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XML Connectivity Guide

Agilent Technologies

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In This Guide...

This guide contains installation and reference information for the XML interface between the Agilent ChemStation and a LIMS system. The Appendixes contain examples of the XML files and the schemas used to generate them.

1 XML in the Agilent ChemStation

This chapter gives an introduction to XML, and describes how the interface is implemented.

2 Enabling XML Functionality

This chapter contains an explanation of how the Agilent ChemStation imports an XML file from the LIMS system.

3 Import Worklist

This chapter describes the changes that have to be made to enable the XML interface functions in the Agilent ChemStation.

4 LIMS Fields: Linking the Sample to the Result File

This chapter describes how the samples and their associated data are uniquely identified in the XML interface.

5 Export Data

This chapter explains how the Agilent ChemStation exports the XML file to the LIMS system.

A Example Result File

This appendix contains an example of a results file in XML format in the form that would be exported to a LIMS system.

B Export File Schema (EXPORT.XSD)

In this appendix, the schema that is used to produce the results file for export is listed.

C Sample Worklist File

This appendix gives an example of a worklist file of the type that would be imported into the Agilent ChemStation.

D Worklist Schema (WORKLIST.XSD)

This appendix lists the schema that is used to produce the worklist XML file.

Contents

1 XML in the Agilent ChemStation

This chapter gives an introduction to XML, and describes how the interface is implemented.

What is XML?

XML (eXtensible Markup Language) is a protocol for structuring data in pure text format; the XML file contains data with embedded structural information and, being pure text, it can be edited with a simple editor like Notepad. XML has become a very flexible and portable format especially for exchanging data between different systems.

XML in the Agilent ChemStation

Because of its flexibility and portability, XML can provide the interconnectivity between the Agilent ChemStation and a LIMS system. The workflow that describes the connectivity can be divided into the five sequential activities shown in Figure 1:

1. the sample list is generated by the LIMS system in an XML format
2. it is imported by the Agilent Chemstation
3. samples are analyzed
4. the results of the analysis are exported to an XML results file
5. the XML results file is transferred back to the LIMS system (manually or automatically)

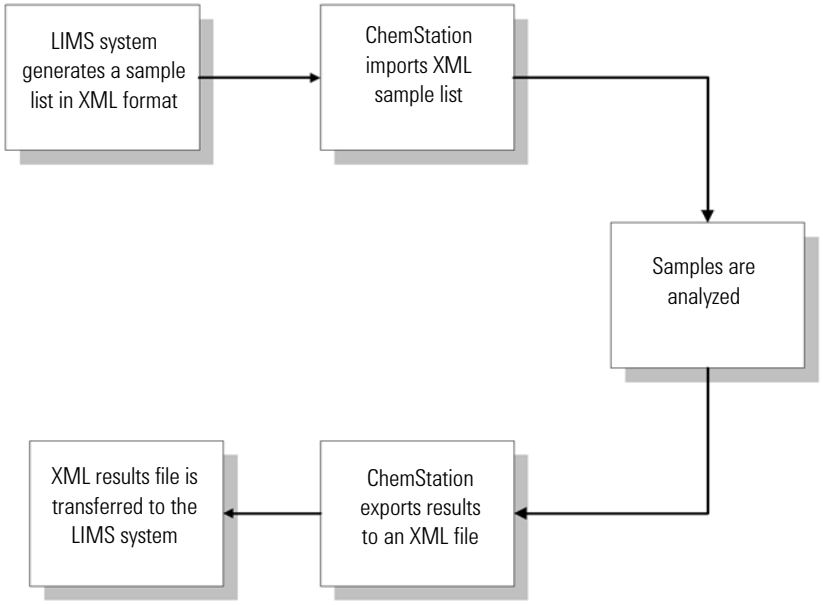

Figure 1 Workflow for XML in the Agilent ChemStation

The Agilent ChemStation XML interface manages two tasks:

- import a worklist containing a sequence in XML format
- export a result file in XML format either manually or automatically

Agilent ChemStation XML support uses XSD templates to describe the document schemas.

2
Enabling XML Functionality

Making Entries in the ChemStation.ini-File

XML functionality in the Agilent ChemStation is enabled by entries in the CHEMSTATION.INI file. The file is located in the windows directory; c:\WINDOWS. Two entries in the [PCS] section of the CHEMSTATION.INI file enable the complete XML export/import functionality. These entries are not written to the CHEMSTATION.INI file during installation, but must be added manually by the system administrator.

[PCS]

XMLEnableImport=1

XMLEnableExport=1

The lack of the entry, or *entry=0* turns off the functionality.

Import-Related Entries

In the section for each instrument, [PCS,n], a variable specifies the default directory for importing files. This is the directory in which the import file dialog opens, and where the manual import function looks for a file with no specified path.

[PCS,n]

XMLImportPath$=d:\xml\wrkl

Export-Related Entries

Instrument-specific entries ([PCS,n] section)

[PCS,n]

XMLExportDestUNC$=\\server\share\directory

XMLExportDestUNC$ describes a path to a remote directory to which the result files will be copied when AUTOMATION mode is enabled. It can be a UNC path.

System-specific entries ([PCS] section)

[PCS]

XMLAutomation=1

XMLAutomation enables the AUTOMATION mode, in which the XML results file is copied automatically from the local raw datafile directory to a remote location during the running of a sequence with Data Analysis.

[PCS]

XMLExportCopyWaitTime=3

XMLExportCopyTries=10

XMLExportCopyTries and *XMLExportCopyWaitTime* specify the number of times the copying application tries to copy the results file to a remote location (*XMLExportDestUNC$*), and the time (in seconds) it should wait between successive tries.

[PCS]

XMLExportLocalRecovPath$=c:\Chem32\recovery

When all the tries of copying fail, *XMLExportLocalRecovPath$* specifies the recovery directory to which the XML file is copied. This must be a local directory.

[PCS]

XML_ExportOnPrint=1

XML_ExportOnPrint enables an update of the result xml file each time a report of the corresponding data file is printed.

NOTE If export of the result.xml on report printing is enabled the result file is not automatically uploaded to a remote location even if *XMLAutomation* is enabled.

[PCS]

XML_ExportAlwaysExtPerf=1

XML_ExportAlwaysExtPerf enables the export of all extended performance parameters that are available with the Extended Performance report style of the ChemStation, independently of the report style that is actually selected. If this option is disabled the extended performance parameters will only be exported when Extended Performance is selected as report style (see page 34 for more information about the various report styles in ChemStation).

3 Import Worklist

The XML-formatted worklist is imported into Chemstation as a sequence table. Two modes of import are provided:

- manual/interactive: a menu item allows the user to select the file to be imported
- automatic: a macro function is used to import the file.

General

The XML file is transformed into an intermediate format using an XSL stylesheet and an external application, which uses Windows MSXML libraries for the transformation.

The application needs a Windows MSXML library of version 3.0 or later. Earlier versions of the library, which do not support XSL transformation, must be updated to the newer version. Updates are readily available for free download from the Microsoft web site.

NOTE

It is possible to run \Chem32\CORE\XML2CSV.EXE from the command line without any parameters. The first line of the output *"Agilent (R) XML Transformer - using MSXML library version 3.0"* specifies the currently used MSXML version.

Format of the Worklist File

The worklist file is an XML file formatted as defined by an XML schema file. The schema file describes the structure of the worklist and may be used as a template for creating correct worklist files. The XML schema for worklists to import is stored as "\Chem32\CORE\worklist.xsd". The complete schema is shown in Appendix D. An example XML worklist file is shown in Appendix C.

The connectivity between the LIMS systems and Agilent ChemStation software has been achieved by introducing three additional columns: LimsID, LimsKField2, and LimsKField3. These are described in detail in "LIMS Fields: Linking the Sample to the Result File" on page 27.

Manual/Interactive Import

Sequence Menu

An additional item, Import XML Worklist, appears in the Sequence menu (full menus) in the Method and Run Control view (see Figure 2). The menu item appears only when *XMLEnableImport=1*.

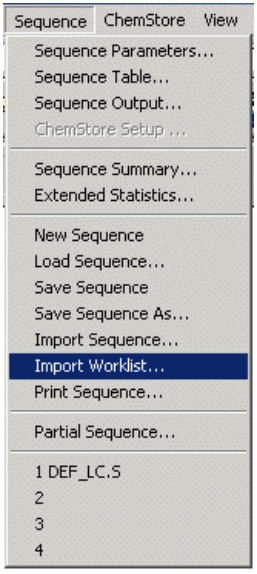

Figure 2 Sequence menu with XML Import

In GC ChemStation, there are two entries for import of worklists for both the front and the back injector.

Import XML Worklist displays the Import XML File dialog box (see Figure 3 on page 19), which allows the user to select an XML-formatted worklist to import. The default directory for each instrument is specified separately in the relevant [PCS,n] section of CHEMSTATION.INI. If the variable is not properly specified, or not specified at all, the default directory is _EXEPATH$.

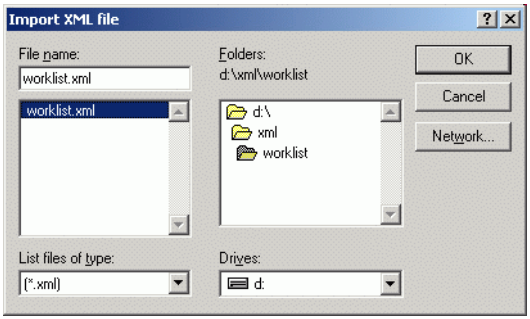

Figure 3 The Import XML File dialog box

XML Import Table

If the file has been read successfully, the XML Import table is displayed (see Figure 4 on page 20). It presents a preview of the rows to import. It does not show all fields comprising the worklist, but shows the following columns:

- Line Number
- Vial
- Sample Name
- Method
- Sample Type
- Sample Info
- LimsID

The window is not resizable; the first three columns are fixed, the horizontal scroll bar allows access to columns at the right of the table.

At this level, no error checking is provided. The table shows all strings as they are, without interpretation. It is the user's responsibility to discard obviously invalid rows.

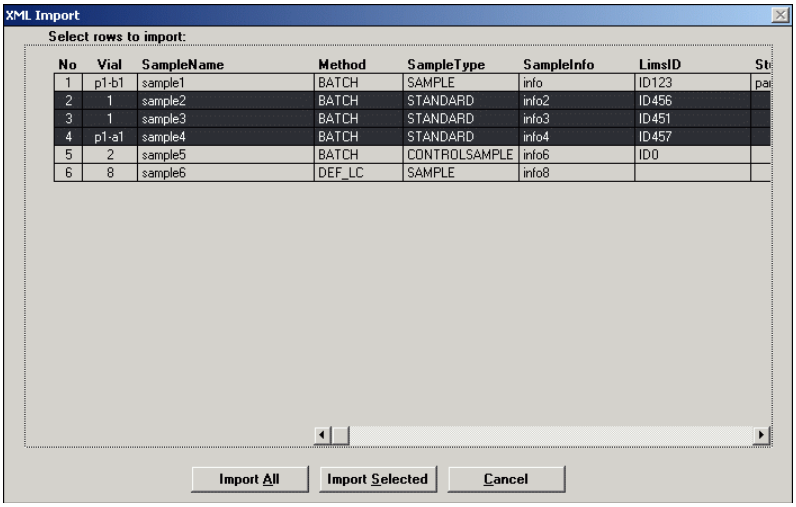

Figure 4 The XML Import Table

Selection of multiple rows is possible. The buttons give possibilities to **Import All** rows, **Import Selected** rows and to **Cancel** the import process.

Import Process

The interactive import always works in *replace* mode: it replaces the current sequence table with the imported one. All the fields are imported in accordance with Import Sequence rules. They are string columns with the maximum size of 40 characters. The corresponding values are imported from the XML worklist input file.

All the columns are checked for correctness but are always imported (even with errors, as Import Sequence does). It is the user's responsibility to make a decision if the worklist should be imported, based on the information shown in the Import Summary (see Figure 5 on page 22).

The columns imported are:

- Location
- Sample Name
- Method

- Number Of Injections
- SampleType
- Cal Level
- Update RF
- Update RT
- Interval
- Sample Amount
- ISTD Amount
- Multiplier
- Dilution
- Data Filename
- Injection Volume
- Sample Info
- LimsID

The second and third LIMS fields, LimsKField2 and LimsKField3, are also imported, but are not displayed in the sequence table as columns.

Import Summary

The Import Summary dialog box works the same way as in Import Sequence. As the import progresses, it shows the current status of the process, and all the errors encountered. The dialog box buttons are inactive until the import is finished.

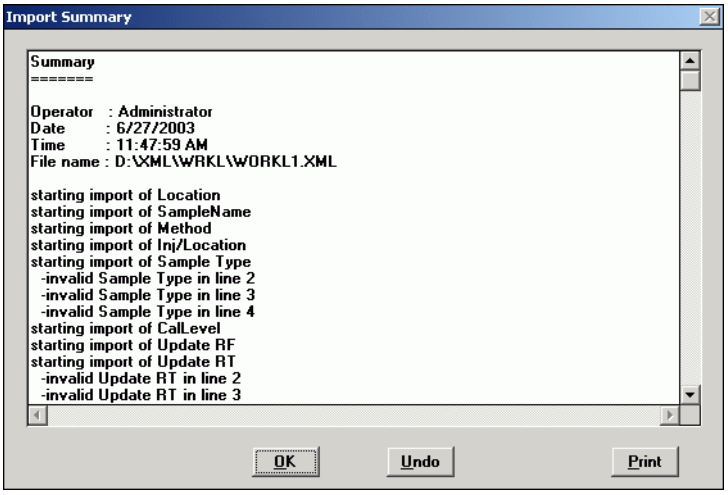

Figure 5 The Import Summary

When the import is complete, the imported sequence table is still a temporary one, and the user has the possibility of confirming the import. The **OK** button exchanges the current sequence table for the imported one; **UNDO** abandons the whole process (the current sequence table remains unchanged); **PRINT** prints the content of the window.

If the input XML file is wrongly formatted, or contains no data, the message **Nothing imported!** is displayed. In this case, both the **OK** and **UNDO** buttons simply close the dialog box, and the current sequence table remains unchanged. Please check that the MSXML libraries are installed.

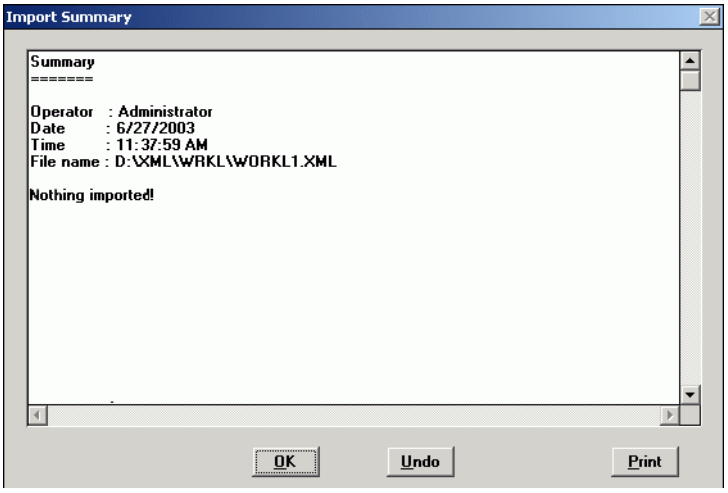

Figure 6 The Import Summary with no import

Common Sequence Information

In addition to the columns mentioned above, the worklist schema allows to import a table of general sequence information. This table is independent of the sequence table, but can easily be correlated to the sequence table rows if necessary.

The Common Sequence Information consists of both rows and header items in the following structure (for a complete example of a worklist.xml see Appendix C, “Sample Worklist File”):

```
<CommonInformation Type="HEADER">
    <Name>MyHeader</Name>
    <Value>TextMyHeader</Value>
</CommonInformation>
<CommonInformation Type="ROW">
    <Name>MyRow1</Name>
    <Value>ValueMyRow1</Value>
</CommonInformation>
<CommonInformation Type="ROW">
    <Name>MyRow2</Name>
    <Value>ValueMyRow2</Value>
</CommonInformation>
```

The information in the *CommonInformation* node of the worklist is not automatically exported to the result.xml’s custom table. Because the Common Information is stored in a register of the sequence file, this can achieved with an additional macro employing the XML_PreExport hook. See “Hooks and Custom Results Table” on page 49 for more details.

Automated Import

Automated import enables non-interactive import of an XML worklist to the current sequence table. It can be used in any batch process when no interaction is needed or indeed when any interaction is unwelcome.

The macro function that imports the worklist uses the following parameters:

Name XML_ImportWorklist

Parameter ImportFileName$

Parameter boErrorEnds default 0

Parameter boAppendSequence default 0

Parameter boRowSelection default 0

Parameter boSumLog default 0

ImportFileName$

A string describing the full path to the XML worklist to import. If no full path is given, the file is searched in the default XMLImportPath$ directory.

boErrorEnds

A 0/1 variable. 0 is the default setting; the import is not stopped by an error; every value gets imported, even when incorrect, and only the notifications are shown in the summary. 1 stops the import function when it encounters an error.

boAppendSequence

A 0/1 variable. 0 is the default *replace* state. 1 switches to *append* mode, in which the imported data is appended to the current sequence table.

CAUTION The maximum number of rows in the sequence table is 999. Any rows that exceed this number are not imported.

boRowSelection

A 0/1 variable. 0 is the default setting, which disables row selection in the import table, as described in “XML Import Table” on page 19. 1 enables interactive row selection.

boSumLog

A 0/1 variable. 0 is the default setting, which suppresses the Import Summary: no summary is produced after having the rows imported, and there is no possibility to undo the import. 1 enables the Import Summary.

The return value describes the last encountered error (when in “boErrorEnds=0” mode) or the error causing the import to stop (when in “boErrorEnds=1” mode). The error code is a combined float value, where the integer part indicates the error type and the fractional part indicates the row number where the error occurred.

Error codes:

0 – no error

1 - wrong type

2 - exceeds the max length

3 - out of range

4 - invalid chars

5 - invalid value

6 - file doesn't exist

7 - seq is running

8 - XML file in invalid format

The error value 2.34 describes that some value in the 34th row exceeded the maximum length limit.

The most frequently used form of the command may look like this:

Val = XML_ImportWorklist(“worklist.xml”)

This imports the file from the default import directory, does not stop on any error, replaces the current sequence table, does not show row selection, and suppresses the Import Summary.

4 LIMS Fields: Linking the Sample to the Result File

One of the main objectives of the implementation of the XML import/export mechanism is the continuity of sample identity in the flow of data between the Agilent ChemStation and the LIMS system. This chapter describes how the samples and their associated data are uniquely identified in the XML interface.

Workflow

The XML import/export function can be envisaged as four separate sub-tasks:

1. The user exports a worklist from a LIMS system.
2. The worklist is imported into the Agilent ChemStation's sequence table.
3. Every sample of the worklist is analyzed by the Agilent ChemStation.
4. The result datafile is exported back to LIMS system.

The main issue is to establish a correspondence between the imported sample information in the worklist and the results exported to the LIMS.

LIMS IDs and the Sequence Table

"Import Process" on page 20 contains a list of the imported columns. Three new columns are introduced: LimsID, LimsKField2, and LimsKField3. Every sample in the worklist may contain additional data in these three fields. The fields can be used, for example, to unambiguously identify the samples in the LIMS system, or for any other LIMS-related purpose.

When the worklist is imported, three additional fixed-length string columns are created in the first sequence table (SeqTable1) of the _SEQUENCE registry. They are given the names of the fields in the worklist: LimsKField1 (displayed as LimsID), LimsKField2, and LimsKField3. For every imported sequence line, appropriate values for the LIMS fields are imported into the sequence table.

Additional File in the Raw Data File Directory

In Agilent ChemStation, the raw data files are not bound to the sequence table data; once the data has been acquired and analyzed, it has no direct relationship with the sample described as a row of the sequence table. The additional LimsKFields imported to the sequence table have to be stored along with the raw datafile, otherwise they will not be linked to the output data.

An additional XML file (limsinf.xml) is created in a raw datafile directory. The XML export uses the values to insert the LIMS information into the exported result file. The file has a very simple structure:

<?xml version="1.0" encoding="UTF-8"?>

<SampleLimsInfo xmlns:xsi="http:\\www.w3.org\2001\
XMLSchema-instance">

<LimsKField1>1</LimsKField1> (displayed as LimsID)

<LimsKField2>2</LimsKField2>

<LimsKField3>3</LimsKField3>

</SampleLimsInfo>

It contains the values of the sequence table's LimsKFieldN column for the corresponding sample.

The file is created at two hooks, only when a sequence is running and when the LIMS columns exist in the sequence table:

PostACQ (executed after DATA ACQUISITION)

PostDA (executed after DATA ANALYSIS)

The file can be overwritten when reprocessing the data. This is intentional: the user is allowed to change at least LimsKField1 value using the sequence table editor.

For the user, this means that after changing the LimsID in the sequence table, the sequence has to be reprocessed, so that the correct values get written into limsinf.xml.

The LIMS Fields Idea in Summary

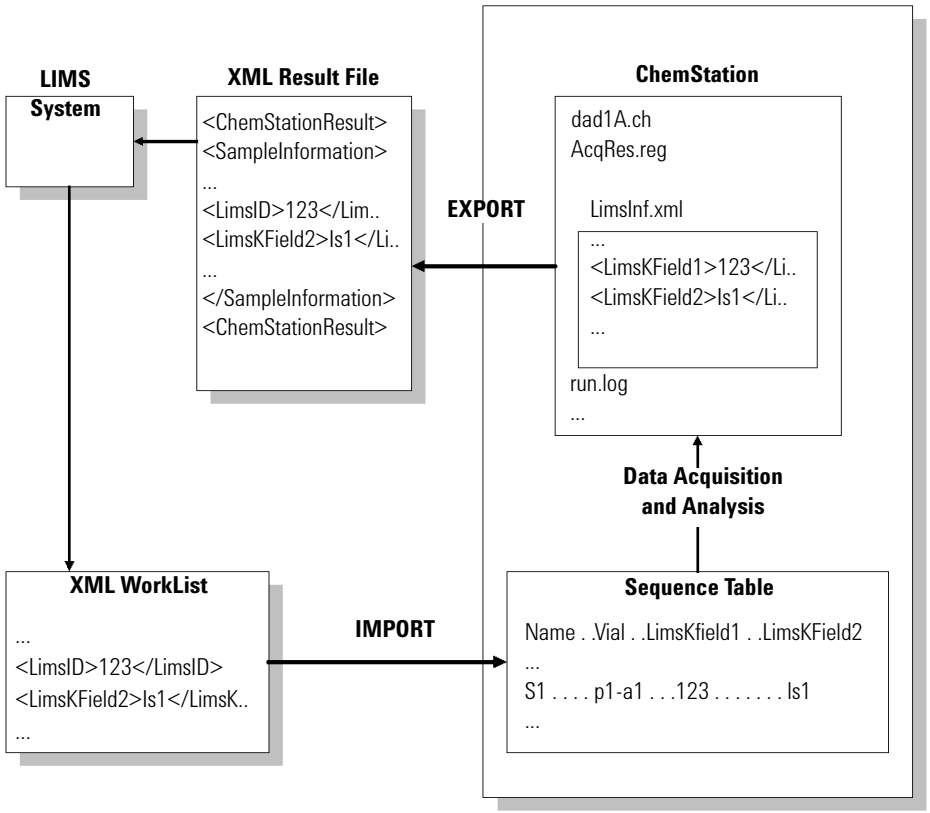

Figure 7 Persistence of the LIMS fields

5 Export Data

The XML-formatted result file is exported from the Agilent ChemStation and uploaded to the remote location if so configured. There are two modes:

- manual/interactive: a menu item and a button allow the user to export current results to an XML file and upload it to a remote directory
- automatic: the XML results file is generated automatically while a sequence is running and the file is copied to a remote directory if configured

The file is protected by a checksum, and the user has a possibility to check the integrity of the datafile with a command-line tool. If the first attempt at copying to the remote location fails, more attempts are made. If all attempts fail, the file is copied to the local directory.

General

The export process is driven by a macro that creates an XML file containing values taken from the CHROMREG and CHROMRES registers. The file is created either automatically (after the data analysis while the sequence is running) or manually (in Data Analysis view) using a button/menu item. The file is created in an appropriate raw datafile directory and copied to a remote location if *XMLAutomation*=1.

The report type is determined by the **Specify Report** settings of the method. The following settings affect the export file:

- Style: Short, Detail, Header+Short, GLP+Short, GLP+Detail, Short+Spectrum, Detail+Spectrum, Full and Library Search all generate the same standard style of export file.
  Performance styles add an amount of complementary detail in accordance with the style name.
  None means that no quantitative Results section is included in the export file.
- Report Layout For Uncalibrated Peaks: Do Not Report means that no uncalibrated peaks are included in the Results section of the export file. The other options are treated identically: uncalibrated peaks are included.

In addition, the option *XML_ExportAlwaysExtPerf=1* enables an export of the extended set of performance parameters as provided by the Extended Performance report style independent of the actual report style selected.

Manual Export

There is an additional menu entry in Data Analysis View, available only in Full Menu mode. It is present only when *XMLEnableExport*=1.

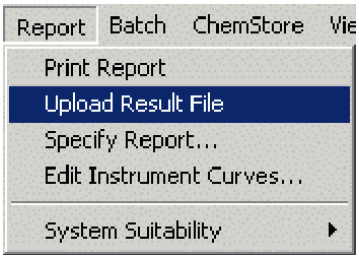

Figure 8 The Report menu for XML export

For the user's comfort, a tool is also available in the report section of the toolbar. It appears along with the other buttons of the section only when in Calibration Task or Integration Task mode. It also works in BATCH mode.

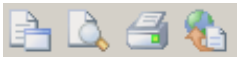

Figure 9 XML tool

The actions are undertaken in three phases:

1 identify and calculate peaks.

If this is successful:

2 create the XML results file (result.xml) in the current raw datafile directory (the directory current data registers are loaded from).

If this is successful:

3 upload the file to the remote location. For this step, the Automation mode has to be switched, and a remote location has to be specified in the ChemStation.ini file. See "Export-Related Entries" on page 13 for more details.

Automatic Export

The automatic export is done after data analysis for every sequence run, which means that if Data Analysis is not a part of the method, the file is not created.

The file (result.xml) is created in a current raw datafile directory and if *XMLAutomation*=1 it is uploaded to the remote directory in accordance with the settings in CHEMSTATION.INI. No user interface is necessary for automatic export.

The Format of the XML Results File

The result file includes the following sections:

- Acquisition parameters
- Module information
- Sample information
- Chromatograms
- Calibration information
- Results (Compound table)
- Fraction information
- Custom fields
- Custom results

Acquisition

Contains the version number of the acquisition software, instrument name, and method modification data:

```
<Acquisition>
        <Version>Rev. A.02.02 Copyright (c) Hewlett Packard 1990-2003</Version>
        <InstrumentName>HP LC 1050</InstrumentName>
          ...
</Acquisition>
```

Module Information

Contains a list of modules including: module name, serial number, firmware revision:

```
<ModuleInformation>
    <Module>
        <Number>1</Number>
        <NumberInModule>1</NumberInModule>
        <ModuleName>Analog/digital converter</ModuleName>
            ...
    </Module>
    <Module>
        <Number>2</Number>
            ...
    </Module>
    ...
</ModuleInformation>
```

Sample Information

Contains software revision description, fields from a sequence table line belonging to the sample plus method path and description and injection date/time:

```
<SampleInformation>
    <Version>Rev. C.01.01 [xxxx] Copyright © Agilent Technologies</Version>
    <VialUnused>0</VialUnused>
    <SequencePath/>
    <Dilution>-1</Dilution>
    <InjVolume>2</InjVolume>
      ...
</SampleInformation>
```

Chromatograms

Grouped by signals:

```
<Chromatograms>
        <Signal>
            <Title>DAD1 A, Sig=254,4 Ref=550,100 (DEMO\005-0102.D)</Title>
            <Description>DAD1 A, Sig=254,4 Ref=550,100</Description>
            …
            <IntegrationResults>
                <RetTime Unit="min">0.74711</RetTime>
                <Area Unit="mAU*s">300.036407</Area>
                …
            </IntegrationResults>
            <IntegrationResults>
            …
            </IntegrationResults>
        </Signal>
        <Signal>
            <Title>DAD1 B, Sig=230,4 Ref=550,100 (DEMO\005-0102.D)</Title>
            …
        </Signal>
</Chromatograms>
```

Each SIGNAL group contains signal descriptions (i.e. title, detector, signal id, operator, X and Y Axis units etc.) and all integrated peaks of the signal (INTEGRATIONRESULTS) with a thorough description of each peak: RT, Area, Area%, Width.

If the “Performance+Noise” report style is used, the SIGNAL node contains also a group called NOISE, built of NOISEPERIOD subnodes. They hold all the noise data generated by “Performance+Noise” report style.

```
<Chromatograms>
        <Signal>
            <Title>DAD1 A, Sig=254,4 Ref=550,100 (DEMO\005-0102.D)</Title>
            …
                <Noise>
              <NoisePeriod>
                <TimeFrom Unit="min">0</TimeFrom>
```

```
                    <TimeTo Unit="min">0.5</TimeTo>
                    <Noise6SD Unit="mAU">0.300586</Noise6SD>
                    <NoisePToP Unit="mAU">0.192784</NoisePToP>
                    <NoiseASTM Unit="mAU">0</NoiseASTM>
                    <Wander Unit="mAU">0</Wander>
                    <Drift Unit="mAU/h">16.720044</Drift>
                  </NoisePeriod>
                  <NoisePeriod>
                  ...
                  </NoisePeriod>
                </Noise>
                <IntegrationResults>
                ...
                </IntegrationResults>
              </Signal>
              ...
</Chromatograms>
```

Calibration Information

Contains the calibration settings. The three basic items describe

- the title of the calibration settings
- behavior if calibrated peaks are missing
- usage of multipliers and dilution factors with the ISTD compounds

```
<CalibrationInformation>
        <Title>Default Calibration</Title>
        <PartialCalibrationIfPeaksMissing correctallRTs="false">true</PartialCali-
brationIfPeaksMissing>
        <UseMultiAndDilutFactorWithISTDs>true</UseMultiAndDilutFactorWith-
ISTDs>
        <RecalibrationSettings>
          ...
        </RecalibrationSettings>
        <ISTD>
          ...
        </ISTD>
        <Signal>
          ...
        </Signal>
        <Compound>
          ...
        </Compound>
```

The RECALIBRATIONSETTINGS node contains the settings for recalibration.

```
<RecalibrationSettings>
        <AverageResponse Type="AVERAGEALLCALIBRATIONS" />
        <AverageRT Type="FLOATINGAVERAGENEW">75</AverageRT>
</RecalibrationSettings>
```

The ISTD node is only present if at least one compound is set up as internal standard (ISTD). For each ISTD compound there is a separate node.

```
<ISTD>
        <ISTDID>1</ISTDID>
        <Amount Unit="wt%">0.0900000000</Amount>
        <CompoundID>1</CompoundID>
        <Name>Dimethylphthalate</Name>
</Signal>
```

The SIGNAL nodes describe the signals that are calibrated and how any uncalibrated peaks in each signal are treated.

```
<Signal>
        <SignalID>1</SignalID>
        <SignalDesc>DAD1 A, Sig=254,4 Ref=550,100</SignalDesc>
        <UncalibratedPeaks />
</Signal>
```

The COMPOUND nodes describe for each of the calibrated compounds the related information from the calibration table, e.g. name, amount limits, information about ISTD usage, etc..

```
<Compound>
        <CompoundID>1</CompoundID>
        <Name>Dimethylphthalate</Name>
        <AmountLimitLow>0.0000000000</AmountLimitLow>
        <AmountLimitHigh>0.0000000000</AmountLimitHigh>
        <Multiplier>1.0000000000</Multiplier>
        <IsTimeReference>false</IsTimeReference>
        <IsISTD>true</IsISTD>
        <ISTDID>1</ISTDID>
        <CompoundSignal>
        ...
        </CompoundSignal>
</Compound>
```

For each of the signals assigned to the compound there is a node COMPOUNDSIGNAL. It contains information about the signal description, the usage of the peak in this signal, the details of the calibration curve, etc.

```
<CompoundSignal>
        <SignalID>1</SignalID>
        <SignalDesc>DAD1 A, Sig=254,4 Ref=550,100</SignalDesc>
        <ExpRetTime>0.7470206469</ExpRetTime>
        <RTWindowLow>0.7283451308</RTWindowLow>
        <RTWindowHigh>0.7656961631</RTWindowHigh>
        <PeakUsage>MAIN</PeakUsage>
        <Curve>
            <Correlation>1.0000000000</Correlation>
            <Origin>INCLUDE</Origin>
            <Type>LINEAR</Type>
            <Formula>
                <Text>y = mx + b</Text>
                <Parameter>
                    <Symbol>m</Symbol>
                    <Value>3303.5863623254</Value>
                </Parameter>
                <Parameter>
                    <Symbol>b</Symbol>
                    <Value>0.0000000000</Value>
                </Parameter>
            </Formula>
            <Weight>EQUAL</Weight>
        </Curve>
        <Level>
        ...
        </Level>
</CompoundSignal>
```

For each of the levels calibrated in the signal there is a separate LEVEL node containing all the level specific information:

```
<Level>
        <LevelID>1</LevelID>
        <Amount Unit="wt%">0.0900000036</Amount>
        <Area>297.3227844238</Area>
        <ResponseFactor>0.0003027013</ResponseFactor>
        <RefAmount>0.0900000036</RefAmount>
        <RespPercent>100.0000000000</RespPercent>
</Level>
```

Results

Contains the result of quantitative calculations, according to the current report settings. The two basic items describe:

- the type of calculation (Percent, ISTD,...)
- the base for calculation (Area, Height)

```
<Results>
   <QuantCalc>ESTD</QuantCalc>
   <QuantBase>Area</QuantBase>
   <ResultsGroup>
   ...
   </ResultsGroup>
   <ResultsGroup>
   ...
   </ResultsGroup>
</Results>
```

The RESULTSGROUP nodes contain peak groups.

When the calculation is of a percent type, peaks are grouped by signals. The group description is a particular signal description then.

```
   <ResultsGroup>
      <ResultsGroupDescription>DAD1 A, Sig=254,4 Ref=550,100</ResultsGroup-
Description>
      <Peak>
      ...
      </Peak>
      <Peak>
      ...
      </Peak>
   </ResultsGroup>
   <ResultsGroup>
      <ResultsGroupDescription>DAD1 C, Sig=280,4 Ref=550,100</ResultsGroup-
Description>
      <Peak>
      ...
      </Peak>
      <Peak>
      ...
```

```
        </Peak>
    </ResultsGroup>
```

When the calculation is of any other type, there is only one group, called MAIN. It contains all the calculated peaks.

```
<ResultsGroup>
        <ResultsGroupDescription>MAIN</ResultsGroupDescription>
        <Peak>
        ...
        </Peak>
        <Peak>
        ...
        </Peak>
</ResultsGroup>
```

PEAK node represents a single peak/compound (in the “Percent” calculations all of the integrated peaks are the part of the result file, not only found compounds).

```
 <Peak>
        <SignalDesc>DAD1 A, Sig=254,4 Ref=550,100</SignalDesc>
        <PeakType>BB </PeakType>
        <ExpRetTime Unit="min">0.747087</ExpRetTime>
        <MeasRetTime Unit="min">0.74711</MeasRetTime>
        <Area Unit="mAU*s">300.036407</Area>
        <Height Unit="mAU">106.920616</Height>
        <Width Unit="min">0.044739</Width>
        <Symmetry>0.716419</Symmetry>
        <Name>Dimethylphthalate</Name>
        <Amount Unit="wt%">0.0905459542</Amount>
</Peak>
```

Apart from the basic data (the Signal it belongs to, Peak type, RT, Area, Height, ...), each peak contains the “amount” field which presents the result of the current quantitative calculations, and the name of the found compound (if the method supports calibration table with compound names).

In calculations of other type (not Percent) only compounds with the amount >0.0 are presented.

When a “Performance“-like results XML file is generated, additional nodes appear in a PEAK section:

```
<Peak>
    ...
    <kPrime>5.42268</kPrime>
    <PlatesHalfWidth>4080.07502</PlatesHalfWidth>
    <ResolutionHalfWidth>11.903108</ResolutionHalfWidth>
    <Selectivity>3.48661</Selectivity>
    <Skew>1.039269</Skew>
    <Excess>1.564137</Excess>
    ...
    and other performance results
</Peak>
```

When System Suitability -> Performance Limits are set the information about them appears as an attribute at the value affected by the limits.

A value is higher than the higher limit:

```
<kPrime Suitability=”>”>5.42268</kPrime>
```

A value is lower than the lower limit:

```
<PlatesHalfWidth Suitability=”<”>4080.07502</PlatesHalfWidth>
```

A value is between the limits:

```
<ResolutionHalfWidth Suitability=”=”>11.903108</ResolutionHalfWidth>
```

Fraction Information

Contains the fraction collection settings and information about the fractions collected in the data file, including information about the recovery locations.

In the COLLECTION section information is provided about the fraction trigger mode and the criteria for fraction collection:

```
<Collection>
    <Type>PEAK</Type>
    <Criteria>
        <Name>MaximumPeakDuration</Name>
        <Value Unit="min">0.5</Value>
    </Criteria>
</Collection>
```

The DATA section contains information about the collected fractions and the recovery locations:

```
<Data>
    <Fractions>
        <Fraction>
            <Frac>1</Frac>
            <Well>1</Well>
            <Location>1-P1-A-01</Location>
            <Volume Unit="microliter">89.791664</Volume>
            <BeginTime Unit="min">4.009667</BeginTime>
            <EndTime Unit="min">4.08445</EndTime>
            <Reason>DAD1</Reason>
        </Fraction>
        ...
    </Fractions>
    <RecoveryLocations>
        <RecoveryLocation>
            <Recovery>1</Recovery>
            <Location>2-Vial 1</Location>
            <Volume Unit="microliter">191.0625</Volume>
        </RecoveryLocation>
        ...
    </RecoveryLocations>
</Data>
```

Custom results

Contains custom results from “XmlCustom” table.

Hooks and Custom Results Table

The XML results file supports custom results. This means that the exported file can contain the custom values structured in a simple tabular form.

Three additional hooks are available to the user:

XML_PreExport: executed just before the values from the CHROMREG/CHROMRES registers are exported.

XML_PostExport: executed after the XML results file has been created; checksum has not been created yet.

XML_PostUpload: executed after creation of the checksum and after the XML results file has been uploaded to a remote directory

At the beginning of the export process, an empty *XmlCustom* table is created in the CHROMRES register. It contains two text columns (*Item* and *Text*):

XMLCUSTOM

Item	Text
...	...

Immediately after the table has been created, the *XML_PreExport* hook is triggered. It is intended to give the user an opportunity to fill the *XmlCustom* table with his/her own values.

Example of the macro:

Name *XML_FillCustomTableExample*

InsTabRow *ChromRes, "XmlCustom", 1:2*

SetTabText *ChromRes, "XmlCustom", 1, "Item", "ItemExample1"*

SetTabText *ChromRes, "XmlCustom", 1, "Text", "TextExample1"*

SetTabText *ChromRes, "XmlCustom", 2, "Item", "ItemExample2"*

SetTabText *ChromRes, "XmlCustom", 2, "Text", "TextExample2"*

EndMacro

A command:

SetHook *"XML_PreExport", " XML_FillCustomTableExample "*

sets the *XML_FillCustomTableExample* macro to be executed every time before exporting the file.

If the table is not empty, the following sections are created as a part of the XML results file:

```
...
<CustomResults>
        <Info>
            <Item>ItemExample1</Item>
            <Text>TextExample1</Text>
        </Info>
        <Info>
            <Item>ItemExample2</Item>
            <Text>TextExample2</Text>
        </Info>
</CustomResults>
...
```

Having created the file, the exporting process executes the *XML_PostExport* hook and deletes the *XmlCustom* table.

The Custom Results table can also be used to export the Common Sequence Information (see “Common Sequence Information” on page 24) of the imported worklist into the result.xml file using the XML_PreExport hook

Example of a macro:

Name *ExportSeqCommonInfoToXML*

Local *hdrnr,hdrcnt,rownr,rowcnt,newrow,hdrname$*

If *RegSize(ChromRes)* < *1* **Then**

Return

EndIf

```
If ObjHdrType(ChromRes,XmlCustom) <> 4 or
ObjHdrType(_sequence,commoninfo) <> 4 Then
    Return
EndIf
hdrnr = TabHdrVal(_sequence,commoninfo,"NumberOfHead")
If hdrnr > 4 Then
    For hdrcnt = 5 To hdrnr
      InsTabRow chromres,"xmlcustom"
      newrow = TabHdrVal(ChromRes,xmlcustom,"NumberOfRows")
      hdrname$ = TabHdrName$(_sequence,commoninfo,hdrcnt)
     SetTabText chromres,"xmlcustom",newrow,"item","HEADER_NAME: "
+ hdrname$
     SetTabText chromres,"xmlcustom",newrow,"text","HEADER_TEXT: " +
TabHdrText$(_sequence,commoninfo,hdrname$)
    Next hdrcnt
EndIf
rownr = TabHdrVal(_sequence,commoninfo,"NumberOfRows")
If rownr > 0 Then
    For rowcnt = 1 To rownr
      InsTabRow chromres,"xmlcustom"
      newrow = TabHdrVal(ChromRes,xmlcustom,"NumberOfRows")
      SetTabText chromres,"xmlcustom",newrow,"item","ROW_NAME: " +
TabText$(_sequence,commoninfo,rowcnt,"Name")
      SetTabText chromres,"xmlcustom",newrow,"text","ROW_VALUE: " +
TabText$(_sequence,commoninfo,rowcnt,"Value")
    Next rowcnt
EndIf
EndMacro
```

sethook *"XML_PreExport","ExportSeqCommonInfoToXML"*

Uploading the File: The Copying Process

The external application is responsible for copying an XML results file from the current raw datafile directory to a remote location. \Chem32\CORE\Filecopy.exe is a 32-bit command line application that can operate on UNC paths as well as on local directories. It is used indirectly only by macros creating result files when the *XMLAutomation* variable exists and is equal to 1.

First, it tries to copy the file to the *XMLExportDestUNC$* directory. If this fails, the application sleeps for *XMLExportCopyWaitTime* seconds and tries again. The process is repeated *XMLExportCopyTries* times. If the copying is still unsuccessful, it copies the file to *XMLExportLocalRecovPath$* directory (if it exists).

The appropriate messages are logged in the Instrument's Log Book, informing about the result of copying process and sources of errors.

The Name of the File

The name of the results file in the raw datafile directory is always the same: result.xml. The file is copied to the remote directory under a different name so as to:

1. make sure that the names are unique, since the files are copied to the same directory
2. make the names meaningful

The name is constructed as:

InstrumentName_SampleName_YYMMDDHHmmSS.xml

where the time included is the time of creating the file.

All the spaces in the instrument or sample's name are replaced with underscore "_"

Example:

HP_LC_1050_Isocratic_Std._1_030213111701.xml

NOTE

It is possible to use different naming convention for the name of the XML result file spooled to the remote directory. Two macros are available in the User Contributed Library (UCL) on the OpenLAB ChemStation Core Disk DVD that allow the user to choose between the following option:

LIMSID_DATE_TIME.xml or **DATE_TIME_LIMSID.xml**

Both solutions are based on macro usage. The installation and instructions to run the macros are documented in the readme.txt along with the macro.

Checksums

The checksum for the XML file is calculated using the MD5 algorithm. The checksum is inserted into the file as a root node attribute:

<ChemStationResult checksum="ce117a6da2eaa3a91d92d6ba9699a0fb">

It is a hexadecimal form of 128 bits value, always containing 32 characters of [0-9a-f] range.

Just after the XML results file has been created, the line above contains the checksum attribute equal to: checksum="00000000000000000000000000000000". The external \Chem32\CORE\ checksum.exe application calculates the 128 bits value for the file and then replaces the sequence of zeros with the calculated value.

The user is provided with the \Chem32\CORE\chkfile.exe command line tool to check the integrity of the XML results file. The tool extracts the checksum attribute from the XML file, replaces it temporarily with a sequence of zeros, calculates the checksum and compares it with the extracted one. If they are equal, it means that the XML file hasn't been changed since it was created. The message is printed to the standard output of application.

A
Example Result File

This appendix contains an example of a results file that includes extended results.

Special Formatting:

Body Objects (located directly under <Body>) appear green.

References to Body Objects (consisting of ID and Revision) appear blue.

Embedded Body Objects (types that could also be located directly under <Body>) appear red.

Embedded Sample Objects (located directly under <Sample>) appear brown.

```
<?xml version = "1.0" encoding="ISO-8859-1"?>
  <ChemStationResult xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xsi:noNamespace-
SchemaLocation="C:\Chem32\CORE\export.xsd" checksum="d50fb25d668361554903d6bb6a88f600">
    <Acquisition>
      <Version>Rev. A.02.02 Copyright (c) Hewlett Packard 1990-1993</Version>
      <InstrumentName>HP LC 1050</InstrumentName>
      <MethodPath/>
      <InjectionTime>1:00:00 AM</InjectionTime>
      <MethodLastModifiedTime>1:00:00 AM</MethodLastModifiedTime>
      <MethodLastModifiedBy/>
      <MethodModifiedAtRun>0</MethodModifiedAtRun>
```

```
</Acquisition>
<ModuleInformation>
 <Module>
  <Number>1</Number>
  <NumberInModule>1</NumberInModule>
  <ModuleName>Analog/digital converter</ModuleName>
  <SerialNumber/>
  <FirmwareRevision>Rev C.01.00</FirmwareRevision>
 </Module>
 <Module>
  <Number>2</Number>
  <NumberInModule>1</NumberInModule>
  <ModuleName>Pump</ModuleName>
  <SerialNumber/>
  <FirmwareRevision>3.1</FirmwareRevision>
 </Module>
 <Module>
  <Number>3</Number>
  <NumberInModule>1</NumberInModule>
  <ModuleName>Autosampler</ModuleName>
  <SerialNumber/>
  <FirmwareRevision>4.0</FirmwareRevision>
 </Module>
 <Module>
  <Number>4</Number>
  <NumberInModule>1</NumberInModule>
  <ModuleName>Diode array detector</ModuleName>
  <SerialNumber/>
  <FirmwareRevision>1.0</FirmwareRevision>
 </Module>
</ModuleInformation>
<SampleInformation>
 <Version>Rev. B.03.01 [xxx] Copyright © Agilent Technologies</Version>
 <VialUnused>0</VialUnused>
 <SequencePath/>
 <Dilution>-1</Dilution>
 <InjVolume>2</InjVolume>
 <ActInjVolume>2</ActInjVolume>
 <AcqInstName>HP LC 1050</AcqInstName>
 <SeqLine>1</SeqLine>
 <Location>Vial 5</Location>
```

```
    <Inj>2</Inj>
    <Method>DEMO.M</Method>
    <Operator>a.g.h.</Operator>
    <InjectionDateTime>4/19/94 7:52:24 AM</InjectionDateTime>
    <SampleName>Isocratic Std. 1</SampleName>
    <SampleInfo/>
    <IstdNum>1</IstdNum>
    <InternalStandardAmount>-1</InternalStandardAmount>
    <SampleAmount>-1</SampleAmount>
    <Multiplier>-1</Multiplier>
    <MethodInfo/>
    <CalMethod>C:\Chem32\1\METHODS\BATCH.M</CalMethod>
    <ResModDateTime>Thursday, February 01, 2007 1:28:51 PM</ResModDateTime>
    <LimsID>LF12</LimsID>
    <LimsKField2>LF22</LimsKField2>
    <LimsKField3>LF32</LimsKField3>
</SampleInformation>
  <Chromatograms>
    <Signal>
      <Title>DAD1 A, Sig=254,4 Ref=550,100 (DEMO\005-0102.D)</Title>
      <Description>DAD1 A, Sig=254,4 Ref=550,100</Description>
      <Detector>DAD1</Detector>
      <SignalId>A</SignalId>
      <Operator>a.g.h.</Operator>
      <DateTime>4/19/94 7:52:24 AM</DateTime>
      <DerivOrder>0</DerivOrder>
      <RawdataFile>C:\Chem32\1\DATA\DEMO\005-0102.D</RawdataFile>
      <Start>0.002083</Start>
      <End>6.962083</End>
      <XUnits>min</XUnits>
      <YUnits>mAU</YUnits>
      <IntegrationResults>
        <RetTime Unit="min">0.74711</RetTime>
        <Area Unit="mAU*s">300.036407</Area>
        <AreaPercent Unit="%">29.85427</AreaPercent>
        <AreaSum Unit="mAU*s">1005.003326</AreaSum>
        <Height Unit="mAU">106.920616</Height>
        <HeightPercent Unit="%">46.40455</HeightPercent>
        <HeightSum Unit="mAU">230.409767</HeightSum>
        <Width Unit="min">0.044739</Width>
        <Symmetry>0.716419</Symmetry>
```

```
  <Baseline>0.039978</Baseline>
  <TimeStart Unit="min">0.695417</TimeStart>
  <LevelStart>0.230399</LevelStart>
  <BaselineStart>0.027093</BaselineStart>
  <TimeEnd Unit="min">0.922083</TimeEnd>
  <LevelEnd>0.24495</LevelEnd>
  <BaselineEnd>0.083591</BaselineEnd>
</IntegrationResults>
<IntegrationResults>
  <RetTime Unit="min">1.022115</RetTime>
  <Area Unit="mAU*s">275.973206</Area>
  <AreaPercent Unit="%">27.45993</AreaPercent>
  <AreaSum Unit="mAU*s">1005.003326</AreaSum>
  <Height Unit="mAU">79.915726</Height>
  <HeightPercent Unit="%">34.684175</HeightPercent>
  <HeightSum Unit="mAU">230.409767</HeightSum>
  <Width Unit="min">0.052289</Width>
  <Symmetry>0.699074</Symmetry>
  <Baseline>0.108524</Baseline>
  <TimeStart Unit="min">0.96202</TimeStart>
  <LevelStart>0.550645</LevelStart>
  <BaselineStart>0.093545</BaselineStart>
  <TimeEnd Unit="min">1.18875</TimeEnd>
  <LevelEnd>0.212814</LevelEnd>
  <BaselineEnd>0.150059</BaselineEnd>
</IntegrationResults>
<IntegrationResults>
  <RetTime Unit="min">2.569072</RetTime>
  <Area Unit="mAU*s">176.769363</Area>
  <AreaPercent Unit="%">17.588933</AreaPercent>
  <AreaSum Unit="mAU*s">1005.003326</AreaSum>
  <Height Unit="mAU">26.735945</Height>
  <HeightPercent Unit="%">11.603651</HeightPercent>
  <HeightSum Unit="mAU">230.409767</HeightSum>
  <Width Unit="min">0.101136</Width>
  <Symmetry>0.62962</Symmetry>
  <Baseline>-0.038655</Baseline>
  <TimeStart Unit="min">2.455417</TimeStart>
  <LevelStart>0.13536</LevelStart>
  <BaselineStart>-0.036177</BaselineStart>
  <TimeEnd Unit="min">2.86875</TimeEnd>
```

```
    <LevelEnd>0.077134</LevelEnd>
    <BaselineEnd>-0.045186</BaselineEnd>
   </IntegrationResults>
   <IntegrationResults>
    <RetTime Unit="min">5.849135</RetTime>
    <Area Unit="mAU*s">252.22435</Area>
    <AreaPercent Unit="%">25.096867</AreaPercent>
    <AreaSum Unit="mAU*s">1005.003326</AreaSum>
    <Height Unit="mAU">16.837481</Height>
    <HeightPercent Unit="%">7.307624</HeightPercent>
    <HeightSum Unit="mAU">230.409767</HeightSum>
    <Width Unit="min">0.222766</Width>
    <Symmetry>0.669291</Symmetry>
    <Baseline>-0.049734</Baseline>
    <TimeStart Unit="min">5.605175</TimeStart>
    <LevelStart>0.233419</LevelStart>
    <BaselineStart>-0.06446</BaselineStart>
    <TimeEnd Unit="min">6.38875</TimeEnd>
    <LevelEnd>0.138756</LevelEnd>
    <BaselineEnd>-0.017162</BaselineEnd>
   </IntegrationResults>
  </Signal>
  <Signal>
   <Title>DAD1 B, Sig=230,4 Ref=550,100 (DEMO\005-0102.D)</Title>
   <Description>DAD1 B, Sig=230,4 Ref=550,100</Description>
   <Detector>DAD1</Detector>
   <SignalId>B</SignalId>
   <Operator>a.g.h.</Operator>
   <DateTime>4/19/94 7:52:24 AM</DateTime>
   <DerivOrder>0</DerivOrder>
   <RawdataFile>C:\Chem32\1\DATA\DEMO\005-0102.D</RawdataFile>
   <Start>0.002083</Start>
   <End>6.962083</End>
   <XUnits>min</XUnits>
   <YUnits>mAU</YUnits>
   <IntegrationResults>
    <RetTime Unit="min">0.74713</RetTime>
    <Area Unit="mAU*s">653.132202</Area>
    <AreaPercent Unit="%">36.775681</AreaPercent>
    <AreaSum Unit="mAU*s">1775.989422</AreaSum>
    <Height Unit="mAU">301.804749</Height>
```

```
    <HeightPercent Unit="%">53.555611</HeightPercent>
    <HeightSum Unit="mAU">563.535254</HeightSum>
    <Width Unit="min">0.036068</Width>
    <Symmetry>0.919298</Symmetry>
    <Baseline>56.379501</Baseline>
    <TimeStart Unit="min">0.698083</TimeStart>
    <LevelStart>-48.939671</LevelStart>
    <BaselineStart>52.960743</BaselineStart>
    <TimeEnd Unit="min">0.810568</TimeEnd>
    <LevelEnd>-42.619328</LevelEnd>
    <BaselineEnd>60.80143</BaselineEnd>
  </IntegrationResults>
  <IntegrationResults>
    <RetTime Unit="min">1.022128</RetTime>
    <Area Unit="mAU*s">608.131226</Area>
    <AreaPercent Unit="%">34.241827</AreaPercent>
    <AreaSum Unit="mAU*s">1775.989422</AreaSum>
    <Height Unit="mAU">223.176926</Height>
    <HeightPercent Unit="%">39.603011</HeightPercent>
    <HeightSum Unit="mAU">563.535254</HeightSum>
    <Width Unit="min">0.045415</Width>
    <Symmetry>0.81026</Symmetry>
    <Baseline>40.815121</Baseline>
    <TimeStart Unit="min">0.810568</TimeStart>
    <LevelStart>-24.324389</LevelStart>
    <BaselineStart>42.506493</BaselineStart>
    <TimeEnd Unit="min">1.464386</TimeEnd>
    <LevelEnd>-36.989391</LevelEnd>
    <BaselineEnd>37.279369</BaselineEnd>
  </IntegrationResults>
  <IntegrationResults>
    <RetTime Unit="min">2.568969</RetTime>
    <Area Unit="mAU*s">50.427227</Area>
    <AreaPercent Unit="%">2.839388</AreaPercent>
    <AreaSum Unit="mAU*s">1775.989422</AreaSum>
    <Height Unit="mAU">7.624327</Height>
    <HeightPercent Unit="%">1.352946</HeightPercent>
    <HeightSum Unit="mAU">563.535254</HeightSum>
    <Width Unit="min">0.101163</Width>
    <Symmetry>0.628476</Symmetry>
    <Baseline>0.063173</Baseline>
```

```
    <TimeStart Unit="min">2.463123</TimeStart>
    <LevelStart>0.103844</LevelStart>
    <BaselineStart>0.074115</BaselineStart>
    <TimeEnd Unit="min">2.802083</TimeEnd>
    <LevelEnd>0.115898</LevelEnd>
    <BaselineEnd>0.039075</BaselineEnd>
  </IntegrationResults>
  <IntegrationResults>
    <RetTime Unit="min">5.848876</RetTime>
    <Area Unit="mAU*s">464.298767</Area>
    <AreaPercent Unit="%">26.143104</AreaPercent>
    <AreaSum Unit="mAU*s">1775.989422</AreaSum>
    <Height Unit="mAU">30.929253</Height>
    <HeightPercent Unit="%">5.488433</HeightPercent>
    <HeightSum Unit="mAU">563.535254</HeightSum>
    <Width Unit="min">0.223136</Width>
    <Symmetry>0.66407</Symmetry>
    <Baseline>0.116811</Baseline>
    <TimeStart Unit="min">5.58875</TimeStart>
    <LevelStart>0.233893</LevelStart>
    <BaselineStart>0.094171</BaselineStart>
    <TimeEnd Unit="min">6.42875</TimeEnd>
    <LevelEnd>0.157922</LevelEnd>
    <BaselineEnd>0.167281</BaselineEnd>
  </IntegrationResults>
</Signal>
<Signal>
  <Title>DAD1 C, Sig=280,4 Ref=550,100 (DEMO\005-0102.D)</Title>
  <Description>DAD1 C, Sig=280,4 Ref=550,100</Description>
  <Detector>DAD1</Detector>
  <SignalId>C</SignalId>
  <Operator>a.g.h.</Operator>
  <DateTime>4/19/94 7:52:24 AM</DateTime>
  <DerivOrder>0</DerivOrder>
  <RawdataFile>C:\Chem32\1\DATA\DEMO\005-0102.D</RawdataFile>
  <Start>0.002083</Start>
  <End>6.962083</End>
  <XUnits>min</XUnits>
  <YUnits>mAU</YUnits>
  <IntegrationResults>
    <RetTime Unit="min">0.747073</RetTime>
```

```
    <Area Unit="mAU*s">159.286362</Area>
    <AreaPercent Unit="%">35.755745</AreaPercent>
    <AreaSum Unit="mAU*s">445.484665</AreaSum>
    <Height Unit="mAU">57.07592</Height>
    <HeightPercent Unit="%">50.930406</HeightPercent>
    <HeightSum Unit="mAU">112.066494</HeightSum>
    <Width Unit="min">0.044559</Width>
    <Symmetry>0.725186</Symmetry>
    <Baseline>0.107379</Baseline>
    <TimeStart Unit="min">0.695417</TimeStart>
    <LevelStart>0.166858</LevelStart>
    <BaselineStart>0.105893</BaselineStart>
    <TimeEnd Unit="min">0.882083</TimeEnd>
    <LevelEnd>0.222046</LevelEnd>
    <BaselineEnd>0.111263</BaselineEnd>
  </IntegrationResults>
  <IntegrationResults>
    <RetTime Unit="min">1.022065</RetTime>
    <Area Unit="mAU*s">144.066391</Area>
    <AreaPercent Unit="%">32.339248</AreaPercent>
    <AreaSum Unit="mAU*s">445.484665</AreaSum>
    <Height Unit="mAU">42.16349</Height>
    <HeightPercent Unit="%">37.623636</HeightPercent>
    <HeightSum Unit="mAU">112.066494</HeightSum>
    <Width Unit="min">0.051863</Width>
    <Symmetry>0.713981</Symmetry>
    <Baseline>0.115291</Baseline>
    <TimeStart Unit="min">0.962083</TimeStart>
    <LevelStart>0.296515</LevelStart>
    <BaselineStart>0.113565</BaselineStart>
    <TimeEnd Unit="min">1.175417</TimeEnd>
    <LevelEnd>0.142557</LevelEnd>
    <BaselineEnd>0.119703</BaselineEnd>
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  <IntegrationResults>
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    <Area Unit="mAU*s">37.495598</Area>
    <AreaPercent Unit="%">8.41681</AreaPercent>
    <AreaSum Unit="mAU*s">445.484665</AreaSum>
    <Height Unit="mAU">5.66039</Height>
    <HeightPercent Unit="%">5.050921</HeightPercent>
```

```
      <HeightSum Unit="mAU">112.066494</HeightSum>
      <Width Unit="min">0.101282</Width>
      <Symmetry>0.627049</Symmetry>
      <Baseline>0.013593</Baseline>
      <TimeStart Unit="min">2.463229</TimeStart>
      <LevelStart>0.071826</LevelStart>
      <BaselineStart>0.019464</BaselineStart>
      <TimeEnd Unit="min">2.802083</TimeEnd>
      <LevelEnd>0.083288</LevelEnd>
      <BaselineEnd>0.000635</BaselineEnd>
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    <IntegrationResults>
      <RetTime Unit="min">5.848838</RetTime>
      <Area Unit="mAU*s">104.636314</Area>
      <AreaPercent Unit="%">23.488197</AreaPercent>
      <AreaSum Unit="mAU*s">445.484665</AreaSum>
      <Height Unit="mAU">7.166694</Height>
      <HeightPercent Unit="%">6.395037</HeightPercent>
      <HeightSum Unit="mAU">112.066494</HeightSum>
      <Width Unit="min">0.226338</Width>
      <Symmetry>0.69496</Symmetry>
      <Baseline>0.031643</Baseline>
      <TimeStart Unit="min">5.588574</TimeStart>
      <LevelStart>0.061248</LevelStart>
      <BaselineStart>-0.010528</BaselineStart>
      <TimeEnd Unit="min">6.242084</TimeEnd>
      <LevelEnd>0.281816</LevelEnd>
      <BaselineEnd>0.095362</BaselineEnd>
    </IntegrationResults>
  </Signal>
</Chromatograms>
<CalibrationInformation>
  <Title>Default Calibration</Title>
  <PartialCalibrationIfPeaksMissing correctallRTs="false">true</PartialCalibrationIfPeaksMissing>
  <UseMultiAndDilutFactorWithISTDs>true</UseMultiAndDilutFactorWithISTDs>
  <RecalibrationSettings>
    <AverageResponse Type="AVERAGEALLCALIBRATIONS" />
    <AverageRT Type="FLOATINGAVERAGENEW">75</AverageRT>
  </RecalibrationSettings>
  <Signal>
    <SignalID>1</SignalID>
```

```
    <SignalDesc>DAD1 A, Sig=254,4 Ref=550,100</SignalDesc>
    <UncalibratedPeaks />
  </Signal>
  <Compound>
    <CompoundID>1</CompoundID>
    <Name>Dimethylphthalate</Name>
    <AmountLimitLow>0.0000000000</AmountLimitLow>
    <AmountLimitHigh>0.0000000000</AmountLimitHigh>
    <Multiplier>1.0000000000</Multiplier>
    <IsTimeReference>false</IsTimeReference>
    <IsISTD>false</IsISTD>
    <CompoundSignal>
      <SignalID>1</SignalID>
      <SignalDesc>DAD1 A, Sig=254,4 Ref=550,100</SignalDesc>
      <ExpRetTime>0.7470206469</ExpRetTime>
      <RTWindowLow>0.7283451308</RTWindowLow>
      <RTWindowHigh>0.7656961631</RTWindowHigh>
      <PeakUsage>MAIN</PeakUsage>
      <Curve>
        <Correlation>1.0000000000</Correlation>
        <Origin>INCLUDE</Origin>
        <Type>LINEAR</Type>
        <Formula>
          <Text>y = mx + b</Text>
          <Parameter>
            <Symbol>m</Symbol>
            <Value>3303.5863623254</Value>
          </Parameter>
          <Parameter>
            <Symbol>b</Symbol>
            <Value>0.0000000000</Value>
          </Parameter>
        </Formula>
        <Weight>EQUAL</Weight>
      </Curve>
      <Level>
        <LevelID>1</LevelID>
        <Amount Unit="wt%">0.0900000036</Amount>
        <Area>297.3227844238</Area>
        <ResponseFactor>0.0003027013</ResponseFactor>
        <RefAmount>0.0900000036</RefAmount>
```

```
      <RespPercent>100.0000000000</RespPercent>
    </Level>
  </CompoundSignal>
</Compound>
<Compound>
  <CompoundID>2</CompoundID>
  <Name>Diethylphthalate</Name>
  <AmountLimitLow>0.0000000000</AmountLimitLow>
  <AmountLimitHigh>0.0000000000</AmountLimitHigh>
  <Multiplier>1.0000000000</Multiplier>
  <IsTimeReference>false</IsTimeReference>
  <IsISTD>false</IsISTD>
  <CompoundSignal>
    <SignalID>1</SignalID>
    <SignalDesc>DAD1 A, Sig=254,4 Ref=550,100</SignalDesc>
    <ExpRetTime>1.0218706429</ExpRetTime>
    <RTWindowLow>0.9963238768</RTWindowLow>
    <RTWindowHigh>1.0474174090</RTWindowHigh>
    <PeakUsage>MAIN</PeakUsage>
    <Curve>
      <Correlation>1.0000000000</Correlation>
      <Origin>INCLUDE</Origin>
      <Type>LINEAR</Type>
      <Formula>
        <Text>y = mx + b</Text>
        <Parameter>
          <Symbol>m</Symbol>
          <Value>2980.5489945194</Value>
        </Parameter>
        <Parameter>
          <Symbol>b</Symbol>
          <Value>0.0000000000</Value>
        </Parameter>
      </Formula>
      <Weight>EQUAL</Weight>
    </Curve>
    <Level>
      <LevelID>1</LevelID>
      <Amount Unit="wt%">0.0900000036</Amount>
      <Area>268.2494201660</Area>
      <ResponseFactor>0.0003355087</ResponseFactor>
```

```
      <RefAmount>0.0900000036</RefAmount>
      <RespPercent>100.0000000000</RespPercent>
     </Level>
    </CompoundSignal>
   </Compound>
   <Compound>
    <CompoundID>3</CompoundID>
    <Name>Biphenyl</Name>
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    <AmountLimitHigh>0.0000000000</AmountLimitHigh>
    <Multiplier>1.0000000000</Multiplier>
    <IsTimeReference>false</IsTimeReference>
    <IsISTD>false</IsISTD>
    <CompoundSignal>
     <SignalID>1</SignalID>
     <SignalDesc>DAD1 A, Sig=254,4 Ref=550,100</SignalDesc>
     <ExpRetTime>2.5681717396</ExpRetTime>
     <RTWindowLow>2.5039674461</RTWindowLow>
     <RTWindowHigh>2.6323760331</RTWindowHigh>
     <PeakUsage>MAIN</PeakUsage>
     <Curve>
      <Correlation>1.0000000000</Correlation>
      <Origin>INCLUDE</Origin>
      <Type>LINEAR</Type>
      <Formula>
       <Text>y = mx + b</Text>
       <Parameter>
        <Symbol>m</Symbol>
        <Value>29407.0355720207</Value>
       </Parameter>
       <Parameter>
        <Symbol>b</Symbol>
        <Value>0.0000000000</Value>
       </Parameter>
      </Formula>
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     </Curve>
     <Level>
      <LevelID>1</LevelID>
      <Amount Unit="wt%">0.0060000001</Amount>
      <Area>176.4422149658</Area>
```

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      <ResponseFactor>0.0000340055</ResponseFactor>
      <RefAmount>0.0060000001</RefAmount>
      <RespPercent>100.0000000000</RespPercent>
    </Level>
  </CompoundSignal>
</Compound>
<Compound>
  <CompoundID>4</CompoundID>
  <Name>o-Terphenyl</Name>
  <AmountLimitLow>0.0000000000</AmountLimitLow>
  <AmountLimitHigh>0.0000000000</AmountLimitHigh>
  <Multiplier>1.0000000000</Multiplier>
  <IsTimeReference>false</IsTimeReference>
  <IsISTD>false</IsISTD>
  <CompoundSignal>
    <SignalID>1</SignalID>
    <SignalDesc>DAD1 A, Sig=254,4 Ref=550,100</SignalDesc>
    <ExpRetTime>5.8460775614</ExpRetTime>
    <RTWindowLow>5.6999256223</RTWindowLow>
    <RTWindowHigh>5.9922295004</RTWindowHigh>
    <PeakUsage>MAIN</PeakUsage>
    <Curve>
      <Correlation>1.0000000000</Correlation>
      <Origin>INCLUDE</Origin>
      <Type>LINEAR</Type>
      <Formula>
        <Text>y = mx + b</Text>
        <Parameter>
          <Symbol>m</Symbol>
          <Value>13970.0730297663</Value>
        </Parameter>
        <Parameter>
          <Symbol>b</Symbol>
          <Value>0.0000000000</Value>
        </Parameter>
      </Formula>
      <Weight>EQUAL</Weight>
    </Curve>
    <Level>
      <LevelID>1</LevelID>
      <Amount Unit="wt%">0.0179999992</Amount>
```

```
        <Area>251.4613037109</Area>
        <ResponseFactor>0.0000715816</ResponseFactor>
        <RefAmount>0.0179999992</RefAmount>
        <RespPercent>100.0000000000</RespPercent>
       </Level>
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   </Compound>
 </CalibrationInformation>
 <Results>
   <QuantCalc>ESTD</QuantCalc>
   <QuantBase>Area</QuantBase>
   <ResultsGroup>
     <ResultsGroupDescription>MAIN</ResultsGroupDescription>
     <Peak>
       <SignalDesc>DAD1 A, Sig=254,4 Ref=550,100</SignalDesc>
       <PeakType>BB  </PeakType>
       <ExpRetTime Unit="min">0.747087</ExpRetTime>
       <MeasRetTime Unit="min">0.74711</MeasRetTime>
       <Area Unit="mAU*s">300.036407</Area>
       <Height Unit="mAU">106.920616</Height>
       <Width Unit="min">0.044739</Width>
       <Symmetry>0.716419</Symmetry>
       <Name>Dimethylphthalate</Name>
       <Amount Unit="wt%">0.0905459542</Amount>
       <kPrime>0.867774</kPrime>
       <PlatesHalfWidth>1266.536758</PlatesHalfWidth>
       <ResolutionHalfWidth/>
       <Selectivity/>
       <Skew>1.226811</Skew>
       <Excess>3.487737</Excess>
       <WidthHalfHeight>0.049412</WidthHalfHeight>
       <Width5Sigma>0.10902</Width5Sigma>
       <WidthTangent>0.075845</WidthTangent>
       <WidthTailing>0.106667</WidthTailing>
       <USPTailing>1.098393</USPTailing>
       <TimeIncrement Unit="msec">800</TimeIncrement>
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       <StatisticalMoment0>296.804047</StatisticalMoment0>
       <StatisticalMoment1>0.752654</StatisticalMoment1>
       <StatisticalMoment2>0.000491</StatisticalMoment2>
       <StatisticalMoment3>0.000013</StatisticalMoment3>
```

```
  <StatisticalMoment4>1.566e-006</StatisticalMoment4>
  <PlatesTangent>1552.502327</PlatesTangent>
  <Plates5Sigma>1174.085003</Plates5Sigma>
  <PlatesStatistical>1153.031523</PlatesStatistical>
  <ResolutionTangent/>
  <Resolution5Sigma/>
  <ResolutionStatistical/>
 </Peak>
 <Peak>
  <SignalDesc>DAD1 A, Sig=254,4 Ref=550,100</SignalDesc>
  <PeakType>BB  </PeakType>
  <ExpRetTime Unit="min">1.022054</ExpRetTime>
  <MeasRetTime Unit="min">1.022115</MeasRetTime>
  <Area Unit="mAU*s">275.973206</Area>
  <Height Unit="mAU">79.915726</Height>
  <Width Unit="min">0.052289</Width>
  <Symmetry>0.699074</Symmetry>
  <Name>Diethylphthalate</Name>
  <Amount Unit="wt%">0.0917111781</Amount>
  <kPrime>1.555287</kPrime>
  <PlatesHalfWidth>1718.169915</PlatesHalfWidth>
  <ResolutionHalfWidth>3.007242</ResolutionHalfWidth>
  <Selectivity>1.792272</Selectivity>
  <Skew>0.864925</Skew>
  <Excess>1.360217</Excess>
  <WidthHalfHeight>0.058039</WidthHalfHeight>
  <Width5Sigma>0.131765</Width5Sigma>
  <WidthTangent>0.089452</WidthTangent>
  <WidthTailing>0.127843</WidthTailing>
  <USPTailing>1.206689</USPTailing>
  <TimeIncrement Unit="msec">800</TimeIncrement>
  <DataPoints>23</DataPoints>
  <StatisticalMoment0>270.771027</StatisticalMoment0>
  <StatisticalMoment1>1.029706</StatisticalMoment1>
  <StatisticalMoment2>0.000668</StatisticalMoment2>
  <StatisticalMoment3>0.000015</StatisticalMoment3>
  <StatisticalMoment4>1.944e-006</StatisticalMoment4>
  <PlatesTangent>2088.99101</PlatesTangent>
  <Plates5Sigma>1504.323467</Plates5Sigma>
  <PlatesStatistical>1587.931583</PlatesStatistical>
  <ResolutionTangent>3.327396</ResolutionTangent>
```

```
  <Resolution5Sigma>2.855306</Resolution5Sigma>
  <ResolutionStatistical>2.885621</ResolutionStatistical>
 </Peak>
 <Peak>
  <SignalDesc>DAD1 A, Sig=254,4 Ref=550,100</SignalDesc>
  <PeakType>BB  </PeakType>
  <ExpRetTime Unit="min">2.568847</ExpRetTime>
  <MeasRetTime Unit="min">2.569072</MeasRetTime>
  <Area Unit="mAU*s">176.769363</Area>
  <Height Unit="mAU">26.735945</Height>
  <Width Unit="min">0.101136</Width>
  <Symmetry>0.62962</Symmetry>
  <Name>Biphenyl</Name>
  <Amount Unit="wt%">0.0060074120</Amount>
  <kPrime>5.42268</kPrime>
  <PlatesHalfWidth>4080.07502</PlatesHalfWidth>
  <ResolutionHalfWidth>11.903108</ResolutionHalfWidth>
  <Selectivity>3.48661</Selectivity>
  <Skew>1.039269</Skew>
  <Excess>1.564137</Excess>
  <WidthHalfHeight>0.094667</WidthHalfHeight>
  <Width5Sigma>0.266667</Width5Sigma>
  <WidthTangent>0.163861</WidthTangent>
  <WidthTailing>0.26</WidthTailing>
  <USPTailing>1.51771</USPTailing>
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  <DataPoints>40</DataPoints>
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  <StatisticalMoment1>2.588773</StatisticalMoment1>
  <StatisticalMoment2>0.002983</StatisticalMoment2>
  <StatisticalMoment3>0.000169</StatisticalMoment3>
  <StatisticalMoment4>0.000041</StatisticalMoment4>
  <PlatesTangent>3932.966028</PlatesTangent>
  <Plates5Sigma>2320.358549</Plates5Sigma>
  <PlatesStatistical>2246.776872</PlatesStatistical>
  <ResolutionTangent>12.213776</ResolutionTangent>
  <Resolution5Sigma>9.706547</Resolution5Sigma>
  <ResolutionStatistical>9.689001</ResolutionStatistical>
 </Peak>
 <Peak>
  <SignalDesc>DAD1 A, Sig=254,4 Ref=550,100</SignalDesc>
```

```
      <PeakType>BB  </PeakType>
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      <MeasRetTime Unit="min">5.849135</MeasRetTime>
      <Area Unit="mAU*s">252.22435</Area>
      <Height Unit="mAU">16.837481</Height>
      <Width Unit="min">0.222766</Width>
      <Symmetry>0.669291</Symmetry>
      <Name>o-Terphenyl</Name>
      <Amount Unit="wt%">0.0180363758</Amount>
      <kPrime>13.622837</kPrime>
      <PlatesHalfWidth>4270.722925</PlatesHalfWidth>
      <ResolutionHalfWidth>12.622513</ResolutionHalfWidth>
      <Selectivity>2.512196</Selectivity>
      <Skew>0.870258</Skew>
      <Excess>1.019275</Excess>
      <WidthHalfHeight>0.210667</WidthHalfHeight>
      <Width5Sigma>0.608</Width5Sigma>
      <WidthTangent>0.370535</WidthTangent>
      <WidthTailing>0.592</WidthTailing>
      <USPTailing>1.487052</USPTailing>
      <TimeIncrement Unit="msec">800</TimeIncrement>
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      <StatisticalMoment1>5.890457</StatisticalMoment1>
      <StatisticalMoment2>0.01364</StatisticalMoment2>
      <StatisticalMoment3>0.001386</StatisticalMoment3>
      <StatisticalMoment4>0.000748</StatisticalMoment4>
      <PlatesTangent>3986.992494</PlatesTangent>
      <Plates5Sigma>2313.748386</Plates5Sigma>
      <PlatesStatistical>2543.872414</PlatesStatistical>
      <ResolutionTangent>12.275778</ResolutionTangent>
      <Resolution5Sigma>9.37518</Resolution5Sigma>
      <ResolutionStatistical>9.631284</ResolutionStatistical>
    </Peak>
  </ResultsGroup>
</Results>
<CustomResults>
  <Info>
    <Item>HEADER_NAME: MyHeader</Item>
    <Text>HEADER_TEXT: TextMyHeader</Text>
  </Info>
```

```
    <Info>
      <Item>ROW_NAME: MyRow1</Item>
      <Text>ROW_VALUE: ValueMyRow1</Text>
    </Info>
    <Info>
      <Item>ROW_NAME: MyRow2</Item>
      <Text>ROW_VALUE: ValueMyRow2</Text>
    </Info>
  </CustomResults>
</ChemStationResult>
```

B
Export File Schema (EXPORT.XSD)

This appendix lists the schema that is used to produce the results file for export.

```
<?xml version="1.0" encoding="ISO-8859-1"?>
<!-- edited with XMLSpy v2007 sp2 (http://www.altova.com) by Maciej Tokarski (Agilent Technologies Germany) -->
<!-- edited with XMLSPY v5 rel. 4 U (http://www.xmlspy.com) by Reiner Lange (Agilent Technologies) -->
<xs:schema xmlns:xs="http://www.w3.org/2001/XMLSchema" elementFormDefault="qualified" attributeFormDefault="unqualified">
    <xs:element name="ChemStationResult">
        <xs:complexType>
            <xs:sequence>
                <xs:element name="Acquisition">
                    <xs:complexType>
                        <xs:complexContent>
                            <xs:extension base="AcquisitionType"/>
                        </xs:complexContent>
                    </xs:complexType>
                </xs:element>
                <xs:element name="ModuleInformation">
                    <xs:complexType>
                        <xs:sequence>
                            <xs:element name="Module" minOccurs="0" maxOccurs="unbounded">
                                <xs:complexType>
```

```
                        <xs:complexContent>
                            <xs:extension base="ModuleType"/>
                        </xs:complexContent>
                    </xs:complexType>
                </xs:element>
            </xs:sequence>
        </xs:complexType>
    </xs:element>
    <xs:element name="SampleInformation">
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                <xs:extension base="SampleInformationType"/>
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        </xs:complexType>
    </xs:element>
    <xs:element name="Chromatograms">
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            <xs:sequence>
                <xs:element name="Signal" minOccurs="0" maxOccurs="unbounded">
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                        <xs:complexContent>
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                        </xs:complexContent>
                    </xs:complexType>
                </xs:element>
            </xs:sequence>
        </xs:complexType>
    </xs:element>
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    <xs:element name="Results" type="ResultsType"/>
    <xs:element name="FractionInformation" minOccurs="0">
        <xs:complexType>
            <xs:complexContent>
                <xs:extension base="FractionInformationType"/>
            </xs:complexContent>
        </xs:complexType>
    </xs:element>
    <xs:element name="CustomResults">
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```

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                        </xs:complexType>
                    </xs:element>
                </xs:sequence>
            </xs:complexType>
        </xs:element>
    </xs:sequence>
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  </xs:complexType>
</xs:element>
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  <xs:sequence>
    <xs:element name="Version"/>
    <xs:element name="InstrumentName"/>
    <xs:element name="MethodPath"/>
    <xs:element name="InjectionTime"/>
    <xs:element name="MethodLastModifiedTime"/>
    <xs:element name="MethodLastModifiedBy"/>
    <xs:element name="MethodModifiedAtRun"/>
  </xs:sequence>
</xs:complexType>
<xs:complexType name="IntegrationResultsType">
  <xs:sequence>
    <xs:element name="RetTime" type="xs:double"/>
    <xs:element name="Area" type="xs:double"/>
    <xs:element name="AreaPercent" type="xs:double"/>
    <xs:element name="AreaSum" type="xs:double"/>
    <xs:element name="Height" type="xs:double"/>
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    <xs:element name="Symmetry" type="xs:double"/>
    <xs:element name="Baseline" type="xs:double"/>
    <xs:element name="TimeStart" type="xs:double"/>
    <xs:element name="LevelStart" type="xs:double"/>
    <xs:element name="BaselineStart" type="xs:double"/>
    <xs:element name="TimeEnd" type="xs:double"/>
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  </xs:sequence>
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  <xs:sequence>
    <xs:element name="Version"/>
    <xs:element name="VialUnused"/>
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```
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            <xs:element name="InjVolume"/>
            <xs:element name="ActInjVolume"/>
            <xs:element name="AcqInstName"/>
            <xs:element name="SeqLine"/>
            <xs:element name="Location"/>
            <xs:element name="Inj"/>
            <xs:element name="Method"/>
            <xs:element name="Operator"/>
            <xs:element name="InjectionDateTime"/>
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            <xs:element name="SampleInfo"/>
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            <xs:element name="SampleAmount"/>
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            <xs:element name="MethodInfo"/>
            <xs:element name="CalMethod"/>
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            <xs:element name="LimsID" minOccurs="0"/>
            <xs:element name="LimsKField2" minOccurs="0"/>
            <xs:element name="LimsKField3" minOccurs="0"/>
        </xs:sequence>
    </xs:complexType>
    <xs:complexType name="ModuleType">
        <xs:sequence>
            <xs:element name="Number"/>
            <xs:element name="NumberInModule"/>
            <xs:element name="ModuleName"/>
            <xs:element name="SerialNumber"/>
            <xs:element name="FirmwareRevision"/>
            <xs:element name="BuildNumber" minOccurs="0"/>
            <xs:element name="PartNumber" minOccurs="0"/>
        </xs:sequence>
    </xs:complexType>
    <xs:complexType name="SignalType">
        <xs:sequence>
            <xs:element name="Title"/>
            <xs:element name="Description"/>
            <xs:element name="Detector"/>
            <xs:element name="SignalId"/>
            <xs:element name="Operator"/>
            <xs:element name="DateTime"/>
            <xs:element name="DerivOrder"/>
            <xs:element name="RawdataFile"/>
```

```
            <xs:element name="Start"/>
            <xs:element name="End"/>
            <xs:element name="XUnits"/>
            <xs:element name="YUnits"/>
            <xs:element name="Noise" minOccurs="0">
                <xs:complexType>
                    <xs:sequence maxOccurs="unbounded">
                        <xs:element name="NoisePeriod" minOccurs="0">
                            <xs:complexType>
                                <xs:sequence>
                                    <xs:element name="TimeFrom" type="Value"/>
                                    <xs:element name="TimeTo" type="Value"/>
                                    <xs:element name="Noise6SD" type="Value"/>
                                    <xs:element name="NoisePToP" type="Value"/>
                                    <xs:element name="NoiseASTM" type="Value"/>
                                    <xs:element name="Wander" type="Value"/>
                                    <xs:element name="Drift" type="Value"/>
                                </xs:sequence>
                            </xs:complexType>
                        </xs:element>
                    </xs:sequence>
                </xs:complexType>
            </xs:element>
            <xs:element name="IntegrationResults" type="IntegrationResultsType" minOccurs="0" maxOc-
curs="unbounded"/>
        </xs:sequence>
    </xs:complexType>
    <xs:complexType name="CompoundType">
        <xs:sequence>
            <xs:element name="CompoundID" type="xs:integer" minOccurs="0"/>
            <xs:element name="SignalDesc"/>
            <xs:element name="PeakType" type="xs:anySimpleType"/>
            <xs:element name="ExpRetTime">
                <xs:complexType>
                    <xs:simpleContent>
                        <xs:extension base="xs:double">
                            <xs:attribute name="Unit" type="xs:string"/>
                        </xs:extension>
                    </xs:simpleContent>
                </xs:complexType>
            </xs:element>
            <xs:element name="MeasRetTime">
                <xs:complexType>
                    <xs:simpleContent>
                        <xs:extension base="xs:double">
```

```
                    <xs:attribute name="Unit" type="xs:string"/>
                </xs:extension>
            </xs:simpleContent>
        </xs:complexType>
    </xs:element>
    <xs:element name="Area">
        <xs:complexType>
            <xs:simpleContent>
                <xs:extension base="xs:double">
                    <xs:attribute name="Unit" type="xs:string"/>
                </xs:extension>
            </xs:simpleContent>
        </xs:complexType>
    </xs:element>
    <xs:element name="Height">
        <xs:complexType>
            <xs:simpleContent>
                <xs:extension base="xs:double">
                    <xs:attribute name="Unit" type="xs:string"/>
                </xs:extension>
            </xs:simpleContent>
        </xs:complexType>
    </xs:element>
    <xs:element name="Width">
        <xs:complexType>
            <xs:simpleContent>
                <xs:extension base="xs:double">
                    <xs:attribute name="Unit" type="xs:string"/>
                </xs:extension>
            </xs:simpleContent>
        </xs:complexType>
    </xs:element>
    <xs:element name="Symmetry" type="xs:double"/>
    <xs:element name="Name"/>
    <xs:element name="Amount">
        <xs:complexType>
            <xs:simpleContent>
                <xs:extension base="xs:double">
                    <xs:attribute name="Unit" type="xs:string"/>
                </xs:extension>
            </xs:simpleContent>
        </xs:complexType>
    </xs:element>
    <xs:sequence minOccurs="0">
        <xs:element name="kPrime" type="xs:double"/>
```

```
                <xs:element name="PlatesHalfWidth" type="xs:double"/>
                <xs:element name="ResolutionHalfWidth" type="xs:double"/>
                <xs:element name="Selectivity" type="xs:double"/>
                <xs:element name="SignalNoiseRatio" type="xs:double" minOccurs="0"/>
                <xs:sequence minOccurs="0">
                    <xs:element name="Skew" type="xs:double"/>
                    <xs:element name="Excess" type="xs:double"/>
                    <xs:element name="WidthHalfHeight" type="xs:double"/>
                    <xs:element name="Width5Sigma" type="xs:double"/>
                    <xs:element name="WidthTangent" type="xs:double"/>
                    <xs:element name="WidthTailing" type="xs:double"/>
                    <xs:element name="USPTailing" type="xs:double"/>
                    <xs:element name="TimeIncrement" type="xs:double"/>
                    <xs:element name="DataPoints" type="xs:double"/>
                    <xs:element name="StatisticalMoment0" type="xs:double"/>
                    <xs:element name="StatisticalMoment1" type="xs:double"/>
                    <xs:element name="StatisticalMoment2" type="xs:double"/>
                    <xs:element name="StatisticalMoment3" type="xs:double"/>
                    <xs:element name="StatisticalMoment4" type="xs:double"/>
                    <xs:element name="PlatesTangent" type="xs:double"/>
                    <xs:element name="Plates5Sigma" type="xs:double"/>
                    <xs:element name="PlatesStatistical" type="xs:double"/>
                    <xs:element name="ResolutionTangent" type="xs:double"/>
                    <xs:element name="Resolution5Sigma" type="xs:double"/>
                    <xs:element name="ResolutionStatistical" type="xs:double"/>
                </xs:sequence>
            </xs:sequence>
        </xs:sequence>
    </xs:complexType>
    <xs:complexType name="CustomResultsType">
        <xs:sequence>
            <xs:element name="Info" type="InfoType" minOccurs="0" maxOccurs="unbounded"/>
        </xs:sequence>
    </xs:complexType>
    <xs:complexType name="InfoType">
        <xs:sequence>
            <xs:element name="Item"/>
            <xs:element name="Text"/>
        </xs:sequence>
    </xs:complexType>
    <xs:complexType name="ResultsType">
        <xs:sequence>
            <xs:element name="QuantCalc" type="xs:string"/>
            <xs:element name="QuantBase" type="xs:string"/>
            <xs:element name="ResultsGroup" minOccurs="0" maxOccurs="unbounded">
```

```
                <xs:complexType>
                    <xs:sequence>
                        <xs:element name="ResultsGroupDescription"/>
                        <xs:element name="Peak" type="CompoundType" minOccurs="0" maxOc-
curs="unbounded"/>
                    </xs:sequence>
                </xs:complexType>
            </xs:element>
        </xs:sequence>
    </xs:complexType>
    <xs:complexType name="Value">
        <xs:attribute name="Unit" type="xs:string" use="optional"/>
        <xs:attribute name="Suitability" type="xs:string" use="optional"/>
    </xs:complexType>
    <xs:complexType name="FractionInformationType">
        <xs:sequence>
            <xs:element name="PurifyStudy" minOccurs="0"/>
            <xs:element name="PurifyDataPath" minOccurs="0"/>
            <xs:element name="Collection" type="CollectionType"/>
            <xs:element name="Data" type="FractionDataType"/>
        </xs:sequence>
    </xs:complexType>
    <xs:complexType name="CollectionType">
        <xs:sequence>
            <xs:element name="Type"/>
            <xs:sequence maxOccurs="2">
                <xs:element name="Criteria">
                    <xs:complexType>
                        <xs:sequence>
                            <xs:element name="Name"/>
                            <xs:element name="Value"/>
                        </xs:sequence>
                    </xs:complexType>
                </xs:element>
            </xs:sequence>
        </xs:sequence>
    </xs:complexType>
    <xs:complexType name="FractionsType">
        <xs:sequence minOccurs="0" maxOccurs="unbounded">
            <xs:element name="Fraction">
                <xs:complexType>
                    <xs:sequence>
                        <xs:element name="Frac"/>
                        <xs:element name="Well"/>
                        <xs:element name="Location"/>
```

```
                        <xs:element name="Volume"/>
                        <xs:element name="BeginTime"/>
                        <xs:element name="EndTime"/>
                        <xs:element name="Reason"/>
                        <xs:element name="Mass" minOccurs="0"/>
                    </xs:sequence>
                </xs:complexType>
            </xs:element>
        </xs:sequence>
    </xs:complexType>
    <xs:complexType name="RecoveryLocationsType">
        <xs:sequence minOccurs="0" maxOccurs="unbounded">
            <xs:element name="RecoveryLocation">
                <xs:complexType>
                    <xs:sequence>
                        <xs:element name="Recovery"/>
                        <xs:element name="Location"/>
                        <xs:element name="Volume"/>
                    </xs:sequence>
                </xs:complexType>
            </xs:element>
        </xs:sequence>
    </xs:complexType>
    <xs:complexType name="FractionDataType">
        <xs:sequence>
            <xs:element name="Fractions" type="FractionsType"/>
            <xs:element name="RecoveryLocations" type="RecoveryLocationsType"/>
        </xs:sequence>
    </xs:complexType>
    <xs:complexType name="CalibrationInformationType">
        <xs:sequence>
            <xs:element name="Title" type="xs:string"/>
            <xs:element name="PartialCalibrationIfPeaksMissing">
                <xs:complexType>
                    <xs:simpleContent>
                        <xs:extension base="xs:boolean">
                            <xs:attribute name="correctallRTs" type="xs:boolean" use="optional"
default="false"/>
                        </xs:extension>
                    </xs:simpleContent>
                </xs:complexType>
            </xs:element>
            <xs:element name="UseMultiAndDilutFactorWithISTDs" type="xs:boolean"/>
            <xs:element name="RecalibrationSettings">
                <xs:complexType>
```

```
            <xs:sequence>
                <xs:element name="AverageResponse">
                    <xs:complexType>
                        <xs:simpleContent>
                            <xs:extension base="xs:string">
                                <xs:attribute name="Type" use="required">
                                    <xs:simpleType>
                                        <xs:restriction base="xs:string">
                                            <xs:enumeration value="NOUPDATE"/>
                                            <xs:enumeration value="AVERAGEALLCALIBRATIONS"/>
                                            <xs:enumeration value="FLOATINGAVERAGENEW"/>
                                        </xs:restriction>
                                    </xs:simpleType>
                                </xs:attribute>
                            </xs:extension>
                        </xs:simpleContent>
                    </xs:complexType>
                </xs:element>
                <xs:element name="AverageRT">
                    <xs:complexType>
                        <xs:simpleContent>
                            <xs:extension base="xs:string">
                                <xs:attribute name="Type" use="required">
                                    <xs:simpleType>
                                        <xs:restriction base="xs:string">
                                            <xs:enumeration value="NOUPDATE"/>
                                            <xs:enumeration value="AVERAGEALLCALIBRATIONS"/>
                                            <xs:enumeration value="FLOATINGAVERAGENEW"/>
                                        </xs:restriction>
                                    </xs:simpleType>
                                </xs:attribute>
                            </xs:extension>
                        </xs:simpleContent>
                    </xs:complexType>
                </xs:element>
            </xs:sequence>
        </xs:complexType>
    </xs:element>
    <xs:element name="ISTD" minOccurs="0" maxOccurs="unbounded">
        <xs:complexType>
            <xs:sequence>
                <xs:element name="ISTDID" type="xs:integer"/>
                <xs:element name="Amount">
                    <xs:complexType>
                        <xs:simpleContent>
```

```
                        <xs:extension base="xs:double">
                            <xs:attribute name="Unit" type="xs:string" use="optional"/>
                        </xs:extension>
                    </xs:simpleContent>
                </xs:complexType>
            </xs:element>
            <xs:choice>
                <xs:element name="CompoundID" type="xs:integer"/>
                <xs:element name="GroupID" type="xs:integer"/>
            </xs:choice>
            <xs:element name="Name" type="xs:string"/>
        </xs:sequence>
    </xs:complexType>
</xs:element>
<xs:element name="Signal" maxOccurs="unbounded">
    <xs:complexType>
        <xs:sequence>
            <xs:element name="SignalID" type="xs:integer"/>
            <xs:element name="SignalDesc">
                <xs:complexType>
                    <xs:simpleContent>
                        <xs:extension base="xs:string"/>
                    </xs:simpleContent>
                </xs:complexType>
            </xs:element>
            <xs:element name="UncalibratedPeaks" nillable="true">
                <xs:complexType>
                    <xs:choice minOccurs="0">
                        <xs:element name="UsingCompound">
                            <xs:complexType>
                                <xs:sequence>
                                    <xs:element name="CompoundID" type="xs:integer"/>
                                    <xs:element name="CompoundName" type="xs:string"/>
                                </xs:sequence>
                            </xs:complexType>
                        </xs:element>
                        <xs:sequence>
                            <xs:element name="RspFactor" type="xs:double"/>
                            <xs:element name="UseISTD" minOccurs="0"/>
                        </xs:sequence>
                    </xs:choice>
                </xs:complexType>
            </xs:element>
        </xs:sequence>
    </xs:complexType>
```

```
</xs:element>
<xs:element name="Compound" minOccurs="0" maxOccurs="unbounded">
    <xs:complexType>
        <xs:sequence>
            <xs:element name="CompoundID" type="xs:integer"/>
            <xs:element name="Name" type="xs:string"/>
            <xs:element name="AmountLimitLow" type="xs:double"/>
            <xs:element name="AmountLimitHigh" type="xs:double"/>
            <xs:element name="Multiplier" type="xs:double"/>
            <xs:element name="IsTimeReference" type="xs:boolean"/>
            <xs:element name="IsISTD" type="xs:boolean"/>
            <xs:element name="ISTDID" type="xs:integer" minOccurs="0"/>
            <xs:element name="GroupID" type="xs:integer" minOccurs="0"/>
            <xs:element name="CompoundSignal" maxOccurs="unbounded">
                <xs:complexType>
                    <xs:sequence>
                        <xs:element name="SignalID" type="xs:integer"/>
                        <xs:element name="SignalDesc" type="xs:string"/>
                        <xs:element name="ExpRetTime" type="xs:double"/>
                        <xs:element name="RTWindowLow" type="xs:double"/>
                        <xs:element name="RTWindowHigh" type="xs:double"/>
                        <xs:element name="PeakUsage">
                            <xs:simpleType>
                                <xs:restriction base="xs:string">
                                    <xs:enumeration value="MAIN"/>
                                    <xs:enumeration value="QUALIFIER"/>
                                    <xs:enumeration value="IGNORE"/>
                                </xs:restriction>
                            </xs:simpleType>
                        </xs:element>
                        <xs:element name="Curve" type="CalibrationCurveType"/>
                        <xs:element name="Level" maxOccurs="unbounded">
                            <xs:complexType>
                                <xs:sequence>
                                    <xs:element name="LevelID" type="xs:integer"/>
                                    <xs:element name="Amount">
                                        <xs:complexType>
                                            <xs:simpleContent>
                                                <xs:extension base="xs:double">
                                                    <xs:attribute name="Unit" type="xs:string"/>
                                                </xs:extension>
                                            </xs:simpleContent>
                                        </xs:complexType>
                                    </xs:element>
                                    <xs:choice>
```

```
                                        <xs:element name="Area" type="xs:double"/>
                                        <xs:element name="Height" type="xs:double"/>
                                    </xs:choice>
                                    <xs:element name="ResponseFactor" type="xs:double"/>
                                    <xs:element name="RefAmount" type="xs:double"/>
                                    <xs:element name="RespPercent" type="xs:double"/>
                                    <xs:element name="LevelWeight" type="xs:double" minOccurs="0"/>
                                </xs:sequence>
                            </xs:complexType>
                        </xs:element>
                    </xs:sequence>
                </xs:complexType>
            </xs:element>
        </xs:sequence>
    </xs:complexType>
    <xs:complexType name="CalibrationCurveType">
        <xs:sequence>
            <xs:element name="Correlation" type="xs:double"/>
            <xs:element name="Origin">
                <xs:simpleType>
                    <xs:restriction base="xs:string">
                        <xs:enumeration value="IGNORE"/>
                        <xs:enumeration value="INCLUDE"/>
                        <xs:enumeration value="FORCE"/>
                        <xs:enumeration value="CONNECT"/>
                    </xs:restriction>
                </xs:simpleType>
            </xs:element>
            <xs:element name="Type">
                <xs:simpleType>
                    <xs:restriction base="xs:string">
                        <xs:enumeration value="PIECEWISE"/>
                        <xs:enumeration value="LINEAR"/>
                        <xs:enumeration value="QUADRATIC"/>
                        <xs:enumeration value="CUBIC"/>
                        <xs:enumeration value="EXPONENTIAL"/>
                        <xs:enumeration value="LOGARITHMIC"/>
                        <xs:enumeration value="POWER"/>
                        <xs:enumeration value="AVERAGE_RSP_AMNT"/>
                    </xs:restriction>
                </xs:simpleType>
            </xs:element>
```

```
            <xs:element name="Formula" type="CalibrationCurveFormulaType"/>
            <xs:element name="Weight">
                <xs:simpleType>
                    <xs:restriction base="xs:string">
                        <xs:enumeration value="EQUAL"/>
                        <xs:enumeration value="NOFCALIBRATIONS"/>
                        <xs:enumeration value="LINEAR_AMNT"/>
                        <xs:enumeration value="QUADRATIC_AMNT"/>
                        <xs:enumeration value="LINEAR_RESP"/>
                        <xs:enumeration value="QUADRATIC_RESP"/>
                    </xs:restriction>
                </xs:simpleType>
            </xs:element>
        </xs:sequence>
    </xs:complexType>
    <xs:complexType name="CalibrationCurveFormulaType">
        <xs:sequence>
            <xs:element name="Text"/>
            <xs:element name="Parameter" maxOccurs="unbounded">
                <xs:complexType>
                    <xs:sequence>
                        <xs:element name="Symbol" type="xs:string"/>
                        <xs:element name="Value" type="xs:double"/>
                    </xs:sequence>
                </xs:complexType>
            </xs:element>
        </xs:sequence>
    </xs:complexType>
</xs:schema>
```

C
Sample Worklist File

This appendix gives an example of a worklist file of the type that would be imported into the Agilent ChemStation. Note that the values contained in this file are not real; they are there only to demonstrate the format.

```
<Samples xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance" xsi:noN-
amespaceSchemaLocation="d:\lego\cpext\txt_imp\xml-templates\worklist.xsd">
    <Sample>
        <Number>1</Number>
        <Location>p1-b1</Location>
        <Name>sample1</Name>
        <CDSMethod>BATCH</CDSMethod>
        <numberOfInj>6</numberOfInj>
        <sampleType>SAMPLE</sampleType>
        <CalLevel>8</CalLevel>
        <calibration>BRACKET</calibration>
        <UpdateRT>NO UPDATE</UpdateRT>
        <Interval>0</Interval>
        <sampleAmount>1</sampleAmount>
        <ISTDAmount>9</ISTDAmount>
        <Multipliers>7</Multipliers>
        <Dilution>7</Dilution>
        <DataFilename>005-0101</DataFilename>
        <InjectionVolume>7</InjectionVolume>
        <description>info</description>
        <StudyName>part 11 demo</StudyName>
        <LimsID>fr37238723</LimsID>
        <LimsKField2>12</LimsKField2>
```

```
        <LimsKField3>KF31</LimsKField3>
        <CustomField>
            <Name>Wish List</Name>
            <Value>3</Value>
        </CustomField>
        <CustomField>
            <Name>Price</Name>
            <Value>5</Value>
        </CustomField>
    </Sample>
    <Sample>
        <Number>2</Number>
        <Location>p1-a1</Location>
        <Name>sample2</Name>
        <CDSMethod>BATCH</CDSMethod>
        <numberOfInj>1</numberOfInj>
        <sampleType/>
        <CalLevel/>
        <calibration/>
        <UpdateRT/>
        <Interval/>
        <sampleAmount>1</sampleAmount>
        <ISTDAmount>2</ISTDAmount>
        <Multipliers>3</Multipliers>
        <Dilution/>
        <DataFilename>005-0102</DataFilename>
        <InjectionVolume>7</InjectionVolume>
        <description>info1</description>
        <StudyName/>
        <LimsID>fr234322</LimsID>
        <LimsKField2>23</LimsKField2>
        <LimsKField3>KF32</LimsKField3>
        <CustomField>
            <Name>Price</Name>
            <Value>6</Value>
        </CustomField>
    </Sample>
    <CommonInformation Type="Header">
        <Name>MyHeader</Name>
        <Value>TextMyHeader</Value>
    </CommonInformation>
```

```
    <CommonInformation Type="ROW">
        <Name>MyRow1</Name>
        <Value>ValueMyRow1</Value>
    </CommonInformation>
    <CommonInformation Type="ROW">
        <Name>MyRow2</Name>
        <Value>ValueMyRow2</Value>
    </CommonInformation>
</Samples>
```

C Sample Worklist File

D
Worklist Schema (WORKLIST.XSD)

This appendix lists the schema that is used to produce the worklist XML file.

```
<?xml version="1.0" encoding=" ISO-8859-1"?>
<xs:schema xmlns:xs="http://www.w3.org/2001/XMLSchema" elementFormDefault="qualified" attrib-
uteFormDefault="unqualified">
    <xs:element name="Samples">
        <xs:annotation>
            <xs:documentation>worklist for ChemStation sequence import</xs:documentation>
        </xs:annotation>
        <xs:complexType>
            <xs:sequence>
                <xs:element name="Sample" maxOccurs="unbounded">
                    <xs:complexType>
                        <xs:sequence>
                            <xs:element name="Number" type="xs:integer"/>
                            <xs:element name="Location" type="xs:string"/>
                            <xs:element name="Name" type="xs:string"/>
                            <xs:element name="CDSMethod" type="xs:string"/>
                            <xs:element name="numberOfInj" type="xs:string"/>
                            <xs:element name="sampleType">
                                <xs:simpleType>
                                    <xs:restriction base="xs:string">
                                        <xs:enumeration value="CONTROLSAMPLE"/>
                                        <xs:enumeration value="SAMPLE"/>
                                        <xs:enumeration value="CALIBRATION"/>
                                        <xs:enumeration value="UNKNOWN"/>
                                        <xs:enumeration value="STANDARD"/>
                                        <xs:enumeration value="QUALITYCONTROL"/>
                                        <xs:enumeration value="BLANK"/>
```

```
                <xs:enumeration value="DOUBLEBLANK"/>
                <xs:enumeration value="SOLVENT"/>
                <xs:enumeration value=""/>
            </xs:restriction>
        </xs:simpleType>
    </xs:element>
    <xs:element name="CalLevel" type="xs:string"/>
    <xs:element name="calibration">
        <xs:simpleType>
            <xs:restriction base="xs:string">
                <xs:enumeration value="NO UPDATE"/>
                <xs:enumeration value="REPLACE"/>
                <xs:enumeration value="BRACKET"/>
                <xs:enumeration value="DELTA%"/>
                <xs:enumeration value="AVERAGE"/>
                <xs:enumeration value=""/>
            </xs:restriction>
        </xs:simpleType>
    </xs:element>
    <xs:element name="UpdateRT">
        <xs:simpleType>
            <xs:restriction base="xs:string">
                <xs:enumeration value="NO UPDATE"/>
                <xs:enumeration value="REPLACE"/>
                <xs:enumeration value="BRACKET"/>
                <xs:enumeration value="DELTA%"/>
                <xs:enumeration value="AVERAGE"/>
                <xs:enumeration value=""/>
            </xs:restriction>
        </xs:simpleType>
    </xs:element>
    <xs:element name="Interval" type="xs:string"/>
    <xs:element name="sampleAmount" type="xs:string"/>
    <xs:element name="ISTDAmount" type="xs:string"/>
    <xs:element name="Multipliers" type="xs:string"/>
    <xs:element name="Dilution" type="xs:string"/>
    <xs:element name="DataFilename" type="xs:string"/>
    <xs:element name="InjectionVolume" type="xs:string"/>
    <xs:element name="description" type="xs:string"/>
    <xs:element name="StudyName" type="xs:string"/>
    <xs:element name="LimsID" type="xs:string"/>
    <xs:element name="LimsKField2" type="xs:string"/>
    <xs:element name="LimsKField3" type="xs:string"/>
    <xs:element name="CustomField" minOccurs="0" maxOccurs="unbounded">
        <xs:complexType>
```

```
                        <xs:sequence>
                            <xs:element name="Name" type="xs:string"/>
                            <xs:element name="Value" type="xs:string"/>
                        </xs:sequence>
                    </xs:complexType>
                </xs:element>
            </xs:sequence>
        </xs:complexType>
    </xs:element>
    <xs:element name="Commoninformation" minOccurs="0" maxOccurs="unbounded">
        <xs:complexType>
            <xs:complexContent>
                <xs:extension base="CustomFieldType">
                    <xs:attribute name="Type" use="optional" default="ROW">
                        <xs:simpleType>
                            <xs:restriction base="xs:string">
                                <xs:enumeration value="ROW"/>
                                <xs:enumeration value="HEADER"/>
                            </xs:restriction>
                        </xs:simpleType>
                    </xs:attribute>
                </xs:extension>
            </xs:complexContent>
        </xs:complexType>
    </xs:element>
</xs:sequence>
</xs:complexType>
</xs:element>
<xs:complexType name="CustomFieldType">
    <xs:sequence>
        <xs:element name="Name" type="xs:string"/>
        <xs:element name="Value" type="xs:string"/>
    </xs:sequence>
</xs:complexType>
</xs:schema>
```

D Worklist Schema (WORKLIST.XSD)

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In This Book

This Guide describes the implementation of the XML interface between the Agilent OpenLAB CDS ChemStation Edition and a LIMS system. It also contains examples of import and export XML files, as well as their associated schemas.

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