

# The CompTox Chemistry Dashboard: Helping researchers ID unknown contaminants

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## Video Abstract

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## Abstract

For researchers, identifying sources of environmental contamination can be like trying to find a needle in a haystack. And that's if they're lucky. Because in some cases, they may not even know what to look for. In this line of work, known as non-targeted analysis, high-powered detection technology is critical to generating chemical fingerprints for unknown compounds. Just as important, however, is an expansive database that matches those fingerprints to the correct compounds. But bigger isn't necessarily better. Researchers from the United States Environmental Protection Agency have shown that a promising new resource called the CompTox Chemistry Dashboard can actually outperform larger, well-established chemical databases, pointing to streamlined approaches to ID-ing potentially harmful contaminants. The CompTox dashboard uses a ranking approach similar to that of the popular database ChemSpider. Both order search results according to how frequently a target compound occurs in different data sources, including scientific articles and patents. The difference lies in how those data sources are managed. The Dashboard's highly curated database is limited to chemicals relevant to environmental health science, whereas ChemSpider caters to all walks of chemistry. That contrast is reflected in the number of chemicals in each database: 720,000 versus over 50 million. As a result, the researchers saw that although the CompTox dashboard generated fewer results for a given compound, the target candidate consistently ranked closer to the top than in ChemSpider. Fewer entries, of course, could mean that some compounds won't be captured by the dashboard. But it could also mean fewer dead-ends to muddle through in any given search. Because the key is to quickly but accurately identify potentially harmful compounds, future work will be dedicated to growing the database with high-quality data sources and to refining the built-in search tool. Tapping into results generated by popular internet search engines, for example, could be one way to improve accuracy. But already the approach in the Dashboard appears promising. Built by environmental scientists for environmental scientists, the CompTox Dashboard could provide much needed guidance in non-targeted analysis, helping researchers and decision-makers assess the risks posed by unknown contaminants.