Organic and Biological Analytical Chemistry Group

Machine learning, the separation scientist acolyte for innovative method development

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Acknowledgements

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What is a separation scientist acolyte?

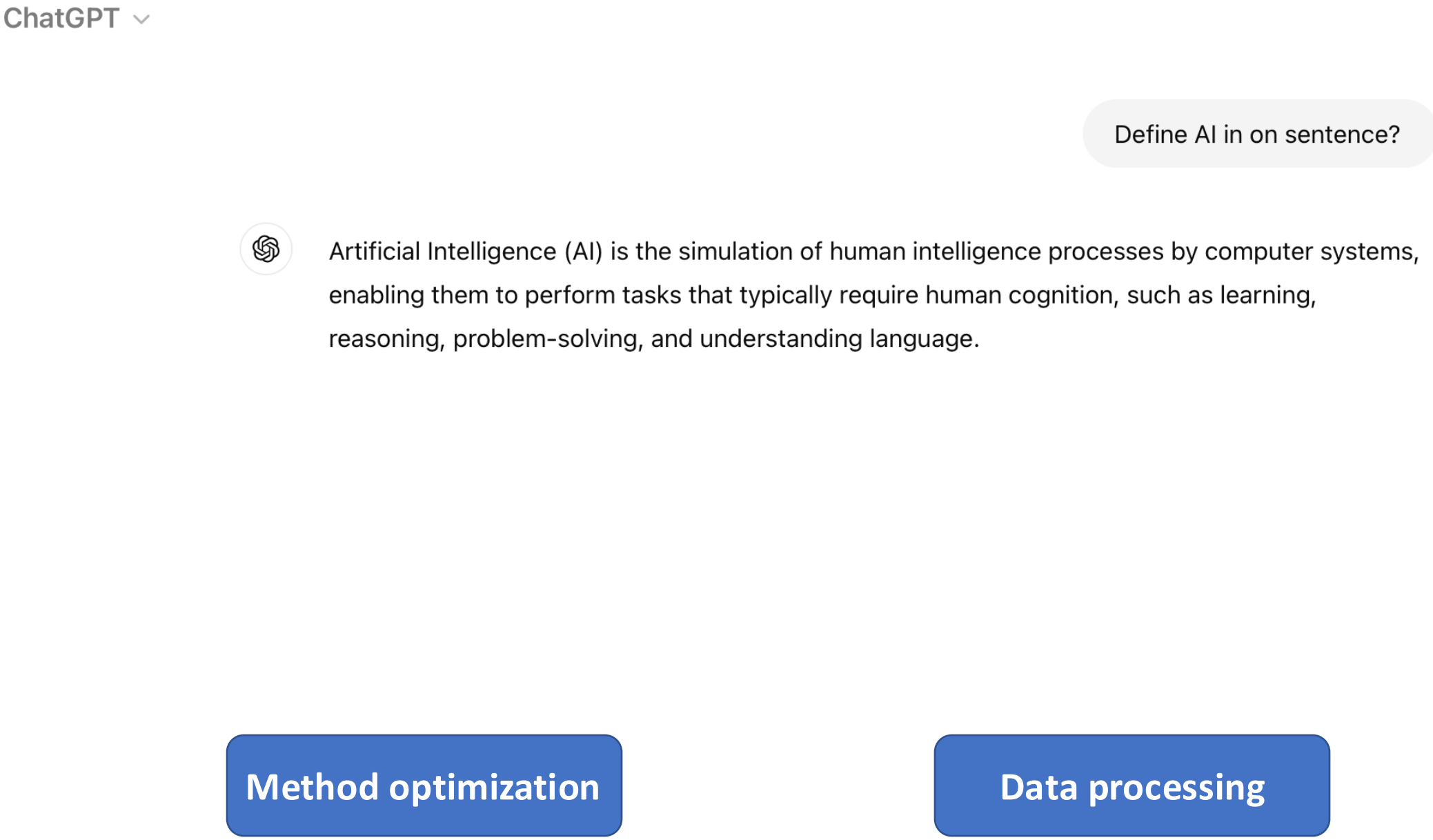
*An **acolyte** refer to a devoted follower or **assistant of a prominent figure**. An acolyte is someone who **supports and learns from a more experienced person**, sometimes in political, academic, or professional environments.*

*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



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GPT concept

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

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

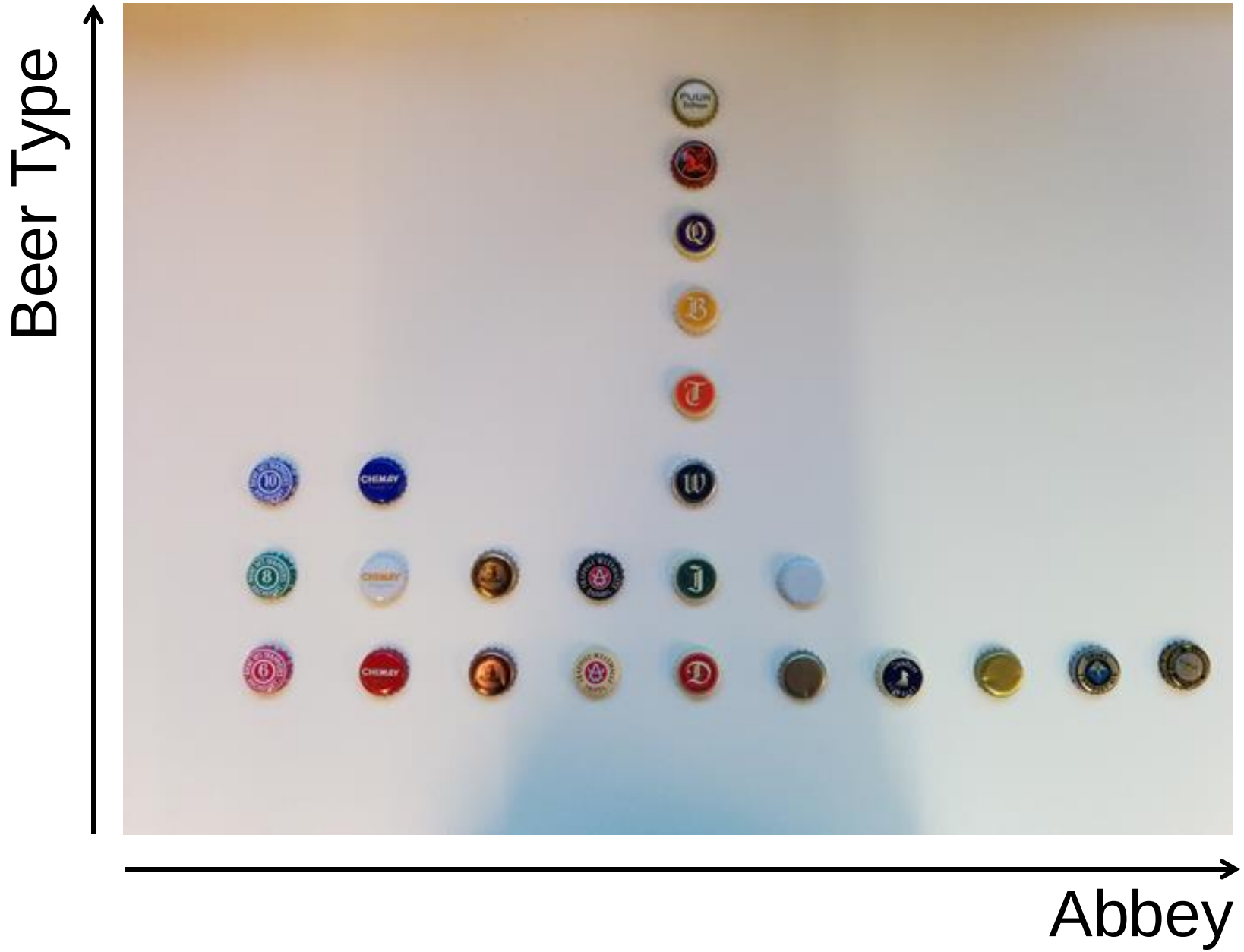
Pre-trained: *The model has been trained on a large amount of data* → The quality of the training

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

GC×GC-TOFMS: the principle

The sample

Abbey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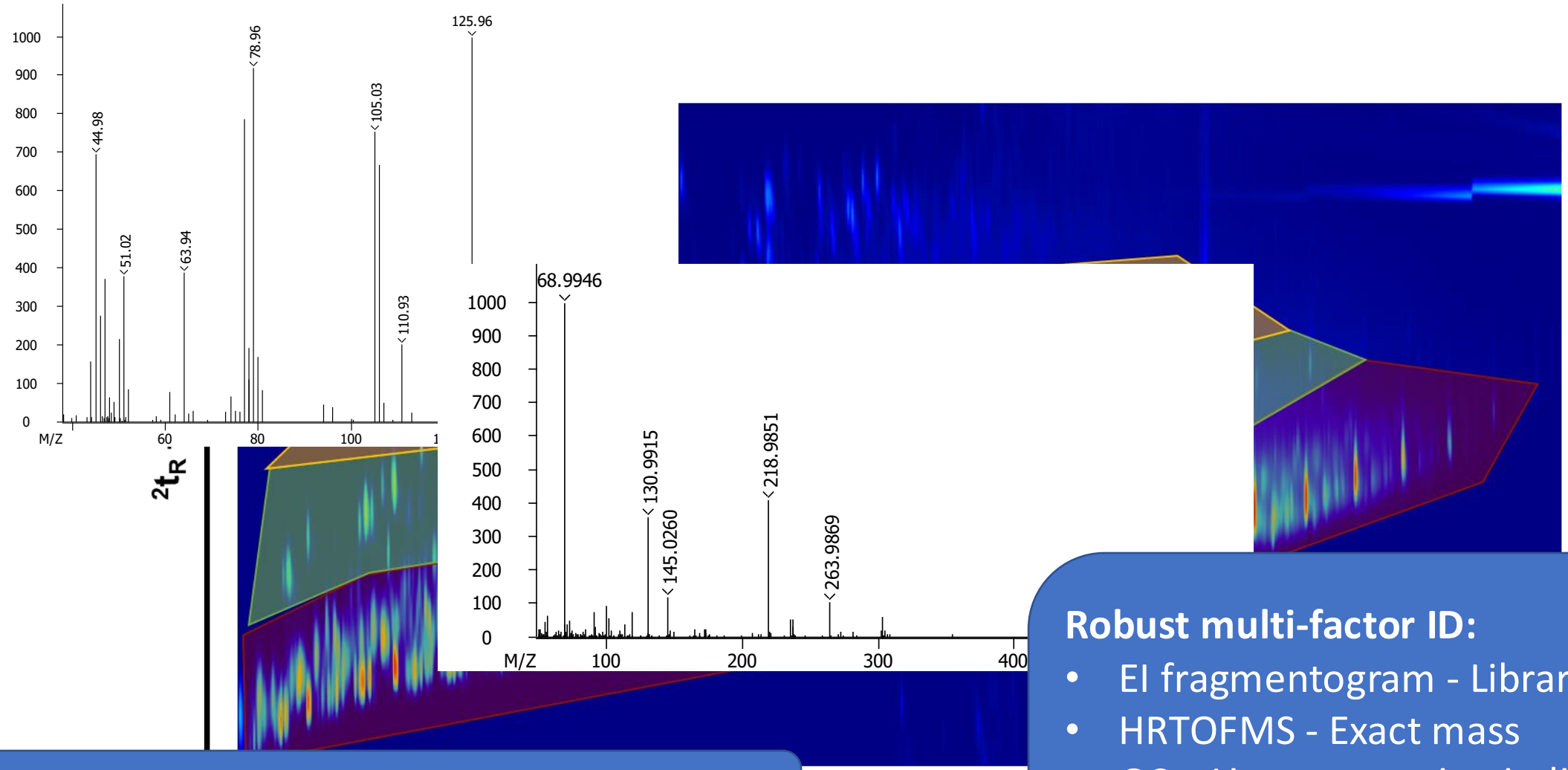


How to handle the method development?

How to manage the data processing?

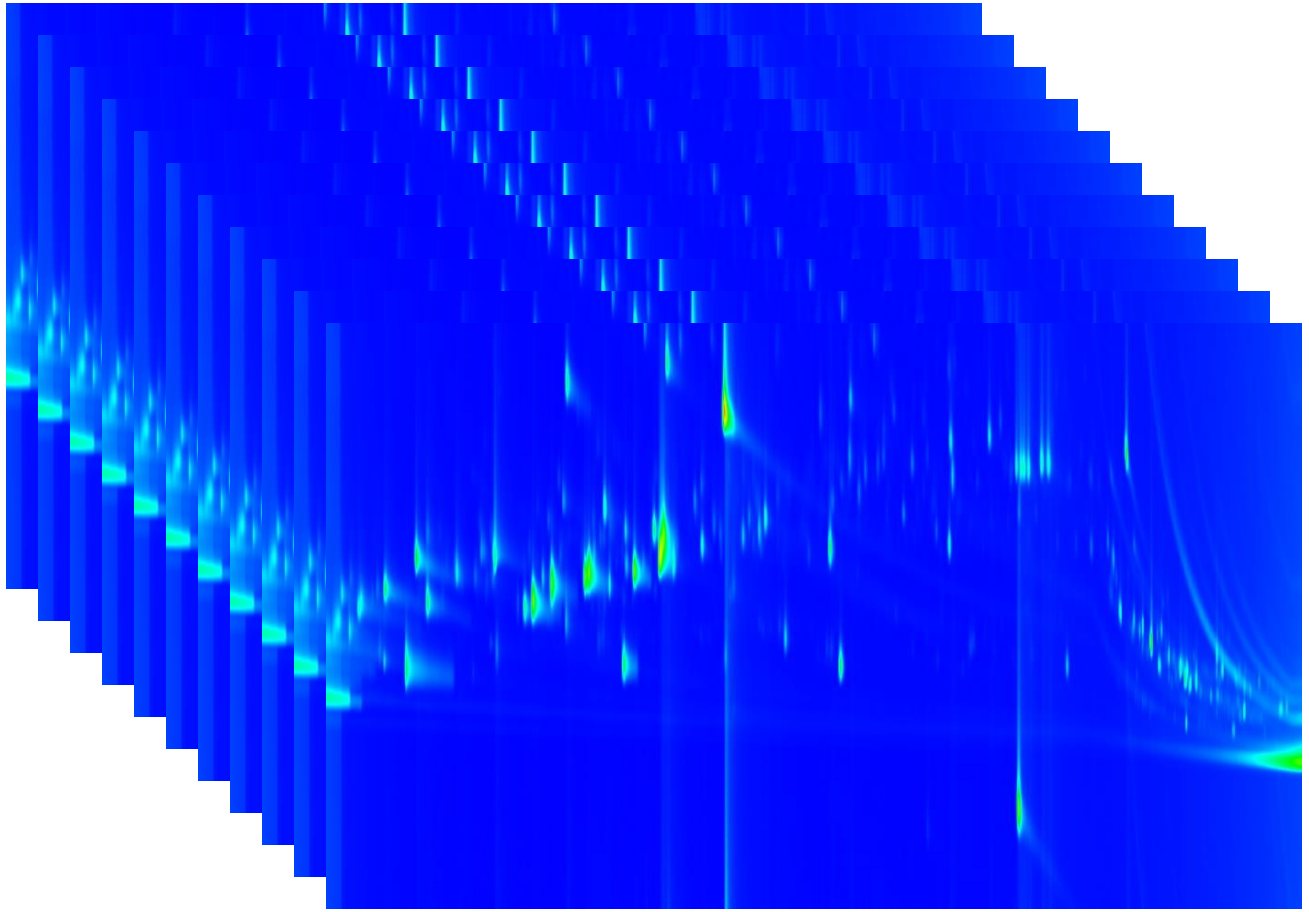
Robust multi-factor ID:

- EI fragmentogram - Library match
- HRTOFMS - Exact mass
- GC – Linear retention indices
- GCxGC – Elution pattern

→ **Level 2 MSI ID**

Generative I: Method optimization

LECO Simply GC×GC®



Generative I: Method optimization

analytical chemistry

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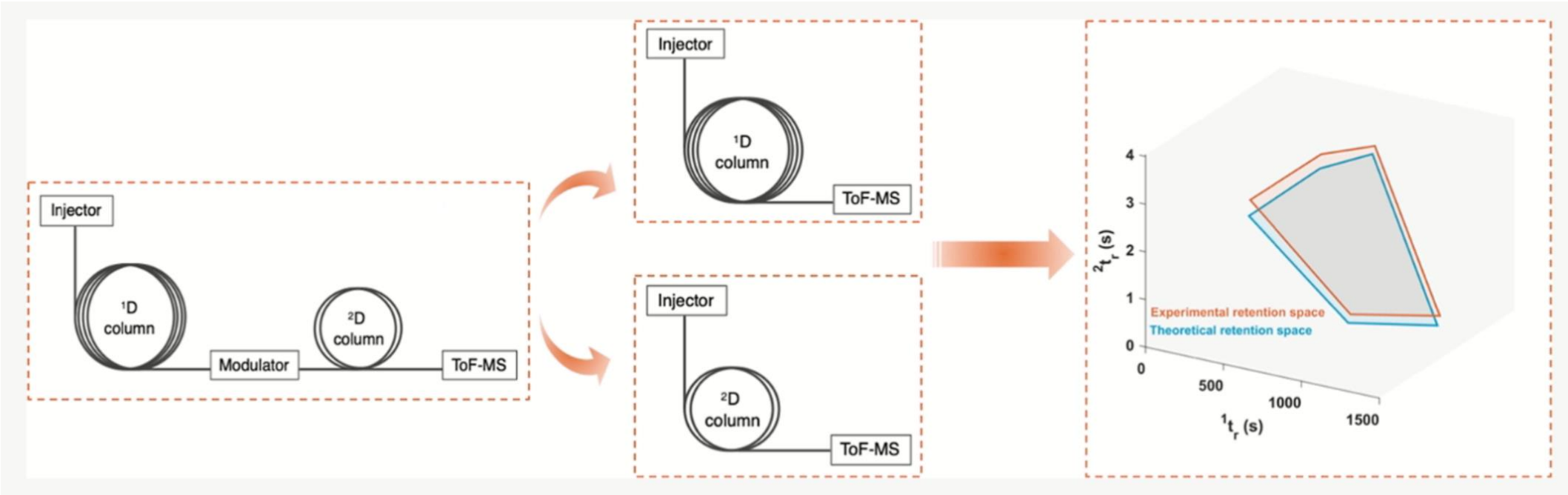
Top-Down Approach to Retention Time Prediction in Comprehensive Two-Dimensional Gas Chromatography–Mass Spectrometry

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

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



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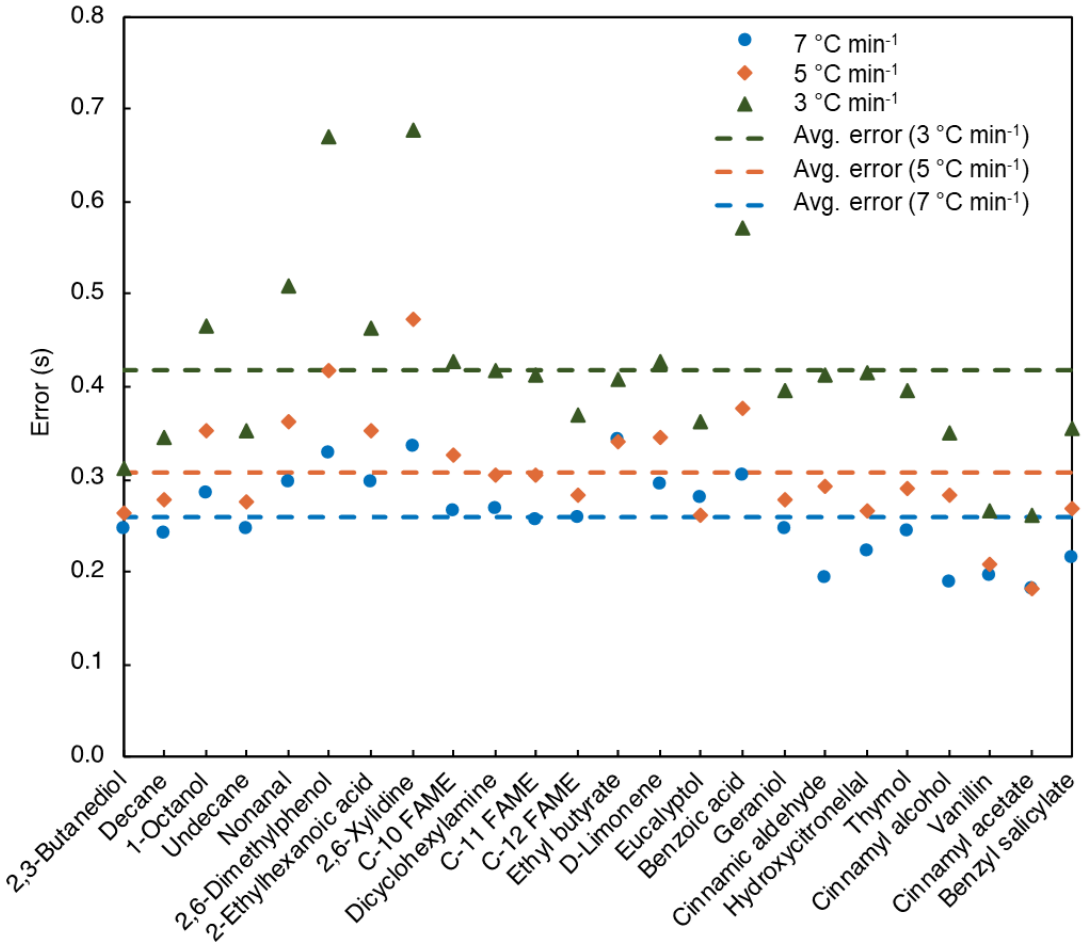

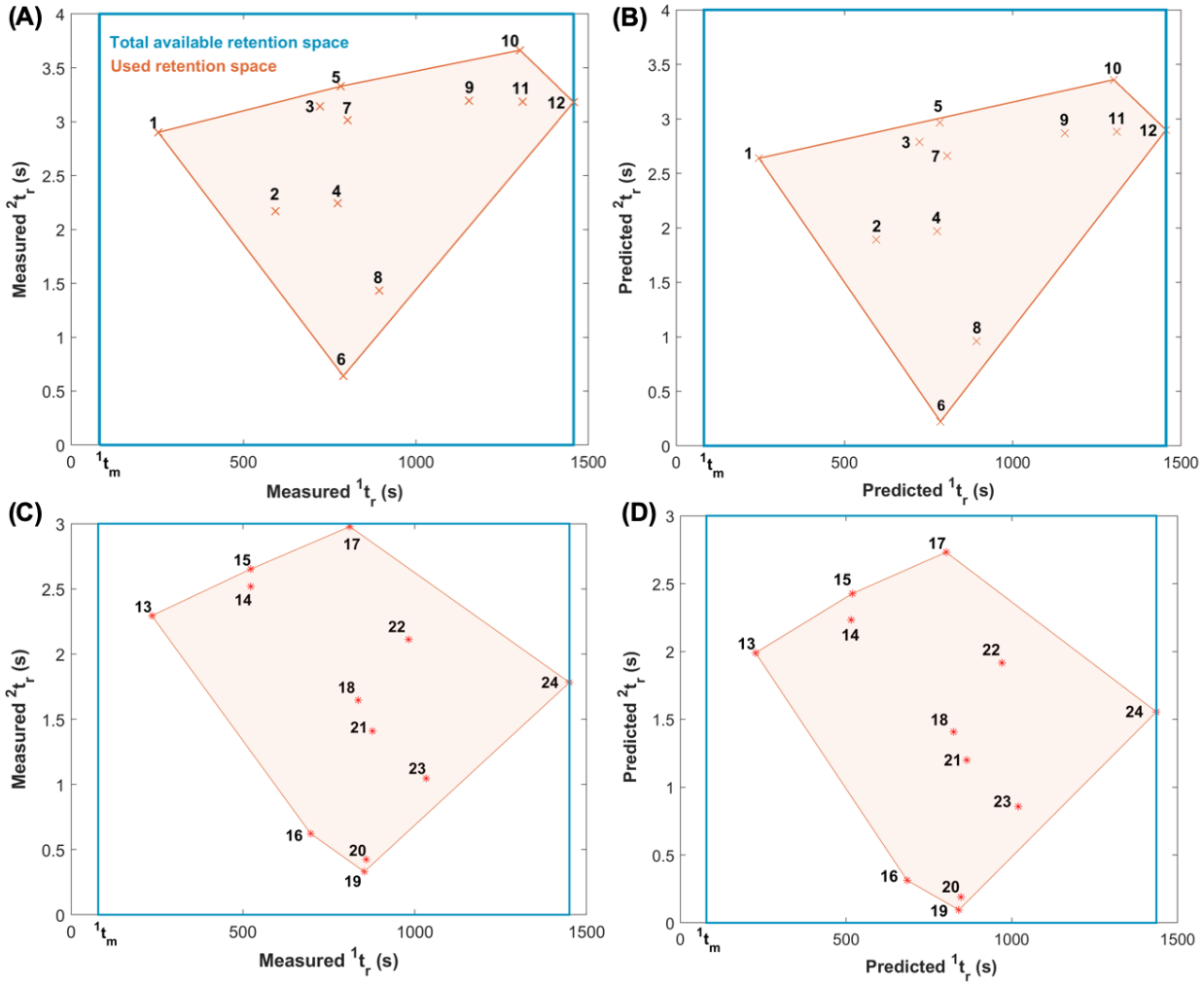

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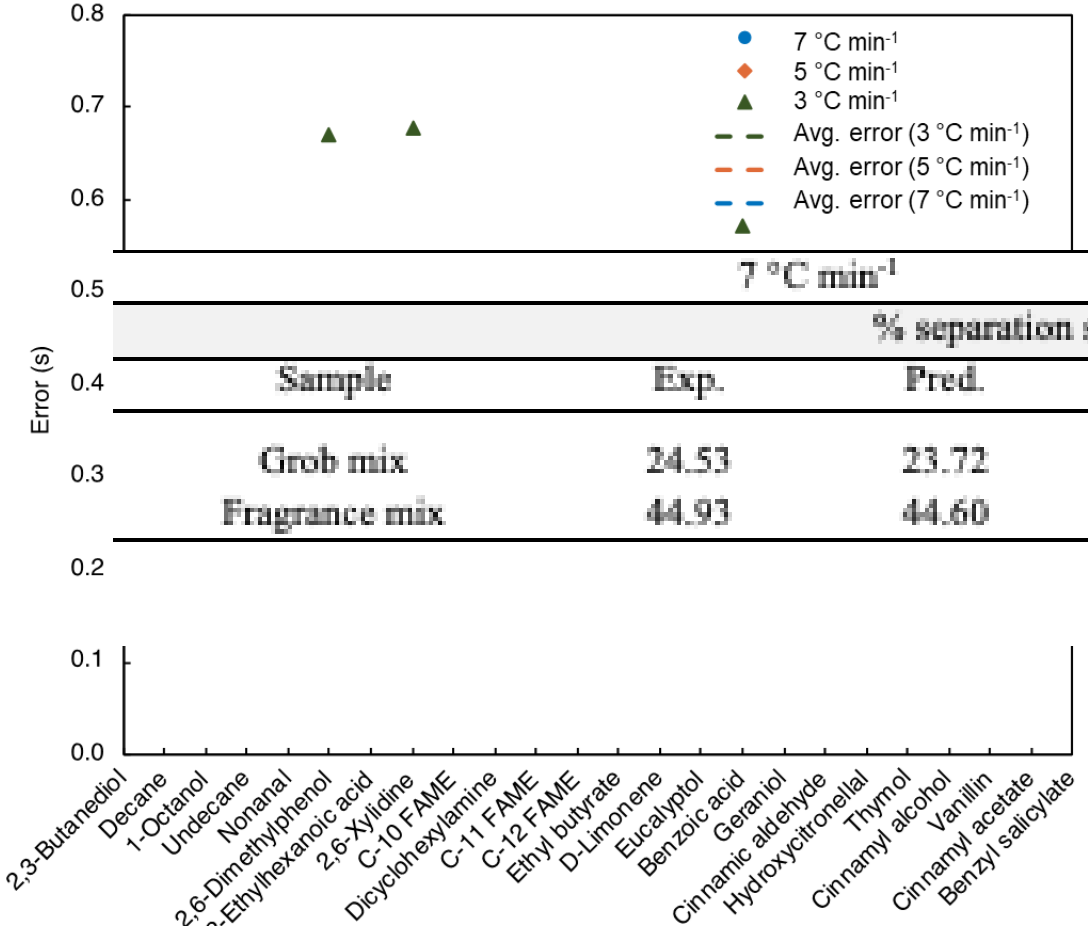
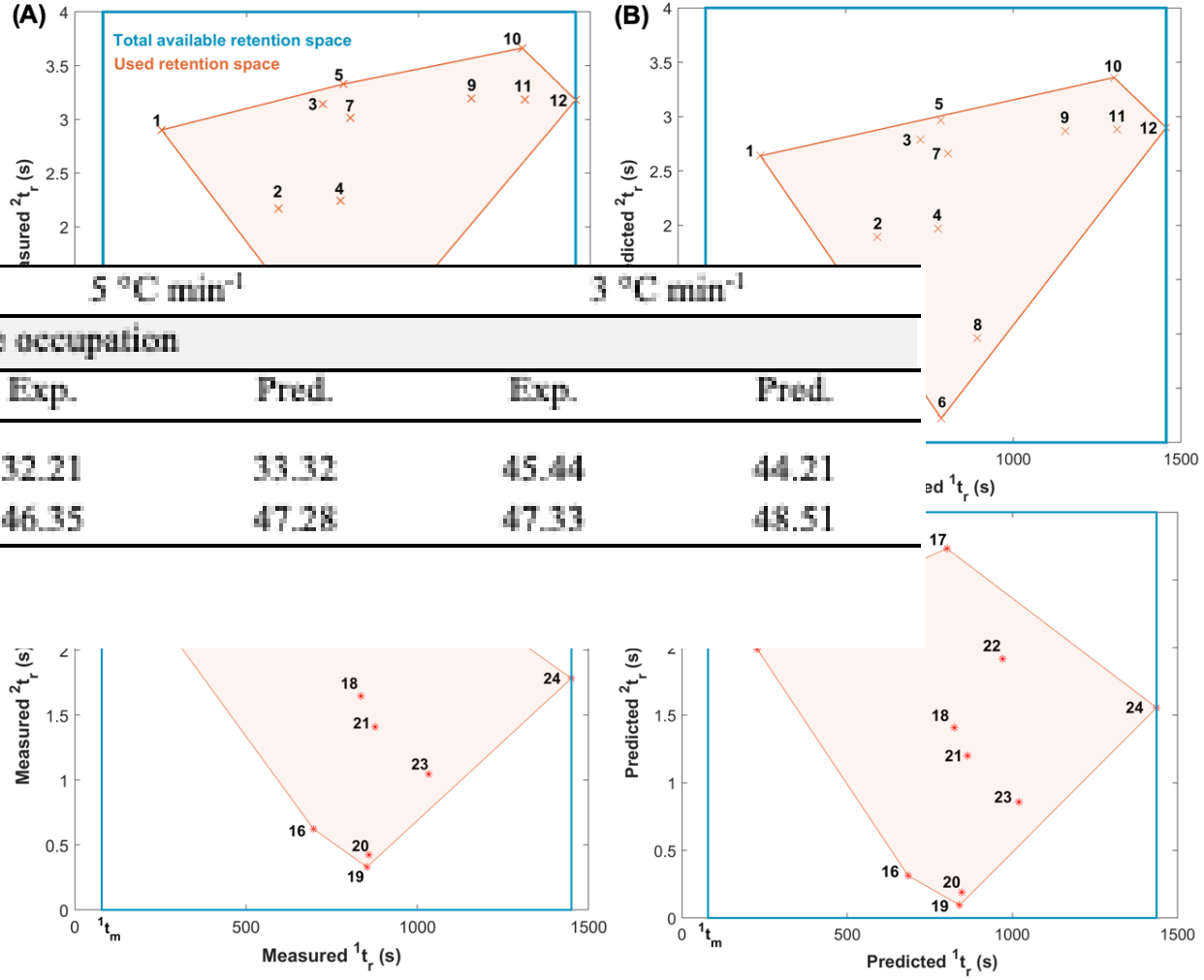


% separation space occupation						
	7 °C min^{-1}		5 °C min^{-1}		3 °C min^{-1}	
Sample	Exp.	Pred.	Exp.	Pred.	Exp.	Pred.
Grob mix	24.53	23.72	32.21	33.32	45.44	44.21
Fragrance mix	44.93	44.60	46.35	47.28	47.33	48.51



Generative I: Method optimization

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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*

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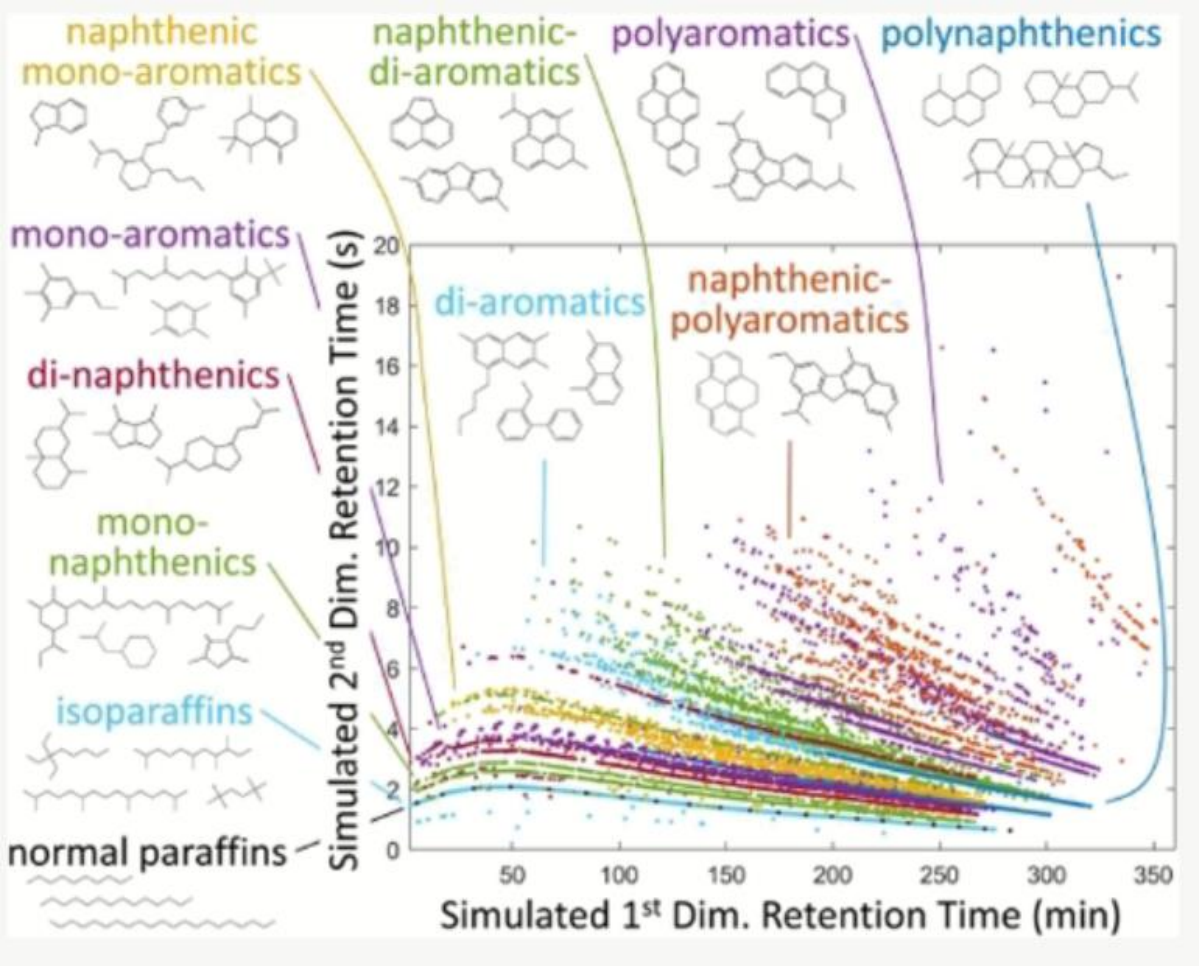

Bringing AI in the game!

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

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

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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

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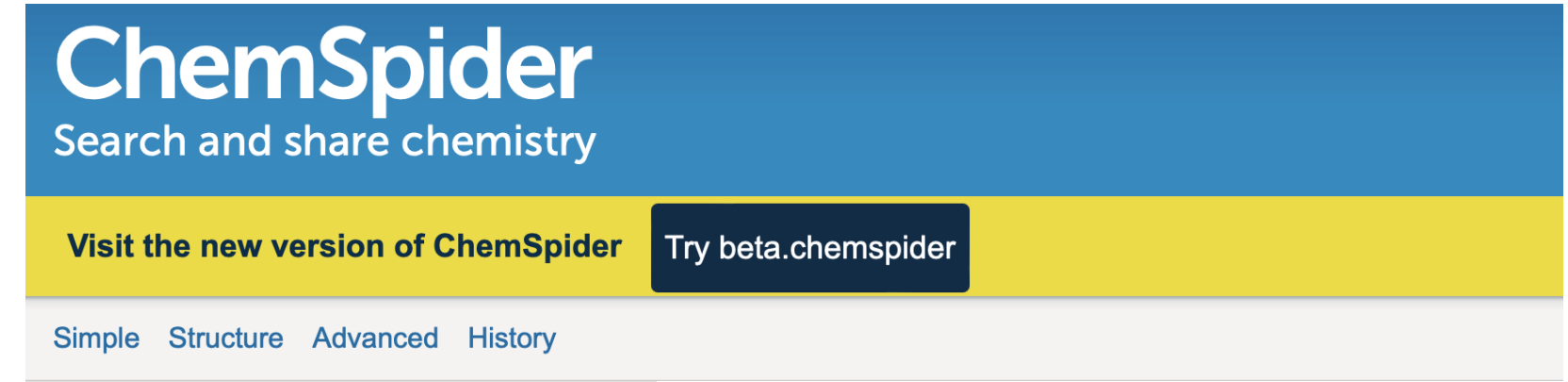
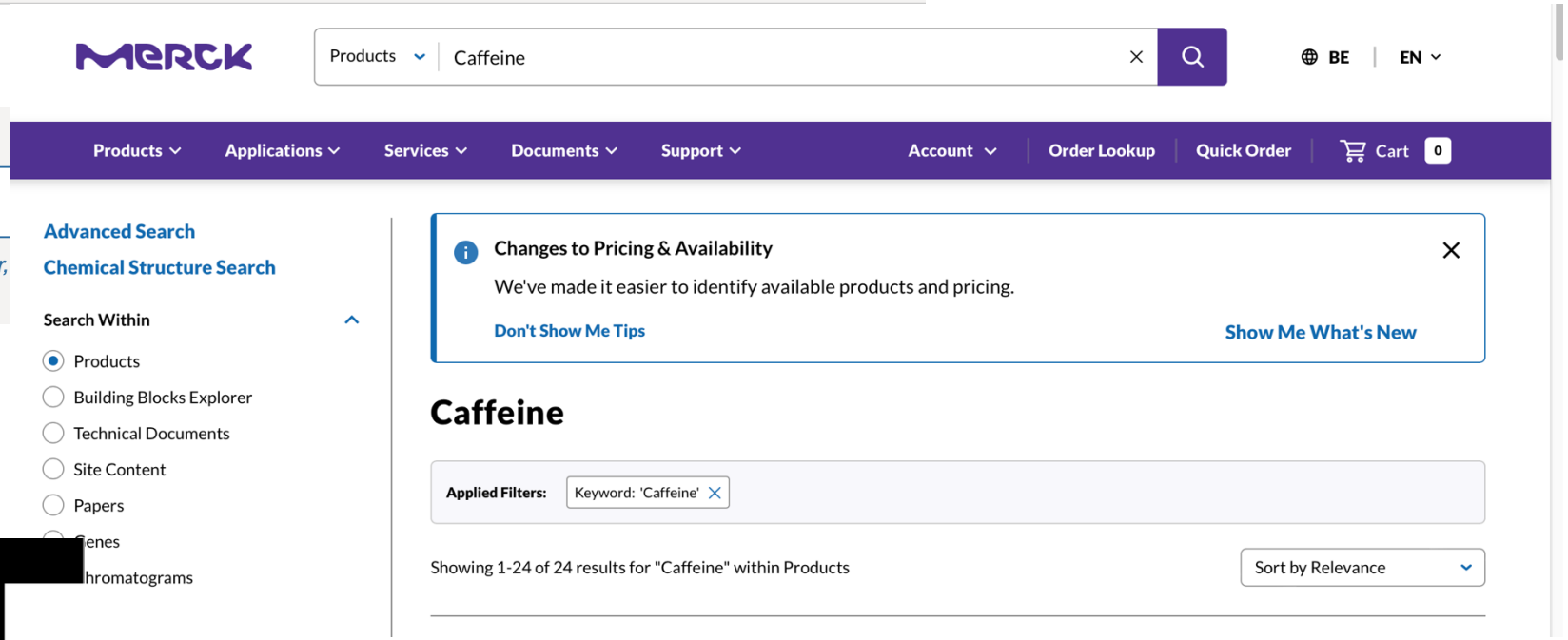
Pre-trained: we need large data!





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**

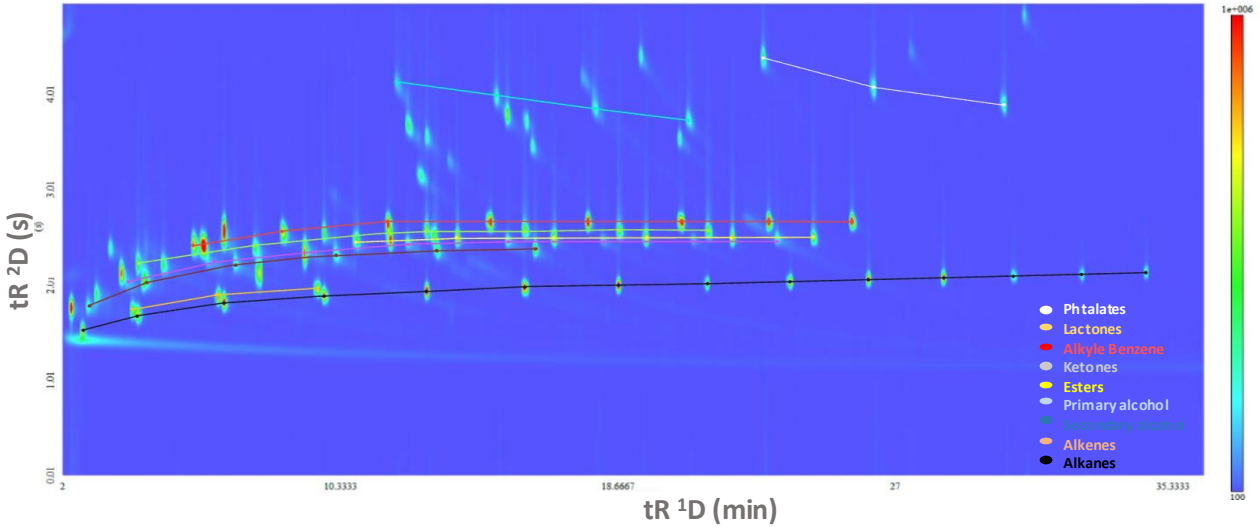
Polarity	Apolar	Mid-Polar	Polar
Apolar			
Mid-Polar			
Polar			

Normal orthogonality

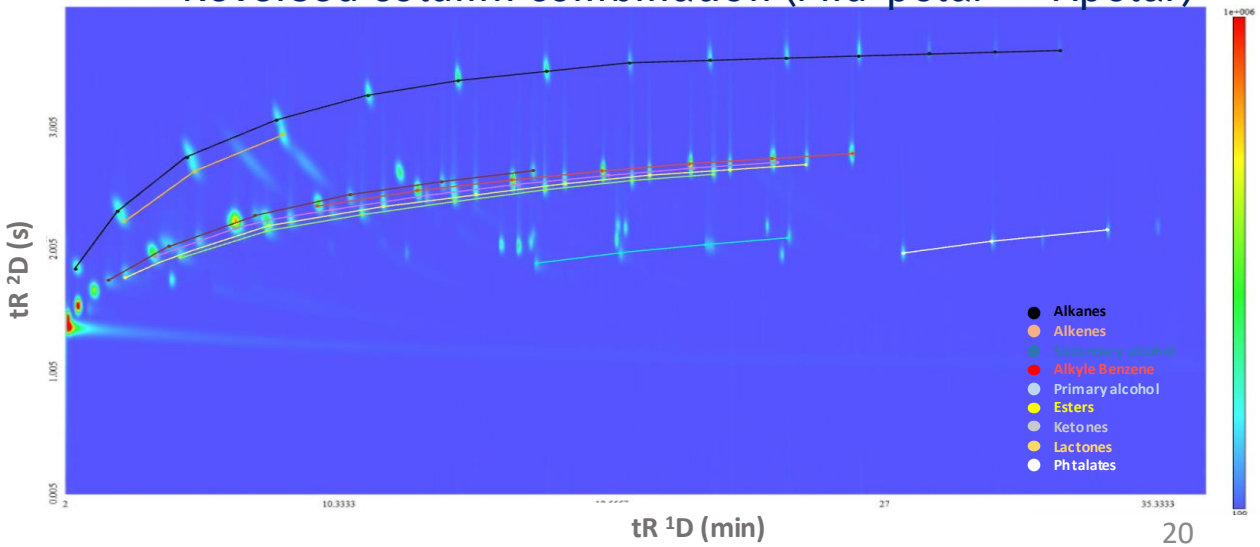
Non-orthogonal

Reversed orthogonality

Normal column combination (Apolar × Mid-polar)



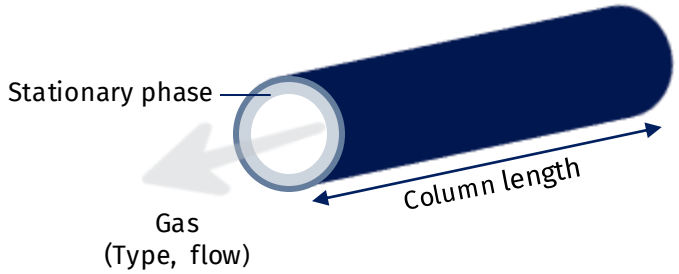
Reversed column combination (Mid-polar × Apolar)



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)

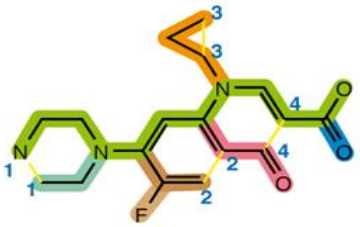


2 – Data Collection

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

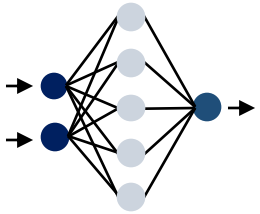
3 – Modelisation-Prediction

Retention indices prediction

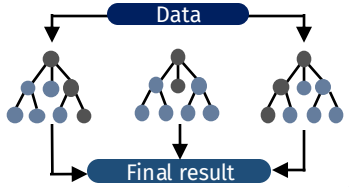
(System-independent constants)

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

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