s13.m37.o4 **Buy one, get one free - redefining the role of service crystallography in a pharmaceutical environment.** Trixie Wagner and Lukas Oberer, *Novartis Institutes for BioMedical Research, Switzerland.*
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Keywords: Service crystallography; Instrumentation; Pharmaceutical industry

Maintaining a dedicated small molecule x-ray facility in a pharmaceutical company is not a compelling necessity anymore. Alternative analytical methods such as NMR, IR, and MS have become so powerful over the past years that an ever increasing percentage of full structure proof requests can be handled based on their contributions alone. One possible way out of this dilemma is to utilize rather non-scientific marketing instruments such as rebates and discounts. A second, and maybe in the long run more beneficial approach is to focus on complementary aspects and at the same time emphasize the unique advantages that still distinguish x-ray methods from all other analytical techniques: In many cases, e.g., a single crystal structure analysis is the only method to identify the chirality of a sample. For unknown samples and/or certain classes of compounds x-ray crystallography allows the most reliable assignment of atom types. And last but not least x-ray coordinates still provide a very good approximation to a realistic 3-dimensional model of the molecule of interest, indispensable in an industrial branch living off structure-based drug design. If time and cost-effectiveness are issues to consider, too, it seems only natural to additionally take advantage of the facts that a) the technical developments of the past 5-10 years have eliminated the need for an x-ray experiment to take up several days and b) the variability of modern machines (in our case a CCD area detector on a three-circle goniometer with Cu-K(α) radiation from a sealed tube source) allows the experimental parameters to be flexibly adapted to actual needs of a structure request. Based on some representative examples we will show how a very efficient use of beamtime can be realized: preliminary results (on a proof of constitution level) are available within 30 to 60 minutes, and routine structure determinations can then, depending on the crystal symmetry, be completed within 4-12 hours, with data quality and refinement results in perfect compliance with the standards defined by the IUCr. In cases of doubt we have the option to immediately match our refinement results with additional data from the adjacent NMR, MS, or HPLC departments. Decisions on the continuation and/or design of an experiment are then made on the fly to obtain as much data as possible but not more than necessary. In more complex cases such as stereochemical assignments when oxygen is the heaviest atom present more elaborate data collection strategies are needed and can be employed very easily. Here, too, speed is the key to success, this time, however, it is utilized to significantly improve data quality by exploiting the additional information of highly redundant measurements. This way it is possible to achieve standard deviations for the Flack x parameter smaller than the generally acknowledged limit of 0.10. In combination with the purity figures from HPLC data stereochemical problems can then be addressed very reliably. Our tailored-to-fit-approach makes even non-automated crystallography based on Cu radiation a highly valuable add-on for an analytical department, especially when drug substances are the subject of investigation and a careful balance between quality, unambiguousness, and speed is vital.

s13.m37.o5 **Single-crystal x-ray diffraction studies of light-activated molecular species**. J. M. Cole[a], [a]*Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge, CB2 1EW. UK. E-mail: jmc61@cam.ac.uk*

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Light-activated processes in various materials have attracted a wide level of interest over recent years on account of the very applied nature of their light emissive properties: e.g. for non-linear optical components, optical storage devices, and light-emitting diodes. The origin of these properties lies in the structural perturbations caused by the application of light. Such structural manifestations typically comprise a temporal redistribution of electrons in a molecule compared with their original ground state. Therefore, if one can probe the electronic structure of the light-induced state, one can understand better the physical properties of a given material. Understanding of this inherent structure-property relationship leads to the ultimate goal of being able to tailor materials for a given photonic device.

In order to obtain the most direct and quantitative three-dimensional picture of excited-states, we are using (laser)pump-(X-ray)probe single-crystal diffraction methodologies, investigating materials that undergo metastable and time-resolved light-activated structural changes whilst retaining their single-crystal form. The development of the experimental x-ray diffraction techniques, the complementary laser spectroscopy that needs to be performed in tandem with such experiments, and results obtained thus far are presented. Such results derive from work that has been carried out in the USA [1], France [2] and the UK [2,3] on materials with photo-induced lifetimes ranging from the metastable (long-lived), through to those with a lifetime of nanoseconds.

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