

Sample Preparation Protocol - BioAccord Target Confirmation

Please aim the concentration of analyte in the range **1 - 10 μM** . Depending on the ionisation of your compound of interest, you may need to adjust the concentration. Do not submit samples which have a concentration greater than **50 μM** as you will likely damage the instrument.

Over concentrated samples will be flagged to MS Staff and will lead to **increased chemical noise, poor mass resolution, blockage in the sample delivery lines and contamination of the mass spectrometer**. 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 **pre-slit septum** on the top of the lid should be used. The vials are available from CRL stores. No taller vials or vials with hard lids can be used.

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:

1. *Dissolve the sample in organic solvent (e.g., DCM, CHCl_3 , EtOAc, MeCN, MeOH) or H_2O to a concentration of 1 mg/mL. Please **do not use low vapour pressure solvents**, such as DMSO.*
2. *Take 1 - 10 μL of this solution and dilute it with 1 mL 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 2 mL mass spec sample vial** with a screw cap lid and pre-slit 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** (or any other ion-pairing agents) these will contaminate all subsequent samples run on the system.*