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CHEMISTRY

Comparing the EPA CompTox Dashboard with ChemSpider for MS-based Structure Identification

ANTONY WILLIAMS

CORRESPONDENCE:
tony27587@gmail.com

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It's almost ten years, this April, since ChemSpider was released to the public at the 233rd ACS meeting in Chicago. For two years, prior to being acquired by RSC in May 2009, we worked very closely with a number of mass spectrometry vendors including Waters (Micromass), Thermo and Agilent. I always considered that the work that we did with ChemSpider could be highly valued by the mass spectrometry community. This was especially true after we published the work for the identification of known unknowns with James Little (http://link.springer.com/article/10.1007/s13361-011-0265-y) Certainly ChemSpider has become highly recognized, and used, by an increasing number of mass spectrometry vendors (through the ChemSpider Web Services).

A few months ago Andrew McEachran joined our team as a postdoc. Combining my experience with bringing ChemSpider to bear for the purpose of structure identification, his mass spectrometry skills and experience, and our tremendous development team to the development of the CompTox Chemistry Dashboard, we were able to make some further advances in the "identification known unknowns". Our efforts were recently reported in this publication "Identifying known unknowns using the US EPA's CompTox Chemistry Dashboard" (http://link.springer.com/article/10.1007%2Fs00216-016-0139-z). Readers are pointed to the summary tables in the article (results) demonstrating the improved performance of the CompTox Chemistry Dashboard based on high quality data sources and new approaches to rank ordering results based on formula and mass searching.

We recently rolled out new functionality and "MS-Ready structure batch-based searching" to offer even greater support for MS-structure identification . We will report on further extensions to this work at the Spring ACS Meeting.

The AltMetrics for the Article are shown below