CONFIDENTIAL

FINAL REPORT

Grant Agreement Number:	285045
Project Acronym:	Sniffles
Project Title:	Artificial sniffer using linear ion trap technology
Funding Scheme:	SEC-2011.3.4-2 Seventh Framework Programme
Date of latest version of Annex I against which the assessment will be made:	26-01-2015
Period covered	10 January 2012 to 31 July 2015
Version number	2
Last date modified	31-10-2015
Name, title and organisation of the scientific representative of the project's coordinator[1]:	Dr Carl Hauser, Principal Project Leader, Yorkshire Laser Additive Manufacture Electron Beam, Friction and Laser Processes Group (EFL) TWI. Technology Centre (Yorkshire) Ltd Wallis Way Catcliffe Rotherham S60 5TZ
Tel:	Tel:+44 (0)114 2699046
E-mail:	Carl.hauser@twi.co.uk,
Project website[2] address:	http://www.sniffles.eu/
Project Document Reference	
Author	Carl Hauser

[1] Usually the contact person of the coordinator as specified in Art.1 of the grant agreement.
[2] The home page of the website should contain the generic European flag and the FP7 logo which are available in electronic format at the Europa website (logo of the European flag: http://europa.eu/abc/symbols/emblem/index_en.htm;
logo of the 7th FP: http://ec.europa.eu/research/fp7/index_en.cfm?pg=logos). The area of activity of the project should also be mentioned.

Contents

Glossary of Terms

AM	Additive Manufacturing
CNC	Computer Numerical Control
CBRNe or CBRN	Chemical, Biological, Radiological, Nuclear
CPO	Charged Particle Optics
Da	Unified atomic mass unit
DAPCI	Desorption atmospheric pressure chemical ionization
DAPI	Discontinuous Atmospheric Pressure Inlet
DART	Direct Analysis in Real Time
DLP	Digital Light Processing
ECU	Electronic Control Unit
EI	Electron Impact
GUI	Graphical User Interface
HUP	Hot Uniaxial Pressing
LE	Large Enterprise
LIT	Linear Ion Trap
LTP	Low Temperature Probe
NEG	Non Evaporable Getter
MS	Mass Spectrometry
OEM	Original Equipment Manufacturer.
PIM	Powder Injection Moulding
SME	Small to Medium Enterprise
SMEi	H2020: Small to Medium Enterprise INSTRUMENT
TMP	Turbomolecular Pump
VIM	Vacuum Induction Melting

1 Executive Summary

The Sniffles project aimed to develop a universal gas sensor using modular technologies to function as an artificial sniffer. The device would detect a range of substances, including but not limited to people, drugs, explosives (including weapons) and CBRNe. The technology will complement trained sniffer dogs. The technology proposed was based on linear ion trap (LIT) mass spectrometry (MS). Sniffles was initially a 36 month project but following three amendments at M25, M35 and M38 the final project duration was 43 months. In this report, work is aligned to the third revision of the grant agreement and the date of preparation of Annex 1 of the consortium agreement dated 2015-01-26.

MS techniques have been increasingly deployed in security sniffing applications. MS is a non-intrusive, high-resolution technique able to detect single atoms and complex molecules through their charged species (ions) or fragmentation pattern. The technique is capable of detecting an extremely wide range of substances rapidly, with high accuracy and with a stand-off capability – critically it is able to detect trace levels below parts per million. Once the MS fingerprint of an unknown substance is measured it can be compared online with a database of known substances and rapid identification can be made on the spot in real time.

The Sniffles project aimed to develop a LIT MS based device that had a mass range larger than other comparable MS techniques (2000amu). However, this was revised to 500amu during the M18 DOW and consortium agreement amendment. 500amu mass range was still deemed suitable to allow detection of the types of substances described above. Table 1 gives the system specification targets as described in Annex 1. Table 2 shows the achieved specifications of the Sniffles Rover 2000 (known herein as Beta system). Figure 1 show images of the integrated Beta system complete with docking station and one method of person transportation.

Technology development focused towards the Sniffles Beta system included (1) Development low cost 3D printed plastic parts for the ion trap electrodes and housing (2) development of simulation software (LIT2) that has allowed the development of novel trap operating schemes (the ramped pulse method of trap excitation), (3) electronic control unit with simplified design and lower cost and volume due to non-scanning mode of operation that isolates only specific ion masses, (4) Stable and miniaturised source of electrons for ionisation (GDES cell), with electron kinetic energy characterisation, (5) a DAPCI handheld ionisation source , (6) a reduced dimension vacuum pumping system and (7) new Getter alloys for an improved Getter vacuum pumping system.

The above development allowed integration of a portable MS system with overall dimensions of 400mm x 300mm x 170mm. The unit weight was 16Kg which was twice the target weight. This was largely dictated by off-the-shelf products (ion pump, battery, vacuum flanges, peli case) which would require further significant developments and additional partners.

The technology developments were validated and tested for hidden people, drug simulants (Methyl benzoate, Acetic acid) and explosive simulants (2-nitrotoluene, Cyclohexanone).

Two patent applications have been submitted on a glow discharge ion source and non-evaporable Getter alloys suitable for hydrogen and carbon monoxide sorption and a trademark (ZAO) newly developed Getter alloy. There has also been the development of a handheld DAPCI ion source for sample inlets into portable and other MS systems. As part of the exploitation plan for Sniffles, a continuation project (ChemSniff) funded under the H2020 SME instrument will begin and is focused on reducing system weight and volume and improve reliability, taking the device to TRL7 and closer to commercialisation.

Table 1: Sniffles Rover 2000 system specifications.

Manufacturer/Model	Detection speed	Dimensions	Weight	Analyser type	Mass range	Resolution	Cost
SNIFFLES/ Rover 2000	< 5 sec	40 cm x 30 cm x 10 cm	< 8 kg	Hyperbolic linear ion trap	50-500 amu	< 1 amu	€25,000

Table 2: Sniffles Beta system alignment to project specifications.

Achieved in beta-testing unit	End user requirement
Detection of explosives, drugs, CBRNEs, hidden persons	✓Able to screen, but also target search.
Detection speed < 5 sec	✓adequate for needs.
Dimensions, (x) 400 x (y)300 x (z)170 mm	× adequate for needs but failed to meet depth (z) specifciation due to oversized battery and ECU3 dimensions. Further, the power supply to drive the ion pump had to be fixed to the outside of the carry case
Weight, 16 kg	× too heavy, target < 8kg.
Mass range, 50 – 500 amu Non-scanning Resolution	✓more than adequate for several markets. ✓ < 1 amu, FWHM
Estimated sales price, €25k	✓ competitive for most of minature/portable market.
Power consumption, 75 W ⇨ ~ 4 hrs use	✓adequate for several applications but battery was larger to give greater usage (<50W would be preffered allowing smaller/lighter battery.
Designed to be used by a trained, but non-specialist operator.	✓User-friendly
Pre-concentrator	✓Detection of very low concentration. A concentration factor of 1000 is achievable

Figure 1: Sniffles Rover 2000 Beta System.

2 Project Context and main objectives

When it comes to the difficulties of effective European border control the numbers speak for themselves: With 42,672 km of external sea borders and 8,826 km of land borders, the Schengen free-movement area within the EU-27 enabling free internal travel for the population (half a billion people). The numbers are staggering, with 160M crossings by EU citizens and 120M by non-EU citizens. There are an estimated 8M illegal immigrants in the EU, half of whom came in legally but overstayed. To cope with the migration of people the EU has 1,792 designated controlled border crossing points; 871 sea borders, 665 air borders and 246 land borders.

However, it is not just people that cross borders; the EU also imports 3.9 billion tonnes of goods each year, including machinery, alcohol and tobacco, all of which is subject to customs duty and tax. For this very reason, goods are smuggled into, out of and around the EU every year from foodstuffs, technology and drugs, to endangered species, firearms and explosives. Not only is the range of smuggled goods diverse, but also extensive; for example, the UN estimates a global annual turnover of $400 billion as a direct result of illegal drugs trafficking.

As EU populations continue to increase, all of these figures are expected to rise. Hence there is a growing need for new and/or improved technologies to ensure that the EU's borders remain permeable and efficient for legitimate travellers and goods, while being an effective barrier to cross-border crime.

The Sniffles project aimed to develop a universal gas sensor using modular technologies to function as an artificial sniffer. The focus was the detection of a range of substances, including but not limited to people (e.g. through CO_2 detection), drugs, explosives (including weapons) and CBRNe. The technology proposed was based on linear ion trap (LIT) mass spectrometry (MS) and its mode of operation would ensure complementary operation with trained detection dogs.

2.1 Mass Spectrometry

MS techniques have been increasingly deployed in security sniffing applications. MS is a non-intrusive, high-resolution technique able to detect single atoms and complex molecules through their charged species (ions) or fragmentation pattern. The technique is capable of detecting an extremely wide range of substances rapidly, with high accuracy and with a stand-off capability – critically it is able to detect trace levels below parts per million. Once the MS fingerprint of an unknown substance is measured it can be compared online with a database of known substances and rapid identification can be made on the spot and in real time. Figures 2 and 3 show concept diagrams (given at the proposal stage) for the Sniffles device and its means of portability. Figure 2(i) depicts an entire LIT Mass Spectrometer system (including a vacuum system and handheld PC) housed in a case to make a portable sniffer instrument. Figure 2(ii) shows a possible sample inlet that can be used for sampling vapours with and operational control provided via the ergonomic handset. Figure 2 shows two options for carrying the portable LIT-based sniffer instrument; by hand or in a custom-made backpack.

In the case of an unknown vapour analyte, a sample is introduced into an ion source via a capillary tube (the sample inlet), and ionised (e.g. by Electron Impact). Ions may be collimated using a series of Einzel (electrostatic) lenses and injected into an ion trap (ion storage region) which acts as an 'electronic test tube'. Ions are then selectively ejected (rapidly) and detected with a multiplier detector and high gain amplifier. The resulting mass spectrum is thus a unique 'fingerprint' of the unknown analyte vapour, which may then be identified by comparison with known mass spectra from an existing database of substances. Sample injection, ionisation, capture and ejection takes less than 1 second. Analyte identification typically takes a further few seconds depending upon the substance and speed of access to the database.

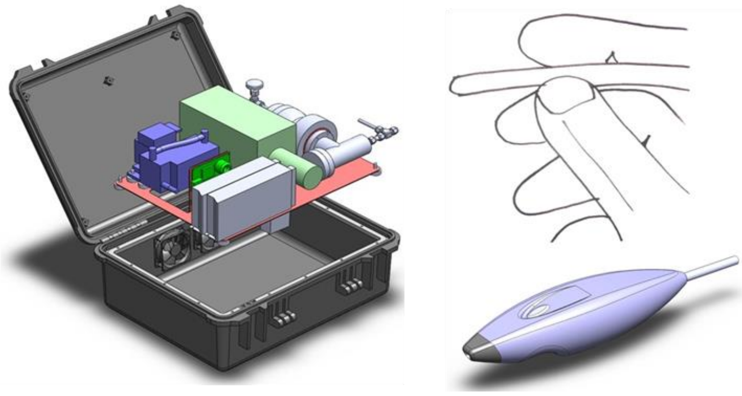


Figure 2: Sniffles device concept drawing.

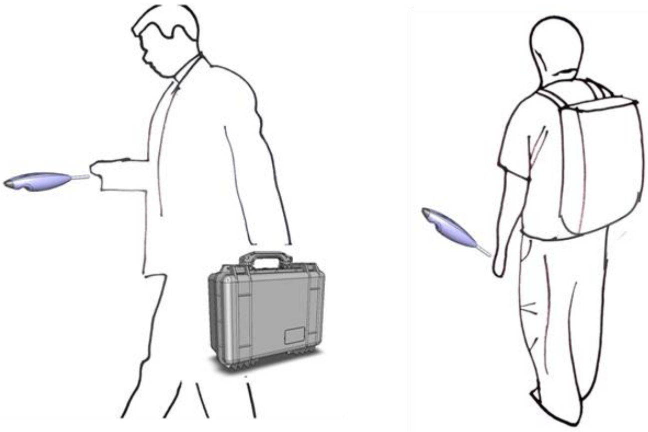


Figure 3: Concept of Sniffles device modes of portability.

In the case of a solid analyte e.g. particulates of drugs or explosives on banknotes or clothing, such samples maybe analysed by first vaporising the particulate using a cool microplasma. The vapourised sample is admitted into the ion trap via a carrier gas (can be air). In this case the sample inlet takes the form of a microplasma torch in addition to the capillary tube.

However, MS implementation requires suitable methods of ion generation, ion analysis, and ion detection. The Sniffles consortium will address each of these processes, developing unique solutions for an integrated all-encompassing portable detection device.

Table 1 below gives the primary specifications of the sniffles systems requirements as described in Annex 1 of the consortium agreement. The one revision to the table occurred at M18 where the mass range was revised from 2000 to 500 amu. A mass range of 500amu mass range was deemed more appropriate for the detection of substances described above.

2.2 Technical Barriers

The ability to sense a wide range of illegal substances (including weapons, drugs, explosives, CBRNE threats and hidden persons) is linked to a very high sensitive detection device. Only traces or ultra-traces are present at ambient pressure and at room temperature as the major part of these substances have very low vapour pressure.

Consequently a highly sensitive mass spectrometer device is required if a direct vapour inlet is used. With ion creation at ambient atmosphere (for example DART), more ions can be then created, however the poor efficiency of ions introduction requires also a high sensitivity mass spectrometer.

In order to deliver this cutting edge artificial detection system, there are a number of technical barriers which have until now, prevented the previous development of a Sniffles type device:

1. There is no single country (in Europe or elsewhere) which has the range of technology or expertise necessary to achieve all of the sub-system component parts.
2. To deliver a cost-effective LIT MS detector there are a number of sub-systems (LIT, ionisation, sample inlet, vacuum system, software and packaging) which require, considerable research effort to develop and optimise the solution while maintaining a focus towards a portable and cost effective device:
3. The sample inlet forms the interface between the real world and the vacuum system in which the mass spectrometer operates. In recent years many types of inlet have been introduced, but most of these are unsuitable for a handheld portable MS sniffer. There remains a clear need for development work to miniaturise and couple an inlet adapted for low levels of illegal vapours and solid analytes into a portable sniffer instrument – especially one that is non-obtrusive within the context of border control.
4. Usually the most expensive, bulky and heavy part of any portable MS device is the vacuum system, which effectively determines the system cost. Existing turbo molecular and bellows pumps are too heavy and/or power hungry for mobile applications. There is a need to find a low cost, lightweight and low power vacuum system coupled to a miniature MS in such a way that the overall system performance is not compromised. Novel getter pumps are the answer because they are low weight, high vacuum potential and capable of running at low power, but still require development to further increase their pumping capacity and ruggedness and to further reduce total weight and volume, power consumption and cost.
5. The requirements needed for the Electronic Control Unit for such a sniffer are particularly demanding: small footprint, low power, high sensitivity, stable and precise RF and DC voltages alongside sub-picoamp measurement and data recording in the same package. While units are available, most are supplied from within US; there is a need to develop a generic/low-cost ECU which is specifically tuned for optimal performance of a LIT.
6. The LIT is complex in design; containing electrodes with precisely positioned and shaped contours, the housing which must support electrodes with high positional accuracy yet allow for communication of services (electrical signals), and it must operate under high vacuum and at elevated temperatures. Thus, the method of manufacture of the LIT is a key consideration; not only to give freedom of design, choice of suitable materials and dimensional and surface accuracy, but it must also be cost effective and rapid. Digital Light Processing (DLP) is an ideal method that can meet these needs, but requires specific developments on system resolution and improved performance of material systems (high temperature stability >150 degrees) with improved mechanical properties with to allow successful implementation.
7. In order to be successful within a border control setting, the operating procedures of the LIT MS – Sniffles device – needs to be carefully considered, including; operation procedures, gas loadings, integration of novel sub-system technologies, space constraints and portability and ergonomic design. Ultimately the device needs to perform within this environment, be easy to operate by non-technical end users and show identical or superior (complementary) detection compared to existing sniffer dogs.

2.3 Objectives

Considering the technical barriers given previously, the following objectives have been defined which form the basis for the R&D content of the SNIFFLES project.

System Objectives:

1. To design, simulate, build and validate through field testing, an artificial sniffer with the ability to sense a wide range of illegal substances up to 500 amu and including, but not limited to, cannabis, cocaine, Methyl salicylate, dimethyl methyl phosphate (DMMP), RDX (i.e. cyclotrimethylenetrinitramine) and TNT (Trinitrotoluene).
2. To provide a portable, easy-to-use (by non-specialist personnel) device through integration of various technologies being developed across the EU (LIT, Vacuum system, methods of Ionisation).
3. To be able to detect the specified threats/substances rapidly (<1 sec) and continuously, with stand-off capability (< 300mm), at low levels (less that parts per million) and accurately (a false positive rate of <2%).
4. A target price for a single unit of the sniffer device is <25k euros.
5. The portable system will fit inside a briefcase sized holdall of dimensions 40 cm x 30 cm x 10 cm and will have an operational weight < 8kg.
6. Specification of border control operating procedures which incorporate the new Sniffles detector, showing secure operation and complementary (synergistic) operation with sniffer dogs – achieved through demonstration of controlled smuggling tests (i.e. information on substance type and concentrations) of controlled substances than existing border control operations)

Device Objectives:

7. Produce a prototype device which integrates each sub-system and is capable of demonstrating the performance characteristics listed in objectives 1-5, within the context of a border control checkpoint trials.
8. To demonstrate that the Sniffles artificial sniffer device has suitable cost (<€25,000) and can be manufacturing by a scalable route (i.e. capable of >500 units per year within 5 years of market introduction).

Sub-System Objectives:

9. Small, lightweight and low cost Ion trap, yet capable of achieving the required mass range (500 Da), resolution (<1 Da) and high sensitivity (at sub-parts per million trace levels).
10. Sample inlet: able to accept all vapours and solids of interest (threat analytes).
11. Ionisation methodology: optimised and suited to achieve the most efficient coupling of sample inlet to ion trap in a miniature volume.
12. Dynamic range of detector at operating vacuum with a maximum signal to noise ratio.
13. Electronic Control Unit (ECU): miniaturised and operating at low power (<25W).
14. Portable getter pump vacuum system: capable of handling required load of inlet gas (at atmospheric pressure) and sample.
15. Develop the use of silver nano-particulate inks to form low ohmic LIT electrodes that are hyperbolic (or other) in shape for cost effective (<€10 per electrode) replaceable (disposable) electrode.
16. Handheld PC: able to couple to the firmware of the ECU and provide a user friendly interface for operation of the Artificial Sniffer by trained but non-specialist personnel (e.g. police and/or customs officials). PC to provide rapid identification of threat substances via on board data base and access to mass spectral libraries in real time.

3 Sniffles Partnership

The Sniffles project beneficiary list is given in Table 3 and a pan European map showing beneficiary locations is given in Figure 4. Please note that beneficiary 4 (omitted from Table 3), DSM Research - Technology and Analysis Geleen, left the project at M18 and was immediately replaced by Da Vinci Laboratory solutions BV. The Sniffles consortium consisted of specialists in complementary fields particularly well qualified for the development of portable MS instrumentation (UoL, Qtec, DVLS), sample inlets (Qtec), Ion sources (AMU), vacuum technology (SAES), control software (TWI, SAES, DVLS), 3D printing manufacturing technologies (TWI, Xaarjet), testing and simulation (DVLS, UoL, Qtec, AMU) and demonstration and validation of the technologies (DVLS, WAG) within the border security and customs control environment.

Table 3: Sniffles Consortium

Participant no.	Participant organisation name	Short Name	Country
1 (Coordinator)	TWI LTD	TWI	UK
2	The University of Liverpool	UoL	UK
3	Aix-Marseille Université	AMU	France
5	Q-Technologies Ltd	QTec	UK
6	SAES Getters S.p.A	SAES	Italy
7	Envisiontec GbmH	Env	Germany
8	Xaar Jet AB	Xaar	Sweden
9	Wagtail UK Ltd	WAG	UK
10	Da Vinci Laboratory solutions BV	DVLS	Netherlands

Figure 4: Sniffles European Collaboration.

4 Science and Technology Results

The overall work plan strategy for the Sniffles project is given in the PERT diagram in Figure 5. The different micro collaborations between beneficiaries in each work package are given in Figure 6.There were 3 phases to the project: Road-mapping (and device creation), Integration (and device optimisation) and Testing and Validation. The activities within each of these phases of work are outlined below:

Phase 1: Project Road-mapping (and device creation): This phase provided a holistic overview of the gas sensor device development, within the context of creating a robust and reliable artificial sniffer for border control. This was mainly controlled and managed in work package 1. The performance of the device was defined in line with objectives given in 3.3

Device and Subsystem creation

Ion Trap (WP2): To ensure a highly sensitive artificial sniffer device with a small footprint operated under vacuum conditions, it is essential that the ion trap design is optimised through simulations of linear ion traps to enhance performance (e.g. sensitivity, resolution). In this initial phase, LIT's were built using CNC manufactured electrodes and housing for the purpose of performance benchmarking and validation.

ECU (WP3): The electronic control unit (ECU) is an essential part of the proposed artificial sniffer. It provides (i) the RF excitation necessary for the trap to function; (ii) the DC excitation for electron/ion production and focussing; (iii) the detection electronics for accurate measurement of ion current and mass spectra (analyte fingerprint); (iv) firmware to provide an interface of the above functions to a display system e.g. PC. The creation of a Graphical User interface to communicate with the ECU firmware was also included in this work package. In this phase, a first prototype ECU1 was built for integration into the pre-prototype unit (WP7 – Phase 2).

Optimisations of operating conditions (WP4): Investigation will be conducted by AMU to increase the performances of each stage of the mass spectrometer (ion creation at low pressure in the vacuum chamber, injection, confinement and mass analysis) and define the optimal operating conditions.

Sample Inlet (WP5): To ensure a versatile artificial sniffer capable of detection a wide range of substances including drugs and explosives an inlet which efficiently couples an analyte into the ionisation region of the ion trap was developed. 2 sample inlets based upon the most common ambient techniques: DAPI and DAPT were developed and tested for samples contain in vapour and on solid surface.

Vacuum System (WP6): In order to guarantee the expected spectrometer performances, a suitable vacuum level must be achieved. State of the art technologies will be applied in order to design and construct a first vacuum system (pre-prototype) and a docking station, fulfilling the stringent specifications of this project. The pre-prototype had the following characteristics: (1) Non evaporable Getter pump, (2) Sputter Ion pump and (3) initial vacuum chamber layout to ensure require pumping speed/pressures.

Phase 2: Integration (and device optimisation): This phase built upon the developments of phase 1 and integrated a first prototype device to gain understanding of the potential for the Sniffles technologies. It incorporated the technical and practical operating parameters achievable, including operating procedures and interaction with sniffer dogs. As part of this phase, WP2-6 continued to run, but focussed on optimisation and manufacturing of the various device subsystems, culminating in a prototype system followed by three beta testing units for testing and validation.

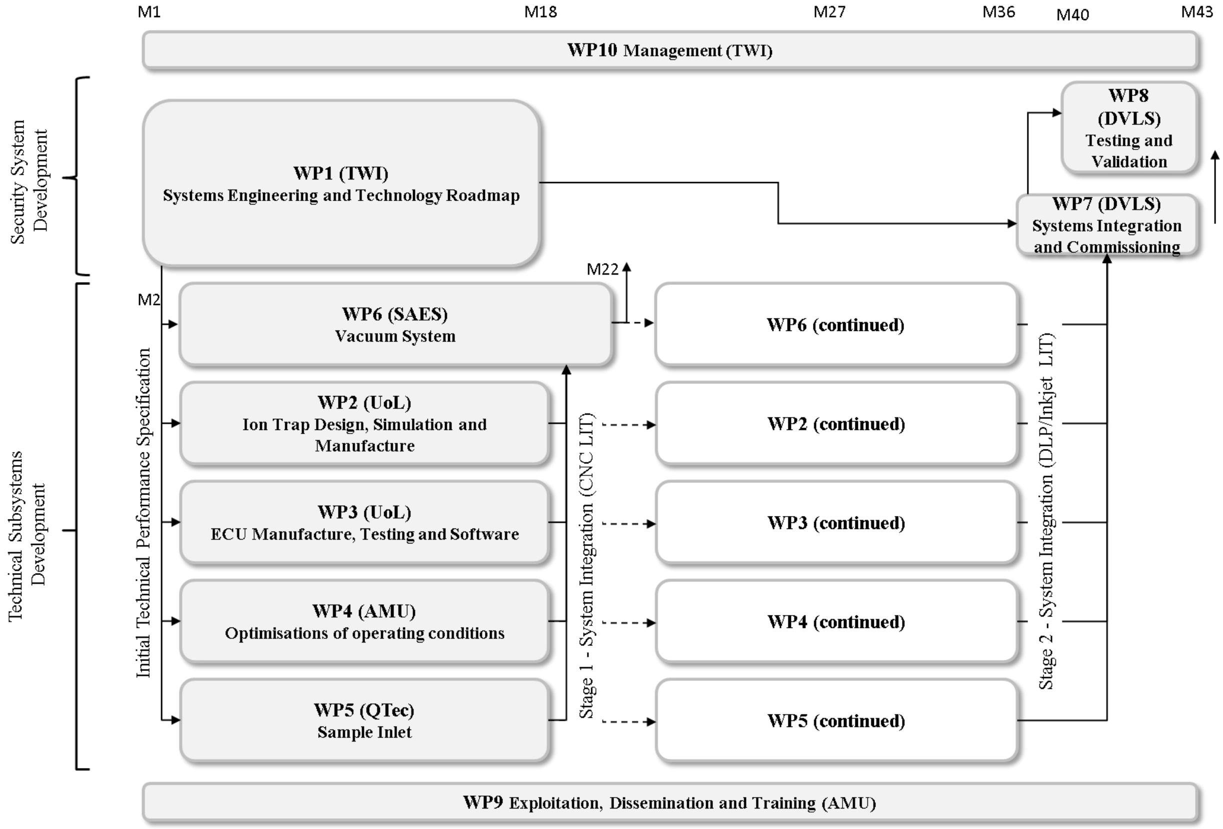


Figure 5: Sniffles Work packages and work package flow.

Device and Subsystem Optimisation:

Ion Trap (WP2): New, faster and lower cost manufacturing methods were developed for the LIT analyser (1) Digital light processing – a polymer based 3D printing technology and (2) inkjet printing of conducting silver inks for coatings. At each stage, the design of the ion trap required optimisation and simulation and benchmarked against the CNC manufactured LIT.

ECU (WP3): In this phase further development and refinement of the ECU took place (reducing, size and weight and increasing functionality). This resulted in delivery of ECU 2 for testing purposes in WP4 and ECU3 for integration into the beta testing units.

Optimisations of operating conditions (WP4): Work continued in this work package looking at system performance increases.

Sample Inlet (WP5): The DART inlet developed in phase 1 was then superseded by a desorption atmospheric pressure chemical ionization (DAPCI) system for the analysis of complex molecules including samples of explosives. This is a more effective method of DART realisation. The complete handheld DAPCI ion source, including the air pump, battery and electronic circuitry was enclosed in a 3D printed plastic enclosure and was validated with the use of explosives substances.

Vacuum System (WP6): In parallel to the development of the pre-prototype vacuum system, new Getter materials able to better suit the specific need of this application (i.e. high capacity for N_2 and oxygen at “low” temperature) were successfully developed and innovative methods of manufacturing explored with the aim of decreasing the process cost, increasing the degrees of freedom as far as the getter material geometry is concerned and increasing Getter performance in a portable MS device. This culminated in the manufacture of an advanced vacuum system that was integrated into the beta system.

System Integration (WP7): This work packaged involved the integration of technical outputs from work packages 2-6, firstly as a pre-prototype system and then as three beta systems for systems testing and validation in WP8

<u>Phase 3: Testing and Validation:</u> This phase is the final culmination of activities on the project and used the optimised Sniffles beta units for device testing.

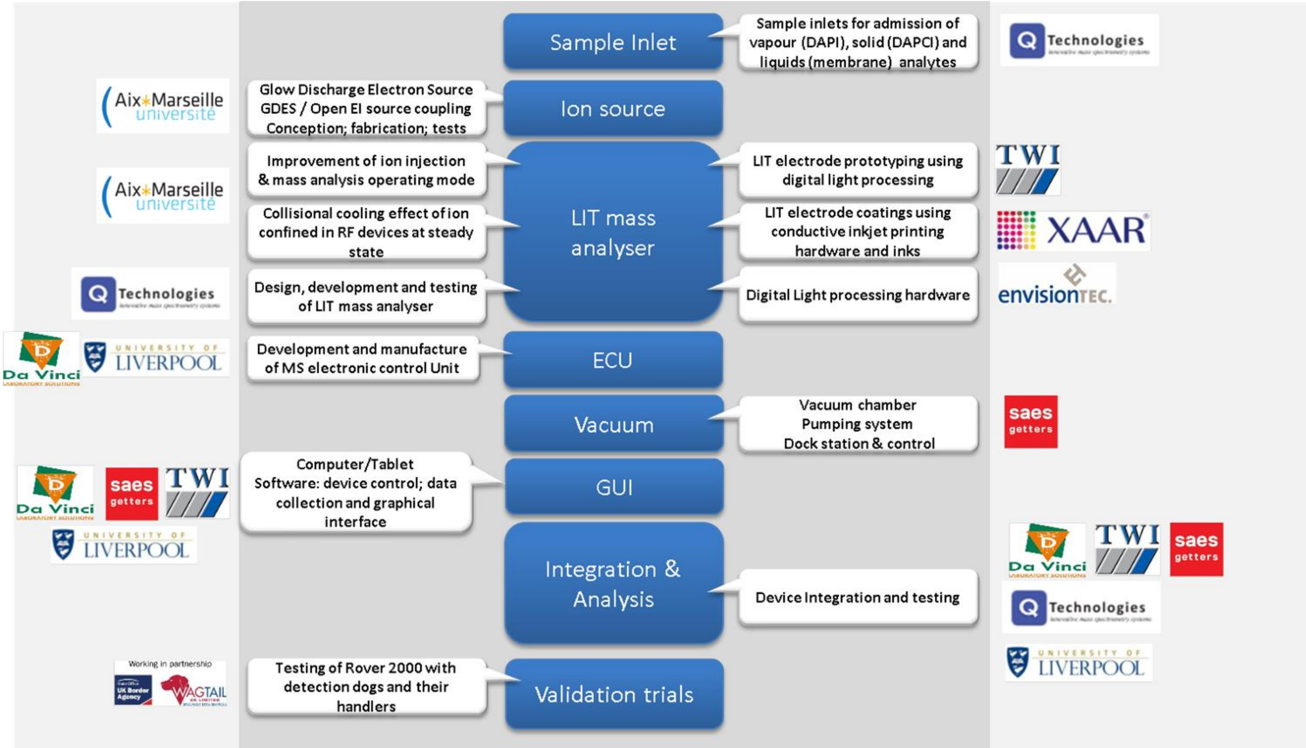


Figure 6: Sniffles technology development collaborations.

4.1 Work Package 1: Systems Engineering and Technology Roadmap

Start month: ***Month 1***
Schedule Completion: ***Month 18***
Status: Completed

Task	Task Title	Start Month	Scheduled End Month	Status
1.1	Artificial Sniffer operation procedures	1	3	Complete
1.2	Gas load evaluation	1	4	Complete
1.3	Vacuum system functional specification definition:	1	4	Complete
1.4	Vacuum system space constraints definition (Proximity constraints definition)	1	5	Complete
1.5	Vacuum system concept definition:	1	5	Complete
1.6	Interfacing Specification	1	5	Complete
1.7	Ergonomic Design Constraint Specification	1	6	Complete
1.8	Sensor performance metric	1	18	Complete

Deliverable	Deliverable Title	Status
D1.1	Report on gas sensor operational procedures and functional specification (SNIFFLES Roadmap)	Complete
D1.2	Report on Interfacing specifications and GUI operations	Complete
D1.3	Report on gas sensor ergonomic design outline	Complete
D1.4	Report on metric to asses sensor performance	Complete

Within Work Package 1 all tasks consisted of studies and discussions to provide a holistic overview of the gas sensor device development, within the context of creating a robust and reliable artificial sniffer for border control. Initially within this period the specification of the device performance was defined. This task finished at the end or reporting period 1. However, for completeness, a summary of work package 1 has been included in this final report.

Task 1.1: Artificial Sniffer operation procedures
The procedures for operating a linear ion trap mass spectrometry (LIT MS) unit have been developed. These procedures were developed with input from all beneficiaries concerning the operation of a portable unit with the objectives of the project in mind. Input from WAG was important in changing the procedures so that the unit follows those currently employed by dog search teams at border crossings. The beneficiaries have determined and defined the initialisation protocols and procedures necessary for ‘turn-key’ operation of the sensor system and use by non-specialised personnel. This allowed D1.1 to be completed.

Task 1.2 and 1.3: Gas load evaluation and Vacuum system functional specification definition
An initial gas load evaluation was carried out based on the experience of the beneficiaries involved. This has defined the amount of entry gas per gas sample and the life cycle of the final product in service. This can change throughout the project as more of the sub systems are defined and the whole device is developed. This in turn allowed for the vacuum system functional specification to be defined allowing the development of the getter alloy material and the sintering technologies to meet this specification. With these other tasks being defined this allowed for the appraisal of the space constraints of the vacuum system This constraint is constantly re-evaluated with reference to the

development of the gas load / inlet designs, also the development of the getter alloy and sintering technologies.

Task 1.4, Task 1.5 and Task 1.6: Vacuum system space constraints definition, Vacuum system concept definition and Interfacing specification
The output from all the tasks in work package 1 allowed for the concept of the vacuum system to be formed. This design is constantly updated with the development of the inlet devices in WP5 affecting the vacuum system. This in turn allowed for the interfacing specification to be defined. This details methods of communication and interfacing between the various technologies sub-systems. This allowed for the completion of D1.2.

Task 1.7: Ergonomic Design Constraint Specification
The ergonomic design of the gas sensor has been considered in relation to the needs of the end user and the workplace for purposes of storage, carrying and handling, interactions and use. One of the key inputs was from WAG having defined the environment that the device will be expected to work under. The ergonomic outline will aid in the design of the Sniffles device after highlighting a number of areas that will need detailed consideration. It allows other work packages to understand the design requirements and the environment that the device is expected to be used in. The handler also needs rest and breaks from searching as this can be very strenuous activity and may involve the handler working in severe weather conditions. These constraints would be applied to the final testing of the device. This resulted in the completion of D1.3.

Task 1.8: Sensor performance metric
The performance of how the system will be assessed in relation to the types of components that the device will need to be able to detect has been analysed. For real life testing of Drugs; cocaine, XTC, methamphetamine and heroin are the main target compounds. For real life testing of explosive, there are 3 main test compounds. For real life testing for human presence, lactic and/or propanoic acids are the target compounds.

As most of these compounds are difficult to obtain alternative compounds are proposed for instrument laboratory testing. Limonene is proposed as the main test compound. It is often present as a contaminant in drugs. Methyl benzoate, 2-nitrotoluene Cyclohexanone, DMMP and CEES are proposed as other alternative testing compounds.

For testing of the mass range of the instrument Perfluorotributylamine (PFTBA) is proposed, covering a broad mass range. Beside the target compounds, the sampling area itself is of importance in the following aspects:

- Surface – direct sampling, headspace or swabs. Swabs can directly be heated or be extracted with a solvent). For surface testing, caffeine is proposed as the main target compound. Headspaces can be sampled as a gas.
- Liquids – direct sampling with an injector or headspace sampling like gases. Toluene and methyl benzoate are the preferred target compounds.
- Gases – direct gas inlet, Toluene in air is the main target sample.

D1.4 was completed from the output from this task. All deliverables for work package 1 are all complete and submitted.

4.2 Work Package 2: Ion Trap: Design, Simulation and Manufacture

Start month: ***Month 2***
Schedule Completion: ***Month 28***
Status: Complete

Task	Task Title	Start Month	Scheduled End Month	Status
2.1	Ion Trap Design and Simulation:	2	10	Complete
2.2	Manufacture by CNC:	2	12	Complete
2.3	Manufacture by DLP	2	12	Complete
2.4	Manufacture by Enhanced DLP	12	18	Complete
2.5	Manufacture by Inkjet Printing	16	24	Complete

Deliverable	Deliverable Title	Status
D2.1	Report on Ion trap design and simulation	Complete
D2.2	Creation of CNC LITs for testing at UoL	Complete
D2.3	Creation of DLP LITs for testing at UoL	Complete
D2.4	Creation of Inkjet LIT electrodes for testing at UoL	Complete
D2.5	D2.5 Creation of 3 LIT-MS systems	Complete

4.2.1 Objectives

The key objectives for this work package were:

- Design and simulations of linear ion traps (LITs) to enhance performance of the mass analyser (e.g. sensitivity, resolution),
- Fabricate most suitable LITs using three manufacturing techniques: computer numerical control (CNC) machining, digital light processing (DLP) and inkjet printing.

4.2.2 Key Technical Achievements

<u>Creation of digital light processing (DLP) LITs (TWI, Env and UoL)</u>
Digital Light Processing (DLP) is a low-cost, high resolution 3D layer based additive manufacturing (AM) technique. In this project DLP was used to successfully manufacture the LITs for the Sniffles Beta system for which UoL already holds a patent (S. Taylor, P. R. Chalker, C. J. Sutcliffe, UK Patent application: GB2009/051119, MS fabrication using rapid prototyping (2008). At the start of the project, CNC manufactured LITs were used for benchmarking the system (electrodes and housing). However, they are heavy and the complex shape of the LIT's are difficult and time consuming to manufacture using CNC, and hence high cost (€470 a set based on delivery of+20 sets). The machine used for the construction of the LIT was an Envisiontec Perfactory DLP system which employs a dynamic masking technique to selectively cure a photosensitive polymer resin. Several polymer resins were investigated but HTM140 v2 was finally chosen for the electrodes and housing based on its resolution and high temperature sensitivity. The DLP electrode surfaces are rendered conducting via a secondary step through the deposition of a layer of gold by thermal evaporation techniques (see Figure 7). The manufacturing cost for the DLP housing, 4 electrodes and gold coating was €130.

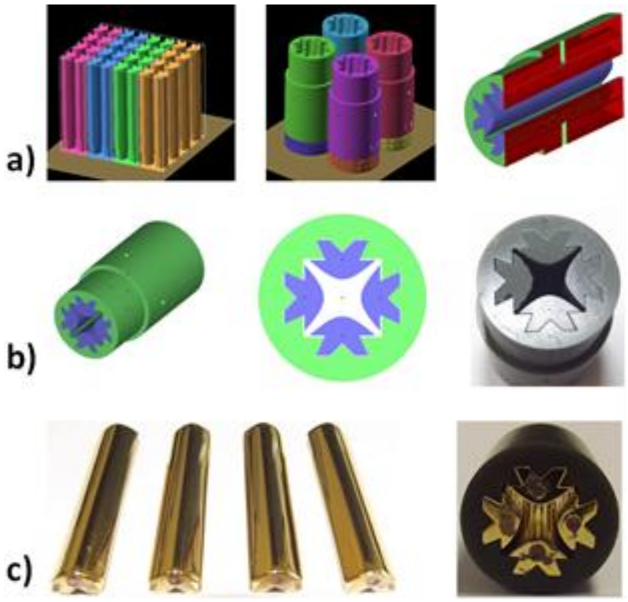


Figure 7: Design, fabrication and assembly of DLP linear ion trap: a) fabrication design stack of DLP LIT rods and housings on a machine build envelope with vertical cross section of LIT assembly, b) fabrication design of LIT assembly with non-coated prototype, c) electroplated LIT rods and final rod assembly in ceramic resin housing.

<u>Creation of inkjet printed LITs (Xaar, TWI, UoL)</u>
The desire to have a truly interconnected device to include internal features for communication of services (i.e. electrical connectivity to the electrodes) would be impossible to do by CNC and very difficult to achieve using DLP. The final DLP LIT's rely on metallic screws to communicate voltages from the gold conducting surfaces. For this reason, the use of inkjet printing of conducting inks was investigated in the hope to give greater flexibility in a low weight and size integrated sensor.

Three layers of Ag nano-particle ink (SunChemical's Suntronic U5603) at a total of 0,6 µm thickness showed a sufficiently low electrical resistivity to function as the desired electrode layer on DLP produced polymeric LIT electrodes. The sintered Ag nano-particle ink did not contaminate the vacuum in the LIT when tested. The cost to inkjet print 4 DLP electrodes was 0.24 €. This was based on inks costs of 10K € with5% solid content of Ag in the ink, 5 cm^2 surface area per electrode (20 cm^2 for a full set of 4 electrodes) and a 0.6 µm Ag electrode thickness. This gives an ink usage of 24mm^3. However, this route was not without problems. Firstly, it was attempted to achieve electrical connection to the Ag-electrodes with metal screws mechanically impressing through the housing but no sufficient low resistance connection could be achieved. This was caused by the screws penetrating the sub-micrometer thick Ag film on the (soft) polymeric DLP bodies. Additionally, Ag paint was used to connect the printed electrodes with the screws but a sufficiently low resistance could not be achieved. The silver paint also caused contamination of the LIT vacuum. In an attempt to resolve the connectivity issue

DLP electrode bodies were produced, which contained a hole to insert a copper wire, and a via-hole with access from the top side to the copper wire. The idea was to inkjet print Ag-ink into the via-hole, forcing a connection between the Ag-electrode and the copper wire. However, this also did not work out positively due to the limited precision of the hole and the via-holes in the DLP-bodies. Both holes were too large so that the inkjeted Ag-ink receded into the capillaries. A further problem could have been that the oxide layer on the copper wire prevented good electrical contact to the inkjeted Ag-ink in the via hole.

Table 4: Cost and weight comparison of LIT manufactured using different methods explored and developed in Sniffles.

Methods	CNC Electrode rods (set of 4) €	DLP Electrode rods (set of 4) €	DLP housing €	Metalise™ gold coating method from 3DDC Ltd (set of 4 electrodes) €	Inkjet printed silver coating (set of 4 electrodes) €	Weight Kg	**Total Cost €**
CNC electrodes + DLP housing	450	-	20	-	-	0.2	**470**
DLP electrodes and housing and gold plated	-	10	20	90	-	0.015	**130**
DLP electrodes and housing and inkjet coated with silver	-	10	20	--	20	0.015	**50**

LIT-MS implementation (UoL)

Three types of LIT-MS instruments were fully assembled and wired for use in: pre-prototype, prototype and beta portable MS systems . The pre-prototype LIT-MS was assembled on a standard CF40 vacuum flange with stainless steel pins together with low pressure electron multiplier detector and electron impact (EI) ion source. It was made in two copies – one containing CNC LIT and the other preliminary DLP LIT. The prototype LIT-MS was built on a custom CF40 flange with gold plated pins and better pin isolation for minimizing noise on the output. It contained CNC LIT, low pressure electron multiplier and GDES/EI source. Beta LIT-MS was built in three identical copies on a custom CF40 flange with high enhanced DLP LIT, high pressure electron multiplier and EI source.

Development of a novel LIT simulation software LIT2 (UoL)

LIT2 is unique simulation package that includes:

- Non-scanning LIT support for different electrode geometries.
- Boundary element method for more accuracy in solving electromagnetic field calculations,
- Separate field solving program for faster computation,
- Large number of ions (500k ions),
- Buffer gas cooling effect for sensitivity enhancement,
- Ramped pulse method support for resolution enhancement (optional).

Development of a ramped pulse method for resolution enhancement (UoL)

A novel voltage control method was developed to improve resolution of the LIT analyser using in-house simulation software LIT2 mentioned previously. Standard non-scanning method of LIT operation gives 4 Da mass peak width, while with the new ramped pulse method, peak width is reduced to 1 Da (unit resolution) within 500 Da mass range.

4.2.3 Deviations from work plan

A deviation from the original work plan was usage of DLP LITs for beta units rather than inkjet LITs, whose cost is significantly lower than for both CNC and DLP. Due to difficulty to manufacture 3D hyperbolic electrodes using inkjet printing, it was decided to use this technique only for low-cost coating of DLP electrodes. However, as mentioned previously, a good electrical contact could not be applied to inkjet coated rods, which resulted in using electroplating coating technique for DLP rods.

4.2.4 Progress beyond current state of art

TWI and EnvisionTec worked to improve the software and build files of the EnvisionTec Perfactory hardware in an attempt to build LIT-MS electrodes with increased resolution i.e. finer layer thickness from 25µm down to 15 µm. This enhanced method of building was successful and will give greater functionality and improved resolution for future commercial DLP systems. However, the improved resolution (in z direction) gave no noticeable improvement to gold plated electrodes or positioning/ sizing accuracy of vias for inkjet printing. A novel polymer coating method, Metalise^{TM} from 3DDC Ltd, has been used to coat the DLP rods with gold. Development of novel ion trap simulation software (LIT2) that has allowed the development of novel trap operating schemes (the ramped pulse method of trap excitation).

4.2.5 Future Work

<u>Creation of inkjet printed LITs</u>
It has been proposed that a better dimensioned DLP body with a tight-fitting hole for a metal wire, and a series of up to 10 via holes along the wire, with the via hole diameter of size equal to half the diameter of the wire be produced. Gold wires would then be interested in the holes of the DLP electrodes and the hold filled with inkjet Ag ink. This should then be followed by photonic sintering or very low heat oven sintering. Xaar have used inkjet to successfully contact LED's buried into flat substrates by way on inkjet printing Ag-ink into vias.

<u>Advanced simulations</u>
Using LIT2 simulation package, a number of effects will be investigated for enhancement of LIT sensitivity and resolution. These will include different buffer gas temperatures, fringing field effects between LIT endcap (z-electrodes) and LIT rods (x,y-electrodes), ramped pulse optimization and manufacturing errors.

4.3 Work Package 3: ECU Manufacture, Testing and Software

Start month: ***Month 2***
Schedule Completion: ***Month 28***
Status: On-going

Task	Task Title	Start Month	Scheduled End Month	Status
3.1	ECU manufacture	2	12	Complete
3.2	Testing for MS functionality	3	13	Complete
3.3	Capability Testing	9	18	Complete
3.4	Instrument Development	10	19	Complete
3.5	Software GUI	11	24	Complete

Deliverable	Deliverable Title	Status
D3.1	Creation of ECU for Sniffer development to AMU and UoL and validation to RESOLVE	Complete
D3.2	Report on artificial Sniffer Stage 1 (CNC LIT) test results	Complete
D3.3	Creation of software (GUI and application interfaces)	Complete
D3.4	Creation tested artificial Sniffer Stage 2 (DLP LIT)	Complete
D3.5	Tested artificial Sniffer Stage 3 (Inkjet LIT)	Complete
D3.6	Creation of 3 ECU beta units	Complete

4.3.1 Objectives

The key objectives for this work package were:

- Design, build and test three types of electronic control unit (ECU) to drive LIT-MS: ECU1 (pre-prototype), ECU2 (prototype) and ECU3 (beta unit).
- Develop graphical user interface (GUI) that will communicate with ECU to control its power, input parameters and output data.

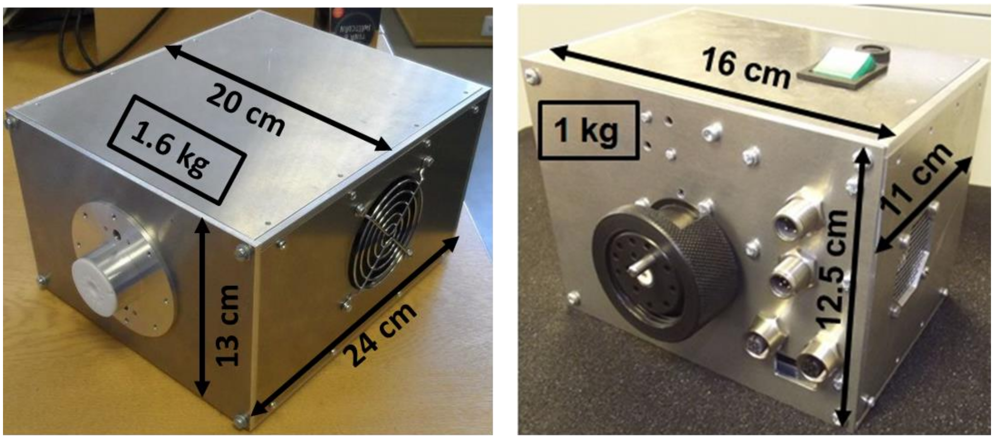
4.3.2 Key Technical Achievements

<u>Creation and testing of ECU1 (UoL)</u>
ECU1 was the pre-prototype electronic unit that was used to test LIT-MS with CNC, DLP and inkjet coated LITs. It was also integrated into the Sniffles pre-prototype system (see Section 4.7). It consisted of 5 PCBs that were used to power and control the key components of LIT-MS: EI ion source, LIT and electron multiplier detector. It was tested for MS functionality with CNC, DLP and inkjet coated LITs using krypton and xenon gases showing reliable results for CNC and DLP LITs, but no output signal on inkjet LITs. ECU1 was also used with DLP LIT for capability tests for a number of simulants of drugs, explosives and CWAs including real samples of drugs and explosives.

<u>Creation and testing of ECU2 (UoL)</u>
ECU2 was made as a part of the prototype system with a GDES/EI ion source (see Sections 4.4 and 4.7). The overall design is identical as the one in ECU1 with additional PCB to control the GDES/EI source. ECU2 has only been tested for control of GDES/EI source showing a reliable electron emission inside the GDES cell. Experiments with ECU2 coupled to LIT-MS with GDES/EI source are planned after ECU2 is properly tuned and calibrated for the prototype LIT-MS.

Creation and testing of ECU3 (UoL)

ECU3 was made as an integrative part of the beta unit (see Section 4.7). It was reduced in size by a factor of two compared to the ECU1. It consists of 8 PCBs that provide additional improvements and functionality options compared to the ECU1. These are: fully shielded RF circuit for stability of mass peaks, ramped pulse voltage control for resolution enhancement, control of HV valve and sample pump for safe operation of the getter vacuum system, communication support for the I/O controller and built-in battery power input. After implementation, the ECU3 was tested with beta LIT-MS for functionality using krypton and xenon gases. It was also successfully tested for capability and limit of detection (LOD) using limonene as well as for a number of real substances that were provided at the final review meeting. Figure 8 shows fully assembled and encased ECU3.



(a) (b)

Figure 8: Fully assembled (a) ECU1 and (b) ECU3 with front panel connectors and power switch.

Creation of GUI (TWI and UoL)

Two types of graphical user interfaces were developed for the ECU3. One was a test GUI for technical users that allowed low-level testing of the ECU for performance optimization. The other was end-user GUI for high level control of substance detection and communication with the I/O controller of the beta unit (see Figure 9).

Figure 9: Fully functioning GUI shown on a Tablet and tested in docked mode.

4.3.3 Deviations from work plan

A major deviation from the work plan was that ECU3 was used to control LIT-MS with a standard EI source rather than with a novel GDES/EI source. This was due to insufficient time to test a miniaturised GDES/EI source for functionality and capability. There were also delays in the delivery of a fully functioning ECU which reduced the time for device integration into the Sniffles Beta system in Work package 7.

4.3.4 Progress beyond current state of art

Compared to existing commercial electronic units, ECU3 has simplified design and lower cost due to non-scanning mode of operation that isolates only specific ion masses. This does not require a ramping circuit for doing mass scanning across the whole mass range. It also has a built-in support for voltage control with a unique ramped pulse method for enhancement of mass resolution.

4.3.5 Future Work

Future work will include further experimental investigation of the ramped pulse method, ionisation and mass fragmentation tests at 70eV, and development of automated method of mass calibration using PFTBA.

4.4 Work Package 4: Optimisations of operating conditions

Start month: ***Month 2***
Schedule Completion: ***Month 28***
Status: Complete but with revisions

Task	Task Title	Start Month	Scheduled End Month	Status
4.1	Glow Discharge Electron Source (GDES)	2	5	Complete
4.2	GDES EI ion source	2	5	Complete
4.3	Injection and focussing in the LIT of ions created at atmospheric pressure:	2	18	Complete
4.4	Improvement of the Ion preparation in the LIT	2	18	Complete
4.5	Mass analysis operating mode	2	18	Complete
4.6	Ion Source design and Manufacture	3	38	Complete

Deliverable	Deliverable Title	Status
D4.1	Report on simulation results from Task 4.1 and 4.2	Complete
D4.2	Report on simulation and experimental results from Task 4.3-4.5	Complete
D4.3	Delivery of Ion Source	Complete
D4.4	Delivery of Miniaturised Ion Source	Complete

4.4.1 Objectives

WP4 concerns the development of an EI positive ion source to be coupled to the mass spectrometer (Tasks 4.1, 4.2 and 4.6) and (2) the determination then optimisation of operating conditions of ion injection and confinement in a LIT operated a non-scanning mode (Tasks 4.3, 4.4 and 4.5).

4.4.2 Key Technical Achievements

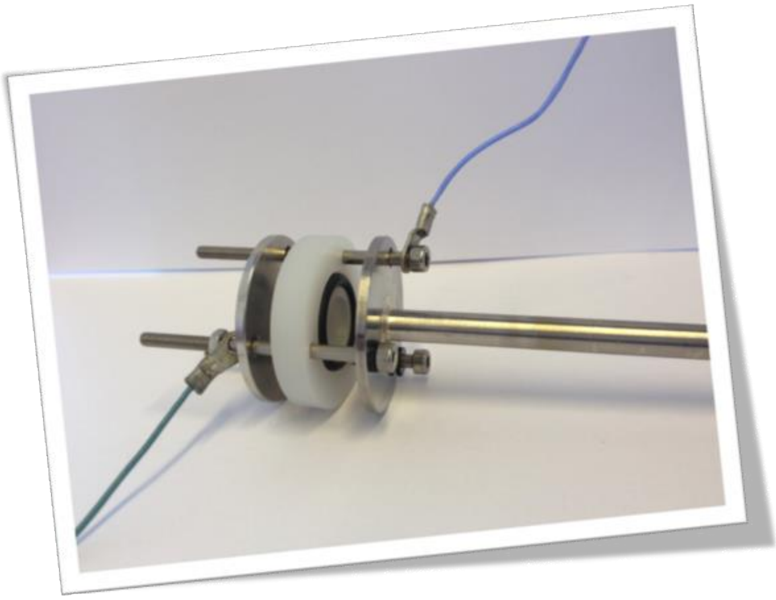


Figure 10: GDES developed in Sniffles

Task 4.1: GDES cell (electron source) (AMU)
The Glow Discharge Electron Source (GDES) cell produces an electron beam from a plasma discharge in glow regime. Two testing cells and a miniaturised cell (Figure 10) to be implemented in mass spectrometer have been fabricated.

GDES cells have been implemented in an offline vacuum chamber to be tested with ECU2 (Sniffles Prototype). The characteristics and operating mode and conditions of the glow discharge have been determined. The main operating conditions are:

- Gas load for vacuum chamber: gas throughput of pumping system must be ≥ 5 10^{-6} torr x m^3/s
- Discharge sustaining power supply:
    - V = 500 V; I = 50 µA (at discharge brakdown)
    - V = 420 V; I = 0.7mA; Power consumption = 0.3 W (Typical operating values, when discharge operates in glow regime)

The characteristics of the beam of emitted electrons available for substance ionisation have been determined:

- Electron beam intensity = 0.2 µA for typical operating values.
- Electron beam kinetic energy at anode orifice of GDES cell ranging between 0 to c.a. 20 eV.

Task 4.2: GDES EI ion source (AMU)
This task concerns the conception and development of an EI positive ion source using the GDES cell as source of electron. The electron kinetic energy is well defined at impact with neutrals. The operating conditions and characterisation of the electron current and ion signal have been determined and compared with a conventional EI source using a filament. The ion source has been tested with Faraday cup detector as ion detector of N_2 of ambient air.

Task 4.6: Delivery of Miniaturised Ion Source (AMU, UoL)
The discharge is constricted in the GDES cell. However, the size of the discharge could have been reduced and a miniaturised GDES EI ion source has been developed. Optimisations of operating conditions and improvements of the performances have been done with the aim of in-the-field device implementation. The principle of use, and mechanical and electrical implementations in SNIFFLES prototype or in other mass spectrometer have been then proposed. A running miniaturised GDES EI ion source for a mass spectrometer has been delivered and tested as part of the Sniffles prototype system with ECU2.

The "miniaturised GDES EI ion source" has been submitted to apply for a patent.

4.4.3 Deviations from work plan

Due to time delays in the miniaturisation of the GDES, it was not implemented on the final Sniffles Beta system. Instead, integration and testing took place on the Sniffles prototype with ECU2.

4.4.4 Progress beyond current state of art

Stable and miniaturised source of electrons for ionisation (GDES cell), with electron kinetic energy characterisation was delivered. This included:

- Miniaturised GDES EI ion source for vapour ionisation
- Ion position and velocity distribution in the LIT operated with non-scanning mode (ion injection with switched potentials)
- Characterisation of sensitivity and resolution of LIT non-scanning operating mode
- Position and velocity distribution at equilibrium of confined ions subjected to collisions with cooling buffer gas in RF traps (Numerical Methode)

4.4.5 Future Work

The EI fragmentation pattern of molecules depends on the initial electron kinetic energy. The MS characterisation of positive ions created by GDES EI ion source will be of a great concern.

The aim of new research works is to study how the initial kinetic energy of the electrons is distributed inside the molecule (when electrons impact molecules in an EI source) leading to different fragmentation pathways according to this initial kinetic energy. Threshold Ionisation Mass Spectrometry (TIMS) seems to be the best technique to perform these studies. With TIMS, the fragmentation spectra of the molecule are recorded for different values of the mean kinetic energy of the impacting electron. For instance, the application could concern detection by handled mass spectrometry of explosive and synthesis by-products, more volatile than some types of explosive (plastic, for instance). These works could lead to an increase of detection sensitivity by further optimisation of the detected ion signal corresponding to the 2-4 majors fragments used to identify a targeted substance in the portable MS.

From position and velocity distribution at equilibrium, it will be then possible to estimate the reduction of the extension of the ion cloud after cooling, as well as the cooling time to set the optimal time of the cooling stage.

The beneficiaries AMU and UoL pursue these simulation works on ion cooling by buffer gas of ions confined in a LIT and the results will be compared to results of experiments. Experiments will be conducted with the LIT-MS and ECU2 prototype implemented in AMU vacuum chamber, described in WP7 (see Section 4.7).
.

4.5 Work Package 5: Sample Inlet

Start month: ***Month 2***
Schedule Completion: ***Month 28***
Status: Complete

Task	Task Title	Start Month	Scheduled End Month	Status
5.1	Sample inlet using DAPI	2	24	Complete
5.2	Sample inlet using DART	2	24	Complete

Deliverable	Deliverable Title	Status
D5.1	Creation of DAPI inlets for testing at UoL and AMU	Complete
D5.2	Creation of DART inlets for testing at UoL and AMU	Complete
D5.3	Sample Inlet Development	Complete

4.5.1 Objectives

WP5 concerns the design, development and manufacture of suitable sample inlets for admission of vapour (DAPI) and solid (DAPCI) analytes into the Sniffles portable MS Sniffer.

4.5.2 Key Technical Achievements

5.1 Creation of DAPI (Qtec):
A DAPI inlet with user programmable valve opening and closing times has been designed, built and tested with a portable QMS and vacuum system (see Figure 11a). The purpose of the DAPI inlet is to provide a discontinuous but user programmable supply of an analyte sample of gas (e.g. from atmospheric ambient) into a vacuum system (e.g. of the linear ion trap (LIT) mass spectrometer). The inlet of sample gas was provided by the sequential switching of the two solenoid pinch valves with user programmable on-off times provided via a commercially obtainable programmable logic controller (PLC). The DAPI housing is custom 3D printed enclosure and houses the valve(s) Arduino microcontroller board and associated circuitry.

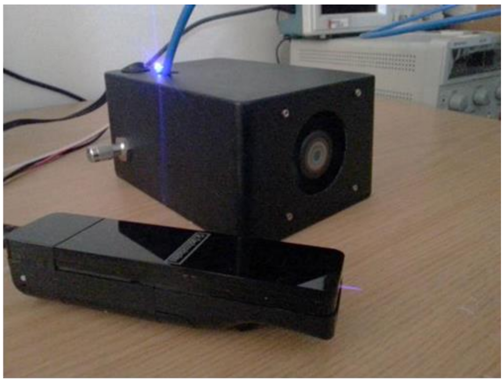
The most recent iteration of the DAPI has been to modify the original design by making it smaller (suitable for 1 pinch valve), lighter and lower cost. In this configuration (but depending upon vacuum system pumping speed etc.) the single valve is of a type with a lower leakage flow rate when in the normally closed position.

5.2 Creation of DART (Qtec)::
A low power, low voltage (12V) ambient ion source using a low temperature plasma (LTP) suitable for DART, has been designed, built and tested (see Figure 11b). The principle of operation using inductively coupled plasma with helium as the carrier gas has been successfully achieved. Safe operation of the LTP source has been demonstrated against the skin of a human subject. The LTP source is capable of vaporising paracetamol and other (similar) pharmaceutical solids. The source was tested using a commercial QMS (MKS Microvision 2) and vacuum system. No mass spectra were obtained for the range of solid samples tested due to the difficulties of ion transmission into the QMS. The experiments were repeated with a nonionizing handheld laser. The laser was also capable of producing a vapour plume from paracetamol and other solid samples. No mass spectra were obtained using this arrangement either for the same reason.. It was decided to resume the testing of the DART source, coupled to the DAPI inlet, and directly into the GDES and /or the LIT directly, as the prototype of the LIT becomes available from UoL. In the meantime other methods of ambient ionisation were investigated and developed

5.3 Sample Inlet Development (Qtec, UoL):

A battery operated, handheld ionisation source (DAPCI) has been developed for point-and-shoot chemical analysis (see Figure 11c). The entire arrangement including battery and pump weighs <0.2kg and fits in the palm of one's hand. The battery allows for ~5 hours of continuous use and is rechargeable. The handheld DAPCI has an adjustable voltage regulator to allow operation over a wide range of voltages (positive or negative HVDC to 5kV). The handheld DAPCI allows a variable pump speed to be set by the user (Mk#1 uses a fixed pump speed). The miniature pump has an integrated airline that pumps ambient air directly; alternatively connection can be made to an external gas supply. The ability to analyse different explosives and drugs of abuse has also been demonstrated using the DAPCI with a several larger MS instruments such as the Waters Q-TOF. A range of different explosive simulants and drugs of abuse stimulants have been successfully tested using the DAPCI approach and mass spectra have been obtained.

(a)



(b)

(c)

Figure 11: Sample Inlets (a) DAPI, (b) DART and (c) DAPCI.

4.5.3 Deviations from work plan

It was decided to move away from the low temperature plasma, as used in D5.2, and achieve Direct Analysis in Real Time using the DAPCI inlet. This was to do with difficulties that arose when using the plasma to vaporise samples so that they could be ionised and tested. DAPCI sufficiently fulfils the initial parameters without the drawbacks of the earlier DART system. The work was published in Analytical Chemistry journal in September 2015.

4.5.4 Progress beyond current state of art

The DART inlet valve system and the handheld DAPCI represent progress beyond state of the art. The DAPCI handheld ionisation source represents a key technological advance directly resulting from the SNIFFLES project.

4.5.5 Future Work

Future work remains to test the DAPCI coupled to ECU3 in field conditions.

4.6 Work Package 6: Vacuum System

Start month: ***Month 2***
Schedule Completion: ***Month 28***
Status: Complete

Task	Task Title	Start Month	Scheduled End Month	Status
6.1	Mechanical, electrical/electronic design	2	12	Complete
6.2	Prototype assembly and Software Development	3	18	Complete
6.3	Test bed design and assembling	2	19	Complete
6.4	Prototype characterization on test bed	18	25	Complete
6.5	Screening of new getter materials	2	28	Complete
6.6	Screening of sintering technologies and development of new getter elements	2	28	Complete
6.7	Design and Prototyping of advanced getter pump and vacuum system	19	28	Complete
6.8	Advanced prototype characterization on test bed	19	30	Complete

Deliverable	Deliverable Title	Status
D6.1	Creation of vacuum system prototype	Complete
D6.2	Creation of advanced vacuum system prototype	Complete

4.6.1 Objectives

WP6 concerns the design, development and manufacture of a complete vacuum system:

- Portable instrument, operated by battery
- Docking station for pump-down, getter pump reactivation and battery recharging
- Development of new getter solutions (alloys, sintered elements)

4.6.2 Key Technical Achievements

The main technical results can be divided into two parts:

1. **Vacuum System:** Solutions for the vacuum system (VS) design and operation (task 6.1 - 6.4 and 6.7, 6.8)
2. **Getter Alloys:** New getter alloy and sintering process (task 6.5, 6.6)

Vacuum system (SAES, DVLS, UoL, Qtec)**:**
The VS has been designed taking into account the requirements for LIT operation and the estimated gas load, and it consists of two parts: the Rover, i.e. the portable sniffer (see Figure 12), and the docking station (DS). The latter is equipped with a Turbo molecular pump (TMP) used to pump down the Rover from atmosphere to a pressure suitable for operation and to regenerate the Non Evaporable Getter (NEG) pump.

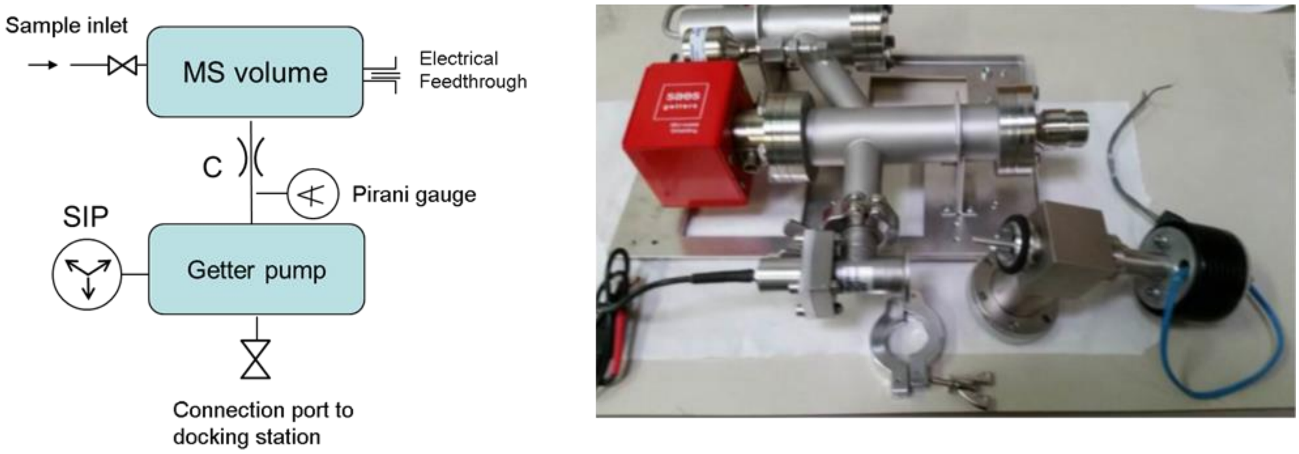


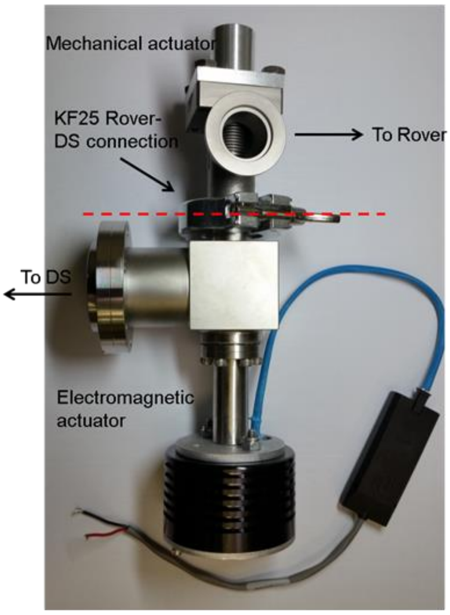
Figure 12: Left: scheme of the Sniffles vacuum system. Right: picture of the vacuum chambers during assembling.

The following technical solutions have been implemented in the Sniffles Beta system:

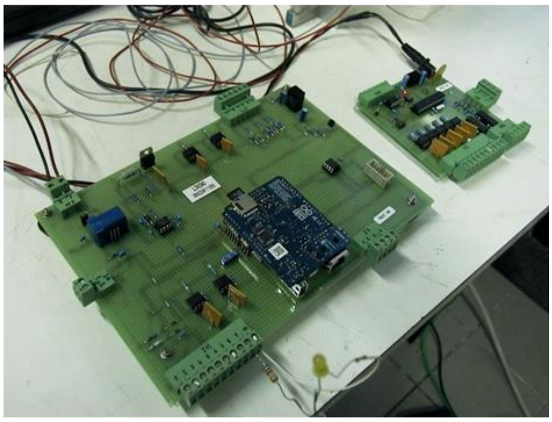
- The pumps and the LIT have been mounted in two chambers separated by suitable tubing so that a constant and known pumping speed is available in the mass spectrometer chamber.
- A small Sputter-ion pump (SIP) has been included to pump inert gases, which are not pumped by the NEG. The latter consist of 39 sintered getter disks and an internal heater for getter operation
- The custom quick-connection valve (Figure 13a) has been designed to reduce space and weight, placing the actuator on the DS. In this way the system is protected against accidental venting, since the valve can be opened only when the Rover is docked.
- The control electronics and software (Figure 13b) has been developed to carry out the following tasks: i) automatic control of the Rover and DS (pumps, valves, gauges); ii) interfacing the ECU with the GUI; iii) provide Wi-Fi communication with the tablet.
- The Rover is powered by Li-ion battery enabling about 6 hours of continuous operation.

The key VS performances have been successfully characterized with DAPI. In particular:

- A base pressure in the low 10^{-7} - 10^{-8} mbar range was achieved, by far compatible with LIT operation
- A pumping speed of 10 l/s has been measured, in line with specifications
- Accidental venting test have been performed showing no safety issues
- Full automatic operation of the system was achieved



(a)



(b)

Figure 13: (a) picture of the custom quick-connection valve and (b) Rover and DS control boards.

Getter Alloys (SAES):

A new family of alloys, named ZAO®, has been developed for this application and a patent application has been sought. In combination with the development of new production processes for getter sintered bodies, the new NEG disks show a significant improvement of the capacity for nitrogen, oxygen and CO, CO_2 with respect to the current solution (St172® disks). This makes possible the use of NEG pumps in applications characterized by a high gas load, like portable MS. Based on the gas amount introduced by the DAPI and the hypothesis of 12 analyses/hour, 10h/day, 365 days/year, the pump is expected to be reactivated about once a month and cover at least one year of work before cartridge replacement is required. In comparison with existing materials, the St172® pump would last not more than 2 months before replacement. In addition, ZAO® presents much increased safety against unwanted air inrush when operating at high temperature.

4.6.3 Deviations from work plan

The main deviations from the original work plan were related to the time needed for the electronics/ software development and testing. Final version of the software was available only a couple of months before the end of the project. This did not allow enough time for further optimization of the hardware in terms of weight and size.

4.6.4 Progress beyond current state of art

The technical solutions implemented in the VS represent an improvement with respect to the state of the art with respect to the following aspects:

- The Rover pumping system has reduced dimensions and is much more robust with respect to TMP-based systems, thanks to the high performance-to-size ratio of NEGs and the absence of moving parts.
- The pumping system based on SIP and NEG is operated with only 5W, allowing a significant power saving and therefore prolonged battery lifetime.
- The properties of the new getter solution enable operation for reasonable times before cartridge replacement against high air load, which would not be possible with standard getter materials available on the market.

4.6.5 Future Work

Several improvements of the VS can be envisaged aimed at reducing the weight and the size of the device. From a general point of view, the prototype was assembled with components available on the market, so there is room for finding smarter and more specific solutions. Some examples are listed below:

- The current case weights about 3 kg: in the next re-engineering phase a custom structure to hold and protect the different components will be designed, with the objective of reducing space and weight. A 30% reduction can be envisaged. This could include using additive manufacture technologies (3D printing) for the manufacture of more complex and lightweight geometric structures.
- The current electronic hardware of the VS is still in a prototype stage. Following the positive tests here reported, definitive printed boards will have less than a half size.
- There is significant room for reduction of the weight of the vacuum chambers, using aluminium, reducing the wall thickness and adopting sealing techniques other than standard UHV CF flanges. Weight saving up to 40% seems reasonable (i.e. more than 1 kg less).

Even if a more quantitative estimation will be possible only in the near future, when the next re-engineering will actually take place, weight reduction of the complete portable system down to 12 kg or below can be considered a reasonable target.

4.7 Work Package 7: System Integration

Start month: ***Month 18***
Schedule Completion: ***Month 36***
Status: Semi- Complete

Task	Task Title	Start Month	Scheduled End Month	Status
7.1	Making of pre-prototype ('functional design')	18	23	Complete
7.2	Conversion of pre-prototype into a working prototype	23	27	Complete
7.3	Building of the beta-testing device	27	36	Complete

Deliverable	Deliverable Title	Status
D7.1	Functional design / pre-prototype	Complete
D7.2	Creation of advanced vacuum system prototype	Complete
D7.3	Prototype M33	Complete
D7.4	3 beta-testing units	Complete
D7.5	Report on feasibility of Alpha beta-testing unit	Complete
D7.6	I/O controller delivery	Complete

4.7.1 Objectives

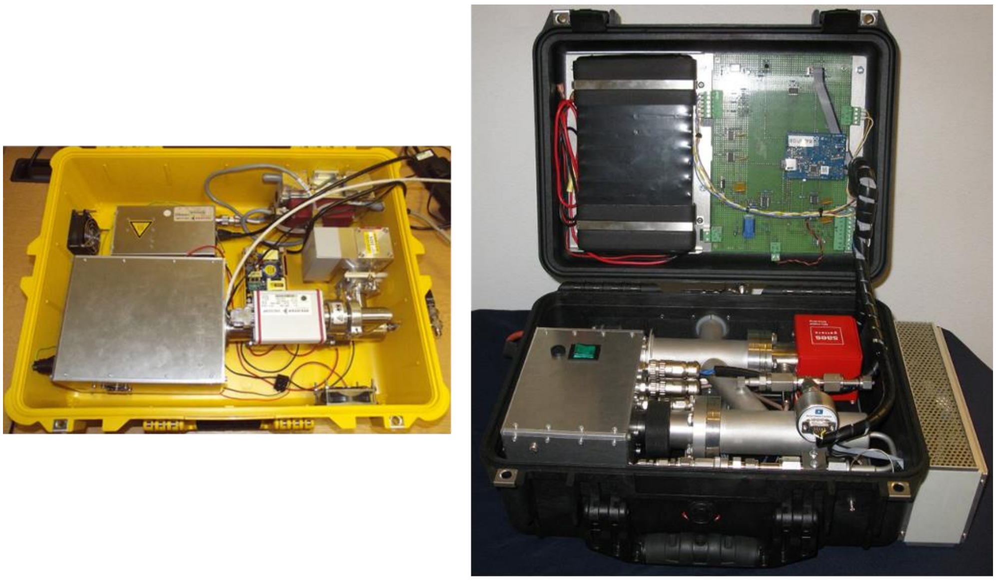
WP7 concerns the integration of all the Sniffles technologies defined and developed in work packages 1-6. The objective was to deliver a fully operational portable gas sensor suitable for end user trials. This was underpinned by three key device development activities:

- Integration of a Pre-Prototype System
- Integration of a prototype system
- Integration of sniffles beta system for end user trials

Pre-prototype system (see Figure 14a):
The pre-prototype system was driven by ECU1 (see section 4.3) and included a Pfeifer miniature vacuum system consisting of a diaphragm pump (MVP 006-4) and a turbomolecular pump (iPace 10). It also included an EI source – Electron impact (EI) ion source with a three-lens system and dual thoria filaments which is used for ionisation. A CNC LIT built onto a CF40 vacuum flange was also used (see Section 4.2)

Prototype system:
The prototype system consisted of the miniaturised Glow Discharge Electron Source (or GDES) cell coupled and tested offline with ECU2 (WP3), a DLP manufactured LIT mass analyser (WP2) and a vacuum system located at AMU.

Beta system (see Figure 14b):
The beta system included ECU3 (WP3), the advanced Getter vacuum system (WP6) and a DLP manufactured LIT mass analyser (WP2) all integrated into a dockable carry case. The dimensions of the Beta system were within specification for x and y (400mm and 300mm) but the depth of the unit was 170mm (target > 100mm). It was not possible to achieve the intended dimension due to the available choice of peli case (an off the shelf product where nearest suitable dimensions were chosen) coupled with the final dimensions of the electronic control unit (ECU3) and the battery. The ion pump power pack also had to be mounted on the outside of the peli case. The system was also to heavy at 16Kg (Target <8Kg), almost twice the weight of the intended system. Most notable, the ECU3, battery, vacuum system, pumps and case were significant elements adding to the overall weight. The battery is purposefully oversized in both weight and dimension, but was chosen to give added longevity during validation of the portable device (estimated at 4 hours continuous use). There is still extensive scope to reduce system weight (and also volume) but these developments require significant additional work, primarily on non-critical components (i.e. flanges, vacuum tubes and enclosure of ECU3) and/or bespoke development of third party products (i.e. batteries, couplings etc.). Hence, additional weight and volume reduction activity, although important, would consume extensive resource not available in Sniffles.



(a) (b)

Figure 14: (a) Sniffles pre-prototype system and (b) Sniffles Beta system fully integrated unit including I/O controller.

4.7.2 Key Technical Achievements

The main technical results can be divided into four parts:

- Sniffles Technologies 'system' integration
- Sample introduction
- Docking station
- Pre-concentrator

Sniffles Technologies 'System ' integration (DVLS and all partners):
During the Sniffles project, several sub developments (see previous WPs) took place. Some examples of these are the development of a getter based pumping system to achieve the system vacuum, a linear ion-trap mass spectrometer (LIT-MS), an electronic control unit (ECU) and a general user interface (GUI). In the end, all developments have to be brought together and integrated to one system. The main challenge during system integration is to fit all parts in one case to make the system portable. In common MS systems is the vacuum chamber made from a large amount of stainless steel, large and in a straight orientation, where the parts are fitted as best as possible before enclosing in a suitable cover. The challenge in this work was the fact that the system had to fit in a commercially available Peli-case.

The fact that the dimensions of the Peli-case are fixed, the way of working had to start from the case. All the parts out of the sub developments had to be placed in the case together with a vacuum chamber. The outcome is a vacuum chamber, built from a minimal amount of stainless steel tubes welded into an H-shape geometry. A special designed electronic valve makes it possible to connect/disconnect the system from/to a docking station used for regeneration of the vacuum system and loading the battery pack.

The result is a portable LIT-MS based artificial sniffer, containing an electron-impact ionisation source, a DLP linear ion-trap mass spectrometer, a getter ion pump, and an electronic control unit, All of this is controlled from a tablet containing the general user interface software (developed in WP3).

Sample Introduction (DVLS, SAES, UoL):
Since the system will be carried on the back of the operator, there is a relative long transfer line between the sniffing point and the ion source of the mass spectrometer. This causes a potential delay in sample detection. Because of this, a special sampling device was developed. Sample is pumped continuously through the transfer line. Once the system is ready for the next "sniff", there is always a fresh sample at the membrane inlet. To prevent for dead volumes, the transfer capillary is feed through a T-piece all the way to the membrane. When the system is not sniffing, a pump removes the sample along the outside of the transfer line through the T-piece. Figure 15 shows a schematic of the sampling device.

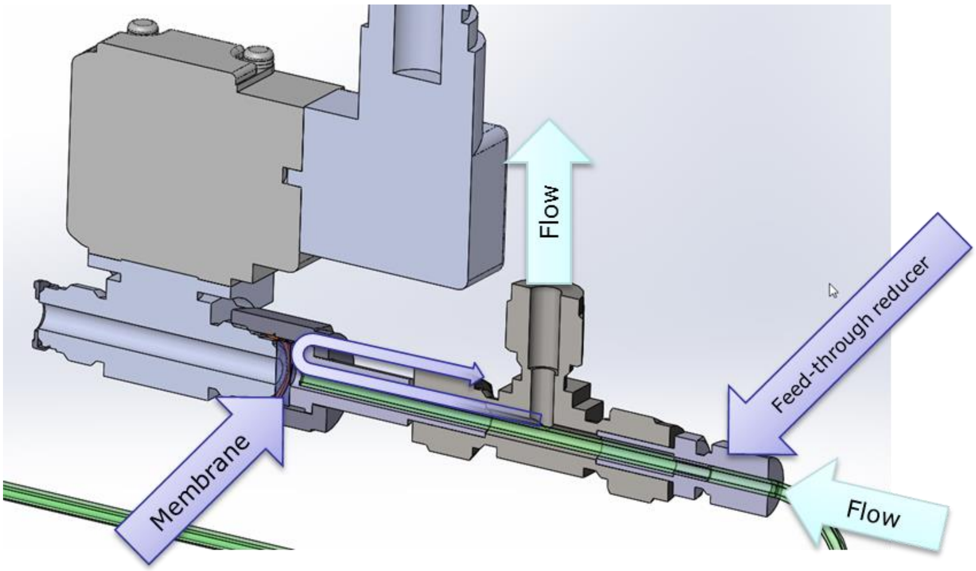


Figure 15: Schematic of sample inlet device.

<u>Docking station (SAES, DVLS):</u>
Because the Sniffles Beta system is battery operated and making use of a solid state Getter-pump based vacuum system, the system needs to get recharged/regenerated after operation. Also, following a service, the system has to be evacuated. To enable regeneration and to prime the vaccum system a docking station was built. The docking station consists of a diaphragm pump combined with a turbo molecular pump, control electronics and a special developed high-vacuum valve. Figure 16 shows pictures of the Sniffles beta system on the docking station.

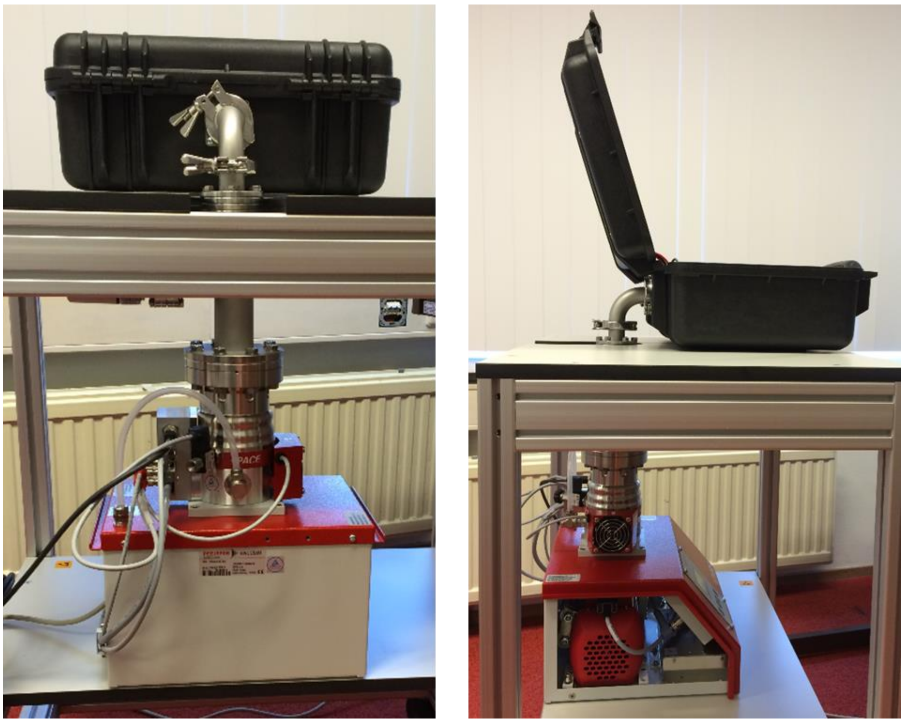


Figure 16: Sniffles Beta system connected to the docking station.

Pre-concentrator (DVLS):
During the feasibility tests of the system, it became obvious that the Sniffles Beta system might not be able to meet the requirements for sensitivity. It was therefore decided to build a pre-concentrator to place in front of the LIT-MS. Pre-concentrator systems are well known from the world of gas chromatography (GC) and several devices are commercially available. These pre-concentrator systems usually use coolants as forced air, compressed CO_2 or liquid nitrogen. Heating of these pre-concentrators is usually done using with a lot of electrical power. In GC laboratories are both coolants and electricity widely available. However, the consumption of these is far too much for battery operation.

A low consuming pre-concentrator has been developed based on commercially available parts. Compounds are trapped on a short length of capillary GC column coated with PoraPlot-Q material, using a small pump. During sampling, the trap is cooled with a very small ventilator. For release of the compounds, the trap is coiled with resistive wire causing flash heating for a very short period of time. Switching between the sampling flow and the carrier flow is done using a very small 2/3 valve. The enriched compounds can be carried to the LIT-MS simply using the vacuum of the system, eventually by a carrier gas from a small tank. The whole is controlled using a small programmable logic controlling (PLC) device.

-	Trap	Capillary, 15 cm x 0.53 mm ID x 20 µm PoraPlot-Q
-	Heater	2.5 Ω; 80 coils resistance wire, constantane alloy, 0.3 mm, 6.93Ω/m
-	Power	7.6 W
-	Sampling flow	25 ml/min
-	Sampling time	<75 sec
-	Linearity	0 – 300< ppm acetone, R2=0.9994
-	%RSD	0.8%
-	Concentration factor	1000

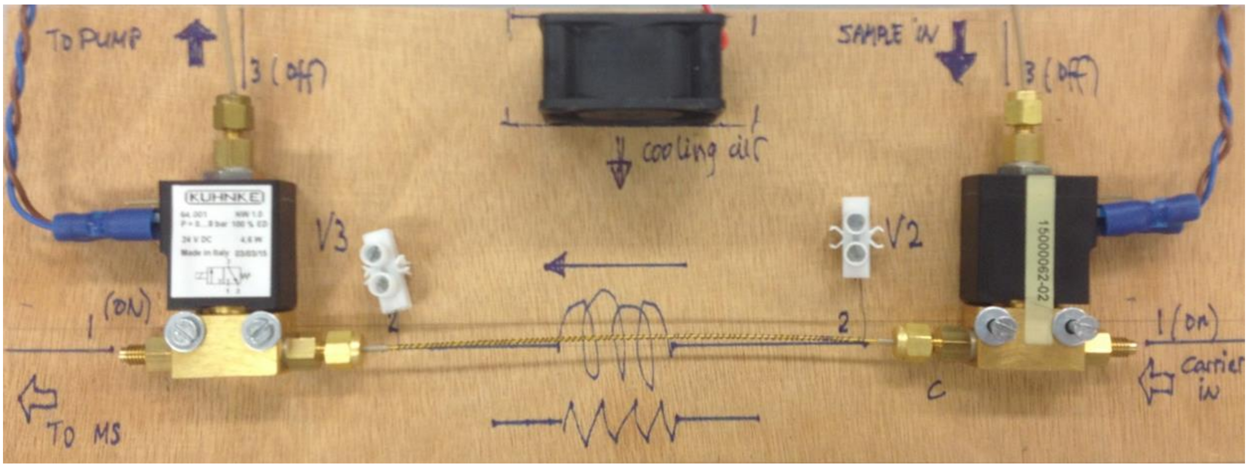


Figure 17: Functional design of a miniaturised PLC controlled pre-concentrator.

4.7.3 Deviations from work plan

The main deviations from the original work plan were related to the time due to delays in previous WPs primarily focussed on the development and delivery of ECU3.

4.7.4 Future Work

By the delivery of the Sniffles beta system, the system has some shortcomings; weight, sensitivity, robustness. On the side of the weight there are two important factors; battery and pumping system. As with the continued improvements on battery technology, it is expected that on short time batteries will become available on the market with much lower weight although the same or even better performing. Also is it expected that the vacuum system can reduce weight in a next generation (see WP6). Electronics are continuously under investigation. Out of this, it is expected that improvements will be made both on the side of sensitivity as well as the system robustness.

Table 5: Sniffles beta system final user specifications.

Rover 2000 beta-testing unit	Achieved in beta-testing unit	End user requirement
 	Detection of explosives, drugs, CBRNEs, hidden persons	✓Able to screen, but also target search compounds to ppb level.
	Detection speed < 5 sec	✓adequate for needs. × requires improved sampling system for more versatile use.
	Dimensions, 400 x 300 x 170 mm	✓adequate for needs. × smaller unit would be better (e.g. 400 x 300 x 100 mm).
	Weight, 16 kg	× too heavy, target < 8kg.
	Mass range, 50 – 500 amu Non-scanning Resolution < 1 amu, FWHM	✓more than adequate for several markets including border security (including human trafficking) and drug detection × e.g. for military environments this needs to be enhanced via MS^n capability.
	Estimated sales price, €25k	✓ competitive in comparison to most of the miniature/portable MS market.
	Power consumption, 75 W ⇨ ~ 4 hrs use	✓adequate for many applications × aim to reduce below 50W (target <25W) to give >4h continuous usage.
	Designed to be used by a trained, but non-specialist operator.	✓User-friendly software uses 'traffic light' warning and alarm system
	Pre-concentrator	✓Detection of very low concentrations possible due to LOD enhancement by 1000x e.g to ppt levels × with short analysis times

4.8 Work Package 8: Testing and Validation

Start month: ***Month 27***
Schedule Completion: ***Month 36***
Status: Not Complete

Task	Task Title	Start Month	Scheduled End Month	Status
8.1	Testing of the pre-prototype	23	27	Complete
8.2	Pumping system characterization with pre-prototype	27	30	Complete
8.3	Check different Electrode Layouts	30	33	Complete
8.4	Testing of the prototype	33	36	Complete
8.5	Testing and validation of the beta-testing unit	31	35	Complete
8.6	Field/Beta testing	33	36	Complete

Deliverable	Deliverable Title	Status
D8.3	Testing/validation report of beta-testing unit	Complete
D8.4	Field testing reports of beta-testing unit	Complete
D8.5	List of end user requirements	Complete

4.8.1 Objectives

WP8 concerns the testing and validation of the Sniffles portable MS systems. Specifically:

- To test the gas sensor according to specifications
- Validate gas sensor against current high end state-of-the-art lab equipment
- Field test the analyser together with a selected number of end users

4.8.2 Key Technical Achievements

<u>Pre-prototype:</u>

- Pre-prototype was able to scan for individual mass fragments for multiple compounds at the level of 5 ppm (Methyl benzoate (m/z 136), Acetic acid (m/z 60), 2-nitrotoluene (m/z 137) and Cyclohexanone (m/z 98)). The Sniffles pre-prototype system without a heated sample probe is expected to be 2 decades less sensitive than the benchmark system (portable membrane inlet quadrupole mass spectrometer (MIMS)) with no heated probe and 3 decades less sensitive than the benchmark system with a heated probe.
- Prone to disturbances and malfunction
- After a while ECU1 became a non-traceable malfunction

<u>Prototype:</u>
The prototype Sniffles device consisted of the Glow Discharge Electron Source (or GDES) cell, LIT mass analyser (WP2), ECU2 (WP3) and a vacuum system located at AMU. Unfortunately, due to complications with ECU2, the system was not able to be tested as an integrated piece of equipment. The Sniffles consortium made a decision to concentrate efforts with ECU3 (implemented in Sniffles Beta system) rather than losing momentum on ECU2.

<u>Sniffles Beta System:</u>

For field testing of the beta-testing unit, the first step was to compare with sniffer dogs. This was done in cooperation with Sniffles partner Wagtail (UK). Tests were done using a portable quadrupole mass spectrometer containing a heated membrane inlet. This system is relatively closely related to the Sniffles Beta-system system. However, it contains a turbo molecular pump-based vacuum system and a quadrupole analyser. The materials included:

- Drug simulants
  - Methyl benzoate (CAS# 93-58-3)
  - Acetic acid (CAS# 64-19-7)
- Explosive simulants
  - 2-nitrotoluene (CAS# 88-72-2)
  - Cyclohexanone (CAS# 108-94-1)

From the measurements, it was shown that dogs are 17 to 20 times more sensitive in detecting the examined compounds compared to the QT200+ triple quadrupole MS portable analytical instrumentation (membrane inlet triple filter quadrupole mass spectrometer), whereas they present very fast detection times (few seconds) and the ability to localise the target scent accurately. It was concluded that the Sniffles pre-prototype is 3 – 4 decades less sensitive than the QT200+ MIMS system. This means that it is to be expected that the Sniffles alpha-beta system will be 4 – 5 orders less sensitive than sniffer dogs. Additionally, the fact that the Sniffles beta system has a cold membrane inlet means that the rise and fall times will be slower than for the QT200+ MIMS system, and much slower than a sniffer dog.

4.8.3 Deviations from work plan

The main deviations from the original work plan were related to significant time delays in the delivery and integration of ECU3.

4.8.4 Future Work

The Sniffles Beta system has been demonstrated, but it is currently not robust or portable enough (too large and too heavy - 14Kg - and too much power consumption), all of which are based on specifications that were devised 4 years ago. Nevertheless, the work in Sniffles has provided a solid foundation on which to exploit the developed technology and focus on a commercial drive. This will be achieved through a recently awarded 2 year project funded by Horizon 2020's SME instrument. This phase 2 demonstration, market replication and R&D project will start in October 2015 will focus on improving the reliability of the Sniffles beta system as well as reducing its size and weight. The Getter pump developed in Sniffles will also become integral to the improved ChemSniff device. The project will involve the miniaturisation of the current Sniffles device through further developments, improvement and integration of ECU, LIT-MS device, a more compact a fully integrated vacuum system (topology optimised and 3D printed vacuum parts), software interface and tablet, carry case and inlets. The ChemSniff project will take the technology from readiness level 4-5 to level 7. Ultimately this project will enable the launch of the DVLS-QT-LIT-MS system to market.

5 Achievement of Project Objectives

System Objectives	Achievement Metric
To design, simulate, build and validate through field testing, an artificial sniffer with the ability to sense a wide range of illegal substances up to 500 amu.	This was achieved with the manufacture of the pre-prototype and sniffles beta system.
To provide a portable, easy-to-use (by non-specialist personnel) device through integration of various technologies being developed across the EU (LIT, Vacuum system, methods of Ionisation).	Degree of automation: main system tasks (e.g. pump down, NEG activation etc), self-diagnistics and error management (refers to easiness of use by non-specialist personnel)
To be able to detect the specified threats/substances rapidly (<1 sec) and continuously, with stand-off capability (< 300mm), at low levels (less that parts	This has been demonstrated in WP7/8.

per million) and accurately (a false positive rate of <2%).	
A target price for a single unit of the sniffer device is <25k euros.	DVLS are still confident the Sniffles Beta system could meet the target price.
The portable system will fit inside a briefcase sized holdall of dimensions 40 cm x 30 cm x 10 cm and will have an operational weight < 8kg.	The final Sniffles system was housed in a case of dimension dimensions 40 cm x 30 cm x 17 cm. The extra dimension was due to an oversized battery giving increase use between recharges and the dimensions of the ECU3. System weight was 16Kg.
Specification of border control operating procedures which incorporate the new Sniffles detector, showing secure operation and complementary (synergistic) operation with sniffer dogs	This was developed as part of the Sniffles system specification document (Deliverable 1.1)
Device Objectives	Achievement Metric
Produce a prototype device which integrates each sub-system and is capable of demonstrating the performance characteristics listed in objectives 1-5, within the context of a border control checkpoint trials.	This was demonstrated in the integration of the Sniffles Beta system. Unfortunately, due to delays with ECU3, full validation and field trials were not possible with ECU3. However, validation has been reported with ECU1.
To demonstrate that the Sniffles artificial sniffer device has suitable cost (<€25,000) and can be manufacturing by a scalable route (i.e. capable of >500 units per year within 5 years of market introduction).	Current production scale of components I mean that to my knowledge all components (except LIT), or equivalent ones (e.g. similar chambers/electronics/pumps), are already produced on large scale, so it is feasible once provided adequate infrastructures and manpower…
Sub-system Objectives	Achievement Metric
Small, lightweight and low cost Ion trap, yet capable of achieving the required mass range (500 Da), resolution (<1 Da) and high sensitivity (at sub-parts per million trace levels).	The LIT electrodes and housing were successful developed and validated for use in the Sniffles MS system. This gave a considerable reduction in both weight and cost over CNC machined parts.
Sample inlet: able to accept all vapours and solids of interest (threat analytes).	The DART inlet valve system and the handheld DAPCI represent progress beyond state of the art. The DAPCI handheld ionisation source represents a key technological advance directly resulting from the SNIFFLES project.
Ionisation methodology: optimised and suited to achieve the most efficient coupling of sample inlet to ion trap in a miniature volume. Dynamic range of detector at operating vacuum with a maximum signal to noise ratio.	Stable and miniaturised source of electrons for ionisation (GDES cell), with electron kinetic energy characterisation was delivered.
Electronic Control Unit (ECU): miniaturised and operating at low power (<25W).	ECU3 was reduced in size and weight by almost half when compared to the ECU1 which was developed at the start of the project.
Portable getter pump vacuum system: capable of handling required load of inlet gas (at atmospheric pressure) and sample.	Test of pump capacity and comparison with expected gas load (see D6.1, D6.2)
Develop the use of silver nano-particulate inks to form low ohmic LIT electrodes that are hyperbolic (or other) in shape for cost effective (<€10 per electrode) replaceable (disposable) electrode.	Silver inks were successfully deposited onto DLP produced LIT electrodes with required electrical conductivity. The issue was making an electrical connection to the printed surface which proved difficult within project time lines.
Handheld PC: able to couple to the firmware of the ECU and provide a user friendly interface for operation of the Artificial Sniffer by trained but non-specialist personnel (e.g. police and/or customs officials). PC to provide rapid identification of threat	This has been demonstrated in WP3 with the development of a GUI that operates the Sniffles Beta system in docked mode.

substances via on board data base and access to mass spectral libraries in real time.	

6 Project Impact, wider social implications and exploitation and dissemination

The dissemination actions of Sniffles have taken place through various available media: scientific journals; conferences; workshops and Sniffles project website. The targeted topics have been: security and detection of illicit substances and hidden persons, mass spectrometry (more precisely, instrumentation, in-the-field, miniature and/or micro engineered), analytical physical-chemistry and vacuum technology.

A scientific/technical innovation, a positive ion source for portable instrument and Getter materials for a vacuum system has been protected and valorised by submission of patent proposals.

Two Ph.D. students have been involved in the application context of mass spectrometry research topics, building up general knowledge, experience, and confidence to become young researchers.

A final public workshop was not organised due to a lack of robustness of the Sniffles beta device. Hence, it was not ready for public dissemination to potential stakeholders. For this reason Sniffles beneficiaries (DVLS, QTec and TWI) have recently written and been awarded a two year EC funded project (ChemSniff), coordinated by DVLS, within Horizon 2020's SME instrument. This phase 2 demonstrations, market replication and R&D project will start in October 2015 and will run for 2 years and will focus on improving the reliability of the Sniffles beta system as well as reducing its size and weight. The Getter pump developed in Sniffles will also become integral to the improved ChemSniff device. The project will involve the miniaturisation of the current Sniffles device through further developments, improvement and integration of ECU, LIT-MS device, a more compact a fully integrated vacuum system (topology optimised and 3D printed vacuum parts), software interface and tablet, carry case and inlets. The ChemSniff project will take the technology from readiness level 4-5 to level 7. Ultimately this project will enable the launch of the DVLS-QT-LIT-MS system to market.

6.1 Project Impact

Beneficiary 1 TWI

- TWI has benefitted from the development of new processing parameters for digital light processing and new and improved techniques for metalising DLP surfaces. This has enabled capability for the manufacture of different conducting structures for TWI members.
- The inclusion of TWI as a subcontractor within the ChemSniff project will enable TWI to gain a better understanding of the performance of additive manufacture metallic components for vacuum applications.
- Inclusion for further development in the ChemSniff project.
- New appointment PL and an apprenticeship to work on ChemSniff project.

Beneficiary 2 UoL

- LIT2 software development is exploitable via ChemSniff follow on project
- Future patent applications for RPM but further research needed to establish parameters. FOR RPM
- Novel method of trap operation (rpm) has potential impact beyond ChemSniff (i.e. to other ion trap instruments).

Beneficiary 3 AMU

- Patent application for GDES

- Computation by invariance method of distributions at steady state of ions confined in RF devices and subjected to collisions with buffer gas. The study of collisional cooling of confined ions and the knowledge of kinetic energy distributions at steady state of ions confined are of great interest for the scientific community.
- Initial ion distributions at confinement in trap operated switched-potential operating mode. Through the SNIFFLES programme, the application of this method has been extended to a LIT operated a Single Ion Monitoring Mode.
- Ion Confinement in a LIT close to the apex. This method has been used in submitted paper No. 9 (see table A2) to estimate the performances of the mass analyser. It has allows us the modification of the operating mode sequence. This method should be applied to 2D ion traps having other electrode shapes.

Beneficiary 4 QTec
- Development of handheld DAPI units and handheld DAPCI ion source for sample inlets into portable and other MS systems
- Inclusion for further development in the ChemSniff project – able to retain key staff that worked on Sniffles (Boris Brkic).

Beneficiary 5 SAES
- SAES has benefitted from the development of new getter alloys with improved capacity, which extend the application of NEG materials beyond UHV (below 1e-8 Torr) into the HV pressure range (1e-8 – 1e-6 Torr). A patent has been filed on the alloys composition (see section 1.1.6) and a new series of pumps is being commercialized.
- Participation to the Sniffles project (and in future to the ChemSniff as subcontractor), increased the knowhow in the field of portable MS.
- Collaboration with the beneficiaries enlarged SAES network, in particular in the security area, otherwise difficult to reach. This may create conditions for future market enlargement or partnership, both commercial and scientific.

Beneficiary 6 Env
- New commercial applications for its range of 3D printers
- Improved process parameter set for Envisiontec perfactory through increased resolution capability in z direction during a build. Env are looking to offer this as an enhanced operation mode in future hardware sales.

Beneficiary 7 Xaar
- Developed new printing techniques to coat 3D printed polymer parts (DLP system) with conformal surfaced using nano silver inks.

Beneficiary 8 WAG
- Introduction and attendance at security events that have, historically, proven difficult to gain attendance outside of Sniffles (e.g. Frontex events).
- Had a unique opportunity to gain a better understanding of different artificial Sniffer technologies and make direct comparisons with working dogs.
- Gained experience of being able to use technology alongside dogs during in-field validation trials.

Beneficiary 9 DVLS
- Development of a low power consuming pre-concentrator which has been developed based on commercially available parts. This has the potential to become a commercial product but requires further development in ChemSniff project.

6.2 Website

The project website is available at http://www.sniffles.eu/. It allows the public dissemination of the SNIFFLES programme and the controlled exchange of documents between beneficiaries via a secure login page.

6.3 Journal articles

The publication of research articles is essential for academic beneficiaries and R&D departments of industrial beneficiaries as this primarily contributes to the impartial evaluation of the research work..

During the Sniffles project, six papers have been published and three are under peer review. The targeted journals have high Impact Factors. The mean Impact Factor of published papers is 3.126.

The list of the published and submitted papers sorted by release date in tabulated in appendix A1.

6.4 Conference participations

Conference participations included preferential oral presentations, poster presentations and proceedings. Many conference papers were reviewed according to conference regulations. All of the Sniffles beneficiaries are main authors regarding the scientific and technical themes addressed in the conference. The total score is 14 participations at international conferences, with:

- 5 oral presentations at international conferences
- 1 oral presentation at workshop
- 5 proceedings (with review) at international conferences
- 8 poster presentations at international conferences
- poster presentations at national conferences
- 2 banners at international conferences
- 1 poster presentation at workshop
- 1 press release.

The list of dissemination activities generated by the Sniffles project is tabulated in appendix A2.

6.5 PhD thesis

The two academic beneficiaries (AMU and UoL) have hosted two Ph.D. students whose the thesis have been funded by the SNIFFLES programme:

- Achouack Chalkha, "Glow discharge electron impact ionisation and improvements of linear ion trap operating mode for in-the-field detection of illegal substances", Ph.D. thesis defended February 17th 2015 (Confidential thesis manuscript for two years), Aix-Marseille Université, Marseille, France.
- Stamatios Giannoukos, "Portable mass spectrometry for artificial sniffing", Ph.D. thesis defended March 18th 2015, University of Liverpool, Liverpool, UK.

6.6 Scientific recognition

Sniffles works have received the recognition of the Scientific Community.

Paper no. 5 of AMU, "An historical approach to the effects of elastic collisions in radiofrequency devices and recent developments", by Jacques André, Aurika Janulyte and Yves Zerega, is an Invited Paper in a special issue of International Journal of Mass Spectrometry entitled "Mass Spectrometry Entering its Second Century: 1960's Concepts to the Present" (Editors Jean Futrell &

Mike Bowers), in recognition of the centenary of Sir J. J. Thomson's monograph "Rays of Positive Electricity and Their Application to Chemical Analyses", published October 4th, 1913.

Stamatios Giannoukos, UoL PhD student, is winner of the 6th Journal of Mass Spectrometry Postgraduate Award for presentation "Membrane Inlet Mass Spectrometry for In-Field Security Applications" at 20th International Mass Spectrometry Conference (IMSC), August 24 and 29, 2014, Geneva, Switzerland.

6.7 Exploitation

The Sniffle Beta system has been demonstrated, but it is currently not robust or portable enough (too large and too heavy - 14Kg - and too much power consumption), all of which are based on specifications that were devised 4 years ago. Nevertheless, the work in Sniffles has provided a solid foundation on which to exploit the developed technology and focus on a commercial drive. This will be achieved through a recently awarded 2 year project funded by Horizon 2020's SME instrument. This phase 2 demonstrations, market replication and R&D project will start in October 2015 will focus on improving the reliability of the Sniffles beta system as well as reducing its size and weight. The Getter pump developed in Sniffles will also become integral to the improved ChemSniff device. The project will involve the miniaturisation of the current Sniffles device through further developments, improvement and integration of ECU, LIT-MS device, a more compact a fully integrated vacuum system (topology optimised and 3D printed vacuum parts), software interface and tablet, carry case and inlets. The ChemSniff project will take the technology from readiness level 4-5 to level 7. Ultimately this project will enable the launch of the DVLS-QT-LIT-MS system to market.

The newly developed Getter alloys by SAES are already planned for implementation in new vacuum products from 2016.