Electronic Supplementary Material (ESI) for Soft Matter.

Supporting Information

Metal–ligand complexation and clustering in mussel-inspired side-chain functionalized supramolecular hydrogels

Amir Jangizehi[a], Mostafa Ahmadi[a], Sarah Pschierer[a], Paola Nicolella[a], Hailong Li[b], Katrin Amann-Winkel[b], and Sebastian Seiffert[a]*

[a] Johannes Gutenberg University Mainz, Department of Chemistry, Duesberweg 10–14, D-55128 Mainz, Germany

[b] Max Planck Institute for Polymer Research, D-55128 Mainz, Germany

Email: Sebastian.seiffert@uni-mainz.de

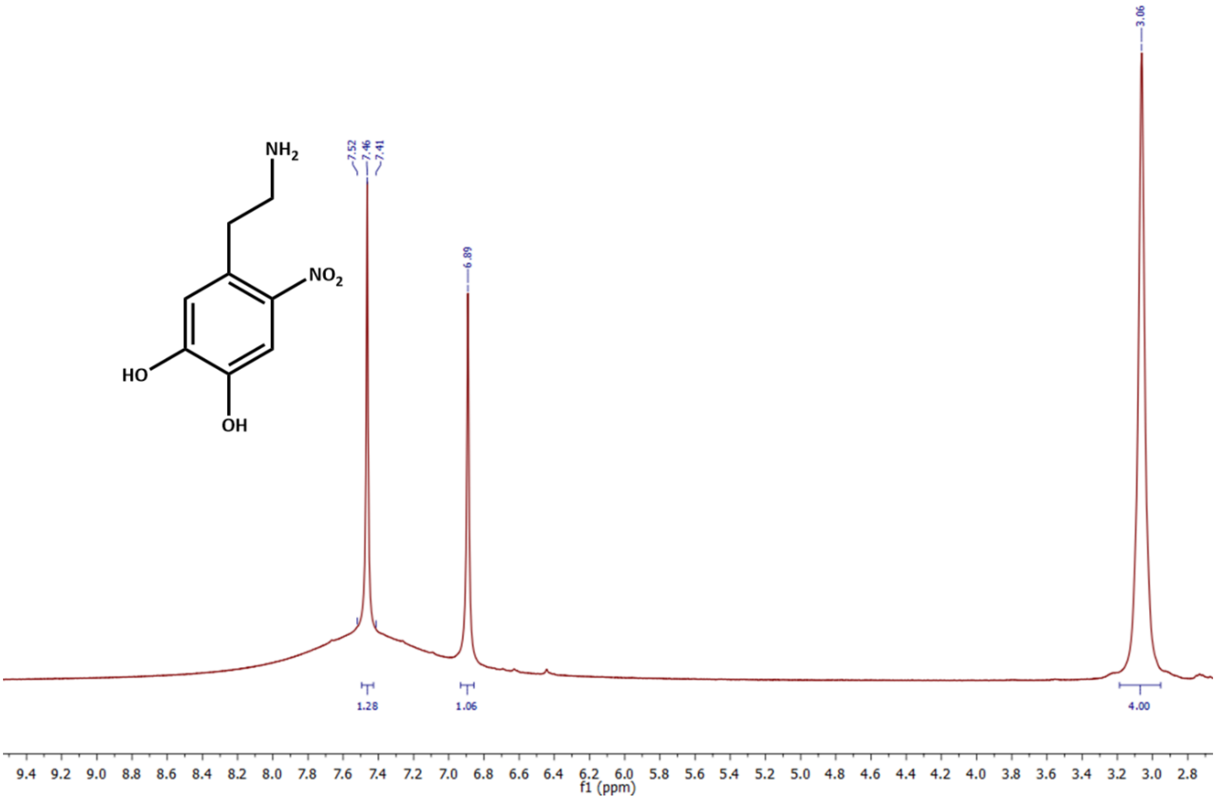

Figure S 1. ^{1}H NMR spectrum of nitrodopamine hydrogen sulfate

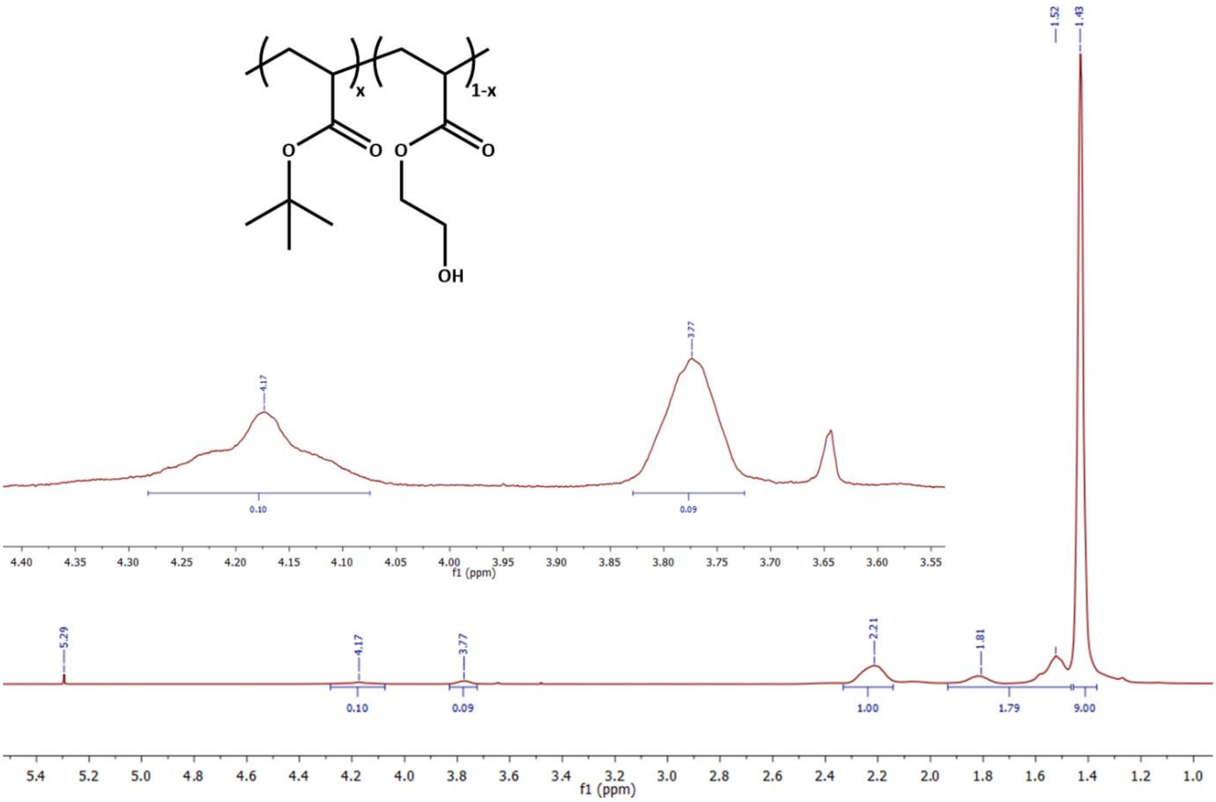

Figure S 2. ^{1}H NMR spectrum of poly(*tert*-butyl acrylate-*ran*-hydroxyethyl acrylate)

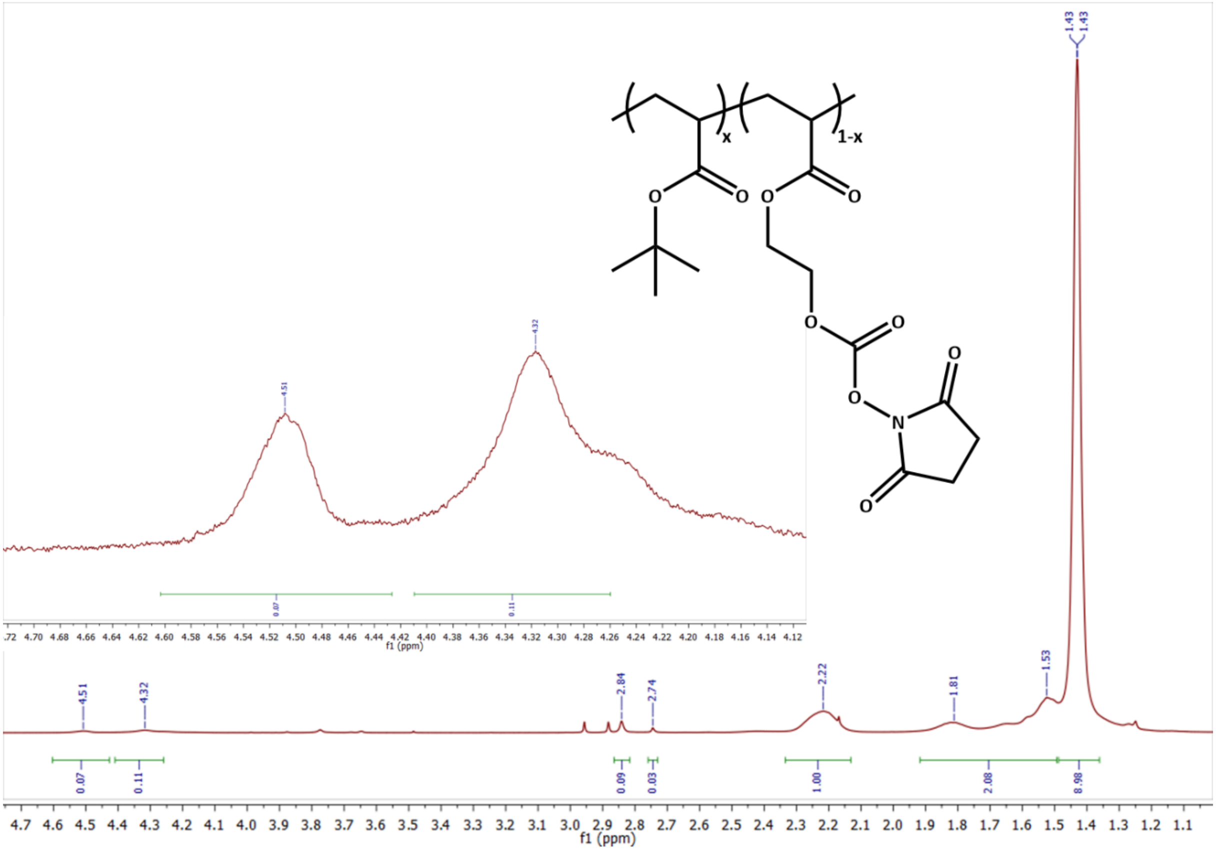

Figure S 3. [1]H NMR spectrum of poly(*tert*-butyl acrylate-*ran*-NHS-ethyl acrylate)

+

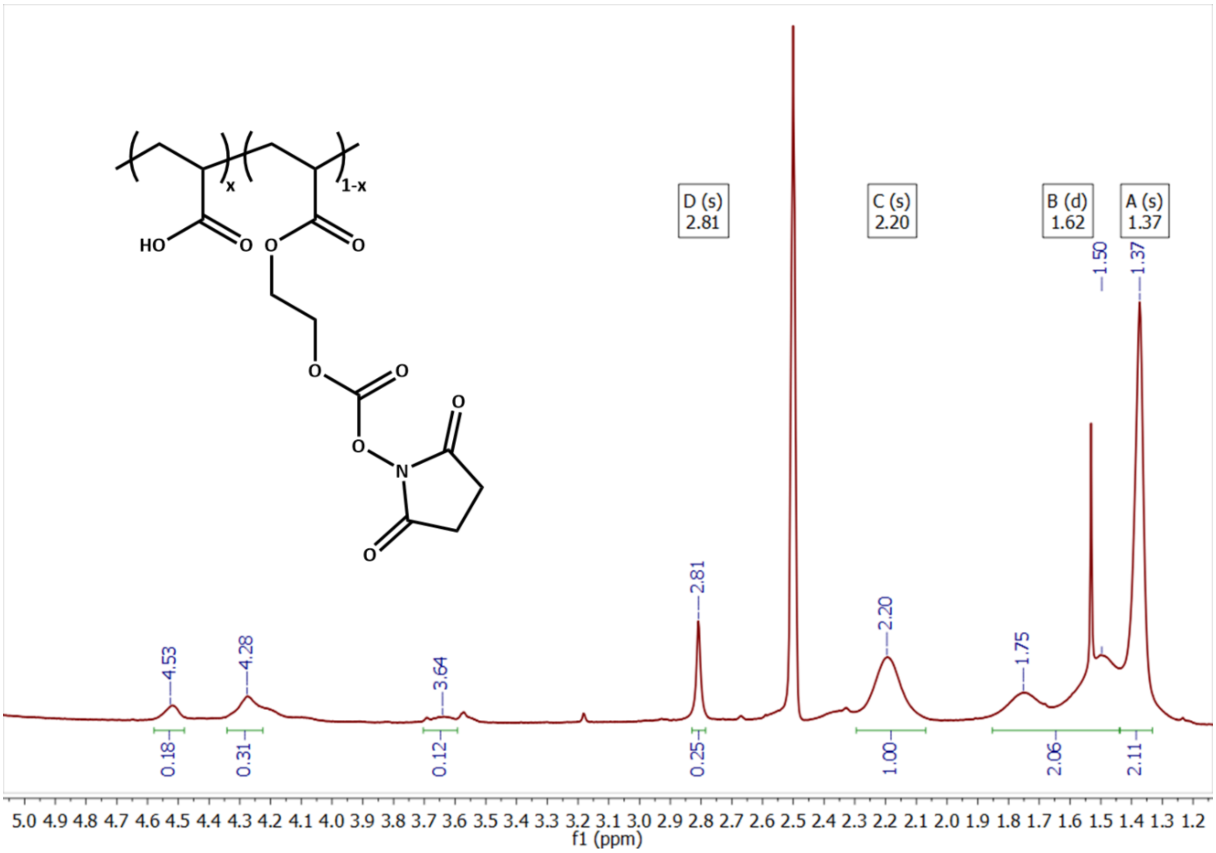

Figure S 4. [1]H NMR spectrum of poly(AAc-*ran*-NHS-ethyl acrylate)

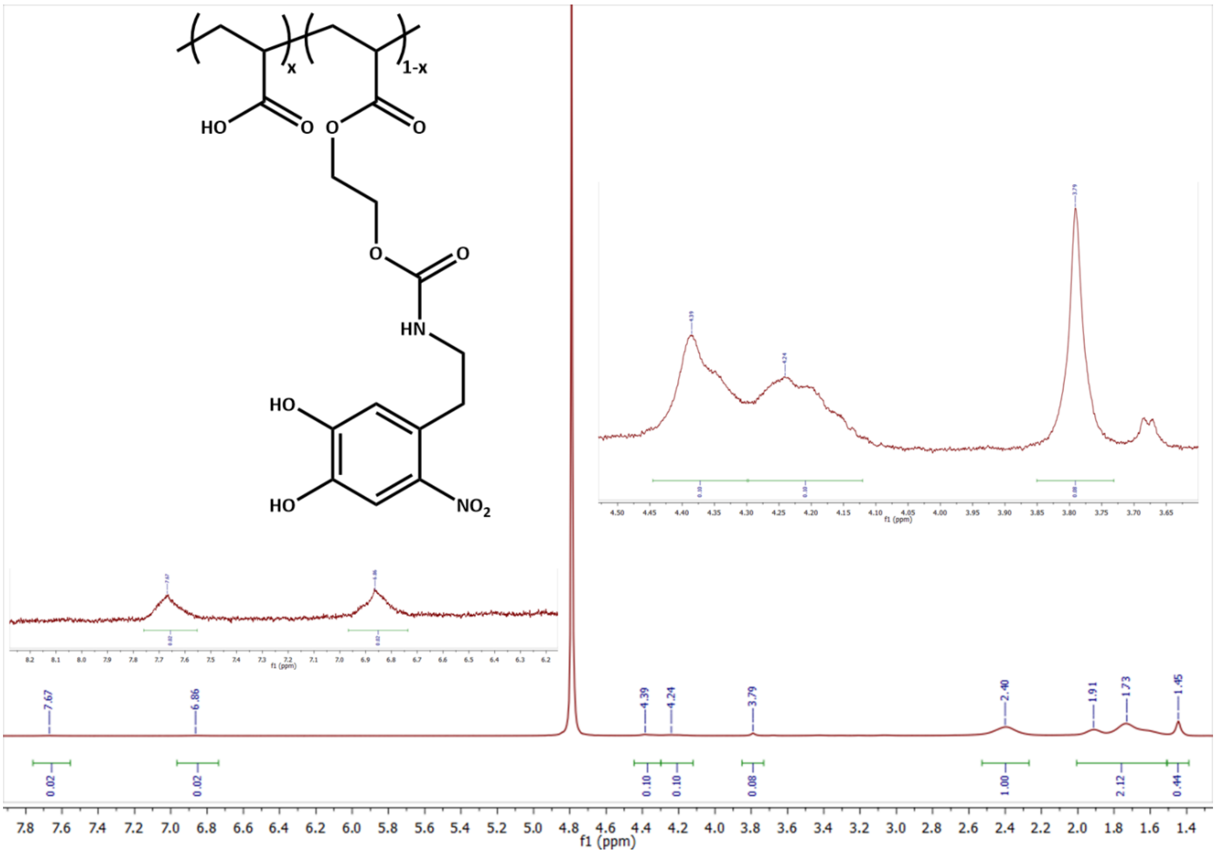

Figure S 5. [1]H NMR spectrum of Poly(acrylic acid-*ran*-NHS-ethyl acrylate)

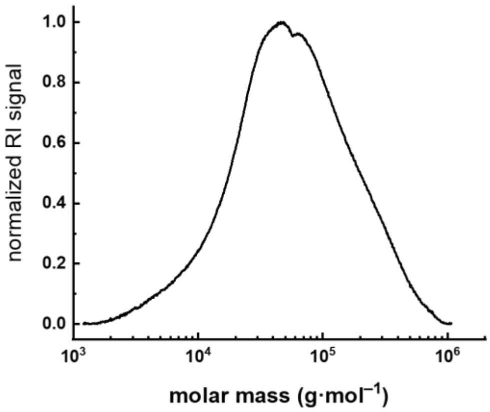

Figure S 6. GPC spectrum of of poly(*tert*-butyl acrylate-*ran*-hydroxyethyl acrylate). The polydispersity index (M_w/M_n) is 3.16.

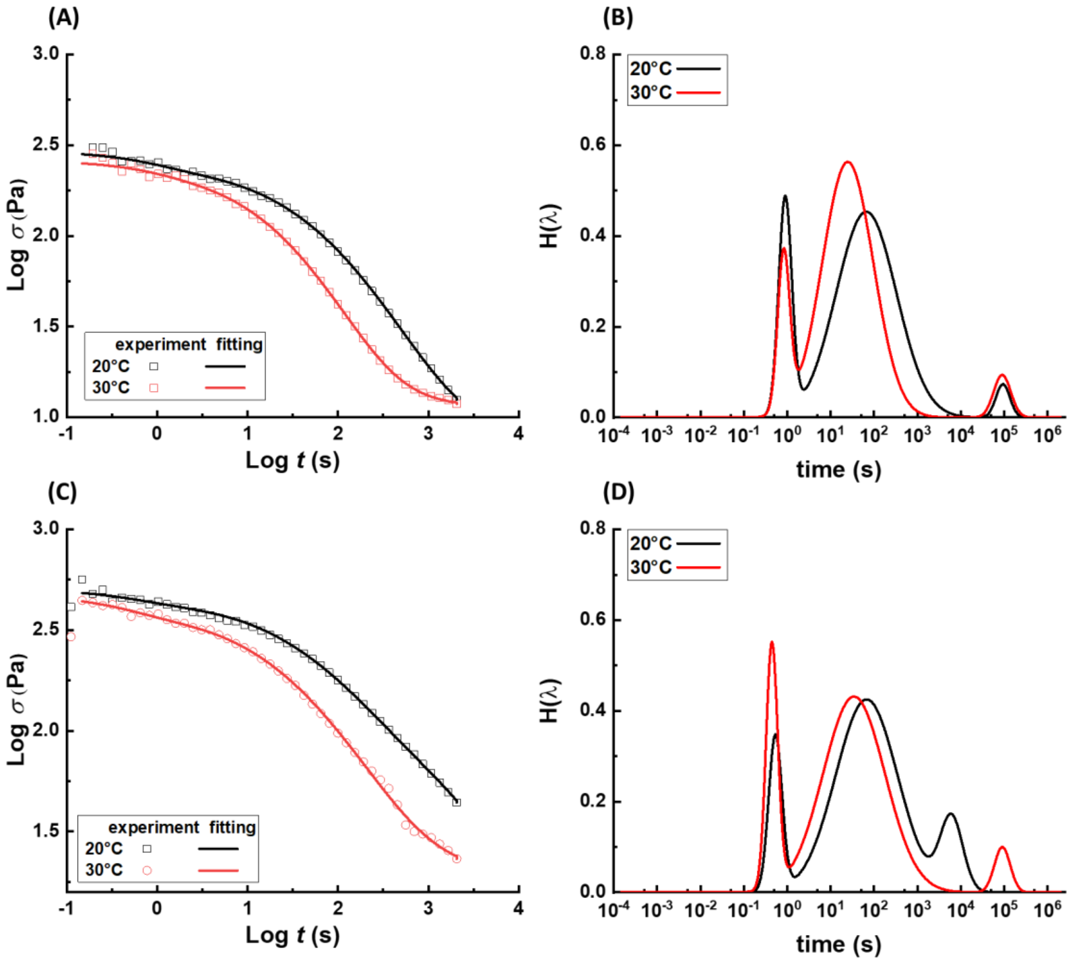

Figure S 7. (A) Comparison of the experimentally and calculated stress relaxation data for sample 153 at 20°C and 30°C. (B) The relaxation time spectrum for this sample at 20°C and 30°C, obtained from the fitting of stress relaxation data by considering three relaxation modes. (C) and (D) demonstrate similar data for sample 203.

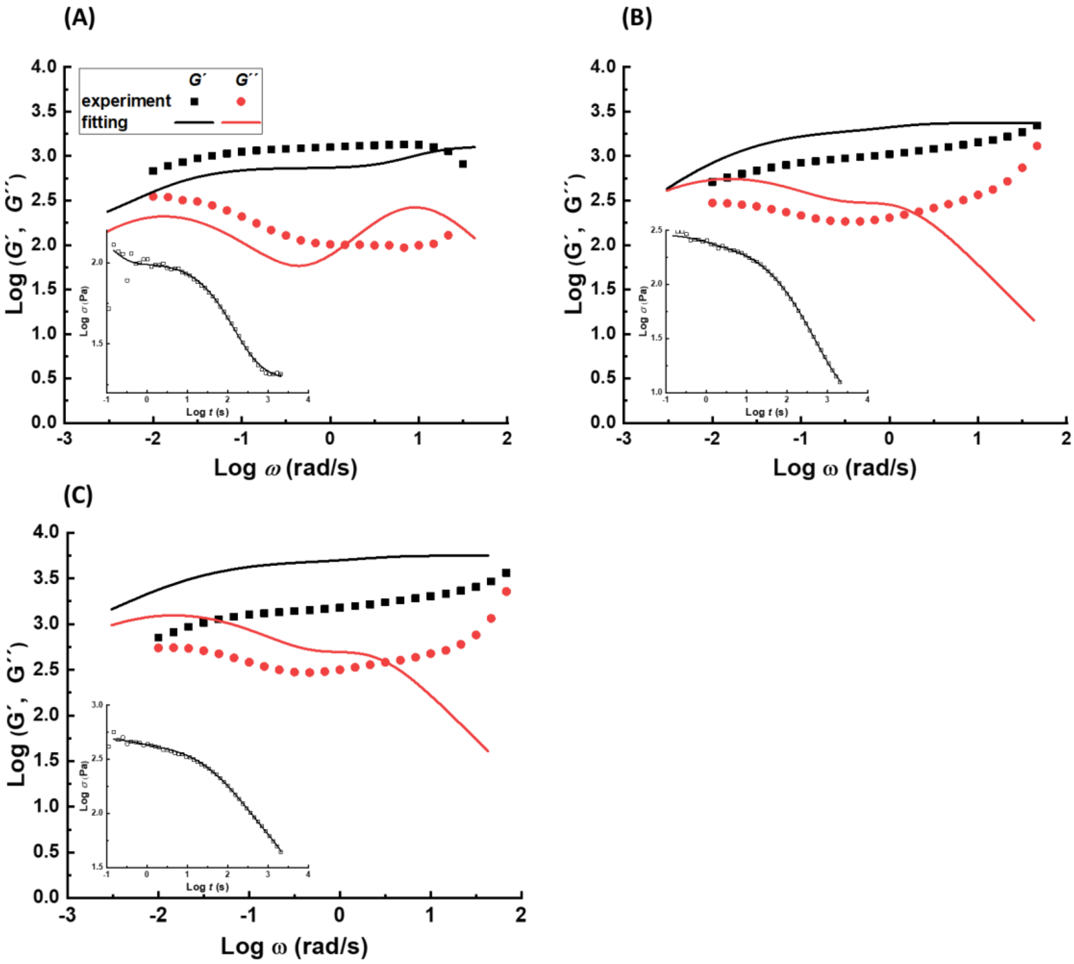

Figure S 8. Experimental and calculated frequency sweep data for samples (A)103, (B)153, and (C)203 at 20 °C. Insets represent the experimental and calculated stress relaxation for the corresponding samples.

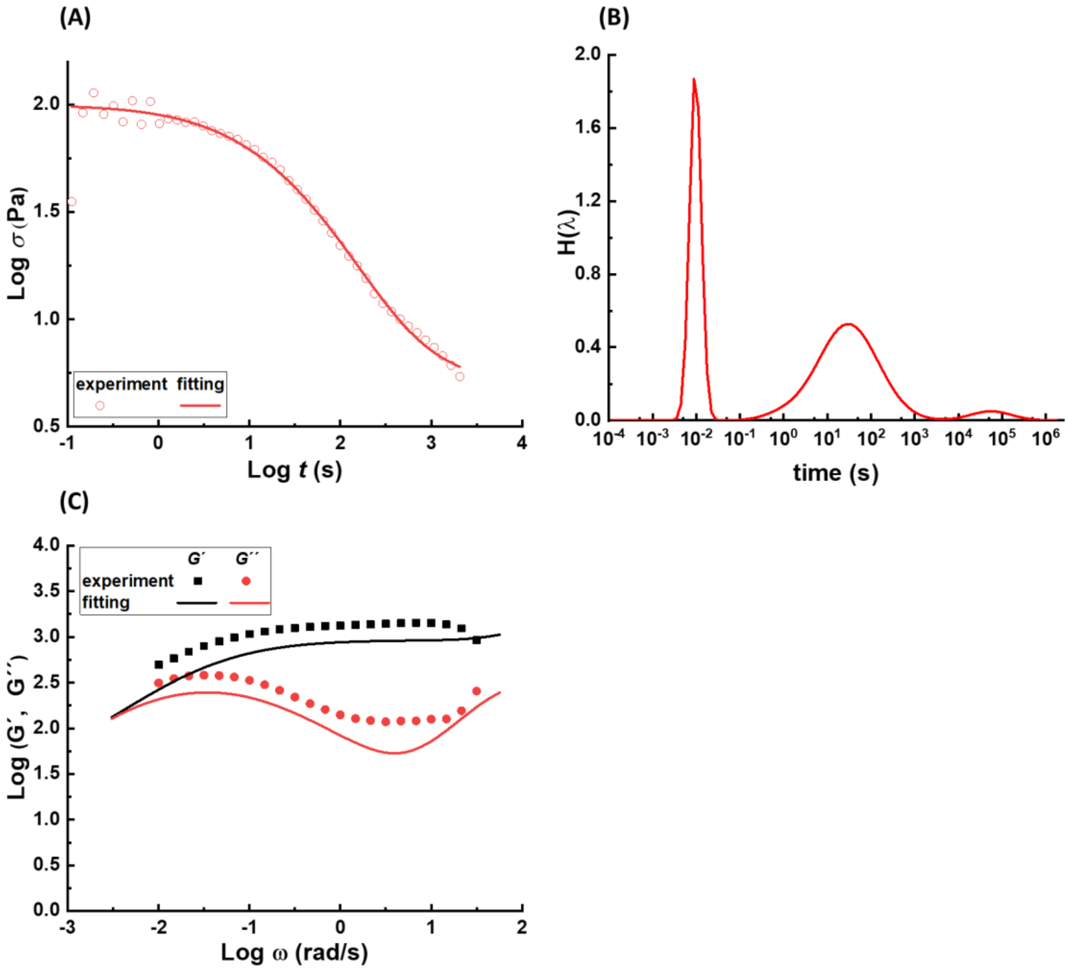

Figure S 9. (A) experimental and fitted stress relaxation data, (B) relaxation time spectrum, and (C) experimental and fitted frequency sweep data of sample pAA10_NC3 at 30 °C. The fitted data and the relaxation time spectrum are obtained by considering 4 relaxation modes. The relaxation time, PDI, and weight of this additional relaxation mode are 0.01 s, 1.1, and 0.17%, respectively. The results show a better agreement between experimental and fitted frequency sweep data. In addition, the overlap of the first two relaxation peaks in the relaxation time spectrum, are not observed anymore.

Table S 1. The fit parameters obtained from the fitting of stress relaxation data by considering three relaxation modes

Sample	Temperature (°C)	τ_1 (s)	τ_2 (s)	τ_3 (s)	PDI_1	PDI_2	PDI_3	W_1	W_2	W_3
pAA10_NC3	20	0.11540335	135.908963	98058.3934	1.12910878	3.24042403	0.11540335	0.200828	0.652633	0.146539
pAA15_NC3	20	0.95084939	238.298881	99981.2396	1.12887548	12.9346649	0.95084939	0.047073	0.944791	0.008136
pAA20_NC3	20	0.56614133	260.647505	7285.95638	1.13376895	14.9579503	0.56614133	0.03434	0.918718	0.046942
pAA20_NC2	20	0.04419676	157.339386	99927.0757	4.49637966	8.19549413	0.04419676	0.068011	0.921135	0.010853
pAA20_NC4	20	2.59499925	402.229326	97962.0004	14.0694403	11.7006265	2.59499925	0.523271	0.425209	0.05152
pAA10_NC3	30	1.51128225	105.076205	98993.8364	2.76340974	12.2678436	3.174689	0.020335	0.938479	0.041186
pAA15_NC3	30	0.86975655	62.2622439	99973.608	1.10795724	6.29986096	1.227472	0.032761	0.949597	0.017642
pAA20_NC3	30	0.46327881	133.736008	98847.1463	1.10076295	14.9996929	1.19056	0.041849	0.944096	0.014055
pAA20_NC2	30	1.70488554	68.7749853	99999.957	4.41635968	14.9999624	1.219071	0.000167	0.99649	0.003343
pAA20_NC4	30	4.95779499	253.865403	90209.8432	4.92751198	12.2286889	4.462901	0.440849	0.511226	0.047926