

Potential new drugs: 970 million and still counting

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There are more than 970 million chemicals suitable for study as new drugs, according to a new study. Credit: Wikimedia Commons

Like astronomers counting stars in the familiar universe of outer space, chemists in Switzerland are reporting the latest results of a survey of chemical space -- the so-called chemical universe where tomorrow's miracle drugs may reside. The scientists conclude, based on this phase of the ongoing count, that there are 970 million chemicals suitable for study as new drugs.

Scheduled for the July 1 issue of the [Journal of the American Chemical Society](#), the study represents the largest publicly available database of

virtual molecules ever reported, the researchers say.

Jean-Louis Reymond and Lorenz Blum point out that the rules of chemical bonding allow simple elements such as carbon, hydrogen, oxygen, nitrogen and fluorine to potentially form millions of different molecules. This so-called “chemical universe” or “chemical space” has an enormous potential for [drug](#) discovery, particularly for identifying so-called “small molecules” -- made of 10 to 50 atoms. Most of today’s medicines consist of these small molecules. Until now, however, scientists had not attempted a comprehensive analysis of the molecules that populate chemical space.

In the report, Reymond and Blum describe development of a new searchable database, GDB-13, that scientists can use in the quest for new drugs. It consists of all molecules containing up to 13 atoms of carbon, nitrogen, oxygen, sulfur, and chlorine under rules that define chemical stability and synthetic feasibility. The researchers identified more than 970 million possible structures, the vast majority of which have never been produced in the lab. Some of these molecules could lead to the design and production of new drugs for fighting disease, they say.

More information: *Journal of the American Chemical Society*, Journal Article: “970 Million Druglike Small [Molecules](#) for Virtual Screening in the Chemical Universe Database GDB-13”

Source: American Chemical Society ([news](#) : [web](#))

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