Reaxys®

Where curiosity and scientific rigor lead to greener chemistry

Reaxys® is the foundation and gateway of discovery for a lab reimagining chemistry in Argentina

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Around the world, research groups explore avenues to revamp industrial chemistry into a productive and environmentally conscious enterprise. One group in La Plata, Argentina, reaches deep into the properties and reactions data of Reaxys to redesign manufacturing processes. The group leader, Dr. Gustavo Pablo Romanelli, describes how they uncover novel solvents, reagents, catalysts and energy sources for a greener future.

Dr. Gustavo Pablo Romanelli, GISOE Group Leader

Learn about his work on Scopus,
scopus.com/authid/detail.uri?authorId=7005511248

As the second largest country of South America, Argentina is a significant contributor to the chemical and petrochemical production of the continent. The industry accounts for approximately 9% of the nation's gross domestic product[1] with exports totaling 1.68 billion Euros in 2020.[2] Argentina is also a country rich in natural resources and unique ecosystems that is actively pursuing sustainable change in manufacturing.[3]

Government, private sector and academia all play a role in this effort. Among them, the Eco-efficient Organic Synthesis Group at CINDECA (Center for Research and Development in Applied Sciences "Dr. Jorge J. Ronco," affiliated with Universidad Nacional de La Plata (UNLP) and CONICET — National Scientific and Technical Research Council) is an intellectual powerhouse revamping the production of high-value chemical products according to the principles of green chemistry. The group is led by Dr. Gustavo Pablo Romanelli, who is also a professor of organic chemistry in the Faculty of Agricultural and Forestry Sciences at UNLP. Dr. Romanelli's work spans multiple sectors. "Our work is relevant in generating compounds of interest in the pharmaceutical, paint, fragrances and food industries," he shares. Constant in his work, however, is the goal to create more environmentally friendly processes that generate less waste and valorize compounds found in biomass. To that end, the group taps into historical and new chemistry knowledge using Reaxys.

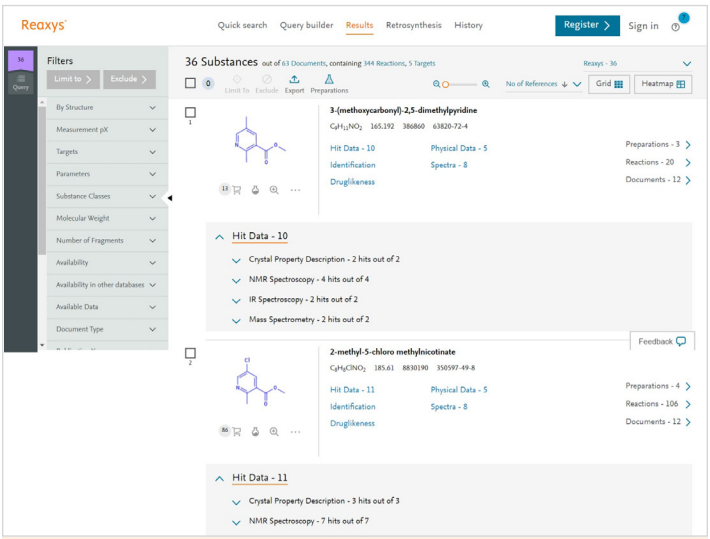
An extensive toolbox for cleaner chemistry

Dr. Romanelli leverages every strategy at his disposal to redesign existing chemical manufacturing processes. Being able to visualize existing routes in Reaxys helps him to quickly evaluate ideas towards that redesign. "There is so much we can do!" he says. "We replace toxic reaction solvents with environmentally friendlier ones that can be derived from biomass, or we remove the solvents altogether. We seek less toxic reagents and better catalysts. We also drive processes with alternative energy sources, like microwave, ultrasound and mechanochemistry. Finally, we employ multicomponent processes of high atomic economy with the aim of reducing the E factor[4] — the mass ratio of waste to product."

Noteworthy among his group's research projects is the development of numerous novel materials that act as catalysts in organic transformations. "One of the fundamental pillars in our redesign of processes is the use of solid catalysts," explains Dr. Romanelli. "They allow us to model reaction conditions as well as maximize yields and selectivity of the different transformations. Plus, they are easily recovered and reused."

Access to the global landscape of chemical synthesis

At a fundamental level, Dr. Romanelli and his students count on Reaxys to accelerate their research by simplifying the search for specific information. Publishing research on synthesized compounds, he explains, requires an extensive search of the literature to determine if a compound has already been described. "Reaxys allows you to verify that. If the compound is undoubtedly new, a full characterization must be made. If it is known, a more targeted characterization can be compared to existing data that are also easily found in Reaxys, like physical and spectroscopic properties including UV, IR, ^{1}H-NMR and ^{13}C-NMR."



Number of physical and spectra data identified from documents in Reaxys, including number of reactions and targets.

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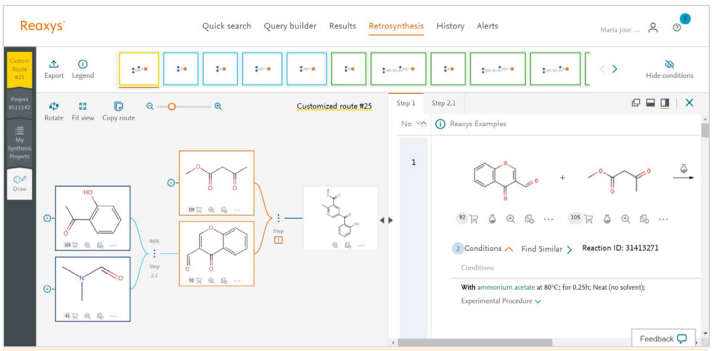
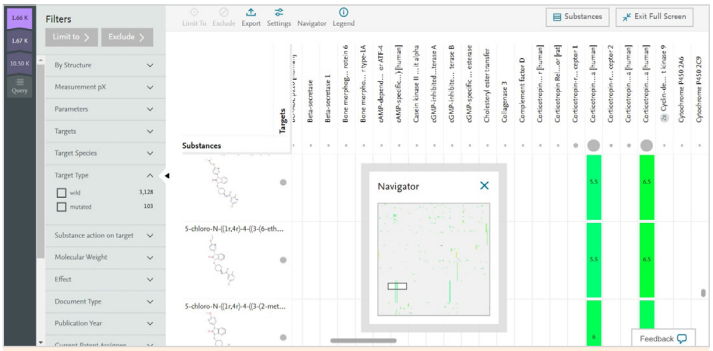
Dr. Romanelli also uses Reaxys to gain insights into existing reactions and potential synthetic routes. “Many times, when synthesizing a compound, we have open questions about routes to pursue. With Reaxys, we can quickly and efficiently find answers to questions about a route and any alternatives. This saves a lot of time compared to searching other databases.” He adds: “Also very helpful is the single-click access to the primary bibliography, plus information on sourcing and cost of reagents to perform a synthesis.”



A custom route using the Reaxys Retrosynthesis module.

Anticipating room for innovation

The information that the group garners from Reaxys also reveals answers that advance innovations. Dr. Romanelli highlights one example: “You can visualize products from reaction sequences that many times are unforeseen. Once, in preparing dihydropyridines using formylchromones as a starting material, a simple search in Reaxys delivered the main reaction product, and it was not what I expected.” The work resulted in a clean alternative synthetic method that yields 60–99% functionalized pyridines.[5]



Normalized bioactivity data visualization in Reaxys.

In addition to pyridines, Dr. Romanelli and his lab work with flavones, coumarins, pyrimidines and quinoxalines, all of which are used as or in the production of pharmaceuticals. Thus, the group also employs bioactivity data in Reaxys to conduct theoretical quantitative structure-activity relationship (QSAR) studies. “With Reaxys,” Dr. Romanelli describes, “it’s fast and efficient to achieve the large amount of correlated data that are needed.” To gather and evaluate data on compounds, Dr. Romanelli uses the chemical structure, sub-structure and related structure search options of Reaxys. “With a simple and quick molecular drawing, you can know with great precision whether a compound is described and find a range of relevant property data.”

Training information-savvy green chemists

Dr. Romanelli has been training master’s and doctoral students for over 20 years. Reaxys is an integral component of the skills and expertise that he wants students to acquire. “Efficiency of research and the ability to recognize novel areas of investigation that build on what is known are two essential learnings for postgraduate students. Only so can they move fluidly within and contribute to the chemistry research community at large. Reaxys is, in my opinion, the most complete database that allows a researcher to access the vast corpus of chemistry knowledge quickly and accurately. My students learn to answer questions with Reaxys — from how a compound is synthesized to which reagents are missing in the lab to perform a synthesis and what are the characteristics of our target compounds. In a few words, the great advantage of using Reaxys is being able to make decisions.”

Inspired to do things better

One of the core objectives of CINDECA is to provide solutions to regional and national challenges, supporting the sustainable development of Argentina and fostering recognition of scientific and technological contributions. Researchers and students at CINDECA work steeped in a tradition of scientific inquisitiveness that is seen as an important catalyst of Argentina’s future. The zeal to uncover better ways of doing things — the motivation behind CINDECA and inspiration for the Eco-efficient Organic Synthesis Group — reaches even Dr. Romanelli’s use of Reaxys. “Day in and day out, I continue to discover new functionalities in Reaxys that facilitate the efficiency of my work, and I can count on Reaxys to keep pace with my science.”

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August 2022