Supplementary Information

for

Acetyl-Protected Cytosine- and Guanine-Containing Acrylics for Supramolecular Adhesives

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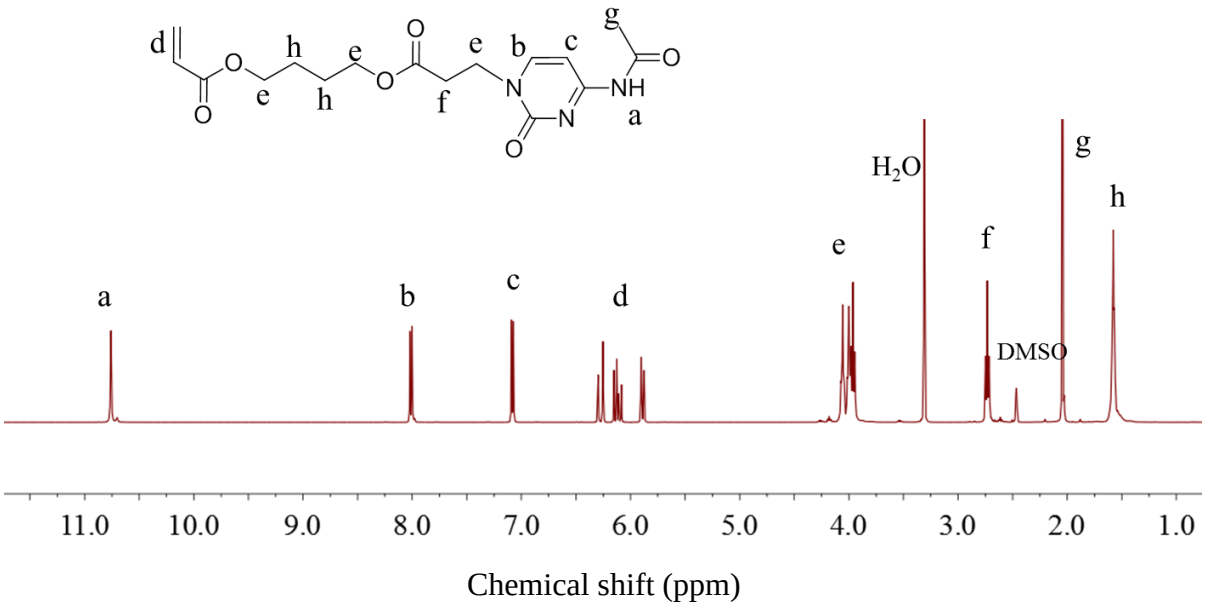


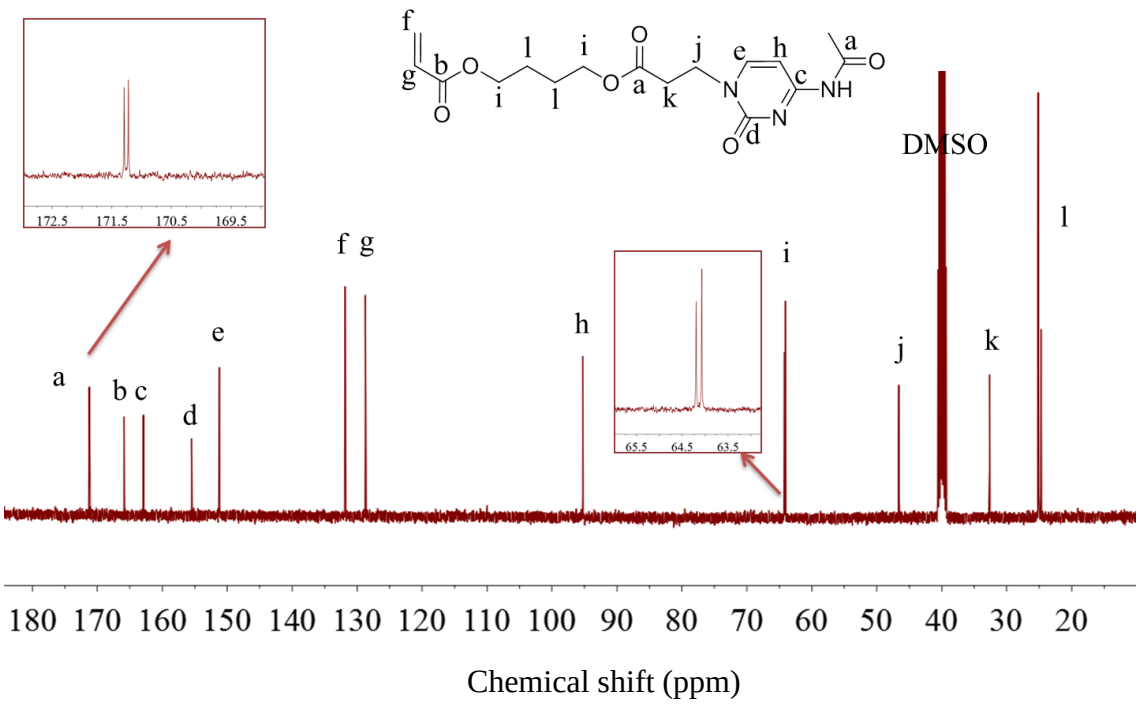


Figure S1. ^{1}H NMR and ^{13}C NMR spectra of *N*2-acetylcytosine acrylate (ACyA).

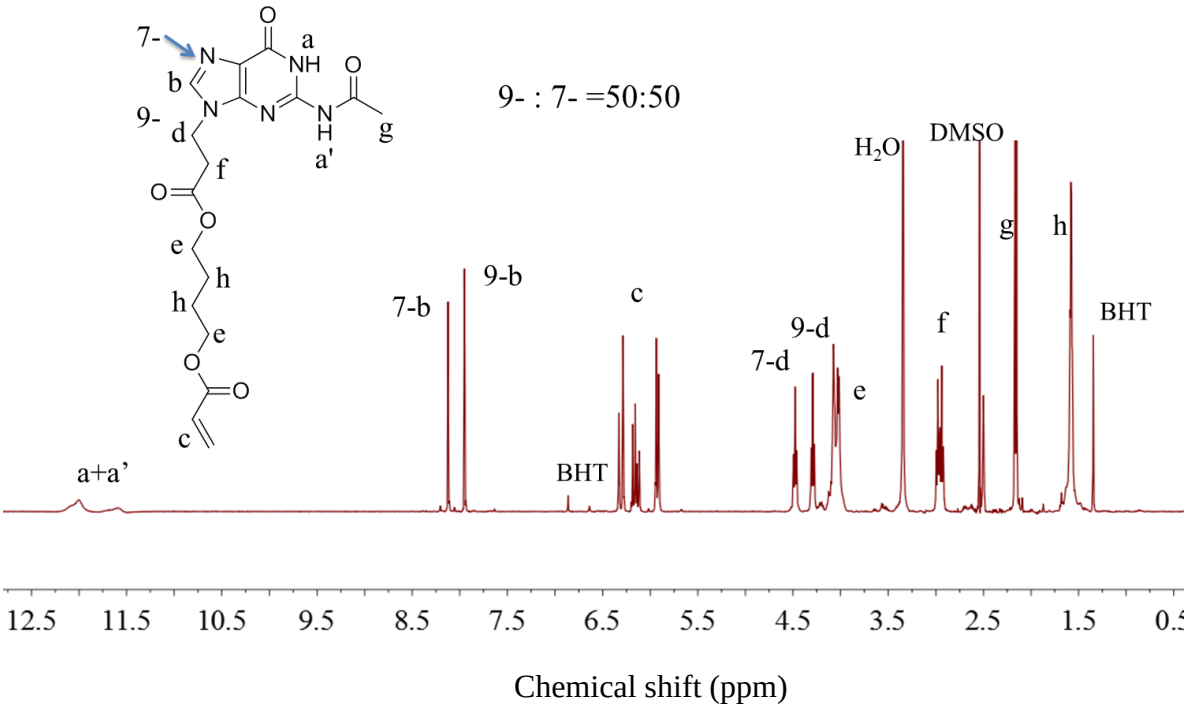


Figure S2. ^{1}H NMR spectrum of the 9- and 7-isomer mixture of *N*4-acetylguanine acrylate (AGuA).

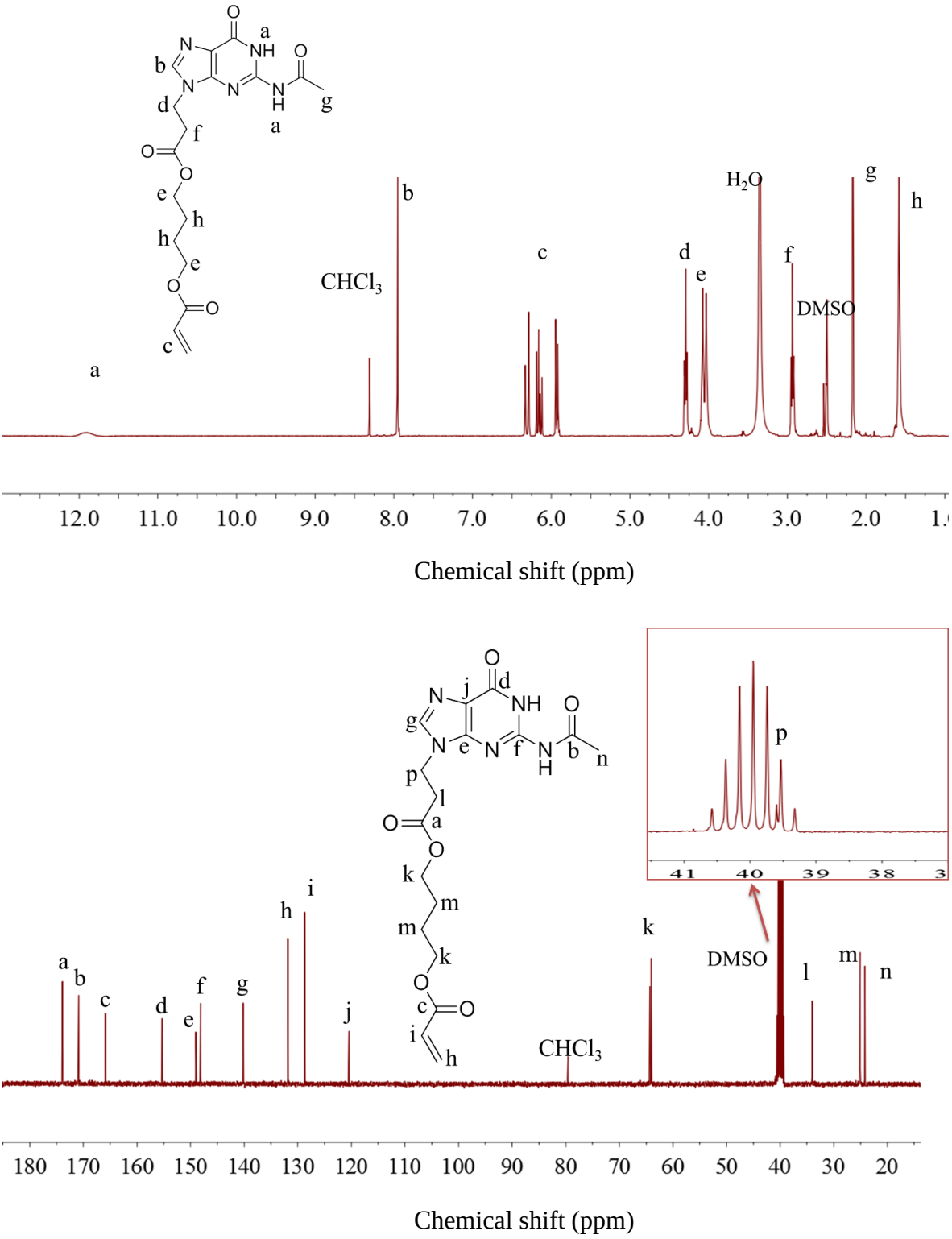


Figure S3. ^{1}H NMR and ^{13}C NMR spectra of 9-isomer of *N*4-acetylguanine acrylate (AGuA).

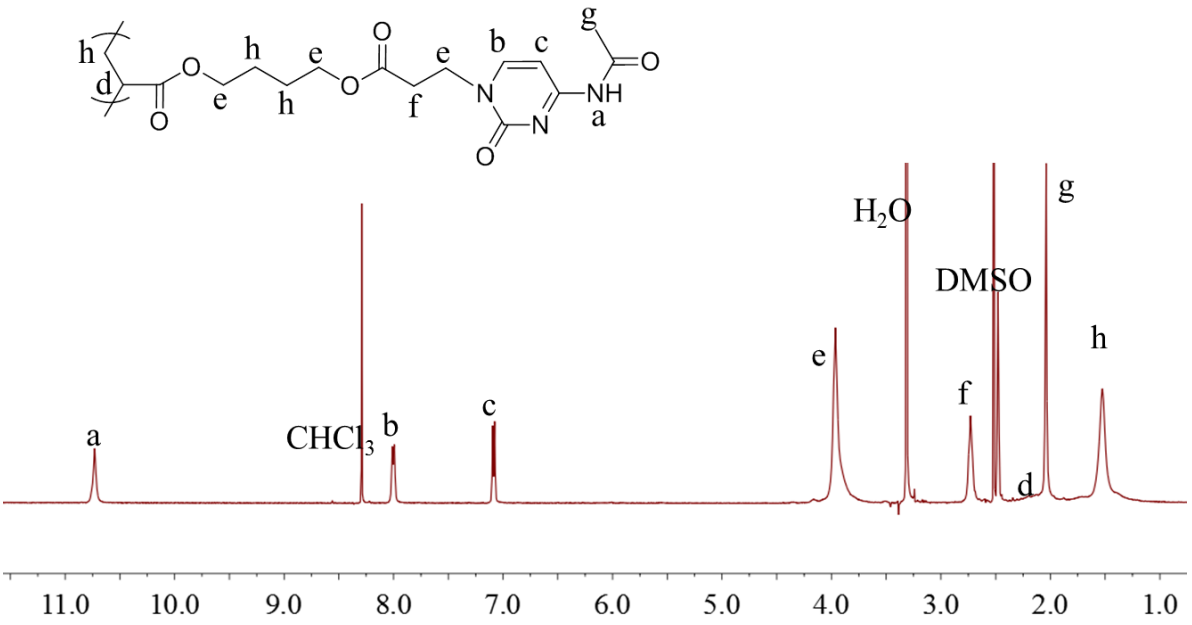


Figure S4. ^{1}H NMR spectrum of poly (ACyA).

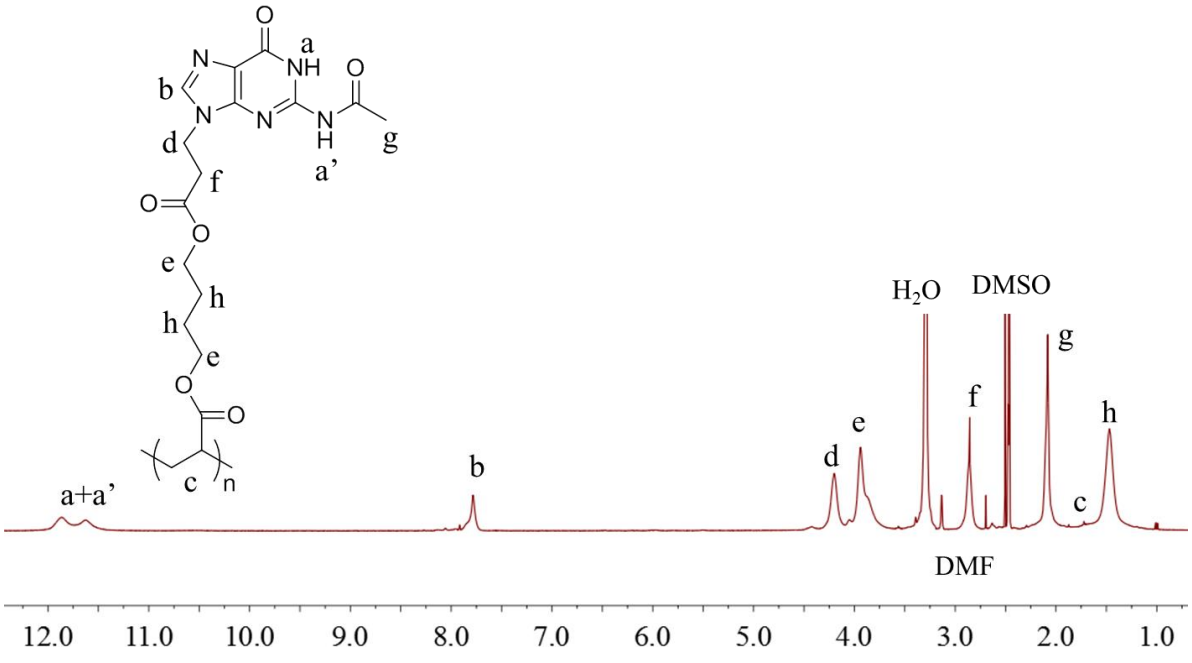


Figure S5. ^{1}H NMR spectrum of poly (AGuA).

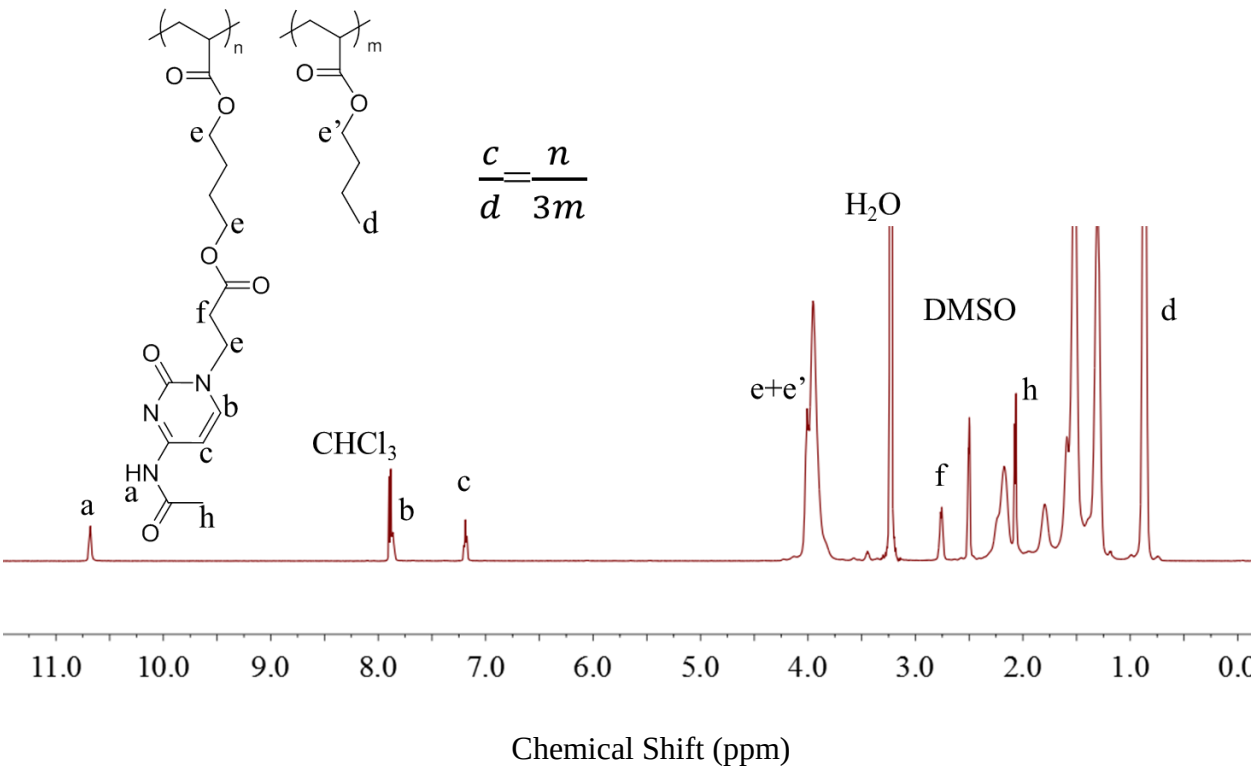
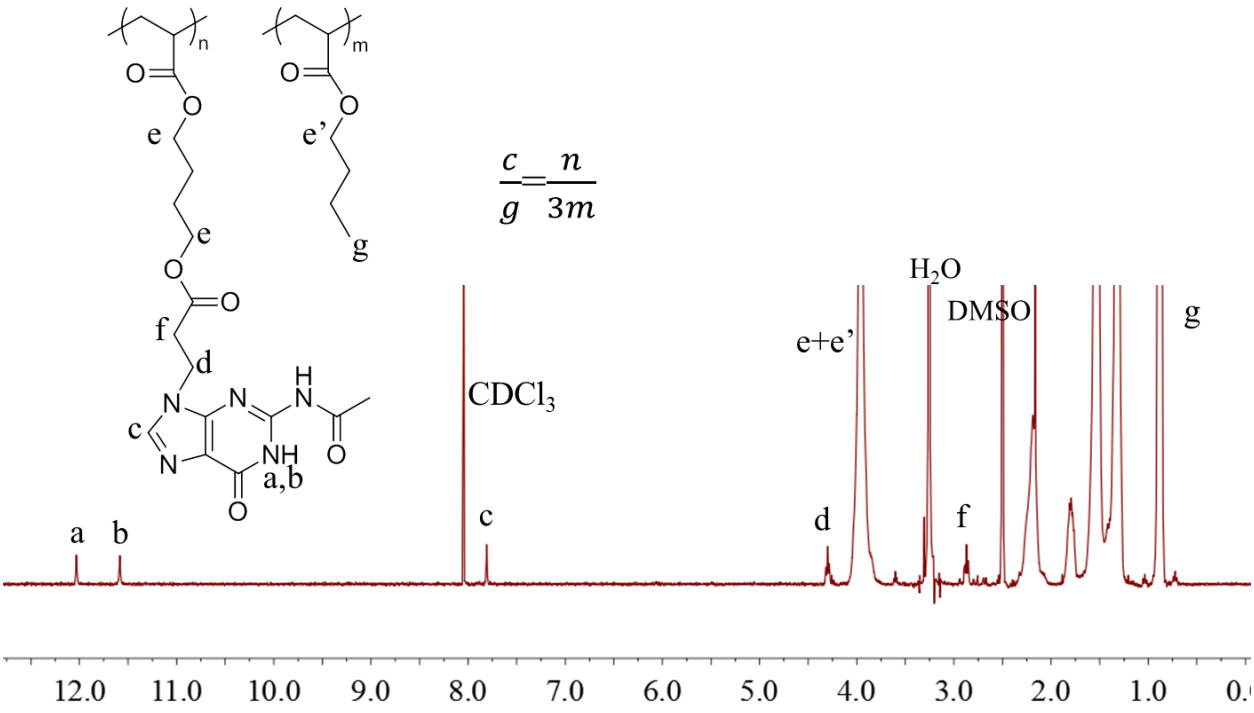
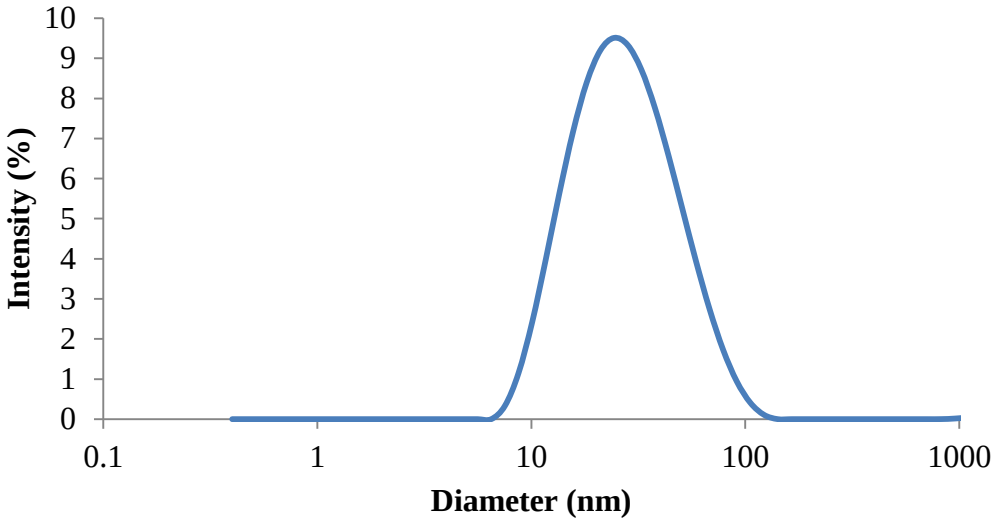


Figure S6. ^{1}H NMR spectrum of poly(ACyA-*co*-*n*BA) in a mixture of $CDCl_3$ and DMSO-d_6.



Chemical Shift (ppm)

Figure S7. ^{1}H NMR spectrum of poly(AGuA-*co*-*n*BA) in a mixture of $CDCl_3$ and DMSO-d_6.



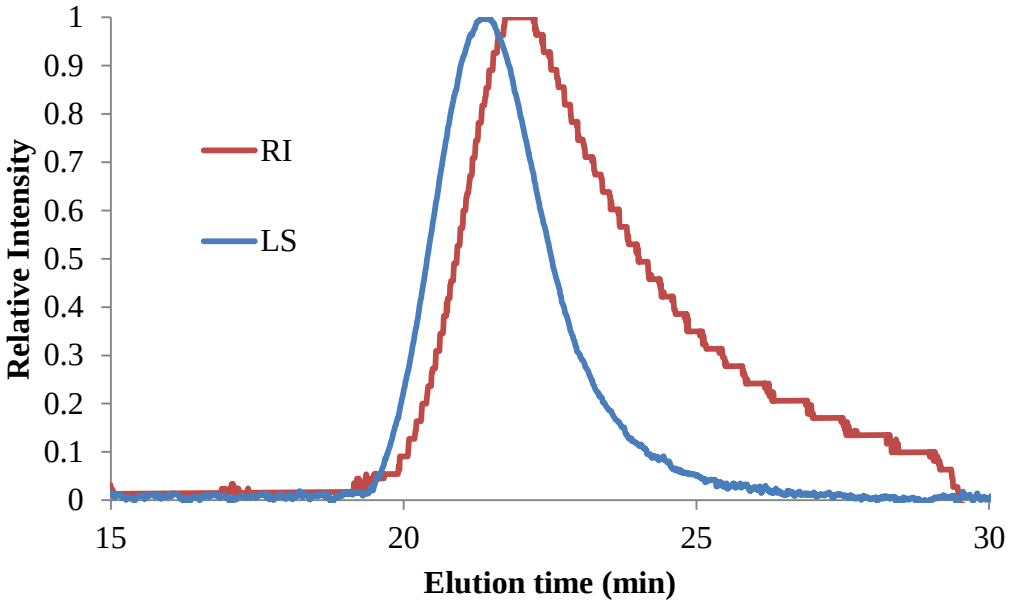


Figure S8. Representative DLS and SEC traces of poly(ACyA-*co*-*n*BA) in DMF 0.05 M LiBr at 50 °C.

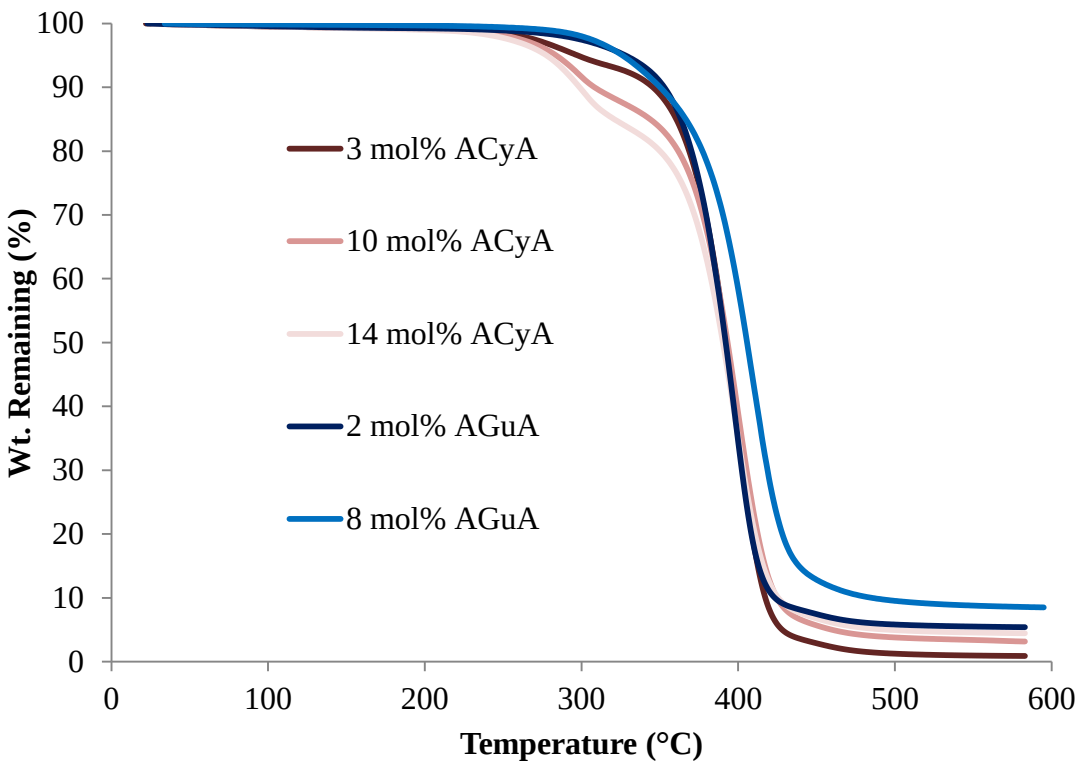
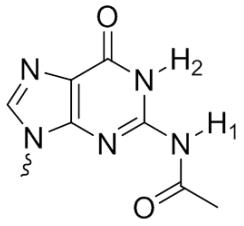


Figure S9. Representative TGA thermograms of poly(ACyA-*co*-*n*BA) and poly(AGuA-*co*-*n*BA) under nitrogen purge.

$$[H]_0 = \frac{\frac{1}{K} - [G]_0\left(\frac{\delta_i}{\delta_c} - 1\right)}{\frac{\delta_c}{\delta_i} - 1}$$

$[G]_0$= 0.002 M

Host ACyA
Guest AGuA



Δδ1 K=265 M^{-1}, δ_c=1.18 ppm

Δδ2 K=252 M^{-1}, δ_c=2.69 ppm

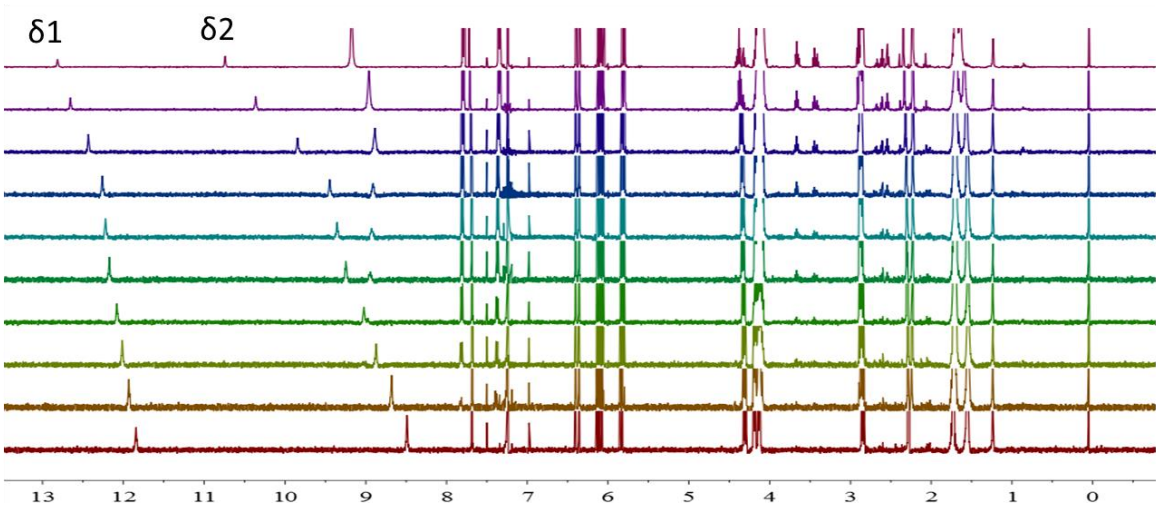


Figure S10. ^{1}H NMR spectra of the ACyA and AGuA mixture with varying ratios in $CDCl_3$ for the titration experiment.

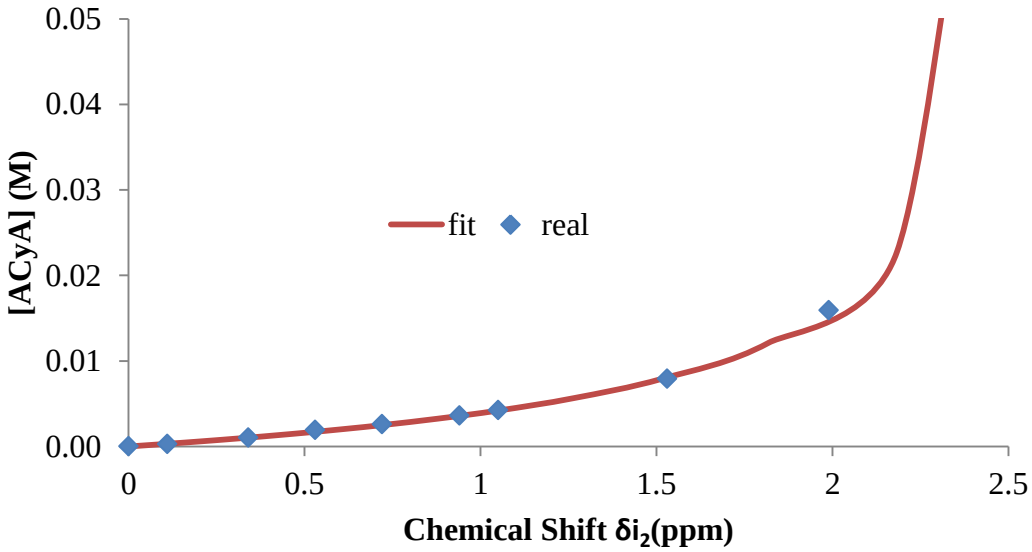


Figure S11. Non-linear fitting of NMR titration results for number two proton on AGuA to determine the binding constant of ACyA and AGuA in $CDCl_3$ at 22 °C.

In equation S1, $[H]_0$ and $[G]_0$ represent the concentration of ACyA (host) and AGuA (guest), respectively. δ_c defines the proton chemical shift difference between completely bonded AGuA and free AGuA, and δ_i defines the proton chemical shift difference between observed AGuA and the free AGuA. The titration experiment included a sequence of solution in $CDCl_3$ with constant AGuA concentration and varying ACyA concentration. The chemical shift of hydrogen bonded proton on AGuA shifted from high field to low field with increasing ACyA concentration.

$$[H]_0 = \frac{\frac{1}{K} - [G]_0\left(\frac{\delta_i}{\delta_c} - 1\right)}{\frac{\delta_c}{\delta_i} - 1} \qquad \text{(S1)}$$

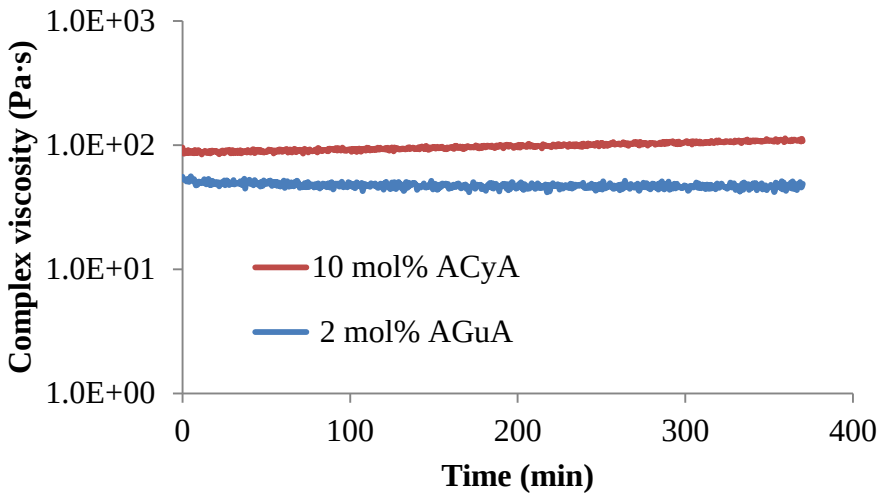


Figure S12. Isothermal time sweep of nucleobase-containing acrylics at 130 °C for 6 h.