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第 25 回 葉山セミナー / The 25th Hayama Seminar

2025. Dec. 3rd (13:00 – 14:30) (at: Room 310, Hybrid Style)

AI and machine learning for proteomics: Orthurus and Anubis enable improved metaproteomics discovery and protein authentication

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Abstract:

AI and machine learning have emerged as transformative tools for proteomics sequencing, biomarker discovery, and therapeutic modelling. Here I introduce two bioinformatics pipelines for species identification in metaproteomics and the chemistry-augmented authentication of ancient proteins. Firstly, Orthurus is a two-pronged, hybrid sequencing workflow combining *de novo* sequencing without reference databases and conventional database searching. Benchmarked against established search engines including PEAKS and MaxQuant, Orthurus demonstrates increased proteome coverage and improved taxonomic resolution for one million, mixed coprolite data. Secondly, Anubis leverages a random forest classifier trained on a wide range of physico-chemical and mass spectrometry-based features. Using a combination of ancient and experimentally degraded milk data, Anubis distinguishes a putative ancient dairy protein from potential contaminants based on position-specific deamidation rates and clusters of relative deamidation patterns. Together, Orthurus and Anubis illustrate how AI and machine learning can empower the analysis of challenging metaproteomics and palaeoproteomics data.

(Host: Asst. Prof. Tsutaya)