Major Contaminants and Their Sources

This document lists some major contaminants in UPLC/MS, HPLC/MS, and UPC²/MS systems, along with their sources and spectra.

Polyethylene glycol (PEG) or PEG-like materials

PEG is a synthetic polymer produced in a range of molecular weights. Common sources of PEG contamination include:

1. Organic solvents
   - Methanol
   - 2-propanol
   - Acetonitrile
   - Water

2. Mass spectrometer calibration solution

3. Hand cream

4. Detergent
   - Triton X-100, etc.
   - Glassware detergents

5. Cutting solutions in machining

6. Column manufacturing

Figure 3 shows a typical PEG spectrum, exhibiting a series of mass peaks separated by 44 Da.
**Metal ions**

Metal ions such as lithium (Li), sodium (Na), potassium (K), copper (Cu), platinum (Pt), and iron (Fe) can be sources of contamination.

For example, iron forms adducts with varying numbers of acetate in acetic acid or acetate mobile phases. Iron can contaminate an UPC²/MS system through the following sources:

- Solvents such as water and acetonitrile
- Acetic acid (lower in formic acid)
- Formic acid
- Non-passivated stainless steel parts
- Titanium or inert metal parts fabricated with steel tools

Figure 4 shows the typical pattern of Fe-acetate cluster spectra. The strongest ion (base peak intensity, or BPI) mass may be different, depending on the number of acetates in the cluster. The upper spectra are based on the MassLynx isotope model.

![Figure 4 - Fe Contamination Spectra](image)

**Phthalates**

Phthalates are chemical compounds used chiefly as plasticizers, and can cause contamination. The compounds can be detected on a wide range of laboratory materials, including water and other solvents, laboratory air, and plastic materials such as tubing and water storage containers. Common phthalates include di-2-ethyl hexyl phthalate (DEHP), diisodecyl phthalate (DIDP), diisononyl phthalate (DINP), and diisooctyl phthalate (DIOP).
Diisooctylphthalates can form the following adducts:

- \([M+H]^+ = 391\)
- \([M+Na]^+ = 413\)
- \([M+K]^+ = 429\)
- \([2M+NH_4]^+ = 798\)
- \([2M+Na]^+ = 803\)

**Slip agents (amides)**

Avoid using components packed in plastic bags containing slip agents, or amides. The three most commonly used amides are:

- Oleamide \(([M+H]^+ = 282)\)
- Stearamide \(([M+H]^+ = 284)\)
- Erucamide \(([M+H]^+ = 338)\)

*Figure 5* shows a spectrum revealing amide contamination.