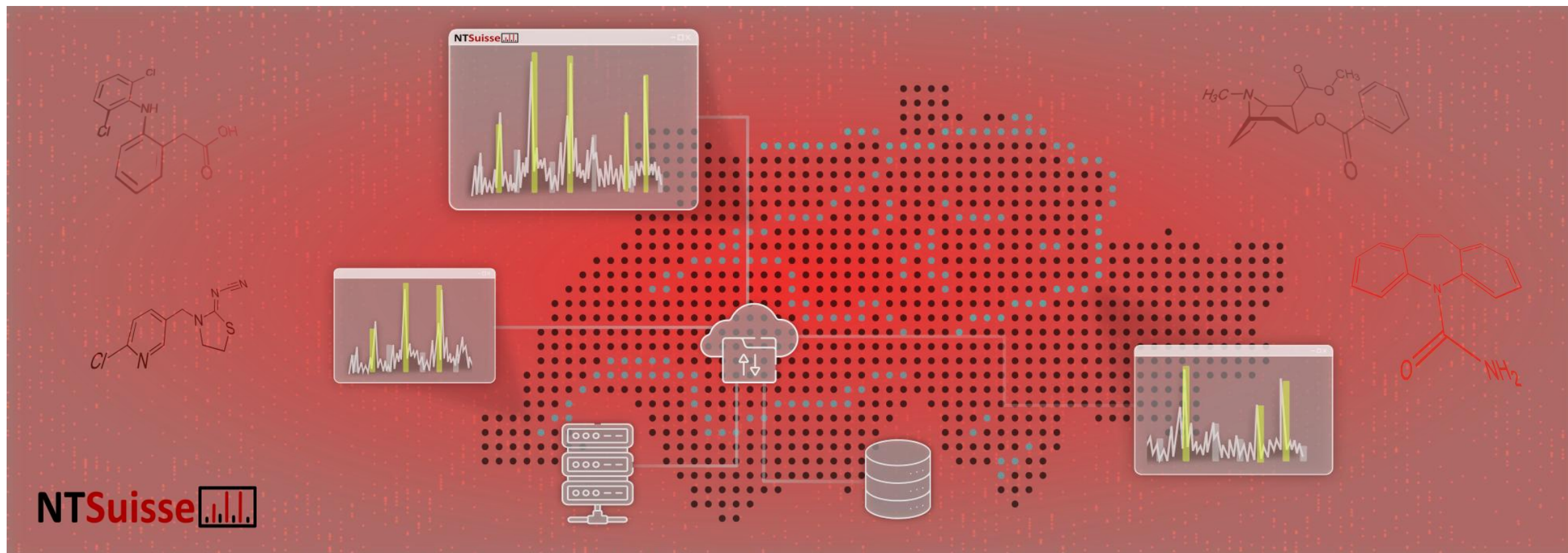


NTSuisse: A Web Platform for Centralized Automatic Processing and Evaluation of Swiss LC-HRMS Surface Water Data



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31.08.2025



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Kanton Basel-Stadt



Kanton Bern
Canton de Berne



Stadt Zürich

eawag
aquatic research

Introduction

- Part 1
 - Project Overview
 - Software Architecture
 - Development
- Part 2
 - AI Usage in NTSuisse

Project Goals & Overview

- 10 Partners (and counting)
 - Cantonal water protection labs
 - Cantonal water suppliers
 - BAFU/FOEN
 - Eawag
- Provide a more comprehensive understanding of chemical pollution of Swiss surface waters
- Compare & exchange data between cantons using a harmonized measurement method

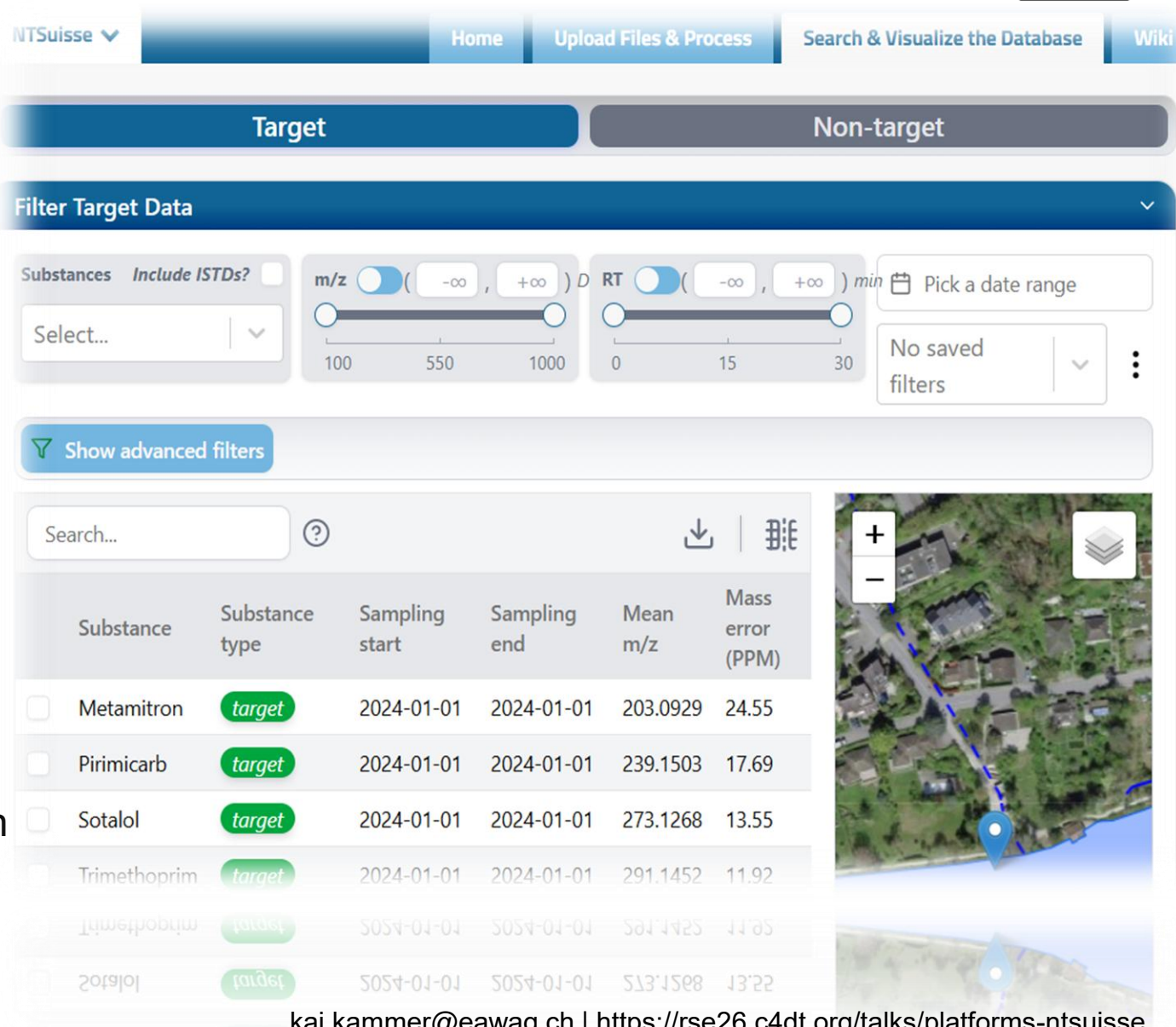


The Web Platform

- *Simple* web platform of Swiss LC-HRMS surface water data
- Uploading and storage
- Centralized automatic processing
- Target screening & non-target views
- Evaluation and visualization capabilities
- Retrospective screening of new targets

Non-goals

- Real-time & alarm monitoring
- Replacement of in-house target quantification



NTSuisse ▾ Home Upload Files & Process Search & Visualize the Database Wiki

Target Non-target

Filter Target Data ▾

Substances Include ISTDs? ☐

Select... ▾

m/z ☐ (-∞ , +∞) D RT ☐ (-∞ , +∞) min Pick a date range

100 550 1000 0 15 30

No saved filters ▾ ⋮

Show advanced filters

Search... ? ⬇ ⌘

	Substance	Substance type	Sampling start	Sampling end	Mean m/z	Mass error (PPM)
☐	Metamitron	target	2024-01-01	2024-01-01	203.0929	24.55
☐	Pirimicarb	target	2024-01-01	2024-01-01	239.1503	17.69
☐	Sotalol	target	2024-01-01	2024-01-01	273.1268	13.55
☐	Trimethoprim	target	2024-01-01	2024-01-01	291.1452	11.92
☐	Trimethoprim	target	2024-01-01	2024-01-01	291.1452	11.92
☐	Sotalol	target	2024-01-01	2024-01-01	273.1268	13.55

Map view showing a location with a blue pin and a dashed line.

NTSuisse Time Schedule

2023 2025 2027 2029 2031

Development

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

Piloting

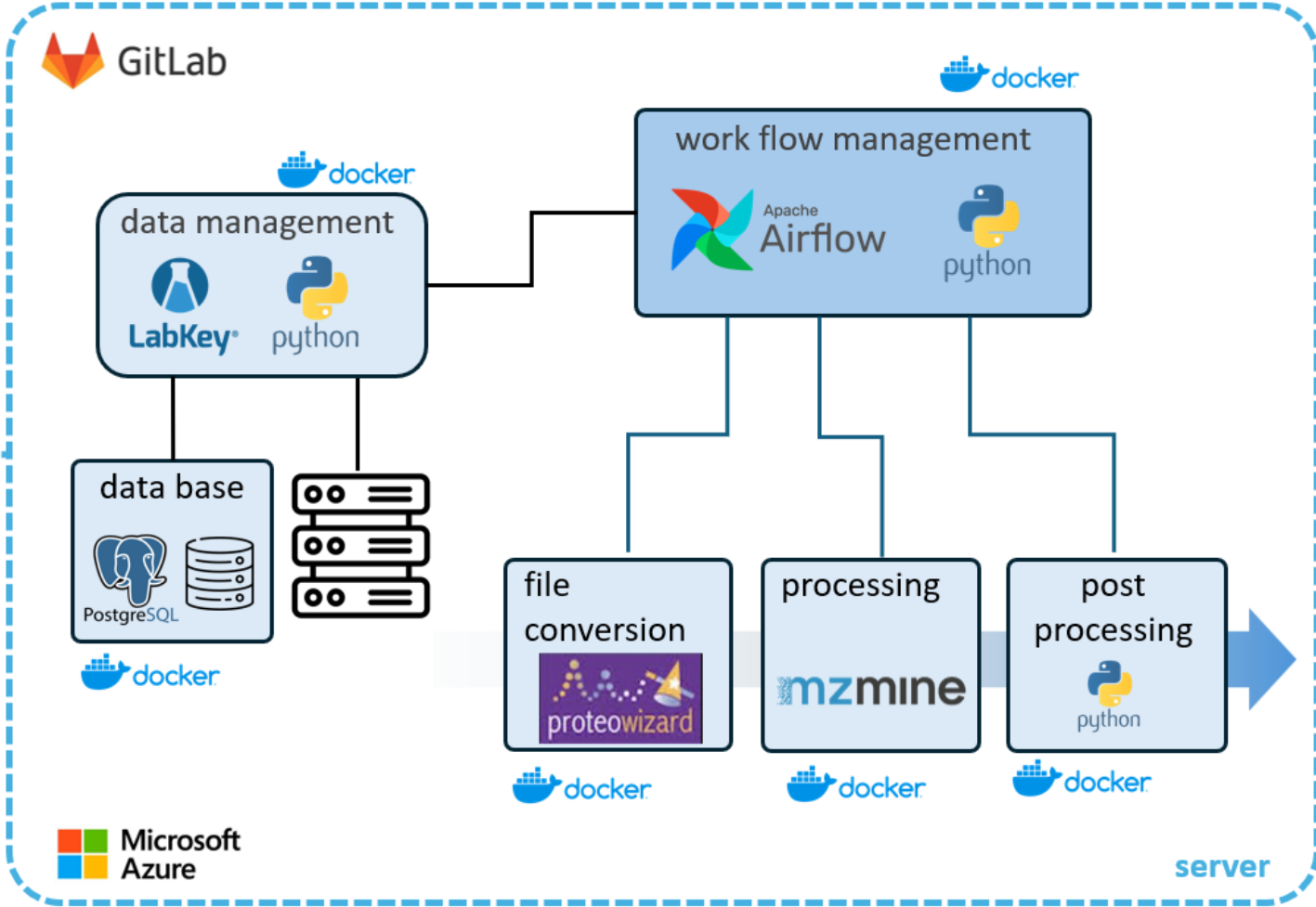
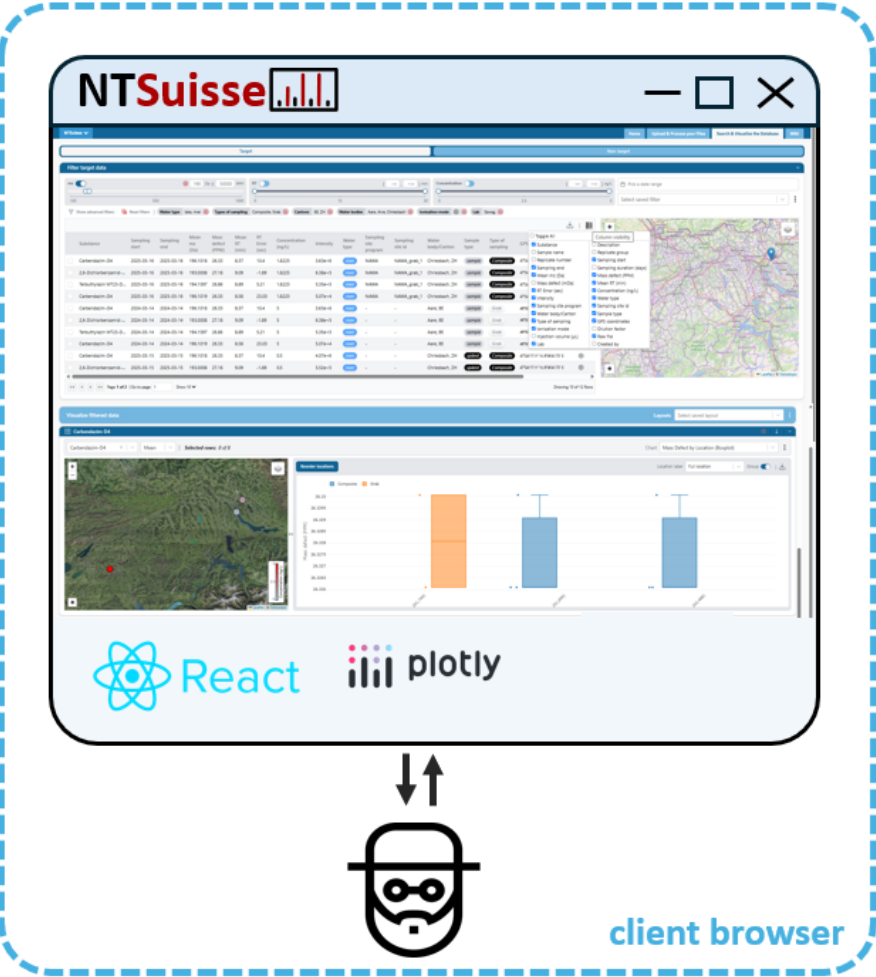
- Real-scale testing
- Performance & cost optimization

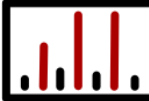
Operation

- Regular maintenance



Platform Architecture – Technology



NTSuisse 

Method Side

- Harmonized measurement method
- Requirements regarding samples
- Method continuously optimized

**Developed
together**



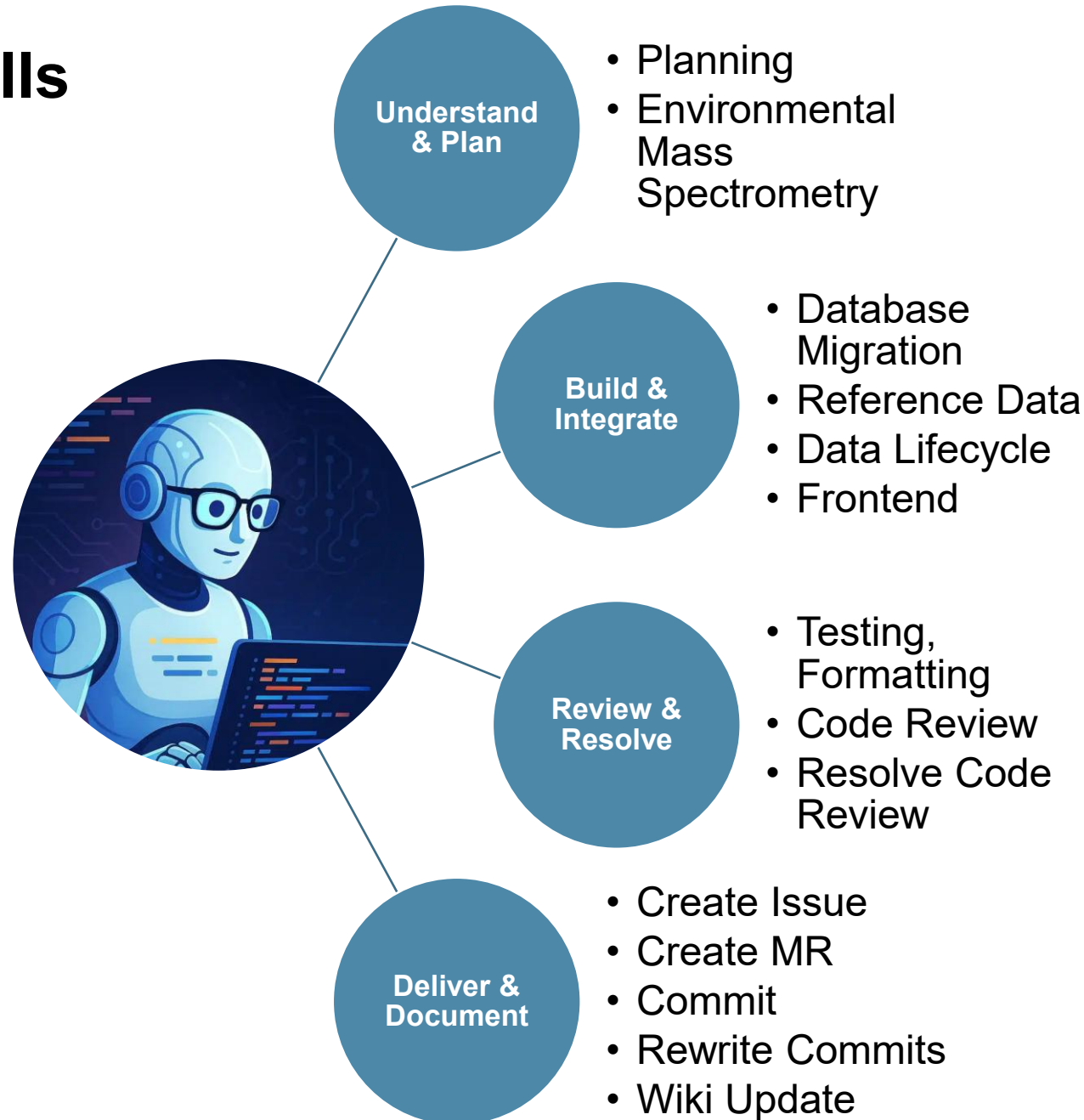
**User
Meetings**

Platform Side

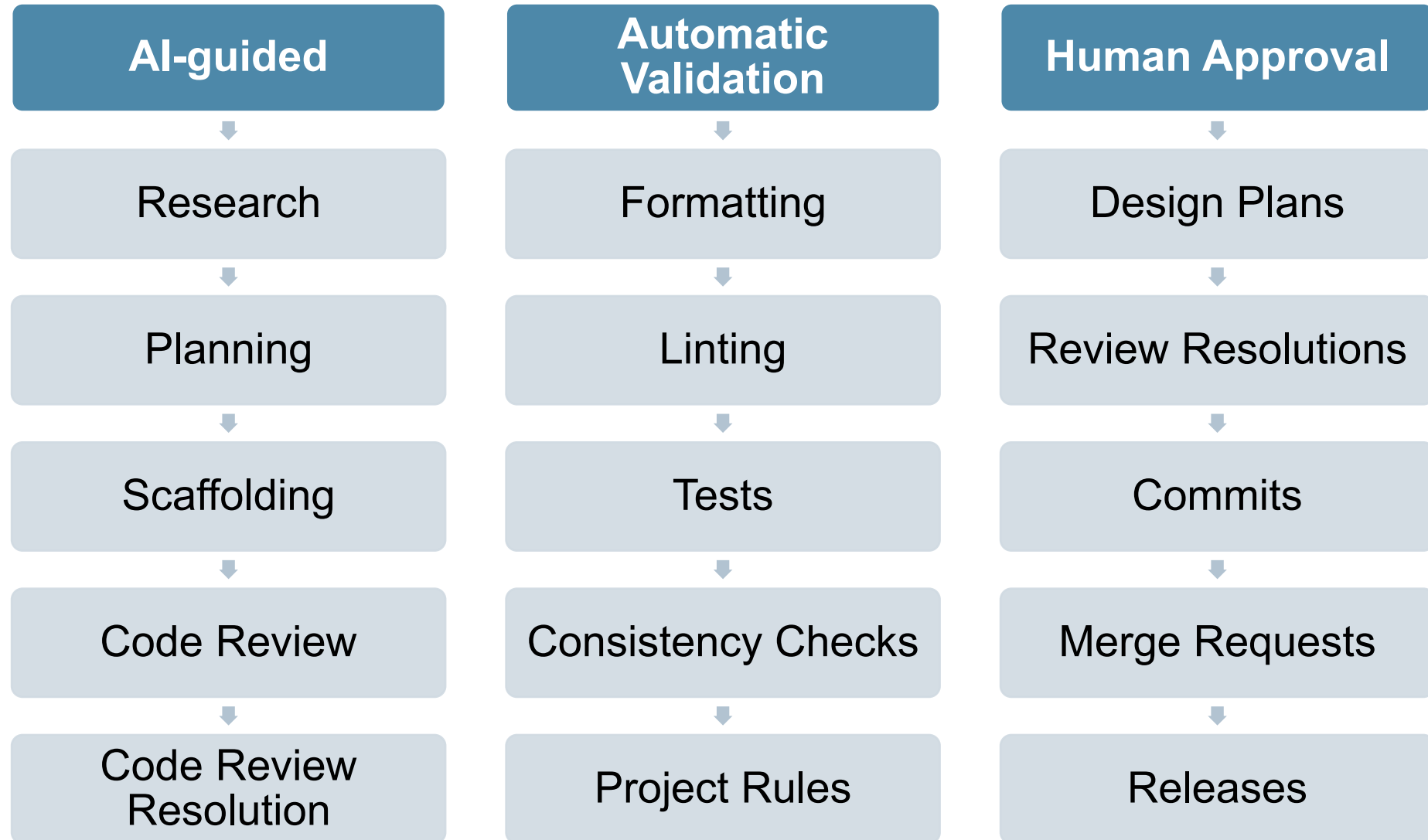
- Upload & storage management
- React UI & backend
- Data processing
- Parameters optimized along with method development

Project AI Skills

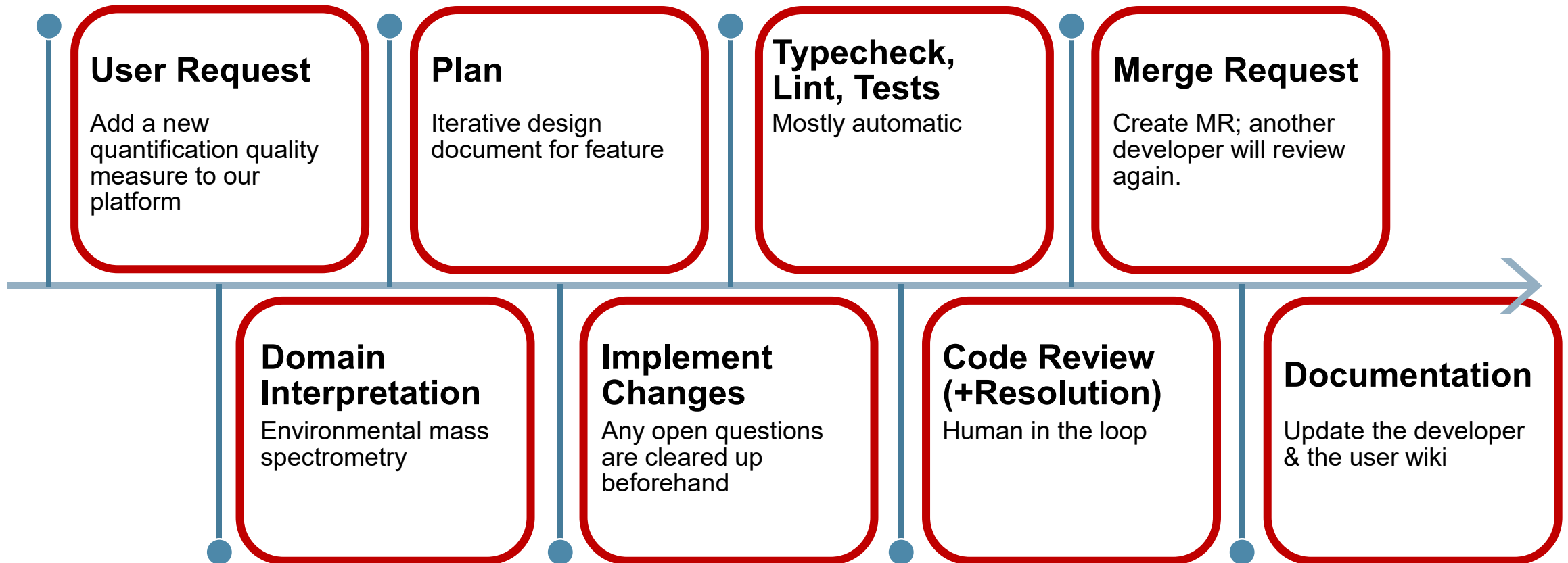
Overall Instructions
+ 13 Skills In Total



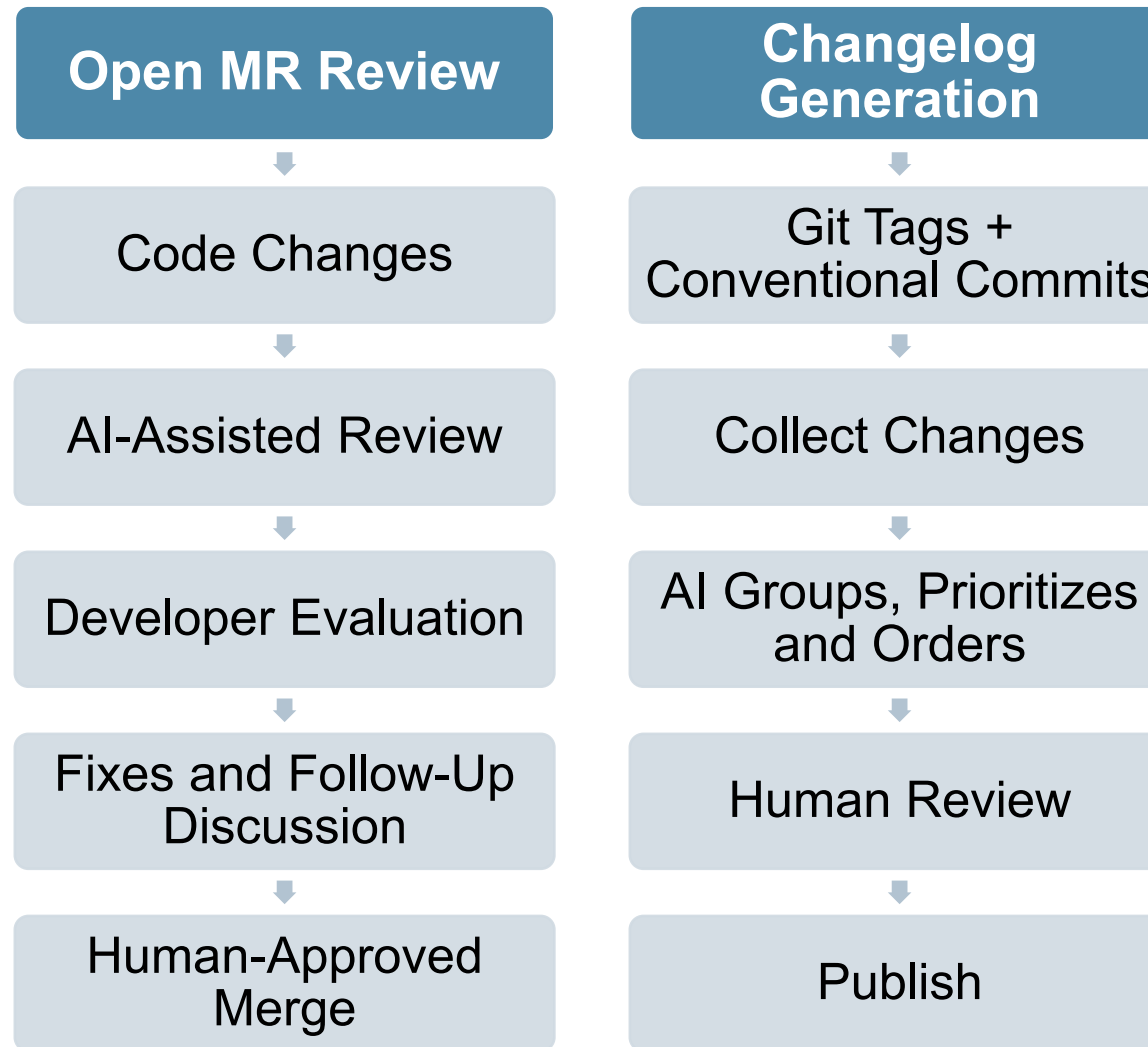
AI Within Our Engineering Guardrails



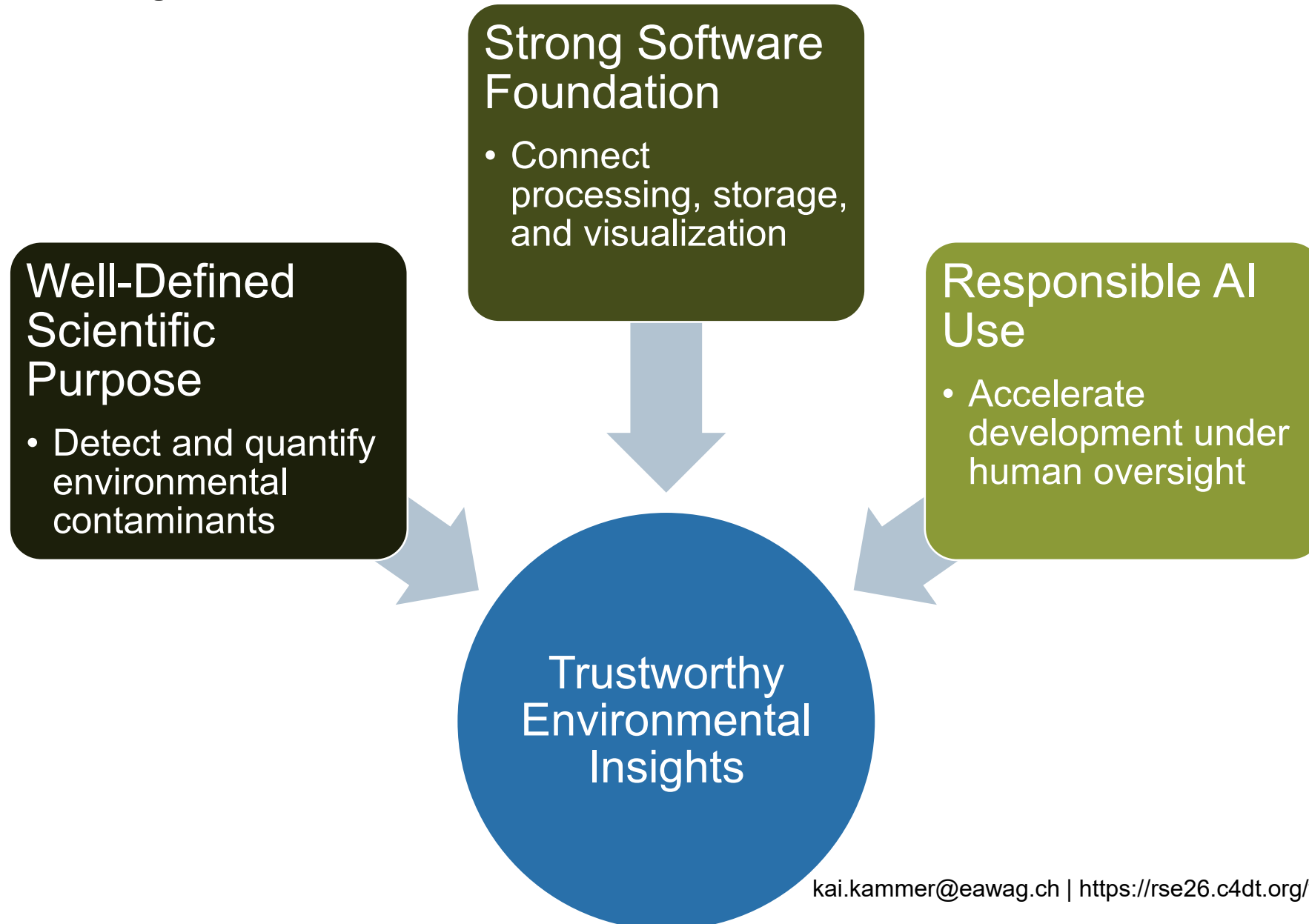
Example: Adding a Quantification Quality Field



WIP: AI-Assisted CI/CD



Key Takeaways



Thank you!

- **Current & Former Developers: Johannes Boog, Benjamin Schwalb, Fernando Calvo, Sebastian Salzmann, Michele Stravs**
- **Special thanks to Carolin Huber and Philipp Longree at UChem**
- **All our platform partners & mzmine team**
- **The whole UChem department @eawag**
- **Thank you for your attention!**



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