

Sequence Summary Report (Extended)



Agilent Technologies

Sequence name: SingleSample
Description:
Acquisition date: 2021-03-02 10:13:21+02:00
Acquired by: fatma
Data path: d:\CDSPProjects\Fatma\Results\Agilent HPLC-2021-03-02 10-13-20+02-00.sirslt

Approved by:

Signature:

Date:

Sequence Summary Report (Extended)



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Sequence Table:

Bracketing Mode: None

Seq. Line: 1

Location: P1-A2

Sample name: Crude 2

Sample info:

Acq. Method: Marwa Elhawary2-3-21.amx

Data file: Agilent HPLC-2021-03-02 10-13-20+02-00.dx

Injection #: 1 of 1

Inj. volume: 80.000

Proc. Method: 3D UV
Quantitative_DefaultMethod.p
mx

Sample amount: 0.000

Sample type: Sample

Dilution: 1

Calibration level:

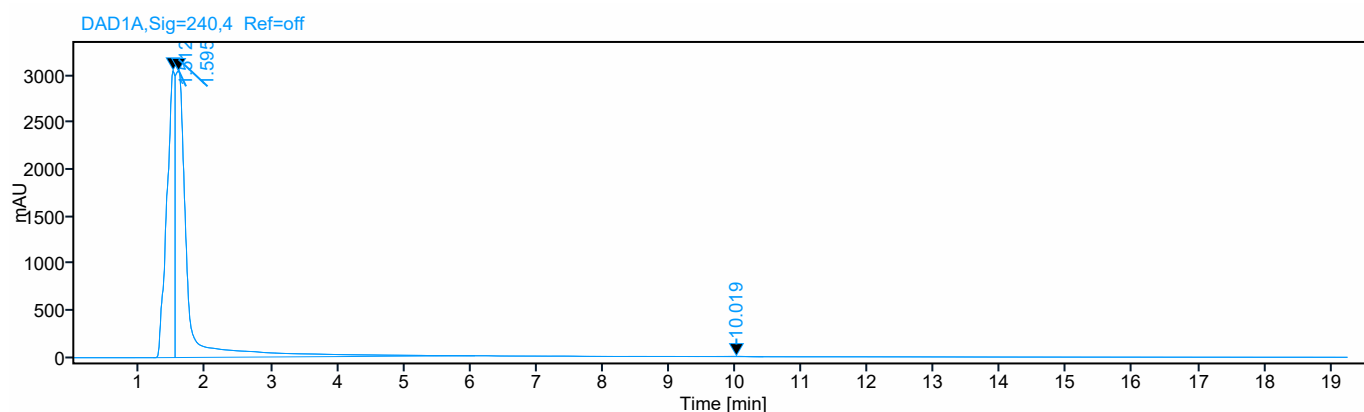
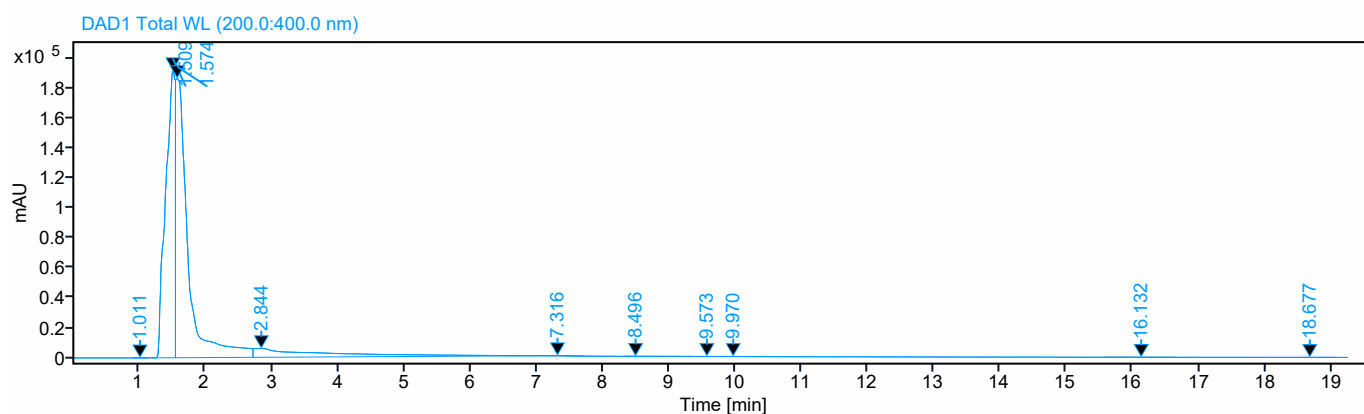
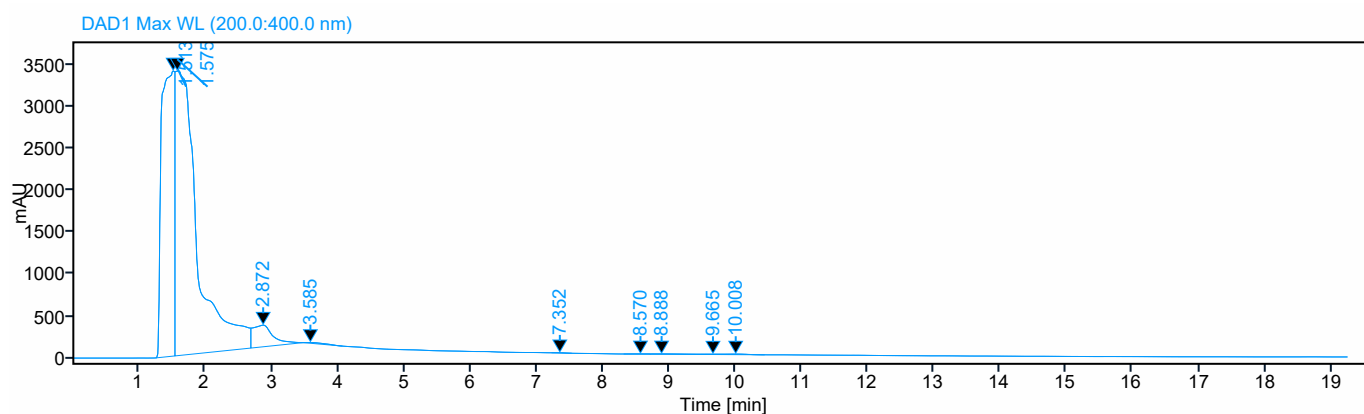
Multiplier: 1

Sequence Summary Report (Extended)



Agilent Technologies

Sample name: Crude 2
Data file: Agilent HPLC-2021-03-02 10-13-20+02-00.dx
Operator: fatma
Instrument: Agilent HPLC
Injection date: 2021-03-02 10:15:06+02:00
Inj. volume: 80.000
Location: P1-A2
Acq. method: Marwa Elhawary2-3-21.amx
Type: Sample
Processing method: 3D UV
 Quantitative_DefaultMethod.pmx
Sample amount: 0.00
Manually modified: None



RT [min]	Signal	Type	Area	Amount ☐	Conc. ☐	Name
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**Method Summary**

Processing method: 3D UV Quantitative_DefaultMethod.pmx

Method version: 2021-0228-0814-48778

Line#	Location	Sample Name	Injection modified	Acq. Method	ACQ Method Version
1	P1-A2	Crude 2	2021-03-02 10:35:51+02:00	Marwa Elhawary2-3- 21.amx	2021-0302-0756- 23650

Calibration standard statistics:

Sample statistics:

**Acquisition method:**

Acquisition Method: Marwa Elhawary2-3-21.amx
Path: d:\CDSPProjects\Fatma\Results\Agilent HPLC-2021-03-02 10-13-20+02-00.sirsl

Method Information

Last Saved As: d:\CDSPProjects\Fatma\Methods\Marwa Elhawary2-3-21.amx Modified: 2021-03-02 09:56:23+02:00
Modifier: fatma Created: 2021-03-02 09:56:23+02:00
Creator: fatma Description:
Version: 2021-0302-0756-23650

Method Properties

Instrument Liquid Chromatography
Technique:

Schema version

Schema version: 2.3

Quat. Pump Method

Flow: 1.000 mL/min Low Pressure Limit: 0.00 bar
High Pressure Limit: 600.00 bar Maximum Flow Gradient: 100.000 mL/min²
Primary Channel: Automatic Module Display Name: Quat. Pump
Module Type: G7111B Order: 1

Solvent Composition

Row ID	Channel	Name 1	Used	Percent (%)
1	A		Yes	0.0
2	B		Yes	50.0
3	C		Yes	50.0
4	D		No	

Timetable

Row ID	Time (min)	A (%)	B (%)	C (%)
1	20.00	0.0	50.0	50.0

Row ID	D (%)	Flow (mL/min)	Pressure (bar)
1	0.0	---	---

Stroke

Automatic Stroke Calculation: Yes

Compress

Compressibility Mode: Compressibility Value Set Compressibility: 100 10e-6/bar

Stop Time

Stoptime Mode: No limit

**Post Time**

Posttime Mode: Off

Sampler MethodModule Display Name: Sampler
Order: 1

Module Type: G7129A

Auxiliary

Draw Speed: 200 µL/min

Eject Speed: 400 µL/min

Wait Time After Draw: 1.2 s

Needle Height Offset: 0.0 mm

Injection

Injection Mode: Injection with needle wash

Injection Volume: 80.00 µL

Needle Wash

Needle Wash Location: P1-A1

Needle Wash Location: Wash Vial

Wash Cycles: 3

High throughput

Sample Flush-Out Factor: 5.0

Injection Valve to Bypass for Delay Volume Reduction: No

Overlapped Injection

Overlapped Injection Mode: Off

Stop Time

Stoptime Mode: As pump/No limit

Post Time

Posttime Mode: Off

Column Oven MethodModule Display Name: Column Oven
Order: 1

Module Type: G7130A

Temperature Control

Temperature Control Mode: Not Controlled

Temperature Not Ready LimitTemperature Not Ready Limit On: Yes
Temperature Equilibration Time: 0.0 min

Temperature Not Ready Limit Value: 0.8 °C

Enforce column for run

Enforce column for run enabled: No

Stop Time

Stoptime Mode: As pump/injector

Post Time

Sequence Summary Report (Extended)



Agilent Technologies

Posttime Mode: Off

DAD Method

Peakwidth: > 0.1 min (2 s response time) (2.5 Hz) Slit: 4 nm
UV Lamp Required: Yes Vis Lamp Required: Yes
Module Display Name: DAD Module Type: G7115A
Order: 1

Analog Output

Analog Zero Offset: 5 % Analog Attenuation: 1000 mAU

Signals

Signal table

Row ID	Acquire	Signal	Wavelength (nm)	Bandwidth (nm)
1	Yes	Signal A	240	4
2	No	Signal B		
3	No	Signal C		
4	No	Signal D		
5	No	Signal E		
6	No	Signal F		
7	No	Signal G		
8	No	Signal H		

Row ID	Use Ref.
1	No
2	
3	
4	
5	
6	
7	
8	

Prepare Mode

Margin for negative Absorbance: 100 mAU

Autobalance

Autobalance Prerun: Yes Autobalance Postrun: Yes

Spectrum

Spectrum Range WL 190 nm Spectrum Range WL 400 nm
from: to:
Spectrum Step: 2.0 nm Spectrum Store: All

Stoptime

Stoptime Mode: As pump/injector

**Posttime**

Posttime Mode: Off

**Processing method:**

Data Analysis Method: 3D UV Quantitative_DefaultMethod.pmx
Path: d:\CDSPProjects\Fatma\Methods

Method Information

Last Saved As:	d:\CDSPProjects\Fatma\Methods\3D UV Quantitative_DefaultMethod.pmx	Modified:	2021-02-28 10:19:05+02:00
Modifier:	fatma	Created:	2020-12-16 10:10:44+02:00
Creator:	fatma	Description:	
Version:	2021-0228-0814-48778	Type:	3D UV Quantitative

Method Parameters**Chromatogram extraction****MS Chromatogram extraction parameters**

Single m/z width:	0.5 mda	Asymmetric m/z width low:	0.3 mda
Asymmetric m/z width high:	0.7 mda	Single ppm width:	100.0
Single m/z expansion mode:	Asymmetric (m/z)	Absolute RT window :	0.000 min
Relative RT window :	0.0 percent		

UV Chromatogram extraction parameters**Total wavelength chromatogram**

Is extracted:	Yes	Restricted range:	Yes
Minimum wavelength:	200.0 nm	Maximum wavelength:	400.0 nm

Maximum wavelength chromatogram

Is extracted:	Yes	Restricted range:	Yes
Minimum wavelength:	200.0 nm	Maximum wavelength:	400.0 nm

Spectrum extraction**MS Spectrum extraction parameters**

Start time:	0.000 min	End time:	0.000 min
Use external time range:	No	Background Source Type:	None
Spectrum type:	Peak apex spectrum	Extract spectra from integrated peaks on reprocessing:	No

UV Spectrum extraction parameters

Start time:	0.000 min	End time:	0.000 min
Use external time range:	Yes	Background Source Type:	Spectrum at peak start and end

Signals**Blank Subtraction**

Blank subtraction:	None	Used blank:	Defined in sequence
Specific blank path:		Specific blank:	

Sequence Summary Report (Extended)



Agilent Technologies

Subtract blank if data rates are different: No

Signal matching mode:

Perform blank subtraction if signal names match

Signal alignment

Use delay: Yes

Detector: DAD1

RT : 0.000 min

Delay : 0.000 min

Chromatogram Smoothing

Smoothing algorithm: None

Number of points: 5

Number of passes: 1

ChemStation integrator

ChemStation integrator parameters

Tangent skim mode: Standard

Baseline correction: Advanced

Front peak skim height ratio: 0.00

Tail peak skim height ratio: 0.00

Skim valley ratio: 20.00

Peak to valley ratio: 500.00

Initial timed events

Row ID	Use	Time (min)	Event	Value
1	Yes	0.000	Slope sensitivity	1
2	Yes	0.000	Peak width	0.02
3	Yes	0.000	Area reject	1
4	Yes	0.000	Height reject	1.7
5	Yes	0.000	Shoulders mode	Off
6	Yes	0.000	Area% reject	0

Compound parameters

Include ISTD Amount: No

Is normalized: No

Level count: 5

ISTD method: No

Use time references: No

Use relative retention time: No

Norm amount: 100.0 percent

Response factor calculation mode: Response per amount

Use individual points: No

Concentration calculation: Amount * Multipliers * Dil. factor

Calculate mass %: No

Qualifier count: 2

Qualifier RT Window: 0.010 min

Qualifier response window: 20.0 percent

Response Window Type: Relative

Automatic spectra extraction parameters

Impurity check parameters

Peak purity parameters

Calculate peak purity: No

Use wavelength range low: No

Use wavelength range high: No

Wavelength range low value: 0.00

Wavelength range high value: 0.00

Sensitivity not identified peaks: 50.00

Threshold exceptions: 0



UV spectra confirmation settings

UV confirmation spectra parameters

Baseline subtraction:	Yes	Match factor limit:	0.0
Minimum wavelength:	nm	Maximum wavelength:	nm
Wavelength range low:	No	Wavelength range high:	No
UV reference spectrum exist:	No		

MS purity check parameters

MS peak purity parameters

Calculate MS peak purity:	No	Top (n) ions to extract:	10
Minimum peak purity (%):	95		

System Suitability

EP:	No	Column performance:	None
JP:	No	USP:	No
Signal to noise:	None	Noise calculation:	P2P
Use blank reference for noise:	on blank	Calculate noise before or after peak:	before peak start
Range mode for Noise Selection:	Automatic	Noise range end time:	0.60
Noise range start time:	0.50	Noise range relative end time:	0.40
Noise range relative start time:	0.00	Name:	
Overwrite column parameters:	No	Serial number:	
Particle size:		Void time *:	
Length *:		Particle size unit:	µm
Diameter:		Column length unit:	m
Dead volume:			

Custom calculations

Last imported file:	Embedded file:	No
Created by:	Creation date:	
Last modified by:	Last modified date:	
File version:	Custom calculations file:	

Reporting parameters

From time:	To time:
From response:	To response:

General reporting parameters

Row ID	Report template	Do print	Do create file	Printer name
1		No	No	
2		No	No	



Sequence name: SingleSample
Description:
Acquisition date: 2021-02-28 09:49:07+02:00
Acquired by: fatma
Data path: d:\CDSPProjects\Fatma\Results\Agilent HPLC-2021-02-28 09-49-07+02-00.sirslt

Approved by:

Signature:

Date:

**Sequence Table:****Bracketing Mode:** None**Seq. Line:** 1**Location:** P1-A2**Sample name:** Crude 1**Sample info:****Acq. Method:** Marwa Elhawary28-2-21.amx**Data file:** Agilent HPLC-2021-02-28 09-49-07+02-00.dx**Injection #:** 1 of 1**Inj. volume:** 80.000**Proc. Method:** *3D UV
Quantitative_DefaultMethod.p
mx**Sample amount:** 0.000**Sample type:** Sample**Dilution:** 1**Calibration level:****Multiplier:** 1

Sequence Summary Report (Extended)



Agilent Technologies

Sample name: Crude 1

Data file: Agilent HPLC-2021-02-28 09-49-07+02-00.dx

Operator: fatma

Instrument: Agilent HPLC

Injection date: 2021-02-28 09:50:53+02:00

Inj. volume: 80.000

Location: P1-A2

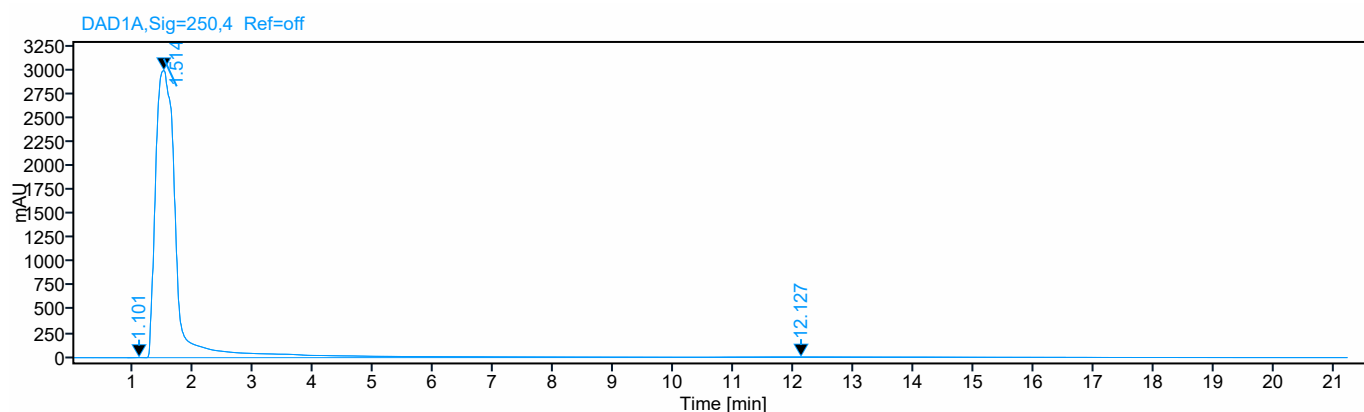
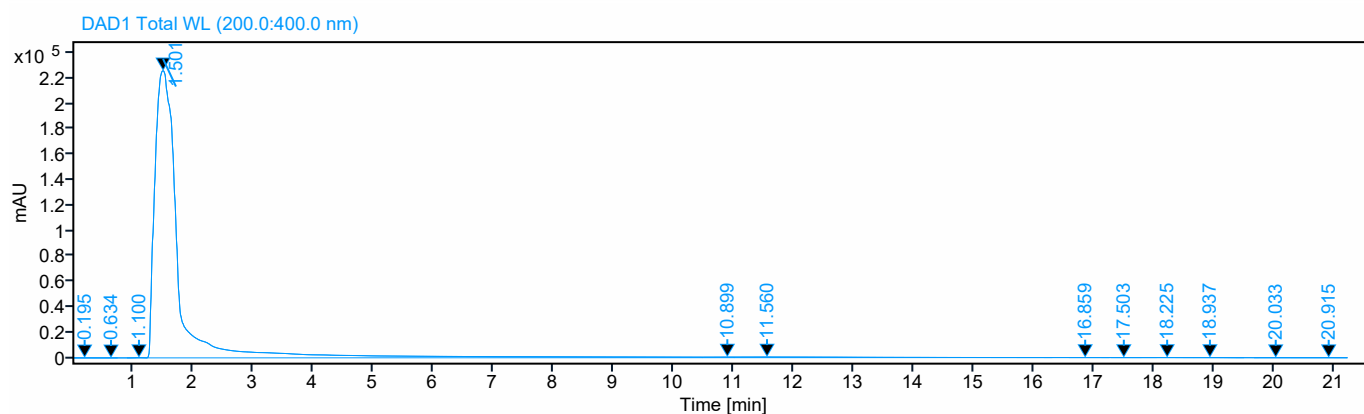
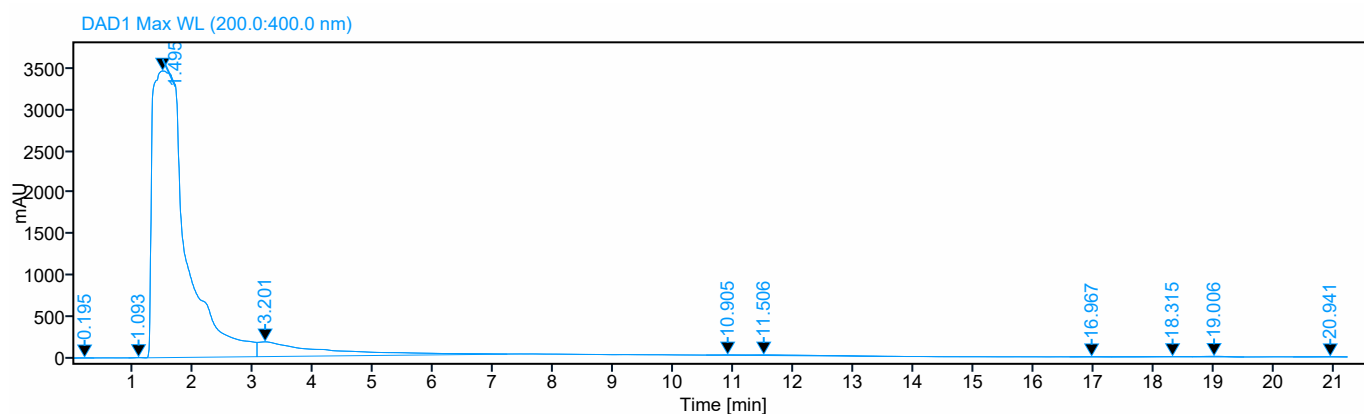
Acq. method: Marwa Elhawary28-2-21.amx

Type: Sample

Processing method: *3D UV
Quantitative_DefaultMethod.pmx

Sample amount: 0.00

Manually modified: None



RT [min]	Signal	Type	Area	Amount ☐	Conc. ☐	Name
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**Method Summary****Processing method:** *3D UV Quantitative_DefaultMethod.pmx**Method version:** 2021-0228-0814-48778

Line#	Location	Sample Name	Injection modified	Acq. Method	ACQ Method Version
1	P1-A2	Crude 1	2021-02-28 10:21:28+02:00	Marwa Elhawary28-2- 21.amx	2021-0228-0749- 07094

Calibration standard statistics:**Sample statistics:**

**Acquisition method:**

Acquisition Method: Marwa Elhawary28-2-21.amx
Path: d:\CDSPProjects\Fatma\Results\Agilent HPLC-2021-02-28 09-49-07+02-00.sirslt

Method Information

Last Saved As: d:\CDSPProjects\Fatma\Methods\Marwa Elhawary28-2-21.amx Modified: 2021-02-28 09:49:07+02:00
Modifier: fatma Created: 2021-02-28 09:47:28+02:00
Creator: fatma Description:
Version: 2021-0228-0749-07094

Method Properties

Instrument Liquid Chromatography
Technique:

Schema version

Schema version: 2.3

Quat. Pump Method

Flow: 1.000 mL/min Low Pressure Limit: 0.00 bar
High Pressure Limit: 600.00 bar Maximum Flow Gradient: 100.000 mL/min²
Primary Channel: Automatic Module Display Name: Quat. Pump
Module Type: G7111B Order: 1

Solvent Composition

Row ID	Channel	Name 1	Used	Percent (%)
1	A		Yes	0.0
2	B		Yes	40.0
3	C		Yes	60.0
4	D		No	

Timetable

Row ID	Time (min)	A (%)	B (%)	C (%)
1	20.00	0.0	40.0	60.0

Row ID	D (%)	Flow (mL/min)	Pressure (bar)
1	0.0	---	---

Stroke

Automatic Stroke Calculation: Yes

Compress

Compressibility Mode: Compressibility Value Set Compressibility: 100 10e-6/bar

Stop Time

Stoptime Mode: No limit

**Post Time**

Posttime Mode: Off

Sampler MethodModule Display Name: Sampler
Order: 1

Module Type: G7129A

Auxiliary

Draw Speed: 200 µL/min

Eject Speed: 400 µL/min

Wait Time After Draw: 1.2 s

Needle Height Offset: 0.0 mm

Injection

Injection Mode: Injection with needle wash

Injection Volume: 80.00 µL

Needle Wash

Needle Wash Location: P1-A1

Needle Wash Location: Wash Vial

Wash Cycles: 3

High throughput

Sample Flush-Out Factor: 5.0

Injection Valve to Bypass for Delay Volume Reduction: No

Overlapped Injection

Overlapped Injection Mode: Off

Stop Time

Stoptime Mode: As pump/No limit

Post Time

Posttime Mode: Off

Column Oven MethodModule Display Name: Column Oven
Order: 1

Module Type: G7130A

Temperature Control

Temperature Control Mode: Not Controlled

Temperature Not Ready LimitTemperature Not Ready Limit On: Yes
Temperature Equilibration Time: 0.0 min

Temperature Not Ready Limit Value: 0.8 °C

Enforce column for run

Enforce column for run enabled: No

Stop Time

Stoptime Mode: As pump/injector

Post Time

Sequence Summary Report (Extended)



Agilent Technologies

Posttime Mode: Off

DAD Method

Peakwidth: > 0.1 min (2 s response time) (2.5 Hz) Slit: 4 nm
UV Lamp Required: Yes Vis Lamp Required: Yes
Module Display Name: DAD Module Type: G7115A
Order: 1

Analog Output

Analog Zero Offset: 5 % Analog Attenuation: 1000 mAU

Signals

Signal table

Row ID	Acquire	Signal	Wavelength (nm)	Bandwidth (nm)
1	Yes	Signal A	250	4
2	No	Signal B		
3	No	Signal C		
4	No	Signal D		
5	No	Signal E		
6	No	Signal F		
7	No	Signal G		
8	No	Signal H		

Row ID	Use Ref.
1	No
2	
3	
4	
5	
6	
7	
8	

Prepare Mode

Margin for negative Absorbance: 100 mAU

Autobalance

Autobalance Prerun: Yes Autobalance Postrun: Yes

Spectrum

Spectrum Range WL 190 nm Spectrum Range WL 400 nm
from: to:
Spectrum Step: 2.0 nm Spectrum Store: All

Stoptime

Stoptime Mode: As pump/injector



Posttime

Posttime Mode: Off

**Processing method:**

Data Analysis Method: 3D UV Quantitative_DefaultMethod.pmx
Path: d:\CDSPProjects\Fatma\Methods

Method Information

Last Saved As:	d:\CDSPProjects\Fatma\Methods\3D UV Quantitative_DefaultMethod.pmx	Modified:	2021-02-28 10:19:05+02:00
Modifier:	fatma	Created:	2020-12-16 10:10:44+02:00
Creator:	fatma	Description:	
Version:	2021-0228-0814-48778	Type:	3D UV Quantitative

Method Parameters**Chromatogram extraction****MS Chromatogram extraction parameters**

Single m/z width:	0.5 mda	Asymmetric m/z width low:	0.3 mda
Asymmetric m/z width high:	0.7 mda	Single ppm width:	100.0
Single m/z expansion mode:	Asymmetric (m/z)	Absolute RT window :	0.000 min
Relative RT window :	0.0 percent		

UV Chromatogram extraction parameters**Total wavelength chromatogram**

Is extracted:	Yes	Restricted range:	Yes
Minimum wavelength:	200.0 nm	Maximum wavelength:	400.0 nm

Maximum wavelength chromatogram

Is extracted:	Yes	Restricted range:	Yes
Minimum wavelength:	200.0 nm	Maximum wavelength:	400.0 nm

Spectrum extraction**MS Spectrum extraction parameters**

Start time:	0.000 min	End time:	0.000 min
Use external time range:	No	Background Source Type:	None
Spectrum type:	Peak apex spectrum	Extract spectra from integrated peaks on reprocessing:	No

UV Spectrum extraction parameters

Start time:	0.000 min	End time:	0.000 min
Use external time range:	Yes	Background Source Type:	Spectrum at peak start and end

Signals**Blank Subtraction**

Blank subtraction:	None	Used blank:	Defined in sequence
Specific blank path:		Specific blank:	

Sequence Summary Report (Extended)



Agilent Technologies

Subtract blank if data rates are different: No

Signal matching mode:

Perform blank subtraction if signal names match

Signal alignment

Use delay: Yes

Detector: DAD1

RT : 0.000 min

Delay : 0.000 min

Chromatogram Smoothing

Smoothing algorithm: None

Number of points: 5

Number of passes: 1

ChemStation integrator

ChemStation integrator parameters

Tangent skim mode: Standard

Baseline correction: Advanced

Front peak skim height ratio: 0.00

Tail peak skim height ratio: 0.00

Skim valley ratio: 20.00

Peak to valley ratio: 500.00

Initial timed events

Row ID	Use	Time (min)	Event	Value
1	Yes	0.000	Slope sensitivity	1
2	Yes	0.000	Peak width	0.02
3	Yes	0.000	Area reject	1
4	Yes	0.000	Height reject	1.7
5	Yes	0.000	Shoulders mode	Off
6	Yes	0.000	Area% reject	0

Compound parameters

Include ISTD Amount: No

Is normalized: No

Level count: 5

ISTD method: No

Use time references: No

Use relative retention time: No

Norm amount: 100.0 percent

Response factor calculation mode: Response per amount

Use individual points: No

Concentration calculation: Amount * Multipliers * Dil. factor

Calculate mass %: No

Qualifier count: 2

Qualifier RT Window: 0.010 min

Qualifier response window: 20.0 percent

Response Window Type: Relative

Automatic spectra extraction parameters

Impurity check parameters

Peak purity parameters

Calculate peak purity: No

Use wavelength range low: No

Use wavelength range high: No

Wavelength range low value: 0.00

Wavelength range high value: 0.00

Sensitivity not identified peaks: 50.00

Threshold exceptions: 0



UV spectra confirmation settings

UV confirmation spectra parameters

Baseline subtraction:	Yes	Match factor limit:	0.0
Minimum wavelength:	nm	Maximum wavelength:	nm
Wavelength range low:	No	Wavelength range high:	No
UV reference spectrum exist:	No		

MS purity check parameters

MS peak purity parameters

Calculate MS peak purity:	No	Top (n) ions to extract:	10
Minimum peak purity (%):	95		

System Suitability

EP:	No	Column performance:	None
JP:	No	USP:	No
Signal to noise:	None	Noise calculation:	P2P
Use blank reference for noise:	on blank	Calculate noise before or after peak:	before peak start
Range mode for Noise Selection:	Automatic	Noise range end time:	0.60
Noise range start time:	0.50	Noise range relative end time:	0.40
Noise range relative start time:	0.00	Name:	
Overwrite column parameters:	No	Serial number:	
Particle size:		Void time *:	
Length *:		Particle size unit:	µm
Diameter:		Column length unit:	m
Dead volume:			

Custom calculations

Last imported file:	Embedded file:	No
Created by:	Creation date:	
Last modified by:	Last modified date:	
File version:	Custom calculations file:	

Reporting parameters

From time:	To time:
From response:	To response:

General reporting parameters

Row ID	Report template	Do print	Do create file	Printer name
1		No	No	
2		No	No	