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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
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Michael A. Nelson

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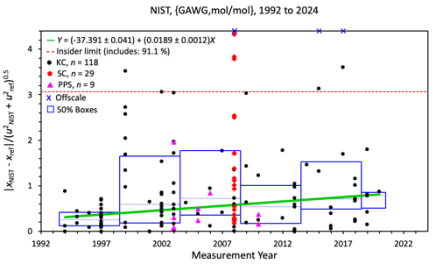

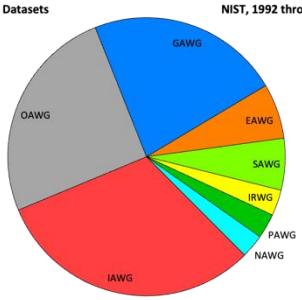

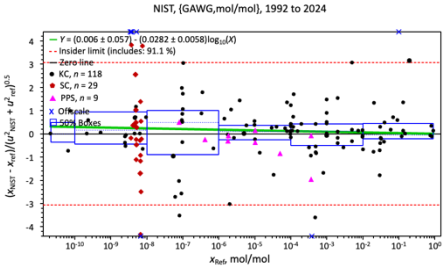

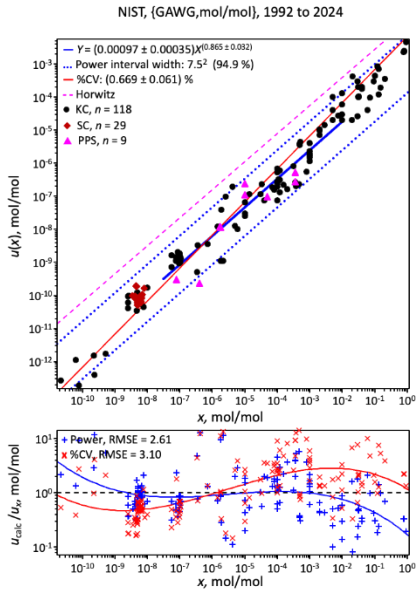

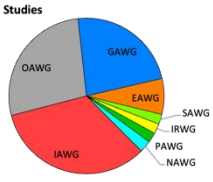

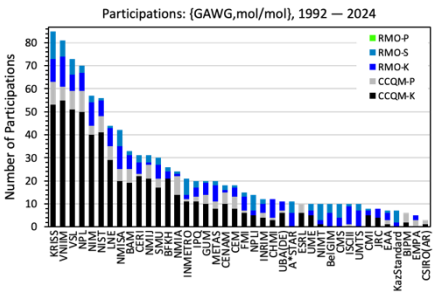

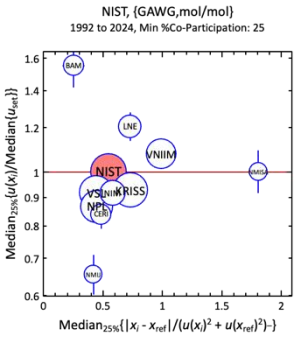

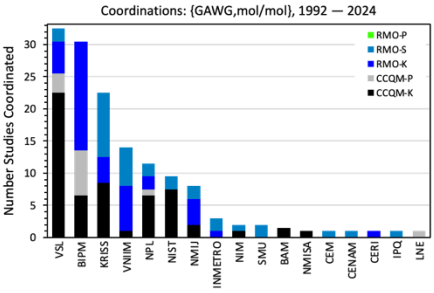

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December 2024

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Abstract

This document is a detailed reference manual for the 1-September-2024 version of the *CCQM_Retrospectoscope* system. The *CCQM_Retrospectoscope* 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. *CCQM_Retrospectoscope* supports a diverse collection of sometimes eye-opening appraisals of participation and measurement performance throughout the history of 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 *CCQM_Retrospectoscope* is implemented in Excel using Microsoft 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 (DI); Electroanalytical Working Group (EAWG); Gas Analysis Working Group (GAWG); graphical data analysis; Inorganic Analysis Working Group (IAWG); Key Comparison (KC); national metrology institute (NMI); Organic Analysis Working Group (OAWG); pilot study; Regional Metrology Organization (RMO); Supplementary Comparison (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 Comparisons, 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*.

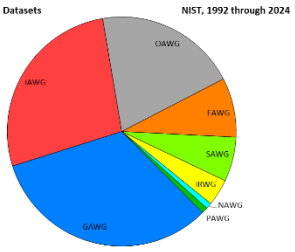
1.1. Analysis Subsystems

The *CCQM_Retrospectoscope* provides fourteen graphical analysis subsystems: five that address individual NMI/DIs, four that address peer relationships among NMI/DIs, and five that address Working Group (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, 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

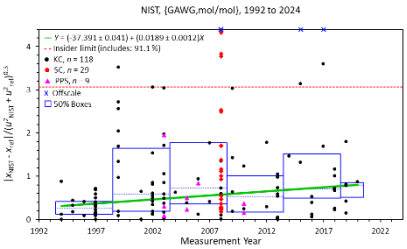
The following five subsystems summarize aspects of a given NMI/DI's participation or measurement performance in CCQM studies.

1.1.1.1. Lab_Activity (Section 4)



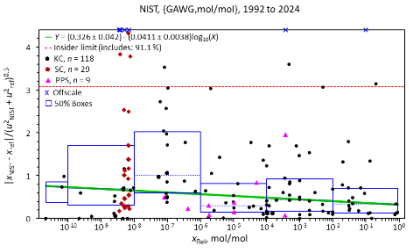
The *Lab_Activity* subsystem displays the relative proportions of the various groups of CCQM datasets and studies that a given NMI/DI participated in, where a group is defined as a unique combination of WG and measurement BaseUnit, {WG, BaseUnit} (Section 2.4.1.3). A table to the right of the charts lists the number of datasets and studies of each group, further categorized by the type of the study (Section 1.5.1). The displays and tables document what types of measurands the NMI/DI is most interested in.

1.1.1.2. Lab_History (Section 5)



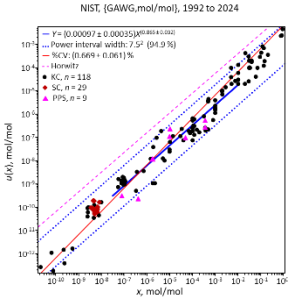
The *Lab_History* subsystem displays a given NMI/DI's performance as a function of time, enabling assessment of past performance in all studies of a given {WG, BaseUnit} that the NMI/DI participated in. The performance metrics are relative to the WG-assigned reference values (RVs), the expanded uncertainties 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)



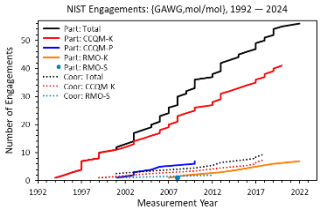
The *Lab_Bias* subsystem displays a given NMI/DI's performance as a function of the dataset's RV. The performance metrics are relative to the WG-assigned RVs and the expanded uncertainties assigned to those values.

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)

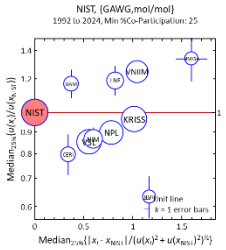


The *Lab_Engagements* subsystem details the number and timing of a given NMI/DI's engagements with the various types of CCQM study, where "engagements" are separated into "participations" (reporting measurement values) and "coordinations" (providing leadership). This subsystem combines results from the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

1.1.2. The "Peer" Subsystems

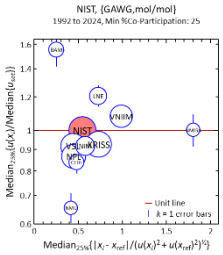
The following four subsystems help identify NMI/DI's that are most similar with respect to measurement performance or shared interests.

1.1.2.1. Peer_Bilateral (Section 9)



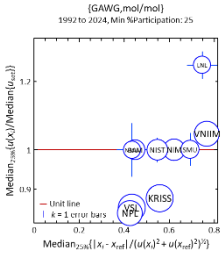
The *Peer_Bilateral* subsystem provides the most direct of three related analysis approaches to identifying the peers of a given NMI/DI based upon participation and measurement performance in the same studies. This approach explores the bilateral differences between the NMI/DI's results and that of co-participants. 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)



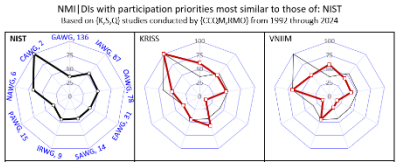
The *Peer_Unilateral* subsystem provides an alternative approach to identifying an NMI/DI's peers. The analysis explores the summary performance relative to unilateral dataset RVs, not bilateral paired differences. Results are displayed for all NMI/DIs that co-participated with the target NM/DI in a 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 RV. 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)

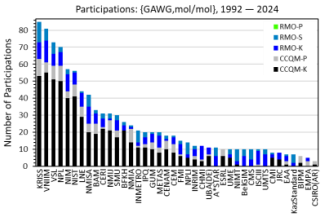


The *Peer_Priorities* subsystem displays the proportions of studies in each of the WGs that a designated NMI/DI has participated in. Similar displays are provided for the eleven NMI/DIs that either have the most similar participation priorities or are members of a designated list.

1.1.3. The "WG" Subsystems

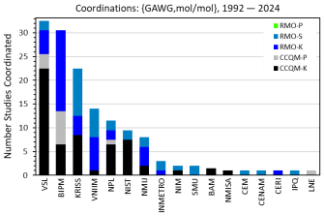
The following five subsystems summarize aspects of the WG communities.

1.1.3.1. WG_Participations (Section 13)



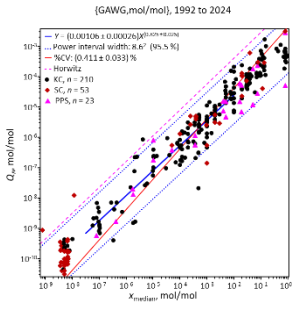
The *WG_Participations* subsystem summarizes the number of WG studies the various NMI/DIs have participated in. This information is mined from the *CCQM_Retrospectoscope* data worksheets ("datasheets"), so excludes pilot studies that did not provide a final report or did not identify the participants.

1.1.3.2. WG_Coordinations (Section 14)



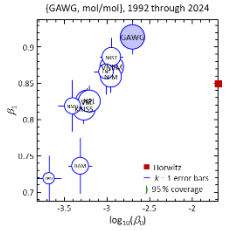
The *WG_Coordinations* subsystem summarizes the number of WG studies various NMI/DIs have coordinated or co-coordinated. This information is mined from summary records maintained at the Bureau International des Poids et Mesures (BIPM), these summaries include all pilot studies, regardless of how (or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

1.1.3.3. WG_Precision (Section 15)



The *WG_Precision* subsystem depicts measurement reproducibility as a function of analyte level for NMI/DI communities. For each {WG, BaseUnit} 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].

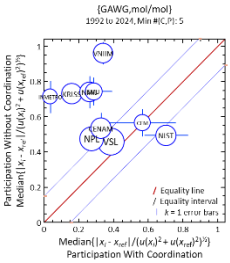
1.1.3.4. WG_Power (Section 16)



The *WG_Power* subsystem displays the power-law coefficients characteristic of a WG (as estimated by the *WG_Precision* subsystem) and for NMI/DIs (as estimated by the *Lab_Uncertainty* subsystem). The NMI/DIs can be identified using the *Peer_Bilateral*, *Peer_Unilateral*, or *Peer_Global* subsystems.

Efficient use of this subsystem requires considerable experience and patience.

1.1.3.5. WG_Diagonal (Section 17)

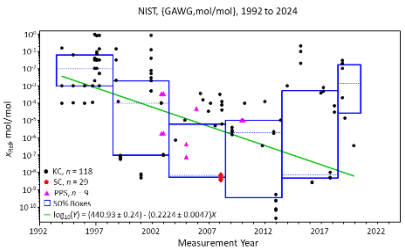


For NMI/DIs that have coordinated CCQM studies, the *WG_Diagonal* subsystem displays their median measurement bias in datasets from studies that they just participated in as a function of the median measurement bias in datasets from studies that they coordinated.

1.2. Other_Tools: Support Systems (Section 18)

The *Other_Tools* dashboard provides access to two auxiliary dataset analysis tools, three dataset support subsystems, two database maintenance subsystems, a benchmarking tool, a worksheet display tool, and three datasheets. Each subsystem is contained on its own worksheet; the benchmarking and display tools do not require their own worksheets.

1.2.1. Study_RefVals (Section 19)

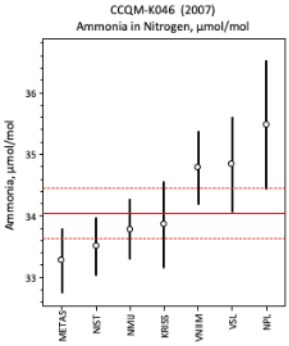


The *Study_RefVals* subsystem displays the RVs for studies of a specified {WG, BaseUnit} in which a given NMI/DI has participated. The RVs are plotted as a function of each study's measurement year.

1.2.2. Study_Locate (Section 20)

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

1.2.3. Dataset_Review (Section 21)



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

1.2.4. Dataset_NMI/DI (Section 22)

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

1.2.5. Dataset_AnalyteFilter (Section 23)

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

1.2.6. TimeTrial (Section 24)

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

1.2.7. Zoom (Section 25)

The *Zoom* tool sets the "zoom" of every worksheet to the zoom of the *Other_Tools* dashboard.

1.2.8. Database_FindNew (Section 26)

The *Database_FindNew* worksheet provides a set of stand-alone tools for identifying new or changed information contained in summary Excel workbooks downloadable from the BIPM's web-system.

1.2.9. Database_Checkup (Section 27)

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

1.2.10. Datasheets (Section 28)

The Other_Tools dashboard also has three buttons that each connect to one of the permanent database worksheets (i.e., "datasheets"):

- *CCQM_KC*, which contains (non-continuous) datasets produced by Key Comparison and Supplementary Comparison datasets.
- *CCQM_PubPilot*, which contains all the publicly available datasets from pilot studies.
- *CCQM_Continuous*, which contains all of the BIPM's continuous bilateral gas analysis Key Comparison datasets.

1.3. ReadMe: Licensing and Contact Information (Section 29)

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

1.4. ChangeLog: Changes to CCQM_Retrospectoscope (Section 30)

A compact listing of bugfixes and updates to the *CCQM_Retrospectoscope* since its initial release.

1.5. 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 RV 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 28.2 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 28.4).

1.5.1. 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]. All CCQM SCs are 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*; 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.

1.5.2. 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 six RMOs currently recognized by the CIPM are pictured in Fig. 1.

Fig. 1. Geographic Areas of Metrological Responsibility.

In addition to its administrative and support roles, the BIPM sponsors ongoing bilateral comparisons of ambient levels of atmospheric gases.

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	57	6	11	95	13	22	1	3	39
BIPM [a]	BIQM	36				36	17				17
CCQM	CCQM	793		238	576	1607	233		73	182	488
COOMET	CoQM	18	14			32	8	6			14
EURAMET [b]	EUQM	17	88			105	9	13			22
GULFMET	GUQM					0					0
SIM	SIQM	9	44			53	5	11			16
	Total	896	203	244	587	1930	286	52	74	185	597

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.

1.5.3. 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	4	8			3	4	7
Electrochemical Analysis	EAWG	100	8	7	41	156	27	2	2	15	46
Gas Analysis	GAWG	365	132	74	7	578	101	31	23	4	159
Inorganic Analysis	IAWG	209	52	28	251	540	66	13	9	76	164
Isotopic Ratio	IRWG	15		39	10	64	5		6	4	15
Nucleic Acid	NAWG	8		10	58	76	4		2	19	25
Organic Analysis	OAWG	137	11	16	181	345	64	6	8	58	136
Protein Analysis	PAWG	9		23	19	51	5		11	4	20
Surface Analysis	SAWG	53		43	16	112	14		10	1	25
	Total	896	203	244	587	1930	286	52	74	185	597

Jointly coordinated studies are assigned to the most appropriate WG on the basis of the units used; 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.

1.5.4. Units and BaseUnits

Some WGs conduct mostly one type of study, with results reported using the same BaseUnit. For instance, most GAWG gas mixture results are reported in terms of mole analyte per mole mixture (mole fraction, mol/mol) and nearly all of the IAWG inorganic measurand results either are or can be readily converted to mass analyte per mass matrix (mass fraction, g/g). Other WGs conduct two or more very different types of study; e.g., the EAWG supports measurements of pH (pH) and electrolytic conductivity (S/m) and the SAWG supports measurements that include adsorption (mol/g), film thickness (m), and pore volume (cm^3/g). Since results reported in different units differ qualitatively, datasets within a WG are grouped by the "BaseUnit" of the measurand.

A BaseUnit 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 BaseUnit of mass. There are also measurement results that cannot be expressed in SI units, including: number of nucleotide base pairs (bp), 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 BaseUnit.

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 in that mass).

1.5.5. 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 as of 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	8		8	7		7
Electrochemical Analysis	EAWG	141	15	156	44	2	46
Gas Analysis	GAWG	304	274	578	126	33	159
Inorganic Analysis	IAWG	130	410	540	54	110	164
Isotopic Ratio	IRWG	15	49	64	4	11	15
Nucleic Acid	NAWG	39	37	76	11	14	25
Organic Analysis	OAWG	68	277	345	37	99	136
Protein Analysis	PAWG	7	44	51	7	13	20
Surface Analysis	SAWG	58	54	112	12	13	25
	Total	770	1160	1930	302	295	597

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.

1.5.6. 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.

1.5.7. 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 21).

Table 4. Number of Datasets Held in the Datasheets.

	Number of Datasets		
Datasheet	Single	Multiple	Total
CCQM_KC	946	113	1059
CCQM_Pilot	584	4	588
CCQM_PubPilot	243		243
CCQM_Continuous	34	2	36
CCQM_KC_Beta	4		4
Total	1811	119	1930

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

Table 5. BaseUnits and Associated Dataset Numbers.

		Number of Usable Datasets									
Measurement	BaseUnit	CAWG	EAWG	GAWG	IAWG	IRWG	NAWG	OAWG	PAWG	SAWG	Total
Massfraction	g/g				511			330	46	2	889
Mole fraction	mol/mol			488	5	4		10		4	511
pH	pH		94								94
Entity fraction	n/n					32	34				66
Length	M									51	51
Entity concentration	n/L	2		10			21				33
Conductivity	S/m		29								29
Isotopic δ-scale	‰ (per mille)					23					23
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		1		6
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	508	516	62	69	340	47	94	1777

1.6. 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, BaseUnit} studies. For each organization in each {WG, BaseUnit}, 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, BaseUnit} and study type as of this document's publication date.

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

	NMI/DIs				Other Organizations			
{WG, BaseUnit}	KC	SC	PPS	PS	KC	SC	PPS	PS
{CAWG,EFF}			9					
{CAWG,n/L}			9	5				
{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	42	33	16	1[a]		7	1
{GAWG,n/L}	8							
{IAWG,g/g}	54	55	27	64	1[a]		18	91
{IAWG,mol/mol}		4						
{IRWG,‰}	8		18	10			6	13
{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}	45	34	18	42		1[a]	4	25
{OAWG,mol/mol}				12				
{PAWG,g/g}	14		20	10			1	
{PAWG,g/L}			4					
{SAWG,a.u.}				6				3
{SAWG,cm^3/g}	6		1					
{SAWG,g/g}	5		5					
{SAWG,m}	12		14				1	
{SAWG,m^2/g}	6		1					
{SAWG,mol/g}	6		1					

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.

1.6.1. 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).

1.6.2. 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.

1.6.3. 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 RVs, their results have been included in the *CCQM_Retrospectoscope* datasets.

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

1.7. 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.

1.8. 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 Gaussian $\mathrm{N}(\hat{\mu}, \hat{\sigma})$ distribution, where $\hat{\mu}$ and $\hat{\sigma}$ are robust estimates of the "true" location (mean) and scale (standard deviation) of the distribution.

1.8.1. 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 Median{*x*}, where *x* is the symbol for a representative value.

1.8.2. 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" (MAD_E) estimator but is considerably more efficient, 88 % compared to the 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.

1.9. Performance Metrics

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

1.9.1. 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 RV, x_{ref}, normalized in different ways to enable comparison across datasets. These bias metrics are: [13]

signed z-score $$z_i = (x_i - x_{\text{ref}})/u(x_i)\ , \quad (1)$$

absolute z-score $$|z_i| = |x_i - x_{\text{ref}}|/u(x_i)\ , \quad (2)$$

signed zeta-score $$\zeta_i = (x_i - x_{\text{ref}})/\sqrt{u^2(x_i) + u^2(x_{\text{ref}})}\ , \quad (3)$$

absolute zeta-score $$|\zeta_i| = |x_i - x_{\text{ref}}|/\sqrt{u^2(x_i) + u^2(x_{\text{ref}})}\ , \quad (4)$$

signed percent difference $$D_i = 100(x_i - x_{\text{ref}})/x_{\text{ref}}\ , \text{ and} \quad (5)$$

absolulte percent difference $$|D_i| = 100|x_i - x_{\text{ref}}|/x_{\text{ref}} \quad (6)$$

where $u(x_i)$ is the standard uncertainty associated with x_i and $u(x_{\text{ref}})$ is the standard uncertainty associated with x_{ref}. The $u(x_{\text{ref}})$ is typically estimated as one-half of the RV's 95 percent level of confidence expanded uncertainty, $U_{95}(x_{\text{ref}})$. Both the signed and absolute values of these metrics are provided since the sign of the difference 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 RV in units of the participant's standard uncertainty. When the RV is "exactly" known (e.g., established by gravimetric preparation rather than consensus estimation), accurately determined x_i values should be within about $2u(x_i)$ 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 RV in units of the root-mean-square error (RMSE) of the participant's standard uncertainty and that of the RV. Since this combined standard uncertainty is always larger than $u(x_i)$, 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 $u(x_{\text{ref}})$ was estimated. CCQM policy (and politics) aside, accurate x_i values are expected to be within the interval $x_{\text{ref}} \pm 2\sqrt{u^2(x_i) + u^2(x_{\text{ref}})}$ 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}. However, correlation exists when x_{ref} is estimated by consensus. Many of the CCQM studies that estimated x_{ref} by consensus have not 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 expected coefficient of variation (%CV, aka percent relative standard deviation).

The six metrics as used in the *Lab_History* subsystem (see Section 1.9.1) 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.

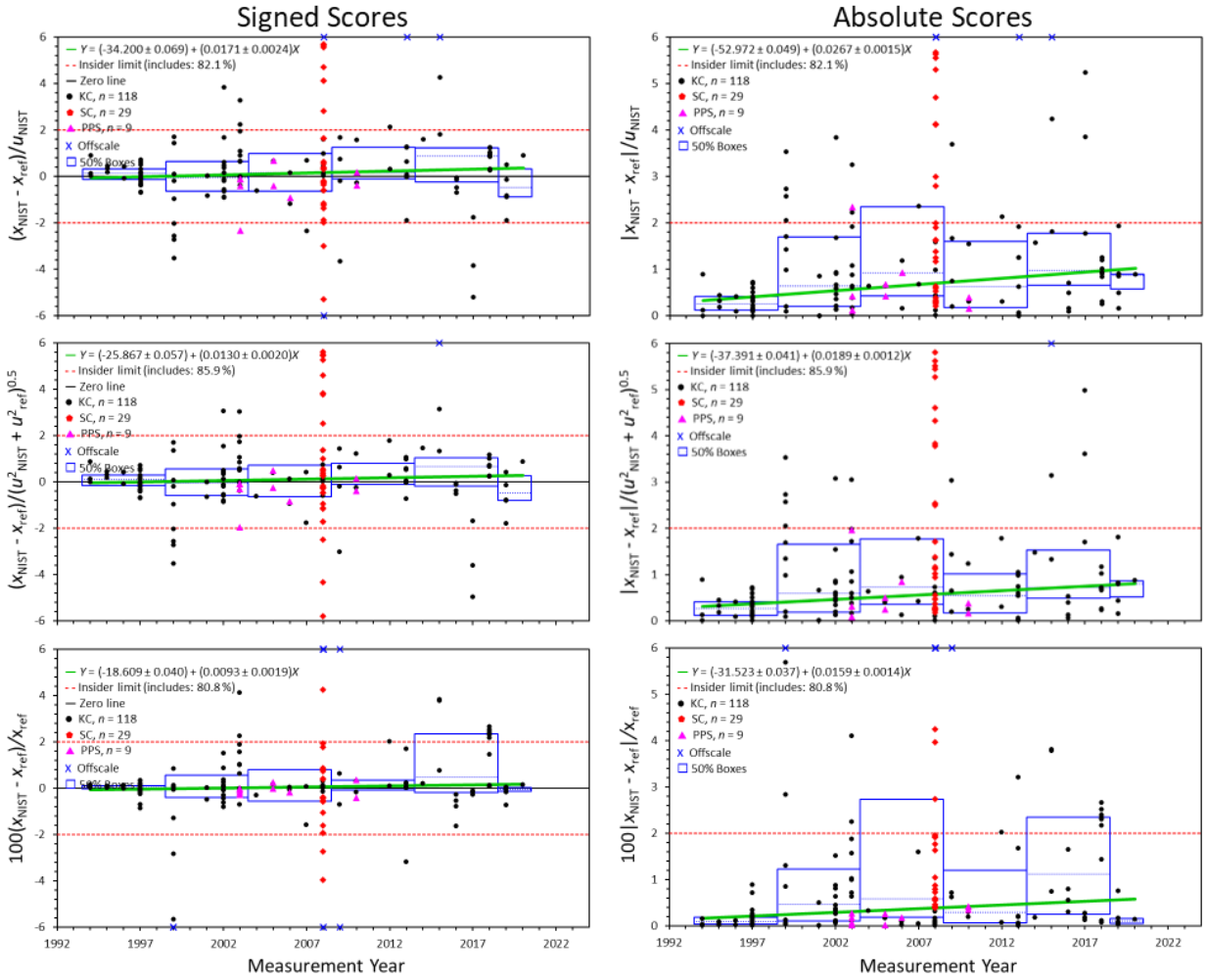


Fig. 2. Comparison of Bias Metrics for the NIST GAWG Data.

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, RVs were (by policy) not reported for many PS datasets. Only relatively recently have x_{ref} and $u(x_{\mathrm{ref}})$ 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 $u(x_{\mathrm{ref}})$ 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.

1.9.2. Relative Uncertainties

Bias metrics have two components, 1) the difference between the laboratory's result and the RV 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 $u(x_i)$ or a composite that incorporates the participant's $u(x_i)$. If the $u(x_i)$ 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 $u(x_i)$ has been correctly estimated that is independent of $x_i - x_{\mathrm{ref}}$. However, a given $u(x_i)$ divided by the median of the standard uncertainties associated with all of the technically valid x_i in the dataset, $\mathrm{Median}\{u_{\mathrm{set}}\}$, is a convenient indicator of whether, relative to the co-participants, participant i under-or-overestimated $u(x_i)$

$$u_{\mathrm{rel}}(x_i) = u(x_i)/\mathrm{Median}\,\{u_{\mathrm{set}}\}\,, \tag{7}$$

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

1.9.3. 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:

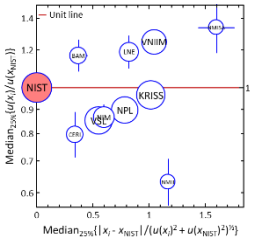
$$\zeta_{ij} = (x_i - x_j)/\sqrt{u^2(x_i) + u^2(x_j)}\,, \text{ and} \tag{8}$$

$$\left|\zeta_{ij}\right| = \left|x_i - x_j\right|/\sqrt{u^2(x_i) + u^2(x_j)}\,. \tag{9}$$

The uncertainty metric of interest for these bias metrics is the ratio of the two uncertainties:

$$u_{\mathrm{rel}}\left(x_i, x_j\right) = u(x_i)/u\left(x_j\right)\,. \tag{10}$$

1.9.4. {Bias, Uncertainty Ratio} Distance



The three "Peer" analysis systems *Peer_Bilateral*, *Peer_Unilateral*, and *Peer_Global* summarize estimates of relative uncertainty as functions of relative bias for NMI/DIs that meet given participation criteria. While the bias metrics are scaled by uncertainty values and so the metrics are not independent, it is convenient to calculate a distance of each pair of {bias, uncertainty ratio} estimates to their RVs.

Since the bias of a RV 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}. Assuming that a factor-of-two in the uncertainty ratio has about the same significance as a bias of 1, the binary logarithm ($\log_2$) of the uncertainty ratio has about the same intrinsic scale as the bias. Since $\log_2(1) = 0$, a practical definition for the {bias, uncertainty ratio} distance is:

$$\Delta_i = \sqrt{X_i^2 + \left(a \times \log_2(Y_i)\right)^2} \tag{11}$$

where X_i is the bias of the i^{th} NMI/DI, Y_i is the uncertainty ratio, and a is user-settable scale factor that has a default value of 1.

The smaller the Δ_i distance, the more similar the NMI/DI's results are to the RVs. The Δ_i values are provided in the **Dist** column of the tables to the right-hand side of the chart.

1.9.5. 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

$$Y = \beta_0 + \beta_1 X \tag{12}$$

can be parameterized using classical least squares regression. The values of the β coefficients are those that minimize 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. For these plots, the *CCQM_Retrospectoscope* uses the robust non-parametric Theil-Sen estimator [14,15] to visualize plausible linear trends. 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 $\text{Median}\{(y_j - y_i)/(x_j - x_i)\}$ for all data pairs where x_j differs from x_i. The intercept, β_0, is estimated as the $\text{Median}\{y_i - \beta_1 x_i\}$. Because the Q_n estimator can become irritatingly slow when applied to a large number of values, the $u(\beta_1)$ is estimated as the MAD_E of the $(y_j - y_i)/(x_j - x_i)$ and $u(\beta_0)$ is estimated as the MAD_E of the $y_i - \beta_1 x_i$.

1.9.5.1. 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:

$$Y = \big(\beta_0 \pm u(\beta_0)\big) + \big(\beta_1 \pm u(\beta_1)\big)X\,. \tag{13}$$

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

$$Y = \big(\beta_0 \pm u(\beta_0)\big) + \big(\beta_1 \pm u(\beta_1)\big)\log_{10}(X)\,. \tag{14}$$

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

$$\log_{10}(Y) = \big(\beta_0 \pm u(\beta_0)\big) + \big(\beta_1 \pm u(\beta_1)\big)X \tag{15}$$

$$Y = 10^{(\beta_0 \pm u(\beta_0)) + (\beta_1 \pm u(\beta_1))X}. \tag{16}$$

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

$$\log_{10}(Y) = \big(\beta_0 \pm u(\beta_0)\big) + \big(\beta_1 \pm u(\beta_1)\big)\log_{10}(X) \tag{17}$$

$$Y = 10^{(\beta_0 \pm u(\beta_0))} X^{(\beta_1 \pm u(\beta_1))} = \big(\beta_0' \pm u(\beta_0')\big) X^{(\beta_1 \pm u(\beta_1))}\,. \tag{18}$$

where $\beta_0' = 10^{\beta_0}$ and $u(\beta_0') \cong \frac{10^{\beta_0 + u(\beta_0)} - 10^{\beta_0 - u(\beta_0)}}{2}$. This "power function" defines a straight line in a scattergram with log-log axes.

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

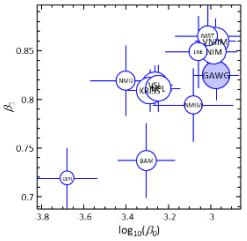
1.9.5.2. Interpreting the Slope Parameter

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 -β_1, is a good indicator of whether the Y increases or decreases, on average, with increasing X. An absolute *t*-statistic

$$|t| = |\beta_1| / u(\beta_1) \tag{19}$$

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

1.9.6. {log10(β0), β1} Distance



The *WG_Power* subsystem displays power function coefficients (Eq. 17) for specified measurement communities.

The distance between the i^{th} and j^{th} pair of $\{\log_{10}(\beta_0), \beta_1\}$ coefficients within a community is estimated as

$$\Delta_{ij} = \sqrt{\left(\frac{\log_{10}(\beta_0)_i - \log_{10}(\beta_0)_j}{\log_{10}(\beta_0)_{\max} - \log_{10}(\beta_0)_{\min}}\right)^2 + \left(\frac{\beta_{1i} - \beta_{1j}}{\beta_{1\max} - \beta_{1\min}}\right)^2} \quad (20)$$

where the "min" and "max" subscripts designate minimum and maximum allowed values.

Since the power function coefficients have different scales, normalizing to the allowed span of the coefficients gives the values equal influence. However, the Δ_{ij} distances will change if one or both spans are changed. To compare Δ_{ij} across different measurement communities, it is thus necessary to use the same allowed spans.

1.10. User-Specified Parameters

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 BaseUnits 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 in the **Use** and **Default** columns. The Use values are displayed in red font.

1.10.1. 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 BaseUnit 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.*

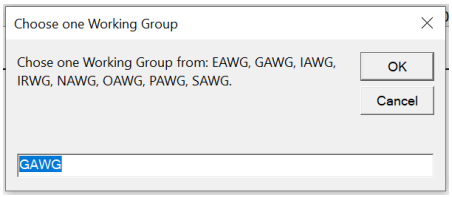
1.10.2. When the Default Value is not *Auto*

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.

1.10.2.1. 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 through:", 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*.

1.10.2.2. 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**.

1.11. 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_Continuous*, 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 RV 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 RVs 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; 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.

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 21).

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.

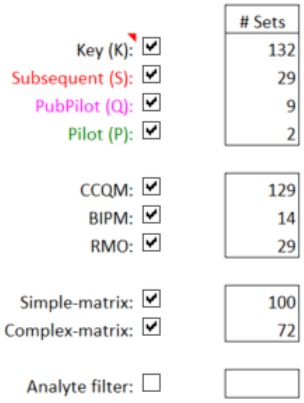
2.1.7. Restore

Clicking the **Restore** button, which is intentionally placed 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



Ten checkboxes are used by many subsystems to specify what datasets are included in the analysis. These checkboxes control the study type (KC, SC, PPS, and PS; see Section 1.5.1), whether studies were conducted by the CCQM , BIPM, or an RMO (Section 1.5.2), whether the sample had a relatively simple or complex matrix (Section 1.5.5), and analytes (Section 1.5.6). 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, placed 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, clicking any one of the first nine dataset selection checkboxes 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, BaseUnit} settings. 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.

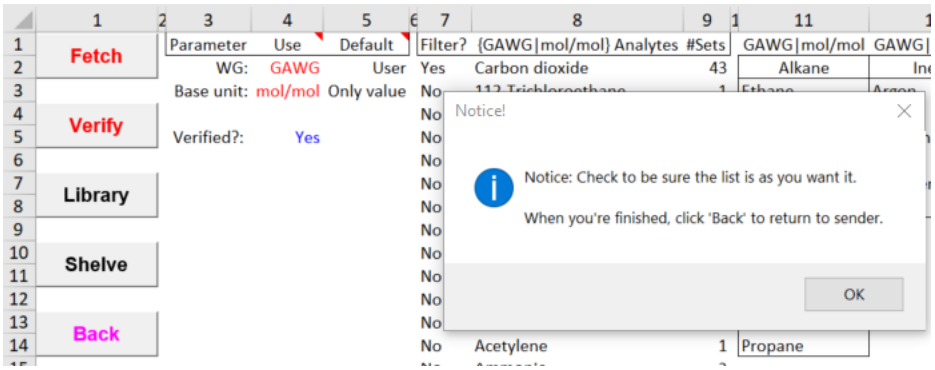


Fig. 3. *Dataset_AnalyteFilter* Confirmation Notice and Prompt.

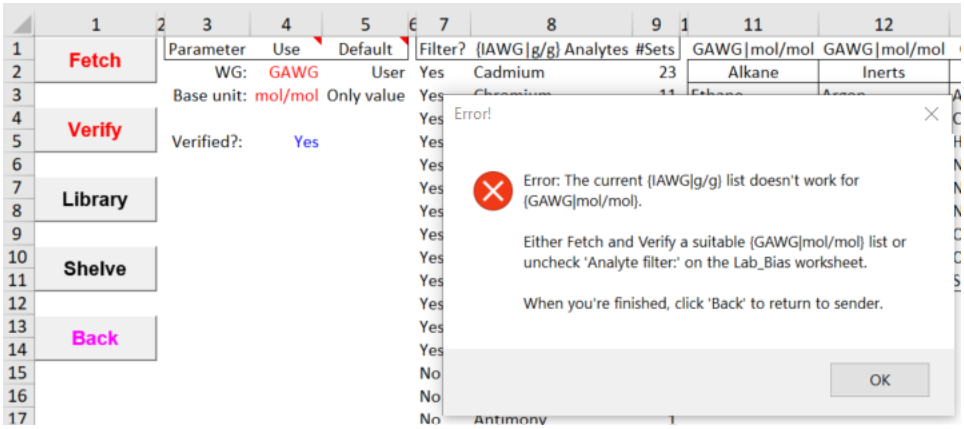


Fig. 4. *Dataset_AnalyteFilter* Error Message and Prompt.

In either case, clicking the **OK** button enables use of the *Dataset_AnalyteFilter* worksheet’s controls. See Section 23 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 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.

2.2.3.2. Title

Clicking the title checkbox toggles display of the chart title.

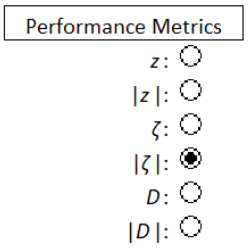
2.2.3.3. Plot area box

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.

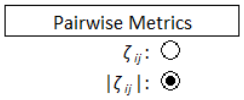
2.3. Radio Buttons

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.

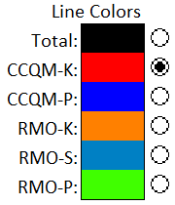
The *Lab_History*, *Lab_Bias*, *Peer_Unilateral*, and *Peer_Global* analysis subsystems use the same series of radio buttons for selecting one of six performance metrics (see Section 1.9.1). Changing the metric on one of these subsystems as no effect on the others.



The *Peer_Bilateral* subsystem uses ratio buttons to select between the two pairwise metrics (see Section 1.9.3).



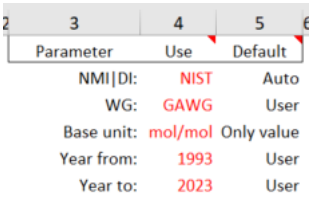
The *Lab_Engagements* subsystem uses radio buttons to select the type of studies to be summarized.



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 1.9.4 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 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 27.4.4). Additionally, for some applications the code *All* can be used to accept results without regard to any particular NMI/DI.

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 1.5.3); however, most datasets are from studies conducted by the EAWG, GAWG, IAWG, and OAWG. Additionally, for some applications the code All can be used to accept results without regard to any particular WG.

2.4.1.3. BaseUnit: 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 1.5.4). This is mostly important for studies conducted by the EAWG since they support two qualitatively different measurement systems: pH and electrolytic conductivity. The default BaseUnits are the units used in the majority of the WG's studies. Additionally, for some applications the code All can be used to accept results without regard to any particular BaseUnit.

2.4.1.4. Year from and Year through: 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 through:” 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 1.7).

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 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.

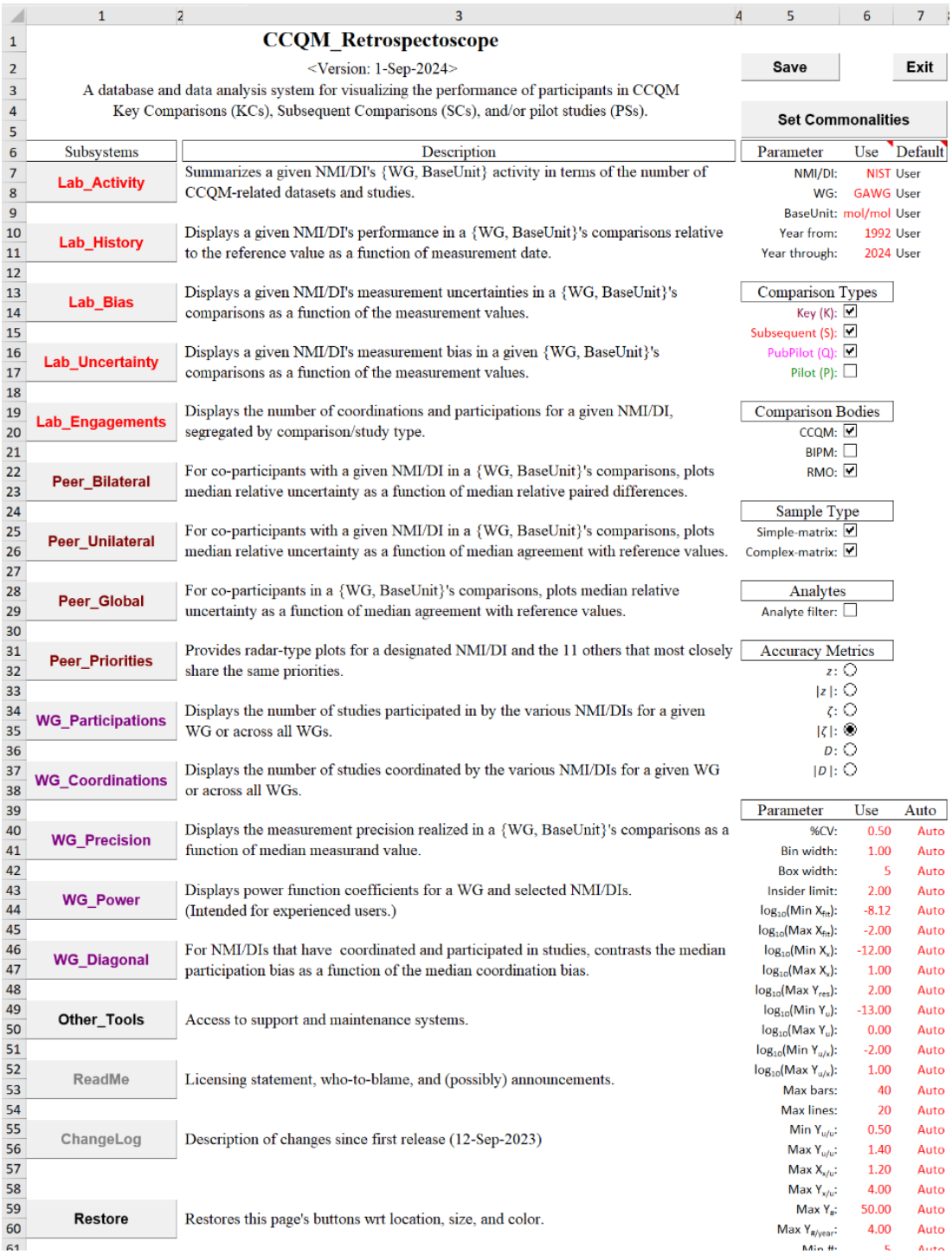


Fig. 5. *Welcome* Dashboard.

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

Clicking the **Other_Tools** button activates the *Other_Tools* worksheet, enabling access to several specialized analysis 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. See Section 29 for details

3.4. ChangeLog

Clicking the **ChangeLog** button activates the *ChangeLog* worksheet which documents the changes made to the *CCQM_Retrospectoscope* since it was first released (12-Sep-2023). See Section 30 for details

3.5. 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>.

3.6. Set Commonalities

Clicking the **Set Commonalities** button transfers the settings of the parameters and controls listed in the **Use** (column 6) and **Default** (column 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.

Commonalities

Parameter	Use	D
NMI|DI:	NIST	
WG:	GAWG	
Base unit:	mol/mol	Auto
Year from:	1993	User
Year to:	2022	User

Values in red font control what data is analyzed.

Commonalities

Parameter	Use	Default
NMI|DI:	NIST	User
WG:	GAWG	User
Base unit:	mol/mol	Auto
Year from:	1993	User
Year to:	2022	User

Set the default to "User" or a specific valid value if you want something other than the **Auto**matric value.

Set Commonalities

Parameter	Use	Default
NMI/DI:	NIST	User
WG:	GAWG	User
BaseUnit:	mol/mol	User
Year from:	1992	User
Year through:	2024	User

Comparison Types

Key (K):	☑
Subsequent (S):	☑
PubPilot (Q):	☑
Pilot (P):	☑

Comparison Bodies

CCQM:	☑
BIPM:	☑
RMO:	☑

Sample Type

Simple-matrix:	☑
Complex-matrix:	☑

Analytes

Analyte filter:	☐

Accuracy Metrics

z:	○
$\|z\|$:	○
ζ:	○
$\|\zeta\|$:	◉
D:	○
$\|D\|$:	○

Parameter	Use	Auto
%CV:	0.50	Auto
Bin width:	1.00	Auto
Box width:	5	Auto
Insider limit:	2.00	Auto
$\log_{10}(\text{Min } X_{fit})$:	-8.12	Auto
$\log_{10}(\text{Max } X_{fit})$:	-2.00	Auto
$\log_{10}(\text{Min } X_u)$:	-12.00	Auto
$\log_{10}(\text{Max } X_u)$:	1.00	Auto
$\log_{10}(\text{Max } Y_{res})$:	2.00	Auto
$\log_{10}(\text{Min } Y_u)$:	-13.00	Auto
$\log_{10}(\text{Max } Y_u)$:	0.00	Auto
$\log_{10}(\text{Min } Y_{u/u})$:	-2.00	Auto
$\log_{10}(\text{Max } Y_{u/u})$:	1.00	Auto
Max bars:	40	Auto
Max lines:	20	Auto
Min $Y_{u/u}$:	0.50	Auto
Max $Y_{u/u}$:	1.40	Auto
Max $X_{x/u}$:	1.20	Auto
Max $Y_{x/u}$:	4.00	Auto
Max $Y_{\#}$:	50.00	Auto
Max $Y_{\#/year}$:	4.00	Auto
Min #:	5	Auto
Min %:	25	Auto
Power width:	4.00	Auto
Y/X factor:	1.00	Auto

Checkbox	State	Value
%CV lines:	TRUE	
50 % boxes:	TRUE	
All studies:	TRUE	
Color symbols:	TRUE	
Color target:	TRUE	
Ellipse:	TRUE	1
Error bars:	TRUE	1
Horwitz line:	TRUE	
Legend:	TRUE	
Limit line(s):	TRUE	
Mark complex:	TRUE	
Opacity:	TRUE	
Outsider labels:	TRUE	
Plot area box:	TRUE	
Power interval:	TRUE	
Power line:	TRUE	
Title:	TRUE	
Target/All ratio:	TRUE	
Trend line(s):	TRUE	
Yearly average:	TRUE	

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.

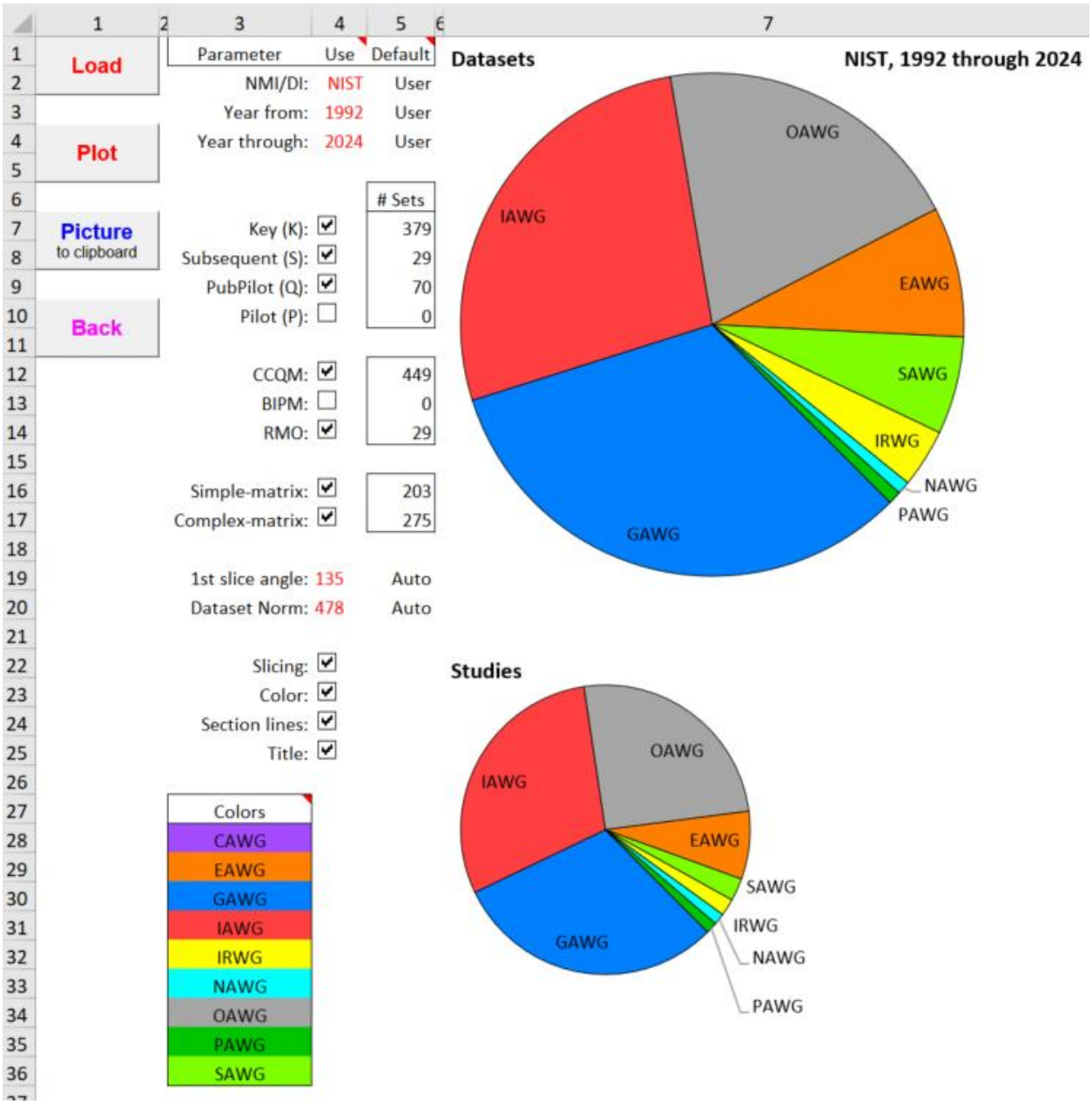


Fig. 6. *Lab_Activity* Dashboard.

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 1.10 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, BaseUnit} "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.

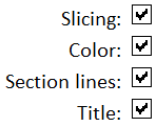
4.2.1. 1st slice angle: Set angle of First Pie Slice

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, BaseUnit} 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 within a 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, BaseUnit}. As displayed in Fig. 7, the identity of the slices can become difficult to discern when there are many {WG, BaseUnit} with relatively few datasets.

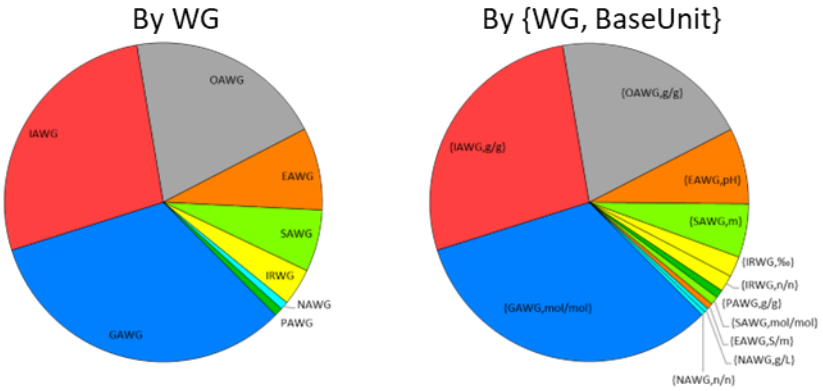


Fig. 7. *Lab_Activity* Chart LA-1 Summarized by WG and by {WG, BaseUnit}.

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, BaseUnit} 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.

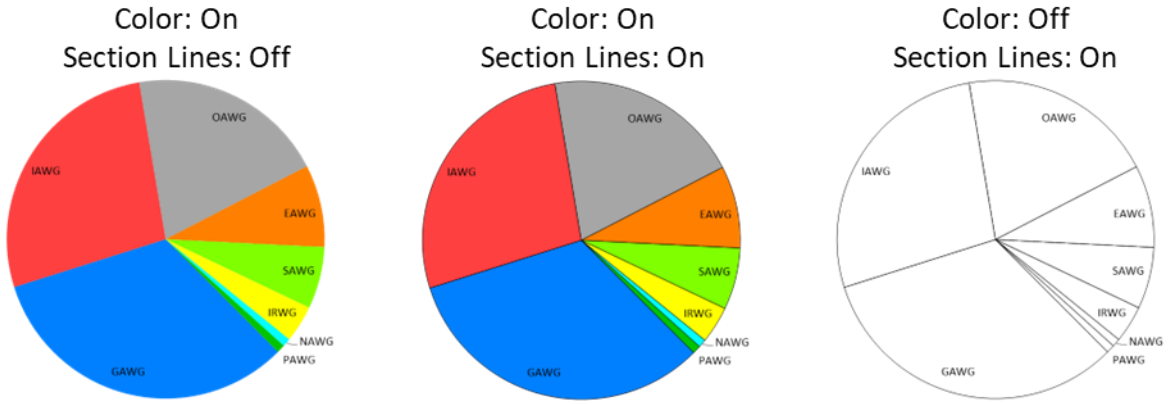


Fig. 8. *Lab_Activity* Chart LA-1 With Color and Section Line Variations.

4.4. Table

The table to the right of chart LA-1, shown in Fig. 9, summarizes the number of datasets and studies for each WG. The **All** columns provide the sum the number of datasets or studies that come from KCs, SCs, PPSs, and PSs (which is also the sum of the CCQM, BIPM, and RMO datasets or studies, which is also the sum of the simple (Smpl) and complex (Cmplx) datasets or studies).

For each WG, the table also provides a robust estimate of the over-all coefficient of variation (CV, the percent relative standard deviation) and the range between the minimum and maximum values (Span) expressed as $\log_{10}$(maximum/minimum) of the NMI/DI's results. The CV and Span calculations exclude results that are less than or equal to zero.

8	9	1	11	12	13	14	15	16	17	18	19	20	2	22	23	24	25	26	27	28	29	30	31	3	33	34
			Number Datasets											Number Studies											Properties	
Slicing By			All	KC	SC	PPS	PS	CCQM	BIPM	RMO	Smpl	Cmplx		All	KC	SC	PPS	PS	CCQM	BIPM	RMO	Smpl	Cmplx		%CV	Span
GAWG			156	118	29	9	0	127	0	29	84	72		48	41	1	6	0	47	0	1	35	13		0.67	10.62
IAWG			130	115	0	15	0	130	0	0	34	96		47	41	0	6	0	47	0	0	16	31		0.74	10.16
OAWG			96	81	0	15	0	96	0	0	11	85		40	33	0	7	0	40	0	0	9	31		1.09	8.56
EAWG			40	40	0	0	0	40	0	0	40	0		12	12	0	0	0	12	0	0	12	0		0.02	3.30
SAWG			30	12	0	18	0	30	0	0	22	8		4	3	0	1	0	4	0	0	2	2		3.38	8.80
IRWG			18	8	0	10	0	18	0	0	12	6		3	1	0	2	0	3	0	0	1	2		0.12	2.63
NAWG			4	4	0	0	0	4	0	0	0	4		2	2	0	0	0	2	0	0	0	2		9.10	7.1
PAWG			4	1	0	3	0	4	0	0	0	4		2	1	0	1	0	2	0	0	0	2		2.34	6.55

Fig. 9. 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.

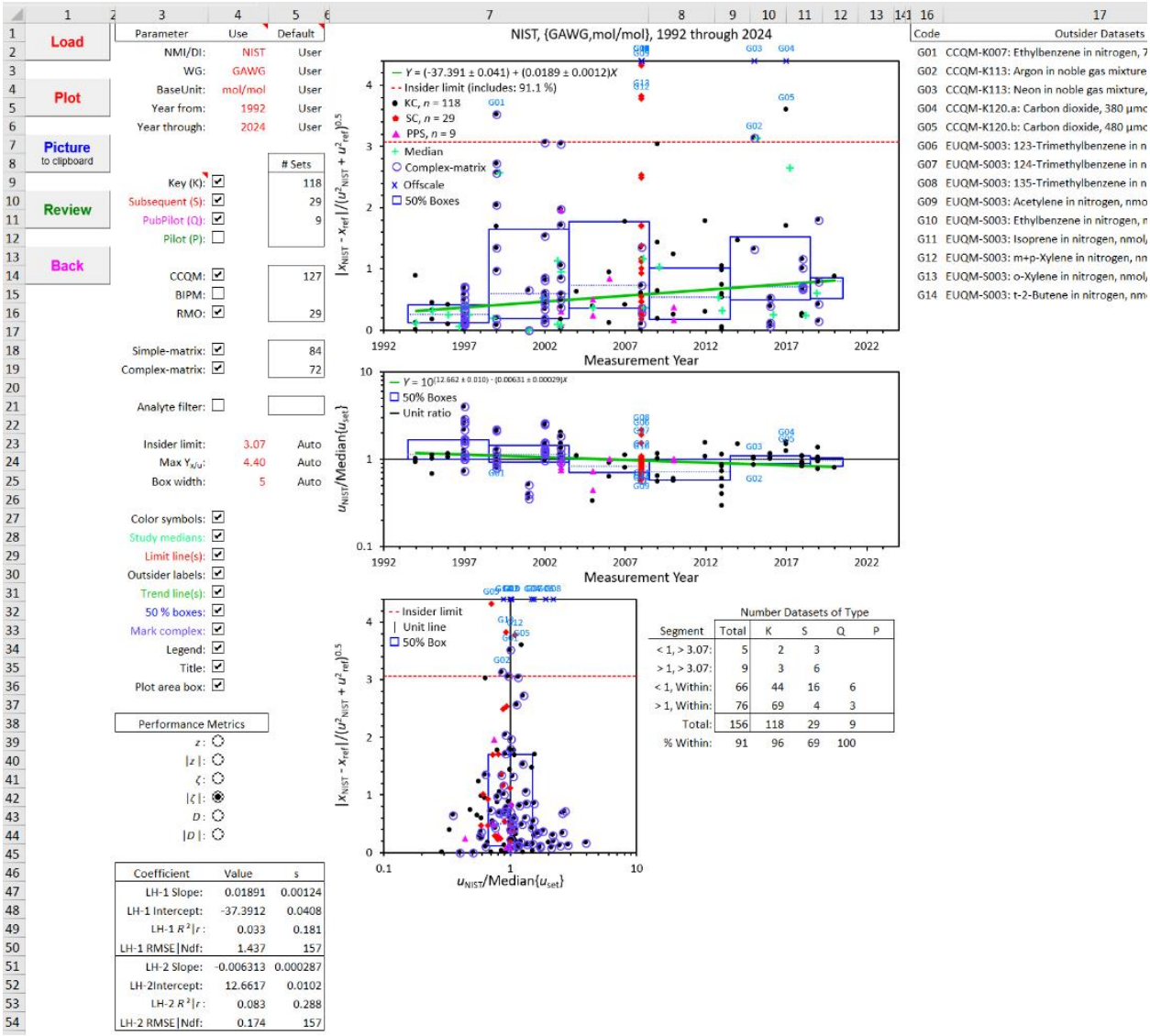


Fig. 10. *Lab_History* Dashboard.

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 1.10 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 plotted as a function of the study's measurement yea. 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 $u_i/\mathrm{median}(u_{\mathrm{set}})$ ratios are of interest and ratios are seldom *very* large or *very* small, the chart's $u_i/\mathrm{median}(u_{\mathrm{set}})$ 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 signed- and absolute value bias metrics with the "50 % Boxes:" and "Limit line(s):" activated are displayed in Fig. 11.

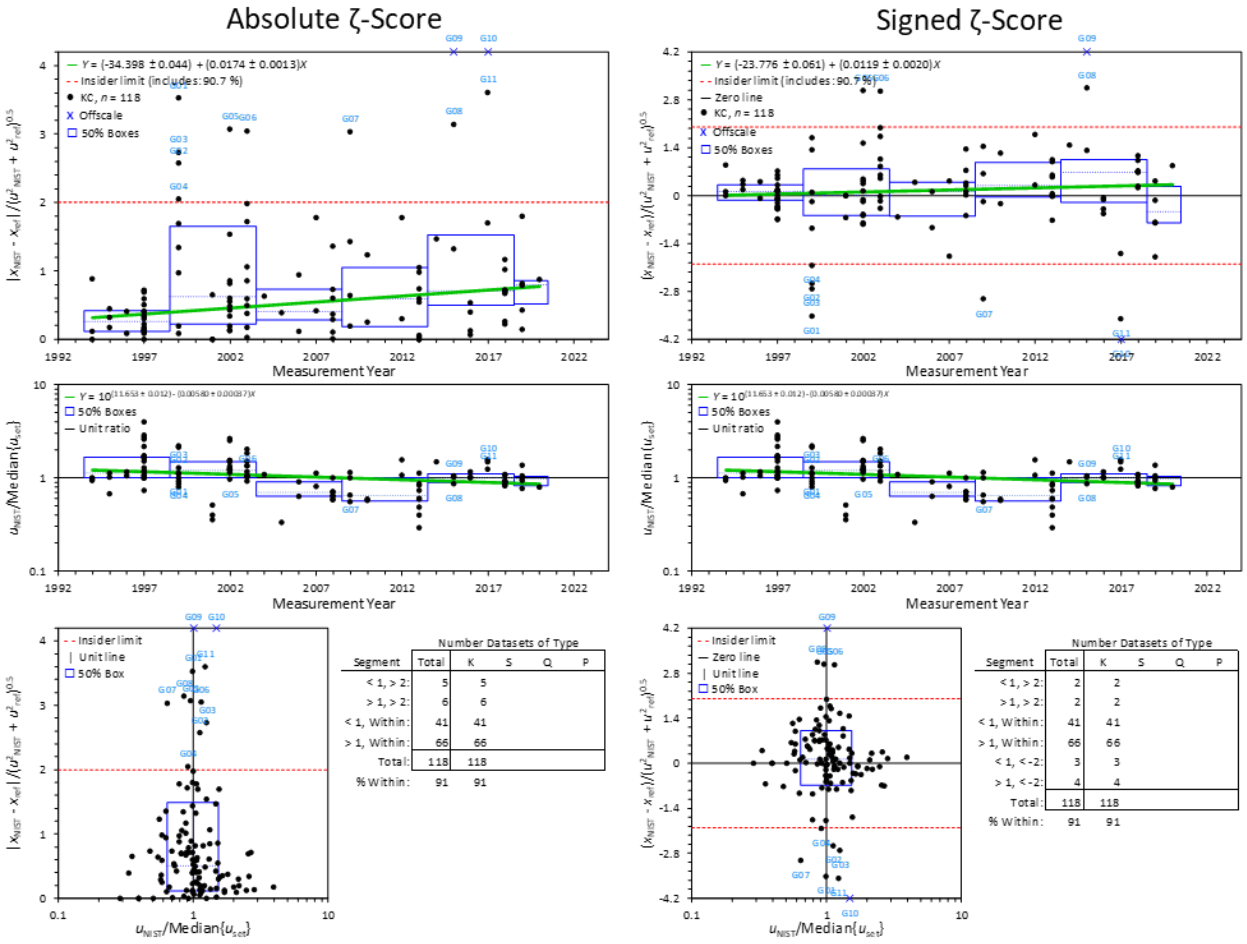


Fig. 11. *Lab_History* Charts with Absolute and Signed Bias Metrics.

5.2. Chart Display Parameters

Insider limit:	3.07	Auto
Max $Y_{x/u}$:	4.50	Auto
Box width:	5	Auto

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: Outsider 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 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).

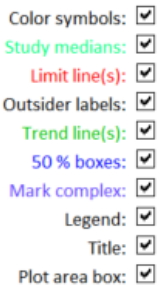
5.2.2. Max $Y_{x/u}$: *y*-Axis Maximum for Charts LH-1 and LH-3

The value of the "Max $Y_{x/u}$:" parameter sets the display range of the *y*-axis (bias) 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

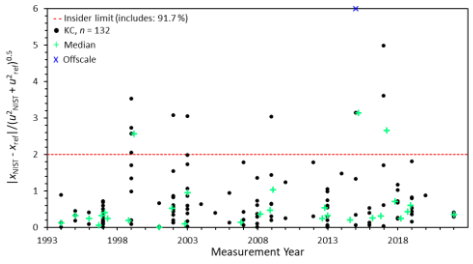


The *Lab_History* worksheet contains seven chart display checkboxes in addition to the three discussed in Section 2.2.3. Clicking a chart display checkbox invokes an immediate change in the chart display.

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 are 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

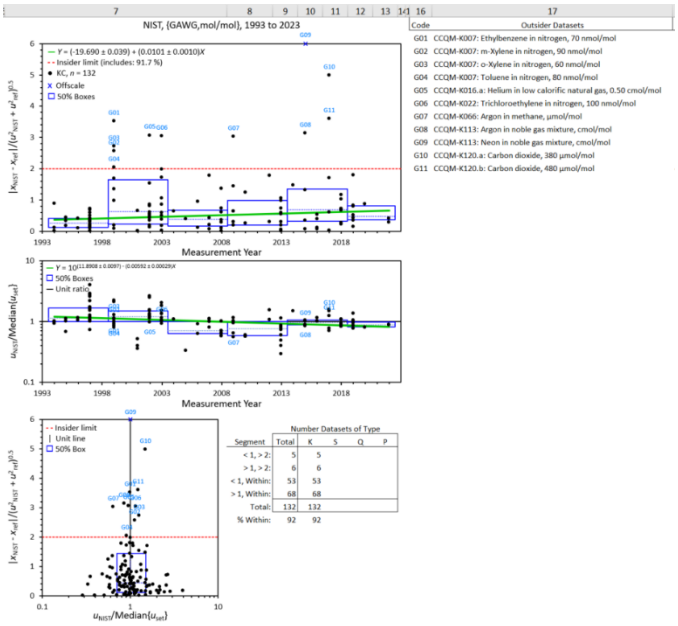


Since many studies evaluate more than one measurand, clicking the "Study medians:" checkbox toggles a display of the median bias of the multi-measurand studies. These values are displayed as green "+"s. They are only displayed in chart LH-1.

5.3.3. Limit line(s)

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

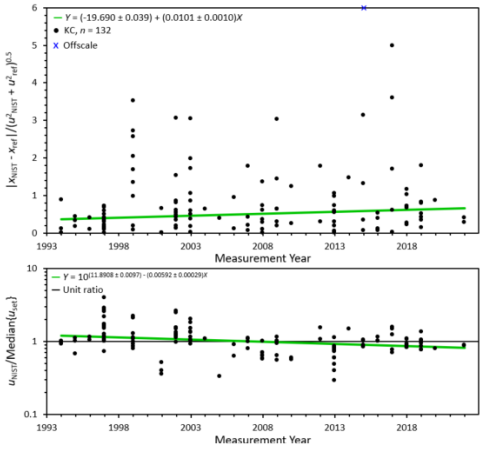
5.3.4. Outsider labels



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

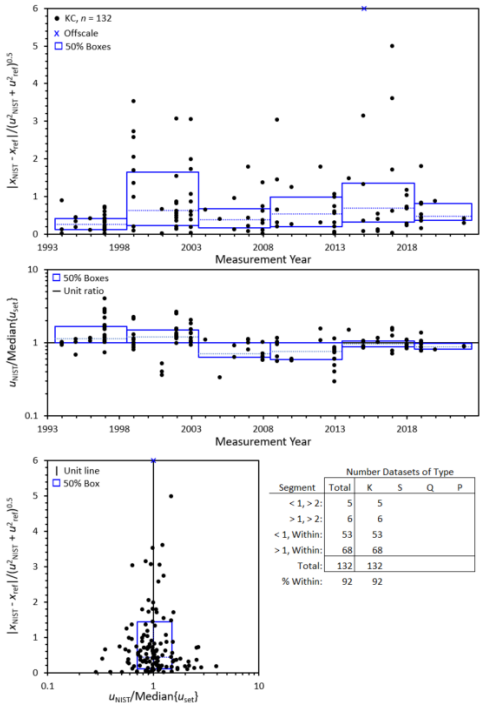
The outsider datasets are identified in the table to the right of the charts. Selecting a cell containing either the code or the dataset name and clicking the **Review** button produces a dot-and-bar chart for that dataset (Section 21).

5.3.5. Trend line(s)



Clicking the “Trend line(s):” checkbox toggles the display of robust Thiel-Sen linear trend lines [14,15] in the LH-1 and LH-2 charts.

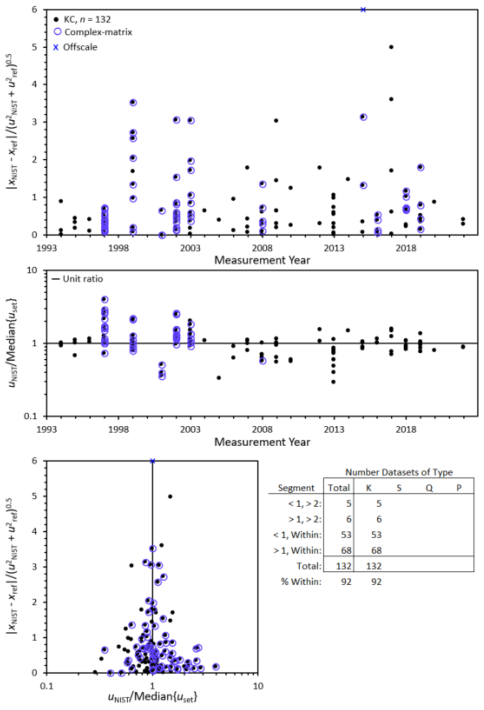
5.3.6. 50 % boxes



For charts LH-1 and LH-2, clicking the "50 % boxes:" checkbox toggles the display of a series of rectangular 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 $100(1\text{-}2*0.146)^2 = 50.1$ %, 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



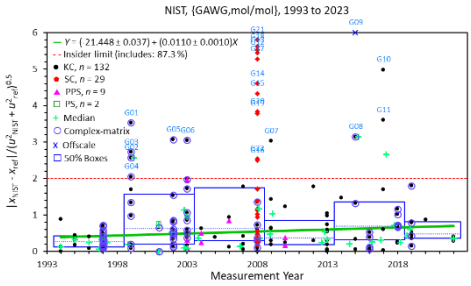
Clicking the "Mark complex:" checkbox toggles the identification of results for complex-matrix materials. This option is only relevant when simple-matrix and complex-matrix datasets are analyzed together. Complex-matrix datasets are identified with a surrounding purple circle.

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.

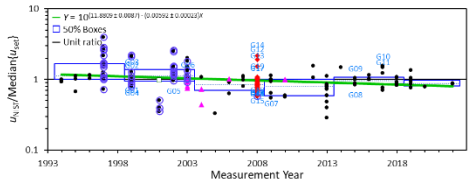
In chart LH-1:

- if “Trend line(s):” is checked the trend equation of the bias metric over time is listed.
- if “Insider limit:” is checked the percentage of results that are inside the Insider limit is listed.
- If the symbols are shown colored, the number of each type of study is listed.

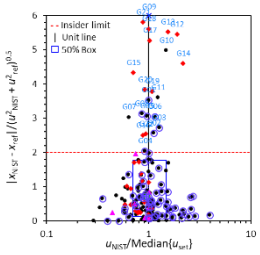


In chart LH-2:

- if “Trend line(s):” is checked the trend equation of the relative uncertainty over time is listed.



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



5.4. Stored Theil-Sen Regression Parameters

The Chart LH-1 and LH-2 trendline slopes, intercepts, Pearson correlation (R^2) of the fit, imputed correlation between the slope and intercept coefficients (r), RMSE, and number of degrees of freedom (ndf) are stored below the radio buttons. These values are generated during the analysis and are stored whether or not the trendlines are displayed.

Coefficient	Value	s
LH-1 Slope:	0.01891	0.00124
LH-1 Intercept:	-37.3912	0.0408
LH-1 R^2|r:	0.033	0.181
LH-1 RMSE|Ndf:	1.437	157
LH-2 Slope:	-0.006313	0.000287
LH-2Intercept:	12.6617	0.0102
LH-2 R^2|r:	0.083	0.288
LH-2 RMSE|Ndf:	0.174	157

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.

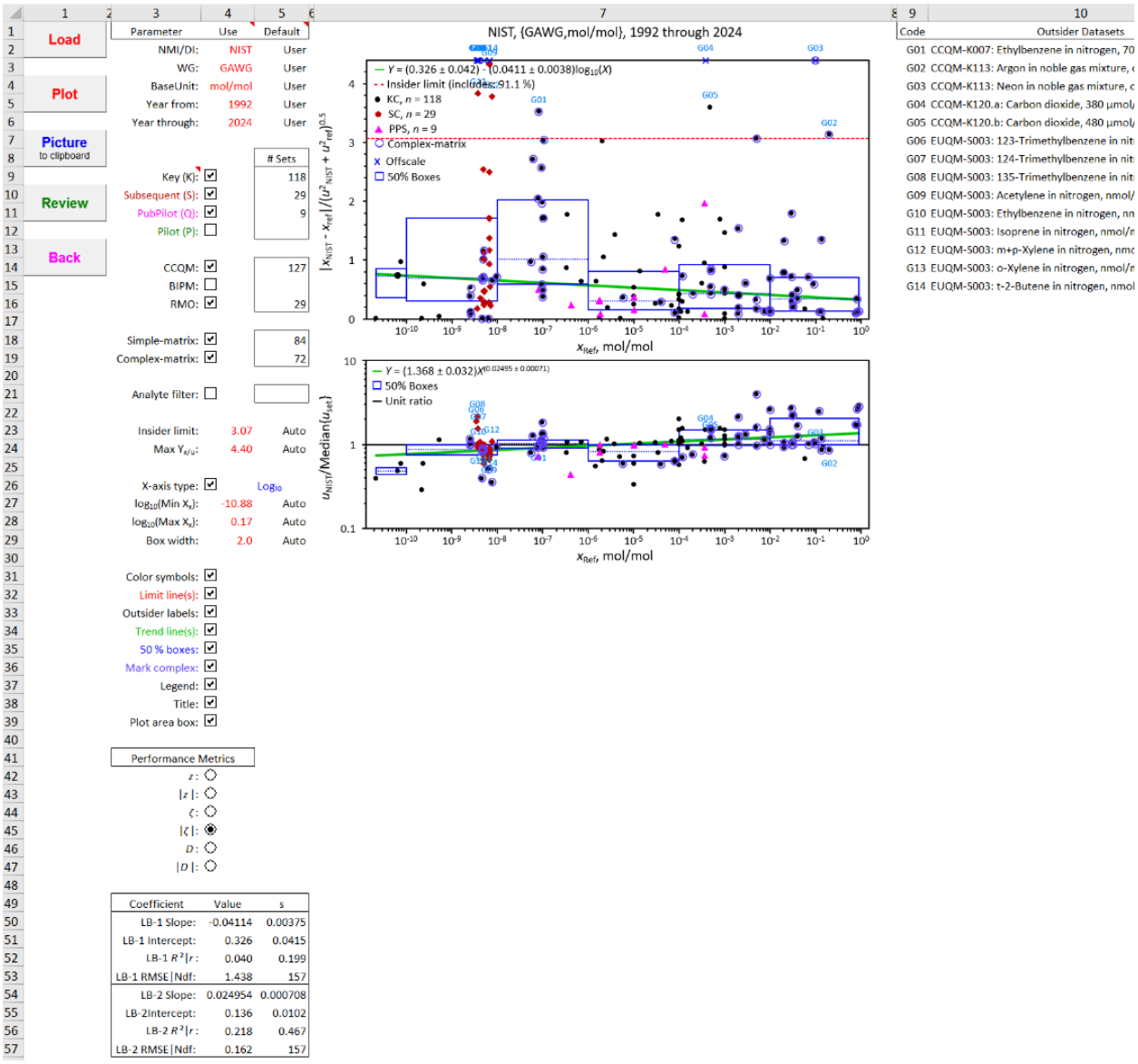


Fig. 12. *Lab_Bias* Dashboard.

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 1.10 for further information.

6.1. Charts

Each symbol in the worksheet's upper 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 study's RV. Likewise, each symbol in the lower chart (chart LB-2) represents the target's relative uncertainty plotted as a function of the study's RV.

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

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.

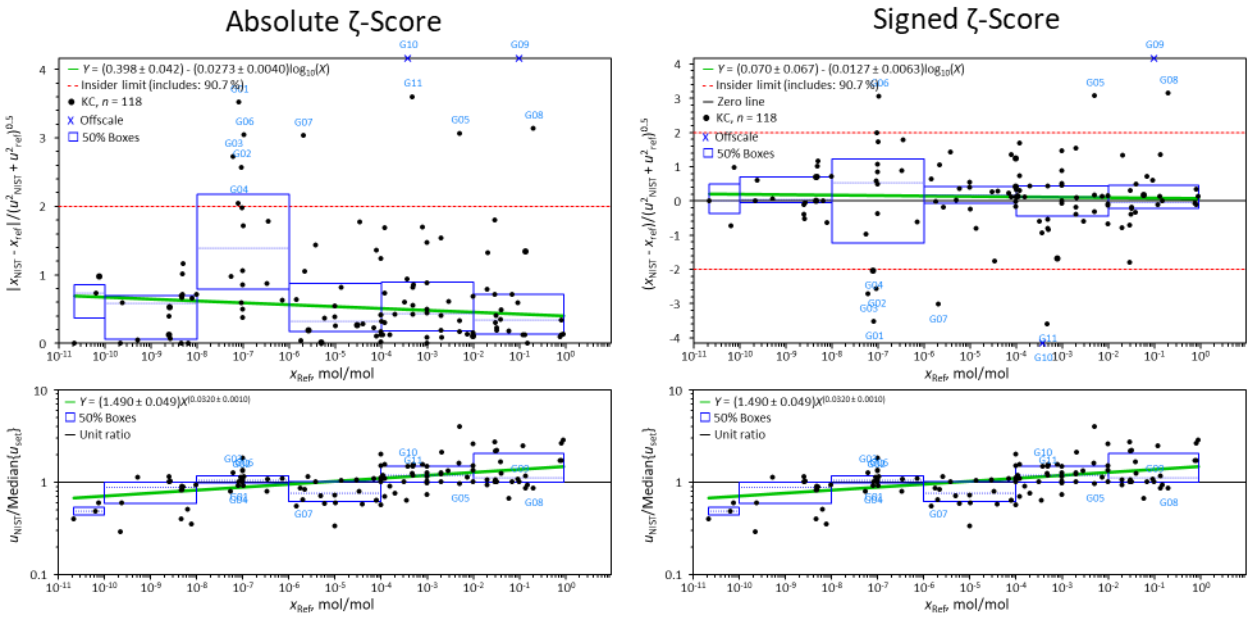


Fig. 13. *Lab_Bias* Charts with Absolute and Signed Bias Metrics.

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: Outsider 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 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*-axis (bias) in chart LB-1. 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: Type of *x*-Axis

The *Lab_Bias* worksheet contains a checkbox toggle and three chart display parameters related to the *x*-axis (reported value). When the "X-axis type:" checkbox is checked, the chart's *x*-axis is $base_{10}$ (decadic) 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 and updates the chart.

6.3.1. Log_{10} X-axis: *x*-Axis Display Limits

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

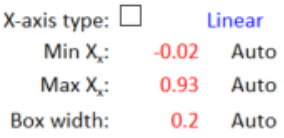
6.3.1.1. $log_{10}(Min\ X_x)$ and $log_{10}(Max\ X_x)$: *x*-Axis Display Limits

The values of the "$log_{10}(Min\ X_x)$:" and "$log_{10}(Max\ X_x)$:" parameters 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 results of the selected data. Modifying these limits does not affect what data are used 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 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 $\mathrm{INT}(\log_{10}(\mathrm{Max\ X_x}) - \log_{10}(\mathrm{Min\ X_x})) + 1$, where INT is the function "convert to integer".

6.3.2. Linear X-axis: *x*-Axis Display Limits



When the "X-axis type:" checkbox is unchecked, the *x*-axis is linear, and the three chart display parameters require linear values.

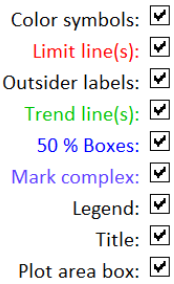
6.3.2.1. Min X_x and Max X_x: *x*-Axis Display Limits

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 results of the selected data. Modifying these limits does not affect what data are used for analysis.

6.3.2.2. Box width: 50 % Box Width

The value of the "Box width:" parameter sets the width of the 50 % boxes, specified in the units of measurement. Its default value is one-fifth of the range (Max X_x) – (Min 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.

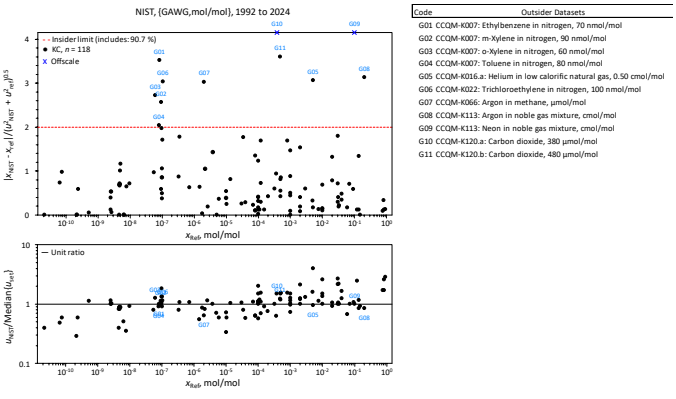
6.4.1. Color symbols

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 are 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 panel of Fig. 13). When an absolute metric is selected, there is only the one horizontal line at the Insider limit (see right panel of Fig. 13).

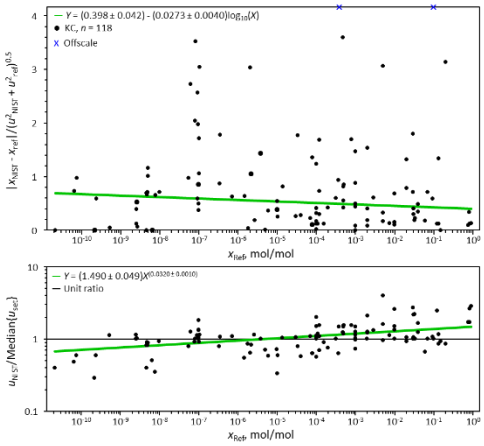
6.4.3. Outsider labels



Clicking the “Outsider labels:” checkbox toggles the display of codes used to identify the outsider datasets in both charts.

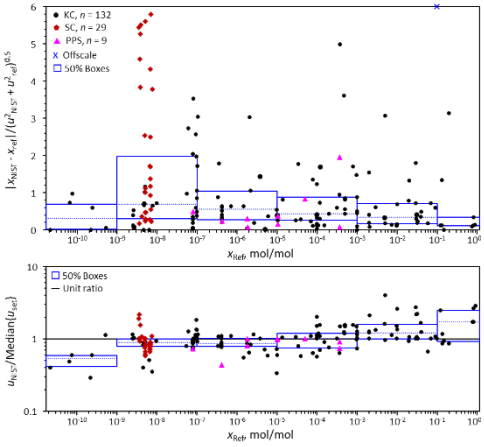
The outsider datasets are identified in the table to the right of the charts. Selecting a cell containing either the code or the dataset name and clicking the **Review** button produces a dot-and-bar chart for that dataset (Section 21).

6.4.4. Trend line(s)



Clicking the “Trend line(s):” checkbox toggles the display of robust Thiel-Sen linear trend lines [14,15] in the LB-1 and LB-2 charts.

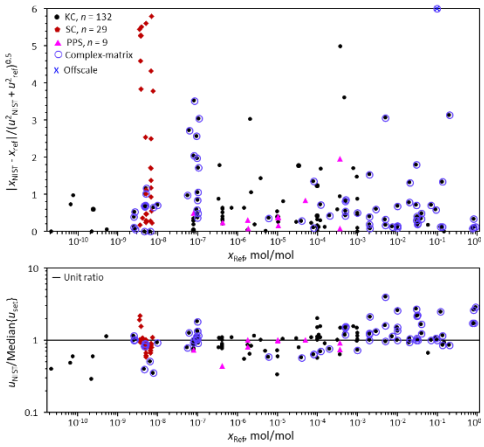
6.4.5. 50 % boxes



Clicking the “50 % boxes:” checkbox toggles the display of a series of rectangular 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:” 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 purple circle.

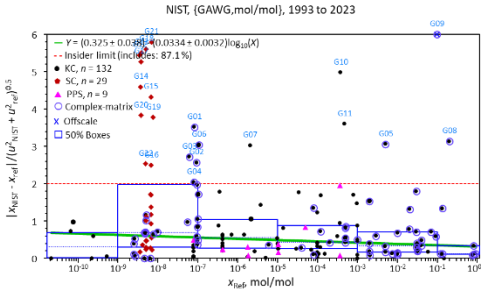


6.4.7. Legend entries

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.

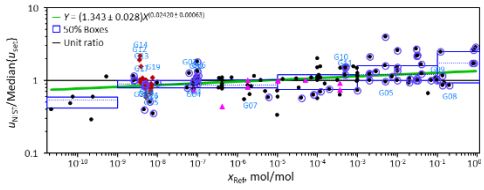
In chart LB-1:

- if “Trend line(s):” is checked the trend equation for the the bias metric as a function of value is listed.
- if “Insider limit:” is checked the percentage of results that are within the Insider limit is listed.
- if the symbols are shown colored, the number of each type of study is listed.



In chart LB-2:

- if “Trend line(s):” is checked the trend equation for the the relative uncertainty as a function of value is listed.



6.5. Stored Theil-Sen Regression Parameters

The Chart LB-1 and LB-2 trendline slopes, intercepts, Pearson correlation (R^2) of the fit, imputed correlation between the slope and intercept coefficients (r), RMSE, and number of degrees of freedom (ndf) are stored below the radio buttons. These values are generated during the analysis and are stored whether or not the trendlines are displayed.

Coefficient	Value	s
LB-1 Slope:	-0.04114	0.00375
LB-1 Intercept:	0.326	0.0415
LB-1 R^2|r:	0.040	0.199
LB-1 RMSE|Ndf:	1.438	157
LB-2 Slope:	0.024954	0.000708
LB-2Intercept:	0.136	0.0102
LB-2 R^2|r:	0.218	0.467
LB-2 RMSE|Ndf:	0.162	157

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. 14. The in-common data selection and chart display parameters and controls are discussed in Section 2.

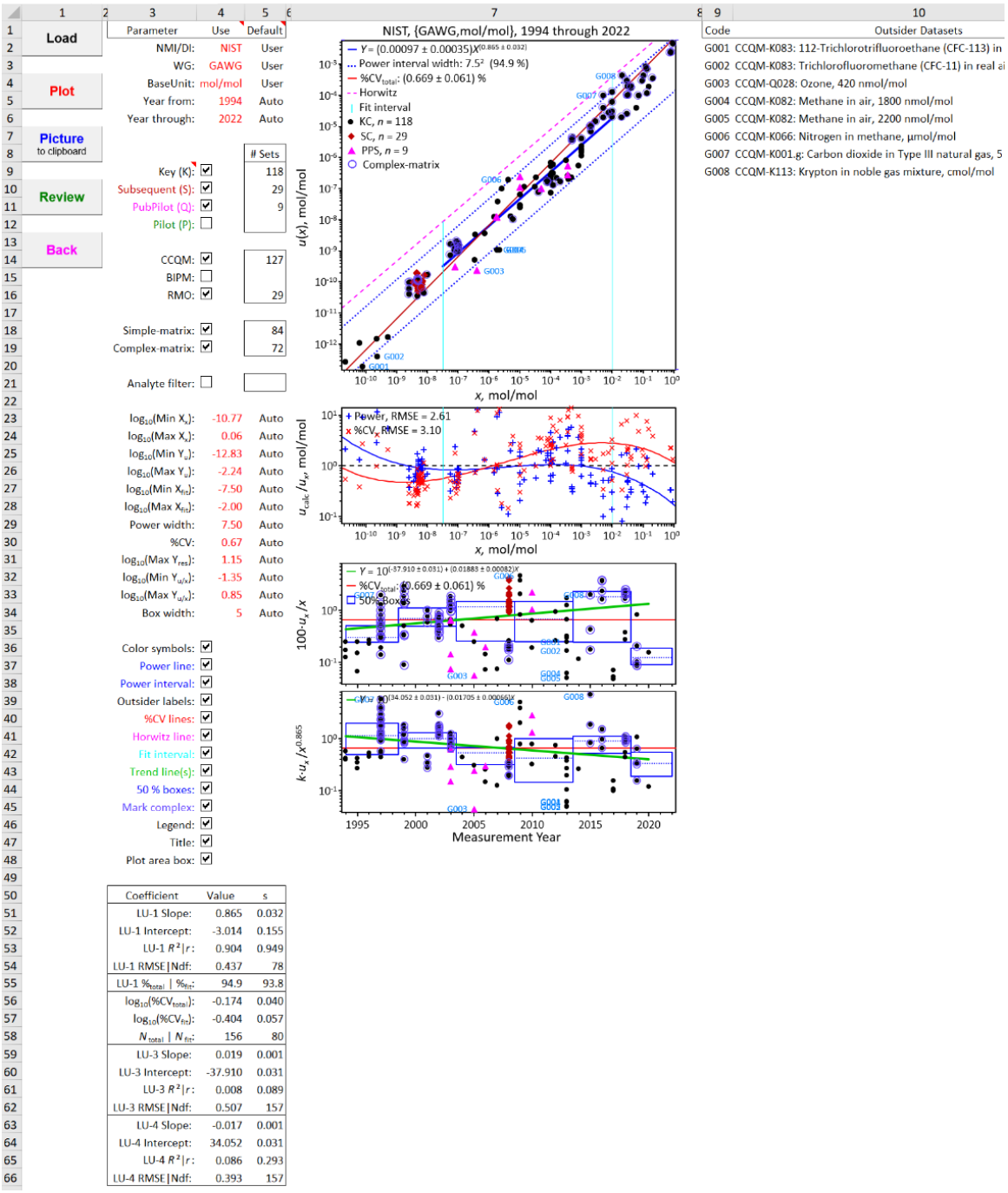


Fig. 14. *Lab_Uncertainty* Dashboard.

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 1.10 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 a measurement result in a single dataset.

The top chart (chart LU-1) displays standard uncertainty, $u(x)$, as a function of the value, x. For many of the {WG, BaseUnit} groups studied by the CCQM, the range of magnitudes is quite large; e.g., the 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 second chart (chart LU-2) displays the residuals between the reported uncertainties and predictions made using two uncertainty function models of the relationship between $u(x)$ and x [2]. The residuals are calculated as $\log_{10}\left(u_{\text{calc}}(x)\right) - \log_{10}\left(u(x)\right)$ and are plotted on a logarithmic *y*-axis labeled with the ratio formulation $u_{\text{calc}}(x)/u(x)$.

The commonly assumed constant coefficient of variation (CV)

$$u_{\text{calc}}(x) = \beta_0 x \tag{21}$$

is a one-parameter power-law function where power is 1 and β_0 is the assumed CV. The two-parameter power-law curve

$$u_{\text{calc}}(x) = \beta_0 x^{\beta_1} \tag{22}$$

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 third chart (chart LU-3) displays the relative reported uncertainty expressed as a percentage (%CV)

$$\%\text{CV} \;=\; 100 \cdot u(x)/x \tag{23}$$

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 %CV

$$\%\text{CV}^{*} \;=\; 100 \cdot u(x)/x^{\beta_1} \tag{24}$$

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, $u(x)/x^{\beta_1}$ 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.

$\log_{10}$(Min X_x):	-12.00	Auto
$\log_{10}$(Max X_x):	1.00	Auto
$\log_{10}$(Min Y_u):	-13.00	Auto
$\log_{10}$(Max Y_u):	0.00	Auto
$\log_{10}$(Min X_{fit}):	-8.12	Auto
$\log_{10}$(Max X_{fit}):	-2.00	Auto
Power width:	4.00	Auto
%CV:	0.50	Auto
$\log_{10}$(Max Y_{res}):	2.00	Auto
$\log_{10}$(Min $Y_{u/x}$):	-2.00	Auto
$\log_{10}$(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):" parameters set the minimum and maximum limits for the *x*-axis (reported 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 used 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 uncertainties) in chart LU-1. The default values for these limits are the $\log_{10}$-transformed minimum and maximum $u(x)$ values. Modifying the limits of either axis does not affect what data are used for analysis.

7.2.3. $\log_{10}$(Min X_{fit}) and $\log_{10}$(Max X_{fit}): *x*-Axis Regression Limits

For some {WG, BaseUnit} 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* used to estimate the power-law curve of $u(x)$ as a function of x. The default values, taken from [16], are -7.5 (a fractional value of ≈3.2 ×10-8) and -2.0 (a fractional value of 0.01).

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: Outsider Identification Interval

One of 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: $\log_{10}\big(u(x)\big) = \log_{10}(\beta_0) + \beta_1 \log_{10}(x)$. The "Power width:" parameter defines a symmetric interval centered on the power-law curve that 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 w of the value predicted by the power-law; i.e., the interval includes the observed $\{x, u(x)\}$ values from$(\beta_0/w)x^{\beta_1}$ to $(\beta_0 \cdot w)x^{\beta_1}$. 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

The "%CV:" parameter defines a robust coefficient of variation (%CV, relative standard deviation expressed as a percentage) characteristic of the selected data. The %CV can be visualized as a line in chart LU-1 and (in derivede form) the other charts. The default value for %CV is 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 used 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 *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 used 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 7.3.6. The default interval is five years.

7.3. Additional Chart Display Checkboxes

The *Lab_Uncertainty* worksheet contains ten 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. 15. 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.

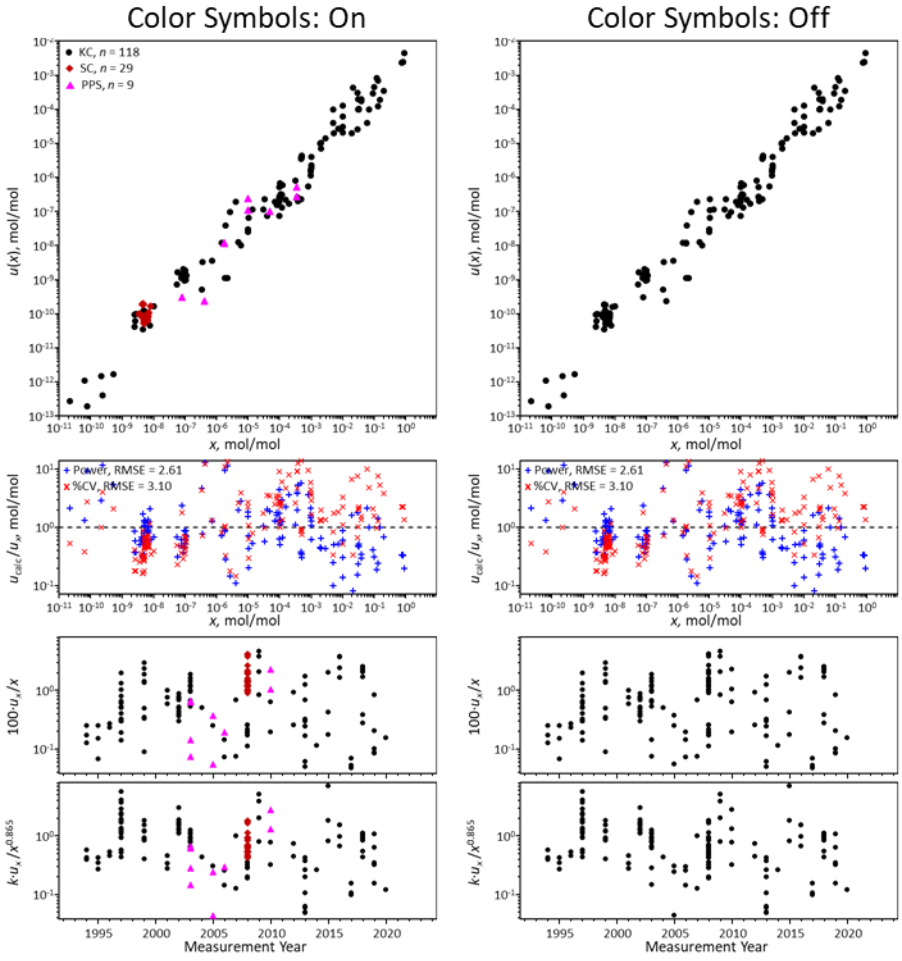
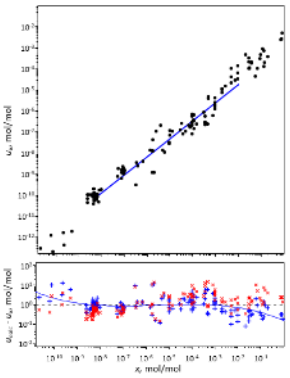


Fig. 15. *Lab_Uncertainty* Charts With Color-Coded and All-Black Symbols.

7.3.2. Power line

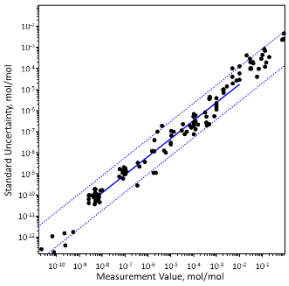


In chart LU-1, clicking the "Power line:" checkbox toggles the display of a regression estimate of the power-law: $u(x) = \beta_0\, x^{\beta_1}$. Since both the *x*- and *y*-axes are logarithmic, this is parameterized as the linear function: $\log_{10}(u(x)) = \log_{10}(\beta_0) + \beta_1 \cdot \log_{10}(x)$.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

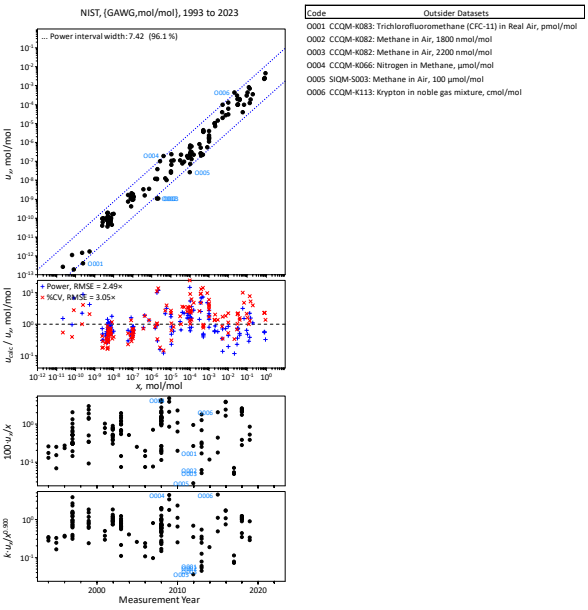
In both chart LU-1 and LU-2, the power-law-derived relationships are displayed as solid blue lines. Charts LU-3 and LU-4 are not affected by this control.

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 $\log_{10}$(Min X_x) to $\log_{10}$(Max X_x) chart display range (Section 7.2.1).

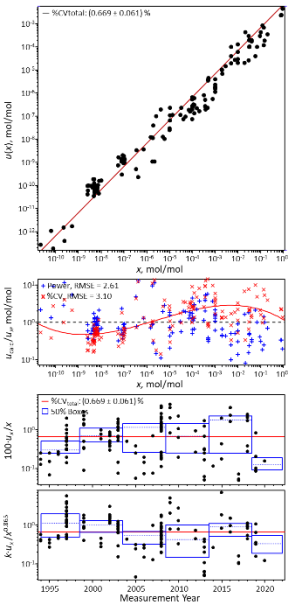
7.3.4. Outsider labels



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 21).

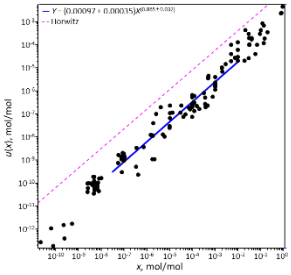
7.3.5. %CV lines



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.

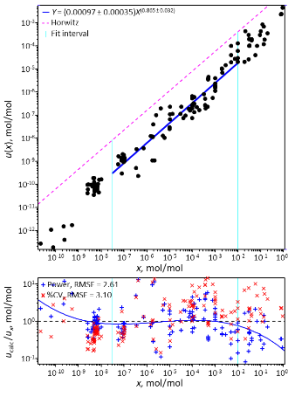
The %CV value is specified by the "%CV:" parameter described in Section 7.2.5.

7.3.6. Horwitz line



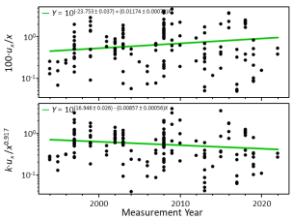
Clicking the "Horwitz line:" checkbox toggles chart LU-1's display of the Horwitz relationship between reproducibility and analyte concentration [3]. The relationship, shown as a dashed magenta line, is a power-law with coefficients $\beta_0 = 0.02$ and $\beta_1 = 0.8495$. These values are derived from 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. Fit interval



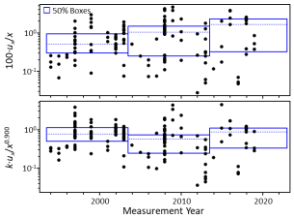
Clicking the "Fit interval:" checkbox toggles display of lines that bound the regression interval, $\log_{10}(\text{Min } X_{fit})$ to $\log_{10}(\text{Max } X_{fit})$, in chart LU-1 and LU-2. Only the $\{x,u(x)\}$ pairs within this interval are used to estimate the power function. To emphasize the interval's Horwitz function origin, in chart LU-1 the upper end of the bounding lines terminate on the Horwitz line.

7.3.8. Trend line(s)



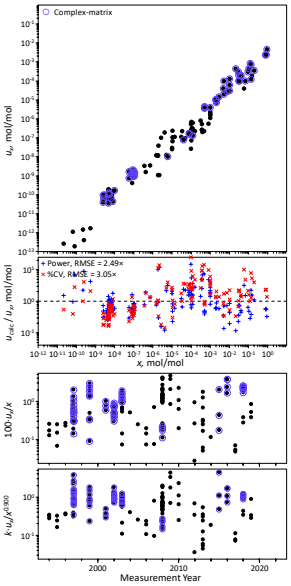
Clicking the "Trend line(s):" checkbox toggles the display of robust Thiel-Sen linear trend lines [14,15] in the LU-3 and LU-4 charts. The regession uses all results displayed in each chart.

7.3.9. 50% Boxes



For charts LU-3 and LU-4, clicking the “50 % boxes:” checkbox toggles the display of a series of rectangular boxes at intervals along the *x*-axis (measurement year). 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).

7.3.10. Mark complex

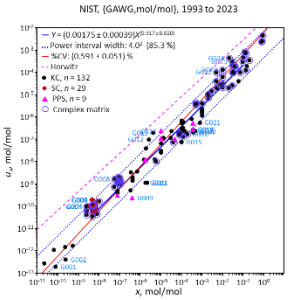


In charts LU-1, LU-3 and LU-4 clicking the “Mark complex:” checkbox toggles the identification of results for complex-matrix materials. This option is only relevant when simple-matrix and complex-matrix datasets are analyzed together. Complex-matrix datasets are identified with a surrounding purple circle.

7.3.11. Legend Entries

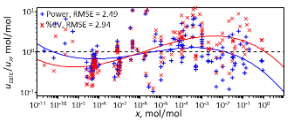
As described in Section 2.2.3.1, clicking the “Legend:” checkbox toggles the display of the legend. The optional features have a legend entry when (and only when) active. In addition to identifying the graphical elements, some of the entries provide quantitative information.

In Chart LU-1:



- if “Power line:” is checked the power-law equation is listed.
- if “Power interval:” is checked the multiplicative width and the percent of the $\{x, u(x)\}$ values within the lines are listed.
- if “%CV:” is checked the median of the $100 \cdot u(x)/x$ values is listed.
- if the symbols are shown colored, the number of each type of study is listed.

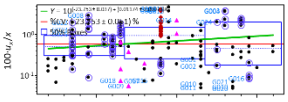
In chart LU-2:



- the RMSE of the power and %CV uncertainty function residuals are displayed. The RMSE is defined as $\sqrt{(\sum_1^n d_i^2)/(n-m)}$,

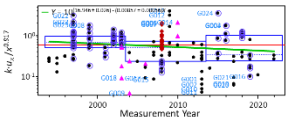
where d_i is the residual for one $\{x, u(x)\}$, n is the number of $\{x, u(x)\}$, and m is the number of parameters in the uncertainty function. For the power-law, m is 2; for %CV, m is 1.

In chart LU-3:



- if "Trend line(s):" is checked the trend equation of $100 \cdot u(x)/x$ over time is listed.
- if "%CV:" is checked the median of the $100 \cdot u(x)/x$ values is listed.

In chart LU-4:



- if "Trend line(s):" is checked the power-law-adjusted linear trend equation of $100 \cdot u(x)/x$ over time is listed.

Coefficient	Value	s
LU-1 Slope:	0.865	0.032
LU-1 Intercept:	-3.014	0.155
LU-1 R^2|r:	0.904	0.949
LU-1 RMSE|Ndf:	0.437	78
LU-1 $\%_{total}$ | $\%_{fit}$:	94.9	93.8
$\log_{10}(\%CV_{total})$:	-0.174	0.040
$\log_{10}(\%CV_{fit})$:	-0.404	0.057
N_{total} | N_{fit}:	156	80
LU-3 Slope:	0.019	0.001
LU-3 Intercept:	-37.910	0.031
LU-3 R^2|r:	0.008	0.089
LU-3 RMSE|Ndf:	0.507	157
LU-4 Slope:	-0.017	0.001
LU-4 Intercept:	34.052	0.031
LU-4 R^2|r:	0.086	0.293
LU-4 RMSE|Ndf:	0.393	157

7.4. Stored Coefficients

The first four lines of the coefficient storage block store the regression coefficients and fit statistics for the Chart LU-1 power function provided by the Excel LINEST function:

- slope and its standard error.
- intercept and its standard error.
- square of the Pearson correlation (R^2) of the fit and the imputed correlation between the slope and intercept (r).
- root-mean square error residual (RMSE) and number of degrees of freedom (ndf).

The fifth line stores the percent of all results that fall within the Chart LU-1 power interval ($\%_{total}$) and the percent of results within the region bounded by the power interval and the regression fit interval ($\%_{fit}$).

The sixth through eighth lines store values related to the coefficient of variation (%CV) that is used (one way or another) in all four charts:

- median and $Q_n/\sqrt{N_{\text{total}}}$ of $\log_{10}(100 \cdot u(x)/x)$ for all N_{total} results displayed.
- median and $Q_n/\sqrt{N_{\text{fit}}}$ of $\log_{10}(100 \cdot u(x)/x)$ for all N_{fit} results that are within the Horwitz regression interval, $\log_{10}(\text{Min X}_{\text{fit}})$ to $\log_{10}(\text{Max X}_{\text{fit}})$. These values are not used by the current *CCQM_Retrospectoscope* system.
- N_{total} and N_{fit}. Note: N_{fit}.should be equal to two more than the regression ndf.

The ninth through twelfth lines store the Chart LU-3 trendline slopes, intercepts, R^2, r, RMSE, and ndf. The last four lines store these parameters for Chart LU-4.

These values are stored below the radio buttons. They are generated during the analysis and are stored whether or not the graphical elements they relate to are displayed.

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. 16.

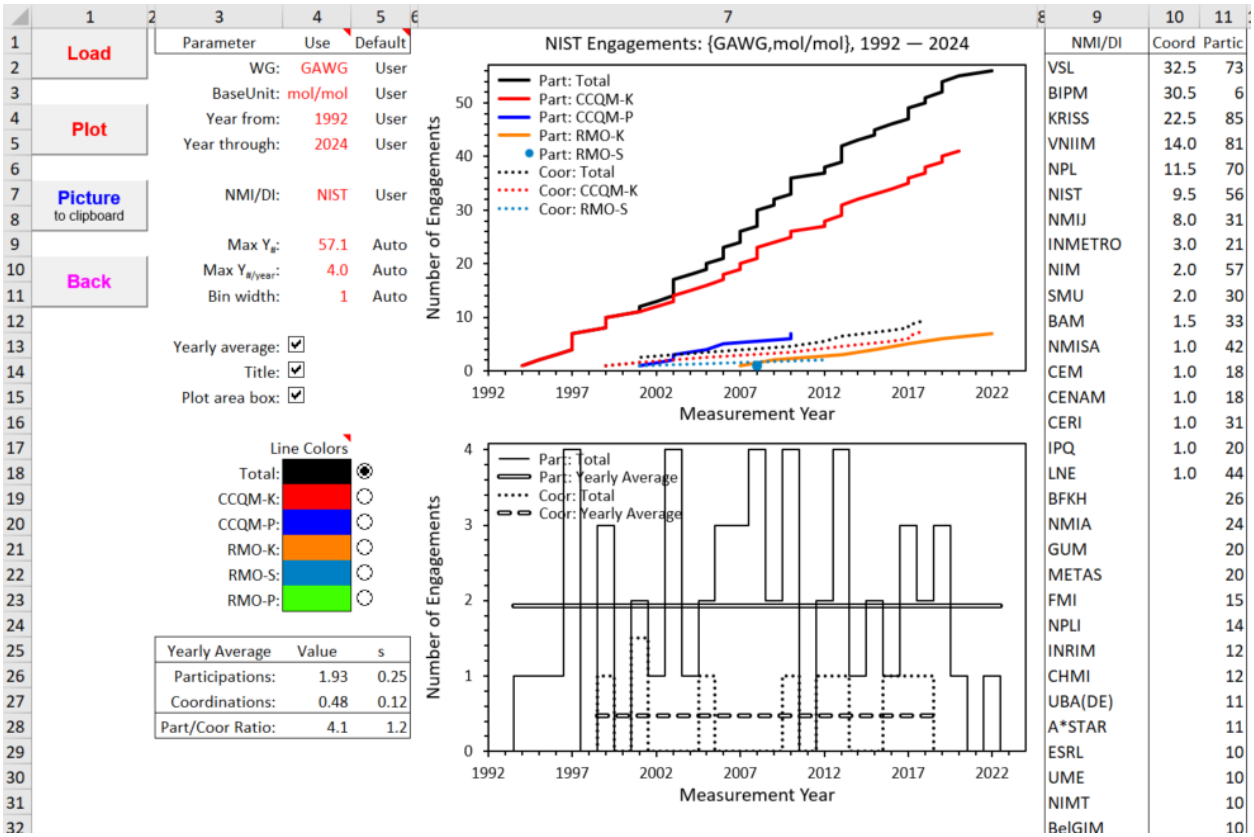


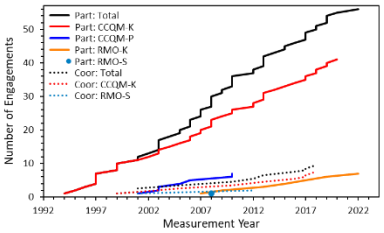
Fig. 16. *Lab_Engagements* Dashboard.

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 1.10 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 focused on just the target NMI/DI.

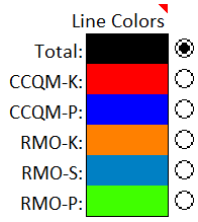
The worksheet's top chart (chart LE-1) displays cumulative distributions for the target NMI/DI's CCQM- and RMO-sponsored engagements. There are twelve possible distributional classes:



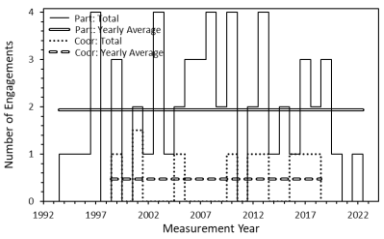
- Part: Total, the total number of participations.
- Part: CCQM-K, the number of CCQM-sponsored KCs.
- Part: CCQM-P, the number of CCQM-sponsored PPSs (and PSs, if in database).
- Part: RMO-K, the number of RMO-sponsored KCs, including the BIPM-sponsored continuous KCs.
- Part: RMO-S, the number of RMO-sponsored 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, including the BIPM-sponsored continuous 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* 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 [17].

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 **BaseUnit** parameters. If a particular **WG** is specified, setting **BaseUnit** 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.

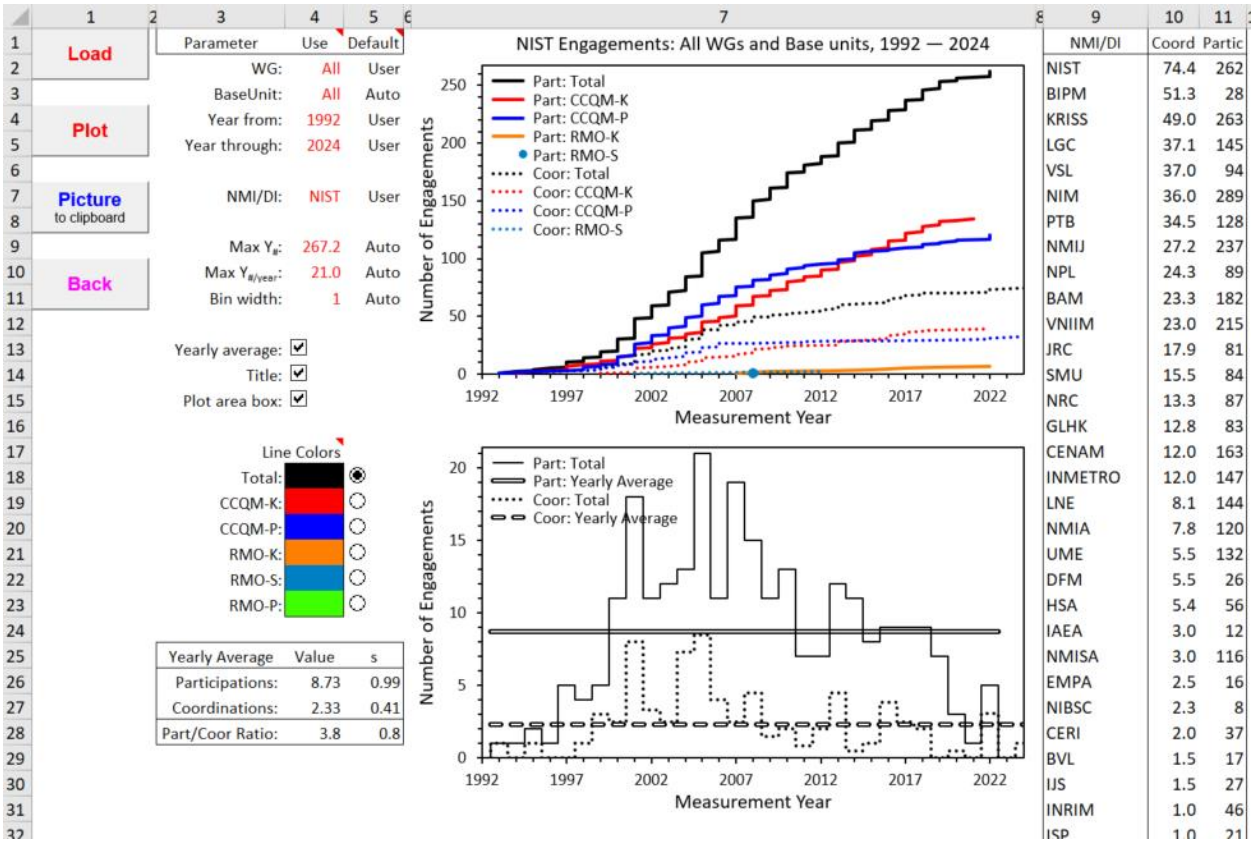


Fig. 17. *Lab_Engagements* Dashboard With WG and BaseUnit Set to *All*.

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 in and/or coordinated at least one study.

8.4. Chart Display Parameters

Max $Y_{\#}$: 267.2 Auto
Max $Y_{\#/year}$: 21.0 Auto
Bin width: 1 Auto

The *Lab_Engagements* worksheet contains three chart display parameters. The first pertains 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 through: *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, BaseUnits}, the "Year from:" value can be set to a value earlier than the earliest of the studies (but not earlier than 1992) and "Year through:" can be set to a value later than the most recent of the studies (but not later than the current year). Note: 1993 is the measurement year of the earliest CCQM study, now attributed to the IAWG.

8.4.2. Max $Y_{\#}$: *y*-Axis Maximum for Chart LE-1

By default, the maximum *y*-axis (number of engagements) 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, BaseUnits}, the value of the "Max $Y_{\#}$:" parameter enables setting the maximum to a specified value. Changing the maximum does not affect what data are used 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, BaseUnits}, 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. 18.

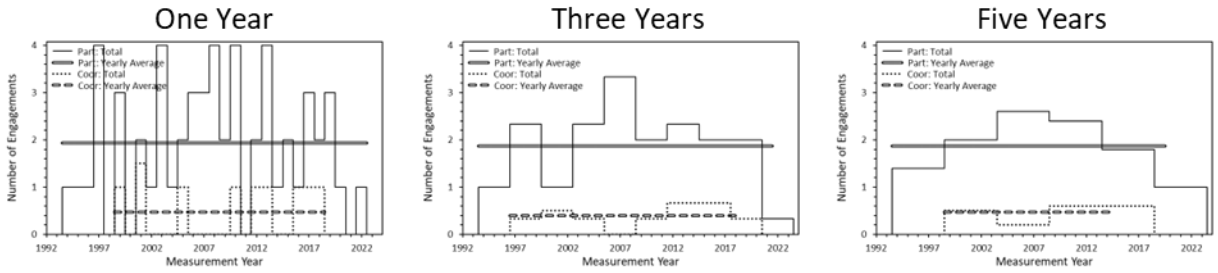
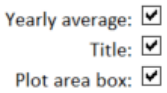


Fig. 18. *Lab_Engagement* Histograms With Different Bin Widths.

8.5. Additional Chart Display Checkbox

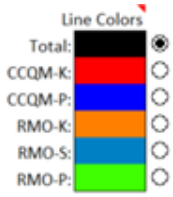
The *Lab_Engagements* worksheet contains one chart display checkbox in addition to two discussed in Section 2.2.3. The worksheet also contains a series of radio buttons. Clicking a chart display checkbox or radio button invokes an immediate change in the chart display.



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. 19. 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).

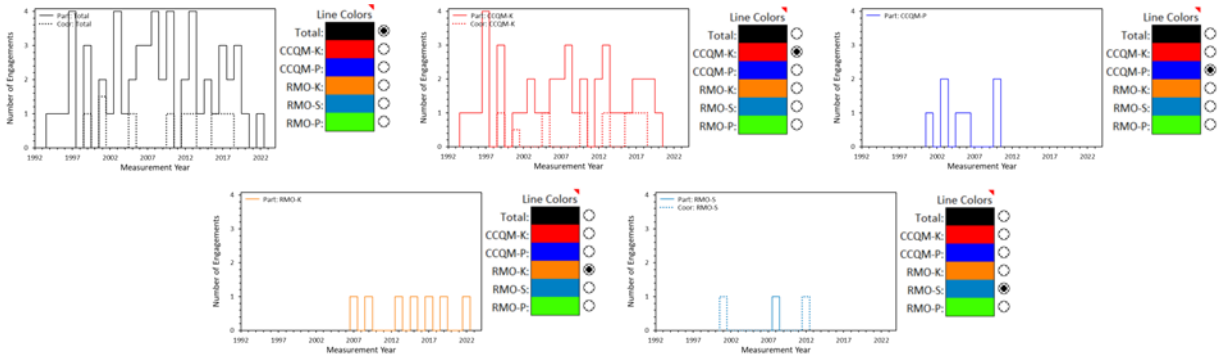


Fig. 19. *Lab_Engagements* Histogram Classes.

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. 20.

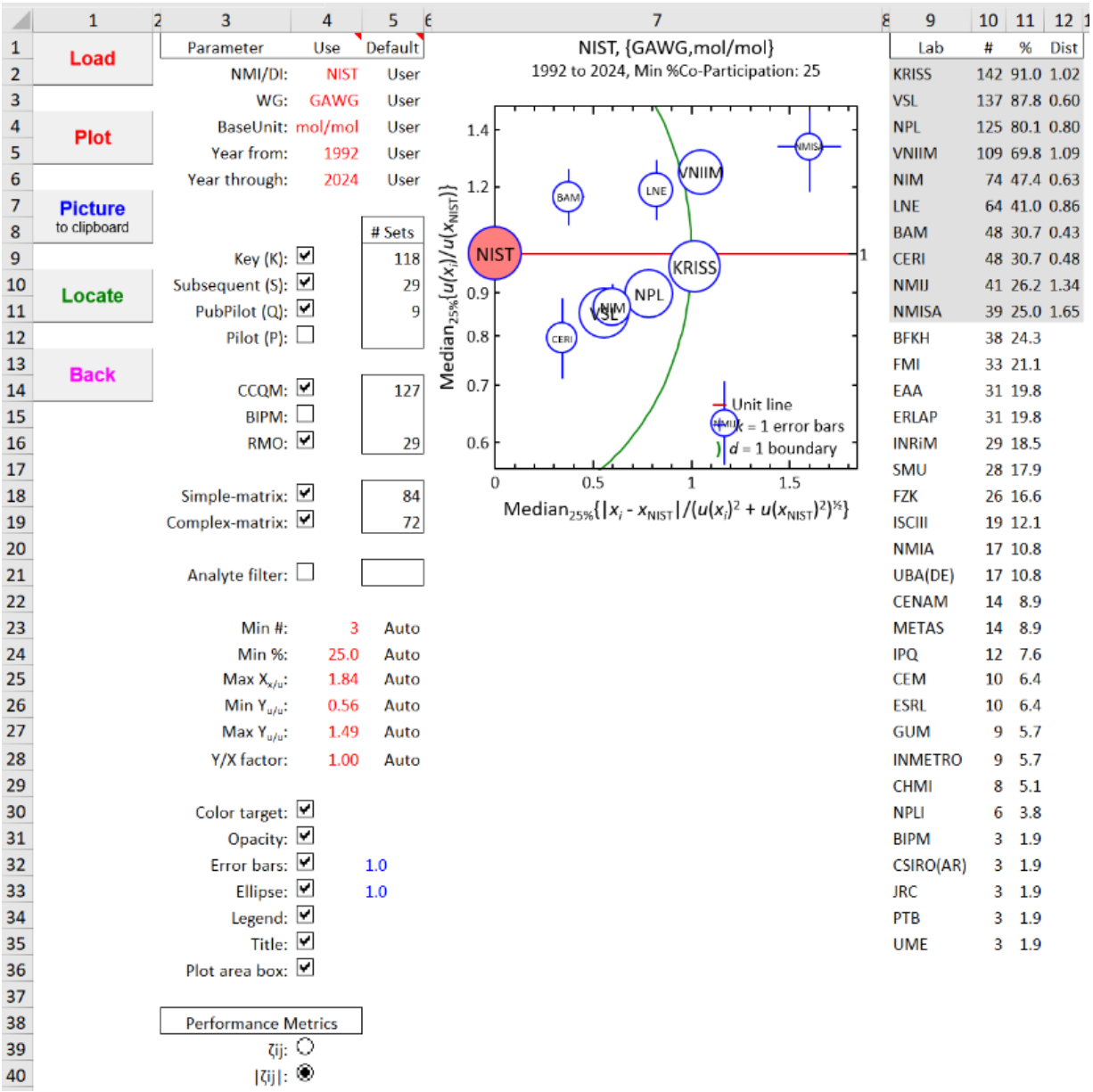


Fig. 20. *Peer_Bilateral* Dashboard.

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 1.10 for further information.

9.1. Chart

The location of each open circle symbol represents the median ratio of the uncertainty reported by a 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. Different co-participants need not share the same datasets.

The symbol for the target NMI/DI is always 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. 21). For the signed difference, it will be in the center (see right panel of Fig. 21).

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: see Fig. 21.

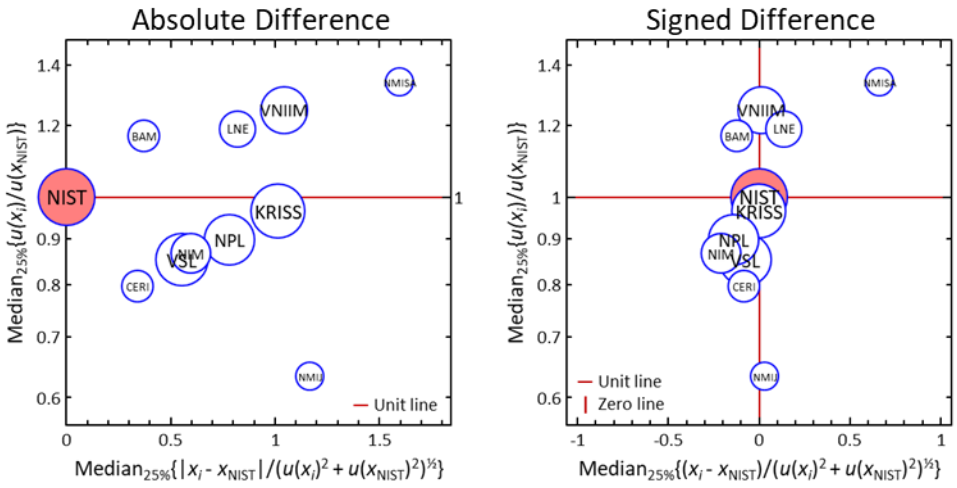


Fig. 21. *Peer_Bilateral* Chart With Absolute and Signed Difference Metrics.

9.2. Chart Display Parameters

The *Peer_Bilateral* worksheet contains six 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 $X_{u/u}$:	1.15	Auto
Min $Y_{u/u}$:	0.71	Auto
Max $Y_{u/u}$:	1.33	Auto
Y/X factor:	1.00	Auto

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 co-participant for differences to be calculated. The number of co-participations is listed in the **#** column (10) of the table to the right of the chart (see Fig. 20). The default 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 the **%** 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. 20). The default value is (an arbitrary) 30 %.

9.2.3. Max $X_{x/u}$: *x*-Axis Limits

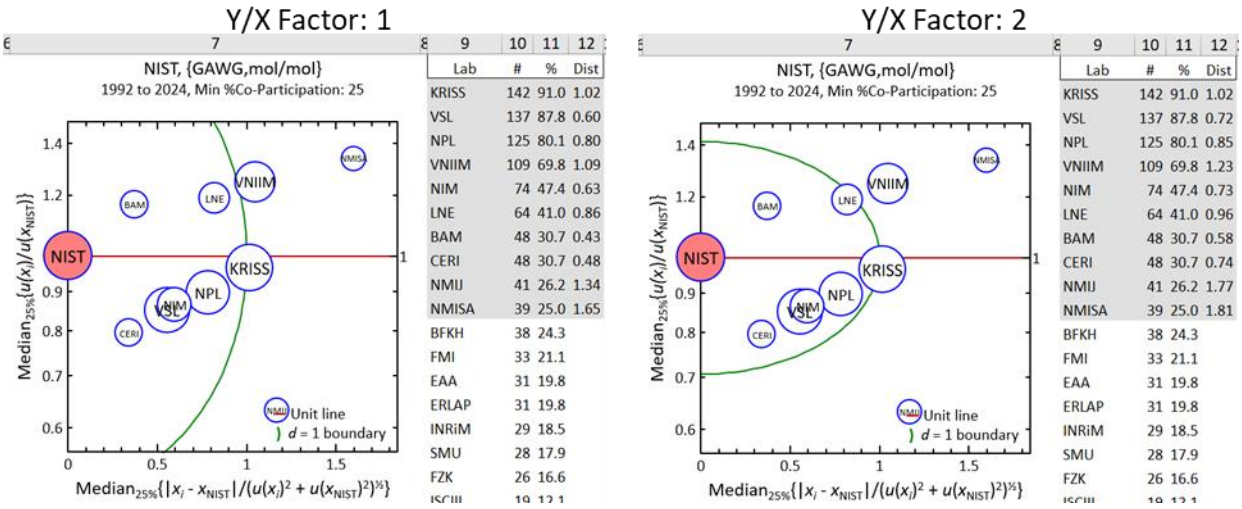
The value of the "Max $X_{x/u}$:" parameter sets the display range of the *x*-axis (difference) of the chart. Its default value is set by the extreme value of the display symbols including their error bars. When the signed difference metric is selected, the range is set to be symmetric about zero.

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 *y*-axis (uncertainty ratio). The default values are set by the extreme values of the displayed symbols including their error bars.

9.2.5. Y/X factor: *y*-Axis Scale Factor

The value of the "Y/X factor:" parameter sets the importance of the *y*-axis (uncertainty ratio) relative to the *x*-axis (difference) for estimating the similarity distance between the target NMI/DI and its co-participants. The default value is 1, which gives equal weight to a factor-of-two relative uncertainty ratio and a unit difference in the uncertainty-scaled difference. The estimated distances are listed in the **Dist** column (12) of the table to the right of the chart: see Fig. 22.



Lab	#	%	Dist
KRISS	142	91.0	1.02
VSL	137	87.8	0.60
NPL	125	80.1	0.80
VNIIM	109	69.8	1.09
NIM	74	47.4	0.63
LNE	64	41.0	0.86
BAM	48	30.7	0.43
CERI	48	30.7	0.48
NMIJ	41	26.2	1.34
NMISA	39	25.0	1.65
BFKH	38	24.3	
FMI	33	21.1	
EAA	31	19.8	
ERLAP	31	19.8	
INRiM	29	18.5	
SMU	28	17.9	
FZK	26	16.6	

Lab	#	%	Dist
KRISS	142	91.0	1.02
VSL	137	87.8	0.72
NPL	125	80.1	0.85
VNIIM	109	69.8	1.23
NIM	74	47.4	0.73
LNE	64	41.0	0.96
BAM	48	30.7	0.58
CERI	48	30.7	0.74
NMIJ	41	26.2	1.77
NMISA	39	25.0	1.81
BFKH	38	24.3	
FMI	33	21.1	
EAA	31	19.8	
ERLAP	31	19.8	
INRiM	29	18.5	
SMU	28	17.9	
FZK	26	16.6	

Fig. 22. *Peer_Bilateral* Chart With Different Y/X Factors.

When the Boundary ellipse (Section 9.3.4) is active, the value of "Y/X factor:" affects the ellipse shape. The ellipse is intended to help visualize the relative influence of the difference- and uncertainty metrics on the estimated distances.

Note: For a given *x*-axis maximum (Max $X_{x/u}$), the signed difference metric, ζ_{ij}, has an *x*-axis span twice that of the absolute difference metric, $|\zeta_{ij}|$. The *apparent* shape of the ellipse therefore changes when switching between the difference metrics, but the coverage remains the same. Of course, changing the difference metric can radically change the co-participant similarity distances. The net differences are illustrated in Fig. 23 for two values of the "Y/X factor:" parameter, using expanded *x*- and *y*-axis spans to facilitate comparisons.

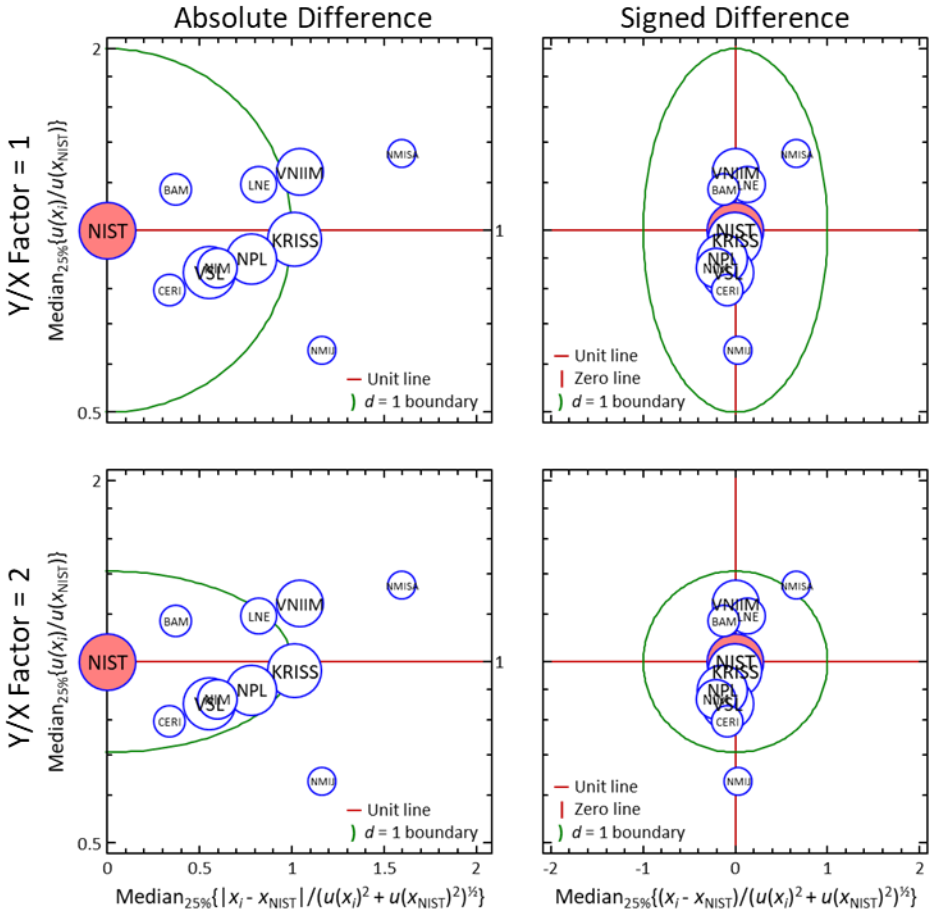


Fig. 23. *Peer_Bilateral* Interaction Between Difference Metric, Y/X Factor, and Ellipse.

9.3. Additional Chart Display Checkboxes

The *Peer_Bilateral* worksheet contains four 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 "Color target:" checkbox toggles the display of the target NMI/DI's symbol from opaque rose to opaque white: see Fig. 24.

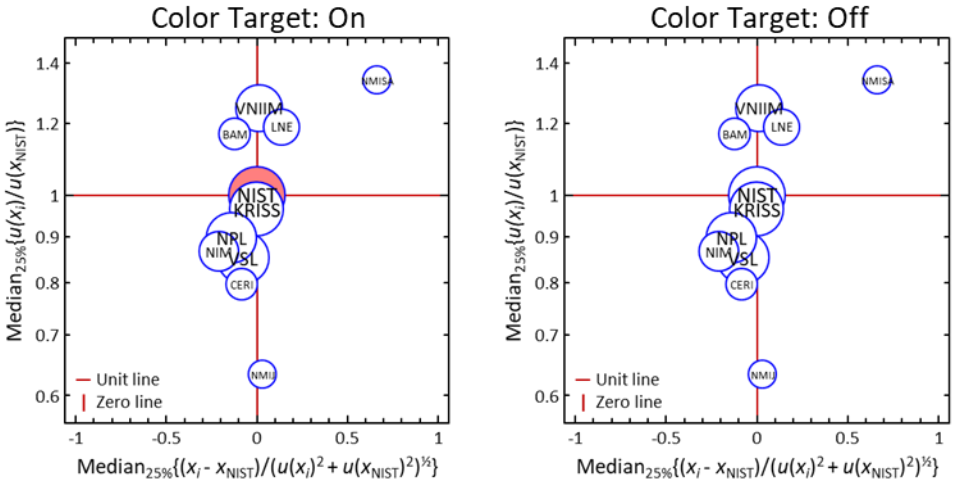


Fig. 24. *Peer_Bilateral* Chart With and Without Target Color.

9.3.2. Opacity

Clicking the "Opacity:" checkbox toggles the display of the symbols used for the co-participants from opaque to transparent: see Fig. 25. This can be useful for visualizing a co-participant's relationship to the target NMI/DI when its symbol is buried beneath others.

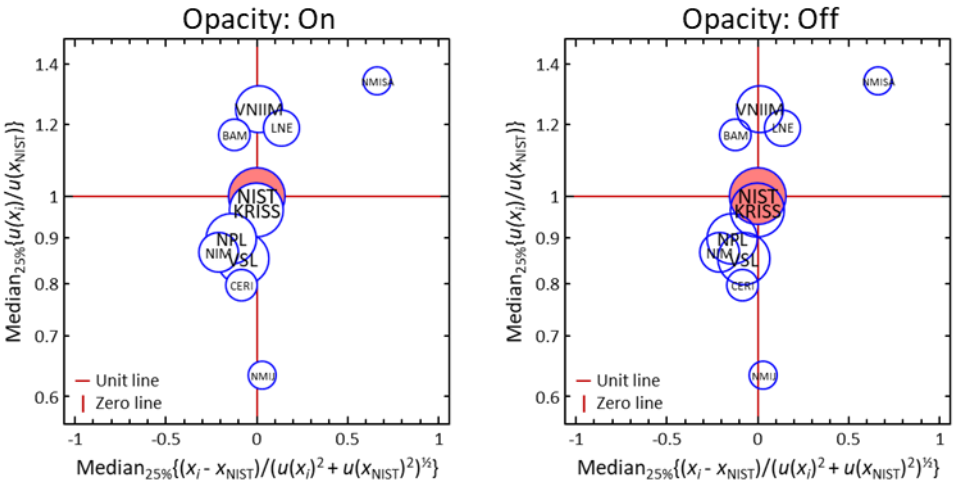


Fig. 25. *Peer_Bilateral* Chart With and Without Symbol Opacity.

9.3.3. Error bars

Clicking the “Error bars:” checkbox toggles the display of the error bars. The error bars span ±(one standard deviation of the mean)×(scale factor) 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 scale factor is a non-negative numeric value between 1 and 6 in cell(32,5) – i.e., the “Error bars:” row and the **Default** parameter column.

The display regions of the difference (*X*) and uncertainty ratio (*Y*) axes are defined by the maximum intervals required to display all the error bars at their specified expansion. These limits are set whether or not the error bars are displayed: see Fig. 26.

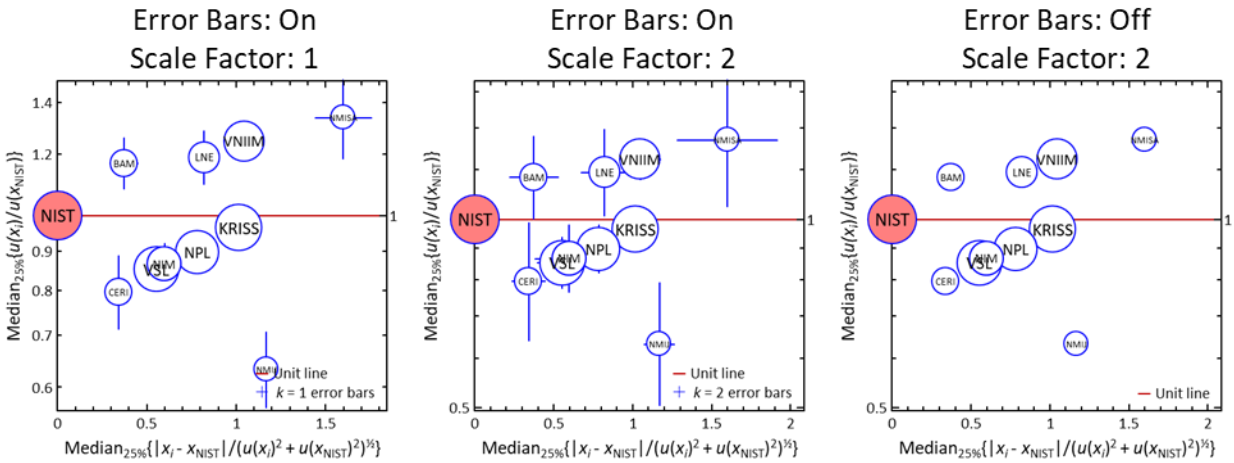


Fig. 26. *Peer_Bilateral* Chart With and Without Error Bars.

Clicking the “Error bars:” checkbox immediately toggles whether the error bars are displayed. However, changing the scale factor has no effect until the **Plot** command button is clicked.

9.3.4. Ellipse

Clicking the “Ellipse:” checkbox toggles the display of an ellipse centered on the target NMI/DI symbol. The ellipse provides a visual similarity distance boundary (proportional to the **Dist** values in column 12) around the target NMI/DI: see Fig. 27.

The size of the ellipse is controlled by the scale factor, a non-negative numeric value between 0.1 and 10 in cell(33,5) – i.e., the “Ellipse:” row and the **Default** parameter column. The default scale factor is 1. The scale factor has no effect on the estimated similarity distances.

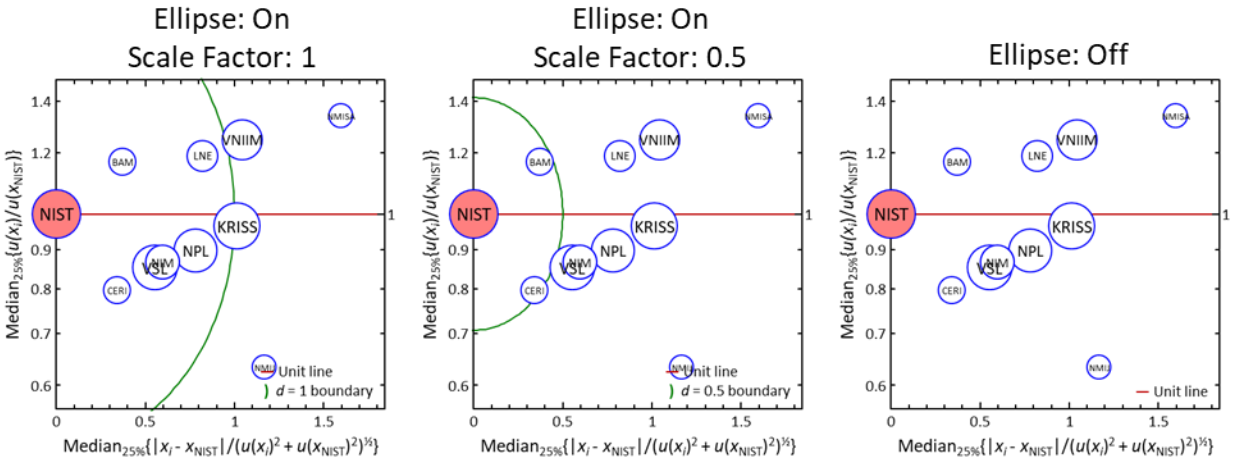


Fig. 27. *Peer_Bilateral* Chart With and Without Ellipse.

Clicking the “Ellipse:” checkbox immediately toggles whether the ellipse is displayed. However, changing the “Ellipse:” scale factor has no effect until the **Plot** command button is clicked.

10. Peer_Unilateral Subsystem

The *Peer_Unilateral* charts, the controls used to specify the datasets evaluated, and the controls used to modify what the charts display are pictured in Fig. 28.

While sharing many of the *Peer_Bilateral* subsystem's features, the performance metrics are estimated relative to the dataset RVs and thus estimate expected measurement accuracy rather than NMI/DI similarity. However, the estimates are calculated using just datasets that contain results reported by the target NMI/DI and that meet all the selection criteria.

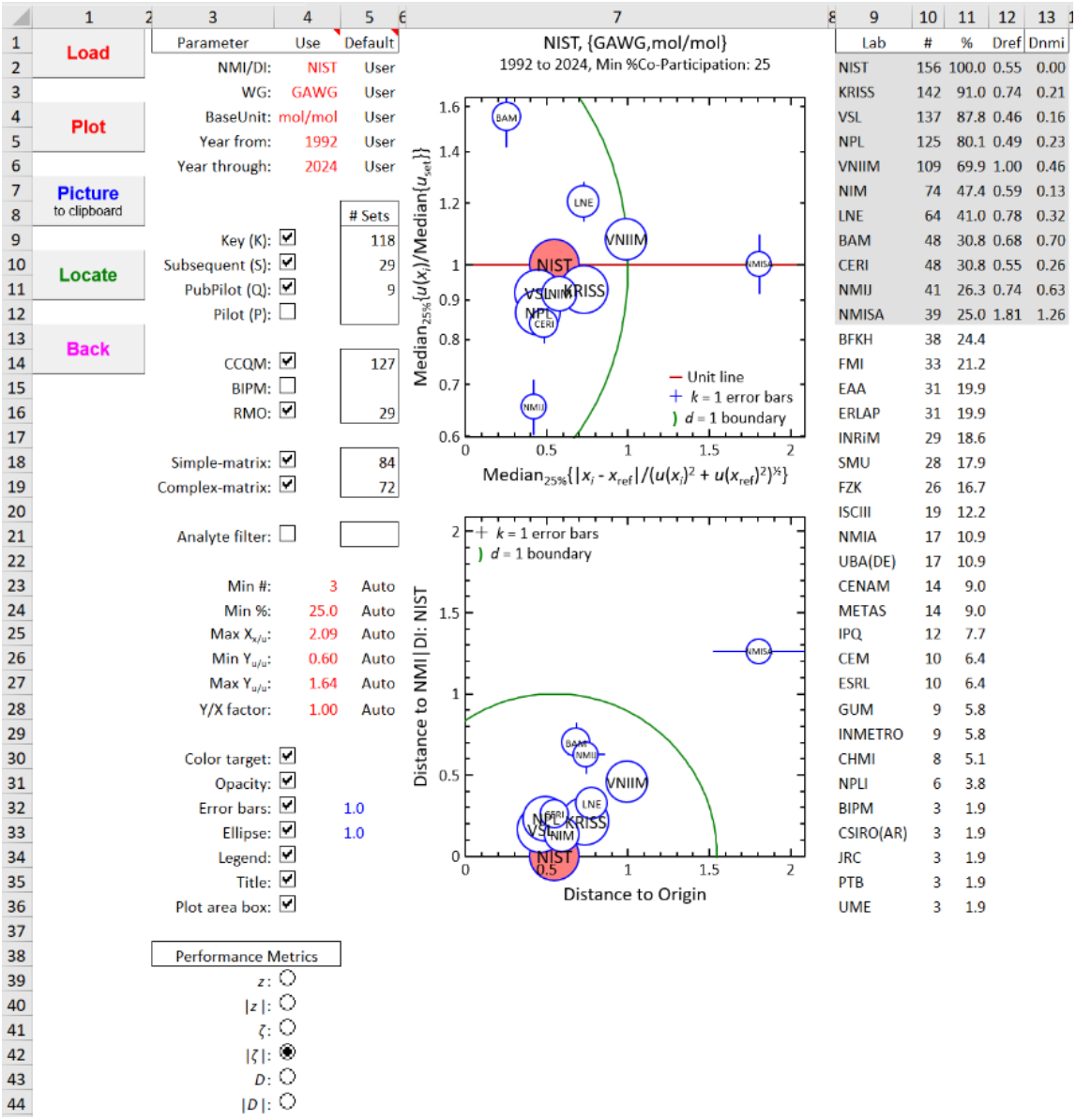


Fig. 28. *Peer_Unilateral* Dashboard.

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 1.10 for further information.

10.1. Charts

The *Peer_Unilateral* worksheet provides two charts that display relationships between the results reported by a target NMI/DI and the target's co-participants. Co-participants need not share the same datasets. The area of each circle in the charts is proportional to the number of datasets shared with the target NMI/DI.

The position of each symbol in the upper chart (chart PU-1) 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 1.9.1). As with the *Peer_Bilateral* analysis, the closer a co-participant's symbol is to the target's, the more similar their measurement results. In contrast to *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 in chart PU-1 is *not* constrained to be at the chart's {0,1} origin: compare the top two panels of Fig. 29 with Fig. 21.

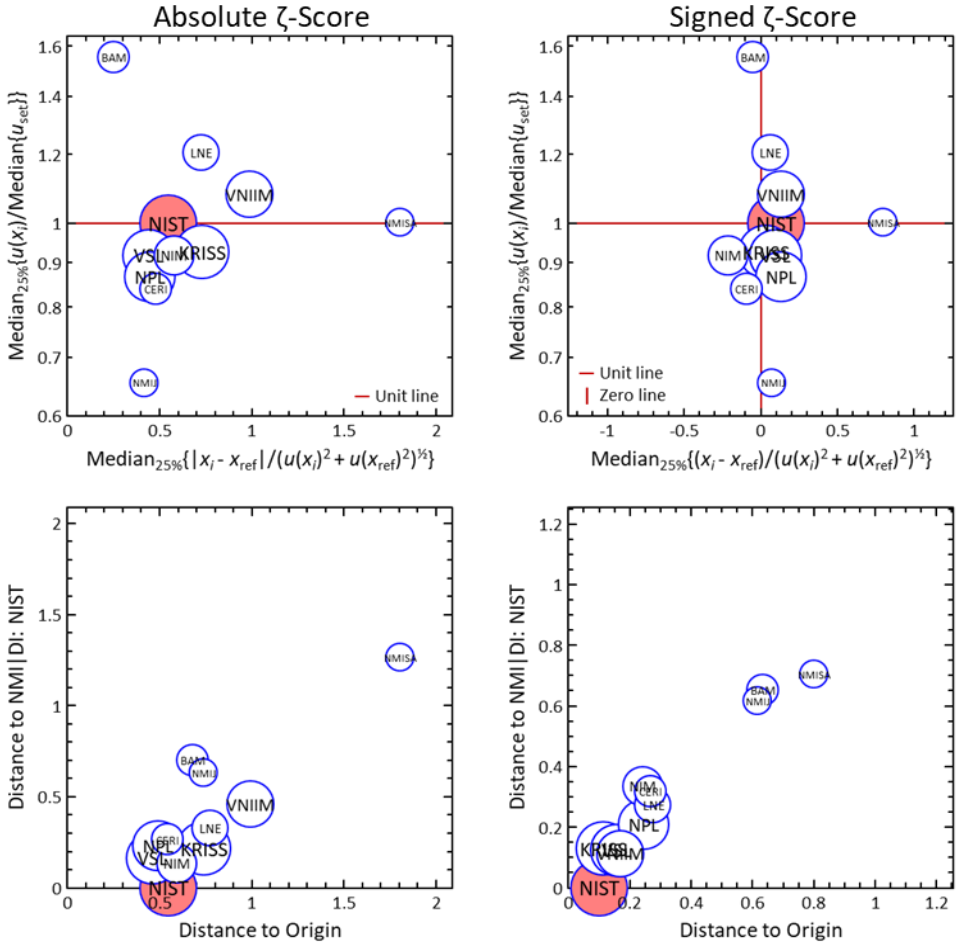


Fig. 29. *Peer_Unilateral* Charts With Absolute and Signed Bias Metrics.

The lower chart (chart PU-2) plots the median distance of the NMI/DI co-participants to the target NMI/DI (**Dnmi**, listed in column 13 of the table to the right of the charts) as a function of

the distance to the dataset references (**Dref**, listed in column 12 of the table). Since the target NMI/DI is at zero distance from itself, its symbol is along the bottom edge of chart PU-2.

10.2. Chart Display Parameters

Min #:	3	Auto
Min %:	30	Auto
Max $X_{x/u}$:	0.47	Auto
Min $Y_{u/u}$:	0.71	Auto
Max $Y_{u/u}$:	1.74	Auto
Y/X factor:	1.00	Auto

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

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 co-participant for differences to be calculated. The number of co-participations is listed in the **#** column (10) of the table to the right of the charts (see Fig. 28). The default is three datasets, the minimum number for the median to have any statistical relevance.

10.2.2. 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 the **%** 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. 28). 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 (bias) 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.

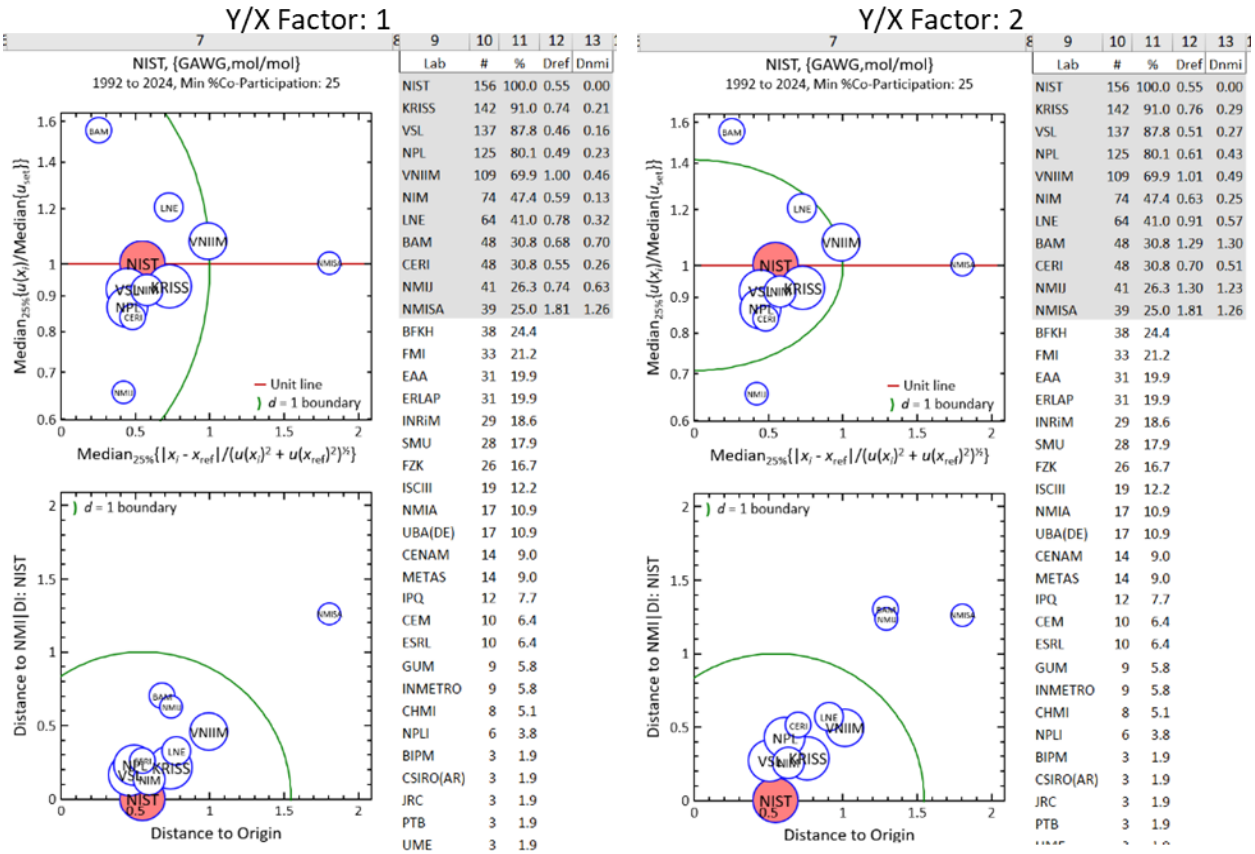
10.2.4. Min $Y_{u/u}$ and Max $Y_{u/u}$: *y*-Axis Limits

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

10.2.5. Y/X Factor: *y*-Axis Scale Factor

The value of the "Y/X factor:" parameter sets the importance of the *y*-axis (uncertainty ratio) relative to the *x*-axis (bias) for estimating the accuracy distance between the reference and the participant values. The default value is 1, which gives equal weight to a factor-of-two relative uncertainty ratio and a unit difference in the uncertainty-scaled bias. The estimated distances are listed in the **Dref** column (12) of the table to the right of the charts: see Fig. 30.

When the ellipse (Section 10.3.4) is active, the value of the "Y/X factor:" parameter affects the ellipse shape in chart PU-1. The ellipse in this chart is intended to help visualize the relative influence of the bias- and uncertainty metrics on the estimated distances. The parameter has no effect on the shape of the ellipse in chart PU-2.



Lab	#	%	Dref	Dnmi
NIST	156	100.0	0.55	0.00
KRISS	142	91.0	0.74	0.21
VSL	137	87.8	0.46	0.16
NPL	125	80.1	0.49	0.23
VNIIM	109	69.9	1.00	0.46
NIM	74	47.4	0.59	0.13
LNE	64	41.0	0.78	0.32
BAM	48	30.8	0.68	0.70
CERI	48	30.8	0.55	0.26
NMIJ	41	26.3	0.74	0.63
NMISA	39	25.0	1.81	1.26
BFKH	38	24.4		
FMI	33	21.2		
EAA	31	19.9		
ERLAP	31	19.9		
INRiM	29	18.6		
SMU	28	17.9		
FZK	26	16.7		
ISCIII	19	12.2		
NMIA	17	10.9		
UBA(DE)	17	10.9		
CENAM	14	9.0		
METAS	14	9.0		
IPQ	12	7.7		
CEM	10	6.4		
ESRL	10	6.4		
GUM	9	5.8		
INMETRO	9	5.8		
CHMI	8	5.1		
NPLI	6	3.8		
BIPM	3	1.9		
CSIRO(AR)	3	1.9		
JRC	3	1.9		
PTB	3	1.9		
UME	3	1.9		

Lab	#	%	Dref	Dnmi
NIST	156	100.0	0.55	0.00
KRISS	142	91.0	0.76	0.29
VSL	137	87.8	0.51	0.27
NPL	125	80.1	0.61	0.43
VNIIM	109	69.9	1.01	0.49
NIM	74	47.4	0.63	0.25
LNE	64	41.0	0.91	0.57
BAM	48	30.8	1.29	1.30
CERI	48	30.8	0.70	0.51
NMIJ	41	26.3	1.30	1.23
NMISA	39	25.0	1.81	1.26
BFKH	38	24.4		
FMI	33	21.2		
EAA	31	19.9		
ERLAP	31	19.9		
INRiM	29	18.6		
SMU	28	17.9		
FZK	26	16.7		
ISCIII	19	12.2		
NMIA	17	10.9		
UBA(DE)	17	10.9		
CENAM	14	9.0		
METAS	14	9.0		
IPQ	12	7.7		
CEM	10	6.4		
ESRL	10	6.4		
GUM	9	5.8		
INMETRO	9	5.8		
CHMI	8	5.1		
NPLI	6	3.8		
BIPM	3	1.9		
CSIRO(AR)	3	1.9		
JRC	3	1.9		
PTB	3	1.9		

Fig. 30. *Peer_Unilateral* Chart With Different Y/X Factors.

Note: For a given *x*-axis maximum (Max $X_{x/u}$), A signed difference metric Has an *x*-axis span twice that of the corresponding absolute difference metric. The *apparent* shape of the ellipse therefore changes when switching between the difference metrics, but the coverage remains the same. Of course, changing the difference metric can radically change the co-participant similarity distances. The net differences are illustrated in Fig. 31 for two values of the "Y/X factor:" parameter, using expanded *x*- and *y*-axis spans to facilitate comparisons.

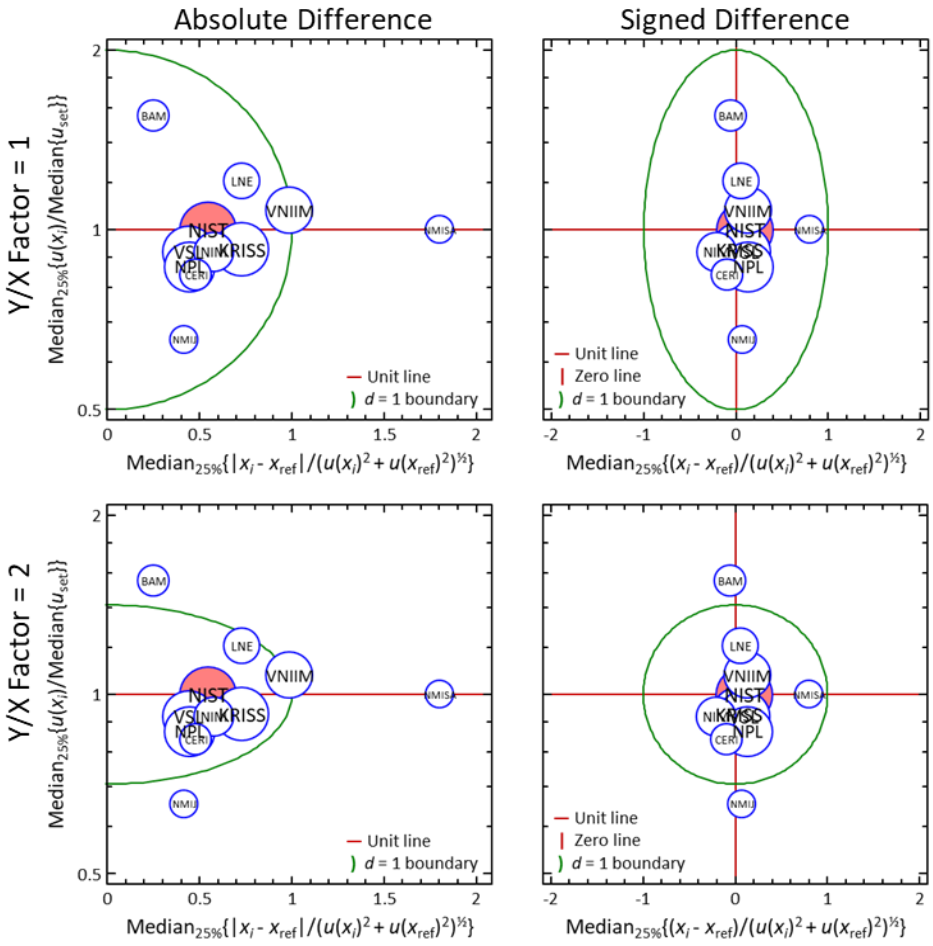


Fig. 31. *Peer_Unilateral* Interaction Between Difference Metric, Y/X Factor, and Ellipse.

10.3. Additional Chart Display Checkboxes

Color target: ☑
Opacity: ☑
Error bars: ☑
Boundary ellipse: ☑
Legend: ☑
Title: ☑
Plot area box: ☑

The *Peer_Unilateral* worksheet contains four chart display checkboxes in addition to those discussed in Section 2.2.3. The changes in chart PU-1 are mirrored in chart PU-2. Clicking a chart display checkbox invokes immediate changes.

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: see Fig. 32.

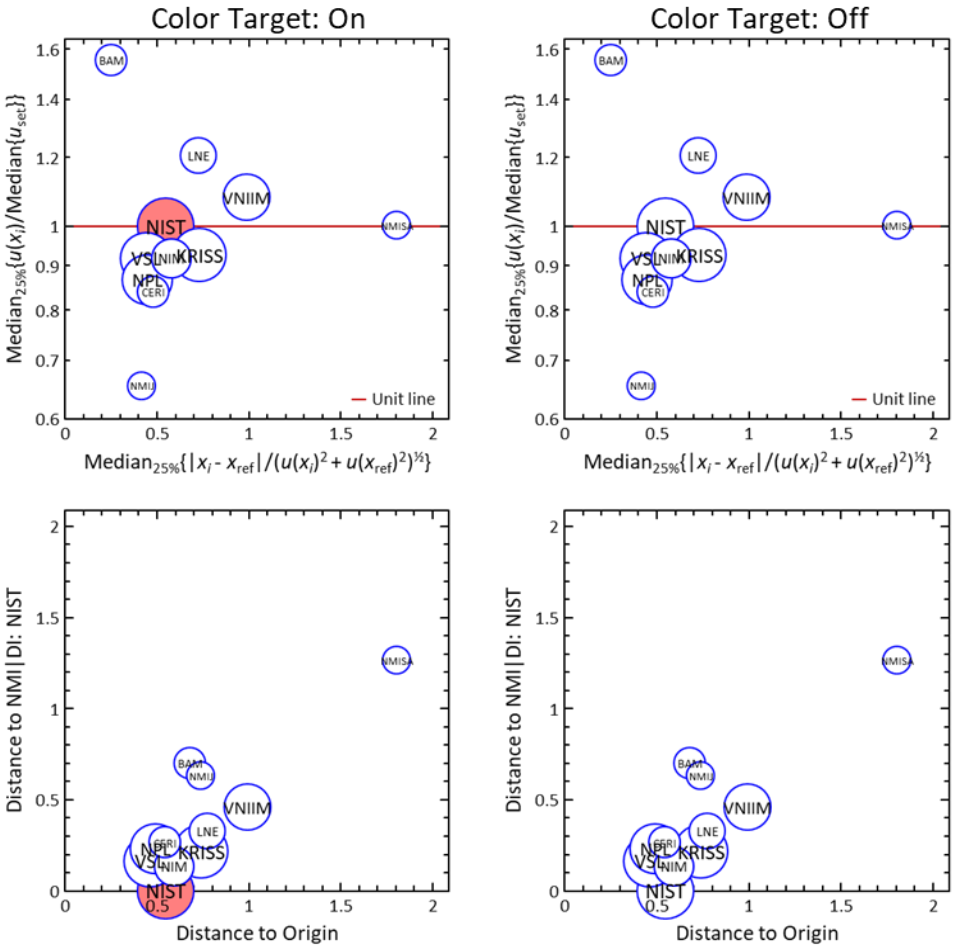


Fig. 32. *Peer_Unilateral* Charts With and Without Target Color.

10.3.2. Opacity

Clicking the “Opacity:” checkbox toggles the display of the symbols used for the co-participants from opaque to transparent: see Fig. 33. 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.

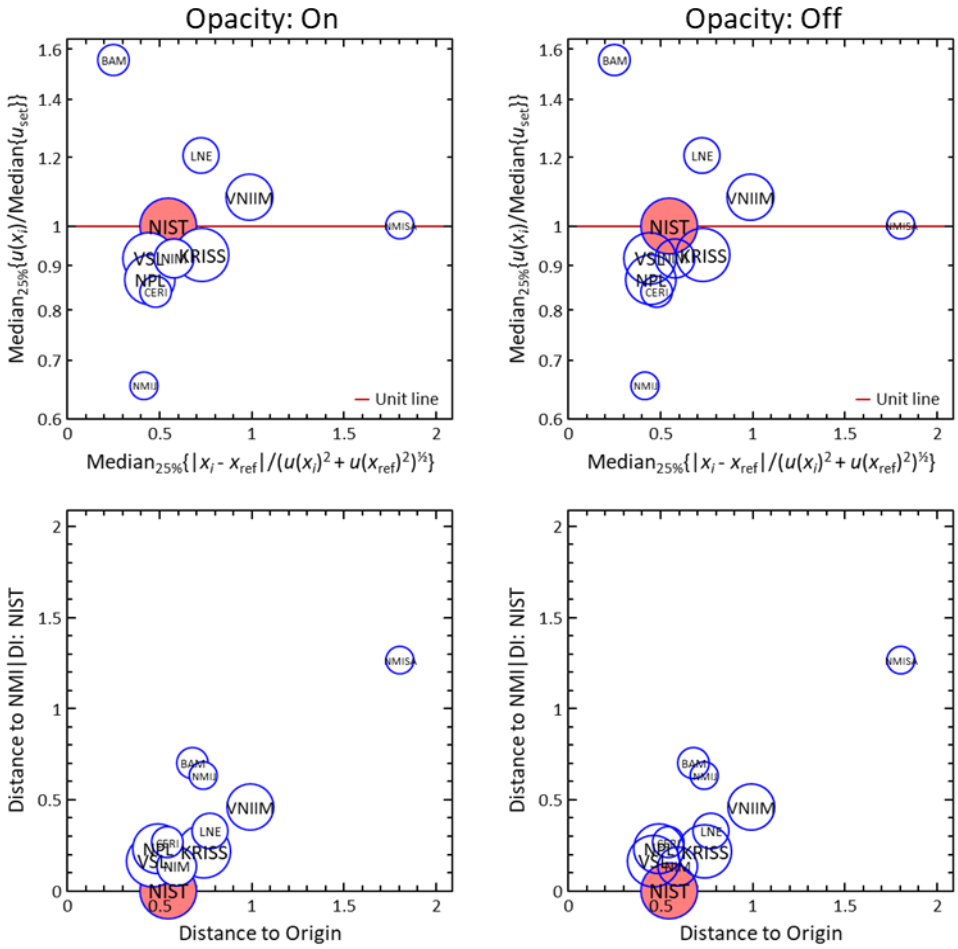


Fig. 33. *Peer_Unilateral* Charts With and Without Symbol Opacity.

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)×(scale factor) 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 scale factor is a non-negative numeric value between 1 and 6 in cell(32,5) – i.e., the “Error bars:” row and the **Default** parameter column.

The display regions of the difference (*X*) and uncertainty ratio (*Y*) axes are defined by the maximum intervals required to display all the error bars at their specified expansion. These limits are set whether or not the error bars are displayed: see Fig. 34.

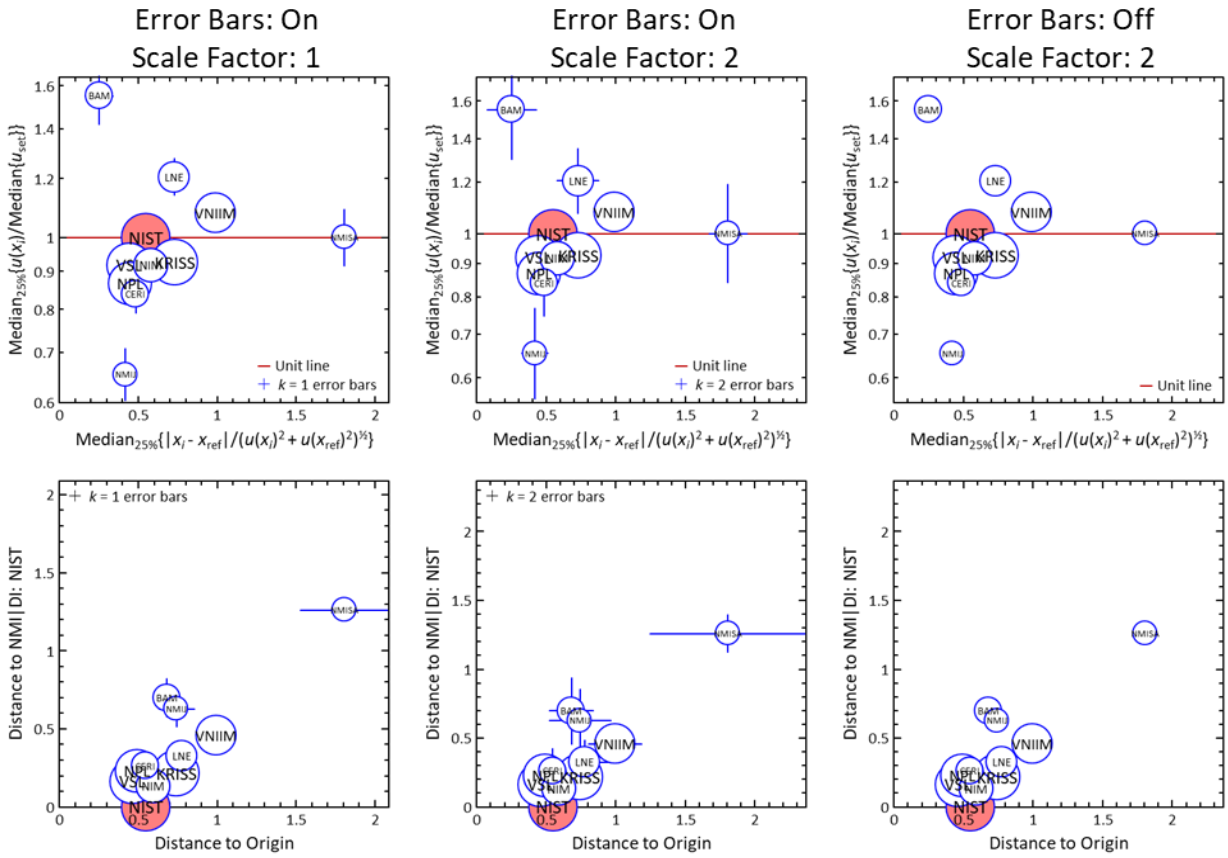


Fig. 34. *Peer_Unilateral* Charts With and Without Error Bars.

Clicking the “Error bars:” checkbox immediately toggles whether the error bars are displayed. However, changing the “Error bars:” scale factor has no effect until the **Plot** command button is clicked.

10.3.4. Ellipse

Clicking the “Ellipse:” checkbox toggles the display of an ellipse in each of the two charts: see Fig. 35. For chart PU-1, the ellipse is centered on the reference parameters and provides a visual accuracy distance boundary (proportional to the **Dref** values in column 12). For chart PU-2, the ellipse is centered on the target NMI/DI and provides an empirical “how close” distance boundary (proportional to the **Dnmi** values in column 13).

The size of the ellipse is controlled by the scale factor, a non-negative numeric value between 0.1 and 10 in cell(33,5) – the “Ellipse:” row and the **Default** parameter column. The default scale factor is 1. The ellipse size has no effect on the estimated similarity distances.

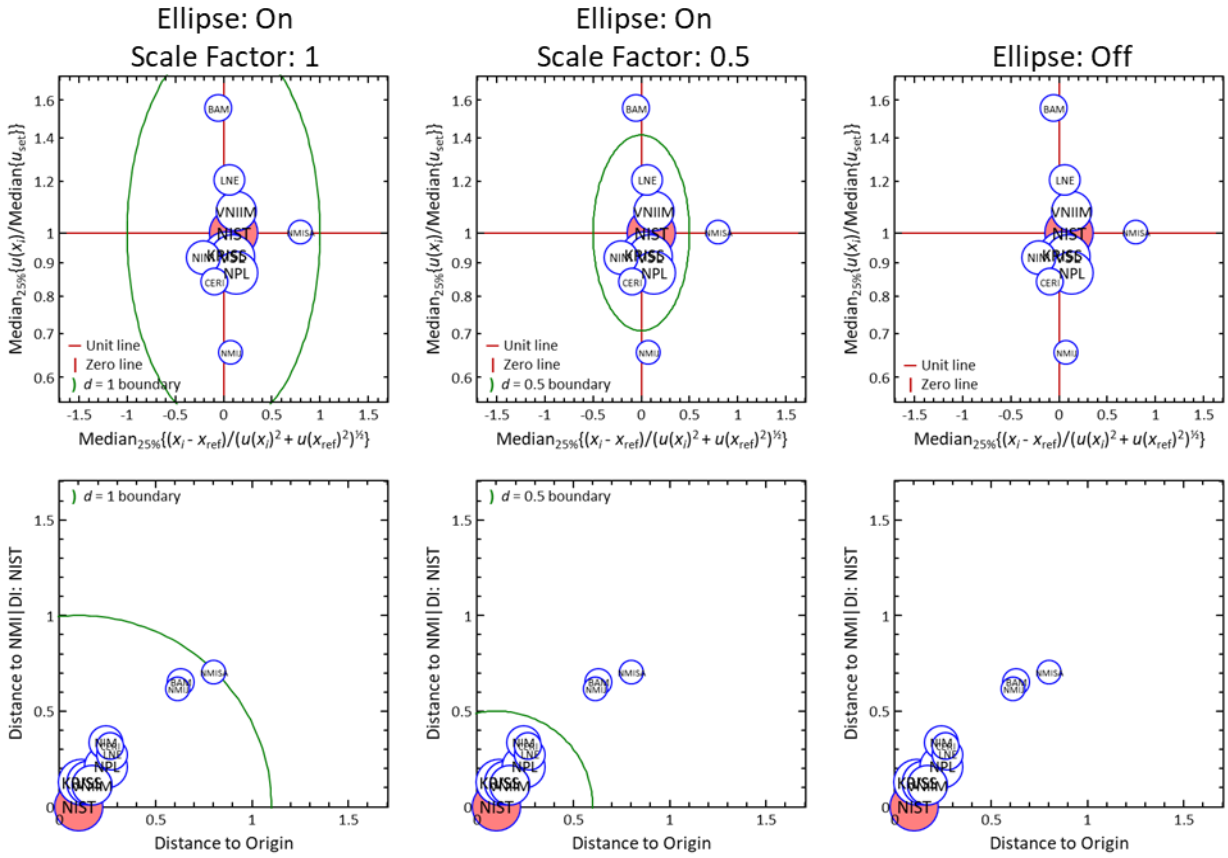


Fig. 35. *Peer_Unilateral* Boundary Ellipses and Distance Values.

Clicking the “Ellipse:” checkbox immediately toggles whether the ellipses are displayed. However, changing the “Ellipse:” scale factor has no effect until the **Plot** command button is clicked.

11. Peer_Global Subsystem

The *Peer_Global* charts, the controls used to specify the datasets evaluated, and the controls used to modify what the charts display are pictured in Fig. 36. This subsystem is identical to *Peer_Unilateral*, except that results for each NMI/DI is calculated using all datasets that meet all the selection criteria.

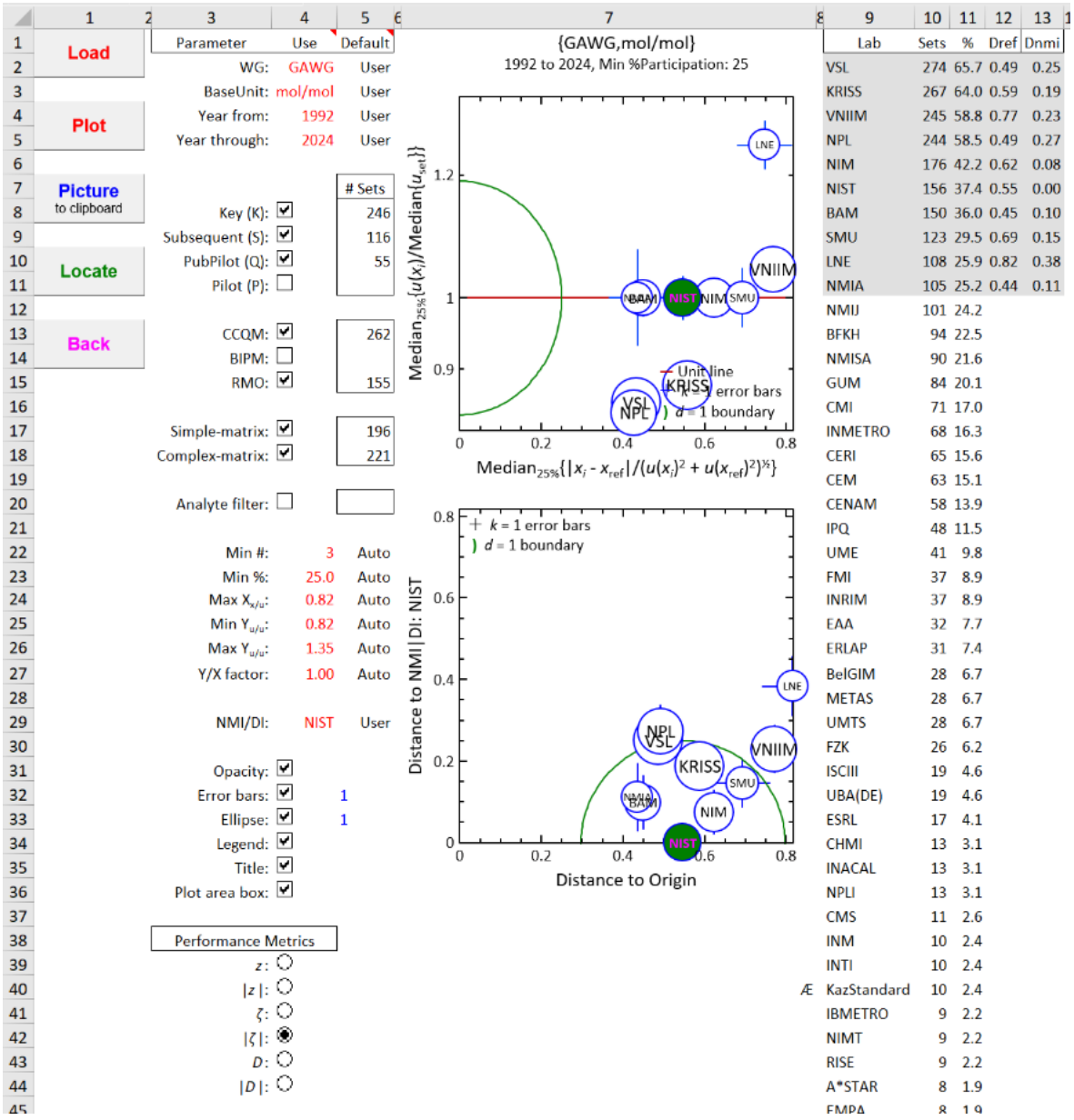


Fig. 36. *Peer_Global* Dashboard.

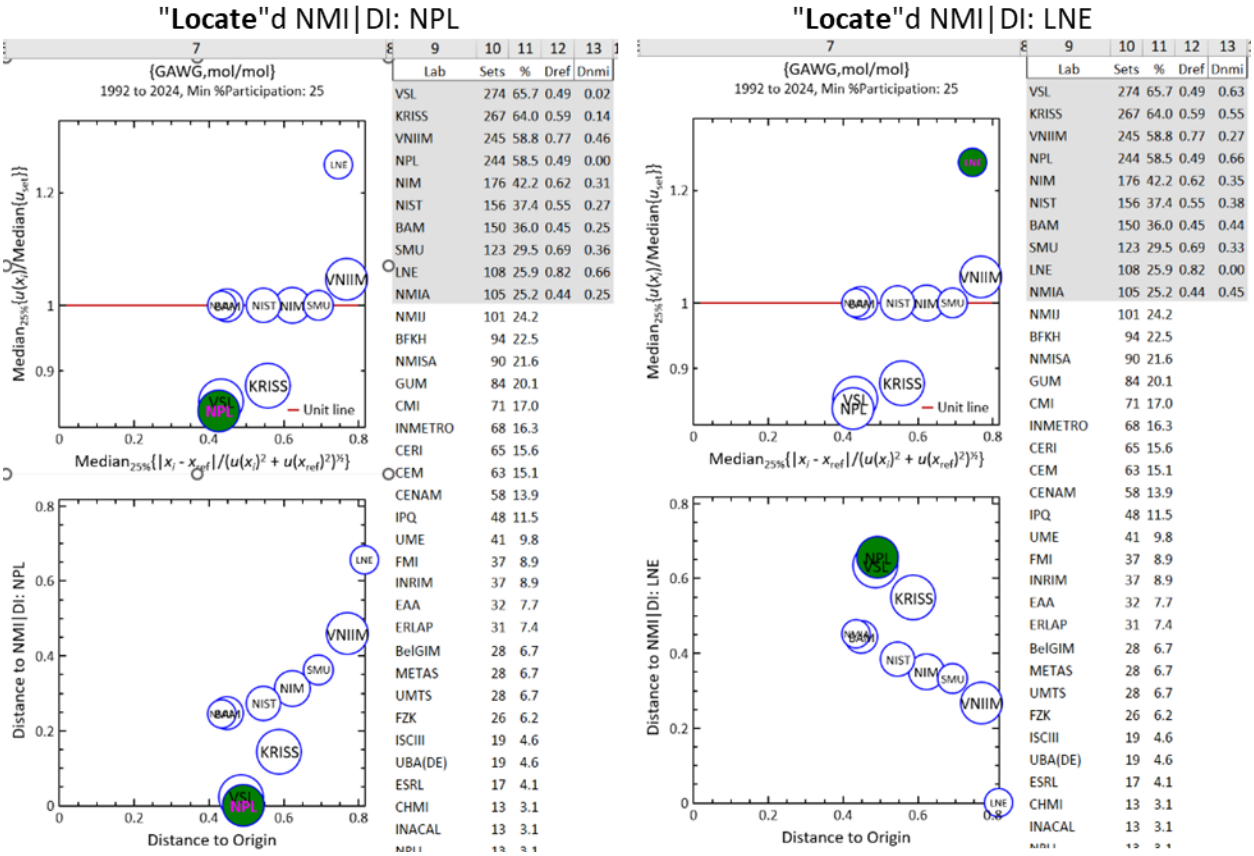
Reminder: A data selection or chart display parameter value listed under the **Use** heading can only be changed when its **Default** value is *User*. See Section 1.10 for further information.

11.1. Charts

Each open circle symbol in the upper chart (PG_1) 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 1.9.1). As in the *Peer_Unilateral* chart, the bias and uncertainty metrics are relative to the dataset references. However, the metric estimates use all of the datasets each NMI/DI has contributed to rather than just the subset in which a target NMI/DI contributed.

The lower chart (PG_2) is populated with symbols representing the distance of other NMI/DIs to a "**Locate**"d NMI/DI (the **Dnmi** values in column 13 of the table to the right of the charts) plotted as a function of their distance to the dataset references (the **Dref** values in column 12.) When no NMIDI has been specified or a specified NMI/DI hasn't contributed to enough datasets, chart PG_2 displays results for the NMI/DI that contributed to the largest proportion of datasets.

In both PG_1 and PG_2. the symbol for the "**Locate**"d NMI/DI is colored dark green: Charts for NPL or LNE are displayed in Fig. 37.



Lab	Sets	%	Dref	Dnmi
VSL	274	65.7	0.49	0.02
KRISS	267	64.0	0.59	0.14
VNIIM	245	58.8	0.77	0.46
NPL	244	58.5	0.49	0.00
NIM	176	42.2	0.62	0.31
NIST	156	37.4	0.55	0.27
BAM	150	36.0	0.45	0.25
SMU	123	29.5	0.69	0.36
LNE	108	25.9	0.82	0.66
NMIA	105	25.2	0.44	0.25
NMIJ	101	24.2		
BFKH	94	22.5		
NMISA	90	21.6		
GUM	84	20.1		
CMI	71	17.0		
INMETRO	68	16.3		
CERI	65	15.6		
CEM	63	15.1		
CENAM	58	13.9		
IPQ	48	11.5		
UME	41	9.8		
FMI	37	8.9		
INRIM	37	8.9		
EAA	32	7.7		
ERLAP	31	7.4		
BelGIM	28	6.7		
METAS	28	6.7		
UMTS	28	6.7		
FZK	26	6.2		
ISCIII	19	4.6		
UBA(DE)	19	4.6		
ESRL	17	4.1		
CHMI	13	3.1		
INACAL	13	3.1		

Lab	Sets	%	Dref	Dnmi
VSL	274	65.7	0.49	0.63
KRISS	267	64.0	0.59	0.55
VNIIM	245	58.8	0.77	0.27
NPL	244	58.5	0.49	0.66
NIM	176	42.2	0.62	0.35
NIST	156	37.4	0.55	0.38
BAM	150	36.0	0.45	0.44
SMU	123	29.5	0.69	0.33
LNE	108	25.9	0.82	0.00
NMIA	105	25.2	0.44	0.45
NMIJ	101	24.2		
BFKH	94	22.5		
NMISA	90	21.6		
GUM	84	20.1		
CMI	71	17.0		
INMETRO	68	16.3		
CERI	65	15.6		
CEM	63	15.1		
CENAM	58	13.9		
IPQ	48	11.5		
UME	41	9.8		
FMI	37	8.9		
INRIM	37	8.9		
EAA	32	7.7		
ERLAP	31	7.4		
BelGIM	28	6.7		
METAS	28	6.7		
UMTS	28	6.7		
FZK	26	6.2		
ISCIII	19	4.6		
UBA(DE)	19	4.6		
ESRL	17	4.1		
CHMI	13	3.1		
INACAL	13	3.1		

Fig. 37. *Peer_Global* Charts with NPL or VNIIM as the "**Locate**"d NMI/DI.

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 differ: see Fig. 38.

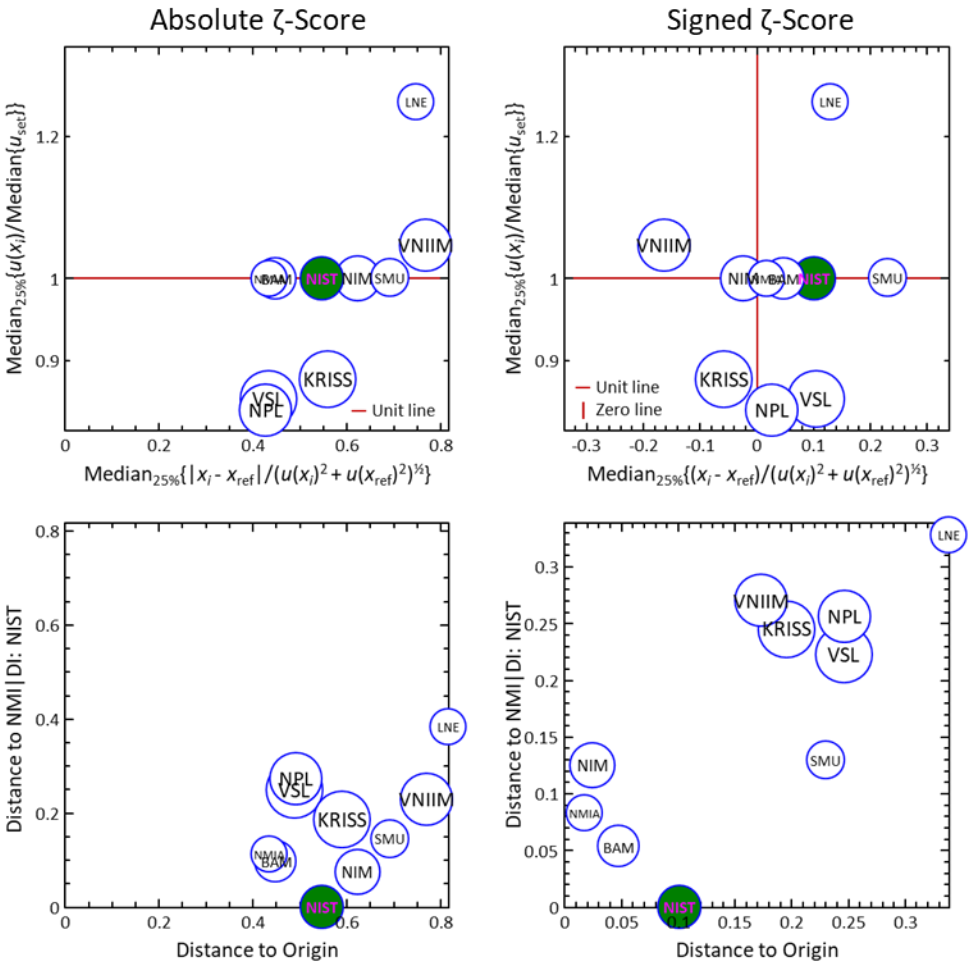


Fig. 38. *Peer_Global* Chart With Absolute and Signed Bias Metrics.

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

Min #:	3	Auto
Min %:	30.0	Auto
Max $X_{x/u}$:	0.25	Auto
Min $Y_{u/u}$:	0.82	Auto
Max $Y_{u/u}$:	1.08	Auto
Y/X scale:	1.00	Auto

The *Peer_Unilateral* worksheet contains six 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 a given participant for that participant to be displayed in the charts. The number of participations is listed in the **Sets** column (10) of the table to the right of the chart (see Fig. 36). The default value is three datasets, the minimum number for the median to have any statistical relevance.

11.2.2. Min %: Minimum Participation

The value of the "Min %:" parameter sets the minimum proportion of 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 the **%** 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. 36). 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 *x*-axis (bias) 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.

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 *y*-axis (uncertainty ratio). The default values are set by the extreme values of the displayed symbols including their error bars.

11.2.5. Y/X Factor: *y*-Axis Scale Factor

The value of the "Y/X factor:" parameter sets the importance of the *y*-axis (uncertainty ratio) relative to the *x*-axis (bias) for estimating the accuracy distance between the reference and the participant values. The default value is 1, which gives equal weight to a factor-of-two relative uncertainty ratio and a unit difference in the uncertainty-scaled bias. The estimated distances are listed in the **Dref** column (12) of the table to the right of the charts: see Fig. 41.

When the ellipse (Section 11.3.3) is active, the value of the "Y/X factor:" parameter affects the ellipse shape in chart PG-1. The ellipse in this chart is intended to help visualize the relative

influence of the bias- and uncertainty metrics on the estimated distances. The parameter has no effect on the shape of the ellipse in chart PG-2.

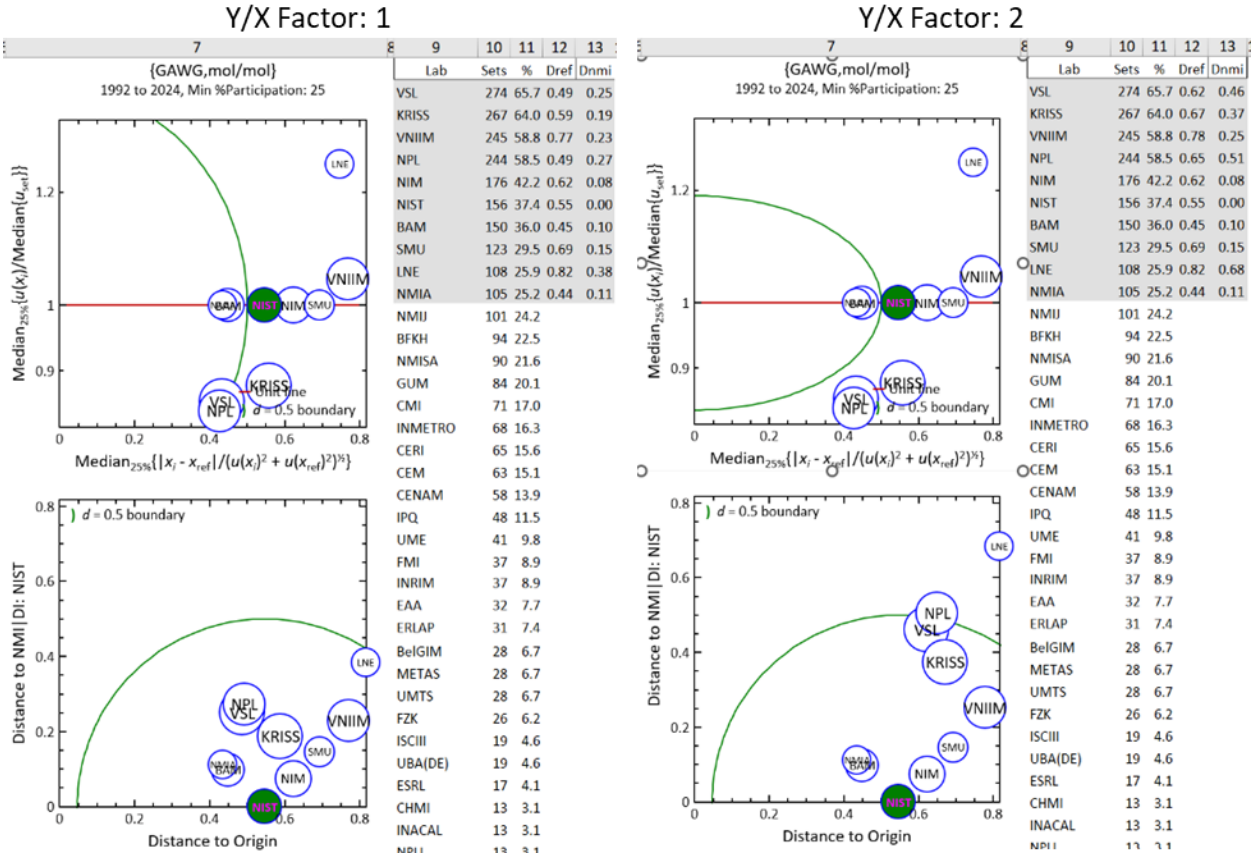


Fig. 39. *Peer_Unilateral* Chart With Different Y/X Factors.

Note: For a given *x*-axis maximum (Max $X_{x/u}$), A signed difference metric has an *x*-axis span twice that of the corresponding absolute difference metric. The *apparent* shape of the ellipse therefore changes when switching between the difference metrics, but the coverage remains the same. Of course, changing the difference metric can radically change the co-participant similarity distances. The net differences are illustrated in Fig. 40 for two values of the "Y/X factor:" parameter, using expanded *x*- and *y*-axis spans to facilitate comparisons.

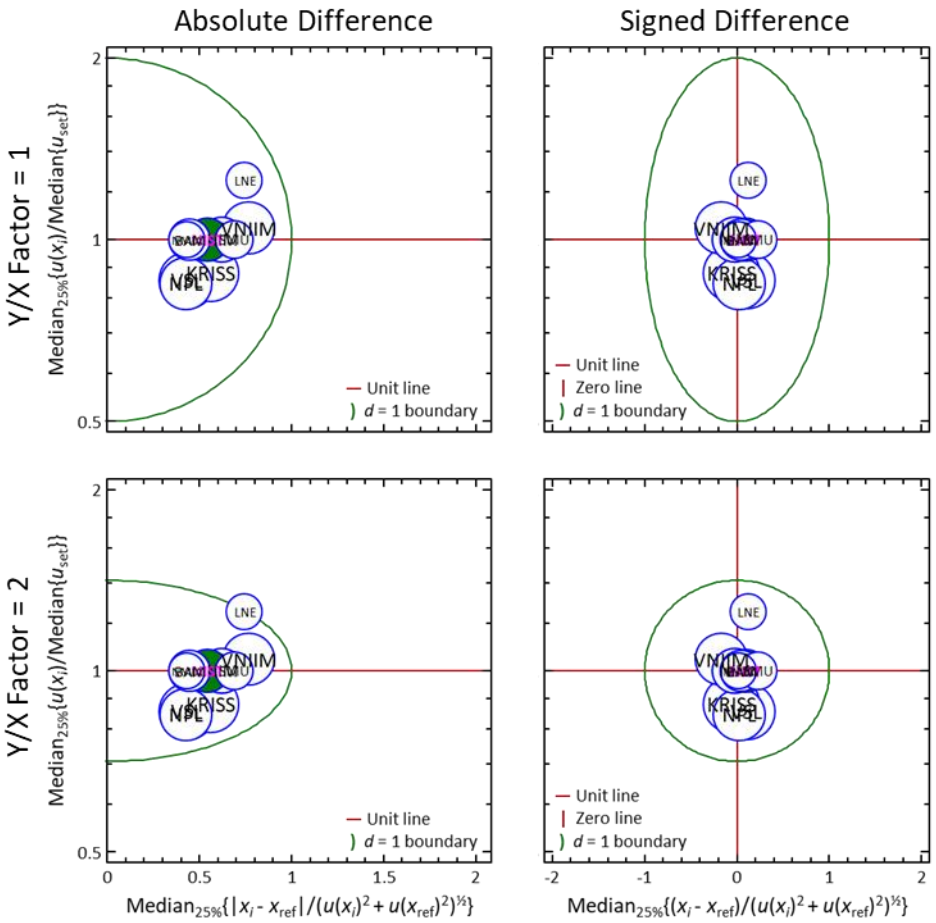
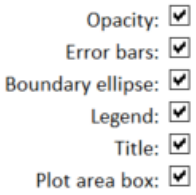


Fig. 40. *Peer_Global* Interaction Between Difference Metric, Y/X Factor, and Ellipse.

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 participants from opaque to transparent: see Fig. 41. This can be useful for visualizing a participant's relationships to the other NMI/DIs when its symbol is buried beneath others.

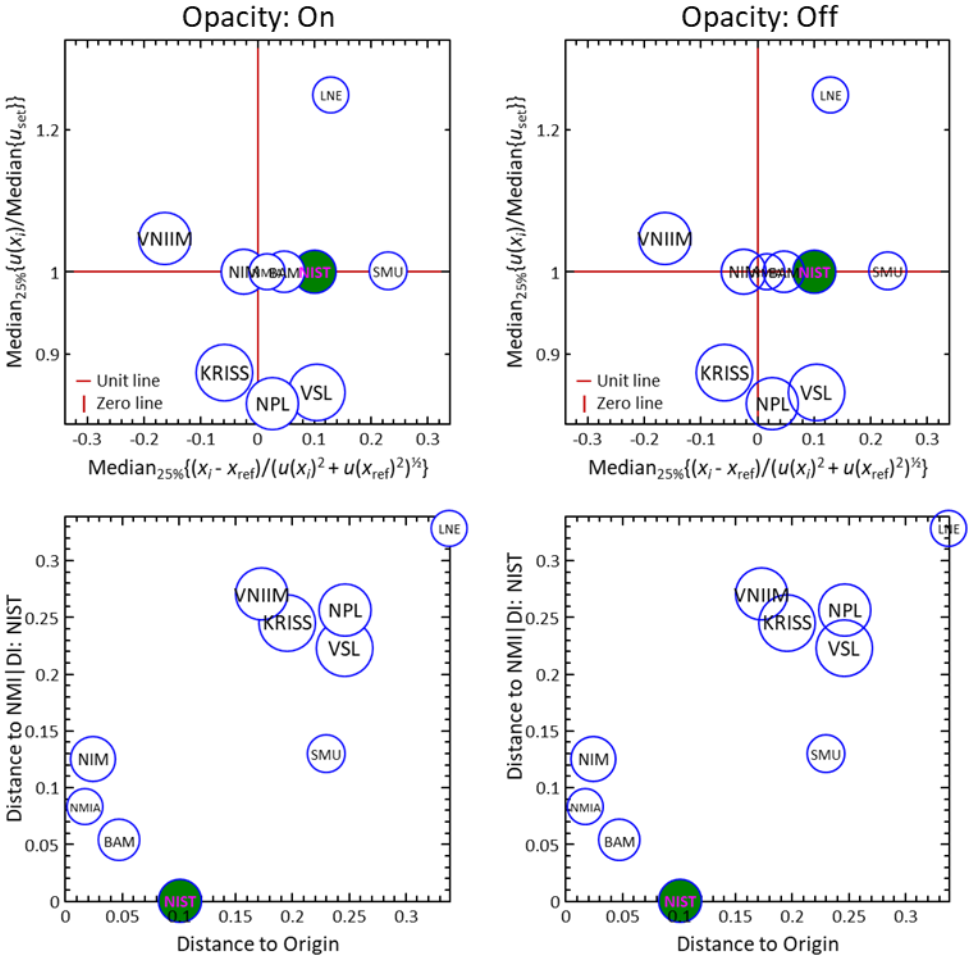


Fig. 41. *Peer_Global* Charts With and Without Symbol Opacity.

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)×(scale factor) 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 scale factor is a non-negative numeric value between 1 and 6 in cell(32,5) – i.e., the “Error bars:” row and the **Default** parameter column.

The display regions of the difference (*X*) and uncertainty ratio (*Y*) axes are defined by the maximum intervals required to display all the error bars at their specified expansion. These limits are set whether or not the error bars are displayed: see Fig. 42.

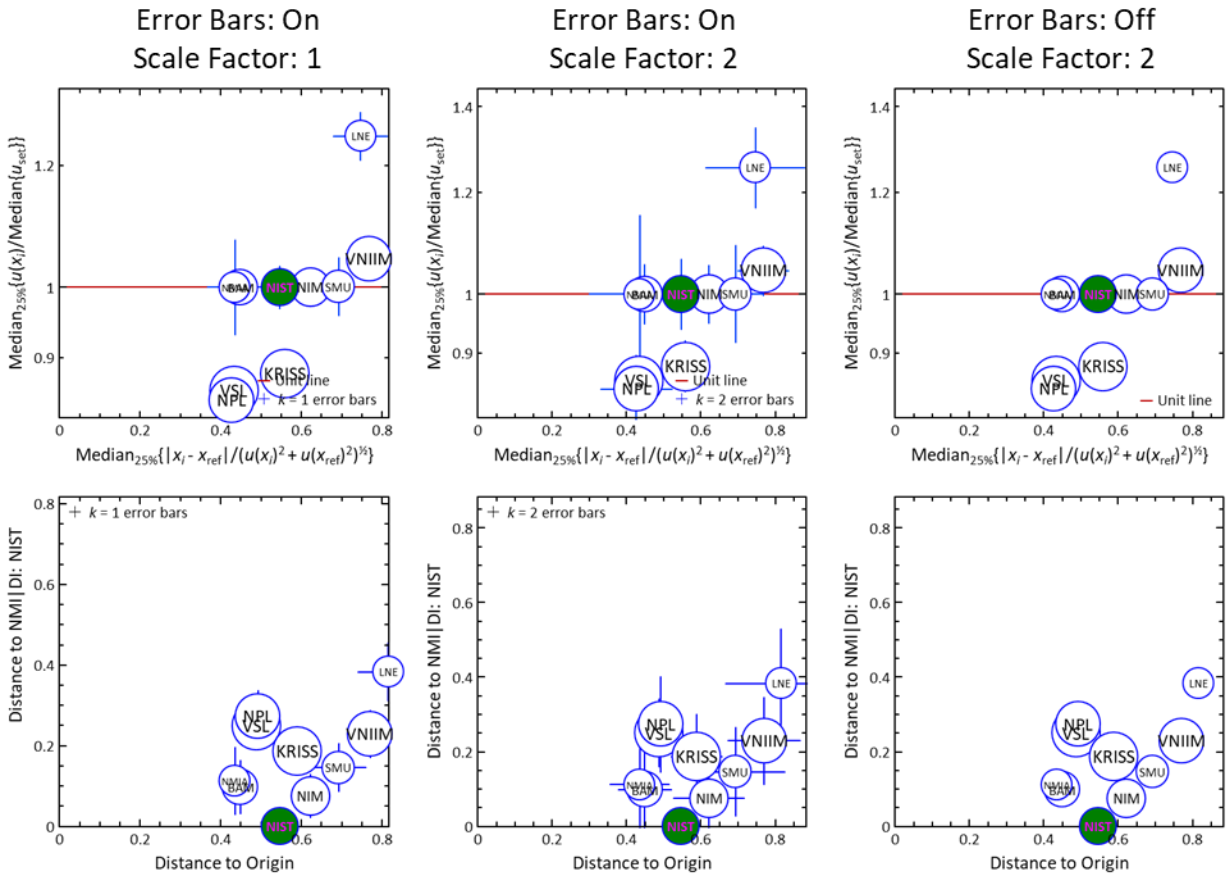


Fig. 42. *Peer_Global* Charts With and Without Error Bars.

11.3.3. Ellipse

Clicking the “Ellipse:” checkbox toggles the display of an ellipse in each of the two charts: see Fig. 43. For chart PG-1, the ellipse is centered on the reference parameters and provides a visual accuracy distance boundary (proportional to the **Dref** values in column 12). For chart PG-2, the ellipse is centered on the “**Locate**”d NMI/DI and provides an empirical “how close” distance boundary (proportional to the **Dnmi** values in column 13).

The size of the ellipse is controlled by the scale factor, a non-negative numeric value between 0.1 and 10 in cell(33,5) – the “Ellipse:” row and the **Default** parameter column. The default scale factor is 1. The ellipse size has no effect on the estimated similarity distances.

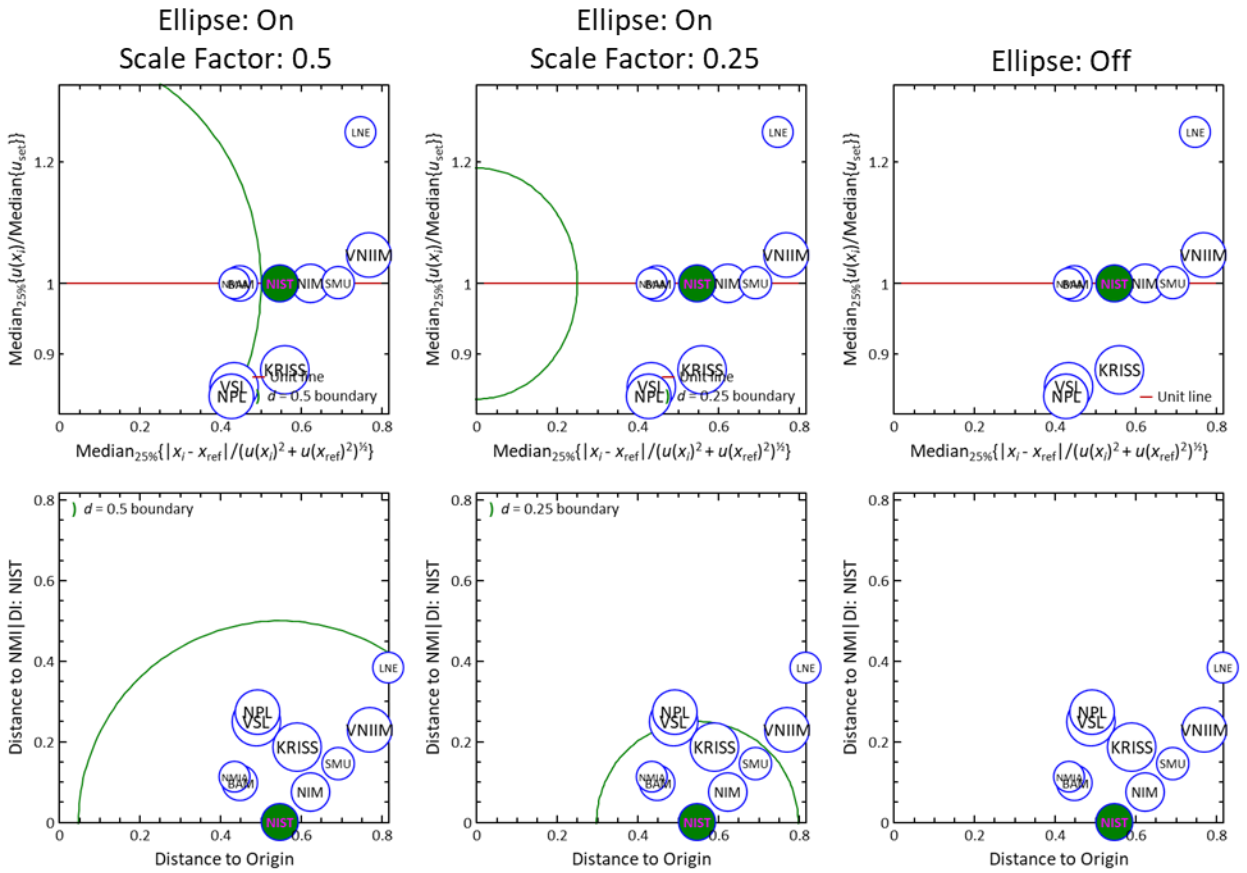


Fig. 43. *Peer_Global* Boundary Ellipses and Distance Values.

Clicking the “Ellipse:” checkbox immediately toggles whether the ellipses are displayed. However, changing the “Ellipse:” scale factor has no effect until the **Plot** command button is clicked.

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. 44.

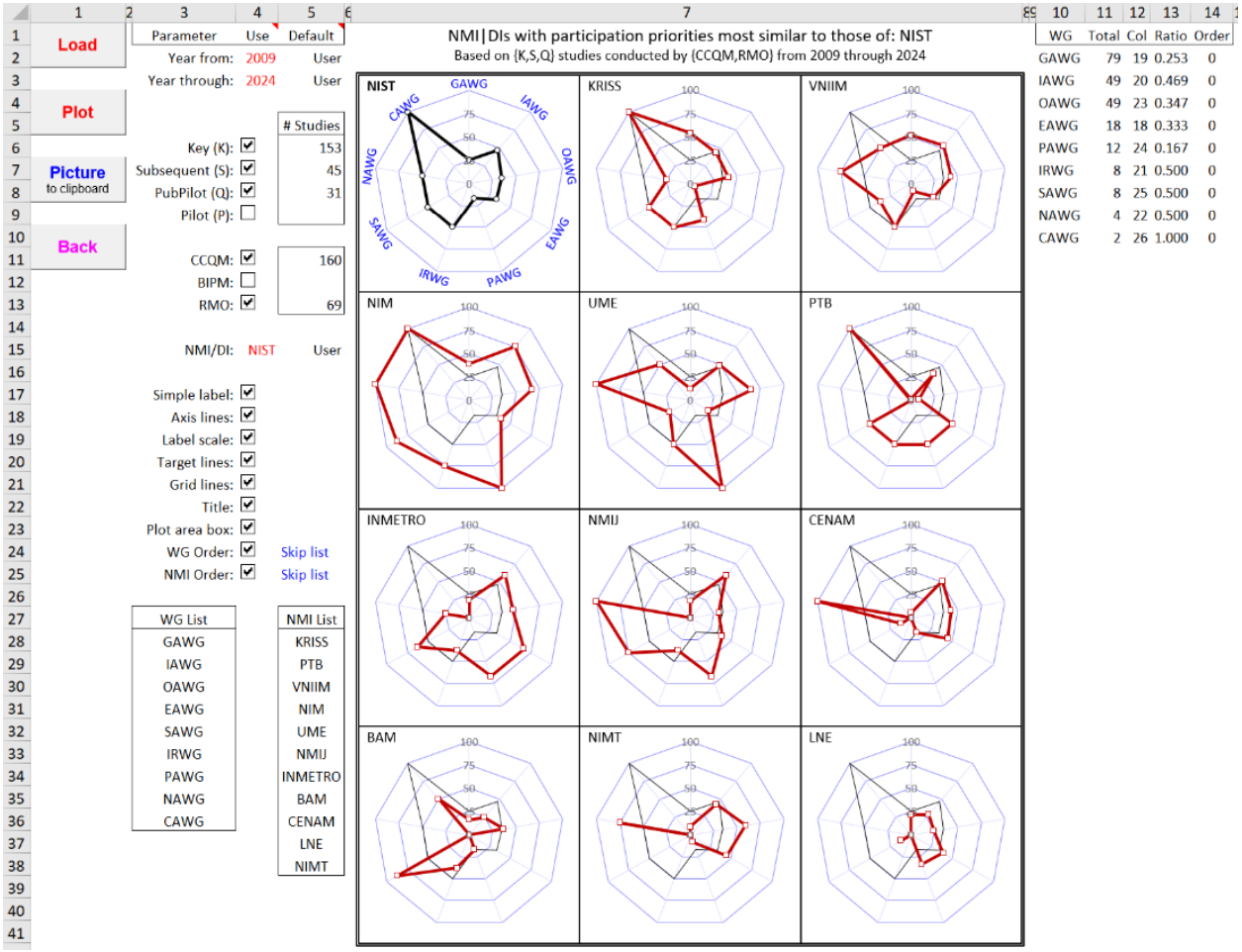


Fig. 44. *Peer_Priorities* Dashboard.

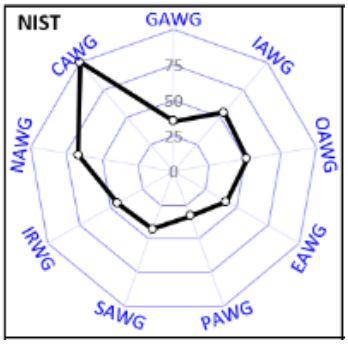
Reminder: A data selection or chart display parameter value listed under the **Use** heading can only be changed when its **Default** value is *User*. See Section 1.10 for further information.

12.1. Chart

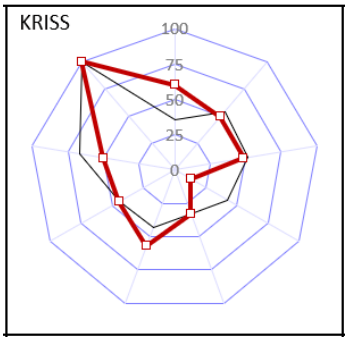
Each segment of the *Peer_Priorities* chart is a radar-style display of WG participation rates for a particular NMI/DI. A WG participation rate is the ratio (expressed as a percentage) of the number of studies in which the particular NMI/DI participated relative to the number of studies sponsored by 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 12.3.10). 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 placed below the "NMI/DI:" parameter. Clicking any one of these checkboxes immediately changes the chart display. 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: see Fig. 45.

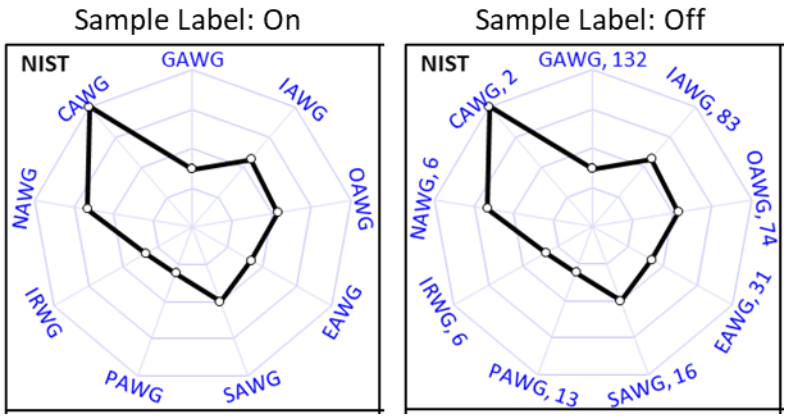


Fig. 45. Target NMI/DI Panel of the *Peer_Priorities* Chart With and Without Simple Label.

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: see Fig. 46.

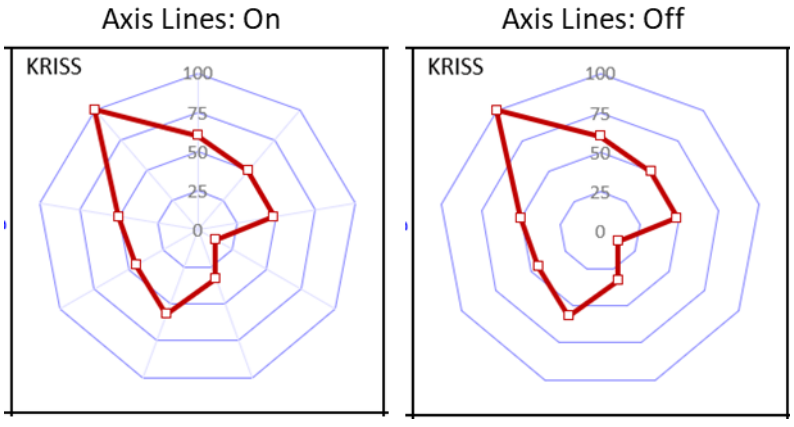


Fig. 46. A Non-Target NMI/DI Panel of the *Peer_Priorities* Chart With and Without Axis Lines.

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: see Fig. 47.

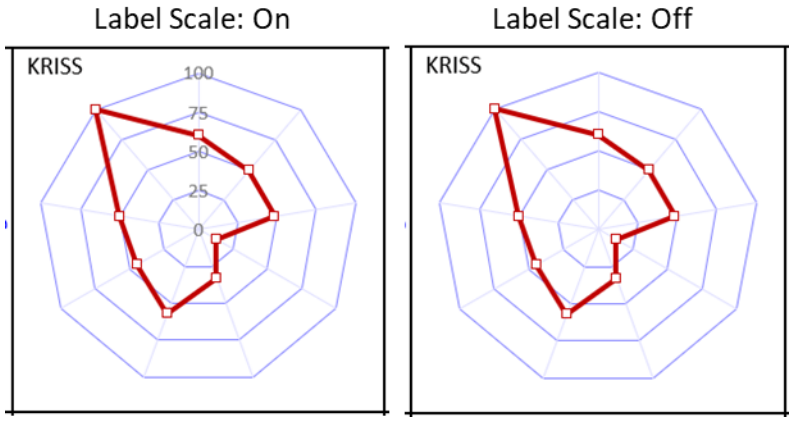


Fig. 47. A Non-Target NMI/DI Panel With and Without Scale Labels.

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: see Fig. 48.

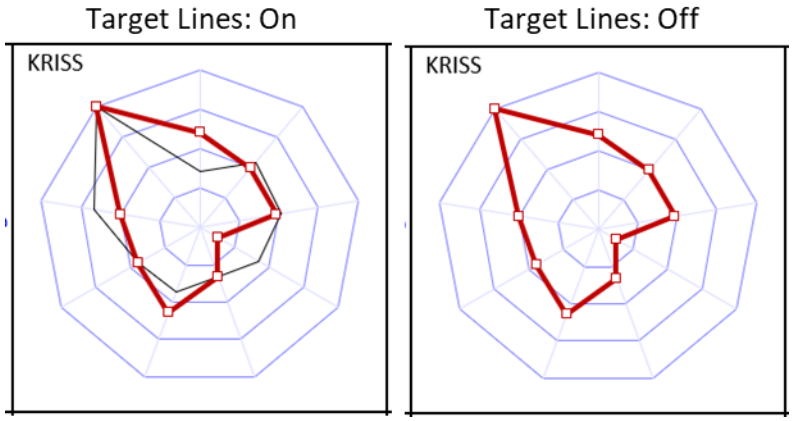


Fig. 48. A Panel With and Without Target Lines.

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: see Fig. 49.

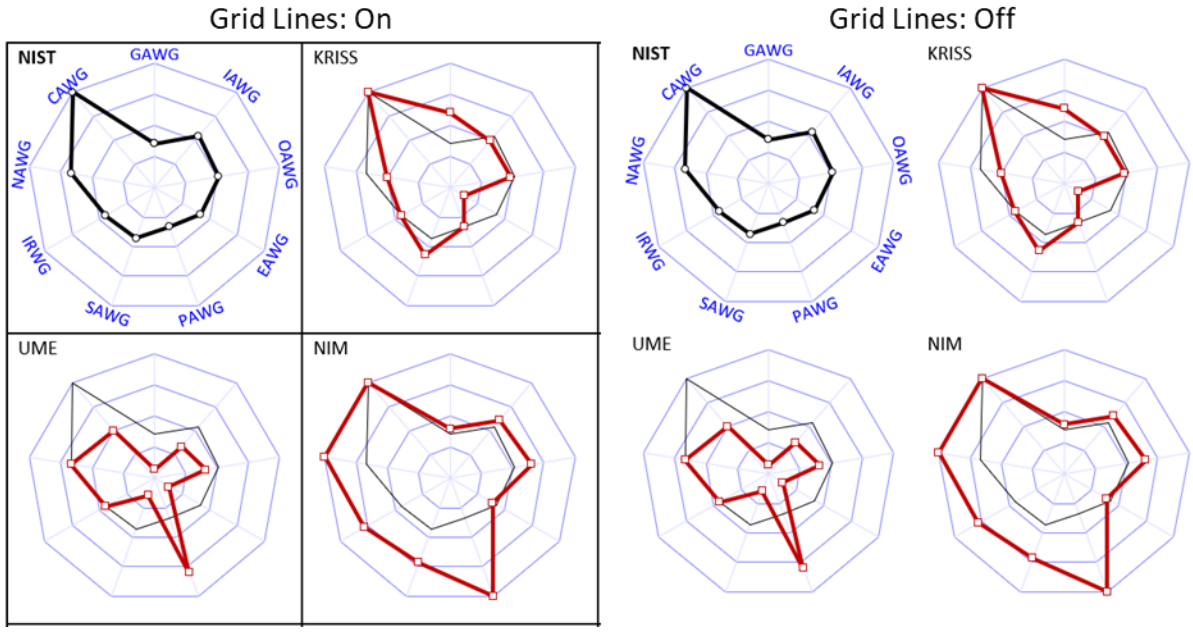


Fig. 49. Panels of the *Peer_Priorities* Chart With and Without Grid Lines.

12.3.6. Title: Chart Title

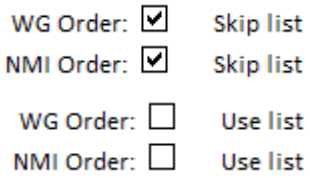
The “Title:” checkbox toggles between displaying and not displaying the chart’s title. When checked the title is displayed. When unchecked the title is not displayed. In addition to identifying the target NMI/DI, the title identifies the studies considered in the analysis by type (K S, Q, and/or P),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



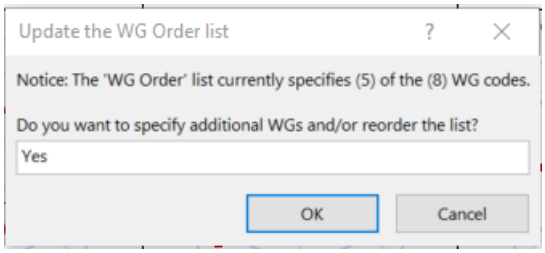
12.3.9. WG Order: Which WGs and in What Order

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. 50. 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. 50.

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. 50.
- If the response is Yes, the subsystem issues a prompt and the focus returns to the user.

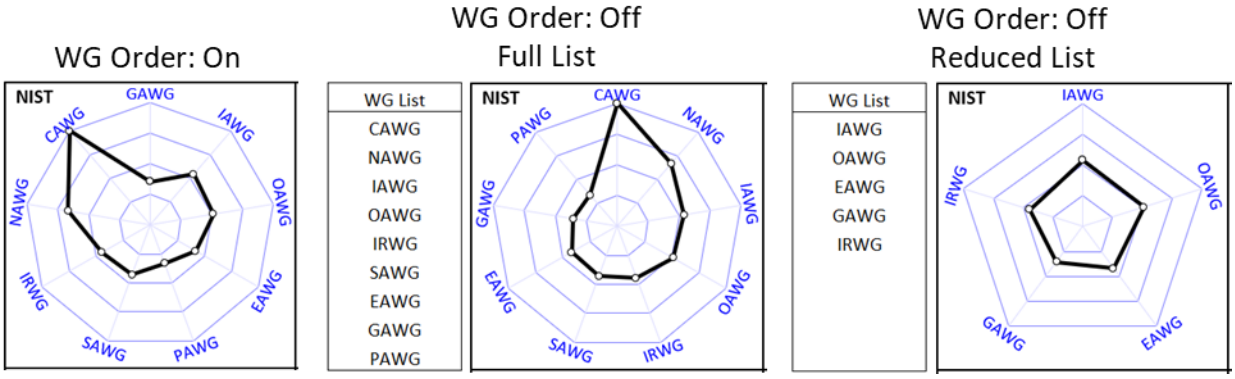


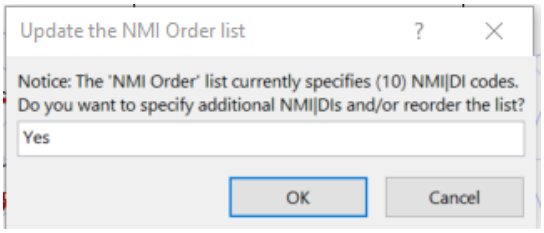
Fig. 50. Target Panels of the *Peer_Priorities* Chart with Various WG Orderings.

12.3.10. 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 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 12.3.10.1), 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 12.3.10.1) to those of the target NMI/DI.
- If the response is Yes, the subsystem issues a prompt and the focus returns to the user.

12.3.10.1. 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, Δ_{other}, across all of the WGs currently included in the analysis:

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

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, $r_{target,i}$ is the target NMI/DI's participation rate in the i^{th} WG, and $r_{other,i}$ is the other NMI/DI's participation rate in the i^{th} WG.

If the "NMI Order:" checkbox is checked, the Δ_{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 Δ_{other}. The *Peer_Priorities* chart displays the participation ratios for the target NMI/DI and the eleven NMI/DIs having the smallest Δ_{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. 51.

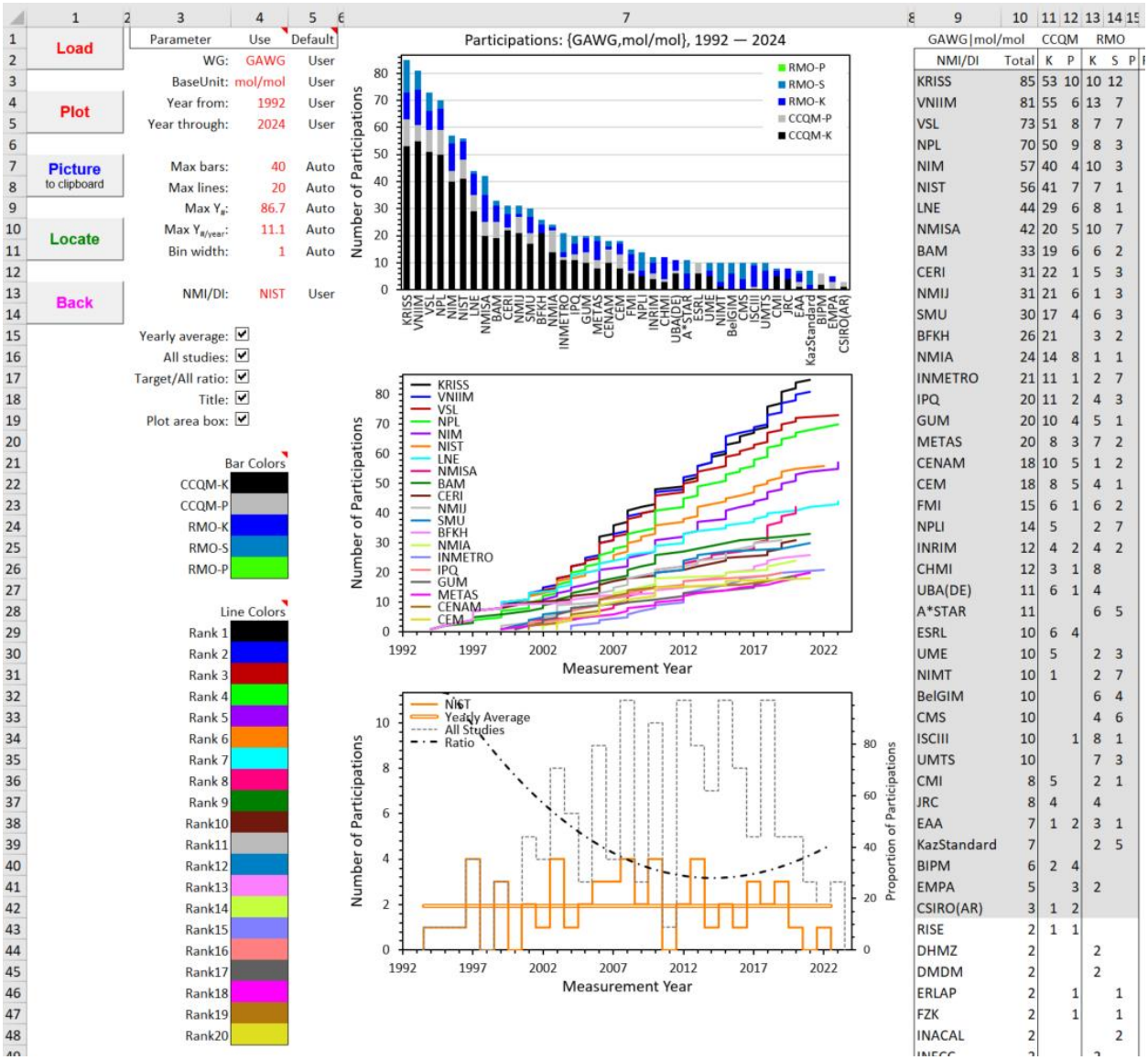


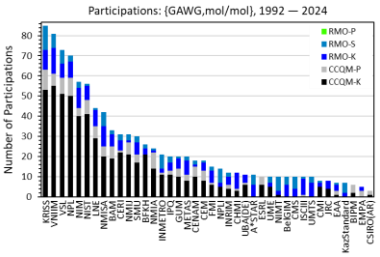
Fig. 51. *WG_Participations* Dashboard.

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 1.10 for further information.

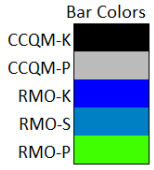
The information displayed in these charts is derived from the *CCQM_Retrospectoscope* datasheets. There is often a lengthy interval between when participants must report their results (the measurement year used by the *CCQM_Retrospectoscope*) and when the report with complete data is published. Participation counts within three years of the current date may thus (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* database. The complete database, including PSs as well as PPSs, is only available at NIST; elsewhere, only PPS participations will be counted.

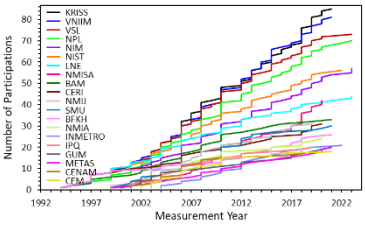
13.1. Charts



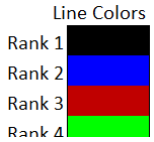
For a given {WG, BaseUnit}, the worksheet's top chart (chart WPa-1) displays the number and type of studies that up-through 40 NMI/DIs have participated in. These data are displayed in the form of a stacked bar chart. Participations are grouped by body (CCQM and RMO, with BIPM here considered to be an 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 ("spilling paint can" in the Font menu of the Home tab).

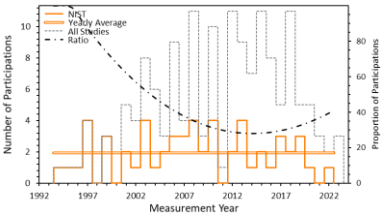


For the up-through-20 NMI/DIs with the most total participations, the middle chart (chart WPa-2) displays the cumulative number of participations as a function of measurement year. As in chart WPa-1, the NMI/DIs are arranged by decreasing number of total participations. The number of NMI/DIs for which 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 **BaseUnit** parameters. If a particular **WG** is specified, setting **BaseUnit** 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. 52.

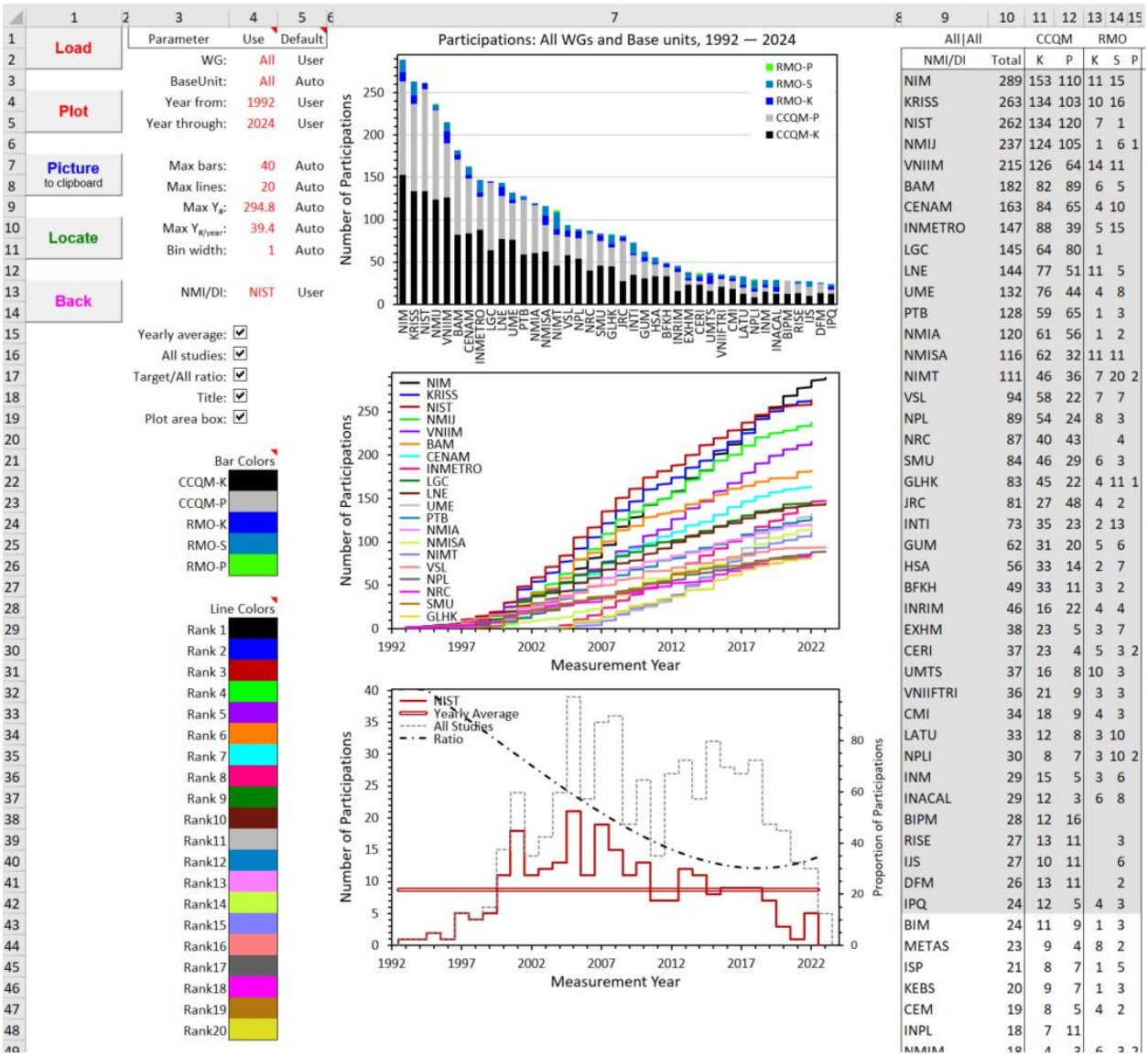


Fig. 52. *WG_Participations* Dashboard With WG and BaseUnit Set to *All*.

13.3. Chart Display Parameters

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

Max bars:	40	Auto
Max lines:	20	Auto
Max $Y_{\#}$:	294.8	Auto
Max $Y_{\#/year}$:	39.4	Auto
Bin width:	1	Auto

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. 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, BaseUnits}, the value of the "Max $Y_{\#:}$" parameter enables setting the maximum to a specified value. Changing the maximum does not affect what data are used for analysis.

13.3.4. 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, BaseUnit}, otherwise it is the largest number of participations by any of the NMI/DIs. However, to facilitate comparisons across different histogram bin widths (Section 13.3.5) and/or {WG, BaseUnits}, 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.

13.3.5. 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. 53.

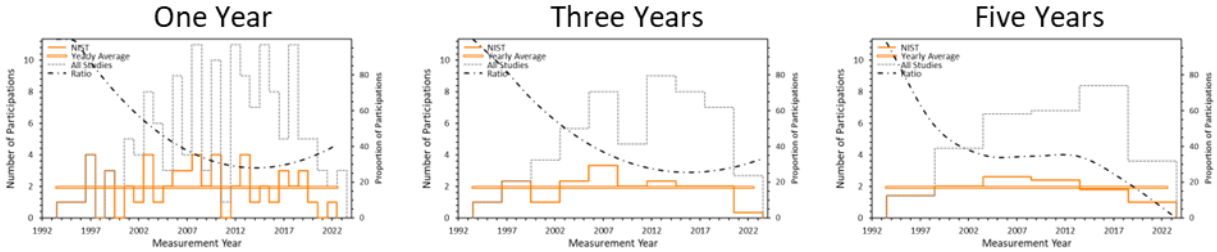


Fig. 53. *WG_Participations* Histograms With Different Bin Widths.

13.4. NMI/DI: Specifying a Target NMI/DI

NMI/DI: NIST User

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 participators, the NMI/DI's bar in chart WPa-1 and cumulative distribution in chart WPa-2 are highlighted. The charts with and without NISTas the target NMI/DI are displayed in Fig. 54.

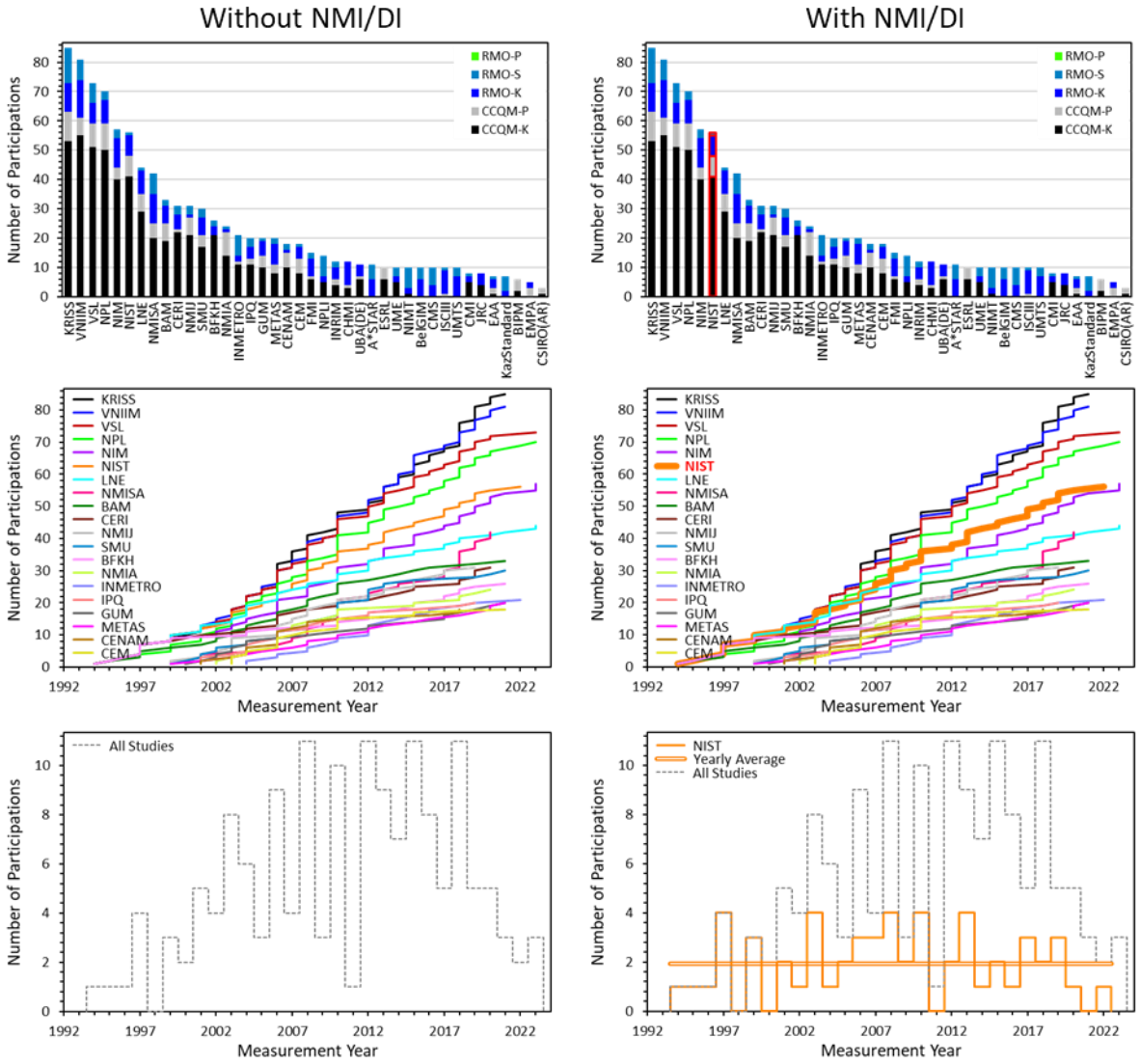


Fig. 54. *WG_Participations* Charts Without and With a "Locate"d NMI/DI.

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.

Yearly average: ☑
All studies: ☑
Target/All Ratio: ☑
Title: ☑
Plot area box: ☑

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. 55.

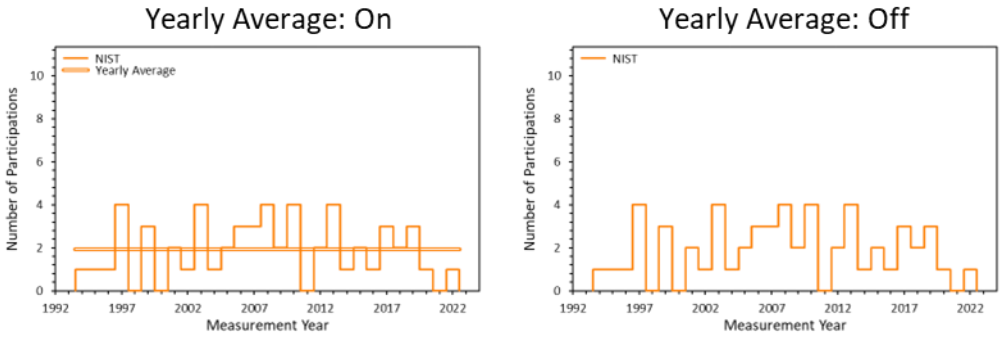


Fig. 55. *WG_Participations* Histograms With and Without Yearly Average.

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, BaseUnit}. This histogram is displayed as a dashed light grey line. NIST’s histogram with and without the All studies histogram is pictured in Fig. 56.

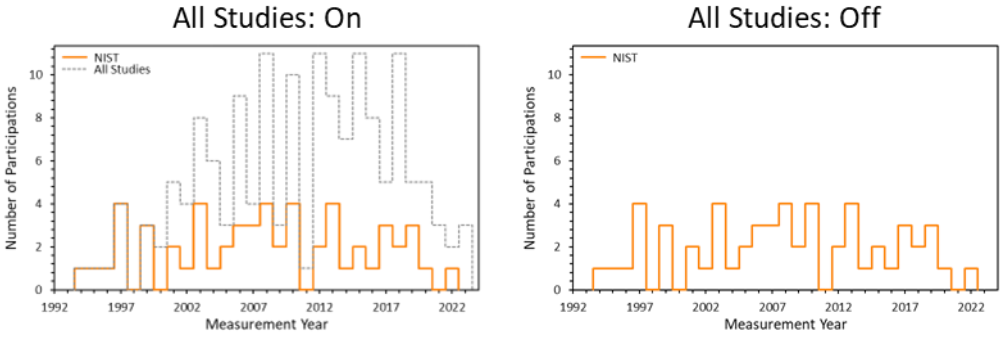


Fig. 56. *WG_Participations* Histograms With and Without All Studies.

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. 57.

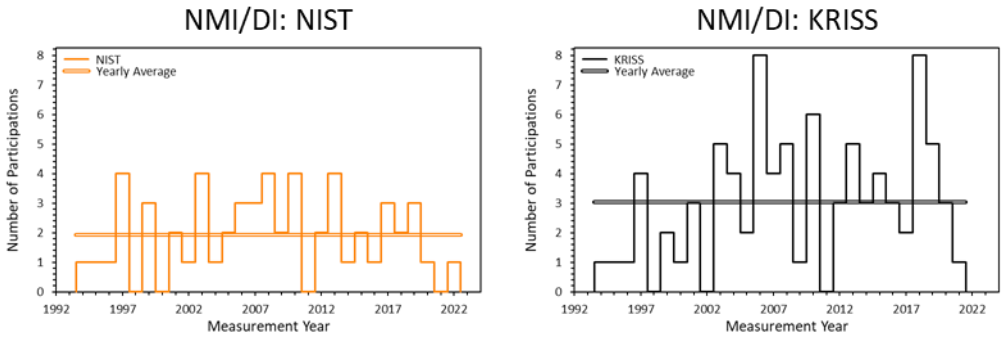


Fig. 57. *WG_Participations* Histograms With Different Target NMI/DIs.

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 trend line 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 13.3.5). This ratio is expressed as a percentage, with the (0 to 100) % scale displayed at the right edge of the chart. The trend line is displayed as a dot-dash black line.

NIST's histogram with and without the Target/All ratio line is pictured in Fig. 58.

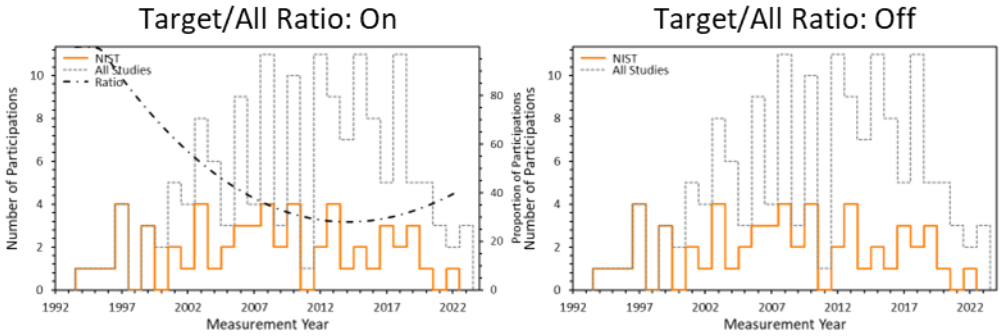
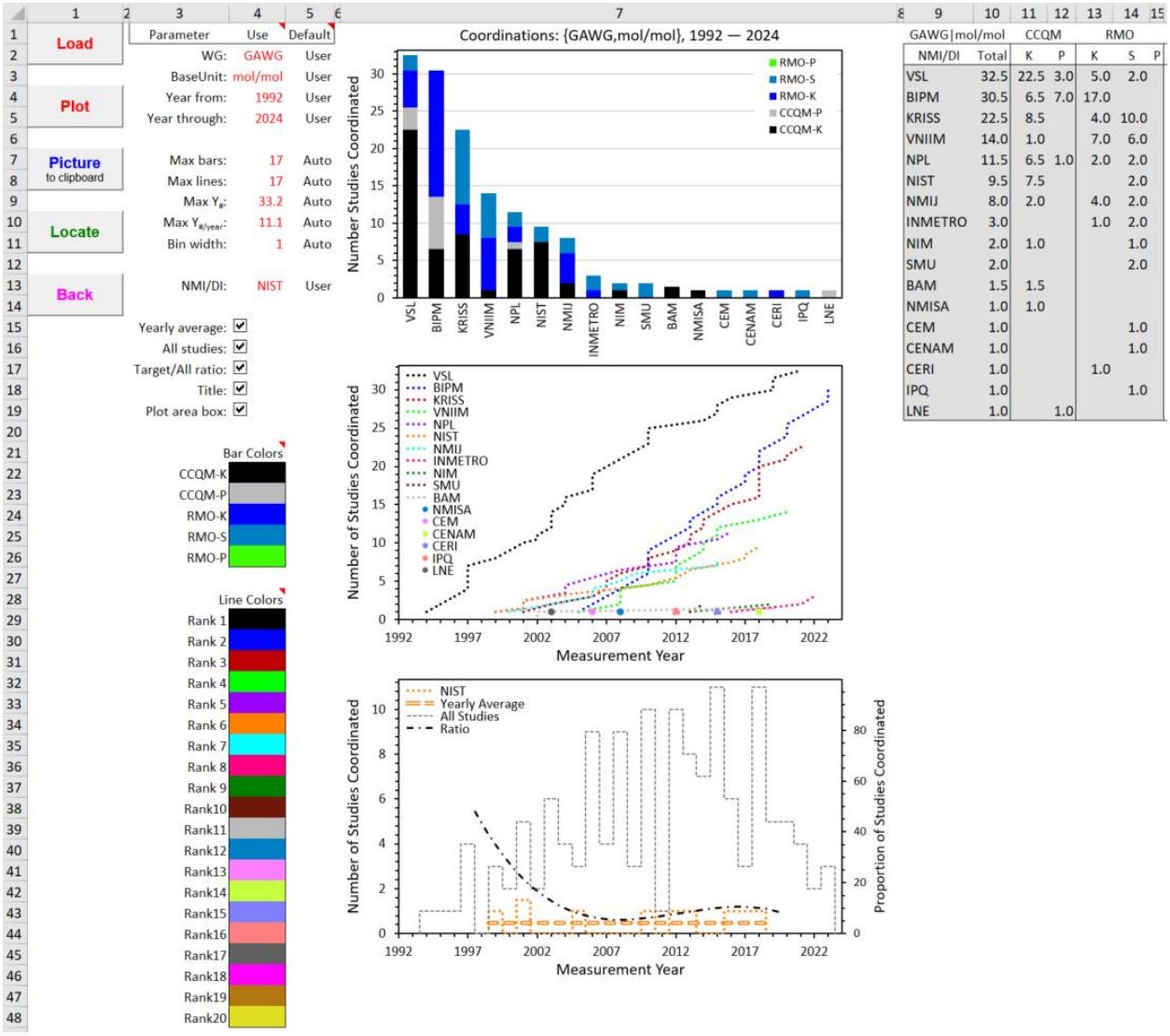


Fig. 58. *WG_Participations* Histograms With and Without the Target/All Ratio Trend Line.

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. 59.



GAWG|mol/mol		CCQM		RMO		
NMI/DI	Total	K	P	K	S	P
VSL	32.5	22.5	3.0	5.0	2.0	
BIPM	30.5	6.5	7.0	17.0		
KRISS	22.5	8.5		4.0	10.0	
VNIIM	14.0	1.0		7.0	6.0	
NPL	11.5	6.5	1.0	2.0	2.0	
NIST	9.5	7.5			2.0	
NMIJ	8.0	2.0		4.0	2.0	
INMETRO	3.0			1.0	2.0	
NIM	2.0	1.0			1.0	
SMU	2.0				2.0	
BAM	1.5	1.5				
NMISA	1.0	1.0				
CEM	1.0				1.0	
CENAM	1.0				1.0	
CERI	1.0			1.0		
IPQ	1.0				1.0	
LNE	1.0		1.0			

Fig. 59. *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 1.10 for further information.

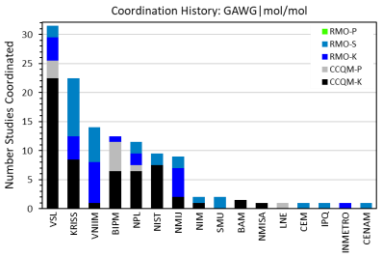
Many studies are co-coordinated. While the effort and resources expended are unlikely to be equally divided among the co-coordinators, there is no practical way to determine who did how much. Therefore, with *n* NMI/DI co-coordinators for a given study, each is assumed to have contributed $1/n^{th}$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

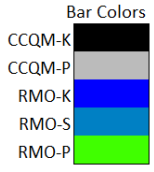
When available, the coordination information is derived from a study's final report, otherwise from the *CCQM_KCs_PSs.xlsx* workbook hosted by the BIPM [17]. Coordination information is stored in the *Datacore_Dates* worksheet. In addition to the information contained within the *CCQM_Retrospectoscope* 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.

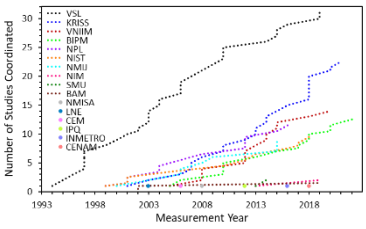
14.1. Charts



For a given {WG, BaseUnit}, 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, with BIPM here considered to be an 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.

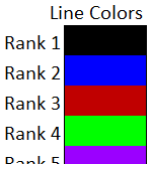


The colors used to distinguish the segments of each NMI/DI's bar are set by the "Bar Colors" area of the worksheet. These colors can be changed at will using Excel's "Fill Color" tool (the "spilling paint can" in the Font menu of the Home tab).

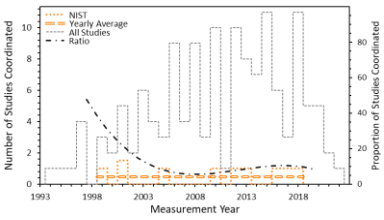


For the up-to-20 NMI/DIs with the most coordinations, the middle chart (chart WC-2) displays the cumulative number of coordinations as a function of measurement year. As in chart WC-1, the NMI/DIs are arranged by decreasing number of total coordinations. The number of NMI/DIs displayed is limited to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

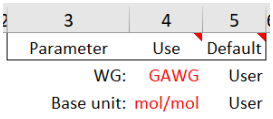
The colors used to distinguish the NMI/DIs are set by the “Line Colors” area of the worksheet. These colors can be changed at will using Excel’s “Fill Color” tool. To help distinguish the cumulative distributions for coordinations from those for participations (see Section 13), the coordination lines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



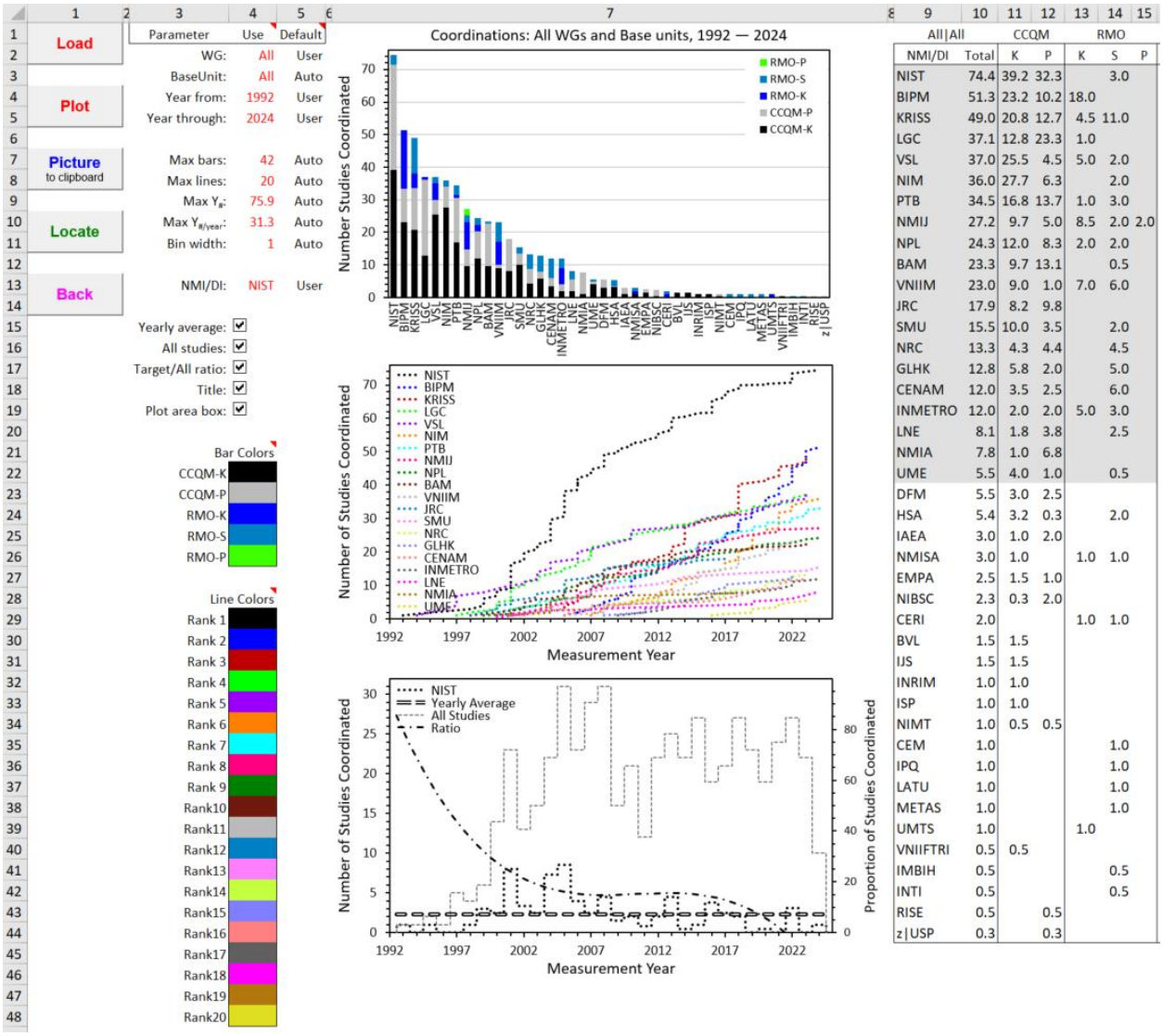
For a given NMI/DI, the bottom chart (chart WC-3) displays the number of coordinations per unit time period as a function of measurement year. The number of possible coordinations (that is, the total number of studies with a measurement year within a specified interval) can be displayed. The data are displaced as histograms. The target’s yearly average number of coordinations can also be displayed, as well as a polynomial trend line 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 BaseUnit parameters. If a particular WG is specified, setting BaseUnit 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. 60.



All|All		CCQM		RMO		
NMI/DI	Total	K	P	K	S	P
NIST	74.4	39.2	32.3		3.0	
BIPM	51.3	23.2	10.2	18.0		
KRISS	49.0	20.8	12.7	4.5	11.0	
LGC	37.1	12.8	23.3	1.0		
VSL	37.0	25.5	4.5	5.0	2.0	
NIM	36.0	27.7	6.3		2.0	
PTB	34.5	16.8	13.7	1.0	3.0	
NMIJ	27.2	9.7	5.0	8.5	2.0	2.0
NPL	24.3	12.0	8.3	2.0	2.0	
BAM	23.3	9.7	13.1		0.5	
VNIIM	23.0	9.0	1.0	7.0	6.0	
JRC	17.9	8.2	9.8			
SMU	15.5	10.0	3.5		2.0	
NRC	13.3	4.3	4.4		4.5	
GLHK	12.8	5.8	2.0		5.0	
CENAM	12.0	3.5	2.5		6.0	
INMETRO	12.0	2.0	2.0	5.0	3.0	
LNE	8.1	1.8	3.8		2.5	
NMIA	7.8	1.0	6.8			
UME	5.5	4.0	1.0		0.5	
DFM	5.5	3.0	2.5			
HSA	5.4	3.2	0.3		2.0	
IAEA	3.0	1.0	2.0			
NMISA	3.0	1.0		1.0	1.0	
EMPA	2.5	1.5	1.0			
NIBSC	2.3	0.3	2.0			
CERI	2.0			1.0	1.0	
BVL	1.5	1.5				
IJS	1.5	1.5				
INRIM	1.0	1.0				
ISP	1.0	1.0				
NIMT	1.0	0.5	0.5			
CEM	1.0				1.0	
IPQ	1.0				1.0	
LATU	1.0				1.0	
METAS	1.0				1.0	
UMTS	1.0			1.0		
VNIIFTRI	0.5	0.5				
IMBIH	0.5				0.5	
INTI	0.5				0.5	
RISE	0.5		0.5			
z|USP	0.3		0.3			

Fig. 60. *WG_Coordinations* Dashboard With WG and BaseUnit Set to *All*.

14.3. Chart Display Parameters

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

Max bars:	17	Auto
Max lines:	17	Auto
Max $Y_{\#}$:	33.2	Auto
Max $Y_{\#/year}$:	11.1	Auto
Bin width:	1	Auto

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. Max $Y_{\#}$: *y*-Axis Maximum for Charts WC-1 and WC-2

By default, the maximum *y*-axis (number of studies) 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, BaseUnits}, the value of the “Max $Y_{\#:}$” parameter enables setting the maximum to a specified value. Changing the maximum does not affect what data are used for analysis.

14.3.4. Max $Y_{\#/year}$: *y*-Axis Maximum for Chart WC-3

By default, the maximum *y*-axis (number ofstudies) 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, BaseUnit}, otherwise it is the largest number of coordinations by any of the NMI/DIs. However, to facilitate comparisons across different “Bin width:” and/or {WG, BaseUnits}, 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.

14.3.5. 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. 61.

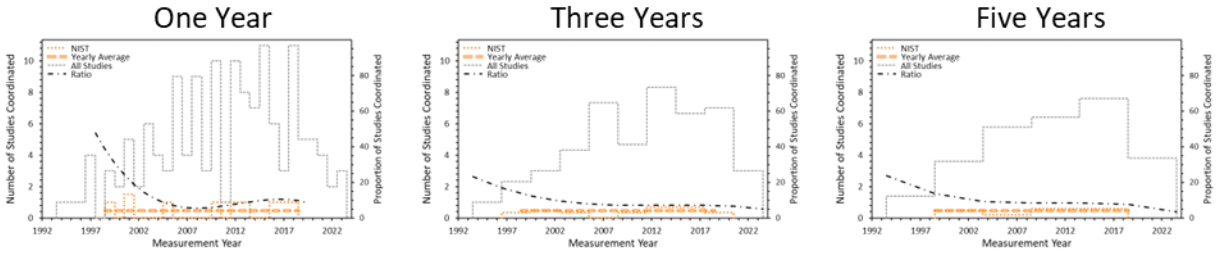


Fig. 61. *WG_Coordinations* Histograms With Different Year Intervals.

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 as the target NMI/DI are displayed in Fig. 62.

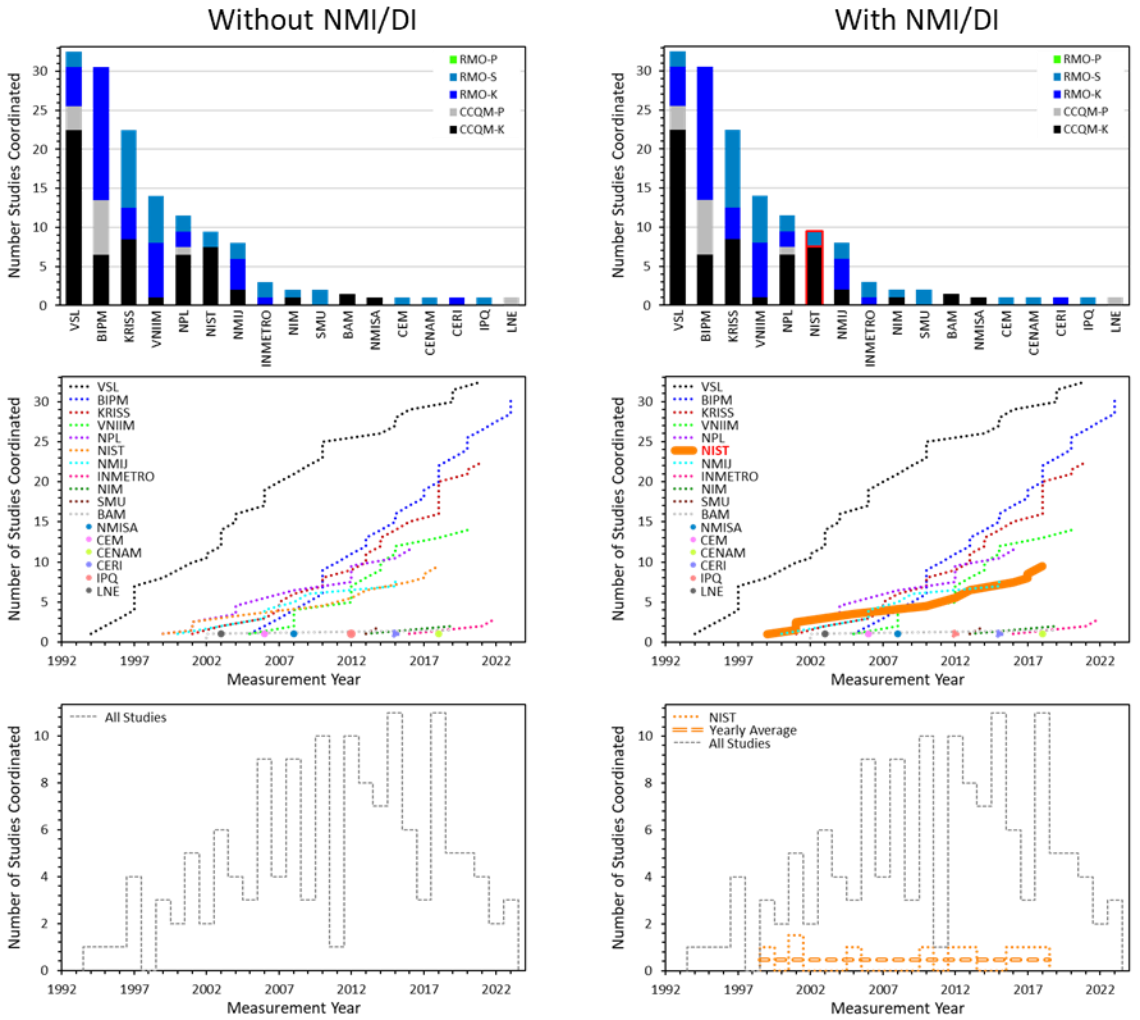


Fig. 62. *WG_Coordinations* Charts With and Without Target NMI/DI Highlighted.

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. 63.

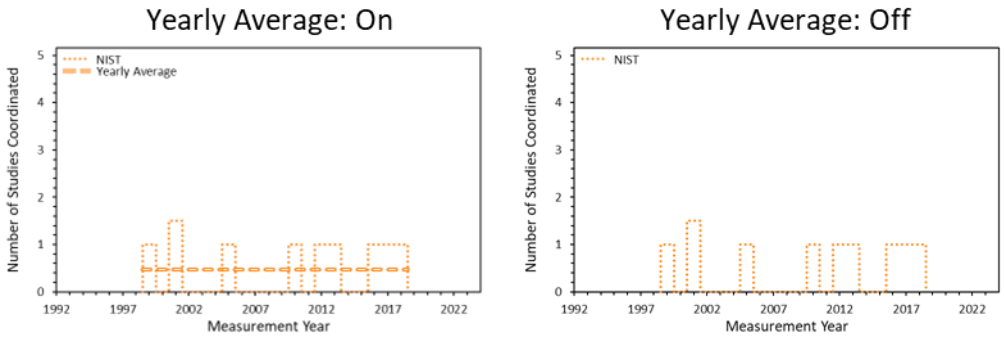


Fig. 63. *WG_Coordinations* Histograms With and Without Yearly Average.

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, BaseUnit}. This histogram is displayed as a dashed light grey line. NIST's histogram with and without the All studies histogram is pictured in Fig. 64.

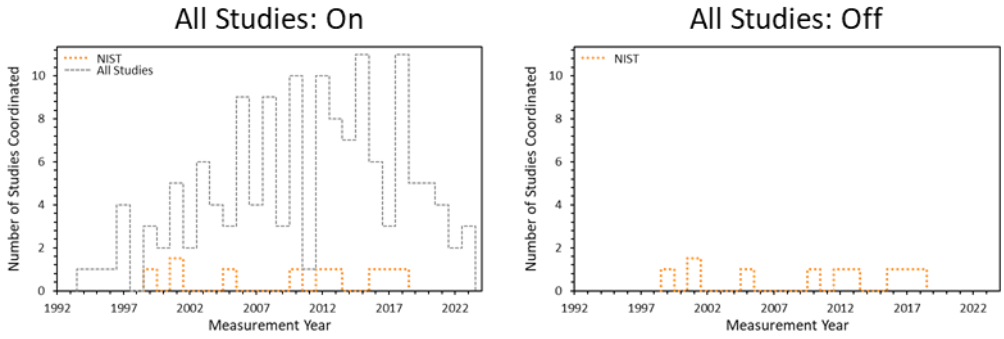


Fig. 64. *WG_Coordinations* Histograms With and Without the All Studies.

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. 59). However, as shown in Fig. 65, KRISS has provided the most within a single measurement year.

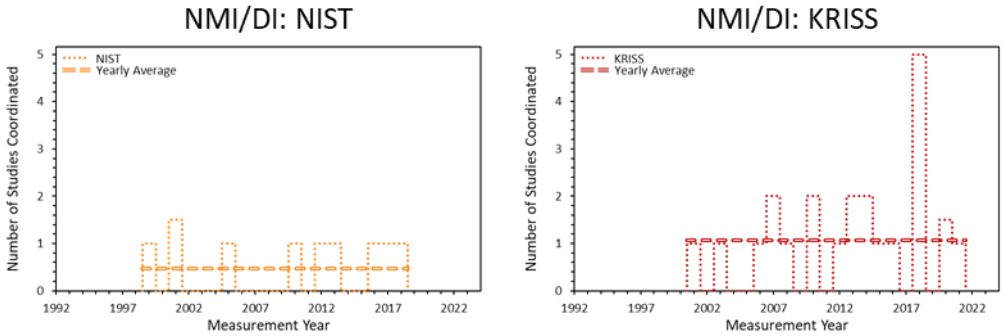


Fig. 65. *WG_Coordinations* Histograms for VSL and KRISS.

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 trend line 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 14.3.5). This ratio is expressed as a percentage, with the (0 to 100) % scale displayed at the right edge of the chart. The trend line is displayed as a dot-dash black line.

NIST’s histogram with and without the Target/All ratio line is pictured in Fig. 58.

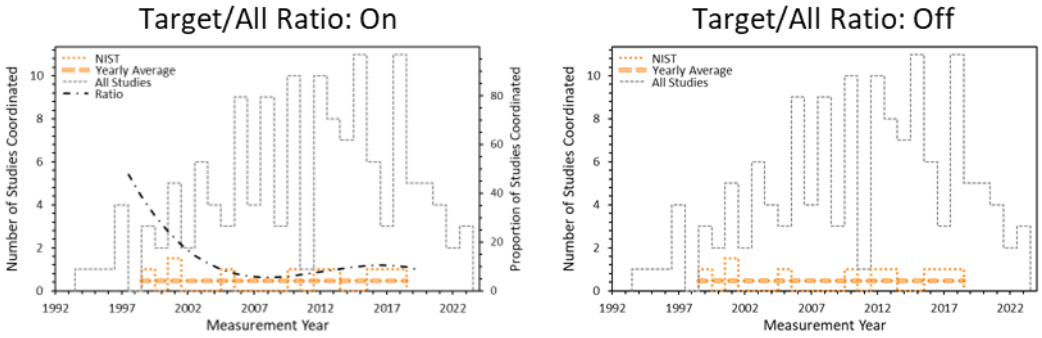


Fig. 66. *WG_Coordinations* Histograms With and Without the Target/All Ratio Trend Line.

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. 67. The in-common data selection and chart display parameters and controls are discussed in Section 2.

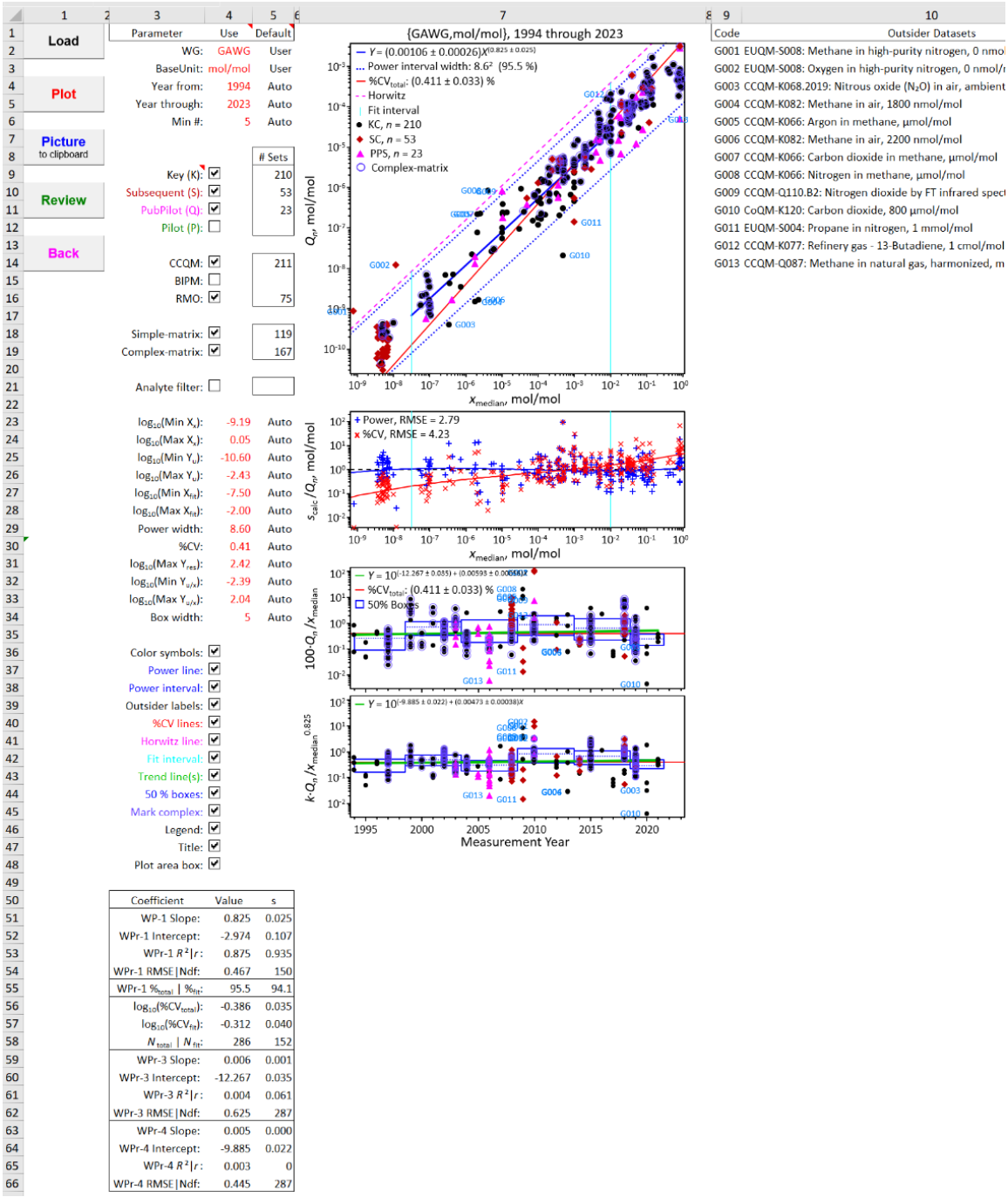


Fig. 67. *WG_Precision* Dashboard.

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 1.10 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 (here defined as $\%\text{CV} = 100 \cdot Q_n/x_{\text{median}}$) 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: $Q_n/x_{\text{median}}^{p}$. Chart WPr-1 visualizes the relevant data and the potential relationships.

The %CV can be expressed as a one-parameter power-law curve, $Q_n = \beta_0 x_{\text{median}}$, where the power is 1 and β_0 is the %CV. The two-parameter power-law curve, $Q_n = \beta_0 x_{\text{median}}^{\beta_1}$, has been observed to describe the relationship between measurement reproducibility and value of the measurand expressed as fractional concentration in many interlaboratory studies of many different measurands [3,4,5]. The chart (chart WPr-2) immediately below chart WPr-1, displays the residuals between the reported uncertainties and predictions made using the two uncertainty function models. The residuals are calculated as $\log_{10}(s_{\text{calc}}) - \log_{10}(Q_n)$; since these differences are plotted on a logarithmic *y*-axis, the axis is labeled with the linearized formulation s_{calc}/Q_n. The values for the parameters of both functions are derived from the results shown in chart WPr-1.

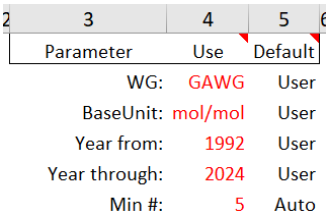
The next chart (chart WPr-3) displays the %CV as a function of measurement year. In addition to visualizing when measurements were made and the median %CV during the specified time period, the chart enables estimating the change in the magnitude of relative reproducibility over time.

The bottom chart (chart WPr-4) displays a value-corrected relative reproducibility expressed as %CV, $Q_n/x_{\text{median}}^{\beta_1}$, 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, $Q_n/x_{\text{median}}^{\beta_1}$ will be larger than Q_n/x_{median}. Since $1^{\beta_1} = 1$ for all exponent values, the difference between $100 \cdot Q_n/x_{\text{median}}$ and $100 \cdot Q_n/x_{\text{median}}^{\beta_1}$ 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, BaseUnit} 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 $\{x_{\text{median}}, Q_n\}$ values, these charts display the $\log_{10}$-transformation of the values.

15.2. Additional Data Specification Parameter

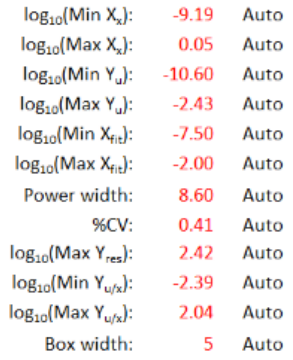


In additional to the four in-common parameters described in Section 2.4.1, there is one additional data specification parameter.

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



The *WG_Precision* worksheet contains twelve 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 areused 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 used for analysis.

15.3.3. $\log_{10}$(Min X_{fit}) and $\log_{10}$(Max X_{fit}): *x*-Axis Regression Limits

For some {WG, BaseUnit} 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 [16], are -7.5 (a fractional value of ≈3.2 ×10^{-8}) and -2.0 (a fractional value of 0.01).

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

15.3.4. Power width: Outsider 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}: $Q_n = \beta_0 x_{\mathrm{median}}^{\beta_1}$ [2]. Parameterization is accomplished by linear regression on $\log_{10}$-transformed values: $\log_{10}(Q_n) = \log_{10}(\beta_0) + \beta_1 \log_{10}(x_{\mathrm{median}})$. The "Power width:" parameter defines a symmetric interval centered on the power-law curve that 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 w) defines an interval about the power-law curve that includes all datasets with Q_n values that are within a factor *w* of the value predicted by the power-law; i.e., the interval includes the observed $\{x_{\mathrm{median}}, Q_n\}$ values from $(\beta_0/w)x_{\mathrm{median}}^{\beta_1}$ to $(\beta_0 \cdot w)x_{\mathrm{median}}^{\beta_1}$. 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 $\{x_{\mathrm{median}}, Q_n\}$ if they are approximately normally distributed. Transformed into a multiplicative factor, the default value of w is $10^{2 \cdot \mathrm{RMSE}}$.

15.3.5. %CV: %CV lines

The "%CV:" parameter defines a robust coefficient of variation (%CV, relative standard deviation expressed as a percentage) characteristic of the selected data. The %CV can be visualized as a line in chart WPr-1 and (in derived form) the other charts. The default value for %CV is the median of all the reported $100 \cdot Q_n/x_{\mathrm{median}}$ 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 used for analysis.

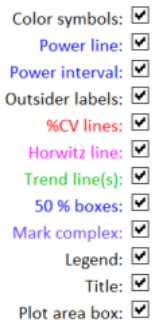
15.3.7. $\log_{10}$(Min $Y_{u/x}$) and $\log_{10}$(Max $Y_{u/x}$): *y*-Axis Limits for WPr-3 and WPr-4

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 (%CV) of chart WPr-3 and the power-law corrected *y*-axis (adjusted %CV) 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 used 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. 68. 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.

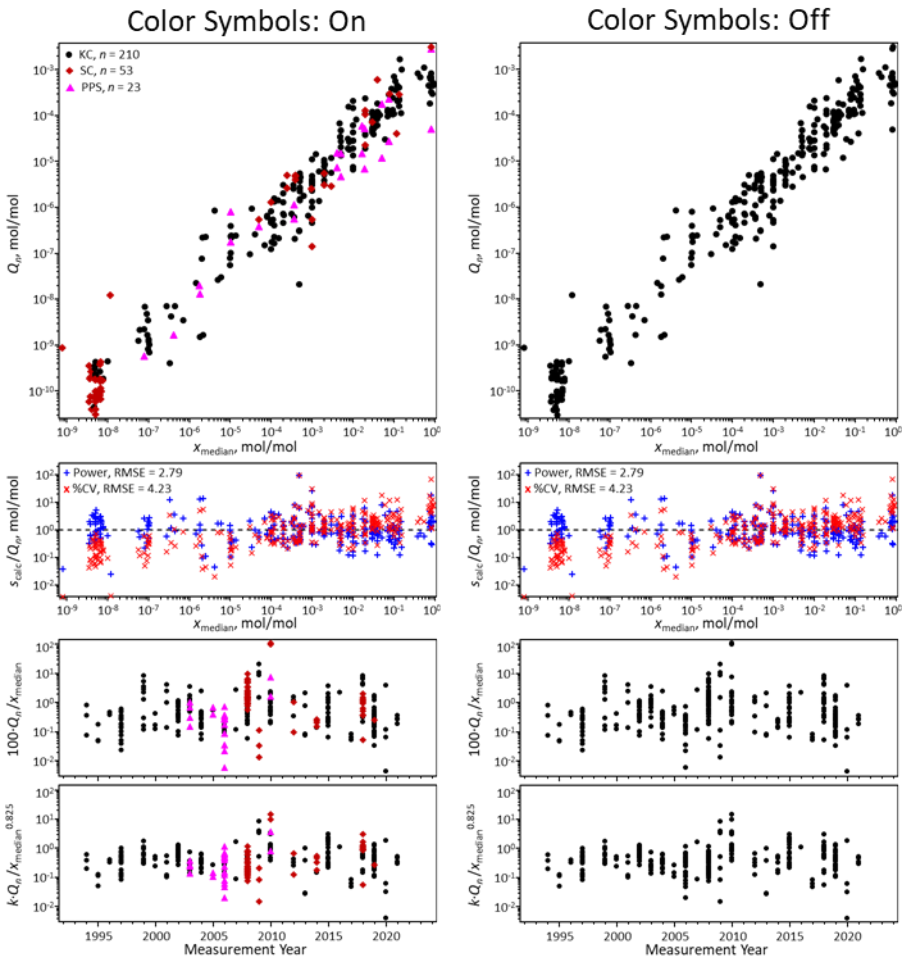
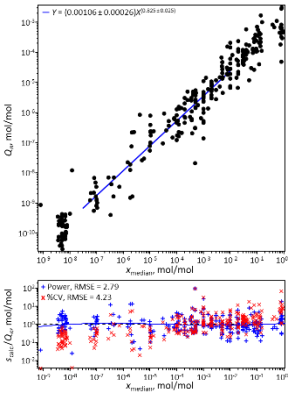


Fig. 68. *WG_Precision* Charts With Color-Coded and All-Black Symbols.

15.4.2. Power line

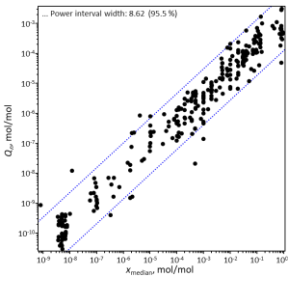


In chart WPr-1, clicking the "Power line:" checkbox toggles the display of a regression estimate of the power-law function: $Q_n = \beta_0 \, x_{\text{median}}^{\beta_1}$. Since both the x_{median} and Q_n axes are logarithmic, this is parameterized as: $\log_{10}(Q_n) = \log_{10}(\beta_0) + \beta_1 \log_{10}(x_{\text{median}})$. 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, $\log_{10}(\beta_0) + \beta_1 \log_{10}(x_{\text{median}}) - \log_{10}(Q_n)$, to $\log_{10}(x_{\text{median}})$. The resulting line is displayed for the entire width of the chart, not just the interval used to parameterize the power-law curve.

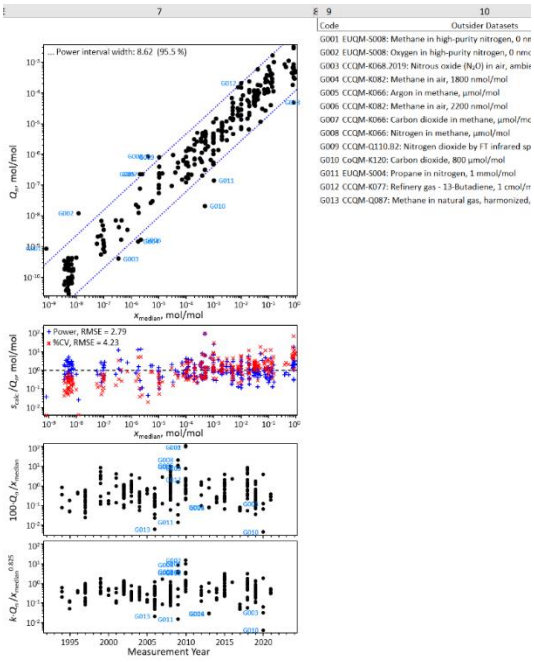
In both chart WPr-1 and WPr-2, the power-law-derived relationships are displayed as solid blue lines. Charts WPr-3 and WPr-4 are not affected by this control.

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 interval:” parameter described in Section 15.3.4. The interval is displayed as two dashed blue lines. Using the default value, about 95 % of the $\{x_{\text{median}}, Q_n\}$ 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).

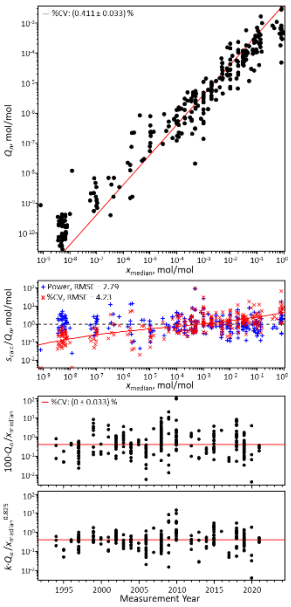
15.4.4. Outsider labels



If there are outsider results (i.e., outside the Power interval), clicking the “Outsider labels:” checkbox toggles their display in charts WPr-1, WPr-3, and WPr-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 21).

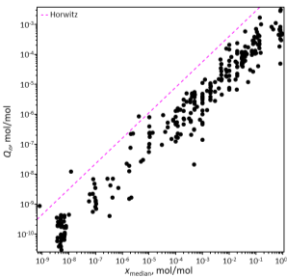
15.4.5. %CV lines



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, $\log_{10}(\%\text{CV} \cdot x_{\text{median}}/100) - \log_{10}(Q_n)$, as a function of $\log_{10}(x_{\text{median}})$. These relationships are displayed as solid red lines.

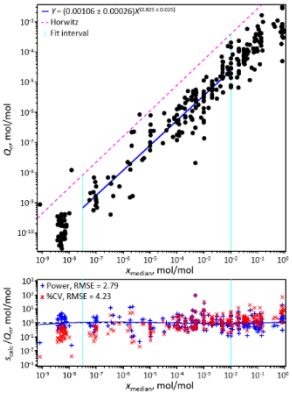
The %CV value is specified by the “%CV:” parameter described in Section 15.3.5.

15.4.6. Horwitz line



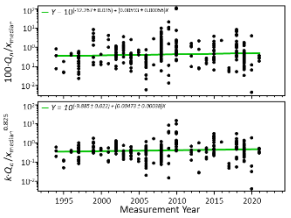
Clicking the "Horwitz line:" checkbox toggles chart WPr-1's display of the Horwitz relationship between reproducibility and analyte concentration [3]. The relationship, shown as a dashed magenta line, is a power-law with coefficients a = 0.02 and b = 0.8495. These values are derived from the rather obscure 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. Fit interval



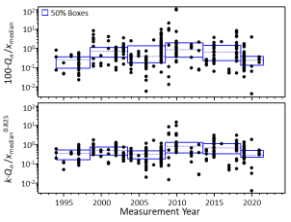
Clicking the "Fit interval:" checkbox toggles display of lines that bound the regression interval, $\log_{10}(\text{Min } X_{fit})$ to $\log_{10}(\text{Max } X_{fit})$, in charts WPr-1 and WPr-2. Only the {Median,Q_n} pairs within this interval are used to estimate the power function. To emphasize the interval's Horwitz function origin, in chart WPr-1 the upper end of the bounding lines terminate on the Horwitz line.

15.4.8. Trend line(s)



Clicking the "Trend line(s):" checkbox toggles the display of robust Thiel-Sen linear trend lines [14,15] in the WPr-3 and WPr-4 charts. The regession uses all results displayed in each chart. In chart WPr-3, the y-axis metric is the estimated %CV. In chart WPr-4, the y-axis metric is the estimated %CV after correcting for the observed power function relationship.

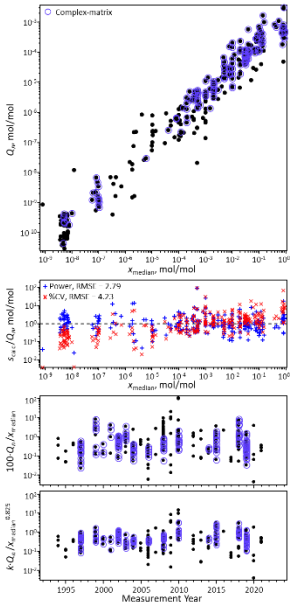
15.4.9. 50 % boxes



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 x-axis (measurement year). 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.

15.4.10. Mark complex

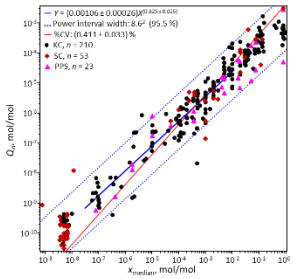
Clicking the “Mark complex:” checkbox toggles the identification of results for complex-matrix materials. This option is only relevant when simple-matrix and complex-matrix datasets are analyzed together. Complex-matrix datasets are identified with a surrounding purple circle.



15.4.11. Legend Entries

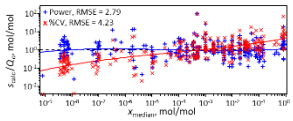
As described in Section 2.2.3.1, clicking the “Legend:” checkbox toggles the display of the legend. The optional features have a legend entry when (and only when) active. In addition to identifying the graphical elements, some of the entries provide quantitative information.

In Chart WPr-1:



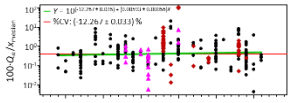
- if “Power line:” is checked the power-law equation is listed.
- if “Power interval:” is checked the multiplicative width and the percent of the $\{x_{\text{median}}, Q_n\}$ values within the lines are listed.
- if "%CV:” is checked the median of the $100 \cdot Q_n/x_{\text{median}}$ values is listed.
- if the symbols are shown colored, the number of each type of study is listed.

In chart WPr-2:



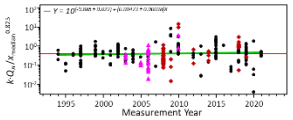
- the RMSE of the power and %CV uncertainty function residuals are displayed. The RMSE is defined as $\sqrt{\sum_1^n d_i^2/(n-m)}$, where d_i is the residual for one $\{x_{\text{median}}, Q_n\}$, n is the number of $\{x_{\text{median}}, Q_n\}$, and m is the number of parameters in the uncertainty function.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

In chart WPr-3:



- if “Trend line(s):” is checked the trend equation for $100 \cdot Q_n/x_{\text{median}}$ over time is listed.
- if “%CV:” is checked the median of the $100 \cdot Q_n/x_{\text{median}}$ values is listed.

In chart WPr-4:



- if “Trend line(s):” is checked the trend equation for the power-law-adjusted $100 \cdot Q_n/x_{\text{median}}$ over time is listed.

15.5. Stored Coefficients

Coefficient	Value	s
WP-1 Slope:	0.825	0.025
WPr-1 Intercept:	-2.974	0.107
WPr-1 $R^2 \mid r$:	0.875	0.935
WPr-1 RMSE|Ndf:	0.467	150
WPr-1 $\%_{total} \mid \%_{fit}$:	95.5	94.1
$\log_{10}(\%CV_{total})$:	-0.386	0.035
$\log_{10}(\%CV_{fit})$:	-0.312	0.040
$N_{total} \mid N_{fit}$:	286	152
WPr-3 Slope:	0.006	0.001
WPr-3 Intercept:	-12.267	0.035
WPr-3 $R^2 \mid r$:	0.004	0.061
WPr-3 RMSE|Ndf:	0.625	287
WPr-4 Slope:	0.005	0.000
WPr-4 Intercept:	-9.885	0.022
WPr-4 $R^2 \mid r$:	0.003	0
WPr-4 RMSE|Ndf:	0.445	287

The first four lines of the coefficient storage block store the regression coefficients and fit statistics for the Chart WPr-1 power function:

- slope and its standard error.
- intercept and its standard error.
- square of the Pearson correlation (R^2) of the fit and the imputed correlation between the slope and intercept (r).
- root-mean square error residual (RMSE) and number of degrees of freedom (ndf).

The fifth line stores the percent of all results that fall within the Chart WPr-1 power interval ($\%_{total}$) and the percent of results within the region bounded by the power interval and the regression fit interval ($\%_{fit}$).

The sixth through eighth lines store values related to the coefficient of variation (%CV) that is used (one way or another) in all four charts:

- median and $Q_n/\sqrt{N_{\text{total}}}$ of $\log_{10}(100 \cdot u(x)/x)$ for all N_{total} results displayed.
- median and $Q_n/\sqrt{N_{\text{fit}}}$ of $\log_{10}(100 \cdot u(x)/x)$ for all N_{fit} results that are within the Horwitz regression interval, $\log_{10}(\text{Min X}_{\text{fit}})$ to $\log_{10}(\text{Max X}_{\text{fit}})$. These values are not used by the current *CCQM_Retrospectoscope* system.
- N_{total} and N_{fit}. Note: N_{fit}.should be equal to two more than the regression ndf.

The ninth through twelfth lines store the Chart WPr-3 trendline slopes, intercepts, R^2, r, RMSE, and ndf. The last four lines store these values for Chart WPr-4.

These values are stored below the radio buttons. They are generated during the analysis and are stored whether or not the graphical elements they relate to are displayed.

15.6. An Additional Filter for the Obsessive

The *WG_Precision* subsystem uses results from datasets that pass selected WG, BaseUnit, year span, study type, sponsoring body, and sample type filters. However, it also supports the capability of filtering on participant code. For each {WG, BaseUnit}, results are accepted only for participants listed in the corresponding column of the *Dataset_NMI/DI* worksheet (see Section 22). 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, 56 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 56 NMI/DIs; for the 14 “Core” NMI/DIs that started participating before 2000 and have participated in a recent study; and for the 42 “Non-Core” NMI/DIs who were not early participants and/or have not recently participated are compared in Fig. 69.

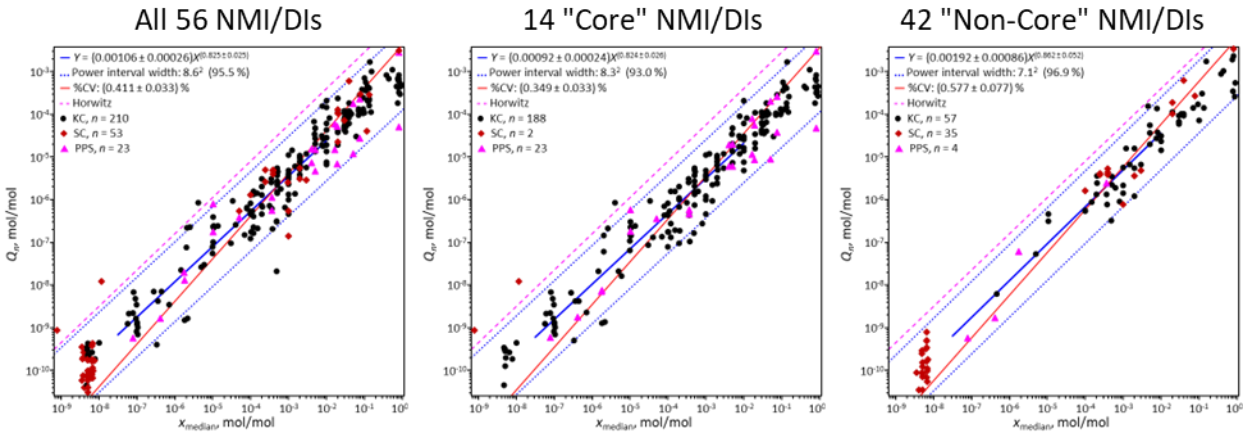


Fig. 69. *WG_Precision* Chart With and Without NMI/DI Filtering.

The similarity in the results for the “All 56” 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 27) 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* 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. 70.

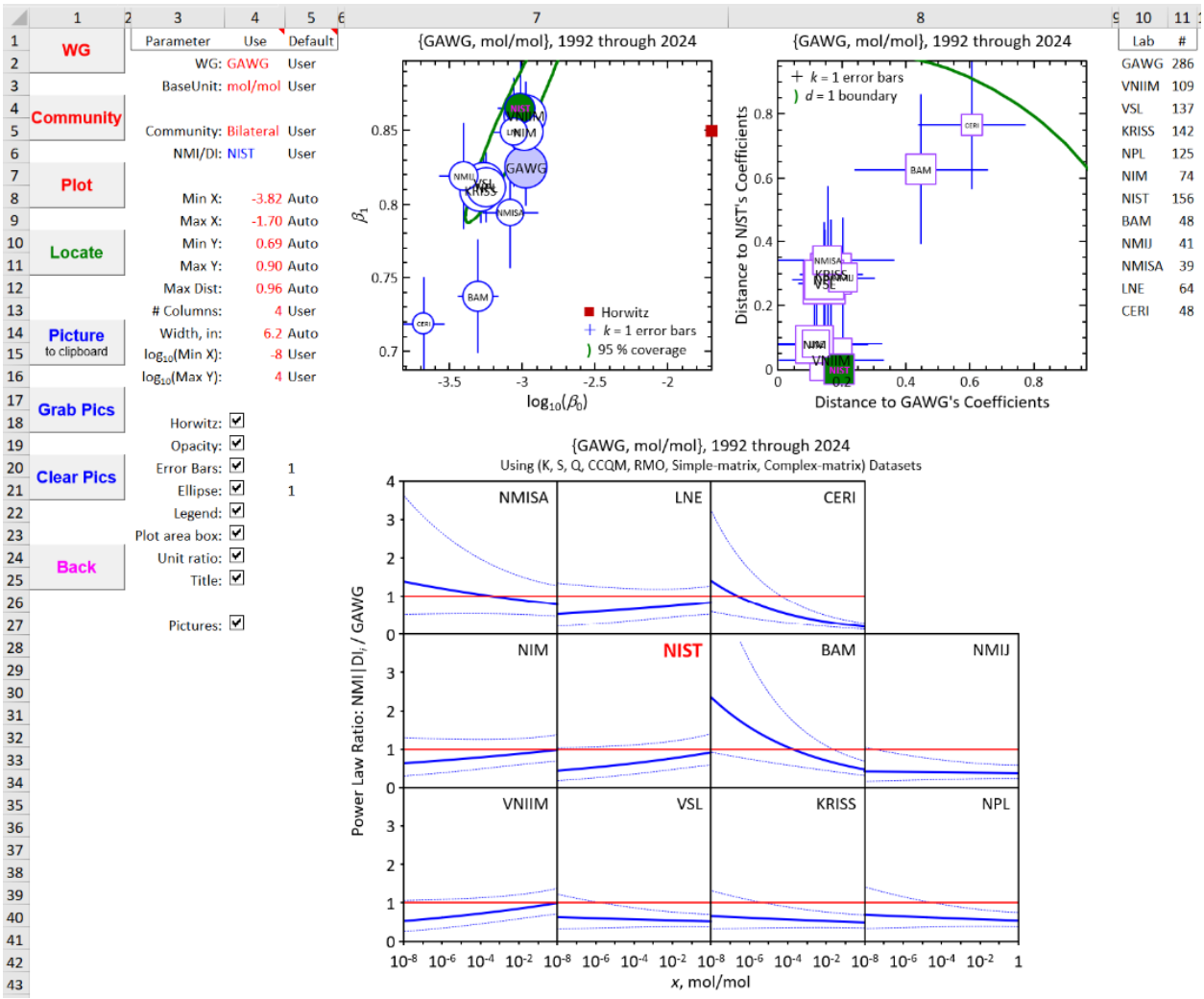
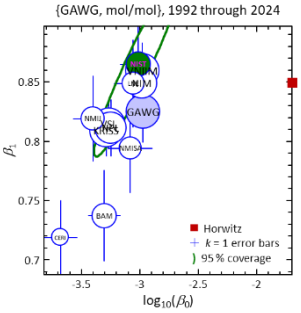


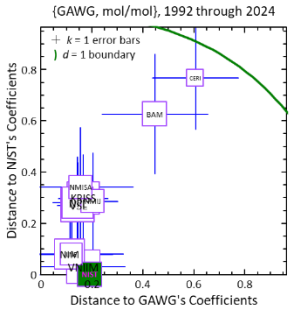
Fig. 70. *WG_Power* Dashboard.

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 1.10 for further information.

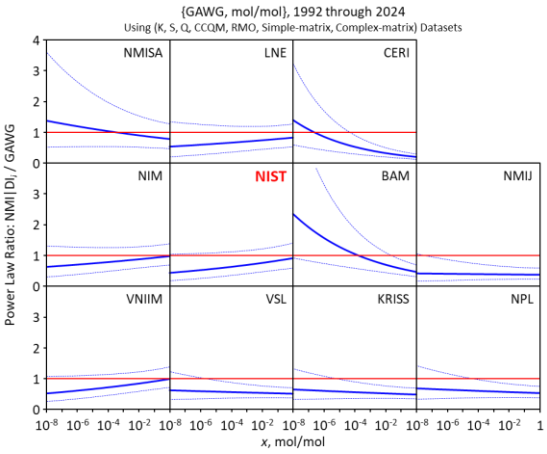
16.1. Charts



The chart to the upper left, WPo-1, plots the power-law exponent, β_1, as a function of the decadic logarithm of the scale factor, $\log_{10}(\beta_0)$. The area of each open circle symbol for a given $\{\log_{10}(\beta_0), \beta_1\}$ pair is proportional to the number of degrees of freedom (heading **ndf**, col 13 in Fig. 70) used in estimating the coefficients. The symbol for the WG's $\{\log_{10}(\beta_0), \beta_1\}$ is colored blue. The symbols for NMI/DIs are uncolored, except that a "**Locate**"d NMI/DI is colored dark green.



The chart to the upper right, WPo-2, plots the empirical Δ_{ij} distance from a "**Locate**"d NMI/DI's $\{\log_{10}(\beta_0), \beta_1\}$ to those of the other NNMI/DIs as a function of the Δ_{ij} distance from the WG's $\{\log_{10}(\beta_0), \beta_1\}$ to the NMI/DIs' coefficients. Since the exponent and decadic logarithm of the scale coefficients have different scale, both parameters are normalized by the range of their values (see Section 1.9.6). To compare results across datasets, it is necessary to specify the value of the "Max Dist:" parameter (see Section 16.5.3).



The lower chart (WPo-3) 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*, $Q_n = \beta_0 x_{\text{median}}^{\beta_1}$. The nominator in each segment is the power-law for one of the NMI/DI from *Lab_Uncertainty*, $u(x) = \beta_0 x^{\beta_1}$. A thick solid blue curve displays the ratio. Lighter dotted curves above and below the ratio represent the one standard uncertainty interval about the ratio, calculated using the regression-estimated standard errors of the parameters. A thin solid rad line displays a unit ratio, where the values estimated by the numerator and denominator functions are equal. Where the ratio (blue line) is below the unit ratio (red line), the NMI/DI's estimated measurement uncertainties are smaller than the WG community's measurement reproducibility.

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 *Peer_Bilateral* 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 *x*-axis (mole fraction or mass fraction) of the bottom row is fully labelled.

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 "BaseUnit:" 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* or *Peer_Global* and then estimates the power-law coefficients for each NMI/DI using the *Lab_Uncertainty* subsystem. Which of *Peer_Bilateral* or *Peer_Global* 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. If the community was identified by *Peer_Bilateral*, the target NMI/DI will be "**Locate**"d.

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.

16.2.4. Clear Pics

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

16.3. Community NMI/DI Selection Parameter

Community: Bilateral User
NMI/DI: NIST

The "Community:" parameter specifies which subsystem is used to identify the NMI/DIs: *Peer_Bilateral* or *Peer_Global*. If "Bilateral" is specified, the community will be defined as the peers of the NMI/DI that is specified in the *Peer_Bilateral* subsystem. The identity of that NMI/DI is echoed as the target NMI/DI immediately beneath the Community keyword. If "Global" is specified, the community is defined without reference to a target NMI/DI and the cell immediately beneath the keyword is set to "Not used". The default value is "Bilateral".

Note: The *Peer_Unilateral* subsystem identifies the same peer NMI/DIs as does *Peer_Bilateral* and thus is not used for community identification.

16.4. Store Pictures Checkbox

Pictures: ☑

The "Pictures:" checkbox controls whether PNG-format pictures of the various analyses are generated and stored in column 101 of the *WG_Power* worksheet. The default value is checked (i.e., *True,* a pictorial record is made).

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".

16.5. Chart Display Parameters

Min X:	-3.82	Auto
Max X:	-1.70	Auto
Min Y:	0.69	Auto
Max Y:	0.90	Auto
Max Dist:	0.96	Auto
# Columns:	4	User
Width, in:	6.2	Auto
$\log_{10}$(Min X):	-8	User
$\log_{10}$(Max Y):	4	User

The *WG_Power* subsystem has nine parameters, four that control the *x*- and *y*-axis limits of chart WPo-1, one that controls the *x*- and *y*-axis limits of chart WPo-2, and four that control the shape, and *x*- and *y*-axis limits of WPo-3.

16.5.1. Min X and Max X: *x*-Axis Limits for Chart WPo-1

The minimum and maximum limits for Chart WPo-1's *x*-axis (power-law scale, $\log_{10}(\beta_0)$), are specified by the values of the "Min X:" and "Max X:" parameters. The default values for these limits are the minimum and maximum of the $\log_{10}(\beta_0) \pm u(\log_{10}(\beta_0))$ estimates. Modifying the limits does not affect what data are used for analysis.

The span defined by these parameter values is used to range-scale the $\log_{10}(\beta_0)$ coefficients used in the distances displayed in chart WPo-2 (see Section 1.9.6).

16.5.2. Min Y and Max Y: *y*-Axis Limits for Chart WPo-1

The minimum and maximum limits for Chart WPo-1's *y*-axis (power-law exponent, β_1) are specified by the values of the "Min Y:" and "Max Y:" 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 used for analysis.

The span defined by these parameter values is used to range-scale the β_1 coefficients used in the distances displayed in chart WPo-2 (see Section 1.9.6).

16.5.3. Max Dist: *x*- and *y*-Axis Limits for Chart WPo-2

The maximum for both Chart WPo-2's *x*- and *y*-axes between coefficient distances, Δ_{ij}, is specified by the value of the "Max Dist:" parameter. The default value is the maximum of the $\Delta_{ij} \pm u(\Delta_{ij})$ estimates. The minimum value for both axes is fixed at 0.

16.5.4. # 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.

16.5.5. Width, in: Chart width in Inches

The value of the "Width, in:" parameter sets the horizontal size of chart WPo-3 in inches. Currently, the width must be between (2 and 9) in. The default value is 6.2 in.

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

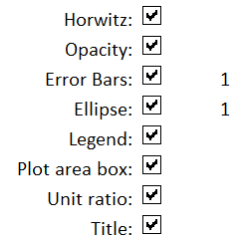
The value of the "$\log_{10}$(Min X):" parameter is the smallest concentration value, X_{min}, for which the power-law ratio is displayed in each segment of chart WPo-2. The currently allowed values are -10, -8, and -6. The default value is -8. The maximum $\log_{10}$(concentration) is fixed at 0.

16.5.7. 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 eight checkboxes that control various chart elements. The first six apply to both WPo-1 and WPo-2, the seventh applies only to chart WPo-3, and the last applies to all three charts.



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}: see Fig. 71. When the “Min X:”, “Max X:”, “Min Y:”, and/or “Max Y:” 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.

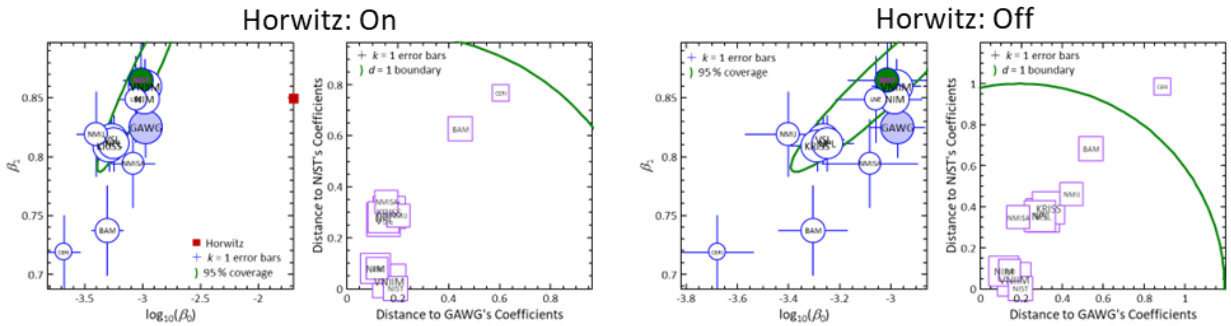


Fig. 71. *WG_Power* Chart WPo-1 With and Without Horwitz Display.

Note: Because the Δ_{ij} distances displayed in chart WPo-2 are estimated from $\{\log_{10}(\beta_0), \beta_1\}$ values normalized by the span of the corresponding axes in chart WPo-1 (see Section 1.9.6), changes in the WPo-1 display can change the WPo-2 distances. To compare results across datasets, it is necessary to specify the value of the “Max Dist:” parameter (see Section 16.5.3).

16.6.2. Opacity

Clicking the “Opacity:” checkbox toggles charts WPo-1 and WPo-2 between displaying opaque and transparent symbols: see Fig. 72. This enables identifying the location of NMI/DI symbols that are hidden under other symbols. The symbol for the WG power-law in chart WPo-1 is always opaque blue. If an NMI/DI has been “**Locate**”d, it’s symbol in both WPo-1 and WPo-2 is opaque dark green.

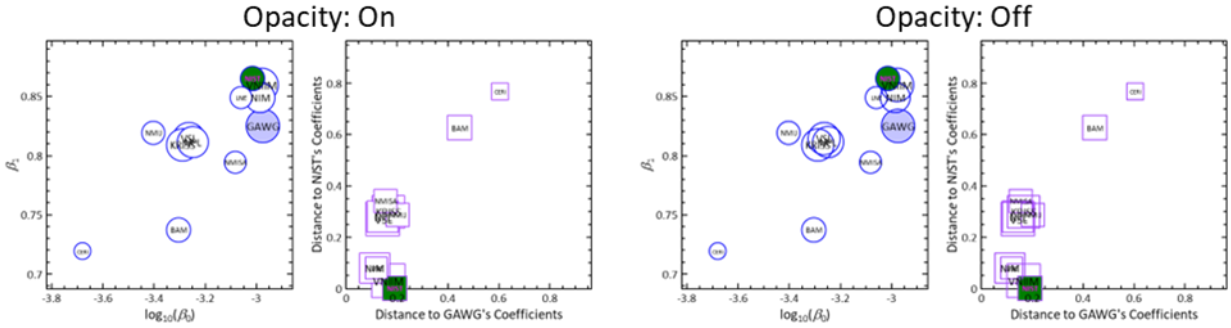


Fig. 72. *WG_Power* Charts WPo-1 WPo-2 With and Without Symbol Opacity.

16.6.3. Error bars

Clicking the “Error bars:” checkbox toggles the display of the error bars: see Fig. 73. The error bars in chart WPo-1 span ±(one standard estimate of error)×(scale factor) about the power function coefficients. The error bars in chart WPo-2 span ±(one standard distance uncertainty)×(scale factor) about the estimated distances. The scale factor is a non-negative numeric value between 1 and 6 in cell(20,5) – i.e., the “Error bars:” row and the **Default** parameter column.

The display regions of the two charts are defined by the maximum intervals required to display all the error bars at their specified expansion. These limits are set whether or not the error bars are displayed.

The distance values in chart WPo-2

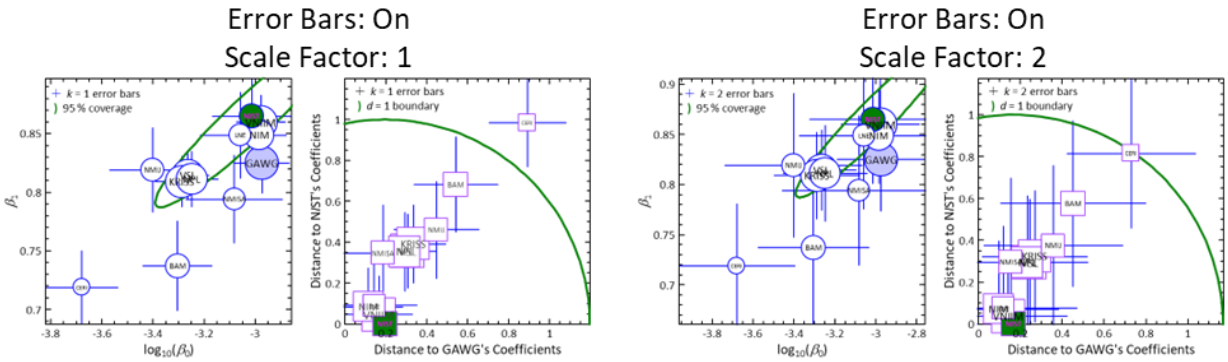


Fig. 73. *WG_Power* Charts WPo-1 and WPo-2 With Error Bars at Scale Factors 1 and 2.

Note: Because the Δ_{ij} distances displayed in chart WPo-2 are estimated from $\{\log_{10}(\beta_0), \beta_1\}$ values normalized by the span of the corresponding axes in chart WPo-1 (see Section 1.9.6), changes in the WPo-1 display can change the WPo-2 distances. To compare results across datasets, it is necessary to specify the value of the “Max Dist:” parameter (see Section 16.5.3).

16.6.4. Ellipse

Clicking the “Ellipse:” checkbox toggles the display of an ellipse in each of the two charts: see: Fig. 74. For chart WPo-1, the ellipse represents an approximate 95 % confidence boundary around the $\{\log_{10}(\beta_0), \beta_1\}$ coefficients of a target NMI/DI. This ellipse is not influenced by the ellipse scale factor.

For chart Wpo-2, the ellipse is centered on a target NMI/DI and provides an empirical “how close” boundary. The *x*-axis location of the target NMI/DI is its estimated distance to the power law coefficients of the WG community. Since the distance of the target to itself is always zero, the y-axis location is zero. The size of this ellipse is controlled by the scale factor, a non-negative numeric value between 0.1 and 10 in cell(21,5) – the “Ellipse:” row and the **Default** parameter column. The default scale factor is 1. The ellipse size has no effect on the estimated similarity distances

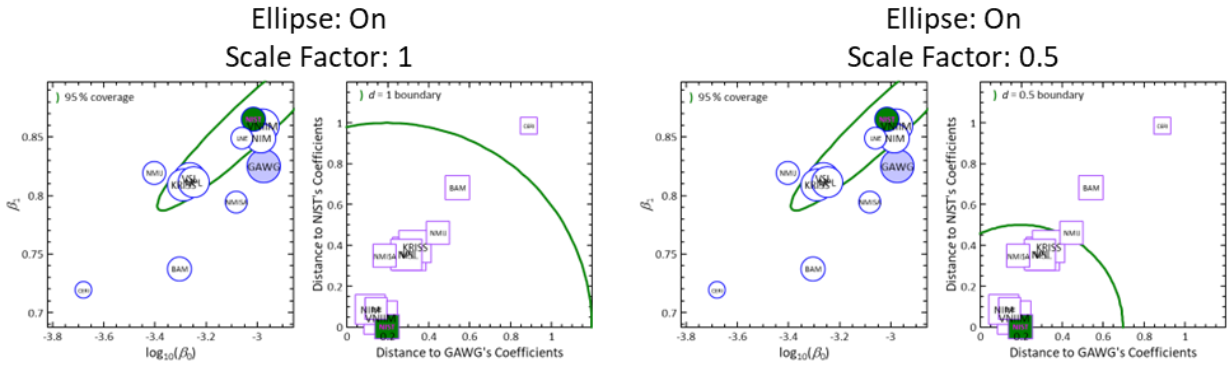


Fig. 74. *WG_Power* Charts WPo-1 and WPo-2 With Ellipses at Scale Factors 1 and 0.5.

Clicking the "Ellipse:" checkbox immediately toggles whether the ellipses are displayed. However, changing the "Ellipse:" scale factor has no effect until the **Plot** button is clicked.

16.6.5. Legend

Clicking the "Legend:" checkbox toggles between displaying and not displaying the legends in WPo-1 and WPo-2: see Fig. 75. It has no effect on the display of the WPo-3 chart.

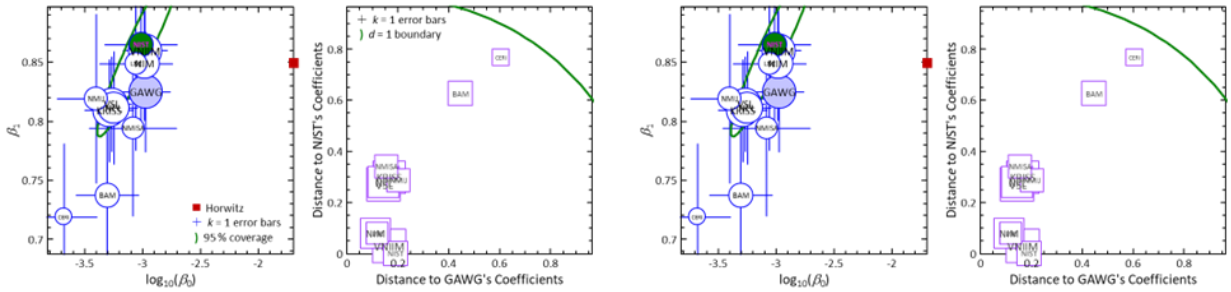


Fig. 75. *WG_Power* Charts WPo-1 and WPo-2 With and Without Legend.

16.6.6. Plot area box

Clicking the "Plot area box:" checkbox toggles between displaying and not displaying the area box lines at the top and right-hand side of charts WPo-1 and WPo-2: see Fig. 76. It has no effect on the display of the WPo-3 chart.

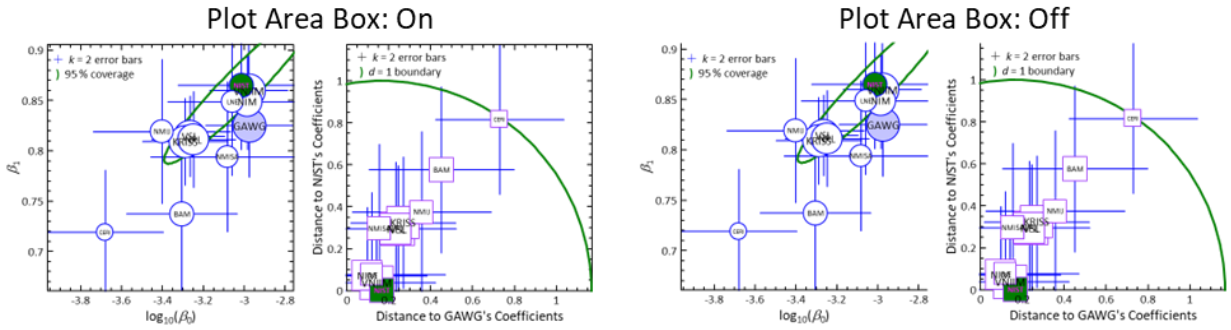


Fig. 76. *WG_Power* Charts With and Without Plot Area Box.

16.6.7. Unit ratio

Clicking the “Unit ratio:” checkbox toggles between displaying and not displaying a line denoting the unit ratio (i.e., a ratio of 1) in each segment of the WPo-3 multiplot: see Fig. 77.

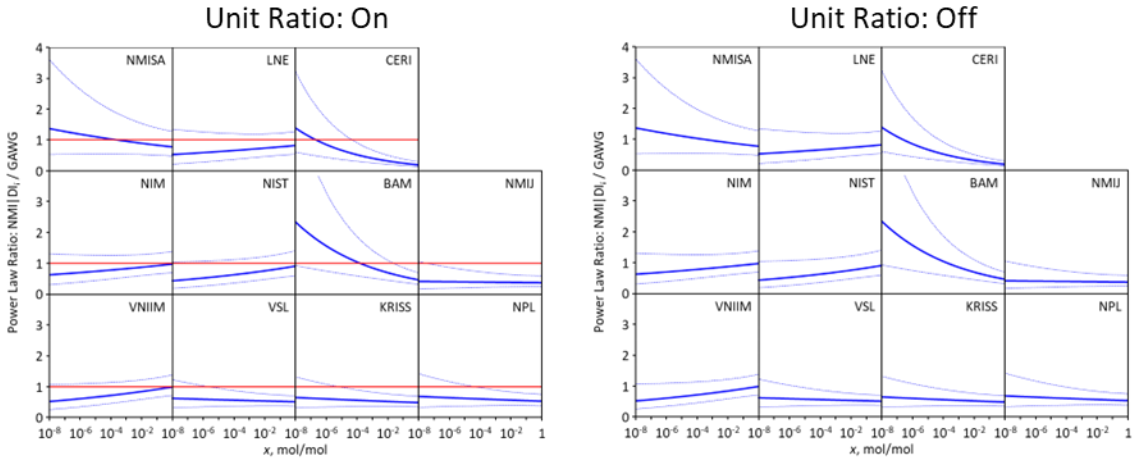


Fig. 77. *WG_Power* Chart WPo-3 With and Without Unit Ratio.

16.6.8. Title

Clicking the “Title:” checkbox toggles between displaying and not displaying the title lines.

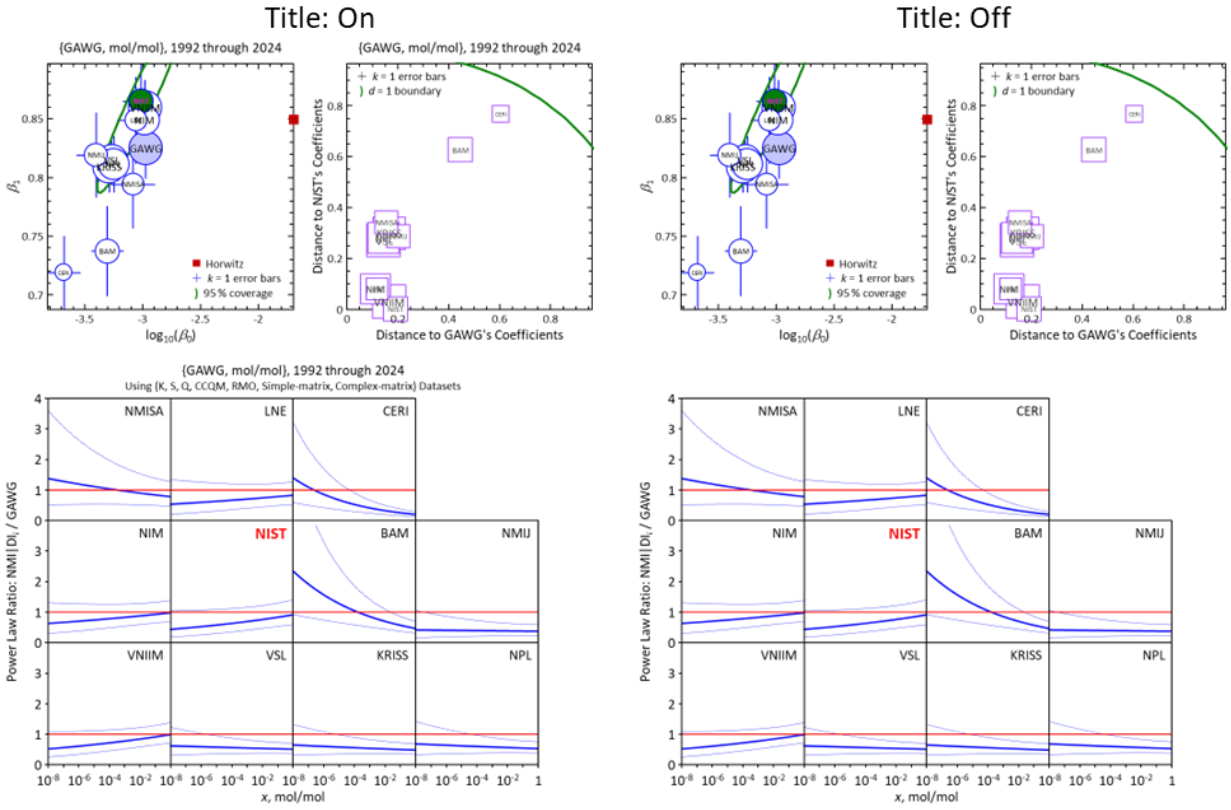


Fig. 78. *WG_Power* Charts With and Without Titles.

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. 79.

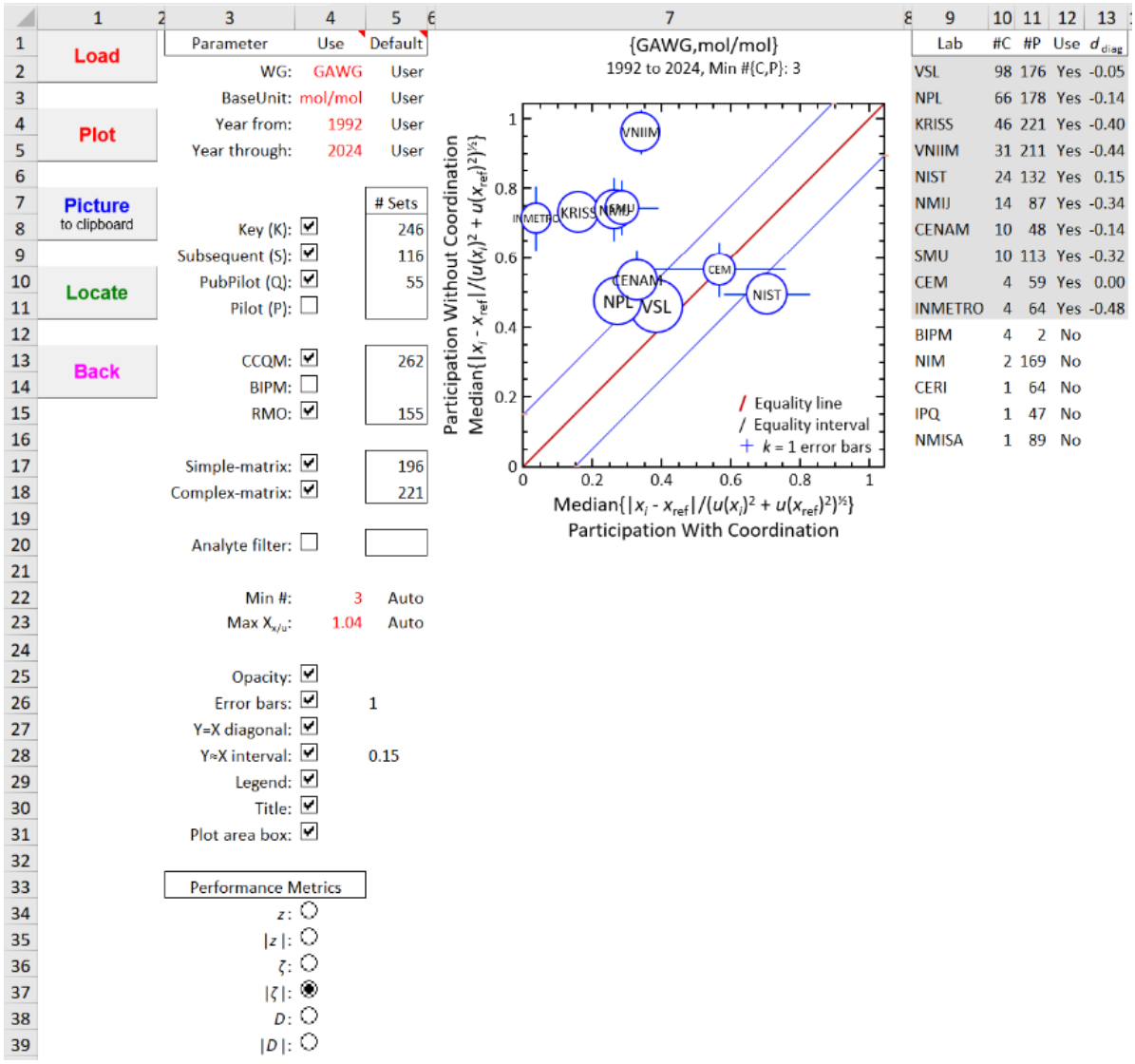


Fig. 79. *WG_Diagonal* Dashboard.

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 1.10 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 RVs.

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. 80.

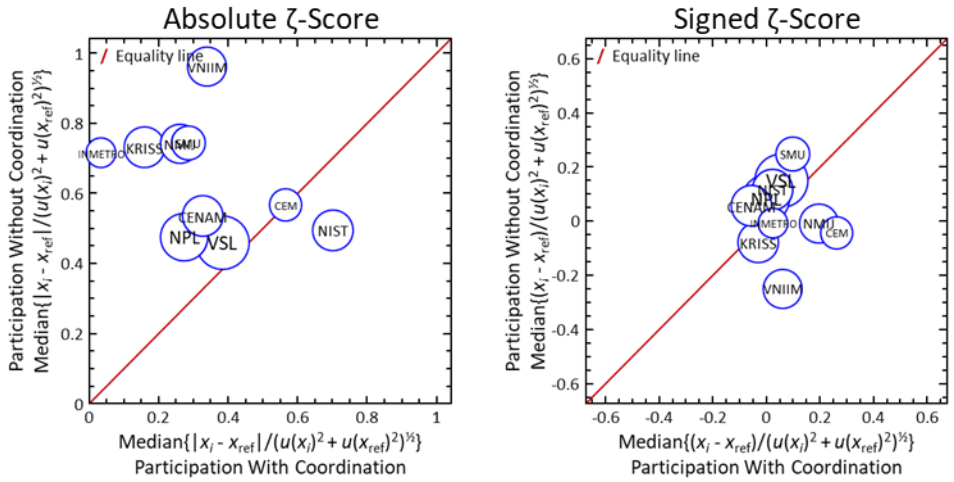


Fig. 80. *WG_Diagonal* Chart With Absolute and Signed Bias Metrics.

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 in which 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 $X_{x/u}$:	1.04	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.

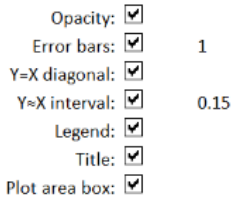
17.2.1. Min #: Minimum Participation

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. 79). The default value is (a more-or-less arbitrary) 3 datasets.

17.2.2. Max $X_{x/u}$: *x*- and *y*-Axis Limit

The value of the "Max $X_{x/u}$:" parameter sets the display range of the biases; the default value is set by the extreme value of the display symbols including their error bars. The same value 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.

17.3. Additional Chart Display Checkboxes



The *WG_Diagonal* worksheet contains four chart display checkboxes in addition to three 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 transparent: see Fig. 81. This enables identifying the location of NMI/DI symbols that are hidden under other symbols.

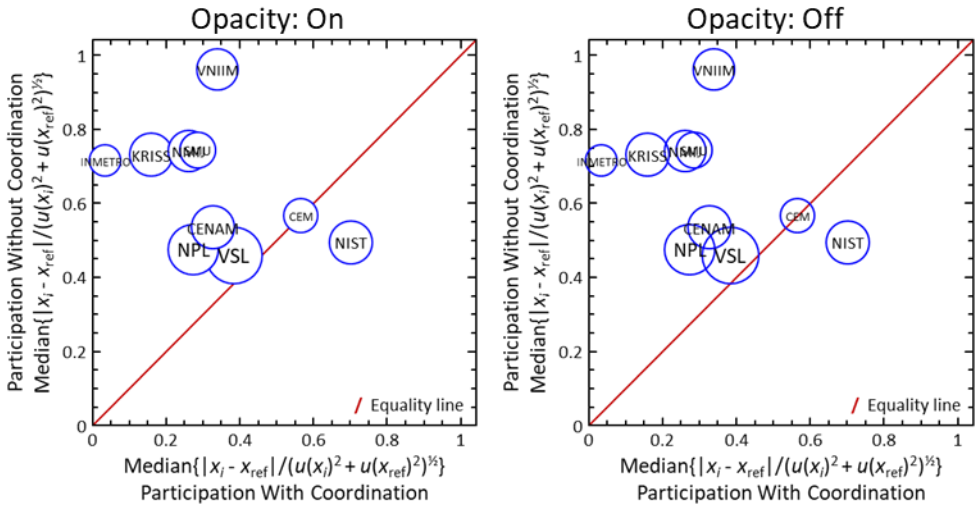


Fig. 81. *WG_Diagonal* Chart With and Without Symbol Opacity.

17.3.2. Error bars

Clicking the “Error bars:” checkbox toggles the display of the error bars: see Fig. 82. The error bars span ± (one standard deviation of the mean)×(scale factor) 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 scale factor is a non-negative numeric value between 1 and 6 in cell(26,5) – i.e., the “Error bars:” row and the **Default** parameter column.

The display region is defined by the maximum interval required to display all the error bars at their specified expansion. These limits are set whether or not the error bars are displayed.

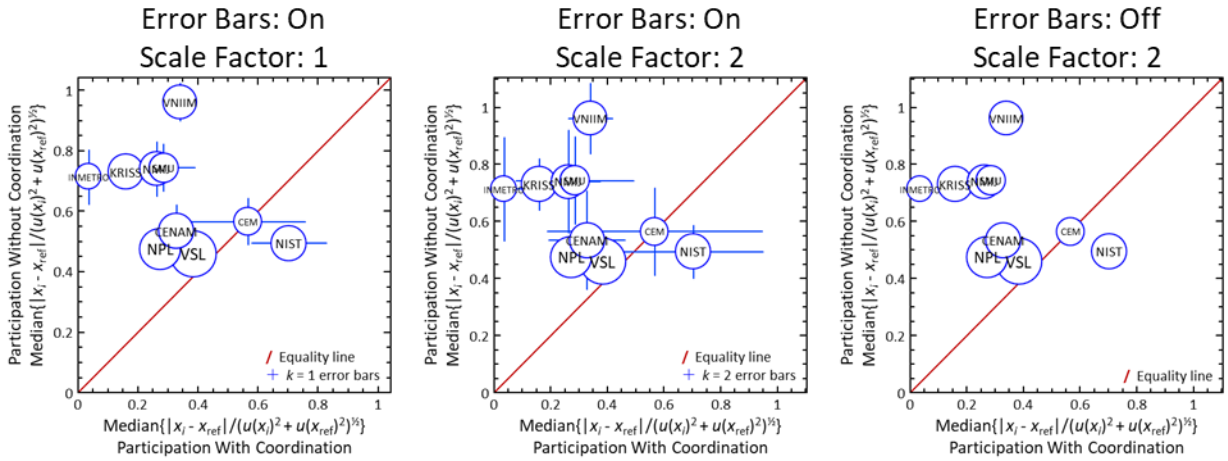


Fig. 82. *WG_Diagonal* Chart With and Without Error Bars.

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: see Fig. 83. 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.

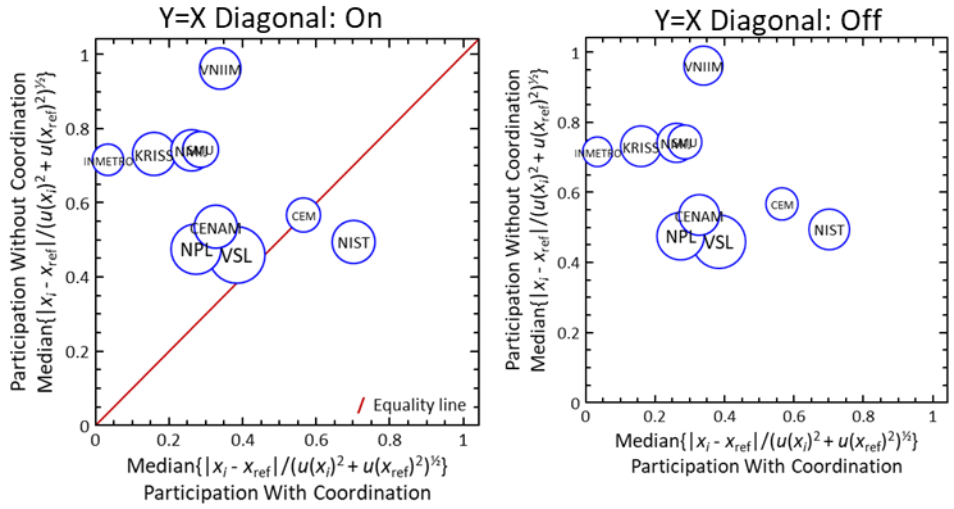


Fig. 83. *WG_Diagonal* Chart With and Without the Y=X Diagonal Equality Line.

17.3.4. Y≈X Interval

Clicking the "Y≈X interval:" checkbox toggles between displaying and not displaying two diagonal lines that symmetrically border the Y=X diagonal line: see Fig. 84. The bordering lines are offset from the equality line by a user-specified bias. The bias is a non-negative numeric value between 0.05 and 1 in cell(28,5) – i.e., the "Y≈X interval:" row and the **Default** parameter column.

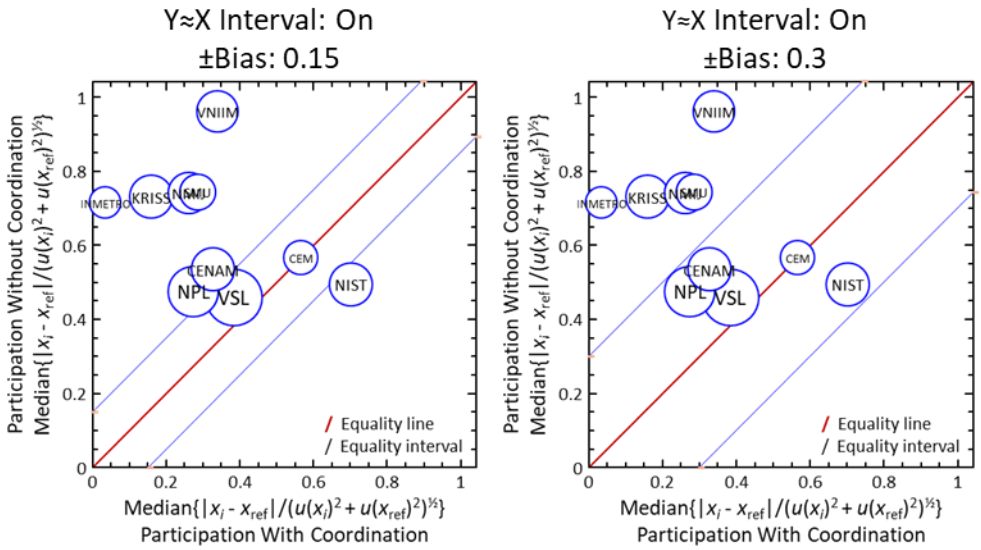
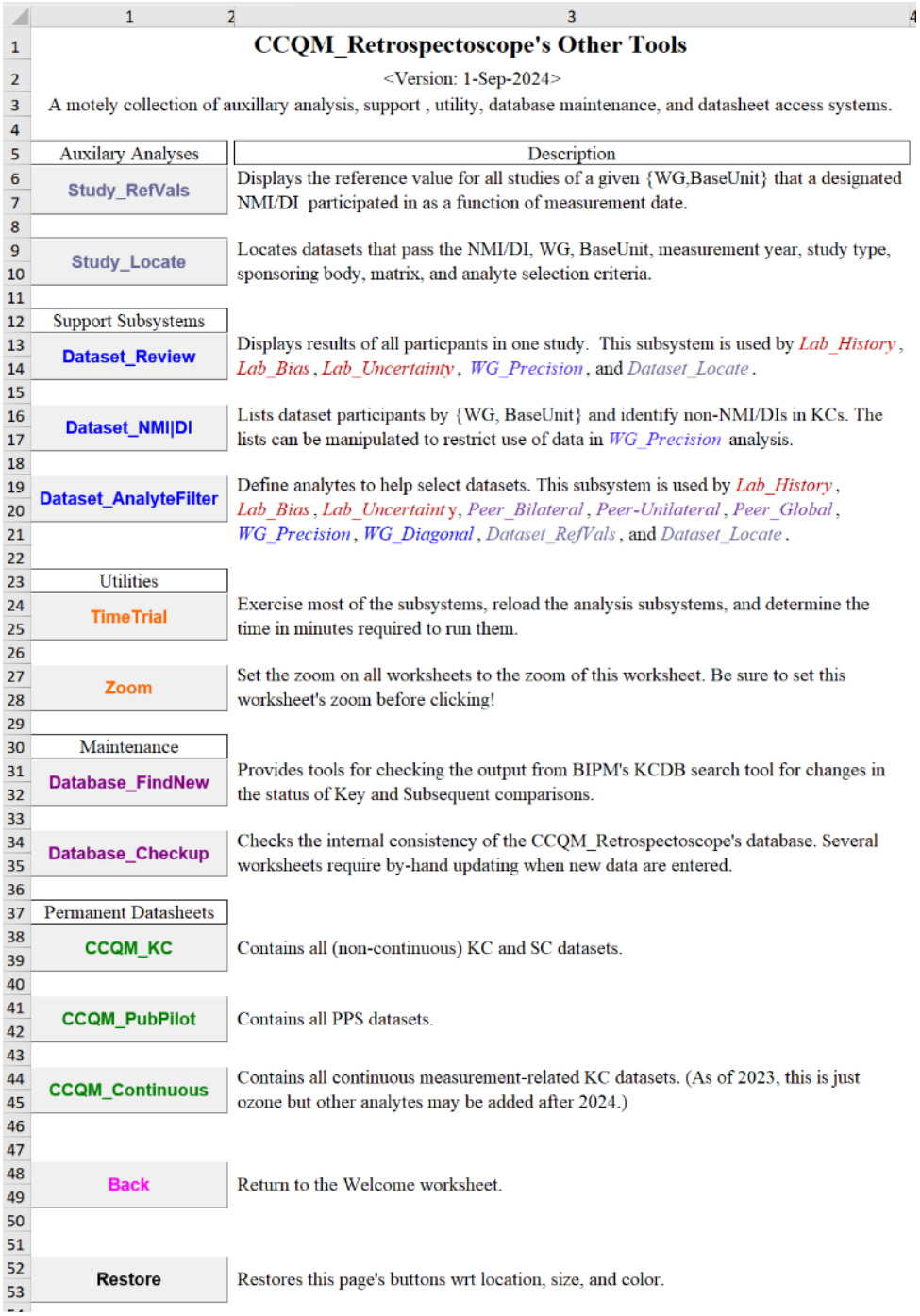


Fig. 84. *WG_Diagonal* Chart With and Without the Y≈X Interval Lines.

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 two auxiliary analysis subsystems, three analysis support subsystems, two user-oriented utilities, two database-maintenance support subsystems, and links to the three datasheets that hold publicly available comparison results. The controls used to access these functions are pictured in Fig. 85.



CCQM_Retrospectoscope's Other Tools

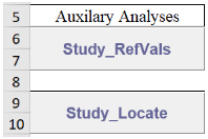
<Version: 1-Sep-2024>

A motely collection of auxillary analysis, support , utility, database maintenance, and datasheet access systems.

Auxilary Analyses	Description
Study_RefVals	Displays the reference value for all studies of a given {WG,BaseUnit} that a designated NMI/DI participated in as a function of measurement date.
Study_Locate	Locates datasets that pass the NMI/DI, WG, BaseUnit, measurement year, study type, sponsoring body, matrix, and analyte selection criteria.
Support Subsystems	
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, BaseUnit} and identify non-NMI/DIs in KCs. The lists can be manipulated to restrict use of data in *WG_Precision* analysis.
Dataset_AnalyteFilter	Define analytes to help select datasets. This subsystem is used by *Lab_History*, *Lab_Bias*, *Lab_Uncertainty*, *Peer_Bilateral*, *Peer-Unilateral*, *Peer_Global*, *WG_Precision*, *WG_Diagonal*, *Dataset_RefVals*, and *Dataset_Locate*.
Utilities	
TimeTrial	Exercise most of the subsystems, reload the analysis subsystems, and determine the time in minutes required to run them.
Zoom	Set the zoom on all worksheets to the zoom of this worksheet. Be sure to set this worksheet's zoom before clicking!
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-continuous) KC and SC datasets.
CCQM_PubPilot	Contains all PPS datasets.
CCQM_Continuous	Contains all continuous measurement-related KC datasets. (As of 2023, this is just ozone but other analytes may be added after 2024.)
Back	Return to the Welcome worksheet.
Restore	Restores this page's buttons wrt location, size, and color.

Fig. 85. *Other_Tools* Dashboard.

18.1. Auxiliary Analysis Subsystems

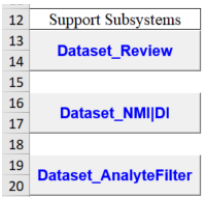


The *Study_RefVals* subsystem visualizes the dataset RVs for datasets that the target NMI/DI (or the WG, if *All* is specified) has contributed to.

The *Study_Locate* subsystem facilitates identifying datasets with specific characteristics.

Clicking these buttons activates the corresponding worksheet; it does not initiate the actions implemented in that worksheet.

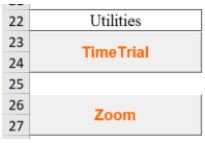
18.2. Support Subsystems



The *Dataset_Review*, *Dataset_NMI/DI*, or *Dataset_AnalyteFilter* subsystems support dataset selection or visualization in one or more of the analysis subsystems.

Clicking these buttons activates the corresponding worksheet; it does not initiate the actions implemented in that worksheet.

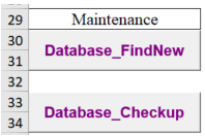
18.3. Utilities



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

Clicking the **Zoom** button sets the zoom (the viewable size of a worksheet on your display device) on all of the *CCQM_Retrospectoscope* worksheets to the current zoom setting of the *Other_Tools* worksheet.

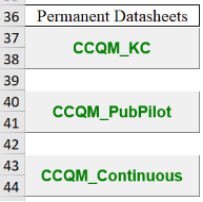
18.4. Maintenance Systems



The *Database_FindNew* subsystem facilitates identifying newly approved studies. The *Database_Checkup* subsystem facilitates ensuring the integrity of added data. These subsystems are intended to be used by the unfortunate(s) tasked with maintaining the *CCQM_Retrospectoscope* database. However, the output from successful completion of *Database_Checkup* is useful in documenting the number of datasets and studies having a variety of characteristics.

Clicking these buttons activates the corresponding worksheet; it does not initiate the actions implemented in that worksheet.

18.5. Database Worksheets



Clicking the **CCQM_KC, CCQM_PubPilot,** or **CCQM_Continuous** button activates the corresponding datasheet. It does not initiate any other action.

19. Study_RefVals Subsystem

The *Study_RefVals* chart, the controls used to specify the datasets evaluated, and the controls used to modify what the chart displays are pictured in Fig. 86. The in-common data selection, bias metrics, and chart display controls are discussed in Section 2.

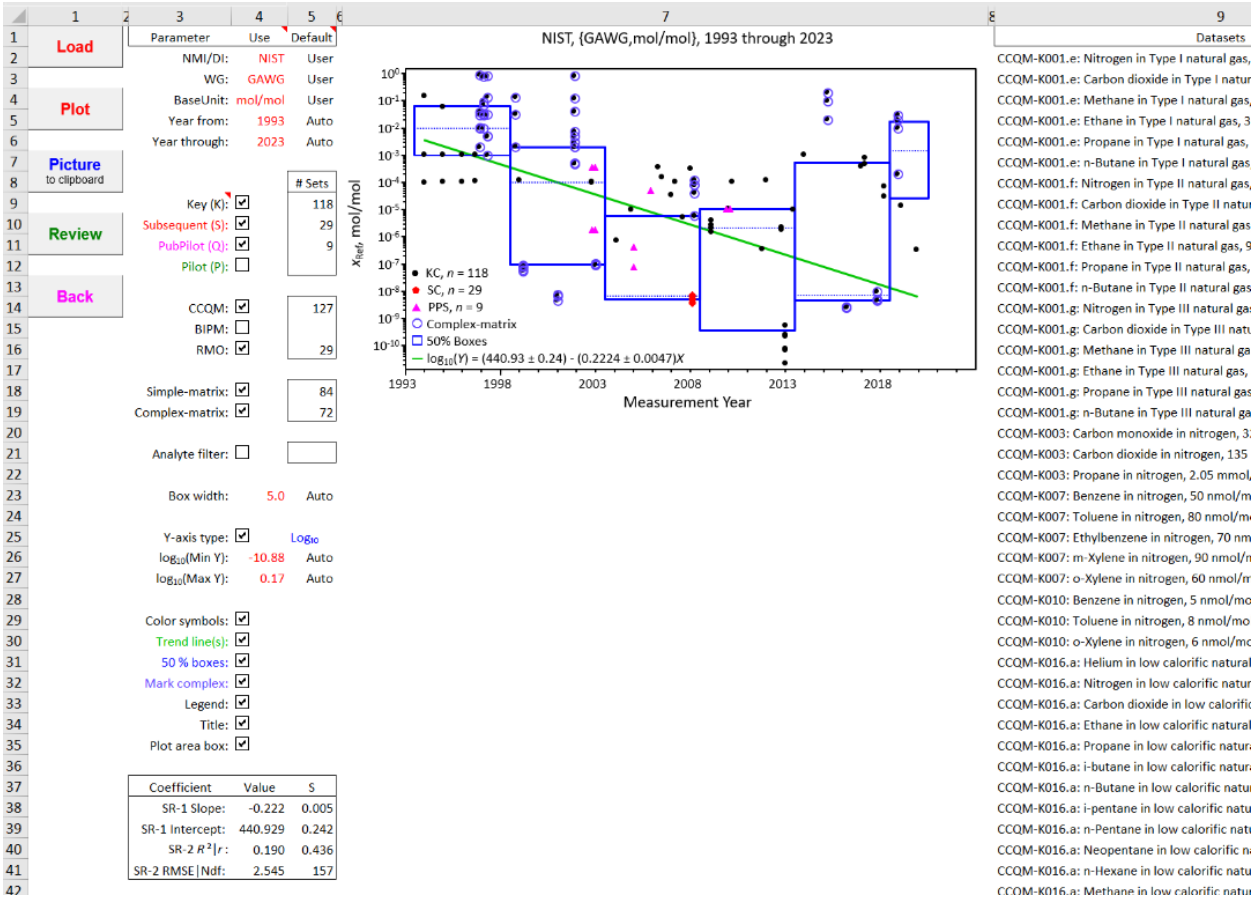


Fig. 86. *Study_RefVals* Dashboard with a Specified NMI/DI.

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 1.10 for further information.

19.1. Chart

Each symbol in the worksheet's chart represents the RV for one dataset in which the target NMI/DI has contributed a result, plotted as a function of measurement year. This may be useful in discovering the measurement challenges an NMI/DI was interested in.

Additionally, as displayed in Fig. 87 the NMI/DI code *All* can be used to visualize all RVs associated with a given {WG, BaseUnit}. This may be useful in accessing the measurement challenges a WG's measurement community was interested in.

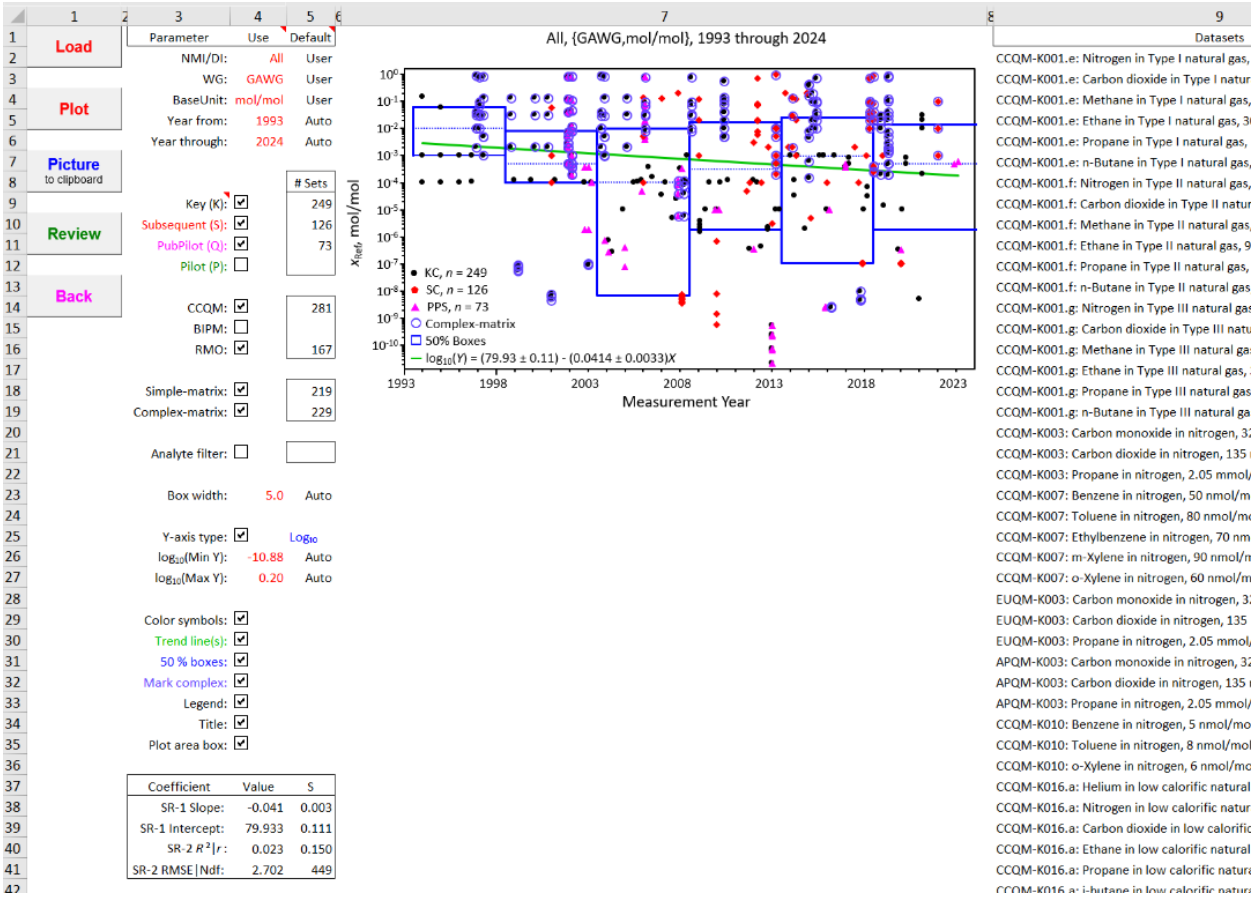


Fig. 87. *Study_RefVals* Dashboard With the NMI/DI Parameter set to *All*.

19.2. Chart Display Parameters

Box width: 5.0 Auto

19.2.1. Box width: 50 % Box Width

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 19.3.3. The default interval is five years.

19.2.2. Y-axis type: Checkbox

The *Study_RefVals* worksheet contains a checkbox toggle and two chart display parameters related to the *y*-axis. When the "Y-axis type:" checkbox is checked, the chart's *y*-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 *y*-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.

19.2.2.1. Log_{10} Y-axis: *y*-Axis Display Limits

When the "Y-axis type:" checkbox is checked, the *y*-axis is $base_{10}$-logarithmic. The values of the "log_{10}(Min Y):" and "log_{10}(Max Y):" parameters set the minimum and maximum limits for the $base_{10}$ logarithmic *y*-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 used for analysis.

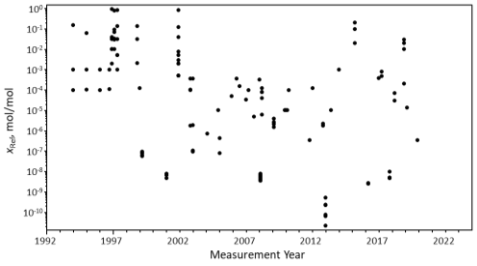
19.2.2.2. Linear *y*-axis: *y*-Axis Display Limits

When the "Y-axis type:" checkbox is unchecked, the *y*-axis is linear. The values of the "Min Y:" and "Max Y:" parameters set the minimum and maximum limits for the linear *y*-axis. The default values for these limits are the minimum and maximum values of *Y* among the selected data. Modifying these limits does not affect what data are used for analysis.

19.3. Additional Chart Display Checkboxes

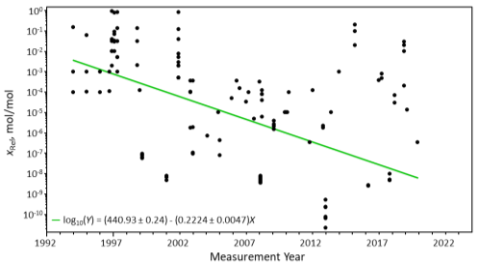
The *Study_RefVals* worksheet contains four chart display checkboxes in addition to the three discussed in Section 2.2.3. Clicking a chart display checkbox invokes an immediate change in the chart display.

19.3.1. Color symbols



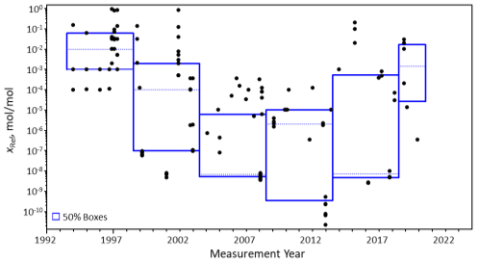
Clicking the "Color symbols:" checkbox toggles the charts between the colored symbols displayed in Fig. 82 and all-black symbols as displayed in the thumbnail to the right. The colors used for the four study types are dictated by the font colors of the checkbox labels. When colored, KC results are solid circles, SC results are solid diamonds, PPS results are solid triangles, and PS results are open squares. When black, all symbols are solid circles.

19.3.2. Trend line(s)



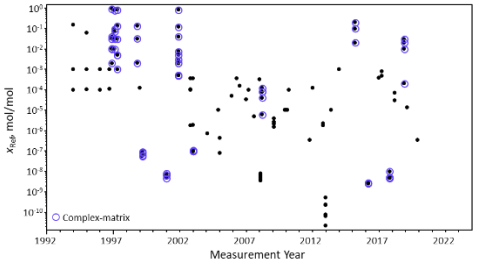
Clicking the "Trend line(s):" checkbox toggles the display of the robust Thiel-Sen linear trend line [14,15], $Y = \beta_0 + \beta_1 X$ or $\log_{10}(Y) = \beta_0 + \beta_1 X$, where *X* is the date in years and *Y* is the RV in units of the specified BaseUnit.

19.3.3. 50 % boxes



Clicking the "50 % boxes:" checkbox toggles the display of a series of rectangular boxes at intervals along the *x*-axis (measurement year). Each box is bounded with solid blue lines. The width of each box is set by the "Box width:" parameter (Section 19.2.1). 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).

19.3.4. 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 purple circle.

19.4. Review Command Button

While the function of the **Review** command button in this subsystem is as described in Section 2.1.4 (displaying a dot-and-bar chart of all results of a selected study), the *Study_RefVals* subsystem supports an additional method of specifying which study to display: selecting a single symbol from the data series on the chart before clicking the button. Since there is no other convenient way to connect a symbol with its study, this facilitates exploring the data.

However, it is all too easy to inadvertently damage the chart while attempting to select one particular symbol, so the selection must be done with care. (It's not difficult, but it does take some practice.) If damage occurs, clicking <ctrl-Z> will generally "undo" the misstep. If the damage appears permanent, close CCQM_Retrospectoscope without saving and begin anew.

19.5. Stored Theil-Sen Regression Parameters

Coefficient	Value	S
SR-1 Slope:	-0.222	0.005
SR-1 Intercept:	440.929	0.242
SR-2 $R^2\|r$:	0.190	0.436
SR-2 RMSE|Ndf:	2.545	157

The chart's trendline slope, intercept, Pearson correlation (R^2) of the fit, imputed correlation between the slope and intercept coefficients (r), RMSE, and number of degrees of freedom (ndf) are stored below the radio buttons. These values are generated during the analysis and are stored whether or not the trendline is displayed.

20. Study_Locate Subsystem

The *Study_Locate* subsystem facilitates identifying datasets having specific characteristics. The commands and controls for this subsystem are pictured in Fig. 91.

	1	2	3	4	5	6	7	8	9
1	Load		Parameter	Use	Default		Matching Datasets	Analyte	Year
2			WG:	GAWG	User		EUQM-S003: 123-Trimethylbenzene in nitrogen, nmol/mol	123-Trimethylbenzene	2008
3			BaseUnit:	mol/mol	User		EUQM-S003: 124-Trimethylbenzene in nitrogen, nmol/mol	124-Trimethylbenzene	2008
4	Find		Year from:	1992	User		CCQM-K022: 12-Dichloroethane in nitrogen, 100 nmol/mol	12-Dichloroethane	2003
5			Year through:	2024	User		EUQM-S003: 135-Trimethylbenzene in nitrogen, nmol/mol	135-Trimethylbenzene	2008
6							CCQM-K022: 13-Butadiene in nitrogen, 100 nmol/mol	13-Butadiene	2003
7	Review		NMI/DI:	NIST	User		EUQM-S003: 13-Butadiene in nitrogen, nmol/mol	13-Butadiene	2008
8							CCQM-K121: 18-Cineole in nitrogen, 2.5 nmol/mol	18-Cineole	2016
9					# Sets		EUQM-S003: 1-Butene in nitrogen, nmol/mol	1-Butene	2008
10	Back		Key (K): ☑		118		EUQM-S003: 1-Pentene in nitrogen, nmol/mol	1-Pentene	2008
11			Subsequent (S): ☑		29		CCQM-K121: 3-Carene in nitrogen, 2.5 nmol/mol	3-Carene	2016
12			PubPilot (Q): ☑		9		EUQM-S003: Acetylene in nitrogen, nmol/mol	Acetylene	2008
13			Pilot (P): ☐				CCQM-K046: Ammonia in nitrogen, µmol/mol	Ammonia	2007
14							CCQM-K117: Ammonia in nitrogen, 14 µmol/mol	Ammonia	2019
15			CCQM: ☑		127		CCQM-K066: Argon in methane, µmol/mol	Argon	2009
16			BIPM: ☐				CCQM-K113: Argon in noble gas mixture, cmol/mol	Argon	2015
17			RMO: ☑		29		CCQM-K007: Benzene in nitrogen, 50 nmol/mol	Benzene	1999
18							CCQM-K010.2018: Benzene in nitrogen, 5 nmol/mol	Benzene	2018
19			Simple-matrix: ☑		84		CCQM-K010: Benzene in nitrogen, 5 nmol/mol	Benzene	2001
20			Complex-matrix: ☑		72		CCQM-K022: Benzene in nitrogen, 100 nmol/mol	Benzene	2003
21							EUQM-S003: Benzene in nitrogen, nmol/mol	Benzene	2008
22			Analyte filter: ☐				EUQM-S003: c-2-Butene in nitrogen, nmol/mol	c-2-Butene	2008
23							CCQM-K001.h: Carbon dioxide in nitrogen, 100 µmol/mol	Carbon dioxide	1994

Fig. 88. *Study_Locate* Dashboard with NIST as 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 1.10 for further information.

20.1. Additional Command Button: Find

Find is the only command button on the *Study_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 finds all datasets that match the current selection criteria and lists their titles and many of their characteristics in columns 7 to 18.

20.2. Dataset Selection Parameters: NMI/DI

NMI|DI: NIST User

NMI/DI has 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. The result of clicking the **Find** button with 'NMI/DI:" set to *All* is displayed in Fig. 89.

	Load	Parameter	Use	Default	Matching Datasets	Analyte	Year
2		WG:	GAWG	User	APQM-S014: 112-Trichloroethane in nitrogen, 100 nmol/mol	112-Trichloroethane	2020
3		BaseUnit:	mol/mol	User	APQM-S014: 11-Dichloroethane in nitrogen, 100 nmol/mol	11-Dichloroethane	2020
4	Find	Year from:	1992	User	EUQM-S003: 123-Trimethylbenzene in nitrogen, nmol/mol	123-Trimethylbenzene	2008
5		Year through:	2024	User	EUQM-S003: 124-Trimethylbenzene in nitrogen, nmol/mol	124-Trimethylbenzene	2008
6					CCQM-K022: 12-Dichloroethane in nitrogen, 100 nmol/mol	12-Dichloroethane	2003
7	Review	NMI/DI:	All	User	EUQM-S003: 135-Trimethylbenzene in nitrogen, nmol/mol	135-Trimethylbenzene	2008
8					APQM-S014: 13-Butadiene in nitrogen, 100 nmol/mol	13-Butadiene	2020
9				# Sets	CCQM-K022: 13-Butadiene in nitrogen, 100 nmol/mol	13-Butadiene	2003
10	Back	Key (K):	☑	249	CCQM-K077: Refinery gas - 13-Butadiene, 1 cmol/mol	13-Butadiene	2010
11		Subsequent (S):	☑	126	EUQM-S003: 13-Butadiene in nitrogen, nmol/mol	13-Butadiene	2008
12		PubPilot (Q):	☑	74	EUQM-S006: 1,3-Butadiene in hydrocarbon mixture, cmol/mol	13-Butadiene	2012
13		Pilot (P):	☐		CCQM-K121: 18-Cineole in nitrogen, 2.5 nmol/mol	18-Cineole	2016
14					CCQM-Q177: 18-Cineole in nitrogen, 2.5 nmol/mol	18-Cineole	2016
15		CCQM:	☑	282	CCQM-K077: Refinery gas - 1-Butene, 0.5 cmol/mol	1-Butene	2010
16		BIPM:	☐		CCQM-K119: 1-Butene in Liquified Petroleum Gas (LPG), cmol/mol	1-Butene	2015
17		RMO:	☑	167	CoQM-S004: 1-Butene in Liquified Petroleum Gas (LPG), cmol/mol	1-Butene	2018
18					EUQM-S003: 1-Butene in nitrogen, nmol/mol	1-Butene	2008
19		Simple-matrix:	☑	220	EUQM-S006: 1-Butane in hydrocarbon mixture, cmol/mol	1-Butene	2012
20		Complex-matrix:	☑	229	EUQM-S003: 1-Pentene in nitrogen, nmol/mol	1-Pentene	2008
21					CCQM-K121: 3-Carene in nitrogen, 2.5 nmol/mol	3-Carene	2016
22		Analyte filter:	☐		CCQM-Q177: 3-Carene in nitrogen, 2.5 nmol/mol	3-Carene	2016

Fig. 89. *Study_Locate* Dashboard Without a Specified NMI/DI.

20.3. Dataset Selection Checkbox: Analyte filter

"Analyte filter:" also has some functionality beyond that described for other subsystems (Section 2.2.1). 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. The result of clicking the **Find** button with the "Analyte filter:" active and set to {GAWG, mol/mol} Inerts (see Section 23) is displayed in Fig. 90.

	Load	Parameter	Use	Default	Matching Datasets	Analyte	Year
2		WG:	GAWG	User	CCQM-K066: Argon in methane, µmol/mol	Argon	2009
3		BaseUnit:	mol/mol	User	CCQM-K113: Argon in noble gas mixture, cmol/mol	Argon	2015
4	Find	Year from:	1992	User	CCQM-K016.a: Helium in low calorific natural gas, 0.50 cmol/mol	Helium	2002
5		Year through:	2024	User	CCQM-K113: Krypton in noble gas mixture, cmol/mol	Krypton	2015
6					CCQM-K113: Neon in noble gas mixture, cmol/mol	Neon	2015
7	Review	NMI/DI:	NIST	User	CCQM-K001.e: Nitrogen in Type I natural gas, 40 mmol/mol	Nitrogen	1997
8					CCQM-K001.f: Nitrogen in Type II natural gas, 70 mmol/mol	Nitrogen	1997
9				# Sets	CCQM-K001.g: Nitrogen in Type III natural gas, 135 mmol/mol	Nitrogen	1997
10	Back	Key (K): ☑		10	CCQM-K016.a: Nitrogen in low calorific natural gas, 12.0 cmol/mol	Nitrogen	2002
11		Subsequent (S): ☑			CCQM-K066: Nitrogen in methane, µmol/mol	Nitrogen	2009
12		PubPilot (Q): ☑					
13		Pilot (P): ☐					
14							
15		CCQM: ☑		10			
16		BIPM: ☐					
17		RMO: ☑					
18							
19		Simple-matrix: ☑		2			
20		Complex-matrix: ☑		8			
21							
22		Analyte filter: ☑		10			
23		Nitrogen		5			
24		Argon		2			
25		Helium		1			
26		Krypton		1			
27		Neon		1			
28		Xenon		0			

Fig. 90. *Study_Locate* Dashboard with NIST as NMI/DI Using an Analyte Filter.

21. 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*, *Study_Locate*, or the *datasheets*. 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. 91.

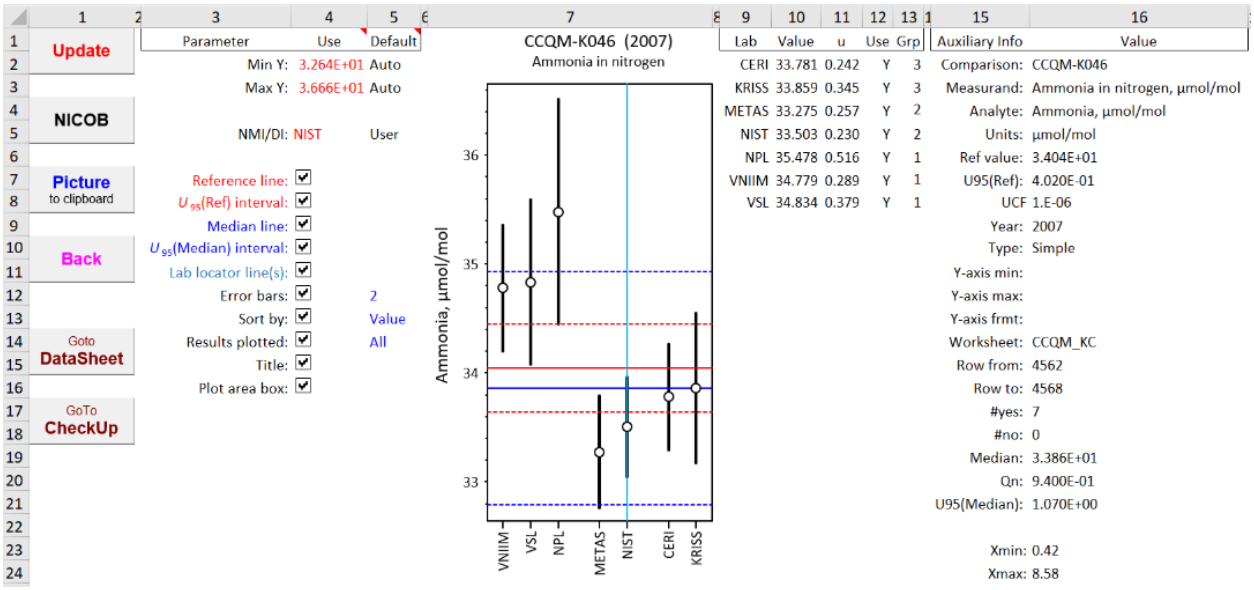


Fig. 91. *Dataset_Review* Dashboard with an Example Dataset.

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 1.10 for further information.

Note: The dataset, International Comparison CCQM-K46 – Ammonia in Nitrogen [18], 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.

21.1. 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 plotted along the *y*-axis (reported value) directly above the code. Participant results flagged “Y” are displayed as open circles with black error bars; results flagged “N” or “Z” are displayed as solid red circles with red error bars. Section 28.2.4 describes how these flags are defined and used.

The chart size can be adjusted as needed. The adjusted size will be maintained until the **Restore** function is invoked. The default chart size is shown in Fig. 92.

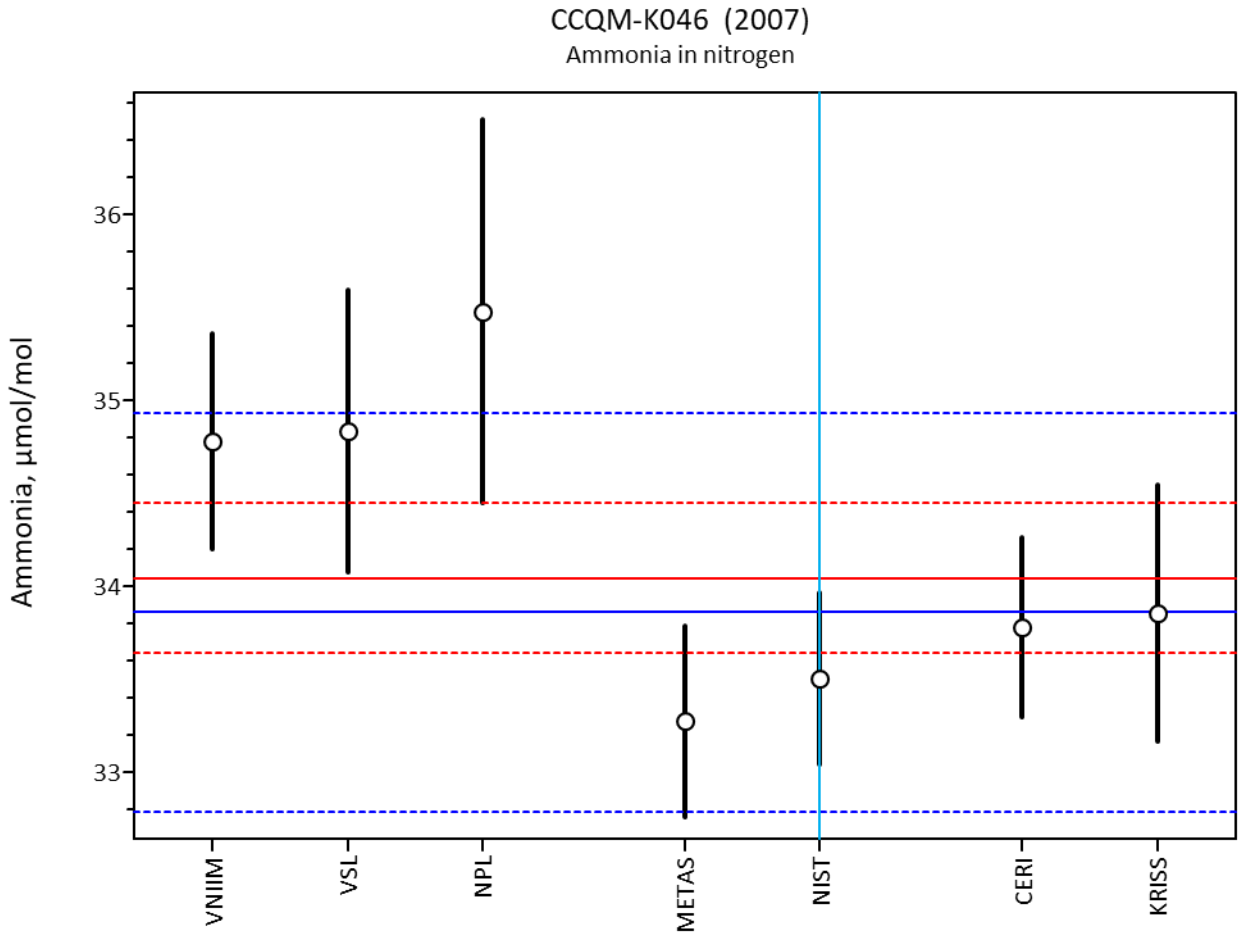


Fig. 92. Default size of the *Dataset_Review* Chart.

21.2. 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*.

21.2.1. Update

When the **Update** button is clicked, the chart displays the dataset results using the scaling defined by the “Min Y:” and “Max Y:” parameters (Section 21.3.1).

21.2.2. NICOB

NICOB is the acronym for the NIST Consensus Builder, a system designed to provide statistically defensible consensus estimates for interlaboratory study results [19]. Clicking the **NICOB** button causes dataset results to be output in the NICOB-friendly format shown in Fig. 93. 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. 93. 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 RVs that were assigned using other estimation techniques.

Note: the NIST Decision Tree (NDT) is a recently developed expert system for the analysis of interlaboratory study results [20]. The data provided in columns 9 through 11 (headings **Lab**, **Value**, and **u**: see Fig. 91) are suitable input for the NDT system.

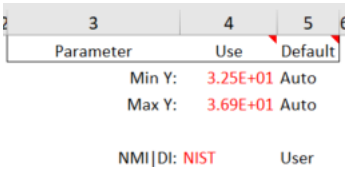
21.2.3. Goto Datasheet

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.

21.2.4. 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.

21.3. 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.

21.3.1. Min Y and Max Y: *y*-Axis Display Limits

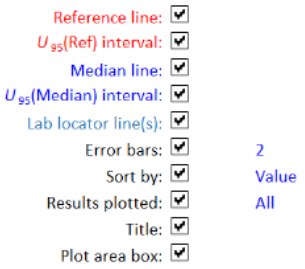
The “Min Y:” and “Max Y:” parameter values set the display range of the *y*-axis (reported value). The default values are set by the extreme values of the results using the “Error bars: “ scale factor times the standard uncertainties or by the values of the “Y-axis min:” and “Y-axis max:” parameters in the **Auxiliary Info** block (cells (11,16) and (12,16).

21.3.2. 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 21.4.3) is active, the symbols for those values will be bisected by a thin blue line. The default target NMI/DI is, of course, NIST.

21.4. Additional Chart Display Checkboxes

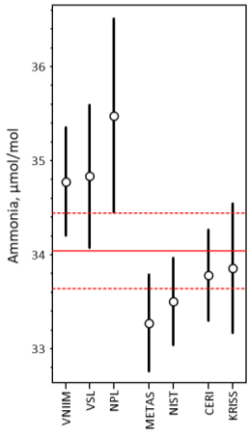
The *Dataset_Review* worksheet contains eight chart display checkboxes in addition to the “Title:” and “Plot area box:” that are discussed in Section 2.2.3.



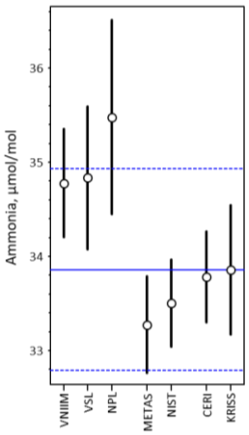
21.4.1. Reference Line and U_{95}(Ref) Interval

Clicking the “Reference line:” checkbox toggles the display of a sold red horizontal line that represents the dataset’s assigned RV.

Clicking the “U_{95}(Ref) interval:” toggles the display of two dotted red lines that represent the assigned approximate 95 % confidence region around the RV.



21.4.2. Median Line and U_{95}(Median) Interval

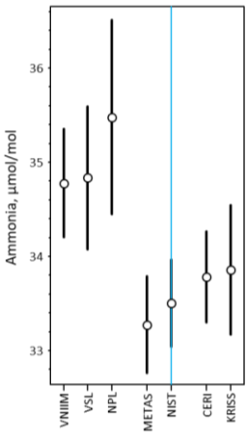


Clicking the "Median line:" checkbox toggles the display of a solid blue horizontal line that represents the median of the values considered valid by the coordinating WG (that is, are flagged as "Y").

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 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 that of the mean:

$$U_{95}(X_{\text{median}}) = 1.24(t_{1-0.05,n-1})Q_n/\sqrt{n} \quad (25)$$

21.4.3. Lab locator line(s)



When a data set contains one or more values reported by the NMI/DI specified by the "NMI/DI:" parameter (Section 21.3.2), clicking the "Lab locator line(s):" checkbox toggles display of thin cyan vertical line(s) that connect the dot-and-bar symbols to the participant code.

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

21.4.4. Error bars

Clicking the "Error bars:" checkbox toggles display of error bars. When the checkbox is checked, each participant's reported $x \pm ku(x)$ results are displayed. When the checkbox is unchecked, only the x values are displayed. The "k" factor is set by the scale factor associated with the checkbox. It is a non-negative numeric value between 1 and 6 in cell(12,5) – i.e., the "Error bars:" row and the **Default** parameter column.

The "Errorbars:" scale parameter has two functions, setting the length of the error bars and setting the default y-axis span. When *Dataset_Review* is invoked from one of the analysis subsystems or datasheets, the scale factor is set to 2. This sets the chart so that the displayed error bars for each participant are $x \pm 2 \cdot u(x)$ and the default y-axis limits are set by the span required to fully display all resulting error bars.

When invoked directly by the *Dataset_Review* **Update** command, the scale factor likewise sets both the axis and bar scales, but the value of the parameter is set by the user. When the "Error bars:" checkbox is toggled, the scale factor only sets the length of the bars. This can facilitate examination of datasets that contain extreme outsider results. The various display options are illustrated in Fig. 94.

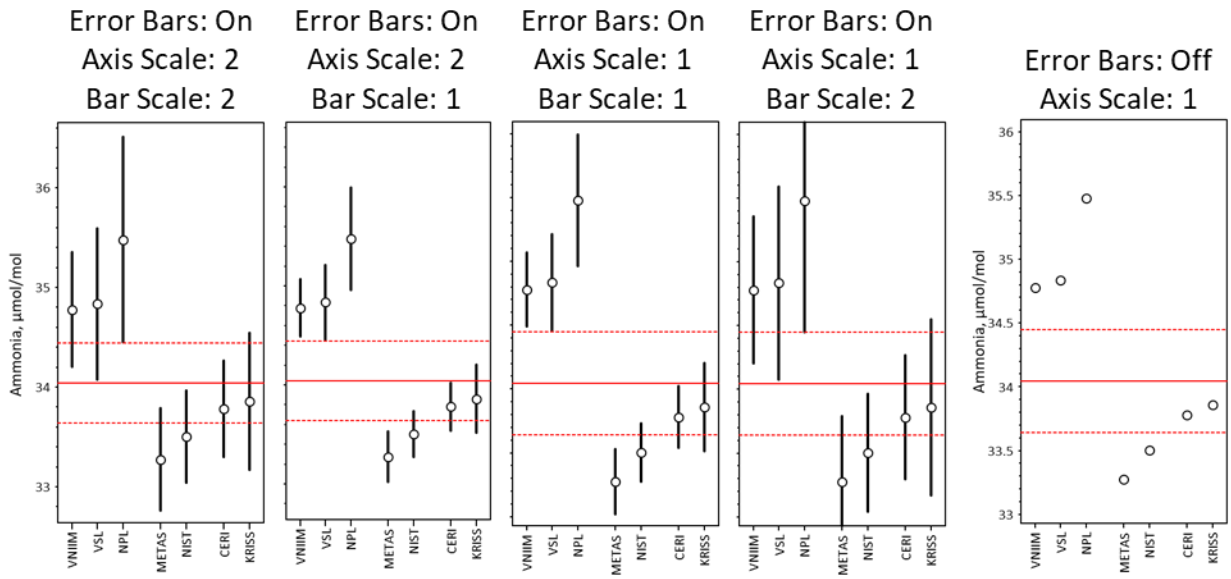


Fig. 94. *Dataset_Review* Chart with Various Error Bar Options.

21.4.5. 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 1.24, the results are sorted in order of increasing value: see the left two panels of Fig. 95. When the results are grouped, they are ordered first by their Group designation and then by *Alpha* or *Value* with a wider gap between the groups than between the results within a group: see the right two panels of Fig. 95.

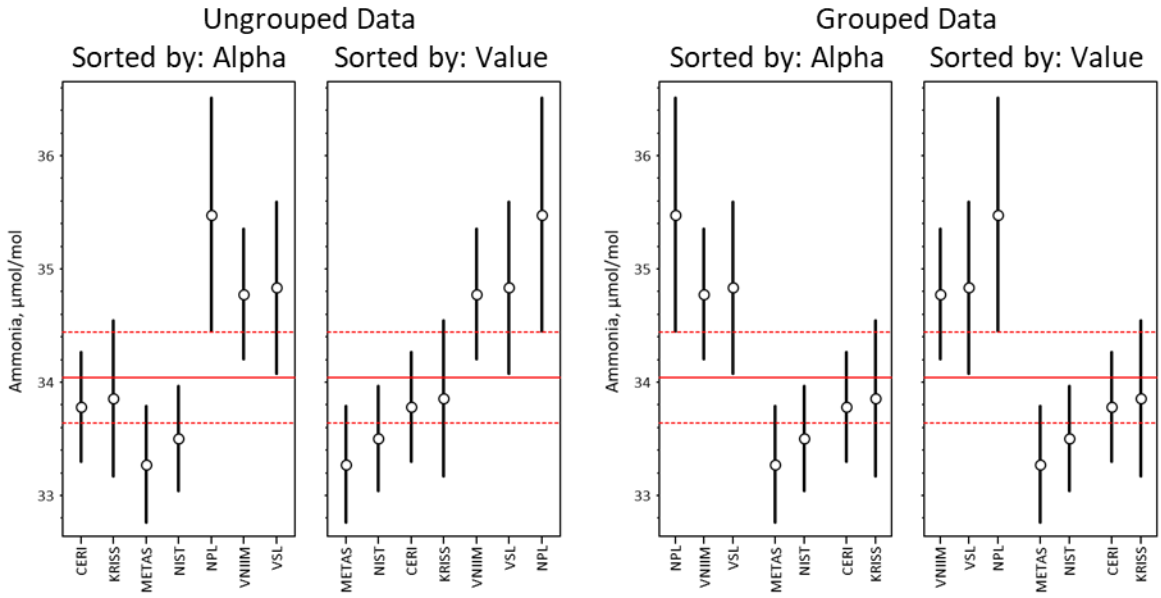


Fig. 95. *Dataset_Review* Chart With Group Results Sorted Alphabetically and By Value.

Note: The codes used for many NMI/DIs are not consistent over time or in different studies (see Section 27.4.4). Alphabetical sorting by the NMI/DI codes used in the *CCQM_Retrospectoscope* may produce orderings that differ from those used by the study coordinators.

Note: Grouping is controlled by the values in the *Dataset_Review* worksheet's column 13 (**Grp**). As displayed in Fig. 91, column 13 contains the method-related assignments 1", "2", and "3". These assignments drive the ordering in the right two panels of Fig. 95. The ordering in the left two panels were generated by clearing the grouping assignments and then clicking the "Results plotted:" checkbox (Section 21.4.6).

21.4.6. Results plotted

To enable visualizing dataset changes without modifying the original data, clicking the "Results plotted:" checkbox transfers values from the *Dataset_Review* worksheet's columns 9 through 13 to columns 18 through 22. When the checkbox is checked, all of the dataset's results are transferred. When unchecked, just the results used to estimate the median and its 95 % confidence interval (i.e., those flagged "Y" and "Z") are transferred: see Fig. 96.

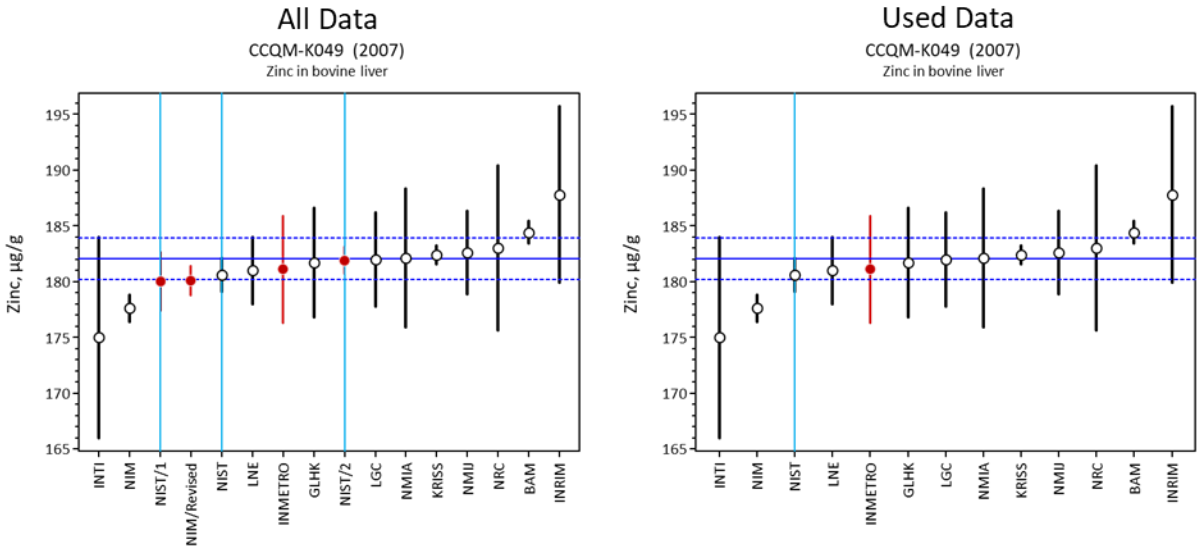


Fig. 96. *Dataset_Review* Chart Displaying All Available and Only Used Results.

21.5. Data

When invoked from one of the *CCQM_Retrospectoscope* subsystems or a datasheet, dataset information from the datasheet is copied onto the *Dataset_Review* worksheet. While the copied data can be modified, any changes are not propagated back into the datasheets.

21.5.1. Columns 9 through 13, Participant results

Columns 9 through 13 contain the specified dataset's **Lab**, **Value**, **u**, **Use**, and **Grp** values. However, these values are not directly displayed in the chart. Any changes to these data are not implemented until the "Results plotted:" checkbox is clicked (Section 21.4.6).

21.5.2. 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 7 describes the information stored.

Table 7. *Dataset_Review* Auxiliary Information.

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

22. Dataset_NMI/DI Subsystem

The *Dataset_NMI/DI* subsystem has informative, data quality, and dataset selection functions. First and foremost, for each {WG, BaseUnit} it lists the participating organizations that reported a result in at least one {WG, BaseUnit} 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 22).

The worksheet's commands, parameters, and summary table are pictured in Fig. 97. The table lists the current **{WG, BaseUnit}** combinations and the number of organizations that are not (**No Fill**) and are (**Highlighted**) currently flagged in yellow (see Sections 22.1.2 and 22.1.3).

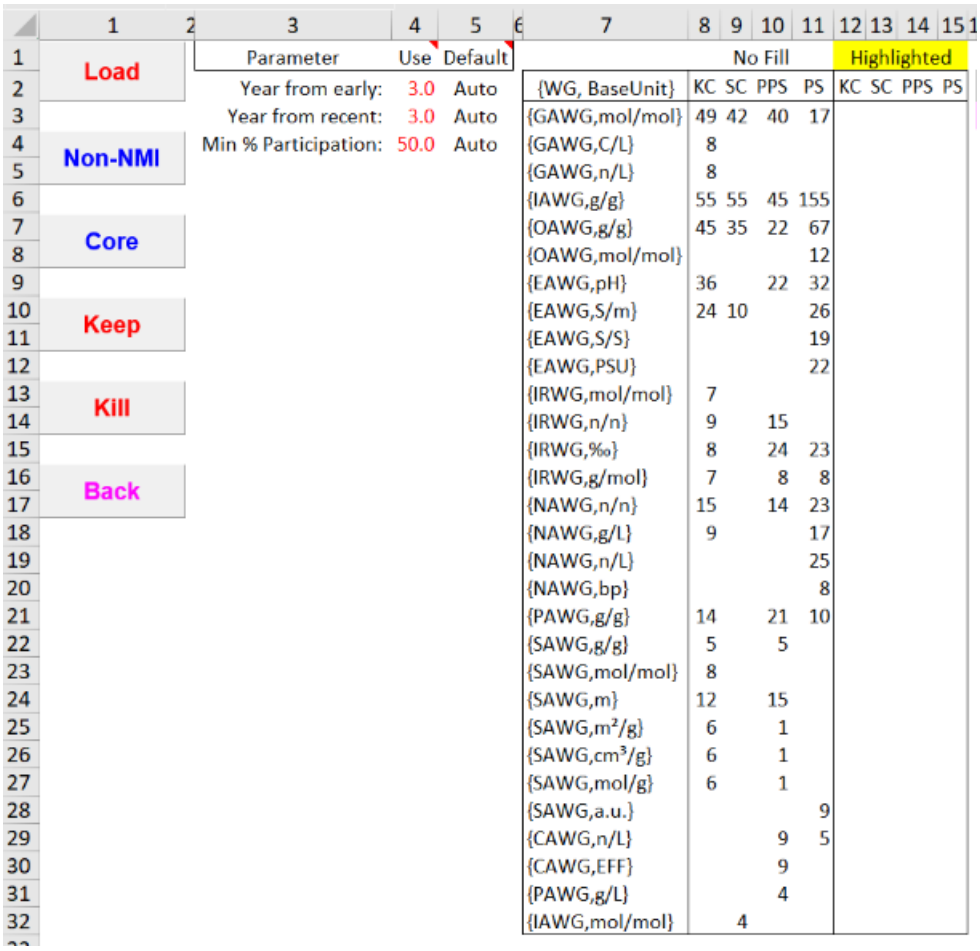


Fig. 97. Basic *Dataset_NMI/DI* Dashboard.

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 1.10 for further information.

An exemplar header of the tables generated for each {WG, BaseUnit} is pictured in Fig. 98. 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.

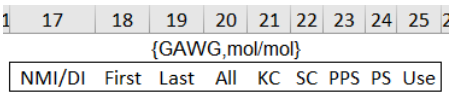


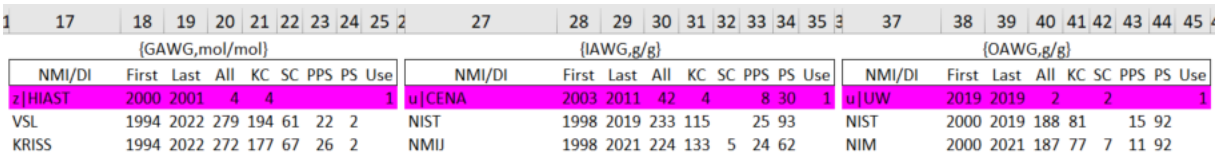
Fig. 98. Exemplar {WG, BaseUnit} Table Header.

22.1. 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).

22.1.1. Load

Clicking the **Load** 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, BaseUnit} list. A representative portion of the output is pictured in Fig. 99.



{GAWG,mol/mol}

NMI/DI	First	Last	All	KC	SC	PPS	PS	Use
z|HIAST	2000	2001	4	4				1
VSL	1994	2022	279	194	61	22	2	
KRISS	1994	2022	272	177	67	26	2	

{IAWG,g/g}

NMI/DI	First	Last	All	KC	SC	PPS	PS	Use
u|CENA	2003	2011	42	4		8	30	1
NIST	1998	2019	233	115		25	93	
NMIJ	1998	2021	224	133	5	24	62	

{OAWG,g/g}

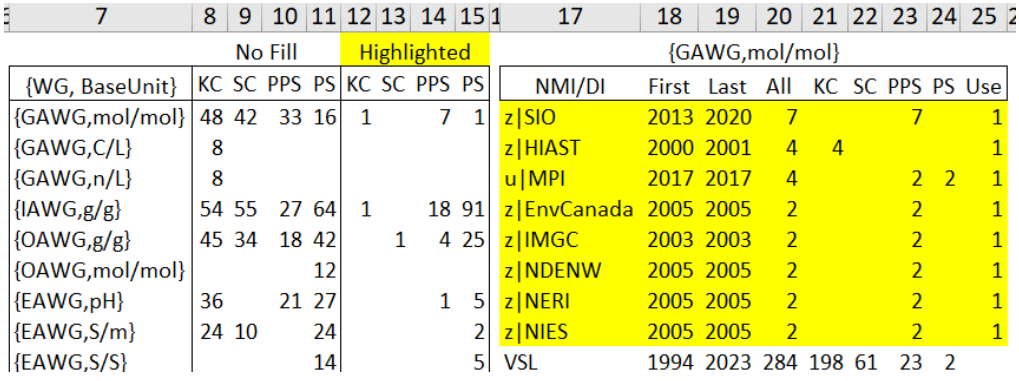
NMI/DI	First	Last	All	KC	SC	PPS	PS	Use
u|UW	2019	2019	2		2			1
NIST	2000	2019	188	81		15	92	
NIM	2000	2021	187	77	7	11	92	

Fig. 99. Exemplar {WG, BaseUnit} 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.

22.1.2. 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, BaseUnit} lists. A representative portion of the output is pictured in Fig. 100.



	No Fill				Highlighted			
{WG, BaseUnit}	KC	SC	PPS	PS	KC	SC	PPS	PS
{GAWG,mol/mol}	48	42	33	16	1		7	1
{GAWG,C/L}	8							
{GAWG,n/L}	8							
{IAWG,g/g}	54	55	27	64	1		18	91
{OAWG,g/g}	45	34	18	42		1	4	25
{OAWG,mol/mol}				12				
{EAWG,pH}	36		21	27			1	5
{EAWG,S/m}	24	10		24				2
{EAWG,S/S}				14				5

{GAWG,mol/mol}

NMI/DI	First	Last	All	KC	SC	PPS	PS	Use
z|SIO	2013	2020	7			7		1
z|HIAST	2000	2001	4	4				1
u|MPI	2017	2017	4			2	2	1
z|EnvCanada	2005	2005	2			2		1
z|IMGC	2003	2003	2			2		1
z|NDENW	2005	2005	2			2		1
z|NERI	2005	2005	2			2		1
z|NIES	2005	2005	2			2		1
VSL	1994	2023	284	198	61	23	2	

Fig. 100. Exemplar {WG, BaseUnit} 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 managed in the *Datacore_Codes* worksheet (see Section 27.4.4).

22.1.3. 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, BaseUnit} with yellow highlight and sorts them to the top of the lists. Fig. 101 displays a representative portion of the {WG, BaseUnit} lists after clicking **Core**.

7	8	9	10	11	12	13	14	15	17	18	19	20	21	22	23	24	25
	No Fill				Highlighted				{GAWG,mol/mol}								
{WG, BaseUnit}	KC	SC	PPS	PS	KC	SC	PPS	PS	NMI/DI	First	Last	All	KC	SC	PPS	PS	Use
{GAWG,mol/mol}	29	24	21	4	20	18	19	13	VSL	1994	2023	284	198	61	23	2	7
{GAWG,C/L}					8				KRISS	1994	2021	276	181	67	26	2	7
{GAWG,n/L}					8				NPL	1994	2023	256	188	42	24	2	7
{IAWG,g/g}	31	34	24	131	24	21	21	24	VNIIM	1994	2021	253	217	15	19	2	7
{OAWG,g/g}	29	25	9	51	16	10	13	16	NIM	1994	2023	185	159	21	4	1	7
{OAWG,mol/mol}				12					NIST	1994	2022	172	132	29	9	2	7
{EAWG,pH}	22		11	19	14		11	13	BAM	1994	2021	158	127	7	21	3	7
{EAWG,S/m}	15	6		17	9	4		9	SMU	1999	2021	125	106	14	3	2	7
{EAWG,S/S}				19					LNE	1994	2023	118	92	5	18	3	7
{EAWG,PSU}				22					NMIA	2002	2020	107	63	1	43		7
{IRWG,mol/mol}					7				NMIJ	1999	2019	103	78	3	20	2	7
{IRWG,n/n}	6		12		3		3		NMISA	2000	2020	100	71	23	6		7
{IRWG,‰}	6		22	21	2		2	2	BFKH	1994	2021	97	93	4			7
{IRWG,g/mol}			3	2	7		5	6	GUM	2000	2021	87	61	1	23	2	7
{NAWG,n/n}	9		8	17	6		6	6	CERI	1994	2020	65	56	8	1		7
{NAWG,g/L}	3			11	6			6	CEM	2003	2021	63	39	4	20		7
{NAWG,n/L}				25					IPQ	2000	2019	50	40	7	1	2	7
{NAWG,bp}				8					METAS	1999	2021	38	27	6	3	2	7
{PAWG,g/g}	11		18	7	3		3	3	UBA(DE)	1999	2019	25	23		2		7
{SAWG,g/g}					5		5		CHMI	2000	2021	23	21		2		7
{SAWG,mol/mol}					8				INMETRO	2004	2022	74	40	29	5		6

Fig. 101. Exemplar {WG, BaseUnit} 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 early:", "y from recent:", and "% Participation:". Starting from the score Use = 0:

- If the organization's initial participation was no more than "y from early:" years after the most recent of the earliest 25 % of {WG, BaseUnit} datasets, Use = Use +1.
- If the organization's most recent participation was no more than "y from recent:" years before the earliest of the most recent 25 % of {WG, BaseUnit} datasets, Use = Use + 2.
- If the organization has participated in at least "% Participation:" of the {WG, BaseUnit} 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, BaseUnit} list.

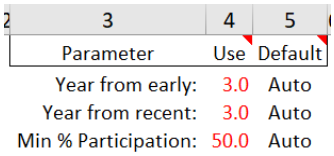
22.1.4. Keep

The **Non-NMI** and **Core** commands just highlight the {WG, BaseUnit} 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.

22.1.5. Kill

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

22.2. 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.

22.2.1. Year from early: Number of Years Elapsed from Early Studies

For an NMI/DI to be considered a Core organization, the “y from early:” parameter specifies the maximum number of years that can have elapsed between an organization’s first participation and the measurement year of the most recent of the {WG, BaseUnit}’s first 25 % datasets.

22.2.2. Year from recent: Number of Years Elapsed from Recent Studies

For an NMI/DI to be considered a Core organization, the “y from recent:” parameter specifies the maximum number of years that can have elapsed between an organization’s most recent participation and the measurement year of the earliest of the {WG, BaseUnit}’s most recent datasets.

22.2.3. Min % Participation: Minimum Participation Proportion

For an NMI/DI to be considered a Core organization, the “Min % Participation:” parameter specifies the minimum percentage of the {WG, BaseUnit}’s datasets that the organization must have contributed to.

23. 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, BaseUnit}. 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. 102.

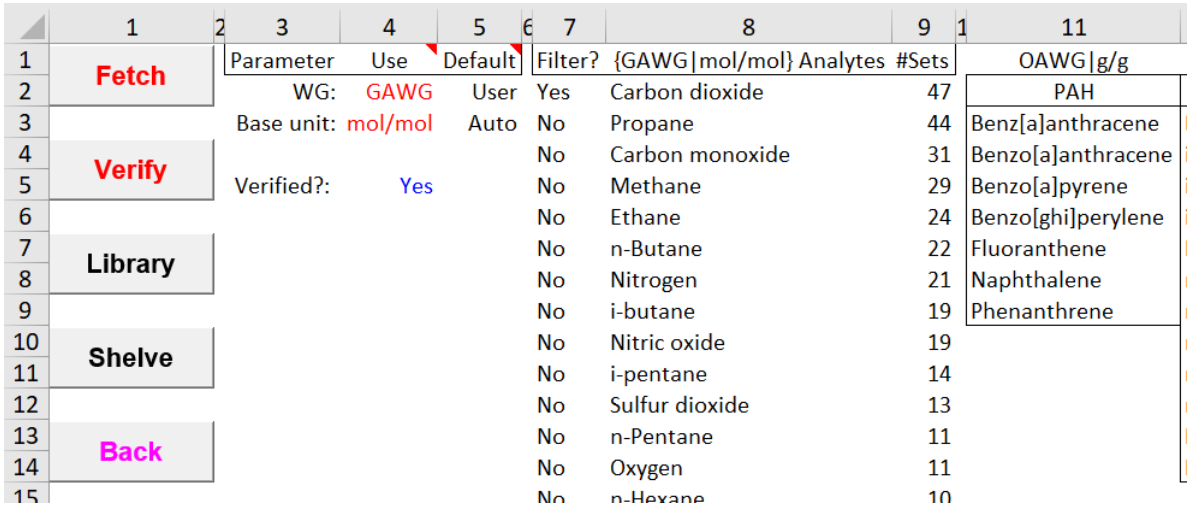


Fig. 102. *Dataset_AnalyteFilter* Worksheet with an Exemplar {GAWG, mol/mol} List.

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 1.10 for further information.

23.1. 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).

23.1.1. Fetch

Clicking the **Fetch** button populates column 8 with all the analytes for which the specified {WG, BaseUnit} 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.

23.1.2. 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, BaseUnit} results in the error message and prompt shown in Fig. 103. A list is considered to be inappropriate when the specified {WG, BaseUnit} doesn't match that specified in the header of column 8, cell(1,8).

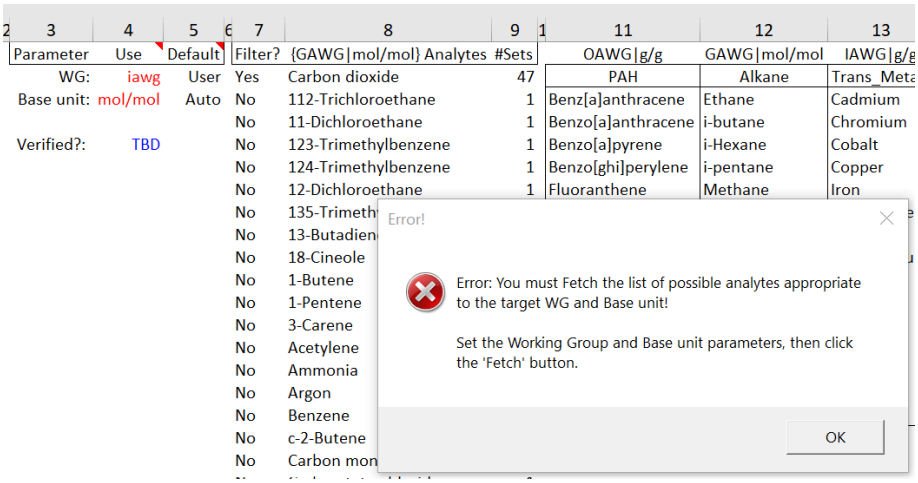


Fig. 103. Error Message and Prompt for an Inappropriate List.

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. 104.

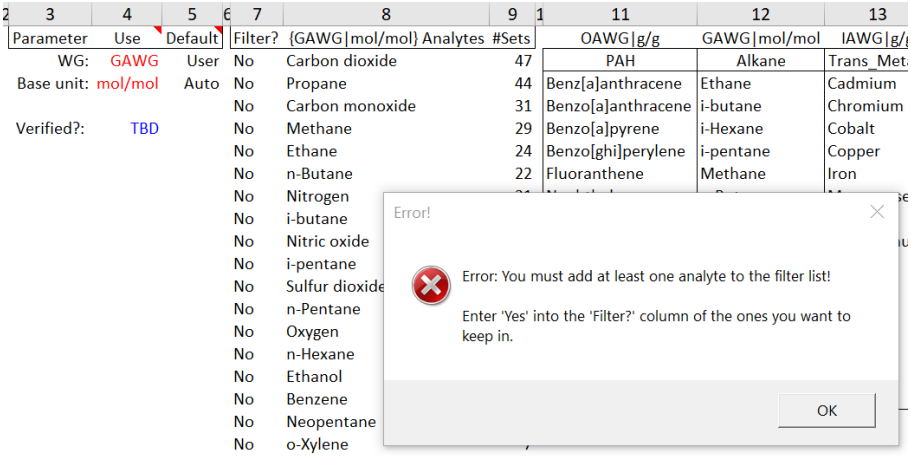


Fig. 104. Error Message and Prompt for an Inactive List.

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.

23.1.3. 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, BaseUnit}.

The notification response if there is no appropriate library list is pictured in Fig. 105.

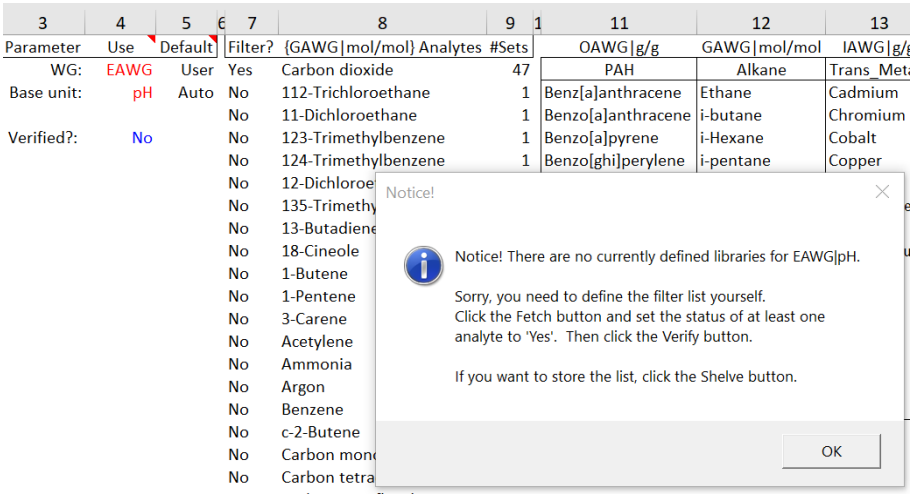


Fig. 105. Notification Response When There Is No Appropriate Library List.

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. 106. 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.

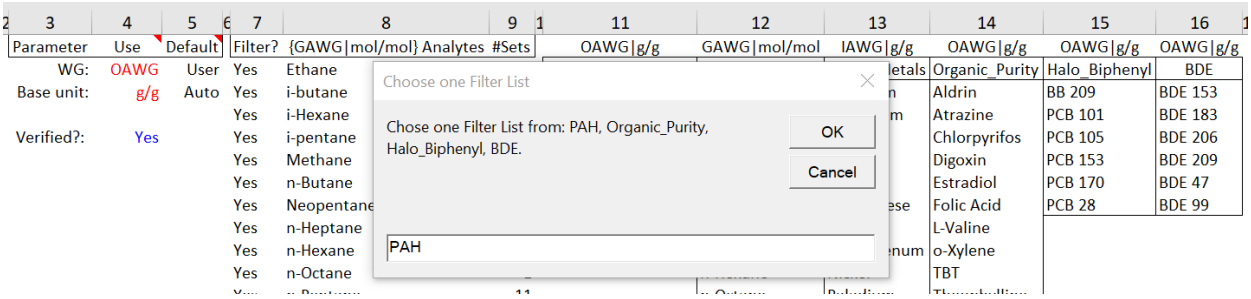


Fig. 106. Exemplar Input Box When There Are Two or More Appropriate Filter Lists.

Once a library list has been specified, the entire set of analytes appropriate to the specified {WG, BaseUnit} 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.

23.1.4. Shelve

The **Shelve** command allows users to 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. 107.

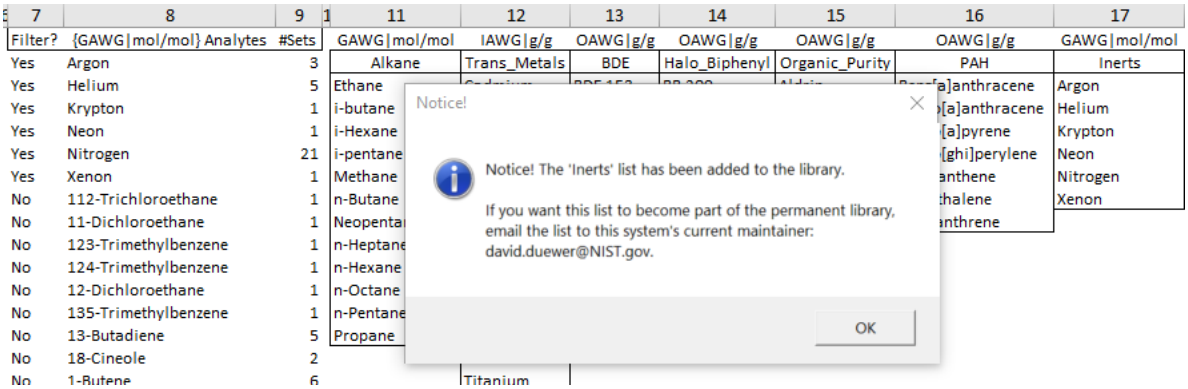
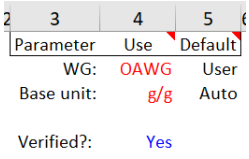


Fig. 107. Notification and Prompt When the Filter List Is Successfully Shelved.



23.2. Parameters

"WG:" and "BaseUnit:" 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.

23.3. Structure of a Library List

Library lists have the following defined structure:

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

24. 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.

This subsystem does not have its own worksheet. As displayed in Fig. 108, 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.

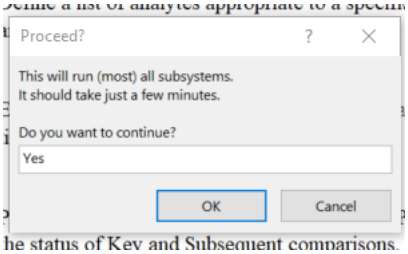


Fig. 108. *TimeTrial* Dialog Box.

If *TimeTrial* finishes without error, as shown in Fig. 109, 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.

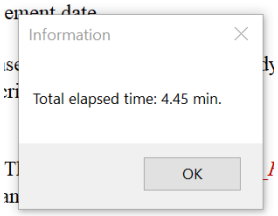


Fig. 109. *TimeTrial* Successful Completion Notification Box.

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.

24.1. 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.

24.2. 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	4.5
HP 350 G1, Intel COREi3, 1.70 GHz, 6 GB, Windows 10 Home	Microsoft Office Home and Student 2013	8.2
MacBook Air 2020, Apple M1, 3.2 GHz, 16 GB, Ventura 13.51	Microsoft 365 Subscription Excel for Mac	3.2

As shown in Fig. 110, 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.

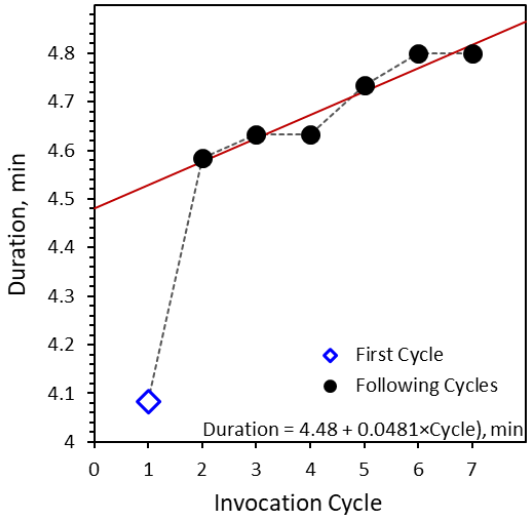


Fig. 110. *TimeTrial* Duration as a Function of Invocation Cycle on the Dell 7490 Platform.

The clock-time required by most *CCQM_Retrospectoscope* subsystems to load and evaluate the default data (GAWG, NIST, 1993 to 2024) on the Dell 7490 is displayed in Fig. 111. These summary statistics are for cycles following the initial invocation.

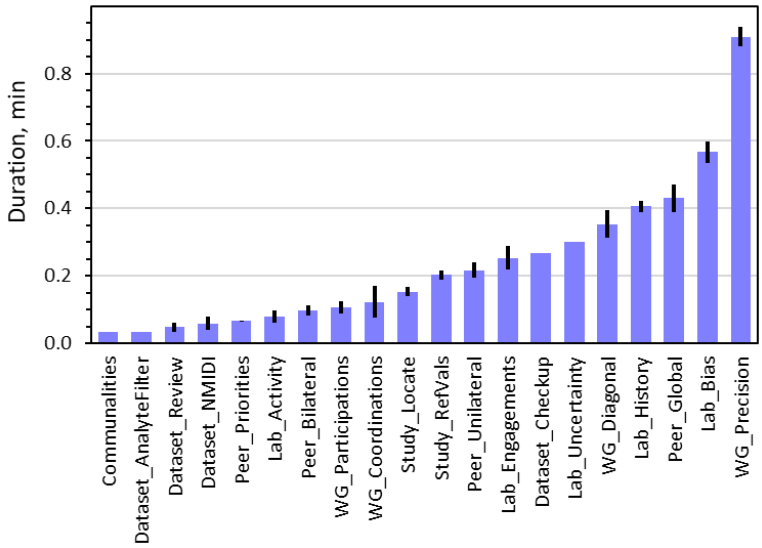


Fig. 111. Average Subsystem "Following Cycle" Duration on the Dell 7490.

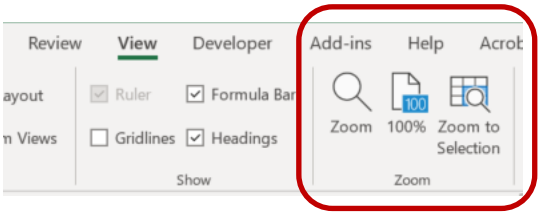
Error bars represent approximate 95 % confidence intervals on the mean durations.

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 or Peer_Global*) and number-of-peer-NMI/DIs × *Lab_Uncertainty*.

25. Zoom

Display screens of different physical size, pixel resolution, and/or portrait/landscape orientation can vary in how much of a worksheet they show. And it is sometimes useful to enlarge what is displayed at the expense of displaying less content – or to shrink what is displayed to see more of the content. Since having to independently resize each worksheet of interest can become irritating, the **Zoom** command is provided to set the display size (the worksheet "zoom") for *all* worksheets in the *CCQM_Retrospectoscope* system to the zoom of the *Other_Tools* worksheet.

You can set the zoom for the *Other_Tools* worksheet (or any other worksheet) using:



- the tools in the Zoom panel of the ribbon's View tab

and/or

- the slider control at the bottom right of the active window. Slide to the percentage zoom setting that you want. Click the "-" or "+" symbols at the ends of the slider to zoom in gradual increments.

This subsystem does not have its own worksheet. Clicking the **Zoom** button invokes a simple macro program that quickly does its job and returns control back to the *Other_Tools* worksheet when finished.

Clicking the **Zoom** button before you've modified the worksheet's zoom setting does no harm, but it doesn't accomplish much beyond ensuring that all of the worksheets have the same zoom.

26. Database_FindNew

The *Database_FindNew* worksheet provides seven standalone tools for identifying newly available studies or for identifying changes in study status. The worksheet's command button and output format are shown in Fig. 120.

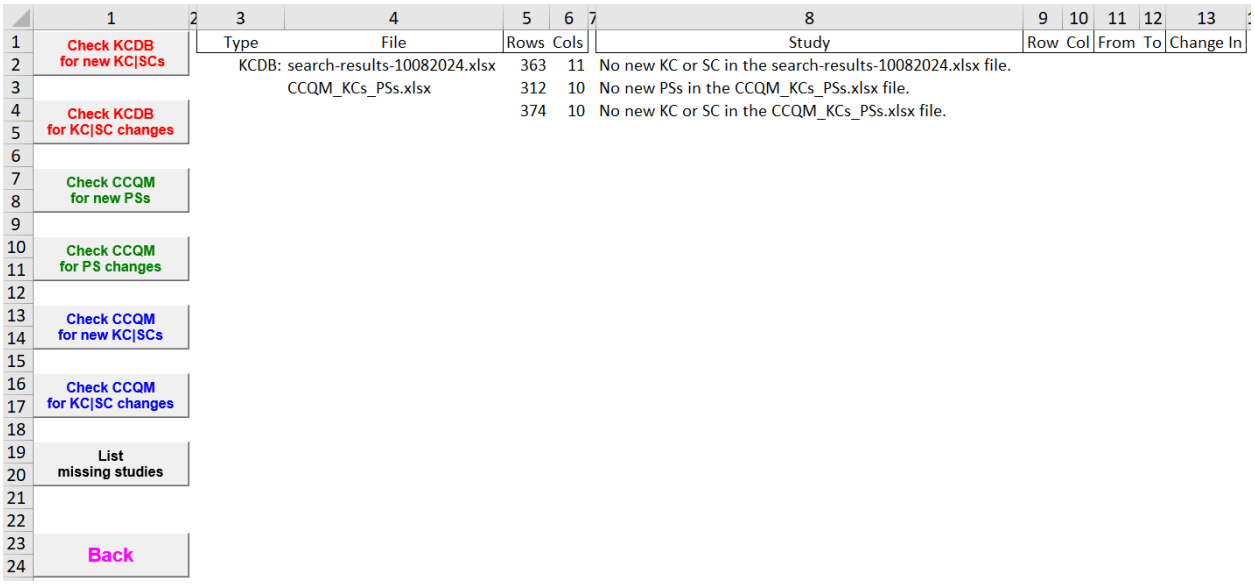


Fig. 112. *Database_FindNew* Dashboard After Clicking the **Check for New KC|SC** Button.

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.

26.1. Additional Command Buttons

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

26.1.1. Check KCDB for New KC|SCs

Clicking the **Check KCDB for New KC|SCs** button compares the list of KC and SC studies maintained in the *Datacore_Dates* worksheet with that provided in a KCDB "search-results" workbook. The name of the KCDB-generated workbook must be specified in row 2 column 4 of the *Database_FindNew* worksheet. 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 26.2.1 for how to obtain a current KCDB "search-results" workbook.

26.1.2. Check KCDB for KC|SC Changes

Clicking the **Check KCDB 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" workbook (see Section 26.1.1). 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.

26.1.3. Check CCQM for New PSs

Clicking the **Check CCQM for New PSs** button compares the list of pilot studies (PPS and PS) maintained in the *Datacore_Dates* worksheet with that provided in "Pilot Studies" worksheet of the CCQM's study-tracking workbook, currently named "*CCQM_KCs_PSs.xlsx"* [17]. The workbook is a summary of all CCQM studies, is updated at infrequent intervals, and has accumulated numerous minor errors. While the name of this workbook has not changed since it was upgraded from ".xls" to ".xlsx" format, the current name must be specified in row 3 column 4 of the *Database_FindNew* worksheet. 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 26.3.1 for how to obtain a current *CCQM_KCs_PSs.xlsx* workbook.

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.

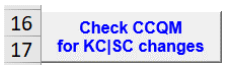
26.1.4. Check CCQM for PS Changes

Clicking the **Check CCQM for PS 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_KCs_PSs.xlsx* studt-tracking workbook (see Section 26.1.3). Changes in these status values are listed in column 8 to 12 of the *Database_FindNew* worksheet. Confirmed differences must be by-hand added to the *Datacore_Dates* worksheet.

26.1.5. Check CCQM for new KC|SCs

Clicking the **Check CCQM for new KC|SCs** button compares the list of KCs and SCs maintained in the *Datacore_Dates* worksheet with that provided in the "Key Comparisons" worksheet of the *CCQM_KCs_PSs.xlsx* stufy- tracking workbook (see Section 26.1.3). The study existence information in this worksheet is less authoritative than that in the KCDB, but it provides a cross-check that occasionally identifies a study not yet in the KCDB. 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.

26.1.6. Check CCQM for KC|SC Changes



Clicking the **Check CCQM for KC|SC 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 "Key Comparisons" worksheet of the *CCQM_KCs_PSs.xlsx* study-tracking workbook (see Section 26.1.3). The status information in this worksheet is *much* less authoritative than that in the KCDB and should not be used without independent confirmation. Differences in status values are listed in column 8 to 12 of the *Database_FindNew* worksheet. Any confirmed changes must be by-hand added to the *Datacore_Dates* worksheet.

26.1.7. List Missing Studies

Clicking the **List missing studies** button lists the studies identified in the *Datacore_Dates* worksheet as finalized but without datasets or an explanation for the absence of results. As of this document's publication date, there are four missing pilot study reports; Fig. 113 lists the available information on these studies.

8	9	10	11	12	13
Study	Row	Col	WG	Year	Comment
CCQM-P045: Purity of parent gases including water	394	1	GAWG	(2002)	
CCQM-P137: Activity of α-amylase in human serum	498	1	PAWG	(2015)	
CCQM-P164: Human growth hormone in serum	524	1	PAWG	(2017)	
CCQM-P202: Mass fraction of leucine, phenylalanine in pooled	555	1	OAWG	(2019)	|| to: CCQM-K159

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

Fig. 113. *Database_FindNew* Output After Clicking the **List Missing** Button.

26.2. *search-results-ddmmyyyy.xlsx* Workbook

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 workbook named *search-results-ddmmyyyy.xlsx* where ddmmyyyy is the current day-month-year date. The KCDB webpage is https://www.bipm.org/kcdb/.

26.2.1. Obtaining the search-results-ddmmyyyy.xlsx Workbook

The current *search-results-ddmmyyyy.xlsx* workbook is obtained using the KCDB's "Key and supplementary comparisons" "Advanced search" function. The function is accessed by clicking the "Advanced search" link placed just below the "Key and supplementary comparisons" search box at the bottom right of the KCDB dashboard, shown in Fig. 121.

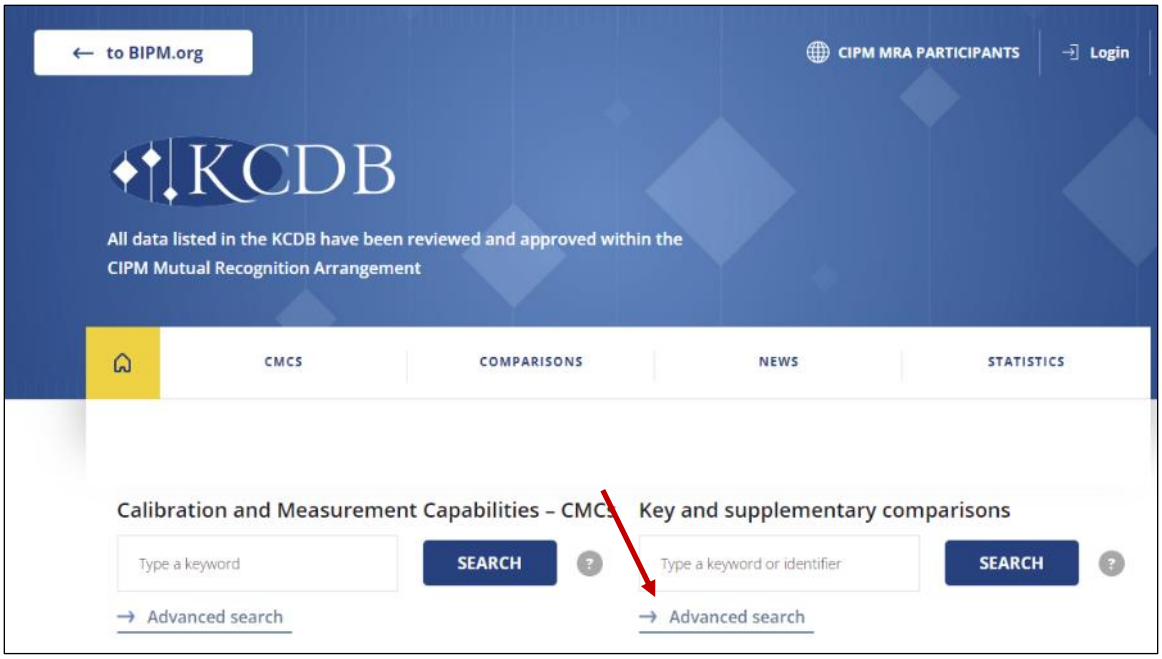


Fig. 114. Image of the BIPM's KCDB Dashboard.

Clicking the "Advanced search" link activates the BIPM's "COMPARISON ADVANCED SEARCH" dashboard, shown in Fig. 122. 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 (356 as of this document's publication date) and the start of a listing as shown in Fig. 116.

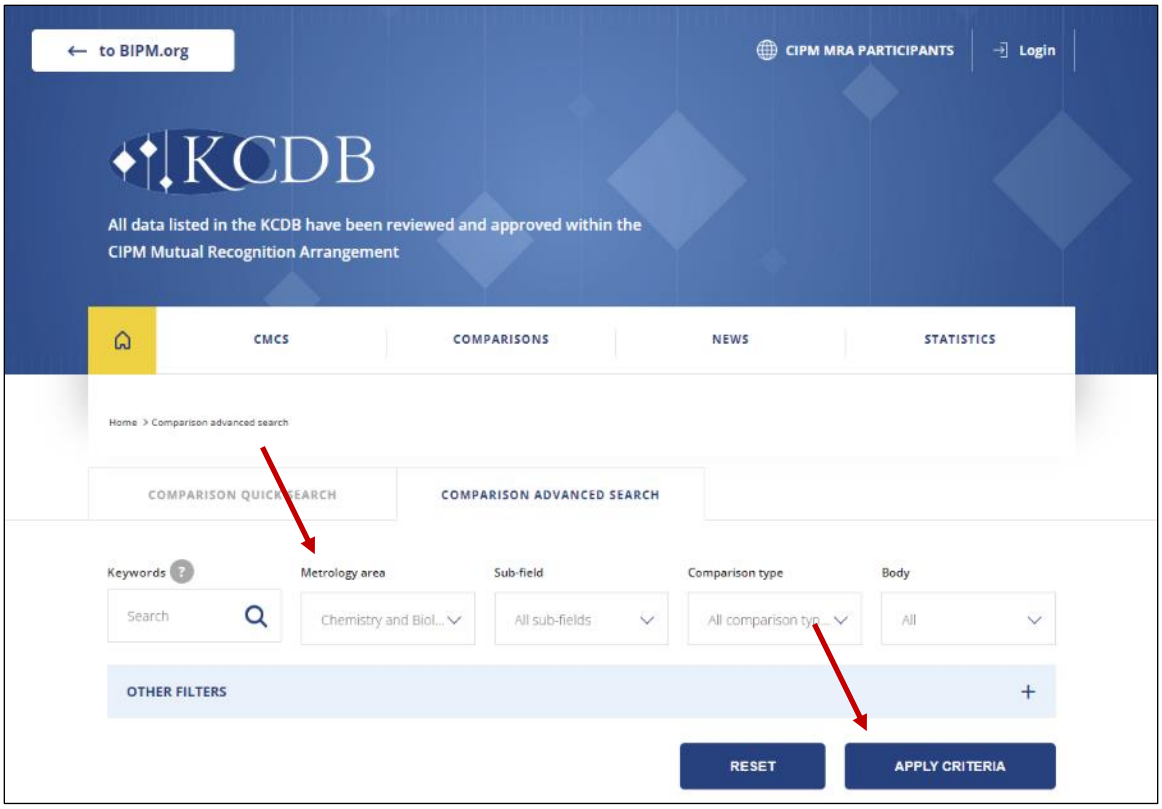


Fig. 115. Image of the KCDB "COMPARISON ADVANCED SEARCH" Dashboard.

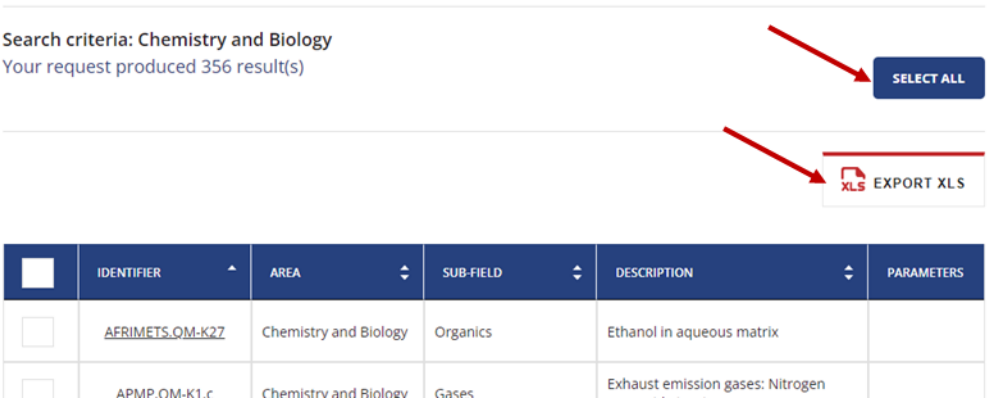


Fig. 116. Image of an Example Advanced Search Output.

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* workbook.

26.2.2. Making Use of the search-results-ddmmyyyy.xlsx Workbook

Move the *search-results-ddmmyyyy.xlsx* workbook into the folder that holds *CCQM_Retrospectoscope* and activate the *Database_FindNew* worksheet. Modify the workbook

designation in row 2 of column 4 as needed. If the system can't find the workbook, you will be prompted to supply the correct name.

Click the **Check KCDB for New KC|SCs** 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 KCDB for New KC|SCs** button produces the message "No new KC or SC in the search-results-10082024.xlsx file."

Click the **Check KCDB 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 KCDB for KC|SC Changes** button either produces the message "No KC/SC-relevant WG, pilot lab, measurement date, or status changes were identified." or the indicated changes are determined to be unnecessary.

26.3. *CCQM_KCs_PSs.xlsx* Workbook

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. This workbook is by-hand curated (and has accumulated a number of minor misspellings and out-of-date information over the years). Nevertheless, the "Pilot Study" worksheet in this workbook is the primary source of PS information. The information in the workbook's "Key Comparison" worksheet is sometimes worth checking, but should be independently verified before use

26.3.1. Obtaining the *CCQM_KCs_PSs.xlsx* Workbook

As of this document's publication date, the *CCQM_KCs_PSs.xlsx* workbook can be retrieved using the BIPM's search function (https://www.bipm.org/en/search) as shown in Fig. 117. The search also finds documents that mention the workbook.

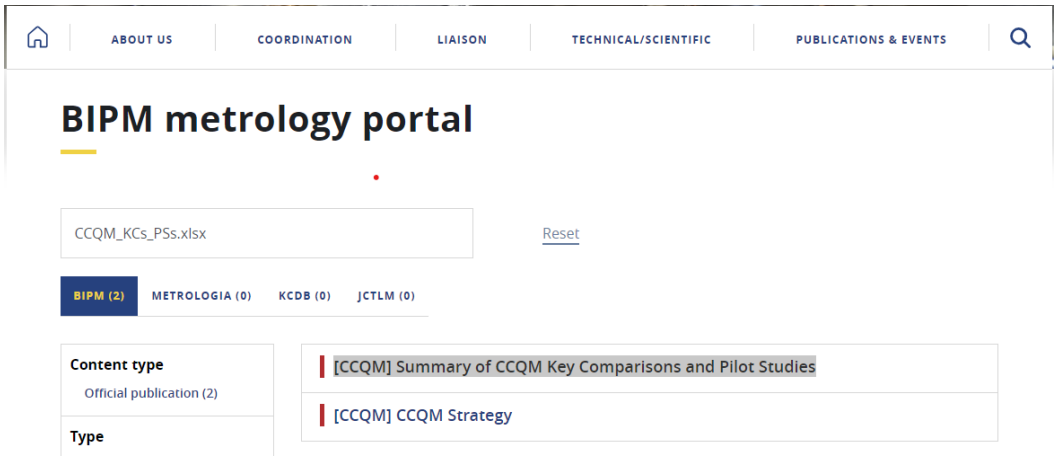


Fig. 117. Results of BIPM Search for *CCQM_KCs_PSs.xlsx*.

The worksheets in this workbook specify the date they were last updated in row 3 column 2: see Fig. 118. As of this document's publication date, the workbook was last updated 12/14/2023.

	1	2	3	4	5	6	
1	**CCQM Pilot Studies**						
2							
3	**Date updated**	**4 December 2023**					
4							
5	**WG**	**Reference No.**	**Description**	**Coordinating Laboratory**	**Start date**	**Status**	**Comments**
6	IAWG	CCQM-P1	Trace elements in water Pb	NIST	1997	Completed 1998	
7	OAWG	CCQM-P2	p,p'-DDE in isooctane	LGC	1997	Completed	

Fig. 118. Header of the *Pilot Studies* Worksheet of the *CCQM_KCs_PSs.xlsx* Workbook.

26.3.2. Making Use of the *CCQM_KCs_PSs.xlsx* Workbook

Move the *CCQM_KCs_PSs.xlsx* workbook into the folder that holds *CCQM_Retrospectoscope* and activate the *Database_FindNew* worksheet. If necessary, modify the workbook designation in row 3 of column 4. If the system can't find the workbook, you will be prompted to supply the correct name.

Click the **Check CCQM for New PSs** 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 CCQM for New PSs** button produces the message "No new PSs in the *CCQM_KCs_PSs.xlsx* file."

Click the **Check CCQM for PS 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 CCQM for PS Changes** button either produces the message "No PS-relevant WG, pilot lab, measurement date, or status changes were identified." or the indicated changes are determined to be unnecessary.

Click the **Check CCQM for New KC/SCs** button. In the unlikely case that 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 CCQM for New KC/SCs** button produces the message "No new KC or SC in the *CCQM_KCs_PSs.xlsx* file."

Click the **Check CCQM for KC/SC Changes** button. Many differences will be identified, mostly due to the much more frequent updating of the KCDB. However, occasionally the *CCQM_KCs_PSs.xlsx* is more up-to-date than the current KCDB "search results" workbook. When there is evidence that measurement results may be available in a Draft A or Draft B, it may be useful to try to obtain a copy. Other changes should be reviewed, but not added to the *Datacore_Dates* worksheet without strong evidence that the KCDB holds incorrect information. Non-trivial KCDB corrections should be reported to the WebMaster@bipm.org.

26.4. 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.

26.4.1. 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 find 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.

26.4.2. 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".

26.4.3. 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.

26.5. Addressing Input File Disagreements

When any of the six "Check" buttons are clicked and a deficiency in the *CCQM_Retrospectoscope* database is identified, there is a non-zero chance that the problem is with the information in the BIPM-provided *search-results-ddmmyyyy.xlsx* or *CCQM_KCs_PSs.xlsx* workbooks. 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. 119.

Study Name Change		#
From	To	K P
CCQM-K120	CCQM-K120.a	1
CCQM-P020.e.1	CCQM-Q020.e	1
CCQM-P041	CCQM-Q041.1	1
CCQM-P110	CCQM-Q110.B1	1
CCQM-P189	CCQM-Q189	1
CCQM-P204	CCQM-Q204	1
CCQM-P212	CCQM-Q212	1
CCQM-P216	CCQM-Q216.1	1

WG Change		#
Study	WG	K P
CCQM-K034	IAWG	5
CCQM-K048	IAWG	2
CCQM-K073	IAWG	5
CCQM-K096	IAWG	4
CCQM-K169	IAWG	1
CCQM-K173	IAWG	2

Coordinator Change		#
Study	Pilot	K P
CCQM-K027.1	NIST	1
CCQM-K030.1	ISP	1
CCQM-P012.2	ISP	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-P197	NPL,NIST	1
CCQM-P205	NIM,NIST	1
CCQM-P217	LGC,NIBSC,NIST,PTB	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
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
NIMChina	NIM	1
NIMJ	NMIJ	2
NIMT,TUBITAKUME	NIMT,UME	1
NMi	VSL	1
NML,LGC,NIMC,NIBSC,NIST	LGC,NIM,NIBSC,NIST	1
NML@LGC	LGC	1
NRCCRM	NIM	1
SE	UMTS	1
UME,KISS	UME,KRISS	1
UNIIM	VNIIM	2 3
UNIIM,BAM	VNIIM,BAM	1

Date Changes			#
Study	Type	Year	K P
APQM-S003	First	2008	1
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
CCQM-K160	Last	6-May-2022	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-P226	First	2022	1
CCQM-Q058.1	First	2011	1
CCQM-Q102	First	Oct-2011	1
CCQM-Q204	First	1-Apr-2022	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
SIQM-S006	Last	2022	1

Fig. 119. 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 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 KCDB for New KC|SCs** and **Check KCDB for KC|SC Changes** commands, the **#P** columns are populated during execution of the **Check CCQM for New PSs** and **Check CCQM for PS 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 change counts are reset when "**Check KCDB for New KC|SCs**" is executed.

Note: these changes were originally hard coded in the *Database_FindNew* subsystem. They were implemented in their current form to make life a little easier for any future system maintainer.

27. 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. 120.

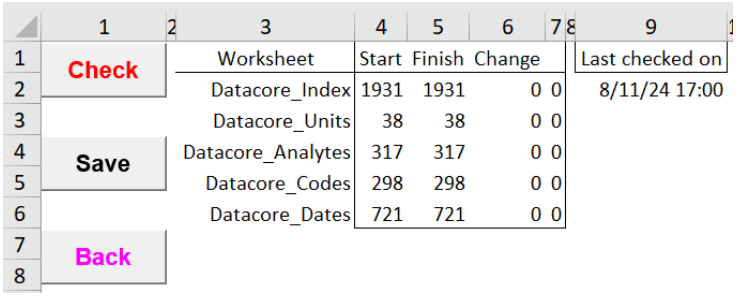


Fig. 120. Basic *Database_Checkup* Dashboard.

27.1. 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 *Datacore_Index* row lists the total number of datasets in the *CCQM_Retrospectoscope* datasheets,
- the *Datacore_Units* row lists the number of unique BaseUnits,
- the *Datacore_Analytes* row lists the number of unique analytes,
- the *Datacore_Codes* row lists the number of unique participating organization code names, and
- the *Datacore_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.

27.2. 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. 121.

1	11	12	13	14	1	16	17	18	19	20	21	2	23	24	25	26	27	28	2	30	31	32	33	3
		Datasets					DataSets							Datasets							Datasets			
	Datasheet	Single	Multiple	Total		Body	KC	SC	PPS	PS	Total		WG	KC	SC	PPS	PS	Total		WG	Smpl	Cmplx	Total	
	CCQM_KC	946	113	1059		AFRIMETS	2				2		CAWG			4	4	8		CAWG	8		8	
	CCQM_Pilot	585	4	589		APMP	21	57	6	11	95		EAWG	100	8	7	41	156		EAWG	141	15	156	
	CCQM_PubPilot	243		243		BIPM	36				36		GAWG	365	132	74	7	578		GAWG	304	274	578	
	CCQM_Continuous	34	2	36		CCQM	793		238	577	1608		IAWG	209	52	28	252	541		IAWG	131	410	541	
	CCQM_KC_Beta	4		4		COOMET	18	14			32		IRWG	15		39	10	64		IRWG	15	49	64	
	Total	1812	119	1931		EURAMET	17	88			105		NAWG	8		10	58	76		NAWG	39	37	76	
						SIM	9	44			53		OAWG	137	11	16	181	345		OAWG	68	277	345	
						Total	896	203	244	588	1931		PAWG	9		23	19	51		PAWG	7	44	51	
													SAWG	53		43	16	112		SAWG	58	54	112	
						Studies							Total	896	203	244	588	1931		Total	771	1160	1931	
						Body	KC	SC	PPS	PS	Total		Studies							Studies				
						AFRIMETS	1				1		WG	KC	SC	PPS	PS	Total		WG	Smpl	Cmplx	Total	
						APMP	13	22	1	3	39		CAWG			3	4	7		CAWG	7		7	
						BIPM	17				17		EAWG	27	2	2	15	46		EAWG	44	2	46	
						CCQM	233		73	183	489		GAWG	101	31	23	4	159		GAWG	126	33	159	
						COOMET	8	6			14		IAWG	66	13	9	77	165		IAWG	55	110	165	
						EURAMET	9	13			22		IRWG	5		6	4	15		IRWG	4	11	15	
						SIM	5	11			16		NAWG	4		2	19	25		NAWG	11	14	25	
						Total	286	52	74	186	598		OAWG	64	6	8	58	136		OAWG	37	99	136	
													PAWG	5		11	4	20		PAWG	7	13	20	
													SAWG	14		10	1	25		SAWG	12	13	25	
													Total	286	52	74	186	598		Total	303	295	598	

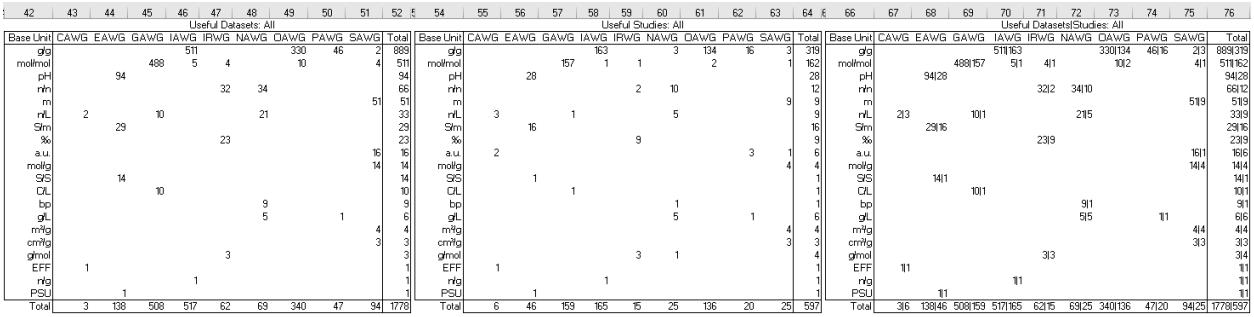
Fig. 121. *Database_Checkup* Datasheet, Body, and WG Tables.

A part of the table that summarizes the number of datasets containing given numbers of valid (Nok) data is pictured in Fig. 122. The first row, where Nok is 0 and the numbers are in red font, accounts for the composite datasets and datasets for which a RV and/or its uncertainty could not be assigned.

35	36	37	38	39	40	4
	Datasets					
Nok	KC	SC	PPS	PS	Total	
0	110	6	11	26	153	
1	17	10	27	58	112	
2	33	20	32	44	129	
3	32	29	21	30	112	
4	43	26	23	42	134	
5	72	11	8	33	124	
6	57	9	2	45	113	
7	88	23	14	64	189	
8	100	10	11	42	163	
9	95	9	6	45	155	
10	70	18	25	51	164	
11	26	5	12	23	66	
12	21	3	8	23	55	
13	28	5	8	20	61	
14	17	2	15	9	43	
15	21	7	15	6	49	
16	36	5		8	49	
17	12	5		5	22	
18	9		4	3	16	
19	3			3	6	
20	1			3	4	
22			2	3	5	
23	1			1	2	
24	1			1	2	
25	3				3	
Total	896	203	244	588	1931	

Fig. 122. *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 BaseUnits is pictured in Fig. 123. 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				511				330	46	2 889
mol/mol			488	5	4		10			4 511
pH		94								94
nln					32	34				66
m										51 51
nL	2		10			21				33
S/m		29								29
‰					23					23
a.u.										16 16
mol/g										14 14
S/S		14								14
C/L			10							10
bp						9				9
g/L						5		1		6
m²/g									4	4
cm³/g									3	3
g/mol					3					3
EFF	1									1
n/g				1						1
PSU		1								1
Total	3	138	508	517	62	69	340	47	94	1778

Useful Studies: All

Base Unit	CAWG	EAWG	GAWG	IAWG	IRWG	NAWG	OAWG	PAWG	SAWG	Total
g/g				163		3	134	16	3	319
mol/mol			157	1	1		2		1	162
pH		28								28
nln					2	10				12
m									9	9
nL	3		1			5				9
S/m		16								16
‰					9					9
a.u.	2							3	1	6
mol/g									4	4
S/S		1								1
C/L				1						1
bp						1				1
g/L						5		1		6
m²/g									4	4
cm³/g									3	3
g/mol					3	1				4
EFF	1									1
n/g				1						1
PSU		1								1
Total	6	46	159	165	15	25	136	20	25	597

Useful Datasets|Studies: All

Base Unit	CAWG	EAWG	GAWG	IAWG	IRWG	NAWG	OAWG	PAWG	SAWG	Total
g/g				511|163			330|134	46|16	2|3	889|319
mol/mol			488|157	5|1	4|1		10|2		4|1	511|162
pH		94|28									94|28
nln						32|2	34|10				66|12
m										51|9	51|9
nL	2|3		10|1			21|5					33|9
S/m		29|16									29|16
‰						23|9					23|9
a.u.										16|1	16|6
mol/g										14|4	14|4
S/S		14|1									14|1
C/L			10|1								10|1
bp							9|1				9|1
g/L							5|5		1|1		6|6
m²/g										4|4	4|4
cm³/g										3|3	3|3
g/mol						3|3					3|4
EFF	1|1										1|1
n/g				1|1							1|1
PSU		1|1									1|1
Total	3|6	138|46	508|159	517|165	62|15	69|25	340|136	47|20	94|25	1778|597

Fig. 123. Exemplar *Database_Checkup* {WG, BaseUnit} Tables.

27.3. 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.

27.3.1. 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.

27.3.2. 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.

27.4. Datacore Worksheets

The five *Datacore* worksheets store information essential to *CCQM_Retrospectoscope* 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.

27.4.1. 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.

27.4.2. Datacore_Units

The *Datacore_Units* worksheet lists all the measurement units used and connects the units-as-used to their BaseUnits (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 28.

27.4.3. 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 28.

27.4.4. 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 organization's 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 28.3). 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.

27.4.5. 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 28.2.7).

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 study 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* workbooks. 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.

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.

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, “pilot labs”). This information is used by the *WG_Coordinations* subsystem.

28. Database Worksheets

There are three database worksheets that contain publicly accessible CCQM measurement information: *CCQM_KC*, *CCQM_PubPilot*, and *CCQM_Continuous*. These 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 of the database worksheets have the same basic format. They differ only in the type of study they support.

28.1. Command buttons

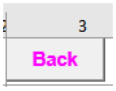
Each datasheet provides two command buttons, **Review** and **Back**, placed at the top left of the worksheet. To provide access to these commands regardless of what dataset is being examined, the default worksheet view is frozen such that row 1 and columns 1 to 3 are always visible.

28.1.1. 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 21).

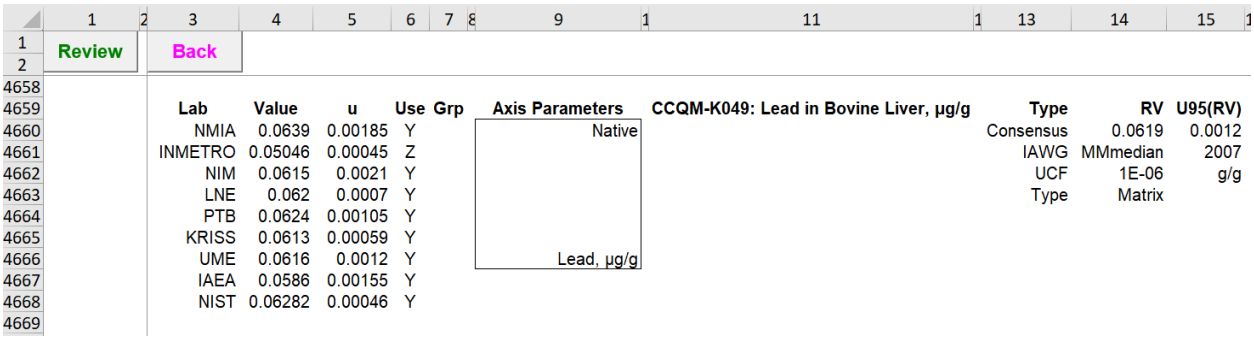
28.1.2. Back

Clicking the **Back** button causes the focus to be returned to whatever worksheet invoked the dataset Review.



28.2. Dataset Format

A representative dataset is pictured in Fig. 124. 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.



	Lab	Value	u	Use	Grp	Axis Parameters	CCQM-K049: Lead in Bovine Liver, µg/g	Type	RV	U95(RV)
4659										
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. 124. Standard Dataset Storage Format.

28.2.1. 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.

28.2.2. 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.

28.2.3. 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.

28.2.4. 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.

28.2.5. 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.

28.2.6. Column 9, Axis Parameters

This is the most clunky bit. The older system supported a variety of *y*-axis (reported value) 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* 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.

28.2.7. 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 1.5.2)
- Type of study (“K”) (see Section 1.5.1)
- Assigned numeric index (“100: ”) This index may be followed by various modifiers.
- Measurand (“Copper in Ethanol,”)
- Units (“µg/g”) (see Section 1.5.4)

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 the (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.

28.2.8. Column 13, Type

The cell in the first row beneath the **Type** header describes the "type" of RV, 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.

28.2.9. Column 14, RV

The cell in the first row beneath the **RV** header defines the RV 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 RV 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 BaseUnit (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.

28.2.10. Column 15, U95(RV)

The cell in the first row beneath the **U95(RV)** header is the 95 % expanded uncertainty on the RV.

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 BaseUnit. The *Database_Checkup* subsystem checks this assignment for consistency with the units stated in both the dataset title and the *y*-axis title.

28.3. Auxiliary Information, Columns 18 to 29

The values under the **Lab**, **Value**, **u**, and **Use** headers (columns 3 through 6) contain the values that the *CCQM_Retrospectoscope* uses, but these values are transferred from data held in other columns (Fig. 125). This indirect approach is used because there isn't a one-size-fits-all method for documenting the results of a study.

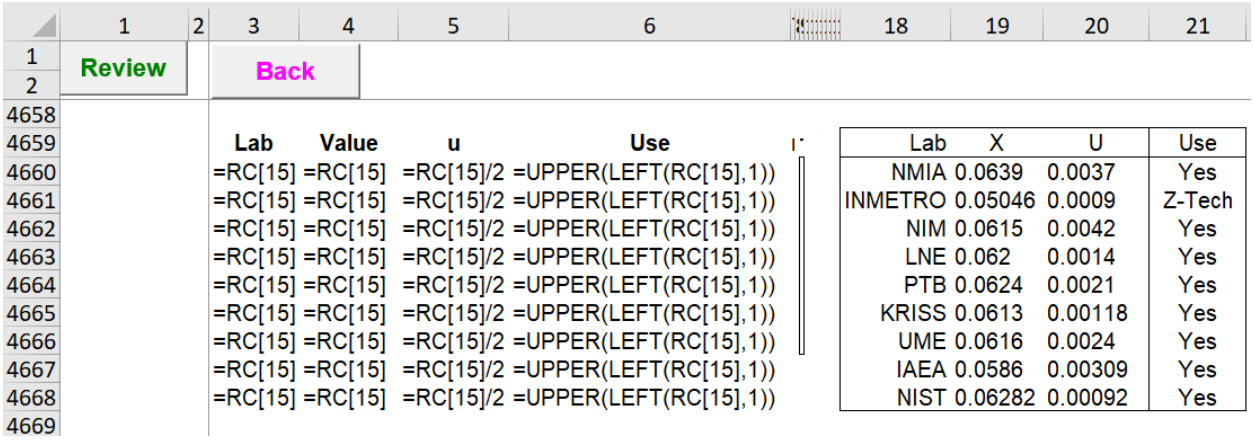


Fig. 125. Where the Raw Data is Stored.

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.

28.3.1. 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.

28.3.2. 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 RVs. Converting them to a common reference require the transformation:

$$w_i \pm u(w_i) \;=\; y_{\mathrm{nom}} \cdot (x_i \pm u(x_i))/(y_i \pm u(y_i))$$

where: y_{nom} is the nominal concentration of the measurand and $y_i \pm u(y_i)$ is the RV and its standard uncertainty.

The *CCQM_Retrospectoscope* datasheets calculate y_{nom} as the arithmetic mean of the individual RVs; its 95 % expanded uncertainty, $U_{95}(y_{\mathrm{nom}})$, is calculated as the twice the pooled standard uncertainty of the individual RVs. When the multiple uncertainty components are provided (e.g., u_{prep} and u_{verify}), only the combined standard uncertainty, $u(x_{\mathrm{ref}})$, 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.

28.3.3. 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:

$$w_i = x_{\mathrm{ref}}(1 + \%DoE_i/100);\ u(w_i) = w_i \cdot u(\%DoE_i)/100$$

Results expressed as values with units of the measurement, $\%DoE_i \pm u(\%DoE_i)$, have been transformed:

$$w_i = x_{\mathrm{ref}} + DoE_i;\ u(w_i) = u(DoE_i)$$

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}:

$$u(x_{\mathrm{ref}}) = x_{\mathrm{ref}} \cdot u_{\mathrm{repeat}}$$

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.

28.3.4. *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 "$v = \mathrm{large}$" 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* 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, 95 expanded uncertainty/2), while an imperfect remedy, at the very least gives rise to 95 % error bars of the correct length.

28.3.5. 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: $u = (u(lo) + u(hi))/2$.

28.3.6. "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 RV 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 RV 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.

28.3.7. 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, “Z-SO” indicates that the result was declared to be a “statistical outlier” by the coordinating WG, “Z-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”, “Y”, or “Z” since that what is captured by the transfer function.

28.4. 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 RV to the RV 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 RV 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.

28.5. Creating New Datasets

Once new data results have been found, updating the *CCQM_Retrospectoscope* is generally straight forward - but it requires attention to detail and careful validation.

In each new report, find the tables that list the study timeline, the measurement results, and the RVs and uncertainties. While it’s efficient to hand-transfer simple values like the measurement year and RVs, 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 28.2 and 28.3 and ensuring that the measurement results are accessible:

- Find 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 28.2 and 28.3!). 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 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.

28.6. 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 order.

29. 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* is 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. 126.

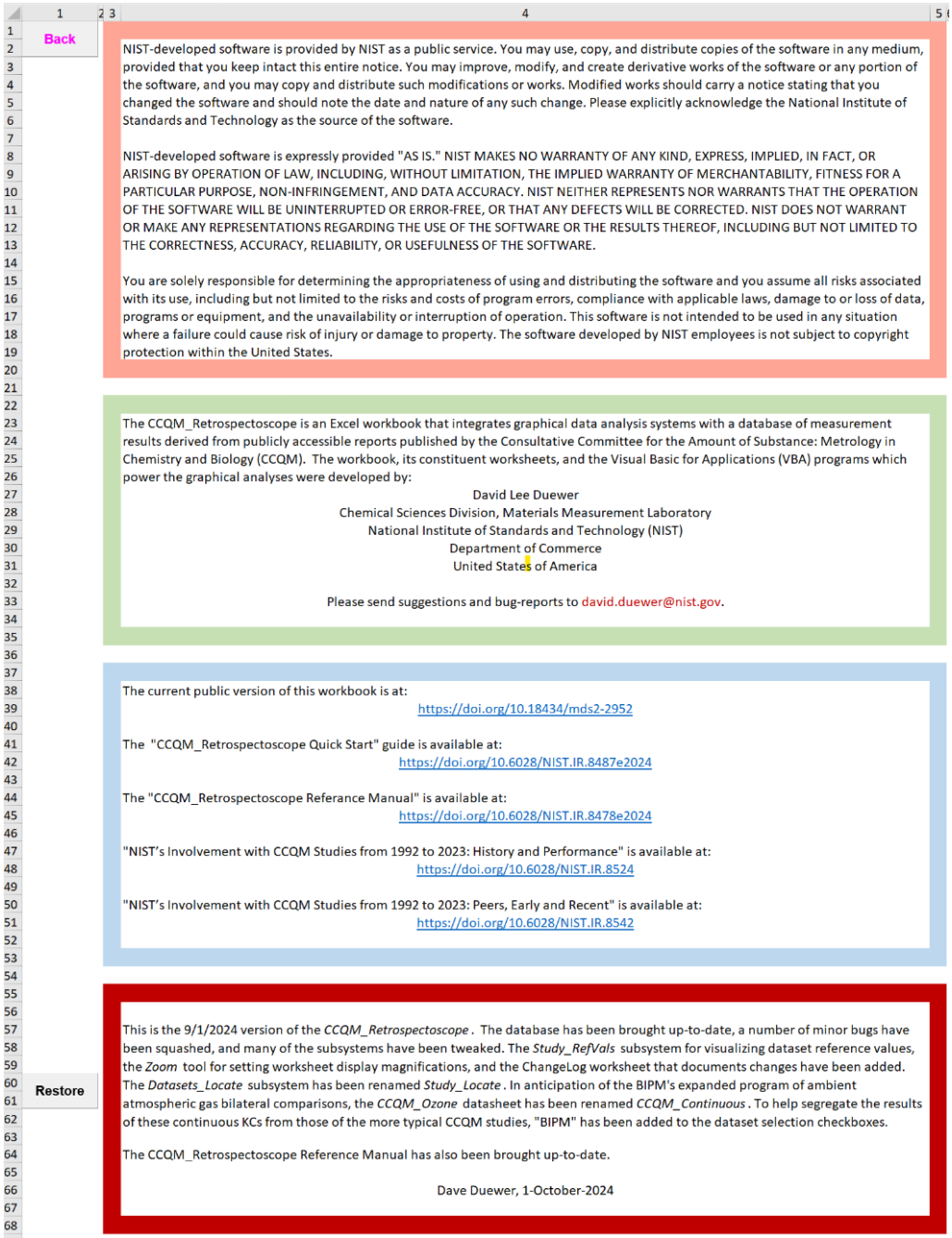


Fig. 126. *ReadMe* Worksheet.

30. The ChangeLog Worksheet

The *ChangeLog* worksheet is activated when the **ChangeLog** button on the *Welcome* worksheet is clicked. The worksheet is pictured in Fig. 127.

	Date	Type	Where	Problem	Fix
Back	9/14/2023	Upgrade	Workbook	Need to keep track of changes to Master version	Added "ChangeLog" worksheet
	9/14/2023	Bugfix	QMRS_DSReview_DataLoad	Datasets with one or more "na" uncertainties would not plot.	Any "na" now replaced by 2xMAX(other uncertainties) in chart.
	9/18/2023	New capability	Dataset_RefVals worksheet	Need plot of reference values as function of measurement date (john Molloy)	Added the Dataset_RefVals subsystem and various linkages to it.
	9/18/2023	Upgrade	Lab_Activity to Lab_Coordinations	Changeable colored elements did not have helper comments.	Added helper comments
	10/5/2023	Upgrade	CCQM_KC	Periodic check of BIPM website	CCQM-K168 and SIQM-S017
	10/5/2023	New capability	Other_Tools	Optimal Zoom differs among display devices	Added utility to set zoom for all worksheets to zoom of Other_Tools.
	10/6/2023	Bugfix	QMRS_Utility_GetLab	List with more than 255 characters aborted user input.	Replaced "Application.Inputbox" with "Inputbox" , list sorted by number datasets.
	10/8/2023	Upgrade	CCQM_KC	Periodic check of BIPM website	CCQM-K156.1
	10/12/2023	Bugfix	CCQM_KC	TEXT(X,"0.x") fatal for versions that use "," not "." (Michal Mariassy)	Deleted TEXT truncations (not needed, and inconsistently appled in any case)
	10/16/2023	Upgrade	CCQM_Ozone	BIPM adding on-going KC Gas analytes in 2024. (Joele VIALLON)	Changed worksheet name to "CCQM_Continuous" and updated linkage.
	10/19/2023	Bugfix	Many modules	"FullSeriesCollection" not compatble with pre-2010 Excel (Michal Mariassy)	Replaced with "SeriesCollection" which is compatible and fit-for-purpose.
	11/26/2023	Upgrade	CCQM_KC	Periodic check of BIPM website	EUQM-K003.2019, SIQM-S006, SIQM-S009
	11/26/2023	Bugfix	CCQM_KC	"Auto exhaust" used as matrix in K003-related datasets	Replaced "auto emmission" with "nitrogen" as matrix.
	1/15/2024	Bugfix	Datacore_Codes	Miss-spelling of the full names of several NMIs (Ken Pratt)	Corrected spelling.
	1/17/2024	Upgrade	CCQM_Continuous	New BIPM.QM-K1 measurements available	Added them. Checked that all results from posted studies are loaded.
	1/18/2024	Upgrade	Database_FindNew	The CCQM_KCs_PSs.xlsx workbook lists some KC and SC not in the KCDB.	Added ability to evaluate "Key Comparisons" as well as "Pilot Studies" worksheet.
	1/22/2024	Upgrade	Dataset_Locate	Only finds studies for one WG at a time	Allowed WG to be specified as "All", enabling finding all studies regardless of WG.
	1/30/2024	Upgrade	CCQM_KC	Periodic check of BIPM website	APQM-S019, SIQM-S012
	1/30/2024	BugFix	QMRS_DSAnalyteFilter_List	Run-time error when only one entry in list	Added tests to ensure there's at least one "Yes" else an error message and termination
	1/31/2024	Bugfix	QMRS_GetSortedListNMI	Duplicate "Key1" & "order1" in sort (Macintosh error)	Changed 2nd occurence to "key2" and "order2"
	1/31/2024	Bugfix	WGPower_LabUncertainty	Assigned the "show the title" flag to the wrong worksheet	Replaced "WSwpr" with "WSlun"
	3/27/2024	New capability	QMRS_DSLocate	Useful to have counts of datasets and studies along with lists	Added QMRS_DSLocate_Make_Summaries (used to catch bug in Lab_Activity)
	3/28/2024	BugFix	QMRS_LabActivity_Find_Combinations	Incorrect count of CAWG, IRWG studies in when not interested in baseunits	Revised sort to insure all datasets from same study stay together
	3/29/2024	Bugfix	QMRS_Diagonal	Tried to use data having 'zero' (empty) u(value)	Revised QMRS_WGDiagonal_Filter_GetList to ignore u(value)=0
	3/29/2024	Bugfix	QMRS_Welcome	QMRS_Dataset_RefVal was not being set to Communal values	Revised QMRS_Welcome_Commonalities to include Dataset_RefVal
	3/31/2024	Bugfix	QMRS_Dataset_RefVals	Review wasn't recognizing study selection by active cell	Updated and robustified the dataset-to-display specification code
	4/4/2024	Bugfix	Participation, Coordination, Engagement	Year range ignored; plots always showed smallest -1 to largest +1	Plots now provide info only for the range of years
	4/12/2024	Upgrade	Peer subsystem distances	The u(x)/u(ref) Y-axis was on a linear scale, distorting distances	Y-axis on log-scale, so distance between 0.5 and 1 is same as between 1 and 2.
	4/12/2024	Upgrade	Peer subsystem distances	Distances scaled by axis range: enabled user-weighting but cryptic.	Added user-defined weighting factor.
	4/19/2024	Upgrade	Peer_Unilateral & Global	Distance to target or Located NMI|DI also of interest	Added distance-to-target/Located NMI|DI graph & augmented table
	4/25/2024	Upgrade	Subsystems with CCQM/RMO checkboxes	BIPM's "continual" studies can distort analyses	Replaced CCQM/RMO with CCQM/BIPM/RMO control boxes
	4/29/2004	Upgrade	CCQM_KC	Periodic check of BIPM website	CCQM-K73.2018.2, CCQM-K160
	5/8/2024	Upgrade	Peer_Unilateral & Global	Chart element changes took too much time to execute	Chart element toggles changed to direct-call subroutines
	5/17/2024	Bugfix	Lab_Engagement	"Total" lines redundant when only one P/C type contributes (Jennifer Benkstein)	"Total" line(s) suppressed when only one P-and/or-C type active.
	5/23/2024	Upgrade	Peer subsystem axis titles	"Median(" didn't convey the % minimum subset requierment	Added %minium co-participation between "Median" and "(" as subscript
	5/23/2024	Bugfix	Datacore_Codes	Chile's CMQ was replaced by ISP in 2023 (for water and food-related measurands)	Converted all CMQ to ISP
	6/1/2024	Upgrade	WG_Power (Lab_Unc & WG_Pre)	Slope and intercept parameters are strongly correlated	Added ability to visualize 95% joint coverage ellipse to "located" organization
	6/13/2024	Upgrade	CCQM_KC	Periodic check of BIPM website	Added CCQM-K161, four status updates
	7/8/2024	Upgrade/Bugfix	QMRS_Welcome	Miss-spelling and some clumsy wording	Corrected and simplified descriptions
	7/8/2024	Upgrade	QMRS_Welcome, ReadMe, ChangeLog	Missing access functions	Added ChangeLog buttom to Welcome, Restore to ReadMe and ChangeLog
	7/12/2024	Upgrade	Bivariate charts (Peer_*, WG_Power)	Needed way to visualize "closeness to reference"	Added ability to plot unit ellipse
	7/23/2024	Upgrade/Bugfix	Dataset_NMI|DI	Parameters used to define Core organizations too restrictive	Changed earliest & latest to most recent of earliest 25% & earliest of most recent 25% datasets
	8/1/2024	Upgrade	Database_Checkup	Needed prefix for 10^0.	Added CCQM-P194. Added prefixes "F", "G", and "T" to anticipate future needs.
	8/5/2024	Upgrade	Peer, Power, Diagonal chart legends	Baddly positioned and don't inform errorbar or ellipse factors	Updated legends. Legend moved to bottom of top chart, added to bottom charts.
	8/12/2024	Upgrade	All subsystems	Needed more storage rows above "Restore" for Lab_Uncertainty & WG_Precision	Relocated Restore buttons (and "Used Parameters" if present) to row 70
	8/12/2024	Upgrade	Lab_Uncertainty and WG_Precision	%CV estimated as median of all results may be biased	Added %CV calculated over same range as power function to enable comparison
	8/15/2024	Upgrade	Subsystems that use Theil-Sen regression	No quality metrics for Theil-Sen regressions.	Added correlation, RMSE, and ndf calculations and storage
	8/27/2024	Upgrade/Bugfix	Study_Locate	"#use" was count of all "Y" + "Z" regardless of NMI/DI status.	Changed "#use" to "#yes" and added true "#use" (for median and Qn estimates)

Fig. 127. *ChangeLog* Worksheet.

The ChangeLog does not document minor “esthetic” changes to worksheet dashboards. These changes do not impact the *CCQM_Retrospectoscope*’s function but (hopefully) they facilitate its use.

References

[1] CIPM-MRA-2003. Mutual recognition of national measurement standards and of calibration and measurement certificates issued by national metrology institutes, Paris, 14 October 1999. Technical Supplement revised in October 2003 (pages 38-41). https://www.bipm.org/documents/20126/43742162/CIPM-MRA-2003.pdf. Accessed: 6/15/2023.

[2] Thompson M. Uncertainty functions, a compact way of summarising or specifying the behaviour of analytical systems. TrACs Trends Anal Chem 2011;30(7):1168-1175. https://doi.org/10.1016/J.TRAC.2011.03.012.

[3] Horwitz W. Evaluation of Analytical Methods Used for Regulation of Foods and Drugs. Anal Chem 1982;54:67A-76A. https://doi.org/10.1021/ac00238a002.

[4] Thompson M, Lowthian PJ. The Horwitz Function Revisited. J AOAC Int 1997;80(3):676-679. https://doi.org/10.1093/jaoac/80.3.676.

[5] Thompson M. Towards an explanation of the Horwitz function. Anal Bioanal Chem 2022;414:1671-1676. https://doi.org/10.1007/s00216-021-03791-w.

[6] CIPM MRA-G-11, Measurement comparisons in the CIPM MRA. https://www.bipm.org/documents/20126/43742162/CIPM-MRA-G-11.pdf Accessed: 6/15/2023.

[7] KCDB. https://www.bipm.org/kcdb/. Accessed: 6/15/2023.

[8] JCGM/WG2. 2012. JCGM 200:2012 International vocabulary of metrology – Basic and general concepts and associated terms (VIM). https://www.bipm.org/en/publications/guides/vim.html.

[9] Andrews DF, Bickel PJ, Hampel FR, Huber PJ, Rogers WH, Tukey JW. Robust Estimates of Location. Princeton University Press, 1972

[10] Rousseeuw PJ, Croux C. Alternatives to Median Absolute Deviation. J Am Stat Assoc. 1993;88:1273-83. https://doi.org/10.1080/01621459.1993.10476408.

[11] Wilrich P-Th. Robust estimates of the theoretical standard deviation to be used in interlaboratory precision experiments. Accred Qual Assur. 2007;12:231–40. https://doi.org/10.1007/s00769-006-0240-7.

[12] Wikipedia. Robust measures of scale. https://wikipedia.org/wiki/Robust_measures_of_scale. Accessed: 6/15/2023.

[13] ISO/IEC 17043:2010 Conformity assessment – General requirements for proficiency testing. International Standards Organization International Standard, 2010. Geneva, CH.

[14] Sen PK (1968) Estimates of the Regression Coefficient Based on Kendall's Tau, JASA 63(324):1379-1389. https://doi.org/10.1080/01621459.1968.10480934.

[15] Theil-Sen estimator. https://en.wikipedia.org/wiki/Theil-Sen_estimator. Accessed: 6/15/2023.

[16] Thompson M, Sykes M, Mathieson K, Wood R (2022) Comparison of reproducibility precision on mass fraction in some interlaboratory studies of methods of food analysis. Anal Bioanal Chem 414:1105-1114. https://doi.org/10.1007/s00216-021-03736-3.

[17] The Excel workbook *CCQM_KCs_PSs.xlsx* lists all registered CCQM comparisons and pilot studies and is periodically updated. As of 7/17/2024, the workbook is available at https://www.bipm.org/documents/20126/48101949/CCQM_KCs_PSs.xlsx/eaf57589-7beb-52d0-60c6-ca8e21481c03. If this URL has expired, try searching the web for "*CCQM_KCs_PSs".* If multiple versions exist, use the most recently updated. As of 7/17/2024, there are at least two versions: the most recent was updated 12/4/2023.

[18] van der Veen AMH, Nieuwenkamp G, Wessel RM, Maruyama M, Heo GS, Kim Y-d, Moon DM, Niederhauser B, Quintilii M, Milton MJT, Cox MG, Harris PM, Guenther FR, Rhoderick GC, Konopelko LA, Kustikov YA, Pankratov VV, Selukov DN, Petrov VA, Gromova EV. International comparison CCQM-K46: Ammonia in nitrogen. Metrologia 2010;47:08023. https://doi.org/10.1088/0026-1394/47/1A/08023.

[19] Koepke A, Lafarge TV, Possolo A, Toman B. 2020. NIST Consensus Builder. User's Manual and program available at: https://consensus.nist.gov/app/nicob.

[20] Possolo A, Koepke A, Newton D, Winchester MR (2021) Decision Tree for Key Comparisons. NIST JRES 126; 126007. https://doi.org/10.6028/jres.126.007. User's Manual and program available at: https://decisiontree.nist.gov/.

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

a	user-settable value
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: $D_i = 100(x_i - x_{\mathrm{ref}})/x_{\mathrm{ref}}$
$\lvert D_i \rvert$	absolute percent difference score: $\lvert D_i \rvert = 100\lvert x_i - x_{\mathrm{ref}} \rvert/x_{\mathrm{ref}}$
DoE_i	reported degree of equivalence for participant value x_i
$\%DoE_i$	reported percent relative degree of equivalence for participant value x_i
Δ_i	distance between values for a given NMI/DI and reference values
Δ_{ij}	distance between values for a given pair of NMI/DIs
Δ_{other}	composite distance between WG participation rates of a target and another NMI/DI
i	index
j	index
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
$r_{\mathrm{other},i}$	participation rate of the "other" NMI/DI in the i^{th} WG
$r_{\mathrm{target},i}$	participation rate of the target NMI/DI in the i^{th} WG
$\lvert t \rvert$	absolute value of a Student's *t* metric
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_{set}	all of the valid $u(x_i)$ in a given dataset
$u(\cdot)$	standard uncertainty for a specified value
$u_{\mathrm{rel}}(\cdot)$	relative standard uncertainty for a specified value
$U_{95}(\cdot)$	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

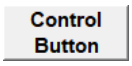
$X_{\min}$	minimum *x*-axis value
y_i	assigned reference value for a given gas cylinder
y_{nom}	nominal reference value for a set of gas cylinders
Y	dependent variable, plotted on *y*-axis of a scattergram
$Y_{\max}$	maximum *y*-axis value
$Y_{\min}$	minimum *y*-axis value
z_i	z-score: $z_i = (x_i - x_{\text{ref}})/u(x_i)$
$\lvert z_i \rvert$	absolute z-score: $\lvert z_i \rvert = \lvert x_i - x_{\text{ref}} \rvert / u(x_i)$
ζ_i	zeta-score: $\zeta_i = (x_i - x_{\text{ref}})/\sqrt{u^2(x_i) + u^2(x_{\text{ref}})}$
$\lvert \zeta_i \rvert$	absolute zeta-score: $\lvert \zeta_i \rvert = \lvert x_i - x_{\text{ref}} \rvert / \sqrt{u^2(x_i) + u^2(x_{\text{ref}})}$
ζ_{ij}	zeta-score between two participants: $\zeta_{ij} = (x_i - x_j)/\sqrt{u^2(x_i) + u^2(x_j)}$
$\lvert \zeta_{ij} \rvert$	absolute zeta-score between two participants: $\lvert \zeta_{ij} \rvert = \lvert x_i - x_j \rvert / \sqrt{u^2(x_i) + u^2(x_j)}$

A.3. Functions

INT	integer part of a real number
$\log_2$	binary logarithm
$\log_{10}$	decadic logarithm
Median	middle value of a set of values

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 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 option. Only one of the 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 studies.

Workbook
A spreadsheet system 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.

Appendix C. Change Log

5-Oct-2023: Added the description of the *Zoom* subsystem (Section 25) and the associated description and adjustments in the Other_Tools overview (Section 18.)

16-Oct-2023: Added the description of the *Study_RefVals* subsystem (Section 19) and the associated description and adjustments in the Other_Tools overview (Section 18.)

Jul/Aug-2024 Editorial corrections, clarifications, and updates throughout document.

28-Aug-2024 Addition of "Coefficient Storage" details to *Lab_History* (Section 5) , *Lab_Bias* (Section 6), *Lab_Uncertainty* (Section 6.5), *WG_Precision* (Section 15), and *Study_RefVals* (Section 19).