'Digital chemistry' breakthrough turns words into molecules

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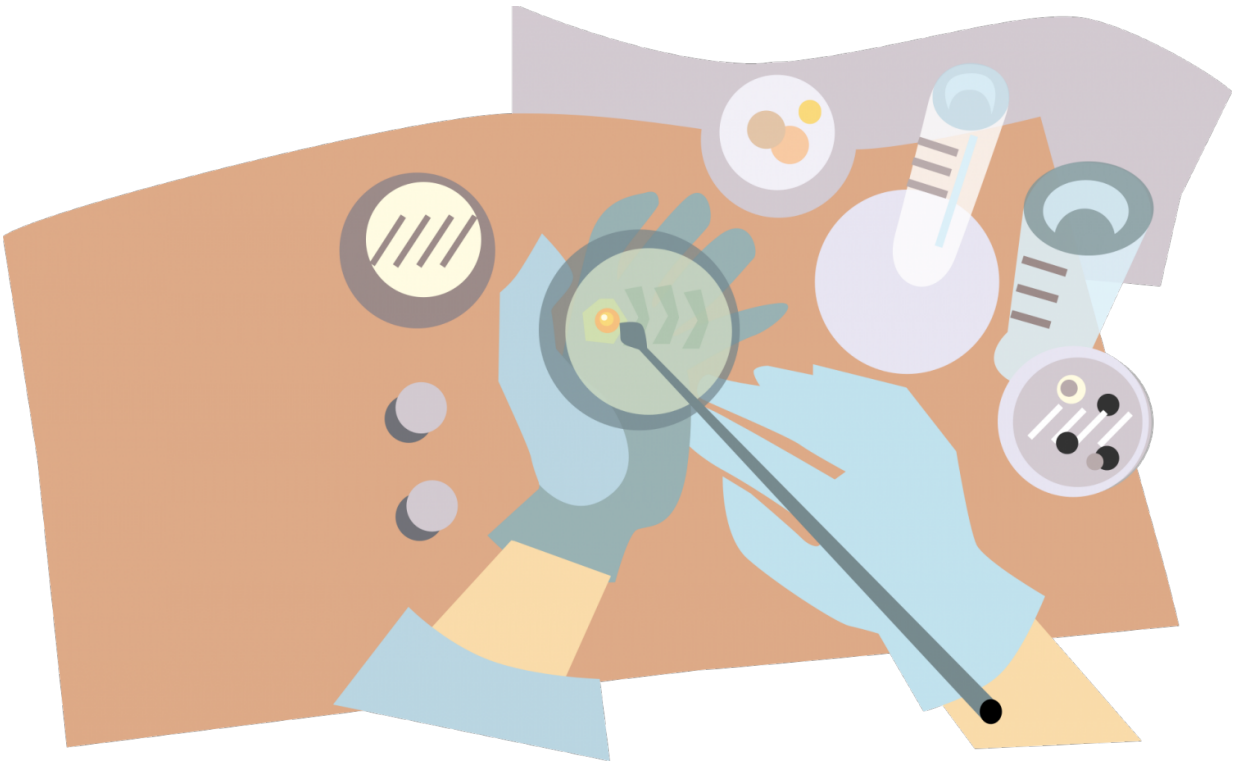

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A new system capable of automatically turning words into molecules on demand will open up the digitisation of chemistry, scientists say.

Researchers from the University of Glasgow's School of Chemistry, who

developed the system, claim it will lead to the creation of a "Spotify for chemistry"—a vast online repository of downloadable recipes for important molecules including drugs.

The creation of such a system could help developing countries more easily access medications, enable more efficient international scientific collaboration, and even support the human exploration of space.

The Glasgow team, led by Professor Lee Cronin, have laid the groundwork for digital chemistry with the development of what they call a "chemical processing unit"—an affordable desktop-sized robot chemist which is capable of doing the repetitive and time-consuming work of creating chemicals. Other robot chemists, built with different operating systems, have also been developed elsewhere.

Up until now, those robot chemists have required a massive amount of programming from their human counterparts, with detailed instructions. The problem is there is currently no standard programming language for chemistry, meaning that programs made for one robot do not work on any other type.

In a new paper published in the journal *Science*, the Glasgow researchers describe a universal approach to digitizing chemistry, including a programming system which could remove the vast majority of the effort required to program the robots.

They have found a way to create new sets of instructions for robot chemists by harnessing the power of natural language processing. They developed a computer program called SynthReader to scan through scientific papers and recognize sections which outline procedures for organic and inorganic chemical synthesis. Synthreader automatically breaks those procedures down to simple instructions and stores them in a format the team call Chemical Description Language, or XDL, which is

a new open source language for describing chemical and material synthesis.

Those XDL files are chemical instructions which can in principle be read any chemical robot in. The team built an easy-to-use interface called ChemIDE to integrate with any robotic chemist system and allow the XDL instructions to be turned into chemicals. The only human input required is ensuring that the equipment the robot needs to make the molecules is set up correctly.

The paper describes how the team used their system to scan scientific papers and produce 12 different molecules using their chemical processing unit, including the analgesic lidocaine, the Dess-Martin periodinane oxidation reagent, and the fluorinating agent AlkylFluor.

Professor Lee Cronin, Regius Professor of Chemistry at the University of Glasgow, said: "What we've managed to do with the development of our 'Chemical Spotify' is something similar to ripping a compact disc into an MP3. We take information stored in a physical format, in this case a scientific paper, and pull out all the data we need to create a digital file which can be played on any system, in this case any robot chemist, including our robotic system which is an order of magnitude lower cost than any other similar robot. We're hoping that the system we've built will massively expand the capabilities of robot chemists and allow the creation of a huge database of molecules drawn from hundreds of years' worth of scientific papers. Our system, which we're calling Chemify, can read and run XDL files which have been shared among users. Putting that kind of knowledge directly in the hands of people with access to robot chemists could help doctors make drugs on demand in the future. It could even mean that future manned missions to Mars could take raw chemical materials with them and make whatever they need right there on the red planet."

More information: A universal system for digitization and automatic execution of the chemical synthesis literature. *Science*. DOI: 10.1126/science.abc2986

Chemify: www.chemify.org/

Provided by University of Glasgow