Data Review Stations 2024

ACTRIS CiGas QA/QC workshop

07.04.2024

Stefan Reimann, Livia Schneider, Pascal Rubli, Zoé Le Bras

Agenda

- Overview of the data submission for 2024

- General feedback from the external QC conducted by Empa for 2024 data (highlights and/or lessons learned)

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Data review for each station (20 min / station) :

- Brief station presentation by station operators (~ 5 min)

- Feedback from the data reviewer with selected examples

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- Further improvment of the external QC/outlook

Station order for this morning's data review
Beromünster
Jungfraujoch
Auchencorth
Chibolton
Pallas
Monte Cimone
Cape Verde
Kosetice
Hohenpeissenberg FID
Hohenpeissenberg TOF
Puy de Dôme
Sirta
Zeppelin
Hyytiala

Overview data review station

Station	In EBAS	External QC feedback sent	Comment
Beromünster	yes	yes	
Jungfraujoch	yes	yes	
Auchencorth Moss	yes	yes	
Chibolton	yes	yes	
Pallas	yes	yes	
Monte Cimone	yes	yes	
Cape Verde	yes	yes	
Kosetice	yes	yes	
Hohenpeissenberg	yes	yes	April-July and Dec data will be sent by 31.05.25
Puy de Dôme	yes	Yes	Only sorbent tube, no online GC-data
SIRTA (Gif-sur-Yvette)	yes	yes	
Zeppelin	yes	yes	
Hyytiälä	no	-	

Next steps:

1. Data providers sends feedback in the NILU Tracker for the external QC conducted with updated .nas file when required (if samples are modified, flags added)

2. Feedback from external QC

3. External QC approved (if not, repeat 1. and 2.)

Feedback from the external QC (Empa)

- Overall, data sent to EBAS are already in a good shape

- It seems that the local event flag has been used with caution

- Flags "check data" (2.000) exported from @VOC@ tool after the external QC and added to NILU Tracker (more tomorrow with Ralf and Peeyush's discussion at the CiGas community meeting) – is this helpful for the data provider?

Keep in mind:

- Consistent data submission year to year (same unit for concentration, name conventions, ...)

- Mention of new compounds in the NILU Tracker to include them in the external QC process

- After calibration/downtime of instrument, don't forget to flag the data generously (carryover)

Ethyne concentration
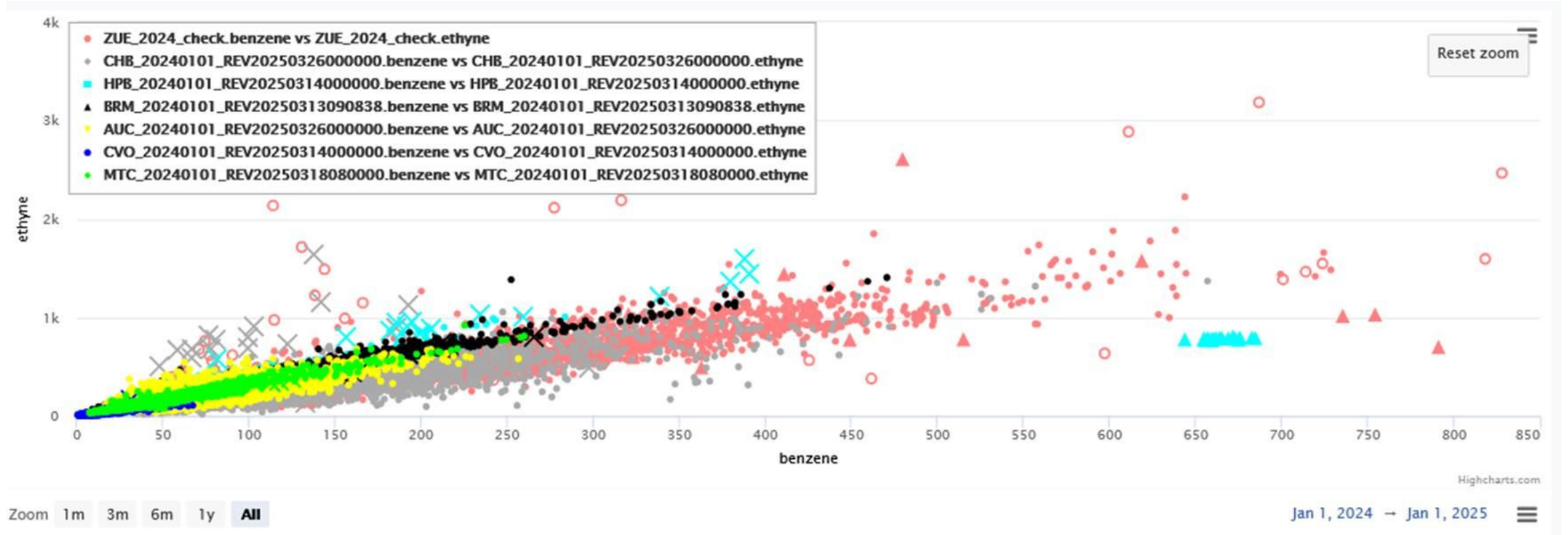
AUC, CHB: ethyne calibrated with NPL-Std, carbon response factor of ethyne affected in the calibration cylinder but not in ambient air; exclude ethyne calibration if carbon response off and older calibration used

ZUE, BRM: ethyne calibrated with NPL-Std. In the past, corrected according to the response factor of the other VOCs in the NPL-Std, now ethyne integration adapted

HBP: issues to measure ethyne from NPL-Std, use of average carbon response for alkane for ethyne calibration

→ Issues with ethyne observed this year at Cape Verde

Beromünster

Station presentation by Operator: Stefan Reimann
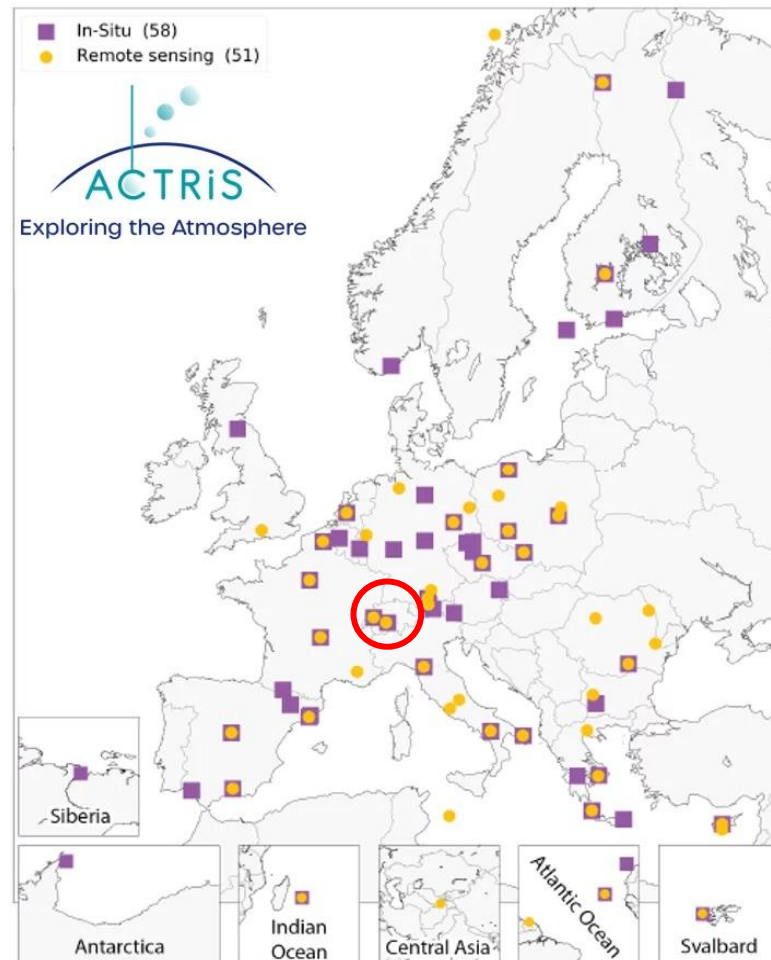
General/Flags:

Feedback QC

Example plots for probably wrong set flags OR issue with the QA tool?
Since the y axis always is fixed it is almost impossible to check the time series like in this case.
Use of 9999.999 and 99999.999 as missing flag - > suggest to use only 99999.999
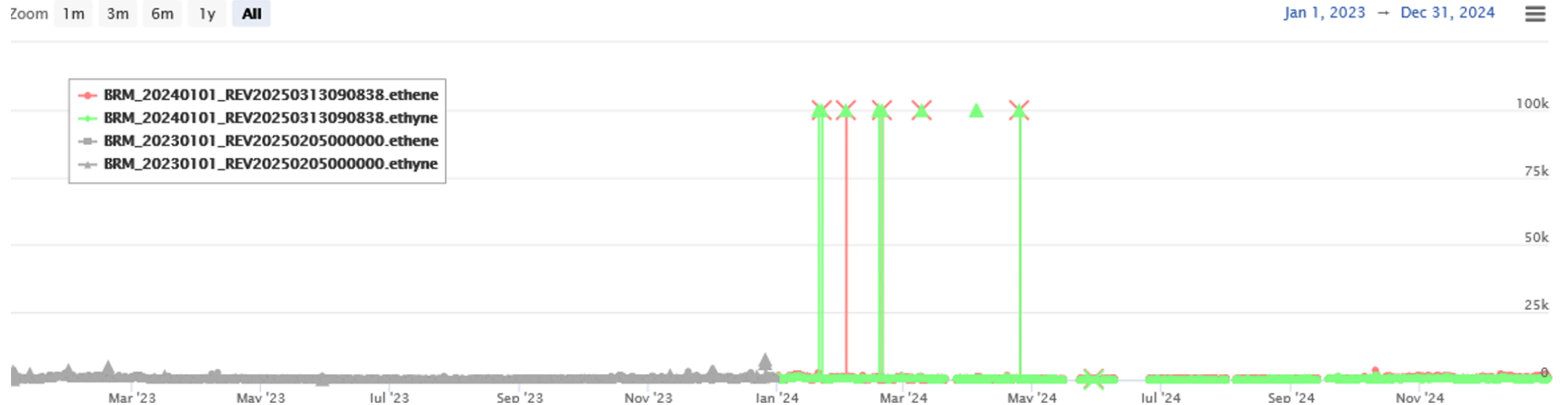
m-p-xylene

Feedback QC

Are you sure that p+m-xylene was not integrated with split peak? For the flagged data points, the ratio between o-xylene and p+m xylene is ~1 while the "regularly" observed ratio is >=2? Data shows 'jumping' concentrations.

Beromünster

Alcohols:

Negative trend? Lower values observed in 2024.
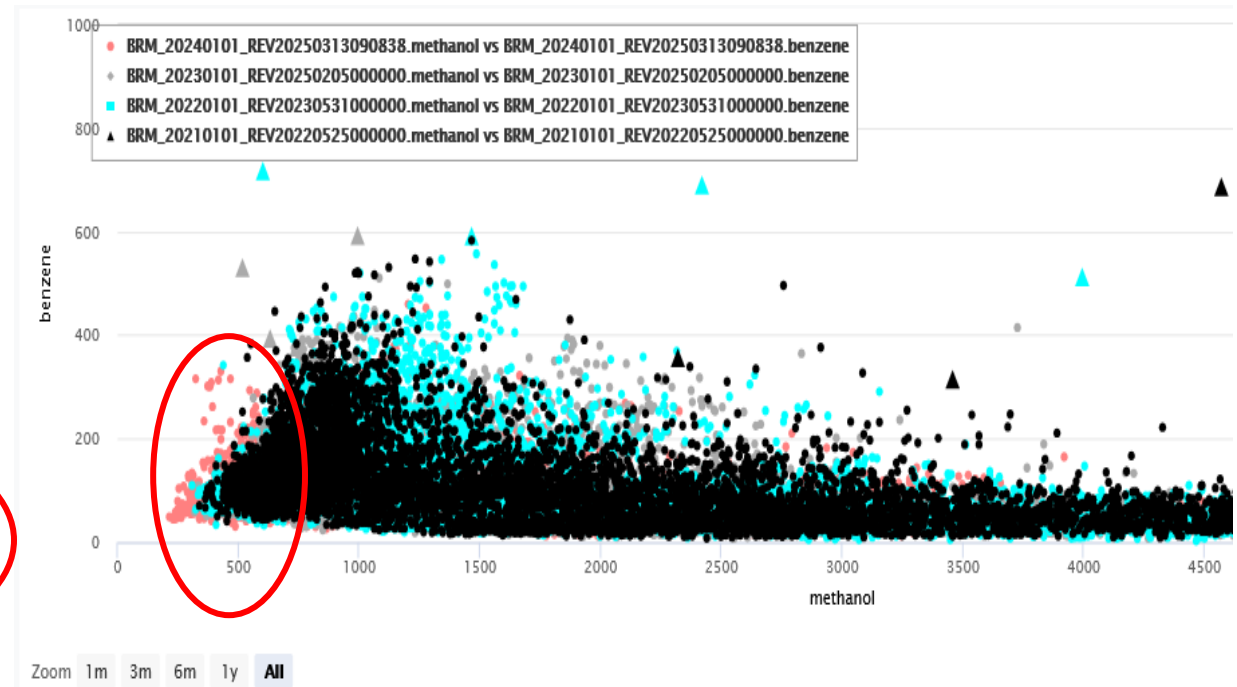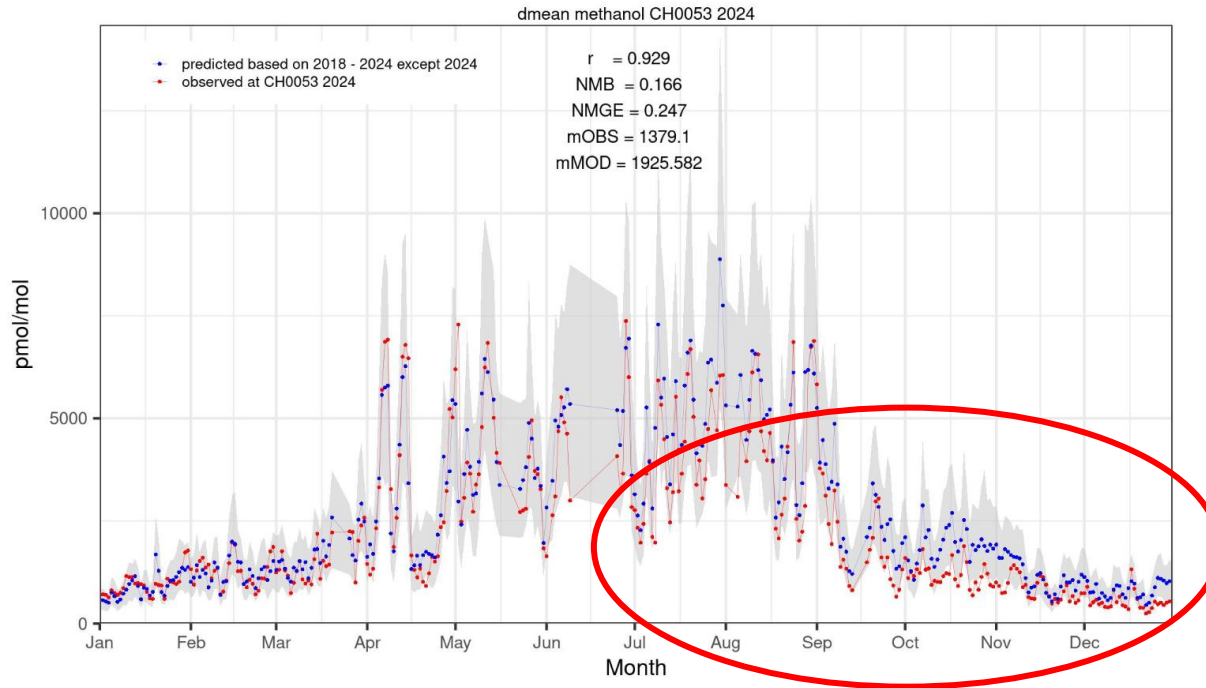
Ethane/Propane:

Feedback QC

Interesting feature: Ethane vs propane for and respective time series for BRM, JFJ and HPB. After October~ 21st the time series start to show more deviations.
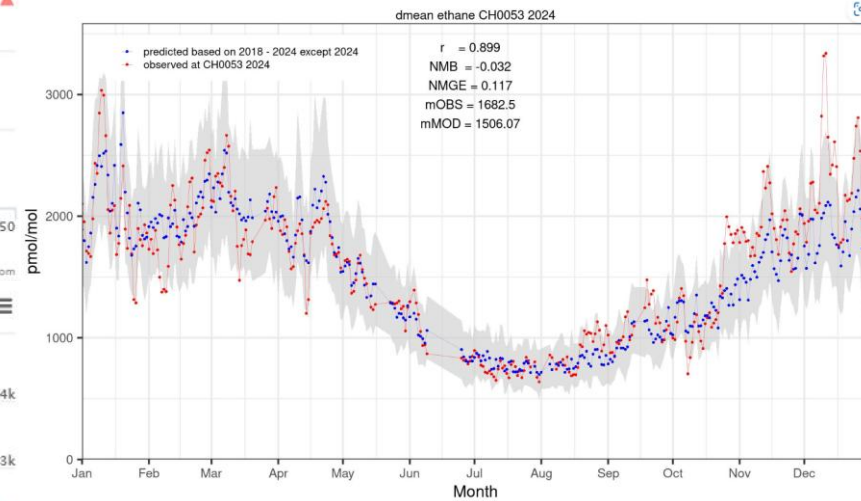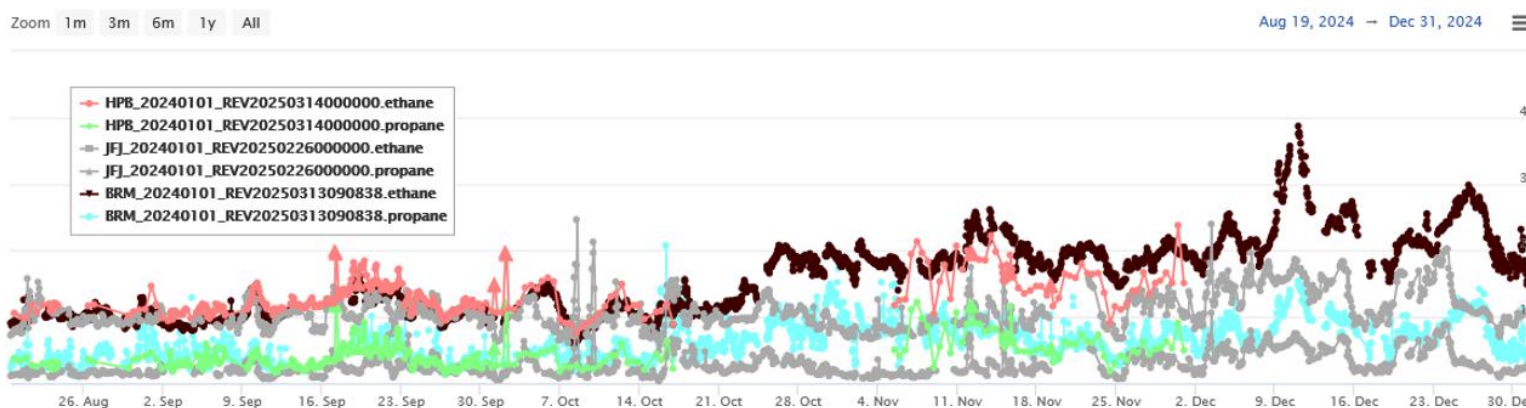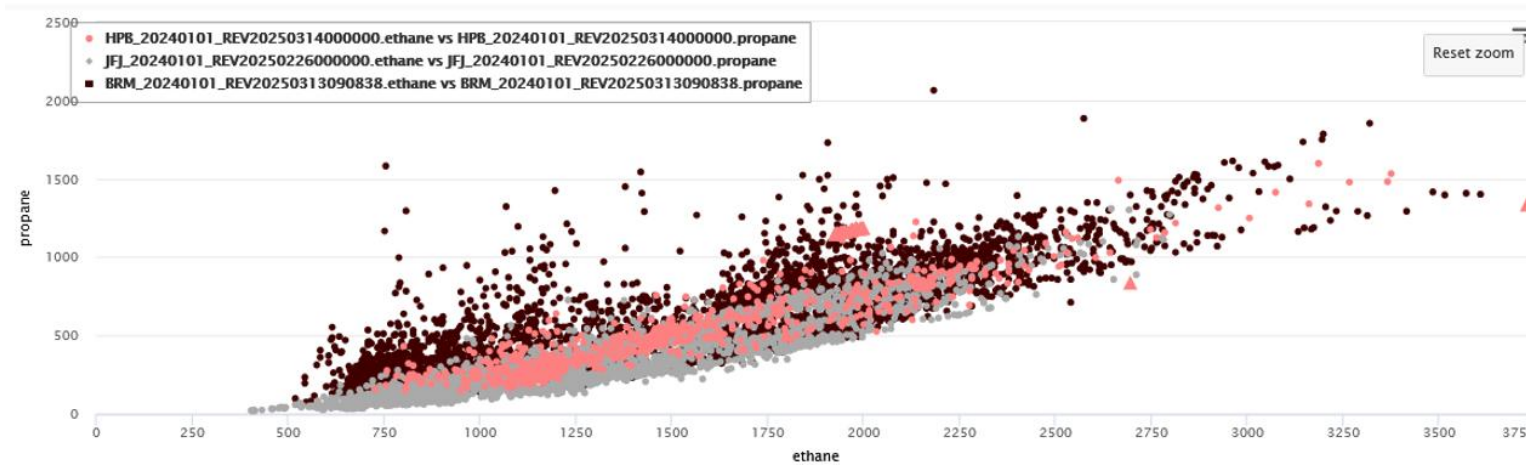
Jungfraujoch

Station presentation by Operator: Stefan Reimann
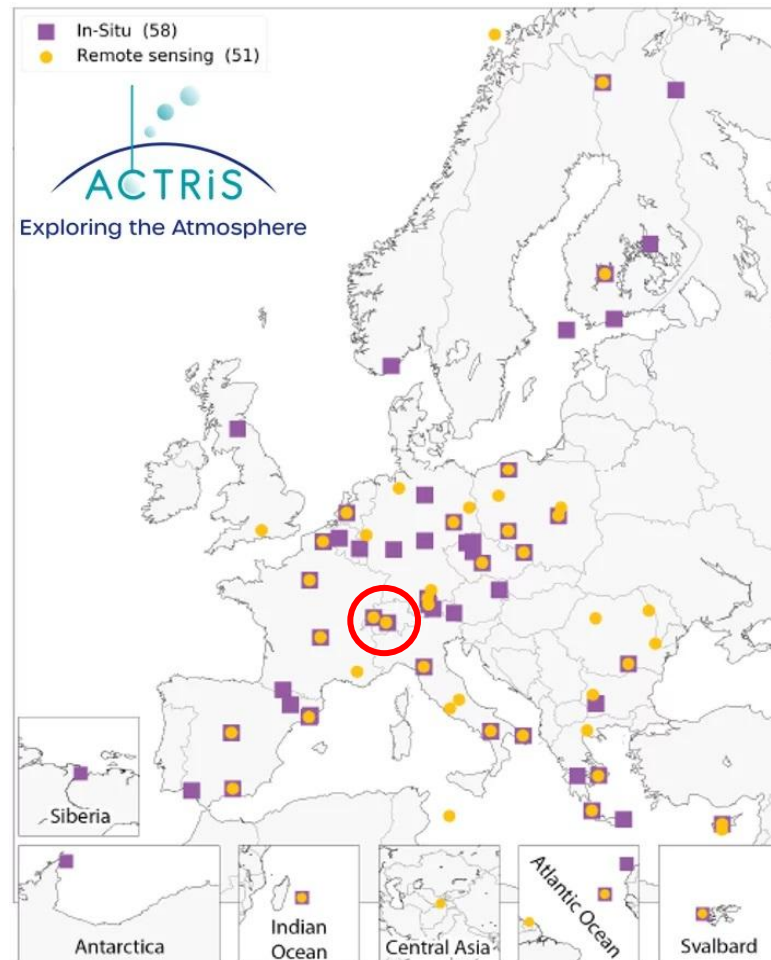
Jungfraujoch

n-butane (n-butane vs ethane correlation plot)

Feedback QC

Strong scatter of data observed in 2024 in comparison to 2023 and 2022 in the n-butane vs ethane correlation plot. Most events occur in the "summer" season between May until October. Also observed in the correlation of n-butane vs propane

Feedback from the station (06.04.2025)

There are indeed high local laboratory values for n-butane at Jungfraujoch, frequently reaching values of a few thousand ppt, with maximum at about 60'000 ppt. This may have resulted in some contamination of the ambient air sample analysis. As a consequence, the suspicious data points were removed.

JFJ 2022
JFJ 2023
JFJ 2024

In the time series analysis, difference is more pronounced in May for n-butane.

n-butane (n-butane vs propane correlation plot)

Feedback QC

In the correlation of n-butane vs propane the same flagged data also show the strong scatter.
Furthermore, some more n-butane data points stick out versus propane (red filled circles below). This is linked to 3 events in Feb, May and Nov.
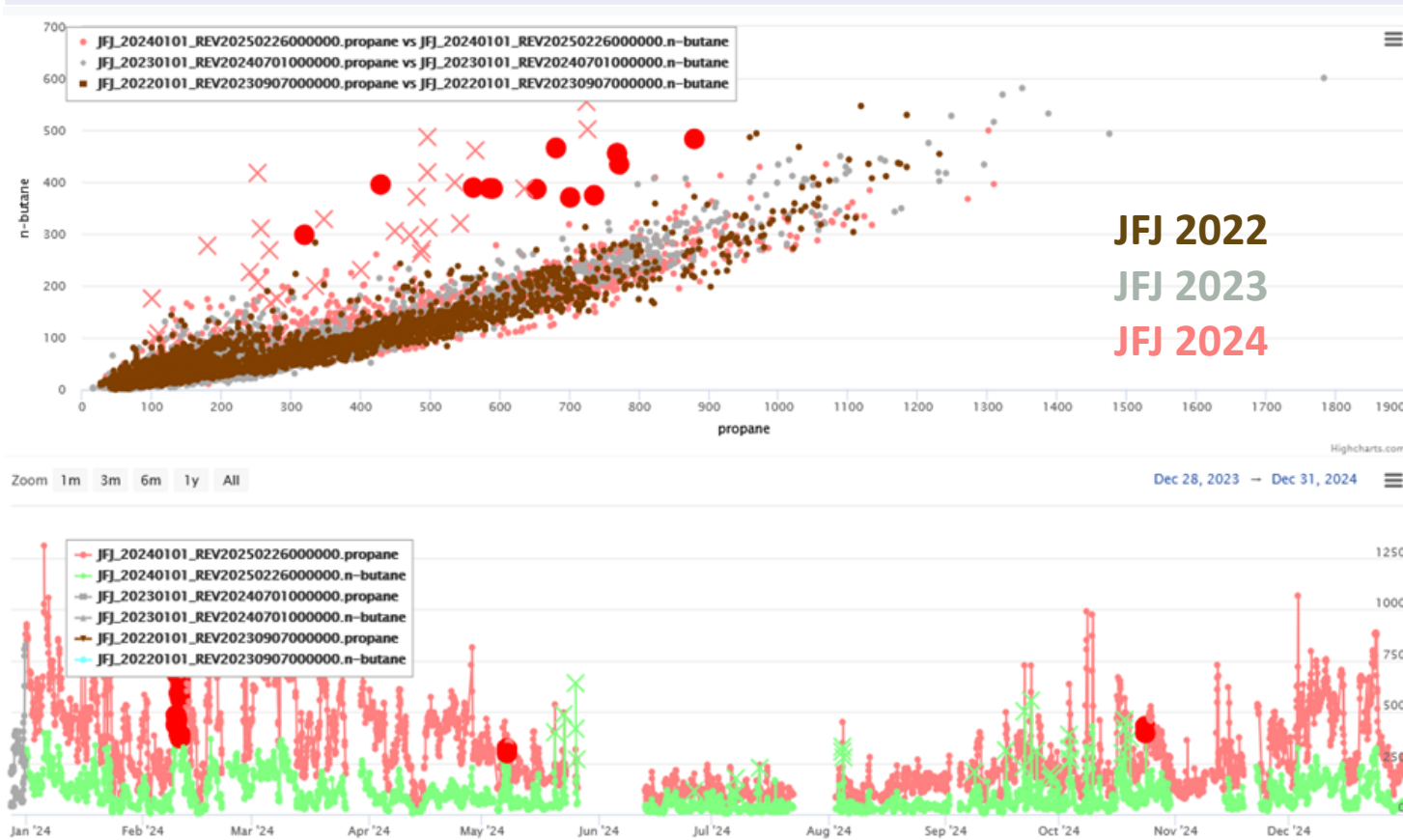
2-methylpropane

- n-butane / 2-methylpropane correlation shows larger scatter compared to 2023
- 2-methylpropane elevated versus 2-methylbutane – this seems to be the case during the same events when n-butane was elevated. Similar samples were not observed during the previous years.

Feedback from the station (06.04.2025)

- 2-methylpropane is often also elevated in the Jungfraujoch laboratory air, however, not as strongly as n-butane. Nevertheless, suspicious 2-methylpropane measurements were now also removed from the 2024 record.
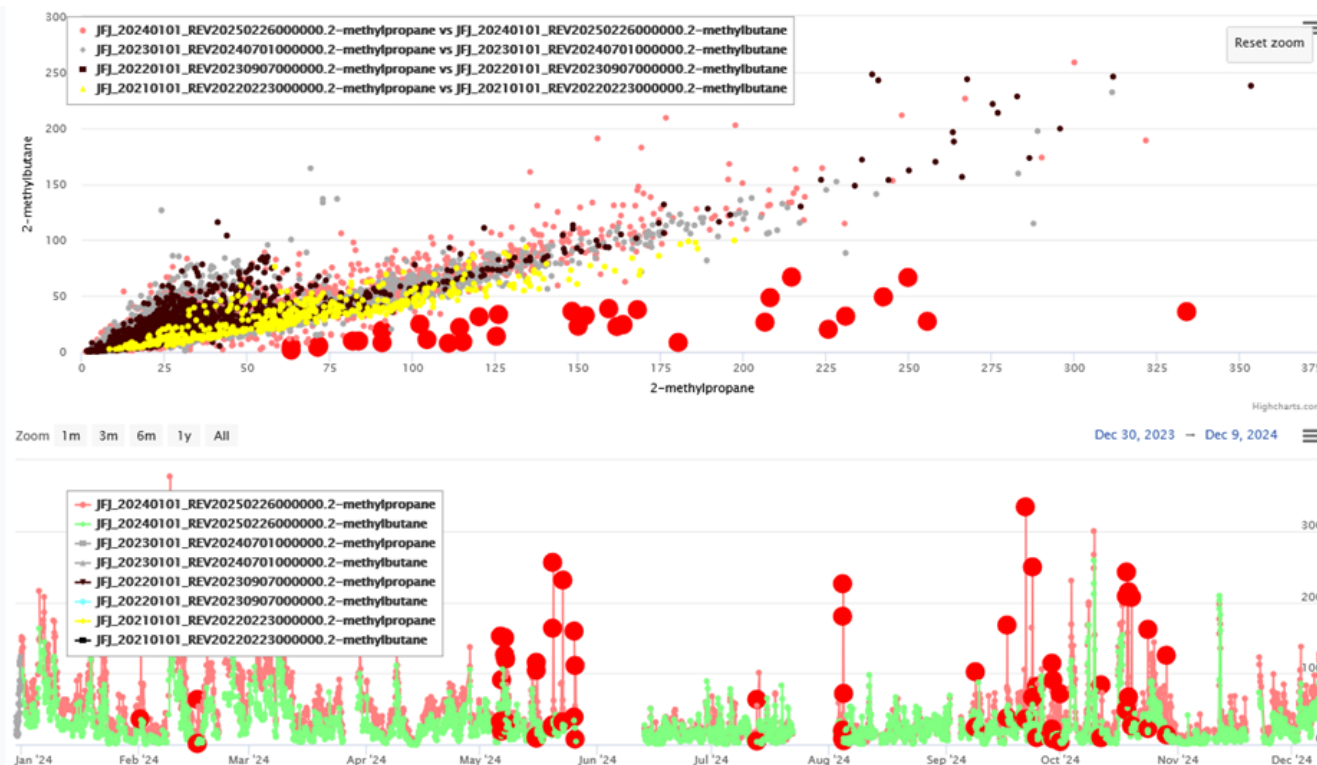
JFJ 2021
JFJ 2022
JFJ 2023
JFJ 2024

Change in the station setting/activity in the summer (new local source?), that may have led to the larger variability and scatter in the correlation specifically for n-butane (and i-butane)?

Propane

Feedback QC from Sverre

- A comparison of the 2024 data vs the previous 5 years is given in the box plots. Seems to be well in line with previous levels except perhaps slightly higher levels of propane in 2024.
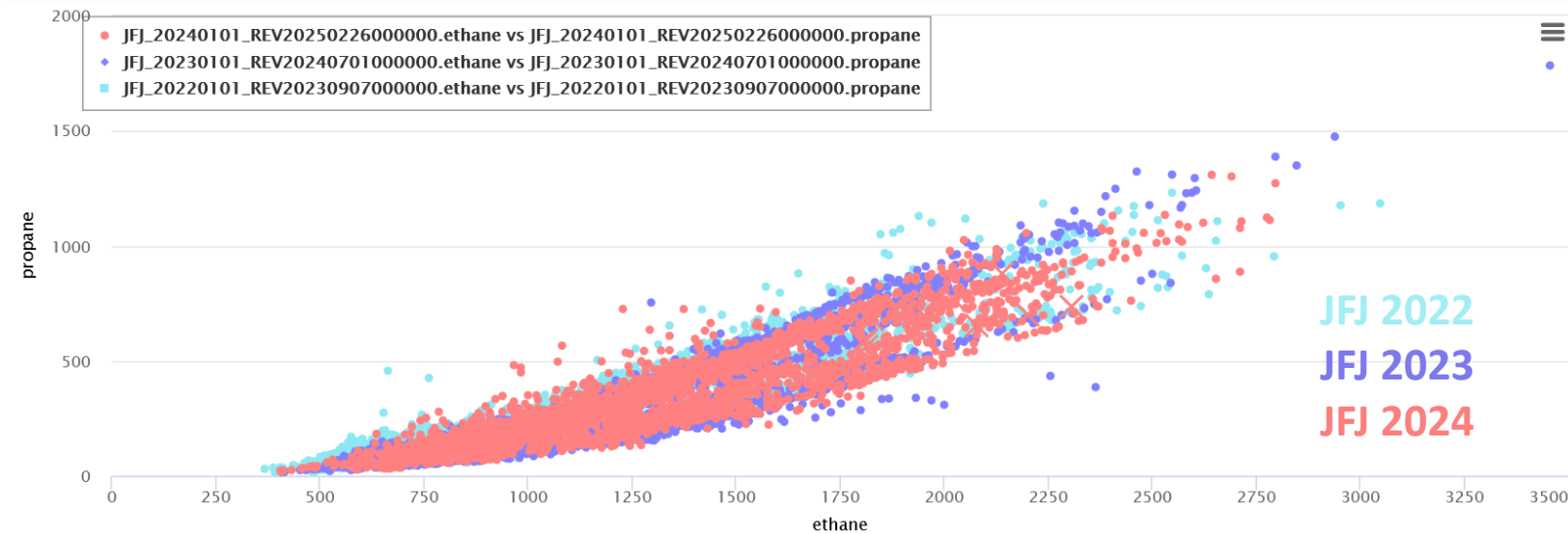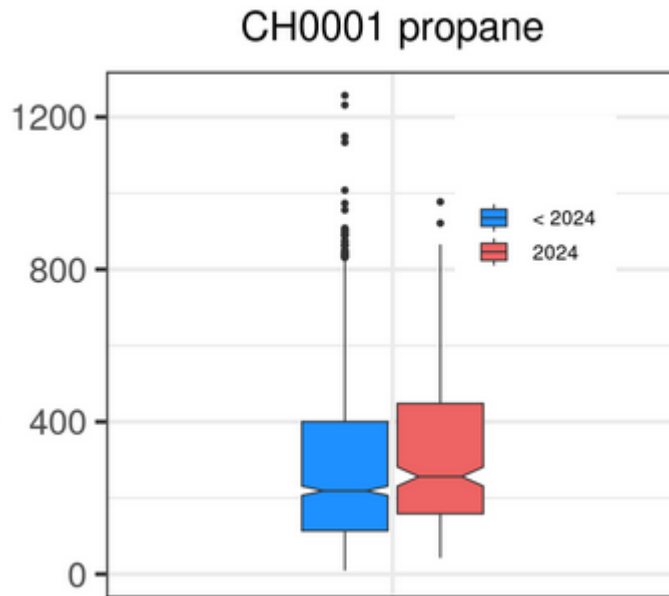
In @VOC@, the slight increase in the propane median concentration in 2024 is not obvious.

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Auchencorth Moss

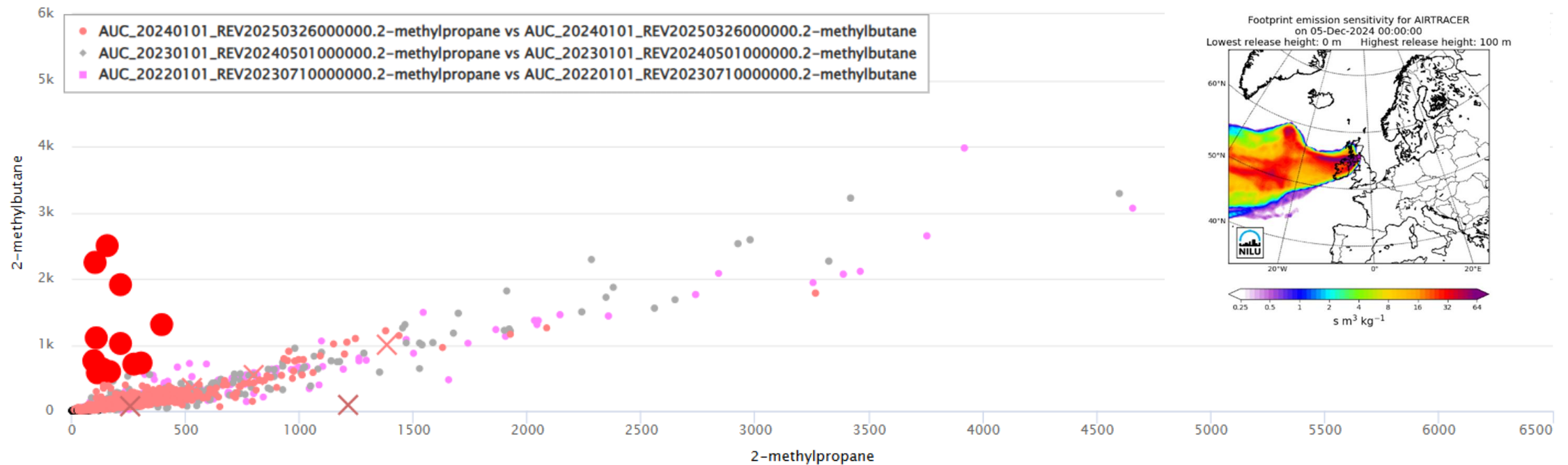Station presentation by Operator: James Dernie
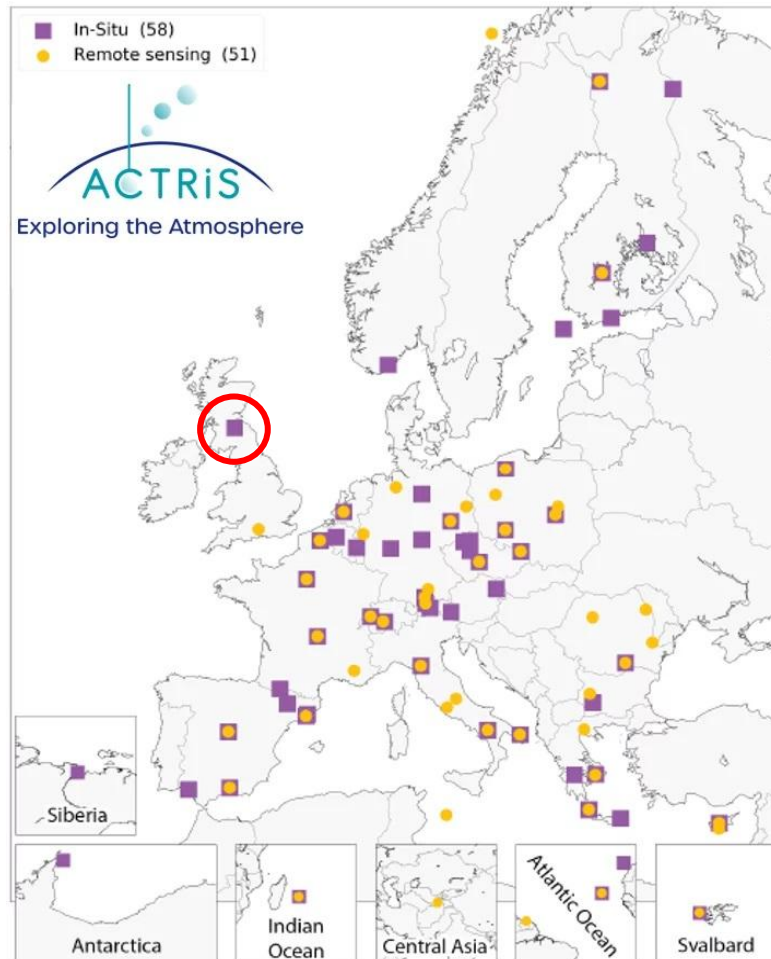
Auchencorth Moss

2-methylpropane / 2-methylbutane

Feedback QC

Elevated concentrations of 2-methylbutane, out of the correlation between substances. Is it real/local event? According to the footprint, the air mass comes from the west.

2-methylbutane / n-pentane

Feedback QC

2-methylbutane event without elevated concentrations of n-pentane. Maybe linked to a local event?
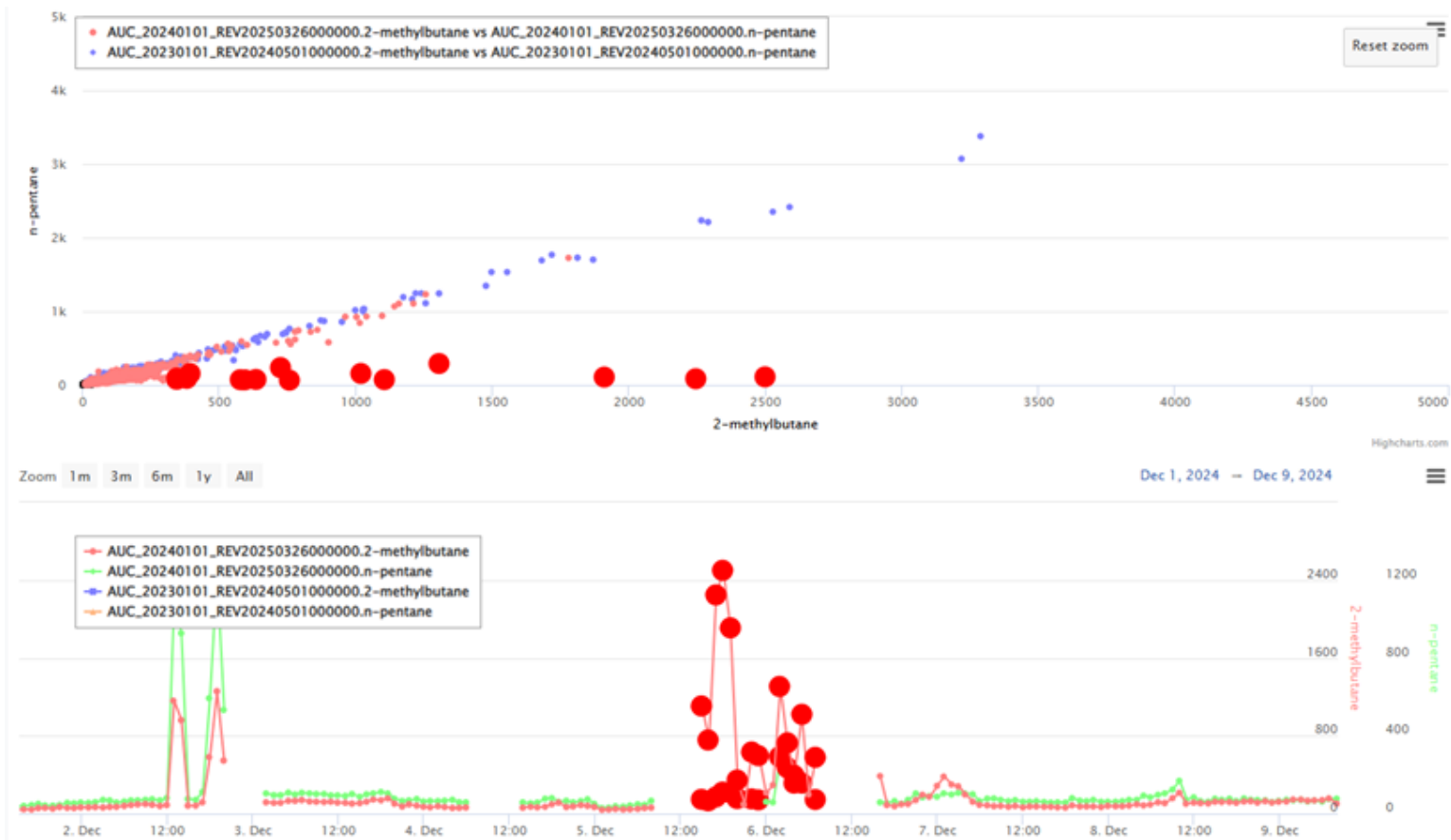
benzene / ethyne

Feedback QC

The lowest concentrations measured in 2024 are higher than those measured in 2023. Is it linked to a change in the detection limit/higher background in the system in 2024?
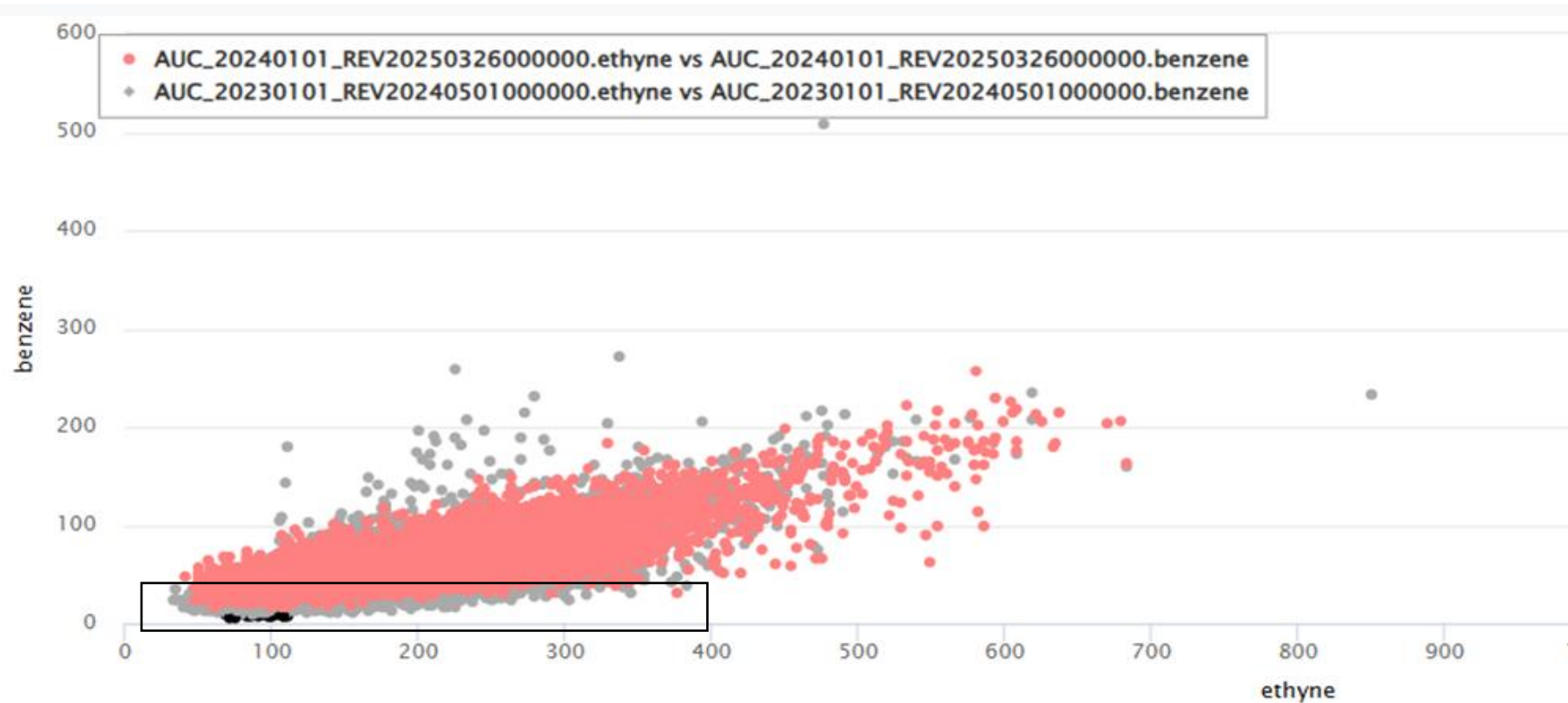
Chilbolton

Station presentation by Operator: James Dernie
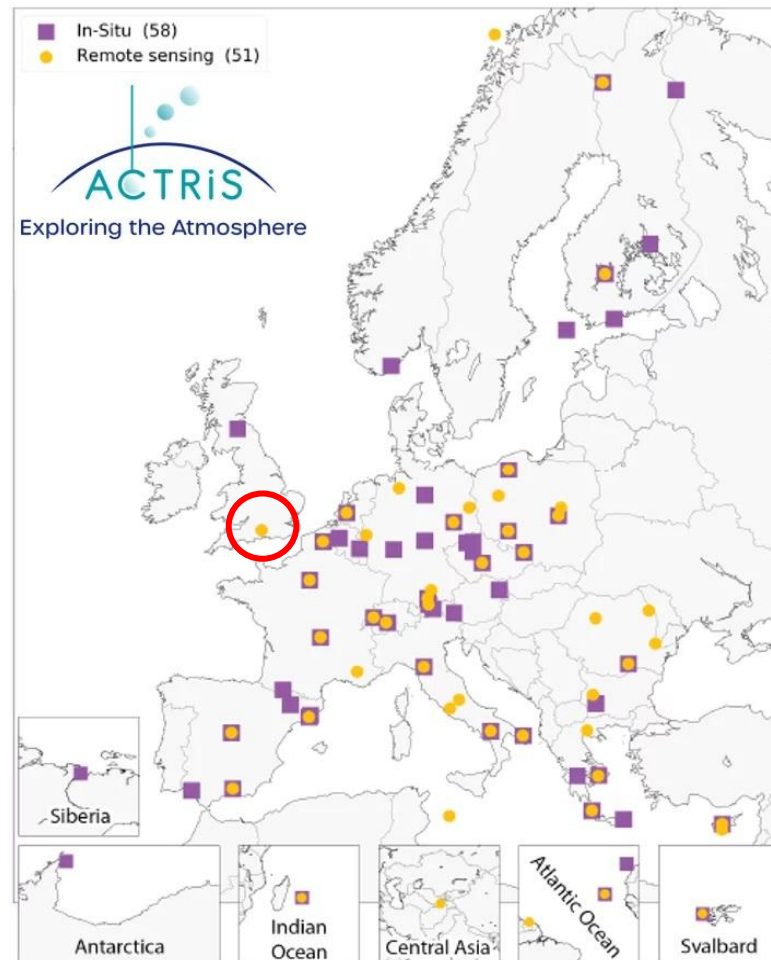
Ethane / n-butane

Feedback QC
Suspicious spikes which seem to be artifacts and also out of correlation between substances. Real or maybe local events?

Generally a good, clean dataset. Here and there a few suspicious spikes for some substances.
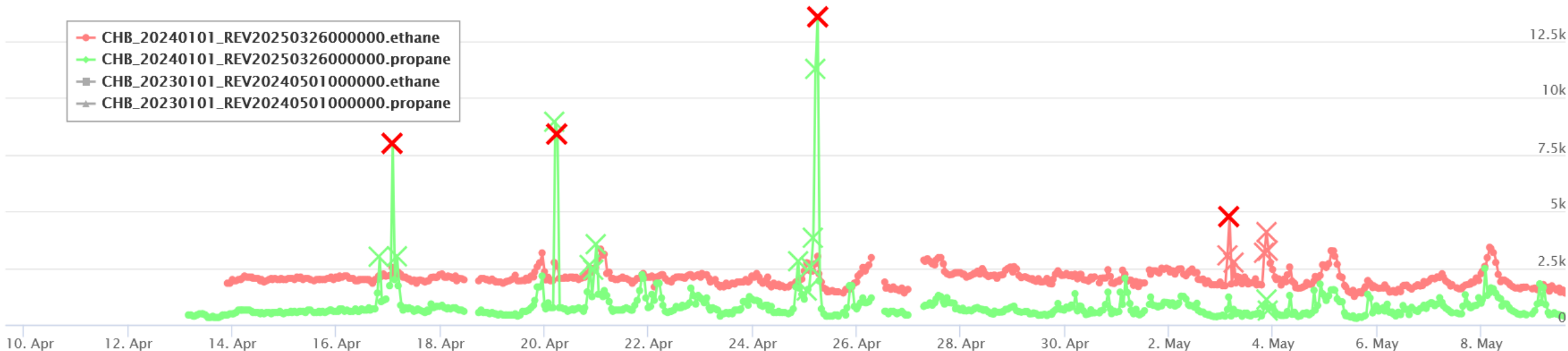
Pallas

Station presentation by Operator: Heidi Hellén
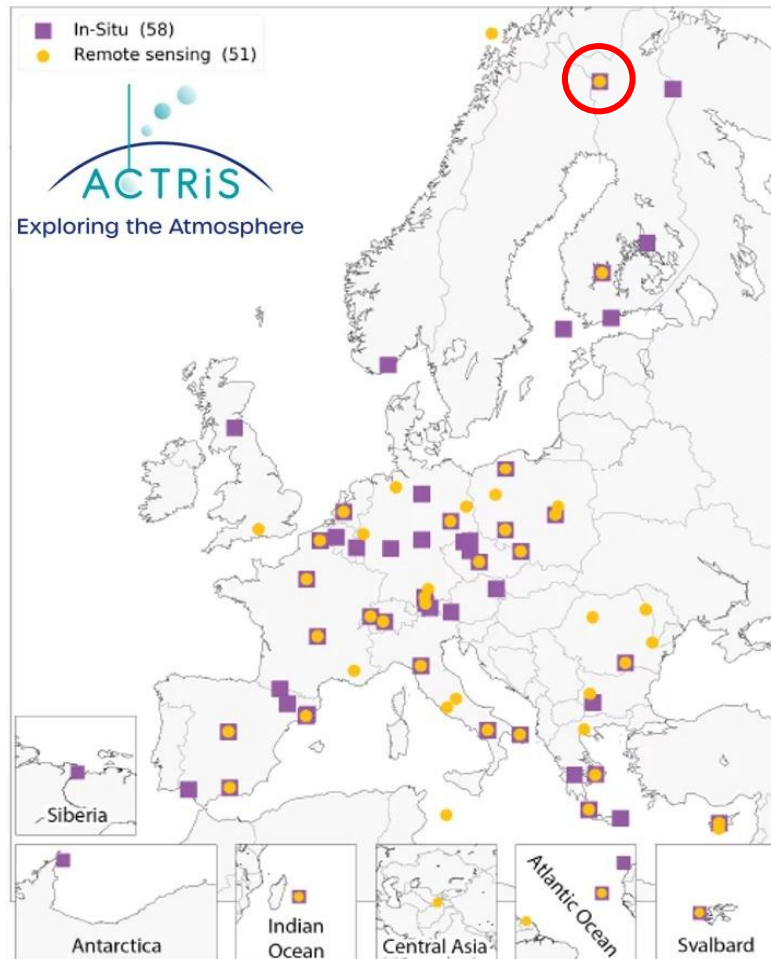
Pallas

Ethane

Sudden low concentration observed in the time series for ethane. Please recheck if the peaks are well integrated
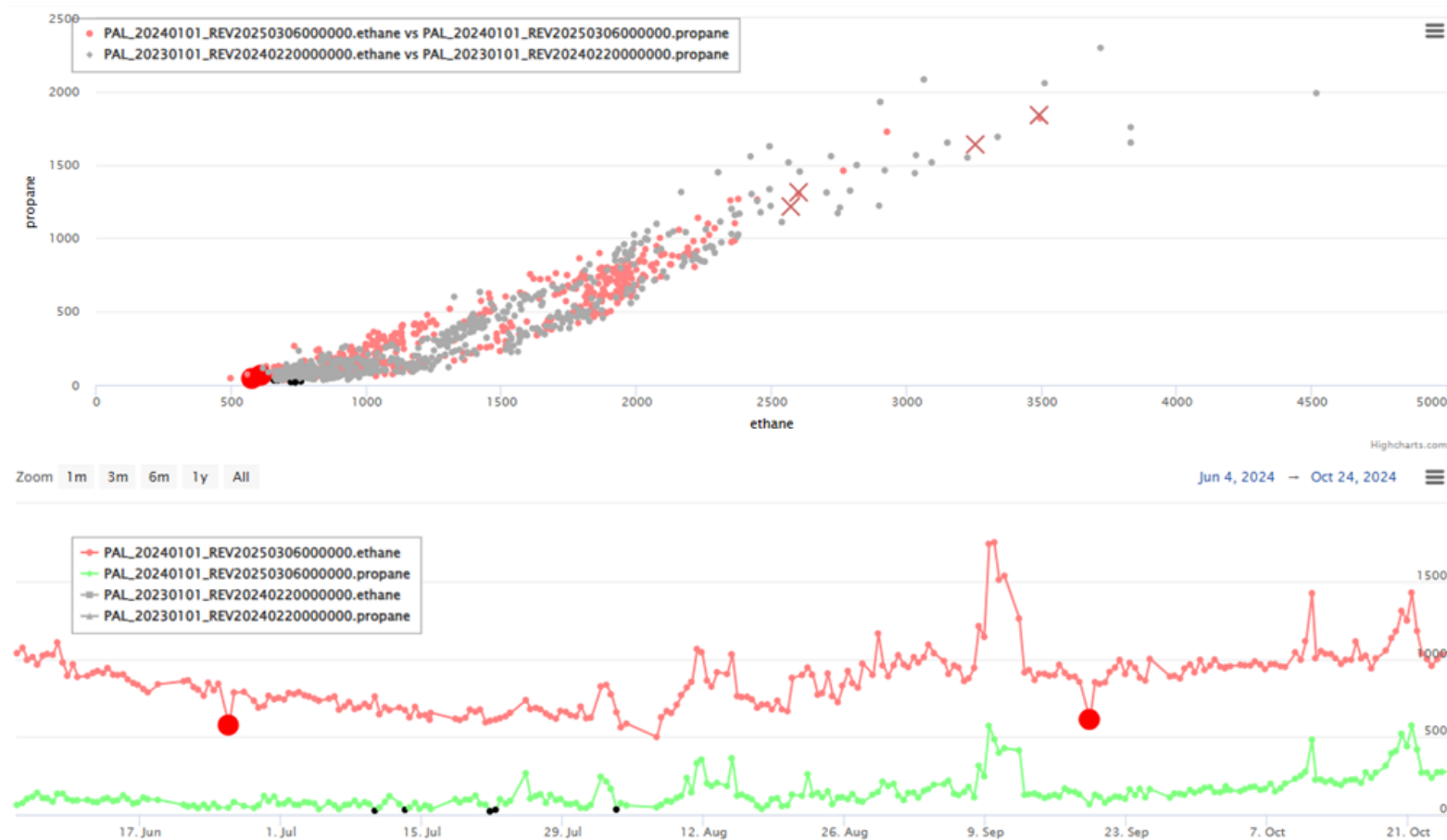
Monte Cimone
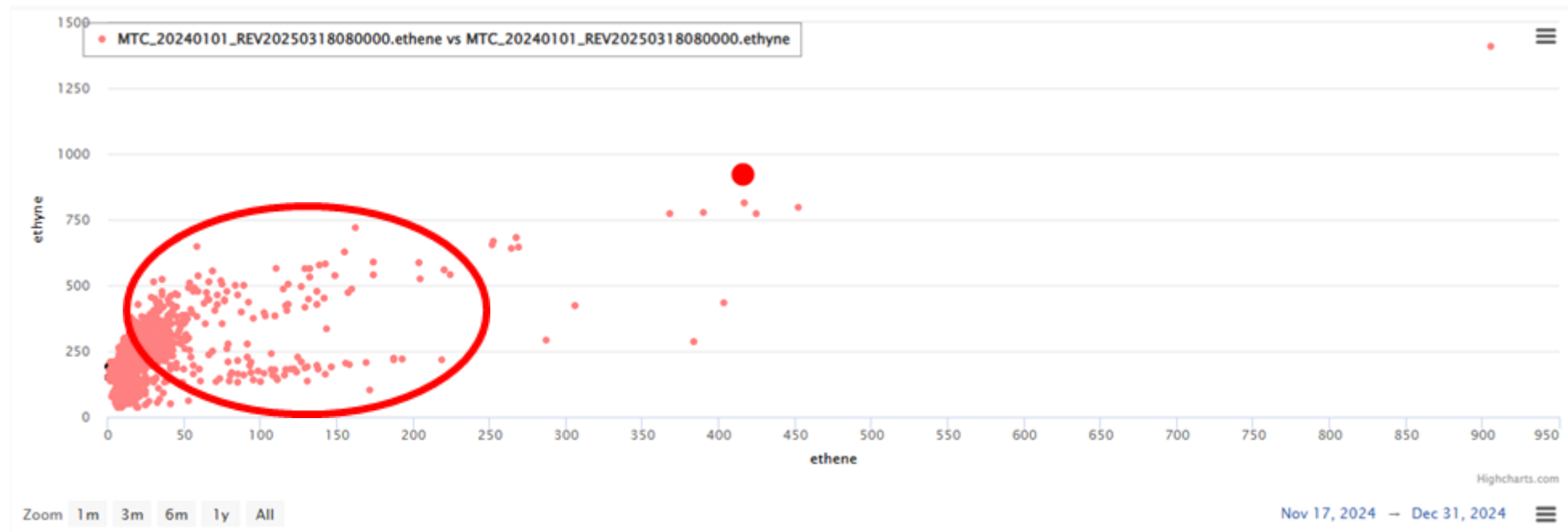
Station presentation by Operator: Jgor Arduini
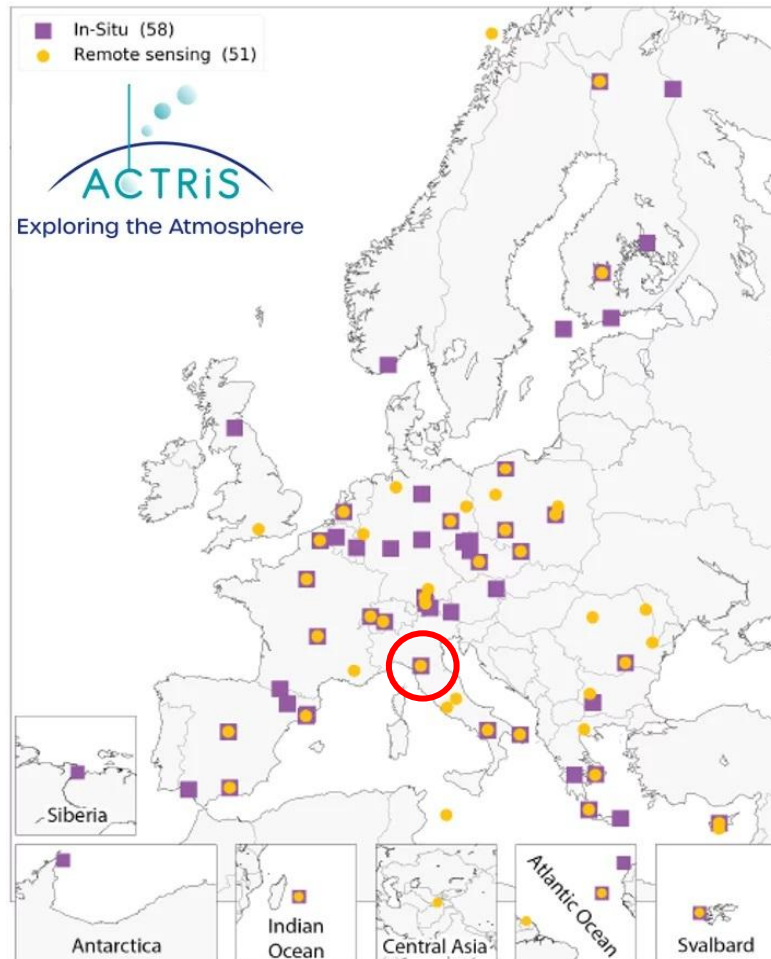
Monte Cimone

Ethene / ethyne

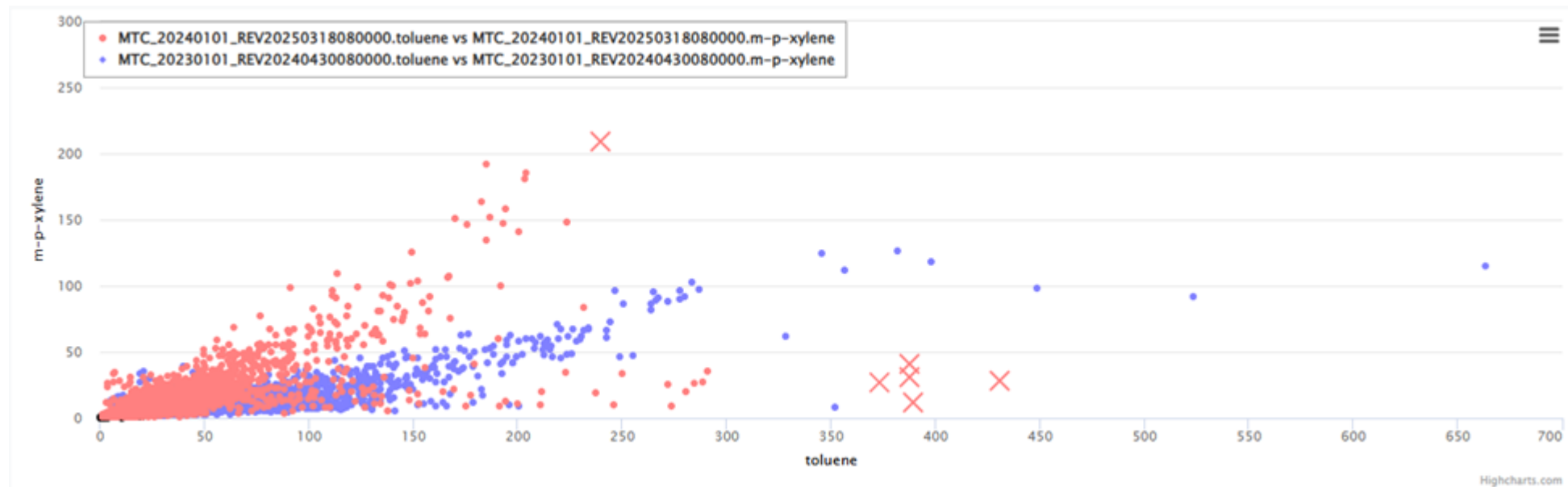Shift in the slope end of November. Has the calibration changed?

Monte Cimone

m-p-xylene / toluene

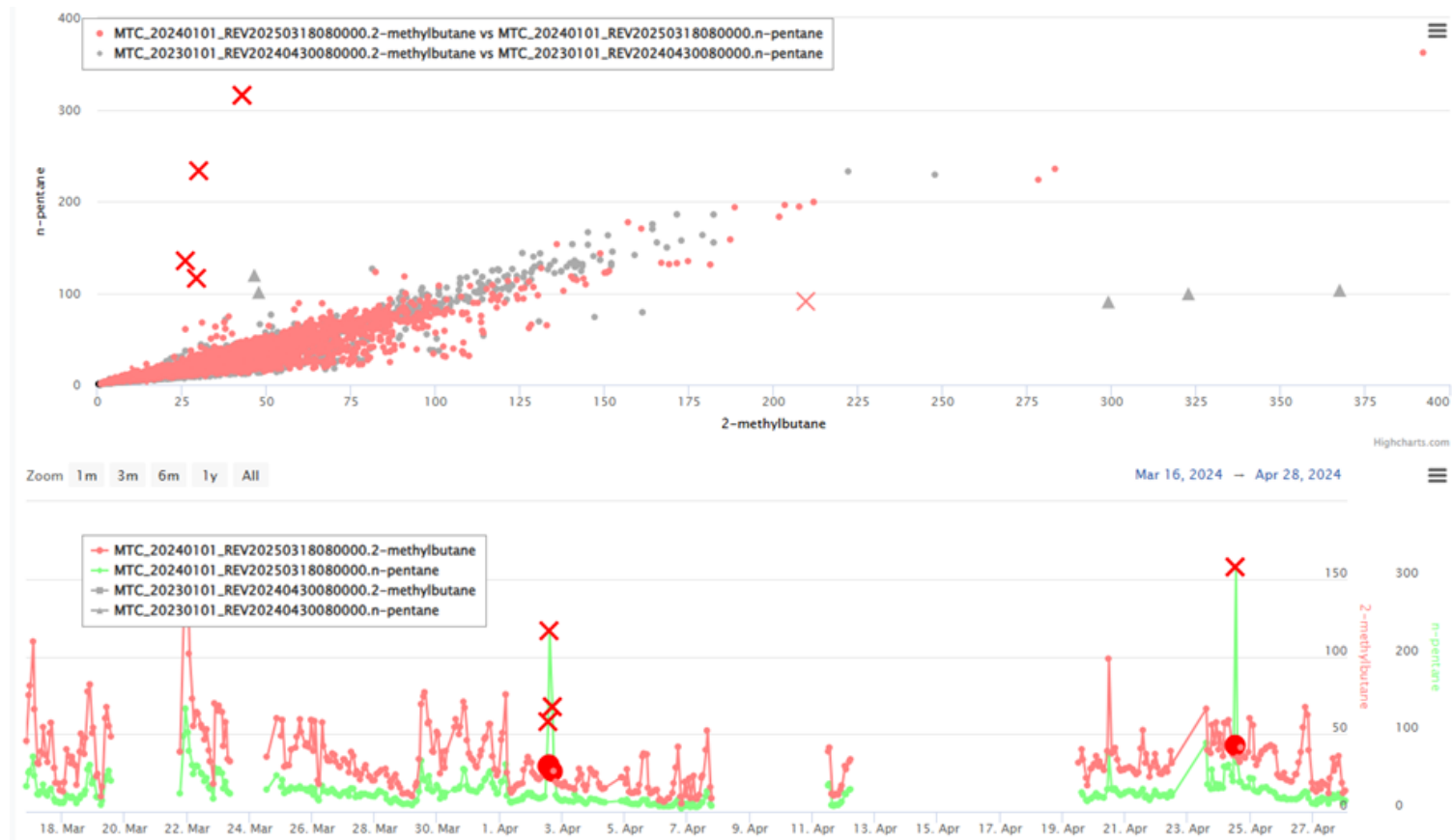Shift in the slope compared to the data from 2023. Has the calibration changed?

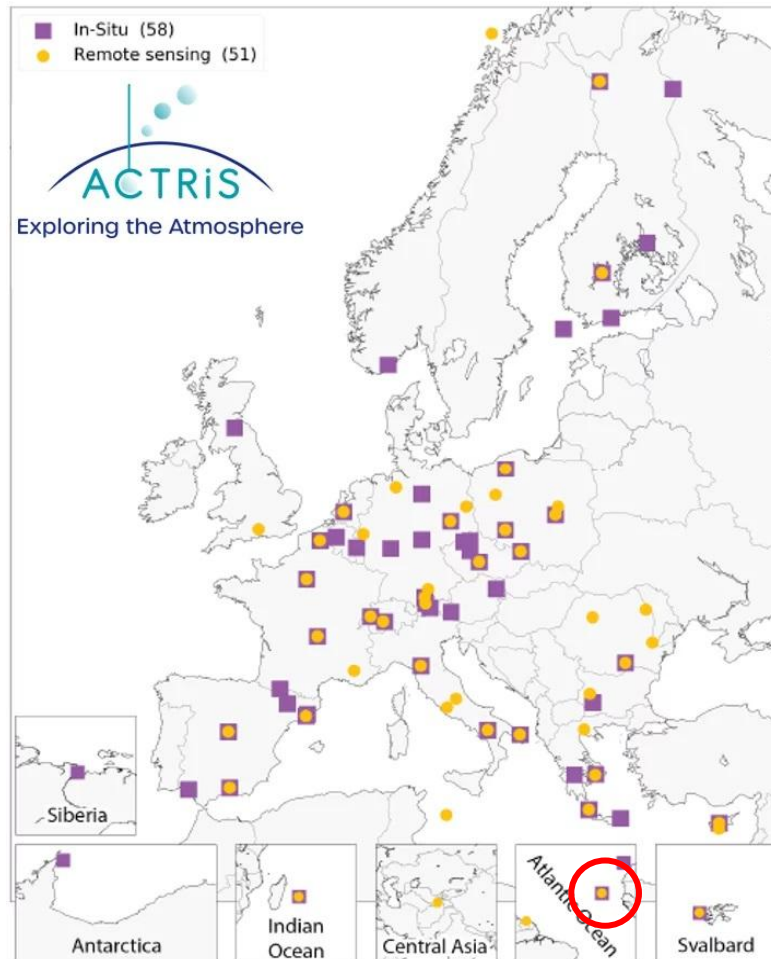# Monte Cimone

2-methylbutane / n-pentane

Feedback QC

Elevated concentrations of n-pentane, out of the general trend. Linked to a local event?

Cape Verde

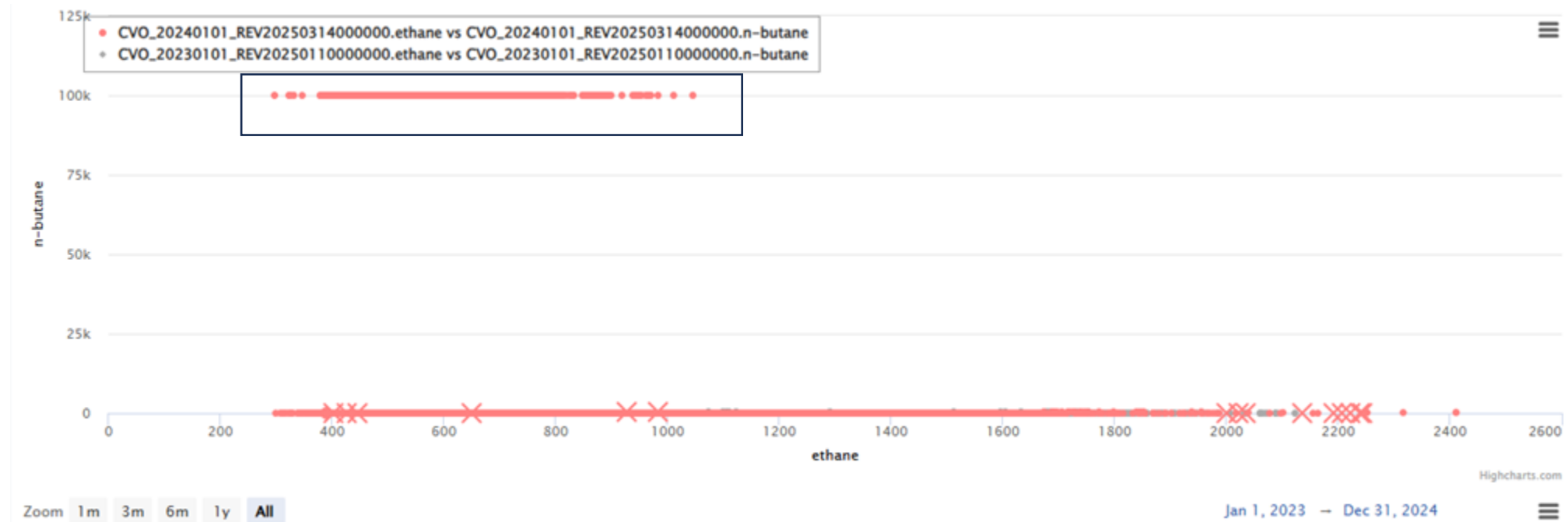Station presentation by Operator: Beth Nelson

General comment

In @VOC@, values 99999.99 observed for some compounds and flagged as valid (000). Please check that the invalid flag (999) is correctly implemented in the .nas file
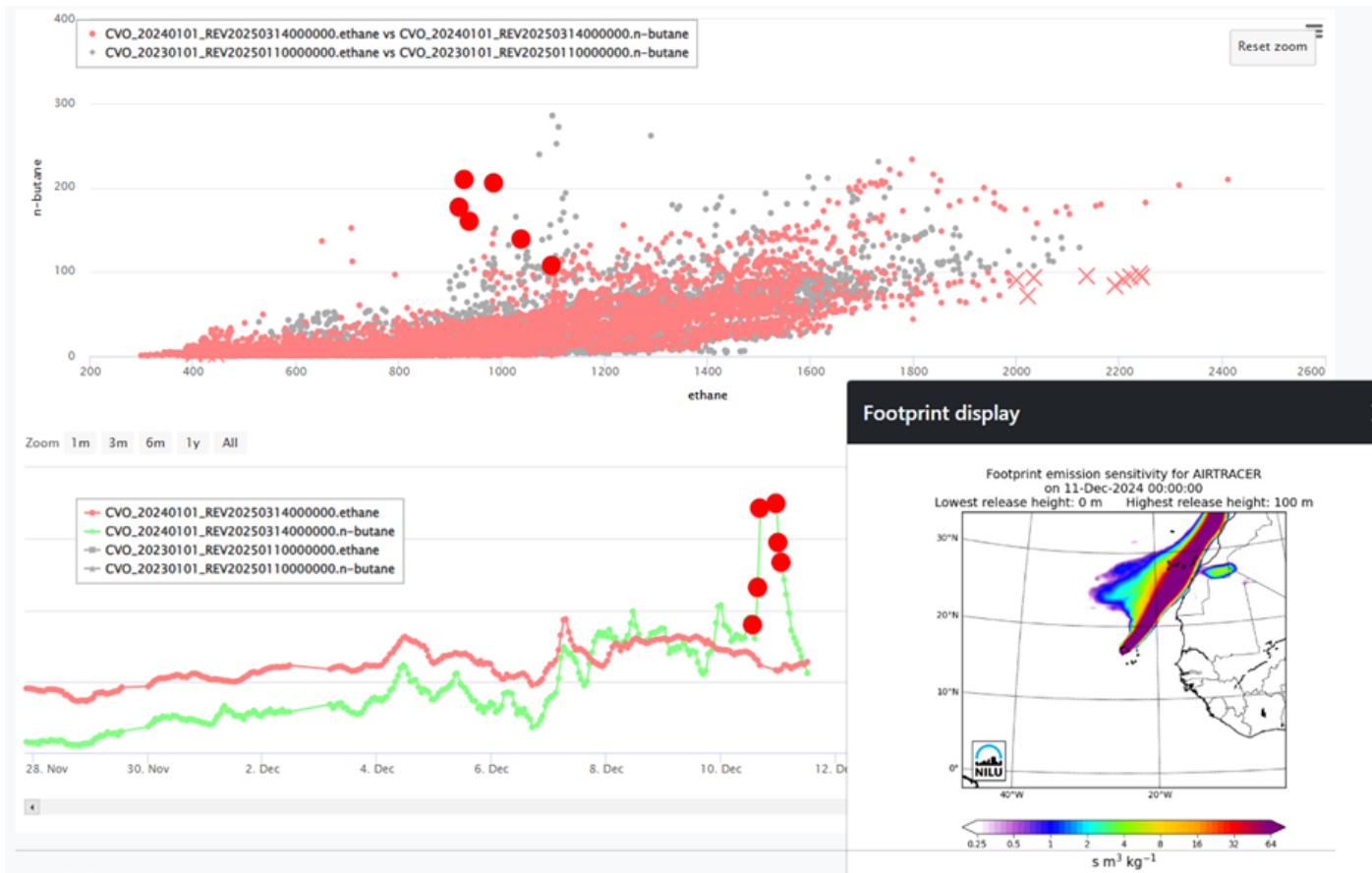
n-butane

High concentration observed for n-butane. Seems to be linked to air masses coming from north-east. Looks like a real event.

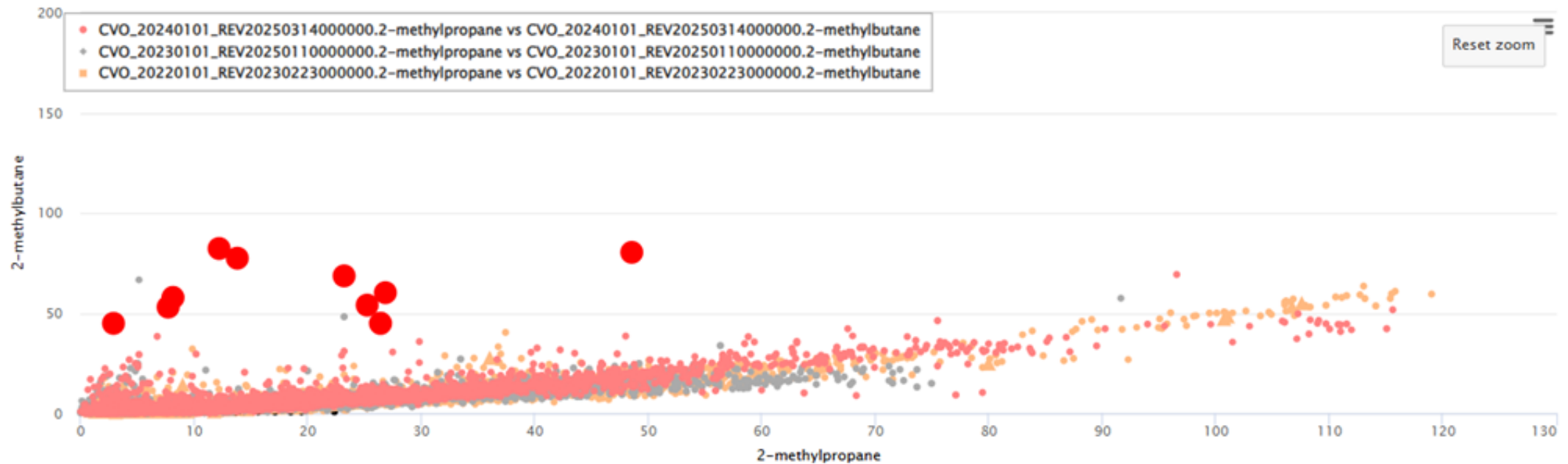## 2-methylbutane vs 2-methylpropane

<table>
<tr><td>Feedback QC</td></tr>
</table>

Samples out of the general trend when comparing to 2023 and 2022. Is it linked to something specific? The air footprint is mostly coming from east, NE. By looking at n-pentane vs 2-methylbutane, these samples are also linked to high n-pentane levels.
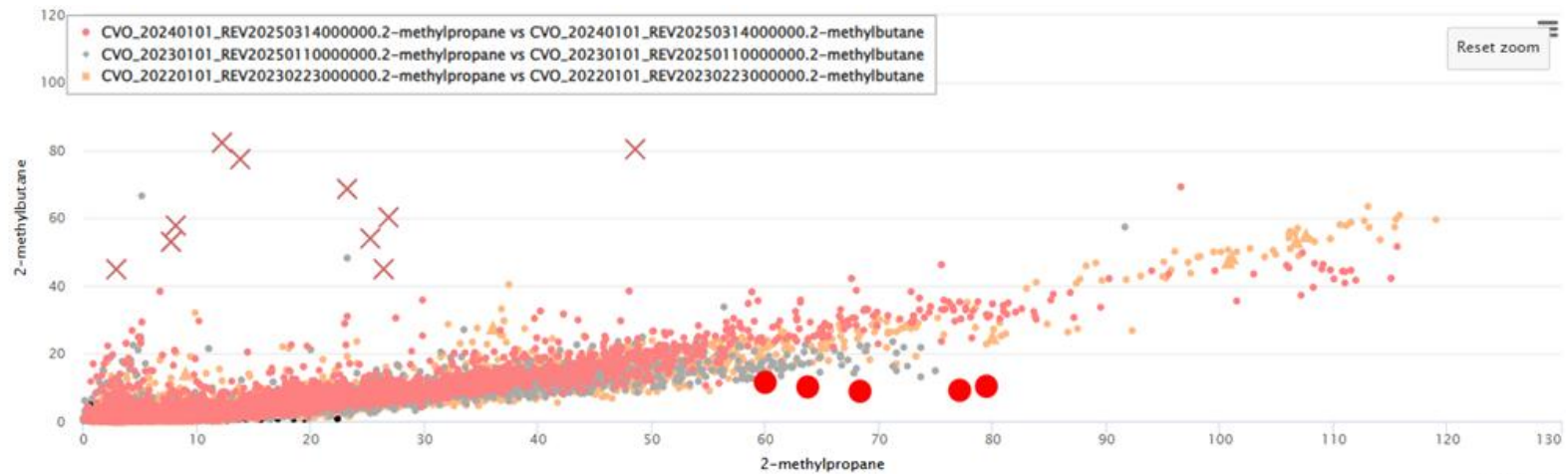
2-methylbutane vs 2-methylpropane

Feedback QC

Higher values expected for 2-methylpropane. Is it real?
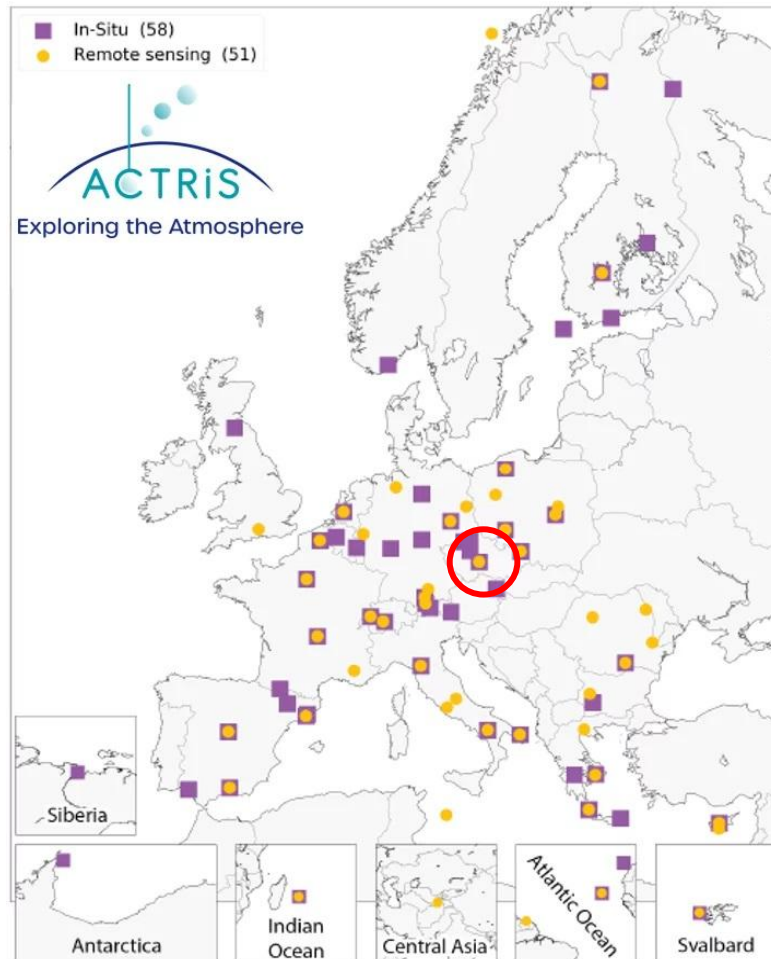
ethyne vs ethene; ethyne vs benzene

Feedback QC

Lower levels observed in 2024 (red in the plot below) for ethyne. Did you change something for the calibration, integration of the ethyne peak?

Kosetice
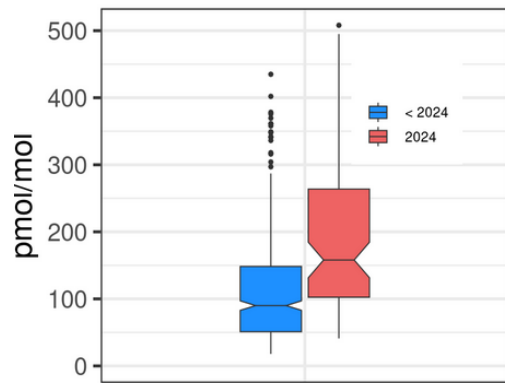
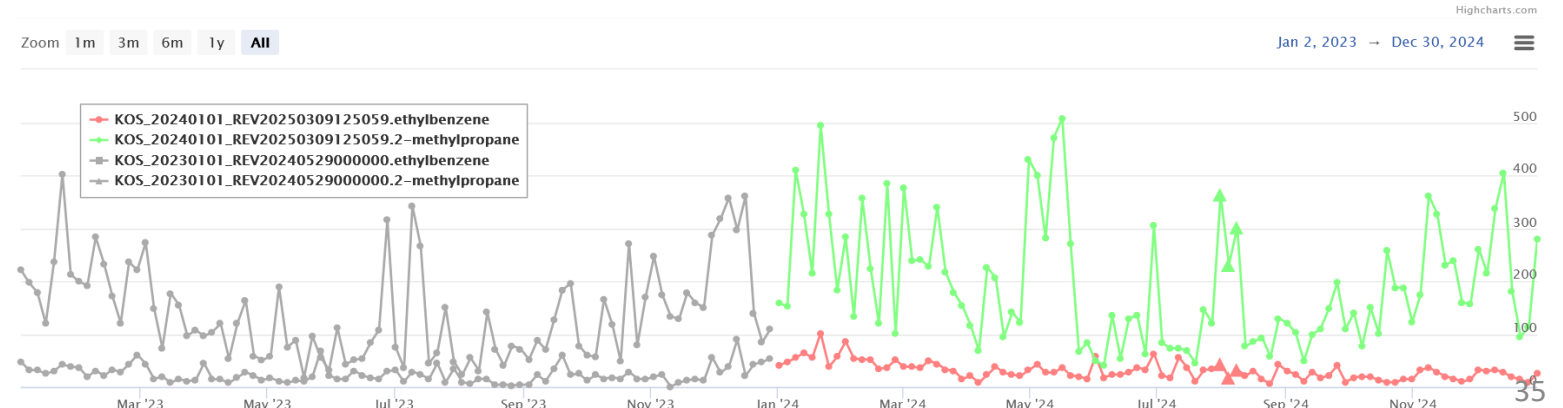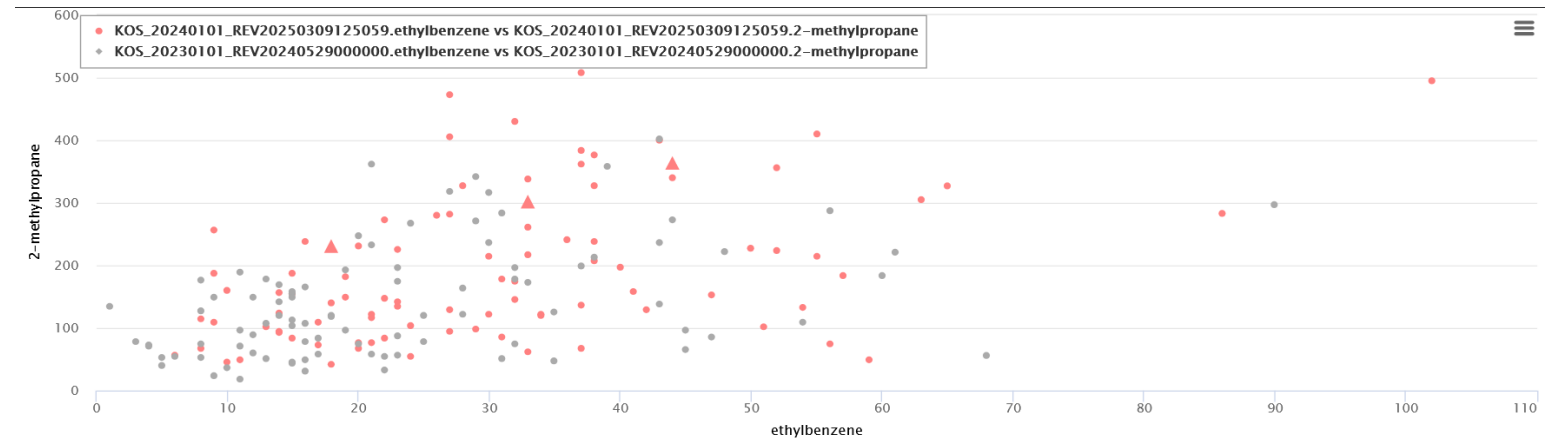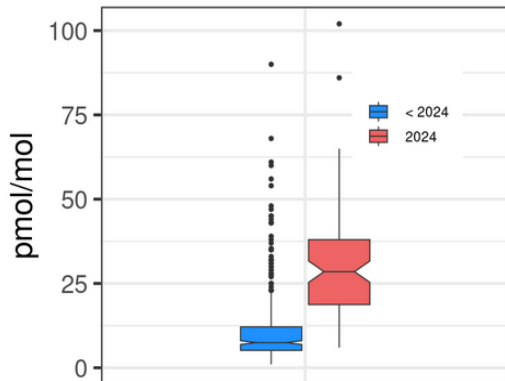Station presentation by Operator: Lucie Školoudová

Various substances

Generally higher concentrations observed in 2024. Is this real or due to earlier outliers?
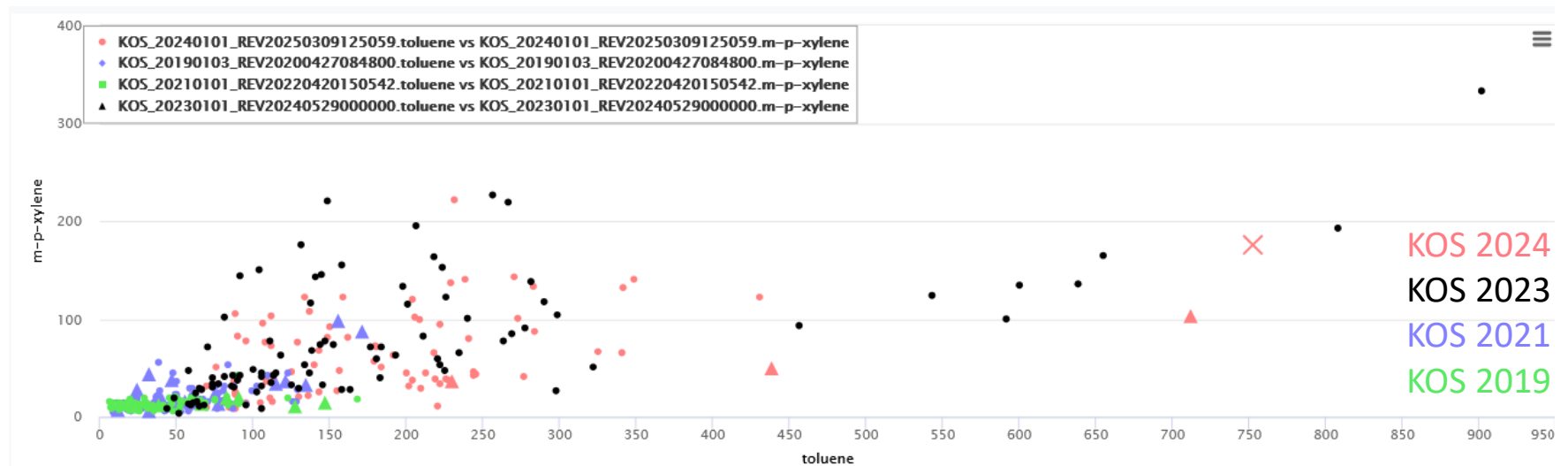-> Was hard to spot during Empa QA!

Sverre's box plots:

Example with m-p-xylene vs toluene

Feedback QC

Generally higher concentrations observed in 2024 and 2023 and in comparison to other ACTRIS Stations.
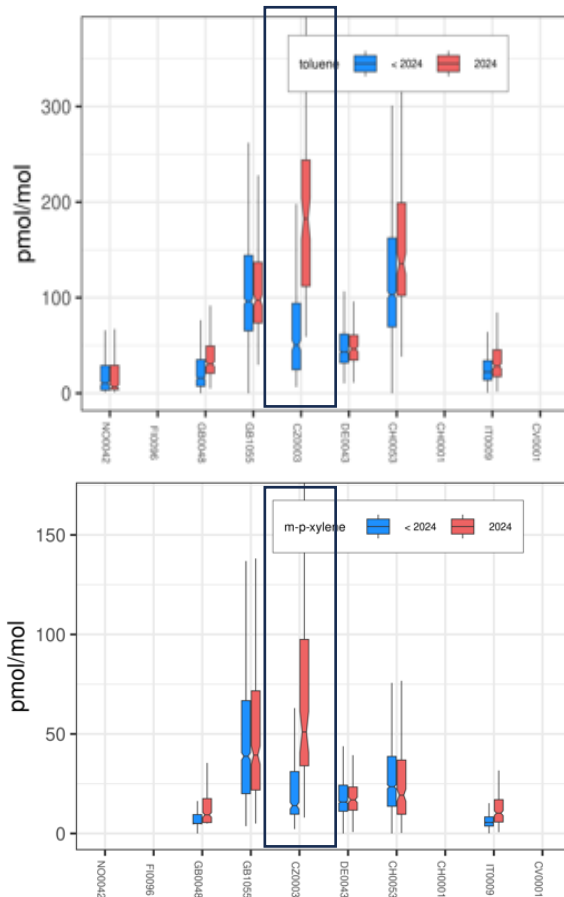
Comments from the station (04.04.2024): Calibration and integration workflow remains the same as since 2022. The only significant change in our workflow is the new process of cleaning canisters used since 5.9.2024. Now we are using TO-Clean – Automated Canister Cleaner (Wasson - ECE).

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Hohenpeissenberg

Station presentation by Operator: Anja Claude / Felix Klein
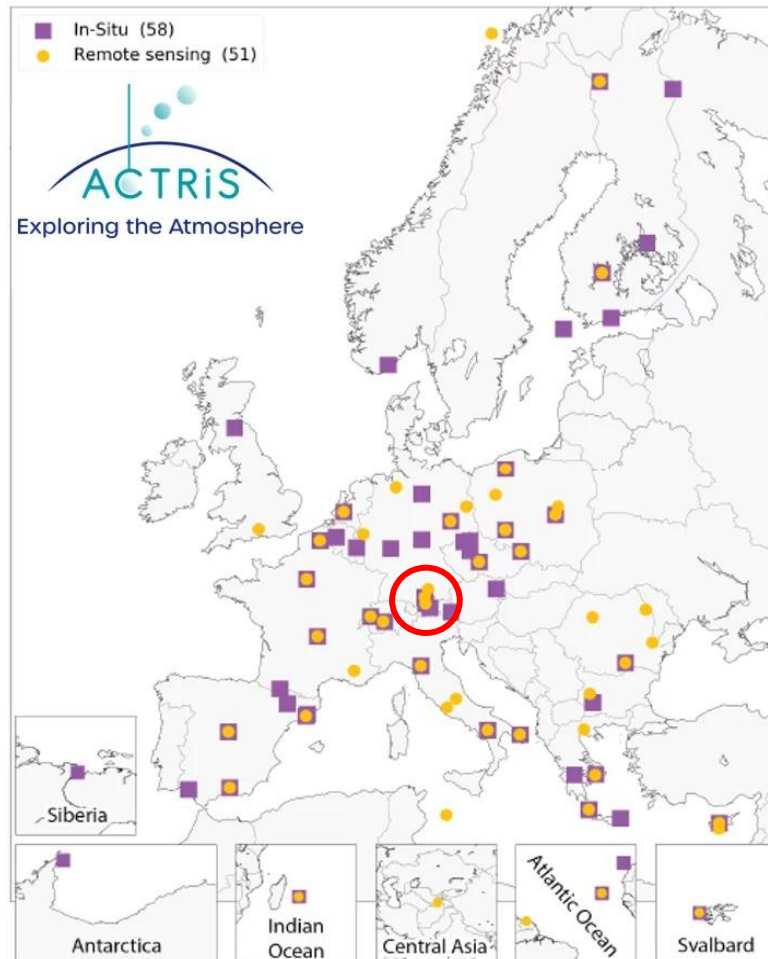
ethane / propane

Feedback QC

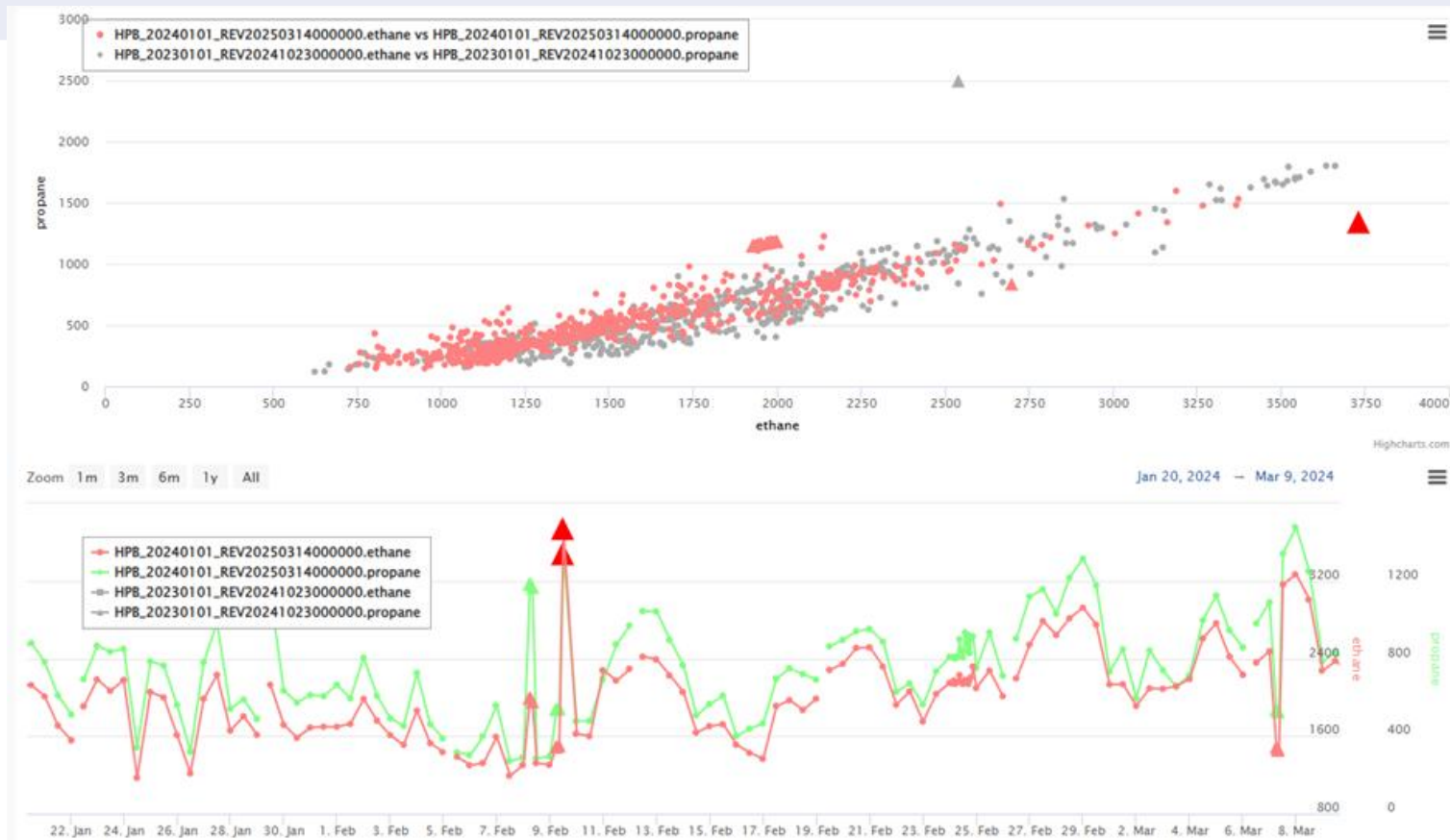Elevated concentrations of ethane and propane. Looks real, just out of curiosity, why was it flagged as local event?
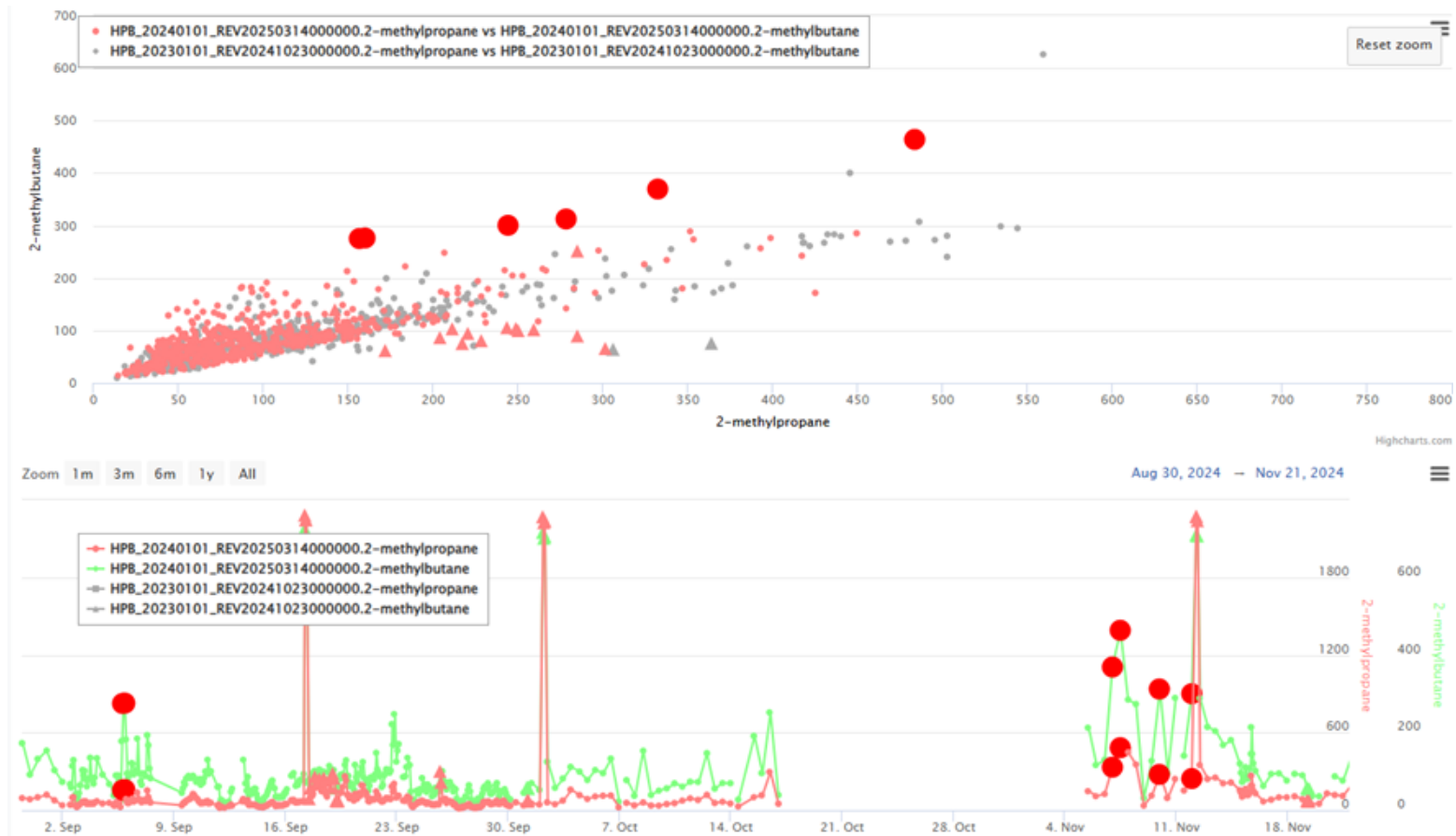
2-methylpropane / 2-methylbutane

Feedback QC

Periodic elevated concentrations of 2-methylbutane. Is it related to a specific event?

Various substances, most pronounced for DMS

Feedback QC

There is a periodic feature of peaking data observed in the data, which is most pronounced in Dimethylsulfide data, but also observed for mass 121 or even volatile compounds such as isoprene. Spiking values followed by a decaying signal. Is this a real feature or caused by calibration carryover/background subtraction or e.g. a sticky gas? -> This should be carefully assessed!
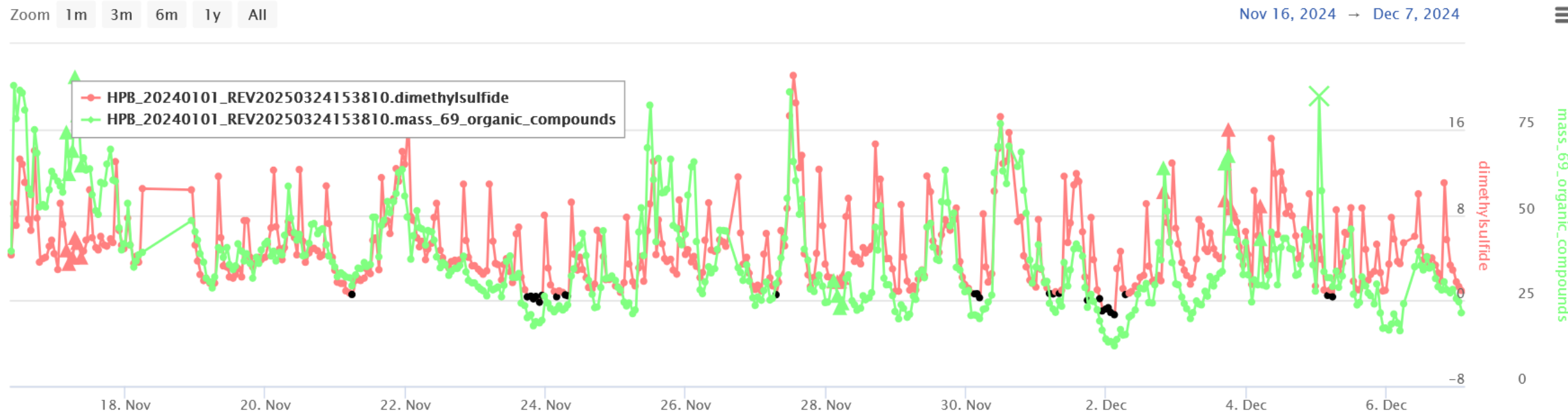
Puy de Dôme
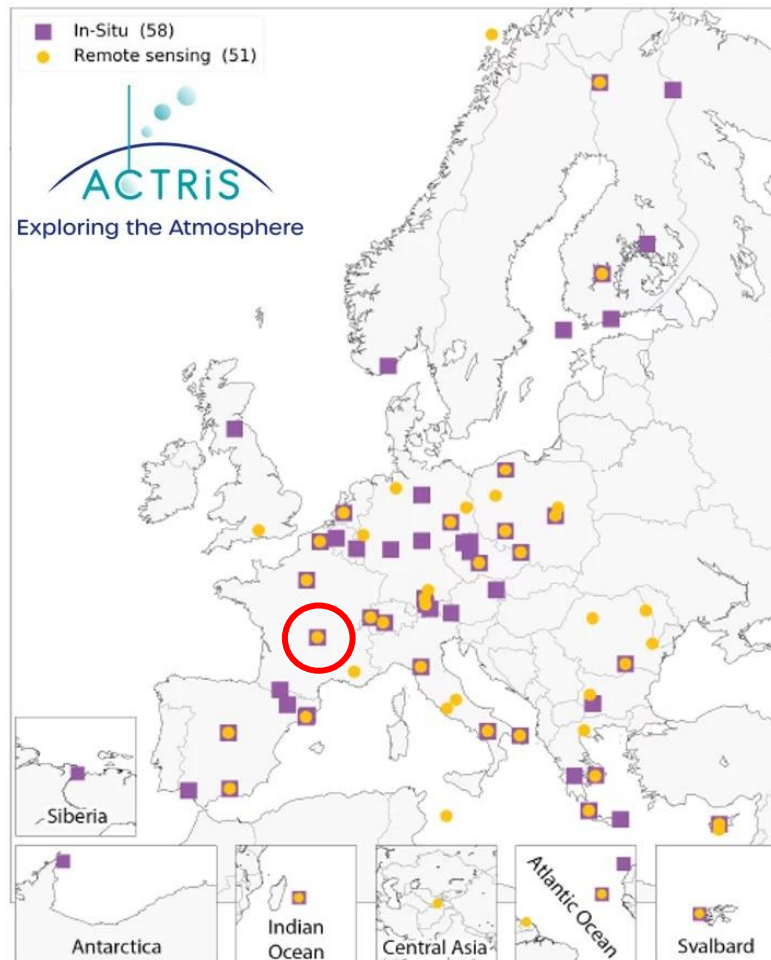
Station presentation by Operator: Aurélien Chevigné

alpha-pinene vs beta-pinene

Feedback QC

Shift in the general trend between 2023 and 2024. Did you change something for the calibration?
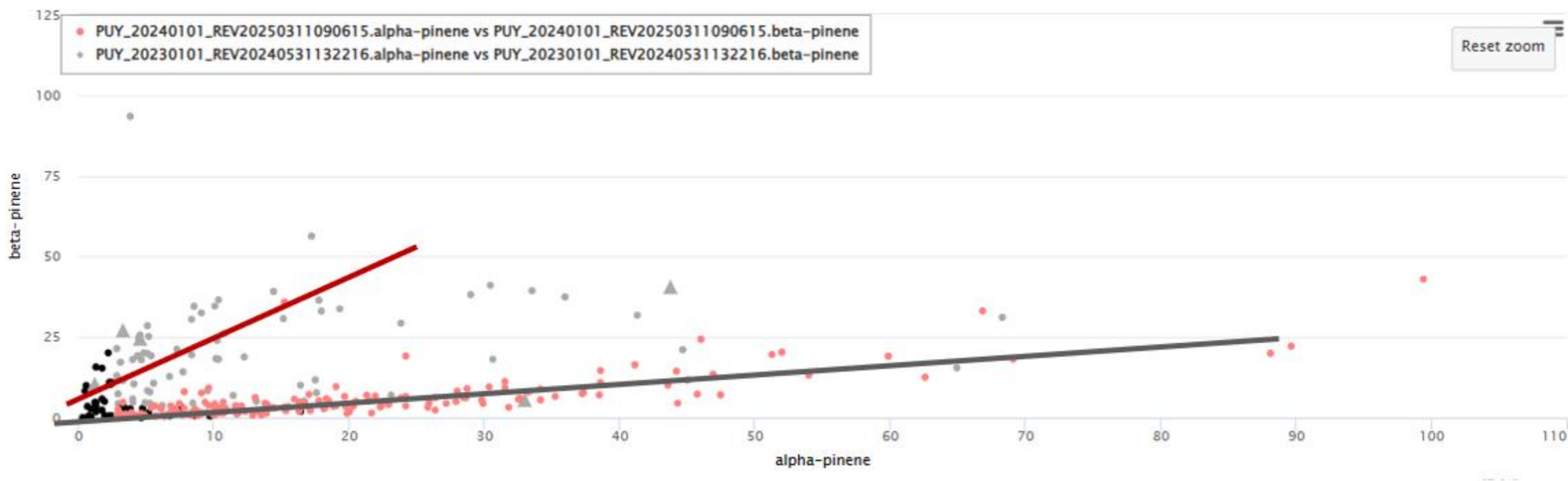
SIRTA (Gif-sur-Yvette)

Station presentation by Operator: Aurélien Chevigné
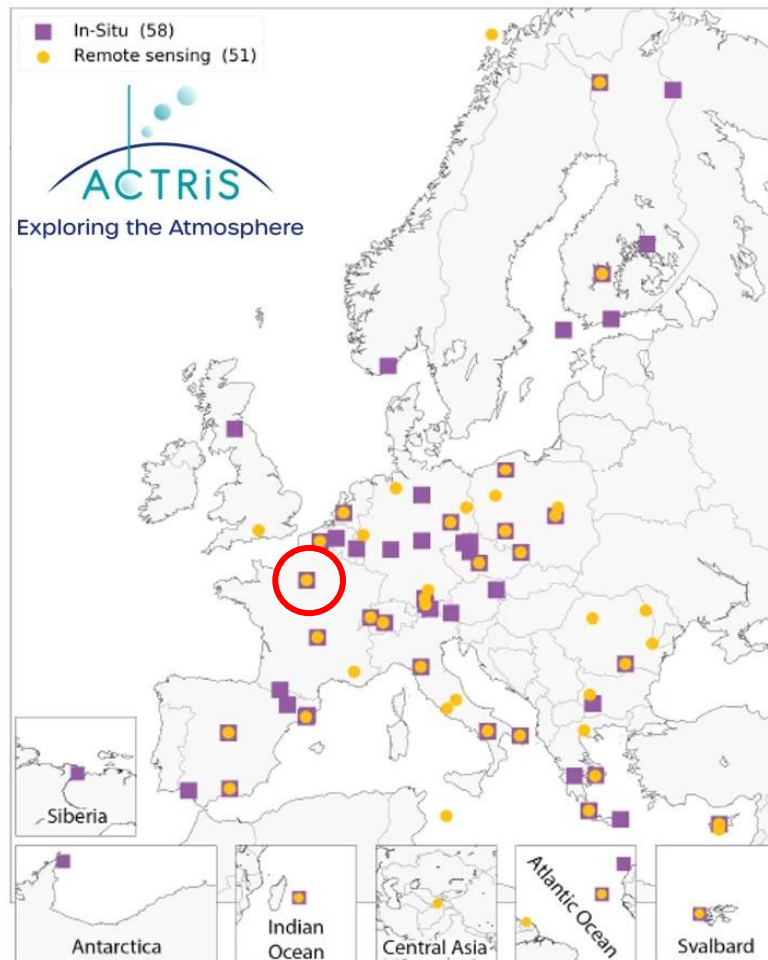
Methanol

Feedback QC

High concentrations after measurement break (calibration?). Possible carryover?

Generally: Concentration unit differs from previous year (ppb instead of ppt), otherwise a good dataset.
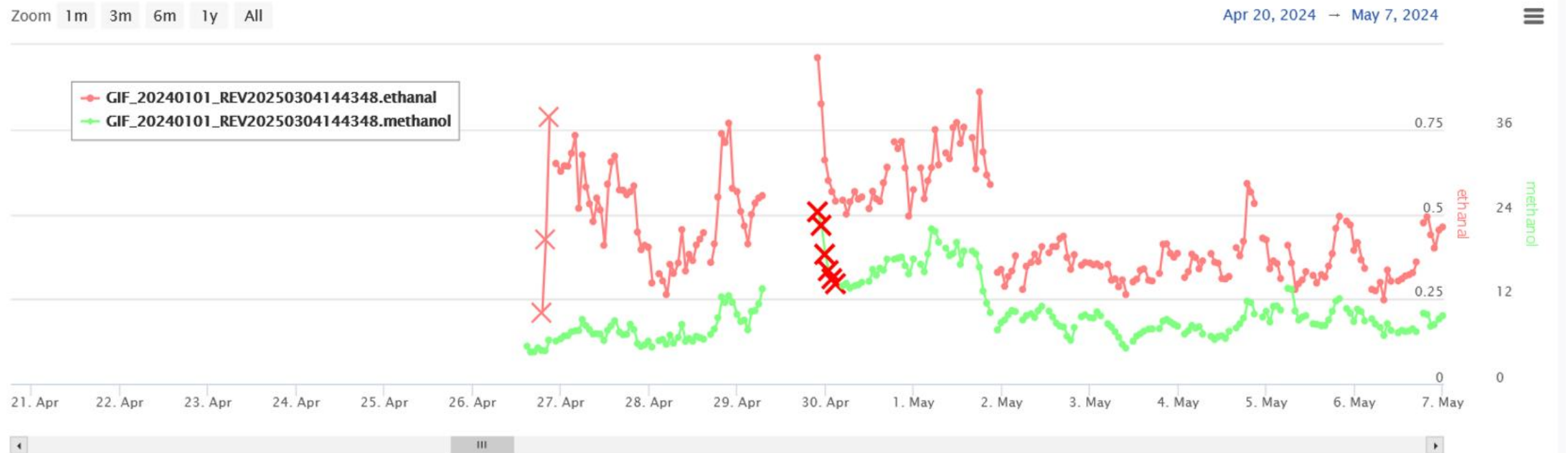
Zeppelin

Station presentation by Operator: Chris Lunder

Zeppelin

Benzene / toluene

Concentration of toluene is higher than expected. Is it a pollution event/contamination?

Hyytiälä

Station presentation by Operator: Ilona Ylivinkka

- Who is using the @VOC@ tool for QC for data level 2?

  → Discussion on external QC improvments tomorrow by Ralf and Peeyush

- Request for the external QC: access to the metadata of .nas file (potential change in detection limits, calibration levels...)
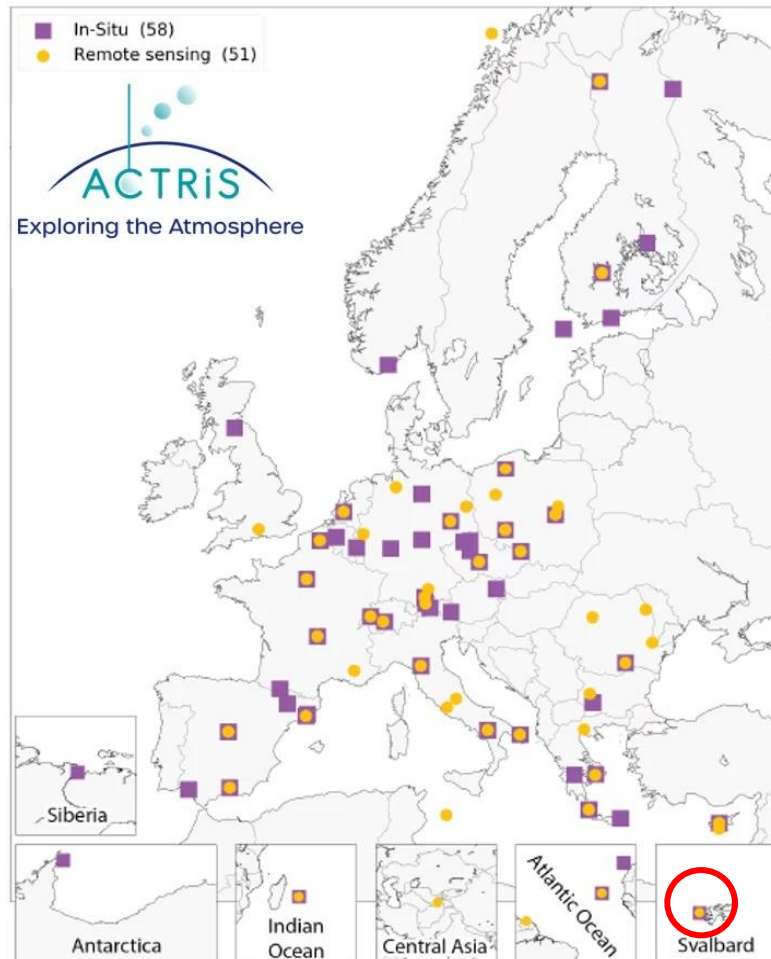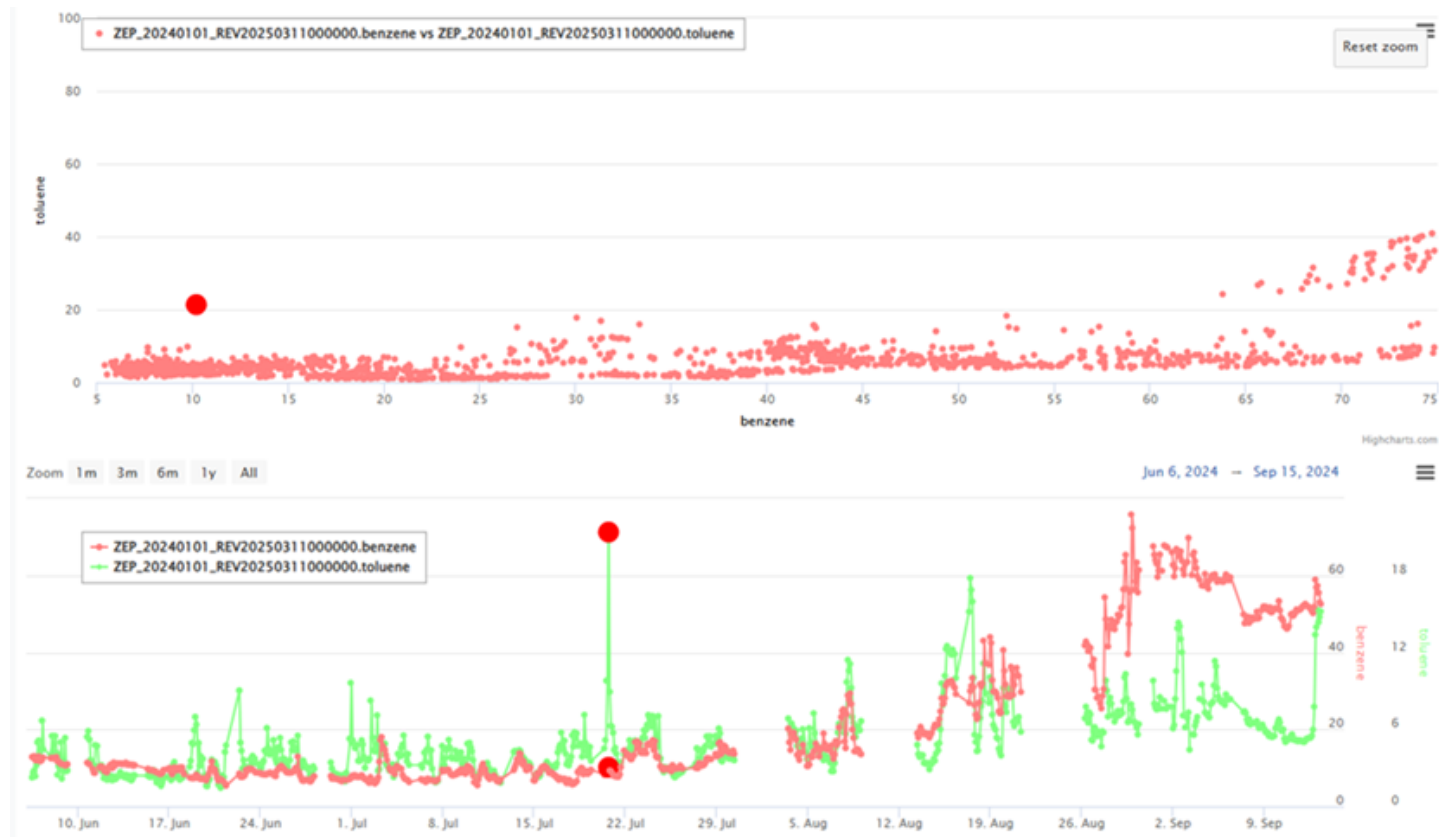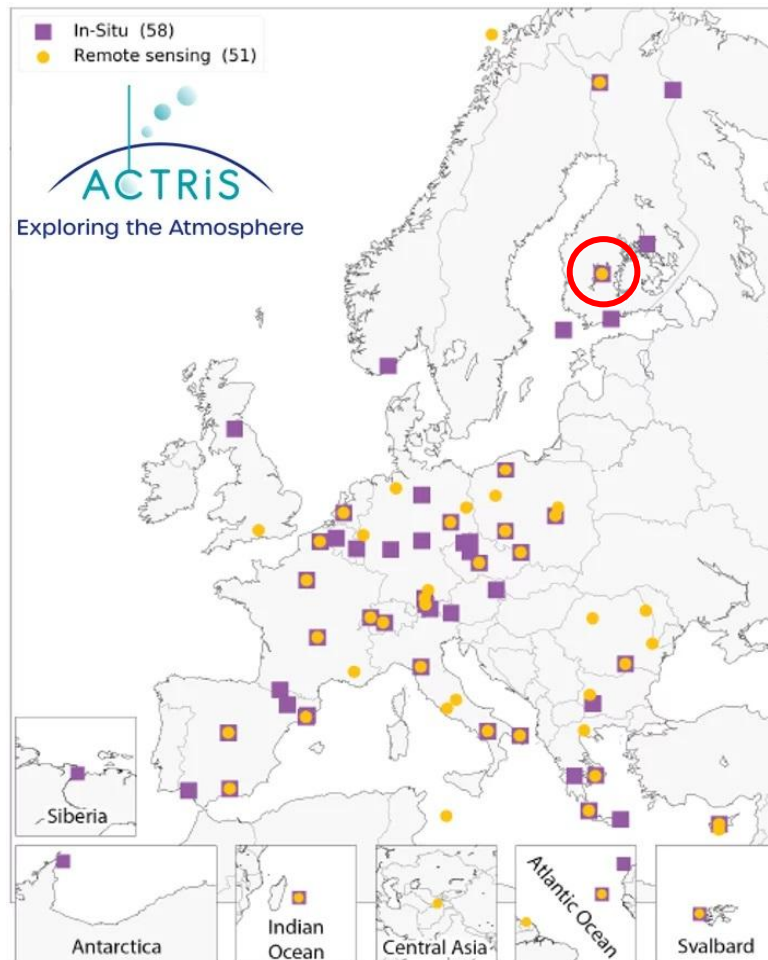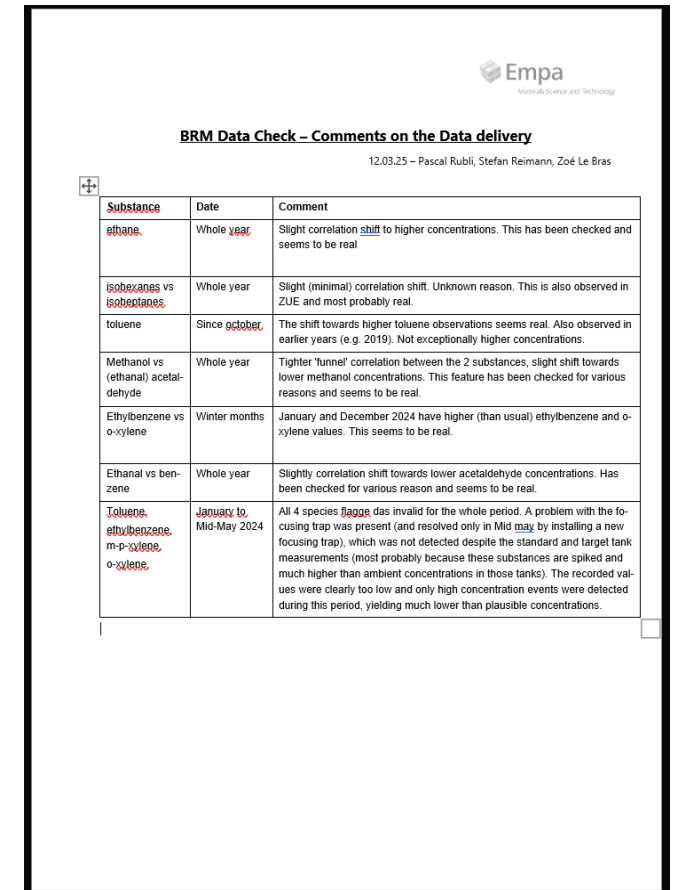
- High-resolution data (PTR-MS): indication of calibration and blank measurement period for external QC

- Optimisation of data delivery: general comments on the data set for external QC on problems, observations, already flagged data at the station during the year, indication on the stability of the instrument

  → Should a template be provided for external QC?

- Any suggestions for further improvements of the data submission/external QC?

BRM Data Check – Comments on the Data delivery

12.03.25 – Pascal Rubli, Stefan Reimann, Zoé Le Bras

Substance	Date	Comment
ethane	Whole year	Slight correlation shift to higher concentrations. This has been checked and seems to be real
isohexanes vs isoheptanes	Whole year	Slight (minimal) correlation shift. Unknown reason. This is also observed in ZUE and most probably real.
toluene	Since october	The shift towards higher toluene observations seems real. Also observed in earlier years (e.g. 2019). Not exceptionally higher concentrations.
Methanol vs (ethanal) acetaldehyde	Whole year	Tighter 'funnel' correlation between the 2 substances, slight shift towards lower methanol concentrations. This feature has been checked for various reasons and seems to be real.
Ethylbenzene vs o-xylene	Winter months	January and December 2024 have higher (than usual) ethylbenzene and o-xylene values. This seems to be real.
Ethanal vs benzene	Whole year	Slightly correlation shift towards lower acetaldehyde concentrations. Has been checked for various reason and seems to be real.
Toluene, ethylbenzene, m-p-xylene, o-xylene	January to Mid-May 2024	All 4 species flagge das invalid for the whole period. A problem with the focusing trap was present (and resolved only in Mid may by installing a new focusing trap), which was not detected despite the standard and target tank measurements (most probably because these substances are spiked and much higher than ambient concentrations in those tanks). The recorded values were clearly too low and only high concentration events were detected during this period, yielding much lower than plausible concentrations.

Example of the comments of the station added to the NILU Tracker for Beromünster (Nilu Tracker: 5191)