# Supporting Informations for Detection of post-translational modification in a peptide with single-amino acid resolution using a graphyne nanopore: findings from molecular dynamics simulations

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## I. IONIC CURRENT ANALYSIS AT DIFFERENT BIAS VOLTAGES

In addition to the 3.0 and 4.0 V bias voltage results presented in the main text, we performed similar calculations for other bias voltages to provide a comprehensive understanding of how the ionic current varies under different conditions. Using the same ion trajectories extracted from molecular dynamics simulations, we calculated the ionic current as described in Equation 1. The outcomes for various amino acids positioned at the nanopore were obtained and analyzed.

The results, depicted in Supplementary Figures S1-S4, reveal distinct patterns in both the average ionic current and its fluctuations for each amino acid under varying bias conditions. These differences highlight the ionic current's sensitivity to the specific amino acid at the pore and the applied bias voltage.

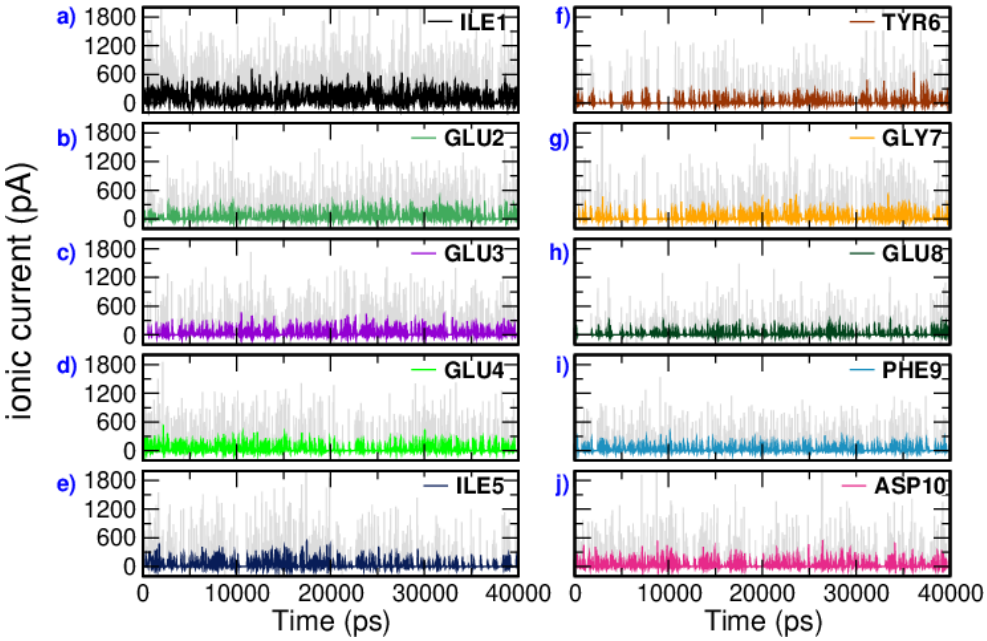


**FIG. S1.** Raw (gray) and LPF occupied-pore currents for simulations with various amino acids positioned at the center of the nanopore, computed based on ion trajectories for IEEEIYGEFD peptide at a bias voltage of 1.0 V.

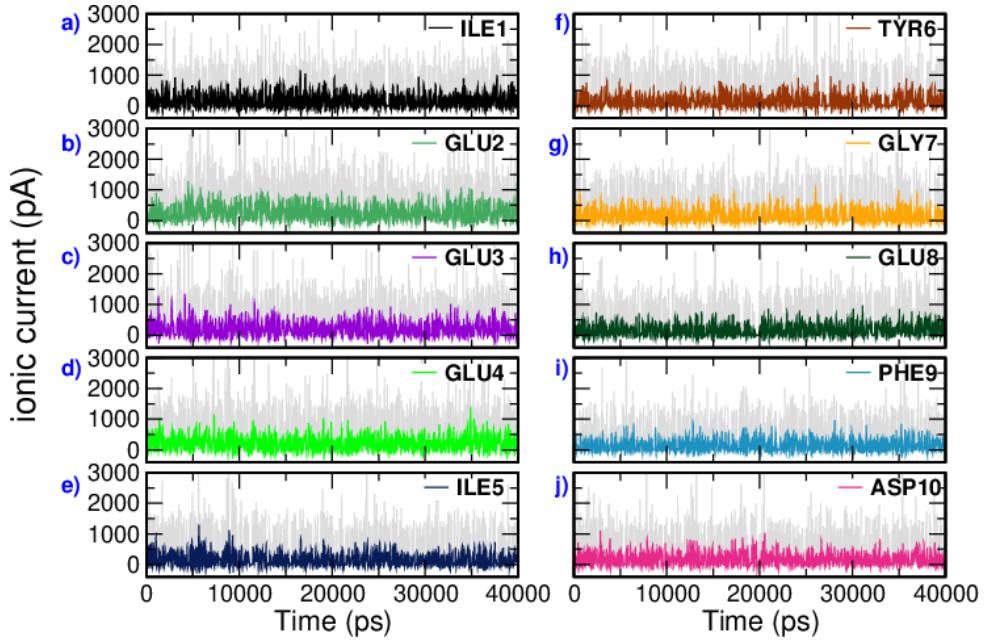


**FIG. S2.** Raw (gray) and LPF occupied-pore currents for simulations with various amino acids positioned at the center of the nanopore, computed based on ion trajectories for IEEEIYGEFD peptide at a bias voltage of 2.0 V.

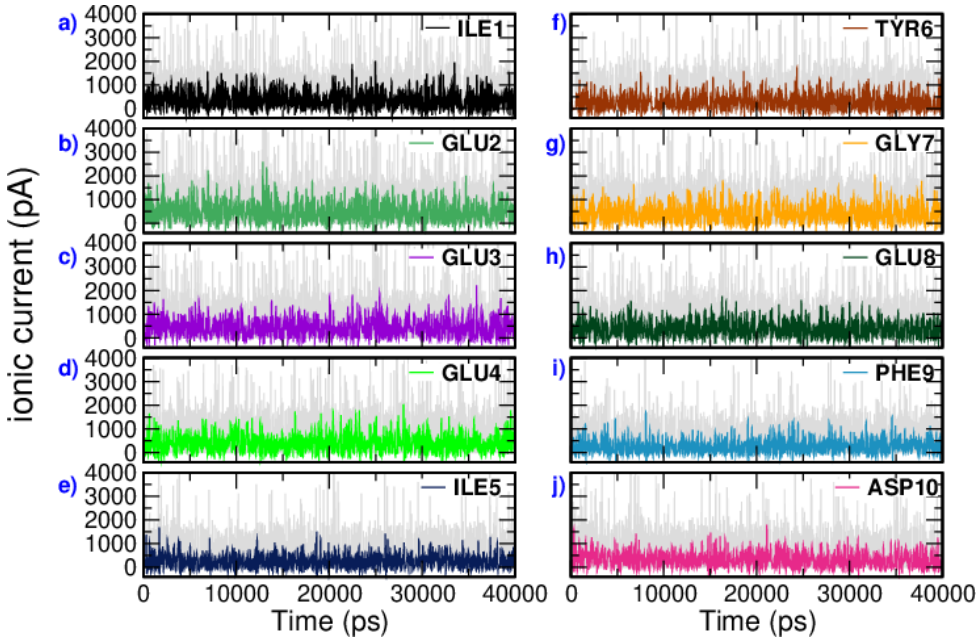


**FIG. S3.** Raw (gray) and LPF occupied-pore currents for simulations with various amino acids positioned at the center of the nanopore, computed based on ion trajectories for IEEEIYGEFD peptide at a bias voltage of 3.0 V.

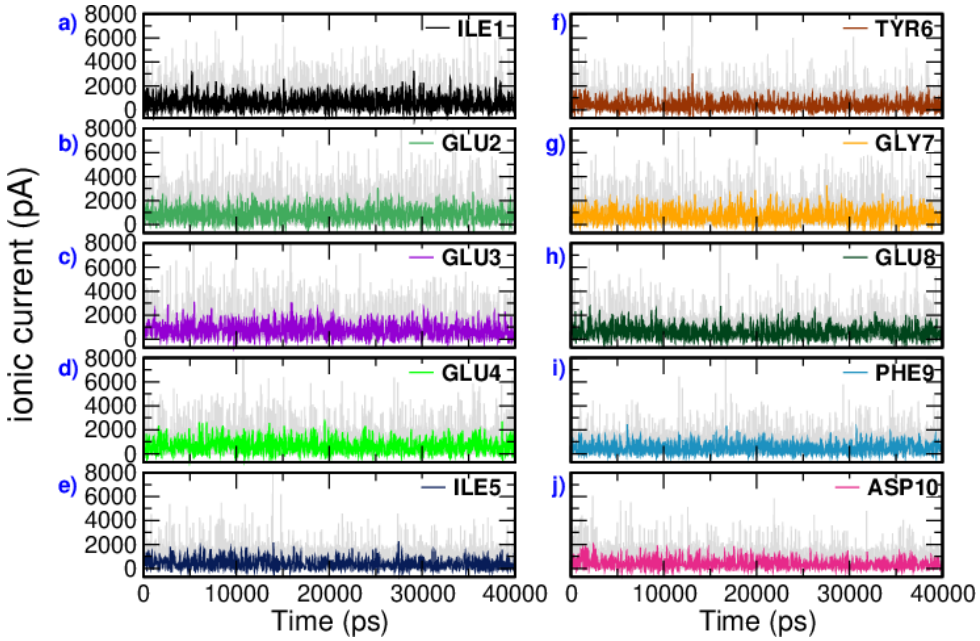


**FIG. S4.** Raw (gray) and LPF occupied-pore currents for simulations with various amino acids positioned at the center of the nanopore, computed based on ion trajectories for IEEEIYGEFD peptide at a bias voltage of 4.0 V.

## II. AMINO ACID POSITIONS

**TABLE S1.** The initial position of each amino acid's center of mass from IEEEIYGEFD sequencing during the blocked pore ionic current simulation. The positions are in units of nm.

| Amino | Position 1 | Position 2 | Position 3 | Position 4 |
|---|---|---|---|---|
| **ILE1** | 4.01 | 4.10 | 4.04 | 4.13 |
| **GLU2** | 4.14 | 4.04 | 4.09 | 4.18 |
| **GLU3** | 4.08 | 4.13 | 4.10 | 4.06 |
| **GLU4** | 4.10 | 4.04 | 4.12 | 4.06 |
| **ILE5** | 4.09 | 4.01 | 4.05 | 4.14 |
| **TYR** | 4.06 | 3.97 | 4.01 | 4.15 |
| **GLY** | 4.10 | 4.06 | 4.08 | 4.15 |
| **GLU8** | 4.13 | 4.05 | 4.06 | 4.11 |
| **PHE** | 4.09 | 3.97 | 4.03 | 4.15 |
| **ASP10** | 4.07 | 4.12 | 4.03 | 4.10 |

**TABLE S2.** The initial position of each amino acid's center of mass from IEEEIpYGEFD sequencing during the blocked pore ionic current simulation. The positions are in units of nm.

| Amino | Position 1 | Position 2 | Position | Positon4 |
|---|---|---|---|---|
| **ILE1** | 4.10 | 4.15 | 4.04 | 4.07 |
| **GLU2** | 4.08 | 4.11 | 4.23 | 4.15 |
| **GLU3** | 4.18 | 4.17 | 4.02 | 4.09 |
| **GLU4** | 4.16 | 4.09 | 4.04 | 4.17 |
| **ILE5** | 4.13 | 4.20 | 4.05 | 4.09 |
| **TYR** | 4.09 | 4.25 | 4.04 | 4.16 |
| **GLY** | 4.16 | 4.22 | 4.07 | 4.09 |
| **GLU8** | 4.09 | 4.22 | 4.05 | 4.15 |
| **PHE** | 4.13 | 4.17 | 4.06 | 4.10 |
| **ASP10** | 4.11 | 4.17 | 4.04 | 4.54 |

## III. PORE AREA CALCULATION

The accessible area of the bare pore was assessed by considering the Van der Waals radius of atoms surrounding the pore area. Subsequently, this area was determined by processing the image with a MATLAB code, with the resulting value taken as a reference ($A_{bare}$). The final snapshot of each voltage drop simulation was captured, and the XY-plane view was generated by considering only the atoms within a distance of 1 nm from the graphyne sheet.

The accessible area, denoted as $A_{\text{acess}}$, was computed, and the normalized area $A_n$ was introduced, defined as $A_n = \frac{A_{\text{acess}}}{A_{\text{bare}}}$. Given that the amino acid extremities are fixed, we only considered the final snapshot.