Laboratory Automation

Weighing, Dosing
Titration, Karl Fischer
pH Measurement
UV/VIS Spectroscopy
Density & Refractometry
Melting & Dropping Point
Thermal Analysis

Single & Multiple
Sample Automation

Lab Automation Guide

Efficiency, Reproducibility and Safety

METTLER TOLEDO

Content

1. Introduction

The application of automation technology in today's laboratories is required to achieve timely progress and to remain competitive. The goal of laboratory automation is to:

- increase productivity
- elevate experimental data quality
- increase safety
- or enable experimentation that otherwise would be impossible

The term automation is open for interpretation and covers a wide range of technical possibilities. The most widely known application of laboratory automation is laboratory robotics. More generally, the field of laboratory automation comprises many different automated laboratory instruments, devices (the most common being autosamplers) and software algorithms. It also includes methodologies used to enable, expedite and increase the efficiency and effectiveness of scientific research in laboratories. This guide lists and describes all types of automation, starting from solutions that are not generally thought of when talking about automation, through to big sample changers.

Important: Besides sample changers and sophisticated software, this guide shall shed light on smaller solutions. Simple peripherals such as a stirrer, printer or bar code scanner also elevate the degree of automation of a specific step within a routine workflow. There are many examples of auxiliary devices and internal functions that automate certain parts of an analysis. In the following chapters these solutions are called Single Sample Automation (SSA).

The sample robot automates DSC increasing efficiency and avoiding sample reaction before measurement

The degree of automation that is implemented is a personal decision. Some users might want to only work with automated systems, while other users might prefer to use it only in certain cases. As a rule of thumb, single sample automation makes sense when analyzing more than 10 samples a day. Investing in multiple sample automation pays back when 30 or more samples are measured a day. Automation can make life easier, safer and often healthier, be it from an ergonomic or from a toxicological point of view. This aspect is covered in table 1 under "safety and comfort" and explained in more detail in chapter 3, Multiple Sample Automaton.

pH measurements can be run with just one click thanks to InMotion™ autosamplers and LabX® laboratory software

Undoubtedly, automation adds to safety and comfort, increases efficiency and enhances the precision of measurements, hence increases the reproducibility. Automation makes analyses less dependent on people, on individual working styles. Automation helps get consistent results from various labs, sometimes far apart. This is important in ringtests. In addition, chosing the right service solution for an automated system significantly optimizes uptime. The various automation options and their benefit can be summarized as shown in table 1.

	Manual, no automation <10 samples per day	**Single sample automation** 10–30 samples per day	**Multiple sample automation** >30 samples per day
Safety and comfort	–	★	★★★
Efficiency	–	★	★★★★
Reproducibility	–	★★	★★★

Table 1: Overview of recommendations and benefits of automation solutions (the benefits are rated from 1 to 4).

2. Single Sample Automation

The main difference between single sample automation and an autosampler is that with single sample automation there is at least one manual step between the analyses of each sample. The sample is manually attached to the titrator, placed under the pH sensor, placed in DSC or placed on the refractometer etc. each time. Despite not using an autosampler, many steps can be automated using peripheral devices, pre-programmed methods, customized algorithms, clever accessories, PC software etc.

Here are some examples of single sample automation:

Touchless operation and ErgoSense™
Excellence analytical balances have a single sample automation feature that is truly tried and trusted: SmartSens™ sensors allow you to operate your balance with the wave of a hand, making weighing tasks easier and avoiding cross-contamination issues. ErgoSens is an infrared sensor for hands-free operation of Excellence density meters and refractometers.

One Click™ operation
One Click is an intuitive usability concept designed to add standardization and a sense of ease to every-day laboratory work: Users are able to customize their screen and create short-cuts to start analyses and customized workflows quickly and easily. The ease in operating METTLER TOLEDO's Excellence instruments results in less errors and higher efficiency in the laboratory.

PC software EasyDirect™ and LabX®
When using simple data dump software like EasyDirect results are automatically transferred to MS Excel, avoiding transcription errors. The results can easily be further processed or archived. With the more sophisticated PC software LabX more steps can be automated. For instance, the correct formulation recipe can be applied; raw results can be re-evaluated etc.

Barcode scanner and SmartCodes™
The barcode scanner ScanStraight™ is a strong example of single sample automation: Just scan the barcode of your single sample for error-free acquisition of information like serial, batch or identification number. In addition, when using SmartCodes the correct method on the titrator or density meter is automatically activated.

SmartSample™
Gain efficiency and security for weighing titration samples with SmartSample. At the balance all the information is automatically added to the beaker tag keeping the sample ID, weight and weighed sample together. Via the InMotion™ autosampler the titrator automatically reads all sample information from the beaker tag for efficient and secure analysis.

uMix™ Stirrer

One very effective way to increase repeatability and reproducibility of e.g. pH, conductivity or ion readings is to use a stirrer. The stirrer provides identical conditions in the media being measured independent of the user. When using the uMix stirrer the duration and stirring speed can be linked to a specific application, making it the perfect single sample automation peripheral.

FillPal™ Sampling pumps

These pumps can be used for the DM density meters and RM refractometers and are suitable for all applications where the samples to be measured are of a similar nature and no intermediate complete drying of the measuring cell is required. The sampling pumps replace the syringe for density measurement, available as FillPal Food and FillPal Chem.

LevelSens

After a titration or density/refractive index measurement, waste solution is often pumped into a waste bottle. LevelSens is installed at the waste bottle and interrupts the series when the waste bottle is full. Overflow is reliably prevented, increasing security in the laboratory, fully automatically. The user can then empty the waste bottle and continue the interrupted task.

SC1 single sample automation

The SC1 single sample automation solution runs fully automated density measurements, saving time and improving the repeatability of the results. The SC1 performs sample delivery with pressurized air, automatic rinsing with two different solvents and complete drying with a desiccator. It also allows contamination free sample recovery for retained samples.

Quantos single sample automation

Quantos is ideal for automatic weighing of fine, fluffy, static, compacted, granular, and heterogeneous substances. Thousands of substances have been tested: Nanoparticles, fine powders, granules and heterogeneous mixtures are suitable for dispensing. Automated liquid dispensing is also possible: dispense from 1 mg to grams of liquids in seconds.

Printer

One of the oldest yet still most reliable peripheral devices to automate documentation is a printer. Transcription errors are reduced, particularly if the results do not have to be transferred from the printed slip of paper to a final destination. Mistakes based on illegible handwriting are avoided fully. METTLER TOLEDO offers a whole range of professional printers with and without clock, statistics etc.

3. Multiple Sample Automation

Laboratories devoted to activities such as high-throughput screening, combinatorial chemistry, automated clinical and analytical testing, diagnostics, large scale biorepositories, and many others, would not exist without advanced laboratory automation. But also labs with relatively low sample throughput might consider investing in multiple sample automation. Sometimes automation enables experimentation that otherwise would be impossible, be it due to the lack of resources, not achieving the required precision or the high toxicity of the substances involved.

3.1. Multiple Determination and Reproducibility

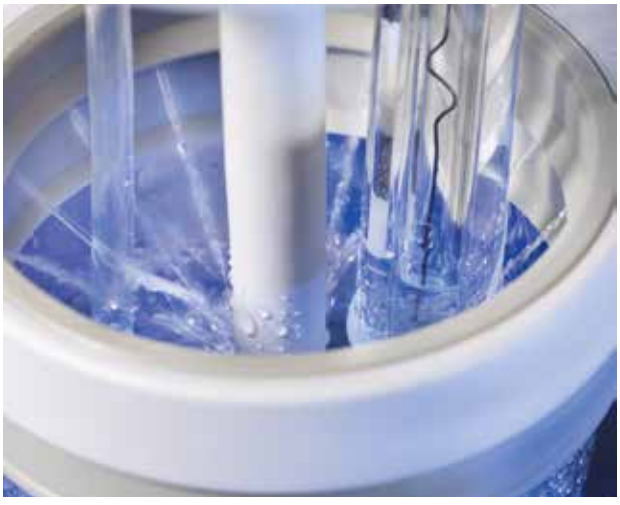
A survey conducted by Nature in 2016 asked over 1500 scientists in an online questionnaire about the state of reproducibility in research. Strikingly, the survey reveals that more than 70% of the researchers have attempted but failed to reproduce another scientist's experiments, and more than half even admitted having failed to reproduce their own experiments. Together with superior chemistries, lab automation can eliminate operator-to-operator variations in your experiment and increase robustness as well as reproducibility, thus making your results worth sharing with peers.

Multiple sample automation is the ideal setup to run sample series, so if the same sample shall be measured multiple times for statistical evaluation. Typically, higher precision is achieved by using a sample changer. This leads to more reliable, less people dependent results with better reproducibility.

3.2. Avoiding Contact with Harmful or Toxic Substances

InMotion autosampler with CoverUp

Do you have volatile or strong smelling samples and would like to avoid using expensive hood space? Do you want to protect your samples from contamination while they are waiting to be analyzed? CoverUp™, the automation accessory for InMotion™, is the device of choice. Samples are covered before, after and during titration, resulting in minimal exposure to the environment, and increasing user safety by reducing solvent exposure. Build your autosampler according to your sample needs with modular boards for extra pumps, CoverUp™ system for protecting your samples and operators as well as the water bath sample trays for temperature control of your samples.



PowerShower rinsing in action

Intuitive and flexible programming in our instruments allows for tailored workflows of your samples. Use the PowerShower™ and conditioning sequences for effective cleaning and to maintain sensors for secure operations or parallel tasks for ultimate efficiency. The well-proven PowerShower rinsing offers a fully automated and highly effective cleaning mechanism. Carryover is eliminated thanks to a strong solvent stream that cleans the electrode, stirrer and tubes from top to bottom.

3.3 Solutions for Multiple Sample Automation

The maximum number of samples varies from instrument to instrument, InMotion™ can take up to 303 samples when using 25 mL vials. METTLER TOLEDO offers the following autosamplers.

Product	Solution	Supported Parameters	Max. number of samples
	**InMotion** Designed to maximize throughput in the minimal space, InMotion Autosamplers increase productivity without sacrificing laboratory bench space. The innovative robotic arms of the Pro and Max series reach into the sample tray optimizing space.	Titration, pH/conductivity/ion, density, refractive index, UV/VIS spectrophotometry	303
	**Rondolino** Rondolino is a carroussel-type titration stand for METTLER TOLEDO general titrators used to automate titrations. It can be loaded with up to 9 sample beakers and one conditioning beaker in an unique position.	Titration, pH/conductivity/ion	9
	**KF InMotion** Karl Fischer sample changer with integrated oven for water extraction. Up to 26 samples can be placed on a compact platform, just 25 cm in diameter, maximising the space in your laboratory.	Karl Fischer titration	26/120

Product	Solution	Supported Parameters	Max. number of samples
	**SC30** The SC30 is a sample changer with 30 positions. It performs sample delivery with pressurized air, automatic rinsing with two different solutions and complete drying with a desiccator. Contamination free sample recovery for retained samples.	Density, refractive index	30
	**CuvetteChanger** The CuvetteChanger allows efficient automatic measurement of series of up to 8 cuvettes for both standard measurements with blank subtraction or complex kinetic applications. An external thermostat makes it possible to cool and heat the cuvettes within a range of 10–80 °C.	UV/VIS spectrophotometry	8
	**Quantos** Autosampler allows up to 30 samples to be dispensed in one completely unattended run. From 1 mg up to several grams of powder can be weighed out automatically into containers of your choice. Add the liquid dispensing module to prepare solutions.	Weighing and dosing (solids and liquids)	30
	**TA Robot** The sample robot is very robust and operates reliably 24 hours a day and throughout the whole year. It offers up to 34 sample positions.	DSC, TGA	34

Table 2: METTLER TOLEDO's offering of autosamplers.

3.4. Software Automation

Automation increases efficiency and thus also the amount of created data. LabX® PC software can connect to multiple METTLER TOLEDO laboratory instruments and supports you in all data management tasks, ensuring full traceability. Furthermore, the software enables you to automate complete SOP workflows, guiding users through every step. All data, resources and users are managed centrally.

LabX laboratory software provides instrument connectivity, user guidance and data handling for seamless compliance.

Data management automation

LabX provides you with full data management, from automatic and complete data collection and storage up to data analysis, reporting and export to your ELN or LIMS. The software has all technical controls in place to support your laboratory with regulatory compliance, such as 21 CFR part 11 or FDA ALCOA+ data integrity requirements.

Full workflow automation

With LabX you can program complete workflows/SOPs into so called methods. These methods guide users step-by-step through the workflow directly at the instrument, what makes them work faster and more precise. A workflow can even consist of steps performed at different instruments. All results are captured centrally in the LabX software.

Explore our Services
For Quality, Efficiency and Productivity

Find more information on
www.mt.com/Service

We assist you globally to achieve excellency:

- Increased productivity through equipment reliability
- Enhanced efficiency due to improved operator skills and process optimization
- Measurement accuracy thanks to regular maintenance and calibration
- Calibration while taking into account regulatory requirements relevant to your industry
- Audit-proof documentation covering process and risk assessment

www.mt.com
For more information

METTLER TOLEDO Group
Laboratory Weighing
Local contact: www.mt.com/contacts

Global MarCom 2397 RK/MD, L00855EN A