The Bridge for SFE/GC Configurations

User's Guide

The Bridge for SFE/GC Configurations

Safety Information

The HP 7680 Supercritical Fluid Extractors (SFE) have been designed and tested in accordance with IEC Publication 348, “Safety Requirements for Electronic Measuring Apparatus” as a safety class 1 instrument and CSA C22.2 no. 151-M1986, “Laboratory Equipment”. The manuals supplied with the extractor contain information and warnings that must be followed by the user to ensure safe operation and maintain the extractor in safe condition.

The extractor has been designed for indoor use. It may be shipped and stored for brief intervals at temperatures between −40°C and +70°C without degradation of its safety.

Before switching the extractor on, ensure that it is connected to a source of power for which it is rated. The power cord shall only be inserted in a socket outlet provided with a protective earth (ground) contact. The protective action of this connection must not be negated by the use of an extension cord without a ground conductor.

Whenever it is likely that the protective mechanisms of the HP 7680 SFE have been impaired, the extractor shall be made inoperative and be secured against any unintended operation. Protective mechanisms are likely to be impaired if, for example, the extractor:

— Shows visible damage.

— Fails to perform the intended functions.

— Has been subjected to prolonged storage under unfavorable conditions.

— Has been subjected to severe transport stresses.

Safety Symbols

This manual contains safety information that should be followed by the user to ensure safe operation.

WARNING A Warning calls attention to a condition or possible situation that could cause injury to the user.

Caution A Caution calls attention to a condition or possible situation that could damage or destroy the product or the user's work.

Warranty

The information contained in this document is subject to change without notice.

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1

Introduction

Introduction

The Bridge is a software/hardware package that enables you to link your HP 7680T Supercritical Fluid Extractor (SFE) to your HP 6890 Series or HP 5890 Series II Gas Chromatograph (GC).

With the Bridge, you will have an uninterrupted and fully automated chain of sample extraction and analysis from your SFE to your GC (or GC/MS if you are using a Mass Selective Detector). This automation eliminates operator intervention and hand transfers of vials between instruments. Because vials are transferred to the GC as the SFE produces them, no efficiency is lost.

Basically, the Bridge automation package provides:

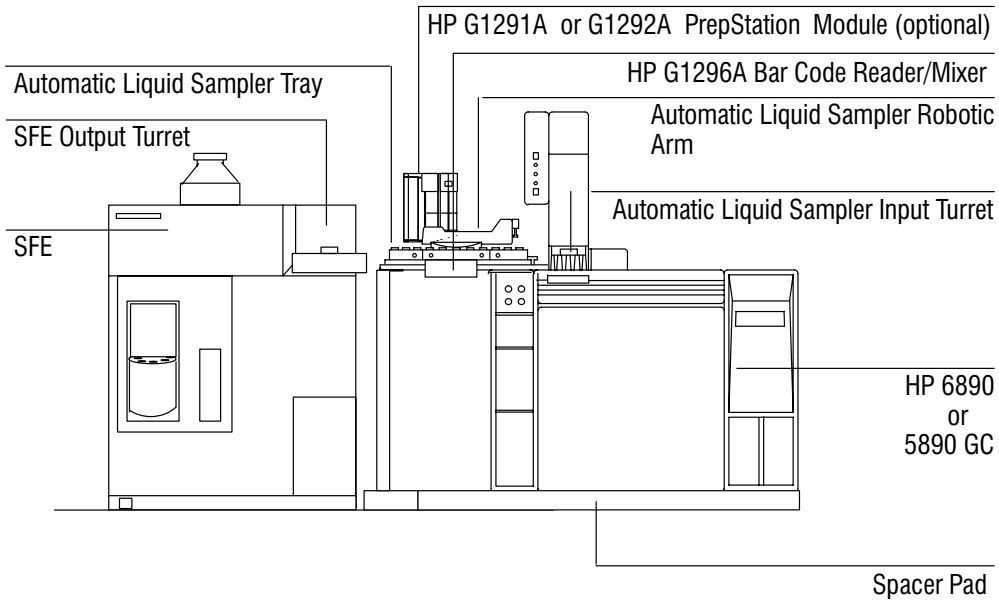
- Fully automated coordination of all instrument activities, sequencing, run control, and resource tracking, through the Bench Supervisor software. (You will need to re-enter SFE and ChemStation sequences as Bench Supervisor sequences.)
- Automatic vial transfer by the HP Automatic Liquid Sampler robotic arm between the SFE output turret, the sampler tray and the sampler input turret
- Simultaneous sample extraction and analysis which the Bench Supervisor software oversees
- Sample preparative capability prior to analysis using HP PrepStation modules
- Mixing and bar code reading of extracted analytes using the HP Bar Code Reader/Mixer

What is in this manual

This manual provides detailed instructions for the installation and basic functions of two Bridge configurations; SFE/GC Bridge and SFE/MS Bridge. Which chapters you should read depends on the configuration you will be using. For the specifics on which chapters apply to which configuration, read the information below.

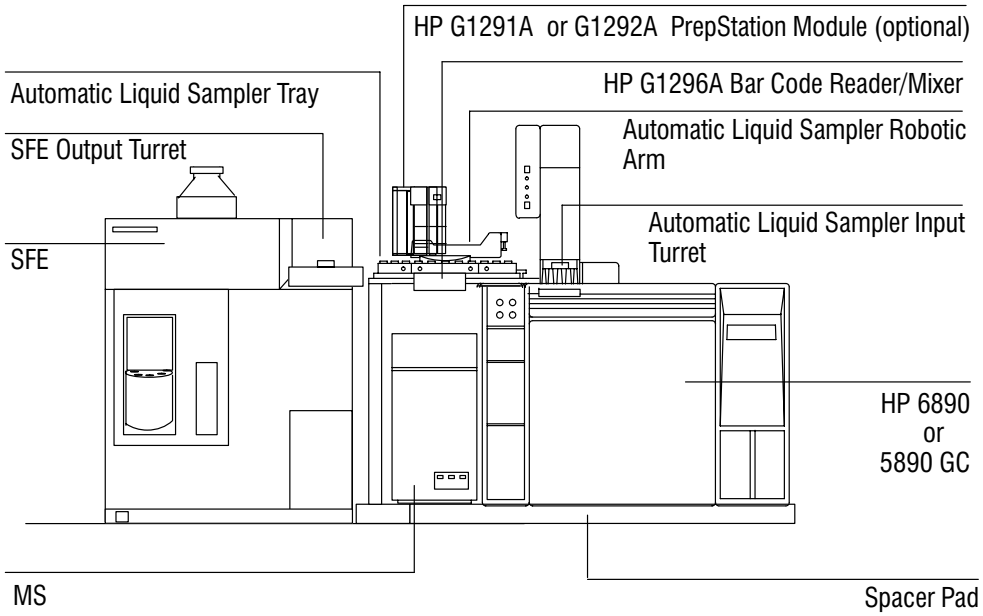
SFE/GC Bridge configuration (no mass selective detector) — Read chapters 2, 3, 4, 5, and 10 for information on the configuration and operation of your Bridge hardware and software. Chapter 10 contains information on troubleshooting that is the same for both configurations.

SFE/GC Bridge configuration



SFE/MS Bridge configuration — Read chapters 6, 7, 8, 9, and 10 for information on the configuration and operation of your Bridge hardware and software. Chapter 10 contains information on troubleshooting that is the same for both configurations.

SFE/MS Bridge configuration



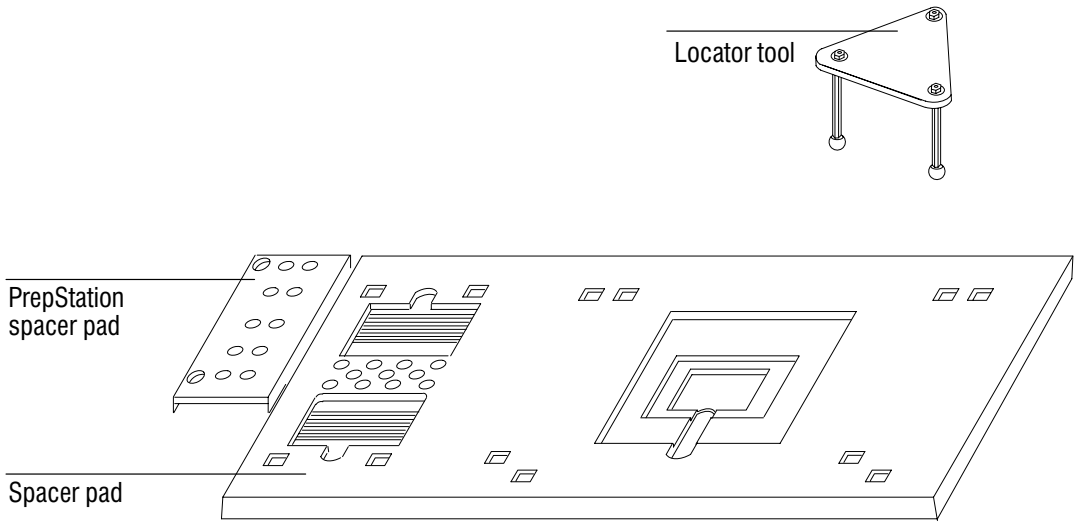
How the Bridge works

The Bridge uses both hardware and software to allow the SFE, PrepStation and GC instruments to transfer vials back and forth.

The hardware

The hardware that makes up the Bridge is very simple. Each Bridge installation kit includes a spacer pad on which the GC (and MS if it is present) will sit, a spacer pad for the PrepStation support legs (if a PrepStation is present), adhesive-backed metal shims for leveling purposes, and a locator tool for lining up the SFE and Automatic Liquid Sampler robotic arm for proper transfer of vials.

The spacer pads and the locator tool



The software

The Bridge comes with the Bench Supervisor software. The Bench Supervisor oversees the activities of the instruments: tracking all resources such as vials and data files, and coordinating the timing of the instrument methods to allow for efficient extraction and sample analysis processing.

The kit also includes a Bridge installation diskette. This software allows Bench Supervisor to control the SFE.

2

SFE/GC Bridge Installation

SFE/GC Bridge Installation

This chapter provides you with the information necessary to properly install the hardware and software that enables your system to operate in a Bridge configuration.

After you have completed these installation and configuration procedures, you will be ready to control your SFE and GC modules through Bench Supervisor, and to pass vials automatically between them.

Parts

See the contents sheet for parts included in this kit.

Hardware and software specifications

You will need the following hardware and software in addition to your SFE/GC Bridge accessory kit:

- HP 6890 GC and Automatic Liquid Sampler, or HP 5890/II GC, with HP 7673 Automatic Liquid Sampler and Injector (only 18596B tray module and 18594B controller module with serial number 3138A26712 or greater supported; see your local HP service representative for an EPROM upgrade)
- HP G2070AA ChemStation software for 6890 GC, or HP 3365 GC ChemStation software for 5890 Series II GC. Ensure that you have the correct version of the software.
- HP G1291A or G1292A PrepStation module, if installing one
- HP 1926A Bar Code Reader/Mixer
- HP 7680T SFE
- DOS-based computer capable of running the ChemStation software (Recommended minimum configuration: 486 IBM-compatible computer with 8 MB RAM, 80 MB hard drive with DOS 6 or higher and Windows™ 3.1 or higher.)
- Latest version of HP G1225C SFE software (included with Bridge kit)

See the installation instructions in this chapter before installing or attempting to run the Bridge.

This hardware will typically occupy the maximum bench space of:

193 cm W $\times$ 61 cm D $\times$ 93 cm H.

The setup will be slightly shorter if you are not using a PrepStation module. Running in a Bridge configuration will add slightly to the height of the GC and PrepStation, due to the spacer pad, but will not otherwise effect the dimensions of your bench setup.

The bench should be capable of supporting a minimum of 156 Kg (the weight of the system) with no noticeable deflection or vibration.

Before you begin

Perform the steps below before installing any software or hardware for the Bridge configuration.

NOTE: If you are using Windows EMM386 Memory Manager, you must modify the device line in the `config.sys` file to include the underlined information in the line below, in order for the HP-IB board to work properly:

`DEVICE=C:\WINDOWS (or DOS)\EMM386.EXE . . . X=DC00-DFFF`

Use a text editor, such as the DOS Edit command or Windows NotePad to make the modification.

1. Determine which HP-IB addresses are currently in use on your system and be sure to select available addresses for the instruments you are installing. System communication errors will result if you assign more than one instrument to an HP-IB address. Refer to the manual set for each instrument for information on how to read and select the appropriate HP-IB addresses. Also, use the information in the `DEVICE` lines in the PCS section of your `win.ini` file to record the instrument addresses for previously installed instruments, where:

   `DEVICEN=X,ADDRESS,DEVICE NAME`

NOTE: The ChemStation software will not accept HP-IB addresses greater than 29.

2. Perform any of the following that apply before installing the software:
   - Back up any methods you wish to keep.
   - Back up the `sfe1`, `sfe2` (if you have one) and `hpchem` directories. Once backed up, delete the `sfe1`, `sfe2` and `hpchem` directories from the hard drive.
   - Back up and modify the `autoexec.bat` file with the following changes, using a text editor, such as the DOS Edit command or Windows NotePad:
     a. Remove `c:\hpchem` from the path line.
     b. Remove the TEMP directory designation line.
   - Back up the `win.ini` file, then delete all PCS sections from it, again using a text editor. The PCS sections contain the line [PCS] as their first line. There may be numbers after the [PCS] in some PCS sections. Delete these numbered sections as well.
   - Select the ChemStation program group icon, then press <Delete> on the keyboard. Confirm the deletion by pressing <Enter>. Repeat this process for all ChemStation group icons.
3. Reboot the computer to allow the current path designations to take effect.
4. Prior to installing any software, be sure that the following items are **NOT** present in the computer system:
   - `c:\hpchem` directory and its subdirectories
   - `c:\hpchem` in the path and in the TEMP directory designation, as seen in the `autoexec.bat` file
   - PCS sections in the `win.ini` file
   - Windows program groups for any previously installed ChemStation applications

Hardware installation

Follow the procedures below to set up your SFE and gas chromatograph in a Bridge configuration.

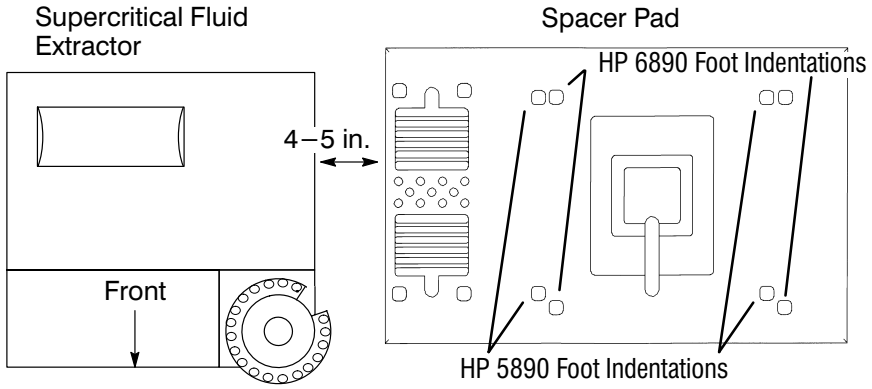
WARNING Have an assistant available to help you with the following installation procedures. The SFE and the GC are heavy. Moving either device is a two-person job!

Setting up the GC

This procedure sets up the GC in close proximity to your SFE in preparation for the final alignment of the two instruments.

1. Place the Bridge spacer pad on the right side of the SFE in the orientation shown below.

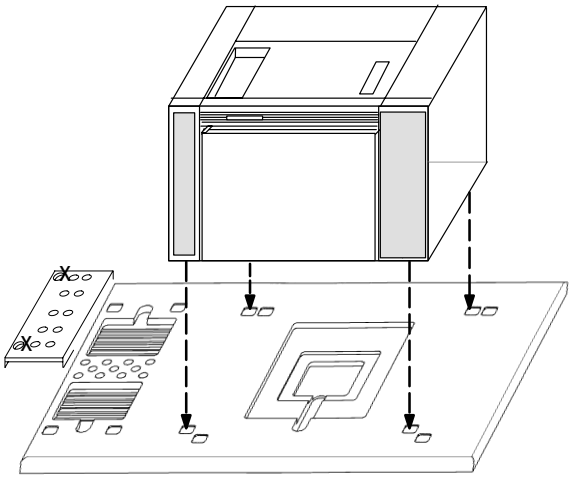
Overhead View



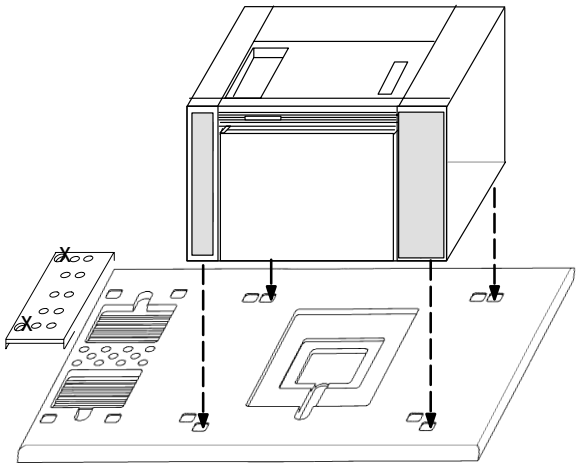
2. Remove the protective paper tape from the adhesive on the back of four of the metal shims and place a shim in each one of the GC foot indentations on the Bridge spacer pad for 5890 or 6890 locations. To begin with, place at least one metal shim in each foot indentation. You may need to place more, depending on your particular hardware.

3. With your assistant, lift and place the GC on the pad so that the GC's feet rest on the metal shims in the foot indentations.

Placing 5890 GC on spacer pad



Placing 6890 GC on spacer pad



4. Install the automatic liquid sampler hardware (bracket, tray, injector(s) and bar code reader/mixer) if you have not already done so. If you have one, install the HP G1291A or G1292A PrepStation on the bracket, as described in the PrepStation documentation. The legs for the PrepStation should be positioned just to the right of the leg locator slots on the PrepStation spacer pad, as indicated by Xs on the illustration above.

Software installation

After setting up the hardware, install and configure the software necessary to run the SFE/GC Bridge. Follow the steps below to install the software properly.

NOTE: You must install the software in the correct order. Installing the software out of order will prevent the Bridge configuration from operating properly. Locate your ChemStation, PrepStation, Tray and SFE floppy disks to perform this installation.

1. Install and configure the GC ChemStation Analyzer software according to the instructions in your ChemStation documentation and verify that the GC is operating normally. Ensure that the ChemStation has added `c:\hpchem` to the path in your `autoexec.bat` file. If it has not, add it using a text editor.

2. Exit Windows and reboot your computer to allow the change to the path designation to take effect, then re-enter Windows.

3. If your software does not create program and group icons for your ChemStation, follow the instructions in your ChemStation manual for creating a new program group under Windows, and for creating new items in that group for ChemStation and Configuration Editor. Set up and save the GC using the Configuration Editor, as follows:

   Instrument Type: 6890 or 5890 GC
   Instrument Name: GC
   Initially Start Instrument Session: No
   Initial Screen Window Size: Normal
   HPIB Address for GC: Your Instrument # for the GC
   HPIB Address for Sampler: Your Instrument # for the Sampler

   When prompted, “ADD” the HP Automatic Liquid Sampler.

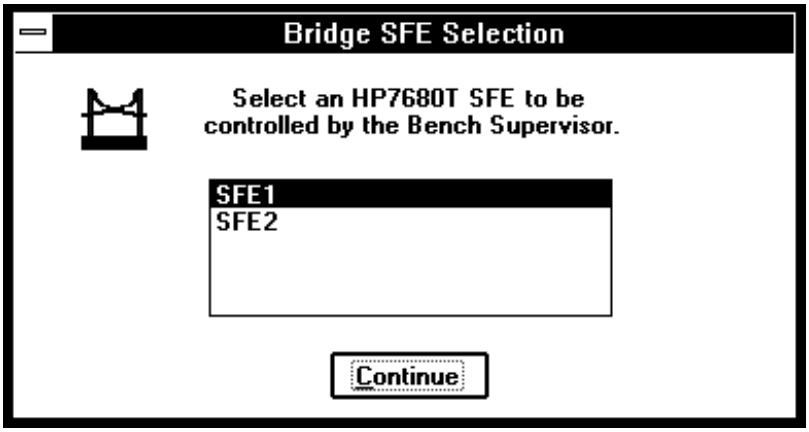
4. Verify that the ChemStation is operating correctly.

4. Close the ChemStation software, then exit and reenter Windows before proceeding with the installation, to avoid causing an APG_VGA.FON error.
5. After exiting and restarting Windows, install the SFE software according to the instructions in your SFE documentation and verify that the SFE is operating normally.
6. Close the SFE software before continuing with the installation.

   NOTE: When using the Configuration Editor to configure instruments, be aware of the following restrictions:

   - You can only configure up to four instruments using the Configuration Editor.
   - Do not use the Configuration Editor to add a second non-Bridge SFE.
   - You will be unable to change modifier pump settings with the Configuration Editor due to the file structure of methods that incorporate the pump. To change modifier pump settings, you will need to reinstall the SFE software and change the Modifier Pump as needed. Note that SFE methods for a configuration with no modifier pump are unusable under a configuration that includes a modifier pump, and vice versa.
   - Do not use the Configuration Editor to change from a single-channel modifier pump to a quaternary pump; reinstall the SFE software to do this.
7. Install the Bench Supervisor software according to the instructions in the *Bench Supervisor Operating Manual*.
8. If you will be using a PrepStation, install PrepStation software as described in the *PrepStation Site Prep and Installation Manual*.
9. Install the Tray software as described in the *Bench Supervisor Operating Manual*.
10. Verify that Bench Supervisor control of the GC, PrepStation and Tray is operating normally.

11. Close the Bench Supervisor software before continuing with the installation.
12. Install the Bridge software as described below. This software enables the Bench Supervisor to control the SFE application.
    a. From the Windows Program Manager, select `File`, then `Run` to access the Run dialog box.
    b. Put the Bridge Installation disk in drive `A:` and type "A:\setup" in the Run dialog box. (If you are using drive `B:`, type "B:\setup" instead.) Follow the instructions on your screen to complete the installation.
    c. When the "Bridge SFE Selection" window appears, select the SFE that Bench Supervisor will control, then select `Continue`. If you have installed only one SFE on the system, only one will appear in the message box.



    d. Select `Continue` when the system prompts you, then select `OK` when the installation is complete.
    e. For additional information on the Bridge installation, read the `ins_note.wri` file displayed at the end of the Bridge installation procedure. The installation software will place this file in your root directory.

Aligning and checking out the instruments

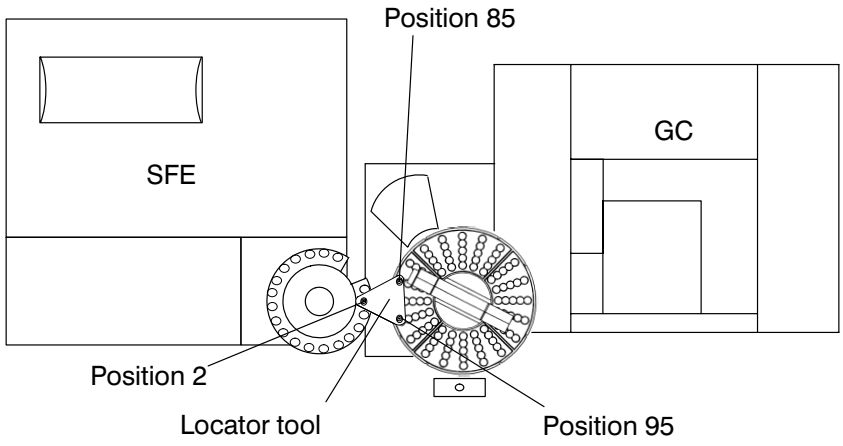
After setting up the hardware and installing the software for the SFE/GC Bridge, align the instruments to ensure proper transfer of vials, then run checkout tests to verify everything is functioning properly.

Aligning the instruments

Use the locator tool to align the SFE and automatic liquid sampler for precise vial transfers, as follows.

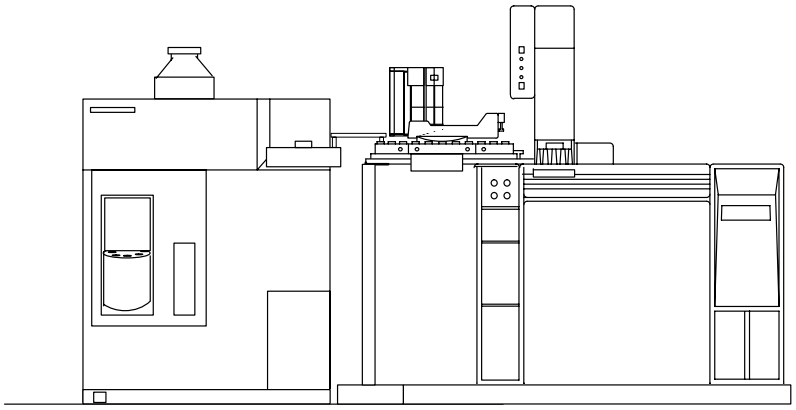
1. Start up the SFE software.
2. Select `Run` from the SFE menu bar, then select the `Maintenance and Test` option. Select `Rotate tray: vial #2 side`. This command rotates the SFE output turret clockwise so that position 2 is nearest to the sampler tray.
3. Place the locator tool so that two of the legs rest in vial positions 85 and 95 on the sampler tray and the leg indicated by a hole rests on the SFE output turret, as shown in the illustration below.

Overhead View



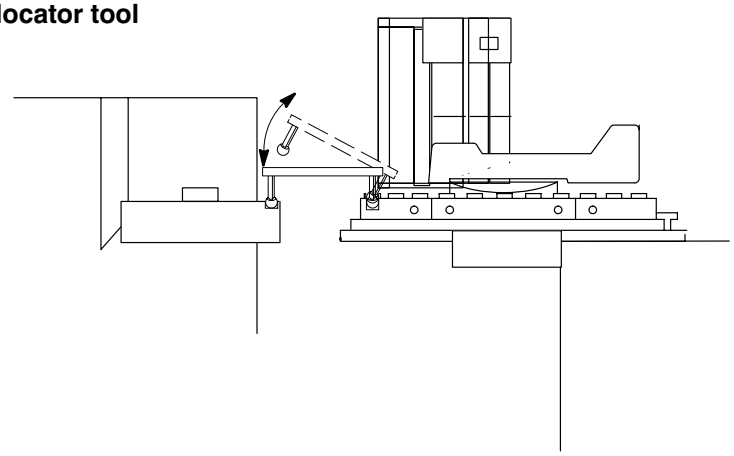
4. Reposition the Bridge spacer pad so that the leg of the locator tool resting on the SFE output turret drops into vial position 2 on the turret.
5. The locator tool should appear level with respect to the SFE and the sampler tray, as shown below. If it is not level, have your assistant lift the corners of the GC while you add or remove metal shims as needed, and adjust the lengths of the PrepStation legs if you have a PrepStation installed.

Checking the SFE and Automatic Liquid Sampler alignment



6. Pivot the locator tool to make sure it can move freely in and out of vial position 2 on the SFE output turret, as shown below. If you encounter resistance, reposition the Bridge spacer pad until you can pivot the locator tool freely.

Pivoting the locator tool



When the locator tool pivots freely, the automatic liquid sampler and the SFE are perfectly aligned for vial transfers.

WARNING If you align the sampler tray and SFE improperly, the robotic arm may drop or eject the vials when retrieving them from the SFE output turret for placement in the sampler tray.

Checking out the instruments

After you have set up the hardware and installed the software, check to be sure the instruments are operating properly. Perform checkout tests using each instrument and its software to verify that the SFE/GC Bridge is functioning normally.

Using the SFE/GC Bridge

Using the SFE/GC Bridge

Once you have installed the Bridge hardware and software, you can begin setting up Bench Supervisor bench methods and bench sequences to automatically run series of extractions and analyses.

This section describes what you need to know to use your SFE, PrepStation and GC in a Bridge configuration. It explains how the Bridge operates and how to use Bench Supervisor to pass vials between your SFE and automatic liquid sampler.

Bridge mode and Local mode

There are two modes for operating the SFE and GC: Bridge and Local.

Bridge mode

If you start an SFE or GC run in the Bench Supervisor software, the instruments are running in Bridge mode. The Bridge mode allows automated transport of vials between the output turret of the SFE and the automatic liquid sampler tray. The sampler tray can then transfer these vials to and from the PrepStation and/or GC for injection. In Bridge mode, the Bench Supervisor software handles all sequencing. You cannot use SFE and ChemStation sequences.

Local mode

If you start a run from the SFE or ChemStation software without Bench Supervisor, the instruments are running in Local mode. In Local mode, you can use all of the features of the SFE and ChemStation software, including sequencing; however, you cannot automatically transfer vials between the SFE and the automatic liquid sampler.

When you are running instruments in Local mode that the Bench Supervisor software normally controls, their Bench Supervisor status will be “Busy.” While the GC, PrepStation and SFE have a status of “Busy,” the Bench Supervisor software cannot run bench methods and bench sequences. Likewise, when you are running bench methods and bench sequences, you cannot use the SFE or PrepStation in Local mode. However, you can run GC instruments in Local mode while running bench methods and sequences. See the following chapter, *Using the GC ChemStation with the Bench Supervisor software*, for details on running multiple ChemStation sessions in Bridge mode. Multiple SFE’s cannot be configured to run under Bench Supervisor.

Vial transport

The Bench Supervisor software coordinates all of your instruments to provide a chain of automation from your extractor to your gas chromatograph. When the SFE is ready to rinse analytes to a vial, the Bench Supervisor software will transport a vial from the sampler tray to the SFE output turret. After the SFE delivers the sample fraction, the Bench Supervisor software returns the vial to the sampler tray, then transports it first to the PrepStation (if specified), then to the injector turret, which injects it into your GC.

Bench Supervisor overrides the vial numbers specified in the SFE method for fraction output and always places vials into position 2 of the SFE’s 21 vial output turret. The automatic liquid sampler robotic arm needs position 1 empty to allow enough clearance to place a vial in vial position 2 of the SFE turret.

NOTE: Be sure to empty vial positions 1 and 2 of the SFE output turret before running SFE methods through the Bench Supervisor software.

Bench methods and sequences

Bench methods

A bench method is a combination of methods from the instruments running under Bench Supervisor. A typical bench method in an SFE/GC configuration consists of an SFE method, PrepStation method, then one or more GC methods to analyze the extracted output.

Bench Supervisor oversees the activities of the individual pieces of equipment and coordinates the automation that permits unattended running of bench methods involving the SFE, PrepStation, bar code reader/mixer and GC. For more information on bench methods, see the examples in Chapter 5, or your *Bench Supervisor Operating Manual*.

Bench sequences

Bench sequences are a grouping of bench methods, and are useful when you need to analyze multiple samples or a range of samples. For more information on bench sequences, see the examples in Chapter 5, or your *Bench Supervisor Operating Manual*.

Quantitative analysis with the Bridge system

The Bridge configuration is designed to provide unattended sample preparation and analysis. If you want to do quantitative work, you must add an internal standard to the sample vials. Add it beforehand to each of the vials that will receive the fraction output from the SFE. After the fraction output vials leave the SFE, they **MUST** be mixed. They will then be ready for injection into the GC without any further manual intervention.

If you will be using PrepStation to add internal standards, consult the PrepStation documentation for additional information and instructions.

SFE methods and sequences

SFE methods

You do not have to make any changes to your SFE methods to run them in Bridge mode. Even though all output fractions go to vial position 2 on the output turret when you are in Bridge mode, you can specify any output vial numbers in your method. These values will be overridden by the Bench Supervisor software when you run the method in Bridge mode. This allows you to use the same SFE methods in Bridge mode as you would when operating the SFE by itself (Local mode).

NOTE: Be sure to empty vial positions 1 and 2 of the SFE output turret before running SFE methods through the Bench Supervisor software, to allow clearance for the automatic liquid sampler robotic arm.

SFE sequences

Do not create SFE sequences to be used in Bridge mode. All sequencing is handled at the Bench Supervisor level. You can, however, still run SFE sequences in Local mode.

Access to the SFE software during a run

During a run, the functionality of the top SFE level screen changes, based on whether you are in Local mode or Bridge mode.

Bridge mode

NOTE: The Bench Supervisor software will not allow you to load or run bench methods or sequences if you leave a dialog box open in the SFE or ChemStation software. The Bench Supervisor software will report the application as "Busy" until you close the dialog box.

When performing a run in Bridge mode, Bench Supervisor displays the Remote keyboard on the screen. All areas of the SFE Top Level screen become grayed out and are inaccessible. You can, however, open the Instrument Status screen from the Run menu and view the Step Setpoints from the Extract menu if you wish.

In Bridge mode, the SFE is under the control of the Bench Supervisor software. Local control returns when the bench method or bench sequence concludes its run or is stopped. For additional information on SFE runs in Bridge mode, see the examples in Chapter 5, or your *Bench Supervisor Operating Manual*.

Local mode

When performing a run in Local mode, only the Thimble View and keyboard areas of the top level screen are active. All other areas are grayed out. You can select `Change Setpoints During Run` to access other areas, but changing the parameters of a run is NOT recommended due to the risk of adding potentially unsafe parameter specifications. For more information on SFE runs in Local mode, see your SFE User's Guide.

Power failure and hardware faults

Power failures and/or hardware faults will render the SFE software status as “Busy” or “Down.” Such events may cause the SFE to set the instrument status to “Failed.” It will be necessary to stop the run and restart all software.

To help avoid aborted runs due to power failures, uninterruptable power supplies (UPS) should be properly sized and added to the main power sources for each instrument and computer in a Bridge configuration.

Aborting or stopping a run

You can abort a bench method from the Bench Supervisor software or the ChemStation software. You can also stop a run from the SFE software.

Aborting from either instrument’s software or from the Bench Supervisor software will cause the entire bench method or bench sequence to abort. The SFE and/or the GC instruments may have to proceed to a safe state before shutting down (i.e., depressurize).

In the event that an SFE run fails due to SFE instrument errors during a run, it may or may not halt other bench activity.

Stopping from the SFE software

Select the `STOP` button on the Remote keyboard. See *Stopping from the Remote keyboard* on the following page for more information about stopping using the Remote keyboard.

Aborting from the ChemStation software

Select `Abort` from the `RunControl` menu. See the *ChemStation* documentation for more information about aborting a run from the software.

Aborting from the Bench Supervisor software

The `Abort` option is on the top level of all four Bench Supervisor menu bars. Select `Abort` from the menu bar to abort a bench sequence or method.

See the *Bench Supervisor Operating Manual* for more information about aborting a run from the software.

Aborting from the PrepStation software

See the *PrepStation Operating Manual* for more information about aborting a run from the software.

Stopping from the Remote keyboard

In Bridge mode, when you launch a bench method or bench sequence from the Bench Supervisor that references an SFE method, a Remote keyboard appears on the screen just before the SFE method begins its run. This keyboard, titled “Remote,” is a replica of the actual keyboard on the SFE instrument and can be moved about the display.

The Remote keyboard looks similar to the keyboard displayed during an SFE run in Local mode, but it does not have a `Start` button because the SFE method is started and controlled remotely by the Bench Supervisor software.

The Remote keyboard does have a `STOP` button that stops the currently running SFE method. If stopped, the extractor is programmed to proceed to a safe condition (depressurized, thimble cooled and containing only pure CO_2) before opening the chamber. This may take as long as 10 minutes. If the output turret has been rotated to the side to receive or return a vial to the sampler tray, the extractor may halt until delivery (or removal) of the vial is completed by Bench Supervisor. While the turret is rotated to the side, the extractor’s error recovery abilities (e.g., depressurization) are limited.

Using the GC ChemStation with the Bench Supervisor software

Using the GC ChemStation with the Bench Supervisor software

If you are used to running the HP ChemStation by itself, there will be some differences when you use it in combination with the Bench Supervisor and another instrument, such as the HP 7680T SFE. You will use the Bench Supervisor software to control the automation between the SFE, PrepStation and the GC, and to create and edit bench methods and sequences. You will, however, continue to use the HP ChemStation for creating and editing GC methods, and for data analysis.

Version

You must have the correct version of the HP G2070AA ChemStation to operate the HP 6890 GC. To operate the HP 5890 Series II GC, you will require the HP 3365 ChemStation at its supported level. Earlier versions will not work properly with the Bench Supervisor software.

Installation and configuration

See Chapter 2 for notes on installing and configuring the HP ChemStation to run with the Bench Supervisor software.

Calibration

See Example 5 in Chapter 5 of this manual, or the *Bench Supervisor Operating Manual*, for information on running calibrations using the Bench Supervisor software.

Multiple GC instruments

This section applies only if you have a version of the ChemStation capable of supporting multiple GCs.

Only one GC can be run by the Bench Supervisor software. However it is possible to run other GC sessions outside of the Bench Supervisor while running one with it. To accomplish this, the `win.ini` file must be set up properly.

Verify that the `[PCS,`*n*`]` of the GC session running with the Bench Supervisor (where *n* is the instrument number of the GC) contains the line `Supervisor=Yes`.

The other sessions can remain unchanged, except that their `Supervisor=` lines must be set to `Supervisor=NO`.

To start multiple GC sessions:

1. Start `apg_top.exe`.
2. Start Bench Supervisor. It will start the GC session that it will use.
3. Use the `APG_TOP` window to start up any other GC sessions that are desired.

Sequencing

While the Bench Supervisor software is running, all sequencing should be done by it. If you run sequences from either the HP 7680T SFE or the ChemStation, you are bypassing the Bench Supervisor software and will not be able pass vials from the SFE to the GC.

***NOTE*:** Unlike the ChemStation software, the sequencing performed by the Bench Supervisor software will not stagger GC methods for optimization when two injectors are used.

Data Analysis

If you open the Data Analysis screen of the ChemStation, the GC instrument's status at the Bench Supervisor level will be reported as "Busy" and you will be unable to perform many Bench Supervisor functions. Be sure to remain in the ChemStation's Top level screen unless you are manually manipulating files in Data Analysis.

Method inputs

When you set up a GC method as part of a bench method, you will see the following Vial, Data and Value inputs at the Bench Supervisor level. The values for these fields are entered through the Bench Supervisor software, which passes them to the ChemStation for use when a run is started. Below are descriptions of each method input and how to use it:

GC Vial

This is the vial that will be injected into the GC.

Sample Name

This is a short name for the sample being analyzed. It will appear in the ChemStation report.

Comment

This is a longer description for the sample being run. It will appear in the ChemStation report. If you set this field to `Track GC Vial` on the `Bench Method/Edit/Data` screen, the report will include a description of any instrument steps that were run on the vial before injection into the GC, such as extraction using the HP 7680T SFE.

Data Directory

This is the subdirectory that stores the data files for the run. This can be either a name supplied by the user, or it can be an *autoname* such as `yymmddss` which will be expanded to create a unique directory for a run based on the date of the run (see the Bench Supervisor documentation for more information on autonames).

GC Raw File Name

This is the name of the file that receives the GC data. You can create your own name, or set up an *autoname* so that the file name is made up of vial number, injector, sequence line, and injection number (see the Bench Supervisor documentation for more information on autonames).

Operator

This is the name of the operator of the system. It is stored in ChemStation data files and printed on the reports.

CalibLine

If the bench method is to be used for a standard to recalibrate the GC method calibration table, this is the line in the Sequence Recalibration table for the GC method to use for this run (see the calibration examples later in this document). If the run is not a recalibration run, the value should be zero.

Multiplier

The multiplier value for this sample. This is only used for calibrated reports.

Sample Amount

The sample amount for this sample. This value is used only in ESTD and ISTD reports. See the ChemStation documentation for more information.

ISTD Amount

The ISTD amount for this sample. This is only used for calibrated ISTD reports. See the ChemStation documentation for more information.

5

Examples of SFE/GC Bridge Operations

Examples of SFE/GC Bridge Operations

This chapter contains five examples to illustrate the use of the Bench Supervisor software with the HP 7680T SFE and the HP ChemStation.

Example 1, *Bench Methods*—Shows you how to set up a simple bench method to run an unattended extraction and analysis using the SFE and the GC. This example is designed to show you the basic steps involved in setting up bench methods to pass fraction output from the SFE to the GC for analysis.

Example 2, *Bench Sequences with a single extraction*—Shows you how set up a simple bench sequence to perform extractions and analyses on multiple samples. In this example, each run of the SFE method performs a single extraction that produces a single sample vial.

Example 3, *Bench Sequences with multiple extractions*—Shows you how to set up a bench sequence to perform extractions and analyses on multiple samples, where each run of the SFE method performs two extractions and produces two sample vials.

Example 4, *Bench Sequences with multiple extractions into a single vial*—Shows you how to set up a bench sequence to perform extractions on two samples and combine them into a single vial for analysis.

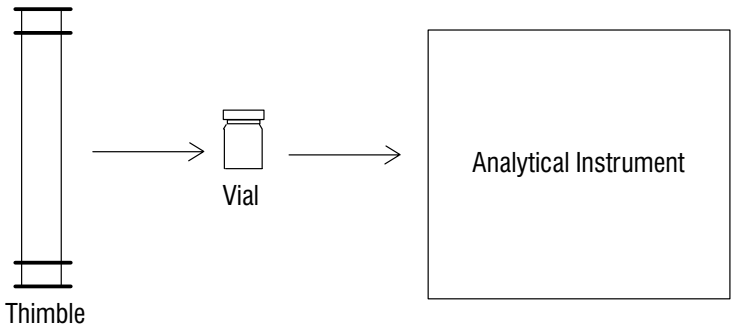
Example 5, *Calibrations using the Bridge*—Shows you how to use the Bridge to perform unattended calibrations of the GC.

Example 1—Setting up a bench method

The example below shows the best way to set up a bench method, in which the SFE outputs one fraction vial to the GC for analysis.

The scenario

For this example, assume you have an SFE method, `SFE1`, that outputs one vial to be analyzed at the end of its run, and you want to analyze this vial with a run of the GC method, `GC1`.

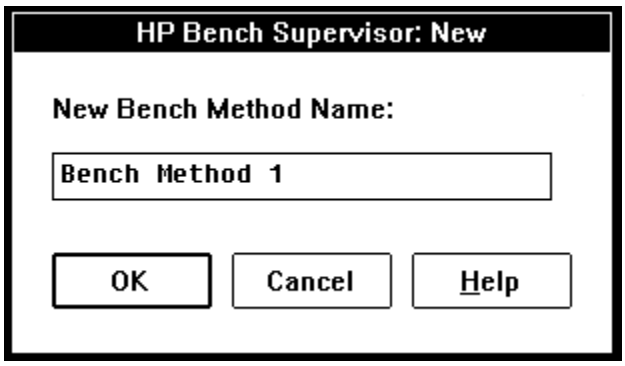


Creating the bench method

The following procedure describes how you would go about setting up the bench method described above to extract a single sample using the SFE and then transfer the sample to the GC for analysis.

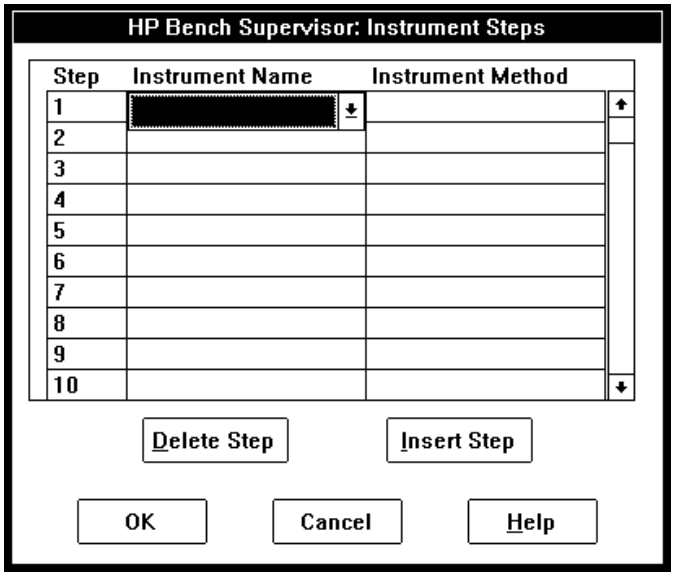
***NOTE*:** This example is provided to show you the steps necessary to set up an SFE/GC bench method. It is not necessary to actually complete the steps shown. The two instrument methods used to create the bench method in this procedure are not provided in the software. Just follow along with the procedure to get an idea of what is required to set up a bench method in Bridge mode.

1. In the Bench Supervisor program, select the `Bench Method` button to load the Bench Method menu bar. From the `File` menu, select `New Bench Method`.



2. Type a name for the bench method and select `OK`. The name can be any size up to the width of the box, and include any letter, number, or symbol, including spaces.

3. From the `Edit` menu, select `Instrument Steps`.



The Instrument Steps dialog box is where you specify the order of the SFE and ChemStation methods you want to run in your bench method.

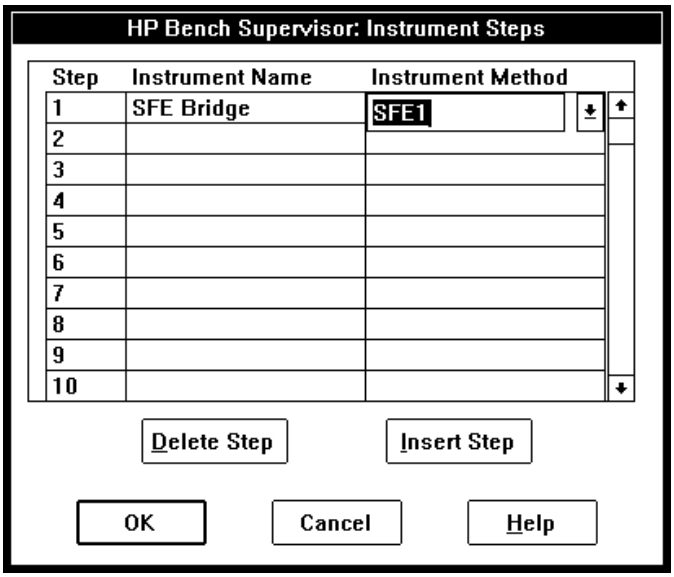
NOTE: You must first create an instrument method using the appropriate instrument software before it will appear in the Instrument Steps dialog box, shown below, for incorporation into a bench method.

4. To make the SFE method `SFE1` the first step in this bench method:

   a. Select `SFE Bridge` from the Instrument Name drop-down list for *step one*.

   b. Select `SFE1` from the Instrument Method drop-down list for *step one*. The dialog box should appear as shown on the following page.

NOTE: SFE Bridge is the default name for the SFE instrument controlled by Bench Supervisor. If the name for the SFE instrument has been changed in the `win.ini` file, it will be different in the drop-down list box also.



NOTE: All quantitative analysis bench methods **MUST** contain a mixing step. If you *do not* have a PrepStation, include this step in the Instrument Steps dialog box, as shown in step 5. If you *do* have a PrepStation, consult your PrepStation documentation for information on vial mixing.

5. To run the bar code method `mix.mth` as the second step in the bench method:

   a. Select `BARCODE` from the Instrument Name drop-down list box for *step two*.

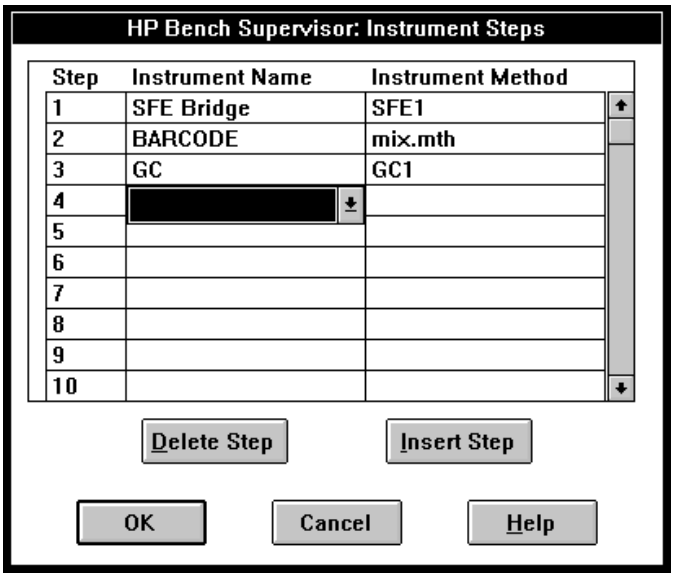
   b. Type `mix.mth` in the Instrument Method column for *step two*. The method name will not appear in the list box, you must type it in.

NOTE: If you also want to use the bar code reader/mixer to read a bar code, select the `BARCODE` instrument name and type `barcode.mth` in the Instrument Method column for the desired step.

6. To run the GC method `GC1` as the third step in the bench method:

   a. Select the name of the GC instrument from the Instrument Name drop-down list box for *step three*. In our example the name of the GC instrument is GC.

   b. Select `GC1` from the Instrument Method list for *step three*.

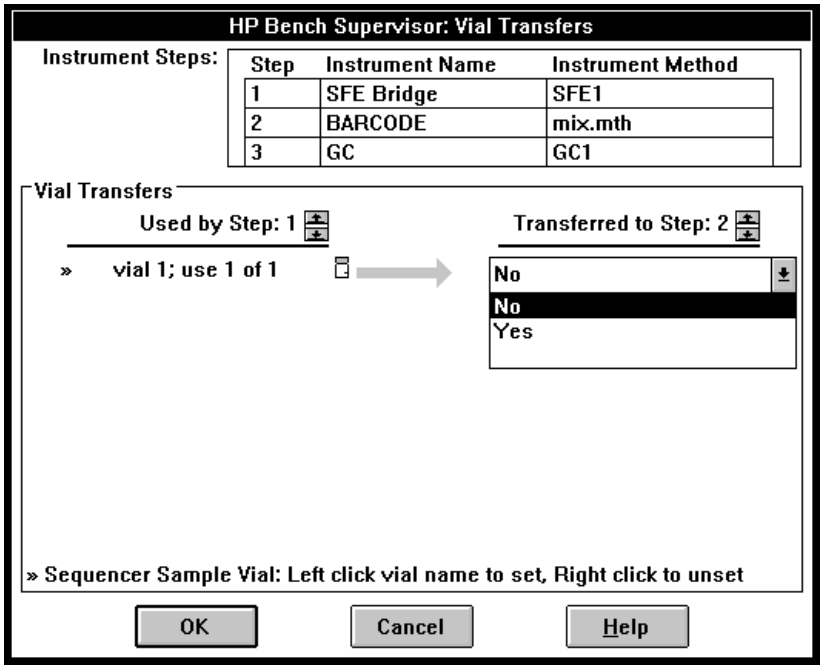


7. Select `OK`. The steps for the bench method are now set. Now you need to tell the Bench Supervisor software where to find the vial to use for each step in the bench method.

Assigning vial transfers

The previous procedure set up a basic three-step bench method with the intention of immediately transferring the fraction output vial as it is produced by the SFE to the mixer, then to the GC for injection. To complete this process, you need to set up a vial transfer between the SFE, bar code reader/mixer and GC, as described in the following procedure:

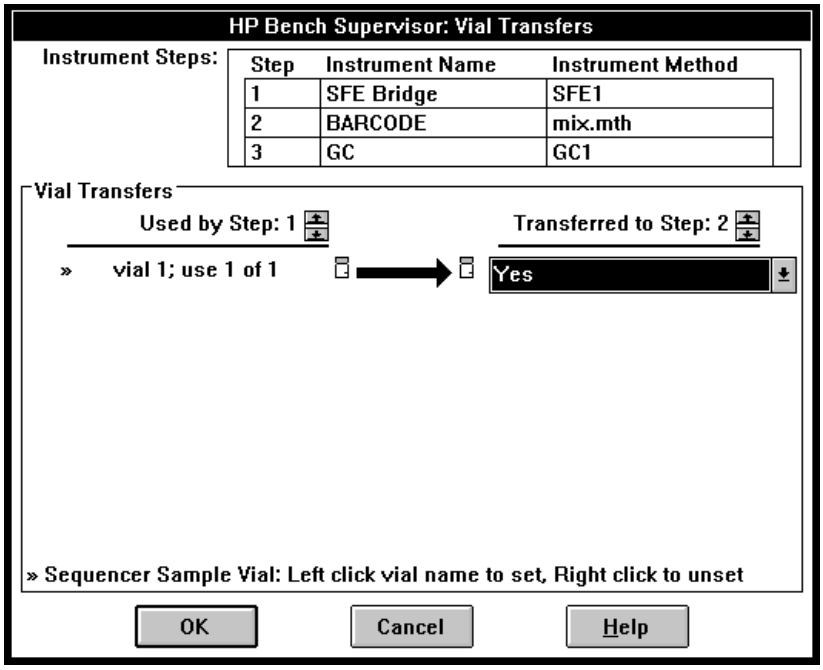
1. If the Vial Transfers dialog box is not open, from the Bench Method menu bar, select the `Edit` menu and then select `Vial Transfers`.



The left side of the dialog box shows the vial output by the SFE in step one. (If the SFE method was set up to produce more fraction output vials, they would also be listed on the left side.) The default name for sample vials is “vial 1; use 1 of 1.” If more than one vial will be used in the method, subsequent vials will have a default name of “vial *n*; use 1 of 1,” where *n* equals the number of the vial.

The right side of the dialog box allows you to specify whether the vial used in step one is to be transferred to the reader/mixer for use in step two.

2. Because we *do* want the fraction output vial from step one to be mixed in step two, we would select `Yes` from the drop down list box on the right side of the dialog box.



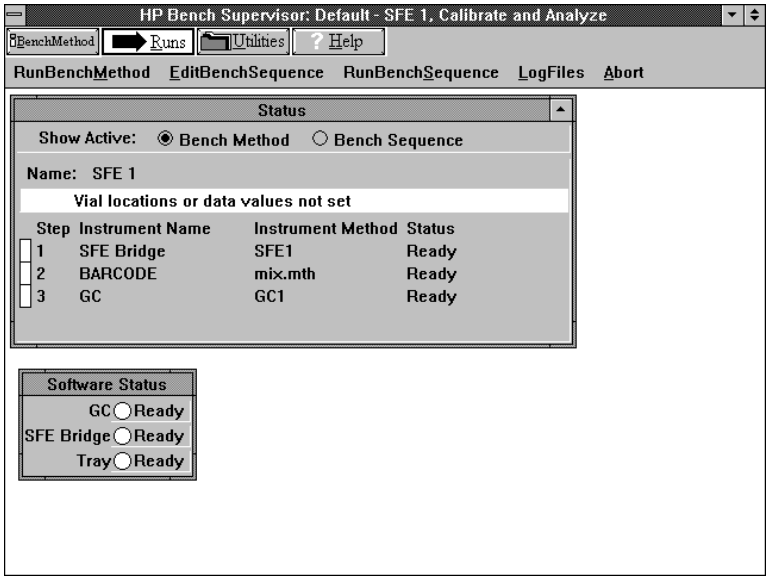
A pair of chevrons (**»**) appears on the Vial Transfers dialog box next to the vial in step one currently designated as the sequencer vial. This is a default designation. Designating a sequencer sample vial in a bench method simplifies data entry on the Sample Queue screen when you want to run the bench method multiple times in a bench sequence. Because we are not concerned with creating a bench sequence at this point, we do not need to worry about the sequencer designation. See the first bench sequence example in this chapter, or your Bench Supervisor documentation, for more information.

3. The next transfer is from the bar code reader/mixer to the GC. Select the “Transferred to Step: (#)” up arrow until it is set to “3”.

4. Select Yes from the drop-down list box to indicate that Bench Supervisor should transfer the vial to the GC after mixing.

NOTE: In the Vial Transfers dialog box, if your bench method contains more than three steps, and the same vial will be used for each of them, when you select “Used by Step: 1” and “Transferred to Step: 3” for vial 1, you will see the “Yes” designation. This does not mean that the vial will be transferred directly from step 1 to step 3, just that Bench Supervisor knows that the same physical vial selected for step one will eventually be in step 3.

5. Select OK. The Status screen will appear within the Bench Supervisor screen, advising you that “Vial locations or data values not set.”

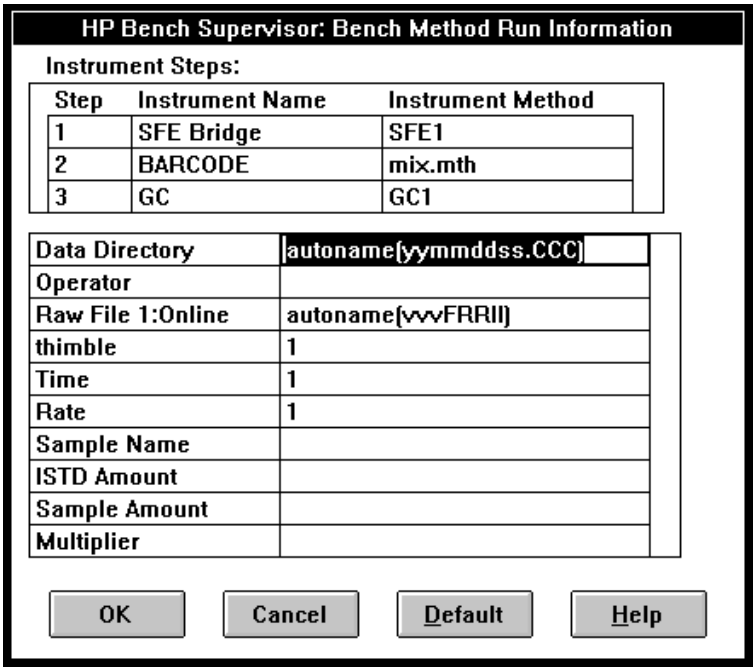


6. Complete the run time data as described on the following page.

Entering run time data information

After you create the bench method and assign vial transfers, as described on the previous pages, enter the run time data for the bench method as follows. Run time data is information required by the instrument software running under the Bench Supervisor software. The information is necessary for the instruments to make their runs.

1. To access the Run Information screen, select the `Runs` button to open up the Runs menu bar. Then, from the `RunBenchMethod` menu, select `Run Info`.



The fields displayed contain information that replaces what would normally be filled out on the ChemStation's Sample Info screen (opened from the `RunControl` menu).

2. Keep the following in mind as you complete each field:

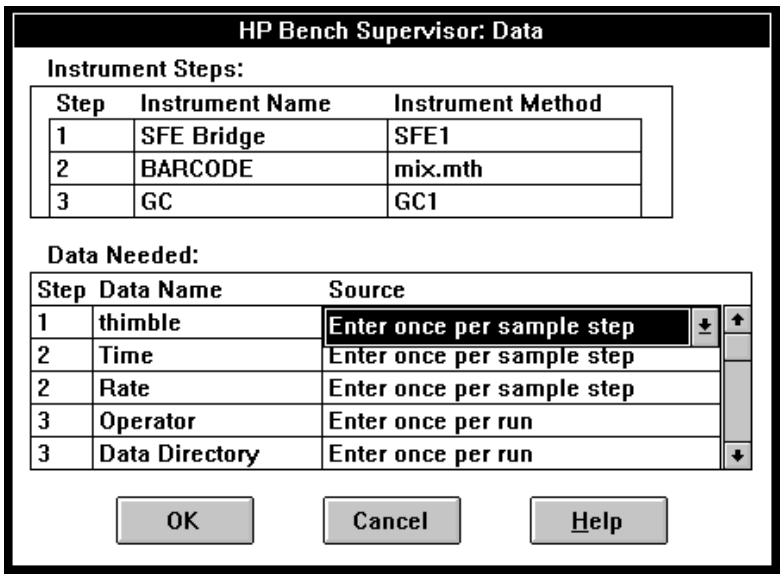
   a. In the Data Directory and Raw File fields, a dialog box opens that allows you to designate an autoname *pattern*. Patterns are a type of code or mask where the number/letter combinations you designate will be replaced at run time with values such as the date, the number of the run, etc. See your Bench Supervisor documentation for more information on patterns.

   b. In the thimble field, you fill in the thimble position in the SFE carousel that contains the appropriate sample.

NOTE: If the thimble designation does not appear in the Run Information dialog box:

   a. Open the Bench Method menu and select Edit, then Data.

   b. Choose “Enter once per sample step” from the Source drop-down list box for the thimble, as shown below. Select OK to close the dialog box.



3. Select `OK` when you are finished with the Run Information dialog box. The Status screen will appear as before, advising you that "Vial locations or data values not set."
4. Set up the tray, as described below, to complete this procedure.

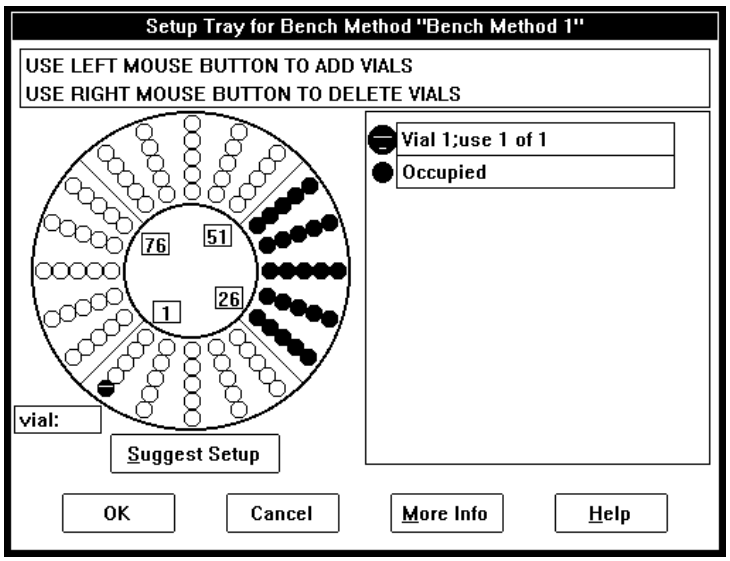
Setting up the tray

The last thing that needs to be done to create this bench method is to put all of the vials in the tray that the method requires. In this case, the method requires only one vial.

1. All of the vials the instrument methods require must start out in the sampler tray on the GC. To be safe, remove all vials from the turrets on the SFE and the AutoInjector tower(s). (You must at least remove vials from positions 1 and 2 in the SFE output turret and position 1 in the AutoInjector, as well as the PrepStation module positions if you have a PrepStation.)

Complete the tray set up for this example as follows:

2. From the Runs menu bar, select `RunBenchMethod` and then `Setup Tray`.

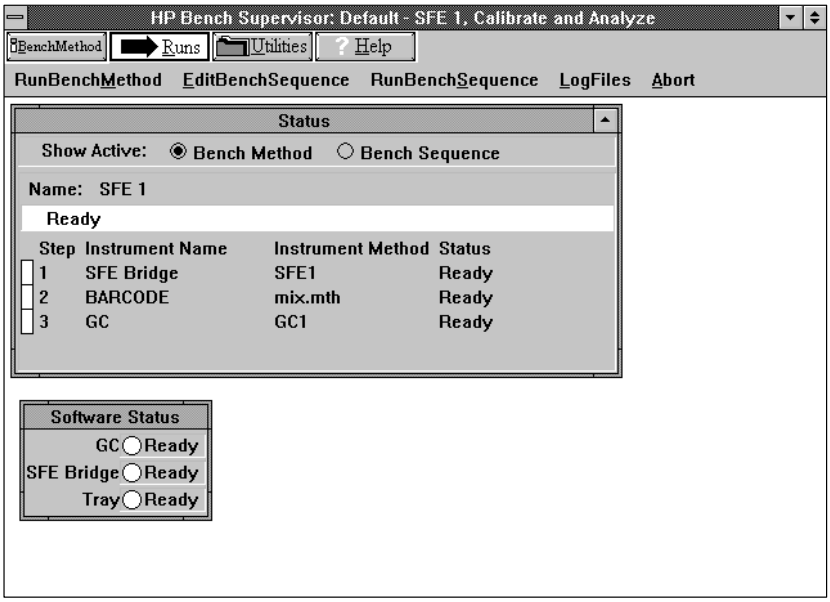


3. Assign the vial for the fraction output to a position in the tray in either one of the following two ways:

   - Use the left mouse button to select the vial's colored circle in the table on the right side of the dialog box and then select the desired position number in the tray.
   - Use the `Suggest Setup` button and let Bench Supervisor assign the vial to a position for you.

   The solid black positions on the Setup Tray screen show vial positions occupied by vials not used in this bench method.

4. Check the sampler tray and verify that the correct vials are in the tray positions you specified, and select `OK`. The Status screen will appear within the Bench Supervisor screen, showing that the method is ready to run.



Running the bench method

After you have set up your method and told the Bench Supervisor software where to find its resources and where to send its output, you can run the bench method.

1. Make sure the thimble and the vial required by the bench method are in their correct positions. Make sure there are no vials in the input turret of the AutoInjector tower(s), positions 1 or 2 of the SFE output turret or the PrepStation module positions, if you have a PrepStation.
2. Make sure you have loaded the correct bench method. Then, select the `Runs` button on the Bench Supervisor screen to open the Runs menu bar.
3. Select `RunBenchMethod` and then `Start`.
4. The Run Info dialog box is opened. Make any necessary changes and select `OK`.
5. The Setup Tray dialog box is opened. Make any necessary changes and select `Start Run`.

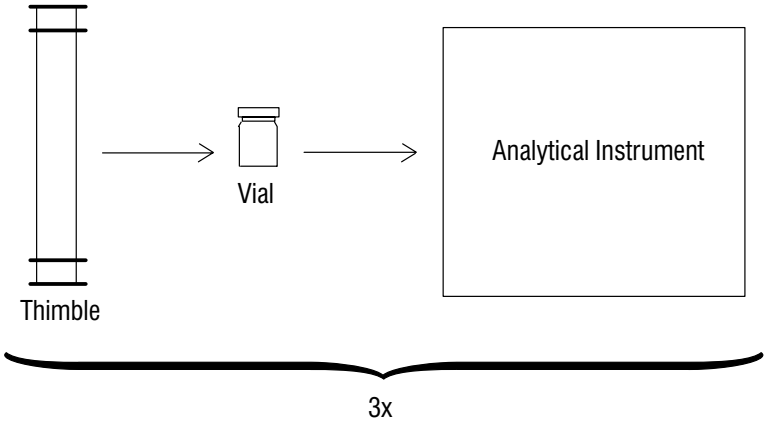
   The Bench Supervisor screen will show the status of the bench method and each instrument method in it. During the run the status will read "Running." After a successful run the status for each instrument will read "Completed."
6. View the status of individual instruments running under Bench Supervisor by selecting the iconized instrument, and using the normal status selection technique for that instrument.

Example 2—Setting up a bench sequence with a single extraction

In the previous example, we created a bench method that would extract a single sample in the SFE and analyze it in the GC. What if you wanted to process five samples? or seven? You could either edit the bench method to process multiple samples, or you could create a *bench sequence*, which is the more reasonable solution.

Bench sequences provide a way to run numerous repetitions of one or more bench methods.

In the original example, we created a bench method to run one repetition of the method *Bench Method 1*. This example shows you how to create a sequence to run this method three times on three different samples.



If you have not read the first example on creating a bench method, do that now. This example assumes you have a familiarity with the steps involved in creating bench methods.

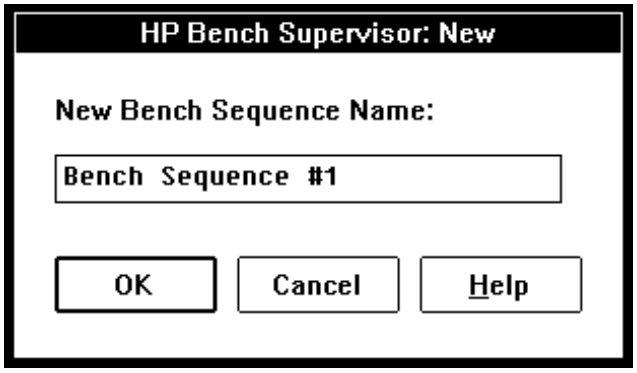
NOTE: All quantitative analysis bench methods **MUST** include a mixing step. For convenience, however, the mixing steps are not included in this example. For information on including the bar code reader/mixer in bench methods, see Example 1 in this chapter.

NOTE: This example is provided to show you the steps necessary to create a bench sequence. It is not necessary to actually complete these steps. The bench method and two instrument methods used to create the bench sequence are not provided in the software. Just follow along with the procedure to get an idea of what is required to set up a bench sequence in Bridge mode.

Creating the bench sequence

1. From the Bench Method menu bar, select `File`, then `Load`, then `Bench Method 1`.
2. Select `Edit` and then `Vial Transfers` to open the Vial Transfers dialog box.

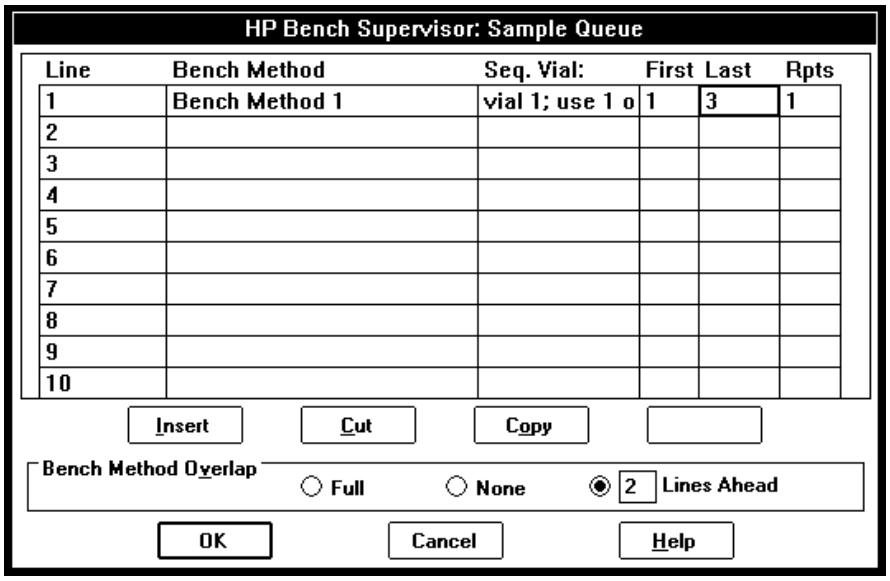
   Verify that the sequencer sample vial is set to `vial 1` in step one. This will allow us to run this bench method multiple times on a range of vials when we create the bench sequence. Select `OK` to proceed. The system will display the Status screen for the bench method.
3. Select the `Runs` button to load the Runs menu bar. Select `Edit Bench Sequence` and then `New`. Name the sequence `Bench Sequence #1`, then select `OK`.



4. From the Runs menu bar, select `Edit Bench Sequence` and then `Sample Queue`.
5. Select `Bench Method 1` from the drop down list for line one. The system automatically enters the method name you selected, the name of the sequencer vial (if any) and the default settings of "1" for the "First," "Last," and "Rpts" columns.

   The "Seq. Vial" (Sequencer Vial) field is set to `vial 1`, as we specified in the Vial Transfers dialog box. The "Rpts" (Repetitions) field identifies the number of times to run the selected bench method on the same vial or range of vials.
6. Leave "First" set to "1," change "Last" to "3," and leave "Rpts" set to "1," then select `OK` .

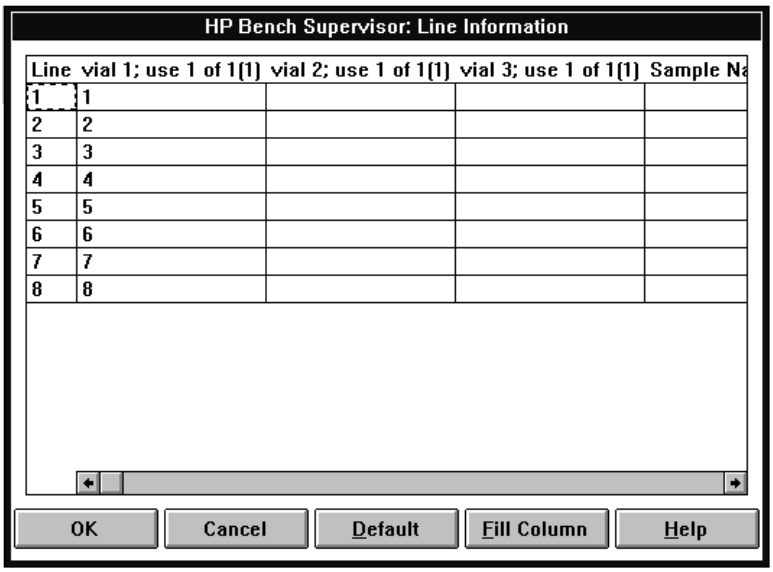
NOTE: When using Bench Supervisor in a Bridge configuration, always leave "Rpts" set to "1".



This tells Bench Supervisor to run `Bench Method 1` first, using the vial in position 1 of the sampler tray, then to run the method two more times using the vials in positions 2 and 3. The First and Last numbers can be any position number in the 100 vial tray.

After selecting OK to close the Sample Queue dialog box, the Line Information dialog box is opened.

The Line Information dialog box determines which thimbles extract and rinse into which vials. The types of fields appearing on the Line Information dialog box may be different for different sequences, depending on the instruments and resources used in the bench methods within the sequence. If a horizontal scroll bar appears, use it to view the additional information in the table.

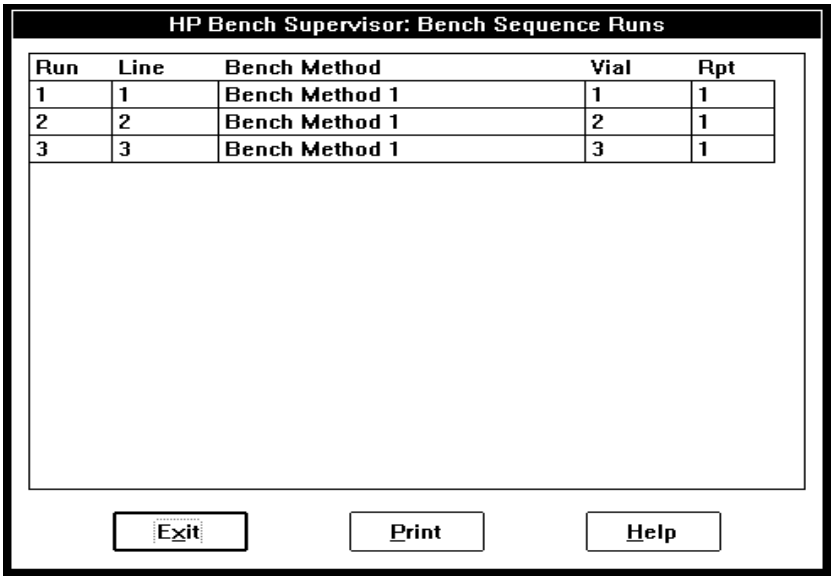


7. Enter the Sample Name and which SFE thimble position to use for each line in the sequence. This designation tells Bench Supervisor which thimble will extract into which vial. In this example, the thimbles in position 1, 2 and 3 will extract and rinse into vials 1, 2 and 3, respectively.

   Select OK to proceed.

8. From the Runs menu bar, select `Edit Bench Sequence` and then `Show All Runs`.

   Notice that we could have created a bench method that would have produced the same results as those in this sequence. The bench sequence, however, provides greater flexibility because just by changing the “First”, “Last” or “Rpts” fields on the Sample Queue dialog box we can extract varying numbers of samples.



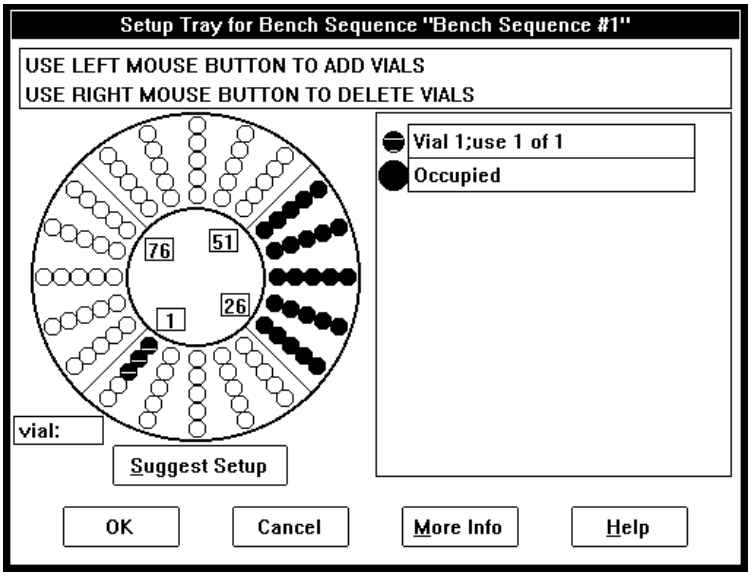
9. Select `EXIT` to return to the Status screen.

Setting up the tray

1. From the Runs menu bar, select `Run Bench Sequence` and then `Setup Tray`. This shows the input vial locations as defined on the Sample Queue screen in step six of the *Creating the bench sequence* portion of this example.

Had there been more than one vial in the bench method example, each would have been listed separately here (with a different color code). In this example, the bench method contains only one vial which will be run three times, so the three vials are not listed separately because each sample is considered to be of the same type.

The solid black vial positions on the Setup Tray screen show vial positions occupied by vials not used in this bench sequence.



2. If you were actually going to run this sequence, at this point you would place empty vials in the positions indicated in the Setup Tray screen and select `OK` to continue.

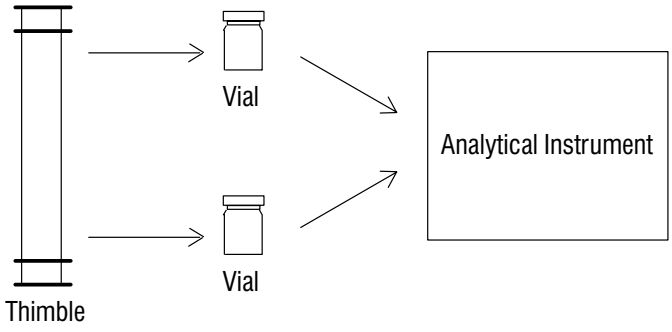
Running the bench sequence

1. To run the bench sequence, you would open the Runs menu bar, select `Run Bench Sequence` and then `Start`. The system will display the Bench Sequence Info Screen. Make any necessary changes and select `OK`.

2. The system will then display the Setup Tray for Bench Sequence screen. Make any necessary changes and select `Start Run`.
3. To view the status of the bench sequence, open the Bench Sequence menu and select `Show Active: Bench Sequence.` The Bench Supervisor screen will display the status of each method and the equipment it uses throughout the run.

Example 3—Setting up a bench sequence with multiple extractions

In the previous example, we created a bench sequence that would extract a single sample in the SFE and analyze it in the GC. This process was repeated three times. What if each run of your SFE method performed more than one extraction, to produce multiple samples? This example shows you how to set up a bench method and bench sequence that contain an SFE method which produces two sample vials.



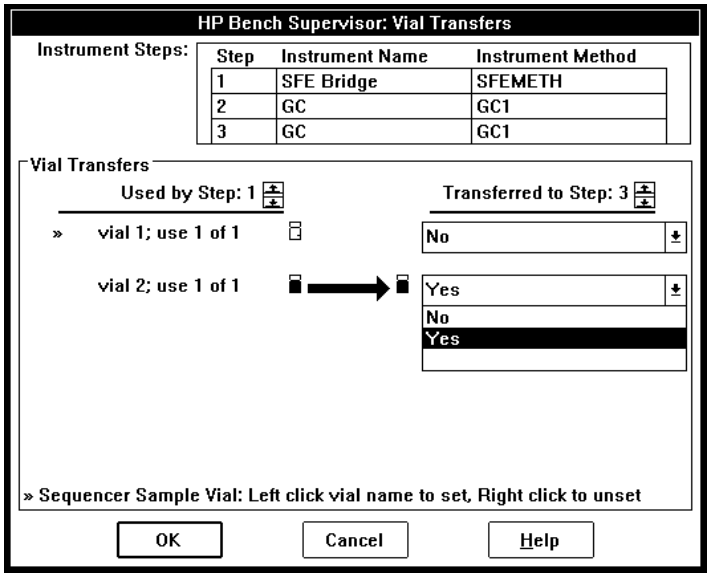
If you have not read the first example on creating a bench method, do that now. This example assumes you have a familiarity with the steps involved in creating bench methods.

NOTE: All quantitative analysis bench methods **MUST** include a mixing step. For convenience, however, the mixing steps are not included in this example. For information on including the bar code reader/mixer in bench methods, see Example 1 in this chapter.

NOTE: This example is provided to show you the steps necessary to create a bench sequence with multiple SFE extractions. It is not necessary to actually complete these steps. The bench method and two instrument methods used to create the bench sequence are not provided in the software. Just follow along with the procedure to get an idea of what is required to set up a bench sequence involving multiple sample vials.

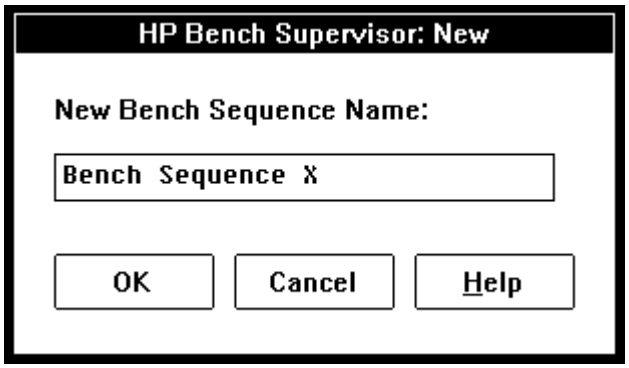
1. From the Bench Method menu bar, select `File`, then `New`.
2. Name the new method `Bench Method Y`.
3. Select `Edit` and then `Instrument Steps`. Enter the following information to set up the three-step bench method:
    a. For *step 1*, select `SFE Bridge` as the Instrument Name and `SFEMETH` as the Instrument Method. `SFEMETH` is a hypothetical method that performs two extractions, with one rinse to a vial per extraction, thus producing two sample vials during each run. See your SFE documentation for more details on how to set up this type of method.
    b. For *step 2* and *step 3*, select `GC` as the Instrument Name, and `GC1` as the Instrument Method. You could list a different method in step 3 if you did not want to analyze both vials with the same method. Note that for each vial to be analyzed there must be a corresponding analysis method in the Instrument Steps dialog box. If you did not wish to analyze the contents of the second vial, you would omit creating a third step.
4. Select `Edit` and then `Vial Transfers` to open the Vial Transfers dialog box, if it is not already open.
5. Select `Yes` to transfer vial 1 to *step 2*.

6. If you wish to analyze the contents of the second vial, select the "`Transferred to Step:` (#)" up arrow to change the designated step to *3*, then select `Yes` to transfer vial 2 to *step 3*, as shown below.



Verify that the sequencer sample vial is set to `vial 1` in step one. This will allow us to run this bench method multiple times on a range of vials when we create the bench sequence. Select `OK` to proceed. The system will display the Status screen for the bench method.

7. Select the Runs button to load the Runs menu bar. Select Edit Bench Sequence and then New. Name the sequence Bench Sequence X, then select OK.



8. From the Runs menu bar, select Edit Bench Sequence and then Sample Queue.
9. Select Bench Method Y from the drop down list for line one. The system automatically enters the method name you selected, the name of the sequencer vial (if any) and the default settings of "1" for the "First," "Last," and "Rpts" columns.

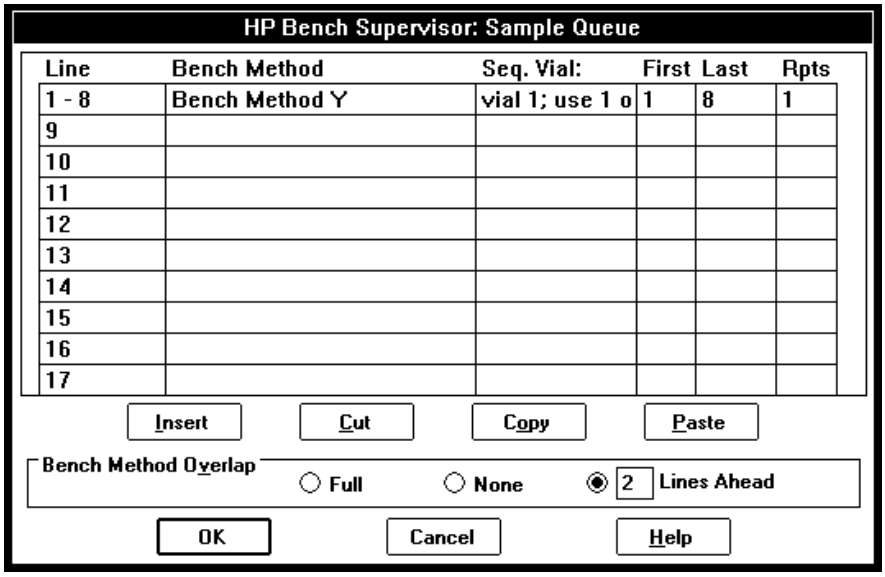
   The "Seq. Vial" (Sequencer Vial) field is set to vial 1, as we specified in the Vial Transfers dialog box.

   The "Rpts" (Repetitions) field identifies the number of times to run the selected bench method on the same vial or range of vials.

10. Leave “First” set to “1,” change “Last” to “8,” and leave “Rpts” set to “1,” then select OK.

NOTE: When using Bench Supervisor in a Bridge configuration, always leave “Rpts” set to “1”.

NOTE: The “First” and “Last” columns indicate the sampler tray locations into which *Vial 1* (the sequencer vial) samples only will be placed. You will designate tray locations for the *Vial 2* samples on the Line Information screen, as described on the following page.

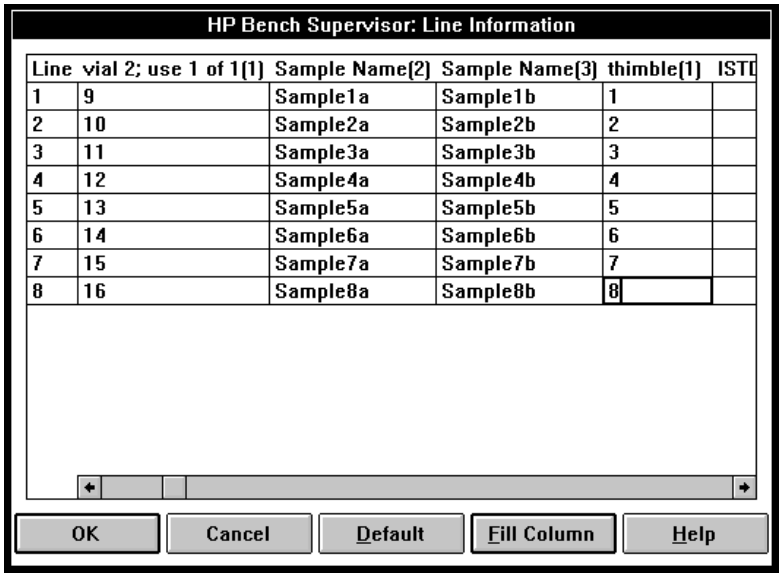


These settings tell Bench Supervisor to run Bench Method Y first, using the vial in position 1 of the sampler tray, then to run the method seven more times using the vials in positions 2 thru 8. The First and Last numbers can be any position number in the 100 vial tray.

After selecting OK to close the Sample Queue dialog box, the Line Information dialog box is opened.

The Line Information dialog box determines which thimbles extract and rinse into which vials. The types of fields appearing on the Line Information dialog box may be different for different sequences, depending on the instruments and resources used in the bench methods within the sequence. If a horizontal scroll bar appears, use it to view additional information on the table.

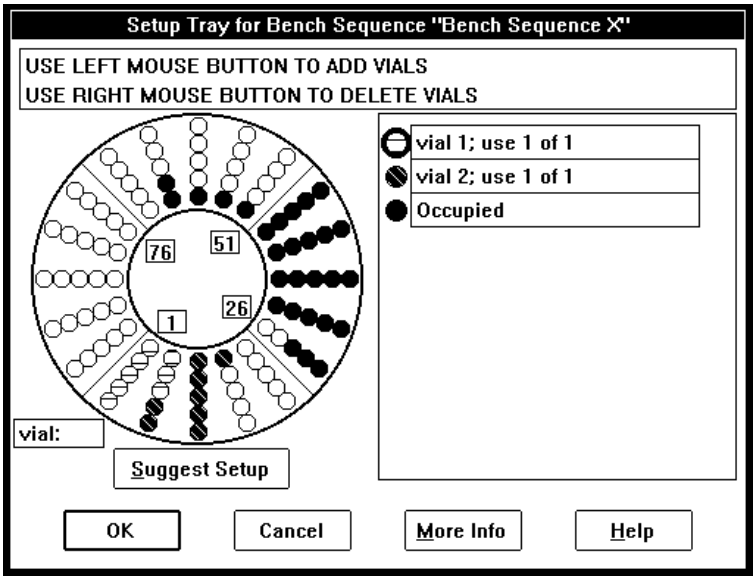
11. Enter the tray locations for the vial 2 samples (locations 9 through 16, as shown below.)



12. Enter the Sample Names and which SFE thimble position to use for each line in the sequence. Since the SFE method produces two vials per run, there are two columns for naming the samples. Select OK to proceed.

13. From the Runs menu bar, select `Edit Bench Sequence` and then `Show All Runs` to view the information for each run in the sequence.
14. Select `Exit` to return to the Status screen.
15. From the Runs menu bar, select `Run Bench Sequence` and then `Setup Tray`. This shows the input vial locations as defined on the Sample Queue screen in step 10 of this example.

    Since there was more than one vial in the bench method example, each is listed separately here (with a different color code). In this example, the bench sequence runs the bench method eight times, producing two vials with each run. The sixteen vials are not listed separately in the column on the right because there are only two sample types.

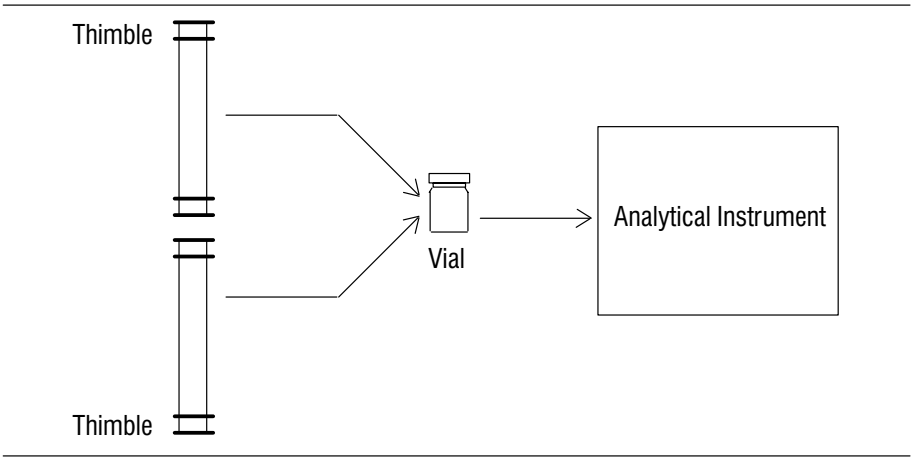


The solid black vial positions on the Setup Tray screen show vial positions occupied by vials not used in this bench sequence.

16. If you were actually going to run this sequence, at this point you would place empty vials in the positions indicated in the Setup Tray screen and select `OK` to continue.
17. To run the bench sequence, you would open the Runs menu bar, select `Run Bench Sequence` and then `Start`. The system will display the Bench Sequence Info Screen. Make any necessary changes and select `OK`.
18. The system will then display the Setup Tray for Bench Sequence screen. Make any necessary changes and select `Start Run`.
19. The Bench Supervisor screen will display the status of each instrument in use and the method it is running.

Example 4—Setting up a bench sequence with multiple extractions into a single vial

In the previous example, we created a bench sequence that would extract multiple samples. This example shows you how to set up a bench method and bench sequence which extract analytes from two thimbles, and combine them into a single vial for analysis.



If you have not read the first example on creating a bench method, do that now. This example assumes you have a familiarity with the steps involved in creating bench methods.

NOTE: This example is provided to show you the steps necessary to create a bench sequence with multiple SFE extractions into a single vial. It is not necessary to actually complete these steps. The bench method and instrument methods used to create the bench sequence are not provided in the software. Just follow along with the procedure to get an idea of what is required to set up a bench sequence that combines multiple extracts into a single vial.

1. In your SFE software, create two SFE methods, as follows:

   a. The first method should have no rinse between thimbles. Name the method `SFE_NO_R`.

   b. The second method should have a rinse step between thimbles. Name the method `SFE_RINS`.

   Consult your SFE documentation if you need additional information to create these methods.

2. In Bench Supervisor, from the Bench Method menu bar, select `File`, then `New`.

3. Name the new method `Bench Method B`.

NOTE: All quantitative analysis bench methods **MUST** contain a mixing step. If you *do not* have a PrepStation, include this step in the Instrument Steps dialog box, as shown in step 4c. If you *do* have a PrepStation, consult your PrepStation documentation for information on vial mixing.

4. Select `Edit` and then `Instrument Steps`. Enter the following information to set up the bench method:

   a. For *step 1*, select `SFE Bridge` for the Instrument Name and `SFE_NO_R` for the Instrument Method.

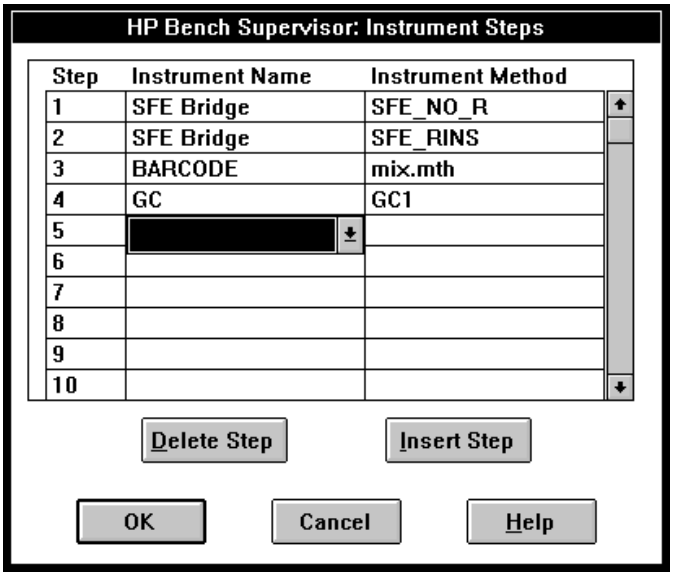
   b. For *step 2*, select `SFE Bridge` for the instrument, and `SFE_RINS` for the method.

   c. For *step 3*, select `BARCODE` as the instrument and type `mix.mth` for the third step in the bench method.

d. For *step 4*, select `GC` as the instrument, and `GC1` for the instrument method.

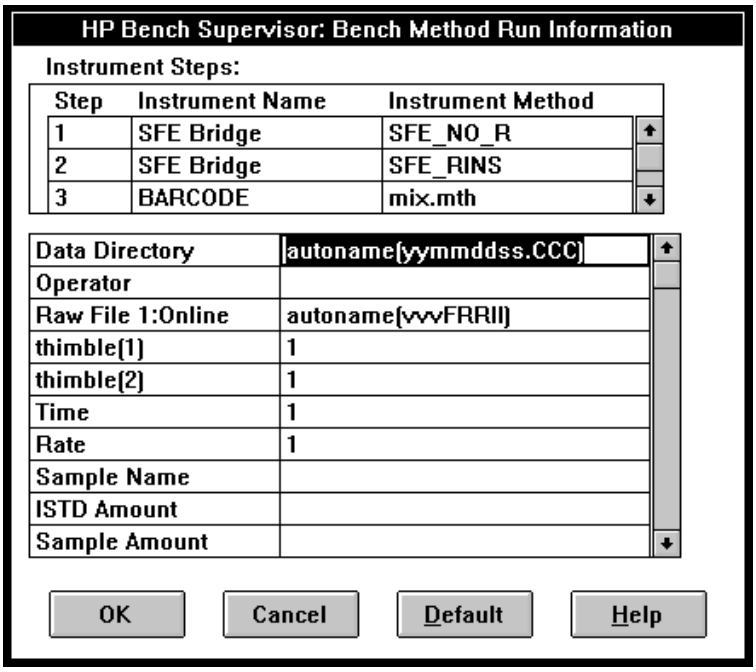
NOTE: If you also want to use the bar code reader/mixer to read a bar code, select `BARCODE` as the Instrument Name and type `barcode.mth` for the Instrument Method.

After completing these steps, the Instrument Steps dialog box should appear similar to the one below.



5. Select `Edit` and then `Vial Transfers` to open the Vial Transfers dialog box, if it is not already open.
6. Select `Yes` to transfer vial 1 to *step 3*.
7. Also select `Yes` to transfer vial 1 to step 4, to tell Bench Supervisor to transfer the vial to the GC after mixing. Select `OK` to proceed. The system will display the Status screen for the bench method.

7. Access the Run Information dialog box by selecting the `Runs` button to open up the Runs menu bar. Then, from the `RunBenchMethod` menu, select `Run Info`.



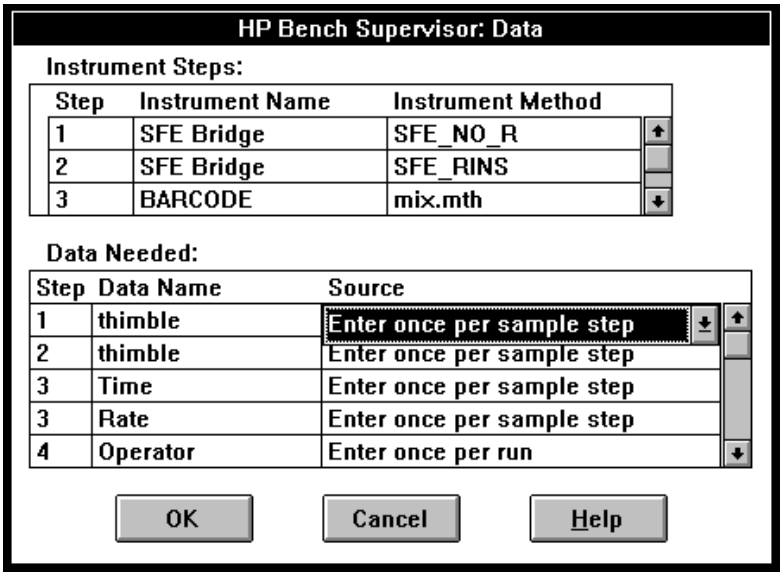
The fields displayed contain information that replaces what would normally be filled out on the ChemStation's Sample Info screen (opened from the `RunControl` menu).

8. In the thimble field, fill in the thimble position in the SFE carousel that contains the appropriate sample. The number immediately following the word `thimble` indicates the bench method step associated with that thimble. For example, the thimble with `(1)` following it is the one that the `SFE_NO_R` method uses in step 1 of the bench method.

NOTE: If the thimble designation does not appear in the Run Information dialog box:

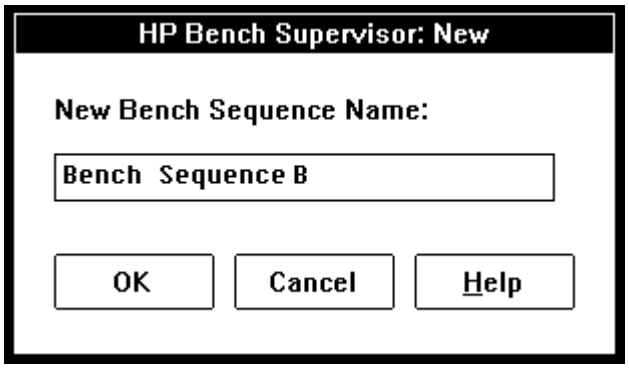
a. Open the Bench Method menu and select Edit, then Data.

b. Choose "Enter once per sample step" from the Source drop-down list box for the thimble, as shown below. Select OK to close the dialog box.



9. Select OK when you are finished with the Run Information dialog box. The Status screen will appear as before, advising you that "Vial locations or data values not set."

10. Select the Runs button to load the Runs menu bar. Select Edit Bench Sequence and then New. Name the sequence Bench Sequence B, then select OK.



11. From the Runs menu bar, select Edit Bench Sequence and then Sample Queue.
12. Select Bench Method B from the drop down list for line one. The system automatically enters the method name you selected, the name of the sequencer vial (if any) and the default settings of "1" for the "First," "Last," and "Rpts" columns.

    The "Seq. Vial" (Sequencer Vial) field is set to vial 1, as we specified in the Vial Transfers dialog box.

    The "Rpts" (Repetitions) field identifies the number of times to run the selected bench method on the same vial or range of vials.

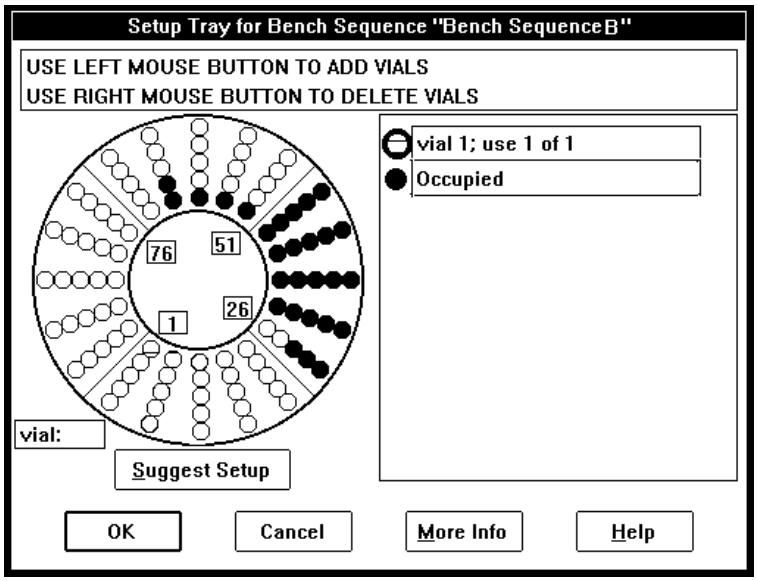
    These settings tell Bench Supervisor to run Bench Method B first, using the vial in position 1 of the sampler tray. The First and Last numbers can be any position number in the 100-vial tray.

    After selecting OK to close the Sample Queue dialog box, the Line Information dialog box is opened.

The types of fields appearing on the Line Info dialog box may be different for different sequences, depending on the instruments and resources used in the bench methods within the sequence. If a horizontal scroll bar appears, use it to view additional information on the table.

13. Enter the Sample Names and which SFE thimble positions to use for each line in the sequence. Select `OK` to proceed.
14. From the Runs menu bar, select `Edit Bench Sequence` and then `Show All Runs` to view the information for the sequence.
15. Select `Exit` to return to the Status screen.
16. From the Runs menu bar, select `Run Bench Sequence` and then `Setup Tray`. This shows the input vial locations as defined on the Sample Queue screen in step 12 of this example.

    In this example, the bench sequence runs the bench method one time, producing one vial.



The solid black vial positions on the Setup Tray screen show vial positions occupied by vials not used in this bench sequence.

17. If you were actually going to run this sequence, at this point you would place empty vials in the positions indicated in the Setup Tray screen and select `OK` to continue.
18. To run the bench sequence, you would open the Runs menu bar, select `Run Bench Sequence` and then `Start`. The system will display the Bench Sequence Info Screen. Make any necessary changes and select `OK`.
19. The system will then display the Setup Tray for Bench Sequence screen. Make any necessary changes and select `Start Run`.
20. The Bench Supervisor screen will display the status of each instrument in use and the method it is running.

Example 5—Calibration using the Bridge

The scenario

For this example, assume you have an SFE method, `SFE Extract and Analyze`, that outputs eight vials to be analyzed at the end of its run, and you want to perform a calibration using these vials with a run of the GC method, `BRIDGE`, which contains a three-level calibration table.

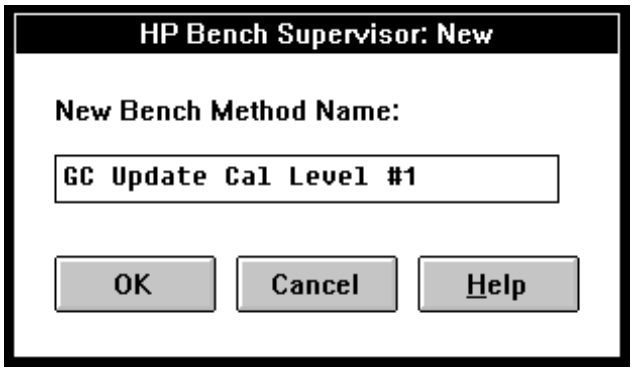
NOTE: This example assumes you are familiar with the steps necessary to create basic bench methods and sequences. If you are not, read the other examples in this chapter before proceeding.

***NOTE*:** This example is provided to show you the steps necessary to set up calibrations using the Bridge. It is not necessary to actually complete the steps shown. The instrument methods used to create the bench methods in this procedure are not provided in the software. Just follow along with the procedure to get an idea of what is required to set up a calibration in Bridge mode.

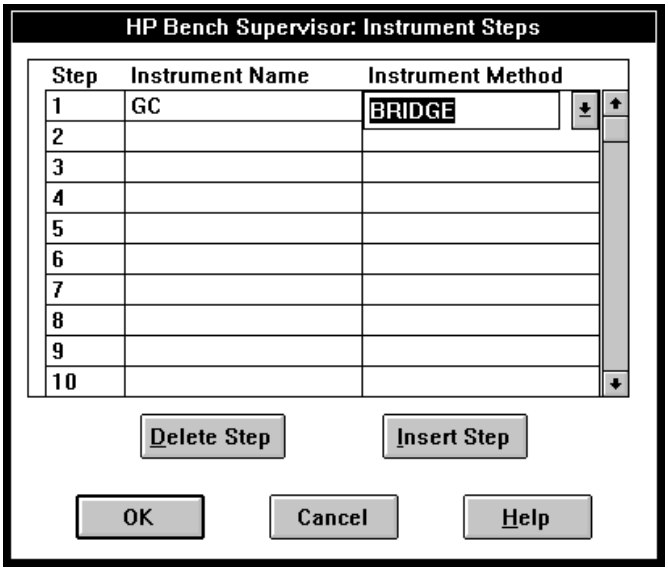
Creating the bench methods

The following procedure describes how you would go about setting up the bench methods needed to perform the calibration described above. You will need to create four bench methods—one to update each level of the calibration table and one to perform the extraction, mixing and analysis.

1. In Bench Supervisor, open the `File` menu and select `New Bench Method`. Name the method `GC Update Cal Level #1,` as shown on the following page. This naming convention will make it easier to determine which vial location in the tray is associated with which calibration standard.

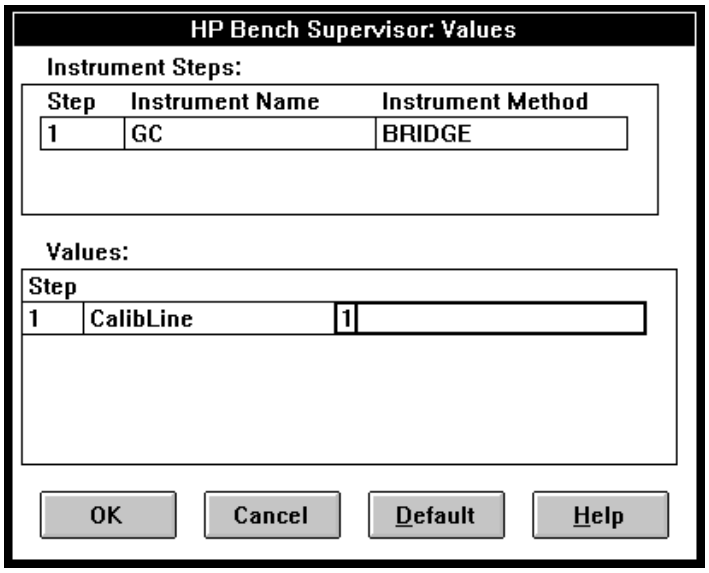


2. From the EDIT menu select `Instrument Steps`. Select `GC` as the Instrument Name and `BRIDGE` as the Instrument Method.



3. From the Bench Method menu, select `Edit`, then `Values`. The Values dialog box will appear.

4. Type “1” in the CalibLine box, as shown below. This value determines which level of the calibration table an instrument line will update. In this case, the method contains only one instrument line, which will update level 1 of the calibration table.



5. Create identical bench methods for the remaining two levels in the calibration table. Name the second method `GC Update Cal Level #2`, and set the CalibLine to 2. Name the third method `GC Update Cal Level #3` and set the CalibLine to 3. The CalibLine number of each method must match the level of the calibration table that the method will update.

6. Now create a bench method that will extract a sample, then mix and analyze the extract. Name the method `SFE Extract and Analyze`.

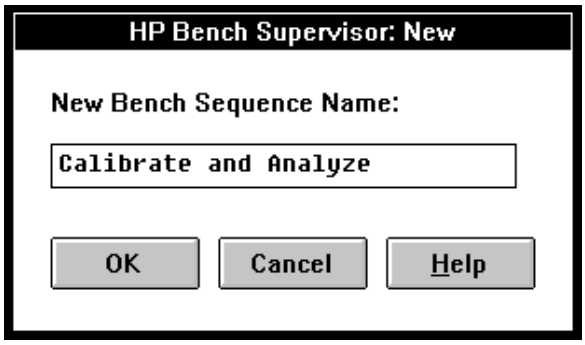
   Leave the CalibLine of this method at the default setting of “0”.

   See *Example 1—Setting up a bench method*, earlier in this chapter, for an example of this type of bench method.

Creating the bench sequence

After creating the bench methods, you need to create a bench sequence that incorporates the three calibration methods, then extracts and analyzes additional samples and produces a quantitative report.

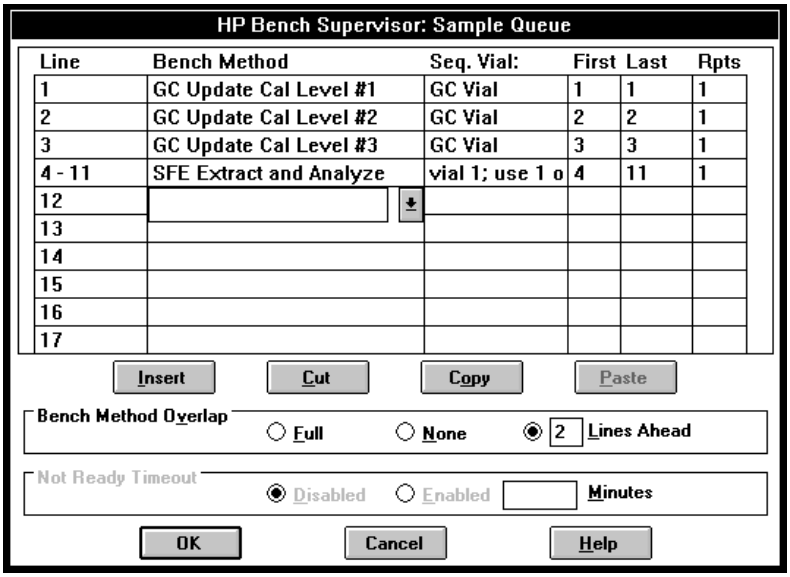
1. From the Bench Sequence menu, create a new bench sequence and name it `Calibrate and Analyze`.



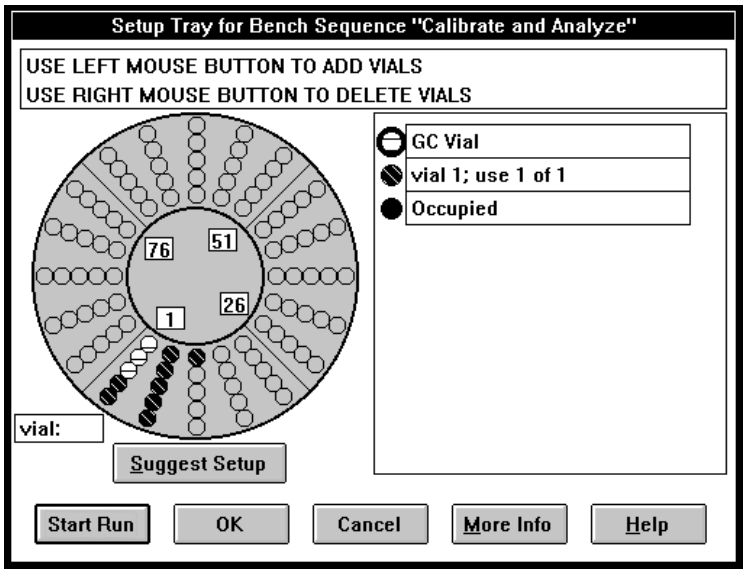
2. In the Sample Queue dialog box for the sequence, list the methods you created earlier in numerical order.
3. In the First/Last columns, designate the vial location of each of the calibration solutions.

NOTE: Verify that each vial location in the Sample Queue dialog box corresponds to the appropriate sample vial and calibration level, to ensure accurate calibration.

4. Add the SFE `Extract and Analyze` Bench Method to the sample queue and close the dialog box, which should appear similar to the one shown below.



5. From the Runs menu bar, select Run Bench Sequence and then Setup Tray. This shows the input vial locations, as defined on the Sample Queue screen.



6

SFE/MS Bridge Installation

SFE/MS Bridge Installation

This chapter provides you with the information necessary to properly install the hardware and software that enables your system to operate in a Bridge configuration.

After you have completed these installation and configuration procedures, you will be ready to control your SFE and GC/MS modules through Bench Supervisor, and to pass vials automatically between them.

Parts

See the contents list in this kit for the parts.

Hardware and software specifications

You will need the following hardware and software in addition to your SFE/MS Bridge accessory kit:

- HP 6890 GC and Automatic Liquid Sampler, or HP 5890/II GC with HP 7673 Automatic Liquid Sampler and Injector (only 18596B tray module and 18594B controller module with serial number 3138A26712 or greater supported; see your local HP service representative for an EPROM upgrade.)
- HP 5971 or 5972 MSD
- HP G1291A or G1292A PrepStation module, if installing one
- HP 1926A Bar Code Reader/Mixer
- HP 7680T SFE
- DOS-based computer capable of running the MS ChemStation software (Recommended minimum configuration: 486 IBM-compatible computer with 8 MB RAM, 80 MB hard drive with DOS 6 or higher and Windows™ 3.1 or higher.)

- Correct version of the HP G1034C MS ChemStation software, for HP 5890 Series II GC. If operating a 6890 GC, ensure that you have the correct product number and version of the ChemStation software.
- Latest version of HP G1225C SFE software (included with Bridge kit)

See the installation instructions in this chapter before installing or attempting to run the Bridge.

This hardware will typically occupy the maximum bench space of:

193 cm W $\times$ 61 cm D $\times$ 93 cm H.

Running in a Bridge configuration will add slightly to the height of the GC and MS, due to the spacer pad, but will not otherwise effect the dimensions of your bench setup. The height of the set up will be slightly less if your configuration does not include a PrepStation.

The bench should be capable of supporting a minimum of 160 Kg (the weight of the system) with no noticeable deflection or vibration.

Before you begin

Perform the steps below before installing any software or hardware for the Bridge configuration.

Caution

Vent the MSD before disconnecting or moving it per the instructions in your *MSD Manual Set*. Failure to do so may damage the MSD.

NOTE: If you are using Windows EMM386 Memory Manager, you must modify the device line in the `config.sys` file to include the underlined information in the line below, in order for the HP-IB board to work properly:

`DEVICE=C:\WINDOWS (or DOS)\EMM386.EXE . . . X=DC00-DFFF`

Use a text editor, such as the DOS Edit command or Windows NotePad to make the modification.

1. Determine which HP-IB addresses are currently in use on your system and be sure to select available addresses for the instruments you are installing. System communication errors will result if you assign more than one instrument to an HP-IB address. Refer to the manual set for each instrument for information on how to read and select the appropriate HP-IB addresses. Also, use the information in the `DEVICE` lines in the PCS section of your `win.ini` file to record the instrument addresses for previously installed instruments where:

   `DEVICEN=X,ADDRESS,DEVICE NAME`

NOTE: The ChemStation software will not accept HP-IB addresses greater than 29.

2. Perform any of the following that apply before installing the software:
   - Back up any methods you wish to keep.
   - Back up the `sfe1`, `sfe2` (if you have one) and `hpchem` directories. Once backed up, delete the `sfe1`, `sfe2` and `hpchem` directories from the hard drive.
   - Back up and modify the `autoexec.bat` file with the following changes, using a text editor, such as the DOS Edit command or Windows NotePad;
     a. Remove `c:\hpchem` from the path line.
     b. Remove the TEMP directory designation line.
   - Back up the `win.ini` file, then delete all PCS sections from it, again using a text editor. The PCS sections contain the line [PCS] as their first line. There may be numbers after the [PCS] in some PCS sections. Delete these numbered sections as well.
   - Select the ChemStation program group icon, then press <Delete> on the keyboard. Confirm the deletion by pressing <Enter>. Repeat this process for all ChemStation group icons.
3. Reboot the computer to allow the current path designations to take effect.

4. Prior to installing any software, be sure that the following items are **NOT** present in the computer system:
   - `c:\hpchem` directory and its subdirectories
   - `c:\hpchem` in the path and in the TEMP directory designation, as seen in the `autoexec.bat` file
   - PCS sections in the `win.ini` file
   - Windows program groups for any previously installed ChemStation applications

Hardware installation

Follow the procedures below to set up your Supercritical Fluid Extractor, Mass Selective Detector and Gas Chromatograph in a Bridge configuration.

WARNING Have an assistant available to help you with the following installation procedures. The SFE and the GC are heavy. Moving either device is a two-person job!

Disconnecting the GC and MS

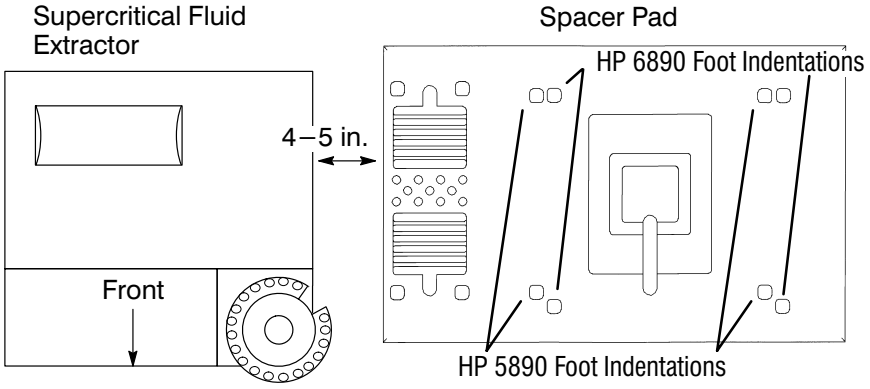
WARNING See your HP 5971 or 5972 *MSD Hardware Manual* for information on this procedure, to protect the MS and column. Be sure you disconnect the MS and GC instruments before moving either of them.

Setting up the MS

This procedure sets up the MS and the Bridge spacer pad, in preparation for the placement of the GC.

1. Place the Bridge spacer pad on the right side of the SFE in the orientation shown below.

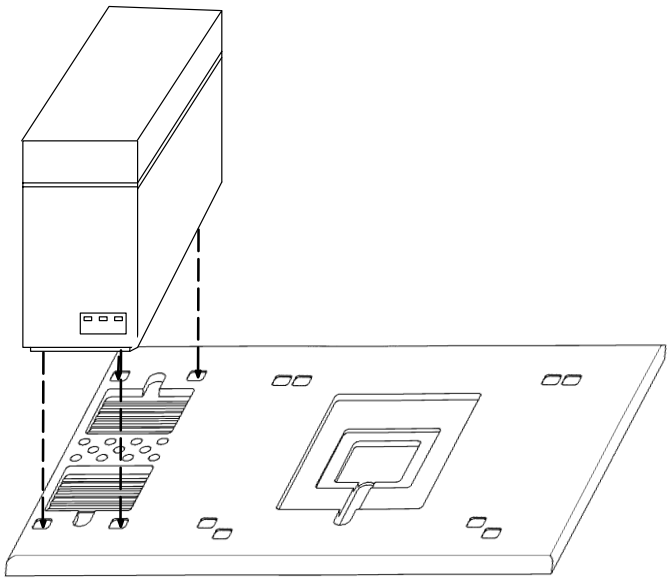
Overhead View



2. Remove the protective paper tape from the adhesive on the back of four of the metal shims and place a shim in each one of the MS foot indentations on the Bridge spacer pad. To begin with, place at least one metal shim in each foot indentation. You may need to place more, depending on your particular hardware.

3. Place the MS on the metal shims in the indentations closest to the SFE, as shown below.

Placing MS on spacer pad

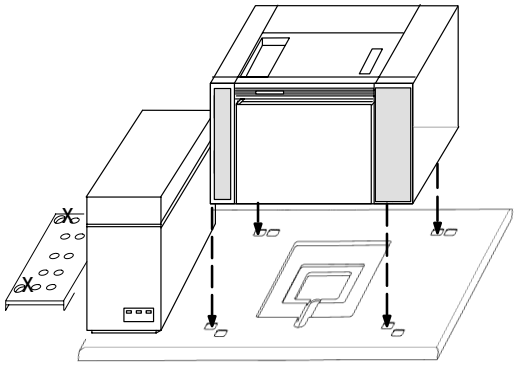


Setting up the GC

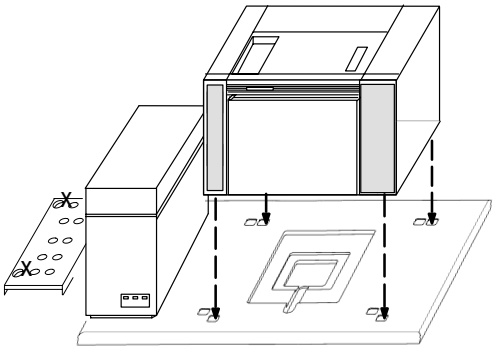
This procedure sets up the GC in close proximity to your SFE in preparation for the final alignment of the two instruments and for the GC's reconnection to the MS.

1. Remove the protective paper tape from the adhesive on the back of four of the metal shims and place a shim in each one of the GC foot indentations on the Bridge spacer pad. To begin with, place at least one metal shim in each foot indentation. You may need to place more, depending on your particular hardware.
2. With your assistant, lift and place the GC on the pad so that the GC's feet rest on the metal shims in the foot indentations.

Placing 5890 GC on spacer pad



Placing 6890 GC on spacer pad



3. Reconnect the GC and MS according to your MS User's Guide.

4. Install the automatic liquid sampler hardware (bracket, tray, injector(s) and bar code reader/mixer) if you have not already done so. If you have one, install the HP G1291A or G1292A PrepStation on the bracket, as described in the PrepStation documentation. The legs for the PrepStation should be positioned just to the right of the leg locator slots on the PrepStation spacer pad, as indicated by Xs on the illustration on the previous page.

Software installation

After setting up the hardware, install and configure the software necessary to run the SFE/MS Bridge. Follow the steps below to install the software properly.

NOTE: The software must be installed in the correct order. Installing the software out of order will prevent the Bridge configuration from operating properly. Locate your ChemStation, PrepStation, Tray and SFE floppy disks to perform this installation.

1. Install and configure the MS ChemStation Analyzer software according to the instructions in your ChemStation documentation and verify that the MS/GC is operating normally. Ensure that the ChemStation has added `c:\hpchem` to your `autoexec.bat` file. If it has not, add it using a text editor.
2. Exit Windows and reboot your computer to allow the change to the path designation to take effect, then re-enter Windows.
3. If your software does not create program and group icons for your ChemStation, follow the instructions in your ChemStation manual for creating a new program group under Windows, and for creating new items in that group for ChemStation and Configuration Editor.
4. Verify that the ChemStation is operating correctly.
5. Close the MS ChemStation software before continuing with the installation.

6. Exit and reenter Windows before proceeding with the installation, to avoid causing an APG_VGA.FON error.
7. After exiting and restarting Windows, install the SFE software according to the instructions in your SFE documentation and verify that the SFE is operating normally.
8. Close the SFE software before continuing with the installation.

NOTE: When using the Configuration Editor to configure instruments, be aware of the following restrictions:

- You can only configure up to four instruments using the Configuration Editor.
- Do not use the Configuration Editor to add a second non-Bridge SFE.
- You will be unable to change modifier pump settings with the Configuration Editor due to the file structure of methods that incorporate the pump. To change modifier pump settings, you will need to reinstall the SFE software and change the Modifier Pump as needed. Note that SFE methods for a configuration with no modifier pump are unusable under a configuration that includes a modifier pump, and vice versa.
- Do not use the Configuration Editor to change from a single-channel modifier pump to a quaternary pump; reinstall the SFE software to do this.

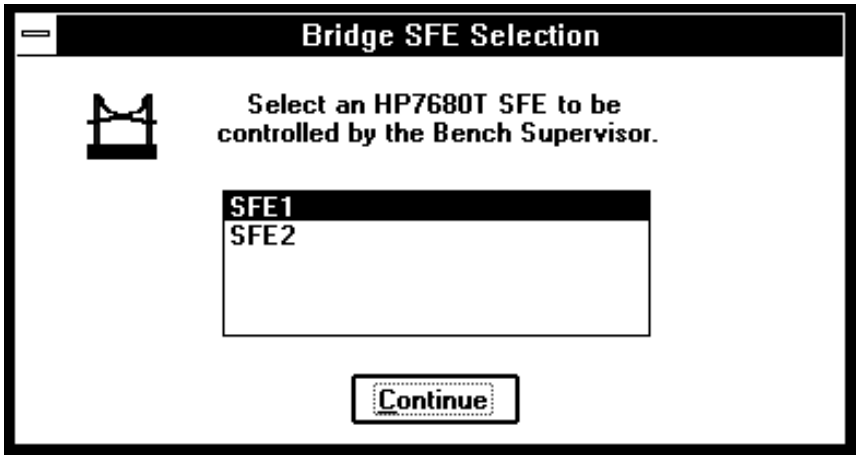
9. Install the Bench Supervisor software according to the instructions in the *Bench Supervisor Operating Manual*. If the software prompts you to replace the ChemStation file `TOP.MAC`, select Overwrite.
10. Install the Tray software as described in the *Bench Supervisor Operating Manual*.
11. Verify that Bench Supervisor control of the GC/MS and Tray is operating normally.
12. Close the Bench Supervisor software before continuing with the installation.

13. Install the Bridge software as described below. This software enables the Bench Supervisor to control the SFE application.

    a. From the Windows Program Manager, select `File`, then `Run` to access the Run dialog box.

    b. Put the Bridge Installation disk in drive `A:` and type "A:\setup" in the Run dialog box. (If you are using drive `B:`, type "B:\setup" instead.) Follow the instructions on your screen to complete the installation.

    c. When the "Bridge SFE Selection" window appears, select the SFE to be controlled by the Bench Supervisor, then select `Continue`. If only one SFE has been installed on the system, only one will appear in the message box.



    d. Select `Continue` when the system prompts you, then select `OK` when the installation is complete.

    e. For additional information on the Bridge installation, read the `ins_note.wri` file displayed at the end of the Bridge installation procedure. The installation software will place this file in your root directory.

Aligning and checking out the instruments

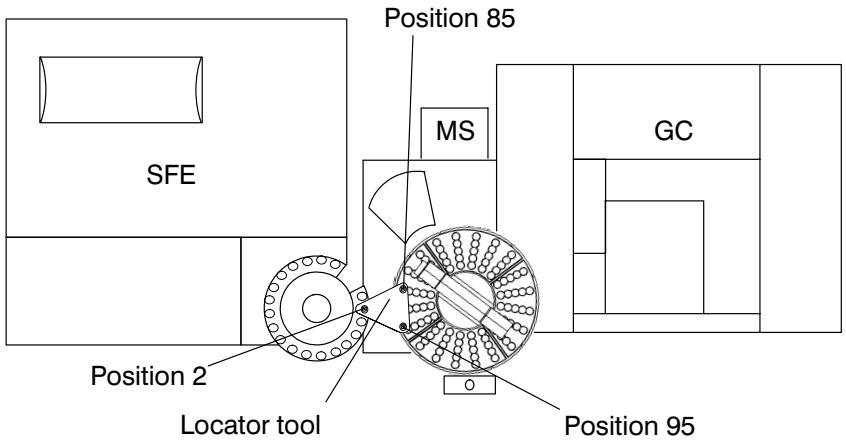
After setting up the hardware and installing the software for the SFE/MS Bridge, align the instruments to ensure proper transfer of vials, then run checkout tests to verify everything is functioning properly.

Aligning the instruments

Use the locator tool to align the SFE and automatic liquid sampler for precise vial transfers, as follows.

1. Start up the SFE software.
2. Select `Run` from the SFE menu bar, then select the `Maintenance and Test` option. Select `Rotate tray: vial #2 side`. This command rotates the SFE output turret clockwise so that position 2 is nearest to the sampler tray.
3. Place the locator tool so that two of the legs rest in vial positions 85 and 95 on the sampler tray and the leg indicated by a hole rests on the SFE output turret, as shown in the illustration below.

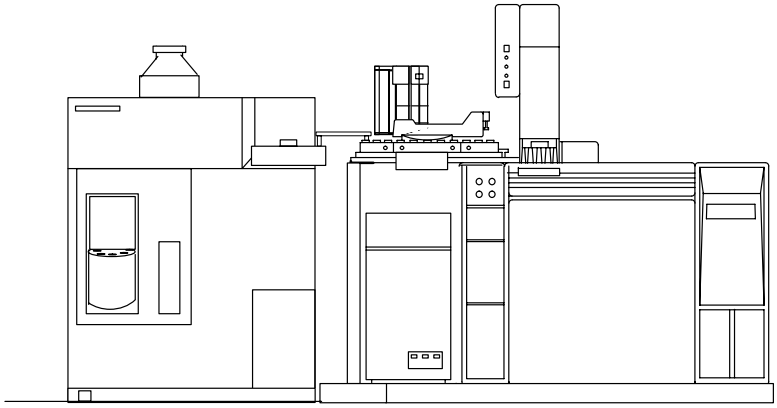
Overhead View



4. Reposition the Bridge spacer pad so that the leg of the locator tool resting on the SFE output turret drops into vial position 2 on the turret.
5. The locator tool should appear level with respect to the SFE and the sampler tray. If it is not level, have your assistant lift the corners of the GC while you add or remove metal shims as needed, and adjust the lengths of the PrepStation legs if you have a PrepStation installed.

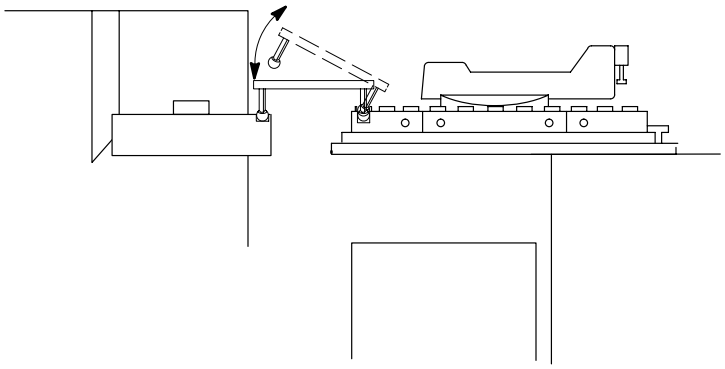
NOTE: If you add or remove any metal shims from beneath the GC, add or remove the same number of shims from beneath the MS to reduce strain on the column connection. Adjust the length of the PrepStation legs as well, if you have one installed.

Checking the SFE and Automatic Liquid Sampler alignment



6. Pivot the locator tool to make sure it can move freely in and out of vial position 2 on the SFE output turret, as shown below. If you encounter resistance, reposition the Bridge spacer pad until you can pivot the locator tool freely.

Pivoting the locator tool



When the locator tool pivots freely, the sampler and the SFE are perfectly aligned for vial transfers.

WARNING If you align the sampler tray and SFE improperly, the robotic arm may drop or eject the vials when retrieving them from the SFE output turret for placement in the sampler tray.

Checking out the instruments

After you have set up the hardware and installed the software, check to be sure the instruments are operating properly. Perform checkout tests using each instrument and its software to verify that the SFE/MS Bridge is functioning normally.

Using the SFE/MS Bridge

Using the SFE/MS Bridge

Once you have installed the Bridge hardware and software, you can begin setting up Bench Supervisor bench methods and bench sequences to automatically run series of extractions and analyses.

This section describes what you need to know to use your SFE and GC/MS in a Bridge configuration. It explains how the Bridge operates and how to use Bench Supervisor to pass vials between your SFE and sampler.

Bridge mode and Local mode

There are two modes for operating the SFE and GC/MS: Bridge and Local.

Bridge mode

If you start an SFE or GC/MS run in the Bench Supervisor software, the instruments are running in Bridge mode. The Bridge mode allows automated transport of vials between the output turret of the SFE and the sampler tray. The sampler tray can then transfer these vials to and from the GC/MS for injection. In Bridge mode, the Bench Supervisor software handles all sequencing. You cannot use SFE and ChemStation sequences.

Local mode

If you start a run from the SFE or ChemStation software without Bench Supervisor, the instruments are running in Local mode. In Local mode, you can use all of the features of the SFE and ChemStation software, including sequencing; however, the system will not be able to transfer vials automatically between the SFE and the sampler.

When you are running instruments in Local mode that are normally controlled by Bench Supervisor, their Bench Supervisor status will be "Busy." While the GC/MS and SFE have a status of "Busy," the Bench Supervisor software cannot run bench methods and bench sequences. Likewise, when you are running bench methods and bench sequences, you cannot use the SFE or PrepStation in Local mode.

Vial transport

The Bench Supervisor software coordinates all of your instruments to provide a chain of automation from your extractor to your gas chromatograph and mass spectrometer. When the SFE is ready to rinse analytes to a vial, the Bench Supervisor software will transport a vial from the sampler tray to the SFE output turret. After the SFE delivers the sample fraction, the Bench Supervisor software returns the vial to the sampler tray, then transports it to the injector turret, which injects it into your GC/MS**.**

Bench Supervisor overrides the vial numbers specified in the method for fraction output and always places vials into position 2 of the SFE's 21 vial output turret. The sampler tray robotic arm needs position 1 of the SFE output turret empty to allow enough clearance for it to place a vial in position 2 of the SFE turret.

NOTE: Be sure to empty vial positions 1 and 2 of the SFE output turret before running SFE methods through the Bench Supervisor software.

Bench methods and sequences

Bench methods

A bench method is a combination of methods from the instruments running under Bench Supervisor. A typical bench method consists of an SFE method followed by one or more GC/MS methods to analyze the extracted output. Bench Supervisor oversees the activities of the individual pieces of equipment and coordinates the automation that permits unattended running of bench methods involving the SFE and GC/MS. For more information on bench methods, see the examples in Chapter 9, or your *Bench Supervisor Operating Manual*.

Bench sequences

Bench sequences are a grouping of bench methods, and are useful when you need to analyze multiple samples or a range of samples. For more information on bench sequences, see the examples in Chapter 9, or your *Bench Supervisor Operating Manual*.

Quantitative analysis with the Bridge system

The Bridge configuration is designed to provide unattended sample preparation and analysis. If you want to do quantitative work, you must add an internal standard to the sample vials. Add it beforehand to each of the vials that will receive the fraction output from the SFE. After the fraction output vials leave the SFE, they **MUST** be mixed. They will then be ready for injection into the GC/MS without any further manual intervention.

If you will be using PrepStation to add internal standards, consult the PrepStation documentation for additional information and instructions.

SFE methods and sequences

SFE methods

You do not have to make any changes to your SFE methods to run them in Bridge mode. Even though all output fractions go to vial position 2 on the output turret when you are in Bridge mode, you can specify any output vial numbers in your method. These values will be overridden by the Bench Supervisor software when you run the method in Bridge mode. This allows you to use the same SFE methods in Bridge mode as you would when operating the SFE by itself (Local mode).

NOTE: Be sure to empty vial positions 1 and 2 of the SFE output turret before running SFE methods through the Bench Supervisor software, to allow clearance for the sampler robotic arm.

SFE sequences

Do not create SFE sequences to be used in Bridge mode. All sequencing is handled at the Bench Supervisor level. You can, however, still run SFE sequences in Local mode.

Access to the SFE software during a run

During a run the functionality of the top SFE level screen changes, based on whether you are in Local mode or Bridge mode.

Bridge mode

NOTE: The Bench Supervisor software will not allow you to load or run bench methods or sequences if you leave a dialog box open in the SFE or ChemStation software. The Bench Supervisor software will report the application as "Busy" until you close the dialog box.

When performing a run in Bridge mode, Bench Supervisor displays the Remote keyboard on the screen. All areas of the SFE Top Level screen become grayed out and are inaccessible. You can, however, open the Instrument Status screen from the Run menu and view the Step Setpoints from the Extract menu if you wish.

In Bridge mode, the SFE is under the control of the Bench Supervisor software. Local control returns when the bench method or bench sequence concludes its run or is stopped. For additional information on SFE runs in Bridge mode, see the examples in Chapter 9, or your *Bench Supervisor Operating Manual*.

Local mode

When performing a run in Local mode, only the Thimble View and keyboard areas of the top level screen are active. All other areas are grayed out. You can select `Change Setpoints During Run` to access other areas, but changing the parameters of a run is NOT recommended due to the risk of adding potentially unsafe parameter specifications. For more information on SFE runs in Local mode, see your SFE User's Guide.

Power failures and hardware faults

Power failures and/or hardware faults will render the SFE software status as “Busy” or “Down.” Such events may cause the SFE to set the instrument status to “Failed.” It will be necessary to stop the run and restart all software .

To help avoid aborted runs due to power failures, uninterrupted power supplies (UPS) should be properly sized and added to the main power sources for each instrument and computer in a Bridge configuration.

Aborting or stopping a run

You can abort a bench method from the Bench Supervisor software or the ChemStation software. You can also stop a run from the SFE software.

Aborting from the instrument software or from the Bench Supervisor software will cause the entire bench method or bench sequence to abort. The SFE and GC/MS instruments may have to proceed to a safe state before shutting down (i.e., depressurize).

In the event that an SFE run fails due to SFE instrument errors during a run, it may or may not halt other bench activity.

Stopping from the SFE software

Select the `STOP` button on the Remote keyboard. See *Stopping from the Remote keyboard* on the following page for more information about this procedure.

Aborting from the ChemStation software

Select `Abort` from the `RunControl` menu. See your *ChemStation* documentation for more information about aborting a run from the software.

While the ChemStation is in a run, there are limits to when it can accept an `ABORT` command from the Bench Supervisor. If you must abort the run immediately, go to the ChemStation and abort it from there.

Aborting from the Bench Supervisor software

The `Abort` option is on the top level of all four Bench Supervisor menu bars. Select `Abort` from the menu to abort a bench sequence or method.

See the *Bench Supervisor Operating Manual* for more information about aborting a run from the software.

Aborting from the PrepStation software

See the *PrepStation Operating Manual* for more information about aborting a run from the software.

Stopping from the Remote keyboard

In Bridge mode, when you launch a bench method or bench sequence from the Bench Supervisor that references an SFE method, a Remote keyboard appears on the screen just before the SFE method begins its run. This keyboard, titled “Remote,” is a replica of the actual keyboard on the SFE instrument and you can move it about the display.

The Remote keyboard looks similar to the keyboard that appears during an SFE run in Local mode, but it does not have a `Start` button because the SFE method is started and controlled remotely by the Bench Supervisor software.

The Remote keyboard does have a `STOP` button that stops the currently running SFE method. If stopped, the extractor is programmed to proceed to a safe condition (i.e., depressurized, thimble cooled and containing only pure CO_2) before opening the chamber. This may take as long as 10 minutes. If the output turret has rotated to the side to receive or return a vial to the sampler tray, the extractor may halt until delivery (or removal) of the vial is completed by Bench Supervisor. While the turret is rotated to the side, the extractor’s error recovery abilities (e.g., depressurization) are limited.

Using the MS ChemStation with the Bench Supervisor software

Using the MS ChemStation with the Bench Supervisor software

If you are used to running the MS ChemStation by itself, there will be some differences when you use it in combination with the Bench Supervisor and another instrument, such as the HP 7680T SFE. You will use the Bench Supervisor software to control the automation between the SFE and the sampler, and to create and edit bench methods and sequences. You will, however, continue to use the MS ChemStation for creating and editing ChemStation methods and for data analysis.

Version

You must have the correct version of the HP G2070AA ChemStation to operate the HP 6890 GC and MS. If you are operating an HP 5890 Series II GC with MS, you must have the HP G1034C ChemStation at its supported level. Earlier versions will not work properly with the Bench Supervisor software.

Installation and configuration

See Chapter 6, *SFE/MS Bridge Installation*, for information on installing and configuring the MS ChemStation to run with the Bench Supervisor software.

Calibration

See Example 5 in Chapter 9 of this manual, or the *Bench Supervisor Operating Manual*, for information on running calibrations using the Bench Supervisor software.

Sequencing

While the Bench Supervisor is running, all sequencing should be done by it. If you run sequences from either the HP 7680T SFE or the MS ChemStation, you are bypassing the Bench Supervisor software and will not be able to pass vials from the SFE to the sampler tray. Also, you will not be able to use other instruments as part of a sequence if you use ChemStation or SFE sequences.

***NOTE*:** Unlike the ChemStation software, the sequencing performed by the Bench Supervisor software will not stagger ChemStation methods for optimization when two injectors are used.

Aborting a run

While the MS ChemStation is in a run, there are limits to when it can accept an ABORT command from the Bench Supervisor. If you must abort the run immediately, go to the ChemStation and abort it from there. See chapter 7, *Using the SFE/MS Bridge*, for more information on aborting or stopping a run.

Method inputs

When you set up an MS method as part of a bench method, you will see the following Vial, Data and Values inputs at the Bench Supervisor level. The values for these fields are entered through the Bench Supervisor, which passes them to the ChemStation for use when a run is started. Below are descriptions of each method input and how to use it.

MS Vial

This is the vial that you will inject into the GC/MS.

Sample Name

This is the name of the sample. It will appear in the ChemStation report.

Misc Info

This is additional information for the sample. It will appear in the ChemStation report.

Sample Track Printout

This field will print a file containing information about steps that the sample went through before injection. If you leave this field set to "Track MS Vial," Bench Supervisor will print a report of this information after the run, and will copy a file with this information to the data file directory as `samptrck.txt`. If you change this field to any other source in the bench method and set its value to "None" (or the name of a non-existent file), Bench Supervisor will not print or copy the information.

Operator

This is the name of the operator of the system. Bench Supervisor stores this information in ChemStation data files and prints it on the reports.

Data Directory

This is the subdirectory that stores the data files for the run. This can be either a name supplied by the user, or it can be an *autoname* such as `yymmddss` which will be expanded to create a unique directory for a run based on the date of the run (see Bench Supervisor documentation for more information on autonames).

MS Raw File Name

This is the name of the file that will receive the MS data. You can create your own file name, or set up an *autoname* so that the file name is made up of vial number, sequence line, and injection number (see the Bench Supervisor documentation for more information on autonames).

Multiplier

The multiplier value for this sample. This value is only necessary for calibrated reports.

Sample Amount

The sample amount for this method. This value is used only in ESTD and ISTD reports. See the ChemStation documentation for more information.

RunType

The type of run to be performed. It should be *S* for samples, *B* for blanks, or *C* for calibration runs.

Level

If `RunType` is a calibration run, this value indicates the level from the quantitation database to recalibrate.

Update RT

If `RunType` is a calibration run, this value indicates how to update retention times. *N* = No Update, *A* = Average, and *R* = Replace.

Update RF

If `RunType` is a calibration run, this value indicates how to update response factors. *N* = No Update, *A* = Average, and *R* = Replace.

Update QI

If `RunType` is a calibration run, this value indicates how to update qualifier ion responses. *N* = No Update and *R* = Replace.

9

Examples of SFE/MS Bridge Operations

Examples of SFE/MS Bridge Operations

This chapter contains five examples to illustrate the use of the Bench Supervisor software with the HP 7680T SFE and the MS ChemStation.

Example 1, *Bench Methods*—Shows you how to set up a simple bench method to run an unattended extraction and analysis using the SFE and the GC/MS. This example is designed to show you the basic steps involved in setting up bench methods to pass fraction output from the SFE to the GC/MS for analysis.

Example 2, *Bench Sequences with a single extraction*—Shows you how set up a simple bench sequence to perform extractions and analyses on multiple samples. In this example, each run of the SFE method performs a single extraction that produces a single sample vial.

Example 3*, Bench Sequences with multiple extractions*—Shows you how to set up a bench sequence to perform extractions and analyses on multiple samples, where each run of the SFE method performs two extractions and produces two sample vials.

Example 4, *Bench Sequences with multiple extractions into a single vial*—Shows you how to set up a bench sequence to perform extractions on two samples and combine them into a single vial for analysis.

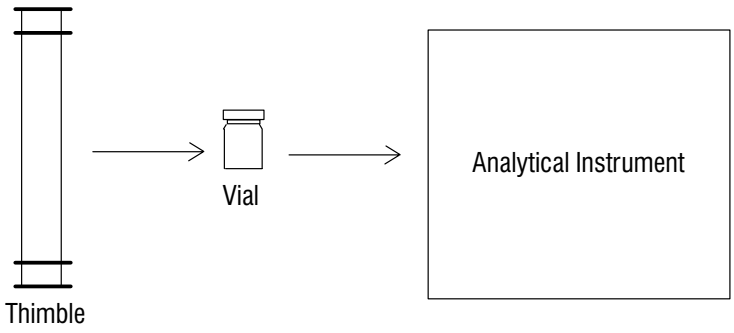
Example 5, *Calibrations using the Bridge*—Shows you how to use the Bridge to perform unattended calibrations of the GC/MS.

Example 1—Setting up a bench method

The following example shows the best way to set up a bench method, in which the SFE outputs one fraction vial to the GC/MS for analysis.

The scenario

For this example, assume you have an SFE method, `SFE1`, that outputs one vial to be analyzed at the end of its run, and you want to analyze this vial with a run of the GC/MS method, `MS1.M`.

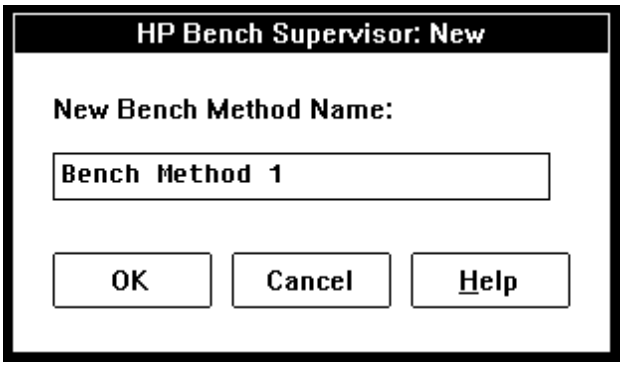


Creating the bench method

The following procedure describes how you would go about setting up the bench method described above to extract a single sample using the SFE and then transfer the sample to the GC/MS for analysis.

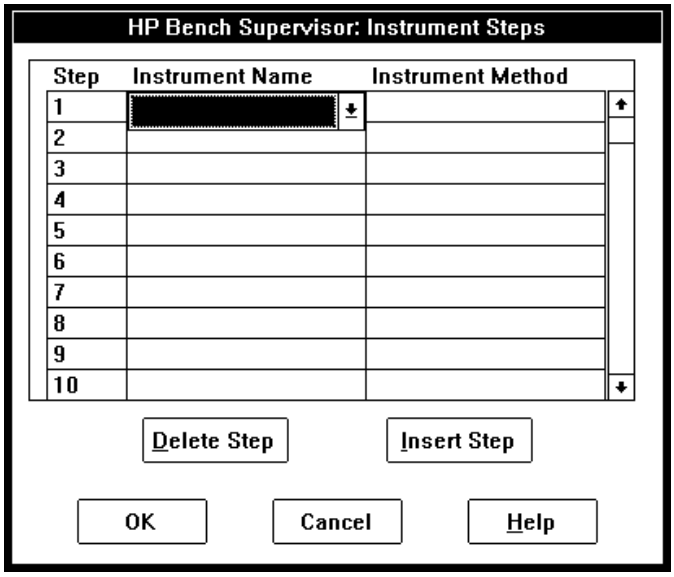
***NOTE*:** This example is provided to show you the steps necessary to set up a bench method. It is not necessary to actually complete the steps shown. The two instrument methods used to create the bench method in this example are not provided in the software. Just follow along with the procedure to get an idea of what is required to set up a bench method in Bridge mode.

1. In the Bench Supervisor program, select the `Bench Method` button to load the Bench Method menu bar. From the `File` menu, select `New Bench Method`.



2. Type a name for the bench method and select `OK`. The name can be any size up to the width of the box, and include any letter, number, or symbol, including spaces.

3. From the `Edit` menu, select `Instrument Steps`.

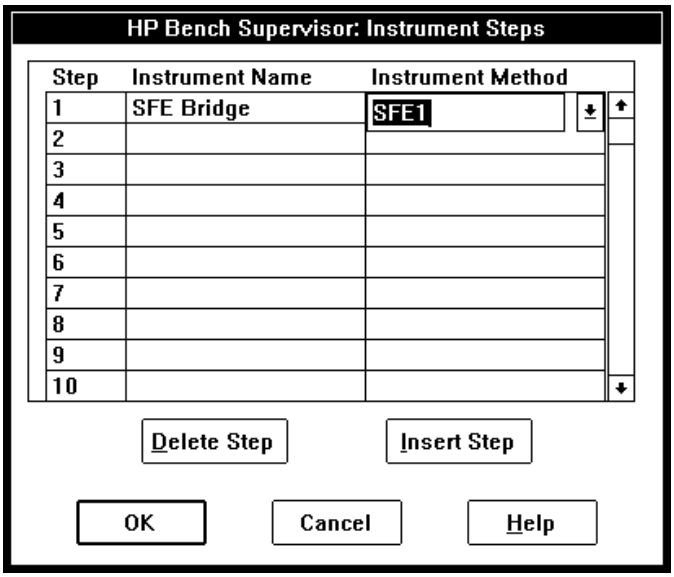


The Instrument Steps dialog box is where you specify the order of the SFE and ChemStation methods you want to run in your bench method.

NOTE: You must first create an instrument method using the appropriate instrument software before it will appear in the Instrument Steps dialog box, shown below, for incorporation into a bench method.

4. To make the SFE method `SFE1` the first step in this bench method:
   a. Select `SFE Bridge` from the Instrument Name drop-down list for *step one*.
   b. Select `SFE1` from the Instrument Method drop-down list for *step one*. The dialog box should appear as shown on the following page.

NOTE: SFE Bridge is the default name for the SFE instrument controlled by Bench Supervisor. If the name for the SFE instrument has been changed in the `win.ini` file, it will be different in the drop-down list box also.



NOTE: All quantitative analysis bench methods **MUST** contain a mixing step. If you *do not* have a PrepStation, include this step in the Instrument Steps dialog box, as shown in step 5. If you *do* have a PrepStation, consult your PrepStation documentation for information on vial mixing.

5. To run the bar code method `mix.mth` as the second step in the bench method:

   a. Select `BARCODE` from the Instrument Name drop-down list box for *step two*.

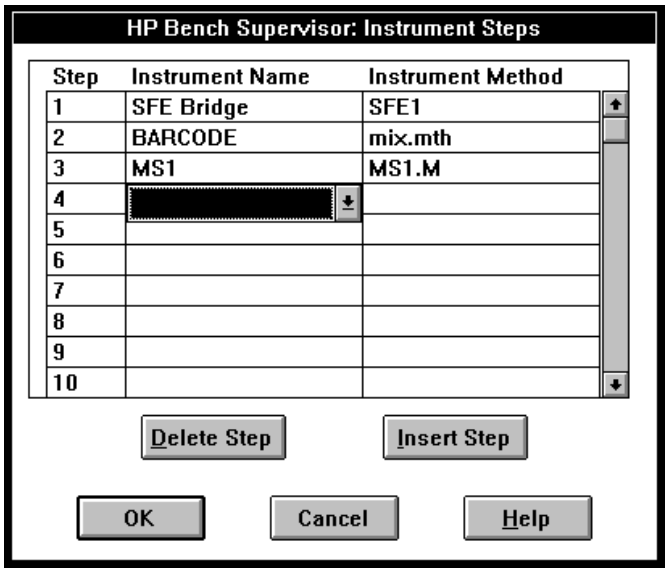
b. Type `mix.mth` in the Instrument Method column for *step two*. The name will not appear in the list box. You will have to type it in.

NOTE: If you also want to use the bar code reader/mixer to read a bar code, select the `BARCODE` instrument name and type `barcode.mth` in the Instrument Method

6. To run the MS method `MS1.MTH` as the third step in the bench method:

   a. Select `MS1`, the name of the MS instrument, from the Instrument Name drop-down list box for *step three*.

   b. Select `MS1.M` from the Instrument Method list for *step three*.

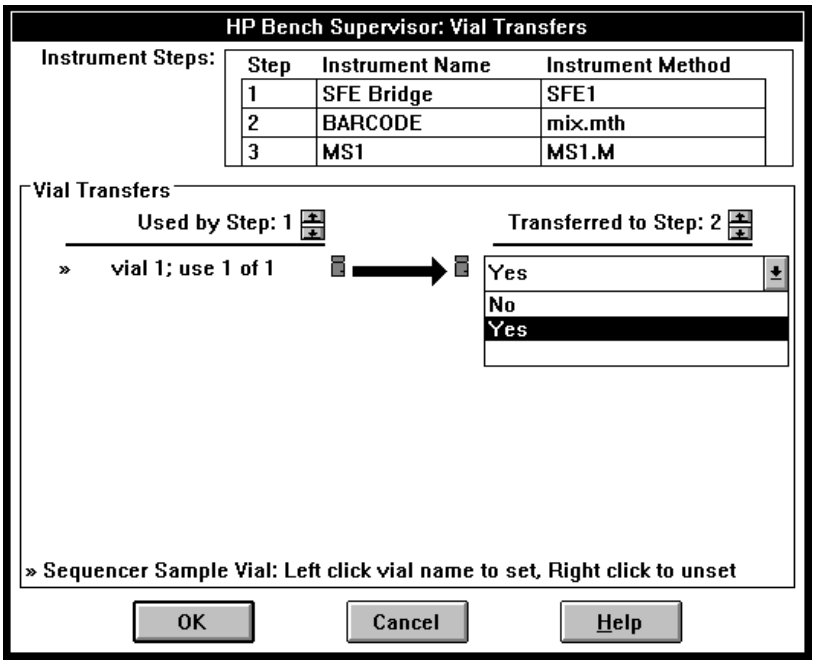


7. Select `OK`. The steps for the bench method are now set. Now you need to tell the Bench Supervisor software where to find the vial to use for each step in the bench method.

Assigning vial transfers

The previous procedure set up a basic three-step bench method with the intention of immediately transferring the fraction output vial as it is produced by the SFE to the mixer, then to the GC/MS for injection. To complete this process, you need to set up a vial transfer between the SFE, bar code reader/mixer and GC/MS, as described below:

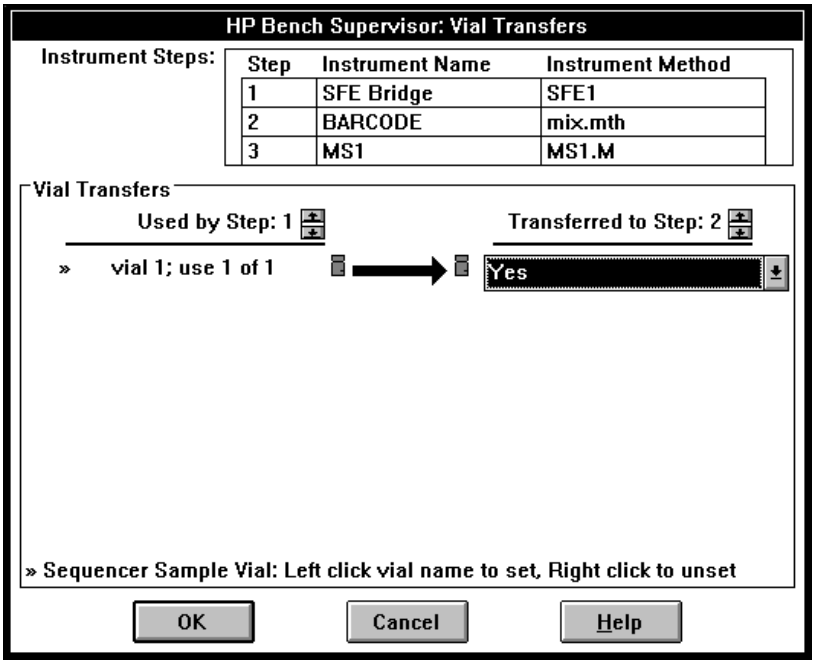
1. If the Vial Transfers dialog box is not open, from the Bench Method menu bar, select the `Edit` menu and then select `Vial Transfers`.



The left side of the dialog box shows the vial output by the SFE in step one. (If the SFE method was set up to produce more fraction output vials, they would also be listed on the left side.) The default name for sample vials is "vial 1; use 1 of 1." If more than one vial will be used in the method, subsequent vials will have a default name of "vial *n*; use 1 of 1," where *n* equals the number of the vial.

The right side of the dialog box allows you to specify whether the vial used in step one is to be transferred to the reader/mixer for use in step two.

2. Because we *do* want the fraction output vial from step one to be mixed in step two, we would select `Yes` from the drop down list box on the right side of the dialog box.

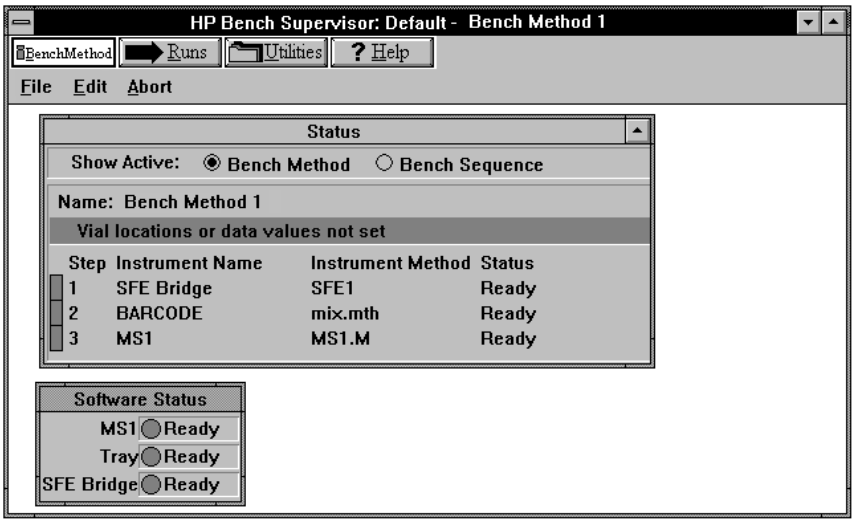


A pair of chevrons (**»**) appears on the Vial Transfers dialog box next to the vial in step one currently designated as the sequencer vial. This is a default designation. Designating a sequencer sample vial in a bench method simplifies data entry on the Sample Queue screen when you want to run the bench method multiple times in a bench sequence. Because we are not concerned with creating a bench sequence at this point, we do not need to worry about the sequencer designation. See the first bench sequence example in this chapter, or your Bench Supervisor documentation for more information about sequencer sample vials.

3. The next transfer is from the bar code reader/mixer to the GC/MS. Select the “Transferred to Step: (#)” up arrow until it is set to “3”.
4. Select Yes from the drop-down list box to indicate that Bench Supervisor should transfer the vial to the GC after mixing.

NOTE: In the Vial Transfers dialog box, if your bench method contains more than three or more steps, and the same vial will be used for each of them, when you select “Used by Step: 1” and “Transferred to Step: 3” for vial 1, you will see the “Yes” designation. This does not mean that the vial will be transferred directly from step 1 to step 3, just that Bench Supervisor knows that the same physical vial selected for step one will eventually be in step 3.

5. Select OK. The Status screen will appear within the Bench Supervisor screen, advising you that “Vial location or data values not set.”

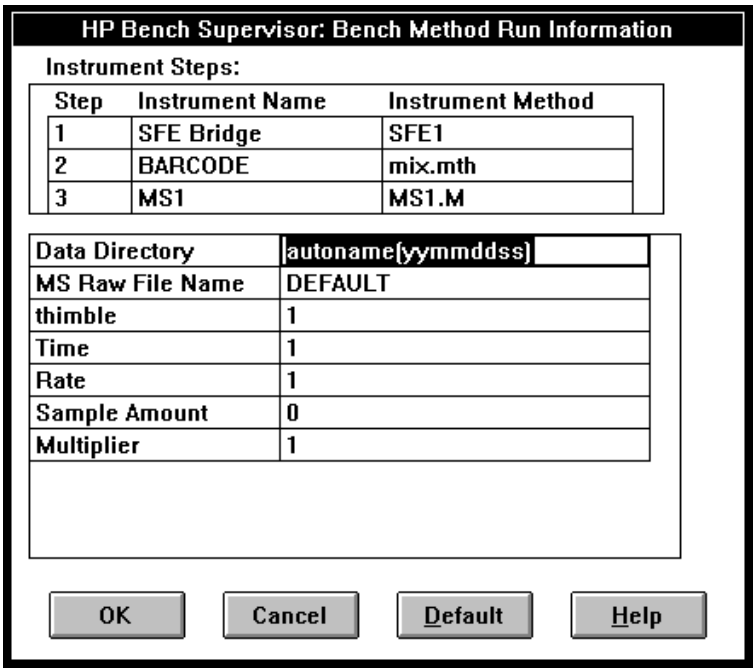


6. Complete the run time data as described on the following page.

Entering run time data information

After you create the bench method and assign vial transfers, as described on the previous pages, enter the run time data for the bench method as follows. Run time data is information required by the instrument software running under the Bench Supervisor software. The information is necessary for the instruments to make their runs.

1. To access the Run Information screen, select the `Runs` button to open up the Runs menu bar. Then, from the `RunBenchMethod` menu, select `Run Info`.



The fields displayed contain information that replaces what would normally be filled out on the ChemStation's Sample Info screen (opened from the `RunControl` menu).

2. Keep the following in mind as you complete each field:

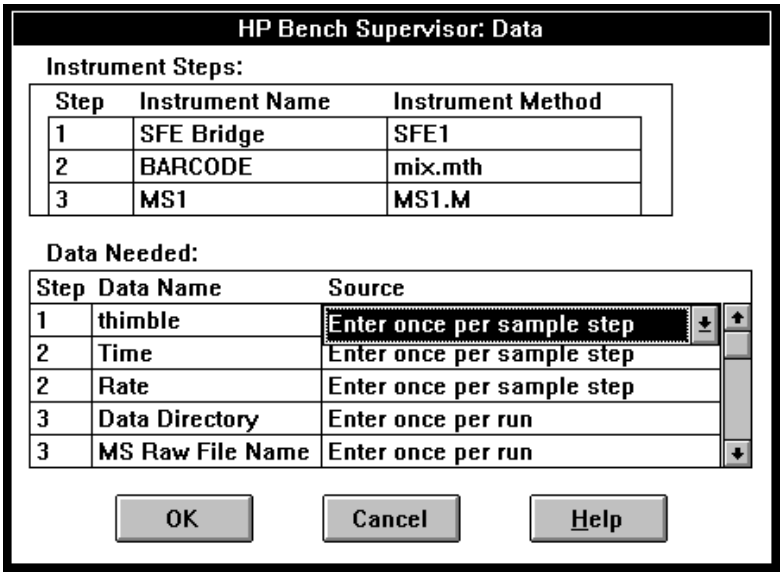
   a. In the Data Directory and Raw File fields, a dialog box opens that allows you to designate an autoname *pattern*. Patterns are a type of code or mask where the number/letter combinations you designate will be replaced at run time with values such as the date, the number of the run, etc. See your Bench Supervisor documentation for more information on patterns.

   b. In the Thimble field, you fill in the thimble position in the SFE carousel that contains the appropriate sample.

NOTE: If the thimble designation does not appear in the Run Information dialog box:

   a. Open the Bench Method menu and select Edit, then Data.

   b. Choose “Enter once per sample step” from the Source drop-down list box for the thimble, as shown below. Select OK to close the dialog box.



3. Select `OK` when you are finished. The Status screen will appear as before, advising you that "Vial locations or data values not set."
4. Set up the tray, as described below, to complete this procedure.

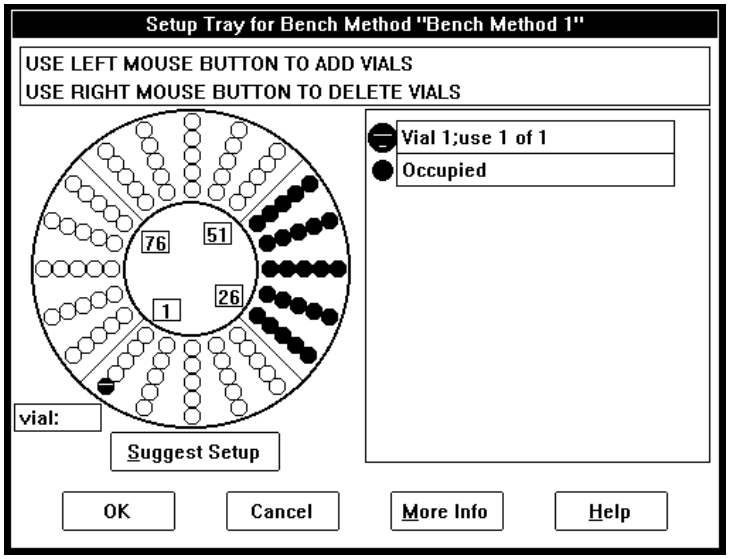
Setting up the tray

The last thing that needs to be done to create this bench method is to put all of the vials in the tray that the method requires. In this case, the method requires only one vial.

1. All of the vials the instrument methods require must start out in the sampler tray on the GC. To be safe, remove all vials from the turrets on the SFE and the AutoInjector tower(s). (You must at least remove vials from positions 1 and 2 in the SFE output turret, position 1 in the AutoInjector and the PrepStation module positions if you have a PrepStation.)

Complete the tray set up for this example as follows:

2. From the Runs menu bar, select `RunBenchMethod` and then `Setup Tray`.

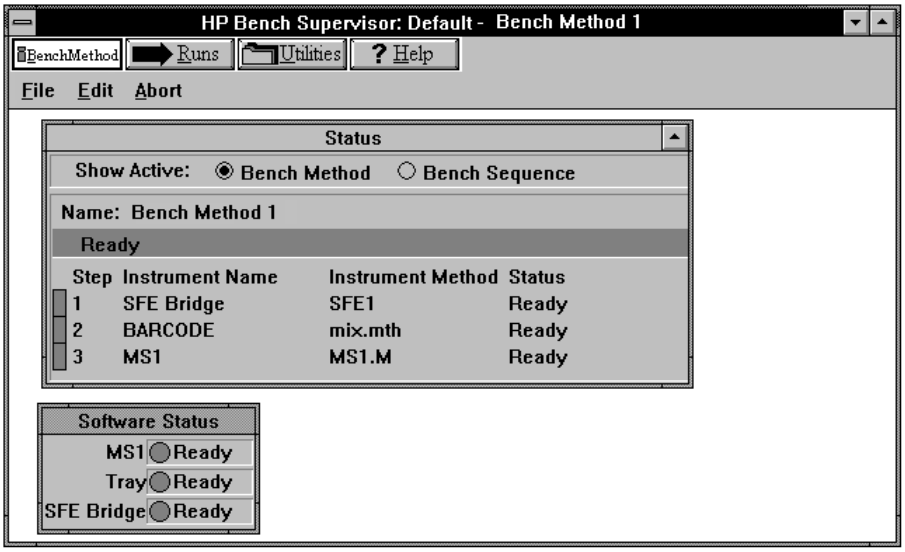


3. Assign the vial for the fraction output to a position in the tray in either one of the following two ways:

   - Use the left mouse button to select the vial's colored circle in the table on the right side of the dialog box and then select the desired position number in the tray.
   - Use the `Suggest Setup` button and let Bench Supervisor assign the vial to a position for you.

   The solid black positions on the Setup Tray screen show vial positions occupied by vials not used in the bench method.

4. Check the sampler tray and verify that the correct vials are in the tray positions you specified, and select `OK`. The Status screen will appear within the Bench Supervisor screen, showing that the method is ready to run.



Running the bench method

After you have set up your method and told the Bench Supervisor software where to find its resources and where to send its output, you can run the bench method.

1. Make sure the thimble and the vial required by the bench method are in their correct positions. Make sure there are no vials in the input turret of the AutoInjector tower(s), positions 1 or 2 of the SFE output turret, or the PrepStation module positions, if you have a PrepStation.
2. Make sure you have loaded the correct bench method. Then, select the `Runs` button on the Bench Supervisor screen to open the Runs menu bar.
3. Select `RunBenchMethod` and then `Start`.
4. The Run Info dialog box is opened. Make any necessary changes and select `OK`.
5. The Setup Tray dialog box is opened. Make any necessary changes and select `Start Run`.

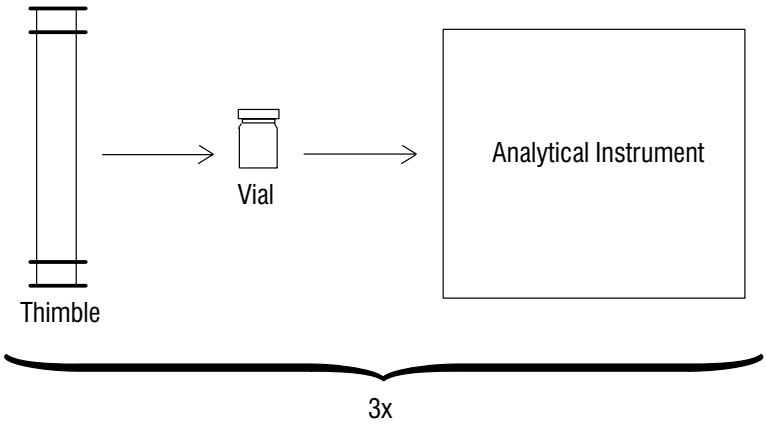
   The Bench Supervisor screen will show the status of the bench method and each instrument method in it. During the run the status will read "Running." After a successful run the status for each instrument will read "Completed."
6. View the status of individual instruments running under Bench Supervisor by selecting the iconized instrument, and using the normal status selection technique for that instrument.

Example 2—Setting up a bench sequence with a single extraction

In the previous example, we created a bench method that would extract a single sample in the SFE and analyze it in the GC/MS. What if you wanted to process five samples? or seven? You could either edit the bench method to process multiple samples, or you could create a *bench sequence*, which is the more reasonable solution.

Bench sequences provide a way to run numerous repetitions of one or more bench methods.

In the original example, we created a bench method to run one repetition of the method *Bench Method 1*. This example shows you how to create a sequence to run this method three times on three different samples.



If you have not read the first example on creating a bench method, do that now. This example assumes you have a familiarity with the steps involved in creating bench methods.

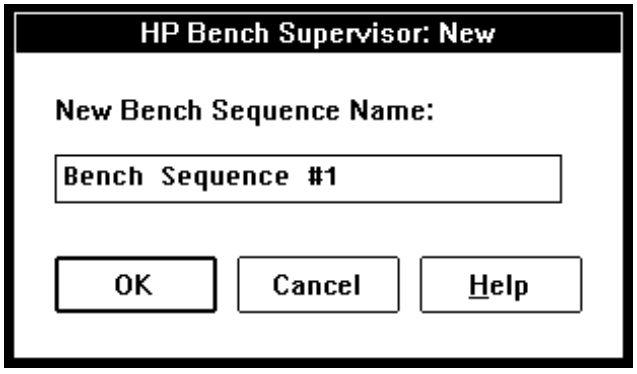
NOTE: All quantitative analysis bench methods **MUST** include a mixing step. For convenience, however, the mixing steps are not included in this example.

NOTE: This example is provided to show you the steps necessary to create a bench sequence. It is not necessary to actually complete these steps. The bench method and two instrument methods used to create the bench sequence are not provided in the software. Just follow along with the procedure to get an idea of what is required to set up a bench sequence in Bridge mode.

Creating the bench sequence

1. From the Bench Method menu bar, select `File`, then `Load`, then `Bench Method 1`.
2. Select `Edit` and then `Vial Transfers` to open the Vial Transfers dialog box.

   Verify that the sequencer sample vial is set to `vial 1` in step one. This will allow us to run this bench method multiple times on a range of vials when we create the bench sequence. Select `OK` to proceed. The system will display the Status screen for the bench method.
3. Select the `Runs` button to load the Runs menu bar. Select `Edit Bench Sequence` and then `New`. Name the sequence `Bench Sequence #1`, then select `OK`.



4. From the Runs menu bar, select `Edit Bench Sequence` and then `Sample Queue`.

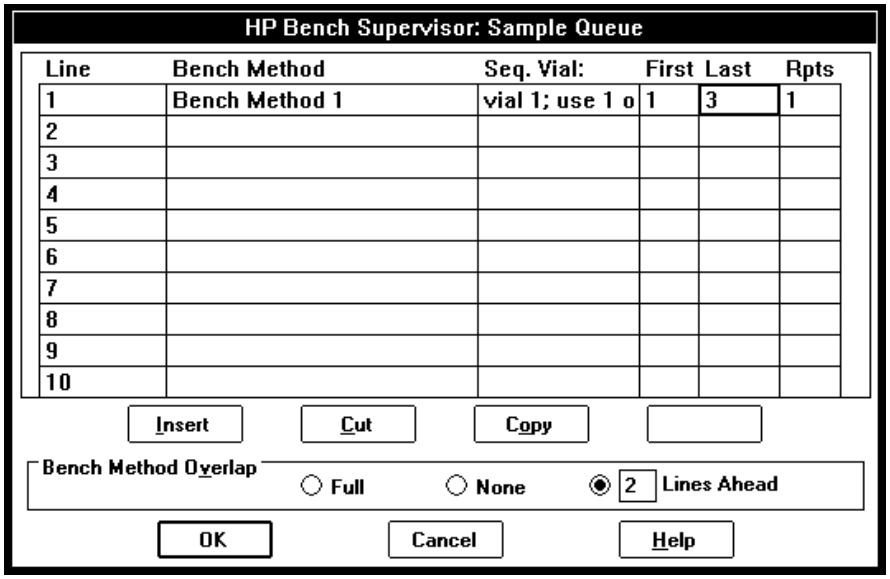
5. Select `Bench Method 1` from the drop down list for line one. The system automatically enters the method name you selected, the name of the sequencer vial (if any), and the default settings of "1" for the "First," "Last," and "Rpts" columns.

   The "Seq. Vial" (Sequencer Vial) field is set to `vial 1`, as we specified in the Vial Transfers dialog box.

   The "Rpts" (Repetitions) field identifies the number of times to run the selected bench method on the same vial or range of vials.

6. Leave "First" set to "1," change "Last" to "3," and leave "Rpts" set to "1," then select `OK`.

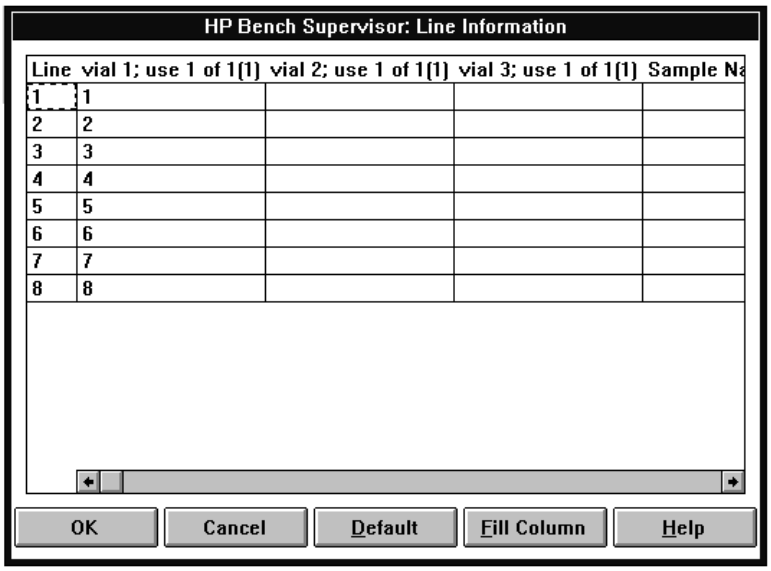
NOTE: When using Bench Supervisor in a Bridge configuration, always leave "Rpts" set to "1".



This tells Bench Supervisor to run `Bench Method 1` first, using the vial in position 1 of the AutoSampler tray, then to run the method two more times using the vials in positions 2 and 3. The First and Last numbers can be any position number in the 100 vial tray.

After selecting OK to close the Sample Queue dialog box, the Line Information dialog box is opened.

The Line Information dialog box determines which thimbles extract and rinse into which vials. The types of fields appearing on the Line Information dialog box may be different for different sequences, depending on the instruments and resources used in the bench methods within the sequence. If a horizontal scroll bar appears, use it to view the additional information in the table.

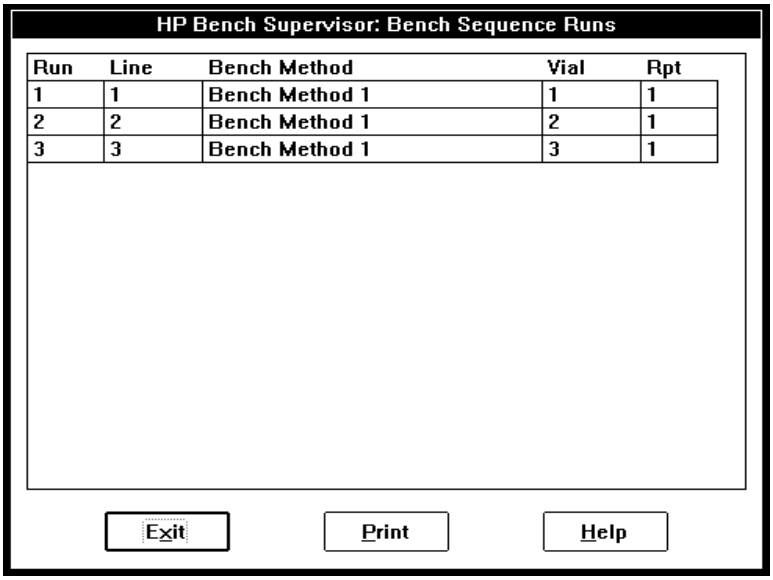


7. Enter the Sample Name and which SFE thimble position to use for each line in the sequence. This designation tells Bench Supervisor which thimble will extract into which vial. In this example, the thimbles in position 1, 2, and 3 will extract and rinse into vials 1, 2, and 3, respectively.

   Select OK to proceed.

8. From the Runs menu bar, select `Edit Bench Sequence` and then `Show All Runs`.

   Notice that we could have created a bench method that would have produced the same results as those in this sequence. The bench sequence, however, provides greater flexibility because just by changing the “First”, “Last” or “Rpts” fields on the Sample Queue dialog box we can extract varying numbers of samples.



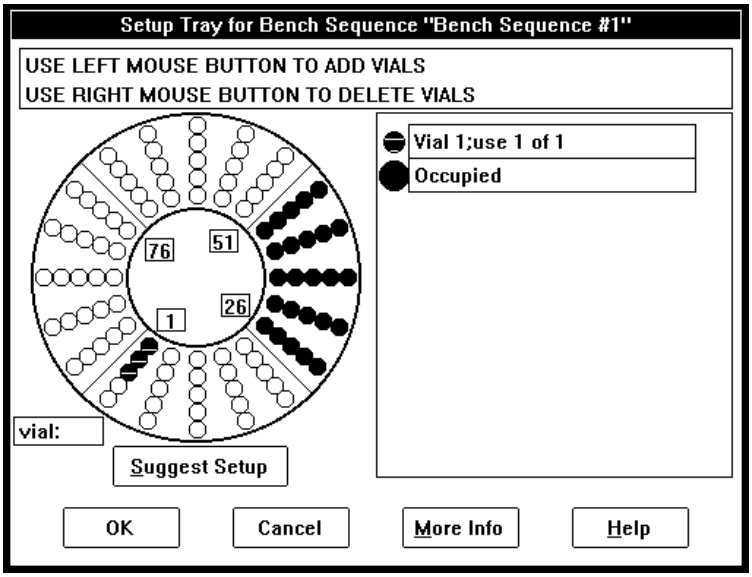
9. Select `EXIT` to return to the Status screen.

Setting up the tray

1. From the Runs menu bar, select `Run Bench Sequence` and then `Setup Tray`. This shows the input vial locations as defined on the Sample Queue screen in step six of the *Creating the bench sequence* portion of this example.

Had there been more than one vial in the bench method example, each would have been listed separately here (with a different color code). In this example, the bench method contains only one vial which will be run three times, so the three vials are not listed separately because each sample is considered to be of the same type.

The solid black vial positions on the Setup Tray screen show vial positions occupied by vials not used in this bench sequence.



2. If you were actually going to run this sequence, at this point you would place empty vials in the positions indicated in the Setup Tray screen and select `OK` to continue.

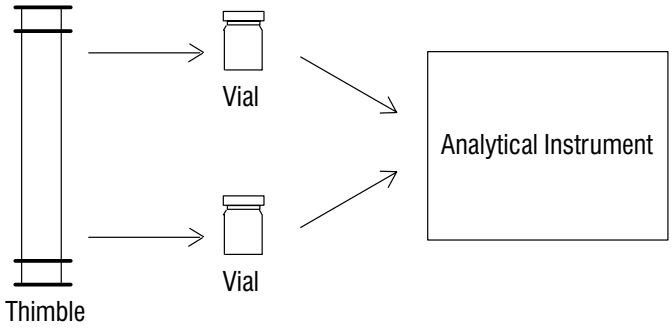
Running the bench sequence

1. To run the bench sequence you would open the Runs menu bar, select `Run Bench Sequence` and then `Start`. The system will display the Bench Sequence Info Screen. Make any necessary changes and select `OK`.

2. The system will then display the Setup Tray for Bench Sequence screen. Make any necessary changes and select `Start Run`.
3. To view the status of the bench sequence, open the Bench Sequence menu and select `Show Active: Bench Sequence`. The Bench Supervisor screen will display the status of each method and the equipment it uses throughout the run.

Example 3—Setting up a bench sequence with multiple extractions

In the previous example, we created a bench sequence that would extract a single sample in the SFE and analyze it in the GC/MS. This process was repeated three times. What if each run of your SFE method performed more than one extraction, to produce multiple samples? This example shows you how to set up a bench method and bench sequence that contain an SFE method which produces two sample vials.



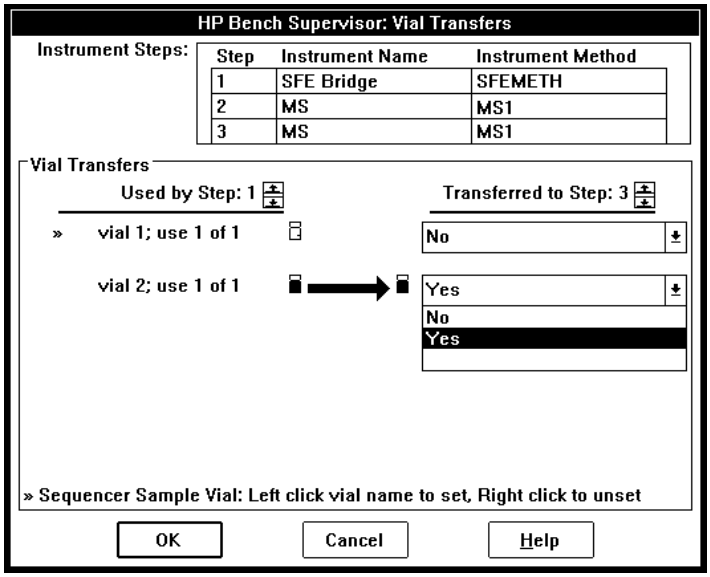
If you have not read the first example on creating a bench method, do that now. This example assumes you have a familiarity with the steps involved in creating bench methods.

NOTE: All quantitative analysis bench methods **MUST** include a mixing step. For convenience, however, the mixing steps are not included in this example. For information on including the bar code reader/mixer in bench methods, see Example 1 in this chapter.

NOTE: This example is provided to show you the steps necessary to create a bench sequence with multiple SFE extractions. It is not necessary to actually complete these steps. The bench method and two instrument methods used to create the bench sequence are not provided in the software. Just follow along with the procedure to get an idea of what is required to set up a bench sequence involving multiple sample vials.

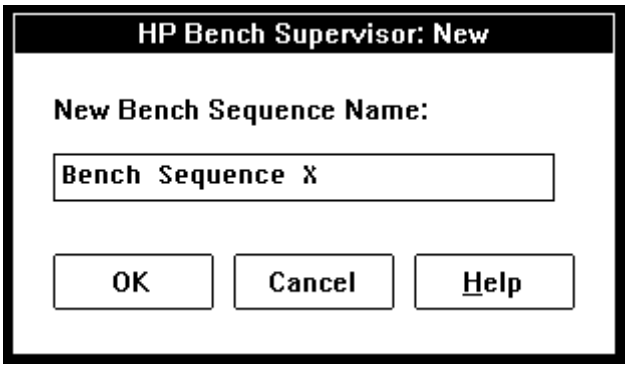
1. From the Bench Method menu bar, select `File`, then `New`.
2. Name the new method `Bench Method Y`.
3. Select `Edit` and then `Instrument Steps`. Enter the following information to set up the three-step bench method:
    a. For *step 1*, select `SFE Bridge` as the Instrument Name and `SFEMETH` as the Instrument Method. `SFEMETH` is a hypothetical method that performs two extractions, with one rinse to a vial per extraction, thus producing two sample vials during each run. See your SFE documentation for more details on how to set up this type of method.
    b. For *step 2* and *step 3*, select `MS` as the Instrument Name, and `MS1` as the Instrument Method. You could list a different method in step 3 if you did not want to analyze both vials with the same method. Note that for each vial to be analyzed there must be a corresponding analysis method in the Instrument Steps dialog box. If you did not wish to analyze the contents of the second vial, you would omit creating a third step.
4. Select `Edit` and then `Vial Transfers` to open the Vial Transfers dialog box, if it is not already open.
5. Select `Yes` to transfer vial 1 to *step 2*.

6. If you wish to analyze the contents of the second vial, select the "`Transferred to Step:` (#)" up arrow to change the designated step to *3*, then select `Yes` to transfer vial 2 to *step 3*, as shown below.



Verify that the sequencer sample vial is set to `vial 1` in step one. This will allow us to run this bench method multiple times on a range of vials when we create the bench sequence. Select `OK` to proceed. The system will display the Status screen for the bench method.

7. Select the Runs button to load the Runs menu bar. Select Edit Bench Sequence and then New. Name the sequence Bench Sequence X, then select OK.



8. From the Runs menu bar, select Edit Bench Sequence and then Sample Queue.
9. Select Bench Method Y from the drop down list for line one. The system automatically enters the method name you selected, the name of the sequencer vial (if any) and the default settings of “1” for the “First,” “Last,” and “Rpts” columns.

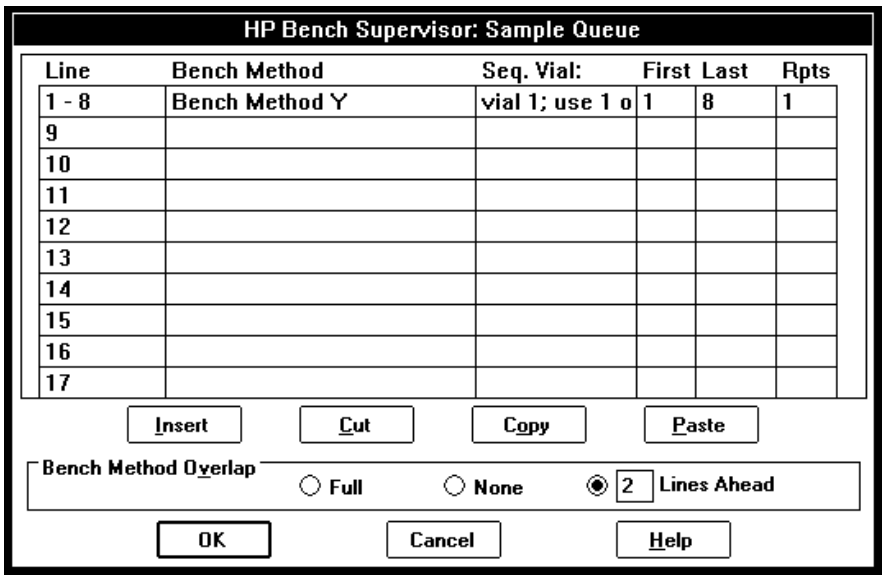
   The “Seq. Vial” (Sequencer Vial) field is set to vial 1, as we specified in the Vial Transfers dialog box.

   The “Rpts” (Repetitions) field identifies the number of times to run the selected bench method on the same vial or range of vials.

10. Leave “First” set to “1,” change “Last” to “8,” and leave “Rpts” set to “1,” then select OK.

NOTE: When using Bench Supervisor in a Bridge configuration, always leave “Rpts” set to “1”.

NOTE: The “First” and “Last” columns indicate the AutoSampler tray locations into which *Vial 1* (the sequencer vial) samples only will be placed. You will designate tray locations for the *Vial 2* samples on the Line Information screen, as described on the following page.

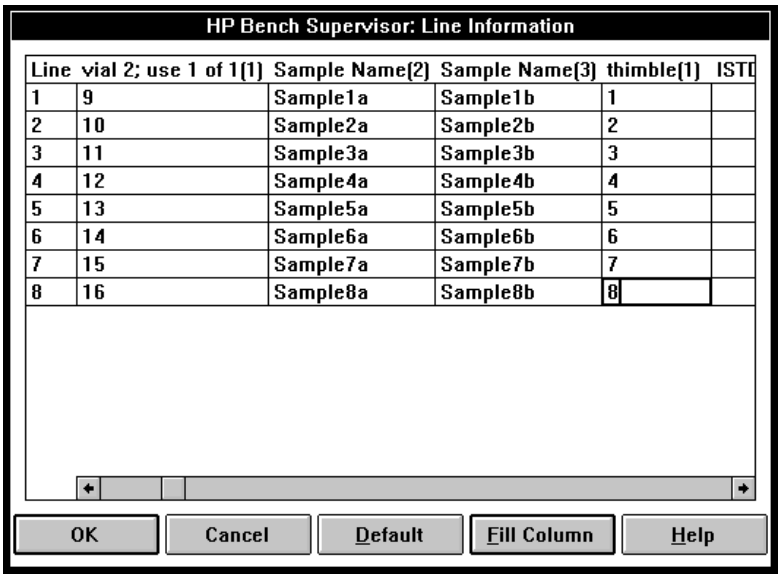


These settings tell Bench Supervisor to run Bench Method Y first, using the vial in position 1 of the AutoSampler tray, then to run the method seven more times using the vials in positions 2 thru 8. The First and Last numbers can be any position number in the 100 vial tray.

After selecting OK to close the Sample Queue dialog box, the Line Information dialog box is opened.

The Line Information dialog box determines which thimbles extract and rinse into which vials. The types of fields appearing on the Line Information dialog box may be different for different sequences, depending on the instruments and resources used in the bench methods within the sequence. If a horizontal scroll bar appears, use it to view additional information on the table.

11. Enter the tray locations for the vial 2 samples (locations 9 through 16, as shown below.)

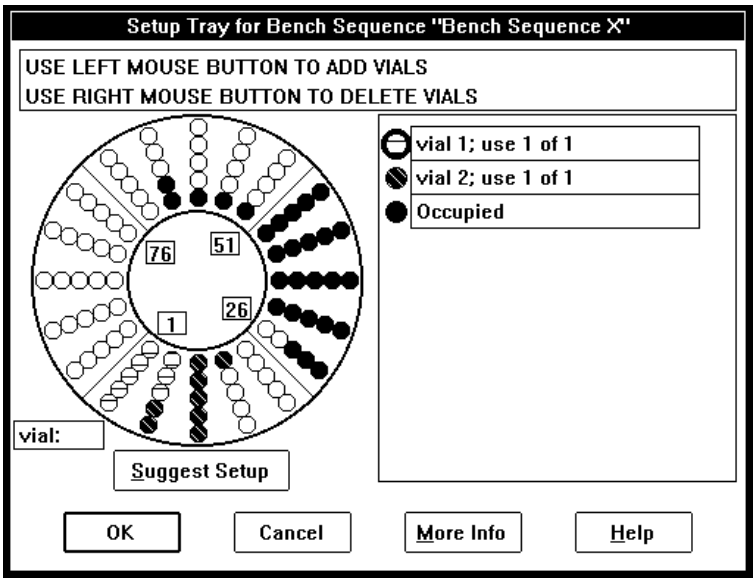


12. Enter the Sample Names and which SFE thimble position to use for each line in the sequence. Since the SFE method produces two vials per run, there are two columns for naming the samples. Select `OK` to proceed.

13. From the Runs menu bar, select `Edit Bench Sequence` and then `Show All Runs` to view the information for each run in the sequence.

14. Select `Exit` to return to the Status screen.
15. From the Runs menu bar, select `Run Bench Sequence` and then `Setup Tray`. This shows the input vial locations as defined on the Sample Queue screen in step 10 of this example.

    Since there was more than one vial in the bench method example, each is listed separately here (with a different color code). In this example, the bench sequence runs the bench method eight times, producing two vials with each run. The sixteen vials are not listed separately in the column on the right because there are only two sample types.

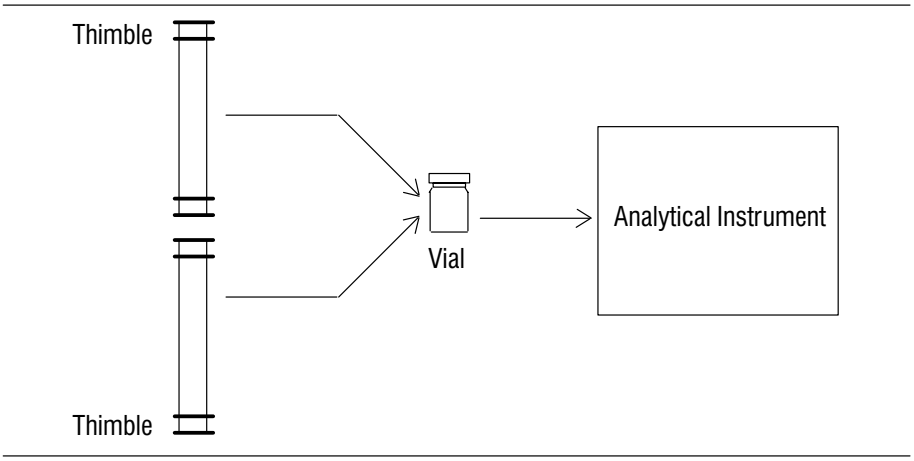


The solid black vial positions on the Setup Tray screen show vial positions occupied by vials not used in this bench sequence.

16. If you were actually going to run this sequence, at this point you would place empty vials in the positions indicated in the Setup Tray screen and select `OK` to continue.
17. To run the bench sequence, you would open the Runs menu bar, select `Run Bench Sequence` and then `Start`. The system will display the Bench Sequence Info Screen. Make any necessary changes and select `OK`.
18. The system will then display the Setup Tray for Bench Sequence screen. Make any necessary changes and select `Start Run`.
19. The Bench Supervisor screen will display the status of each instrument in use and the method it is running.

Example 4—Setting up a bench sequence with multiple extractions into a single vial

In the previous example, we created a bench sequence that would extract multiple samples. This example shows you how to set up a bench method and bench sequence which extract analytes from two thimbles, and combine them into a single vial for analysis.



If you have not read the first example on creating a bench method, do that now. This example assumes you have a familiarity with the steps involved in creating bench methods.

NOTE: All quantitative analysis bench methods **MUST** contain a mixing step. If you *do not* have a PrepStation, include this step in the Instrument Steps dialog box, as shown in step 4c. If you *do* have a PrepStation, consult your PrepStation documentation for information on vial mixing.

NOTE: This example is provided to show you the steps necessary to create a bench sequence with multiple SFE extractions into a single vial. It is not necessary to actually complete these steps. The bench method and instrument methods used to create the bench sequence are not provided in the software. Just follow along with the procedure to get an idea of what is required to set up a bench sequence that combines multiple extracts into a single vial.

1. In your SFE software, create two SFE methods, as follows:

   a. The first method should have no rinse between thimbles. Name the method `SFE_NO_R`.

   b. The second method should have a rinse step between thimbles. Name the method `SFE_RINS`.

   Consult your SFE documentation if you need additional information to create these methods.

2. In Bench Supervisor, from the Bench Method menu bar, select `File`, then `New`.

3. Name the new method `Bench Method B`.

4. Select `Edit` and then `Instrument Steps`. Enter the following information to set up the bench method:

   a. For *step 1*, select `SFE Bridge` for the Instrument Name and `SFE_NO_R` for the Instrument Method.

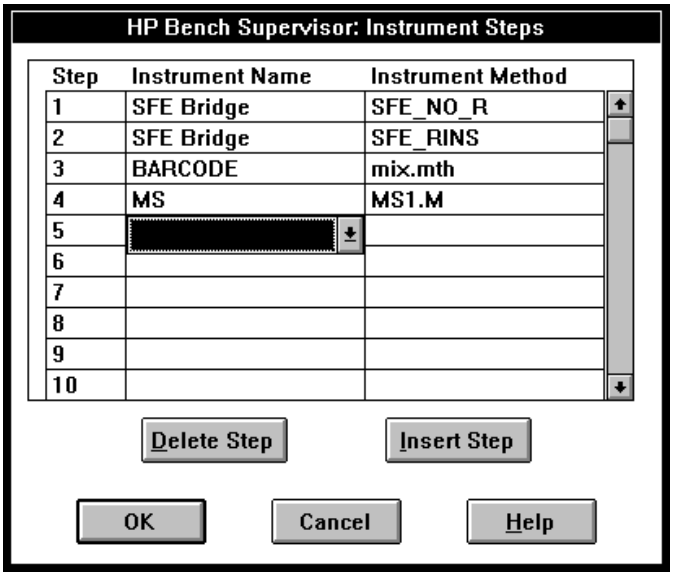
   b. For *step 2*, select `SFE Bridge` for the instrument, and `SFE_RINS` for the method.

   c. For *step 3*, select `BARCODE` as the instrument and type `mix.mth` for the third step in the bench method.

d. For *step 4*, select `MS` as the instrument, and `MS1` for the instrument method.

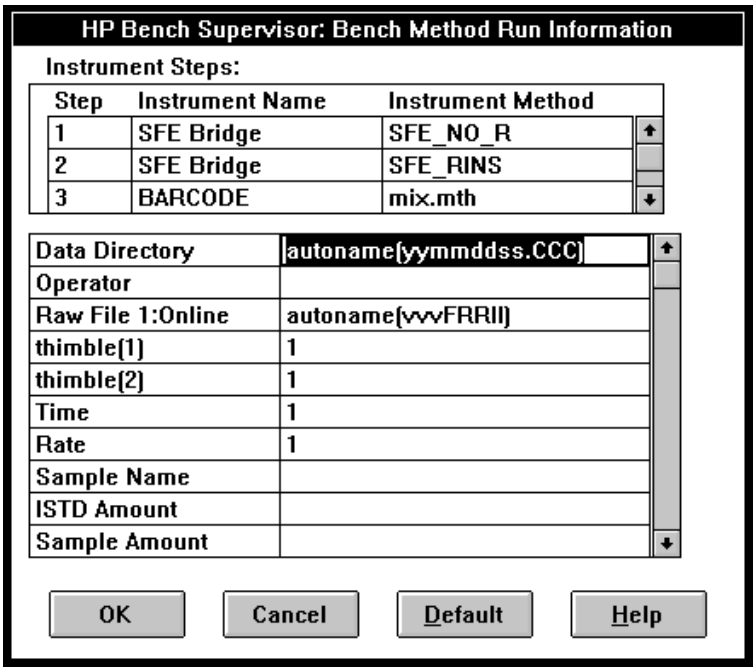
NOTE: If you also want to use the bar code reader/mixer to read a bar code, select `BARCODE` as the Instrument Name and type `barcode.mth` for the Instrument Method.

After completing these steps, the Instrument Steps dialog box should appear similar to the one below.



5. Select `Edit` and then `Vial Transfers` to open the Vial Transfers dialog box, if it is not already open.
6. Select `Yes` to transfer vial 1 to *step 3*.
7. Also select `Yes` to transfer vial 1 to step 4, to tell Bench Supervisor to transfer the vial to the GC after mixing. Select `OK` to proceed. The system will display the Status screen for the bench method.

7. Access the Run Information dialog box by selecting the `Runs` button to open up the Runs menu bar. Then, from the `RunBenchMethod` menu, select `Run Info`.



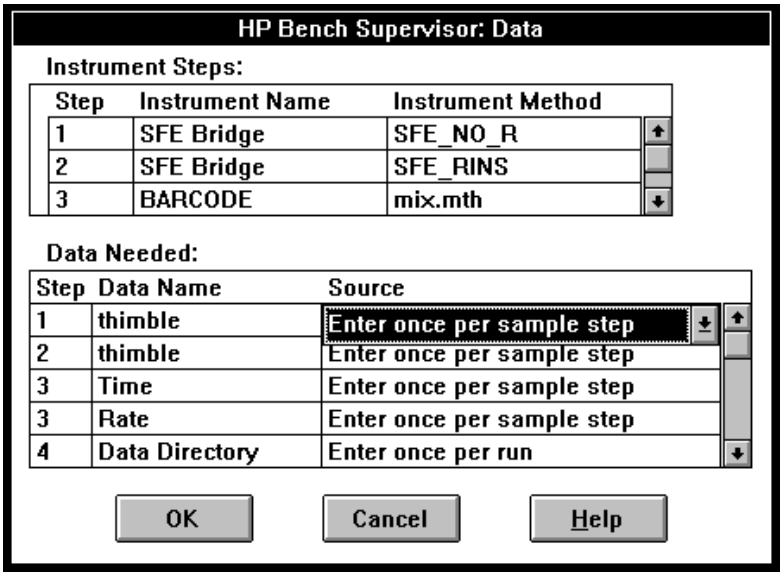
The fields displayed contain information that replaces what would normally be filled out on the ChemStation's Sample Info screen (opened from the `RunControl` menu).

8. In the thimble field, fill in the thimble position in the SFE carousel that contains the appropriate sample. The number immediately following the word `thimble` indicates the bench method step associated with that thimble. For example, the thimble with `(1)` following it is the one that the `SFE_NO_R` method uses in step 1 of the bench method.

NOTE: If the thimble designation does not appear in the Run Information dialog box:

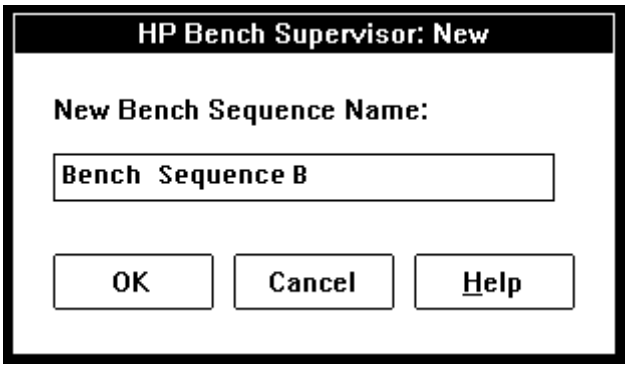
a. Open the Bench Method menu and select Edit, then Data.

b. Choose "Enter once per sample step" from the Source drop-down list box for the thimble, as shown below. Select OK to close the dialog box.



9. Select OK when you are finished with the Run Information dialog box. The Status screen will appear as before, advising you that "Vial locations or data values not set."

10. Select the Runs button to load the Runs menu bar. Select Edit Bench Sequence and then New. Name the sequence Bench Sequence B, then select OK.



11. From the Runs menu bar, select Edit Bench Sequence and then Sample Queue.
12. Select Bench Method B from the drop down list for line one. The system automatically enters the method name you selected, the name of the sequencer vial (if any) and the default settings of “1” for the “First,” “Last,” and “Rpts” columns.

    The “Seq. Vial” (Sequencer Vial) field is set to vial 1, as we specified in the Vial Transfers dialog box.

    The “Rpts” (Repetitions) field identifies the number of times to run the selected bench method on the same vial or range of vials.

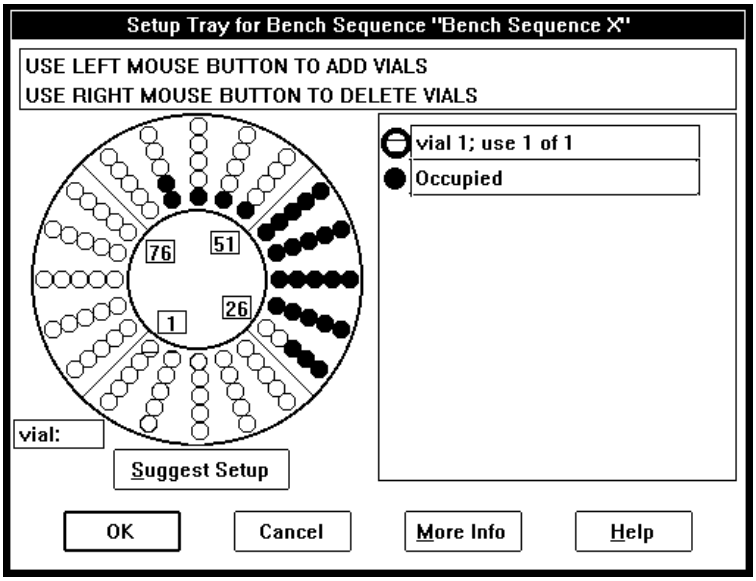
    These settings tell Bench Supervisor to run Bench Method B first, using the vial in position 1 of the AutoSampler tray. The First and Last numbers can be any position number in the 100 vial tray.

    After selecting OK to close the Sample Queue dialog box, the Line Information dialog box is opened.

The types of fields appearing on the Line Info dialog box may be different for different sequences, depending on the instruments and resources used in the bench methods within the sequence. If a horizontal scroll bar appears, use it to view additional information on the table.

13. Enter the Sample Names and which SFE thimble positions to use for each line in the sequence. Select `OK` to proceed.
14. From the Runs menu bar, select `Edit Bench Sequence` and then `Show All Runs` to view the information for the sequence.
15. Select `Exit` to return to the Status screen.
16. From the Runs menu bar, select `Run Bench Sequence` and then `Setup Tray`. This shows the input vial locations as defined on the Sample Queue screen in step 12 of this example.

    In this example, the bench sequence runs the bench method one time, producing one vial.



The solid black vial positions on the Setup Tray screen show vial positions occupied by vials not used in this bench sequence.

17. If you were actually going to run this sequence, at this point you would place empty vials in the positions indicated in the Setup Tray screen and select OK to continue.
18. To run the bench sequence, you would open the Runs menu bar, select Run Bench Sequence and then Start. The system will display the Bench Sequence Info Screen. Make any necessary changes and select OK.
19. The system will then display the Setup Tray for Bench Sequence screen. Make any necessary changes and select Start Run.
20. The Bench Supervisor screen will display the status of each instrument in use and the method it is running.

Example 5—Calibration using the Bridge

The scenario

For this example, assume you have an SFE method, `SFE Extract and Analyze`, that outputs eight vials to be analyzed at the end of its run, and you want to perform a calibration using these vials with a run of the GC/MS method, `BRIDGE`, which contains a three-level calibration table.

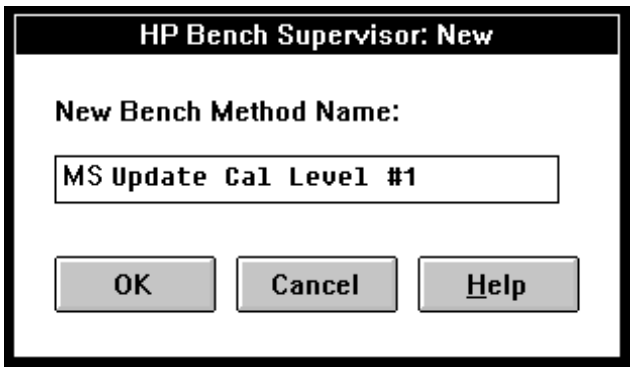
NOTE: This example assumes you are familiar with the steps necessary to create basic bench methods and sequences. If you are not, read the other examples in this chapter before proceeding.

***NOTE*:** This example is provided to show you the steps necessary to set up calibrations using the Bridge. It is not necessary to actually complete the steps shown. The instrument methods used to create the bench methods in this procedure are not provided in the software. Just follow along with the procedure to get an idea of what is required to set up a calibration in Bridge mode.

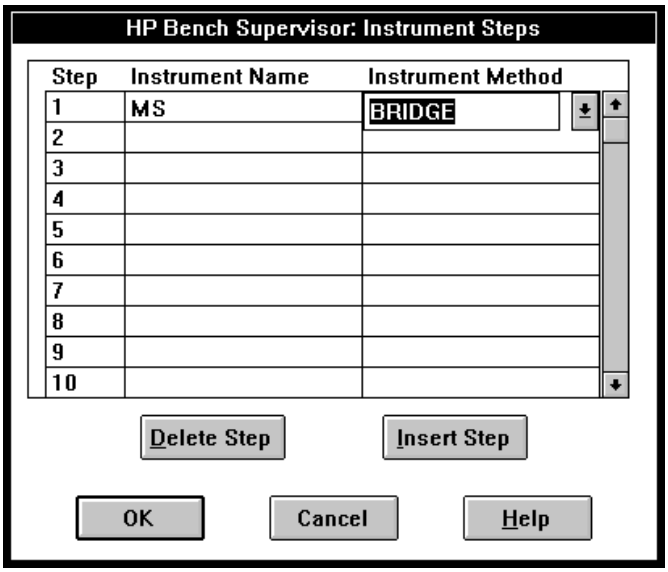
Creating the bench methods

The following procedure describes how you would go about setting up the bench methods needed to perform the calibration described above. You will need to create four bench methods—one to update each level of the calibration table and one to perform the extraction, mixing and analysis.

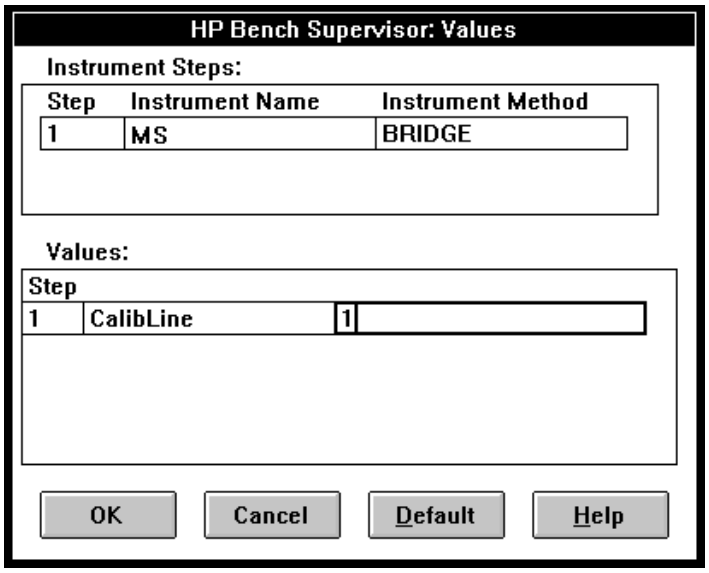
1. In Bench Supervisor, open the `File` menu and select `New Bench Method`. Name the method `MS Update Cal Level #1,` as shown on the following page. This naming convention will make it easier to determine which vial location in the tray is associated with which calibration standard.



2. From the `EDIT` menu select `Instrument Steps`. Select `MS` as the Instrument Name and `BRIDGE` as the Instrument Method.



3. From the Bench Method menu, select `Edit`, then `Values`. The Values dialog box will appear.
4. Type “1” in the CalibLine box, as shown below. This value determines which level of the calibration table an instrument line will update. In this case, the method contains only one instrument line, which will update level 1 of the calibration table.



5. Create identical bench methods for the remaining two levels in the calibration table. Name the second method `GC Update Cal Level #2`, and set the CalibLine to 2. Name the third method `GC Update Cal Level #3` and set the CalibLine to 3. The CalibLine number of each method must match the level of the calibration table that the method will update.

6. Now create a bench method that will extract a sample, then mix and analyze the extract. Name the method `SFE Extract and Analyze`.

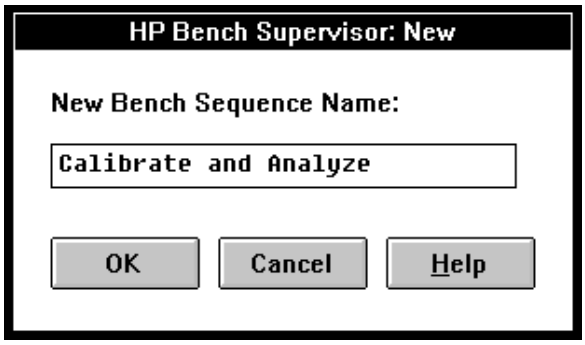
   Leave the CalibLine of this method at the default setting of "0".

   See *Example 1—Setting up a bench method*, earlier in this chapter, for an example of this type of bench method.

Creating the bench sequence

After creating the bench methods, you need to create a bench sequence that incorporates the three calibration methods, then extracts and analyzes additional samples and produces a quantitative report.

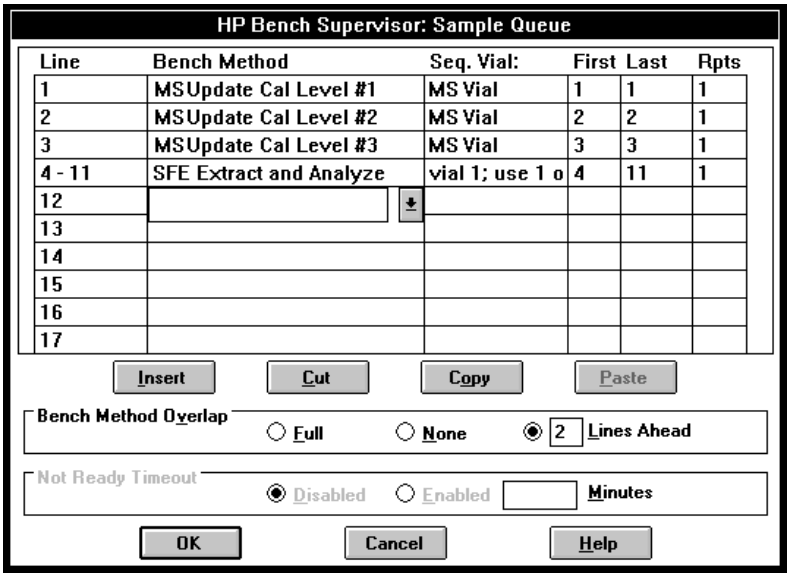
1. From the Bench Sequence menu, create a new bench sequence and name it `Calibrate and Analyze`.



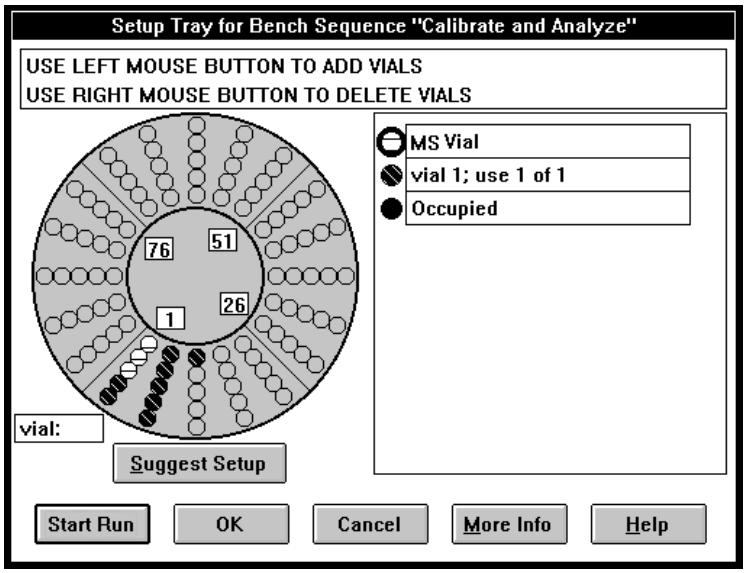
2. In the Sample Queue dialog box for the sequence, list the methods you created earlier in numerical order.
3. In the First/Last columns, designate the vial location of each of the calibration solutions.

NOTE: Verify that each vial location in the Sample Queue dialog box corresponds to the appropriate sample vial and calibration level, to ensure accurate calibration.

4. Add the SFE `Extract and Analyze` Bench Method to the sample queue and close the dialog box, which should appear similar to the one shown below.



5. From the Runs menu bar, select Run Bench Sequence and then Setup Tray. This shows the input vial locations, as defined on the Sample Queue screen.



Troubleshooting/ System Messages

Troubleshooting/System Messages

This chapter describes some potential problems you might encounter while running in a Bridge configuration, their possible causes and their solutions.

In addition, this chapter covers the various system messages relating to the Bridge, what they mean, and how to deal with them if they occur.

Vial transfer problems

Automatic liquid sampler arm fails to successfully deliver or remove a vial from the SFE output turret.

A vial was left in vial position 1 or 2 of the SFE output turret. Remove any vials from positions 1 and 2 and rerun the bench method.

The SFE and the sampler tray are out of alignment. Use the locator tool to check their alignment. If they are out of alignment, realign the instruments as described in the *Aligning the instruments* procedure in the *Installation* chapter appropriate to your configuration, and rerun the bench method.

System messages

Message: `Remote connection terminated—returning to LOCAL control`

The STOP button on the Remote keyboard was selected or the bench method or sequence was stopped from within the Bench Supervisor software.

When this happens, all runs are terminated and communication between Bench Supervisor and the SFE is shut down. The extractor may need to depressurize before it can release the thimble currently in the chamber. If necessary, run a cleanup method to purge the lines of any sample material, modifiers, or rinse solvents. Be sure to place vials in the correct positions in the SFE output turret if you will be using the SFE in Local mode.

Bench Supervisor may resume communications with the SFE unless the status for the SFE in the Bench Supervisor Software status box is “Down” or “Communications Error.” If communication is not re-established, close the SFE and Bench Supervisor software and restart Bench Supervisor.

Error: `Vial not loaded from Remote`

Either the sampler tray robotic arm failed to deliver a vial to the output turret, or was not able to retrieve a vial from the output turret.

The tray or the SFE may have become misaligned or a vial was removed from position 2 of the SFE output turret.

Check the alignment of the SFE relative to the sampler tray with the locator tool. Realign the SFE and sampler if necessary, as described in the *Installation* chapter.

To resume operation—This is a fatal error for the SFE software. Other applications linked to the Bench Supervisor software may continue running unless they require the missing vial. You may wait until these finish if desired before restarting.

1. Abort the bench method or bench sequence.
2. Close the Bench Supervisor software.
3. Restart the Bench Supervisor software.
4. Remove any vials from positions 1 and 2 in the SFE output turret and from all positions in the AutoInjector turret(s).
5. Load the sampler tray with any vials necessary and rerun the bench method or bench sequence.

Appendix A

WIN.INI PCS Sections

Appendix A

WIN.INI PCS Sections

The following are typical examples of the [PCS] sections of your `win.ini` files, which contain parameter information for the server. Any application that uses the server requires a [PCS, *n*] section. The following table lists the PCS parameters and their function.

[PCS] – The section for the server software

Parameter	Description
Path=C:\HPCHEM	The path file where APG_TOP.EXE and the .INI files are located. An .INI file is necessary for each APG application (with the exception of MDS).
Instruments=1,5,6	Identifies all the instrument IDs which will run under the server. A [PCS,*n*] section must exist for each instrument identified by this statement.
Applications=HP3365,hp7680,TRAY	List of the PCS applications. An .INI file is necessary for each APG application (with the exception of MDS).
Link1=HPIB,1,7,0,3	Interface type, SelectCode, DMAChannel, Interrupt
Links=1	Specifies which link *n* to look for
Device1=1,15,5890	link, HP-IB address, device type
Device2=1,8,7673	link, HP-IB address, device type
Device3=1,4,7680	link, HP-IB address, device type
Devices=1,2,3	Indicates which Device *n* lines to look for

[PCS,1] —The section for the first APG instrument ,“GC”

Parameter	Description
Program=C:\HPCHEM\HP3365.EXE	Higher level programs use these lines when calling this application. The line used depends on the program calling the application. Path\executable PCS # (This line starts the application—the # is needed.)
Program1=c:\hpchem\bs\vi3365.exe 1 /a	
InstName=GC	The instrument name
InstType=5890	The instrument type
Path=C:\HPCHEM\1	The directory path for the program
Supervisor=yes	Tells Bench Supervisor to start this program, if Bench Supervisor is reading this PCS section
Start=no	Tells the server (APG_TOP) whether or not to start this instrument
Devices=1,2	The devices that this instrument uses (relates to [PCS] section)
jconbmp=c:\hpchem\bs\gc.bmp	Bitmap used for this instrument in the JCON window
WinSize=normal	Specifies window size
DataPath=C:\HPCHEM\1\DATA	Specifies the instrument data path
MethPath=C:\HPCHEM\1\METHODS	Specifies the instrument method path
SeqPath=C:\HPCHEM\1\SEQUENCE	Specifies the instrument sequence path
Method=C:\HPCHEM\1\METHODS\QUICK.MTH	The last method this application used
Sequence=C:\HPCHEM\1\SEQUENCE\DEFAULT.SEQ	The last sequence this application used
DEBackground=255 255 255	These lines determine the RGB colors of the specified areas
DEChromatogram=0 0 255	
DEAxes=0 0 0	
DETitle=0 0 0	
DERtimes=255 0 0	
DEBaselines=255 0 255	
DEAnnotation=255 0 0	
DEFrame=255 0 0	

[PCS,2] —The section for the second APG instrument, “Analyzer 2”

Parameter	Description
InstName=Analyzer2	The instrument name
InstType=offline	The instrument type. This instrument will run offline
Supervisor=no	Tells Bench Supervisor not to start this program, if Bench Supervisor is reading this PCS section
Start=no	Tells the server (APG_TOP) whether or not to start this instrument
WinSize=min	Specifies window size

[PCS,3] —The section for the third APG instrument, “Analyzer 3”

Parameter	Description
InstName=Analyzer3	The instrument name
InstType=offline	The instrument type. This instrument will run offline
Supervisor=no	Tells Bench Supervisor not to start this program, if Bench Supervisor is reading this PCS section
Start=no	Tells the server (APG_TOP) whether or not to start this instrument
WinSize=min	Specifies window size

[PCS,4] —The section for the fourth APG instrument, “Analyzer 4”

Parameter	Description
InstName=Analyzer4	The instrument name
InstType=offline	The instrument type. This instrument will run offline.
Supervisor=no	Tells Bench Supervisor not to start this program, if Bench Supervisor is reading this PCS section
Start=no	Tells the server (APG_TOP) whether or not to start this instrument
WinSize=min	Specifies window size

[PCS,5] —The section for the fifth APG instrument, “SFE Bridge”

Parameter	Description
Program=C:\HPCHEM\hp7680.exe	Higher level programs use these lines when calling this application. The line used depends on the program calling the application. Path\executable PCS # (This line starts the application—the # is needed.)
Program1=c:\hpchem\hp7680.exe 5 /a	
InstName=SFE Bridge	The instrument name
InstType=7680	The instrument type
Path=C:\SFE1	The directory path for the instrument
Supervisor=yes	Tells Bench Supervisor to start this program, if Bench Supervisor is reading this PCS section
Start=no	Tells the server (APG_TOP) whether or not to start this instrument
Devices=3	The devices that this instrument uses (relates to [PCS] section)
jconbmp=c:\hpchem\hp7680.bmp	Bitmap used for this instrument in the JCON window
WinSize=normal	Specifies window size
Method=C:\SFE1\method.ext	The instrument method file path

[PCS,6] —The section for the sixth APG instrument, “Tray”

Parameter	Description
InstName=Tray	The instrument name
InstType=Tray	The instrument type
Path=c:\hpchem\bs	The directory path for the instrument
Program=c:\hpchem\bs\gcmstray.exe 6	path\executable PCS # (This line starts the application—the # is needed)
Devices=2	The device that this instrument uses (relates to [PCS] section
Supervisor=yes	Tells Bench Supervisor to start this program, if Bench Supervisor is reading this PCS section
Start=no	Tells the server (APG_TOP) whether or not to start this instrument
WinSize=min	Specifies window size
WinShow=hide	The icon and program for this application will be hidden
Bracket=prep	Specifies the type of bracket the tray is on

[PCS_BS] —The section for Bench Supervisor

Parameter	Description
Controllers=5,6,1	Specifies which PCS sections Bench Supervisor reads
Path=C:\HPCHEM\bs\database	Specifies the Bench Supervisor data path, which Bench Supervisor will create
Tray=gc	Specifies the TRAY orientation. Valid types are GC, LC and GCMS.
ShowTrayInsts=no	Tells Bench Supervisor not to display the Tray instrument window
Holder=Holder	Designates the holder location
Manual=TRAY	The tray will place vials in the analyzer.
Hide=Tray, Manual, Holder	Bench Supervisor will hide the icon and program for these applications

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