ICFO

SPECIFICATION SHEET

SUPPLY, INSTALLATION AND COMMISSIONING OF AN "ION CHROMATOGRAPHY – MASS SPECTROMETRY SYSTEM" FOR THE LABORATORY OF THE INSTITUT DE CIÈNCIES PHOTONIQUES, THROUGH AN OPEN PROCEDURE NOT SUBJECT TO HARMONIZED REGULATION

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CLAUSE 1. Object of the contract

The purpose of this contract is the supply, installation and commissioning of an "*Ion chromatography-mass spectrometry (IC-MS) system*" for the ICFO laboratory.

The types of items supplied are linked to the CPV (Common Public Procurement Vocabulary), 38430000-8 – Detection and analysis apparatus; 38432200-4 Chromatographs; 38433100-0 – Mass spectrometers.

CLAUSE 2. Needs to satisfy

Ion chromatography-mass spectrometry (IC-MS) combines ion chromatography (IC) and mass-spectroscopy (MS) to address analytical tasks which cannot be adequately handled by IC alone. IC is a robust, easy-to-use, selective, and sensitive technique for the determination of inorganic anions like sulphate, nitrate, nitrite, ammonium etc., and alkali or alkaline earth metal cations. IC is also very sensitive and selective towards polar organic compounds like organic acids, haloacetic acids, oxyhalides, and urea even in its different ionic forms. The integration if IC and MS, further enables the mass-selective detection of MS helps to identify the compounds in ppb levels.

Liquid chromatography with mass spectroscopy (HPLC-MS) is also robust and sensitive. However, it faces several difficulties in separating highly ionic compounds due to their weak interactions in liquid with the stationary phase. On the other hand, IC can separate any kind of ionic compound in different ionic forms with specific columns tailored for ion separations. For instance, IC can separate sulphur in different ionic forms like sulphate, sulphite, thiocyanate etc. Other typical ions like different forms of nitrogen (nitrite, nitrate, azide, ammonium) can also be easily separated by IC which is a drawback of HPLC.

The mass spectroscopy serves as a secondary detector for IC, recording the mass-to-charge ratios of specific analytes of interest. In this way, MS detection verifies the identification of compounds present in the complex matrices, ensuring accurate results. It is also possible to quantify co-eluting components and significantly improve detection limits.

We are looking to purchase an equipment that combines an IC with a MS system in a tandem IC-MS configuration, for the identification and quantification of products like urea, nitrite, ammonium, formate, acetate, and other ionic compounds generated during electrochemical reactions, down to ppb levels. These requirements are detailed in the next section. In particular, our applications require an IC system comprising two separation systems (both anionic and cationic columns in parallel) that operate simultaneously, and that can be individually connected to the MS system.

CLAUSE 3. Technical requirements

3.1. Requirements for the ionic chromatography system and associated modules

- Conductivity detectors
  - Two detectors (at least one detector per channel)
  - Digital signal processing
  - Cell volume: 0.3 µl
  - Range: 0…15000 µS/cm
  - Non-transferable electronic card for software control, monitoring and traceability
- Pumping systems
  - Two systems
  - High pressure

- Flow: 0.001…20 ml/min
- Binary gradient system
- Non-transferable electronic card for software control, monitoring, traceability and control of maintenance intervals
- Vacuum microchamber system for degassing of samples and eluents

- Column ovens:
  - At least two independent and thermostatted compartments
  - Temperature range: at least +5ºC to +80ºC
  - Automatic cleaning and regeneration of the chromatographic columns
  - Automatic column recognition system

- Sequential chemical suppression for anion detection:
  - Chemical suppression module consisting of three cation exchange cartridges in a rotor. This system allows the regeneration and rinsing of the chemical suppressor externally to the chromatographic circuit
  - No memory effects between different chromatograms
  - Low background noise (< 0.2 nS/cm in the conductivity detector).
  - Compatibility with organic solvents and pH from 0 to 14
  - Possibility of working with and without chemical suppression depending on the analytical application
  - Vacuum microchamber CO_2 suppressor

- Columns:
  - Column for detection of anions and organic acids:
    - One guard column to prevent column damage and sample contamination
    - Stationary phase based on surface-functionalized polystyrene-divinylbenzene copolymer
    - Intrinsic and non-transferable electronic card for storing its usage history (LPG functions)
    - Automatic column recognition
    - One additional guard and one additional column replacement included

  - Column for detection of cations and urea:
    - One guard column to prevent column damage and sample contamination
    - Stationary phase based on silica gel
    - Intrinsic and non-transferable electronic card for storing its usage history (LPG functions)
    - Automatic column recognition
    - One additional guard and one additional column replacement included

- Autosampler:
  - Capacity > 96 sample vials, volume 2 ml
  - Different injection modes:
    - Full loop
    - Partial loop
    - Pick-up mode
  - 1 µl precision for aspiration and dosing of the liquids
  - 4-channel selection
  - Programmable washing of the injection circuit

- Possibility of cooling the samples down to at least 4ºC
- Multiple injections without filter replacement
- Filtration of the in-line samples with standard 0.20 µm and 47 mm filters

3.2. Requirements for the mass spectrometer to be coupled to the ion chromatographer

- Ionization source
  - Atmospheric pressure electrospray ionization (API-ESI)
  - Possibility to work in both positive and negative modes
  - Disassembly without venting
  - Nebulizer connected to ground, orthogonal to the MS inlet

- Single quadrupole mass analyzer
  - Mass range: 10 – 2000 m/z
  - Hyperbolic quadrupole
  - Fragmentation
  - Sensitivity S/N > 100:1
  - Mass accuracy: ≤ ± 0.005 Da
  - Working in full range and single ion modes

3.3. Requirements for the software:

- Data acquisition, evaluation, reprocessing, overlay, and import and export functions in a single software
- Automatic and manual integration algorithms
- Quantification by calibration curves with external (ESTD) and internal (ISTD) standards
- Possibility of data analysis of unfinished chromatograms
- Lifetime license, including software updates, that could be portable to a new workstation if needed.

CLAUSE 4. Power distributions and safety

- The system should be configured for EU (Spain) power grid (voltage, sockets, etc.) and be CE marked.
- The system will be fully protected against unexpected power cuts and, in that case, will be fully safe for the operators. A quick and easy turning on of the system has to be possible after a power cut.

CLAUSE 5. System components, layout and services

- The system should include a workstation for full control of the entire ion chromatography system coupled to mass spectrometry, with a single control and data acquisition software, two conductivity detectors, two independent column ovens, two columns for anion detection with two guard columns, two columns for cation detection with two guard columns, and all necessary instruments for the maintenance of the system (wrenches, screwdrivers, hex keys, etc.), as well as all necessary technical information (manuals, technical sheets, catalogues etc.)

- The proposal will include a complete set of pictures, drawings and layouts of the system, including dimensions, location and details of the different components.
- The proposal **will include full installation and start-up requirements** (power, water, compressed air, process gases, etc), clearly specifying connection type, tubing materials, pressures, flows, etc, for the specific configuration of the offered system.

CLAUSE 6. Transportation, installation, start-up and training

- The proposal will include transportation to ICFO's facilities including insurance and all export/import and customs duties. **DAP incoterm will apply.**
- The machine will be placed in the selected location by ICFO. Contract winner will cover all costs, organization and coordination of machine placement, including any required specialized equipment or vehicle, and any required component disassembly and reassembly for system unloading and transportation inside the building to the target lab location.
- Onsite system startup included followed by the acceptance tests specified below.
- System training to ICFO personnel included. The number of training days and approximate schedule will be specified in the proposal

CLAUSE 7. Acceptance test

Test Parameter specifications:

1. **System sensitivity to urea (MS detector)**
   - 1.1. Sample = 5 ppb urea in [0.1M $KHCO_3$ + 5mM KNO_3] electrolyte
   - 1.2. Test procedure = measure signal-to-noise ratio of the urea peak
   - 1.3. Eluent = 3.0 mM oxalic acid
   - 1.4. Flow rate = 0.9 ml/min
   - 1.5. Injection volume = 100 µl
   - 1.6. Column temperature = 30ºC
   - 1.7. Recording time = 7 min
   - 1.8. Test results
     - 1.8.1. SNR ≥ 10:1 for the urea peak

2. **System sensitivity to ammonium (conductivity detector)**
   - 2.1. Sample = 0.05 mM NH_4^+ in [0.1M $KHCO_3$ + 5mM KNO_3] electrolyte
   - 2.2. Test procedure = measure signal-to-noise ratio of the NH_4^+peak
   - 2.3. Eluent = 3.0 mM oxalic acid
   - 2.4. Flow rate = 0.9 ml/min
   - 2.5. Injection volume = 100 µl
   - 2.6. Column temperature = 30ºC
   - 2.7. Recording time = 7 min
   - 2.8. Test results
     - 2.8.1. SNR ≥ 10:1 for the NH_4^+ peak

3. **Chromatographic peak resolution for cations (MS detector and conductivity detector)**
   - 3.1. Sample = 1 ppm urea + 0.5 mM NH_4^+ in [0.1M $KHCO_3$ + 5mM KNO_3] electrolyte

3.2. Test procedure = measure chromatographic peak resolution
3.3. Eluent = 3.0 mM oxalic acid
3.4. Flow rate = 0.9 ml/min
3.5. Injection volume = 100 µl
3.6. Column temperature = 30ºC
3.7. Recording time = 30 min
3.8. MS mode: **single ion**
3.9. Test results
3.9.1. Fully resolved urea, NH_4^+, K^+ and Na^+ peaks (Rs > 1.5, mutual overlap < 0.15%)

4. Chromatographic peak resolution for cations in full-range MS mode
4.1. Sample = 1 ppm urea + 0.5 mM NH_4^+ in [0.1M $KHCO_3$ + 5mM KNO_3] electrolyte
4.2. Test procedure = measure chromatographic peak resolution
4.3. Eluent = 3.0 mM oxalic acid
4.4. Flow rate = 0.9 ml/min
4.5. Injection volume = 100 µl
4.6. Column temperature = 30ºC
4.7. Recording time = 30 min
4.8. MS mode: **full range**
4.9. Test results
4.9.1. Fully resolved urea, NH_4^+, K^+ and Na^+ peaks (Rs > 1.5, mutual overlap < 0.15%)

5. Limit of detection for cations in single-ion MS mode
5.1. Samples = {1 ppb; 100 ppb; 1 ppm urea} + {0.05 µM; 0.5 µM; 5 µM NH_4^+} in [0.1M $KHCO_3$ + 5mM KNO_3] electrolyte
5.2. Test procedure = measure the limit of detection for urea and NH_4^+
5.3. Eluent = 3.0 mM oxalic acid
5.4. Flow rate = 0.9 ml/min
5.5. Injection volume = 100 µl
5.6. Column temperature = 30ºC
5.7. Recording time = 30 min
5.8. MS mode: **single ion**
5.9. Test results
5.9.1. LOD ≤ 1 ppb for each compound

6. Limit of detection for cations in full-range MS mode
6.1. Samples = {5 ppb; 50 ppb; 500 ppb; 5 ppm urea} + {0.25 µM; 2.5 µM; 2.5 mM NH_4^+} in [0.1M $KHCO_3$ + 5mM KNO_3] electrolyte
6.2. Test procedure = measure chromatographic peak resolution
6.3. Eluent = 3.0 mM oxalic acid
6.4. Flow rate = 0.9 ml/min
6.5. Injection volume = 100 µl
6.6. Column temperature = 30ºC
6.7. Recording time = 30 min
6.8. MS mode: **full range**
6.9. Test results
6.9.1. LOD ≤ 50 ppb for each compound

7. **Chromatographic peak resolution for anions (conductivity detector)**
   7.1. Sample = 0.1 mM formate + 0.05 mM acetate + 0.5 mM NO_2^- in [0.1M $KHCO_3$ + 5mM KNO_3] electrolyte
   7.2. Test procedure = measure chromatographic peak resolution
   7.3. Eluent = 3.0 mM oxalic acid
   7.4. Flow rate = 0.9 ml/min
   7.5. Injection volume = 100 µl
   7.6. Column temperature = 30ºC
   7.7. Recording time = 30 min
   7.8. Test results
      7.8.1. Fully resolved formate, acetate and nitrite peaks (Rs > 1.5, mutual overlap < 0.15%)

8. **Calibration curve for urea**
   8.1. Sample = 1, 5, 10, 100 and 1000 ppb of urea in [0.1M $KHCO_3$ + 5mM KNO_3] electrolyte
   8.2. Test procedure = build a calibration curve
   8.3. Eluent = 3.0 mM oxalic acid
   8.4. Flow rate = 0.9 ml/min
   8.5. Injection volume = 100 µl
   8.6. Column temperature = 30 ºC
   8.7. Recording time = 7 min
   8.8. Test results
      8.8.1. LOD ≤ 1 ppb
      8.8.2. Linear calibration curve with R^2 > 0.999

CLAUSE 8. Warranty and Follow-on Support

- **Two-year Full Warranty** on all parts and components of the system irrespective of the manufacturer. The warranty will include the replacement of any faulty or damaged part(s) during normal use of the system, no matter the manufacturer of the component(s). It will cover any cost related with the disassembly, transportation, reparation and re-assembly of the damaged component(s), including all travelling and living costs of the required service engineer(s). An on-site repair, or a justified alternative to reduce the system down time to the minimum, will always be the first service option. A team of properly qualified and skilled service engineers will have to be available.
- Spare parts, components and subsystems (no matter the manufacturer) will be available during, at least, 10 years after system supply.
- System lifetime support:
  - By phone and e-mail with a response within two working days.
  - Emergency visit after a system breakdown within 10 working days.
- The technical service team must be based in Europe and ideally in Spain.

CLAUSE 9. Delivery and Installation Time

The system must be delivered at ICFO within a maximum period of 12 weeks. Delivery time is defined as the time elapsed since the signature of the contract until the system delivery at ICFO facilities. It includes the manufacture of the system, the transportation, the installation and the acceptance test at ICFO's premises.

CLAUSE 10. Target price

- The target price for the system is 197.000€ (VAT excluded).
- Payment terms:
    - 30% upon order,
    - 20% upon shipment from manufacturer,
    - 50% after installation training and acceptance.

Castelldefels, on the date of its digital signature

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GL CO2MAP