



## 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	7
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 offered the possibility to all applicants 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	
First name	Nathalie
Family name	Hayeck
Nationality	Lebanese
Activity domain <sup>1</sup>	Physics; Chemistry, Earth Sciences & Environment
Home institution	CNRS, IRCELYON
Institution legal status <sup>2</sup>	Public research Organisation
Email	Nathalie.hayeck@ircelyon.univ-lyon1.fr
Gender	female
User status <sup>3</sup>	Postdoctoral researcher
New user	Yes

User 1 Information <sup>4</sup>	
First name	Cornelia
Family name	Amarandei
Nationality	Romanian
Activity domain	Physics; Chemistry, Earth Sciences & Environment
Home institution	CERNESIM
Institution legal status	University
Email	cornelia.amarandei@yahoo.com
Gender	female
User status	Postgraduate
New user	Yes

User 2 Information	
First name	Teresa
Family name	Vera
Nationality	Spanish
Activity domain	Physics; Chemistry, Earth Sciences & Environment
Home institution	Fundacion CEAM
Institution legal status	Public research Organisation
Email	teresa@ceam.es
Gender	female
User status	Postdoctoral researcher
New user	Yes

<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

<b>User 3 Information</b>	
First name	Georgiana
Family name	Balulescu
Nationality	Romanian
Activity domain	Physics; Chemistry, Earth Sciences & Environment
Home institution	CERNESIM
Institution legal status	University
Email	georgiana.balulescu@gmail.com
Gender	female
User status	Postgraduate
New user	Yes

<b>User 4 Information</b>	
First name	Agata
Family name	Kołodziejczyk
Nationality	Polish
Activity domain	Physics; Chemistry, Earth Sciences & Environment
Home institution	Institute of Physical Chemistry; Polish Academy of Science
Institution legal status	University
Email	agata.d.kolodziejczyk@gmail.com
Gender	female
User status	Postgraduate
New user	Yes

<b>User 5 Information</b>	
First name	Kumar
Family name	Sarang
Nationality	Indian
Activity domain	Physics; Chemistry, Earth Sciences & Environment
Home institution	Institute of Physical Chemistry; Polish Academy of Science, Poland
Institution legal status	University
Email	ksarang@ichf.edu.pl
Gender	male
User status	Postgraduate
New user	Yes

User 6 Information	
First name	Shamjad
Family name	Moosakutty
Nationality	Indian
Activity domain	Physics; Chemistry, Earth Sciences & Environment
Home institution	Aarhus University, Denmark
Institution legal status	University
Email	spm@chem.au.dk
Gender	male
User status	Postdoctoral researcher
New user	New

## 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 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: Nathalie Hayeck**

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

**Campaign name and period: Aerosol particle organic analytical training course, 22.01.-26.01.2018**

**Text:**

#### Introduction and Motivation

Organic compounds make up a large fraction of aerosol particles and vary in composition depending on the meteorological conditions, the sampling location as well as the level of processing. Thus aerosol particles contain hundreds of different compounds affecting both chemical and physical properties and, through this, human health, environmental impact 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 sequence of 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 though many groups are working on the detection and quantification of marker compounds general guideline and standard operation procedures are largely missing. Thus OGTAC CC as the first CC for organic marker compounds worldwide provides a strong 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.

For the first OGTAC CC activity the topic of Liquid Chromatography coupled with Mass Spectrometry (LC/MS) was selected as this is the most dominating technique for the target analysis of atmospheric relevant tracer compounds. Through the use of 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 atmospherically 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 ACD published about 20 first-author papers with 380 citations dealing solely with the development of new methods or improvements of existing methods (e.g. Ref. 1-9). The large array 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. A series of lectures in sample collection and basics on separation techniques as well as approaches for quantification were given. Correspondingly, the applicants achieved a high level of hands-on training during sample extraction and sample analysis. The schedule of the complete 5-days training course is given in Figure 1.

	Monday	Tuesday	Wednesday	Thursday	Friday
9:00 – 10:00		Group A: Filter extraction	Group B: Filter extraction	LC/MS-based strategies and approaches for the analysis of OA filter samples	Presentation by the participants
10:00-10:30	Welcome + OGTAC CC presentation	Group B: Preparation of dilution series	Group A: Preparation of dilution series		
10:30-12:30	General Introduction;  Filter material, collection, artefacts, extraction, storage	Group A: Hands-on Training at the LC- $\mu$ TOF  Group B: Hands-on Training at the Synapt	Group A: Hands-on Training at the Synapt  Group B: Hands-on Training at the LC- $\mu$ TOF	Matrix effects	Presentation by Waters  Closing with Summary and Feedback
12:30-13:30	Lunch	Lunch	Lunch	Lunch	13:00 Lunch
13:30-14:30	Enrichment procedures	Group A: Hands-on Training at the LC- $\mu$ TOF  Group B: Hands-on Training at the Synapt	Group A: Hands-on Training at the Synapt  Group B: Hands-on Training at the LC- $\mu$ TOF	Applications of LC/MS	
14:30-15:30	Break	Break	Break	Visit TROPOS New Laboratory building	
15:30-17:00	LC Basics  Ionization and detection techniques	Hands-on Training Open questions	Hands-on Training Open questions		
19:00				Joint Dinner (voluntary)	

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 foundation for atmospheric studies and for the subsequent analytically oriented technical work. As the applicants had various levels of previous knowledge these lectures brought all participants on a similar level of knowledge.

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 brought, OGTAC-CC with TROPOS ACD provided filter from the aerosol chamber LEAK 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. At the same time, the second group prepared 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 5 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.

On the 4<sup>th</sup> day a lecture was given about LC/MS-based strategies and approaches for the analysis of OA filter samples. This lecture gave 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 first lecture was followed by presentations regarding different applications of LC/MS, in particular « Chemical characterisation of amino acids as part of marine organic matter using LC/MS » and « Elucidating the composition of humic-like substances in the atmospheric aerosol via 2D-liquid chromatographic fractionation and ultra-high resolution mass spectrometry ». Furthermore, all applicants got the chance to present their own work and discuss their results with the community. A co-worker of the company 'Waters' as one of the world leading manufacturers gave an overview talk on evolving mass spectrometric techniques, joined the discussions with the participants and finally provided very good feedback to the presentations of the participants.

#### User feedback

Users were asked to answer a feedback questionnaire including the following points: overall impression, organisation, balance between theory and practical work, structure of the course, content, oral presentations, and practical part. Everybody could rate between 1 (excellent), 2 (very good), 3 (good), 4 (fair) and 5 (poor). All participants joint the questionnaire and an average rating of 1.8 was achieved, which can be counted as very good. Finally, the participants were asked if they

would recommend this course. In this case a unanimously result was obtained as all participants would recommend the course.

#### Future perspective

The knowledge obtained during the course is broad and can be applied by all participants during their daily laboratory work. Thus, it will probably improve the daily laboratory work. 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 the 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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