User manual and instructions for Agilent 6530 UHPLC-QTOF

with Agilent 1290 UHPLC



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1. Contact information

In case of assistance or support needs with the instrument contact primarily to Staff scientist Anniina Kiesilä. For needs with permissions, data interpretation or method development, please contact primarily Lab manager Elina Kalenius. If you notice shortage in N2 collision gas, please inform Lab manager or staff scientist or contact directly Hannu Salo.

Lab Manager: Elina Kalenius YSK517 tel. +358 40 805 4474 elina.o.kalenius@jyu.fi Staff Scientist: Anniina Kiesilä YO405 tel. +358 50 576 4752 anniina.m.kiesila@jyu.fi Gas delivery: Hannu Salo YSK343 tel. +358 40 805 3709 hannu.t.salo@jyu.fi

2. Sample preparation

For sample preparation use the balance and solvents found in MS laboratory (O309) (instructions to use balance are found in MS lab General Instructions document). Weigh an exact amount of sample and prepare a 1-5 mM stock solution. Then dilute the sample to appropriate concentration, recommendation is to start with 50 μ M concentration. The samples can be prepared to MeCN or H₂O. Last and most importantly, **filter all the samples through 0.2 \mum filter to remove any solids which might block the analytical column used. For samples in H₂O syringe filters can be used, for organic solvents use centrifuge filters. Both filters and syringes can be found in MS laboratory.**

Note that with 6530 instrument it is allowed to measure organic compounds only! Metal complexes and other metal containing compounds should be measured with other instruments. If you are unsure about your compound, please contact lab manager or staff scientist.

3. Opening the software

Make sure that all the compartments are shown in green in the Instrument status slide. If not, put the instrument on by pressing *on* in Instrument status. In case any of the compartments are shown in red (error) contact staff scientist or lab manager.



4. Logbook

Fill the logbook during the measurements. Before starting the measurements, check the gases and mark their pressures into the logbook. The CID N_2 bottle should have more than 20 bar and nitrogen generator should give 80-100 psi for normal operating pressure. If you notice that the gas pressure is not sufficient for your measurements, inform the staff scientist or manager.

5. Solvent lines

Normal user:

Before starting, plan that which solvents you are going to use

Line A: H₂O/MeCN 90/10

Line B: MeCN

Line C: H₂O + 0.1% TFA (Trifluoroacetic acid)

Line D: H₂O + 0.1% FA (Formic acid)

Check that solvent lines have enough solvent for your runs. Check the seal wash and flush port bottles, both must have > 50 ml of solvent. If the needed solvent levels are low for your runs, ask MS lab personnel to fill them.

Bottle Fillings	-		\times								
Solvent Bottle											
Fillings											
Actual Volume	Total Volume										
A: 0.46 🛟 liter	1.00	liter									
B: 0.59 -	1.00	liter									
C: 0.38 -	0.50	liter									
D: 0.27 _ liter	0.50 🛟	liter									
Actions											
Prevent analysis if level falls below	w	0.02 📫	iter								
 Turn pump off if running out of sol 	vent										
Waste Bottle											
Filling											
Actual Volume	Tel	al Volume									
Actual Volume	10										
Waste bottle: 0.08	liter	5.00 🛟	liter								
Actions											
Actions											
Prevent analysis if level raises at	ove	5.00 📫	iter								
 Turn pump off if waste volume has 	s reached maximur	n limit									
	Ok	Cancel	He	lp							

Instrument has a constant flow from lines A and B, but if you will take into use line C or D, you need to **purge the line C or**

D before use. Right click on top of Quat Pump icon \rightarrow Prepare pump. Choose the line that you wish to purge by changing its composition to 100%, then purge that line 5 minutes with the rate of 5 ml/min by pressing start.

Advanced user:

Check the solvents for UHPLC in lines A-D. Estimate the solvent consumption of your runs and fill the bottles if needed. Sonicate all added solvents.

Record the solvent level to the software in *bottle fillings*. Right click on top of Quat Pump icon \rightarrow Bottle fillings. The pump will turn off automatically if the solvent bottle filling information gets below 20 ml. Remember to leave at least ~100ml of solvent to line A at the end of the measurements! (~250ml over the weekend).

Solvents should be changed if instrument has been long time unused or solvents are older than 1 month.

Check the seal wash and flush port bottles. If bottle has < 50 ml left, prepare a new one. Seal wash: H_2O / IPA 9:1, Flush port: H_2O /MeCN 50:50.

🧾 Pr	epare Pump	-	D X
	Purge		
	Use for changing mobile phases, drawing solv	rent or for removing air bubb	bles.
	Duration: 10.00 📫 min Co	mposition A: 50.00 ‡	%
۲	Flow: 5.000 + mL/min Co	mposition B: 50.00 🛟	%
	Co	mposition C: 0.00 📫	%
	Co	mposition D: 0.00 📫	%
	Conditioning		
	Minimize the pressure ripple by dissolving air	bubbles in the pump heads	
0	Note: Solvents will flow through the LC s Method parameters are applied for flow r pressure.	ystem and column. ate, composition and max.	
	Duration: 15.00 📜 min		
	Prime		
0	Draws solvent into (both) pump heads for rem head and particles from valves. Flow goes to	oving air bubbles from the p waste.	ump
	Do not use the Prime function for filling the sol solvent type.	vent lines or changing the	
	/	\frown	
	(Start Cancel	Help

Check the waste bottle under the table. If the waste can is almost full, replace it with new one. Remember to update this action in *bottle fillings*! The pump will automatically turn off if waste bottle gets full.

Purge the lines you are going to use from *Prepare pump*. Right click on top of Quat Pump icon \rightarrow Prepare pump. Choose the lines that you wish to purge, then purge each line at least 5 minutes with the rate of 5 ml/min.

To prepare a new eluent:

Take a new solvent bottle. Rinse the bottle few times with small amount of solvent that you are going to use as an eluent. Add the solvent and mark the date and solvent to the bottle. Sonicate the eluent ~10 minutes prior to use to homogenize it and to remove air bubbles.

To replace an eluent:

If you are going to replace the bottle with the same solvent, remove the sinter from the old bottle and insert it directly into the new one. If you are going to change the eluent to a different one (also if the old one had any additive, and new one does not!), then rinse the sinter in a 50 ml beaker filled with the new eluent and start the purge from beaker before inserting it into the new bottle. Discard the old eluent in the fume hood, wash the bottle and leave it dry.

To prepare a buffer:

Prepare the buffer and adjust the pH. Check column specifications to make sure that the column can be operated in that pH! Filter the buffer through $0.25\mu m$ filter paper (whatman 42) and sonicate the buffer 15 – 30 minutes prior to use.

6. Equilibration of the column

The stand by flow to the instrument is 95:5 A:B ($H_2O+MeCN / MeCN$) with 0.05 ml/min flowrate. Check that the LC flow goes to the waste and calibrant is off.

Right click on top of QTOF icon \rightarrow LC flow \rightarrow waste.



Start increasing the flow gradually (Method editor \rightarrow Quat pump \rightarrow flow rate) 0.1ml/min at the time until you reach the target flow rate, for example 0.5 ml/min if you are using one of the General methods. Each time you change the flowrate, press *apply* to send information to instrument. Follow the pressure of the column constantly. The maximum flowrate is 0.5 ml/min. Finally, open the method you want to use in the runs, for example General method or General method_TFA or _FA. Let the column stabilize at least 10-15 minutes before starting the measurements.

If you need to change the eluent ratio, change it gradually 5-10% at the time. Follow the pressure. If you do any changes to the methods, save them with your name to your own folder.

			-		- E				
				\sim _					
Properties DA Sampler Sampler Pretreatment Quat. Pump Colum	nn Ov	en VWD	Q-TOP	-					
0.05D 🔶 mL min	^	Advanced							
	1	▲ Timetable	(15/1	00 events)					
Solvents									
Enable Blend Assist									
L Enable Blend Assist A: 95.00 ℃ % 100.0 % Water V.03 ▼ H2O + 0.1%		Time [min]	Δ	A [%]	B [%]	C [%]	D [%]	Flow [mL/min]	Max. Pressure Limit [bar]
		Time [min]	۵ 0.00	A [%] 95.00	B [%] 5.00	C [%] 0.00	D [%] 0.00	Flow [mL/min] 0.050	Max. Pressure Limit [bar] 1000.00
L hable blend Assist A: 95.00 1 % 100.0 % Water V.03 ▼ H2O + 0.1% B: ✓ 5.00 1 % 100.0 % Acetonitrile V.03 ▼ ACN		Time [min]	△ 0.00 1.00	A [%] 95.00 95.00	B [%] 5.00 5.00	C [%] 0.00 0.00	D [%] 0.00 0.00	Flow [mL/min] 0.050 0.500	Max. Pressure Limit [bar] 1000.00 1000.00
L brable blend Assist A: 95.00 ; 1 % 100.0 % Water V.03 ▼ H2O + 0.1% B: ✓ 5.00 ; 1 % 100.0 % Acetonitrile V.03 ▼ ACN		Time [min]	△ 0.00 1.00 6.00	A [%] 95.00 95.00 20.00	B [%] 5.00 5.00 80.00	C [%] 0.00 0.00 0.00	D [%] 0.00 0.00 0.00	Flow [mL/min] 0.050 0.500 0.500	Max. Pressure Limit [bar] 1000.00 1000.00 1000.00
L Enable Blend Assist A: 95.00 : % 100.0 % Water V.03 ▼ B: ✓ 5.00 : % 100.0 % Acetonitrile V.03 ▼ C: ✓ 0.00 : % 100.0 % Water V.03 ▼		Time [min]	 0.00 1.00 6.00 6.50 	A [%] 95.00 95.00 20.00 20.00	B [%] 5.00 5.00 80.00 80.00	C [%] 0.00 0.00 0.00 0.00	D [%] 0.00 0.00 0.00 0.00	Flow [mL/min] 0.050 0.500 0.500 0.500	Max. Pressure Limit [bar] 1000.00 1000.00 1000.00 1000.00
L Enable Blend Assist A: 95.00 1 % 100.0 % Water V.03 ▼ B: ✓ 5.00 1 % 100.0 % Acetonitrile V.03 ▼ A: 0.00 1 % 100.0 % Acetonitrile V.03 ▼ A: ✓ D: ✓ 100.0 % Acetonitrile V.03 ▼ ACN C: ✓ 0.00 1 % 100.0 % Water V.03 ▼		Time [min]	 0.00 1.00 6.00 6.50 8.00 	A [%] 95.00 95.00 20.00 95.00	B [%] 5.00 5.00 80.00 80.00 5.00	C [%] 0.00 0.00 0.00 0.00 0.00	D [%] 0.00 0.00 0.00 0.00 0.00	Flow [mL/min] 0.050 0.500 0.500 0.500 0.500	Max. Pressure Limit [bar] 1000.00 1000.00 1000.00 1000.00 1000.00

7. Generating new method

The general method uses: $H_2O+MeCN / MeCN$ (lines A and B) General method_TFA: $H_2O + 0.1\%$ TFA / MeCN (lines B and C) and General method_FA: $H_2O + 0.1\%$ FA / MeCN (lines B and D) All methods have a similar gradient and parameters

Time (min)	H ₂ O (+ acid) %	MeCN %
0	95	5
1	95	5
6	20	80
6.5	20	80
8	95	5
10	95	5

The flow rate is 0.5 ml/min, run time 10 minutes, no post time, injection volume 5 μ l, needle wash from flush port (15 s with 3 reps), column oven 30 ° C. Ion source parameters are the following:

Gas Temp 325 °C, Drying gas 10 l/min, Nebulizer 20 psi, Sheath gas Temp 325 °C, Sheath gas flow 11 l/min, VCap 4000 V, Nozzle 2000 V, Frag 200 V, Skimmer 60 V, Oct 1 RF Vpp 750 V.

(+)ESI-MS, *m/z* 50-2000

You can build your own method using one of the methods as a starting point. Remember, that **if you do any changes to these methods, save the modified method as a new method** with your own name to your own folder!

Advanced user: If you need to **increase the temperature** in the method, let the column stabilize longer (at least 30 minutes) before runs. Create new end methods suitable to your method, where you let the column to cool down. Book enough time, and make sure the column is equilibrated back to 30 °C after your measurements. Cooling of the column might take 30-60 minutes, and let column stabilize at least 30 minutes in 30 °C before the next user.

8. Use of UV detector

If you are not using UV detection, move to the next chapter.

If you want to also measure UV, choose the VWD from method editor. Choose the wavelength(s) you want to acquire. Tick Lamp on required for acquisition. Note that general method does not have UV chosen, and you will have to save the modified method with your own name to your folder!

Method Editor			
+ Cp 💾 💾 General AB 051223.m	$\cdot \checkmark $		
Properties DA Sampler Sampler Pretreatment Quat. Pump Column	Oven VWD Q-TOF		
Dual-Wavelength Settings	Advanced		
✓ Enable Dual-Wavelength			
	۲	Positive (+)	
Wavelength	0	Negative (-)	
Signa B: 320 - nn	Miscellaneous		
Peakwidth: < 0.4 min (4 s resp. time) (2.5 Hz)			
Stoptime Posttime			Lamp on required for acquisition
As Pump/Injector Off			ican Range: 190 to 400 mm
			Step: 2 m

After this turn the UV lamp on from VWD. Right click on top of the icon, and choose switch on. The UV-lamp needs to warm up for \sim 15-20 minutes before the runs.



9. Calibrating the instrument

Check that Calibrant B bottle has calibrant. If calibrant runs out, inform the Staff scientist.

From Acquisition context move to Tune (up in the left corner).

From *Instrument state*, choose the Standard 3200 *m/z* mass range. Fast polarity switching should be disabled and High resolution chosen.

Home	
Acquisition Tune	Status
Context	Li
For Help, Press	F1

on Polarity	C Positive	€ Ne	gative		
Ion Source Dual ESI Gas Temp Drying Gas	▼ 325 5	329	°C I/min	TOFMassCalibration-3200mzRange.tun TOFMassCalibration-3200mzRange.tun Save Save As Load	
VCap Chamber	3500	20 / 5.636 0.32	μΑ μΑ	Fast Polarity Switching Disabled	
				In the Control of	
Calibrant Bott	tle (🖲 None	CAC	в	Advanced Control	
LC Flow to	Waste	C MS			Apply

In *Tune & Calibration*, choose the polarities where you want to calibrate (positive, negative or both) choose Mass Calibration/Check and press Start TOF Mass Calibration. After calibration Tune reports are displayed.

Tune File: TOF	MassCalibration	3200mzRa	ange.tun	Ture & Calibration Instrument State	
Ion Polarity	C Positive	€ Ne	gative	Q-TDF: Standard (3200 m/z) High Resolution	
Ion Source				Positive Negative Negative	
Dual ESI Gas Temp	325	328	°C	Fragile Ions	
Drying Gas	5	5.0	1/min		
Nebulizer	20	20	psi	A	
VCap	3500 V	5.592	μA	Begin session Running TOF Check Tune in Positive Polarity	
Chamber		0.33	μA	Begin Running Mass Calibration(Positive Polarity) Start for Mass Backup All Parameters Calibration	
				Spraying Calibrant Solution Setup Dual ESI Source to Achieve Stable Signals for Auto Tune	
				Waiting for Calibrant to Elute	
				Signal Intensity and Stability Satisfied Auto Tune Requirements	
				Check Ion Source Actuals for Auto Tune Tune Tune Report	
Calibrant Bol	ttle 💽 None	OAO	в	Waiting for Gas Temp to reach its set point 325, current actual value 330	
LC Flow to	Waste	C MS		,	Apply

9. Acquisition of the data

When calibration is finished, move back to *Acquisition* context. Now the LC flow starts flow directly to the MS (if it does not, switch it by right click QTOF icon and change the LC flow from waste to MS).

From Method editor, move to the Worklist Pane.

Method Editor							_
					\checkmark) ≍	
Properties DA Sampler Sampler Pretreatment Quat Pump Colu	imn Oʻ	ven	VWD	Q-TOF			
Solvents	^	Þ	Advanc	ed			
Enable Blend Assist			Timetab	ole (15/10	0 events)		
A: 95.00 ℃ % 100.0 % Water V.03 ▼ + 0.1 % TFA							
B: □ 5.00 ¹ % 100.0 % Acetonitrile V 0.3 ▼							
	- 1			0.00	95.00	5.00	
C 🔽 0.00 ÷ % 100.0 % Water V.03 ▼				1.00	95.00	5.00	I
	_			2.00	95.00	5.00	I
D: 🗸 0.00 + % 100.0 % Acetonitrile V.03 💌 + 0.1 % TEA				3.00	95.00	5.00	I
	•			4.00	95.00	5.00)
				5.00	95.00	5.00	J
Pressure Limite							
Pressure Limits	~						
Method Edito. Worklist Pane Sample Run							

In Worklist, create a new list (or open your former modified list) and add your sample(s) to the list. Place the vials to the multisampler and add the locations to the list accordingly. The locations have to be in form P1-A1 (P1 = plate 1 or 2, A1 = coordinate of your sample in the plate). If there are old samples inside multisampler, place them to measured MS samples tray on the table.

Choose the method you want to use for each sample. In data file, choose your folder as location! Create a new folder to your data folder and name it YEARMMDD_yourname. Save all your data to this folder. Note that you must name all your data files with different name or number. If you are measuring multiple samples, and want the instrument to go standby after them, add the end methods at the end of the worklist (see next chapter). If there are reservations after you, you must run the end methods before the next user! The duration of the end methods is 25 minutes in total. When the worklist is ready, or just to run a single sample, choose the correct row(s) you want to run, and press run worklist.

Work	list Pa	ne							
면 및 수 오 및 후 않 볼 볼 년									
	<	Status	Sample Name	Sample Position	Method	Data File	Sample Type	Level Name	Inj Vol (μl)
1	✓	Pending	sample 1	P1-A1	LC_General method.m	WorklistData-0001.d	Sample		As Method
2	✓	Pending	TES-65 fr 7	P1-A2	LC_General method.m	WorklistData-0002.d	Sample		As Method
3	-	Pending	sample xx	P1-A3	LC_General method.m	WorklistData-0003.d	Sample		As Method

10. Ending the experiments

After your last sample, or at the end of the worklist, add three more samples. For all samples choose "no injection" as sample position. For first row, choose method LC_wash. For second, choose the method LC_Flow down. For third use the method LC_Standby. If you have already started to run your worklist, you can press pause button on top of the worklist. The worklist is then paused after the current run, and you can add the methods to the queue. Then run the whole worklist. Pick up your samples after all the runs are finished or on the following day. Inform the Staff Scientist if you need longer storage for the samples, normally they will be stored only few days.

Work	/orklist Pane														
Ê7 (þ 🗋		∥ 🖨		E	⊒ : ∓ []• Q € [[
	 Image: A second s	Status	Sample Name	Sample Position	Method	Data File	Sample Type	Level Name	lnj Vol (μl)	Comment	Sample Group	Info.			
1	\checkmark	Completed	Blank	P1-A1	LC_General method.m	D:\Projects\Research\Data\Pihko\Veera	Sample		As Method						
2	\checkmark	Completed	Aspartaami	P1-A2	LC_General method.m	D:\Projects\Research\Data\Pihko\Veera	Sample		As Method						
3>	 ✓ 	Acquiring	wash	No Injection	LC_wash.m	WorklistData-0003.d	Sample		As Method						
4	-	Pending	flow down	No Injection	LC_flow down.m	WorklistData-0004.d	Sample		As Method						
5	\checkmark	Pending	stand by	No Injection	LC_standby.m	WorklistData-0005.d	Sample		As Method						

11. Data analysis

Data analysis can be done either in laboratory or using remote Data-PC (please see the separate Data-PC instructions).

Open Qualitative Analysis B.09.00.

Open your data file. With mouse left button, choose the area that you want to extract from the chromatogram, and press right button of the mouse \rightarrow Extract MS Spectrum.

Chro	natog	ram F	Results	(zoom	ed)																	
2 ↔	\$	Q	1	\$ V	☆	<u> </u>	Ð	G	з 👻	H			t 🖉	Ж	%	‰ 🖏	⊉	>	Minute	s		• 4
x10 ²	+ESI	TIC S	can Fra	g=200.	OV Nay	/te_1.d																
1.3-	1																					
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1.1-																						
1-																						
0.9-																						
0.8-																						
0.7-																						
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0.5-																Extract	MS Sp	ectrur	n to Ba	ckaroun	ıd	
0.4 -																Extract	Peak S	pectri	ım			
0.3-																Extract	Chrom	atogr	ams			hand
0.2-																Extract	Additio	onal C	hromat	tograms		
0.1-												-	m	m h		Use Hig	ghlighte	ed Ch	romato	grams	÷	
0-	u same	l.	· ·····	south a	-wa	mprov	*	ng ang ang ang ang ang ang ang ang ang a	igna san din	*****	new Autor					Extract	FBF Ma	anual	Compo	ound(s)		
		0	5	1		1.5		2		2.5		3		3.5		Integra	te Chro	mato	nram			Ġ

Analyse the spectrum. If you observe your compound, you can generate the accurate mass report. To get the report for accurate mass, open from the method editor (down on the left) Data_Analysis_Qual method.

Reskaround Spectra						0.0															
Compounds		🛐 Open Meth	od					×													
			Look in: Aet	thods		3	<u>r</u>	##													
B		Recent Items	6530_Accu 6530_Accu 6530_Sens																		
Method Editor: Generate Form	ulas		6530_Sens	itivity_msms.m																	
1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	🕑 Ge	3	Data_Analy	/sis_Qual.m																	
Method Automation	Allowed	Documents	iii_LCexerci	se1.m																	
Chromatograms	Charge																				
Spectra		Deskton																			
Identification	× +	Deskip																			
Identification Workflow		× +	¥	×+	×+	×+ ×	×+ ×+	×+ ×+	×+ ×+	× +	⊻ + ∑ +	× ×	⊻ + ∑ +								
Database Search Settings		This PC																			
Library Search Settings			File name:	Data_Analysis_Qual.m		`	-	Open	1												
Generate Formulas		1	Files of type:	Method Files (*.m)		,	~	Cancel													
	MS ion	Network						Help													
	Gr	bap into mur oanne		ant onargo oarrioroj		1.05-	-														
	Eleme	nents and limits																			
	EI	ement	Minimum	Maximum		0.9															
) C		8	34		0.8-	-														

From Identification \rightarrow Generate formulas \rightarrow Allowed species: choose the limits for your target compound and the ions it could form (negative, positive, how you expect it to ionize).

Method Editor: Generate Form	nulas			×				
🕼 🕒 🖬 🌠 🤌 • (* •	🕑 Generate F	Formulas from Spectru	m Peaks 🔻					
Method Automation	Allowed Species	Limits Charge State	Fragment Formulas					
Workflow	Charge carrier	to be assumed if not know	wn					
Additional Chromatograms	Positive ions:	Ne	egative ions:					
Paparts	-electron	^	+electron					
	✓ +Na		□ +CI					
Export	✓ +K		+Br					
Chromatograms	+C2H5							
	+C3H5	×	+CF3C00					
Identification		• × •						
Identification Workflow	MS ion electron state: even electron ~							
Database Search Settings	Group hits	with same formula (but o	different charge carriers)					
Library Search Settings	Elements and I							
Generate Formulas	Element	Minimum	Maximum					
	▶ C	8	34					
	н	5	42					
	0	2	10					
	N	2	5					
	S	2	4					
		* X						

In Limits, determine the maximum molecular weight for your compound.

📓 Method Editor: Generate Formulas										
🕼 😕 🌆 🌠 🍯 🕶 🍽 🔹 🕟 Generate Formulas from Spectrum Peaks 🔹										
Method Automation	Allowed Species Limits Charge State Fragment Formulas									
Workflow	Limits on input masses									
Additional Chromatograms	calculated:									
Reports	Limits on results									
Export	Minimum overall score per 75.000									
Chromatograms	Maximum MS mass error 7.5000 ppm V									
Spectra	Require DBE from 0.0 to 50.0									
Identification	Maximum number of hits per 5									
Identification Workflow										
Database Search Settings										
Library Search Settings										
Generate Formulas										

In charge state, choose the appropriate Isotope model and charge states.

Method Editor: Generate Forr	nulas	×
Method Editor: Generate Formula	₃ 🕑 Generate Formulas from Spectrum Peaks 🔹	
Method Automation	Allowed Species Limits Charge State Fragment Formulas	
Workflow	Isotope grouping	
Additional Chromatograms	Isotope model: Common organic molecules ~	
Reports	Charge state	
Export	✓ Limit assigned charge states to a range of: 1-2	
Chromatograms	Report single ions or single-ion features with charge state z=1	
Identification		
Identification Workflow		
Database Search Settings		
Library Search Settings		
Generate Formulas		

Make sure the correct spectrum is chosen active, and press Generate Formulas from Spectrum Peaks. Spectrum Identification Results appear. Choose the one matching to your compound.

J	Spectrum Identification Results: + Scan (rt: 3.779-3.928 min)															
Ì	j	네 対	🛱 👰 🍕	l 👧 🛃												
	Be	st ⊽+⊐	ID Source 🛛 🕇	Name 🖓 🕁	Formula	7-Þ	Species	ΥÞ	m/z	∀≠	Score 🖓 🏹	+⊐ Score (RT) 🟹 +=	RT Diff マ+	Diff (ppm) 🍸	Þ Diff (mDa) 🕻	▼ + Score
\triangleright	•	0	MFG		C29 H41 N	O2 S2	(M+H)+ (M+	Na)+	556.2775	578.2587	84.45			-0.75	-0.42	
\triangleright	(D	MFG		C29 H38 N4	O2 S2	(M+NH4)+		556.2775		84.29			0.47	0.25	

In Method Automation \rightarrow Reports \rightarrow Destination \rightarrow Save report \rightarrow At specified directory and navigate to your own folder!

Method Editor: Reports		×						
🕼 🕒 🖬 🌠 🤊 • ((ii -	Print Workflow Report •						
Method Automation	A	Destination Templates Layout Contents						
Workflow	▲	Print report						
Additional Chromatograms	▲	Printer name:						
Reports		Corauly						
Export		Save report						
Chromatograms	4	Inside data file's reports subdirectory						
Spectra		At specified directory:						
Identification		D:\Projects\My test project						
		If report file already exists						
		 Overwrite existing report 						
		 Auto-generate new report file name 						

In templates, check that you have Qual\10.0\en-US\Letter chosen as shown in the figure. Press Print Workflow Report.

Reports			×						
🕼 🕼 🖪 🖌 🏓 •	(°I -	● Print Workflow Report ▼							
Method Automation	A	Destination Templates Layout Contents							
Workflow	۸								
Additional Chromatograms	4	Use PDF Report Builder							
Reports		⊖ Use Microsoft Excel®							
Export		Report template folder							
Chromatograms	۸	D:\MassHunter\Report Templates\Qual\10.0\en-US\Lett							
Spectra									
+ Identification		Report templates							
		Target Screening :							
		TargetScreening.template.xml 🗸							
		Sample Purity :							
		SamplePurity.template.xml							
		Compound Discovery -							

Cannot find the compound from chromatogram?

Calculate theoretical m/z value for the ion, for example by using Isotope distribution calculator with icon:



Right click the mouse on top of chromatogram, and choose Extract chromatograms.



Choose EIC as Type. Write the accurate m/z value you want to extract from the chromatogram and press OK.

Extract Chromatograms		\times
List of opened data files	Type: EIC Integrate when extracted MS Chromatogram Advanced Excluded Masses	
	MS level: All Polarity: Positive Scans: All scan types m/z of interest: Any m/z value(s): 195.0877 Merge multiple masses into one chromatogram	
	OK Cancel	

If an ion with similar m/z is found, you will see its retention time in extracted ion chromatogram. Right click on top of the chromatogram and choose Smooth chromatogram. Then from smoothed chromatogram extract the MS spectrum and see if your compound can be found in the spectrum.



12. Use of S-Drive

If you need more time to analyse your data, please move your data to S-drive and book the Data-PC from infrabooking. The same softwares for data analysis are available on Data-PC. See also instructions for the use of Data-PC, which can be used remotely.

To transfer your data to S-drive:

On top of This PC, press mouse right and choose Map network drive.

V D This DC	N	msuser (r
> 3	Collapse	
> 🗖 D	Manage	
> 😭 D	Pin to Start	
> _ D	Map network drive	
	Open in new window	
	Pin to Quick access	
	Disconnect network drive	
> 📑 V — > 🟪 W	Add a network location	
> _ D	Delete	
> S	Rename	
🗸 🔜 Sea	Properties	

On Map Network Drive, choose the following options and press Finish.

			×	
\leftarrow	왻 Map Net	work Drive		
	What net	work folder would you like to map? Irive letter for the connection and the folder that you want to connect to:		
	Drive: Folder:	S: ~ \\fileservices.ad.jyu.fi\commonshare ~ Browse		
		Example: \\server\share		
		Connect using different credentials		
		Finish Cance	I	

Write your username and password. Note: the username has to be in the form username@ad.jyu.fi

	Windows Security	×								
Enter network credentials										
Enter your credentials to connect to: fileservices.ad.jyu.fi										
	anmajoki@ad.jyu.fi									
Password										
	Remember my credentials									
	ОК	Cancel								

After pressing OK the connection to S-drive opens. When you have transferred your data to S-drive, take care to disconnect the S-drive!

On top of This PC, press mouse right and choose Disconnect network drive.



Select the network drive, and press OK.

ОК

Cancel

Disconnect Network Drives	
elect the network drive(s) you want to disconnect, then click OK.	
letwork Drives:	
commonshare (\\fileservices.ad.jyu.fi) (S:)	