Summary
Time is a precious commodity for Dr. Carsten Schauerte, who oversees daily operations and customer acquisition at the “chemical sleuthing” company solid-chem GmbH. We gave him access to Reaxys and asked him to see if using this powerful chemistry research solution could help save him time and advance the scientific work at solid-chem. Two weeks later, he shared his thoughts on ways in which Reaxys meets his research and business needs.
Operating out of the Biotech Industry Park at the Ruhr-University Bochum in Germany, solid-chem GmbH is a provider of analytical services for solid-state chemistry. Professor Dr. Roland Boese and Dr. Carsten Schauerte lead a team of scientists and technicians to extend the investigative arm of mostly pharmaceutical customers by sleuthing the composition, quantity and form of materials, as well as advising on formulations and synthesis strategies. Dr. Boese is a world-leading expert in questions related to crystal engineering and crystal structure prediction, and is often called upon to testify in patent litigations. Dr. Schauerte has managed the business aspects and the analytical services at solid-chem for 7 years. With in-depth knowledge of analytical methodologies, he tailors and orchestrates commissioned analyses to leverage the methods that deliver the most impactful answers for customer questions.

Challenge
solid-chem uses a broad spectrum of analytical techniques to examine chemical samples from customers. To that end, Dr. Schauerte and his team gather as much information about the properties of substances relevant to a project. They query multiple databases, sift through literature and patents, and explore any system that gives them concrete, experimentally determined data. The information they find is essential to decide which analytical techniques to pursue. It enables solid-chem to deliver impactful answers and use resources optimally. Efficiencies in technique and resource use drive their business success and create added value for customers. However, the process of finding information is complex and time-intensive.

Solution
With the clear objective of improving the efficiency in searching and using existing substance property information, Dr. Schauerte agreed to an experiment with Reaxys. Unfamiliar with Reaxys, he was given a 15-minute tour of the user interface and then asked to use the solution in his day-to-day work. Two weeks later, he told us about his experiences.

“Reaxys fits well to solid-chem because it encompasses the diverse spectrum of analytical techniques and substance properties that are at the core of what we do.”
—Dr. Carsten Schauerte, Managing Director of solid-chem GmbH
Have you used Reaxys in the last two weeks?

I am starting to think about what I’d do if I didn’t have access to Reaxys! Properties are the foundation of our work. From my exploration of the content of Reaxys so far, I have found it to have an amount and diversity of substance properties unlike any other tool I’ve used. It cannot entirely replace the multiple information research platforms we use, but it has proven to save us time by simplifying the overall search for answers. Reaxys collates information from multiple sources, which I would normally have to interrogate separately. Being able to go into Reaxys and in just a few clicks see what is even out there—be it in the literature, in patents or tabulated in the Substance Records—has been a great experience.

Can you tell us about your exploration of Reaxys?

Deformulations are among the most common commissions that solid-chem receives. Companies owning proprietary drug formulations may want us to test a competitor compound to exclude the possibility of patent infringement. Other companies may want to know what polymorphs are contained in a formulation or answer questions about freedom to operate. Others may contract solid-chem to investigate and solve problems in manufacturing. Determining the composition of customer samples requires knowing existing property values for substances measured by the extensive range of analytical methods we offer. The type of information we can find plays a role in determining what methods we implement. And since it is my goal to keep analyses cost-effective, I invest a lot of time and energy into finding property data.

Take polymorphism analysis. The U.S. Food & Drug Administration requires a polymorphism screening with the submission of a drug for approval. Why? Because different polymorphs exhibit different properties and that conversely impacts the efficacy of a drug. Carbamazepine is a medication used to treat epilepsy and neuropathic pain. The active pharmaceutical ingredient is known to have 5 different polymorphs—maybe more—including the dihydrate form, which is significantly less soluble than the others. Storing the medication in a moist medical cabinet could trigger conversion to the dihydrate and reduce efficacy.

Getting information about polymorphic states of crystals can be difficult and takes a long time. I resort to several sources but most are very specific or require very specific input to get an answer. The Cambridge Structural Database, for example, has over 875,000 entries from X-ray and neutron diffraction analyses. It is a very powerful system, but it builds on single-crystal X-ray diffraction, and I don't always have that information nor can I easily perform the analysis.

So, to get a feel for the content of Reaxys, I explored the property data for carbamazepine to see what I could find about its polymorphic states. Its Substance Record includes a broad range of property information. The amount of data probably exceeds what I have found for other polymorphic systems, and because the collated data were determined using multiple techniques, Reaxys eliminates restrictions I have experienced with other platforms.

Without any previous knowledge about this active ingredient, the tabulated data immediately indicates possible polymorphism. First, the variation in melting point is obvious because the excerpted data are listed right there in the record, and they suggest that the compound may have more than one form.
Tabulated melting points for carbamazepine in Reaxys. Excerpted data are collated within a Substance Record and listed with corresponding sources.

Second, further down the list of physical properties we find specific crystal properties and there is a set of references categorized under the description Polymorphism. Clearly, carbamazepine has polymorphs and now I have a manageable set of references that I can examine to learn more. Finally, the property field Crystal System also provides proof of polymorphism since the listed references report different system forms!

Another thing I like about Reaxys is that it sometimes lists where to find information in a source, so I know from the get-go what paragraph to look for in a patent or if I need to download supplementary documentation.
An organized subset of references from which information about the polymorphism of carbamazepine was excerpted. Reaxys also houses an extensive literature database that can be searched for additional information.
Information excerpted from references presenting evidence of different crystal system forms of carbamazepine. The column Location can assist in finding the specific position of information in a source.

When we perform deformation of a medicinal tablet, we resort to several techniques. For example, infrared (IR) and RAMAN spectroscopy come into play to resolve ambiguous signals from powder X-ray diffraction, or when a sample includes amorphous material. For that purpose we need to know what to expect from IR and RAMAN spectra of substances, and in Reaxys we find several references from which we can glean information.

Information about spectroscopic studies on carbamazepine is also excerpted and collated in its Substance Record.
Do you think Reaxys can positively impact your daily work?

Definitely. Starting with our deformulation service, which is such an important part of our business: Reaxys can help us standardize and streamline our workflow. Our scientists routinely use powder X-ray diffraction, IR spectroscopy, RAMAN spectroscopy and other techniques to find out what is in a formulation. Beyond the active ingredient, a medicine tablet contains a vast number of auxiliary materials, so-called excipients. They improve the physical, chemical and biological properties of the active ingredient, like solubility, bioavailability, shelf-life or even manufacturability. To elucidate the precise composition of the tablet, we compare analytical data to an in-house database of approximately 200 substances that commonly occur in materials from customers and for which we have systematically collected reference data over the years. The signals of matching substances are subtracted from the overall analytical profile of the tablet and whatever is left, needs to be further identified. Naturally, there we need lots of information. While the steps that we follow in the procedure are permanently improved, they are also impacted by the existing property data that we can find in literature, patents and databases. Having access to a system like Reaxys will necessarily influence how we setup the process and has the potential to streamline things by better informing our analytical strategy and experiment planning.

Business Impact

Have you used Reaxys for commissions that your team is currently working on?

Yes, of course; but due to confidentiality agreements, I am not at liberty to discuss the details. Reaxys is helping us optimize the analyses we perform. We are excited about the content we are finding and about the ease with which we can find relevant hits. Data we are finding in Reaxys help ensure that my staff does not waste time on wrong or redundant analyses, that our equipment is used efficiently, and that we maximize our output. This ultimately translates to shorter delivery times and lower costs for our customers because we are better able to focus on the essential ingredients and most telling analyses in each commission.

The functionality of Reaxys also helps make our search for properties easier. I’m impressed with the linking from Reaxys to sources, especially to patent content because navigating the different patent systems can be very time-consuming. I have also rediscovered Scopus. Prior to using Reaxys, Scopus was not really on my radar as a tool for my work. The interoperability with Scopus gives me valuable information—with a click, I can see where references appear in other publications and that is an important part of the research we do.

Will you continue to use Reaxys?

Absolutely. It occurs to me that I need to be smarter about my searches. I see that I can set up very complex searches in Reaxys, using operators and the various query fields for properties. That is my next goal: to explore other substance property fields in Reaxys and dig deeper by building better queries. There are a few property fields that I want to look into, like Enthalpy of Fusion and Transition Point of Crystalline Modification. The latter is of importance for the manufacturing of solid-state chemicals, where solid-chem is often asked to support troubleshooting and optimizing processes. The data and references in that field could be instrumental in advising customers on how to direct synthesis toward a desired polymorph without inadvertently causing transformation to a form from which it would be difficult to return.

All in all, I see a distinct advantage to using Reaxys, especially as a first search point that guides any subsequent information research, whether in Reaxys or in the other systems we use. Reaxys fits well to solid-chem because it encompasses the diverse spectrum of analytical techniques and substance properties that are at the core of what we do. From my perspective, I continuously balance guiding the scientific work of my team with acquiring customers, planning projects, reporting results, and the day-to-day business aspects of the company. Reaxys allows me to accomplish more; and if something saves me time without compromising quality, I want to use it.
Reaxys

Reaxys helps chemical companies develop commercially successful products by providing chemists the shortest path to data for synthesis optimization and the identification of desirable chemical properties in intermediate and end products.

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