NIST Internal Report
NIST IR 8478

CCQM_Retrospectoscope Reference Manual

A detailed reference to the CCQM_Retrospectoscope, a suite of graphical tools for the meta-analysis of measurement results from CCQM studies

David L. Duewer
Michael A. Nelson
Christina E. Cecelski

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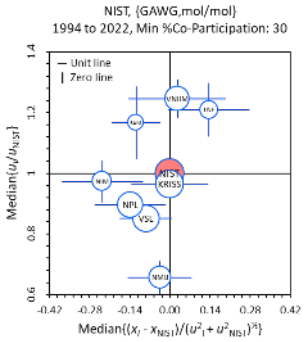

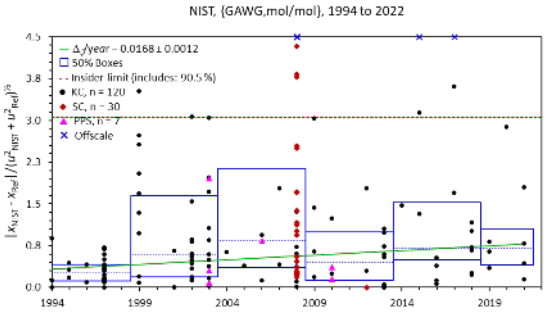

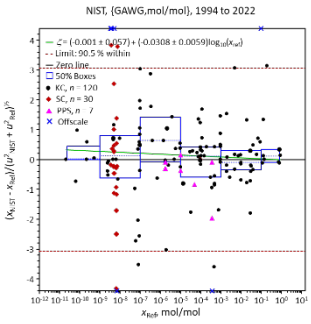

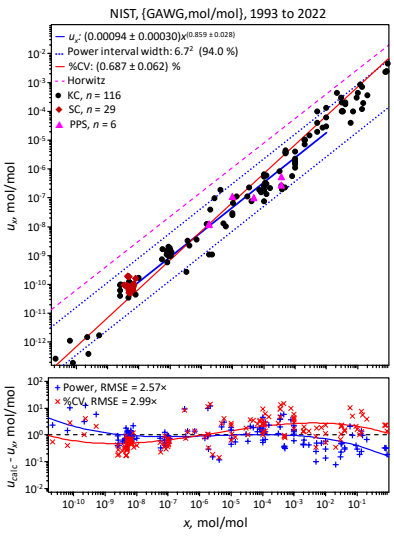

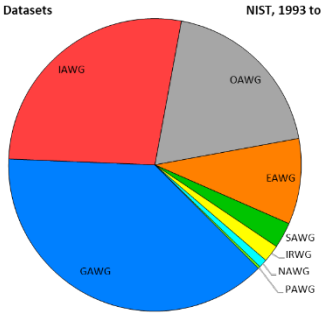

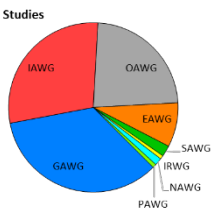

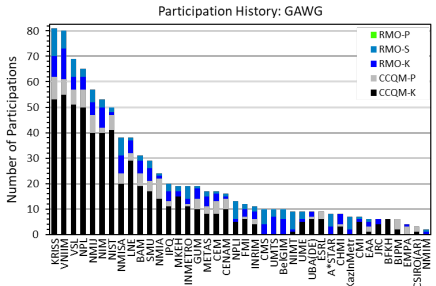

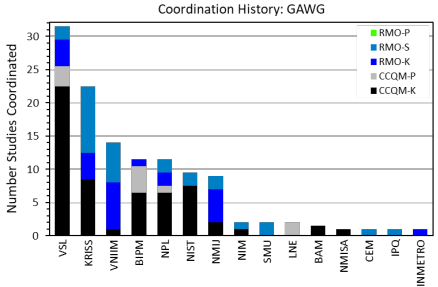

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Abstract

The *CCQM_Retrospectoscope* system combines a nominally complete database of results from Consultative Committee for the Amount of Substance: Metrology in Chemistry and Biology (CCQM) studies with a number of graphical tools for trying to make sense of the data. This system supports a diverse collection of often eye-opening appraisals of participation and measurement performance throughout the history of the CCQM activities. The appraisals include the bias, uncertainty, and degrees of equivalence of results submitted by individual national metrology or designated institutes (NMI|DIs); the relative performance of NMI|DIs, and the uncertainty function characteristic of entire Working Groups (WGs). The system is implemented in Excel using Microsoft's Visual Basic for Applications (VBA) programs. It runs on both Windows and Macintosh platforms.

Keywords

Consultative Committee for the Amount of Substance: Metrology in Chemistry and Biology (CCQM); designated institute; Electroanalytical Working Group (EAWG); Gas Analysis Working Group (GAWG); graphical data analysis; Inorganic Analysis Working Group (IAWG); Key Comparisons (KC); national metrology institute (NMI); Organic Analysis Working Group (OAWG); pilot studies; Supplementary Comparisons (SC).

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Acknowledgements

The *CCQM_Retrospectoscope* database evolved from the Senior Author's (Dave Duewer) *PDF_Maker*, a system used to explore various proposed estimators for assigning Key Comparison Reference Values (KCRVs). *PDF_Maker* was initiated in 2003 with the encouragement of Willie E. May, then Director of NIST's Chemical Science and Technology Laboratory and Chairperson of the Consultative Committee for the Amount of Substance: Metrology in Chemistry and Biology (CCQM)'s Organic Analysis Working Group (OAWG). Quite a number of CCQM participants used one of several versions of *PDF_Maker* over the years, offering suggestions for improving the analysis and correcting errors and oversights in the data: Michal Máriássy, Gavin O'Conner, Reenie Parris, and Kenneth Pratt are among the more influential critics.

In August 2020, what has become *CCQM_Retrospectoscope* was started as a major upgrade of *PDF_Maker*. As the database became more complete, the potential utility of the data for assessing measurement performance characteristics of CCQM study participants and their Working Group communities became apparent. With the encouragement of Carlos Gonzalez, Chief of the Chemical Sciences Division (CSD), in December of 2020 the "upgrade" evolved into *CCQM_Retrospectoscope*. Comments and suggestions provided by CSD staff Christina Cecelski, Mike Epstein, Mike Nelson, and Melissa Phillips have greatly helped debug the system and expand its capabilities.

Mike Nelson's and Christina Cecelski's repeated review and edits of this Reference Manual have made it more accessible, complete, and consistent. Remaining documentary errors and infelicities are, however, solely the responsibility of the (very) Senior Author.

1. Overview

CCQM_Retrospectoscope is an Excel workbook-based data analysis system for visualizing the participation and performance of national metrology and designated institute (NMI|DI) participants in Consultative Committee for the Amount of Substance: Metrology in Chemistry and Biology (CCQM) Key and Supplementary Comparisons and pilot studies. The CCQM operates under the authority of the Comité International des Poids et Mesures (CIPM). CCQM studies are governed by the CIPM's Mutual Recognition Arrangement (CIPM MRA) [1].

In this document, Key Comparisons, Supplementary Comparisons, and pilot studies are collectively termed "studies."

The *CCQM_Retrospectoscope* system contains a curated database of the publicly accessible CCQM studies, current as of the system's Version date. The master database maintained at NIST also contains *CCQM Confidential* datasets from completed pilot studies and provisionally curated data from Key and Supplementary Comparisons that are still under review. These non-public datasets are excluded from the publicly accessible versions of the *CCQM_Retrospectoscope*.

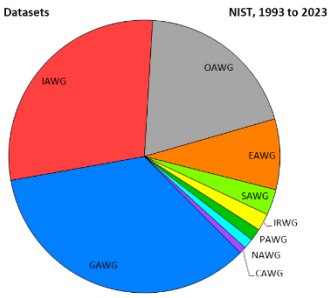
1.1. Analysis Subsystems

The *CCQM_Retrospectoscope* provides thirteen graphical analysis subsystems: five that focus on individual NMI|DIs, four that focus on the peer relationships among NMI|DIs, and four that focus on the WG communities. Each subsystem is contained on its own worksheet. These subsystems support ways of filtering the database for datasets of interest that include some or all: NMI|DI, Working Group (WG), base measurement units, measurement year, and analyte. The subsystems also support several performance metrics and optional graphical elements.

1.1.1. The "Lab" Subsystems

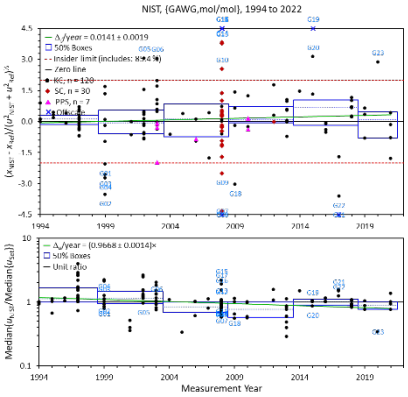
The following five subsystems summarize aspects of a given NMI|DIs participation or measurement performance in CCQM studies.

1.1.1.1. Lab_Activity (Section 4)



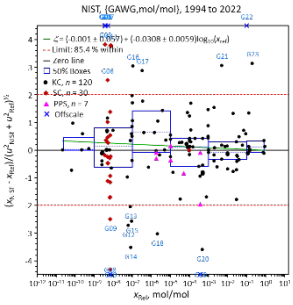
The *Lab_Activity* subsystem displays the relative proportions of the various groups of CCQM datasets and studies that a given NMI|DI participated in, where a group is defined as a unique combination of WG and measurement Base unit, {WG, Base unit} (Section 2.4.1.3). A table to the right of the charts lists the number of datasets and studies of each group, further categorized by the type of the study (Section 1.4.1). The displays and tables document what types of measurands the NMI|DI is most interested in.

1.1.1.2. Lab_History (Section 5)



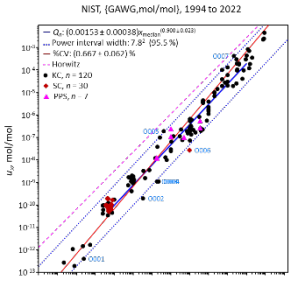
The *Lab_History* subsystem displays a given NMI|DI's performance as a function of time, enabling assessment of past performance in all studies of a given {WG, Base unit} that the NMI|DI participated in. The performance metrics are relative to the WG-assigned reference values, the expanded uncertainties assigned to those values, and the median of the measurement uncertainties reported by the study's participants.

1.1.1.3. Lab_Bias (Section 6)



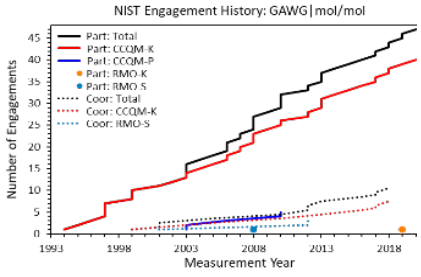
The *Lab_Bias* subsystem displays a given NMI|DI's performance as a function of the dataset's reference value. The performance metrics are relative to the WG-assigned reference values and the expanded uncertainties assigned to those values.

1.1.1.4. Lab_Uncertainty (Section 7)



The *Lab_Uncertainty* subsystem displays a given NMI|DI's reported standard uncertainties as a function of measurement value, enabling assessment of the NMI|DIs characteristic uncertainty function [2]. Datasets with unusually large or small standard uncertainties for a given measurement value are identified to assist in evaluating unusual measurement behavior.

1.1.1.5. Lab_Engagements (Section 8)

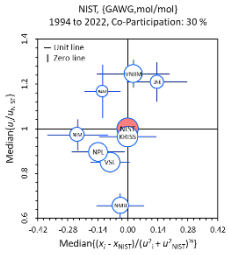


The *Lab_Engagements* subsystem details the number and timing of a given NMI|DI's engagements with the various types of CCQM study, where "engagements" are separated into "participations" (reporting measurement values) and "coordinations" (providing leadership). This subsystem combines results from the *WG_Participations* and *WG_Coordinations* subsystems.

1.1.2. The "Peer" Subsystems

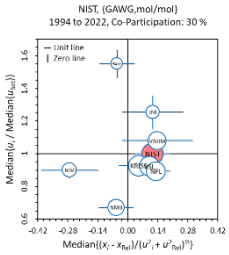
The following four subsystems summarize aspects one or more NMI|DIs activity or measurement performance relative to other NMI|DIs.

1.1.2.1. Peer_Bilateral (Section 9)



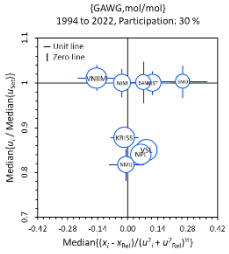
The *Peer_Bilateral* subsystem provides the most direct of three related analysis approaches to identifying the "peers" of a given NMI|DI based upon participation and measurement performance in the same studies. This approach explores the bilateral differences between the NMI|DI's results and that of co-participants. The summaries are of the paired differences in all the selected datasets where both participated. Summary results are reported for all NMI|DIs that co-participated in a specified minimum proportion of the datasets. Each bilateral assessment is independent; different co-participants having participated in different subsets of the selected datasets.

1.1.2.2. Peer_Unilateral (Section 10)



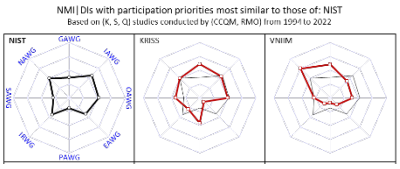
The *Peer_Unilateral* subsystem provides an alternative approach to identifying an NMI|DI's "peers". The analysis explores the summary performance relative to unilateral dataset reference values, not bilateral paired differences. Results are displayed for all NMI|DIs that co-participated with the target NM/DI in a given minimum proportion of datasets. Each unilateral assessment is independent; different co-participants having participated in different subsets of the selected datasets.

1.1.2.3. Peer_Global (Section 11)



The *Peer_Global* subsystem generalizes the approach used in *Peer_Unilateral* for identifying "peer" NMI|DIs. Rather than exploring the performance of NMI|DIs relative to a target participant, *Peer_Global* summarizes their performance in each dataset relative to the dataset's reference value. The chart displays results for all NMI|DIs that participated in a specified proportion of the selected datasets. These summaries illuminate the measurement bias in all the datasets that each NMI|DI contributed to during the specified years. The assessments are independent, NMI|DIs having participated in different subsets of the selected datasets.

1.1.2.4. Peer_Priorities (Section 12)

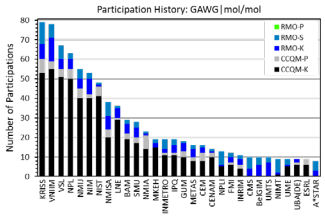


The *Peer_Priorities* subsystem displays the proportions of studies in each of the WGs that a designated NMI|DI has participated in. Similar displays are provided for the eleven NMI|DIs that either have the most similar participation priorities or are members of a designated list.

1.1.3. The "WG" Subsystems

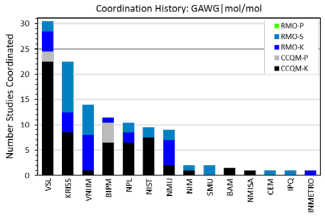
The following five subsystems summarize aspects of the WG communities.

1.1.3.1. WG_Participations (Section 13)



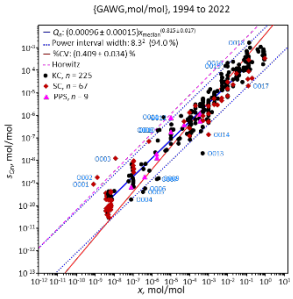
The *WG_Participations* subsystem summarizes the number of WG studies the various NMI|DIs have participated in. This information is mined from the *CCQM_Retrospectoscope* data worksheets ("datasheets"), so excludes pilot studies that did not provide a final report or did not identify the participants.

1.1.3.2. WG_Coordinations (Section 14)



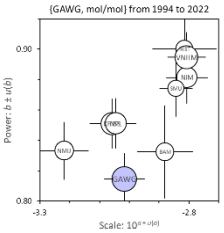
The *WG_Coordinations* subsystem summarizes the number of WG studies various NMI|DIs have coordinated or co-coordinated. This information is mined from summary records maintained at the Bureau International des Poids et Mesures (BIPM), these summaries include all pilot studies, regardless of how (or if) the results of the study were reported.

1.1.3.3. WG_Precision (Section 14.5.3)

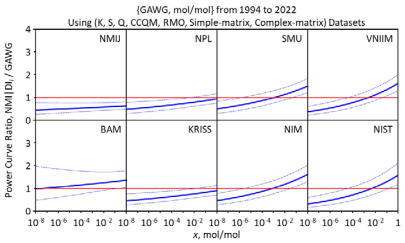


The *WG_Precision* subsystem depicts measurement reproducibility as a function of analyte level for NMI|DI communities. For each {WG, Base unit} group during a given range of measurement years, a robust estimate of the standard deviation of the reported results is plotted against the median of those results. The resulting precision function is analogous to the results from Horwitz's and Thompson's analyses of measurement reproducibility as functions of analyte concentration [2,3,4,5].

1.1.3.4. WG_Power (Section 16)

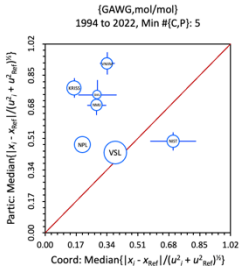


The *WG_Power* subsystem displays the power-law coefficients characteristic of a WG as estimated by the *WG_Precision* subsystem and those for peer NMI|DIs identified by *Peer_Bilateral*, *Peer_Unilateral*, or *Peer_Global* and by the *Lab_Uncertainty* subsystem. It also displays the ratios between the WG's function and those of the identified NMI|DIs, with the WG function as denominator and the NMI|DI functions as numerator.



Efficient use of this subsystem requires considerable experience and patience.

1.1.3.5. WG_Diagonal (Section 17)



For NMI|DIs that have coordinated studies, the *WG_Diagonal* subsystem displays their median measurement bias in datasets from studies that they just participated in as a function of the median measurement bias in datasets from studies that they coordinated.

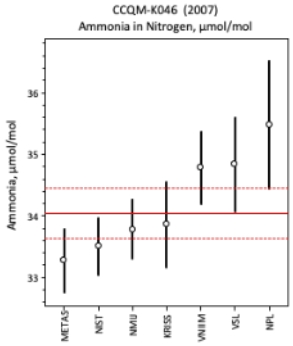
1.2. Other_Tools: Support Systems (Section 18)

The *Other_Tools* dashboard provides access to four dataset support subsystems, two database maintenance subsystems, and one platform benchmarking tool. Each subsystem is contained on its own worksheet; the benchmarking tool does not require its own worksheet.

1.2.1. Dataset_Locate (Section 19)

The *Dataset_Locate* subsystem enables identifying datasets of particular interest and facilitates their visualization.

1.2.2. Dataset_Review (Section 20)



The *Dataset_Review* subsystem displays the results of a selected study as a dot-and-bar chart, along with the reference value and selected summary statistics.

1.2.3. Dataset_NMI|DI (Section 21)

The *Dataset_NMI|DI* subsystem can filter data used to estimate the reproducibility precision associated with a specified {WG, Base unit}.

1.2.4. Dataset_AnalyteFilter (Section 22)

The *Dataset_AnalyteFilter* subsystem is used to filter data by a specified analyte or groups of analytes.

1.2.5. TimeTrial (Section 23)

The *TimeTrial* benchmarking tool explores the integrity of (much of) the *CCQM_Retrospectoscope*'s VBA code and benchmarks its clock-time performance on whatever Windows or Macintosh computer that is being used.

1.2.6. Database_FindNew (Section 24)

The *Database_FindNew* worksheet provides a set of stand-alone tools for identifying new or changed information on KCs, SCs, and PSs contained in summary files downloadable from the BIPM's web-system.

1.2.7. Database_Checkup (Section 25)

The *Database_Checkup* subsystem checks the consistency of the datasheets and documents in detail the number of datasets having selected attributes.

1.3. ReadMe: Licensing and Contact Information (Section 27)

The *Readme* worksheet lists the NIST software license statement and disclaimer, contact information, and where the CCQM_Retrospectoscope documentation lives.

1.4. Datasets

The *CCQM_Retrospectoscope* system contains as complete and up to date a collection of results from CCQM studies as the Senior Author has had the time and wit to assemble. Each dataset contains the results reported by the study's participants for one measurand, a unique title which provides a description of the measurand, and (when provided) a reference value and its associated expanded uncertainty as agreed to by the study's sponsoring body.

Many studies provide results for multiple measurands. The title for all datasets derived from a given study contains the study's designation. See Section 26.2 for database format details.

There are two types of datasets: single-study and multiple-study. Single-study datasets contain results from one study. The *CCQM_Retrospectoscope* analyses only use single-study datasets. Multiple-study datasets contain results from two or more studies, with results adjusted to have a common scale. These datasets enable consolidated display of results from related studies but are not otherwise used (see Section 26.4).

1.4.1. Study Types

The CIPM MRA recognizes three types of measurement comparison: Key Comparisons (KCs), Supplementary Comparisons (SCs), and pilot studies (PSs).

When sponsored by one of the CIPM's Consultative Committees or by the BIPM, KCs "test the principal techniques and methods in the field" and when sponsored by one of the Regional Metrology Organizations (RMOs) they "extend the coverage of CIPM key comparisons regionally" [6]. Since there are relatively few national measurement standards for chemical and biological measurands, KCs for these measurands actually test the measurement capabilities of the participants. Results from completed KCs are (eventually) published with full attribution in the key comparison database (KCDB) [7].

SCs are intended to "meet needs not covered by key comparisons" [6]. As of this document's publication date, all CCQM SCs have been sponsored by RMOs, typically addressing measurement issues of importance to the smaller and less experienced NMI|DIs within the

RMO's geographical region of responsibility. Like KCs, results from completed SCs are published in the KCDB with full attribution.

PSs "establish measurement parameters for a 'new' field or instrument, or as a training exercise" [6]. Unlike KCs and SCs, results from PSs need not be made publicly available. The results from some PSs have been disclosed only to the study's participants. However, with the agreement of all participants (and the sponsoring body) results can be published. There is no standard format for published PSs; the information disclosed ranges from text-only summaries to complete and fully attributed tabular results.

KCs are coded as type "K" in both the KCDB and *CCQM_Retrospectoscope*; likewise SCs are coded as type "S". All PSs are assigned the code "P" when initiated but in the *CCQM_Retrospectoscope* the "P" code is used only for unpublished PSs. Results from published PS are coded "Q" and are referred to as "published pilot studies" (PPSs). Results from unpublished PS are *CCQM-Confidential* and are not included in the public version of the *CCQM_Retrospectoscope*.

Note: The term "subsequent comparison" is sometimes used for a CCQM study that addresses the same measurement challenge as an earlier KC, typically to enable one or more of the participants in the earlier KC to demonstrate improved measurement performance. Such subsequent comparisons are KCs, not SCs.

1.4.2. Sponsoring Bodies

Not all the world's NMI|DIs participate directly in CCQM studies, which are typically reserved for the more experienced NMI|DIs of the larger economies. RMOs are responsible for supporting the NMI|DIs of the economies within their regions with KCs, SCs, and PSs. The geographic regions covered by the five RMOs that have sponsored studies present in the CCQM_Retrospectoscope database are pictured in Fig. 1.

Fig. 1. Geographic Areas of Metrological Responsibility.

Image courtesy of Victor Korniyenko, Creative Commons Attribution-Share Alike 3.0 Unported license
https://commons.wikimedia.org/wiki/File:Regional_metrological_organizations.jpg

Table **1** lists the number of datasets and studies in the CCQM_Retrospectoscope database as of this document's publication date, itemized by the sponsoring body.

Table 1. Number of Datasets and Studies Attributable to Different Sponsoring Bodies.

		Number of Datasets					Number of Studies				
Body	Code	KC	SC	PPS	PS	Total	KC	SC	PPS	PS	Total
AFRIMETS	AFQM	2				2	1				1
APMP	APQM	21	53	6	11	91	13	21	1	3	38
BIPM [a]	BIQM	34				34	16				16
CCQM	CCQM	778		218	555	1551	226		69	175	470
COOMET	CoQM	18	14			32	8	6			14
EURAMET [b]	EUQM	13	88			101	8	13			21
SIM	SIQM	11	31			42	6	7			13
	Total	877	186	224	566	1853	278	47	70	178	573

a In addition to its administrative responsibilities, the BIPM conducts a "continuous" KC for atmospheric ozone that involves periodic comparison of participant ozone photometers with the BIPM's reference instrument.

b The direct successor to what was named EUROMET prior to 2007. Be aware that the KCDB regards these as separate organizations.

1.4.3. Working Groups

Within the CCQM, responsibilities for the diverse types of chemical and biological measurands are spread among various Working Groups (WGs). RMO Technical Committees (TCs) coordinate studies using the same division of responsibilities. The *CCQM_Retrospectoscope* system regards TCs as extensions of the WGs.

Table 2 lists the number of datasets and studies in the CCQM_Retrospectoscope database as of this document's publication date, itemized by WG.

Table 2. Number of Datasets and Studies Attributable to Different CCQM Working Groups.

Working Group		Number of Datasets					Number of Studies				
Responsibility	Code	KC	SC	PPS	PS [c]	Total	KC	SC	PPS	PS [c]	Total
Cell Analysis	CAWG			4	1	5			3	1	4
Electrochemical Analysis	EAWG	100	8	7	41	156	27	2	2	15	46
Gas Analysis	GAWG	359	129	72	7	567	99	30	21	4	154
Inorganic Analysis	IAWG	200	40	43	230	513	63	10	11	72	156
Isotopic Ratio	IRWG	15		31	13	59	5		4	4	13
Nucleic Acid	NAWG	8		10	58	76	4		2	19	25
Organic Analysis	OAWG	133	9	16	181	339	61	5	8	58	132
Protein Analysis	PAWG	9		21	19	49	5		9	4	18
Surface Analysis	SAWG	53		20	16	89	14		10	1	25
	Total	877	186	224	566	1853	278	47	70	178	573

Jointly coordinated studies are assigned to the most appropriate WG on the basis of the units used to report results; e.g., results from joint Inorganic Analysis Working Group (IAWG) and Electrochemical Analysis Working Group (EAWG) studies that were reported in units of mass fraction are assigned to the IAWG.

The Isotopic Ratio Working Group (IRWG) was split from the IAWG in 2018 and reported the results of its first official study in March 2020. However, the IAWG carried out a number of earlier studies that are now within the remit of the IRWG. For the purposes of this analysis system, these have been (retrospectively) assigned to the IRWG.

The Bioanalysis Working Group (BAWG) was the original WG devoted to biological measurements. It was transformed in 2015 into the Cell Analysis (CAWG), Nucleic Acid (NAWG), and Protein Analysis (PAWG) Working Groups. Many of the datasets (retrospectively) attributed to the CAWG, NAWG, and PAWG are from BAWG studies that addressed cell-, nucleotide-, or protein-related measurands.

1.4.4. Units and Base units

The GAWG, with responsibilities for measuring gases in a gas mixture, uniformly describes the results of its studies in terms of mole analyte per mole mixture (mole fraction, mol/mol). Likewise, the IAWG, with responsibilities for measuring elemental composition in solid and liquid matrices uniformly describes results in terms that either are or can be readily converted to mass analyte per mass matrix (mass fraction, g/g). However, other WGs have responsibilities in several measurement domains; e.g., the EAWG supports measurements of pH (pH), conductivity (S/m and S/S), and purity of primary calibrators (g/g). Since these measurement areas differ qualitatively, datasets within a WG are grouped by the "Base unit" of the measurand.

A Base unit is the unit of measure stripped of prefixes: M, d, c, m, µ, n, p, and f. With apologies to the General Conference on Weights and Measures (CGPM), the keepers of the Système international d'unités (SI), "g" is therefore used rather than "kg" as the Base unit of mass. There are also measurement results that cannot be expressed in SI units: pH, number of nucleotide base pairs (bp), the isotopic delta scale (‰), effective fluorescence (EFF), and practical salinity (PSU). There are also a few PS and PPS datasets, mostly representing qualitative method comparison studies, which use "arbitrary unit" (a.u.) as a placeholder Base unit.

Where practical, results published in units of molality (mol/kg) have been transformed into mass fraction (g/g) through division by the molecular mass of the analyte (without worrying about the uncertainty in that mass). Likewise, results for dilute analytes in water reported in units of amount-of-substance concentration (mol/L) have been transformed to g/g assuming 1 L = 1000 g (again without worrying about the uncertainty ln that mass).

1.4.5. Sample Matrix Types

The sample materials evaluated in most CCQM studies can be broadly classified as having simple or complex matrices. The *CCQM_Retrospectoscope* system identifies datasets that report results for analytes in a relatively complex sample matrix as "Complex" datasets and those in a relatively simple matrix as "simple" datasets.

Table 3 lists the number of datasets and studies in the CCQM_Retrospectoscope database this document's publication date, itemized by the sponsoring body and sample matrix type.

Table 3. Number of Dataset Sample Types Evaluated by CCQM Working Groups.

		Number of Datasets			Number of Studies		
Responsibility	Code	Simple	Complex	Total	Simple	Complex	Total
Cell Analysis	CAWG	5		5	4		4
Electrochemical Analysis	EAWG	141	15	156	44	2	46
Gas Analysis	GAWG	296	271	567	122	32	154
Inorganic Analysis	IAWG	116	397	513	50	106	156
Isotopic Ratio	IRWG	15	44	59	4	9	13
Nucleic Acid	NAWG	39	37	76	11	14	25
Organic Analysis	OAWG	65	274	339	35	97	132
Protein Analysis	PAWG	7	42	49	7	11	18
Surface Analysis	SAWG	35	54	89	12	13	25
	Total	719	1134	1853	289	284	573

What constitutes a "relatively simple matrix" varies by WG and is somewhat subjective. It is most straightforward in the IAWG and Organic Analysis Work Group (OAWG) when "simple" samples are titled as calibration solutions or pure materials and "Complex" samples are (relatively) "natural" inorganic or organic materials. Few if any of the Gas Analysis Working Group (GAWG) samples are truly real-world complex mixtures. Most are mixtures of one or two targeted analytes in a non-reactive balance gas (typically nitrogen) or (relatively) non-reactive "synthetic air"; these have been classified as Simple. However, natural-like mixtures of multiple analytes, such as synthetic "natural gas" or "auto exhaust", have been classified as Complex. Virtually all the EAWG samples are aqueous solutions of simple salts and so are classified as Simple, with only a few studies in (synthetic) sea water classified as Complex.

Note: That a dataset that has been classified as Simple because the sample matrix is "relatively simple" does **not** imply that the measurement processes used to produce the results were **not** difficult or challenging.

1.4.6. Analytes

Each dataset consists of measurement results for a specified chemical or physicochemical name (analyte) and sample matrix. While the International Vocabulary of Metrology (VIM) [8] defines "the quantity intended to be measured" as the "measurand" and goes on to note that "In chemistry, 'analyte', or the name of a substance or compound, are terms sometimes used for 'measurand'. This usage is erroneous because these terms do not refer to quantities." However, *CCQM_Retrospectoscope* cheerfully ignores this distinction since it works by mashing together results for different analytes in different sample matrices. All datasets identified with the same analyte name are regarded as if they addressed the same measurand.

Different chemical traditions sometimes use different names for the same chemical entity; multiple names are particularly common for organic compounds. The Senior Author has attempted to standardize the names according to his own tradition.

1.4.7. Usable Datasets

A "usable dataset" has a numeric reference uncertainty and reports values from a single study rather than a composite of values from multiple related studies, typically a CCQM KC and one or more derivative RMO KCs. Table 4 lists the number of single-study and multiple-study datasets in the database as of this document's publication date. Multiple-study datasets are not used in any of the *CCQM_Retrospectoscope* analyses, other than for viewing using the *Dataset_Review* subsystem (Section 20).

Table 4. Number of Datasets Held in the Datasheets.

	Number of Datasets		
Datasheet	Single	Multiple	Total
CCQM_KC	911	112	1023
CCQM_Pilot	563	4	567
CCQM_PubPilot	221		221
CCQM_Ozone	34	2	36
CCQM_KC_Beta	6		6
Total	1735	118	1853

Table 5 lists the number of usable datasets in the database as of this document's publication date, itemized by the Base unit and WG. In addition to 116 composite datasets, there is one dataset for which no meaningful reference uncertainty can be assigned.

Table 5. Base Units and Associated Dataset Numbers.

		Number of Usable Datasets									
Measurement	Base unit	CAWG	EAWG	GAWG	IAWG	IRWG	NAWG	OAWG	PAWG	SAWG	Total
Mass fraction	g/g				489			325	45	2	861
Mole fraction	mol/mol			477		4		10		4	495
pH	pH		94								94
Entity fraction	n/n					32	34				66
Entity concentration	n/L	2		10			21				33
Conductivity	S/m		29								29
Length	m									27	27
Isotopic δ-scale	‰ (per mille)					18					18
Arbitrary units	a.u.									16	16
Specific adsorption	mol/g									14	14
Conductivity ratio	S/S		14								14
Charge concentration	C/L			10							10
Base pair "size"	bp						9				9
Mass concentration	g/L						5				5
Specific surface area	m^2/g									4	4
Specific pore volume	cm^3/g									3	3
Relative molecular mass	g/mol					3					3
Effective fluorescence	EFF	1									1
Practical salinity	PSU		1								1
	Total	3	138	497	489	57	69	335	45	70	1703

1.5. Participating Organizations

The *Datacore_Codes* worksheet provides a complete list of the current code used for every (identified) participant in a CCQM study along with known variants. This worksheet must be curated "by hand" when a new organization participates in a CCQM study or when the code used in a report differs from the current *CCQM_Retrospectoscope* standard.

The *Dataset_NMI|DI* worksheet lists the organizations that have participated in the various {WG, Base unit} studies. For each organization in each {WG, Base unit}, the worksheet provides the initial and most recent measurement year of their participation and the number of their datasets of the four study types (KC, SC, PPS, and PS). Table 6 lists the number of participants in each {WG, Base unit} and study type as of this document's publication date.

Table 6. Number of Participants in {WG, Base unit} Studies.

	NMI|DIs				Other Organizations			
{WG, Base unit}	KC	SC	PPS	PS	KC	SC	PPS	PS
{CAWG,EFF}			9					
{CAWG,n/L}			9					
{EAWG,pH}	36		21	27			1	5
{EAWG,PSU}				13				9
{EAWG,S/m}	24	10		24				2
{EAWG,S/S}				14				5
{GAWG,C/L}	8							
{GAWG,mol/mol}	48	41	33	16	1[a]		7	1
{GAWG,n/L}	8							
{IAWG,g/g}	55	50	31	65	1[a]		18	87
{IRWG,‰}	8		6	16			14	4
{IRWG,g/mol}	7		8	8				
{IRWG,mol/mol}	7							
{IRWG,n/n}	9		6				9	
{NAWG,bp}				8				
{NAWG,g/L}	9			17				
{NAWG,n/L}				22				3
{NAWG,n/n}	15		14	22				1
{OAWG,g/g}	47	30	18	42		1[a]	4	25
{OAWG,mol/mol}				12				
{PAWG,g/g}	14		20	10			1	
{PAWG,mol/g}								
{SAWG,a.u.}				6				3
{SAWG,cm³/g}	6		1					
{SAWG,g/g}	5		5					
{SAWG,m}	12		14				1	
{SAWG,m²/g}	6		1					
{SAWG,mol/g}	6		1					
{SAWG,mol/mol}	8							
{CAWG,EFF}			9					
{CAWG,n/L}			9					

a Non-NMI|DIs have occasionally participated unofficially in KCs or SCs. The results from these participants are not used in any summary calculation; they are kept in the *CCQM_Retrospectoscope* datasets for historical completeness.

1.5.1. NMI|DIs

The code names used to designate NMI|DIs are (generally) those most recently used by the NMI|DI. These codes are updated as necessary when new studies are added to the datasheets. However, in the interests in brevity some codes are modified; e.g., Turkey's TÜBITAK Ulusal Metroloji Enstitüsü (TÜBITAK UME) is coded UME.

Results from institutions that once participated independently but have been incorporated into larger entity have been recoded; e.g., results reported from Japan's National Institute of Advanced Industrial Science and Technology (AIST) are now assigned to the National Metrology Institute of Japan (NMIJ) and results from Russia's Ural'skiy Nauchno-Issledovatel'skiy Institute Metrologii (UNIIM) are assigned to D. I. Mendeleev Institute for Metrology (VNIIM).

1.5.2. International Organizations

Measurement laboratories associated with several international organizations are official participants in selected studies and for the purposes of the *CCQM_Retrospectoscope* are considered to be NMI|DIs. These laboratories include the International Atomic Energy Agency (IAEA) for selected inorganic measurands, World Meteorology Organization (WMO) designees for atmospheric gases, and the BIPM for organic purity.

1.5.3. University and Industrial Participants

While participation in CCQM KCs and SCs is restricted to NMI|DIs, a number of university and commercial laboratories participate in pilot studies. Some of these pilot studies have been published with full attribution of all participants. Very occasionally a non-NMI|DI has been an "unofficial" participant in a KC or SC. While results from such participants are not used to assign reference values, their results have been included in the *CCQM_Retrospectoscope*'s datasets.

University participant codes have the prefix "u|", commercial codes have the prefix "z|".

1.6. Measurement Years

The (approximate) year assigned to a dataset is (generally) the year of the "results must be reported by" date given in the study's report. However, many reports for early CCQM studies did not provide this information. When dates were not explicitly provided or could not be inferred from the reports, they have been assigned based on information provided in the KCDB.

A complete list of CCQM studies and their measurement dates is maintained in the *Datacore_Dates* worksheet. This worksheet must be curated "by hand" when reports for new studies are added to the database.

1.7. Summary Statistics for Characterizing Distributions

Given the typically small number of results in CCQM datasets, the *CCQM_Retrospectoscope* summarizes sets of values assuming that at least the majority of the values can be usefully described as following a "normal" $\mathrm{N}(\hat{\mu}, \hat{\sigma})$ distribution, where $\hat{\mu}$ and $\hat{\sigma}$ are robust estimates of the "true" location (mean) and scale (standard deviation) of the distribution.

1.7.1. Median as a Robust Estimate of Location

The median is a widely used robust (fairly insensitive to atypical values) estimator of the central location of unimodal distributions that is reasonably statistically efficient (provides values close to the true value when applied to truly normally distributed values) [9]. It is calculated as the middle value of the set of values. The median has a breakdown point (that is, it ceases to provide a useful estimate) when the proportion of atypical values exceeds 50 %.

Results summarized using the median estimator are designated in the *CCQM_Retrospectoscope* system as $\mathrm{Median}\{x\}$, where x is the symbol for a representative value.

1.7.2. Q_n as a Robust Estimate of Scale

The Q_n is a robust and efficient estimator of scale for unimodal distributions [10]. Q_n is the name assigned by its developer. It is calculated from the first quartile (smallest 25 %) of the absolute pairwise differences between values, scaled by a function of the number of values being summarized. The Q_n has been proposed as the most generally useful scale estimator for characterizing interlaboratory precision studies [11].

While the standard deviation is extremely sensitive to atypical values (it has a breakdown point of 0 %, potentially ceasing to provide a meaningful summary when there is even one atypical value), the Q_n has the same 50 % breakdown point as the median. The Q_n shares this robust breakdown with the more commonly encountered "adjusted median absolute deviation from the median" ($\mathrm{MAD_E}$) estimator but is considerably more efficient, 88 % compared to the $\mathrm{MAD_E}$'s 37 % [12].

Results summarized using the Q_n estimator are designated in the *CCQM_Retrospectoscope* system as $Q_n\{x\}$, where x is the symbol for a representative value.

1.8. Performance Metrics

The *CCQM_Retrospectoscope* system uses a number of participant performance metrics.

1.8.1. Measurement Bias

The bias of the result reported by the i^{th} NMI|DI in a dataset is calculated as the difference between the NMI|DI's result, x_i, and the dataset's reference value, x_{ref}, normalized in different ways to enable comparison across datasets. These bias metrics are:

- $z_i = (x_i - x_{ref})/u_i$, where u_i is the standard uncertainty associated with x_i. This is a form of a "z-score" [13].
- $|z_i| = |x_i - x_{ref}|/u_i$, the absolute value of z_i.
- $\zeta_i = (x_i - x_{ref})/\sqrt{u_i^2 + u_{ref}^2}$, where u_{ref} is the standard uncertainty associated with x_{ref}. The u_{ref} is estimated as one-half of the reference value's U_{95} expanded uncertainty. This is a form of ζ (zeta)-score [13].
- $|\zeta_i| = |x_i - x_{ref}|/\sqrt{u_i^2 + u_{ref}^2}$, the absolute value of ζ_i.
- $D_i = 100(x_i - x_{ref})/x_{ref}$, the percent difference, sometimes designated $D_{\%}$ [13].
- $|D_i| = 100|x_i - x_{ref}|/x_{ref}$, the absolute value D_i.

Both the signed and absolute values of these metrics are provided since the sign of the difference (greater than or less than x_{ref}) may-or-may-not be of interest for a given analysis.

The z_i and $|z_i|$ metrics report the bias between a participant's result and the reference value in units of the participant's standard uncertainty. When the reference value is "exactly" known (e.g., established by gravimetric preparation rather than consensus estimation), accurately determined x_i values should be within about 2 u_i units of x_{ref} about 95 % of the time.

The ζ_i and $|\zeta_i|$ metrics report the bias between the participant's result and the reference value in units of the root-mean-square error (RMSE) of the participant's standard uncertainty and that of the reference value. Since this combined standard uncertainty is always larger than u_i, the values of the ζ_i and $|\zeta_i|$ metrics will always be smaller (i.e., closer to x_{ref}) than the analogous z_i and $|z_i|$ values. Whether these more forgiving scores are realistic depends upon how u_{ref} was estimated. CCQM policy (and politics) aside, accurate x_i values are expected to be within the interval $x_{ref} \pm 2(u^2_i + u^2_{ref})^{½}$ about 95 % of the time.

A ζ_i is equivalent to the "unilateral degree of equivalence (DoE)" when there is no correlation between x_i and x_{ref}. This correlation arises when x_{ref} is estimated by consensus. The impact of the correlation decreases as the number of results used to estimate x_{ref} increases. Many of the CCQM studies that estimated x_{ref} by consensus have not properly included correlation in their published DoE estimates.

The D_i and $|D_i|$ metrics are independent of the reported uncertainties and report in units of percent difference from x_{ref}. These metrics are most appropriate for studies that do not collect measurement uncertainty information – or the uncertainty information that is collected is not trustworthy. Whether the latter situation is applicable to CCQM studies is a matter of some debate. In any case, the metrics provide objective estimation of the average percent relative standard deviation (CV).

The six metrics as used in the *Lab_History* subsystem (see Section 1.8.1) are illustrated in Fig. 2. The ≈ 10% of values above or below the dotted red lines are labelled as "outsiders" to facilitate review of the more interesting/disturbing datasets.

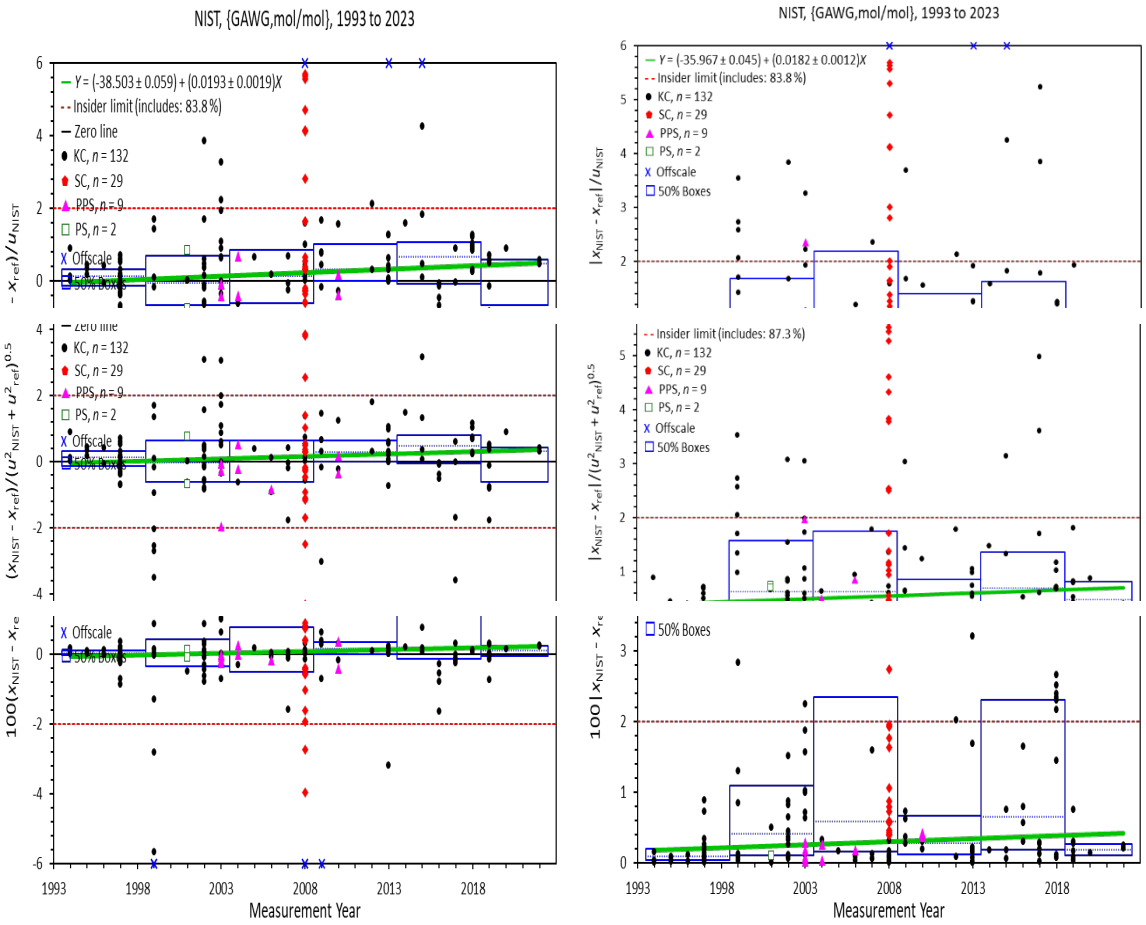


Fig. 2. Comparison of Bias Metrics for the NIST GAWG Data.

Note: Exercise judgement, caution (and compassion) when interpreting PS and PPS results. Since most PSs have been designed to address measurement problems, compare techniques, or assess community capabilities rather than access the capabilities of individual participants, reference values were (by policy) not reported for many PS datasets. Only relatively recently have x_{ref} and u_{ref} begun to be included in the PS reports provided by study coordinators.

To enable use within some of the CCQM_Retrospectoscope subsystems, reference-less datasets have been assigned x_{ref} as the median value of all accepted results and u_{ref} assigned as their Q_n divided by the square-root of the number of valid results. PS results typically vary considerably among participants, rendering unproductive the use of more complex and/or uncertainty-using estimators.

1.8.2. Relative Uncertainties

Bias metrics have two components, 1) the difference between the laboratory's result and the reference value and 2) the normalization factor used to enable comparison across studies. For the z- and ζ-based metrics, the normalization factor is either the participant's u_i or a composite that incorporates the participant's u_i. If the u_i is too small, then (for a given difference from x_{ref}) the value provided by the bias metric will be too large.

Unfortunately, there is no way of determining whether u_i has been correctly estimated that is independent of $(x_i - x_{ref})$. However, a given u_i divided by the median of the standard uncertainties associated with all of the technically valid x_i in the dataset, Median$\{u_{set}\}$, is a convenient indicator of whether, relative to the co-participants, participant i under-or-overestimated u_i: $u_{rel,i} = u_i/\text{Median}\{u_{set}\}$.

Uncertainties that are small relative to those of the co-participants will have $u_{rel,i}$ less than one; those that are large will have $u_{rel,i}$ greater than one. A small $u_{rel,i}$ that is associated with a very large (absolute) or "outsider" bias estimate suggests that the u_i was not evaluated correctly. A large $u_{rel,i}$ associated with an outsider suggests that the x_i is significantly inaccurate. A large $u_{rel,i}$ associated with an x_i that is very close to zero suggests that the u_i is overestimated.

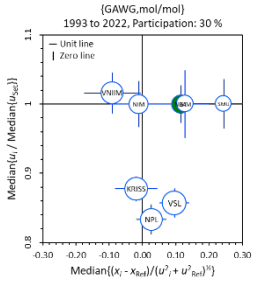
1.8.3. Bilateral Agreement

While having the form of a ζ-score, the metrics used to characterize the normalized differences between the i^{th} and the j^{th} participants in a study estimate the relative agreement between the participants rather than to the dataset RV:

- $\zeta_{ij} = (x_i - x_j)/\sqrt{u_i^2 + u_j^2}$
- $|\zeta_{ij}| = |x_i - x_j|/\sqrt{u_i^2 + u_j^2}$, the absolute value of ζ_{ij}.

The relative uncertainty of interest for this metric is the ratio of the two uncertainties: $u_{rel,ii} = u_i/u_j$.

1.8.4. {Bias, Uncertainty Ratio} Distance



Three "Peer" analysis systems summarize estimates of relative uncertainty as functions of relative bias for NMI|DIs that meet given participation criteria. It is convenient to quantify the distance of each pair of {bias, uncertainty ratio} estimates to their reference values. Since the bias of a reference value to itself is zero and the ratio of the reference uncertainty to itself is 1, the origin for plots of these values is {0,1}.

Since the bias metrics are scaled by uncertainty values, the metrics are not independent. This complicates defining a scale-independent distance. However, range-scaling by the length of the X- and Y-axes used in the graphical analysis provides a practical definition:

$$\Delta_i = \sqrt{\left(\frac{X_i - 0}{X_{max} - X_{min}}\right)^2 + \left(\frac{Y_i - 1}{Y_{max} - Y_{min}}\right)^2}$$

where X_i is the bias of the i^{th} NMI|DI, Y_i is the uncertainty ratio, X_{min} and X_{max} are the minimum and maximum of the X-axis used to display the data, and Y_{min} and Y_{max} are the minimum and maximum of the Y-axis used to display the data. The smaller this distance, the more similar the NMI|DI's results are to the reference {bias, uncertainty ratio} values.

This definition represents the Cartesian plane distance between a {bias, uncertainty ratio} value and the {0, 1} origin as it could be measured with a ruler. As long as the same X- and Y-axis limits are used, comparisons between distance estimates are valid. However, modifying the scale of either or both axes may change the Δ_i values.

The Δ_i values for the NMI|DIs shown in the chart are provided in the "Dist" column of the tables to the right-hand side of the chart.

1.8.5. Trend Analysis

For fairly consistent sets of $\{x_i, y_i\}$ data and assuming that (1) the uncertainties in the x_i are small relative to those of the y_i and (2) the uncertainties in the y_i are all about the same magnitude, linear trends of Y as a function of X

$$Y = \beta_0 + \beta_1 X$$

can be parameterized using classical least squares regression. The values of the β coefficients are those that minimize the root-mean-squared-error (RMSE) between the observed and predicted Y values. The "standard error" of the parameters, $u(\beta_0)$ and $u(\beta_1)$, express the uncertainty in the estimated value of their coefficient at about a 68 % level of confidence.

The power-law evaluations in the *Lab_Uncertainty* and *WG_Precision* subsystems are accomplished using classical least-squares regression as implemented in Excel's LINEST function. The {log(concentration), log(uncertainty) or log(reproducibility)} data used typically have few extreme "outsiders" and classical regression appears to work well.

Since classical regression is sensitive to extreme values, evaluating trends in data that has a high proportion of apparent "outsider" values (e.g., the bias and relative uncertainty Y values in *Lab_History* and *Lab_Bias*) requires use of robust techniques. The *CCQM_Retrospectoscope* uses the robust non-parametric Theil-Sen estimator [14,15] to visualize plausible linear trends except when both the independent and dependent variables are on logarithmic scales. Whether the data are appropriately characterized as showing a linear trend is, of course, for the user to determine.

The Theil-Sen slope parameter, β_1, is estimated as the Median$\{(y_j - y_i)/(x_j - x_i)\}$ for all data pairs where x_j differs from x_i. The intercept, β_0, is estimated as the Median$\{y_i - \beta_1 x_i\}$. The $u(\beta_1)$ is estimated as the MAD_E of the $(y_j - y_i)/(x_j - x_i)$; $u(\beta_0)$ is estimated as the MAD_E of the $y_i - \beta_1 x_i$.

1.8.5.1. Prediction Equations

While the *CCQM_Retrospectoscope* system characterizes linear trends with intercept and slope parameters, the form of the equation used to predict Y values using those two parameters depends on whether they are applied to logarithmically transformed X and/or Y values. The equations used to predict Y values in their native (untransformed) form are as follows.

- If both X and Y were untransformed:

$$Y = (\beta_0 \pm u(\beta_0)) + (\beta_1 \pm u(\beta_1))X\,.$$

- If $\log_{10}(X)$ is the independent variable (plotted along a scattergram X-axis) and Y is untransformed:

$$Y = (\beta_0 \pm u(\beta_0)) + (\beta_1 \pm u(\beta_1))\log_{10}(X)\,.$$

- If $\log_{10}(Y)$ is the dependent variable (plotted along a scattergram Y-axis) and X is untransformed:

$$\log_{10}(Y) = (\beta_0 \pm u(\beta_0)) + (\beta_1 \pm u(\beta_1))X$$
$$Y = 10^{(\beta_0 \pm u(\beta_0)) + (\beta_1 \pm u(\beta_1))X}.$$

- If $\log_{10}(X)$ is the independent variable and $\log_{10}(Y)$ is the dependent variable:

$$\log_{10}(Y) = (\beta_0 \pm u(\beta_0)) + (\beta_1 \pm u(\beta_1))\log_{10}(X)$$
$$Y = 10^{(\beta_0 \pm u(\beta_0))} X^{(\beta_1 \pm u(\beta_1))}$$
$$Y = (\beta_0' \pm u(\beta_0'))X^{(\beta_1 \pm u(\beta_1))}$$

  where $\beta_0' = 10^{\beta_0}$ and $u(\beta_0') \cong \frac{10^{\beta_0 \pm u(\beta_0)} - 10^{\beta_0 - u(\beta_0)}}{2}$.

  This "power function" defines a straight line in a scattergram with log-log axes.

The *CCQM_Retrospectoscope* system reports these equations with the $\beta_0 \pm u(\beta_0)$ and $\beta_1 \pm u(\beta_1)$ values rounded to two significant digits of the standard uncertainties.

1.8.5.2. Interpreting the Slope Parameter

The slope parameters (β_1) in the four equations are not directly comparable. Further, when the data are "noisy" enough to require use of a robust regression technique, the slope and intercept parameters and their standard uncertainties should be regarded with more than a pinch of salt. However, the sign of the slope, $+\beta_1$ or $-\beta_1$, is a good indicator of whether the Y increases or decreases, on average, with increasing X. An absolute value of the t-statistic

$$|t| = |\beta_1|/u(\beta_1)$$

greater than at least two suggests that the slope may be "significantly" different from zero with the significance level increasing as $|t|$ increases.

1.9. User-Specified Parameters

2	3	4	5	6
	Parameter	Use	Default	
	NMI|DI:	NIST	Auto	
	WG:	GAWG	Auto	
	Base unit:	mol/mol	Only value	
	Year from:	1993	User	
	Year to:	2023	User	

Several parameters used to select datasets require the user to specify a value from a sizable list (e.g., NMI|DI, WG, and Base units codes) or to specify a quantity value (e.g., measurement years, the minimum number of NMI|DI participant results for a dataset to be used, the minimum number or proportion of datasets required for an NMI|DI to be included in the analysis). Parameters used to control how graphics are displayed also require the user to specify quantities (e.g., axis minimum or maximum). The values used to define the parameters are located in the **Use** and **Default** columns. The Use values are displayed in red font.

1.9.1. When the Default Value is "Auto"

When the parameter value in the **Default** column is "Auto", the value of the parameter in the **Use** column is determined by *CCQM_Retrospectoscope*. These default values are set in different ways, ranging from parochial (e.g., NIST as target NM|DI), through arbitrary (e.g., GAWG as the WG) and best-guesses (e.g., minimum numbers of datasets required for analysis) to data-driven (e.g., the Base unit most frequently used in a WG's studies).

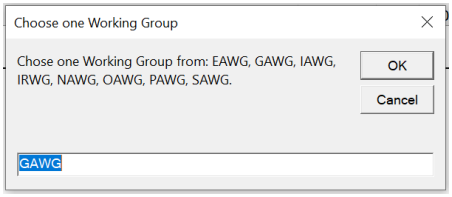
Warning: As long as the value in the **Default** column is "Auto", *the values used in the analysis are determined by the system regardless of whatever value is originally in the* **Use** *column.*

1.9.2. When the Default Value is *not* "Auto"

For a user-supplied value not to be over-written by the system default, the Auto codeword must be replaced by "User" or some other value. The value that is ultimately assigned to the parameter depends upon the contents of the **Use** and **Default** columns and the values that have been assigned to other parameters.

1.9.2.1. When There is No Valid Default Value

If there is a valid **Use** value, the **Default** will be set to "User" and the **Use** value will be… used.



For alphanumeric lists (e.g., WG), if there is no **Use** value or the **Use** value is not a recognized member of the list, the user is asked to choose one element from the list. If no element is selected (by clicking the **Cancel** button rather than the **OK** button), an informative message is issued, and the subsystem stops.

For numeric parameters (e.g., Year from), if the **Use** value is a valid number (a numeric value between the smallest and largest acceptable values), the **Default** will be set to "User" and the **Use** value will be… used. If there is no **Use** value or the **Use** value isn't a valid number, The **Default** will be set to "Auto" and the **Use** value replaced with the system default.

Note: What constitutes "the smallest and largest acceptable values" depends on context. For "Year from", the earliest date is 1993, the year of the first CCQM study; the latest is five years before the current date. For "Year to", the earliest date is five years after whatever was specified for "Year From" to the current calendar year. Percentages are constrained to be between 0 and 100; values without intrinsic boundaries are in general constrained by what the Senior Author considers to be the smallest and largest "reasonable" values. **Use** values that are smaller than the smallest reasonable value are set to the smallest reasonable value; values larger than the largest reasonable value are set to the largest reasonable value; in both circumstances the **Default** is set to "Auto".

1.9.2.2. When the Default Value is Valid or "User"

If there is a valid **Use** value, the **Default** will be left alone, and the **Use** value will be… used. If the **Use** value is not valid, the **Use** value will be set to the **Default**.

1.9.3. When There Is Only One Valid Value

The sizes of the NMI|DI and WG lists are fixed – the number of items in each list does not depend upon the value assigned to other parameters. However, the size of the Base unit list depends on the value assigned to the WG parameter. For WGs with datasets that are always reported in the same Base unit (e.g., the GAWG datasets are always recorded in mol/mol), the Base unit list consists of a single item. In such cases, the **Use** value is set to that single item and the **Default** is set to "Only value". Only for WGs that report measurements with different Base units (e.g., EAWG datasets are reported in pH, S/m, or S/S) will the contents of the **Use** and **Default** columns be used to assign the Base unit parameter.

1.10. Datasheets

The *CCQM_Retrospectoscope* datasets are stored in several worksheets, the name of each beginning "CCQM_". Three datasheets contain finalized results extracted from reports that are publicly available.

- *CCQM_KC*, datasets from KCs and SCs that have been reviewed and approved by the CIPM and published in the KCDB.
- *CCQM_PubPilot*, datasets from PPSs that have been journal-published or otherwise made public. Most PPSs have been published in the journal Metrologia, although several are documented in the report of a parallel or successor KC.
- *CCQM_Ozone*, datasets from the QM.BIPM-K1 bilateral comparisons of ozone photometers with a reference instrument maintained at the BIPM. Unlike all other CCQM studies, this is a continuous process with some NMI|DIs (such as NIST) participating many times. In addition to a composite dataset of results from each participant's most recent comparison, datasets consisting of all bilateral comparison performed during each year from 2007 to this document's publication date are provided to enable evaluation of performance over time.

Two worksheets contain results from preliminary reports of KCs and SCs. The datasets contained in these datasheets are *CCQM Confidential*.

- *CCQM_KC_Beta*, datasets from KCs and SCs that are not yet published but for which a "Draft B" report is available. The results in Draft B reports have been reviewed by the WG, but issues regarding how the reference value and its uncertainties should be evaluated may remain. Datasets within this worksheet are promoted, after suitable review, to the *CCQM_KC* when the Final report becomes available.
- *CCQM_KC_Alpha*, datasets from KCs and SCs that are not yet published but for which a "Draft A" report is available. The results in Draft A reports have been reviewed by the participants but have not been fully interpreted by the WG. Results from assessments of outsider results may not be included and reference values are not assigned. Datasets within this worksheet are promoted, after suitable review, to the *CCQM_KC_Beta* worksheet when a Draft B report becomes available.

One worksheet contains results from Pilot studies that have not been made publicly available. The datasets in this datasheet are *CCQM Confidential.*

- *CCQM_Pilot*, datasets from PSs that have not been made public. The datasets have been extracted from the most recent report issued by the coordinating WG (not always a "Final" or even "Draft B" document). Not all possible PS datasets are present in this worksheet since some available PS reports do not attribute results and others have not been made available outside of the WG that carried out the study.

Note: The *CCQM_KC_Beta, CCQM_KC_Alpha*, and *CCQM_Pilot* worksheets are available only in the master system maintained at NIST. These non-public datasets are excluded from the publicly accessible versions of the *CCQM_Retrospectoscope*.

2. In-Common Features

The *CCQM_Retrospectoscope* subsystems are each implemented in their own worksheet. Analyses are performed by interacting with a variety of controls and user-settable parameters. Many of the control features are shared among the worksheets.

2.1. Command Buttons

Command buttons are used to start specific programs written in Microsoft Virtual Basic for Applications (VBA); click them and the program that is associated with the button starts its work.

2.1.1. Load

Clicking the **Load** button produces a fresh evaluation of all the datasets stored in any of the workbook's CCQM datasheets. After completing the refresh, the charts on the worksheet are themselves refreshed using all the currently defined options. It is only necessary to invoke this command when one or more of the datasheets has been added to or otherwise modified, although invocation does no harm other than taking a bit of time.

2.1.2. Plot

Clicking the **Plot** button updates the charts to satisfy the current data-selection and chart element criteria.

2.1.3. Picture

Clicking the **Picture** button places a picture of the charts and information identifying outsider studies onto the clipboard. This picture can be placed wherever pasting from the clipboard is valid; however, the picture is not automatically saved within the *CCQM_Retrospectoscope* system.

2.1.4. Review

Clicking the **Review** button when a cell listing the code or title of dataset has been selected produces a dot-and-bar chart of that study's results in the *Dataset_Review* subsystem (see Section 20).

2.1.5. Locate

Clicking the **Locate** button when a cell listing one of the NMI|DIs has been selected highlights the location of that NMI|DI in one or more of the subsystem's charts. Unless a different cell has been selected, clicking the button a second time removes the highlight.

2.1.6. Back

Clicking the **Back** button causes the worksheet that invoked the active worksheet to become active.

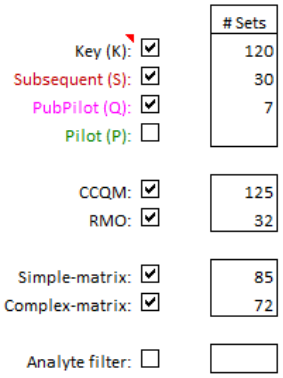
2.1.7. Restore

Clicking the **Restore** button, which is intentionally located below the others because it should seldom be needed, restores the location and size of all the subsystem's control and graphical elements. When the *CCQM_Retrospectoscope* (and Excel) are behaving themselves, a **Restore** *should* take only a few seconds.

2.2. Checkboxes

Checkboxes provide two functions: they 1) toggle between values of *True* (checkmark visible) and *False* (empty box) and 2) invoke a VBA program when clicked.

2.2.1. Dataset Selection Checkboxes



Nine checkboxes are used by many subsystems to specify what datasets are included in the analysis. These checkboxes control the study type (KC, KC, PPS, and PS; see Section 1.4.1), whether studies were conducted by the CCQM or an RMO (Section 1.4.2), whether the sample had a relatively simple or complex matrix (Section 1.4.5), and analytes (Section 1.4.6). The table to the right of the checkboxes lists the number of datasets displayed for each study type, conducting body, and type of sample. Due to subsystem-specific requirements, these numbers are not necessarily the same across the different subsystems.

In both the *Lab_Uncertainty* and *WG_Precision* worksheets, the colors of the symbols representing performance for the four study types is set by the color of the checkbox label, located to the immediate left of the checkbox. To change the color of the symbol used for a given study type, change the label's font color.

To avoid a series of one-at-a-time changes, except for "Analyte filter", clicking a dataset selection checkbox invokes worksheet recalculation rather than reanalysis. The *True*/*False* state of each of the boxes is queried when the **Plot** button is clicked.

2.2.2. Analyte filter Checkbox

Unlike the other dataset selection checkboxes, clicking the "Analyte filter" checkbox invokes the *Dataset_AnalyteFilter* subsystem which checks if the filter is compatible with the analysis subsystem's {WG, Base unit}. The confirmation notice generated if the current filter is appropriate is displayed in Fig. 3; the error message and prompt if the current filter is not appropriate is displayed in Fig. 4.

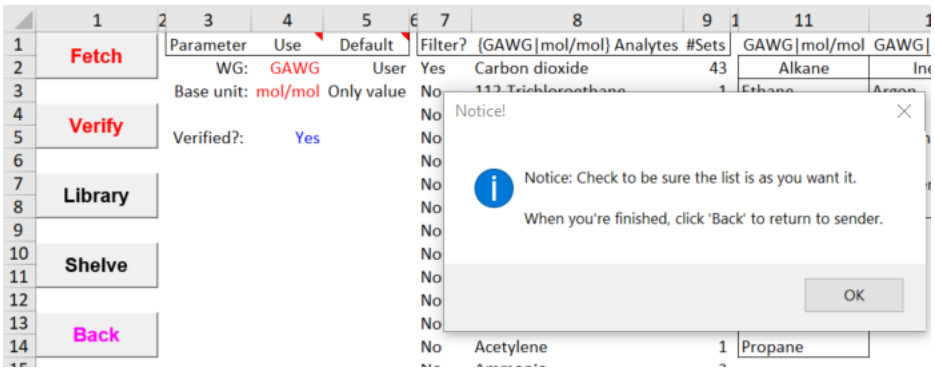


Fig. 3. *Dataset_AnalyteFilter* Confirmation Notice and Prompt.

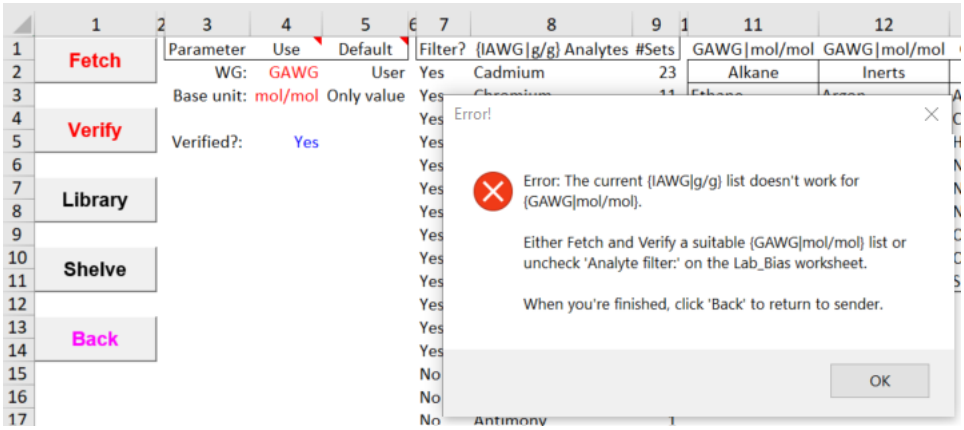


Fig. 4. *Dataset_AnalyteFilter* Error Message and Prompt.

In either case, clicking the **OK** button enables use of the *Dataset_AnalyteFilter* worksheet's controls. See Section 22 for detailed information about these controls if the filter needs to be modified or replaced. Otherwise, clicking the **Back** button returns the focus to the data analysis subsystem.

2.2.3. Chart Display Checkboxes

Legend: ☐
Title: ☐
Plot area box: ☐

All the graphic analysis subsystems provide a series of chart display checkbox controls that toggle on/off selected graphical elements. Many of these controls are used with most charts, including display of legends, chart titles, and the top and right-side plot-area boundary lines. Unlike the dataset selection checkboxes, clicking a chart display checkbox invokes an immediate change in the chart display.

2.2.3.1. Legend

Clicking the Legend checkbox toggles display of the chart legend. The legend is always placed at the top left corner of the chart area box.

2.2.3.2. Title

Clicking the title checkbox toggles display of the chart legend. The title is always placed above the area box of the main chart.

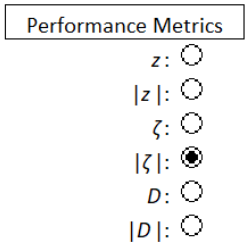
2.2.3.3. Plot area box

Clicking the title checkbox toggles display of the chart area box lines at top and right-hand side of the chart. The bottom and left-hand side lines are provided by the X- and Y-axes.

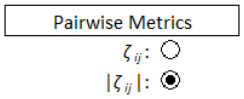
2.3. Radio Buttons

Radio buttons also provide two functions: they 1) allow a user to choose one of a predefined set of mutually exclusive options and 2) invoke a VBA program when clicked. As with the chart display checkboxes, clicking a radio button invokes an immediate change in the chart display.

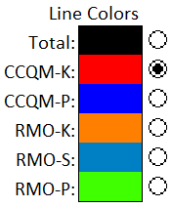
The *Lab_History*, *Lab_Bias*, *Peer_Unilateral*, and *Peer_Global* analysis subsystems use the same series of radio buttons for selecting one of six performance metrics (see Section 1.8.1). Changing the metric on one of these subsystems as no effect on the others.



The *Peer_Bilateral* subsystem uses ratio buttons to select between the two pairwise metrics (see Section 1.8.3).



The *Lab_Engagements* subsystem uses radio buttons to select the type of studies to be summarized.

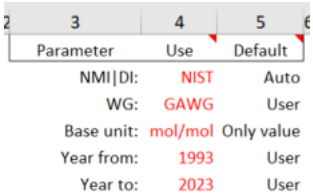


2.4. Parameters

Text-based parameters are used to specify the data to be analyzed and some chart display properties. None of the specifications are evaluated or acted upon until the **Plot** (or **Load)** button is clicked. Parameter values stated are in red font, with a short description to their left and a default to their right. See Section 1.8.5 for how parameter values can be modified.

2.4.1. Data Specification Parameters

The data analysis worksheets share a number of user-must-specify dataset selection parameters. These are always located in the first rows of the worksheet. The following are used in many of the subsystems.



2.4.1.1. NMI|DI: Target Institution

The value of this parameter specifies which NMI|DI is the target of the analysis. The codes accepted are those listed in the *Datacore_Codes* worksheet (see Section 25.4.4).

2.4.1.2. WG: Working Group

The value of this parameter specifies which WG's datasets are evaluated. Some data are currently available from the EAWG, GAWG, IAWG, IRWG, NAWG, OAWG, and SAWG (see Section 1.4.3); however, most datasets are from studies conducted by the EAWG, GAWG, IAWG, and OAWG.

2.4.1.3. Base unit: Basic Unit of Measurement

The value of this parameter defines the basic unit of measurement for a dataset to be included in the analysis (see Section 1.4.4). This is mostly important for studies conducted by the EAWG since they support three qualitatively different measurement systems: pH, conductivity, and the purity of primary calibrators. The default Base units are the units used in the majority of the WG's studies.

2.4.1.4. Year from and Year to: Measurement Dates

The values of these two parameters define the span of measurement years for datasets to be included in the analysis. The default values for the Year from and Year to parameters are the measurement years of the earliest and most recent studies conducted by the specified WG. The minimum interval between the two values is five years.

Since the participants in any given study do not all make their measurements at the same time nor necessarily within the same calendar year, the dataset's "measurement year" is defined by the study's final "on time" submission date (see Section 1.6).

2.4.2. Chart Display Parameters

The charts in the various subsystems are associated with user-modifiable parameters that help control the chart displays. Some parameters are used in only one subsystem while others are used in several subsystems. These are always located below the data selection checkboxes.

3. The Welcome Worksheet

When the *CCQM_Retrospectoscope* system is initialized, the *Welcome* worksheet is activated. All the analysis, database worksheets, and support functions provided by the system can be accessed from here. The controls used to access these functions are pictured in Fig. 5.

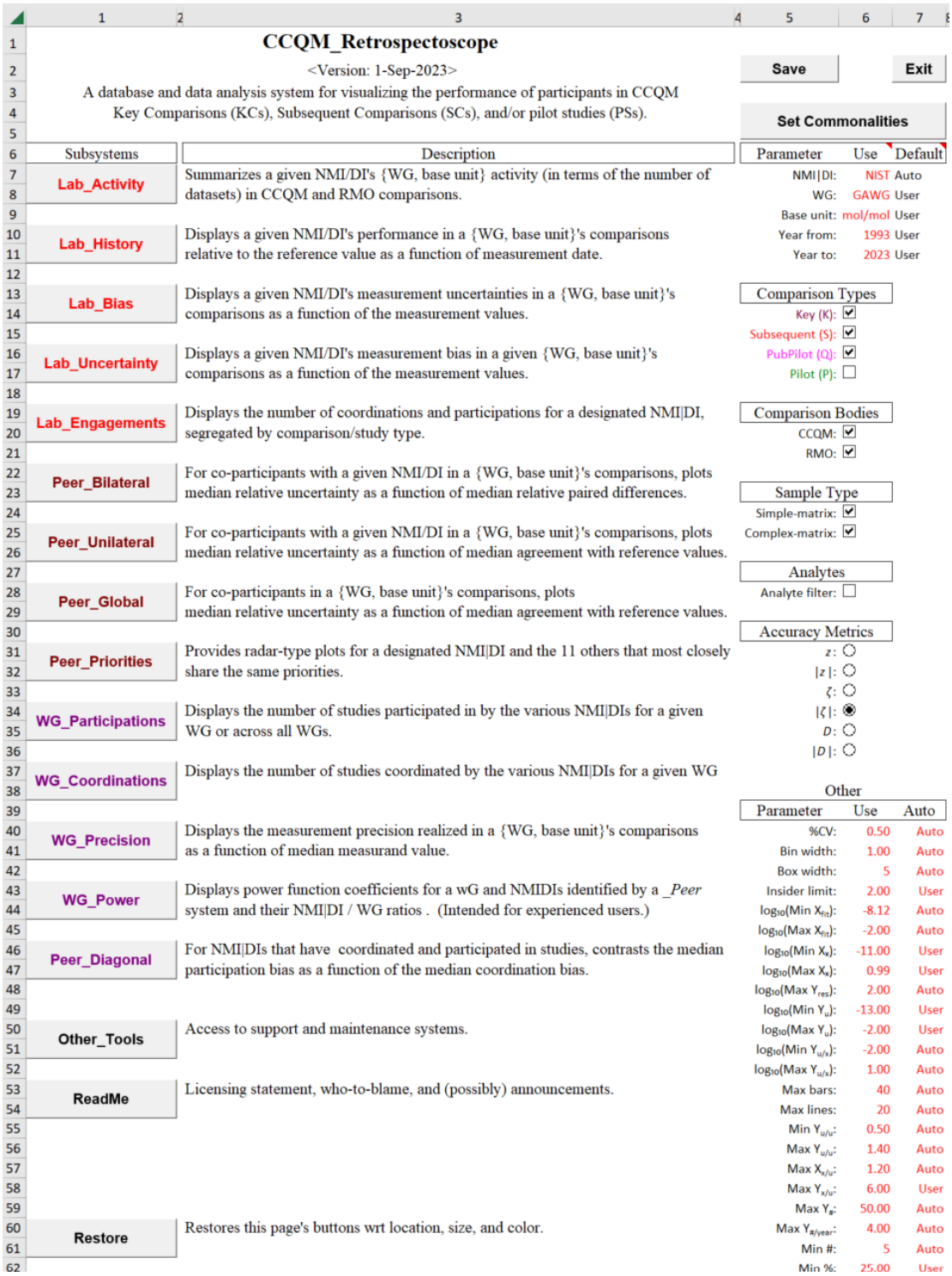


Fig. 5. The *Welcome* Dashboard.

3.1. Analysis Subsystems

Clicking the one of the buttons with a label prefix of **Lab_**, **Peer_**, or **WG_** activates the corresponding analysis worksheet. It does not initiate the analysis system implemented in that worksheet.

3.2. Other_Tools (Provides Access to Specialized Systems)

Clicking the **Other_Tools** button activates the *Other_Tools* worksheet, enabling access to several specialized or system-support subsystems. See Section 18 for details.

3.3. ReadMe

Clicking the **ReadMe** button activates the *ReadMe* worksheet which provides licensing and contact information.

3.4. Save and Exit

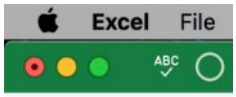
The **Save** and **Exit** buttons at the top right-hand corner of the worksheet are reminders that if any changes are to be saved, users need to do it for themselves. Users are **not** given the option of saving when the workbook is closed.

While convenient, these functions are supernumerary: the user can save the current state of the workbook at any time using Excel's *Save* or *Save As* File-tab options. There are also shortcut keys: <Ctrl+S> with Windows and <Command+S> with Macintosh. The workbook can be closed at any time (without saving) by:

- Windows – clicking the "×" at the far upper-right of the window or with <Ctrl+W>

or

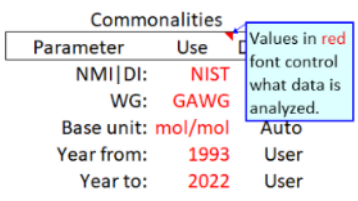
- Macintosh – clicking the red dot at the upper left of the window or with <Command+W>.

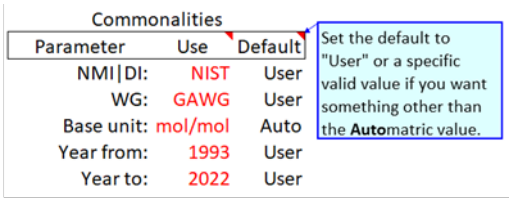


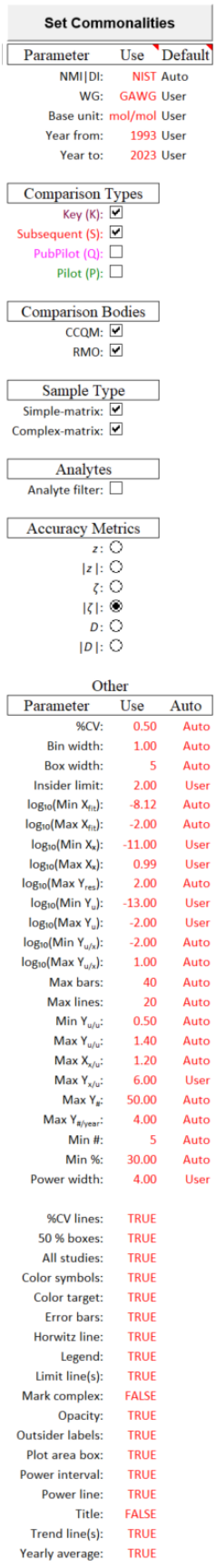
3.5. Set Commonalities

Clicking the **Set Commonalities** button transfers the settings of the parameters and controls listed in columns 6 and 7 of the *Welcome* worksheet to the appropriate analysis subsystems. Transferring the settings does not cause any reanalysis based on those settings. The user must explicitly invoke each desired analysis.

Note: Hovering the cursor over a red triangle in the top-right corner of a cell invokes a comment that is intended to remind the user what information is being requested. The "Use" and "Default" columns on this worksheet and other worksheets provide the following guidance.







4. Lab_Activity Subsystem

The *Lab_Activity* subsystem provides an overview of a given NMI|DI's CCQM activities, in terms of the number of datasets and the number of studies that the NMI|DI contributed to. The two pie charts, the controls used to specify the datasets evaluated, and the controls used to modify the displays are pictured in Fig. 6. The in-common data selection and chart display parameters and controls are discussed in Section 2.

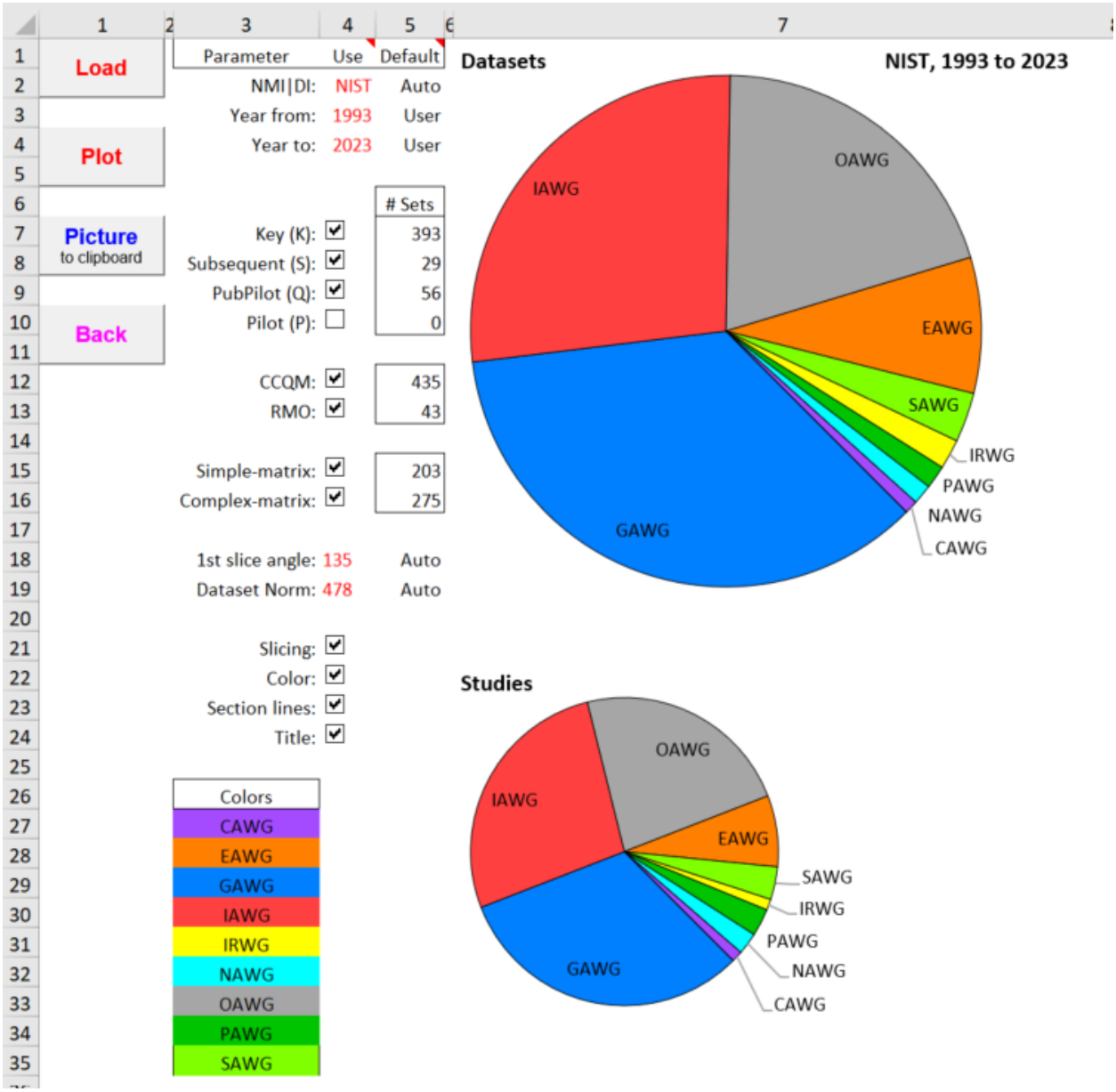


Fig. 6. The *Lab_Activity* Dashboard.

Reminder: A data selection or chart display parameter value listed under the "Use" heading can only be changed when its "Default" value is "User". See Section 1.9 for further information.

4.1. Charts

The worksheet's top chart (chart LA-1) displays the proportion of datasets in each of the various WG or {WG, Base unit} "pie slices" that contain a result provided by the NMI|DI.

The bottom chart (chart LA-2) displays the proportion of the total number of studies attributed to each group. The radius of chart LA-2 is proportional to the square-root of the ratio between the total number of studies and the total number of datasets.

The slices are ordered by decreasing numbers of datasets.

4.2. Chart Display Parameters

The *Lab_Activity* worksheet contains two chart display parameters. These values are not acted upon until the **Plot** button is clicked.

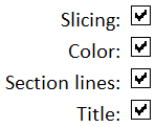
4.2.1. 1st slice angle: Set angle of First Pie Slice

The value of the "1st slice angle" parameter sets the angle where the first (largest proportion) begins. This is important only in that it determines the location of the labels for slices that are too thin to accommodate the {WG, Base unit} identifier inside the pie. The default value is 135 °, which generally puts the small-proportion labels in the white space to the bottom right of the pie. However, the "best fit" function that Excel uses sometimes does odd things.

4.2.2. Dataset Norm: Reduce chart Area

By default, the width of chart LA-1 (Dataset) is about 4.5 in. regardless of the number of datasets summarized. The areas of the LA-1 and LA-2 "pies" can't be increased; however, it is sometimes convenient to reduce them. Specifying a value of the "Dataset Norm" parameter that is larger than the number of datasets reduces the areas proportionally to the ratio between the (number of datasets) and the (Dataset Norm). Setting the norm to the largest number of datasets contributed by an NMI|DI withing a selected group of NMI|DIs can facilitate comparisons.

4.3. Additional Chart Display Checkboxes



The *Lab_Activity* worksheet contains three chart display checkboxes in addition to the *Title* checkbox described in Section 2.2.3.

4.3.1. Slicing

Clicking the "Slicing" checkbox toggles the pie charts between summarizing the datasets and studies by WG and by {WG, Base unit}. As displayed in Fig. 7, the identity of the slices can become difficult to discern when there are many {WG, Base unit} with relatively few datasets.

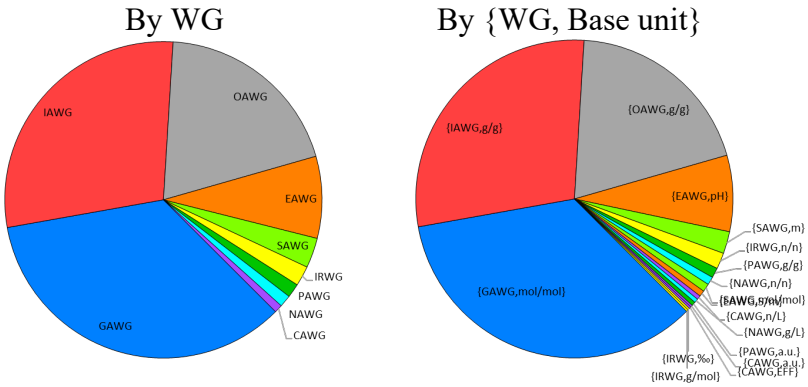


Fig. 7. *Lab_Activity* Chart LA-1 Summarized by WG and by {WG, Base unit}.

4.3.2. Color

Clicking the "Color" checkbox toggles the pie charts between colored slices and colorless slices (compare the first and third panels of **Fig. 8**). To ensure that every WG or {WG, Base unit} has the same color across NMI|DIs, the slice color for the WGs is defined in the strip of cells starting at row 27 of column 3. The slice colors can be changed by changing the highlight color of the cell and re-**Plot**ting.

4.3.3. Section Lines

Clicking the "Section lines" checkbox toggles a thin black line around each of the slices (compare the first and second panels of **Fig. 8**). The section lines are automatically turned on when the slice colors are turned off.

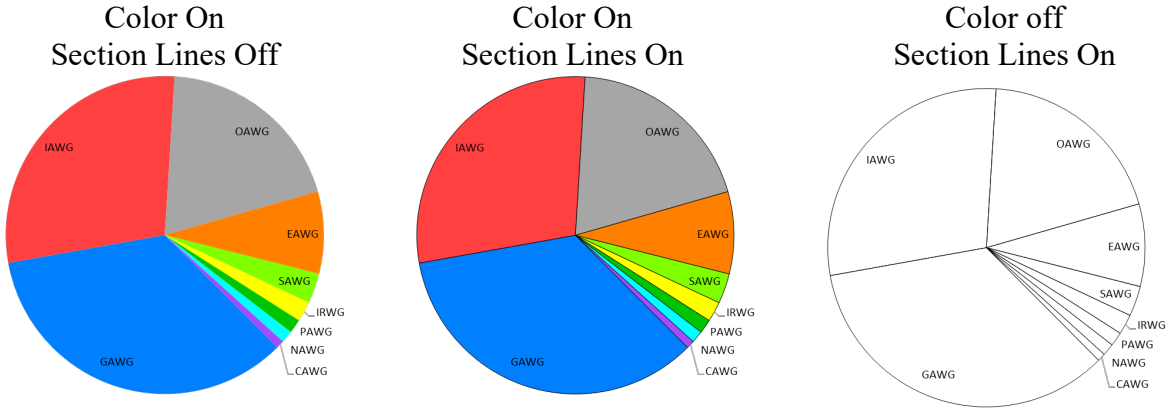


Fig. 8. *Lab_Activity* Chart LA-1 With Color and Section Line Variations.

4.4. Table

The table to the right of chart LA-1, shown in Fig. 9, provides the total number of datasets and studies for each WG groups. This "All" total is supplemented with the number of the datasets and studies that come from KCs, SCs, PPSs, and PSs as well as sponsored by the CCQM and by RMOs. In addition, the table lists a robust estimate of the over-all percent relative standard deviation (coefficient of variation, CV) and the range between the minimum and maximum value (Span) in slice, expressed logarithmically as $\log_{10}$(maximum/minimum - 1).

		Number Datasets									Number Studies									Properties	
Slicing By	All	KC	SC	PPS	PS	CCQM	RMO	Smpl	Cmplx	All	KC	SC	PPS	PS	CCQM	RMO	Smpl	Cmplx	CV	Span
GAWG	170	132	29	9	0	127	43	98	72	55	48	1	6	0	47	8	42	13	0.59	10.62
IAWG	141	115	0	26	0	141	0	34	107	47	41	0	6	0	47	0	16	31	0.82	10.16
OAWG	96	81	0	15	0	96	0	11	85	40	33	0	7	0	40	0	9	31	1.09	8.56
EAWG	41	40	0	1	0	41	0	41	0	13	12	0	1	0	13	0	13	0	0.02	3.30
SAWG	15	12	0	3	0	15	0	7	8	6	3	0	3	0	6	0	4	2	2.49	8.71
IRWG	10	8	0	2	0	10	0	4	6	3	1	0	2	0	3	0	0	3	0.02	
PAWG	7	1	0	6	0	7	0	3	4	5	1	0	4	0	5	0	3	2	1.81	9.07
NAWG	6	4	0	2	0	6	0	1	5	4	2	0	2	0	4	0	1	3	3.08	8.56
CAWG	4	0	0	4	0	4	0	4	0	2	0	0	2	0	2	0	2	0	0.00	

Fig. 9. The Dataset and Study Activity Table for NIST.

5. Lab_History Subsystem

The *Lab_History* chart, the controls used to specify the datasets evaluated, and the controls used to modify what the chart displays are pictured in Fig. 10. The in-common data selection, bias metrics, and chart display controls are discussed in Section 2.

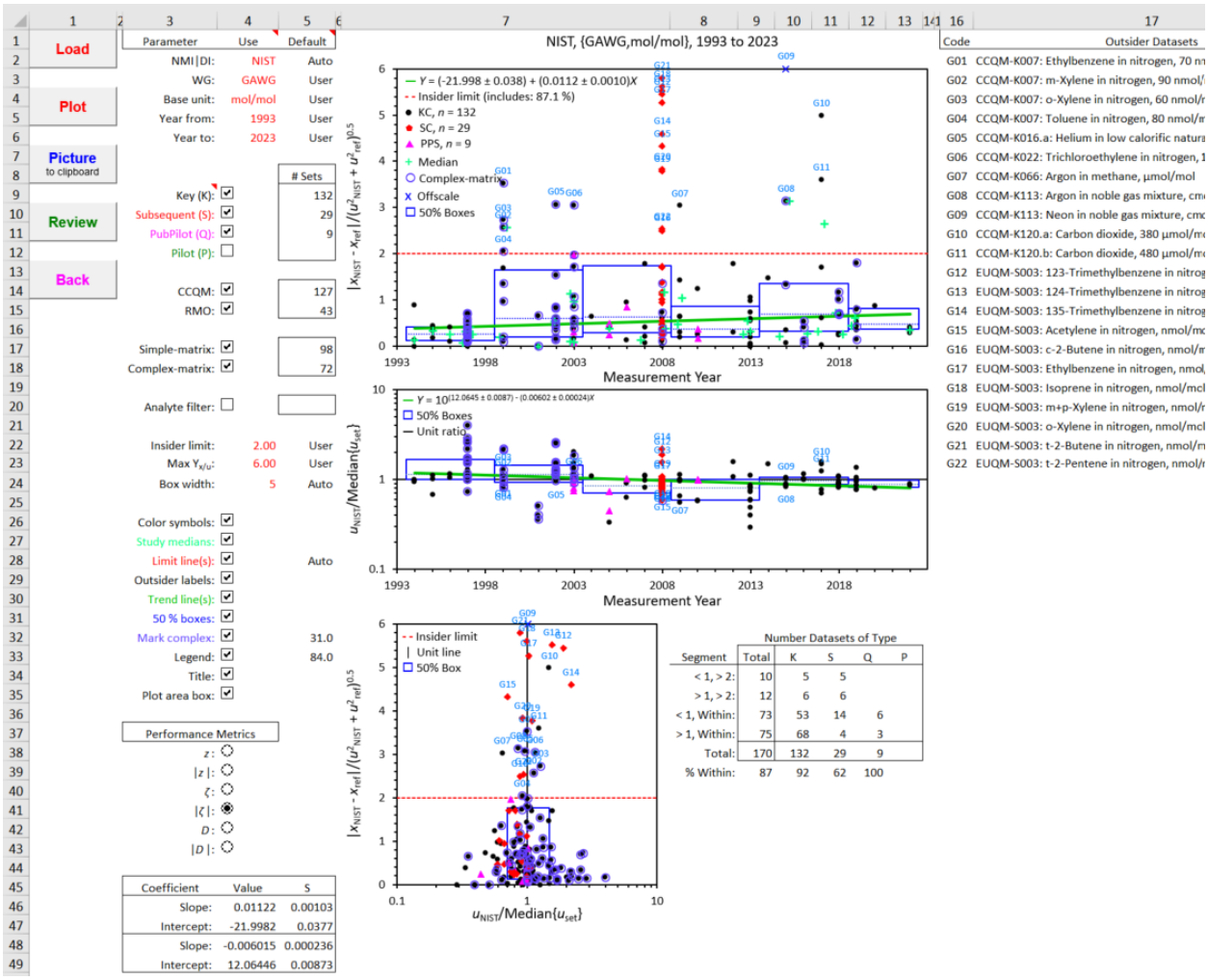


Fig. 10. The *Lab_History* Dashboard.

Reminder: A data selection or chart display parameter value listed under the "Use" heading can only be changed when its "Default" value is "User". See Section 1.9 for further information.

5.1. Charts

Each symbol in the worksheet's top chart (chart LH-1) represents the value of the active bias metric for the target NMI|DI in one dataset, plotted as a function of the study's measurement year. Likewise, each symbol in the center chart (chart LH-2) represents the target's relative uncertainty. The symbols in the bottom chart (chart LH-3) represent the values of the bias metric plotted as a function of the relative uncertainty.

Changing the bias metric does not affect the position of chart LH-2's symbols, but the datasets identified as outsiders will change to match the identifications established in chart LH-1. Since large and small u_i/median(u_{set}) ratios are of interest and ratios are seldom *very* large or *very* small, the chart's u_i/median(u_{set}) axis is logarithmic with a range from 0.1 to 10.

Chart LH-3 provides a direct visualization of the interaction between the two metrics, at the expense of losing the measurement date dependence. The table to the right of chart LH-3 lists the number of each type of study (Key, Supplementary, PubPilot, and Pilot) that fall within each segment of the chart, where the segments are defined by the unit-ratio and outsider limit lines. When one of the absolute value metrics is active, there are four segments; when a signed-value metric is active, there are six segments. When the value of a metric is outside the displayed range along a chart axis, the value is displayed as a "×" at the axis limit.

Versions of the *Lab_History* charts using absolute and signed bias metrics are displayed in Fig. 11.

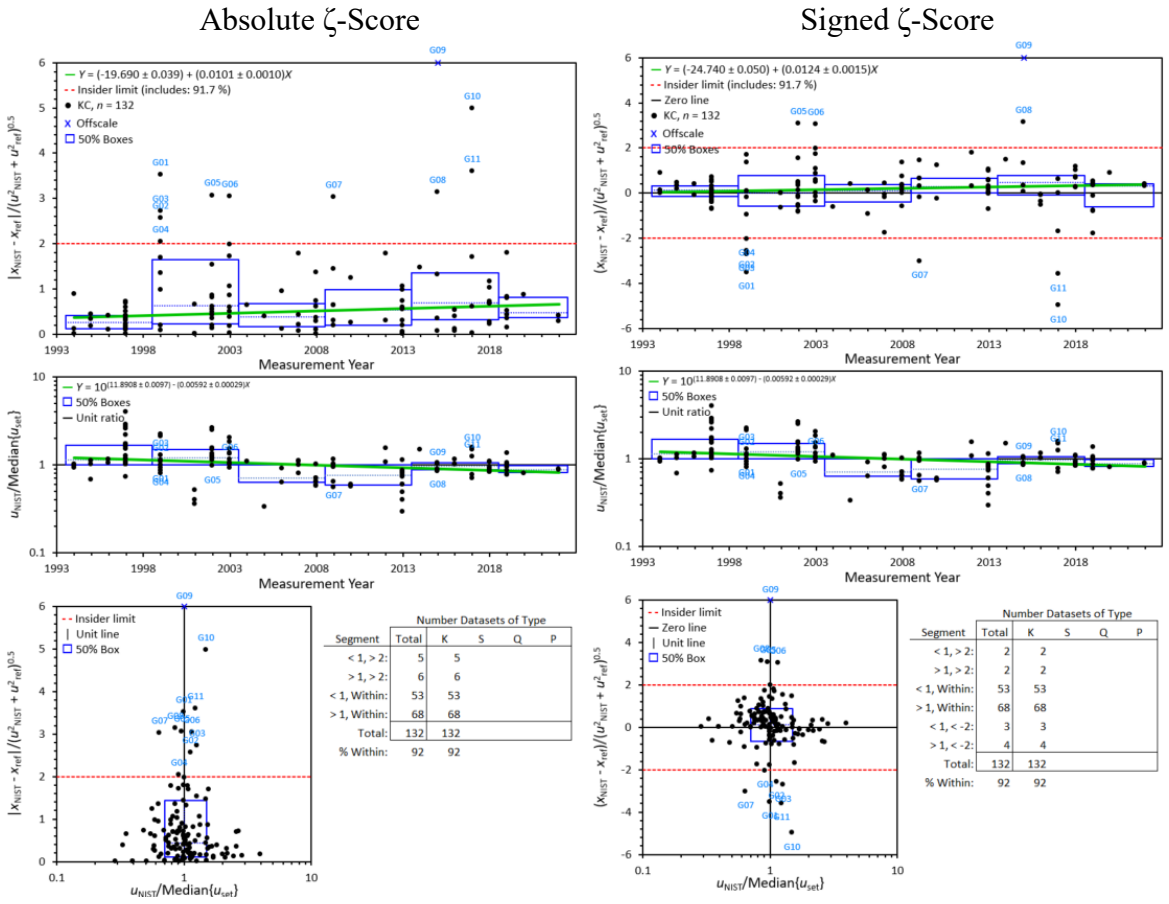
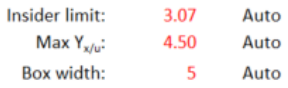


Fig. 11. The *Lab_History* Charts with Absolute and Signed Bias Metrics.

5.2. Chart Display Parameters



The *Lab_History* worksheet contains three chart display parameters. Changes to these values are not evaluated or implemented until the **Plot** button is clicked.

5.2.1. Insider limit: Outlier Identification Interval

The value of the "Insider limit" parameter determines the value of the bias metric that is used to identify outsider datasets. The default is the value that identifies about 10 % of the datasets. The value is represented in charts LH-1 and LH-3 of Fig. 11 as red dashed horizontal lines. If the absolute value of the selected bias metric exceeds this value, the result will be tagged as an outsider and the name of the study will be listed to the right of the charts (see Fig. 10).

5.2.2. Max $Y_{x/u}$: Y-axis Maximum for Charts LH-1 and LH-3

The value of the "Max $Y_{x/u}$" parameter sets the display range of the Y (bias)-axis of charts LH-1 and LH-3. Its default value includes at least 95 % of the datasets. When a signed metric is selected, the range is set to be symmetric about zero and, if necessary, the parameter value is rounded up to produce a symmetric distribution of tic-labels.

5.2.3. Box width: 50 % Box Width for Charts LH-1 and LH-2

The value of the "Box width" parameter sets the number of (contiguous) measurement years included in each segment of the optional "50 % boxes" element described in Section 5.3.6. The default interval is five years.

5.3. Additional Chart Display Checkboxes

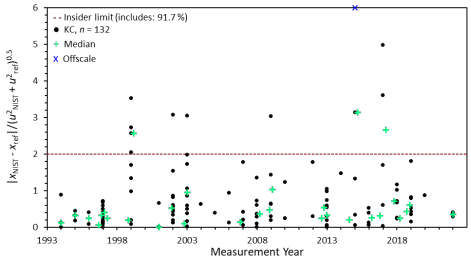
The *Lab_History* worksheet contains seven chart display checkboxes in addition to the three discussed in Section 2.2.3. Clicking a chart display checkbox invokes an immediate change in the chart display.

5.3.1. Color symbols

Clicking the "Color symbols" checkbox toggles the charts between the colored symbols displayed in Fig. 10 and the all-black symbols of Fig. 11. The colors used for the four study types is dictated by the font colors of the checkbox labels. When colored, KC results are solid circles, SC results are solid diamonds, PPS results are solid triangles, and PS results are open squares. When black, all symbols are solid circles.

5.3.2. Study medians

Since many studies evaluate more than one measurand, clicking the "Study medians" checkbox toggles a display of the median bias of the multi-measurand studies. These values are displayed as green "+"s. They are only displayed in chart LH-1.



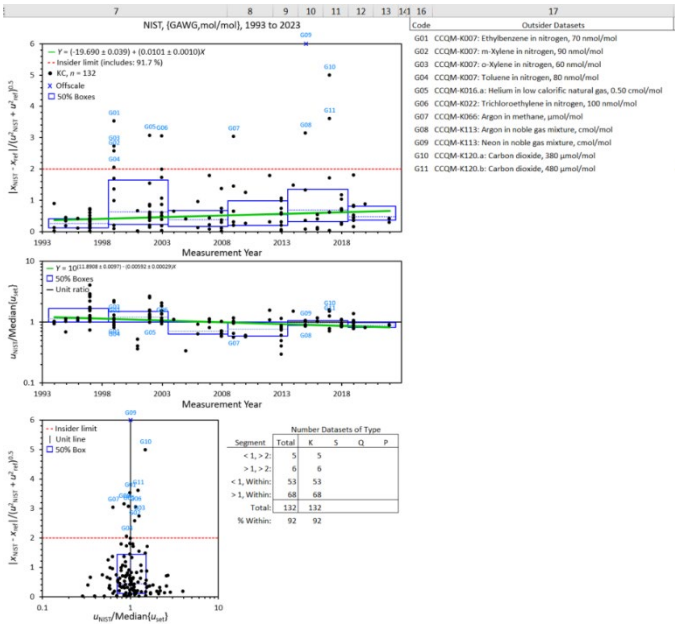
5.3.3. Limit line(s)

Clicking the "Limit line(s)" checkbox toggles the display of the red dashed horizontal "*Limit line(s)"* in charts LH-1 and LH-3 (see Fig. 11).

5.3.4. Outsider labels

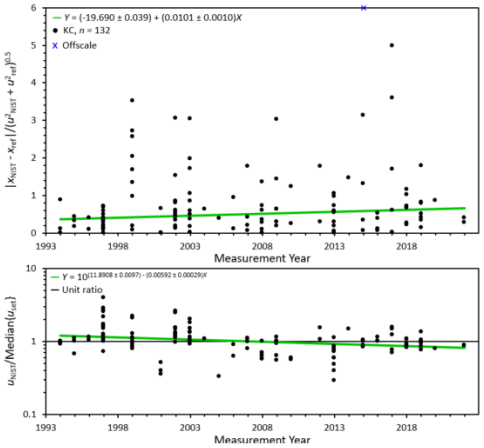
Clicking the "Outsider labels" checkbox toggles the display of codes used to identify the outsider datasets in all three of the charts.

The outsider datasets are identified in the table to the right of the charts. Selecting a cell containing either the code or the dataset name and clicking the **Review** button produces a dot-and-bar chart for that dataset (Section 20).



5.3.5. Trend line(s)

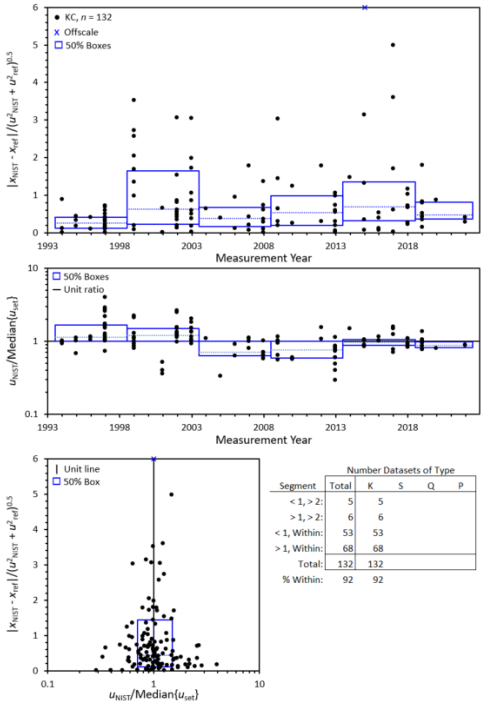
Clicking the "Trend lines" checkbox toggles the display of robust Thiel-Sen linear trend lines [14,15], $Y = \beta_0 + \beta_1 X$ (where X is the date in years and Y is the metric identified in the chart's Y-axis title), in the LH-1 and LH-2 charts.



5.3.6. 50 % boxes

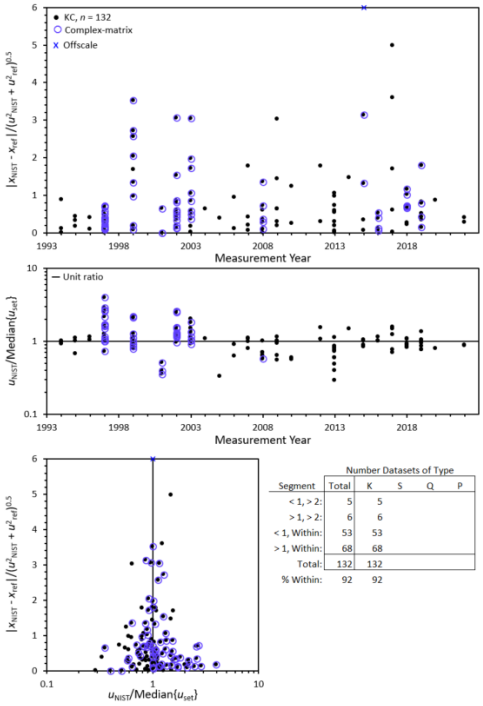
For charts LH-1 and LH-2, clicking the "50 % boxes" checkbox toggles the display of a series of 50 % boxes at intervals along the measurement year axis. Each box is bounded with solid blue lines. The width of each box is set by the "Year interval" parameter (Section 5.2.3). The top line represents the 75th percentile of all results within the interval, the bottom line the 25th percentile, and the dotted blue centerline represents the median (50th percentile).

In chart LH-3, the bottom and top lines mark the 14.6 % and 85.4 % percentiles of the data along the Y-axis while the left and right lines mark the 14.6 % and 85.4 % percentiles of the data along the X-axis. The joint probablilty of enclosure is $100(1-2*0.146)^2 = 50.1$ %, hence the resulting box should enclose the central 50% of the datasets. The central cross marks the median (50 % percentile) of both metrics.



5.3.7. Mark complex

Clicking the "Mark complex" checkbox toggles the identification of results for complex-matrix materials. This option is only relevant when simple-matrix and complex-matrix datasets are analyzed together. Complex-matrix datasets are identified with a surrounding blue circle.

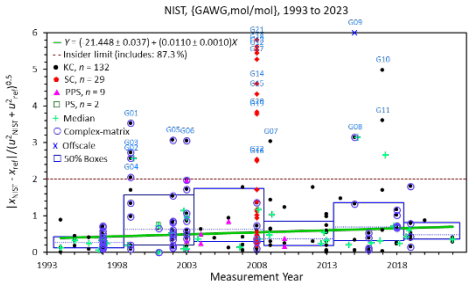


5.3.8. Legend entries

As described in Section 2.2.3.1, clicking the "Legend" checkbox toggles the display of the legend. The optional features have a legend entry when (and only when) active. In addition to identifying the graphical elements, some of the entries provide quantitative information.

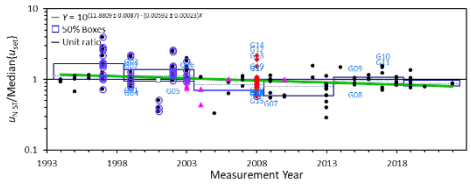
In chart LH-1:

- "Trend lines" states the linear trend of the selected bias metric over time.
- "Insider limit" states the percentage of results that are inside the Insider limit.
- If the symbols are shown colored, the number of each type of study is displayed.

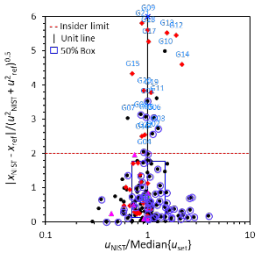


In chart LH-2:

- "Trend lines" states linear trend of the relative uncertainty over time as a multiplicative factor.



The legend for LH-3 provides only non-quantitative information.



6. Lab_Bias Subsystem

The *Lab_Bias* charts, the controls used to specify the datasets evaluated, and the controls used to modify what the chart displays are pictured in Fig. 12. The in-common data selection, bias metrics, and chart display controls are discussed in Section 2.

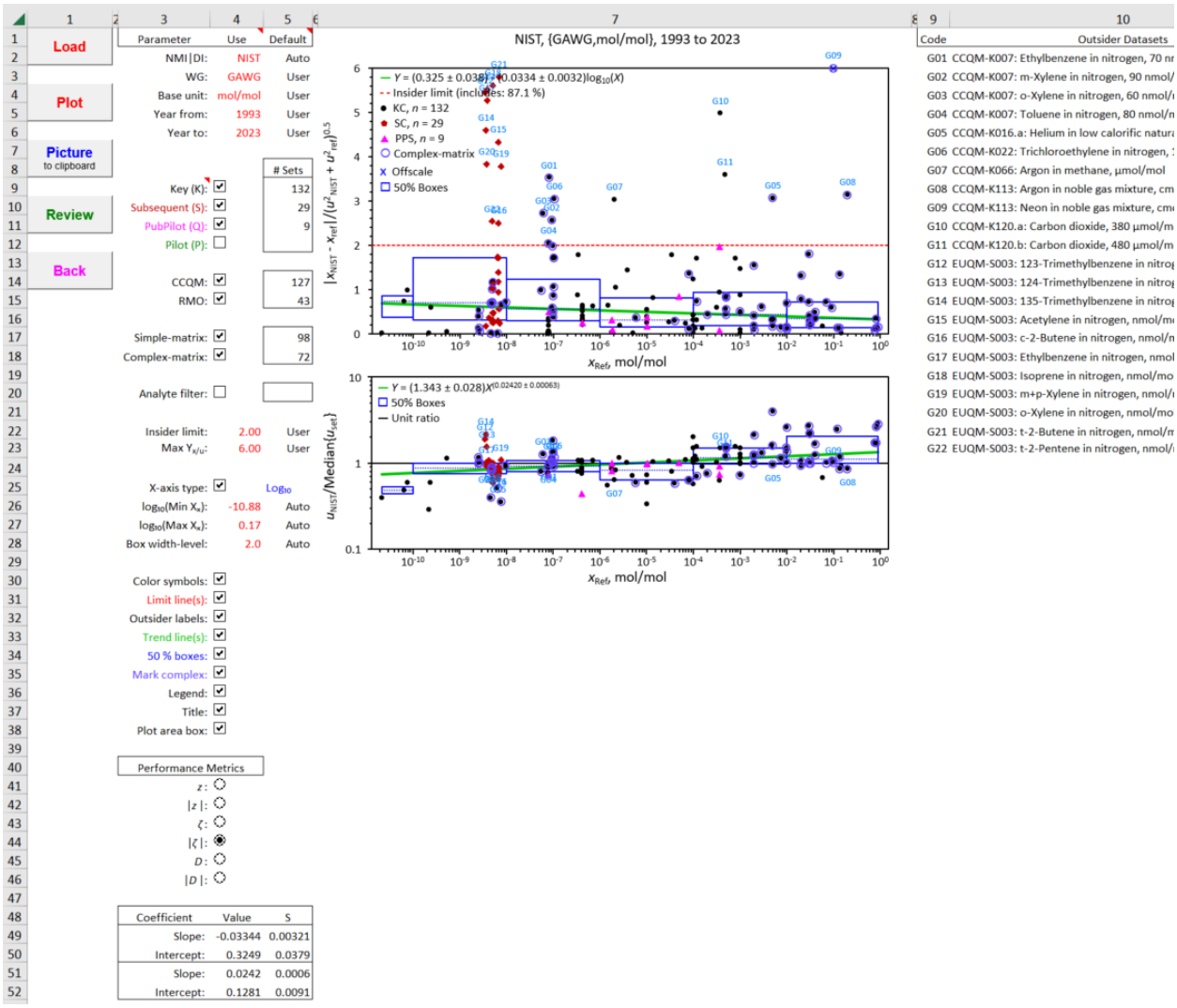


Fig. 12. The *Lab_Bias* Dashboard.

Reminder: A data selection or chart display parameter value listed under the "Use" heading can only be changed when its "Default" value is "User". See Section 1.9 for further information.

6.1. Chart

Each symbol in the worksheet's chart (chart LB-1) represents the value of the active bias metric for the target NMI|DI in one dataset, plotted as a function of the dataset's reference value.

When the value of a metric is outside the displayed range along a chart axis, the value is displayed as a "×" at the axis limit.

Versions of the signed- and absolute value bias metrics with the "50 % Boxes" and "Limit line(s)" activated are displayed in Fig. 13.

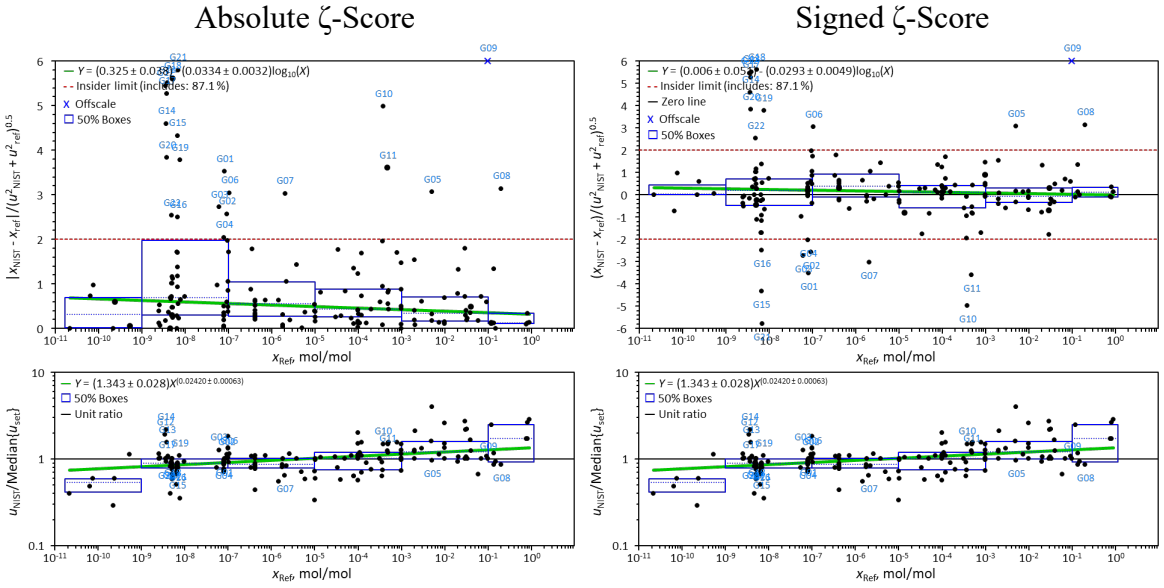


Fig. 13. The *Lab_Bias* Charts with Absolute and Signed Bias Metrics.

6.2. Chart Display Parameters: Y-Axis

Insider limit:	2.00	User
Max $Y_{x/u}$:	6.00	User

The *Lab_Bias* worksheet contains two chart display parameters that control the display of the Y-axis . Changes to these values are not evaluated or implemented until the **Plot** button is clicked.

6.2.1. Insider limit: Outlier Identification Interval

The value of the "Insider limit" parameter determines the value of the bias metric that is used to identify outsider datasets. The default is the value that identifies about 10 % of the datasets. The value is represented as red dashed horizontal lines. If the absolute value of the selected bias metric exceeds this value, the result will be tagged as an outsider and the dataset name will be listed to the right of the charts (see Fig. 12).

6.2.2. Max $Y_{x/u}$: Y-axis Maximum

The value of the "Max $Y_{x/u}$" parameter sets the display range of the Y (bias)-axis. Its default value includes at least 95 % of the datasets. When a signed metric is selected, the range is set to be symmetric about zero.

6.3. Chart Display Parameters: X-Axis type

The *Lab_Bias* worksheet contains a checkbox toggle and three chart display parameters related to the X-axis. When the "X-axis type" checkbox is checked, the chart's X-axis is $base_{10}$-logarithmic which facilitates evaluating results that span several orders-of-magnitude (e.g., mass and mole fraction). When the checkbox is unchecked, the chart's X-axis is linear which enables evaluation of negative-value results (e.g., isotopic δ-scales) and facilitates display of results that span only a narrow range (e.g., pH).

Clicking the checkbox resets the display parameters to their default values. Changes to these values do not affect the chart display until the **Plot** button is clicked.

6.3.1. Log_{10} Xaxis: X-axis Display Limits

When the checkbox is checked, the X-axis is $base_{10}$-logarithmic and the three chart display parameters require log_{10}-based values.

6.3.1.1. log10(Min X_x) and log10(Max X_x): X-axis Display Limits

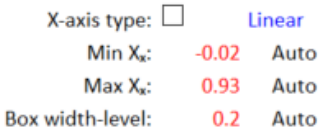
The values of the "log_{10}(Min X_x)" and "log_{10}(Max X_x)" parametes set the minimum and maximum limits for the $base_{10}$ logarithmic X-axis. The default values for these limits are the log_{10}-transformed minimum and maximum result values of the selected data. Modifying these limits does not affect what data are selected for analysis.

6.3.1.2. Box width: 50 % Box Width

The value of the "Box width" parameter sets the width of the 50 % boxes, specified in numbers of factors-of-10. Its default value is 2; that is, the default width of each 50 % box is two factors of 10: $10^2 = 100$. The value is constrained to be an integer within the range 1 to INT(log_{10}(Max X_x) - log_{10}(Min X_x))) + 1, where INT is the function "convert to integer".

6.3.2. Linear X-axis: X-axis Display Limits

When the checkbox is unchecked, the X-axis is linear and the three chart display parameters require linear values.



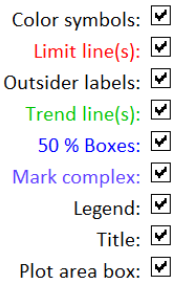
6.3.2.1. Min X_x and Max X_x: X-axis Display Limits

The values of the "Min X_x" and "Max X_x" parameters set the minimum and maximum limits for the linear X-axis. The default values for these limits are the minimum and maximum values of X_x among the selected data. Modifying these limits does not affect what data are selected for analysis.

6.3.2.2. Box width-level: 50 % Box Width

The value of the "Box width-level" parameter sets the width of the 50 % boxes, specified in the units of measurement. Its default value is one-fifth of the range X_x - X_x, rounded to one significant figure.

6.4. Additional Chart Display Checkboxes



The *Lab_Bias* worksheet contains six chart display checkboxes in addition to the three discussed in Section 2.2.3. Clicking a chart display checkbox invokes an immediate change in the chart display.

6.4.1. Color symbols

Clicking the "Color symbols" checkbox toggles the charts between the colored symbols displayed in Fig. 12 and the all-black symbols of Fig. 13. The colors used for the four study types is dictated by the font colors of the checkbox labels. When colored, KC results are solid circles, SC results are solid diamonds, PPS results are solid triangles, and PS results are open squares. When black, all symbols are solid circles.

6.4.2. Limit line(s)

Clicking the "Limit line(s)" checkbox toggles the display of the red dashed horizontal lines that represent the "Insider limit" parameter. When a signed metric is selected, there are horizontal lines across the chart at 0 ± Insider limit (see left-hand panel of Fig. 13). When an absolute metric is selected, there is only the one horizontal line at the Insider limit (see right-hand panel of Fig. 13).

6.4.3. Outsider labels

Clicking the "Outsider labels" checkbox toggles the display of codes used to identify the outsider datasets. Charts with and without the "Outsider labels" activated are displayed in Fig. 14.

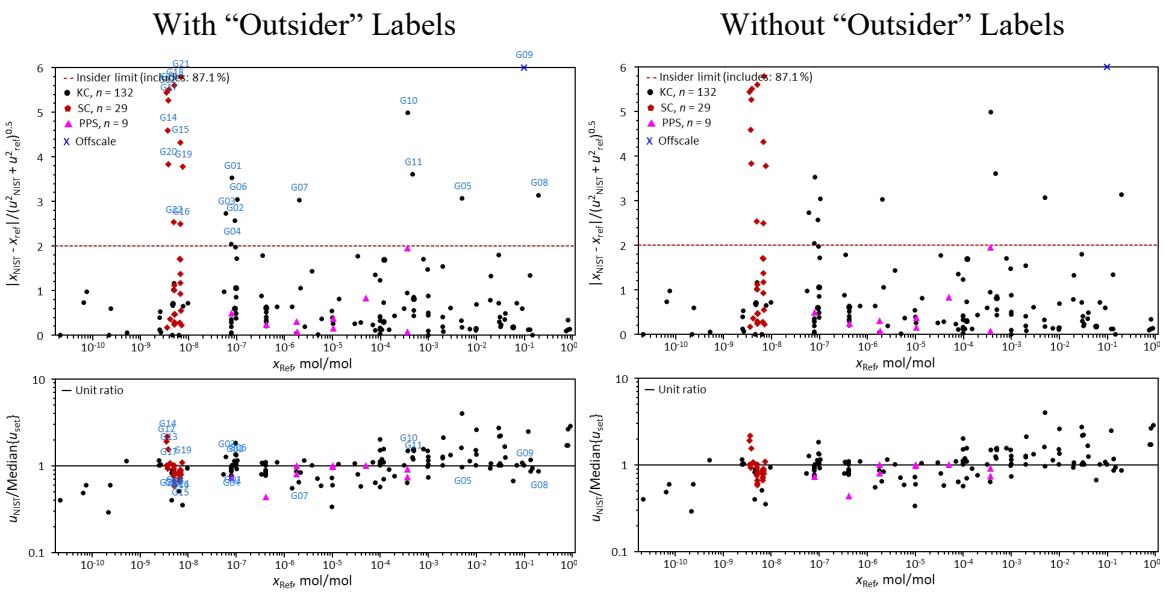
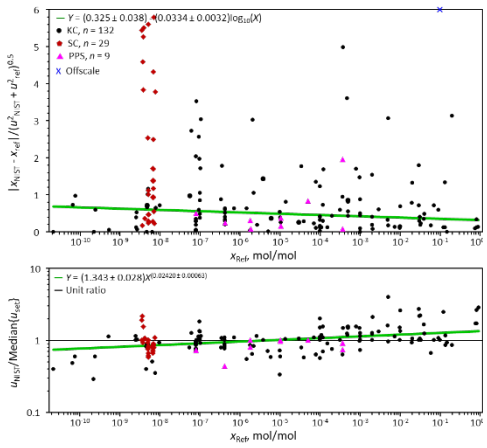


Fig. 14. The *Lab_Bias* Chart With and Without "Outsider labels".

The outsider datasets are identified in the table to the right of the charts (see Fig. 12). Selecting a cell containing either the code or the dataset name and clicking the **Review** button produces a dot-and-bar chart for that dataset (Section 20).

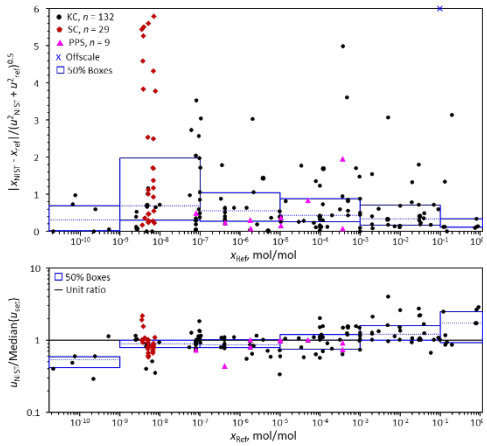
6.4.4. Trend lines



Clicking the "Trend lines" checkbox toggles the display of a robust Thiel-Sen linear trend line [14,15], $Y = \beta_0 + \beta_1 \log_{10}(x_{\text{ref}})$, where Y is the metric identified in the chart's Y-axis title.

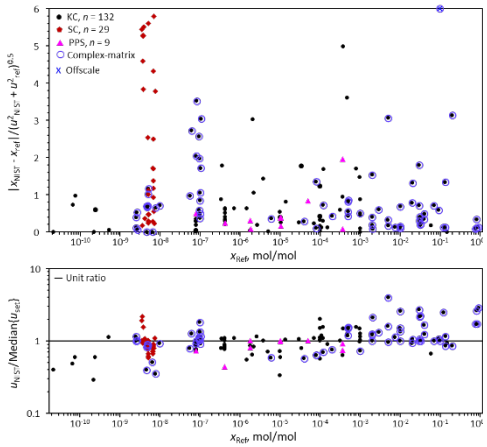
6.4.5. 50 % boxes

Clicking the "50 % boxes" checkbox toggles the display of a series of 50 % boxes at intervals along the measurement axis. Each box is bounded with solid blue lines. The width of each box is set by the "Box width-level" parameter (Section 6.3). The top line represents the 75th percentile of all results within the interval, the bottom line the 25th percentile, and the dotted blue centerline represents the median (50th percentile).



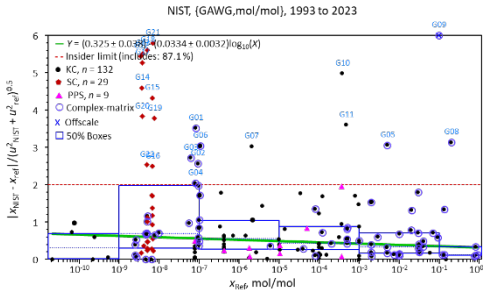
6.4.6. Mark complex

Clicking the "Mark complex" checkbox toggles the identification of results for complex-matrix materials. This option is only relevant when simple-matrix and complex-matrix datasets are analyzed together. Complex-matrix datasets are identified with a surrounding blue circle.



6.4.7. Legend entries

As described in Section 2.2.3.1, clicking the "Legend" checkbox toggles the display of the legend. The optional features have a legend entry when (and only when) active. In addition to identifying the graphical elements, some entries provide quantitative information.

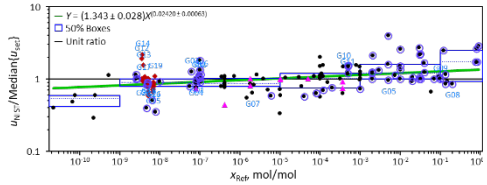


In chart LB-1:

- "Trend line" states the linear trend of the selected bias metric as a function of $\log_{10}(x_{ref})$.
- "Insider limit" states the percentage of results that are within the Insider limit.
- If the symbols are shown colored, the number of each type of study is displayed.

In chart LB-2:

- "Trend lines" states linear trend of the relative uncertainty over time as a multiplicative factor.



7. Lab_Uncertainty Subsystem

The *Lab_Uncertainty* charts, the controls used to specify the datasets evaluated, and the controls used to modify what's displayed are pictured in Fig. 15. The in-common data selection and chart display parameters and controls are discussed in Section 2.

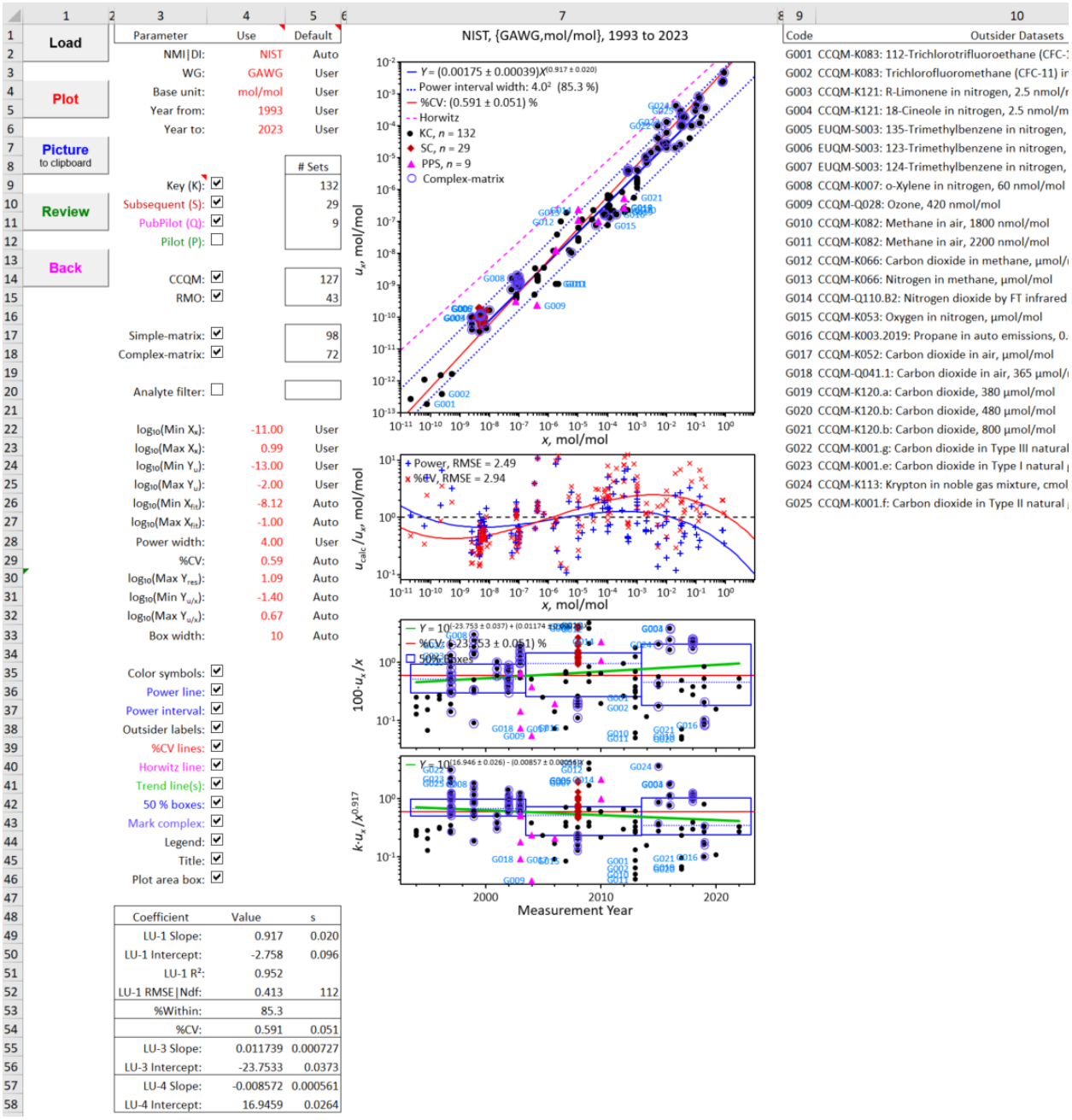


Fig. 15. The *Lab_Uncertainty* Dashboard.

Reminder: A data selection or chart display parameter value listed under the "Use" heading can only be changed when its "Default" value is "User". See Section 1.9 for further information.

7.1. Charts

The *Lab_Uncertainty* worksheet provides four charts for results that meet all the selection criteria. Each symbol in a chart represents measurement results for a single dataset.

The top chart (chart LU-1) displays reported standard uncertainty, u_x, as a function of the reported value, x. For many of the {WG, Base unit} groups studied by the CCQM, the range of magnitudes is quite large; e.g., exemplar GAWG data span eleven orders-of-magnitude. To enable visualizing the entire range of $\{x,u_x\}$ values, the chart displays the $\log_{10}$-transformation of the values.

The chart (chart LU-2) located immediately below chart LU-1 displays the residuals between the reported uncertainties and predictions made using two uncertainty function models for the relationship between u_x and x [2]. The residuals are calculated as $\log_{10}(u_{calc})$ - $\log_{10}(u_x)$; since these differences are plotted on a logarithmic Y-axis, the axis is labeled with the linearized formulation u_{calc}/u_x.

The commonly assumed "constant coefficient of variation" (CV), $u_X = \beta_0 x$, is a one-parameter power-law curve where the power is 1 and β_0 is the assumed CV. The two-parameter power-law curve, $u_x = \beta_0 x^{\beta_1}$ has been observed to describe the relationship between measurement reproducibility and the value of the measurand expressed as mass- or mole-fraction in many interlaboratory studies of many different measurands [3,4,5]. The values for the parameters of both functions are derived from the results shown in chart LU-1.

The next chart (chart LU-3) displays the relative reported uncertainty, $100 \cdot u_x/x$, as a function of measurement year. In addition to visualizing when measurements were made and the median relative uncertainty during the specified time period, the chart enables estimating the change in the magnitude of relative uncertainty over time.

The bottom chart (chart LU-4) displays a value-corrected relative uncertainty expressed as %CV, $100 \cdot u_x/x^{\beta_1}$ as a function of year, where the value of the β_1 exponent is derived from the results shown in chart LU-1. If the two-parameter power-law curve is an appropriate uncertainty function for the selected data, the scatter and any observed rate of change should be somewhat reduced from that displayed in chart LU-3.

Note: For β_1 less than one, u_x/x^{β_1} will be larger than u_x/x. Since $1^{\beta_1} = 1$ for all values of β_1, the difference between $100 \cdot u_x/x$ and $100 \cdot u_x/x^{\beta_1}$ will increase as x increasingly differs from 1. This complicates comparing the results displayed in charts LU-3 and LU-4, hence the transformed results displayed in chart LU-4 are scaled by a constant factor to have the same %CV as the results displayed in chart LU-3.

7.2. Chart Display Parameters

The *Lab_Uncertainty* worksheet contains 12 chart display parameters. The first two of these pertain to charts LU-1 and LU-2; the next six control elements of chart LU-1 (but impact the data displayed in charts LU-2 to LU-4), the ninth pertains solely to chart LU-2, and the last three pertain to charts LU-3 and LU-4. Changes to these values are not evaluated or implemented until the **Plot** button is clicked.

$\log_{10}(\text{Min } X_x)$:	-12.00	User
$\log_{10}(\text{Max } X_x)$:	1.00	User
$\log_{10}(\text{Min } Y_u)$:	-13.00	User
$\log_{10}(\text{Max } Y_u)$:	0.00	User
$\log_{10}(\text{Min } X_{fit})$:	-8.12	Auto
$\log_{10}(\text{Max } X_{fit})$:	-2.00	Auto
Power width:	4.00	Auto
%CV:	0.50	Auto
$\log_{10}(\text{Max } Y_{res})$:	2.00	Auto
$\log_{10}(\text{Min } Y_{u/x})$:	-2.00	Auto
$\log_{10}(\text{Max } Y_{u/x})$:	1.00	Auto
Box width:	5	Auto

7.2.1. $\log_{10}$(Min X_x) and $\log_{10}$(Max X_x): X-axis Limits for Charts LU-1 and LU-2

The values of the "$\log_{10}$(Min X_x)" and "$\log_{10}$(Max X_x)" parametes set the minimum and maximum limits for the X-axis (reported x values) in charts LU-1 and LU-2. The default values for these limits are the $\log_{10}$-transformed minimum and maximum x of the selected data. Modifying these limits does not affect what data are selected for analysis.

7.2.2. $\log_{10}$(Min Y_u) and $\log_{10}$(Max Y_u): Y-axis Limits for Chart LU-1

The values of the "$\log_{10}$(Min Y_u)" and "$\log_{10}$(Max Y_u)" parameters set the minimum and maximum display limits for the Y-axis (reported standard uncertainty, u_x) in chart LU-1. The default values for these limits are the $\log_{10}$-transformed minimum and maximum u_x values of the selected data. Modifying the limits of either axis does not affect what data are selected for analysis.

7.2.3. $\log_{10}$(Min X_{fit}) and $\log_{10}$(Max X_{fit}): X-axis Regression Limits

For some {WG, Base unit} groups, the measurement processes used for the major component in relatively "pure" materials differ qualitatively from those for minor components; likewise, the reproducibility of very low quantity values may not follow the trend shown by middling values [4]. The values of the "$\log_{10}$(Min X_{fit})" and "$\log_{10}$(Max X_{fit})" parameters specify the lower and upper bounds on the x_i used to estimate the power-law curve of u_x as a function of x. The default values, taken from [4], are -8.12 (a fractional value of $\approx 7.6 \times 10^{-9}$) and -1.0 (a fractional value of 0.1).

Modifying these regression limits only affects which data are used to estimate the power-law curve, it does not affect the display of the $\{x,u_x\}$ data.

7.2.4. Power width: Outlier Identification Interval

One of the chart LU-1's optional elements is a least-squares fit of u_x as a power-law function of x: $u_x = \beta_0 x^{\beta_1}$ [2]. Parameterization is accomplished by regression on $\log_{10}$-transformed values: $\log_{10}(u_x) = \log_{10}(\beta_0) + \beta_1 \log_{10}(x)$. A symmetric interval centered on the power-law curve is used to identify outsider results.

Since the chart displays $\log_{10}$-transformed data, the value of the "Power width" parameter specifies the width of the interval as a multiplicative factor. A width value (call it w) defines an interval about the power-law curve that includes all datasets with u_x values that are within a factor f of the value predicted by the power-law; i.e., the interval includes the observed $\{x,u_x\}$ values from $(\beta_0 x^{\beta_1})/w$ to $w(\beta_0 x^{\beta_1})$. The total width of the interval is thus a factor of w^2.

The default power width is twice the RMSE of the power-law fit, a value that is expected to provide an interval that includes about 95 % of the $\{x,u_x\}$ if they are approximately normally distributed. Transformed into a multiplicative factor, the default value of w is $10^{(2 \cdot \mathrm{RMSE})}$.

7.2.5. %CV: %CV lines

An optional element in all four charts are lines representing either the %CV, $100 \cdot u_x/x$, or (for chart LU-2) the predicted difference between (%CV/100)x and u_x. The default value for the "%CV" parameter is Median{%CV}, the median of all the reported $100 \cdot u_x/x$ values that meet the selection criteria.

7.2.6. $\log_{10}$(Max Y_{res}): Y-axis Limits for Chart LU-2

The value of the "$\log_{10}$(Max Y_{res})" parameter sets the minimum and maximum for the Y-axis (residuals) of chart LU-2. Representing the value as g, these endpoints are at $10^{(0 \pm g)}$. The default value for g is the largest absolute residual value for either of the uncertainty functions. Modifying the width of this interval does not affect what data are selected for analysis.

7.2.7. $\log_{10}$(Min $Y_{u/x}$) and $\log_{10}$(Max $Y_{u/x}$): Y-axis Limits for Charts LU-3 and LU-4

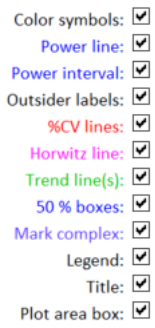
The values of the "$\log_{10}$(Min $Y_{u/x}$)" and "$\log_{10}$(Max $Y_{u/x}$)" parameters set the minimum and maximum display limits for the Y-axis of chart LU-3 and the power-law corrected %CV Y-axis of chart LU-4. The default values for these limits are the minimum and maximum $\log_{10}$-transformed %CV values of the selected data. Modifying the axis limits of does not affect what data are selected for analysis.

7.2.8. Box width: 50 % Box Width for Charts LU-3 and LU-4

The value of the "Box width" parameter sets the number of (contiguous) measurement years included in each segment of the optional "50 % boxes" element described in Section 7.3.7. The default interval is five years.

7.3. Additional Chart Display Checkboxes

The *Lab_Uncertainty* worksheet contains nine chart display checkboxes in addition to the three discussed in Section 2.2.3. Clicking a chart display checkbox invokes an immediate change in the chart display.



7.3.1. Color symbols

Clicking the "Color symbols" checkbox toggles between color-coded and all-black symbols: see Fig. 16. The colors used for the four study types are dictated by the font colors of the labels for the study type checkboxes (see Section 2.2). When colored, KC results are solid circles, SC results are solid diamonds, PPS results are solid triangles, and PS results are open squares. When black, all symbols are solid circles.

The colors of the uncertainty function residuals shown in chart LU-2 are not affected by this control.

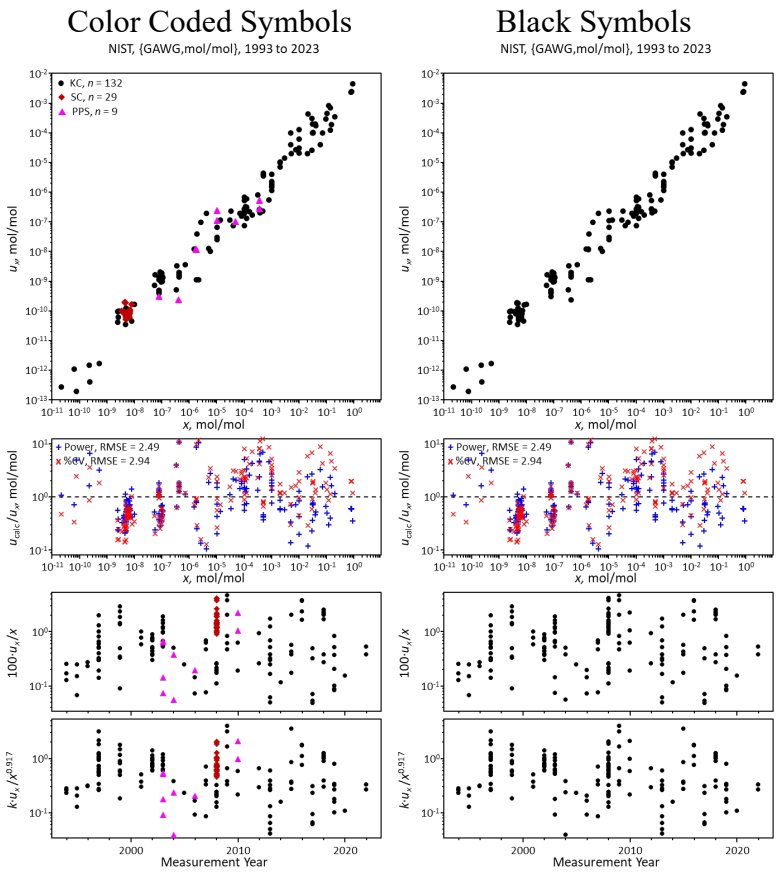
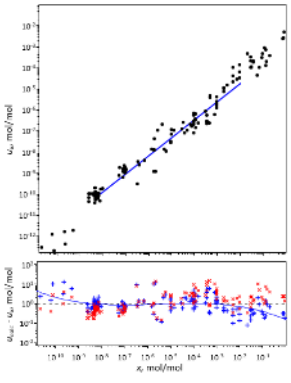


Fig. 16. *Lab_Uncertainty* Charts With Color-Coded and All-Black Symbols.

7.3.2. Power line



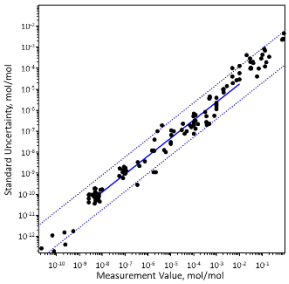
In chart LU-1, clicking the "Power line" checkbox toggles the display of a regression estimate of the power-law: $u_x = \beta_0\, x^{\beta_1}$. Since both the x (X) and u_x (Y) axes are logarithmic, this is parameterized as the linear function: $\log_{10}(u_x) = \log_{10}(\beta_0) + \beta_1 \cdot \log_{10}(x)$. The X-axis limits of the power-law curve are set by the values of the $\log_{10}(\text{Min } X_{fit})$ and $\log_{10}(\text{Max } X_{fit})$ parameters described in Section 7.2.3.

In chart LU-2, clicking the checkbox enables display of a cubic polynomial fit of the residual, $\log_{10}(\beta_0) + \beta_1 \cdot \log_{10}(x) - \log_{10}(u_x)$, to $\log_{10}(x)$. The resulting line is displayed for the entire width of the chart, not just the interval used to parameterize the power-law curve.

In both chart LU-1 and LU-2, the power-law-derived relationships are displayed as solid blue lines. Charts LU-3 and LU-4 are not affected by this control.

7.3.3. Power interval

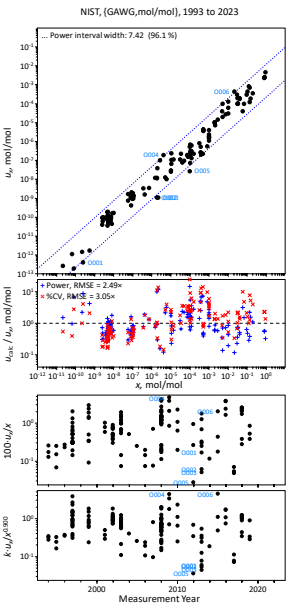
Clicking the “Power interval” checkbox toggles the display of two dotted blue lines in Chart LU-1. These lines define a symmetric interval centered on the power-law curve. This interval has the multiplicative factor width defined by the value of the “Power width” parameter described in Section 7.2.4. Using the default value, about 95 % of the $\{x,u_x\}$ values should be between the two lines. The power interval lines cover the entire $\log_{10}(\text{Min } X_x)$ to $\log_{10}(\text{Max } X_x)$ chart display range (Section 7.2.1).



7.3.4. Outsider labels

If there are outsider results (i.e., outside the Power interval), clicking the “Outsider labels” checkbox toggles their display in charts LU-1, LU-3, and LU-4. The display consists of a three-character code and an index that connects the code to the name of the outsider dataset listed in the table to the right of the chart.

Selecting a cell containing either the code or the dataset name and clicking the **Review** button produces a dot-and-bar chart for that dataset (Section 20).

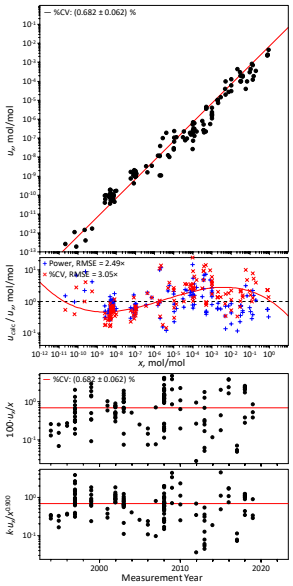


Code	Outsider Datasets
0001	CCQM-K083: Trichlorofluoromethane (CFC-11) in Real Air, pmol/mol
0002	CCQM-K082: Methane in Air, 1800 nmol/mol
0003	CCQM-K082: Methane in Air, 2200 nmol/mol
0004	CCQM-K066: Nitrogen in Methane, µmol/mol
0005	SIQM-S003: Methane in Air, 100 µmol/mol
0006	CCQM-K113: Krypton in noble gas mixture, cmol/mol

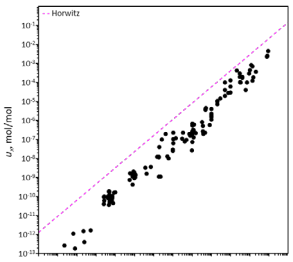
7.3.5. %CV lines

Clicking the “%CV lines” checkbox toggles the display of a constant %CV line in charts LU-1, LU-3, and LU-4. In chart LU-2, clicking the checkbox enables display of a cubic polynomial regression fit of the residual, $\log_{10}((\%CV/100)x) - \log_{10}(u_x) = (\%CV/100)x)/u_x)$, to $\log_{10}(x)$. These relationships are displayed as solid red lines.

The CV value is specified by the “%CV” parameter described in Section 7.2.5.

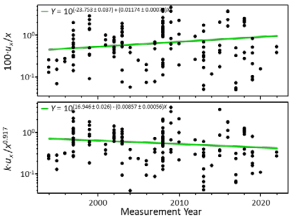


7.3.6. Horwitz line



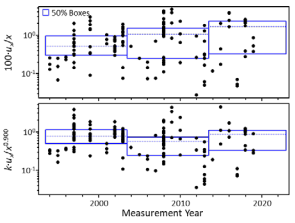
Clicking the "Horwitz line" checkbox toggles chart LU-1's display of the Horwitz relationship between reproducibility and analyte concentration [3]. The relationship, shown as a dashed magenta line, is a power-law with coefficients $\beta_0 = 0.02$ and $\beta_1 = 0.8495$. These values are derived from the rather obscure form originally described in the early 1980's from interlaboratory food-analysis studies: $100 \cdot u/C = 2^{[1-0.5 \cdot \log 10^{C}]}$ where u represents a standard deviation (estimated using some form of outlier rejection) and C a rather nebulously defined estimate of fractional concentration [4].

7.3.7. Trend lines



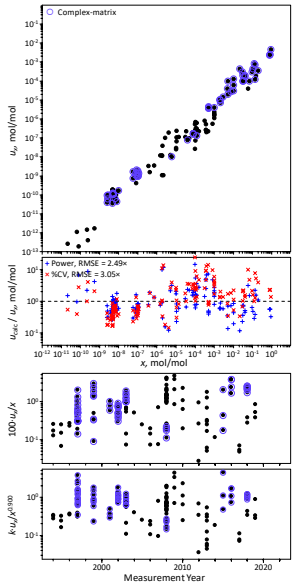
Clicking the "Trend lines" checkbox toggles the display of robust Thiel-Sen linear trend lines [14,15], $Y = \beta_0 + \beta_1 X$, in the LU-3 and LU-4 charts. The regession uses all results displayed in each chart, where X is the date in years and Y is the metric identified in the chart's Y-axis title. In chart LU-3, the metric is the estimated %CV. In chart LU-4, the metric is the estimated %CV after correcting for the observed power function relationship documented in LU-1

7.3.8. 50% Boxes



For charts LU-3 and LU-4, clicking the "50 % boxes" checkbox toggles the display of a series of 50 % boxes at intervals along the measurement year axis. Each box is bounded with solid blue lines. The width of each box is set by the "Year interval" parameter (Section 7.2.8). The top line represents the 75th percentile of all results within the interval, the bottom line the 25th percentile, and the dotted blue centerline represents the median (50th percentile).

7.3.9. Mark complex

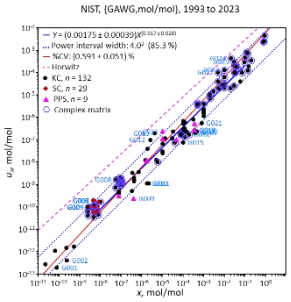


In charts LU-1, LU-3 and LU-4 clicking the "Mark complex" checkbox toggles the identification of results for complex-matrix materials. This option is only relevant when simple-matrix and complex-matrix datasets are analyzed together. Complex-matrix datasets are identified with a surrounding blue circle.

7.3.10. Legend Entries

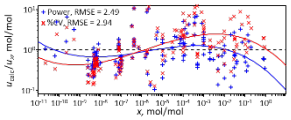
As described in Section 2.2.3.1, clicking the "Legend" checkbox toggles the display of the legend. The optional features have a legend entry when (and only when) active. In addition to identifying the graphical elements, some of the entries provide quantitative information.

In Chart LU-1:



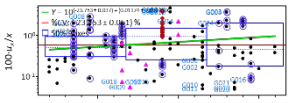
- "Power line" states the coefficients of the power-law.
- "Power interval" states the multiplicative width and the percent of the $\{x,u_x\}$ values within the lines.
- %CV states the median of the $100 \cdot u_x/x$ values
- If the symbols are shown colored, the number of each type of study is displayed.

In chart LU-2:



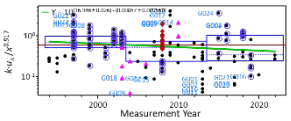
- The RMSE of the power and %CV uncertainty function residuals are displayed. The RMSE is defined as $\sqrt{(\sum_1^n d_i^2)/(n-m)}$, where d_i is the residual for one $\{x,u_x\}$, n is the number of $\{x,u_x\}$, and m is the number of adjustable parameters in the uncertainty function. For the power-law, m is 2; for %CV, m is 1.

In chart LU-3:



- "Trend lines" states linear trend of $100 \cdot u_x/x$ over time.
- %CV states the median of the $100 \cdot u_x/x$ values.

In chart LU-4:



- "Trend lines" states the power-law-adjusted linear trend of $100 \cdot u_x/x$ over time.

8. Lab_Engagements Subsystem

For a target NMI|DI, the *Lab_Engagements* subsystem combines and repackages results produced by the *WG_Participations* and *WG_Coordinations* subsystems to provide graphical summaries of when and how that NMI|DI engaged with the CCQM. The *Lab_Engagements* charts, the controls used to specify the datasets evaluated, and the controls used to modify what the charts display are pictured in Fig. 17.

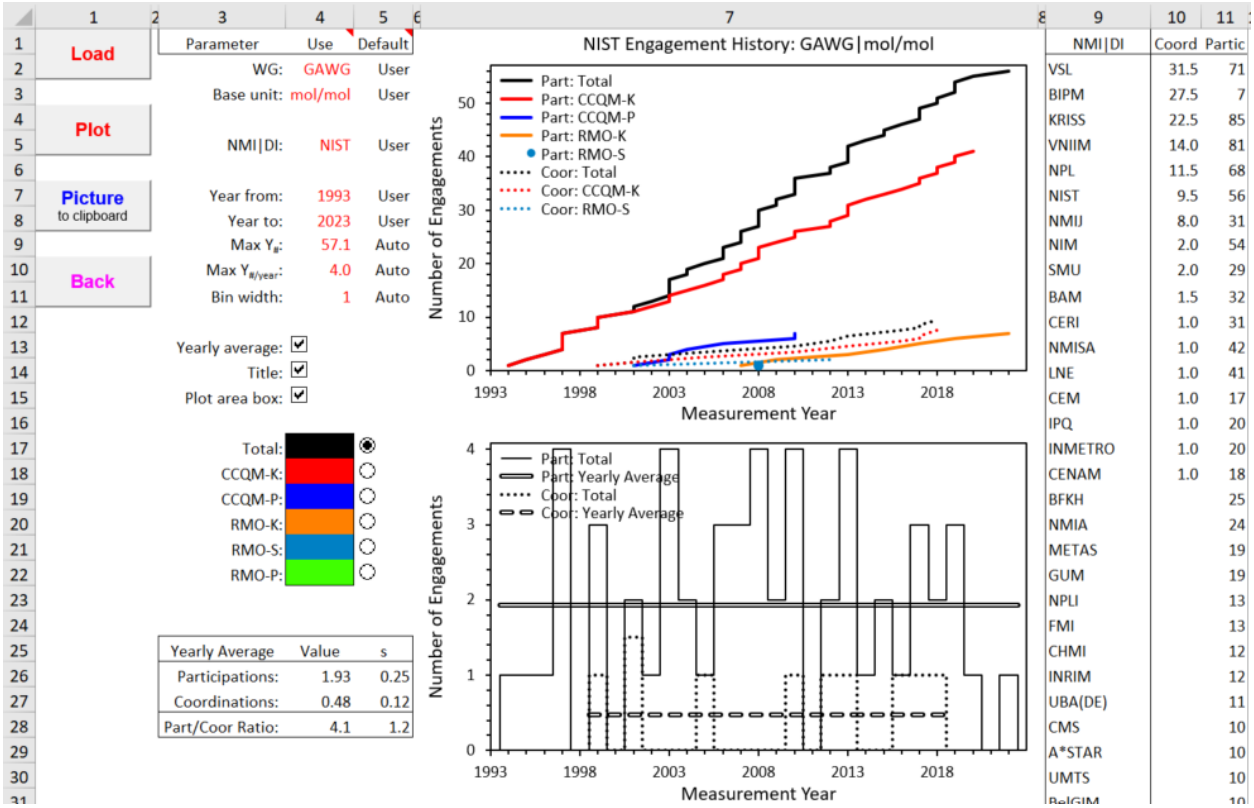
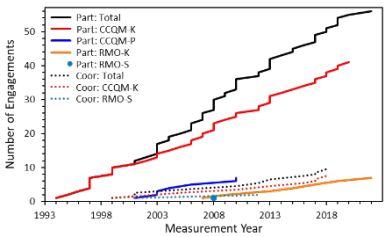


Fig. 17. The *Lab_Engagements* Dashboard.

Reminder: A data selection or chart display parameter value listed under the "Use" heading can only be changed when its "Default" value is "User". See Section 1.9 for further information.

8.1. Charts

While produced in the *WG_Presentations* and *WG_Coordinations* subsystems, the information displayed in the *Lab_Engagements* charts is combined and displayed in much greater detail than in its natal systems.

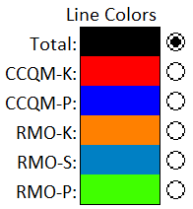


The worksheet's top chart (chart LE-1) displays cumulative distributions for the target NMI|DI's CCQM- and RMO-sponsored engagements. There are twelve possible distributional classes:

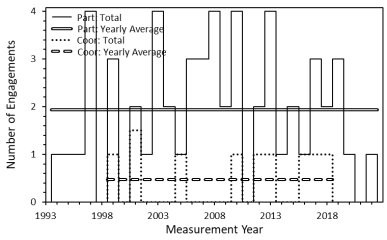
- Part: Total, the total number of participations
- Part: CCQM-K, the number of CCQM-sponsored KCs.
- Part: CCQM-P, the number of CCQM-sponsored PPSs (and PSs, if in database).
- Part: RMO-K, the number of RMO-sponsored KCs.
- Part: RMO-S, the number of RMO-sponsored SCs.
- Part: RMO-P, the number of RMO-sponsored PPSs (and PSs, if in database).
- Coor: Total, the total number of coordinations
- Coor: CCQM-K, the number of CCQM-sponsored KCs.
- Coor: CCQM-P, the number of CCQM-sponsored PPSs and PSs.
- Coor: RMO-K, the number of RMO-sponsored KCs.
- Coor: RMO-S, the number of RMO-sponsored SCs.
- Coor: RMO-P, the number of RMO-sponsored PPSs and PSs.

The count of PS participations requires the presence of the non-published studies in the *CCQM_Retrospectoscope*'s database. The complete database is only available at NIST. The count of coordinations is derived from public information provided in the *CCQM_KCs_PSs.xlsx* workbook hosted by the BIPM [16].

The participation information is displayed as solid lines, the coordinations as dotted lines. The colors used to distinguish the distributions are set by the "Line Colors" area of the worksheet. These colors can be changed at will using Excel's "Fill Color" tool (the "spilling paint can" in the Font menu of the Home tab).



The worksheet's bottom chart (chart LE-2) displays the number of participations and coordinations per unit time period as functions of measurement year. The class of the histogram displayed is specified by the radio buttons to the right-side of the Line Colors area. The yearly averages can also be displayed. The color of the lines is set by the color associated with the selected class.



8.2. Engagement Selection Parameters

In addition to the options described in Sections 2.4.1.2 and 2.4.1.3, this subsystem supports use of "All" settings for the **WG** and **Base unit** parameters. If a particular **WG** is specified, setting **Base unit** to "All" will include coordinations in all the studies coordinated by that WG regardless of the measurement units. Setting **WG** to "All" includes all coordinations regardless of WG or measurement units.

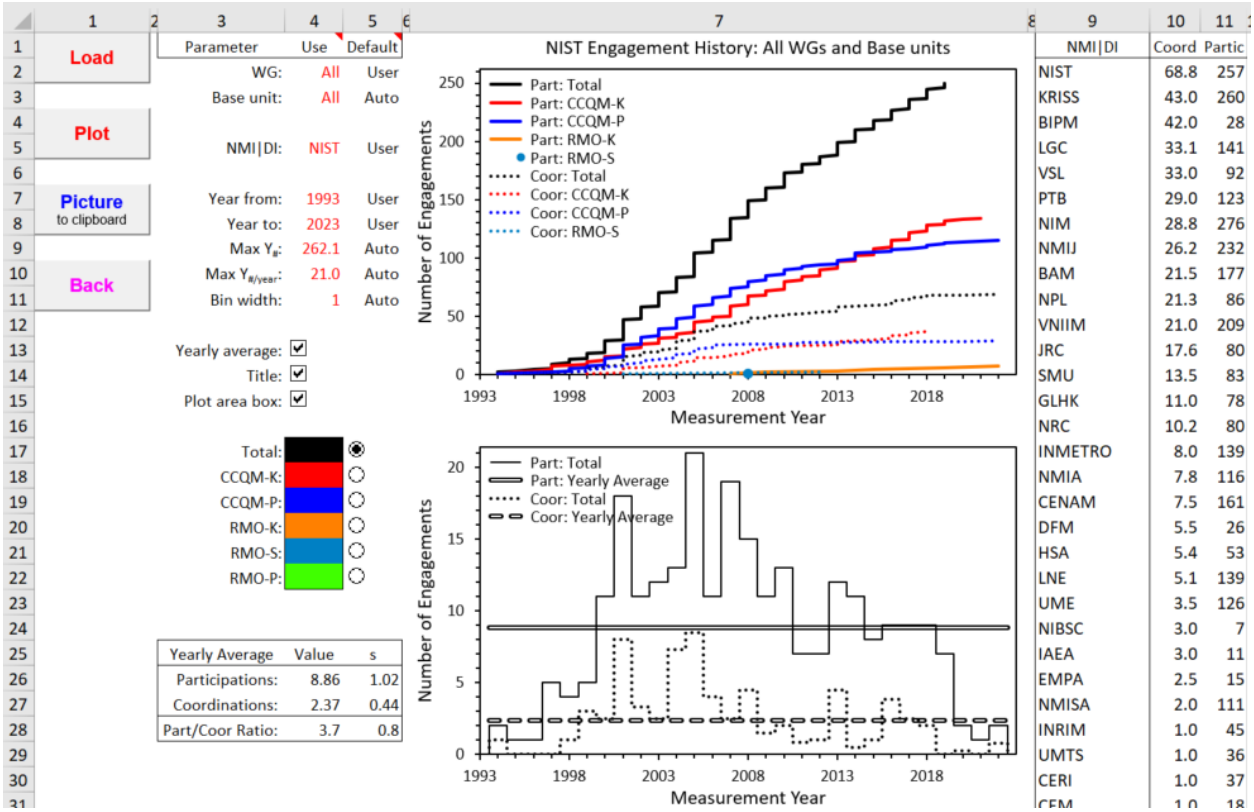


Fig. 18. The *Lab_Engagements* Dashboard With WG and Base Unit Set to "All".

8.3. NMI|DI: Specifying the Target NMI|DI

NMI|DI: NIST User

Charts LE-1 and LE-2 display results for the targeted NMI|DI. The targeted NMI|DI must have participated and/or coordinated at least one study.

8.4. Chart Display Parameters

Year from: 1993 User
Year to: 2022 User
Max Y#: 50.0 Auto
Max Y#/year: 4.0 Auto
Bin width: 1 Auto

The *Lab_Engagements* worksheet contains five chart display parameters. The first pertain to both charts LE-1 and LE-2, the next to chart LE-1; and the last two to chart LE-2. Changes to these values are not evaluated or implemented until the **Plot** button is clicked.

8.4.1. Year from and Year to: X-Axis Display Dates

By default, the minimum and maximum measurement years displayed in the charts are those of the earliest and most recent of the selected studies. However, to facilitate comparisons across {WG, Base units}, the "Year from" value can be set to a value earlier than the earliest of the selected studies (but not earlier than 1993) and "Year to" can be set to a value later than the most recent of the selected studies (but not later than the current year). Note: 1993 is the measurement year of the earliest CCQM studies, now attributed to the GAWG and IAWG.

8.4.2. Max $Y_{\#}$: Y-axis Maximum for Chart LE-1

By default, the maximum Y-axis value for chart LE-1 is set by the target NMI|DI's total number of engagements. However, to facilitate comparisons across NMI|DIs and {WG, Base units}, the value of the "Max $Y_{\#}$" parameter enables setting the maximum to a specified value. Changing the maximum does not affect what data are selected for analysis.

8.4.3. Max $Y_{\#/year}$: Y-axis Maximum for Chart LE-2

By default, the maximum Y-axis value for chart LE-2 is set by the bin of the currently selected histogram class that contains the largest number of engagements. However, to facilitate comparisons across different {WG, Base units}, NMI|DIs, "Year interval" values (histogram bin widths), or distribution classes, the value of the "Max $Y_{\#/year}$" parameter enables setting the maximum to a specified value. Changing the maximum does not affect what data are available for display.

8.4.4. Bin interval: Width of the Histogram Bins in Chart LE-2

The value of the "Bin width" parameter sets the number of (contiguous) measurement years included in each bin of the histogram. The default interval is one year; the maximum is five years. The interval must be an integer number of years. NIST's engagements using intervals of one, three, and five years are contrasted in Fig. 19.

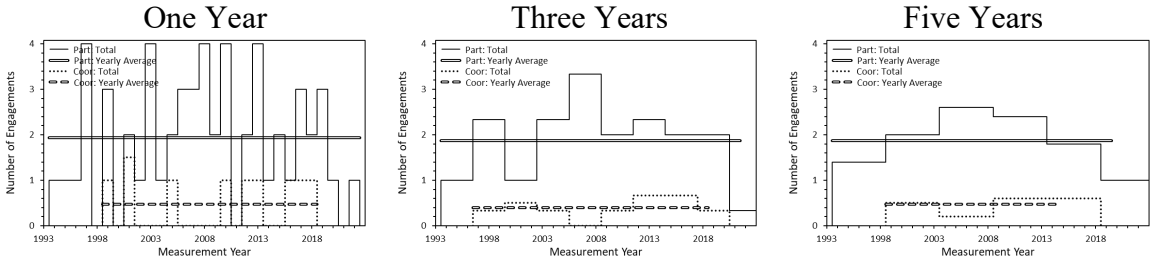
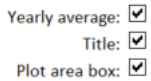


Fig. 19. *Lab_Engagement* Histograms With Different Bin Widths.

8.5. Additional Chart Display Checkbox

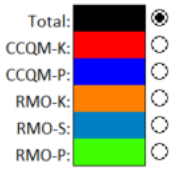


The *Lab_Engagements* worksheet contains one chart display checkbox in addition to two discussed in Section 2.2.3. Clicking a chart display checkbox invokes an immediate change in the chart display.

8.5.1. Yearly average

Clicking the “Yearly average” checkbox toggles the display of the yearly average engagements of the target NMI|DI in chart LE-2. The yearly average participations and coordinations are displayed as horizontal lines stretching from the earliest to the most recent participation and coordination.

8.5.2. Line Color Radio Buttons: Selecting the Engagement Class



The radio buttons to the right-side of the Line Colors area designate which of the six histogram classes is displayed in Chart LE-2. NIST’s engagements for all classes (except RMO pilot studies) are displayed in Fig. 20. There have been only two RMO pilot studies as of this document’s publication date - neither of which NIST participated in nor coordinated. The “RMO-K” participations reflect periodic bilateral ozone photometer comparisons in BIQM-K001 (BIPM.QM-K1).

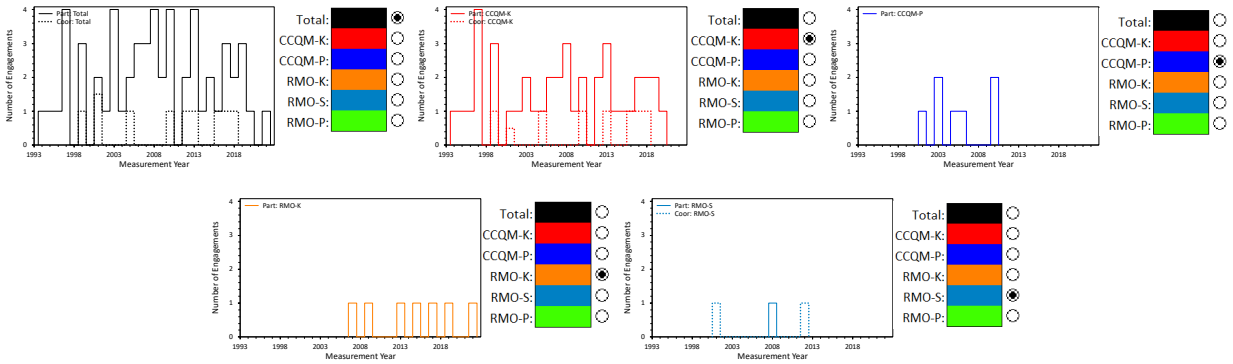


Fig. 20. *Lab_Engagements* Histogram Classes.

The colors assigned to the lines representing the engagement classes in both charts LE-1 and LE-2 are set by the fill color of the cell between the label and the associated radio button. These colors can be changed at will using Excel’s “Fill Color” tool (the “spilling paint can” in the Font menu of the Home tab).

9. Peer_Bilateral Subsystem

The *Peer_Bilateral* chart, the controls used to specify the datasets evaluated, and the controls used to modify what the chart displays are pictured in Fig. 21.

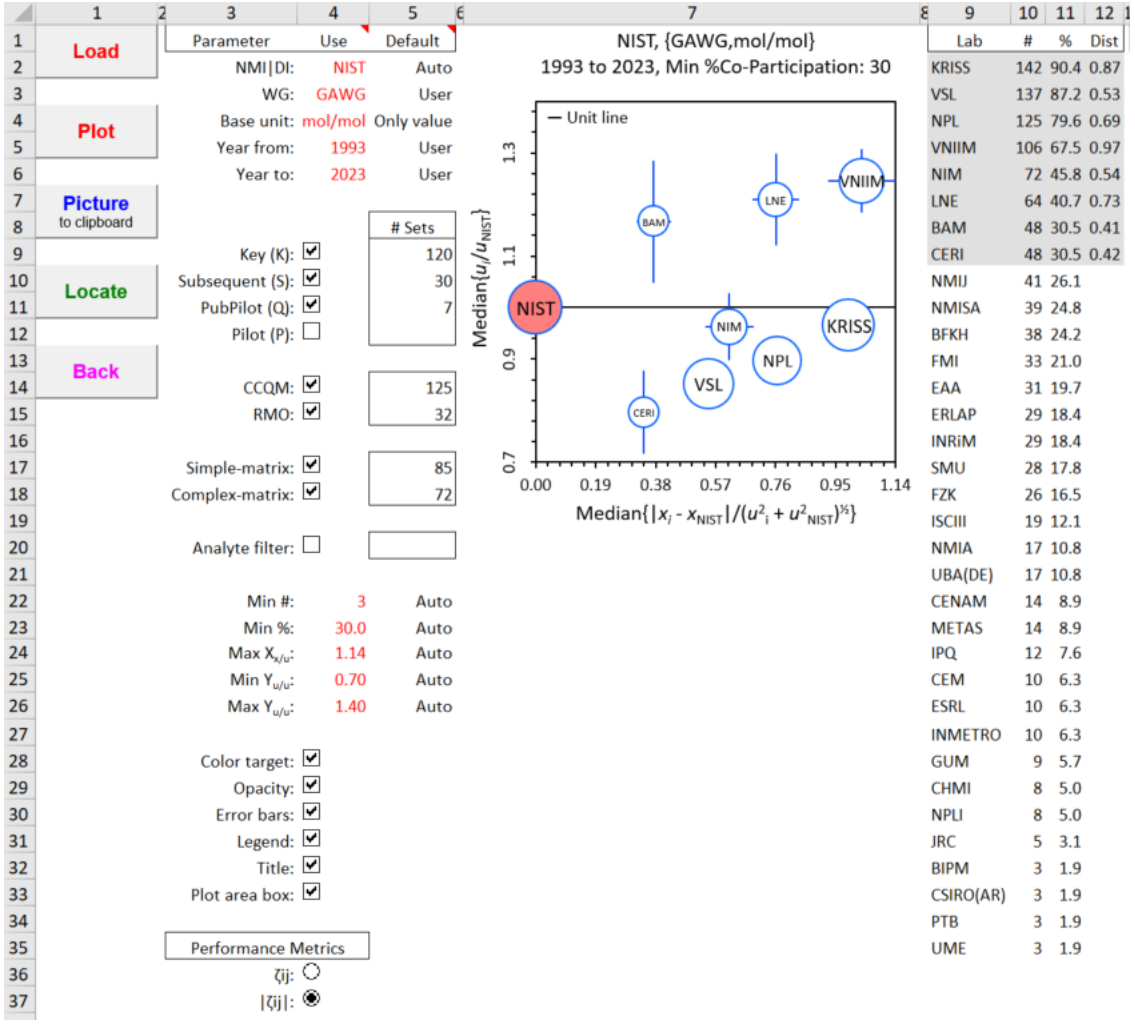


Fig. 21. The *Peer_Bilateral* Dashboard.

Reminder: A data selection or chart display parameter value listed under the "Use" heading can only be changed when its "Default" value is "User". See Section 1.9 for further information.

9.1. Chart

The location of each open circle symbol represents the median ratio of the uncertainty reported by the co-participant and that reported by the target NMI|DI plotted as a function of the median value of the normalized differences between the target and the co-participant. The area of each circle is proportional to the number of datasets shared with the target NMI|DI. Co-participants need not share the same datasets.

The symbol for the target NMI|DI is always located at the intersection of the zero-distance and unit uncertainty ratio lines. For the absolute difference metric, this will be along the left edge of the chart (see left panel of Fig. 22). For the signed difference, it will be in the center (see right panel of Fig. 22).

The closer the co-participant's circle is to the target's, the more similar their measurement results. But since approximately equal numbers of large positive and negative differences can average to zero, the relationships suggested by the signed- and absolute value metrics can significantly differ: compare the panels of Fig. 22.

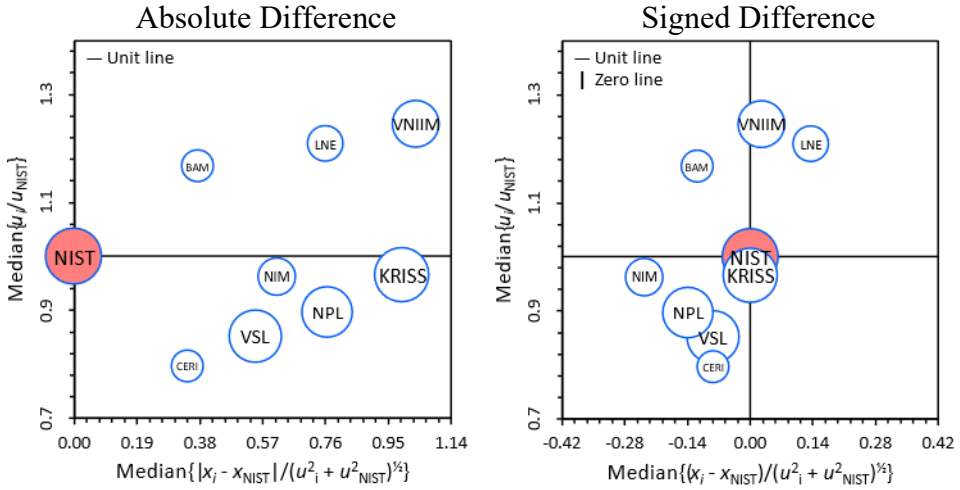


Fig. 22. Comparison of *Peer_Bilateral* Chart With Absolute and Signed Difference Metrics.

9.2. Chart Display Parameters

Min #:	3	Auto
Min %:	30.0	Auto
Max $X_{x/u}$:	0.42	Auto
Min $Y_{u/u}$:	0.50	Auto
Max $Y_{u/u}$:	1.40	Auto

The *Peer_Bilateral* worksheet contains five chart display parameters. Changes to these values are not evaluated or implemented until the **Plot** button is clicked.

9.2.1. Min #: Minimum Number of In-Common Datasets

The value of the "Min #" parameter sets the minimum number of datasets that contain results from both the target and a given co-participant required for differences to be calculated. The number of co-participations is listed in column 10 of the table to the right of the chart (see Fig. 21). The default value is three datasets, the minimum number for the median to have any statistical relevance.

9.2.2. Min %: Minimum Co-Participation Proportion

The value of the "Min %" parameter sets the minimum proportion of co-participation, expressed as a percentage of the target NMI|DI's datasets, for the summary statistics to be evaluated and the results displayed in the chart. The percentage is listed in column 11 of the table to the right of the chart; the co-participants with at least the minimum proportion are identified with grey shading (see Fig. 21). The default value is (an arbitrary) 30 %.

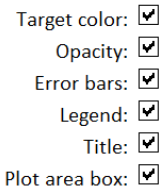
9.2.3. Max $X_{x/u}$: X-axis Limits

The value of the "Max $X_{x/u}$" parameter sets the display range of the difference (X) axis of the chart. Its default value is set by the extreme value of the display symbols including their error bars. When the signed bias metric is selected, the range is set to be symmetric about zero and, if necessary, the parameter value is rounded up to produce a symmetric distribution of tic-labels.

9.2.4. Min $Y_{u/u}$ and Max $Y_{u/u}$: Y-axis Limits

The values of the "Min $Y_{u/u}$" and "Max $Y_{u/u}$" parameters set the display range of the uncertainty ratio (Y) axis. The default values are set by the extreme values of the displayed symbols including their error bars.

9.3. Additional Chart Display Checkboxes



The *Peer_Bilateral* worksheet contains three chart display checkboxes in addition to the three discussed in Section 2.2.3. Clicking a chart display checkbox invokes an immediate change in the chart display.

9.3.1. Target color

Clicking the "Target color" checkbox toggles the display of the target NMI|DI's symbol from opaque rose to opaque white: compare the panels of Fig. 23.

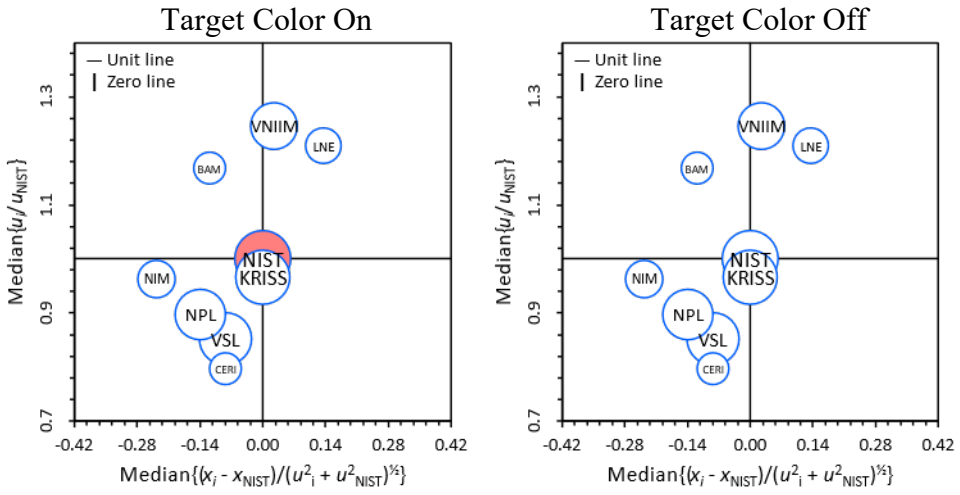


Fig. 23. Comparison of *Peer_Bilateral* Chart With and Without Target Color.

9.3.2. Opacity

Clicking the "Opacity" checkbox toggles the display of the symbols used for the co-participants from opaque white to transparent: compare the panels of Fig. 24. This can be useful for visualizing a co-participant's relationship to the target NMI|DI when its symbol is "buried" beneath others. The **Locate** button (Section 2.1.4) can be used to color a co-participant's symbol opaque green, but that doesn't help if the green isn't visible.

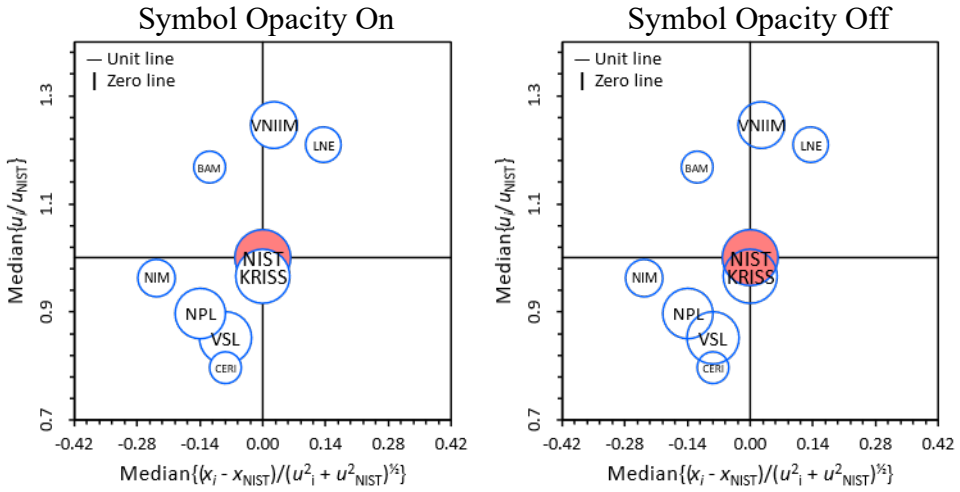


Fig. 24. Comparison of *Peer_Bilateral* Chart With and Without Symbol Opacity.

9.3.3. Error bars

Clicking the "Error bars" checkbox toggles the display of the error bars: compare the panels of Fig. 25. The error bars span ± one standard deviation of the mean ("standard error") about the median value. A standard deviation of the mean is estimated from the Q_n robust standard deviation of set of values divided by the square root of the number of values in the set. The display regions of the bias and uncertainty ratio axes are not affected by whether the error bars are displayed.

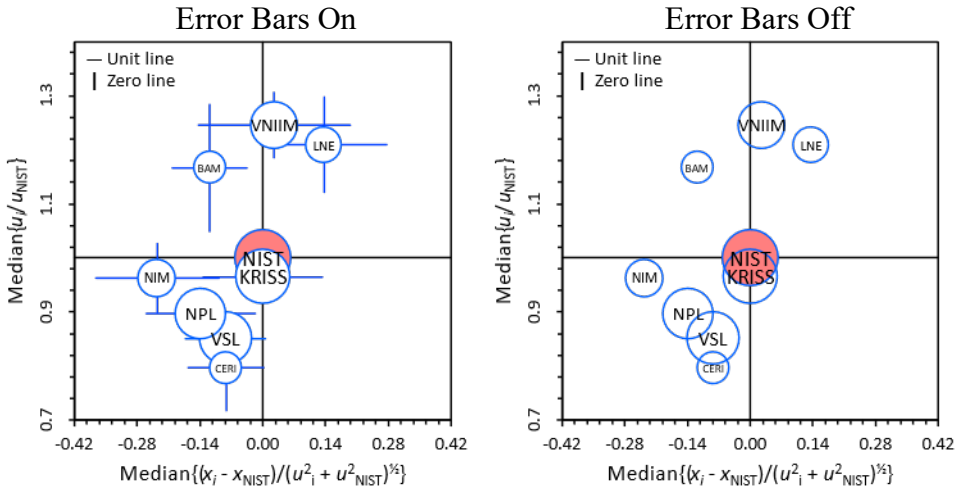


Fig. 25. Comparison of *Peer_Bilateral* Chart With and Without Error Bars.

10. Peer_Unilateral Subsystem

The *Peer_Unilateral* chart, the controls used to specify the datasets evaluated, and the controls used to modify what the chart displays are pictured in Fig. 26.

While sharing many of the *Peer_Bilateral* subsystem's features, the performance metrics are estimated relative to the dataset reference values and median measurement uncertainty, rather than the values reported by the target NMI|DI. However, the estimates are calculated using just datasets that contain results reported by the target and that meet all the selection criteria.

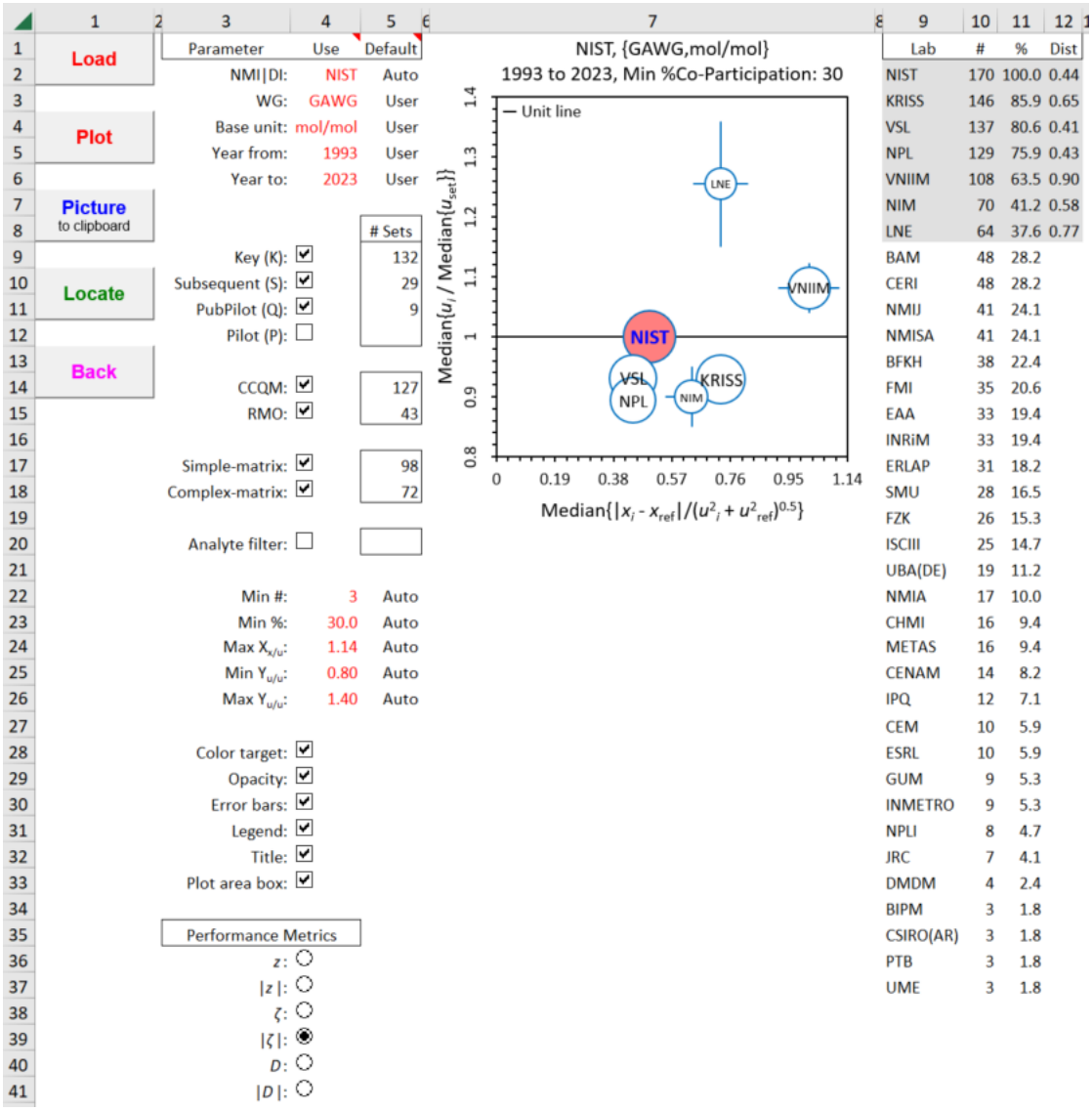


Fig. 26. The *Peer_Unilateral* Dashboard.

Reminder: A data selection or chart display parameter value listed under the "Use" heading can only be changed when its "Default" value is "User". See Section 1.9 for further information.

10.1. Chart

The location of each open circle symbol represents the median of the set of relative standard uncertainties associated with all of the technically valid x_i in the dataset (Section 1.1.3.1) plotted as a function of the median of the set of one of the bias metrics (Section 1.8.1). In contrast to the chart in the *Peer_Bilateral*, the bias and uncertainty metrics are relative to the dataset references rather than to the target NMI|DI's measurements. Therefore, the symbol for the target NMI|DI is *not* constrained to be located at the chart {0,1}: compare Fig. 27 with Fig. 22.

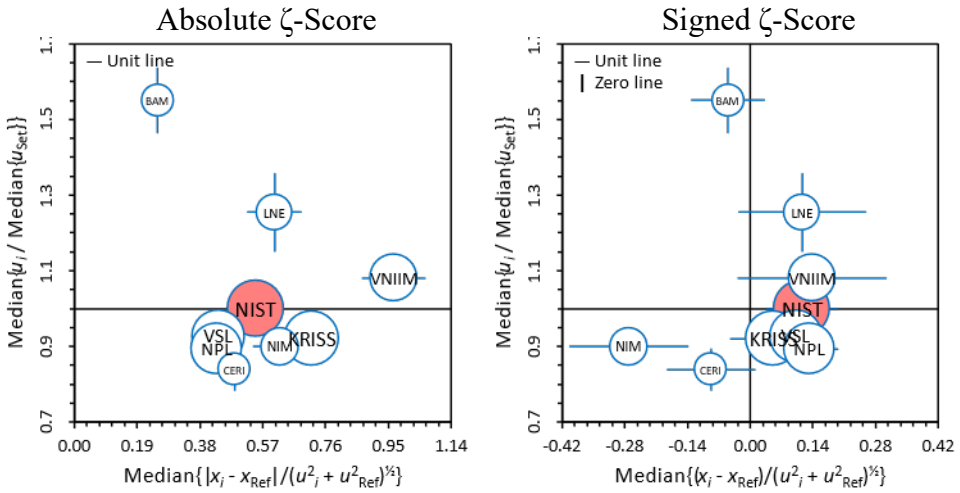


Fig. 27. Comparison of *Peer_Unilateral* Chart With Absolute and Signed Bias Metrics.

As with the *Peer_Bilateral* analysis, the closer a co-participant's circle is to the target's, the more similar their measurement results. But since approximately equal numbers of large positive and negative differences can average to zero, the relationships suggested by signed- and absolute value metrics can significantly differ: compare the panels of Fig. 27.

The area of each circle is proportional to the number of datasets shared with the target NMI|DI. Co-participants need not share the same datasets.

10.2. Chart Display Parameters

The *Peer_Unilateral* worksheet contains four chart display parameters. Changes to these values are not evaluated or implemented until the **Plot** button is clicked.

Min #:	3	Auto
Min %:	30.0	Auto
Max $X_{x/u}$:	0.42	Auto
Min $Y_{u/u}$:	0.50	Auto
Max $Y_{u/u}$:	1.40	Auto

10.2.1. Min #: Minimum Number of In-Common Datasets

The value of the "Min #" parameter sets the minimum number of datasets that contain results from both the target and a given co-participant required for differences to be calculated. The number of co-participations is listed in column 10 of the table to the right of the chart (see Fig. 26). The default value is three datasets, the minimum number for the median to have any statistical relevance.

10.2.2. Min %: Minimum Co-Participation Proportion

The "Min %" parameter has the same function as described for *Peer_Bilateral* (Section 9.2.2), the value of the parameter setting the minimum proportion of co-participation for a co-participant to be displayed in the charts. However, here it only impacts the display rather than the dataset selection. The percentage of co-participation is listed in column 11 of the table to the right of the charts; the co-participants with at least the minimum proportion are identified with grey shading (see Fig. 26). The default value is (an arbitrary) 30 %.

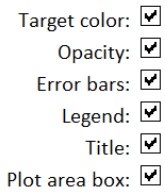
10.2.3. Max $X_{x/u}$: X-axis Limits

The value of the "Max $X_{x/u}$" parameter sets the display range of the X-axis of the chart. Its default value is set by the extreme value of the displayed symbols including their error bars. When the signed bias metric is selected, the range is set to be symmetric about zero and, if necessary, the parameter value is rounded up to produce a symmetric distribution of tic-labels.

10.2.4. Min $Y_{u/u}$ and Max $Y_{u/u}$: Y-axis Limits

The values of the "Min $Y_{u/u}$" and "Max $Y_{u/u}$" parameters set the display range of the uncertainty ratio (Y) axis. The default values are set by the extreme values of the displayed symbols including their error bars.

10.3. Additional Chart Display Checkboxes



The *Peer_Unilateral* worksheet contains three chart display checkboxes in addition to those discussed in Section 2.2.3. These are identical to those described for the *Peer_Bilateral* worksheet (see Section 9.3). Clicking a chart display checkbox invokes an immediate change in the chart display.

10.3.1. Target color

Clicking the "Target color" checkbox toggles the display of the target NMI|DI's symbol from opaque rose to opaque white.

10.3.2. Opacity

Clicking the "Opacity" checkbox toggles the display of the symbols used for the co-participants from opaque white to transparent. This can be useful for visualizing a co-participant's relationship to the target NMI|DI when its symbol is "buried" beneath others. The **Locate** button (Section 2.1.4) can be used to color a co-participant's symbol opaque green, but that doesn't help if the green isn't visible.

10.3.3. Error bars

Clicking the “Error bars” checkbox toggles the display of the error bars. The error bars span ± one standard deviation of the mean (“standard error”) about the median value. A standard deviation of the mean is estimated from the Q_n robust standard deviation of set of values divided by the square root of the number of values in the set. The X- and Y-axis spans are not affected by whether the error bars are displayed.

11. Peer_Global Subsystem

The *Peer_Global* charts, the controls used to specify the datasets evaluated, and the controls used to modify what the chart displays are pictured in Fig. 28. This subsystem is identical to *Peer_Unilateral*, except that there is no target NMI|DI. The estimate for each NMI|DI is calculated using all datasets that meet all the selection criteria.

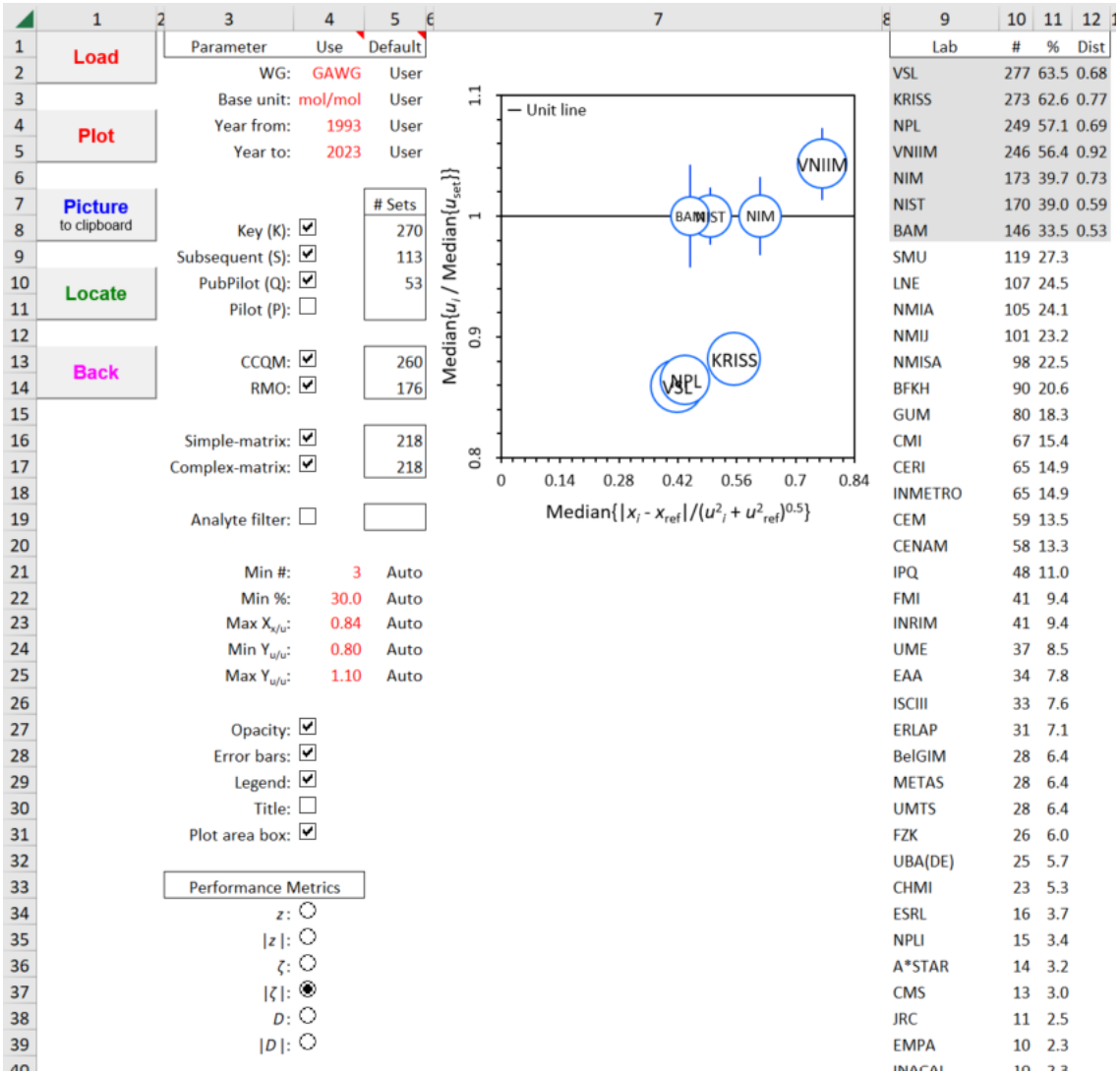


Fig. 28. The *Peer_Global* Dashboard.

Reminder: A data selection or chart display parameter value listed under the "Use" heading can only be changed when its "Default" value is "User". See Section 1.9 for further information.

11.1. Charts

As in the *Peer_Unilateral* worksheet, the location of each open circle symbol in the chart represents the median of the set of relative standard uncertainties associated with all of the technically valid x_i in the dataset (Section 1.1.3.1) plotted as a function of the median of the selected bias metrics (Section 1.8.1). As in the *Peer_Unilateral* chart, the bias and uncertainty metrics are relative to the dataset references. However, the estimates use all the datasets each NMI|DI has contributed to.

As with the *Peer_Bilateral* and *Peer_Unilateral* analyses, the closer symbols are together, the more similar the measurement results reported by the respective NMI|DIs. But since approximately equal numbers of large positive and negative differences can average to zero, the relationships suggested by signed- and absolute-value metrics can significantly differ: compare the panels of Fig. 29.

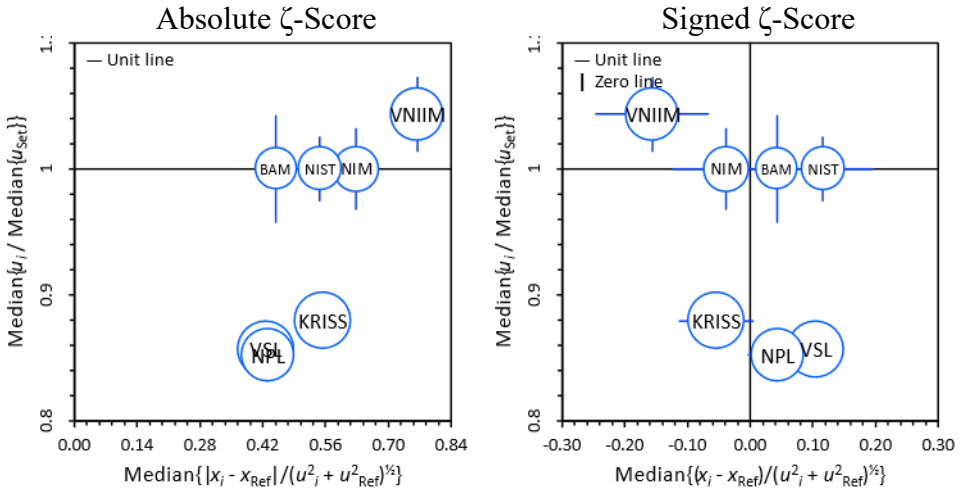
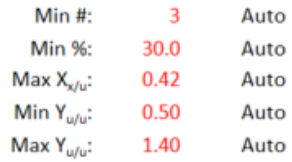


Fig. 29. Comparison of *Peer_Global* Chart With Absolute and Signed Bias Metrics.

The area of each symbol is proportional to the number of eligible datasets that contain a result from the associated NMI|DI.

11.2. Chart Display Parameters



The *Peer_Unilateral* worksheet contains four chart display parameters. Changes to these values are not evaluated or implemented until the **Plot** button is clicked.

11.2.1. Min #: Minimum Number of Datasets

The value of the "Min #" parameter sets the minimum number of datasets that contain results from given participant required for differences to be calculated. The number of participations is listed in column 10 of the table to the right of the chart (see Fig. 28). The default value is three datasets, the minimum number for the median to have any statistical relevance.

11.2.2. Min %: Minimum Participation

The "Min %" parameter has a similar function to that described for the "Min %" parameter in *Peer_Bilateral* (Section 9) and *Peer_Unilateral* (Section 10), the value of the parameter setting the minimum participation for an NMI|DI to be displayed in the charts. Here, participation is defined relative to the total number of datasets that meet the selection criterion rather than to co-participation with some target NMI|DI. The participation percentage is listed in column 11 of the table to the right of the charts; the participants with at least the minimum proportion are identified with grey shading (see Fig. 28). The default value is (an arbitrary) 30 %.

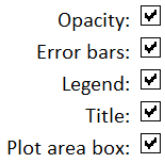
11.2.3. Max $X_{x/u}$: X-axis Limits

The value of the "Max $X_{x/u}$" parameter sets the display range of the bias (X) axis of the chart. Its default value is set by the extreme value of the display symbols including their error bars. When the signed bias metric is selected, the range is set to be symmetric about zero and, if necessary, the parameter value is rounded up to produce a symmetric distribution of tic-labels.

11.2.4. Min $Y_{u/u}$ and Max $Y_{u/u}$: Y-axis Limits

The values of the "Min $Y_{u/u}$" and "Max $Y_{u/u}$" parameters set the display range of the uncertainty ratio (Y) axis. The default values are set by the extreme values of the displayed symbols including their error bars.

11.3. Additional Chart Display Checkboxes



The *Peer_Global* worksheet contains two chart display checkboxes in addition to the three discussed in Section 2.2.3. Clicking a chart display checkbox invokes an immediate change in the chart display.

11.3.1. Opacity

Clicking the "Opacity" checkbox toggles the display of the symbols used for the co-participants from opaque white to transparent.

11.3.2. Error bars

Clicking the "Error bars" checkbox toggles the display of the error bars. The error bars span ± one standard deviation of the mean ("standard error") about the median value. A standard deviation of the mean is estimated from the Q_n robust standard deviation of set of values divided by the square root of the number of values in the set. The X- and Y-axis spans are not affected by whether the error bars are displayed.

12. Peer_Priorities Subsystem

The *Peer_Priorities* subsystem displays the participation rates for a target NMI|DI and eleven other NMI|DIs in the studies sponsored by each WGs. The participation rates are displayed as individual "radar" plots within a 12-panel multiplot. The studies considered can be selected by measurement year interval, study type, and sponsoring body. The *Peer_Priorities* chart, the controls used to specify the datasets evaluated, and the controls used to modify what the chart displays are pictured in Fig. 30.

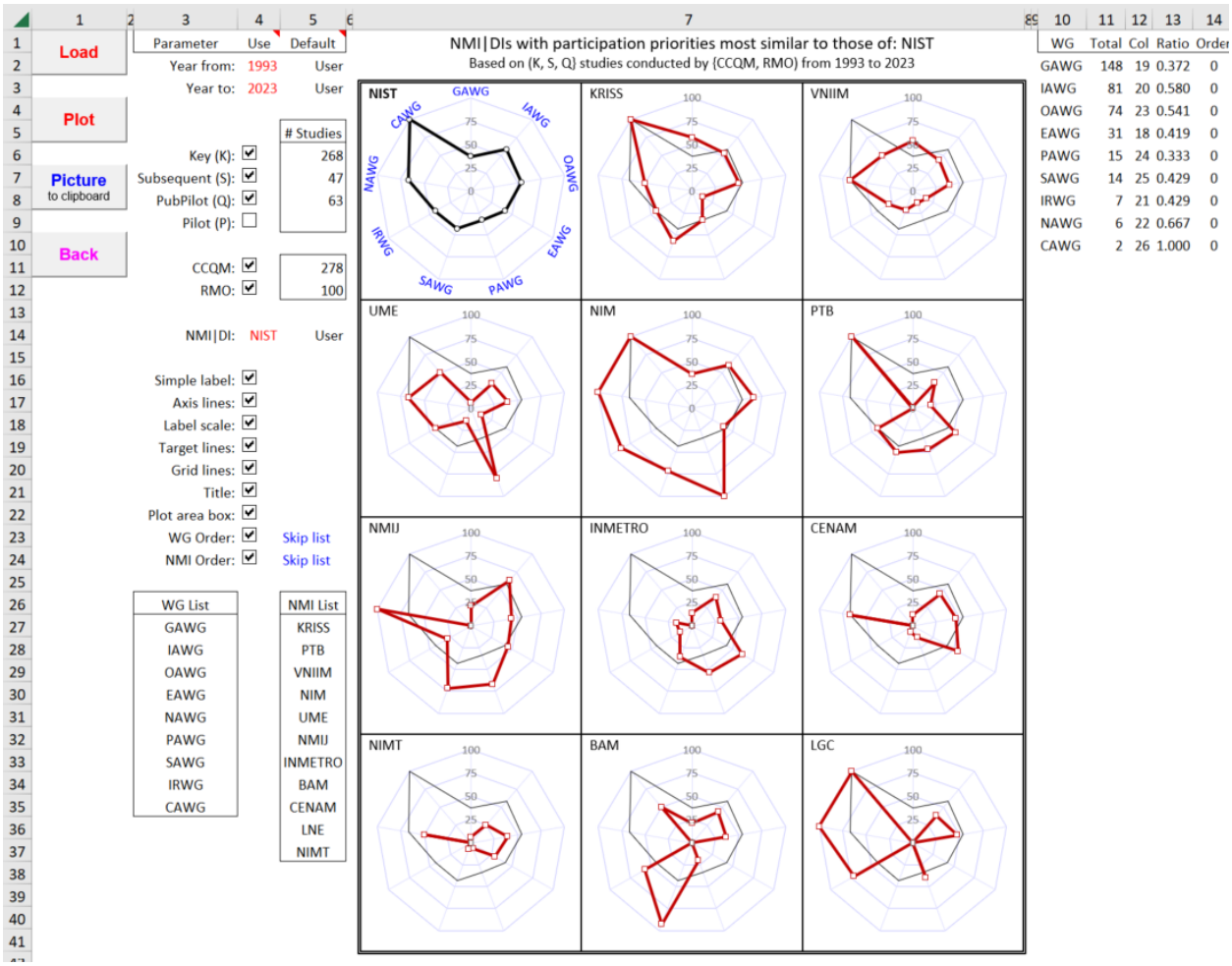


Fig. 30. The *Peer_Priorities* Dashboard.

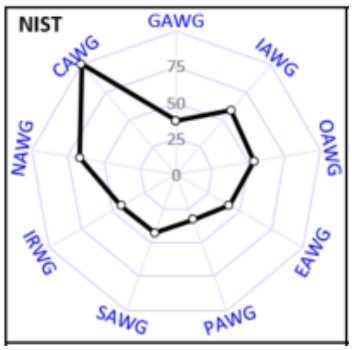
Reminder: A data selection or chart display parameter value listed under the "Use" heading can only be changed when its "Default" value is "User". See Section 1.9 for further information.

12.1. Chart

Each segment of the *Peer_Priorities* chart is a radar-style display of WG participation rates for a particular NMI|DI. A WG participation rate is the ratio (expressed as a percentage) of the number of studies in which the particular NMI|DI participated relative to the number of studies sponsored by the WG in which at least one NMI|DI participated. The studies are selected on the basis of measurement year, study type, and sponsoring body.

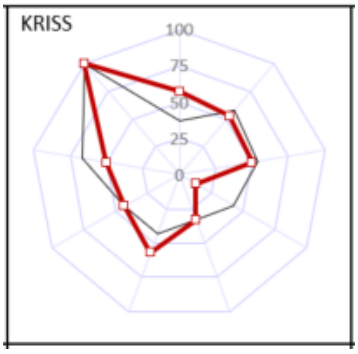
The *Peer_Priorities* chart is divided into two-inch square segments to provide suitable graphical resolution while allowing a reasonable number of comparisons. The twelve segments provided by the four-row by three-column layout fits comfortably on a single portrait-oriented page.

The upper-left corner of each segment identifies the NMI|DI. The center of each set of nested polygons within a segment represents zero participation by the NMI|DI. The vertices of the outer polygon represent participation in every available study. The inner polygons denote WG participation rates of 0.75, 0.50, and 0.25. The center denotes no participation.



The segment to the top left of the multiplot displays the rates for the "target" NMI|DI as open black circles connected with a thick black line. This segment also provides labels for each axis.

Each of the other eleven segments display the WG-participation rates for another NMI|DI, either defined by the degree of participation priorities they share with the target NMI|DI (see Section 12.2 or by a pre-selected list (see Section 12.3.9). The rates are displayed as open red squares connected by a thick red line. As an option, the rates for the target NMI|DI can also be shown via a thin black line where the rates are the vertices of the polygon.



12.2. NMI|DI: Specifying the Target NMI|DI

The values of the "NMI|DI:" parameter specifies the particular NMI|DI that provides the target for the target plots. The participation ratios for this NMI|DI are displayed in the top-left segment. The ratios for the other eleven segments can be chosen based upon the similarity of their ratios to the target NMI|DI.

12.3. Chart Display Checkboxes

There are nine chart display checkboxes located below the "NMI|DI:" parameter. Clicking any one of these checkboxes results in an immediate change to the chart display. The first seven of these are simple toggles, the last two control the number and order of WG display and which of the other NMI|DIs are displayed and in what order.

12.3.1. Simple label: Axis Label Style

The “Simple label:” checkbox toggles between two styles of axis label. When “checked” the axes in the top-left segment are labelled with the four-character WG acronym. When “unchecked” the number of studies of the specified type that the WG sponsored during the specified time period are concatenated with the acronym: compare the panels of Fig. 31.

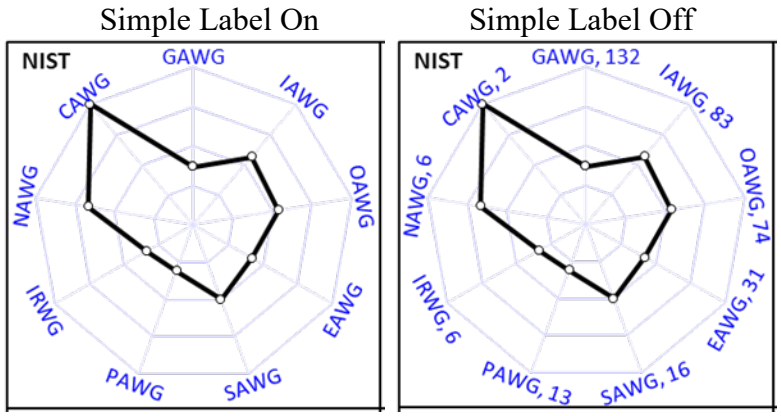


Fig. 31. The Target NMI|DI Panel of the *Peer_Priorities* Chart With and Without Simple Label.

12.3.2. Axis lines: Radial Lines

The “Axis lines:” checkbox toggles between displaying and not displaying the radial line between the center of the polygon and its vertices. When “checked” the axis lines are displayed in all twelve segments. When “unchecked” no axis lines are displayed: compare the panels of Fig. 32.

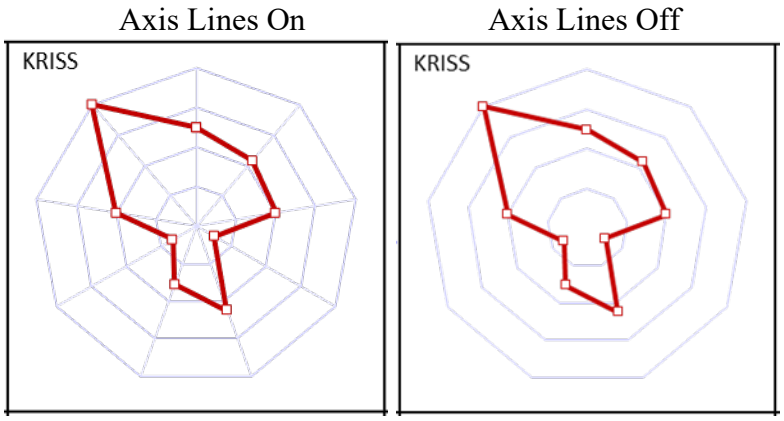


Fig. 32. A Non-Target NMI|DI Panel of the *Peer_Priorities* Chart With and Without Axis Lines.

12.3.3. Label scale: Participation Rate Scale

The “Label scale:” checkbox toggles between labeling and not labeling the participation rate denoted by the center and each of the polygons. When “checked” the rates are displayed are displayed along the zero-degree axis. When “unchecked” the rates are not displayed: compare the panels of Fig. 33.

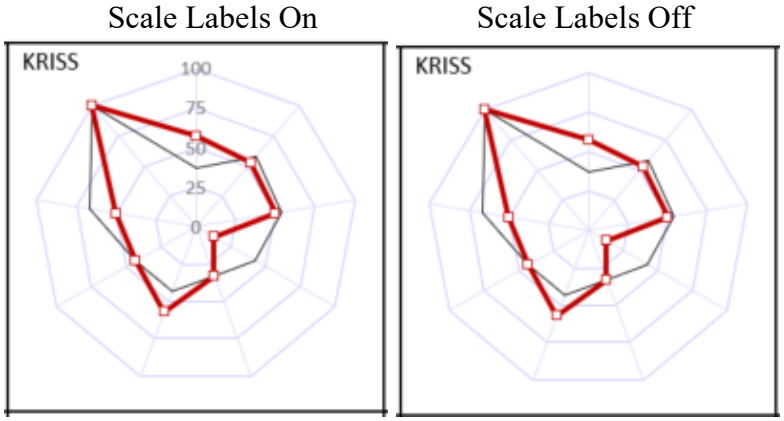


Fig. 33. A Non-Target NMI|DI Panel With and Without Scale Labels.

12.3.4. Target lines: Comparison to Target

The “Target lines:” checkbox toggles between displaying and not displaying the participation rates for the target NMI|DI in the other segments. When “checked” the target NMI|DIs rates are displayed via a thin black line in the other segments. When “unchecked” the target NMI|DI’s rates are displayed only in the top-left segment: compare the panels of Fig. 34.

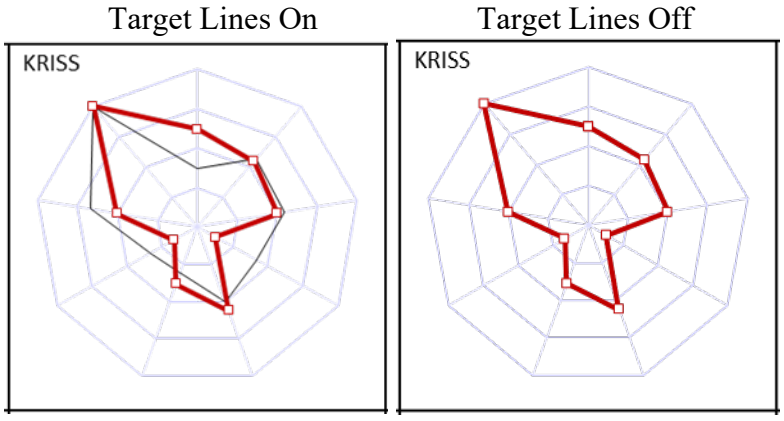


Fig. 34. A Panel With and Without Target Lines.

12.3.5. Grid Lines: Segment Boundaries

The “Grid lines:” checkbox toggles between displaying and not displaying bounding lines around each segment. When “checked” the lines are displayed. When “unchecked” the lines are not displayed: compare the panels of Fig. 35.

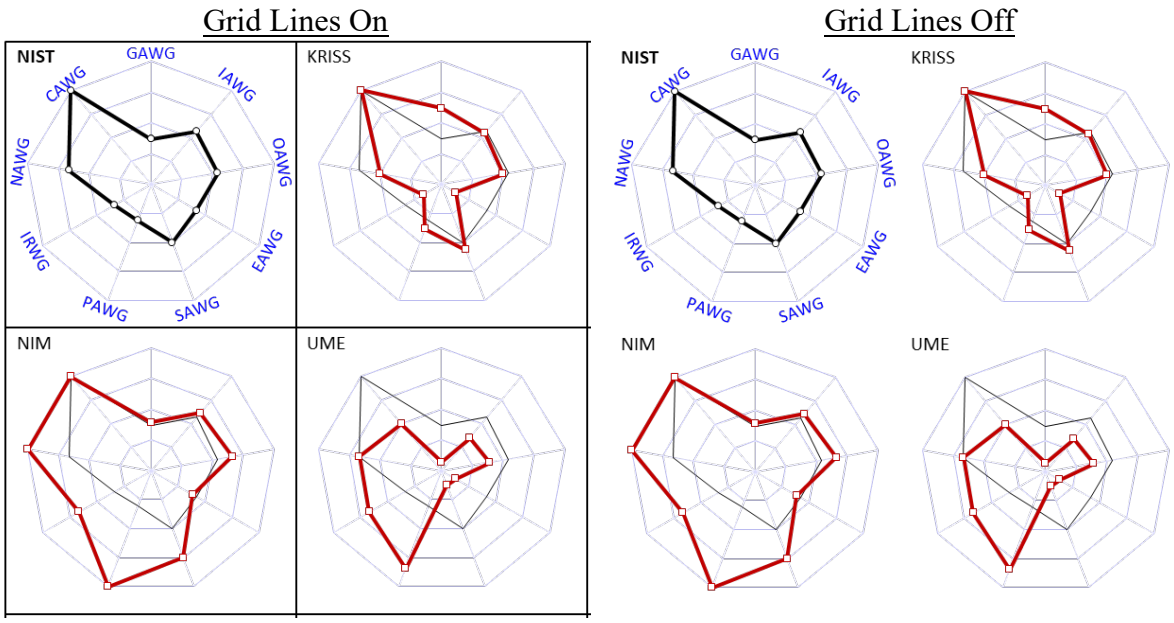


Fig. 35. Panels of the *Peer_Priorities* Chart With and Without Grid Lines.

12.3.6. Title: Chart Title

The “Title:” checkbox toggles between displaying and not displaying the chart’s title. When “checked” the title is displayed. When “unchecked” the title is not displayed. In addition to identifying the target NMI|DI, the title identifies the studies considered in the analysis by type (K S, Q, and/or P), conducting body (CCQM and/or RMO), and the measurement date interval.

12.3.7. Plot area box: Boundary Lines

Clicking the “Plot area box:” checkbox toggles between displaying and not displaying the plot area boundary lines.

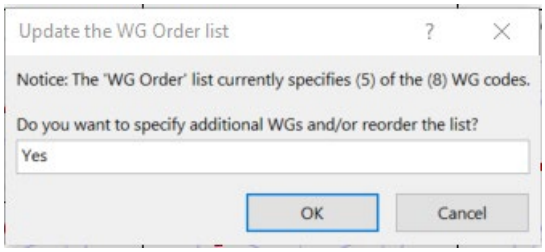
12.3.8. WG Order: Which WGs and in What Order

The "WG Order:" checkbox interacts with "WG List" to enable specifying which participation ratios are displayed and in what order.

When checked, WG List is ignored and participation ratios are displayed for every WG for which at least one study of a selected type was sponsored during the specified time interval. The ratios for these WGs are arranged in clockwise order by decreasing number of studies: see the left panel of Fig. 36. When unchecked, WG List sets which participation ratios are displayed. The ratios for the WGs are displayed clockwise in the list's order: see the middle panel of Fig. 36.

If the *CCQM_Retrospectoscope* database contains results from at least one study sponsored by a WG, the polygon will include a vertex for a listed WG even if no suitable studies were sponsored during the specified time period. Since a triangle is the least complex polygon, at least three WGs must be specified.

Participation ratios for WGs that are not in the "WG Order" list are not displayed. If not all the WGs are in the list, the subsystem will ask whether the user wants to add to the list:



- If the response is No, the subsystem proceeds with the analysis: see the right panel of Fig. 36.
- If the response is Yes, the subsystem issues a prompt and the focus returns to the user.

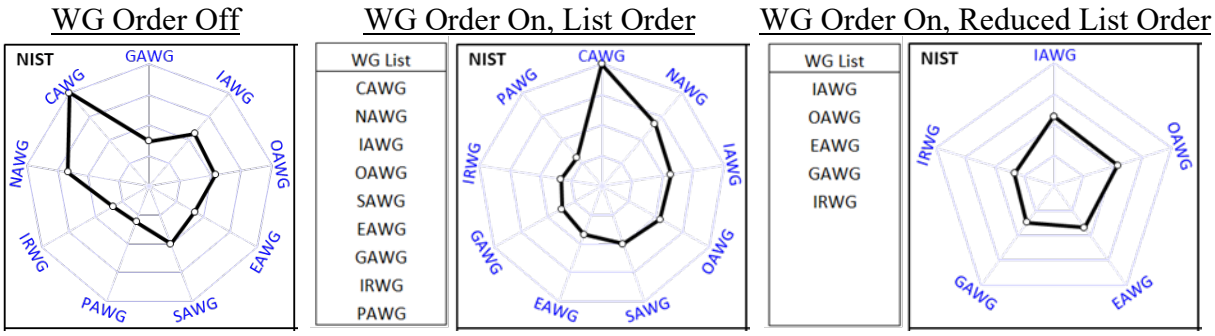
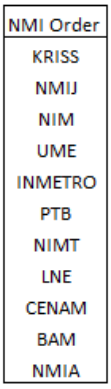


Fig. 36. Target Panels of the *Peer_Priorities* Chart with Various WG Orderings.

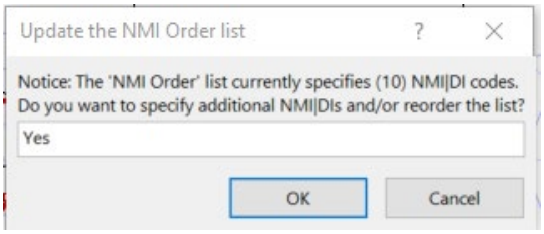
12.3.9. NMI Order: Which NMI|DIs and in What Order



The "NMI Order:" checkbox interacts with "NMI List" to enable specifying which eleven of the other NMI|DIs are displayed and the order in which they are displayed. This option is intended to facilitate changes in participation priorities among a fixed group of NMI|DIs over time.

When "checked", NMI List is ignored and ratios are displayed for the eleven NMI|DIs with participation priorities that are most similar to those of the target NMI|DI. The Segments for these NMI|DIs are arranged in order of decreasing similarity (see Section 12.4), with the most similar in the middle of the top row and the eleventh-most-similar to the right in the bottom row.

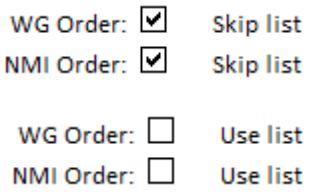
When not "checked", the NMI List sets which NMI|DIs are displayed, with the segments running from the top middle to the bottom right. As long as the *CCQM_Retrospectoscope* database contains results submitted by an NMI|DI in at least one study, the NMI|DI's participation ratios will be displayed even if the NMI|DI did not participate during the specified time period.



Because the *Priorities* chart is divided into twelve segments and the first segment is reserved for the target NMI|DI, the "NMI Order" list holds a maximum of eleven entries. Since the target NMI|DI cannot be a member of the list, the list may need to be updated when the target NMI|DI is changed. If the new target NMI|DI is a member of the list, it is deleted from the list and the subsystem will ask whether the user wants to add to the list:

- If the response is No, the subsystem first displays the results for the NMI|DIs in the list and fills out the available segments with the unlisted NMI|DI(s) that have participation priorities most similar (see 12.4) to those of the target NMI|DI.
- If the response is Yes, the subsystem issues a prompt and the focus returns to the user.

12.3.10. WG Order and NMI Order Status Indicators



As an aid to keeping track of whether the WG and NMI Lists dictate which WGs and NMIs are being displayed, the status of each list is displayed to the right of the corresponding checkbox. When "checked", the lists are ignored. When not "checked", the lists are used.

12.4. Participation Priority Metric

All of the NMI|DIs that have participated in at least one of the selected studies are arranged by the similarity of their participation priorities to those of the target NMI|DI. To facilitate ordering from closest to least close, the ordering metric is estimated as a composite distance, D_{other}, across all of the WGs currently included in the analysis:

$$D_{\text{other}} = n_{\text{unshared}} + \sqrt{\sum_{i}^{n_{\text{shared}}} \left(r_{\text{target},i} - r_{\text{other},i}\right)^2} \Big/ n_{\text{shared}}$$

where n_{unshared} is the number of WGs in which either the target NMI|DI participates and the other NMI|DI does not or the target NMI|DI does not participate and the other NMI|DI does, n_{shared} is the number of WGs in which either both NMI|DIs participate or neither does, i indexes across the WGs, $r_{\text{target},i}$ is the target NMI|DI's participation rate in the i^{th} WG, and $r_{\text{other},i}$ is the other NMI|DI's participation rate in the i^{th} WG.

If the "NMI Order:" checkbox is checked, the D_{other} value for each of the listed NMI|DIs is replaced by its rank within the list divided by 1000. This ensures that the listed NMI|DIs are listed before any non-listed NMI|DI if the NMI List contains fewer than 11 NMI|DIs.

The NMI|DIs are sorted by increasing D_{other}. The *Peer_Priorities* chart displays the participation ratios for the target NMI|DI and the eleven NMI|DIs having the smallest D_{other}.

13. WG_Participations Subsystem

The *WG_Participations* subsystem provides graphical summaries of the number of studies NMI|DIs have participated in. Every study in which an NMI|DI contributed at least one measurement result defines a single participation. This includes results reported in a "parallel pilot study" by NMI|DIs that also reported results in the connected KC or SC. The *WG_Participations* charts, the controls used to specify the datasets evaluated, and the controls used to modify what the charts display are pictured in Fig. 37.

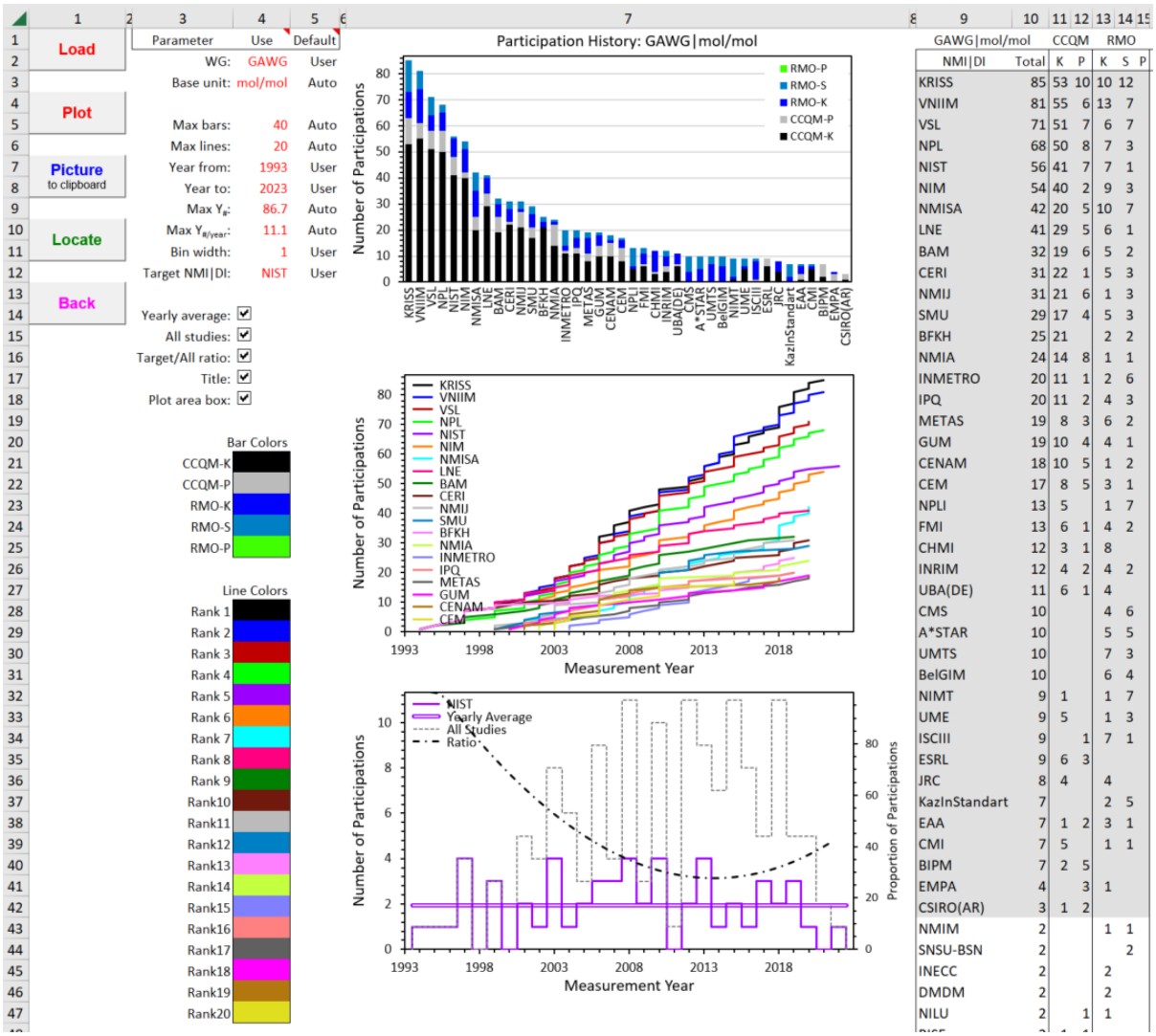


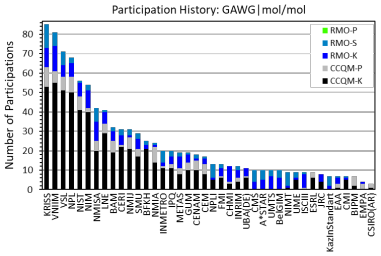
Fig. 37. The *WG_Participations* Dashboard.

Reminder: A data selection or chart display parameter value listed under the "Use" heading can only be changed when its "Default" value is "User". See Section 1.9 for further information.

The information displayed in these charts is derived from the *CCQM_Retrospectoscope*'s datasheets. Keep in mind that there is often a lengthy interval between when participants must report their results (the "measurement year" used by the *CCQM_Retrospectoscope*) and when the report with complete data is published. Participation counts within three years of the current date may (and likely do) under-estimate the number of participations during this period.

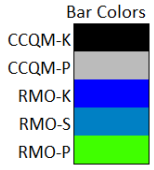
The count of pilot study (P) participations requires that studies be present in the *CCQM_Retrospectoscope*'s database. The complete database, including PSs as well as PPSs, is only available at NIST; elsewhere, only PPS participations will be counted.

13.1. Charts

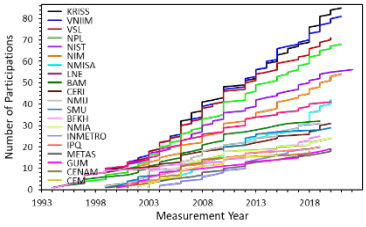


For a given {WG, Base unit}, the worksheet's top chart (chart WPa-1) displays the number and type of studies that the NMI|DIs have participated in. These data are displayed in the form of a stacked bar chart. Participations are grouped by body (CCQM and RMO) and type (Key Comparison, K, Supplementary Comparison, S, and pilot study, P). No distinction is made between pilot studies that have been published in the open literature and those that have not. The NMI|DIs are arranged by decreasing number of participations.

The colors used to distinguish the segments of each NMI|DI's bar are set by the "Bar Colors" area of the worksheet. These colors can be changed at will using Excel's "Fill Color" tool (the "spilling paint can" in the Font menu of the Home tab).

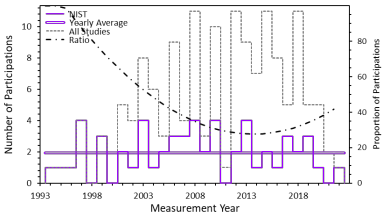


For the up-through-20 NMI|DIs with the most total participations, the middle chart (chart WPa-2) displays the cumulative number of participations as a function of measurement year. As in chart WPa-1, the NMI|DIs are arranged by decreasing number of total participations. The number of NMI|DIs for which a cumulative distribution is displayed is limited to 20 by the space available for the chart legend.

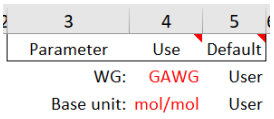


The colors used to distinguish the NMI|DIs are set by the "Line Colors" area of the worksheet. These colors can be changed at will using Excel's "Fill Color" tool.

For a given NMI|DI, the bottom chart (chart WPa-3) displays the number of participations per unit time period as a function of measurement year. As options, the NMI|DI's yearly average participation and the histogram for all possible participations (that is, the total number of studies with a measurement year within a specified interval) can also be displayed. The data are displayed as histograms. The color of the histogram for the specified NMI|DI is the color used for that NMI|DI in chart WPa-2.



13.2. Participation Selection Parameters



In addition to the options described in Sections 2.4.1.2 and 2.4.1.3, this subsystem supports use of "All" settings for both the **WG** and **Base unit** parameters. If a particular **WG** is specified, setting **Base unit** to "All" will include participations in all of the WG's studies regardless of the measurement units. Setting **WG** to "All" includes all participations regardless of WG or measurement units, as shown in Fig. 38.

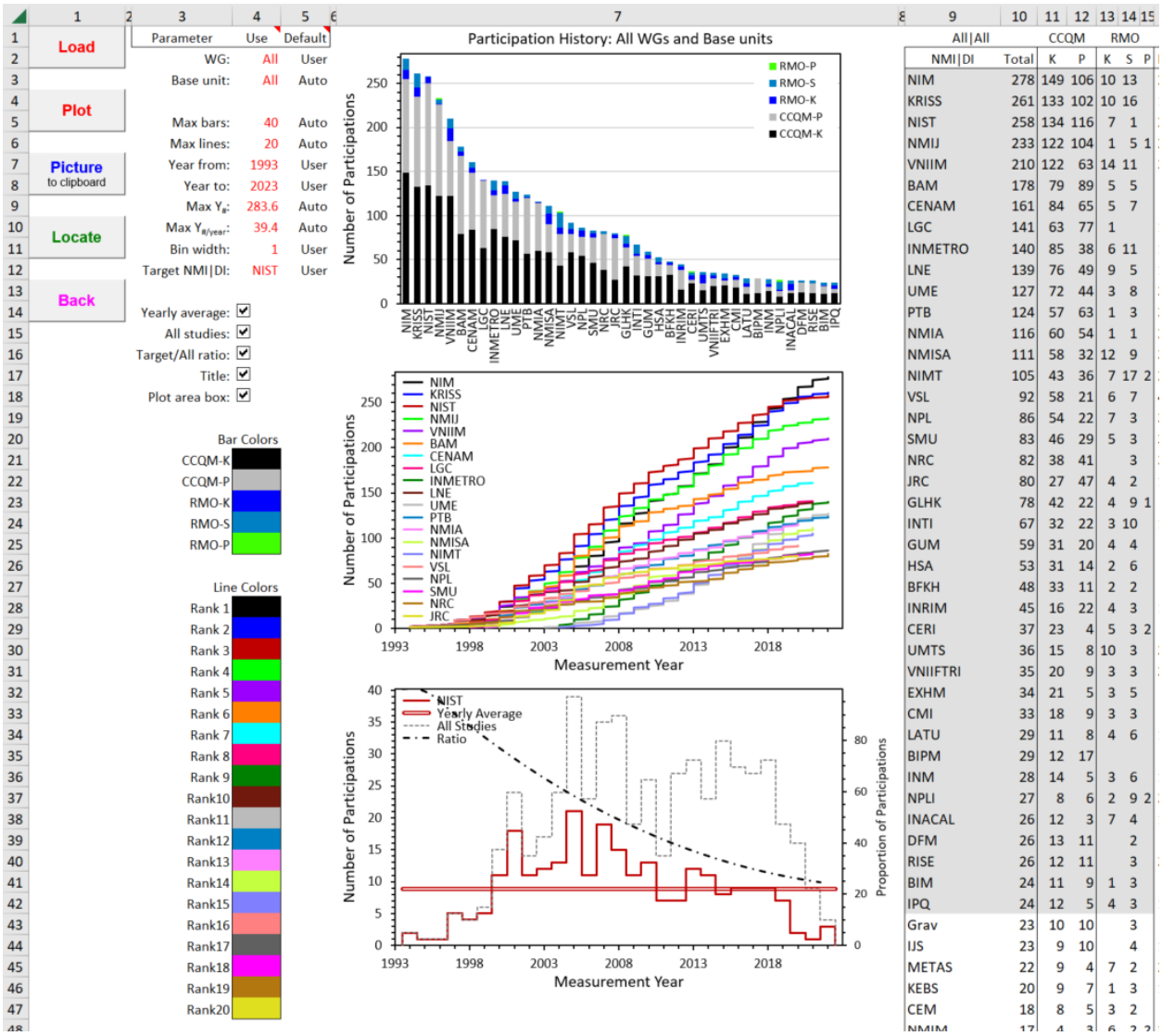


Fig. 38. The *WG_Participations* Dashboard With WG and Base Unit Set to "All".

13.3. Chart Display Parameters

The *WG_Participations* worksheet contains eight chart display parameters. Changes to these values are not evaluated or implemented until the **Plot** button is clicked.

13.3.1. Max bars: Number of NMI|DIs Displayed in Chart WPa-1

While there is no maximum number of NMI|DIs that have participated in at least one study, there is a maximum number that can be meaningfully displayed (about 40). The value of the "Max bars" parameter enables displaying fewer bars.

13.3.2. Max lines: Number of NMI|DIs Displayed in Chart WPa-2

At its current 3-inch height, chart WPa-2 accommodates showing labels of the cummulative distributions for at most 20 NMI|DIs. The value of the "Max lines" parameter enables displaying fewer lines.

13.3.3. Year from and Year to: X-Axis Display Dates

By default, the minimum and maximum measurement years displayed in charts WPa-2 and WPa-3 are those of the earliest and most recent of the selected studies. However, to facilitate comparisons across {WG, Base units}, values of the "Year from" and "Year to" parameters enable setting the values to specified values with the proviso that the interval defined by user-specified values must include the interval from the earliest to the latest of the selected studies.

13.3.4. Max $Y_{\#}$: Y-axis Maximum for Charts WPa-1 and WPa-2

By default, the maximum Y-axis value for charts WPa-1 and WPa-2 is set by the NMI|DI having the largest number of participations. However, to facilitate comparisons across {WG, Base units}, the value of the "Max $Y_{\#}$" parameter enables setting the maximum to a specified value. Changing the maximum does not affect what data are selected for analysis.

13.3.5. Max $Y_{\#/year}$: Y-axis Maximum for Chart WPa-3

By default, the maximum Y-axis value for chart WPa-3 is set by the bin of the histogram that contains the largest number of participations. If "All studies" is active (Section 13.5.2), this is the largest number of possible studies having the specified {WG, Base unit}, otherwise it is the largest number of participations by any of the NMI|DIs. However, to facilitate comparisons across different histogram bin widths (Section 13.3.6) and/or {WG, Base units}, the value of the "Max $Y_{\#/year}$" parameter enables setting the maximum to a specified value. Changing the maximum does not affect what data are available for display.

13.3.6. Bin width: Width of the Histogram Bins

The value of the "Bin width" parameter sets the number of (contiguous) measurement years included in each bin of the histogram. The default interval is one year; the maximum is five years. The interval must be an integer number of years. Intervals of one, three, and five years are displayed in Fig. 39.

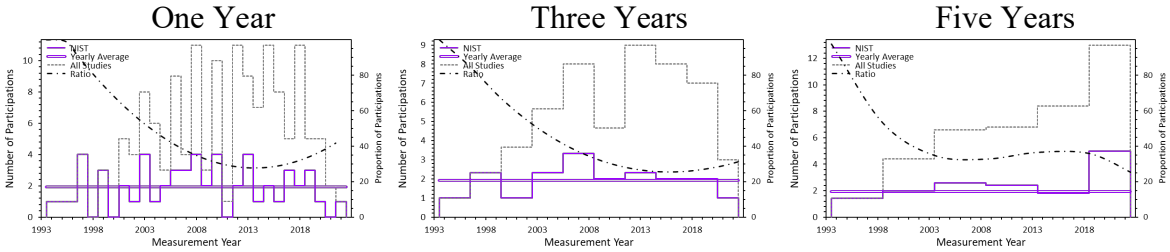


Fig. 39. *WG_Participations* Histograms With Different Bin Widths.

13.4. Target NMI|DI: Specifying the Target NMI|DI

Charts WPa-1 and WPa-2 display results for all NMI|DIs without reference to a targeted NMI|DI, except when the **Locate** button is clicked. When clicked, and if the targeted NMI|DI is among the top 20 participators, the NMI|DI's bar in chart WPa-1 and cumulative distribution in chart WPa-2 are highlighted. The charts with and without NIST selected at the target NMI|DI are displayed in Fig. 40.

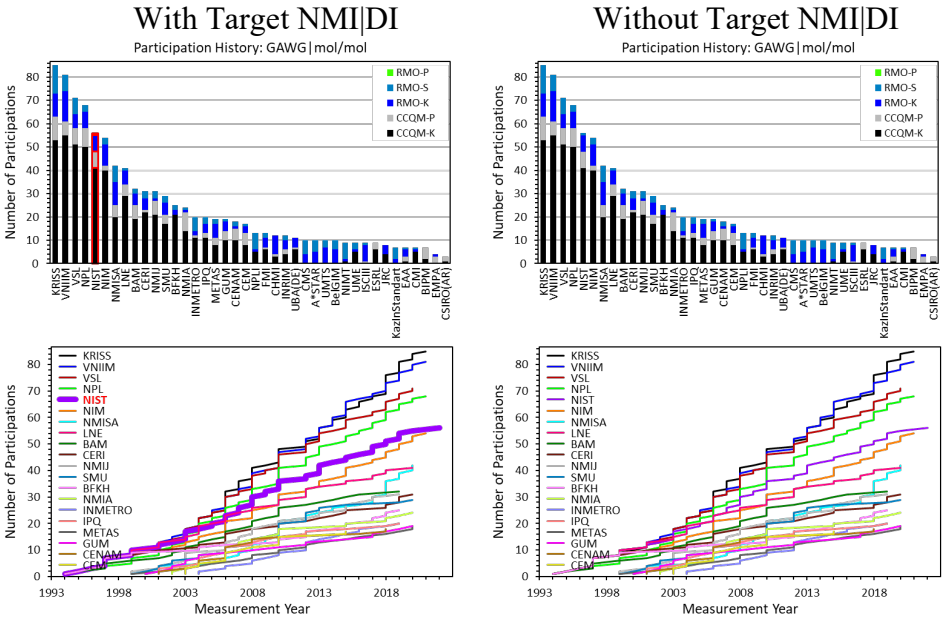


Fig. 40. *WG_Participations* Charts With and Without Target NMI|DI Highlighted.

13.5. Chart Display Checkboxes

The *WG_Participations* worksheet contains three chart display checkboxes in addition to two discussed in Section 2.2.3. Clicking a chart display checkbox invokes an immediate change in the chart display.

13.5.1. Yearly Average

Clicking the "Yearly average" checkbox toggles the display of the yearly average number of participations by the target NMI|DI as a horizontal line stretching from the earliest to the most recent participation. The line shares the color of the histogram, which is the same as the color for the NMI|DI's cumulative distribution in chart WPa-2. NIST's histogram with and without the Yearly Average is pictured in Fig. 41.

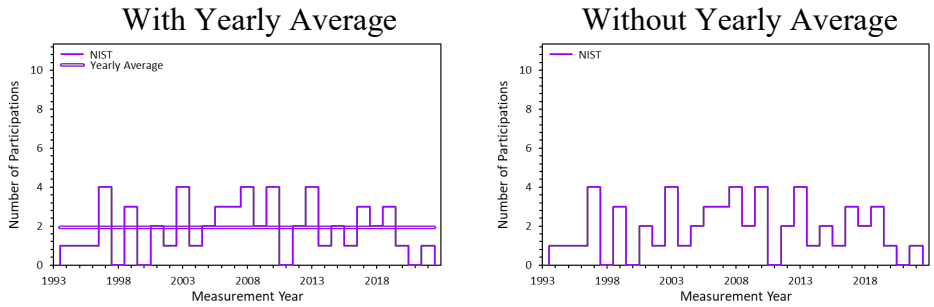


Fig. 41. *WG_Participations* Histograms With and Without Yearly Average.

13.5.2. All studies

Clicking the "All studies" checkbox toggles the display of the histogram of the maximum possible participations for the specified {WG, Base unit}. This histogram is displayed as a dashed light grey line. NIST's histogram with and without the All studies histogram is pictured in Fig. 42.

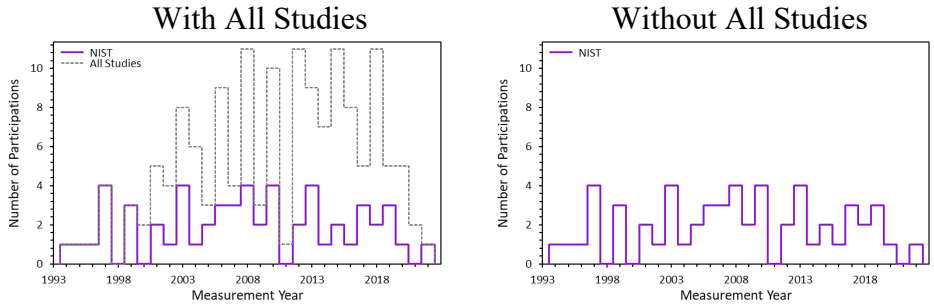


Fig. 42. *WG_Participations* Histograms With and Without All Studies.

Note: When the All studies histogram is toggled off, the default Y-axis scale of chart WPa-3 is set by the NMI|DI with the greatest number of participations within an interval, not by the target NMI|DI. For {GAWG, mol/mol}, the scale-setter is South Korea's Korea Research Institute of Standards and Science (KRISS), as displayed Fig. 43.

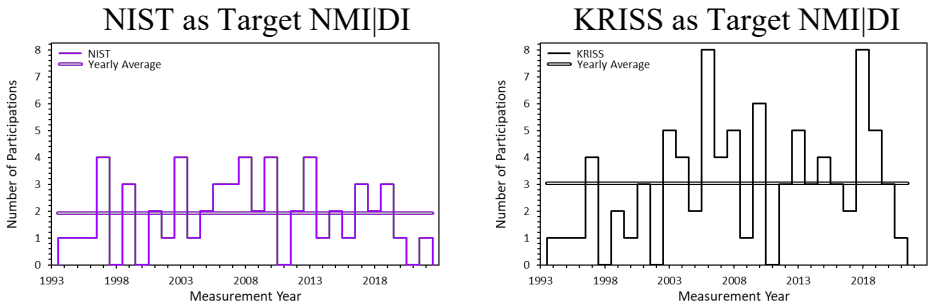


Fig. 43. *WG_Participations* Histograms With Different Target NMI|DIs.

13.5.3. Target/All ratio

Clicking the "Target/All ratio" checkbox when the "All studies" histogram is displayed toggles the display of a polynomial trendline fit to the (number of participations of the target NMI|DI) divided by the (number of possible participations) over the time interval set by the "Bin width" chart display parameter (Section 13.3.6). This ratio is expressed as a percentage, with the (0 to 100) % scale displayed at the right edge of the chart. The trendline is displayed as a dot-dash black line.

NIST's histogram with and without the Target/All ratio line is pictured in Fig. 44.

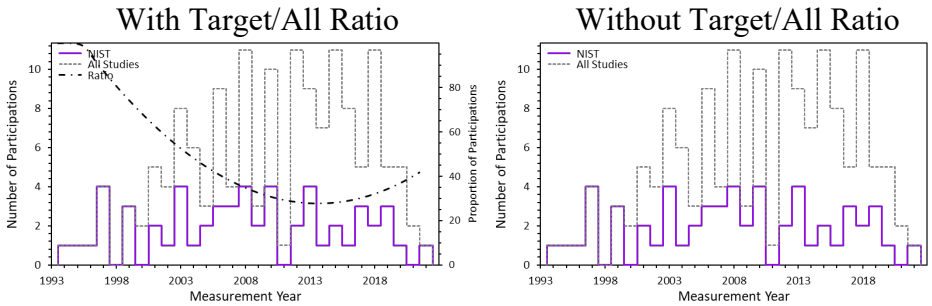


Fig. 44. *WG_Participations* Histograms With and Without the Target/All Ratio Trendline.

14. WG_Coordinations Subsystem

The *WG_Coordinations* subsystem provides graphical summaries of the number of studies NMI|DIs have coordinated (aka "piloted") or co-coordinated. The *WG_Coordinations* charts, the controls used to specify the datasets evaluated, and the controls used to modify what the charts display are pictured in Fig. 45.

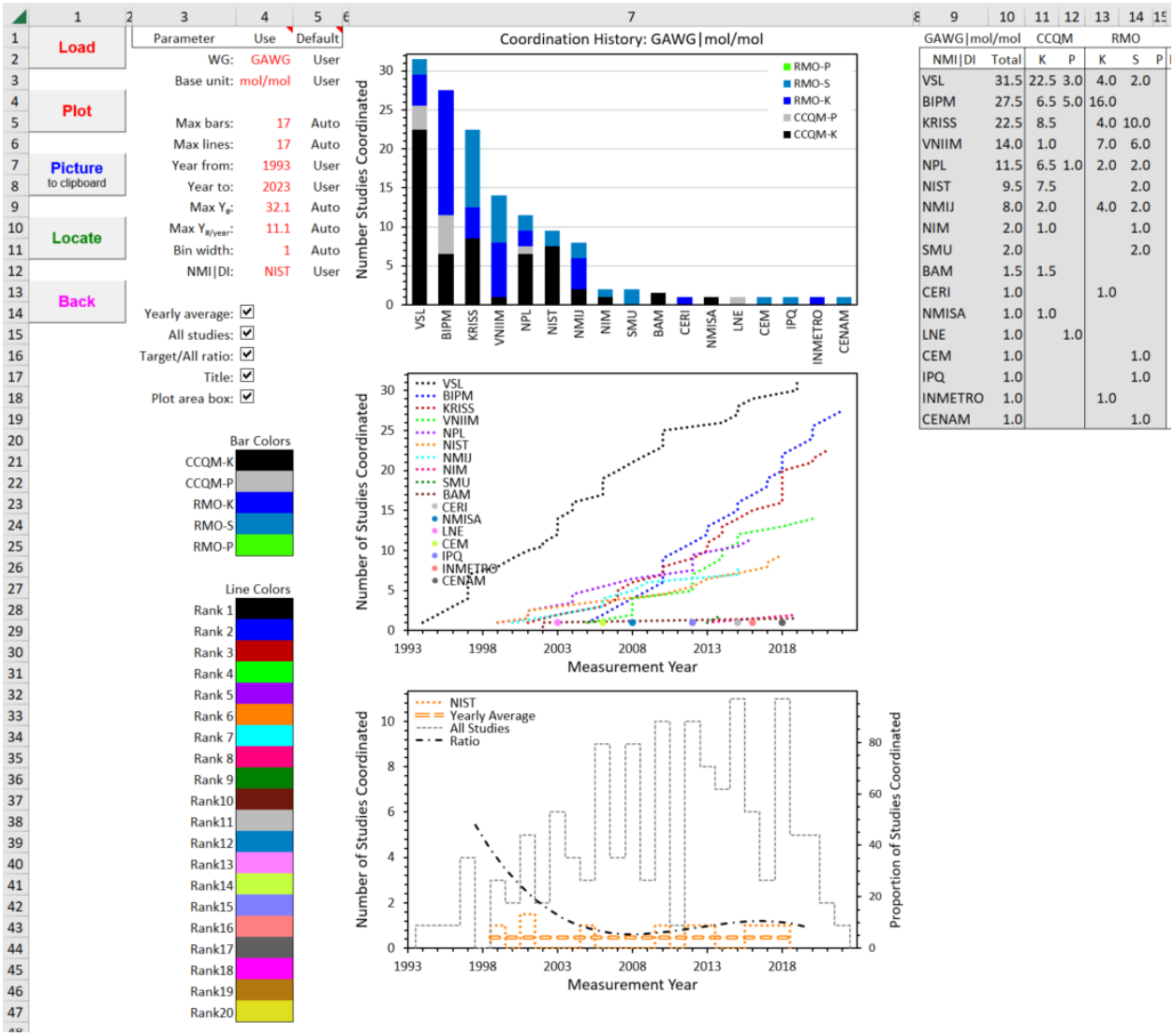


Fig. 45. The *WG_Coordinations* Dashboard.

Reminder: A data selection or chart display parameter value listed under the "Use" heading can only be changed when its "Default" value is "User". See Section 1.9 for further information.

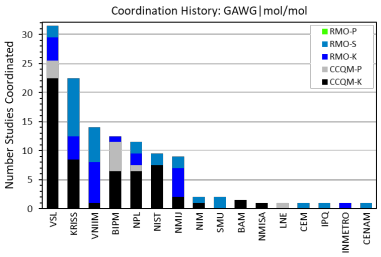
Many studies are co-coordinated. While the effort and resources expended are unlikely to be equally divided among the co-coordinators, there is no practical way to determine who did how much. Therefore, with n NMI|DI co-coordinators for a given study, each is assumed to have contributed $1/n^{th}$ of the effort.

Regardless of when a study was initiated nor how long it took to complete, coordinations are associated only with the year that results were required to be officially submitted.

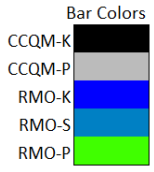
When available, the coordination information is derived from a study's final report, otherwise from the *CCQM_KCs_PSs.xlsx* workbook hosted by the BIPM [16]. Coordination information is stored in the *Datacore_Dates* worksheet. In addition to the information contained within the *CCQM_Retrospectoscope*'s datasheets, the *Datacore_Dates* worksheet includes information about studies that did not publish results, published anonymous results, or have been registered but not yet completed.

In contrast to the definition of participation, parallel pilot studies do not contribute to the coordination count. While such parallel studies do require effort and resources beyond those for just the study that they are allied with, the increase is small compared to the effort required for a truly separate study.

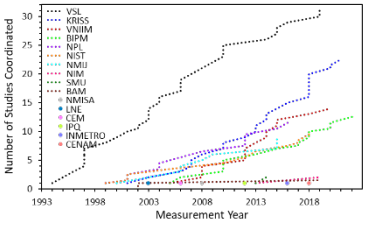
14.1. Charts



For a given {WG, Base unit}, the worksheet's top chart (chart WC-1) displays the number and type of studies that the NMI|DIs coordinated. These data are displayed in the form of a stacked bar chart. Coordinations are grouped by body (CCQM and RMO) and type (Key Comparison, K, Supplementary Comparison, S, and pilot study, P). No distinction is made between pilot studies that have been published in the open literature and those that have not. The NMI|DIs are arranged by decreasing number of total coordinations.

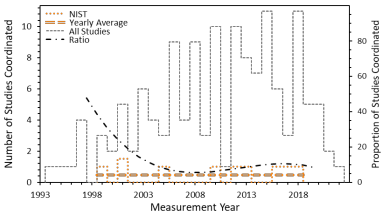


The colors used to distinguish the segments of each NMI|DI's bar are set by the "Bar Colors" area of the worksheet. These colors can be changed at will using Excel's "Fill Color" tool (the "spilling paint can" in the Font menu of the Home tab).



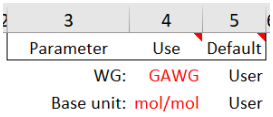
For the up-to-20 NMI|DIs with the most coordinations, the middle chart (chart WC-2) displays the cumulative number of coordinations as a function of measurement year. As in chart WC-1, the NMI|DIs are arranged by decreasing number of total coordinations. The number of NMI|DIs displayed is limited to 20 by the space available for the chart legend.

The colors used to distinguish the NMI|DIs are set by the "Line Colors" area of the worksheet. These colors can be changed at will using Excel's "Fill Color" tool. To help distinguish the cumulative distributions for coordinations from those for participations (see Section 13), the coordination lines are dotted rather than solid.



For a given NMI|DI, the bottom chart (chart WC-3) displays the number of coordinations per unit time period as a function of measurement year. The number of possible coordinations (that is, the total number of studies with a measurement year within a specified interval) can be displayed. The data are displaced as histograms. The target's yearly average number of coordinations can also be displayed, as well as a polynomial trendline fit to the ratio between the number of the target's participations and the number of possible coordinations. The color of the histogram and yearly average for the target NMI|DI is the color used for that NMI|DI in chart WC-2.

14.2. Coordination Selection Parameters



In addition to the options described in Sections 2.4.1.2 and 2.4.1.3, this subsystem supports use of "All" settings for both the WG and Base unit parameters. If a particular WG is specified, setting Base unit to "All" will include coordinations in all the studies coordinated by that WG regardless of the measurement units. Setting WG to "All" includes all coordinations regardless of WG or measurement units, as shown in Fig. 46.

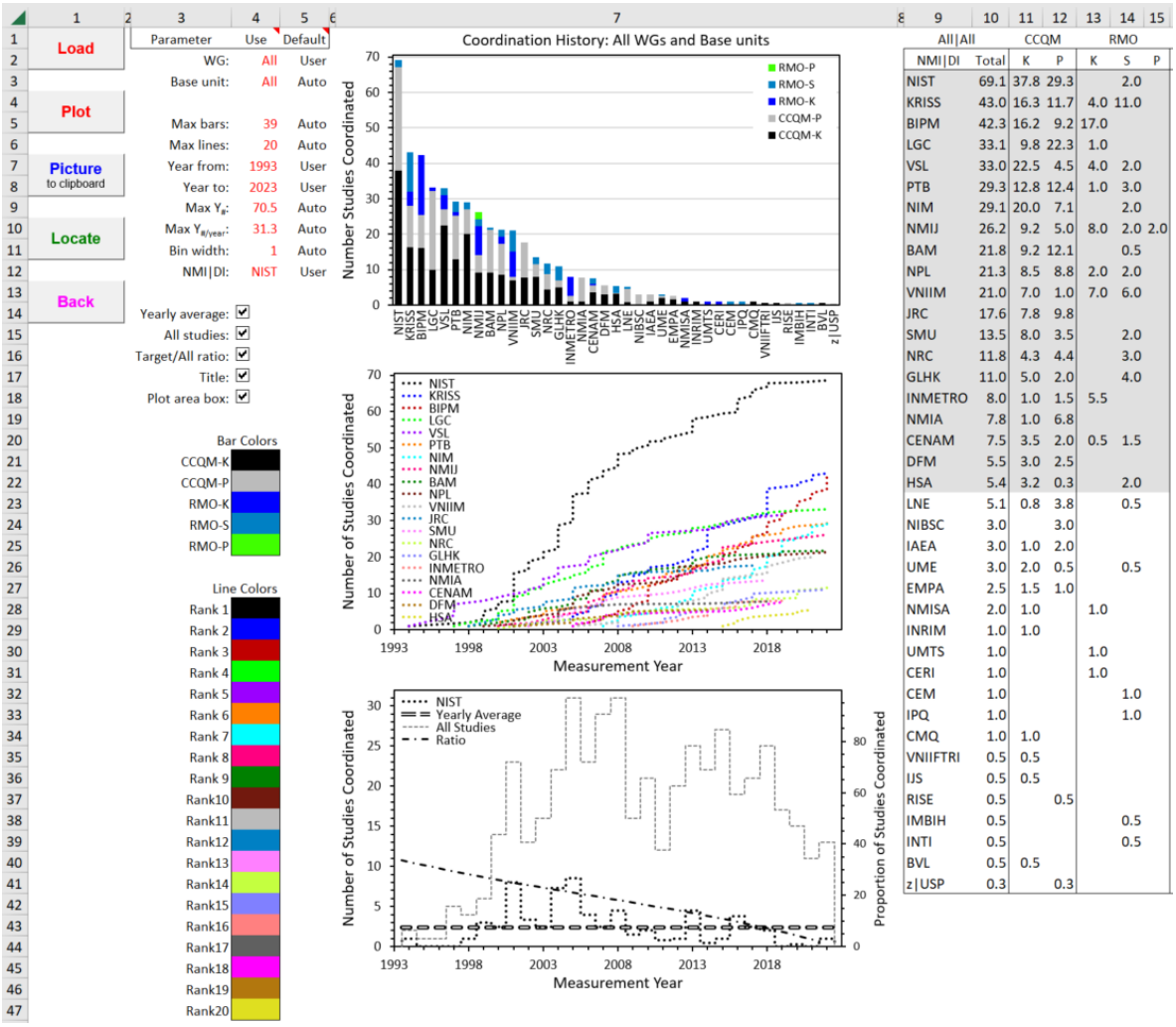


Fig. 46. The *WG_Coordinations* Dashboard With WG and Base Unit Set to "All".

14.3. Chart Display Parameters

The *WG_Coordinations* worksheet contains six chart display parameters. Changes to these values are not evaluated or implemented until the **Plot** button is clicked.

14.3.1. Max bars: Number of NMI|DIs Displayed in Chart WC-1

While there is no maximum number of NMI|DIs that have coordinated at least one study, there is a maximum number that can be meaningfully displayed (about 40). The value of the "Max bars" parameter enables enables displaying fewer bars.

14.3.2. Max lines: Number of NMI|DIs Displayed in Chart WC-2

At its current 3-inch height, chart WC-2 accommodates showing cummulative distributions for at most the 20 NMI|DIs that have coordinated the most studies. The value of the "Max lines" parameter enables enables displaying fewer lines.

14.3.3. Year from and Year to: X-Axis Display Dates

By default, the minimum and maximum measurement years displayed in charts WC-2 and WC-3 are those of the earliest and most recent of the selected studies. However, to facilitate comparisons across {WG, Base units}, values of the "Year from" and "Year to" parameters enable setting the values to specified values with the proviso that the interval defined by user-specified values must include the interval from the earliest to the latest of the selected studies.

14.3.4. Max $Y_{\#}$: Y-axis Maximum for Charts WC-1 and WC-2

By default, the maximum Y-axis value for charts WC-1 and WC-2 is set by the NMI|DI having the largest number of coordinations. However, to facilitate comparisons across {WG, Base units}, the value of the "Max $Y_{\#}$" parameter enables setting the maximum to a specified value. Changing the maximum does not affect what data are selected for analysis.

14.3.5. Max $Y_{\#/year}$: Y-axis Maximum for Chart WC-3

By default, the maximum Y-axis value for chart WC-3 is set by the bin of the histogram that contains the largest number of coordinations to be displayed. If "All studies" is active (Section 14.5.2), this is the largest number of possible sponsored by the specified {WG, Base unit}, otherwise it is the largest number of coordinations by any of the NMI|DIs. However, to facilitate comparisons across different "Year intervals" (histogram bin widths, Section 14.3.6) and/or {WG, Base units}, the value of the "Max $Y_{\#/year}$" parameter enables setting the maximum to a specified value. Changing the maximum does not affect what data are available for display.

14.3.6. Bin width: Width of the Histogram Bins

The value of the "Bin width" parameter sets the number of (contiguous) measurement years included in each bin of the histogram. The default interval is one year; the maximum is five years. The interval must be an integer number of years. Intervals of one, three, and five years are displayed in Fig. 47.

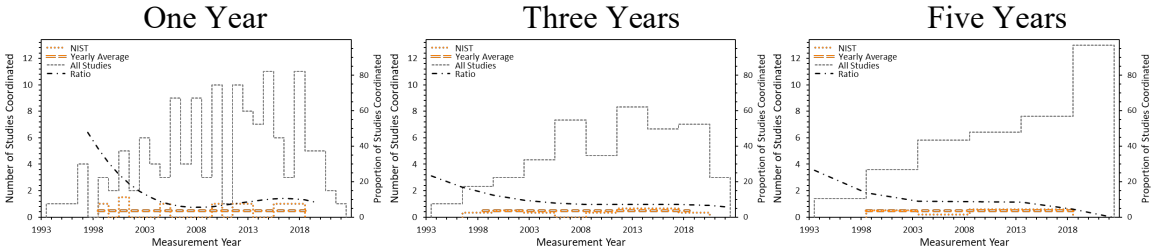


Fig. 47. *WG_Coordinations* Histograms With Different Year Intervals.

14.4. NMI|DI: Specifying the Target NMI|DI

NMI|DI: NIST User

Charts WC-1 and WC-2 display results for all NMI|DIs without reference to a targeted NMI|DI, except when the **Locate** button is clicked. When clicked, and if the targeted NMI|DI is among the top 20 participators, the NMI|DI's bar in chart WC-1 and cumulative distribution in chart WC-2 are highlighted. The charts with and without NIST selected at the target NMI|DI are displayed in Fig. 48.

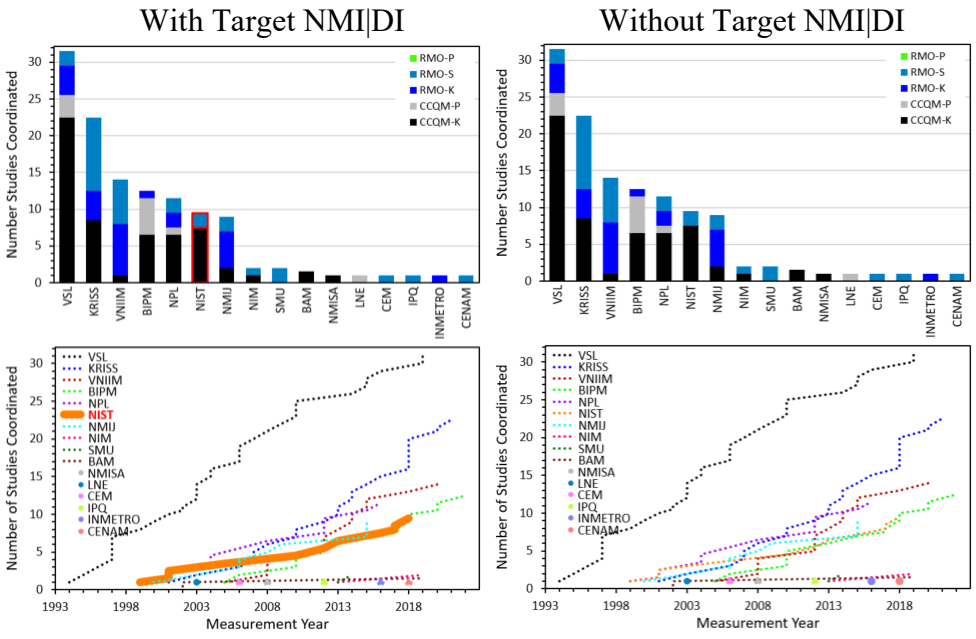


Fig. 48. *WG_Coordinations* Charts With and Without Target NMI|DI Highlighted.

14.5. Chart Display Checkboxes

The *WG_Coordinations* worksheet contains three chart display checkboxes in addition to two discussed in Section 2.2.3. Clicking a chart display checkbox invokes an immediate change in the chart display.

14.5.1. Yearly Average

Clicking the "Yearly average" checkbox toggles the display of the yearly average number of coordinations by the target NMI|DI as horizontal line stretching from the earliest to the most recent coordination. The line shares the color of the histogram, which is the same as the color for the NMI|DI's cumulative distribution in chart WC-2. NIST's histogram with and without the Yearly Average is pictured in Fig. 49.

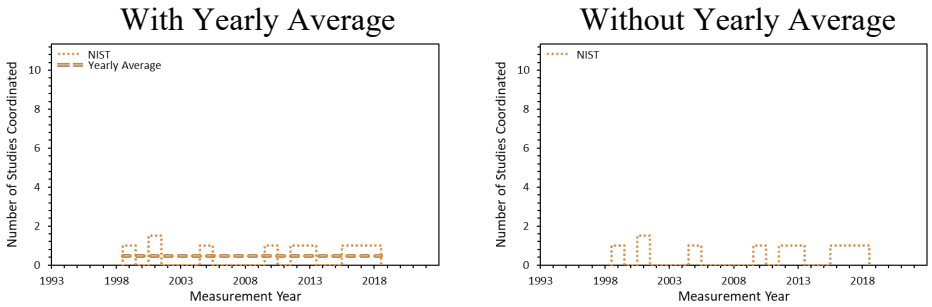


Fig. 49. *WG_Coordinations* Histograms With and Without Yearly Average.

14.5.2. All studies

Clicking the "All studies" checkbox toggles the display of the histogram of the maximum possible coordinations for the specified {WG, Base unit}. This histogram is displayed as a dashed light grey line. NIST's histogram with and without the All studies histogram is pictured in Fig. 50.

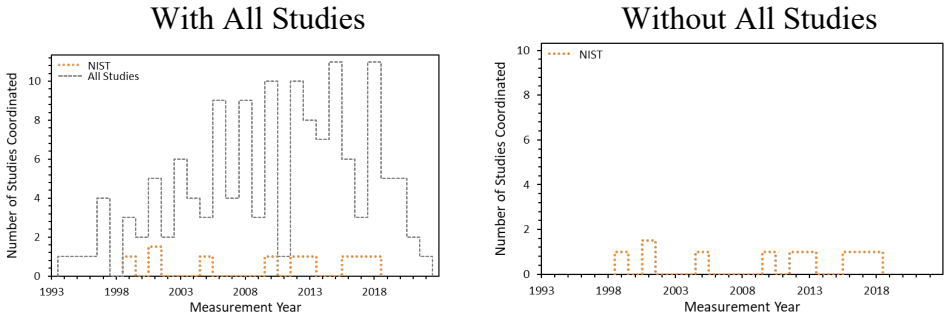


Fig. 50. *WG_Coordinations* Histograms With and Without the All Studies.

Note: When the All studies histogram is inactive, the Y-axis scale of chart WC-3 is set by the NMI|DI with the greatest number of coordinations within an interval, not by the target NMI|DI. This is not necessarily the NMI|DI that has coordinated the most studies. For {GAWG, mol/mol} the Netherland's Van Swinden Laboratorium (VSL) has provided the most coordinations (see Fig. 45). However, as shown in Fig. 51, KRISS has provided the most within a single measurement year.

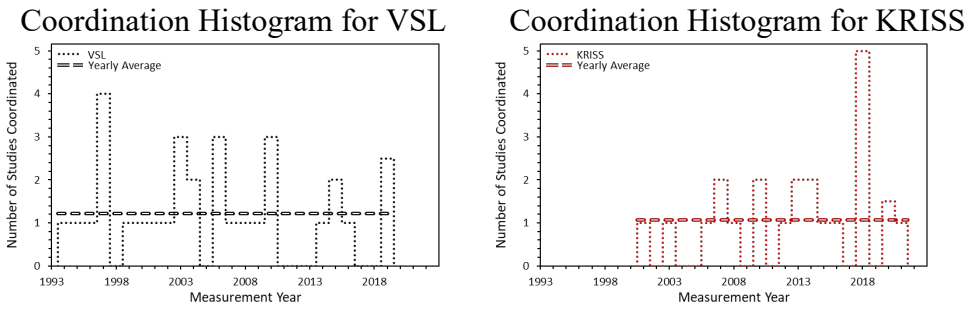


Fig. 51. *WG_Coordinations* Histograms for VSL and KRISS.

14.5.3. Target/All ratio

Clicking the "Target/All ratio" checkbox when the "All studies" histogram is displayed toggles the display of a polynomial trendline fit to the (number of coordinations of the target NMI|DI) divided by the (number of possible coordinations) over the time interval set by the "Bin width" chart display parameter (Section 14.3.6). This ratio is expressed as a percentage, with the (0 to 100) % scale displayed at the right edge of the chart. The trendline is displayed as a dot-dash black line.

NIST's histogram with and without the Target/All ratio line is pictured in Fig. 44.

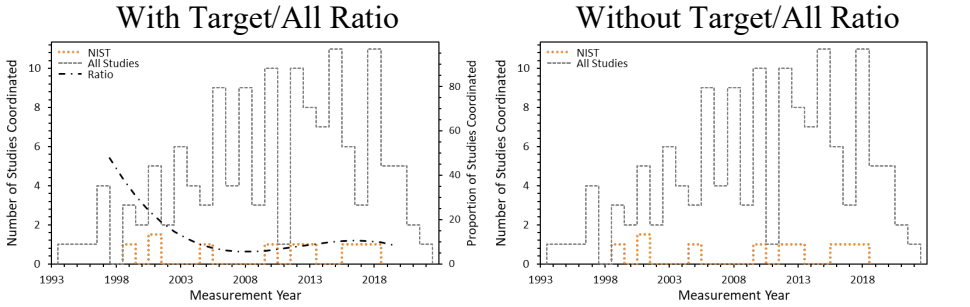


Fig. 52. *WG_Coordinations* Histograms With and Without the Target/All Ratio Trendline.

15. WG_Precision Subsystem

The *WG_Precision* charts, the controls used to specify the datasets evaluated, and the controls used to modify what the charts display are pictured in Fig. 53. The in-common data selection and chart display parameters and controls are discussed in Section 2.

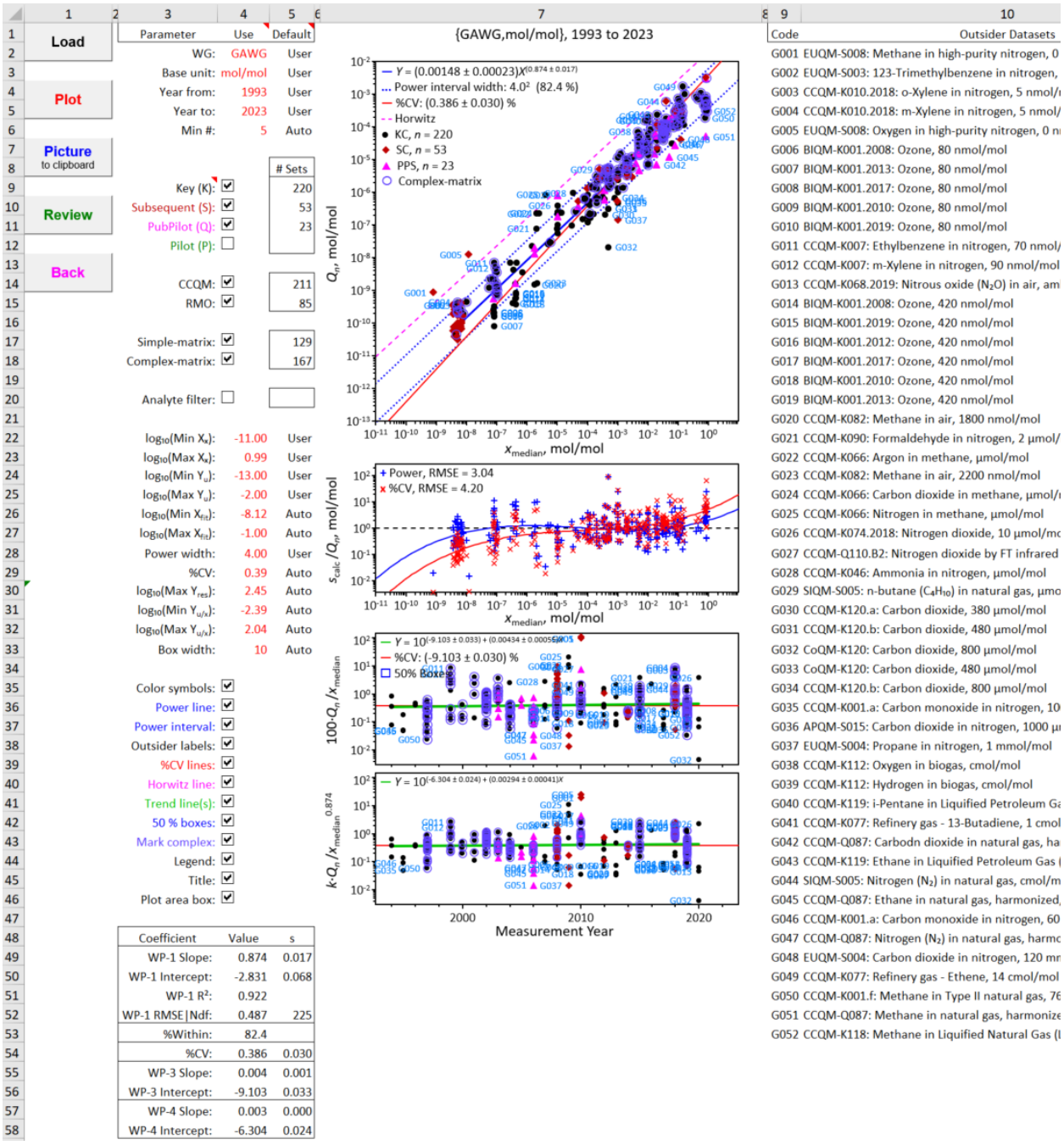


Fig. 53. The *WG_Precision* Dashboard.

Reminder: A data selection or chart display parameter value listed under the "Use" heading can only be changed when its "Default" value is "User". See Section 1.9 for further information.

While similar to *Lab_Uncertainty*, this subsystem characterizes interlaboratory reproducibility for a given WG as a function of consensus location rather than a given NMI|DI's reported standard uncertainty as a function of reported value. The reproducibility standard deviation is estimated as the robust Q_n and location as the robust median, x_{median}.

15.1. Charts

The *WG_Precision* worksheet provides four charts for datasets that meet all the selection criteria. Each symbol in a chart represents measurement results for a single dataset.

The top chart (chart WPr-1) displays the robust Q_n, as a function of x_{median}. Reproducibility for many chemical measurements is often assumed to be proportional to the analyte concentration; i.e., the relative reproducibility (%CV, here defined as %CV = $100 \cdot Q_n / x_{median}$) is assumed to be constant. Horwitz [3] and Thompson [4,2] observed that the relationship is better described as proportional to concentration raised to a power, p, less than one: Q_n / x_{median}^{p}. Chart WPr-1 visualizes the relevant data and the potential relationships.

The chart (chart WPr-2) located immediately below chart WPr-1, displays the residuals between the reported uncertainties and predictions made using two uncertainty function models for the relationship between Q_n and x_{median} [2]. The residuals are calculated as $\log_{10}(s_{calc}) - \log_{10}(Q_n)$; since these differences are plotted on a logarithmic Y-axis, the axis is labeled with the linearized formulation s_{calc}/Q_n.

The commonly assumed "constant coefficient of variation (%CV), $Q_n = \beta_0 \, x_{median}$, is a one-parameter power-law curve where the power is 1 and β_0 is the assumed %CV. The two-parameter power-law curve, $Q_n = \beta_0 \, x_{median}^{\beta_1}$ has been observed to describe the relationship between measurement reproducibility and value of the measurand expressed as a mass- or mole-fraction in many interlaboratory studies of many different measurands [3,4,5]. The values for the parameters of both functions are derived from the results shown in chart WPr-1.

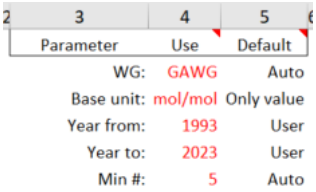
The next chart (chart WPr-3) displays the relative reported uncertainty, $100 \cdot Q_n / x_{median}$, as a function of measurement year. In addition to visualizing when measurements were made and the median %CV during the specified time period, the chart enables estimating the change in the magnitude of relative reproducibility over time.

The bottom chart (chart WPr-4) displays a value-corrected relative reproducibility expressed as %CV, $100 \cdot Q_n / x_{median}^{\beta_1}$, as a function of year, where the value of the β_1 exponent is derived from the results shown in chart WPr-1. If the two-parameter power-law curve is an appropriate uncertainty function for the selected data, the scatter and any observed rate of change should be somewhat reduced from that displayed in chart WPr-3.

Note: For β_1 less than one, Q_n / x_{median}^{p} will be larger than Q_n / x_{median}. Since $1^{\beta_1} = 1$ for all exponent values, the difference between $100 \cdot Q_n / x_{median}$ and $100 \cdot Q_n / x_{median}^{\beta_1}$ will increase as x_{median} increasingly differs from 1. This complicates comparing the results displayed in charts WPr-3 and WPr-4, hence the transformed results displayed in chart WPr-4 are scaled by a constant factor to have the same %CV as the results displayed in chart WPr-3.

For many of the {WG, Base unit} groups studied by the CCQM, the range of magnitudes is quite large; e.g., exemplar GAWG data span eleven orders-of-magnitude. To enable visualizing the entire range of $\{x_{median}, Q_n\}$ values, these charts display the $\log_{10}$-transformation of the values.

15.2. Additional Data Specification Parameter



Parameter	Use	Default
WG:	GAWG	Auto
Base unit:	mol/mol	Only value
Year from:	1993	User
Year to:	2023	User
Min #:	5	Auto

In additional to the four in-common parameters described in Section 2.4.1, there is one additional data specification parameter.

15.2.1. Min #: Minimum Number of Datasets Required

The "Min #" parameter sets the minimum number of valid values for a dataset to be included in the *WG_Precision* analysis. This enables restricting the analysis to datasets that provide enough information for (reasonably) reliable precision estimates. The smallest allowed value for this parameter is 3; the default value is 5. The is no upper bound, but the larger the number of valid values required the fewer the number of suitable datasets.

15.3. Additional Chart Display Parameters

$\log_{10}$(Min X_x):	-12.00	User
$\log_{10}$(Max X_x):	1.00	User
$\log_{10}$(Min Y_u):	-13.00	User
$\log_{10}$(Max Y_u):	0.00	User
$\log_{10}$(Min X_{fit}):	-8.12	Auto
$\log_{10}$(Max X_{fit}):	-1.00	Auto
Power width:	8.20	Auto
%CV:	0.44	Auto
$\log_{10}$(Max Y_{res}):	2.39	Auto
$\log_{10}$(Min $Y_{u/x}$):	-2.36	Auto
$\log_{10}$(Max $Y_{u/x}$):	2.04	Auto
Box width:	10	Auto

The *WG_Precision* worksheet contains 12 chart display parameters. The first two of these controls pertain to charts WPr-1 and WPr-2; the next six pertain solely to chart WPr-1, the ninth pertains solely to chart WPr-2, and the last three pertain to charts WPr-3 and WPr-4. Changes to these values are not evaluated or implemented until the **Plot** button is clicked.

15.3.1. $\log_{10}$(Min X_x) and $\log_{10}$(Max X_x): X-axis Limits for Charts WPr-1 and WPr-2

The minimum and maximum limits for the X-axis (consensus location calculated using the robust median estimator) in charts WPr-1 and WPr-2 are specified by the values of the "$\log_{10}$(Min X_x)" and "$\log_{10}$(Min X_x)" parameters. The default values for these limits are the $\log_{10}$-transformed minimum and maximum medians of the selected data. Modifying the limits of either axis does not affect what data are selected for analysis.

15.3.2. $\log_{10}$(Min Y_u) and $\log_{10}$(Max Y_u): Y-axis Limits for Chart WPr-1

The minimum and maximum display limits for the Y-axis (reproducibility standard deviation calculated using the robust Q_n estimator) are specified by the values for the "$\log_{10}$(Min Y_u)" and "$\log_{10}$(Max Y_u)" parameters. The default values for these limits are the $\log_{10}$-transformed minimum and maximum Q_n values of the selected data. Modifying the limits of either axis does not affect what data are selected for analysis.

15.3.3. $\log_{10}$(Min X_{fit}) and $\log_{10}$(Max X_{fit}): X-axis Regression Limits

For some {WG, Base unit} groups, the measurement processes used for the major component in relatively "pure" materials differ qualitatively from those for minor components; likewise, the reproducibility of very low quantity values may not follow the trend shown by middling values [4]. The values of the "$\log_{10}$(Min X_{fit})" and "$\log_{10}$(Max X_{fit})" parameters specify the lower and upper bounds on the values used to estimate the power-law curve relating Q_n as a function of x_{median}. The default values, taken from [4], are -8.12 (a fractional value of $\approx 7.6 \times 10^{-9}$) and -1.0 (a fractional value of 0.1).

Modifying these regression limits does not affect the display of the $\{x_{median}, Q_n\}$ data, but does affect which data are used to estimate the power-law curve.

15.3.4. Power width: Outlier Identification Interval

One of the optional elements for chart WPr-1 is a least-squares fit of Q_n as a power-law function of x_{median}: $Q_n = \beta_0 \, x_{median}^{\beta_1}$ [2]. Parameterization is accomplished by linear regression on $\log_{10}$-transformed values: $\log_{10}(Q_n) = \log_{10}(\beta_0) + \beta_1 \log_{10}(x_{median})$. A symmetric interval centered on the power-law curve is used to identify outsider datasets. Results within this interval can be considered as having "routine" reproducibility, results below it identify datasets where the participants' results are in exceptionally good agreement, and results above it identify datasets where the results are in relatively poor agreement.

Since the chart displays $\log_{10}$-transformed data, the value of the "Power width" parameter specifies the width of the interval as a multiplicative factor. A width value (call it f) defines an interval about the power-law curve that includes all datasets with Q_n values that are within a factor f of the value predicted by the power-law; i.e., the interval includes the observed $\{x_{median}, Q_n\}$ values from $(\beta_0 \, x_{median}^{\beta_1})/f$ to $f(\beta_0 \, x_{median}^{\beta_1})$. The total width of the interval is thus a factor of f^2.

The default power width is twice the RMSE of the power-law fit, a value that is expected to provide an interval that includes about 95 % of the $\{x_{median}, Q_n\}$ if they are approximately normally distributed. Transformed into a multiplicative factor, the default value of f is $10^{(2 \cdot \mathrm{RMSE})}$.

15.3.5. %CV: %CV lines

An optional element in all four charts are lines representing either the %CV, $100 \cdot Q_n / x_{median}$, or (for chart WPr-2) the predicted difference between $(\%\mathrm{CV}/100) x_{median}$ and Q_n. The default value for %CV is Median{%CV}, the median of all the reported $100 \cdot Q_n / x_{median}$ values that meet the selection criteria.

15.3.6. $\log_{10}$(Max Y_{res}): Y-axis Limits for Chart WPr-2

The value of the "$\log_{10}$(Max Y_{res})" parameter sets the minimum and maximum for the Y-axis (residuals) of chart WPr-2. Representing the value as g, these endpoints are at $10^{(0 \pm g)}$. The default value for g is the largest absolute residual value for either of the uncertainty functions. Modifying the width of this interval does not affect what data are selected for analysis.

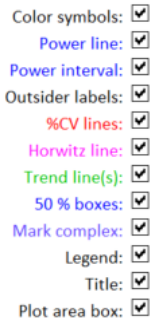
15.3.7. $\log_{10}$(Min $Y_{u/x}$) and $\log_{10}$(Max $Y_{u/x}$): Y-axis Limits for WPr-3 and WPr-4

The values of the "$\log_{10}$(Min $Y_{u/x}$)" and "$\log_{10}$(Max $Y_{u/x}$)" parameters set the minimum and maximum display limits for the Y-axis of chart WPr-3 and the power-law corrected %CV Y-axis of chart WPr-4. The default values for these limits are the minimum and maximum $\log_{10}$-transformed Q_n values of the selected data. Modifying the limits of either axis does not affect what data are selected for analysis.

15.3.8. Box width: 50 % box width for Charts WPr-3 and WPr-4

The value of the "Box width" parameter sets the number of (contiguous) measurement years included in each segment of the optional "50 % boxes" element described in Section 15.3.8. The default interval is five years.

15.4. Additional Chart Display Checkboxes



The *WG_Precision* worksheet contains nine chart display checkboxes in addition to the three discussed in Section 2.2.3. Clicking a chart display checkbox invokes an immediate change in the chart display.

15.4.1. Color symbols

Clicking the "Colored symbols" checkbox enables the toggling between the colored symbols and tall-black symbols: see Fig. 16. The colors used for the four study types are dictated by the font colors of the labels for the study type checkboxes (see Section 2.2). When colored, KC results are solid circles, SC results are solid diamonds, PPS results are solid triangles, and PS results are open squares. When black, all symbols are solid circles.

The colors of the uncertainty function residuals shown in chart WPr-2 are not affected by this control.

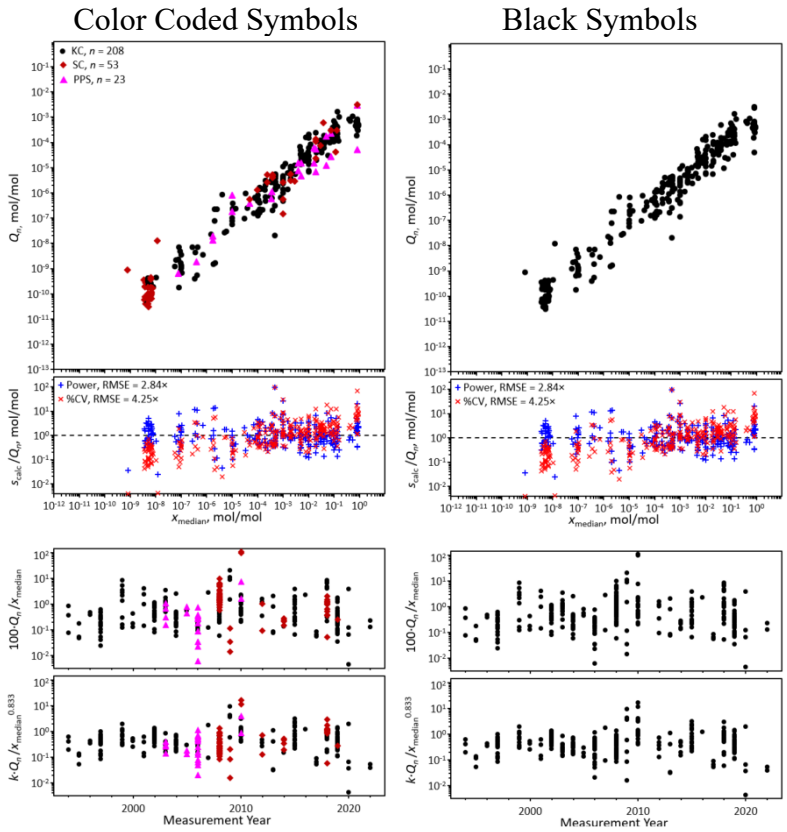
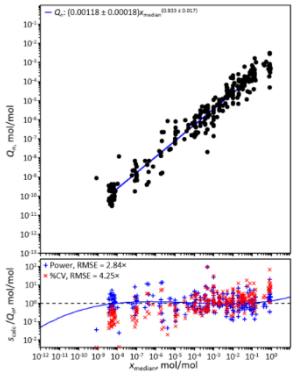


Fig. 54. *WG_Precision* Charts With Color-Coded and All-Black Symbols.

15.4.2. Power line

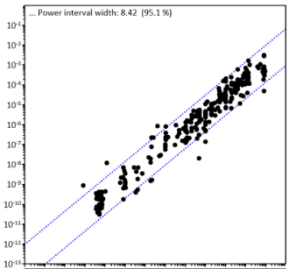


In chart WPr-1, clicking the "Power line" checkbox toggles the display of a regression estimate of the power-law function: $Q_n = \beta_0 \, x_{median}^{\beta_1}$. Since both the x_{median} (X) and Q_n (Y) axes are logarithmic, this is parameterized as: $\log_{10}(Q_n) = \log_{10}(\beta_0) + \beta_1 \cdot \log_{10}(x_{median})$. The X-axis limits of the power-law curve are set by the values of the $\log_{10}$(Min X_{fit}) and $\log_{10}$(Max X_{fit}) parameters described in Section 15.3.3.

In chart WPr-2, clicking the checkbox enables display of a cubic polynomial regression fit of the residual ($\log_{10}(\beta_0) + \beta_1 \cdot \log_{10}(x_{median})$ - $\log_{10}(Q_n)$) to $\log_{10}(x_{median})$. The resulting line is displayed for the entire width of the chart, not just the interval used to parameterize the power-law curve.

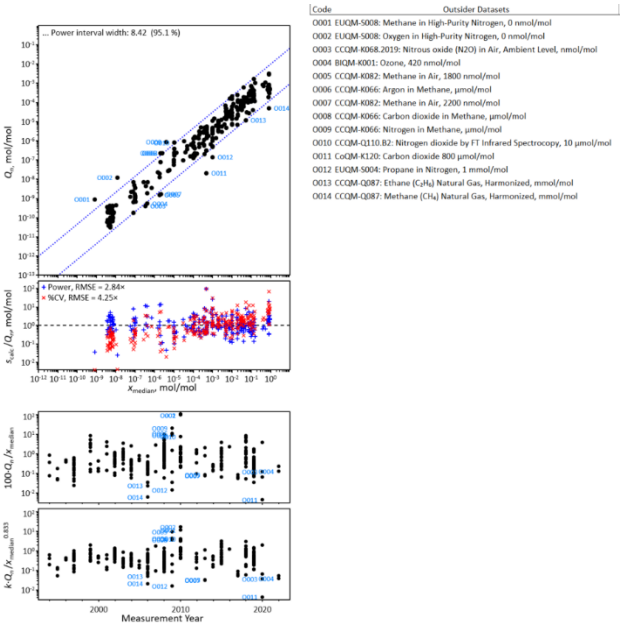
In both chart WPr-1 and WPr-2, the power-law-derived relationships are displayed as solid blue lines. Charts WPr-3 and WPr-4 are not affected by this control.

15.4.3. Power interval



Clicking the “Power interval” checkbox toggles the display of two dotted blue lines in Chart WPr-1. These lines define a symmetric interval centered on the power-law curve. This interval has the multiplicative factor width defined by the value of the “Power width” parameter described in Section 15.3.4. The interval is displayed as two dashed blue lines. Using the default value, about 95 % of the $\{x_{median}, Q_n\}$ values should be between the two lines. The power interval lines cover the entire $\log_{10}(\text{Min } X_x)$ to $\log_{10}(\text{Max } X_x)$ chart display range (Section 15.3.1).

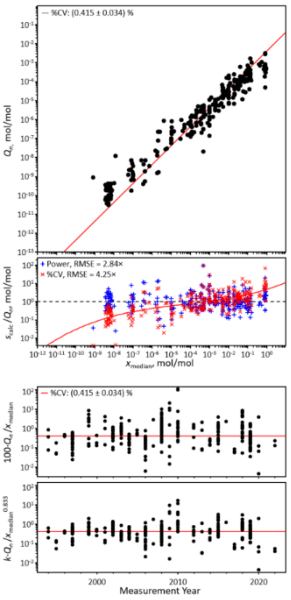
15.4.4. Outsider labels



Code	Outsider Datasets
0001	EUQM-S008: Methane in High-Purity Nitrogen, 0 nmol/mol
0002	EUQM-S008: Oxygen in High-Purity Nitrogen, 0 nmol/mol
0003	CCQM-K068.2019: Nitrous oxide (N2O) in Air, Ambient Level, nmol/mol
0004	BIQM-K001: Ozone, 420 nmol/mol
0005	CCQM-K082: Methane in Air, 1800 nmol/mol
0006	CCQM-K066: Argon in Methane, µmol/mol
0007	CCQM-K082: Methane in Air, 2200 nmol/mol
0008	CCQM-K066: Carbon dioxide in Methane, µmol/mol
0009	CCQM-K066: Nitrogen in Methane, µmol/mol
0010	CCQM-Q110.B2: Nitrogen dioxide by FT Infrared Spectrocopy, 10 µmol/mol
0011	CCQM-K120: Carbon dioxide 800 µmol/mol
0012	EUQM-S004: Propane in Nitrogen, 1 mmol/mol
0013	CCQM-Q087: Ethane (C_2H_6) Natural Gas, Harmonized, mmol/mol
0014	CCQM-Q087: Methane (CH_4) Natural Gas, Harmonized, mmol/mol

Selecting a cell containing either the code or the dataset name and clicking the **Review** button produces a dot-and-bar chart for that dataset (Section 20).

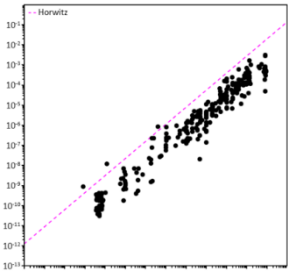
15.4.5. %CV lines



Clicking the “%CV lines” checkbox toggles the display of a constant %CV line in charts WPr-1, WPr-3, and WPr-4. In chart WPr-2, clicking the checkbox enables display of a cubic polynomial regression fit of the residual, $\log_{10}((\%CV/100)x_{median}) - \log_{10}(Q_n) = (\%CV/100)x_{median})/Q_n$, to $\log_{10}(x_{median})$. These relationships are displayed as solid red lines.

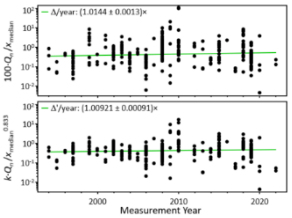
The CV value is specified by the “%CV” parameter described in Section 15.3.5.

15.4.6. Horwitz line



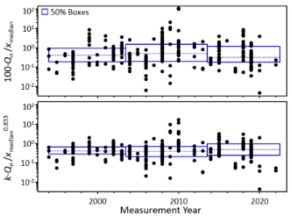
Clicking the "Horwitz line" checkbox toggles chart WPr-1's display of the Horwitz relationship between reproducibility and analyte concentration [3]. The relationship, shown as a dashed magenta line, is a power-law with coefficients $a = 0.02$ and $b = 0.8495$. These values are derived from the rather obscure form originally described in the early 1980's from interlaboratory food-analysis studies: $100 \cdot u/C = 2^{[1-0.5 \cdot \log_{10}(C)]}$ where u represents a standard deviation (estimated using some form of outlier rejection) and C a rather nebulously defined estimate of fractional concentration [4].

15.4.7. Trend lines



Clicking the "Trend lines" checkbox toggles the display of robust Thiel-Sen linear trend lines [14,15], $Y = \beta_0 + \beta_1 X$, in the WPr-3 and WPr-4 charts. The regession uses all results displayed in each chart, where X is the date in years and Y is the metric identified in the chart's Y-axis title. In chart WPr-3, the metric is the estimated %CV. In chart WPr-4, the metric is the estimated %CV after correcting for the observed power function relationship documented in WPr-1.

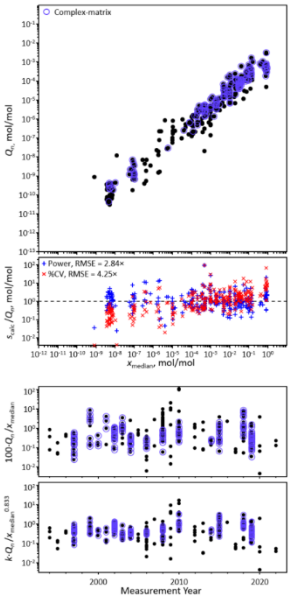
15.4.8. 50 % boxes



For charts WPr-3 and WPr-4, clicking the "50 % boxes" checkbox toggles the display of a series of 50 % boxes at intervals along the measurement year axis. Each box is bounded with solid blue lines. The width of each box is set by the "Year interval" parameter (Section 15.3.4). The top line represents the 75th percentile of all results within the interval, the bottom line the 25th percentile, and the dotted blue centerline represents the median (50th percentile).

In chart WPr-3, the legend states the net change per year, Δ/year, as a multiplicative factor. In chart WPr-4, the legend states the net power-law-adjusted change, Δ'/year, also as a multiplicative factor.

15.4.9. Mark complex

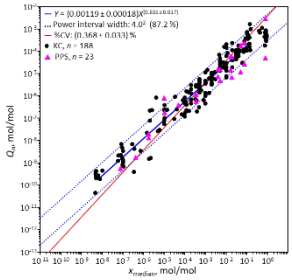


Clicking the "Mark complex" checkbox toggles the identification of results for complex-matrix materials. This option is only relevant when simple-matrix and complex-matrix datasets are analyzed together. Complex-matrix datasets are identified with a surrounding blue circle.

15.4.10. Legend Entries

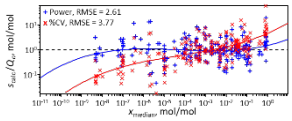
As described in Section 2.2.3.1, clicking the "Legend" checkbox toggles the display of the legend. The optional features have a legend entry when (and only when) active. In addition to identifying the graphical elements, some of the entries provide quantitative information.

In Chart WPr-1:



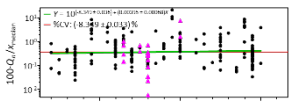
- "Power line" states the coefficients of the power-law.
- "Power interval" states the multiplicative width and the percent of the $\{x_{median}, Q_n\}$ values within the lines.
- %CV states the median of the $100 \cdot Q_n / x_{median}$ values
- If the symbols are shown colored, the number of each type of study is displayed.

In chart WPr-2:



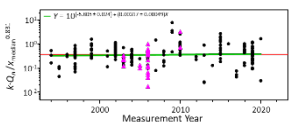
- The RMSE of the power and %CV uncertainty function residuals are displayed. The RMSE is defined as $\sqrt{\sum_1^n d_i^2/(n-m)}$, where d_i is the residual for one $\{x_{median}, Q_n\}$, n is the number of $\{x_{median}, Q_n\}$, and m is the number of adjustable parameters in the uncertainty function. For the power-law, m is 2; for %CV, m is 1.

In chart WPr-3:



- "50 % boxes" states linear trend of $100 \cdot Q_n / x_{median}$ over time as a multiplicative factor.
- %CV states the median of the $100 \cdot Q_n / x_{median}$ values.

In chart WPr-4:



- "50 % boxes" states the power-law-adjusted linear trend of $100 \cdot Q_n / x_{median}$ over time as a multiplicative factor.

15.5. An Additional Filter for the Obsessive

The *WG_Precision* subsystem uses results from datasets that pass selected WG, Base unit, year span, study type, sponsoring body, and sample type filters. However, it also supports the capability of filtering on participant code. For each {WG, Base unit}, results are accepted only for participants listed in the corresponding column of the *Dataset_NMI|DI* worksheet (see Section 21). These lists can be manipulated to include or exclude particular organizations. This manipulation is intended to support studies of performance by different participant subsets.

For example, 55 NMI|DIs have participated at least once in GAWG KC, SC, and/or PPS studies, however only 14 have participated (relatively) regularly from near the start of GAWG studies to recent times. The results for all 55 NMI|DIs; for the 14 "Core" NMI|DIs that started participating before 2000 and have participated in a recent study; and for the 41 "Non-Core" NMI|DIs who were not early participants and/or have not recently participated are compared in Fig. 55.

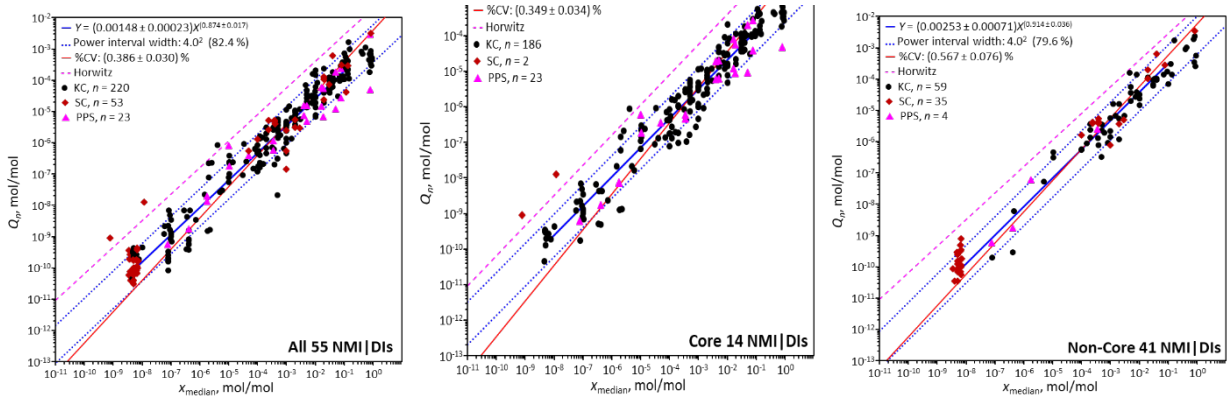


Fig. 55. Comparison of Results With and Without NMI|DI Filtering.

The similarity in the results for the "All 55" and the "Core 14" suggests that this analysis is relatively robust to changes in the pool of study participants.

The complete participant lists in the *Dataset_NMI|DI* worksheet are restored whenever the *Database_Checkup* subsystem (Section 25) is invoked.

16. WG_Power Subsystem

The *WG_Power* subsystem is not self-contained but rather (reasonably) efficiently collects and compares the power-law results provided by *WG_Precision* with those provided by *Lab_Uncertainty* for NMI|DIs identified by the *Peer_Bilateral*, *Peer_Unilateral*, or *Peer_Global* subsystems. Successful use requires familiarity with all the *CCQM_Retrospectoscope* analysis subsystems.

The *WG_Power* charts, the controls used to specify which WG and NMI|DIs are included, and the controls used to modify the chart structure are pictured in Fig. 56.

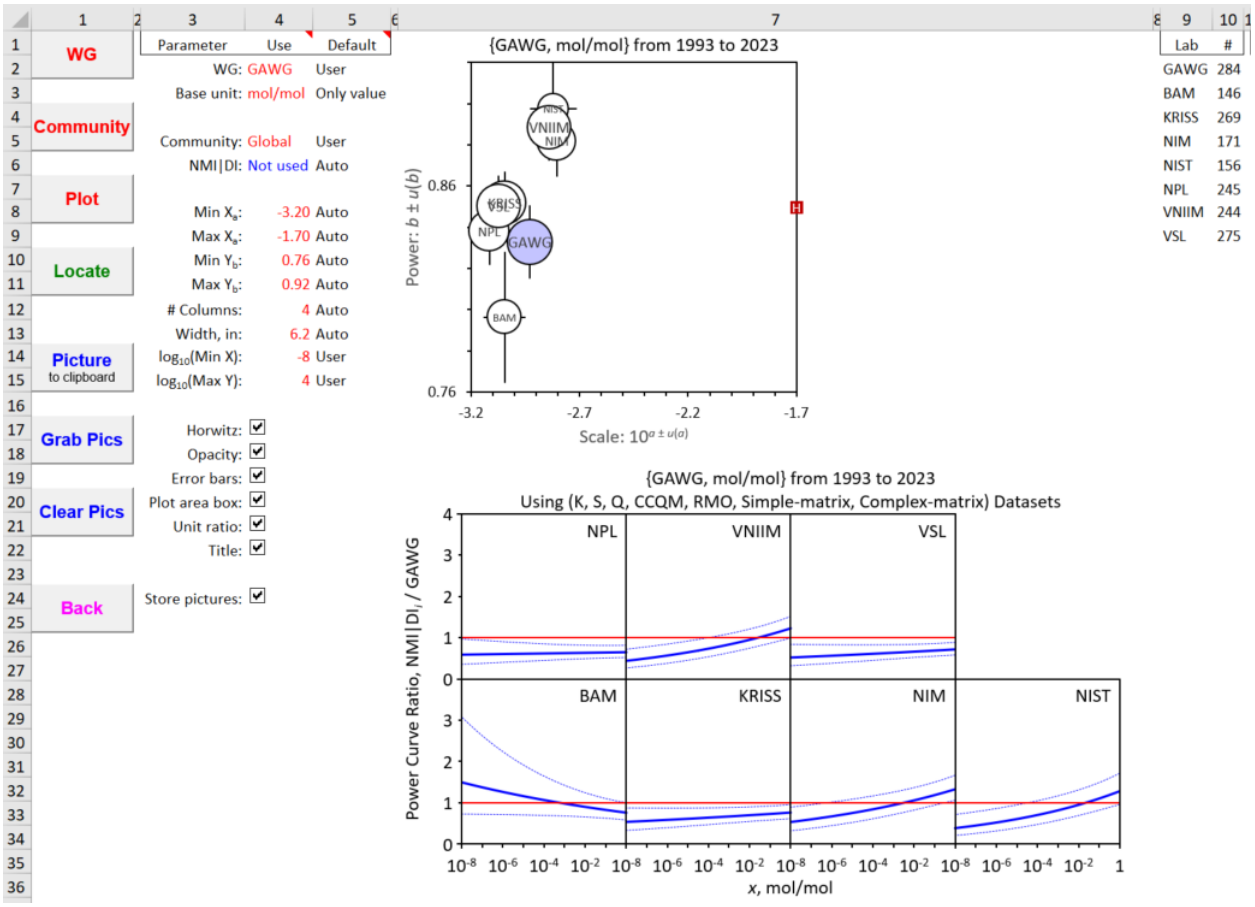


Fig. 56. The *WG_Power* Dashboard.

Reminder: A data selection or chart display parameter value listed under the "Use" heading can only be changed when its "Default" value is "User". See Section 1.9 for further information.

16.1. Charts

The lower chart (WPo-2) is a "multiplot", each segment displaying the ratio of two power-law curves over a range of analyte concentration expressed as a fraction. The denominator in each segment is the power-law from *WG_Precision*, $Q_n = \beta_0 \cdot x_{median}^{\beta_1}$ calculated as $\log_{10}(Q_n) = \log_{10}(\beta_0) + \beta_1 \cdot \log_{10}(x_{median})$. The nominator in each segment is the power-law for a selected NMI|DI from *Lab_Uncertainty*, $u_x = \beta_0 x^{\beta_1} \cdot$ calculated as $\log_{10}(u_x) = \log_{10}(\beta_0) + \beta_1 \cdot \log_{10}(x)$. A thick solid blue curve displays the ratio. Lighter dotted curves above and below the ratio represent the "one sigma" standard uncertainty interval about the ratio, calculated using the regression-estimated "standard errors" of the parameters.

Each of the multiplot segments is approximately square. The number of segments in the chart is controlled by the number of NMI|DIs identified using one of the "*Peer_*" subsystems: *Peer_Bilateral*, *Peer_Unilateral*, or *Peer_Global*. The number of rows, the physical dimension of the chart, the minimum of the analyte concentration range, and the maximum of the ratio range are controlled by chart display parameters (Section 16.5). The multiplot segments are ordered alphabetically by NMI|DI code, with "A" to the bottom left and "Z" to the top right. This ordering ensures that the concentration axis of the bottom row is fully labelled.

The upper chart (WPo-1) plots the power-law exponent (β_1) as a function of the scale factor (β_0). The area of each symbol representing a given $\{\beta_0, \beta_1\}$ pair is proportional to the number of datasets used in estimating the function. The symbol for the WG's $\{\beta_0, \beta_1\}$ is colored blue.

16.2. Additional Command Buttons

The *WG_Power* worksheet has nine command buttons; five of which (**Plot**, **Locate**, **Picture**, **Back**, and **Restore**) have functions in common with other subsystems (Section 2.1).

16.2.1. WG: Denominator Definition

The denominator power-law is defined by clicking the **WG** button; this

- clears any prior *WG_Power* results;
- sets the "WG:" and "Base unit:" parameters in the *WG_Precision* subsystem to the values specified by those parameters in *WG_Power*;
- sets all parameters in the *Lab_Uncertainty* subsystem that are in common with those in *WG_Precision* to have the same values as those in *WG_Precision*;
- runs *WG_Precision*, storing the resulting power-law parameter values and optionally storing a picture of the *WG_Precision* charts.

16.2.2. Community: Numerator Definition

Defining which NMI|DIs will be included in the analysis is accomplished by clicking the **Community** button. This first identifies the peer NMI|DIs for which power-law parameters are to be estimated using *Peer_Bilateral*, *Peer_Unilateral*, or *Peer_Global* and then estimates the power-law coefficients for each NMI|DI using the *Lab_Uncertainty* subsystem. Which of the *Peer_* subsystem is used is controlled by the setting of the "Community:" parameter (Section 16.3).

Clicking the **Community** button:

- transfers the settings for all relevant parameters from *WG_Precision* to the designated *Peer_* subsystem;
- runs the designated *Peer_* subsystem, storing the identified NMI|DIs and optionally storing a picture of the chart that results from the *Peer_* analysis;
- runs *Lab_Uncertainty* for each of the identified NMI|DIs, storing the resulting power-law parameter values, and optionally storing a picture of the *Lab_Uncertainty* charts; and
- creates the *WG_Power* charts and optionally stores pictures of them.

17 Grab Pics
18

16.2.3. Grab Pics

Clicking the **Grab Pics** button copies to the clipboard all stored pictures that that are on the worksheet. This facilitates transferring the pictures to MS Word or PowerPoint documents.

20 Clear Pics
21

16.2.4. Clear Pics

Clicking the **Clear Pics** button deletes any stored pictures that may be on the worksheet.

Community: Global User
NMI|DI Target Not used

16.3. Community NMI|DI Selection Parameter

The "Community:" parameter specifies which subsystem is used to identify the NMI|DIs: *Peer_Bilateral*, *Peer_Unilateral*, or *Peer_Global*. If "Bilateral" or "Unilateral" are specified, the community will be defined as the peers of the NMI|DI that is specified in the selected subsystem. The identity of that NMI|DI is echoed as the NMI|DI Target immediately beneath the Community keyword. If "Global" is specified, there is no NMI|DI target.

The default value is "Global".

Store pictures: ☑

16.4. Store Pictures Checkbox

The "Store Pictures:" checkbox controls whether PNG-format pictures of the various analyses are stored in column 57 of the *WG_Power* worksheet. The default value is "checked" (i.e., *True*).

Note: Very occasionally, Excel's PasteSpecial function hiccups and causes VBA programs to cease operation. The *CCQM_Retrospectoscope* should be hiccup-protected, but the glitch has occurred so infrequently that it's hard to confirm that "should" can be replaced by "is".

Min X_a:	-3.30	Auto
Max X_a:	-1.70	Auto
Min Y_b:	0.80	Auto
Max Y_b:	0.93	Auto
# Columns:	4	User
Width, in:	6.2	Auto
$\log_{10}$(Min X):	-8	User
Max Y:	4	User

16.5. Chart Display Parameters

The *WG_Power* subsystem has eight parameters, four that control to X- and Y-axis limits of chart WPo-1, two that define the shape and size of the chart WPo-2, and two that control the X- and Y-axis limits of each segment of WPo-2.

16.5.1. Min X_a and Max X_a: X-axis Limits for Chart WPo-1

The minimum and maximum limits for the X-axis for the power-law scale parameter, a, in chart WPo-1 are specified by the values of the "Min X_a" and "Max X_a" parameters. The default values for these limits are the minimum and maximum of the $a \pm u(a)$ estimates. Modifying the limits does not affect what data are selected for analysis.

16.5.2. Min Y_b and Max Y_b: Y-axis Limits for Chart WPo-1

The minimum and maximum limits for the Y-axis for the power-law exponent, β_1, in chart WPo-1 are specified by the values of the "Min Y_b" and "Max Y_b" parameters. The default values for these limits are the minimum and maximum of the $\beta_1 \pm u(\beta_1)$ estimates. Modifying the limits does not affect what data are selected for analysis.

16.5.3. # Columns: Number of Segment Columns

The value of the "# Columns" parameter sets the number of segment columns, N_{col}, displayed in chart WPo-2 The number of segment rows is set by the ratio between the number of identified NMI|DIs and N_{col}. Currently, N_{col} must be 2, 3, 4, or 5. The default value is 4.

16.5.4. Width, in: Chart width in Inches

The value of the "Width, in:" parameter sets the horizontal size of chart WPo-2 in inches. Currently, the width must be between (2 and 9) in. The default value is 6.2 in.

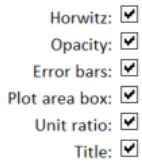
16.5.5. $\log_{10}$(Min X): Minimum Concentration

The value of the "$\log_{10}$(Min X):" parameter is the smallest concentration value, X_{min}, for which the power-law ratio is displayed in each segment of chart WPo-2. The currently allowed values are -10, -8, and -6. The default value is -8. The maximum $\log_{10}$(concentration) is fixed at 0.

16.5.6. Max Y: Maximum Ratio

The value of the "Max Y:" parameter is the largest ratio that will be displayed n each segment of chart WPo-2. The currently allowed maximum ratios are the integers 3, 4, 5, and 6. The default value is 4. The minimum ratio is fixed at 0.

16.6. Chart Display Checkboxes



The *WG_Power* subsystem has six checkboxes that control chart elements. The first four of which only apply to the WPo-1 scatterplot, the fifth applies only to the WPo-2 multiplot, and the sixth applies to both the WPo-1 and WPo-2 charts. parameters,

16.6.1. Horwitz

Clicking the "Horwitz:" checkbox toggles chart WPo-1 between displaying and not displaying the Horwitz power-law coefficients, {-1.7, 0.8495}. When the X1min, X1max, Y1min, and/or Y1max parameters are set to *Auto*, the Horwitz parameters are included in the assessment of the axis limits. When the checkbox is checked, the location of the Horwitz coefficients is denoted by a solid red square labeled "H". The chart appearance with the checkbox checked and unchecked is contrasted in Fig. 57.

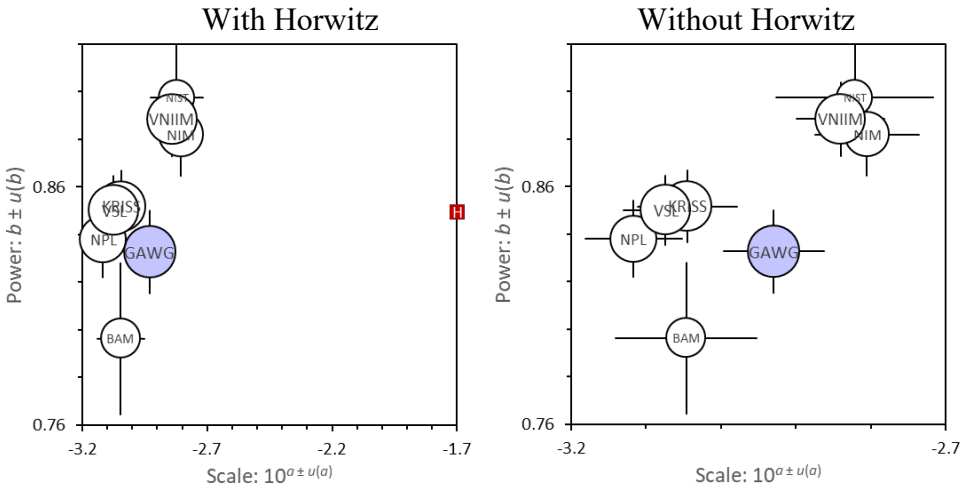


Fig. 57.The *WG_Power* Chart WPo-1 With and Without Horwitz Display.

16.6.2. Opacity

Clicking the "Opacity:" checkbox toggles chart WPo-1 between displaying the symbols for the NMI|DI power-law coefficients between opaque white and clear. This enables identifying the location of NMI|DI symbols that are hidden under other symbols. The symbol for the WG power-law is always opaque blue.

16.6.3. Error bars

Clicking the "Error bars:" checkbox toggles chart WPo-1 between displaying and not displaying error bars. The error bars span $\beta_0 \pm u(\beta_0)$ and $\beta_1 \pm u(\beta_1)$, where the uncertainties are the "standard errors" of the regression coefficients.

16.6.4. Plot area box

Clicking the "Error bars:" checkbox toggles between displaying and not displaying the area box lines at the top and right-hand side of chart WPo-1. It has no effect on the display of the WPo-2 chart.

16.6.5. Unit ratio

Clicking the “Unit ratio:” checkbox toggles between displaying and not displaying a line denoting ratio 1 in each segment of the WPo-2 multiplot., where the values estimated for the numerator and denominator functions are equal. The chart appearance with both checkboxes checked and both unchecked is contrasted in Fig. 58.

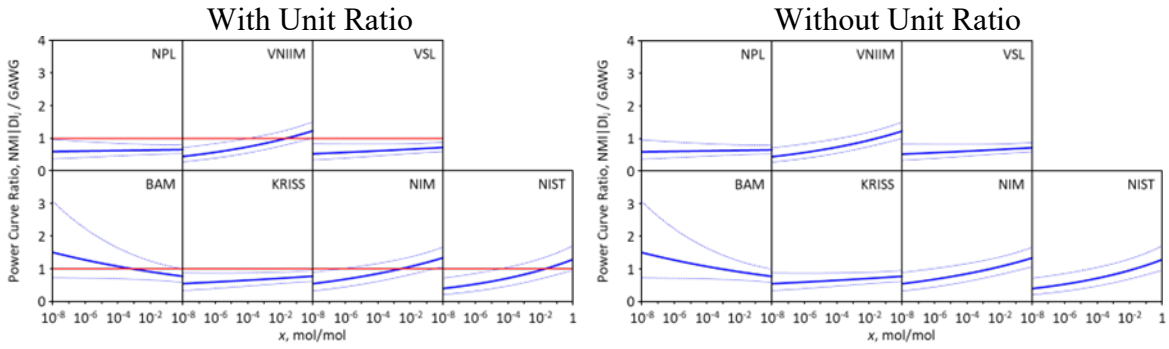


Fig. 58. Comparison of Chart Display With and Without Unit Ratio.

16.6.6. Title

Clicking the “Title:” checkbox toggles between displaying and not displaying the title lines above the WPo-1 and WPo-2 charts.

17. WG_Diagonal

The *WG_Diagonal* chart, the controls used to specify the datasets evaluated, and the controls used to modify what the chart displays are pictured in Fig. 59.

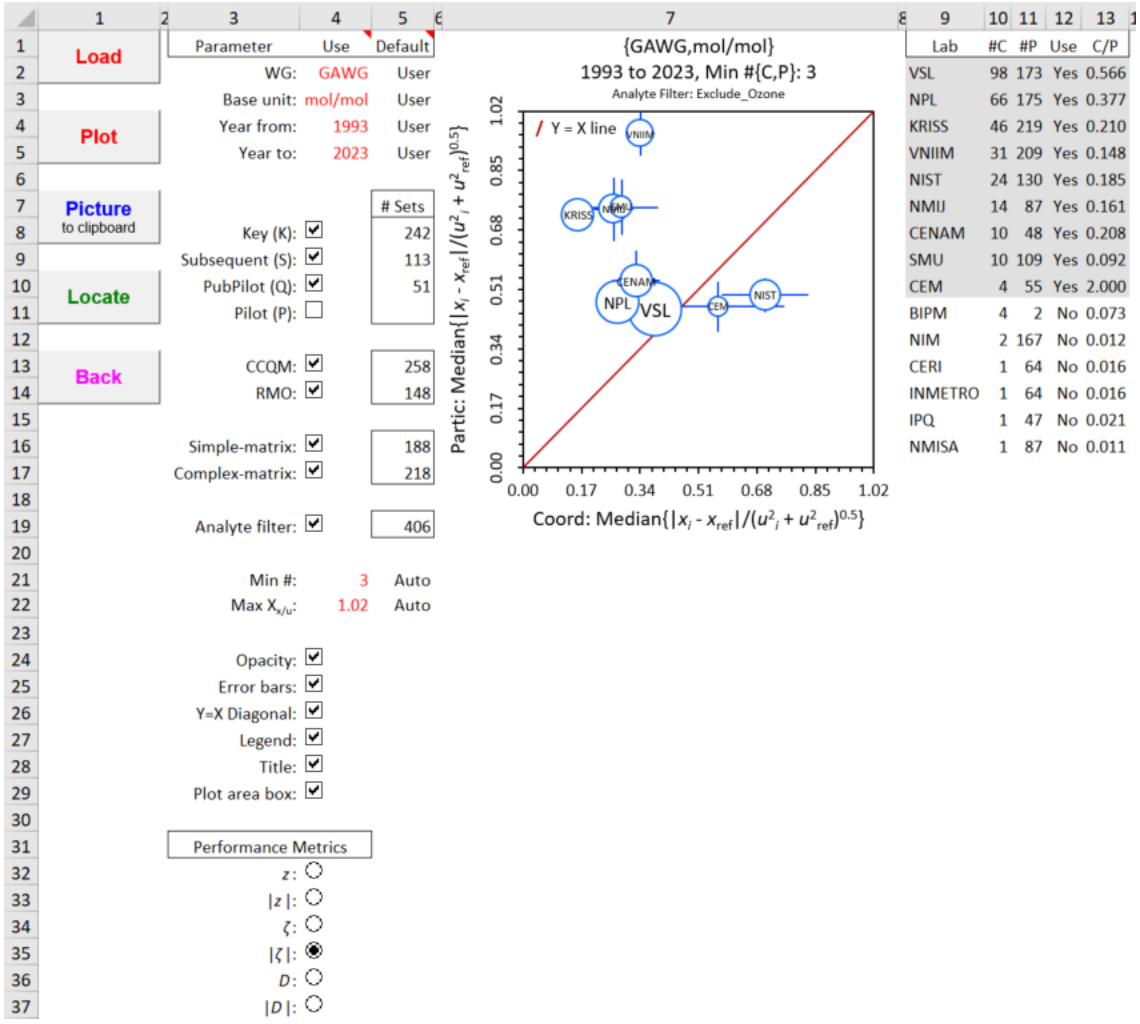


Fig. 59. The *WG_Diagonal* Dashboard.

Reminder: A data selection or chart display parameter value listed under the "Use" heading can only be changed when its "Default" value is "User". See Section 1.9 for further information.

17.1. Chart

For each NMI|DI that has coordinated enough studies, the chart displays the median measurement bias in studies that it did *not* coordinate as a function of the median bias in studies that it *did* coordinate. The median estimates are calculated using all datasets that meet the selection criteria. The more similar the magnitude of the two bias estimates, the less likely that coordination of a study influences the NMI|DI's values relative to the assigned reference values.

However, since approximately equal proportions of large positive and large negative differences can average to zero, the relationships suggested by signed- and absolute-value bias metrics can significantly differ: compare the panels of Fig. 60.

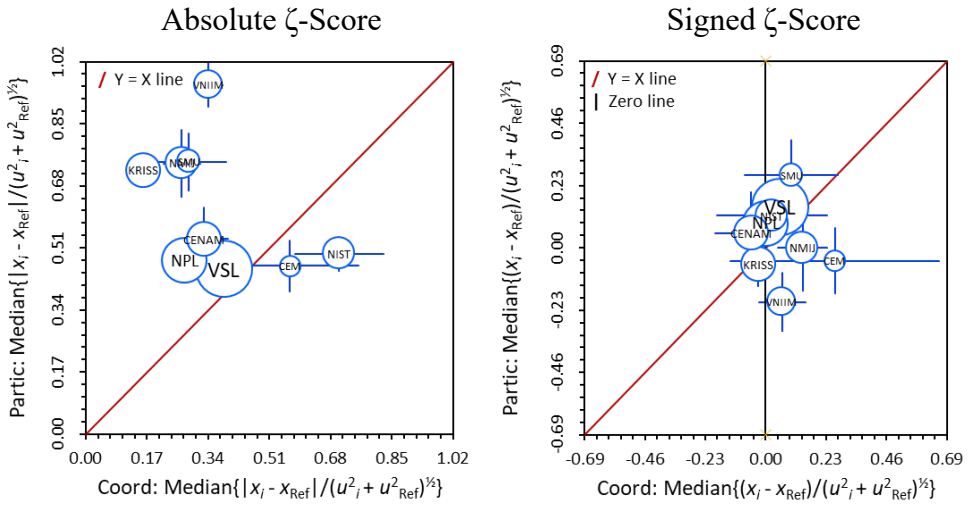


Fig. 60. Comparison of *WG_Diagonal* Chart With Absolute and Signed Bias Metrics.

The area of each symbol is proportional to the ratio between the number of datasets from studies the NMI|DI coordinated and the number of datasets from studies the NMI|DI only participated in (*i.e.*, did not coordinate). This ratio, denoted C/P, is normalized to the largest C/P value of the NMI|DIs that have reported values in at least the specified minimum number of datasets from studies that they coordinated and from studies that they did not coordinate.

17.2. Chart Display Parameters

Min #:	3	Auto
Max $X_{x/u}$:	1.02	Auto

The *WG_Diagonal* worksheet contains two chart display parameters. Changes to these values are not evaluated or implemented until the **Plot** button is clicked.

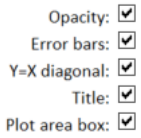
17.2.1. Min #: Minimum Participation

The value of the "Min #" parameter sets the minimum number of datasets there must be from studies the NMI|DI coordinated and from studies the NMI|DI did not coordinate for the NMI|DI to be displayed in the chart. Here, participation is defined relative to the total number of datasets that meet the selection criterion rather than to co-participation with some target NMI|DI. The coordination and participation numbers are listed in columns 10 and 11 of the table to the right of the chart; the NMI|DIs with at least the minimum numbers are identified with grey shading (see Fig. 59). The default value is (a more-or-less arbitrary) 3 datasets.

17.2.2. Max $X_{x/u}$-axis: X- and Y-axis Limit

The value of the "Max $X_{x/u}$" parameter sets the display range of the biases. Its default value is set by the extreme value of the display symbols including their error bars. The same limit is applied to both the X- and the Y-axis. When a signed bias metric is selected, the range is set to be symmetric about zero and, if necessary, the parameter value is rounded up to produce a symmetric distribution of tic-labels.

17.3. Additional Chart Display Checkboxes



The *WG_Diagonal* worksheet contains three chart display checkboxes in addition to two discussed in Section 2.2.3. Clicking a chart display checkbox invokes an immediate change in the chart display.

17.3.1. Opacity

Clicking the "Opacity:" checkbox toggles between displaying the symbols between opaque white and clear. This enables identifying the location of NMI|DI symbols that are hidden under other symbols.

17.3.2. Error bars

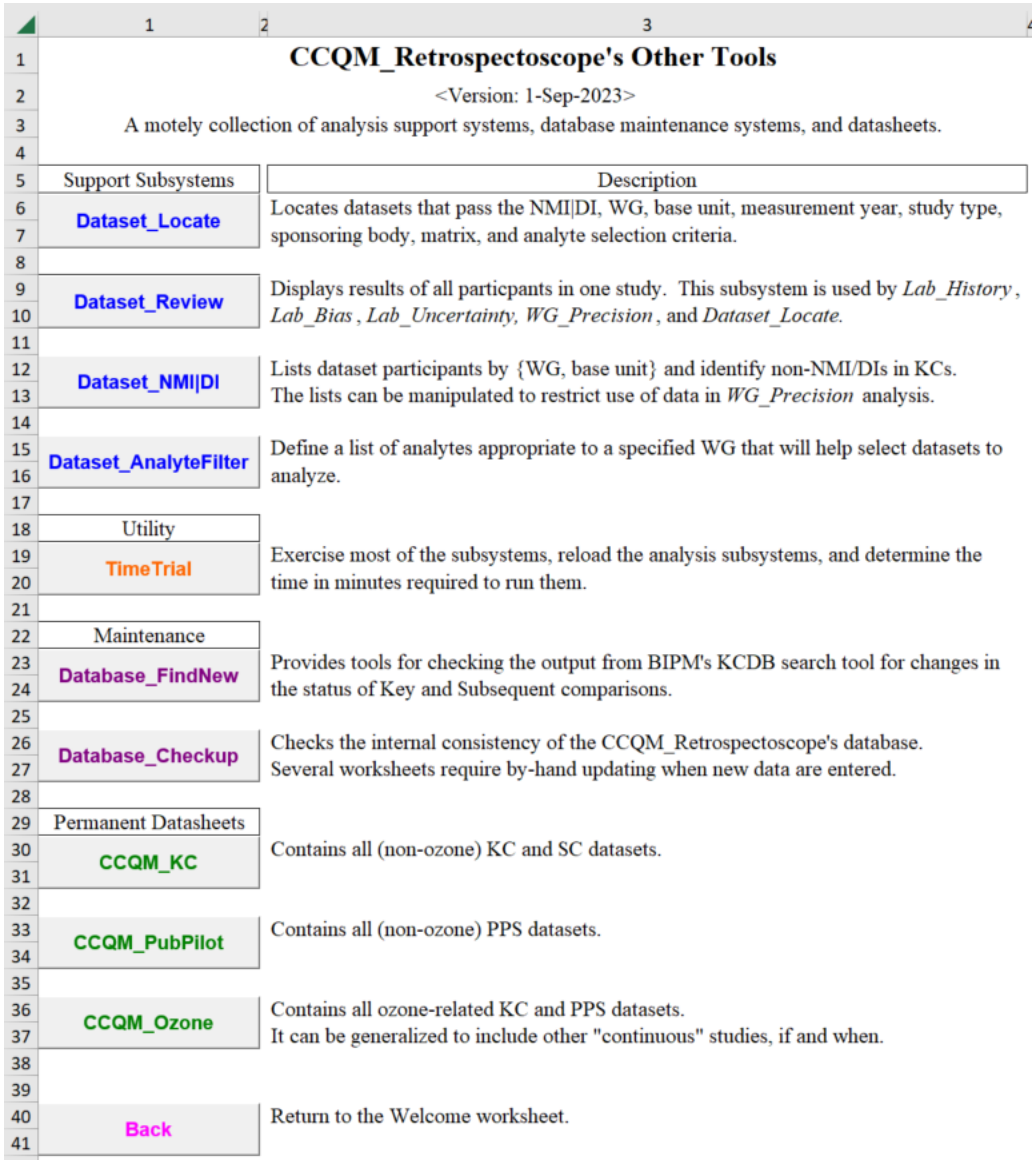
Clicking the "Error bars:" checkbox toggles between displaying and not displaying error bars. The error bars span ± one standard deviation of the mean ("standard error") about the median value. A standard deviation of the mean is estimated from the Q_n robust standard deviation of set of values divided by the square root of the number of values in the set. The X- and Y-axis spans are not affected by whether the error bars are displayed.

17.3.3. Y=X diagonal

Clicking the "Y=X diagonal:" checkbox toggles between displaying and not displaying a diagonal line that runs from the lower-left to the upper-right corners. Symbols above this diagonal line suggest that an NMI|DI's measurement bias in studies that they did not coordinate is larger than it is in studies they did coordinate. Symbols below this line suggest that an NMI|DI's measurement bias in studies that they did coordinated is larger than it is in studies they did not coordinate.

18. The Other_Tools Worksheet

The *Other_Tools* worksheet is activated when the **Other_Tools** button on the *Welcome* worksheet is clicked. This worksheet provides access to five specialized analysis subsystems, four support subsystems, and a utility that invokes all the *CCQM_Retrospectoscope*'s subsystems and the clock-time they take to complete. The controls used to access these functions are pictured in Fig. 61.



CCQM_Retrospectoscope's Other Tools

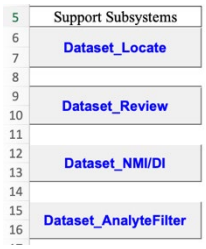
<Version: 1-Sep-2023>

A motely collection of analysis support systems, database maintenance systems, and datasheets.

Support Subsystems	Description
Dataset_Locate	Locates datasets that pass the NMI|DI, WG, base unit, measurement year, study type, sponsoring body, matrix, and analyte selection criteria.
Dataset_Review	Displays results of all particpants in one study. This subsystem is used by *Lab_History*, *Lab_Bias*, *Lab_Uncertainty*, *WG_Precision*, and *Dataset_Locate*.
Dataset_NMI|DI	Lists dataset participants by {WG, base unit} and identify non-NMI/DIs in KCs. The lists can be manipulated to restrict use of data in *WG_Precision* analysis.
Dataset_AnalyteFilter	Define a list of analytes appropriate to a specified WG that will help select datasets to analyze.
Utility	
TimeTrial	Exercise most of the subsystems, reload the analysis subsystems, and determine the time in minutes required to run them.
Maintenance	
Database_FindNew	Provides tools for checking the output from BIPM's KCDB search tool for changes in the status of Key and Subsequent comparisons.
Database_Checkup	Checks the internal consistency of the CCQM_Retrospectoscope's database. Several worksheets require by-hand updating when new data are entered.
Permanent Datasheets	
CCQM_KC	Contains all (non-ozone) KC and SC datasets.
CCQM_PubPilot	Contains all (non-ozone) PPS datasets.
CCQM_Ozone	Contains all ozone-related KC and PPS datasets. It can be generalized to include other "continuous" studies, if and when.
Back	Return to the Welcome worksheet.

Fig. 61. The *Other_Tools* Dashboard.

18.1. Support Subsystems



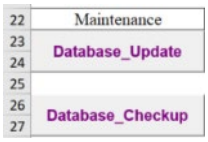
Clicking the any of the buttons with a label prefix of **Dataset_** activates the corresponding worksheet. It does not initiate the actions implemented in that worksheet.

While the four of these subsystems can be directly accessed from their worksheets, *Dataset_Review*, *Dataset_NMI|DI*, and *Dataset_AnalyteFilter* subsystems support dataset selection or visualization in one or more of the analysis subsystems. The *Dataset_Locate* subsystem facilitates identifying datasets with specific characteristics.

18.2. Utility

Clicking the **TimeTrial** button invokes a subsystem that exercises all the *CCQM_Retrospectoscope* analysis and support subsystems and reports the clock time required.

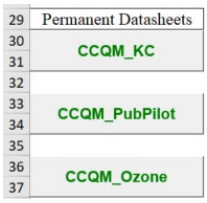
18.3. Maintenance Systems



Clicking the **Database_FindNew** or **Database_Checkup** button activates the corresponding worksheet. It does not initiate the actions implemented in that worksheet.

These systems facilitate the identification of newly available CCQM studies and the validation of newly entered datasets. They are intended to be used only by the unfortunate(s) tasked with maintaining the *CCQM_Retrospectoscope*'s database.

18.4. Database Worksheets



Clicking the **CCQM_KC, CCQM_PubPilot,** or **CCQM_OZONE** button activates the corresponding worksheet.

19. Dataset_Locate subsystem

The *Dataset_Locate* subsystem facilitates identifying datasets having specific characteristics. The commands and controls for this subsystem are pictured in Fig. 64.

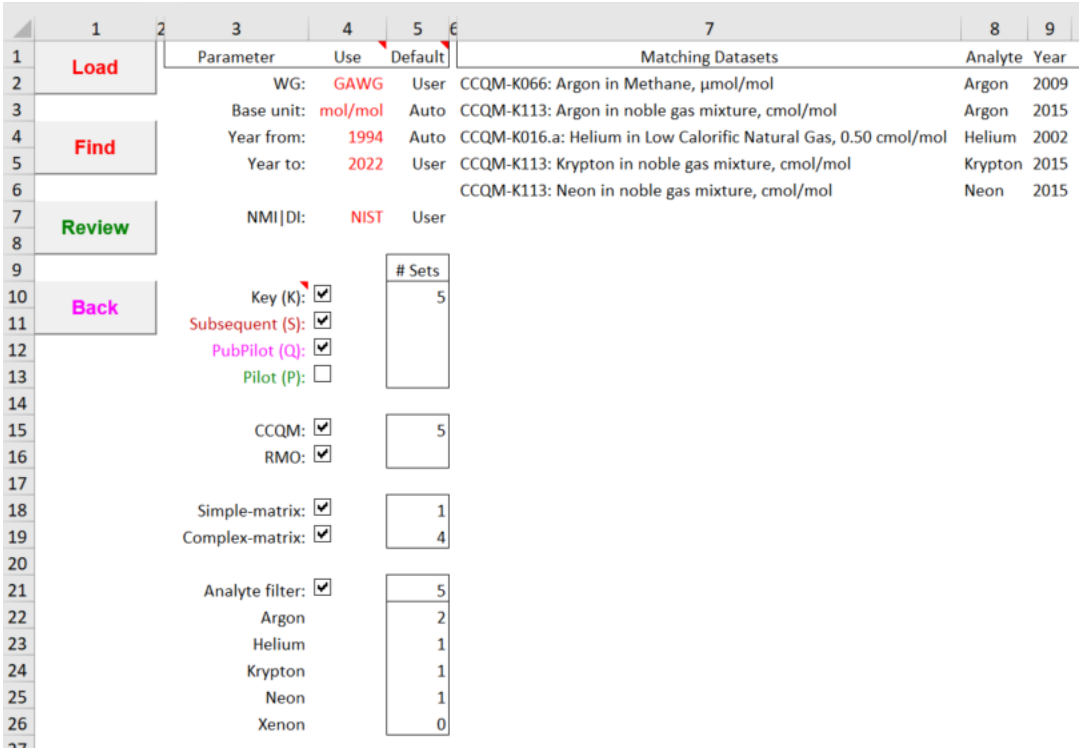
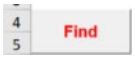


Fig. 62. The *Dataset_Locate* Dashboard With a Specified NMI|DI.

Reminder: A data selection or chart display parameter value listed under the "Use" heading can only be changed when its "Default" value is "User". See Section 1.9 for further information.

19.1. Additional Command Button: Find

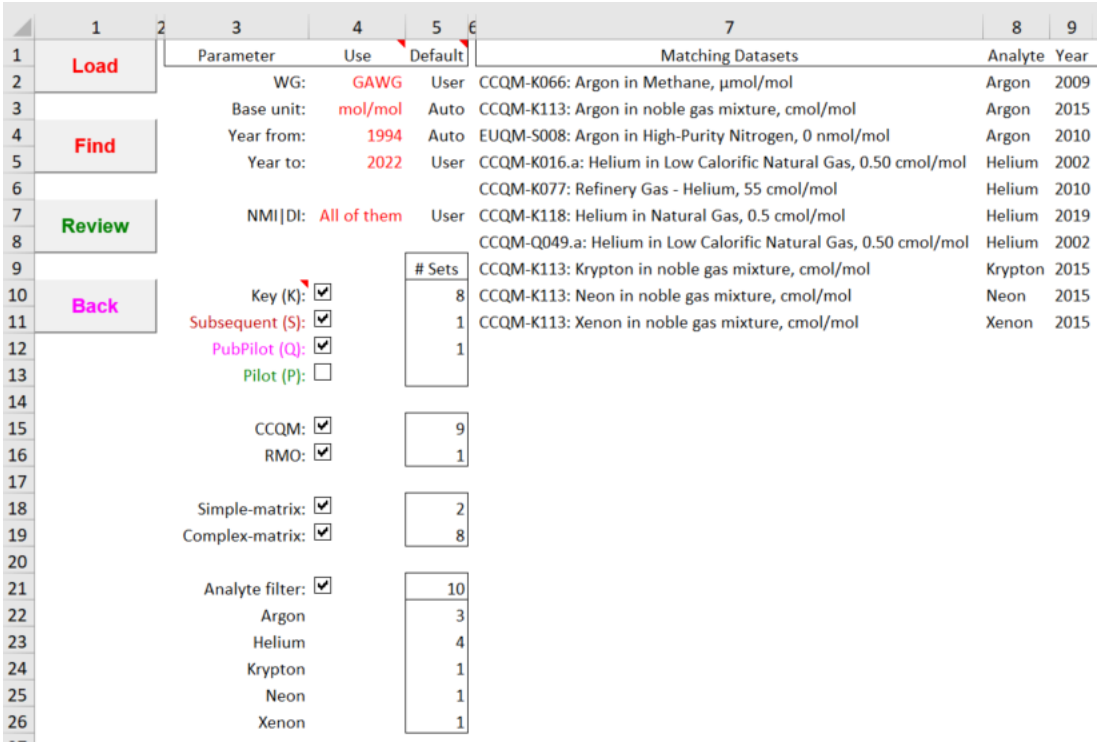


Find is the only command button on the *Dataset_Locate* worksheet that is not in-common with other subsystems (Section 2.1). However, **Find** is analogous to the **Plot** button in subsystems that provide their results as charts.

Clicking the **Find** button locates all datasets that match the current selection criteria and lists their titles and many of the characteristics in columns 7 to 18.

19.2. Dataset Selection Parameters: NMI|DI

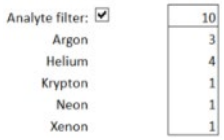
NMI|DI is the only dataset selection parameter having some functionality that is not described in Section 2.4.1. In addition to allowing datasets to be restricted to those in which a specified NMI|DI participated, leaving the parameter empty (or specifying "All") disables the NMI|DI selection criterion. Fig. 63 displays the result of clicking the **Find** button with all parameters as shown in Fig. 64 except for NMI|DI.



	Load	Parameter	Use	Default	Matching Datasets	Analyte	Year
2		WG:	GAWG	User	CCQM-K066: Argon in Methane, µmol/mol	Argon	2009
3		Base unit:	mol/mol	Auto	CCQM-K113: Argon in noble gas mixture, cmol/mol	Argon	2015
4	Find	Year from:	1994	Auto	EUQM-S008: Argon in High-Purity Nitrogen, 0 nmol/mol	Argon	2010
5		Year to:	2022	User	CCQM-K016.a: Helium in Low Calorific Natural Gas, 0.50 cmol/mol	Helium	2002
6					CCQM-K077: Refinery Gas - Helium, 55 cmol/mol	Helium	2010
7	Review	NMI|DI:	All of them	User	CCQM-K118: Helium in Natural Gas, 0.5 cmol/mol	Helium	2019
8					CCQM-Q049.a: Helium in Low Calorific Natural Gas, 0.50 cmol/mol	Helium	2002
9				# Sets	CCQM-K113: Krypton in noble gas mixture, cmol/mol	Krypton	2015
10	Back	Key (K): ☑		8	CCQM-K113: Neon in noble gas mixture, cmol/mol	Neon	2015
11		Subsequent (S): ☑		1	CCQM-K113: Xenon in noble gas mixture, cmol/mol	Xenon	2015
12		PubPilot (Q): ☑		1			
13		Pilot (P): ☐					
14							
15		CCQM: ☑		9			
16		RMO: ☑		1			
17							
18		Simple-matrix: ☑		2			
19		Complex-matrix: ☑		8			
20							
21		Analyte filter: ☑		10			
22		Argon		3			
23		Helium		4			
24		Krypton		1			
25		Neon		1			
26		Xenon		1			

Fig. 63. The *Dataset_Locate* Worksheet Without a Specified NMI|DI.

19.3. Dataset Selection Checkbox: Analyte filter



Analyte filter: is the only dataset selection checkbox that differs in any way from its presentation in other subsystems (Section 2.2.1). While its function is unchanged, successfully selected analytes are listed immediately below the Analyte filter. After clicking the **Find** button, the number of datasets for each analyte is provided, along with the routine total number output.

20. Dataset_Review subsystem

The *Dataset_Review* subsystem displays the results and auxiliary information present in one dataset. This subsystem is most typically invoked from the *Lab_History*, *Lab_Bias*, *Lab_Uncertainty*, *WG_Precision,* or *Dataset_Locate,* or the database worksheets. Clicking the **Review** button from these worksheets causes the information for a selected dataset to be loaded and displayed. *Dataset_Review* can also be invoked from the *Other_Tools* worksheet, allowing interaction with whatever dataset was most recently visualized.

The *Dataset_Review* commands, chart, controls, and auxiliary information are pictured in Fig. 64.

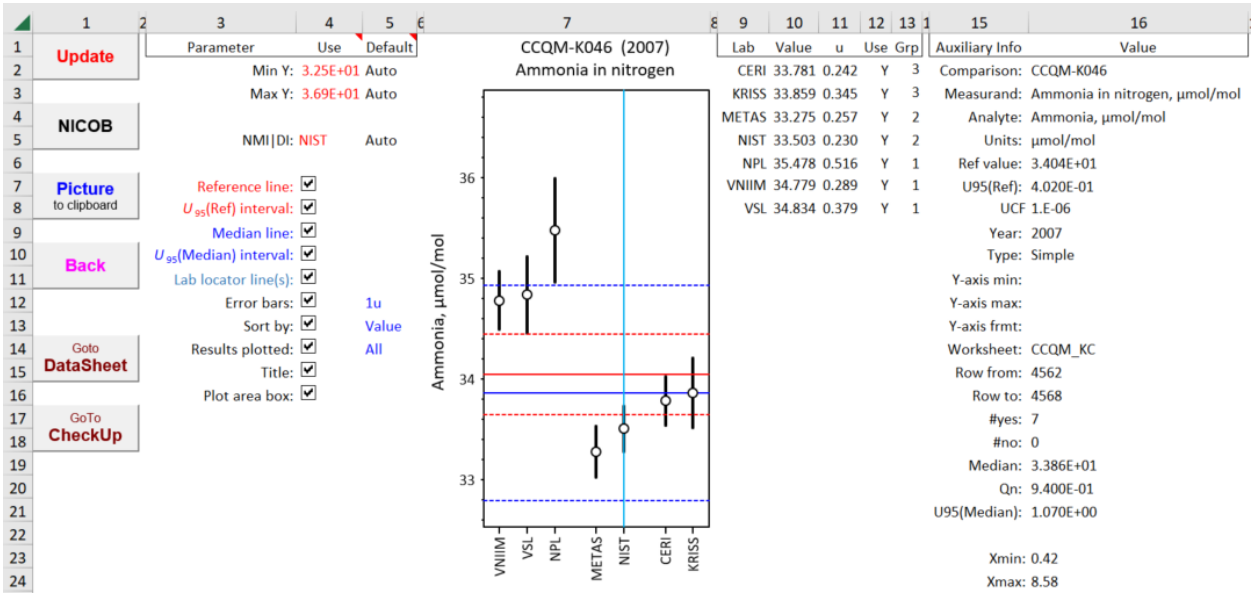


Fig. 64. The *Dataset_Review* Dashboard with an Example Dataset.

Reminder: A data selection or chart display parameter value listed under the "Use" heading can only be changed when its "Default" value is "User". See Section 1.9 for further information.

Note: The dataset, International Comparison CCQM-K46 – Ammonia in Nitrogen [17], was chosen as the example because (unusually for CCQM studies) the results turned out to be method-dependent. The discordance between the methods facilitates display of optional chart elements. The NMI|DIs are here grouped by the method used.

20.1. Chart

Participant results are displayed as "dot and bar" symbols where the value part the results are shown as "dots" and an associated measurement uncertainty as "bars". The code names of the participants are arranged along the X-axis with their reported results are plotted along the value (Y) axis directly above the code.

The chart size can be "by-hand" adjusted as needed. The adjusted size will be maintained until the **Restore** function is invoked, either by clicking the worksheet's **Restore** button or running the *TimeTrial* system (Section 23). The default chart size is shown in Fig. 65.

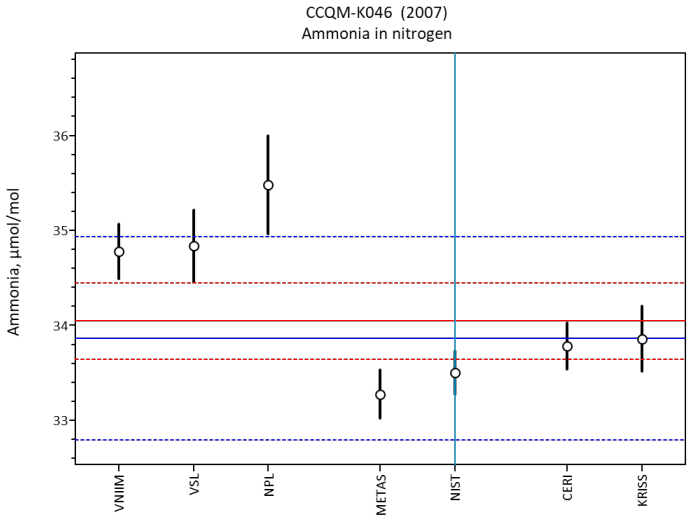


Fig. 65. The Default size of the *Dataset_Review* Chart.

20.2. Additional Command buttons

The *Dataset_Review* worksheet has seven command buttons; three of which (**Picture**, **Back**, and **Restore**) have functions in common with other subsystems (Section 2.1). Clicking the **Back** button returns the *CCQM_Retrospectoscope* focus to the button that invoked the present instance of *Dataset_Review*.

20.2.1. Update

When the **Update** button is clicked, the chart displays the dataset results using either default scaling or the scaling defined under the dataset's "Axis Parameters" header. Clicking the Update command implements the value (Y) axis scaling defined by the "Min Y" and "Max Y" chart display parameters (Section 20.3.1).

20.2.2. NICOB

NICOB is the acronym for the NIST Consensus Builder, a system designed to provide statistically defensible consensus estimates for interlaboratory study results [18]. Clicking the **NICOB** button causes dataset results to be output in the NICOB-friendly format shown in Fig. 66. The output is generated in the rows below the chart.

Data formated for input into the NIST Concensus Builder
NPL, VNIIM, VSL, METAS, NIST, KRISS, NMIJ
35.478, 34.779, 34.834, 33.275, 33.503, 33.859, 33.781
0.516, 0.289, 0.379, 0.257, 0.23, 0.345, 0.242
µmol/mol

Fig. 66. Example of Dataset Information Output in NICOB-Friendly Format.

The NICOB capability is provided to facilitate addressing issues that may arise about the appropriateness of reference values that were assigned using other estimation techniques.

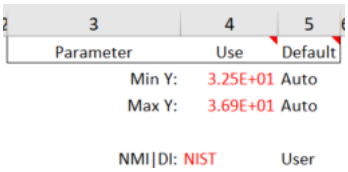
20.2.3. Goto Datasheet

Clicking the **Goto Datasheet** button activates the database worksheet that holds the displayed dataset, with the first row of the dataset selected. This facilitates database access: it is intended primarily for use by database maintainers during the addition of new datasets or the correction of identified errors.

20.2.4. Goto Checkup

Clicking the **Goto Checkup** button activates the *DataBase_Checkup* worksheet. This is intended for use by database maintainers to validate the *CCQM_Retrospectoscope* database after new datasets have been added or existing datasets have been modified.

20.3. Chart Display Parameters



The *Dataset_Review* worksheet contains three chart display parameters. Changes to these values are not evaluated or implemented until the **Update** button is clicked.

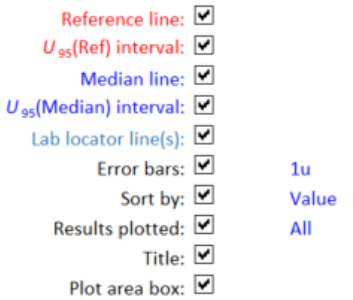
20.3.1. Min Y and Max Y: Y-axis Display Limits

The "Min Y" and "Max Y" values set the display range of the value (Y) axis. The default values are set by the extreme values of the results using "2u" error bars (Section 20.4.4) or by the values in the cells in the second and third rows of the dataset's "Axis Parameter" header (Section 26.2.6).

20.3.2. Target NMI|DI: Participant of Particular Interest

This parameter is provided as an aid to spotting the value or values submitted by a given target NMI|DI. If the target has one or more values in the dataset and the "Lab locator line(s)" checkbox (Section 20.4.3) is active, the symbols for those values will be bisected by a thin blue line. The default target NMI|DI is, of course, NIST.

20.4. Additional Chart Display Checkboxes



The *Dataset_Review* worksheet contains seven chart display checkboxes in addition to the "Title" and "Plot area box" that are discussed in Section 2.2.3.

20.4.1. Reference Line and Interval

Clicking the "Reference line" checkbox enables the toggling display of a sold red horizontal line that represents the dataset's reference value. Clicking the "U_{95}(Ref) interval" toggles the display of two dotted red lines that represent the approximate 95 % confidence region around the reference value. The left-hand panel of Fig. 67 displays these two graphical elements.

20.4.2. Median Line and Interval

Clicking the “Median line” checkbox enables the toggling display of a solid blue horizontal line that represents the median of the values considered valid by the coordinating WG (that is, are flagged as “Y”). Clicking the “U_{95}(Median) interval” toggles the display of two dotted blue lines that represent an approximate 95 % confidence region around the median value. The middle panel of Fig. 67 displays these two graphical elements.

The ” U_{95}(Median) interval” is estimated from the Q_n robust standard deviation, the number of valid values (n), the appropriate Student’s t factor, and the median’s 1.24-fold additional variance relative to the mean: $U_{95}(\text{Median}) = (1.24)(t_{1\text{-}0.05,n\text{-}1})(Q_n)/\sqrt{n}$.

20.4.3. Lab locator line(s)

When a data set contains one or more values reported by the NMI|DI specified by the “Target Lab” parameter (Section 20.3.2), clicking the “Lab locator line(s)” checkbox enables the toggling display of thin cyan vertical lines that connect the dot-and-bar symbols to the participant code. The right-hand panel of Fig. 67 displays this graphical element when these is one and only one result for the target NMI|DI.

If the target NMI|DI doesn’t have a value in the dataset, clicking the checkbox has no effect.

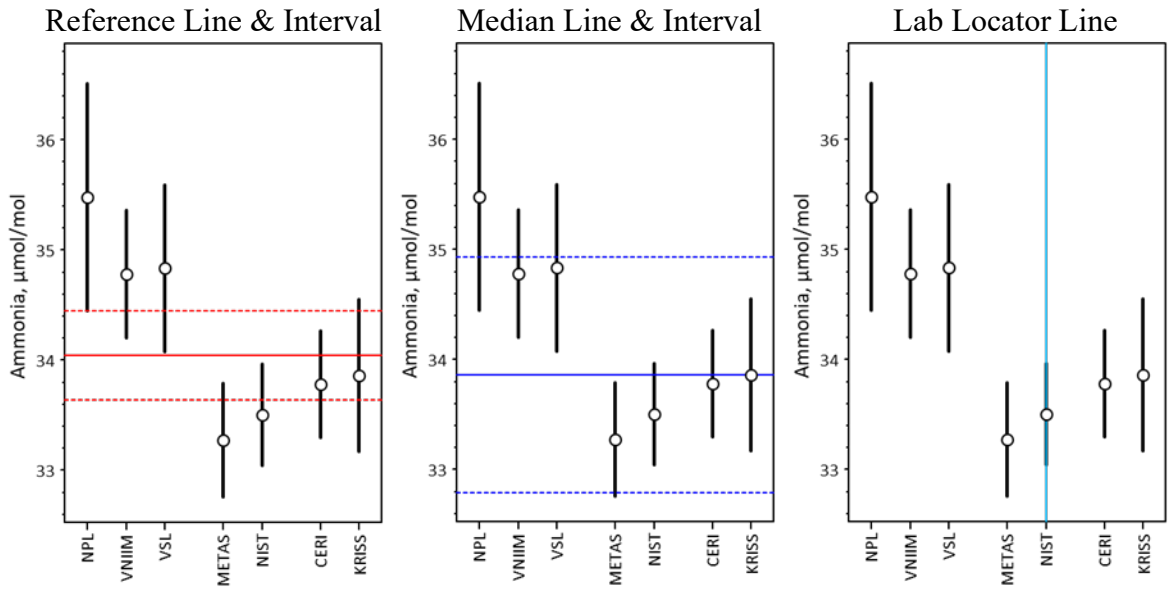


Fig. 67. The *Dataset_Review* Chart With Optional Line Elements.

20.4.4. Error bars

Clicking the “Error bar:” checkbox toggles the display of the error bars between “2u” and “1u”; i.e., between twice the standard uncertainty and one standard uncertainty. Since the standard uncertainties stored under the dataset’s “u” header are preferentially defined as one-half of the reported expanded uncertainty (Section 26.3.4), the “2u” bars represent 95 % level of confidence intervals.

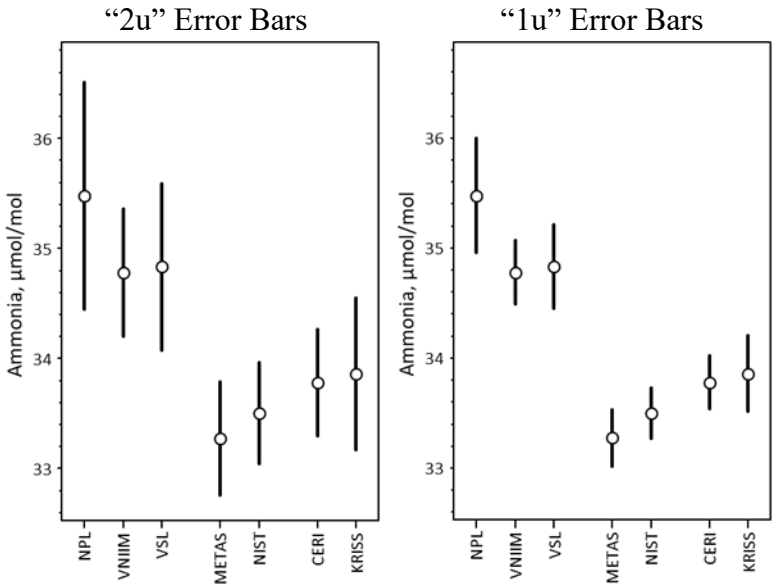


Fig. 68. The *Dataset_Review* Chart With u" and "1u" Error Bars.

20.4.5. Sort by

Clicking the "Sort by:" checkbox toggles the order in which the participant results are displayed between "Alpha" and "Value". When "Alpha", they are sorted in the alphabetical order of the NMI|DI code. When "Value", the results are sorted in order of increasing value. When the results are grouped, they are ordered first by their Group designation and then by "Alpha" or "Value": see Fig. 69.

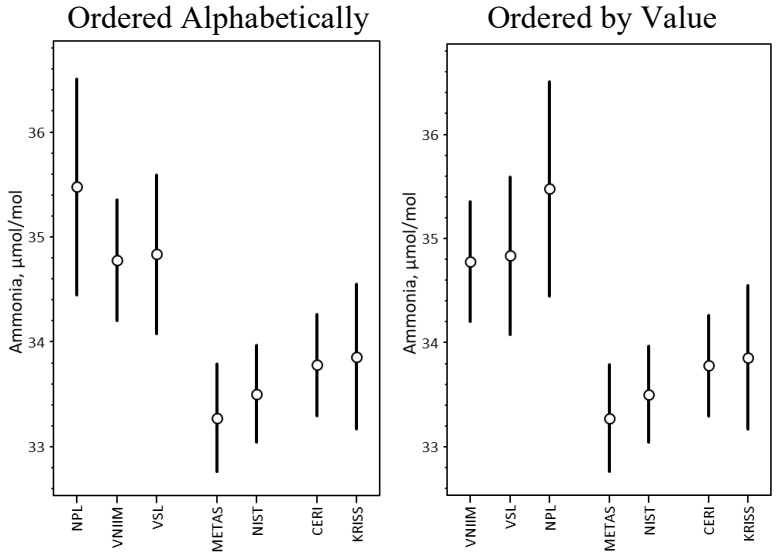


Fig. 69. The *Dataset_Review* Chart With Group Results Sorted Alphabetically and By Value.

Ordering by value generally facilitates visualizing differences between participants while ordering alphabetically facilitates locating results from given NMI|DIs: compare the panels of Fig. 70, showing the results for the exemplar dataset without grouping.

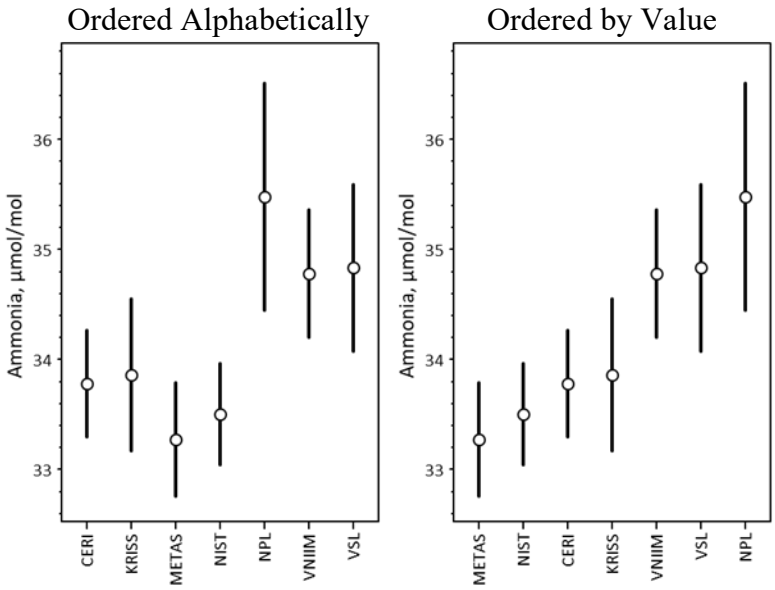


Fig. 70. The *Dataset_Review* Chart With Results Sorted Alphabetically and By Value.

Note: the codes used for many NMI|DIs are not consistent over time or in different studies (see Section 25.4.4). Alphabetical sorting by NMI|DI may produce orderings that differ from those used by the study coordinators.

20.4.6. Results plotted

Clicking the "Results plotted:" checkbox toggles the display between showing all available results and just the results used to estimate the median and its 95 % confidence interval (i.e., those flagged "Y" and "Z", excluding "N"). Compare the panels of Fig. 71.

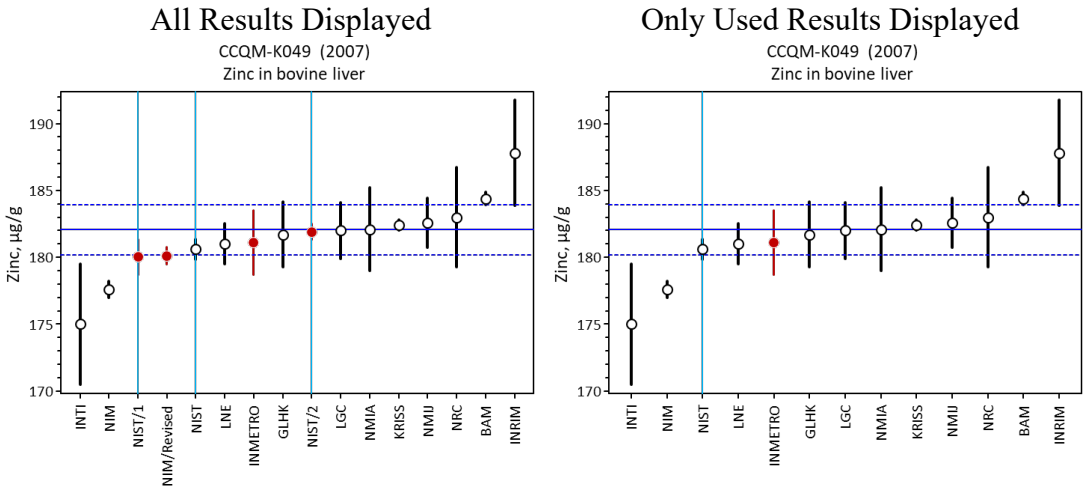


Fig. 71. The *Dataset_Review* Chart Displaying All Available and Only Used Results.

20.5. Auxiliary Columns

In addition to the chart, dataset information from the datasheet is copied onto the *Dataset_Review* worksheet. It is this data that is used in the chart. While these data can be modified, the changes are not propagated back into the datasheets.

20.5.1. Columns 9 to 13, Participant results

The datasets “Lab”, “Value”, “u”, “Use”, and “Grp” from the datasheet are copied into the cells in these columns without modification.

While not shown in this example, results that are associated with a “N” or “Z” in the “Use” column are shown as solid dark red circles with dark red error bars.

Note that in Fig. 64 the cells under the “GRP” header contain the group assignments 1”, “2”, and “3”. This results in the participant’s results being ordered first by the group assignment, with a wider gap between the groups than between the results within a group. The panels in Fig. 70 were generated by clearing these values and then clicking the “Sort by…” checkbox.

20.5.2. Columns 15 and 16, Dataset Descriptors

The cells under the column 15’s “Auxiliary Info” header are labels for the values listed in the cells under column 16’s “Value” header. Table 7describes the information stored.

Table 7. *Dataset_Review* Auxiliary Information.

Row	Label	Description	Source
2	Comparison:	CCQM-assigned designation	Dataset title
3	Measurand:	Description of measurand	Dataset title
4	Analyte:	Name of analyte	Axis Parameters
5	Units:	Measurement units	Axis Parameters
6	Ref value:	WG-assigned reference value	RV column
7	U95(Ref):	95 % expanded uncertainty,	U95(RV) column
8	UCF	Units conversion factor,	RV column
9	Year:	Measurement year	*Datacore_Dates*
10	Type:	Simple or complex matrix	RV column
11	Y-axis min:	Minimum value for the chart Y-axis	Axis Parameters
12	Y-axis max:	Maximum value for the chart Y-axis	Axis Parameters
13	Y-axis frmt:	Display format for the Y-axis labels	Axis Parameters
14	Worksheet:	Name of the worksheet dataset is stored in	Worksheet
15	Row from:	First row of dataset in the worksheet	Worksheet
16	Row to:	Last row of dataset in the worksheet	Worksheet
17	#yes:	Number of results used in consensus calculations	Counted
18	#no:	Number of results not used in the calculations	Counted
19	Median:	Median of the “Yes” results	Calculated
20	Qn:	Qn of the “Yes” results	Calculated
21	U95(Median):	95 % level of confidence expanded uncertainty	Calculated
23	Xmin:	The chart’s current minimum X-axis value	Calculated
24	Xmax:	The chart’s current maximum X-axis value	Calculated

21. Dataset_NMI|DI Subsystem

The *Dataset_NMI|DI* subsystem has informative, data quality, and dataset selection functions. First and foremost, for each {WG, Base unit} it lists the participating organizations that reported a result in at least one {WG, Base unit} dataset. Its data-quality purpose is the identification of non-NMI|DIs that have participated in KCs. The *WG_Precision* subsystem uses the contents of this worksheet to filter results by participant code (see Section 21).

The worksheet's commands, parameters, and summary table are pictured in Fig. 72. The summary lists the current {WG, Base unit} combinations and the number of organizations that are not (No Fill) and are (Highlighted) currently flagged in yellow (see Sections 21.1.2 and 21.1.3).

Load
Non-NMI
Core
Keep
Kill
Back

Parameter	Use	Default
Year from first:	5.0	Auto
Year from last:	3.0	Auto
Min % Participation:	50.0	Auto

	No Fill				Highlighted			
{WG, base unit}	KC	SC	PPS	PS	KC	SC	PPS	PS
{GAWG,mol/mol}	49	41	36	17				
{IAWG,g/g}	56	50	49	154				
{OAWG,g/g}	47	31	22	67				
{EAWG,pH}	36		22	32				
{EAWG,S/m}	24	10		26				
{EAWG,S/S}				19				
{EAWG,PSU}				22				
{IRWG,mol/mol}	7							
{IRWG,n/n}	9		15					
{IRWG,‰}	8		20	7				
{IRWG,g/mol}	7			8				
{NAWG,n/n}	15		14	23				
{NAWG,g/L}	9			17				
{NAWG,n/L}				19				
{OAWG,mol/mol}				12				
{PAWG,g/g}	14		18	9				
{SAWG,g/g}	5		5	10				
{SAWG,mol/mol}	8							
{SAWG,m}	12		15					
{SAWG,mol/kg}	6		1					
{SAWG,m^2/g}	6		1					
{SAWG,cm^3/g}	6		1					
{IAWG,m}								
{IAWG,mol/kg}								
{IAWG,m^2/g}								
{IAWG,cm^3/g}								
{CAWG,n/L}			9					
{CAWG,EFF}			9					
{SAWG,Uno}				9				
{CAWG,pH}								
{NAWG,bp}				8				
{NAWG,%}								
{PAWG,Uno}			6	2				
{OAWG,n/n}								
{NAWG,cn/n}								
{NAWG,ng/g}								
{NAWG,g/mol}								
{NAWG,Uno}								
{NAWG,m}								
{CAWG,Uno}			8	3				
{IAWG,ng/g}				9				
{SAWG,g/mol}			8					
{PAWG,mol/kg}				9				

Fig. 72. The Basic *Dataset_NMI|DI* Dashboard.

Reminder: A data selection or chart display parameter value listed under the "Use" heading can only be changed when its "Default" value is "User". See Section 1.9 for further information.

An exemplar header of the tables generated for each {WG, Base unit} is pictured in Fig. 73. Each table lists the organizations ("NMI|DI"), the first and last measurement years during which the organization participated ("First" and "Last"), the total number of datasets it contributed to ("Tot"), and the number of KC, SC, PPS, and PS data sets it contributed to. It also contains a "Use" column that is used for sorting purposes.

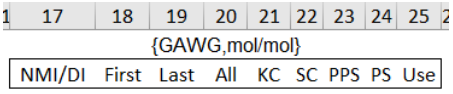


Fig. 73. Exemplar {WG, Base unit} Table Header.

21.1. Additional Command Buttons

The *Dataset_NMI|DI* worksheet supports five command buttons in addition to the usual **Back** (Section 2.1.5) and **Restore** (Section 2.1.7).

21.1.1. Fetch

Clicking the **Fetch** button produces a fresh evaluation of all the datasets present in any of the workbook's CCQM datasheets. Any non-NMIs that contributed "unofficial" results in a KC are flagged with magenta highlight and sorted to the top of the {WG, Base unit} list. A representative portion of the **Fetch** output is pictured in Fig. 74.

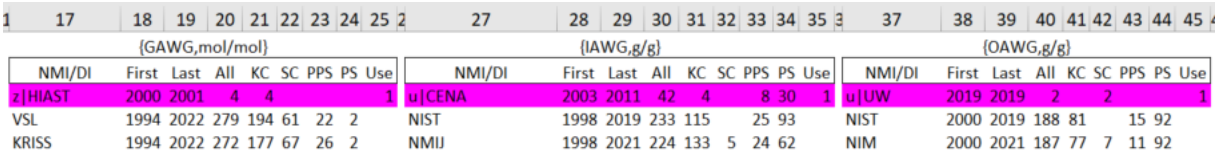


Fig. 74. Exemplar {WG, Base unit} Tables After Clicking Fetch.

The flagged participations should be investigated to ensure that they aren't entry mistakes but reflect the content of the study's official report.

21.1.2. Non-NMI

Clicking the **Non-NMI** button flags all participating organizations that are not NMI|DIs (or international organizations) with yellow highlight and sorts them to the top of the {WG, Base unit} lists. A representative portion of the {WG, Base unit} lists after clicking **Non-NMI** is pictured in Fig. 75.

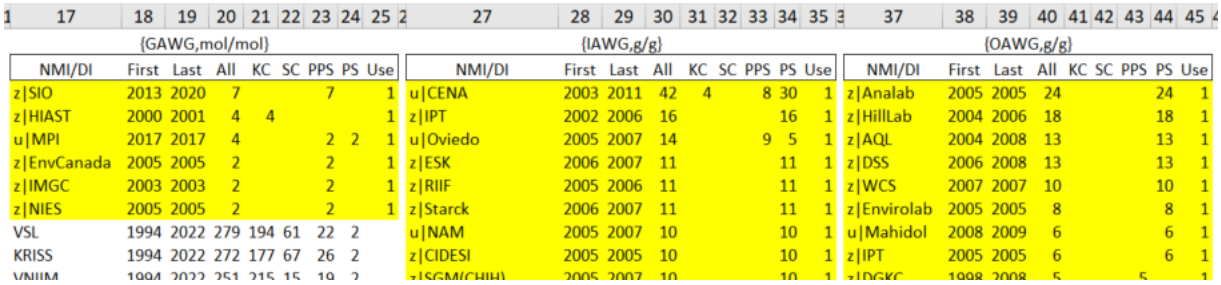


Fig. 75. Exemplar {WG, Base unit} Lists After Clicking Non-NMI.

The "Use" column is used to identity non-NMI|DIs and enable sorting them to the top of the lists. The *CCQM_Retrospectoscope* database codes non-NMI|DIs with the prefix "u|" for academic and "z|" for non-academic participants. These assignments are maintained in the *Datacore_Codes* worksheet (see Section 25.4.4).

21.1.3. Core

On the basis of the three selection criteria specified by the parameter values, clicking the **Core** button flags the most active ("Core") organizations in each {WG, Base unit} with yellow highlight and sorts them to the top of the lists. Fig. 76 displays a representative portion of the {WG, Base unit} lists after clicking **Core**.

1	17	18	19	20	21	22	23	24	25	2	27	28	29	30	31	32	33	34	35	3	37	38	39	40	41	42	43	44	45	4
	{GAWG,mol/mol}										{IAWG,g/g}										{OAWG,g/g}									
	NMI/DI	First	Last	All	KC	SC	PPS	PS	Use		NMI/DI	First	Last	All	KC	SC	PPS	PS	Use		NMI/DI	First	Last	All	KC	SC	PPS	PS	Use	
	VSL	1994	2022	279	194	61	22	2	7		NIST	1998	2019	233	115		25	93	7		NIST	2000	2019	188	81		15	92	7	
	KRISS	1994	2022	272	177	67	26	2	7		NMIJ	1998	2021	224	133	5	24	62	7		NIM	2000	2021	187	77	7	11	92	7	
	VNIIM	1994	2022	251	215	15	19	2	7		NIM	2000	2021	207	123	17	26	41	7		NMIJ	2000	2019	155	69		7	79	7	
	NPL	1994	2022	249	182	42	23	2	7		VNIIM	2000	2021	203	93	13	19	78	7		BAM	2000	2019	151	61	2	6	82	7	
	NIM	1994	2022	179	155	21	2	1	7		BAM	2000	2021	195	70	9	19	97	7		KRISS	2000	2019	150	72	3	8	67	7	
	NIST	1994	2022	159	120	30	7	2	7		CENAM	2000	2021	158	76	14	14	54	7		CENAM	2002	2019	118	68	1	6	43	7	
	BAM	1994	2019	153	123	7	21	2	7		KRISS	1998	2020	147	89	7	13	38	7		LGC	2000	2019	114	59		13	42	7	
	SMU	1999	2020	121	102	14	3	2	7		LNE	1998	2019	125	65	9	24	27	7		JRC	2001	2019	98	34	1	4	59	7	
	LNE	1994	2022	106	84	5	15	2	7		PTB	1998	2019	125	54	10	22	39	7		VNIIM	2000	2019	92	62		3	27	7	
	NMIJ	1999	2019	103	78	3	20	2	7		NRC	1998	2018	122	56	12	23	31	7		LNE	2002	2019	91	39	2		50	7	
	BFKH	1994	2019	93	89	4			7		LGC	1998	2018	116	53		24	39	7		NMIA	2000	2019	68	42		7	19	7	
	CERI	1994	2020	65	56	8	1		7		NMISA	2000	2020	81	46	4	1	30	7		NRC	2000	2021	43	24		7	12	7	
	METAS	1999	2022	30	19	6	3	2	7		JRC	1998	2018	75	34	3	10	28	7		GLHK	2007	2019	97	45	5		47	6	
	UBA(DE)	1999	2022	21	19		2		7		NMIA	2000	2018	70	41		10	19	7		UME	2009	2021	69	50	6		13	6	
	NMIA	2004	2020	107	63	1	43		6		SMU	2000	2021	51	26		9	16	7		NMISA	2004	2021	64	43	2	2	17	6	
	NMISA	2000	2022	94	65	23	6		6		UME	2005	2019	143	98	9	1	35	6		INMETRO	2007	2021	59	44	1		14	6	

Fig. 76. Exemplar {WG, Base unit} Lists After Clicking Core.

The "Use" column is used to assess the Core organizations. The values contained in this column are calculated using the three parameters: "y from first", "y from last", and "% Participation". Starting from the score Use = 0:

- If the organization's initial participation was no more than "y from first" years after the measurement year of the earliest {WG, Base unit}, Use = Use +1;
- If the organization's most recent participation was no more than "y from last" years before the measurement year of the latest {WG, Base unit}, Use = Use + 2;
- If the organization has participated in at least "% Participation" of the {WG, Base unit} datasets, Use = Use + 4.

The lowest score is thus 0 and the maximum 7. The Core organizations are those that share the largest Use score within the {WG, Base unit} list.

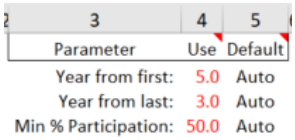
21.1.4. Keep

The **Non-NMI** and **Core** commands just highlight the {WG, Base unit} entries. Clicking the **Keep** button deletes all entries that *are not* yellow high-lighted. The remaining entries are sorted into ascending order by organization code.

21.1.5. Keep and Kill

The **Non-NMI** and **Core** commands just highlight the {WG, Base unit} entries. Clicking the **Kill** button deletes all entries that *are* yellow high-lighted. The remaining entries are sorted into ascending order by organization code.

21.2. Parameters



The *Dataset_NMI|DI* worksheet contains three parameters that control how the most active NMI|DIs are identified. Changes to these values are not evaluated until the **Core** button is clicked. Based on these three parameters, participants are assigned a cumulative "Use" score: +1 for participating relatively early, +2 for participating relatively recently, and +4 for contributing to at least a minimum proportion of the datasets.

The sum of these scores constitutes a binary code that facilitates identification of Core participants. By default, only the NMI|DIs with a Use score of seven are considered Core. However, all participants are sorted in order of decreasing Use score, facilitating refining the parameter values.

21.2.1. y from first: Number of Years Elapsed From First Dataset

The "y from first" parameter specifies the maximum number of years that can have elapsed between an organization's first participation and the measurement year of the {WG, Base unit}'s earliest dataset.

21.2.2. y from last: Number of Years Elapsed from Most Recent Dataset

The "y from last" parameter specifies the maximum number of years that can have elapsed between an organization's most recent participation and the {WG, Base unit}'s most recent dataset.

21.2.3. % Participation: Minimum Participation Proportion

The "% Participation" parameter specifies the minimum percentage of the WG's datasets that the organization must have contributed to.

22. Dataset_AnalyteFilter Subsystem

When the "Analyte filter:" option is active in any of the primary data analysis subsystems, that system only uses datasets for the analytes marked "Yes" in columns 7 and 8 of the *Dataset_AnalyteFilter* worksheet. This subsystem is designed to be activated when the status of the "Analyte filter:" checkbox in one of the data analysis subsystems is active.

However, the *Dataset_AnalyteFilter* worksheet can also be accessed directly to facilitate defining, validating, and re-using lists appropriate to a specified {WG, Base unit}. The worksheet set to limit the analysis of {GAWG, mol/mol} results to datasets that report results for measurements of carbon dioxide, along with one pre-defined filter-list for {OAWG, g/g} datasets, is pictured in Fig. 77.

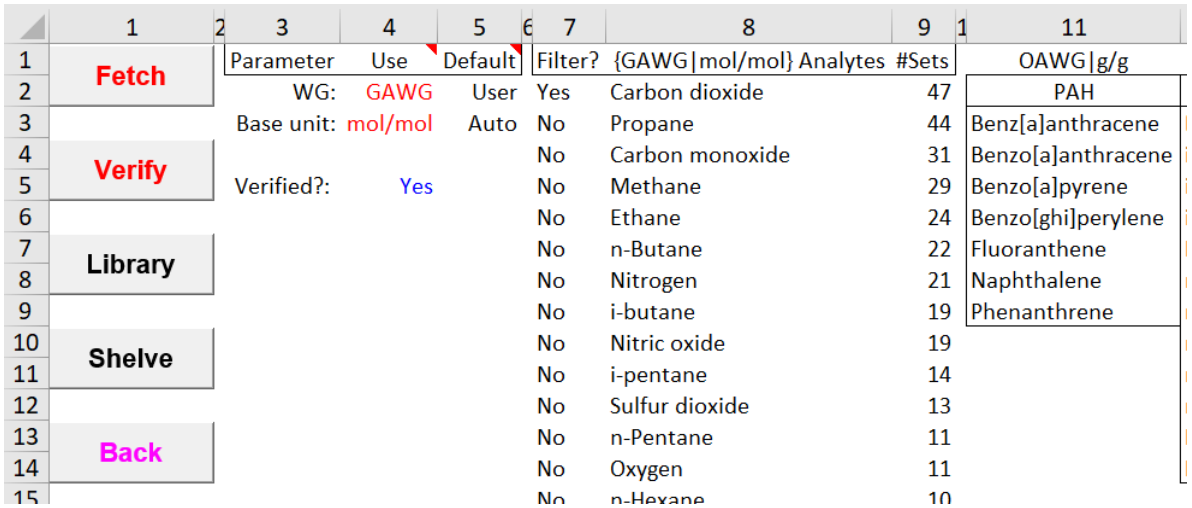


Fig. 77. *Dataset_AnalyteFilter* Worksheet with an Exemplar {GAWG, mol/mol} List.

Reminder: A data selection or chart display parameter value listed under the "Use" heading can only be changed when its "Default" value is "User". See Section 1.9 for further information.

22.1. Additional Command Buttons

The *Dataset_AnalyteFilter* worksheet supports four command buttons in addition to the usual **Back** (Section 2.1.5) and **Restore** (Section 2.1.7).

22.1.1. Fetch

Clicking the **Fetch** button populates column 8 with all the analytes for which the specified {WG, Base unit} has at least one dataset. The analytes are sorted by declining number of datasets. The status for all the analytes, along with the "Verified?" status of the total filter, is initially set to "No" (which excludes the dataset from use) by default.

22.1.2. Verify

To be used as a filter, the status for at least one of the analytes in the list must be set to "Yes." This is accomplished by replacing the default "No" with "Yes" (or any character or symbol string that does not start with "n", "N", or "0"). Clicking the **Verify** button sorts all the "Yes" analytes to the top of the list and sets the "Verified?" status to "Yes".

Clicking **Verify** without a list of analytes that is appropriate for the specified {WG, Base unit} results in the error message and prompt shown in Fig. 78. A list is considered to be inappropriate when the specified {WG, Base unit} doesn't match that specified in the header of column 8, cell(1,8).

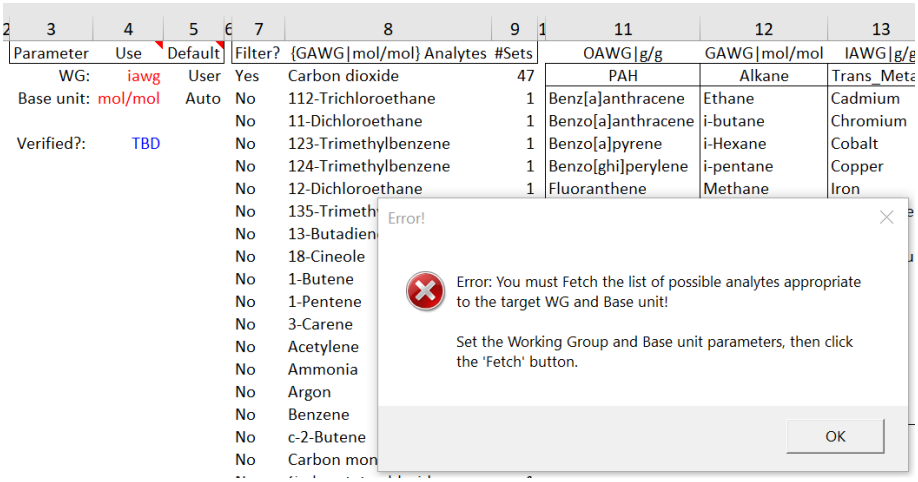


Fig. 78. Error Message and Prompt for an Inappropriate List.

Clicking **Verify** when the list is appropriate but the status of all the analytes in the list is "No" results in the error message and prompt displayed in Fig. 79.

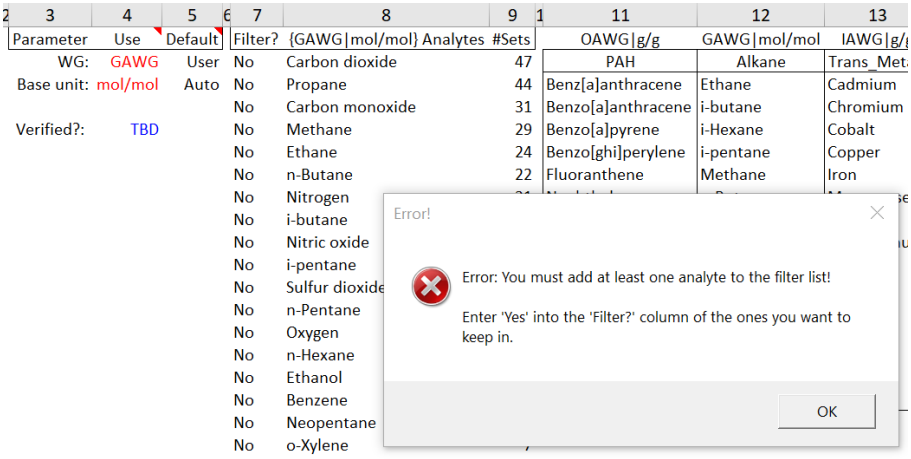
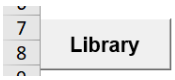


Fig. 79. Error Message and Prompt for an Inactive List.

In either case, click the **OK** button and follow the instructions provided in the prompt. Or click the worksheet's **Back** button and deselect the Analyte filter option.

22.1.3. Library



Rather than just filtering on single analytes, the filter can be on multiple analytes up to and including the entire list (although "filtering" on the full list would slow the data analysis). Lists of analytes that are considered to be related, either physiochemically (e.g., polyaromatic hydrocarbons) or metrologically (e.g., used in organic purity assessment studies) can be stored for efficient recall. Clicking the **Library** button allows the user to select one of the library lists that is appropriate for the specified {WG, Base unit}.

The notification response if there is no appropriate library list is pictured in Fig. 80.

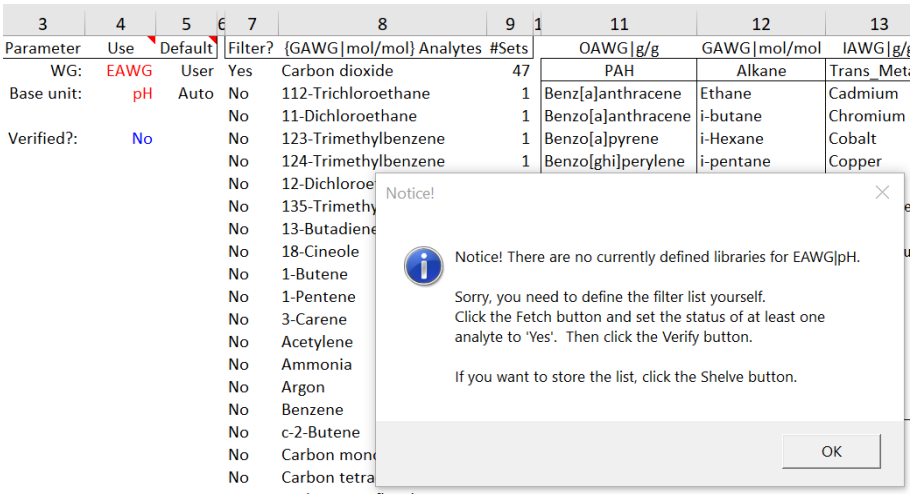


Fig. 80. Notification Response When There Is No Appropriate Library List.

If there is one and only one appropriate library list, that list is loaded as the filter list.

An exemplar input box when there is more than one appropriate library list to choose from is pictured in Fig. 81. Either specify one of the available lists and click the **OK** button or abort the selection by clicking the **Cancel** button or closing the input box.

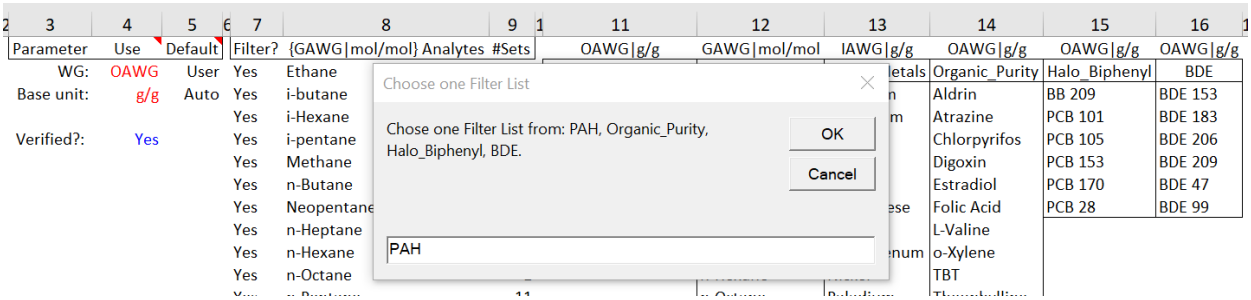


Fig. 81. Exemplar Input Box When There Are Two or More Appropriate Filter Lists.

Once a library list has been specified, the entire set of analytes appropriate to the specified {WG, Base unit} is loaded, the status of the analytes in the specified library list set to "Yes", and the status of the resulting filter list set to "Yes".

The inactive analytes are sorted alphabetically; they should be quickly examined to ensure that all analytes of the desired grouping are active. If the status of any analyte must be changed, the revised list must be re-**Verify**-ed.

22.1.4. Shelve

The **Shelve** command allows users to specify and save custom analyte Filter Lists to the Library. If the current filter list contains more than one active analyte, has been successfully verified, and is given a name that does not conflict with previously defined library lists, then clicking the **Shelve** button stores the active members of the list in the next available empty column.

There are a number of validation tests performed and a unique name must be given to the list before the it is added to the library. The notification and prompt when the filter list has been successfully shelved in the library is pictured in Fig. 82.

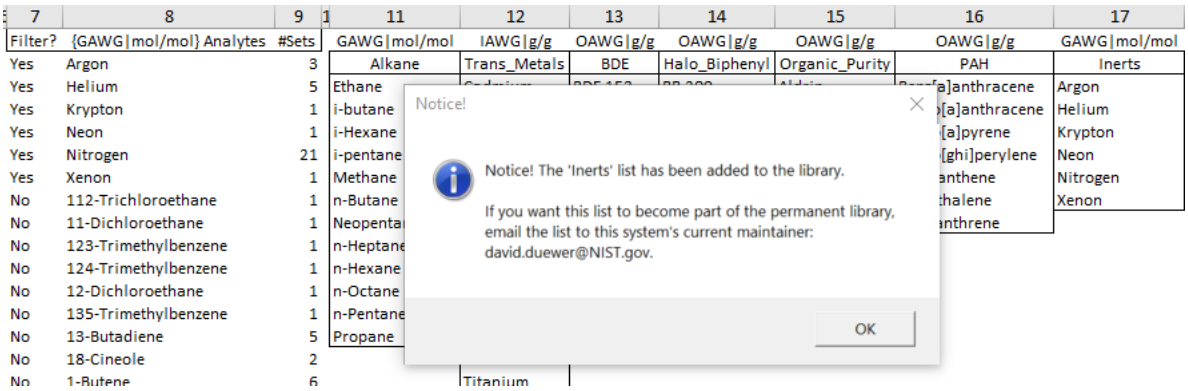
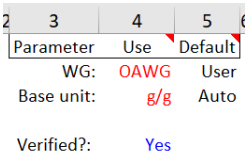


Fig. 82. Notification and Prompt When the Filter List Is Successfully Shelved.

22.2. Parameters



WG: and **Base unit:** are the only input parameters (see Sections 2.4.1.2 and 2.4.1.3). However, **Verified?:** is a critical output parameter. Until the status of this parameter is "Yes", the Analyte filter cannot be applied. This parameter can only be successfully set by using the **Verify** command.

22.3. Structure of a Library List

Library lists have the following defined structure:

- Row 1 (header). The {WG, Base unit} appropriate to the analytes. This is specified as the four-character acronym (e.g., GAWG), the vertical line character (|), and the Base unit (e.g., mol/mol).
- Row 2 (list name). A unique name, a short description that should be readily recognizable.
- Rows 3 to … (analytes). The analyte names, as used in the datasets.

23. TimeTrial

The *TimeTrial* benchmarking tool exercises most of the *CCQM_Retrospectoscope* analysis and support subsystems. If it successfully completes, it reports the elapsed time. The primary utility of this subsystem is to confirm that everything is working, secondarily to provide a clock-time performance benchmark for a given computing platform.

Unlike other subsystems, this subsystem does not have its own worksheet. As displayed in Fig. 83, clicking the **TimeTrial** button invokes an input box that gives due warning about the likely time required and waits for a user response. Clicking the **OK** button with the response set to "Yes" starts the trial; setting the response to "No", clicking the **Cancel** button, or closing the input box aborts the trial.

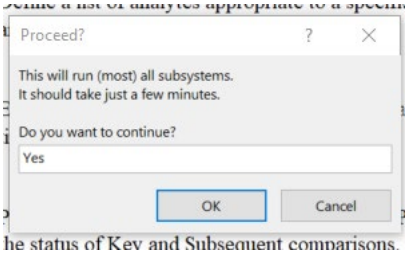


Fig. 83. *TimeTrial* Dialog Box.

If *TimeTrial* finishes without error, as shown in Fig. 84, the only output is a notification box that displays the elapsed clock time, in minutes, from the start of the trial. Clicking the **OK** button returns control to the user.

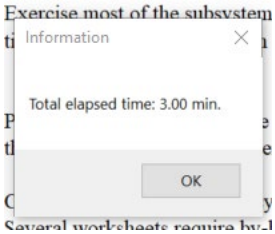


Fig. 84. *TimeTrial* Successful Completion Notification Box.

If the *CCQM_Retrospectoscope* maintainer has done his/her/their job properly, it is unlikely that *TimeTrial* will terminate with either a datasheet or programmatic error. However, Excel's VBA programs are prone to various "real time" errors that can be erratic and may be computer specific.

23.1. What To Do If TimeTrial Does Not Successfully Complete

If *TimeTrial* does not complete, please do the following:

- Close Excel (and all other open apps) and restart your computer. This (sometimes) clears corrupted registry and temporary files that cause real-time overflow errors.
- Restart a clean copy of the current *CCQM_Retrospectoscope* and rerun *TimeTrial*. Hopefully, it will finish normally. However, if it halts again then…
- Take a screenshot of whatever error message the Excel engine provide. With Windows systems, use the keyboard <shift+PrtScn> combination or the Snip & Sketch utility; with

Macintosh, use <Shift+Command+3> to capture the entire screen (or <Shift+Command+5> to define a smaller region) or use the Image Capture utility.

- Email the image to david.duewer@nist.gov or whoever the current maintainer may be, along with a description of your computing platform and Excel version.

23.2. Tested Platforms and Performance Metrics

Table 8 lists some of the computing platforms that the *CCQM_Retrospectoscope* has been tested on and the time (in minutes) required by *TimeTrial* to exercise all the system's major functionalities.

Table 8. Computing Platforms and Time Required to Complete *TimeTrial*.

Platform	Excel	Minutes
Dell 7490, Intel COREi7, 1.90 GHz, 8 GB, Windows 10 Enterprise	Microsoft 365 Apps for Enterprise	3.0
HP 350 G1, Intel COREi3, 1.70 GHz, 6 GB, Windows 10 Home	Microsoft Office Home and Student 2013	5.6
MacBook Pro10,1, Intel COREi7, 2.3 GHz, 16 GB, Catalina 10.15.7	Microsoft 365 Subscription Excel for Mac	8.1
MacBook Air 2020, Apple M1, 3.2 GHz, 16 GB, Ventura 13.51	Microsoft 365 Subscription Excel for Mac	2.2

As shown in Fig. 85, the initial invocation requires less time than do following invocations, evidence of some as-yet unexplained parasitic overhead. While the magnitude of the duration difference is sensitive to what else on the platform is competing with *CCQM_Retrospectoscope* for resources, the increased clock time for following invocations is consistent across the Windows and Macintosh platforms evaluated.

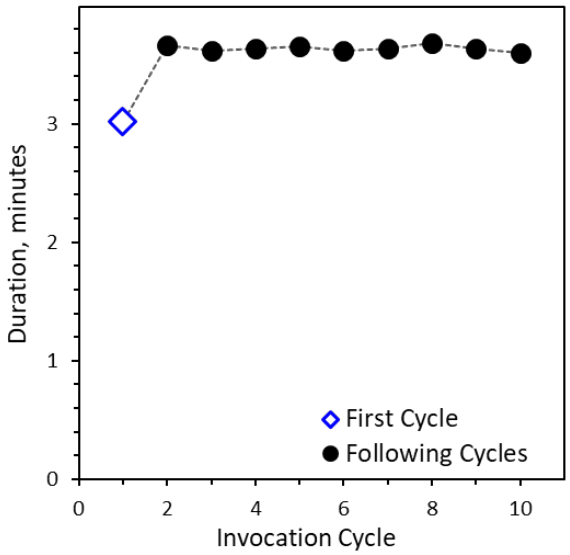


Fig. 85. *TimeTrial* Duration as a Function of Invocation Cycle on the Dell 7490 Platform.

The clock-time required by most of *CCQM_Retrospectoscope*'s subsystems to load and evaluate the default data (GAWG, NIST, 1993 to 2023) on the Dell 7490 is displayed in Fig. 86. These summary statistics are for cycles following the initial invocation.

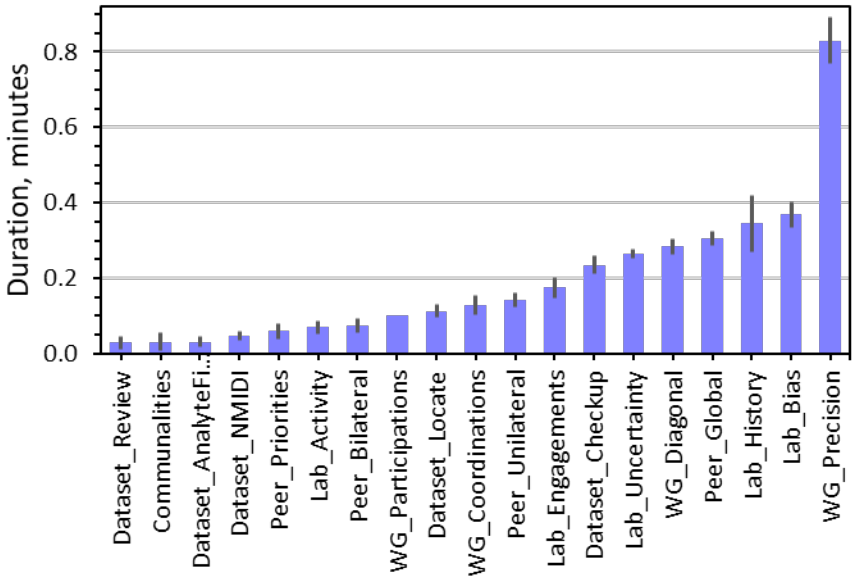


Fig. 86. Average Subsystem "Following Cycle" Duration on the Dell 7490.

Error bars represent approximate 95 % confidence intervals on the mean durations.

The time required by *WG_Power* is not displayed as it requires somewhat more than the sum of the times required by its component invocations: *WG_Precision*, (*Peer_Bilateral*, *Peer_Unilateral, or Peer_Global*) and number-of-peer-NMI|DIs × *Lab_Uncertainty*.

24. Database_FindNew

The *Database_FindNew* worksheet provides five standalone tools for identifying newly available studies and for identifying changes in study status. The worksheet's command buttons and output format are shown in Fig. 95.

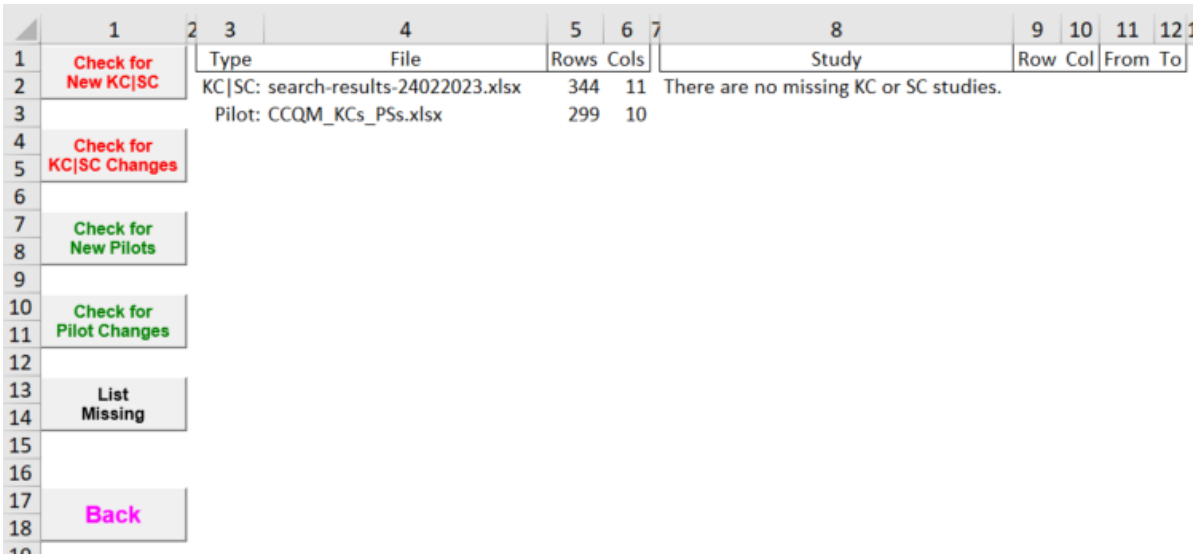


Fig. 87. *Database_FindNew* Dashboard After Clicking the **Check for New KC|SC** Button.

Note: These tools only identify newly available studies or changes in their status. Adding summary information to the *Datacore_Dates* worksheet, downloading newly available final reports, and adding new datasets to the *CCQM_Retrospectoscope* datasheets must be done "by hand" (sometimes accompanied by considerable head-scratching) by the system maintainer.

24.1. Additional Command Buttons

The *Dataset_AnalyteFilter* worksheet supports five command buttons in addition to the usual **Back** (Section 2.1.5) and **Restore** (Section 2.1.7).

24.1.1. Check for New KC|SC

Clicking the **Check for New KC|SC** button compares the list of KC and SC studies maintained in the *Datacore_Dates* worksheet with that provided in a KCDB "search-results" file specified in row 2 of column 4. The KCDB provides status information for all authorized KC and SCs and is updated as new information is becomes available. Newly authorized studies are listed in column 8 of the *Database_FindNew* worksheet. These studies and their characteristics must be "by hand" added to the *Datacore_Dates* worksheet.

See Section 24.2.1 for how to obtain a current KCDB "search-results" file.

24.1.2. Check for KC|SC Changes

Clicking the **Check for KC|SC Changes** button compares the study dates, WG, coordinator(s), and status of KC and SC studies as maintained in the *Datacore_Dates* worksheet with that provided in a KCDB "search-results" file specified in row 2 of column 4. Changes in these values are listed in column 8 to 12 of the *Database_FindNew* worksheet. These changes must be "by hand" added to the *Datacore_Dates* worksheet.

See Section 24.2.1 for how to obtain a current KCDB "search-results" file.

24.1.3. Check for New Pilots

Clicking the **Check for New Pilots** button compares the list of pilot studies (PPS and PS) maintained in the *Datacore_Dates* worksheet with that provided in the CCQM's master tracking file: *CCQM_KCs_PSs.xlsx* [**Error! Bookmark not defined.**], specified in row 3 o f column 4. This file is a summary of all CCQM studies, is updated at infrequent intervals, and has accumulated numerous minor errors. Newly authorized studies are listed in column 8 of the *Database_FindNew* worksheet. These studies and their characteristics must be "by hand" added to the *Datacore_Dates* worksheet.

See Section 24.3.1 for how to obtain a current *CCQM_KCs_PSs.xlsx* file.

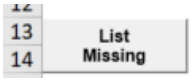
Note: The existence of pilot studies is publicly accessible information, although the results of the studies may not be. The summary information stored in the *Datacore_Dates* worksheet is used by the *Peer_Priorities* and *WG_Coordinations* subsystems.

24.1.4. Check for Pilot Changes

Clicking the **Check for Pilot Changes** button compares the study dates, WG, coordinator(s), and status of pilot studies (PPS and PS) as maintained in the *Datacore_Dates* worksheet with that provided in the CCQM's master tracking file: *CCQM_KCs_PSs.xlsx* [**Error! B ookmark not defined.**] specified in row 3 of column 4. Changes in these values are listed in column 8 to 12 of the *Database_FindNew* worksheet. These changes must be "by hand" added to the *Datacore_Dates* worksheet.

See Section 24.3.1 for how to obtain a current *CCQM_KCs_PSs.xlsx* file.

24.1.5. List Missing



Clicking the **List Missing** button lists the studies identified in the *Datacore_Dates* worksheet as finalized but with no datasets in the CCQM_Retrospectoscope database and no explanatory comment. As of this document's publication date, there are six missing pilot study reports; Fig. 88 lists the available information on these studies.

H	I	J	K	L	M
Study	Row	Col	From	To	Comments
CCQM-P045: Purity of parent gases including water	375	1	GAWG	(2002)	
CCQM-P137: Activity of α-amylase in human serum	479	1	PAWG	(2015)	
CCQM-P164: Human growth hormone in serum	505	1	PAWG	(2017)	
CCQM-P202: Mass fraction of leucine, phenylalanine in pooled	536	1	OAWG	(2019)	|| to: CCQM-K159
CCQM-P212: Carbon isotope delta measurements	544	1	IRWG	(2020)	|| to: CCQM-K167/P211
CCQM-P214: Trans-zearalenone in maize powder	545	1	OAWG	(2020)	|| to: CCQM-K168

6 finalized pilot studies are missing.
Good luck in finding the data!

Fig. 88. *Database_FindNew* Output After Clicking the **List Missing** Button.

24.2. *search-results-ddmmyyyy.xlsx* File

The BIPM's KCDB can output summary information (designation, title, WG, coordinator(s), start year, and current status) about all of the CCQM's KCs and SCs as an Excel file named *search-results-ddmmyyyy.xlsx* where ddmmyyyy is the current day-month-year date. The KCDB webpage is https://www.bipm.org/kcdb/.

24.2.1. Obtaining the *search-results-ddmmyyyy.xlsx* File

The current *search-results-ddmmyyyy.xlsx* file is obtained using the KCDB's "Key and supplementary comparisons" "Advanced search" function. The function is accessed by clicking the "Advanced search" link located just below the "Key and supplementary comparisons" search box at the bottom right of the KCDB dashboard, shown in Fig. 96.

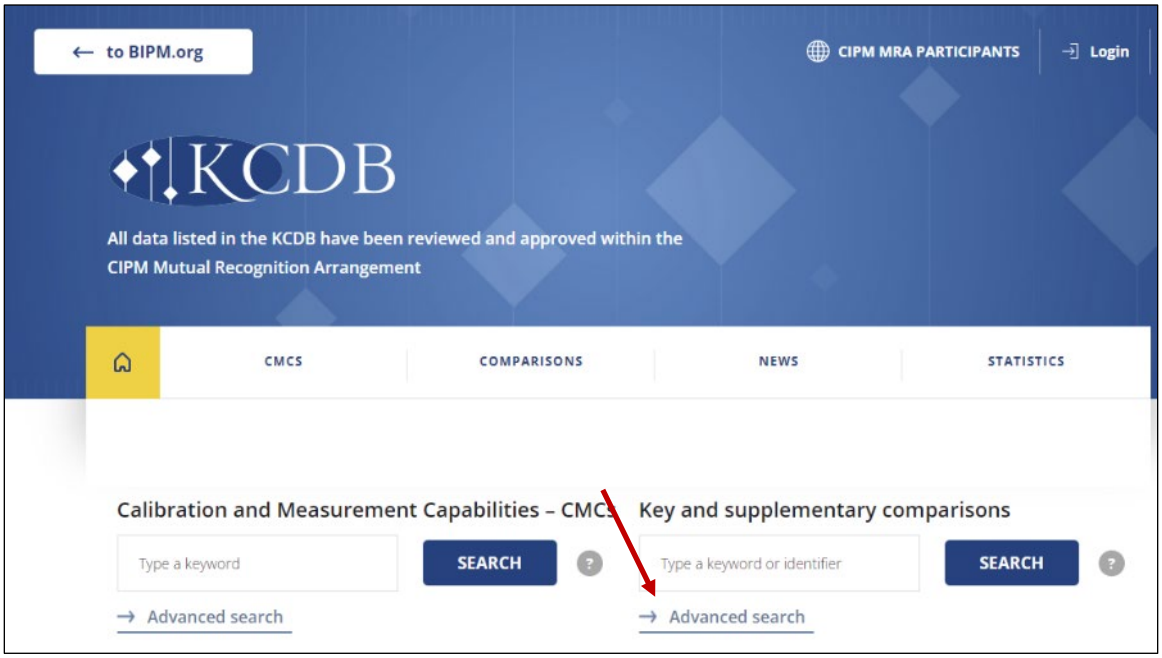


Fig. 89. Image of the BIPM's KCDB Dashboard.

The "Advanced search" function is accessed by clicking the link indicated by the red arrow.

Clicking the “Advanced search” link activates the BIPM’s “COMPARISON ADVANCED SEARCH” dashboard, shown in Fig. 97. As of this document’s publication date, this webpage could be accessed at https://www.bipm.org/kcdb/comparison/advanced-search.

Select “Chemistry and Biology” from the list provided in this dashboard’s “Metrology area” field. All other fields should be left at their default values. Clicking the “APPLY CRITERIA” button should generate a message reporting the total number of CCQM KC and SC studies (342 as of this document’s publication date) and the start of a listing as shown in Fig. 91.

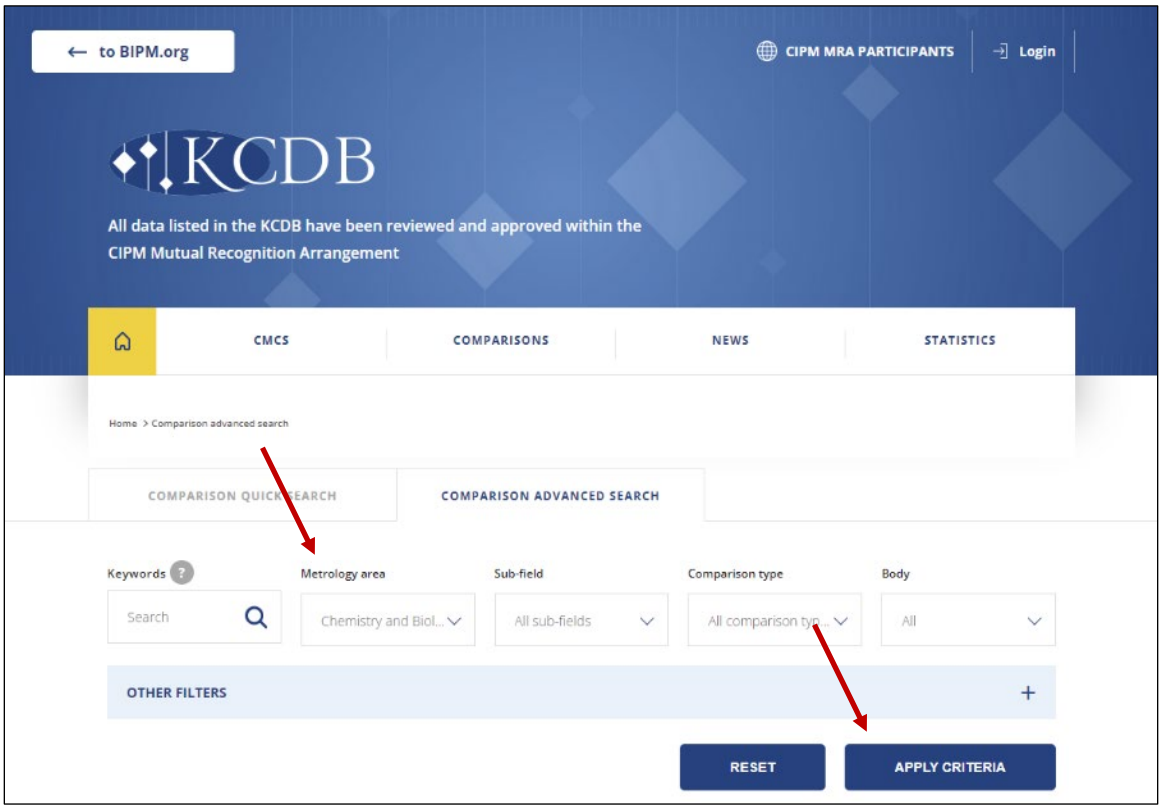


Fig. 90. Image of the KCDB “COMPARISON ADVANCED SEARCH” Dashboard.

The red arrow to the left points to the Metrology area field. The search is initiated by clicking the APPLY CRITERIA button pointed to by the red arrow to the right.

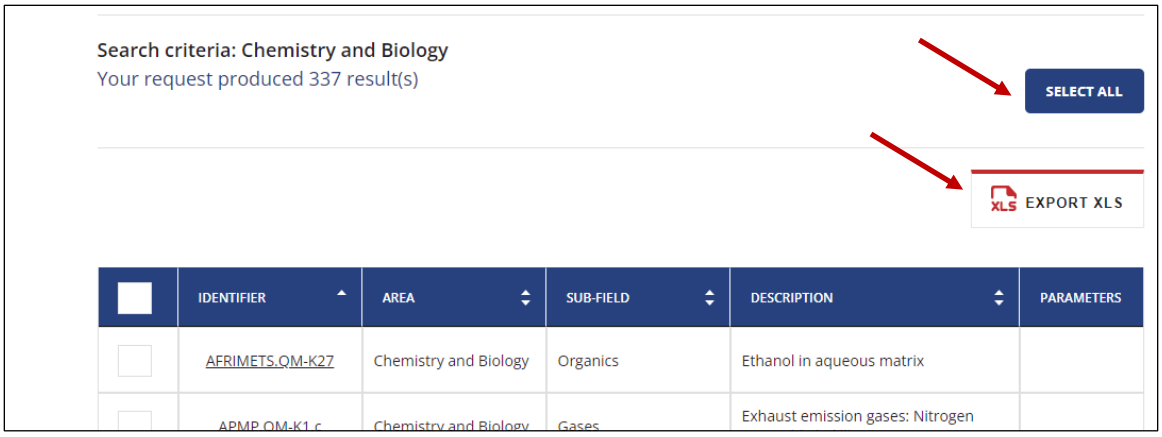


Fig. 91. Image of an Example Advanced Search Output.

The upper red arrow points to the Select All button. The lower arrow points to the "EXPORT XLS" link.

Clicking the "SELECT ALL" button loads the summary information on all of the studies; this sometimes takes several seconds. Clicking the "EXPORT XLS" link downloads the *search-results-ddmmyyyy.xlsx* file.

24.2.2. Making Use of the *search-results-ddmmyyyy.xlsx* File

Move the *search-results-ddmmyyyy.xlsx* file into the folder that holds *CCQM_Retrospectoscope* and activate the *Database_FindNew* worksheet. Modify the file designation in row 2 of column 4 as needed. If the system can't find the file, you will be prompted to supply the correct name.

Click the **Check for New KC|SC** button. If any new studies are identified, add the information to the *Datacore_Dates* worksheet. This step is not automated to force the system maintainer to cross-check and think before typing, hopefully helping maintain database integrity. Do not proceed until clicking the **Check for New KC|SC** button produces the message "There are no missing KC or SC studies."

Click the **Check for KC|SC Changes** button. If changes are identified, change the information in the *Datacore_Dates* worksheet. This step is not automated to force the system maintainer to cross-check and think before typing, hopefully helping maintain database integrity. Do not proceed until clicking the **Check for KC|SC Changes** button either produces the message "No WG, pilot lab, measurement date, or status changes were identified" or the indicated changes are determined to be unnecessary.

24.3. *CCQM_KCs_PSs.xlsx* File

All approved studies are summarized in the *CCQM_KCs_PSs.xlsx* workbook hosted by the BIPM. This workbook contains separate worksheets for KCs and PSs, along with worksheets that list the KCs for each WG. Since this workbook is hand-curated (and has accumulated a number of minor misspellings and out-of-date information over the years), only the "Pilot Study" worksheet is of interest since the *search-results-ddmmyyyy.xls* files are a primary source for the KC and SC summary information.

24.3.1. Obtaining the *CCQM_KCs_PSs.xlsx* File

As of this document's publication date, the *CCQM_KCs_PSs.xlsx* file can be located and retrieved using the BIPM's search function (https://www.bipm.org/en/search) as shown in Fig. 92. The search also locates documents that mention the file.

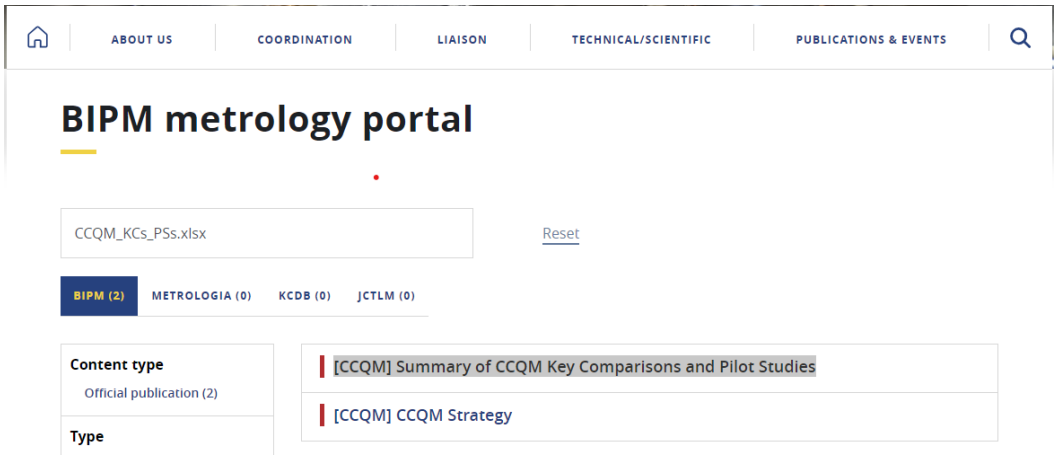


Fig. 92. Results of BIPM Search for *CCQM_KCs_PSs.xlsx*.

The worksheets in this files specify the date they were last updated in row 3 column 2: see Fig. 93. As of this document's publication date, the workbook was last updated January 27, 2023.

	1	2	3	4	5	6
1	CCQM Pilot Studies					
2						
3	Date updated	20 July 2022				
4						
5	WG	Reference No.	Description	Coordinating Laboratory	Start date	Status
6	IAWG	CCQM-P1	Trace elements in water Pb	NIST	1997	Completed 1998

Fig. 93. Header of the *Pilot Studies* Worksheet of the *CCQM_KCs_PSs.xlsx* Workbook.

24.3.2. Making Use of the *CCQM_KCs_PSs.xlsx* File

Move the *CCQM_KCs_PSs.xlsx* file into the folder that holds *CCQM_Retrospectoscope* and activate the *Database_FindNew* worksheet. If necessary, modify the file designation in row 3 of column 4. If the system can't find the file, you will be prompted to supply the correct name.

Click the **Check for New Pilots** button. If any new studies are identified, add the information to the *Datacore_Dates* worksheet. This step is not automated to force the system maintainer to cross-check and think before typing, hopefully helping maintain database integrity. Do not proceed until clicking the **Check for New Pilots** button produces the message "There are no missing Pilot studies."

Click the **Check for Pilot Changes** button. If changes are identified, change the information in the *Datacore_Dates* worksheet. This step is not automated to force the system maintainer to

cross-check and think before typing, hopefully helping maintain database integrity. Do not proceed until clicking the **Check for Pilot Changes** button either produces the message "No WG, pilot lab, measurement date, or status changes were identified" or the indicated changes are determined to be unnecessary.

24.4. Obtaining Reports

Once new studies have been identified and their status suggests reports are (or may be) available, the reports that provide the data and their interpretation needed to update the CCQM_Retrospectoscope must be obtained.

24.4.1. Obtaining "Draft" Reports and Preliminary Presentations

Get the documents and reports that contain the data from your local CCQM WG contacts. Not every contact within a WG gets such reports automatically, so you may need to ask them to search their WG's "Members Only" site.

It's difficult to locate non-Final reports from RMO studies unless your NMI|DI has "skin in the game" (i.e., participating in the study and being on the draft report distribution list). Searching RMO websites and/or the general web can be productive. But you need to know the official designation of any study to have any real chance of finding interesting data.

24.4.2. Obtaining KC and SC Final Reports

Once a KC has been "Approved for Equivalence" or an SC has been "Approved", the final report can be obtained using the KCDB dashboard's "Key and supplementary comparisons" search function. Type the study identifier (in the BIPM format; that is, without leading "0"s) into the search field and click the SEARCH button. For RMO KCs and SC's. recall the differences between the BIPM and CCQM_Retrospectoscope designations: e.g., "COOMET.QM-K120" becomes "CoQM-K120" and "EURAMET.QM-S9" become "EUQM-S009".

24.4.3. Obtaining Pilot Study Results

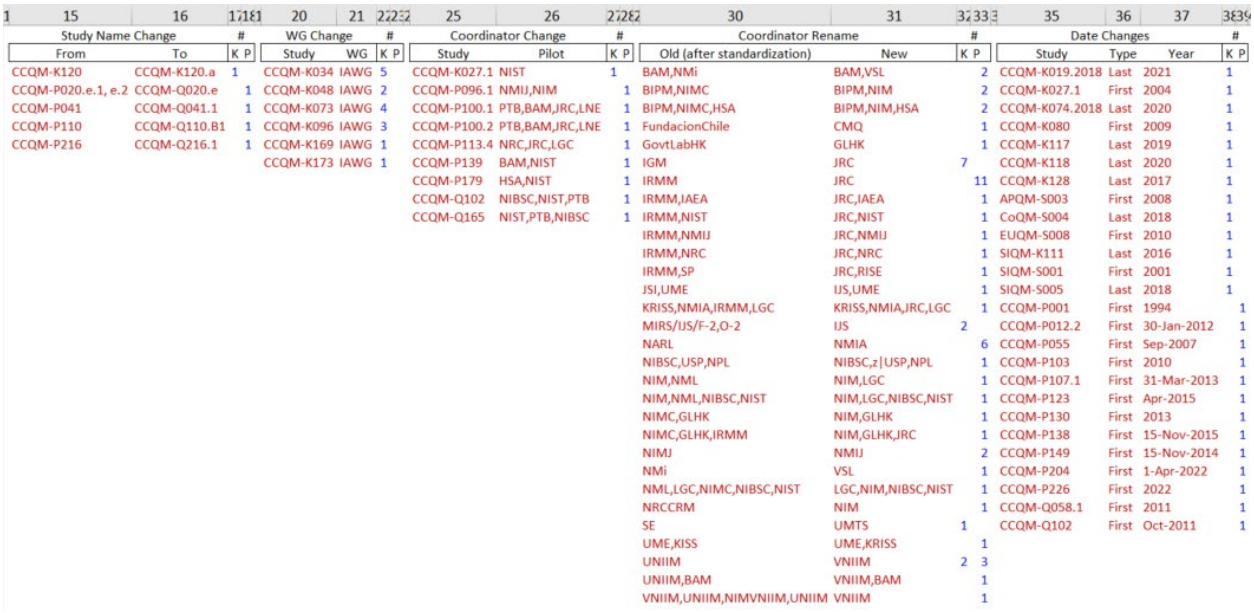
Many PPS are listed on the BIPM's *https://www.bipm.org/en/committees/cc/ccqm/pilot-studies* website in declining order of publication date. The listings provide links to final reports. As of this document's publication date there is no simple way to export a summary file from this webpage. Identifying newly available PPS requires visual comparison of the listings against what's documented in the *Datacore_Dates* worksheet. PPS are coded in the CCQM_Retrospectoscope as "CCQM-Qxxx" (and xxx is always three digits with leading zeros as needed) rather than the official "CCQM-Px" (no leading zeros).

Results from parallel PSs are often provided only in preliminary presentations or "Draft A" reports, in which case the results cannot be made public. However, occasionally parallel pilot results are published as part of the KC's final report and are therefore publicly accessible.

Since the results from some pilot studies have been described in specialist publications, it's always worth searching the internet.

24.5. Addressing Input File Disagreements

When any of the four "Check for" buttons are clicked and a deficiency in the *CCQM_Retrospectoscope*'s database is identified, there is a non-zero chance that the problem is with the information in the BIPM-provided *search-results-ddmmyyyy.xlsx* (for KCs and SCs) or *CCQM_KCs_PSs.xlsx* (for PPSs and PSs) files. These discrepancies include differences in study names, WG assignments, coordinating laboratories, NMI acronyms, and study dates. The changes required as of this document's publication date are listed in Fig. 94.



Study Name Change		#	
From	To	K	P
CCQM-K120	CCQM-K120.a	1	
CCQM-P020.e.1, e.2	CCQM-Q020.e	1	
CCQM-P041	CCQM-Q041.1	1	
CCQM-P110	CCQM-Q110.B1	1	
CCQM-P216	CCQM-Q216.1	1	

WG Change		#	
Study	WG	K	P
CCQM-K034	IAWG	5	
CCQM-K048	IAWG	2	
CCQM-K073	IAWG	4	
CCQM-K096	IAWG	3	
CCQM-K169	IAWG	1	
CCQM-K173	IAWG	1	

Coordinator Change		#	
Study	Pilot	K	P
CCQM-K027.1	NIST	1	
CCQM-P096.1	NMIJ,NIM	1	
CCQM-P100.1	PTB,BAM,JRC,LNE	1	
CCQM-P100.2	PTB,BAM,JRC,LNE	1	
CCQM-P113.4	NRC,JRC,LGC	1	
CCQM-P139	BAM,NIST	1	
CCQM-P179	HSA,NIST	1	
CCQM-Q102	NIBSC,NIST,PTB	1	
CCQM-Q165	NIST,PTB,NIBSC	1	

Coordinator Rename		#	
Old (after standardization)	New	K	P
BAM,NMi	BAM,VSL		2
BIPM,NIMC	BIPM,NIM		2
BIPM,NIMC,HSA	BIPM,NIM,HSA		2
FundacionChile	CMQ		1
GovtLabHK	GLHK		1
IGM	JRC	7	
IRMM	JRC		11
IRMM,IAEA	JRC,IAEA		1
IRMM,NIST	JRC,NIST		1
IRMM,NMIJ	JRC,NMIJ		1
IRMM,NRC	JRC,NRC		1
IRMM,SP	JRC,RISE		1
JSI,UME	IJS,UME		1
KRISS,NMIA,IRMM,LGC	KRISS,NMIA,JRC,LGC		1
MIRS/IJS/F-2,O-2	IJS	2	
NARL	NMIA		6
NIBSC,USP,NPL	NIBSC,z|USP,NPL		1
NIM,NML	NIM,LGC		1
NIM,NML,NIBSC,NIST	NIM,LGC,NIBSC,NIST		1
NIMC,GLHK	NIM,GLHK		1
NIMC,GLHK,IRMM	NIM,GLHK,JRC		1
NIMJ	NMIJ		2
NMi	VSL		1
NML,LGC,NIMC,NIBSC,NIST	LGC,NIM,NIBSC,NIST		1
NRCCRM	NIM		1
SE	UMTS	1	
UME,KISS	UME,KRISS		1
UNIIM	VNIIM	2	3
UNIIM,BAM	VNIIM,BAM		1
VNIIM,UNIIM,NIMVNIIM,UNIIM	VNIIM		1

Date Changes			#
Study	Type	Year	K P
CCQM-K019.2018	Last	2021	1
CCQM-K027.1	First	2004	1
CCQM-K074.2018	Last	2020	1
CCQM-K080	First	2009	1
CCQM-K117	Last	2019	1
CCQM-K118	Last	2020	1
CCQM-K128	Last	2017	1
APQM-S003	First	2008	1
CoQM-S004	Last	2018	1
EUQM-S008	First	2010	1
SIQM-K111	Last	2016	1
SIQM-S001	First	2001	1
SIQM-S005	Last	2018	1
CCQM-P001	First	1994	1
CCQM-P012.2	First	30-Jan-2012	1
CCQM-P055	First	Sep-2007	1
CCQM-P103	First	2010	1
CCQM-P107.1	First	31-Mar-2013	1
CCQM-P123	First	Apr-2015	1
CCQM-P130	First	2013	1
CCQM-P138	First	15-Nov-2015	1
CCQM-P149	First	15-Nov-2014	1
CCQM-P204	First	1-Apr-2022	1
CCQM-P226	First	2022	1
CCQM-Q058.1	First	2011	1
CCQM-Q102	First	Oct-2011	1

Fig. 94. Changes Required to the BIPM-Provided Information.

As new information becomes available, it is probable that additional changes will be required. But before adding to any of these lists, confirm that the information in the CCQM_Retrospectoscope's *Datacore_Dates* worksheet accurately reflects what's in the study's primary documentation (typically the Final Report).

The "#K" columns in the above image are populated during execution of the "Check For New KC|SC" and "Check for "KC|SC Changes" commands, the "#P" columns are populated during execution of the "Check for New Pilots" and "Check for Pilot Changes" commands. These columns count the number of records changed. This facilitates checking that the listed changes have been appropriately implemented. Be aware that none of the listed changes are pertinent to all four commands, but some of the changes are pertinent to more than one command.

The all of the change counts are reset when "Check For New KC|SC" is executed.

Note: these changes were originally "hard coded" in various VBA subroutines in the *Database_FindNew* subsystem. They were implemented in their current "soft" form to make life a little easier for any future system maintainer.

25. Database_Checkup

The *Database_Checkup* subsystem checks the datasets stored in all the CCQM datasheets for validity and the supporting information for completeness and consistency. The *Database_Checkup* commands and monitor table are pictured in Fig. 95.

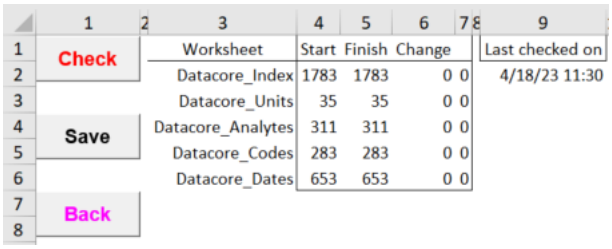


Fig. 95. The Basic *Database_Checkup* Dashboard.

25.1. Monitor Table

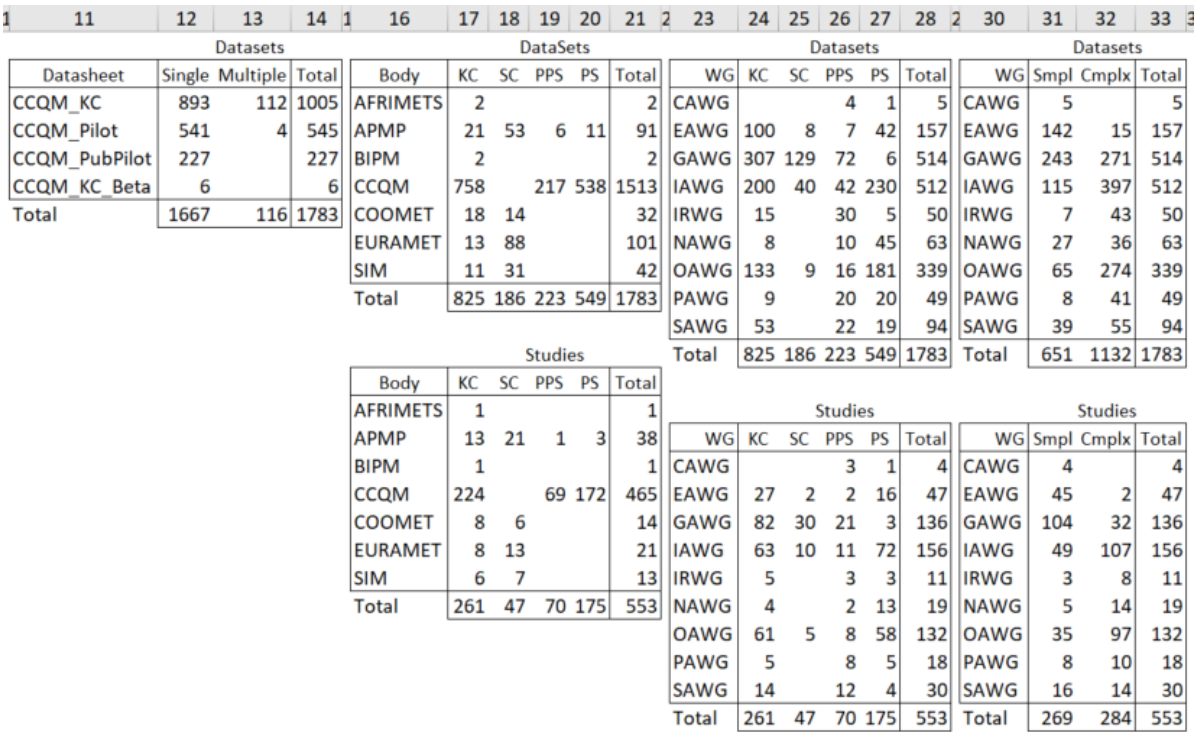
The small table to the right of the command buttons is used to monitor the number of various database elements before and after updates, any change in those numbers, and the number of flagged issues. This table has five rows:

- the *Index* row lists the total number of datasets in the *CCQM_Retrospectoscope* datasheets,
- the *Units* row lists the number of unique Base units,
- the *Analytes* row lists the number of unique analytes,
- the *Codes* row lists the number of unique participating organization code names, and
- the *Dates* row lists the number of different CCQM studies. Not all these studies are associated with datasets: many authorized studies are not complete (or even started), a goodly number of authorized Pilot studies had no participants or only reported anonymized results and a few studies have been abandoned or renamed.

Immediately to the right of this table is the date and time of the latest checkup.

25.2. Summary Tables

If there are no issues, the subsystem creates a series of summary tables. The tables that list the number and types of datasets within the various datasheets, sponsored by the various bodies, and coordinated by the various WGs are pictured in Fig. 96.



Datasets

Datasheet	Single	Multiple	Total
CCQM_KC	893	112	1005
CCQM_Pilot	541	4	545
CCQM_PubPilot	227		227
CCQM_KC_Beta	6		6
Total	1667	116	1783

DataSets

Body	KC	SC	PPS	PS	Total
AFRIMETS	2				2
APMP	21	53	6	11	91
BIPM	2				2
CCQM	758		217	538	1513
COOMET	18	14			32
EURAMET	13	88			101
SIM	11	31			42
Total	825	186	223	549	1783

Studies

Body	KC	SC	PPS	PS	Total
AFRIMETS	1				1
APMP	13	21	1	3	38
BIPM	1				1
CCQM	224		69	172	465
COOMET	8	6			14
EURAMET	8	13			21
SIM	6	7			13
Total	261	47	70	175	553

Datasets

WG	KC	SC	PPS	PS	Total
CAWG			4	1	5
EAWG	100	8	7	42	157
GAWG	307	129	72	6	514
IAWG	200	40	42	230	512
IRWG	15		30	5	50
NAWG	8		10	45	63
OAWG	133	9	16	181	339
PAWG	9		20	20	49
SAWG	53		22	19	94
Total	825	186	223	549	1783

Studies

WG	KC	SC	PPS	PS	Total
CAWG			3	1	4
EAWG	27	2	2	16	47
GAWG	82	30	21	3	136
IAWG	63	10	11	72	156
IRWG	5		3	3	11
NAWG	4		2	13	19
OAWG	61	5	8	58	132
PAWG	5		8	5	18
SAWG	14		12	4	30
Total	261	47	70	175	553

Datasets

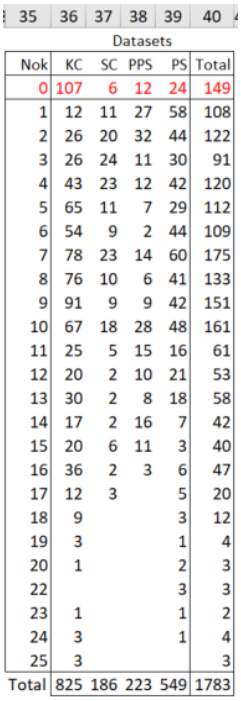
WG	Smpl	Cmplx	Total
CAWG	5		5
EAWG	142	15	157
GAWG	243	271	514
IAWG	115	397	512
IRWG	7	43	50
NAWG	27	36	63
OAWG	65	274	339
PAWG	8	41	49
SAWG	39	55	94
Total	651	1132	1783

Studies

WG	Smpl	Cmplx	Total
CAWG	4		4
EAWG	45	2	47
GAWG	104	32	136
IAWG	49	107	156
IRWG	3	8	11
NAWG	5	14	19
OAWG	35	97	132
PAWG	8	10	18
SAWG	16	14	30
Total	269	284	553

Fig. 96. The *Database_Checkup* Datasheet, Body, and WG Tables.

A part of the table that summarizes the number of datasets containing given numbers of valid (Nok) data is pictured in Fig. 97. The first row, where Nok is 0 and the numbers are in red font, accounts for the composite datasets and datasets for which a reference value and/or its uncertainty could not be assigned.

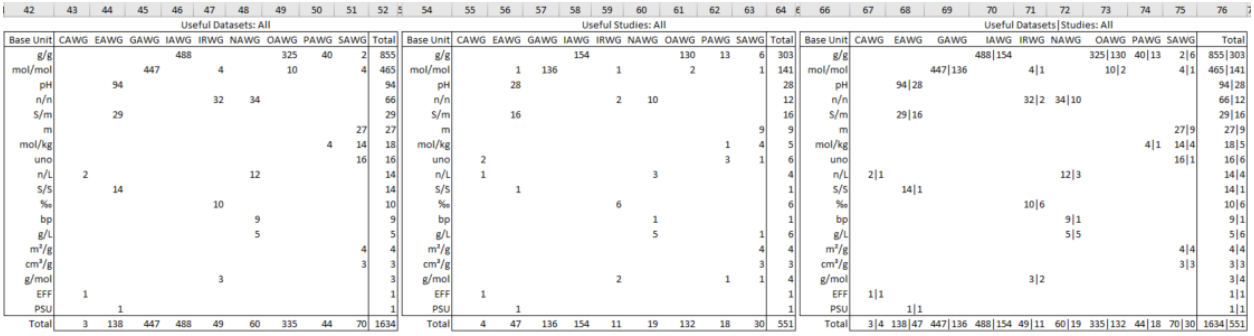


Datasets

Nok	KC	SC	PPS	PS	Total
0	107	6	12	24	149
1	12	11	27	58	108
2	26	20	32	44	122
3	26	24	11	30	91
4	43	23	12	42	120
5	65	11	7	29	112
6	54	9	2	44	109
7	78	23	14	60	175
8	76	10	6	41	133
9	91	9	9	42	151
10	67	18	28	48	161
11	25	5	15	16	61
12	20	2	10	21	53
13	30	2	8	18	58
14	17	2	16	7	42
15	20	6	11	3	40
16	36	2	3	6	47
17	12	3		5	20
18	9			3	12
19	3			1	4
20	1			2	3
22				3	3
23	1			1	2
24	3			1	4
25	3				3
Total	825	186	223	549	1783

Fig. 97. The *Database_Checkup* Distribution of Valid Values Table.

A portion of the tables that list the number of usable datasets, studies, and the combination of datasets and studies coordinated by the various WGs for the various Base units is pictured in Fig. 98. In addition to the "All" tables shown, tables are provided for KC, SC, PPS, P, and the publicly available data (KC, SC, and PPS). A "usable dataset" has both a numeric reference uncertainty and measurement year.



Useful Datasets: All

Base Unit	CAWG	EAWG	GAWG	IAWG	IRWG	NAWG	OAWG	PAWG	SAWG	Total
g/g				488			325	40	2	855
mol/mol			447		4		10		4	465
pH		94								94
n/n					32	34				66
S/m		29								29
m									27	27
mol/kg								4	14	18
uno									16	16
n/L	2					12				14
S/S		14								14
‰					10					10
bp						9				9
g/L						5				5
m²/g									4	4
cm²/g									3	3
g/mol					3					3
EFF	1									1
PSU		1								1
Total	3	138	447	488	49	60	335	44	70	1634

Useful Studies: All

Base Unit	CAWG	EAWG	GAWG	IAWG	IRWG	NAWG	OAWG	PAWG	SAWG	Total
g/g				154			130	13	6	303
mol/mol		1	136		1		2		1	141
pH		28								28
n/n						2	10			12
S/m		16								16
m									9	9
mol/kg								1	4	5
uno	2							3	1	6
n/L	1						3			4
S/S		1								1
‰						6				6
bp							1			1
g/L							5		1	6
m²/g									4	4
cm²/g									3	3
g/mol						2		1	1	4
EFF	1									1
PSU		1								1
Total	4	47	136	154	11	19	132	18	30	551

Useful Datasets|Studies: All

Base Unit	CAWG	EAWG	GAWG	IAWG	IRWG	NAWG	OAWG	PAWG	SAWG	Total
g/g				488|154			325|130	40|13	2|6	855|303
mol/mol			447|136		4|1		10|2		4|1	465|141
pH		94|28								94|28
n/n					32|2	34|10				66|12
S/m		29|16								29|16
m									27|9	27|9
mol/kg								4|1	14|4	18|5
uno									16|1	16|6
n/L	2|1					12|3				14|4
S/S		14|1								14|1
‰					10|6					10|6
bp						9|1				9|1
g/L						5|5				5|6
m²/g									4|4	4|4
cm²/g									3|3	3|3
g/mol					3|2					3|4
EFF	1|1									1|1
PSU		1|1								1|1
Total	3|4	138|47	447|136	488|154	49|11	60|19	335|132	44|18	70|30	1634|551

Fig. 98. Exemplar *Database_Checkup* {WG, Base unit} Tables.

25.3. Additional Command Buttons

Of the four command buttons present on the *Database_Checkup* worksheet, only the **Check** and **Save** buttons are not described in Section 2.1.

25.3.1. Check

Clicking the **Check** button initiates the checkup. If issues are identified, they must be completely resolved – and the **Check** button clicked again – before the summary tables are generated. There are three types of issues that this subsystem identifies:

- Duplicate NMI|DI codes and non-numeric values within a dataset. The affected dataset is made visible, the suspect values are identified with red highlight, a message describing the problem is issued, and processing terminates. The maintainer is instructed to correct the problem and "try again."
- Duplicate dataset titles, inconsistencies in the auxiliary information, and missing measurement year. The issues are identified in column 16 of the *Datacore_Index* worksheet, the affected dataset entries are sorted to the top and identified with yellow highlight. Fixing the problems is the maintainer's responsibility.
- New analytes, codes, and units. These may well represent legitimate additions, but they need to be checked to ensure that they aren't misspellings (e.g., NSIT for NIST) or alternate designations (e.g., g/kg for mg/g, 2-Methylbutane for *i*-Pentane). Clicking **Check** again accepts them as valid additions.

25.3.2. Save

Clicking the **Save** button saves the workbook. Since it's really irritating to fail to save a completed update, this function is provided here for convenience and as a reminder that updates must be explicitly saved.

25.4. Datacore Worksheets

The five *Datacore* worksheets store information essential to *CCQM_Retrospectoscope*'s operation. These worksheets are updated from the *CCQM* datasheets whenever the *Database_Checkup* subsystem successfully completes. The *Datacore_Units, Datacore_Analytes*, and *Datacore_Codes* worksheets require curation by the system maintainer when new units, analytes, or participant code names are encountered. The *Datacore_Dates* worksheets requires curation when new studies are identified.

25.4.1. Datacore_Index

The content of the *Datacore_Index* worksheet is completely regenerated by the *Database_Checkup* subsystem. Every dataset in the *CCQM_Retrospectoscope* system is listed, one dataset per row. The information stored in this worksheet is used to identify duplicate datasets, datasets that aren't listed in the *Datacore_Dates* worksheet, datasets with inconsistent auxiliary information, and datasets with new NMI|DI, analyte, or measurement units. Datasets identified during the checking process as having one or more of these issues are flagged with yellow highlight and sorted to the top of the worksheet.

All flagged issues must be resolved by the system maintainer for the CCQM_Retrospectoscope to function optimally.

25.4.2. Datacore_Units

The *Datacore_Units* worksheet lists all the measurement units used and connects the units-as-used to their Base units (e.g., mg/g to g/g). New unit designations are flagged with yellow highlight. Additions should be checked for validity before re-invoking the **Check** function. Invalid unit designations must be corrected in the datasets: see Section 26.

25.4.3. Datacore_Analytes

The *Datacore_Analytes* worksheet lists all the analytes. It also separately lists the analytes used in studies by WG. New analytes are flagged with yellow highlight. Additions should be checked for validity (particularly spelling and alternative names) before re-invoking the *Check* function. Incorrect or duplicative analyte names must be corrected in the datasets: see Section 26.

25.4.4. Datacore_Codes

The *Datacore_Codes* worksheet lists all the participant code names used in any of the datasets. Codes are assigned four groups: NMI|DIs (flag: aNMI|DI), international organizations (flag: eIntOrg), other organizations such as universities and companies (flag: mOther), and values from other sources (flag: zCodeword). These particular flag words were chosen to structure the sorting order. Purely for esthetic reasons, the first character of these flags is in white font.

New code names are sorted to the bottom of the worksheet and flagged with yellow highlight. They should be checked for validity (particularly with regard to spelling and alternative names). When an apparently new code name matches one of the many aliases previously encountered, the possible match will be proposed in column four. If the "new" code is an archaic form (if in doubt, search the web to find out), change the code in the new dataset. However, if the new code reflects an organization's change in name, the code used in the earlier datasets should be changed. If the code is validly new, the organizations nationality should be entered into column 2 and its formal name into 4 before re-invoking the *Check* function.

The code names for "other organizations" have either a "u|" (for universities) or a "z|" prefix (for industries and non-NMI|DI institutes). Very occasionally, one of these organizations is raised to NMI|DI status. If that is the case, the code name used in the earlier datasets should be updated.

Note: In the CCQM datasheets the code names are stored as values in auxiliary column 18, not in column 3 (Section 26.3). The spreadsheet system's "Find and Replace" function used when column 18 is selected is the most efficient way of updating the codes. But do so with care; given the similarities among many of the code names, it's rather easy to change more than what was intended. "Replace all" is not necessarily your friend.

25.4.5. Datacore_Dates

Along with the datasheets themselves, the *Datacore_Dates* worksheet requires diligent and thoughtful curation by the system maintainer. The information provided in this worksheet is essential for several of the analysis subsystems.

Column 1: CCQM-authorized study codes. New (or otherwise unrecognized) codes are sorted to the bottom of the worksheet and flagged with yellow highlight. They should be checked for validity (recall that the *CCQM_Retrospectoscope* system codes the numeric part of the code as three digits: it's "K009" not "K9" and uses the first two characters of the sponsoring bodies name followed by "QM" rather than the full name followed by ".QM", see Section 26.2.7).

Column 2: The datasheet containing the first-encountered dataset of each study. This information is updated each time the *Database_Checkup* subsystem is invoked.

Column 3: The nominal date of the study measurements, typically the date by which participant reports had to be submitted to the Coordinator. This can differ from the year that the study was officially approved that is listed in the *search-results-ddmmyyyy.xls*x and *CCQM_KCs_PSs.xlsx* files. The dates must be entered by the database maintainer as strings, not numbers – that is with a leading single quote ('), with the four-digit year in the last four digits of the string. This information is used in several of the analysis subsystems.

Column 4: A short (no more than 50 characters) description of each study. This information is for the convenience of the system maintainer.

Column 5: The status of the study. This information is used by the *Database_FindNew* tools.

Column 6: Cross-references to parallel studies, if any. This information is for the convenience of the system maintainer.

Column 7: Comments, including explanations of why some study results have not been entered into the *CCQM_Retrospectoscope* database. This information is used by the *Database_FindNew* tools.

Column 8: The sponsoring WG. This information is used by the *WG_Participations* subsystem.

Column 9: The study Coordinator(s) (aka, “pilots”). This information is used by the *WG_Coordinations* subsystem.

26. Database Worksheets

There are two database worksheets that contain publicly accessible CCQM measurement information: *CCQM_KC* and *CCQM_PubPilot*. These two worksheets are a permanent part of the *CCQM_Retrospectoscope* system.

There are three database worksheets that are only available in the master system maintained at NIST: *CCQM_Alpha*, *CCQM_Beta*, and *CCQM_Pilot*. *CCQM_Alpha* and *CCQM_Beta* are used to temporarily store data that has been gleaned from *CCQM Confidential* "alpha" and "beta" reports in order to make the data available for examination while avoiding mixing it with public information. The *CCQM_Pilot* worksheet stores results from *CCQM Confidential* pilot studies. These three worksheets are not present in publicly accessible versions of the *CCQM_Retrospectoscope* system.

All five of the database worksheets have the same basic format. They differ only in the type of study they support.

26.1. Command buttons

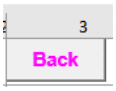
Each datasheet provides two command buttons, **Review** and **Back**, located at the top left of the worksheet. To provide access to these commands regardless of what dataset is being examined, the default worksheet view is "frozen" such that row 1 and columns 1 to 3 are always visible.

26.1.1. Review

Clicking the **Review** button when a cell within the rows used to store a given dataset produces a dot-and-bar chart of that study's results (see Section 20).

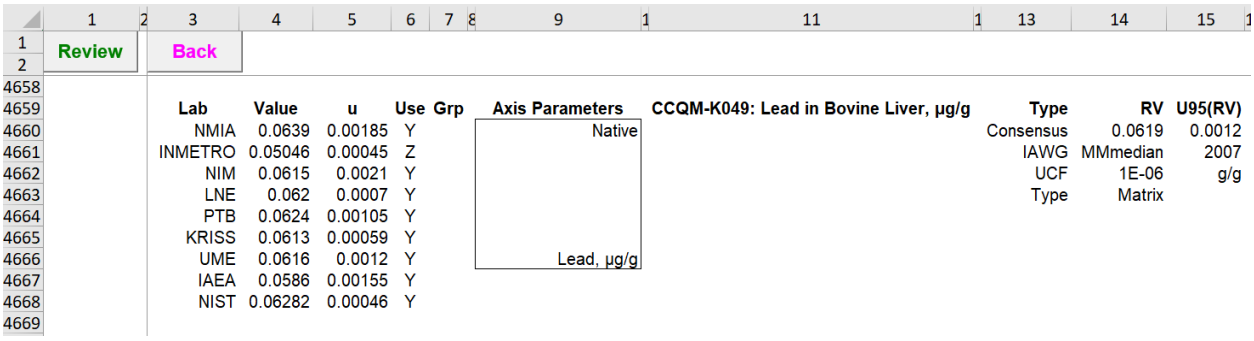
26.1.2. Back

Clicking the **Back** button causes the focus to be returned to whatever worksheet invoked the dataset Review.



26.2. Dataset Format

A representative dataset is pictured in Fig. 99. The basic format was developed for an older system (PDF_Maker) and is a bit clunky, however it is fit-for-purpose and is (reasonably) easy to maintain. The dataset consists of all the information provided between a row with "Lab" in column 3 (in this picture, row 4659) and an empty row (here, row 4669). The minimum of nine rows per dataset is needed to accommodate auxiliary information, regardless of the number of participants.



	Review	Back													
4658															
4659		Lab	Value	u	Use	Grp	Axis Parameters	CCQM-K049: Lead in Bovine Liver, µg/g			Type		RV	U95(RV)
4660		NMIA	0.0639	0.00185	Y		Native				Consensus		0.0619	0.0012
4661		INMETRO	0.05046	0.00045	Z						IAWG		MMmedian	2007
4662		NIM	0.0615	0.0021	Y						UCF		1E-06	g/g
4663		LNE	0.062	0.0007	Y						Type		Matrix	
4664		PTB	0.0624	0.00105	Y									
4665		KRISS	0.0613	0.00059	Y									
4666		UME	0.0616	0.0012	Y		Lead, µg/g							
4667		IAEA	0.0586	0.00155	Y									
4668		NIST	0.06282	0.00046	Y									
4669														

Fig. 99. Standard Dataset Storage Format.

26.2.1. Column 3, “Lab”

The acronymic code names of the contributors to the dataset are entered beneath the “Lab” header. The known codes are listed in the *Datacore_Codes* worksheet. Unrecognized codes will be flagged when the *Database_Checkup* subsystem is invoked. Every code in this column must be unique; only one value per participant will be used in the various graphical analysis subsystems.

However, if a participant submits more than one result (e.g., from different measurement approaches, a corrected calculation or other revision submitted after the study’s results have been discussed), such “unofficial” results can be designated using the construction “Code/Digit”, where Code is the acronym and digit is a number. The data associated with a code containing a “/” are ignored by the analysis subsystems but are displayed in the *Dataset_Review* chart.

26.2.2. Column 4, “Value”

The results used in all the *CCQM_Retrospectoscope* analyses are entered beneath the “Value” header. There must be a fully numeric value associated with each code name provided. Upper or lower bound (<, ≤, ≥, and > values) are not supported, nor is any “not available” text.

26.2.3. Column 5, “u”

The standard uncertainties associated with the reported results are entered beneath the “u” header. When the study report provides 95 % expanded uncertainties, these “u” values are assigned as one-half of the expanded uncertainty regardless of whether the standard uncertainties are also provided.

Unlike the values, a missing uncertainty can be reported as “na”, although the associated value will not be used in any consensus calculation.

26.2.4. Column 6, “Use”

Results that were used in consensus calculations are flagged “Y”. Officially accepted results that were identified as technically or statistically suspect by the WG that conducted the study and excluded from consensus calculations are flagged “Z”. Unofficial results (e.g., provided for information purposes or submitted after the final reporting date) are flagged “N”.

The *CCQM_Retrospectoscope* analysis systems do not distinguish between "Y" and "Z" results and do not use "N" results. However, the *Dataset_Review* dot-and-bar chart displays "Y" results as black symbols, "Z" and "N" as red.

26.2.5. Column 7, "Grp"

Occasionally, a dataset may contain results that are best displayed as members of two or more groups; e.g., from different measurement approaches. For display purposes only, such results can be visually grouped by providing alphanumeric categorical values in this column.

26.2.6. Column 9, "Axis Parameters"

This is the most clunky bit. The older system supported a variety of value (Y)-axis formatting options that are no longer relevant. However, the cells in three of the seven rows beneath the "Axis Parameters" header are used:

- Row 2: Y-axis minimum value
- Row 3: Y-axis maximum value
- Row 7: Y-axis title, formatted as: Analyte, units

The Y-axis minimum and maximum (second and third rows beneath the header) are only useful when the dataset contains extreme values that cause the default scaling of the *Dataset_Review*'s chart to misbehave. The *Dataset_Review* subsystem does not add or change the values in these rows. Their presence or absence of these values has no impact on any other *CCQM_Retrospectoscope* subsystem.

The Y-axis title in the cell of the seventh row (bottom row of the bordered box beneath the header) is used by the *Dataset_Review* and *Database_Checkup* subsystems. The unit specification in this chart-title is checked for consistency against that in the dataset title.

26.2.7. Column 11, Dataset Title

Each dataset has a unique title, e.g., "CCQM-K100: Copper in Ethanol, µg/g". Dataset titles are always in the dataset's header row. Dataset titles have five components:

- Sponsoring body ("CCQM-") (see Section 1.4.2)
- Type of study ("K") (see Section 1.4.1)
- Assigned numeric index ("100: ") This index may be followed by various modifiers.
- Measurand ("Copper in Ethanol,")
- Units ("µg/g") (see Section 1.4.4)

The first three of these components ("CCQM-K100: ") constitute a study-specific "prefix" that is derived from the designation assigned by the CCQM when the study is given permission to proceed. This prefix is in a one-to-one relationship with that used in the KCDB but can differ in two aspects:

- the code used to designate the sponsoring body and
- the format of the numeric index.

Whereas the KCDB prefix uses the formalism (sponsoring body).QM-(type of study)(index in as few digits as possible), to facilitate meaningful sorting the *CCQM_Retrospectoscope* uses (first two characters of the sponsoring body's acronym)QM-(type of study)(index in three digits). That is, the KCDB's study prefix "APMP.QM-K1.c" is "APQM-K001.c" in the *CCQM_Retrospectoscope* system.

Note that the prefixes are identical for studies sponsored by the CCQM with numeric indices in the range 100 to 999. Since the indices for currently planned studies only range into the low 200's, it is likely that the three-digit coding will suffice for the useful lifetime of this analysis system.

The rows beneath the title may contain database-maintenance notes; e.g., the table or tables in the study report that provided the listed values. However useful these notes may be for folk entering and checking the recorded values, they are not used by the system's programs. However, to avoid confusing the algorithm used to detect the dataset's end, any such notes should be confined to the first seven rows beneath the title.

26.2.8. Column 13, "Type"

The cell in the first row beneath the "Type" header describes the "type" of reference value, although codes used haven't been sufficiently standardized to be of much use. They are not currently used by any *CCQM_Retrospectoscope* subsystem.

The cell in the second row specifies the WG that sponsored the study. The *Database_Checkup* subsystem checks this assignment for consistency with the assignment in the *Datacore_Dates* worksheet.

The cell in the third row should always contain the initials "UCF" (acronym for "Units Conversion Factor"). It is only a label for the value in the cell to its immediate right.

The cell in the fourth row should always contain the word "Type." It is only a label for the value in the cell to its immediate right.

The cell in the fifth row may contain the words "Units Factor", again only a label for the value to its immediate right.

26.2.9. Column 14, "RV"

The cell in the first row beneath the "RV" header defines the reference value for the dataset. This is used in many of the *CCQM_Retrospectoscope*' s subsystems.

The cell in the second row is generally used to describe how the reference value was estimated, but like the first row under the "Type" header the codes used haven't been sufficiently standardized to be of much use. In any case, they are not currently used by any *CCQM_Retrospectoscope* subsystem.

The cell in the third row is the UCF used to transform the results as listed to have the scale expressed in the Base unit (e.g., 5.1 mg/g with a UCF of 1E-03 is 5.1×10^{-3} g/g). The *Database_Checkup* subsystem checks this value for consistency with the units stated in both the dataset title and the Y-axis title.

The cell in the fourth row is the sample type designation, either Simple or Complex.

When present, the cell in the fifth row is the Units factor used to transform the units used in the report into units used in the *CCQM_Retrospectoscope* (e.g., the units factor 65.4 g/mol converts 0.35 µmol/g zinc to (65.4)(0.35) = 22.9 µg/g zinc). The transformation is embedded "by hand" in the datasheet using the usual worksheet functions.

26.2.10. Column 15, "U95(RV)"

The cell in the first row beneath the "U95(RV)" header is the 95 % expanded uncertainty on the reference value.

The cell in the second row is the measurement year. The *Database_Checkup* subsystem checks this assignment for consistency with the year stated in the *Datacore_Dates* worksheet.

The cell in the third row is the Base unit. The *Database_Checkup* subsystem checks this assignment for consistency with the units stated in both the dataset title and the Y-axis title.

26.3. Auxiliary Information, Columns 18 to 29

The values under the "Lab", "Value", "u", and "Use" headers (columns 3 to 6) contain the values that the *CCQM_Retrospectoscope* uses, but these values are transferred from data held in other columns (Fig. 100). This indirect approach is used because there isn't a one-size-fits-all method for documenting the results of a study.

	1	2	3	4	5	6	18	19	20	21
1	Review		Back							
2										
4658										
4659			Lab	Value	u	Use	Lab	X	U	Use
4660			=RC[15]	=RC[15]	=RC[15]/2	=UPPER(LEFT(RC[15],1))	NMIA	0.0639	0.0037	Yes
4661			=RC[15]	=RC[15]	=RC[15]/2	=UPPER(LEFT(RC[15],1))	INMETRO	0.05046	0.0009	Z-Tech
4662			=RC[15]	=RC[15]	=RC[15]/2	=UPPER(LEFT(RC[15],1))	NIM	0.0615	0.0042	Yes
4663			=RC[15]	=RC[15]	=RC[15]/2	=UPPER(LEFT(RC[15],1))	LNE	0.062	0.0014	Yes
4664			=RC[15]	=RC[15]	=RC[15]/2	=UPPER(LEFT(RC[15],1))	PTB	0.0624	0.0021	Yes
4665			=RC[15]	=RC[15]	=RC[15]/2	=UPPER(LEFT(RC[15],1))	KRISS	0.0613	0.00118	Yes
4666			=RC[15]	=RC[15]	=RC[15]/2	=UPPER(LEFT(RC[15],1))	UME	0.0616	0.0024	Yes
4667			=RC[15]	=RC[15]	=RC[15]/2	=UPPER(LEFT(RC[15],1))	IAEA	0.0586	0.00309	Yes
4668			=RC[15]	=RC[15]	=RC[15]/2	=UPPER(LEFT(RC[15],1))	NIST	0.06282	0.00092	Yes
4669										

Fig. 100. Where the Raw Data is Stored.

Many of the as-reported values must be transformed to be fully useful. These transformations are much more conveniently performed using values stored in separate cells rather than as hand-entered values in complex single-cell calculations. Most importantly, the input data stored in individual cells can be easily checked against the values as listed in the reports.

26.3.1. Molality to Mass Fraction: mol/g to g/g

For values reported in units of molality, mol/g, comparing reproducibility as a function of concentration across similar studies requires transforming them to mass fraction, g/g:

$$w_i \pm u(w_i) \;=\; M \cdot (x_i \pm u(x_i))$$

where M is the relative molecular mass of the analyte (perhaps scaled to be able to state results in a manageable magnitude) and $x_i \pm u(x_i)$ is the value and associated standard uncertainty as reported by the participant.

26.3.2. Individual Reference Values to Single Reference Value

Many GAWG studies involve multiple gas cylinders, each with a very similar-but-slightly-different gas mixture and thus different reference values. Converting them to a common reference require the transformation:

$$w_i \pm u(w_i) \;=\; y_{nom} \cdot (x_i \pm u(x_i))/(y_i \pm u(y_i))$$

where: y_{nom} is the nominal concentration of the measurand and $y_i \pm u(y_i)$ is the reference value and its standard uncertainty.

The *CCQM_Retrospectoscope* datasheets calculate y_{nom} as the arithmetic mean of the individual reference values; its 95 % expanded uncertainty, $U_{95}(y_{\text{nom}})$, is calculated as the twice the pooled standard uncertainty of the individual reference values. When the multiple uncertainty components are provided (e.g., u_{prep} and u_{veriffy}), only the combined standard uncertainty, u_{ref}, is stored and used.

The y_{nom} uncertainty is used in the *CCQM_Retrospectoscope* analyses but doesn't enter into the transformation since y_{nom} is only a scale factor that applies uniformly to all the dataset values.

26.3.3. Degree of Equivalence to Single Reference Value

Several studies involving CRMs or calibration solutions summarize each participant's performance in terms of a DoE that combines results for several materials. Results expressed as percent relative values, $\%DoE_i \pm u(\%DoE_i)$, have been transformed:

$$w_i = x_{ref}(1 \;+\; \%DoE_i/100);\; u(w_i) \;=\; w_i \cdot u(\%DoE_i)/100$$

Results expressed as values with units of the measurement, $DoE_i \pm u(DoE_i)$, have been transformed:

$$w_i = \; x_{ref} + DoE_i;\; u(w_i) \;=\; u(DoE_i)$$

In both cases, x_{ref} is estimated as the median of the values for all the materials used in the study. The uncertainty assigned to this x_{ref} is estimated from the pooled relative uncertainty of the repeatability measurements, u_{repeat}:

$$u(x_{ref}) = x_{ref} \cdot \; u_{repeat}$$

This uncertainty is not included in the z_i estimation since the uncertainties assigned to the DoE include the measurement component.

Since the materials used in the study can have very different analyte levels, there is no simple transformation that will completely represent measurement reproducibility as a function of analyte level. Defining x_{ref} as the median (probably) minimizes the distortion.

26.3.4. $u = U_{95}/2$

Two functions are used to transfer the "*u*" information from the auxiliary column to column 5. When the study report only lists standard uncertainties, the function is an unadorned transfer "=RCxx", where "xx" is a column designation. When the report provides expanded uncertainties, the function is "=RCxx/2".

There are three pragmatic reasons for defining the standard uncertainty as half of the expanded uncertainty:

- Most CCQM expanded uncertainties are estimated as twice the experimentally determined standard uncertainty. This implicitly asserts that standard uncertainty estimate is associated with "large" degrees of freedom, *v*. For these values, the division is "exact" - even though the one-sided Student's t_{95} becomes less than 2.0 only for $v \geq 61$, so it is unlikely that the "*v* = large" assertion is always justified.
- For uncertainties estimated using an appropriate Student's *t* expansion factor, the division by 2 results in the assignment of standard uncertainties larger than those used by the WGs to calculate degrees of equivalence (DoE). Since a larger standard uncertainty produces a more favorable DoE, this does not disadvantage the affected NMI|DIs.
- Statistically rigorous calculations would require storage and use of the expansion factors. While adding this information would be tedious, it certainly could be done and the increased storage readily accommodated. However, given the limitations of graphical analysis and the vagaries of summarizing distributions with two (too?) simple robust estimators, actually making use of the *v* information in the *CCQM_Retrospectoscope*'s metrics would add considerable complexity for little benefit.

There is also a philosophical reason. If a measurement result is envisioned as representing a center-symmetric probability distribution, it is punitive to treat a result that is implicitly defined as a Student's t (mean, standard uncertainty, *v*) as a Gaussian (mean, standard uncertainty). Treating it as a Gaussian (mean, expanded uncertainty / 2), while an imperfect remedy, at the very least gives rise to 95 % error bars of the correct length.

26.3.5. Asymmetric Uncertainties

A very few CCQM results have been reported as asymmetric distributions: $x^{+u(\mathrm{hi})}_{-u(\mathrm{lo})}$. Lacking the infrastructure to make full use of this information the uncertainty recorded in the *CCQM_Retrospectoscope* datasheets is the average: $u = (u(\mathrm{lo}) + u(\mathrm{hi}))/2$.

26.3.6. "Anchor" Results

"Anchor" results are provided by one or more experienced NMI|DIs used to enable connecting the results of participants in a SC to the reference value of the parent KC. The Anchor NMI|DI(s)

are not participants in the study and do not necessarily perform their analyses under the same constraints of time and sample quantity as do the participants. Further, since their results are used to establish the connection, their results will axiomatically be "more accurate" than they would be if the study's reference value was determined by consensus of all technically valid results performed under the same constraints.

The results for Anchor NMI|DIs are therefore not included in the dataset results, although they are included in the calculations carried out in the auxiliary columns.

26.3.7. Other Issues

There are other issues that are best handed in these auxiliary columns, such as:

- combining uncertainties expressed as expanded uncertainties with those expressed as standard uncertainties,
- for Pilot studies, combining multiple measurements from one participant into a single "representative" value, and
- adjusting values in SCs to be comparable to the parent KC using results reported by one or more "anchor" NMI|DIs.

The auxiliary columns can contain additional information that may be of interest to a database maintainer. The cells in column 21 indicate why a value is not used in consensus calculations: e.g., "N-Info" indicates that the result is unofficial and was reported to provide information about some aspect of a measurement process, "N-SO" indicates that the result was declared to be a "statistical outlier" by the coordinating WG, "N-Tech" indicates that the submitting organization identified a technical flaw in the reported measurement value of uncertainty. The only critical element of these codes is the leading character, "n" or "y", since that what is captured by the transfer function.

26.4. Multiple-Study Datasets

The datasets used by the *CCQM_Retrospectoscope* analysis systems each contain the information from only one study. However, there have been quite a number of RMO SCs (and CCQM special-purpose follow-on KCs that are SCs in all but designation) that trace their reference value to the reference value of a prior study. In addition to being present as single-study datasets, the datasheets include an additional multiple-study dataset for each of these parent-child groups. These composite datasets are identified by the presence of "&" in the dataset title. For the convenience of the database maintainer, these titles are listed in **dark red** font and the titles of the component single-study datasets are listed in **blue** font.

The multiple-study datasets are present mostly to facilitate visualization of all the related data using the *Dataset_Review* subsystem. However, for "child" studies that derived their reference value from the parent study via results provided by anchor NMI|DIs, the calculations required are performed in the auxiliary columns of the multiple-study dataset. The results of these calculations are transferred (as values, not formulae) to the single-study components.

26.5. Creating New Datasets

Once new data results have been located, updating the CCQM_Retrospectoscope is generally straight forward - but it requires attention to detail and careful validation.

In each new report, locate the tables that list the study timeline, the measurement results, and the reference values and uncertainties. While it's efficient to hand-transfer simple values like the measurement year and reference values, avoid transcription errors by copying-and-pasting the measurement results.

Most CCQM reports are distributed in portable document format (pdf). Some of these are either locked to copying or the tables aren't organized for easy data extraction. You can generally get around this by saving report as a Microsoft Word ".docx" document. The tables in such converted files are generally well organized for copy-and-paste. If the .pdf is locked to format conversion, scan the useful pages into high-quality pdf format, use character recognition to make the text accessible, then *Save As* a .docx file. Worse-comes-to-worst, hand transfer the relevant data – but obsessively validate the transferred results.

After reviewing Sections 26.2 and 26.3 and ensuring that the measurement results are accessible:

- Locate an already-entered dataset of a study that is similar to the new study. Copy all the rows of the dataset and paste it into the last row plus one of an appropriate database worksheet.
- Replace all of the old data with the new measurement results and auxiliary information. (Figuring out what needs to be replaced where is why you need to be familiar with Sections 26.2 and 26.3!). Make sure that all the measurement results from column 18 (and beyond) are properly linked to the corresponding rows of columns 2 to 6.
- Check the validity by selecting the new dataset's first row and clicking the **Review** button located in row 1 of column 3 of the datasheet.
- Correct any glaring oversights. When all such are corrected, click the **Check** button on the *Database_Checkup* worksheet.
- Correct any deficiencies. Keep clicking the **Check** button until all issues are resolved.
- Save the updated workbook as *CCQM_Retrospectoscope.xlsm.*
- Repeat as needed for each analyte in the new study.
- Once validation is complete, move the datasets to their expected location with the proper datasheet. Click the **Check** button on the *Database_Checkup* worksheet one last time – just to make sure.

26.6. Storage Order

The order in which datasets are organized within the datasheets is mostly for the benefit of the database maintainer. In general, they are in sequential order by their CCQM-assigned code. CCQM studies are listed before those sponsored by the RMOs or the BIPM. Datasets from RMO and BIPM studies are listed in alphabetical order after the CCQM datasets. Datasets for different measurands of the same study are listed in the order used by the study's report.

However, all the component datasets of a multiple-study are stored immediately following the multiple-study dataset. The parent study is listed first, followed by its children in alphabetical

27. The ReadMe Worksheet

The *ReadMe* worksheet is activated when the **ReadMe** button on the *Welcome* worksheet is clicked. This worksheet lists the standard NIST software license statement (as long as you acknowledge NIST as the source, the workbook and all of the underlying code is yours to use) and disclaimer (the *CCQM_Retrospectoscope* provided AS IS, use it at your own risk), who to send your suggestions, bugs reports, and irate complaints to, and where the *CCQM_Retrospectoscope* documentation lives. The worksheet is pictured in Fig. 101.

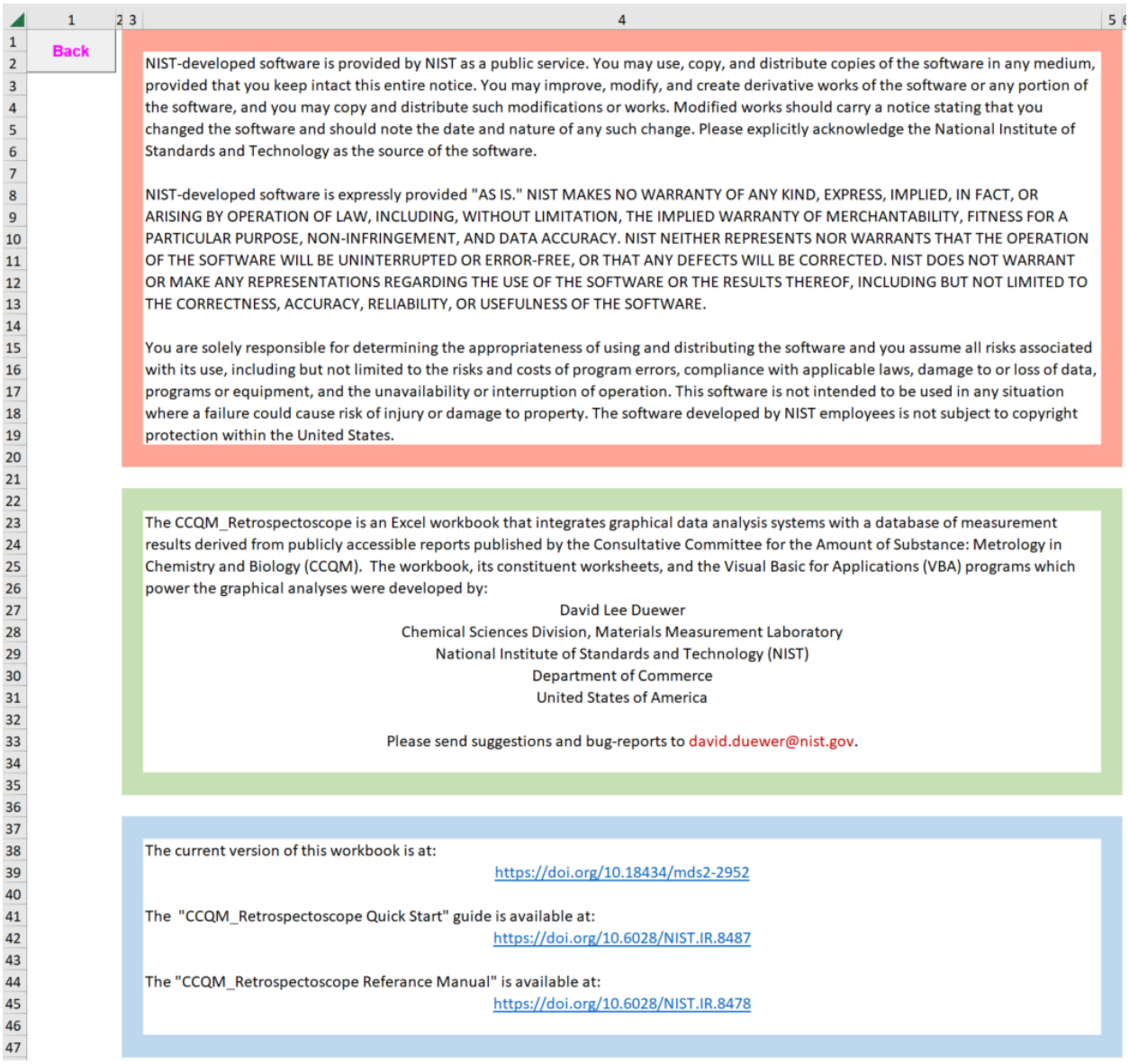


Fig. 101. The *ReadMe* Worksheet.

The only control on the worksheet is the **Back** command button, which when clicked returns control to the *Welcome* worksheet.

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Appendix A. List of Acronyms and Symbols

A.1. Acronyms

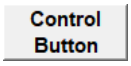
BAWG	Bioanalysis Working Group
BIPM	Bureau International des Poids et Mesures
CAWG	Cell Analysis Working Group
CCQM	Originally "Consultative Committee for the Quantity of Matter"; now "Consultative Committee for the Amount of Substance: Metrology in Chemistry and Biology"
CIPM	Comité International des Poids et Mesures
CV	coefficient of variation (relative standard deviation) expressed as a percentage
DI	designated institute, an organization having the responsibility for a specified aspect of a nation's measurement infrastructure
DoE	degree of equivalence
EAWG	Electrochemical Analysis Working Group
GAWG	Gas Analysis Working Group
IAWG	Inorganic Analysis Working Group
IRWG	Isotope Ratio Working Group
KC	Key Comparison
KCDB	Key Comparison Database, a web-based data source maintained by the BIPM
KRISS	Korea Research Institute of Standards and Science, South Korea's NMI
NAWG	Nucleic Acid Working Group
NICOB	NIST Consensus Builder
NIST	National Institute of Standards and Technology, USA's NMI
NMI	national metrology institute, an organization having the responsibility for all a nation's measurement infrastructure not delegated to a DI.
NMI|DI	national metrology institutes and designated institutes, the organizations that participate in CCQM KCs
OAWG	Organic Analysis Working Group
PAWG	Protein Analysis Working Group
pdf	portable document format (pdf)
PS	pilot study
PPS	published pilot study
RMO	Regional Metrology Organization
RMSE	root-mean square error
RV	reference value
SAWG	Surface Analysis Working Group
SC	Supplementary Comparison
TC	Technical Committee (of an RMO)
VBA	Microsoft Virtual Basic for Applications
WG	Working Group

A.2. Symbols

β_0	intercept of a linear function, scale factor of a power-law
β_1	slope of a linear function, exponent of a power-law
%CV	coefficient of variation, the relative standard deviation expressed as a percentage
d_i	difference between a calculated and observed value
D_i	percent difference score: $D_i = 100(x_i - x_{ref})/x_{ref}$
$\|D_i\|$	absolute percent difference score: $\|D_i\| = 100\|x_i - x_{ref}\|/x_{ref}$
DoE_i	reported degree of equivalence for participant value x_i
$\%DoE_i$	reported percent relative degree of equivalence for participant value x_i
D_{other}	average distance between WG participation rates of a target and "other" NMI|DI
Δ_i	range-scaled distance of point $\{X_i,Y_i\}$ to a chart's $\{0,1\}$ origin
INT	function: return the integer part of a real number
i	participant index
j	participant index
$\log_{10}$	function: decadic logarithm
m	number of adjustable parameters
M	relative molar mass (molecular weight)
n	number of values
n_{shared}	number of WGs in which a target and "other" NMI|DI either both participate of don't participate
$n_{unshared}$	number of WGs in which only one of the target and "other" NMI|DI participate
Q_n	a robust and efficient estimate of the standard deviation of a set of values
p	exponent of a power-law
$r_{other,i}$	participation rate of the "other" NMI|DI in the i^{th} WG
$r_{target,i}$	participation rate of the target NMI|DI in the i^{th} WG
t	Student's t distribution
u_i	standard uncertainty associated with participant value x_i
u_i	standard uncertainty associated with participant value x_i
u_j	standard uncertainty associated with participant value x_j
u_{prep}	standard uncertainty associated with gas cylinder preparation
u_{repeat}	standard uncertainty associated with measurement repeatability
u_{verify}	standard uncertainty associated with gas cylinder verification
u_{ref}	standard uncertainty associated with reference value x_{ref}
$u_{rel,ii}$	relative standard uncertainty of the ratio u_i/u_j
u_{set}	all of the valid u_i in a given dataset
$u(\cdot)$	standard uncertainty for a specified variable
$U_{95}(\cdot)$	expanded uncertainty providing approximately a 95 % level of confidence
v	degrees of freedom for a specified value
w_i	transformed measurement value
x_i	value reported by participant i for a given measurand in a given study
x_j	value reported by participant j for a given measurand in a given study
x_{median}	median of a set of values
x_{ref}	reference value for a given measurand in a given study

X	independent variable, plotted on X-axis of a scattergram
X_{max}	maximum X-axis value
X_{min}	minimum X-axis value
y_i	assigned reference value for a given gas cylinder
y_{nom}	nominal reference value for a set of gas cylinders
Y	dependent variable, plotted on Y-axis of a scattergram
Y_{max}	maximum Y-axis value
Y_{min}	minimum Y-axis value
z_i	z-score: $z_i = (x_i - x_{ref})/u_i$
$\|z_i\|$	absolute z-score: $z_i = \|x_i - x_{ref}\|/u_i$
ζ_i	zeta-score: $\zeta_i = (x_i - x_{ref})/(u_i^2 + u_{ref}^2)^{0.5}$
$\|\zeta_i\|$	absolute zeta-score: $\|\zeta_i\| = \|x_i - x_{ref}\|/(u_i^2 + u_{ref}^2)^{0.5}$
ζ_{ij}	zeta-score between two participants: $\zeta_{ij} = (x_i - x_j)/(u_i^2 + u_j^2)^{0.5}$
ζ_{ij}	absolute zeta-score between two participants: $\zeta_{ij} = \|x_i - x_j\|/(u_i^2 + u_j^2)^{0.5}$

Appendix B. Glossary

Command button


A control object that invokes action by a given computer program. Command buttons are labeled. When referred to in the text of this document, the button labels are in bold roman font.

Checkbox

A control object that acts as an off-and-on switch. It may or may not invoke action by a given computer program when its state is changed.

Dashboard
In *CCQM_Retrospectoscope* usage, the graphical user interface part of a worksheet.

Dataset
All of the measurement results, reference value, name, and other ancillary information for a given analyte in a given CCQM multi-laboratory study.

Datasheet


A worksheet that contains datasets. The names of *CCQM_Retrospectoscope* datasheets all begin "CCQM_" and the tabs are colored green.

Focus
The active or selected cell on the active worksheet.

Radio button

A control object that, when grouped with a set of radio buttons, is used to specify a particular discrete options. Only one of the set of radio buttons is active at any given time. It may or may not invoke action by a given computer program when its state is changed.

Subsystem
A collection of computer programs that can be used to accomplish a given task. In the *CCQM_Retrospectoscope* system, each subsystem is instantiated in one worksheet. The subsystem and its worksheet have the same name. When referred to in this document, the worksheet name is in *black italic* font while subsystem is in *colored italic* font.

System
The *CCQM_Retrospectoscope* is a collection of relatively independent subsystems and curated data into a system for the graphical analysis of results from CCQM-sponsored multi-laboratory studies.

Workbook
A spreadsheet program file containing one or more worksheets. The *CCQM_Retrospectoscope* system is instantiated in the Excel workbook *CCQM_Retrospectoscope.xlsm*.

Worksheet
A matrix of rows and columns of cells that can contain numbers, formulas, charts, and various sorts of control objects. Each worksheet has a unique name, displayed in the worksheet tab at the bottom of the spreadsheet window. When referred to in this document, a worksheet name is in *black italic* font.