

Utilization of chromic polydiacetylene assemblies as a platform to probe specific binding between drug and RNA

Anothai Kamphan^{a,b}, Changjun Gong^c, Krishnagopal Maiti^c, Souvik Sur^c, Rakchart Traiphol^{a,b,d} and Dev P. Arya^{c*}*

^a Department of Chemistry, Faculty of Science, Naresuan University, Phitsanulok 65000, Thailand.

^b Laboratory of Advanced Polymers and Nanomaterials, School of Materials Science and Engineering and Center of Excellence for Innovation in Chemistry, Faculty of Science, Mahidol University at Salaya, Phutthamonthon 4 Road, Salaya, Nakhon Pathom 73170, Thailand.

^c Laboratories of Medicinal Chemistry, Department of Chemistry, Clemson University, Clemson, South Carolina 29634, United States.

^d NANOTEC-MU Excellence Center on Intelligent Materials and Systems, Faculty of Science, Mahidol University, Rama 6 Road, Ratchathewi, Bangkok 10400, Thailand.

*Corresponding author emails: (D. P. Arya) dparya@clemson.edu and (R. Traiphol) rakchart.tra@mahidol.ac.th

Supporting Information

Contents

Figures	Page
Figure S1. MALDI-TOF spectrum of 5	3
Figure S2. ^1H NMR spectrum of 5	3
Figure S3. ^{13}C NMR spectrum of 5	4
Figure S4. MALDI-TOF spectrum of Neo-PCDA1	4
Figure S5. ^1H NMR spectrum of Neo-PCDA1	5
Figure S6. ^{13}C NMR spectrum of Neo-PCDA1	5
Figure S7. MALDI-TOF spectrum of 6	6
Figure S8. ^1H NMR spectrum of 6	6
Figure S9. ^{13}C NMR spectrum of 6	7
Figure S10. HMQC NMR spectrum of 6	8
Figure S11. MALDI-TOF spectrum of Neo-PCDA2	9
Figure S12. ^1H NMR spectrum of Neo-PCDA2	9
Figure S13. ^{13}C NMR spectrum of Neo-PCDA2	10
Figure S14. Absorption spectrum of poly(PCDA)/Neo-PCDA assembly upon testing with poly(rA)-poly(rU)	11
Figure S15. Absorption spectrum of poly(PCDA)/Neo-PCDA assembly upon increasing temperature	12

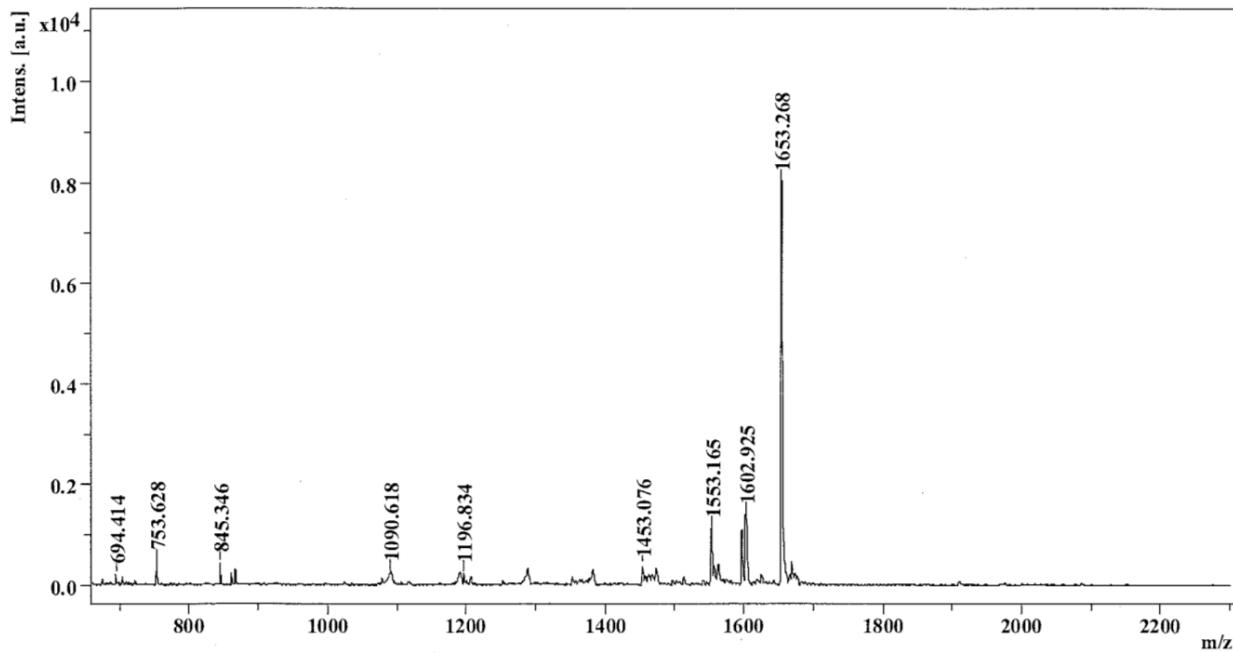


Figure S1. MALDI-TOF spectrum of compound **5**.

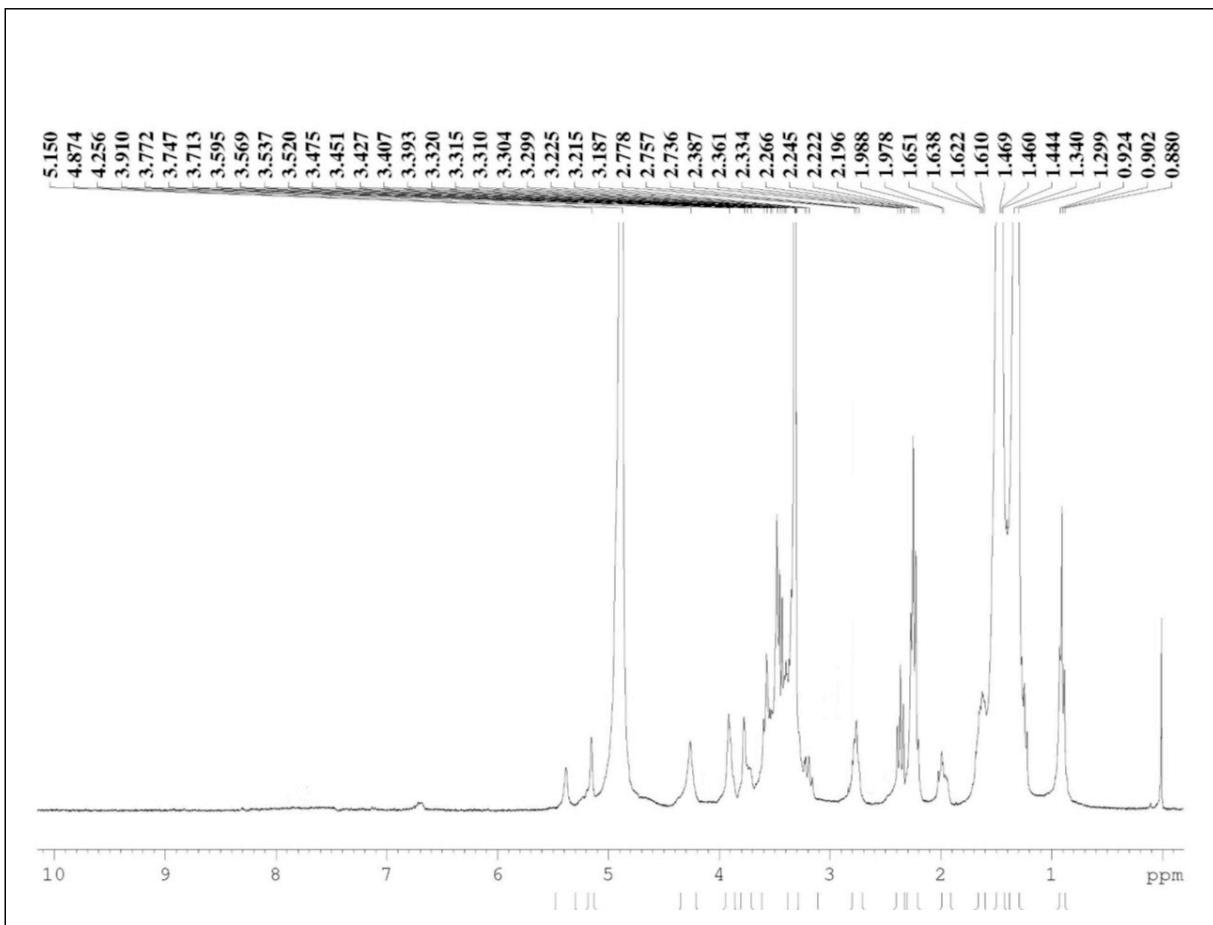


Figure S2. ^1H NMR spectrum of compound **5** (CD_3OD , 300 MHz).

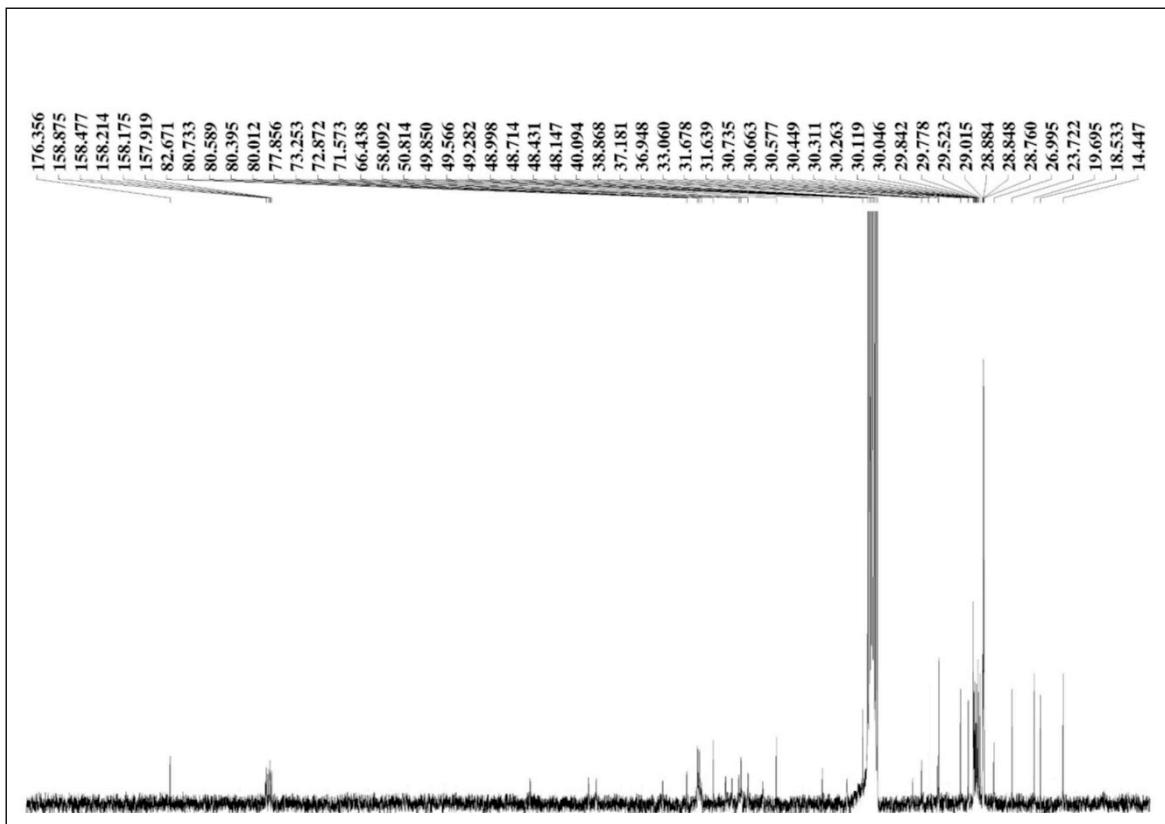


Figure S3. ¹³C NMR spectrum of compound 5 (CD₃OD, 75 MHz).

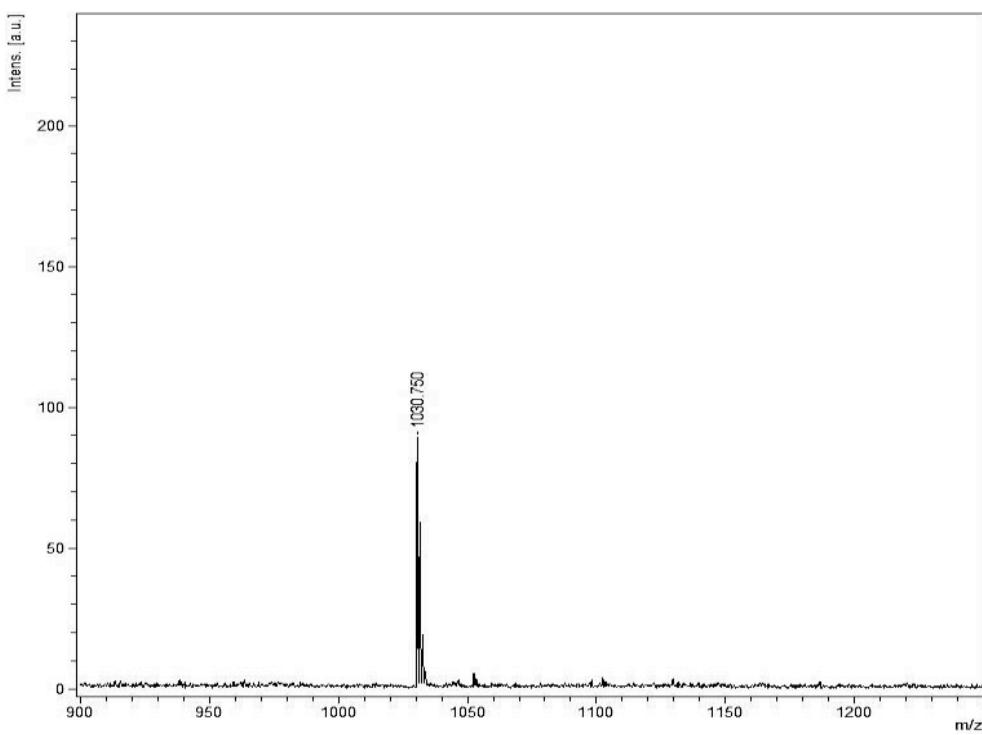


Figure S4. MALDI-TOF spectrum of Neo-PCDA1.

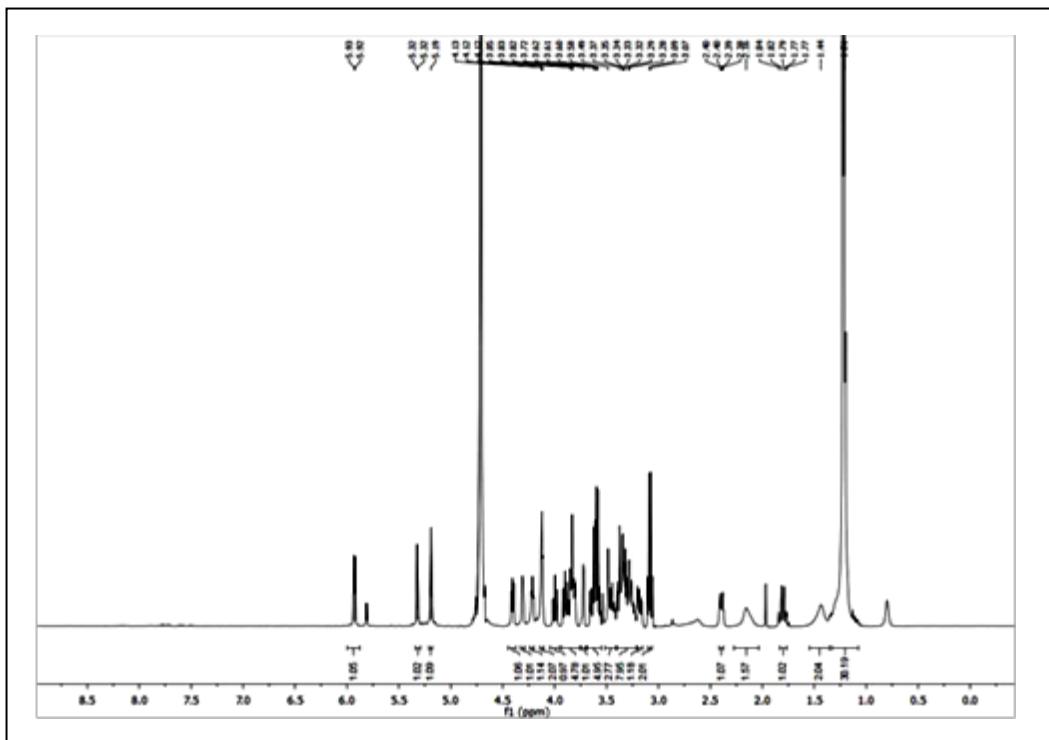


Figure S5. ¹H NMR spectrum of Neo-PCDA1 (D_2O , 500 MHz).

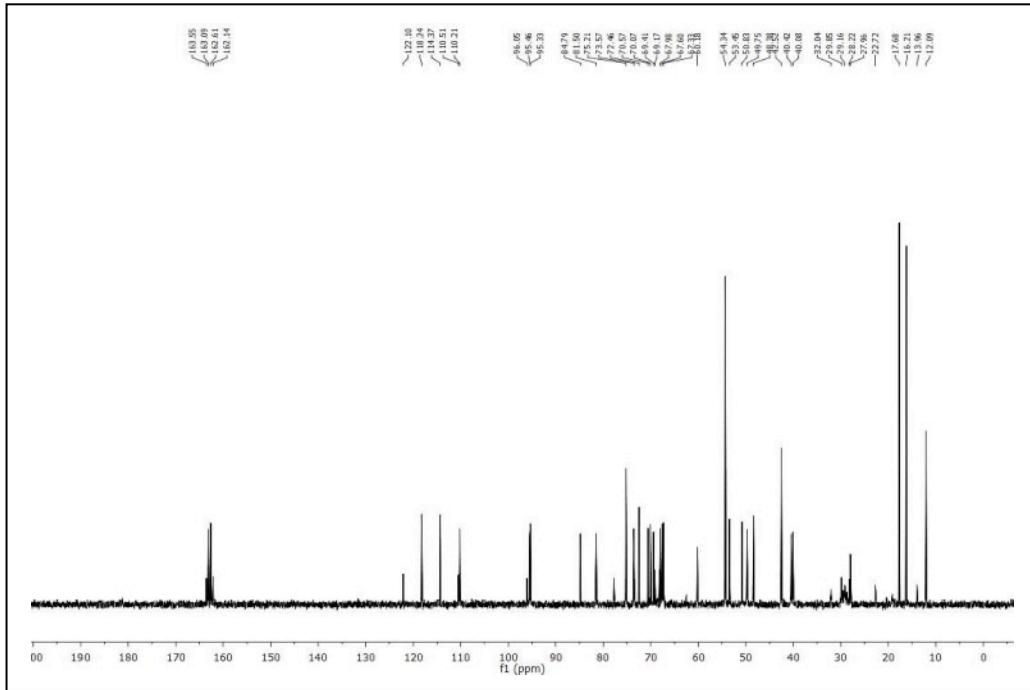


Figure S6. ¹³C NMR spectrum of Neo-PCDA1 (D_2O , 75 MHz).

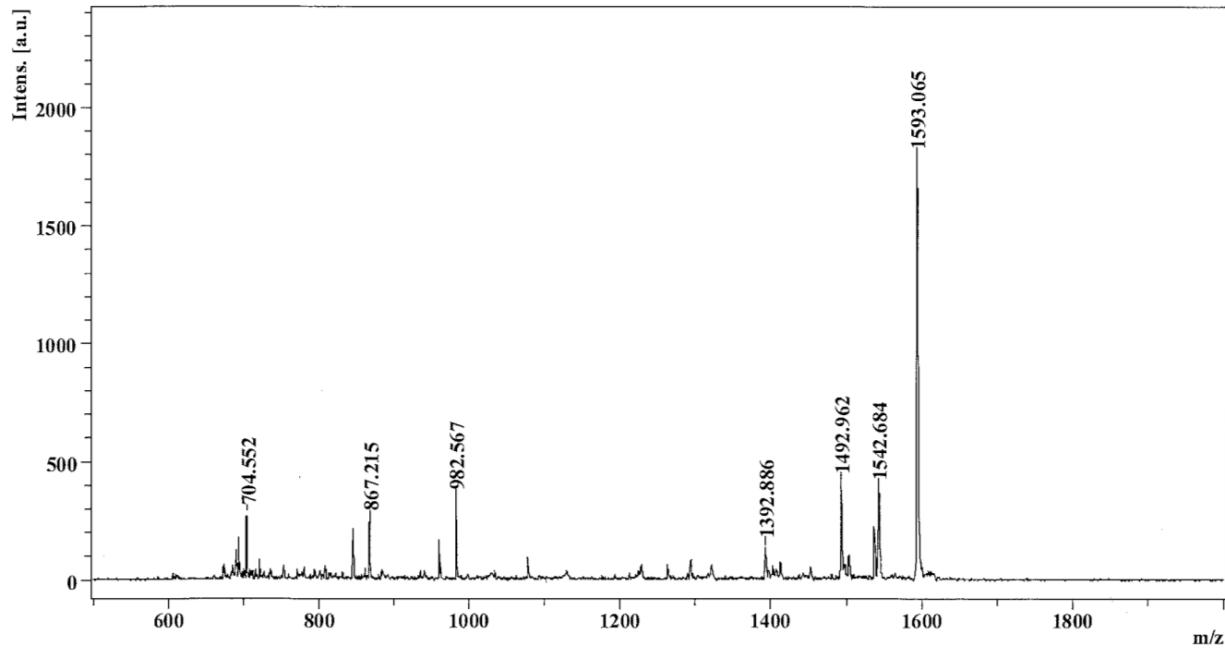


Figure S7. MALDI-TOF spectrum of compound **6**.

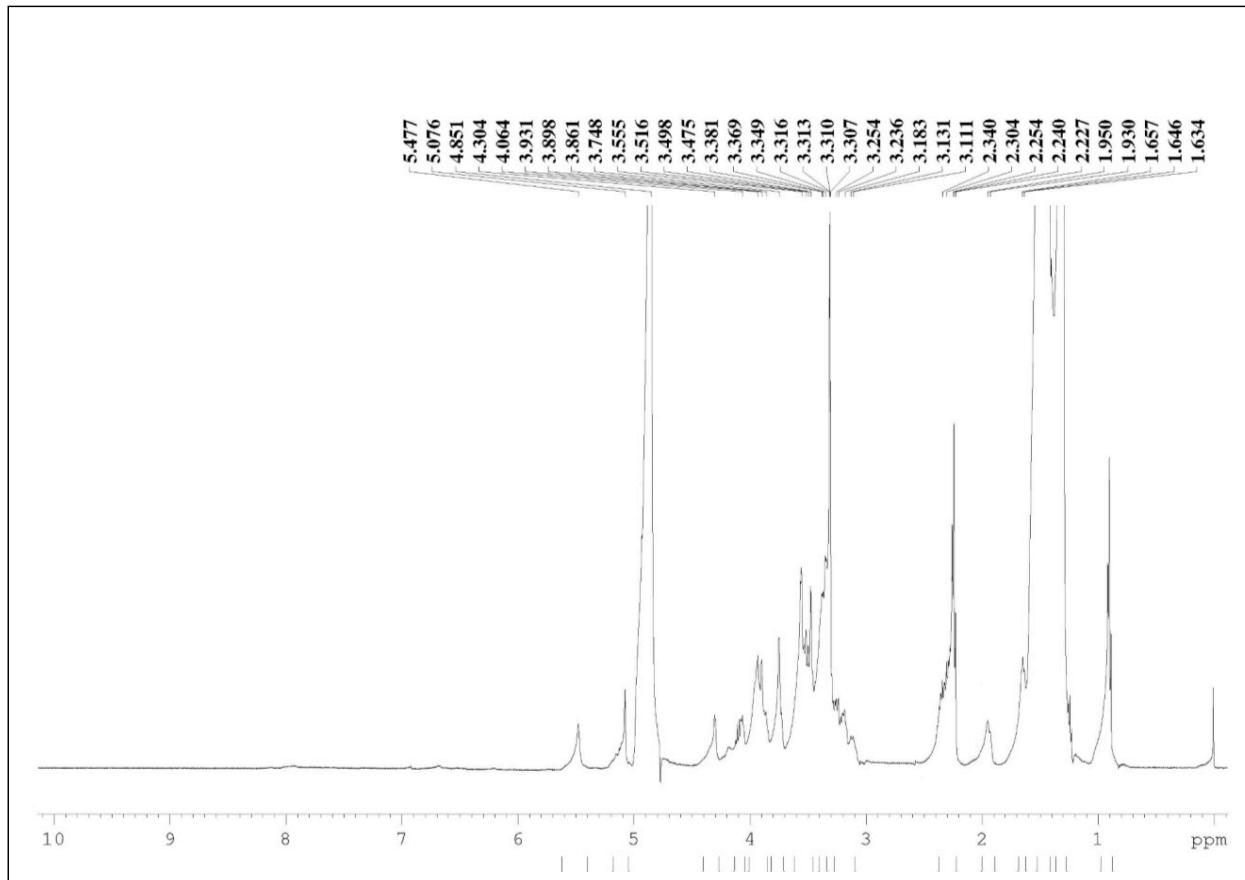


Figure S8. ^1H NMR spectrum of compound **6** (CD_3OD , 500 MHz).

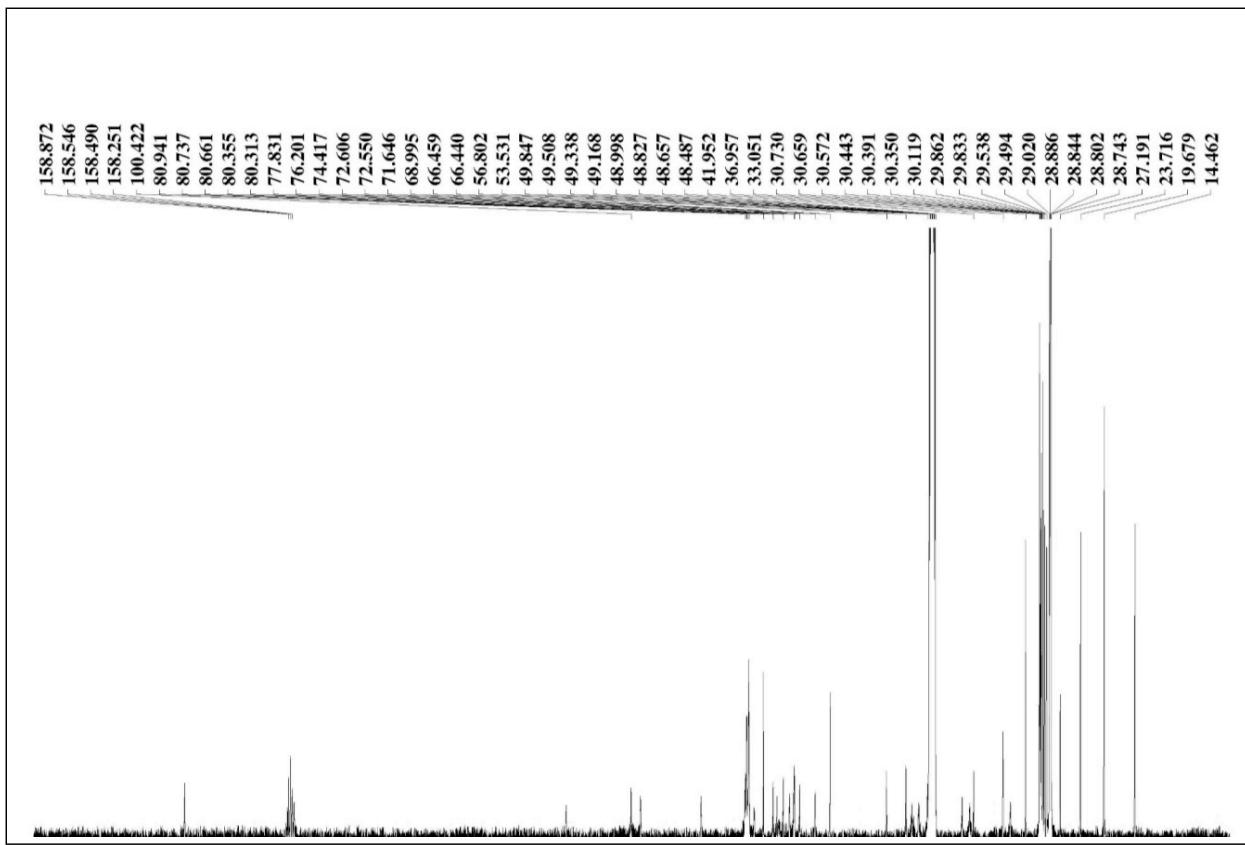


Figure S9. ¹³C NMR spectrum of compound **6** (CD₃OD, 125 MHz).

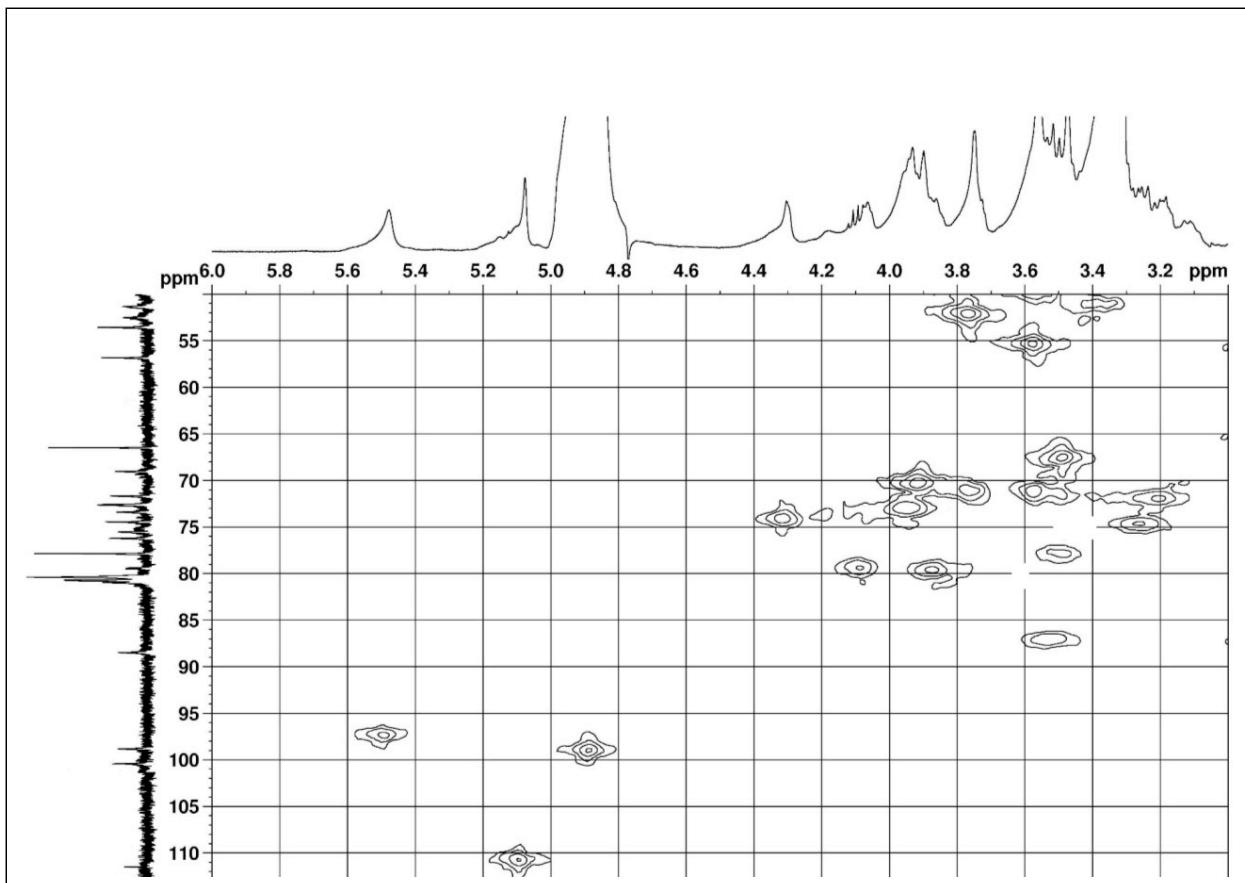


Figure S10. HMQC NMR spectrum of compound **6** (CD_3OD , 500 and 125 MHz).

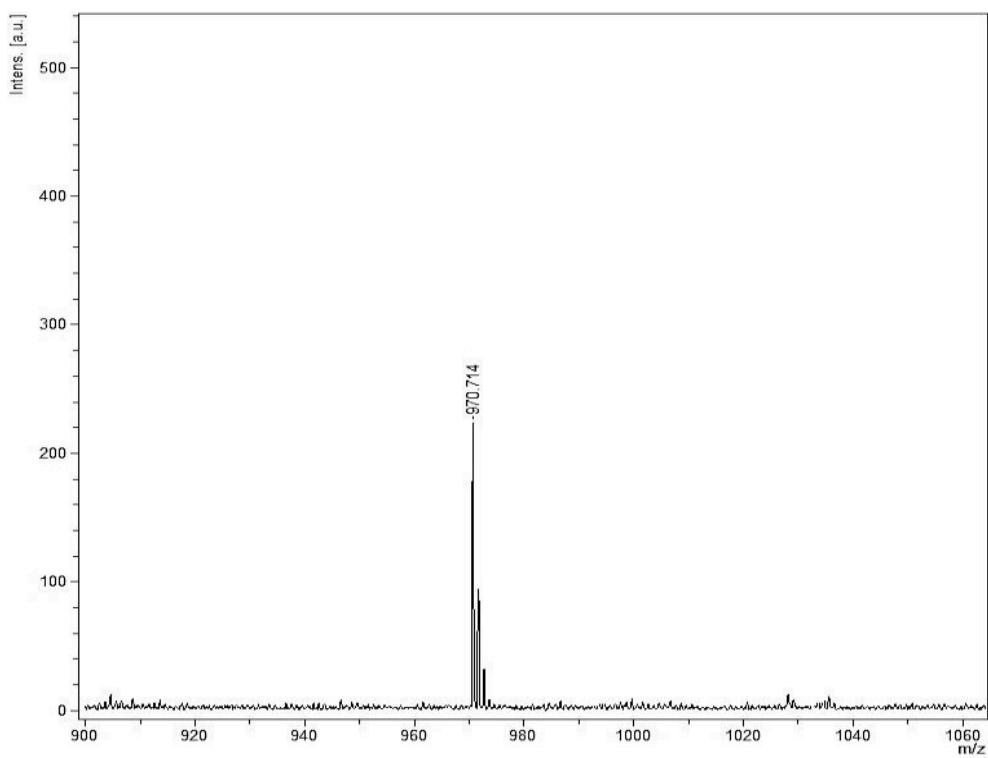


Figure S11. MALDI-TOF spectrum of Neo-PCDA2.

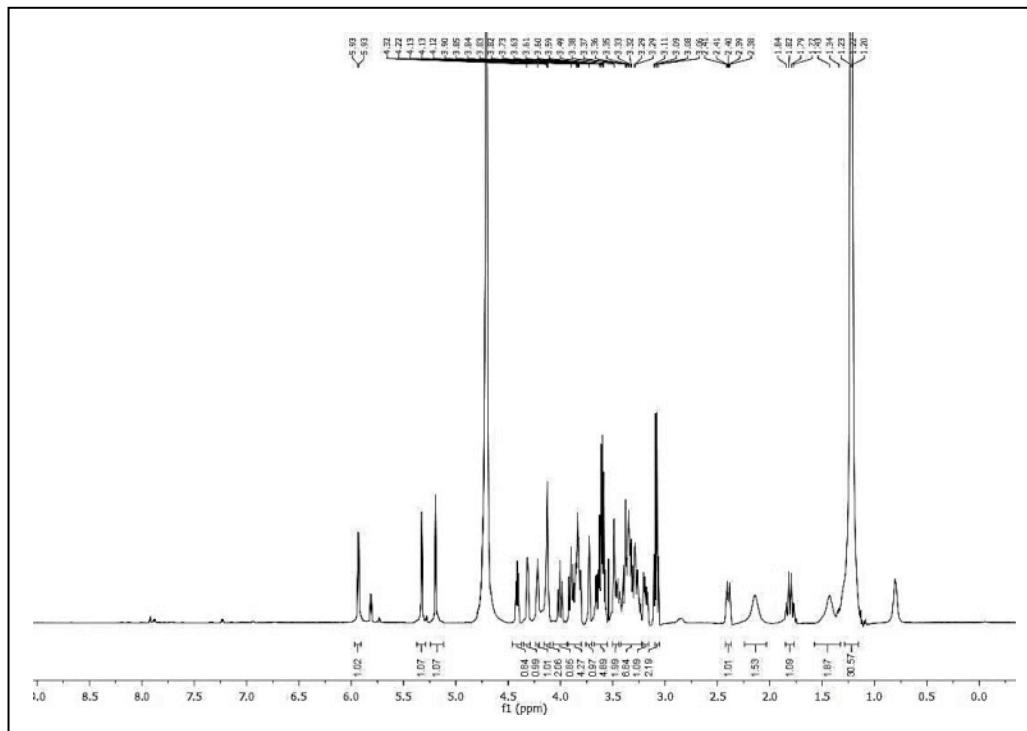


Figure S12. ^1H NMR spectrum of Neo-PCDA2 (D_2O , 500 MHz).

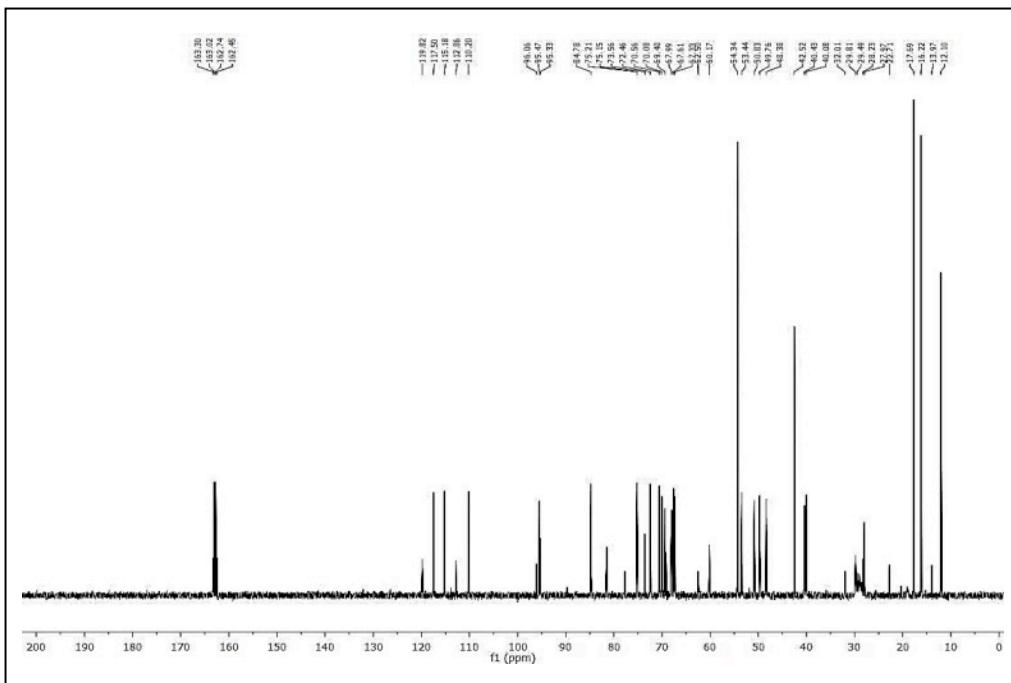


Figure S13. ^{13}C NMR spectrum of Neo-PCDA2 (D_2O , 125 MHz).

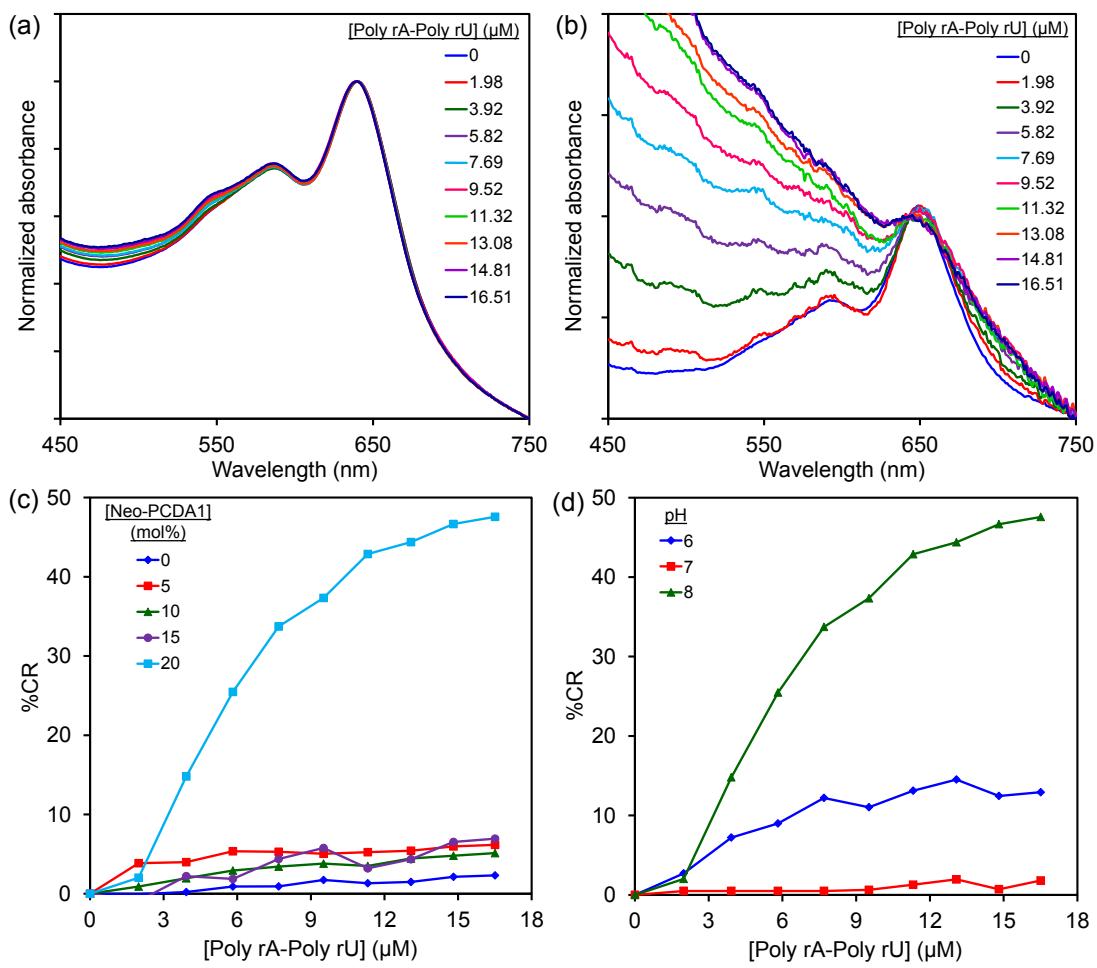


Figure S14. Absorption spectra of (a) pure poly(PCDA) and (b) poly(PCDA)/Neo-PCDA1 (20 mol% Neo-PCDA1) upon testing with poly (rA) - poly (rU). The %CR curves of poly(PCDA)/Neo-PCDA1 upon the variations of (c) Neo-PCDA1 concentration and (d) pH of medium. (The assemblies were prepared under the conditions: (c) 4 mM PBS buffer pH 8, (d) mixed with 20 mol% Neo-PCDA1 in 4 mM PBS buffer).

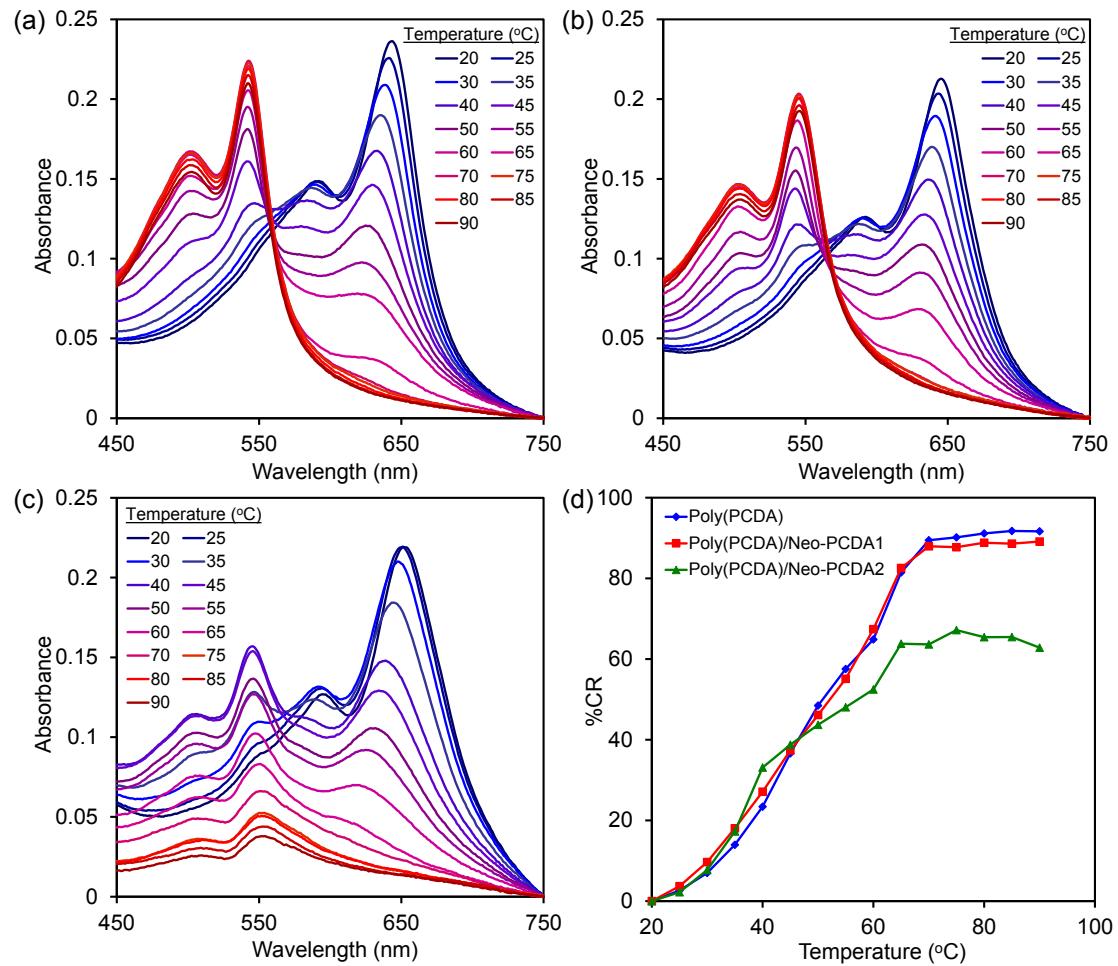


Figure S15. Absorption spectra of (a) pure poly(PCDA) and poly(PCDA)/Neo-PCDA prepared by mixing with 10 mol% of (b) Neo-PCDA1 and (c) Neo-PCDA2 measured upon increasing temperature. (d) Colorimetric response to temperature of these three systems.