

GCMSsolution

# AOC-6000 Control Software

## Instruction Manual

Read the manual thoroughly before you use the product.

Keep this manual for future reference.

This page is intentionally left blank.

# Introduction

Read this Instruction Manual thoroughly before using the product.

Thank you for purchasing Shimadzu analytical instrument workstation AOC-6000 Software for GCMSsolution.

This manual describes the procedures for operating this product. Read this manual thoroughly before using the product and operate the product in accordance with the instructions in this manual.

Also, keep this manual for future reference.

This manual assumes that the reader is knowledgeable of basic operations of Windows. For the operation of Windows, refer to the instruction manual that comes with that product.

## Important

- If the user or installation location changes, ensure that this Instruction Manual is transferred with the product.
- If this manual is lost or damaged, immediately contact your Shimadzu representative to request a replacement.
- To ensure safe operation, contact your Shimadzu representative for product installation, adjustment, or reinstallation (after the product is moved).

## Notice

- Information in this manual is subject to change without notice and does not represent a commitment on the part of the vendor.
- Any errors or omissions which may have occurred in this manual despite the utmost care taken in its production will be corrected as soon as possible, although not necessarily immediately after detection.
- All rights are reserved, including those to reproduce this manual or parts thereof in any form without written permission from Shimadzu Corporation.
- Microsoft and Windows are registered trademarks of Microsoft Corporation in the United States and/or other countries. Other company names and product names mentioned in this manual are trademarks or registered trademarks of their respective companies. The TM and ® symbols are omitted in this manual.
- Microsoft Windows 10 Operating System is referred to as "Windows 10".

© 2016-2022 Shimadzu Corporation. All rights reserved.

Original version is approved in English.

# Warranty

Shimadzu provides the following warranty for this product.

- 1. Period:** Please contact your Shimadzu representative for information about the period of this warranty.
- 2. Description:** If a product/part failure occurs for reasons attributable to Shimadzu during the warranty period, Shimadzu will repair or replace the product/part free of charge (including USB dongles). However, in the case of products which are usually available on the market only for a short time, such as personal computers and their peripherals/parts, Shimadzu may not be able to provide identical replacement products.
- 3. Limitation of Liability**
  1. In no event will Shimadzu be liable for any lost revenue, profit or data, or for special, indirect, consequential, incidental or punitive damages, however caused regardless of the theory of liability, arising out of or related to the use of or inability to use the product, even if Shimadzu has been advised of the possibility of such damage.
  2. In no event will Shimadzu's liability to you, whether in contract, tort (including negligence), or otherwise, exceed the amount you paid for the product.
- 4. Exceptions:** Failures caused by the following are excluded from the warranty, even if they occur during the warranty period.
  1. Improper product handling
  2. Repairs or modifications performed by parties other than Shimadzu or Shimadzu designated companies
  3. Product use in combination with hardware or software other than that designated by Shimadzu
  4. Computer viruses leading to device failures and damage to data and software, including the product's basic software
  5. Power failures, including power outages and sudden voltage drops, leading to device failures and damage to data and software, including the product's basic software
  6. Turning OFF the product without following the proper shutdown procedure leading to device failures and damage to data and software, including the product's basic software
  7. Reasons unrelated to the product itself
  8. Product use in harsh environments, such as those subject to high temperatures or humidity levels, corrosive gases, or strong vibrations
  9. Fires, earthquakes, or any other act of nature, contamination by radioactive or hazardous substances, or any other force majeure event, including wars, riots, and crimes
  10. Product movement or transportation after installation
  11. Consumable items

Note: Recording media such as CD-ROMs are considered consumable items.

- If there is a document such as a warranty provided with the product, or there is a separate contract agreed upon that includes warranty conditions, the provisions of those documents shall apply.
- Warranty periods for products with special specifications and systems are provided separately.

## Indications Used in This Instruction Manual

Warnings, Cautions and Notes are indicated using the following conventions, and the following symbols are used in this manual:

Indication	Meaning
 <b>CAUTION</b>	Indicates a potentially hazardous situation which, if not avoided, may result in minor to moderate injury or equipment damage.
 <b>NOTE</b>	Emphasizes additional information that is provided to ensure the proper use of this product.
 <b>Reference</b>	Indicates the location of related reference information.
[ ]	Indicates the names of buttons, menu options, setting options, windows/sub-windows, and icons that are displayed in a window.  Example: Click [OK].

# Contents

1	Description.....	1
2	Installing .....	2
2.1	Installing the Software .....	2
2.2	Uninstalling the Software.....	6
3	Initial Setting.....	8
3.1	Connecting AOC-6000 Series with a Computer.....	8
3.2	Setting the Configuration.....	9
3.3	Changing the Ready Signal Setting .....	13
3.4	Changing the Style of Batch Tables.....	14
3.5	When the AOC-6000 Series Configuration Is Changed.....	17
3.5.1	Changing a Syringe Tool .....	17
3.5.2	Change a Tray Type .....	17
4	Method Settings .....	19
4.1	Setting AOC-6000 Parameters.....	19
4.2	Printing AOC-6000 Parameters.....	23
4.2.1	Printing from the [GCMS Real Time Analysis] Program.....	23
4.2.2	Printing from the [GCMS Postrun Analysis] Program.....	24
5	Measuring Samples.....	26
6	Measuring a Series of Samples Continuously .....	29
7	Advanced Operations.....	32
7.1	Confirming the Tray Name .....	32
7.2	Confirming the Location Where AOC-6000 Methods Are Saved.....	34
7.3	Protecting Method Files and AOC-6000 Methods.....	35
7.4	Checking Programs .....	36
8	Troubleshooting.....	38
8.1	Connection to the AOC-6000 Series Failed .....	38
8.2	Data Acquisition Does Not Start.....	38
8.3	AOC-6000 Series Status Remains [Run] .....	42

# Contents

Appendix – Method Parameters for Each Injection Method .....	43
AOC-6000 Method List .....	44
Parameter Groups .....	44
Method Parameters for Liquid Injection Methods .....	45
Method Parameters for Headspace Methods .....	50
Method Parameters for SPME Methods .....	54
Method Parameters for SPME Arrow Methods.....	58
Method Parameters for ITEX Methods .....	61

This page is intentionally left blank.

# 1 Description

This software installs Instrument Control Solution. Instrument Control Solution enables method development and analysis using the AOC-6000 Series (AOC-6000 Plus, AOC-6000) with GCMSsolution.

## NOTE

- This software can be used in the following instrument environment. This software requires the same computer environment as GCMSsolution.

Sampler:	AOC-6000 Plus, AOC-6000
GC-MS:	GCMS-NX Series, GCMS-QP2020, GCMS-QP2010 Series, GCMS-TQ Series
Workstation:	GCMSsolution Ver. 4.30 or later
OS:	Windows 10 Professional 64bit or Microsoft Windows 7 Professional SP1 .NET Framework 4
Firmware:	Refer to the table below.

Correspondence table between AOC-6000 Control Software, Instrument Control Solution, and Firmware  
(✓:Compatible, -:Not compatible)

AOC-6000 Control Software	Instrument Control Solution	Firmware				
		AOC-6000			AOC-6000 Plus	
		2.1.3	2.2.8	2.3.7	3.1.6.2	3.1.6.3
Ver. 1.0	3.0.143.0	✓	-	-	-	-
Ver. 1.1	3.0.158.0	-	✓	-	-	-
Ver. 1.2	3.1.31.0	-	✓	-	-	-
Ver. 1.3	3.1.31.0	-	-	✓	-	-
Ver. 2.0	3.2.2.0	-	-	✓	✓	✓
Ver. 2.1	3.2.3.1	✓	✓	-	-	-
	3.2.4.0	-	-	✓	✓	✓

- Ecology mode, which saves electric power and carrier gas during idle time, is not applicable for AOC-6000 Series. Please set a temperature of a syringe, an agitator, the SPME fiber conditioning during idle time, "Standby Temperature", in the PAL terminal of AOC-6000 Series.
- Controlling the AOC-6000 Series increases the load on the computer. When using the AOC-6000 Series continuously, reboot the computer approximately once every two weeks.

# 2 Installing



### NOTE

GCMSSolution Ver. 4.30 or later must already be installed and firmware of AOC-6000 Series must already be updated to the version described in "1. Description" before the AOC-6000 software is installed.

This software and the AOC-5000 Plus control software cannot be installed on one computer. If the AOC-5000 Plus control software is installed, uninstall it and then install this software.

When using a computer on which .NET Framework has not been installed, the installation program of this software automatically installs .NET Framework. It is not necessary to perform a procedure to install .NET Framework separately.

Also, the software will not run by simply copying the contents of the CD-ROM to the computer hard drive. Be sure to install the software using the proper method.

## 2.1 Installing the Software

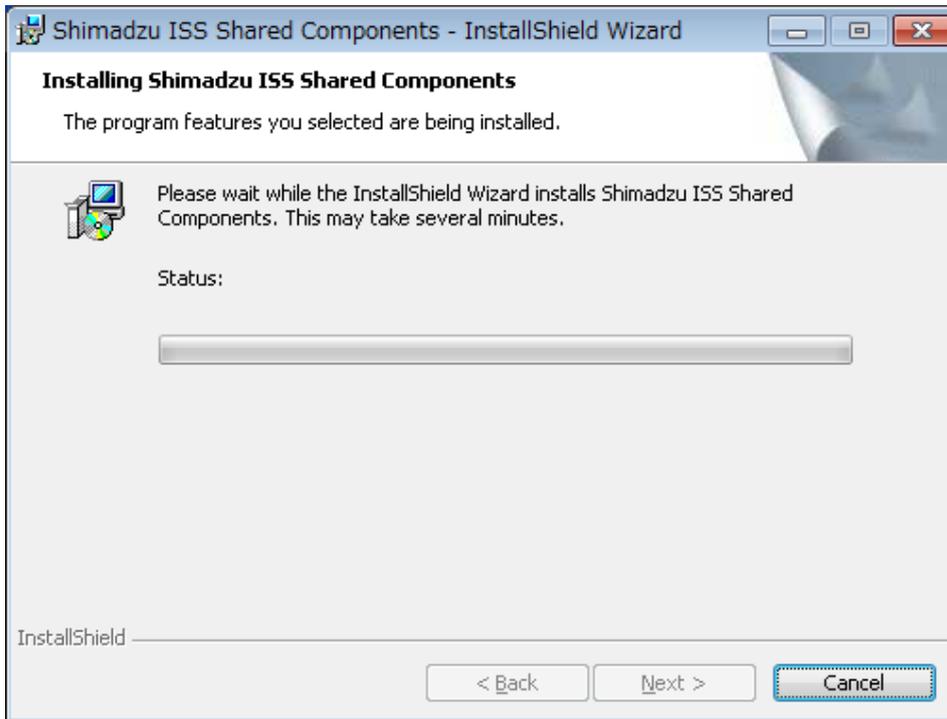
- 1) Exit the GCMSSolution.
- 2) Insert AOC-6000 control software installation disk into the CD-ROM drive. This automatically starts the installation program. If the "Do you want the following program to allow changes to this computer?" message appears, click [Continue].



### NOTE

- If the installation program does not start, click [Start] on the taskbar, point to [All Programs] and [Accessories], and click [Run].
- In the [Run] sub-window that is displayed, enter "E:\AUTORUN.EXE" in the [Open] text box, then click [OK]. (Specify the applicable CD-ROM drive for the "E:" portion.)

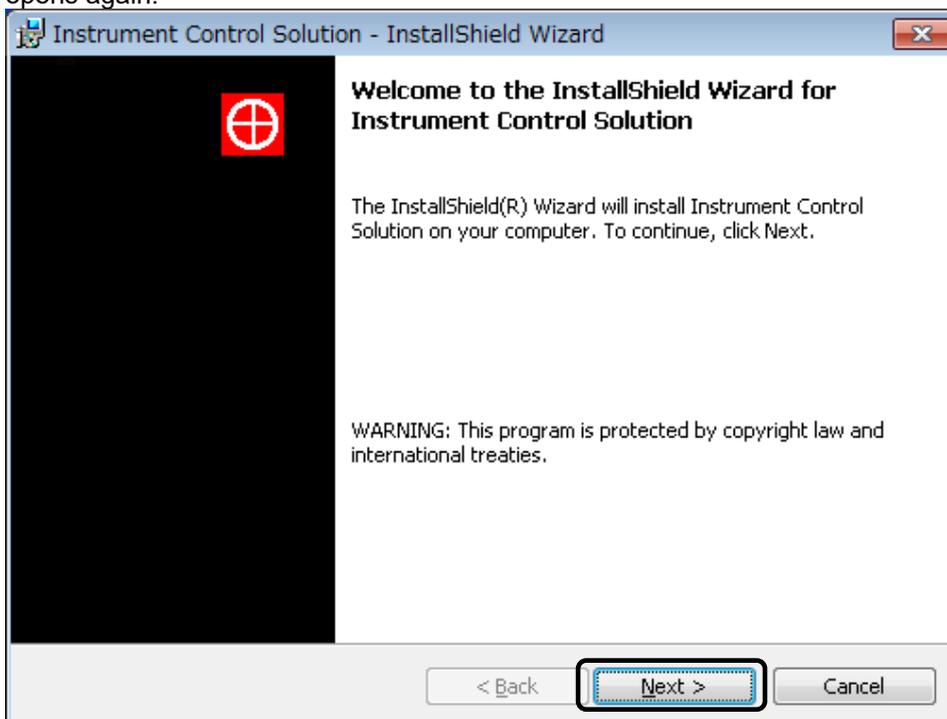
- 3) The [Shimadzu ISS Shared Components] program is automatically installed.



 **NOTE**

It takes a while to install the [Shimadzu ISS Shared Components] program. Do not click the [Cancel] button during installation.

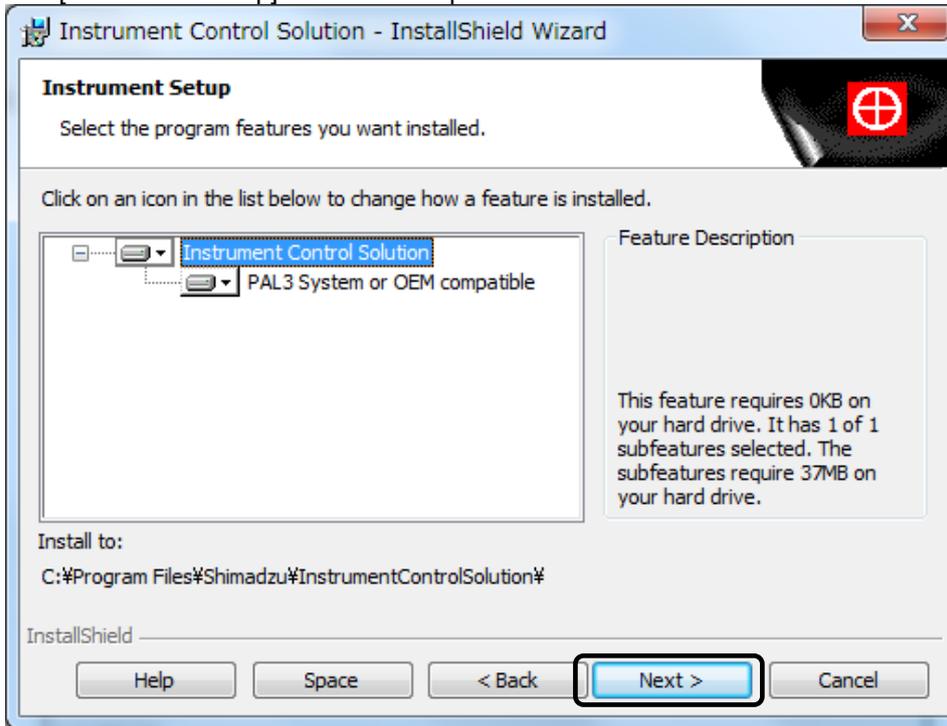
After a while, the [Welcome to the InstallShield Wizard for Instrument Control Solution] sub-window opens again.



## 2 Installing

---

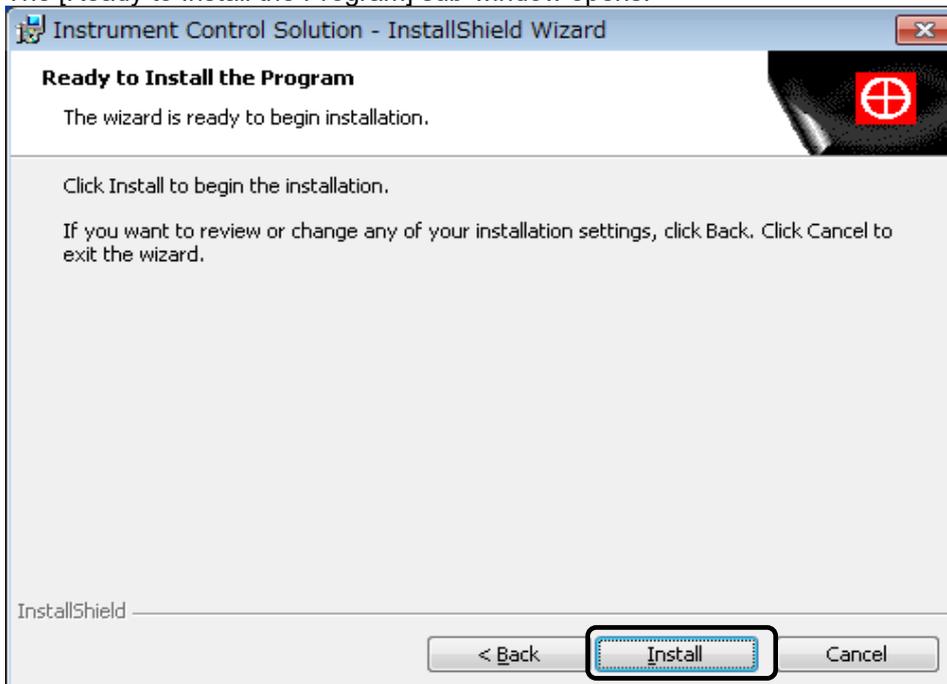
- 4) Click [Next >].  
The [Instrument Setup] sub-window opens.



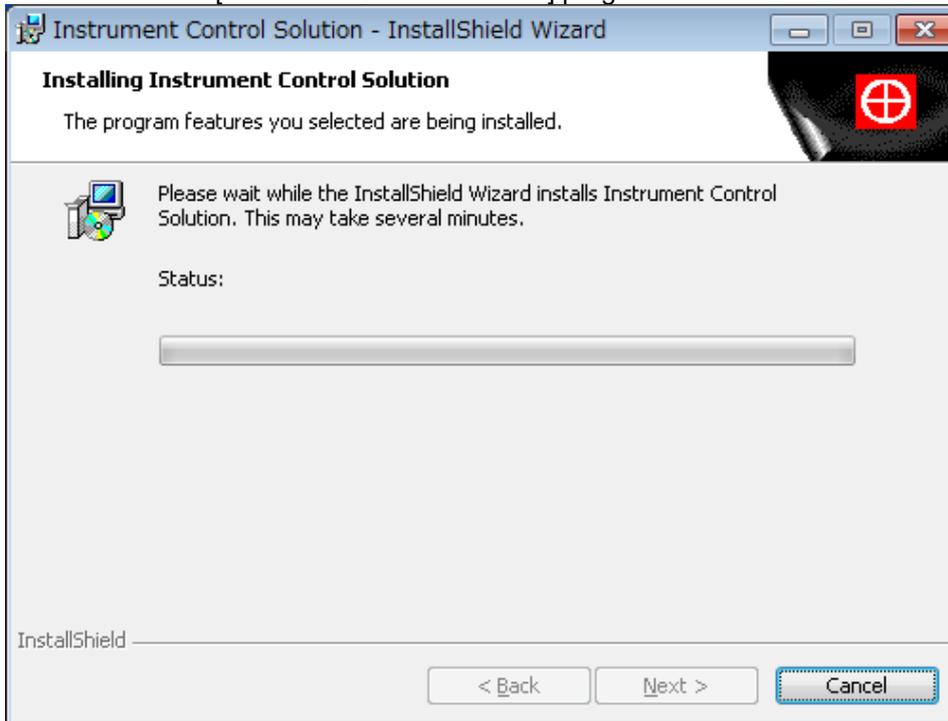
### NOTE

Do not change the settings in this sub-window.

- 5) Click [Next >].  
The [Ready to Install the Program] sub-window opens.



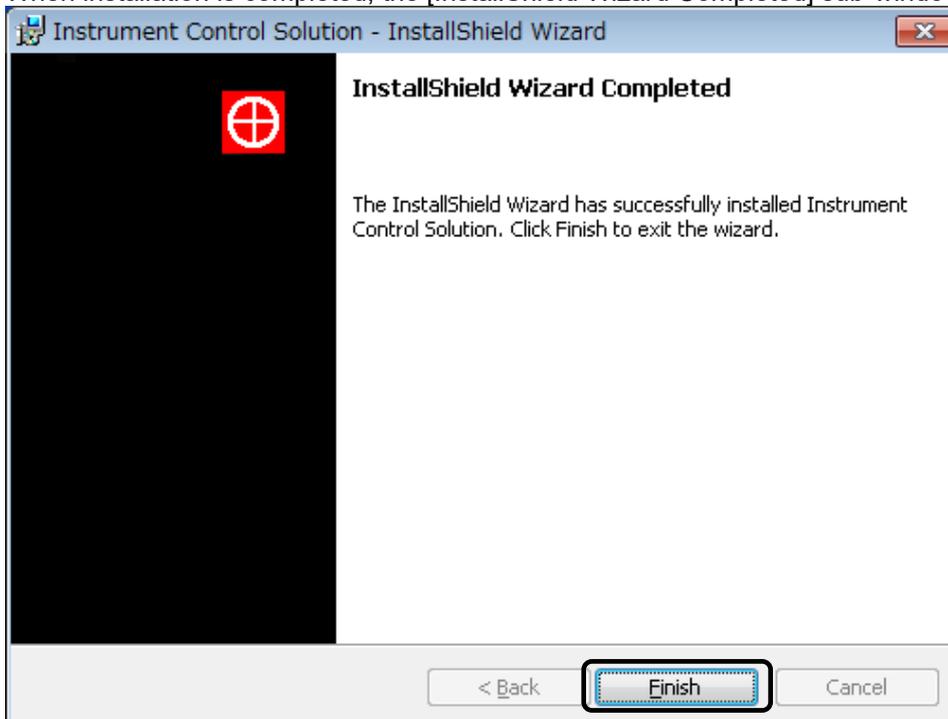
- 6) Click [Install].  
Installation of the [Instrument Control Solution] program starts.



 **NOTE**

It takes a while to install the [Instrument Control Solution] program.

When installation is completed, the [InstallShield Wizard Completed] sub-window opens.

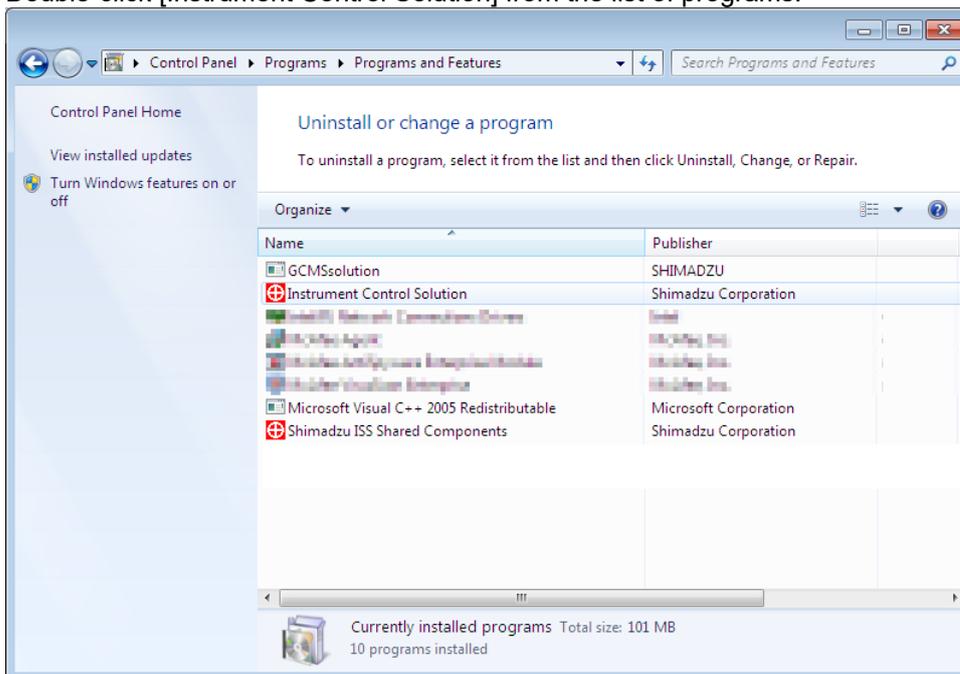


- 7) After confirming that "InstallShield Wizard Completed" is displayed, Click [Finish].

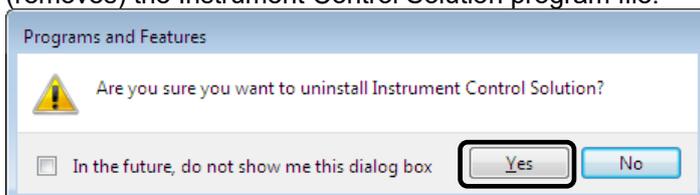
### 2.2 Uninstalling the Software

When uninstalling AOC-6000 control software, be sure to uninstall 2 programs.

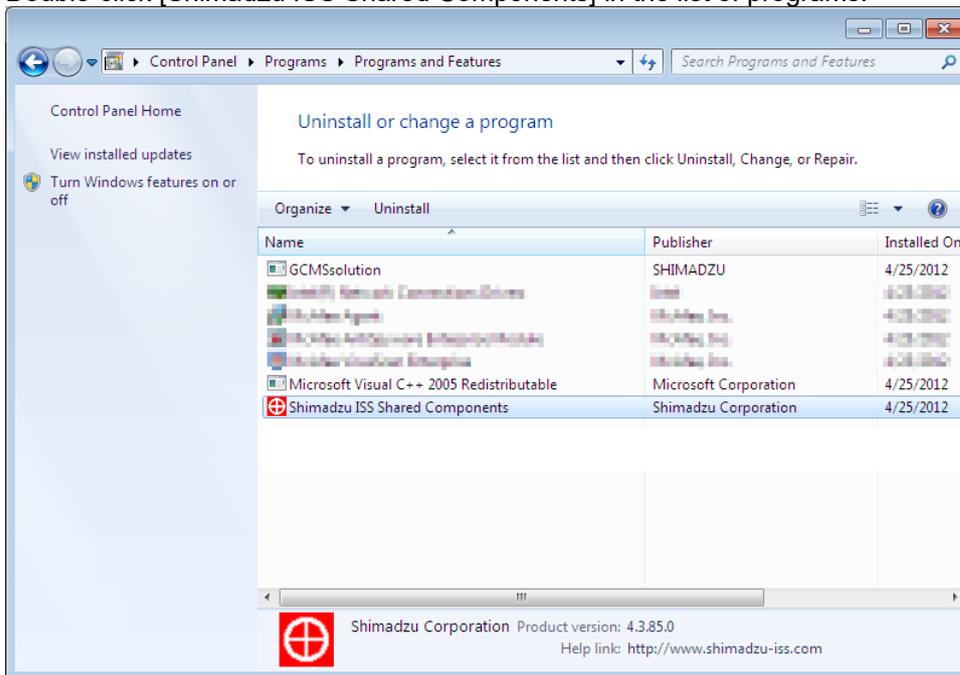
- 1) Select [Control Panel] on the [Start] menu.  
The [Control Panel] sub-window opens.
- 2) Click [Programs and Features].
- 3) Double-click [Instrument Control Solution] from the list of programs.



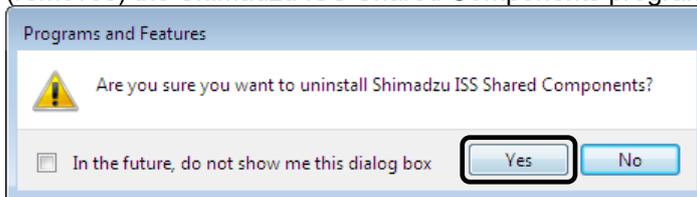
- 4) A message appears to confirm uninstalling (removing) the program. Clicking [Yes] uninstalls (removes) the Instrument Control Solution program file.



- 5) Double-click [Shimadzu ISS Shared Components] in the list of programs.



- 6) A message appears to confirm uninstalling (removing) the program. Clicking [Yes] uninstalls (removes) the Shimadzu ISS Shared Components program file.



# 3 Initial Setting

## 3.1 Connecting AOC-6000 Series with a Computer

Connect the AOC-6000 Series with a computer via Ethernet using a LAN cable.

 **NOTE**

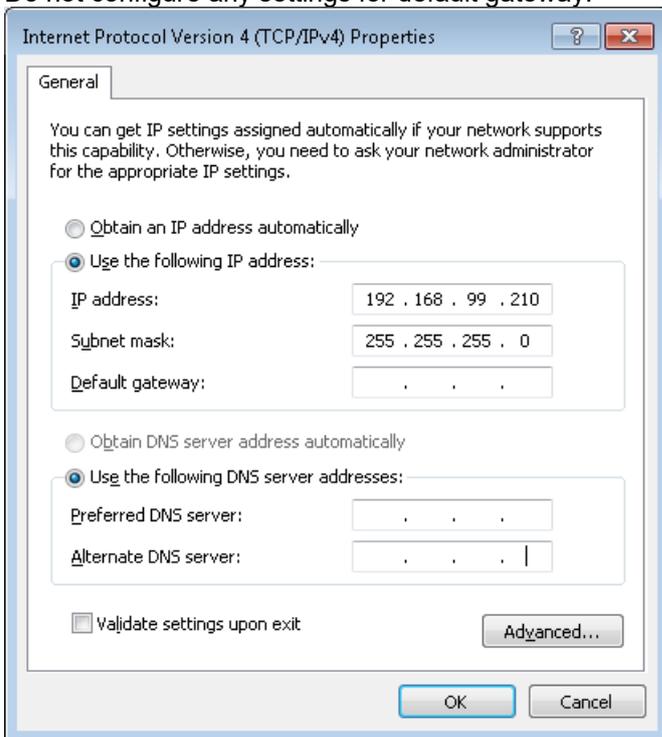
- If the computer is not connected to the backbone LAN, setting the following IP addresses is recommended.

	AOC-6000 Series	Computer
<b>IP Address</b>	192.168.99.230	192.168.99.210
<b>Subnet Mask</b>	255.255.255.0	255.255.255.0
<b>Default Gateway</b>	No setting	No setting

- For the connection to the backbone LAN, the IP address, subnet mask, and default gateway need to be set. For their settings, consult with the network administrator.

Below is the procedure to directly connect the AOC-6000 Series with a computer (peer-to-peer connection).

- 1) Switch the AOC-6000 Series power ON. Wait until the LED on the AOC-6000 Series turns green and the PAL terminal presents the initial display.
- 2) Connect the AOC-6000 Series and a computer using the provided LAN cable (crossover cable).
- 3) Configure LAN settings on the computer.  
Select [Internet Protocol Version 4 (TCP/IPv4)] from [Local Area Connection] and click [Properties].  
Do not configure any settings for default gateway.



## 3.2 Setting the Configuration

Make the following settings to enable controlling the AOC-6000 Series from GCMSsolution.

### NOTE

- Be sure to set configuration settings before using the AOC-6000 Series for the first time. As long as the AOC-6000 Series system configuration is not changed, these settings do not need to be changed each time.



- 1) Double-click the  (GCMS Real Time Analysis) icon on the desktop. The [Login] sub-window opens.
- 2) Set the user ID and password, and click [OK]. The [GCMS Real Time Analysis] program starts up.

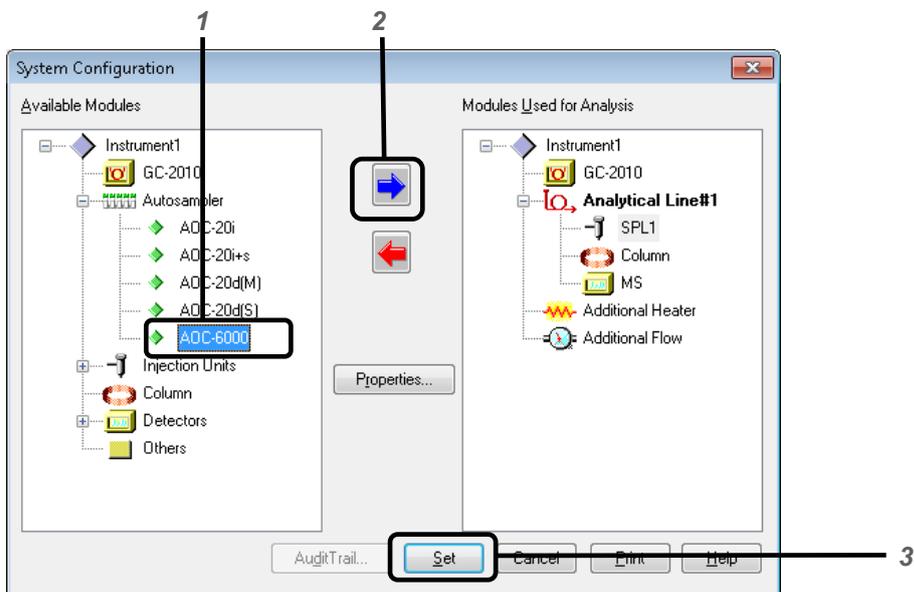


- 3) Click the [System Configuration] icon on the [Real Time] assistant bar. The [System Configuration] sub-window opens.



### 3 Initial Setting

- 4) Add AOC-6000 to [Modules Used for Analysis].



- 1 Select [AOC-6000] at [Available Modules].

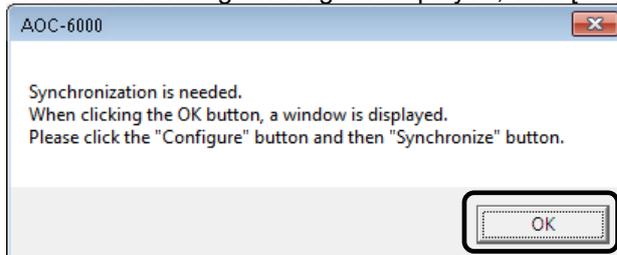


#### NOTE

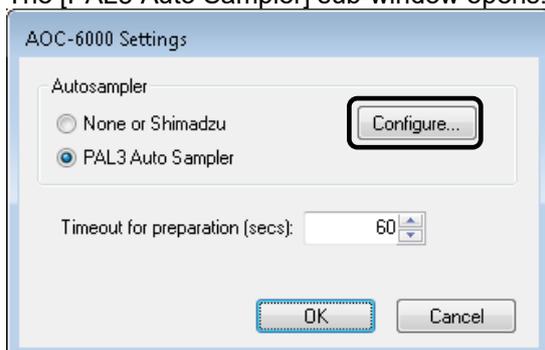
AOC-6000 can be selected only when the AOC-6000 control software has been installed.

- 2 Click  to add AOC-6000 to [Modules Used for Analysis].
- 3 Click [Set].  
The [System Configuration] sub-window closes.

- 5) When the following message is displayed, click [OK].



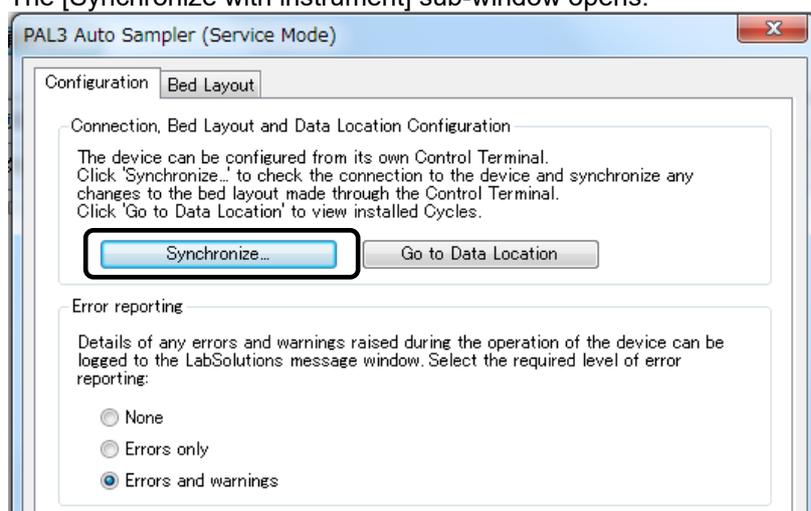
- 6) The [AOC-6000 Settings] sub-window opens. Click [Configure].  
The [PAL3 Auto Sampler] sub-window opens.



**NOTE**

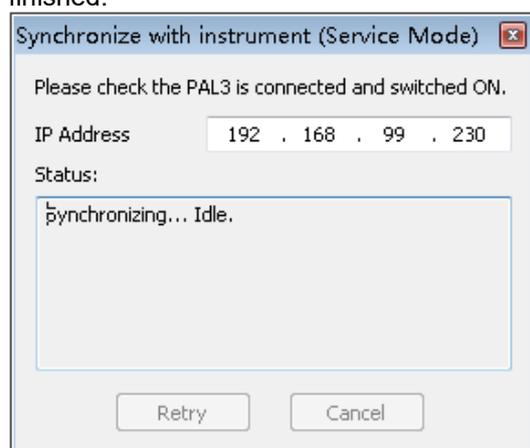
Do not change the initial [Autosampler] and [Timeout for preparation] settings. The initial settings are [PAL3 Auto Sampler] and [60], respectively.

- 7) Click [Synchronize] on the [Configuration] tab page.  
The [Synchronize with instrument] sub-window opens.

**NOTE**

Select the [Errors and warnings] at the [Error reporting] in the [PAL3 Auto Sampler] sub-window. When not selected, it may cause that error and warning log is not saved correctly and data measurement doesn't stop.

- 8) This sub-window automatically closes when communication with the AOC-6000 Series is successfully finished.

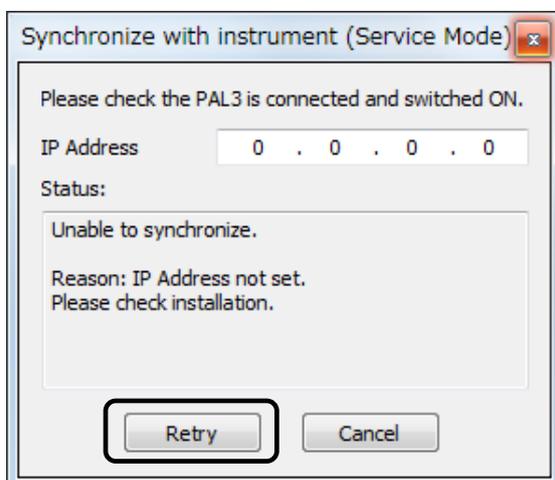


### 3 Initial Setting

---

 **NOTE**

If communication to the AOC-6000 Series cannot be established, [IP Address] may be set. Enter the IP address set for the AOC-6000 Series unit (see NOTE in 3.1) and click [Retry]. For the procedure to set/check the IP address of the AOC-6000 Series unit, refer to the PAL3 RTC/RSI User Manual.



- 9) Click [OK] in the [PAL3 Auto Sampler] sub-window.
- 10) Click [OK] in the [Edit AOC-6000 Config] sub-window.
- 11) Confirm the AOC-6000 status in the instrument monitor.

 **NOTE**

It takes about one minute for the status to change to [Ready].



 **NOTE**

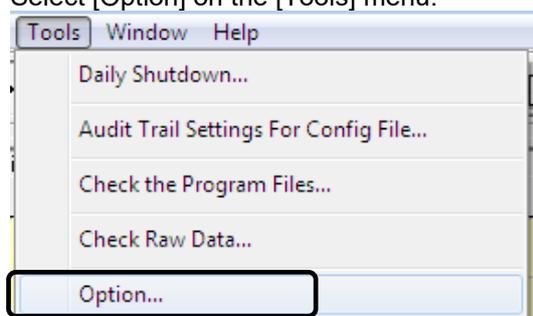
If the [Synchronize] button is clicked without switching the AOC-6000 Series power ON, an error is displayed in the [Synchronize with instrument] sub-window. If that occurs, follow the procedure below.

- 1 Switch the AOC-6000 Series power ON. Wait until the LED on the AOC-6000 Series turns green and the PAL terminal presents the initial display.
- 2 Click [Retry] in the [Synchronize with instrument] sub-window.

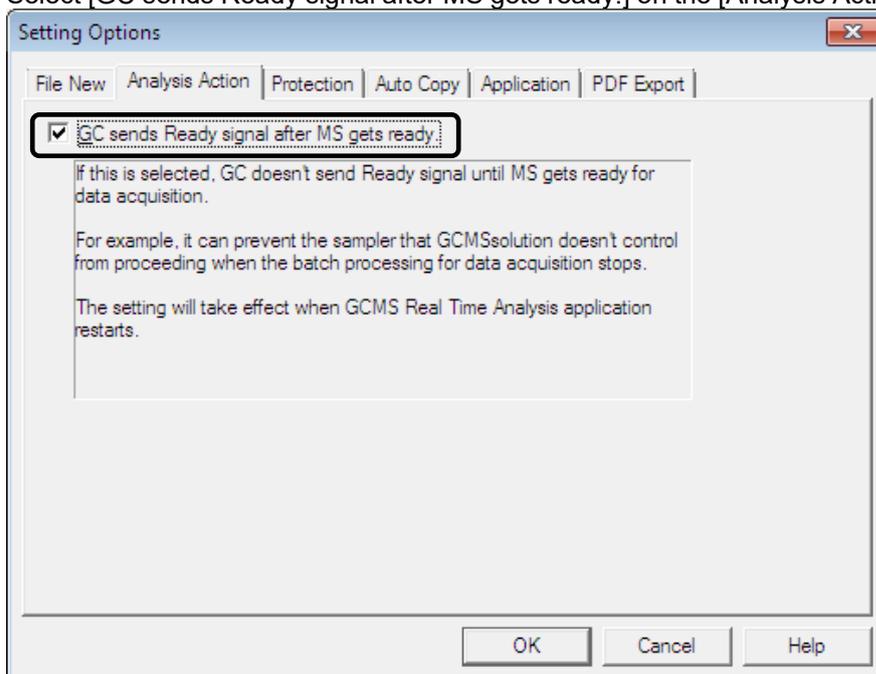
### 3.3 Changing the Ready Signal Setting

If an error occurs in the GC/MS system, the GC Ready signal is controlled to prevent the AOC-6000 Series from injecting subsequent samples into the GC unit.

- Open the [Acquisition] window from the [GCMS Real Time Analysis] program.
- Select [Option] on the [Tools] menu.



- Select [GC sends Ready signal after MS gets ready.] on the [Analysis Action] tab page, and click [OK].

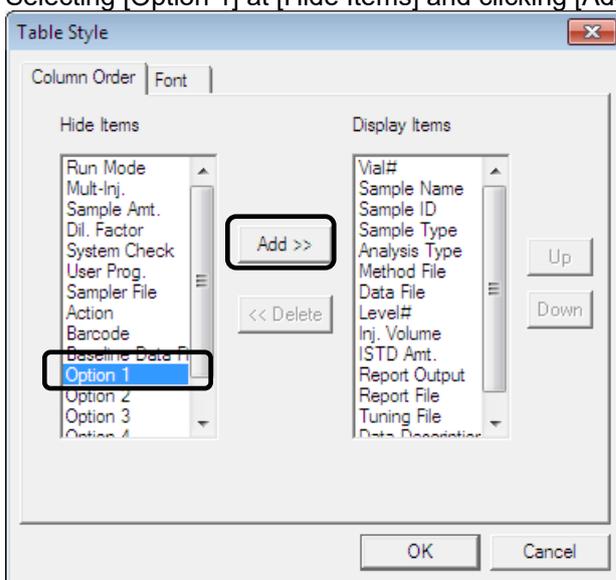


- Restart the [GCMS Real Time Analysis] program.

#### 3.4 Changing the Style of Batch Tables

To use the AOC-6000 Series for continuous data acquisition requires setting the tray names in a Batch Table. In default GCMSsolution settings, the column for setting tray names is not displayed. This section describes how to display a tray name column in a Batch Table and save the Batch Table as a template, then use that template for creating new batch files.

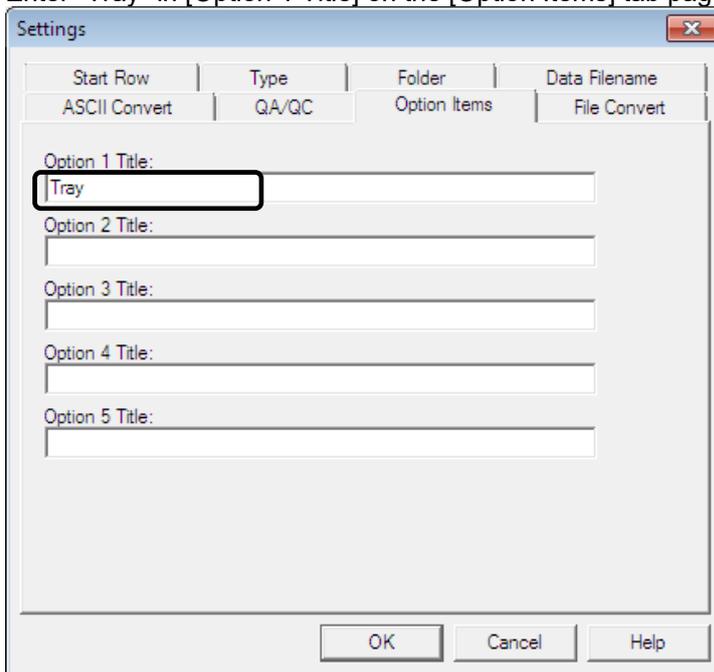
- 1) Right-click on the Batch Table, and click [Table Style] on the popup menu. The [Table Style] sub-window opens.
- 2) Selecting [Option 1] at [Hide Items] and clicking [Add >>] moves [Option 1] to [Display Items].



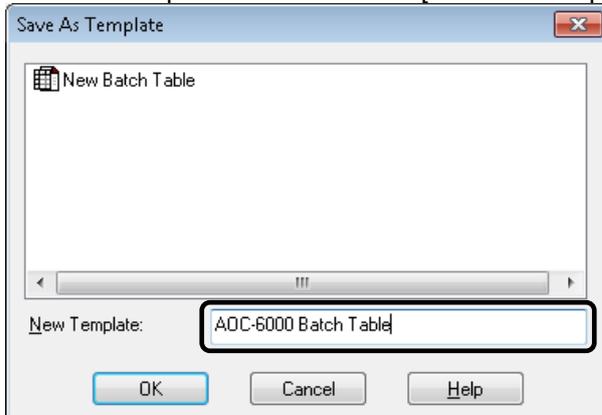
- 3) Click [Up] repeatedly to move [Option 1] to the top of the [Display Items] list.
- 4) Click [OK].
- 5) To change the title for the [Option 1] column, click the [Settings] icon on the [Batch] assistant bar.



- 6) Enter "Tray" in [Option 1 Title] on the [Option Items] tab page in the [Settings] sub-window. Click [OK].



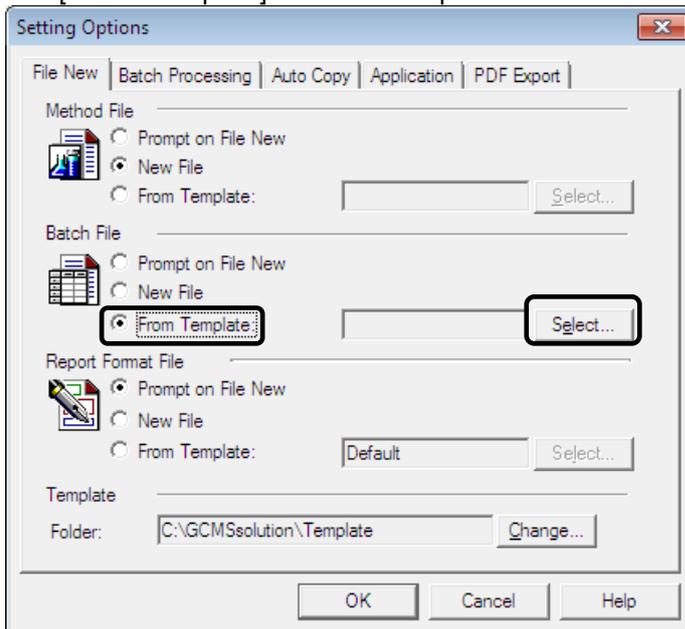
- 7) To save this Batch Table as a template so that the template is used to create new batch files, click [Save Batch As Template] on the [File] menu.
- 8) Enter the template file name in the [Save As Template] sub-window, and click [OK].



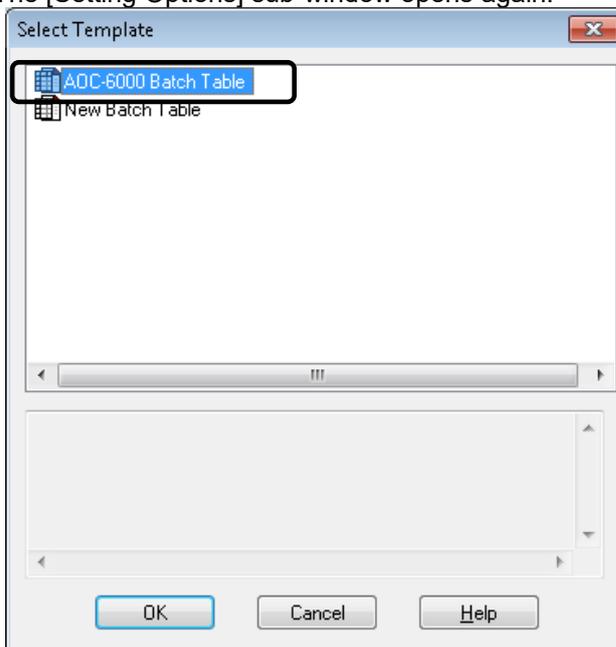
- 9) Select [Option] on the [Tools] menu.  
The [Setting Options] sub-window opens.

### 3 Initial Setting

- 10) Select [From Template] at [Batch File] on the [File New] tab page, and click [Select].  
The [Select Template] sub-window opens.



- 11) Select the template file name saved at step 8), and click [OK].  
The [Setting Options] sub-window opens again.



- 12) Clicking [OK] returns to the Batch Table.

With the above procedure, the column for setting the tray name is displayed when creating new batch files.



#### NOTE

Tray name is needed for AOC-5000 Series or AOC-6000 Series. It is not necessary to enter anything to the [Tray] when the other sampler is operated

## 3.5 When the AOC-6000 Series Configuration Is Changed

### 3.5.1 Changing a Syringe Tool

The AOC-6000 Series enables liquid injection, headspace injection, and solid phase micro extraction (SPME) injection, as well as SPME Arrow injection, and ITEX injection. Exchange the syringe tool depending on the injection method.

If the type of syringe tool is changed when GCMSsolution is running, the link between the GCMSsolution and AOC-6000 Series must be reconnected. Exit and restart the [GCMS Real Time Analysis] program.

#### Reference

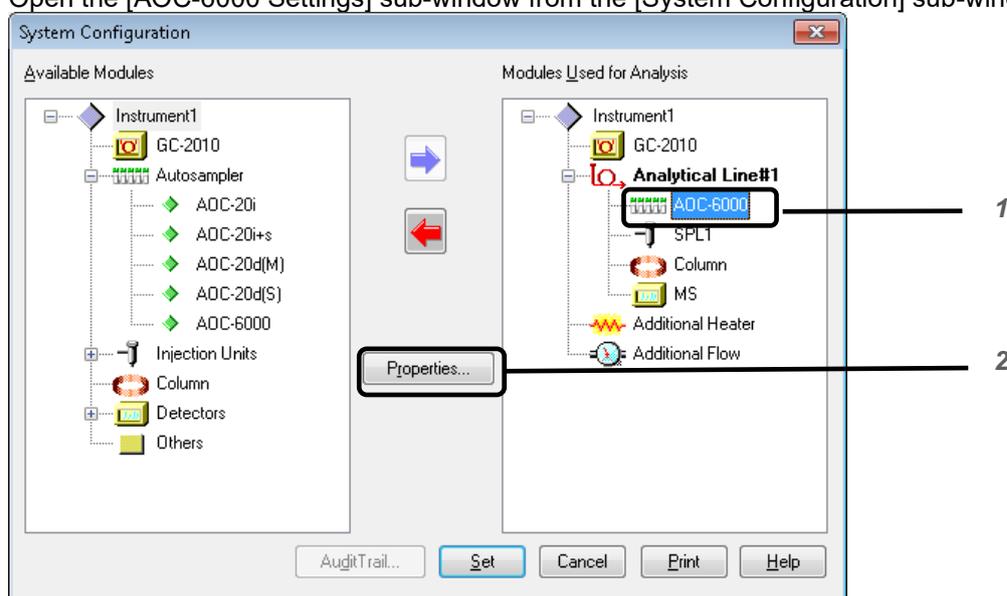
For instructions on attaching or removing syringe tools, refer to the PAL3 RTC/RSI User Manual.

On the AOC-6000 Series with RTC(Robotic Tool Change), syringe tools are replaced automatically. Replacement with a syringe tool set on the park station is done when necessary according to the syringe tool type specified in the method. There is no need to reconnect GCMSsolution and the AOC-6000 Series.

### 3.5.2 Change a Tray Type

Tray type can be changed in accordance with vial size on AOC-6000 Series PAL terminal. When a tray type is changed, synchronization is needed after restarting the [GCMS Real Time Analysis] program.

- 1) Open the [System Configuration] sub-window. To open the [System Configuration] sub-window, see "3.2 Setting the Configuration."
- 2) Open the [AOC-6000 Settings] sub-window from the [System Configuration] sub-window.

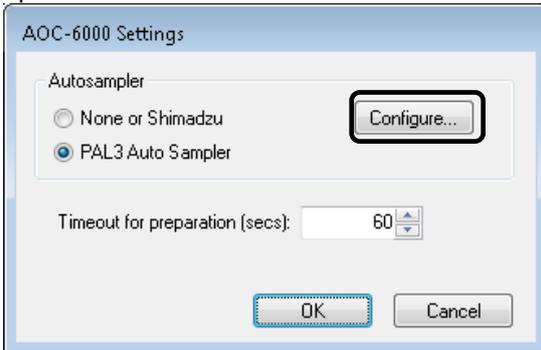


- 1 Select [AOC-6000] at [Modules Used for Analysis].
- 2 Click [Properties].

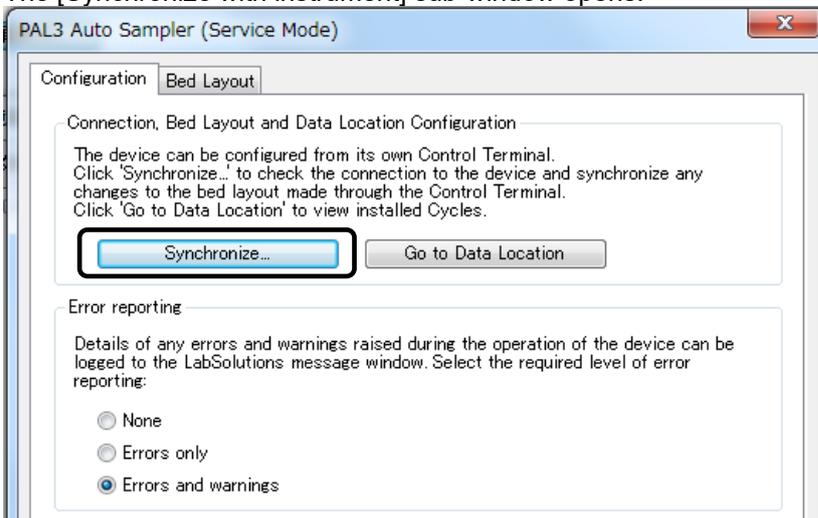
### 3 Initial Setting

---

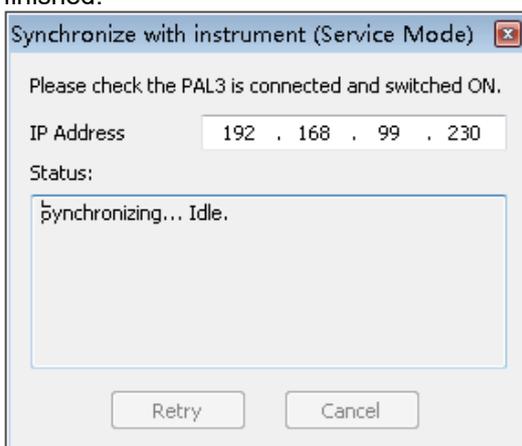
- 3) Click [Configure] in the [AOC-6000 Settings] sub-window. The [PAL3 Auto Sampler] sub-window opens.



- 4) Click [Synchronize] on the [Configuration] tab page. The [Synchronize with instrument] sub-window opens.



- 5) This sub-window automatically closes when communication with the AOC-6000 Series is successfully finished.



- 6) Click [OK] in the [PAL3 Auto Sampler] sub-window.
- 7) Click [OK] in the [AOC-6000 Settings] sub-window.

# 4 Method Settings

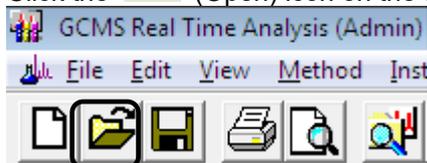
Only users with the [Edit Method (Instrument Parameters)] system administration rights can change AOC-6000 method settings.

## 4.1 Setting AOC-6000 Parameters

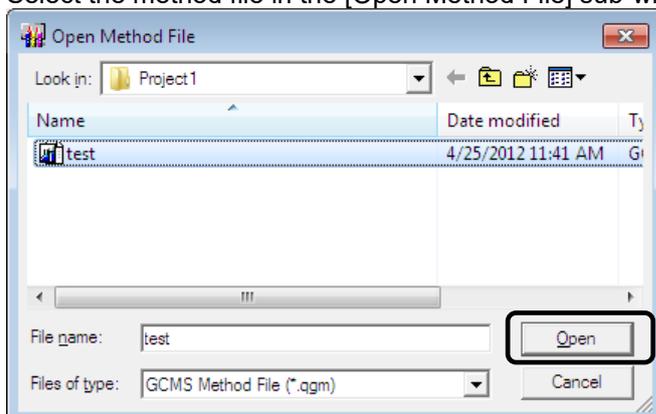
- 1) Click the [Data Acquisition] icon on the [Real Time] assistant bar in the [GCMS Real Time Analysis] program.  
The [Acquisition] window opens.



- 2) Click the  (Open) icon on the toolbar.



- 3) Select the method file in the [Open Method File] sub-window, and click [Open].



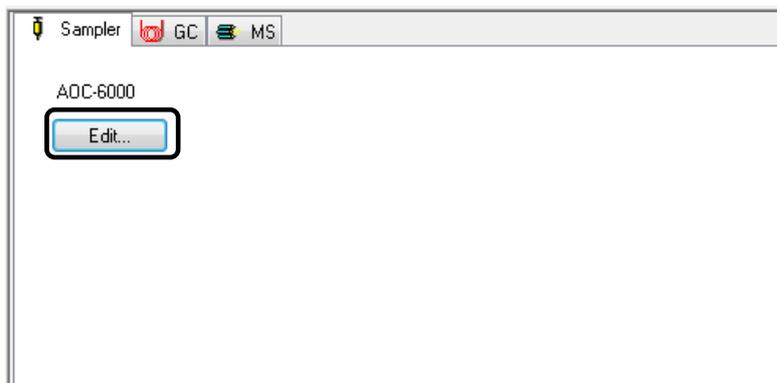
- 4) Click [Edit] on the [Sampler] tab page in [Instrument Parameters View].  
The [Method Parameters] sub-window opens.

## 4 Method Settings



### NOTE

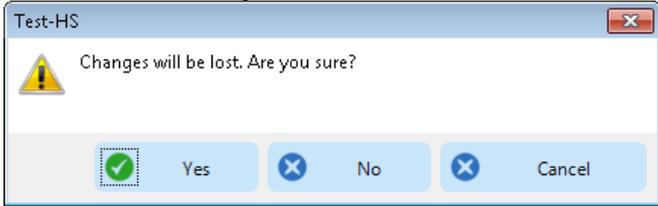
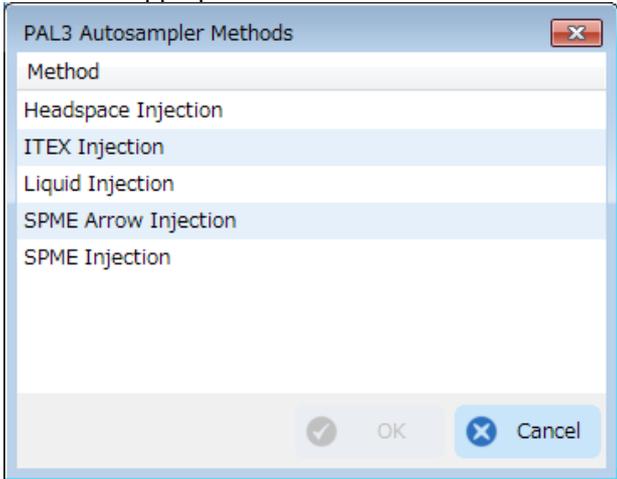
- Only one [Method Parameters] sub-window can be opened. If it was already opened from a different sub-window, then that sub-window must first be closed before clicking [Edit].
- The [Edit] button is grayed out during data measurements and cannot be clicked.



5) Set the AOC-6000 parameters.

The screenshot shows the 'Test-HS - Method Parameters' dialog box. At the top, there are three buttons: 'Apply' (1), 'Print' (2), and 'Methods' (3). Below these buttons is a section titled 'Headspace Injection' containing a table of parameters. The table has three columns: 'Parameter', 'Value', and 'Unit'. The 'Analysis' section is expanded, showing various parameters and their current values. At the bottom of the dialog, there are two callouts: '4' pointing to the 'Parameter' column and '5' pointing to the 'Value' column.

Parameter	Value	Unit
<b>Setup</b>		
<b>Analysis</b>		
Syringe Tool	HS 1	
Incubation Temperature	40	°C
Incubation Time	5	min
Syringe Temperature	60	°C
Agitator Speed	250	rpm
Pre Purge Time	5	s
Injector	Injector 1	
Injection Flow Rate	10	mL/min
Post Purge Time	10	s
Analysis Time	15	min
<b>Advanced</b>		

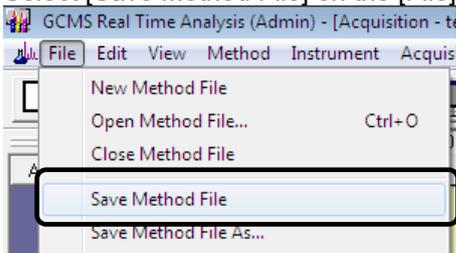
No.	Item	Explanation
①	Apply	<p>After setting the parameters, click [Apply] to determine the settings before closing the sub-window.</p> <p> <b>NOTE</b> If you try to close the sub-window without clicking [Apply], a warning message is displayed. Go back to the [Method Parameters] sub-window and check the contents if necessary.</p> 
②	Print	<p>Print out the AOC-6000 parameters.</p> <p> <b>NOTE</b> AOC-6000 parameters cannot be printed out together with other method parameters.</p>
③	Methods	<p>Select an AOC-6000 method. This software incorporates typically used AOC-6000 methods.</p> <p>Click [Methods] to display the [PAL3 Autosampler Methods] sub-window. Select the appropriate AOC-6000 method and click [OK].</p>  <p>If you click [▼] on the right of the [Methods] button, the list of available methods is displayed on a drop-down list. You can also select a method from this list.</p> <p>The name of the selected AOC-6000 method is displayed at the top of the parameter table.</p>
④	Parameter	<p>The list of parameters of the selected AOC-6000 method is shown. Parameters are categorized into several groups (e.g. "Analysis" group, "Setup" group). The parameters in each group can be displayed and hidden by clicking the arrow on the left side of the group name.</p> <p> <b>Reference</b> For details, see "Appendix – Method Parameters for Each Injection Method."</p>

## 4 Method Settings

5	Value Unit	<p>Set each parameter. Click the [Value] cell for the parameter to be set. Enter a value for parameters that need numerical value entry. For tools that are incorporated in the AOC-6000 such as syringes, select an item in the list box displayed.</p> <p> <b>NOTE</b></p> <ul style="list-style-type: none"><li>• Enter a value within the range allowable for the type of the tools.</li><li>• Parameters with the  icons require setting.</li></ul> <p>When the  icon is displayed, the [Apply] and [Print] buttons remain gray and they cannot be clicked.</p> <p> <b>Reference</b> For details, see "Appendix – Method Parameters for Each Injection Method."</p>
---	------------	--

6) Click  to close the [Method Parameters] sub-window.

7) Select [Save Method File] on the [File] menu.



 **NOTE**

- Methods can also be created in the [Acquisition] sub-window in the [GCMS Analysis Editor] program.
- The computer must be connected to the AOC-6000 Series unit to specify AOC-6000 methods. Methods cannot be created on other computers using a secondary license program.

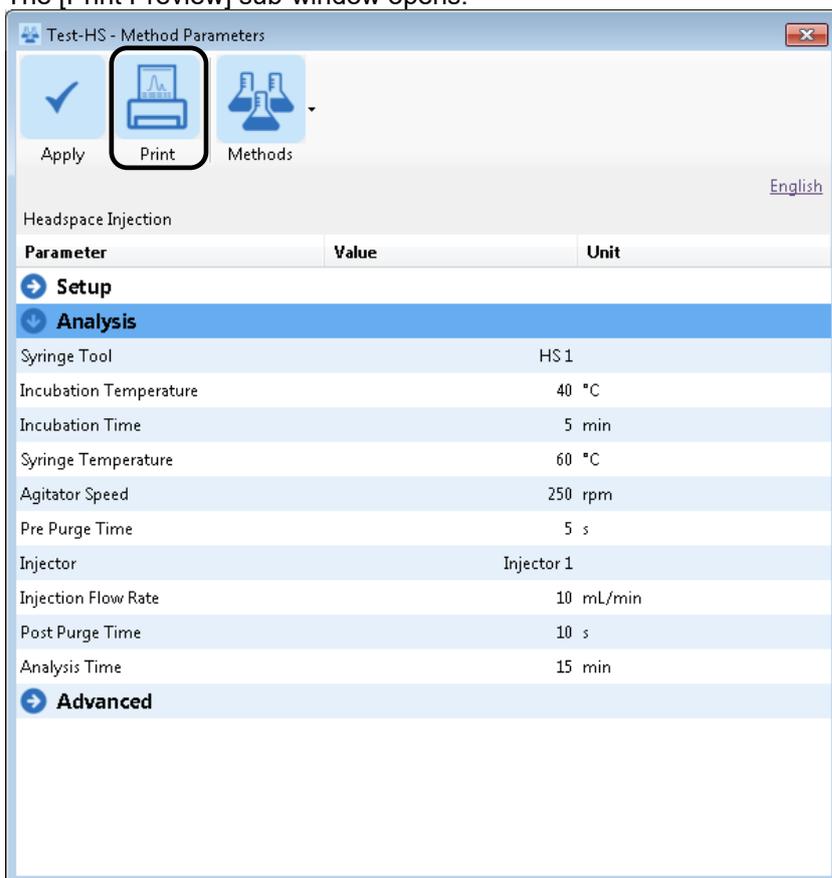
## 4.2 Printing AOC-6000 Parameters

### 4.2.1 Printing from the [GCMS Real Time Analysis] Program

- 1) Open the method file in the [Acquisition] window.
- 2) Click [Edit] on the [Sampler] tab page in [Method Parameters].  
The [Method Parameters] sub-window opens.

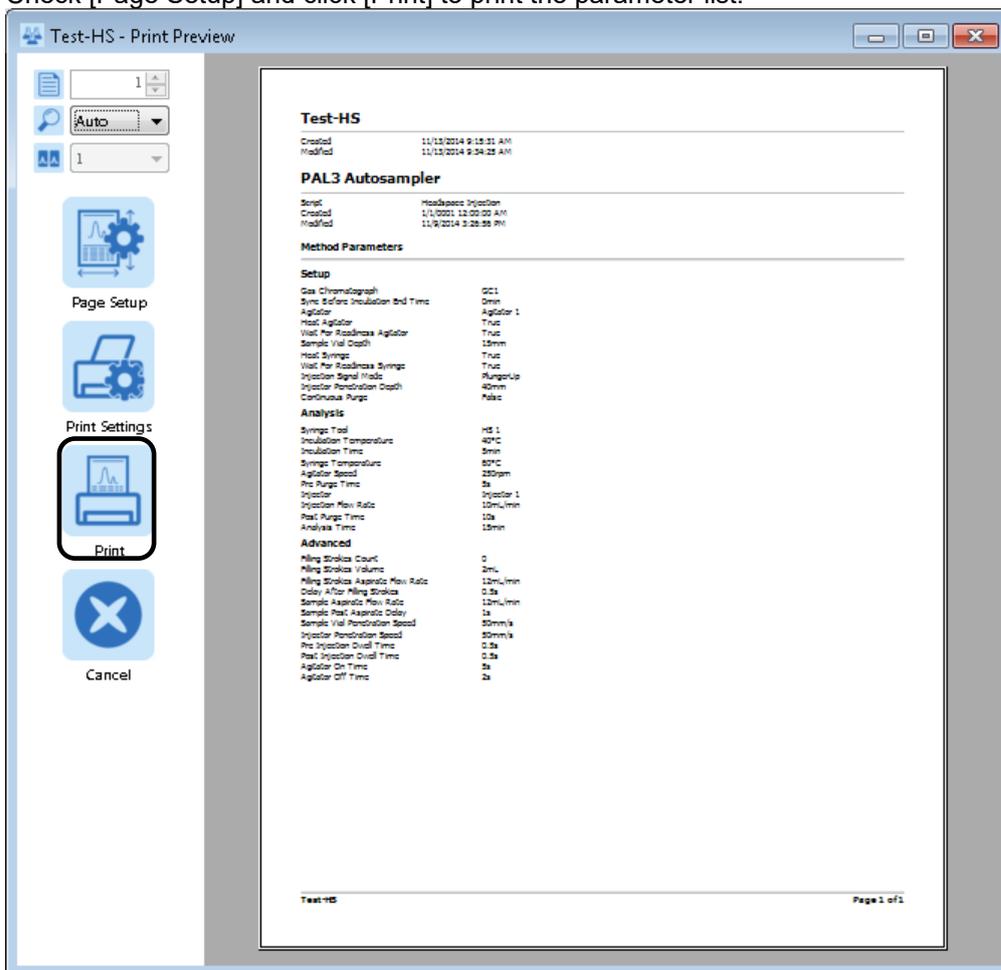


- 3) Click [Print].  
The [Print Preview] sub-window opens.



## 4 Method Settings

- 4) Check [Page Setup] and click [Print] to print the parameter list.



### NOTE

AOC-6000 parameters can't be printed together with GC/MS instrument parameters.

### 4.2.2 Printing from the [GCMS Postrun Analysis] Program

- 1) Open the data file in the [Data Analysis] window.
- 2) Select [Data Acquisition Settings] on the [View] menu, and click [Instrument Parameters]. The [Data Acquisition Parameters] sub-window opens.
- 3) Click [Edit] on the [Sampler] tab page. The [Print Preview] sub-window opens.

4) Click [Print].

**Test-HS**  
 Created 11/13/2014 9:15:31 AM  
 Modified 11/13/2014 9:34:25 AM

**PAL3 Autosampler**  
 Script HeadSpace Injection  
 Created 11/1/2001 12:00:00 AM  
 Modified 11/9/2014 2:36:26 PM

**Method Parameters**

**Setup**

Gas Chromatograph	GC1
Time Before Inoculation End Time	0min
Agitator	Agitator 1
Head Agitator	True
Wait For Roadmax Agitator	True
Sample Vial Depth	15mm
Head Syringe	True
Wait For Roadmax Syringe	True
Injection Signal Mode	PurgeUp
Injector Penetration Depth	40mm
Continuous Purge	None

**Analysis**

Syringe Tool	HS 1
Inoculation Temperature	40°C
Inoculation Time	3min
Syringe Temperature	50°C
Agitator Speed	250rpm
Pre Purge Time	5s
Injector	Injector 1
Injection Flow Rate	10mL/min
Post Purge Time	10s
Analysis Time	15min

**Advanced**

Mixing Stroke Count	0
Mixing Stroke Volume	2mL
Mixing Stroke Aspirate Flow Rate	12mL/min
Delay After Mixing Stroke	0.5s
Sample Aspirate Flow Rate	12mL/min
Sample Post Aspirate Delay	1s
Sample Vial Penetration Speed	50mm/s
Injector Penetration Speed	50mm/s
Pre Injection Dwell Time	0.5s
Post Injection Dwell Time	0.5s
Agitator On Time	5s
Agitator Off Time	2s

Test-HS Page 1 of 1

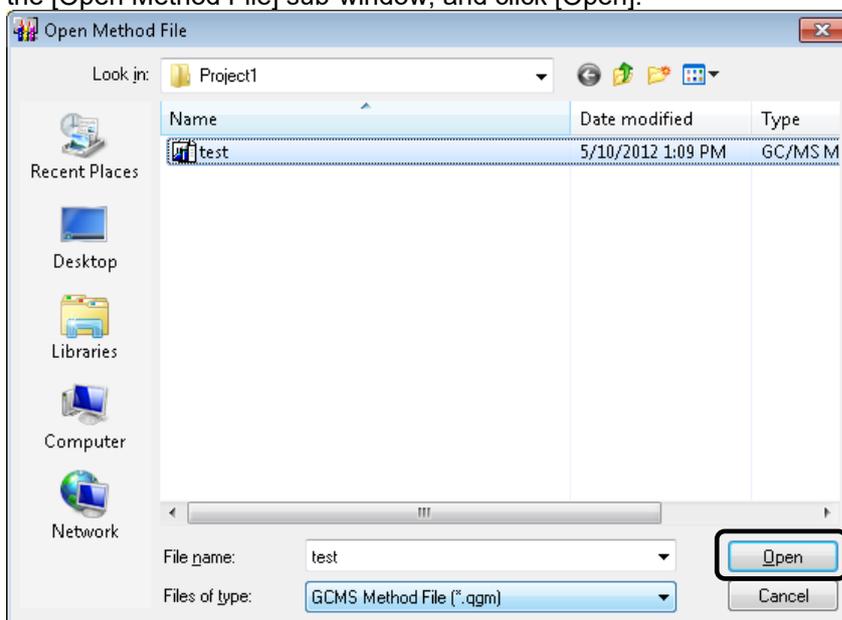


**NOTE**

AOC-6000 parameters can't be printed together with GC/MS instrument parameters.

# 5 Measuring Samples

- 1) Click the  (Open) icon on the toolbar in the [Acquisition] window. Select the method file to use in the [Open Method File] sub-window, and click [Open].



### NOTE

Confirm that the type of syringe tool attached to the AOC-6000 Series matches the syringe size setting for [Syringe Tool] in AOC-6000 parameters in the specified method file. See "4.1 Setting AOC-6000 Parameters" to confirm AOC-6000 parameters.

- 2) Click the [Sample Login] icon on the [Acquisition] assistant bar. The [Sample Login] sub-window opens.



- 3) Click [AOC-6000 Settings].  
The [AOC-6000 Settings] sub-window opens.

Sample Login - C:\GCMSsolution\Data\Project1\Test-HS.qgm

Line1

Acquisition Information

Sample Name :

Sample ID :

Data File : Data001.qgd

Baseline Data :

Data Description :

Sampler

Vial # :

Injection Volume :  uL Syringe Capacity :  uL

Multi Inj. Times :

Tuning File :

- 4) In [Tray], select the name of the tray where vials will be placed. If the appropriate tray name is not listed in the drop-down list, enter the name directly. This setting is case-sensitive. Enter a space between "Rack" and the number.

Click [OK] to go back to the [Sample Login] sub-window again.

AOC-6000 Settings

Tray:

**NOTE**

- Specify the tray name which has been set on the AOC-6000 Series unit. Default settings are as follows.

Rack: Rack 1, Rack 2, Rack 3, .....

- The specified tray name is recorded in the data file. Load the data on the [GCMS Postrun Analysis] program, select [Data File Properties] from the [File] menu, and check the tray name on the [Option Info.] tab page

- 5) Enter the data file name, vial number, injection volume, and other settings, then click [OK].  
The [Acquisition] window opens again.

**NOTE**

- Vial numbers cannot be set to 0 or -1.
- Injection volume settings are in terms of  $\mu\text{L}$  units. If a headspace syringe tool is used, use caution specifying the injection volume. Set an injection volume of 1 for SPME syringe tools or SPME Arrow syringe tools.
- Enter vial number and injection volume values that are within a normal range.

## 5 Measuring Samples

---

- 6) Arrange the specified vials in the tray.

 **CAUTION**

- Be careful not to forget placing the vials.
- If any vials are remaining in the agitator, they must be removed.
- If an error occurs during data acquisition, the analytical process is stopped.

- 7) Click the [Standby] icon on the [Acquisition] assistant bar.  
When the GC and MS units are restored to ready state, data acquisition starts automatically.



**NOTE**

Vials left in the agitator will cause an error the next time data is acquired. Remove vials manually.

 **CAUTION**

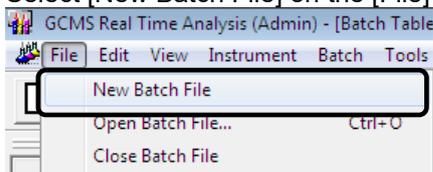
The agitator can become very hot. Therefore, be very careful not to get burned when removing the vials.

# 6 Measuring a Series of Samples Continuously

- 1) Click the [Batch Processing] icon on the [Real Time] assistant bar in the [GCMS Real Time Analysis] program.  
The [Batch Table] window opens.



- 2) Select [New Batch File] on the [File] menu.



- 3) Enter the sample type, method file name, data file name, vial number, injection volume, and other information.



## NOTE

- Confirm that the type of syringe tool attached to the AOC-6000 Series matches the syringe size setting for [Syringe Tool] in AOC-6000 parameters in the specified method file. See "4.1 Setting AOC-6000 Parameters" to confirm AOC-6000 parameters.
- Note the following precautions regarding vial numbers and injection volume values.
  - Injection volume settings are in terms of  $\mu\text{L}$  units. If a headspace syringe tool is used, use caution specifying the injection volume. Set an injection volume of 1 for SPME syringe tools or SPME arrow syringe tools.
  - If a headspace syringe tool or ITEX syringe tool is used, specify the same injection volume values in a batch file. To use a combination of different injection volumes, use a batch queue.
  - Vial numbers cannot be set to 0 or -1.
- Specify method files that contain the identical AOC-6000 parameters and the identical initial GC/MS temperature like injection unit when using headspace, SPME, SPME arrow and ITEX syringe tool. Different parameters could cause an error to occur during batch processing and stop measurements. To use different parameters, use a batch queue.

## 6 Measuring a Series of Samples Continuously

- 4) Set the rack name by entering "Rack 1" if using rack 1 and "Rack 2" if using rack 2. Enter a space between "Rack" and the number. This setting is case-sensitive. Make sure it is set correctly.

Folder: C:\GCMSsolution\Data\Project1

	Tray	Vial#	Sample Name	Sample ID	Sample Type	Analysis Type	Method File	Data File
1	Rack 1	1			0:Unknown	IT QT	Test-HS.qgm	UNK-001.qgd
2	Rack 1	2			0:Unknown	IT QT	Test-HS.qgm	UNK-001.qgd
3	Rack 1	3			0:Unknown	IT QT	Test-HS.qgm	UNK-001.qgd
4	Rack 1	4			0:Unknown	IT QT	Test-HS.qgm	UNK-001.qgd
5	Rack 1	5			0:Unknown	IT QT	Test-HS.qgm	UNK-001.qgd



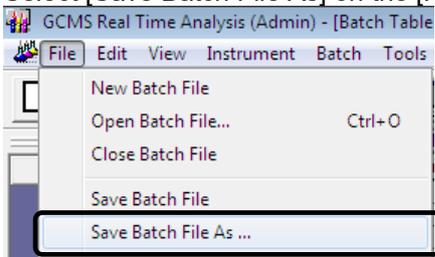
### NOTE

• Specify the tray name which has been set on the AOC-6000 Series unit. Default settings are as follows.

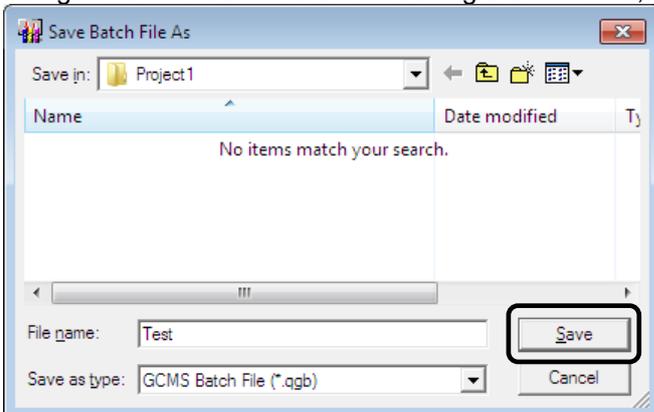
Rack: Rack 1, Rack 2, Rack 3, .....

• The specified tray name is recorded in the data file. Load the data on the [GCMS Postrun Analysis] program, select [Data File Properties] from the [File] menu, and check the tray name on the [Option Info.] tab page

- 5) Select [Save Batch File As] on the [File] menu.



- 6) Navigate to the desired folder for saving the batch file, then enter the file name and click [Save].



- 7) Arrange the specified vials in the tray.



### CAUTION

- Be careful not to forget placing the vials.
- If any vials are remaining in the agitator, they must be removed.
- If an error occurs during data acquisition, the analytical process is stopped.

- 8) Click the [Start] icon on the [Batch] assistant bar to start batch processing.



### NOTE

- When headspace, SPME, SPME arrow or ITEX syringe are used, the following vials are incubated during data acquisition (overlapped incubation).
- In batch processing, data acquisition can be performed on up to 60 samples at one time. To perform data acquisition on more samples, create a new batch file and run data acquisition using a batch queue.
- On the AOC-6000 Series with RTC (Robotic Tool Change), syringes are replaced automatically. However, on a batch file, use one syringe for data acquisition. For example, to establish a TwinLineMS system and perform batch processing while switching between headspace and SPME, create a batch file each for headspace and SPME, register one of them to a batch queue, and run data acquisition.



### NOTE

- Note the following precautions to stop or pause batch processing.
  - To stop batch processing, click the [Stop] icon on the [Batch] assistant bar. If a batch is stopped, samples in the agitator are not injected.
  - If any vials remain in the agitator, an error occurs when analysis is started the next time. If there are any remaining vials, manually remove them.
  - When a method file that specifies an AOC-6000 method for headspace, SPME, SPME arrow or ITEX is used, then the batch process cannot be paused.
- When a method file or AOC-6000 has an issue like no vial or wrong syringe adapter, an error message is displayed and batch processing is stopped. When vials are left in agitator, remove them.
- Don't open the method file used in ongoing batch processing in the [GCMS Analysis Editor] program and the [Calibration Curve] window of the [GCMS Postrun Analysis] program. It may cause an error and the batch processing stopped.



### CAUTION

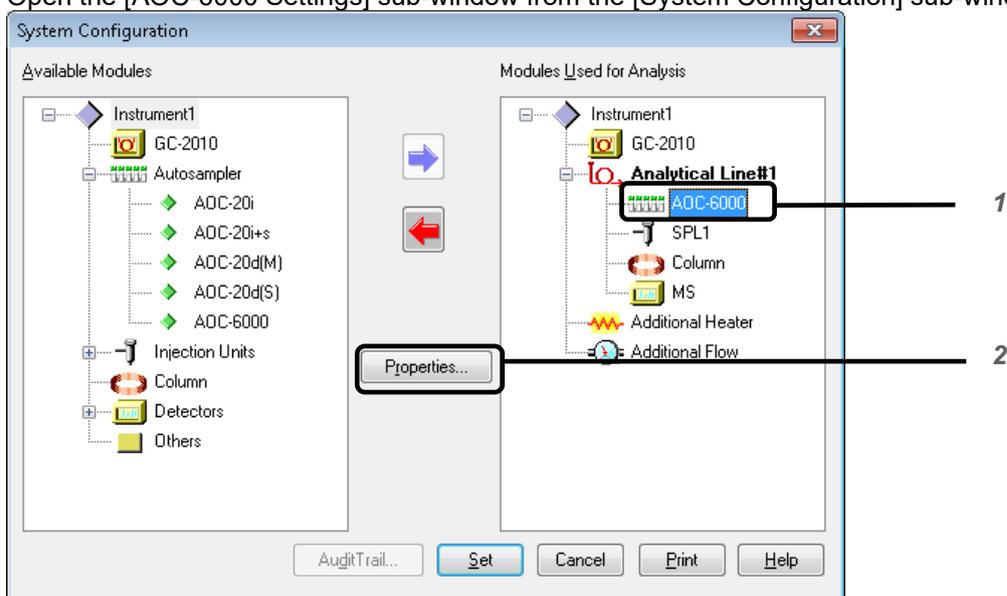
The agitator can become very hot. Therefore, be very careful not to get burned when removing the vials.

# 7 Advanced Operations

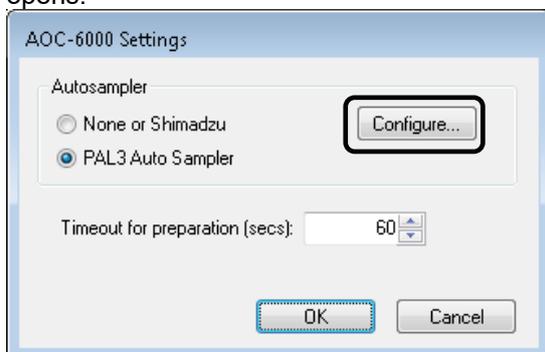
## 7.1 Confirming the Tray Name

Display the tray names registered in the AOC-6000 Series. During measurements, the specified tray names must be the same as names displayed here.

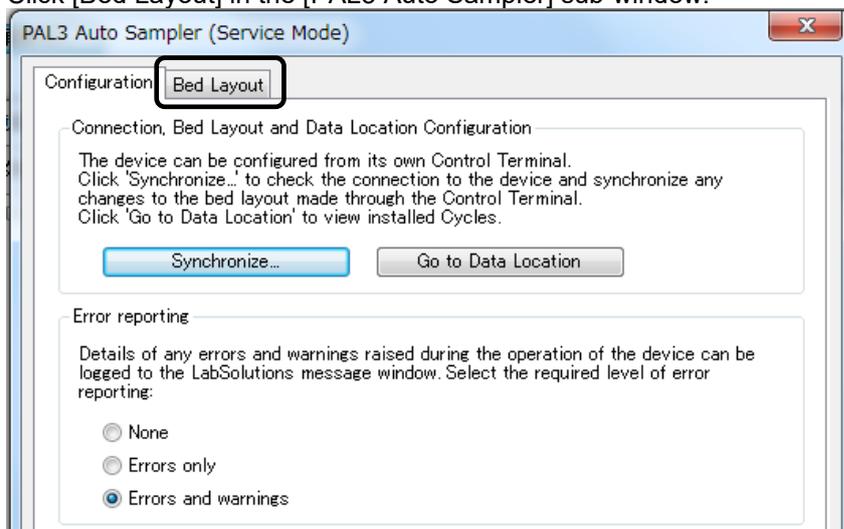
- 1) Open the [System Configuration] sub-window. To open the [System Configuration] sub-window, see "3.2 Setting the Configuration."
- 2) Open the [AOC-6000 Settings] sub-window from the [System Configuration] sub-window.



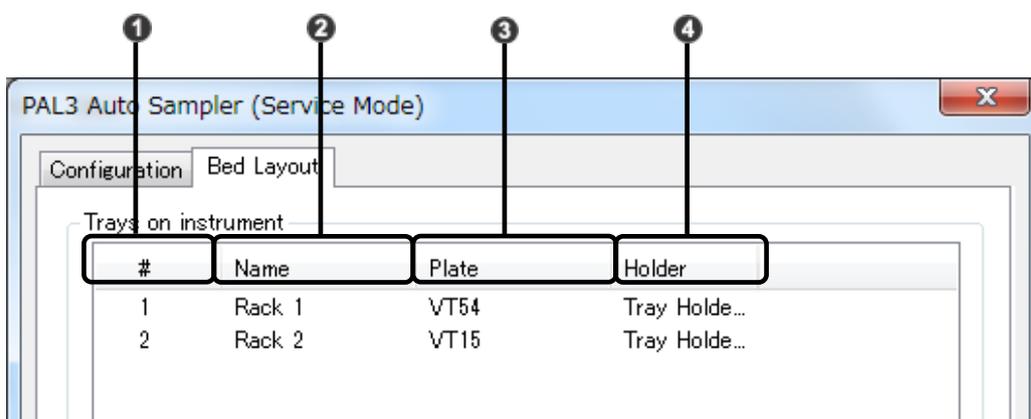
- 1) Select [AOC-6000] at [Modules Used for Analysis].
  - 2) Click [Properties].
- 3) Click [Configure] in the [AOC-6000 Settings] sub-window. The [PAL3 Auto Sampler] sub-window opens.



- 4) Click [Bed Layout] in the [PAL3 Auto Sampler] sub-window.



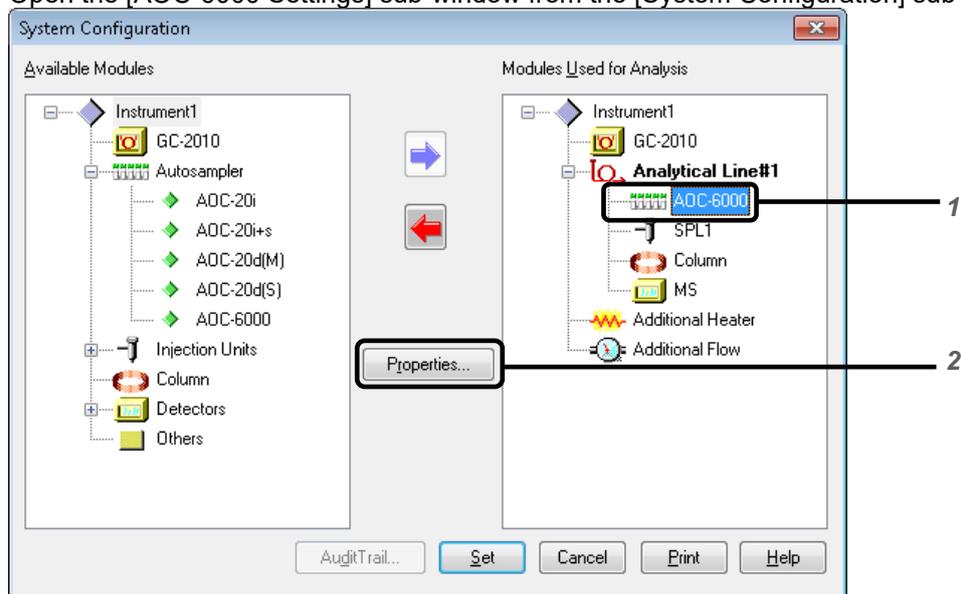
The tray names registered in the AOC-6000 are displayed.



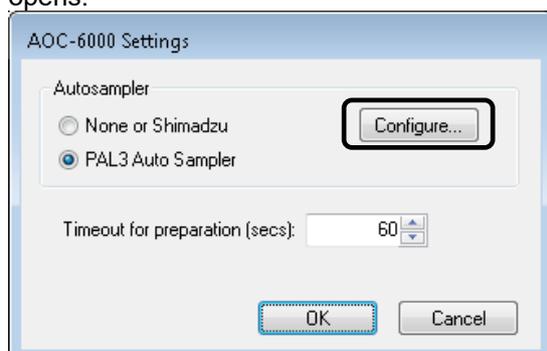
No.	Item	Explanation
①	#	Displays the tray numbers.
②	Name	Displays the names of the trays. These character strings are used for tray name set during measurements
③	Plate	Displays the type of tray attached to the tray holder.
④	Holder	Displays the names of the tray holders.

### 7.2 Confirming the Location Where AOC-6000 Methods Are Saved

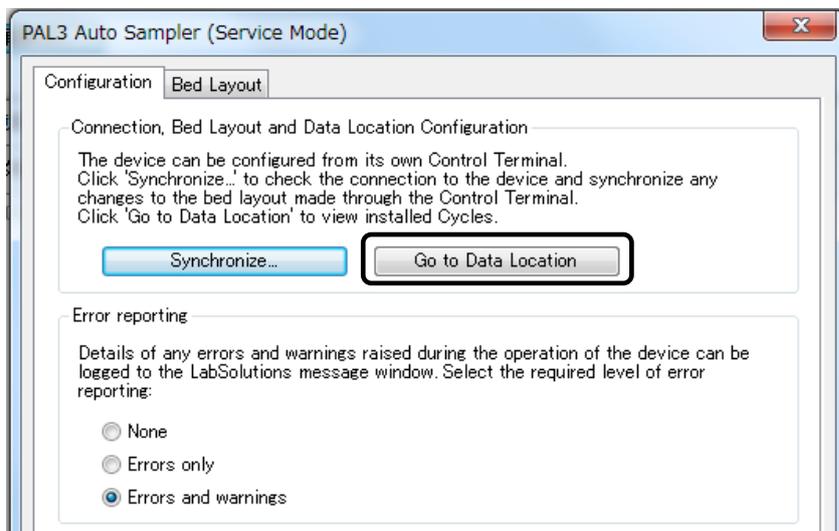
- 1) Open the [System Configuration] sub-window. To open the [System Configuration] sub-window, see "3.2 Setting the Configuration."
- 2) Open the [AOC-6000 Settings] sub-window from the [System Configuration] sub-window.



- 1 Select [AOC-6000] at [Modules Used for Analysis].
- 2 Click [Properties].
- 3) Click [Configure] in the [AOC-6000 Settings] sub-window. The [PAL3 Auto Sampler] sub-window opens.



- 4) Click [Go to Data Location] on the [Configuration] tab page in the [PAL3 Auto Sampler] sub-window. The default folder where AOC-6000 methods should be saved is opened in Windows Explorer.



### 7.3 Protecting Method Files and AOC-6000 Methods

To ensure method files and AOC-6000 methods can be used in a safe environment, use GCMSsolution system administration to specify appropriate operating policies and manage users. This software enables using GCMSsolution functionality to do the following. For more details, refer to the GCMSsolution Instruction Manual or the [Help] menu.

- System administration [Edit Method (Instrument Parameters)] rights can restrict users from changing method files. This prevents unauthorized users from making accidental changes.
- If the audit trail function is enabled, any changes made to method files can be verified. If an AOC-6000 parameter is changed, the method file audit trail saves a record of the fact that a change was made. However, it does not record how individual parameters were changed.

To prevent accidental changes to AOC-6000 method, assign that right to the user that logs into Windows, so that only specified users can change the file. Refer to the Windows [Help] menu or other sources regarding how to set user rights. However, note the following precautions.

- For instructions on how to open the folder, see "7.2 Confirming the Location Where AOC-6000 Methods Are Saved."
- The names of files and folders that should have restricted access are indicated below.

Folder/File Name	Type	User/Group Right (for example)
Shimadzu	Folder	[Delete subfolders and files], [Delete] and [Change permissions] are not allowed.
Shimadzu\InstrumentControl	Folder	[Delete subfolders and files], [Delete] and [Change permissions] are not allowed.
Shimadzu\*** (Folder other than InstrumentControl)	Folder	Full control
Shimadzu\InstrumentControl\	Folder	[Delete subfolders and files], [Delete] and [Change

## 7 Advanced Operations

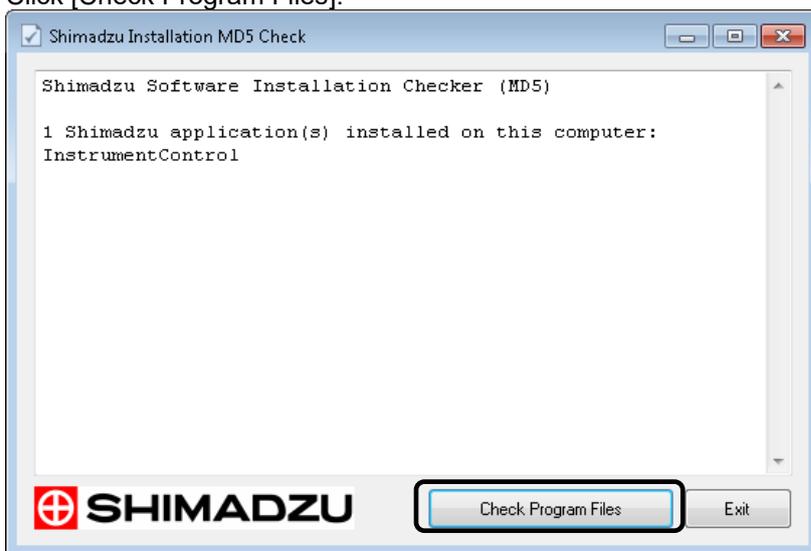
---

PAL3		permissions] are not allowed.
Shimadzu\InstrumentControl\ PAL3\Scripts	Folder	[Delete subfolders and files], [Delete] and [Change permissions] are not allowed.
Shimadzu\InstrumentControl\ PAL3\***.***	File	Full control
Shimadzu\InstrumentControl\ PAL3\Scripts\***.xml	File	[Create files / write data], [Delete] and [Change permissions] are not allowed.

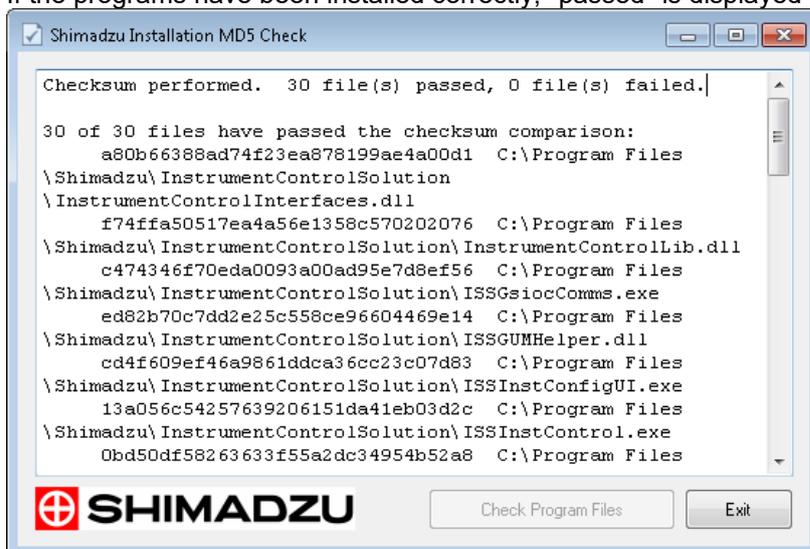
### 7.4 Checking Programs

The following enables checking that a program was installed correctly.

- 1) Start up the Windows Explorer.
- 2) Double-click the [Check the Program Files] program (ShimadzuMD5Check.exe).  
The [Check the Program Files] program is in the following location.  
32-bit PC C:\Program Files\Shimadzu\InstrumentControlSolution\ShimadzuMD5Check.exe  
64-bit PC C:\Program Files (x86)\Shimadzu\InstrumentControlSolution\ShimadzuMD5Check.exe
- 3) Click [Check Program Files].



- 4) If the programs have been installed correctly, "passed" is displayed for all programs.



# 8 Troubleshooting

## 8.1 Connection to the AOC-6000 Series Failed

When the [GCMS Real Time Analysis] program is started, the AOC-6000 Series status remains [Not Connected] in the instrument monitor.

Error Message	Probable Cause	Corrective Measure
None	Connection to the AOC-6000 Series is taking a long time.	Wait for a while. It takes about 1 minute for the status to change to [Ready] after starting the [GCMS Real Time Analysis] program.
Error has occurred in instruments. (The Driver is currently not connected)	The communication cable is disconnected between the AOC-6000 Series and computer.	Make sure the communication cable is connected properly.
	The AOC-6000 Series power is OFF.	Switch the AOC-6000 Series power ON and wait for AOC-6000 Series initialization to finish before starting the [GCMS Real Time Analysis] program.
	Multiple instances of the program were launched internally.	Restart the computer.
	An incorrect IP address is set.	Check the IP address of the instrument and computer.
Error has occurred in instruments. (There is already a listener on IP endpoint 127.0.0.1:64001. Make sure that you are not trying to use this endpoint multiple times in your application and that there are no other applications listening on this endpoint.)	The AOC-6000 Series and computer could not be connected when the [GCMS Real Time Analysis] program was started.	Exit the [GCMS Real Time Analysis] program, wait for approximately ten seconds, and restart the program.

## 8.2 Data Acquisition Does Not Start

An error occurs if data acquisition is started.

Error Message	Probable Cause	Corrective Measure
Cannot stand by (Invalid injection volume.)	Appropriate injection volume is not specified.	Specify an injection volume ( $\mu\text{L}$ ) consistent with the syringe tool setting in the method.

Error Message	Probable Cause	Corrective Measure
	Appropriate AOC-6000 Series syringe tool is not specified in method.	In methods, specify the syringe tool actually installed on the instrument.
	The value specified in method parameters is outside the specified range.	See "Method Parameters for Each Injection Method " and enter a [Value] setting that is within the input range specified for the instrument
Cannot stand by (Incorrect tray number)	The tray name specified for the tray is not correct.	Specify the correct tray name. Tray names are case-sensitive. <ul style="list-style-type: none"> <li>For continuous data acquisition, confirm the Option 1 (Tray) setting for the batch file.</li> <li>For data acquisition analyses, confirm the tray name registered in sample registration.</li> </ul>
	Synchronization was not performed. Synchronization is required before initial use after changing tray information in the AOC-6000 Series unit or after installation.	Click the [Configure] button in the AOC-6000 properties ([Edit AOC-6000 Config]) in the [System Configuration] sub-window, and click the [Synchronize] button in the window that is displayed.
Error has occurred in instruments. (Number of samples exceeds the upper limit. This system allows up to 60 samples.)	The number of samples registered to the batch file is over the upper limit. This system can perform data acquisition on up to 60 samples.	Limit the number of samples registered to the batch file to 60 at the maximum. To measure more samples, create a new batch file for them and register the file to a batch queue.
Error has occurred in instruments. (Cannot aspirate requested volume. Total volume exceeds syringe volume. Requested: X $\mu$ L; Currently available)	The aspiration volume is over the allowable volume for the syringe.	Reduce the aspiration volume for the wash solvent, internal standard, and pumping in the AOC-6000 method. Or, reduce the injection volume during data acquisition.
	The value set for the internal standard penetration depth is too small.	Set a larger value for the internal standard penetration depth in the AOC-6000 method.
Error has occurred in instruments. (Cannot change the Tool. There is no free Slot in any configured Tool Change Station.)	The syringe tool cannot be changed because the park station has no free slot.	Remove unnecessary syringe tools from the park station.
Error has occurred in instruments. (Cannot move to target Vial with current needle guide type)	The vial cannot be moved because of incorrect needle guide type setting in tool setting on the AOC-6000 Series.	Set the needle guide type on the AOC-6000 Series correctly according to the size of the vial used and the cap type.

## 8 Troubleshooting

Error Message	Probable Cause	Corrective Measure
Error has occurred in instruments. (Cannot transport the vial. Vial and destination is incompatible. Check the configuration.)	The type of vial in the agitator is different from the vial actually used.	Specify the type of the vial set on the rack for the type of vial in the agitator on the AOC-6000 Series unit.
Error has occurred in instruments. (Collision occurred on 'Plunger Drive 1' (force limit exceeded))	A collision was detected during operation of the syringe plunger.	Remove the foreign object.
	One batch file is being used for data acquisition using different syringes.	Use the same syringe for one batch file. To perform data acquisition with switching syringes, create a batch file for each syringe, register one of them to a batch queue, and run data acquisition.
Error has occurred in instruments. (Collision occurred on 'Z Drive X' (force limit exceeded).)	Data acquisition was started with a vial remaining in the agitator.	Remove vials from the agitator. Also, remove any vials from the injection tool (PAL head).
	The syringe tool collided with a vial placed behind the specified vial. This error occurs, for example, when a rack for 20 mL vials is placed behind a rack for 2 mL vials.	Place a rack for tall vials in the front.
	Tray type is wrong.	Set correct tray type in PAL terminal on AOC-6000 Series. Then conduct synchronization. Click the [Configure] button in the AOC-6000 properties ([Edit AOC-6000 Config]) in the [System Configuration] sub-window, and click the [Synchronize] button in the window that is displayed.
	Interference occurred between a vial and another vial placed on the rack when the vial was returning to the rack from the agitator or other part.	Remove both vials that interfered. Check for problems in vial or rack settings and teaching. If the injection unit (PAL head) did not go back to its home position, shut down the AOC-6000 Series and restart it. For the shutdown procedures, refer to the PAL3 RTC/RSI User Manual.
Error has occurred in instruments. (Error: Error while validating script.)	The AOC-6000 method settings or the AOC-6000 unit settings are insufficient or incorrect.	Check the AOC-6000 method settings or the AOC-6000 unit settings.
Error has occurred in instruments. (LS X has not been calibrated with RobotArmLeft yet.)	The LS X tool position has not been calibrated.	Calibrate the LS X tool position from the PAL terminal.

Error Message	Probable Cause	Corrective Measure
Error has occurred in instruments. (Rack item type of Rack X is not set.)	There is not sufficient information about the rack used on the AOC-6000.	Specify the rack item for the rack to be used on the AOC-6000 Series.
Error has occurred in instruments. (Requested penetration depth X (incl. position above the target) is $\geq$ Maximum tool penetration depth Y)	The penetration depth is over the allowable amount for the syringe.	Set a smaller penetration depth value in the AOC-6000 method.
Error has occurred in instruments. (Specified Flow Rate exceeds maximum allowed plunger speed.)	The sample aspiration/injection speed is over the allowable rate for the syringe.	Set a smaller flow rate value in the AOC-6000 method.
Error has occurred in instruments. (Target Object Injector X, Index X could be detected but it was outside the allowed range.)	The injector's injection position is incorrect. The adapter may not be placed on the GC injection unit.	Place the adapter on the GC injection unit. If it has been already placed, perform teaching for the injector's injection position again.
Error has occurred in instruments. (Target Object PosX, Index X could not be detected.)	Vials such as wash vial, internal standard vial, and waste solution vial are not detected.	Place the vials at the specified positions.
Error has occurred in instruments. (Target vial could not be detected. This might be caused by a missing or a wrong vial.)	Vials were not placed in the rack.	Place vials in the specified rack.
	An incorrect rack type is specified.	Register the correct rack for the vial size on the AOC-6000 Series unit.
	The vial moves unintentionally because no use of magnetism is specified for a vial cap that uses magnetism.	For a vial cap that uses magnetism, select "Magnetic" in rack item setting for the rack on the AOC-6000 Series unit.
	The specified tray name is incorrect.	Specify the name of the tray where vials were actually placed. <ul style="list-style-type: none"> <li>For continuous data acquisition, confirm the Option 1 (Tray) setting for the batch file.</li> <li>For data acquisition analyses, confirm the tray name registered in Sample Login.</li> </ul>
	The rack position is not set correctly.	Perform teaching for the rack position again.
Error has occurred in instruments. (Unable to use PAL method)	There is no syringe tool to be used.	Attach a syringe tool to be used or place it in the park station. Then, run [Synchronize] in the [GCMS Real Time Analysis] program.

## 8 Troubleshooting

---

Error Message	Probable Cause	Corrective Measure
Error has occurred in instruments. (X Drive 1 is not homed.)	The injection unit (PAL Head) has been returned to its home position.	Turn OFF and then ON the AOC-6000 Series. If the error still occurs, turn OFF the power and then manually move the injection unit to its home position.
Error has occurred in instruments. (General_SmartObjectStatus Defect)	The status of the Smart Syringe attached to the head of the AOC-6000 Plus or that of the SPME fiber or SPME Arrow is "Defective".	Perform replacement with a new Smart Syringe, SPME fiber, or SPME Arrow. Change the status to "OK" or "Suspect" at the PAL terminal.
Error has occurred in instruments. (Smart Object Plunger not present)	The plunger of the Smart Syringe is broken.	Replace with a new Smart Syringe.

If GCMSsolution is unintentionally closed, be sure to restart the computer. Otherwise, the AOC-6000 Series cannot be controlled correctly.

If the injection unit (PAL head) does not go back to its home position after an error occurs, shut down the AOC-6000 Series first and restart it.

For the shutdown procedures, refer to the PAL3 RTC/RSI User Manual.

### 8.3 AOC-6000 Series Status Remains [Run]

If the automatic recovery function of the AOC -6000 Series does not work due to an unexpected error during the analysis (for example, the AOC -6000 Series status remains [Run]), restart the computer.

# Appendix – Method Parameters for Each Injection Method

The following describes the parameters and reference values used in methods for each injection method. Since the optimal parameter values vary depending on the type and quantity of sample, optimize parameter values by eventually measuring samples.

 **NOTE**

- In methods for which the temperature of the sample can be maintained during data measurement including headspace methods, injection operation does not start until the state of the GC unit becomes Ready. Therefore, set the [Analysis Time ] parameter value that allows plenty of time.

 **NOTE**

- From AOC-6000 Control Software Ver.2.0, the default values of the method parameters of Liquid Injection, Headspace Injection and SPME Arrow Injection have been changed. For details, see NOTE for each method parameter.

 **NOTE**

- In AOC-6000 control software Ver. 2.1 and later, the upper settings limit for the heating temperature of a sample vial with an agitator is restricted to 80 °C. This ensures that the internal vial pressure does not become too high when a low boiling point solvent such as hexane is used as the sample solvent. Use a method for high boiling point solvents if heating the vial higher than 80 °C. In a method for high boiling point solvents, the temperature can be set up to 200 °C. However, please set the temperature to a maximum of the solvent boiling point +10 °C.

### AOC-6000 Method List

The following methods are available for use when the AOC-6000 control software is installed.

Method Name	Application	Syringe (example)	Details
Liquid Injection	For liquid injection methods	10 $\mu$ L	A syringe for injecting liquids is used to inject samples.
SPME Injection	For SPME methods	Fiber	Samples adsorbed to SPME fiber are injected. Samples are adsorbed by heating reagents in an agitator while stirring. After injecting samples, fibers are conditioned in a bakeout station.
(For High Boiling Solvent) SPME Injection For High Boiling Solvent			
Headspace Injection	For headspace methods	2.5mL-HS	A headspace syringe is used to inject samples.
(For High Boiling Solvent) Headspace Injection For High Boiling Solvent			
SPME Arrow Injection	For SPME Arrow methods	Arrow	Samples adsorbed to SPME arrow are injected. After the reagent is heated while being stirred by the agitator, samples are adsorbed while being agitated by the Heatex Stirrer. After injecting samples, fibers are conditioned in a bakeout station.
(For High Boiling Solvent) SPME Arrow Injection For High Boiling Solvent			
ITEX Injection	For ITEX DHS methods	ITEX	The reagent is heated while being stirred by the agitator. The headspace portion is pumped multiple times, and samples are adsorbed by the adsorbent inside the syringe.
(For High Boiling Solvent) ITEX Injection For High Boiling Solvent			

### Parameter Groups

Parameters of methods are categorized into the following groups.

Group Name	Description
Analysis	Parameters in this group need to be set to appropriate values according to the target sample to be measured.
Setup	Parameters in this group are determined by the selection of instrument configuration or the instrument selected. When selected the new method, be sure to specify instrument configuration first. They rarely need to be changed once they have been set.
Advanced	Parameters in this group are expanded parameters. Basically keep the initial values and only change them when necessary.

#### NOTE

- When the [Method Parameters] sub-window is opened, parameters in the [Setup] group and [Advanced] group are hidden. Click the arrow on the left side of the group name to display the parameters.

### Method Parameters for Liquid Injection Methods

Parameter Name	Description	Default	Settable Range	Remarks
<b>Analysis Group</b>				
Syringe Tool	Specifies the syringe tool for liquid injection.			Select one from the list of syringe tools for injection connected to the instrument (e.g. LS1, LS2).
Pre Wash Cycles	Number of cycles to wash the syringe before sampling	3	0-15	
Sample Rinse Cycles	Number of cycles to rinse with the sample before sampling	1	0-10	
Sample Aspirate Flow Rate	Speed to take up the sample to be injected	1uL/s	0.1-100uL/s	
Sample Post Aspirate Delay	Waiting time from when the sample to be injected is collected until the syringe is pulled out from the sample vial	2s	0-10s	
Injector	Specifies the injector name.			Select one from the list of the injectors connected to the instrument (e.g. Injector1, Injector2).
Injection Flow Rate	Speed to inject the sample	50uL/min	1-250uL/min	
Post Wash Cycles	Number of cycles to wash the syringe after sample injection	3	0-15	
<b>Setup Group</b>				
Gas Chromatograph	Specifies the GC unit to be used.			Select one from the list of GC units connected to the instrument (e.g. GC1).
Cooled Stack 1	Specifies this item only when using the cooled stack.			Select one from the pull-down list.
Cooled Stack 1 Temperature	Temperature of cooled stack 1	20°C	4-40°C	
Cooled Stack 2	Specifies this item only when using the cooled stack.			Select one from the pull-down list.
Cooled Stack 2 Temperature	Temperature of cooled stack 2	20°C	4-40°C	
Pre Wash Station	Specifies the wash station to be used to wash the syringe before sampling.			Select one from the list of wash stations connected to the instrument.
Post Wash Station	Specifies the wash			Select one from the list

## Appendix – Method Parameters for Each Injection Method

Parameter Name	Description	Default	Settable Range	Remarks
	station to be used to wash the syringe after sampling.			of wash stations connected to the instrument.
Wash Vial Depth	Depth to insert the syringe into the wash solution bottle	40mm	20-73mm	See Note 3.
Waste Port Depth	Depth to insert the syringe into the waste solution bottle	10mm	10-45mm	See Note 3.
Sample Vial Depth	Depth to insert the syringe into the sample vial	30mm	1-45mm	
Bottom Sense Sample Vial	Specifies whether or not to use the bottom sensing function when the syringe is inserted into the sample vial.	Off	On Off	This parameter is only used in the AOC-6000 with RTC(Robotic Tool Change). In the other model, please use the initial value(Off), Not to damage the syringe.
Height From Bottom Sample Vial	Depth to insert the syringe into the sample vial (height from the bottom)	3mm	0-32mm	
Injection Mode	Injection mode of the GC unit	Normal	Normal Fast	When "Fast" is selected, injection is performed at the maximum registered value.
Injection Signal Mode	Timing to send the Start signal	PlungerDown	PreInject PlungerUp PlungerDown None	PreInject: Before the syringe is inserted into the injector PlungerUp: When the syringe is pulled out from the injector PlungerDown: When the plunger is pressed down and the sample is injected None: The Start signal is not output.
Injector Penetration Depth	Depth to insert the syringe into the injector	40mm	10-73mm	
Pre Ahead Option	Specifies the timing to wait for the GC Ready signal.	Disabled	Disabled  After sample rinse  After bubble elimination  After sample asp. In home	Disabled: Standby before washing the syringe which is performed before sampling After sample rinse: Standby after sample rinse (before pumping the sample in and out)

## Appendix – Method Parameters for Each Injection Method

Parameter Name	Description	Default	Settable Range	Remarks
				After bubble elimination: Standby after pumping the sample in and out (before sampling) After sample asp. In home: Standby after sampling (before injection to GC)
<b>Advanced Group</b>				
Pre Wash Solvent Volume	Volume of the wash solvent used for washing the syringe before sampling	8uL	0.1-1000uL	
Pre Wash Solvent Position Step 1	Index of the pre wash station used for the first wash	1	0-4	Set "0" when not using the wash solvent.
Pre Wash Solvent Position Step 2	Index of the pre wash station used for the second wash	0	0-4	Set "0" when not using the wash solvent.
Pre Wash Solvent Position Step 3	Index of the pre wash station used for the third wash	0	0-4	Set "0" when not using the wash solvent.
Pre Wash Solvent Position Step 4	Index of the pre wash station used for the fourth wash	0	0-4	Set "0" when not using the wash solvent.
Pre Wash Aspirate Flow Rate	Speed to collect the wash solvent for washing the syringe before sampling	1uL/s	0.1-100uL/s	
Sample Vial Penetration Speed	Speed to insert the syringe into the sample vial	50mm/s	1-75mm/s	
Sample Rinse Volume	Volume of the solvent used for rinsing with the sample before sampling	3uL	0-1000uL	
Filling Strokes Count	Number of cycles to pump the sample in and out when sampling	5	0-15	
Filling Strokes Volume	Volume of the sample to be pumped in and out when sampling	3uL	0-1000uL	
Filling Strokes Aspirate Flow Rate	Speed to take up the sample by pumping the sample in and out when sampling	5uL/s	2-100uL/s	See Note 2.
Filling Strokes Post Aspirate Delay	Waiting time from when the sample is taken up until it is	0.2s	0-10s	

8.4

## Appendix – Method Parameters for Each Injection Method

Parameter Name	Description	Default	Settable Range	Remarks
	discharged by pumping the sample in and out when sampling			
Filling Strokes Post Dispense Delay	Waiting time from when the sample is discharged until it is taken up next time by pumping the sample in and out when sampling	0.5s	0-10s	
Delay After Filling Strokes	Waiting time after pumping the sample in and out until the sample for injection is collected	0.5s	0-10s	
Air Gap Volume	Volume of the air to be taken up after sampling.	1uL	0-1000uL	
Injector Penetration Speed	Speed to insert the syringe into the injector	100mm/s	2-200mm/s	
Pre Injection Dwell Time	Waiting time from when the syringe is inserted into the injector until the sample is injected	0s	0-15s	
Post Injection Dwell Time	Waiting time from when the sample is injected until the syringe is pulled out	0.3s	0-15s	
Post Wash Solvent Volume	Volume of the wash solvent collected for washing the syringe after sample injection	8uL	0.1-1000uL	
<b>Post Wash Solvent Position Step 1</b>	Index of the post wash station used for the first wash	1	0-4	Set "0" when not using the wash solvent.
<b>Post Wash Solvent Position Step 2</b>	Index of the post wash station used for the second wash	0	0-4	Set "0" when not using the wash solvent.
<b>Post Wash Solvent Position Step 3</b>	Index of the post wash station used for the third wash	0	0-4	Set "0" when not using the wash solvent.
<b>Post Wash Solvent Position Step 4</b>	Index of the post wash station used for the fourth wash	0	0-4	Set "0" when not using the wash solvent.
Post Wash Aspirate Flow Rate	Speed to collect the wash solvent for washing the syringe after the sample injection	1uL/s	0.1-100uL/s	

8.4

## Appendix – Method Parameters for Each Injection Method



### NOTE

1. When changing the syringe tool to a tool with a different syringe size, change the corresponding parameters ([...Volume], [...Flow Rate]) settings to appropriate values.
2. When performing liquid injection with a gas-tight syringe (syringe with a plunger tip), change the value of [Filling Stroke Aspirate Flow Rate] from 5 uL/s to 2 uL/s. This changes the settings so that the sample is suctioned slowly, to prevent bubbles forming inside the syringe.
3. If a metal plate for fastening the vials is attached to the standard wash module, change the value of [Wash Vial Depth] from 40 mm to 44 mm, and change the value of [Waste Port Depth] from 10 mm to 20 mm.
4. Since AOC-6000 Control Software Ver.2.0, the default values of the following method parameters of Liquid Injection have been changed. Please be careful when upgrading from your software version 2.0 or earlier.

Group	Parameter Name	Default	
		Ver.2.0 or later	~ Ver.1.3
Analysis	Injection Flow Rate	50uL/s	100uL/s
Advanced	Pre Wash Aspirate Flow Rate	1uL/s	5uL/s
	Sample Rinse Volume	3uL	6uL
	Filling Strokes Volume	3uL	6uL
	Air Gap Volume	1uL	0uL
	Post Wash Aspirate Flow Rate	1uL/s	5uL/s

### Method Parameters for Headspace Methods

Parameter Name	Description	Default	Settable Range	Remarks
<b>Analysis Group</b>				
Syringe Tool	Specifies the name of the syringe tool for HS			Select one from the list of syringe tools for HS connected to the instrument (e.g. HS1, HS2).
Incubation Temperature	Incubation temperature for sample vials in the agitator	80°C	(Headspace Injection Method) 30-80°C	
			(Headspace Injection For High Boiling Solvent Method) 30-200°C	
Incubation Time	Time to incubate sample vials in the agitator	45min	0.1-600min	
Syringe Temperature	Temperature to heat the syringe	100°C	(Headspace Injection Method) 40-100°C	To prevent deterioration of the syringe, set the syringe temperature at about 30°C at the PAL terminal except during analysis.
			(Headspace Injection For High Boiling Solvent Method) 40-150°C	
Agitator Speed	Agitator's rotating speed	250rpm	250-750rpm	
Pre Purge Time	Time of syringe purge performed before sampling	0s	0-60s	
Injector	Specifies the injector name.			Select one from the list of the injectors connected to the instrument (e.g. Injector1, Injector2).
Injection Flow Rate	Speed of sample injection	25mL/min	1-100mL/min	
Post Purge Time	Time of syringe purge performed after sample injection	60s	0-600s	
Analysis Time	Interval to repeat analysis	15min	0-600min	The time is the total of the GC program time, cooling time, equilibration time, plus some additional time.
<b>Setup Group</b>				
Gas Chromatograph	Specifies the GC unit to be used.			Select one from the list of GC units connected to the instrument (e.g. GC1).

## Appendix – Method Parameters for Each Injection Method

Parameter Name	Description	Default	Settable Range	Remarks
Sync Before Incubation End Time	Specifies the time to start the Cryo Trap operation by using the time before sample vial incubation ends.	0min	0-600min	Use this parameter when Cryo Trap is installed on the GC unit. Set "0 min" when Cryo Trap is not used.
Agitator	Specifies the agitator.			Select one from the list of trays connected to the instrument.
Do Agitation	Specifies whether or not to vibrate (rotate) the agitator.	True	True False	
Heat Agitator	Specifies whether or not to heat the agitator.	True	True False	
Wait For Readiness Agitator	Specifies whether or not to wait until the actual temperature reaches the set value when setting the temperature of the agitator.	True	True False	
Sample Vial Depth	Depth to insert the syringe into the sample vial	15mm	10-50mm	
Heat Syringe	Specifies whether or not to heat the headspace syringe.	True	True False	
Wait For Readiness Syringe	Specifies whether or not to wait until the actual temperature reaches the set value when setting the temperature of the headspace syringe.	True	True False	
Injection Signal Mode	Timing to send the Start signal	PlungerUp	PreInject PlungerUp	PreInject: Before the syringe is inserted into the injector PlungerUp: When the syringe is pulled out from the injector
Injector Penetration Depth	Depth to insert the syringe into the injector	40mm	15-50mm	
Continuous Purge	Specifies whether or not to purge the syringe continuously except during sampling to injection.	False	True False	Select "True" to perform purge. In this case, the parameter set for Pre/Post Purge Syringe is ignored.
<b>Advanced Group</b>				
Enable Pre Filling	Specifies whether or not to pressure the vial before sampling	True	True False	In the script of the previous version of AOC-6000 control software, it was False internally.

## Appendix – Method Parameters for Each Injection Method

---

Parameter Name	Description	Default	Settable Range	Remarks
Filling Strokes Count	Number of times to pump the sample in and out when sampling	5	0-15	
Filling Strokes Volume	Volume of pumping the sample in and out when sampling	1.2mL	0-2.2mL	
Filling Strokes Aspirate Flow Rate	Speed to take up the sample by pumping the sample in and out	6mL/min	1-100mL/min	
Delay After Filling Strokes	Waiting time after the sample is pumped in and out until the sample for injection is collected	30s	0-60s	
Sample Aspirate Flow Rate	Speed to take up the sample to be injected	6mL/min	1-100mL/min	
Sample Post Aspirate Delay	Waiting time from when the sample is collected until the syringe is pulled out from the sample vial	0s	0-600s	
Sample Vial Penetration Speed	Speed to insert the syringe into the sample vial	25mm/s	1-75mm/s	
Injector Penetration Speed	Speed to insert the syringe into the injector	25mm/s	1-100mm/s	
Pre Injection Dwell Time	Waiting time from when the syringe is inserted into the injector until the sample is injected	3s	0-60s	
Post Injection Dwell Time	Waiting time from when the sample is injected until the syringe is pulled out	10s	0-60s	
Agitator On Time	Time of the agitator's rotation	5s	1-600s	
Agitator Off Time	Time that the rotation of the agitator is stopped	2s	0-600s	

## Appendix – Method Parameters for Each Injection Method

 **NOTE**

1. Since AOC-6000 Control Software Ver.2.1, the default values of the following method parameters of Headspace Injection have been changed. Please be careful when upgrading from your software version 2.0.

Group	Parameter Name	Default	
		Ver.2.1 or later	Ver.2.0
Analysis	Syringe Temperature	100°C	105°C

2. Since AOC-6000 Control Software Ver.2.0, the default values of the following method parameters of Headspace Injection have been changed. Please be careful when upgrading from your software version 2.0 or earlier.

Group	Parameter Name	Default	
		Ver.2.0 or later	~Ver.1.3
Analysis	Incubation Temperature	80°C	40°C
	Incubation Time	45min	5min
	Syringe Temperature	105°C	60°C
	Pre Purge Time	0s	5s
	Injection Flow Rate	25mL/min	10mL/min
	Post Purge Time	60s	10s
Advanced	Enable Pre Filling	True	Set to "False" inside the method.
	Filling Strokes Count	5	0
	Filling Strokes Volume	1.2mL	2mL
	Filling Strokes Aspirate Flow Rate	6mL/min	12mL/min
	Delay After Filling Strokes	30s	0.5s
	Sample Aspirate Flow Rate	6mL/min	12mL/min
	Sample Post Aspirate Delay	0s	1s
	Sample Vial Penetration Speed	25mm/s	50mm/s
	Injector Penetration Speed	25mm/s	50mm/s
	Pre Injection Dwell Time	3s	0.5s
Post Injection Dwell Time	10s	0.5s	

**Method Parameters for SPME Methods**

Parameter Name	Description	Default	Settable Range	Remarks
<b>Analysis Group</b>				
Fiber Tool	Specifies the name of the syringe tool for SPME.			Select one from the list of syringe tools for SPME connected to the instrument.
Conditioning Port	Specifies the fiber conditioning port.			Select one from the pull-down list.
Conditioning Temperature	Temperature for fiber conditioning	40°C	40-350°C	
Pre Conditioning Time	Time of fiber conditioning performed before extraction	0min	0-600min	
Incubation Temperature	Incubation temperature for sample vials in the agitator	40°C	(SPME Injection Method) 30-80°C	
			(SPME Injection For High Boiling Solvent Method) 30-200°C	
Incubation Time	Time to incubate sample vials in the agitator	5min	0-600min	
Agitator Speed	Agitator's rotating speed	250rpm	250-750rpm	
Sample Vial Depth	Depth to insert the fiber needle into the sample vial	22mm	8-70mm	See Note.
Sample Extract Time	SPME time	10min	0-600min	
Injector	Specifies the injector name.			Select one from the list of the injectors connected to the instrument (e.g. Injector1, Injector2).
Sample Desorb Time	Desorption time	1min	0-600min	
Post Conditioning Time	Time of fiber conditioning performed after desorption	3min	0-600min	
Analysis Time	Interval to repeat analysis	15min	0-600min	The time is the total of the GC program time, cooling time, equilibration time, plus some additional time.
<b>Setup Group</b>				
Gas Chromatograph	Specifies the GC unit to be used.			Select one from the list of GC units connected to the instrument (e.g. GC1).
Sync Before Extraction End	Specifies the time to start the Cryo Trap	0min	0-600min	Use this parameter when Cryo Trap is installed on

## Appendix – Method Parameters for Each Injection Method

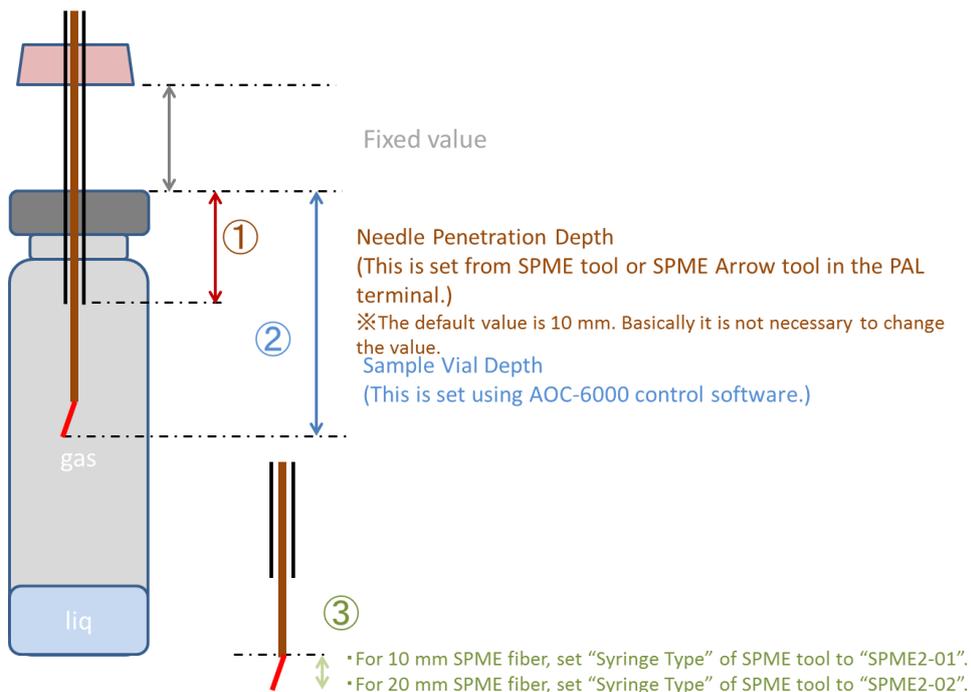
Parameter Name	Description	Default	Settable Range	Remarks
Time	operation by using the time before SPME ends.			the GC unit. Set "0 min" when Cryo Trap is not used.
Agitator	Specifies the agitator.			Select one from the list of trays connected to the instrument.
Do Agitation	Specifies whether or not to vibrate (rotate) the agitator.	True	True False	
Heat Agitator	Specifies whether or not to heat the agitator.	True	True False	
Wait For Readiness Agitator	Specifies whether or not to wait until the actual temperature reaches the set value when setting the temperature of the agitator.	True	True False	
Internal Standard Station	Specifies the position to place the internal standard solution vial.			Select one from the pull-down list.
Internal Standard Position	Specifies the index on the station for internal standard solution vial.	1	1-70	
Injector Penetration Depth	Depth to insert the fiber needle into the injector	54mm	15-70mm	
Injection Signal Mode	Timing to send the Start signal	Before Expose	Before Expose After Expose	Before Expose : The Start signal is output when SPME is injected. After Expose : The Start signal is output when desorption starts.
<b>Advanced Group</b>				
Internal Standard Adsorb Time	Time for the internal standard solution to adsorb	0min	0-600min	
Internal Standard Penetration Depth	Depth to insert the fiber needle into the internal standard solution vial	32mm	10-70mm	
Sample Vial Penetration Speed	Speed to insert the syringe into the sample vial	20mm/s	2-75mm/s	
Injector Penetration Speed	Speed to insert the syringe into the injector	100mm/s	2-200mm/s	
Agitator On Time	Time of the agitator's rotation	5s	0-600s	
Agitator Off Time	Time that the rotation of the agitator is stopped	2s	0-600s	

### NOTE

1. In this software, the definition of [Penetration Depth], which is the depth that the fiber needle penetrates for absorption and desorption of the sample in SPME or SPME Arrow, is the **distance between the reference position and the tip when the fiber is pulled out.**

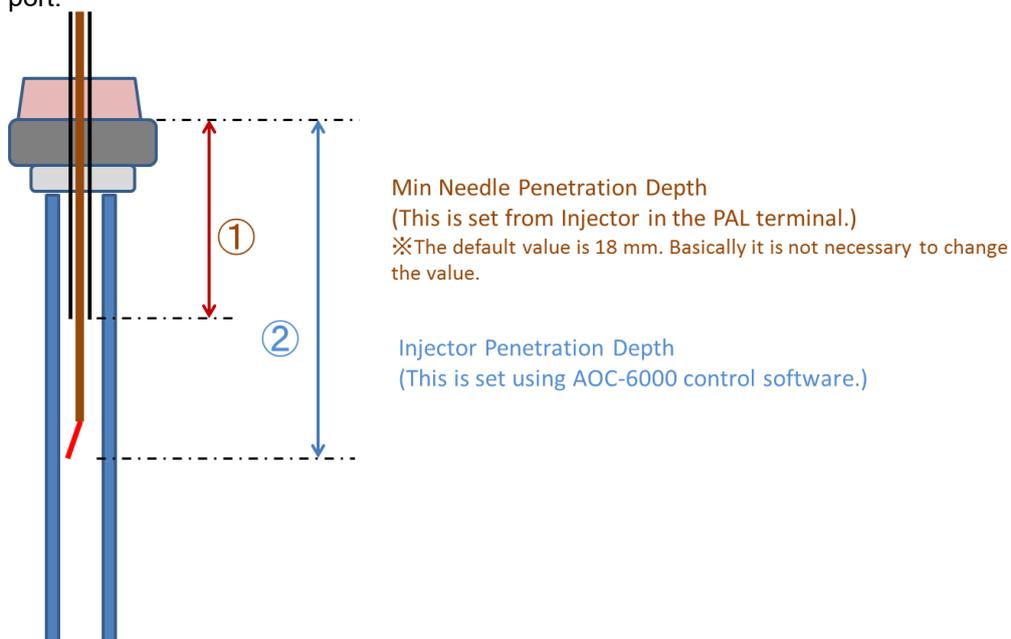
#### ■ Sample Absorption

In sample absorption, the settings are configured as per the figure below.



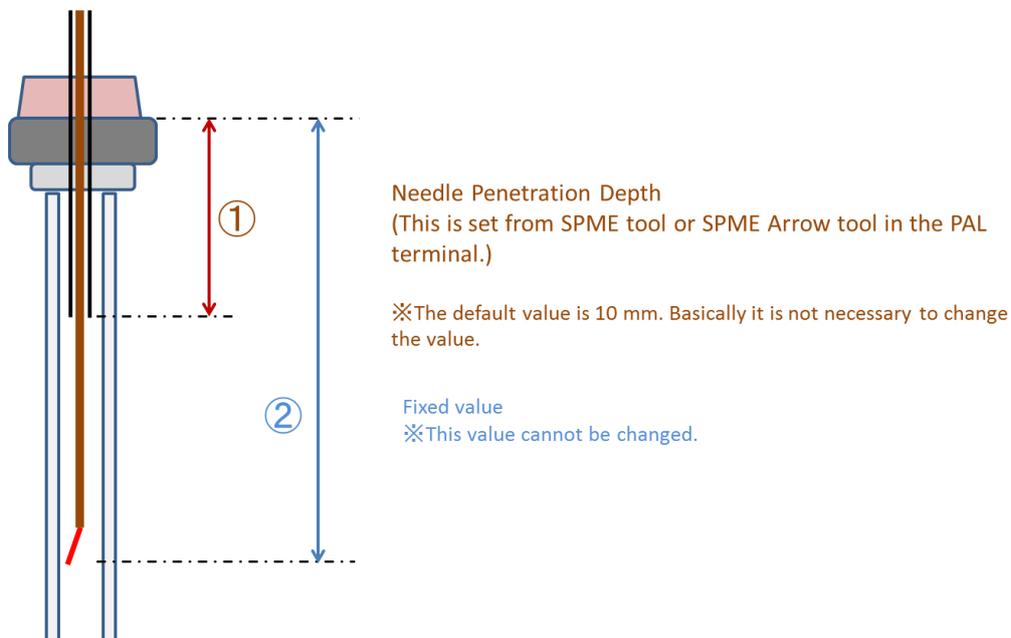
#### ■ Sample Desorption at the Injection Port

The settings are configured as per the figure below in the case of sample desorption at the injection port.



### ■ Conditioning

The settings are configured as per the figure below in the case of SPME fiber and SPME Arrow conditioning.



2. The table below shows the recommended sample volume for SPME and SPME Arrow methods by vial size.

- SPME Injection

([Sample Vial Depth] is set to 22 mm when the fiber length is 10 mm and 31 mm when the fiber length is 20 mm.)

Vial Size	Headspace Extraction		Immersion Extraction	
	Fiber Length 10 mm	Fiber Length 20 mm	Fiber Length 10 mm	Fiber Length 20 mm
10 mL	6 mL max	Not recommended	9 mL	Not recommended
20 mL	15 mL max.	13 mL max.	18 mL	18 to 19 mL

- SPME Arrow Injection

Vial Size	Headspace Extraction	Immersion Extraction
10mL	Not recommended	Not recommended
20mL	13mL max	18 to 19 mL

### Method Parameters for SPME Arrow Methods

Parameter Name	Description	Default	Settable Range	Remarks
<b>Analysis Group</b>				
SPME Arrow Tool	Specifies the name of the syringe tool for SPME Arrow.			Select one from the list of syringe tools for SPME Arrow connected to the instrument.
Conditioning Port	Specifies SPME Arrow conditioning port.			Select one from the pull-down list.
Conditioning Temperature	Temperature for SPME Arrow conditioning	40°C	40-350°C	
Pre Conditioning Time	Time of SPME Arrow conditioning performed before extraction	0min	0-600min	
Incubation Temperature	Incubation temperature for sample vials in the agitator and Stirrer	40°C	(SPME Arrow Injection Method) 30-80°C	
			(SPME Arrow Injection For High Boiling Solvent Method) 30-200°C	
Incubation Time	Time to incubate sample vials in the agitator	5min	0-600min	
Agitator Speed	Agitator's rotating speed	250rpm	250-750rpm	
Stirrer Speed	Stirrer's rotating speed	250rpm	0-1600rpm	
Sample Vial Depth	Depth to insert the fiber needle into the sample vial	33mm	8-70mm	See Note.
Sample Extract Time	SPME Arrow sampling time	10min	0-600min	
Injector	Specifies the Arrow injector name.			Select one from the list of the Arrow injectors connected to the instrument (e.g. Arrow Injector1, Arrow Injector2).
Sample Desorb Time	Desorption time	2min	0-600min	
Post Conditioning Time	Time of SPME Arrow conditioning performed after desorption	3min	0-600min	
Analysis Time	Interval to repeat analysis	15min	0-600min	
<b>Setup Group</b>				
Gas Chromatograph	Specifies the GC unit to be used.			
Wash Station	Specifies the wash station to use for the			Select one from the pull-down list.

## Appendix – Method Parameters for Each Injection Method

Parameter Name	Description	Default	Settable Range	Remarks
	SPME Arrow solvent wash before extraction			
Do Pre Wash	Specifies whether to perform the SPME Arrow solvent wash before extraction	False	True False	
Agitator	Specifies the agitator.			Select one from the pull-down list.
Stirrer	Specifies the stirrer.			Select one from the pull-down list.
Do Agitation	Specifies whether or not to vibrate (rotate) the agitator and stirrer.	True	True False	
Heat Agitator and Stirrer	Specifies whether or not to heat the agitator and stirrer.	True	True False	
Internal Standard Station	Specifies the position to place the internal standard solution vial.			Select one from the pull-down list.
Internal Standard Position	Specifies the index on the station for internal standard solution vial.	1	1-70	
Injector Penetration Depth	Depth to insert the fiber needle into the injector	54mm	15-70mm	
Injection Signal Mode	Timing to send the Start signal	Before Expose	Before Expose After Expose	Before Expose : The Start signal is output when SPME is injected. After Expose : The Start signal is output when desorption starts.
Do Post Wash	Specifies whether to perform the SPME Arrow solvent wash after desorption	False	True False	
<b>Advanced Group</b>				
Pre Solvent Index	Index for the wash station used in the solvent wash before extraction	1	1-4	
Pre Wash Time	Solvent wash time before extraction	0min	0-10min	
Pre Wash Vial Depth	SPME Arrow insertion depth with respect to the wash vial for the solvent wash before extraction	35mm	10-35mm	
Internal Standard Adsorb Time	Time for the internal standard solution to adsorb	0min	0-600min	

## Appendix – Method Parameters for Each Injection Method

Parameter Name	Description	Default	Settable Range	Remarks
Internal Standard Penetration Depth	Depth to insert the SPME Arrow needle into the internal standard solution vial	32mm	10-70mm	
Sample Vial Penetration Speed	Speed to insert the syringe into the sample vial	20mm/s	2-75mm/s	
Injector Penetration Speed	Speed to insert the syringe into the Arrow injector	100mm/s	2-200mm/s	
Post Solvent Index	Index for the wash station used in the solvent wash after desorption	1	4	
Post Wash Time	Solvent wash time after desorption	0min	0-10min	
Post Wash Vial Depth	SPME Arrow insertion depth with respect to the wash vial for the solvent wash after desorption	35mm	10-35mm	

### NOTE

1. Since AOC-6000 Control Software Ver.2.0, the default values of the following method parameters of SPME Arrow Injection have been changed. Please be careful when upgrading from your software version 2.0 or earlier.

Group	Parameter Name	Default	
		Ver.2.0 or later	~Ver.1.3
Analysis	Stirrer Speed	250rpm	1000rpm
	Sample Vial Depth	33mm	40mm

### Method Parameters for ITEX Methods

Parameter Name	Description	Default	Settable Range	Remarks
<b>Analysis Group</b>				
ITEX Tool	Specifies the name of the syringe tool for ITEX			Select one from the list of syringe tools for ITEX connected to the instrument (e.g. ITEX1, ITEX2).
Trap Pre Cleaning Temperature	Trap cleaning temperature before extraction	250°C	100-350°C	
Trap Pre Cleaning Time	Trap cleaning time before extraction	300s	0-86400s	
Incubation Temperature	Incubation temperature for sample vials in the agitator	40°C	(ITEX Injection Method) 30-80°C	
			(ITEX Injection For High Boiling Solvent Method) 30-200°C	
Incubation Time	Time to incubate sample vials in the agitator	5min	0.1-600min	
Agitator Speed	Agitator's rotating speed	700rpm	250-750rpm	
Syringe Temperature	Syringe Temperature	70°C	(ITEX Injection Method) 40-110°C	
			(ITEX Injection For High Boiling Solvent Method) 40-150°C	
Trap Extraction Temperature	Trap temperature during extraction	40°C	30-150°C	
Extraction Strokes	Number of strokes during extraction	10	0-99	
Injector	Specifies the injector name.			Select one from the list of the injectors connected to the instrument (e.g. Injector1, Injector2).
Injector Aspirate Flow Rate	Intake flow rate at the injection port	10µL/s	1-1000µL/s	
Desorb Temperature	Trap temperature during desorption	250°C	50-350°C	
Desorb Flow Rate	Injection flow rate during desorption	100µL/s	5-1000µL/s	
Trap Post Cleaning Temperature	Trap cleaning temperature after desorption	250°C	100-350°C	
Trap Post Cleaning Time	Trap cleaning time after desorption	0s	0-86400s	
Analysis Time	Analysis time	15min	0-600min	
<b>Setup Group</b>				
Gas Chromatograph	Specifies the GC unit to be used.			Select one from the list of GC units connected to

## Appendix – Method Parameters for Each Injection Method

Parameter Name	Description	Default	Settable Range	Remarks
				the instrument (e.g. GC1).
Sync Before Incubation	Specifies the time to start the Cryo Trap operation by using the time before sample vial incubation ends.	0min	0-600min	Use this parameter when Cryo Trap is installed on the GC unit. Set "0 min" when Cryo Trap is not used.
Agitator	Specifies the agitator.			Select one from the pull-down list.
Heat Agitator	Specifies whether or not to heat the agitator.	True	True False	
Sample Vial Depth	Depth to insert the syringe into the sample vial	15mm	10-35mm	
Water Removal	Specifies whether to perform water removal	Disable	Disable Enable	
Water Removal Position	Specifies the waste liquid bottle for dispensing the removed water			Select one from the pull-down list.
Injection Signal Mode	Timing to send the Start signal	PlungerUp	PreInject PlungerUp PlungerDown	
Injector Penetration Depth	Depth to insert the syringe into the injector	33mm	10-35mm	
<b>Advanced Group</b>				
Extraction Volume	Sample aspiration volume during extraction	1000µL	0-1300µL	
Extraction Aspirate Flow Rate	Sample aspiration flow rate during extraction	100µL/s	10-1000µL/s	
Extraction Dispense Flow Rate	Sample dispensing flow rate during extraction	100µL/s	10-1000µL/s	
Sample Prefill Rate	Rate of aspiration volume from the sample after extraction	40%	0-100%	
Water Removal Trap Temperature	Trap temperature during water removal	60°C	40-150°C	
Water Removal Purge Time	Purge time during water removal	0s	0-600s	
Injector Penetration Speed	Speed to insert the syringe into the injector	50mm/s	1-100mm/s	
Post Inject Delay	Waiting time from when the sample is injected until the syringe is pulled out	0s	0-600s	

The typical sequence for the ITEX method is shown below.

