

# Simplifying the Screening Workflow for Extractables Testing

The structural elucidation of unknown compounds found in packaging is a complex and time-consuming process. Waters™ **UNIFI™ Scientific Information System** provides a simple workflow including scientific library creation, multivariate statistical analysis, elucidation, and reporting.

[www.waters.com/extractables](http://www.waters.com/extractables)

## 1. COMPLEX MS DATA

Data acquired on ToF mass spectrometry instruments from complex matrices can yield an overwhelming amount of raw data.



## 2. TARGETED SCREENING

User generated library with retention time, fragment, collision cross section (CCS) information can be used to confirm the presence of compounds in the sample. Concentrations can be determined with calibration standards.



## 3. NON-TARGETED SCREENING/ WHAT ELSE IS IN THE SAMPLE?

Comparison and statistical analysis tools can be used to discover other compounds of interest present in the sample.

IRGANOX 1098  
SALICYLIC ACID  
TRIBUTYL PHOSPHATE  
DIETHANOLAMINE  
NABUMETONE  
HEXAMETHYLENETETRAMINE  
SUDAN I

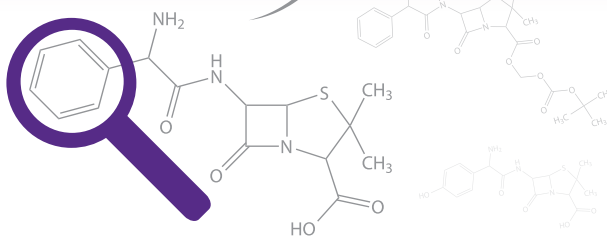


MELAMINE  
TETRABROMOBISPHENOL A (TBBPA)  
CIPROFLOXACIN  
2-HYDROXYETHYL STEARATE  
DIETHYL PHTHALATE (DEP)  
CYASORB 3638  
TRIPHENYL PHOSPHATE (TPP/TPHP)

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SCIENTIFIC INFORMATION SYSTEM

## 4. IDENTIFYING COMPOUNDS

Combining the accurate mass and fragment information with structural database search can yield the identity of these compounds.



## 5. REPORT

A customized report can be generated that includes analysis method, processing parameters, chromatograms, spectra, and identified compound summary tables.

