

Marie Curie Early Stage Researcher Positions Available for 2016 10 Early Stage Researcher Positions within a MARIE SKŁODOWSKA-CURIE ACTIONS Innovative Training Network

"IMPACT"

Ion-Molecule Processes for Analytical Chemistry Technologies
A Research and Technological Driven Programme
Early Call for Applications
Expected Start Date: 1st July – 1st September 2016 (but flexible)

The Ion Molecule Processes for Analytical Chemistry Technologies (IMPACT) Innovative Training Network (ITN) is a multidisciplinary EU-funded H2020-MSCA-ITN-2015 program, specially designed to provide scientific, research and transferable skill training and career development for Early Stage Researchers (ESRs) in the field of Soft Chemical Ionization Mass Spectrometry. IMPACT consists of ten full partners and twelve associated partners from nine different countries and from various sectors (commercial, academic and governmental). The network is being coordinated by Dr. Chris Mayhew, University of Birmingham, UK.

Each full partner institute will be hosting one ESR. Thus the **IMPACT network** invites applications for 10 **full-time research vacancies** for highly motivated **ESRs**. Selected researchers must be able to work independently and as part of multidisciplinary teams. ESRs will undertake an **Individual Research Project** at one of the partner institutions, as well as participate in a joint network training programme and secondments at other establishments. ESRs will be hired at the full partners under employment contracts. The maximum duration of the employment is 36 months.

An ESR is a researcher who, at the time of the recruitment, has not yet been awarded a doctorate degree and is in the first four years (full-time equivalent) of their research careers, including the research training period that would entitle them to a doctorate. Each ESR position includes a PhD.

IMPACT - Program Summary

Soft chemical-ionization mass-spectrometry (SCIMS) is an exquisitely sensitive analytical technique with applications to health, the environment and security that are vital to the EU. However, the recent, rapid and widespread adoption of this technique has caught Europe unprepared. The resultant shortage in analytical chemical expertise has created an urgent need for highly skilled young researchers to be trained in the wide variety of SCIMS methods. IMPACT addresses this skills' shortage by establishing an intersectoral and multidisciplinary SCIMS training network. IMPACT also brings cohesion to the fragmented SCIMS research and development activities within the EU. To date, most SCIMS developments have been driven not by users but by manufacturers, whose main focus has been on increased sensitivity. However, just as crucial is improved selectivity. Indeed, many users consider improved selectivity to be the key to taking SCIMS technology to a whole new level. Instead of private and public sectors working independently, we need a fresh, intersectoral approach. IMPACT will achieve this through intersectoral work packages and multidisciplinary research projects. In place of major and costly changes in instrumental design, IMPACT's projects will focus on developing new methods for improved chemical specificity by manipulating ion chemistry. Hence, IMPACT's fresh approach will produce a step change in SCIMS instrumentation to deliver both economic and societal benefit to the EU. Specifically, IMPACT will train 10 ESRs within an integrated partnership of commercial, governmental and academic organisations, with planned secondments, Advanced Training Courses, interactive Complementary Skills Workshops, and ESR Centred Research Meetings, IMPACT will therefore provide Europe with both a world-class capability in SCIMS technology and a cohort of highly trained researchers who will bring the benefits of that technology to citizens across the EU.

Positions

ESR positions are available for ten research projects contained within three interlinking work packages:

Work Package 1 - Fundamental Science of SCIMS (ESRs 1 and 2)

Project 1: Scientific Underpinning of Ion-Molecule Processes and their use as Analytical Probes for SCIMS (University of Birmingham, UK, Supervisor: Dr. Chris Mayhew, c.mayhew@bham.ac.uk).

Project 2: Advanced Evaluation of Product Ion Branching Ratios in the Presence of Water Vapour (J. Heyrovsky Institute of Physical Chemistry, Czech Republic, Supervisor: Professor Patrik Spanel, spanel@jh-inst.cas.cz).

Work Package 2 - SCIMS Instrumental & Software Development (ESRs 3 and 4)

Project 3: Measures for Improved Substance Identification (IONICON Analytik GmbH., Austria, Supervisors: Drs Simone Jürschik and Philipp Sulzer, simone.juerschik@ionicon.com).

Project 4: Production of Thermal Desorption Unit and Electronic Devices for Improved Selectivity (KORE Technology Ltd., UK, Supervisor: Dr. Fraser Reich, dfr@kore.co.uk).

Work Package 3: SCIMS Applications Research Programmes

(i) Homeland Security (ESR 5)

Project 5: Homeland Security Applications: Improved Selectivity for IMS-MS and Limits of Detection (Comenius University, Slovakia, Supervisor: Professor Stefan Matejcik, matejcik@fmph.uniba.sk).

(ii) Environmental Sciences (ESRs 6 and 7)

Project 6: Biogenic Volatile Organic Compounds: Characterization in Various (agro) Ecosystems (Centre de la Recherche Scientifique, France, Supervisor: Professor Valerie Gros, valerie.gros@lsce.ipsl.fr).

Project 7: OH Reactivity and other Integrative Techniques using SCIMS (Max Planck Gesellschaft zur Förderung der Wissenschaften E.V., Germany, Supervisor: Professor Jonathan Williams, jonathan.williams@mpic.de).

(iii) Bioscience (ESRs 8-10)

Project 8: Applications of SCIMS Techniques in Biosciences (Radboud University of Nijmegen, Netherlands, Supervisor: Dr. Simona Cristescu, s.cristescu@science.ru.nl).

Project 9: SCIMS for Metabolic Profiling in Health and Disease (Universität Medizin Rostock, Germany, Supervisor: Professor Jochen Schubert, jochen.schubert@uni-rostock.de)

Project 10: Improved Breath and Skin Emanation Sampling Techniques (Universität Innsbruck, Austria, Supervisor: Professor Karl Unterkofler, karl.unterkofler@fhv.at).

More detailed descriptions on the projects are supplied at the end.

General Requirements

- A Master's degree in a physical science or engineering discipline is desirable.
- Language skills (English compulsory).
- Networking and communication skills (to be evaluated in the interview).

Eligibility

The Post is offered in the context of a Marie Curie ITN and transnational mobility is a key element of eligibility. Nationals from any country may apply. Researchers must not have carried out their main activities in the country where they will perform their studies for more than 12 months in the 3 years prior to the start of the fellowship. An ESR can only be employed in the country of his/her own nationality if he/she has spent more than four of the five years prior to the appointment in a non-EU country. Early Stage Researchers must hold a Master degree (e.g. Master of Science or an equivalent diploma) which qualifies them to embark onto a doctoral degree. It is required that the degree has been acquired not more than 4 years earlier to the envisaged starting date. (Non-research work after acquiring a Master's degree is not counted in the four years of the research career; certificates on the nature of tasks in non-research employment will be requested for shortlisted

candidates.) Applicants should also have a good knowledge of English, as the successful candidate will be asked to submit project reports and a doctoral thesis in English.

Salary and Benefits

Researchers employed by IMPACT will receive salary and benefits at the rates stipulated by the European Commission for Marie Curie ESRs. ESRs will be employed via full employment contracts with the respective institutions, carrying social benefits such as pension and social security, but also subject to normal taxes.

How to Apply

Initial enquiries of interest and any questions can be directed initially to the co-ordinator of IMPACT: Dr. Chris Mayhew (c.mayhew@bham.ac.uk). Interest in particular projects can be directed to the appropriate supervisor.

If you are interested in applying for an ESR position please supply Dr. Mayhew with a curriculum vitae, which should include details on Personal Information, Work Experience, Education and Training, Skills and Competences, and the contact details of two referees. You should state your interest in at least one of the research projects and explain your choice, but also state two more alternative projects (by order of preference). All material should be e-mailed as a single pdf with "IMPACT ESR Position" in the subject line. Final applications will be completed entirely online at each of the individual partners' organisations once the positions are officially advertised. We particularly encourage female candidates to apply for these positions.

Estimated Recruitment Calendar:

- Early Applications of Interest and General Enquiries 1st October 2015 1st April 2016
- Institutional Deadline for Applications 30thApril 2016
- Notification of candidates to be shortlisted: 15th May 2016
- Interviews with shortlisted candidates: May-June
- Notification of selected candidates: 1st July 2016
- Contract begins 1st July 30th September 2016 (or as soon after). (Ideally ESRs should start as close to the 1st September for training purposes. All ESRs to be in place no later than the 1st November 2016.)

IMPACTS Full Partners:

- 1. University of Birmingham (UoB), UK
- 2. KORE Technology Ltd. (KORE), UK
- 3. IONICON Analytik GmbH (ION), Austria
- 4. Univerzita Komenskeho V Bratislave (CU), Slovakia
- CentreNational de la Recherche Scientifique (CNRS) CNRS participates with the Laboratoire des Sciences du Climat et de l'Environnement, France
- 6. Universitäts Medizin Rostock (UMR), Germany
- 7. Max Planck Gesellschaft zur Förderung der Wissenschaften E.V. (MPG), Germany
- 8. Universität Innsbruck (UIBK), Austria
- 9. Stichting Katholieke Universiteit (RUN), Netherlands
- 10. Ustav Fyzikalni Chemie J. Heyrovskeho AV CR, v. v. i. (HIPC), Czech Republic

IMPACTS Associate Partners:

- 1. Defence Science and Technology Laboratory (Dstl), UK
- 2. FZMB GmbH (FZMB), Germany
- 3. MaSa Tech s.r.o. (MASA), Slovakia
- 4. Open University (OU), UK
- 5. OWLSTONE (OWL), UK
- 6. Smiths Detection Ltd (Smiths), UK
- 7. Syft Technologies Ltd. (Syft), New Zealand
- 8. Tracer Measurement Systems Ltd. (TMS), UK
- 9. Waters Corporation (Waters), UK
- 10. Wehrwissenschaftliches Institut für Schutztechnologien (WIS), Germany
- 11. Business Consultant: Anna Buxaderas Riorola, Spain
- 12. Scriptoria (transferable skills training), UK

Brief Summary of Individual Research Projects

Fellow ESR 1 Host institution UoB

Project Title: Scientific Underpinning of Ion-Molecule Processes and their use as Analytical Probes for SCIMS (WP 1, ROs 1 & 2)

Objectives: (1) An improved scientific underpinning of the chemistry involved with SCIMS through a deeper understanding of the inherent ion-molecule reactions through experimental and computational investigations exploring the fundamental processes involved. (2) A strengthened knowledge and database for specific ion-molecule reaction processes and their dependences on temperature, humidity, reduced electric field strengths, pressure, dopants, gas flow rates, collisional induced processes etc., and how they can be used to improve selectivity for compounds of relevance to WP 2 (ESRs 5-10). (3) Characterisation of (a) an Ion-Funnel System (WP 3 with ESR 4 and 8) for PTR/SRI systems, (b) a Fast GC-MS (WP 3) PTR/SRI, IMS and SIFT-MS systems, (c) a Thermal Desorption Unit (WP 3, with ESR 4 and 8) for PTR/SRI, IMS and SIFT-MS systems and (d) a Multiple Reagent Ion Source (with ESR 3 (WP 3))

Expected Results: (a) An improved understanding of how to control and exploit IM chemistry occurring in SCIMS systems for improving selectivity of SCIMS for testing in WP2 projects and for commercial exploitation by the private sector in WP3 projects. (b) A Roadmap on how SCIMS instruments can be used to identify trace chemicals with high levels of confidence.

Proposed Secondments: *TMS*, Y2, 1 month, selectivity techniques adapted for SIFDT-MS systems based on homeland security applications; *KORE*, Y2, 2 months, training on and use of (i) Ion-Funnel Systems and *E/N* changes relating to selectivity innovation; *CU*, Y3, 1 month (i) atmospheric pressure ion chemistry by IMS and different types of ionisation sources (coronal discharge vs. radioactive), (ii) separation of isomers with IMS and (iii) laser desorption IMS for explosive detection.

Fellow ESR 2

Host institution HIPC

Project Title: Advanced Evaluation of Product Ion Branching Ratios in the Presence of Water Vapour (WP 1, ROs 1 & 2)

Objectives: (1) Mathematical description of the experimentally obtained dependencies of relative ion signals of product ions, their fragments and hydrates on water vapour concentration, electrical field and pressure in the SCIMS tube reactors. (2) Formulation and analytical validation of advanced algorithms resolving mass spectral overlaps of isobaric product and fragment ions based on two dimensional data analyses (*m*/*z* versus reduced electric field, *E*/*N*, with ESR 1). (3) Characterisation of a Thermal Desorption Unit (TDU) developed for PTR-MS used with SIFT-MS (with ESR 1 (WP 1), ESR 4 (WP 3) and 8 (WP 2). (4) Formulation and analytical validation of algorithms for analyses of desorption temperature resolved TDU-SIFT-MS data with improved selectivity. (5) Testing methods in clinical breath analysis (with ESR 8) and environmental science (with ESR 6).

Expected Results: (1) Knowledge and data on variation of SCIMS relative mass spectral ion intensities with humidity and electric field. (2) New mathematical algorithms for calculations of VOC concentrations from mass spectral SCIMS data accounting for ion overlaps. (3) Original interdisciplinary results in the areas of breath analysis and environmental science.

Proposed Secondments: *KORE*, Y2, 1 month, PTR-MS instrumental development. *OWL*, Y3, 1 month, Training on FAIMS/IMS and comparison with SIFT-MS for Homeland Security, *MASA*, Y3, 1 month, IMS-MS and Homeland Security comparison with SIFT-MS and IMS-MS.

Fellow ESR 3

Host institution ION

Project Title: Measures for Improved Substance Identification (WP 3, RO3)

Objectives: (1) Investigate the advantages and disadvantages of multiple reagent ions compared to switching reagent ions in terms of time per analysis, accuracy of identification (particularly for isobaric & isomeric compounds) and user-friendliness (with ESR 1 (WP 1)). (2) Deducing detection algorithms from these investigations, which can be utilized for creating a software package with a simple graphical user interface. (3) Detailed studies using a novel fast GC inlet system for PTR-MS: applicability to low vapour pressure compounds, separation capabilities concerning isomeric compounds (e.g. new psychoactive substances which are isomers of illicit drugs), minimum amount of gas necessary for one fast GC run. (4) Comparing SRI/PTR-MS with more compact IMS, (with ESR 5 (WP 2)).

Expected Results: (a) Knowledge on the best method / setup for highly selective substance identification in near real-time using switchable and/or multiple reagent ions including algorithm for implementing the method into user-friendly software. (b) Comparison of this method to PTR-MS equipped with a fast GC inlet system in terms of speed, selectivity, sensitivity, maintenance, reliability, etc.; which SCIMS fields can benefit most from which technology?

Proposed Secondments: Y1 HIPC, 1 month, SIFT-MS Training; Y2 UoB, 1 month, IMS-MS training, Y3 MASA, 1 month, IMS Studies and comparison with PTR/SRI-MS; DSTL/WIS, 1 month, Homeland Security comparative studies of IMS &SRI-MS.

Fellow ESR 4

Host institution KORE

Project Title: Production of Thermal Desorption Unit and Electronic Devices for Improved Selectivity (WP 3, RO3)

Objectives: (1) Development and characterisation of new thermal desorption unit for specific use on SCIMS instruments to improve and provide efficient sampling and pre-concentration systems and to achieve fast cycle-times (with ESRs 1 (WP 1), 5 and 8 (WP 2). (2) Development and characterisation of ion-funnel technology and novel manipulation of electric field (collisional energy) to improve selectivity and distinguish between isobaric/isomeric compounds (with ESRs 1 (WP 1) and 8 (WP 2)).

Expected Results: (a) A Thermal Desorption Unit that can be easily interfaced to SCIMS (b) Technology to allow novel changes in operational parameters for improved selectivity.

Planned Secondments: *MPG*, Y1 1 month, Applications of PTR/SRI-MS to the Environmental Sciences, *Smiths*, Y2, 1 month, IMS Training; *OWL*, Y2, 1 month FAIMS training, *TMS*, Y3, 1 month SIFDT-MS, calibration diffusion tubes.

Fellow ESR 5

Host institution CU

Project Title: Homeland Security Applications: Improved Selectivity for IMS-MS and Limits of Detection (WP2 iii, ROs1&3)

Objectives: Improvement of understanding in different aspects of SCIMS methods regarding selectivity and the limits of detection for compounds relevant to homeland security and other potential applications: 1) the influence of different SCIMS ionisation schemes on the selectivity and sensitivity of detection (different reagent ions, polarity of the ions, operational parameters) (with ESR 1 (WP 1)); 2) understanding the influence of the physical parameters (drift gases, humidity of gases, gas temperature, electric field homogeneity, ion gate design) on the selectivity of detection (with ESR 1); 3) exploration of different sampling methods for IMS and IMS-MS for improved sensitivity of SCIMS techniques – thermal desorption (with ESR 4 (WP 3)), laser desorption, liquid sampling (with ION); 4) application of IMS-MS technique for identification of the products ions generated in chemical ionisation ion sources.

Expected Results: a) Improvement in the understanding of atmospheric pressure ionisation sources and their operation for selective formation of reagent ions; (b) training in different sampling methods for homeland security relevant compounds from different phases; c) gain experience in the quantitative analysis of the selectivity of analytical methods and a determination of the limits of detection.

Proposed Secondments: Y1 OWL, 1 month, FAIMS and Homeland Security (comparing IMS-MS systems); Y2 ION 1 month, training on PTR/SRI-ToF-MS; Y3 HIPC, 1 month, SIFT-MS and Homeland Security, Smiths, 1 month, IMS and Explosive Detection.

Fellow ESR 6

Host institution CNRS

Project Title: Biogenic Volatile Organic Compounds: Characterization in Various (agro) Ecosystems (WP 2 i, RO2)

Objectives: (1) Optimized systems for measurements of BVOC (Biogenic Volatile Organic Compounds) and of OH reactivity at the leaf-scale (within a small enclosure chamber) and at the canopy scale (with ESR 7 (WP 2)); (2) Utilisation of the SRI-MS and PTR-MS in order to measure additional compounds (e.g. ammonia); (3) Deployment of the experimental systems on the field (various ecosystems – forests and cultures will be investigated); (4) Determination of BVOCs fingerprints and OH reactivity of the studied ecosystems and their impact on secondary pollutants (ozone, aerosols) (with ESR 7 (WP 2)).

Expected Results: 1) Improved analytical systems (BVOCs and reactivity OH) for field measurements at the source (from the branch to the canopy level), (2) An investigation into BVOCs emissions and OH reactivity of forested/agricultural sources (representative of European vegetation/cultures) not or poorly characterized so far. (3) Feedback to WP1 and WP 3 regarding speciation.

Proposed Secondments: *Waters* Y2, 1 month, IMS and IMS-MS Training; *MPG*, Y2, 3 months, PTR/SRI-MS collaborative OH reactivity measurements; *HIPC*, Y3, 1 month, Training on SIFT-MS.

Fellow ESR 7

Host institution MPG

Project Title: OH Reactivity and other Integrative Techniques using SCIMS (WP 2 i, ROs 2 and 3)

Objectives: (1) To establish an improved method for OH reactivity (with ESR 6 (WP 2)). (2) To establish a method for chlorine reactivity. (3) To explore the use of new SCIMS techniques in integrative measurements. (4) To make measurements of OH and Cl reactivity simultaneously under field conditions. (5) To develop OH reactivity suitable for commercialization (with KORE (WP 3).

Expected Results: (a) An improved OH reactivity method with lower detection limits, greater duty cycle, variety of reagents, and more inert inlets. (b) A field measurement dataset for OH reactivity and Cl reactivity. (c) A design recommendation for commercialization of OH reactivity as an instrument. (d) Feedback to WP1 and WP 3 regarding speciation (with KORE).

Proposed Secondments: *HIPC*, Y1, 1 month SIFT-MS training, *MASA*, Y2, 1 month IMS comparative studies; *KORE*, Y3, 3 months Instrumental development for the environmental sciences in the commercial sector

Fellow ESR 8

Host institution RUN

Project Title: Applications of SCIMS Techniques in Biosciences (WP 2 ii, RO2)

Objectives: (1) Applications of PTR-MS (with ion-funnel) & PIT-MS to the biosciences, predominantly on the use of breath analysis for medical diagnosis (with KORE (WP 3)). (2) WP2 collaboration with UMR & UIBK on development of standard breath sampling procedures to better compare SCIMS instruments. (3) Collaborate as part of with KORE (WP 3) and UoB (WP 1) on the ion-funnel & thermal desorption unit for use in biosciences. (4) Feedback to WPs1 & 3 regarding speciation, detection and general problems encountered applying SCIMS techniques to biosciences. (5) Testing developments from WPs 1 & 3 for improved selectivity.

Expected Results: a) Research covering biosciences applications of SCIMS techniques; (b) Standardised breath sampling technique; (c) Validation of improvements in speciation and usability of SCIMS instruments for biosciences applications.

Proposed Secondments: *UMR*, Y1, 2 months, Collaborative projects on breath sampling techniques and data analysis training using PTR/SRI-ToF-MS; *FZMB*, Y2, 1 month IMS use in breath analysis; *OWL*, Y2, 1 month, Training and IMS techniques for use in the biosciences.

Fellow ESR 9

Host institution UMR

Project Title: SCIMS for Metabolic Profiling in Health and Disease (WP 2 ii, RO2)

Objectives: (1) Application of real-time SCIMS to metabolic monitoring during exercise and under diseased conditions (e.g. insulinand non-insulin dependent diabetes mellitus (DM)). (2) Optimization of breath resolved sampling in spontaneously breathing participants. Solving the problem of high respiratory rates under (exhaustive) exercise (with ESR 10, WP 2)). (3) Planning of clinical studies in healthy volunteers and DM patients: Standardization of nutritional and environmental conditions; Preparation of study protocols and ethical proposals. (4) Training in execution of clinical studies in the hospital (dealing with patients, obtaining informed consent). Acquiring basic understanding of the involved pathologies. (5) Cross evaluation of SCIMS with lab-based methods such as GC-MS and GCxGC-MS. Using adequate preconcentration techniques (SPME, NTME). (6) Testing of drift-tube switching and multiple reagent ion procedures being developed in WP 1 and 3 for improved breath VOC selectivity (with ESRs 1, 2 and 4).

Expected Results: (a) A strengthened knowledge on interdisciplinary application of SCIMS in life sciences. (b) Improved understanding of specific problems occurring in medicine: ethical issues, technical and safety requirements of instrumentation used at/near the bedside. (c) An introduction into planning and execution of clinical studies in the way that meaningful results can be obtained and potential commercial exploitation can be assessed, specifically improved selectivity.

Planned Secondments: *Waters*, Y2, 1 month, Training of IMS systems used for breath analysis & collaborative project comparing IMS and PTR-MS for breath analysis; *FZMB*, Y3, 1 month IMS & breath analysis for disease detection; *UIBK* 2 months breath sampling.

Fellow ESR 10 Host institution UIBK

Project Title: Improved Breath and Skin Emanation Sampling Techniques (WP 2 ii, RO2)

Objectives: To develop and optimize sampling techniques for exhaled breath and skin emanations using IMS-MS, but which can be used by all of the SCIMS techniques (with ESR 9, WP 2). A database of VOCs, carefully identified by parallel SRI-TOF-MS and GC-TOF-MS measurements, will be established (WP 1). For selected biomarker VOCs, exhalation concentration patterns under different protocols (also during exertion of an effort) will be determined. Release rates for exhaled breath & skin emanations will be determined. Preliminary work on the human volatilome (with 1764 compounds) has recently been published by UIBK and its partners.

Expected Results: (a) improved sampling protocols for VOCs in exhaled breath and in skin emanations. (b) Exhalation concentration patterns under different protocols (also during exertion of an effort). (c) Release rates (in nmol/min/person for exhaled breath and in fmol/cm²/min/person for skin emanations). (d) Establishment of a database of volatile compounds appearing in exhaled breath and from skin emanations with typical exhalation rates of chosen biomarker candidates.

Proposed Secondments: *ION*, Y1, 3 months, PTR-MS and the biosciences; *FZMB*, Y2, 1 month IMS and breath analysis for disease detection; *UMR*, Y2, 1 month, PTR-MS and breath analysis.