Deliverable D3.1:
An expert workshop to determine the targeted set of OA tracers

This document was prepared by Erik Swietlicki (ULUND) after consultation with relevant ACTRIS partners

Work package no	**WP3**
Deliverable no.	**D3.1**
Lead beneficiary	**Partner 20 (ULUND)**
Deliverable type	☑ R (Document, report) ☐ DEC (Websites, patent fillings, videos, etc.) ☐ OTHER: please specify **..**
Dissemination level	☑ PU (public) ☐ CO (confidential, only for members of the Consortium, incl Commission)
Estimated delivery date	**Month 6**
Actual delivery date	***26/04/2016***
Version	**1**
Comments	*Delayed due to:* *(i) Expert workshop decided to be held in connection with WP3 Meeting in Athens (M7) for logistical reasons.* *(ii) Prolonged discussions on selection of new OA tracer following Athens meeting (in M7).* *(iii) Additional tests performed on MBTCA analysis before decision.*

1 Background – Task 3.1 subtask on organic aerosol tracers

This deliverable deals with Task 3.1 of WP3 (“Improvement of instrumentation, standardization and quality assessment of essential climate and air quality variables”). This task within ACTRIS-2 includes, among other variables, also selected Organic Aerosol (OA) tracer compounds. The OA tracer subtask aims to establish a set of common European Standard Operating Procedures (SOP) for sampling and analysis of a selection of organic tracers, in order to facilitate their subsequent implementation at several ACTRIS sites for the purpose of organic aerosol (OA) source apportionment across Europe. The work on OA tracers in Task 3.1 is a continuation of that performed within the EU FP7 Infrastructure Project ACTRIS (Task 3.3b).

According to the ACTRIS-2 Grant Agreement, Task 3.1 including the OA tracer part aims:

- to increase the amount and quality of delivered data,
- to control implementation of existing Standard Operation Procedures (SOP), and
- to eventually propose revisions.

This will be achieved (here only that relevant for OA tracers) via:

- inter-laboratory comparison exercises (round-robin),
- use of ACTRIS TNA (WP8).

In addition to core variables controlled in EU FP7 ACTRIS, which already includes SOPs for OC/EC and specific organic tracers, ACTRIS-2 will

- **implement control procedures** for **one additional organic tracer** for which SOPs were recently agreed upon in ACTRIS.

This means that within ACTRIS-2, inter-laboratory comparison (ILC) studies will be performed for anhydrous sugars (levoglucosan, mannosan, galactosan) since these were identified in EU FP7 ACTRIS as suitable tracers for biomass burning, and Draft SOPs were presented.

In addition to the implementation of control procedures for the anhydrous sugars, the ACTRIS-2 Grant Agreement further specifies that ILC studies will be performed to support the establishment of SOPs for variables not already addressed by EU FP7 ACTRIS, such as:

- tracers for primary and secondary OA from biogenic sources, as well as
- traffic OA.

The ILC will use both synthetic standards and ambient air test samples and will determine the quality performance of the participating laboratories.

This deliverable D3.1 describes how these objectives will be achieved and presents recommendations for which OA tracers that will be selected during ACTRIS 2.

2 Outline of the road forward for OA tracers in ACTRIS

The ACTRIS-2 WP3 Task 3.1 deliverables related to the work on Organic tracers are:

- Expert workshop to determine the targeted set of OA tracers (D3.1, public report, M6)
- Inter-laboratory comparison (ILC) studies for the targeted set of OA tracers (D3.10, confidential, M24)
- Standard Operating Procedures (SOPs) for the targeted set of OA Tracers (D3.15, public report, M36)

The deliverables are planned to follow a logical chain of events that, at the end of ACTRIS-2, will lead us further towards our final aim of achieving a comprehensive and informative source apportionment of the organic aerosol at ACTRIS sites across Europe. It will also provide quality-assured data for development and evaluation of chemical transport models. The combination of a validated OA source apportionment and modelling framework will, in turn, eventually be used to support political decision-making that aims to safe-guard human health and mitigate climate change in the EU member states.

The chain of events is:

i. Selection of additional candidate OA tracers;
ii. Performing ILC for the selected candidate OA tracers to estimate their applicability with ACTRIS;
iii. Establishing new SOPs for the suitable OA tracers for subsequent implementation in ACTRIS;
iv. Establishing control procedures for the suitable OA tracers (merging SOPs and ILC procedures);
v. Implementing the control procedures for the OA tracers at regular time intervals to ensure data quality and operability at ACTRIS sites.

Once completed for each candidate OA tracer, this procedure can then be repeated for additional tracers until an adequate, yet minimum, number of OA tracers are established and implemented within ACTRIS.

As noted already in EU FP7 ACTRIS Deliverable D3.19, intercomparison studies (ILC) are essential elements of the ACTRIS concept, since they are the tool by which to determine the applicability of a certain SOP and to establish control procedures that will ensure the quality and intercomparability of the acquired data across the ACTRIS network.

Regular ILC therefore form a vital part of the control procedures for the OA tracers as they enter into the more operational stage of implementation within the ACTRIS network. For comparison, this was the case already in EU FP7 ACTRIS for OC/EC.

An **ACTRIS control procedure** for a specific OA tracer is the combination of the SOP and a predefined schedule for ILC studies to be performed at regular time intervals. It also describes how the ILC should be carried out (ambient air test samples, synthetic standards, reference standards, blanks, instructions for handling, evaluation and reporting etc).

Two intercomparison studies for organic tracers were performed within EU FP7 ACTRIS. Both of these (for levoglucosan and 14C) were carried out with the intention to establish a sound basis for new SOPs.

EU FP7 ACTRIS concluded that there was adequate information regarding the interlaboratory applicability and suitability of anhydrous sugars (levoglucosan, mannosan, galactosan) as tracers for biomass burning for ACTRIS to suggest Draft SOPs for these compounds using GC, LC and HPAEC analytical techniques. More information can be found in EU FP7 ACTRIS Deliverable D3.19, and Draft

SOPs are publically available on the ACTRIS-2 webpage (http://www.actris.net/language/en-GB/ProjectResults/QualityStandards.aspx; then under >In-situ aerosol measurements >Organic tracers).

In performing the ILC, the **applicability of the SOPs for the anhydrous sugars was established**. In ACTRIS-2, the **next step is then to establish and implement control procedures** for these OA tracers to ensure the quality and intercomparability of the acquired data across the ACTRIS network.

As stated in the Grant Agreement, Task 3.1 will also conduct further ILC studies to support the **establishment of SOPs for additional OA tracers**, such as tracers for primary and secondary OA from biogenic sources, as well as traffic OA. For these new OA tracers however, no control procedures will be determined or implemented within the ACTRIS-2 timeframe.

For the anhydrous sugars, the steps in the chain of events that have already been completed are
(i) Selection, (ii) ILC performed, and (iii) Draft SOPs established. What remains are steps (iv) Establishing control procedures, and (v) Implementing the control procedures.

For additional candidate OA tracers, all five steps remain to be fulfilled, of which steps (i) to (iii) will be accomplished within the ACTRIS-2 timeframe.

It should be noted that it is the aim of this WP3 activity to apportion only the carbonaceous aerosol material (expressed as OA, TC, OC, EC) and not PM (Particulate Matter given as PM10, PM2.5 or PM1).

Ultimately, the European-scale OA source apportionment will be significantly supported by ACTRIS-2 Task 3.2.1 ("Development of a measurement standardization and data submission protocol for aerosol particle mass spectroscopy based on Aerosol Chemical Speciation Monitor (ACSM) products"). A large network of ACSM instruments are now being deployed across the ACTRIS station network, providing highly time-resolved OA concentration data that will be used also for source apportionment (see https://www.psi.ch/acsm-stations/about-actris). Due to the large differences in working principles, the OA source apportionment based on ACSM versus that based on OA tracers (derived from analytical chemistry) will differ. This does not mean that one is better that the other. They should be seen instead to provide equally important yet different views on the impact of various OA sources on a given receptor site. Indeed, the methods are highly complementary, for reasons that would lead too far to be discussed here.

It should also be noted here that ACTRIS-2 has no ambitions to further develop or recommend source-receptor models for OA source apportionment (Hopke, JAWMA 2016). Instead, we refer to the extensive work carried out within the FAIRMODE network (the European networks in the field of air quality modelling) coordinated by JRC (see http://fairmode.jrc.ec.europa.eu/wg3.html, and the European Reference Website for source apportionment http://source-apportionment.jrc.ec.europa.eu/). A thorough examination of the currently available source-receptor models can be found in the report entitled "European guide on air pollution source apportionment with receptor models" (Belis et al., 2014; available at http://source-apportionment.jrc.ec.europa.eu/Docu/EU_guide_on_SA.pdf). This report contains a guide and a European harmonised protocol prepared within the framework of the JRC initiative for the harmonisation of source apportionment using receptor models.

3 Time plan for OA tracers activities

The time plan for the activities related to organic tracers are essentially determined by the timing of the relevant ACTRIS-2 WP3 Task 3.1 deliverables (see Table 1 below).

Table 1. Time plan for OA tracer activities in ACTRIS-2.

ACTRIS Year >	Year 1				Year 2				Year 3				Year 4			
Calender Year >		2015	|		2016		|		2017		|		2018		|	2019
Activity↓/ Month >	MJJ	ASO	NDJ	FMA	MJJ	ASO	NDJ	FMA	MJJ	ASO	NDJ	FMA	MJJ	ASO	NDJ	FMA
WP3 workshops	KOM		‖				‖				‖				‖	
Selection of new OA tracers		D3.1	Select	Select												
ILC-1 BSOA tracers					Prep	Prep	ILC-1	D3.10								
New SOPs and Control Procedures									CP SOP	CP SOP	CP SOP	D3.15				
ILC-2 Levoglucosan													ILC2	ILC-2	ILC-2	
Final Reporting																FR

For **additional candidate OA tracers**, (including BSOA tracers), an ILC (ILC-1) will be carried out during M19-24 and reported in D3.10 (M24, confidential). The ILC will be preceded by a preparation phase during M13-18. The preparations include distribution of tasks, selection of samples and of standards, instructions for sample handling and reporting.

ILC-1 will result in the drafting of SOPs for those new OA tracers that fulfilled the applicability and quality requirements (M25-36), and reported in D3.15 (M36).

For the **anhydrous sugars** (including levoglucosan), control procedures (CP) will be established during M25-36, and reported in D3.15 (M36). The control procedures will then be implemented in the form of an ILC (ILC-2) during M37-45, and reported in the Final Report (prepared M46-48).

4 Selection of additional candidate OA tracers

During the EU FP7 ACTRIS project, the community focusing on organic tracers discussed a wide range of potential tracer compounds than might qualify for recommendation by ACTRIS. These are discussed in ACTRIS Deliverables D3.14 and D3.19 and are publically available at http://www.actris.net/language/en-GB/ProjectResults/QualityStandards.aspx.

Also during EU FP7 ACTRIS, several SOPs were received from the project partners, covering not only the anhydrous sugars, but also fungal spore tracers (arabitol, mannitol and trehalose), PAHs, tracers for gasoline and diesel traffic sources (hopanes and steranes), organic acids, organosulfates and radiocarbon. For many of these OA tracers, several SOPs were collected using different analytical techniques for the same tracer.

A recent review paper on “The Molecular Identification of Organic Compounds in the Atmosphere: State of the Art and Challenges” (Nozière et al, 2015) provides additional essential input to the discussion.

During the WP3 workshop in Athens 9-12 November 2015, the discussions on OA tracers were continued with the aim to draw up the plans for this activity within ACTRIS-2, and to select a targeted set of suitable OA tracers to be pursued for an ILC study and SOP. The conclusions of that expert workshop, complemented by ensuing discussions, are summarized in this deliverable.

Biogenic SOA tracers

One important legacy of ACTRIS is that the SOPs are implemented also in regular European air quality monitoring networks, such as EMEP. Traditionally, these activities have focused on anthropogenic pollutants, and air quality issues related to human health have lately been the main motivation for EU member states to fund such activities. What are then the arguments for proposing Biogenic SOA (BSOA) tracers for implementation in ACTRIS?

Firstly, OA constitutes a major mass fraction of the European aerosol. This has been clearly demonstrated, both using thermo-optical OC data vs PM, and with what is now becoming an extensive database from the ACTRIS ACSM network.

Secondly, through 14C (radiocarbon) analysis it has been clearly demonstrated that the fraction of the carbonaceous aerosol originating from non-fossil sources is equal to, or in many cases larger than, the fossil carbonaceous mass fraction.

Thirdly, a large portion of modern OA is caused by biomass burning, for which ACTRIS has identified levoglucosan as a suitable tracer. The remaining modern OA mass fraction is of biogenic origin, both primary and secondary in nature.

Emissions of α-pinene and other biogenic VOCs are likely to increase as a result of climate change (Hermansson et al, 2014; Kulmala et al, 2015). This biogenic response to a warming climate in Europe has been shown to provide a negative (cooling) feedback mechanisms, as observed at several ACTRIS sites (Paasonen et al, 2013).

As fossil fuels will be rapidly phased as a consequence of the COP21 Paris agreement, modern-carbon sources of SOA will tend to dominate in the near future, at least at remote ACTRIS sites. In parallel, emissions of SO_2, NOx and anthropogenic fossil VOC are also projected to decrease as a result of imposing even more stringent UN-ECE CLTRAP protocols and EU NEC directives. Of course, biogenic VOC (BVOC) emissions are not regulated, and instead increase as a result of climate change. As a result, future air quality issues will increasingly be related to BVOC and BSOA, meaning that they will not only be of interest to the climate science community.

Transportation is still a major SOA source, and it would be advantageous to be able to observe the diminishing importance of fossil fuels used for transportation and the gradual transition towards renewable fuels. Doing so would offer a way to safeguard the quality of the national emissions reports compiled by each EU member state and track the rate of progress towards a completely fossil-free transportation system.

There is still a large uncertainty what types of renewable fuels (biogas, ethanol, methanol, various biodiesel fuels etc) and combustion and exhaust cleaning techniques that will be available in the future. Most likely, a variety of renewable fuels and energy sources will be used in the coming decades in the transportation sector. Hopefully some of them will not even produce any OA at all (electric vehicles, hydrogen fuel cells). Therefore, it is not possible now to select a renewable fuel OA tracer.

Unfortunately, there are no really good candidates for OA tracers for oil-based gasoline and diesel fuels. Hopanes and steranes are readily quantifiable in urban air, but experience from the French station network shows that their low background concentrations often prohibit detection and analysis. This is partly due to the fact that they are fairly reactive, which also limits their use as OA tracers. PAHs are emitted from all (hydrocarbon) combustion sources, including biomass burning: therefore they are not unique traffic tracers, even though the relative PAH contributions differ between source categories. Radiocarbon (14C) analysis will show how much of the carbon is from modern versus fossil sources, not from which source.

In conclusion, tracers for biogenic sources of OA would be a preferred choice to complement levoglucosan, which is a (primary) tracer for biomass combustion.

The biogenic sources of modern OA are biogenic SOA and biogenic primary OA (or BPAP; biogenic primary aerosol particles). ACTRIS-2 has decided to focus on biogenic SOA.

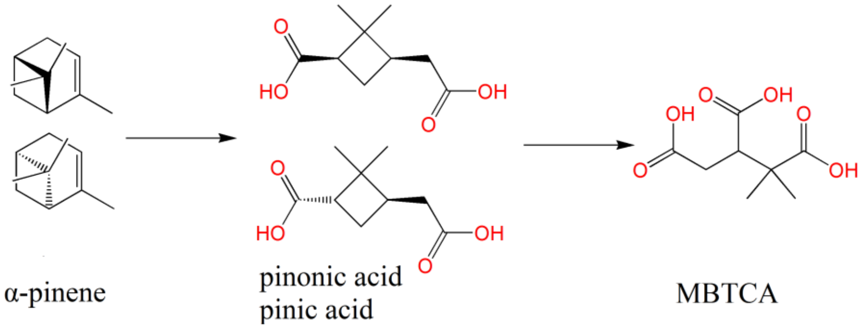
Although Aerosol Mass Spectrometers (AMS and ACSM) are used for OA source apportionment using PMF analysis, they are unable to separate the BSOA mass fraction, only biomass burning (BBOA) and cooking OA. BSOA will show up as part the low-volatility oxidized OA (LV-OOA) mass fraction.

Biogenic SOA are oxidation products of biogenic VOC (BVOC) that are emitted from vegetation. See Tables 7-9 in Nozière et al (2015) for an overview of BSOA products of various important BVOC.

The BSOA compound selected by the ACTRIS community is **3-methyl-1,2,3-butanetricarboxylic acid (3-MBTCA)**, which has been shown to be a unique tracer compound for terpene BSOA (Müller et al, 2012). More specifically MBTCA is a unique oxidation product of α-pinene, with reaction pathways through pinonic acid. Owing to the three carboxyl groups, and despite the loss of two carbon atoms, this $C_8H_{12}O_6$ compound is a low-volatility product which means that it partitions completely to the particle phase, forming OA.

Compared to the atmospheric lifetimes of SOA from most VOC precursors, including isoprene, monoterpenes, and aromatics (1 day or less), MBTCA is a fairly long-lived SOA product with an estimated atmospheric lifetime on the order of 10 days (Nozière et al 2015, figure 2).

MBTCA is in many ways an excellent surrogate for LV-OOA measured by Aerosol Mass Spectrometers (AMS, ACSM), since it has similar (low) volatility, O:C atomic ratio (MBTCA O:C = 0.75) and average carbon oxidation state (0 for MBTCA) as the highly oxidized LV-OOA.



In the smog chamber study of Müller et al (2012), MBTCA was observed and characterized by liquid chromatography-ESI-mass spectrometry after collection on filter. They concluded that the formation of MBTCA explains about 10% of the newly formed SOA mass, and the experimental yield was determined to be about 0.6 %.

Ever since the first observation (Kubátová et al, 2000) and clear identification of MBTCA (Jaoui et al, 2005), this compound has been observed and quantified in a variety of environments.

In field studies at the Melpitz ACTRIS site in Germany in July 2013 and May 2014, a number of BSOA marker compounds and oxidation product of α-pinene, β-pinene and Δ3-carene could readily be quantified using LC-MS, including MBTCA (TROPOS).

GC-MS has also been shown to be a suitable analytical technique for MBTCA, although it requires derivatization using BSTFA (Ekman Hyberg, 2016; Ding et al, 2014; Shen et al, 2015; Fu et al, 2014; Kourtchev et al, 2011).

Hollow fibre liquid phase micro-extraction (HF-LPME) was recently demonstrated as a suitable technique for enrichment of MBTCA by a factor of ~2000 (Ekman Hyberg, 2016; Lund University). The optimized

HF-LPME enrichment technique was also applied to quartz filter samples collected at the Swedish ACTRIS site Vavihill and resulted in significantly improved detection limits for MBTCA.

For primary tracers, such as levoglucosan for biomass burning, the observed concentrations are the result of a chain of events:

Emissions → Atmospheric transport, dilution and deposition → Concentration at receptor site

For secondary tracers, such as MBTCA for biogenic sources, a number of additional chemical and physical processes influence the concentrations at the receptor site:

Emissions → Atmospheric transport, dilution, *chemical/physical transformation* and deposition → Concentration at receptor site

In order to determine the amount of terpene BSOA in the total OA, the mass fraction of MBTCA in terpene BSOA will then have to be known over a range of atmospheric conditions. This requires estimates of the yields – through chemical and physical processes – of the tracer as well as all SOA produced from VOCs emitted from that source. Even though the yields are constrained from smog chamber studies, the chamber BSOA yields may still differ significantly from ambient BSOA. This remains an issue for MBTCA, but similar uncertainties are also found for the primary tracers, for instance uncertainties in the emitted mass fraction of levoglucosan in biomass burning OA.

In conclusion, MBTCA yields from α-pinene are constrained through chamber experiments and MBTCA is present at ACTRIS sites, at least during the warmer part of the year when BVOC emissions are significant.

Furthermore, a standardized analytical procedure for MBTCA is available (LC-ESI-MS), and GC-MS can also be used following derivatization. Also the MBTCA compound was recently made commercially available by Toronto Research Chemicals Inc. and can be used as a pure MBTCA standard in ILC studies.

A summary of the reasons for selecting MBTCA as a BSOA tracer for ACTRIS-2 are:

- BVOC emissions are expected to increase as a result of climate change, which will likely lead to increased atmospheric concentrations of MBTCA;
- Phasing out of fossil fuels will gradually increase the relative contribution of BSOA to total OA.
- MBTCA is a unique oxidation product of α-pinene, a major BVOC;
- MBTCA yields from α-pinene are constrained, both absolute and relative to other BSOA products;
- MBTCA shows near-complete partitioning to the particle phase (low volatility);
- MBTCA has a long atmospheric lifetime (~10 days) compared to other BSOA compounds;
- Several analytical techniques exist for MBTCA that can form the basis for SOPs;
- The required analytical instrumentation is already available in most well-equipped analytical chemistry laboratories, also within ACTRIS;
- Extraction techniques are available for pre-concentration of MBTCA in aerosol samples;
- Standards (reference material) of MBTCA are available, both in the pure form and on filters (NIST);
- It has been shown, also at ACTRIS sites, that it is possible to sample and analyze MBTCA with reasonable accuracy, precision and cost.
- Other OA tracers can be quantified simultaneously with MBTCA in many cases.

ACTRIS-2 therefore selects **3-methyl-1,2,3-butanetricarboxylic acid (3-MBTCA)** for further work in the WP3 Task 3.1 subtask on OA tracers in order to establish this compound as a new OA tracer for biogenic (monoterpene) biogenic secondary organic aerosol in Europe.

5 Inter-laboratory comparison exercises for OA tracers

The Task 3.1 ILC exercises on OA tracers are not explicitly supported by ACTRIS TNA (WP8) as is the case for OC/EC. In the context of OA tracers in Task 3.1, TNA can only be used for OA sampling. Furthermore, there are no ACTRIS funds allocated specifically for organizing OA ILCs. Instead, these have to be performed on a voluntary basis.

Fortunately, ACTRIS partners have volunteered to arrange the BSOA ILC (INERIS, France) and the anhydrous sugars ILC (LGGE, France). The contact information to these organizations are found below:

Contact information ILC-1:
Alexandre Albinet
INERIS/LCSQA
DRC/CARA/CIME
Parc technologique Alata, BP 2
60550 Verneuil-en-Halatte, France
Tel : +33 3 44 55 64 85
e-mail: alexandre.albinet@ineris.fr

Contact information ILC-2:
Jean-Luc Jaffrezo
Directeur du LGGE
Laboratoire de Glaciologie et Géophysique de l'Environnement
(http://www-lgge.obs.ujf-grenoble.fr/)
54 Rue Molière, BP 96
38 402 St Martin d'Hères Cedex, France
Tel: +33 4 76 51 44 92
e-mail: jaffrezo@lgge.obs.ujf-grenoble.fr

Additional information can be obtained from the subtask coordinator.

Coordinator of the ACTRIS-2 Task 3.1 subtask on OA tracers:
Erik Swietlicki
Div. of Nuclear Physics, Dept. of Physics, Lund University
PO Box 118, SE-221 00, Lund, Sweden
Tel : +46 46 22 96 80, +46 709 92 45 12
e-mail: erik.swietlicki@nuclear.lu.se

ILC-1 on BSOA tracers

This section outlines the proposed time schedule and tasks for ILC-1 and drafting of SOPs for biogenic SOA tracers, with special emphasis on MBTCA.

Proposed time schedule ILC-1 (BSOA):
Preparations for ILC-1: May-October 2016 (M13-18)
Announcing ILC-1 to potential participants: June 2016 (M14)
Communicating ILC procedures to participants: November-December 2016 (M19-20)
Sending the samples to participants: January 2017 (M21)
Analysis by participants: January – March 2017 (M21-23)
Preliminary report prepared (confidential, D3.10): April 2017 (M24).

The ILC will be preceded by a preparation phase during which first the distribution of tasks will be settled and a call will be issued to the community for participation in the ILC. The selection of samples and standards will be done and instructions for sample handling and reporting will be provided to the participants.

In order to have a significant statistical analysis for the ILC evaluation, the number of participants needs to be at least 10 and preferably higher (up to 20). The call should therefore be enlarged to the international level in order to get the requested minimum number of participants. This is not unrealistic, since the required analytical techniques involved (LC-ESI-MS and GC-MS) are typically already available in most well-equipped analytical chemistry laboratories.

A variety of samples should be provided for the ILC. These could include:

- 2 PM10 aerosol samples
- 1 PM10 field blank filter
- 1 Fortified sample extract
- 1 standard solution
- 1 SRM

PM10 samples are to be collected on quartz filters using a Hi-Vol sampler. One filter should be collected during the winter (or at least colder) period and one from the summer period. Several punches are prepared from the exposed filters. Sampling locations are to be defined, but should preferably include ACTRIS sites.

The fortified sample extract is a PM aerosol filter sample extract that is spiked using a solution of standards. INERIS already has several native standards of SOA markers including MBTCA and DHOPA (a tracer of anthropogenic aromatic SOA). The final composition of the spiking solution will be determined during the ILC-1 preparation phase.

INERIS is currently collaborating with NIST in order to determine reference values on different SOA markers in standard reference materials (SRM). If this work will prove to be successful during the ILC-1 preparation phase, then it is the ambition to also include a NIST SRM in ILC-1, although still in the test phase. This would open up for future ILC world-wide and greatly facilitate the spreading of best practices regarding SOA tracer analysis.

ILC-1 will not only on focus on MBTCA, even though this will be the main objective.

Instead, ILC-1 should grasp the opportunity to work on a series of different SOA markers (tracers) commonly reported in the literature (see Nozière et al 2015 and references therein). Apart from MBTCA, other biogenic SOA markers would be of considerable interest, including pinic acid, pinonic acid, alpha-methylglyceric acid, succinic acid, etc.).

DHOPA (2,3-dihydroxy-4-oxopentanoic acid) is widely considered to be an anthropogenic SOA tracer, being a result of atmospheric oxidation of aromatics, including toluene. Typically, DHOPA exhibited higher levels at urban sites than at remote sites (Shen et al, 2014).

The list of targeted compounds, biogenic and anthropogenic, will be defined during the ILC-1 preparation phase. Also a decision will be taken on which compounds that should be compulsory or reported on a voluntary basis. Consideration should be given to ensure that several analytical techniques can be employed.

ILC-1 will result in the drafting of SOPs for those new OA tracers that fulfilled the applicability and quality requirements (M25-36), and reported in D3.15 (M36).

In doing so, the first three steps in the chain of events aiming to establish a new organic tracer will be accomplished [(i) Selection, (ii) ILC performed, and (iii) Draft SOPs established]. The remaining two steps will not be performed within ACTRIS-2, in accordance with the Grant Agreement.

5 Establishing and implementing control procedures for anhydrous sugars

This section outlines the proposed time schedule and tasks for establishing ACTRIS control procedures and, as a first step towards implementing these procedures, performing an ILC-2 for the anhydrous sugars as tracers for biomass burning.

Proposed time schedule for establishing control procedures for anhydrous sugars and for ILC-2:

Establishing Control Procedures: May 2017 - April 2018 (M25-36)
Reporting Control Procedures for implementation in ILC-2 (D3.15): April 2018 (M36)

Preparations for ILC-2: May – July 2018 (M37-39)
Sending the samples to participants: August 2018 (M40)
Analysis by participants: September – November 2018 (M41-43)
Preliminary ILC-2 report prepared (confidential): December 2018 – January 2019 (M44-45).

Final report summarizing all results from the WP3.1 subtask on OA Tracer: December 2018 – January 2019 (M46-48).

This time schedule will fulfil the two remaining steps [(iv) Establishing control procedures, and (v) Implementing the control procedures] in the chain of events towards a full establishment of the anhydrous sugars as tracers for biomass burning within ACTRIS. In doing so, ACTRIS-2 will have developed the tools needed to ensure the quality and intercomparability of the acquired data across the network for these OA tracers. This is in accordance with the Grant Agreement.

References

Belis C.A., B.R. Larsen, F. Amato, I. El Haddad, O. Favez, R.M. Harrison, P.K. Hopke, S. Nava, P. Paatero, A. Prévôt, U. Quass, R. Vecchi, M. Viana (2014) European Guide on Air Pollution Source Apportionment with Receptor Models, Reference Report by the Joint Research Centre of the European Commission. doi: 10.2788/9307. http://source-apportionment.jrc.ec.europa.eu/Docu/EU_guide_on_SA.pdf

Ding, X., Q.-F. He, R.-Q. Shen, Q.-Q. Yu, and X.-M. Wang (2014), Spatial distributions of secondary organic aerosols from isoprene, monoterpenes, β-caryophyllene, and aromatics over China during summer, J. Geophys. Res. Atmos., 119, 11,877–11,891, doi:10.1002/2014JD021748.

Ekman Hyberg P. (2016) Method optimization for quantitative analysis of 3-methyl-1,2,3-butanetricarboxylic acid using hollow fiber liquid phase microextraction and gas chromatography mass spectrometric detection. Master Thesis in Analytical Chemistry, Centre for Analysis and Synthesis, Department of Chemistry, Lund University, Sweden.

Fu P. Q., K. Kawamura, Y. F. Cheng, S. Hatakeyama, A. Takami, H. Li, and W. Wang (2014) Aircraft measurements of polar organic tracer compounds in tropospheric particles (PM10) over central China. Atmos. Chem. Phys., 14, 4185–4199, doi:10.5194/acp-14-4185-2014.

Glasius, M., Lahaniati, M., Calogirou, A., Di Bella, D., Jensen, N.R., Hjorth, J., Kotzias, D., and Larsen, B. R.: Carboxylic acids in secondary aerosols from oxidation of cyclic monoterpenes by ozone, Environ. Sci. Technol., 34, 1001–1010, 2000.

Hermansson, E., Roldin, P., Rusanen, A., Mogensen, D., Kivekäs, N., Väänänen, R., Boy, M., and Swietlicki, E.: Biogenic SOA formation through gas-phase oxidation and gas-to-particle partitioning – a comparison between process models of varying complexity, Atmos. Chem. Phys., 14, 11853-11869, doi:10.5194/acp-14-11853-2014, 2014.

Hopke P.K. (2016) Review of receptor modeling methods for source apportionment, Journal of the Air & Waste Management Association, 66:3, 237-259, DOI:10.1080/10962247.2016.1140693.

Jaoui M, Kleindienst TE, Lewandowski M, Offenberg JH, Edney EO (2005) Identification and quantification of aerosol polar oxygenated compounds bearing carboxylic or hydroxyl groups: 2 organic tracer compounds from monoterpenes. Environ Sci Technol 39:5661–5673.

Kourtchev I., S. Hellebust, J.M. Bell, I.P. O'Connor, R.M. Healy, A. Allanic, D. Healy, J.C. Wenger, J.R. Sodeau (2011) The use of polar organic compounds to estimate the contribution of domestic solid fuel combustion and biogenic sources to ambient levels of organic carbon and PM2.5 in Cork Harbour, Ireland, Science of the Total Environment 409 (2011) 2143–2155.

Kubátová A, Vermeylen R, Claeys M, Cafmeyer J, Maenhaut W, Roberts G, Artaxo P (2000). Carbonaceous aerosol characterization in the Amazon basin, Brasil: novel dicarboxylic acids and related compounds. Atmos Environ 34:5037–5051

Kulmala M., Tuomo Nieminen, Anna Nikandrova, Katrianne Lehtipalo, Hanna E. Manninen, Maija K.Kajos, Pasi Kolari, Antti Lauri, Tuukka Petaja, Radovan Krejci, Hans-Christen Hansson, Erik Swietlicki, Anders Lindroth, Torben R. Christensen, Almut Arneth, Pertti Hari, Jaana Back, Timo Vesala, Veli-Matti Kerminen (2014) CO2-induced terrestrial climate feedback mechanism: From carbon sink to aerosol source and back, Bor. Env. Res. 19(2014)122.

Müller L, Reinnig M-C, Naumann KH, Saathoff H, Mentel TF, Donahue N, Hoffmann T (2011) Formation of 3-methyl-1,2,3-butanetricarboxylic acid via gas phase oxidation of pinonic acid – a mass spectrometric study of SOA aging. Atmos Chem Phys Discuss 11:19443–19476.

Nozière B., M. Kalberer, M. Claeys, J. Allan, B. D'Anna, S. Decesari, E. Finessi, M. Glasius, I. Grgić, J. F. Hamilton, T. Hoffmann, Y. Iinuma, M. Jaoui, A. Kahnt, C. J. Kampf, I. Kourtchev, W. Maenhaut, N. Marsden, S. Saarikoski, J. Schnelle-Kreis, J.D. Surratt, S. Szidat, R. Szmigielski, and A. Wisthaler (2015) The Molecular Identification of Organic Compounds in the Atmosphere: State of the Art and Challenges, Chem. Rev., 2015, 115 (10), pp 3919–3983, DOI: 10.1021/cr5003485.

Paasonen P., Ari Asmi, Tuukka Petaja, Maija K. Kajos, Mikko Aijala, Heikki Junninen, Thomas Holst,

Jonathan P. D. Abbatt, Almut Arneth, Wolfram Birmili, Hugo Denier van der Gon, Amar Hamed, Andras Hoffer, Lauri Laakso, Ari Laaksonen, W. Richard Leaitch, Christian Plass-Duelmer, Sara C. Pryor, Petri Raisanen, Erik Swietlicki, Alfred Wiedensohler, Douglas R. Worsnop, Veli-Matti Kerminen, Markku Kulmala (2013) Warming-induced increase in aerosol number concentration likely to moderate climate change, Nature Geoscience, DOI: 10.1038/NGEO1800.

Shen R.-Q., X. Ding, Q.-F. He, Z.-Y. Cong, Q.-Q. Yu, and X.-M. Wang (2015) Seasonal variation of secondary organic aerosol tracers in Central Tibetan Plateau, Atmos. Chem. Phys., 15, 8781–8793, 2015, www.atmos-chem-phys.net/15/8781/2015/, doi:10.5194/acp-15-8781-2015

Szmigielski, R.; Surratt, J. D.; Gómez-González, Y.; Van der Veken, P.; Kourtchev, I.; Vermeylen, R.; Blockhuys, F.; Jaoui, M.; Kleindienst, T. E.; Lewandowski, M.; Offenberg, J. H.; Edney, E. O.; Seinfeld, J. H.; Maenhaut, W.; Claeys, M. (2007) 3-Methyl-1,2,3-Butanetricarboxylic Acid: An Atmospheric Tracer for Terpene Secondary Organic Aerosol. Geophysical Research Letters, 34 (24), doi:10.1029/2007GL031338.