



# NIST Internal Report NIST IR 8487e2024

## CCQM\_Retrospectroscope Quick Start

*A beginner's guide to a data analysis system for visualizing results from CCQM studies*

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1 CCQM_Retrospectroscope	
2 <Version: 1-Sep-2024>	
3 A database and data analysis system for visualizing the performance of participants in CCQM	
4 Key Comparisons (KCs), Subsequent Comparisons (SCs), and/or pilot studies (PSs).	
5 Subsystems	6 Description
7 <b>Lab_Activity</b>	Summarizes a given NMI/DI's (WG, BaseUnit) activity in terms of the number of CCQM-related datasets and studies.
8	
9 <b>Lab_History</b>	Displays a given NMI/DI's performance in a (WG, BaseUnit)'s comparisons relative to the reference value as a function of measurement date.
10	
11 <b>Lab_Bias</b>	Displays a given NMI/DI's measurement uncertainties in a (WG, BaseUnit)'s comparisons as a function of the measurement values.
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14	
15 <b>Lab_Engagements</b>	Displays the number of coordinations and participations for a given NMI/DI, segregated by comparison/study type.
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17 <b>Peer_Bilateral</b>	For co-participants with a given NMI/DI in a (WG, BaseUnit)'s comparisons, plots median relative uncertainty as a function of median relative paired differences.
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19 <b>Peer_Unilateral</b>	For co-participants with a given NMI/DI in a (WG, BaseUnit)'s comparisons, plots median relative uncertainty as a function of median agreement with reference values.
20	
21 <b>Peer_Global</b>	For co-participants in a (WG, BaseUnit)'s comparisons, plots median relative uncertainty as a function of median agreement with reference values.
22	
23 <b>Peer_Priorities</b>	Provides radar-type plots for a designated NMI/DI and the 11 others that most closely share the same priorities.
24	
25 <b>WG_Participations</b>	Displays the number of studies participated in by the various NMI/DIs for a given WG or across all WGs.
26	
27 <b>WG_Coordinations</b>	Displays the number of studies coordinated by the various NMI/DIs for a given WG or across all WGs.
28	
29 <b>WG_Precision</b>	Displays the measurement precision realized in a (WG, BaseUnit)'s comparisons as a function of median measurand value.
30	
31 <b>WG_Power</b>	Displays power function coefficients for a WG and selected NMI/DIs. (Intended for experienced users.)
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33 <b>WG_Diagonal</b>	For NMI/DIs that have coordinated and participated in studies, contrasts the median participation bias as a function of the median coordination bias.
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35 <b>Other_Tools</b>	Access to support and maintenance systems.
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1 CCQM_Retrospectroscope's Other Tools	
2 <Version: 1-Sep-2024>	
3 A motley collection of auxiliary analysis, support, utility, database maintenance, and dataset access systems.	
4	
5 Auxiliary Analyses	6 Description
7 <b>Study_RefVals</b>	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.
8	
9 <b>Study_Locate</b>	Locates datasets that pass the NMI/DI, WG, BaseUnit, measurement year, study type, sponsoring body, matrix, and analyte selection criteria.
10	
11 <b>Support Subsystems</b>	
12 <b>Dataset_Review</b>	Displays results of all participants in one study. This subsystem is used by <i>Lab_History</i> , <i>Lab_Bias</i> , <i>Lab_Uncertainty</i> , <i>WG_Precision</i> , and <i>Dataset_Locate</i> .
13	
14 <b>Dataset_NMI/DI</b>	Lists dataset participants by (WG, BaseUnit) and identify non-NMI/DIs in KCs. The lists can be manipulated to restrict use of data in <i>WG_Precision</i> analysis.
15	
16 <b>Dataset_AnalyteFilter</b>	Define analytes to help select datasets. This subsystem is used by <i>Lab_History</i> , <i>Lab_Bias</i> , <i>Lab_Uncertainty</i> , <i>Peer_Bilateral</i> , <i>Peer_Unilateral</i> , <i>Peer_Global</i> , <i>WG_Precision</i> , <i>WG_Diagonal</i> , <i>Dataset_RefVals</i> , and <i>Dataset_Locate</i> .
17	
18 <b>Utilities</b>	
19 <b>TimeTrial</b>	Exercise most of the subsystems, reload the analysis subsystems, and determine the time in minutes required to run them.
20	
21 <b>Zoom</b>	Set the zoom on all worksheets to the zoom of this worksheet. Be sure to set this worksheet's zoom before clicking!
22	
23 <b>Maintenance</b>	
24 <b>Database_FindNew</b>	Provides tools for checking the output from BPM's KCDB search tool for changes in the status of Key and Subsequent comparisons.
25	
26 <b>Database_Checkup</b>	Checks the internal consistency of the CCQM_Retrospectroscope's database. Several worksheets require by-hand updating when new data are entered.
27	
28 <b>Permanent Datasheets</b>	
29 <b>CCQM_KC</b>	Contains all (non-continuous) KC and SC datasets.
30	
31 <b>CCQM_PubPilot</b>	Contains all PPS datasets.
32	
33 <b>CCQM_Continuous</b>	Contains all continuous measurement-related KC datasets. (As of 2023, this is just ozone but other analytes may be added after 2024.)
34	
35 <b>Back</b>	Return to the Welcome worksheet.
36	
37 <b>Restore</b>	Restores this page's buttons wrt location, size, and color.
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December 2024

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## Abstract

This revised and updated “Quick Start” guide is intended to introduce potential users to the 1-Sep-2024 version of the *CCQM\_Retrospectroscope* system. The *CCQM\_Retrospectroscope* system combines a 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. The *CCQM\_Retrospectroscope* system supports fairly comprehensive and potentially novel appraisals of participation and measurement performance throughout the history of the CCQM activities. The appraisals include the bias, uncertainty, and degrees of equivalence of results submitted by individual national metrology or designated institutes (NMI/DIs); the relative performance of NMI/DIs, and the uncertainty function characteristic of entire Working Groups (WGs).

## Keywords

Consultative Committee for the Amount of Substance: Metrology in Chemistry and Biology (CCQM); Key Comparison (KC); national metrology institute or designated institute (NMI/DI); pilot study; Supplementary Comparison (SC).

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## Acknowledgements

We thank our colleagues Melissa Phillips for identifying the need for this guide and Michael Epstein for asking interesting questions.

## 1. Introduction

The *CCQM\_Retrospectroscope* system [1] combines a complete\* database of results from Consultative Committee for the Amount of Substance: Metrology in Chemistry and Biology (CCQM) studies with a number of graphical tools for trying to make sense of the data. This currently unique system supports fairly comprehensive 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) [2]; the relative performance of NMI/DIs [3], and the uncertainty functions characteristic of individual NMI/DIs and entire Working Groups (WGs) [4].

This “Quick-Start” Guide is intended to help users familiar with the CCQM get started using the *CCQM\_Retrospectroscope* to explore results from Key Comparisons (KCs), Supplementary Comparisons (SCs) and/or pilot studies (PSs) without having to first wade through the 200+ page **CCQM\_Retrospectroscope Reference Manual** [5]. Interpreting CCQM data requires some familiarity with what KCs, SCs, PSs, WGs, and Regional Metrology Organizations (RMOs) are. If you are not familiar with this jargon, please read the Introductory sections of the **Reference Manual** (pages 1 to 23) before attempting to use the *CCQM\_Retrospectroscope*.

### 1.1. Setup

The *CCQM\_Retrospectroscope* system is implemented in Excel using Microsoft’s Visual Basic for Applications (VBA) macro programs. It runs on both Windows and Macintosh platforms.

If your version of Excel is not already set to allow macros to run, you will need to set the “Macro Security” option to “Disable VBA macros with notification.” For Windows, find it under File > Options > Trust Center > Trust Center Settings > Macro Settings. For MacOS, find it under Excel > Preferences > Security > Macro Security. This should be a once-only hassle, although you will have to grant permission every time you invoke *CCQM\_Retrospectroscope*.

Large and complicated Excel workbooks like *CCQM\_Retrospectroscope.xlsm* are prone to various odd interactions with operating systems, other applications, and user-inputs. Minimize the number of open applications when you are using the system. Do not attempt to use the *CCQM\_Retrospectroscope* while downloads or virus scans are in progress. While the system is generally responsive, it can become quite irritatingly slow when competing for computational resources.

Always keep an unused, “clean” copy of the *CCQM\_Retrospectroscope.xlsm* workbook safe and accessible in case the workbook is compromised during use or recovery.

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\* As complete as earnest and somewhat tedious effort can provide. We believe the database includes all quantitative results from studies that have produced publicly accessible documentation as of this document’s publication date.

## 1.2. Welcome to *Welcome*

When you invoke the *CCQM\_Retrospectroscope*, you will be taken to the *Welcome* worksheet. This worksheet is the system's primary user-interface (dashboard). If you have a large enough screen in portrait orientation, it should look like Fig. 1. If you're using a smallish screen, you will need to scroll to reach some of the buttons.

**CCQM\_Retrospectroscope**  
<Version: 1-Sep-2024>

A database and data analysis system for visualizing the performance of participants in CCQM  
Key Comparisons (KCs), Subsequent Comparisons (SCs), and/or pilot studies (PSs).

**Subsystems**

Subsystems	Description
<b>Lab_Activity</b>	Summarizes a given NMI/DI's {WG, BaseUnit} activity in terms of the number of CCQM-related datasets and studies.
<b>Lab_History</b>	Displays a given NMI/DI's performance in a {WG, BaseUnit}'s comparisons relative to the reference value as a function of measurement date.
<b>Lab_Bias</b>	Displays a given NMI/DI's measurement uncertainties in a {WG, BaseUnit}'s comparisons as a function of the measurement values.
<b>Lab_Uncertainty</b>	Displays a given NMI/DI's measurement bias in a given {WG, BaseUnit}'s comparisons as a function of the measurement values.
<b>Lab_Engagements</b>	Displays the number of coordinations and participations for a given NMI/DI, segregated by comparison/study type.
<b>Peer_Bilateral</b>	For co-participants with a given NMI/DI in a {WG, BaseUnit}'s comparisons, plots median relative uncertainty as a function of median relative paired differences.
<b>Peer_Unilateral</b>	For co-participants with a given NMI/DI in a {WG, BaseUnit}'s comparisons, plots median relative uncertainty as a function of median agreement with reference values.
<b>Peer_Global</b>	For co-participants in a {WG, BaseUnit}'s comparisons, plots median relative uncertainty as a function of median agreement with reference values.
<b>Peer_Priorities</b>	Provides radar-type plots for a designated NMI/DI and the 11 others that most closely share the same priorities.
<b>WG_Participations</b>	Displays the number of studies participated in by the various NMI/DIs for a given WG or across all WGs.
<b>WG_Coordinations</b>	Displays the number of studies coordinated by the various NMI/DIs for a given WG or across all WGs.
<b>WG_Precision</b>	Displays the measurement precision realized in a {WG, BaseUnit}'s comparisons as a function of median measurand value.
<b>WG_Power</b>	Displays power function coefficients for a WG and selected NMI/DIs. (Intended for experienced users.)
<b>WG_Diagonal</b>	For NMI/DIs that have coordinated and participated in studies, contrasts the median participation bias as a function of the median coordination bias.
<b>Other_Tools</b>	Access to support and maintenance systems.
<b>ReadMe</b>	Licensing statement, who-to-blame, and (possibly) announcements.
<b>ChangeLog</b>	Description of changes since first release (12-Sep-2023)
<b>Restore</b>	Restores this page's buttons wrt location, size, and color.

**Set Commonalities**

Parameter	Use	Default
NMI/DI:	NIST	User
WG:	GAWG	User
BaseUnit:	mol/mol	User
Year from:	1992	User
Year through:	2023	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|:
- z':
- |z'|:
- D:
- |D|:

**Parameter Use Default**

Parameter	Use	Auto
%CV:	0.50	Auto
Bin width:	1.00	Auto
Box width:	5	Auto
Insider limit:	2.00	Auto
log <sub>10</sub> (Min X <sub>0</sub> ):	-7.50	User
log <sub>10</sub> (Max X <sub>0</sub> ):	-2.00	User
log <sub>10</sub> (Min X <sub>0</sub> ):	-11.70	User
log <sub>10</sub> (Max X <sub>0</sub> ):	0.20	User
log <sub>10</sub> (Max Y <sub>00</sub> ):	3.10	User
log <sub>10</sub> (Min Y <sub>0</sub> ):	-12.99	User
log <sub>10</sub> (Max Y <sub>0</sub> ):	-1.60	User
log <sub>10</sub> (Min Y <sub>00</sub> ):	-2.70	User
log <sub>10</sub> (Max Y <sub>00</sub> ):	2.70	User
Max bars:	40	Auto
Max lines:	20	Auto
Min Y <sub>00</sub> :	0.50	Auto
Max Y <sub>00</sub> :	1.40	Auto
Max X <sub>00</sub> :	1.20	Auto
Max Y <sub>00</sub> :	4.00	Auto
Max Y <sub>0</sub> :	50.00	Auto
Max Y <sub>000</sub> :	4.00	Auto

Fig. 1. The *Welcome* Worksheet as Displayed on a Large Portrait Screen.

### 1.2.1. Graphical Analyses

Control  
Button

The *CCQM\_Retrospectroscope*'s subsystems are intended to be accessed by clicking the *Welcome* worksheet's command buttons. Clicking one of the first 14 command **buttons** along the worksheet's left edge of the worksheet activates a *worksheet* (of the same name) that hosts a graphical analysis *subsystem* (of the same name) that visualizes the performance of individual NMI/DIs, peer groups of NMI/DIs, or aspects of WG measurement communities.

- **Lab\_Activity** activates the *Lab\_Activity* worksheet. This analysis system reveals what measurement areas an NMI/DI has been interested in.
- **Lab\_History** activates the *Lab\_History* worksheet. This analysis system displays an NMI/DI's measurement accuracy as a function of time.
- **Lab\_Bias** activates the *Lab\_Bias* worksheet. This analysis system displays an NMI/DI's measurement bias as a function of measurement value.
- **Lab\_Uncertainty** activates the *Lab\_Uncertainty* worksheet. This analysis system displays an NMI/DI's reported uncertainties as a function of measurement value.
- **Lab\_Engagements** activates the *Lab\_Engagements* worksheet. This analysis system details the number and timing of an NMI/DI's engagements with CCQM, where "engagements" are separated into "participations" (reporting measurement values) and "coordinations" (providing leadership).
- **Peer\_Bilateral** activates the *Peer\_Bilateral* worksheet. This analysis system defines an NMI/DI's peers by how closely their measurements agree.
- **Peer\_Unilateral** activates the *Peer\_Unilateral* worksheet. This analysis system defines an NMI/DI's peers by how closely their measurements agree with reference values in studies they both participated in.
- **Peer\_Global** activates the *Peer\_Global* worksheet. This analysis system defines a group of peer NMI/DIs by how closely the individual NMI/DI measurements agree with reference values.
- **Peer\_Bilateral** activates the *Peer\_Priorities* worksheet. This analysis system defines an NMI/DI's peers by their measurement communities.
- **WG\_Participations** activates the *WG\_Participations* worksheet. This analysis system displays which and when NMI/DIs have participated in a measurement community's studies.
- **WG\_Coordinations** activates the *WG\_Coordinations* worksheet. This analysis system displays which and when NMI/DIs have coordinated a measurement community's studies.
- **WG\_Precision** activates the *WG\_Precision* worksheet. This analysis system depicts measurement reproducibility as a function of analyte level for NMI/DI communities.

- **WG\_Power** activates the *WG\_Power* worksheet. This analysis system displays relationships between NMI/DI uncertainty functions and their measurement community's reproducibility function.
- **WG\_Diagonal** activates the *WG\_Diagonal* worksheet. This analysis system displays relationships between NMI/DI measurement accuracy in studies they have participated in relative to studies they have coordinated.

### 1.2.2. Other Buttons

Clicking any of the four buttons at the bottom of the *Welcome* worksheet's left-edge invokes a non-analysis worksheet or action:

- **Other\_Tools** activates the *Other\_Tools* auxiliary dashboard, described in Section 3. Visit these tools only after you have familiarized yourself the *Welcome* worksheet's other buttons.
- **ReadMe** activates the *Readme* worksheet, pictured in Section 4, that displays a disclaimer message. It is important to read only if you intend to distribute the system or publish results obtained through use of the system.
- **ChangeLog** activates the *ChangeLog* worksheet that summarizes the various bugfixes, upgrades, and additions to the *CCQM\_Retrospectroscope* since it's 2023 public release.
- **Restore** resets the *Welcome* worksheet's column width, command button, radio button, and checkbox formats.

The three buttons at the top-right invoke utilities.

- **Save** saves *CCQM\_Retrospectroscope.xlsm* in its current state. You will not be prompted with a pop-up window providing the option to save the workbook when you close it, so if you want to save its current state you should click this button or use your platform's "save" function.
- **Exit** closes the *CCQM\_Retrospectroscope* workbook. This is provided only as a convenience; you can use your platform's usual method(s) of closing Excel workbooks.
- **Set Commonalities** sets the parameters and controls listed along the *Welcome* worksheet's right edge in all relevant *CCQM\_Retrospectroscope* worksheets. Using this common subset of values and control settings facilitates comparing and combing the analyses provided by the subsystems. When you start to analyze data, using this utility is often a time and/or sanity saver.

## 2. Getting Started

### 2.1. Get Ready

The graphical analysis systems are by far the most important for getting a sense of what the *CCQM\_Retrospectroscope* can do. A good first step would be to visit these buttons and:

- read the brief description to the right of the button,
- click the button,
- invest a moment or two looking at the worksheet you were (should have been) taken to,
- click worksheet's **Back** button (see Figure 2) to get back to the *Welcome* worksheet, and
- repeat until you have:
  - clicked all the buttons,
  - become bored, or
  - gotten interested in analyzing some data.

### 2.2. Get Set

Simply activating a worksheet does not initiate an analysis!

Starting an analysis requires a bit more clicking. But before you start, you need to set some parameter values and checkbox settings. The *Lab\_Activity* system is both (relatively) simple to use and provides results of general interest so it is a good place to start learning how to specify parameters and settings. Once you click the **Lab\_Activity** button on the *Welcome* worksheet (or activate the *Lab\_Activity* worksheet directly), you should see something like Fig. 2.

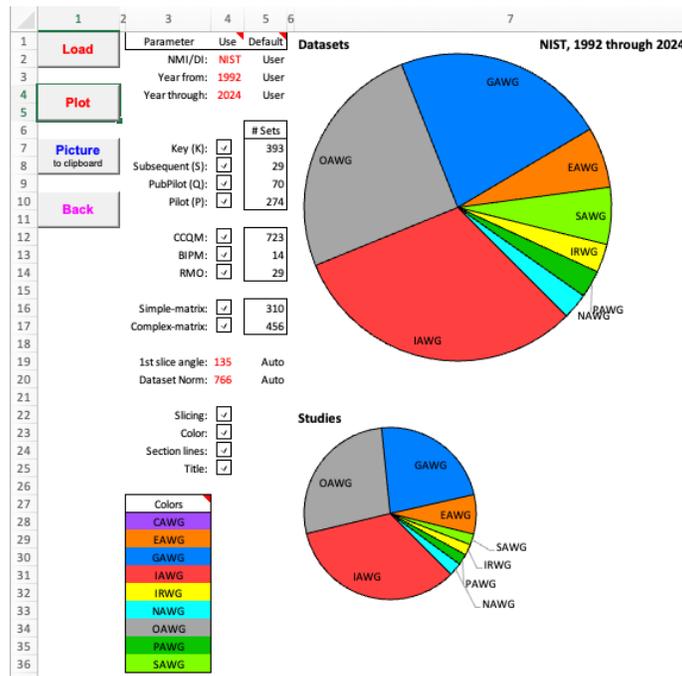


Fig. 2. The *Lab\_Activity* Analysis Subsystem.

### 2.2.1. Parameters

Parameter values are in red font and are located under the “Use” header (column 4).

When the “Default” setting to the right of a parameter value (column 5) is “User”, *CCQM\_Retrospectroscope* checks the validity of the parameter’s value and at need will either present a list of valid entries (e.g., NMI/DI:) or will use a (reasonably) reasonable default (e.g., Year from: and Year through:). When the “Default” value is “Auto” the default value for the parameter will be used regardless of the “Use” value.

Thus to use other than a parameter’s default value, you must set the associated “Default” setting to “User”. (Heeding this warning can prevent considerable frustration!)

#### 2.2.1.1. Data Specification Parameters

Three parameters that specify what data gets used are in column 4, rows 2 through 4:

- NMI/DI, the NMI/DI of interest (here, NIST),
- Year from, the earliest measurement year of interest (here, 1992), and
- Year through, the most recent measurement year of interest (here, 2024).

#### 2.2.1.2. Display Parameters

Two parameters that specify how the selected data are displayed are in column 4, rows 18 and 19:

- 1<sup>st</sup> slice angle, the angle where the biggest pie slice begins (here, 135°). This angle helps put the labels for the smallest slices in an esthetically pleasing location.
- Dataset Norm, the number of datasets that correspond to a full-sized pie (here, 766, the number of KC, SC, and PS datasets NIST contributed to from 1992 through 2024). This facilitates scaling pies for different times and/or NMI/DIs relative to some larger reference number of datasets.

### 2.2.2. Checkboxes



Checkboxes have two states: checked (with a logical value of TRUE) and unchecked (logical value of FALSE). In *Lab\_Activity* they are used in two applications: for specifying which types of dataset are analyzed and switching on-and-off selected graphical elements.

#### 2.2.2.1. Data specification Checkboxes

Checkboxes that control the dataset types that are included in *Lab\_Activity* analyses are located in column 4, rows 7 through 16. Datasets of a given type are included when the checkbox is checked, excluded when unchecked. The number of datasets of the given type that are included is listed in the cell to the immediate right of the checkbox. The types that can be considered for use in *Lab\_Activity* (and most of the other analysis systems) are:

- study type – KCs, SCs, and PSs that have been published, and PSs that have not been published. Results from unpublished PSs are not included in the publicly accessible version of the *CCQM\_Retrospectroscope*.
- sponsoring body – CCQM WGs, BIPM (for continuous bilateral gas mixture comparisons), and RMO Technical Committees.
- sample matrix – Simple and Complex. These terms indicate the composition of the sample materials analyzed, not the difficulty of analyzing them!

Changes to the state of these checkboxes are only implemented when the chart is renewed by clicking the **Plot** or **Load** button (see Section 2.3) or clicking one of the display checkboxes.

#### 2.2.2.2. Display Checkboxes

The checkboxes located in column 4, rows 21 through 24, control the display of some of the chart elements:

- Slicing – checked, the pie is sliced by WG regardless of the units used the report the study values. Unchecked, there is a pie for every combination of WG and reporting unit.
- Color – checked, slices are colored. Unchecked, they are not.
- Section lines – checked, slices are bounded with a black line. Unchecked, they are not.
- Title – checked, titles for the two pies are displayed. Unchecked, they are not.

Clicking any of these checkboxes immediately implements the change, as well as any changes to the parameters or data specification checkboxes.

### 2.2.3. Colors

Don't like the pie-slice color scheme? Change it! The scheme is defined by the "Fill Color" of the cells in column 3, rows 27 through 35.

Colors
CAWG
EAWG
GAWG
IAWG
IRWG
NAWG
OAWG
PAWG
SAWG

#### 2.2.4. Radio Buttons



While not used in *Lab\_Activity*, radio buttons are used by several of the graphical analysis systems to select one option from a set of mutually exclusive options. Pressing one of the buttons selects the associated option and invokes an immediate change in the chart display.

#### 2.3. Go

Change the parameters and the checkbox states as you will, then click the **Plot** command button and observe the changes. Except for the display checkboxes, changes are implemented when the **Plot** button is clicked.

The above descriptions and the labels to the left of the parameters and checkboxes are intended to be descriptive, but the simplest way to find what they do is to fiddle the value or the control's state and click the **Plot** button. But fiddle patiently, allowing each set of changes to take effect before re-clicking to avoid overtaxing your computing platform.

You do not need to bother with the **Load** button, but it does no harm to click it – other than taking a bit of time. The **Load** function is only necessary after the system's database has been modified. Best to leave that to the system's maintainers – or *really* experienced and adventuresome users.

If you want to obtain an image of the charts, click the **Picture** button. It places a PNG-format image of the charts onto your systems clipboard. This image can then be pasted into your choice of (open) document.

To return to the *Welcome* worksheet, click the **Back** button.

To confirm your understanding of the parameters or if doubt remains, the *Reference Manual* [5] describes and illustrates all parameters and controls. It has a detailed Table of Contents to make finding stuff a bit easier.

### 3. Other Tools

When you click the **Other\_Tools** button on the *Welcome* worksheet, control is transferred to the *Other\_Tools* auxiliary dashboard/worksheet as shown in Fig. 3.

	1	2	3	4
1	<b>CCQM_Retrospectroscope's Other Tools</b>			
2	<Version: 1-Sep-2024>			
3	A motely collection of auxillary analysis, support , utility, database maintenance, and datasheet access systems.			
4				
5	Auxiliary Analyses	Description		
6	<b>Study_RefVals</b>	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.		
7				
8				
9	<b>Study_Locate</b>	Locates datasets that pass the NMI/DI, WG, BaseUnit, measurement year, study type, sponsoring body, matrix, and analyte selection criteria.		
10				
11				
12	Support Subsystems			
13	<b>Dataset_Review</b>	Displays results of all participants in one study. This subsystem is used by <i>Lab_History</i> , <i>Lab_Bias</i> , <i>Lab_Uncertainty</i> , <i>WG_Precision</i> , and <i>Dataset_Locate</i> .		
14				
15				
16	<b>Dataset_NMI DI</b>	Lists dataset participants by {WG, BaseUnit} and identify non-NMI/DIs in KCs. The lists can be manipulated to restrict use of data in <i>WG_Precision</i> analysis.		
17				
18				
19	<b>Dataset_AnalyteFilter</b>	Define analytes to help select datasets. This subsystem is used by <i>Lab_History</i> , <i>Lab_Bias</i> , <i>Lab_Uncertainty</i> , <i>Peer_Bilateral</i> , <i>Peer-Unilateral</i> , <i>Peer_Global</i> , <i>WG_Precision</i> , <i>WG_Diagonal</i> , <i>Dataset_RefVals</i> , and <i>Dataset_Locate</i> .		
20				
21				
22				
23	Utilities			
24	<b>TimeTrial</b>	Exercise most of the subsystems, reload the analysis subsystems, and determine the time in minutes required to run them.		
25				
26				
27	<b>Zoom</b>	Set the zoom on all worksheets to the zoom of this worksheet. Be sure to set this worksheet's zoom before clicking!		
28				
29				
30	Maintenance			
31	<b>Database_FindNew</b>	Provides tools for checking the output from BIPM's KCDB search tool for changes in the status of Key and Subsequent comparisons.		
32				
33				
34	<b>Database_Checkup</b>	Checks the internal consistency of the CCQM_Retrospectroscope's database. Several worksheets require by-hand updating when new data are entered.		
35				
36				
37	Permanent Datasheets			
38	<b>CCQM_KC</b>	Contains all (non-continuous) KC and SC datasets.		
39				
40				
41	<b>CCQM_PubPilot</b>	Contains all PPS datasets.		
42				
43				
44	<b>CCQM_Continuous</b>	Contains all continuous measurement-related KC datasets. (As of 2023, this is just ozone but other analytes may be added after 2024.)		
45				
46				
47				
48	<b>Back</b>	Return to the Welcome worksheet.		
49				
50				
51				
52	<b>Restore</b>	Restores this page's buttons wrt location, size, and color.		
53				

**Fig. 3. The *Other\_Tools* Auxiliary Dashboard.**

While clicking through all of these buttons is a good familiarization idea, be aware that some of the systems and utilities accessed through this dashboard are of more use to system maintainers than to casual users. The buttons and their functions are:

- **Study\_RefVals** activates the *Study\_RefVals* worksheet. This graphical analysis system displays dataset reference values as a function of measurement year.
- **Study\_Locate** activates the *Study\_Locate* worksheet. This system enables locating datasets that have specified attributes, including specific analytes or groups of analytes.
- **Dataset\_Review** activates the *Dataset\_Review* worksheet. When this utility is invoked from an analysis subsystem or a datasheet, it supports visualization of all results in a specified dataset. When invoked directly, it can be used to modify the display of the last-loaded dataset.
- **Dataset\_NMI|DI** activates the *Dataset\_NMI/DI* worksheet. When this utility is invoked from an analysis subsystem, it supports the exclusion of results contributed by selected NMI/DIs. When invoked directly, it can be used to select which NMI/DIs are selected.
- **Dataset\_AnalyteFilter** activates the *Dataset\_AnalyteFilter* worksheet. When this utility is invoked from an analysis subsystem, it supports specifying which analyte or groups of analytes will be used in an analysis. When invoked directly, it can be used to select which analytes are used.
- **TimeTrial** invokes the *TimeTrial* utility that evaluates the clock-time performance of a computing platform by exercising the *CCQM\_Retrospectroscope's* subsystems.
- **Zoom** invokes a utility that sets the “zoom” (worksheet magnification factor) of all of the *CCQM\_Retrospectroscope's* worksheets to the “zoom” of the **Other\_Tools** worksheet.
- **Database\_FindNew** activates the *Database\_FindNew* worksheet. This worksheet hosts functions that facilitate discovery of new information about CCQM studies. These functions are intended to be used by system maintainers.
- **Database\_Checkup** activates the *Database\_Checkup* worksheet. This worksheet hosts functions that support the evaluation of dataset data and metadata consistency. These functions are intended to be used by system maintainers.
- **CCQM\_KC** activates the *CCQM\_KC* datasheet. This is the *CCQM\_Retrospectroscope* datasheet for KC and SC results.
- **CCQM\_PubPilot** activates the *CCQM\_PubPilot* datasheet. This is the *CCQM\_Retrospectroscope* datasheet for published PSs results.
- **CCQM\_Continuous** activates the *CCQM\_Continuous* datasheet. This is the *CCQM\_Retrospectroscope* datasheet for BIPM-coordinated bilateral comparisons of ambient atmospheric gases.
- **Back** activates the *Welcome* worksheet.

For further information, please consult the Reference Manual [5].

#### 4. ReadMe

The *ReadMe* worksheet is activated when the **ReadMe** button on the *Welcome* worksheet is clicked. This worksheet lists the standard NIST software license statement and disclaimer, who to send your suggestions, bug reports, and irate complaints to, and where the *CCQM\_Retrospectroscope* documentation lives. The worksheet is pictured in Fig. 4.

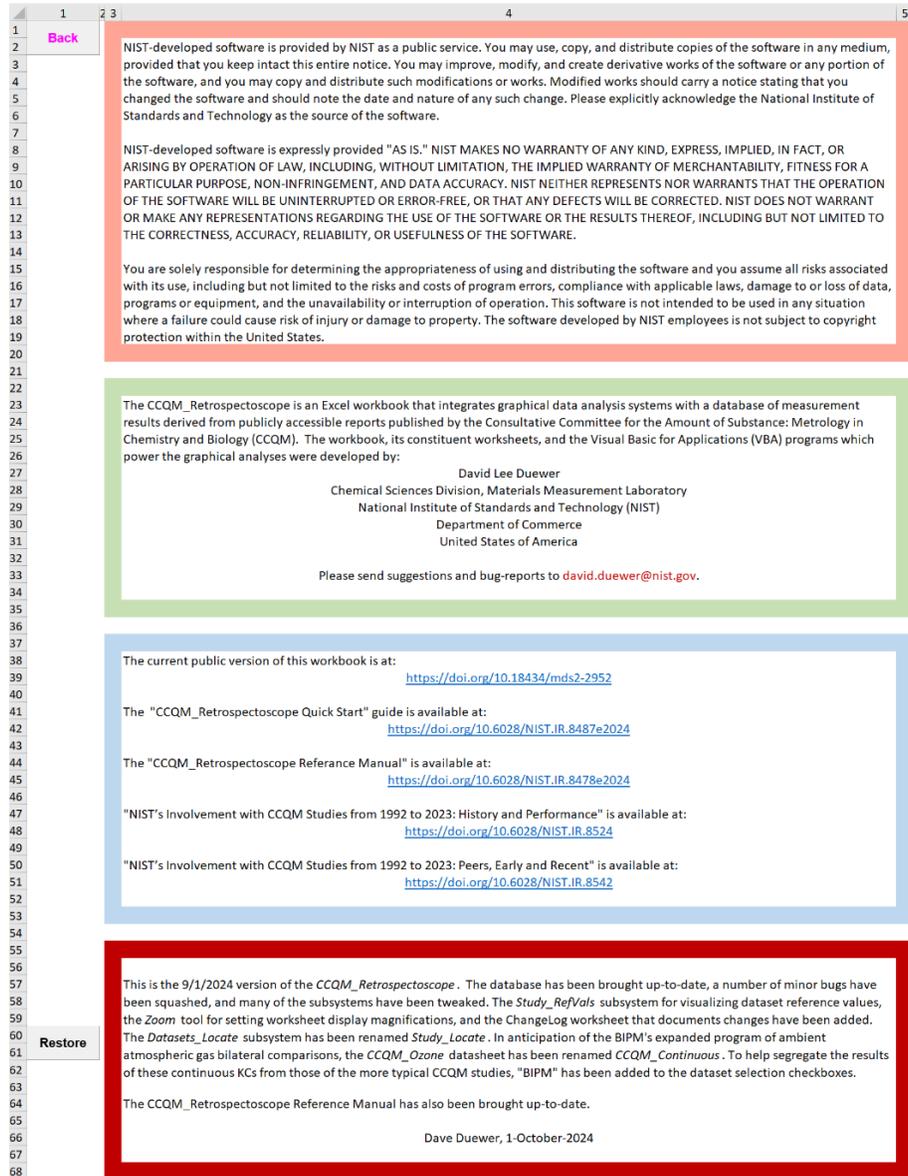


Fig. 4. The *ReadMe* Worksheet.

When clicked, the **Back** command button returns control to the *Welcome* worksheet. When clicked, the **Restore** button standardizes the worksheet's format.

## 5. Problems?

### 5.1. Analysis Doesn't Stop

If what should be a quick operation (like *Restore*) takes so long that you grow seriously impatient, then you should abort the session and attempt to identify whatever is competing with Excel for system resources.

- On Windows-based platforms, the performance of executing programs can be visualized and (if needed) ended using Task Manager, an app in the Windows System folder in the Windows Toolbar. Task Manager can be invoked directly with <Ctrl+Shift+Esc> or indirectly through the more familiar <Ctrl+Alt+Delete> keystroke.
- On Mac systems, you can force programs to quit using the <Command+Option+Esc> keystroke. To monitor activity, use the Activity Monitor app which lives in the Finder > Applications > Utilities folder.

Once you have wrested control back from Excel, make quite sure that there are no competing processes – such as background system updates or virus checking. Once your system is quiet, cross your fingers, invoke a clean version of *CCQM\_Retrospectoscope*, and try again.

If the above doesn't clear the problem, email [david.duewer@NIST.gov](mailto:david.duewer@NIST.gov) with as complete a description as you can come up with, including details on your computing platform and Excel version.

### 5.2. Analysis Stops Prematurely

Congratulations, you've potentially discovered a new "bug". To be sure:

- Note down what you were attempting to do (what subsystem, dataset selection options, parameter settings, etc.) Take and store a screenshot of whatever the *CCQM\_Retrospectoscope* is showing.
- Close the *CCQM\_Retrospectoscope*, shut down your computer, restart your computer, wait a bit to let startup processes (virus checkers, updates, etc.) complete, then invoke a clean version of the *CCQM\_Retrospectoscope*.
- Redo the analysis that generated the problem.

If the analysis again aborts, please email [david.duewer@NIST.gov](mailto:david.duewer@NIST.gov) with as complete a description of what you were attempting to do as you can come up with, including diagnostic screen-shots.

## References

- [1] Duewer DL (2023) CCQM\_Retrospectroscope, an Excel workbook-based suite of graphical meta-analysis tools for the exploration of measurement results from Consultative Committee for the Amount of Substance: Metrology in Chemistry and Biology (CCQM)-sponsored multi-site studies. (National Institute of Standards and Technology, Gaithersburg, MD), <https://doi.org/10.18434/mds2-2952>.
- [2] Duewer DL, Cecelski CE, Cleveland MH, Lin NJ, Lippa KA, Mann JL, Molloy JL, Nelson MA, Norris JE, Pratt KW, Rhoderick GC, Sarkar S, Schantz MM, Watters RL, Windover DA (2024) NIST's Engagement with CCQM Studies from 1992 to 2023: History and Performance. (National Institute of Standards and Technology, Gaithersburg, MD), NIST Internal Report (NIST IR) NIST.IR.8524. <https://doi.org/10.6028/NIST.IR.8524>.
- [3] Duewer DL (2024) NIST's Engagement with CCQM Studies from 1992 to 2023: Peers, Early and Recent. (National Institute of Standards and Technology, Gaithersburg, MD), NIST Internal Report (NIST IR) NIST.IR.8542. <https://doi.org/10.6028/NIST.IR.8542>.
- [4] Duewer DL (2024) NIST's Engagement with CCQM Studies from 1992 to 2023: Uncertainty Scaling Relationships. With luck, it will "soon" be another NIST IR; try googling for it.
- [5] Duewer DL, Nelson MA, Cecelski CE (2024) CCQM\_Retrospectroscope Reference Manual. A detailed reference to the CCQM\_Retrospectroscope, a suite of graphical tools for the meta-analysis of measurement results from CCQM studies. (National Institute of Standards and Technology, Gaithersburg, MD), NIST Internal Report (NIST IR) NIST.IR.8478e2024. <https://doi.org/10.6028/NIST.IR.8478e2024>.

## **Appendix A. List of Acronyms**

CCQM	Originally “Consultative Committee for the Quantity of Matter”; now “Consultative Committee for the Amount of Substance: Metrology in Chemistry and Biology”
KC	Key Comparison
NIST	National Institute of Standards and Technology
NMI/DI	national metrology institutes and/or designated institutes
PS	pilot study
RMO	Regional Metrology Organization
SC	Supplementary Comparison
VBA	Microsoft Virtual Basic for Applications
WG	Working Group

## 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.

A rectangular button with a grey background and a thin black border. The text "Control Button" is centered on the button in a bold, black, sans-serif font.

### Checkbox

A control object that acts as an off-and-on switch. It may or may not invoke action when its state is changed.



### Dashboard

In *CCQM\_Retrospectroscope* usage, the graphical user interface part of a worksheet.

### Dataset

All of the measurement results, reference value, name, and other ancillary information for a given analyte in a given CCQM multi-laboratory study.

### Datasheet

A worksheet that contains datasets. The names of *CCQM\_Retrospectroscope* datasheets all begin "CCQM\_" and the tabs are colored green.



### Radio button

A control object that, when grouped with a set of radio buttons, is used to specify a particular discrete options. Only one of the set of radio buttons is active at any given time. It typically invokes action when its state is changed.



### Subsystem

A collection of computer programs that can be used to accomplish a given task. In the *CCQM\_Retrospectroscope* 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\_Retrospectroscope* is a collection of relatively independent subsystems and curated data into a system for the graphical analysis of results from CCQM-sponsored multi-laboratory studies.

### Workbook

A spreadsheet program file containing one or more worksheets. The *CCQM\_Retrospectroscope* system is instantiated in the Excel workbook *CCQM\_Retrospectroscope.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**

4-Sep-2024 Added “NIST’s Engagement with CCQM Studies from 1992 to 2023” series of NIST Internal Reports references. Added descriptions of the *Study\_RefVals* subsystem and the *Zoom* utility. Added this “Change Log” appendix.

5-Sep-2024: Editorial clarifications and updates throughout document.