



Operation Walkthrough

Head Space Gas Chromatography Mass Spectrometer (HS-GCMS) with Solid Phase Microextraction (SPME)

Melbourne TrACEES Platform



Doc No. WT-GC-SPME-v1.0

Created by: Crystal Hartanto

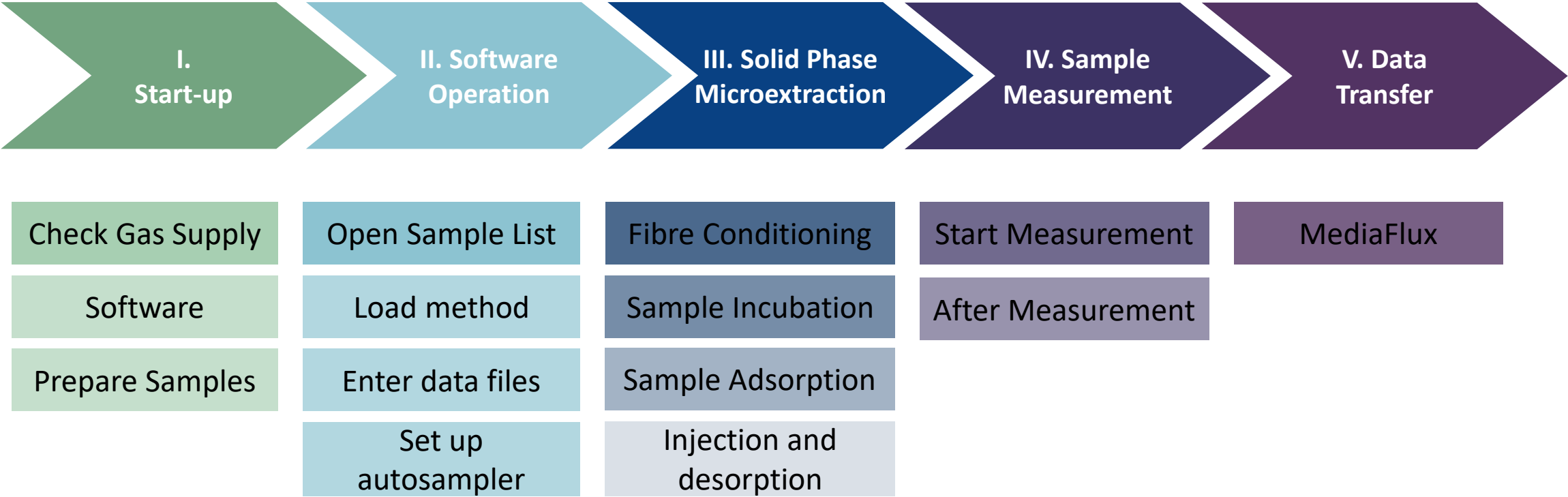
Reviewed by: Alex Duan

Approved by: Alex Duan

Nov 2023, Version 1



GCMS Operation Flow



Operation Flow – Start-up

I.
Start-up

II. Software
Operation

III. Solid Phase
Microextraction

IV. Sample
Measurement

V. Data
Transfer



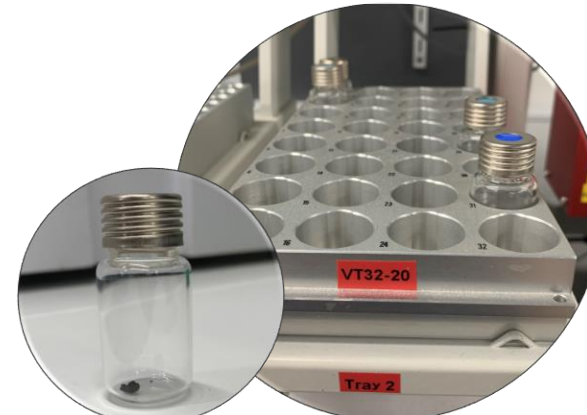
Check Gas Supply

N₂ gas connection is pre-fixed.
Ensure the supply is working
by checking pressure gauge



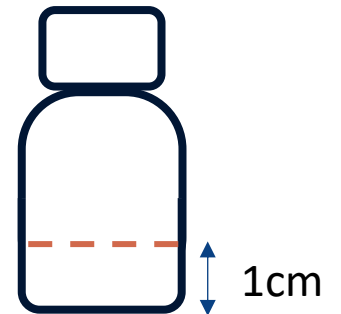
Software

Open **GCMS Real Time Analysis**
and **Cycle Composer** software.
When prompted a login
window, enter “Admin” as
username with no password



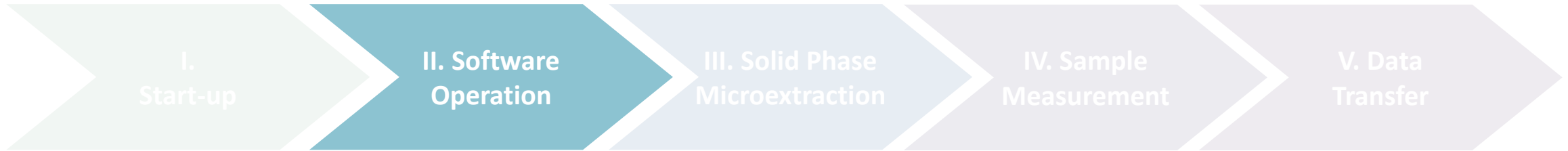
Prepare Samples

Place samples in head
space vials.
Load sample on to
Tray 2



Ensure less
than 1cm

Operation Flow – Use Software

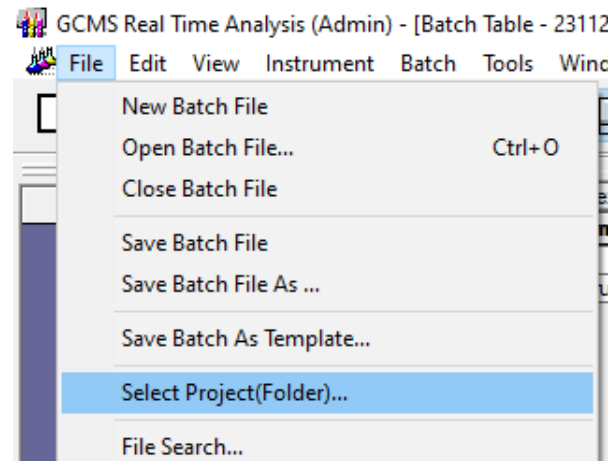


Open Sample List

Load method

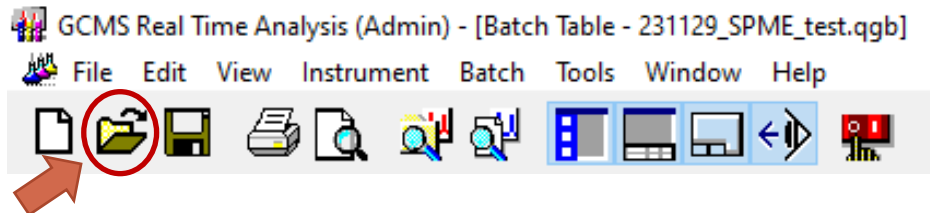
Enter data files

Set up
autosampler



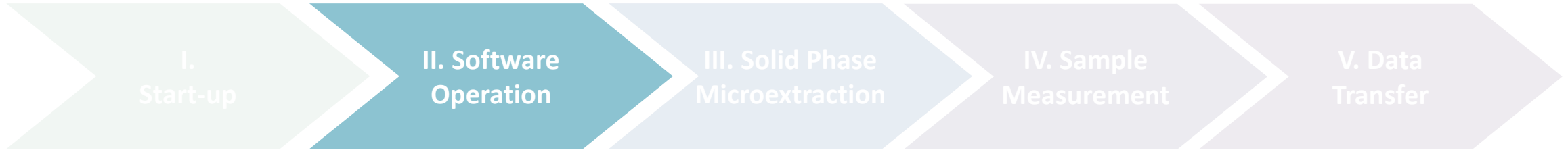
In **GCMS Real Time Analysis**, Click “Select Project(Folder)” under “File” in Menu bar

Select the right folder from the pop-up window



Click “Open” button and load a pre-existing sample list as batch file (*.qgb)

Operation Flow



Open Sample List

Load method

Enter data files

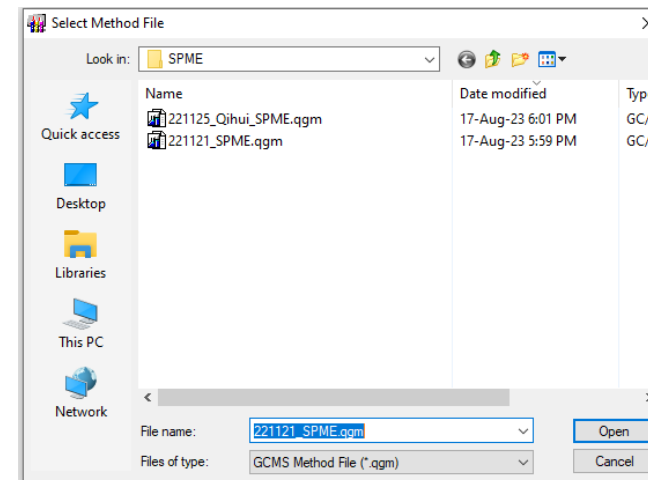
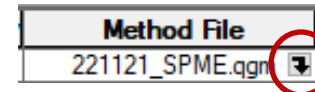
Set up
autosampler

Folder: C:\GCMSsolution\Data\01UOM\AlexDuan\SPME

	Run Mode	Inj. V	Sample Name	Sample Type	Leve	Analysis Ty	Method File	Data File	Report Outp	Report File	Tuning File
1	DL AQ	1	test1	0:Unknown	1	QT ILT	221121_SPME.qgm	1129_SPME_1.qgd	☐ Print	a\l\es\l\es' qual report.qgr	1103_atune.qgt
2	DL AQ	1	test2	0:Unknown	1	QT ILT	221121_SPME.qgm	1129_SPME_2.qgd	☐ Print	a\l\es\l\es' qual report.qgr	1103_atune.qgt

1. Give each sample an appropriate name

2. Select a pre-created GCMS method based on the user's project.



Operation Flow



Open Sample List

Load method

Enter data files

Set up
autosampler

Folder: C:\GCMSsolution\Data\01UOM\AlexDuan\SPME

	Run Mode	Inj. V	Sample Name	Sample Type	Leve	Analysis Ty	Method File	Data File	Report Outp	Report File	Tuning File
1	DL AQ	1	test1	0:Unknown	1	QT ILT	221121_SPME.qgm	1129_SPME_1.qgd	☐ Print	a\l\nes\l\nes' qual report.qgr	1103_atune.qgt
2	DL AQ	1	test2	0:Unknown	1	QT ILT	221121_SPME.qgm	1129_SPME_2.qgd	☐ Print	a\l\nes\l\nes' qual report.qgr	1103_atune.qgt

3. Data files should be unique for each sample.
Operators must ensure data files will not overwrite each other.

Suggested format “[YYMMDD]-[Operator Initial]-[Sample].qgd”, e.g. “231120-AD-sample1.qgd”
Do Not use “space” or any special characters.

5. Use the latest tuning file

4. Click “**Save Batch File As**” under “File” tab with a different batch file name.



Operation Flow



Open Sample List

Load method

Enter data files

Set up
autosampler

1. In **Cycle Composer** software, create an identical sample list to the one in GCMS

Folder: C:\GCMSSolution\Data\01UOM\AlexDuan\SPME

	Run Mode	Inj. V	Sample Name	Sample Type	Leve	Analysis Ty	Method File	Data File
1	DL AQ	1	test1	0:Unknown	1	QT ILT	221121_SPME.qgm	1129_SPME_1.qgd
2	DL AQ	1	test2	0:Unknown	1	QT ILT	221121_SPME.qgm	1129_SPME_2.qgd

PAL Cycle Composer PAL 1 (C:\CTC METHODS)

File Help

Sample List Method Editor

Sample List Name
SPME-test

Start Pause Reset PAL View Log File Append Line Insert Line Delete Line Trays

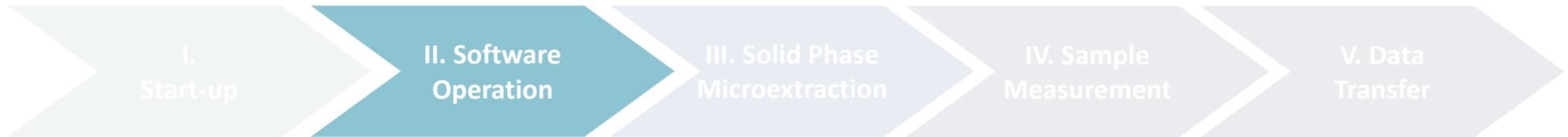
	Status	Method	Volume	Tray	Vial	Sample Type	Sample ID
1		SPME-INJ2	1.0	Tray2	1	Unknown	test1
2		SPME-INJ2	1.0	Tray2	2	Unknown	test2

2. Choose the pre-existing injection method under **Method** column

3. Enter "Tray2" under **Tray** column and the corresponding vial numbers under **Vial** column e.g., 1, 2, ...

4. Give an appropriate name for each sample

Operation Flow



To start measurement, click start button in **GCMS Real Time Analysis**, then start button in **Cycle Composer**

GCMS Real Time Analysis (Admin) - [Batch Table - 231129_SPME_test.qgb]

File Edit View Instrument Batch Tools Window Help

Folder: C:\GCMSsolution\Data\01UOM\AlexDuan\SPME

	Run Mode	Inj. V	Sample Name	Sample Type	Leve	Analysis Ty	Method File	Data File
1	DL AQ	1	test1	0:Unknown	1	QT ILT	221121_SPME.qgm	1129_SPME_1.qgd
2	DL AQ	1	test2	0:Unknown	1	QT ILT	221121_SPME.qgm	1129_SPME_2.qgd

Cycle Composer PAL 1 (C:\CTC METHODS)

File Help

Sample List Method Editor

Sample List Name: SPME-test

Start Pause Reset PAL View Log File Append Line Insert Line Delete Line Trays

	Status	Method	Volume	Tray	Vial	Sample Type	Sample ID
1		SPME-INJ2	1.0	Tray2	1	Unknown	test1
2		SPME-INJ2	1.0	Tray2	2	Unknown	test2

Automation starts now

sit back & relax

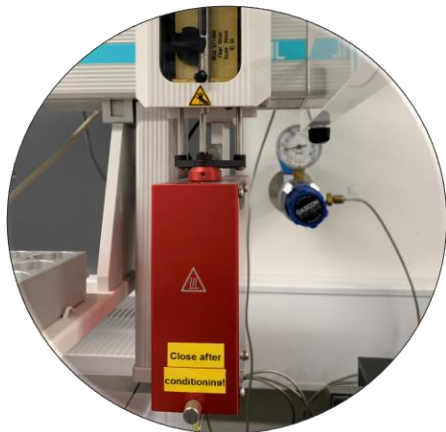
Following slides will show the automated SPME adsorption and desorption process, and GCMS analysis

III. Solid Phase Microextraction

SPME utilises a fine fibre to adsorb volatile compounds in a sample.
Once started, the autosampler fibre will automatically go through:



Fibre Conditioning



Conditioning the
fibre under N₂
at 250 °C

Sample Incubation



Sample vial will be
moved to the incubator
and heated. Temperature
and time are determined
by method

Sample Adsorption



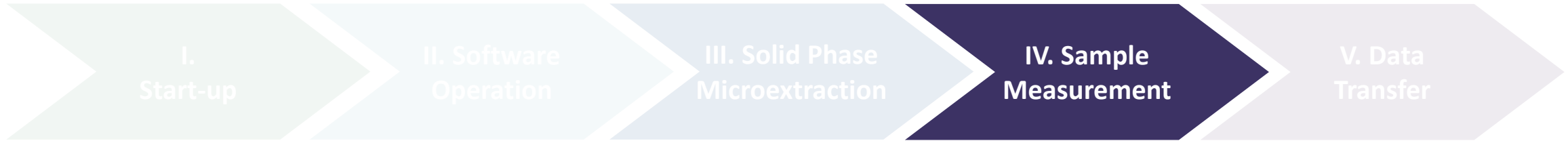
SPME fibre will adsorb
volatile compounds in
the head space of the
sample vial

Injection and Desorption

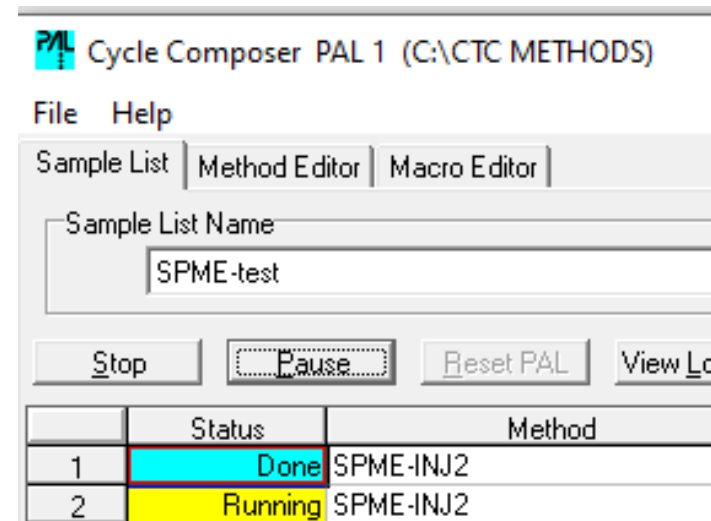
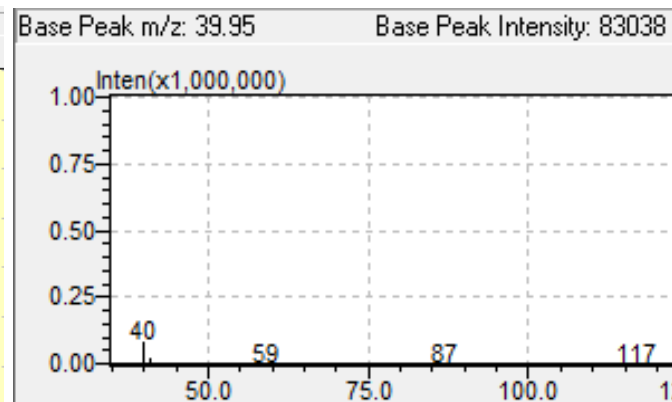
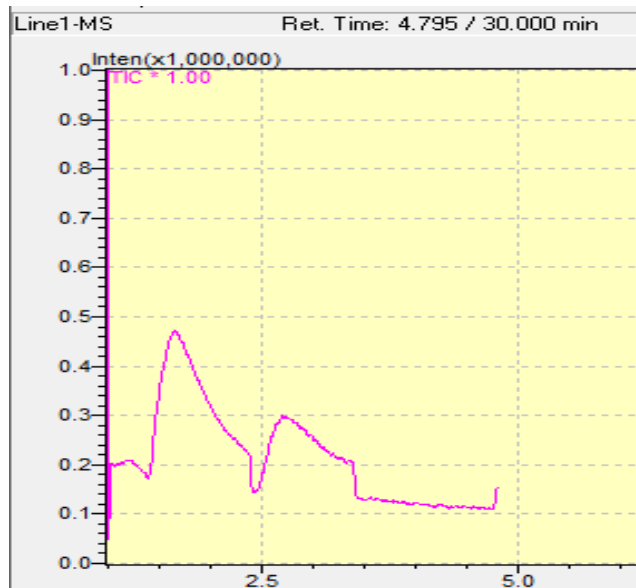


The fibre will be inserted
to the GC injection port.
Compounds will be
desorbed from the fibre
and be analysed

GCMS measurement



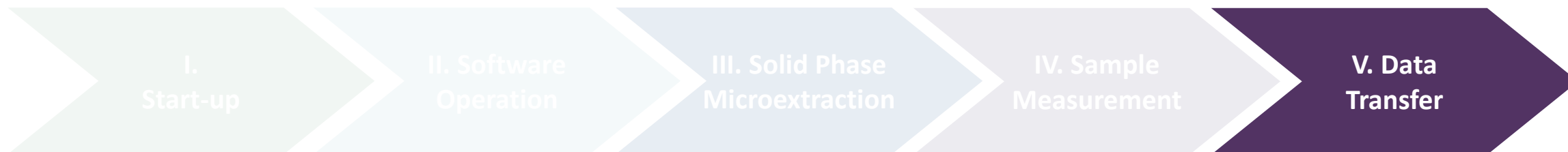
Measurement will automatically start.



GCMS Real Time Analysis shows chromatogram and mass spectrum as the measurement proceeds. **Cycle composer** shows the progress for each sample

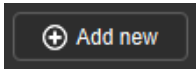
Instrument shutdown is not required once the measurements are completed.
Remove all sample vials from holder and dispose

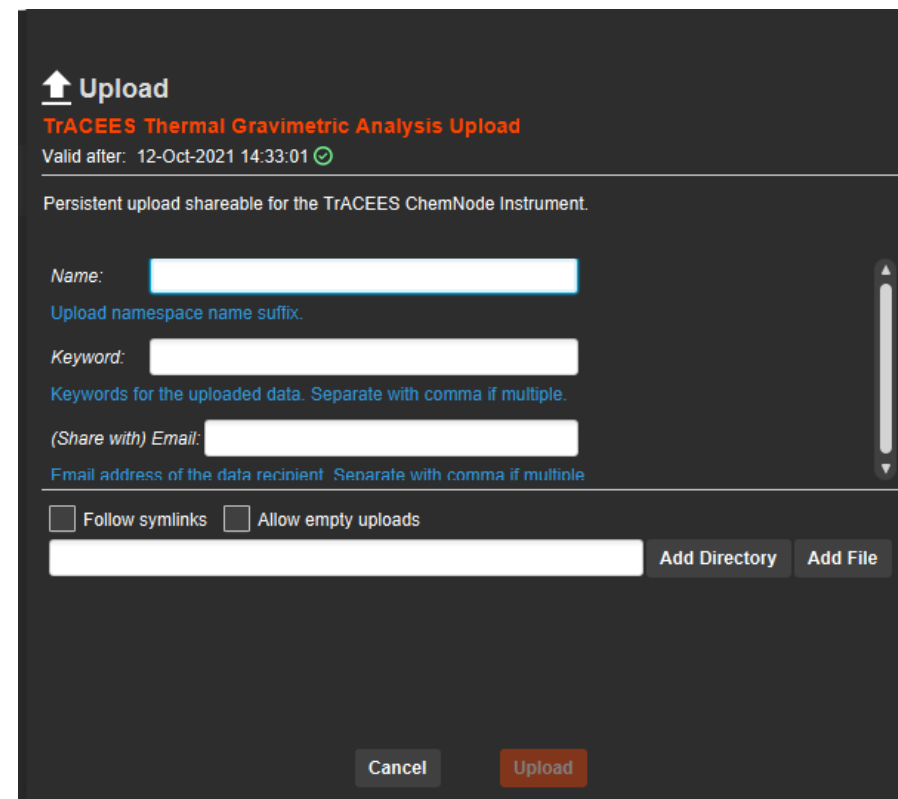
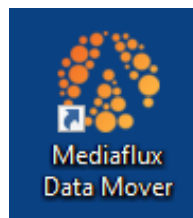
Data transfer



Users shall not bring and use their own data storage device
e.g., USB sticks.

Mediaflux Data Mover is preferred.

1. Open Mediaflux Data Mover from Desktop
2. Click Add new 
3. In **Name** field, enter user's name and date
4. In **Keyword** field, enter technique name, e.g. HS-GCMS
5. Enter recipient (user) email address
6. Click "Add Directory" (to add the entire data folder), or click "Add File" (to select a single file)
7. Click Upload



Upload
TrACEES Thermal Gravimetric Analysis Upload
Valid after: 12-Oct-2021 14:33:01

Persistent upload shareable for the TrACEES ChemNode Instrument.

Name:

Upload namespace name suffix.

Keyword:

Keywords for the uploaded data. Separate with comma if multiple.

(Share with) Email:

Email address of the data recipient. Separate with comma if multiple.

☐ Follow symlinks ☐ Allow empty uploads