

Technical Requirements Documentation

instrumental setup and infrastructure
needed to provide data about particulate organics
(personnel resources not included)

*1st OGTAC-CC community meeting within the framework of the
ECAC-CAIS CF 04/2024*




Technical requirements documentation

Content:

- 1) About this document
- 2) Data Quality Objectives
- 3) Technical requirements for particle sampling
 - 3.1 General aerosol sampling recommendations
 - 3.2 Aerosol particle sampler (offline)
 - 3.3 Filter material and impactor substrate
 - 3.4 Sample pre-treatment, storage and transport
 - 3.5 Sampling system checks and maintenance
 - 3.6 Additional requirements at the field site
 - 3.7 Data resolution, coverage and provision
- 4) Technical requirements for laboratory analysis
 - 4.1 General remarks
 - 4.2 Sample handling and preparation in the laboratory
 - 4.3 Supported analytical techniques
- 5) References
- 6) Appendix

Technical requirements documentation

Content:

- 1) About this document  *List of target compounds and minimum requirements*
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TROPOS

Draft list of supported target compounds

- 7-8 modules
- Min. requirement for label: 2 target compounds from one or more modules
- Opt.: Maximum outcome (from one analytical procedure)

Discussion points:

- Modules OK?
- Missing targets (urgently needed)?
- Min req. realistic?
- ...

Module name	sum formula	Module	SOA - aldehydes	
		1	Vanillin	C8H8O3
		2	Syringaldehyde	C9H10O4
		3	Coniferyl aldehyde	C10H10O3
		(4	Acetosyringone	C10H12O4)
Module	Biomass burning (Anhydromonosaccharides)			
1	Levoglusosan	C6H5O10		
2	Mannosan	C6H5O10		
3	Galactosan	C6H5O10		
Module	Primary biogenic (pollen / fungal spores)			
1	Erythritol	C4H10O4		
2	Arabitol	C5H12O5		
3	Glucose	C6H12O6		
4	Fructose	C6H12O6		
5	Mannose	C6H12O6		
6	Galactose	C6H12O6		
7	Mannitol	C6H14O6		
8	Ergosterol	C28H44O		
Module	Organic ions (inorganic IC measurement byproducts)			
1	Oxalate	C2O4 ²⁻		
2	Formate	CHO2 ⁻		
3	Methane sulfonic acid	CH4O3S ⁻		
Module	Biogenic SOA - acids			
1	Terebic acid	C7H10O4		
2	Vanillic acid	C8H8O4		
3	Isovanillic acid	C8H8O4		
4	MBTCA	C8H12O6		
5	Norpinonic acid	C9H14O3		
6	Pinic acid	C9H14O4		
7	Pinonic acid	C10H16O3		
Module	SOA - nitroaromatics			
1	4-nitrophenol	C6H5NO3		
2	3-Nitrocatechol	C6H5NO4		
3	4-nitrocatechol	C6H5NO4		
4	2-methyl-4-nitrophenol	C7H7NO3		
5	4-Nitroguaiacol	C7H7NO4		
6	4-Methyl-5-nitrocatechol	C7H7NO4		
7	3-methyl-5-nitrocatechol	C7H7NO4		
Module	16 EPA PAHs			
1	Naphthalene	C10H8		
2	Acenaphthylene	C12H8		
3	Acenaphthene	C12H10		
4	Fluorene	C13H10		
5	Phenanthrene	C14H10		
6	Anthracene	C14H10		
7	Fluoranthene	C16H10		
8	Pyrene	C16H10		
9	Benz(a)anthracene	C18H12		
10	Chrysene	C18H12		
11	Benzo[b]fluoranthene	C20H12		
12	Benzo[k]fluoranthene	C20H12		
13	Benzo[a]pyrene	C20H12		
14	Indeno[1,2,3-cd]pyrene	C22H12		
15	Benzo[ghi]perylene	C22H12		
16	Dibenz[a,h]anthracene	C22H14		
Module	Hopane + Sterane for traffic OA???			

[object group](#) > [organics](#) > [organic tracers](#)

[object of interest](#) > [organics](#) > [organic tracers](#)

PREFERRED TERM

organic tracers 

BROADER CONCEPT

[organics](#)

NARROWER CONCEPTS

[2-methylerythritol](#)

[2-methylthreitol](#)

[cellulose](#)

[fructose](#)

[galactosan](#)

[glucose](#)

[hexahydroxycyclohexane](#)

[levoglucosan](#)

[mannitol](#)

[mannosan](#)

[mannose](#)

[myo-inositol](#)

[sucrose](#)

[trehalose](#)

CONTRIBUTOR

<https://orcid.org/0000-0002-8981-0805>

CREATOR

<https://orcid.org/0000-0002-3380-3470>

<https://orcid.org/0000-0002-8981-0805>

URI

https://dev-voc.actris.nilu.no/actris_vocab/organictracers 

Download this concept:

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TROPOS

DQOs under development/ discussion - more topics or updates possible, if required:

Data quality objectives (DQOs) define the type, quality and quantity required of primary data and derived parameters to yield information that can be used to support decisions. In particular, DQOs specify tolerable levels of uncertainty in the data, required completeness, comparability and representativeness based on the decisions to be made [WMO, 2007].

- Field blank (sampling)
 - Instrument calibration (LOD, LOQ)
 - Reproducibility standard deviations
 - Data coverage
 - Participation in ILCs minimum once per year and stay within the statistical factors
- (1st ILC in autumn 2024 will serve as the base for the first draft of DQO)

Module dependent

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Need to be met by observatories in order to provide particulate organics within ACTRIS

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*All information about general aerosol sampling, aerosol inlet design under consideration of the individual NF circumstances and aerosol conditioning are described in the overall document “**ACTRIS Standard Procedures for In-Situ Aerosol Sampling, Measurements, and Analyses at ACTRIS Observatories**”*

→ See ECAC website

<https://www.actris-ecac.eu/>



ACTRIS Standard Procedures for In-Situ Aerosol Sampling, Measurements, and Analyses at ACTRIS Observatories

ACTRIS-ERIC Version 1.0; January, 2024
Center for Aerosol In-Situ Measurement
European Center for Aerosol Calibration and Characterization (CAIS-ECAC).

TROPOS

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Reference: EN 12341:2023

(Ambient air – Standard gravimetric measurement method for the determination of the PM10 or PM2.5 mass concentration of suspended particulate matter)

TROPOS

Aerosol particle sampler / sampling

Sampler type:

- High volume/ Low volume filter sampler and impactor (Berner, Moudi) are possible
- Up to now no official list of ACTRIS compliant samplers exists
- Overview current NFs:

NF	Birkenes	Zeppelin	Melpitz	Vielsalm	Sonnblick
Filter sampler	Low volume 38.3 L min ⁻¹	High volume 633 L min ⁻¹	High Volume 500 L min ⁻¹	Low volume 38.3 L min ⁻¹	High volume + low volume
Manufacturer	KFG ?	DIGITEL	DIGITEL	DERENDA PNS 16-6-1	?

- *Current CC status: All filter sampler and impactor types are allowed!*

Aerosol particle sampler / sampling

Filter sampler overview:

1		Instrument manufacturer	Instrument model	Extension	Station			
2	LVS	Derenda	LVS3.1					
3	LVS	Derenda	PNS 16T		Cabauw			
4	LVS	Derenda	PNS 18-DM-3.1					
5	LVS	Derenda	PNS 18T-DM-3.1					
6	LVS	Derenda	PNS 24-DM-3.1					
7	LVS	Derenda	PNS 24T-DM-3.1					
8	MVS	Derenda	MVS6.1					
9	MVS	Derenda	PNS 18-DM-6.1					
10	MVS	Derenda	PNS 18T-DM-6.1					
11	MVS	Derenda	PNS 24-DM-6.1					
12	MVS	Derenda	PNS 24T-DM-6.1					
13								
14	HVS	DIGITEL	DA-80		Payerne, Rigi, MSY, Donon, etc...			
15	HVS	DIGITEL	DHA-80		MEL, MSY, OPE, ZEP, Diabla Gora, Zielonka			
16	HVS	DIGITEL	DH-77					
17	HVS	DIGITEL	DS-02					
18	LVS	DIGITEL	DPA14					
19	LVS	DIGITEL	DPA96					
20	LVS	DIGITEL	DPA02					
21								
22	LVS	FAI	SWAM 5A					
23	LVS	FAI	SWAM 5A	Dual Channel	Monte Martano			
24	LVS	FAI	HYDRA	Dual Sampler				
25								

25								
26	LVS	KNF	IP20-T		Pic du Midi, PUY			
27								
28	LVS	Leckel	LVS3		NILU, KOS			
29	LVS	Leckel	SEQ47/49		UBA, Norunda, Iskrba			
30	LVS	Leckel	SEQ47/50	-RV				
31	LVS	Leckel	SEQ47/50	-RV CD				
32	LVS	Leckel	SEQ47/50	-RV 19"				
33	LVS	Leckel	LVS6					
34								
35	HVS	MCV	CAV-A/MSb		MSA, MSY			
36	HVS	MCV	CAV-A/mb					
37								
38	HVS	Tecora	Echo PM					
39	LVS	Tecora	Sentinel					
40	LVS	Tecora	Skypost PM FX					

1		Instrument manufacturer	Instrument model	Extension	Station			
41								
42	LVS	Thermo	Partisol2025		SIRTA			
43	LVS	Rupprecht	Partisol2025		Ispra			
44	LVS	ThermoFisher	Partisol 2025i					
45	LVS	ThermoFisher	Partisol 2025i-D					
46								
47	LVS	Dado lab	Giano	(external mount)				
48	LVS	Dado lab	Giano	(19" rack)				
49	LVS	Dado lab	Gemini	Dual sampler (external mount)				
50	LVS	Dado lab	Gemini	Dual sampler (19" rack)				
51	LVS	Dado lab	1PMx					
52	HVS	Dado lab	1PMx					

TROPOS

Aerosol particle sampler / sampling

Cut off size:

- For OC/EC PM2.5 is required by the EU standard (EN-16909)
- But NF site specifications and their respective scientific scopes will be considered, e.g., applications like source apportionment studies
- Overview current NFs:

NF	Birkenes	Zeppelin	Melpitz	Vielsalm	Sonnblick
Cut off size	PM10	PM10	PM10	PM2.5	PM10 and PM1

- *Current CC status: Size cut off required but the decision for PM10, PM2.5 or PM1 is on the NF and its scientific scope!*
- **Important:** *Note in the standard document at the ECAC website about the need of PM10 is corrected!*

TROPOS

Aerosol particle sampler / sampling

Denuder:

- ACTRIS deliverable 3.19: ACTRIS concludes that a denuder is not needed during the cold season for particulate organics
- KEY at Birkenes is currently running a sampling campaign aiming to test the effect of the EUSAAR-denuder on mass concentration, OC/EC, and organic tracers
- This work is still in progress
- Overview current NFs:

NF	Birkenes	Zeppelin	Melpitz	Vielsalm	Sonnblick
Denuder	Yes/NO	?	No	?	?

- *Current CC status: Still under discussion!*

TROPOS

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Filter material and impactor substrate

- Only two types of filter material are recommended, Teflon filters and quartz fibre filters, according to the WMO/GAW guidelines
- Quartz filter for OC/EC measurements needed (high temperature stability) vs. Teflon
- Other types of filters should not be used, if a station uses other types of filter it is needed to proof the applicability by parallel measurements for a certain timeframe (to be set with the TC unit)
- Impactor substrate is typically aluminum foil, Teflon filters and polycarbonate filters depending on the purpose of sampling
- Documentation important, e.g., manufacturer and batch number

Filter material and impactor substrate

➤ Overview current NFs:

NF	Birkenes	Zeppelin	Melpitz	Vielsalm	Sonnblick
Filter material	quartz	quartz	quartz	Tissuquartz 2500-QAT-UP	quartz
Manufacturer	Pall	Pall	Munktell Ahlstrom	Pall	?

➤ *Current CC status: Quartz or Teflon for filter sampling, aluminum foil, Teflon or polycarbonate filters for impactor!*

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*Content of the measurement guidelines,
but for discussion of the hardware also
included in this section*

Sample pre-treatment, storage and transport

Filter pre-treatment (example from MELPITZ for 150mm quartz filter):

- Bake out at 105°C for 24h (VDI 2463) – oven needed
- 72h equilibration before weighing
- Documentation of T and RH – respective sensors needed
- Transport and storage in aluminum boxes
- Maximum one month before application
- Before transport to the station, filters are transferred in the filter holder and wrapped in aluminum foil
- All samples are transported in a small zarges box, only used for this application

Sample pre-treatment, storage and transport

Storage at measurement station (after sampling) and transport:

- For OC/EC measurements a threshold of T exists based on experimental results → 7 weeks at 25°C does not impact the results
- Module dependend, anhydrosugars on quartz filters are shown to be stable for 12 weeks (DRC-13-136071-08508B)
- Tests for selected organic tracers are currently done at OG-TAC-CC
- Overview current NFs:

NF	Birkenes	Zeppelin	Melpitz	Vielsalm	Sonnblick
Storage at station	5 days at 4°C	At -18°C	Max. 6 days at ambient T	Max. 14 days < 23°C	3 month in freezer/fridge
Transport info	2-3 days at ambient T	2-3 days at ambient T	1h at ambient T	?	In air tight containers

- Fridge or freezer and transport T-controlled?



Sample pre-treatment, storage and transport

Again, example from MELPITZ:

- Filter+filter holder (wrapped in the same aluminum foil as before) transported back in a zarges box
- Stored at 5°C in a **fridge** over night
- Remove the filter holder the next day and store filter in aluminum boxes, typically a unit of 7 of these boxes are wrapped in aluminum foil and stored in a **freezer** at -20°C until the weighing

- After the weighing filters are stored **only** wrapped in aluminum foil **without folding** until punching out the filter spots
- **Important:** Every special event, like small insects on the filter or any damage were documented (including pictures) = part of the measurement guidelines

Sample pre-treatment, storage and transport

Sample storage of filters in the lab:

➤ Overview current NFs:

NF	Birkenes	Zeppelin	Melpitz	Vielsalm	Sonnblick
Storage	Freezer	Freezer	Freezer	Freezer	Freezer
T (°C)	-18	-18	-20	-18	?
Time until analysis	< 6 month	< 6 month	No rule	1 month	?
Covered by...	?	?	Aluminum foil, without folding	?	?

➤ *What is the effect of storing the filters in comparison of storing the filter extracts until the analysis? Tests currently ongoing at OGTAC-CC...*

TROPOS

Sample pre-treatment, storage and transport

General recommendations:

- Minimize filter handling and transport time
- Storage always in the dark, in cleaned boxes/bags
- For daily measurements: recommended to ship a one week supply from the laboratory to the site, and vice versa, once every week, exceptions because of particular NF site conditions possible
- Transfer (back) ideally in cooled containers below 20°C
- Filter manipulation always with new gloves (anti-static and powder free) and cleaned tweezers

- *Current CC status: Still under discussion, but these steps have to be documented in detail!*

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Sampling system checks and maintenance

- Field blanks (at least once a month if daily measurements are performed, preferably once a week) by following the full procedure unless placing the filter holder with the filter into the sampling unit and pump on
- Maintenance of the individual system in accordance with the manufacturer's specifications
- Maintenance of the sampling system: Cleaning of the sampling head (monthly or if an obvious error occurs), sample flow control, control the temperature and pressure sensor (every three months), maintain the sampling pump (yearly)
- Reference: EN 12341:2023 (Ambient air – Standard gravimetric measurement method for the determination of the PM10 or PM2.5 mass concentration of suspended particulate matter)
- *Current CC status: Recommendations set!*

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Additional requirements at the field site

- If any filter manipulation is done at the field site, a clean work area (work bench with clean surface) is required, plus cleaned devices for all performed steps (laboratory standard), ideally in a filtered flow hood or glove box (particle free air)
- Basic laboratory equipment (gloves, tissue, tweezers, etc.) needed
- Equipment for comprehensive documentation of all sampling steps and special occurrences which is needed for reporting and potential flagging of data

- *Current CC status: Recommendations set!*

1 st OGAC-CC community meeting 2024 (online) – Agenda Tuesday April 9	
13:00 - 13:15	Welcome
13:15 - 13:45	Introduction of OGAC-CC
13:45 - 14:30	Presentation of the Tech <ul style="list-style-type: none"> - Draft list of target co - Sampling procedure - Sample pre-treatment - Maintenance (Samp
14:30 - 14:45	Coffee break
14:45 - 15:30	Presentation of the Tech <ul style="list-style-type: none"> - Data resolution, coverage - Sample handling and - Recommended and s
15:30 - 16:00	Outlook on the Measurement Guidelines
16:00 - 16:15	Coffee break
16:15 - 16:45	Introduction ILC autumn 2024
16:45 - 17:00	Time for further discussion



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Data resolution/coverage

- Recommendation to **measure on a continuous basis**
- Minimum requirement is a weekly sample or one sample per week
- Exceptions need to be explained and individually discussed with the CC
- Exception could be an intensive measurement campaign, e.g. minimum 5 samples per campaign but then minimum two of these campaigns per year, ideally in two different seasons
- Coverage? > 80% of planned activity
- Overview current NFs:

NF	Birkenes	Zeppelin	Melpitz	Vielsalm	Sonnblick
Sampling time	One week	One week	24h	24h	One week
Intervall	weekly	weekly	daily	daily	weekly

Data provision (processing and submission)

➤ Overview current NFs:

NF	Birkenes	Zeppelin	Melpitz	Vielsalm	Sonnblick
Analysis	< 6 month after arrival in the lab	< 6 month after arrival in the lab	No internal rule	1 month	3 month

➤ *Current CC status: Data should be provided minimum 6 months after sampling*

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Technical requirements for laboratory analysis – general remarks

“The ACTRIS variable “organic tracers” is measured offline from aliquots filter or impactor substrate samples. For the quantification of organic tracers there are several analytical techniques with different suitable configurations, including detectors or chromatography columns from various suppliers available. OGTAC-CC does not explicitly specify which manufacturers, instruments or chromatographic columns are to be used for laboratory analysis. However, a minimum sensitivity, precision and calibration range for each analyte is defined that must be achieved in order to ensure NFs capabilities to measure typical organic tracer concentrations with appropriate analytical quality. Regular interlaboratory comparisons (ILCs) will be conducted to identify potential methodological deviations between NFs as a measure of quality control.”

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Sample handling and preparation in the laboratory

*This paragraph lists necessary **equipment** for all steps after the sample arrival at the laboratory until its chemical analysis, including storage, transfer and filtration.*

- Clean laboratory rooms for trace level chemical analysis
- Dedicated laboratory equipment (e.g., gloves, glassware) and workplaces to avoid cross contamination with potentially highly concentrated substances
- Dedicated space in a fridge or freezer for sample storage
- Samples must not be stored together with volatile substances or samples that may contain such components to avoid cross contamination
- A supply of ultra pure water ($R > 18.2$ megohm) is required for sample preparation steps and cleaning procedures

Sample handling and preparation in the laboratory

- Syringes, filters, vials, caps, pipette tips etc.

(All disposables in contact with samples can be a significant source of contamination and can have severe influence on the final results → Article number, batch numbers and supplier have to be documented → measurement guidelines)

- High quality solvents, standards (commercially available) or derivatization reagents
- Ultrasonication (*not recommended*) or shaking device
- Evaporator or vacuum concentrator, other enrichment devices if needed
- **Important:** document each step in detail!
- ILC to investigate also the impact of the type of sample treatment prior analysis → measurement guidelines
- Technical requirements updated accordingly

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Supported analytical techniques

- Recommended and supported analytical techniques and figures of merit to be met for the determination of particulate organics:

Target compound	Sum formula	IUPAC name	CAS number	Recommended and supported analytical technique	Analytical figures of merit
		Example for BB Module			
Levoglucosan	C ₆ H ₅ O ₁₀	(1R,2S,3S,4R,5R)-6,8-dioxabicyclo[3.2.1]octane-2,3,4-triol	498-07-7	HPAEC-PAD (HPLC-PAD)	...
Mannosan	C ₆ H ₅ O ₁₀	(1R,2S,3S,4S,5R)-6,8-dioxabicyclo[3.2.1]octane-2,3,4-triol	14168-65-1	HPAEC-PAD (HPLC-PAD)	...
Galactosan	C ₆ H ₅ O ₁₀	(1R,2R,3S,4R,5R)-6,8-dioxabicyclo[3.2.1]octane-2,3,4-triol	644-76-8	HPAEC-PAD (HPLC-PAD)	...
...

- Other analytical methods applicable, participation in ILC will demonstrate capabilities (quality control)
- Intensive exchange between the NF and the CC for 1st time documentation

The technical requirements document provides a comprehensive summary about the necessary hardware to determine organic tracers from filters following the requirements of the CC providing ACTRIS compliant data

- Sampler / Sampling unit
- Filter / impactor substrate
- Sample handling and transport
- Dedicated laboratory workplace, equipment and consumables
- Dedicated space in a fridge or freezer for sample storage
- Analytical measurement setup consisting of separation and detection unit
- Sufficient IT power for data storage and processing
- **Careful documentation → Any changes have to be announced to the CC!**

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13:00 - 13:15	Welcome
13:15 - 13:45	Introduction of OGTAC-CC
13:45 - 14:30	Presentation of the Technical Requirements and discussion part 1
	- Draft list of target compounds
	- Sampling procedure
	- Sample pre-treatment, storage and transport
	- Maintenance (Sampling)
14:30 - 14:45	Coffee break
14:45 - 15:30	Presentation of the Technical Requirements and discussion part 2
	- Data resolution, coverage and provision
	- Sample handling and preparation in the laboratory
	- Recommended and supported analytical techniques
15:30 - 16:00	Outlook on the Measurement Guidelines
16:00 - 16:15	Coffee break
16:15 - 16:45	Introduction ILC autumn 2024
16:45 - 17:00	Time for further discussion

