

NTSuisse: Re-imagining LC-HRMS Data Sharing



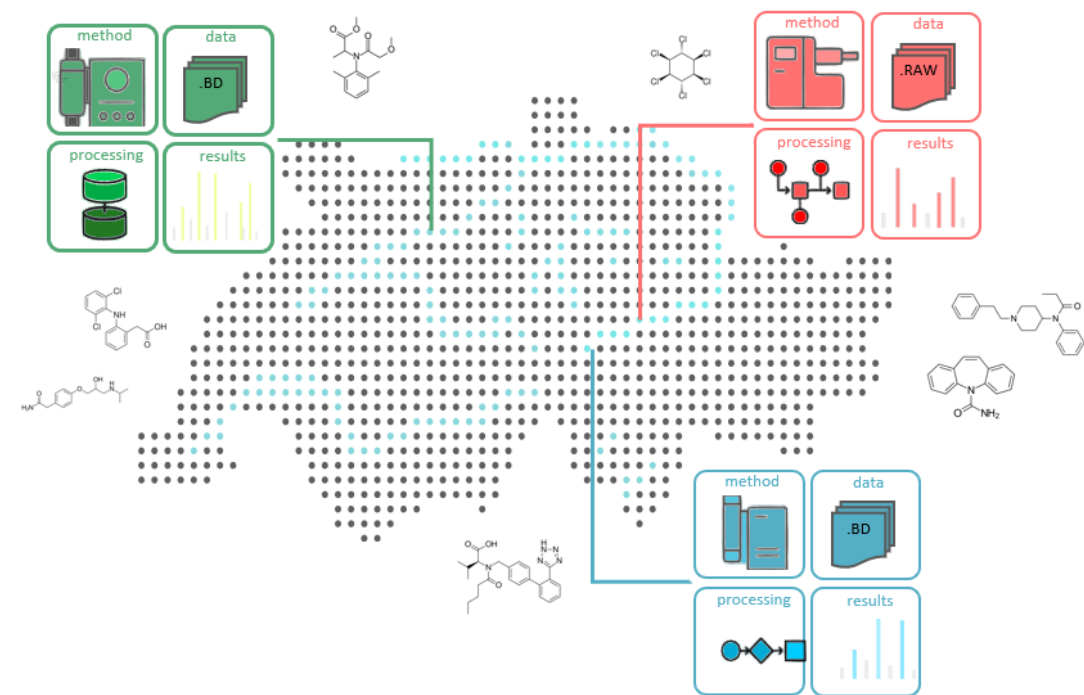
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ccCTA Scientific Days, 3.10.2025

Background

- Problematic micropollutants: pesticides, pharmaceuticals, industrial chemicals
- National monitoring plans by FOEN
- (Non) target analysis of Swiss water bodies by cantonal labs and water suppliers
- Contamination hotspots & trends?
- Need: advance data analysis & sharing



Loger et al, 2014

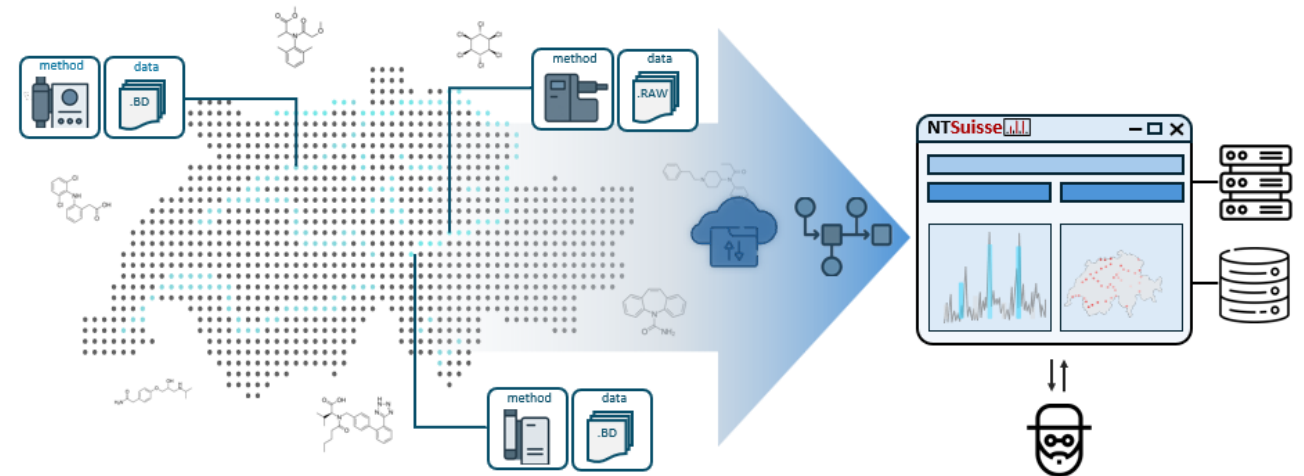
Problem

- **FAIR** data
- Lab-specific analytical measurement & data processing
- Data interoperability and interchangeability difficult
- **No infrastructure** for data processing & sharing **available**



Solution

- Harmonization of measurement method
- Building a web platform
 - Automated data processing
 - Target & non-target analysis
 - Spatial data visualization
 - Sharing across labs



Measurement Harmonization

- LC-HRMS
- Global internal standard and target list

6. Liquid Chromatography

Analytical column:	Agilent Zorbax Eclipse Plus C18, 95 Å, 2.1 mm x 150 mm, 3.5 µm	
Pre-column:	Agilent HPLC Guard Cartridge Zorbax Eclipse Plus C18, 95 Å, 2.1 x 12.5 mm	
Pre-column holder:	High performance Zorbax guard fittings kit (ZGC), Part # 820999-901	
Eluent A:	Ultrapure water + 0.1 % (v/v) formic acid	
Eluent B:	Methanol LC-MS + 0.1 % (v/v) formic acid	
Flow:	300 µL/min	
Gradient:	<i>Time</i>	<i>Eluent B</i>
	0 min	2 %
	1 min	2 %
	20 min	98 %
	25 min	98 %
	25.5 min	2 %
	30 min	2 %
Column temperature:	40 °C	
Injection volume:	50 - 250 µL	

7. High-resolution Mass Spectrometry (Orbitrap or Q-TOF)

The essential MS parameters for Orbitrap and Q-TOF instruments are summarized in the following, while the remaining parameters are more device-specific and should be selected accordingly. As a reference, the complete settings for a representative instrument of each type are provided in Appendix B. Since samples measured in polarity switching mode cannot be processed on the platform, all samples must be measured separately in positive and negative polarity modes.

Mandatory MS Settings

Orbitrap

Source Settings

Source Type	ESI
Sheath Gas (psi)	40
Aux Gas (psi)	10
Spray Voltage (V)	Instrument-specific default values for multi-methods
Probe Heater Temp. (°C)	150
Capillary Temp. (°C)	320

Full Scan Settings

Resolution	≥ 120'000 at m/z 200
Scan Range (m/z)	100 - 1000
S-Lens RF Level (%)	Instrument-specific default value for multi-methods

AGC-Values	1E+06 (pos) 5E+05 (neg)
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Max. Injection time (ms)	50
Number of Microscans	1

MS2 Settings

Resolution	Lowest resolution
Acquisition Mode	DDA
AGC-Values	2E+05 (pos) 1E+05 (neg)
Dynamic Exclusion (s)	After 1 occurrence for 5 s
Max. Injection Time (ms)	60
Isolation window (m/z)	1
Max. Cycle Time (s)	~ 0.8
Collision Energy (NCE)	Stepped: 20, 40, 80

Q-TOF

Source Settings

Source Type	Turbo V with ESI twin
Gas 1 (psi)	60
Gas 2 (psi)	70
Curtain Gas (psi)	35
CAD Gas (psi)	7
Temperature (°C)	550
Spray Voltage (V)	5000 (pos) - 4500 (neg)

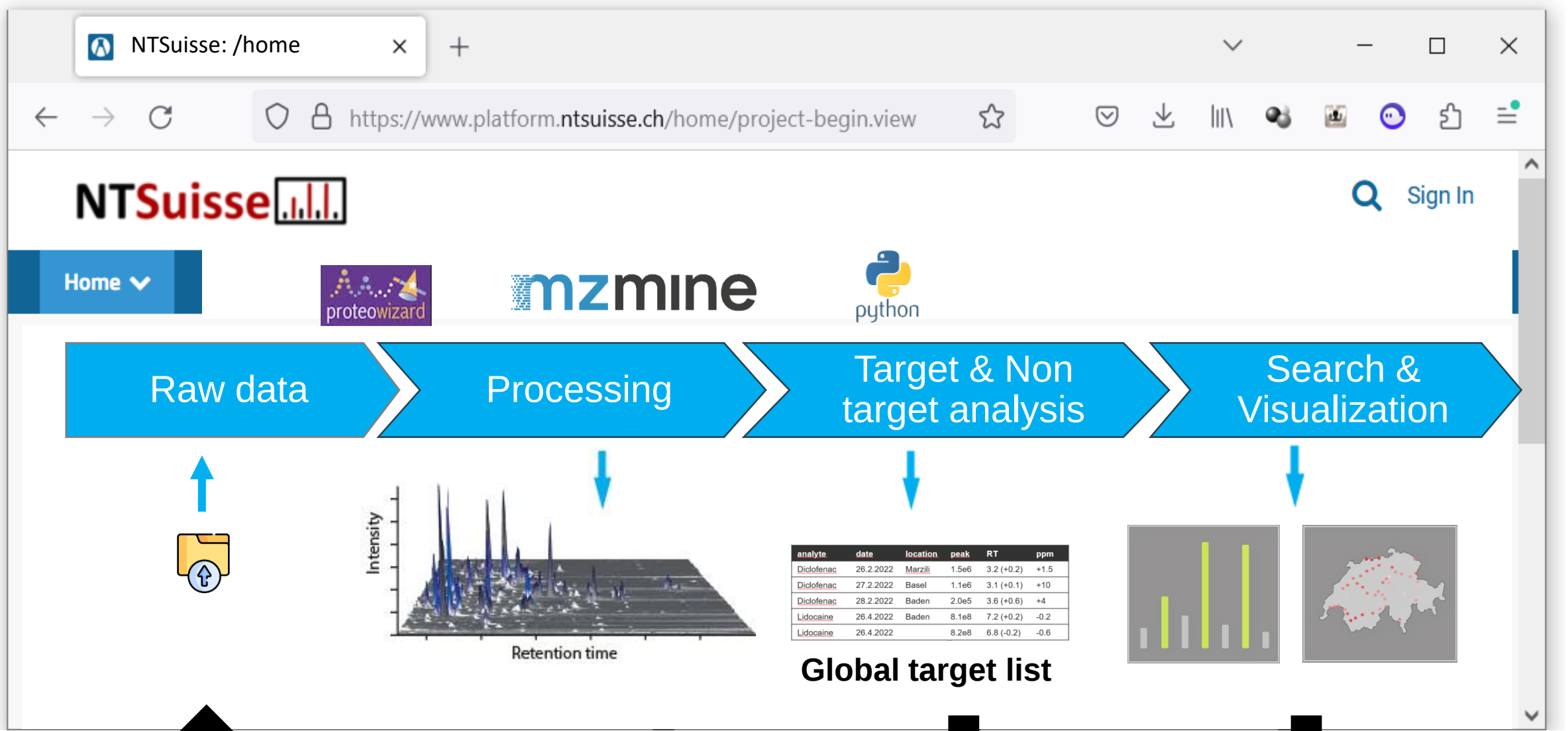
Full Scan Settings

Start – Stop Mass (Da)	100 - 1000
Accumulation Time (s)	0.08

MS2 Settings

Experiment	IDA (Small Molecule)
Max. Cycle Time (s)	~ 0.8
Dynamic Exclusion (s)	After two occurrences for 3 s
Start – Stop Mass (Da)	50 – 1000
Accumulation Time (s)	0.05
CE / CE spread (V)	35 / 15
Q1 Resolution	Unit

The Web platform: Workflow



Live Demo

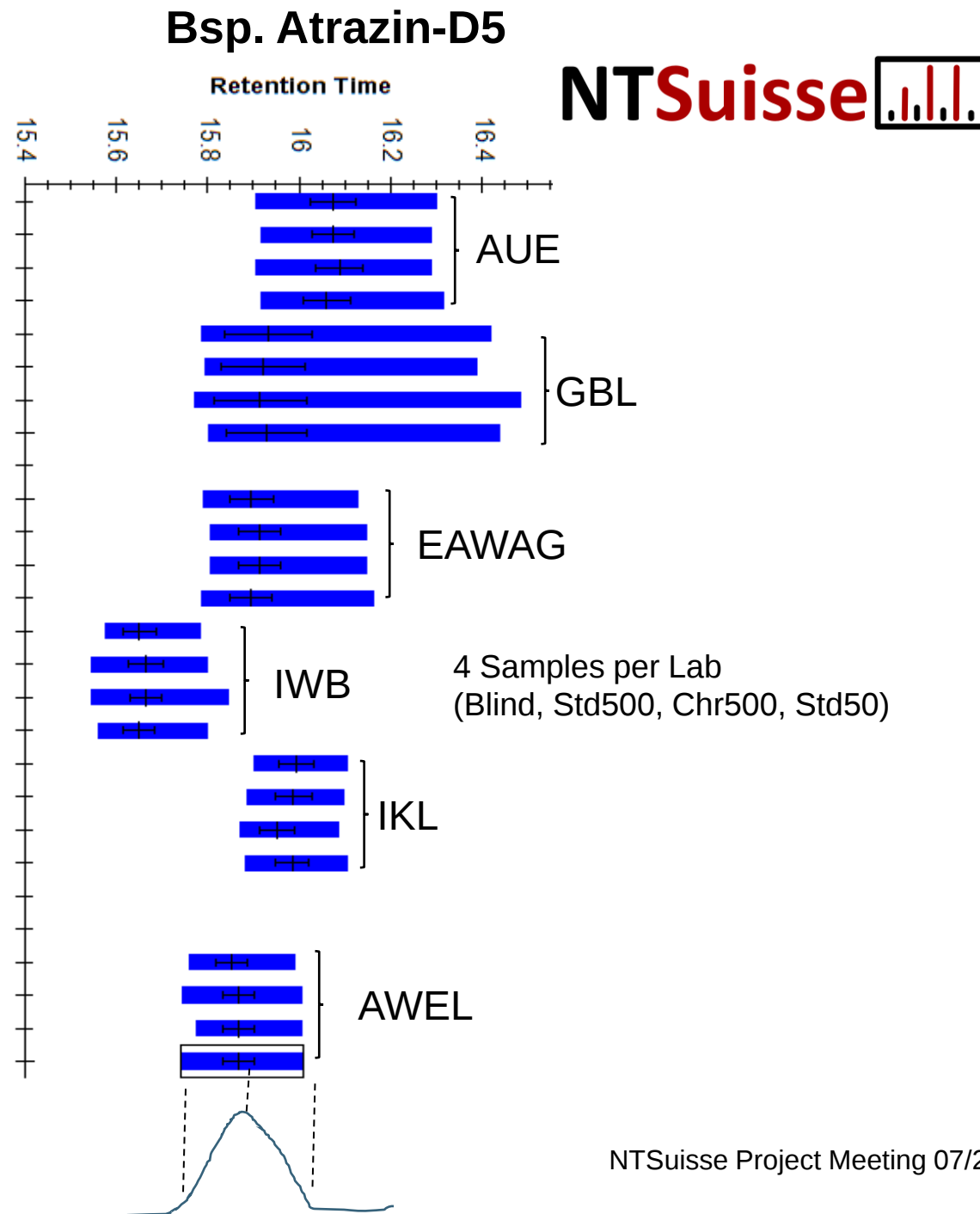
Finger's crossed it is actually working...

1st Evaluation – Round Robin Test

- **How much do retention time shift?**
- **Can we use a global target list?**
- **Are the results reliable and comparable?**

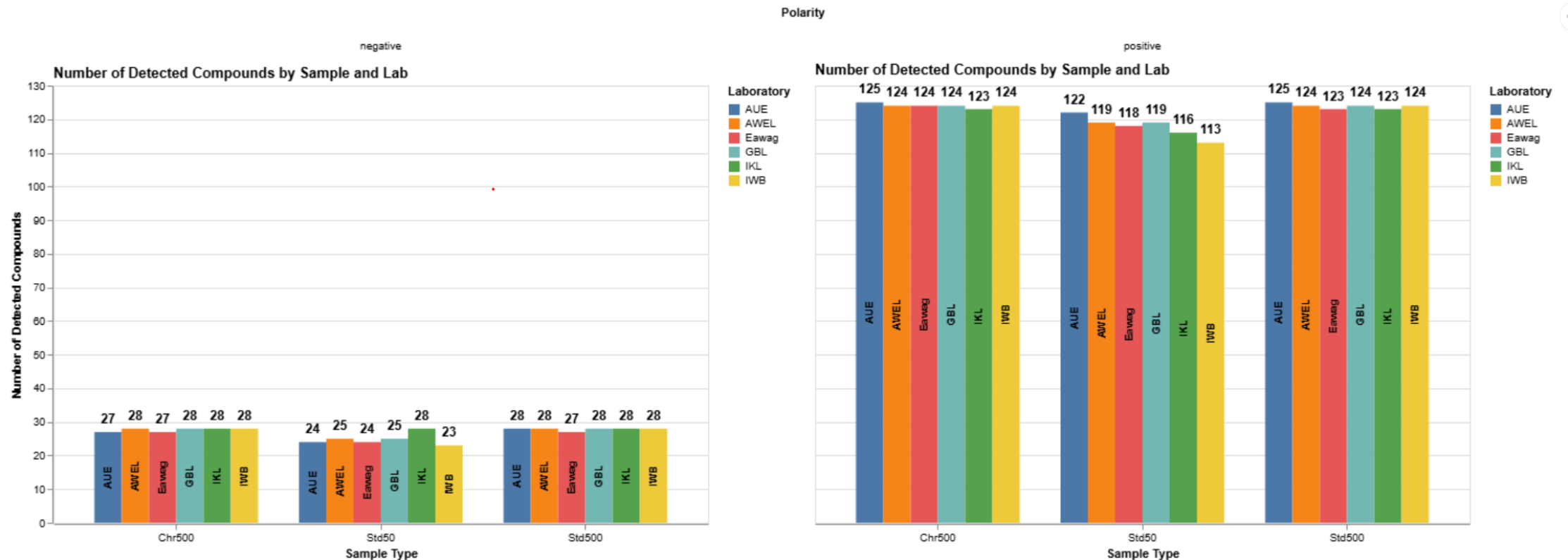
Retention Time

- Lower retention times IWB
- Broader peaks GBL



Manually detected Targets (Skyline)

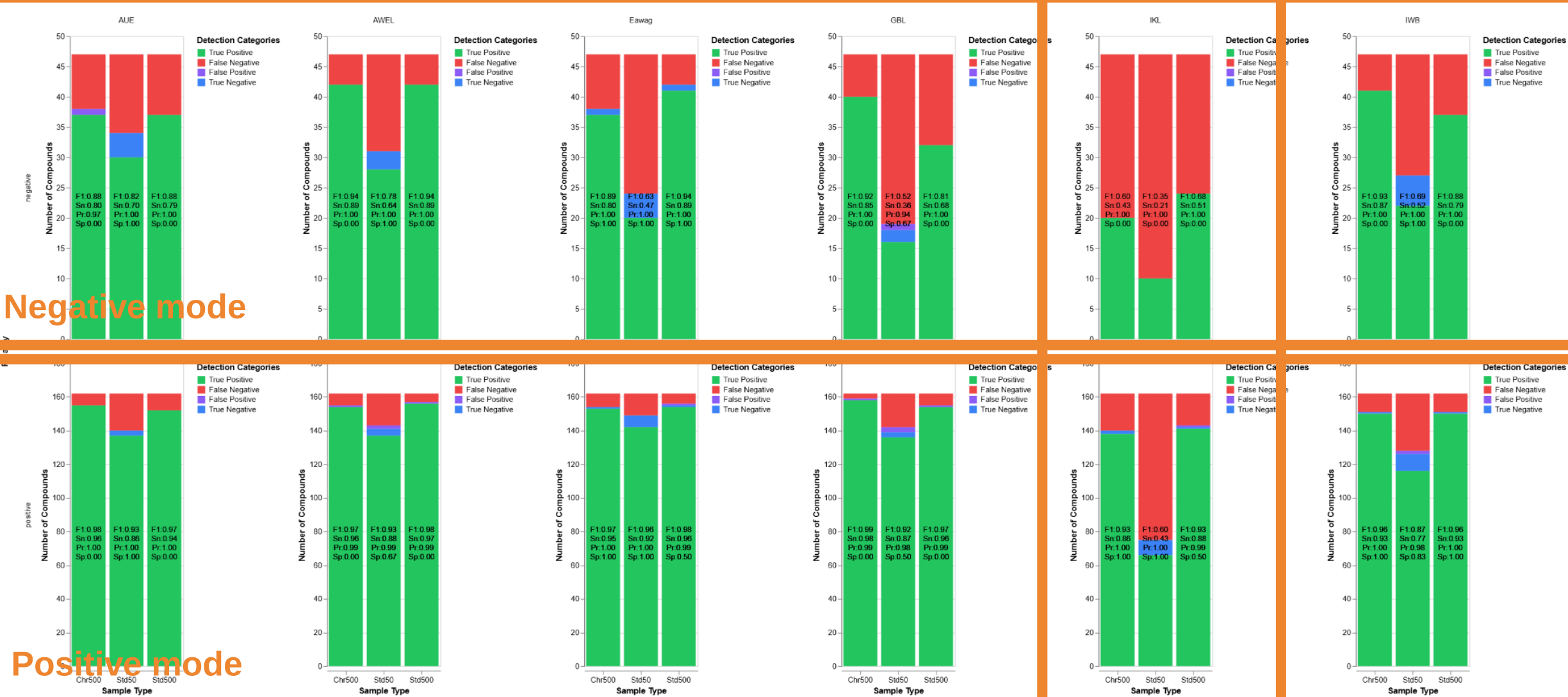
- Ground truth for automated processing



Automatically detected Targets (MZmine)

QToF

Detection Categories by Sample, Lab, and Polarity (Number of Compounds)



NTSuisse Time Schedule

2023 2025 2027 2029 2031

Development

- Measurement harmonization
- Web app conceptual design
- Implementation
- Basic monitoring & (user) testing

Piloting

- Real-scale testing
- Performance & cost optimization

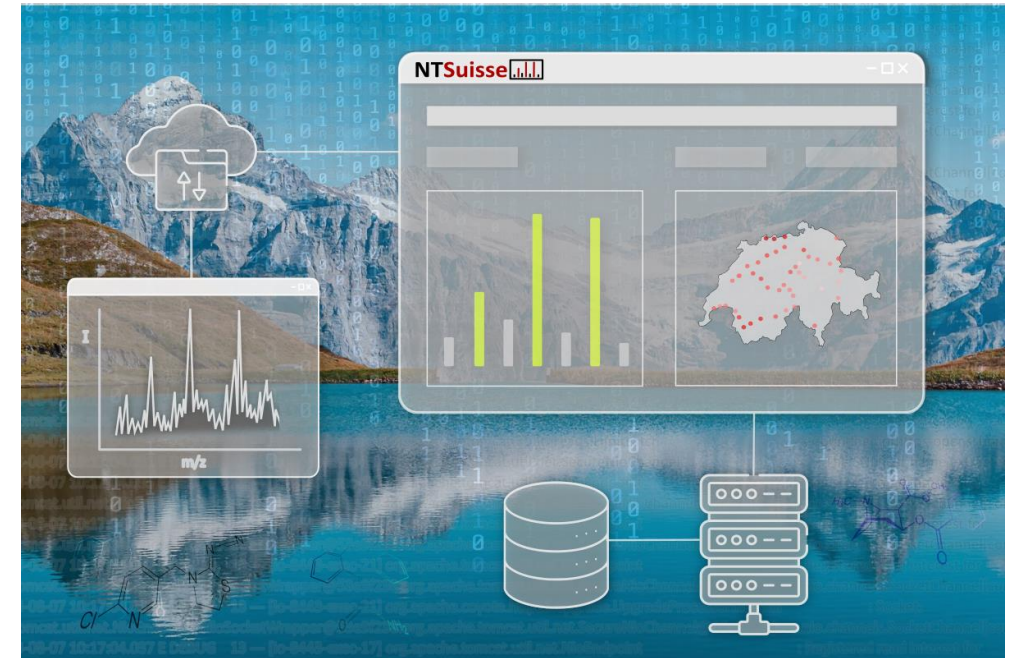
Operation

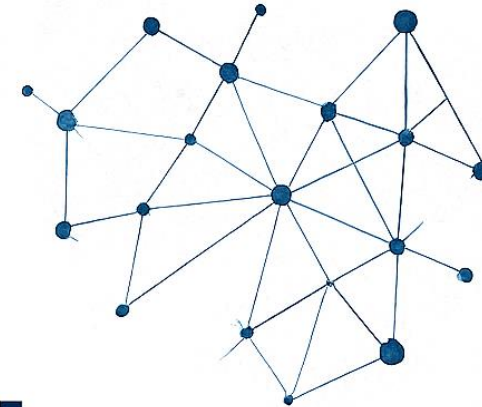
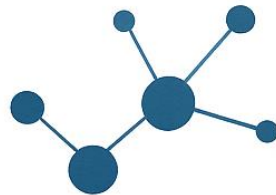
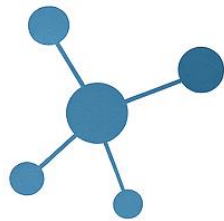
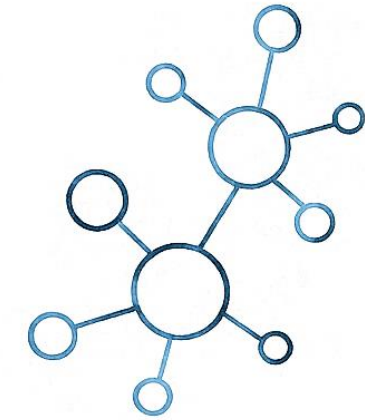
- Regular maintenance



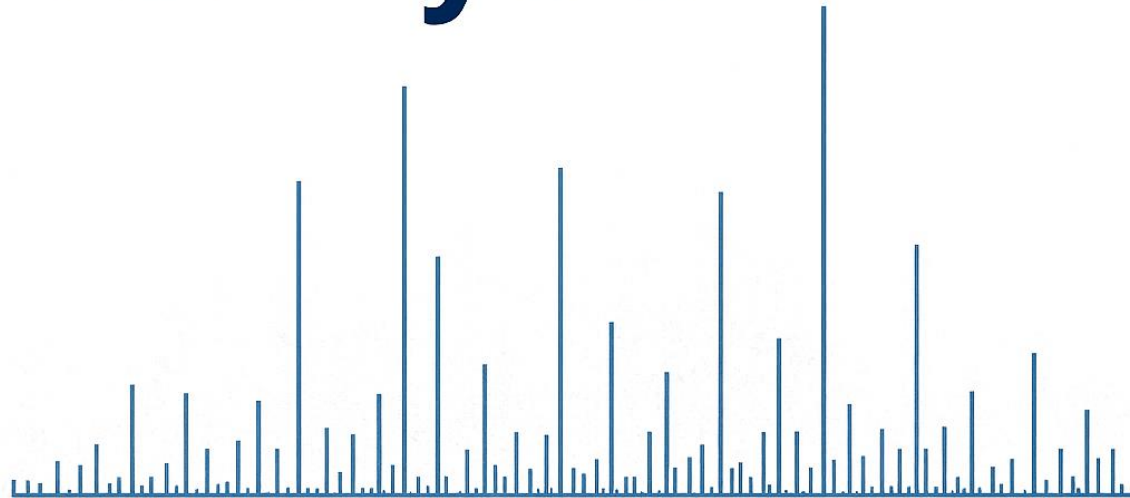
Take Home

- Harmonized measurement & data processing is challenging
- Manual target detection as ground truth is key
- Retention time alignment has to be explored
- Specific parametrization for polarization modes and instruments required
- User experience is key
- More data analysis features will come in the future

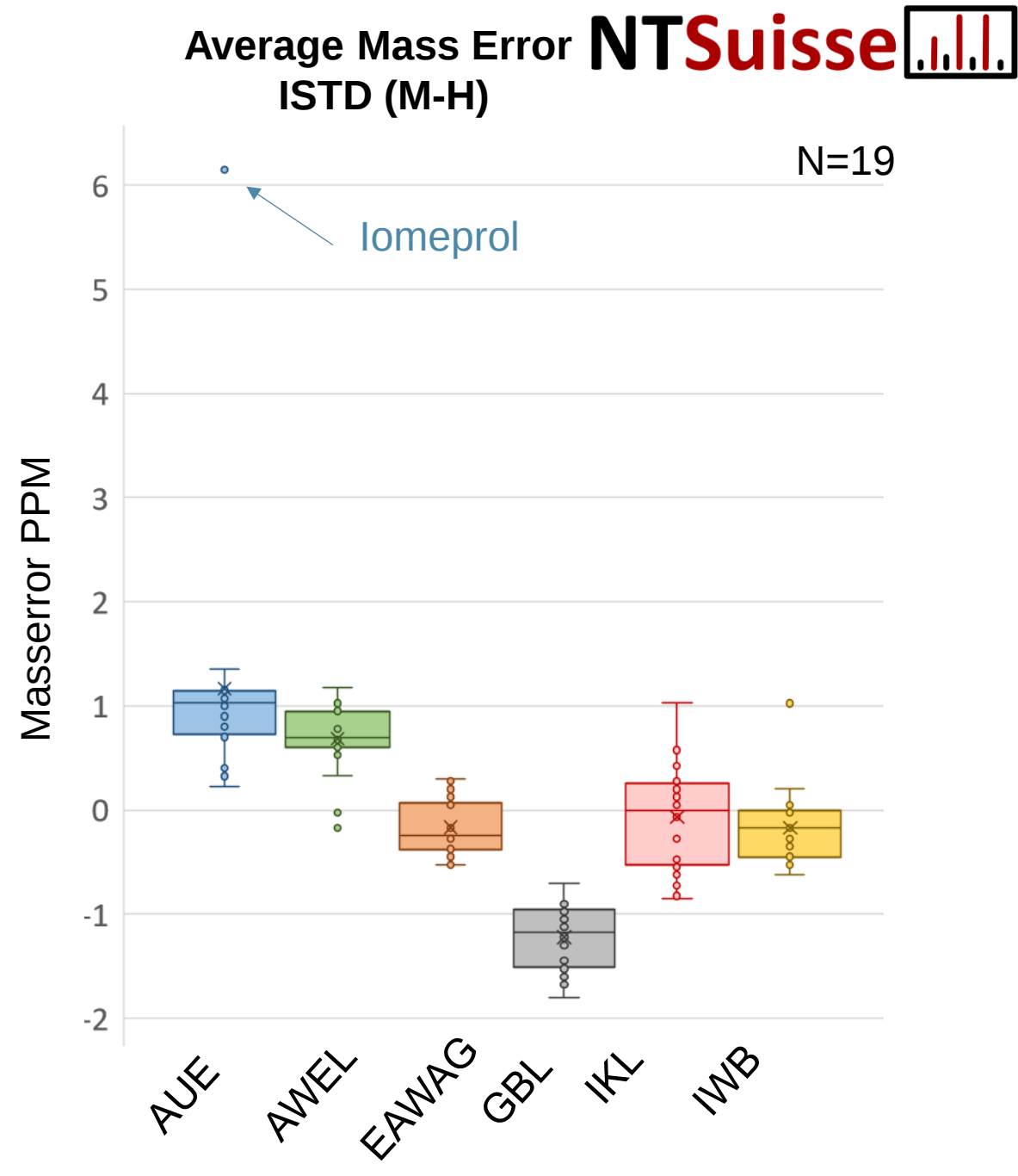
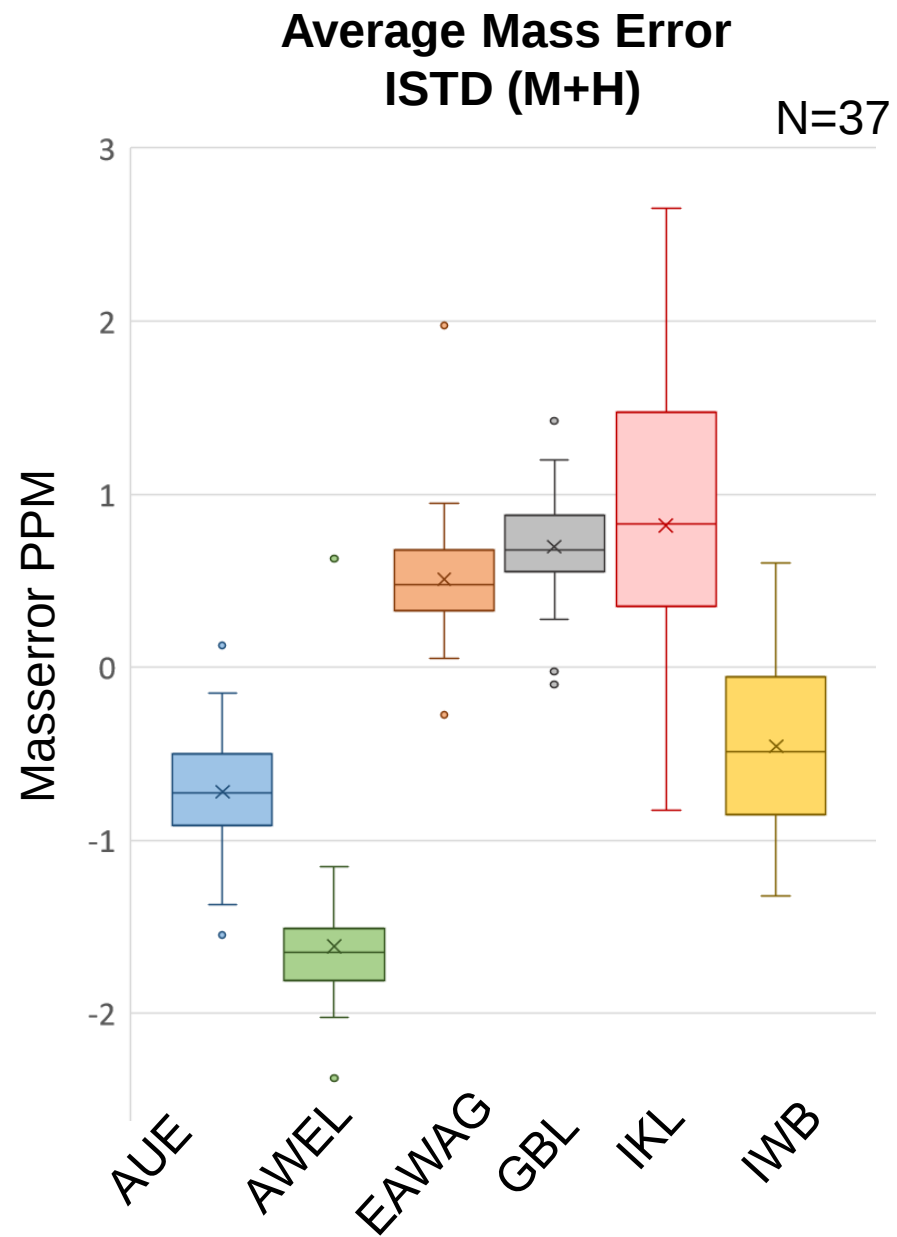




Thank you



Mass Error



Platform Architecture – Technology

