

## GC/MS sample preparation guidelines

### Sample Components to Avoid Completely

The following should never be injected: metals, strong acids or bases, salts, oligomeric and polymeric material. These classes of compounds are unsuitable for gas chromatography, and can damage the GC column. Do not dissolve samples in water, DMSO, or DMF.

### Overview

Volatile analyte (boiling point < 300°C)

0.5 – 2 mL in volume

<< 100 ppm

Volatile, organic solvent

**FILTER TO REMOVE PARTICULATE MATTER**

### Concentration

Mass spectrometry is several orders of magnitude more sensitive than NMR, so please do not use the same samples you have prepared for NMR analysis for MS analysis. The upper limit of concentration needed is 100 ppm. If you introduce a more concentrated sample, you will damage the EI filament. **WHEN IN DOUBT, DILUTE!**

$$\text{Recall, } ppm = \frac{mg}{L} = \frac{\mu g}{mL}$$

To prepare 1.00 mL of a 25 ppm solution,  $\frac{25 \mu g}{mL} \times 1.00 mL \times \frac{1g}{10^6 \mu g} = 2.5 \times 10^{-5} g$  is needed.

For a compound MW of 200 g/mol, the molarity is  $2.5 \times 10^{-5} g \times \frac{mol}{200g} \times \frac{1}{0.001L} = 1.25 \times 10^{-4} M$ .

### Solvents

Hexane, acetone, and methanol are the recommended solvents for sample preparation. Other acceptable options are benzene, ethers, and methylene chloride. Do not use DMSO and DMF. Do not use water.