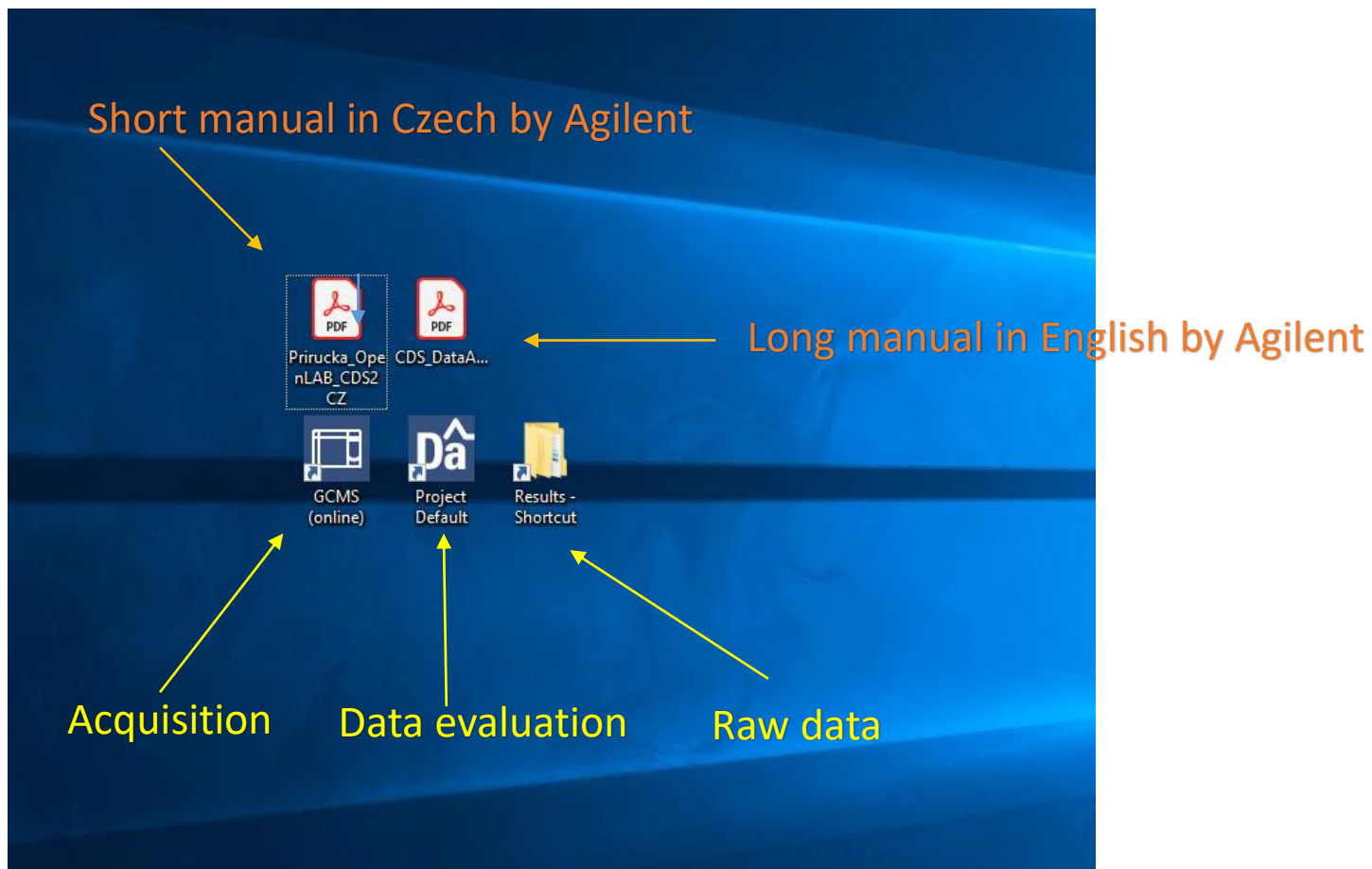


Software instruction for open access GC/MS

10.3. 2022

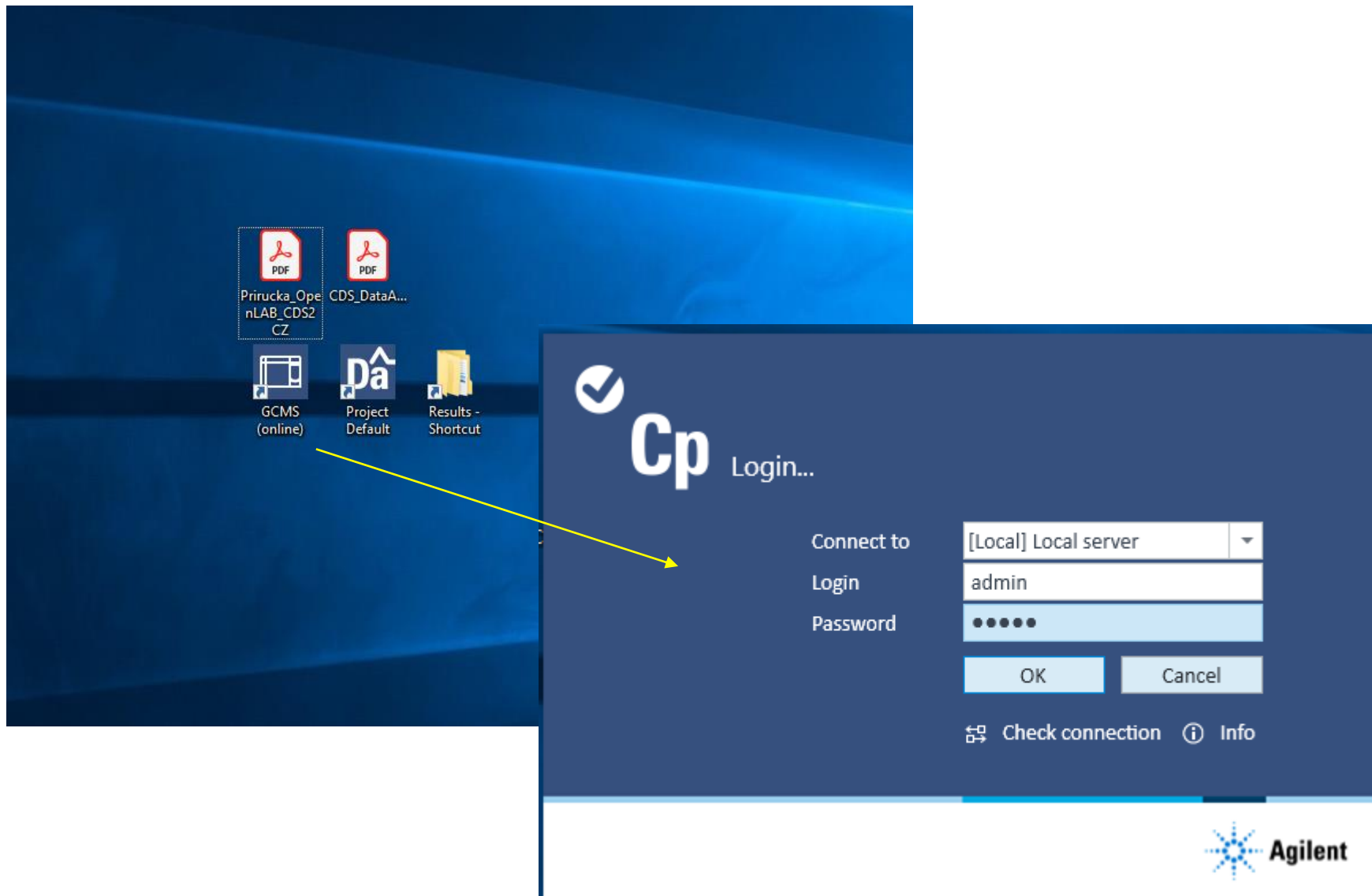
OpenLAB

OpenLAB



Acquisition

Acquisition login



Load your sequence

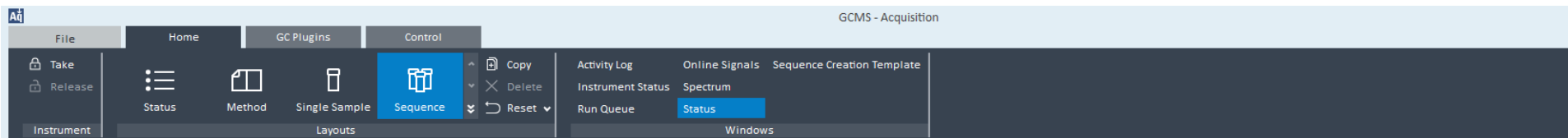
1.

2.

The screenshot displays the Agilent software interface. The top bar includes tabs for File, Home, GC Plugins, and Control. The 'Control' tab is active, showing buttons for Take, Release, Status, Method, Single Sample, and Sequence. The 'Sequence' button is highlighted with a red arrow labeled '1.'. Below the top bar, the 'Sequence - Untitled' window is open, showing a table with two rows. A red arrow labeled '2.' points to the 'Sequence - Untitled' window title bar.

	☒	Action	Vial	Sample type	Acq. method
1	☒	Inject	101	Sample	AS_M_low-C_high_waxeter.amx
2	☒	Inject	101	Sample	

Fill table



Sequence – Untitled

General
Properties
Run Options
Injections
Table

	Action	Vial	Sample type	Acq. method	Proc. method	Inj/Vial	Injection source	Sample name	Data file
1	☒ Inject	101	Sample	AS_M_low-C_high_waxeter.amx	OpenAccess.pmx	1	GC Injector - Front	VV<DS>	<S>
2	☒ Inject	101	Sample			1	GC Injector - Front		

Position of vials in autosampler
(from 101 to 116)

Sample

2 Standard acquisition methods are available

1 Processing method is available

Number of injections from one vial

Sample name

File name

Run

The screenshot shows the GCMS - Acquisition software interface. The 'Sequence - Untitled' window is open, displaying a table of sample data. The 'Result path' and 'Result name' fields are highlighted with a red oval. A red box contains the text '1. Name of your data set (initials in the beginning)!!!' with an arrow pointing to the 'Result name' field. A green box contains the text '2. Run' with an arrow pointing to the 'Run' button.

	Sample type	Vial	Sample name	Acq. method	Data file	Proc. method	Injection source
1	Sample	102	VV	AS_M_high-C_high.amx	VV181126b1	OpenAccess.pmx	GC Injector - Fr...
2	Sample	102	VV	AS_M_high-C_high.amx	VV181126b2	OpenAccess.pmx	GC Injector - Fr...
3	Sample	103	VV	AS_M_high-C_high.amx	VV181126b3	OpenAccess.pmx	GC Injector - Fr...

Result path: C:\CDSP\Projects\User\Results

Result name: VV181126

1. Name of your data set (initials in the beginning)!!!

2. Run

Run

Status

Stop the sequence

Status

The screenshot shows the GCMS - Acquisition software interface. The top menu bar includes File, Home, Control, and GC Plugins. The GC Plugins menu is open, showing options like Activity Log, Spectrum, Run Queue, Status, Online Signals, and Windows. The Run Queue panel displays a table of sequences. The Instrument Status panel shows various parameters like Tune file, Idle, Temperature, Voltage, Pressure, and a progress bar. The Online Signals panel shows a plot of Signal 2: test plot, Signal 1: test plot, and TIC. The Spectrum panel shows a plot of Abundance vs m/z.

Run Queue

State	Type	Result Name	User	Acquisition Method	Details
Completed	Sequence	20181123 081608	admin	AS_M_high-C_high.amx	Details
Completed	Sequence	20181123 095249	admin	AS_M_low-C_high.amx	Details
Acquiring	Sequence	VV181126	user	AS_M_high-C_high.amx	Details

Instrument Status

Dashboard | Agilent 6890 GC | MSD

MSD

Tune file: atune

Idle 0 μ A [#1]

230°C [230°C] 0V

100.0% 1.08E-05 Torr

0.00 / 0.00

Instrument Prerun [i] [On] [Off]

Online Signals

Signal Selection

Signal 2: test plot Signal 1: test plot TIC

Time (minutes)

Spectrum

MSD

Abundance

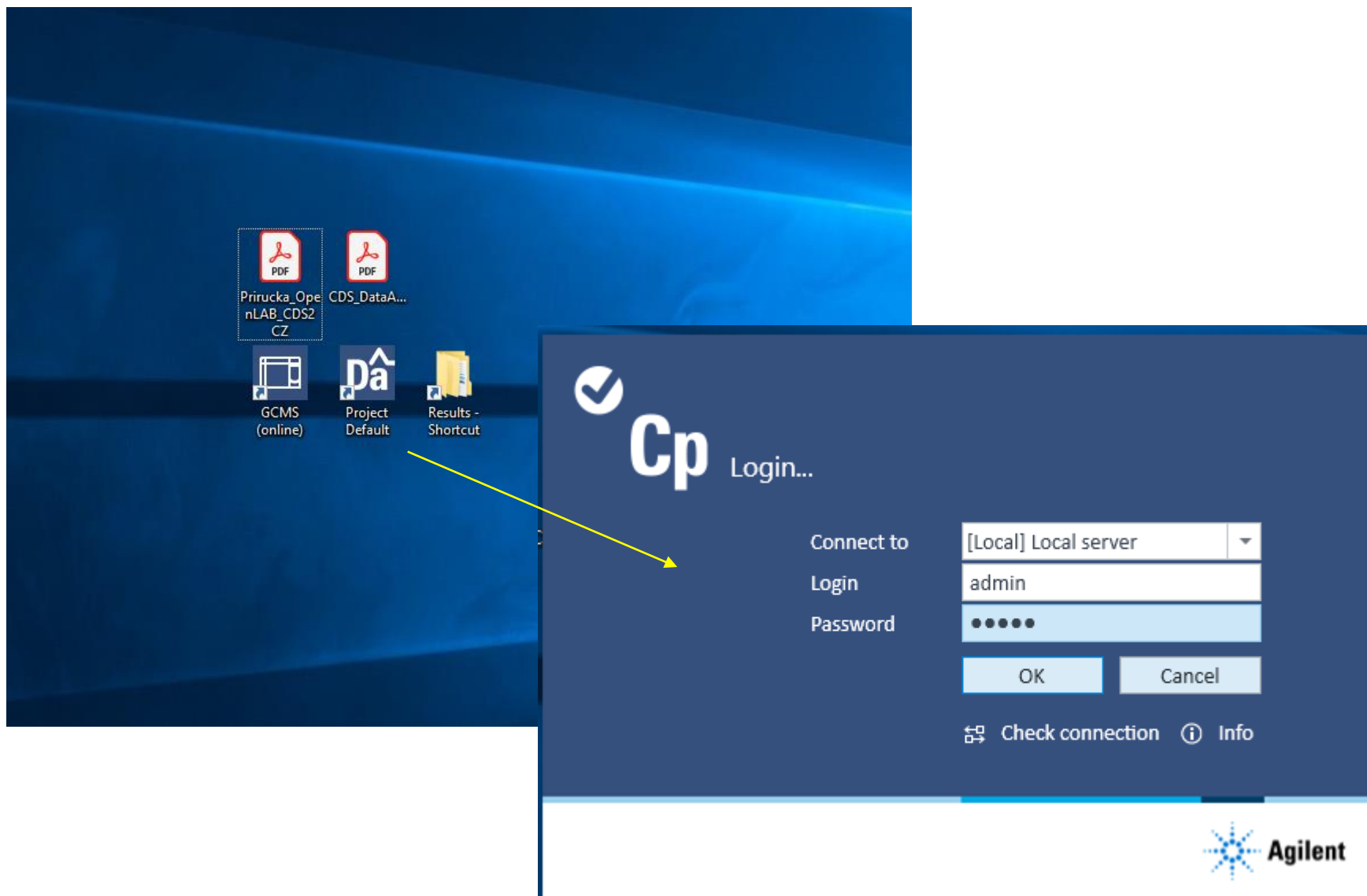
m/z

Current user: user, Active project: User

9:34 AM 11/26/2018

Data Analysis

Data Analysis login



Right click

Current user: admin

Windows taskbar showing the following open applications: Admin, Google Calendar - ..., Document1 - Word, GCMS - Acquisition, User - Data Analysis, Default - Data Anal... The system clock shows 10:54 AM on 10/26/2018.

Zooming

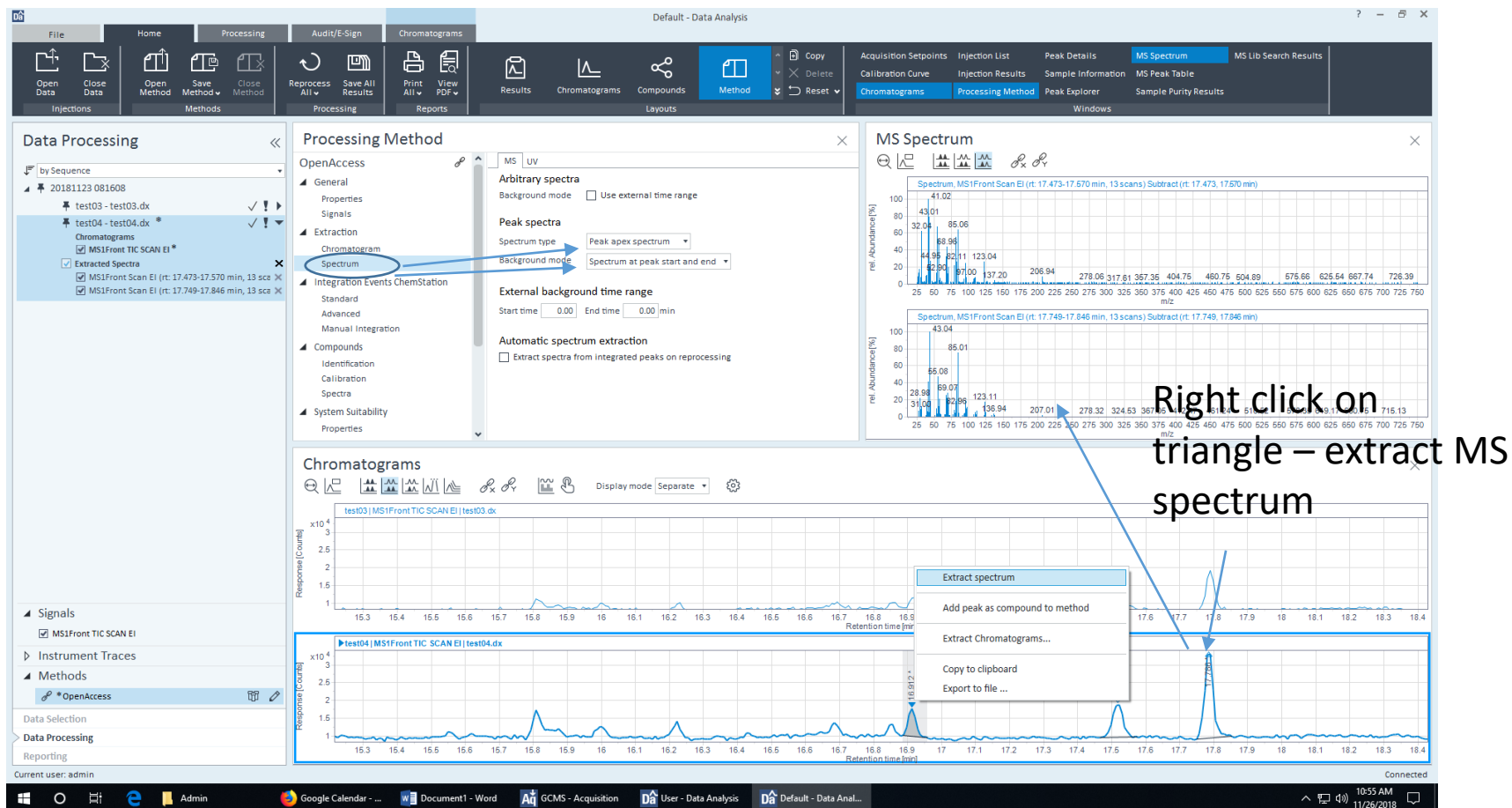
The screenshot displays the Data Analysis software interface, specifically the 'Default - Data Analysis' window. The interface is divided into several sections:

- Top Menu Bar:** Includes File, Home, Processing, Audit/E-Sign, and Chromatograms.
- Top Toolbar:** Contains icons for Open Data, Close Data, Open Method, Save Method, Close Method, Reprocess All, Save All Results, Print All, View PDF, Results, Chromatograms, Compounds, Method, Copy, Delete, and Reset.
- Left Panel (Data Processing):** Shows a list of data files and processing methods. The 'test04 - test04.dx' file is selected, and the 'MS1Front TIC SCAN EI' method is highlighted. The 'Data Processing' section is circled in red.
- Processing Method Panel:** Displays the 'OpenAccess' method settings. The 'Chromatogram' tab is selected, showing the 'Single m/z expansion chromatograms' and 'EIC extraction retention time window for target compounds'.
- Chromatograms Panel:** Shows a list of chromatograms. The 'test04 - test04.dx' file is selected, and the 'MS1Front TIC SCAN EI' method is highlighted. The 'Chromatograms' section is circled in red.
- MS Spectrum Panel:** Displays two mass spectra. The top spectrum is titled 'Spectrum, MS1Front Scan EI (rt: 17.473-17.570 min, 13 scans) Subtract (rt: 17.473, 17.570 min)'. The bottom spectrum is titled 'Spectrum, MS1Front Scan EI (rt: 17.749-17.846 min, 13 scans) Subtract (rt: 17.749, 17.846 min)'. Both spectra show relative abundance (%) on the y-axis and m/z on the x-axis.
- Main Plot Area:** Displays a chromatogram titled 'test04 | MS1Front TIC SCAN EI | test04.dx'. The y-axis is 'rel. Response [%]' and the x-axis is 'Time [min]'. A peak is visible at approximately 17.5 minutes, with a label '17.516' and a value '16.912'.

Annotations and labels on the image:

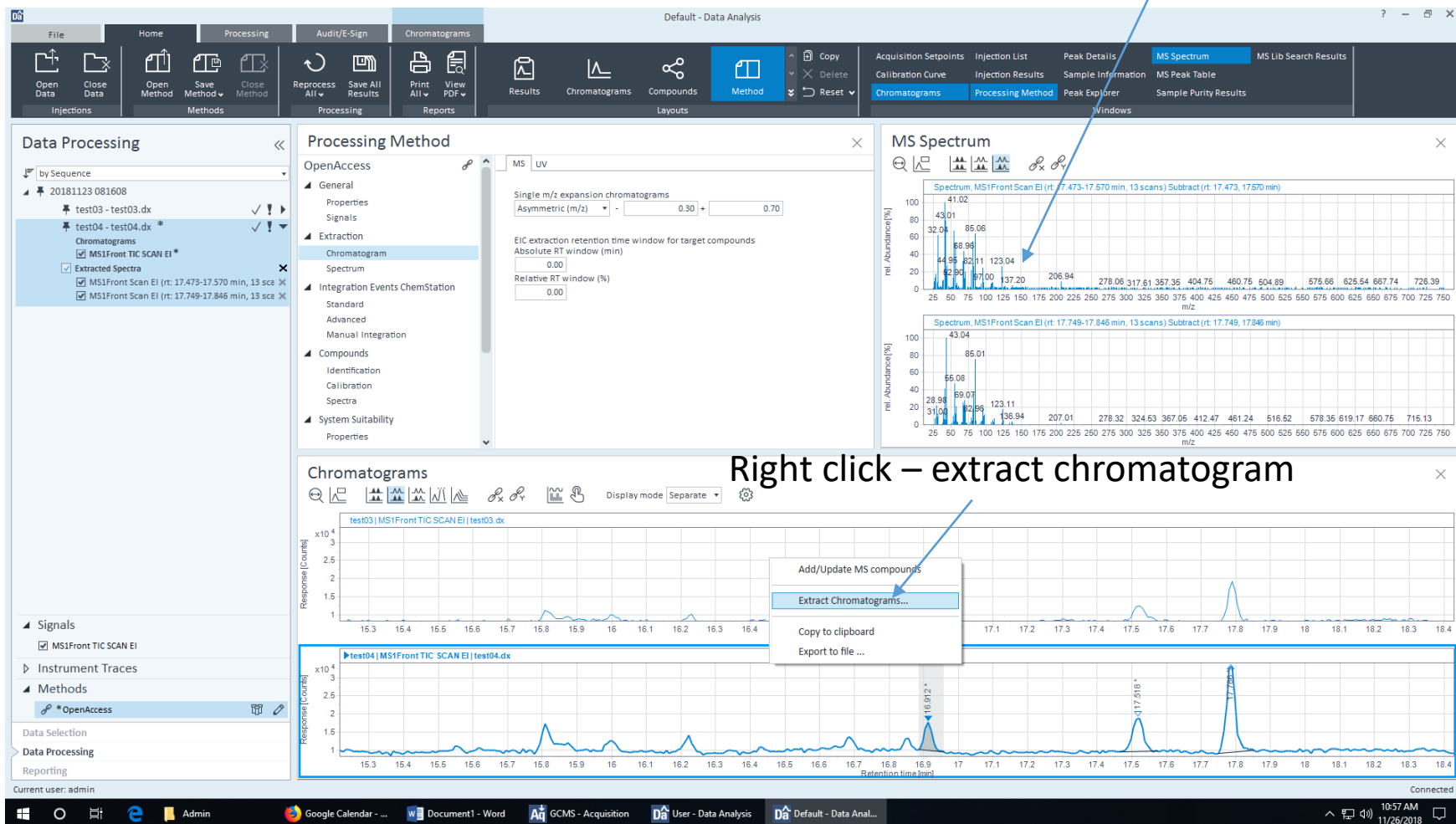
- Restore all:** A blue arrow points to the 'Restore all' button in the 'Chromatograms' panel.
- Tool for zooming:** A blue arrow points to the 'Zoom' icon in the 'Chromatograms' panel.
- Left mouse - rectangle:** A blue arrow points to the 'Zoom' icon in the 'Chromatograms' panel.
- Mouse under axis with or without Shift:** A blue arrow points to the 'Zoom' icon in the 'Chromatograms' panel.

Spectra with background extraction



Extract chromatogram

Click to m/z and extract chromatogram



Extract chromatogram

The screenshot displays the 'Default - Data Analysis' software interface. The 'Processing Method' window is open, showing the 'Extraction' tab. A blue circle highlights the 'Single m/z expansion chromatograms' section, which includes a dropdown menu set to 'Asymmetric (m/z)' and two input fields with values '0.30' and '0.70'. Below this, the 'EIC extraction retention time window for target compounds' is shown with 'Absolute RT window (min)' set to '0.00' and 'Relative RT window (%)' set to '0.00'. A blue arrow points from the 'Scan m/z value(s)' field in the 'Extract Chromatograms' dialog box to the 'm/z' label in the 'Fill in m/z' text. The 'Extract Chromatograms' dialog box also shows 'Signal type' as 'Scan', 'Polarity' as 'Positive', and 'Ionization' as 'EI'. The 'Chromatograms' window at the bottom shows a chromatogram plot with 'Response (Count)' on the y-axis and 'Retention time [min]' on the x-axis. Two peaks are labeled with their retention times: '16.912' and '17.518'. The 'MS Spectrum' window at the top right shows two mass spectra plots with 'rel. Abundance [%]' on the y-axis and 'm/z' on the x-axis. The top spectrum is for 'Spectrum, MS1Front Scan EI (rt: 17.473-17.570 min, 13 scans) Subtract (rt: 17.473, 17.570 min)' and the bottom spectrum is for 'Spectrum, MS1Front Scan EI (rt: 17.749-17.846 min, 13 scans) Subtract (rt: 17.749, 17.846 min)'. Both spectra show peaks at various m/z values, with the top spectrum having a peak at 41.02 and the bottom spectrum having a peak at 43.04.

Default - Data Analysis

File Home Processing Audit/E-Sign Chromatograms

Open Data Close Data Open Method Save Method Close Method

Reprocess All Save All Results Print All View PDF

Results Chromatograms Compounds Method

Acquisition Setpoints Injection List Peak Details MS Spectrum MS Lib Search Results

Calibration Curve Injection Results Sample Information MS Peak Table

Chromatograms Processing Method Peak Explorer Sample Purity Results

Windows

Data Processing

by Sequence

20181123 081608

test03 - test03.dx

test04 - test04.dx

Chromatograms

MS1Front TIC SCAN EI

Extracted Spectra

MS1Front Scan EI (rt: 17.473-17.570 min, 13 scans)

MS1Front Scan EI (rt: 17.749-17.846 min, 13 scans)

Processing Method

OpenAccess

General

Properties

Signals

Extraction

Chromatogram

Spectrum

Integration Events ChemStation

Standard

Advanced

Manual Integration

Compounds

Identification

Calibration

Spectra

System Suitability

Properties

Extract Chromatograms

Chromatogram extraction parameters

Signal type Scan

Scan m/z value(s) 74.00

Polarity Positive

Ionization EI

Auto re-process when extracted

OK Cancel

Chromatograms

test04 | MS1Front TIC SCAN EI | test04.dx

Response (Count)

Retention time [min]

Fill in m/z

MS Spectrum

Spectrum, MS1Front Scan EI (rt: 17.473-17.570 min, 13 scans) Subtract (rt: 17.473, 17.570 min)

rel. Abundance [%]

m/z

Spectrum, MS1Front Scan EI (rt: 17.749-17.846 min, 13 scans) Subtract (rt: 17.749, 17.846 min)

rel. Abundance [%]

m/z

Current user: admin

Admin

Google Calendar - ...

Document1 - Word

GCMS - Acquisition

User - Data Analysis

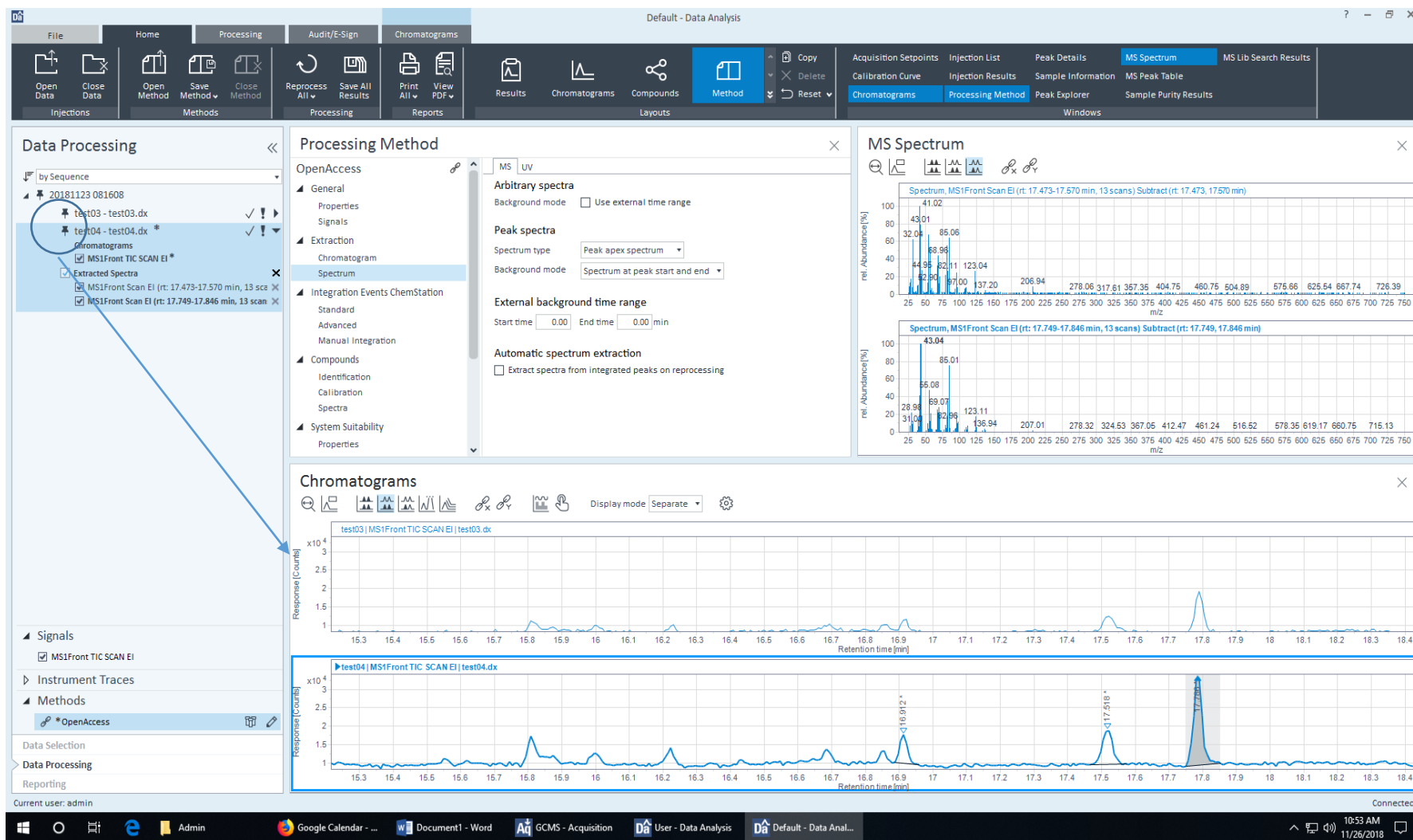
Default - Data Anal...

Connected

10:38 AM

11/25/2018

Overlay chromatogram



NIST search

The screenshot displays the 'Data Analysis' software interface, which is used for processing and analyzing chromatographic data. The interface is divided into several panes and toolbars.

Top Toolbar: Includes icons for File, Home, Processing, Audit/E-Sign, and MS Spectrum. The 'MS Spectrum' tab is currently selected.

Left Pane (Data Processing): Shows a list of data files. The file 'test04 - test04.d' is selected. The 'Chromatograms' section is expanded, showing 'MS1Front TIC SCAN EI' and 'MS1Front EIC(40.7-41.7) EI'.

Processing Method Pane: Contains settings for the processing method. The 'General' section is expanded, showing 'Single m/z expansion chromatograms' and 'EIC extraction retention time window for target compounds'.

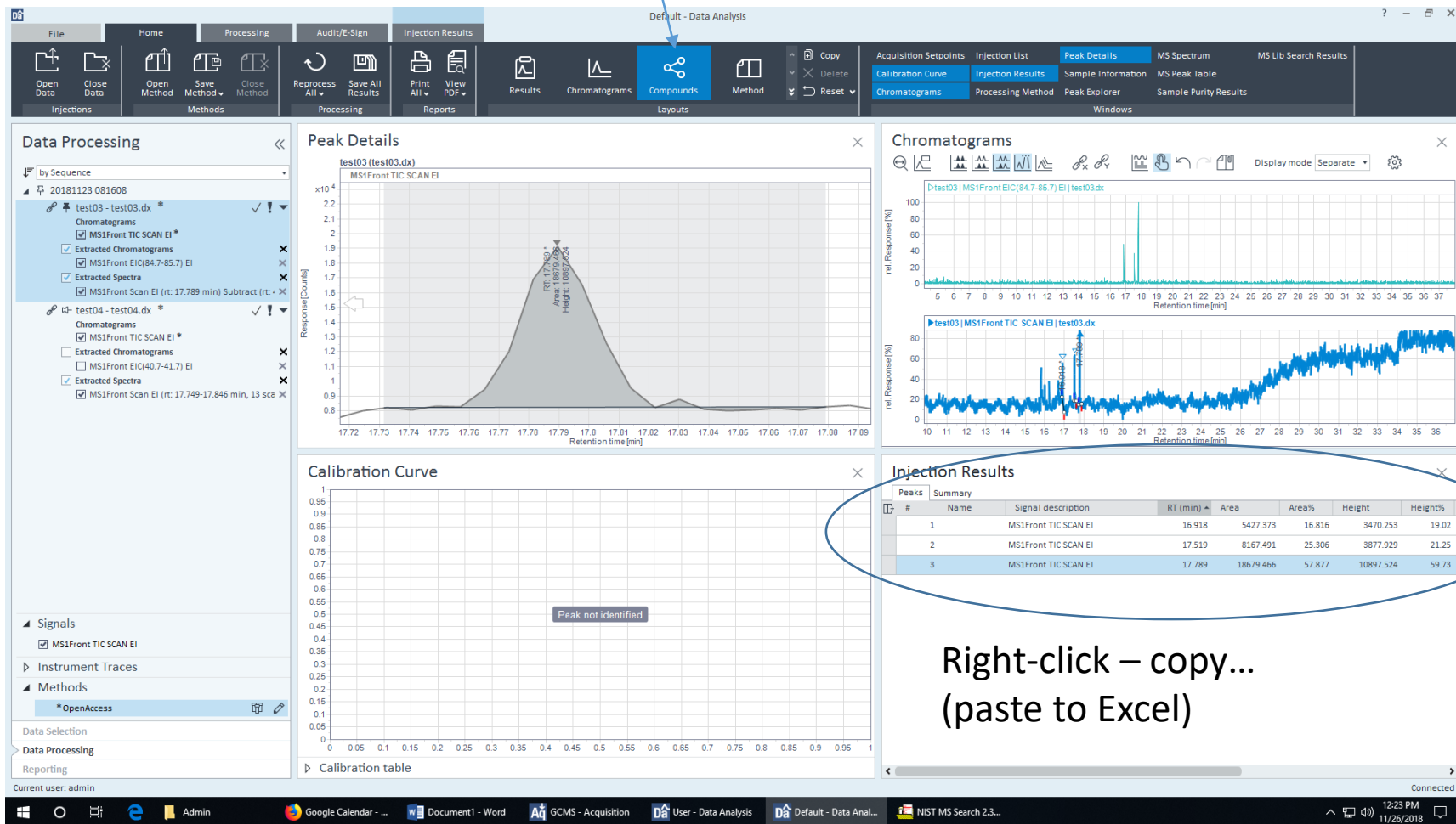
MS Spectrum Pane: Displays two mass spectra. The top spectrum is titled 'Spectrum, MS1Front Scan EI (rt: 17.473-17.570 min, 13 scans) Subtract (rt: 17.473, 17.570 min)'. The bottom spectrum is titled 'Spectrum, MS1Front Scan EI (rt: 17.749-17.846 min, 13 scans) Subtract (rt: 17.749, 17.846 min)'. Both spectra show relative abundance (%) on the y-axis and m/z on the x-axis. A blue arrow points from the 'Right-click on spectra - choose one option' text to the 'Search spectrum in the NIST libraries' button in the top spectrum's context menu.

Chromatograms Pane: Displays two chromatograms. The top chromatogram is titled 'test04 | MS1Front EIC(40.7-41.7) EI | test04.d'. The bottom chromatogram is titled 'test04 | MS1Front TIC SCAN EI | test04.d'. Both chromatograms show relative response (%) on the y-axis and retention time (min) on the x-axis.

Bottom Status Bar: Shows the current user as 'admin' and the current date and time as '11:01 AM 11/26/2018'.

Right-click on spectra - choose one option

Integration results



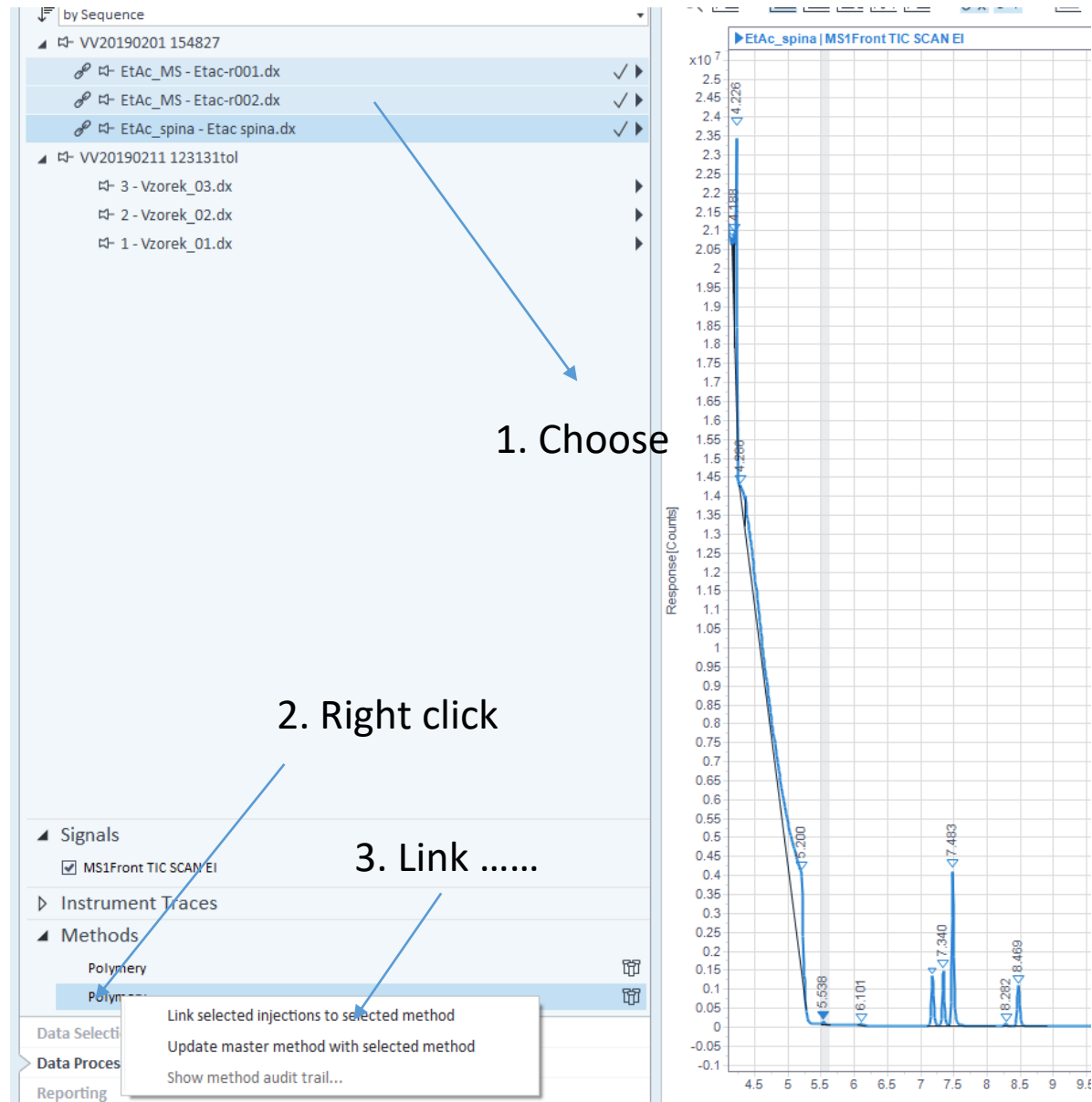
More advanced

Method

The screenshot displays a chromatography software interface with the following components:

- Top Menu Bar:** Includes tabs for File, Home, Processing, Audit/E-Sign, and Injection Tree. The 'Processing' tab is active.
- Processing Tab Sub-Menus:** Contains icons for Open Data, Close Data, Open Method, Save Method, Close Method, Reprocess All, Save All Results, Print All, View PDF, Results, Chromatograms (highlighted), Compounds, Method, and a Copy/Delete/Reset group.
- Data Processing Panel (Left):** Shows a tree view of data files. The 'EtAc_MS - Etac-r002.dx' file is selected and highlighted in blue. Other files include 'EtAc_MS - Etac-r001.dx', 'EtAc_spina - Etac spina.dx', and several 'Vzorek' files.
- Chromatograms Panel (Center):** Displays a plot titled 'EtAc_MS | MS1Front TIC SCAN E'. The y-axis is labeled 'Response (Counts)' and ranges from 0.55 to 2.65. The x-axis represents time in minutes, ranging from 1.05 to 2.65. A sharp peak is visible at approximately 1.45 minutes.
- Open File Dialog (Right):** A modal window titled 'Open File' is open. It shows the 'Project' set to 'Default' and the file path 'C:\CDSProjects\Default\Methods'. The file list includes: '..' (parent directory), 'New method 1.pmx', 'New method 2.pmx', 'Polymery.pmx', and 'rozpoustedla.pmx'. The 'Open' and 'Cancel' buttons are at the bottom right.

Link selected injections to selected method



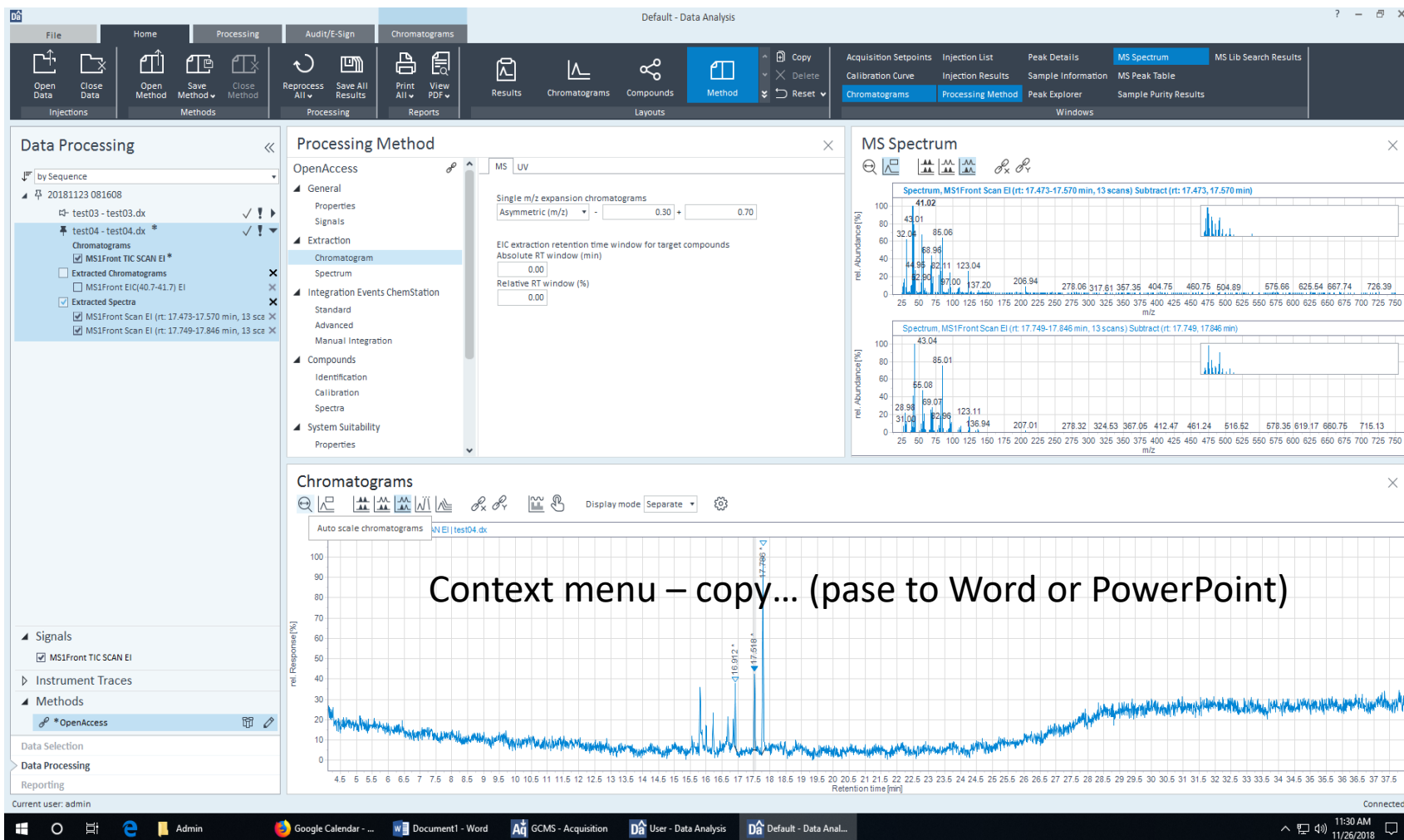
Save result

The screenshot displays the software interface with the following components:

- Top Bar:** Default - Data Analysis
- File Menu:** Open Data, Close Data, Open Method, Save Method, Close Method, Reprocess All, Save All Results, Print All, View PDF.
- Processing Panel:** Data Processing (by Sequence).
 - VV20190201 154837
 - EtAc_MS - Etac-r001.dx ✓▶
 - EtAc_MS - Etac-r002.dx ✓▶
 - EtAc_spina - Etac spina.dx ✓▶
 - VV20190211 123131tol
 - 3 - Vzorek_03.dx ✓▶
 - 2 - Vzorek_02.dx ✓▶
 - 1 - Vzorek_01.dx ✓▶
- Chromatograms Panel:** EtAc_spina | MS1Front TIC SCAN EI. The plot shows relative abundance (%) on the y-axis (1 to 11) and time on the x-axis (1.8 to 2.5 minutes). The display mode is set to Overlaid.

Save and open

Copy chromatogram



Reporting

1 Reprocess and save data before reporting and refresh preview

4 Save report as...

3
Choose report templates

The screenshot displays the GCMS software interface. The top menu bar includes File, Home, and Default - Data Analysis. The Reporting window on the left shows a list of report templates, with 'GCMS_Unknown_Analysis.rdl' selected. The Report Preview window on the right shows the report parameters and a chromatogram plot. The chromatogram plot shows a single peak at 16.918 minutes. The report parameters include Data file: test03.dx, Sequence Name: 20181123 081608, Sample name: test03, Instrument: GCMS, Inj. volume: 1.000, Acq. method: AS_M_high-C_high.amx, Processing method: *OpenAccess.pmx, Project Name: Default, Operator: admin, Acquired on: 2018-11-23 08:17:35+01:00, Location: 101, Type: Sample, and Sample amount: 0.00.

Report Parameters

Reporting Type: Minimum Area % Minimum Value To Be Reported: ACQ

Data file: test03.dx

Sequence Name: 20181123 081608

Sample name: test03

Instrument: GCMS

Inj. volume: 1.000

Acq. method: AS_M_high-C_high.amx

Processing method: *OpenAccess.pmx

Project Name: Default

Operator : admin

Acquired on: 2018-11-23 08:17:35+01:00

Location: 101

Type: Sample

Sample amount: 0.00

MS1Front TIC SCAN EI

Counts x10⁴

Time [min]

Identified peaks from method library

No compound from the identification list had been identified in this analysis

Most abundant unknown peaks library search (peak area at least 15 %)

Retention Time : 16.918 min

Signal Name	Height	Area	Height %	Area %
MS1Front TIC SCAN EI	3470	5427	19	17

Library Search Results :

154.2 164.6 174.6 225.6 230.9 316.4 385.9 416.6 483.7 548.6 614.8 670.6 726.6

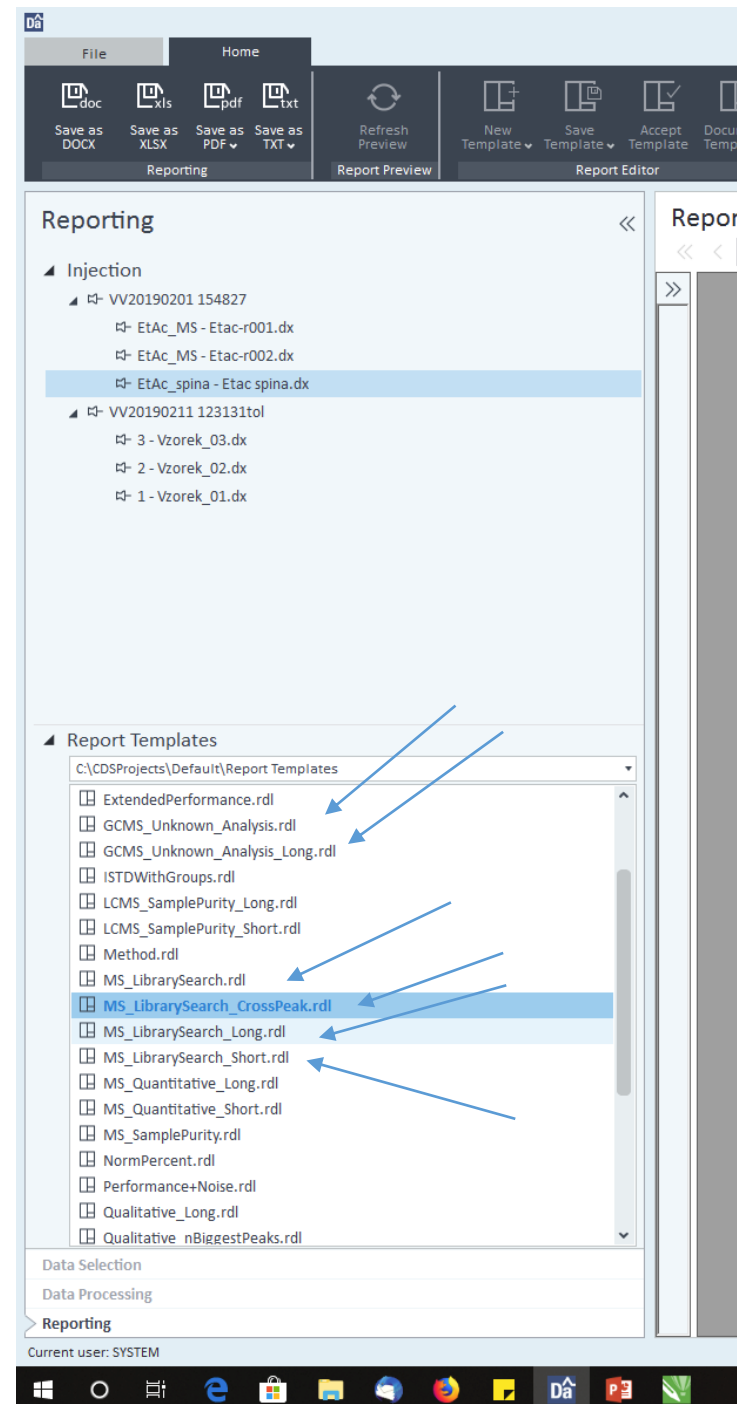
Max : 200

Current user: admin

Connected

12:27 PM 11/26/2018

Useful report layouts



For more information contact Vladimír Vrkoslav

- A.1.85; Tel . 347
- You can get OpenLAB on your computer.
- Back up your data on your computer.
- Write down the sample(s) in the sample book!