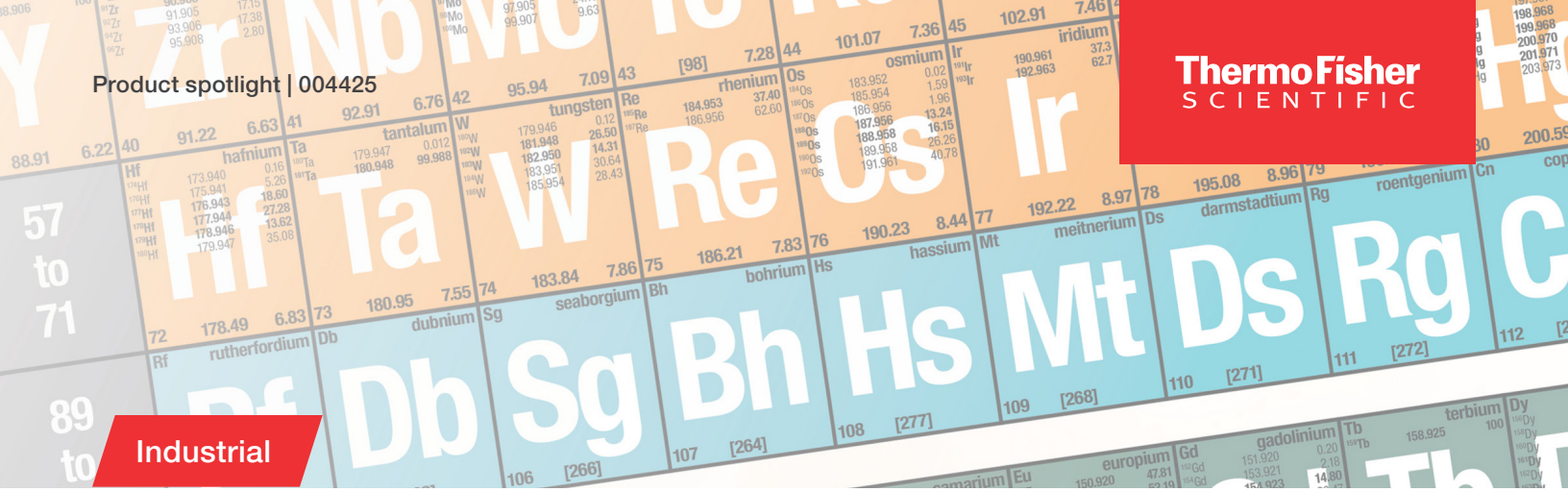


Product spotlight | 004425

Industrial

Qtegra Intelligent Scientific Data Solution Software

Integrated support for high-throughput, intelligent auto dilution with the Elemental Scientific prepFAST 3 system

Thermo Scientific™ Qtegra™ Intelligent Scientific Data Solution Software provides fully integrated support for state-of-the-art peripheral devices from industry-leading suppliers. A dedicated plug-in enables laboratories to add prescriptive and intelligent auto-dilution capabilities to their Thermo Scientific™ iCAP™ PRO Series ICP-OES or Thermo Scientific™ iCAP™ MX Series ICP-MS instrument, delivered by the Elemental Scientific prepFAST3 system.

Adding value

Testing laboratories often face high sample loads and need to analyze a wide range of sample types. This is especially true for laboratories performing environmental monitoring, which therefore need to analyze drinking and/or surface waters as well as soils, effluents, and wastewaters. Typically, such samples need to be diluted prior to analysis to reduce the impact of the matrix on the measurement and also to help ensure consistent performance and uptime of the instrument. The high and often unknown variability of the composition of the samples means that a single dilution cannot be applied to all, and legislation may demand different reporting limits and calibration ranges, depending on the sample type. Additionally, preparation of a series of dilutions of a stock standard is a laborious and potentially error-prone task when done by analysts already tasked with maximizing throughput across multiple instruments in a modern laboratory.

The latest generation of inductively coupled plasma–mass spectrometry (ICP-MS) systems features solutions that significantly improve matrix tolerance and ensure consistent performance. However, in combination with prescriptive and auto dilutions, ICP-MS throughput can be further enhanced. Due to its inherently higher matrix tolerance, data quality in inductively coupled plasma–optical emission spectrometry (ICP-OES) does not immediately suffer from changing matrix composition, and both prescriptive and intelligent auto dilutions can add value, e.g., re-diluting samples that initially fall outside of the calibrated range of an analytical method. For both system types, offline dilutions can be converted to online actions occurring ‘on the fly’ directly before each measurement, ensuring highly reproducible execution every single time.

Working together

Thermo Fisher Scientific and Elemental Scientific have worked together for over 20 years to provide laboratories with advanced hardware and software solutions for routine elemental analysis by ICP-OES and ICP-MS. The very latest Elemental Scientific prep*FAST* 3 auto dilution systems take another significant step forward in automated and unattended operation in high-throughput laboratories. In combination with an extended dilution range of up to 1,000-fold to support the wide range of samples seen in environmental monitoring applications, the entirely new features of the prep*FAST* 3 system, for example anti-clogging filter probes and backflushing capabilities, deliver robust and reliable operation, further minimizing user interaction. Figure 1 shows a screenshot from the Qtegra Intelligent Scientific Data Solution (ISDS) dashboard to show the seamless integration of the Thermo Scientific™ iCAP™ MSX ICP-MS instrument with the prep*FAST* 3 system.



Figure 1. Qtegra ISDS software dashboard view of the prep*FAST* 3 system.

A high-level overview of the hardware is given in Figure 2. The prep*FAST* 3 system can be used in conjunction with the Thermo Scientific™ iCAP™ PRO X, XP, and XPS ICP-OES instrument, as well as the iCAP MSX ICP-MS and the Thermo Scientific™ iCAP™ MTX ICP-MS instruments.

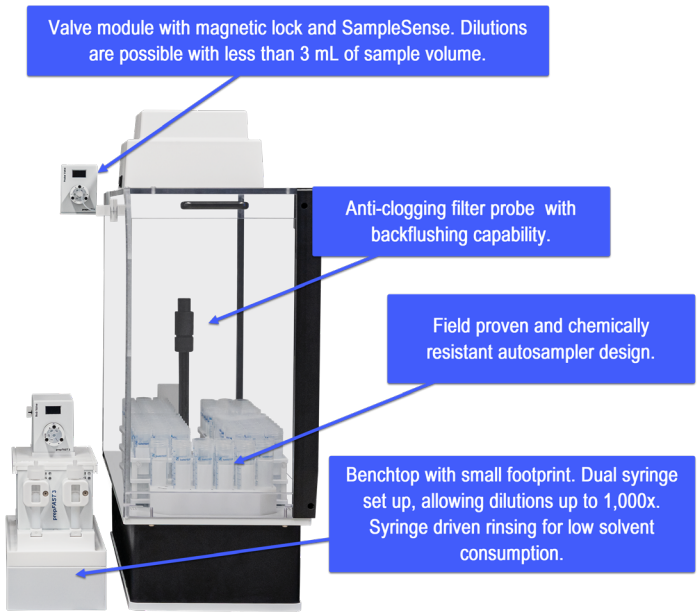


Figure 2: High-level overview of hardware-related capabilities of the prep*FAST* 3 system.

The auto-dilution capabilities provided by the prep*FAST* 3 system can be utilized in two ways, either prescriptive or reactive dilution.

Prescriptive dilution

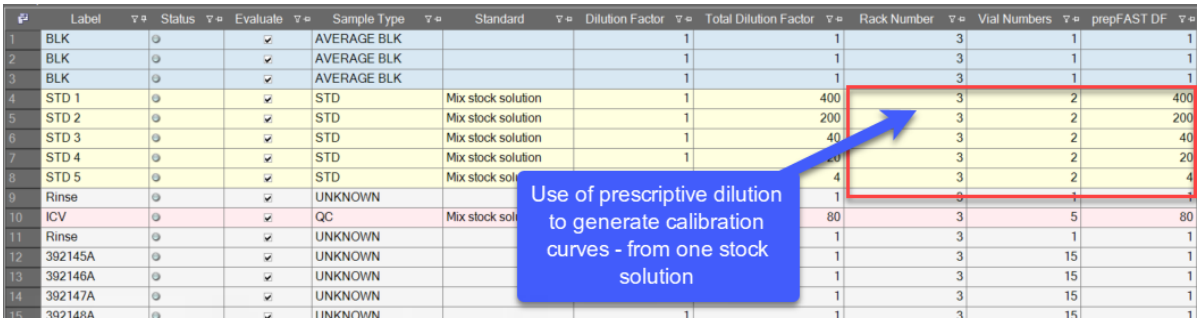
Prescriptive dilution dilutes a sample by a user-defined factor. This allows dilution of a specific sample by a fixed factor before analysis, for example to reduce matrix effects from samples with higher loads of total dissolved solids (TDS). The flexible use of sample-specific dilution factors allows laboratories to easily integrate different sample types within a single series of analyses in a Qtegra ISDS LabBook.

Prescriptive dilution can also be used to generate a calibration curve from a single stock solution prepared at a higher concentration, automating a labor-intensive and error-prone task typically carried out by laboratory personnel.

Reactive dilution

Reactive dilution dynamically adjusts dilution levels according to pre-defined (method or SOP) acceptance criteria (for example internal standard recovery or calibration range) based on an initial reading from a sample. If the acceptance criteria are not met in the first analysis, an automatic dilution is made to bring the result back within the defined limits and a repeat analysis is triggered. All of this is performed without requiring the technician to evaluate the data, spot the outlier, manually re-dilute, and add the repeat sample later in the schedule. Intelligent dilution therefore simplifies the method and, by automating the entire evaluation and re-dilution process, improves reliability and robustness of the analytical method, especially for those outlier samples that often challenge the analytical team.

Prescriptive and reactive dilutions are core capabilities of the Qtegra ISDS software, and the automatic dilution workflows described above are fully supported by the prep*FAST* 3 system. Prescriptive dilution factors can be manually entered in the sample list of a Qtegra ISDS LabBook, as is displayed in Figure 3. Repeated execution of specific dilutions for automatic generation of a calibration curve can be added to a Qtegra template, so that they will be executed every time a new Qtegra LabBook is created. Prescriptive dilution factors can also be directly imported from a Laboratory Information Management System (LIMS) or a simple CSV file.



	Label	Status	Evaluate	Sample Type	Standard	Dilution Factor	Total Dilution Factor	Rack Number	Vial Numbers	prepFAST DF
1	BLK		✓	AVERAGE BLK		1	1	3	1	1
2	BLK		✓	AVERAGE BLK		1	1	3	1	1
3	BLK		✓	AVERAGE BLK		1	1	3	1	1
4	STD 1		✓	STD	Mix stock solution	1	400	3	2	400
5	STD 2		✓	STD	Mix stock solution	1	200	3	2	200
6	STD 3		✓	STD	Mix stock solution	1	40	3	2	40
7	STD 4		✓	STD	Mix stock solution	1	20	3	2	20
8	STD 5		✓	STD	Mix stock sol		4	3	2	4
9	Rinse		✓	UNKNOWN			1	3	1	1
10	ICV		✓	QC	Mix stock sol		80	3	5	80
11	Rinse		✓	UNKNOWN			1	3	1	1
12	392145A		✓	UNKNOWN			1	3	15	1
13	392146A		✓	UNKNOWN			1	3	15	1
14	392147A		✓	UNKNOWN			1	3	15	1
15	392148A		✓	UNKNOWN		1	1	3	15	1

Figure 3: Definition of prescriptive dilution factors for both calibration standards and sample in the sample list of Qtegra ISDS software.

The rules for reactive auto dilution and subsequent actions to ensure method- or SOP-defined data quality requirements are defined in the Qtegra ISDS LabBook method, as displayed in Figure 4. All samples in a LabBook follow these rules with the Qtegra ISDS software assessing the internal standard response and measured concentration with respect to the calibration range. Actions upon failure for both data quality criteria can be independently defined in the method, along with a maximum number of subsequent auto-dilution steps to be performed by the system.

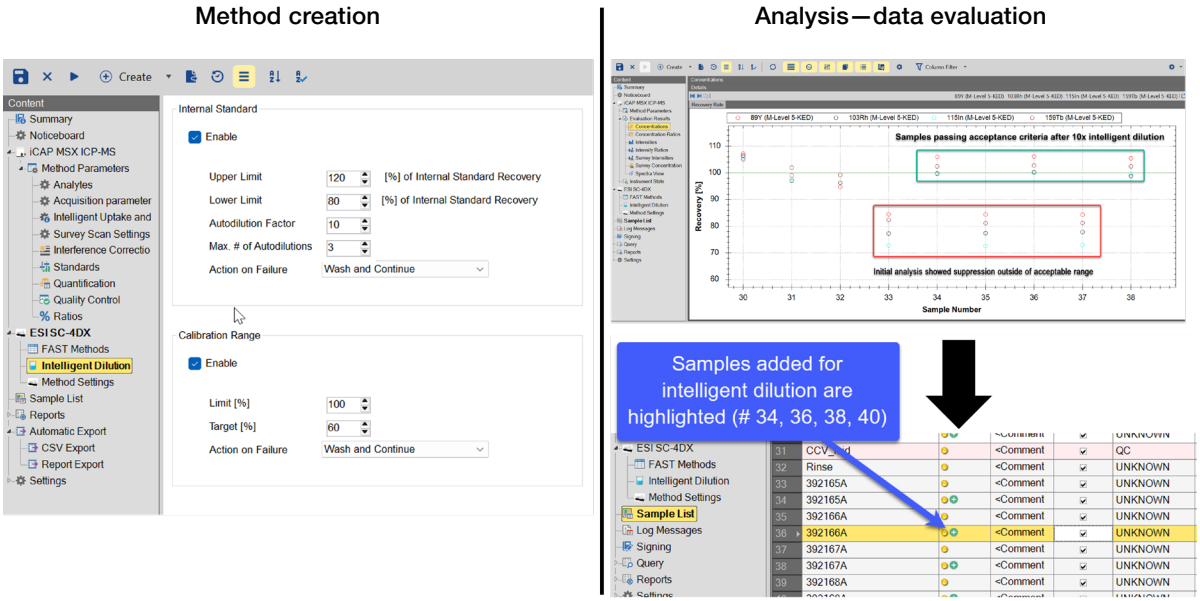


Figure 4: Left: Definition of intelligent auto dilution options with the Qtegra ISDS LabBook, based on either the internal standard response or concentration range, or both. Right: Intelligent auto dilution responding to samples outside the accepted range for internal standard recovery. The automatically added analyses are highlighted in the Qtegra ISDS software sample list.

When the results for a sample fall outside the defined data quality criteria, the sample is automatically re-diluted by the prep*FAST* 3 system and a repeat analysis is inserted into the analysis schedule, which is then immediately processed by the Qtegra ISDS control software.

Increased productivity

The seamless integration between the prep*FAST* 3 system and a compatible Qtegra ISDS-controlled ICP-OES or ICP-MS system alleviates the need for continual monitoring of live results by a technician ready to perform manual dilutions in case of an outlier sample, therefore eliminating labor-intensive and potentially error-prone steps in the workflow. By automating the preparation of calibration standards and eliminating offline dilutions, costly operator time can be saved, and data quality can be improved. Intelligent auto dilution can be combined with other techniques, such as argon gas dilution, for the ultimate in robustness and reliability in busy contract laboratories challenged to maintain throughput in the face of high volume and wide variability in sample types.

Environmental impact

The use of automation helps reduce the amount of plasticware needed in the laboratory, as additional vessels and pipette tips can be omitted. The use of intelligent auto dilution, responsive immediately to the results of a measurement, allows samples to repeat within a sequence, leading to reduced argon consumption by the instrument by an overall shorter runtime (vs. manual dilution and re-analysis).

Conclusion

The use of an auto-dilution system, such as the prep*FAST* 3 system, adds considerable, valuable benefits for busy testing laboratories by reducing workload on laboratory staff and saving costs at the same time. When completely integrated into Qtegra ISDS software, auto-dilution systems streamline workflows and contribute to better data quality for both ICP-OES and ICP-MS analyses.

Learn more at **thermofisher.com/qtegra**

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