A Flexible Learning Infrastructure for Proteomics

Christopher S Wilkins1, Justice Sefas1, Avrett Bilbao1, Richard D Smith1, Lijjana Pasa-Tolic2, Samuel H Payne1, Jared B Shaw2

1Biological Sciences Division, Pacific Northwest National Laboratory, 2Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory

Overview

- FLIP is a modular computational framework for developing and optimizing tandem mass spectrometry (MS/MS) scoring models.
- FLIP enables rapid optimization for new MS/MS methods and experimental conditions that change fragmentation properties.
- Designed to be reused and expanded for integration with new MS/MS identification software.

Methods

Introduction

The development of new MS/MS technologies is driven by the necessity to achieve more complete and confident peptide/protein characterization in proteomics experiments.1

- Mechanisms of fragmentation and the resulting product ion types vary greatly between MS/MS methods.
- Additionally, experimental conditions, such as the presence of TMT/TRAQ, can significantly change MS/MS fragmentation properties.
- Development of MS/MS scoring models has typically been considered part of the software development process and is rarely a user customizable component of peptide identification tools.
- Scoring models are usually hard-coded, hindered optimization and adaptation to new MS/MS methods.
- FLIP’s modular software architecture enables rapid learning and validation of scoring models for MS/MS methods.
- FLIP is trained for new fragment types (UVPD) on both top down and bottom up data.

Results

Our goal was to create a flexible framework capable of adapting to many types of proteomics data. Here we use FLIP to train scoring models for top-down and bottom-up proteomics experiments utilizing UVPD and HCD.

Conclusions

- FLIP is a universal tool for creating scoring models for many types of MS/MS spectra.
- FLIP allows developers to quickly adapt their informatics tools to data with new experimental conditions and fragmentation properties.
- FLIP does not require the user to manually determine fragment ions for training.
- This tool is available as part of the Informed Proteomics software package on Github at http://github.com/PNNL-Comp-Mass-Spec/Informed-Proteomics

Acknowledgments

This research is part of the “High Resolution and Mass Accuracy Capability” development project at EMSL, a Department of Energy (DOE) Office of Science User Facility sponsored by the Office of Biological and Environmental Research and located at the Pacific Northwest National Laboratory (PNNL), a multi-program national laboratory operated by Battelle for the DOE under contract DE-AC05-76RL01830. This project was also supported by the Environmental Research (OBER) Pan-omics program at PNNL.

References:


Contact: Christopher Wilkins
Biological Sciences Division
Pacific Northwest National Laboratory
E-mail: christopher.wilkins@pnnl.gov

Flipping Tandem Mass Spectrometry

Overview

- FLIP is a modular, computational framework for developing and optimizing tandem mass spectrometry (MS/MS) scoring models.
- FLIP enables rapid optimization for new MS/MS methods and experimental conditions that change fragmentation properties.
- Designed to be reused and expanded for integration with new MS/MS identification software.

Methods

Introduction

The development of new MS/MS technologies is driven by the necessity to achieve more complete and confident peptide/protein characterization in proteomics experiments.1

- Mechanisms of fragmentation and the resulting product ion types vary greatly between MS/MS methods.
- Additionally, experimental conditions, such as the presence of TMT/TRAQ, can significantly change MS/MS fragmentation properties.
- Development of MS/MS scoring models has typically been considered part of the software development process and is rarely a user customizable component of peptide identification tools.
- Scoring models are usually hard-coded, hindered optimization and adaptation to new MS/MS methods.
- FLIP’s modular software architecture enables rapid learning and validation of scoring models for MS/MS methods.
- FLIP is trained for new fragment types (UVPD) on both top down and bottom up data.

Results

Our goal was to create a flexible framework capable of adapting to many types of proteomics data. Here we use FLIP to train scoring models for top-down and bottom-up proteomics experiments utilizing UVPD and HCD.

Conclusions

- FLIP is a universal tool for creating scoring models for many types of MS/MS spectra.
- FLIP allows developers to quickly adapt their informatics tools to data with new experimental conditions and fragmentation properties.
- FLIP does not require the user to manually determine fragment ions for training.
- This tool is available as part of the Informed Proteomics software package on Github at http://github.com/PNNL-Comp-Mass-Spec/Informed-Proteomics

Acknowledgments

This research is part of the “High Resolution and Mass Accuracy Capability” development project at EMSL, a Department of Energy (DOE) Office of Science User Facility sponsored by the Office of Biological and Environmental Research and located at the Pacific Northwest National Laboratory (PNNL), a multi-program national laboratory operated by Battelle for the DOE under contract DE-AC05-76RL01830. This project was also supported by the Environmental Research (OBER) Pan-omics program at PNNL.

References:


Contact: Christopher Wilkins
Biological Sciences Division
Pacific Northwest National Laboratory
E-mail: christopher.wilkins@pnnl.gov

Flipping Tandem Mass Spectrometry

Overview

- FLIP is a modular, computational framework for developing and optimizing tandem mass spectrometry (MS/MS) scoring models.
- FLIP enables rapid optimization for new MS/MS methods and experimental conditions that change fragmentation properties.
- Designed to be reused and expanded for integration with new MS/MS identification software.

Methods

Introduction

The development of new MS/MS technologies is driven by the necessity to achieve more complete and confident peptide/protein characterization in proteomics experiments.1

- Mechanisms of fragmentation and the resulting product ion types vary greatly between MS/MS methods.
- Additionally, experimental conditions, such as the presence of TMT/TRAQ, can significantly change MS/MS fragmentation properties.
- Development of MS/MS scoring models has typically been considered part of the software development process and is rarely a user customizable component of peptide identification tools.
- Scoring models are usually hard-coded, hindered optimization and adaptation to new MS/MS methods.
- FLIP’s modular software architecture enables rapid learning and validation of scoring models for MS/MS methods.
- FLIP is trained for new fragment types (UVPD) on both top down and bottom up data.

Results

Our goal was to create a flexible framework capable of adapting to many types of proteomics data. Here we use FLIP to train scoring models for top-down and bottom-up proteomics experiments utilizing UVPD and HCD.

Conclusions

- FLIP is a universal tool for creating scoring models for many types of MS/MS spectra.
- FLIP allows developers to quickly adapt their informatics tools to data with new experimental conditions and fragmentation properties.
- FLIP does not require the user to manually determine fragment ions for training.
- This tool is available as part of the Informed Proteomics software package on Github at http://github.com/PNNL-Comp-Mass-Spec/Informed-Proteomics

Acknowledgments

This research is part of the “High Resolution and Mass Accuracy Capability” development project at EMSL, a Department of Energy (DOE) Office of Science User Facility sponsored by the Office of Biological and Environmental Research and located at the Pacific Northwest National Laboratory (PNNL), a multi-program national laboratory operated by Battelle for the DOE under contract DE-AC05-76RL01830. This project was also supported by the Environmental Research (OBER) Pan-omics program at PNNL.

References:


Contact: Christopher Wilkins
Biological Sciences Division
Pacific Northwest National Laboratory
E-mail: christopher.wilkins@pnnl.gov