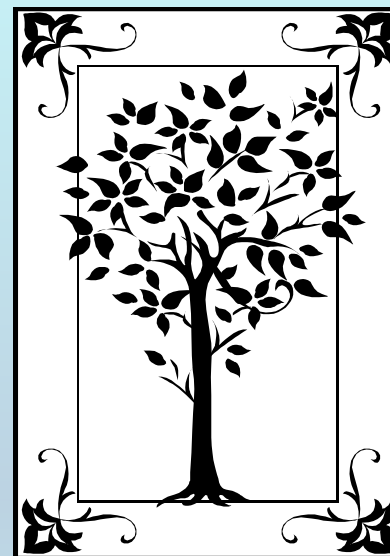


# SAMPLE ENTRY: tutorial (III)

## Guided Data Capture (GDC)



This tutorial demonstrates how to add chemical **SAMPLE** information (i.e., source, purity, etc.) to your file within the Guided Data Capture (GDC) software.

**NOTE:**

The tutorials proceed sequentially to ease the descriptions; however, it is not necessary to enter *all* compounds before entering *all* samples, etc.

Compounds, samples, properties, etc., can be added or modified at any time.

Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reference Compound **Sample** Mixture Reaction Property Data Tables

2002 chi dik 0  
phenylmethane  
pentane  
cyclohexane  
Compound X name

**1. SELECT (i.e., click once) a compound from the list you have entered.**

**2. CLICK *Sample* in the toolbar**

Start | Welcome to MSN.c... | Guided Data Capt... | NATRC DataEntryF... | Microsoft PowerPoi... | 3:45 PM

This form has 2 main sections:

- 1) **The sample *before* purification**; i.e., the original source of the sample, its purity, and the method of purity determination
- 2) **The sample *after* purification**; i.e., the purification method(s), final purity, and method of purity determination (entry of two purities and methods is possible; e.g., fractional melting and glc)

The screenshot shows a software window titled "Sample". At the top, there is a "Compound:" dropdown menu with "phenylmethane" selected and a "Sample #" input field with the value "1". Below this, the form is divided into two main sections. The first section, "Initial sample (before purification)", is highlighted with a red border and contains a "Source of sample:" dropdown menu, an "Initial purity (if reported)" input field with a "mol %" dropdown, and a "Determined by" dropdown menu. The second section, "Sample after purification", is highlighted with a blue border and contains a "Purified by:" label with a list of purification methods: "Chemical reagent treatment", "Crystallization from melt", "Crystallization from solution", "De-gassed by freezing and melting in vacuum", "De-gassed by boiling or ultrasonically", "Dried with chemical reagent", "Dried in a desiccator", and "Dried by oven heating". Below this list are two rows of "Final purity:" and "Another detn." input fields, each with a "mol %" dropdown and a "Determined by" dropdown. At the bottom of the window are "Accept" and "Cancel" buttons.

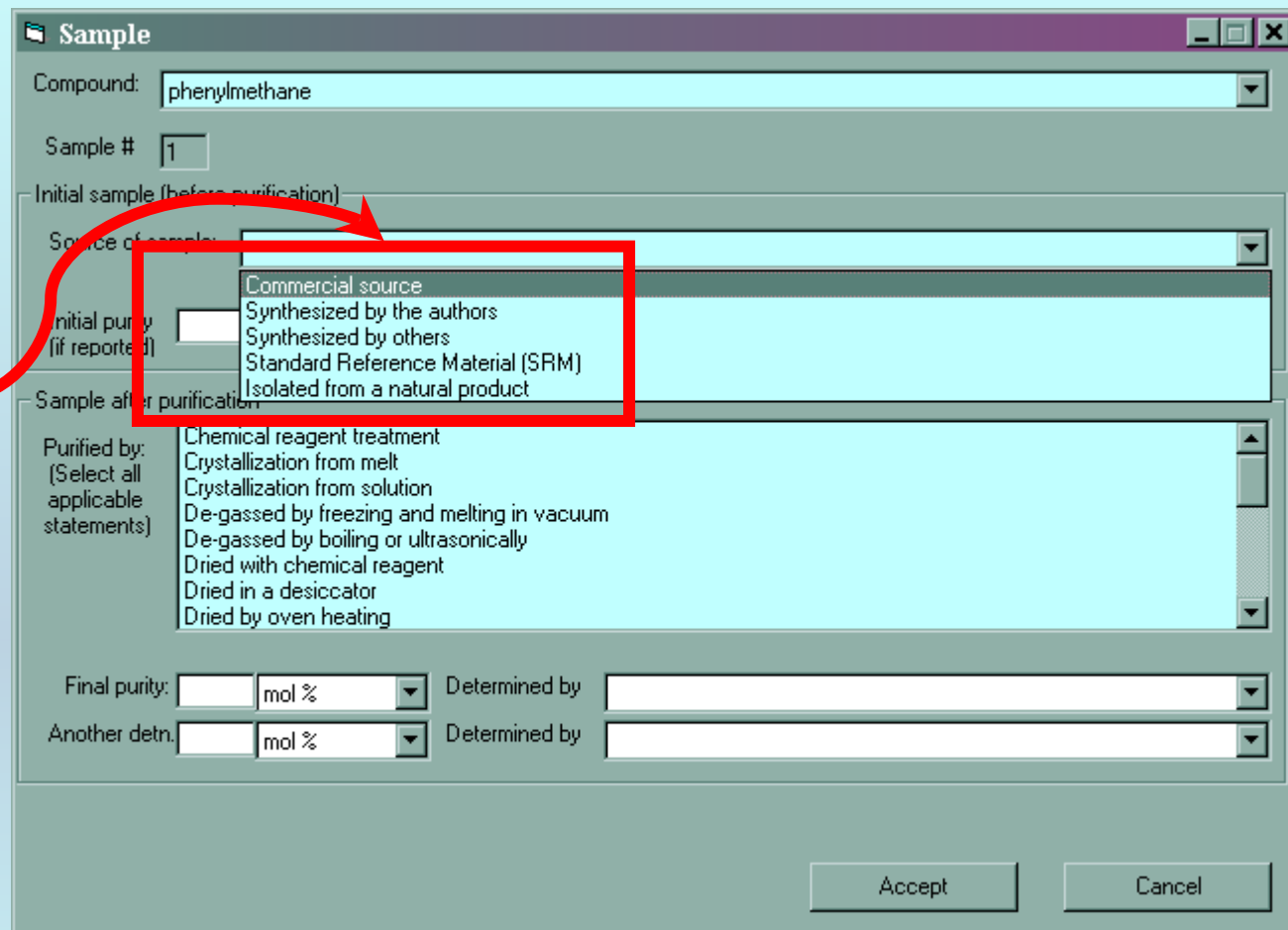
**NOTE:**

Some fields are optional.

Detailed instructions follow...

## Source of Sample:

**SELECT** the source of the original sample from the pulldown list.



The screenshot shows a 'Sample' dialog box with the following fields and options:

- Compound: phenylmethane
- Sample #: 1
- Initial sample (before purification):
  - Source of sample: Commercial source, Synthesized by the authors, Synthesized by others, Standard Reference Material (SRM), Isolated from a natural product
  - Initial purity (if reported):
- Sample after purification:
  - Purified by: (Select all applicable statements)
    - Chemical reagent treatment
    - Crystallization from melt
    - Crystallization from solution
    - De-gassed by freezing and melting in vacuum
    - De-gassed by boiling or ultrasonically
    - Dried with chemical reagent
    - Dried in a desiccator
    - Dried by oven heating
- Final purity:  mol % Determined by
- Another detn.  mol % Determined by

Buttons: Accept, Cancel

**Continue...**

# Initial Purity (if known):

1. TYPE the % purity

2. SELECT its basis from the pulldown list provided.

Sample

Compound: phenylmethane

Sample #: 1

Initial sample (before purification)

Source of sample: Commercial source

Initial purity (if reported): 98 mol %

Determined by:

Sample after purification

Purified by: (Select all applicable statements)

- Chemical water mass %
- Crystallization from melt
- Crystallization from solution
- De-gassed by freezing and melting in vacuum
- De-gassed by boiling or ultrasonically
- Dried with chemical reagent
- Dried in a desiccator
- Dried by oven heating

Final purity: mol %

Determined by:

Another detn.: mol %

Determined by:

Accept Cancel

Continue...

## Method of initial purity determination (if known):

**SELECT** the method from the pulldown list provided.

**Note:** If *Other* is selected, a brief text description will be requested.

The screenshot shows a 'Sample' dialog box with the following fields and options:

- Compound: phenylmethane
- Sample #: 1
- Initial sample (before purification)
  - Source of sample: Commercial source
  - Initial purity (if reported): 98 mol %
  - Determined by: [Dropdown menu]
- Sample after purification
  - Purified by: (Select all applicable statements)
    - Chemical reagent treatment
    - Crystallization from melt
    - Crystallization from solution
    - De-gassed by freezing and melting in vacuum
    - De-gassed by boiling or ultrasonically
    - Dried with chemical reagent
    - Dried in a desiccator
    - Dried by oven heating
  - Determined by: [Dropdown menu]
- Final purity: [ ] mol %
- Another detn.: [ ] mol %
- Determined by: [Dropdown menu]

Buttons: Accept, Cancel

**Continue...**

# Method of purification:

**SELECT**  
from the list  
all methods  
that apply

**Note 1:** If the sample was not further purified, make no selection.

**Note 2:** *Other* is an option here, also.

The screenshot shows a software window titled "Sample" with the following fields and options:

- Compound: phenylmethane
- Sample #: 1
- Initial sample (before purification):
  - Source of sample: Commercial source
  - Initial purity (if reported): 98 mol %
  - Determined by: Not known
- Sample after purification:
  - Purified by: (Select all applicable statements)
    - Solvent extraction
    - Fractional crystallization
    - Fractional distillation
    - Impurity adsorption
    - Liquid chromatography
    - Molecular sieve treatment
    - Preparative gas chromatography
    - Salting out of solution
  - Final purity: [ ] mol %
  - Determined by: [ ]
  - Another detn.: [ ] mol %
  - Determined by: [ ]

Buttons: Accept, Cancel

**Continue...**



# Final purity and method of determination:

1. TYPE the final % purity and SELECT its basis from the pulldown list.

Sample

Compound: phenylmethane

Sample # 1

Initial sample (before purification)

Source of sample: Commercial source

Initial purity (if reported) 98 mol % Determined by Not known

Sample after purification

Purified by: (Select all applicable statements)

- Solvent extraction
- Fractional crystallization
- Fractional distillation
- Impurity adsorption
- Liquid chromatography
- Molecular sieve treatment
- Preparative gas chromatography
- Salt removal from solution

Final purity: 99.8 mol % Determined by

Another detn. mol % Determined by

- Gas chromatography
- HPLC
- DSC
- Fraction melting in an adiabatic calorimeter
- Thermal analysis using temperature-time measurement
- Chemical analysis
- Acid-base titration
- CO<sub>2</sub> yield in combustion products

2. SELECT the method of purity determination from the pulldown list provided. (*Other* is an option.)

Continue...

## Second purity and method of determination:

**1. Add a 2nd  
purity and  
determination  
method, if  
applicable.**

Sample

Compound: phenylmethane

Sample # 1

Initial sample (before purification)

Source of sample: Commercial source

Initial purity (if reported) 98 mol % Determined by Not known

Sample after purification

Purified by: (Select all applicable statements)

- Solvent extraction
- Fractional crystallization
- Fractional distillation
- Impurity adsorption
- Liquid chromatography
- Molecular sieve treatment
- Preparative gas chromatography
- Salting out of solution

Final purity: 99.8 mol % Determined by Gas chromatography

Another detn. mol % Determined by

Accept Cancel

**2. CLICK *Accept* when done.**

**Continue...**

Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reaction Compound Sample Mixture Reaction Property Data Tables

2002  
chi dik 0  
+ benzylmethane  
benzene  
pentane  
cyclohexane  
Compound X name

**A new *node* appears in the navigation tree.**

**CLICK the + sign to expand it.**

**Continue...**

Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reference Compound Sample Mixture Reaction Property Data Tables

2002 cbi dik 0

- phenylmethane
  - Sample 1 [cm,98m%,nc;av,fd,mv;99.8m%,glc]
- pentane
- cyclohexane
- Compound X name

The sample description (in abbreviated notation) now appears below the compound name.

**NOTE:** DOUBLE CLICK the sample description (shown highlighted here) to return to the **Sample** form for editing, if desired.

Continue...

Guided Data Capture - Thermophysical and Thermochemical Data

File Edit Tools Help

Reference Compound Sample Mixture Reaction Property Data Tables

2002 chi dik 0

- phenylmethane
  - Sample 1 (cm,98m%,nc;av,fd,mv;99.8m%,glc)
  - Sample 2 (cm,98m%,nc;dc,mv;99.6m%,glc)
- benzene
- pentane
- cyclohexane
- Compound X name

**NOTE:** It is possible to enter information for more than 1 sample for a given compound.

Start | Welcome to MS... | Guided Data C... | N:\TRC DataEnt... | Microsoft Power... | 4:59 PM

**END**

See **MIXTURE component identification, PROPERTY SELECTION, or REACTION SELECTION** tutorials for the next steps...

The next step will depend upon the type of experimental data you are entering...