UNIVERSITY OF CHEMISTRY AND TECHNOLOGY PRAGUE

Peptide Elongation in Carbon Nanotubes: An Atomistic Approach

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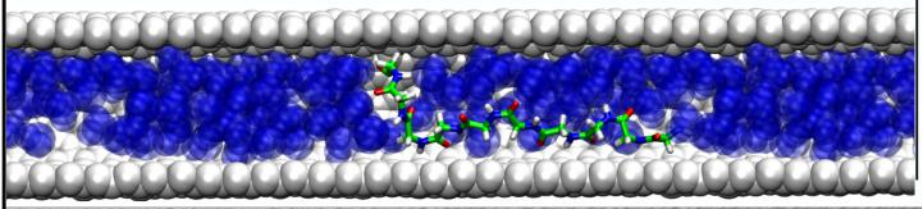
Introduction

What we study:

In the beginning of their existence and at their end, proteins are found in confined spaces. When in such environments, proteins behave differently than the free peptide, adopting disordered states, even proteins with a proper structure. By using a carbon nanotube (CNT) as a confined space environment, it is possible to study the process of protein elongation in such spaces.



Why we study it:

We aim to better understand the mechanics behind protein elongation in confined spaces.

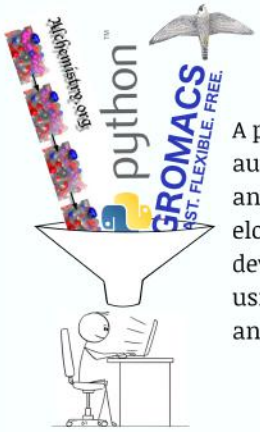
Some specific questions:

- How do proteins move through such confined spaces?

- What molecular interactions are relevant in such ensembles, inter or intramolecular?

Methods and Results

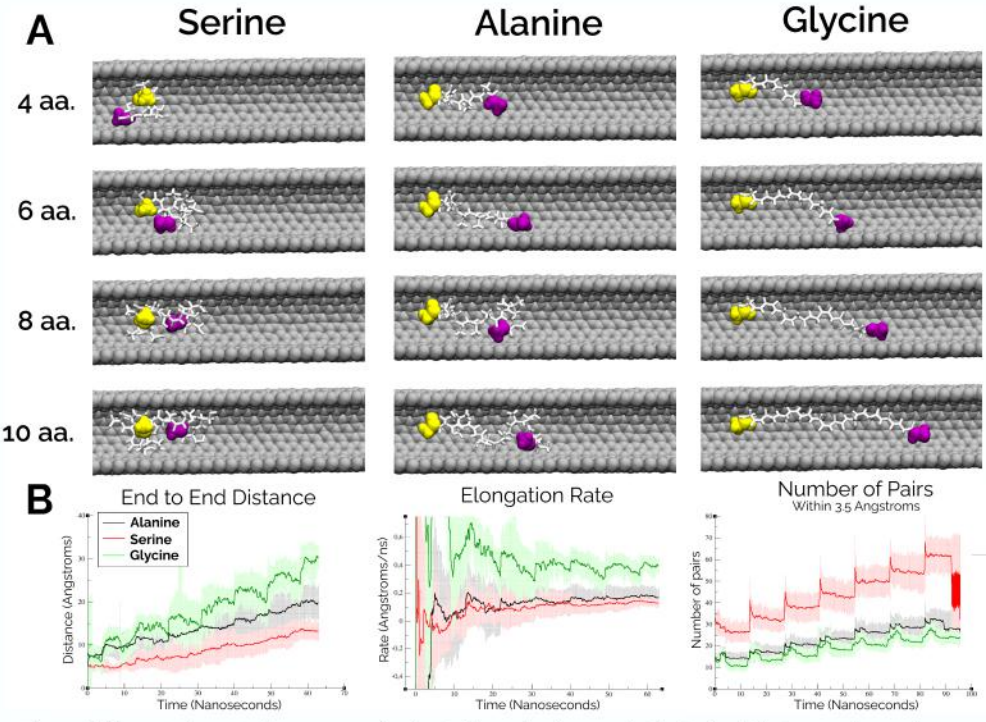
How we study it:



A pipeline for automated simulation and analysis of the elogation process was developed in Python using **Gromacs 2018.8** and **MDAnalysis**.

Each elongation started with 3 amino acids (aa) and finished with **10 aa**. Each added aa was simulated for **10 ns** (totalling **70 ns per elongation**), and each sequence had **12 elongation runs**. The CNT was treated as a **periodic molecule**. Using **amberRibo** with a **tip3p** water model, a **NVT** ensemble was used during the production runs with a **310 K** temperature.

What we learned:



A: Three different elongated sequences (Poly-Serine, Alanine, and Glycine) with the uncharged caps (Yellow: ACE, Purple: NME). B: Average properties from 12 replicates of each sequence. Dotted areas represent the standard deviation.

Take-home message

More intramolecular interactions lead to slower elongation rates and, therefore, to a slower progression of the peptide through the CNT.

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