Demo MDLC method

2D method overview

Fraction	Fractionation (Grad2 method)	Salt injection (AS method)	Conc. of NH_4OAc	pH 10 %B	pH 2 %B	V2 position
0	√	26 min	1000 mM	0-12	/	A / Load
1	√	26 min	1000 mM	12-14	8-20	B / Inject
2	√	26 min	1000 mM	14-16	8-25	A / Load
3	√	26 min	1000 mM	16-19	10-25	B / Inject
4	√	26 min	1000 mM	19-22	10-28	A / Load
5	√	26 min	1000 mM	22-26	12-30	B / Inject
6	√	26 min	1000 mM	26-30	12-32	A / Load
7	√	26 min	1000 mM	30-45	15-35	B / Inject
8	×	/	/	/	20-40	A / Load

3D method overview

Fraction	Fractionation (Grad2 method)	Salt injection (AS method)	Conc. of NH_4OAc	pH 10 %B	pH 2 %B	V2 position
0	√	26 min	20 mM	0-12	/	A / Load
1	√	26 min	20 mM	12-14	5-20	B / Inject
2	×	0 min	100 mM	/	8-20	A / Load
3	×	0 min	100 mM	/	5-20	B / Inject
4	×	0 min	1000 mM	/	8-20	A / Load
5	×	0 min	1000 mM	/	5-20	B / Inject
6	√	26 min	20 mM	14-16	8-20	A / Load
7	√	26 min	20 mM	16-19	8-22	B / Inject
8	×	0 min	100 mM	/	10-25	A / Load
9	×	0 min	100 mM	/	8-22	B / Inject
10	×	0 min	1000 mM	/	10-25	A / Load
11	×	0 min	1000 mM	/	8-22	B / Inject
12	√	26 min	20 mM	19-22	10-25	A / Load
13	√	26 min	20 mM	22-26	12-28	B / Inject
14	×	0 min	100 mM	/	15-32	A / Load
15	×	0 min	100 mM	/	12-28	B / Inject
16	×	0 min	1000 mM	/	15-32	A / Load
17	×	0 min	1000 mM	/	12-28	B / Inject
18	√	26 min	20 mM	26-30	15-32	A / Load
19	√	26 min	20 mM	30-45	20-35	B / Inject
20	×	0 min	100 mM	/	20-35	A / Load
21	×	0 min	100 mM	/	20-35	B / Inject
22	×	0 min	1000 mM	/	20-35	A / Load
23	×	0 min	1000 mM	/	20-35	B / Inject
24	×	/	/	/	20-35	A / Load

Eksigent demo method

Eksigent Injection sequence

Run Table: 2D dualtrap_PPRP_20121220__8F_90mingrad_HENRY.ini

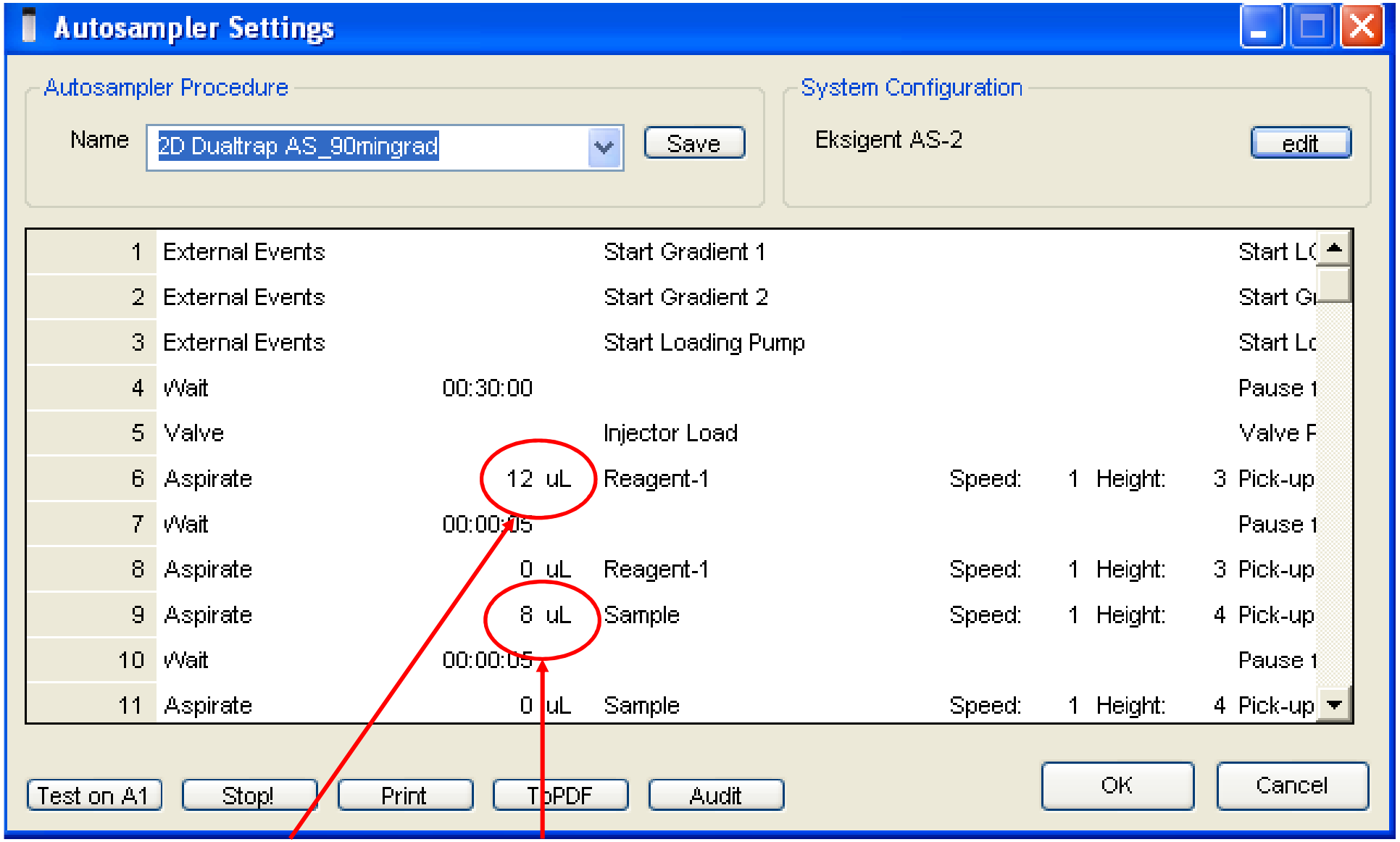
Seq #	Run	Autosampler			LC		
	☑	Method	Tray	Vial	Method	Channel	
1	☑	2D Dualtrap AS_90mingrad	2	A01	2D Dualtrap Grad2_0	Gradient 2	Q
2	☑				2D Dualtrap LoadingPump	Loading Pump	Q
3	☑				2D_C1_P1_90min	Gradient 1	Q
4	☑	2D Dualtrap AS_90mingrad	2	A01	2D Dualtrap Grad2_1_90min	Gradient 2	Q
5	☑				2D Dualtrap LoadingPump_90mingrad	Loading Pump	Q
6	☑				2D_C1_P1_90min	Gradient 1	Q
7	☑	2D Dualtrap AS_90mingrad	2	A01	2D Dualtrap Grad2_2_90min	Gradient 2	Q
8	☑				2D Dualtrap LoadingPump_90mingrad	Loading Pump	Q
9	☑				2D_C2_P1_90min	Gradient 1	Q
10	☑	2D Dualtrap AS_90mingrad	2	A01	2D Dualtrap Grad2_3_90min	Gradient 2	Q
11	☑				2D Dualtrap LoadingPump_90mingrad	Loading Pump	Q
12	☑				2D_C3_P1_90min	Gradient 1	Q
13	☑	2D Dualtrap AS_90mingrad	2	A01	2D Dualtrap Grad2_4_90min	Gradient 2	Q
14	☑				2D Dualtrap LoadingPump_90mingrad	Loading Pump	Q
15	☑				2D_C4_P1_90min	Gradient 1	Q
16	☑	2D Dualtrap AS_90mingrad	2	A01	2D Dualtrap Grad2_5_90min	Gradient 2	Q
17	☑				2D Dualtrap LoadingPump_90mingrad	Loading Pump	Q
18	☑				2D_C5_P1_90min	Gradient 1	Q
19	☑	2D Dualtrap AS_90mingrad	2	A01	2D Dualtrap Grad2_6_90min	Gradient 2	Q
20	☑				2D Dualtrap LoadingPump_90mingrad	Loading Pump	Q

Eksigent Injection sequence (continue)

Run Table: 2D dualtrap_PPRP_20121220__8F_90mingrad_HENRY.ini

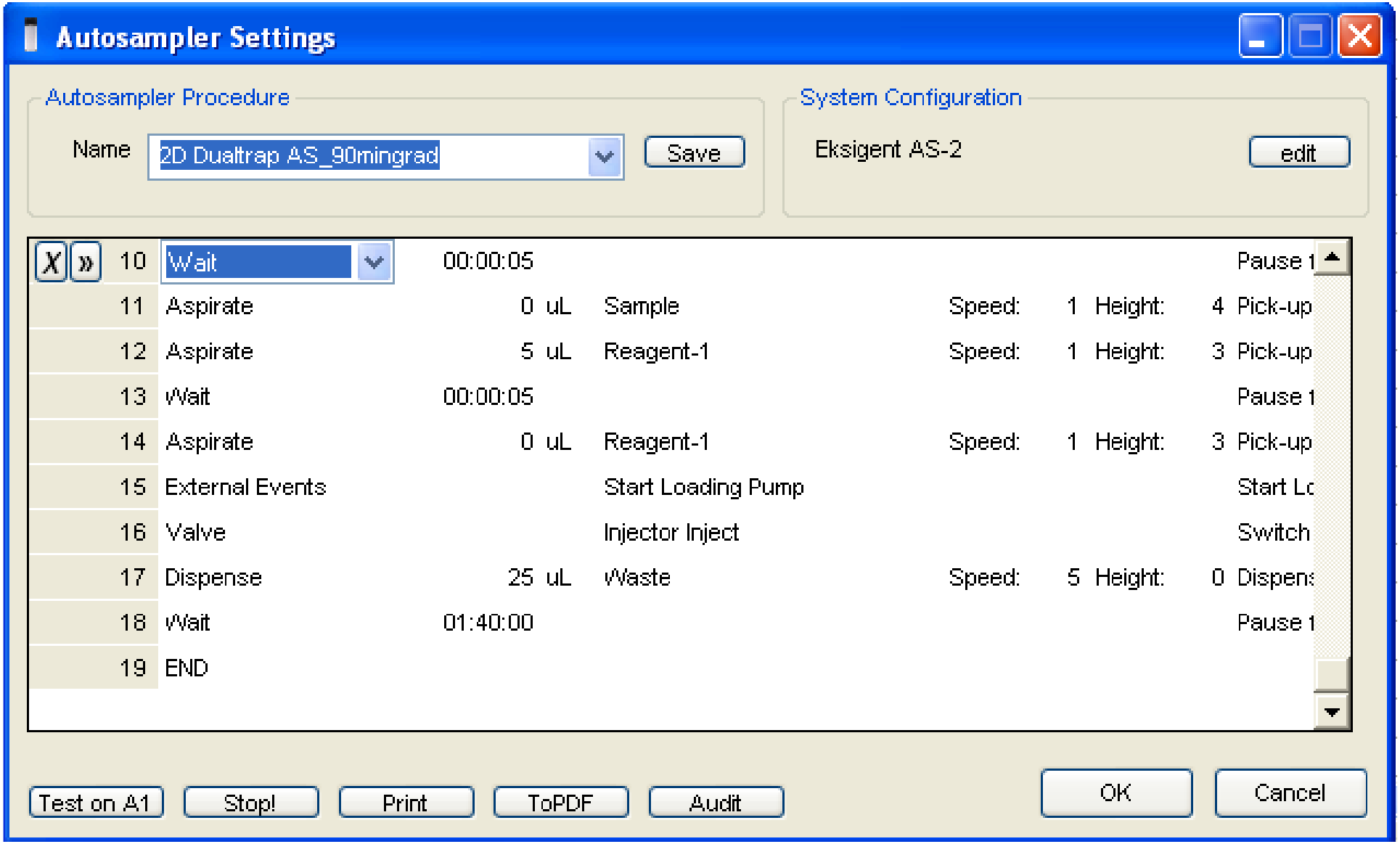
Seq #	Run	Autosampler			LC		h
	☑	Method	Tray	Vial	Method	Channel	at
19	☑	2D Dualtrap AS_90mingrad	2	A01	2D Dualtrap Grad2_6_90min	Gradient 2	Q
20	☑				2D Dualtrap LoadingPump_90mingrad	Loading Pump	Q
21	☑				2D_C6_P1_90min	Gradient 1	Q
22	☑	2D Dualtrap AS_90mingrad	2	A01	2D Dualtrap Grad2_7_90min	Gradient 2	Q
23	☑				2D Dualtrap LoadingPump_90mingrad	Loading Pump	Q
24	☑				2D_C7_P1_90min	Gradient 1	Q
25	☑	2D Dualtrap AS_90mingrad	2	A01	2D Dualtrap Grad2_8_90min	Gradient 2	Q
26	☑				2D Dualtrap LoadingPump_90mingrad	Loading Pump	Q
27	☑				2D_C8_P1_90min	Gradient 1	Q
28	☐						
29	☐						
30	☐						
31	☐						
32	☐						
33	☐						
34	☐						
35	☐						
36	☐						
37	☐						
38	☐						

Autosampler method

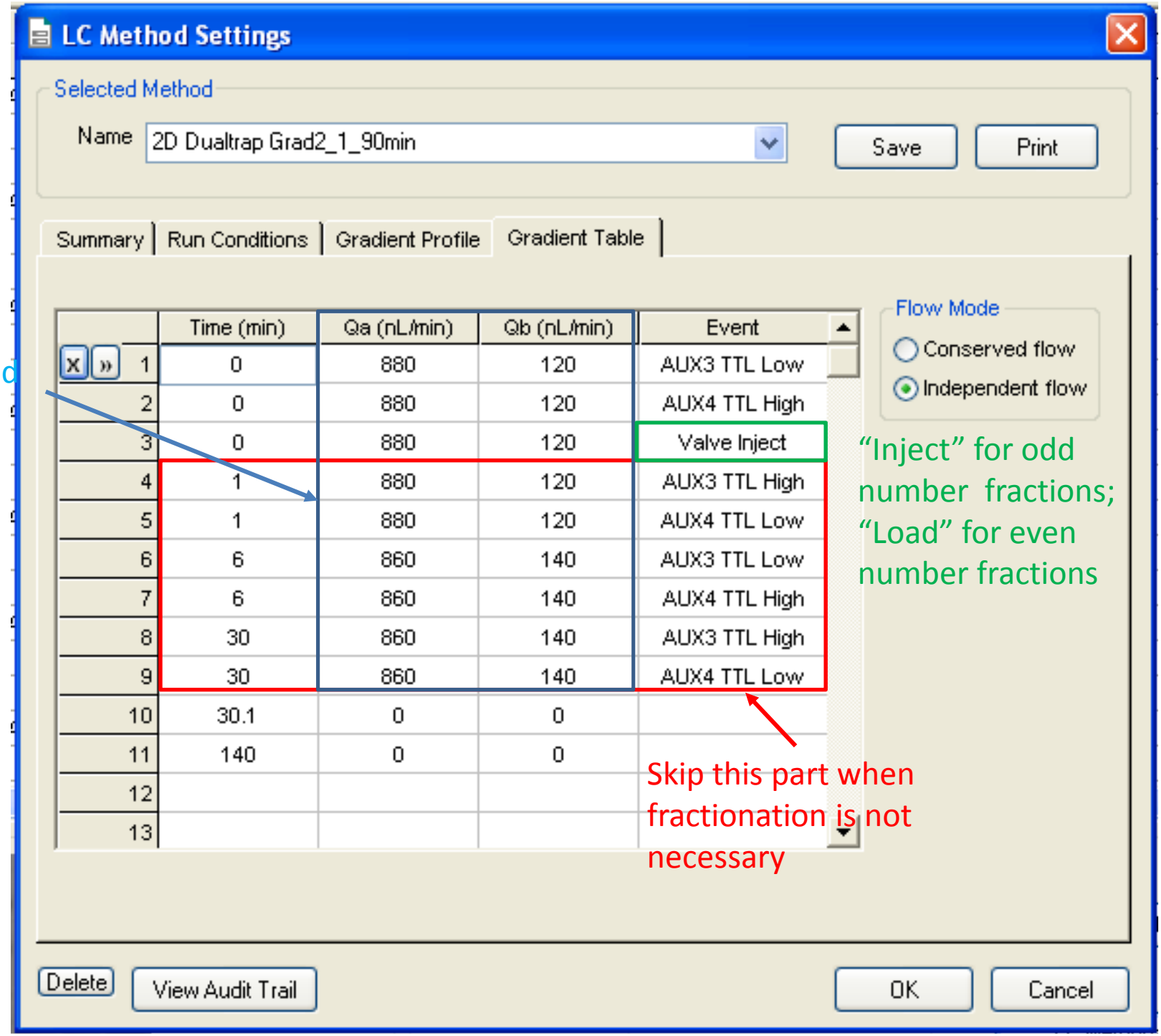


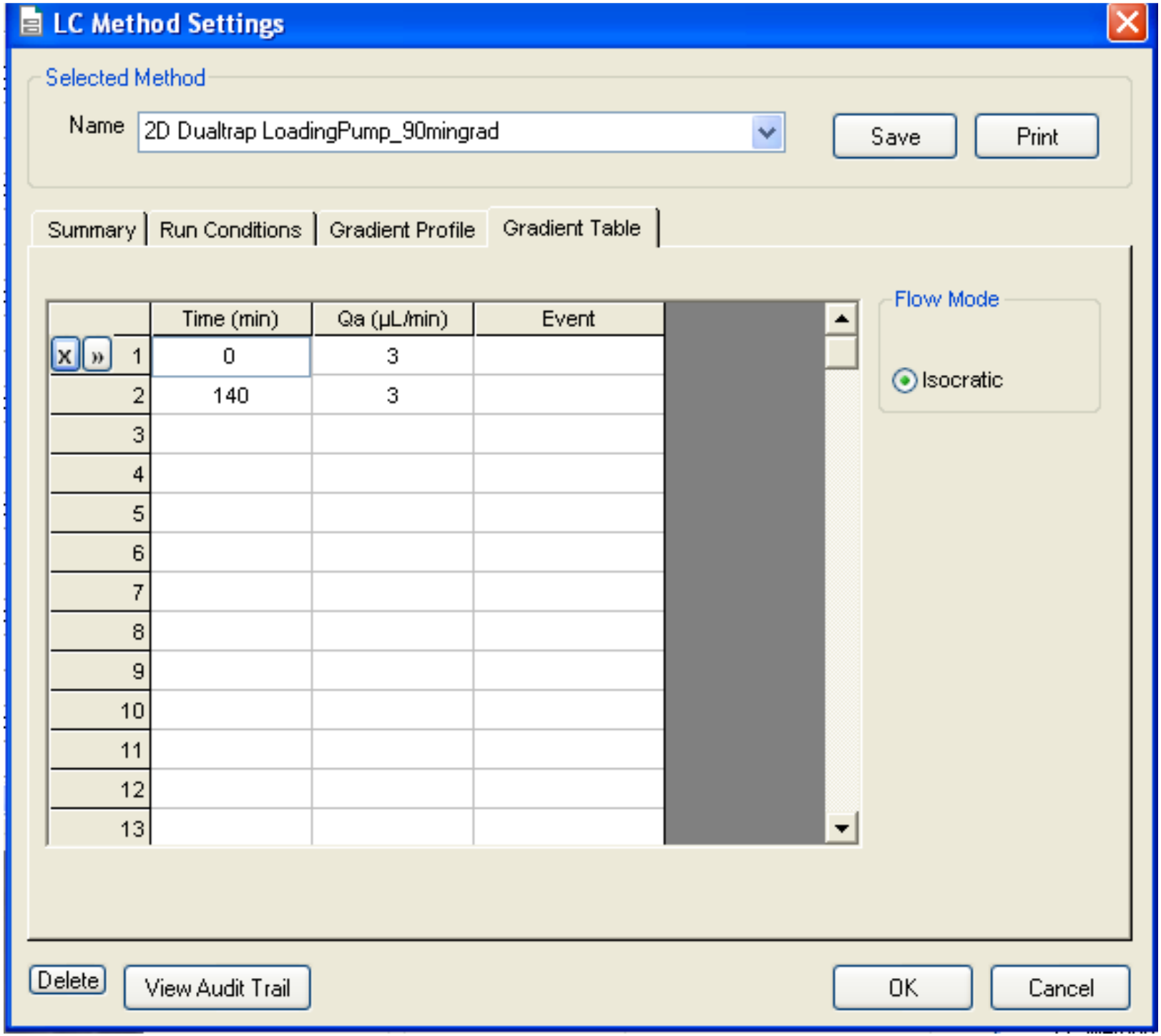
Change into (17, 3) when injecting 20 and 100 mM salt in 3D method

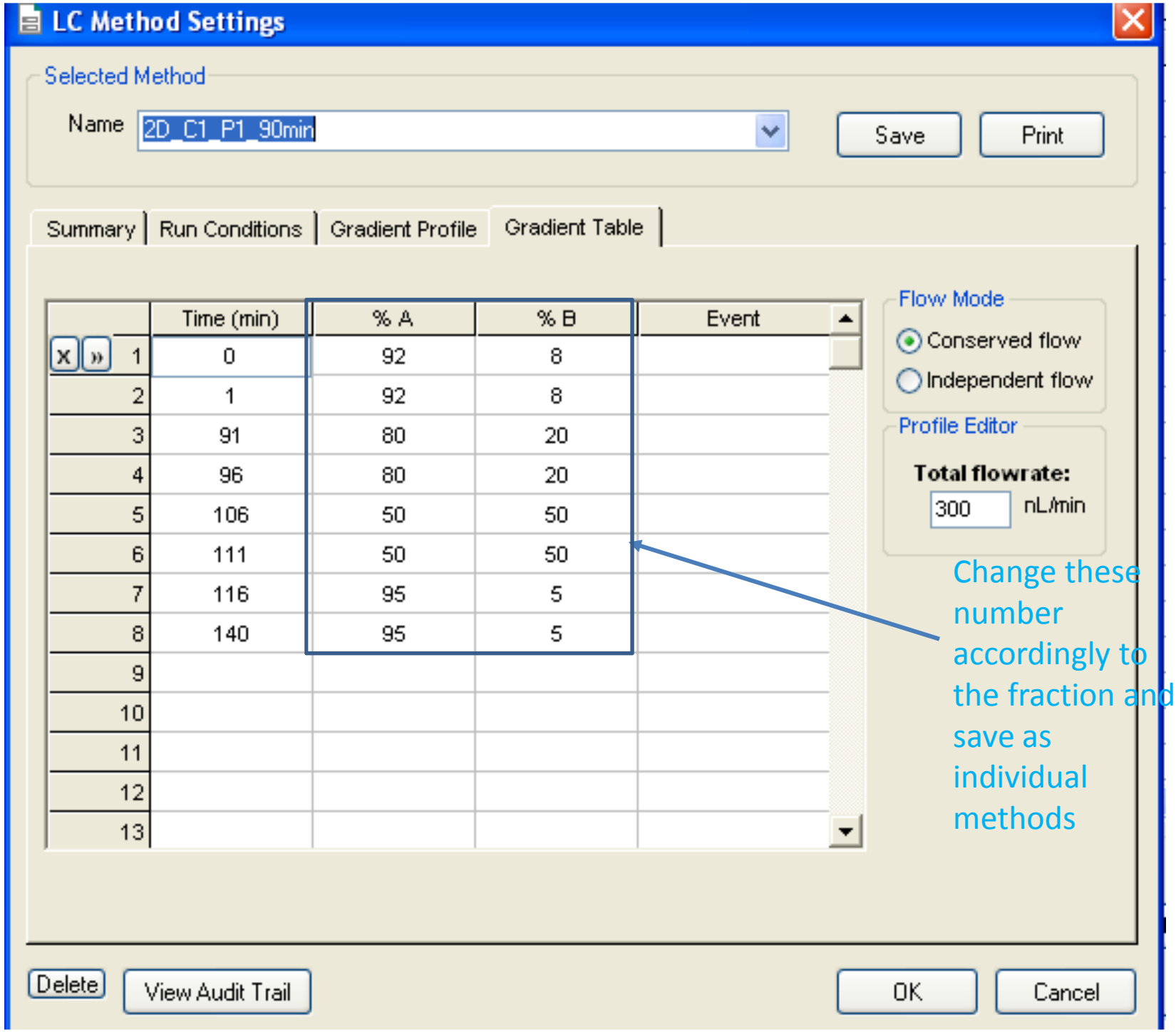
Autosampler method (continue)



Change these number accordingly to the fraction and save as individual methods



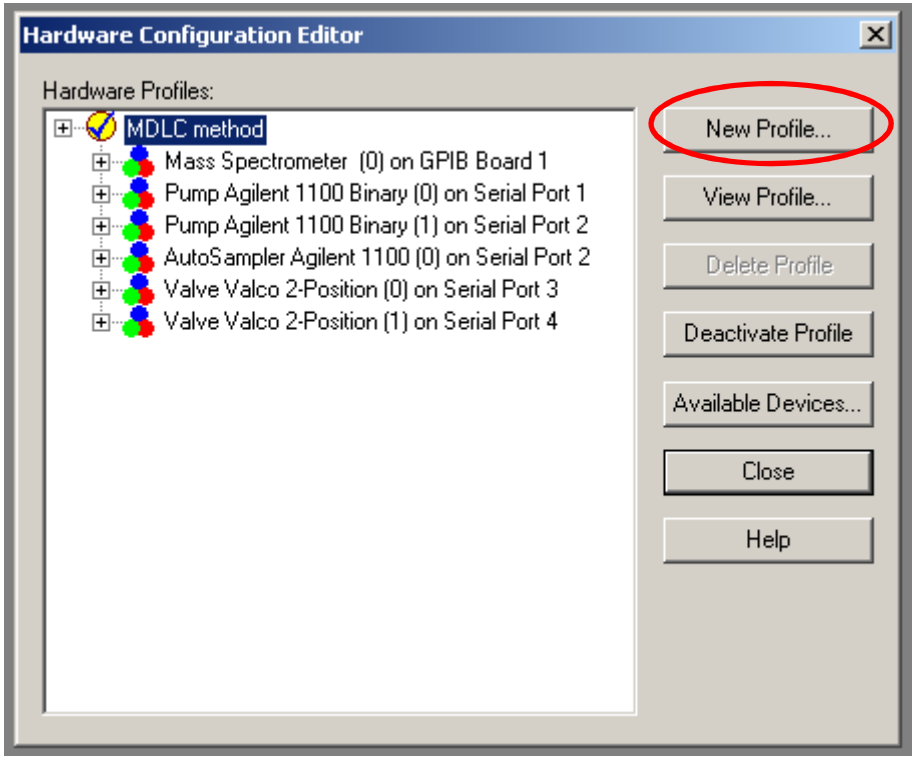

LC Method Settings
Selected Method
Name
2D Dualtrap LoadingPump_90mingrad
Save
Print
Summary
Run Conditions
Gradient Profile
Gradient Table
Time (min)
Qa (µL/min)
Event
1 0 3
2 140 3
3
4
5
6
7
8
9
10
11
12
13
Flow Mode
Isocratic
Delete
View Audit Trail
OK
Cancel


LC Method Settings
Selected Method
Name
2D_C1_P1_90min
Save
Print
Summary
Run Conditions
Gradient Profile
Gradient Table
Time (min)
% A
% B
Event
1 0 92 8
2 1 92 8
3 91 80 20
4 96 80 20
5 106 50 50
6 111 50 50
7 116 95 5
8 140 95 5
9
10
11
12
13
Flow Mode
Conserved flow
Independent flow
Profile Editor
Total flowrate:
300
nL/min
Change these number accordingly to the fraction and save as individual methods
Delete
View Audit Trail
OK
Cancel

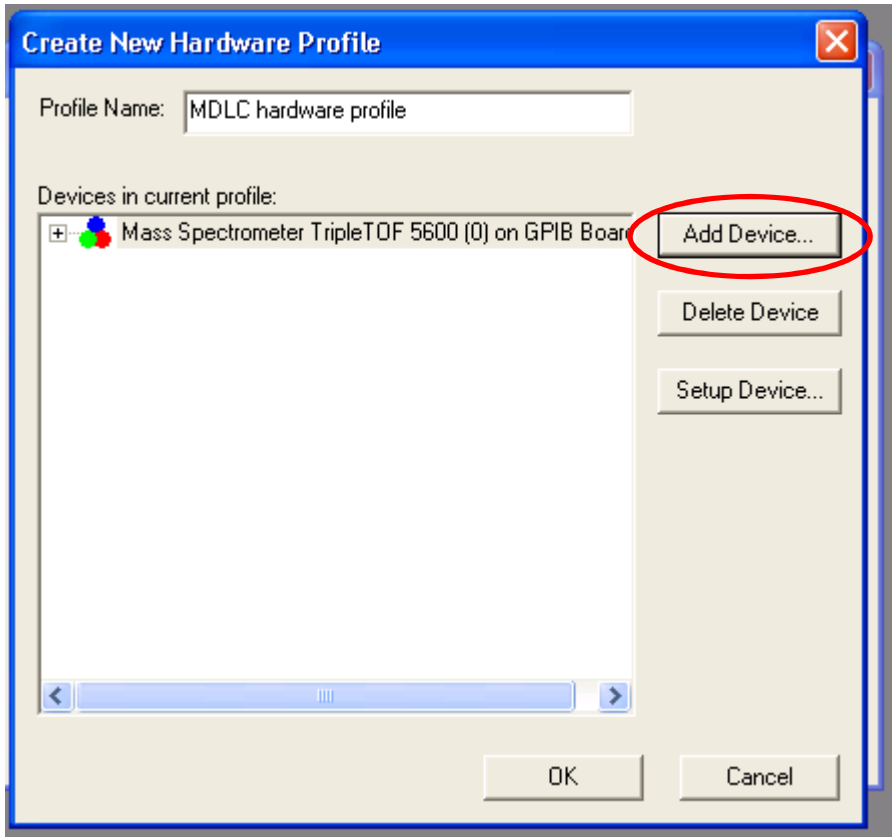
Agilent demo MDLC method

Hardward profile setup guide

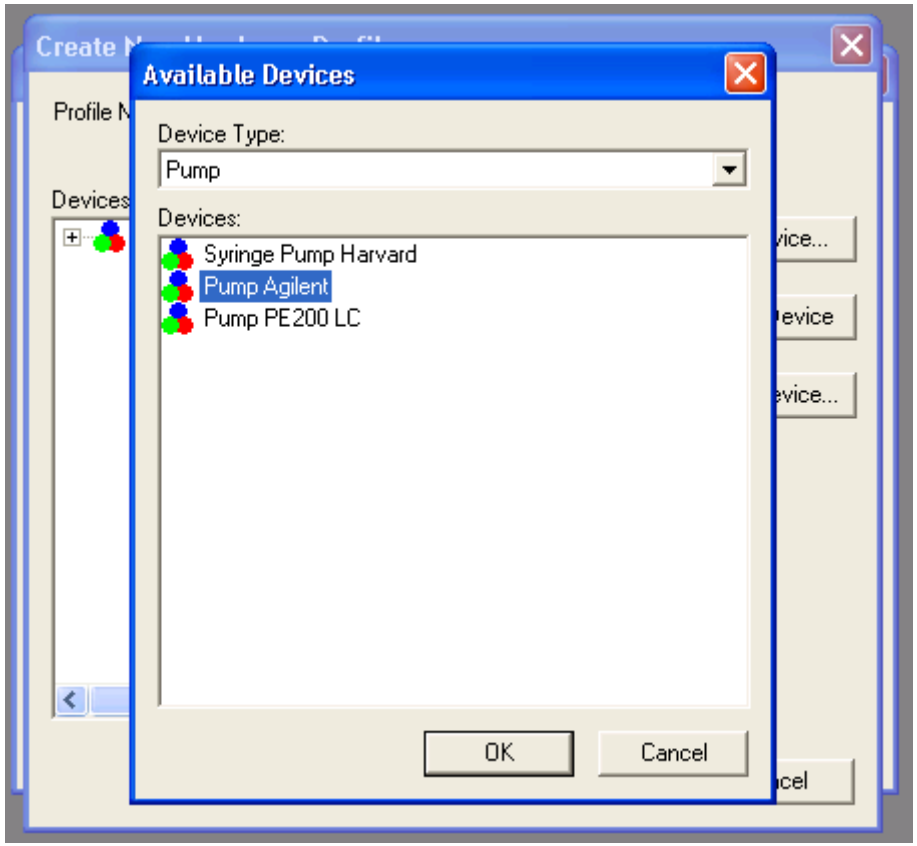
- Click “New Profile”



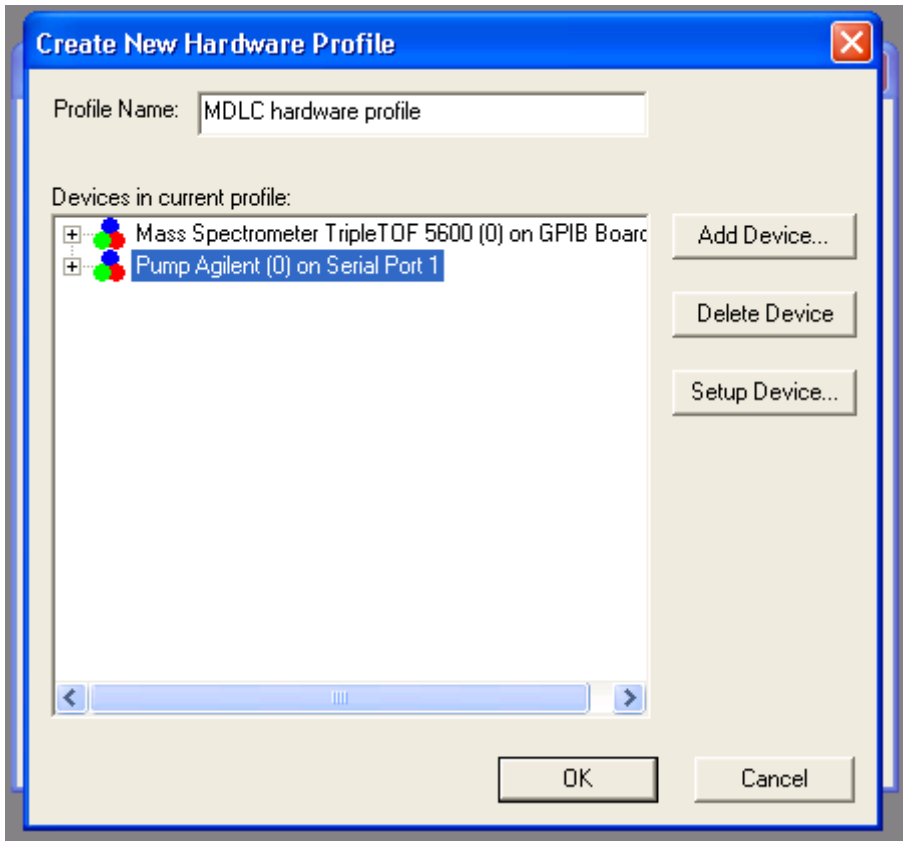
- After adding the mass spectrometer (as instructed as the manufacturer), click “Add Device)



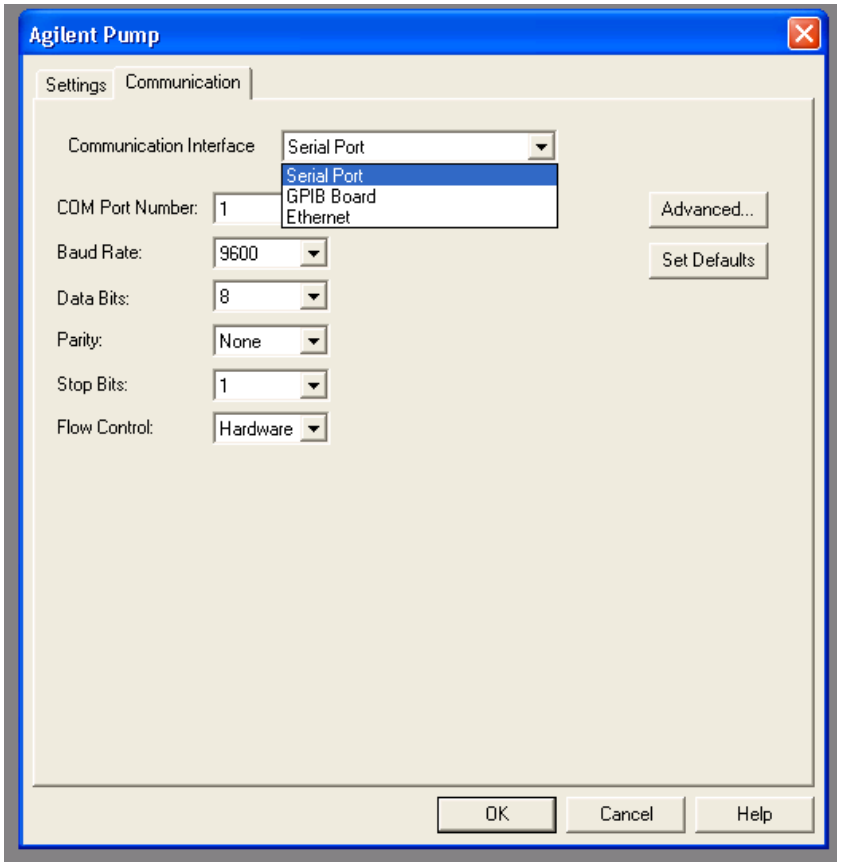
- Choose “Pump” from the drop down list and click “PumpAgilent”, then “ok”



- Click “Setup Device”

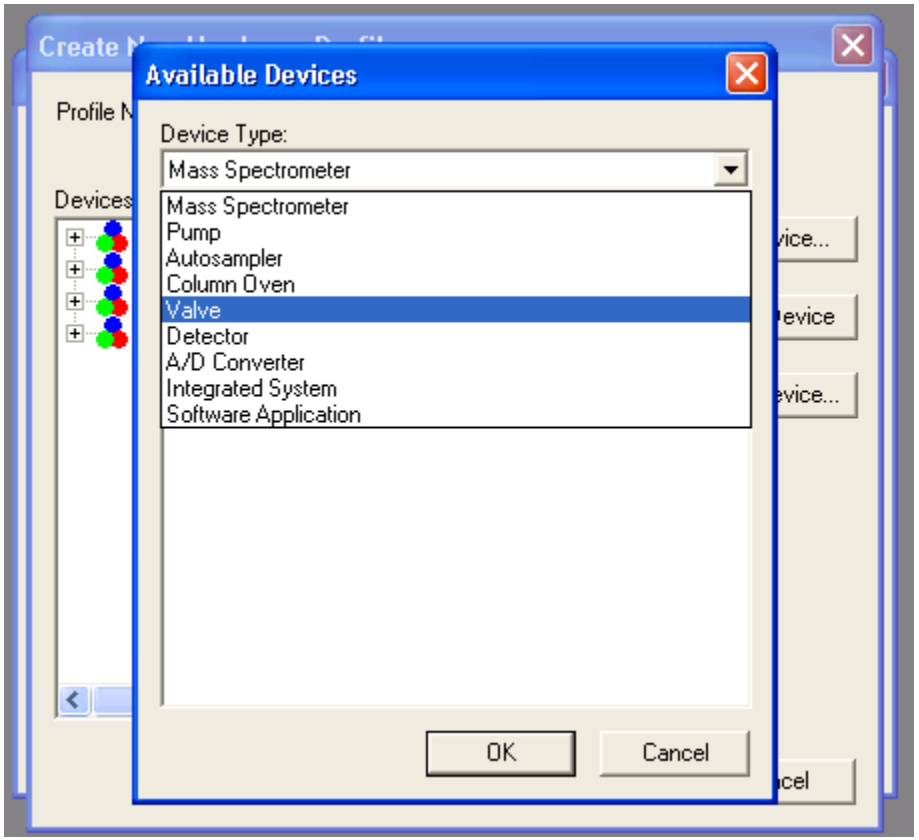


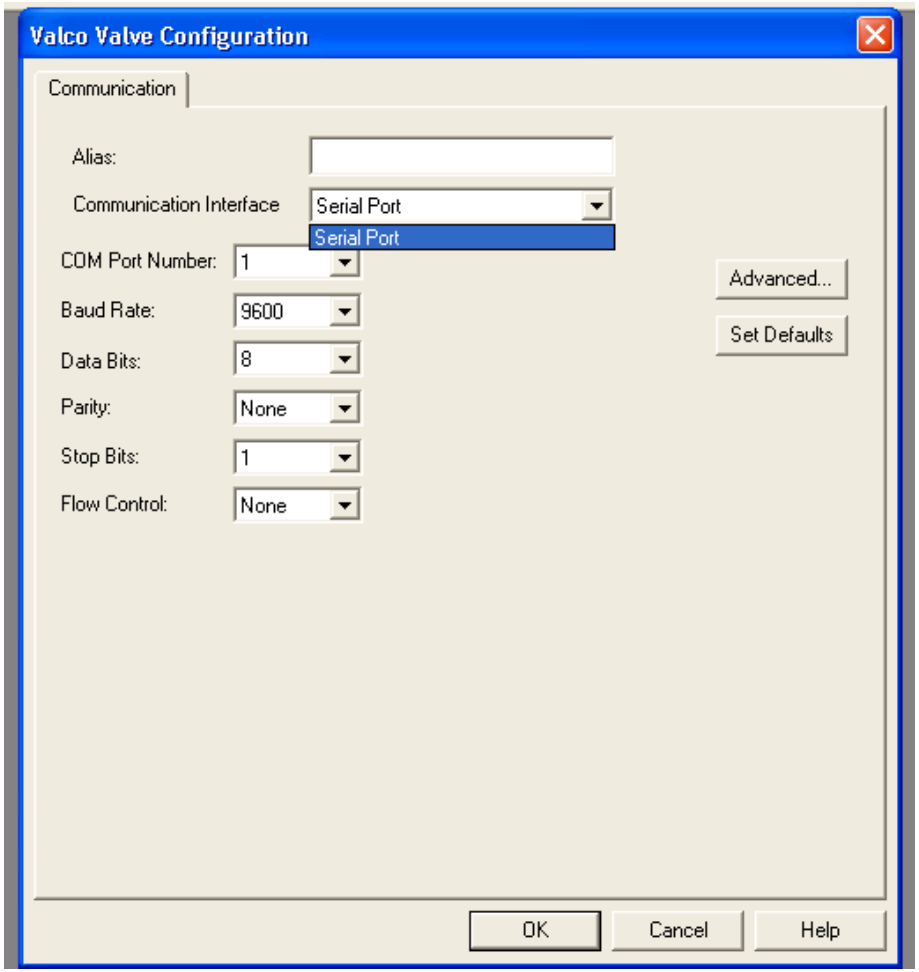
- Choose the communication interface and the port number as the LC is connected. Serial port is suggested



- Add other Agilent components in a similar manner

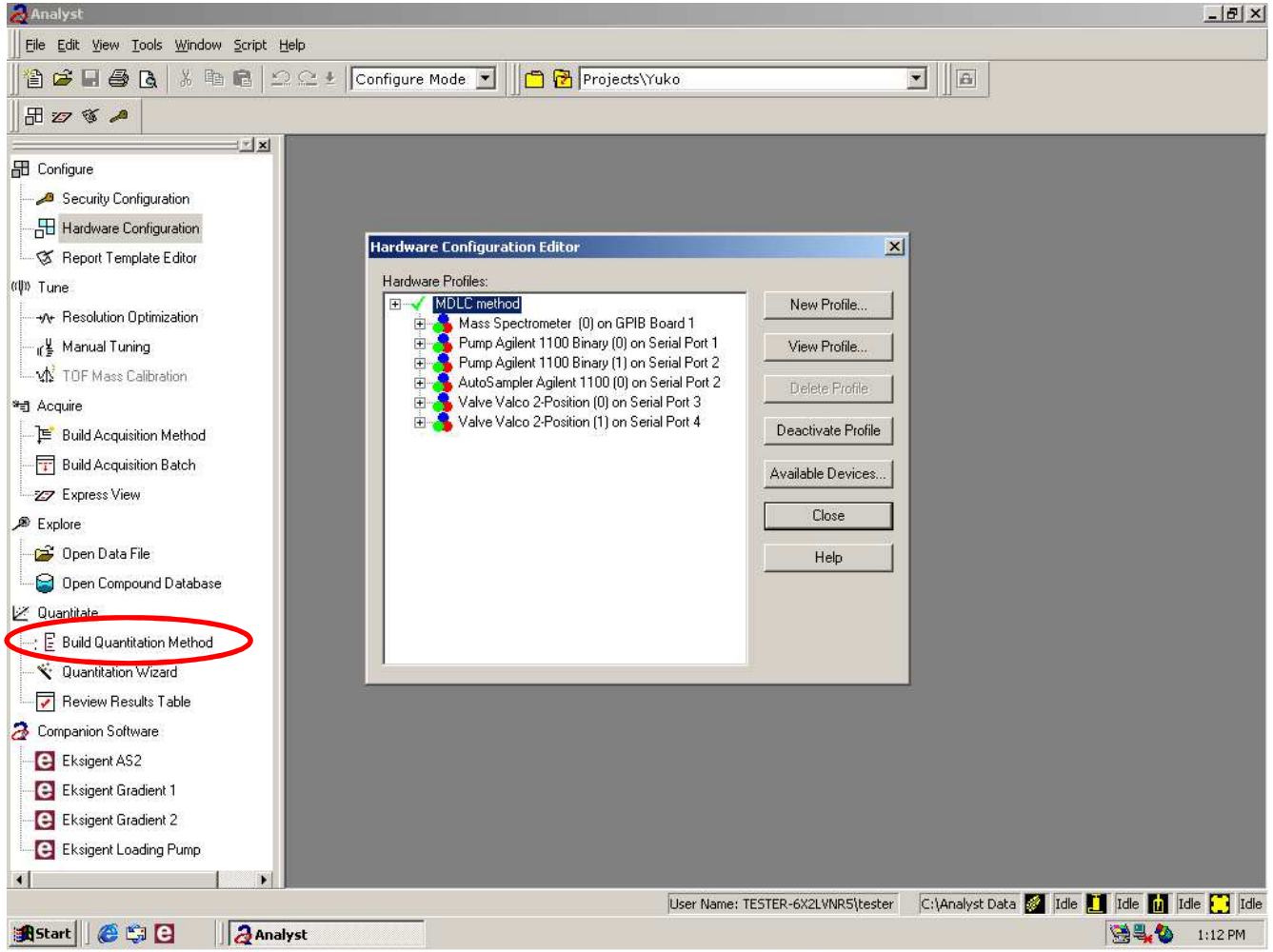
- Valves are added in a similar manner. Choose “Valve” from the drop down list, and choose serial port as communication interface



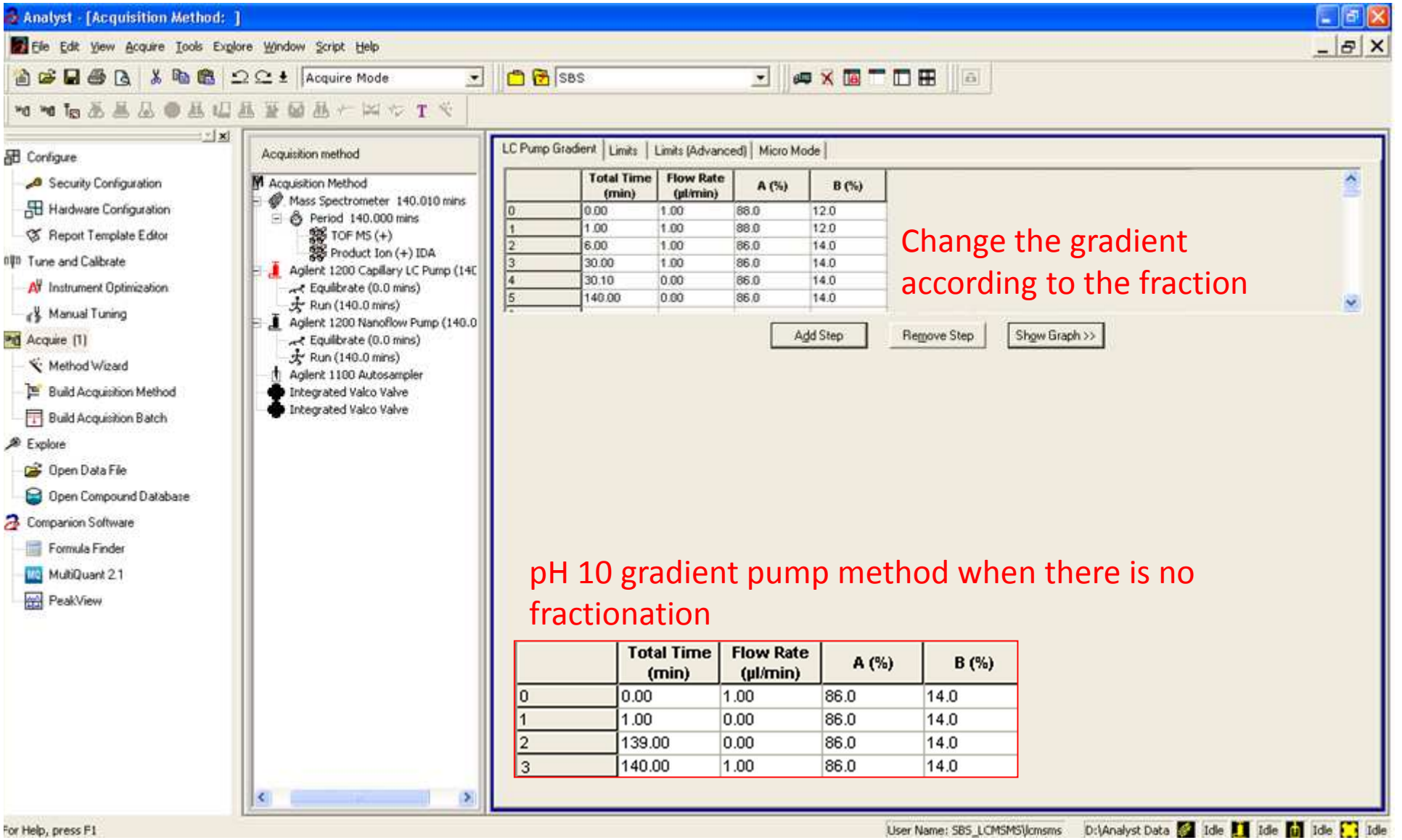


Setting MDLC method for Agilent system

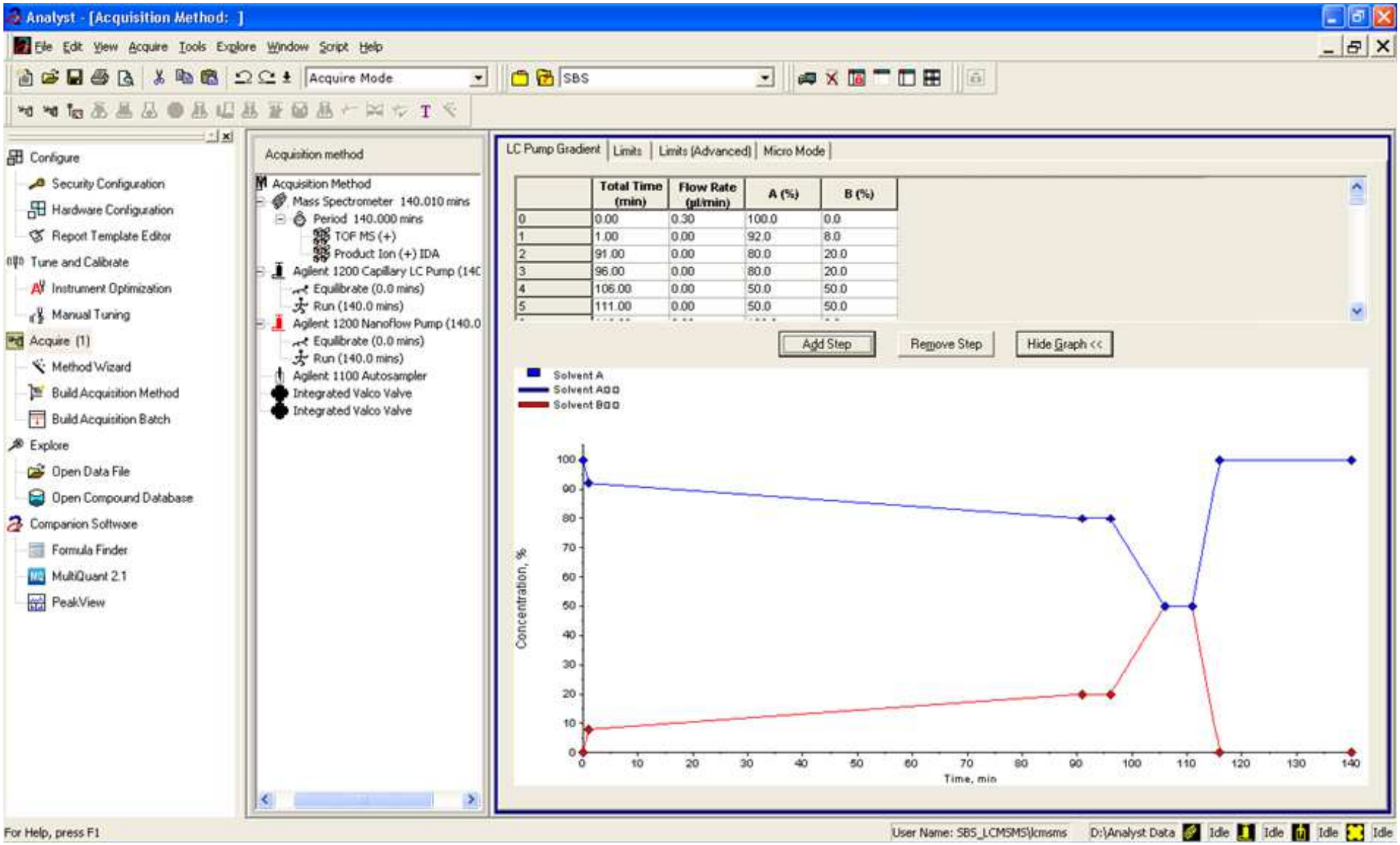
- Double click “Build Acquisition method”

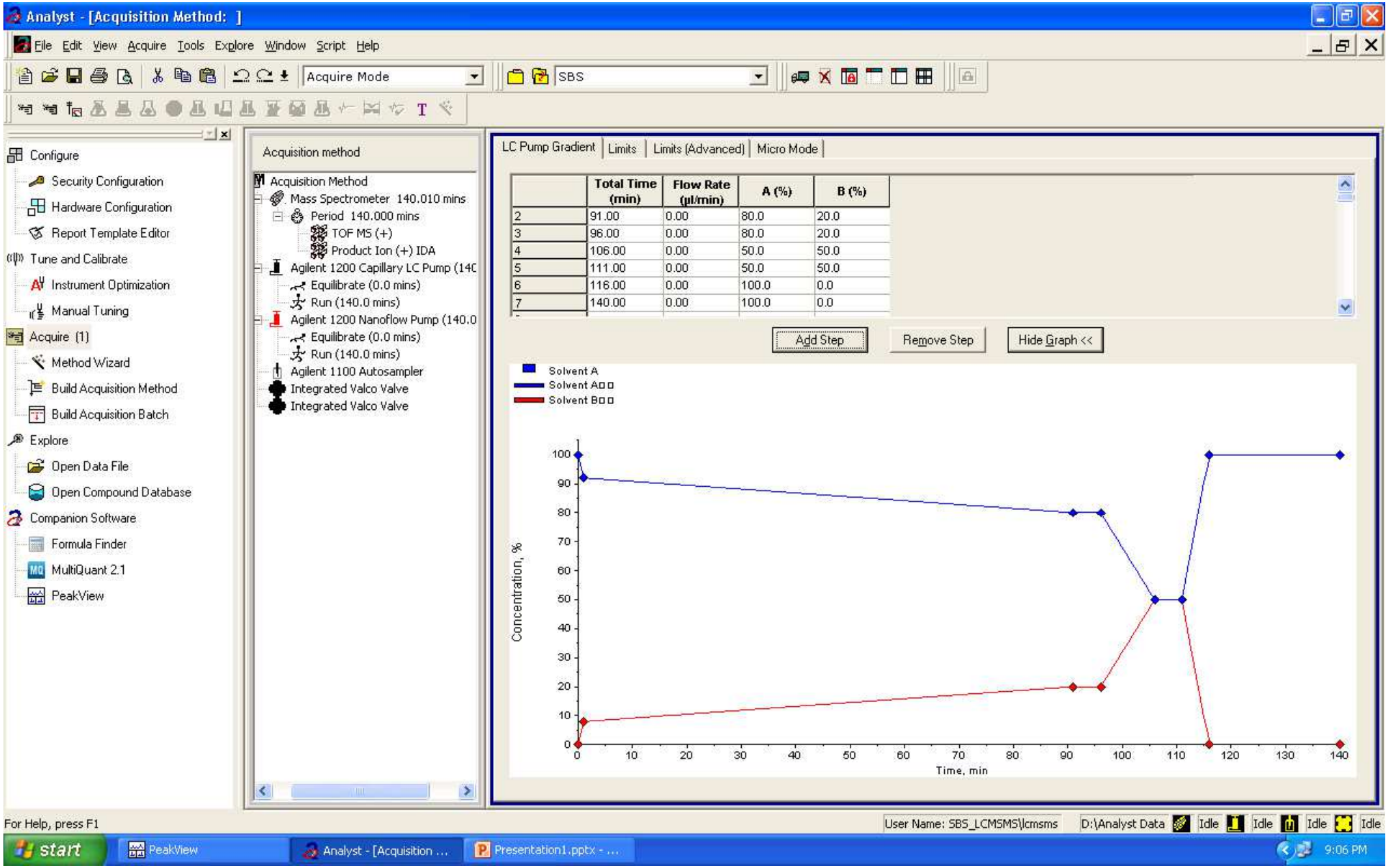


pH 10 gradient pump method

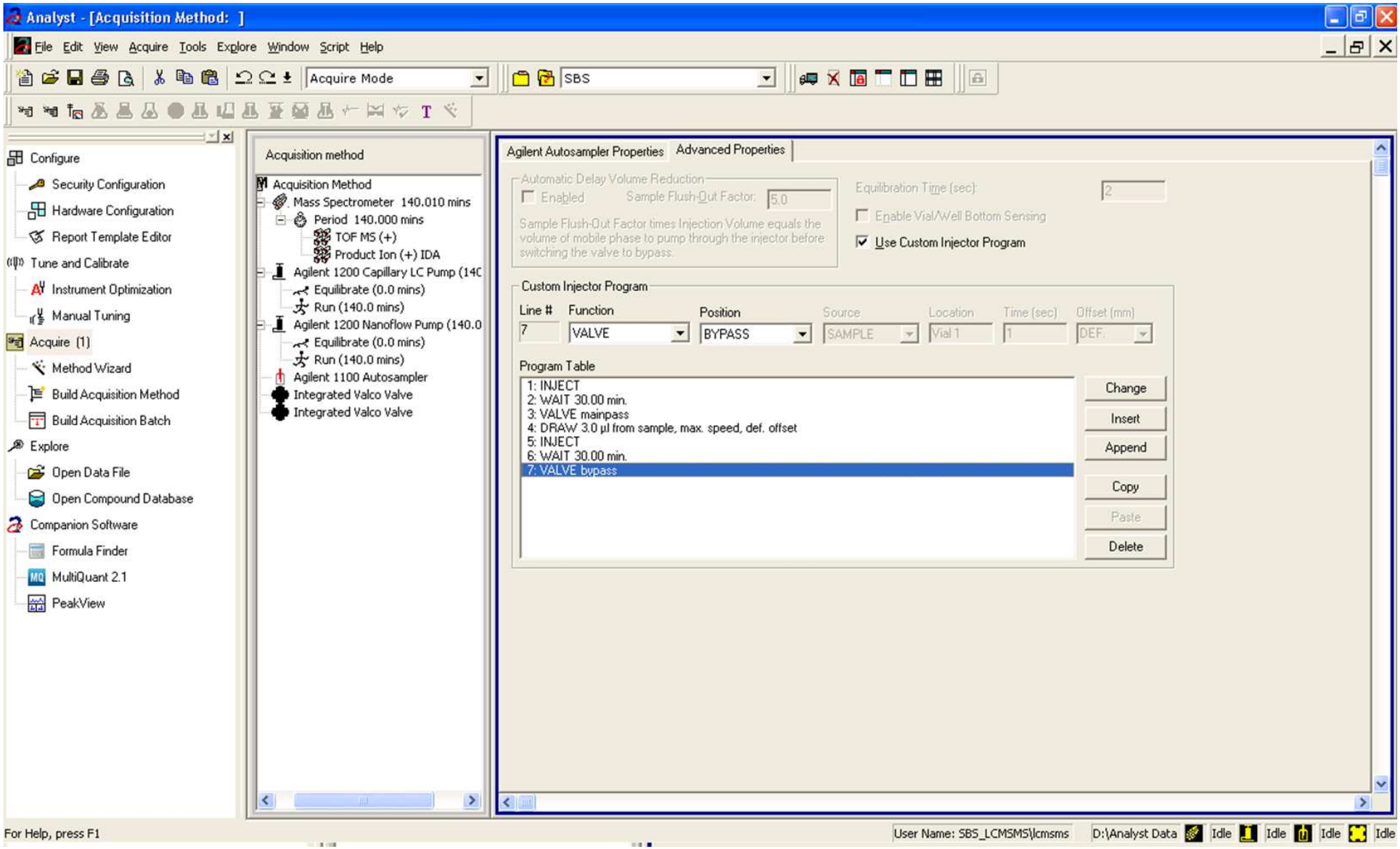


pH 2 gradient pump method

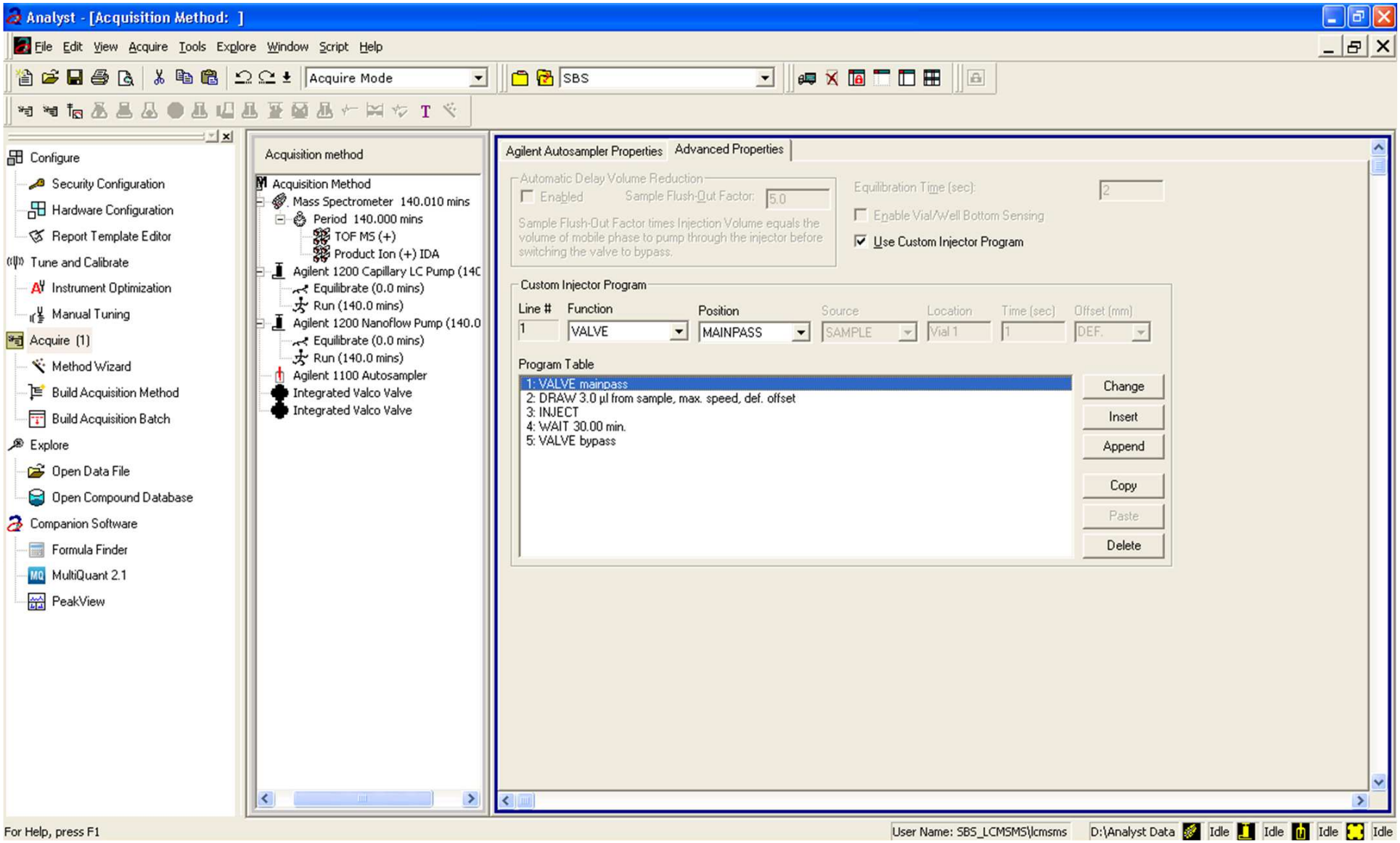



Analyst - [Acquisition Method:]
File Edit View Acquire Tools Explore Window Script Help
Acquire Mode
SBS
Configure
Security Configuration
Hardware Configuration
Report Template Editor
Tune and Calibrate
Instrument Optimization
Manual Tuning
Acquire (1)
Method Wizard
Build Acquisition Method
Build Acquisition Batch
Explore
Open Data File
Open Compound Database
Companion Software
Formula Finder
MultiQuant 2.1
PeakView
Acquisition method
Acquisition Method
Mass Spectrometer 140.010 mins
Period 140.000 mins
TOF MS (+)
Product Ion (+) IDA
Agilent 1200 Capillary LC Pump (140
Equilibrate (0.0 mins)
Run (140.0 mins)
Agilent 1200 Nanoflow Pump (140.0
Equilibrate (0.0 mins)
Run (140.0 mins)
Agilent 1100 Autosampler
Integrated Valco Valve
Integrated Valco Valve
LC Pump Gradient
Limits
Limits (Advanced)
Micro Mode
Total Time (min)
Flow Rate (µl/min)
A (%)
B (%)
2 91.00 0.00 80.0 20.0
3 96.00 0.00 80.0 20.0
4 106.00 0.00 50.0 50.0
5 111.00 0.00 50.0 50.0
6 116.00 0.00 100.0 0.0
7 140.00 0.00 100.0 0.0
Add Step
Remove Step
Hide Graph <<
Solvent A
Solvent A
Solvent B
Concentration, %
Time, min
For Help, press F1
User Name: SBS_LCMSMS\lcmsms
D:\Analyst Data
Idle
Idle
Idle
Idle
start
PeakView
Analyst - [Acquisition ...
Presentation1.pptx - ...
9:06 PM

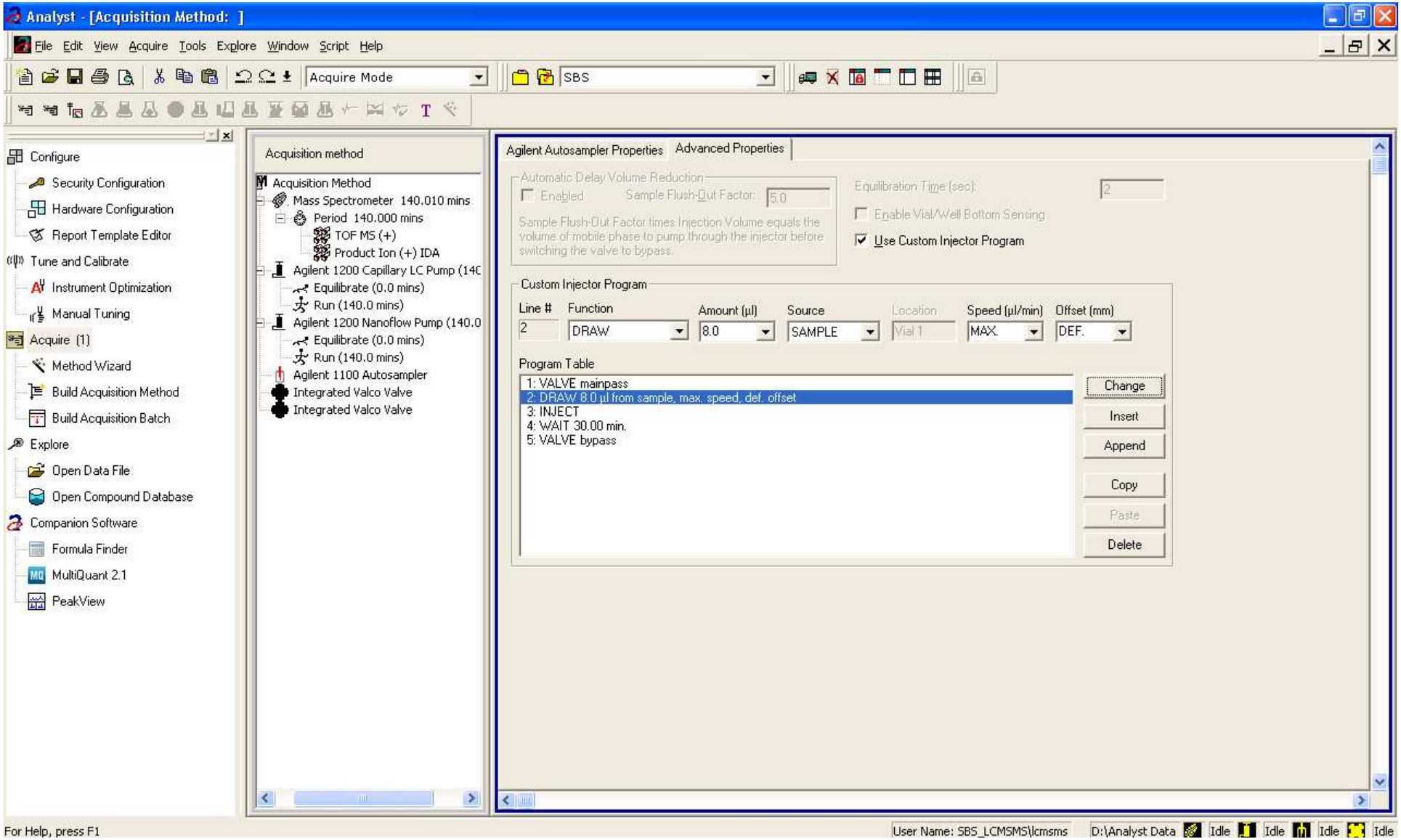
Autosampler method (3D 20 mM/2D 1000 mM)



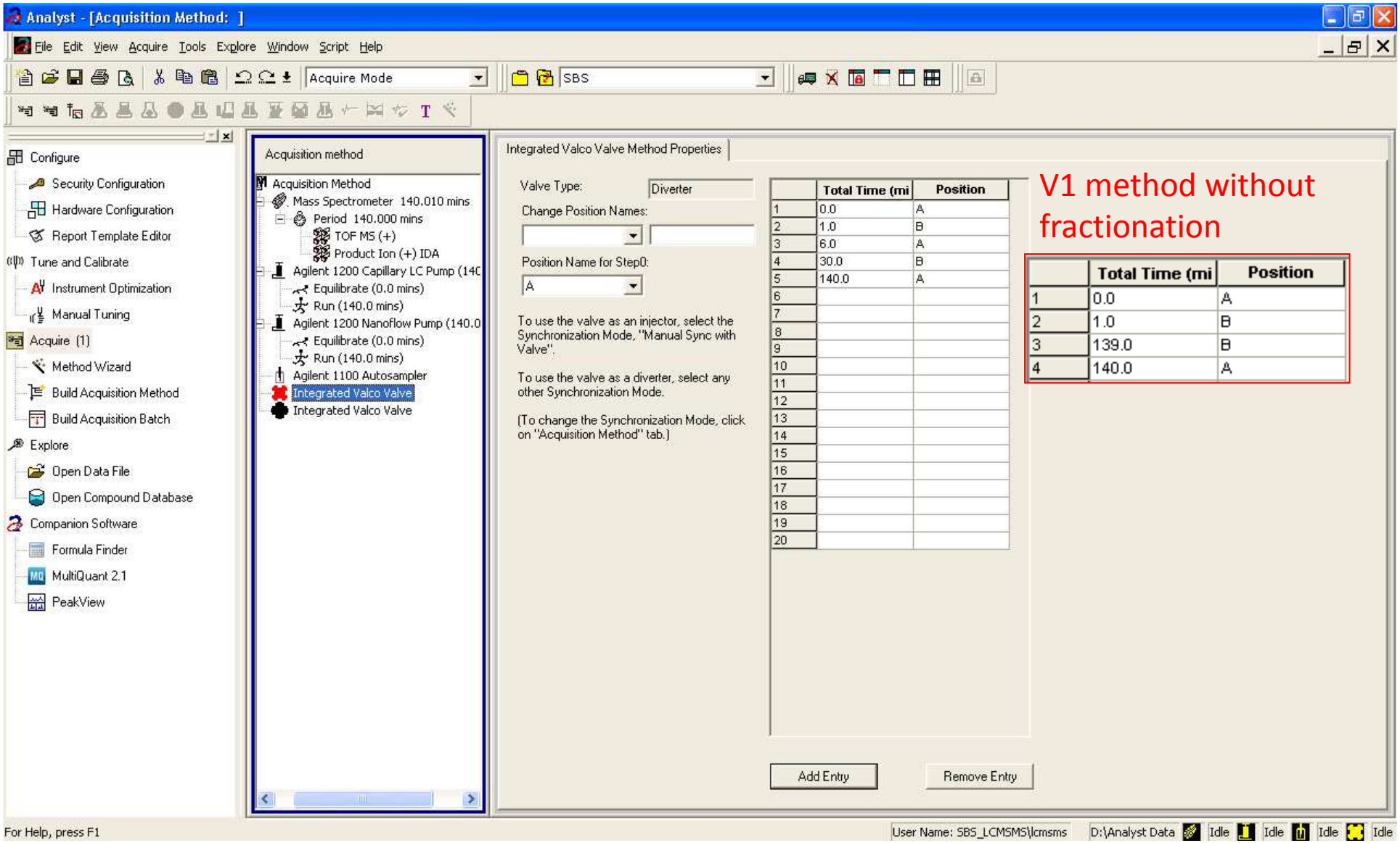
Autosampler method (3D 100 mM)



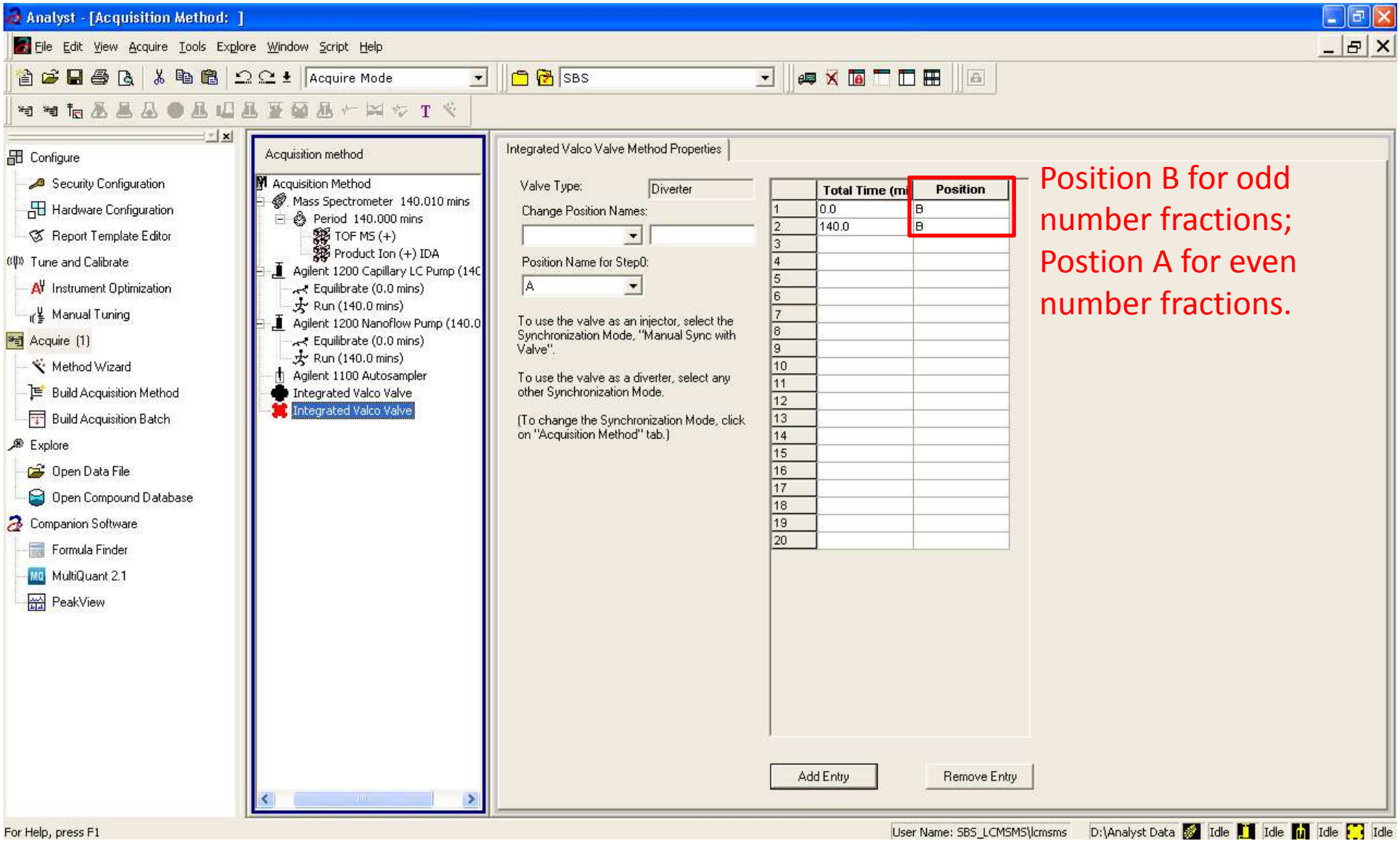
Autosampler method (3D 1000 mM)



V1 method


Analyst - [Acquisition Method:]
File Edit View Acquire Tools Explore Window Script Help
Acquire Mode
SBS
Configure
Security Configuration
Hardware Configuration
Report Template Editor
Tune and Calibrate
Instrument Optimization
Manual Tuning
Acquire (1)
Method Wizard
Build Acquisition Method
Build Acquisition Batch
Explore
Open Data File
Open Compound Database
Companion Software
Formula Finder
MultiQuant 2.1
PeakView
Acquisition method
Acquisition Method
Mass Spectrometer 140.010 mins
Period 140.000 mins
TOF MS (+)
Product Ion (+) IDA
Agilent 1200 Capillary LC Pump (140
Equilibrate (0.0 mins)
Run (140.0 mins)
Agilent 1200 Nanoflow Pump (140.0
Equilibrate (0.0 mins)
Run (140.0 mins)
Agilent 1100 Autosampler
Integrated Valco Valve
Integrated Valco Valve
Integrated Valco Valve Method Properties
Valve Type:
Diverter
Change Position Names:
Position Name for Step0:
A
To use the valve as an injector, select the Synchronization Mode, "Manual Sync with Valve".
To use the valve as a diverter, select any other Synchronization Mode.
(To change the Synchronization Mode, click on "Acquisition Method" tab.)
Total Time (mi
Position
1 0.0 A
2 1.0 B
3 6.0 A
4 30.0 B
5 140.0 A
Add Entry
Remove Entry
V1 method without fractionation
Total Time (mi
Position
1 0.0 A
2 1.0 B
3 139.0 B
4 140.0 A
For Help, press F1
User Name: SBS_LCMSMS\lcmsms
D:\Analyst Data
Idle
Idle
Idle
Idle

V2 method


Analyst - [Acquisition Method:]
File Edit View Acquire Tools Explore Window Script Help
Acquire Mode
SBS
Configure
Security Configuration
Hardware Configuration
Report Template Editor
Tune and Calibrate
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Formula Finder
MultiQuant 2.1
PeakView
Acquisition method
Acquisition Method
Mass Spectrometer 140.010 mins
Period 140.000 mins
TOF MS (+)
Product Ion (+) IDA
Agilent 1200 Capillary LC Pump (140
Equilibrate (0.0 mins)
Run (140.0 mins)
Agilent 1200 Nanoflow Pump (140.0
Equilibrate (0.0 mins)
Run (140.0 mins)
Agilent 1100 Autosampler
Integrated Valco Valve
Integrated Valco Valve
Integrated Valco Valve Method Properties
Valve Type:
Diverter
Change Position Names:
Position Name for Step0:
A
To use the valve as an injector, select the Synchronization Mode, "Manual Sync with Valve".
To use the valve as a diverter, select any other Synchronization Mode.
(To change the Synchronization Mode, click on "Acquisition Method" tab.)
Total Time (mi
Position
1 0.0 B
2 140.0 B
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
Add Entry
Remove Entry
Position B for odd number fractions; Postion A for even number fractions.
For Help, press F1
User Name: SBS_LCMSMS\lcmsms
D:\Analyst Data
Idle
Idle
Idle
Idle