

# Supporting information for

## Persistence Length of $\alpha$ -Helical Poly-L-Lysine

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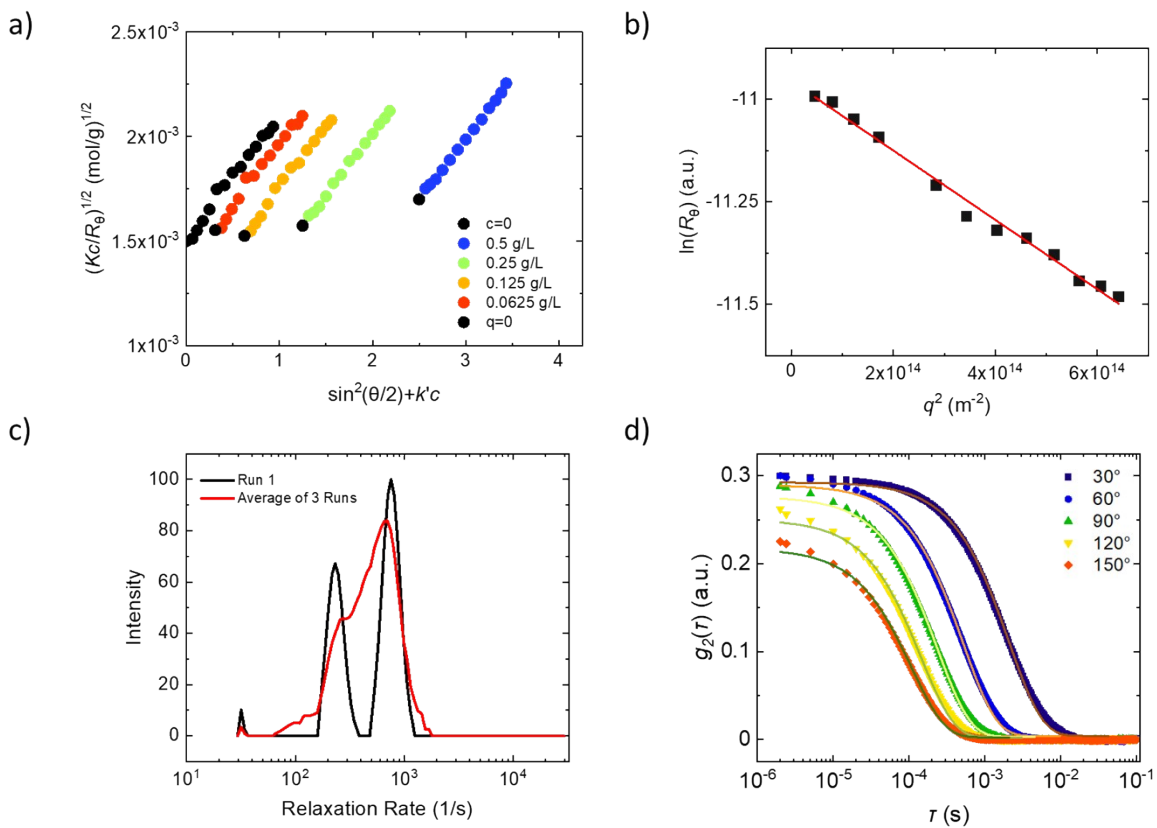


Figure S1: Berry (a), Guinier (b), CONTIN distribution at 90 $^\circ$ , and Correlation Plots of 433,000 g/mol PLL at pH 7.4 and 100 mM.

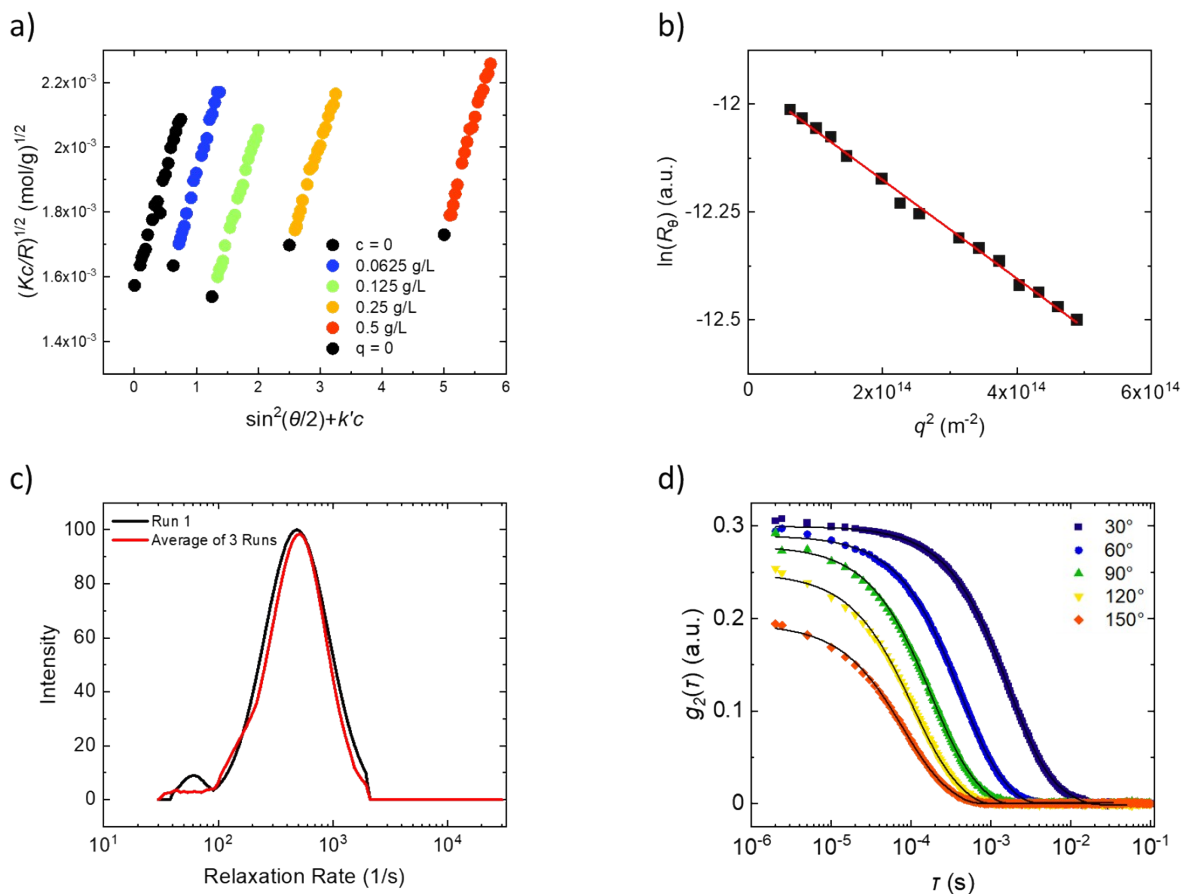


Figure S2: Berry (a), Guinier (b), CONTIN distribution at  $90^\circ$ , and Correlation Plots of 433,000 g/mol PLL at pH 10 and 100 mM.

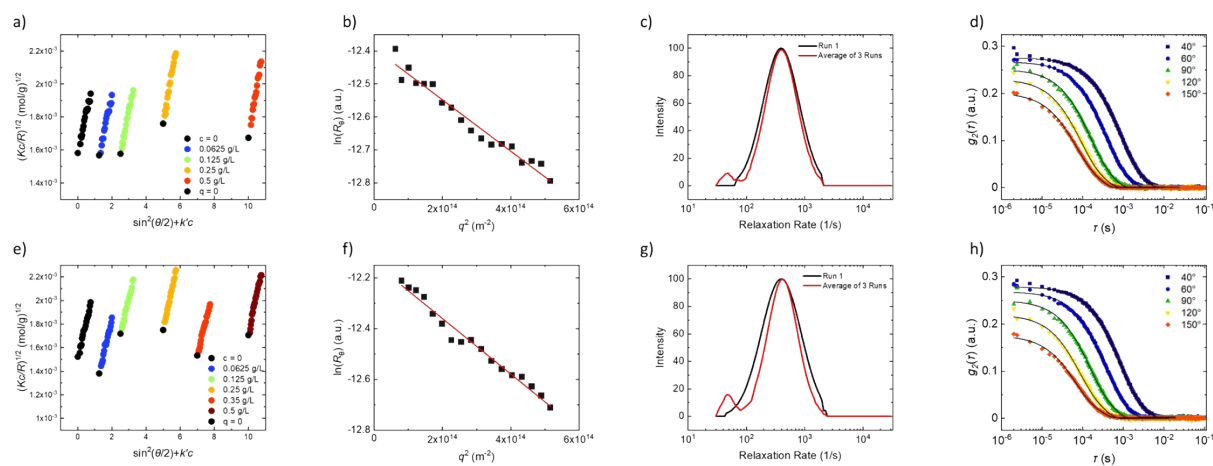


Figure S3: Berry (a), Guinier (b), CONTIN distribution at  $90^\circ$ , and Correlation Plots of 433,000 g/mol PLL at pH 10.2 and 100 mM.

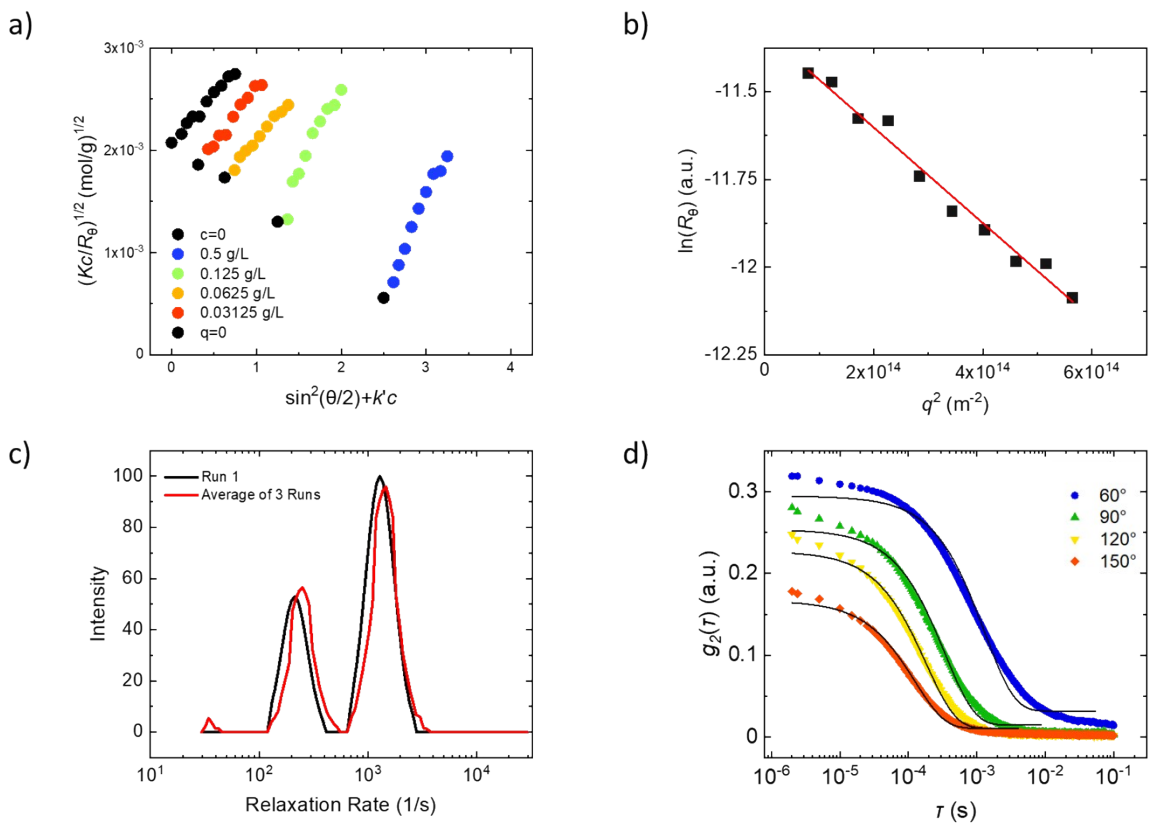


Figure S4: Berry (a), Guinier (b), CONTIN distribution at  $90^\circ$ , and Correlation Plots of 433,000 g/mol PLL at pH 11.4 and 100 mM.

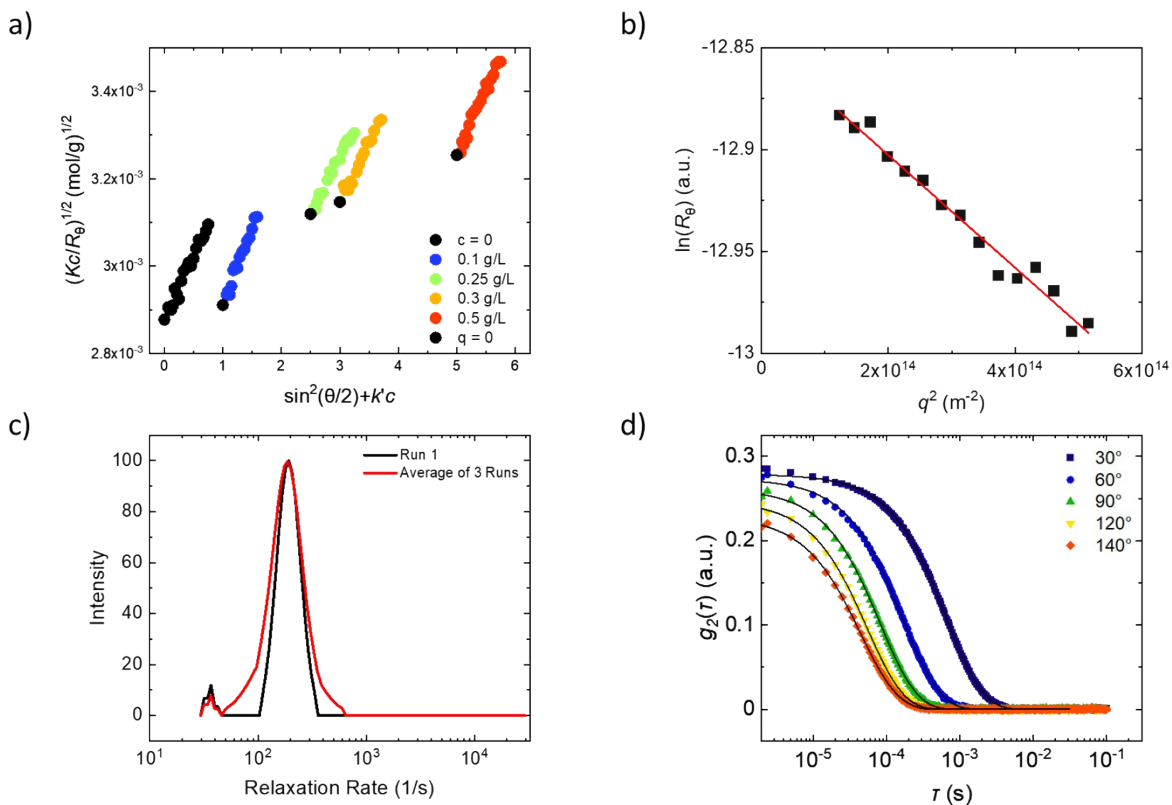


Figure S5: Berry (a), Guinier (b), CONTIN distribution at 90°, and Correlation Plots of 137,000 g/mol PLL at pH 7.4 and 100 mM.

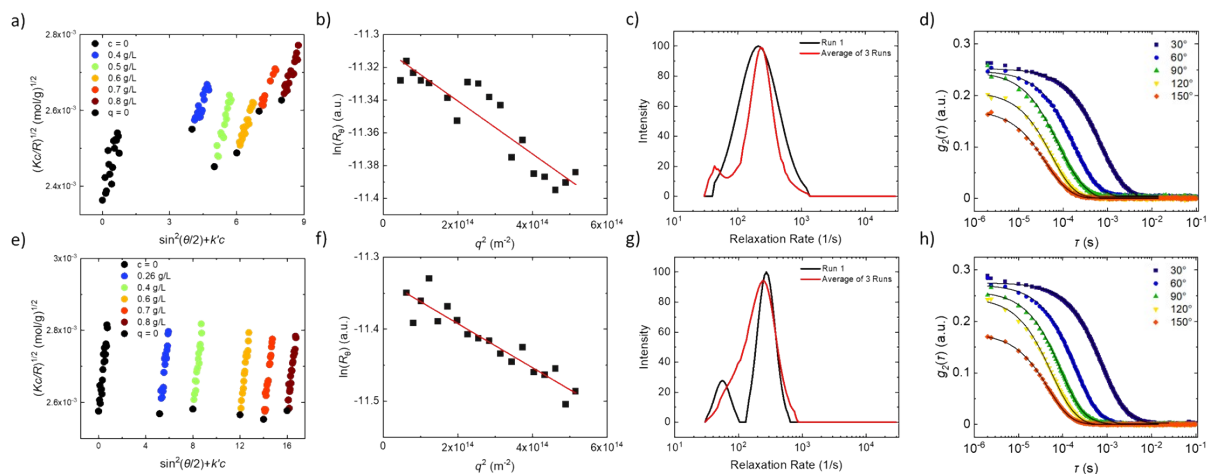


Figure S6: Berry (a), Guinier (b), CONTIN distribution at 90°, and Correlation Plots of 137,000 g/mol PLL at pH 10 and 100 mM.

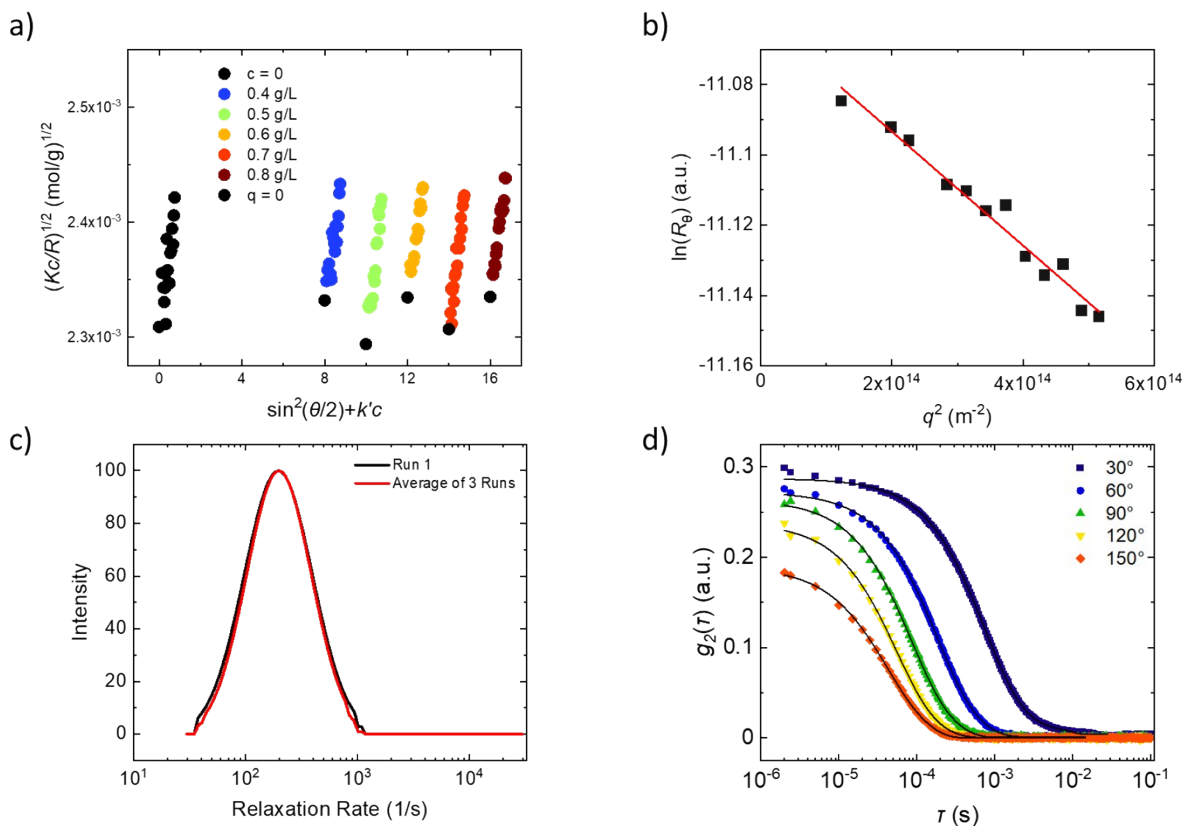


Figure S7: Berry (a), Guinier (b), CONTIN distribution at 90°, and Correlation Plots of 137,000 g/mol PLL at pH 10.2 and 100 mM.

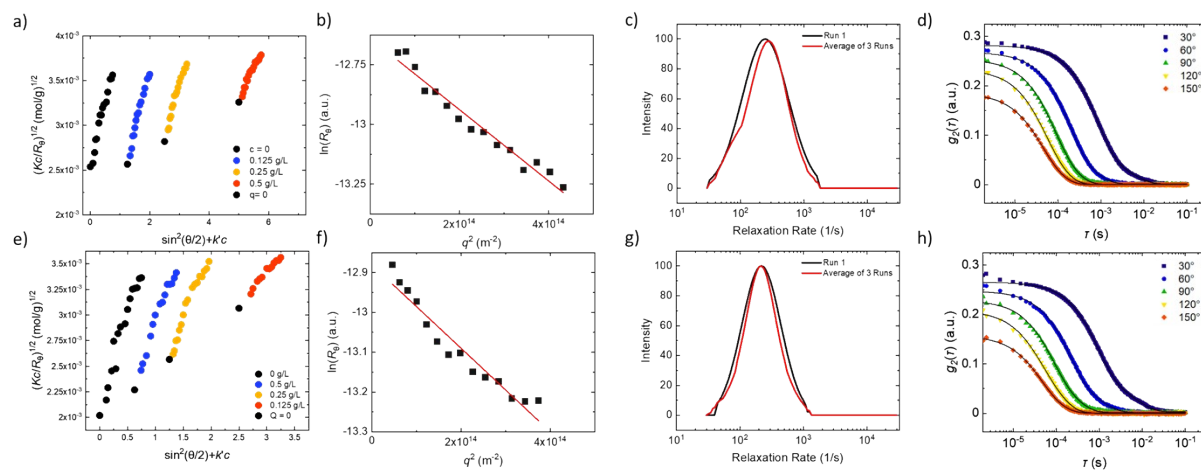


Figure S8: Berry (a), Guinier (b), CONTIN distribution at 90°, and Correlation Plots of 137,000 g/mol PLL at pH 11.4 and 100 mM.

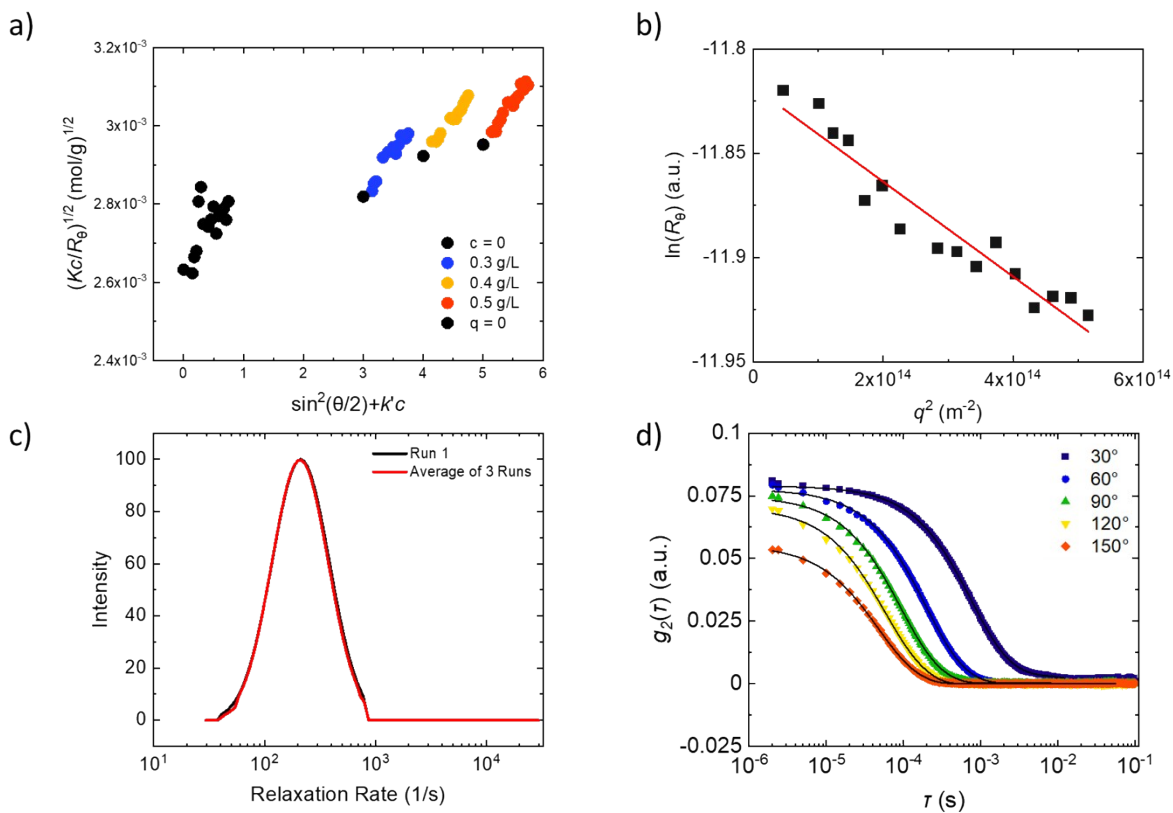


Figure S9 Berry (a), Guinier (b), CONTIN distribution at  $90^\circ$ , and Correlation Plots of 137,000 g/mol PLL at pH 7.4 and 166 mM.

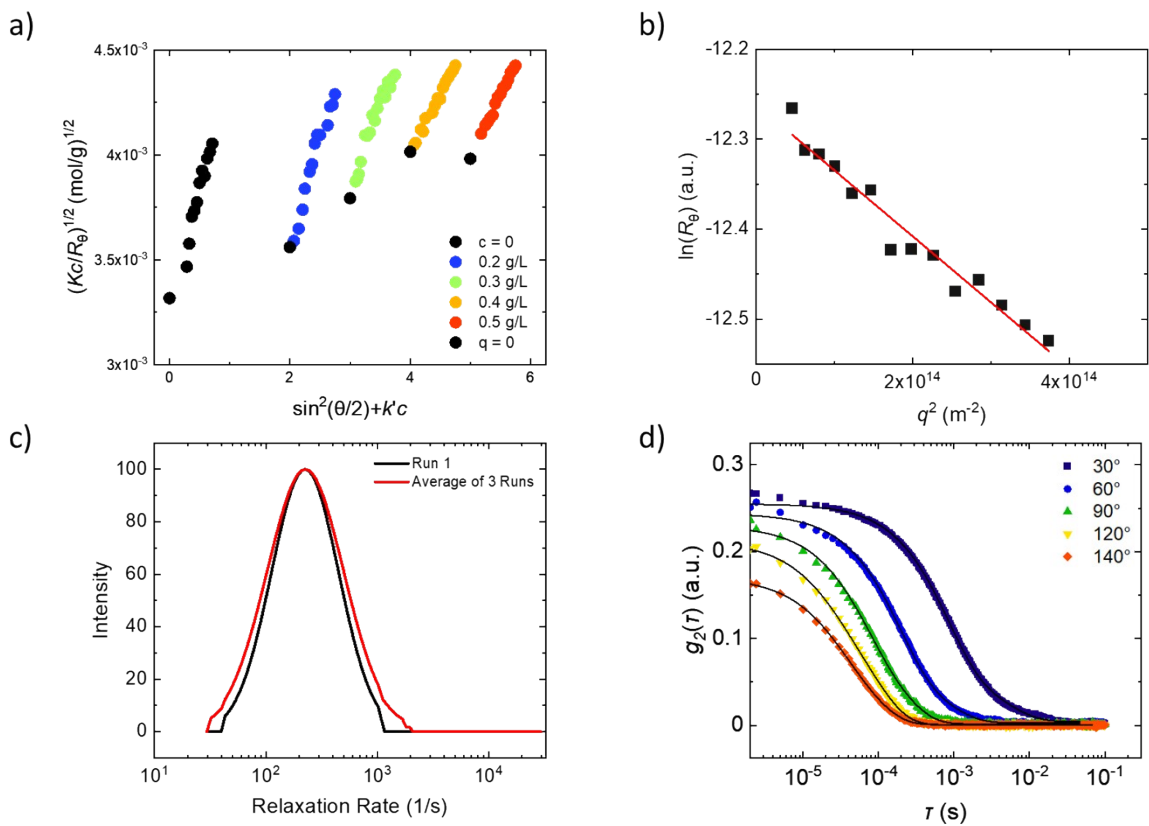


Figure S10: Berry (a), Guinier (b), CONTIN distribution at  $90^\circ$ , and Correlation Plots of 137,000 g/mol PLL at pH 11.4 and 166 mM.

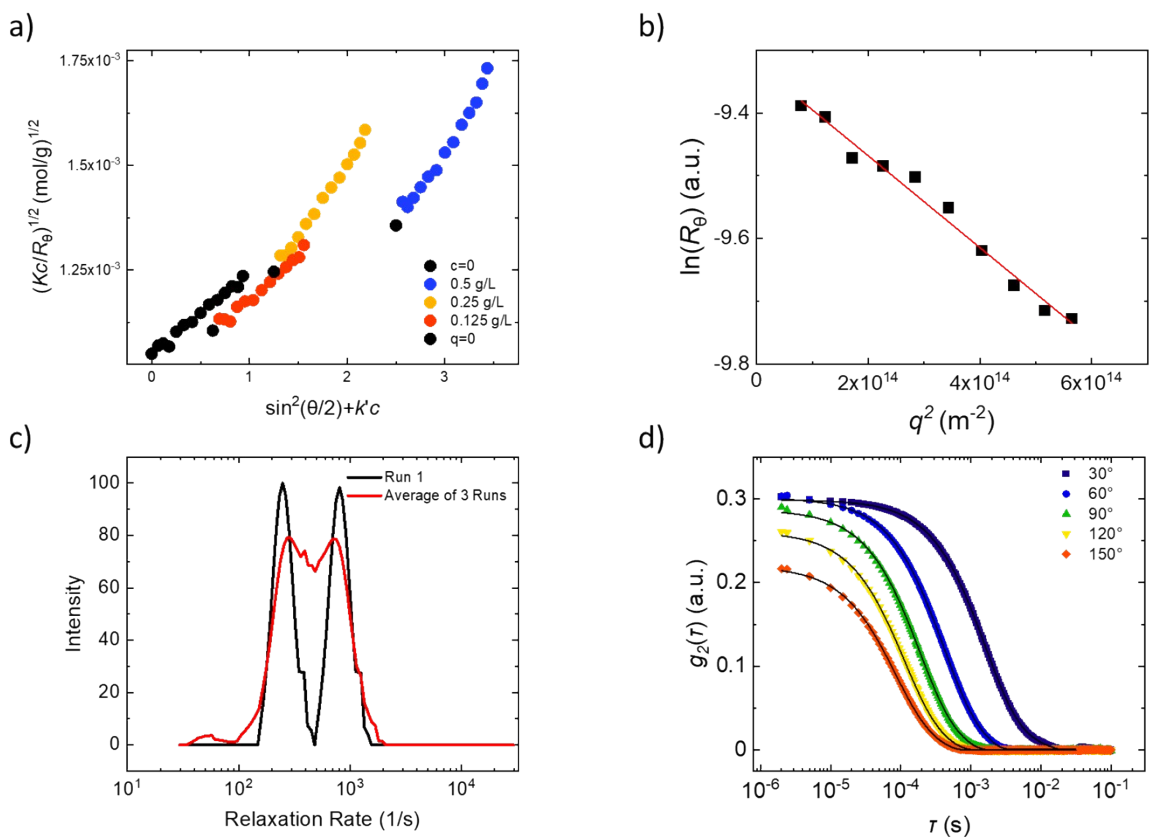


Figure S11: Berry (a), Guinier (b), CONTIN distribution at  $90^\circ$ , and Correlation Plots of 433,000 g/mol PLL at pH 7.4 and 25 mM.

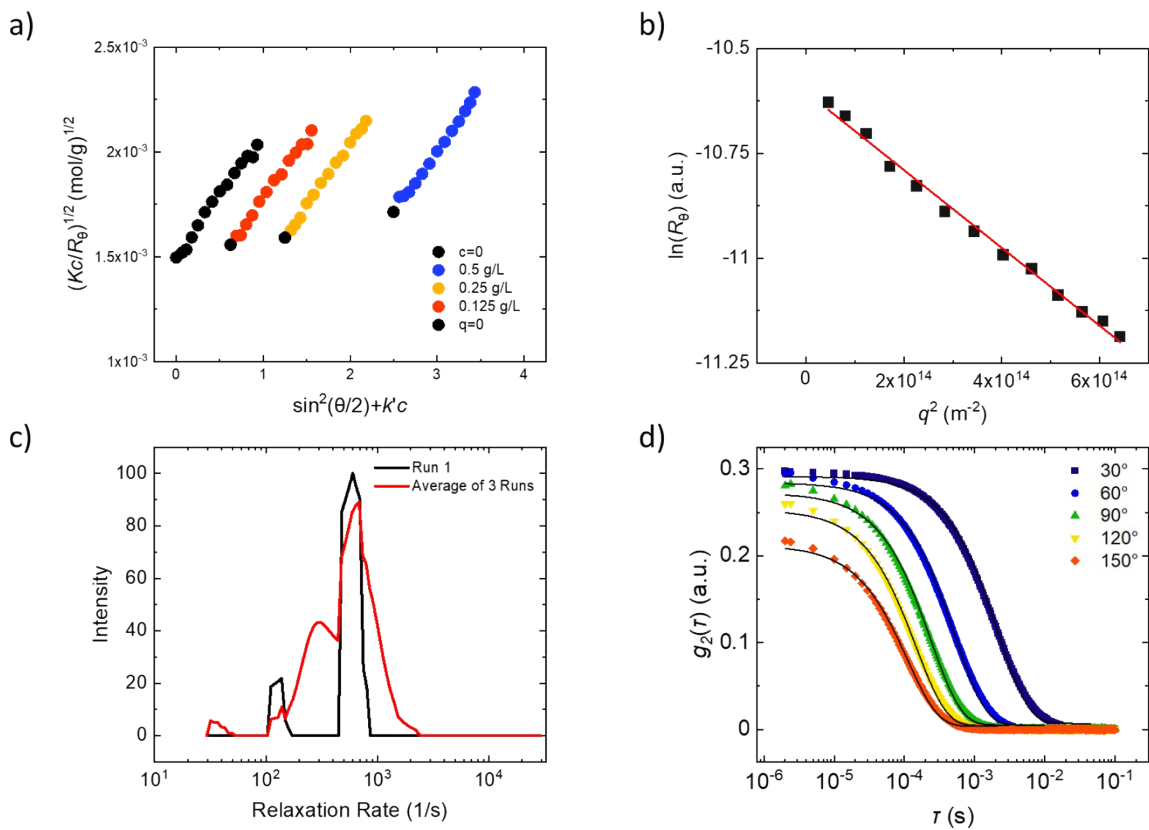


Figure S12: Berry (a), Guinier (b), CONTIN distribution at 90°, and Correlation Plots of 433,000 g/mol PLL at pH 7.4 and 50 mM.

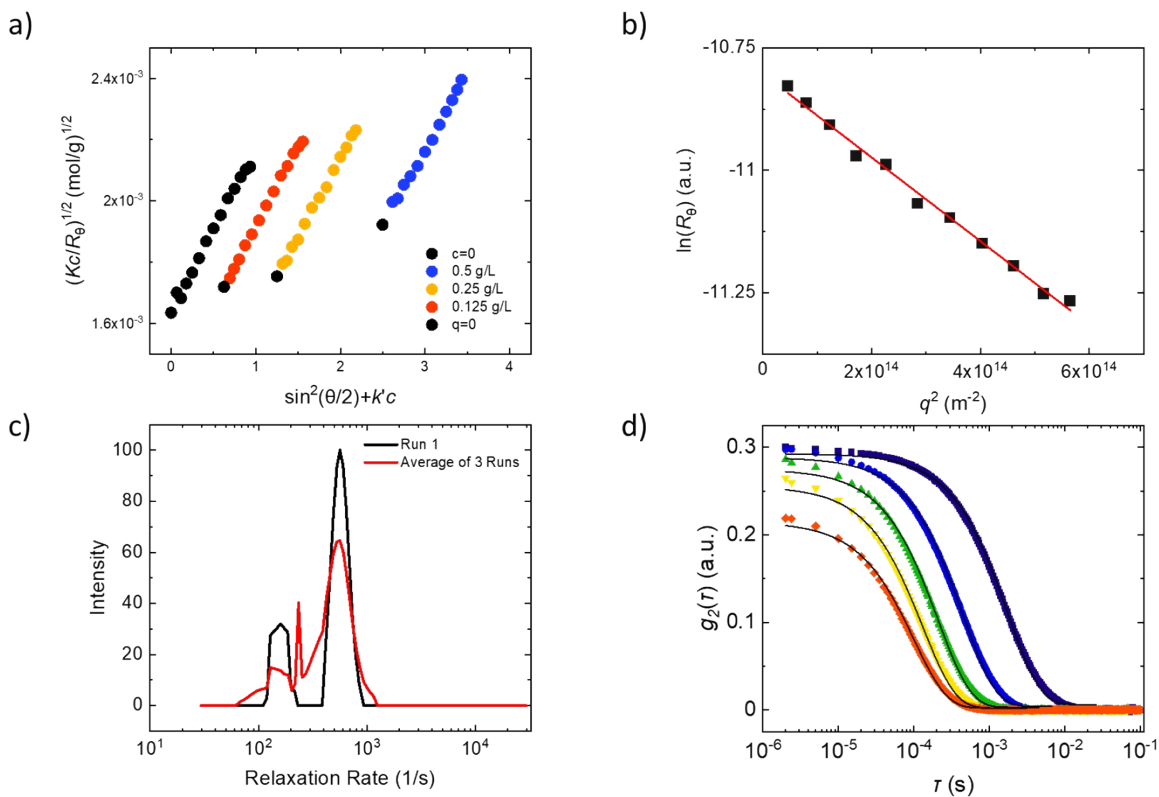


Figure S13: Berry (a), Guinier (b), CONTIN distribution at  $90^\circ$ , and Correlation of 433,000 g/mol PLL at pH 7.4 and 166 mM.

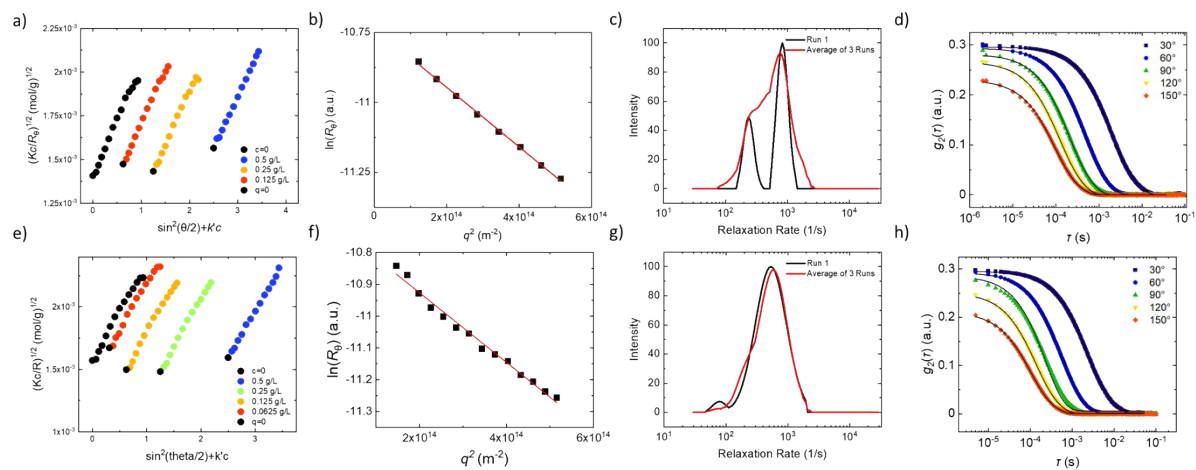


Figure S14: Berry (a), Guinier (b), CONTIN distribution at  $90^\circ$ , and Correlation Plots of 433,000 g/mol PLL at pH 7.4 and 266 mM.

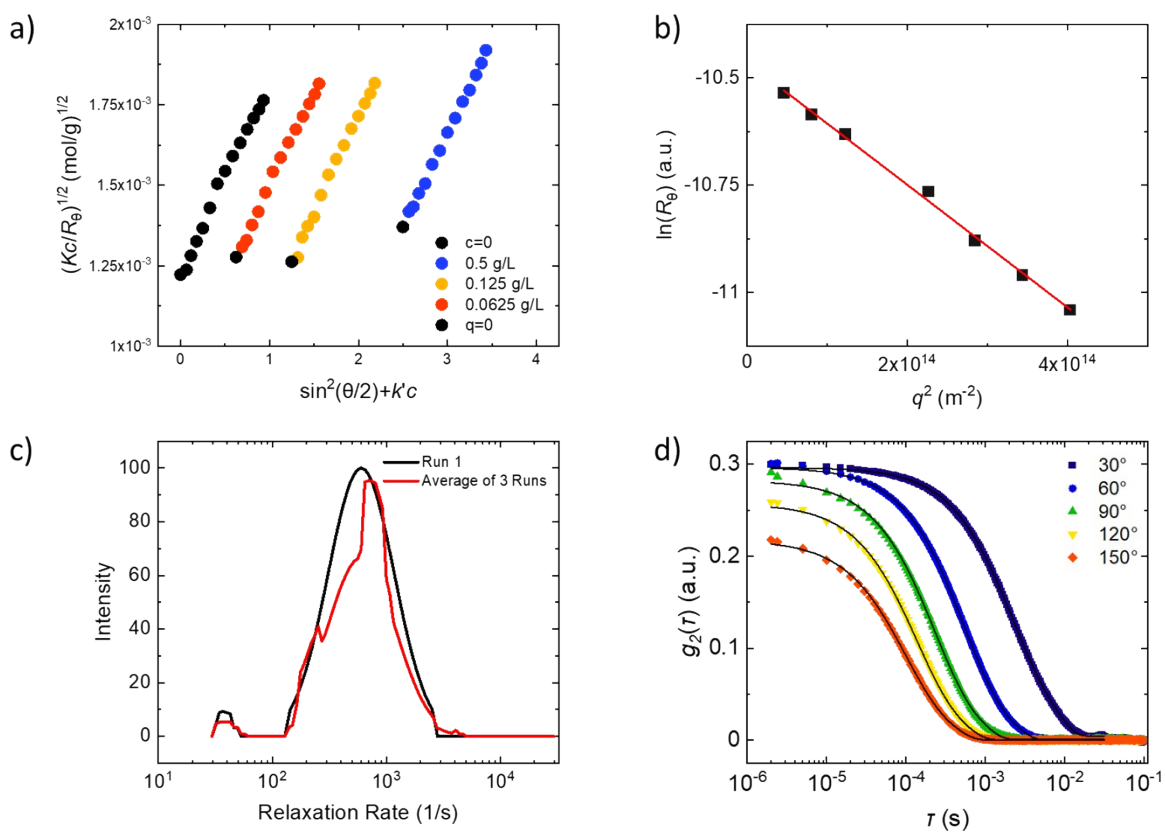


Figure S15: Berry (a), Guinier (b), CONTIN distribution at  $90^\circ$ , and Correlation Plots of 433,000 g/mol PLL at pH 7.4 and 500 mM.

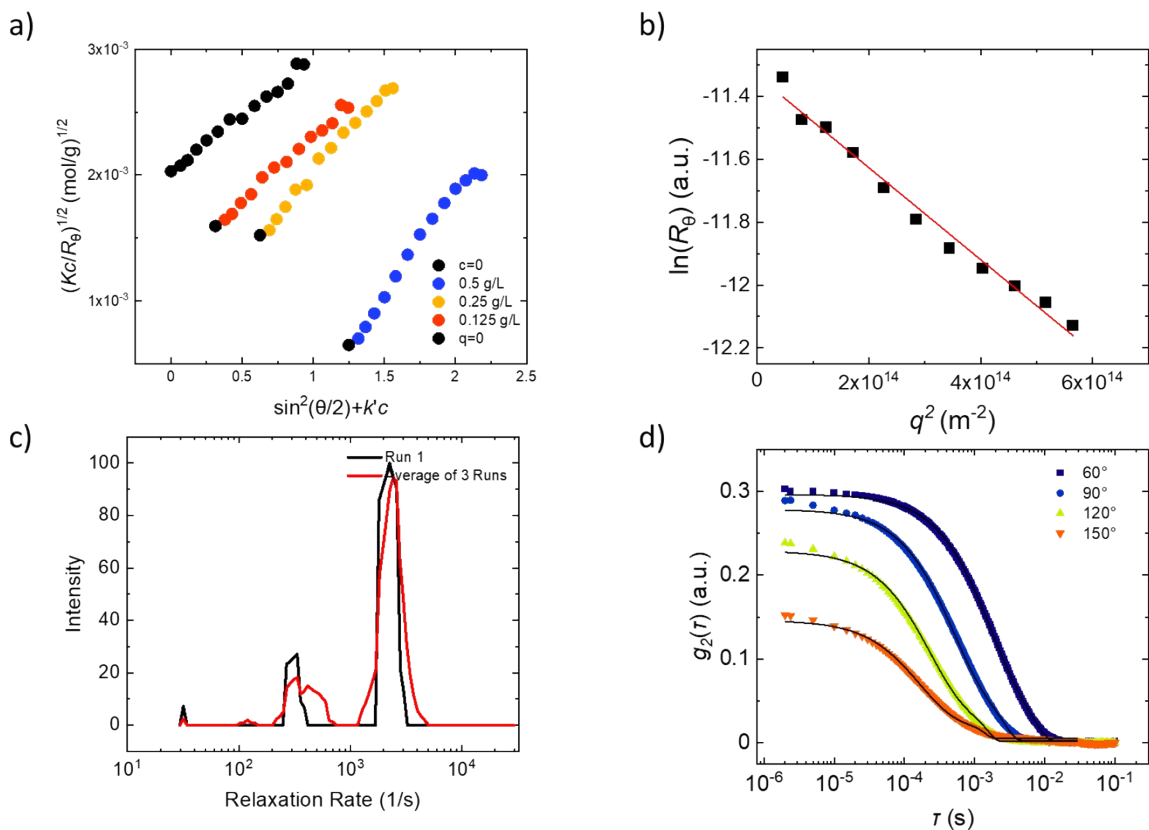


Figure S16: Berry (a), Guinier (b), CONTIN distribution at 90°, and Correlation Plots of 433,000 g/mol PLL at pH 11.4 and 50 mM.

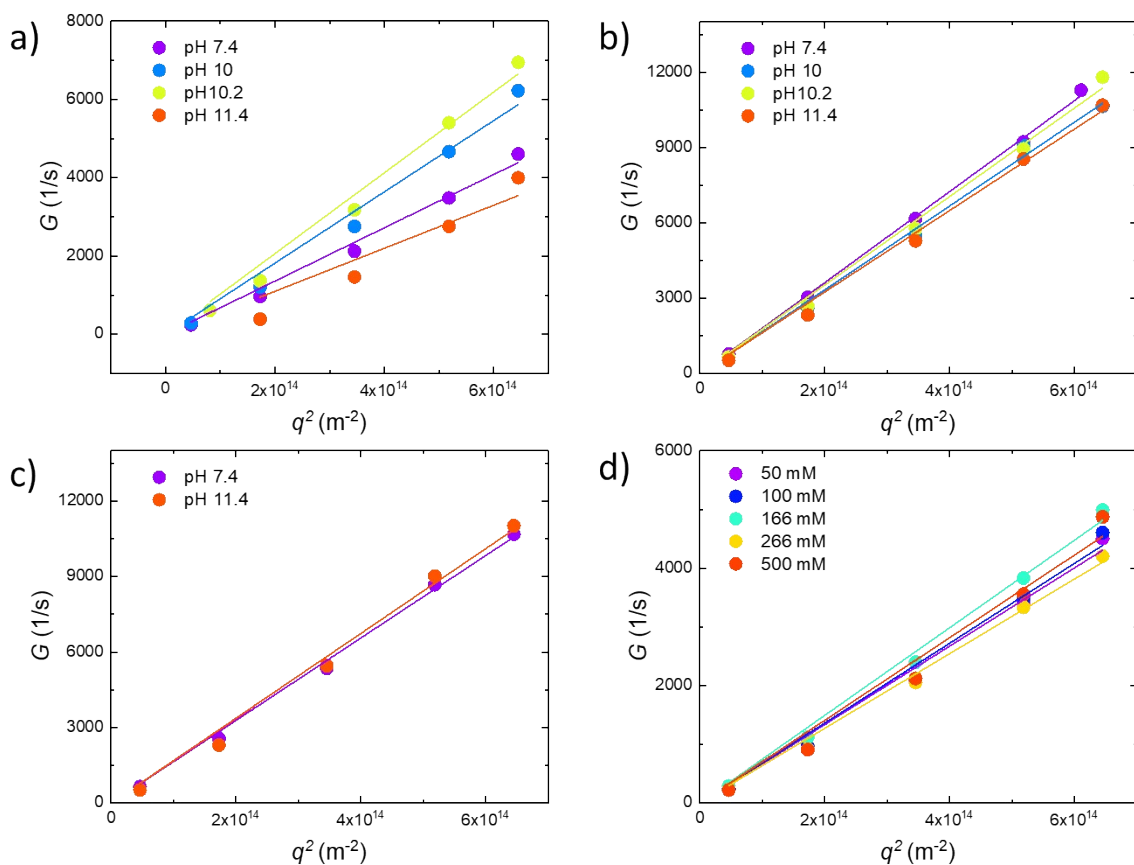


Figure S17: Relaxation rate as a function of the scattering vector squared for a) 433,000 g/mol PLL at 100 mM and various pH b) 137,000 g/mol PLL at 100 mM and various pH c) 137,000 g/mol PLL at 166 mM and various pH d) 433,000 g/mol PLL at pH 7.4 and various ionic strength.

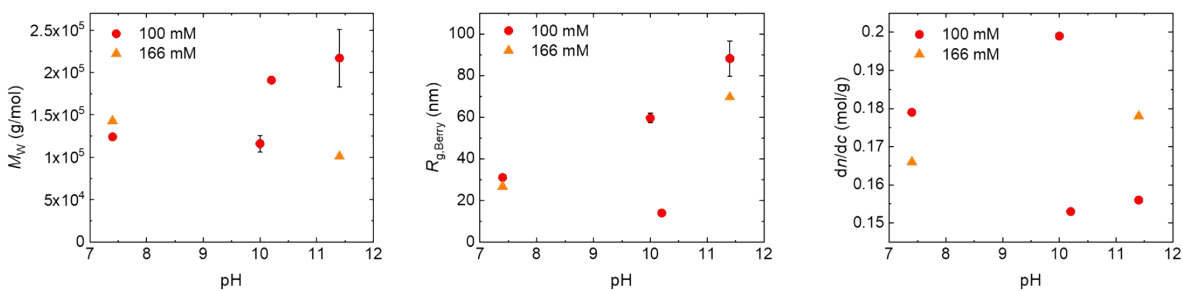


Figure S18: Molecular weight, Berry  $R_g$ , and  $dn/dc$  as a function of pH for 137,000 g/mol PLL at 100 and 166 mM.

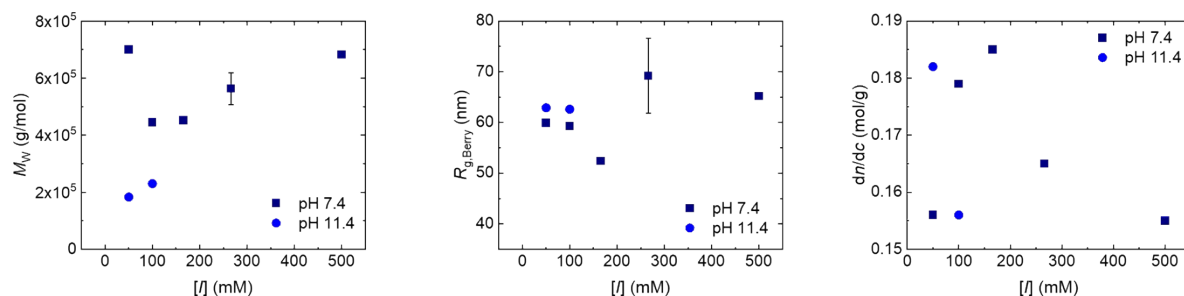


Figure S19: Molecular weight, Berry  $R_g$ , and  $dn/dc$  as a function of ionic strength for 433,000 g/mol PLL at pH 7.4 and 11.4.

The PLL433  $R_g$ ,  $A_2$ , and  $R_g/R_h$  from SLS and DLS experiments and the ellipticity results from CD experiments are shown in Figure S20. Together, these results were used to determine the change in PLL433 structure and interactions as a function of ionic strength in pH 7.4. As the ionic strength increases from 25 mM to 166 mM,  $R_g$  is unchanged, around 50 nm. As the ionic strength is increased to 500 mM,  $R_g$  increases slightly to 65 nm. The  $R_g/R_h$  in Figure 5b similarly increases, from 1.5 in 50 mM to 2.1 in 500 mM, as shown in Figure 5b. As shown in Figure 5c,  $A_2$  decreases as a function of ionic strength from  $1.0 \times 10^{-3}$  mol mL/g<sup>2</sup> in 50 mM to  $1.4 \times 10^{-4}$  mol mL/g<sup>2</sup> in 500 mM. This decrease is consistent with screening of stabilizing charges on the backbone. Consistent with the  $R_g$  results, the mean residue ellipticity does not show a significant change in structure as a function of ionic strength. The random coil peak at 218 nm seems to increase, but because of the high sodium ion concentration, the peaks at 197 nm cannot be accurately compared.<sup>34</sup> Qualitatively, the signal for a random coil orientation increases with increased ionic strength. Overall, the  $A_2$  decreases as a function of ionic strength and indicates increasing attractive backbone interactions in higher ionic strength solutions.

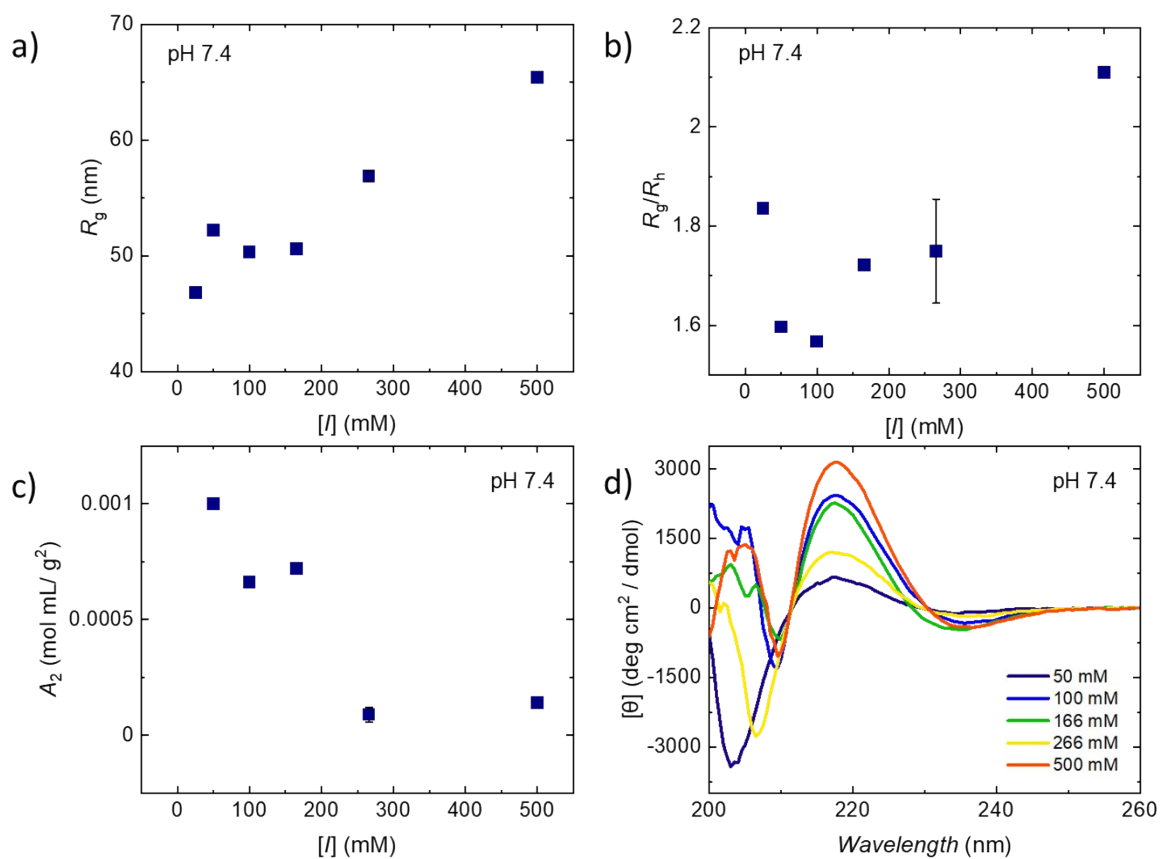


Figure S20: Ionic strength study of 433,000 g/mol PLL. a) Radius of gyration as a function of ionic strength. b) Shape factor as a function of ionic strength. c) Second virial coefficient as a function of ionic strength. d) Mean residue ellipticity as a function of ionic strength for 137,000 g/mol PLL in pH 7.4 solution.

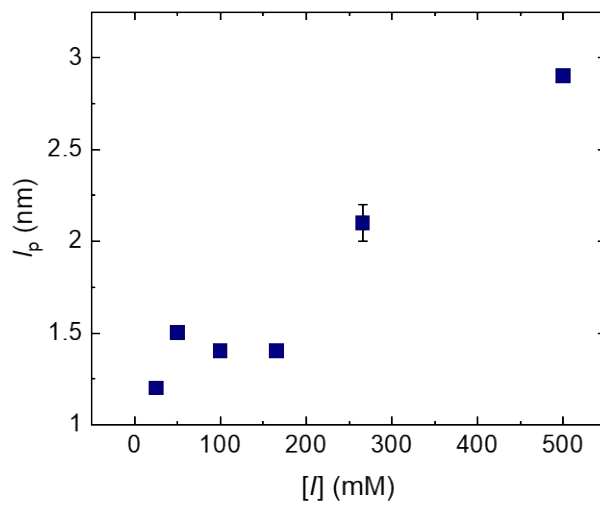


Figure 21: Persistence length as a function of ionic strength for 433,000 g/mol PLL at pH 7.4.

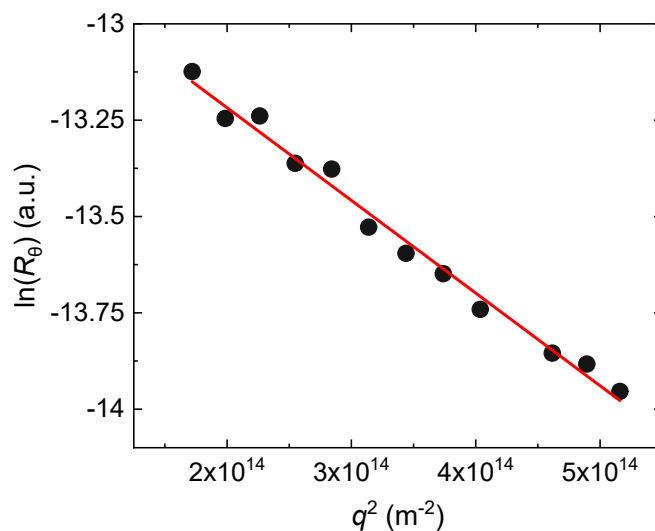


Figure S22: Guinier plot of 433,000 g/mol PLL at pH 12 and 100 mM. As determined from the slope of the Guinier plot,  $R_g$  also increases to 84.9 nm in pH 12; however, PLL did not dissolve easily at this high pH so further concentration experiments could not be performed.

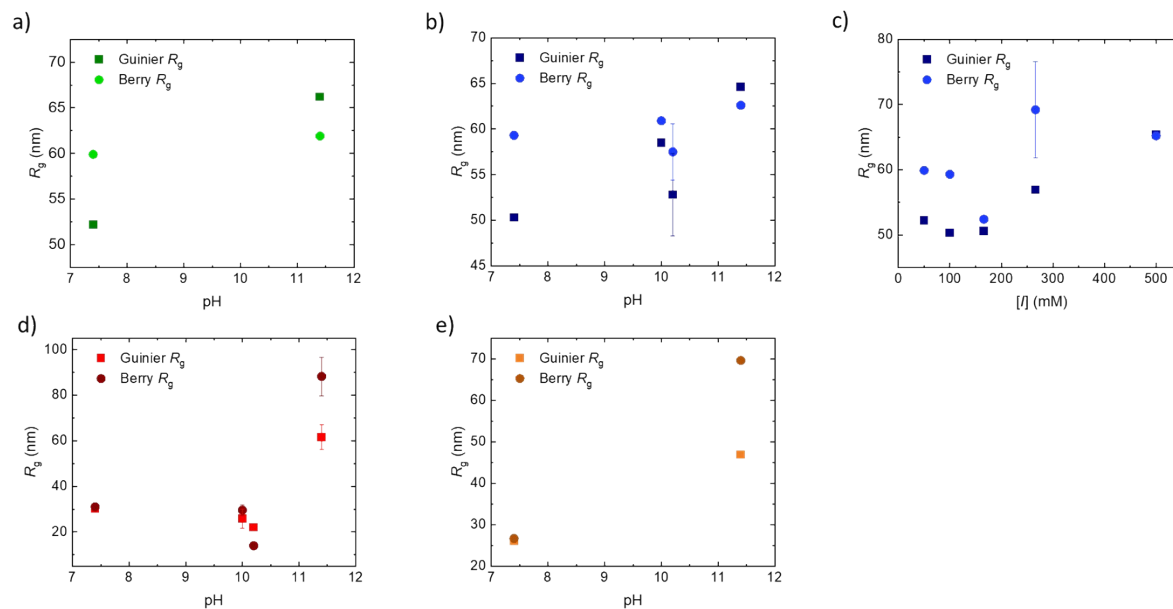


Figure S23: Comparison of  $R_g$ : Top row: PLL433 a) 50mM b) 100 mM c) pH 7.4, Bottom Row: PLL137 d) 100 mM e) 166 mM

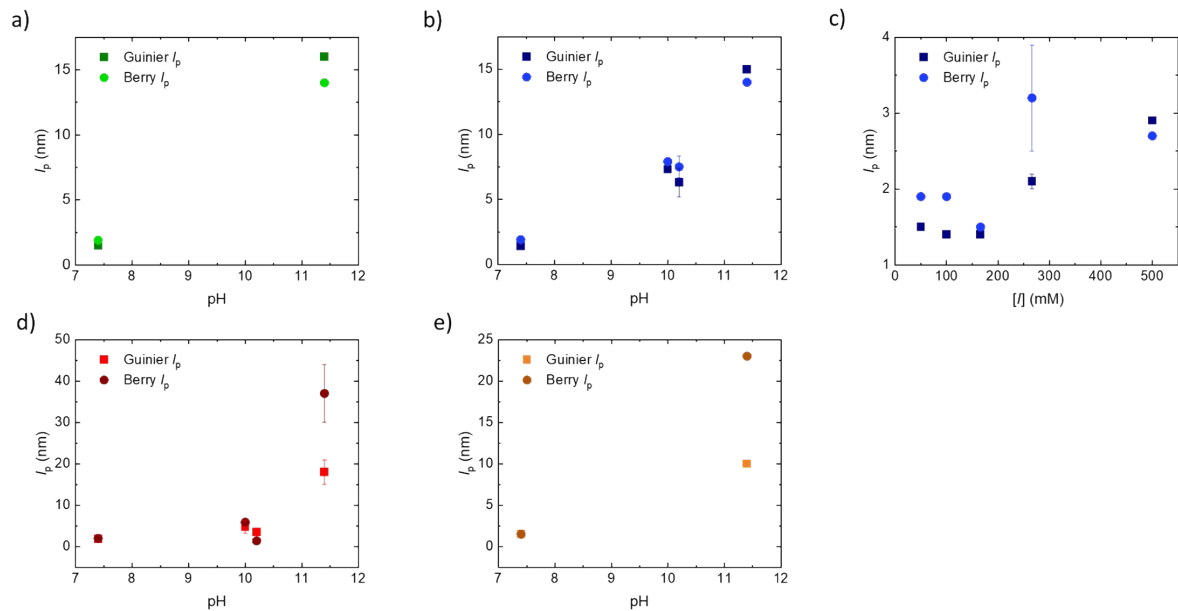


Figure S24: Comparison of  $l_p$ : Top row: PLL433 a) 50mM b) 100 mM c) pH 7.4, Bottom Row: PLL137 d) 100 mM e) 166 mM

pH	[I] (mM)	Buffer Type	$dn/dc$ (mL/g)
7.4	50	PBS	0.156
7.4	100	PBS	0.179
7.4	166	PBS	0.166
7.4	266	PBS	0.165
7.4	266	PBS	0.165
7.4	500	PBS	0.155
10	100	Bicarbonate	0.199
10.2	100	Bicarbonate	0.153
11.4	50	PBS	0.182
11.4	100	PBS	0.156
11.4	166	PBS	0.178

Table S1:  $dn/dc$  Table

<b>pH</b>	<b>[I] (mM)</b>	<b>Buffer Type</b>	<b><math>M_w</math> (g/mol)</b>
7.4	50 PBS		700000
7.4	100 PBS		445000
7.4	166 PBS		452000
7.4	266 PBS		507000
7.4	266 PBS		619000
7.4	500 PBS		682000
11.4	50 PBS		183000
11.4	100 PBS		230000
10	100 Bicarb		398000
10.2	100 Bicarb		420000
10.2	100 Bicarb		442000
10	100 CAPS		232000
10.2	100 CAPS		313000
<b>Avg</b>			<b>432,538.46</b>

Table S2: Higher molecular weight PLL table and average

<b>pH</b>	<b>[I] (mM)</b>	<b>Buffer Type</b>	<b><math>M_w</math> (g/mol)</b>
7.4	100 PBS		124000
7.4	166 PBS		143000
11.4	100 PBS		183000
11.4	100 PBS		250000
11.4	166 PBS		101000
10	100 Bicarb		126000
10	100 Bicarb		106000
10.2	100 Bicarb		191000
10	100 CAPS		145000
10.2	100 CAPS		98000
10	166 CAPS		98000
10.2	166 CAPS		81000
<b>Avg</b>			<b>137,166.67</b>

Table S3: Lower molecular weight PLL table and average