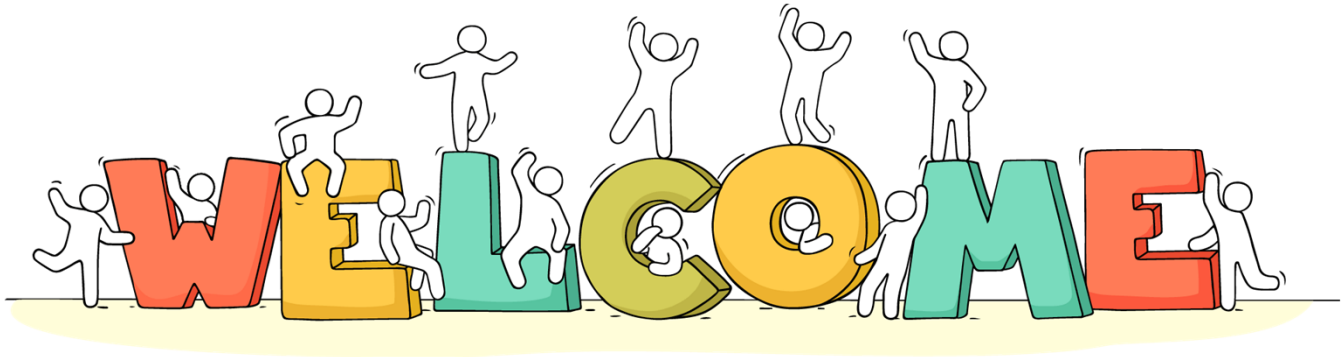
1st OGTAC-CC community meeting
April 09 2024



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(Part of) The TROPOS Atmospheric Chemistry Department (ACD) Team

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Head of ACD analytics

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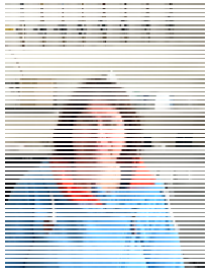

Anke Rödger

Dr. Uwe Käfer

Dr. Andreas Tilgner

Dr. Sebastian Zeppenfeld

Dr. Manuela van Pinxteren

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Participant overview

Country	Name	Affiliation /NF
Austria	Elke Ludewig	Sonnblick Observatory (SBO)
Austria	Anne Kasper-Giebl	Sonnblick Observatory (SBO)
Belgium	Benjamin Bergmans	Vielsalm
Czech Republic	Jaroslav Schwarz	ICPF CAS Prague
France	Jean-Luc Jaffrezo	University Grenoble
France	Aline Gratien	LISA
France	Emmanuelle Mebold	LISA
France	Nicolas Bonnaire	LSCE
France	Olivier Favez	ACMCC
Germany	Alexander Vogel	University Frankfurt
Germany	Laurent Poulain	TROPOS / Melpitz
Greece	Angeliki Matrali	University Patras
Greece	Stergiou Evangelos	University of Crete
Italy	Jean-Philippe Putaud	ERLAP
Norway	Karl-Espen Yttri	NILU - Birkenes / Zeppelin
Sweden	Radovan Krejci	Stockholm University / Zeppelin
Sweden	Margareta Sandahl	Lund University

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Agenda

1st OGTAC-CC community meeting 2024 (online) – Agenda Tuesday April 9	
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
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16:15 - 16:45	Introduction ILC autumn 2024
16:45 - 17:00	Time for further discussion

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Introduction of the OrGanic Tracers and Aerosol Constituents - Calibration Centre (OGTAC-CC)

Falk Mothes and Hartmut Herrmann

Atmospheric Chemistry Department (ACD), Leibniz Institute for Tropospheric Research (TROPOS),
Permoserstraße 15, 04318 Leipzig, Germany

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

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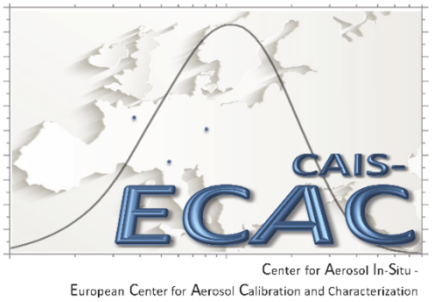
Overview

1) Introduction ACTRIS-D
2) ACTRIS @TROPOS and ACTRIS @Atmospheric Chemistry Department (ACD)
3) Organic Tracers and Aerosol Constituents – Calibration Centre (OGTAC-CC) @ACTRIS
   - Former activities within Eurochamp-2020
   - Ongoing work and current status
   - Planned activities



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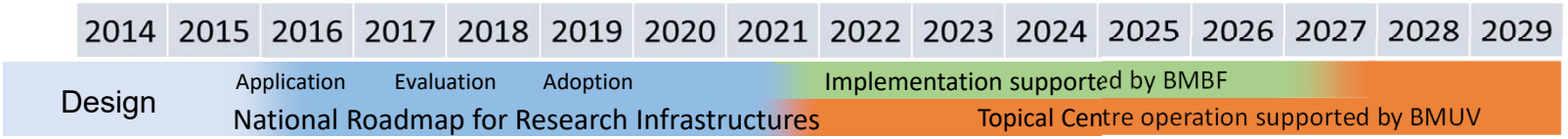
ACTRIS-D

The German contribution to the European Research Infrastructure for aerosol, clouds and trace gases

ACTRIS @TROPOS
ACTRIS @TROPOS ACD

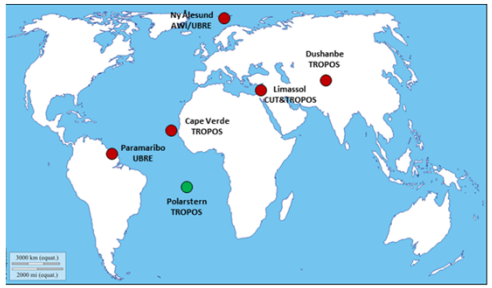
TROPOS

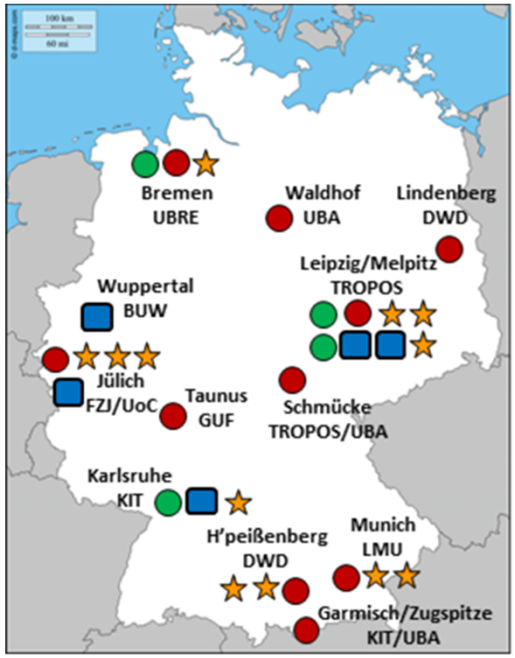
ACTRIS-D



- ACTRIS-D started in 2021 with 11 German partner institutions, led by TROPOS
- Implementation phase 2021-2026 is supported with 86 Mio. Euro by the BMBF (Federal Ministry of Education and Research)
- 27 NFs and 12 TCs in total
  - ➢ 15 Observational platforms
  - ➢ 5 Atmospheric simulation chambers
  - ➢ 7 Mobile platforms

  } Exploratory platfoms





- Operation supported by the BMUV (Federal Ministry for the Environment, Nature, Conservation, Nuclear Safety and Consumer Protection) since the **European Research Infrastructure Consortium (ERIC) was established** in March 2023

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TROPOS facilities

Topic Centre Units

World Calibration Center for Aerosol Physics (WCCAP)

OrGanic Tracers and Aerosol Constituents - Calibration Centre (OGTAC-CC)

Centre for Cloud Water Chemistry (CCWaC)

Observational Platforms

Melpitz Research Station

PollyNET

German Ultrafine Aerosol Network (GUAN)

Cape Verde Atmospheric Observatory (CVAO)

Schmücke Cloud Observatory (SCO)

Exploratory Platforms

Atmospheric Chemistry Department Chamber (ACD-C)

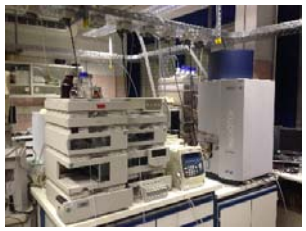
Turbulent Leipzig Aerosol Cloud Interaction Simulator (LACIS-T)

Leipzig Aerosol and Cloud Remote Observations System (LACROS)

Mobile shipborne facility (OCEANET)

Mobile shipborne facility on Polarstern-2 (OCEANET-2)

Aerosol from ground to Cloud Mobile Experiment (ACME)











Overview of former, current and planned activities of the OrGanic Tracers and Aerosol Constituents - Calibration Centre (OGTAC-CC)

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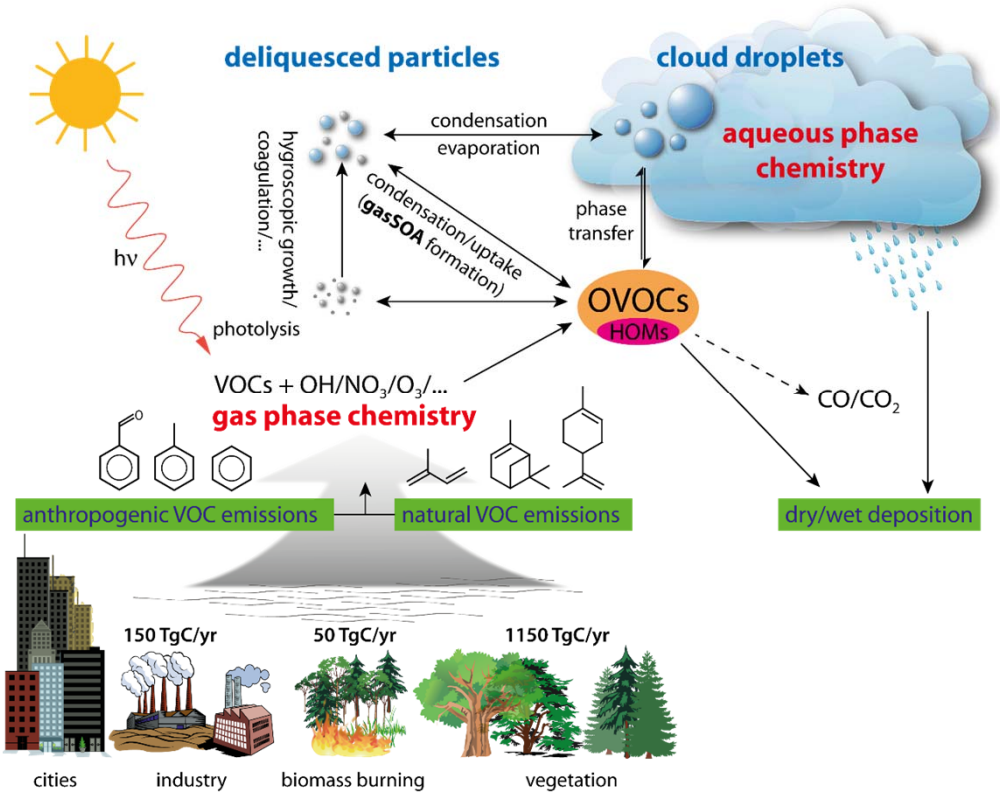
General overview

Why measuring organic tracers and aerosol constituents?

- Aerosol, clouds and trace gas understanding need the information on physical and chemical aerosol properties
- Gain detailed knowledge on aerosol chemical composition
- Improve the understanding on evolution in the atmosphere (transformation processes)
- Provide important compound specific input data for high quality source apportionment of organic aerosol and PM in addition to OC/EC and ACSM/AMS data



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General overview – former activities

Established as training/calibration centre within EUROCHAMP-2020

EUROCHAMP 2020

2 main activities:

- Training
- Interlaboratory comparisons

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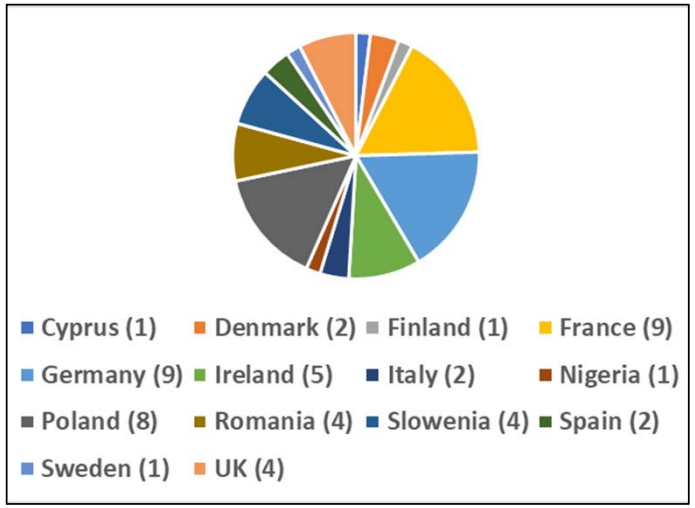
TRAINING

- 14 training sessions conducted within EUROCHAMP-2020 with 53 participants

- Individual trainings via TNAs or group trainings in forms of hands-on training workshops
- Lectures in atmospheric particle related chemical analysis
- Training sessions for the analysis of atmospherically relevant particulate products: filter collection, extraction, derivatization and enrichment procedures, analysis and quantification using state-of the-art instrumentation LC/MS; GC/MS and HPAEC/PAD

- 35% of users from EUROCHAMP partners



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General overview – former activities

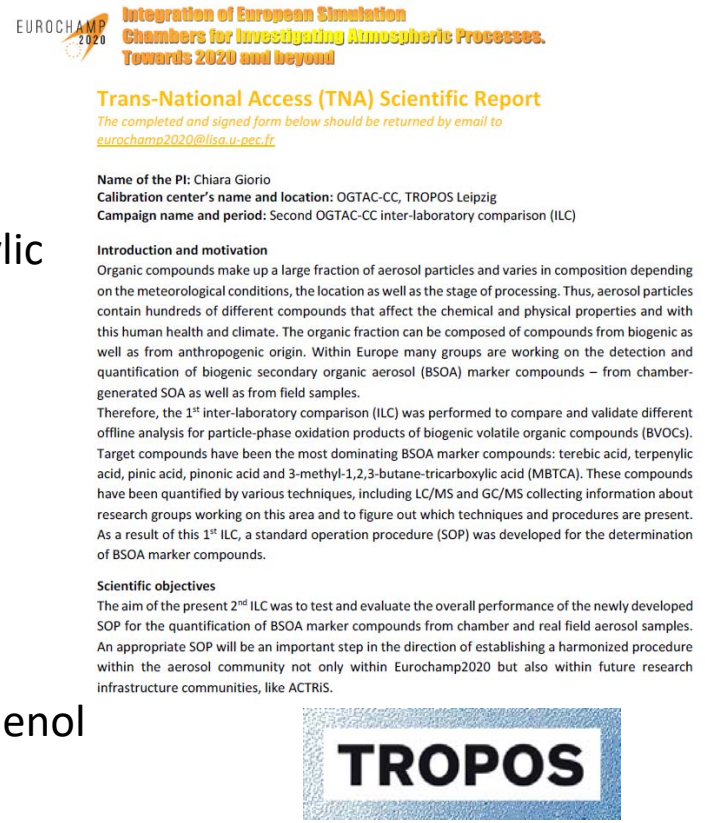
Interlaboratory comparisons (ILCs)

3 ILCs performed within the EUROCHAMP-2020 project:

→ Data evaluation according to ISO 13528 and ISO 5725-2

- **1st ILC on BSOA marker compounds w/o SOP (2018/2019)**
  - 9 participants (6 from Europe and US, 2 from Germany and TROPOS)
  - *MBTCA (3-methyl-1,2,3-butanetricarboxylic acid)*, terebic acid, terpenylic acid, pinic acid and pinonic acid
- **2nd ILC on BSOA marker compounds w/ draft SOP (2019-2021)**
  - 5 participants (4 from Europe and US and TROPOS)
- **3rd ILC on ASOA marker compounds w/o SOP (2021)**
  - 5 participants (4 from Europe and US and TROPOS)
  - syringaldehyde, 4-nitrophenol, 4-nitrocatechol and 2-methyl-4-nitrophenol

Collaboration between EUROCHAMP-2020 and ACTRIS-2 (WP3 Lead Erik Swietlicki (ULUND))



EUROCHAMP 2020 Integration of European Simulation Chambers for Investigating Atmospheric Processes. Towards 2020 and beyond

Trans-National Access (TNA) Scientific Report

The completed and signed form below should be returned by email to eurochamp2020@lisa.u-pec.fr

Name of the PI: Chiara Giorio
Calibration center's name and location: OGTAC-CC, TROPOS Leipzig
Campaign name and period: Second OGTAC-CC inter-laboratory comparison (ILC)

Introduction and motivation

Organic compounds make up a large fraction of aerosol particles and varies in composition depending on the meteorological conditions, the location as well as the stage of processing. Thus, aerosol particles contain hundreds of different compounds that affect the chemical and physical properties and with this human health and climate. The organic fraction can be composed of compounds from biogenic as well as from anthropogenic origin. Within Europe many groups are working on the detection and quantification of biogenic secondary organic aerosol (BSOA) marker compounds – from chamber-generated SOA as well as from field samples.

Therefore, the 1st inter-laboratory comparison (ILC) was performed to compare and validate different offline analysis for particle-phase oxidation products of biogenic volatile organic compounds (BVOCs). Target compounds have been the most dominating BSOA marker compounds: terebic acid, terpenylic acid, pinic acid, pinonic acid and 3-methyl-1,2,3-butane-tricarboxylic acid (MBTCA). These compounds have been quantified by various techniques, including LC/MS and GC/MS collecting information about research groups working on this area and to figure out which techniques and procedures are present. As a result of this 1st ILC, a standard operation procedure (SOP) was developed for the determination of BSOA marker compounds.

Scientific objectives

The aim of the present 2nd ILC was to test and evaluate the overall performance of the newly developed SOP for the quantification of BSOA marker compounds from chamber and real field aerosol samples. An appropriate SOP will be an important step in the direction of establishing a harmonized procedure within the aerosol community not only within Eurochamp2020 but also within future research infrastructure communities, like ACTRiS.

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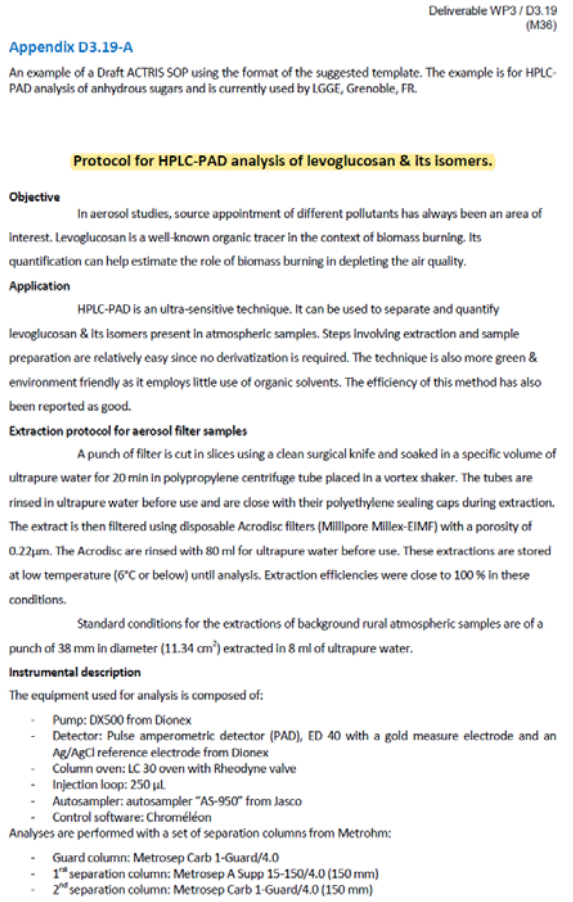
Former ACTRIS activities

By Erik Swietlicki, Karl Espen Yttri, Jean-Luc Jaffrezo et al.

Biomass Burning as source:

- Levoglucosan, Mannosan, Galactosan – ILC performed within ACTRIS-2 [1] → Methods: HPLC/ESI-MS, HPAEC-PAD, GC/MS
- ➢ Analytical methods are significantly different regarding sample preparation (extraction, derivatization), separation and detection
- ➢ All methods seem to be reliable making a general European SOP complex
- ➢ Draft SOP (protocol) available from ACTRIS PPP WP3-NA3 Deliverable D3.19 using HPLC-PAD
- ➢ Publication "An intercomparison study of analytical methods used for quantification of levoglucosan in ambient aerosol filter samples" in AMT 2015



Deliverable WP3 / D3.19
(M36)

Appendix D3.19-A

An example of a Draft ACTRIS SOP using the format of the suggested template. The example is for HPLC-PAD analysis of anhydrous sugars and is currently used by LGGE, Grenoble, FR.

Protocol for HPLC-PAD analysis of levoglucosan & its isomers.

Objective

In aerosol studies, source appointment of different pollutants has always been an area of interest. Levoglucosan is a well-known organic tracer in the context of biomass burning. Its quantification can help estimate the role of biomass burning in depleting the air quality.

Application

HPLC-PAD is an ultra-sensitive technique. It can be used to separate and quantify levoglucosan & its isomers present in atmospheric samples. Steps involving extraction and sample preparation are relatively easy since no derivatization is required. The technique is also more green & environment friendly as it employs little use of organic solvents. The efficiency of this method has also been reported as good.

Extraction protocol for aerosol filter samples

A punch of filter is cut in slices using a clean surgical knife and soaked in a specific volume of ultrapure water for 20 min in polypropylene centrifuge tube placed in a vortex shaker. The tubes are rinsed in ultrapure water before use and are close with their polyethylene sealing caps during extraction. The extract is then filtered using disposable Acrodisc filters (Millipore Millex-EIMF) with a porosity of 0.22µm. The Acrodisc are rinsed with 80 ml for ultrapure water before use. These extractions are stored at low temperature (6°C or below) until analysis. Extraction efficiencies were close to 100 % in these conditions.

Standard conditions for the extractions of background rural atmospheric samples are of a punch of 38 mm in diameter (11.34 cm^2) extracted in 8 ml of ultrapure water.

Instrumental description

The equipment used for analysis is composed of:

- Pump: DX500 from Dionex
- Detector: Pulse amperometric detector (PAD), ED 40 with a gold measure electrode and an Ag/AgCl reference electrode from Dionex
- Column oven: LC 30 oven with Rheodyne valve
- Injection loop: 250 µl
- Autosampler: autosampler "AS-950" from Jasco
- Control software: Chromeleon

Analyses are performed with a set of separation columns from Metrohm:

- Guard column: Metrosep Carb 1-Guard/4.0
- 1st separation column: Metrosep A Supp 15-150/4.0 (150 mm)
- 2nd separation column: Metrosep Carb 1-Guard/4.0 (150 mm)

[1] K.E. Yttri, J. Schnelle-Kreis, W. Maenhaut, G. Abbaszade, C. Alves, A. Bjerke, N. Bonnier, R. Bossi, M. Claeys, C. Dye, M. Evtyugina, D. Garcia-Gacio, R. Hillamo, A. Hoffer, M. Hyder, Y. Iinuma, J.L. Jaffrezo, A. Kasper-Giebl, G. Kiss, P.L. Lopez-Mahia, C. Pio, C. Piot, C. Ramirez-Santa-Cruz, J. Sciare, K. Teinila, R. Vermeylen, A. Vicente, R. Zimmermann, An intercomparison study of analytical methods used for quantification of levoglucosan in ambient aerosol filter samples, Atmos. Meas. Tech., 8 (2015) 125-147.

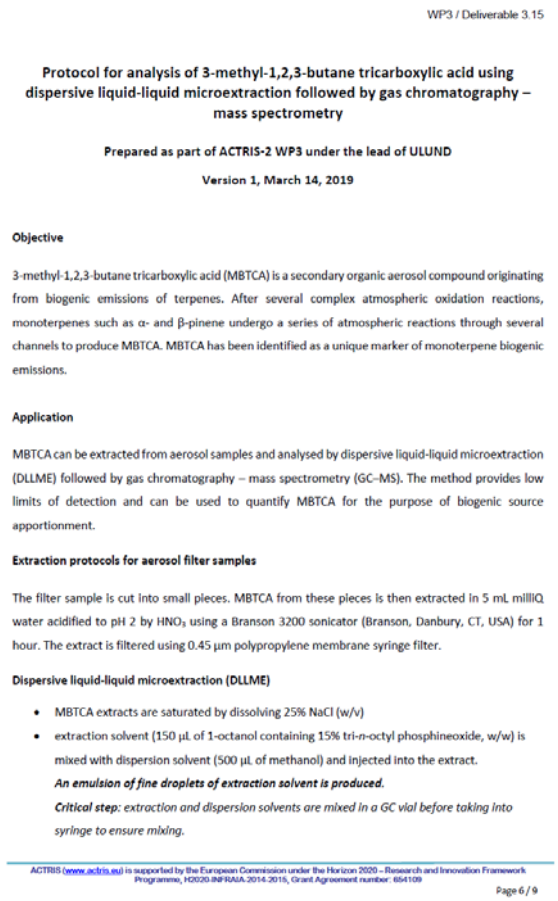
TROPOS

Former ACTRIS activities

By Erik Swietlicki, Karl Espen Yttri, Jean-Luc Jaffrezo et al.

Biogenic secondary organic aerosol (BSOA):

- MBTCA (3-methyl-1,2,3-butanetricarboxylic acid) – 2 ILCs performed in collaboration of EUROCHAMP2020 and ACTRIS-2
- Target compounds besides MBTCA: terebic acid, terpenylic acid, pinonic acid and pinic acid
- Methods: LC/MS, GC/MS
- Draft SOP (protocol) available for MBTCA within ACTRIS-2 WP3 Del. 3.15 using GC/MS after liquid-liquid microextraction
- Draft SOP (protocol) on the full process starting from the filter sample, extraction procedure and final analysis by LC/MS was tested within the 2nd ILC of EUROCHAMP-2020



WP3 / Deliverable 3.15

Protocol for analysis of 3-methyl-1,2,3-butane tricarboxylic acid using dispersive liquid-liquid microextraction followed by gas chromatography – mass spectrometry

Prepared as part of ACTRIS-2 WP3 under the lead of ULUND

Version 1, March 14, 2019

Objective

3-methyl-1,2,3-butane tricarboxylic acid (MBTCA) is a secondary organic aerosol compound originating from biogenic emissions of terpenes. After several complex atmospheric oxidation reactions, monoterpenes such as α- and β-pinene undergo a series of atmospheric reactions through several channels to produce MBTCA. MBTCA has been identified as a unique marker of monoterpene biogenic emissions.

Application

MBTCA can be extracted from aerosol samples and analysed by dispersive liquid-liquid microextraction (DLLME) followed by gas chromatography – mass spectrometry (GC–MS). The method provides low limits of detection and can be used to quantify MBTCA for the purpose of biogenic source apportionment.

Extraction protocols for aerosol filter samples

The filter sample is cut into small pieces. MBTCA from these pieces is then extracted in 5 mL milliQ water acidified to pH 2 by HNO_3 using a Branson 3200 sonicator (Branson, Danbury, CT, USA) for 1 hour. The extract is filtered using 0.45 µm polypropylene membrane syringe filter.

Dispersive liquid-liquid microextraction (DLLME)

- MBTCA extracts are saturated by dissolving 25% NaCl (w/v)
- extraction solvent (150 µL of 1-octanol containing 15% tri-*n*-octyl phosphineoxide, w/w) is mixed with dispersion solvent (500 µL of methanol) and injected into the extract.

An emulsion of fine droplets of extraction solvent is produced.

Critical step: *extraction and dispersion solvents are mixed in a GC vial before taking into syringe to ensure mixing.*

ACTRIS (www.actris.eu) is supported by the European Commission under the Horizon 2020 – Research and Innovation Framework Programme, H2020-INFRAIA-2014-2015, Grant Agreement number: 654109

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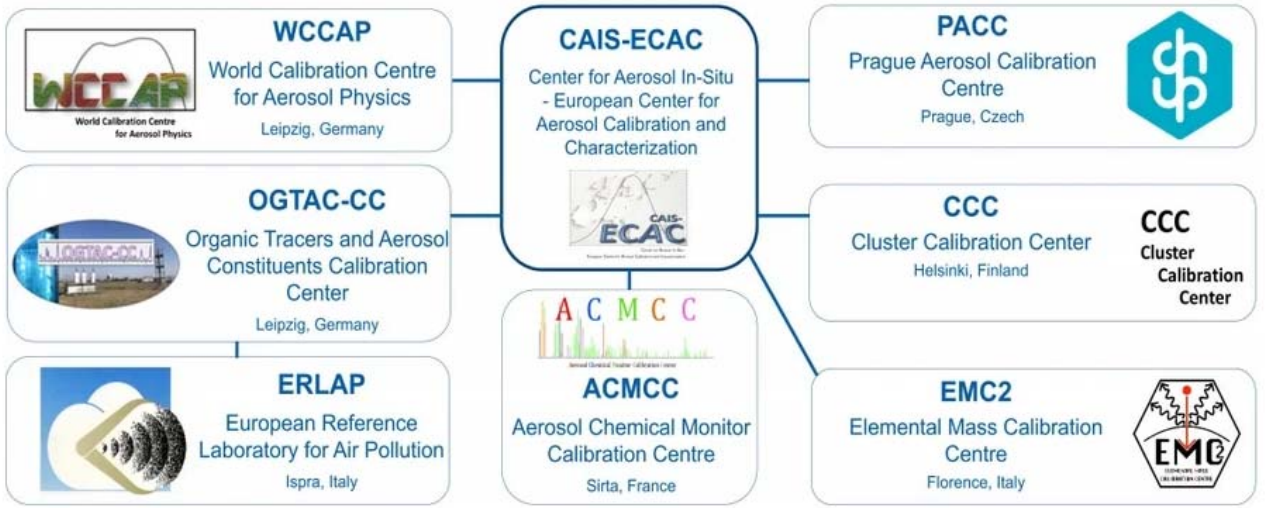
General overview – current status

- Within ACTRIS OGTAC-CC became an Aerosol in situ TC unit as one partner of the Center for Aerosol In Situ-European Center for Aerosol Calibration and Characterizatio (CAIS-ECAC)
- TC parameter: Mass concentration of particulate organic tracer compounds



CAIS-ECAC is a consortium, consisting of seven facilities. The WCCAP (World Calibration Center for Aerosol Physics), PACC (Prague Aerosol Calibration Center), and CCC (Cluster Calibration Center) are responsible for aerosol microphysical and optical aerosol variables. The OCTAC-CC (Organic Tracer and Aerosol Constituents - Calibration Center), ERLAP (European Reference Laboratory for Air Pollution), the ACMCC (Aerosol Chemical Monitor Calibration Center) and EMC2 (Element Mass Calibration Center) are in charge of the chemical & elemental aerosol variables.

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General overview – current status

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).

ACTRIS aerosol in-situ variables

Five out of the 12 ACTRIS aerosol in-situ variables are obligatory for NFs (observatories). The number of obligatory variables for exploratory and mobile platforms may differ and is explained elsewhere.

Obligatory ACTRIS aerosol in-situ variables for observatories:

- Particle number concentration D_{P50} = 10 nm (EN-16976)
- Particle number size distribution – mobility diameter 10 to 800 nm (CEN/TS-17434) [1)]
- Particle light scattering & backscattering coefficient - multi-wavelength [2)]
- Particle light absorption coefficient and/or equivalent black carbon concentration [2)]
- At least one additional variable from the list below, preferably a variable on particle chemical or elemental composition, considering the scientific program of the NF.

TROPOS

General overview – current status

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).

Other ACTRIS aerosol in-situ variables:

- Nano-particle number concentration (D_{P50} < 10 nm)
- Nano-particle number size distribution < 10 nm
- Particle number size distribution - aerodynamic diameter 0.8 to 10 µm [3)]
- Cloud condensation nuclei number concentration
- Mass concentration of particulate organic tracers / unit: (ng m^{-3})
- Mass concentration of particulate organic and elemental carbon [4)]
- Mass concentration of non-refractory particulate organics and inorganics within PM1 fraction [5,6)]
- Mass concentration of particulate elements [2)]

OGTAC-CC @TROPOS

subcontracting

European Reference Laboratory for Air Pollution – ERLAP, Italy

Dr. Fabrizia Cavalli
(fabrizia.cavalli@ec.europa.eu)

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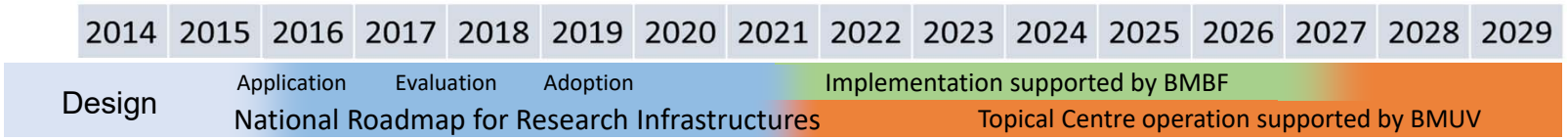
Current status within implementation phase



2 main pillars remain:

1) Training of operators and scientists – operational activity

2) Calibration Centre Activities – task chain

a) implementation → b) operation

\+ Trans National Access (TNA), but currently no official project running

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Hands-on training workshop March and November 2023 @TROPOS ACD, Leipzig (Germany)

1) Training of operators and scientists

1st training within ACTRIS performed in March 2023 @TROPOS

2nd training @TROPOS in November 2023

<u>Topic:</u> Theory and practice - determination of organic tracers and aerosol constituents from sampling to the final result demonstrated for the future ACTRIS platforms Melpitz (observational) and ACD-C (exploratory)

Planned activities within implementation phase

2) Calibration Centre Activities – task chain

- Definition of target compounds, e.g., biomass burning or on secondary organic aerosol constituents of biogenic and anthropogenic origin
- Set up technical requirements, for all steps from sampling to the quantitative result, set Data Quality Objectives (DQO)
- Development of measurement guidelines based on the technical requirements and Interlaboratory Comparisons (ILCs)
- Standard Operating Procedure (SOP) templates needs to be finalized by each NF individually together with the calibration centre
- NF individual SOP will finally need approval by the calibration centre
- Define QA/QC procedures, e.g., performance test by ILCs
- Develop workflow for offline data submission

→ All in close collaboration with the NFs!!!

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Agenda

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	- 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

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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

Leibniz Association

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Technical requirements documentation

Content:

TROPOS

Technical requirements documentation

Content:

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

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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	Biomass burning (Anhydromonosaccharides)	
1	Levoglusosan	$C_6H_5O_{10}$
2	Mannosan	$C_6H_5O_{10}$
3	Galactosan	$C_6H_5O_{10}$
Module	Primary biogenic (pollen / fungal spores)	
1	Erythritol	$C_4H_{10}O_4$
2	Arabitol	$C_5H_{12}O_5$
3	Glucose	$C_6H_{12}O_6$
4	Fructose	$C_6H_{12}O_6$
5	Mannose	$C_6H_{12}O_6$
6	Galactose	$C_6H_{12}O_6$
7	Mannitol	$C_6H_{14}O_6$
8	Ergosterol	$C_{28}H_{44}O$
Module	Organic ions (inorganic IC mesaurement byproducts)	
1	Oxalate	$C_2O_4^{2-}$
2	Formate	CHO_2^-
3	Methane sulfonic acid	$CH_4O_3S^-$
Module	Biogenic SOA - acids	
1	Terebic acid	$C_7H_{10}O_4$
2	Vanillic acid	$C_8H_8O_4$
3	Isovanillic acid	$C_8H_8O_4$
4	MBTCA	$C_8H_{12}O_6$
5	Norpinonic acid	$C_9H_{14}O_3$
6	Pinic acid	$C_9H_{14}O_4$
7	Pinonic acid	$C_{10}H_{16}O_3$

Module	SOA - aldehydes	
1	Vanillin	$C_8H_8O_3$
2	Syringaldehyde	$C_9H_{10}O_4$
3	Coniferyl aldehyde	$C_{10}H_{10}O_3$
(4	Acetosyringone	$C_{10}H_{12}O_4$)
Module	SOA - nitroaromatics	
1	4-nitrophenol	$C_6H_5NO_3$
2	3-Nitrocatechol	$C_6H_5NO_4$
3	4-nitrocatechol	$C_6H_5NO_4$
4	2-methyl-4-nitrophenol	$C_7H_7NO_3$
5	4-Nitroguaiacol	$C_7H_7NO_4$
6	4-Methyl-5-nitrocatechol	$C_7H_7NO_4$
7	3-methyl-5-nitrocatechol	$C_7H_7NO_4$
Module	16 EPA PAHs	
1	Naphthalene	$C_{10}H_8$
2	Acenaphthylene	$C_{12}H_8$
3	Acenapthene	$C_{12}H_{10}$
4	Fluorene	$C_{13}H_{10}$
5	Phenanthrene	$C_{14}H_{10}$
6	Anthracene	$C_{14}H_{10}$
7	Fluoranthene	$C_{16}H_{10}$
8	Pyrene	$C_{16}H_{10}$
9	Benz(a)anthracene	$C_{18}H_{12}$
10	Chrysene	$C_{18}H_{12}$
11	Benzo[b]fluoranthene	$C_{20}H_{12}$
12	Benzo[k]fluoranthene	$C_{20}H_{12}$
13	Benzo[a]pyrene	$C_{20}H_{12}$
14	Indeno[1,2,3-cd]pyrene	$C_{22}H_{12}$
15	Benzo[ghi]perylene	$C_{22}H_{12}$
16	Dibenz[a,h]anthracene	$C_{22}H_{14}$
Module	Hopane + Sterane for traffic OA???	

ACTRIS Vocabulary

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:	RDF/XML TURTLE JSON-LD

TROPOS

Data Quality Objective

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

Module dependent

- 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)

TROPOS

Technical requirements documentation

Content:

1) About this document
2) Data Quality Objectives
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   - 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

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

TROPOS

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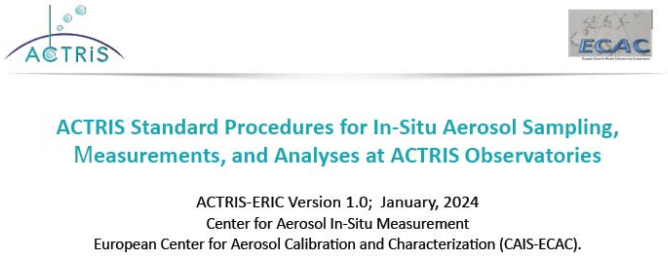
All information about general aerosol sampling, aerosol inlet design under consideration of the individual NF circumstances and aerosol conditioning are described in the overall document ***"ACTRIS Standard Procedures for In-Situ Aerosol Sampling, Measurements, and Analyses at ACTRIS Observatories"***

→ *See ECAC website* https://www.actris-ecac.eu/



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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!*

TROPOS

Aerosol particle sampler / sampling

Filter sampler overview:

		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

Technical requirements documentation

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   - 3.5 Sampling system checks and maintenance
   - 3.6 Additional requirements at the field site
   - 3.7 Data resolution, coverage and provision

TROPOS

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

TROPOS

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!*

TROPOS

Technical requirements documentation

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

TROPOS

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

TROPOS

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 OGTAC-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?

TROPOS

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

TROPOS

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!*

TROPOS

Technical requirements documentation

Content:

TROPOS

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!*

TROPOS

Technical requirements documentation

Content:

TROPOS

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!*

TROPOS

Agenda

1st OGTAC-CC community meeting 2024 (online) – Agenda Tuesday April 9	
13:00 - 13:15	Welcome
13:15 - 13:45	Introduction of OGTAC-CC
13:45 - 14:30	Presentation of the Tech
	- Draft list of target co
	- Sampling procedure
	- Sample pre-treatmer
	- Maintenance (Sampl
14:30 - 14:45	Coffee break
14:45 - 15:30	Presentation of the Tech
	- Data resolution, cove
	- 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

TROPOS

Technical requirements documentation

Content:

TROPOS

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 mimimum 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

TROPOS

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*

TROPOS

Technical requirements documentation

Content:

TROPOS

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."

TROPOS

Technical requirements documentation

Content:

TROPOS

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

TROPOS

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

TROPOS

Technical requirements documentation

Content:

TROPOS

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 Example for BB Module	CAS number	Recommended and supported analytical technique	Analytical figures of merit
Levoglucosan	$C_6H_5O_{10}$	(1R,2S,3S,4R,5R)-6,8-dioxabicyclo[3.2.1]octane-2,3,4-triol	498-07-7	HPAEC-PAD (HPLC-PAD)	…
Mannosan	$C_6H_5O_{10}$	(1R,2S,3S,4S,5R)-6,8-dioxabicyclo[3.2.1]octane-2,3,4-triol	14168-65-1	HPAEC-PAD (HPLC-PAD)	…
Galactosan	$C_6H_5O_{10}$	(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

TROPOS

Summary

The technical requirements document provides a comprehensive summary about the neccessary 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!

TROPOS

Agenda

1st OGTAC-CC community meeting 2024 (online) – Agenda Tuesday April 9	
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

TROPOS

Measurement Guidelines

for the determination of particulate organics

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

Leibniz Association

TROPOS
Leibniz Institute for Tropospheric Research

Outlook Measurement Guidelines

Content:

1) About this document
2) Data Quality Objectives
3) Particle sampling protocol
   - 3.1 General considerations
   - 3.2 Handling aerosol particle sampler (offline)
   - 3.3 Sample pre-treatment, storage and transport
   - 3.4 Documentation of the procedure
   - 3.5 Cleaning and maintenance
   - 3.6 Quality management (field blanks)
4) Laboratory analysis protocol
   - 4.1 Sample preparation
   - 4.2 Analytical procedure
5) Data submission

Module dependent!

TROPOS

Outlook Measurement Guidelines

Content:

1) About this document
2) Data Quality Objectives

Similar and identical to the technical requirements, respectively

3) Particle sampling protocol
   - 3.1 General considerations
   - 3.2 Handling aerosol particle sampler (offline)
   - 3.3 Sample pre-treatment, storage and transport
   - 3.4 Documentation of the procedure
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TROPOS

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4) Laboratory analysis protocol
   - 4.1 Sample preparation
   - 4.2 Analytical procedure
5) Data submission

General recommendations from the CC that can be individually adjusted by the NF (proof of quality required)

TROPOS

Particle sampling protocol

Contains:

- General aerosol particle sampling procedures given in the technical requirements, incl. documentation of experimental parameters (T, RH, flow rate, start end end time, batch numbers, etc.)
- Low-volume sampling following the EUSAAR OC/EC protocol
- High-volume sampling under discussion (cf. technical requirements)
- Filter/ substrate pre-treatment procedure
- Recommendation to minimize transfer steps, transport and storage times, *test experiments on the impact of sample storage currently ongoing (for the BB module)*
- *Maybe module dependent…*

TROPOS

Particle sampling protocol

Contains:

- Maintenance and cleaning procedures
- System checks on a routine basis
- 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

TROPOS

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   - 3.6 Quality management (field blanks)
4) Laboratory analysis protocol
   - 4.1 Sample preparation
   - 4.2 Analytical procedure
5) Data submission

Module dependent

TROPOS

Laboratory analysis protocol

- 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
Levoglucosan	$C_6H_5O_{10}$	(1R,2S,3S,4R,5R)-6,8-dioxabicyclo[3.2.1]octane-2,3,4-triol	498-07-7	HPAEC-PAD (HPLC-PAD)	…
Mannosan	$C_6H_5O_{10}$	(1R,2S,3S,4S,5R)-6,8-dioxabicyclo[3.2.1]octane-2,3,4-triol	14168-65-1	HPAEC-PAD (HPLC-PAD)	…
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…	…	…	…	…	…

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

TROPOS

Sample preparation / extraction procedure

Example BB module – overview current NFs:

NF	Birkenes	Zeppelin	Melpitz	Vielsalm	Sonnblick
Analytical technique	UPLC-Orbitrap MS	UPLC-Orbitrap MS	HPAEC-PAD	GC-MS	HPAEC-PAD
Extraction procedure	Filter sample (1.5 cm^2 or 3.0 cm^2) submerged by precleaned THF (2 mL) in a screw neck brown colored glassware vial, which is subjected to ultrasonic extraction (30 min). The solute is transferred to a centrifuge tube by pipetting. This step is performed twice. The solute is evaporated to 0.4 mL, spun (10 min; 2000 rpm) and transferred to a screw neck brown colored glassware vial to which Milli-Q water (450 µl) is added. The total volume is adjusted to 1 mL by precleaned THF. The sample is whirlmixed before analysis.		3 Spots (diameter 14mm) + 10ml ultrapure water 2h shaking (420rpm) filtration using a 0.45µm syringe filter (IC-Acrodisc, PALL)	We use the entire filter minus 1,5cm^2 for EC/OC. Add levoglucosan d7, Extraction with 5 ml 80/20 dichloromethane/methanol. Ultrasonication 2 times 15 minutes in a bath at 60°C. Add extraction IS at 1 ml extract. Evaporate to dryness, Derivatisation with BSTFA with 1% TMCS and anhydric pyridin, Incubation 1 hour at 80°C. Then add dodécane, Gently evaporation (40°C) and add cyclohexane to 1ml.	punches (PM10: 4,52 cm^2, PM1: 2,26 cm^2) are extracted with ultrapure water (Milli-Q) (PM10: 2 mL, PM1: 3 mL) by ultrasonic agitation (20 min), follwed by centrifugation

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Sample preparation / extraction procedure

Example BB module – recommendation for HPAEC-PAD:

- Use the minimum required filter area to minimize the amount of extraction solvent plus use appropriate labware (e.g., extraction in small Eppendorf vials, plastic labware need to be borate free)
- Document the filter area and the amount of extraction solvent
- Extraction solvent: ultrapure water
- Sample shaking (no ultrasonication), 2h / 420rpm
- *Impact ultrasonication on anhydrosugars - any experience? TROPOS ACD test experiments ongoing together with the federal agency for the environment in Saxony – work in progress!*
- Filtration via 0.45µm PTFE filter (e.g., syringe filter), avoid cellulose filters

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Analytical procedure

Instrument information:

- General type
- Autosampler type
- Injector (amount of injected volume)
- Detection unit
- All linked to the instrument database!
- Separation column (stationary phase)
- Mobile phase

Analytical conditions:

- Flow rate
- Temperature program
- Gradients
- Oven temperature
- Concentrations/mixtures

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Analytical procedure

Calibration:

- External calibration
- Standards; purity and concentration
- Number of standards and repetitions is not yet decided – Should be done for each analytical sequence

Quality management:

- Solvents, Eluents, derivatization reagents and water in sufficient purity
- Gases in sufficient purity

→ Input from the NFs through the ILC

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QA/QC and maintenance of the analytical setup

- QA/QC tests are part of the annual ILC but should be done routinewise minimum 4 times a year in total, including:
  - Recovery control for evaluation of the extraction
  - Repeatability
  - (Reproducibility)

  } *DQOs*

- Data checks on a routine basis

Maintenance example HPAEC-PAD:

- Polishing of the working electrode and rigorous cleaning of the instrument to avoid electrode surface poisoning, e.g. if before high salt containing samples have been analyzed
- Cleaning should include also tubing and fittings

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Outlook Measurement Guidelines

Content:

1) About this document
2) Data Quality Objectives
3) Particle sampling protocol
   - 3.1 General considerations
   - 3.2 Handling aerosol particle sampler (offline)
   - 3.3 Sample pre-treatment, storage and transport
   - 3.4 Documentation of the procedure
   - 3.5 Cleaning and maintenance
   - 3.6 Quality management (field blanks)
4) Laboratory analysis protocol
   - 4.1 Sample preparation
   - 4.2 Analytical procedure
5) Data submission

Data aquisition and processing

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Data aquisition and processing

General:

- Sequence table shall include a defined set of samples, blanks and control standards, e.g. one control standard every 10 samples
- Peak integration should preferably be done automatically (e.g. Chromeleon software)
- Sample results need to be in the calibrated concentration range of the target compound, if not samples need to be diluted
- *Offline data workflow includes preparation, exposure, extraction and analysis protocol (machine readable protocol database)*
  → *see presentation by Markus Fiebig*
- Data provision always as 1) raw data plus the corresponding calibration curves, 2) processed to the level of mass per volume extraction solvent and 3) processed to the level of atmospheric concentration in mass per volume air

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2) Calibration Centre Activities – task chain

- Definition of target compounds, e.g., biomass burning or on secondary organic aerosol constituents of biogenic and anthropogenic origin
- Set up technical requirements, for all steps from sampling to the quantitative result, set Data Quality Objectives (DQO)
- Development of measurement guidelines based on the technical requirements and Interlaboratory Comparisons (ILCs)

Future activities:

- SOP templates needs to be finalized by each NF individually together with the calibration centre containing step by step instructions for a specific sampler/analytical method combination at the respective NF (max. level of detail)
- NF individual SOP will finally need approval by the calibration centre
- Define QA/QC procedures, e.g., performance test by ILCs
- Develop workflow for offline data submission

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Agenda

1st OGTAC-CC community meeting 2024 (online) – Agenda Tuesday April 9	
13:00 - 13:15	Welcome
13:15 - 13:45	Introduction of OGTAC-CC
13:45 - 14:30	Presentation of the Tech
	- Draft list of target co
	- Sampling procedure
	- Sample pre-treatmer
	- Maintenance (Sampl
14:30 - 14:45	Coffee break
14:45 - 15:30	Presentation of the Tech
	- Data resolution, cove
	- 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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1st OGTAC-CC ILC within ACTRIS

Autumn 2024

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

Leibniz Association

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Leibniz Institute for Tropospheric Research

Interlaboratory comparison

General aims:

- Determination of analytical limitations – LOD/LOQ
- Blank characterisation
- Evaluate analytical repeatability and reproducibility standard deviations
- Identification of biases/influencing factors on the quality of the provided data
- Results provide important input for the technical requirements documentation and the measurement guidelines
- 1st QA/QC activity for ACTRIS NFs measuring particulate organic tracers

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Based on the NFs planning to provide data on particulate organics, the 1st ILC will be (minimum) on the compounds from the BB module:

- Levoglucosan
- Mannosan
- Galactosan

→ Participation of the 5 NFs is obligatory
→ 10 participating groups would be optimal
→ Other groups measuring these compounds are very welcome to join!

Limitation is the amount of filter area!

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NF	Birkenes	Zeppelin	Melpitz	Vielsalm	Sonnblick
Target compounds	arabitol, mannitol, fructose, glucose, trehalose, levoglucosan, manonsan, galactosan, 2-methylerythritol, 2-methylthreitol	Arabitol, mannitol, fructose, glucose, trehalose, levoglucosan, mannosan, galactosan, 2-methylerythritol, 2-methylthreitol	Levoglucosan	Levoglucosan, Mannosan and galactosan.	selected carbohydrates (e.g. anhydrosugars, sugar alcohols, monosaccharides)

More compounds resulting from the applied analytical procedure are very welcome for the intercomparison!

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ILC program

- Planned duration of 3 months (e.g., Sept-Nov) for the full program:
  - Send around the test samples
  - Analysis
  - Provision of results
- Participants shall use their individual analytical measurement setup but need to follow the guidelines given by the CC with respect to:
  - Number of injections
  - Number of sample runs (repetitions)
  - Sequence design
  - Documentation

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ILC program

Sample overview and number of measurements:

- 1x field blank filter
- 2x real field samples

→ Triplicate analysis, each sample 3 times full procedure (single injection)

- 2x liquid standard solutions (different concentrations)

→ 3 injections each

Field samples (150mm quartz filter) will be collected using a High Volume Digitel sampler 24h at 500 L min^{-1}

→ Each participant will get a sufficient amount of filter area

→ The CC will store one 10mm punch from each filter area sample as control

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Next to do: Advertisement ☺

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Questions, comments…

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Agenda

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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
	- 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

Thanks for your attention!

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