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Mining Nanopore Big Data to Reveal the Single Entity Heterogeneity

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Abstract:

The recent development of nanopore techniques pushes the envelope in precision and complexity to maximize the information content. However, uncovering the interaction and kinetics of single molecules acquires statistical datasets by thousands of single molecule information.[1-2] The challenge still exists from effectively grouping the time-dependent ionic current trace into subpopulations. In this study, we applied the modified Hidden Markov Model to identify the ionic blockage merging inside current noise, which increase the temporal resolution and current resolution for nanopore techniques.[3-4] Then, we traced the multi-level current variations inside a blockade event by using Markov Chain Model, which reveals the dynamic kinetics for the conversion of multi-intermediates during the folding/unfolding pathways of a biomolecule.[5] Since the ions migrate at different frequency inside nanopore, it acts as the smallest sensor to perceive and feedback the non-covalent interaction into the of ionic current frequency. We further employed Hilbert-Huang transform (HHT) to uncover these varied ionic frequencies which buried in the noise of the ionic current traces.[6] The HHT-based frequency analysis arises a two-dimension signal from time domain (time and current) into a three-dimension spectrum of energy-frequency-time distribution. The frequency-energy spectrum represents the fingerprint spectra for the characterization of non-covalent interaction due to the interaction between residues inside nanopore and the analyte. The very beginning frequency analysis let us mine more information from the data, which could help to unravel different hierarchical pathways and enables to discovery the subpopulations and hidden kinetic during the dynamic motion of single peptides.



References

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主催： 東京大学大学院工学系研究科専攻間横断型教育プログラム 機械システム・イノベーション (GMSI)
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