Purpose

This spreadsheet may be useful to help laboratory analysts and Assessors ensure compliance with ISO/IEC 17025:2017 - It may be useful for the investigation of analytes in solid and aqueous materials in food and environmental samples - Including to prototype extraction methods for new analytes, and to modify new and existing methods to improve their performance for a range of analytes. Several important published methods are included. A particular aim is to help reduce the consumption of chlorinated solvents as required by a number of older established Methods. Methods can be compared using different solvents for similar matrices. "Fine Tuning" is possible by using mixed solvents and different volumes for extraction, and different final solvent volumes for concentration.

It was created using the Apple "Numbers" Version 11, and Microsoft "Excel" 2013 and 2017, spreadsheet programs; using only "Cell Functions"; and does not use any "Code", "Macros" or "Hyperlinks", as as result some compromises have been made to its function and appearance - It should be "Safe" to distribute…

Using the System

The **Main** sheet is used to modify data to investigate changes to selected methods. Subsidiary sheets show relevant data for analytes and solvents, and aqueous matrices. Additional material is included in "Notes". A simple overview of using the controls is below.

Pop Up Menus have coloured backgrounds:

From:

Choose Main Solvent	Choose Main Solvent…
Main Solvent Not Chosen…	None…

No Comparison Run…

To:

Main Solvent Chosen is :	Dichloromethane
Choose 2nd Solvent :	None…

and:

Main Solvent Chosen is :	Dichloromethane
2nd Solvent Chosen is :	Methyl Acetate

Content can change, based on what is Chosen…

Calculated Values :

Matrix Amount mL or g	Solubility in Aqueous	Solvent Volume mL
35	Moderately	2
Left Blank…	Immiscible	1

Data Entry Fields and their Labels are **bold black** (e.g. "2 **Solvent Volume mL**").

Colons (:) at the end of Labels indicates that data entry/choice is done using the next field/pop-up (e.g. "**Choose Method:**"). No colon indicates the data entry field is directly underneath the Label (e.g. "**Solvent Volume mL**"). Data from published/original Methods are shown in Green Headers, borders and Text. Modified Methods are shown with Blue Headers, borders and Text. The section with Cyan borders is a simple tool giving an indication of how an analyte may perform based on the log$_{10}$ of its K$_{ow}$ (n-octanol-water partition coefficient). Warnings and important notifications are shown in Red.

A good place to start might be to look at the established US EPA 3510 method and compare it to the newer 351 method. EPA 3511 is validated specifically for mono- and poly-cyclic aromatic hydrocarbons. This method also may be used to extract selected volatile organic compounds (VOCs) or semivolatile organic compounds (SVOCs) which are slightly soluble or insoluble in water once their extraction performance has been demonstrated to be satisfactory. A number of laboratories are investigating and using this. Further refinements are also better suited to full automation, use small amounts of matrix in 20mL headspace files with low density extraction solvents - A number of instrument manufacturers are actively developing these.

Small Print & Acknowledgements

The author thanks his colleagues at: the UK Ministry of Defence; UK Home Office; British Rail Research; and in particular, the staff and volunteers at NATA Australia.

This spread-sheet is "Public Domain". Anyone is free to copy, modify, publish, use, or distribute it for any purpose, commercial or non-commercial, and by any means. The author has retired from paid work, carrying out "Pro Bono" work only; and does not accept any responsibility for any loss caused by the use of, or failure to use, this spreadsheet.

Please leave My name and Version Number at the bottom of this document.

This is Beta Software   Version 20221030 - © Tim Strutt