

Reaxys®

DRUG DISCOVERY & DEVELOPMENT

Solution Story: Revealing the chemistry of therapeutically important nucleosides

How Reaxys helps to quickly identify the drug-like qualities and feasible synthesis routes for carbocyclic nucleosides



Introduction

Hong-Rae Kim is a research chemist in the lab of Professor Jeong at Seoul National University. His work is focused on the chemistry of carbocyclic nucleosides, which have great potential as therapeutics. Finding the optimal synthesis method for these important compounds can be very challenging, but Reaxys is up to the task.

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—Hong-Rae Kim, research chemist at Seoul National University



Hong-Rae Kim is a researcher in the laboratory of Professor Jeong at Seoul National University. His research is focused on the chemistry of nucleosides that may have potential as therapeutics.



Professor Lak Shin Jeong's laboratory is known for excellence in chemistry and pharmacology that has potential to support medical treatments in innovative ways.

Seoul National University was the first national institution of higher learning in the Republic of Korea. Founded in 1946, it stands on the country's largest campus, with 16 colleges, 1 graduate school and 10 professional schools serving almost 30 thousand students. The faculty are committed to preparing students to work and live in an increasingly competitive global community, but also to create a vibrant intellectual community that will stand strong for democracy, peace and a better future. To remind all staff and students of this goal, the university has the motto “Excellence, honoring public service and pioneering knowledge”.

Professor Lak Shin Jeong runs a research laboratory that certainly bears out this motto, focusing on excellence in chemistry and pharmacology that has potential to support medical treatments in innovative ways. Therapeutics that could be supported by Professor Jeong's group include treatments for strokes, cancer, chronic kidney disease, HIV, herpes and hepatitis B and C.

Hong-Rae Kim is a research chemist on Professor Jeong's team. He agreed to discuss his research experiences with Elsevier and talk about some of the ways that Reaxys and Reaxys Medicinal Chemistry solve his research challenges.

Challenge

Could you tell us about your research project?

My research is focused on complimentary nucleosides with a rotational ring that can exist in two conformations, referred to as the north and south conformations. In solution, it exists in a state of rapid equilibrium between these two forms. It's believed that nucleosides can only bind to a given protein in one of the conformations — for example, the nucleoside analog for HIV reverse transcriptase is thought to interact exclusively in the north conformation. Nucleosides generally only exist in a neutral form that needs activation via phosphorylation. There is considerable interest in creating forms that are locked in one or the other conformation.

Is your focus on the therapeutic applications of these nucleosides?

While I'm certainly interested in the potential applications of locked-conformation nucleosides, my research isn't target oriented. I'm looking at the fundamentals of nucleoside chemistry: I aim to better understand the nature of nucleosides and develop ways to engineer them in forms that can or cannot be recognized, depending on what we want to achieve.

What are the main challenges in your research?

Synthesis itself is probably the greatest challenge. Carbocyclic nucleosides are considered to be among the most difficult substances to synthesize. Nucleoside synthesis strategies often require many steps and are not always economically feasible. Hazardous byproducts are a concern, especially in larger-scale production.

I'm focused on both finding synthesis methods for new locked nucleosides and improving the synthesis of existing ones. Developing or optimizing a synthesis method means spending a lot of time researching reactions. I have to find all the possible reactions that might give the result we want, and that can be a time-consuming process. When I find one that seems economically feasible, I must investigate and test it to see if it will really work. If it doesn't, it's back to the literature again.

Solution

How do you find the reaction information that you need?

I use Reaxys and another research solution to look up reactions. I started with the other research solution when I first joined Professor Jeong's group, but there was a time when I was reading through dozens of papers trying to find one reaction, and I couldn't. Reaxys was recommended to me and I tried it out — I found the reaction and the paper it was sourced from straight away.

The development of the Internet brought us some amazing benefits, but it can be very challenging to find relevance in the noise if you don't use dedicated research solutions.

Reaxys is perfect for me at the moment, especially with the new user interface. The format makes it easier to look up reactions. It's intuitive, it's easy to follow the information. I think information providers don't always realize how important a cleanly formatted interface can be! I'd say that Reaxys currently has the easiest user interface to read.

Another major difference with Reaxys is the focus on excerpted data. Other solutions are more focused on publications. Reaxys lets me directly open the experimental sections and see properties, reaction types and details. That's a huge advantage. And I can always go from the details to the source material.

Reaxys Medicinal Chemistry is also very good for my research. At a glance, I can see what a nucleoside is binding to. The Heatmap shows substance binds to which enzymes, and the information is even quantified with pX values. I can delve into the drug-likeness information.

There's also a great value to seeing the publication numbers for a given substance and target in Reaxys Medicinal Chemistry. That exposes the trends in research focus: who's working on what target inhibition, which targets are in decreasing or increasing focus. That reveals for example, that there might be a side effect of great concern.

Impact

Would you say that Reaxys benefits you in your research?

Absolutely. Reaxys and Reaxys Medicinal Chemistry save us a great deal of time by delivering answers quickly. The user interface is an excellent design, the reaction classifications are exactly what we need, the synthesis information is detailed but well displayed. I find Reaxys wonderful.

Reaxys

Reaxys helps chemical businesses ensure that manufacturing processes are optimized for quality and safety standards by providing chemists working in production the shortest path to data for understanding synthetic routes, manufacturing yield expectations and manufacturing by-products.

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