

Reporting Variable Uncertainty and Statistics Using the *TABLE COLUMN NAME TYPE Key Phrase

New Picklist Entries

Uncertainty--accuracy	[See Note 1]
Uncertainty--precision	[See Note 1]
Uncertainty--confidence interval (+/-)	[See Note 2]
Uncertainty--lower confidence bound	[See Note 2]
Uncertainty--upper confidence bound	[See Note 2]
Uncertainty--combined standard	[Reference 1]
Uncertainty--expanded	[Reference 2]

Statistic--number of observations (N)
Statistic--standard deviation
Statistic--5th percentile
Statistic--95th percentile
Statistic--maximum
Statistic--minimum

FYI: "Detection limit" is already in picklist.

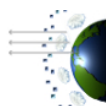
Note 1: Describe accuracy and precision measurements in *TABLE EXPLANATION OF REPORTED UNCERTAINTY key phrase or in companion file.

Note 2: Level of confidence (e.g., 95%) should be stated in *TABLE EXPLANATION OF REPORTED UNCERTAINTY key phrase.

Reference (1): Combined standard uncertainty: standard uncertainty of the result (y) of a measurement when the result is obtained from the values of a number of other quantities, equal to the positive square root of a sum of terms, the terms being the variances or covariances of these other quantities weighted according to how the measurement result varies with these quantities (GUM 2.3.4)

Reference (2): Expanded uncertainty: Quantity defining an interval about the result of a measurement that may be expected to encompass a large fraction of the distribution of values that could reasonably be attributed to the measurand. Obtained by multiplying the combined standard uncertainty by a coverage factor. Usually expressed as 'k'. (GUM 2.3.5)

"Guide to the Expression of Uncertainty in Measurement," ISO, Geneva, Switzerland 1993 (ISBN 92- 67-10188-9). Known as "GUM"

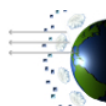


Reporting co-eluting organic compounds

The following strategy has been adopted for reporting co-eluting organic compounds. Note the combined Archive_CAS_values and names. These values should be used in the DES template. Other mixtures, of up to three (3) compounds, can be added to the [reference table](#) as needed.

Archive_CAS	name_9ci	Revision Date
C589-34-4+C96-22-0	Hexane, 3-methyl- and 3-Pentanone	20020829
C100-41-4+C123-19-3	Benzene, ethyl- and 4-Heptanone	20020829
C1071-26-7+C7379-12-6	Heptane, 2,2-dimethyl- and 3-Hexanone, 2-methyl-	20020829
C2216-30-0+C110-12-3	Heptane, 2,5-dimethyl- and 2-Hexanone, 5-methyl-	20020829
C589-53-7+C591-78-6	Heptane, 4-methyl- and 2-Hexanone	20020829
C15869-94-0+C80-56-8	Octane, 3,6-dimethyl- and Bicyclo[3.1.1]hept-2-ene, 2,6,6-trimethyl-	20020829

Common_Name	Comment
Co-eluting compounds	No official CAS number. Systematic Name Source: QSSC. Give retention time in Column Basis.
Co-eluting compounds	No official CAS number. Systematic Name Source: QSSC. Give retention time in Column Basis.
Co-eluting compounds	No official CAS number. Systematic Name Source: QSSC. Give retention time in Column Basis.
Co-eluting compounds	No official CAS number. Systematic Name Source: QSSC. Give retention time in Column Basis.
Co-eluting compounds	No official CAS number. Systematic Name Source: QSSC. Give retention time in Column Basis.
Co-eluting compounds	No official CAS number. Systematic Name Source: QSSC. Give retention time in Column Basis.



Reporting unknown organic compounds

The following strategy has been adopted for reporting unknown organic compounds. Note that unknown compounds for the same analytical method / compound class will have the same *TABLE COLUMN NAME value. *TABLE COLUMN BASIS should be used to provide further information, such as retention time (RT), that will differentiate unknown compounds. *TABLE COLUMN CAS IDENTIFIER should have a value of "None". Unknowns for other compound classes can be added to the [reference table](#) as needed.

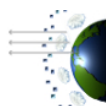
Values currently in Chems without CAS reference table:

- **Unknown: hydrocarbon**
- **Unknown: volatile organic compound (VOC)**
- **Unknown: non-methane hydrocarbon (NMHC)**

*TABLE COLUMN BASIS should be used to provide further information such as retention time (RT). A *TABLE USER NOTE or a *TABLE COLUMN USER NOTE could also be used for text explanation of unknowns.

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Reporting organic compound isomer mixtures

The following strategy has been adopted for reporting organic compound isomer mixtures. Note the combined Archive_CAS_values and the mixture names that were obtained from the EPA CRS. These values should be used in the template. Other mixtures can be added to the [reference table](#) as needed.

SS_Chemical Reference_Tables_20020712, updated July 12, 2002			
Archive_CAS	name_9ci	Revision Date	Common_Name
C108-38-3+C106-42-3	Benzene, 1,3(and 1,4)-dimethyl-	20020712	Xylene: meta and para mixed
C95-47-6+C106-42-3	Benzene, 1,2(and 1,4)-dimethyl-	20020712	Xylene: ortho and para mixed

Comment
No official CAS number. Systematic Source Name: EPA Chemical Registry System
No official CAS number. Systematic Source Name: EPA Chemical Registry System

Two new blue-colored "Bin" Key Phrases

There are two new "blue-colored" Key Phrases that may be used with existing supported template versions (2.212, 2.213, or 2.301):

***TABLE COLUMN BIN (20 characters maximum)** can be used to identify the categories for repetitive measurements. Bins, for example, could carry the values of the mass to charge ratio for single particle mass spec data. Use "Not applicable" as the entry for Site ID: standard, dates and times, etc., and for variables to which it does not apply.

***TABLE COLUMN BIN BASIS (30 characters maximum)** is used to explain the basis for *TABLE COLUMN BIN values.

These key phrases will be documented more fully in a future version of the template. In the meantime, contact the NARSTO QSSC if you have questions about their use.

