Chemical Compound Confidence
Decision Tree

Cambridge Polymer Group

Chemical characterization per ISO 10993-18 → GC-MS/LCMS Data → Full structural identification? → ✓ → Comparison to reference compound? → ✓ → Confirmed identification

Full structural identification? ✗ → Partial structural identification?

Comparison to reference compound? ✗ → Orthogonal Information? AND/OR *a priori* knowledge? → ✓ → Confident identification

Orthogonal Information? AND/OR *a priori* knowledge? ✗ → Tentative identification

Partial structural identification? ✗ → Unknown identification

Partial structural identification? ✓ → Tentative identification

Unknown identification → Additional chemical information needed
- Re-examine data with *a priori knowledge?*
- Re-analysis with different ionization?
- Re-analysis with targeted MS/MS?

Additional chemical information needed → GC-MS/LCMS Data

Tentative identification → Can the structure be assigned to a common group for toxicological risk?

Can the structure be assigned to a common group for toxicological risk? ✓ → Toxicological risk assessment per ISO 10993-17

Can the structure be assigned to a common group for toxicological risk? ✗ → Is the structure a Cohort of Concern compound? AND/OR unexpected from *a priori* information? AND/OR MOS < 1.0

Is the structure a Cohort of Concern compound? AND/OR unexpected from *a priori* information? AND/OR MOS < 1.0 ✓ → Additional chemical information needed

Is the structure a Cohort of Concern compound? ... ✗ → Toxicological risk assessment per ISO 10993-17

Confirmed identification → Toxicological risk assessment per ISO 10993-17
Confident identification → Toxicological risk assessment per ISO 10993-17