

Agilent GC/MSD ChemStation Data Analysis and Reporting

Course Number H4076A

Student Manual





Agilent Technologies

Agilent GC/MSD ChemStation Data Analysis and Reporting

Course Number H4076A

Student Manual

Notice

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

Agilent Technologies makes no warranty of any kind with regard to this material, including but not limited to the implied warranties of merchantability and fitness for a particular purpose.

Agilent Technologies shall not be liable for errors contained herein or for incidental, or consequential damages in connection with the furnishing, performance, or use of this material.

No part of this document may be photocopied or reproduced, or translated to another program language without the prior written consent of Agilent Technologies, Inc.

Agilent Technologies, Inc
3750 Brookside Pkwy
Suite 100
Alpharetta, GA 30022

© 2007 by Agilent Technologies, Inc.

All rights reserved

Printed in the United States of America

Table Of Contents

QUALITATIVE DATA ANALYSIS.....	1
WHAT YOU WILL LEARN.....	2
GENERAL QUALITATIVE PROCEDURES.....	3
NAVIGATION PANEL	4
CONTROL OF TOOL BAR ICONS	5
STANDARD MOUSE FUNCTIONS IN DATA ANALYSIS.....	6
RIGHTCLICK MOUSE FUNCTIONS.....	7
RTE INTEGRATOR.....	8
CHEMSTATION INTEGRATOR	11
SYNCHRONOUS SIM/SCAN DATA.....	14
EASY EICS.....	15
CORRELATION CHROMATOGRAM.....	16
PEAK PURITY	17
ANALYZE MULTIPLE DATA FILES.....	19
ANALYZE MULTIPLE SPECTRA.....	20
CHEMSTATION LIBRARY SEARCH.....	21
WHAT IS A LIBRARY SEARCH?.....	22
PBM LIBRARY SEARCH CONCEPTS.....	23
HOW DOES PBM LIBRARY SEARCH WORK?	25
STEPS IN LIBRARY SEARCHING	26
SELECTING THE LIBRARY(S) TO BE SEARCHED	27
LIBRARY SEARCH STRATEGIES	28
PBM LIBRARY SEARCH RESULTS	31
LIBRARY SEARCH TEXT RESULTS.....	32
LIBRARY SEARCH STATISTICS.....	33
ANNOTATE CHROMATOGRAM WITH LIBRARY SEARCH RESULTS.....	35
AUTOMATED LIBRARY SEARCHING	36
LIBRARY SEARCH REPORT.....	38
FACTORS AFFECTING THE LIBRARY SEARCH	39
PARAMETRIC RETRIEVAL.....	40
PARAMETRIC RETRIEVAL RESULTS.....	42
USER CREATED LIBRARIES	43
STEPS TO CREATE A USER LIBRARY	44
ADDING AND EDITING ENTRIES IN THE USER LIBRARY.....	45
DOSCAN.....	46
METHODS FLOWCHART.....	47
LAB EXERCISE: QUALITATIVE DATA ANALYSIS.....	49
CHROMATOGRAMS AND GRAPHICS.....	50
MASS SPECTRA	52
EASY EICS.....	53
RIGHTCLICK MOUSE FUNCTIONS.....	54

BACKGROUND SUBTRACTION	55
INTEGRATION.....	56
PEAK PURITY ANALYSIS	58
RESIZING WINDOWS	59
LIBRARY SEARCHING.....	60
AUTOMATING LIBRARY SEARCHES.....	62
DOSCAN	64
BUILDING PBM LIBRARIES.....	65
EDITING LIBRARIES.....	67
PARAMETRIC RETRIEVAL.....	68
CREATING SUBSET LIBRARIES	70
ANALYZING MULTIPLE DATA FILES	72
ANALYZING MULTIPLE SPECTRA.....	74
QUANTITATIVE DATA ANALYSIS.....	75
WHAT YOU WILL LEARN.....	76
QUANTITATION CONCEPTS	77
THE QUANTITATION PROCESS.....	78
INTERNAL STANDARDS	79
SETTING UP A QUANTITATION DATABASE.....	80
QUANTITATION DATABASE GLOBALS.....	81
ENTERING COMPOUNDS.....	83
USING THE MOUSE TO ENTER COMPOUNDS.....	84
INTERNAL STANDARDS ORDER IN THE DATABASE.....	86
UPDATE CALIBRATION.....	87
CALIBRATION USING AUTOQUANT.....	89
AUTOQUANT – ADDING COMPOUNDS.....	90
AUTOQUANT – ADDING LEVELS.....	91
COMPOUND INFORMATION – IDENTIFICATION TAB.....	92
COMPOUND INFORMATION – CALIBRATION TAB	93
COMPOUND INFORMATION – USER DEFINED TAB.....	94
COMPOUND INFORMATION – ADVANCED & REPORTING.....	95
QUANTITATION REPORT OPTIONS.....	96
INTERACTIVE QUANTITATION	99
AUTOMATIC QUANTITATION AND REPORTING.....	100
MANUAL REINTEGRATION USING QEDIT	101
CHANGING DATA STATES	103
TROUBLESHOOTING A QUANTITATION DATABASE.....	104
TRACE MODE QUANT	106
LOCATE A COMPOUND / LOCATE ALL COMPOUNDS	108
EASYID.....	109
GLOBAL UPDATE	111
DOLIST	112
SEMIQUANT QUANTITATION	114
AUTOMATION TOOLS: AUTOSIM.....	115
MODIFYING SIM METHOD PARAMETERS	117
EXPORTING REPORTS.....	118

EMETHODS.....	120
METHODS FLOWCHART.....	121
LAB EXERCISE: QUANTITATION OF SIM DATA	123
SETTING QUANTITATION INTEGRATION.....	124
SETTING UP THE CALIBRATION:	127
CREATING A MULTI-LEVEL CALIBRATION DATABASE	133
QUANTITATING AN UNKNOWN.....	135
MANUALLY REQUANTITATING A COMPOUND.....	137
ADDING AUTOMATIC REPORT GENERATION TO A METHOD.....	138
AUTOMATION TOOLS.....	139
CHANGING DATA STATE.....	141
EASYID.....	142
LAB EXERCISE: QUANTITATION OF SCAN DATA.....	145
SETTING UP QUANTITATION INTEGRATION.....	147
SETTING UP THE CALIBRATION:	150
CREATING A MULTI-LEVEL CALIBRATION DATABASE	156
QUANTITATING AN UNKNOWN.....	158
MANUALLY REQUANTITATING A COMPOUND.....	161
ADDING AUTOMATIC REPORT GENERATION TO A METHOD.....	162
AUTOMATION TOOLS.....	163
CHANGING DATA STATE.....	165
EASYID.....	166
CUSTOM REPORTS AND DATABASES	169
WHAT YOU WILL LEARN.....	170
CUSTOM REPORTS MENUS.....	171
CUSTOM REPORTS CONTROL PANEL.....	172
CUSTOM REPORTS WIZARD	174
CUSTOM REPORTS DRAG AND DROP.....	176
CUSTOM REPORTS FORMATTING.....	178
CUSTOM REPORTS PAGE SETUP	180
SAVING THE REPORT TEMPLATE.....	182
INTERACTIVELY PRINTING CUSTOM REPORTS	183
PRINTING MULTIPLE CUSTOM REPORTS	184
DATABASE CONTROL PANEL	186
DATABASE WIZARD.....	188
DATABASE DRAG AND DROP	190
DATABASE FORMATTING.....	192
DATABASE CHARTS	194
SAVING THE DATABASE.....	197
INTERACTIVELY UPDATING THE DATABASE	198
MULTIPLE FILE UPDATING OF THE DATABASE.....	199
METHODS FLOWCHART.....	200

LAB EXERCISE: CUSTOM REPORTS	201
CREATING A TEMPLATE	202
CREATING A DATABASE.....	216
RPN COMMANDS AND MACROS	221
WHAT YOU WILL LEARN.....	222
SYNTAX FOR COMMANDS	223
THE RPN REGISTER STACK	224
THE FILE COMMAND	225
THE TIC COMMAND	227
THE DRAW COMMAND.....	228
THE DRAW COMMAND (CONTINUED).....	230
THE DRAW COMMAND (CONTINUED).....	231
THE RTEINT COMMAND.....	232
THE PEAKNUMBER COMMAND	233
THE PEAKNUMBER COMMAND (CONTINUED)	235
THE EXCHANGE COMMAND.....	236
THE MERGE COMMAND.....	237
THE REMOVE COMMAND.....	238
THE CHROMATOGRAM COMMAND	239
THE SPECTRUM COMMAND.....	241
THE TABULATE COMMAND.....	242
THE TABULATE COMMAND (CONTINUED).....	244
THE TABULATE COMMAND (CONTINUED).....	245
THE TABULATE COMMAND (CONTINUED).....	246
PRINTER OUTPUT COMMANDS	247
GROUP EXERCISE.....	248
MACRO NAMES AND FILES	249
FOUR WAYS TO EXECUTE A MACRO.....	250
CONDITIONAL STATEMENTS	251
VARIABLES	252
EXAMPLE OF VARIABLE USE	253
THE ON_ERROR COMMAND.....	254
CREATIVE MACRO WRITING.....	255
HELPFUL HINTS WHEN WRITING MACROS	256
PREPARING A CUSTOM MACRO FOR DATA ANALYSIS	257
CUSTOM MACROS FOR PRE- AND POST-RUN TASKS	258
MACROS MENU.....	259
METHODS FLOWCHART.....	260
LAB EXERCISE: RPN	261
RPN BASICS	262
REGISTER MANIPULATION	265
VARIABLES	266
SPECTRAL MANIPULATIONS.....	267
EXTRACTED ION CHROMATOGRAMS.....	269

GENERATING OUTPUT TO THE PRINTER	270
LAB EXERCISE: MACROS.....	271
INTRODUCTION TO WRITING MACROS	272
MACRO FORMATTING.....	273
MACRO EXERCISE #1	274
MACRO EXERCISE #2	280
MACRO EXERCISE #3	282
MACRO EXERCISE #4.....	283
MACRO EXERCISE ANSWER.....	284
SEQUENCING.....	287
WHAT YOU WILL LEARN.....	288
WHAT IS A SEQUENCE?	289
CREATING A SEQUENCE	290
CONFIGURING THE SEQUENCE TABLE	292
ASSIGNING DATA FILE NAMES	293
ADDITIONAL SEQUENCING OPTIONS	295
SIMULATING A SEQUENCE	297
RUNNING/REPROCESSING A SEQUENCE	298
VIEWING A SEQUENCE	300
REPROCESSING A SEQUENCE.....	301
IMPORTING SEQUENCE INFORMATION.....	302
SECURED CONTROL	304
SECURED CONTROL ACCOUNTS.....	305
SECURED CONTROL METHODS	307
INSTRUMENT STARTUP/STANDBY METHODS	308
SECURED CONTROL OPERATION	309
SAMPLE-CENTRIC SECURED CONTROL.....	312
ASSIGNING SAMPLE NAMES TO METHODS.....	313
RETENTION TIME LOCKING (RTL).....	314
STEPS IN RETENTION TIME LOCKING (RTL)	316
RELOCKING THE METHOD.....	318
STEPS IN RELocking THE METHOD	319
WHAT IS THE “SAMPLE SCREENER?”	321
STEPS IN CREATING A “SCREENER” METHOD	322
THE RESULTS SCREENER VIEW.....	324
LAB EXERCISE: SEQUENCING, SECURED CONTROL, AND RTL ...	325
SEQUENCING.....	326
IMPORTING INFORMATION FROM A CSV FILE.....	328
SECURED CONTROL	331
SAMPLE-CENTRIC SECURED CONTROL.....	334
RETENTION TIME LOCKING (RTL).....	337