



Guidelines for HRMS analysis request sheet filling and sample preparation

Each sample must be associated to an analysis request sheet. Open the excel file "PC_HRMS 2021" or "MAC_HRMS 2021" and select the tab "HRMS". Please fill all fields electronically and save the file under the name of your sample reference. This way, in case of trouble, you could send it again. **All vial requests must be withdrawn only from Mr Gilles Clodic, after setting an appointment with him (gilles.clodic@sorbonne-universite.fr , 01 44 27 34 09).**

Please pay attention to some important points:

- In the field "Equipe" (Team), choose your corresponding **chef d'équipe (team header)** in the drop-down list. This is a mandatory condition since he will be the payer (if not present, please add it on the second tab of the excel sheet).
- In the field "Responsable de Facturation" (billing contact), indicate the name of the **person in charge of billing** in your team.
- Stock solution of the sample can be prepared in any solvent, but provided for analysis **in solution** in **methanol, acetonitrile, water, dichloromethane** or mixture of them. Please use pure solvents, at least HPLC-grade. If necessary, we will provide the solvent for you. Your sample must appear with a **clear** aspect, i.e. without suspended particles, at a concentration of **10 µg/ml (+/- 20%)**, in a well sized **vial** (11x32mm with a large mouth, blue screw cap and siloxane/PTFE septum) which can be withdrawn from Mr Gilles Clodic. If you want to purchase your own vials, Mr Clodic will give you the reference. Each vial shall be **labelled** with your product reference. The label shall not exceed the surface of the vial to avoid problem with the autosampler. The caps screw very well, so do not use parafilm.
- The best way for **sample preparation**:
 - Prepare a solution at **1 mg/mL in your preferred solvent** (methanol, acetonitrile, water, chloroform, dichloromethane, ethanol, DMSO, etc.). Please avoid the use of pure solvents such as dimethylsulfoxide, dimethylformamide and tetrahydrofuran, they can damage instruments.
 - Fill your analysis vial with **1 mL of HRMS compatible solvent**: methanol, acetonitrile, water, dichloromethane or mixture of them (indicate by using the drop-down list in solvent field).
 - Add **10 µl of your stock solution** at 1 mg/ml to reach a final concentration of about 10 µg/mL. The sample volume must be **1 mL** to ensure detection of losses from potential vapour leaks.
- In the field "Formule brute", input the **raw formula**. Please **remove any counterion** as non-covalent interactions are usually not preserved in ESI mass spectrometry: CH₃COO⁻ or C₂H₅NH₃⁺ for example.
- In the field "Masse exacte", input the **exact mass**, i.e. the mono-isotopic mass of the targeted molecule or ion, with at least two decimal digits. Please use the **coma ","** as decimal separator. To determine the exact mass, you can for example use ChemDraw or an equivalent software. Please remember to select only the target molecule, without counterions.
- When you draw your molecules in ChemDraw or equivalent, enable the window "analysis" and untick the part *Mol. Wt., m/e et Elem. Anal.* Next, paste the formula and exact mass below the structure and paste all, in the corresponding frame of the sheet at the right of "**Structure**".
- The raw formula, exact mass and structure must **correspond**. These three fields are **necessary for a proper spectrum acquisition and data processing**, so please pay a particular attention to them.
- **Make sure all the fields are complete and correct**. Check that you have an internet connexion and click on "Code QR Manuel". Please wait until a web page with your QR code opens. Next, print QR Code picture by a right click (please remove old QR code if still present on your sheet) and paste the new one to the box **A25**. Please check that QR code do not oversized from shaded square.
- Save your sheet, print it under A4 size and tape your vial at the bottom right of the page. Please do not tape your vial on the QR Code or on the information you wrote.