Kruve lab

27èmes Journées Scientifiques

MS2Tox & MS2Quant

Automated detection and identification of TOXIC and HIGH-RISK chemicals

IDA RAHU
Postdoctoral Fellow

Villars-sur-Ollon 2024

INTRODUCTION

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TOXIC and HIGH-RISK chemicals

REAL-WORLD SAMPLES

100+ unidentified chemicals

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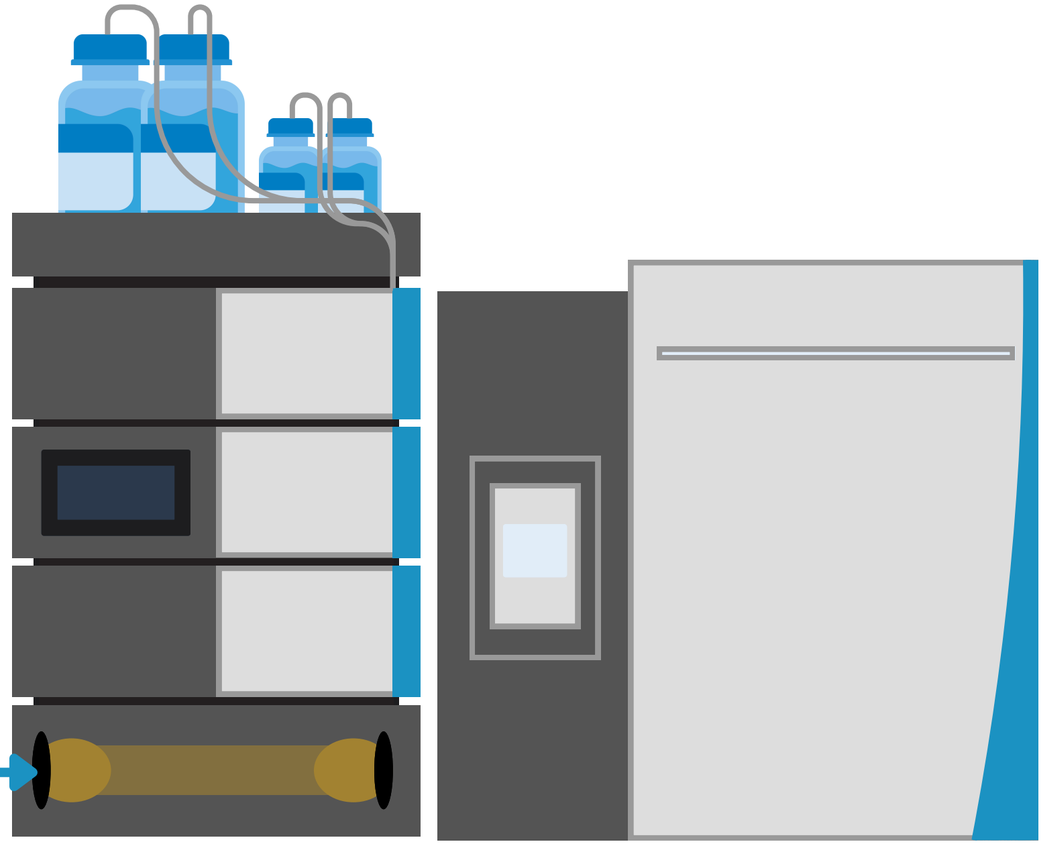
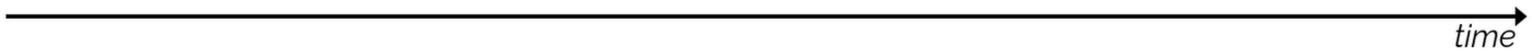


LC/HRMS

NON-TARGETED SCREENING WITH LC/HRMS



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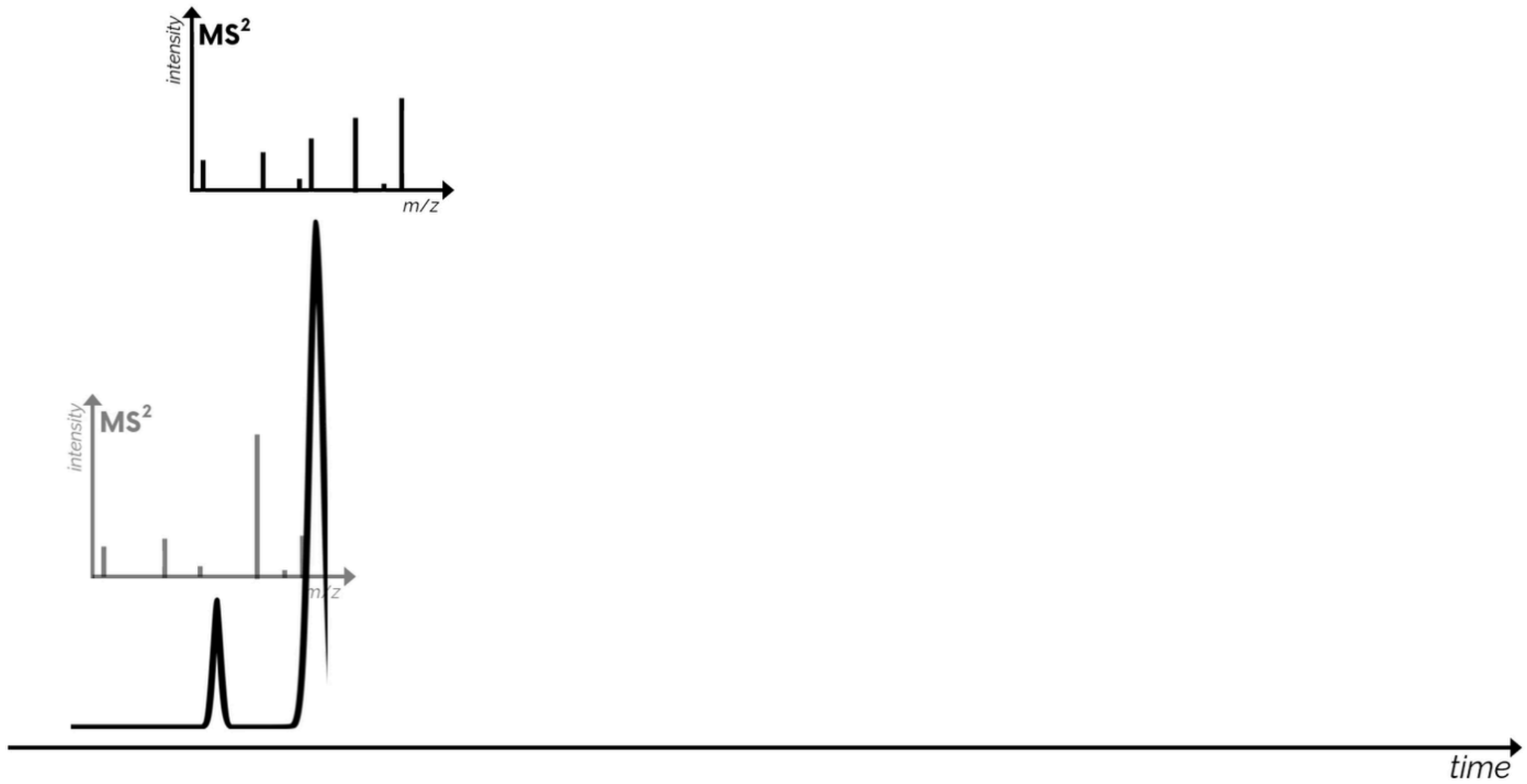

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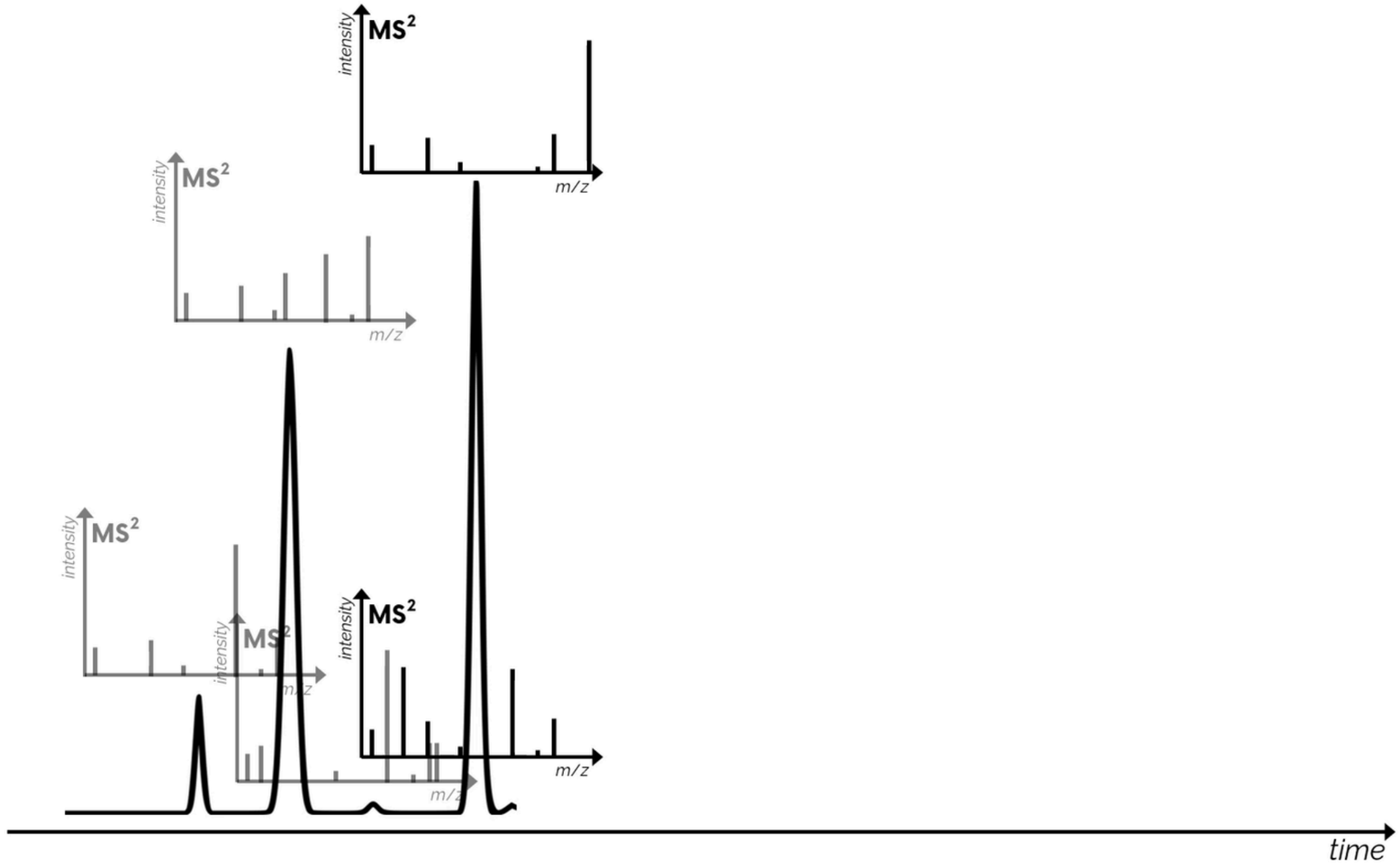

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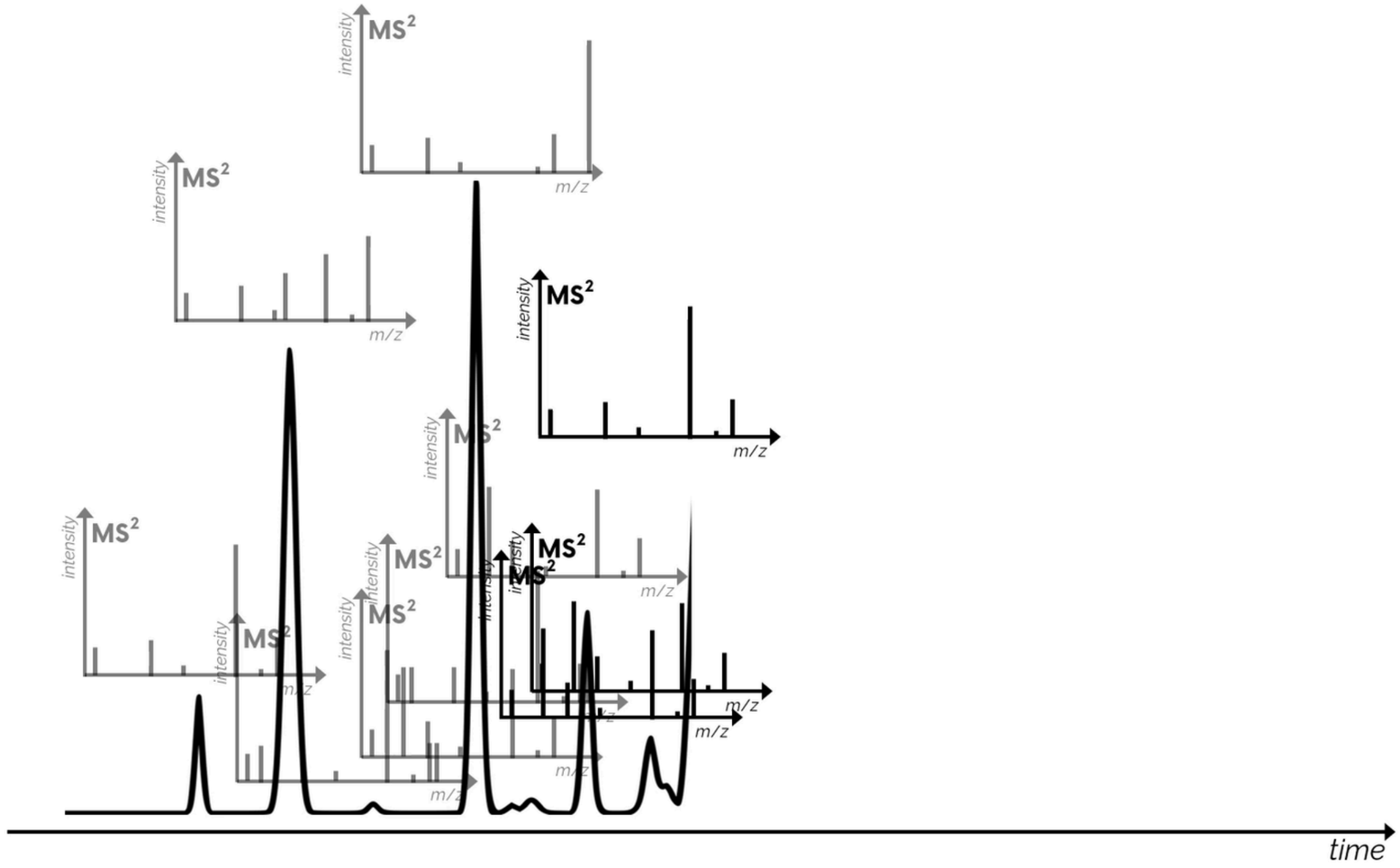

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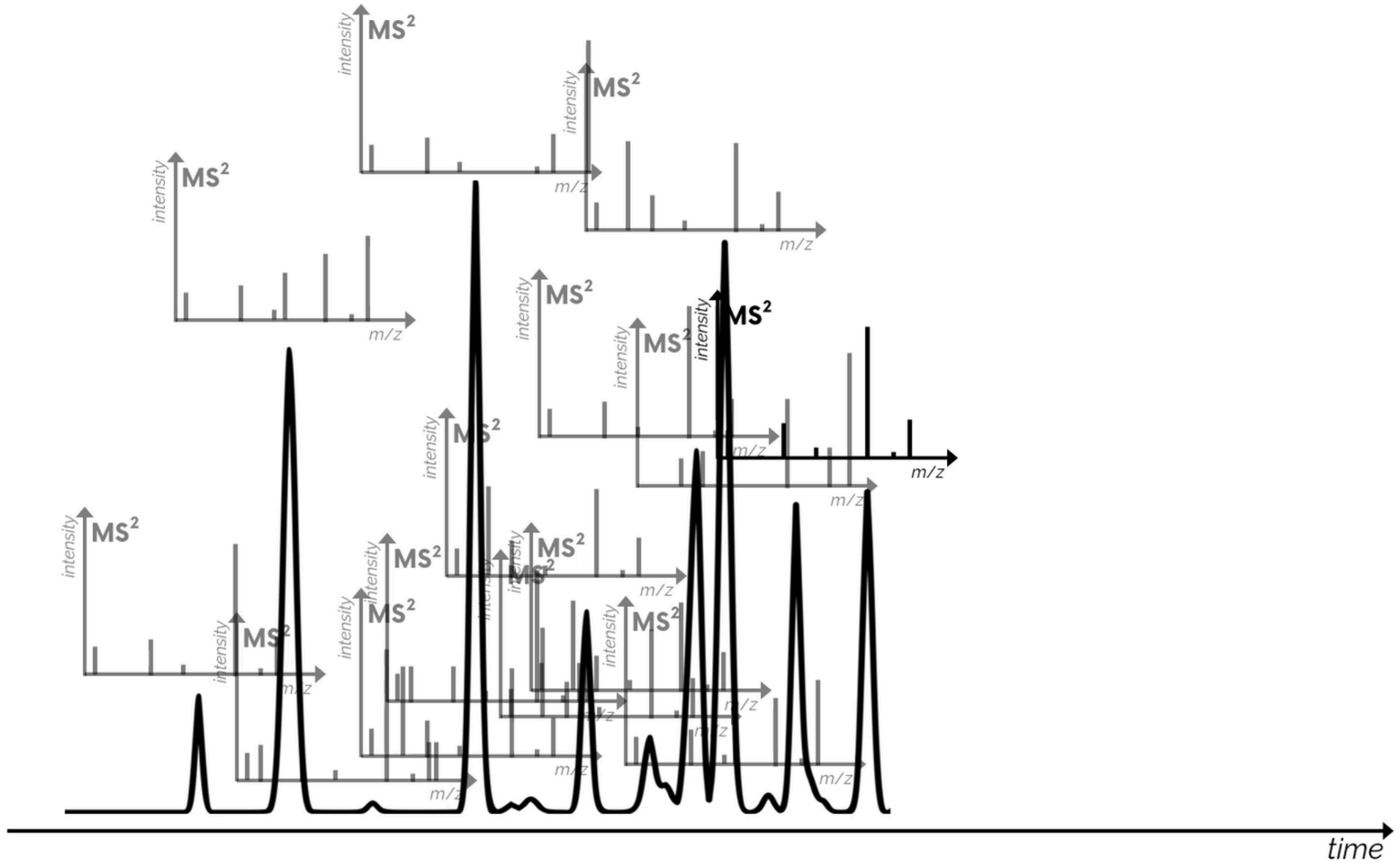

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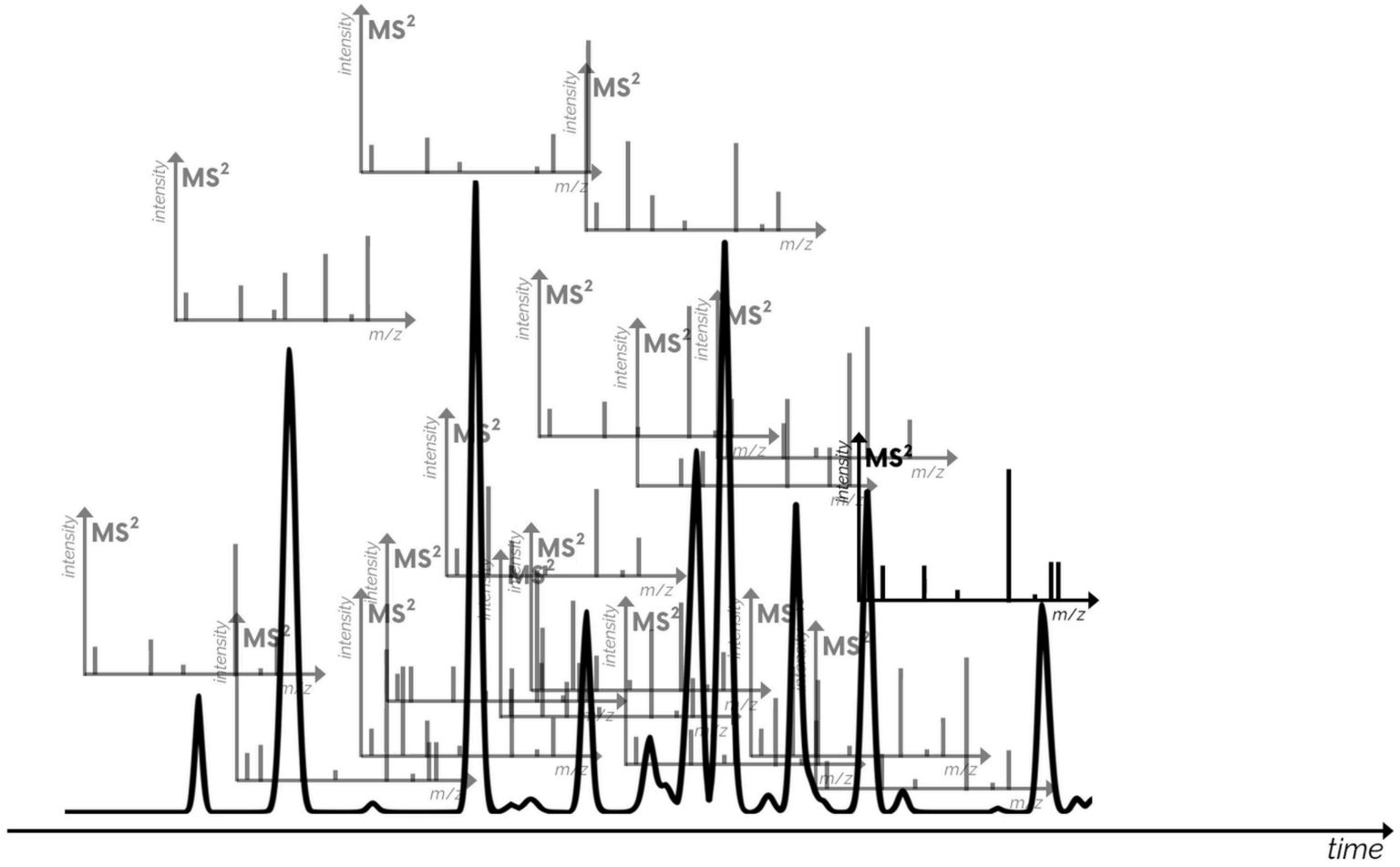

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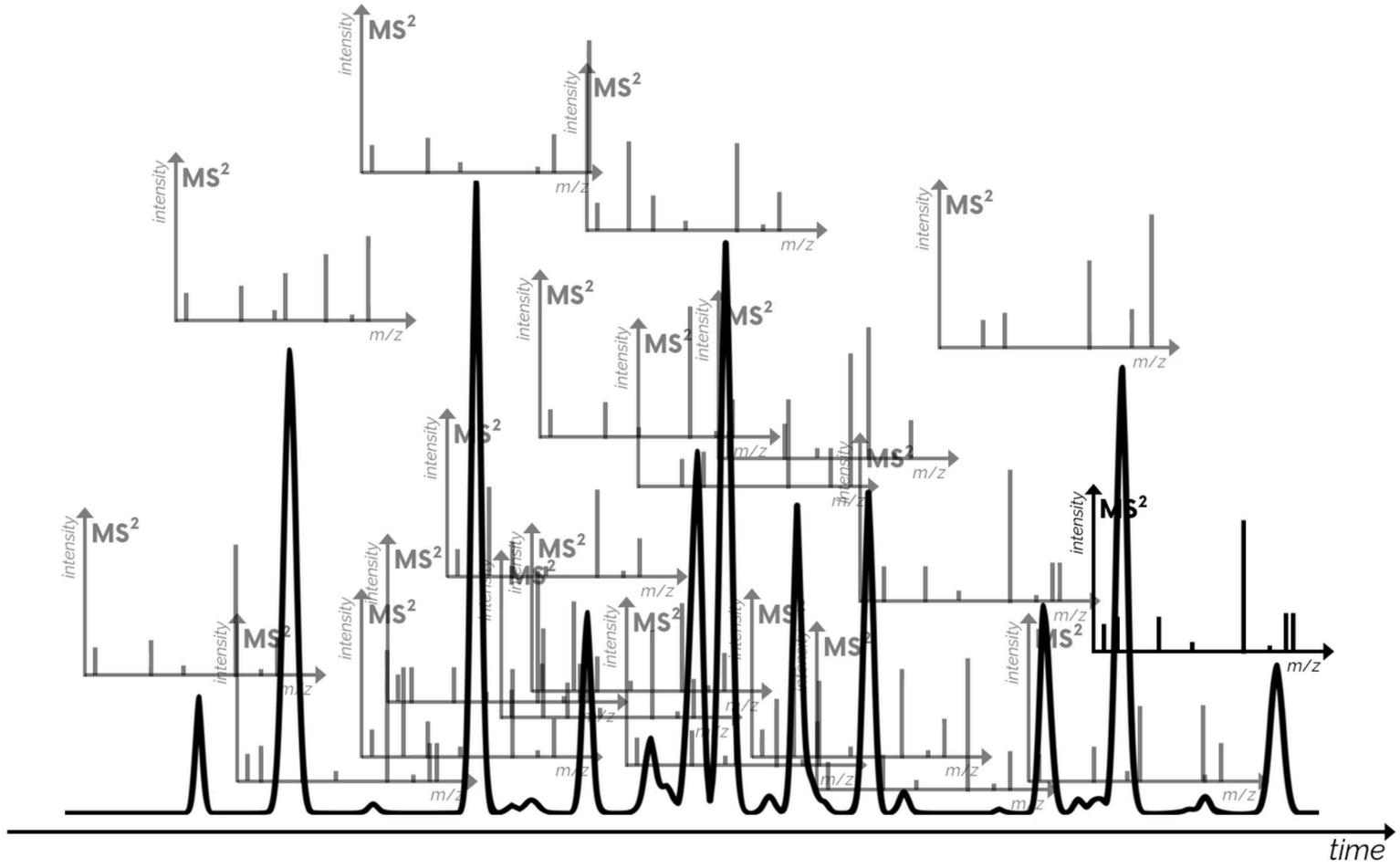

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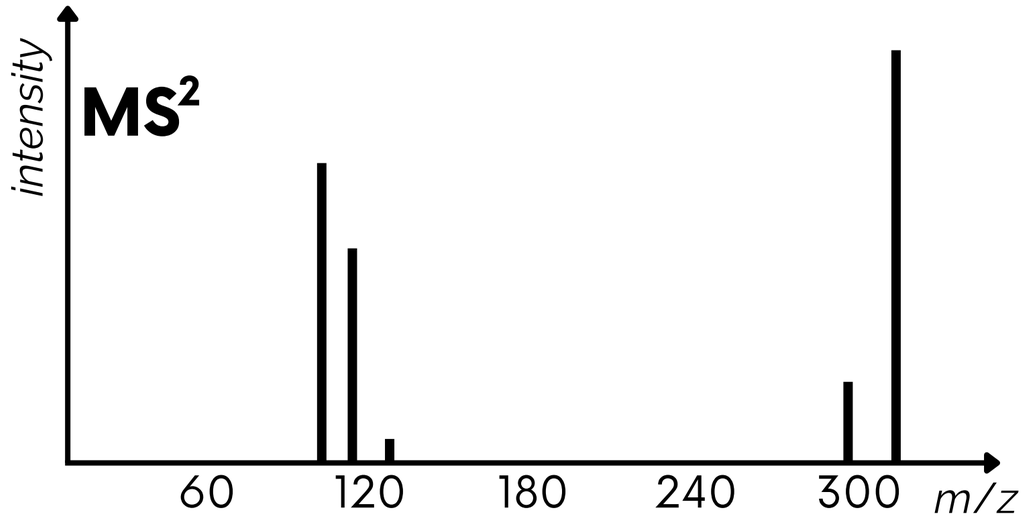

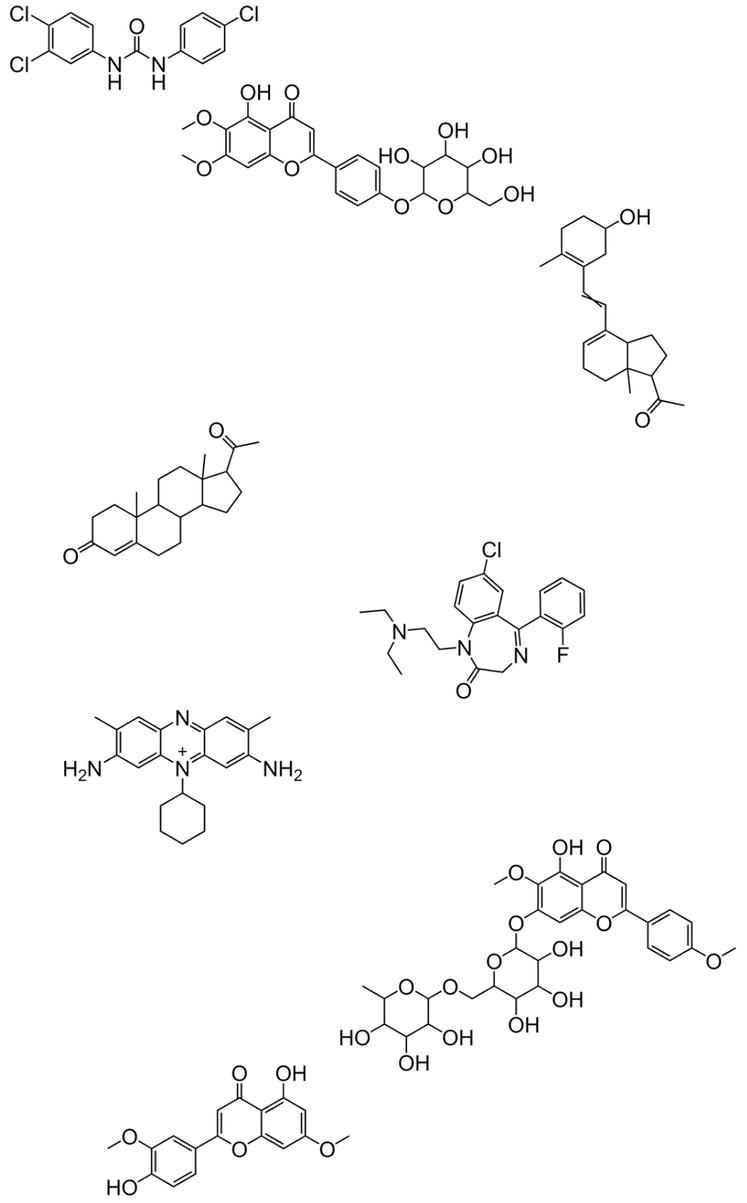

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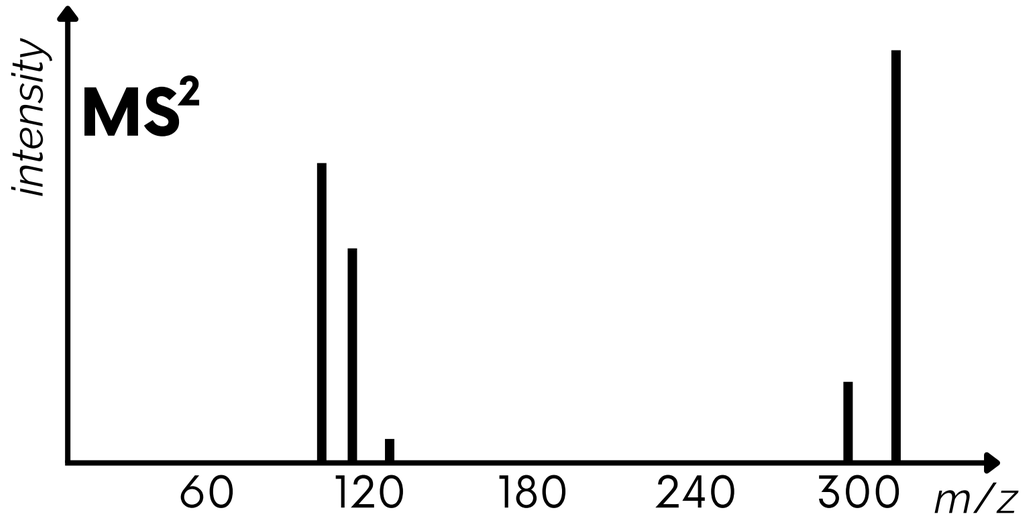

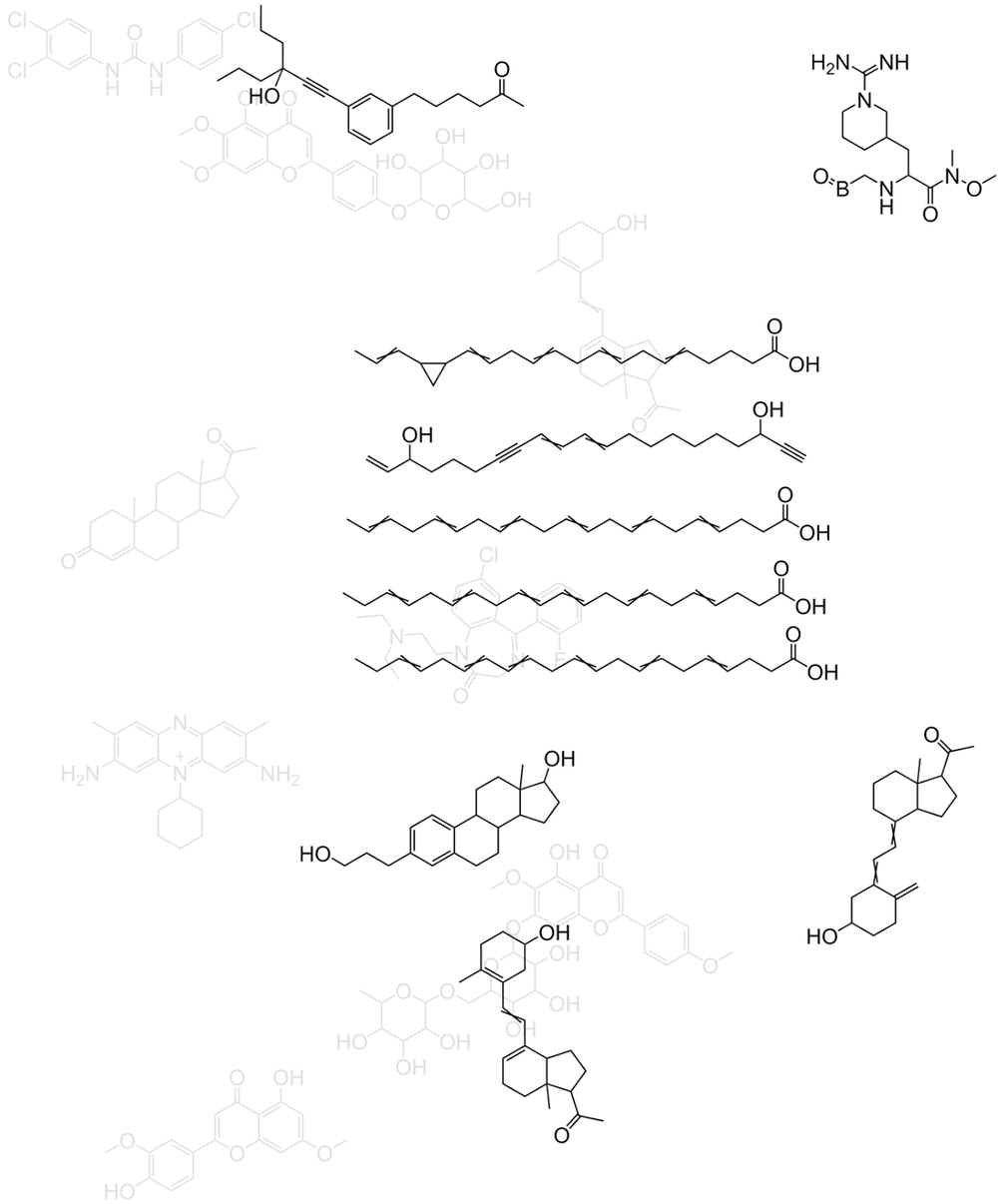

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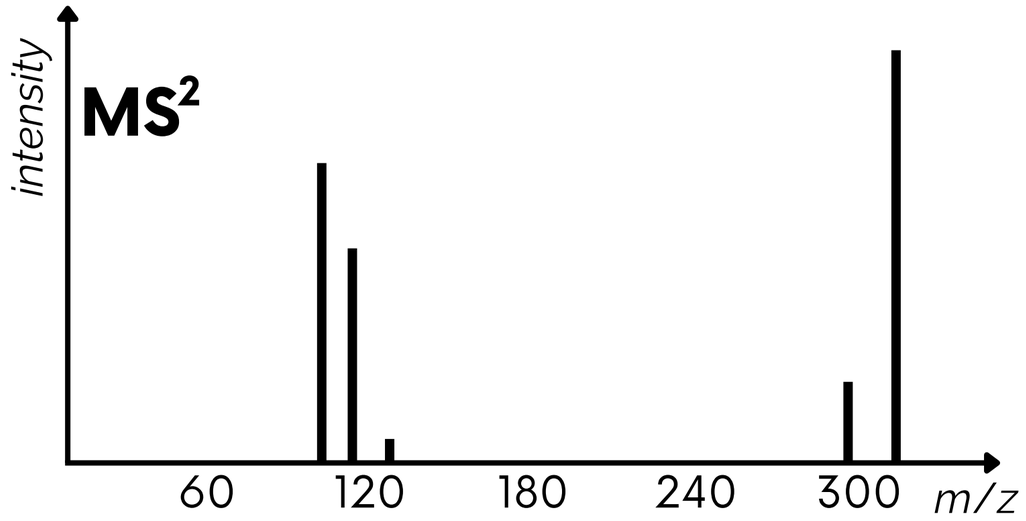

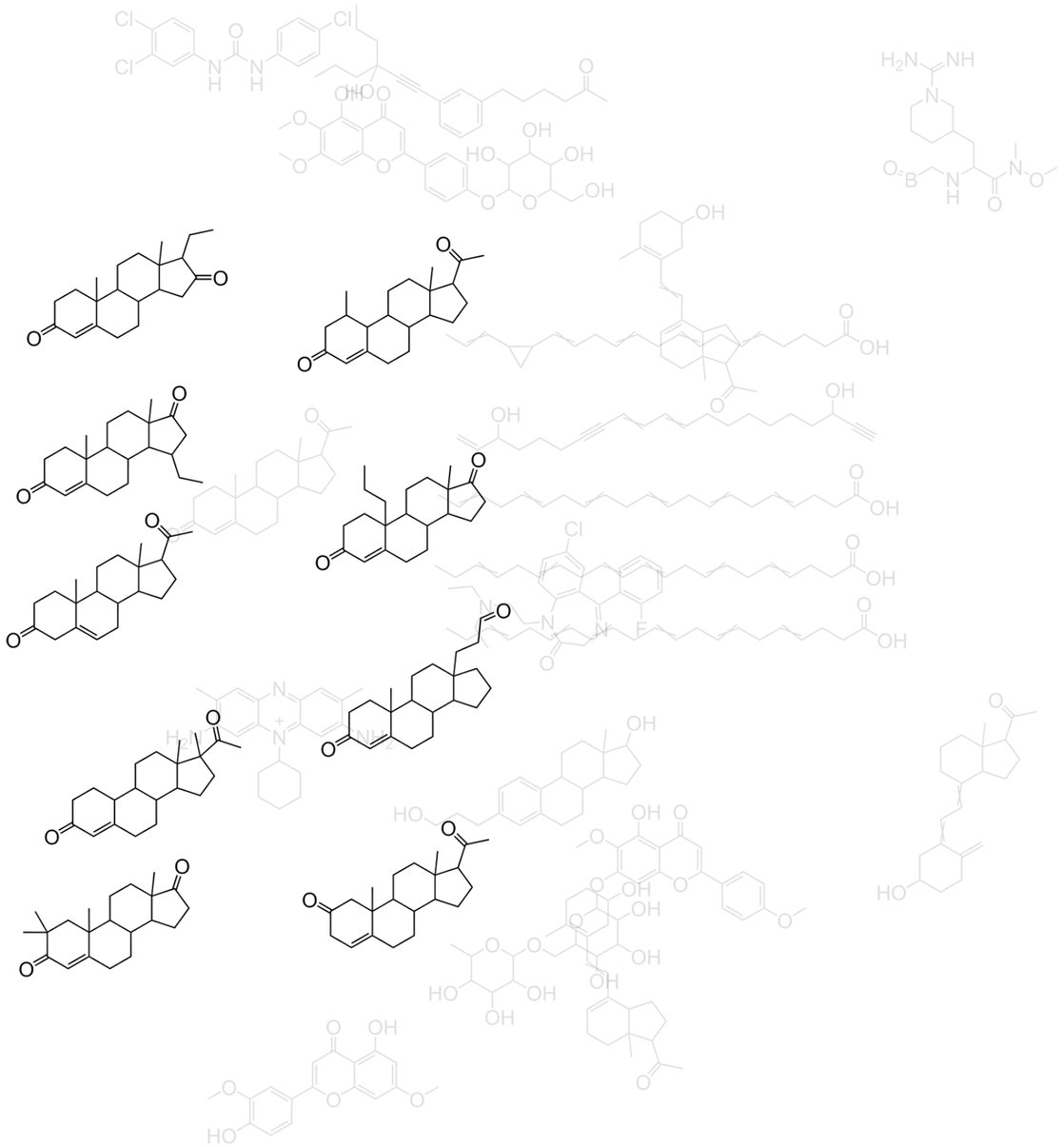

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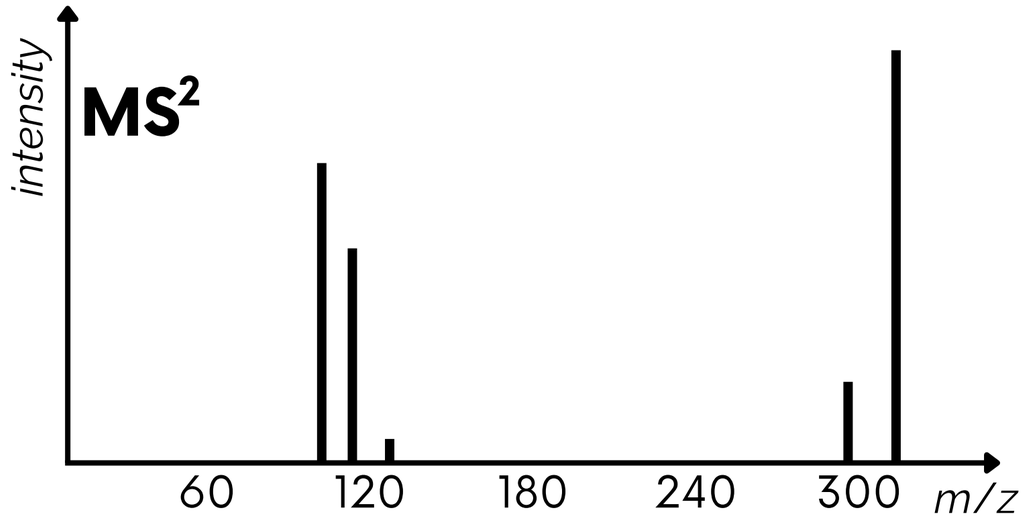

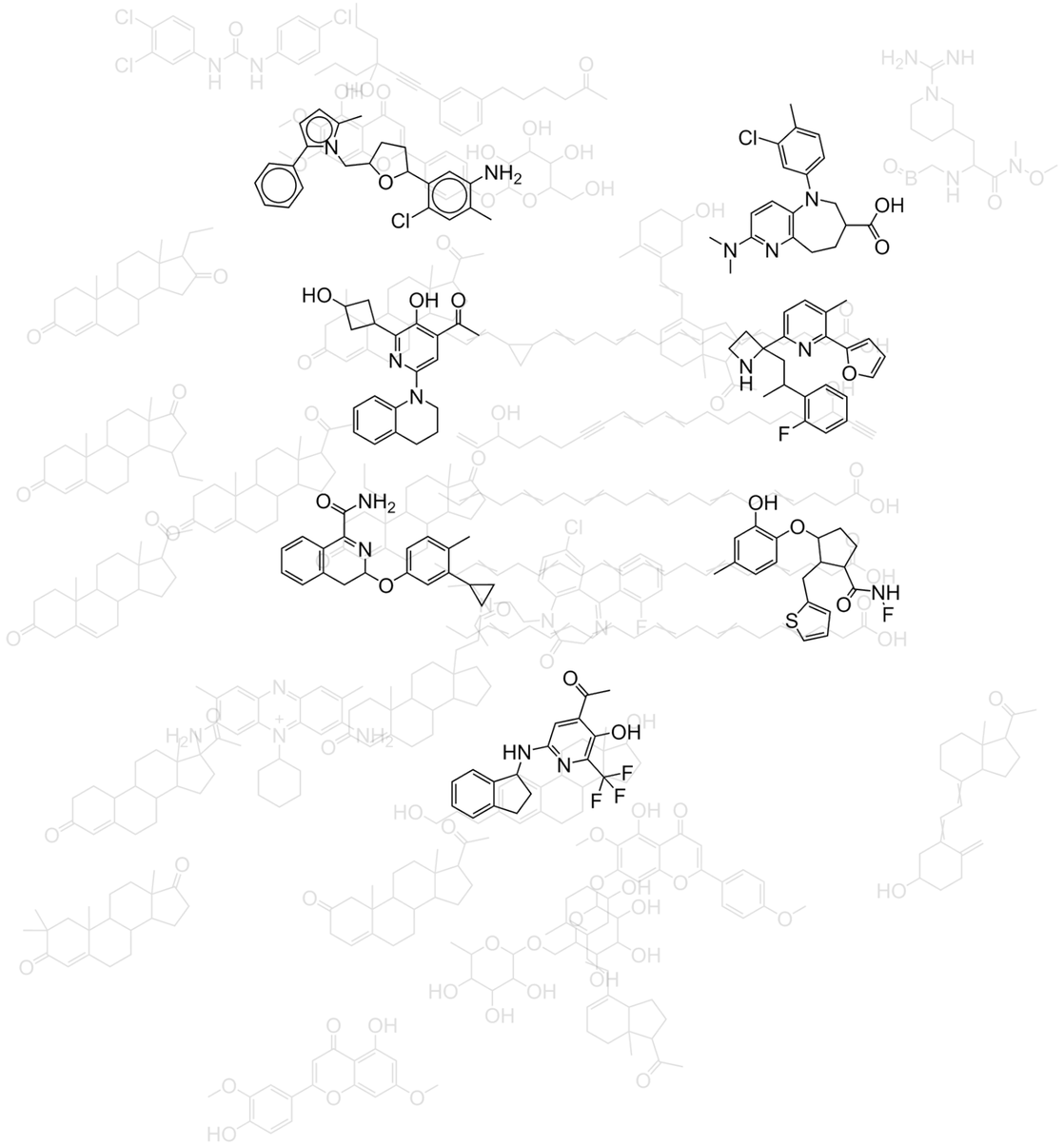

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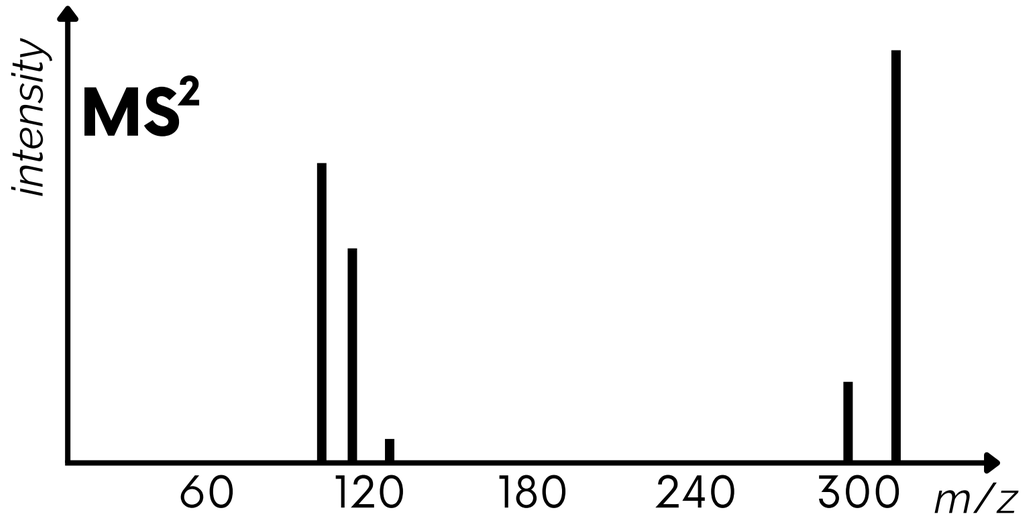

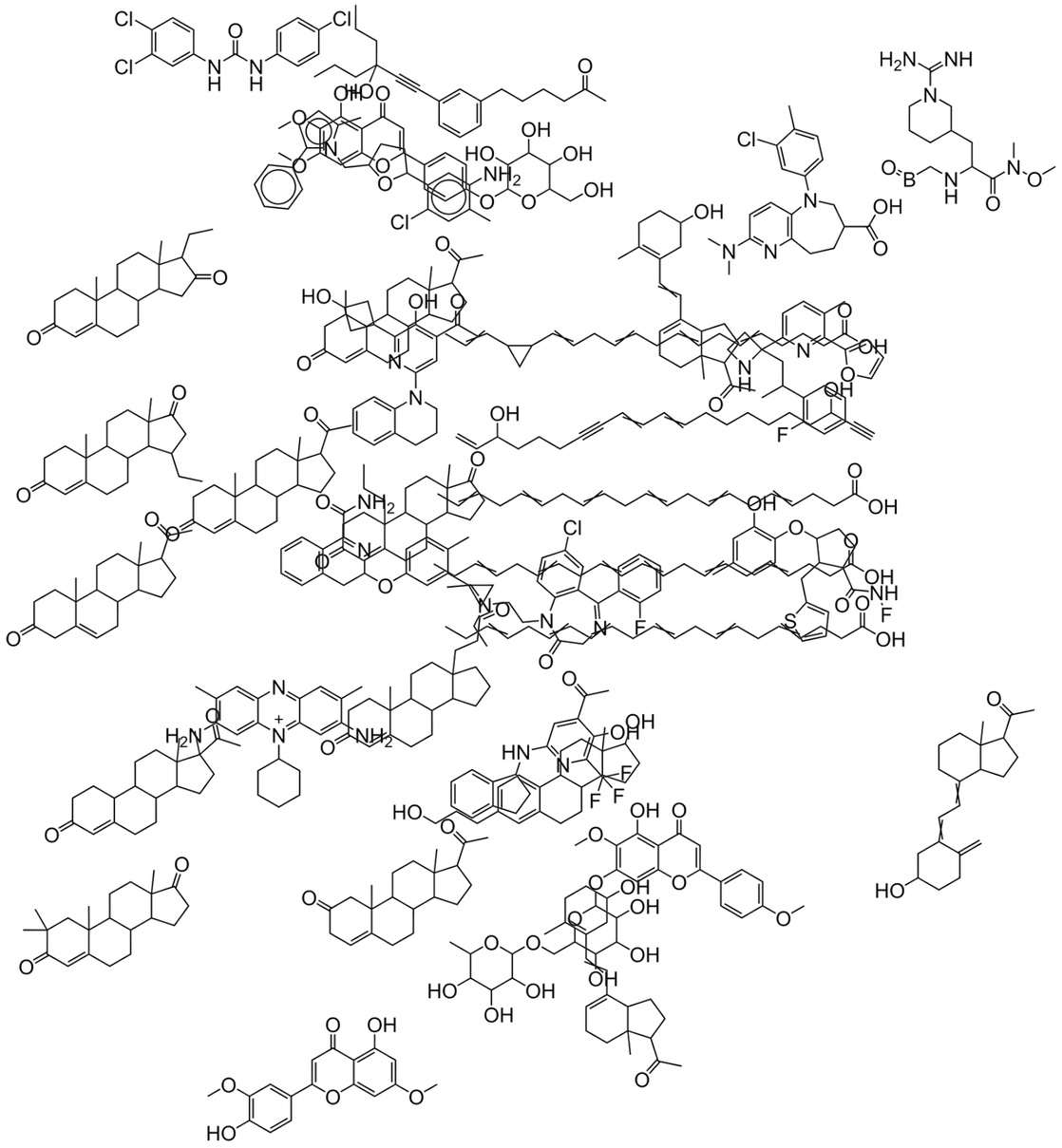

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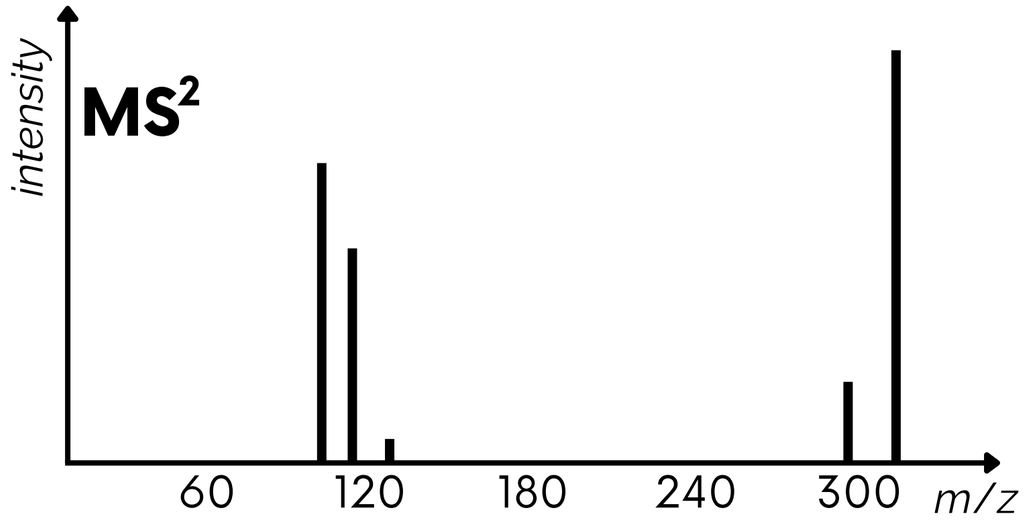
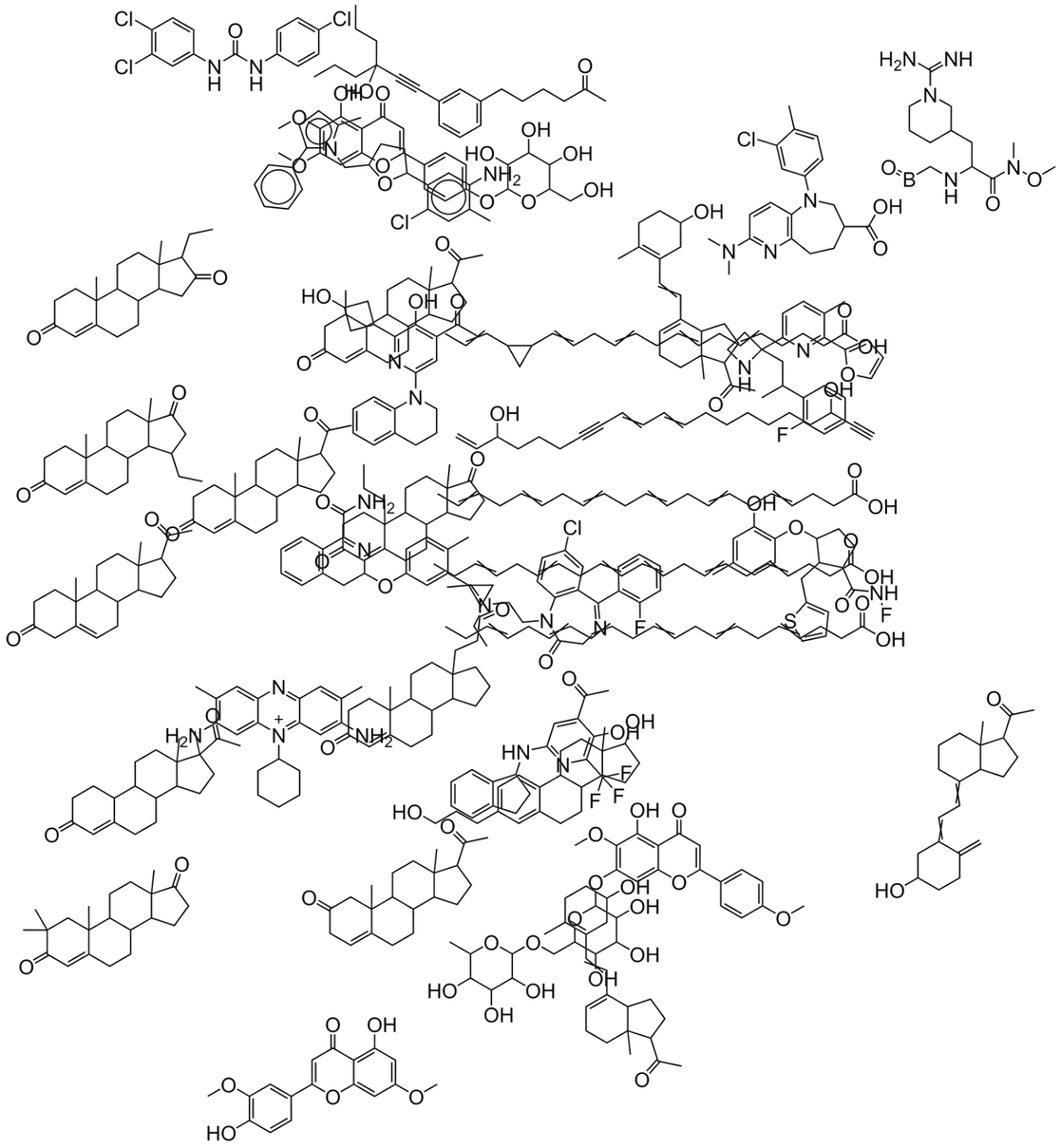
NON-TARGETED SCREENING WITH LC/HRMS

RT = 15.04 min

***CCS* = 178.79 Å^2**





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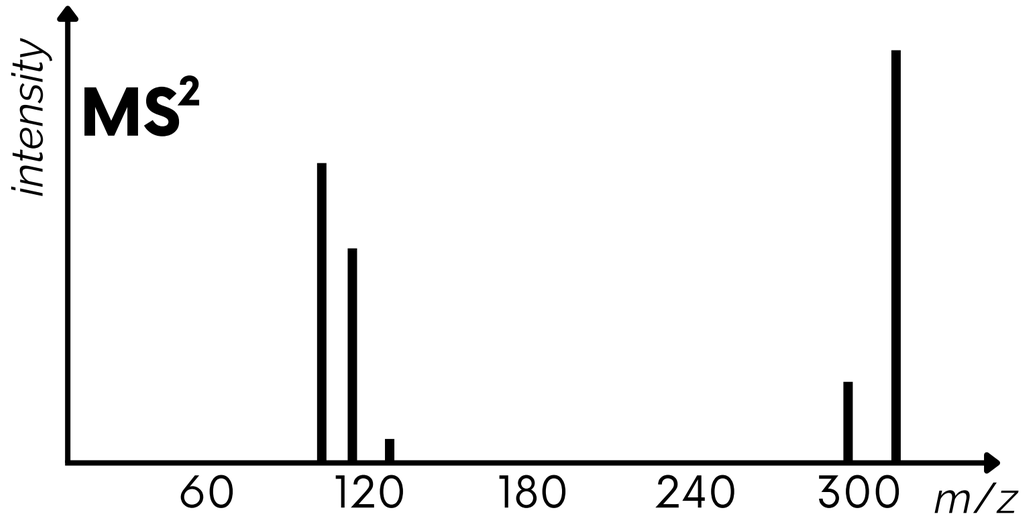

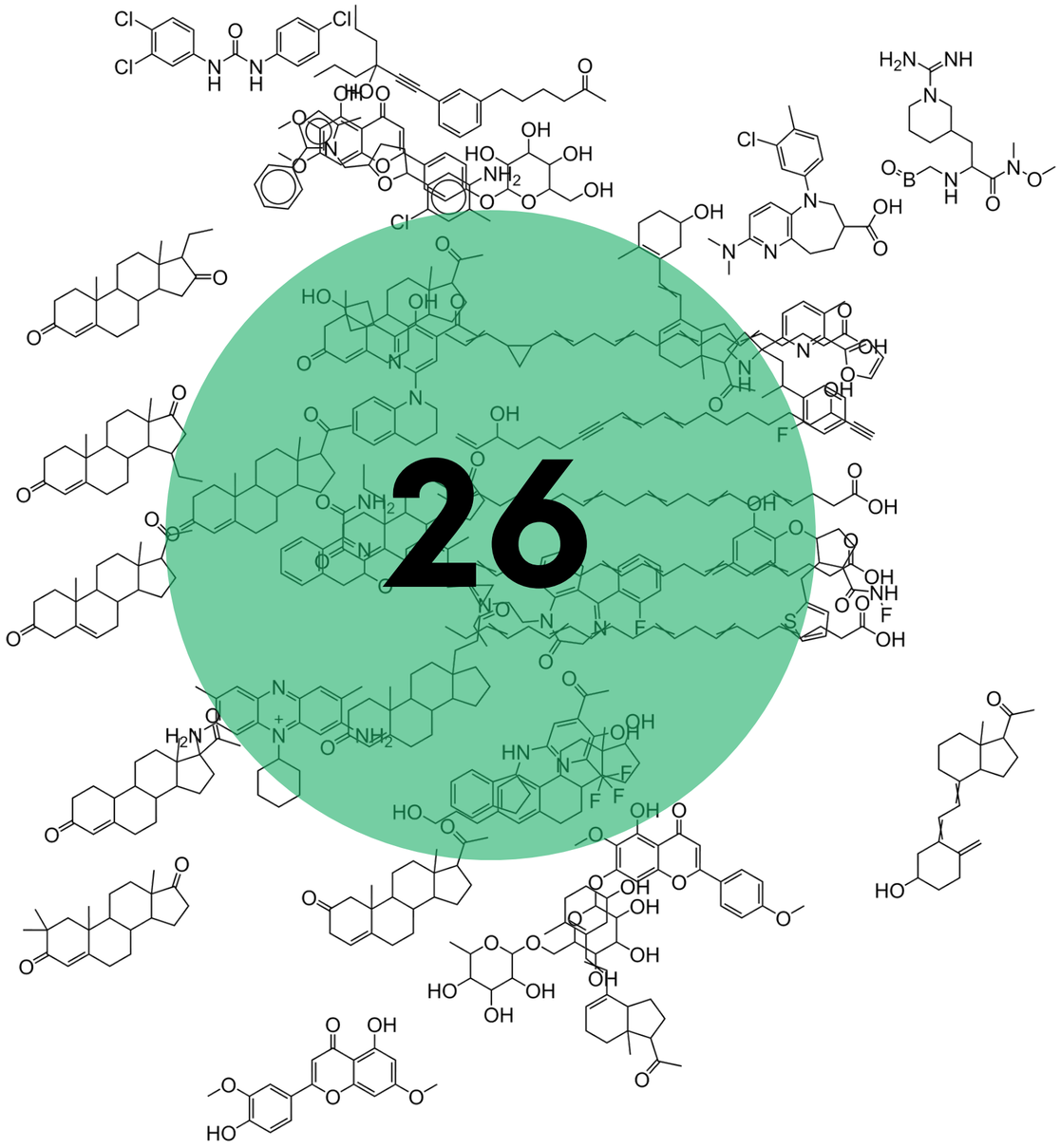

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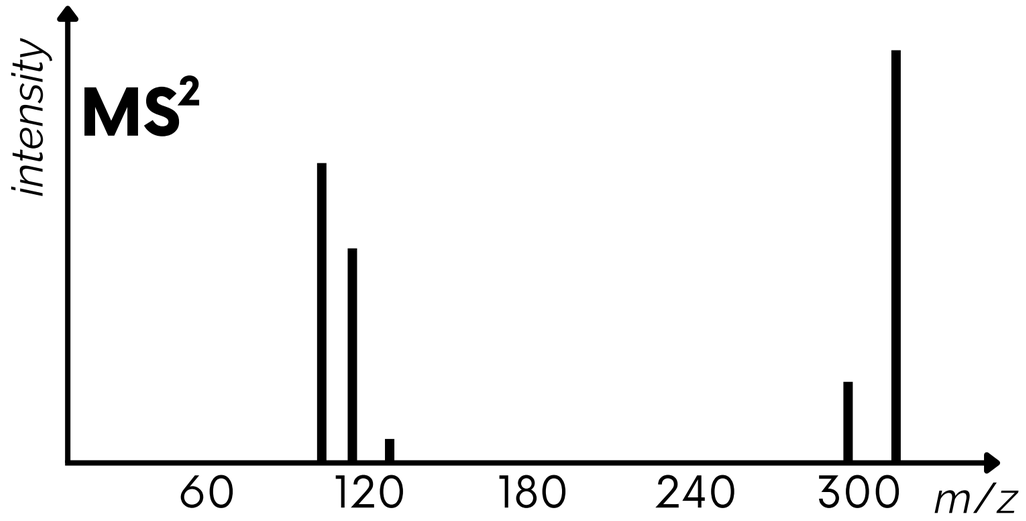

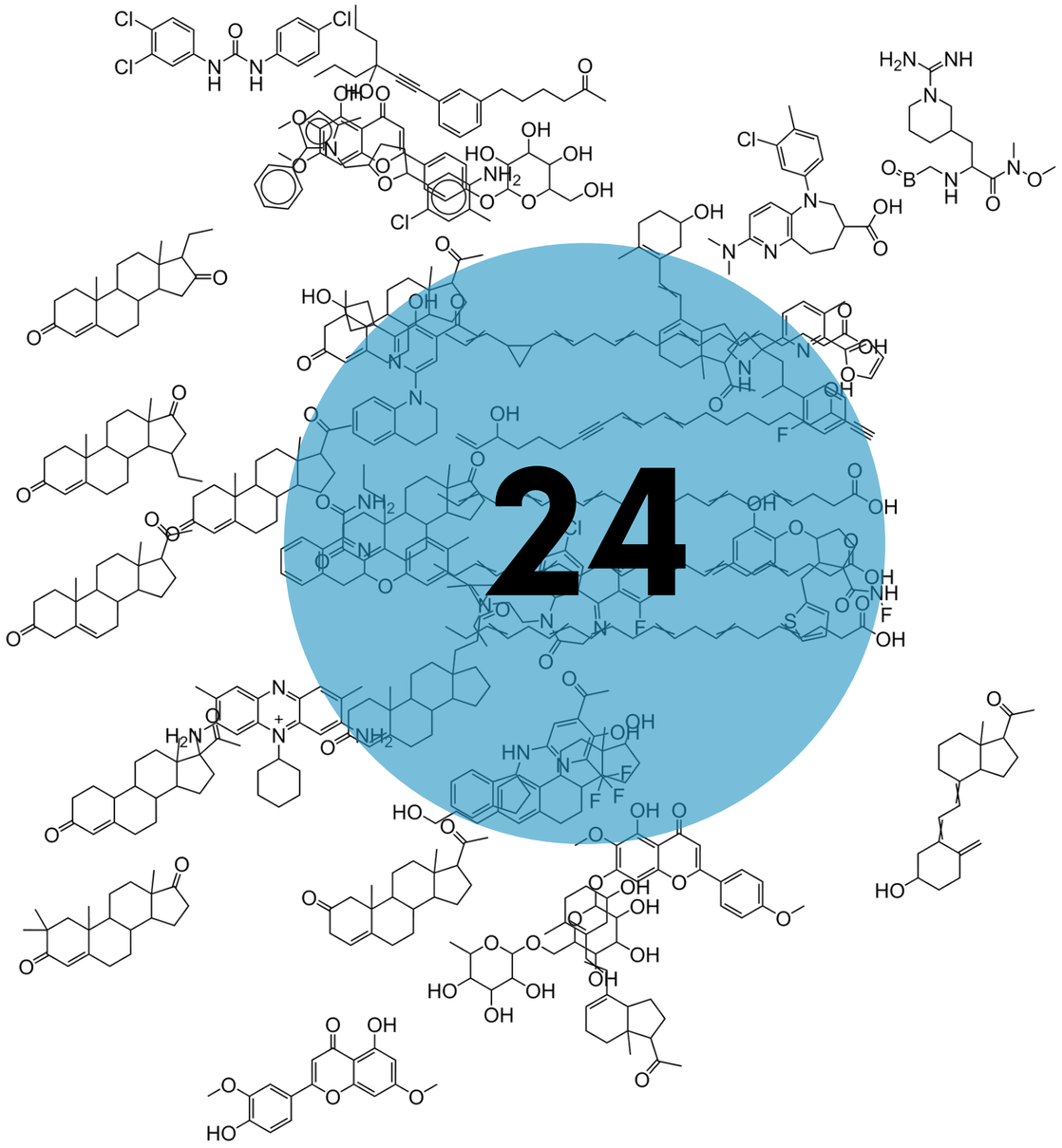

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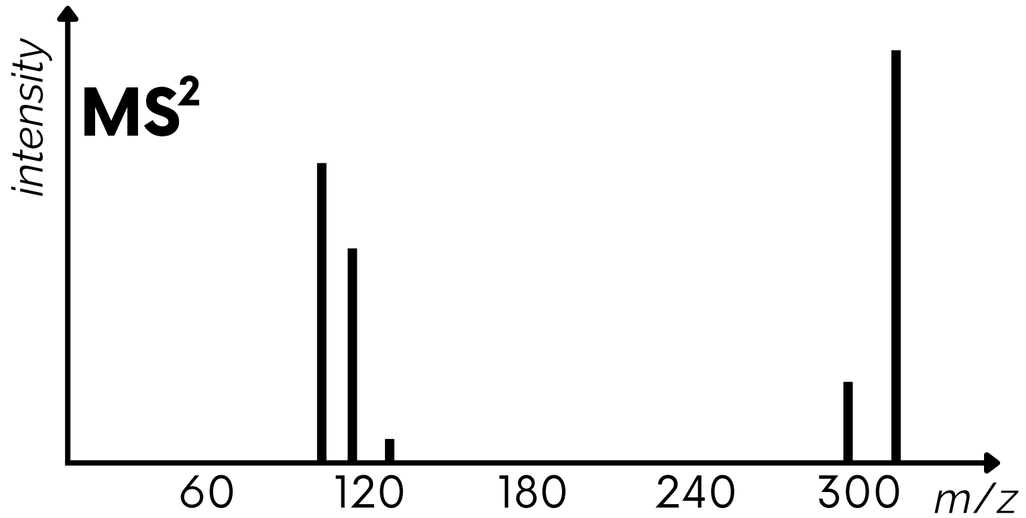

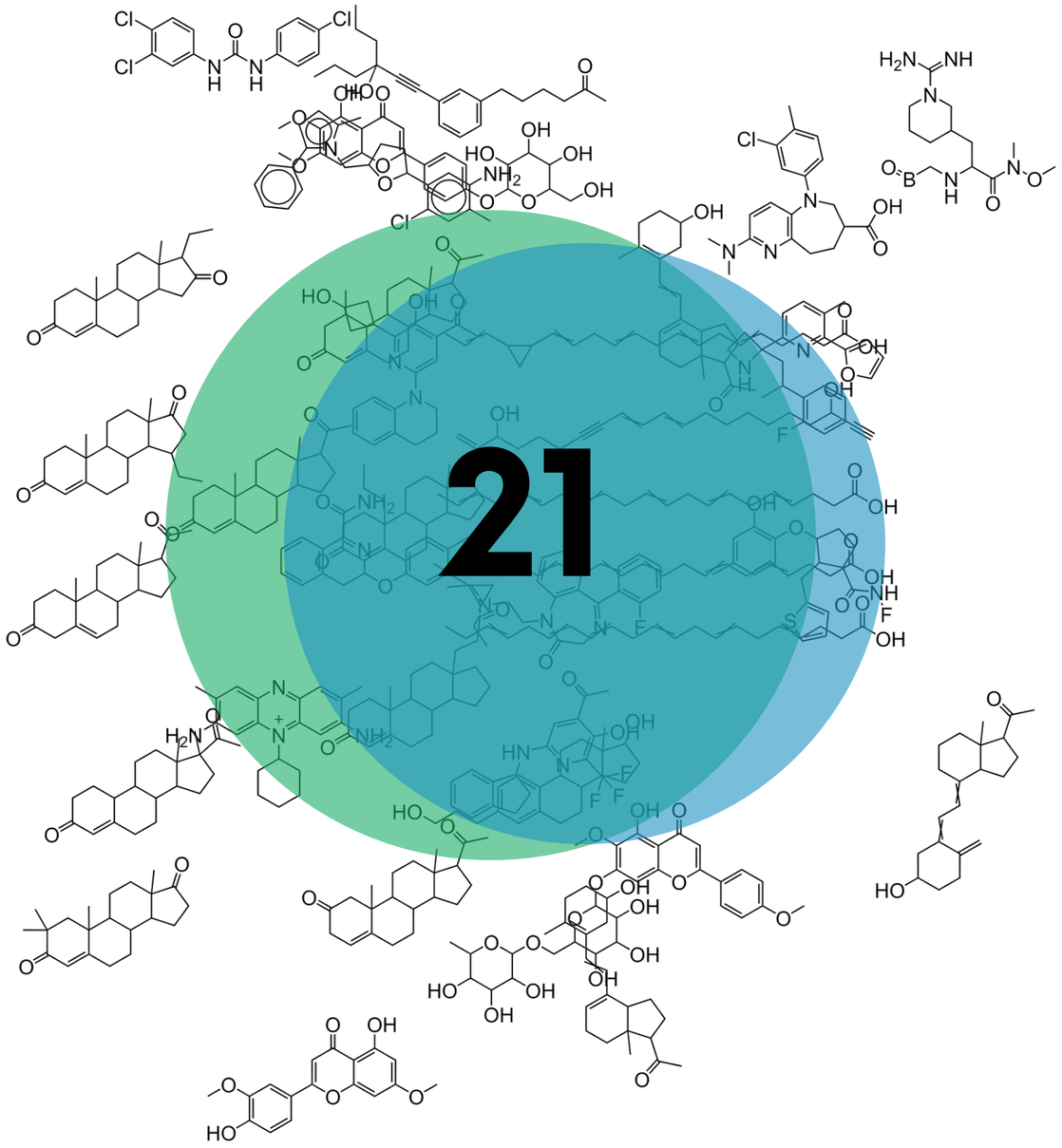

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NON-TARGETED SCREENING WITH LC/HRMS

NORMAN SusDat (*n* = 55793)

T. Hulleman et al., *Environ. Sci. Tech.* (**2023**).

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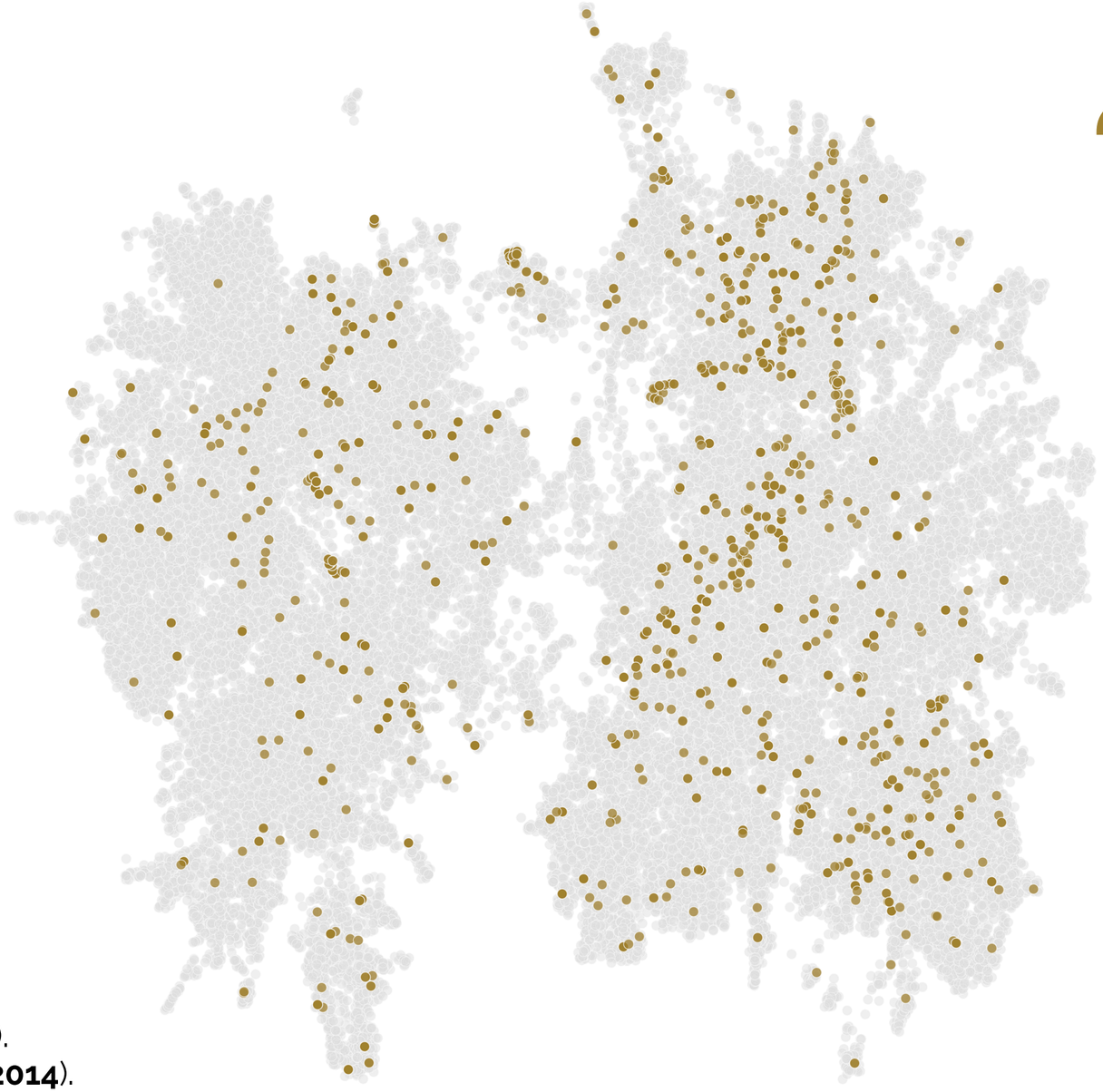
NORMAN SusDat (*n* = 55793)

detected structures (*n* = 1606)

level 1 to 2b identification confidence



~3%

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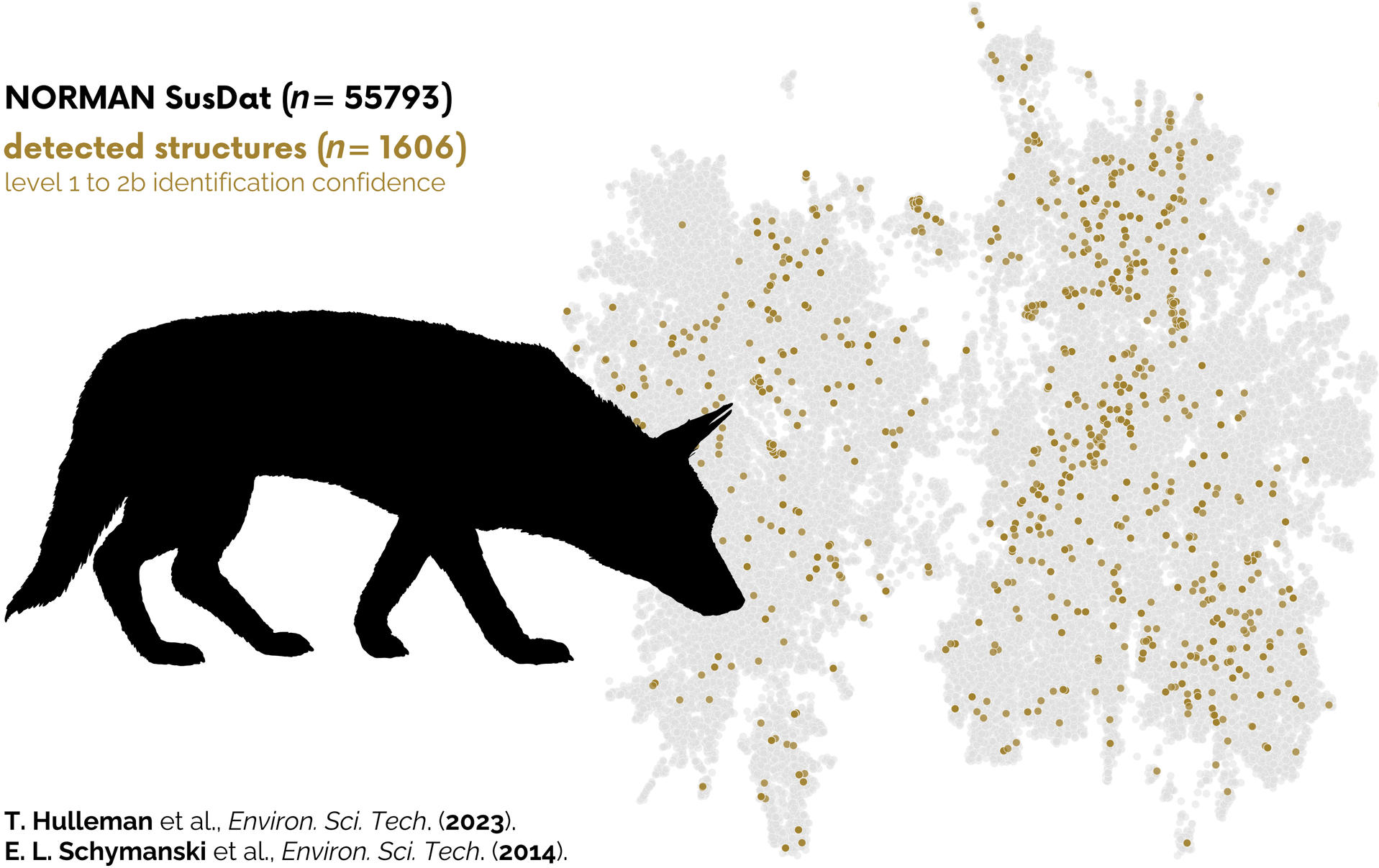

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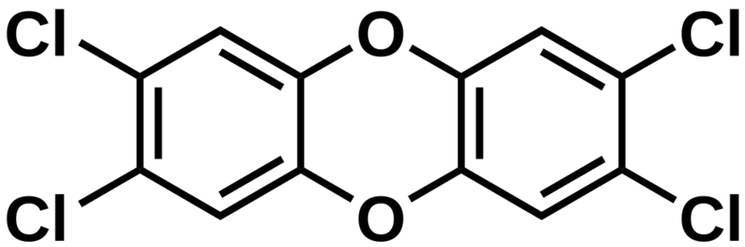
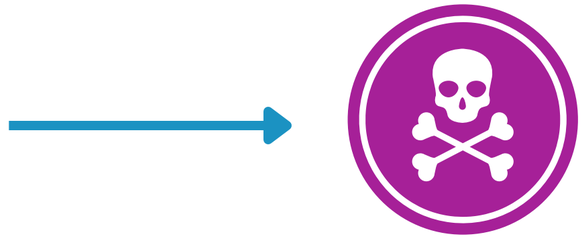
IN SILICO METHODS

in silico tools





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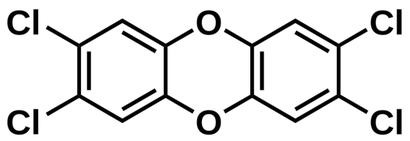

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MOLECULAR REPRESENTATIONS

- fixed representations
- deep representations

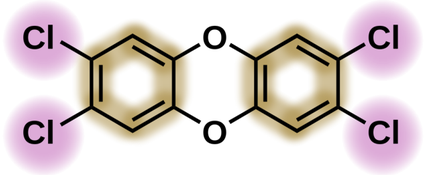
1D
- number of atoms
- number of bonds
- molecular weight
- atomic properties

MW = 321.8936 (g/mol)

2D
- physiological properties
- topological properties
- electrotopological properties
- 2D fingerprints

NumHAcceptors = 2
MACCS keys, ECFP, etc.

0	0	1	...	1	0	0



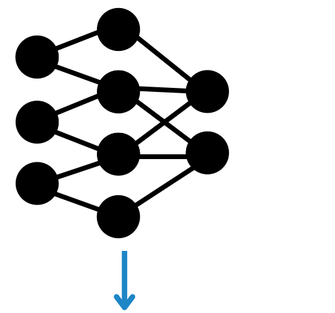
3D
- geometrical properties
- surface properties
- grid properties

TPSA = 18.5 (Å^2)

LINEAR NOTATIONS

SMILES STRINGS

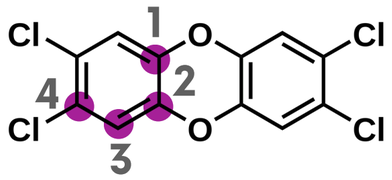
C1=C2C(=CC(=C1Cl)Cl)OC3=CC(=C(C=C3O2)Cl)Cl



VECTOR EMBEDDING

0.8	0.1	0.3	...	0.2	0.2	0.7

MOLECULAR GRAPHS



NODE INDEX

adjacency matrix **(A)**

NODE INDEX	1	2	3	4	...
1	0	1	0	0	...
2	1	0	1	0	...
3	0	1	0	1	...
4	0	0	1	0	...
...	...	...	...	...	...

BOND TYPE

edge features matrix **(E)**

EDGE INDICES	1	2	3	arom
(1, 2)	0	0	0	1
(2, 3)	0	0	0	1
(3, 4)	0	0	0	1
(..., ...)	...	...	...	...

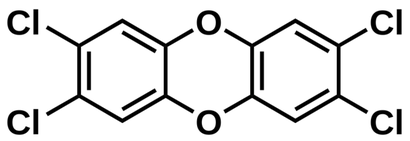
ATOM TYPE | **FORMAL CHARGE** | **IMPLICIT HYDROGENS**

node features matrix **(X)**

NODE INDEX	C	O	Cl	...	-1	0	+1	0	1	2	3
1	1	0	0	...	0	1	0	1	0	0	0
2	1	0	0	...	0	1	0	1	0	0	0
3	1	0	0	...	0	1	0	0	1	0	0
4	1	0	0	...	0	1	0	1	0	0	0
...	...	...	...	...	...	...	...	...	...	...	...

IN SILICO METHODS

in silico tools



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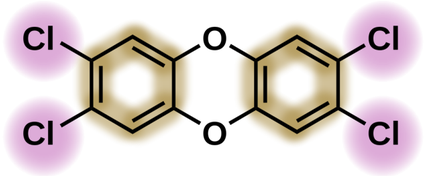

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MOLECULAR GRAPHS

NODE INDEX

NODE INDEX	1	2	3	4	...
1	0	1	0	0	...
2	1	0	1	0	...
3	0	1	0	1	...
4	0	0	1	0	...
...	...	...	...	...	...

adjacency matrix **(A)**

BOND TYPE

EDGE INDICES	1	2	3	arom
(1, 2)	0	0	0	1
(2, 3)	0	0	0	1
(3, 4)	0	0	0	1
(..., ...)	...	...	...	...

edge features matrix **(E)**

VECTOR EMBEDDING

0.8	0.1	0.3	...	0.2	0.2	0.7

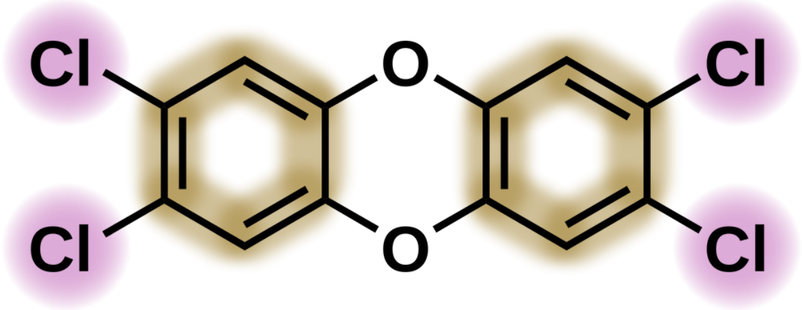
ATOM TYPE / FORMAL CHARGE / IMPLICIT HYDROGENS

NODE INDEX	C	O	Cl	...	-1	0	+1	0	1	2	3
1	1	0	0	...	0	1	0	1	0	0	0
2	1	0	0	...	0	1	0	1	0	0	0
3	1	0	0	...	0	1	0	0	1	0	0
4	1	0	0	...	0	1	0	1	0	0	0
...	...	...	...	...	...	...	...	...	...	...	...

node features matrix **(X)**

IN SILICO METHODS

in silico tools



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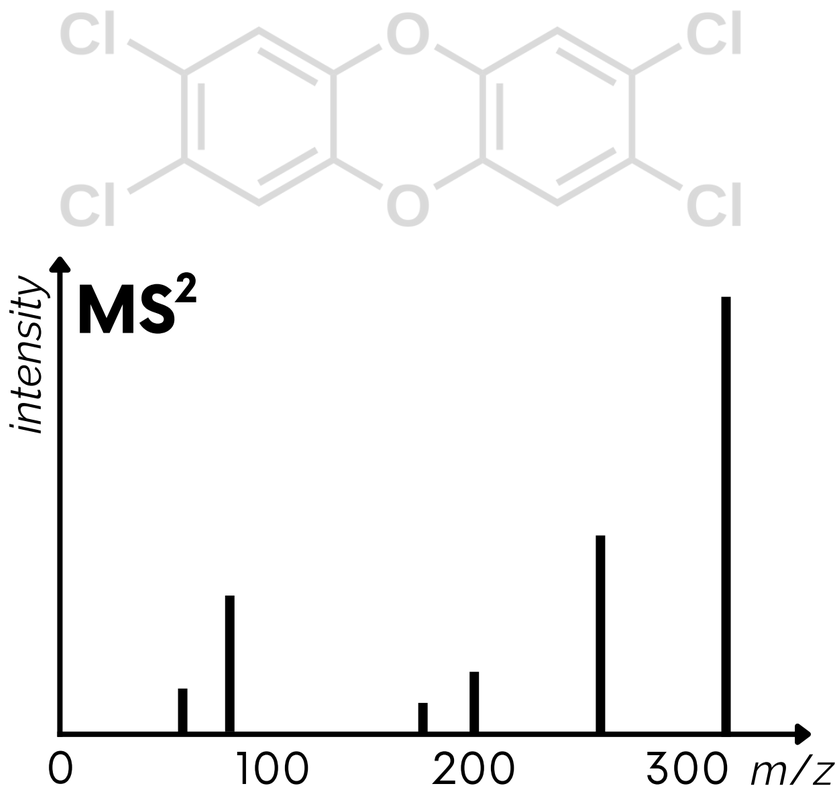
BINARY MOLECULAR FINGERPRINT

0	0	1	...	1	0	0

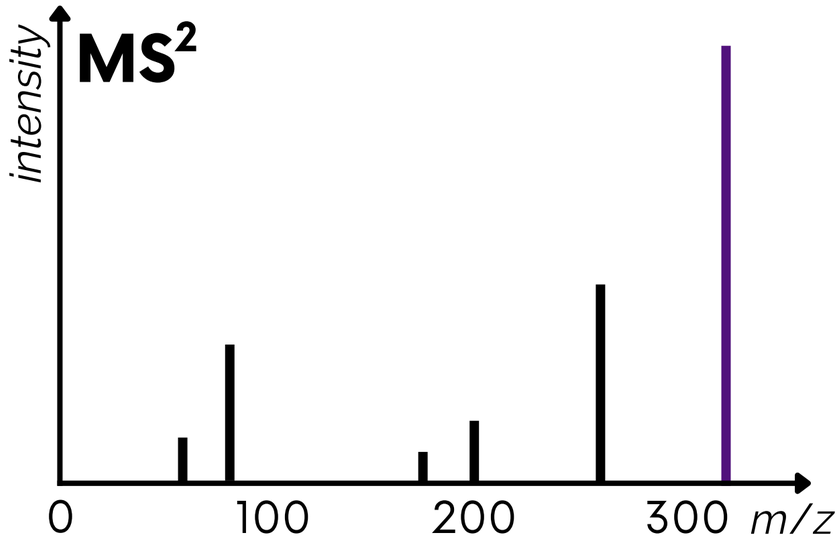
fingerprint feature

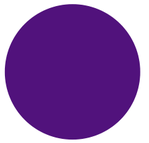
HRMS & SIRIUS+CSI:FINGERID



K. Dührkop et al., *Nat. Methods*. (**2019**).

HRMS & SIRIUS+CSI:FINGERID





$C_{12}H_4Cl_4O_2$

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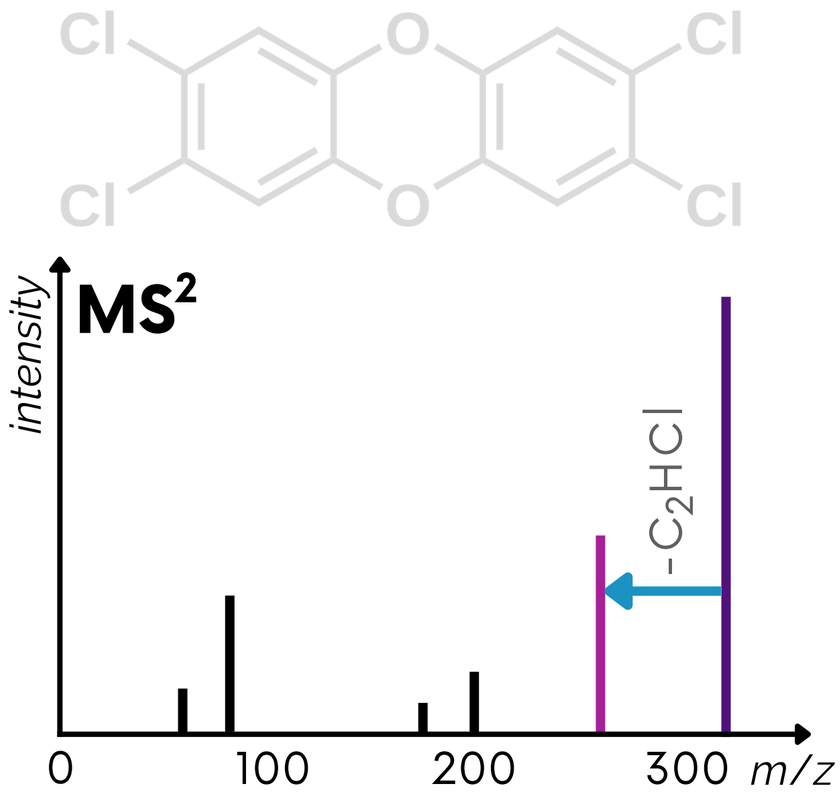

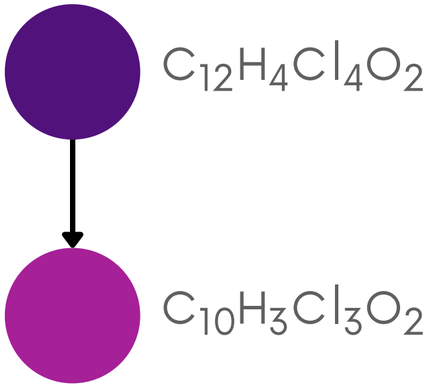

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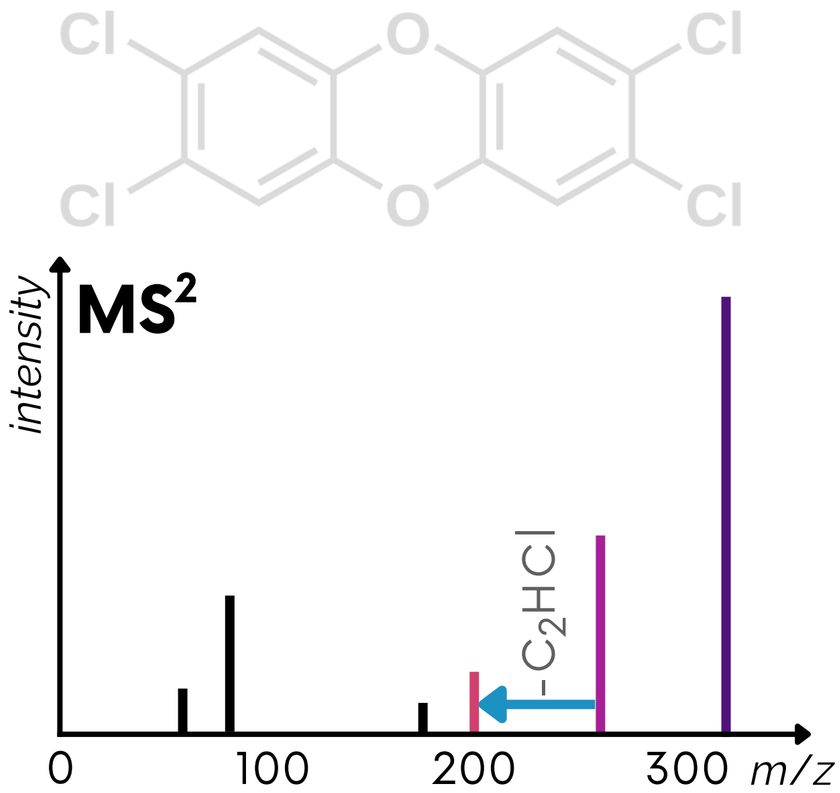
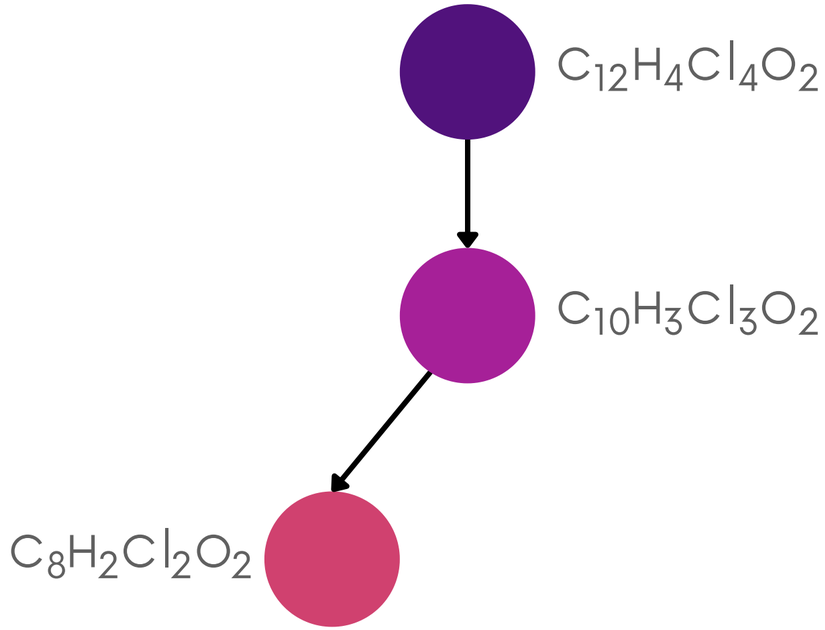
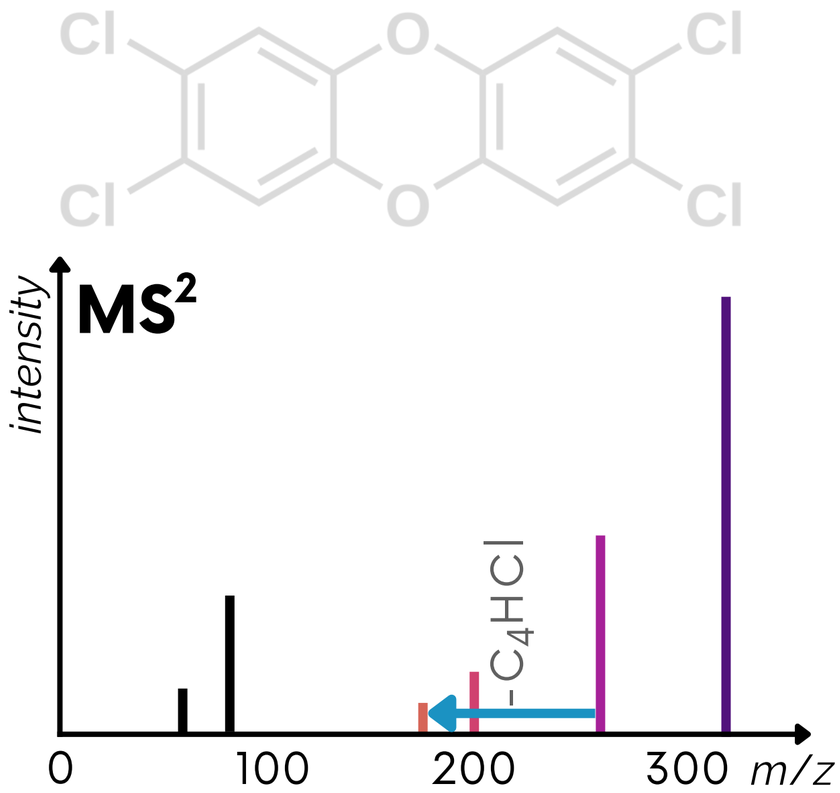
HRMS & SIRIUS+CSI:FINGERID

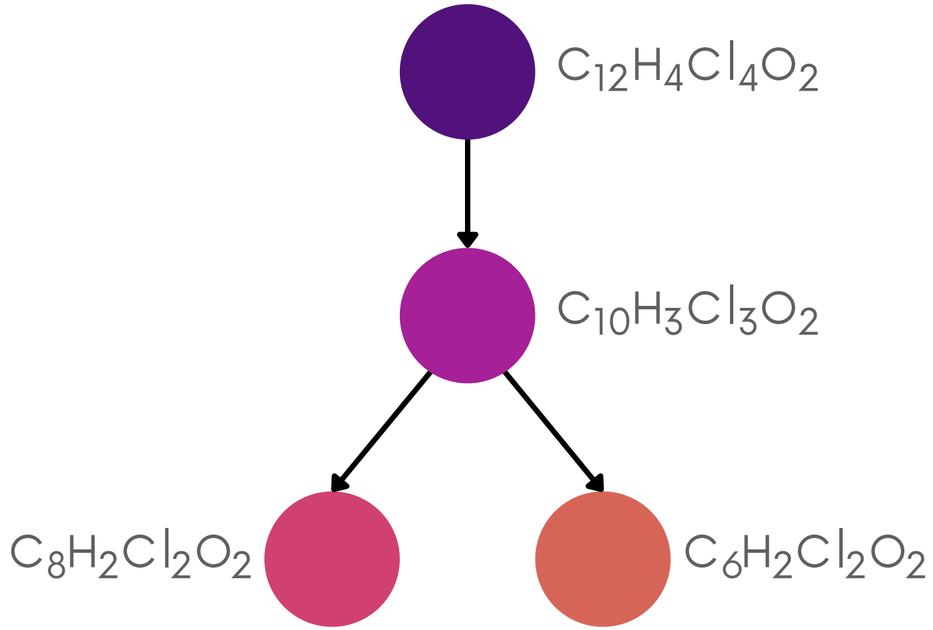




K. Dührkop et al., *Nat. Methods*. (**2019**).

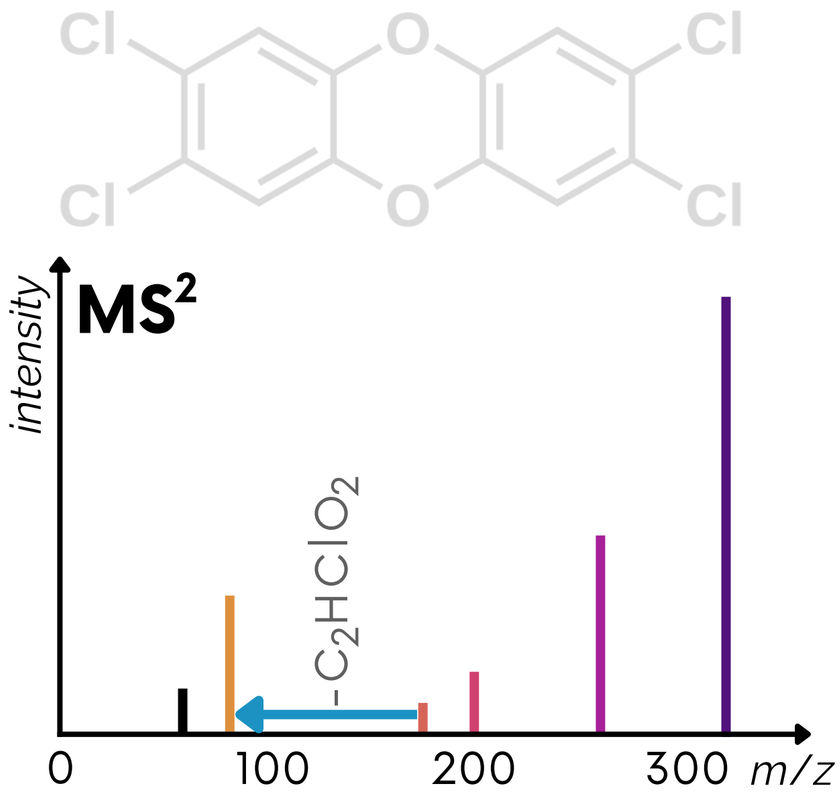
HRMS & SIRIUS+CSI:FINGERID

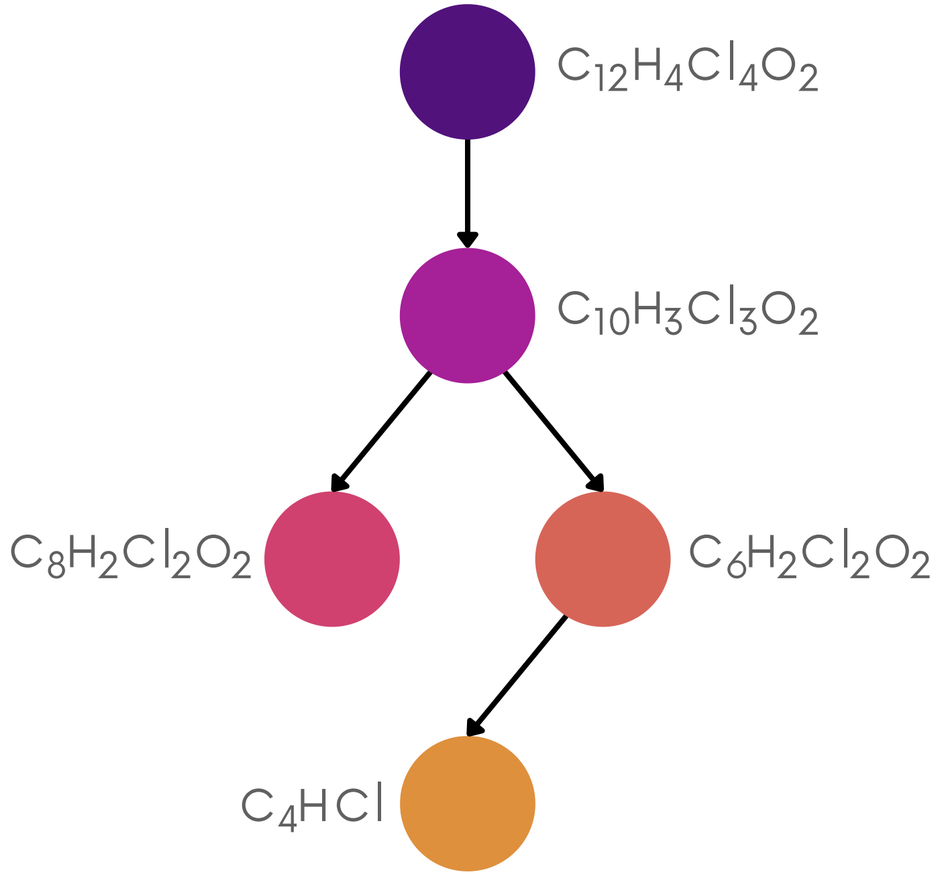




K. Dührkop et al., *Nat. Methods*. (**2019**).

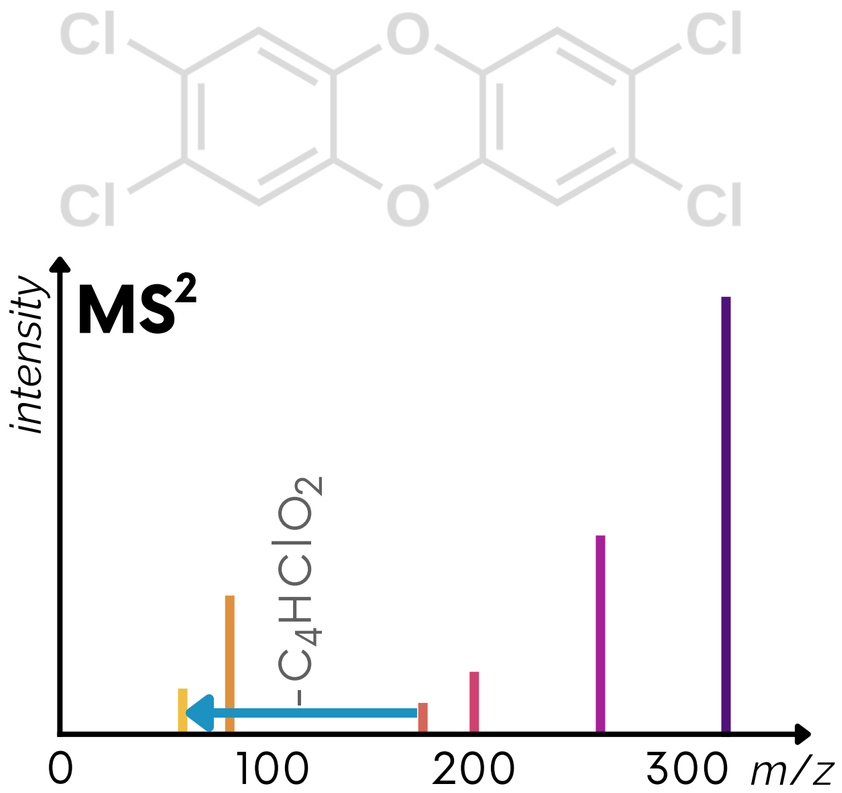
HRMS & SIRIUS+CSI:FINGERID

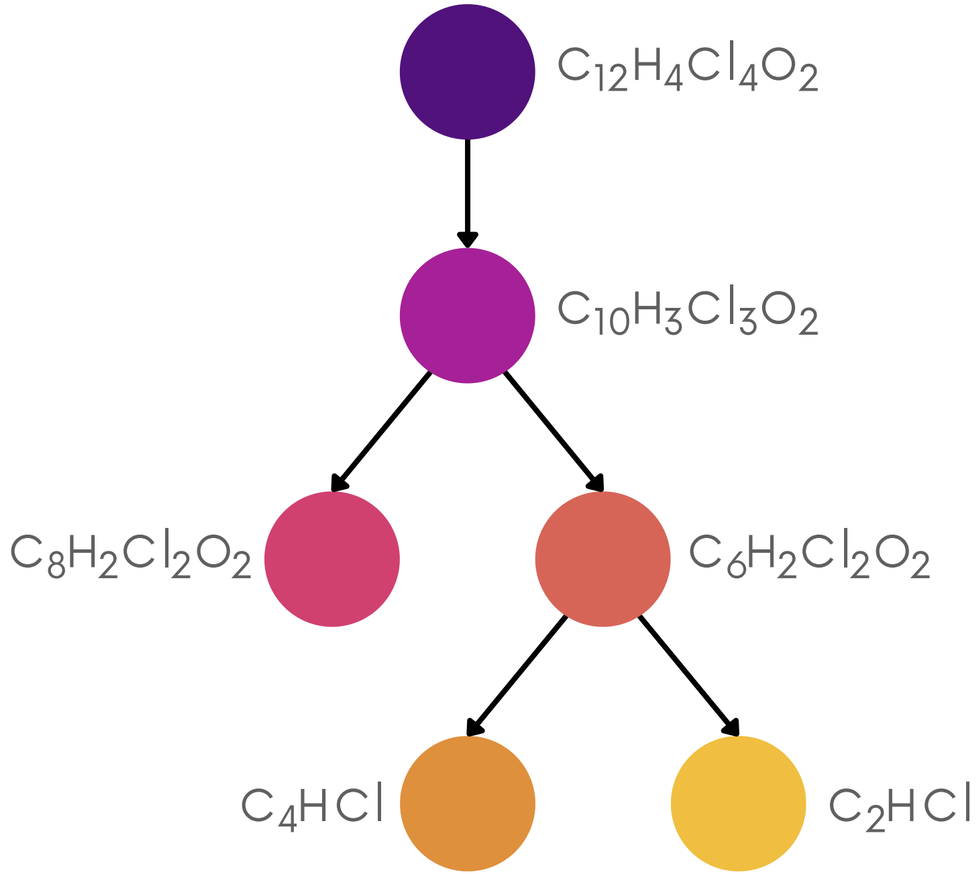




K. Dührkop et al., *Nat. Methods*. (**2019**).

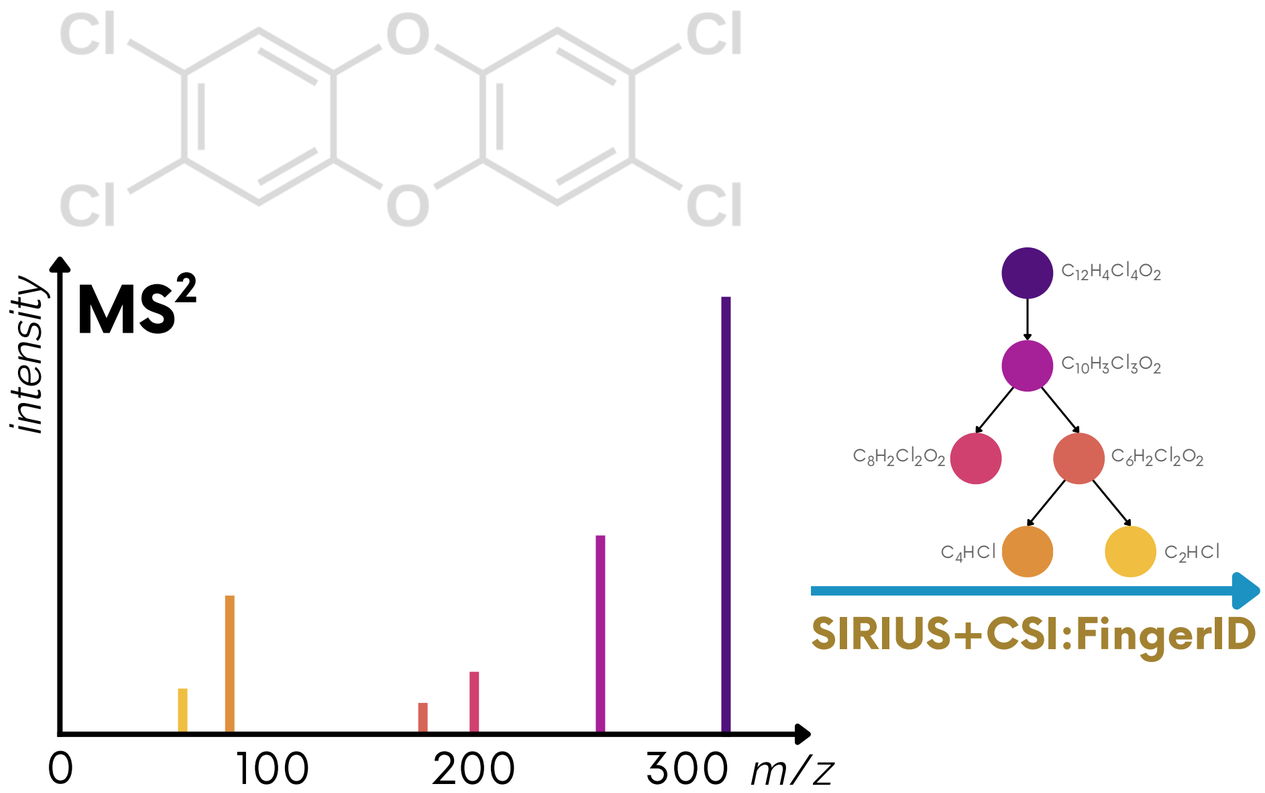
HRMS & SIRIUS+CSI:FINGERID





K. Dührkop et al., *Nat. Methods*. (**2019**).

HRMS & SIRIUS+CSI:FINGERID

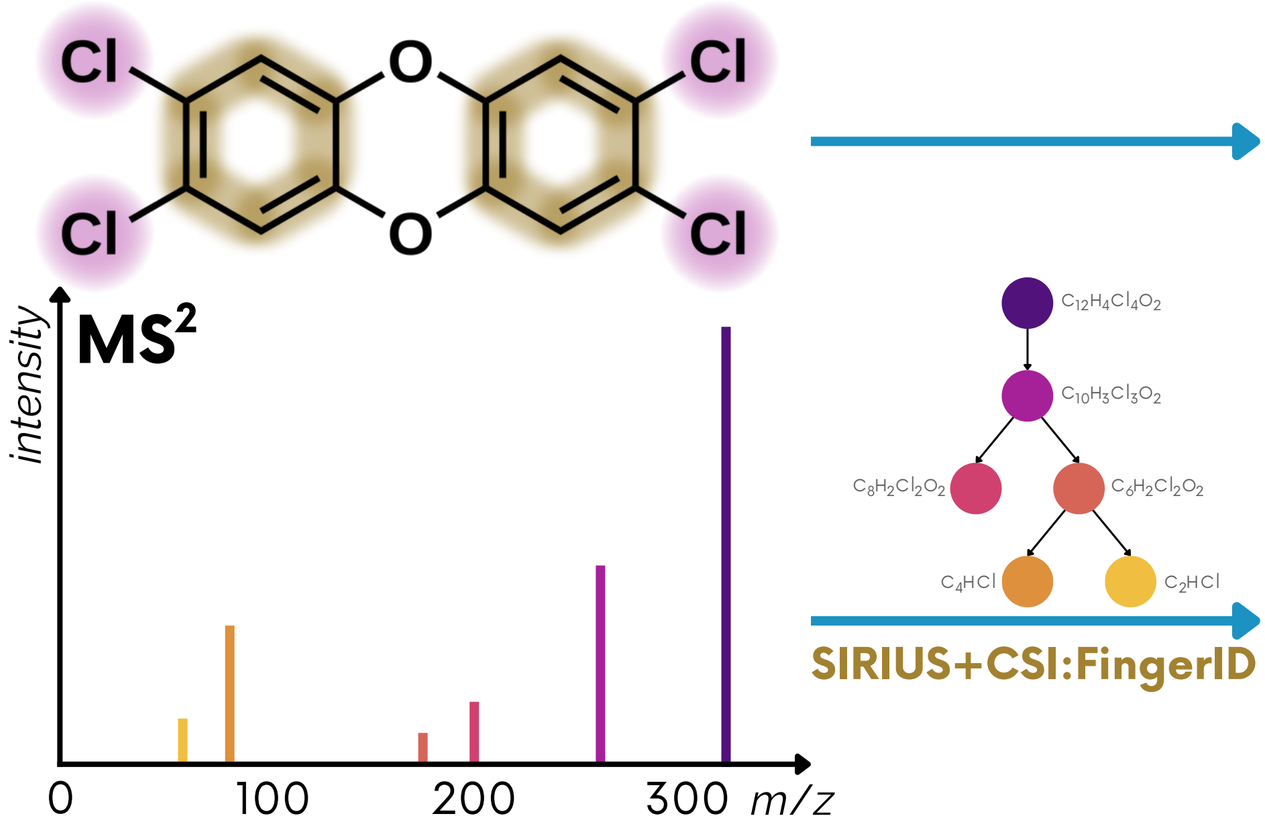


PROBABILISTIC MOLECULAR FINGERPRINT

0.14	0.45	**0.99**	...	**0.71**	0.27	0.08

K. Dührkop et al., *Nat. Methods*. (**2019**).

HRMS & SIRIUS+CSI:FINGERID



BINARY MOLECULAR FINGERPRINT

0	0	**1**	...	**1**	0	0

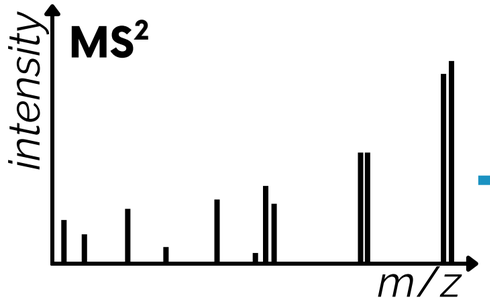
PROBABILISTIC MOLECULAR FINGERPRINT

0.14	0.45	**0.99**	...	**0.71**	0.27	0.08

K. Dührkop et al., *Nat. Methods*. (**2019**).

FIELD OF APPLICATION

TOXIC and HIGH-RISK chemicals



LC/HRMS

REAL-WORLD SAMPLES

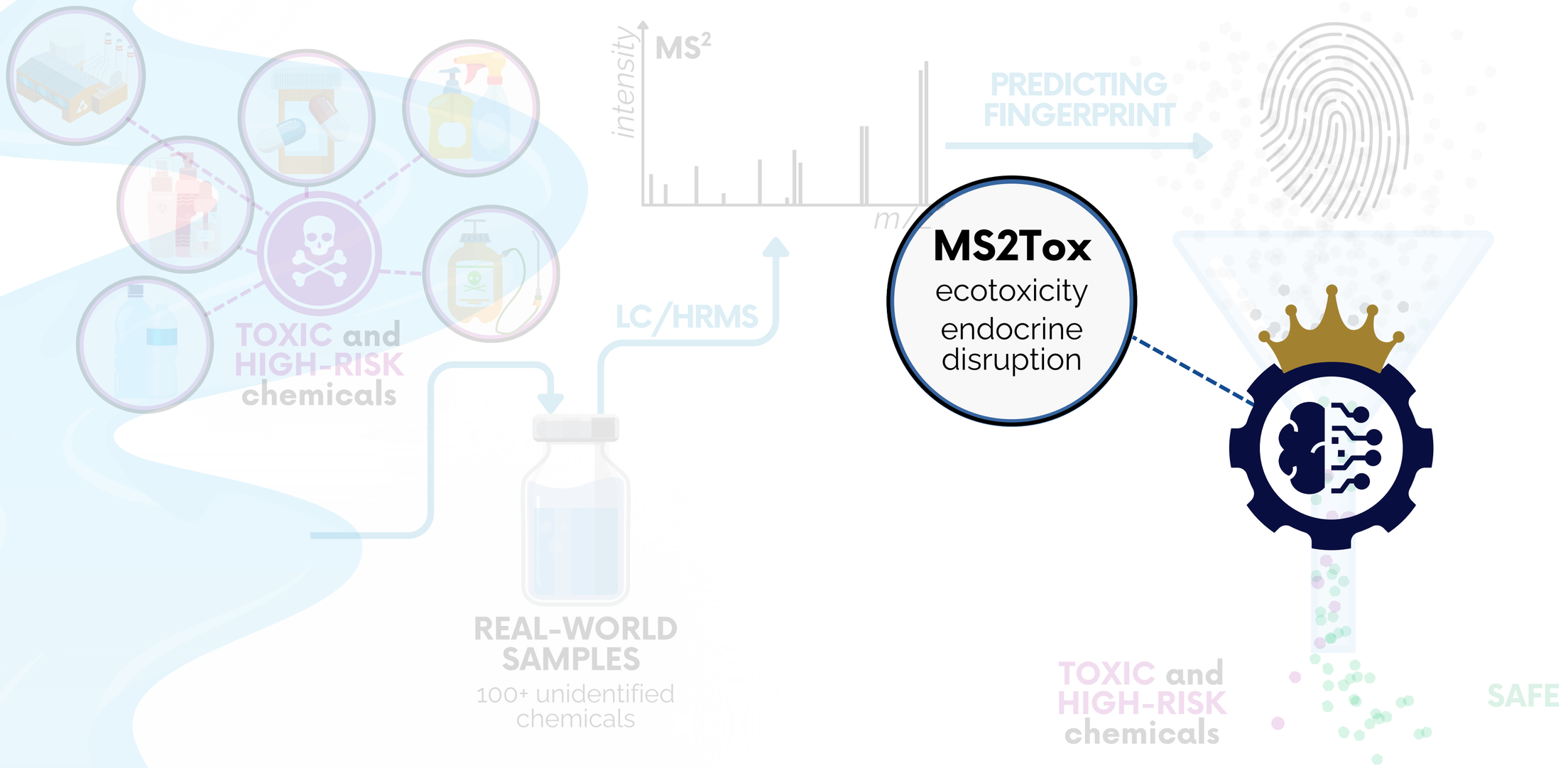
100+ unidentified chemicals

PREDICTING FINGERPRINT

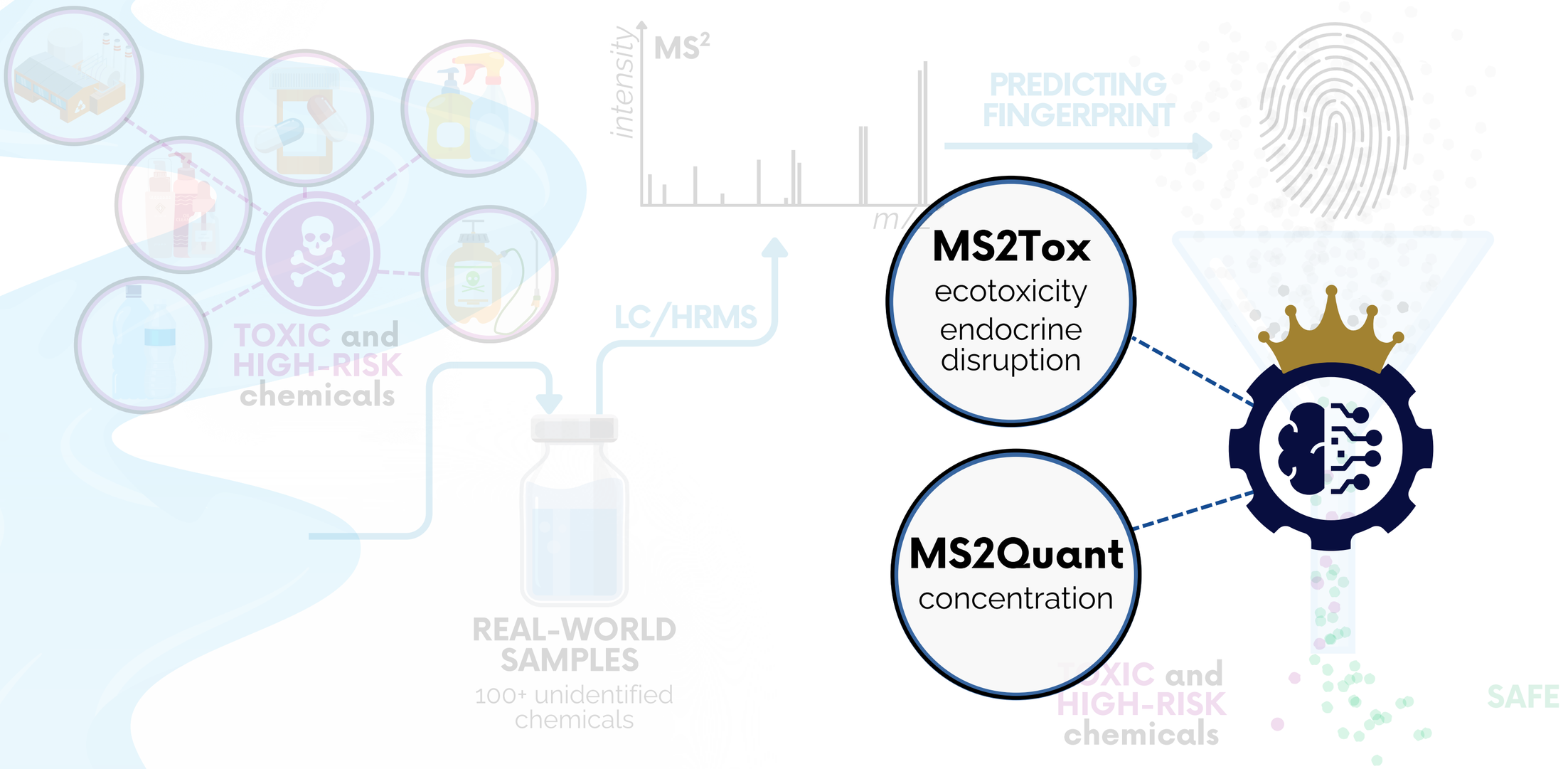
TOXIC and HIGH-RISK chemicals

SAFE

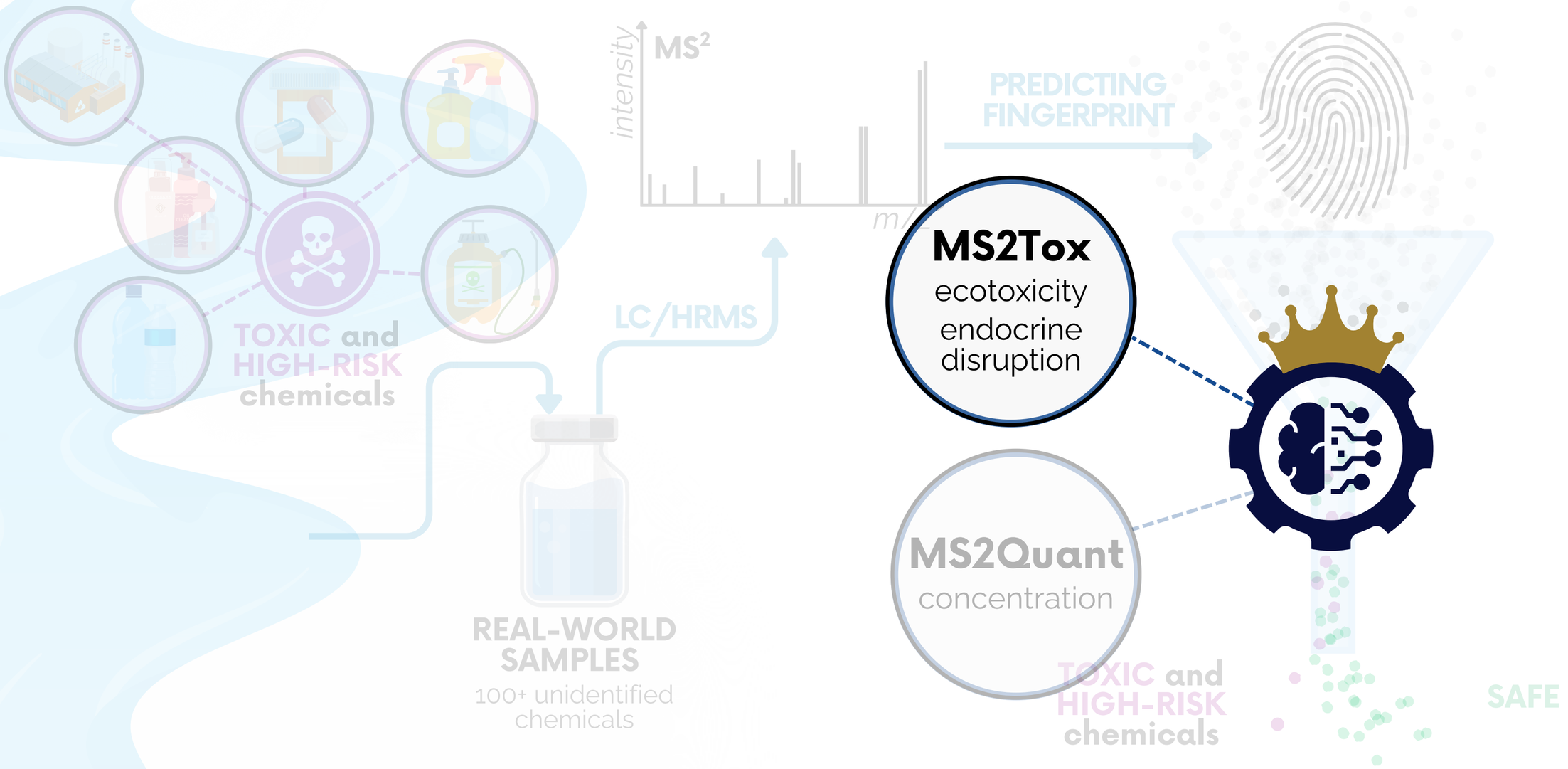
FIELD OF APPLICATION



FIELD OF APPLICATION



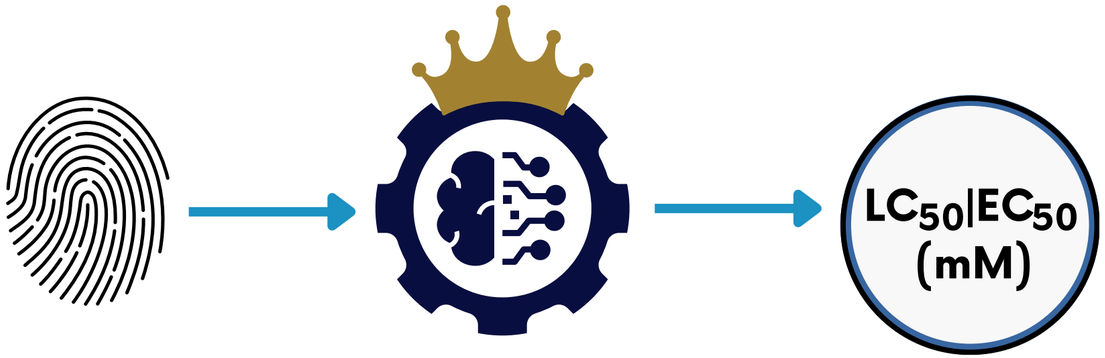
FIELD OF APPLICATION



MS2Tox

ECOTOXICITY

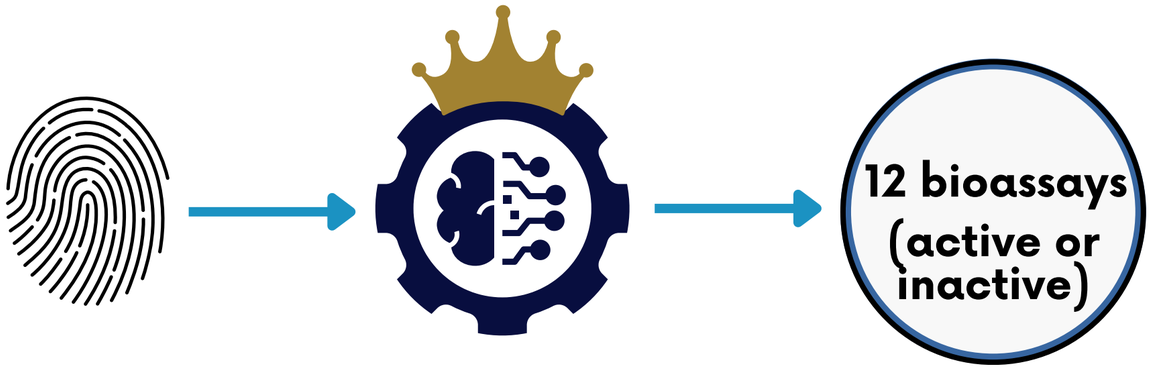
Regression task



P. Peets et al., *Environ. Sci. Tech.* (**2022**).

ENDOCRINE DISRUPTION

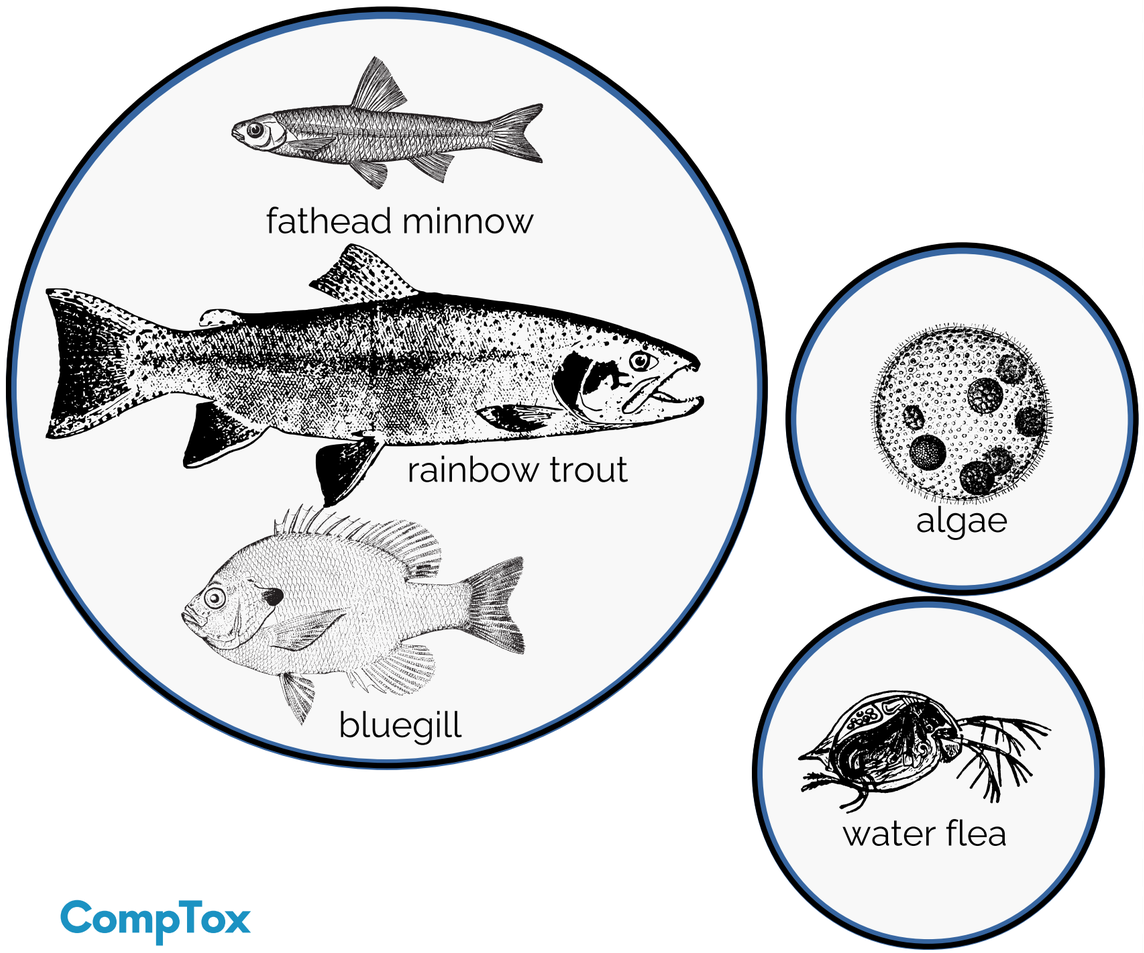
Classification task



I. Rahu et al., *J. Chem. Inf. Model.* (**2024**).

MS2Tox: DATA

ECOTOXICITY



CompTox

P. Peets et al., *Environ. Sci. Tech.* (**2022**).

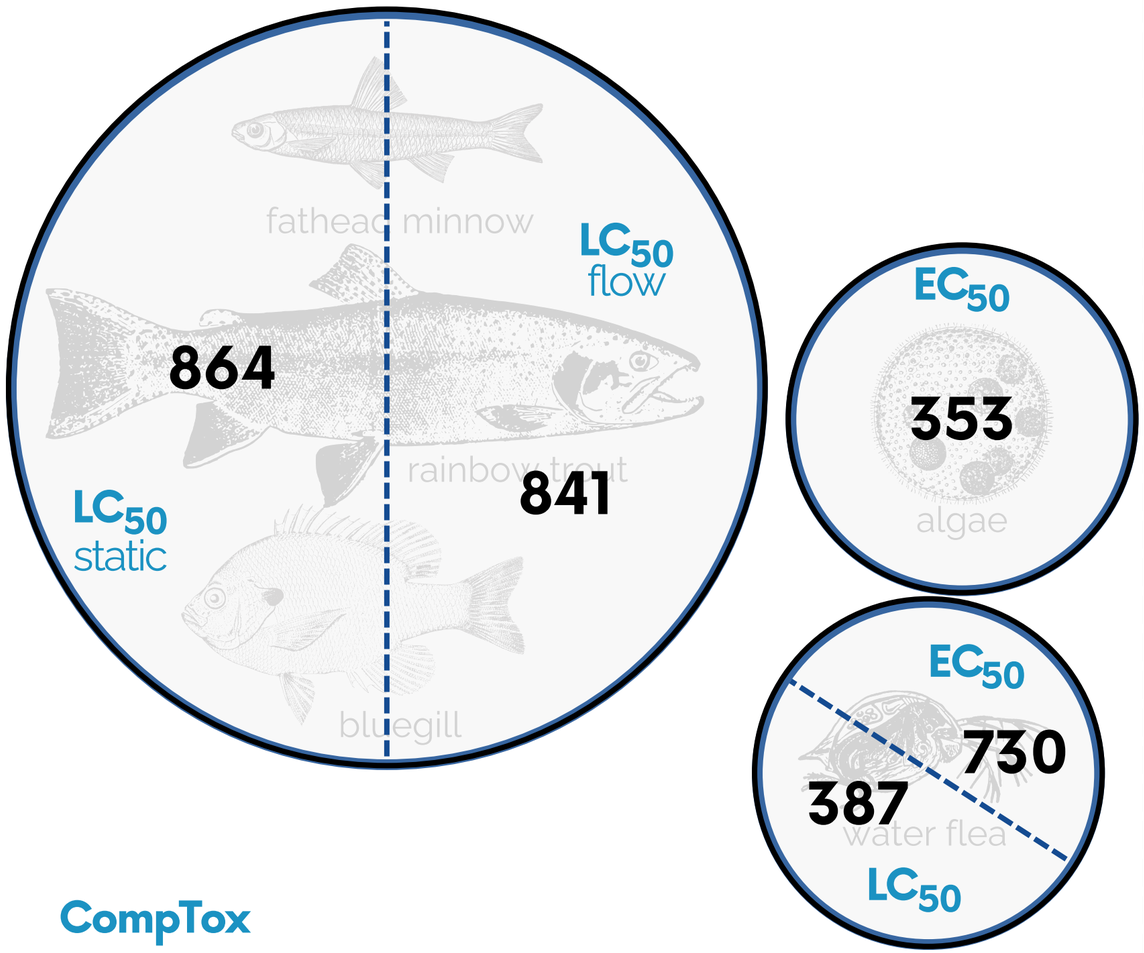
ENDOCRINE DISRUPTION

Classification task

I. Rahu et al., *J. Chem. Inf. Model.* (**2024**).

MS2Tox: DATA

ECOTOXICITY



CompTox

P. Peets et al., *Environ. Sci. Tech.* (**2022**).

ENDOCRINE DISRUPTION

I. Rahu et al., *J. Chem. Inf. Model.* (**2024**).

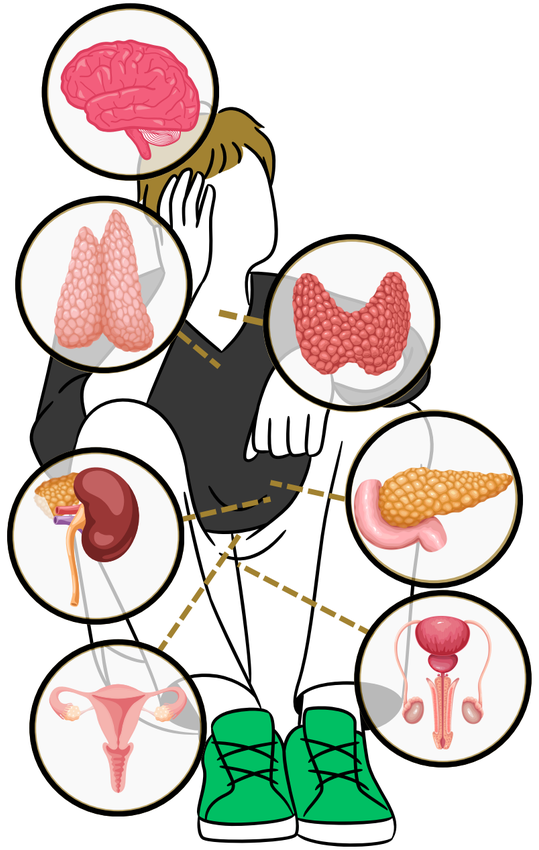
MS2Tox: DATA

ECOTOXICITY

CompTox

P. Peets et al., *Environ. Sci. Tech.* (**2022**).

ENDOCRINE DISRUPTION



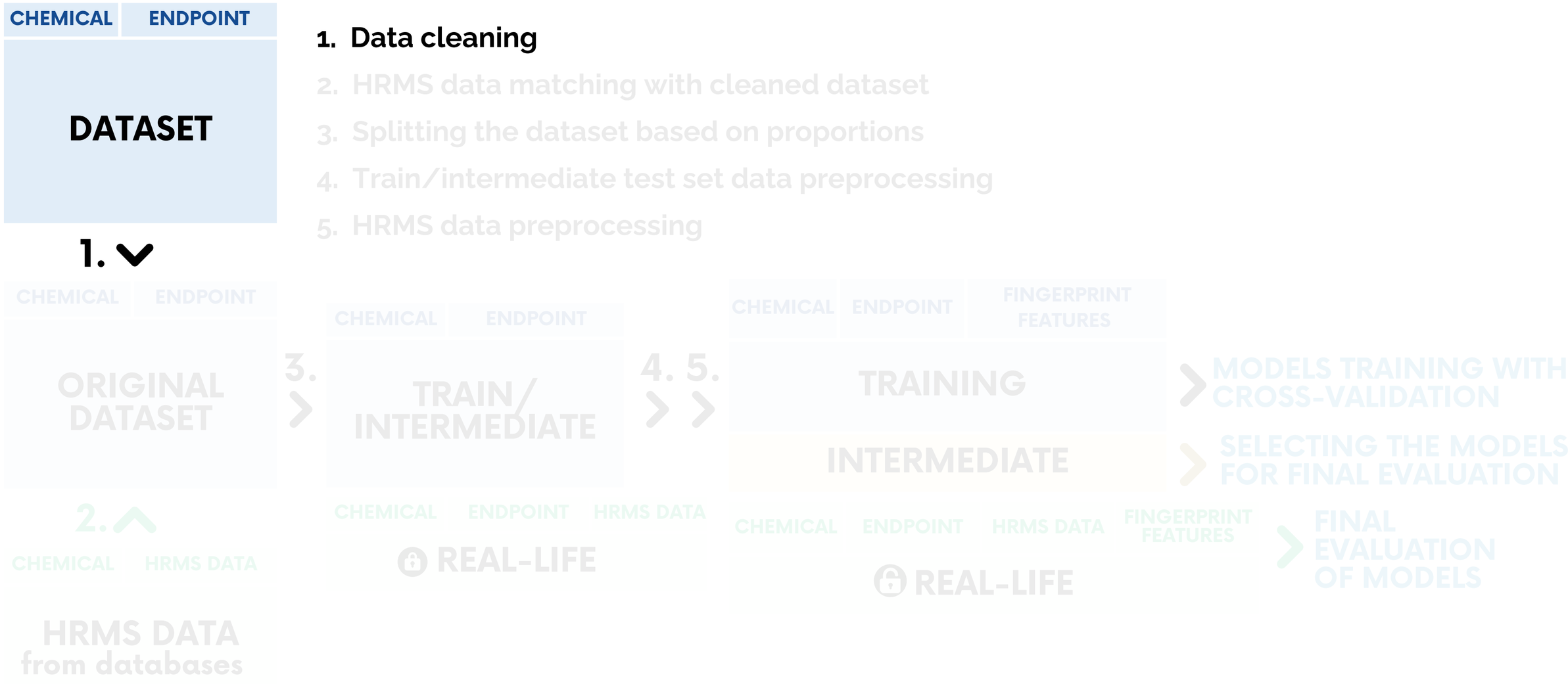
CHEMICAL	12 BIOASSAYS

TOX21
11764 instances

Tox21 Data Challenge dataset

I. Rahu et al., *J. Chem. Inf. Model.* (**2024**).

MS2Tox: WORKFLOW

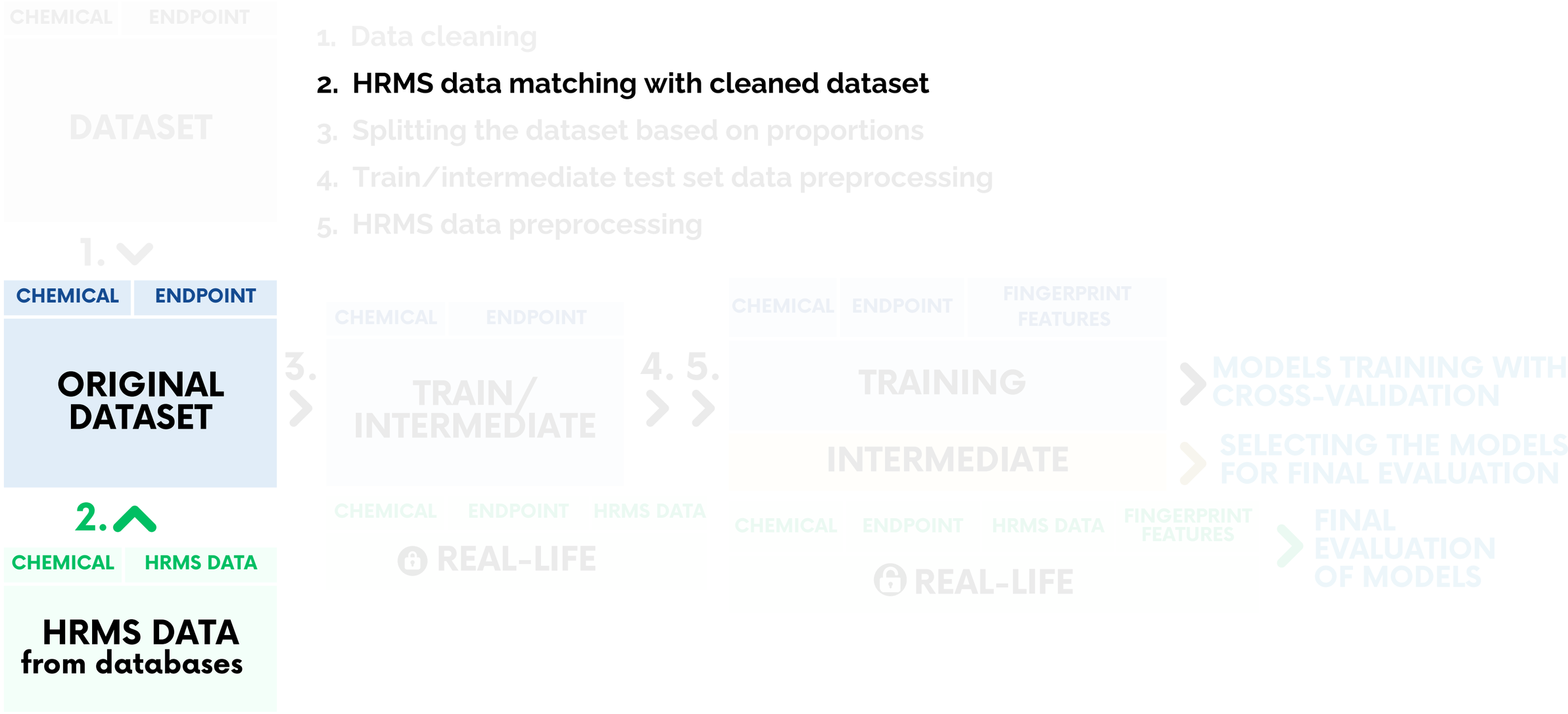


P. Peets et al., *Environ. Sci. Tech.* (**2022**).

I. Rahu et al., *J. Chem. Inf. Model.* (**2024**).

MS2Tox: WORKFLOW

1. Data cleaning
2. **HRMS data matching with cleaned dataset**
3. Splitting the dataset based on proportions
4. Train/intermediate test set data preprocessing
5. HRMS data preprocessing



P. Peets et al., *Environ. Sci. Tech.* (**2022**).

I. Rahu et al., *J. Chem. Inf. Model.* (**2024**).

MS2Tox: WORKFLOW

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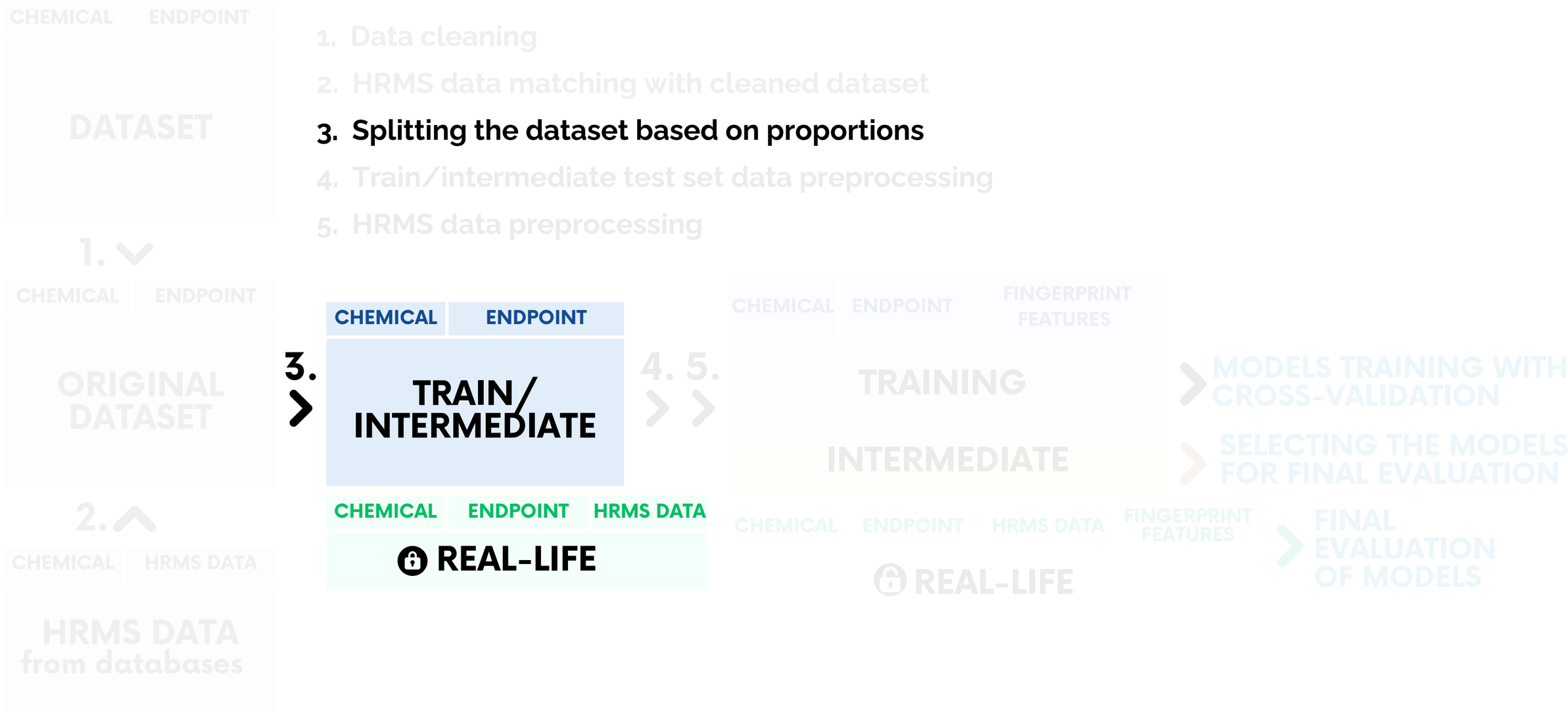

P. Peets et al., *Environ. Sci. Tech.* (**2022**).

I. Rahu et al., *J. Chem. Inf. Model.* (**2024**).

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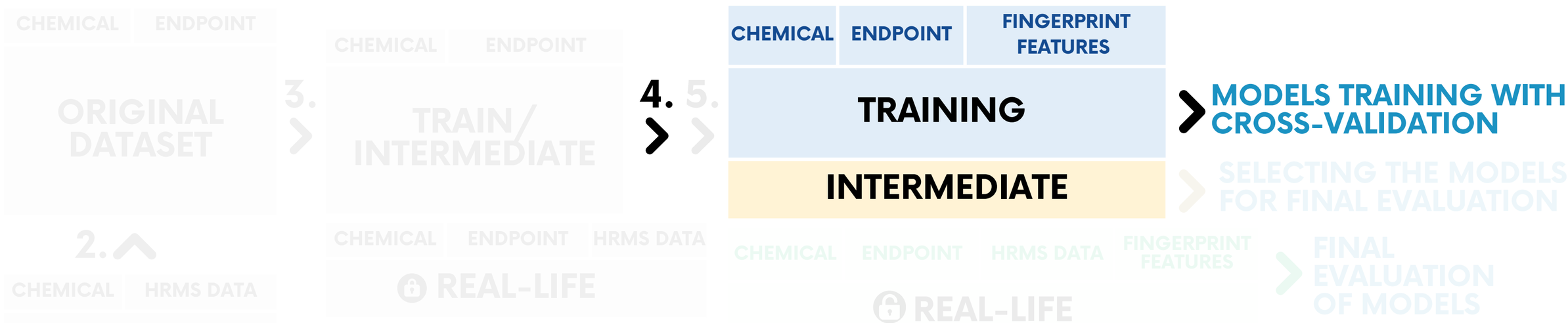

P. Peets et al., *Environ. Sci. Tech.* (**2022**).

I. Rahu et al., *J. Chem. Inf. Model.* (**2024**).

MS2Tox: WORKFLOW

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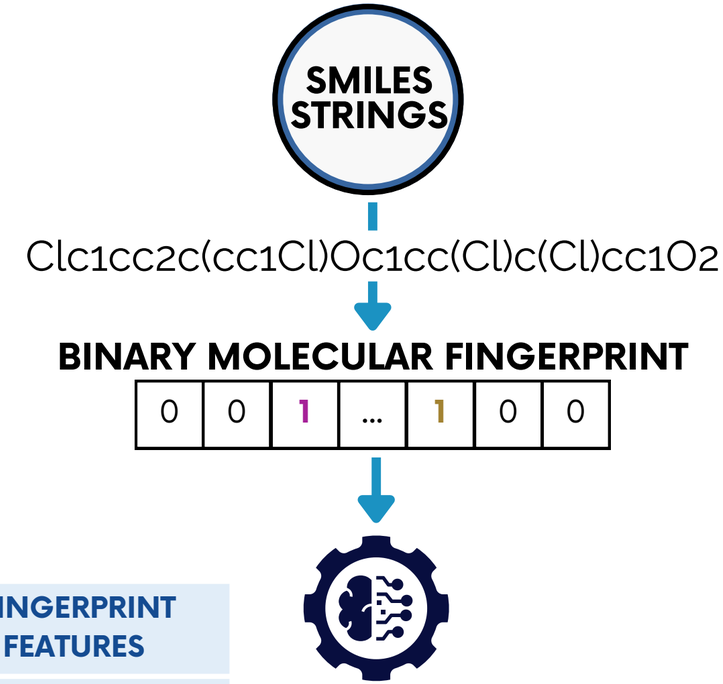

P. Peets et al., *Environ. Sci. Tech.* (**2022**).

I. Rahu et al., *J. Chem. Inf. Model.* (**2024**).

MS2Tox: WORKFLOW

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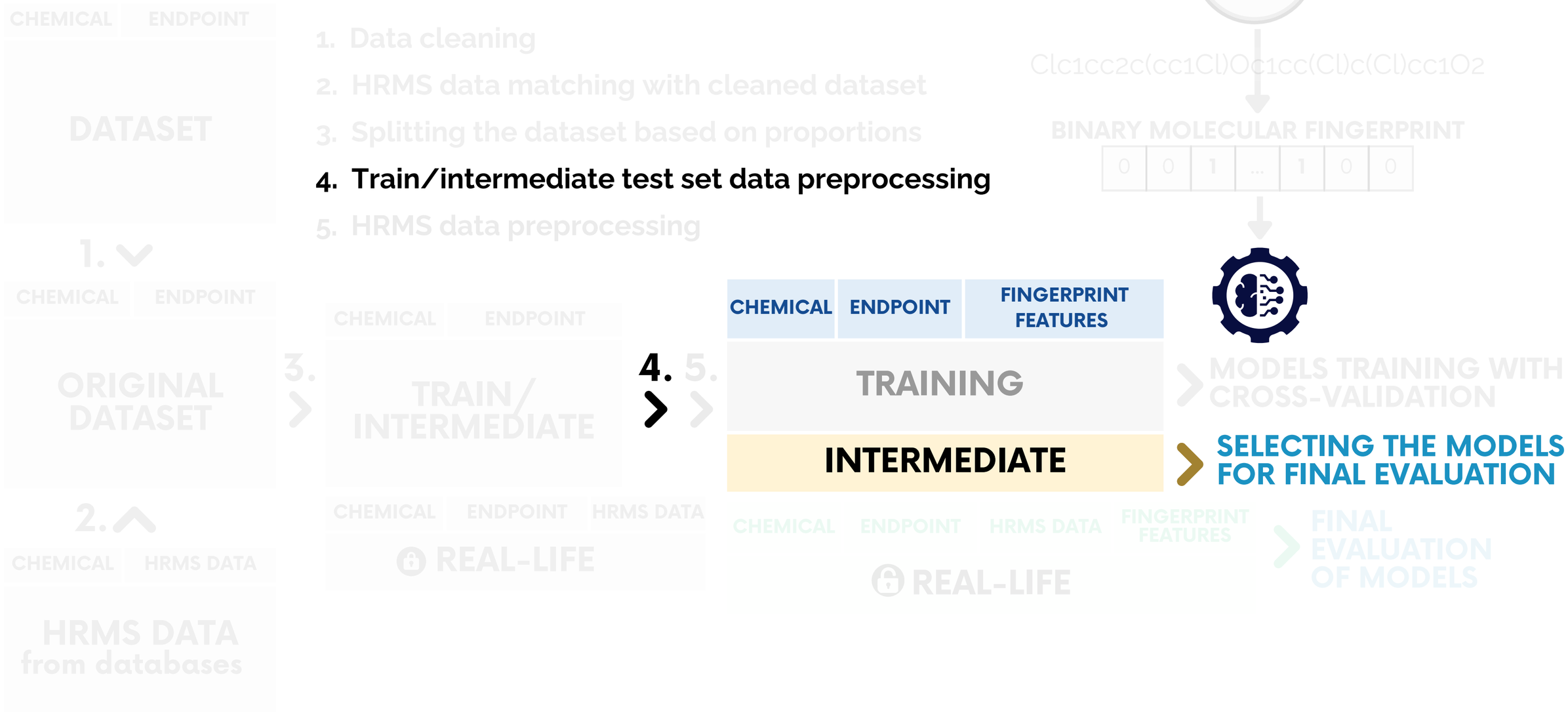

P. Peets et al., *Environ. Sci. Tech.* (**2022**).

I. Rahu et al., *J. Chem. Inf. Model.* (**2024**).

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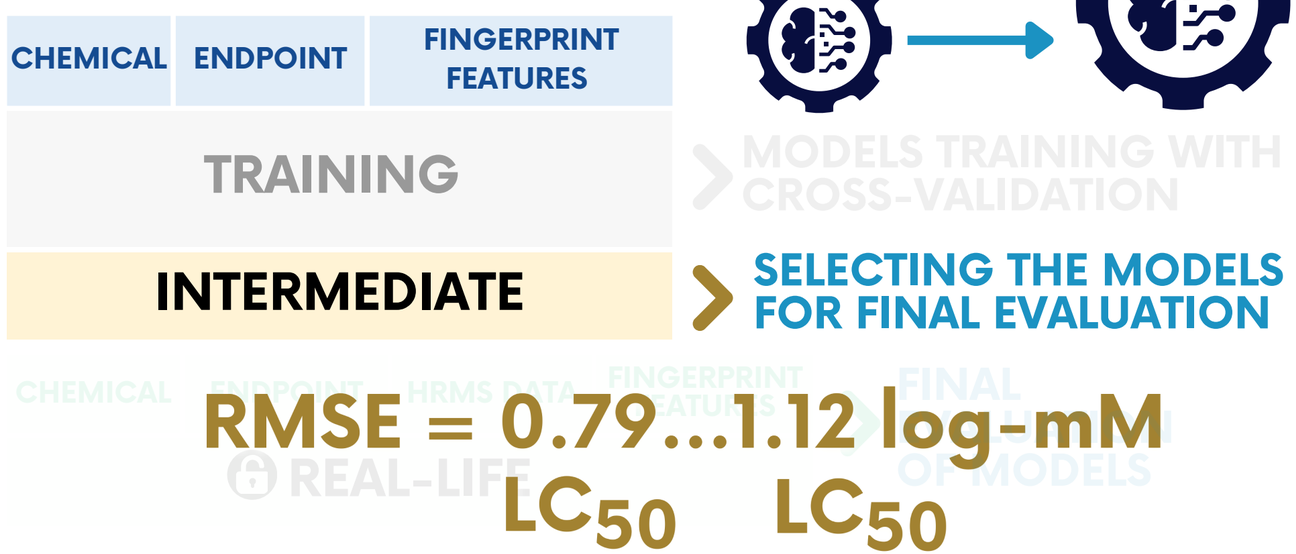
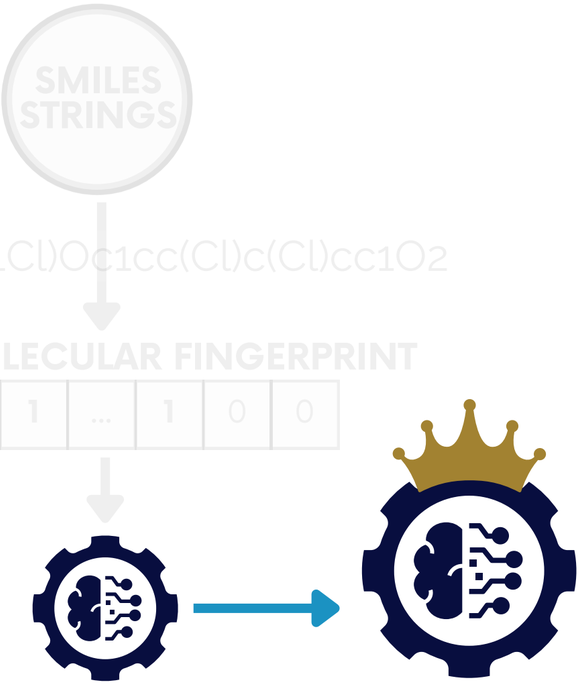




RMSE = 0.79...1.12 log-mM

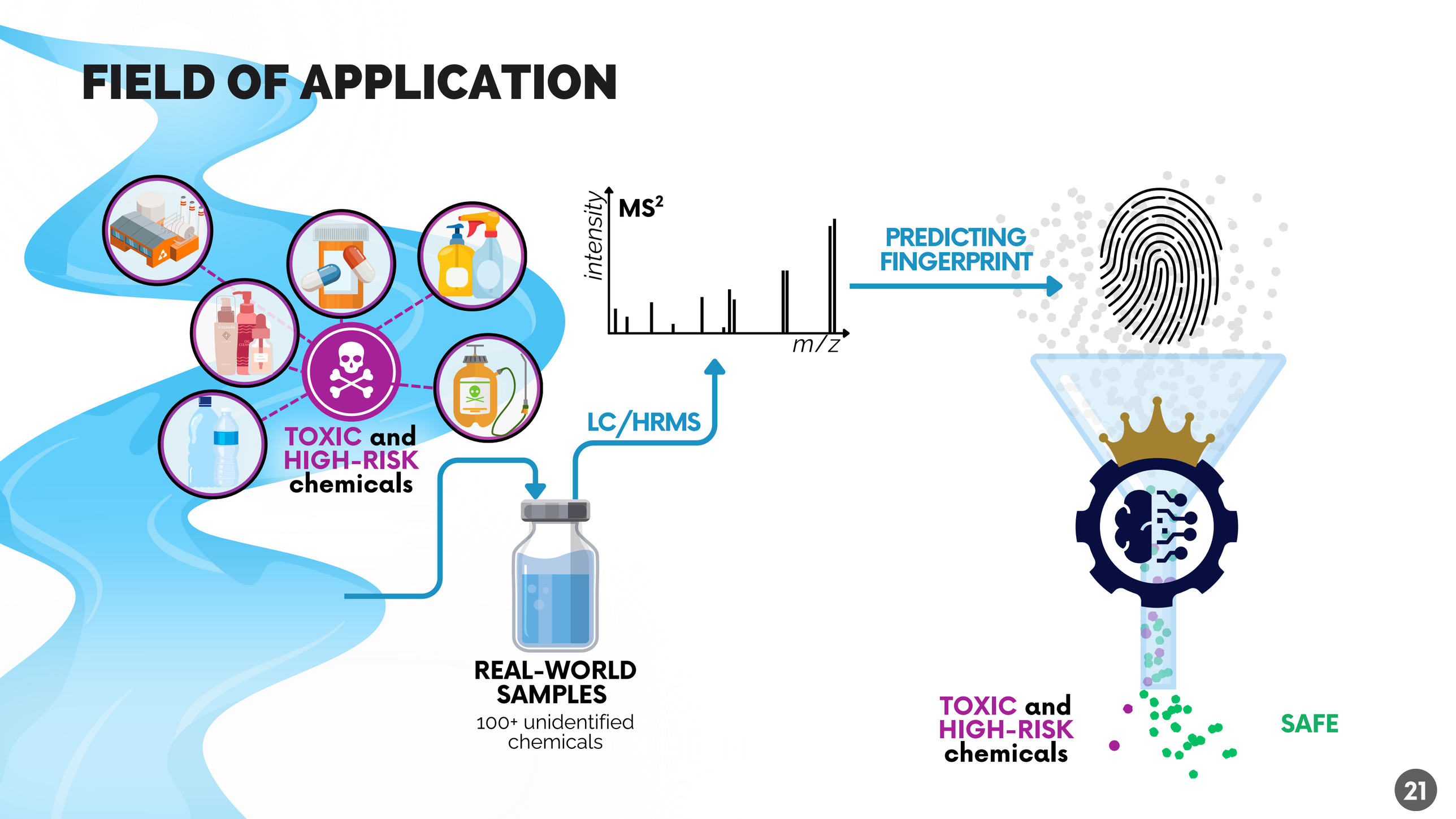
LC_{50} fish (static)

LC_{50} water flea

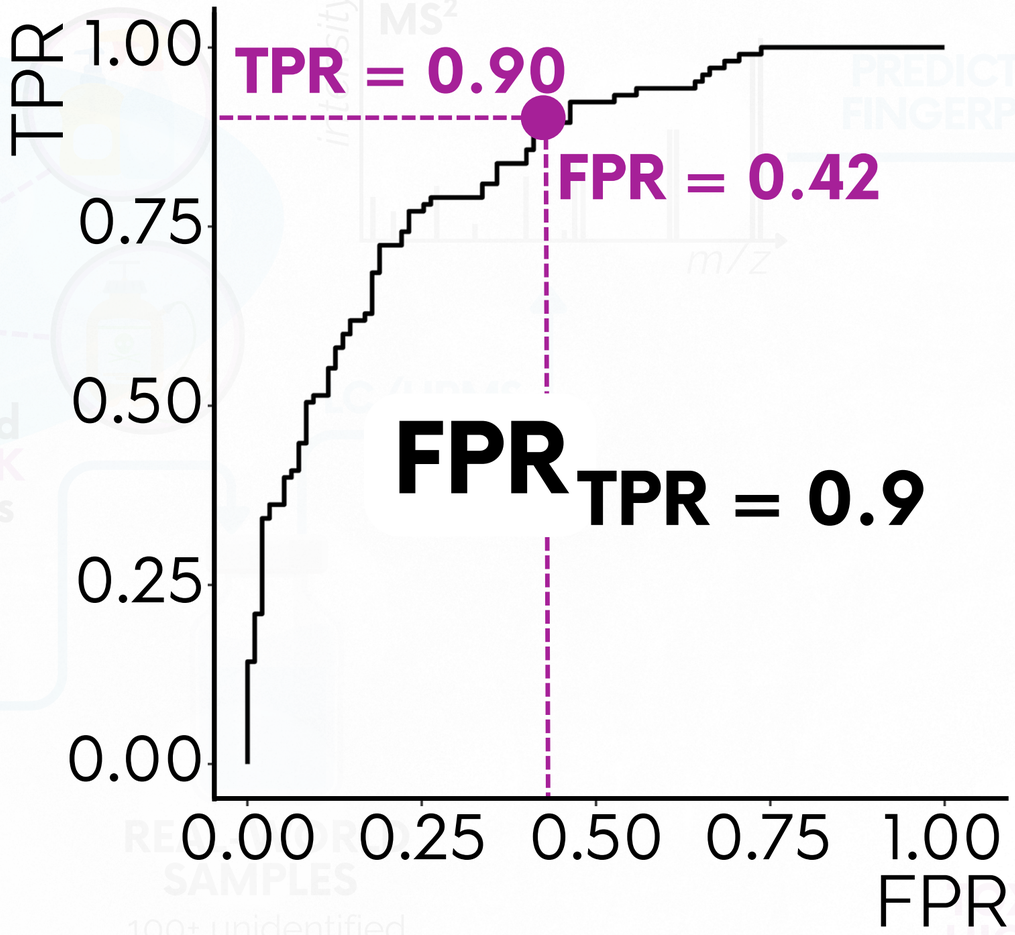
P. Peets et al., *Environ. Sci. Tech.* (**2022**).

I. Rahu et al., *J. Chem. Inf. Model.* (**2024**).

FIELD OF APPLICATION



FIELD OF APPLICATION



MS2Tox: WORKFLOW

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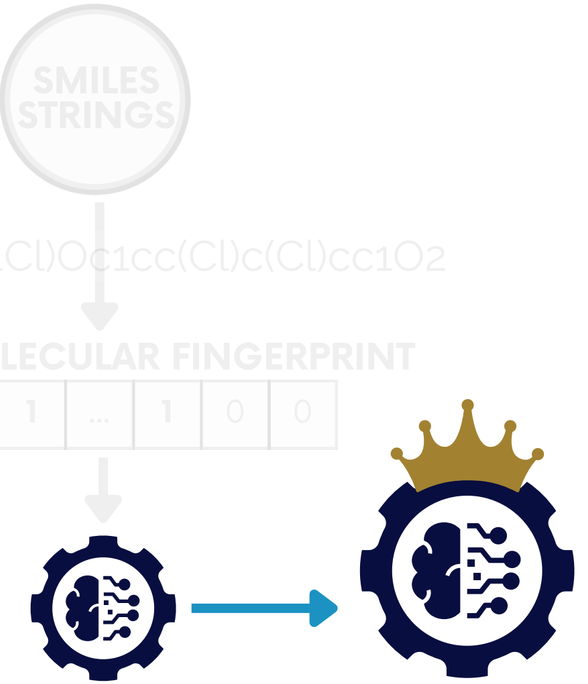


CHEMICAL	ENDPOINT	FINGERPRINT FEATURES
TRAINING		
INTERMEDIATE		

MODELS TRAINING WITH CROSS-VALIDATION

SELECTING THE MODELS FOR FINAL EVALUATION

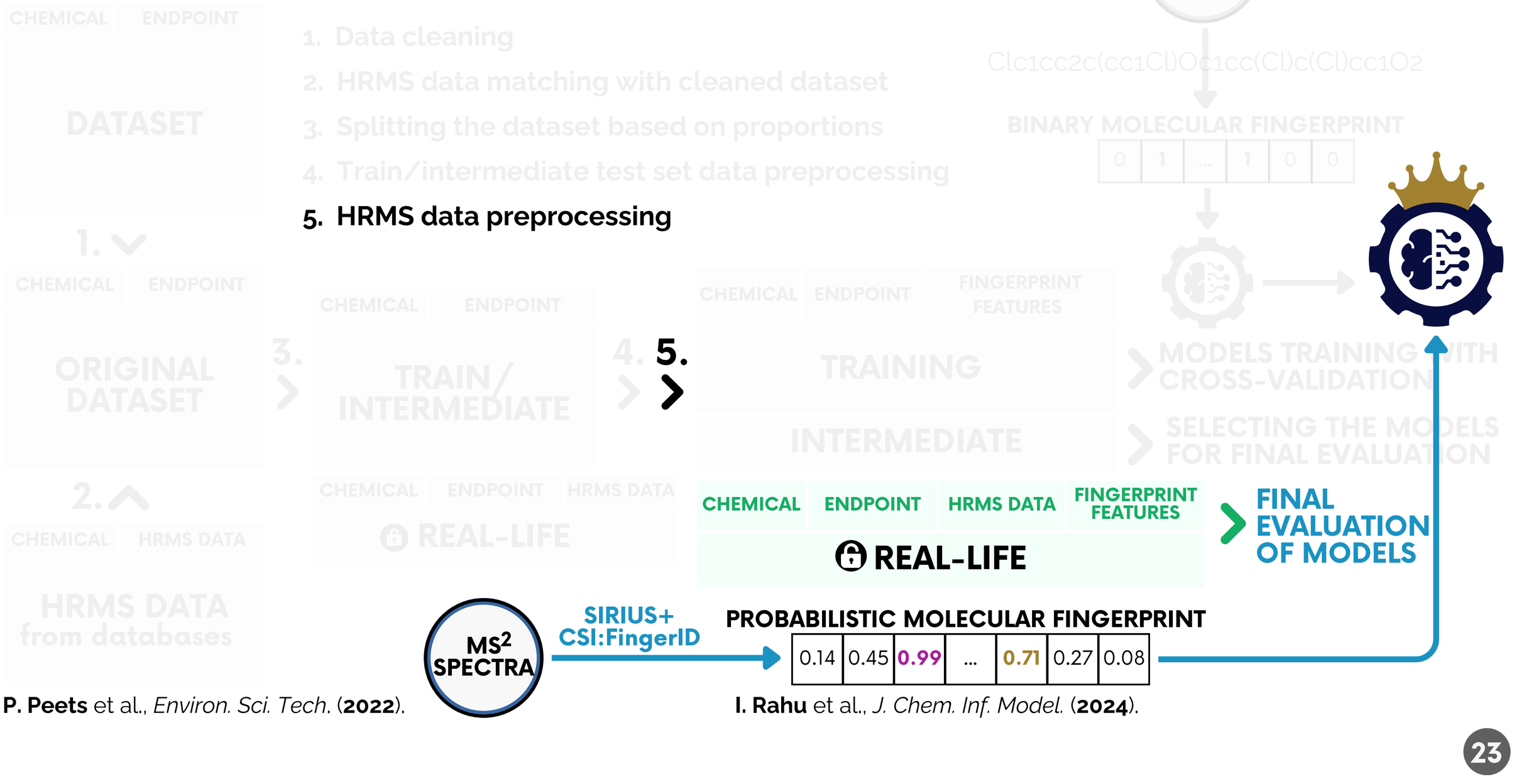
FPR at 90% recall = 0.19...0.69
AHR ER

P. Peets et al., *Environ. Sci. Tech.* (**2022**).

I. Rahu et al., *J. Chem. Inf. Model.* (**2024**).

MS2Tox: WORKFLOW

1. Data cleaning
2. HRMS data matching with cleaned dataset
3. Splitting the dataset based on proportions
4. Train/intermediate test set data preprocessing
5. **HRMS data preprocessing**

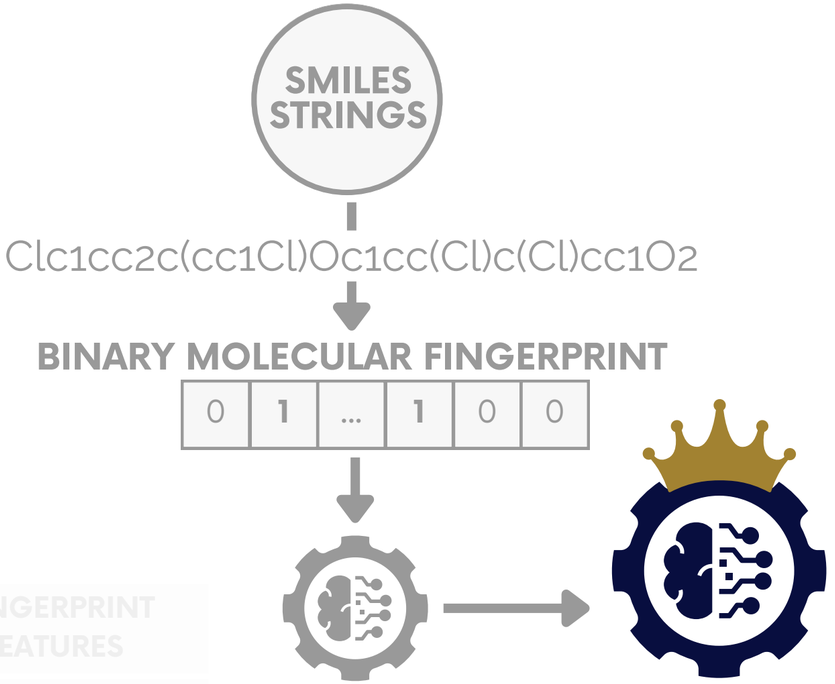


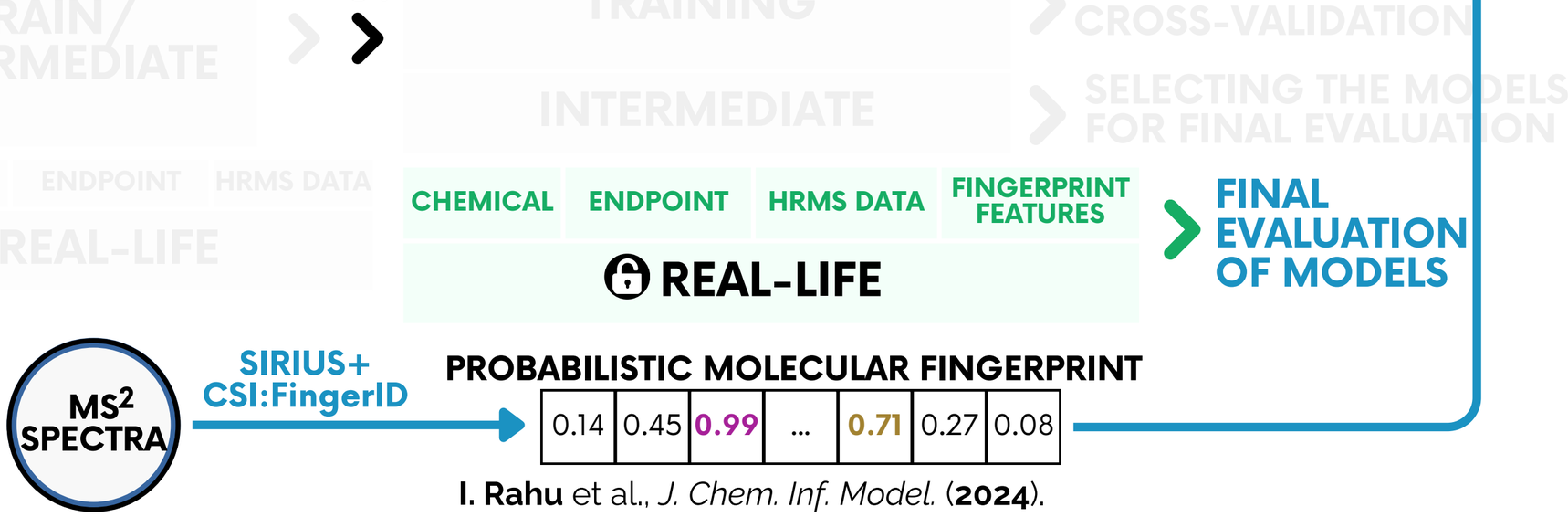
P. Peets et al., *Environ. Sci. Tech.* (**2022**).

I. Rahu et al., *J. Chem. Inf. Model.* (**2024**).

MS2Tox: WORKFLOW

1. Data cleaning
2. HRMS data matching with cleaned dataset
3. Splitting the dataset based on proportions
4. Train/intermediate test set data preprocessing
5. **HRMS data preprocessing**





P. Peets et al., *Environ. Sci. Tech.* (**2022**).

I. Rahu et al., *J. Chem. Inf. Model.* (**2024**).

MS2Tox: WORKFLOW

PROBABILISTIC MOLECULAR FINGERPRINT

0.14	0.45	**0.99**	...	**0.71**	0.27	0.08

P. Peets et al., *Environ. Sci. Tech.* (**2022**).

MS2Tox: WORKFLOW

PROBABILISTIC MOLECULAR FINGERPRINT

0.14	0.45	**0.99**	...	**0.71**	0.27	0.08

THRESHOLD

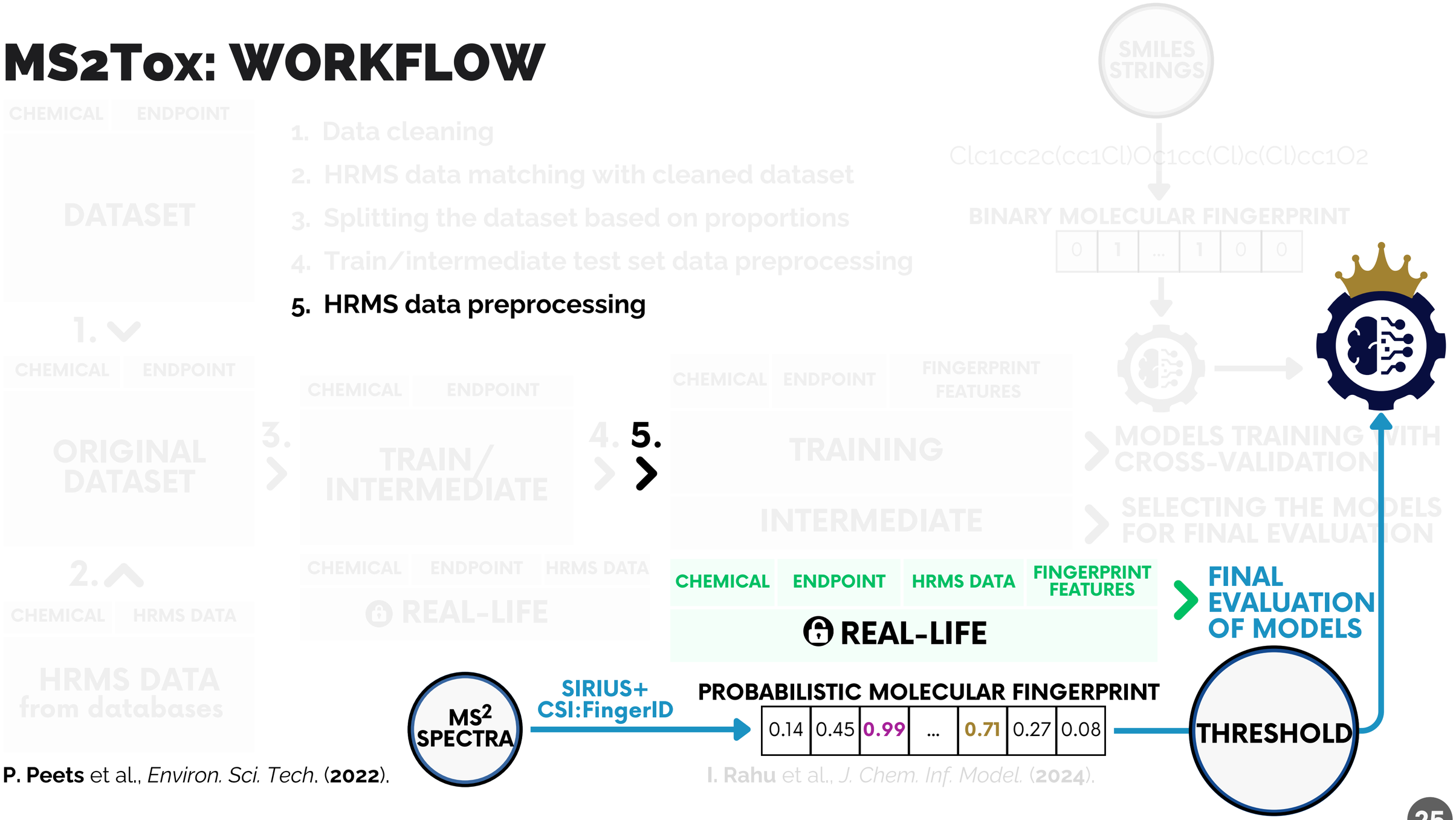
BINARY MOLECULAR FINGERPRINT

0	0	**1**	...	**1**	0	0

P. Peets et al., *Environ. Sci. Tech.* (**2022**).

MS2Tox: WORKFLOW

1. Data cleaning
2. HRMS data matching with cleaned dataset
3. Splitting the dataset based on proportions
4. Train/intermediate test set data preprocessing
5. **HRMS data preprocessing**



P. Peets et al., *Environ. Sci. Tech.* (**2022**).

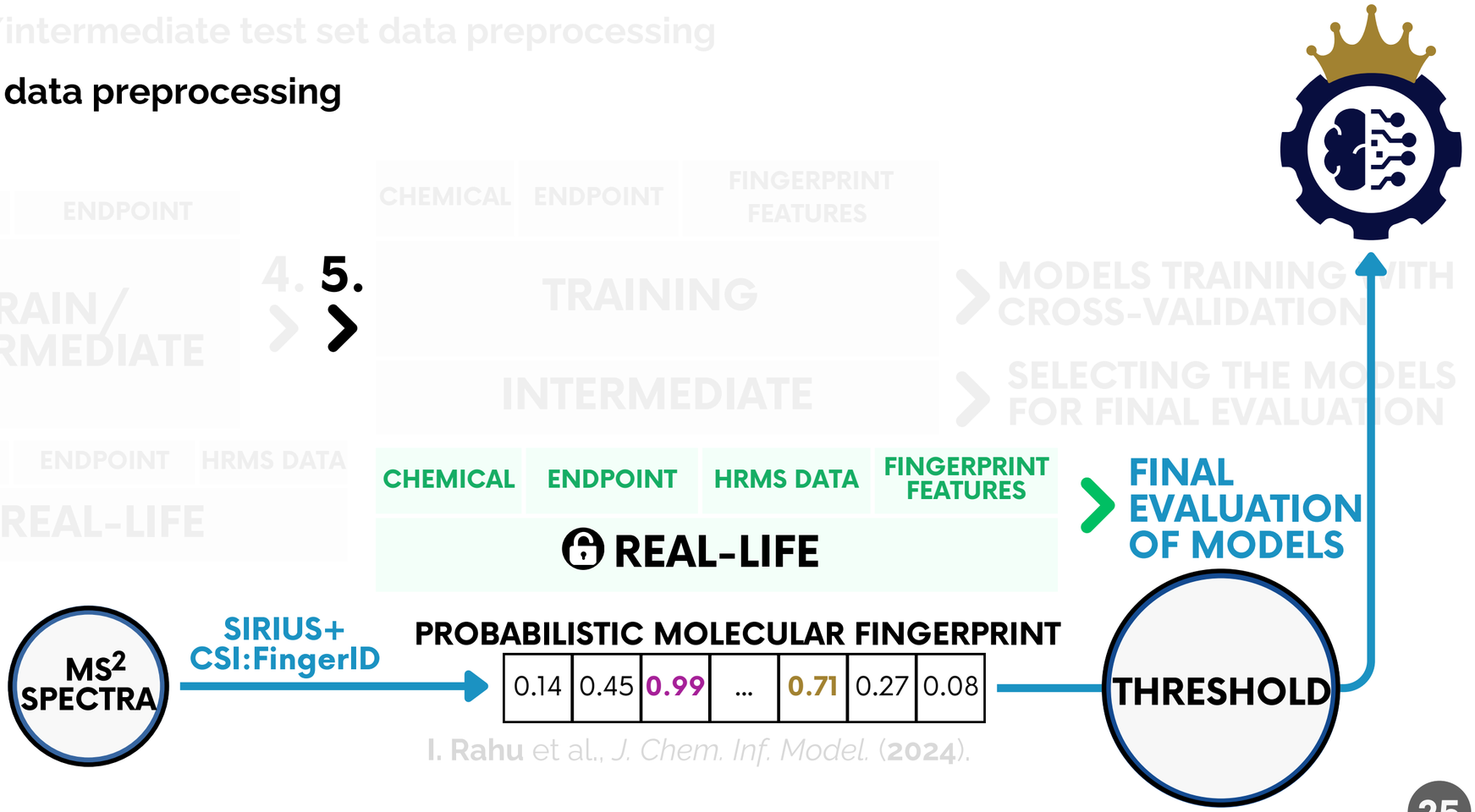
I. Rahu et al., *J. Chem. Inf. Model.* (**2024**).

MS2Tox: WORKFLOW

RMSE = 0.79…1.26 log-mM

EC_{50} water flea EC_{50} algae

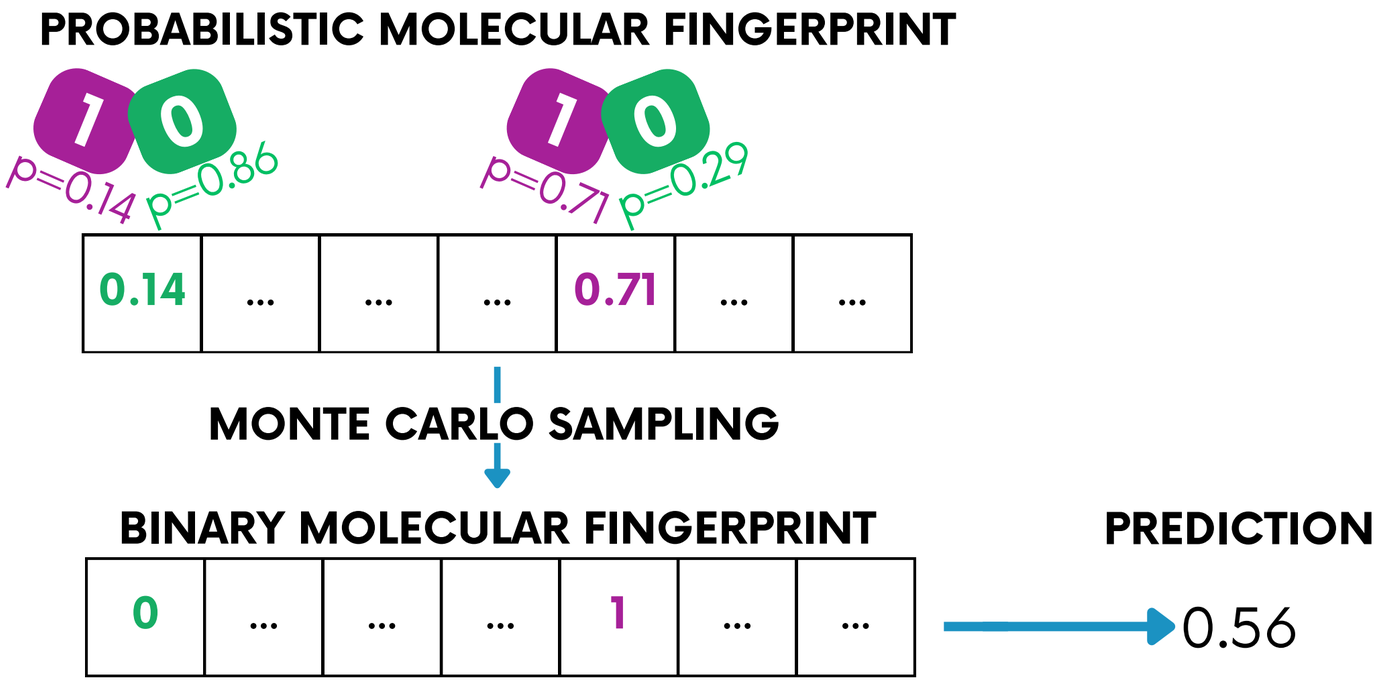
1. Data cleaning
2. HRMS data matching with cleaned dataset
3. Splitting the dataset based on proportions
4. Train/intermediate test set data preprocessing
5. **HRMS data preprocessing**



P. Peets et al., *Environ. Sci. Tech.* (**2022**).

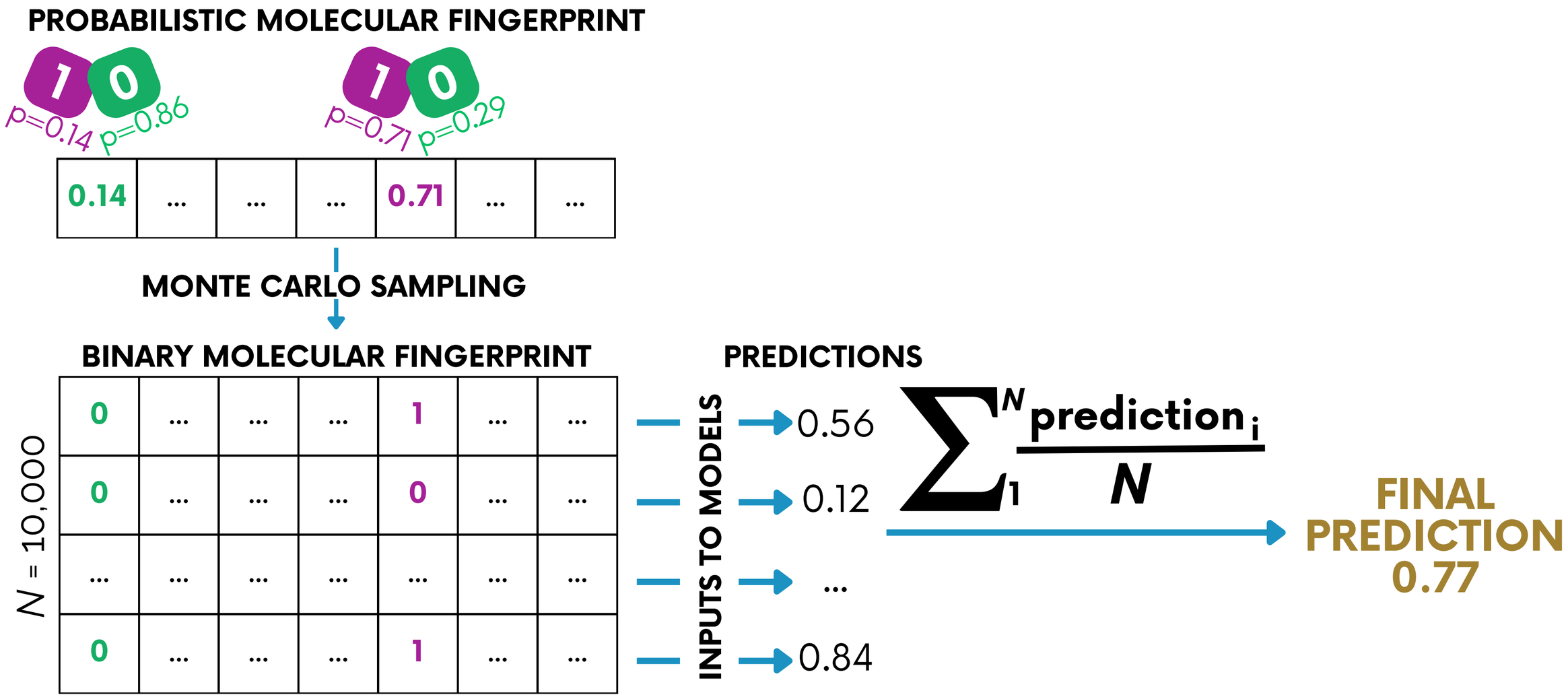
I. Rahu et al., *J. Chem. Inf. Model.* (**2024**).

MS2Tox: WORKFLOW



I. Rahu et al., *J. Chem. Inf. Model.* (**2024**).

MS2Tox: WORKFLOW



I. Rahu et al., *J. Chem. Inf. Model.* (**2024**).

MS2Tox: WORKFLOW

FPR at 90% recall = 0.25...0.85
AHR ER

1. Data cleaning
2. HRMS data matching with cleaned dataset
3. Splitting the dataset based on proportions
4. Train/intermediate test set data preprocessing
5. HRMS data preprocessing

CHEMICAL ENDPOINT FINGERPRINT FEATURES

TRAINING → MODELS TRAINING WITH CROSS-VALIDATION

INTERMEDIATE → SELECTING THE MODELS FOR FINAL EVALUATION

CHEMICAL ENDPOINT HRMS DATA FINGERPRINT FEATURES

REAL-LIFE → FINAL EVALUATION OF MODELS

MS² SPECTRA → SIRIUS+ CSI:FingerID → PROBABILISTIC MOLECULAR FINGERPRINT

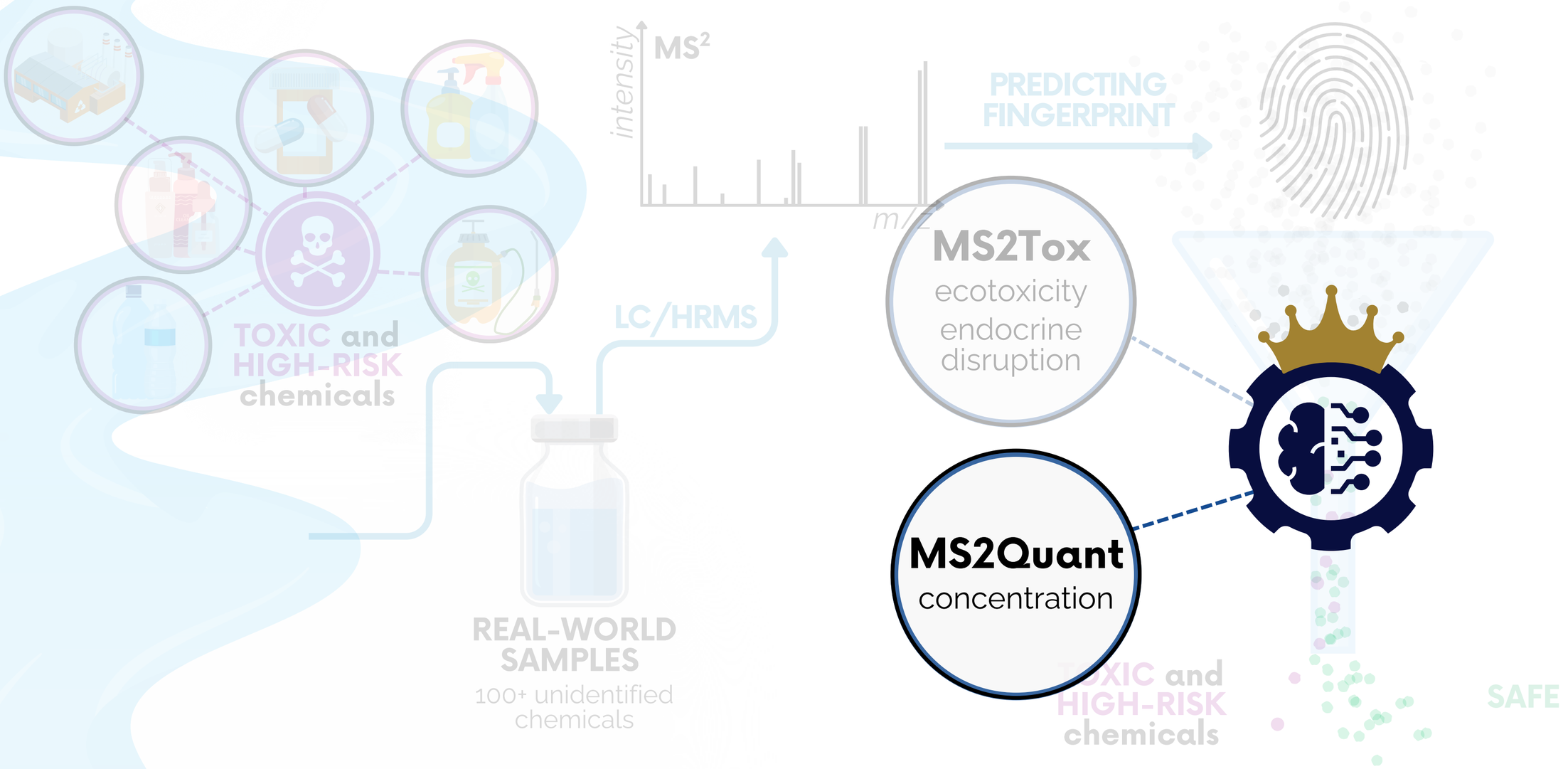
0.14	0.45	0.99	...	0.71	0.27	0.08

MONTE CARLO SAMPLING

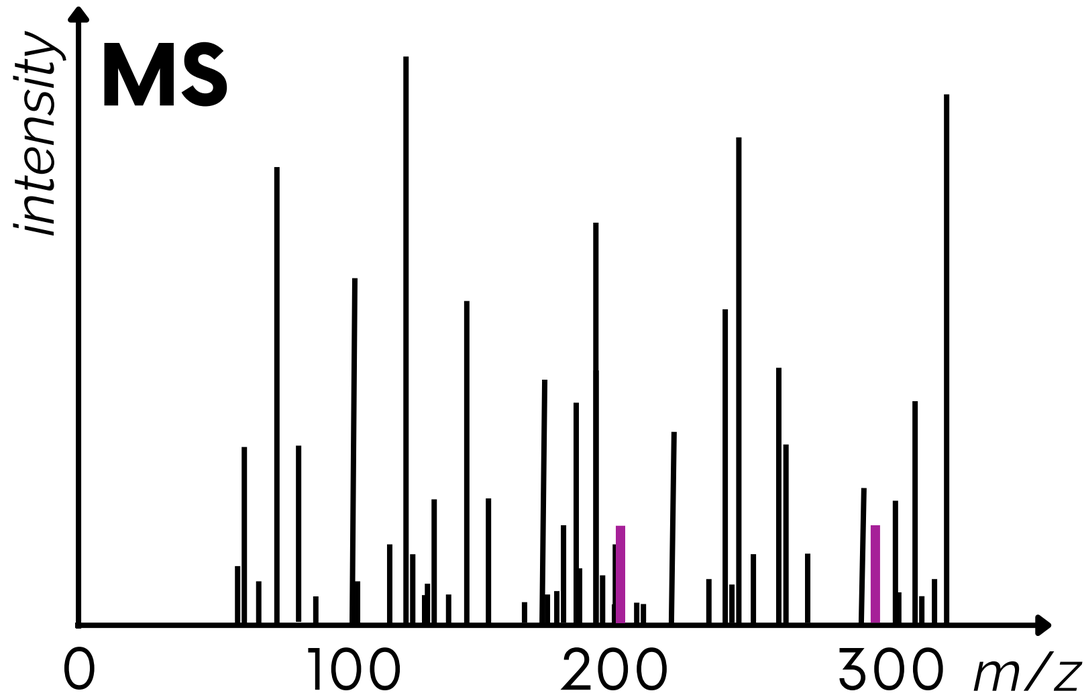
I. Rahu et al., *J. Chem. Inf. Model.* (**2024**).

P. Peets et al., *Environ. Sci. Tech.* (**2022**).

FIELD OF APPLICATION

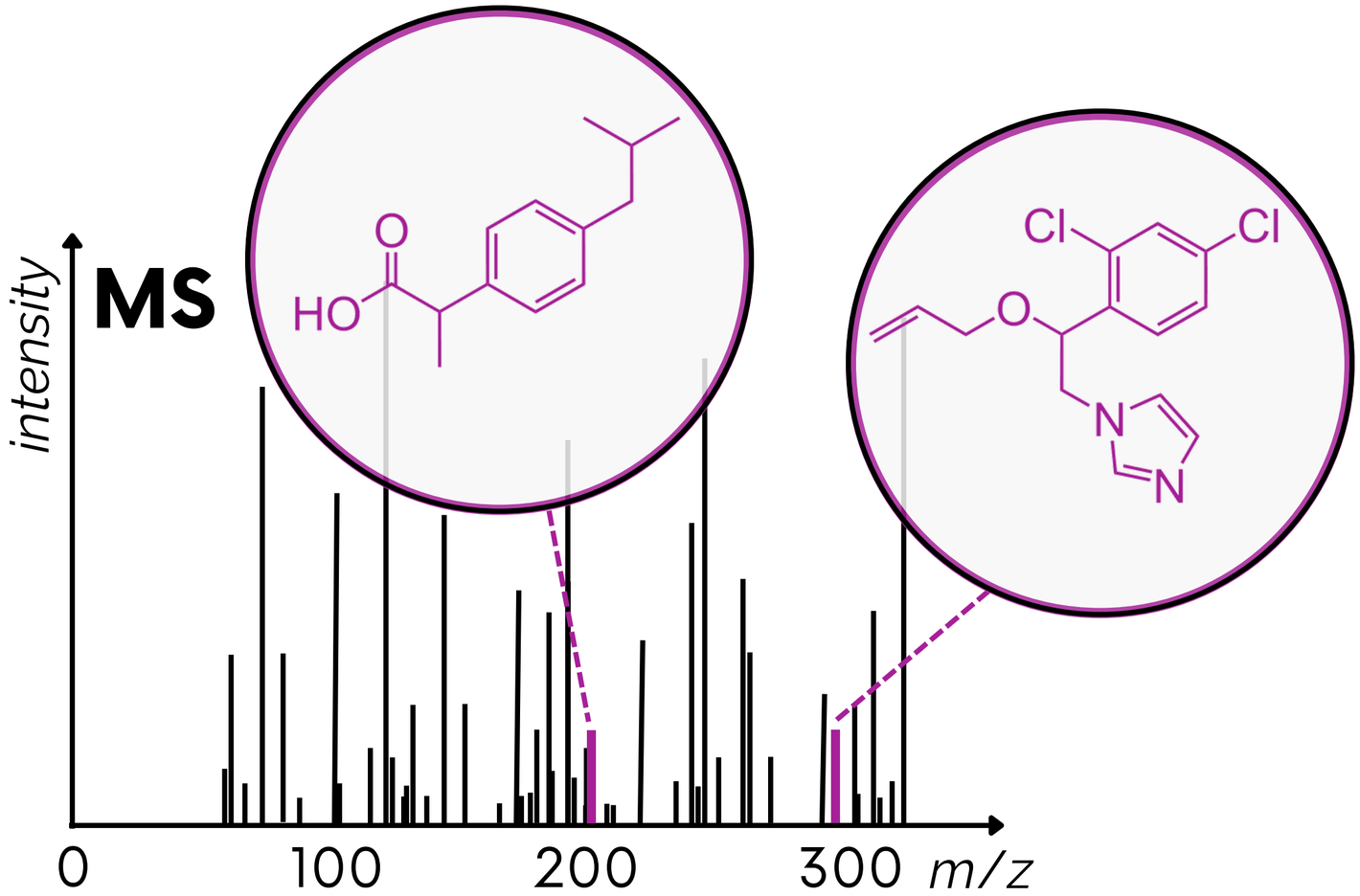


MS2Quant: ESI



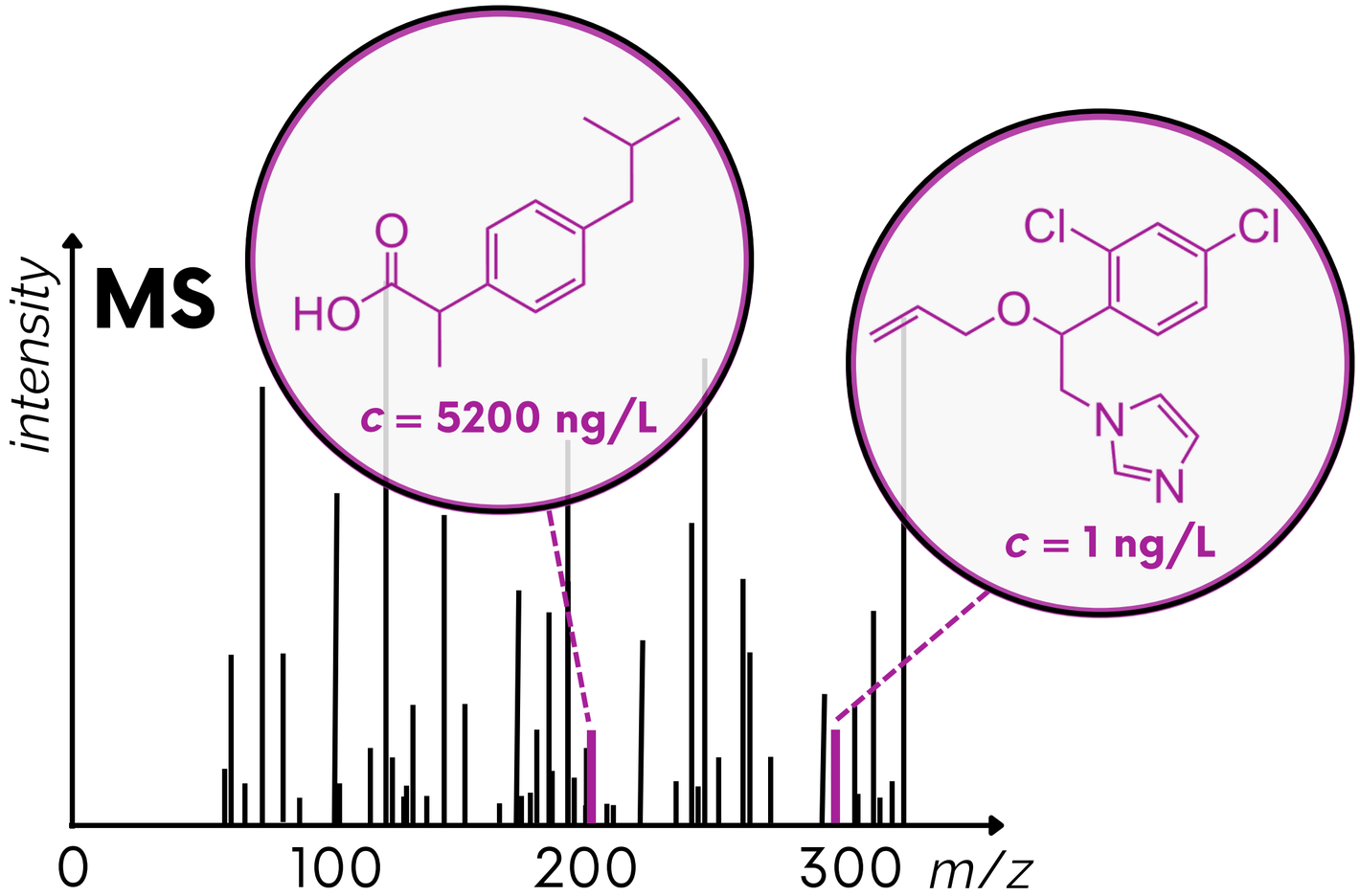
J. Liigand et al., *Sci. Rep.* (**2020**).
L. Malm et al., *Molecules*. (**2021**).

MS2Quant: ESI



J. Liigand et al., *Sci. Rep.* (**2020**).
L. Malm et al., *Molecules*. (**2021**).

MS2Quant: ESI

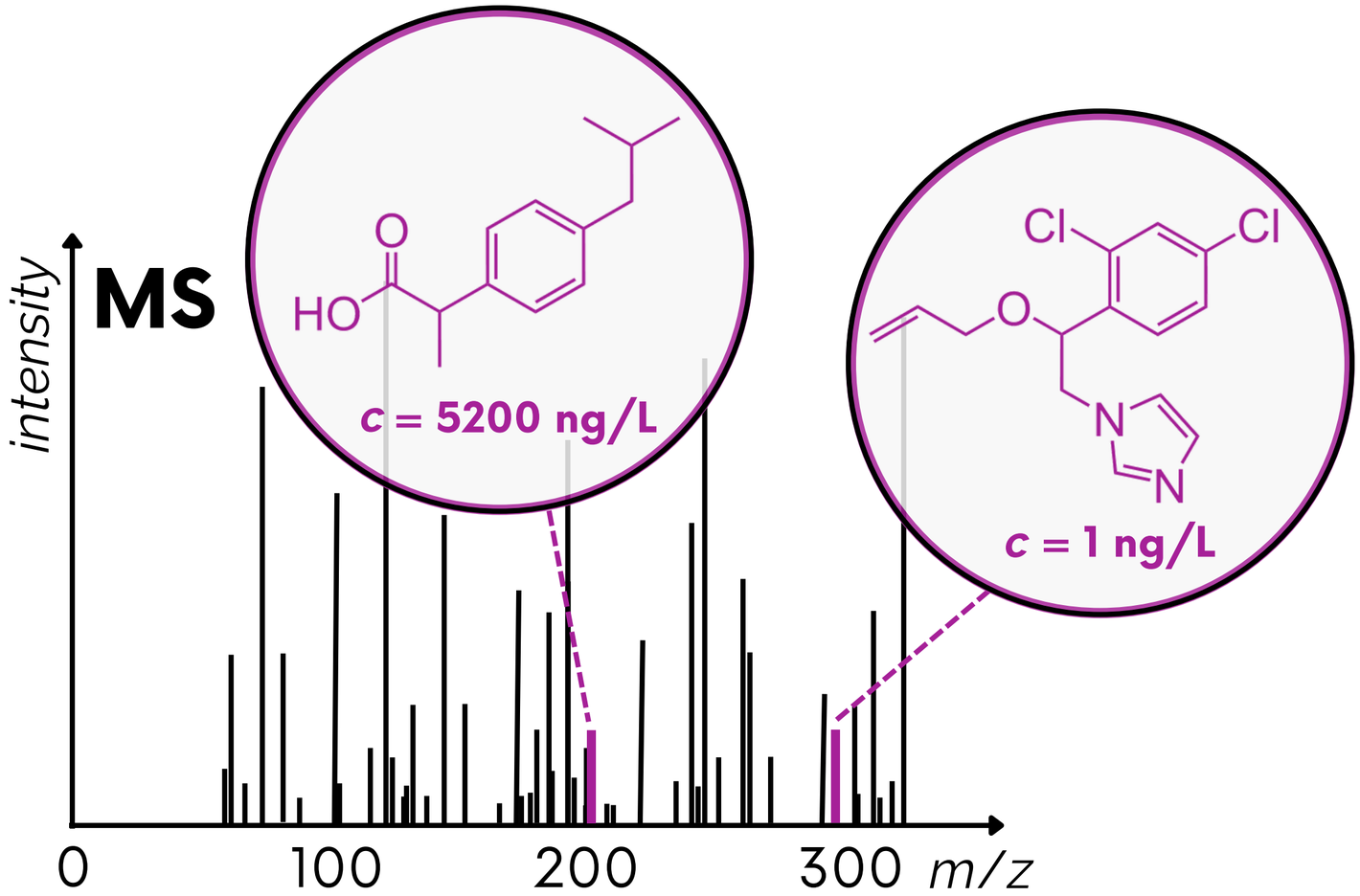


$$\text{RF} = \frac{\text{peak area}}{c}$$

response factor

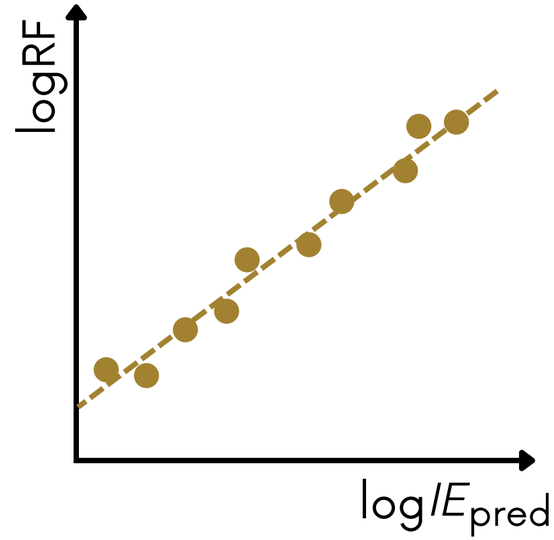
J. Liigand et al., *Sci. Rep.* (**2020**).
L. Malm et al., *Molecules*. (**2021**).

MS2Quant: ESI



$$\text{RF} = \frac{\text{peak area}}{c}$$

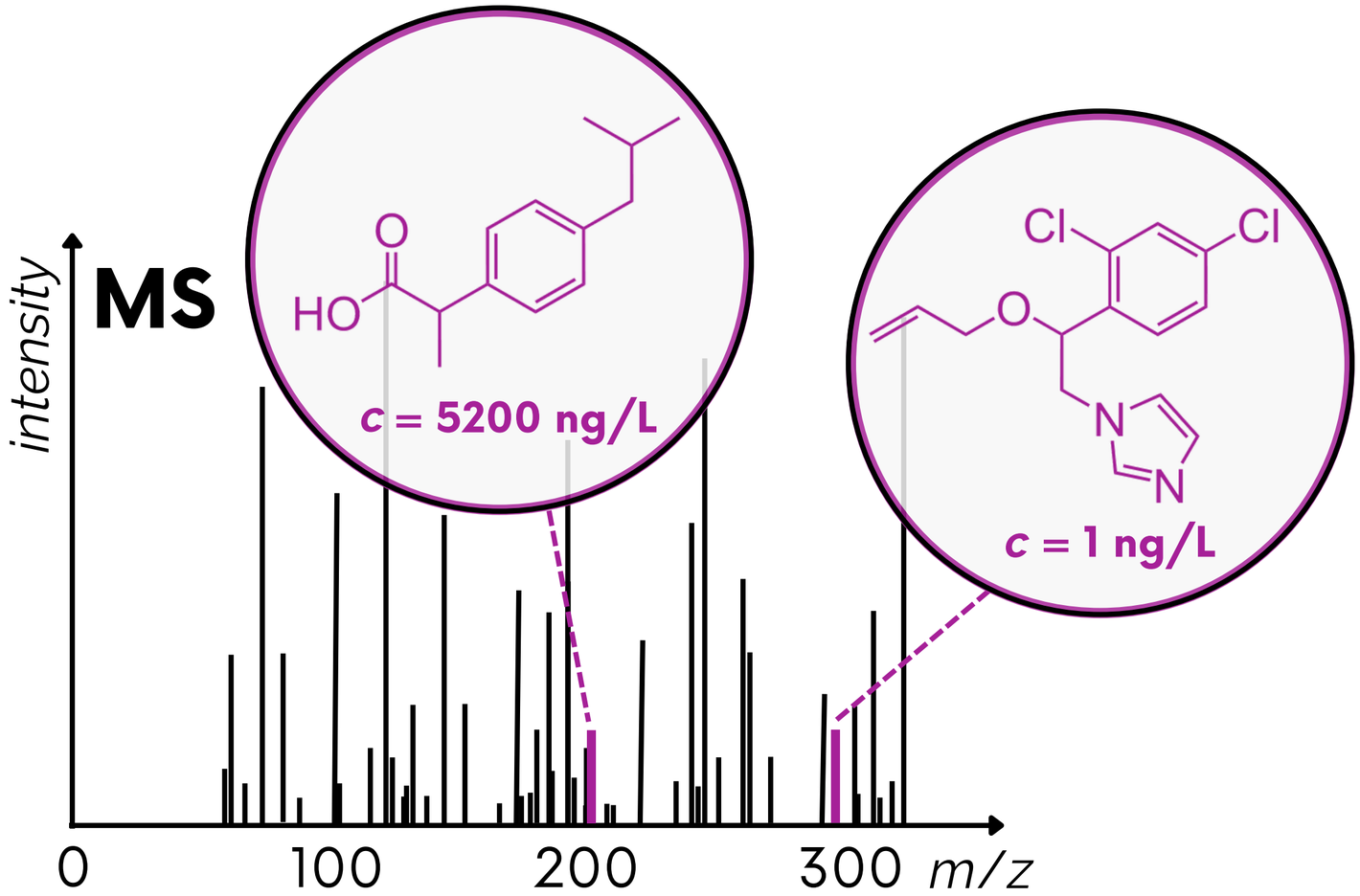
response factor



$$\textbf{logRF}_{\textbf{pred}} = \text{slope} \cdot \textbf{log}\textit{IE}_{\textbf{pred}} + \text{intercept}$$

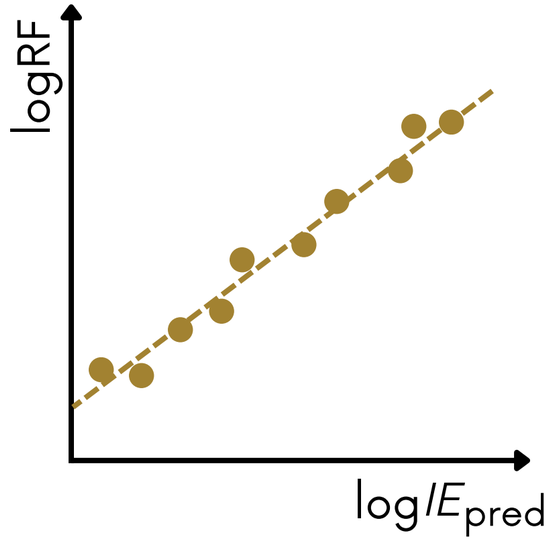
J. Liigand et al., *Sci. Rep.* (**2020**).
L. Malm et al., *Molecules*. (**2021**).

MS2Quant: ESI



$$\text{RF} = \frac{\text{peak area}}{c}$$

response factor

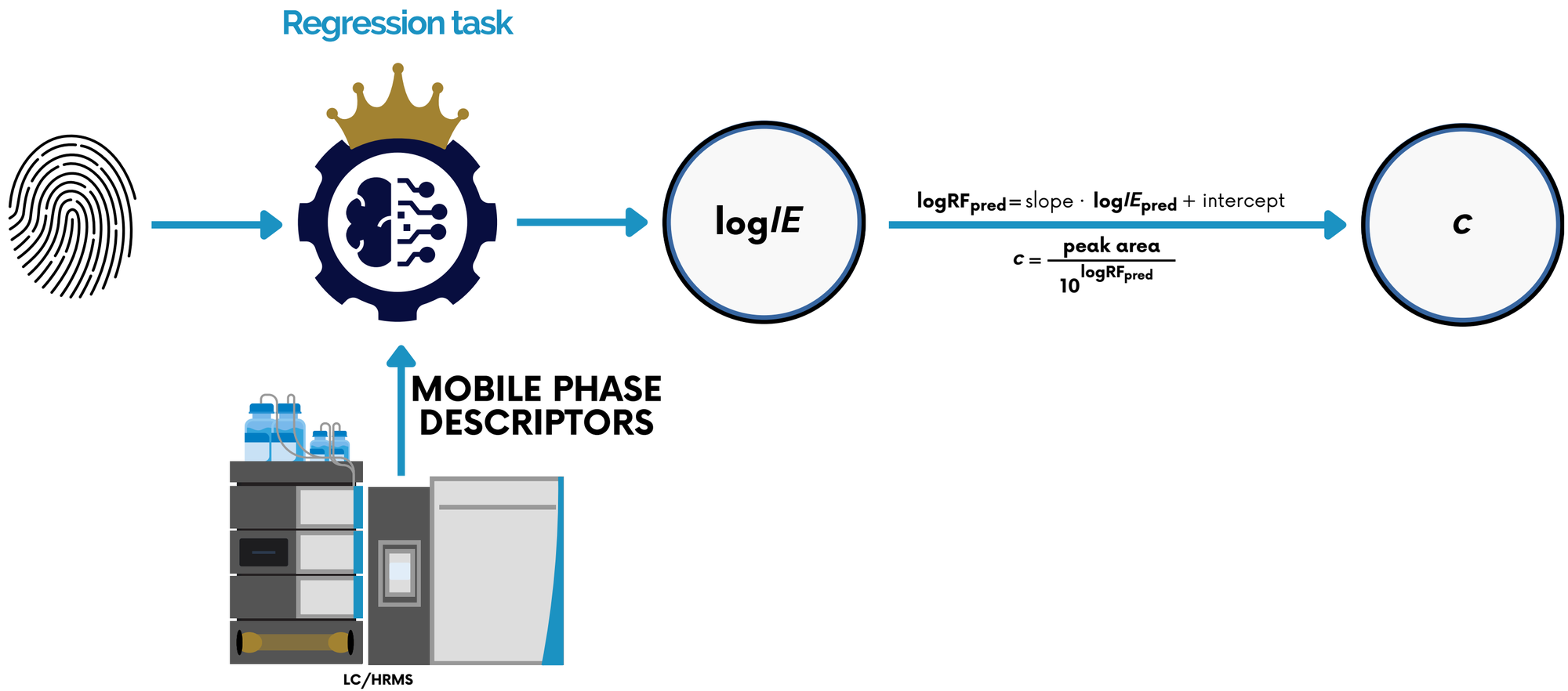


$$\mathbf{logRF_{pred}} = \text{slope} \cdot \mathbf{log}\mathit{IE}_{\mathbf{pred}} + \text{intercept}$$

$$c = \frac{\text{peak area}}{10^{\mathbf{logRF_{pred}}}}$$

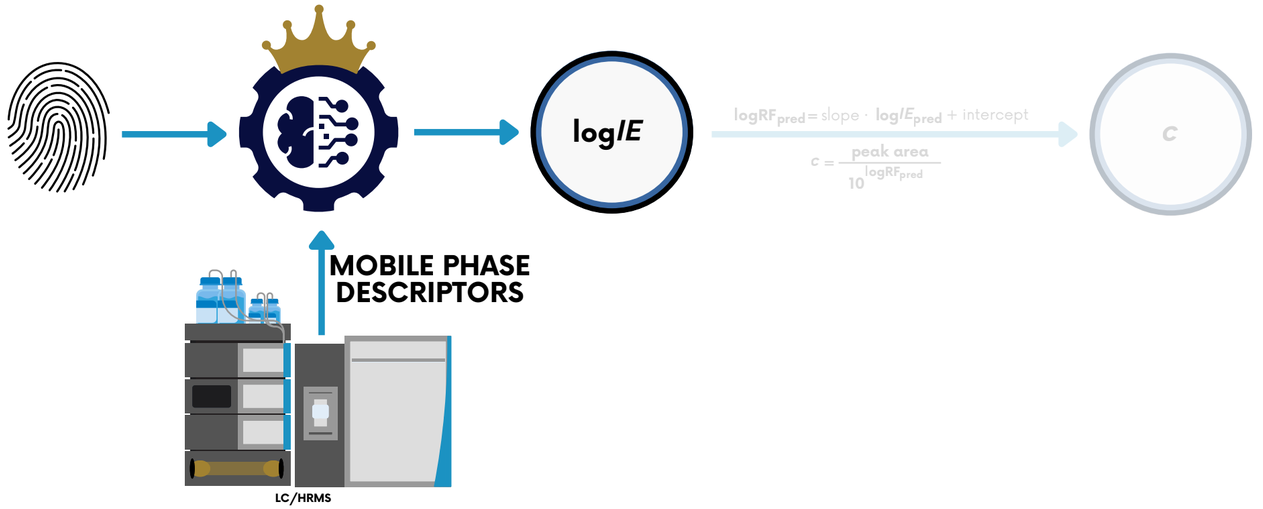
J. Liigand et al., *Sci. Rep.* (**2020**).
L. Malm et al., *Molecules*. (**2021**).

MS2Quant



H. Sepman et al., *Anal. Chem.* (**2023**).

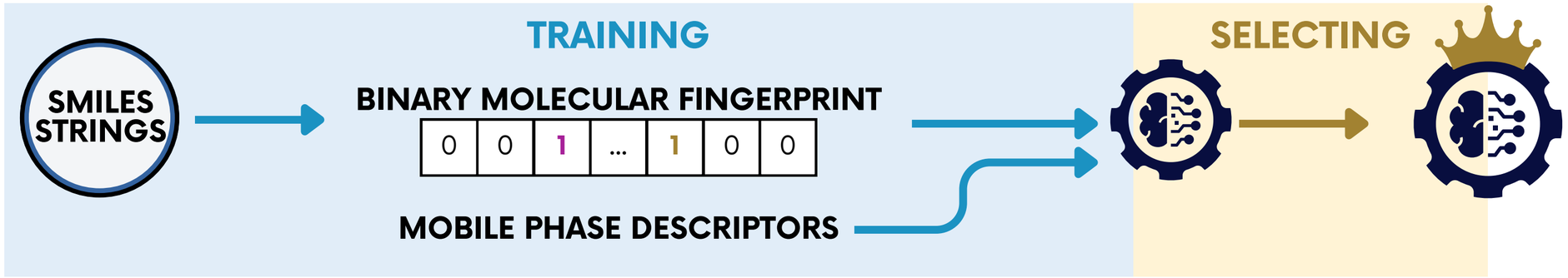
MS2Quant: WORKFLOW



CHEMICAL	log*IE*

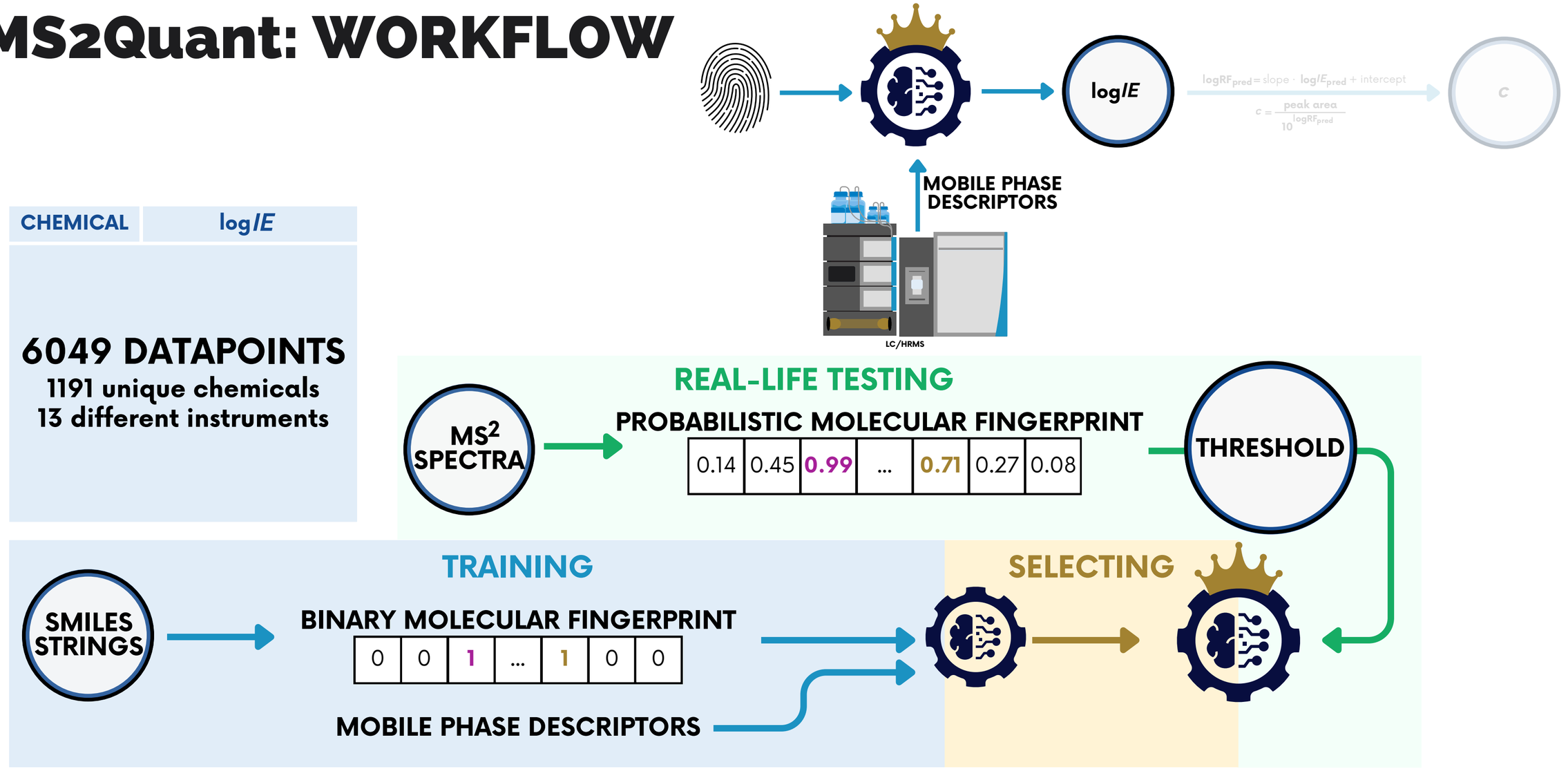
6049 DATAPOINTS
1191 unique chemicals
13 different instruments

RMSE = 0.80 log-units



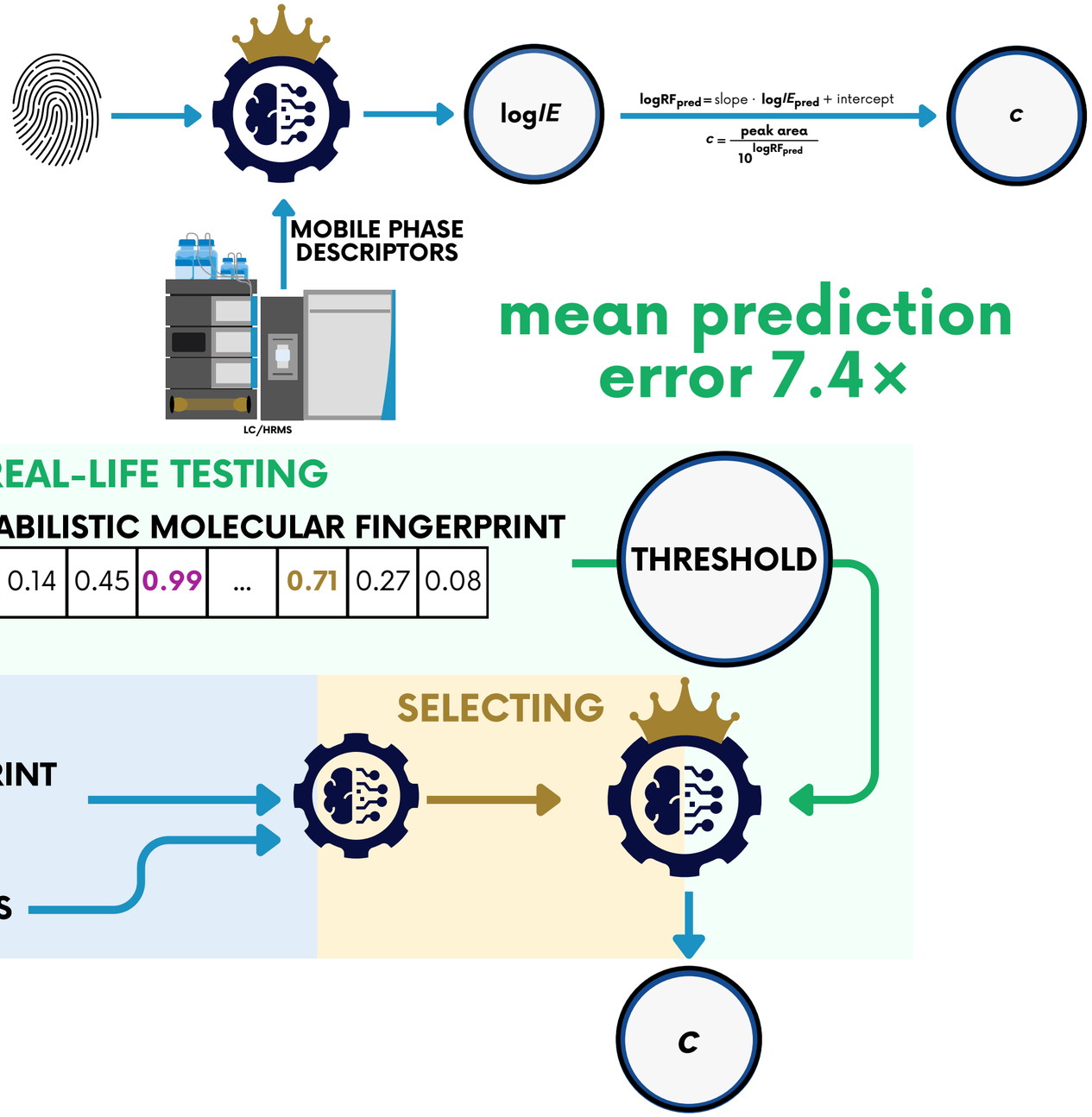
H. Sepman et al., *Anal. Chem.* (**2023**).

MS2Quant: WORKFLOW



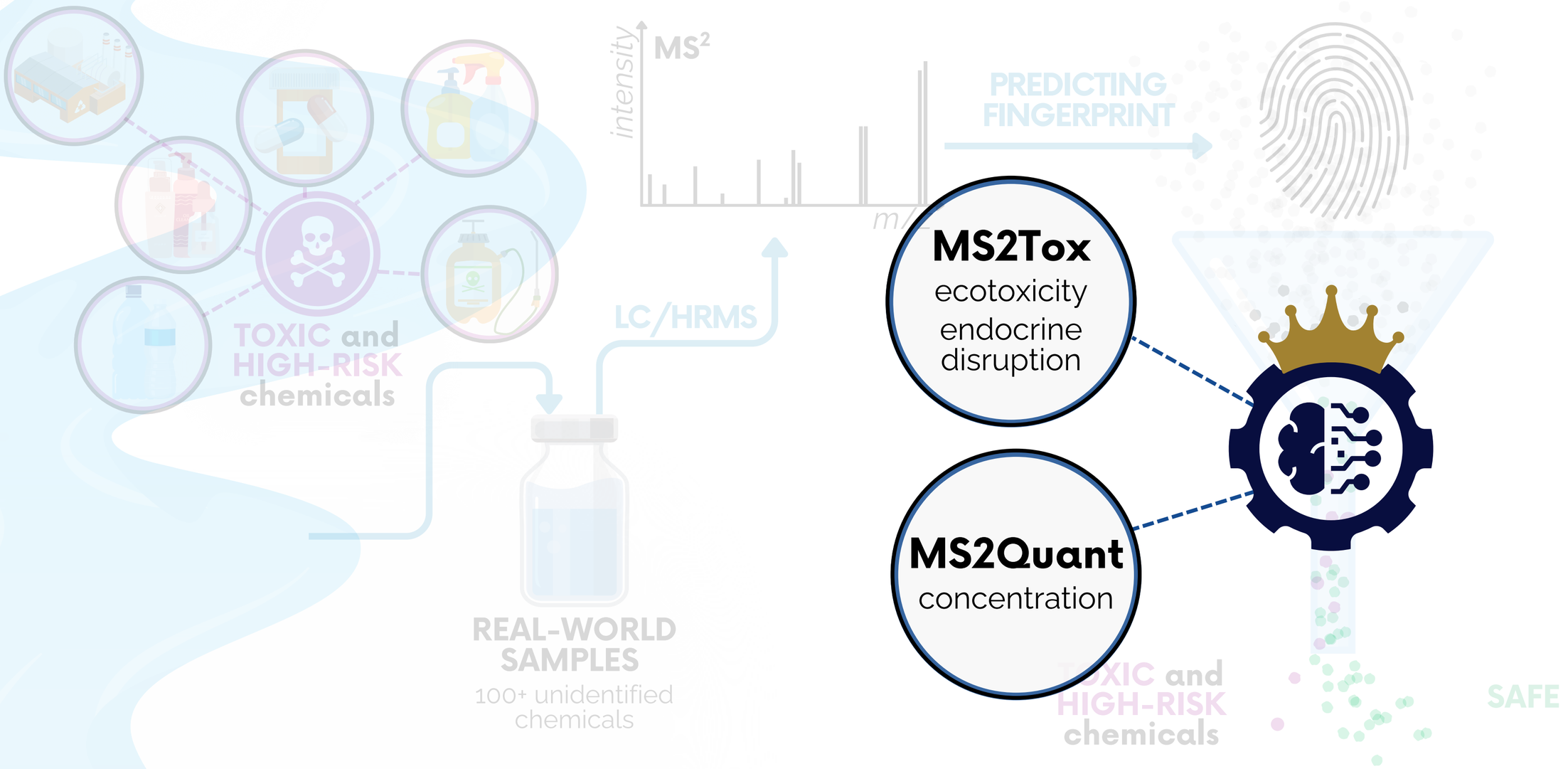
H. Sepman et al., *Anal. Chem.* (**2023**).

MS2Quant: WORKFLOW

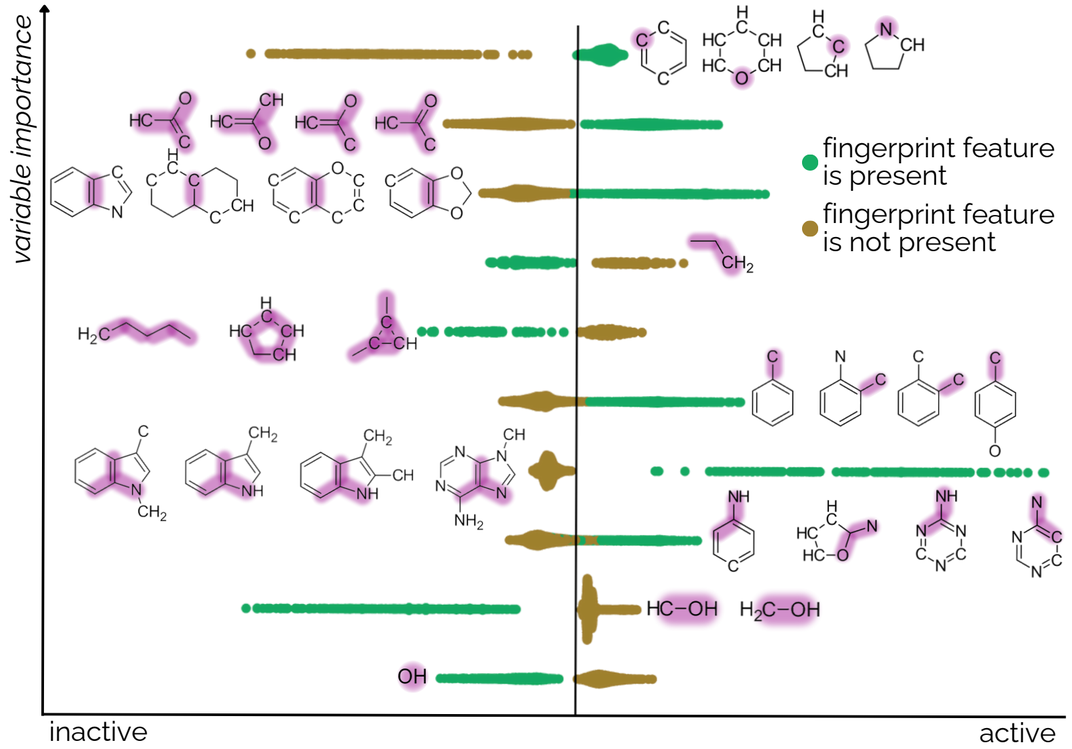


H. Sepman et al., *Anal. Chem.* (**2023**).

FIELD OF APPLICATION



INTERPRETABILITY



AHR

LC_{50}

MOLECULAR MASS

IE

FINGERPRINT FEATURES CONTAINING N

FIELD OF APPLICATION

REAL-WORLD SAMPLES
100+ unidentified chemicals

intensity
MS²
m/z

LC/HRMS

PREDICTING FINGERPRINT

MS2Tox
ecotoxicity
endocrine disruption

MS2Quant
concentration

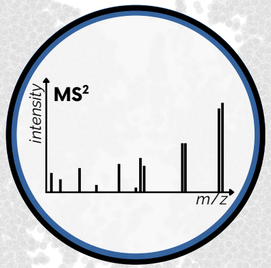
TOXIC and HIGH-RISK chemicals

SAFE

CASE STUDY: RECYCLED TEXTILES

$$\text{priority score} = \frac{\text{predicted concentration (mM)}}{\text{predicted aquatic } LC_{50} \text{ (mM)}}$$

13 RECYCLED PRODUCTS



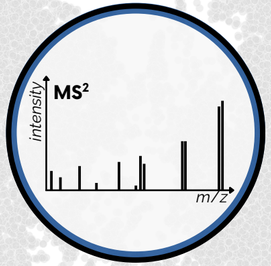
20119
LC/HRMS
FEATURES

D. Szabo et al., *Anal. Chem.* (**2024**).

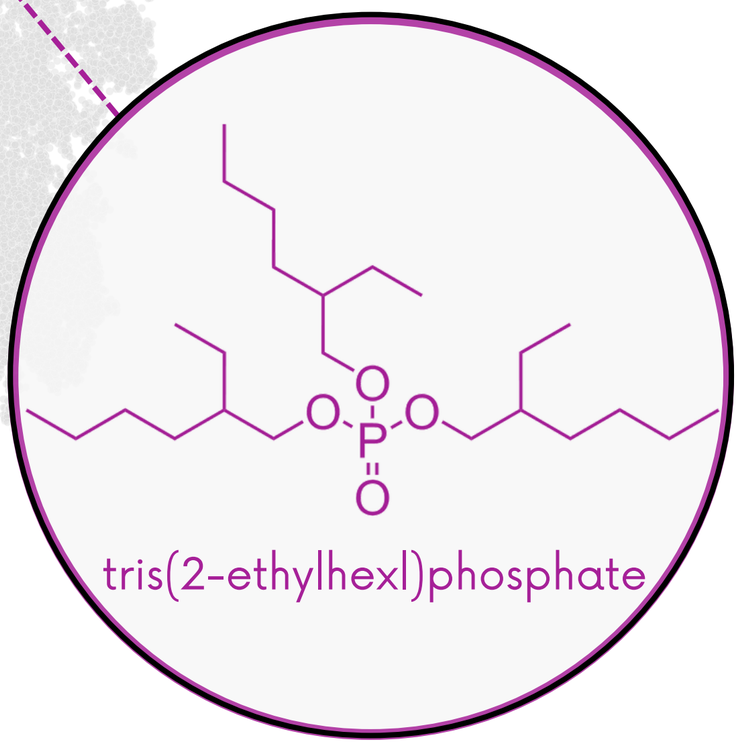
CASE STUDY: RECYCLED TEXTILES

$$\text{priority score} = \frac{\text{predicted concentration (mM)}}{\text{predicted aquatic } LC_{50} \text{ (mM)}}$$

13 RECYCLED PRODUCTS



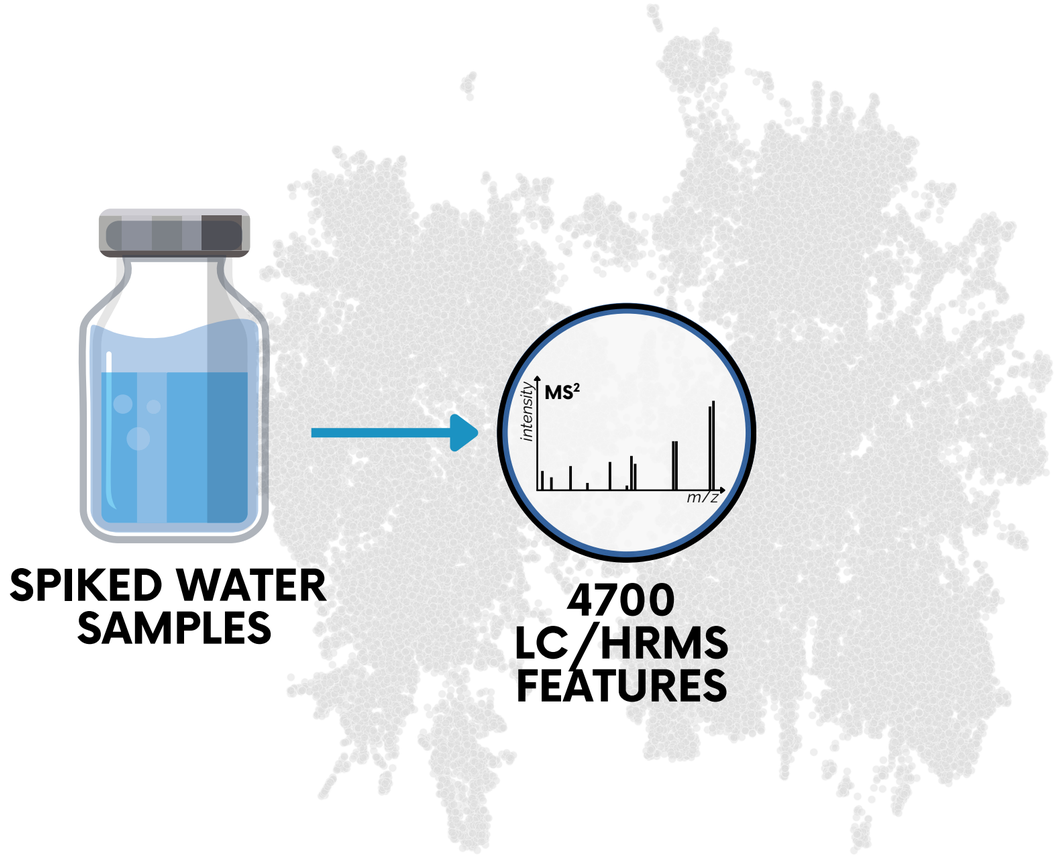
20119 LC/HRMS FEATURES



in TOP 10 by priority score

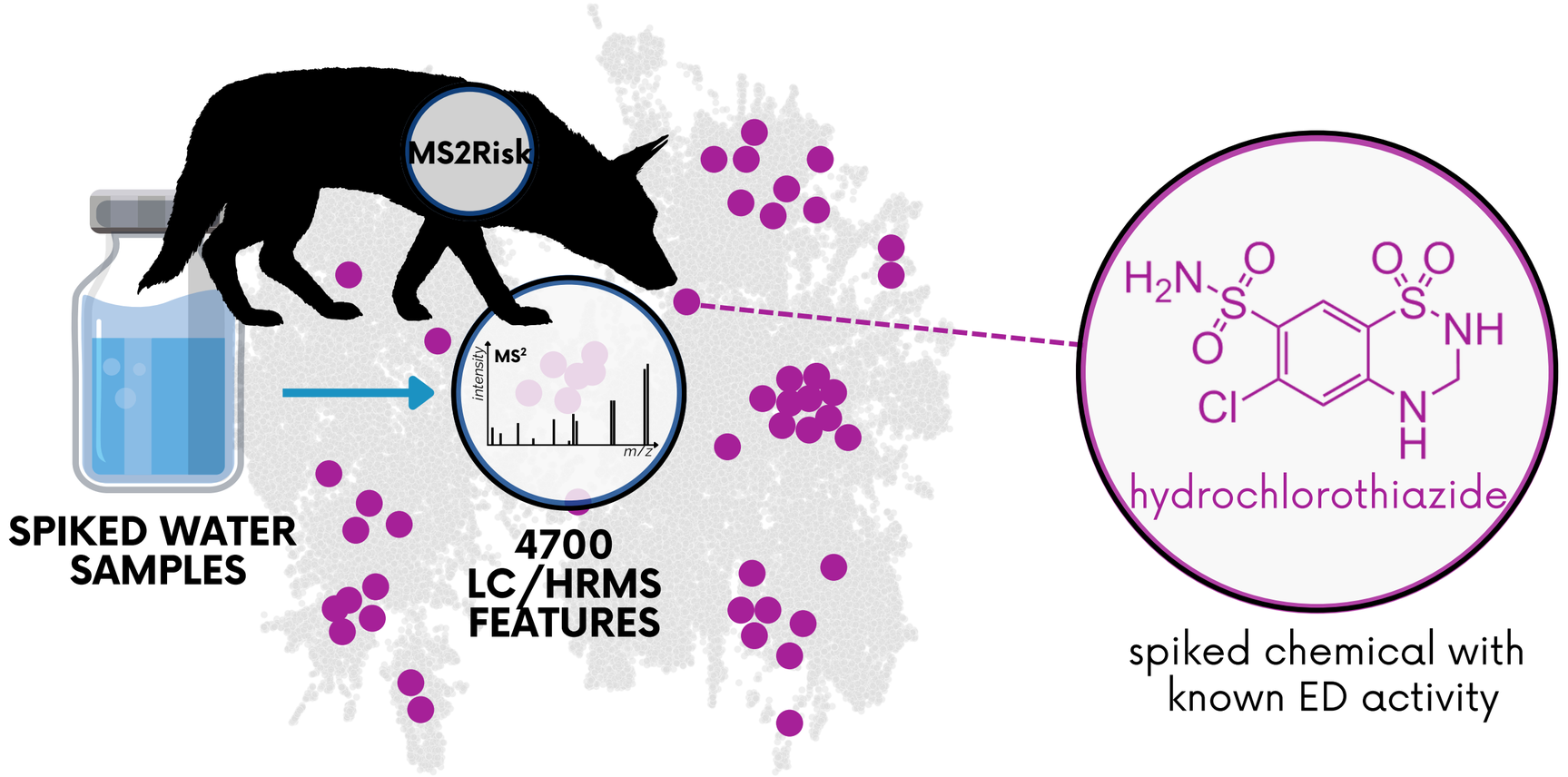
D. Szabo et al., *Anal. Chem.* (**2024**).

CASE STUDY: INTERLABORATORY COMPARISON



I. Rahu, G. Sandberg et al., *in preparation*

CASE STUDY: INTERLABORATORY COMPARISON

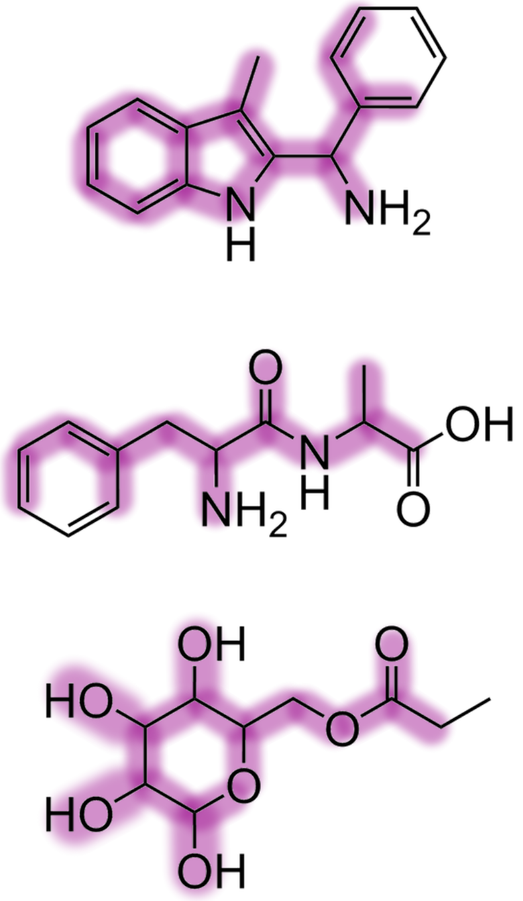


I. Rahu, G. Sandberg et al., *in preparation*

FUTURE PERSPECTIVE: UPDATING MODELS

	SIRIUS5	SIRIUS6
Open Babel FP4	33	8
CDK Substructure	106	77
MACCS	131	68
PubChem	460	161
Klekota Roth	923	898
ECFP	1339	55
custom made SMARTS	266	135
ring systems	236	132
combinatorial fragmenter		3466
NUMBER OF FINGERPRINT FEATURES	**3494**	**5000**

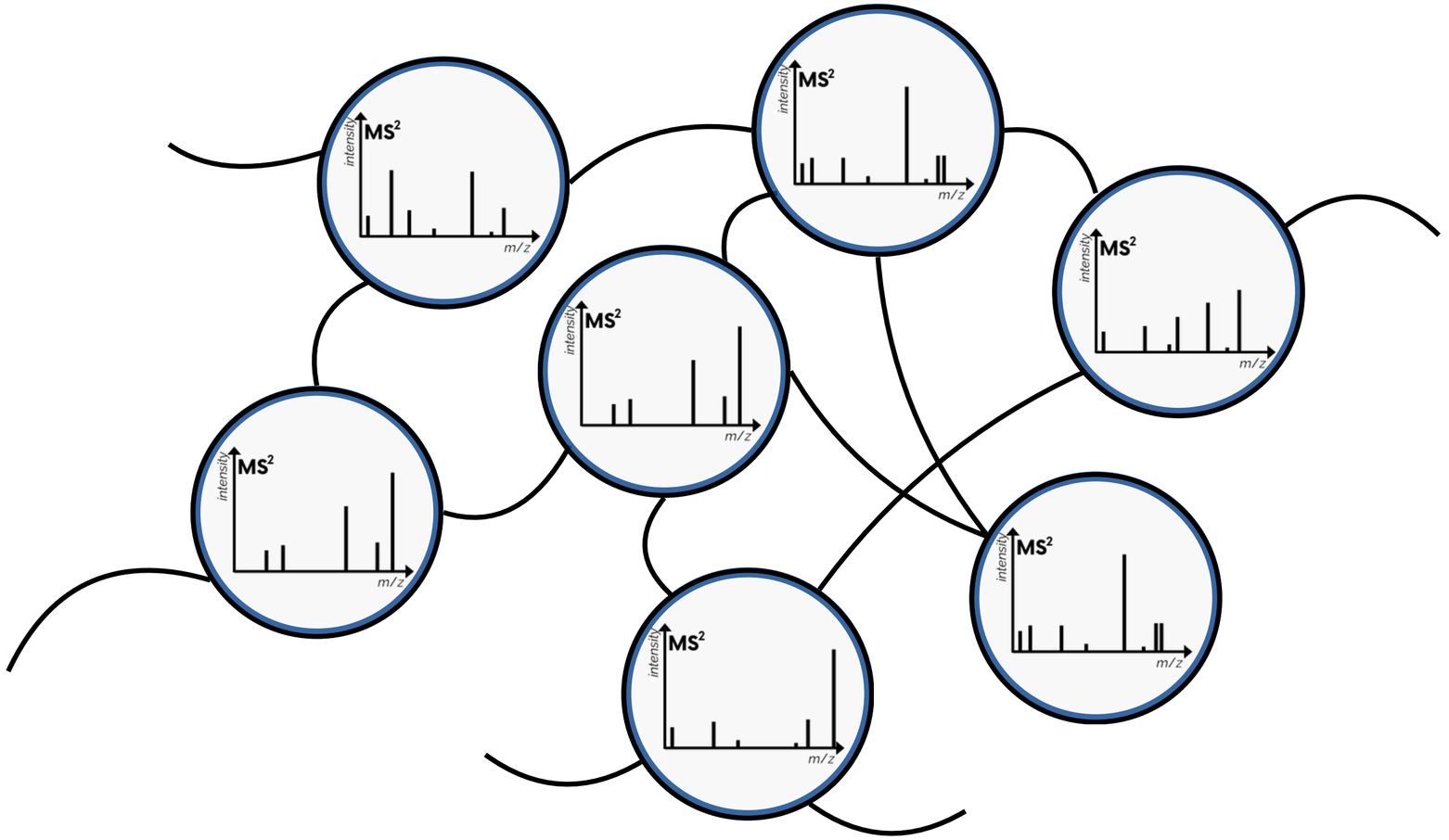
I. Rahu et al., *in preparation*



FUTURE PERSPECTIVE: MS2Quant ESI-

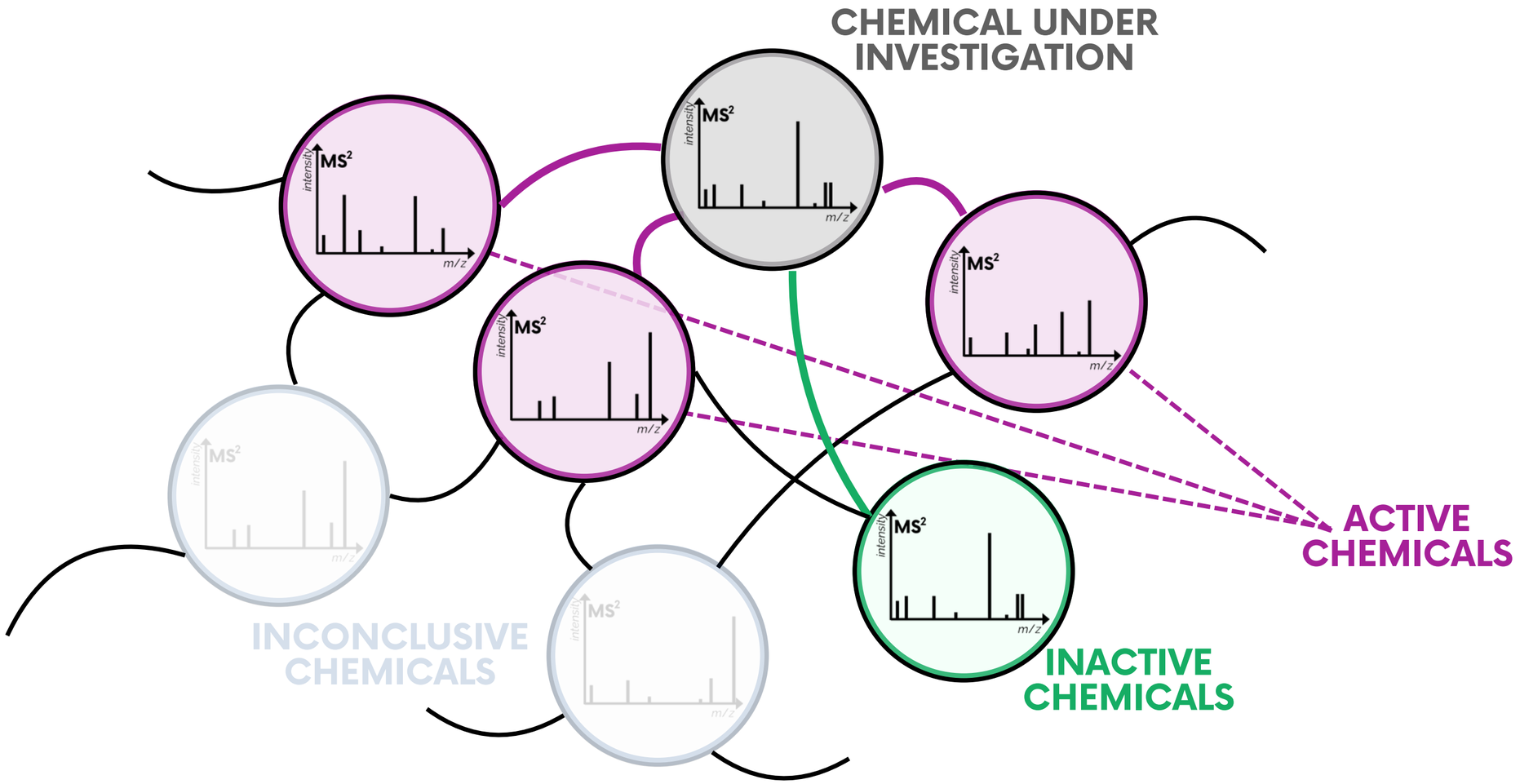
H. Sepman et al., *in preparation*

FUTURE PERSPECTIVE: MOLECULAR NETWORKS



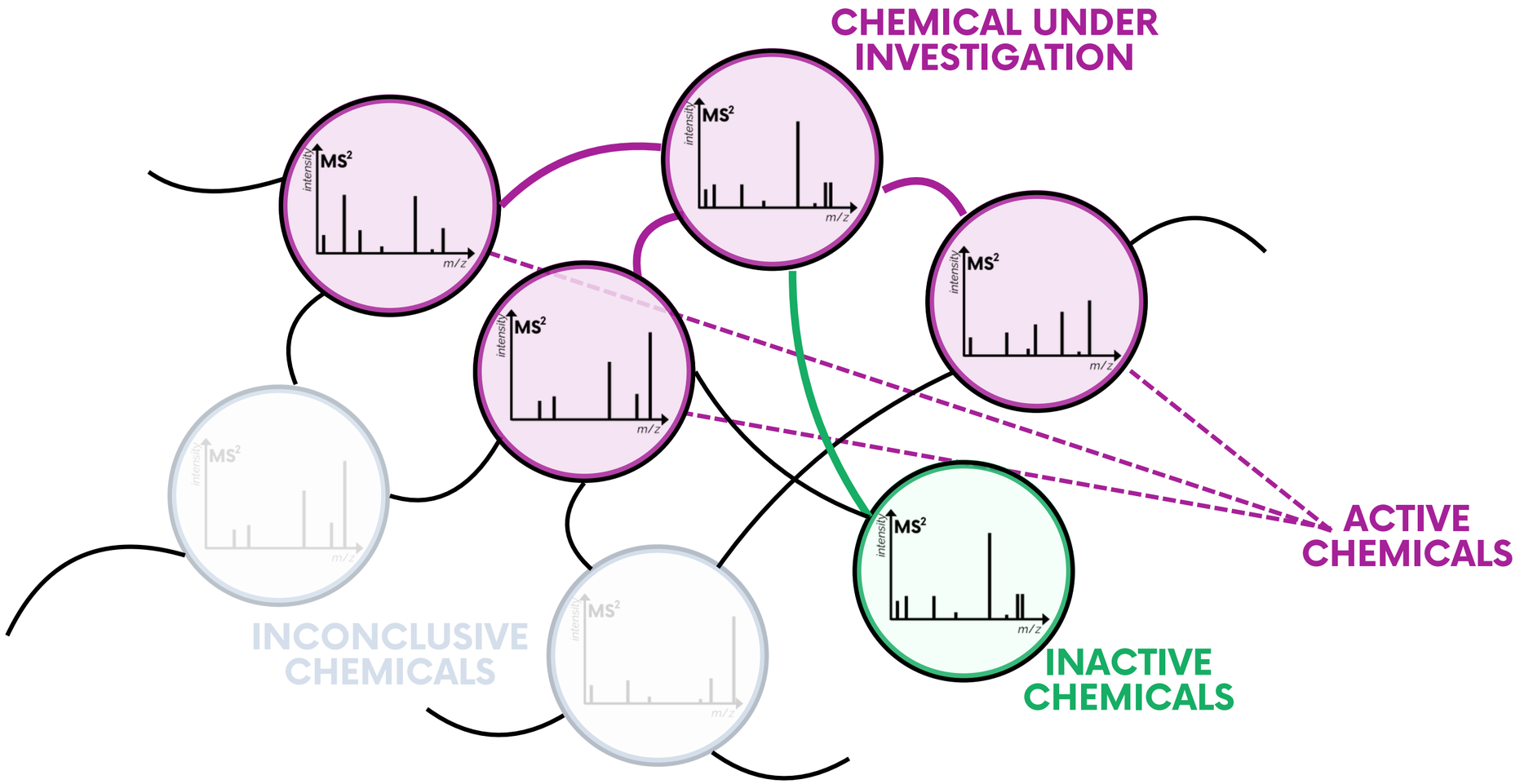
Y. Kreutzer et al., *in preparation*

FUTURE PERSPECTIVE: MOLECULAR NETWORKS



Y. Kreutzer et al., *in preparation*

FUTURE PERSPECTIVE: MOLECULAR NETWORKS



Y. Kreutzer et al., *in preparation*

FORMAS

Wenner-Gren Foundations
Wenner-Gren Stiftelserna

Swedish
Research
Council

Wallenberg Initiative
Materials Science
for Sustainability

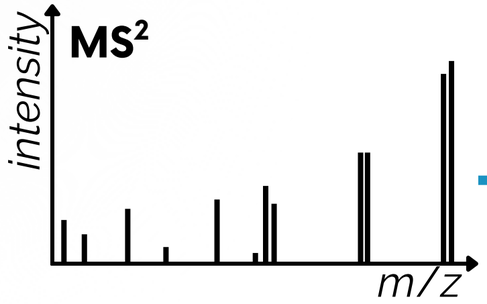
CARL TRYGGERS
STIFTELSE
FÖR VETENSKAPLIG FORSKNING


Kruvelab
Exploring the
research space...

MS2Tox & MS2Quant

Automated detection and identification of TOXIC and HIGH-RISK chemicals

TOXIC and HIGH-RISK chemicals



LC/HRMS

PREDICTING FINGERPRINT

REAL-WORLD SAMPLES

100+ unidentified chemicals

TOXIC and HIGH-RISK chemicals

SAFE