

Increase your HPI IQ with the Agilent iQ

The intelligent LC MS for the HPLC Chemist

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<https://blog.agilent.com/2017/09/26/agilent-drives-a-new-chemical-industry-standard/?from=>

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Agilent
OpenLab

 **Agilent**

Pharmaceutical



Chemical



Food



Academia



Mass confirmation, sample purity, reaction monitoring

Method development

QA/QC

Introducing the InfinityLab LC/MSD iQ

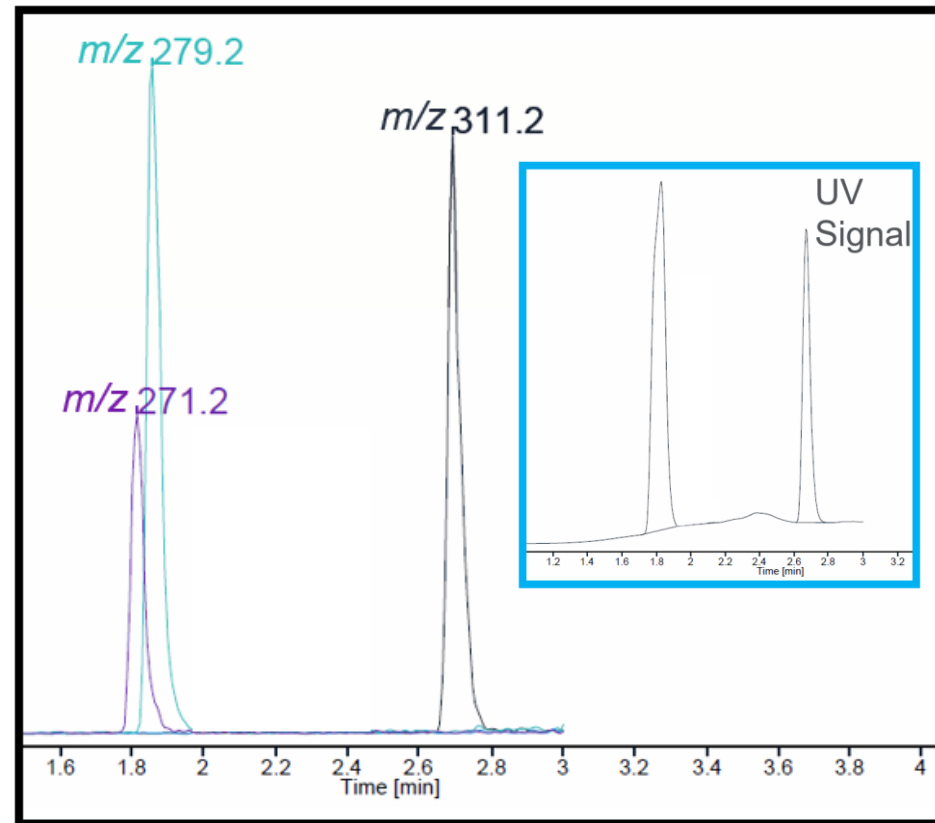
- Intuitive quadrupole
- Self-aware, self-driving
- Robust
- Designed for non-experts



Only **two** peaks are detected in the UV

Sample actually contains **three** compounds

With the ability to extract single ion chromatograms (EIC), the MS can detect separate compounds co-eluting in the UV





- Small and compact
- Same size as LC module
- Integrated with LC stack
- Uses same power outlets as LC modules
- No costly electrical upgrades
- Self-ranging power supply



Add Flexibility and Ergonomics with Flex Bench MS

More ergonomic and convenient access

Movable to key project locations

Extendable shelf for mass spec

Integrated Quiet Cover



Simplified AutoTuning

Scheduled during
instrument idle time

Schedule Tune

Scheduling: Weekly Monthly

Recur every week(s) on:

Monday Tuesday Wednesday Thursday Friday
 Saturday Sunday

Start: Time:

Simple to read reports

MS Checktune Report

Agilent | Trusted Answers

MS Checktune Report - InfinityLab LC/MSD iQ

Instrument Information			
Model	G6180A LC/MSD iQ	Checktune Date	2019-05-07T07:00:53-07:00
Serial Number	SG1901RP08	SW/FW Version	2.3.343/5.47.1
Autotune Version	2.5.23	Last Autotune Date	2019-05-06T08:33:02-07:00
Ion Source	ESI	Overall Result	Passed

Positive Ion Mode	
MS Peak Width: Unit, Scan Speed: Normal	Result: Passed
MS Peak Width: Wide, Scan Speed: Normal	Result: Passed
MS Peak Width: Widest, Scan Speed: Normal	Result: Passed
MS Scan Speed: Fast	Result: Passed
MS Scan Speed: Ultra	Result: Passed

Simplified MS Method Development

Auto Acquire

How can I
make sure I'm
seeing all the
ions?

How high a
voltage do I
need?

How do I
optimize
ionization?

Simplified MS Method Development

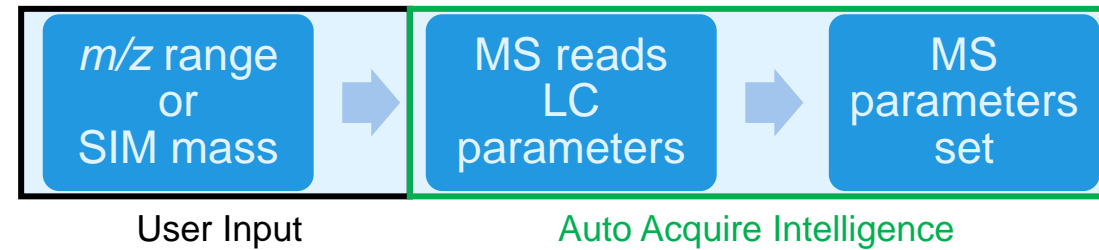
Auto Acquire

Intuitive MS

Auto Acquire simplifies acquisition process

Just enter mass information

Auto Acquire



Acquisition Method – Untitled

General Properties | **Auto Acquire** | Advanced Acquire | Tune

Ion source: ESI | Stop time: As pump/No limit | Limit (min): 1

Acquisition Parameters

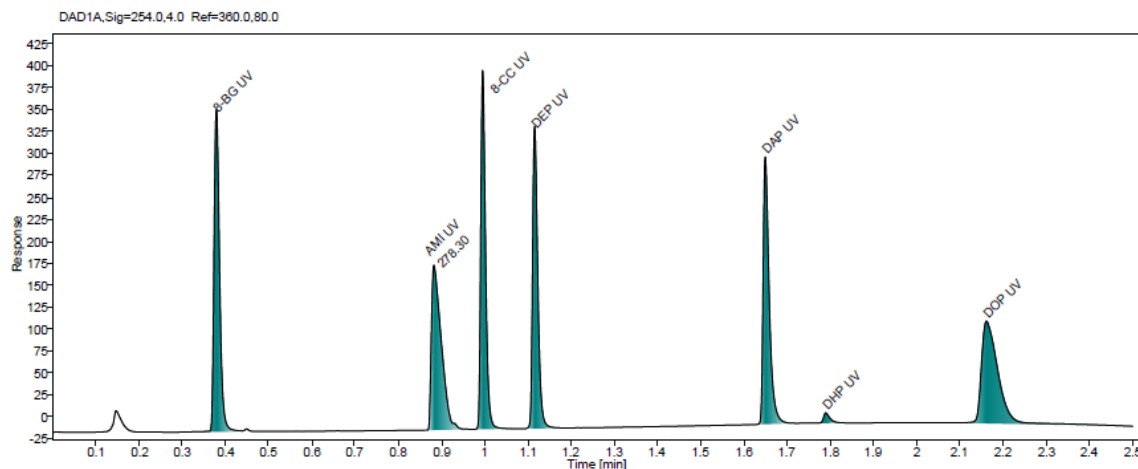
Scan type	Polarity	Compound/Segment name	Mass range start (m/z)	Mass range end (m/z)
▶ Scan	Positive		100	1000
▶ Scan	Negative		100	1000

Targeted points per second (Hz): | Data storage:

Estimated cycle time (ms/cycle): | SIM %:

- Functional test of LC system, column, mass spectrometer and solvents
- Report evaluates sensitivity, peak capacity, peak shape, resolution
- Positive and negative ion mode tested
- Option for full scheduling & automation

Sample name: Agilent Sys Suit	Injection date: 5/16/2019 10:57:34 AM	Acq. operator: Admin
Instrument: 1290 LC/MSD iQ	Location: P1-A4	Injection volume: 0.300
Analysis:	Sample:	Instrument status: Instrument conformity pass



Instrument stability results

Cmp	RT (min)	Ref.	Deviation	Dev. limit	Status
8-BG UV	0.38		0.02	3.00	Pass
8-BG EIC	0.40	Rectangular Smp	0.03	3.00	Pass
AMI UV	0.88		0.33	3.00	Pass
DAP EIC	1.66		0.24	3.00	Pass
DHP EIC	1.80		0.11	3.00	Pass
DOP UV	2.16		0.09	3.00	Pass
DOP EIC	2.19		0.15	3.00	Pass

Peak capacity results

Cmp	Resolution	Ref.	Deviation	Dev. limit	Status
DEP UV	5.850	5.85	0.00	5.00	Pass

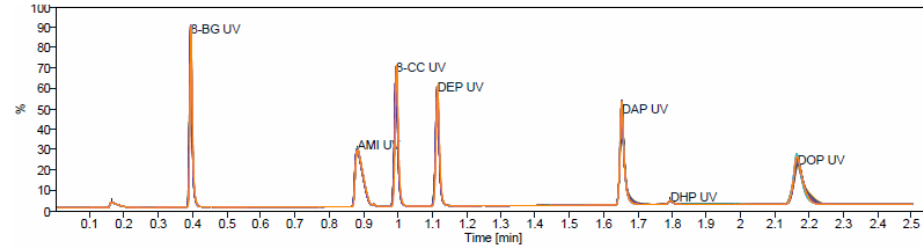
100 injections of system suitability test mix

UV and MS retention time and peak area RSDs

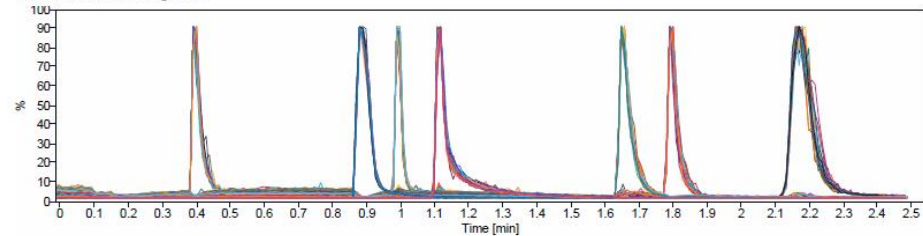
- UV and MS retention time RSDs are <1%
- UV peak area RSDs are <2%
- MS peak area RSDs are <10%

8-BG UV	RT RSD: .14	RT RSD <1%	Peak RSD: 1.274	Peak RSD <2%
AMI UV	RT RSD: .074	RT RSD <1%	Peak RSD: 1.246	Peak RSD <2%
8-CC UV	RT RSD: .058	RT RSD <1%	Peak RSD: 1.243	Peak RSD <2%
DEP UV	RT RSD: .044	RT RSD <1%	Peak RSD: 1.268	Peak RSD <2%
DAP UV	RT RSD: .023	RT RSD <1%	Peak RSD: 1.284	Peak RSD <2%
DHP UV	RT RSD: .028	RT RSD <1%	Peak RSD: 1.984	Peak RSD <2%
DOP UV	RT RSD: .051	RT RSD <1%	Peak RSD: 1.272	Peak RSD <2%
8-BG EIC	RT RSD: .31	RT RSD <1%	Peak RSD: 4.172	Peak RSD <10%
AMI EIC	RT RSD: .197	RT RSD <1%	Peak RSD: 1.702	Peak RSD <10%
8-CC EIC	RT RSD: .139	RT RSD <1%	Peak RSD: 4.345	Peak RSD <10%
DEP EIC	RT RSD: .124	RT RSD <1%	Peak RSD: 4.967	Peak RSD <10%
DAP EIC	RT RSD: .078	RT RSD <1%	Peak RSD: 7.471	Peak RSD <10%
DHP EIC	RT RSD: .081	RT RSD <1%	Peak RSD: 6.895	Peak RSD <10%
DOP EIC	RT RSD: .29	RT RSD <1%	Peak RSD: 6.362	Peak RSD <10%

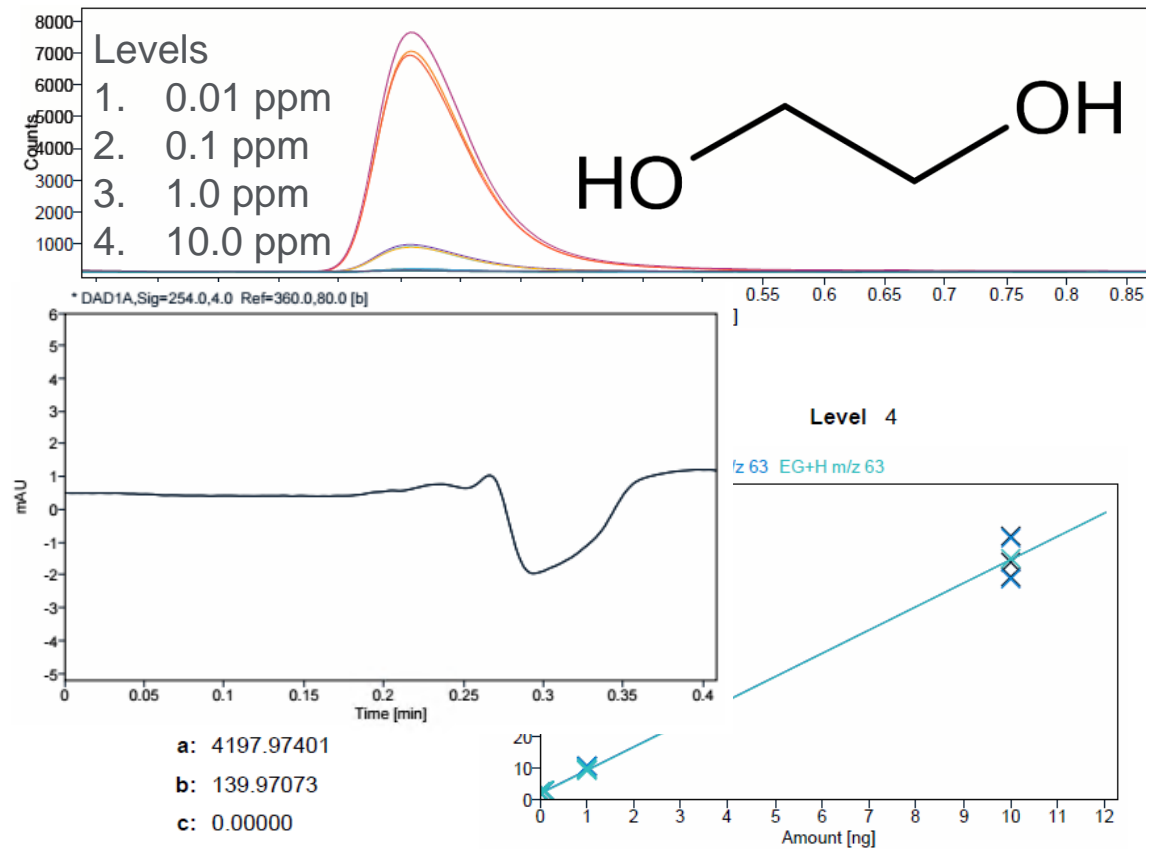
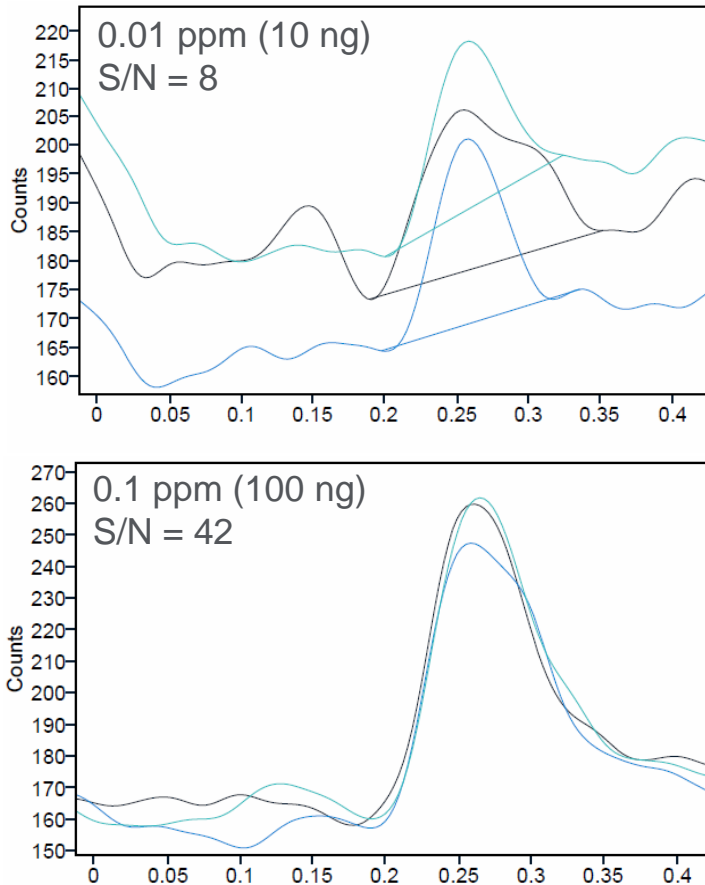
UV Chromatograms



EIC MS Chromatograms



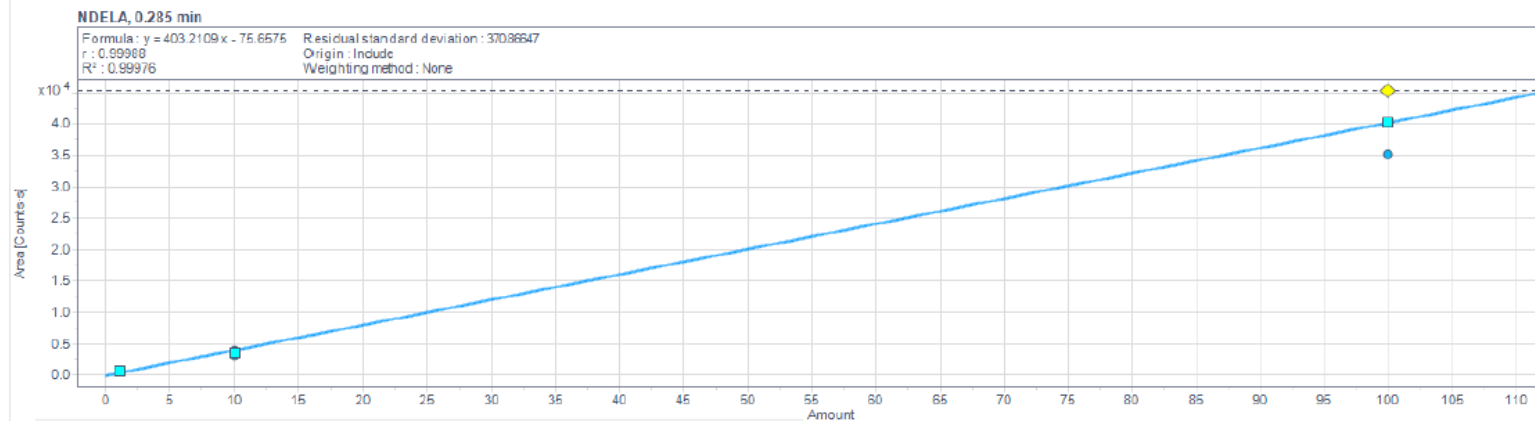
Small Molecule Sensitivity (Ethyhlene Glycol)



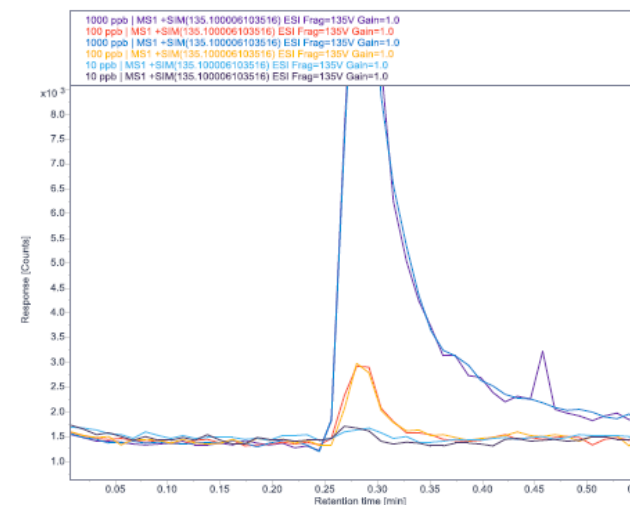
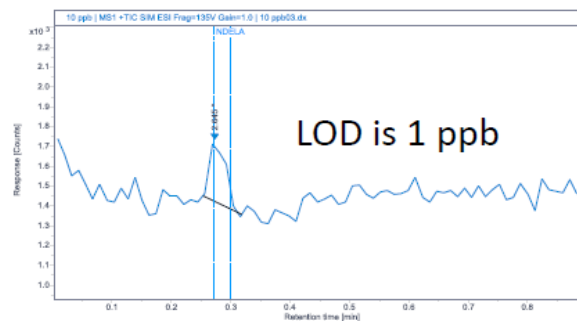
NDELA

N-Nitrosodiethanolamine

Calibration Curve



Order No	Sample name	Vial	Level	Sample type
1	blank	P1-A1		Blank
2	blank 2	P1-A1		Blank
3	1 ppb	P1-A2	1	Cal. Std.
4	1ppb	P1-A2	1	Cal. Std.
5	10 ppb	P1-A3	2	Cal. Std.
6	10 ppb	P1-A3	2	Cal. Std.
7	100 ppb	P1-A4	3	Cal. Std.
8	100 ppb	P1-A4	3	Cal. Std.



100 ppb standard

Sample Purity

With the same data as quantitation

The screenshot displays the Agilent OpenLab software interface for data analysis. The main window is titled "NdelA - Data Analysis". The interface is divided into several panes:

- Data Processing:** A tree view on the left shows a sequence of files, with "10 ppb - 10 ppb04.d" selected. It lists various processing steps like "Chromatograms", "Extracted Chromatograms", and "Extracted Spectra".
- Peak Details:** A central plot shows a chromatogram with a prominent peak at approximately 1.962 minutes. The y-axis is "Response (Counts)" and the x-axis is "Retention time [min]".
- Processing Method:** A panel on the right shows settings for "NDELA purity", including "General", "Positive Ions", and "Negative Ions" sections.
- Sample Purity Results:** A table at the bottom center shows the results for different samples. The "10 ppb" sample is marked as "Impure".
- MS Spectrum:** A panel on the far right shows a mass spectrum with a significant peak at m/z 135.1.

Order	Sample name	Data file	Overall targets found	Overall purity
1	blank	blank01.d	N.A.	N.A.
2	blank 2	blank 202.d	N.A.	N.A.
3	10 ppb	10 ppb03.d	N.A.	N.A.
4	10 ppb	10 ppb04.d	No	Impure
5	100 ppb	100 ppb05.d	N.A.	N.A.
6	100 ppb	100 ppb06.d	N.A.	N.A.
7	1000 ppb	1000 ppb07.d	N.A.	N.A.
8	1000 ppb	1000 ppb08.d	N.A.	N.A.

Name	
Mass	135.10
Formula	
Found	No
Pure	Impure
% Purity	

Walk up software allows anyone to use

Easy sample entry and reporting

Rapid Sample Submission
0
Queue Runtime

Active Samples

User Name:

Password:

Sample Name:

Sample Count:

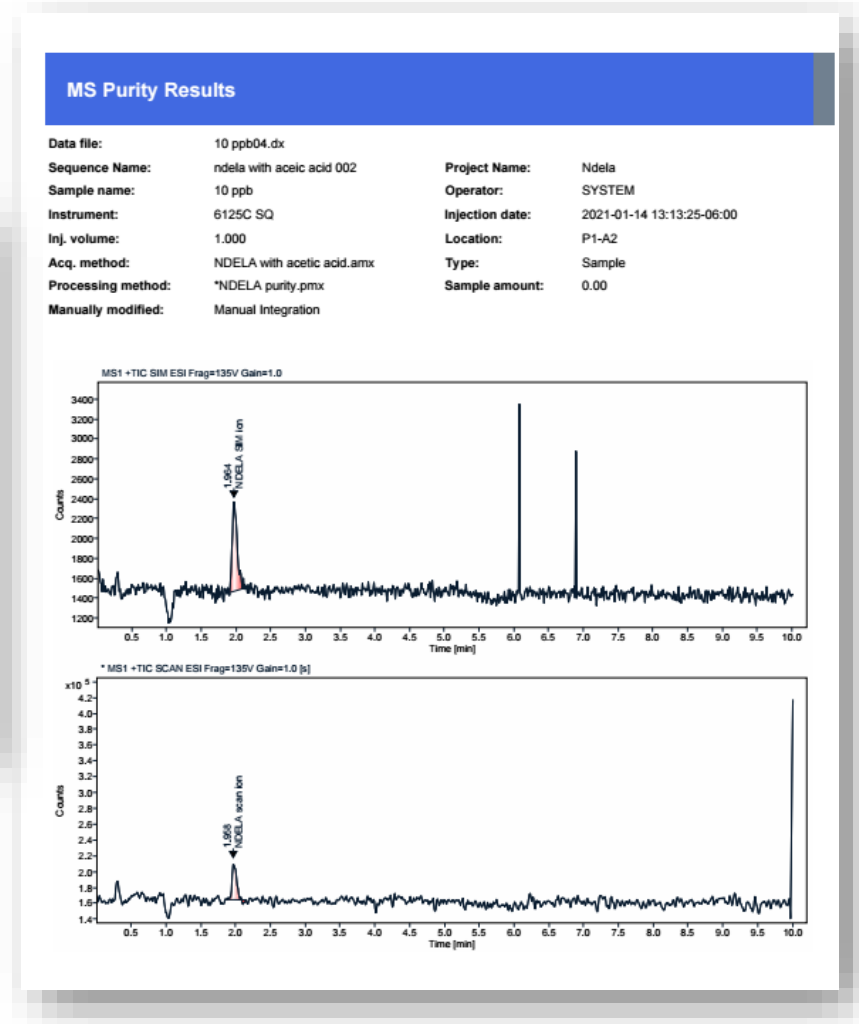
WalkUp Method:

Mass Confirmation:

Select Method

Sample Purity 3 min ACN gradient

Please contact WalkUp Administrator in case of any errors/warnings.
No Samples in Queue







Target found in analysis	Purity (%)	Purity result
Yes	85.44	Impure

Instrument Health Tracking




Early Maintenance Feedback (EMF)



Reports

Detector health	
	Detector lifetime remaining (%) 77.6%
Nebulizer status	
Ion injector status	
Spray stability status	

Summary:

Nebulizer status	
Ion injector status	
Spray stability status	

Maintenance

Early Maintenance Feedback Counters

Autotune

Enable

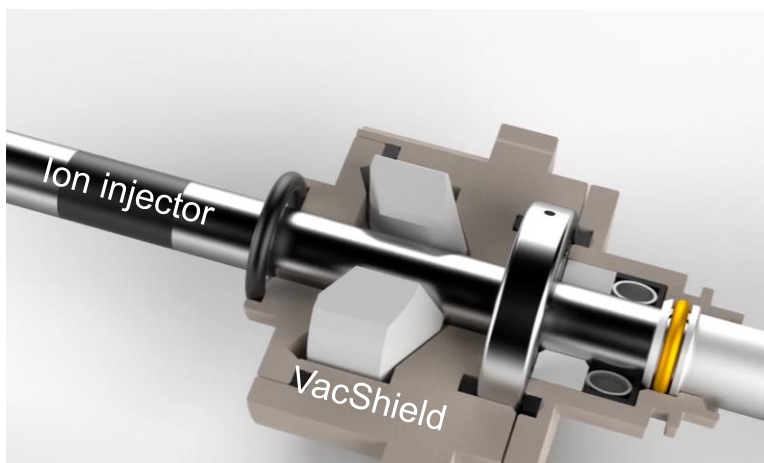
Service Due threshold (Days) 31

Expires on 23-Jun-2019

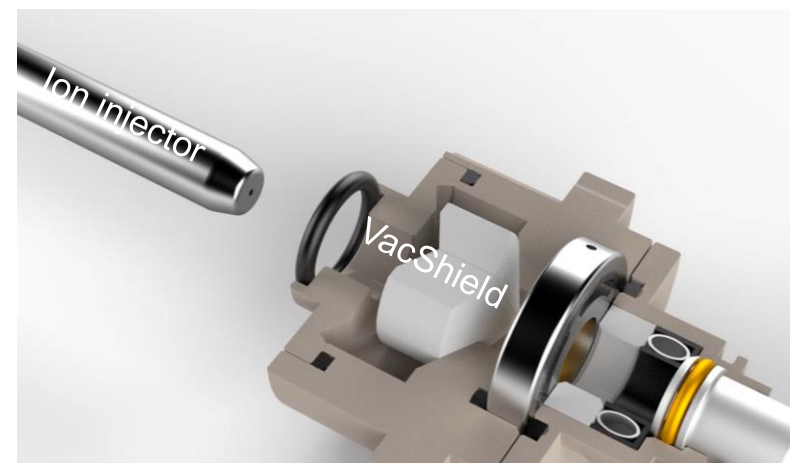
Simple, Rapid, Routine Maintenance with VacShield

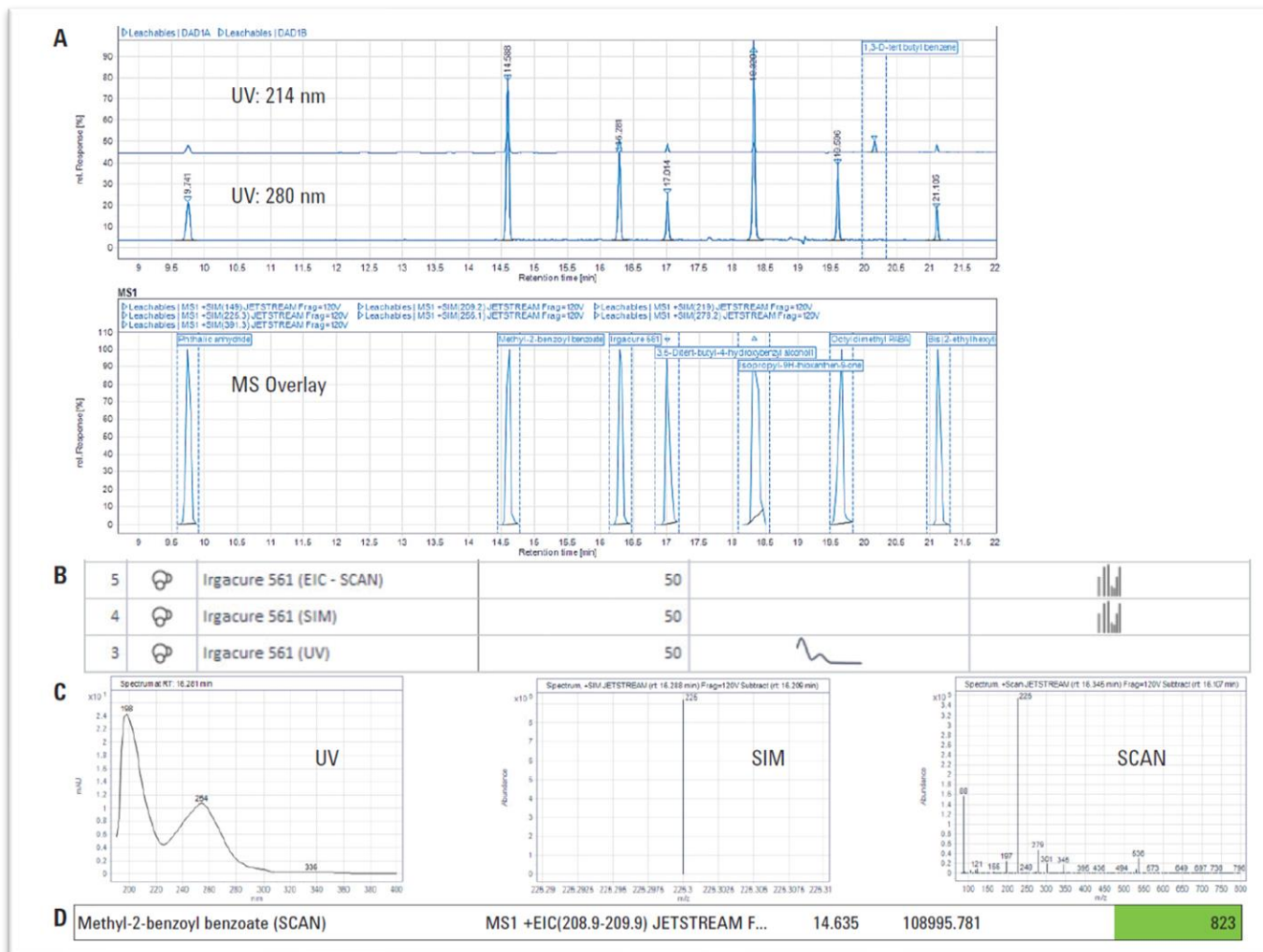
Ion Injector maintenance time reduced to 5 min

VacShield during operation

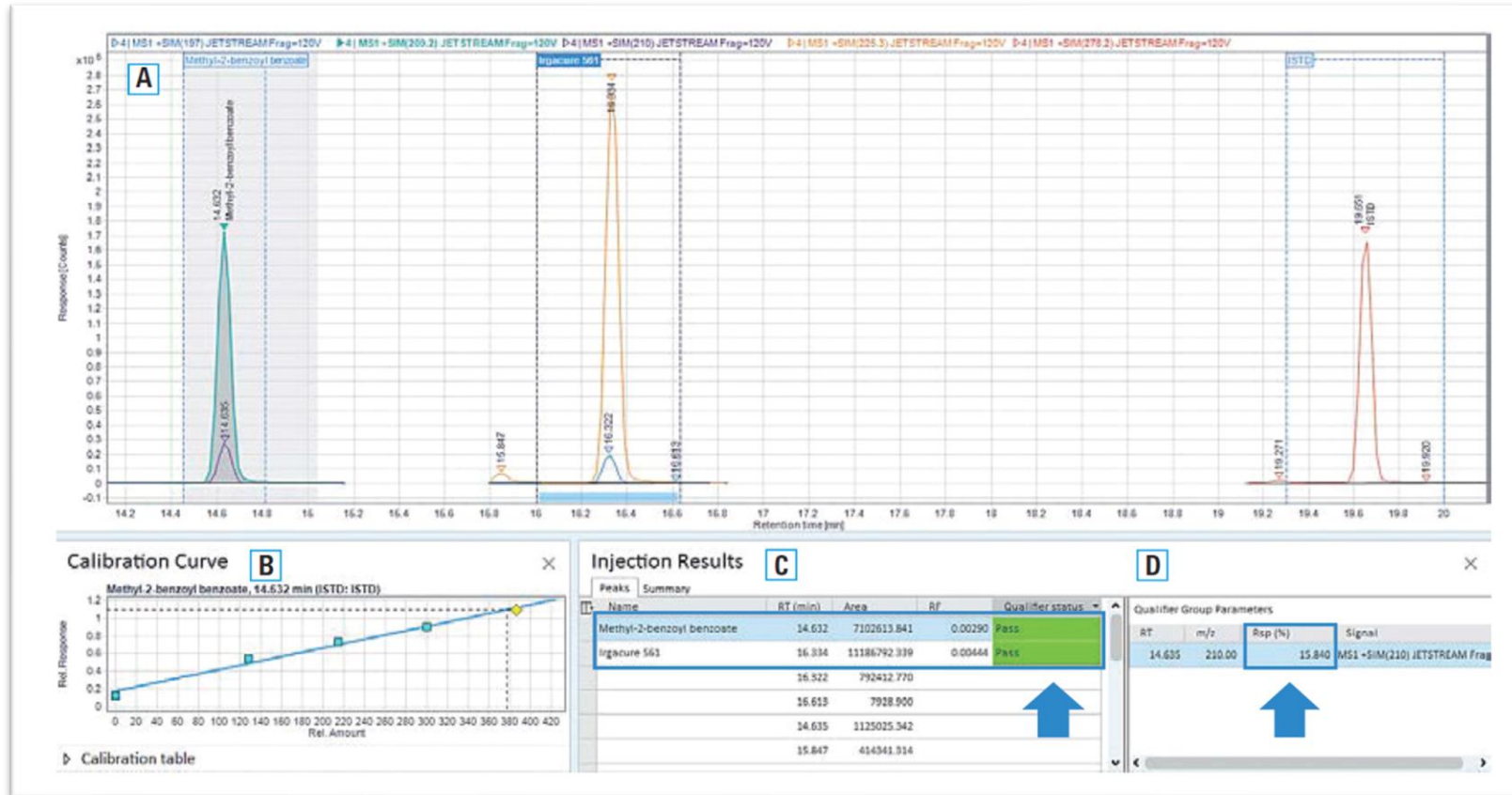


VacShield during maintenance

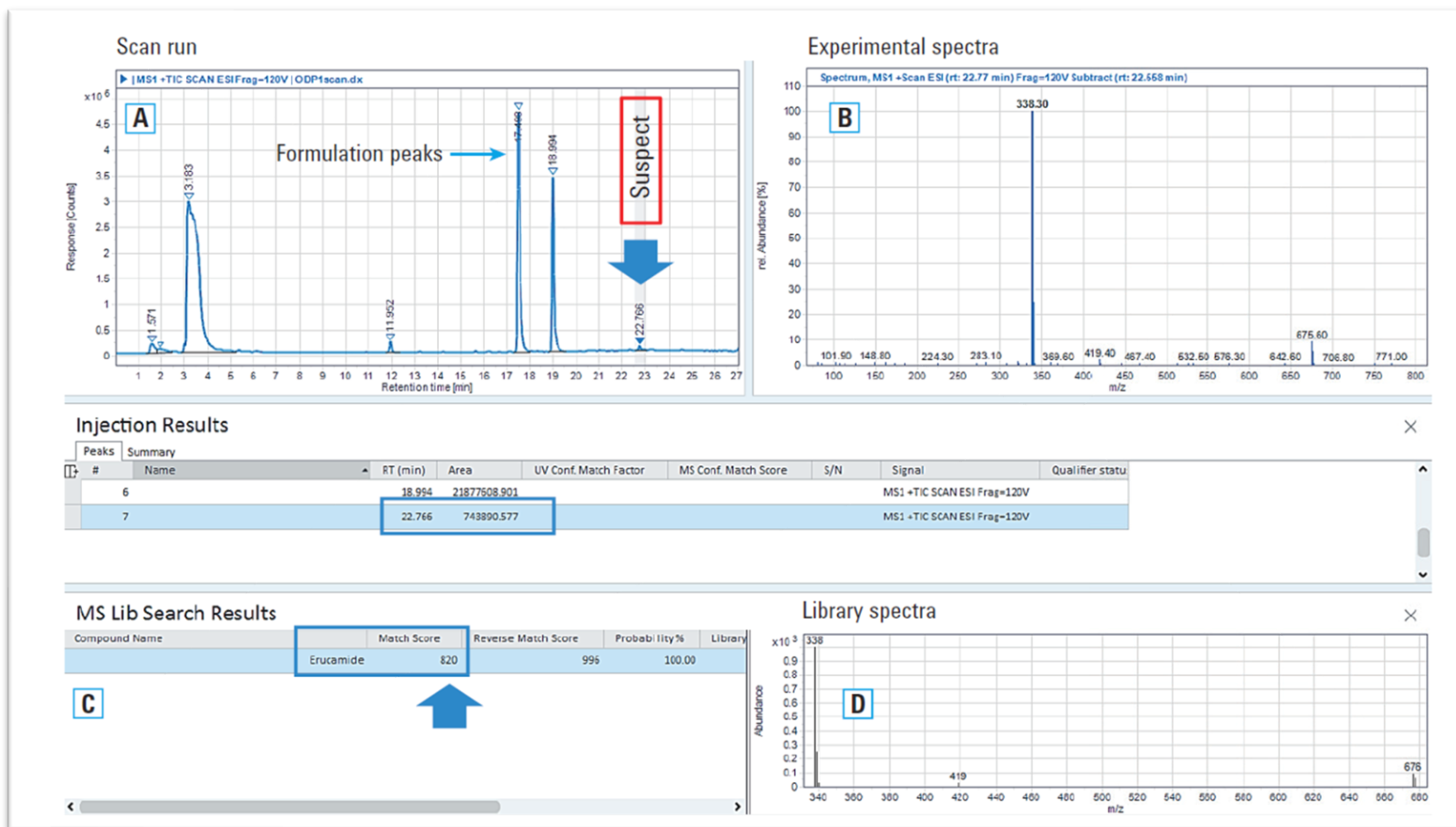




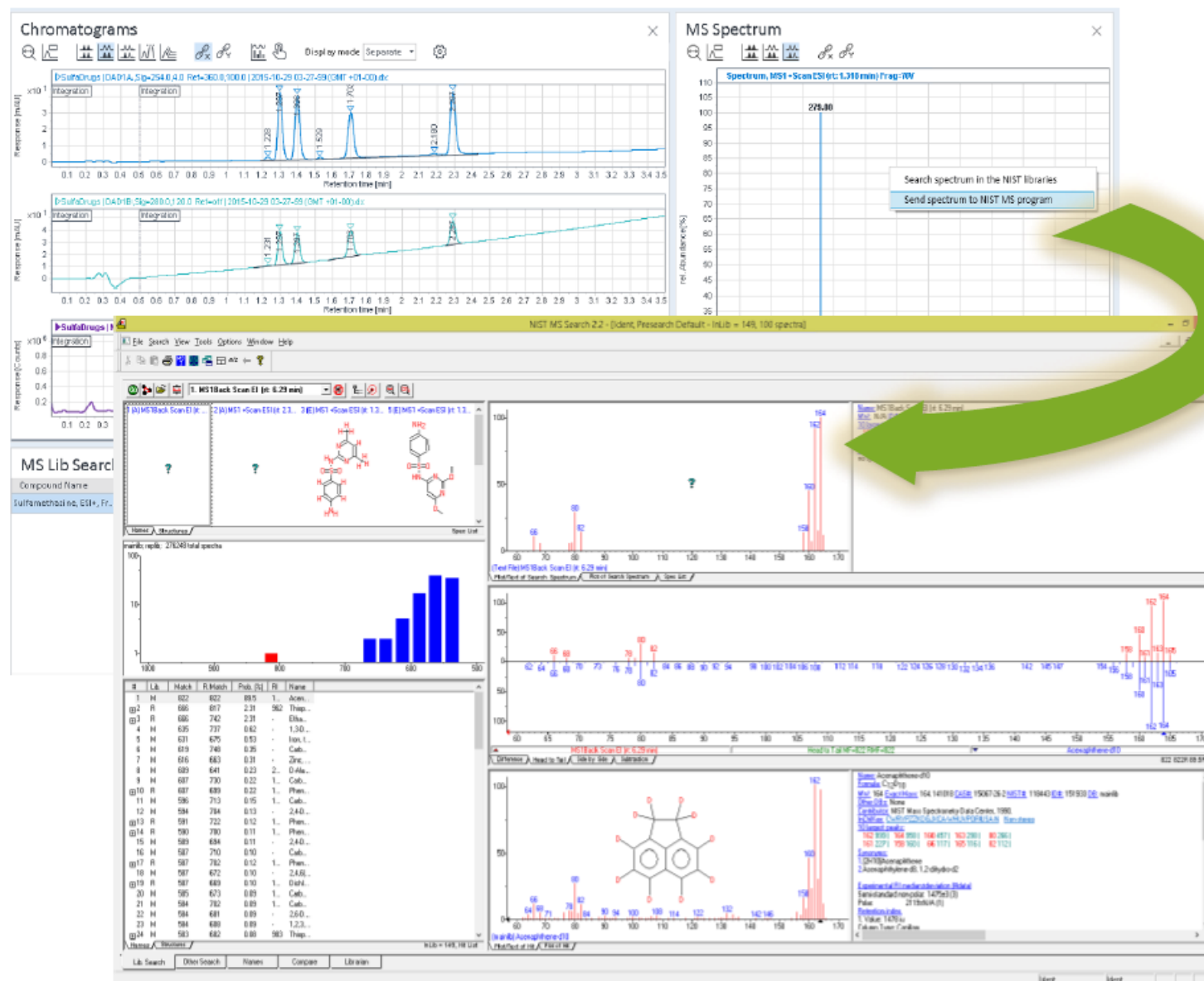
<https://www.agilent.com/cs/library/applications/5991-8088EN.pdf>



A) Drug formulation analysis showing SIM quantifiers of methyl-2-benzoyl benzoate. B) Calibration curve of the standard. C) Results of the analysis along with status of *Pass* for qualifier status. D) The qualifier response percentage achieved.



A suspect peak from the DP sample detected (A) and its mass spectra extracted (B) and library matched to erucamide (C and D).



2D

Agilent
OpenLab



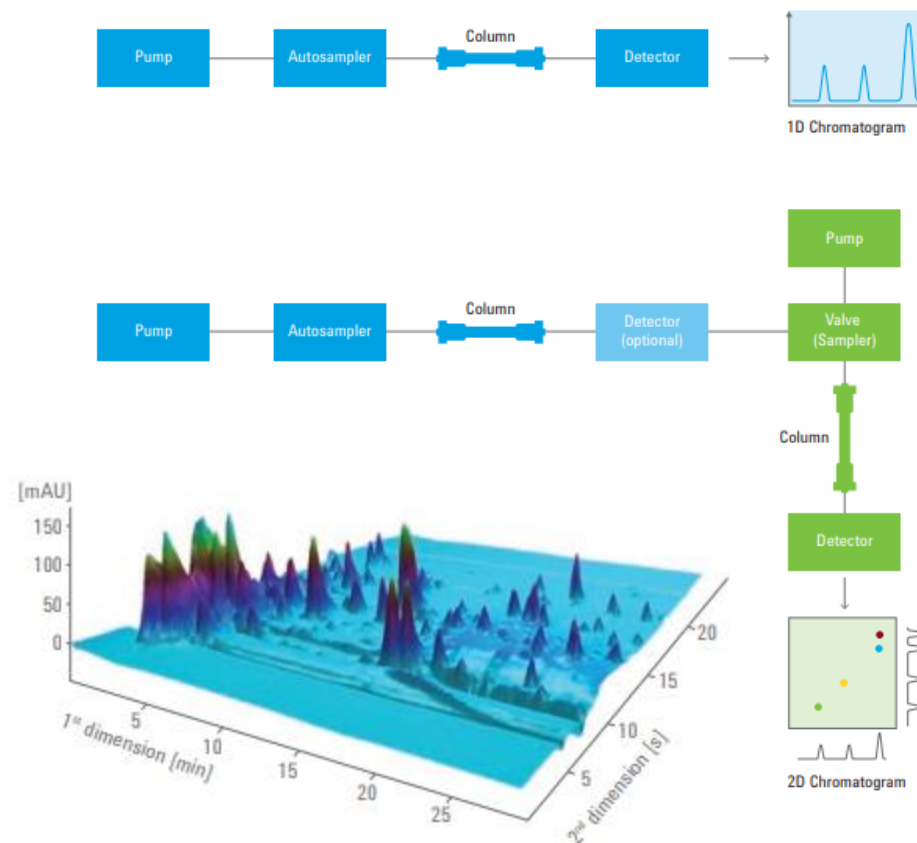
2D control for
OL CDS in
2021

<https://blog.agilent.com/2017/08/17/agilent-and-the-solar-eclipse/?from=>

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Profiling Nonionic Surfactants Applied in Pharmaceutical Formulations by Using Comprehensive Two-Dimensional LC with ELSD and MS Detection

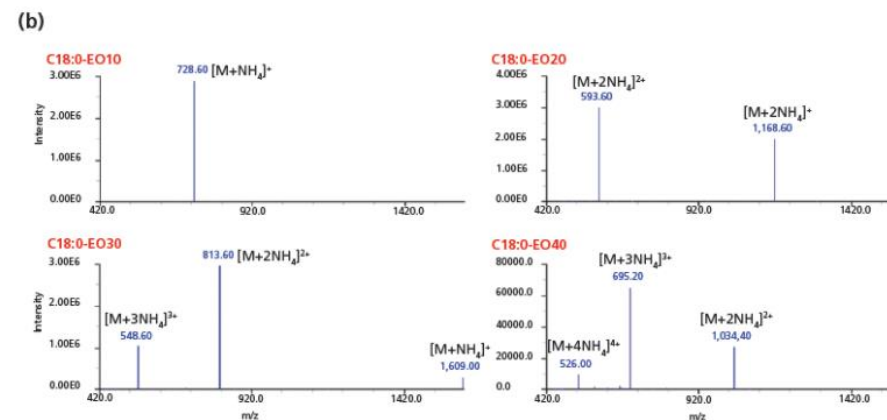
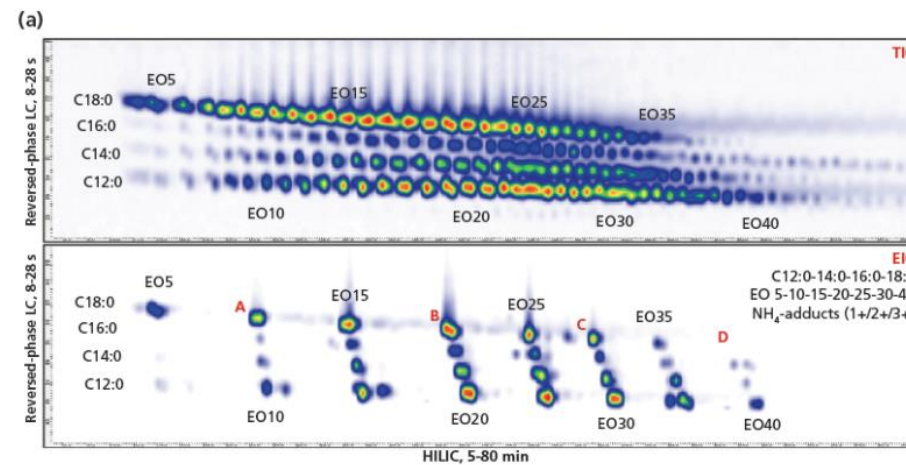
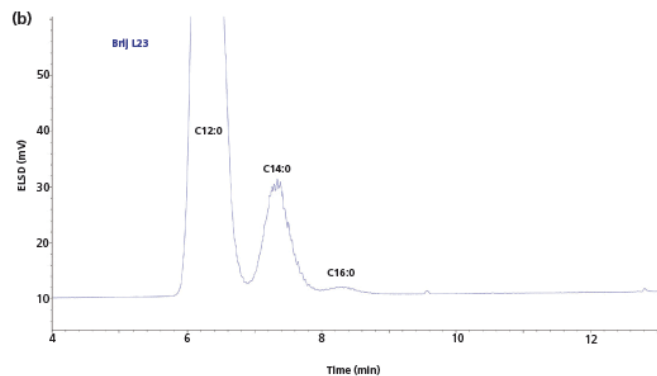
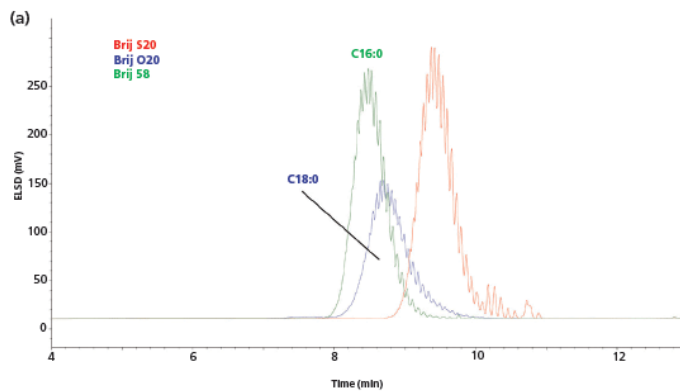
The 2D-LC instrument used for this study was an Agilent 1290 Infinity 2D-LC Solution system. The system comprised the following modules: two binary pumps, a high-performance autosampler, two thermostated column compartments, an external valve drive with a two-position, four-port duo valve equipped with two 20- μ L loops for 2D-LC, and an evaporative light scattering detector (Agilent Technologies). For **LC-MS analysis a G6130B single-quadrupole LC-MS system with an electrospray ionization (ESI) source was used (Agilent Technologies)**. First- and second-dimension columns were a 100 mm \times 2.1 mm, 1.8- μ m Zorbax 300 HILIC RRHD column and a 50 mm \times 2.1 mm, 1.8- μ m Zorbax Eclipse Plus C18 RRHD column (Agilent Technologies), respectively. The second-dimension column effluent was split between ELSD and MS using a zero-dead volume T-piece and two 340 mm \times 0.075 mm stainless steel capillaries. For the one-dimensional reversed-phase screening runs a 150 mm \times 2.1 mm, 1.8- μ m Zorbax Eclipse Plus C18 RRHD column (Agilent Technologies) was used. The method details are summarized in Table II. Instrument control and data analysis were carried out with Agilent OpenLAB chromatography data system (CDS) ChemStation, revision C.01.07 with 2D-LC add-on software (Agilent Technologies) and GC Image LC \times LC Edition Software for 2D-LC data analysis (GC Image, LLC), respectively.



[Koen Sandra](#) , [Pat Sandra](#) , [Gerd Vanhoenacker](#) , [Mieke](#)

[Steenbrink](#), LCGC North America-06-01-2018, Volume 36, Issue 6

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Koen Sandra , Pat Sandra , Gerd Vanhoenacker , Mieke

Steenhake

Questions



[5990-7595EN](#)

The LC Handbook

Guide to LC Columns and Method Development

[5991-2359EN](#)

Two Dimensional Liquid Chromatography

[5990-3777EN](#)

High Performance Capillary Electrophoresis

[5991-5509EN](#)

Supercritical Fluid Chromatography

[5989-6639EN](#)

Principles in Preparative HPLC

[5991-3326EN](#)

Sample Preparation Fundamentals for Chromatography

[5980-1397EN](#)

Fundamentals of UV-visible Spectroscopy



