

Highlights of Analytical Sciences in Switzerland

Division of Analytical Sciences

A Division of the Swiss Chemical Society

RASPP, a Fully Automated Platform Preparing Analytical Samples

Inken Plitzko*, Josef Schneider, Tom Kissling, Christian Bartelmus, Thomas Zumstein, and Roger Steiner

*Correspondence: Dr. I. Plitzko, Roche Pharma Research and Early Development, Roche Innovation Center Basel, F. Hoffmann-La Roche Ltd, Grenzacherstrasse 124, CH-4070 Basel, E-mail: Inken.Plitzko@Roche.com

Keywords: Automation · Robotics · Sample Preparation · SiLA

Up to now automation of laboratory workflows has rarely included preparation of NMR samples. Therefore we developed RASPP (Roche Automated Sample Preparation Platform), a system which prepares three analytical samples (NMR, GC-MS, LC-MS) from one delivery sample (Fig. 1).

A setup of third-party components and in-house developed elements, running on a SiLA-conform scheduling software (Standardization in Lab Automation), allows all steps and challenges of this process to be addressed and to prepare several samples in parallel for optimal time efficiency.

In a first step the sample is identified by its barcode, which connects to the electronic lab notebook (ELN) and to the AWM (Analytical Workflow Manager, Waters®) LIMS system (Fig. 2). In parallel, weighing indicates if the sample comes with (enough) solvent. This allows samples to be processed that are already dissolved, for example those needing solvents other than CDCl_3 or d_6 -DMSO, as they are not provided by RASPP. According to the information extracted, deuterated solvent is then added up to a fixed volume. d_6 -DMSO is dispensed under N_2 flow, since the following high-impact ultrasound treatment which facilitates the dissolution otherwise leads to line-broadening in the NMR spectra. A potential cause is the formation of oxygen radicals and subsequent degradation of DMSO.^[1,2]

Photo documentation of the dissolved sample takes place before the solution is distributed to NMR tubes and GC-LC-MS vials – the LC-MS samples being diluted with MeCN/ H_2O . Noteworthy is that the (de)cappers for those vials were developed in-house and an NMR tube capper is unprecedented (Fig. 3).

A printer labels the prepared samples with their unique LIMS number as they are distributed to respective autosampler racks. This ensures reliable tracking of samples at all times. In the end a CSV (comma-separated values) file is created and (via pipeline pilot script) translated directly into spectrometer work-lists.

Key to the success of this system is the efficient integration of the information flow, providing all information needed for set-up and interpretation of spectra from the ELN of the sample provider to the instrument software and to the LIMS system, in which submissions and finally the results are filed. **RASPP has replaced labor-intensive and error-prone manual sample preparation by a reliable and fully documented process.**

Received: April 5, 2016

References

- [1] C. Mésangeau, S. Yous, B. Pérès, D. Lesieur, T. Besson, *Tetrahedron Lett.* **2005**, *46*, 2465.
- [2] A. Weissler, *J. Am. Chem. Soc.* **1959**, *81*, 1077.

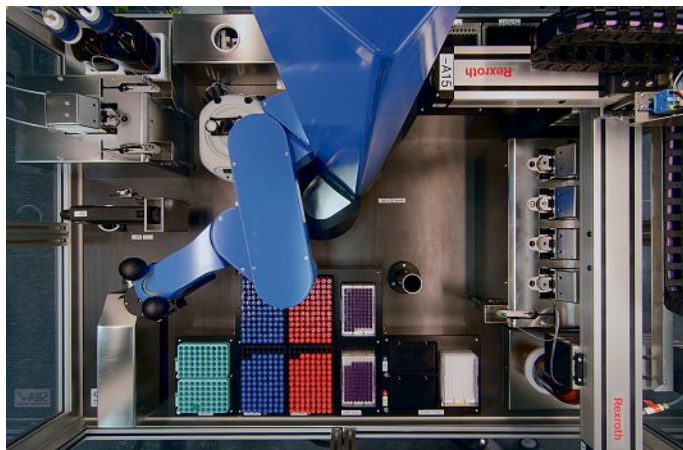


Fig. 1. Birds-eye view of RASPP.



Fig. 2. Barcode reading, weighing, and photo documentation.

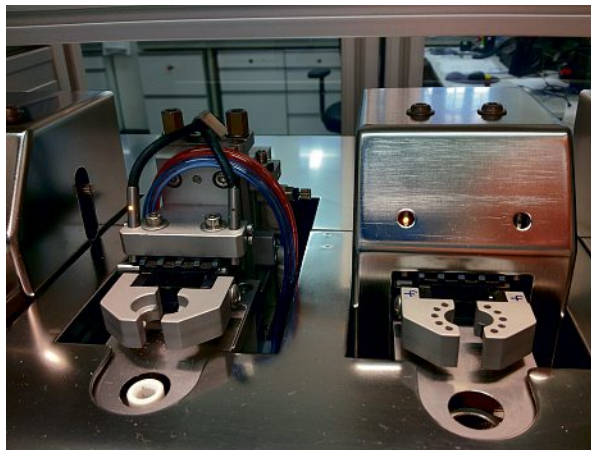


Fig. 3. In-house developed (de)cappers for vials and NMR tubes.

Can you show us your analytical highlight?

Please contact: Dr. Veronika R. Meyer, Unterstrasse 58, CH-9000 St. Gallen
Tel.: +41 71 222 16 81, E-mail: VRMeyer@bluewin.ch