



Characterizing Equilibrium Length of Living Polymers via DOSY-NMR



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OBJECTIVE

To analyze NMR signal intensities for a living polymers to derive the micellar length and diffusion coefficient.

SELF DIFFUSION OF MOLECULES

Self-diffuse of small molecules in solutions occurs due to thermal fluctuations (Fig. 1). Measuring the self-diffusion coefficient gives us the hydrodynamic size of the molecule (Eq.1). Self-diffusion coefficient can be measured with DOSY-NMR technique by imposing a pulse gradient spin echo (Fig.2).

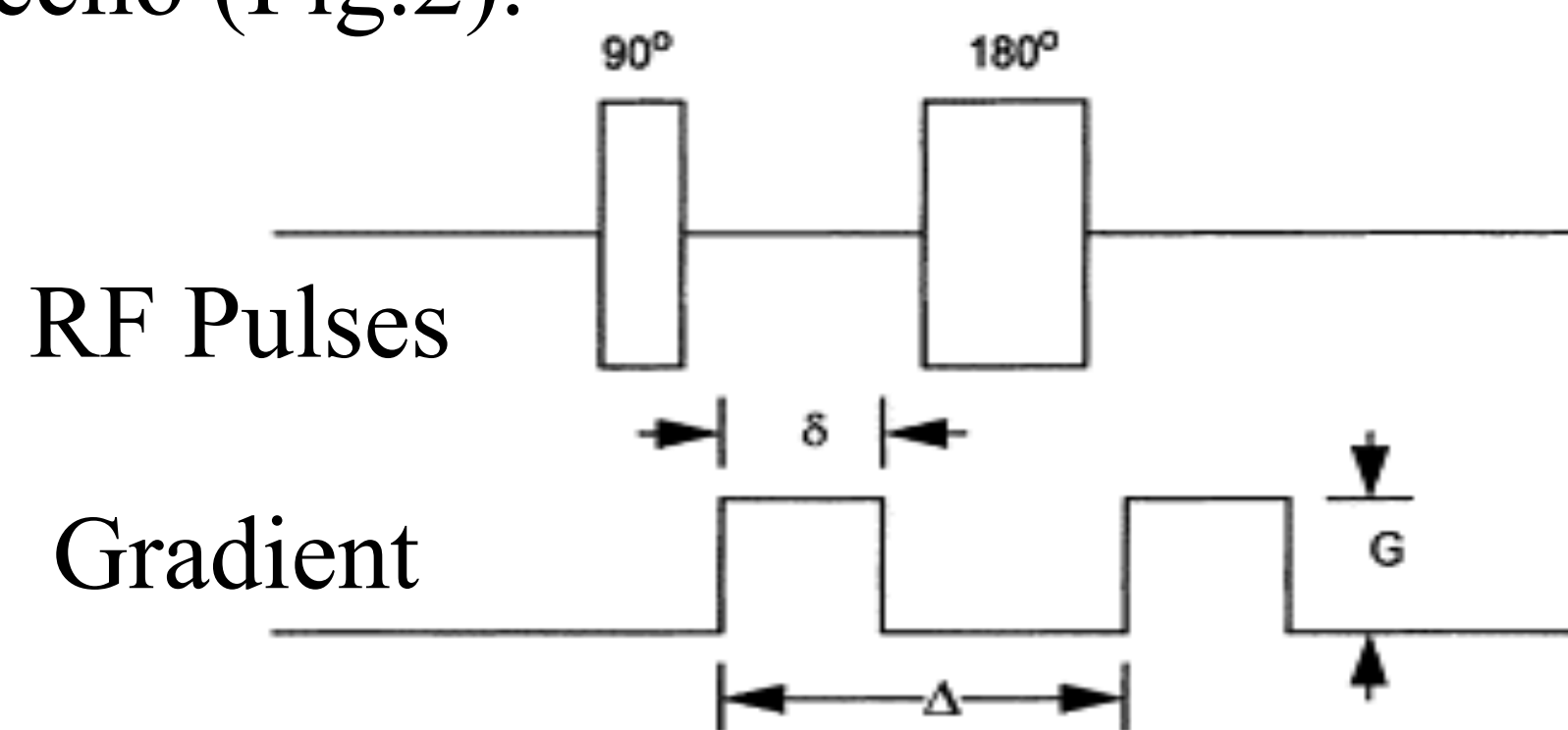
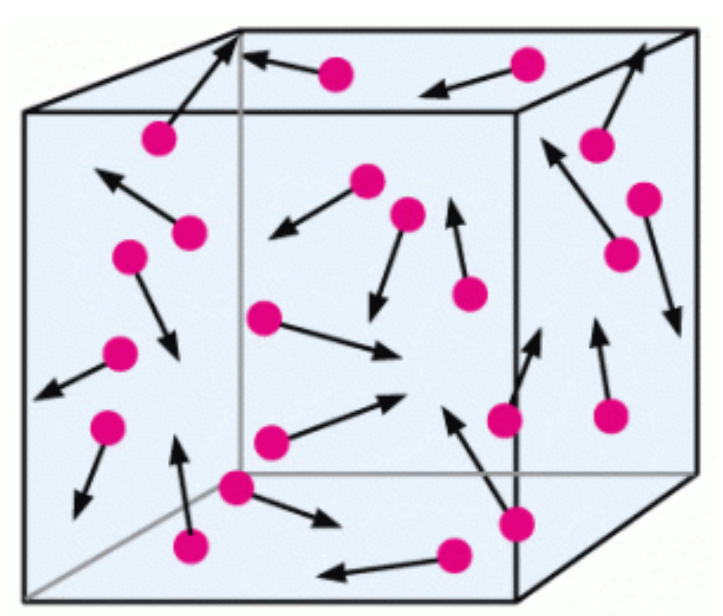


Figure 1; Self-diffusion

Figure 2; Pulse gradient spin echo

$$D = \frac{kT}{6\pi\eta R}$$

Eq.1; Stokes-Einstein Equation,

$$I = I_0 \exp\left[-D\gamma^2 G^2 \delta^2 \left(\Delta - \frac{\delta}{3}\right)\right]$$

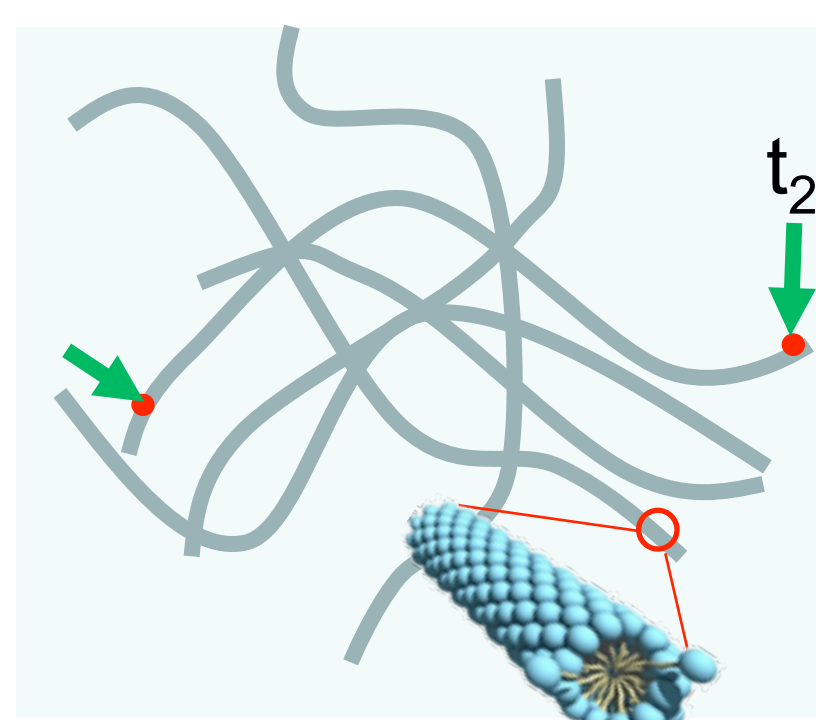
Eq. 2; Stejskal Tanner Equation

RESTRICTED DIFFUSION IN LIVING POLYMERS

$$E(q) = \frac{2(1 - \cos(2\pi qa))}{(2\pi qa)^2} + 4(2\pi qa)^2 \sum_{n=1}^{\infty} \exp\left(-\frac{n^2 \pi^2 D \Delta}{a^2}\right) X \frac{1 - (-1)^n \cos(2\pi qa)}{((-2\pi qa)^2 - (n\pi)^2)^2}$$

$$E(q) = \frac{2(1 - \cos(2\pi qa))}{(2\pi qa)^2} \quad \Delta \gg \frac{a^2}{2D}$$

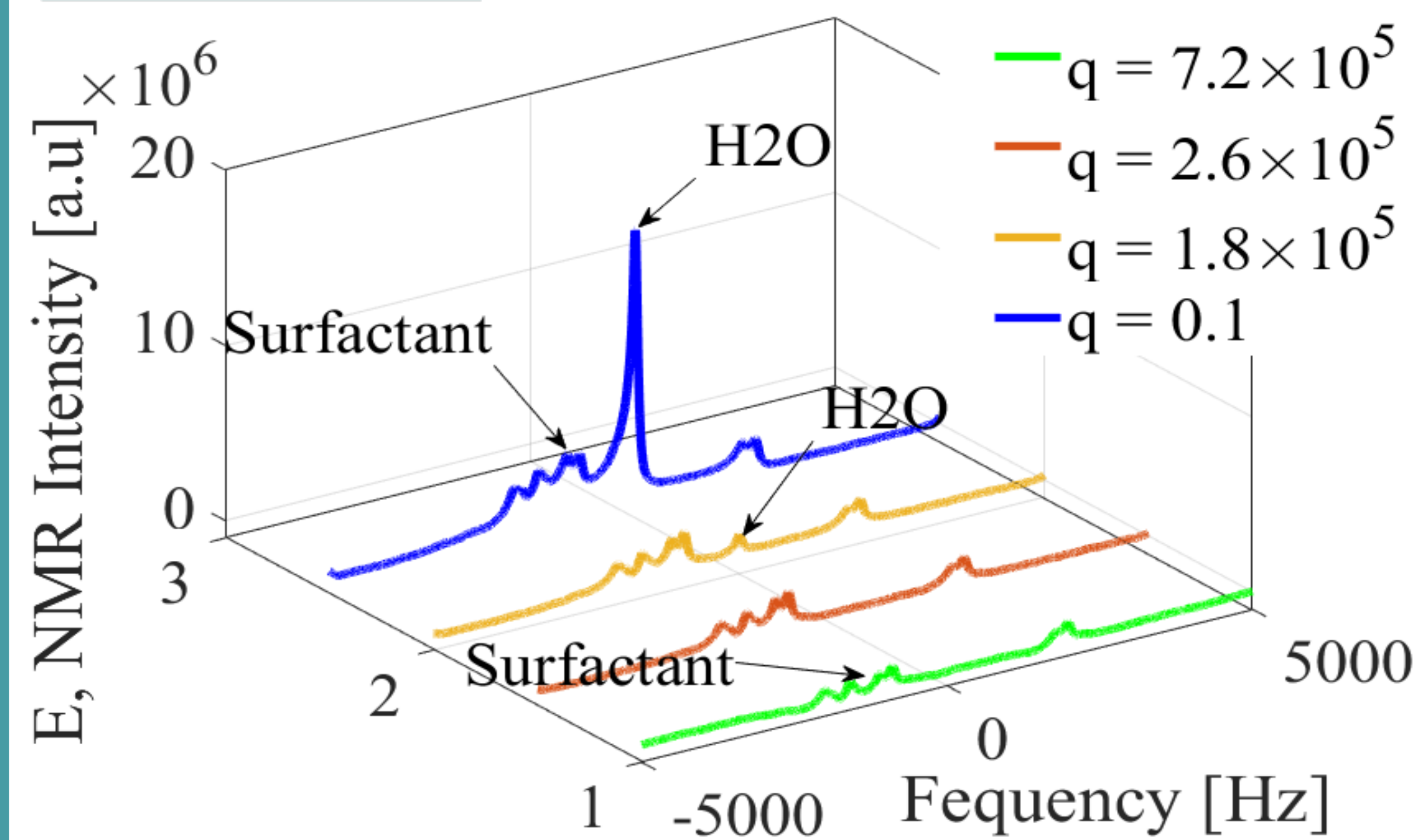
$$E(q) = e^{(-4\pi^2 q^2 D \Delta)} \quad \Delta \ll \frac{a^2}{2D}$$



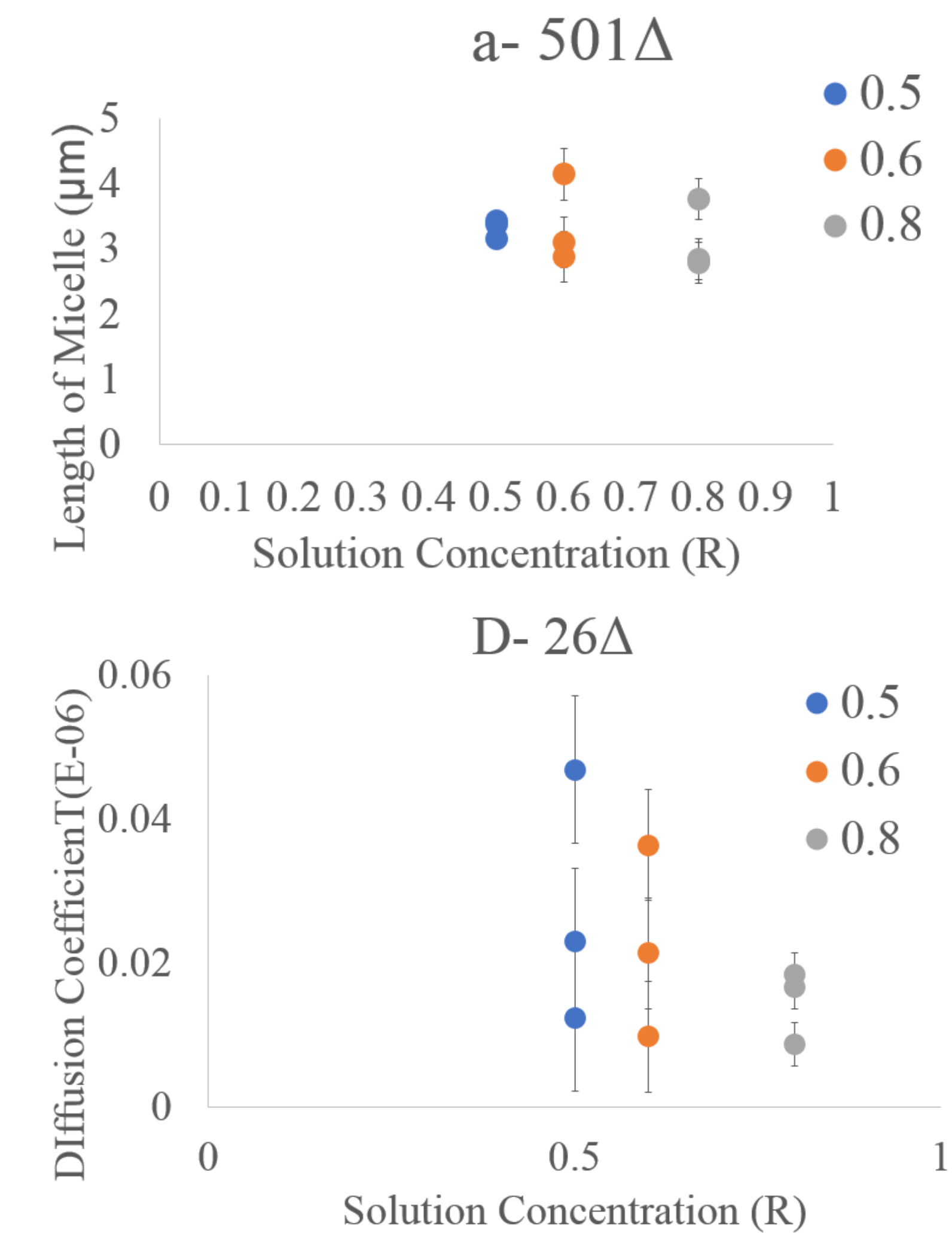
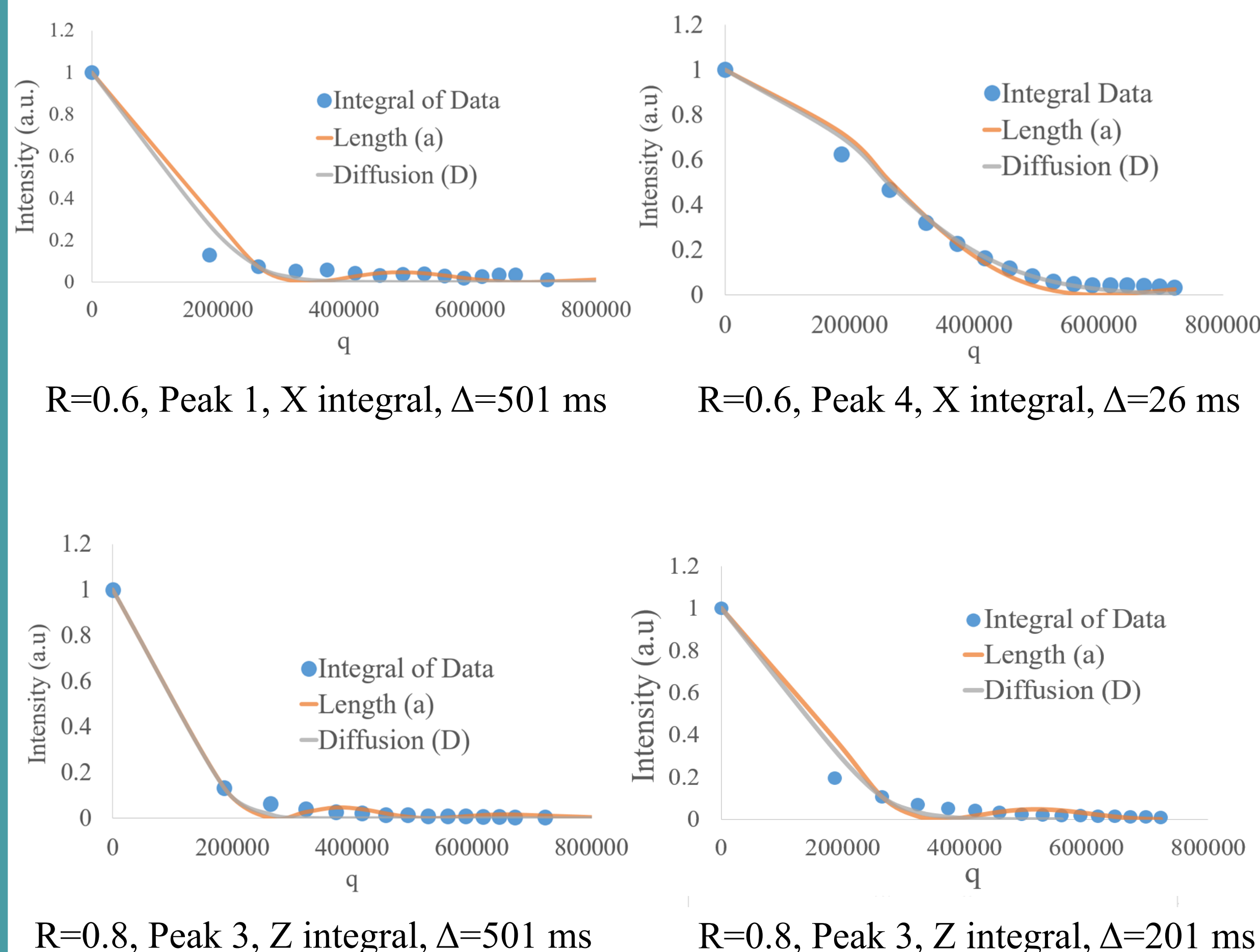
MATERIALS

The solutions used for the experiments are comprised of cetylpyridinium chloride(CPCI) and sodium salicylate (NaSal) in deuterium oxide (D2O). The molar concentration of CPCI was held constant at 100mM, while the NaSal varied from 50mM to 80 mM to make concentration ratios as R=0.5-0.8 ([NaSal]/[CPCI])

RESULTS



ANALYSIS



CONCLUSION

- 1- The diffusion coefficient of surfactants is much lower than the diffusion coefficient of molecules indicating the restricted self-diffusion.
- 2- Microstructure of the wormlike micelles in a living polymer, including their average length, can be characterized using NMR.

REFERENCES

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