CASE STUDY

Reaxys®
Ironwood Pharmaceuticals

Reaxys supports real-time solutions in an entrepreneurial drug discovery and development environment

SUMMARY
Ironwood Pharmaceuticals is an entrepreneurial pharmaceutical company that discovers, develops and intends to commercialize innovative human medicines, particularly in areas in which there are currently unmet medical needs.
Takahashi Nakai, Associate Research Scientist, Medicinal Chemistry at Ironwood Pharmaceuticals talks to us about how Reaxys supports his workflow to perform a multitude of tasks like SAR analyses, propose new targets and as well as their synthetic routes, execute synthesis and characterize compounds.

**Business challenge**
Ironwood tackles the most difficult aspect of drugmaking: the interface of pharmacology and chemistry. The company requires that their programs have a pharmacologically validated mechanism along with robust readouts that are predictive of clinical outcomes. This enables Ironwood’s scientists to rapidly iterate between in vivo models and chemistry to efficiently find lead molecules with clinical promise.

That means that the demand for credible, accurate, easily-accessible chemical information is high. That’s where Reaxys comes in — providing actionable, real-time solutions that help to drive drug discovery and development forward.

“I’m not an encyclopedia of knowledge, so I rely on Reaxys. The benefits from my perspective are that it’s tailored to meet my needs as a chemist and it enables us to get started on our research much more quickly.”

**Solution**
One of Takashi’s primary responsibilities is to develop synthetic routes for targets that he proposes. He and his colleagues increasingly use Reaxys to look up reactions, precedents, starting materials and intermediates in Reaxys.

“Reaxys can quickly lead you to a practical starting point. If you can’t find the exact compound, you just search for similar sequences of reactions to get to the target compounds.”

Used extensively during the synthesis phase and reaction planning, medicinal chemists like Takashi search for structures, specific targets and therapeutic indications, as well as patents and scientific literature. Takashi routinely uses Reaxys to locate relevant patents. He is able to extract critical data in real time. This can circumvent the sometimes lengthy process of having to order patents.

Reaxys has an added benefit over other search engines, in that it provides easy access to published biological data.

“The fact that you can filter your hits by biological data like IC50 and other activity values in a given assay is great. It saves a lot of time by not having to request and read through patents. Additionally I like that we can export data into Excel files.”

It is critical to be able to locate reliable and trustworthy information on commercial availability and pricing of reagents and intermediates. Instead of having to contact vendors either by phone or via their websites, which tends to drag on, links from compounds within

“Reaxys is a powerful and indispensable solution for chemists that has far exceeded my expectations.”

– Takahashi Nakai, Associate Research Scientist
Reaxys to the eMolecules site provide critical sourcing information and real-time pricing. This helps to make quick and sound decisions about which reaction pathways appear to be most promising.

“I think Reaxys saves us a significant amount of time because we don’t have to wait for information to arrive or make repeated phone calls to order a reagent. Using the web link to eMolecules it’s really easy to get the data so we can make a relatively quick judgment regarding whether to pursue a certain path or not. The pricing data is extremely valuable!”

Reaxys provides a depth of information not found in other services. Reaxys covers 400 journals, a portfolio that is constantly reviewed and monitored to ensure relevancy and currency. Data is extracted and presented in a way that makes it readily available and instantly usable.

Outcome
Real-time solutions bring real advantages to the drug discovery and development process. In the highly competitive entrepreneurial environment at Ironwood, decisions need to be made quickly and reliably. Reaxys offers effective workflow solutions and supports real-time decision-making because it goes beyond data and provides insights and ideas that lead to innovation and ultimately, the promise of commercial success.

“In Reaxys you can read the experimental section without having to request an article. This is a major advantage compared to other information resources. It helps us in our endeavor to avoid the mistakes made by others.”

– TAKAHASHI NAKAI, ASSOCIATE RESEARCH SCIENTIST
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