Organic and Biological Analytical Chemistry Group

Machine learning, the separation scientist acolyte for innovative method development

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Organic and Biological Analytical Chemistry Group

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Disclaimer: *This presentation has been generated using AI-Tools*

What is a separation scientist acolyte?

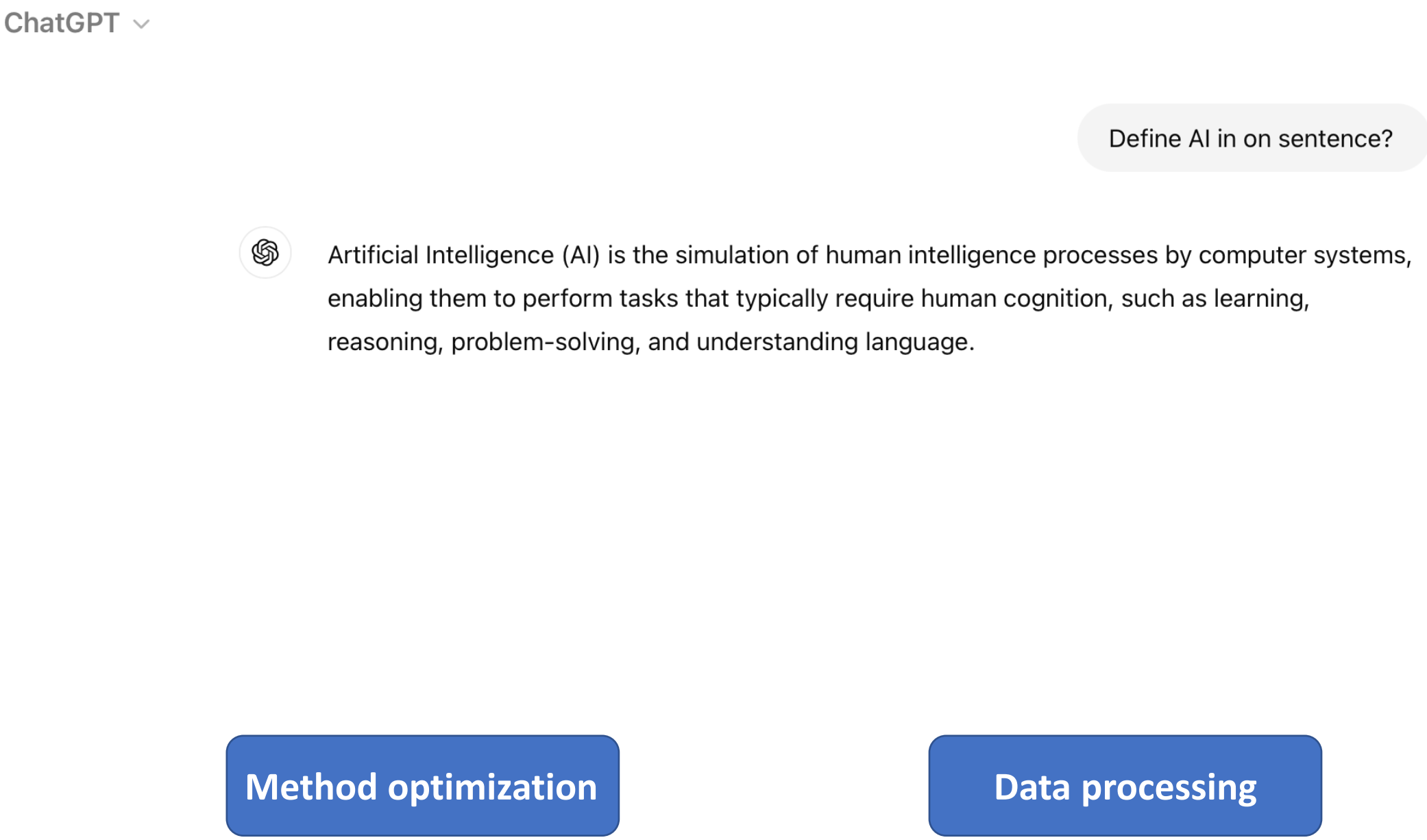
*An **acolyte** refer to a devoted follower or **assistant of a prominent figure**. An acolyte is someone who **supports and learns from a more experienced person**, sometimes in political, academic, or professional environments.*

AI and Machine learning is a support to separation scientist, but it needs to learn from high quality information

ChatGPT

Define AI in on sentence?

Text generated from ChatGPT



Text generated from ChatGPT

GPT concept

GPT: Generative **P**re-trained **T**ransformer

Generative: *The model is generating information* → What we ask

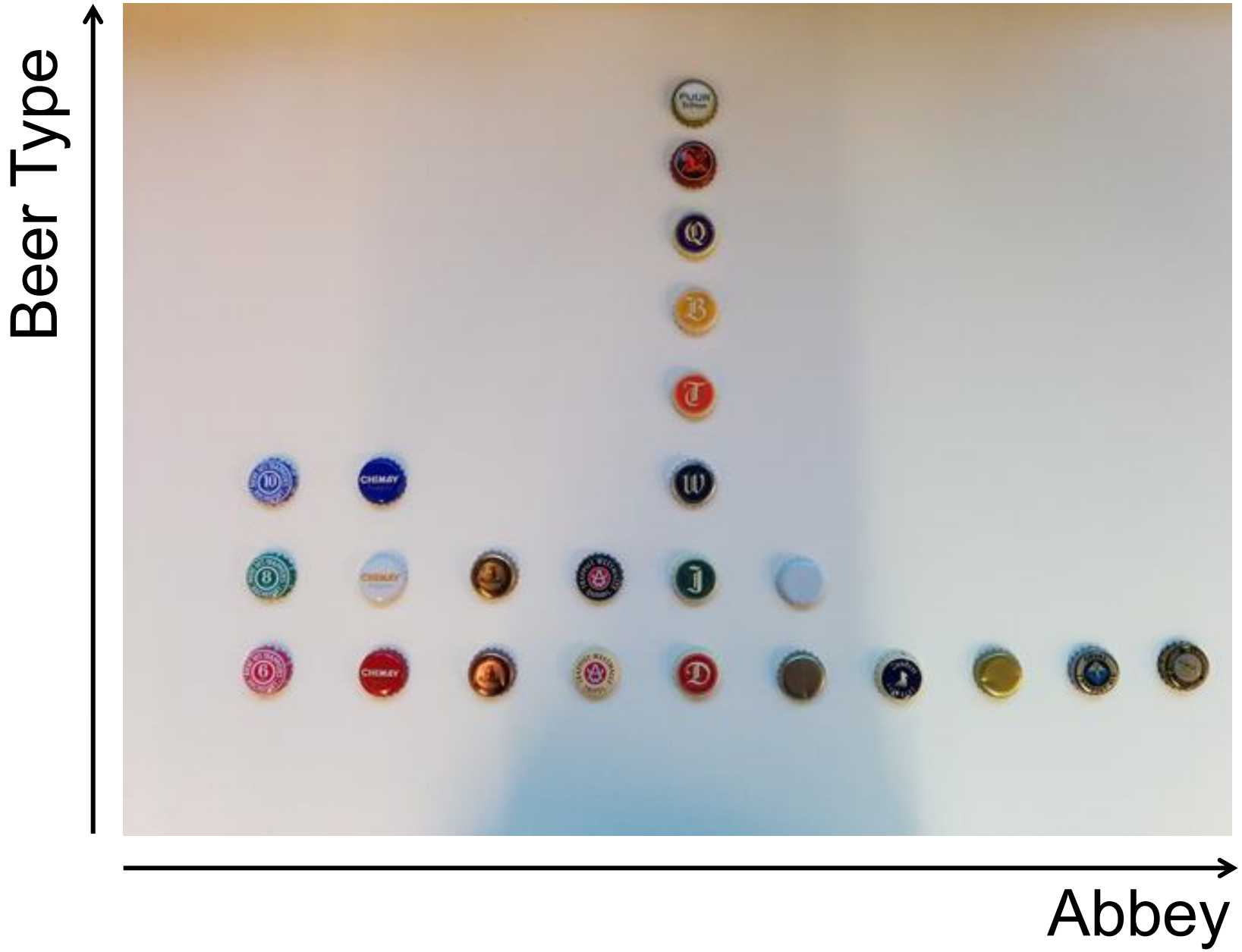
Pre-trained: *The model has been trained on a large amount of data* → The quality of the training

Transformer: *The underlying architecture of neural network model* → The way he manage the information

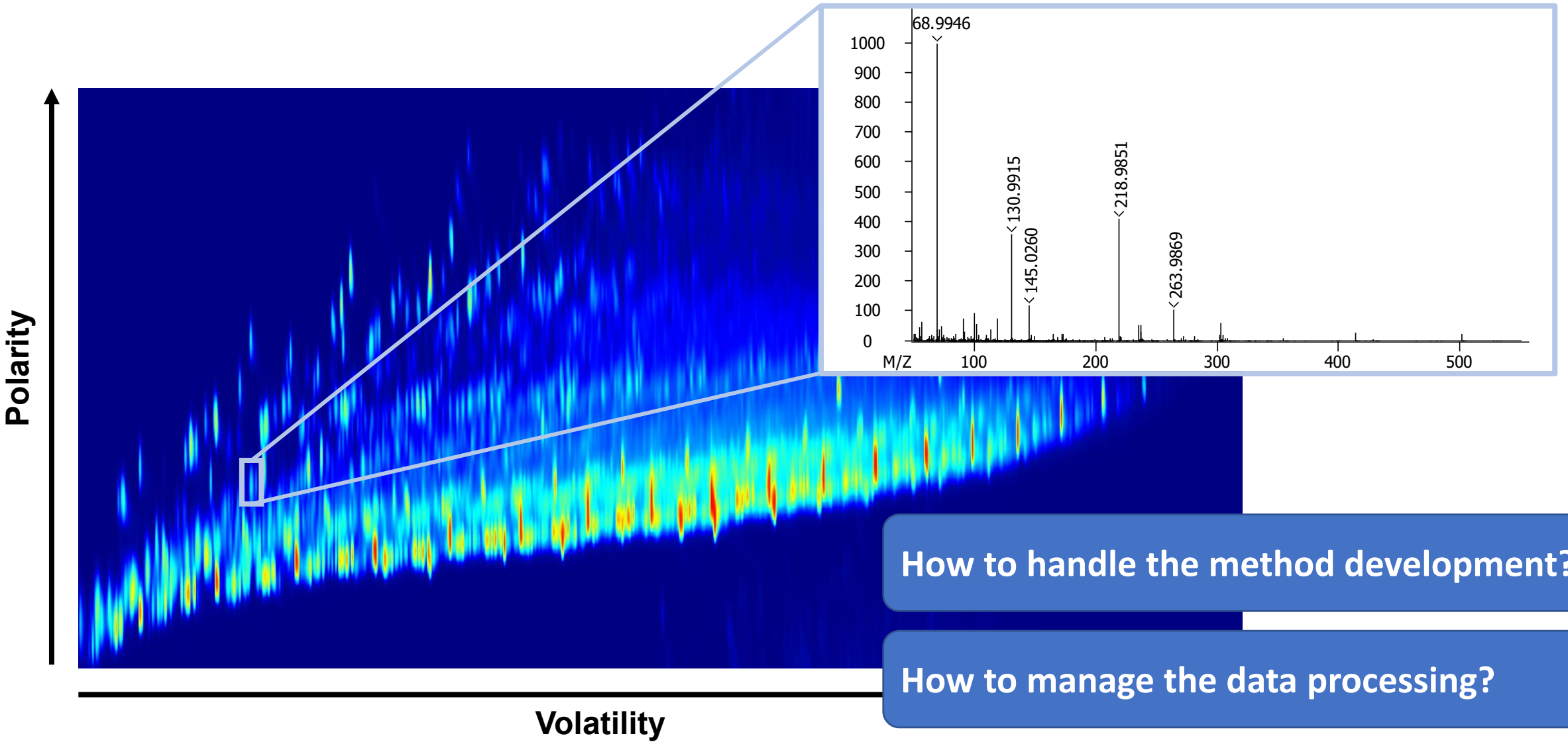
GC×GC-TOFMS: the principle

The sample

Abbey


Beer Type
Abbey

GC×GC-TOFMS: the principle



How to handle the method development?

How to manage the data processing?

Generative I: Method optimization

Generative I: Method optimization

analytical chemistry

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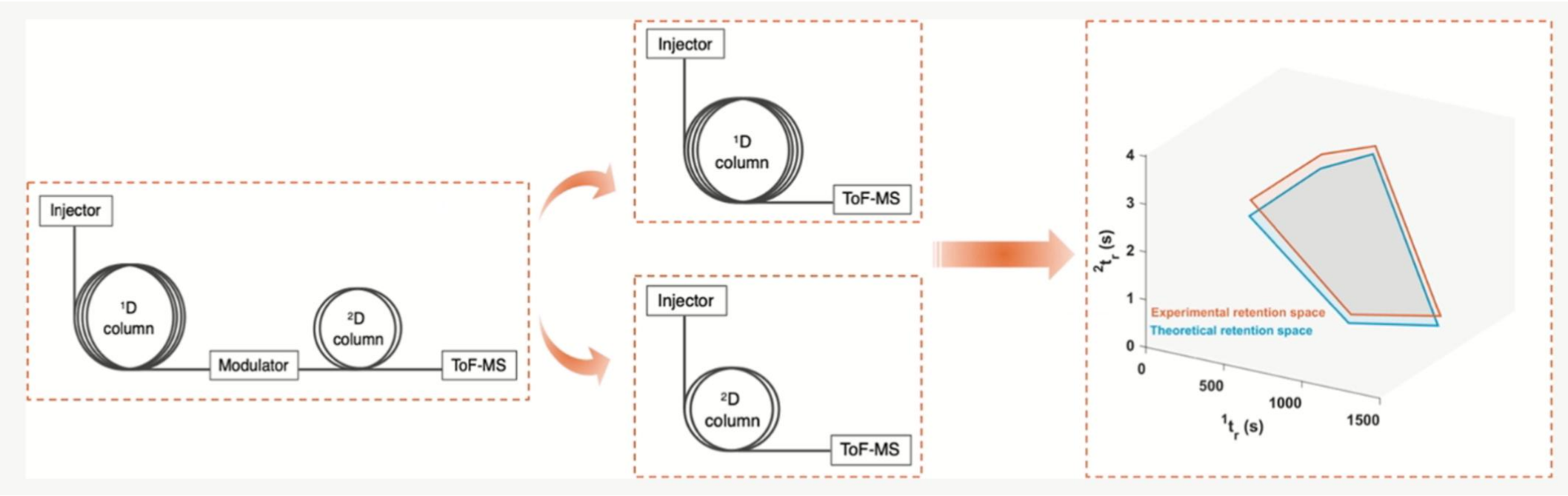
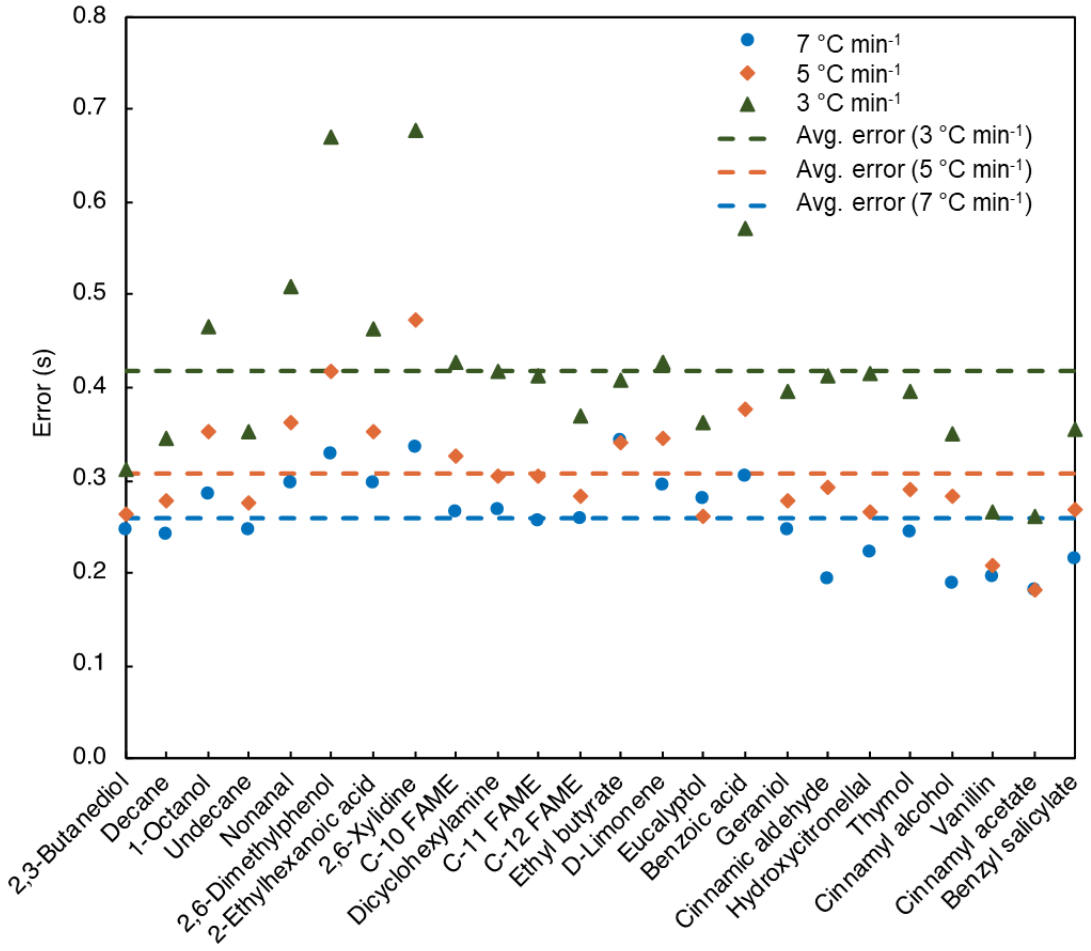
Top-Down Approach to Retention Time Prediction in Comprehensive Two-Dimensional Gas Chromatography–Mass Spectrometry

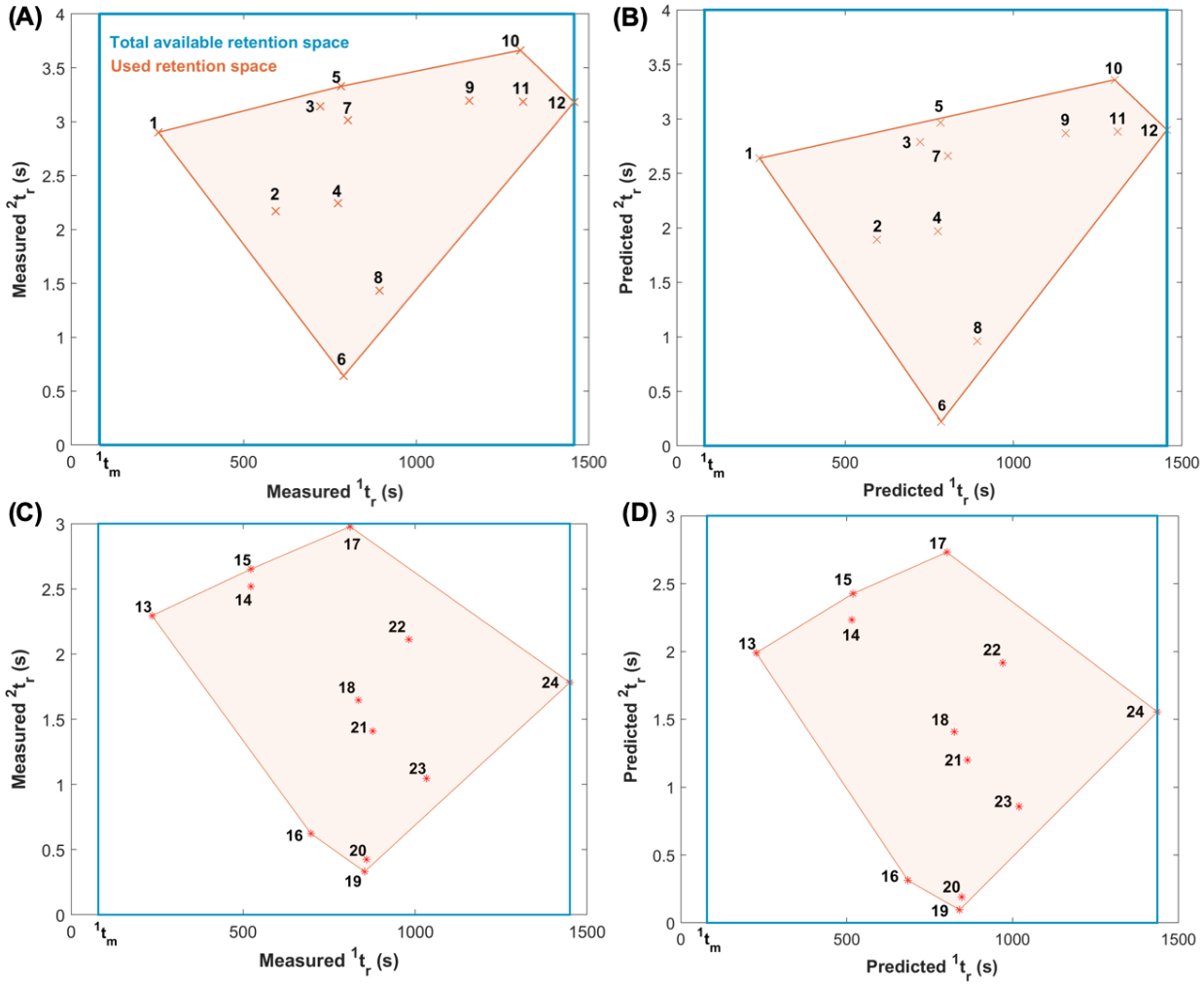
Meriem Gaida,* Flavio A. Franchina, Pierre-Hugues Stefanuto, and Jean-François Focant

Cite This: *Anal. Chem.* 2022, 94, 17081–17089 Read Online

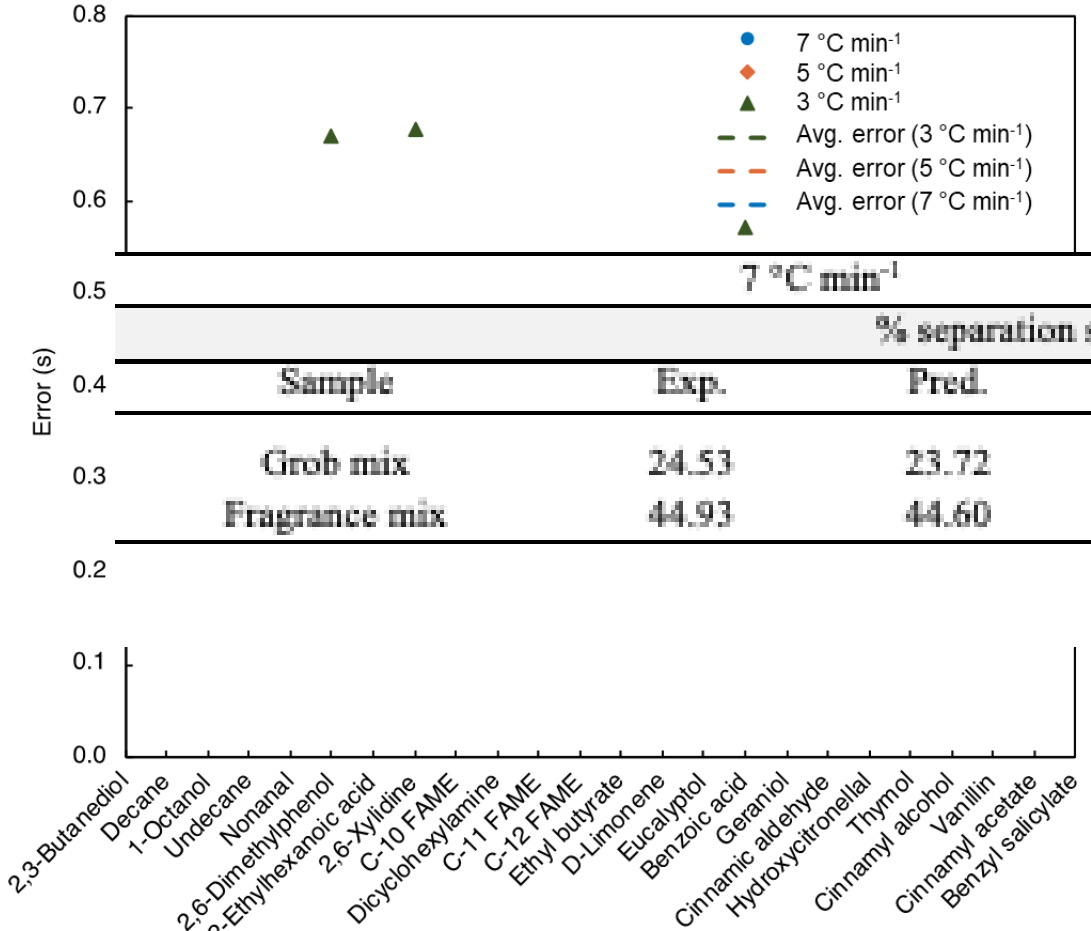


Generative I: Method optimization

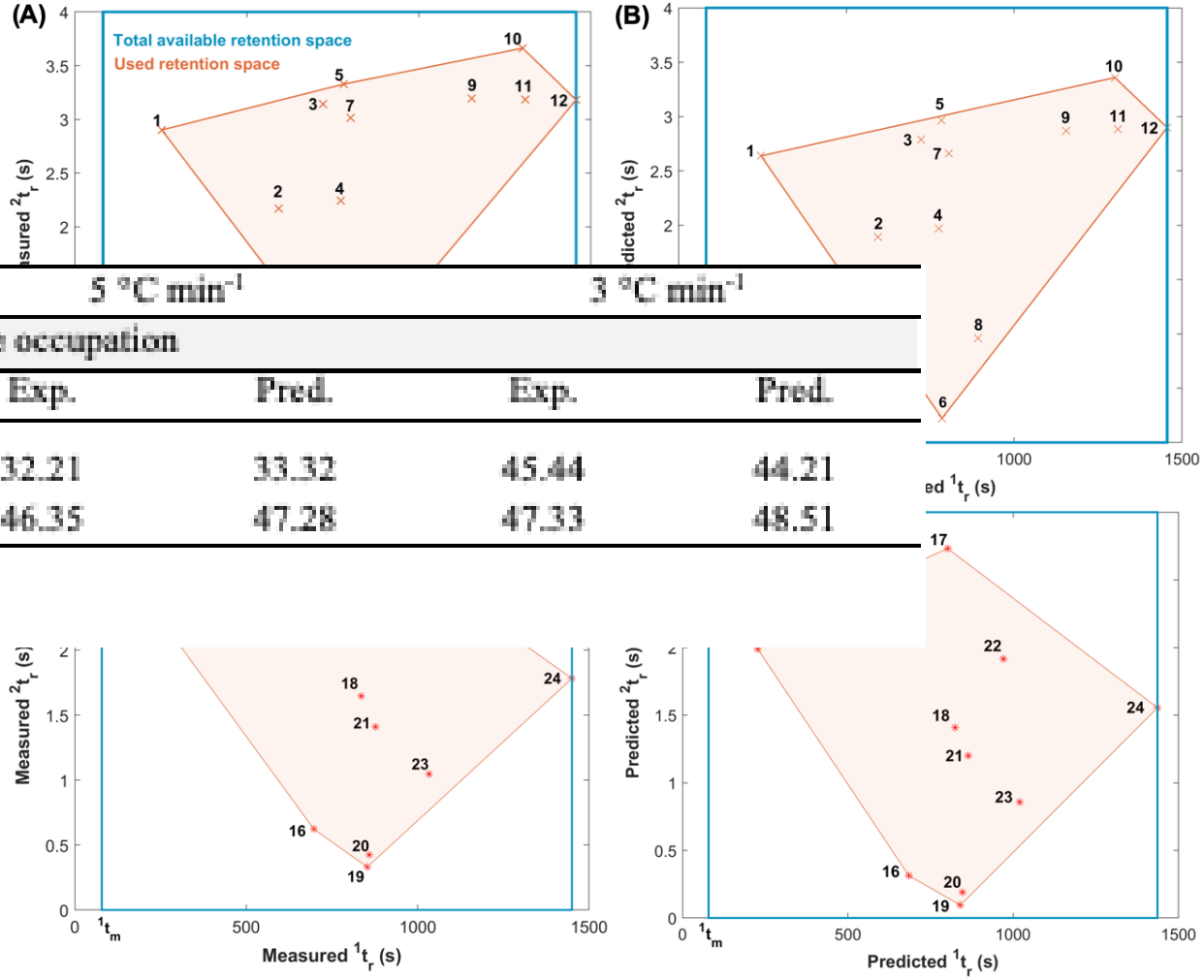




Generative I: Method optimization



% separation space occupation						
	7 °C min^{-1}		5 °C min^{-1}		3 °C min^{-1}	
Sample	Exp.	Pred.	Exp.	Pred.	Exp.	Pred.
Grob mix	24.53	23.72	32.21	33.32	45.44	44.21
Fragrance mix	44.93	44.60	46.35	47.28	47.33	48.51



Generative I: Method optimization

RETURN TO ISSUE | < PREV ECOTOXICOLOGY AND PU... NEXT >

Modeling the GCxGC Elution Patterns of a Hydrocarbon Structure Library To Innovate Environmental Risk Assessments of Petroleum Substances

J. Samuel Arey, Alberto Martin Aparicio, Eleni Vaiopoulou, Stuart Forbes, and Delina Lyon*

Cite this: *Environ. Sci. Technol.* 2022, 56, 24, 17913−17923
Publication Date: December 7, 2022
https://doi.org/10.1021/acs.est.2c06922

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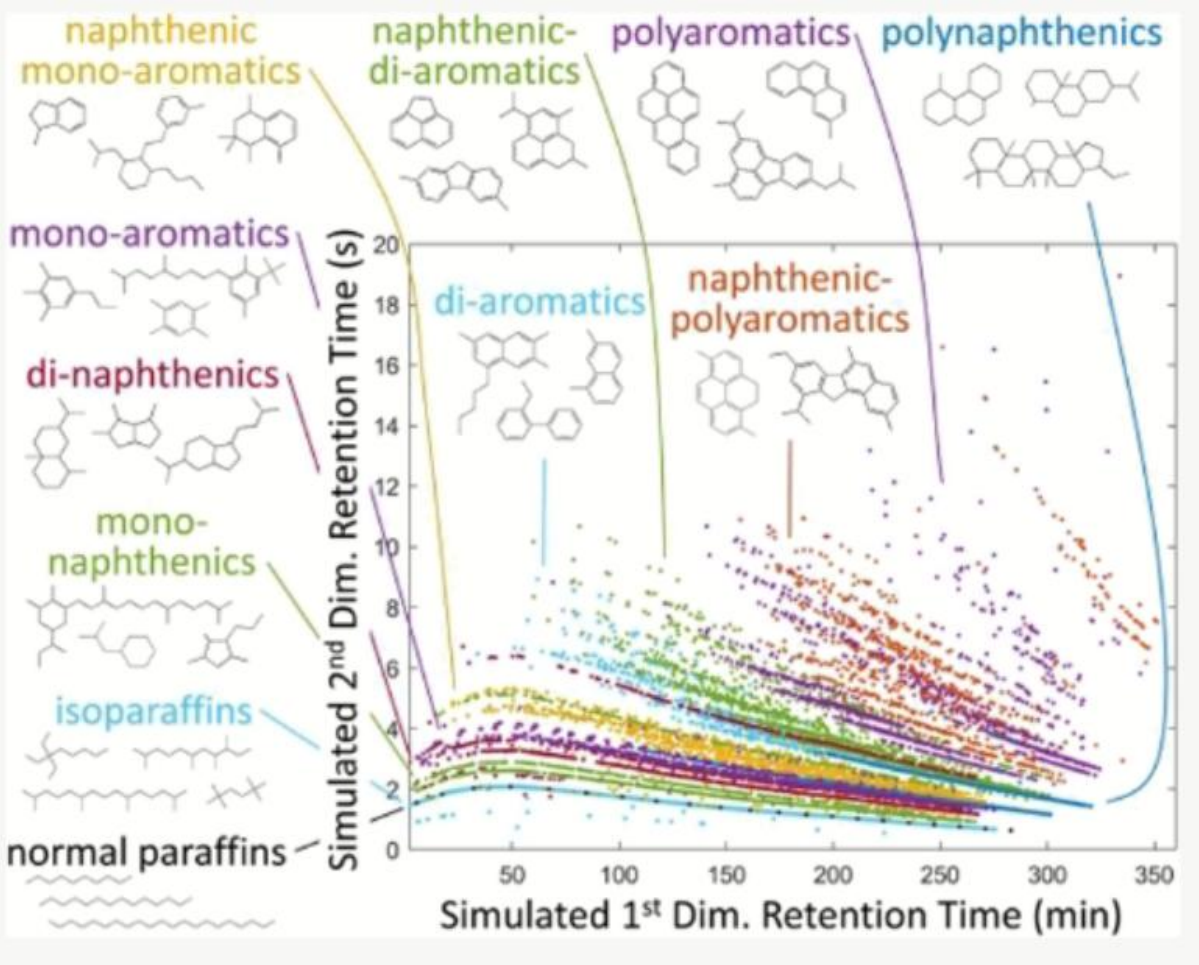

Bringing AI in the game!

Journal of Chromatography A 1612 (2020) 460661

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Journal of Chromatography A

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Steroid identification via deep learning retention time predictions and two-dimensional gas chromatography-high resolution mass spectrometry

Giuseppe Marco Randazzo[a,*], Andrea Bileck[b], Andrea Danani[a], Bruno Vogt[b], Michael Groessl[b,**]

[a] Istituto Dalle Molle di Studi sull'Intelligenza Artificiale (IDSIA), Scuola Universitaria Professionale della Svizzera italiana (SUPSI), Università della Svizzera italiana (USI), CH-6928 Manno, Switzerland
[b] Department of Nephrology and Hypertension and Department of BioMedical Research, Inselspital, Bern University Hospital, University of Bern, Switzerland

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DeepReI: Deep learning-based gas chromatographic retention index predictor

Tomáš Vrzal [a, *], Michaela Malečková [a, b], Jana Olšovská [a]

[a] Research Institute of Brewing and Malting, Plc., Lípová 511/15, 120 44, Prague 2, Czech Republic
[b] Charles University, Faculty of Science, Department of Analytical Chemistry, Albertov 6, 128 43, Prague 2, Czech Republic

Pre-trained: reuse previous data

analytical chemistry

pubs.acs.org/ac Article

Top-Down Approach to Retention Time Prediction in Comprehensive Two-Dimensional Gas Chromatography–Mass Spectrometry

Meriem Gaida,* Flavio A. Franchina, Pierre-Hugues Stefanuto, and Jean-François Focant

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[b] Department of Nephrology and Hypertension and Department of BioMedical Research, Inselspital, Bern University Hospital, University of Bern, Switzerland

Modeling the GCxGC Elution Patterns of a Hydrocarbon Structure Library To Innovate Environmental Risk Assessments of Petroleum Substances

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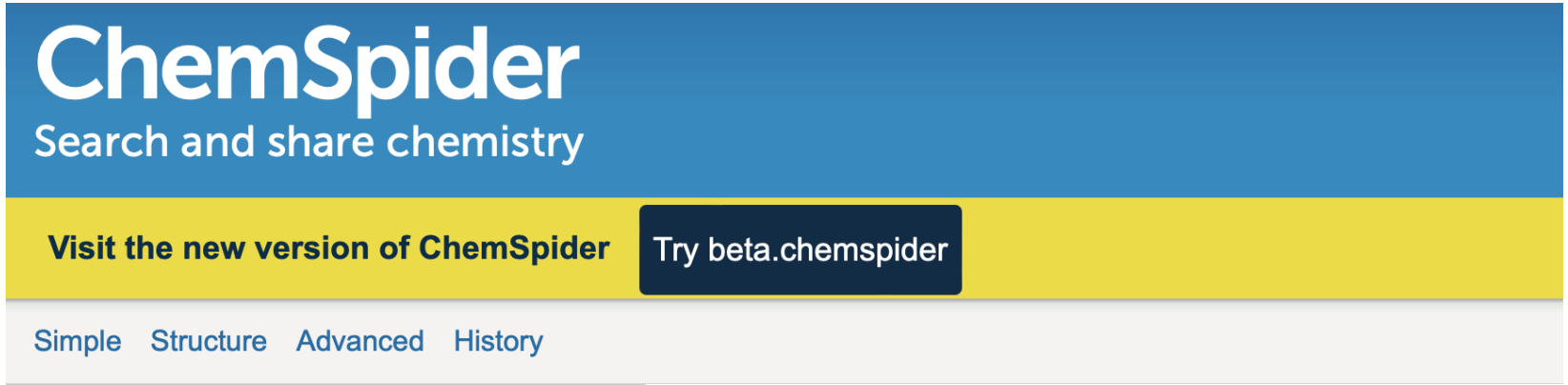
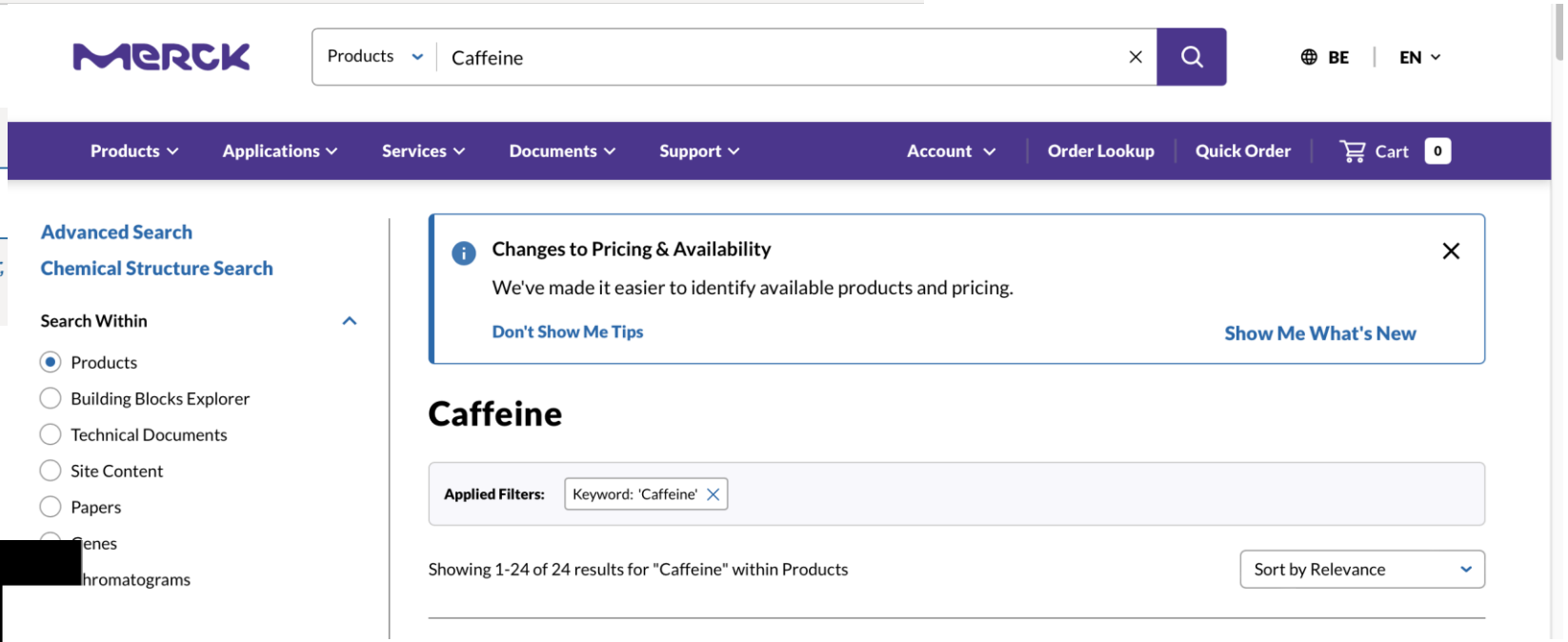
Pre-trained: we need large data!





Pre-trained: **generating data as a community**

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Journal of Chromatography A, 1019 (2003) 261–272

JOURNAL OF CHROMATOGRAPHY A

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Standardized test mixture for the characterization of comprehensive two-dimensional gas chromatography columns: the Phillips mix

Jean-Marie D. Dimandja [a,*], Garrick C. Clouden [b], Ivelisse Colón [c], Jean-François Focant [d], Whitney V. Cabey [a], Ritchard C. Parry [e]

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NIST FDA

Pre-trained: **generating data as a community**

1 – Column classification

- Century mix analysis across **20 Column combinations**

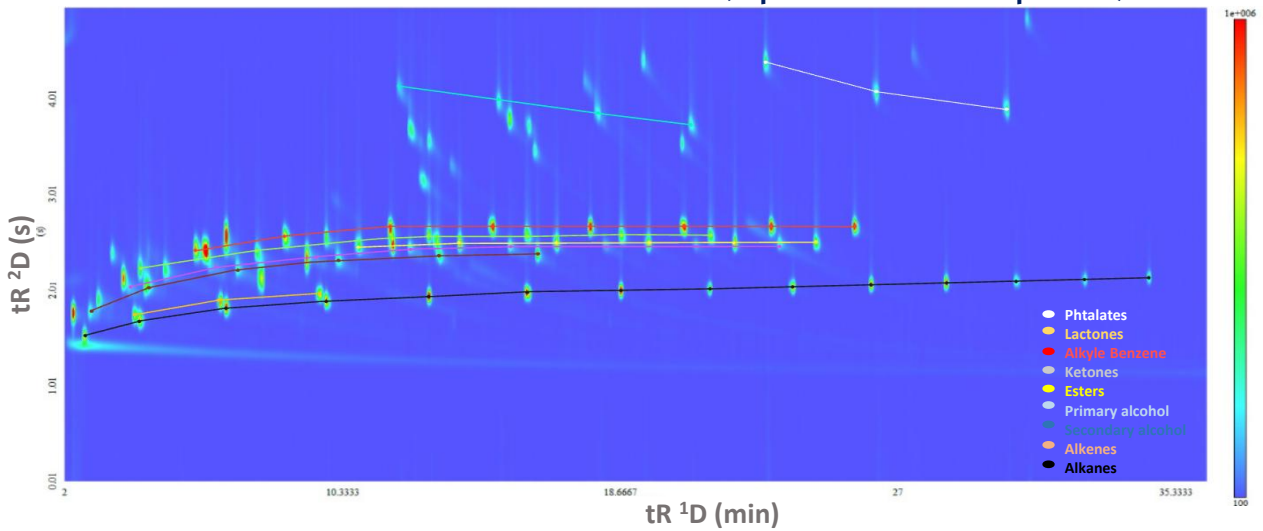
Polarity	Apolar	Mid-Polar	Polar
Apolar			
Mid-Polar			
Polar			

Normal orthogonality

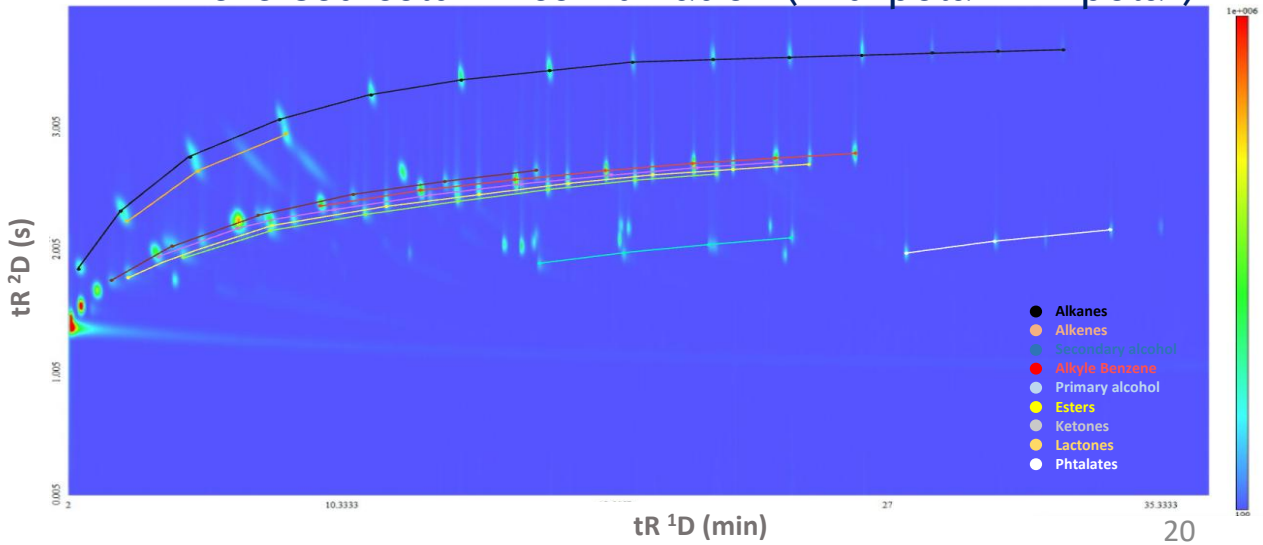
Non-orthogonal

Reversed orthogonality

Normal column combination (Apolar × Mid-polar)



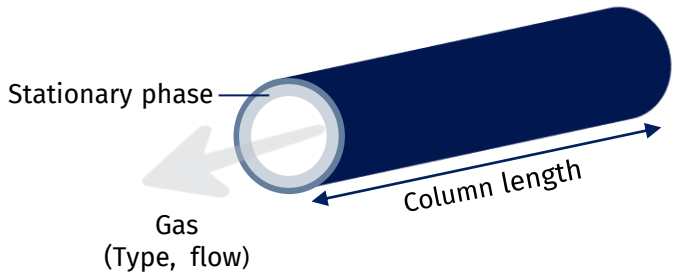
Reversed column combination (Mid-polar × Apolar)



Pre-trained: **generating data as a community**

1 – System evaluation

- Stationary phase film thickness (0.1 à 1.4 µm)
- Temperature ramp (2 à 15 °C/min)
- Gas type (He, H_2, N_2)
- Gas flow (0.8 à 1.5 mL/min)

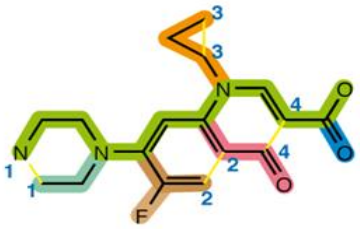


2 – Data Collection

Retention time , elution order , geometric peak repartition Etc

+

Boiling points, polarity moment, **SMILES Annotation**



Ciprofloxacin SMILES Annotation

N1CCN(CC1)C(C(F)=C2)=CC(=C2C4=O)N(C3CC3)C=C4C(=O)O

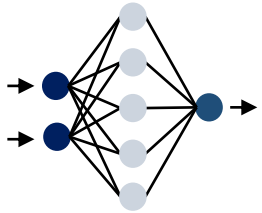
3 – Modelisation-Prediction

Retention indices prediction

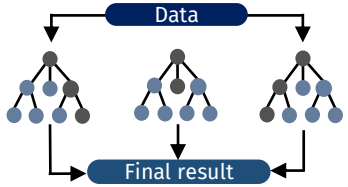
(System-independent constants)

Machine Learning Algorithm

Artificial neural network



Random Forest



Transformer: mostly neural network

Define neural network in one sentence

Text generated from ChatGPT

Deep Learning, a step further for transformers

Machine Learning	Deep Learning
Possible to train with fewer data	Large datasets for training
Statistical algorithms	Artificial Neural Networks (ANN)
Structured data	Unstructured data
Limited tuning capabilities	Can be tuned in multiple ways
Simpler applications	More complex applications

Automation

New methods

Greener methods

Images generated on ideogram.ai

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LIÈGE, BELGIUM

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FREE registration

PRESENTATIONS by key speakers

DISCUSSION on hot topics

POSTER SESSION with awards

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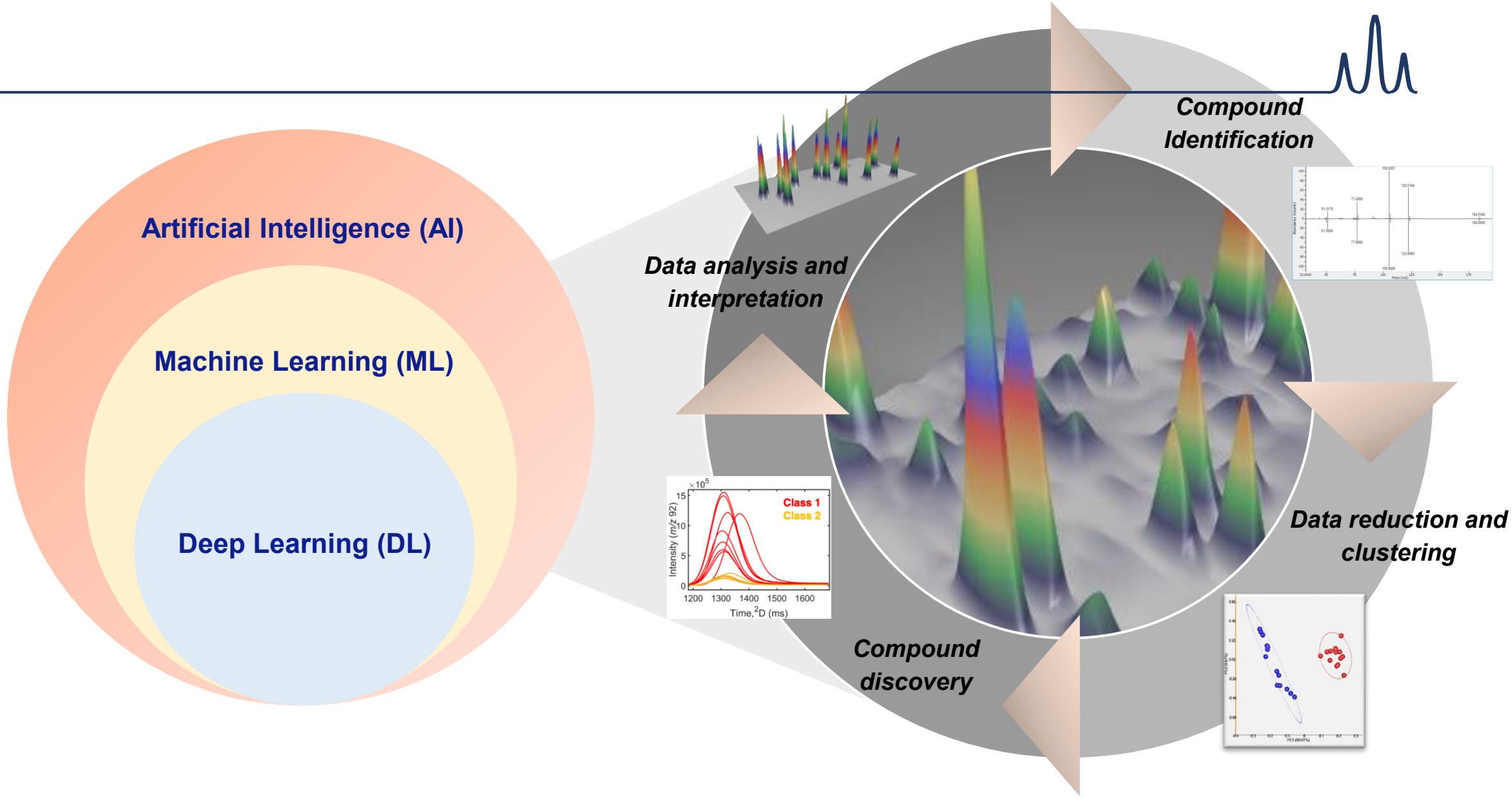
Liège University

Think tank

Networking hub

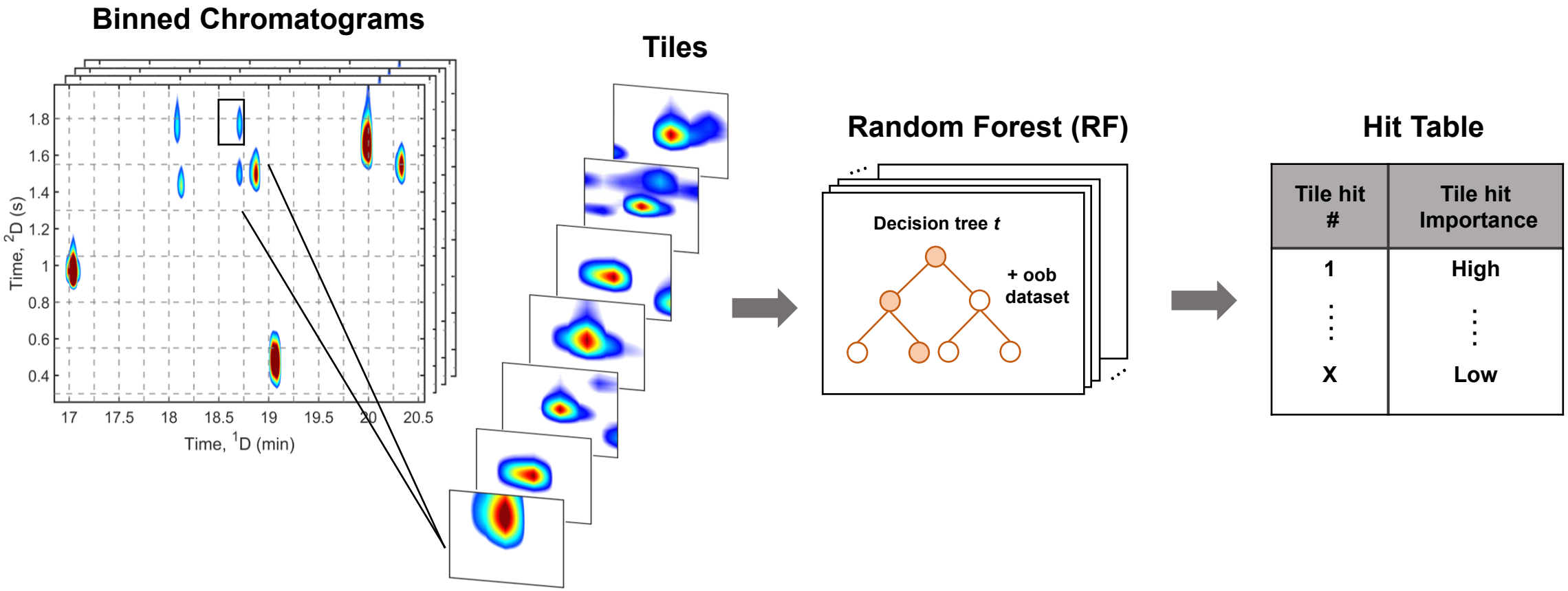
Generative II: Data processing

Can AI help in processing GC×GC data?



Example #1: Tile-based Random Forest Approach

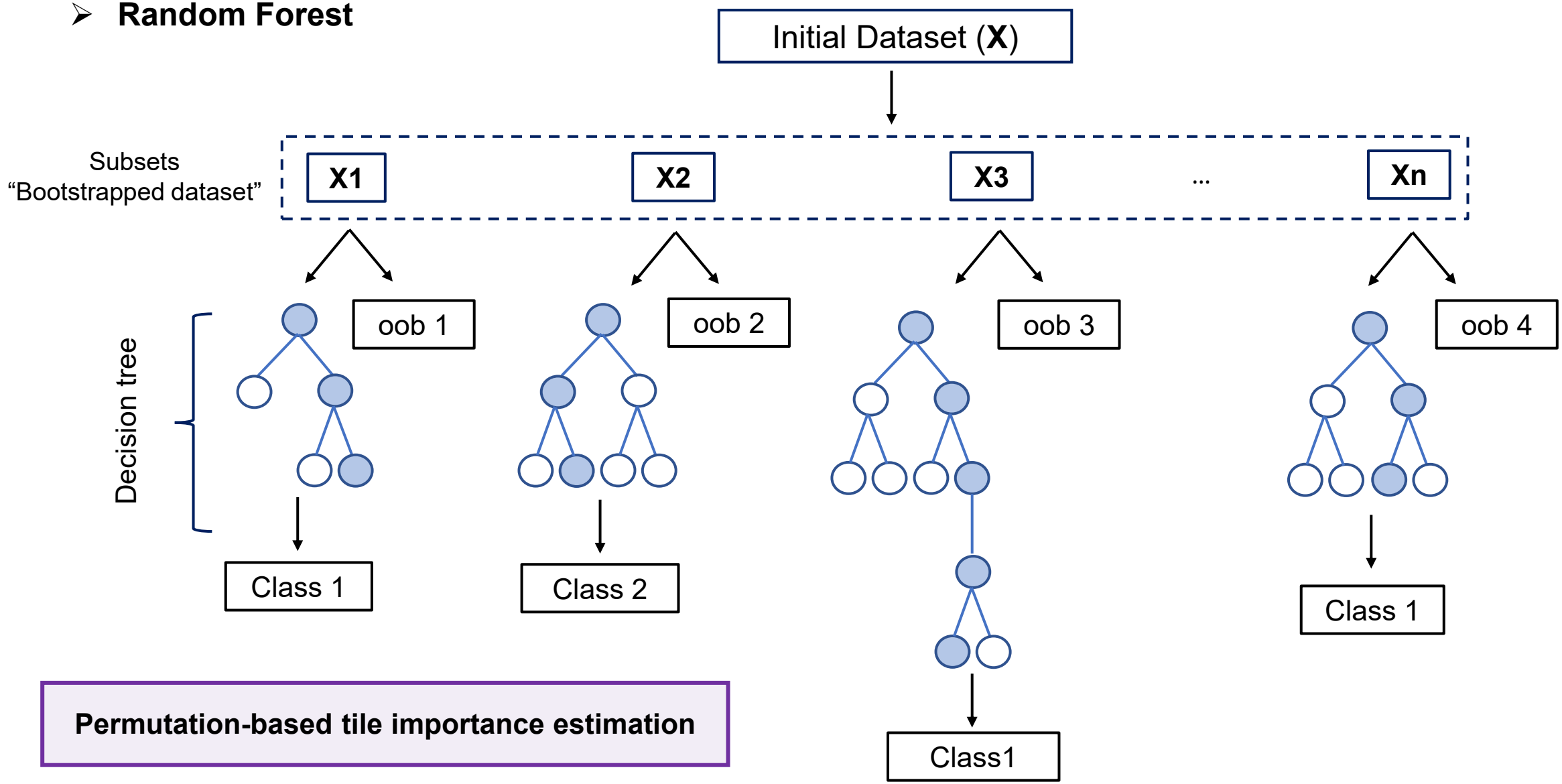
➢ **A novel approach for discovery-based analysis:** alternative to the F-ratio approach for unbalanced datasets.



Gaida, M.; Cain, C. N.; Synovec, R. E.; Focant, J.-F.; Stefanuto, P.-H. ***Anal. Chem.*** 2023.

Example #1: Tile-based Random Forest Approach

➢ **Random Forest**



Permutation-based tile importance estimation

Example #1: Tile-based Random Forest Approach

➢ **Random Forest Advantages**

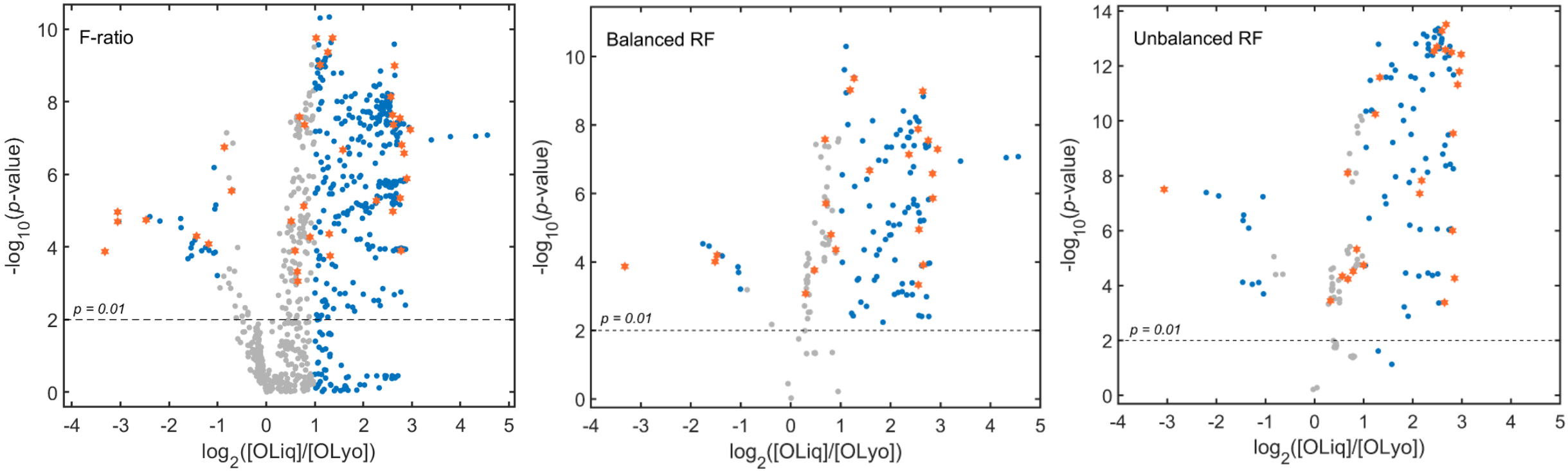
- Efficient for large datasets.
- Good performance for high-dimensional datasets: number of features > number of observations.
- Built-in support for cross-validation (CV) through the oob error calculations.
- Ability to handle multi-class classification problems.

- **Does not require any assumptions about the data distribution.**
- **Stratified sampling when assessing feature/tile importance.**

→ *Each class has an equal chance of being represented avoiding any bias towards the majority class!*

Example #1: Tile-based Random Forest Approach

➢ Volcano Plots



Gray dots: *m/z* with 0.5 < [OLiq]/[OLyo] < 2 (or -1 < $\log_2$ ([OLiq]/[OLyo]) <1)

Orange hexagrams: top purest *m/z* (*p*-value < 10^{-3} and LOF ≤ 10%)

Dashed line: *p*-value = 0.01

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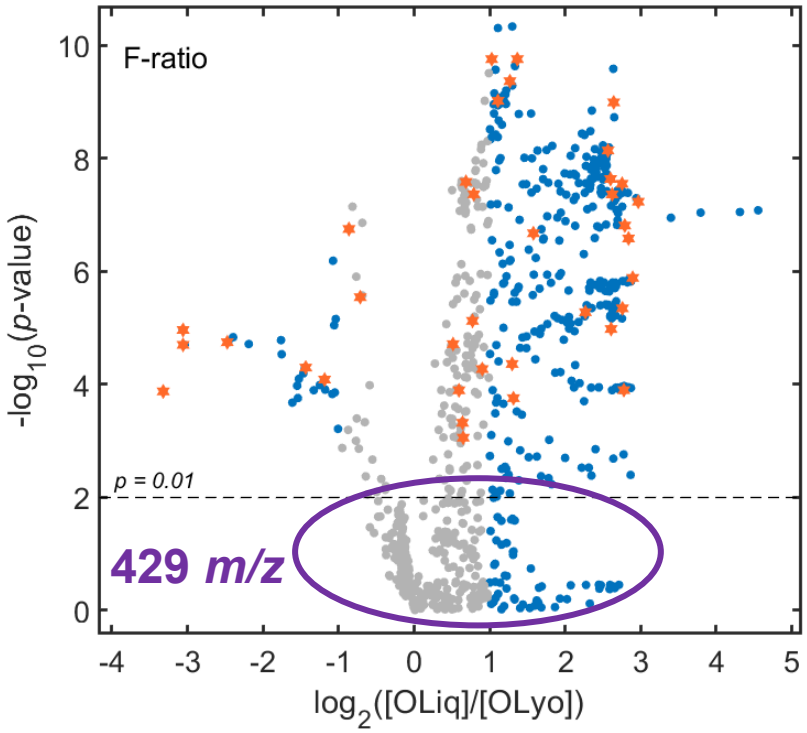
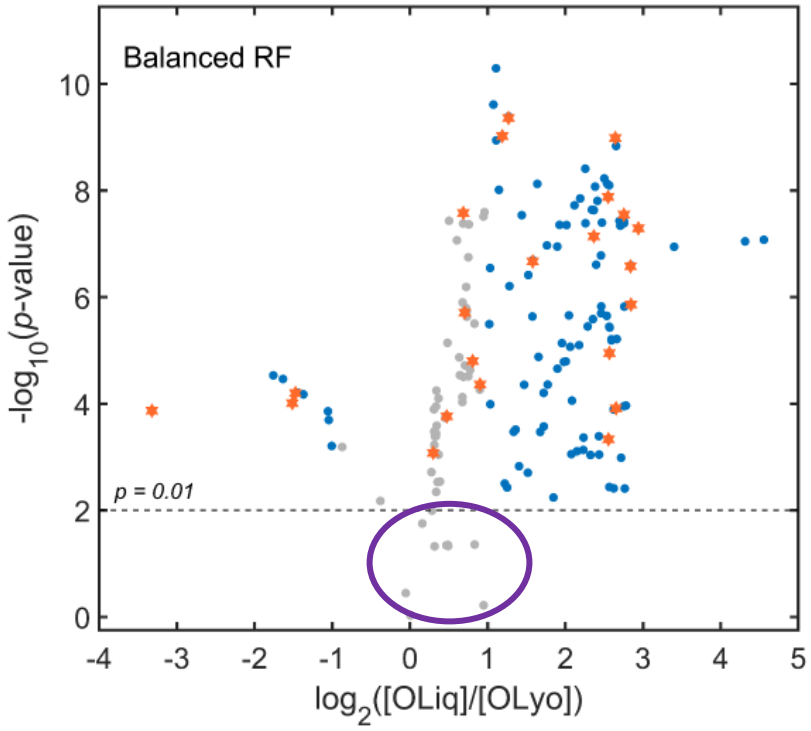
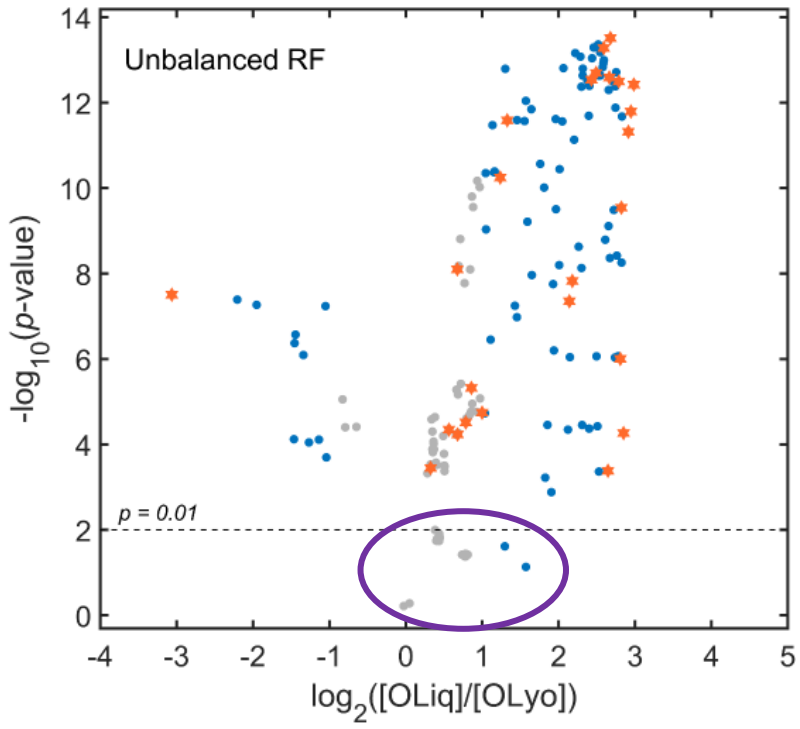


846 *m/z*



169 *m/z*



169 *m/z*

- 50% of the *m/z* discovered by the Fisher-ratio approach correspond to false positives.
- Higher incidence of false positives in the Fisher-ratio approach compared to the Balanced and Unbalanced Random Forest approach.

Gaida, M.; Cain, C. N.; Synovec, R. E.; Focant, J.-F.; Stefanuto, P.-H. ***Anal. Chem.*** 2023.

Example #1: Tile-based Random Forest Approach

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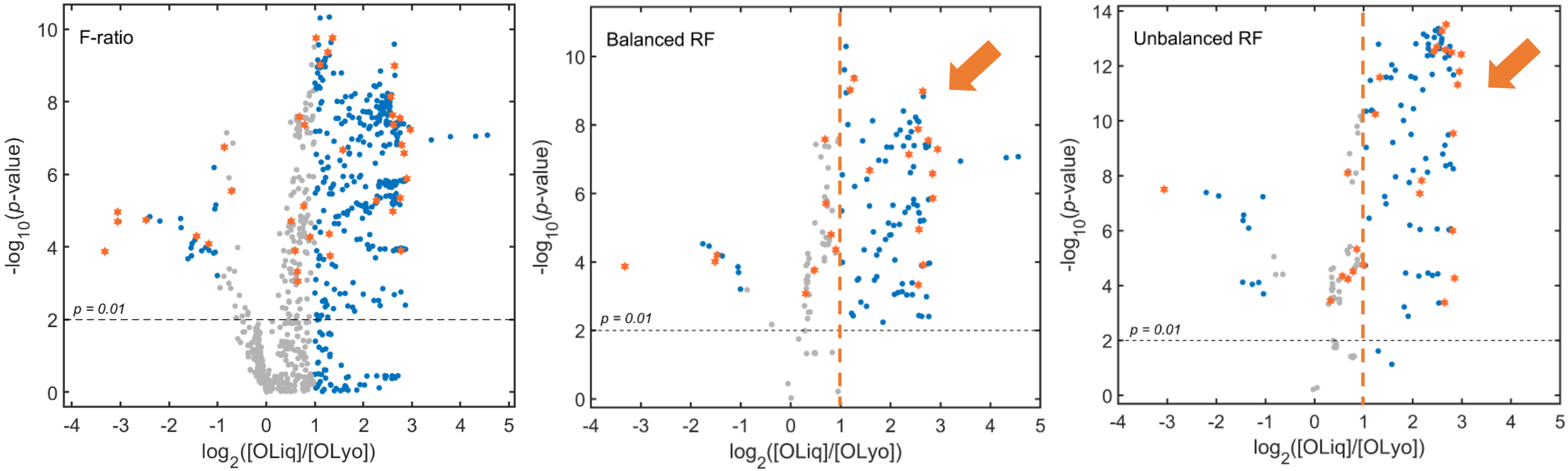

- Most of the *m/z* discovered by the RF analyses have concentration ratios > 2.

The Random Forest approach uses a more stringent feature selection process.

Gaida, M.; Cain, C. N.; Synovec, R. E.; Focant, J.-F.; Stefanuto, P.-H. ***Anal. Chem.*** 2023.

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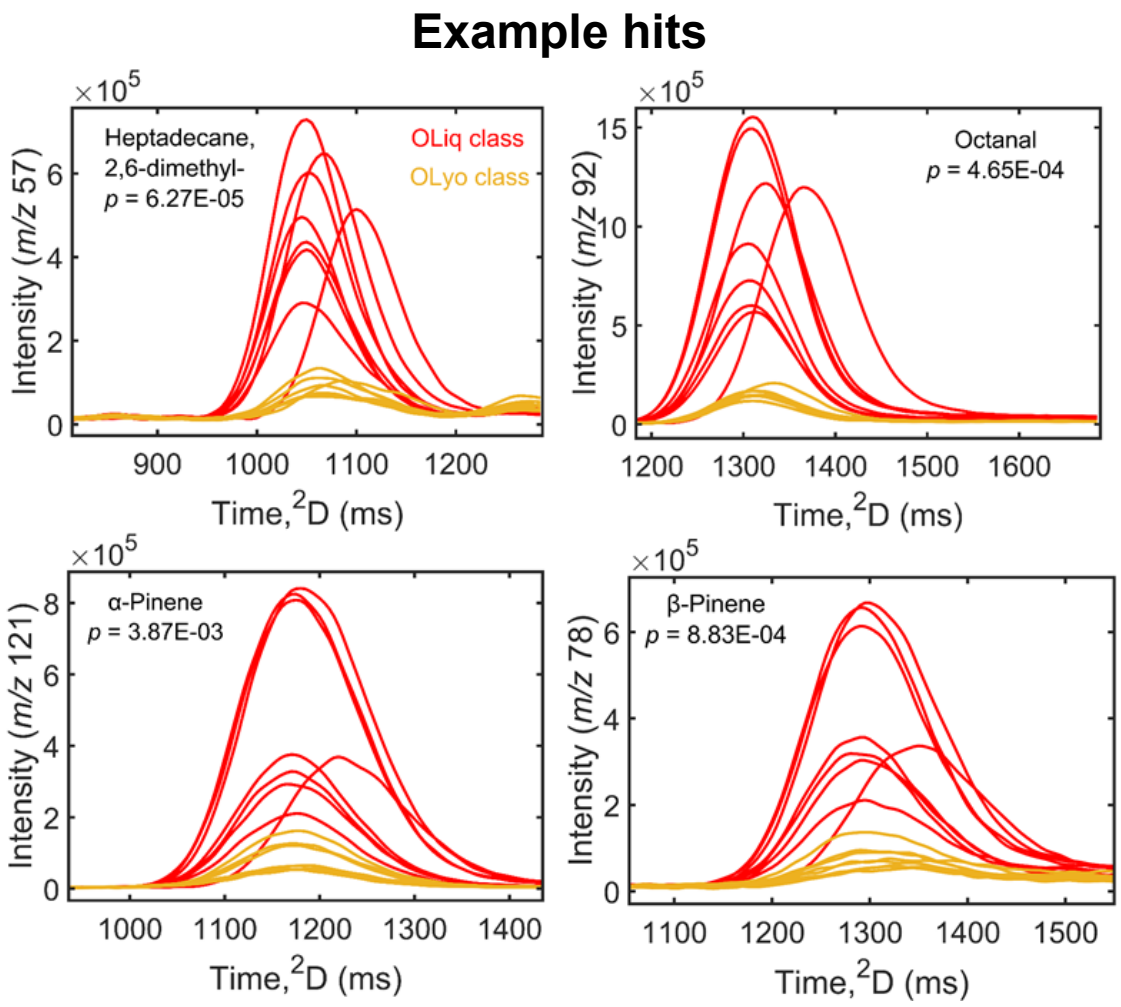


Analytes with high within and between class variance!

$$F - ratio = \frac{Between\ class\ variance}{\sum Within\ class\ variance}$$

Gaida, M.; Cain, C. N.; Synovec, R. E.; Focant, J.-F.; Stefanuto, P.-H. ***Anal. Chem.*** 2023.

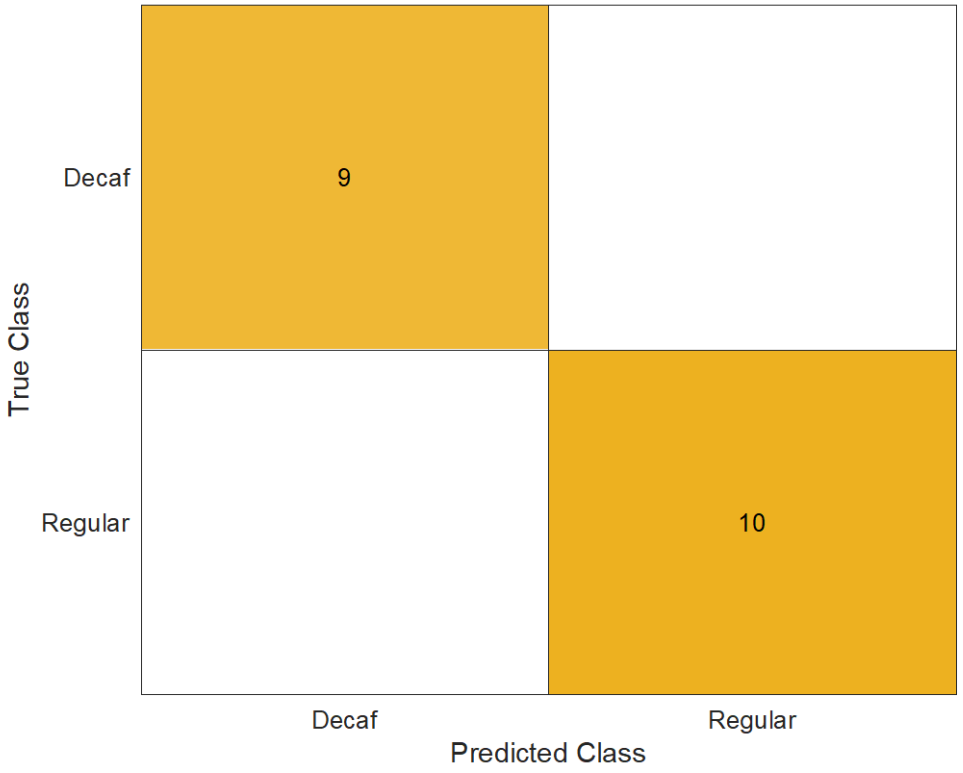
Example #2: Machine Learning for Feature selection and Prediction

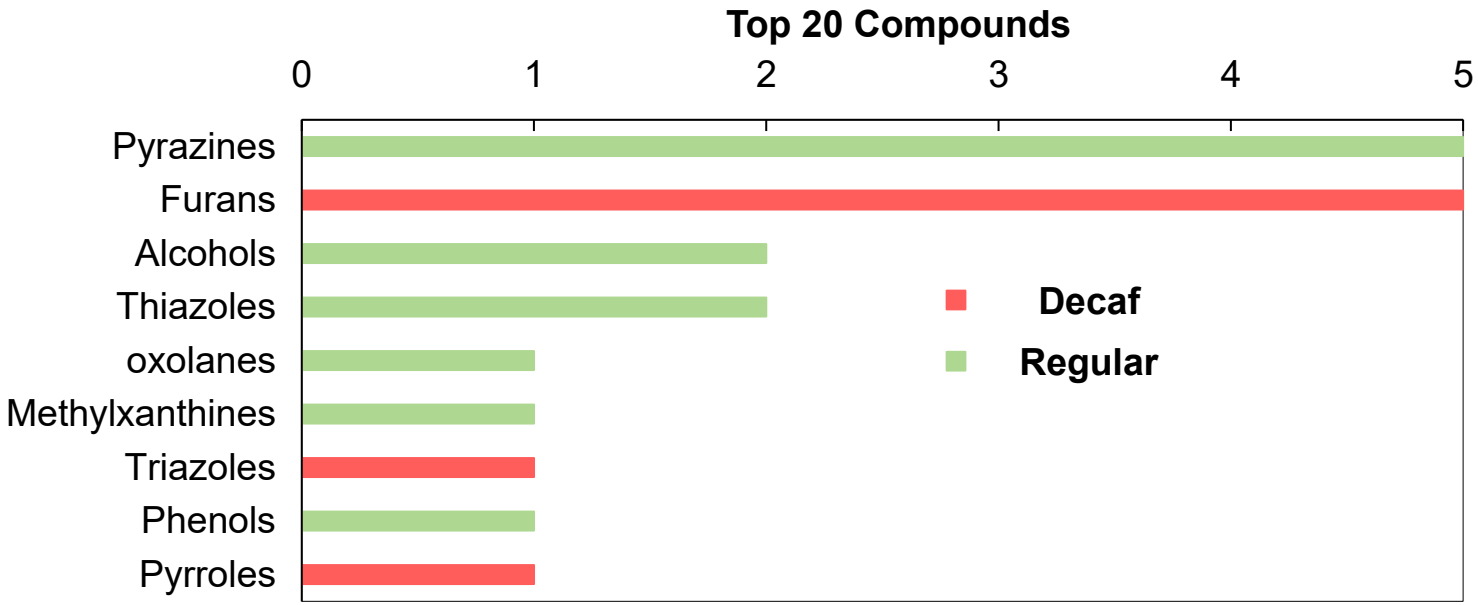
➢ **Untargeted analysis of two different coffee groups: Regular (R) *vs*. Decaf (D)**

- 16 samples (8 R and 8 D) in triplicates.
- *n* = 48 observations and 630 features.
- Selection of **discriminatory features** that are able to distinguish between R and D using a Random Forest classification model.

Example #2: Machine Learning for Feature Selection and Prediction

- 60 % training set (n=29) and 40% validation set (n=19).
- Random Forest is used to select the top 20 discriminatory features.





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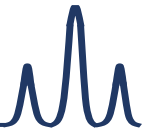
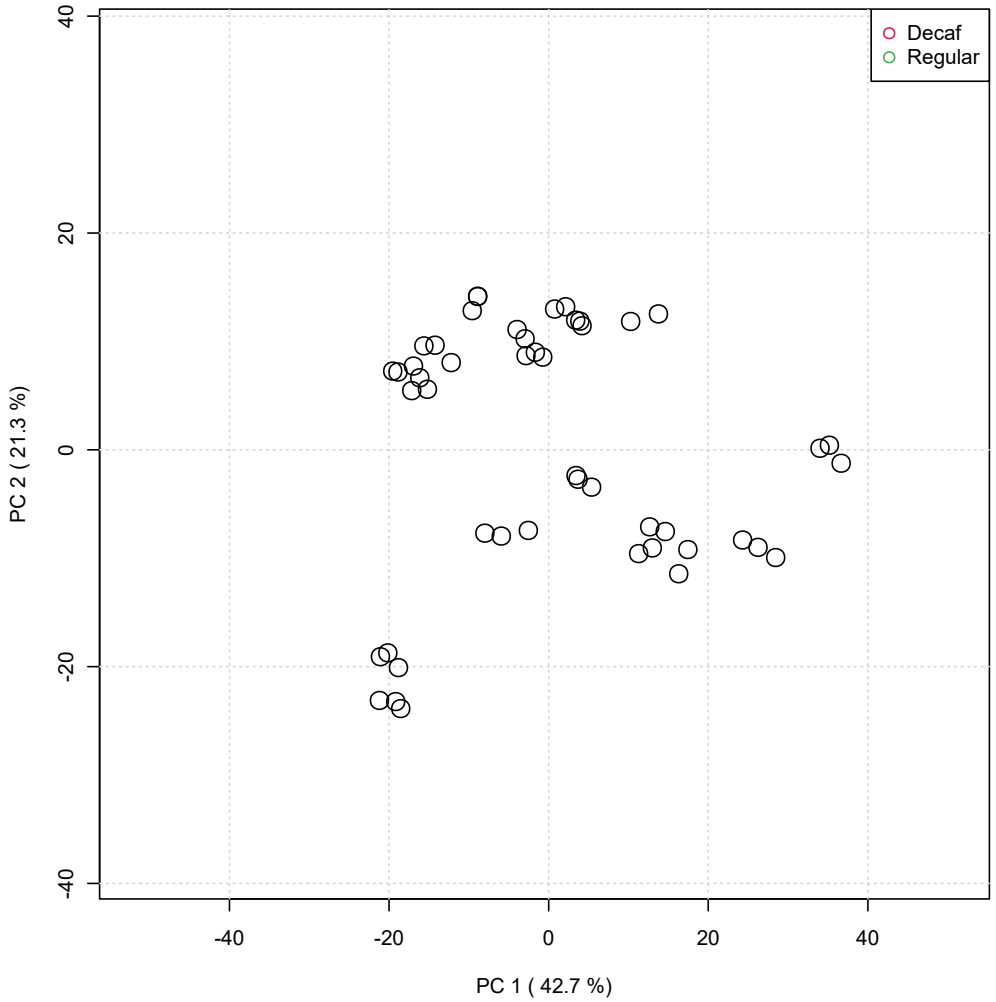
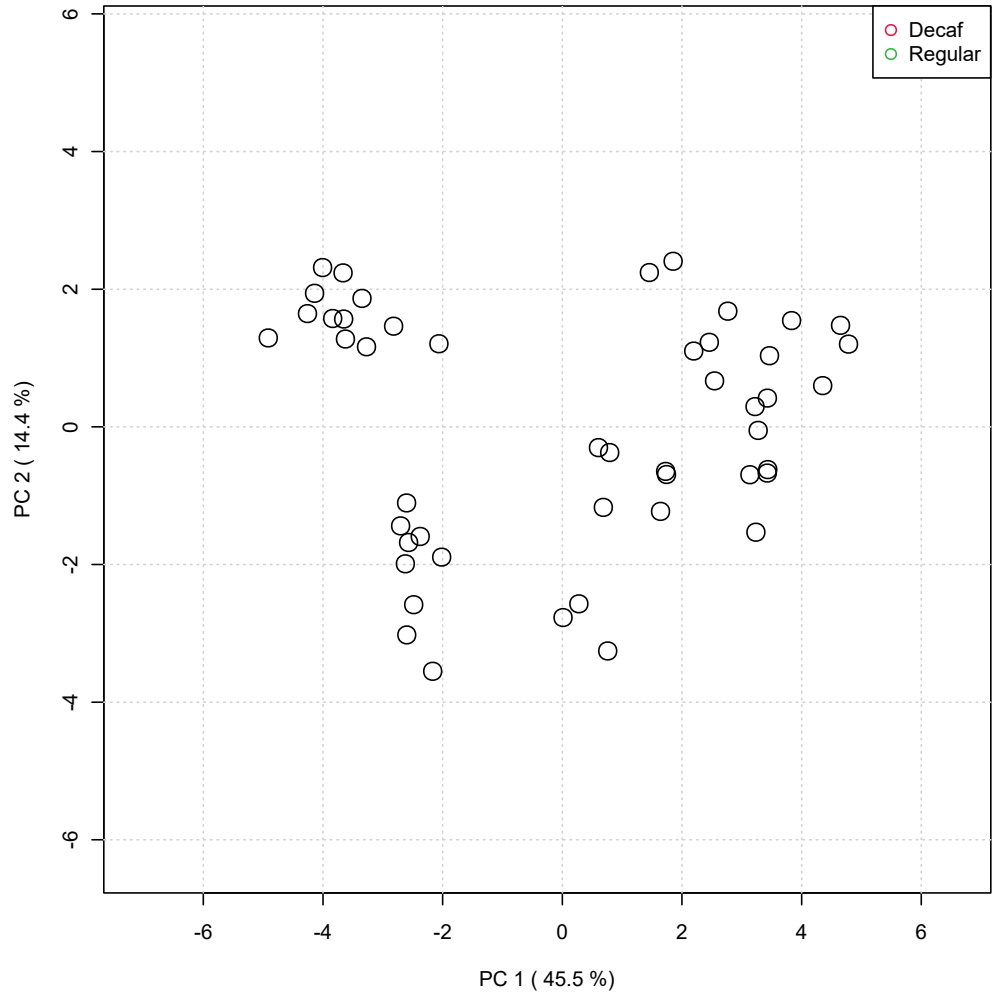


630 features



20 features



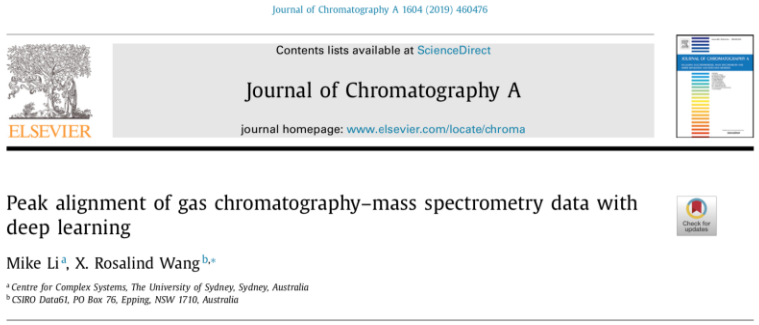
Deep Learning as the '*Next big thing*' in GC×GC Data Processing?

Machine Learning	Deep Learning
Possible to train with fewer data	Large datasets for training
Statistical algorithms	Artificial Neural Networks (ANN)
Structured data	Unstructured data
Limited tuning capabilities	Can be tuned in multiple ways
Simpler applications	More complex applications

Deep Learning as the future in GC×GC Data Processing?

➢ Examples

Example #1: ***Peak alignment***



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Peak alignment of gas chromatography–mass spectrometry data with deep learning

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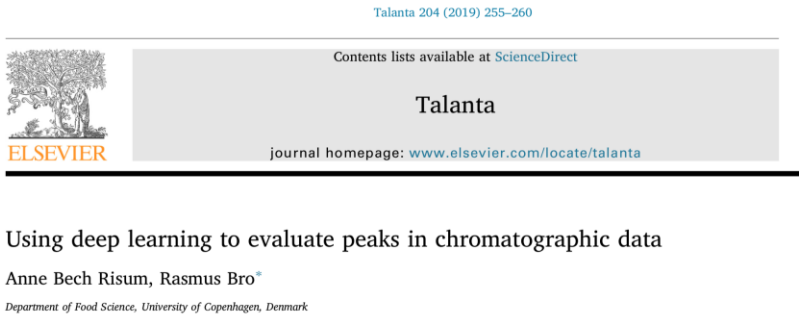
[b] CSIRO Data61, PO Box 76, Epping, NSW 1710, Australia

Example #2: ***Peak quality***



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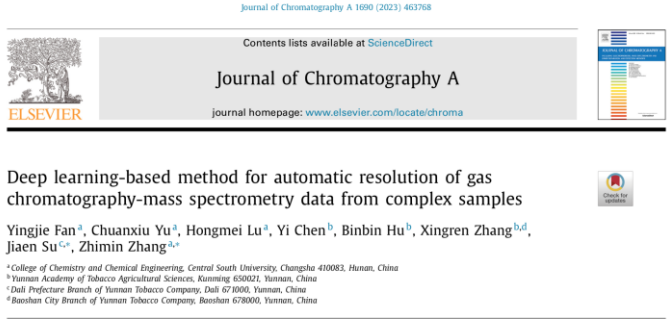
Using deep learning to evaluate peaks in chromatographic data

Anne Bech Risum, Rasmus Bro*

Department of Food Science, University of Copenhagen, Denmark

Example #3: ***Co-elution***



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Deep learning-based method for automatic resolution of gas chromatography-mass spectrometry data from complex samples

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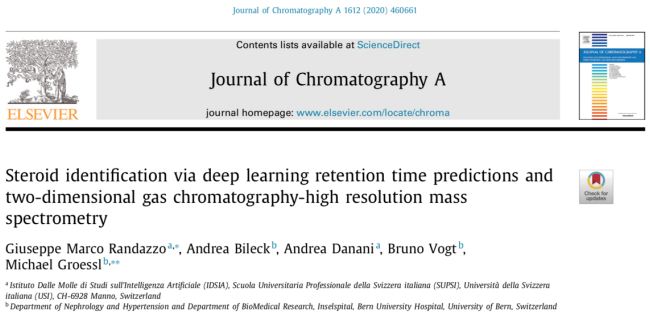
Example #4: ***Retention time and retention index predictions***



Journal of Chromatography A 1612 (2020) 460661

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Steroid identification via deep learning retention time predictions and two-dimensional gas chromatography-high resolution mass spectrometry

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DeepRel: Deep learning-based gas chromatographic retention index predictor

Tomáš Vrzal[a,*], Michaela Malečková[a,b], Jana Olšovská[a]

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Example #5: ***Analyte discovery***

CRISP: a deep learning architecture for GC × GC–TOFMS contour ROI identification, simulation and analysis in imaging metabolomics

Vivek Bhakta Mathema, Kassaporn Duangkumpha, Kwanjeera Wanichthanarak, Narumol Jariyasopit, Esha Dhakal, Nuankanya Sathirapongsasuti, Chagriya Kitiyakara, Yongyut Sirivatanauksorn, and Sakda Khoomrung

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