# TNA User Report

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

| | |
|---|---|
| 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 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 | Elena |
| Family name | Gomez Alvarez |
| Nationality | Spanish |
| Activity domain[1] | Physics; Chemistry, Earth Sciences & Environment |
| Home institution | University College Cork |
| Institution legal status[2] | University |
| Email | elena.gomezalvarez@ucc.ie |
| Gender | female |
| User status[3] | Postdoctoral researcher |
| New user | Yes |

| User 1 Information[4] | |
|---|---|
| First name | Niall |
| Family name | O´Sullivan |
| Nationality | Irish |
| Activity domain | Physics; Chemistry, Earth Sciences & Environment |
| Home institution | University College Cork |
| Institution legal status | University |
| Email | 113379206@umail.ucc.ie |
| Gender | male |
| User status | Postgraduate |
| New user | Yes |

| User 2 Information | |
|---|---|
| First name | Aline |
| Family name | Gratien |
| Nationality | French |
| Activity domain | Physics; Chemistry, Earth Sciences & Environment |
| Home institution | CNRS-LISA |
| Institution legal status | Public research Organisation |
| Email | aline.gratien@lisa.u-pec.fr |
| Gender | female |
| User status | Academic |
| New user | Yes |

[1] Physics; Chemistry, Earth Sciences & Environment; Engineering & Technology; Mathematics; Information & Communication Technologies; Material Sciences; Energy; Social sciences; Humanities.
[2] 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.
[3] UND= Undergraduate; PGR= Post graduate; PDOC= Post-doctoral researcher; RES= Researcher EXP= Engineer; ACA= Academic; TEC= Technician.
[4] Reproduce the table for each user who accessed the infrastructure

| User 3 Information | |
|---|---|
| First name | Cecile |
| Family name | Mirande-Bret |
| Nationality | French |
| Activity domain | Physics; Chemistry, Earth Sciences & Environment |
| Home institution | CNRS-LISA |
| Institution legal status | Public research Organisation |
| Email | Cecile.mirande-bret@lisa.u-pec.fr |
| Gender | female |
| User status | Engineer |
| New user | Yes |

# Trans-National Access (TNA) Scientific Report

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

## 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: Elena Gomez Alvarez**
**Calibration center's name and location: OGTAC CC at TROPOS ACD**
**Campaign name and period:** Aerosol particle organic analytical training course, 29.01.-02.02.2018
**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 a 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 | Data Analysis | 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;<br><br>Filter material, collection, artefacts, extraction, storage | Group A: Hands-on Training at the LC-µTOF<br><br>Group B: Hands-on Training at the Synapt | Group A: Hands-on Training at the Synapt<br><br>Group B: Hands-on Training at the LC-µTOF | LC/MS-based strategies and approaches for the analysis of OA filter samples | 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-µTOF<br><br>Group B: Hands-on Training at the Synapt | Group A: Hands-on Training at the Synapt<br><br>Group B: Hands-on Training at the LC-µTOF | Applications of LC/MS | |
| 14:30-15:30 | Break | Break | Break | Visit TROPOS New Laboratory building | |
| 15:30-17:00 | LC Basics<br><br>Ionization and detection techniques | Hands-on Training<br>Open questions | Hands-on Training<br>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 spend 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$^{th}$ 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.

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 1.9 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

1. Iinuma, Y., G. Engling, H. Puxbaum, and H. Herrmann, A highly resolved anion-exchange chromatographic method for determination of saccharidic tracers for biomass combustion and primary bio-particles in atmospheric aerosol. Atmospheric Environment, 2009. 43(6): p. 1367-1371.
2. Kahnt, A., Y. Iinuma, O. Böge, A. Mutzel, and H. Herrmann, Denuder sampling techniques for the determination of gas-phase carbonyl compounds: A comparison and characterisation of in situ and ex situ derivatisation methods. Journal of Chromatography B, 2011. 879(17-18 (Special Issue)): p. 1402-1411.
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
4. Mutzel, A., M. Rodigast, Y. Iinuma, O. Böge, and H. Herrmann, An improved method for the quantification of SOA bound peroxides (Technical note). Atmospheric Environment, 2013. 67: p. 365-369.
5. Teich, M., D. van Pinxteren, and H. Herrmann, Determination of nitrophenolic compounds from atmospheric particles using hollow-fiber liquid-phase microextraction and capillary electrophoresis/mass spectrometry analysis. Electrophoresis, 2014. 35(9): p. 1353-1361.
6. Rodigast, M., A. Mutzel, Y. Iinuma, S. Haferkorn, and H. Herrmann, Characterisation and optimisation of a sample preparation method for the detection and quantification of atmospherically relevant carbonyl compounds in aqueous medium. Atmospheric Measurement Techniques, 2015. 8: p. 2409-2416.
7. Rodigast, M., A. Mutzel, J. Schindelka, and H. Herrmann, A new source of methylglyoxal in the aqueous phase. Atmospheric Chemistry and Physics, 2016. 16: p. 2689–2702.
8. Teich, M., D. van Pinxteren, S. Kecorius, Z. Wang, and H. Herrmann, First quantification of imidazoles in ambient aerosol particles: Potential photosensitizers, brown carbon constituents and hazardous components. Environmental Science & Technology, 2016. 50: p. 1166-1173.
9. Rodigast, M., A. Mutzel, and H. Herrmann, A quantification method for heat-decomposable methylglyoxal oligomers and its application on 1,3,5-trimethylbenzene SOA. Atmospheric Chemistry and Physics, 2017. 17(6): p. 3929-3943.