



GcDUO: A Batch Processing Framework Integrating PARAFAC and PARAFAC2 for GC×GC-MS Data Analysis

Maria Llambrich, PhD

Frans M. van der Kloet, Lluc Sementé, Anaïs Rodrigues, Saer Samanipour, Pierre-Hugues
Stefanuto, Johan A. Westerhuis, Raquel Cumeras, Jesús Brezmes

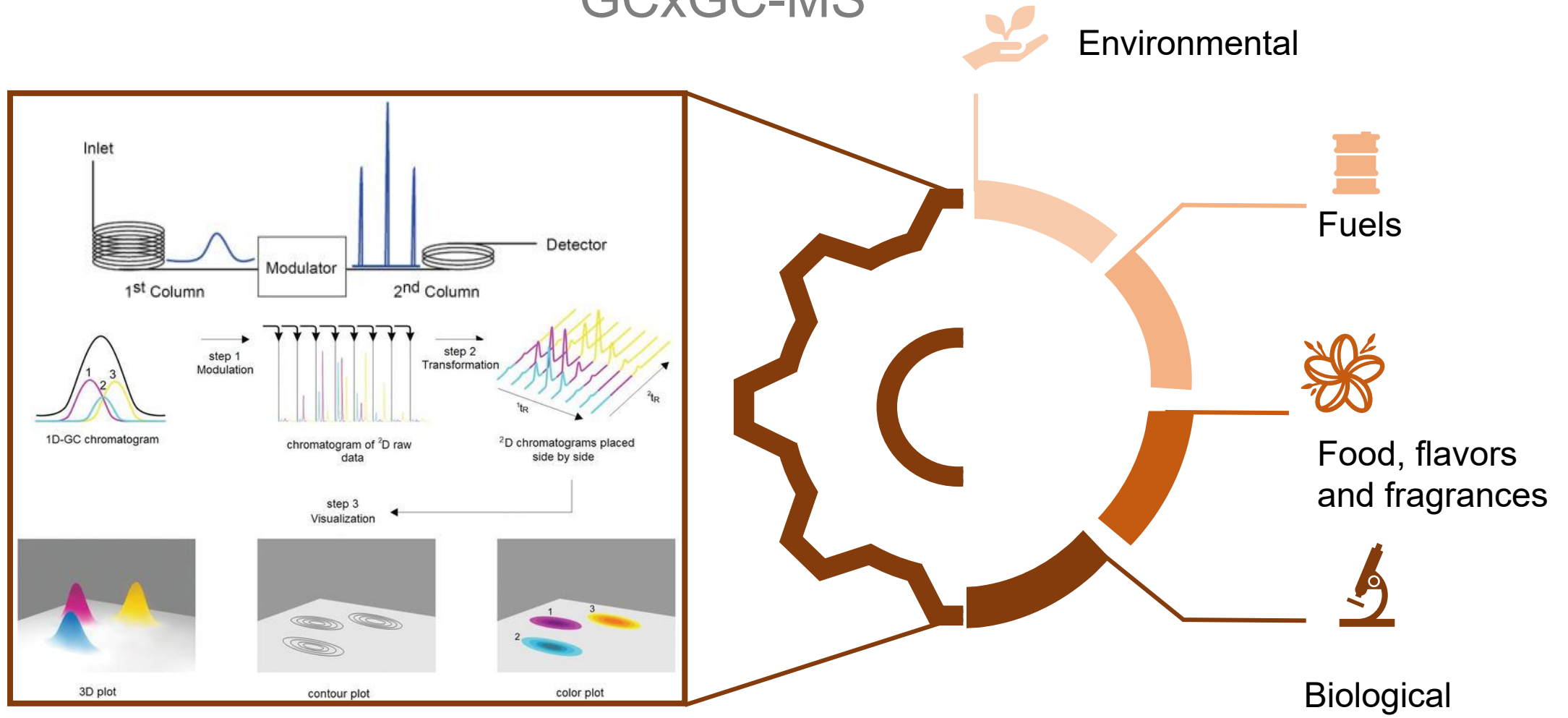
Williamsburg, January 12-15, 2026

Outline

- >> Background
- >> GcDUO algorithm
- >> Results
- >> Conclusions
- >> Acknowledgements

Comprehensive Gas Chromatography – Mass spectrometry

GCxGC-MS



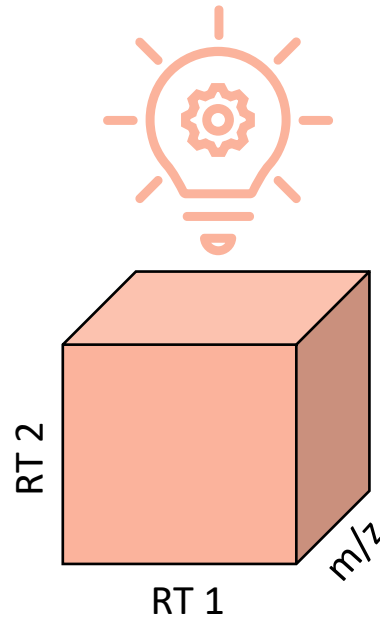
GCxGC-MS data analysis

Third-order tensor

Noise reduction
deconvolution
calibration

Extract relevant
information

Biological meaning



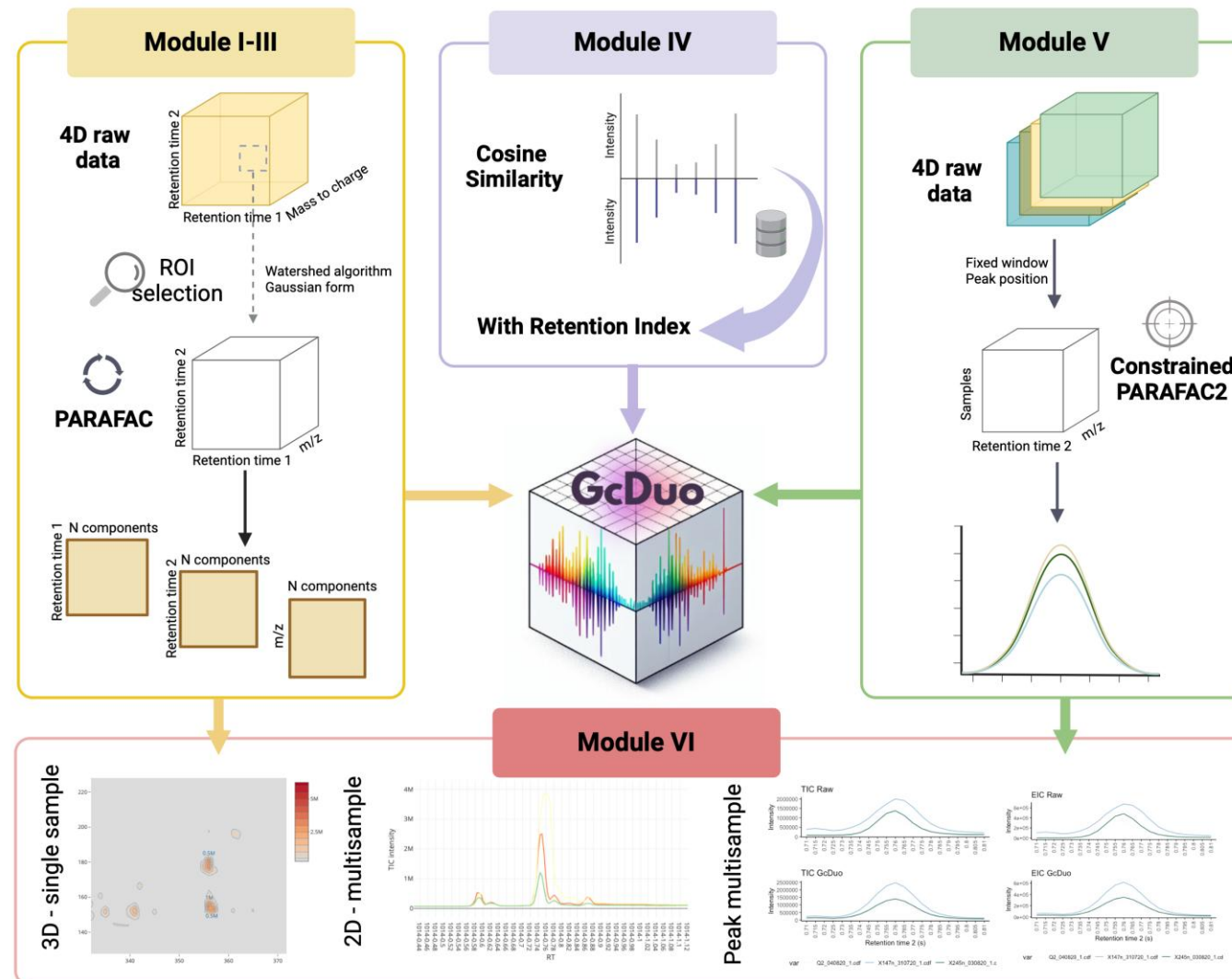
ChromatOF®

GC Image
Software for Multidimensional Chromatography

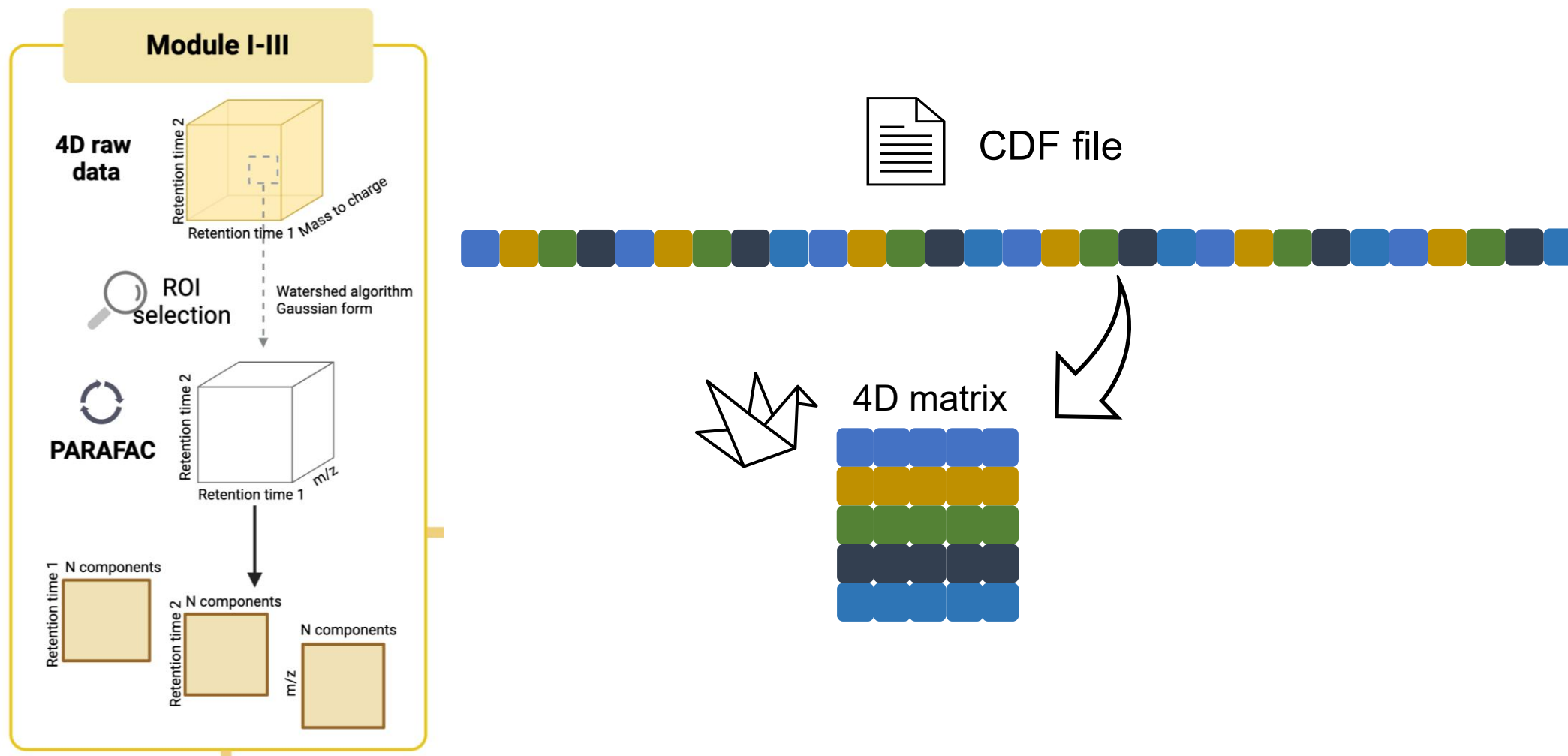
ChromSpace

Limited open source
Non-targeted solution

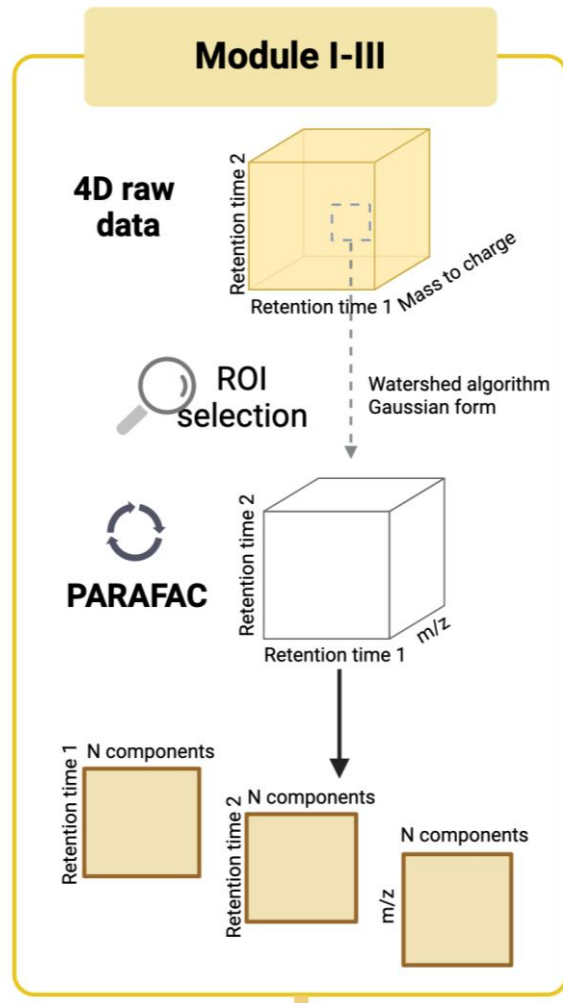
GcDUO architecture



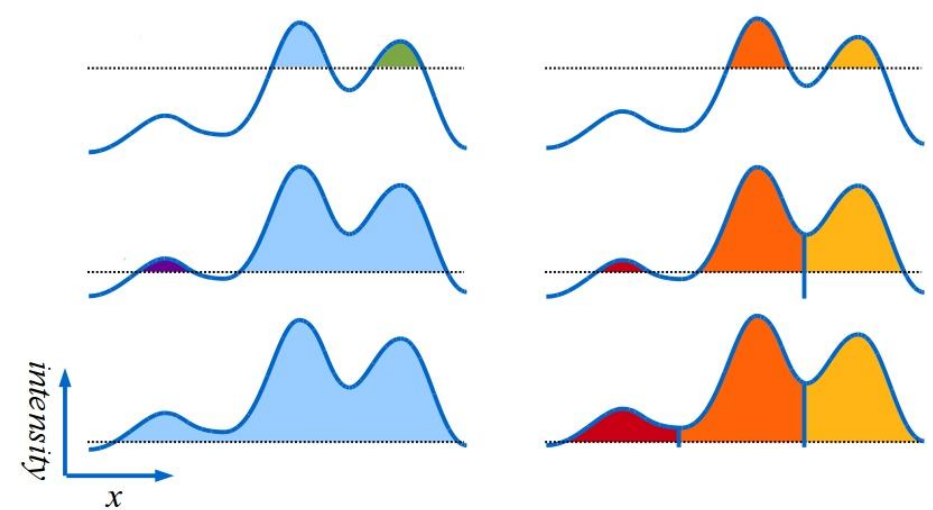
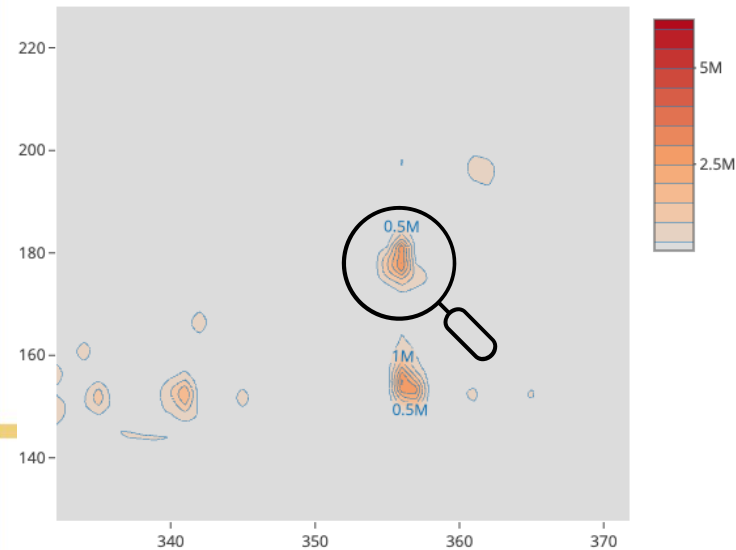
GcDUO architecture



GcDUO architecture

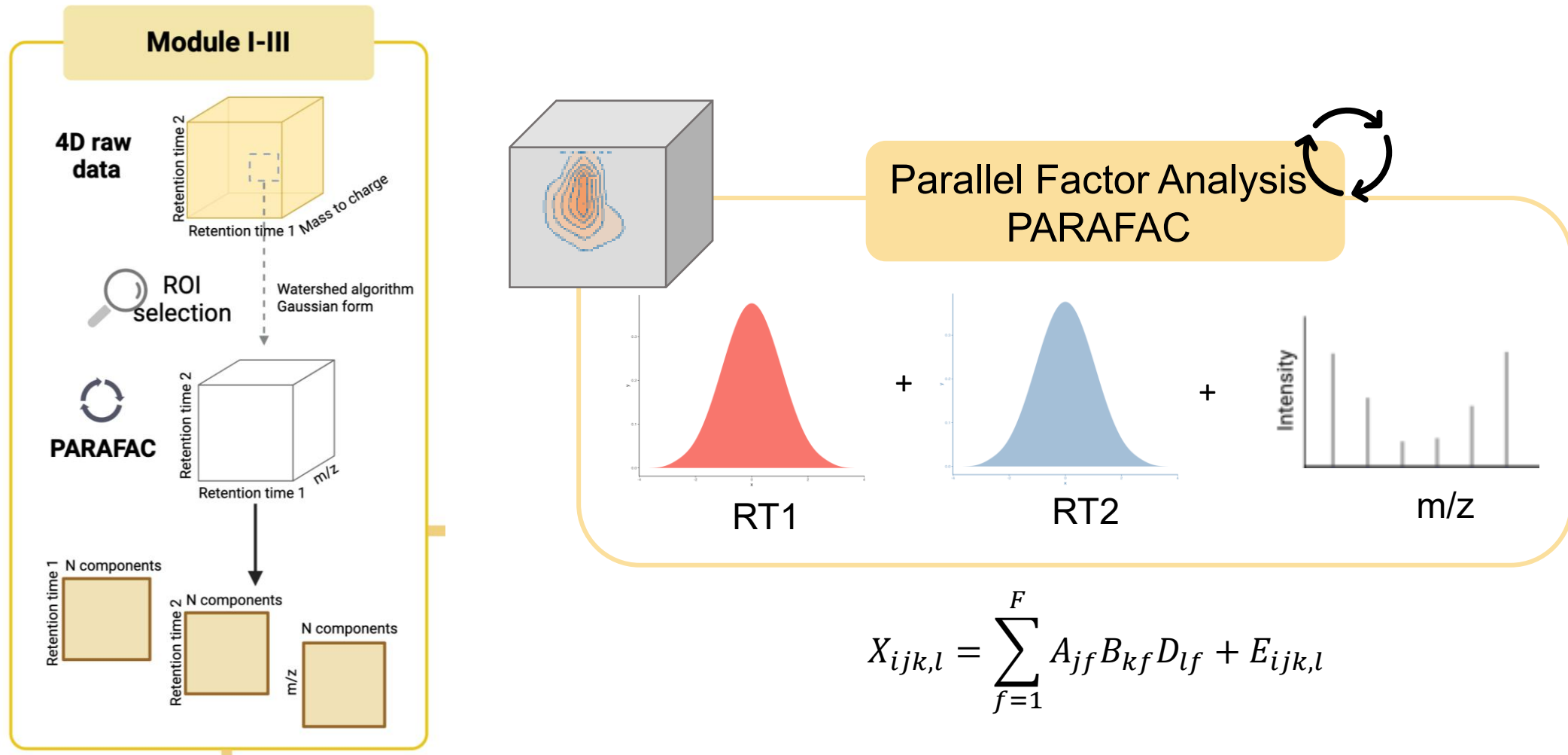


ROI selection – Watershed algorithm

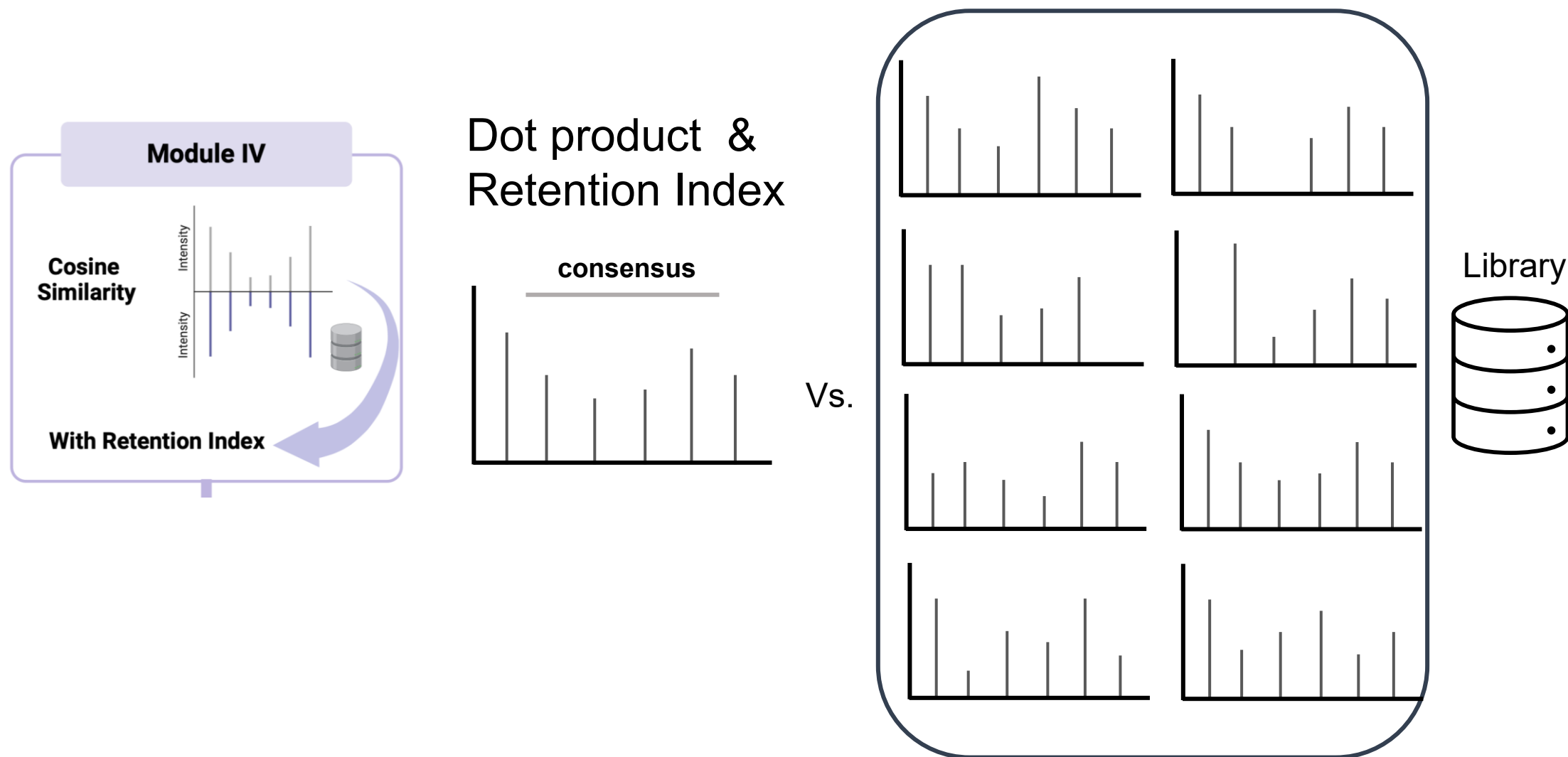


Watershed algorithm procedure

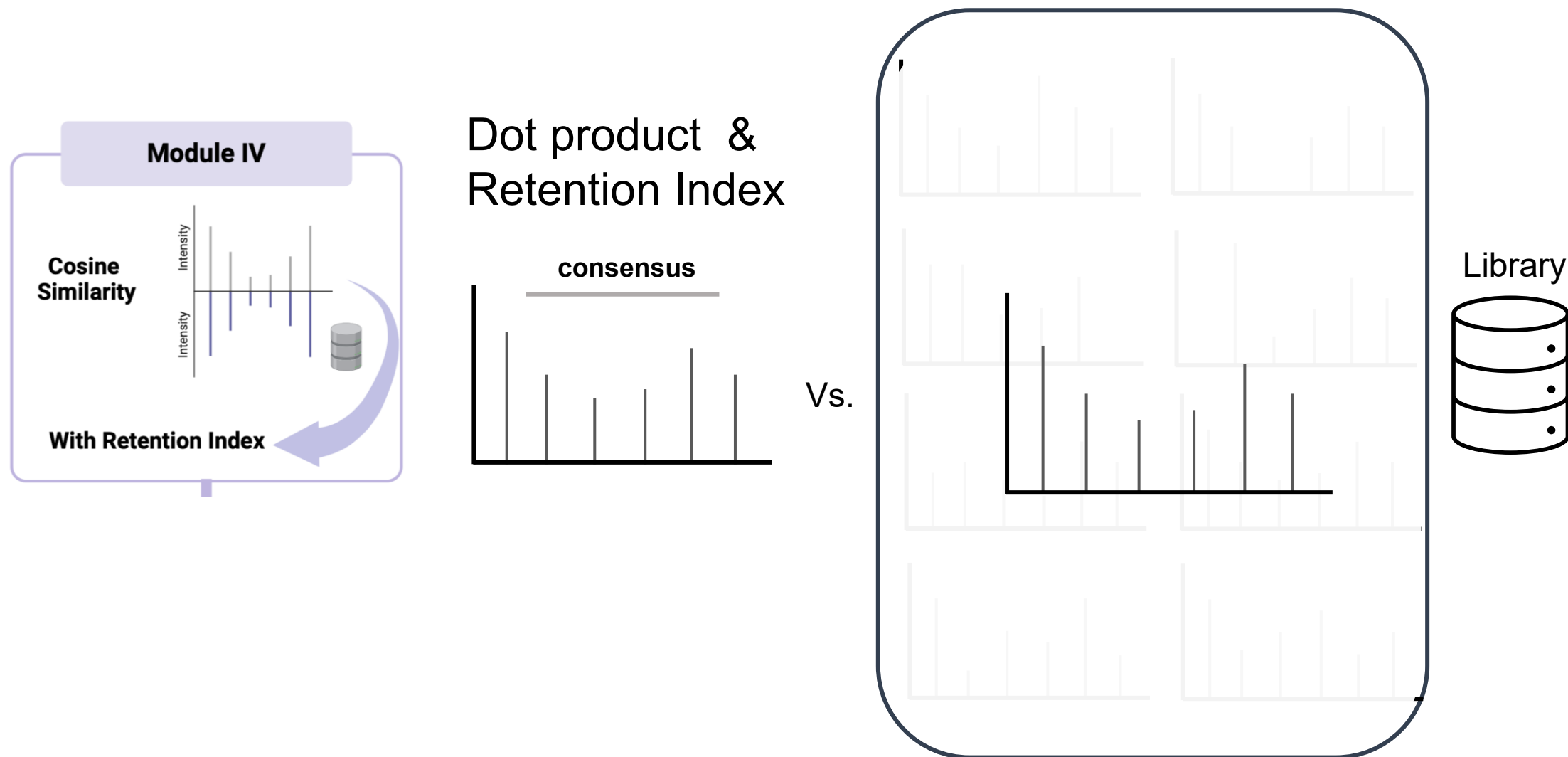
GcDUO architecture



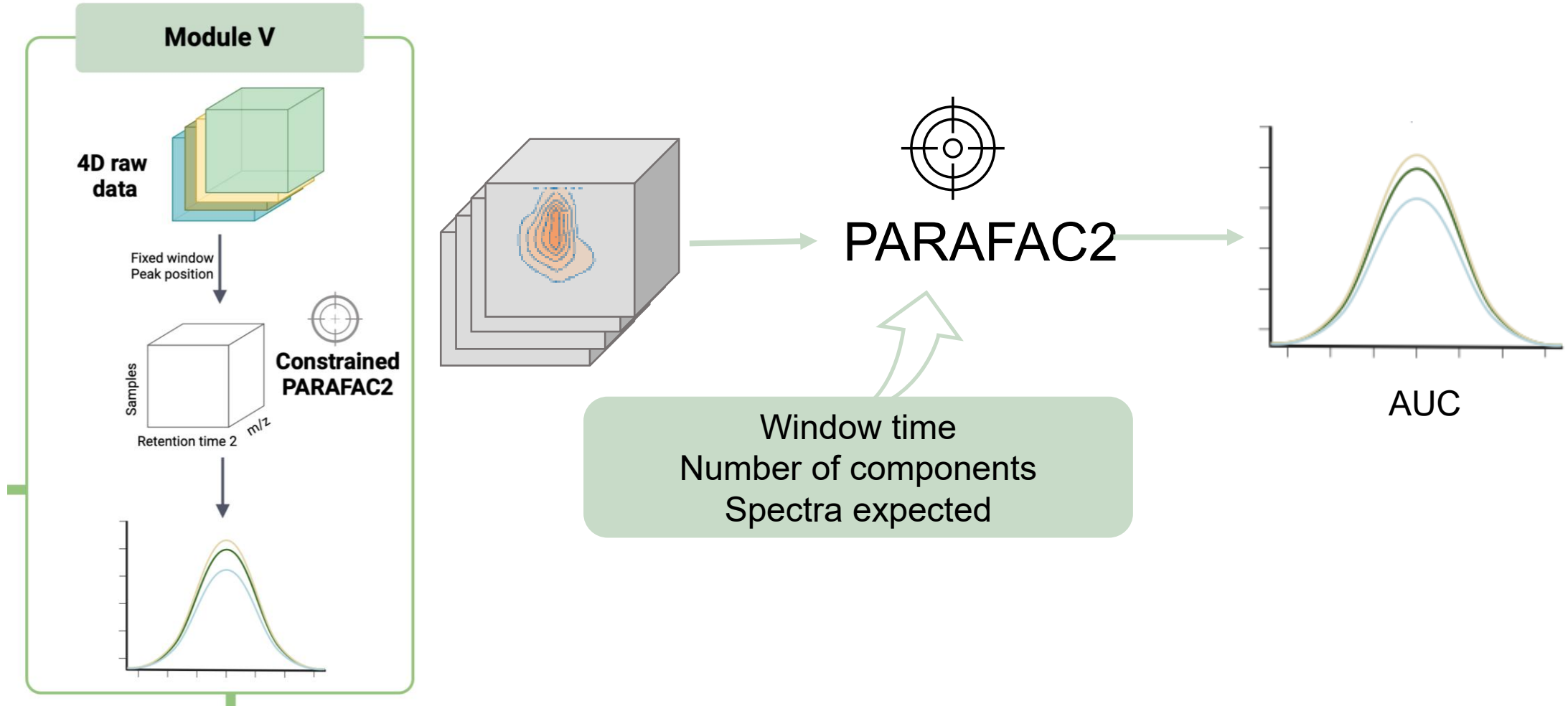
GcDUO architecture



GcDUO architecture



GcDUO architecture



GcDUO results

Training dataset:

 **HARVARD**
Dataverse

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Harvard Dataverse > Dataverse_GCxGC_Benchmarking >

Benchmark GCxGC Data, Standards, Fragrances and Allergens

Version 1.1



Weggler, Benedikt; Dubois, Lena; Gawlitta, Nadine; Gröger, Thomas; Moncur, Jhon; Mondello, Luigi; Reichenbach, Steven; Tranchida, Peter; Zhao, Zhijun; Zimmermann, Ralf; Zoccali, Mariosimone; Focant, Jean-François, 2020, "Benchmark GCxGC Data, Standards, Fragrances and Allergens", <https://doi.org/10.7910/DVN/KA5BTU>, Harvard Dataverse, V1

Cite Dataset ▾ Learn about [Data Citation Standards](#).

Access Dataset ▾

Contact Owner Share

Dataset Metrics ?

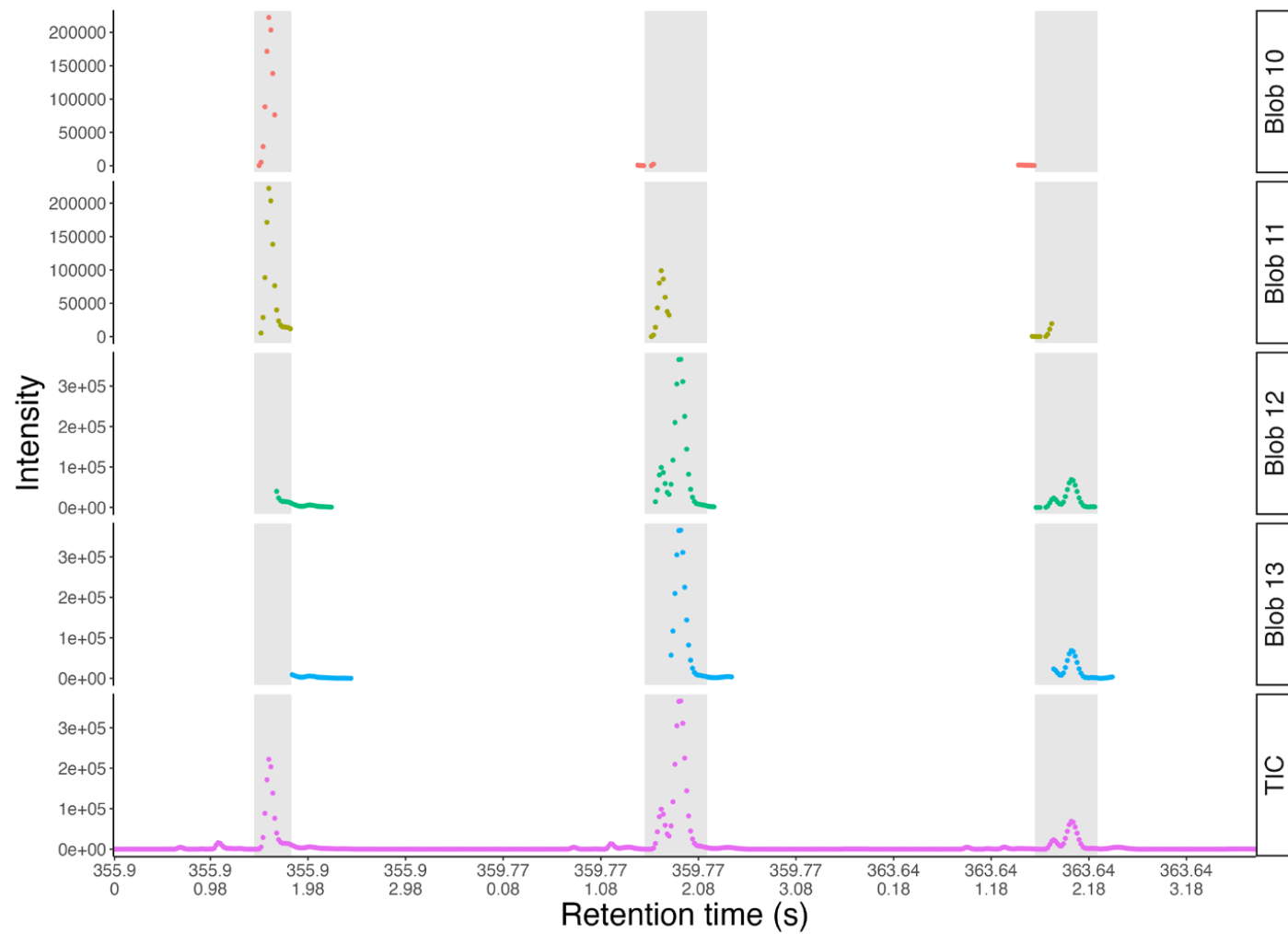
529 Downloads ?

Description ?

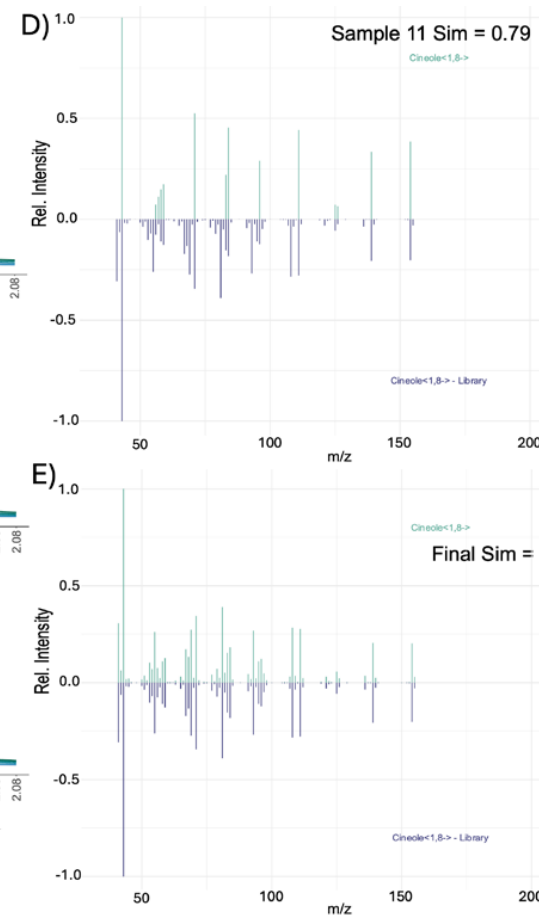
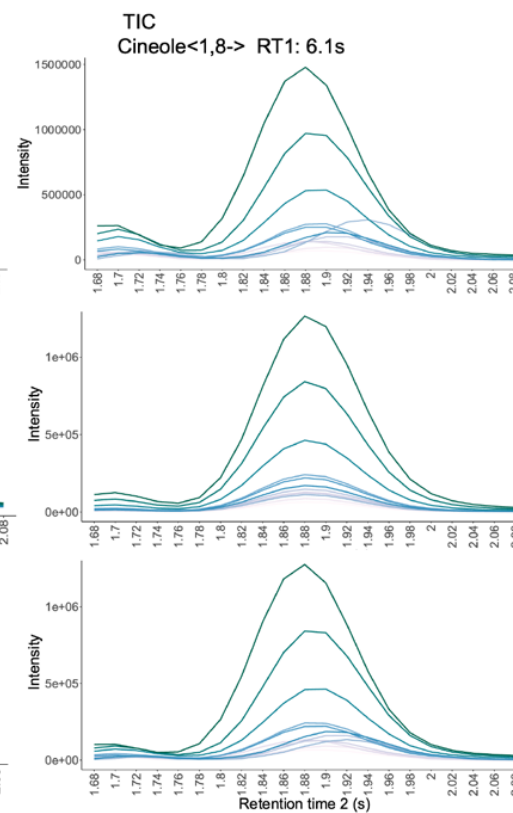
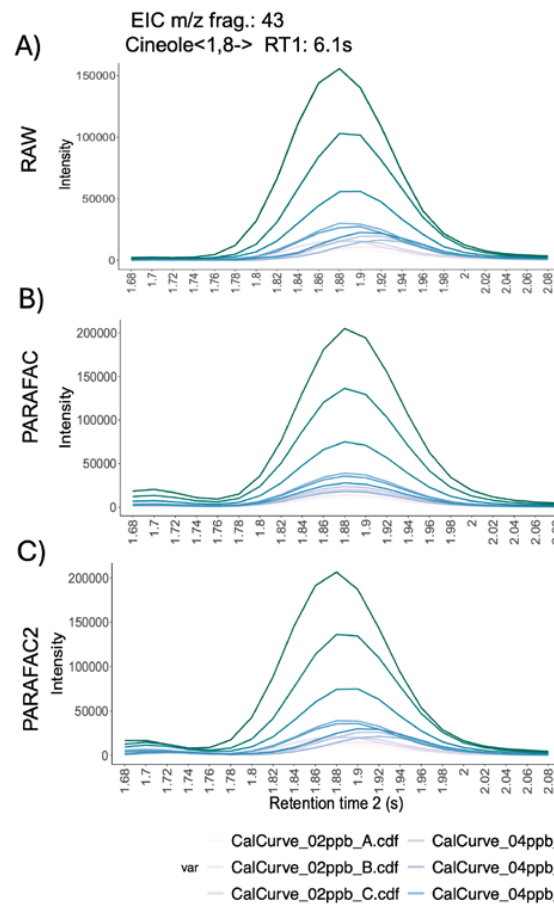
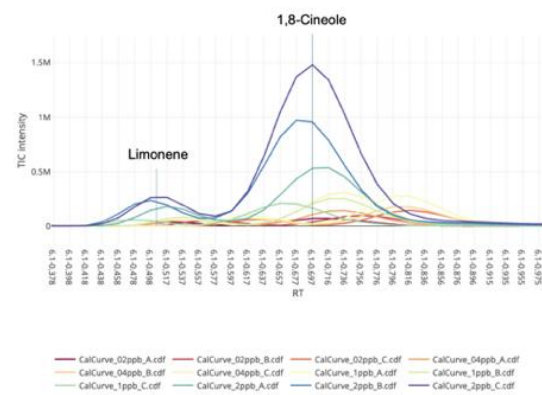
This dataset contains GCGC -ToF/MS data of four concentration of a Fragrance and Allergene Testmixture (Restek, Bellfonte) containing 36 compounds. Additionally 1F-Naphthalene was used as internal Standard and an Alkane Retention Index(C7-C30) mixture was added. Each point was measured in triplicates. Concentration as follows:

1. 2ppb
2. 1ppb
3. 0.4ppb
4. 0.2ppb

GcDUO results



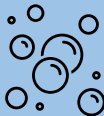
GcDUO results



GcDUO results

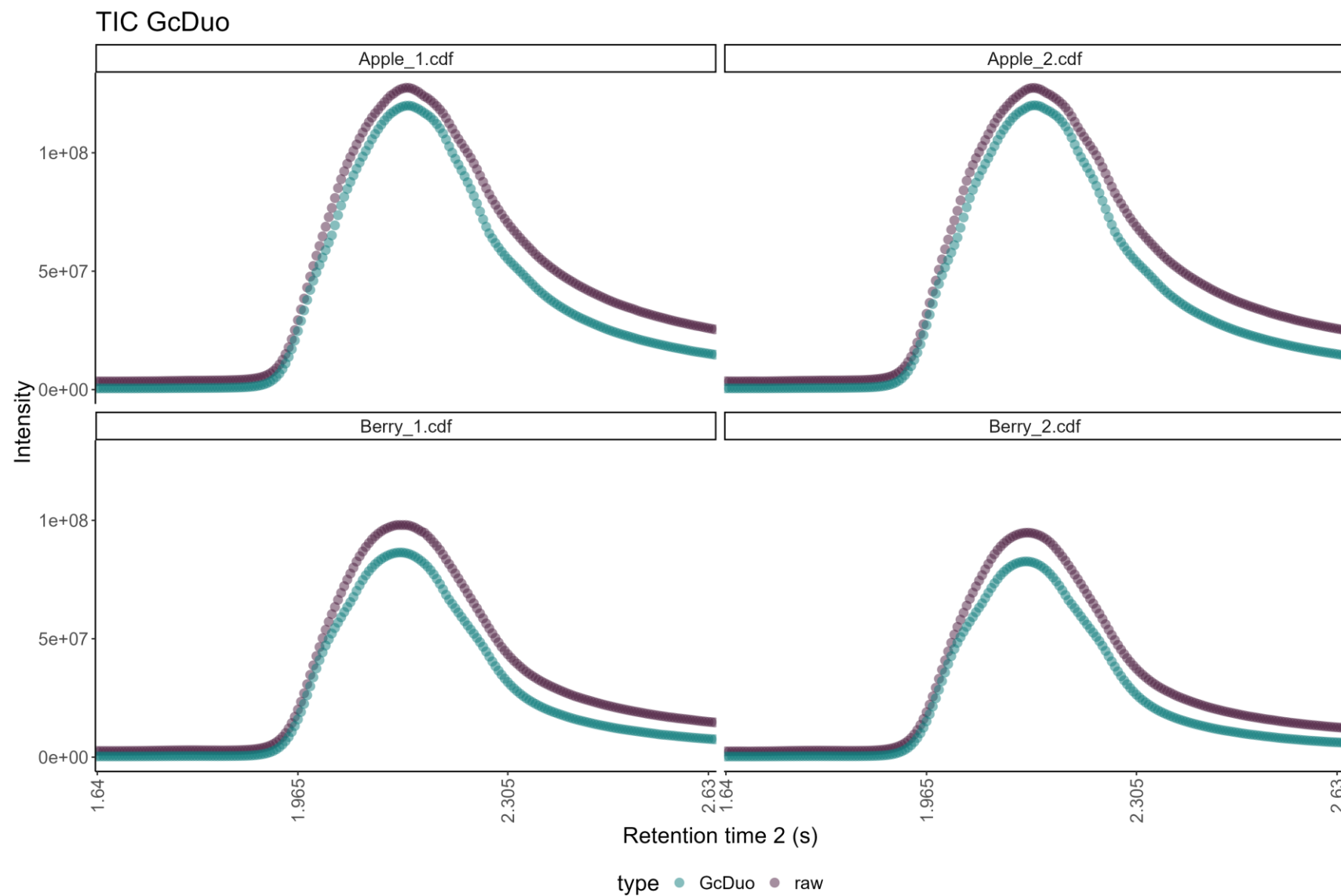
Validation dataset – Detection and Annotation

ID

 FruityBeer	23/27	1 compound missing from the in-house library 3 compounds detected but no match (cosine < 0.7)
 BreathMix	12/12	1 only detected in low signal-to-noise ratio Retention Index used

Data from:  **LIÈGE université** DOI: 10.7910/DVN/RJTYEO (FruityBeer)
OBiAChem DOI: 10.5281/zenodo.13947810 (BreathMix)

GcDUO results



Hexyl acetate

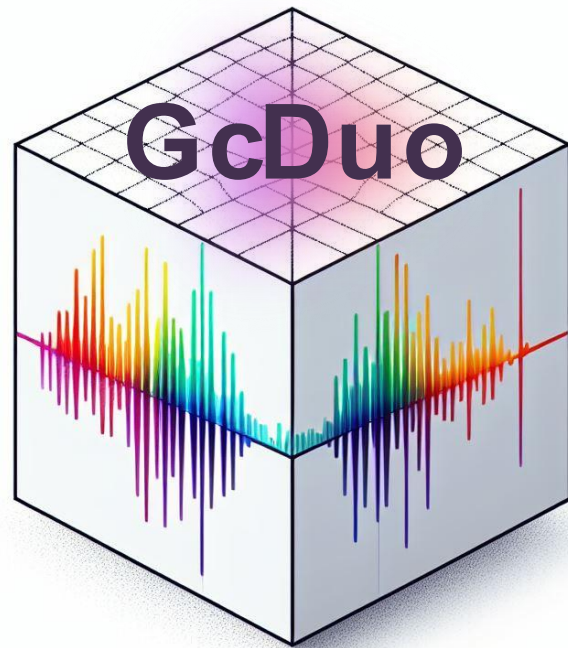
GcDUO results

BreathMix Compound	GcDUO		ChromaTOF	
	RT1, RT2 (s)	Area 1 ppm	RT1, RT2 (s)	Area 1ppm
2-Hexanone	259.98, 1.670	1.11E+07	259.99, 1.660	1.16E+07
Ethylbenzene	374.97, 1.820	1.95E+07	374.98, 1.807	2.44E+07
Cyclohexanone	417.47, 2.465	6.29E+06	417.48, 2.449	8.49E+06
6-Methyl-5-octen-2-one	579.96, 2.070	4.69E+06	579.97, 2.055	4.52E+06
Ethanone, 2-chloro-2,2-difluoro-1-phenyl-	727.45, 0.430	5.90E+06	727.46, 0.419	1.11E+07
Decane	604.80, 1.640	5.09E+05	604.96, 1.392	1.90E+05
Undecane	789.94, 1.430	1.29E+07	789.96, 1.423	9.34E+06
2-Undecene, (Z)-	797.44, 1.960	2.45E+06	797.46, 1.947	2.05E+06
1-Tetradecene	1279.91, 1.575	6.65E+06	1279.93, 1.561	5.17E+06
5,9-Undecadien-2-one, 6,10-dimethyl-, (E)-	1332.41, 2.205	3.27E+06	1332.42, 2.187	1.98E+06
5,9-Undecadien-2-one, 6,10-dimethyl-, (Z)-	1359.91, 2.230	3.71E+06	1359.92, 2.218	3.29E+06
3-HeptaFluorobutyroxytetradecane	1429.90, 1.595	8.25E+06	1429.92, 1.580	5.21E+06

GcDUO summary

GCxGC-MS open-source
tool

No need of
high expertise



Computational cost

Tri-linearity required

Comparable results to
gold-Standard software

<https://github.com/mariallr/GcDuo>

Thank You!

maria.llambrich@iispv.cat



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