



## TNA User Report

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Project title	Aerosol particle organic analytical training course
Name of the accessed calibration center	OGTAC CC (Calibration center for organic tracer and aerosol constituents)
Number of users in the project	4
Project objectives (max 100 words)	The aerosol particle organic analytical training course was focused on the target analysis of atmospheric relevant particle-phase constituents. The training offers all applicants the possibility to get practical training at state of the art instruments, discussions with experts and to strengthen their network.
Description of work (max 100 words):	The 5-day training course was focused on lecturers in atmospheric science, particle collection, sample treatment and target analysis. In the second part of the training, practical experience with the given instrumental analytical equipment of TROPOS ACD was given. Each participant went through the whole proceeding from sample extraction, sample preparation, separation at a LC system and detection and quantification with a mass spectrometer.

Principal Investigator's and group's information	
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User status <sup>3</sup>	PhD
New user	No

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<sup>1</sup> Physics; Chemistry, Earth Sciences & Environment; Engineering & Technology; Mathematics; Information & Communication Technologies; Material Sciences; Energy; Social sciences; Humanities.

<sup>2</sup> UNI= University and Other Higher Education Organisation;

RES= Public Research Organisation (including international research organisations and private research organisations controlled by public authority);

SME= Small and Medium Enterprise;

PRV= Other Industrial and/or Profit Private Organisation;

OTH= Other type of organization.

<sup>3</sup> UND= Undergraduate; PGR= Post graduate; PDOC= Post-doctoral researcher; RES= Researcher EXP= Engineer; ACA= Academic; TEC= Technician.

<sup>4</sup> Reproduce the table for each user who accessed the infrastructure

New user	Yes
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<b>User 3 Information</b>	
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## Trans-National Access (TNA) Scientific Report

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### Instructions

Please limit the report to max 5 pages, you can include tables and figures. Please make sure to address any comments made by the reviewers at the moment of the project evaluation (if applicable, in this case you were informed beforehand). Please do not alter the layout of the document and keep it in Word version. The report will be made available on the [eurochamp.org](http://eurochamp.org) website. Should any information be confidential or not be made public, please inform us accordingly (in this case it will only be accessible by the European Commission, the EUROCHAMP-2020 project partners, and the reviewers). Please include:

- Introduction and motivation
- Scientific objectives
- Reason for choosing the calibration facility
- Method and experimental set-up
- Data description
- Preliminary results and conclusions
- Outcome and future studies
- References

**Name of the PI:** Agata Kołodziejczyk

**Calibration center's name and location:** OGTAC CC at TROPOS ACD

**Campaign name and period:** Aerosol particle organic analytical training course, 02.12.-06.12.2019

**Text:**

#### Introduction and Motivation

Organic compounds makes 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. Due to the different nature of the particulate organic compounds a huge ensemble of instruments is necessary to detect and quantify them. The typical set-up for each kind of group includes a sample preparation, separation of the target compounds, detection of the separated compounds and quantification using authentic standard compounds. Each step will depend on the target compounds and the used technique. Even that many groups are working on the detection and quantification of marker compounds general guideline and standard operation procedures a largely missing. Thus OGTAC CC as first CC worldwide for organic marker compounds provides an enormous benefit for the aerosol community as it harmonizes the analytic of organic particle-phase constituents and builds up a strong network of all groups in Europe working on this area.

This OGTAC CC activity was focused on the Liquid Chromatography coupled with Mass Spectrometry (LC/MS) as is the most dominating technique for the target analysis of atmospheric relevant tracer compounds. Due to various column material for the LC separation and different MS detectors this technique can be applied to a broad spectrum of organic compounds.

### Scientific objectives

The conducted training was focused on the application of LC/MS for the analysis of atmospheric relevant particulate products, in particular High-Performance Liquid Chromatography Electrospray Ionization coupled to Time-of-Flight Mass Spectrometry (HPLC/(-)ESI-TOFMS), Ultra-Performance Liquid Chromatography Electrospray Ionization coupled to Ion-Mobility Mass Spectrometer with a Time-of-Flight Mass Spectrometer (UPLC/ESI-IMS-QTOFMS). The course covered i) dedicated training at the HPLC/ESI-TOFMS and UPLC/ESI-IMS-QTOFMS; ii) Lectures in atmospheric particle related chemical analysis; iii) Practical training for filter collection, extraction, analysis and quantification of target compounds and iv) derivatisation and enrichment procedures. Thus, within one week the participant learned each step from sample collection to quantitative data analysis, with special emphasis for a high level of QA/QC during each phase of sample treatment.

### Reason for choosing the calibration centre

One of the greatest strength of TROPOS ACD is the development and improvement of analytical methods for the detection and quantification of organic compounds in the gas and particle phase. So far TROPOS published about 20 first-author paper with 380 citations dealing solely with the development of new methods or improvements of existing methods (Ref. 1 – 9). The great ensemble of state of the art instruments and methods at TROPOS enables them to cover the majority of organics and to serve many groups that usually use only 1-2 instruments.

### Schedule and Method

The 5-days training is separated into two main sections. Several lectures in sample collection and basics on separation techniques as well as approaches for quantification were given. On the other site, applicants achieved a high level of hands-on training during sample extraction and sample analysis. A schedule for the 5-days training course is given in Figure 1

	Monday	Tuesday	Wednesday	Thursday	Friday
9-10:30		Filter extraction procedure  Preparation of dilution series	<b>Start 9:30</b> Interpretation of PTR-MS and SMPS data	<b>Start 10:00</b> Non-target analysis	<b>Start 9:30</b> Enrichment procedures  Discussion of open topics
10:00-12:30	Welcome Introduction into OGTAC CC and workshop Introduction into chamber Start Chamber experiment		Quantification of filter samples	Applications of LC/MS	Wrap up
12:30-13:30	Lunch	Lunch	Lunch	Lunch	
13:30-15:30	Sampling  Presentation by the participants – Part 1	Presentation by the participants – Part 2  Start Analysis	Introduction into WSOC  Combined interpretation of all results	Application examples Application  Introduction into OC/EC	
	BREAK	BREAK	BREAK	FREE time	
16:00-17:00			Lab tour		

Figure 1. Schedule for the Aerosol particle organic analytical training course at OGTAC CC

Within the first day lectures were given focusing on particle collection, sample treatment, separation and detection techniques. Special emphasis was spent to artefact formation during sampling, selection of filter material and appropriate extraction solvent and technique. Also an overview was given about separation techniques and mass spectrometric detection. This day provided the basement of the subsequent technical work. As the applicants had various levels of previous knowledge these lectures broad all into the same state.

The second and third day was used for the technical work. This included the extraction of filter and the quantification of target compounds, in particular of biogenic SOA compounds. The applicants were invited to bring their own filter. In case that no samples were available TROPOS ACD provided filter from the aerosol chamber ACD-C and/or from the TROPOS research station Melpitz. Each applicant extracted two filter. During the extraction process SOPs for extraction as well as cleaning procedures were discussed. The second group prepared at the same time dilution series and got a lecture on the stoichiometric calculation and approaches for quantification. Subsequently samples were analysed with High-Performance Liquid Chromatography Electrospray Ionization coupled to Time-of-Flight Mass Spectrometer (HPLC/(-)ESI-TOFMS) and Ultra-Performance Liquid Chromatography Electrospray Ionization coupled to Ion-Mobility Mass Spectrometer with a Time-of-Flight Mass Spectrometer (UPLC/ESI-IMS-QTOFMS). The applicants worked in two groups with maximum 2-3 members to ensure the highest level of hands-on experience. From day to day the groups were exchanged to ensure that everybody went through the whole procedure and worked with both instruments.

Within the 4<sup>th</sup> day a lecture is given about LC/MS-based strategies and approaches for the analysis of OA filter samples. This lecture gave the participants a general overview on common instrumental possibilities and procedures used for the analysis of organic aerosol samples. The first part outlined certain features of state-of-the-art mass spectrometers (e.g., Q-MS, TOF-MS, Orbitrap, etc.) and different operation modes (e.g., selected ion monitoring, MS/MS, etc.). Afterwards, common approaches in LC/MS-based analysis strategies were discussed, comprising targeted and untargeted methods as well as examples from the current literature. The third part of the lecture was focusing on data handling and data analysis strategies for LC/MS approaches in organic aerosol analysis.

The lecture is followed by presentations regarding different applications of LC/MS.

Furthermore, all applicants got the chance to present their own work and discuss their results with the community.

#### Future perspective

The knowledge obtained during the course is very general and can be applied by all participants during their daily laboratory work. Thus, it will greatly improve the daily workflow. The practical experience during the hand-on training session can be easily transferred to any other LC/MS system. A special focus during the training sessions was given to the QA/QC techniques (sequence design, preparation of standard solution etc.). This will be employed to each single technique present in the participant's laboratory.

#### References

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3. van Pinxteren, D., M. Teich, and H. Herrmann, Hollow fibre liquid-phase microextraction of functionalised carboxylic acids from atmospheric particles combined with capillary electrophoresis/mass spectrometric analysis. *Journal of Chromatography A*, 2012. 1267(SI): p. 178-188
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