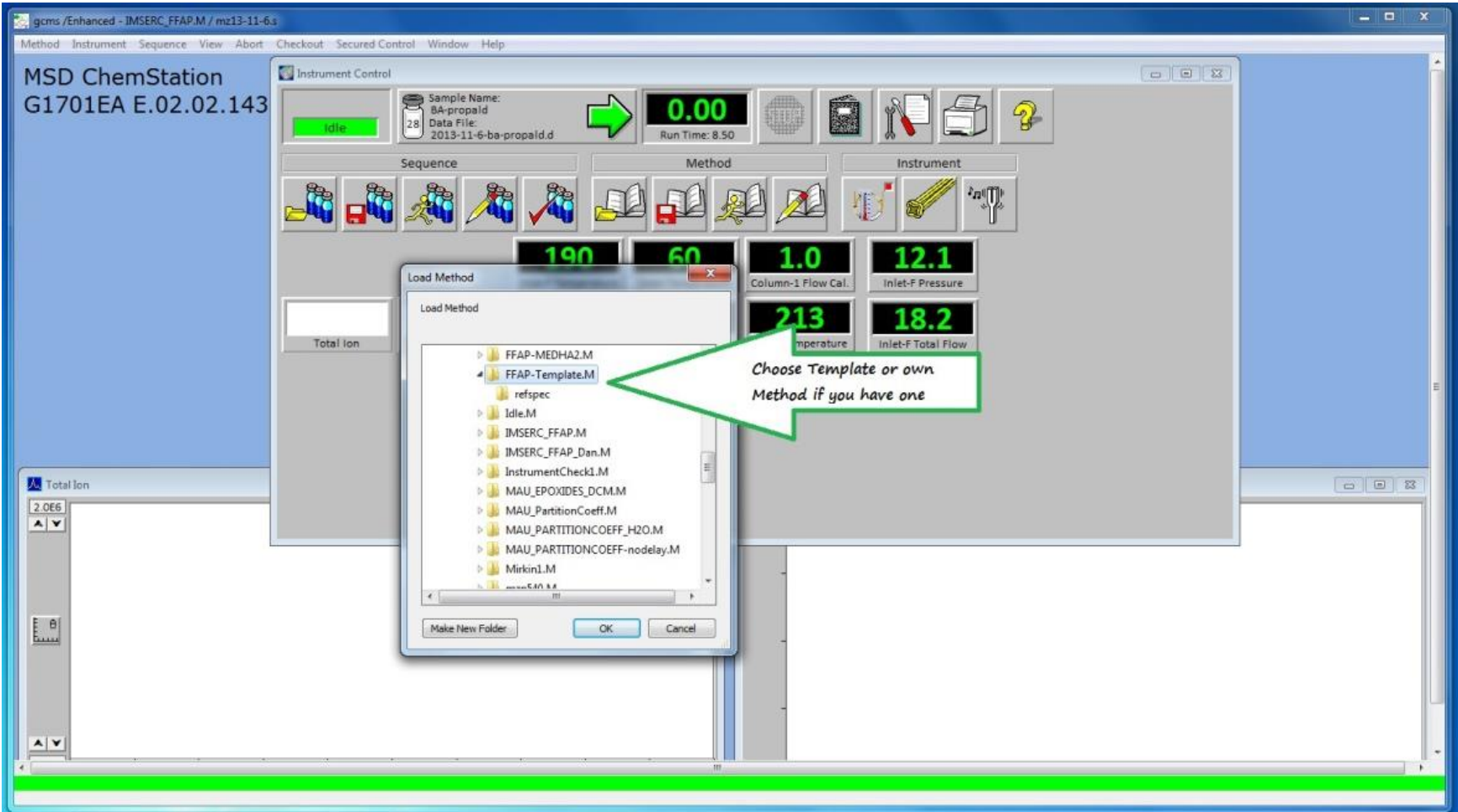


# **Agilent GC-MSD User Manual**

Owen Skinner November 2013





The screenshot displays the MSD ChemStation software interface. The main window is titled "MSD ChemStation G1701EA E.02.02.143" and includes a menu bar with options: Method, Instrument, Sequence, View, Abort, Checkout, Secured Control, Window, and Help.

The "Instrument Control" panel shows the following details:

- Sample Name: BA-propald
- Data File: 2013-11-6-ba-propald.d
- Run Time: 8:50
- Instrument Status: Idle

The "Method" section contains several parameters:

- Inlet-F Temperature: 230
- Oven Temperature: 50
- Column-1 Flow Cal.: 1.0
- MS Source: 230
- MS Quad: 150
- Aux-2 Temperature: 280

The "Instrument" section shows:

- Inlet-F Pressure: 11.6
- Inlet-F Total Flow: 18.2

A green arrow points to the "Edit Method" icon in the Method section, with a callout box containing the text "Select 'Edit Method'".

At the bottom of the interface, a status bar displays the message: "C:\MSDCHEM1\METHODS\FAP-TEMPLATE.M loaded!".

Two data plots are visible at the bottom of the window:

- Total Ion:** A plot with a y-axis ranging from 0.0E0 to 2.0E6 and an x-axis from 0.0 to 12.0. The plot area is currently blank.
- 1.0E5:** A plot with a y-axis ranging from 0.0E0 to 1.0E5 and an x-axis from 0.0 to 480. The plot area is currently blank.

The Windows taskbar at the bottom shows the system clock as 11:30 AM on 11/11/2013.

The screenshot displays the Agilent MSD ChemStation software interface. The main window is titled "MSD ChemStation G1701EA E.02.02.143". The "Instrument Control" panel shows the instrument status as "Idle" with a run time of 8.50. Key parameters are displayed: Inlet-F Temperature (230), Oven Temperature (50), Column-1 Flow Cal. (1.0), Inlet-F Pressure (11.6), and Inlet-F Total Flow (18.2). A "Total Ion" chromatogram is visible at the bottom left, showing a peak at 2.066 minutes. A dialog box titled "Edit Method" is open, with the "Instrument/Acquisition" section selected. A green arrow points to this section with the text "Only select Inst /Acq".

Method Sections to Edit:

- Method Information
- Instrument/Acquisition
- Data Analysis

Buttons: OK, Cancel, Help

Annotation: Only select Inst /Acq

gcms/Enhanced - FFAP-TEMPLATE.M / mz13-11-6.s

Method Instrument Sequence View Abort Checkout Secured Control Window Help

### MSD ChemStation G1701EA E.02.02.143

Instrument Control

Sample Name: BA-propald  
Data File: 2013-11-6-ba-propald.d  
Run Time: 8.50

Sequence Method Instrument

230 50 1.0

Total Ion Spectrum

Inlet and Injection Parameters

Sample Inlet: GC  
Injection Source: GC ALS  
 Use MS

Inlet Location:  Front  Rear  Duct

MS Connected to:  Front Inlet  Rear Inlet

OK Cancel Help

11.6 Inlet-F Pressure  
18.2 Inlet-F Total Flow

Total Ion

2.0E6

0.0E0 0.0 3.0 6.0 9.0 12.0 0.0E0 0.0 120 240 360 480

Confirm these settings and press "OK"

11:37 AM  
11/11/2013

The screenshot displays the GC Edit Parameters window with the following details:

- Graph:** A temperature ramp plot showing temperature (°C) on the y-axis (0 to 250) versus Run Time (min) on the x-axis (0 to 21). The temperature is constant at 50°C until 2 minutes, then ramps up to 230.0°C by 12 minutes, and remains constant thereafter.
- Method:** MSD Chem G1701EA B
- Injection Settings:**
  - Injection Volume: 1.0  $\mu\text{L}$
  - Solvent A Washes: 2
  - Solvent B Washes: 0
- Washes and Pumps:** Includes fields for Preinj and Postinj for Sample Washes and Solvent Pumps.

Hand-drawn annotations include:

- An arrow pointing to the **Injector** tab in the software interface.
- An arrow pointing to the **Injection Volume** field, with the text "Choose Injection Volume (1-5 uL)".
- An arrow pointing to the **Solvent A Washes** and **Solvent B Washes** fields, with the text "Choose Pre- and Post- inject needle washes of Solvent A (MeOH) and B (DCM)".

The screenshot displays the GC Edit Parameters window. At the top, a graph shows the oven temperature ramp over a 21-minute run time. The temperature starts at 50.0 °C, remains constant until 2 minutes, then ramps up to 230.0 °C by 12 minutes, and remains constant thereafter.

Below the graph, the 'Inlet' tab is selected, indicated by a callout arrow. The 'Front Inlet (Split/Splitless Inlet)' section shows the following parameters:

- Temperature: 230.0 °C
- Pressure: 11.6 psi
- Flow: 18.2 mL/min

The 'Split/Splitless Inlet' section is also visible, with the following settings:

- Mode: Split
- Split Ratio: 50.0 : 1 (circled with a callout arrow pointing to the text: "Choose split ratio (1.0-500). If unknown, start at 100")
- Gas Saver:  (After: 2.00 min)

At the bottom of the window, there are 'Apply', 'OK', and 'Cancel' buttons.



Method: Instrument: S...  
MSD Chem  
G1701EA E

Run Time, min

Oven Temperature: 50.0 °C  
Front Inlet (Split/Splitless Inlet):  
Temperature: 230.0 °C  
Pressure: 11.6 psi  
Flow: 18.2 mL/min

**Select "Oven"**

Oven	Rate °C/min	Value °C	Hold Time min	Run Time min
▶ (Initial)		50	2	2
Ramp 1	20	240	10	21.5
*				

**Change GC oven temperature curve here**

Post Run: 0 °C  
Post Run Time: 0.00 min

**Press "OK"**

Apply OK Cancel

11:39 AM  
11/11/2013

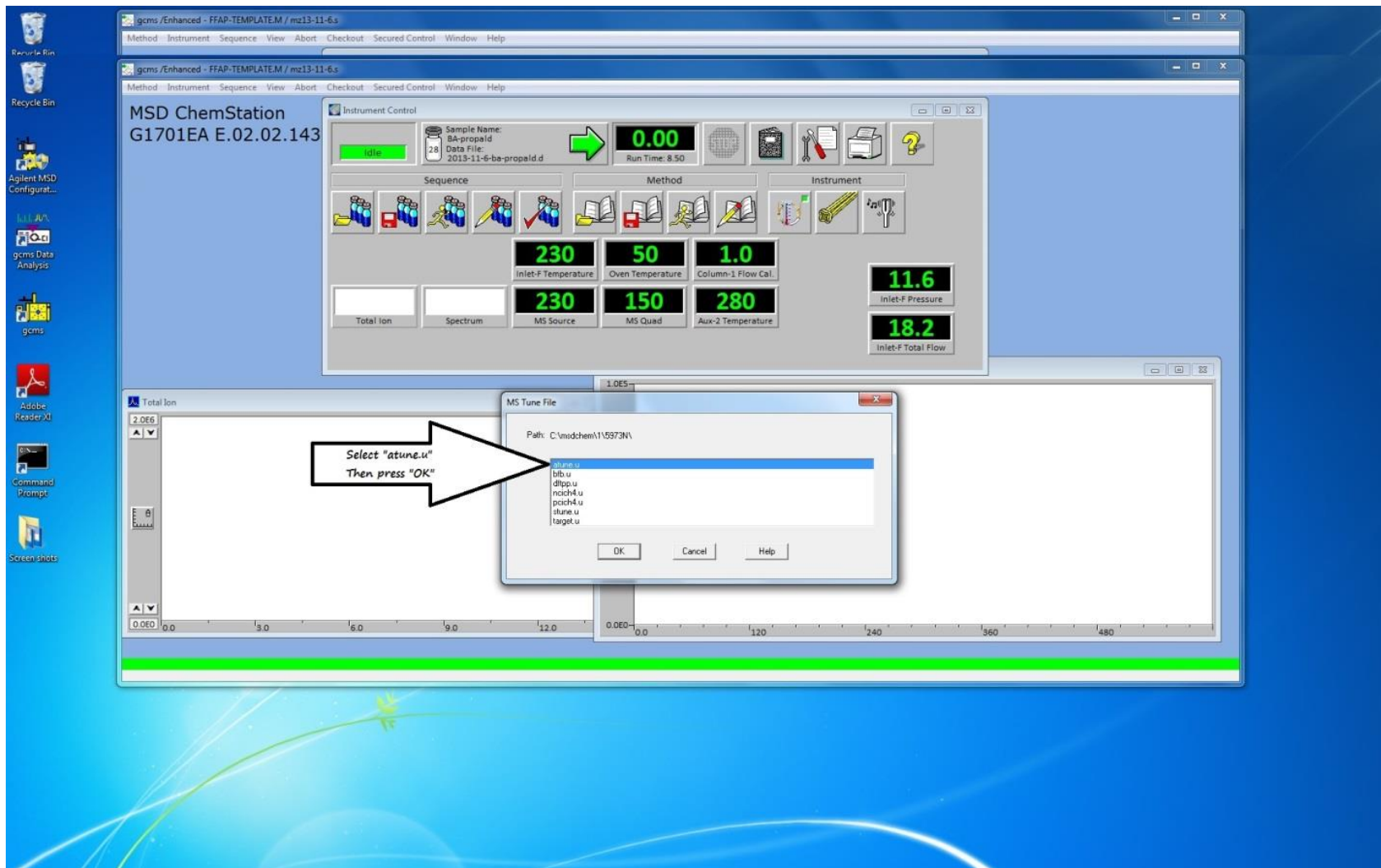
The screenshot displays the Agilent MSD ChemStation software interface. The main window is titled "MSD ChemStation G1701EA E.02.02.143". The "Instrument Control" panel shows the following parameters:

- Sample Name: BA-propald
- Data File: 2013-11-6-ba-propald.d
- Run Time: 8:50
- Inlet-F Temperature: 230
- Oven Temperature: 50
- Column-1 Flow Cal.: 1.0
- MS Source: 230
- MS Quad: 150
- Aux-2 Temperature: 280
- Inlet-F Pressure: 11.6
- Inlet-F Total Flow: 18.2

The "GC Detector Data" dialog box is open, showing settings for Signal 1 and Signal 2:

- Signal 1:  Display, Altr: 0 Z", Offset: 10 %, Time: 5.0 min
- Signal 2:  Display, Altr: 0 Z", Offset: 10 %, Time: 5.0 min

A white arrow points to the "OK" button in the dialog box with the text "Press 'OK'". The background shows a chromatogram plot with a y-axis labeled "Total Ion" and an x-axis with numerical values from 0.0 to 480. The system tray at the bottom right shows the date and time: 11:40 AM, 11/11/2013.

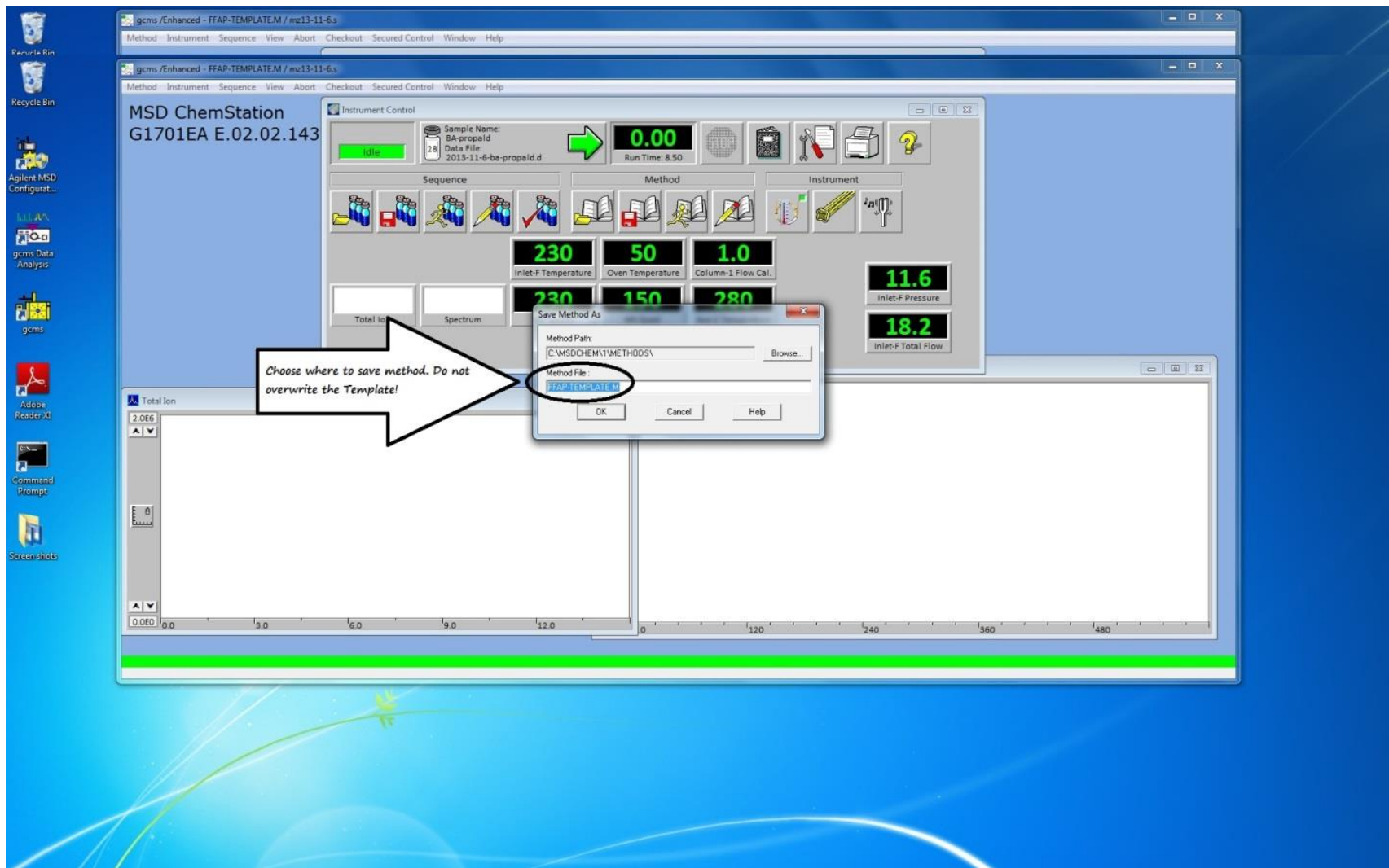


The screenshot displays the Agilent MSD ChemStation software interface. The main window shows the instrument status as "Idle" and a digital display showing "0.00". A dialog box titled "MS SIM/Scan Parameters" is open, with the "Solvent Delay" field set to "3.5" minutes. A green arrow points to the "0.00" display, and another green arrow points to the "Solvent Delay" field. A white arrow points to the "OK" button in the dialog box. The dialog box contains the following information:

- MS Instrument: Sample Inlet: GC
- Solvent Delay: 3.5 min
- EMV Mode: Gain Factor
- Gain Factor: 1.00 +1388 V
- Acq. Mode: Scan
- Real-Time Plot: Time Window: 15 min
- MS Window 1: Plot Type: Total, Y-Scale: 0 to 2000000
- MS Window 2: Plot Type: Spectrum, Y-Scale: 0 to 100000
- Tune File: atune.u
- Valid entries are values between 0.00 and 1440.00 minutes.
- Buttons: Scan Parameters, Zones, Timed Events, OK, Cancel, Help

Annotations include:

- A green arrow pointing to the "0.00" digital display.
- A white arrow pointing to the "Solvent Delay" field with the text "Verify 'Solvent Delay' Start at 3.5 mins".
- A white arrow pointing to the "OK" button with the text "Press 'OK'".



gcms/Enhanced - FFAP-TEMPLATE.M / mz13-11-6.1

Method Instrument Sequence View Abort Checkout Secured Control Window Help

### MSD ChemStation G1701EA E.02.02.143

Instrument Control

Sample Name: BA-propald  
Data File: 2013-11-6-ba-propald.d  
Run Time: 8.50

Idle

Sequence Method Instrument

Inlet-F Temperature: 230  
Oven Temperature: 50  
Column-1 Flow Cal.: 1.0

Total Ion Spectrum MS Source MS Quad Aux-2 Temperature

Inlet-F Pressure: 11.6  
Inlet-F Total Flow: 18.2

Total Ion

2.0E6  
0.0E0

0.0 3.0 6.0 9.0 12.0

1.0E5  
0.0E0

0.0 120 240 360 480

C:\MSDCHEM\1\METHODS\FFAP-TEMPLATE.M loaded!

11:30 AM  
11/11/2013

The screenshot displays the gcms software interface. The main window is titled "MSD ChemStation G1701EA E.02.02.143" and shows the "Instrument Control" panel. The instrument status is "Idle" with a green arrow and a digital display showing "0.00". The "Run Time" is 8.50. A "Load Sequence" dialog box is open, showing a list of sequences. A callout arrow points to the dialog with the text "Select the IMSERC Template or your own sequence if you have it".

**Load Sequence Dialog Box:**

Name	Date modified	Type
Andersen	8/30/2013 10:03 AM	File fol
Medha-Nov2013.s	11/5/2013 11:50 AM	S File
FFAP_Seq_Template.s	11/1/2013 11:22 AM	S File
FFAP-DanS.s	11/1/2013 1:07 PM	S File
C350.s	10/1/2013 1:21 PM	S File
Hupp-Ali.s	10/7/2013 3:11 PM	S File
Jewett	11/1/2013 11:18 AM	File fol
Marks	5/17/2013 1:11 PM	File fol
BFS.s	6/7/2013 2:24 PM	S File
Tyo	11/6/2013 1:16 PM	File fol
default.s	3/13/2013 12:56 PM	S File

File name: FFAP\_Seq\_Template  
Files of type: Custom (\*.S)  
 Open as read-only

**Instrument Control Panel:**

Sample Name: BA-propald  
Data File: 2013-11-6-ba-propald.d  
Run Time: 8.50

**Instrument Status:**

11.6 Inlet-F Pressure  
18.2 Inlet-F Total Flow

**Total Ion Plot:**

Y-axis: 2.0E6  
X-axis: 0.0 to 480

gcms/Enhanced - FFAP-TEMPLATE.M / mz13-11-6.s

Method Instrument Sequence View Abort Checkout Secured Control Window Help

### MSD ChemStation G1701EA E.02.02.143

Instrument Control

Sample Name: BA-propald  
Data File: 2013-11-6-ba-propald.d  
Run Time: 8.50

0.00

Sequence Method Instrument

**230** **50** **1.0**  
Inlet-F Temperature Oven Temperature Column-1 Flow Cal.

**230** **150** **280**  
MS Source MS Quad Aux-2 Temperature

**11.6**  
Inlet-F Pressure

**18.2**  
Inlet-F Total Flow

Total Ion Spectrum

Total Ion

2.0E6

0.0E0

0.0 3.0 6.0 9.0 12.0

1.0E5

0.0E0

0.0 120 240 360 480

C:\MSDCHEM\1\METHODS\FFAP-TEMPLATE.M loaded!

11:30 AM  
11/11/2013





gcms/Enhanced - FFAP-TEMPLATE.M / mz13-11-E.s  
Method Instrument Sequence View Abort Checkout Secured Control Window Help

gcms/Enhanced - FFAP-Template.M / FFAP\_Seq\_Template.s  
Method Instrument Sequence View Abort Checkout Secured Control Window Help

### MSD ChemStation G1701EA E.02.02.143

Instrument Control  
idle Sample Name: 8a-propald Data File: 2013-11-6-ba-propald.d Run Time: 8.50

Sample Log Table

Data Path: C:\MSDCHEM\1\DATA\IMSERC Method Path: C:\MSDCHEM\1\METHODS

Type	Vial	Sample	Method / Keyword	Data File	Comment / KeywordString	Multiplier	Level	Update RF
Blank	84	acetonitrile blank	IMSERC_FFAP_DAN	acetonitrile 11012013A	acetonitrile	1.00000	2	No Update
Blank	84	acetonitrile blank	IMSERC_FFAP_DAN	acetonitrile 11012013B	acetonitrile	1.00000	2	No Update
Sample	85	Test Mix	IMSERC_FFAP			1.00000	2	No Update

Select Data Path

- BFS
- C350
- evaldemo.d
- GCMS\_001.D
- GCMS\_002.D
- Hupp
- IMSERC
- InstrumentCheck
- Jewett
- Kelleher
- Layden
- Markis
- MAU

Make New Folder OK Cancel

Total Ion  
2.0E6  
0.0E0

The screenshot displays the Agilent ChemStation software interface. The main window is titled "MSD ChemStation G1701EA E.02.0". A dialog box is open, showing a table of methods. Handwritten annotations in black ink point to various fields in the dialog box:

- An arrow points to the "Sample Type (Blank or Sample)" dropdown menu.
- An arrow points to the "Sample name" field.
- An arrow points to the "Data file name (when saved)" field.
- An arrow points to the "Vial # of Sample" column header in the table.
- An arrow points to the "Method / Keyword" column header in the table.

The table in the dialog box contains the following data:

	Vial	Method / Keyword	Comment / KeywordString	Multiplier	Level	Update RF	
1	Blank	94 acetone/blank	IMSERC_FFAP_DAN	acetone/blank	1.00000 2	No Update	
2	Blank	94 acetone/blank	IMSERC_FFAP_DAN	acetone/blank	1.00000 2	No Update	
3	Sample	95 Test Mix	IMSERC_FFAP_DAN	TestMix_11012013	MethylSal and Camphor	1.00000 2	No Update
4							
5							
6							
7							
8							
9							
10							
11							
12							
13							
14							
15							
16							
17							
18							
19							
20							
21							
22							
23							

The dialog box also includes a "Run" button with a green arrow, a "Browse..." button, and "OK", "Cancel", and "Help" buttons at the bottom.

gcms /Enhanced - FFAP-TEMPLATE.M / m13-11-6.s

Method Instrument Sequence View Abort Checkout Secured Control Window Help

MSD ChemStation  
G1701EA E.02.02.143

Instrument Control

Sample Name: BA-propald  
Data File: 2013-11-6-ba-propald.d  
Run Time: 8:50

0.00

idle

Select "Run Sequence"

Sequence Method Instrument

Inlet-F Temperature: 230  
Oven Temperature: 50  
Column-1 Flow Cal.: 1.0

MS Source: 230  
MS Quad: 150  
Aux-2 Temperature: 280

Inlet-F Pressure: 11.6  
Inlet-F Total Flow: 18.2

Total Ion

1.0E5

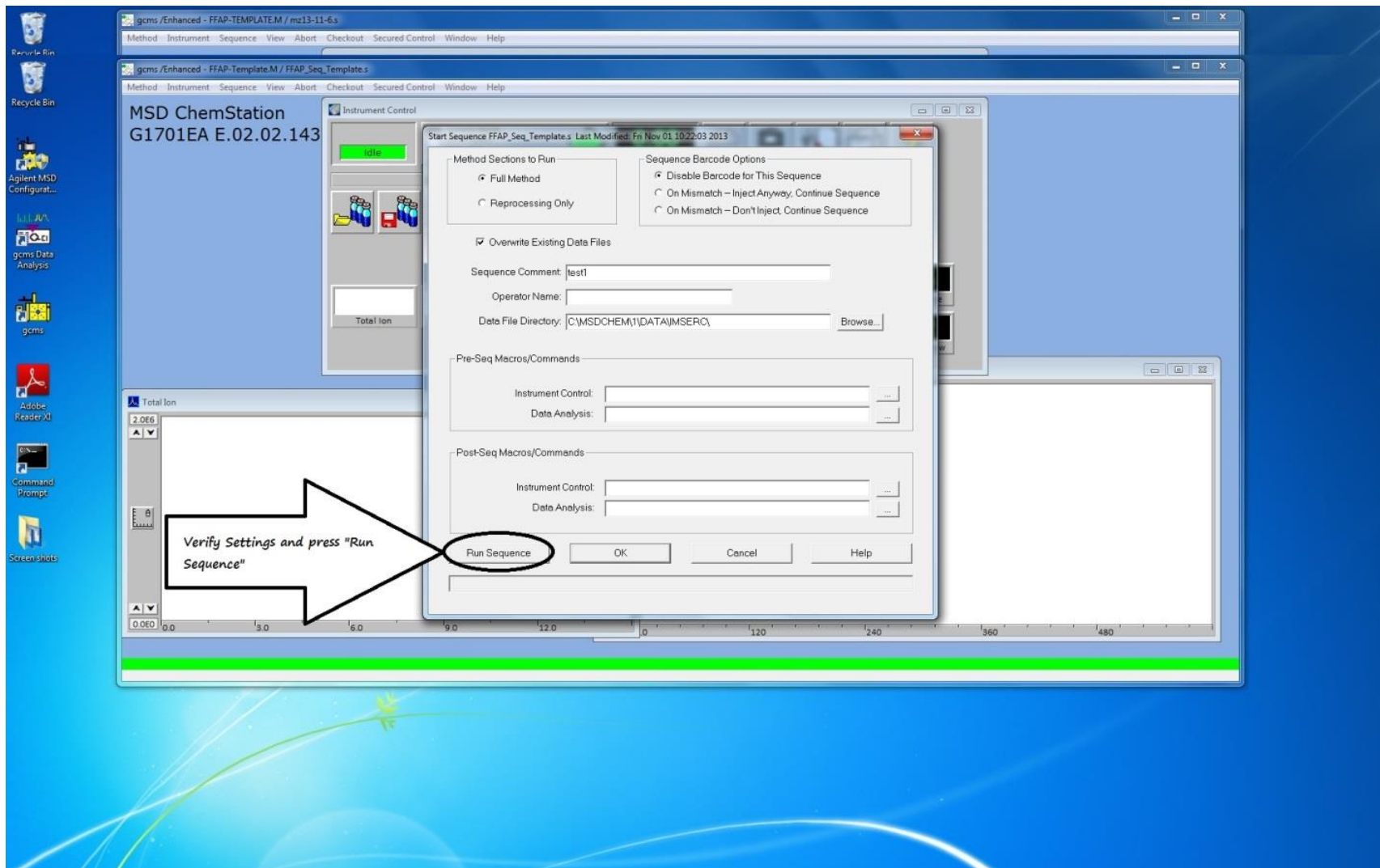
0.0E0

0.0 3.0 6.0 9.0 12.0

0.0 120 240 360 480

C:\MSDCHEM\1\METHODS\FFAP-TEMPLATE.M loaded!

11:30 AM  
11/11/2013



Recycle Bin

Agilent MSD Configur...

gcms Data Analysis

gcms

Adobe Reader

Command Prompt

Screen shots

Acquisition

Override solvent delay (3.50 minutes)?  
Warning: Overriding solvent delay may shorten filament lifetime.

Yes No

Instrument Control

Sample Name: RDK-01-162  
Data File: rdk-01-162\_1.d

0.19  
Run Time: 10.00

STOP

Never override solvent delay:  
Press "No" or do nothing

Inlet-F Temperature: 150  
Oven Temperature: 60  
Column-1 Flow Cal.: 0.9

MS Source: 230  
MS Quad: 150  
Aux-2 Temperature: 280

Inlet-F Pressure: 12.0  
Inlet-F Total Flow: 50.4

Total Ion

2.0E6

Sequence Status: RDK\_sample

Running: 3 of 3 Vial: 99 C:\MSDCHEM\1\DATA\MSRVC\RDK-01-162\_1.D Edit Data Analysis Pause

The injection is done

11:29 AM 11/14/2013