AI FOR COMPUTATIONAL MASS SPECTROMETRY

Wout Bittremieux — 2025/07/03

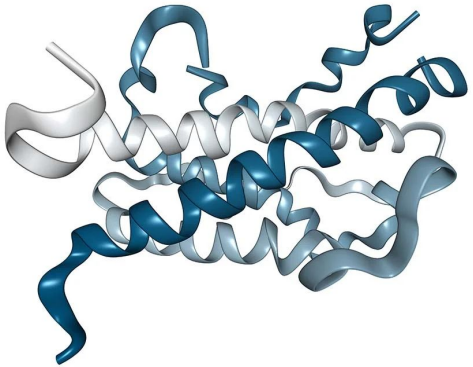
 @wout@sigmoid.social

 bittremieux.be

 wout.bittremieux@uantwerpen.be

WE STUDY THE PROTEOME AND METABOLOME

Proteomics



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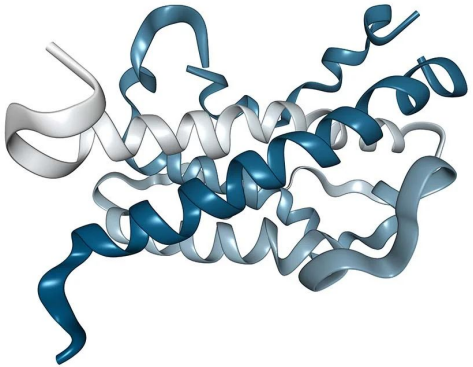
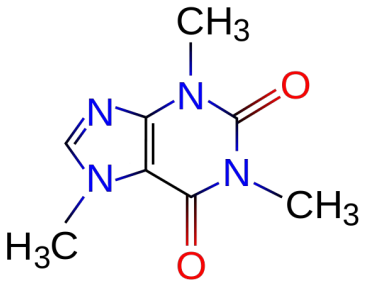
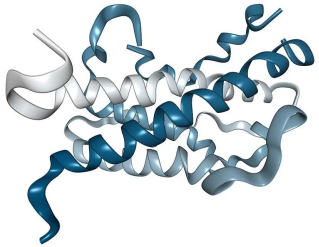
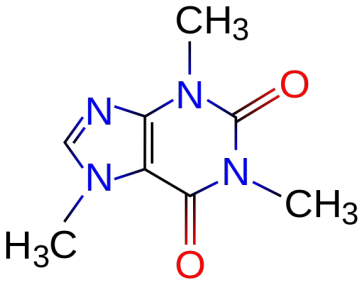


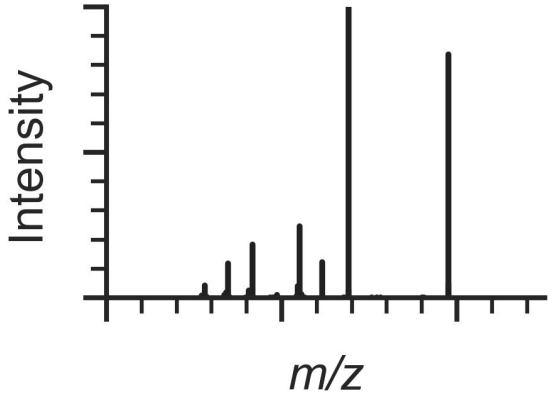
Metabolomics



MASS SPECTROMETRY FOR MOLECULAR DISCOVERY







MOLECULES ARE EVERYWHERE

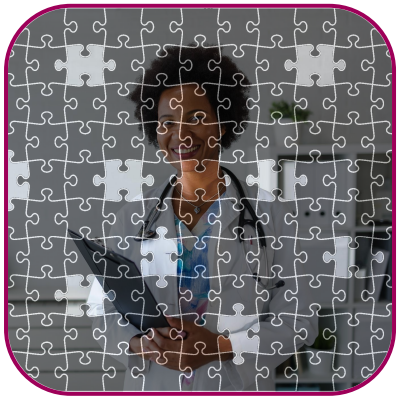
precision medicine

drug discovery

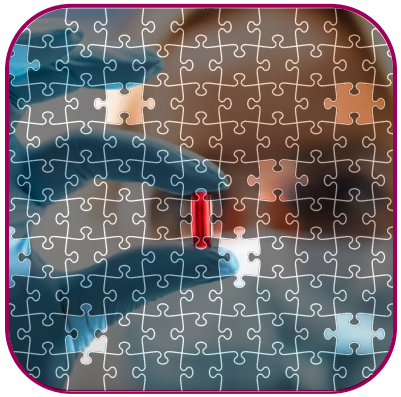
environ-mental

food science

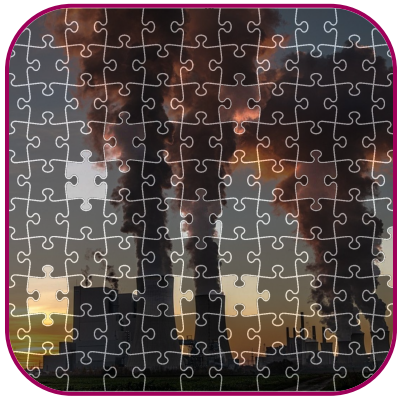
MAJORITY OF MASS SPECTRA REMAIN UNKNOWN



precision medicine



drug discovery



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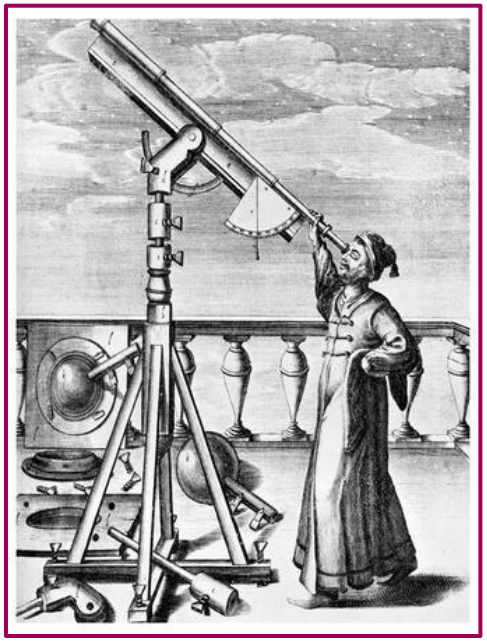
AI TO EXPLORE THE MOLECULAR UNIVERSE



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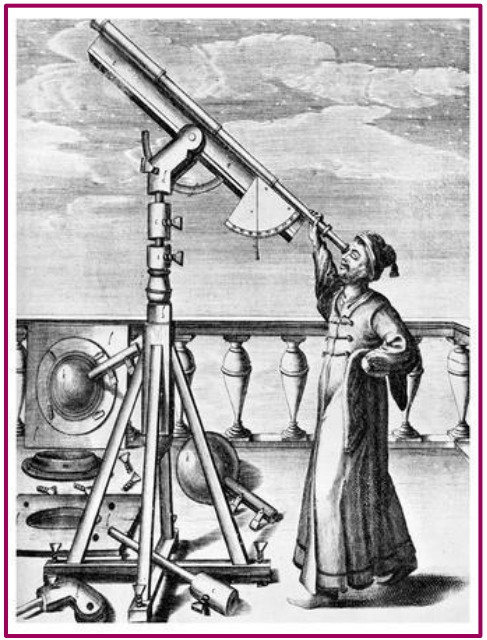

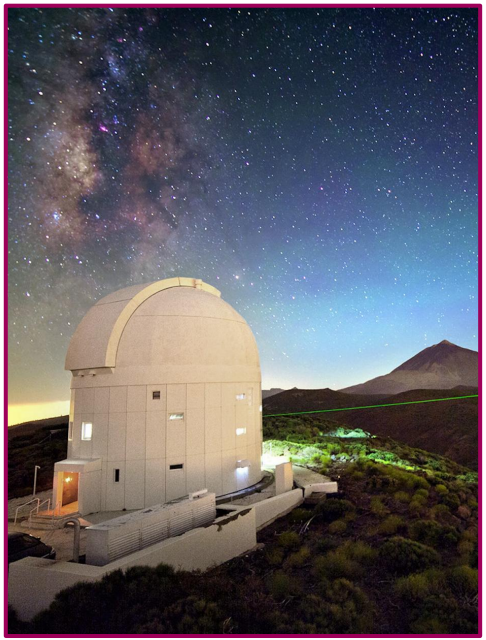

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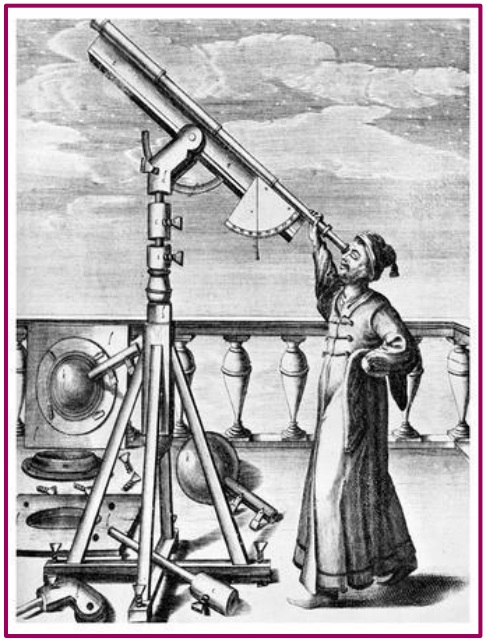
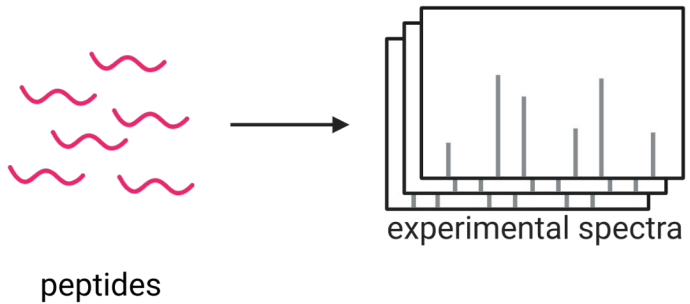


DE NOVO PEPTIDE SEQUENCING AS A TRANSLATION TASK

PEPTIDE DISCOVERY USING *DE NOVO* SEQUENCING

sequence database searching



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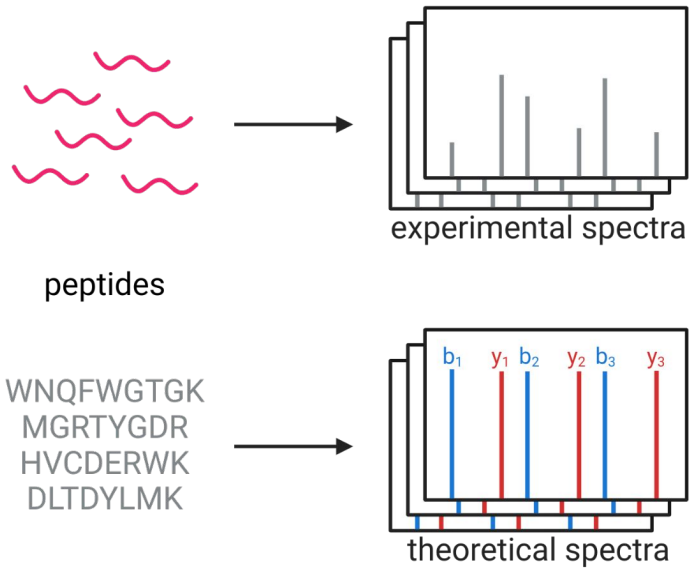

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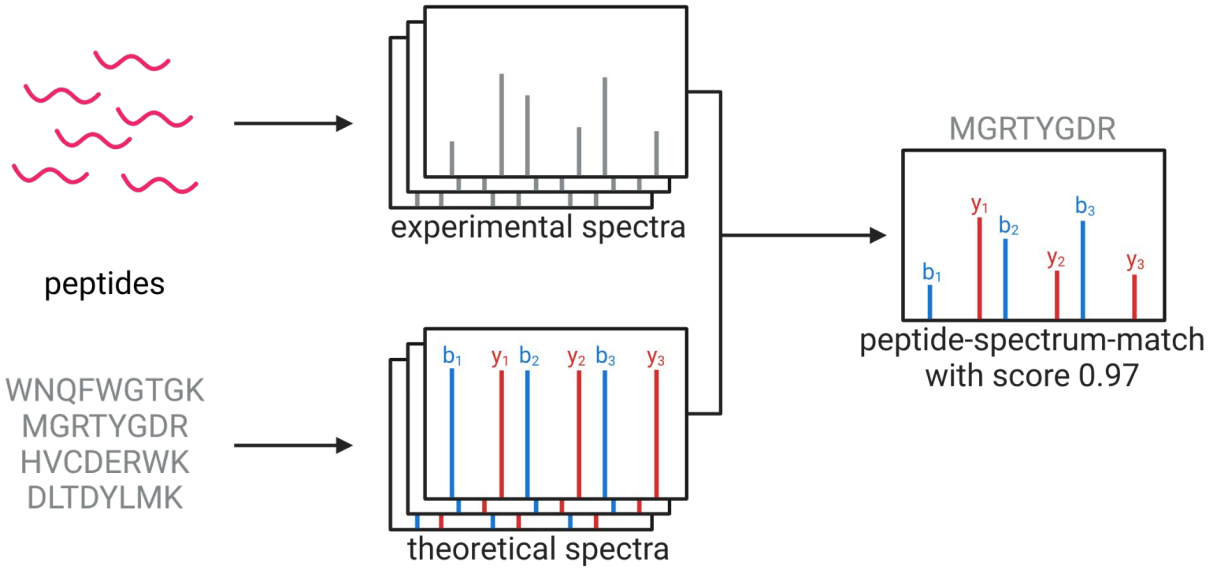

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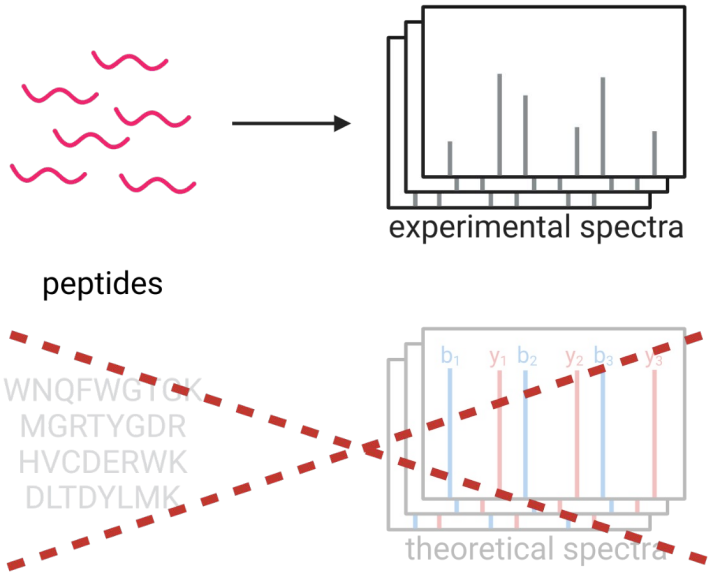
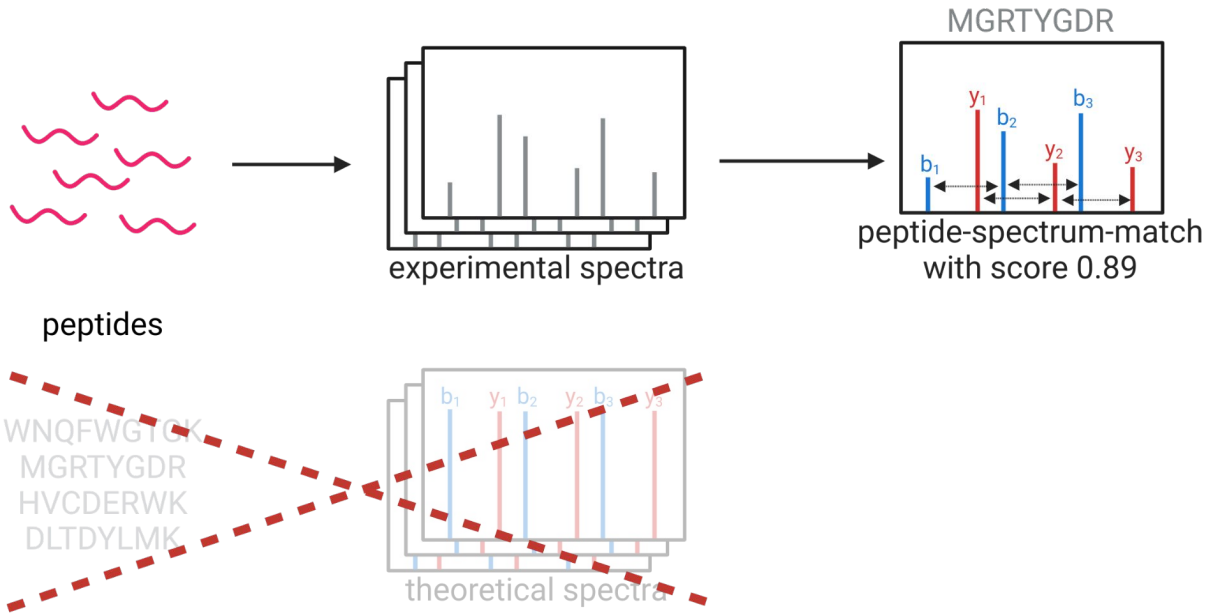
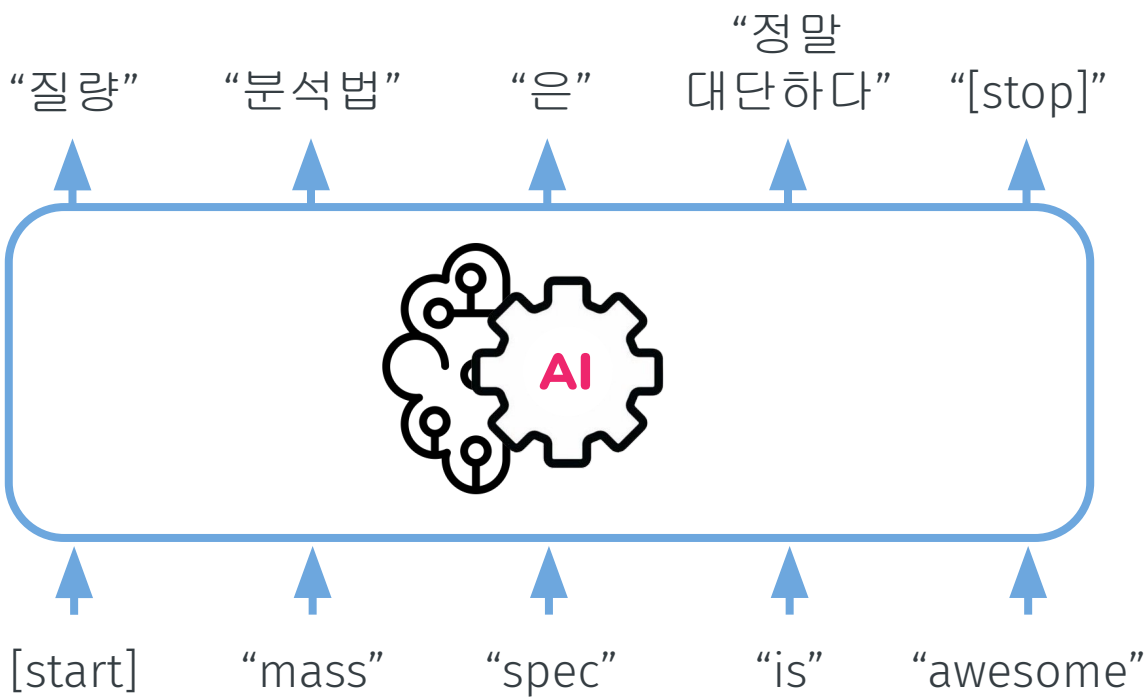


PEPTIDE DISCOVERY USING *DE NOVO* SEQUENCING

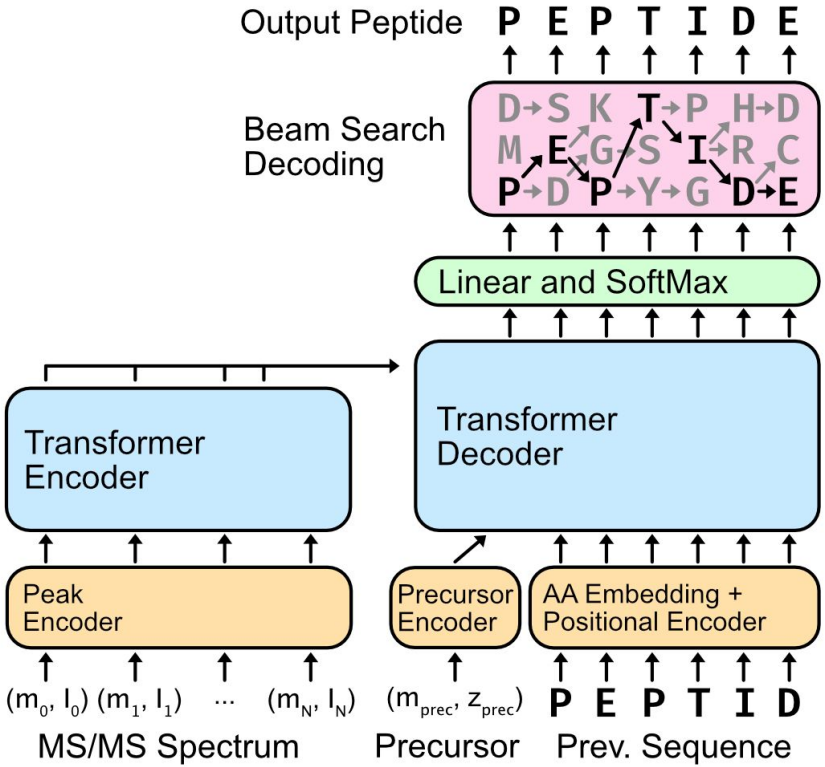
de novo peptide sequencing



PEPTIDE SEQUENCING AS A TRANSLATION PROBLEM



AI FOR *DE NOVO* PEPTIDE SEQUENCING



Yilmaz, M. *et al. Nature Communications* **15**, 6427 (2024).

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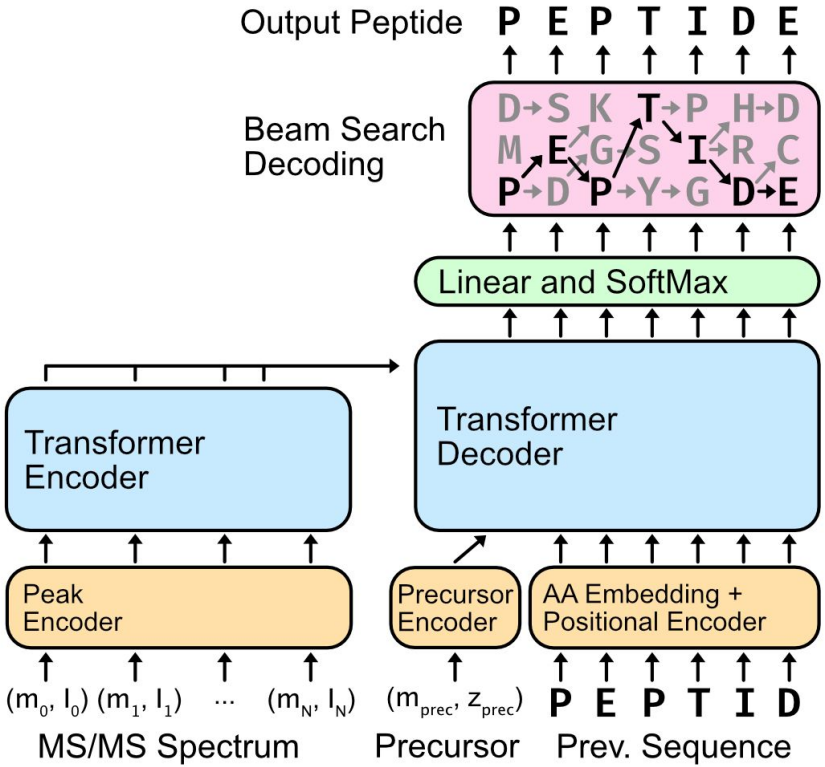

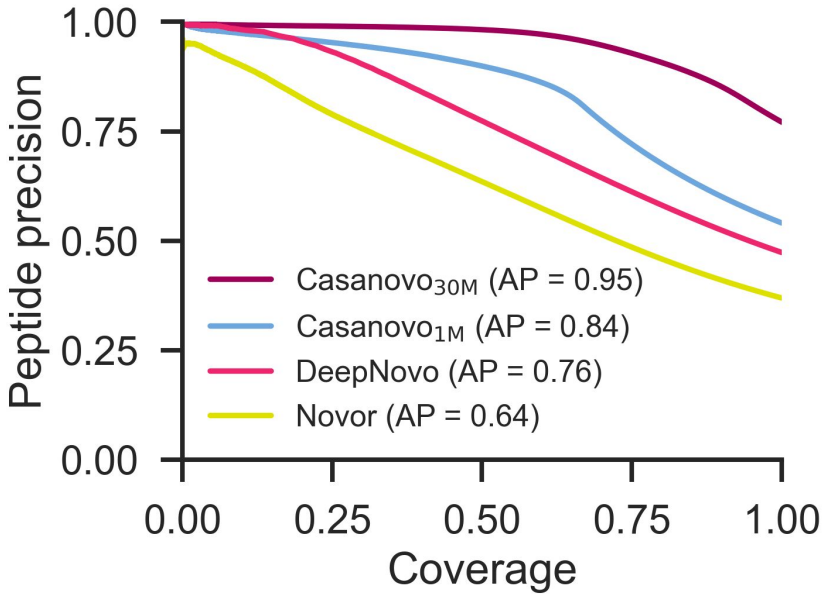

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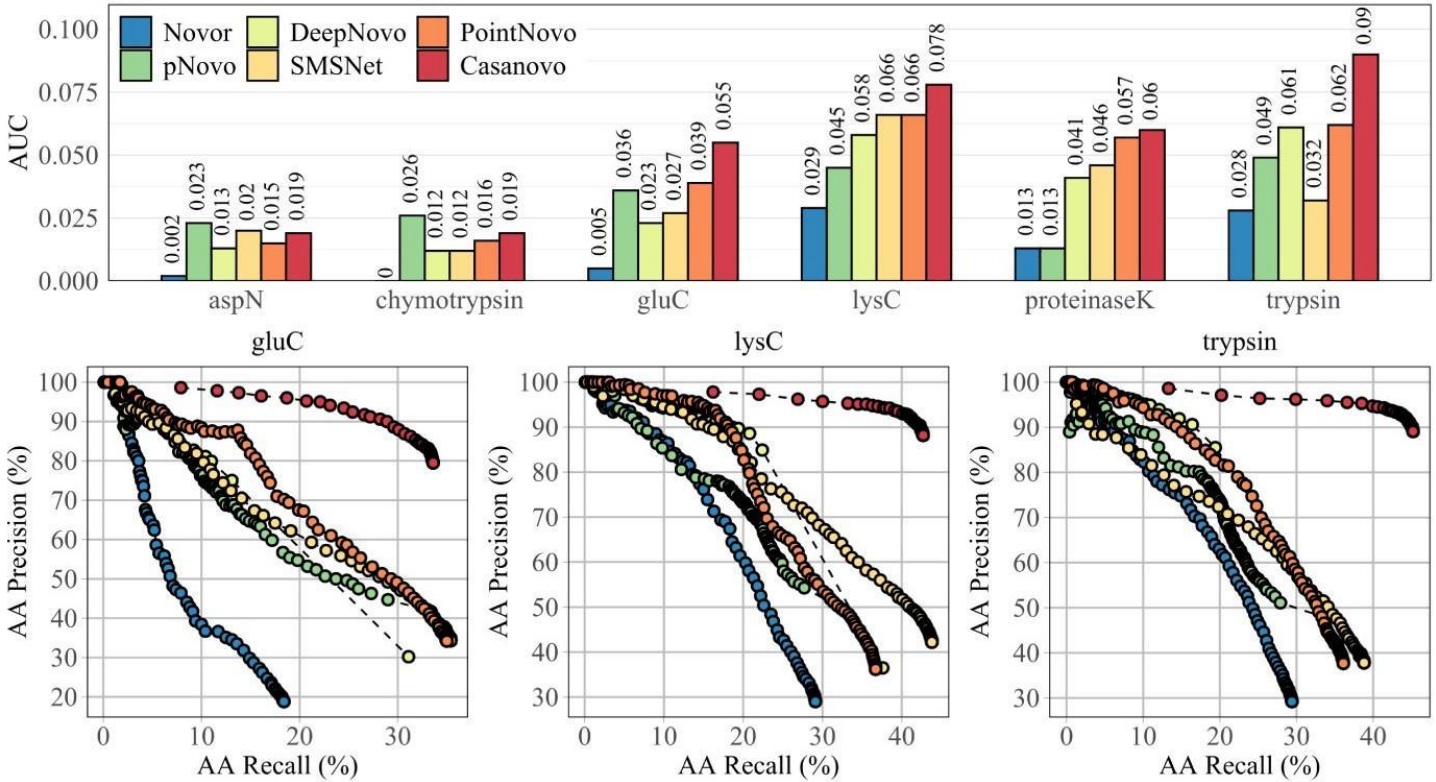
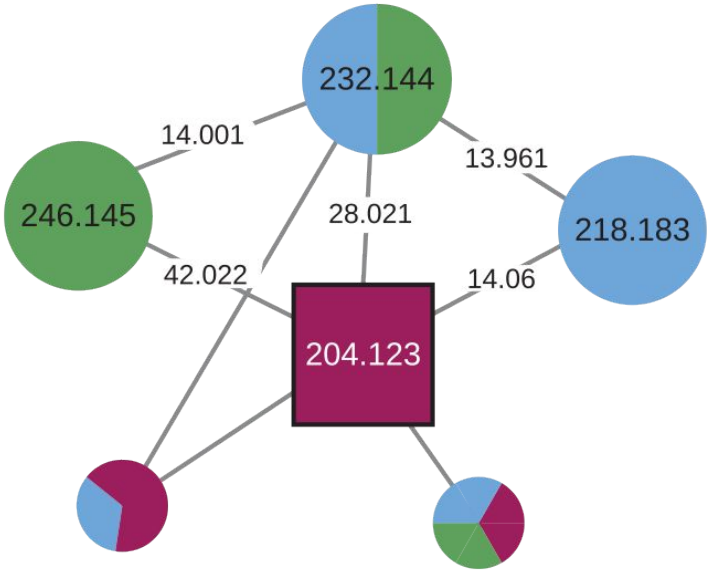
EXTERNAL EVALUATION OF ANTIBODY ASSEMBLY



Beslic, D. *et al. Briefings in Bioinformatics* **24**, bbac542 (2023).

MOLECULAR DISCOVERY FROM MILLIONS OF SMALL MOLECULE MS/MS SPECTRA

MOLECULAR NETWORKING FOR DISCOVERY



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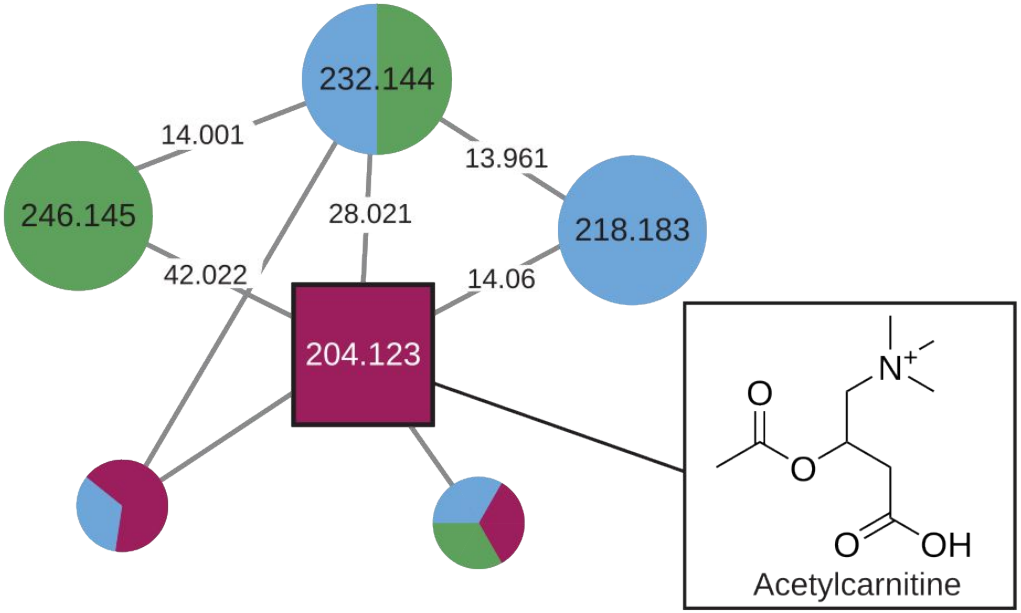

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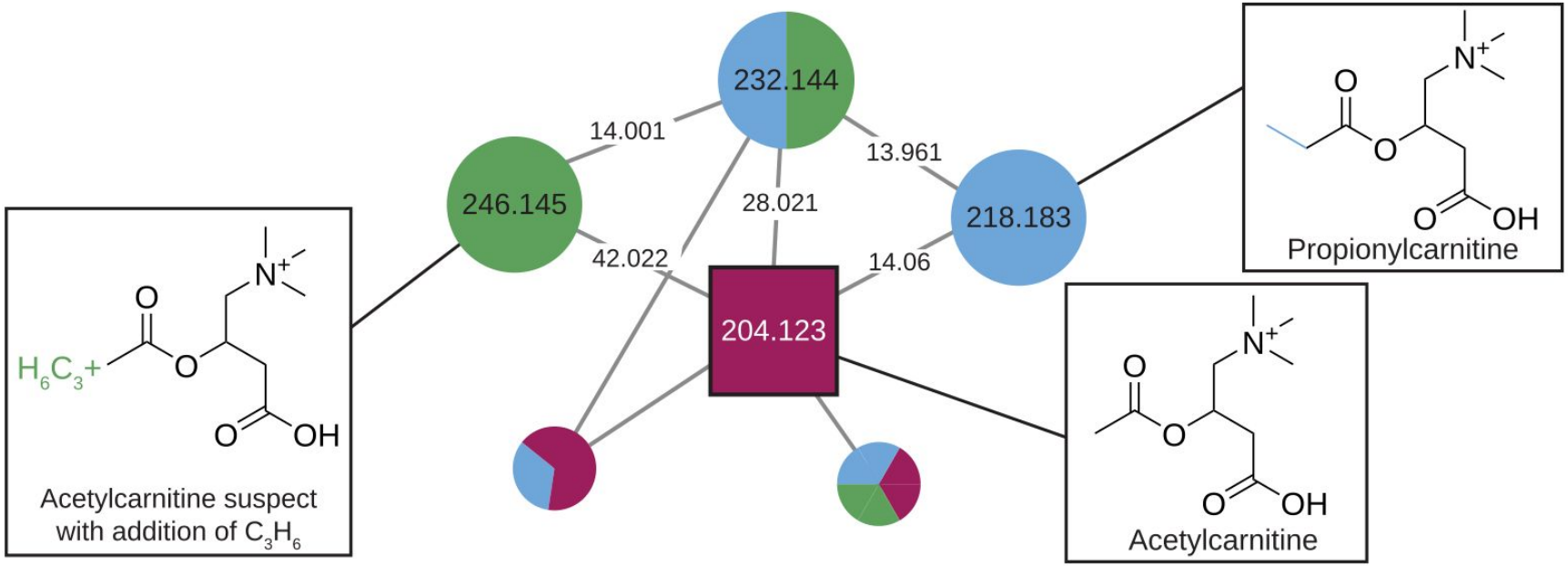
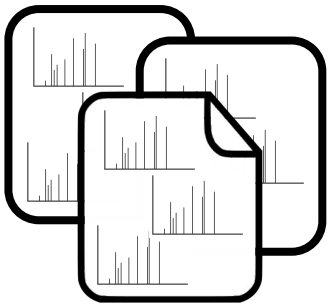


MOLECULAR NETWORKING AT REPOSITORY SCALE



1335 compatible datasets
521 million MS/MS spectra

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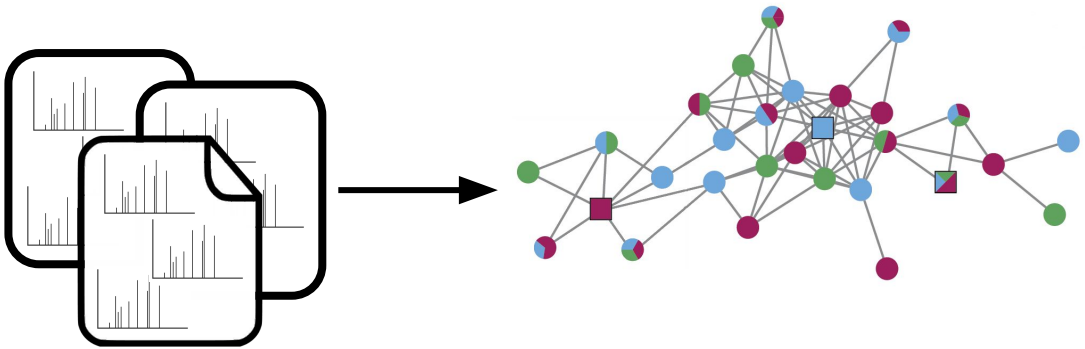

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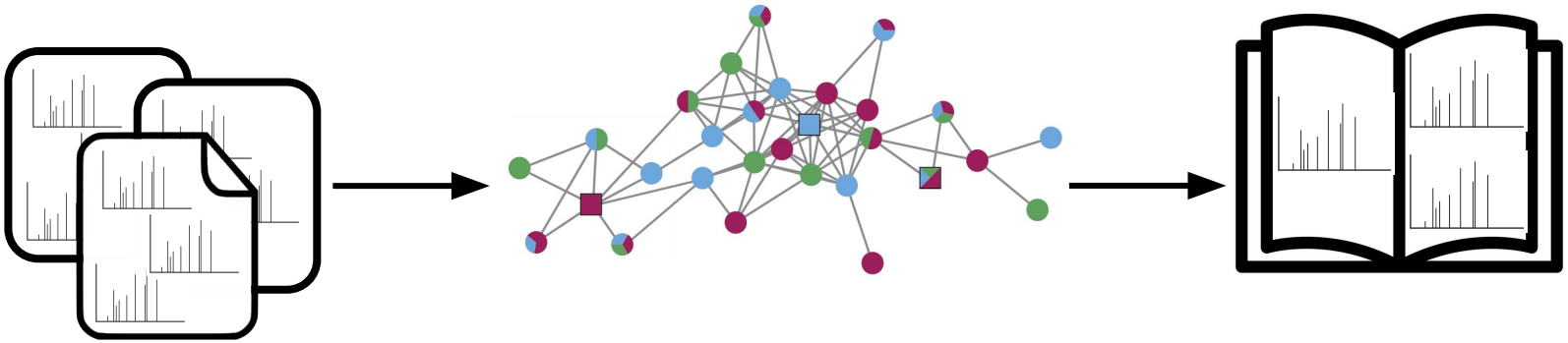

1335 compatible datasets
521 million MS/MS spectra

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13 million edges

suspect library
87,916 unique “suspects”
1350 modifications

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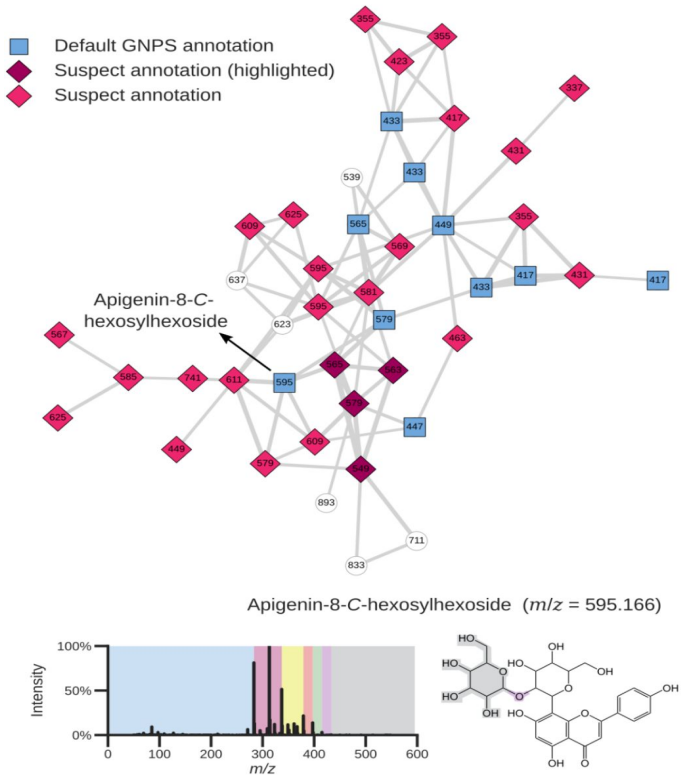
SUSPECTS ANNOTATE NOVEL COMPOUNDS



Data from the Korean Pharmacopeia. Interpretation by Kyo Bin Kang (Sookmyung Women's University).
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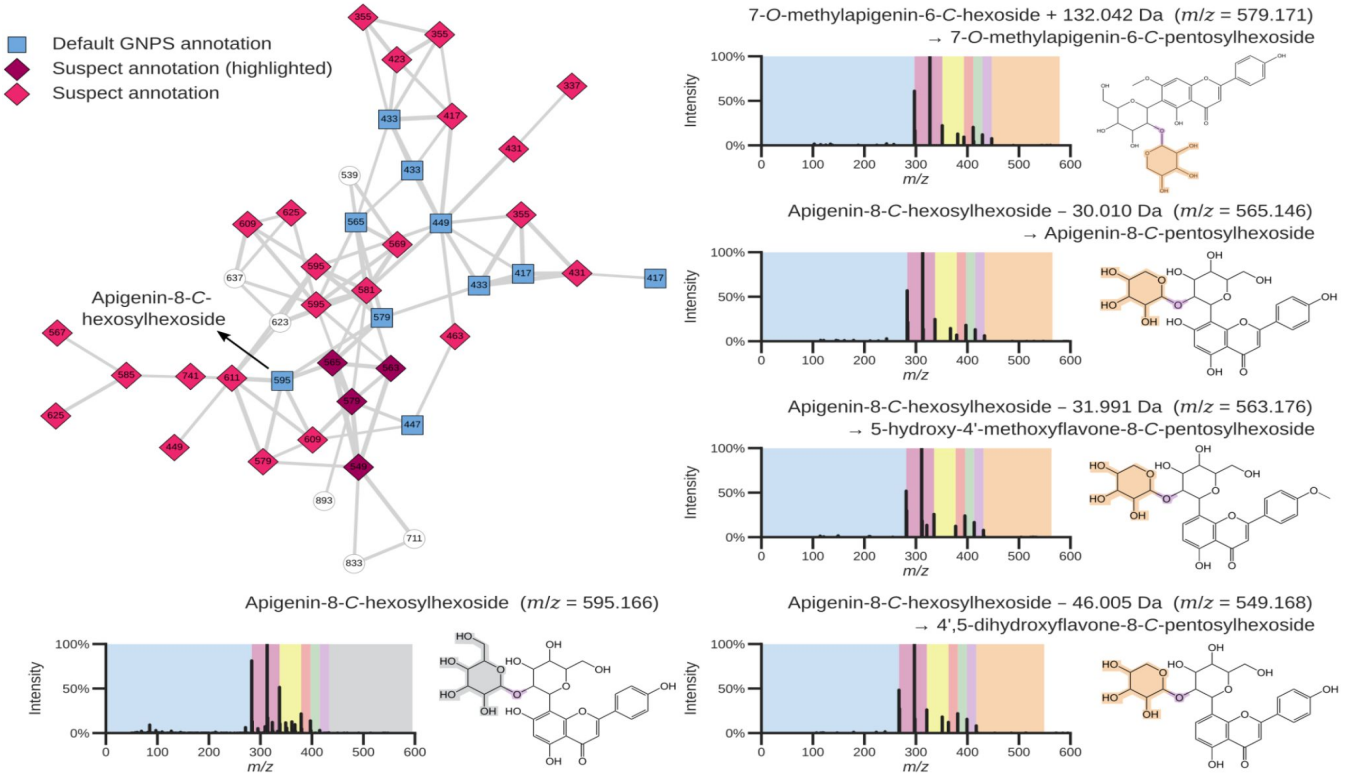

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REFERENCE DATA-DRIVEN METABOLOMICS FOR DIETARY READ-OUTS

ENHANCING METABOLOMICS WITH REFERENCE DATA

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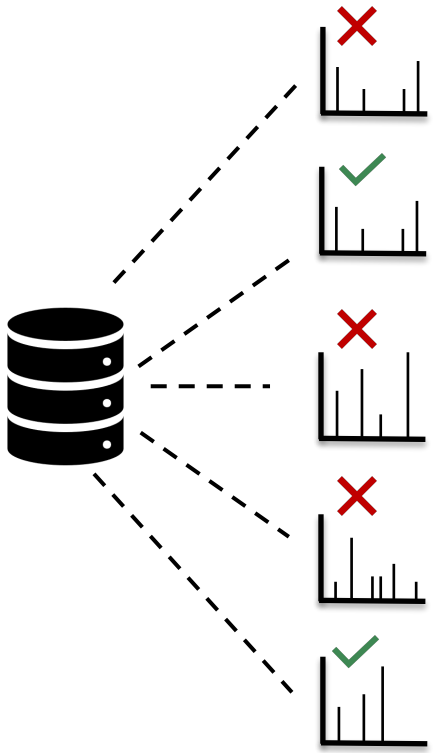

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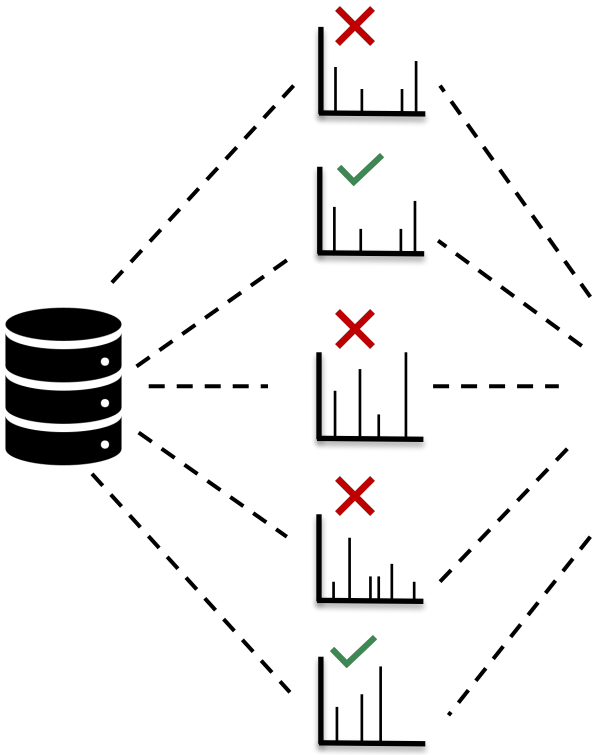
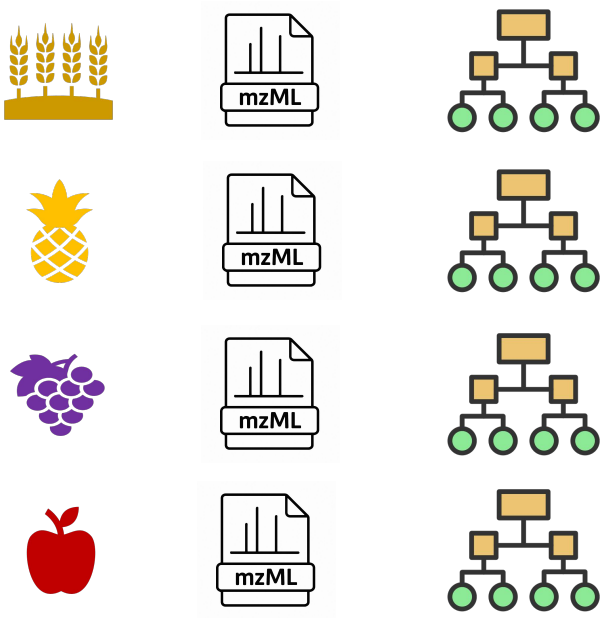
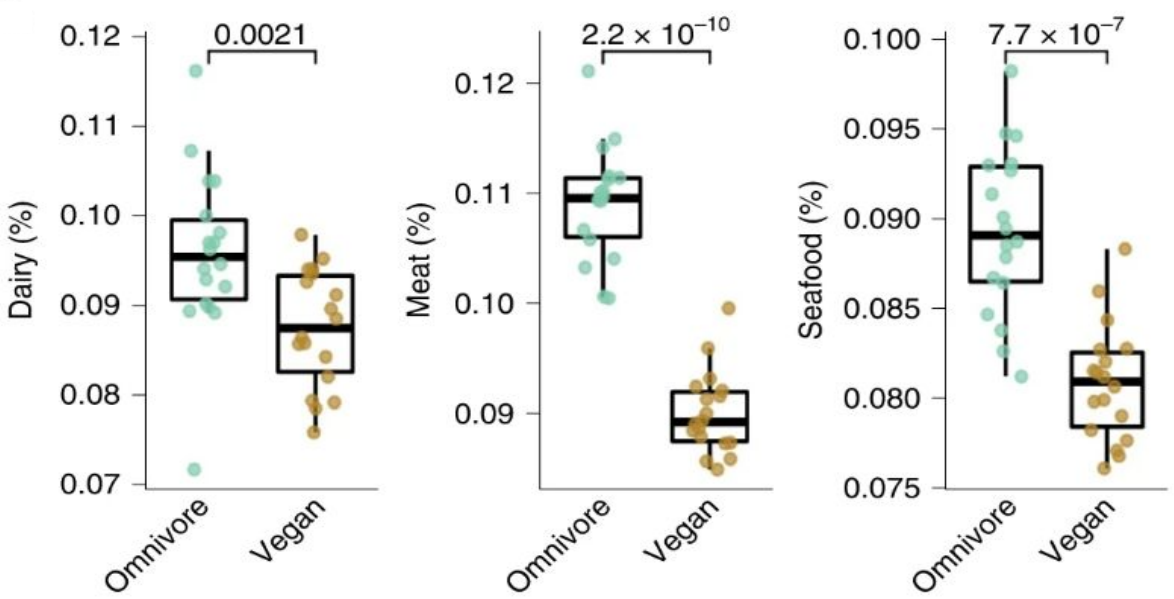


reference MS/MS data + metadata



RDD REVEALS DIETARY SIGNATURES



- NIST Vegan – Omnivore dataset matched with food reference data
- RDD captures dietary intake from distinct groups

Gauglitz, J. *et al. Nature Biotechnology* **40**, 1774–1779 (2022).

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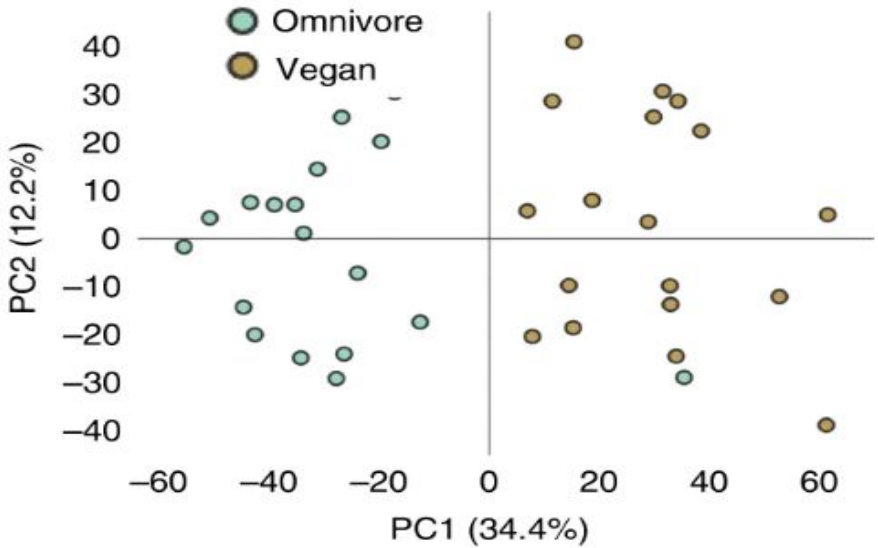

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OVERVIEW

We develop **AI tools**:

- For **computational proteomics and metabolomics**.
- To annotate spectra for molecular discovery.
- To process and learn from massive datasets.
- For quality control in mass spectrometry.
- And many other MS data processing tasks.

ACKNOWLEDGEMENTS

Universiteit Antwerpen


Wout Bittremieux


Sebastian Piedrahita


Ceder Dens


Gaetan De Waele


Moira Breëns


Charlotte Adams


Issar Arab


Madina Bekbergenova


Fatemeh Sarcheshmeh


Samer Makni


Janne Heirman


Alejandro Mendoza Cantu


Marina Pominova


Nikita Kubrakov

FWO

Johnson&Johnson

ThermoFisher SCIENTIFIC