

Supporting Information for

# pH-Induced Changes in Polypeptide Conformation: Force-Field Comparison with Experimental Validation

*Piotr Batys,<sup>a,\*</sup> Maria Morga,<sup>a</sup> Piotr Bonarek<sup>b</sup>, and Maria Sammalkorpi<sup>c,d</sup>*

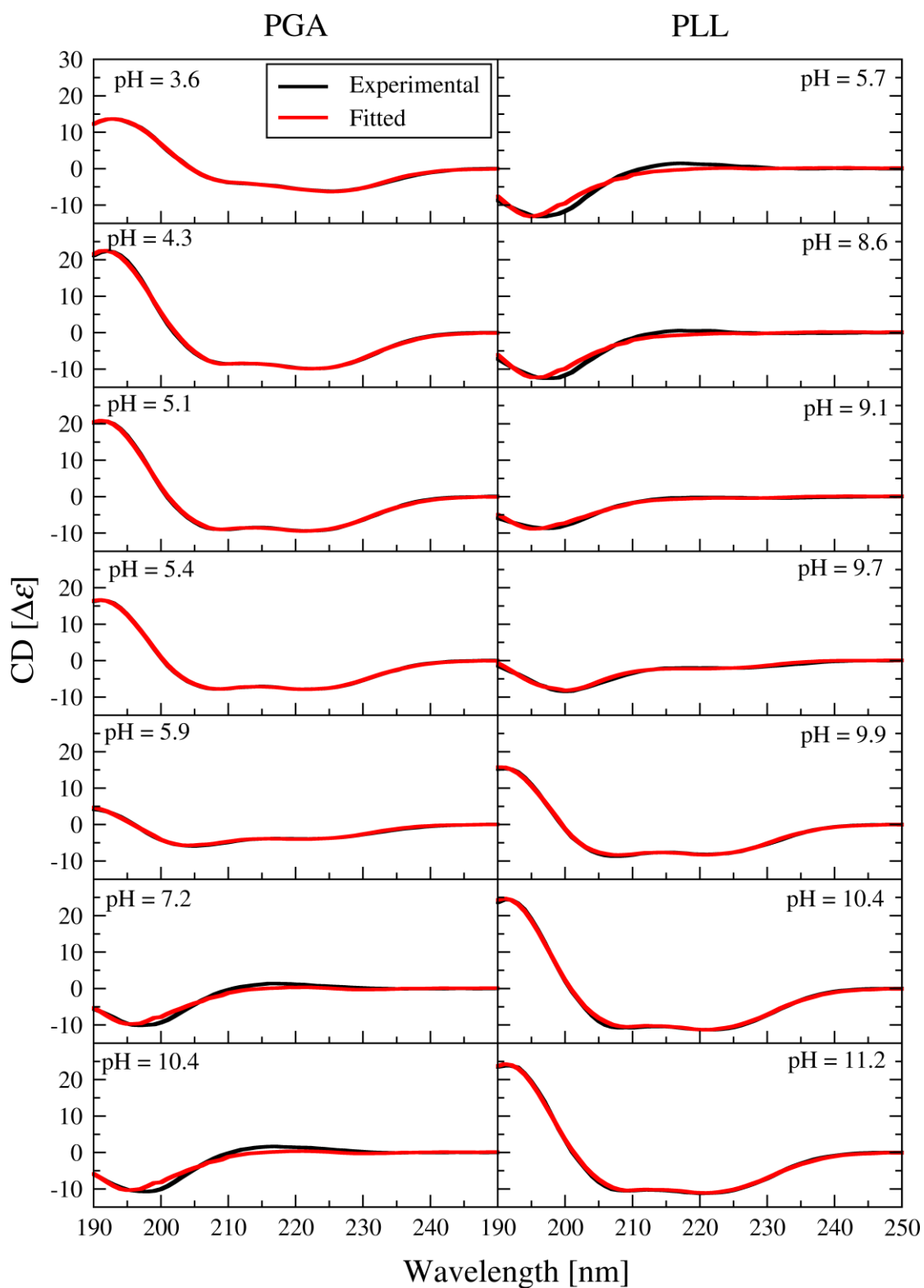
<sup>a</sup>Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences,  
Niezapominajek 8, PL-30239 Krakow, Poland

<sup>b</sup>Department of Physical Biochemistry, Faculty of Biochemistry, Biophysics and  
Biotechnology, Jagiellonian University, Krakow, Poland

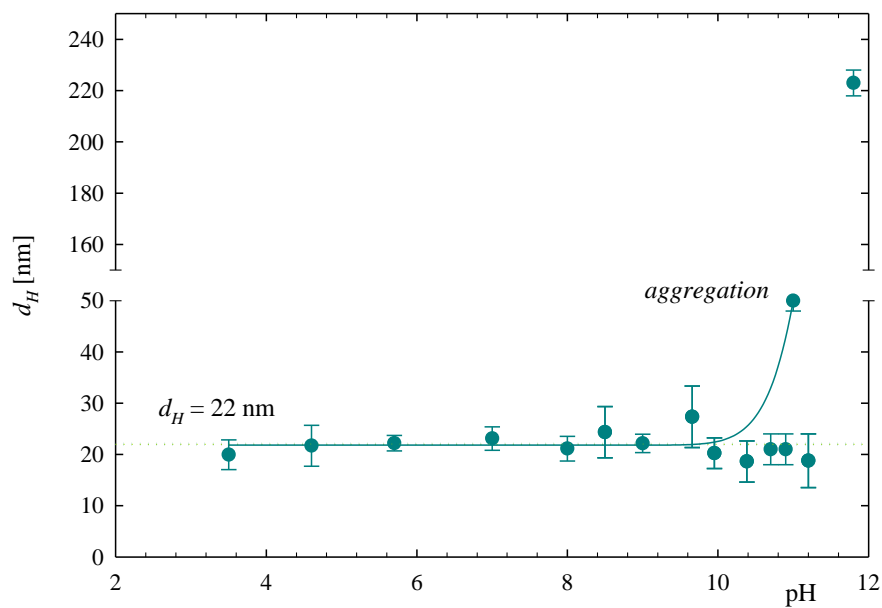
<sup>c</sup>Department of Chemistry and Materials Science, and <sup>d</sup>Department of Bioproducts and  
Biosystems, Aalto University, P.O. Box 16100, 00076 Aalto, Finland

Corresponding author:

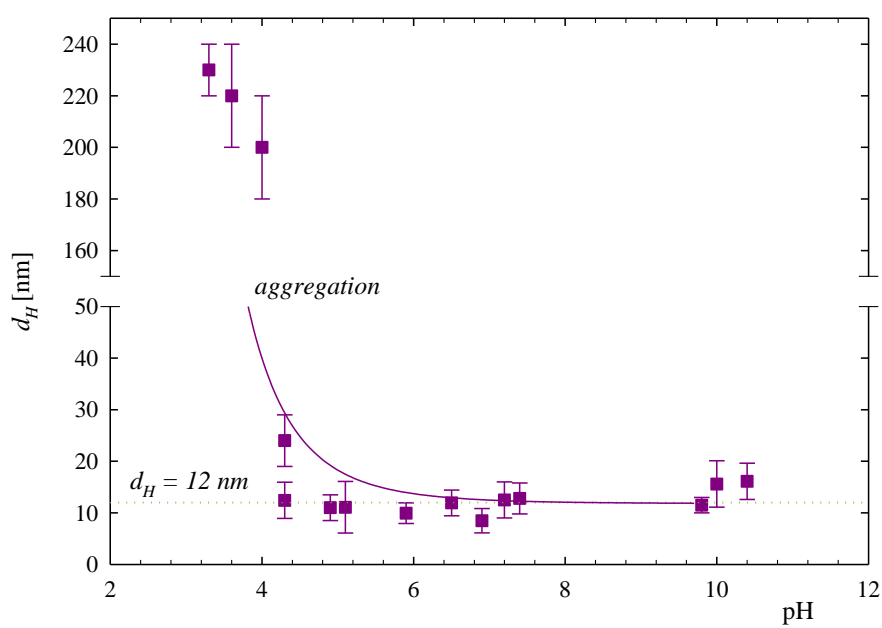
[ncbatys@cyf-kr.edu.pl](mailto:ncbatys@cyf-kr.edu.pl)



**Fig. S1.** CD spectra measured at 293 K for PGA and PLL at different pH values. Ionic strength is  $10^{-2}$  M NaCl. The black and red lines denote the experimental data and the fitted curve using the BeStSel web server, respectively.

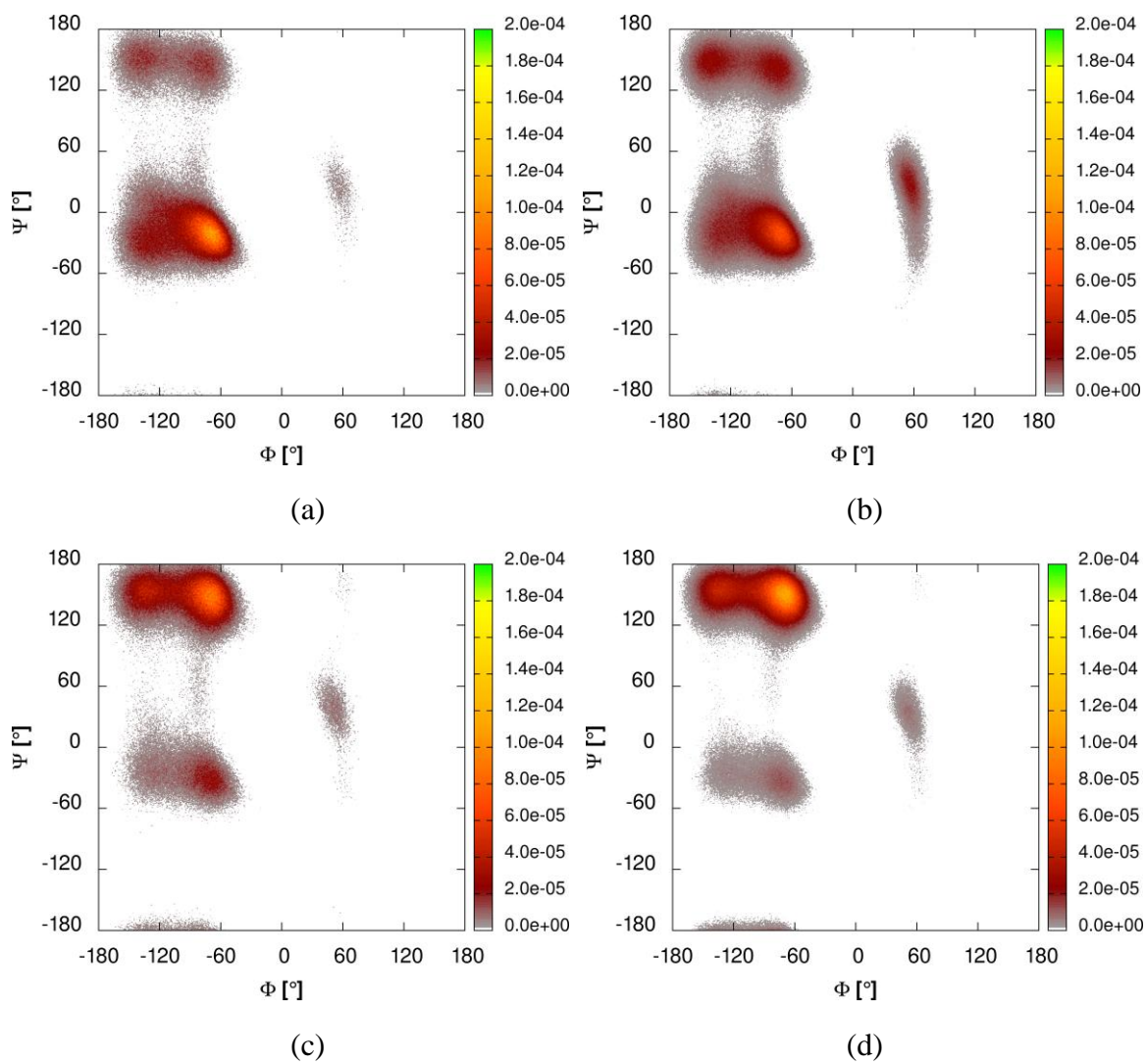


(a)

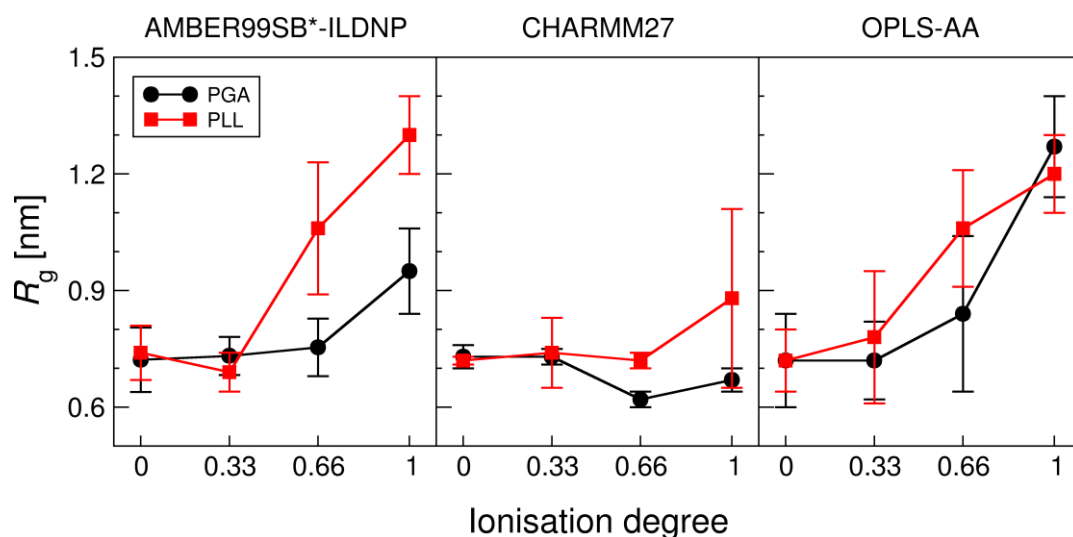


(b)

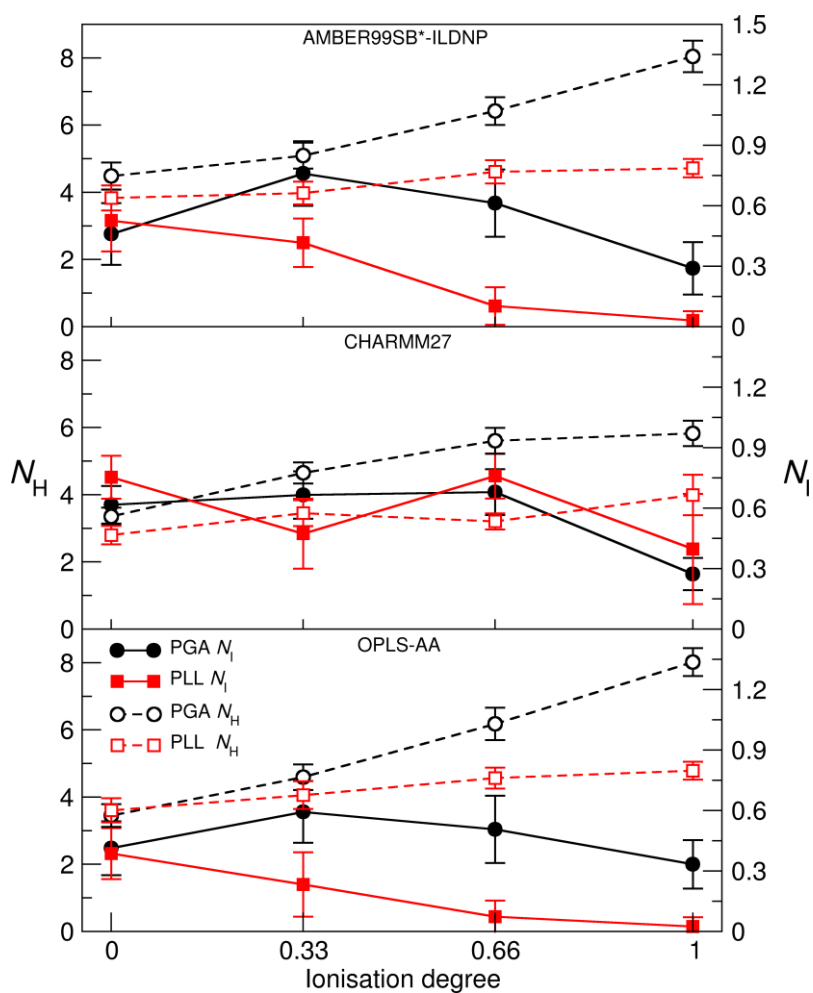
**Fig. S2.** The dependence of the hydrodynamic diameter of (a) PLL molecules and (b) PGA molecules on pH at  $I = 10^{-2}$  M NaCl. The measurements were performed in  $T = 298$  K.



**Fig. S3.** The Ramachandran plots for PGA chains with (a) 5 and (b) 15 amino acids and PLL chains with (c) 5 and (d) 15 amino acids. The ionisation degrees are 1 and the force field used is AMBER99SB\*-ILDNP.



**Fig. S4.** The radius of gyration as a function of ionisation degree and force field type.



**Fig. S5.** The number of internal ( $N_I$ ) and polypeptide-water ( $N_H$ ) hydrogen bonds per single amino acid as a function of the ionisation degree and the force field type.

**Table S1.** Evolution of secondary structure of PGA and PLL with different ionisation degrees (ID) and force fields (FF) in the MD simulations. The examined FFs are AMBER99SB\*-ILDNP (A), CHARMM27 (C), and OPLS-AA (O). The secondary structure classified as  $\alpha$ -helices,  $\beta$ -structure, and other is shown in blue, red, and white, respectively. The y-axis denotes the residue index, and the x-axis is simulation time (single pixel every 2 ns).

