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Ensuring Reliable Results using Agilent's New 7 Analyte System Suitability Standard with WalkUp and the LC/MSD iQ

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Introduction

Every lab must ensure its instruments are calibrated, tuned, and clean everyday to obtain reliable results. Typically, many of the steps are done manually by a lab technician and require special care to review the results and confirm the instrument is ready for use. Agilent's OpenLab CDS and WalkUp software provide a complete data acquisition, data analysis, and reporting platform with fully automated workflows. The instrument will automatically check the tune parameters, and injection events can be scheduled to be performed automatically, all the way to report generation.

To ensure consistency and further reliability of our systems, Agilent co-developed a system suitability standard that enables universal monitoring of all LC/MS components – HPLC pump, autosampler, column, detectors etc.

WalkUp is an open-access add-on control software that provides an additional layer of control over workflows and simplifies sample submission to a single screen

In an open access system, control and simple sample submission are paramount. With WalkUp, results can be obtained from a simple workflow (Fig. 1) that involves no more than walking up to the instrument, submitting the sample, and returning to your desk. All the methods can be locked to specific users/groups, and tasks such as system suitability can be automated.

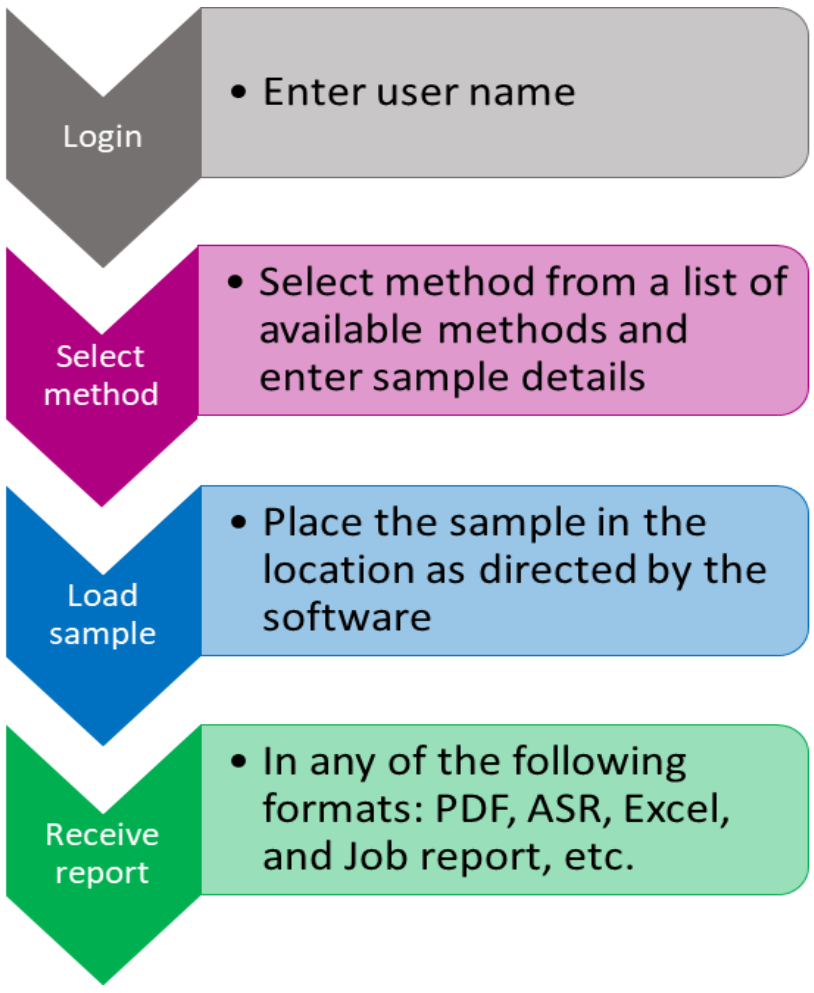


Figure 1. Typical user workflow for the Agilent LC/MSD iQ WalkUp system.

Experimental

Typical WalkUp Instrumentation

The InfinityLab LC/MSD iQ has been designed with a focus on ease-of-use and added flexibility, while maintaining robust and reliable operation. To maximize efficiency and provide chromatographers with an intuitive mass detector, the MS parameters are automatically set based on the LC method and the mass of the target compounds. Early maintenance feedback predicts and notifies users about the need for routine instrument maintenance operations such as a quick check tune or Ion Injector change.

With the addition of the InfinityLab FlexBench MS, the entire LC/MS stack can be converted to a secure mobile lab. Simply wheel the system up to the reaction under study, plug in the bench to power the entire system, and after a short pump-down time the system is ready for analysis. There is easy access to all sides of the modules, including a pull-out bench for the MS, so maintenance can be performed without the burden of unstacking modules and rerunning solvent and waste lines.

The Agilent InfinityLab LC/MSD iQ WalkUp system consists of the following modules:

- Agilent 1290 Infinity II High-Speed Pump (G7120A)
- Agilent 1290 Infinity II Multisampler (G7167B)

  or Agilent 1290 Infinity II Vialsampler (G7129B)
- Agilent 1290 Infinity II Multicolumn Thermostat (G7116B)
- Agilent 1290 Infinity II Diode Array Detector (G7117B)
- Agilent LC/MSD iQ (G6160AA)
- Agilent FlexBench MS (G6015B)

Figure 2. Agilent's LC/MSD iQ with an InfinityLab II HPLC stack

Agilent's 7 Compound System Suitability Mix

Agilent's 7 analyte system suitability standard has been tailored to check an entire LC/MS system from column to mass detector. The 7 compounds within are:

- 8-bromoguanosine (8-BG),
- 4-chlorocinnamic acid (4-CC),
- Amitriptyline HCl (AMI)
- Di-ethyl (DEP), di-amyl (DAP), di-n-hexyl (DHP) and di-octyl (DOP) phthalates.

These compounds cover a wide range of hydrophobicity, contain positive and negative ions, are sensitive to pH and have varied concentrations with a relatively stable shelf life. A single automated microliter injection is all that is needed every morning to check the quality of the instrument.

5191-4544	LCMS 7-Analyte Checkout Standard	1x1mL Vial
5191-4546	LCMS 7-Analyte System Suitability Kit	5x1mL Vials

System Suitability Checkout Method

The Agilent System Suitability checkout method uses an InfinityLab Poroshell 120 EC-C18 column with an ACN gradient. This method can also be optimized for methanol or buffered solutions. A robustness study of 100 injections of the system suitability standard was performed over the course of a week with peak areas and RTs tracked. (Fig. 3)

Parameter	HPLC Set Value	
Column	Agilent InfinityLab Poroshell 120 EC-C18, 2.1 × 50 mm, 1.9 µm at 40 °C (p/n 699675-902)	
Solvent A	0.1% FA in H_2O	
Solvent B	0.1% FA in ACN	
Gradient	Time (min)	%B
	0.00	5
	1.75	90
	2.90	90
	3.00	5
Postrun	0.7 minutes	
Flow rate	0.8 mL/min	
Injection Volume	1 µL	
UV	[254,5 / ref. 360, 80] nm	
MS	2 Scans (+/– 50-600 *m/z*)	

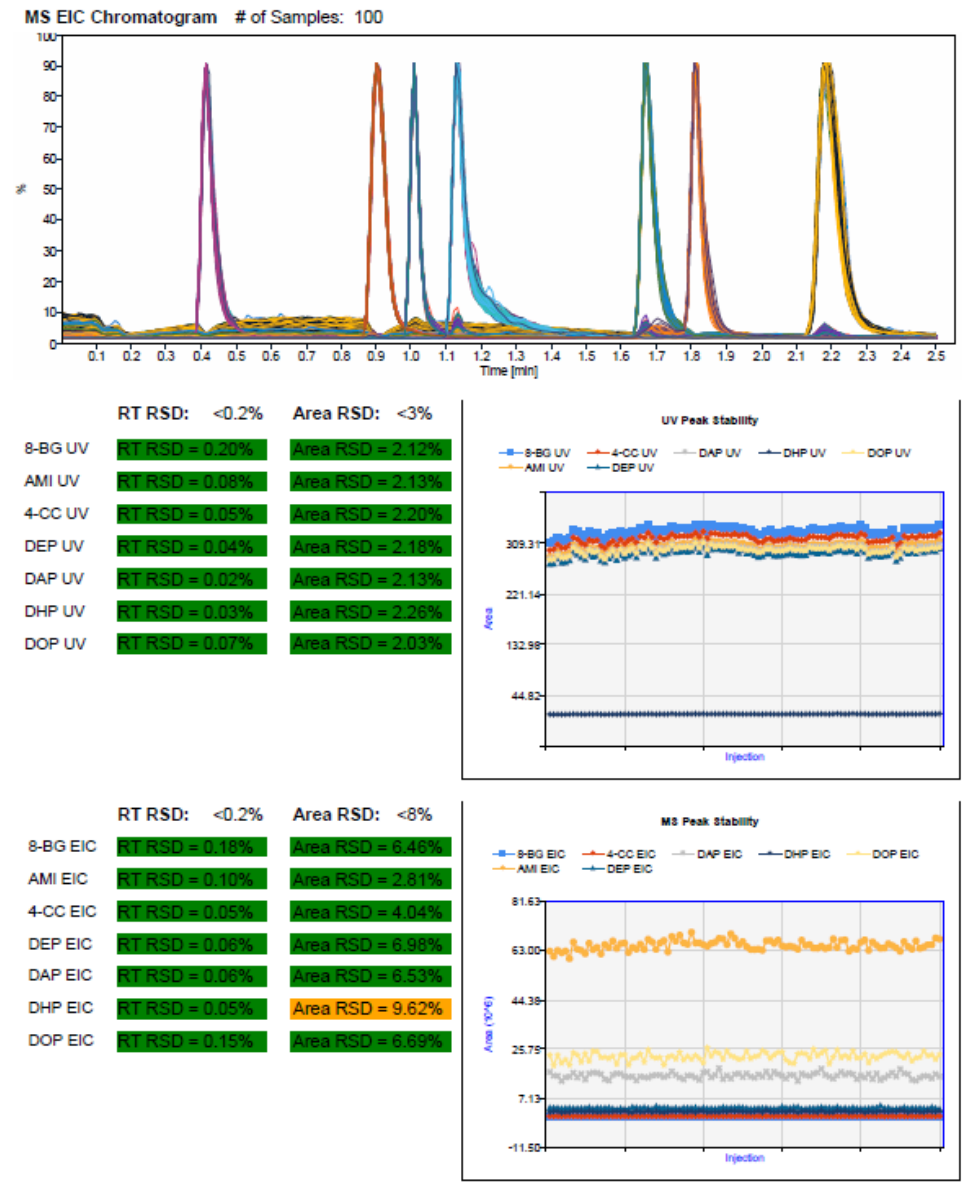


Figure 3. OpenLab CDS template report for trending of 100 injections of system suitability standard across 1 week

The Easiest Sample Submission with WalkUp RSS

Users submit samples through WalkUp's Rapid Sample Submission (RSS). RSS provides the easiest interface to walk up and submit samples. Users sign-in and select a pre-determined method to run their sample. A few inputs are needed and then the user is told where in the tray to submit their samples. This is all done on a single screen and user information can be automatically scanned by a card reader.

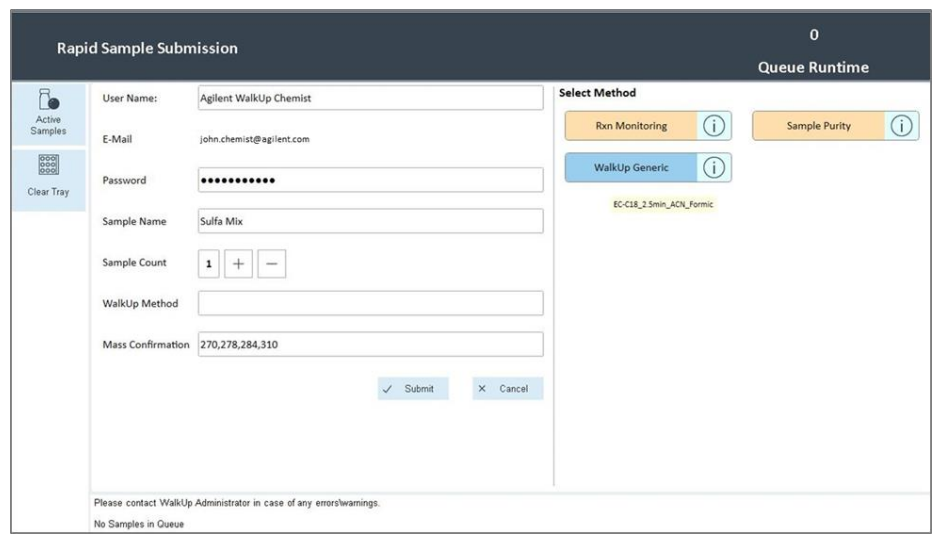


Figure 4. Rapid Sample Submission: all inputs are made from this single screen.

Scheduling Daily Injection Using WalkUp

Key events can be scheduled on a time basis (e.g., every day, week, work day) or sample submission basis (e.g., after a plate is complete, after N runs) (Figure 8). Any number of WalkUp methods can be selected. Sample vials can be stored in reference positions, which are not utilized by the sample queue. Some examples of events that can be scheduled are:

- Running reference standards throughout the work day
- Calibration standards to ensure that reported amounts are on target
- System suitability check for instrument and column stability
- Blank runs to check for carry over or contamination
- Scheduled Autotune or Checktune available with the LC/MSD iQ.

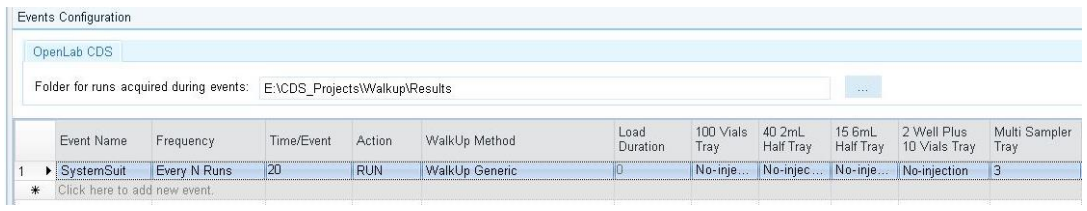


Figure 5. WalkUp Admin Events Screen

Reports and data emailed right to the submitter's inbox

The acquired data is automatically processed by the data analysis method which creates the data analysis report. The administrator then configures what is sent to the submitter (Fig. 6). The submitter receives the report created by the administrator right to their inbox (Fig. 7).

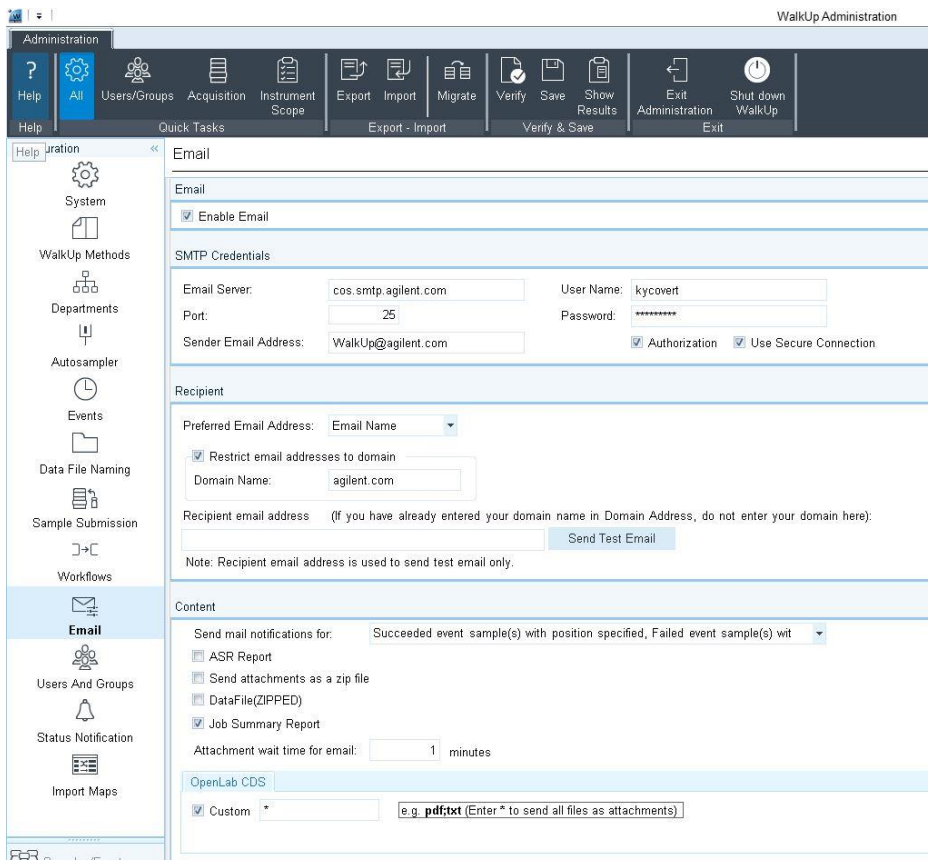
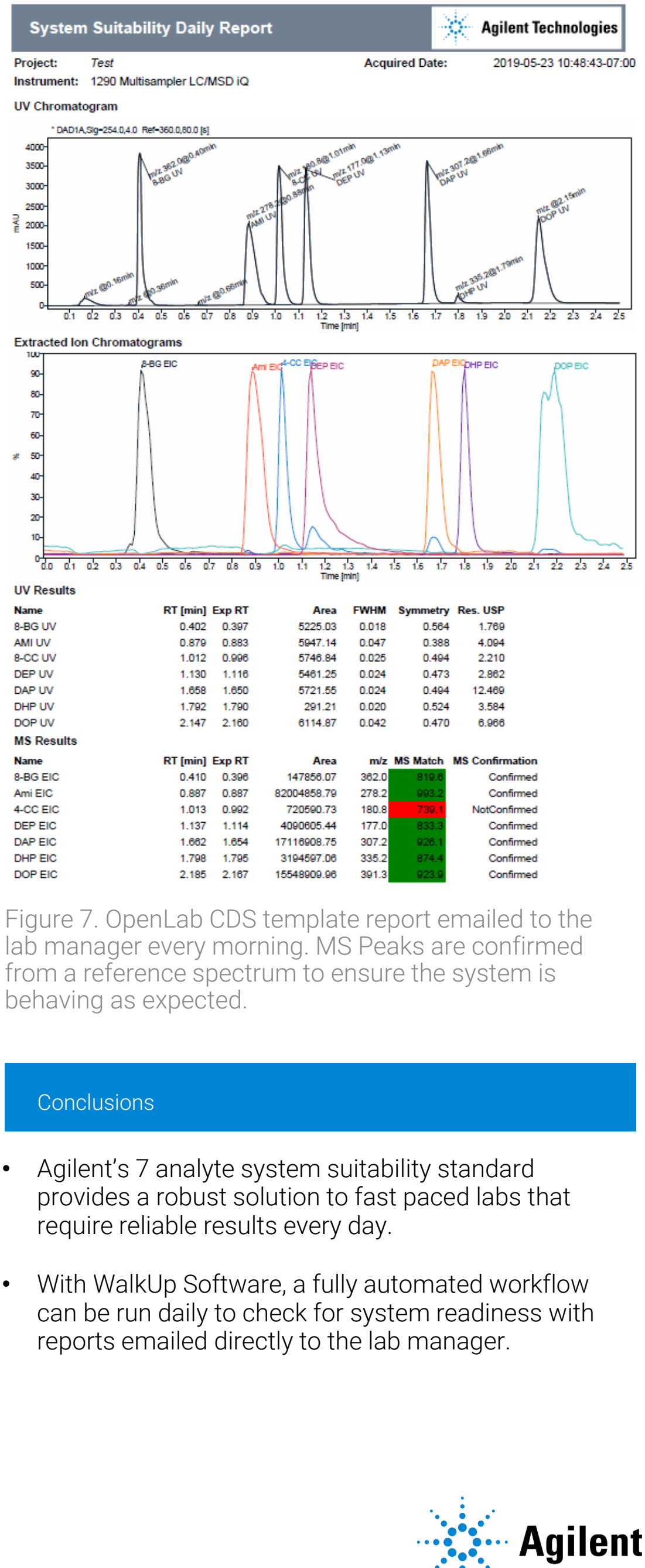


Figure 6. Data files, data analysis reports, and ASR files can be emailed to submitters.



UV Results

Name	RT [min]	Exp RT	Area	FWHM	Symmetry	Res. USP
8-BG UV	0.402	0.397	5225.03	0.018	0.564	1.769
AMI UV	0.879	0.883	5947.14	0.047	0.388	4.094
8-CC UV	1.012	0.996	5746.84	0.025	0.494	2.210
DEP UV	1.130	1.116	5461.25	0.024	0.473	2.862
DAP UV	1.658	1.650	5721.55	0.024	0.494	12.469
DHP UV	1.792	1.790	291.21	0.020	0.524	3.584
DOP UV	2.147	2.160	6114.87	0.042	0.470	6.966

MS Results

Name	RT [min]	Exp RT	Area	m/z	MS Match	MS Confirmation
8-BG EIC	0.410	0.396	147856.07	362.0	819.6	Confirmed
Ami EIC	0.887	0.887	82004858.79	278.2	993.2	Confirmed
4-CC EIC	1.013	0.992	720590.73	180.8	739.1	NotConfirmed
DEP EIC	1.137	1.114	4090605.44	177.0	833.3	Confirmed
DAP EIC	1.662	1.654	17116908.75	307.2	926.1	Confirmed
DHP EIC	1.798	1.795	3194597.06	335.2	874.4	Confirmed
DOP EIC	2.185	2.167	15548909.96	391.3	923.9	Confirmed

Figure 7. OpenLab CDS template report emailed to the lab manager every morning. MS Peaks are confirmed from a reference spectrum to ensure the system is behaving as expected.

Conclusions

- Agilent's 7 analyte system suitability standard provides a robust solution to fast paced labs that require reliable results every day.
- With WalkUp Software, a fully automated workflow can be run daily to check for system readiness with reports emailed directly to the lab manager.

https://explore.agilent.com/asms

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