Varian, Inc.
2700 Mitchell Drive
Walnut Creek, CA 94598-1675/USA

Varian MS Workstation Version 6.5

ToxProPlus Reporting Software Package

QUALITY SYSTEM ISO 9001 CERTIFIED

03-914894-00:Rev. 3

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ToxProPlus Reporting Software Package

Introduction

The ToxProPlus Package generates detailed reports and/or summaries. The package includes three independent templates:

- Screening.mdb
- Ion Ratio Summary .mdb
- MultiCpd.mdb

The ***Screening*** Report presents up to 30 graphic frames, one for each target analytes, per page for rapid graphic review of results.

The ***Ion Ratio Summary*** Report presents the ion ratio results for each analyte in each sample, indicating that the ratio was met or the criteria failed.

The ***Screening*** and ***Ion Ratio Summary*** reports are useful in determining if manual interaction is needed to correct integration imprecision and other processing criteria before detailed reporting with the MultiCpd software can commence.

The ***MultiCpd*** Report presents detailed and complex results in a wide range of formats.

Once the analytical protocols are established, and no further correction is needed, the use of the Screening and Ion Ratio Summary reports may cease and the reporting may take place immediately using the MultiCpd software.

Varian Analytical Instruments
2700 Mitchell Drive
Walnut Creek, CA 94598-1675/USA

Saturn® GC/MS Workstation
Version 6.5

MultiCpd Reports

03-914894-01:Rev. 2

Contents

MultiCpd Reports

Introduction

MultiCpd is a flexible, Microsoft Access 2000 based reporting software package. It allows the generation of numerous graphic and text reports for all kind of analysis. It reports up to 16 graphic displays (peaks and/or spectrum plots) per page, one for each Target Compound or Unknown. Tentatively identified compounds (TICs) may be reported with up to three library search result spectra with associated text fields. The user can design the graphic display and text shown in each report.

MultiCpd reports data from files processed in Varian GCMS Workstation 6.5 and later. Reports can be generated on internal and external standard based calculations.

The reports may be viewed interactively or printed automatically as part of a data acquisition or reprocessing sequence. The text only reports can be saved as text files for later retrieval.

This reporting application is designed to produce useful results within minutes for the new user, yet allow enough flexibility to meet the evolving needs of the more experienced investigator. At the introductory level, it offers several preformatted reports that should cover most routine needs. At the intermediate level, reports can be designed using simple forms to show flexible subsets of data items contained in the quantitated result file. At the advanced level, data is available to Microsoft Office applications for analysis and presentation.

The software allows report generation immediately after a sample analysis is completed, or reports for a sample or sample list can be easily generated as a post run operation.

The report templates can be "cloned" to generate a separate, tailor-made template for each type of reporting requirement.

The template size will increase after the generation of numerous reports; use the Repair/Compact command (last entry in the menu shown when the MS Custom Icon  is pressed in the Toolbar) to restore the original template size.

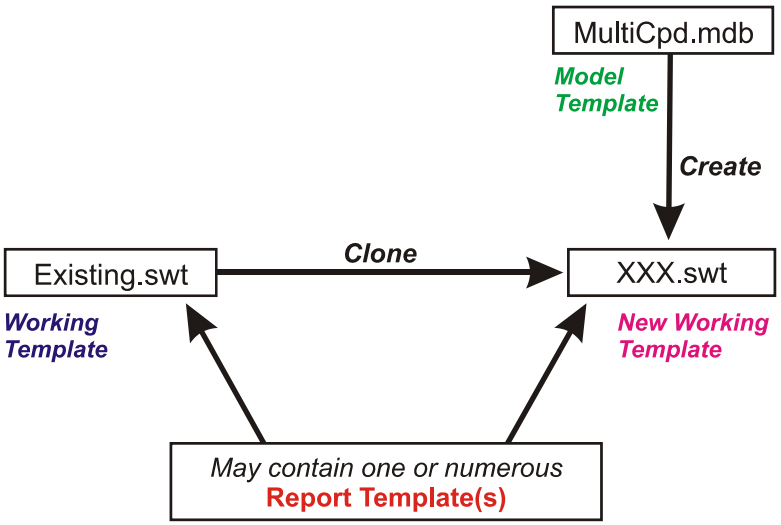
The MultiCpd template presents data already stored in the data file. It does not modify results stored in the data file.

In order for a data file to contain integrated peak information, MS Data Review or System Control must have processed it through peak integration. For a data file to contain quantitated peak information, a data handling method must have been constructed using the Method Editor, and then that method must have been used to process the data file using either MS Data Review or System Control. Changes made to the method only affect reported data file results after the data file has been processed with the changed method. The data file contains copies

of the method, including calibration result information, upon which the reported peak quantitation results are based.

Components of the Software

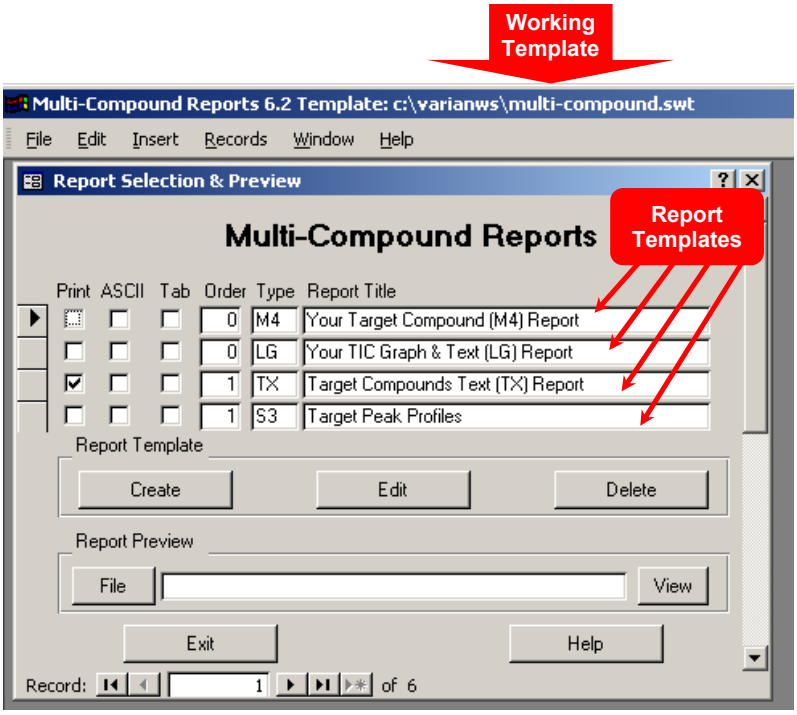
What are the “Templates”?



There are three different templates used within the MultiCpd reporting software. The MultiCpd.mdb is the master template, from which the “Working Template” may be created. The working template also can be “cloned” from an existing, other working template. The working templates have user defined names and .swt extension. Each working template may contain one or several “Report Templates”, each delivering a given type of report. The working template name is used in the AutoLink for automated reporting.

A *Report Template* is the collection of information needed to define the format or layout or presentation of the information in the report. It identifies the subset of information contained in the data file that is to be shown on the report(s). It also defines the placement of each item of information on the report.

There are 19 different Report Templates to choose from, and each of these “base” templates can be formatted in numerous ways to deliver the graphical and numerical information desired in the report. Each report template will have a user-defined title.



Currently Defined Report Templates

The “Multi-Compound Reports” form shows a scrollable list of currently defined report templates. Each Report Template entry shows whether the report will be printed during automated processing by System Control, whether the report will be exported to a text file, the editable report order number, the template type of the report, and the title of the report. The report list can be scrolled using the scroll bar at the right of the form, or using the record selector controls at the bottom left of the form. The currently selected report template is marked by a triangle on the record button at the left edge, and is also indicated by the record number in record selector control at bottom left. This active template is the template affected by the edit or delete keys, and is the template used to generate a report when the view key is clicked.

Types of Report Templates

The Report Template is classified by the type of data it reports. The classifications are:

- Sample (S2, S3, S4)
- Chromatogram (C1, C2, C3)
- Target compounds, graphics only (T2, T3, T4)
- Target compound, graphics and text (M2, M3, M4)
- Target compound, text only (TX)
- Tentatively Identified Compounds (TIC) graphics and text (LG)
- Tentatively Identified Compounds (TIC) text only (LT)
- Unknown, graphics and text (U2, U3, U4)
- Unknown, text only (UT)

Some templates include only text, others only graphics, still others graphic and text information. In the descriptions below, 2 x 2 refers to two rows of two displays each row, etc.

S Sample Report (Text + Graphics)

S2 2 x 2 graphical display, total of 4

S3 3 x 3 graphical display, total of 9

S4 4 x 4 graphical display, total of 16

The selected number of configurable graphics per report includes two configurable lines of text per compound. Included target compounds can be limited to a single group by specifying a matching group name in the data handling method and in the report. The graphic portion of the report is limited to one page only. The first 4 (or 9 or 16) compounds will have graphical display, the others even though they met reporting requirements, will not be printed in graphical form.

C Chromatogram Plots

C1 One chromatogram plot, single section on a single page

C2 One chromatogram, two-section plot on a single page

C3 One chromatogram, three-section plot on a single page

One, two or three configurable chromatogram plot segments on one page.

T Target Compound (Graphics)

T2 2 x 2 graphic display per page (multipage report)

T3 3 x 3 graphic display per page (multipage report)

T4 4 x 4 graphic display per page (multipage report)

The selected number of configurable target compound graphics per page. Only graphical information will be reported. Multipage report, each compound (meeting reporting requirements) will be printed.

M Target Compound (Text + Graphics)

M2 2 x 1 graphic display per page (multipage report)

M3 3 x 2 graphic display per page (multipage report)

M4 4 x 2 graphic display per page (multipage report)

Multipage report containing 2, 6, or 8 graphics plus two configurable text records per compound.

TX Target Compound (Text)

Multipage report consisting of two configurable text records per target compound. Exportable to a text file.

LG Tentatively Identified Compounds (TIC) Summary Report (Graphics)

Shows only peaks receiving 1 or more hits during the automatic library search for the tentatively identified compounds (TIC). The graphical display is pre-determined. For each peak it shows the peak profile, the apex spectrum and the library spectrum for up to three search hits. The report also shows one configurable text record for each peak, and one configurable record for each library search hit (up to 3 hits are reported).

LT Tentatively Identified Compounds (TIC) Report (Text)

Consists of one configurable text record per peak that received at least one hit during the last library search, plus one configurable record for each library search hit up to three per compound. Exportable to a text file.

U Unknowns Report (Graphics)

U2 2 x 2 graphic display per page (multipage report)

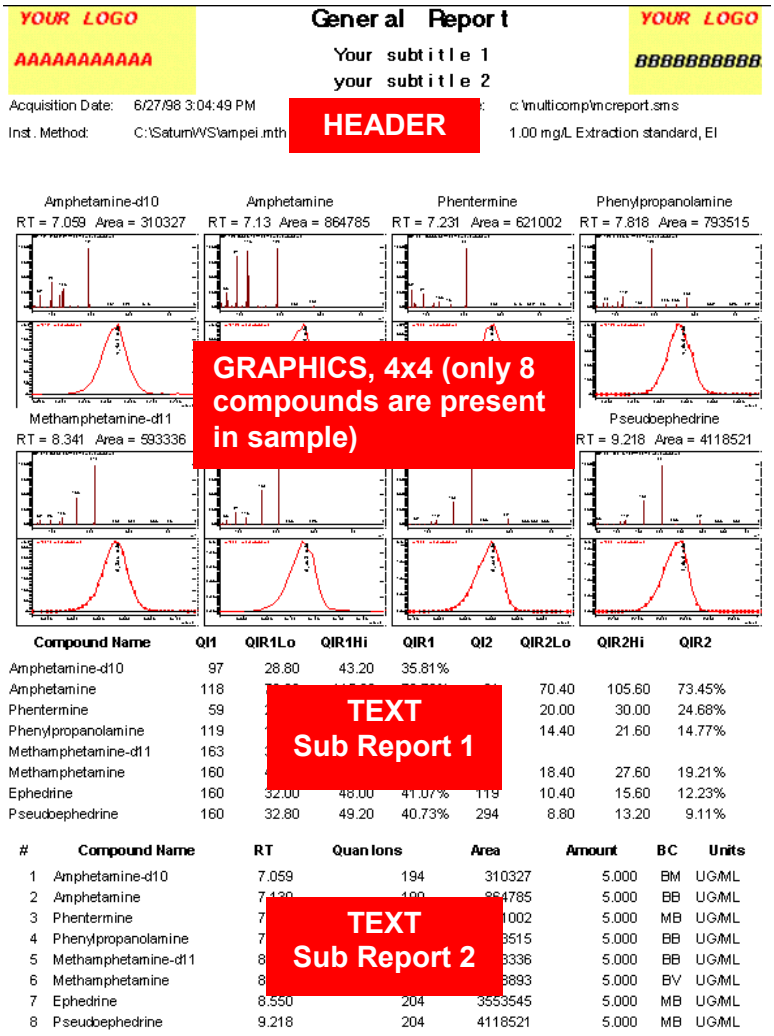
U3 3 x 3 graphic display per page (multipage report)

U4 4 x 4 graphic display per page (multipage report)

Multipage configurable graphics only report of 4, 9 or 16 graphics per page.

UT Unknowns Report (Text)

Shows one configurable record for each tentatively identified compound. Unidentified, and Duplicate peak included in the file. No graphics. Exportable to text files.



Every report may include a title line and two subtitle lines.

Two icons also may be inserted with company logo or other appropriate graphics.

All reports have a header section. The header is user-definable.

Some reports also include a footer.

The graphic and text portion of the reports depend on the report type selected. Furthermore, even the same report type may be configured with different information both in the graphic and text portion, but the overall layout of the report will remain the same.

A summary of the report types is shown below. In the following pages the different graphic and text types are also displayed. These are the building blocks of the reports.

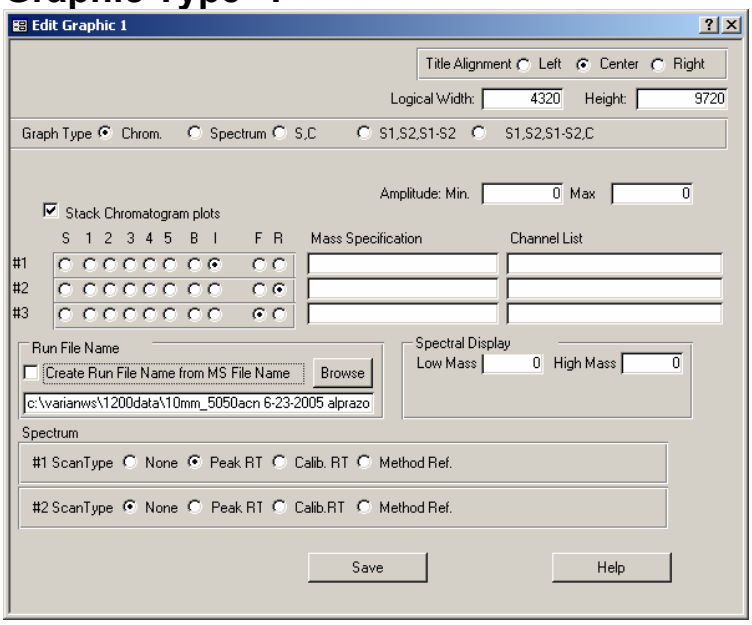
Brief Review of the Different Report Templates

Type of Report	Code	Text		Graphics			Footer	Group	Print to File
		Sub Rep 1	Sub Rep 2	Graphic Type	Number of compound displayed per page	Graphic Size (Pages)			
Sample Graphics and text	S2	A	A	I	2 x 2	1 page only	+	+	
	S3	A	A	I	3x 3	1 page only	+	+	
	S4	A	A	I	4x 4	1 page only	+	+	
Chromatogram	C1			II	1 section	1 page only			
	C2			II	2 sections	1 page only			
	C3			II	3 sections	1 page only			
Target comp. Graphics only	T2			I	2 x 2	Multipage			
	T3			I	3 x 3	Multipage			
	T4			I	4 x 4	Multipage			
Target comp. Graph. and text	M2	A	A	I	2 x 1	Multipage			
	M3	A	A	I	3 x 2	Multipage			
	M4	A	A	I	4 x 2	Multipage			
Target comp. Text only	TX	A	A				+		+
TIC: Graphics and Text	LG	B	C	Pre-defined	3	Multipage			
TIC Text only	LT	B	C				+		+
Unknown Graphics only	U2			III	2 x 2	Multipage			
	U3			III	3 x 3	Multipage			
	U4			III	4 x 4	Multipage			
Unknown Text only	UT	B							+

The full functionality of the options is described in the *Editing an Existing Report Template* Section.

Graphic Types

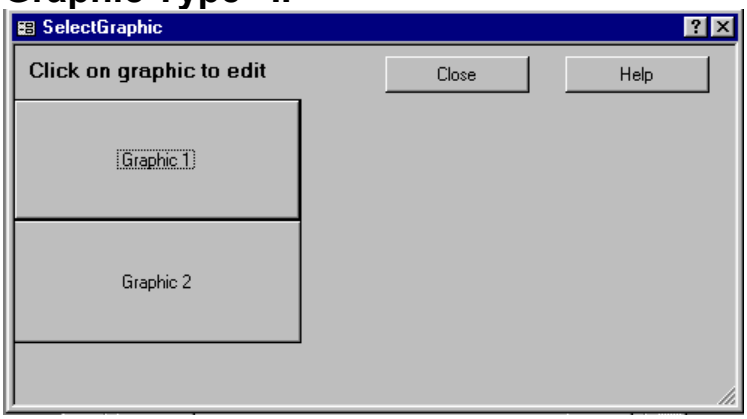
Graphic Type “I”

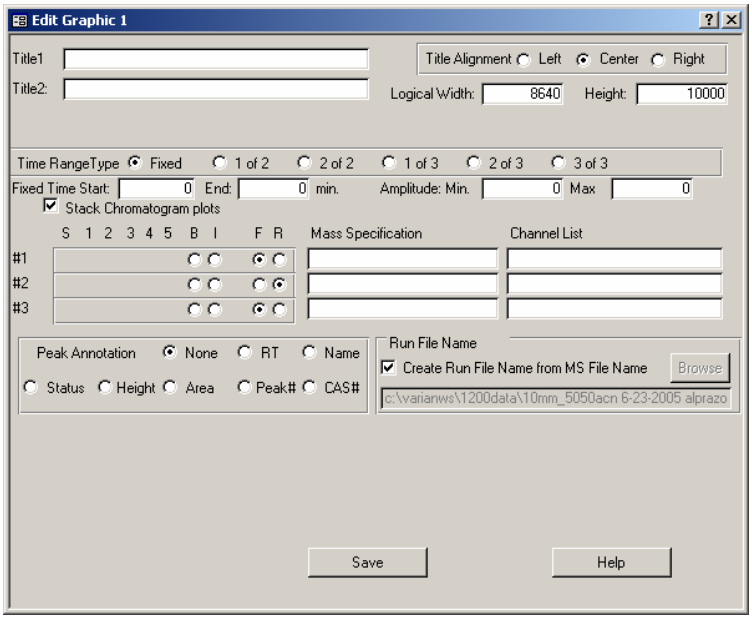


For Report Templates S2, S3, S4, T2, T3, T4, M2, M3 and M4.

This graphic type allows the selection of numerous chromatograms (RIC, unique mass chromatograms, and run file) and sample and reference spectra displays for target compounds.

Graphic Type “II”

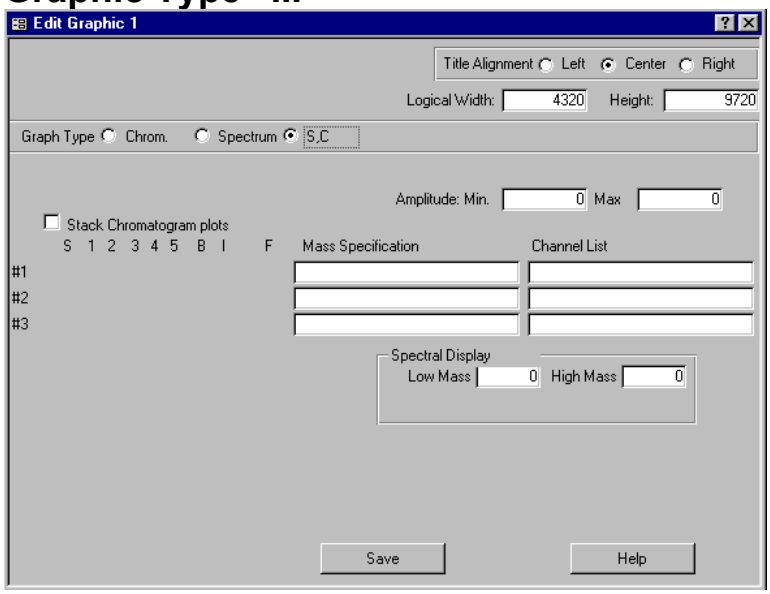




For Report Templates C1, C2, and C3

This page allows the design of the Chromatogram display.

Graphic Type "III"



For Report Templates U2, U3, and U4

This page allows the design of the Unknown compound graphic section.

Text Type

Text Type "A"

The “A” text type is available for Sub Report 1 and Sub Report 2 in Report Templates S2, S3, S4, M2, M3, M4, and TX.

Each sub-report allows a one-line text report for each target compound. The length of the selected fields will determine the number of fields that can be selected.

#
Compound Name
RT
Quan Ion
Area
Area%
Amount
Peak reject
Height
Rmatch
Fit Limit
Calib. RT
Group Name
IS#
IS
BC
Width
Ion Time
Calibration Equation
CAS#
FMatch
Hit Prob
Match
Match Value
Scan
Corr.
RC#
SrchWin
SrchMeth
S/N
Channel
Result Type
RF
RRT
QI1
QIR1Lo
QIR1Hi
QIR1
QI2
QIR21Lo
QIR2Hi
QIR2
QI3
QIR3Lo
QIR3Hi
QIR3
QI4
QIR4Lo
QIR4Hi
QIR4
QI5
QIR5Lo
QIR5Hi
QIR5
Units
Amnt Reject
Error
Status Codes
QIArea1
QIArea2
QIArea3
QIArea4
QIArea5
QIRT1
QIRT2
QIRT3
QIRT4
QIRT5
*
InLib Prob
IntegWin

Text Type “B”

The “B” text type is available for Sub Report 1 in Report Templates LG, LT, and UT.

Each sub-report allows a one-line text report for each target compound. The length of the selected fields will determine the number of fields that can be selected.

Compound Name	CAS#
RT	F Match
Quan Ions	Hit Prob
Area	Match
Area%	Match Value
Amount	RC#
Height	S/N
R Match	Channel
Fit Limit	Result Type
BC	Units
Width	Error
Ion Time	Status Code

Text Type “C”

Text type “C” is available for Sub Report 2, in Report Templates LG and LT.

Each sub-report allows a one-line text report for each target compound. The length of the selected fields will determine the number of fields that can be selected.

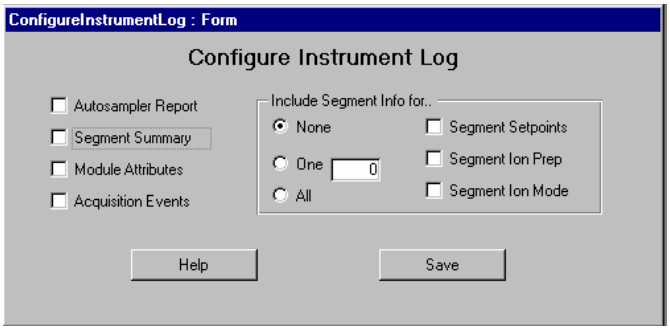
Hit#	R Match
Name	Hit Prob
Library	Match
CAS#	MatchVal
F Match	

Header Option

The Header Option is included with each Report template. The length of the selected field will determine the number of selectable options.

Acquisition Date	Instrument ID
Calculation Date	Peak Measure
Data filename	Calculation Type
Last cal sample	Sample Name
Inst. Method	Calculation Method
Operator Name	Recalc Notes
Inj. Notes	

Footer



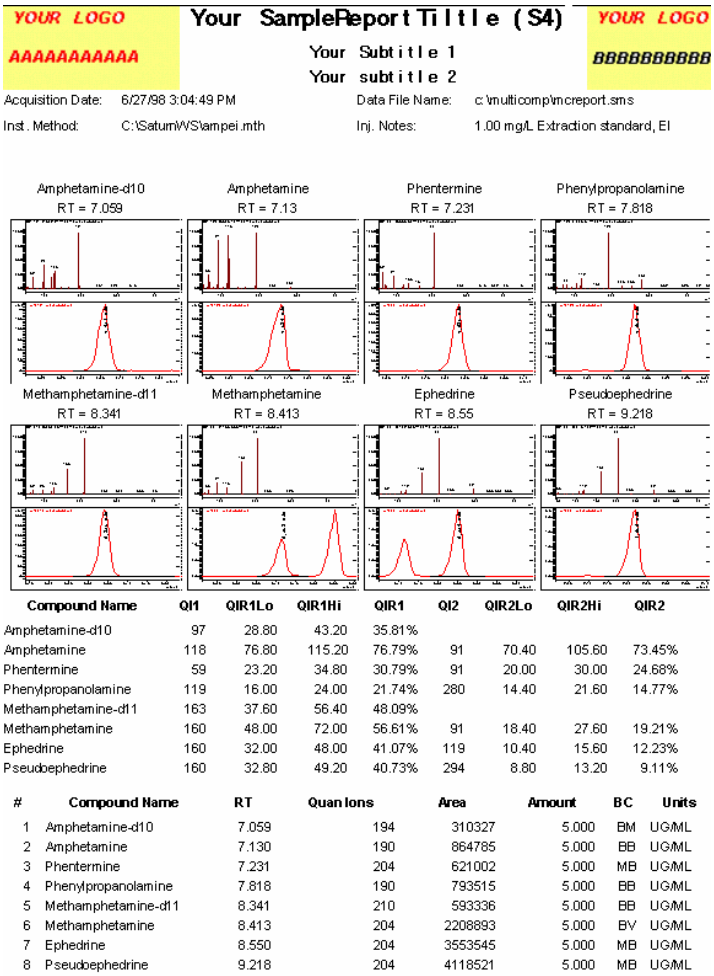
Configuration options for the "Footer" section. The "Footer" section is present only in Report templates S2, S3, S4, TX, LT, and LT.

Report Examples

Sample Reports (S)

S2 (2x2), S3 (3x3), S4 (4x4) differs only in the number of graphic displays on the page.

NOTE: The “S” type report has only 1 graphic page. Analytes identified as a given group may be selected for display; otherwise the first (RT) reported compounds will be printed. (Use the “M” type reports if more than 16 compounds are present and each must have a graphic display.)



YOUR LOGO

AAAAAAAAAA

Your SampleReport Tiltle (S4)

Your Subtitle 1

Your subtitle 2

YOUR LOGO

BBBBBBBBBB

Acquisition Date: 6/27/98 3:04:49 PM

Data File Name: c:\multicomp\mcreport.sms

Inst. Method: C:\SaturnWS\ampei.mth

Inj. Notes: 1.00 mg/L Extraction standard, EI

Amphetamine-d10 RT = 7.059

Amphetamine RT = 7.13

Phentermine RT = 7.231

Phenylpropanolamine RT = 7.818

Methamphetamine-d11 RT = 8.341

Methamphetamine RT = 8.413

Ephedrine RT = 8.55

Pseudoephedrine RT = 9.218

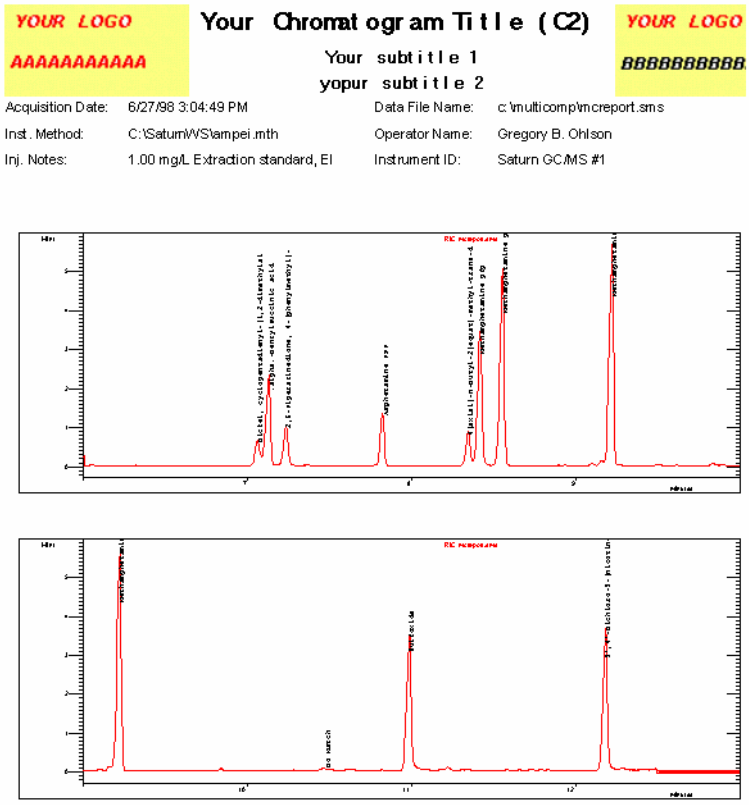
Compound Name	QI1	QIR1Lo	QIR1Hi	QIR1	QI2	QIR2Lo	QIR2Hi	QIR2
Amphetamine-d10	97	28.80	43.20	35.81%				
Amphetamine	118	76.80	115.20	76.79%	91	70.40	105.60	73.45%
Phentermine	59	23.20	34.80	30.79%	91	20.00	30.00	24.68%
Phenylpropanolamine	119	16.00	24.00	21.74%	280	14.40	21.60	14.77%
Methamphetamine-d11	163	37.60	56.40	48.09%				
Methamphetamine	160	48.00	72.00	56.61%	91	18.40	27.60	19.21%
Ephedrine	160	32.00	48.00	41.07%	119	10.40	15.60	12.23%
Pseudoephedrine	160	32.80	49.20	40.73%	294	8.80	13.20	9.11%

#	Compound Name	RT	Quan Ions	Area	Amount	BC	Units
1	Amphetamine-d10	7.059	194	310327	5.000	BM	UG/ML
2	Amphetamine	7.130	190	864785	5.000	BB	UG/ML
3	Phentermine	7.231	204	621002	5.000	MB	UG/ML
4	Phenylpropanolamine	7.818	190	793515	5.000	BB	UG/ML
5	Methamphetamine-d11	8.341	210	593336	5.000	BB	UG/ML
6	Methamphetamine	8.413	204	2208893	5.000	BV	UG/ML
7	Ephedrine	8.550	204	3553545	5.000	MB	UG/ML
8	Pseudoephedrine	9.218	204	4118521	5.000	MB	UG/ML

The sample report uses graphic type “I” and text type “A” for both text sub reports. It also has the “footer”. The graphic display is limited to one page.

Chromatogram Report (C)

C1, C2, C3 differs only in the number of chromatogram segments displayed. To include annotation on target compounds, the “Exclude Duplicates” field in the Varian MS data handling method (calculation set up section) must not be selected.

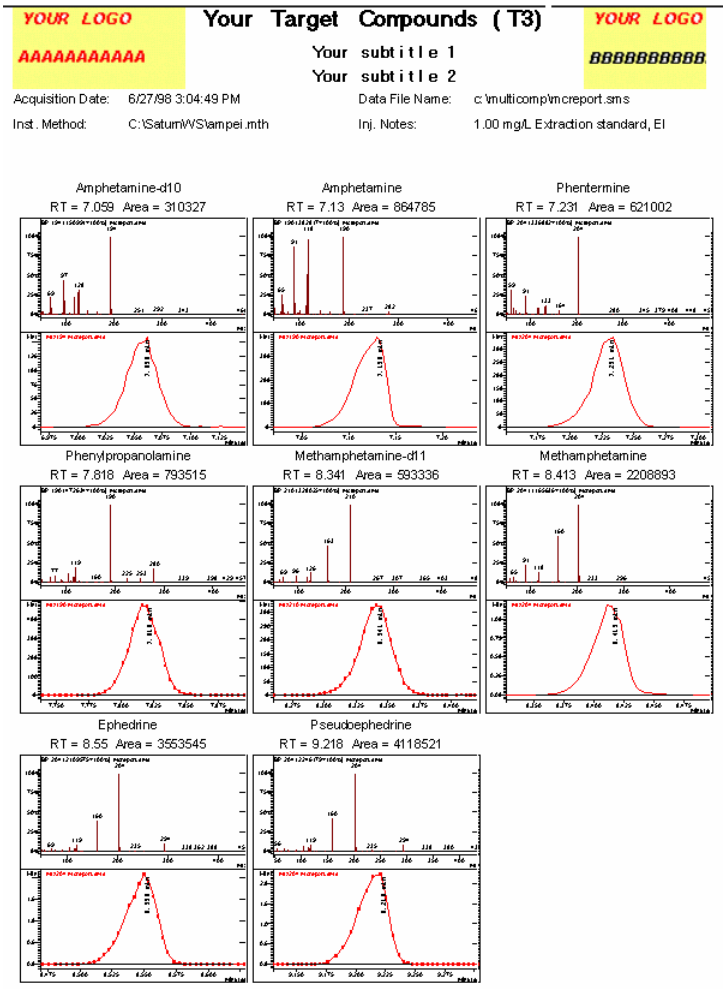


The chromatogram reports use graphic type “II”.

The chromatogram is displayed as one segment in C1, two segments in C2, and three segments in C3. All C reports are 1 page.

Target Report, Graphics Only (T)

T2 (2x2), T3 (3x3), T4 (4x4) differ only in the number of graphic displays on the page. The report has one graphic per target compound, continuing as many pages as necessary to show all compounds. No text report is printed with this template.

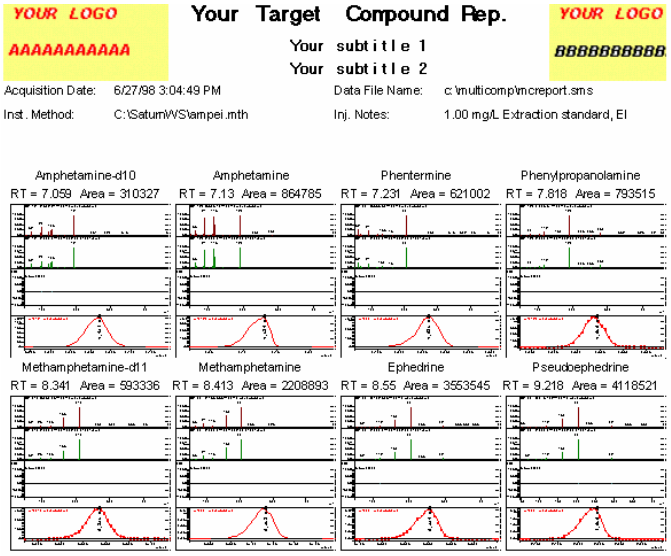


The target (T) reports use graphic type "I" and no text type. This is a multipage report.

Target Report Graphics and Text (M)

M2 (2x1), **M3** (3x2), **M4** (4x2) differ only in the number of graphic displays on the page.

Multiple graphic pages are included if the number of target analytes requires them. Each page contains two text records for each compound graphic shown on the page.



Compound Name	QI1	QIR1Lo	QIR1Hi	QIR1	QI2	QIR2Lo	QIR2Hi	QIR2
Amphetamine-d10	97	28.80	43.20	35.81%				
Amphetamine	118	76.80	115.20	76.79%	91	70.40	105.60	73.45%
Phentermine	59	23.20	34.80	30.79%	91	20.00	30.00	24.68%
Phenylpropanolamine	119	16.00	24.00	21.74%	280	14.40	21.60	14.77%
Methamphetamine-d11	163	37.60	56.40	48.09%				
Methamphetamine	160	48.00	72.00	56.61%	91	18.40	27.60	19.21%
Ephedrine	160	32.00	48.00	41.07%	119	10.40	15.60	12.23%
Pseudoephedrine	160	32.80	49.20	40.73%	294	8.80	13.20	9.11%

#	Compound Name	RT	Quan Ions	Area	Amount	BC	Units
1	Amphetamine-d10	7.059	194	310327	5.000	BM	UG/ML
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4	Phenylpropanolamine	7.818	190	793515	5.000	BB	UG/ML
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6	Methamphetamine	8.413	204	2208893	5.000	BV	UG/ML
7	Ephedrine	8.550	204	3553545	5.000	MB	UG/ML
8	Pseudoephedrine	9.218	204	4118521	5.000	MB	UG/ML

The target compound report with text (M) uses graphic type “I” and text type “A” for both text sub reports. The graphic display is multipage display.

Target Compound Report, Text Only (TX)

YOUR LOGO

AAAAAAAAAAA

Target Compounds text (TX)

Your subtitle 1

Your subtitle 2

YOUR LOGO

BBBBBBBBBB

Acquisition Date: 6/27/98 3:04:49 PM

Data File Name: c:\multicomp\mcreport.sms

Inst. Method: C:\SaturnWS\ampei.mth

Inj. Notes: 1.00 mg/L Extraction standard, EI

Compound Name	QI1	QIR1Lo	QIR1Hi	QIR1	QI2	QIR2Lo	QIR2Hi	QIR2
Amphetamine-d10	97	28.80	43.20	35.81%				
Amphetamine	118	76.80	115.20	76.79%	91	70.40	105.60	73.45%
Phentermine	59	23.20	34.80	30.79%	91	20.00	30.00	24.68%
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Methamphetamine-d11	163	37.60	56.40	48.09%				
Methamphetamine	160	48.00	72.00	56.61%	91	18.40	27.60	19.21%
Ephedrine	160	32.00	48.00	41.07%	119	10.40	15.60	12.23%
Pseudoephedrine	160	32.80	49.20	40.73%	294	8.80	13.20	9.11%

#	Compound Name	RT	Quan Ions	Area	Amount	BC	Units
1	Amphetamine-d10	7.059	194	310327	5.000	BM	UG/ML
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6	Methamphetamine	8.413	204	2208893	5.000	BV	UG/ML
7	Ephedrine	8.550	204	3553545	5.000	MB	UG/ML
8	Pseudoephedrine	9.218	204	4118521	5.000	MB	UG/ML

The Target Compound text only (TX) report uses text type "A" for both text sub reports. It also has the "footer".

Tentatively Identified Compounds (TIC) Report, Graphics and Text (LG)

YOUR LOGO

AAAAAAAAAAA

Your TIC Graph Text (LG) Report

Your subtitle 1

Your subtitle 2

YOUR LOGO

BBBBBBBBBB

Acquisition Date: 6/27/98 3:04:49 PM

Data File Name: c:\multicomp\mcreport.sms

Inst. Method: C:\SaturnWS\ampei.mth

Operator Name: Gregory B. Ohlson

Inj. Notes: 1.00 mg/L Extraction standard, EI

Instrument ID: Saturn GC/MS #1

TIC peak

Apex

Hit #1

Hit #2

Hit #3

RT	Area	Amount	Width	Ion Time	S/N	Units
10.977	9710617	9710617.000	2.0	145	332	Counts

Hit#	Name	CAS#	Fit	RFit	Purity
1	Sulfoxide	120627	777	721	612
2	N-Formyl-3,4-methylenedioxyamphetamine	67669005	790	712	581
3	Methylenedioxyamphetamine acetate	36209719	850	711	646

TIC peak

Apex

Hit #1

Hit #2

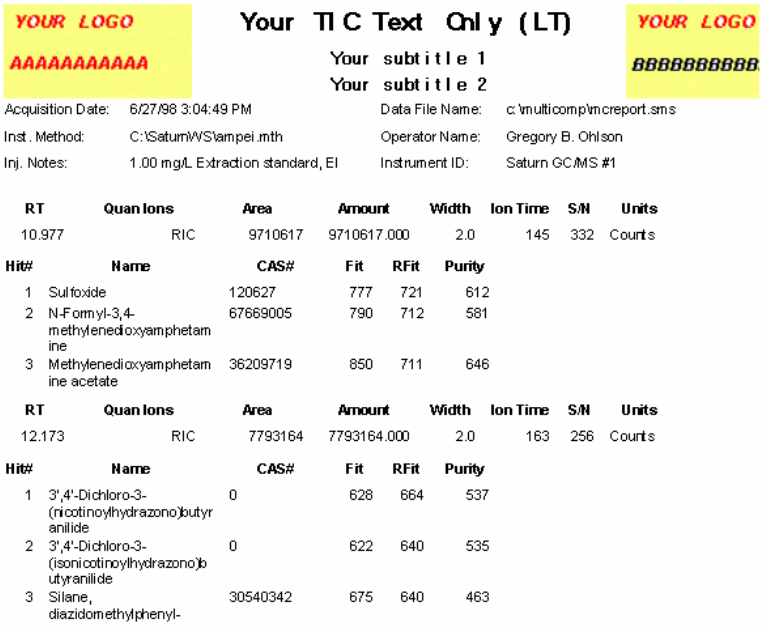
Hit #3

RT	Area	Amount	Width	Ion Time	S/N	Units
12.173	7793164	7793164.000	2.0	163	256	Counts

Hit#	Name	CAS#	Fit	RFit	Purity
1	3',4'-Dichloro-3-(nicotinoylhydrazono)butyranilide	0	628	664	537
2	3',4'-Dichloro-3-(isonicotinoylhydrazono)butyranilide	0	622	640	535
3	Silane, diazidomethylphenyl-	30540342	675	640	463

The TIC Graphic report (LG) has a predefined graphic option as shown above. It uses text type "B" for sub report 1 and Text type "C" for sub report 2. It is a multipage report.

Tentatively Identified Compounds (TIC) Report, Text Only (LT)



YOUR LOGO

AAAAAAAAAA

Your TIC Text Only (LT)

Your subtitle 1

Your subtitle 2

YOUR LOGO

BBBBBBBBBB

Acquisition Date:	6/27/98 3:04:49 PM	Data File Name:	c:\multicomp\mcreport.sms
Inst. Method:	C:\SaturnWS\ampei.mth	Operator Name:	Gregory B. Ohlson
Inj. Notes:	1.00 mg/L Extraction standard, EI	Instrument ID:	Saturn GC/MS #1

RT	Quan Ions	Area	Amount	Width	Ion Time	S/N	Units
10.977	RIC	9710617	9710617.000	2.0	145	332	Counts

Hit#	Name	CAS#	Fit	RFit	Purity
1	Sulfoxide	120627	777	721	612
2	N-Formyl-3,4-methylenedioxyamphetamine	67669005	790	712	581
3	Methylenedioxyamphetamine acetate	36209719	850	711	646

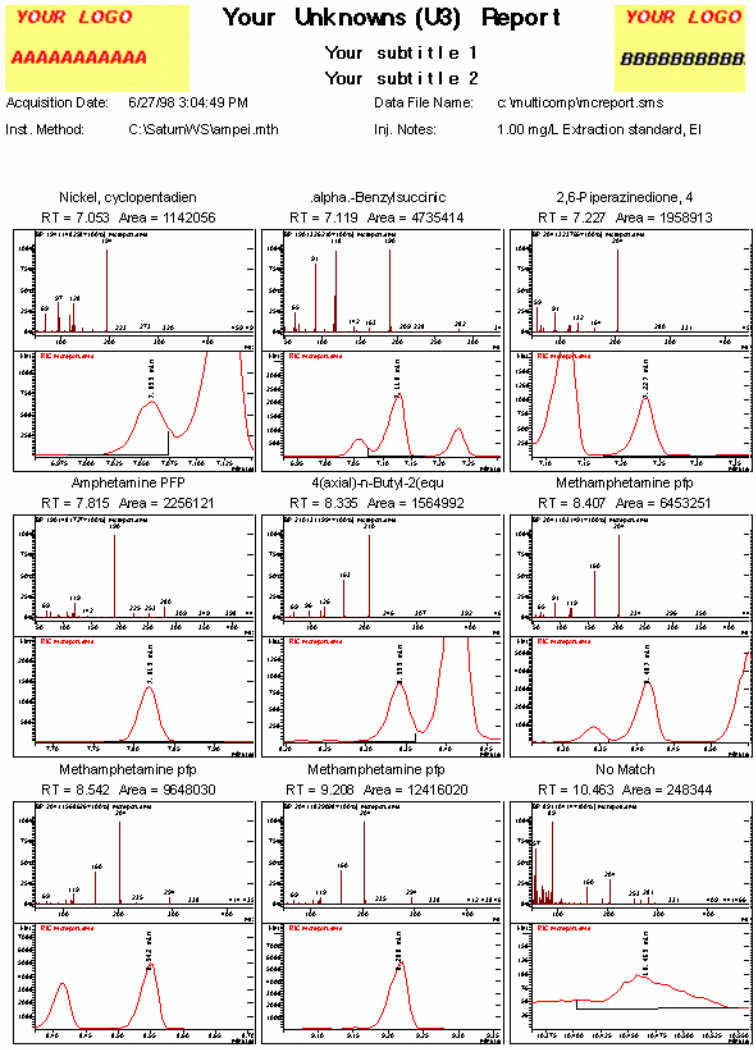
RT	Quan Ions	Area	Amount	Width	Ion Time	S/N	Units
12.173	RIC	7793164	7793164.000	2.0	163	256	Counts

Hit#	Name	CAS#	Fit	RFit	Purity
1	3',4'-Dichloro-3-(nicotinoylhydrazono)butyranilide	0	628	664	537
2	3',4'-Dichloro-3-(isonicotinoylhydrazono)butyranilide	0	622	640	535
3	Silane, diazidomethylphenyl-	30540342	675	640	463

The TIC text only report uses text type "B" for sub report 1 and Text type "C" for sub report 2.

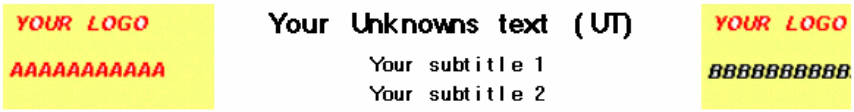
Unknown Report, Graphic and Text (U)

U2 (2x2), **U3** (3x3), **U4** (4x4) differ only in the number of graphic displays on the page. One graphic is shown for each unknown peak.



The Unknown report (U) uses graphic type "III". It is a multipage report.

Unknown Report, Text Only (UT)



Acquisition Date: 6/27/98 3:04:49 PM
Data File Name: c:\multicomp\mcreport.sms
Inst. Method: C:\SaturnWS\ampei.mth
Inj. Notes: 1.00 mg/L Extraction standard, EI

Compound Name	RT	Area	Width	Ion Time	Match	MatchVal	Result Type
Nickel, cyclopentadienyl-(1,2-dimethylal	7.053	1142056	0.8	703	RFit	633	Duplicate
.alpha.-Benzylsuccinic acid	7.119	4735414	2.3	150	RFit	724	Duplicate
2,6-Piperazinedione, 4-(phenylmethyl)-	7.227	1958913	1.7	510	RFit	731	Duplicate
Amphetamine PFP	7.815	2256121	1.6	456	RFit	822	Duplicate
4(axial)-n-Butyl-2(equat)-methyl-trans-d	8.335	1564992	1.6	607	RFit	704	Duplicate
Methamphetamine pfp	8.407	6453251	1.8	150	RFit	865	Duplicate
Methamphetamine pfp	8.542	9648030	2.0	121	RFit	680	Duplicate
Methamphetamine pfp	9.208	12416020	1.9	117	RFit	714	Duplicate
No Match	10.463	248344	0.0	5208	RFit	N/A	Unknown
Sulfoxide	10.977	9710617	2.0	145	RFit	721	TIC
3',4'-Dichloro-3-(nicotinoylhydrazono)bu	12.173	7793164	2.0	163	RFit	664	TIC

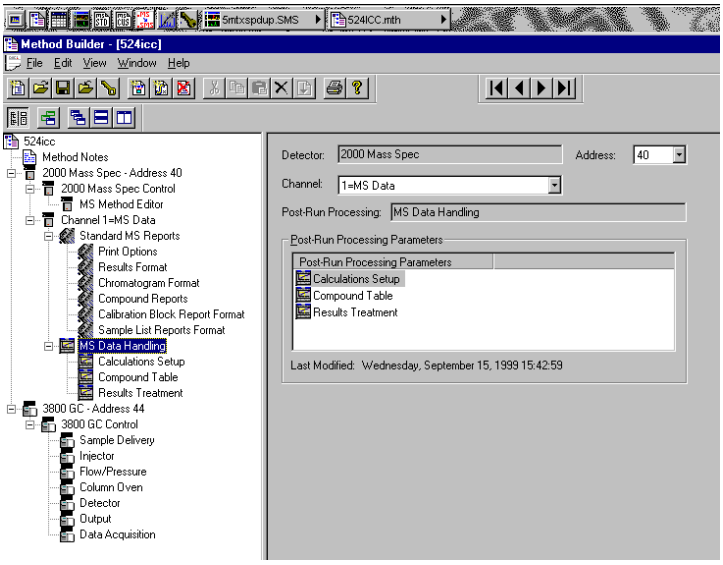
The Unknown text only report (UT) uses text type "B" for Sub report 1. It also includes the "footer".

What You Need to do Before Starting MultiComp

MultiCpd reports the results of datafiles processed in Varian MS Workstation 6.5 or later version. (Data generated with prior versions of the software also can be processed, but first must be converted to version 5.4 or later format.)

The MultiCpd reports the results already stored in the Varian MS workstation data files. It does not calculate or store data itself.

Before using MultiCpd, a Varian MS workstation method (.mth) must be built, calibrated and used to analyze the appropriate samples. The rest of this chapter discusses the use of the Varian MS Workstation Method builder program to build methods for use with MultiCpd.



The data handling section of the method should be built with great care to deliver the best results

In the Compound Table, the compound identification, integration, calculation and quantitation parameters must be optimized to deliver the best results. Review the compound table integration and identification parameters (peak width, slope sensitivity, tangent %, peak window width etc.) before the calibration is carried out. Verify and adjust as necessary the curve fitting options (including the handling of the origin and the regression weighting parameters) to deliver the most accurate results.

The "Calculation Setup" also must be properly completed for the tentatively identified compounds.

Calculations Setup in the Varian MS Workstation (.mth) Method

The following settings are recommended:

General

Measurement Type: Area or Height

Area is the commonly used measurement type.

Calibration type: Internal or External Std

Report Missing peaks: Yes (checked) If not checked, MultiCpd will not report target Compounds which were not found.

Report Unknown peaks: yes if tentatively identified compounds and unknowns are to be reported

Normalize results: no (not checked)

Ignore Calibration data: no (not checked)

Scale Air Flow Samples: no (not checked)

Chromatogram Processing

Tentative Identification

Library Search Unknown peaks: yes if tentatively identified compounds are to be reported

Identify libraries and search parameters as desired.

Specify Quan ion (for tentatively identified compounds this is usually RIC)

Specify Integration Parameters for tentatively identified compounds

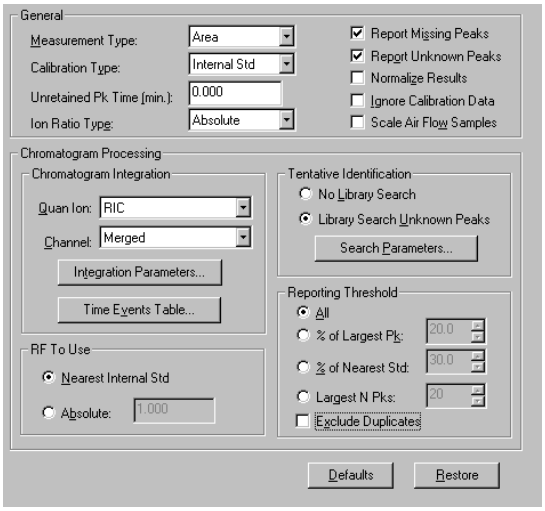
Specify RF to use for tentatively identified compounds

Reporting Threshold

Exclude Duplicates: no (not checked)

If the Duplicates are excluded, the Chromatogram Report will not have annotation on the target compounds. If Duplicates are included, target analytes will be listed as duplicate in the unknown report.

Peaks excluded by the other Report Threshold parameters will be excluded from MultiCpd reports. It may be desirable to increase the peak size threshold here, to limit the number of tentatively identified compound peaks reported



Calculation Setup page of the Data handling section of the .mth method

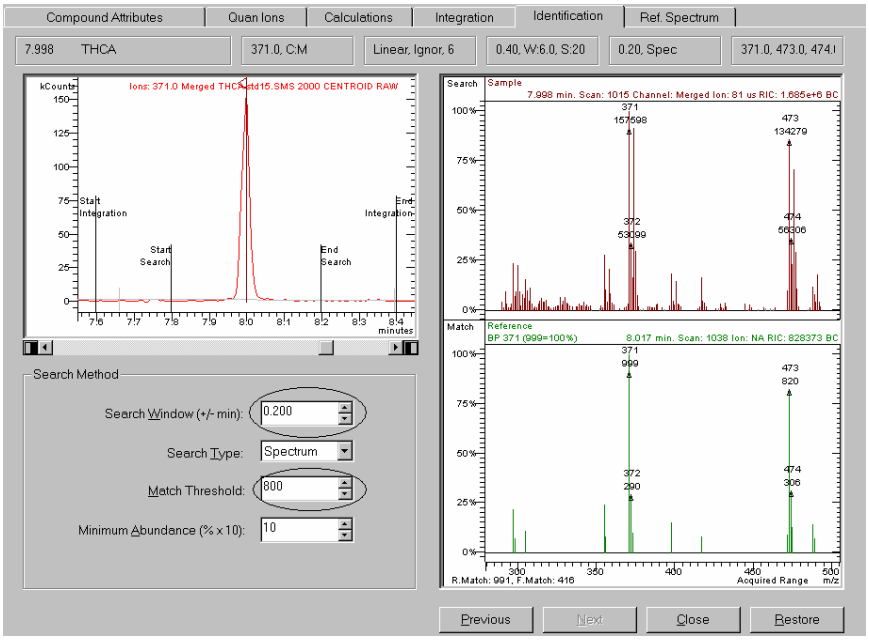
Compound Table Setup in the Varian MS Workstation (.mth) Method

The reporting of target analytes in MutiCpd will be dependent on the parameters set in the Compound table section.

Target compounds excluded by these threshold parameters will be excluded from the reports. These parameters are:

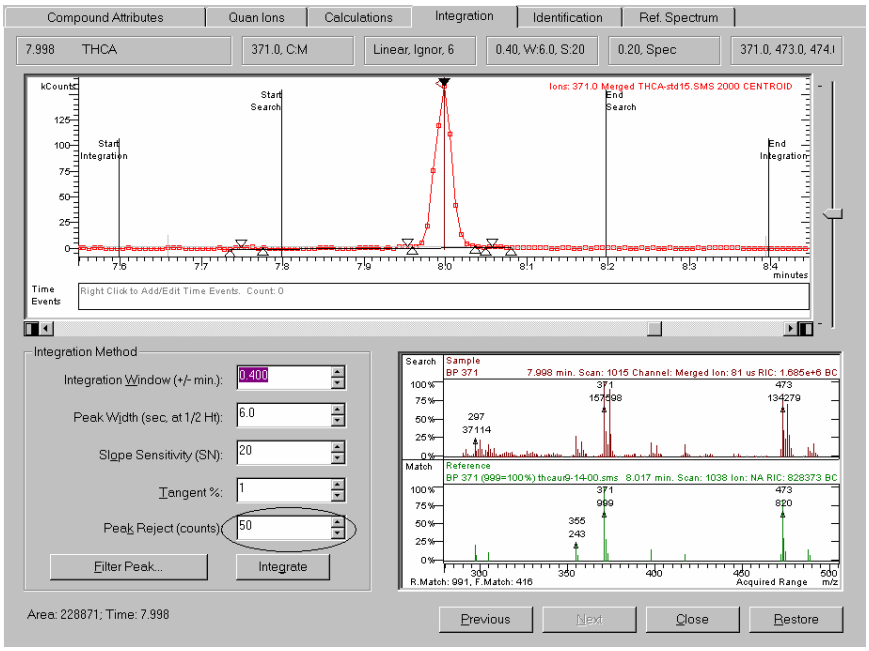
- Search Window
- Identification threshold

- Peak Area/Height rejection threshold
- Report rejection (amount) threshold
- Qualifier Ion Ratios
- Grouping

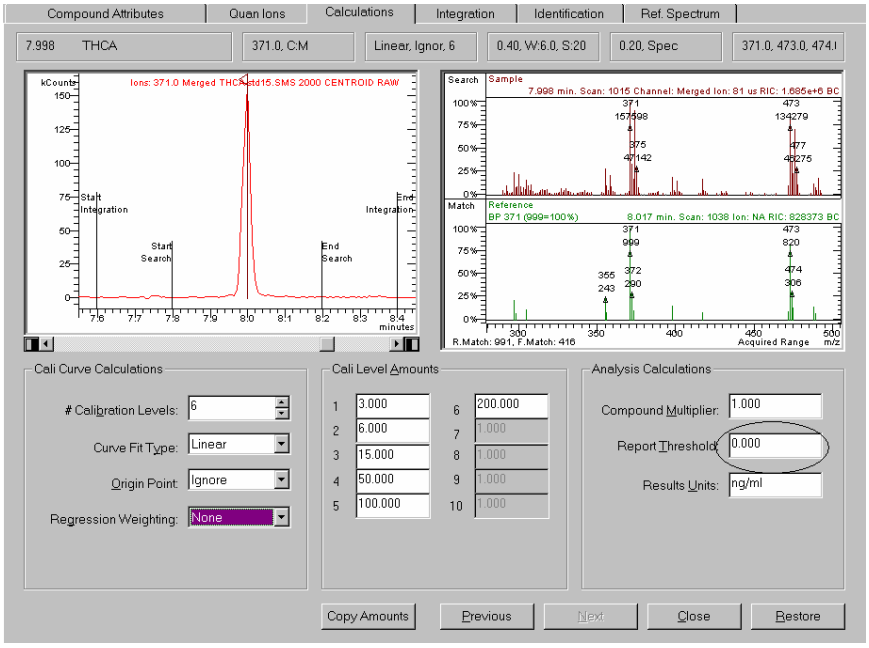


Peak Window +/-. This is the chromatogram segment to be shown for target compound chromatogram plots.

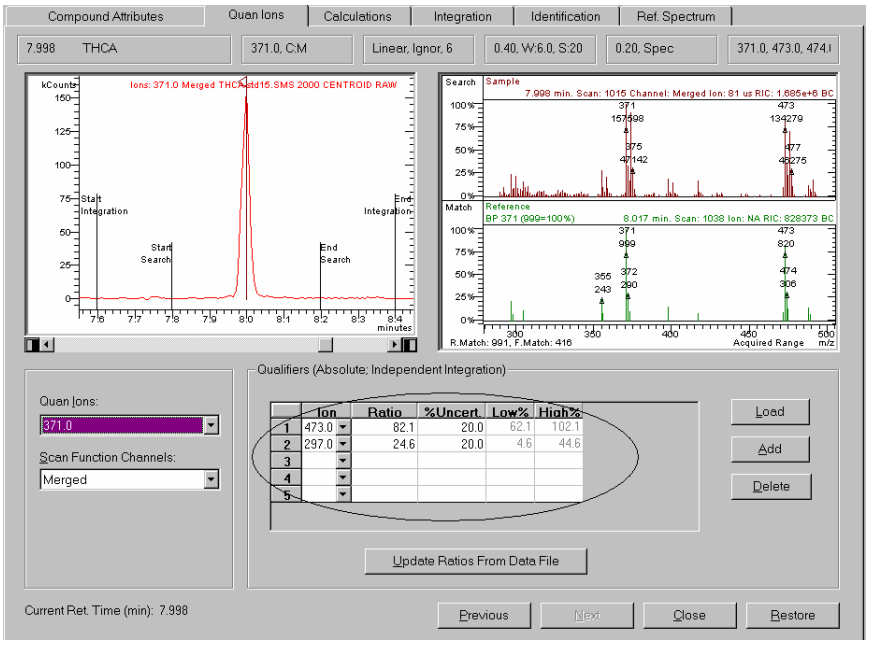
Identification (Match threshold). If the fit is below this number, the peak will be rejected.



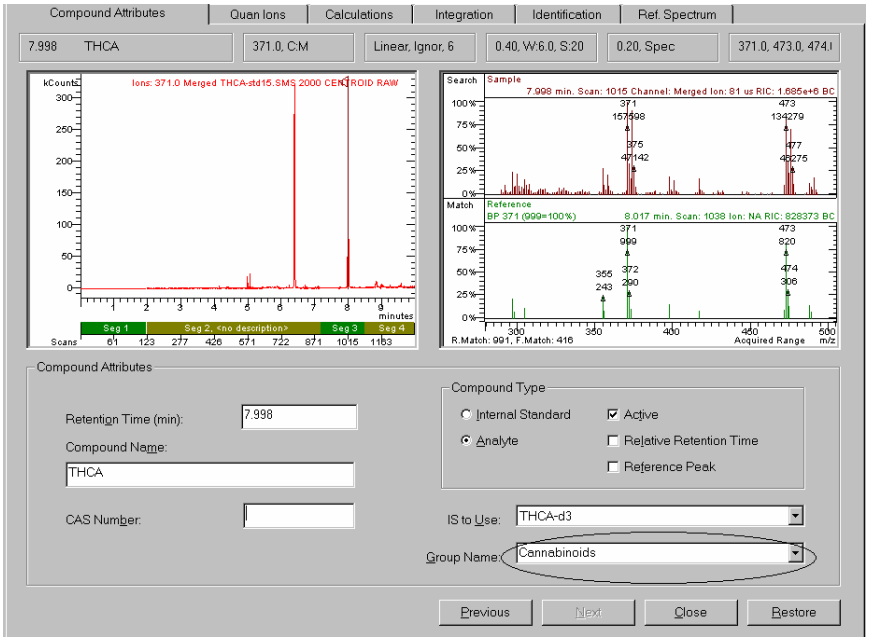
Peak Area/Height Rejection (counts)



Report Threshold (Calculated amount)



Qualifier Ions

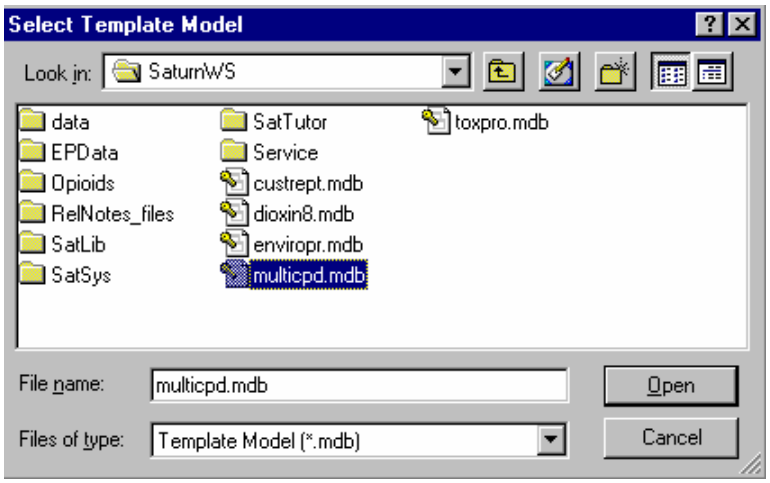


Grouping within the Compound Table

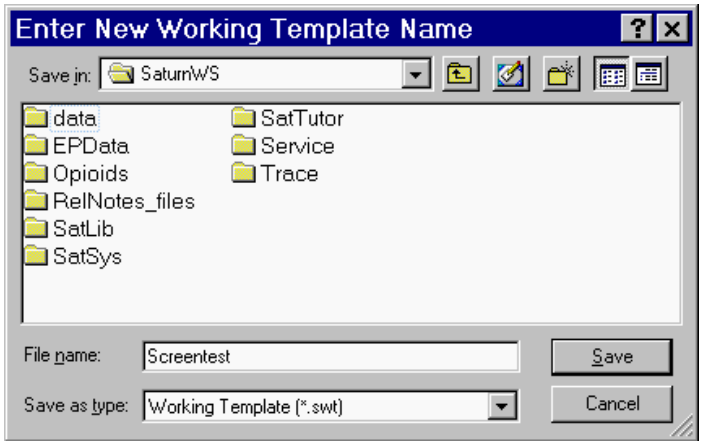
Interactively Reviewing Reports

To use a MultiCpd template to interactively review reports derived from a data file, follow these steps:

1. Prepare the Varian MS (.mth) method. Use MS Data Review in conjunction with the Method Editor to prepare a Varian MS Data Handling method for use in integrating and quantitating the Varian MS Data files of interest.
2. Quantitate the file. Use the method to integrate and quantitate the Varian MS Data file, thereby storing results to report into the data file.
3. Select the printer. The Windows Start-Settings-Printers folder is used to select the default system printer. The printer selected as the "Default System Printer" is used to print Custom MS Reports.
4. Prepare the "swt" file. Open the Star Toolbar and click the "Custom MS Reports" icon. Create a new, MultiCpd derived database (*.swt) file (or select and existing Multicpd template). To create a new template select "new template" and you will see the following (or similar) screen.

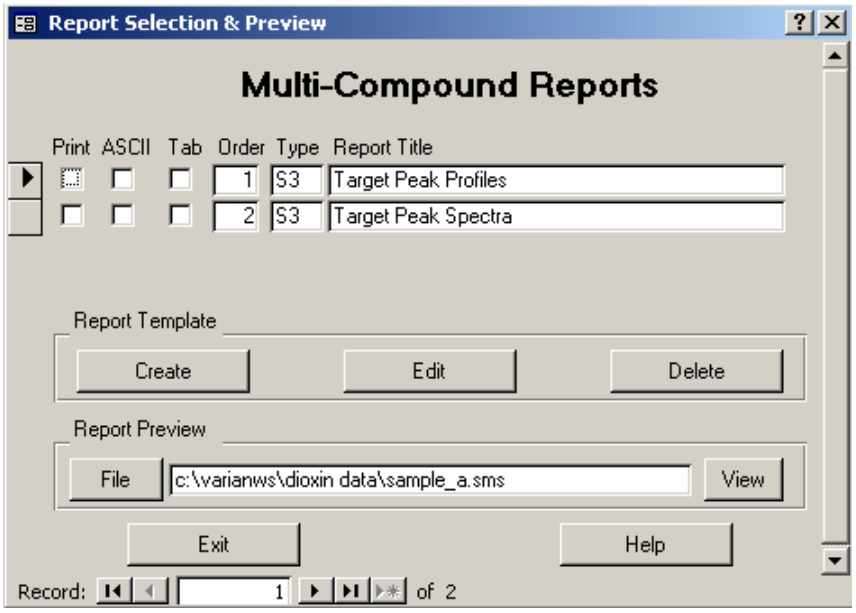


5. Select the "Multicpd.mdb" to be opened.



6. Type the file name you wish to use for this report and select the Save button. The name will be given the extension “swt” as shown in the next screen.

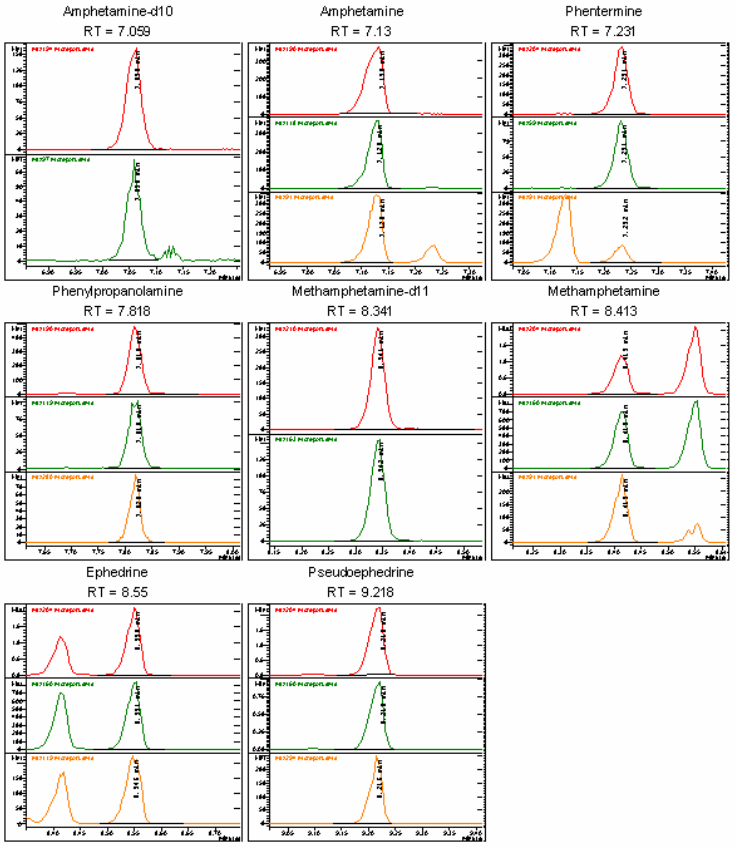
The template box will open. There are two reports already created in this template, the “Target Peak Profiles” and the “Target Peak Spectra”. This is the page where additional reports in the given template may be created or the existing ones edited/deleted. The Edit/create features will be discussed later in the manual.



7. **Select a data file for the report by pressing the “File” button.** An example data (Mcreport.sms) file is located in the Varian MS/MCdata directory.
8. **Select a report template.** To select a report for review based on one of the currently defined reports, click on the far left of the desired report title. A black triangle will indicate the selected report.
9. **View the report.** Click on the “View” button. If the selected report is text only or a Sample type report (S2, S3, or S4) a report image will be shown. If the selected report is a multipage report containing graphics on every page, then a page selection form will appear. To view the report, select the desired page, and then click the “Preview Report” button. While a report is displayed there will be a small toolbar directly above it containing icons to print and zoom the scaling of the report screen image. The record selector structure at the bottom left of the report window can be used to navigate through a multipage report.

Target Peak Profiles

Acquisition Date: 6/27/98 3:04:49 PM Data File Name: c:\multicomp\mcreport.sms
Inst. Method: C:\SaturnWS\ampei.mth Inj. Notes: 1.00 mg/L Extraction standard, EI



Compound Name	#	IS	RT	Quan Ions	Area	Amount	Units
Amphetamine-d10	1		7.059	194	310327	5.000	UG/ML
Amphetamine	2		7.130	190	864785	5.000	UG/ML
Phentermine	3		7.231	204	621002	5.000	UG/ML
Phenylpropanolamine	4		7.818	190	793515	5.000	UG/ML
Methamphetamine-d11	5		8.341	210	593336	5.000	UG/ML
Methamphetamine	6		8.413	204	2208893	5.000	UG/ML
Ephedrine	7		8.550	204	3553545	5.000	UG/ML
Pseudoephedrine	8		9.218	204	4118521	5.000	UG/ML

Compound Name	QI1	QIR1	QIR1Lo	QIR1Hi	QI2	QIR2	QIR2Lo	QIR2Hi
Amphetamine-d10	97	35.81%	28.80	43.20				
Amphetamine	118	76.79%	76.80	115.20	91	73.45%	70.40	105.60
Phentermine	59	30.79%	23.20	34.80	91	24.68%	20.00	30.00
Phenylpropanolamine	119	21.74%	16.00	24.00	280	14.77%	14.40	21.60
Methamphetamine-d11	163	48.09%	37.60	56.40				
Methamphetamine	160	56.61%	48.00	72.00	91	19.21%	18.40	27.60
Ephedrine	160	41.07%	32.00	48.00	119	12.23%	10.40	15.60
Pseudoephedrine	160	40.73%	32.80	49.20	294	9.11%	8.80	13.20

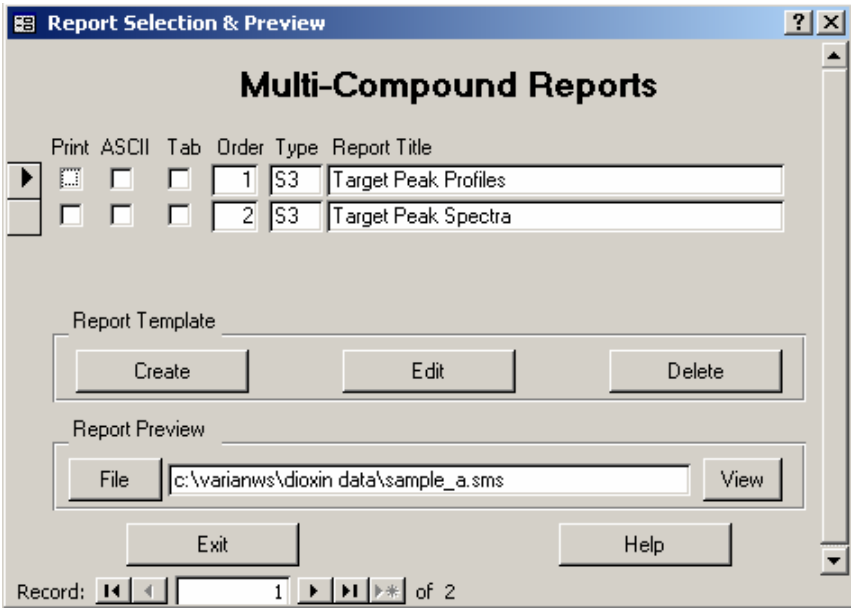
Report generated by the selected template and data file.

10. **Exit Program.** The Working Template (test1.swt in our case) can also be called during automation by using the AutoLink feature in the Sample List.

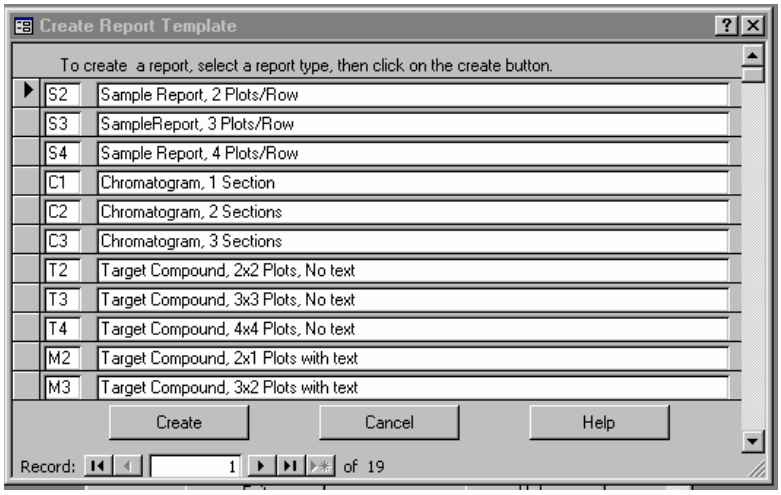
Creating a New Report Template

To create a new report, follow these steps:

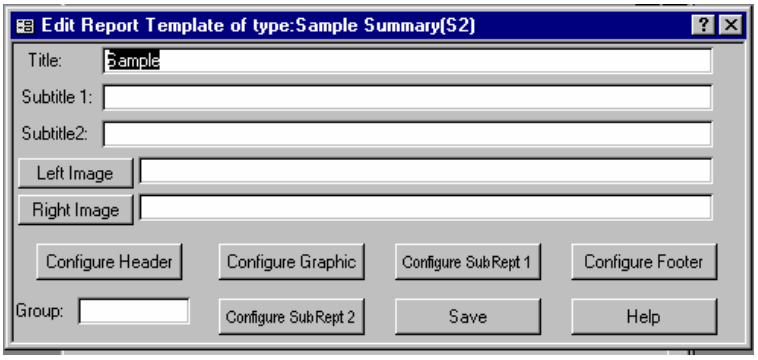
1. Open the appropriate MultiCpd template (x.swt).
2. From the "Multi-Compound Reports" form, click the “Create” button.



3. On the “Create Report” page click the selector button to the left of the report type desired, then click the button.



4. The "Edit Report Template" form will appear. In the top line the type of report created will be indicated. Use this page to customize the default report options, or just click the "Save" button to complete creation of the default report type.



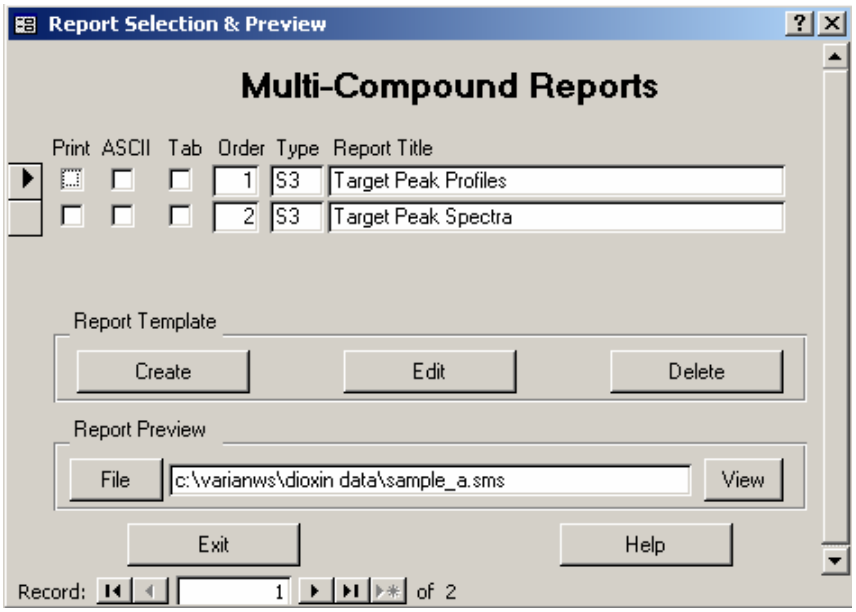
The new report will be listed in the report list shown on the "Multi-Compound Reports" form. It may be necessary to scroll down using the scroll bar on the right of the "Multi-Compound Reports" form for the title of the newly created report to be visible.

When a report is created, its “Print” checkbox is checked, enabling printing during Sample List or Recalc List processing. To disable automatic printing, clear the “Print” check box at the left of the report title on the "Multi-Compound Reports" form. The state of the “Print” checkbox can be changed by clicking the left mouse button while the mouse cursor is over the box.

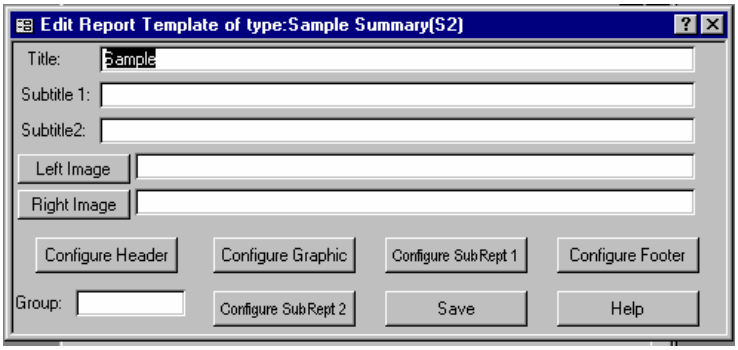
Some report types listed on the Report Creation form have several variants listed in the template list. These variants differ only in the number and/or placement of graphics. Once a report is created, its graphics can be modified to show alternate content, but the number of graphics and their relative placement on the page cannot be changed.

Editing an Existing Report Template

To edit an existing report template, from the "Report Selection & Preview" form, click the “Report Selector” button to the left of the report title of the report to be edited, then click the Edit button.



The "Edit Report Template" form will appear as shown below.



This dialog box can be used to edit the Titles at the top of the report and can also be used to have up to 2 bitmaps appear on the report. This can be a company logo or any picture that you wish to display. Simply type in the file name of the desired bitmap in the Left or Right Image box. Select the “Save” button to exit this dialog box.

Report Titles

The top three fields on the "Edit Report Template" form define the main title and two subtitle lines on the report. These three lines are printed at the top of the report in a fixed position, i.e., leaving them blank does not shorten the length of the report. In those fields you may type in any information that you wish to appear on the top of the report in these fields. It is advisable to edit the main title line to contain a unique title.

Adding Icons or Bitmaps

Three quarters of an inch high by one and a quarter inch wide graphics may be placed to the left and/or right of the Report Title block on a report. If the full pathname of an Icon file (*.ico), a Bitmap file (*.bmp), or a Graphic file (*.gif) is specified in the Left Image and/or Right Image fields of the Edit Report Template form, the corresponding image will be shown on the report.

The specified graphic may be of any native size. It will be scaled, preserving the aspect ratio, so it will fit inside the allotted space.

To browse for an existing graphic file, click the "Left Image" or "Right Image" button. Alternatively, the full pathname may directly entered in the text box.

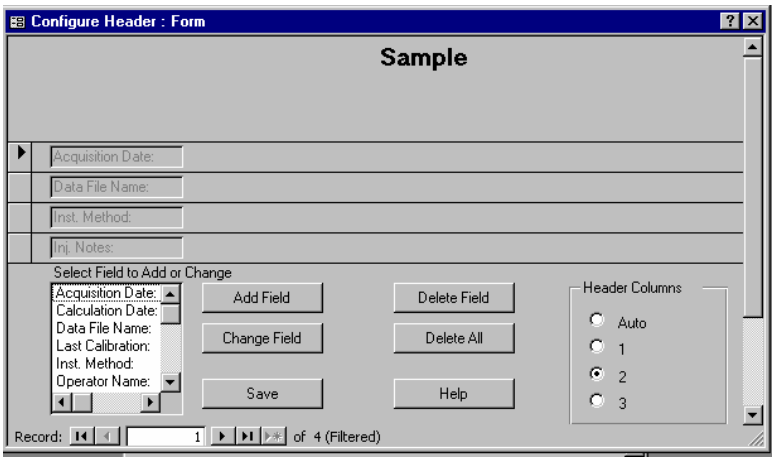
Report Header

The report header follows the title block on the report. It consists of zero to twenty fields, set up on the "Configure Header" form. The selected fields may be listed in a single column, listed in two columns, listed in three columns, or arranged to efficiently fill the space without truncating any fields (Auto). The fields will be listed in the report from left to right, top down in the order specified in the list of selected fields on the "Configure Header" form. A fixed space (0.75 inches high x 6 inches wide) is reserved for the header. It will show about 3 fields vertically or up to about 6 fields in two columns. If additional fields are specified they may be omitted from the report.

Editing the Report Header

To change the report header:

5. From the "Multi-Compound Reports" form, select the report to be edited, then click the "Edit" button to show the "Edit Report Template" form.
6. On the "Edit Report Template" form, click on the "Configure Header" button to show the "Configure Header" form.



The screen shown above is the dialog box that you will see when you select the Configure Header button.

The top of the "Configure Header" form shows the report title and two subtitle lines. This is followed by a scrollable list of fields currently selected for inclusion in the report header. The bottom of the form consists of a list box of all fields available for inclusion in the header, six command buttons and a button group to select the header layout.

- To change the layout format, click on the button corresponding to the desired number of columns.
- To clear the header so no fields are displayed, click the "Delete All" command button.
- To delete a single field from the header, select the field to be deleted by clicking on its selector button then click the "Delete Field" button.
- To change (replace) a field in the header, select the field to be changed, click on the replacement field selection in the list box at the lower left of the form, and then click the "Change Field" command button.
- To add a field to the bottom of the header, click on the field to be added in the list box on the lower left of the form, then click on the "Add Field" command button.

Report Header Fields

The Field List is a list of header items that can be placed on the report. You must use the scroll bar to view the entire list.

Acquisition Date

Time and date that the data file was acquired.

Calculation Date

Time and date that the data file was last processed by data handling.

Data File Name

Full path name of data file.

Last Cal. Sample

Time and date of most recently acquired file listed in the calibration log.

Inst Method

Instrument Method. The full path name of the method used to acquire the data file.

Operator Name

See System Control-Instrument Configuration-Instrument Parameters dialog. This field reports the value of the Operator Name when the data was acquired.

Inj. Notes

See Sample List – Injection Notes in System Control. This field reports the notes made when the data was acquired.

Instrument ID

See System Control-Instrument-Configuration-Instrument Parameters dialog. This field reports the value of the Instrument ID when the data file was acquired.

Peak Measure

"Area", "Height" or "Unknown". Declares the peak measure used to compute RF and Amount fields. Set by data handling based on the method parameter MS Data Handling-Calculation Setup – Measurement Type.

Calculation Type

"Internal Standard", "External Standard", "Area Percent", or "Unknown". Declares the calibration type used to compute RF and Amount. Based on data handling errors, the method parameter MS Data Handling - Calculation Setup - Calibration Type, and influenced by the proper designation and successful identification of internal standard peaks when appropriate.

Sample Name

See Sample List – Sample Name in System Control. This field reports the value of the Sample Name set up when the data was acquired.

Calc Method

Full path name of the method used for last reprocessing of data file by data handling.

Recalc Notes

See Recalc List – Recalc Notes in System Control. This field reports the text of Recalc Notes set when file was last recalculated.

Header Columns

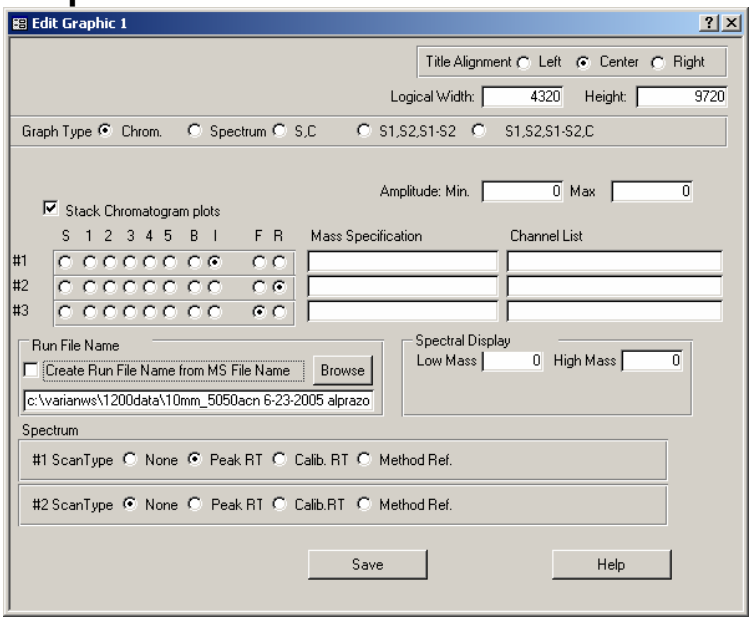
The header fields can be displayed in several ways on the report. Selecting the button for “1” will display all of the information in a single column. Select “2” for two columns and “3” for three columns displayed. The Auto selection will display all of the information using the default settings for spacing of the information.

Graphics

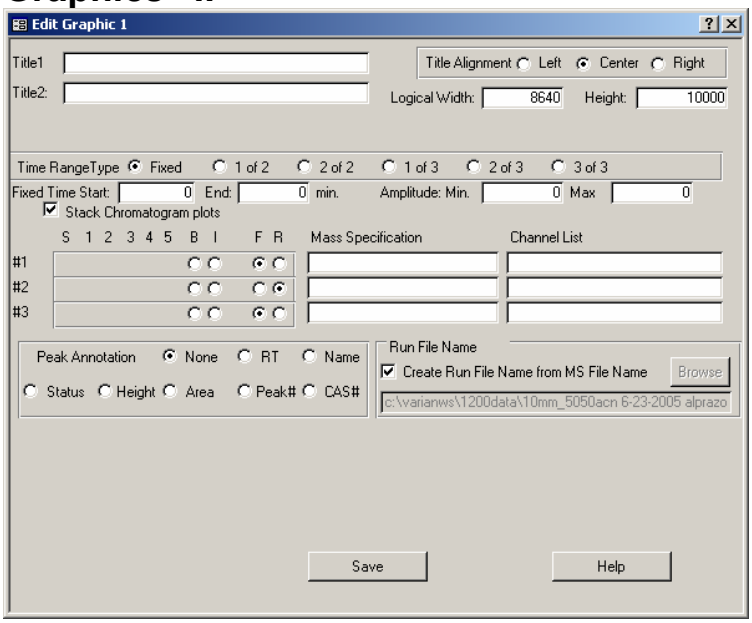
Reports may contain from 0 to 16 chromatogram/spectra frames. The number, relative size, and placement of these frames is determined by the template used to create the report. The content of each frame may be customized in ways that depend on the type of report. To modify a graphic frame:

7. From the "Multi-Compound Reports" form, select the report to be edited, then click the "Edit" button to show the "Edit Report Template" form.
8. On the "Edit Report Template" form, click the "Configure Graphic" button to show the "Select Graphic" form for reports with multiple independent graphics, or to directly open the Edit Graphics form for reports with multiple instances of a single graphic type.
9. The "Select Graphic" form will show buttons whose relative size and position represent the graphic frames present in the report template being edited. Click on the button representing the frame to be edited to open the "EditGraphic" form. This form can be used to configure the content of the graphic frame.

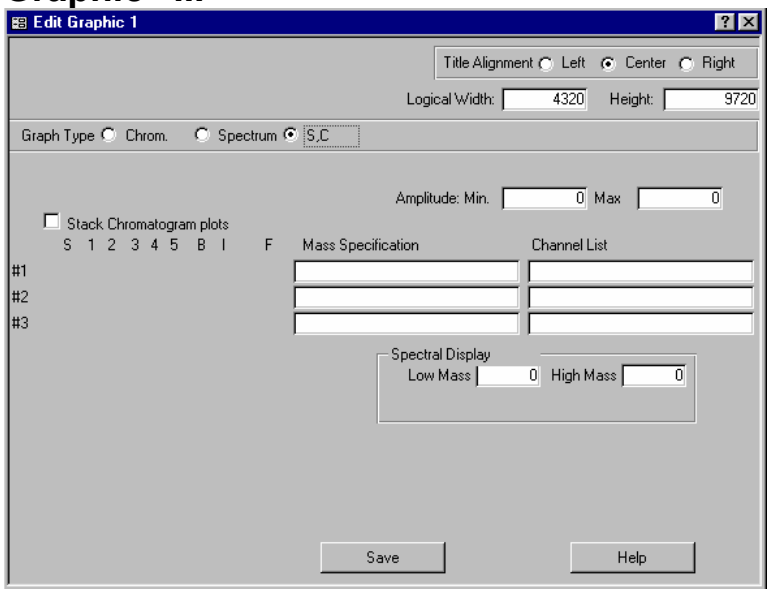
Graphics “I”



Graphics “II”



Graphic “III”



The graphic may be a chromatogram, consisting of between 1 and 3 overlaid or stacked traces; and/or one or three spectra drawn from the chromatogram, the data handling method used to quantitate the chromatogram, the result of a library search, or a combination of these.

Graphic Controls

Some of the parameters described below are not available in all three graphic formats

Title1

Top title line.

Title2

Subtitle line.

Title Alignment

Specifies whether title lines are left, center, or right aligned over graphic.

Logical Width, Logical Height

Width, Height in twips (1440 twips = 1 inch) of graph as drawn. This size is scaled to fit the actual size of the graphic as specified by the report template. The effect of these parameters is primarily to alter the relative size and placement of text on the graphic. Larger values reduce text size.

Graph Type

Select one of the following choices to determine the basic graphic type. Click the button for your choice.

Chrom

Show a chromatogram. One chromatogram is selected. Up to three traces derived from the chromatogram may be shown. The chromatogram segment to be shown will depend on the parameters set for the P*eak Window +/-* parameter in the Varian MS data handling method, identification section.

Spectrum

Show one spectrum. This can be a reference or sample spectrum.

S, C

Show one spectrum over a chromatogram in the same graphic box.

S1, S2, S1-S2

Show two spectra and their difference in the same graphic box.

S1, S2, S1-S2, C

Show two spectra and their difference over a chromatogram in the same graphic box. This can be cluttered due to size restrictions.

Time Range Type (Graphic II)

This selection specifies the time range displayed in the chromatogram.

Fixed

The time range displayed is determined by the content of the Fixed Time Start and End edit boxes.

1 of 2

The first half of the chromatogram is displayed.

2 of 2

The second half of the chromatogram is displayed.

1 of 3

The first third of the chromatogram is displayed.

2 of 3

The middle third of the chromatogram is displayed.

3 of 3

The final third of the chromatogram is displayed.

Amplitude Min., Max.

Specifies the minimum and maximum amplitude of the chromatogram display. If the values are 0, the chromatogram display range will be scaled to the data being displayed. The amplitude minimum and maximum values apply only to MS chromatogram traces, not to .RUN file chromatogram traces.

Stack Chromatogram Plots

Specifies whether multiple chromatogram traces will be overlaid or shown in separate scales stacked one over another.

#1, #2, #3

These lines specify how a chromatogram trace will be constructed. Choices S,1,2,3,4,5, and I are only available for target compound reports. Type R is available only for target compound and chromatogram (TIC) report. The #1 line will always be shown if the chromatogram is part of the graphic. If the selection is F, lines #2 and #3 are shown only if the Mass Specification is not blank.

S The trace will be the sum of Qualifier Ion Intensities.

1 The trace will be the first Qualifier Ion intensity.

2 The trace will be the second Qualifier Ion intensity.

3 The trace will be the third Qualifier Ion intensity.

4 The trace will be the fourth Qualifier Ion intensity.

5 The trace will be the fifth Qualifier Ion intensity.

B The trace will be the intensity of the highest intensity mass at each time.

I The trace will be the sum of intensities of all ions specified in the method for integration of this peak — Quant ions(s).

F The trace will be determined by the content of the Mass Specification and Channel List boxes.

R The trace will come from a standard chromatography .RUN file such as one generated by a UV detector. The name of the .RUN

file to be plotted can either be a fixed file name or it can be the same file name as the current MS file (except with a file extension of .RUN). By default, the first channel of the .RUN file will be plotted, but a different channel can be plotted by entering the desired channel into the Channel List (the first .RUN file channel is 1, the second channel is 2, etc.)

Mass Specification

If this box is blank on line #1, the RIC chromatogram will be displayed. If the boxes on lines #2 or #3 are blank and the trace selector is “F”, the corresponding trace will be omitted. For any line, to specify a specific trace content, enter a specification using one or a combination of the following forms:

- 60:120 to show the sum of intensities of all ions between 60 and 120;
- 60+62+85 to show sum of intensities of masses 60,62 and 85;
- 60 – 81 to show the intensity of m/z 60 minus the intensity of m/z 81;

Channel List

The Channel list is only used for MS/MS data files (MRM or AMD mode files; see MS method editor section) or .RUN files.

For MS data plots, if blank the channel list specification is "merged" data. If the file is MRM or AMD you can select a channel number from 1-10 to display a specific data channel. Enter the expression for the channels to be shown. (It is advisable to test the channel expression in MS Data Review on a file made from the acquisition method used to acquire the files to be reported. Explicitly indicating a channel in the expression which is not present in the file being reported may prevent report graphs from being updated or drawn when the report is printed. The default channel (blank) will never fail.).

For .RUN file plots, if the channel list entry is blank, the first data channel will be plotted. To plot a channel other than the first channel, enter the .RUN file channel number; the first channel is 1, the second channel is 2, etc.

Peak Annotation

This selection determines the type of annotation placed on peaks in the chromatogram window. The annotations can appear only on MS plots and not on .RUN file plots.

- None
- RT
- Name
- Status
- Height
- Area
- Peak #
- CAS #

Spectral Display: Low Mass, High Mass

Specifies the m/z range displayed in spectra windows. If both boxes contain 0, the mass range is determined by the spectrum being displayed.

#1, #2 Scan Type

These lines specify the content of the #1 and #2 spectra. They are used only if the Graph Type specifies that they are visible.

None

If none is selected then no spectral information will appear on the report.

Peak RT

When the Scan Type selection is Peak RT, the spectrum is taken at the time of the observed peak apex.

Calib RT

When the Scan Type option is Calib. RT, the spectrum is taken at the time specified as the retention time in the method. This option is available in Target Compound and Sample Reports.

Method Ref

Spectrum stored in the method for identification of this peak. This option is only available for compound reports.

Run File Name

The controls in this group are used to set the name of the .RUN file to be plotted when at least one of the three chromatogram trace options is set to 'R'.

Create Run File Name from MS File Name

Select the checkbox if the name of the .RUN file to be plotted is the same as the current MS file (except with a file extension of .RUN). Uncheck this option if you want to specify a fixed .RUN file name

Browse

Display a dialog used to select the name of the .RUN file to be plotted. This button is only enabled when the 'Create Run File Name from MS File Name' option is not checked.

Run File Name

This text box contains the name of the .RUN file to be plotted.

Text Report Options

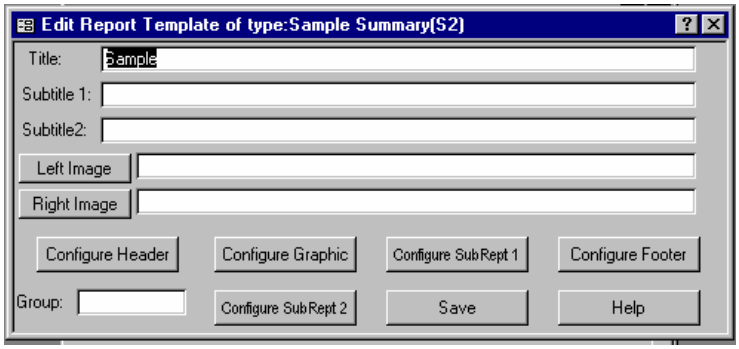
The Text Report section of reports follows the title, header and graphic (when present) sections of the report. It consists of a header line (in bold) followed by one or more data records. The fields available to report depend on the report type. Up to twenty fields may be selected per report record, however fewer than

ten will typically fit on one page. If more fields are specified than fit on the width of one page, the extra fields will be clipped off the report.

The Text Report content is specified on the "Configure Record" form. This form contains a scrollable list of the field captions currently selected for the report, together with the field width of each. A record width box at the bottom right of the form displays the total width of the report. The top field on the list will be at the left edge of the report, with remaining selected fields shown from left to right on the report as the order proceeds from top to bottom on the "Configure Record" form.

To edit a report record:

10. From the "Multi-Compound Report" page, select the report to be modified, then click the "Edit" button to open the "Edit Report Template" form.



11. Click on the "Configure Sub Rep1" or “Configure Sub Rep2” button to open the "Configure Record" form.

The Field List is a list of header items that can be placed on the report. You must use the scroll bar to view the entire list.

Add Field Button

The Add Field button allows you to add a field to the report. To use this feature, select an item in the field list by clicking on it and then select the Add Field button. The item selected will appear at the end of the list above.

Change Field Button

To Change a field you must make 2 selections. First you should select the field that you want to change in the top left list. Click on the record selector for the item that you no longer desire in the list. Next click on the item in the field list that you wish to have in the list. Now select the Change Field button. The old field will be replaced with the newly selected field.

Delete Field Button

The Delete Button is used to remove a field from the list. Click on the record selector on the left side of the header list for the item you wish to delete. Now select the Delete button and that item is removed from the list.

Delete All Button

The Delete All button will delete all of the items from the Header list.

Field Width

The Field Width reports how much space is given to each column in the test report. The dimension is in inches. (This field may not be edited.).

Record Width

The Record Width is the sum of the widths of all of the fields in the report. Watching this number will help you determine if more columns can fit on a particular page.

Save Button

The Save button causes all of the edits to be saved to this file.

Help Button

The Help button will take you to the help pages. All of the Varian MS Writer manual information is included in the help pages.

Field Definitions

The following fields may be selected for inclusion in Sample and Compound reports. The fields marked with (*) may also be included in Unknowns and tentatively identified compound (TIC) reports.

#

Calibration Compound Number: the number of the compound in the method.

Compound Name (*)

Compound name from the method in Target Compound and Sample reports.

Compound name of library search best fit in Unknowns and tentatively identified compound (TIC) reports.

RT (*)

Retention time determined during peak integration, in minutes.

Quan Ions (*)

Ion(s) formula specified in method for integration.

Area (*)

Baseline corrected area determined during integration, in counts.

Area Percent (*)

Area percent computed from the total areas of the peaks included in data file.

Amount (*)

Amount in units of “Units” field, computed from the currently active calibration.

If the Amount field is blank, the actual amount calculated was negative. Examine the calibration results and error codes reported to determine the source of the error.

Peak Reject

Peak Area Reject (in counts) entered in the method.

Height (*)

Peak height determined during integration, in counts.

Fit (*)

Forward Search Fit value.

For Sample, Compound reports: Measures fit to method reference spectrum.

For Unknowns: Measures fit to identified compound in library.

Rmatch (*)

The reverse search fit result for this spectral match.

Fit Limit (*)

Minimum fit value for identification, as set in method. Refers to Fit or Rfit, or Purity as specified in Match field and method, and reported in MatchVal field.

For Sample, Compound reports, refers to fit to compound reference spectrum stored in method.

For Unknowns, tentatively identified compound (TIC) reports, refers to fit to best fit in library search.

Calib RT

Calibration retention time (minutes), as stored in the method used in quantitation.

Group Name

Group Name as stored in the method.

IS#

Internal standard number used to quantitate this peak. This is the calibration record number in the method of the internal standard. This field is meaningless unless the calibration type in the method and the report header is "internal standard".

IS

"Std" if this peak is an internal standard reference, blank if not.

BC (*)

Baseline correction codes from peak integration of the peak. Allowed values are

- BV – Baseline to Valley

- BB – Baseline to Baseline
- MB – Mended End to Baseline
- VB – Valley to Baseline
- VV – Valley to Valley
- MM – Mended End to Mended End
- MV – Mended End to Valley
- TS – Separated Tangent Skim
- TF – Fused Tangent Skim
- GR – Group Peak
- BM – Baseline to Mended End
- VM – Valley to Mended End
- HF – Horizontal Forward
- HB – Horizontal Backward
- HM – Horizontal Minimum

Width (*)

Measured peak width (seconds).

Ion Time (*)

Ionization time of spectrum at peak apex(microseconds).

Calibration Equation

The calibration field consists of two parts. The first piece documents how the origin was treated during computation of the of the calibration equation. This is one of the following options: "Ignore 0", "Force 0", or "Include 0".

The second part is the calibration equation itself. This takes one of the following forms:

- $y = mx + b$
- $y = ax^2 + bx + c$
- "Cubic equation" — where a, b, and c are numerical constants, x is the amount (for external standard) or amount/amount internal standard (for internal standard calibration), and y is area (for external standard) or area/area internal standard (for internal standard calibration).

CAS# (*)

Chemical Abstracts number from the method in the case of Sample or Target Compound reports, or a library match value in the case of Unknowns or tentatively identified compound (TIC) reports.

Fmatch (*)

The forward search fit result for this library match.

HitProb (*)

The probability that the spectrum of the unknown compound arises from the compound in the target list.

Match (*)

The type of fit used to determine the best fit of library or method spectrum to peak apex, ("Fit", "RFit", or "Purity").

Match Val (*)

The best fit value of "Match" type of peak apex to library or method reference spectrum.

Scan

The scan number of the peak apex.

Corr.

The coefficient of determination or correlation coefficient describing the fit of the calibration points to the calibration equation.

RC# (*)

Report compound number.

SrchWin

Search window (minutes) from method.

SrchMeth

Search method type for peak identification (from method). "RT" or "Spectrum"

S/N (*)

Measured signal to noise ratio.

Channel (*)

Channel specification used to integrate peak.

ResultType(*)

The record type of this peak, determined during peak quantitation:

- "Identified" - Peak quantitated using a method compound record. The peak identification tests were passed, as were the minimum size and amount tests.
- "Failed" - Record represents a peak integrated using a method peak specification. The peak failed one or more of the peak criteria for reporting.
- "Missing" - The method could not identify this peak.
- "Tentatively Identified Compound (TIC)" – This peak was integrated using default integration parameters. A library search produced an identification that satisfied the minimum fit criteria for tentative identification.

- "Duplicate" - This peak, integrated using the default integration parameters, appears to be a peak that was also reported using a mass specification from the method.
- "Unknown" - This peak was integrated using default integration parameters, but was not identified as either duplicating a peak integrated using compound specific parameters or matching a compound in a searched library.

RF

Response factor computed using the quantitation criteria. This is either a response factor if the header field "Calculation Type" is "External Standard", or a relative response factor if "Calculation Type" is "Internal Standard". It is computed from areas if the header field "Peak Measure" is "area", or from heights if "Peak Measure" is height.

RRT

Relative Retention Time.

QI1, QI2, QI3, QI4, QI5

Qualifier Ion 1, 2, 3, 4, or 5 from method.

QIR1Lo, QIR2Lo, QIR3Lo, QIR4Lo, QIR5Lo

Qualifier Ion Ratio 1, 2, 3, 4, or 5 Low Limit from method.

QIR1Hi, QIR2Hi, QIR3Hi, QIR4Hi, QIR5Hi

Qualifier Ion Ratio 1, 2, 3, 4, or 5 High Limit from method.

QIR1, QIR2, QIR3, QIR4, QIR5

Actual Qualifier Ion Ratio as determined during quantitation.

Units(*)

Actual units of Amount field, as determined from method "Units" field and the processing results during quantitation. In Unknowns or tentatively identified compound (TIC) reports, units are determined by the data handling processing.

Amnt Reject

The minimum value of the "Amount" field to report as "identified", from the method "Report Threshold" parameter.

Error (*)

Instrument errors that occurred during the run.

Status Codes (*)

Alphanumeric string of status codes set during peak quantitation.

(An “X” is at the start of status codes that represent an error status. Codes S, R, T, and U are advisory codes that do not represent an error condition.

The character codes are interpreted as follows:

R Reference Peak
Factors not updated
***** No result can be calculated
+ More than one result
V Peak fails verification
M Missing Peak
C Result out of calibration range
S Internal Standard peak
U User defined end points
O Saturated Peak Amplitude
T Relative Retention Time peak
D Cannot calibrate -Default to raw peak size
I Invalid scan function channel specification

Weight

The regression weighting used in determining the calibration curve.

QlArea1, QlArea2, QlArea3, QlArea4, QlArea5

Qualifier Ion Area for qualifier ion 1, 2, 3, 4, or 5. The area determined by integrating the qualifier ion intensity.

QlRT1, QlRT2, QlRT3, QlRT4, QlRT5

The retention time obtained for the peak found when integrating qualifier ion 1, 2, 3, 4, or 5.

*****

Qualifier Ion Ratio Test result. Blank if QlRi is between QlRiLo and QlRiHi for i = 1 to 5 where Qli >0. Ratio tests where Qli is 0 are ignored. * is shown in the field if any qualifier ion ratio test fails for a level in which the Qualifier Ion is defined.

InLibProb

In Library Probability-measure of the probability of the compound being in the searched libraries.

IntegWin

The time window within which a peak area is measured.

Field Definitions: Tentatively Identified Compounds (TIC) Subrept2

The following fields are available for library search results shown in Subrept2 of the tentatively identified compound (TIC) reports.

Hit#

The first 60 characters of the compound name in the library record that was matched.

Name

The first 60 characters of the compound name in the library record that was matched.

Library

The full path name of the library containing the record that was matched.

CAS#

The Chemical Abstracts number stored in the library record that was matched.

FMatch

The forward search fit result for this library match.

RMatch

The reverse search fit result for this library match.

HitProb

The purity search fit result for this library match.

Match

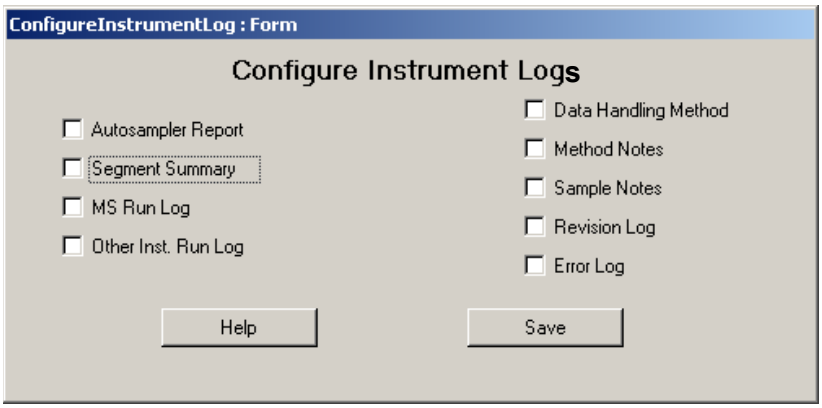
The type of search result used to search the library. (Fit, RFit, Purity)

MatchVal

The search result value of type Match for this library entry.

Configure Report Footer-(Instrument Logs)

To configure the footer, click the "Configure Footer" button on the "Edit Report Template" form to open the "Configure Instrument Log" form. The dialog box below is displayed if you select the configure footer button for the report type in which it is available.



The form's controls are:

Autosampler Report

Presents vial location, injection volume and injection number used by the autosampler.

Segment Summary

Consists of one line per data acquisition segment summarizing the number of groups and the time range of each segment.

MS Run Log

Consists of several pages of instrument settings, including instrument calibration.

Other Inst. Run Log

GC or LC instrument run log.

Other Parameters as Selected in the Check Boxes Listed Below:

- Data Handling Method
- Method Notes
- Sample Notes
- Revision Log
- Error Log

Save Button

The Save button causes all of the edits to be saved to this file.

Help Button

The Help button will take you to the help pages.

Group

The Group Text box is located on the "Edit Report Template" form in the lower left corner. It is visible only when the report type being edited is S2, S3, or S4. If compounds were assigned to a group in the compound table, the name of the group should be entered in the Group Text box. The sample report will then include only those compounds in the group.

Printing Reports Automatically

This section assumes the steps in “Interactively Reviewing Reports” have been done. To prepare and execute printing sets of reports for one or multiple data files, follow these steps:

For each MultiCpd template that will be used to generate reports:

Open the MultiCpd template and select the reports to print. MultiCpd templates are most easily opened from the Star Toolbar “Custom MS Reports” icon. Every report shown on the “Multi-Compound Report” page which has a check in the “Print” column will be printed when a report sequence is printed using this database. The “Print” Checkbox state for any record can be changed by clicking on it.

To print a set of reports for one file using one MultiCpd template database:

Set up the desired working template so that the reports to be printed have their print boxes checked, and close the template. Using the Chromatogram View icon from the Star Toolbar make the data file to be reported the active file. Then left-click on the data file operator button, (it will show the selected file name)

and select the “Print custom report” item. Select the .swt file to be used (it should be already prepared) and all reports marked for printing will be printed.

To print a set of reports for one file using a MultiCpd template database when that file is processed as part of a Sample List or Recalc List.

Enter the name of the MultiCpd template (x.swt) in the AutoLink field in the Sample List or Recalc List on the lines of each data file to be reported.

Note that MultiCpd templates do not follow the Varian MS Workstation System Control flags and parameters. They print to the default system printer, not the workstation printer selections. If a template is invoked, it prints the selected reports, ignoring the Workstation “Enable Automated Printing” flag.

If you wish to print different report sets for different samples, configure different templates to print the different report sets, then invoke the appropriate template for each sample.

Deleting a Report Template

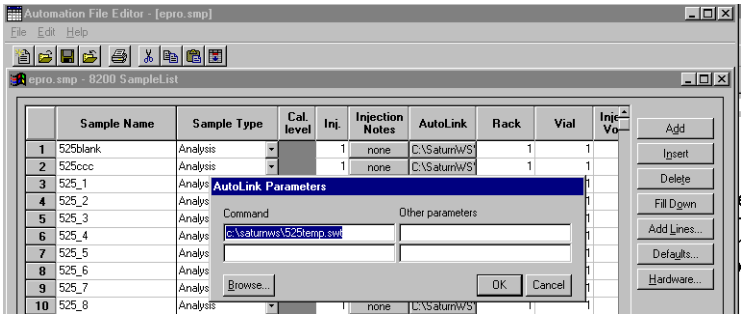
From the "Report Selection and Preview" form, select the report to be deleted by clicking on the record selector button to the left of the report title, then click the "Delete" button in the "Report Template" group.

Automation

Before online reporting can take place, the reporting template (.swt) must be completed. The name of this completed MultiCpd template (.swt) will be used in the Auto Link field of the Sample List of the Varian MS software.

MultiCpd reports may be generated immediately after the file acquisition is completed.

Sample List in the Varian MS Software



List of injections to be executed via System Control (Varian MS software)

Complete the Sample List for data acquisition or recalc as desired. In the Auto Link field enter the name of the MultiCpd template (.swt) to be used for reporting once the acquisition is completed.

Varian, Inc.
2700 Mitchell Drive
Walnut Creek, CA 94598-1675/USA

Varian MS Workstation
Version 6.5

Ion Ratio Summary Report

03-914894-02:Rev. 2

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Contents

Ion Ratio Summary Report

Introduction

This custom report will summarize the data for the calibration and analysis files in a recalculation list. For each analyte in the compound table of a Saturn method, the following information will be listed:

- Area counts for the compound and its internal standard.
- Parameters for the linearity curve (slope, intercept, correlation coefficient).
- The calculated value for each compound in analysis runs
- Ratios for Q_1 (the first qualifier ion) to Q (the quant ion) and Q_2 (the second qualifier ion) to Q, for each compound and its internal standard.*
- The fit of each analyte to its reference spectrum in the compound table.*

The recalculation list must include calibration runs. The mean of the Q_1/Q and Q_2/Q values for the compounds in the calibration runs is calculated. The acceptance limits for each compound are the mean calculated in the calibration runs, plus or minus 20%. The Q_1/Q and Q_2/Q values for the compounds in the sample runs are listed after the calibration runs. Those ratios that are outside of the acceptance limits are printed in red.

* Inclusion of ion ratios and/or fit information is optional.

Using the Ion Ratio Custom Report

Generating a Report

1. Build a recalculation list (Figure 1) for the series of run files that you wish to summarize. (The recalculation list can be built automatically when the sample list is running). Be sure that the recalculation list includes a line for a new calibration block followed by calibration runs.

2. Verify that the Saturn method designates Qualifier ions in the Quant ion section of the compound table.

3. After the data has been processed, click on the custom report ion in the Star Toolbar (Figure 1). Choose “open new template” and select IonRatioReport.mdb. You will be asked to give the report a name.

4. The dialog page appears (Figure 2). Enter any comment that you want included in the report. If you want fit to be on the report check “fit” and if you do not want ion ratios then uncheck “ion ratios”. Click on “Report” and select the Recalculation file that contains the runs that you want summarized. Normally “print to file” * is not checked.

5. The report will be generated (Figure 3) and may be printed. A color printer is recommended since outliers are printed in red.

* “Print to file” enables the user to generate a text file. This can be opened in Excel to generate a report that is editable. The Excel report will require formatting.

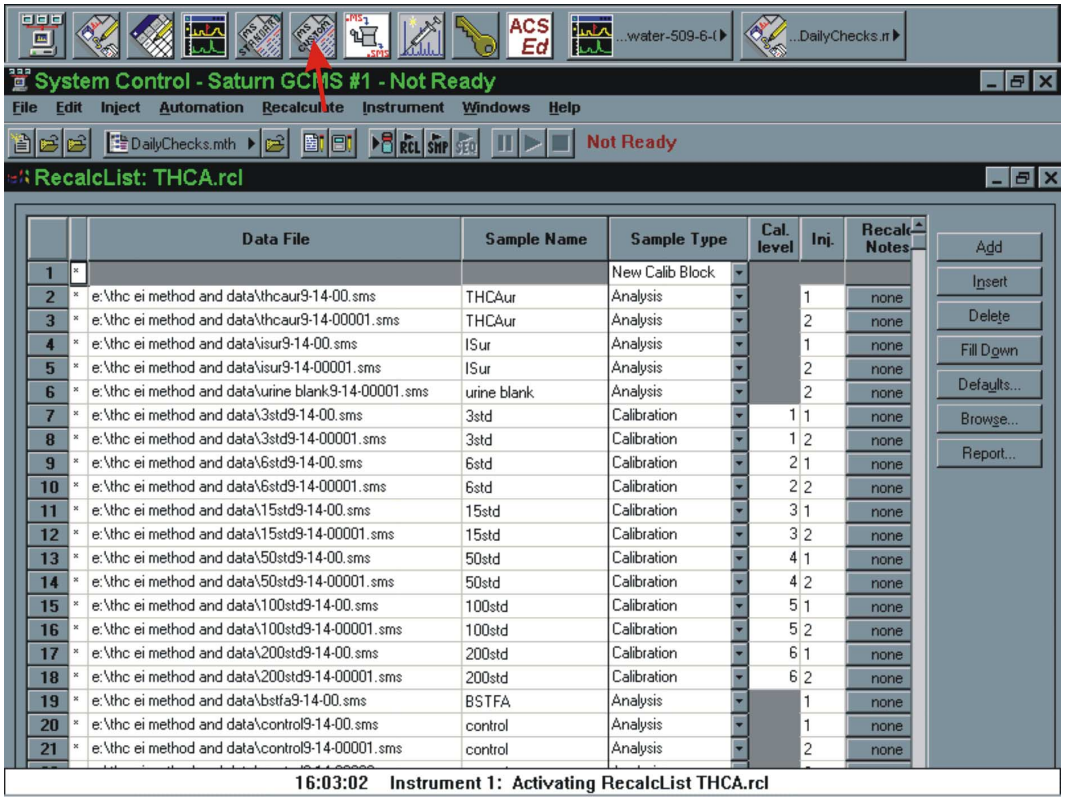


Figure 1. Showing a recalculation list in System Control with the Star Toolbar on top. The arrow points to the custom reports icon on the Star Toolbar.

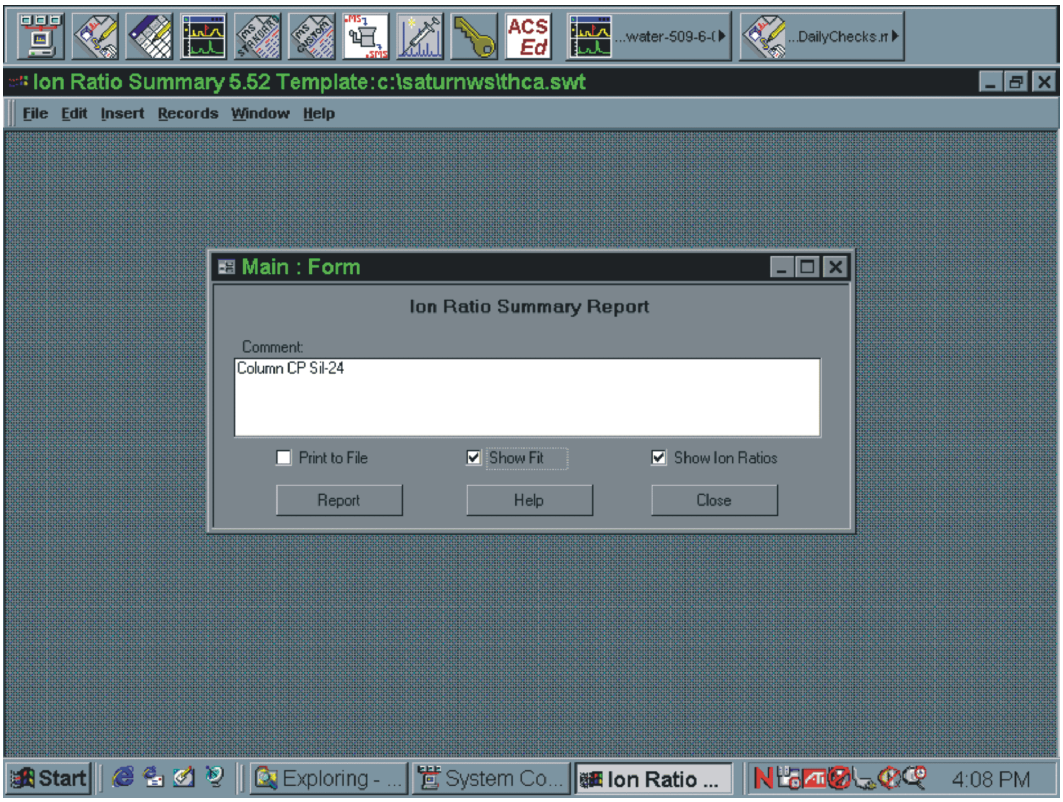
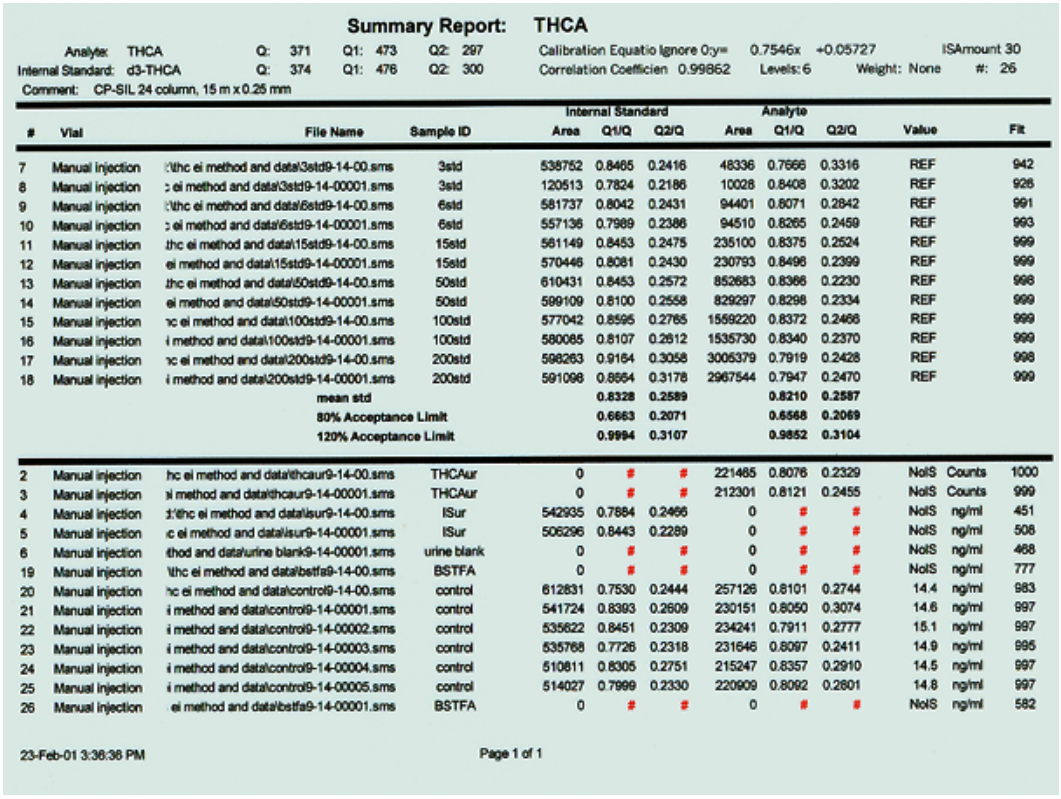


Figure 2. The dialog page in the ion ratio report. In this case, the column that was used for the analysis was entered in the comment section.



Summary Report: THCA

Analyte: THCA Q: 371 Q1: 473 Q2: 297 Calibration Equatio Ignore 0:y= 0.7546x +0.05727 ISAmount 30
Internal Standard: d3-THCA Q: 374 Q1: 476 Q2: 300 Correlation Coefficien 0.99862 Levels: 6 Weight: None #: 26
Comment: CP-SIL 24 column, 15 m x 0.25 mm

#	Vial	File Name	Sample ID	Internal Standard Area	IS Q1/Q	IS Q2/Q	Analyte Area	Analyte Q1/Q	Analyte Q2/Q	Value		Fit
7	Manual injection	\thc ei method and data\3std9-14-00.sms	3std	538752	0.8465	0.2416	48336	0.7666	0.3316	REF		942
8	Manual injection	ei method and data\3std9-14-00001.sms	3std	120513	0.7824	0.2186	10028	0.8408	0.3202	REF		926
9	Manual injection	\thc ei method and data\6std9-14-00.sms	6std	581737	0.8042	0.2431	94401	0.8071	0.2842	REF		991
10	Manual injection	ei method and data\6std9-14-00001.sms	6std	557136	0.7989	0.2386	94510	0.8265	0.2459	REF		993
11	Manual injection	thc ei method and data\15std9-14-00.sms	15std	561149	0.8453	0.2475	235100	0.8375	0.2524	REF		999
12	Manual injection	ei method and data\15std9-14-00001.sms	15std	570446	0.8081	0.2430	230793	0.8496	0.2399	REF		999
13	Manual injection	thc ei method and data\50std9-14-00.sms	50std	610431	0.8453	0.2572	852683	0.8366	0.2230	REF		998
14	Manual injection	ei method and data\50std9-14-00001.sms	50std	599109	0.8100	0.2558	829297	0.8298	0.2334	REF		999
15	Manual injection	c ei method and data\100std9-14-00.sms	100std	577042	0.8595	0.2765	1559220	0.8372	0.2466	REF		999
16	Manual injection	i method and data\100std9-14-00001.sms	100std	580085	0.8107	0.2612	1535730	0.8340	0.2370	REF		999
17	Manual injection	c ei method and data\200std9-14-00.sms	200std	598263	0.9154	0.3058	3005379	0.7919	0.2428	REF		998
18	Manual injection	i method and data\200std9-14-00001.sms	200std	591098	0.8664	0.3178	2967544	0.7947	0.2470	REF		999
		mean std			**0.8328**	**0.2589**		**0.8210**	**0.2587**			
		80% Acceptance Limit			**0.6663**	**0.2071**		**0.6568**	**0.2069**			
		120% Acceptance Limit			**0.9994**	**0.3107**		**0.9852**	**0.3104**			
2	Manual injection	hc ei method and data\thcaur9-14-00.sms	THCAur	0	#	#	221485	0.8076	0.2329	NoIS	Counts	1000
3	Manual injection	i method and data\thcaur9-14-00001.sms	THCAur	0	#	#	212301	0.8121	0.2455	NoIS	Counts	999
4	Manual injection	\thc ei method and data\isur9-14-00.sms	ISur	542935	0.7884	0.2466	0	#	#	NoIS	ng/ml	451
5	Manual injection	c ei method and data\isur9-14-00001.sms	ISur	506296	0.8443	0.2289	0	#	#	NoIS	ng/ml	508
6	Manual injection	thod and data\urine blank9-14-00001.sms	urine blank	0	#	#	0	#	#	NoIS	ng/ml	468
19	Manual injection	\thc ei method and data\bstfa9-14-00.sms	BSTFA	0	#	#	0	#	#	NoIS	ng/ml	777
20	Manual injection	hc ei method and data\control9-14-00.sms	control	612831	0.7530	0.2444	257126	0.8101	0.2744	14.4	ng/ml	983
21	Manual injection	i method and data\control9-14-00001.sms	control	541724	0.8393	0.2609	230151	0.8050	0.3074	14.6	ng/ml	997
22	Manual injection	i method and data\control9-14-00002.sms	control	535622	0.8451	0.2309	234241	0.7911	0.2777	15.1	ng/ml	997
23	Manual injection	i method and data\control9-14-00003.sms	control	535768	0.7726	0.2318	231646	0.8097	0.2411	14.9	ng/ml	995
24	Manual injection	i method and data\control9-14-00004.sms	control	510811	0.8305	0.2751	215247	0.8357	0.2910	14.5	ng/ml	997
25	Manual injection	i method and data\control9-14-00005.sms	control	514027	0.7999	0.2330	220909	0.8092	0.2801	14.8	ng/ml	997
26	Manual injection	ei method and data\bstfa9-14-00001.sms	BSTFA	0	#	#	0	#	#	NoIS	ng/ml	582

23-Feb-01 3:36:36 PM Page 1 of 1

Figure 3. A custom summary report for 9-carboxy-11-nor-Δ^9-tetrahydrocannabinol (THCA). This report includes both fit and ion ratio information. Note that the calibration runs are listed at the top and are separated from the analysis runs by the black line. When several analytes are in a compound table, they will be listed on subsequent pages in order of retention time.

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Varian MS Workstation
Version 6.5

Screening Reports

03-914894-03:Rev. 2

Trademark Acknowledgment

Contents

Screening Reports

Introduction

The Screening template is a supplement to the MultiComp reporting software. It delivers 30 graphic reports per page, based on entries in the data handling method used to process the .sms file. No text report is printed with this software.

The graphics maybe configured to display target chromatogram plots and spectra. Reference spectrum from the data handling method also may be selected for display.

This report will deliver results in a “condensed” way for quick review, and allow data handling improvements (including manual integration) before the final report in the desired format is printed.

"Screening" reports data from files processed in Saturn GCMS Workstation 5.4 or later version. Reports can be generated on internal and external standard based calculations.

The reports may be viewed interactively or printed automatically as part of a data acquisition or reprocessing sequence.

The report templates can be "cloned" to generate a separate, tailor made template for each type of reporting requirement.

The template size will increase after the generation of numerous reports; use the Repair/Compact command (last entry in the menu shown when the MS CUS Icon 

is pressed in the Toolbar) to restore the original template size.

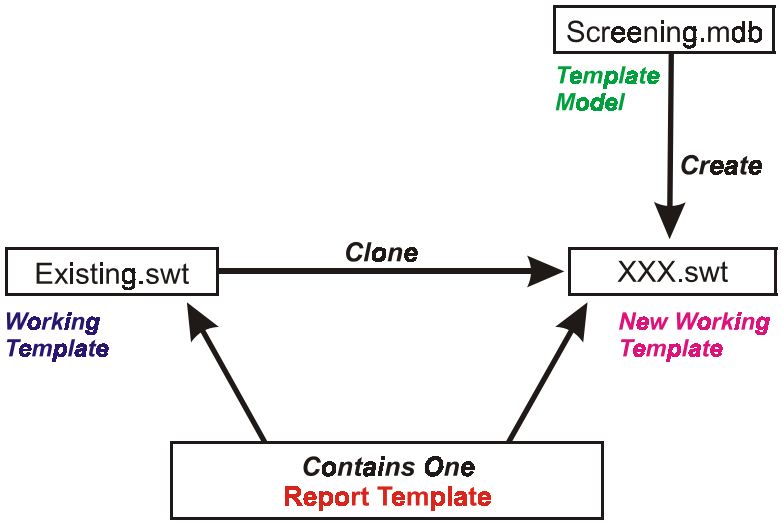
The Screening template presents data already stored in the data file. It does not modify results stored in the data file.

In order for a data file to contain integrated peak information, MS Data Review or System Control must have processed it through peak integration. For a data file to contain quantitated peak information, a data handling method must have been constructed using the Method Editor, and then that method must have been used to quantitate the data file using either MS Data Review or System Control. Changes made to

the method only affect reported data file results after the data file has been reprocessed with the changed method. The data file contains copies of the method, including calibration result information, upon which the reported peak quantitation results are based.

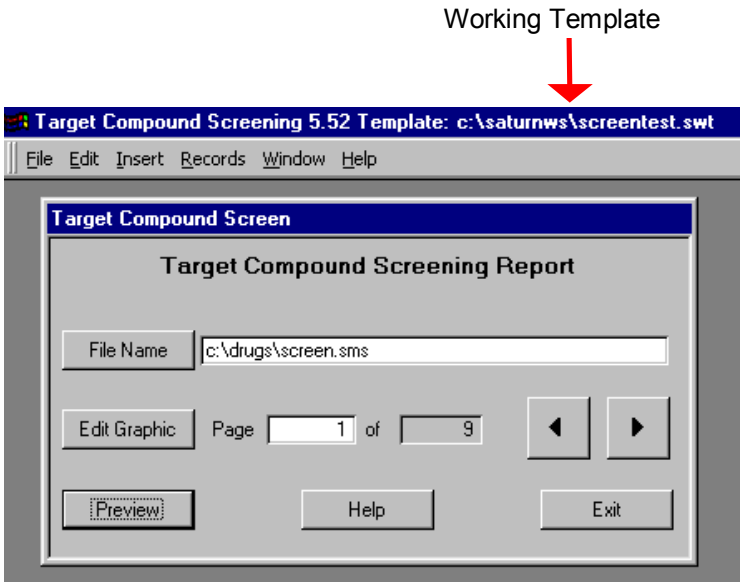
Components of the Software

What are the “Templates”?



There are multiple files used within the Screening reporting software. The file Screening.mdb is the Template Model from which the “Working Templates” may be created. The Working Template also can be “cloned” from an existing, other Working Template. The Working Templates have user defined names and .swt extension. Each Working Template of the Screening software contains one “Report”. The Working Template name is used in the AutoLink for automated reporting.

A *Report Template* is the collection of information needed to define the format or layout or presentation of the information in the report. It identifies the subset of information contained in the data file that is to be shown on the report(s).



Interactively Reviewing Reports

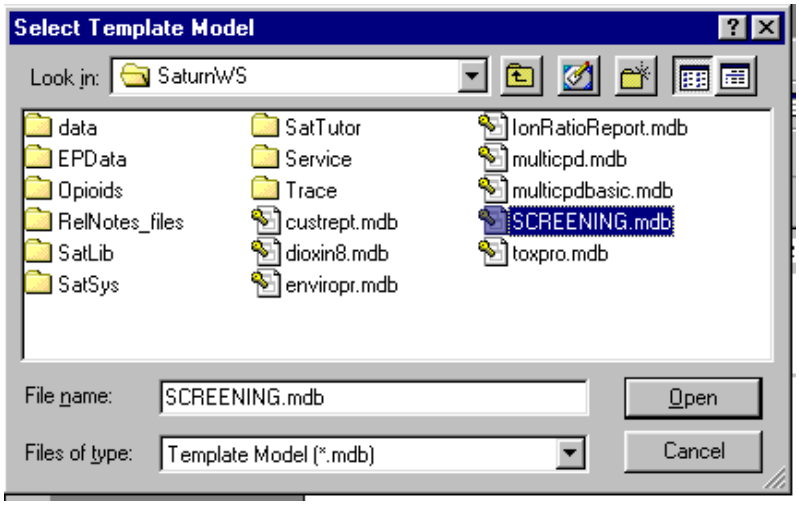
To use the Screening software to interactively review reports derived from a data file, follow these steps:

1. Prepare the MS (.mth) method. Use MS Data Review in conjunction with the Method Editor to prepare a MS Data Handling method for use in integrating and quantitating the MS Data files of interest.

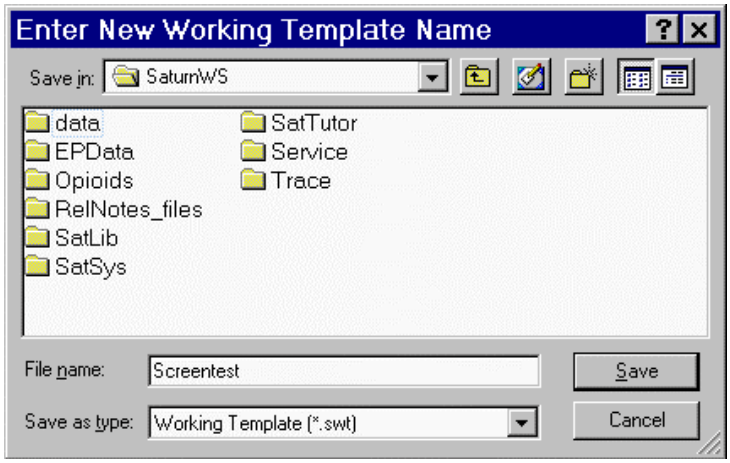
2. Quantitate the file. Use the method to integrate and quantitate the MS Data file, thereby storing results to report into the data file.

3. Select the printer. The Windows Start-Settings-Printers folder is used to select the default system printer. The printer selected as the “Default System Printer” is used to print Custom MS Report Writer reports.

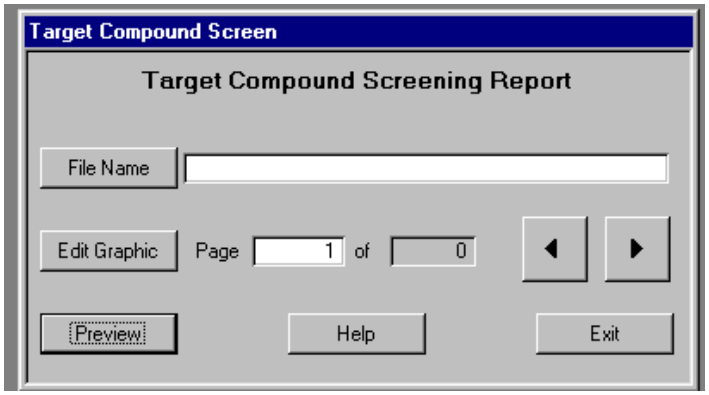
4. Identify a MS Data file to report. Open the Star Toolbar and click the “Custom MS Reports” icon. Create a new, Screening derived database (*.swt) file (or select one of the existing Screening template if exists). To create a new template select “new template” and you will see the following (or similar) screen.



5. Select the “Screening.mdb” to be opened.

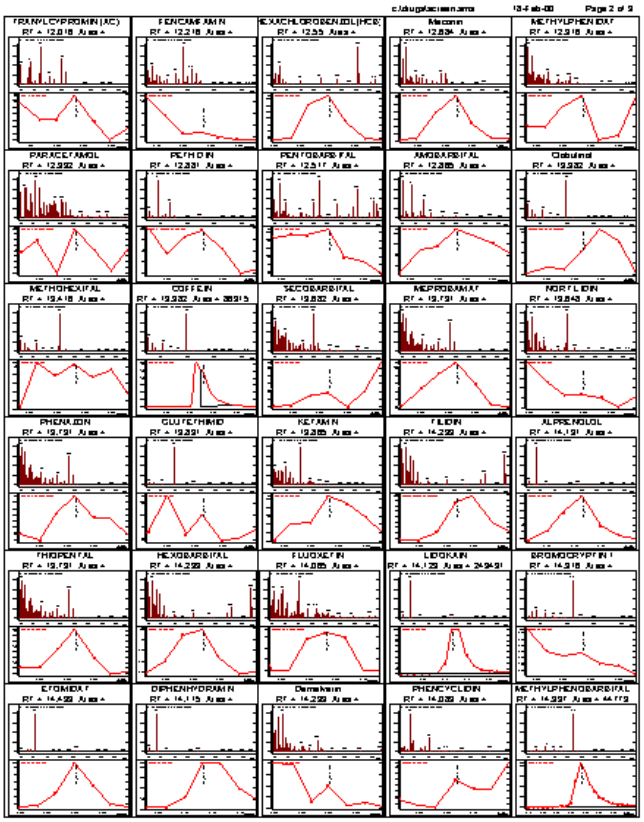


6. Type the file name you wish to use for this report and select the Save button. You will now see the following screen.



7. Select a data file for the report by pressing the “File” button. An example data (Screen.sms) file is located in the SaturnWS/SCdata directory.

8. View the report. Click on the “Preview” button. To view the report, select the desired page either by typing it directly in the Page box or by using the Previous or Next (arrow) button, and then click the “Preview Report” button. While a report is displayed there will be a small toolbar directly above it containing icons to print and zoom the scaling of the report screen image.



Report generated by the selected template and data file

9. Repeat steps 6-7 if necessary.

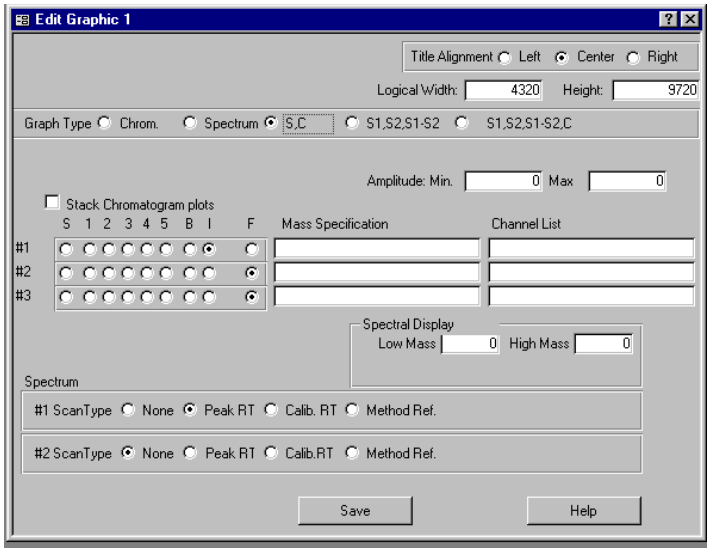
10. Exit program.

The Working Template (Screentest.swt in our case) can also be called during automation by using the AutoLink feature in the Sample List.

Editing an Existing Report Template

Graphics

The reports may contain up to 30 chromatogram/spectra frames per page. The content of each frame may be customized in ways that depend on the type of report. To modify a graphic frame press the Edit Graphic button:



The graphic may be a chromatogram, consisting of between 1 and 3 overlaid or stacked traces; and/or one or three spectra drawn from the chromatogram, the data handling method used to quantitate the chromatogram, the result of a library search, or a combination of these.

Graphic Controls

Logical Width, Logical Height

Width, Height in twips of graph as drawn. This size is scaled to fit the actual size of the graphic as specified by the report template. The effect of these parameters is primarily to alter the relative size and placement of text on the graphic. Larger values reduce text size. 1440 twips = 1 inch.

Graph Type

Select one of the following choices to determine the basic graphic type. Click the radio button for your choice.

Chrom
Show a chromatogram. One chromatogram is selected. Up to three traces derived from the chromatogram may be shown. The chromatogram segment (Rt) to be shown will depend on the parameters

set for the Peak Window +/- parameter in the MS datahandling method, identification section.

Spectrum
Show one spectrum. This can be a reference or sample spectrum.

S, C
Show one spectrum over a chromatogram in the same graphic box.

S1, S2, S1-S2
Show two spectra and their difference in the same graphic box.

S1, S2, S1-S2, C
Show two spectra and their difference over a chromatogram in the same graphic box. This can be cluttered due to size restrictions.

Amplitude Min., Max.

Specifies the minimum and maximum amplitude of the chromatogram display. If the values are 0, the chromatogram display range will be scaled to the data being displayed.

Stack Chromatogram Plots

Specifies whether multiple chromatogram traces will be overlaid or shown in separate scales stacked one over another.

#1, #2, #3

These lines specify how a chromatogram trace will be constructed. Choices S,1,2,3,4,5, and I are only available for Target compound reports. The #1 line will always be shown if the chromatogram is part of the graphic. If the selection is F, lines #2 and #3 are shown only if the Mass Specification is not blank.

S The trace will be the sum of Qualifier Ion Intensities.

1 The trace will be the first Qualifier Ion intensity.

2 The trace will be the second Qualifier Ion intensity.

3 The trace will be the third Qualifier Ion intensity.

4 The trace will be the fourth Qualifier Ion intensity.

5 The trace will be the fifth Qualifier Ion intensity.

B The trace will be the intensity of the highest intensity mass at each time.

I The trace will be the sum of intensities of all ions specified in the method for integration of this peak.

F The trace will be determined by the content of the Mass Specification and Channel List boxes.

Mass Specification

If this box is blank on line #1, the RIC chromatogram will be displayed. If the boxes on lines #2 or #3 are blank and the trace selector is “F”, the corresponding trace will be omitted. For any line, to specify a specific trace content, enter a specification using one or a combination of the following forms:

60:120 to show the sum of intensities of all ions between 60 and 120;

60+62+85 to show sum of intensities of masses 60,62 and 85;

60 – 81 to show the intensity of m/z 60 minus the intensity of m/z 81;

Channel List

The Channel list is only used for MS/MS data files. Specifically it is used if the file is an MRM or AMD mode file. (See MS method editor section)

If blank, the channel list specification is "merged" data. If the file is MRM or AMD you can select a channel number from 1-10 to display a specific data channel. Enter the expression for the channels to be shown. [It is advisable to test the channel expression in MS Data View on a file made from the acquisition method used to acquire the files to be reported. Explicitly indicating a channel in the expression which is not present in the file being reported may prevent report graphs from being updated or drawn when the report is printed. The default channel (blank) will never fail.]

Spectral Display: Low Mass, High Mass

Specifies the m/z range displayed in spectra windows. If both boxes contain 0, the mass range is determined by the spectrum being displayed.

#1, #2 Scan Type

These lines specify the content of the #1 and #2 spectra. They are used only if the Graph Type specifies that they are visible.

None

If none is selected then no spectral information will appear on the report.

Peak RT

When the Scan Type selection is Peak RT, the spectrum is taken at the time of the observed peak apex.

Calib RT

When the Scan Type option is Calib. RT, the spectrum is taken at the time specified as the retention time in the method. This option is available in Target Compound and Sample Reports.

Method Ref

Spectrum stored in the method for identification of this peak. This option is only available for compound reports.

Printing Reports Automatically

This section assumes the steps in “Interactively Reviewing Reports” have been done. To prepare and execute printing sets of reports for one or multiple data files, follow these steps:

To print a set of reports for one file using one Screening template database:
Open the Screening template and select the file to be used. Review the reports and press the print button for each report.

Alternatively, left click on mouse while positioned on the Data File Operations icon, and select Print Custom MS Report. The active file and template will be printed.

To print a set of reports for one file using a Screening template database when that file is processed as part of a Sample List or Recalc List in Saturn GC/MS Workstation System Control:
Enter the name of the Screening template (x.swt) in the AutoLink field in the Sample List or Recalc List on the lines of each data file to be reported.

Note that Screening templates do not follow the Saturn GC/MS Workstation System Control flags and parameters. They print to the default system printer, not the Workstation printer selections. If a template is invoked, it prints the selected reports, ignoring the Workstation “Enable Automated Printing” flag.

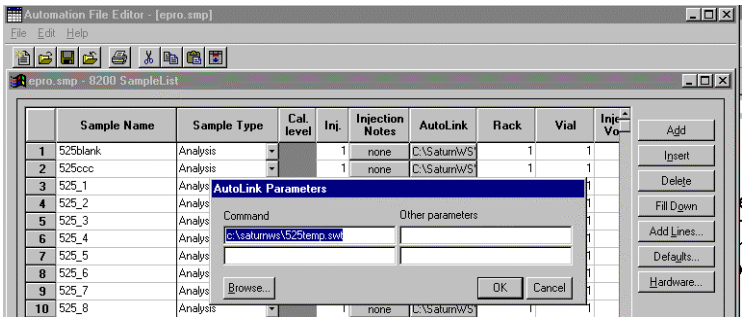
If you wish to print different report sets for different samples, configure different templates to print the different report sets, then invoke the appropriate template for each sample.

Automation

Before online reporting can take place, the working template (.swt) must be completed. The name of this completed Screening template (.swt) will be used in the Auto Link field of the Sample List of the Saturn software.

Screening reports may be generated immediately after the file acquisition is completed.

Sample List in the Saturn Software



List of injections to be executed via System Control (Saturn software)

Complete the Sample List for data acquisition or recalc as desired. In the Auto Link field enter the name of the Screening template (.swt) to be used for reporting once the acquisition is completed.