Sample Preparation Protocol for Open Access Mass Spectrometers

Please aim the concentration of analyte in the range of **100 micrograms per mL (μg/mL) for OA-A** or in the range of **10 μg/mL** for open access **B, C and D instruments.** When analyte concentration could not be estimated, the samples should not be run on the open access MS systems.

Over concentrated samples lead to increased chemical noise, poor mass resolution, blockage in the sample delivery lines and contamination of the mass spectrometer vacuum part. You should be able to see through your sample vial even if the solution is coloured. Please also make sure that there are no hard particles in the solution or precipitation at the bottom of your sample vial, and that the solution is not jelly-like or cloudy.

Only **standard 2 ml Mass Spec sample vials** with a **soft septum** on the top of the lid should be used. The vials are available off-shelf from CRL stores. No taller vials or vials with hard lids can be used.

For **open access C and D (LC/MS analysis)** please submit **an extra blank sample before and after** your samples. Isopropanol is recommended as blank for OA-D (LC/MS of protein). For OA-C (LC/MS of small molecules) please use either the same solvent as in your sample, or isopropanol. Running blank samples is necessary for cleaning the column and to prevent the carrying-over of previous samples.

All open access instruments use **electrospray ionisation** which is only **compatible with volatile organic solvents and water.** Samples have to be cleaned of inorganic salts: **high inorganic salt concentrations are not compatible with ESI.** Please follow the protocol below for sample preparation.

The following approach is recommended for making up samples for open access analysis

1. Dissolve the sample in any organic solvent (e.g., DCM, $CHCl_3$, EtOAc, MeCN, MeOH) or H_2O to a concentration of 1mg/mL. Please ***do not use low vapour pressure solvents***, such as DMSO, or dilute them >20-fold in another solvent.
2. Take 100uL of this solution and dilute it with 1mL of either methanol, acetonitrile or water (or any combination of these solvents).
3. If there is any precipitate in the resulting solution ***it must be filtered*** before running the sample otherwise this is very likely to cause line blockages and delays with sample analysis for all users.
4. Place the solution in ***a standard 2mL sample Mass Spec*** vial with a screw cap lid and soft septum on the top (available from stores).
5. ***Do not use Trifluoroacetic acid (TFA) in your samples***. If you need to acidify your samples use formic acid.
6. ***Do not use Tetrabutyl ammonium (TBA) in your samples*** (also avoid other ion-pairing agents) these will contaminate all subsequent samples run on the system.