

A wide-angle photograph of the TU Wien main building, a grand neoclassical structure with a green copper roof and a central portico with columns. The building is surrounded by lush green trees in the foreground. In the background, the city of Vienna and distant mountains are visible under a clear blue sky.

PET – Pollution Evaluation Tool

*An Open-Source Shiny Application for Scalable Quality Assurance
and Exploration of Transnational River Basin Monitoring Data*

Agenda - PET

01

Context of development

Tethys project & MCC database background

02

Intents of development

Challenges of MCC-DB & PET goals

03

Developed Content

Two modes, features (& live demo)

04

Future Development goals

Ongoing refinement & vision

01

Context of development

Tethys project & MCC database background

Context - The Tethys project

2024 - Launched as EU & Interreg project

13 PP
Project Partners

10 SP
Strategic Partners

CAPACITY BUILDING FOR

Monitoring - Chemical analysis - Data storage - Modelling of hazardous substances in the Danube river basin

OUTPUT
Multi-compartment concentration database (MCC-DB) for pathway-oriented modelling
+
Pollution Evaluation Tool



www.fgg-donau.bayern.de/die_donau/flussgebiet_donau

Context - The MCC database

Tailor-made solution to support state-of-the-art emission modelling (e.g. MoRE)

57

Tables

35

CV registries

17

Import tables

7

Compartments

KEY FEATURES

**Standardized CV
metadata**

**Built-in import
constraints**

**Role-based QA
workflow**

**EU-reporting
harmonized**

FAIR & open-source

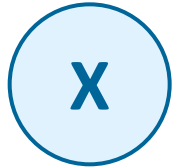
Visit the MCC-DB poster
by Steffen Kittlaus

02

Intents of development

Challenges of MCC-DB & PET goals

Intents - Challenges of the MCC database



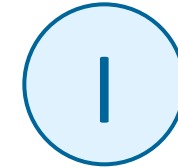
Expert tool

Complex database architecture, that need to be understood



Technical Skills required

Import, validation, curation, maintenance & exploration are technically demanding



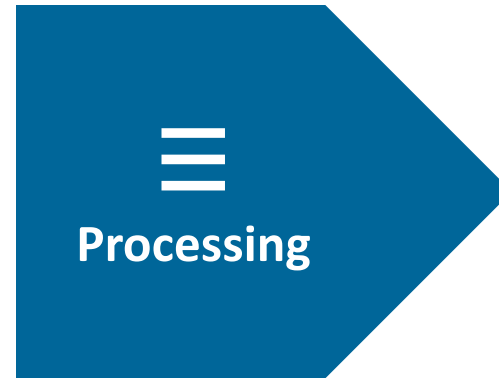
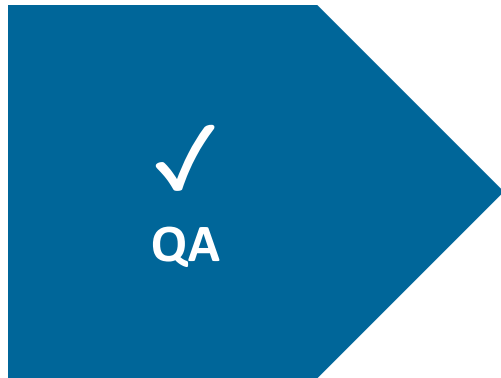
Lack of Overview

Information is spread across many tables, hiding the bigger picture

User-friendly Interface is needed!

Intents - Claim & Goals of PET

Standardized and user-friendly processing system for data governance activities



WITH

Less time

Fewer errors

No coding required

03

Developed Content

Two modes, features (& live demo)

Developed Content - Two modes of PET

✓ QA mode

- Measurement-centred evaluation of compartment-specific project data
- Two filter systems linking the subject of evaluation across all import tables - ONE big picture
- Comparison with already imported data

⚙ Management mode

- Cross-compartment evaluation by controlled vocabulary and spatial dimension
- Filter incl. EU regulatory geodata (WFD water bodies, NUTS regions)
- Data availability, Statistic, CV management, Export & Transfer

(DEMO TIME)

Developed Content - QA: Feature overview

LINKAGE & FILTERING

Fast filter

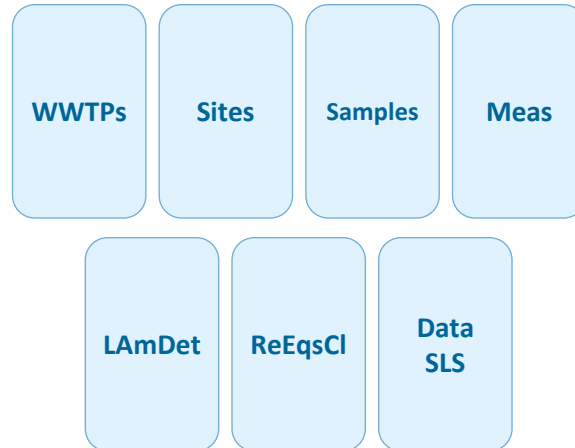
Quick subject lookup

Advanced filter

Precise filter building

PER-TABLE MODULES

SUMMARY - all tables at a glance



ANALYTICS

Key table feature

Controlled vocabulary

Cross-table plots

Grid table plots

Completeness analysis

One big picture of the data - linked across all tables, contextualized for QA

The screenshot displays the 'Sign in' dialog box within the PET (Pollution Evaluation Tool) application. The dialog is centered on a greyed-out background of the application's main interface. The dialog contains the following elements:

- Sign in** title
- How to sign in** — *click to expand* (collapsible section)
- Profile** dropdown menu with options: `Test_user` (selected), `Test_user`, and `Tethys_danube_user`. A [Manage profiles...](#) link is visible to the right.
- Database name** text input field containing `konda_test`.
- Username** text input field containing `sosten`.
- Password** text input field with masked characters (dots).
- Role** dropdown menu with `tethys_user` selected.
- Advanced settings**
- Server ID / Host** text input field containing `10.10.100.20`.
- Port** text input field containing `5432`.
- Save as profile**
- Cancel** and **Connect** buttons at the bottom.

The screenshot displays the PET (Pollution Exposure Tool) interface. The main window shows a 'Fast filter' sidebar on the left with options for Compartment (surfacewater), Sub-compartments (All), Datasource (EU-NORMAN EMPODAT), Determinant class (Choose class(es)), Determinant (Choose determinant(s)), and an Advanced filter section. The main content area is titled 'Summary' and contains a table of data. An 'Advanced datasource filters' dialog box is open in the center, allowing users to define filters for the data. The dialog includes sections for Identifier filters, Controlled vocabulary filters (currently set to 'ss.country'), Sampling time, and Free column filters. A dropdown menu is open for the 'Choose one or more values' field, showing options: AT, DE, HU, SK, and NULL. The dialog has 'Close', 'Apply', and 'Apply & Close' buttons at the bottom.

Fast filter

How the Fast filter works
— click to expand

Compartment

surfacewater

Sub-compartments

All

Datasource

EU-NORMAN-EMPODAT

Determinant class

Choose class(es)

Determinant

Choose determinant(s)

Advanced filter

Configure

Available measurements:
2582

Summary Sites Samples Meas LAmDet ReEqsCl DataSLS

Summary — click to expand

Refresh Close

Search: _____

table	n	n_water	n_spm	n_biota	checked	created_by	last_modified	data_source	license	supplier
All	All	All	All	All	All	All	All	All	All	All
meas	2582	2582	0	0	0	mliu	2025-10-30T09:28:58Z	EU-NORMAN-EMPODAT	CC BY 4.0	Meiqi Liu
samples	1274	1274	0	0	0	mliu	2025-09-29T09:47:35Z	EU-NORMAN-EMPODAT	CC BY 4.0	Meiqi Liu
sampling_sites	271	271	0	0	0	mliu	2026-01-09T11:43:35Z	EU-NORMAN-EMPODAT	CC BY 4.0	Meiqi Liu
determinants	6	6	0	0	4	mliu	2025-09-29T10:21:08Z			
determinants	1	1	0	0	1	rilkanaev	2025-11-07T14:14:09Z			
determinants	22	22	0	0	1	sosten	2025-01-10T16:14:35Z			
analytical_methods	2	2	0	0	0	eeder	2026-01-19T09:23:22Z			
analytical_methods	5	5	0	0	0	mliu	2026-01-19T09:23:22Z			
laboratories	4	4	0	0	3	mliu	2025-10-30T09:32:17Z			
laboratories	1	1	0	0	1	sosten	2025-01-10T14:36:43Z			
classifications	49	49	0	0	49	mliu	2025-11-07T10:36:27Z			
environmental_quality_standards	30	30	0	0	2	sosten	2025-01-10T16:18:24Z			

Showing 1 to 12 of 12 entries

Fast filter

How the Fast filter works — click to expand

Compartment

wastewater

Sub-compartments

All

Datasource

DE-KIT-MPDS

Determinant class

Choose class(es)

Determinant

Choose determinant(s)

Advanced filter

Configure

Available measurements: 79936

Summary WWTPs Sites Samples Meas LamDet ReEqSCI DataSLS

Information Quality Assessment DB-Data

Treatment Overview — click to expand

Treatment Overview

Refresh Close

Applied Not applied No info



Details (click to select):

Controlled Vocabulary — click to expand

Controlled vocabulary of wwtps

Refresh Close

Cross Table — click to expand

Cross table plot

Refresh Severin Ostbrn, 2026

Fast filter

How the Fast filter works
— click to expand

Compartment

surfacewater

Sub-compartment

All

Datasource

EU-NORMAN-EMPODAT

Determinant class

Choose class(es)

Determinant

Choose determinant(s)

Advanced filter

Configure

Available measurements:
2582

Summary Sites Samples Meas LAmDet ReEqsCl DataSLS

Information Quality Assessment DB-Data

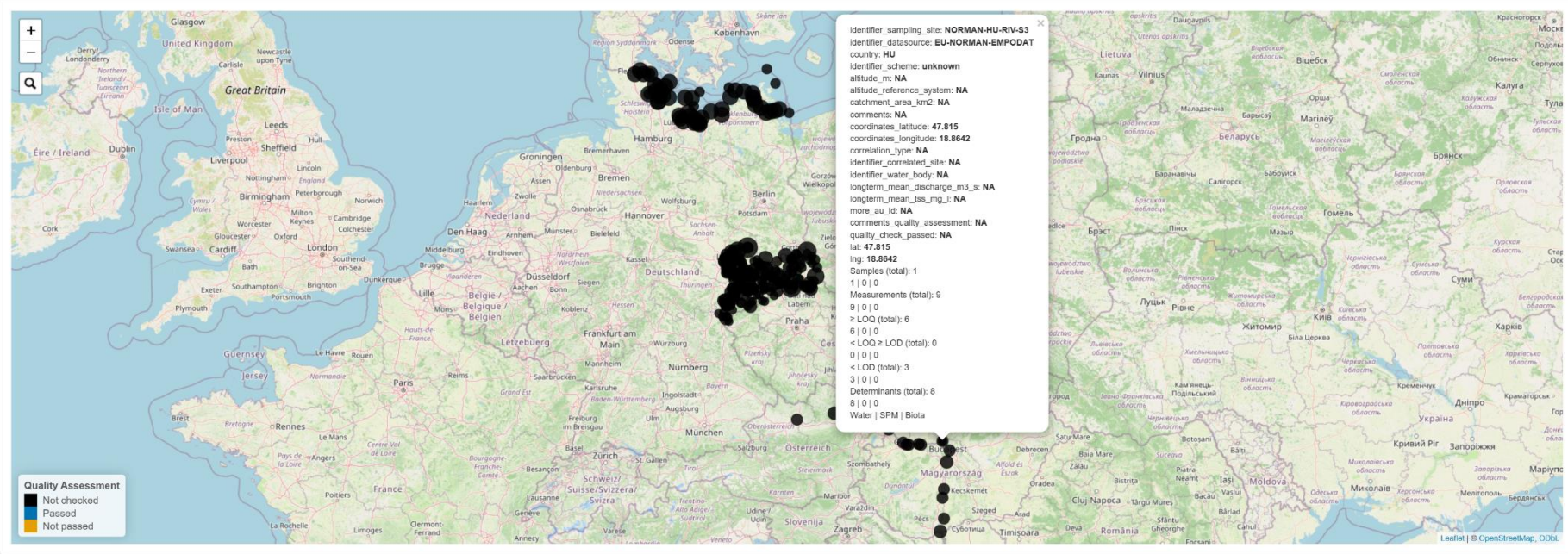
Map — geographic distribution of sampling sites — click to expand

Sampling sites

270 / 271 sampling sites displayed

Refresh

Close



Controlled Vocabulary — click to expand

Controlled vocabulary of sampling_sites

Refresh

Close

Fast filter

How the Fast filter works — click to expand

Compartment

surfacewater

Sub-compartments

All

Datasource

EU-DanubeHazard_m3c

Determinant class

Choose class(es)

Determinant

Choose determinant(s)

Advanced filter

Summary Sites **Samples** Meas LAmDet ReEqSCL DataSLS

Information **Quality Assessment** DB-Data

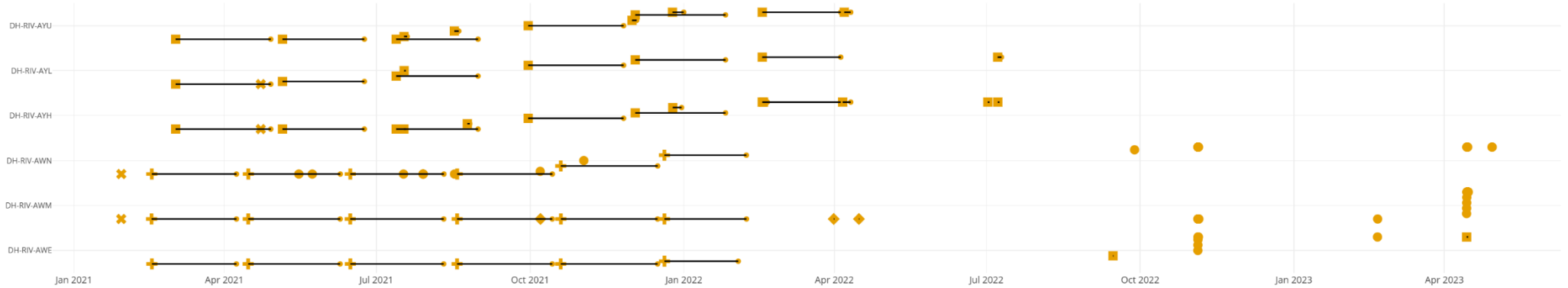
Sample timeline — click to expand

Samples Timeline

Refresh

Close

Method: ● autosampler > vacuum pump ■ composite sampling ◆ composite sampling > flow-proportional + composite sampling > time-proportional ✕ grab sampling QA: ■ Not checked ■ Not passed ■ Passed



Details (click to select):

Fast filter

How the Fast filter works
— click to expand

Compartment
surfacewater

Sub-compartments
All

Datasource
EU-NORMAN-EMPODAT

Determinant class
Choose class(es)

Determinant
Perfluorooctanoic acid

Advanced filter
Configure

Available measurements:
1277

Summary Sites Samples Meas LAmDet ReEqSCL DataSLS

Information Quality Assessment DB-Data

Plot description & legend — click to expand

Violin Plots

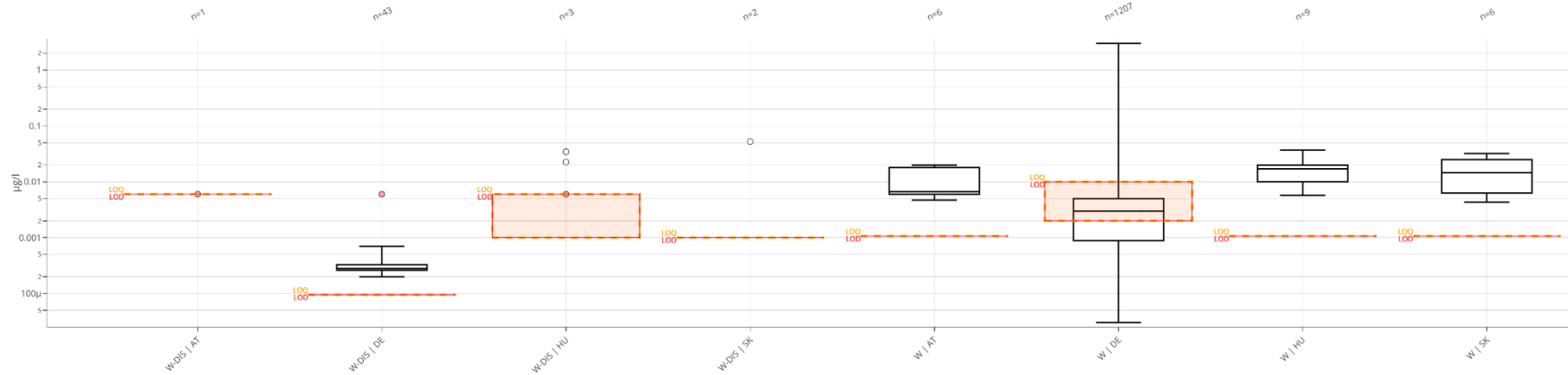
Raw ROS (Helsel, D.R., 2011) 2009/90/EC

ss.country

Refresh Close

Censored value Uncensored value Invalid measurement Hyper-censored measurement Implausible measurement

Perfluorooctanoic acid



Details (click to select):

Controlled Vocabulary — click to expand

Fast filter

How the Fast filter works — [click to expand](#)

Compartment
wastewater

Sub-compartments
All

Datasource
DE-KIT-MPDS

Determinant class
Choose class(es)

Determinant
Choose determinant(s)

Advanced filter
Configure

Available measurements: 79936

Summary WWTPs Sites **Samples** Meas LAmDet ReEqSCL DataSLS

Information **Quality Assessment** DB-Data

Sample timeline — [click to expand](#)

Samples Timeline Refresh Close

Controlled Vocabulary — [click to expand](#)

Controlled vocabulary of samples Refresh Close

All		All		All		All	
compartment	wastewater			2468	valid		
sampling_method	composite sampling			204	valid		
sampling_method	composite sampling > volume-proportional			2010	proposed		
sampling_method	unknown			254	valid		
sampling_point	excess sludge			136	superseded		
sampling_point	inflow			204	superseded		
sampling_point	outflow			2010	superseded		
sampling_point	primary sludge			118	superseded		

Showing 1 to 8 of 8 entries

Cross Table — [click to expand](#)

Fast filter

How the Fast filter works
— click to expand

Compartment
surfacewater

Sub-compartments
All

Datasource
EU-NORMAN-EMPODAT

Determinant class
Choose class(es)

Determinant
Choose determinant(s)

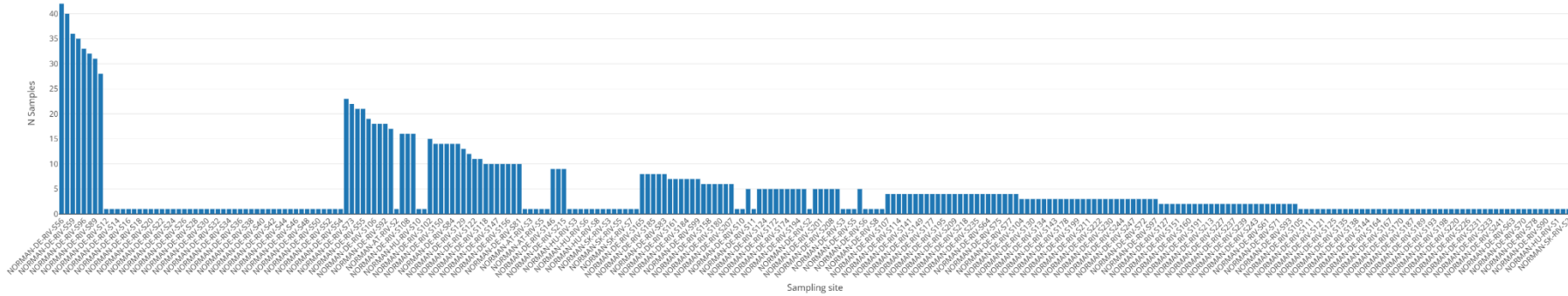
Advanced filter
Configure

Available measurements:
2582

Cross table plots

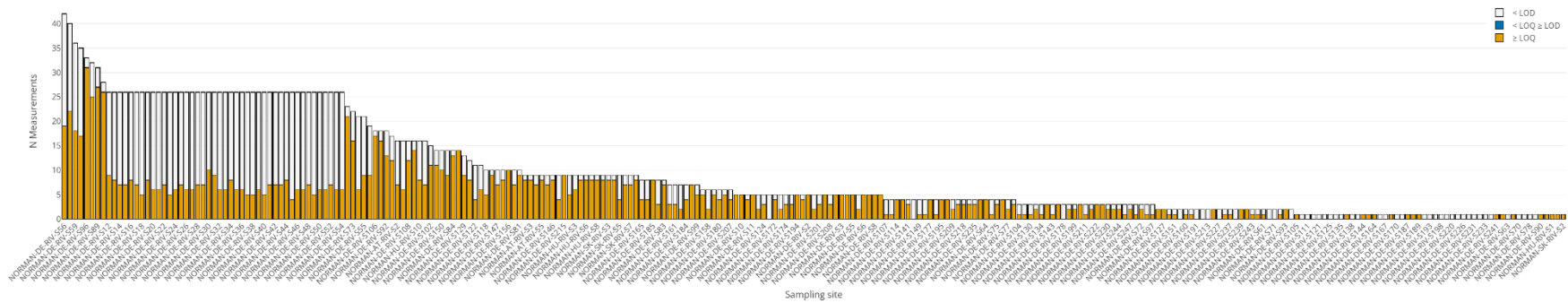
Refresh Close

Sites - Samples



Details (click to select):

Sites - Measurements



Details (click to select):

Fast filter

How the Fast filter works
— click to expand

Compartment

surfacewater

Sub-compartment

All

Datasource

EU-NORMAN-EMPODAT

Determinant class

Choose class(es)

Determinant

Perfluorooctanoic acid

Advanced filter

Configure

Available measurements:
1277

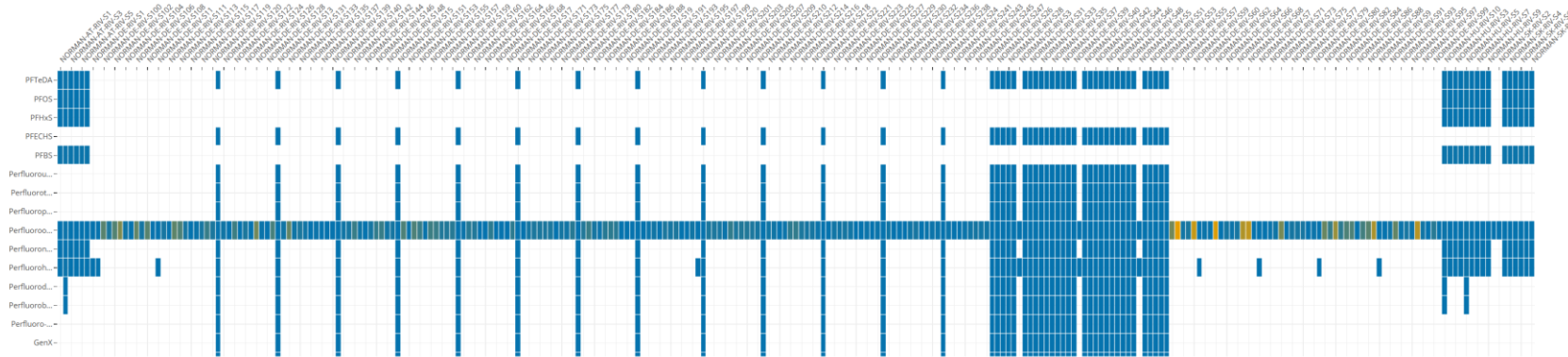
Grid Table — click to expand

Grid table plots

Refresh Close

Sites, Determinants - N Measurements

0 1 42



Details (click to select): identifier_sampling_site: **NORMAN-AT-RIV-S4**

identifier_determinant: **Perfluorooctanoic acid**

identifier_datasource: **EU-NORMAN-EMPODAT**

rel_mean: **0.19**

Samples (total): 1

1 | 0 | 0

Measurements (total): 1

1 | 0 | 0

≥ LOQ (total): 1

1 | 0 | 0

< LOQ ≥ LOD (total): 0

0 | 0 | 0

< LOD (total): 0

0 | 0 | 0

Water | SPM | Biota

Sites, Determinants - relative mean of concentration

0 0.01 rel. mean 35.41 rel. mean

Completeness — click to expand

Completeness overview of samples

Refresh

Close

Vertical completeness

Column name	Completeness
discharge_during_sampling_m3_s	88.57
dry_content_weight_percent	0
igsn_pid	0
organic_content_mgc_per_kg_dry	0
sample_volume_ml	84.44
sampling_method_accruited	100
sampling_method_reported	100
sampling_point_reported	81.44
discharge_during_sampling_m3_s	88.57
igsn_pid	0
sample_volume_ml	84.44
sampling_method_accruited	100
sampling_method_reported	100
sampling_point_reported	81.44

Showing 1 to 14 of 14 entries

Lateral completeness

N ids	Completeness
133	28.57
17	42.86
129	57.14
955	71.43

Showing 1 to 4 of 4 entries

Quality Assessment Management

Fast filter

How the Fast filter works
— click to expand

Compartment
surfacewater

Sub-compartments
All

Datasource
EU-NORMAN-EMPODAT

Determinant class
Choose class(es)

Determinant
Choose determinant(s)

Advanced filter
Configure

Available measurements:
61

Update (filtered)

- compartment * (CV)
Select or type...
- country * (CV)
Select or type...
- identifier_scheme *
Select or type...
- altitude_reference_
Select or type...
- comments
Select or type...
- coordinates_latitud
Select or type...
- correlation_type (CV)
Select or type...
- identifier_water_bo
Select or type...
- longterm_mean_tss
Select or type...
- name
Select or type...
- nuts_2_code
Select or type...
- nuts_version
Select or type...
- geom_point
Select or type...
- quality_check_pass
Select or type...

Confirm UPDATE

Filtered IDs from normal view (ss): 6

Fields to update:

- identifier_correlated_site = NORMAN-AT-RIV-S1

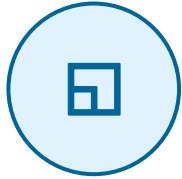
Availability by target table:

- **surfsw.sampling_sites**
update 6 rows, missing 0

Cancel **Commit**

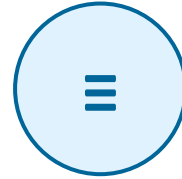
Developed Content - Management: Feature overview

Cross-compartment evaluation with spatial intelligence



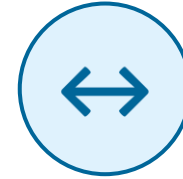
Advanced spatial & data filter

WFD water bodies, NUTS regions, full CV-driven slicing



Summary module

Data availability, Source, License and QA-Status



Compartment comparison plot

Side-by-side measurements across all compartments

TU WIEN
TECHNISCHE UNIVERSITÄT WIEN

Quality Assessment
Management
Structure
Units

PET
Pollution Evaluation Tool

Units: OFF
kenda_test
sosten
tethys_admin
Switch

Active: 1 Radii X 6 GWB X Clear all

Radius in km

Clear all radii

Each click on the map adds a radius.

Controlled vocabulary filters

Schema

CV column

Op

Values

+

-

Sampling time

to

Reset

Determinant filters

Determinant class

Determinant

Search

Compartment	N	Determinant
atdep	57	57
groundw	362	26
sed	0	0
soil	0	0
stormw	0	0
surfw	324	27
wastew	0	0

Spatial filter summary
Refresh
Close

Severin Ostert, 2026

Developed Content - Management: Compartment comparison



04

Future Development goals

Ongoing refinement & vision

Future Development

From pilot to a lasting transnational governance tool

1

Refinement

Bug fixing, usability,
feature requests

2

Task support

Modelling &
management
workflows

3

Insights

Availability, quality,
statistics, CV mgmt

4

Data exchange

Export & transfer
across databases

VISION

PET as the user-friendly gateway to transnational hazardous-substance data

Thank you for your attention

PET - Pollution Evaluation Tool

Severin Osten

Questions & discussion welcome