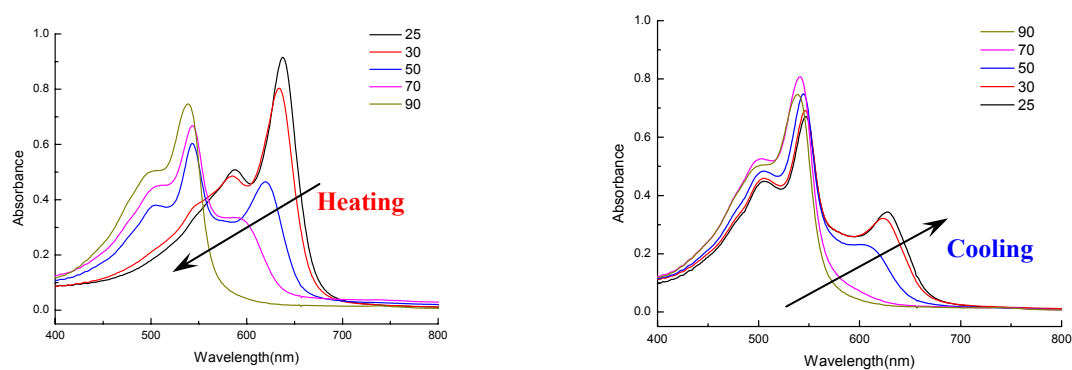


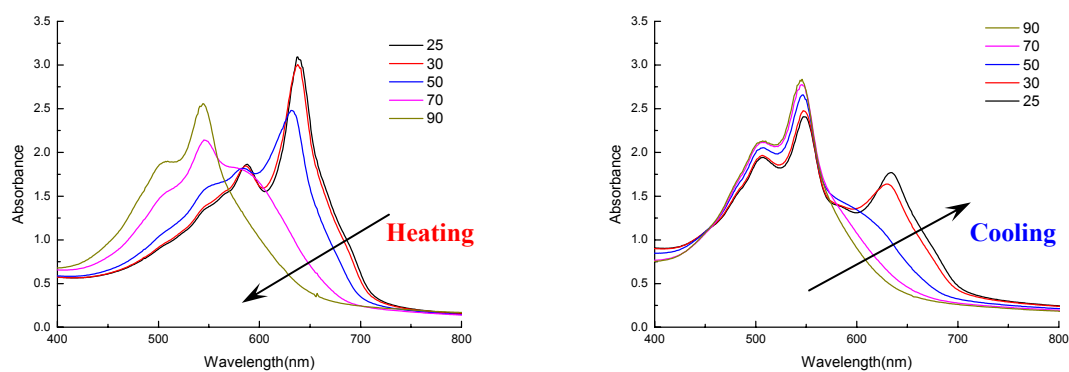
Figure S6. SEM images of polydiacetylene vesicles prepared with PCDA 14.



PCDA-*m*BzA 1

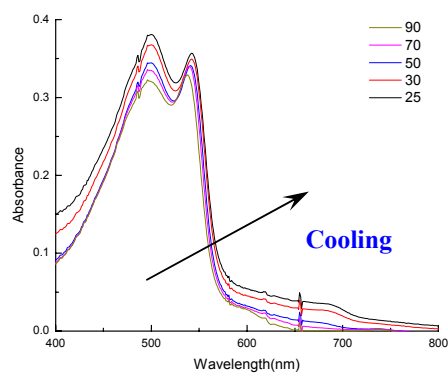
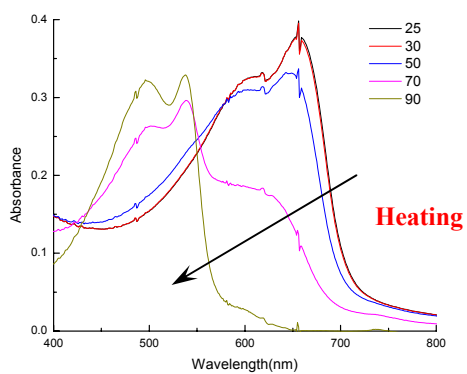


PCDA-*m*CPE 2

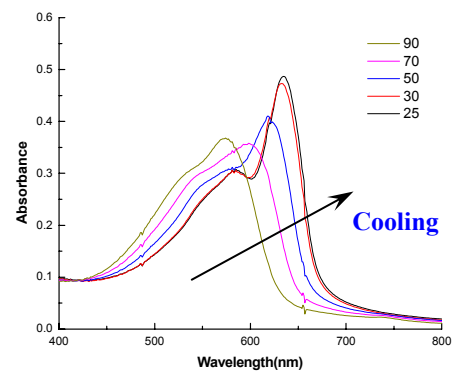
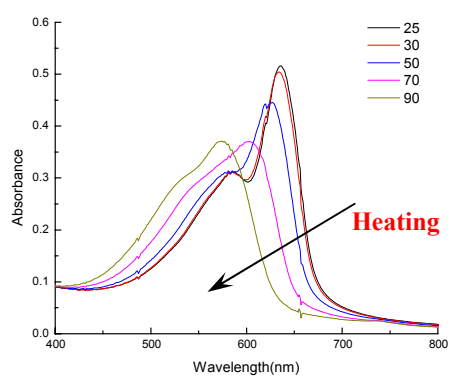


PCDA-ABA 3

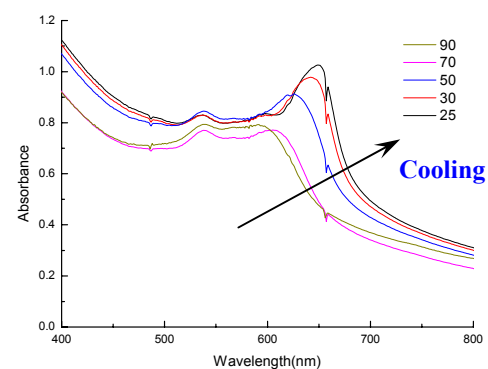
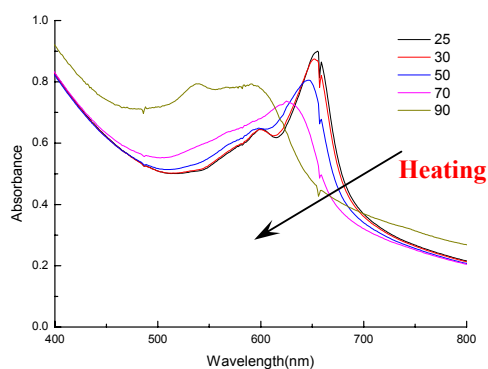
Figure S7. Visible spectral changes of PDA vesicle solutions prepared with PCDA-*m*BzA 1, PCDA-*m*CPE 2, and PCDA-ABA 3 upon heating and cooling process.



PCDA-Gly 4

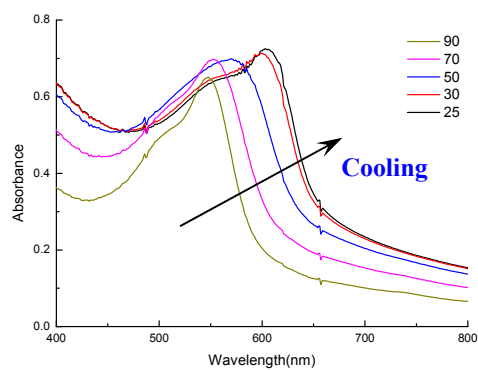
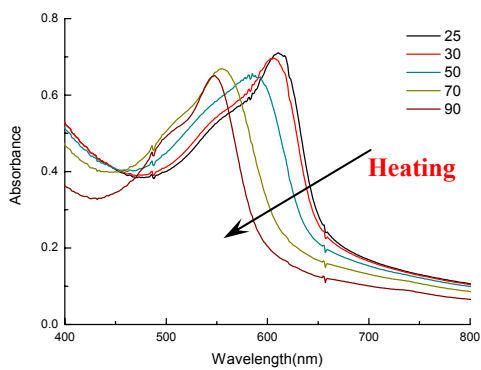


HCDA-mBzA 5

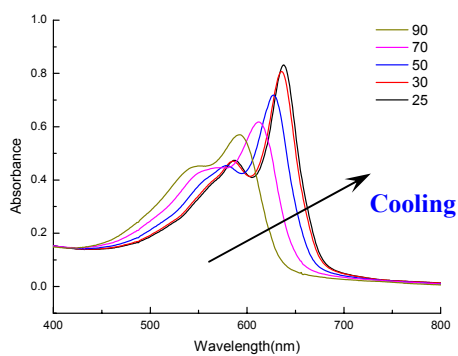
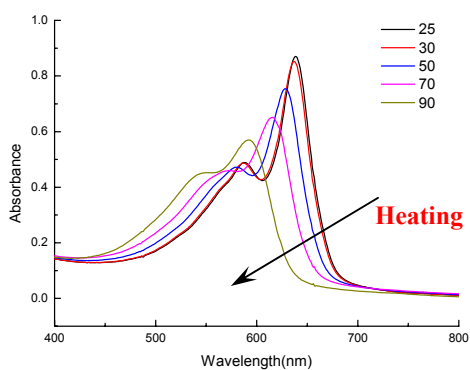


ECDA-mBzA 6

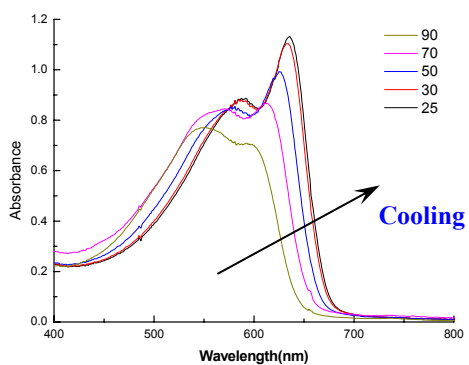
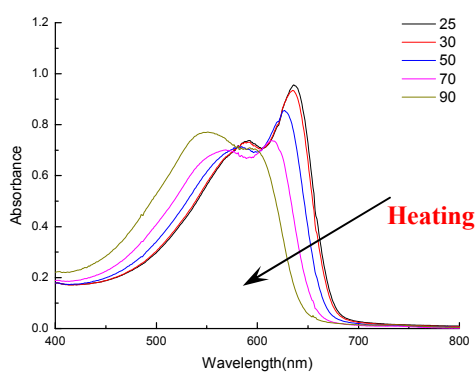
Figure S8. Visible spectral changes of PDA vesicle solutions prepared with PCDA-Gly 4, HCDA-mBzA 5, and ECDA-mBzA 6 upon heating and cooling process.



HDCDA-*m*BzA 7

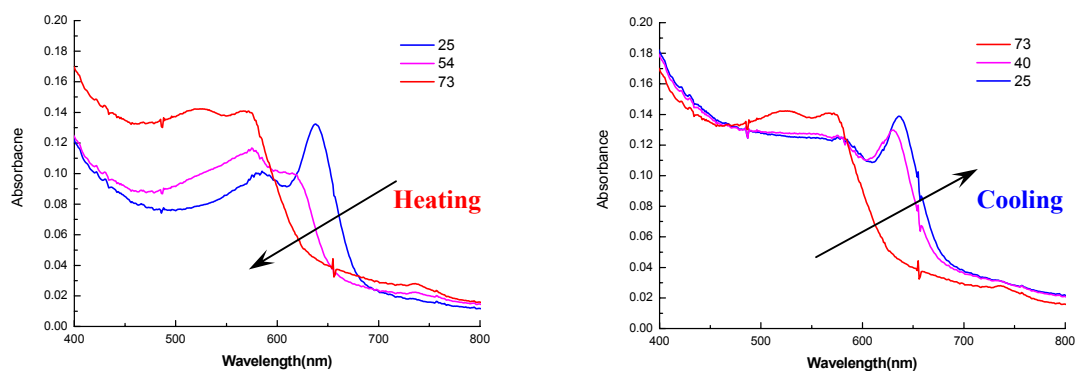


PCDA-*p*BzA 10

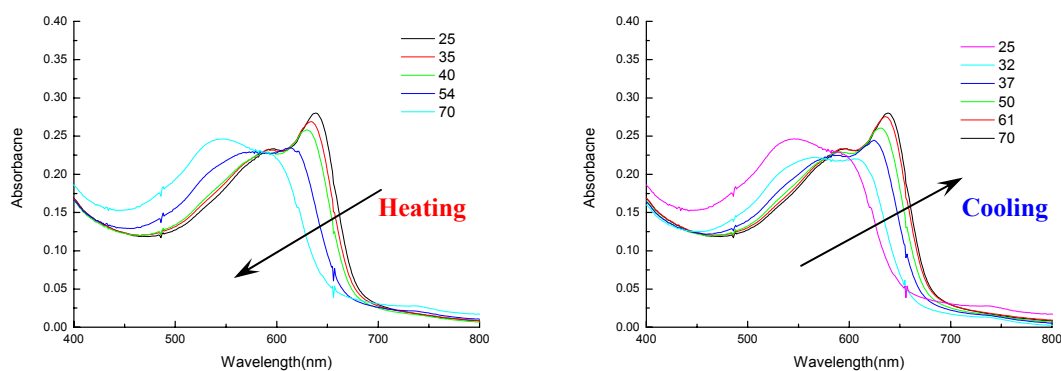


PCDA-NPA 11

Figure S9. Visible spectral changes of PDA vesicle solutions prepared with HDCDA-*m*BzA 7, PCDA-*p*BzA 10, and PCDA-NPA 11 upon heating and cooling process.

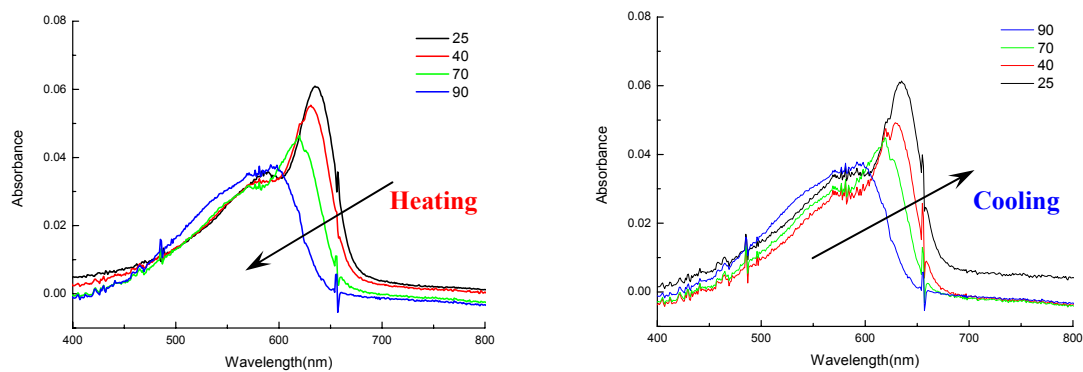


ECDA-NPA 12

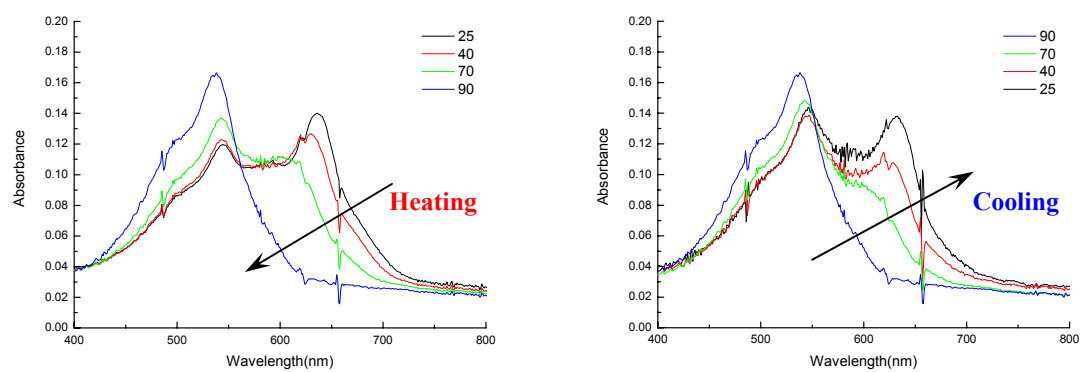


HDCDA-NPA 13

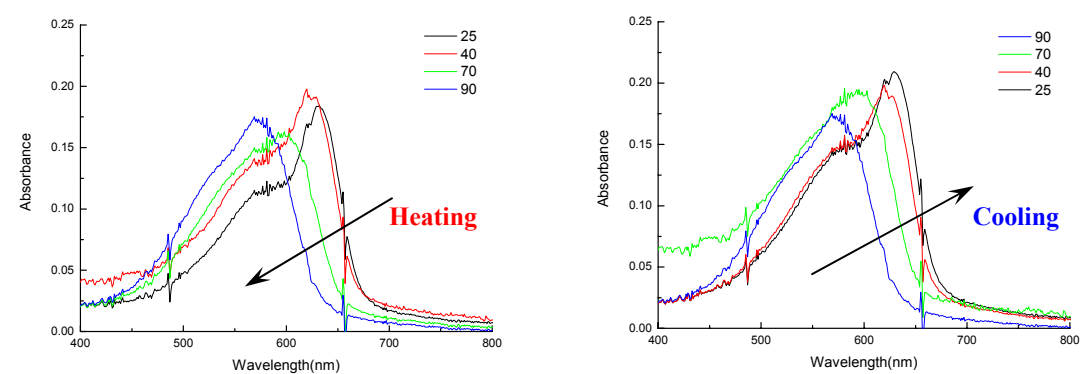
Figure S10. Visible spectral changes of PDA vesicle solutions prepared with ECDA-NPA 12, and HDCDA-NPA 13 upon heating and cooling process.



PCDA-*m*BzA **1**

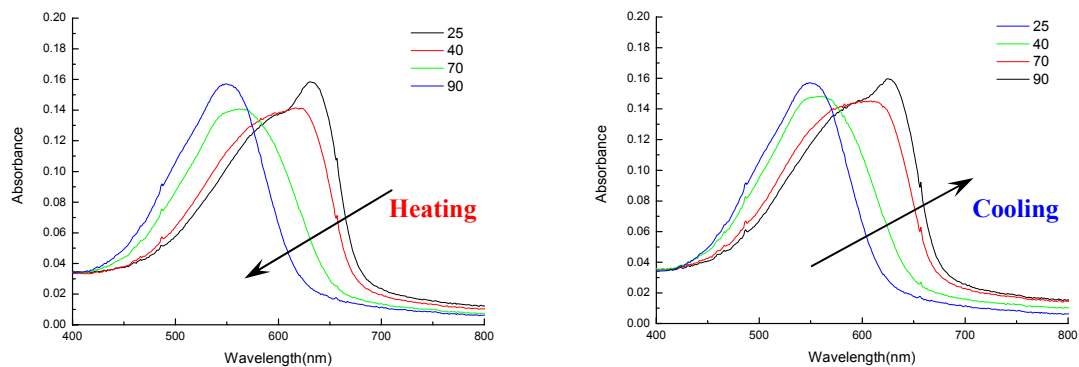


PCDA-*m*CPE **2**

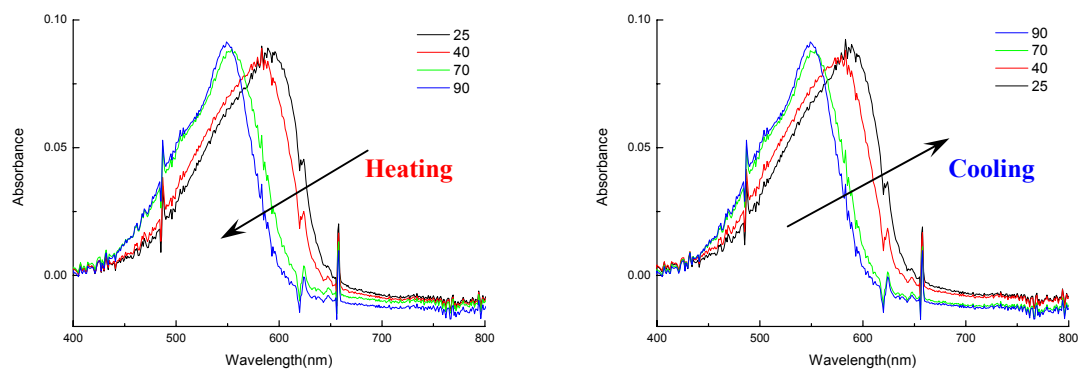


PCDA-*m*BzA **5**

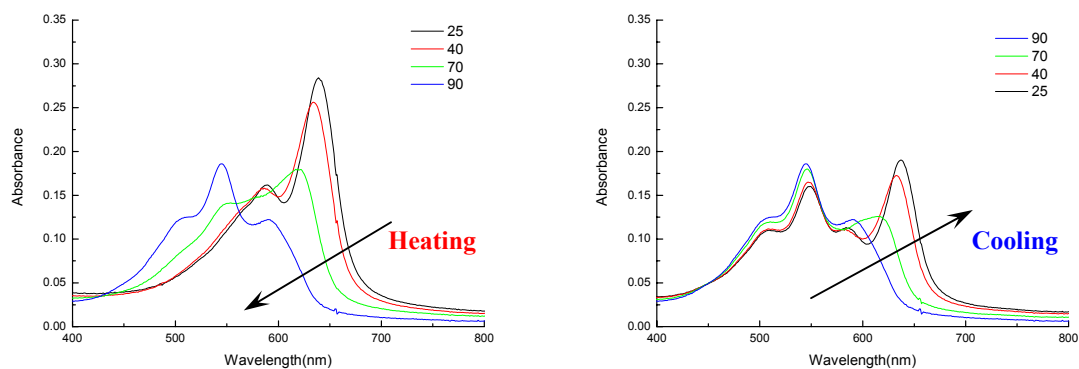
Figure S11. Visible spectral changes of PDA LS films prepared with PCDA-*m*BzA **1**, PCDA-*m*CPE **2**, and PCDA-*m*BzA **5** upon heating and cooling process.



ECDA-*m*BzA **6**

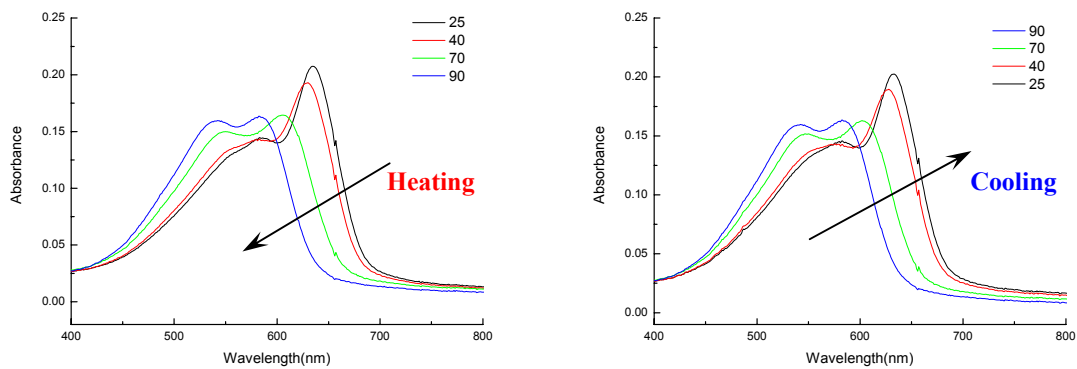


HDCDA-*m*BzA **7**

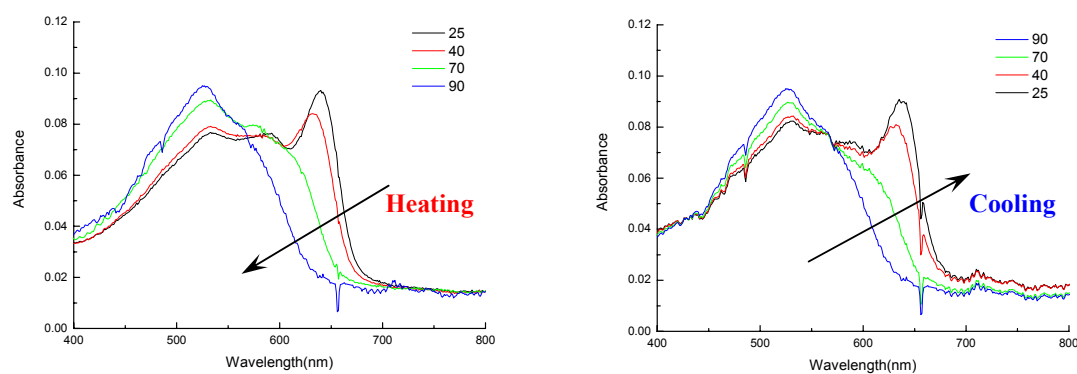


PCDA-Aniline **8**

Figure S12. Visible spectral changes of PDA LS films prepared with ECDA-*m*BzA **6**, HDCDA-*m*BzA **7**, and PCDA-Aniline **8** upon heating and cooling process.

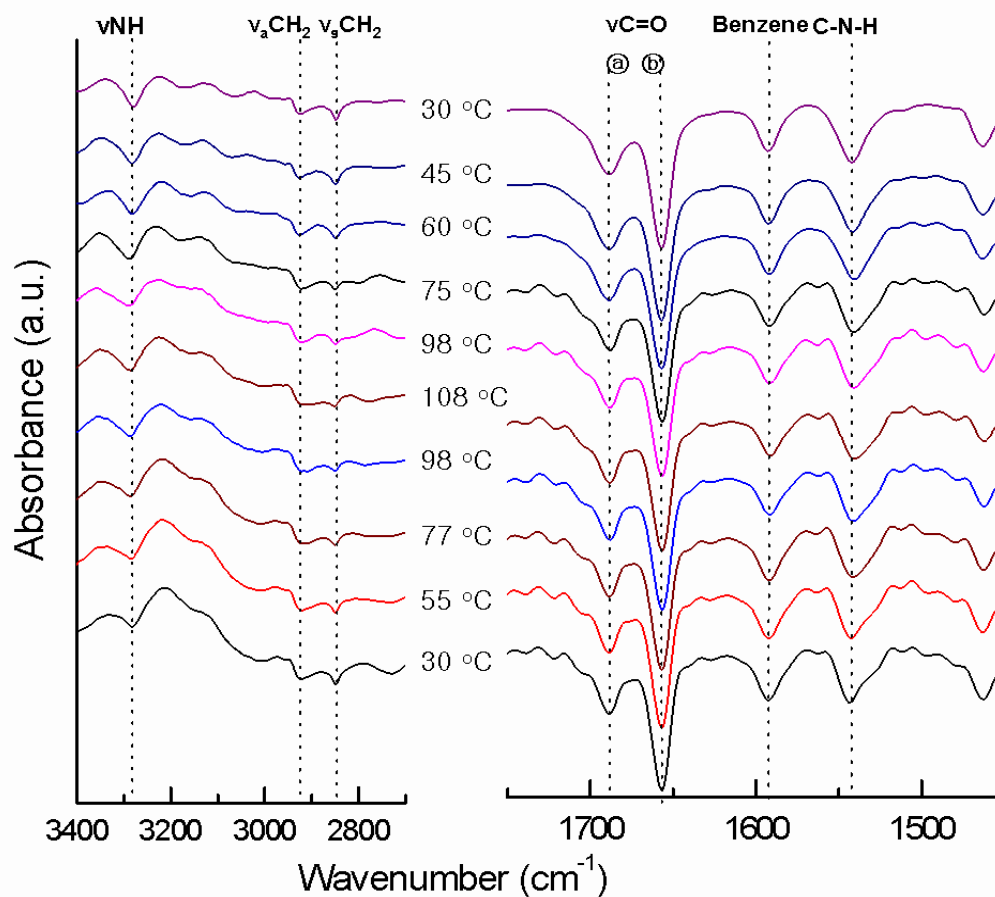


PCDA-*p*BzA 10



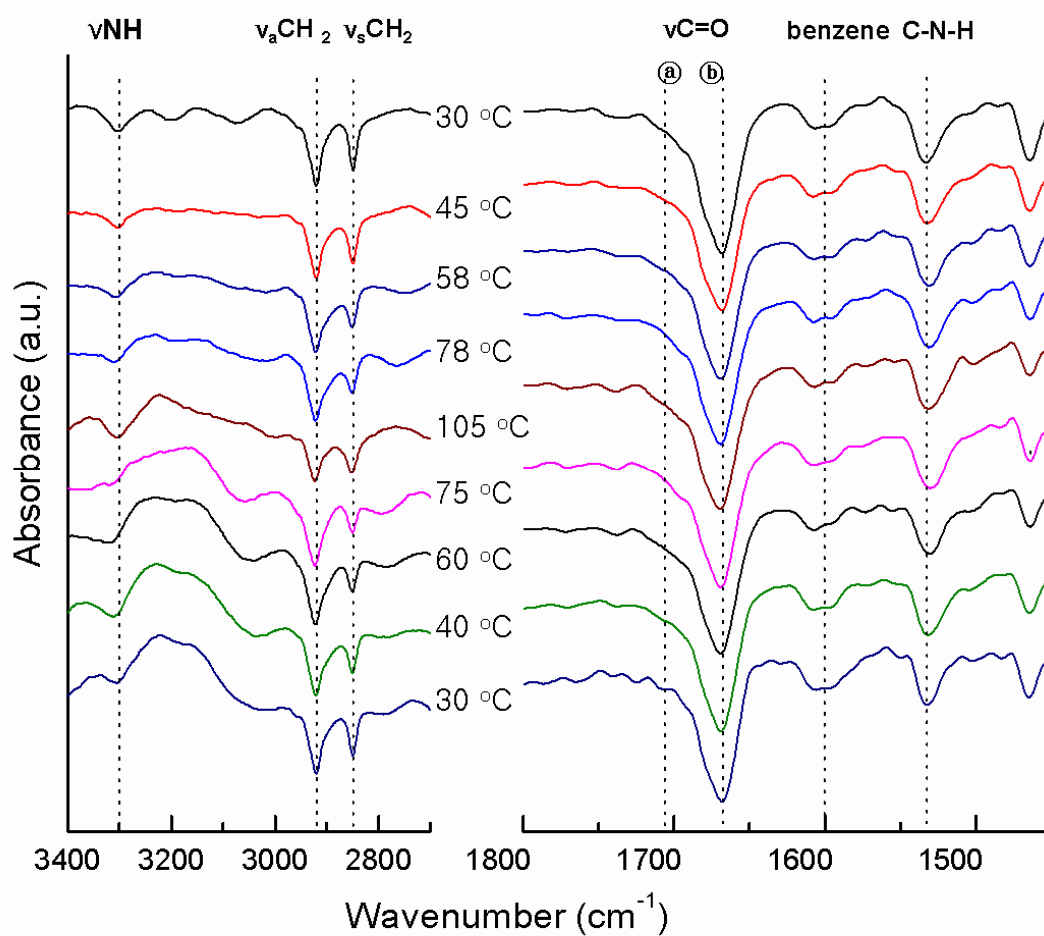
PCDA-NPA 11

Figure S13. Visible spectral changes of PDA LS films prepared with PCDA-*p*BzA 10 and PCDA-NPA 11 upon heating and cooling process.



HCDA-*m*BzA **5**

Figure S14. In-situ near-normal external reflection FTIR spectra of LS films of HCDA-*m*BzA **5** on hydrophobized glasses: $\nu\text{C}=\text{O}$ ① and ② stand for carbonyl stretching bands in terminal carboxyl and amide positions, respectively.



PCDA-*p*BzA **10**

Figure S15. In-situ near-normal external reflection FTIR spectra of LS films of PCDA-*p*BzA **10** on hydrophobized glasses: $\nu\text{C=O}$ ① and ② stand for carbonyl stretching bands in terminal carboxyl and amide positions, respectively.