CHIMIA REPORT/COMPANY NEWS

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Companies present themselves and their products

Interested in a contribution? Please contact
Swiss Chemical Society, info@scg.ch, +41 31 306 92 92

SHIMADZU, Excellence in Science

For more than 140 years, Shimadzu has been servicing science with precise, reliable diagnoses and analyses in a number of industries as well as healthcare markets. The company's inventions and developments have enabled new and more accurate insights, taking analysis, methods and findings to the next level of consumer, patient, environmental and product safety.

Shimadzu Schweiz GmbH – an integral part of the Shimadzu European organization – was founded in 1999 and is responsible for sales and support for the analytical products in Switzerland.

The list of milestones and success stories is long. Many "industry first" products have extended technological boundaries and set new standards; many of them are meanwhile industry benchmarks.

In 2002, there was also the awarding of the Nobel Prize for Chemistry to Shimadzu engineer Koichi Tanaka for his outstanding contributions in the field of mass spectrometry.

The Promise

"Excellence in Science" is the company's brand value proposition and key driver based on increasingly sensitive measuring and diagnostic methods. The new "Laboratory World" in Duisburg, Germany, with a floor space of more than 1500 m^2, is an example of how to fulfill the company's brand promise. Testing and training facilities have been created for the entire product range – from chromatographs, spectrophotometers and TOC analyzers to mass spectrometers and material testing machines.

In the field of analytical instrumentation, a broad variety of products, software solutions and customer services for specific applications, industries and markets is offered. A wide network of sales offices and distributors in most European countries guarantees international and regional service including technical support. For over 45 years the European headquarters has been located in Germany. As a global player, Shimadzu operates production facilities and distribution centers in 76 countries, with more than 10,000 employees worldwide.

Tailor-made Solutions

Customers can choose between many possibilities in order to obtain the solution tailored to their individual needs. In this way, the company has become the only supplier of the whole range of analytical instruments whose product offering has grown constantly. At the same time, Shimadzu is the market or technological leader in many areas.
Driven by globalization, the analyzers and equipment are applied in the chemical, petrochemical and pharmaceutical industry, life sciences, cosmetics, semiconductor and nutrition industry as well as in the flavours and fragrances business. Research institutes, privately run laboratories, administrations and universities complete the list of clients. The systems are used in routine and high-end applications, process and quality control, as well as R&D.

The Mission

When developing products, the company is focused on top quality, including; ease of operation, reliable service and an appropriate high performance/low total cost of ownership ratio. All of the analytical and medical systems are produced according to internationally renowned quality standards, for instance ISO, and enable customers to work under GLP, GMP, FDA and Pharmacopoeia compliance.

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METTLER TOLEDO – Smart Lab Processes

Building on the principles of networked lab processes, METTLER TOLEDO has introduced a variety of smart upgrades which increase data integrity and productivity and support the streamlining of lab processes.

In laboratory environments, data integrity is defined as the completeness, reliability and precision of a data record. Integral results and data must be able to be used for different purposes at any given time in future. METTLER TOLEDO presents the LabX® software which manages all connected instruments and data and centralizes all lab work processes.

The use of just one software package to link multiple laboratory instruments and, additionally, network to the ERP or LIM system, contributes greatly to reducing complexity and encourages implementation of the lean concept throughout the laboratory.

The lean lab principles enable clearly defined, better structured and controlled laboratory processes, delivering more consistent and predictable laboratory performance. It is a case of ensuring that the three parameters – quality, resources and time – are in optimum harmony with each other. The most important lean principles and smart solutions for successful implementation of the lean concept will be illustrated using practical examples from everyday lab work at our exhibit stand.

"Reduce measurement uncertainty": The precision of measurement results must always lie within the specified range. An overview of the calibration and service status of every pipette in use, available at all times, ensures that the instruments are performing correctly and reduces downtimes. The unique smart pipette stand SmartStand™, together with new inventory management software EasyDirect, enables efficient monitoring of all pipettes. With just a few clicks, you can get an immediate overview of which pipettes will need servicing and calibration over the next month, quarter or year. The user immediately learns whether he is working with SOP-compliant pipettes and whether the pipette can actually be used for the task at hand or whether it needs to be recalibrated.

"Avoid mistakes": First, SmartSample™ from METTLER TOLEDO uses radio frequency identification (RFID) technology for contactless transfer of sample data - from the balance to the titrator. The analytical balance transfers sample-specific data to the titration beaker chip and reduces the workflow to a single user interface. The titrator automatically detects the sample and the assigned method, thereby eliminating confusion and mix-ups.

Progress in user-friendly weighing

The new MS-TS balances are designed for everyday work and, thanks to the high-end touch screen, can also be operated through a wide variety of gloves. The interactive user interface makes many routine tasks simpler. With the help of these smart balances, entire workflows and error tolerances can be set automatically. This reduces the risk of human error to a minimum. In combination with the green/red results screen, which clearly indicates if results meet the pass/fail criteria for a process, daily tasks are faster and easier, whilst confidence in results is increased. Standard checks and safety features provide added certainty.

"Simplify processes": In recent years, METTLER TOLEDO has dealt with this complex topic in depth and has focused on simplifying (streamlining) processes.

Thanks to the new FastTrack™ technology, spectroscopic workflows can now be substantially optimized. The models of the new UV/VIS Excellence series (UV5, UV7, UV5Bio, and UV5Nano) have an extremely compact bench space – no larger than a sheet of DIN A4 paper – and provide fast and reliable measurements. Dependable spectroscopic performance is combined with the intuitive and efficient OneClick™ operation. The UV5 provides simplicity in UV/VIS spectroscopy with easy direct measurement applications. The UV7 performance complies with strict EU and US Pharmacopeia requirements and provides advanced automation possibilities. Based on cuvette measurement, the UV5Bio is the ideal instrument for UV/VIS research applications in the life sciences. The UV5Nano provides savings on expensive samples and thanks to the innovative LockPath™ technology, reliably measures a wide range

of concentrations with only 1 µl of sample volume.

A reactor system for optimal synthesis results

The everyday equipment used by an organic synthesis chemist has barely changed in the past 100 years. The simple glass flask still plays the leading role in the synthesis lab. The new EasyMax™ system declutters this area and offers a powerful yet flexible and easy-to-use reactor system. It increases temperature control, reproducibility and information density to levels never seen before. During the course of an experiment, all events and data are automatically recorded. For additional processing or interpretation, it is easy to export the experiment data to iControl™ or Excel®.

"Reduce delays": Automation techniques significantly shorten the throughput times of each analysis.

An automatic pipetting system for precise and consistent aspiration and dosing

BenchSmart combines the speed and flexibility of a manual system with the precision and higher reliability of electronic pipetting. It is particularly suitable for the research environment, where experimental conditions can change quickly and frequent modifications to the study protocol are the norm. Bench-Smart's small footprint also makes it easy to move to wherever it is needed and, unlike fully automated systems, it is so intuitive and easy to operate that anyone in the lab can use it.

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BioSolveIT

The multinational company BioSolveIT develops next generation in silico assistance, fosters understanding & predicting of SAR, properties, peptide design, and more. The services department assists customers with modeling tasks profiting of broad experience and skills.

BioSolveIT focuses on the development of highly efficient and very visual software solutions for the early drug discovery phase. With an immense track record of co-development with Bayer, Roche, Merck, AstraZeneca, Novartis, Boehringer-Ingelheim, Pfizer, BASF, and many others, BioSolveIT software stands out in speed of delivery and visualization. Academic collaborations especially with co-founding Professor Dr. Matthias Rarey, ensure top-notch and up-to-date science behind the tools.

Structure-Based Design

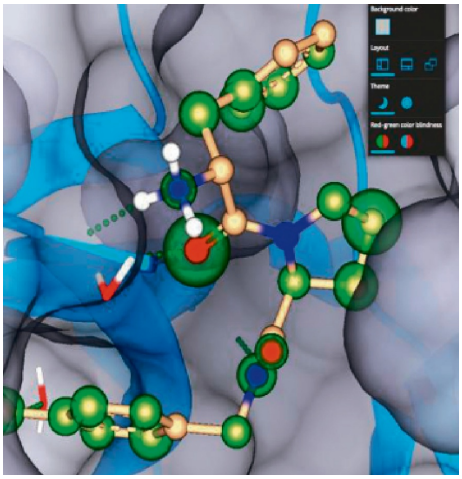
The flexible-ligand docking algorithm FlexX is an industry standard and poses compounds reliably into cavities. Automated detection and proposals of putative binding sites are carried out within seconds, and all insecurities from X-ray relating hydrogen positions, or element assignments are optimized and proposed within milliseconds. This is world speed record – parallelized with high reliability and accuracy. Pharmacophore constraints, filters, and property predictions can be carried out alongside to integrate experimental knowledge.

Award-Winning ΔG Estimates

Collaboration with Bayer in Frankfurt and Hamburg University has delivered a visual and atom-based system to predict affinities (ΔG Free Energies, "HYDE"). This is widely considered a breakthrough since dehydration ("desolvation") effects are taken into account and balanced against hydrogen bonding – without training and thus limitation to any target class. Colored spheres ("Affinity Coronas") on atoms in the 3D design environment let the user directly get into a dialog with the software to optimize the molecule's binding strength to inhibit a target (see picture). With a solid algorithmic background, the software manages to estimate ΔG in a few seconds on a standard laptop; this is very noteworthy since other approaches that are also considered state-of-the-art in the field need hours or massive hardware.

Build and Search Gigantic Chemical Spaces to discover novel compounds

Owing to BioSolveIT's expertise in tree algorithms, the organization has the option to search&find similar molecules in giant chemical spaces of sizes 1016 virtual molecules and larger. Our freely available so-called KnowledgeSpace is defined and built up from chemical reactions so that the results delivered by the software are highly likely to be synthesizable. The respective software "Feature Trees" is unique in being able to visualize why two compounds appear to be similar with an additional colored molecular 2D sketch.



Exploring and Generating New IP by Re-scaffolding

When researchers are stuck with a certain molecular scaffold for IP or toxicity or other reasons, then BioSolveIT can offer a replacement engine that lets clients "google" for replacements in 3D. The software used for this ("ReCore") was developed in collaboration with Hamburg University (Prof. Rarey's lab) and Dr. Martin Stahl's group at Roche in Basel. ReCore exploits indexing techniques and jumps straight to the solutions that fit best – within fractions of a second.

Software Apt for Any Chemist

To make in silico guidance available for non-expert modelers BioSolveIT created front-runner software that can be used by novices right from the start with plenty of the algorithmic 'gems' incorporated. The latest tool has been named "SeeSAR" since it has a pronounced strength in visualizing the structure-activity relationships in 3D; alongside with an editor that delivers changes to ΔG and properties in situ. This helps to streamline the drug development in many companies as computational guidance is easily available for all people in a project.

Service Department

To help drug-design projects succeed BioSolveIT are providing expert computational medicinal chemistry service and help by becoming part of your team. Our service department will carry out your modelling tasks to save precious time while the client gets to learn along the way what the software can do. Especially for small and mid-sized enterprises (SMEs) that often do not have the manpower to employ full-time modeling staff, these services are very useful.

Company History

BioSolveIT GmbH has been established in 2001 as a Fraunhofer Gesellschaft spin-off, and with stakeholders Prof. Dr. Thomas Lengauer PhD (Max-Planck-Institute Saarbrücken), Prof. Dr. Ralf Zimmer (TU Munich), Prof. Dr. Matthias Rarey (Univ. Hamburg), and CEO Dr. Christian Lemmen, the steering board is connected globally and has a wide, cross-disciplinary expertise. Early sales were carried out through Tripos (St. Louis, USA), but from 2004 onwards, BioSolveIT have built up their own distribution force, with a US office, and sales partners in China, India, and Japan. The services department was established in 2013.

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