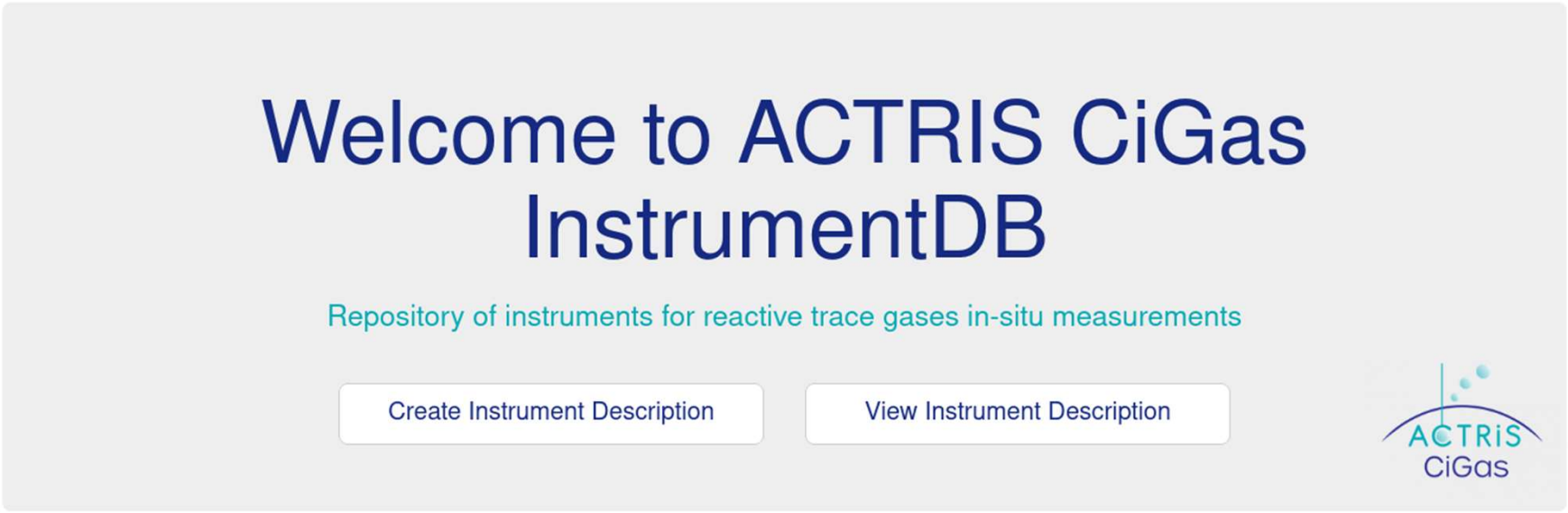
Instrument database - Status, further development

Welcome to ACTRIS CiGas InstrumentDB

Repository of instruments for reactive trace gases in-situ measurements



Roman Romany, Katrin Seemeyer, Ralf Tillmann

Background

- TC responsible for Instrument Meta data base
- Provide FAIR instrument meta data

FAIR meta data (**F**indable: PIDInst (to be implemented) link to Instrument data base; **A**ccessible data via open source DB; **I**nteroperable: Editable by the instrument user, API: Machine readable; Reusable: Usable to all data user

<u>What should the DB do?</u>

- Create header for data submission (optional)
- Create landing page for PIDInst
- Track changes in instrumentation
- Basis for Labelling step 1a

Labelling Workflow

Step 1a: Instrument requirement compliance

- Replaces xls files

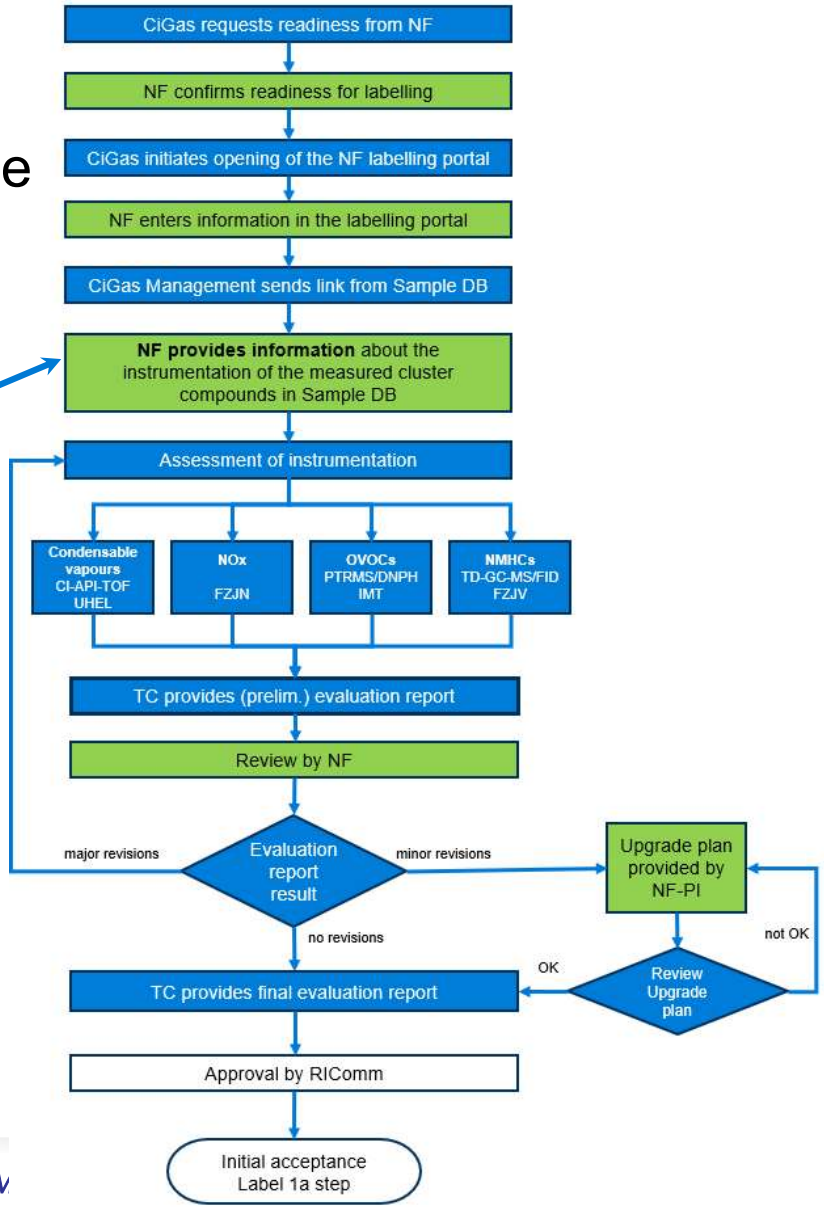
VOC labelling (Online)

CiGas PI for NMHCs:	Ralf Tillmann	r.tillmann@fz-juelich.de	+49 2461
CiGas PI for OVOCs:	Thérèse Salameh	therese.salameh@imt-nord-europe.fr	

Component group specific contact:		
Firstname(s), Lastname(s)	Expertise level	Contact (Email address)
GROS valérie	Scientist	valerie.gros@lsce.ipsl.fr
FOLIOT Lorna	Technician	lorna.foliot@lsce.ipsl.fr
Please fill out	Please select...	Please fill out

Instrument:		
Status:	Operational	
Date of full operation:	January 2020	
Inlet system:		
Measurement height above ground:	9.60 m	
Measurement height above building:	0.85 m	
Distance from NOx inlet:	0.65 m	
Distance from condensables inlet (if applicable):	Please specify [m]	
Distance from ozone inlet:	0.65 m	
Inlet tube material:	Other	PFA
Residence time from the inlet line to entry of sampling device:	3.40 s	
Inlet line heating:	50°C	
Inlet filter:	PTFE	
Inlet filter; mesh size:	0,45 µm	
Sample air flow (select):	Pumping	
Air flow:	8 L/min in sampling line / 0,38 L/min in inlet PTRMS line	
Class of compounds measured (select):	VOC	
Air treatment during sampling (select):		
Water removal:	None	
CO2 removal:	None	
Oxidant removal:	None	
Particle removal:	PTFE	
Other:	Please specify	
Air sampling (select):	Direct feeding to analysis; ion transfer reactions with reagent ion	H3O+
Sampling system manufacturer & model:	Please select...	
Sampling duration:	Please specify [min]	
Sampling volume:	Please specify [L]	

Read me | VOC (online) | VOC (off-line) | NOx | Condensables



Software Architecture

SampleDB

1. PostgreSQL Database for high scaling
2. Templates for creating any kind of Objects
   (e.g. Instrument; calibration data)
3. Version controlled Objects
4. HTTP API with Token System

Gaphical User Interface

1. Python Webserver
2. Template Engine Jinja
3. Individual User and Permission Management

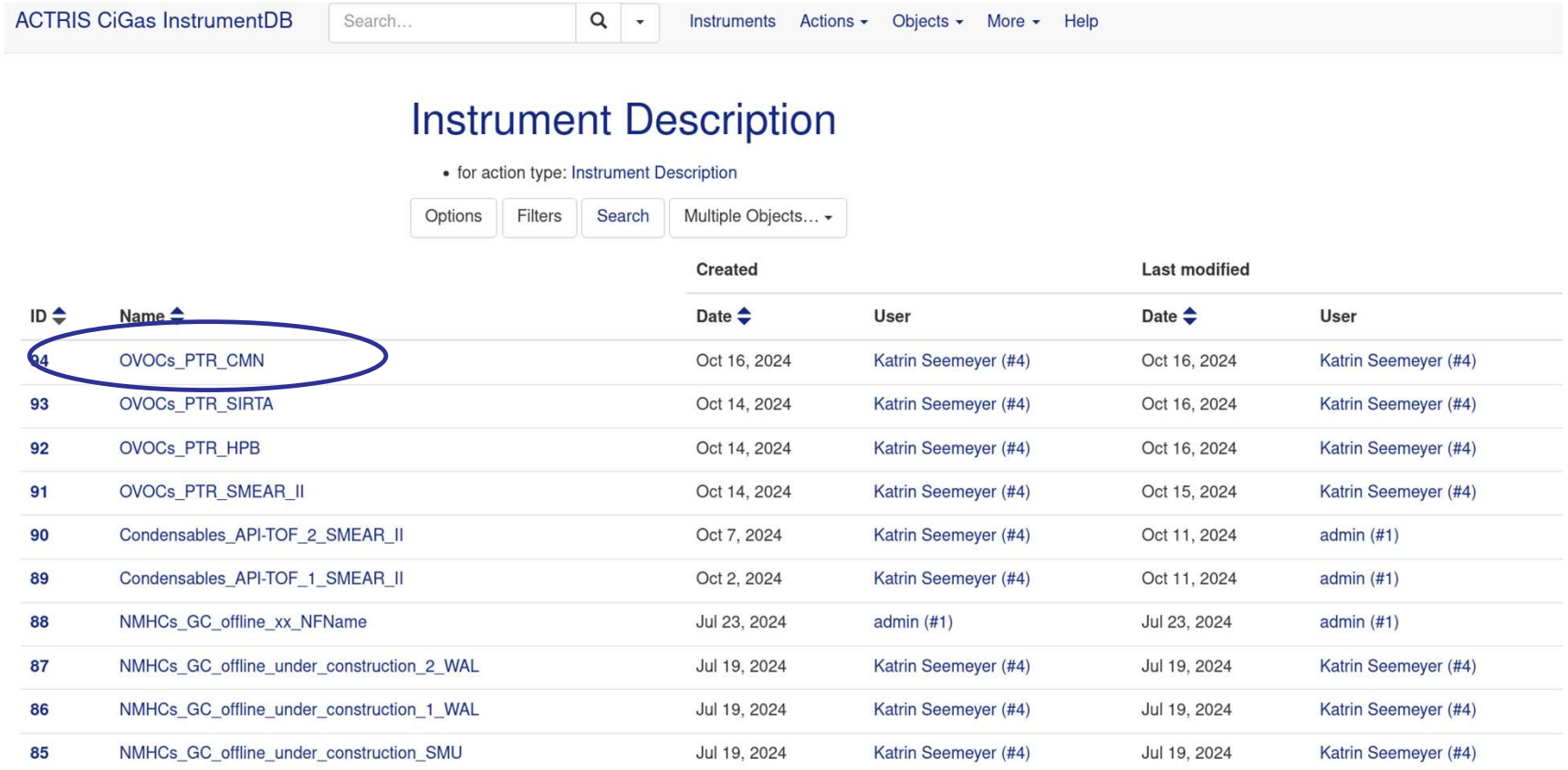
SampleDB Login/Welcome Page

Welcome to ACTRIS CiGas InstrumentDB

Repository of instruments for reactive trace gases in-situ measurements

View Instrument Description

SampleDB Instrument Descriptions



		Created		Last modified	
ID	Name	Date	User	Date	User
94	OVOCs_PTR_CMN	Oct 16, 2024	Katrin Seemeyer (#4)	Oct 16, 2024	Katrin Seemeyer (#4)
93	OVOCs_PTR_SIRTA	Oct 14, 2024	Katrin Seemeyer (#4)	Oct 16, 2024	Katrin Seemeyer (#4)
92	OVOCs_PTR_HPB	Oct 14, 2024	Katrin Seemeyer (#4)	Oct 16, 2024	Katrin Seemeyer (#4)
91	OVOCs_PTR_SMEAR_II	Oct 14, 2024	Katrin Seemeyer (#4)	Oct 15, 2024	Katrin Seemeyer (#4)
90	Condensables_API-TOF_2_SMEAR_II	Oct 7, 2024	Katrin Seemeyer (#4)	Oct 11, 2024	admin (#1)
89	Condensables_API-TOF_1_SMEAR_II	Oct 2, 2024	Katrin Seemeyer (#4)	Oct 11, 2024	admin (#1)
88	NMHCs_GC_offline_xx_NFName	Jul 23, 2024	admin (#1)	Jul 23, 2024	admin (#1)
87	NMHCs_GC_offline_under_construction_2_WAL	Jul 19, 2024	Katrin Seemeyer (#4)	Jul 19, 2024	Katrin Seemeyer (#4)
86	NMHCs_GC_offline_under_construction_1_WAL	Jul 19, 2024	Katrin Seemeyer (#4)	Jul 19, 2024	Katrin Seemeyer (#4)
85	NMHCs_GC_offline_under_construction_SMU	Jul 19, 2024	Katrin Seemeyer (#4)	Jul 19, 2024	Katrin Seemeyer (#4)

View

OVOCs_PTR_CMN

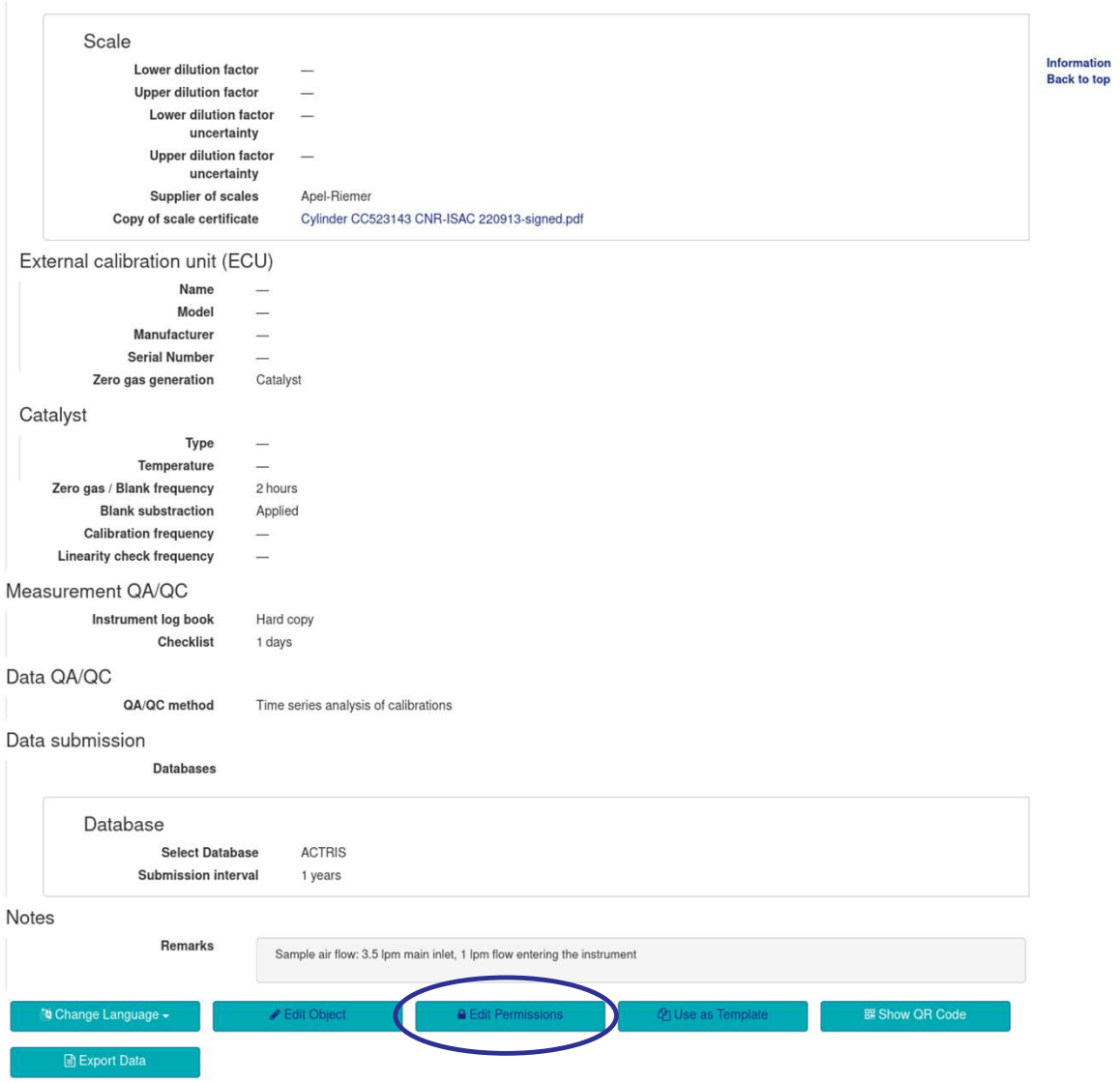
PTRMS instrument description

Instrument name	OVOCs_PTR_CMN
Facility name	CMN-PV (#42)
PID	—
Operator	—
Status	planned
Date of full operation	Jan 1, 2025

Inlet System

Measurement height above ground	2 m
Measurement height above building	7 m
Distance from NOx inlet	0 m
Distance from condensables inlet	—
Distance from ozone inlet	0 m
Distance from GC inlet	—
Inlet tube material	Other
Other tube material	composed inlet: 1 m of Pyrex (main inlet for all the instruments) then PFA tube
Residence time	6 s
Inlet line heating?	✔
Inlet line heating temperature	20 °C
Filter material	None
Oxidant removal	None
Sample flow	—

View



Scale

Lower dilution factor	—
Upper dilution factor	—
Lower dilution factor uncertainty	—
Upper dilution factor uncertainty	—
Supplier of scales	Apel-Riemer
Copy of scale certificate	Cylinder CC523143 CNR-ISAC 220913-signed.pdf

Information
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External calibration unit (ECU)

Name	—
Model	—
Manufacturer	—
Serial Number	—
Zero gas generation	Catalyst

Catalyst

Type	—
Temperature	—
Zero gas / Blank frequency	2 hours
Blank substraction	Applied
Calibration frequency	—
Linearity check frequency	—

Measurement QA/QC

Instrument log book	Hard copy
Checklist	1 days

Data QA/QC

QA/QC method	Time series analysis of calibrations

Data submission

Databases

Database

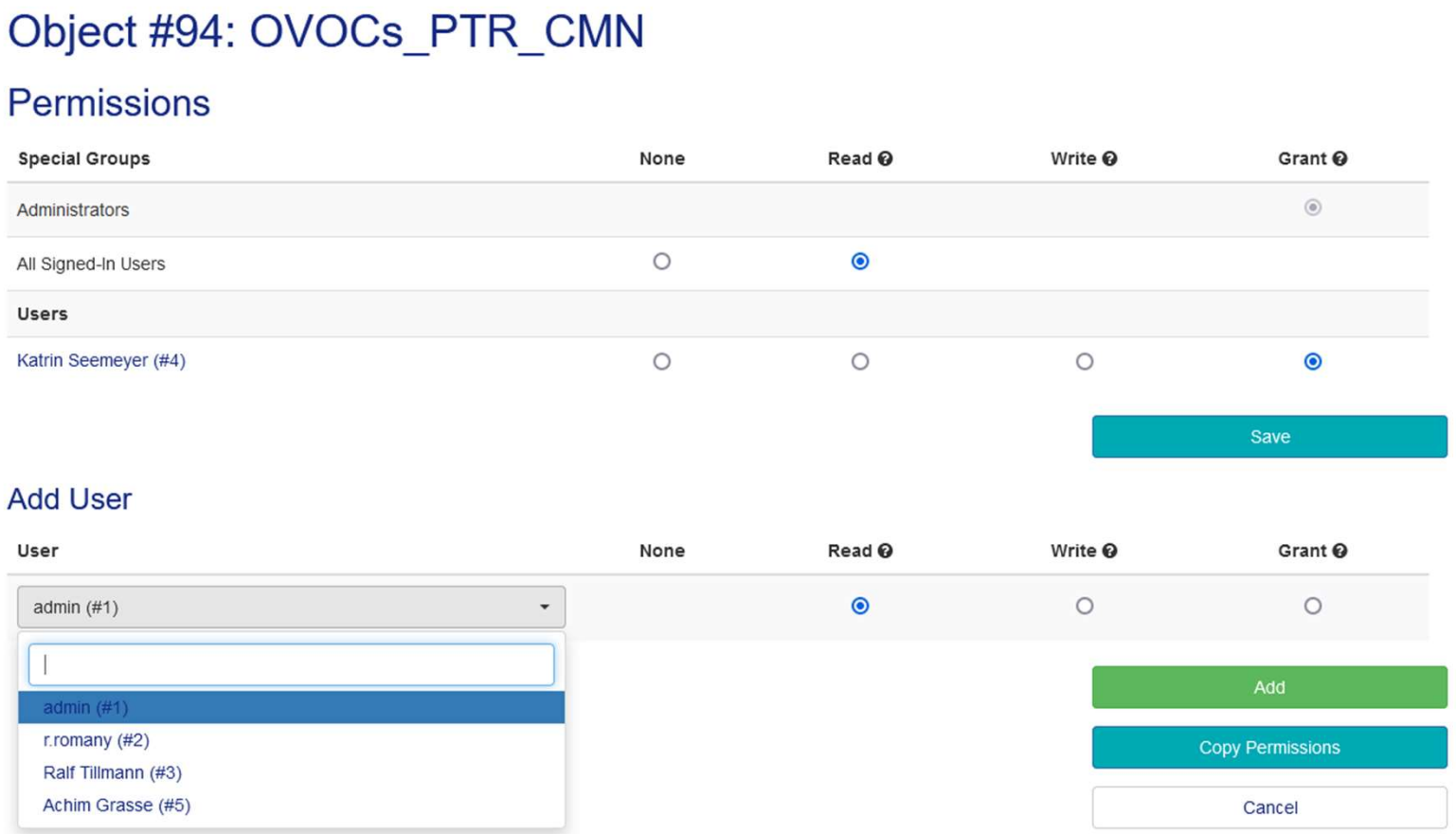
Select Database	ACTRIS
Submission interval	1 years

Notes

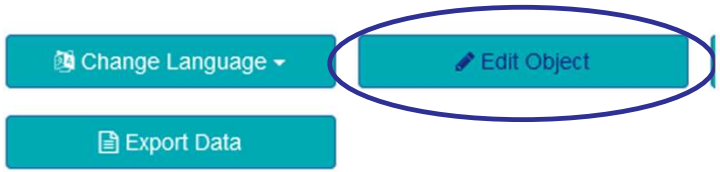
Remarks: Sample air flow: 3.5 lpm main inlet, 1 lpm flow entering the instrument

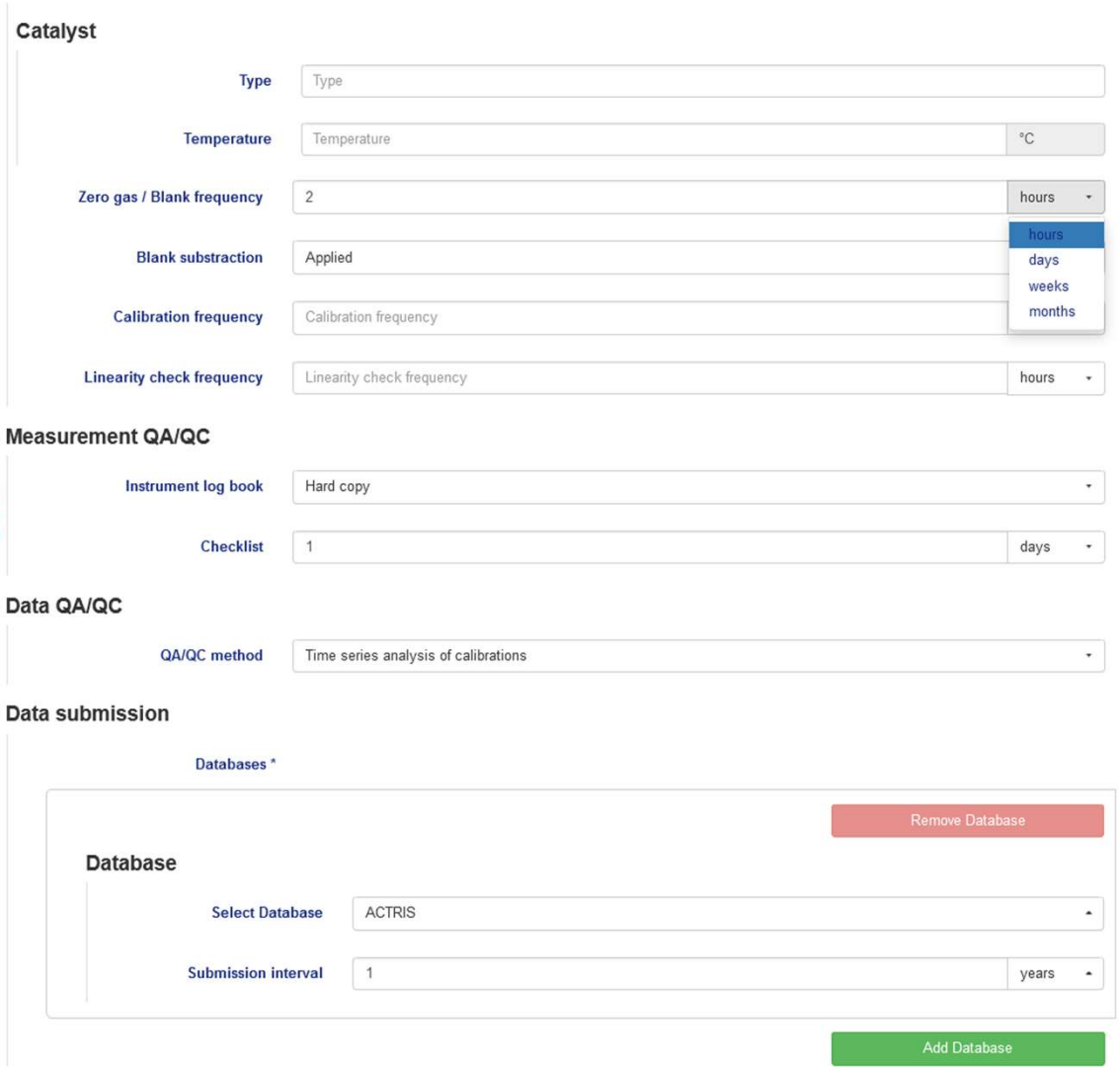
Change Language | Edit Object | Edit Permissions | Use as Template | Show QR Code | Export Data

Permission Management

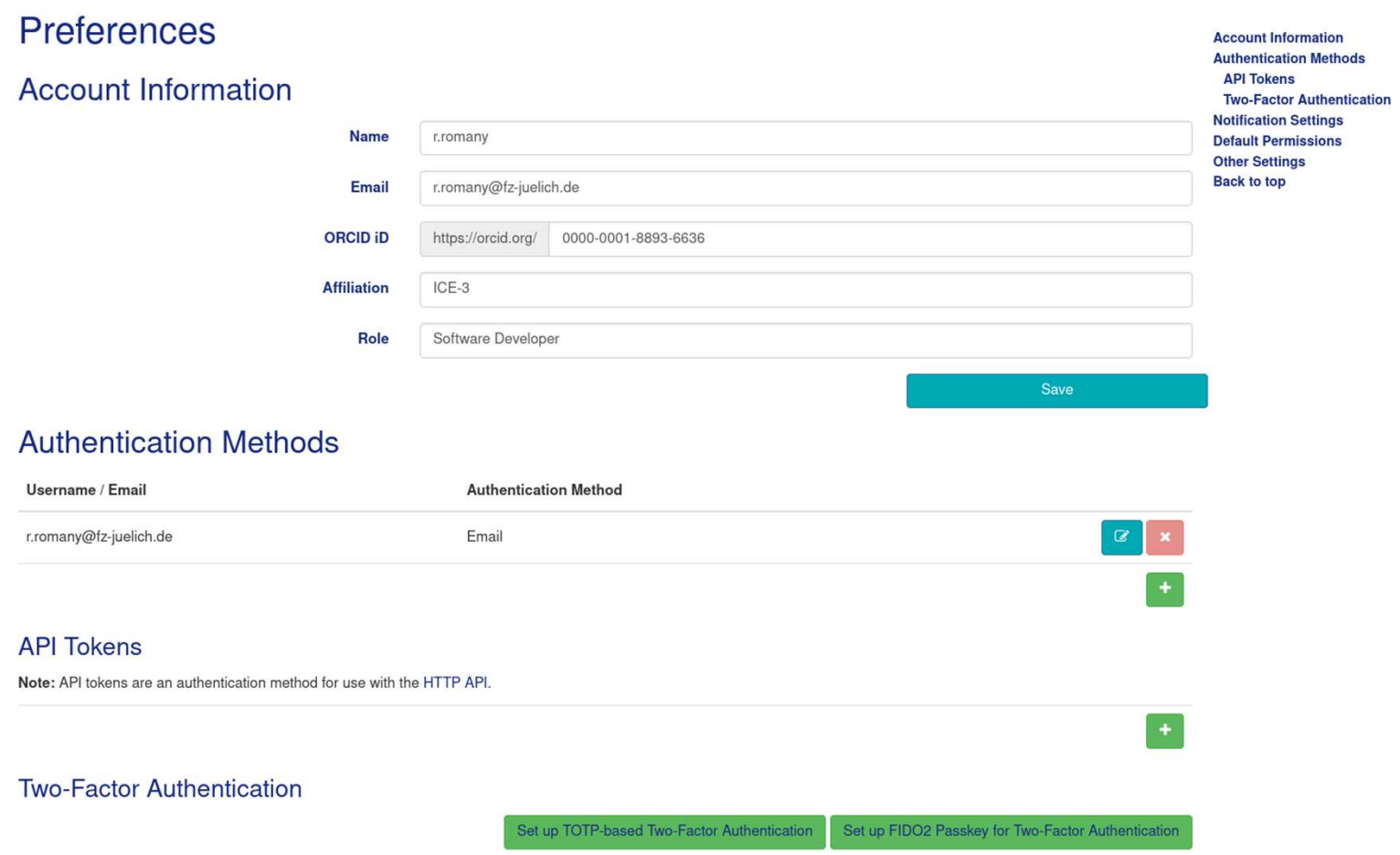


Edit Description





USER Management



Summary SampleDB 

- Traceable metadata
- Machine Readable
- Data units selectable by the user
- Can save almost every file format, including: PDF, PNG
- Login via different Authentication Methods (YubiKey)
- Bot/Token System for Automations
- Export and Import System for Electronic Lab Notebooks (.eln)
- Federation with other SampleDBs (e.g. Simulation Chamber LogBook)
- Comprehensive Documentation (Link)

Outlook

- Implementation of PIDInst → Instrument DB will be the landing page
- Migration to a public server
- Meta data downloadable by ACTRIS data users without registration
- Instrument PI can extend editing rights
- Instrument data management fully in the hand of the NFs
- Already provided Instrument meta data will be transferred by CiGas

<u>Potential features in future:</u>

Incooperation of calibration data

→ Automatic calculation of sensitivities

→ Sensitivity history plot (QC approach)

Landing page with scripts for API Automations

Log book option

CiGas data coverage requirements

Labelling step 1b requirement:

- Observational platforms have to provide at least a **75% data coverage** over a period of 2 years.
- The data have to cover all 4 seasons.

CiGas gas standard requirements

Labelling step 1a requirement:

NFs have to purchase/use laboratory standards

Compound cluster	Amount fraction	Central Calibration Lab (NMI)	Stability
NMHC: 30 component ozone precursor mixture in nitrogen	4 nmol/mol	National Physical Laboratory*)	5 years
Biogenic NMHC	5 nmol/mol	NIST	
NO (NO2 via GPT)	10 µmol/mol	National Physical Laboratory*)	2 years
OVOC: 20 component mixture for PTR-MS calibration	1 µmol/mol	National Physical Laboratory	1 year

*) Coordinated purchase leads to discount