ReadMe_MultiAnalytesMU.pdf: Outline documentation for MS Excel and Apple Notes Spreadsheets

MultiAnalytesMU Spreadsheet - [Notes] This is normally the last sheet - An outline with further details follows on in the next page...

This spreadsheet may be useful to assist Laboratory Analysts and Assessors ensure compliance with ISO/ IEC 17025:2017. The revised standard requires Measurement Uncertainty (MU) of chemical test results to be available. It is designed to help produce necessary information by using sample blanks, spikes, and comparisons with reference materials. Sample "Low Spikes" could be used to determine Recoveries and Method Detection Limits. Spikes establish MUs at different concentrations with different matrices. It may be helpful when developing new methods or for "novel" analytes and matrices.

Created with Apple "Numbers" Version 12.0, and Microsoft "Excel" 2013, spreadsheet programs - Using only "Cell Functions". No "Code", Macros, or Hyperlinks are used - **It should be "Safe" to distribute…**

The spreadsheet uses some **conventions**: In [MainTable] cells where the user is expected to input data have blue text on a white background, **bold blue** indicates that a selection is made from a list**.** Default look-ups are **grey**. Warnings are highlighted with an [**orange background**]; and critical/failure/out-of-range warnings are highlighted with [**red backgrounds**]. **Important** data is purple.

Getting Started: The sheets are [MainTable], [SampleResults], [Distributions], [Units], and **[Notes]**. The last three are "look-ups" or information.
Data should be added or changed as outlined below…

[**MainTable]**: Used to set the parameters of the Test:-
The Test Name that was used to create the results is a "look-up" from the [SamplesResults] sheet.
The Analyte Name is a "look-up" from the [SamplesResults] sheet.
Select Report Type from the drop-down - This will produce different a different [Report] for each type.
Select Units from the drop-down - This will change the Horwitz Ratio (larger concentrations should give higher precision).
Enter 'Spike Value' for each column (Values between 0.00001 and 10,000,000).
MDL (From Mean of Previous Low Spikes) - If a value is entered, it will be used instead of the Results calculation.
Select Number of Significant figures - Usually **2** - 1 may be useful if near Quantitation limits, 3 for special precision.
Horwitz and Outlier fields with coloured backgrounds are not editable, but require consideration - Outliers or errors may well be the cause…
Now go to the [SampleResults] Sheet to check/update outliers as below…

[SampleResults]: Used to add SampleID and Results. There are a number of columns:-.
The First Column is used to Add/Edit **SampleID** (or Paste from another application). ***The 1st Top (Header) row must contain the Test Name. Other Header rows must contain the Analyte Name.*** The other columns are for ***plain numerical*** **Results** (or Paste from another application).
Possible result **Outliers** can be indicated by adding text e.g. Changing 77 to ?77 or 77! Adding text to Outliers will cause it to be ignored by the Horwitz and Grubbs calculations. If pasted results are not plain numbers, cell formatting will be lost.
The sheet can have many rows, but normally 3-11 are used (5, or more recommended).

[Distributions]: Used to calculate Method Detection Limit (t-test) and Grubbs' critical value for 0.05 (95%) level for 1-tail.
This is not editable. It is recommended that the user consults the NIST and RSC papers, referenced in the text at the bottom of the sheet, for further background information.

[Units]: Used to calculate scale of Horwitz values, and in **[Report]** and **[Calculations - Main Table]**:-
It is normally Locked, but any changes must be reflected in **[MU Calculations]** "**Units**" drop-down.

For further information, please consult these References:-
Planning and Reporting Method Validation Studies; Supplement to EURACHEM Guide on the Fitness for Purpose of Analytical Methods, First edition 2019
Blanks in Method Validation, Supplement to EURACHEM Guide The Fitness for Purpose of Analytical Methods, First Edition 2019

The **password** to unlock individual MS Excel sheets and cells is "timstrutt" (no "quotes"). Apple Sheets use Locked "Shapes".

The **[MainTable]** uses "hidden" rows with a *red font* - Changing or deleting them will cause breakages...

Warning: The calculations are based upon standard literature methods, but some approximations have been used. See the references for background information.

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MultiAnalytesMU Spreadsheet - [Main] This is the first sheet - Shows calculations for selected ReportType.

Test Name (TopRow, 1stColumn in SampleResults)	ICP-MS	ICP-MS	ICP-MS	ICP-MS	ICP-MS	ICP-MS	ICP-MS	ICP-MS	ICP-MS	ICP-MS
Analyte (TopRow in SampleResults)	Al	As	B	Ba	Be	Cd	Co	Cr	Cu	Fe
Report Type (Spike, Blank, Ref…)	Low Spike	Low Spike	Low Spike	Low Spike	Low Spike	Low Spike	Low Spike	Low Spike	Low Spike	Low Spike
Units	µg/kg	µg/kg	µg/kg	µg/kg	µg/kg	µg/kg	µg/kg	µg/kg	µg/kg	µg/kg
Low Spike Concentration	95.14	2.2	99	90	92	9	95	90	90	90
MDL - Optional (From Mean of Previous Low Spikes)	11	0.1								
Number of Significant figures	2	2	2	2	2	2	2	2	2	2
Total Number of Results for Analyte	9 (1 Excluded!)	9	9	9	9	9	9	9	9	9
RSD% (CV)	7.7%	8.8%	7.0%	38.2%	9.7%	6.9%	7.1%	12.1%	7.4%	149.9%
bias as %age (100 - Recovery)	12.6%	27.0%	3.7%	-22.2%	11.5%	-3.3%	-2.1%	10.5%	-3.5%	-126.0%
Horwitz Ratio (Ideally 0.3≤ HorRat ≤1)	0.35	0.40	0.32	1.73	0.44	0.31	0.32	0.55	0.34	6.81
Outlier?	0	0	0	220.1	0	0	0	59.97	0	1016
Result to 2 Significant figures	83	1.6	95	110	81	9.3	97	81	93	200
MDL = (MDL Factor x SD)	11	0.10	19	120	23	1.9	20	28	20	880
PQL (Practical Quantitation limit)	33	0.30	58	360	69	5.6	60	85	60	2600
% Recovery	87%	73%	96%	122%	89%	103%	102%	90%	103%	226%
Result Corrected for Recovery	95	2.2	99	90	92	9.0	95	90	90	90
Corrected for Recovery with Uncertainty	95 ± 13 µg/kg	2.2 ± 0.14 µg/kg	99 ± 20 µg/kg	90 ± 100 µg/kg	92 ± 26 µg/kg	9.0 ± 1.8 µg/kg	95 ± 19 µg/kg	90 ± 32 µg/kg	90 ± 19 µg/kg	90 ± 390 µg/kg

This shows an excluded result.
The highlighted result below has been edited by adding "!" which turns it into "nonnumeric".

Grubbs' test indicates analytes have potential outliers.

Typographical error.
Result entered as "1016" instead of the correct 101.6

MultiAnalytesMU Spreadsheet - [Sample Results] Is the second sheet - It contains the data for **[Main]**.

ICP-MS	Al	As	B	Ba	Be	Cd	Co	Cr	Cu	Fe
S1	86.38	1.59	90.21	94.21	86.38	9.03	96	86.38	90	96.1
S2	87.79	1.66	91.3	88.46	87.79	9.11	97	87.79	84	97.2
S3	77.94	1.42	91.88	98.27	77.94	9.24	98	77.94	101	98.2
S4	72.11	1.59	107.83	99.41	72.11	9.35	83	72.11	93	99.3
S5 Duplicate S3	78.56	1.66	94.69	100.24	78.56	9.06	100	78.56	85	100.2
S6	89.84	1.36	85.37	100.91	89.84	9.47	101	89.84	95	101.3
S7	89.3	1.69	99.21	81.31	89.3	9.91	102	89.3	99	102.4
S8	83.42	1.82	96.33	107.18	83.42	8.07	90	83.42	103	1016
S9	!58.97	1.67	101.22	220.1	67.61	10.4	106	59.97	88	119.6

This shows an excluded result.
The highlighted result has been edited by adding "!" which turns it into "nonnumeric".
This is shown above by: 9 (1 Excluded).

Potential Outliers.

Typographical error.

[Sample Results] has no calculated fields. Results are directly pasted, or (with Excel) linked to external data.
Copy cells from other spreadsheets as plain text, otherwise formatting could be lost...

MultiAnalytesMU Spreadsheet - [Distributions] Is the third sheet.

This is used to by **[Main]** look up Horwitz Ratio and Grubbs' test values. It cannot be edited.

MultiAnalytesMU Spreadsheet - [Units] Is the fourth sheet.

It contains many common concentration units. Values cover the range from ~ 10% to Parts-per-Trillion (ppt).

If required additional units may be added; but, as noted "Units" in the **[Main]** sheet must be updated.
