

50 Million Compounds Counting

Paul Livingstone, Senior Editor, R&D Magazine

As of Monday, Sept. 7, 2009, the Chemical Abstracts Service hit a milestone of impressive scale: more than 50 million organic and inorganic compounds are now characterized and catalogued within its database.

It's an impressive number, but not as impressive as the manner in which it was achieved. For more than 100 years—and most diligently in the last 50—CAS has been examining the new particles, small molecules and nanomaterials created through scientific discovery and development. The accelerating quality and quantity of liquid and gas chromatography, mass spectrometry, and x-ray analysis has pushed the patent filings on new compounds into an impressively high gear. CAS has managed to keep up.

Every day—even Labor Day—more than 100,000 compounds are examined—with the help of a distributed computing network—by the 300-400 chemists who work at the Columbus, Ohio, organization to determine whether or not the chemical is actually new. Some 30,000 to 40,000 of them are, which illustrates the pace at which new compounds are being discovered. In the first 33 years since CAS established a comparative archive 10 million compounds were registered, a milestone reached in 1990. Now, just nine months after recording the 40 millionth compound, another 10 million have been recorded.

Cataloging chemicals is not easy work. It's one thing to look at the chemicals as standalone archives, like the entry for “perspicacious” in the dictionary, or the description for “Botswana” in the Encyclopedia Britannica (remember them?). But like these complex objects, molecules also have multiple characteristics that are entwined—bonds, pathways, and more—and must be considered when determining whether a substance is truly unique and whether it's of any use. So, a complex database that can quickly cross-examine each related small molecule is crucial.

Now, the question remains whether this breakneck pace of discovery will continue. According to Dr. Matthew Toussant, a chemist who has been with CAS for many years, the process, contributed to as it is by new methods and new science-based economies in India and China, will likely pick up speed for at least a couple of decades to come. CAS is prepared for the rush—the burden will be on science to find great new uses for these new chemicals.

50 Million Compounds Counting

Published on Chem.Info (<http://www.chem.info>)

Source URL (retrieved on 12/27/2014 - 9:03pm):

<http://www.chem.info/blogs/2009/09/50-million-compounds-counting>