[e0007]

Success with ChemFinder WebServer and ChemDraw Plugin

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Dr. Rob van der Meer is head of the chemical and biological laboratory of the Water Authority Board in the province of Friesland in the Netherlands. He uses the ChemDraw Plugin in conjunction with the ChemFinder WebServer to identify compounds found in waste and surface water, and then post them on a company-wide Intranet.

It all started about a year ago. At that time, the laboratory I headed had analyzed over one thousand samples of waste water, water from our own water treatment plants, and surface water, using the newly acquired GC/MS instruments. Over a span of two years, we had encountered more than two hundred different compounds for which we did not know more than a chemical name and a structure. Most of our colleagues did not know what to do with only a chemical name and structure since the chemical's use, origin, and potential danger to the aquatic ecosystem remained unknown. There was even the possibility that the compound we where looking at were metabolites! I was then asked to shed light on the chemicals found in these water samples.

Looking for Information

Normally, when we encounter a chemical that may be environmentally interesting, we go to the library and try to find the chemical name that the library of our GC/MS systems came up with in the chemical abstracts. That is a very laborious task because the name given by the GC/MS system is most often a synonym. With over two hundred different compounds, that task would take me over a year! Because I was responsible for finding this information, I knew there had to be a better way--if there wasn't, I was out of business. So, at that time, I decided to give the Internet a try.

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Trying the Internet

On the Internet, I was accustomed to search engines like Alta Vista or Lycos. Typing in some of the names found with our GC/MS system indeed yielded some information about the chemical in question. Unfortunately, most of the information found in this way concerned pesticides and how well these pesticides worked. For the most part, information about how these chemicals came in the environment in the first place, could not be found.

ChemFinder WebServer & ChemDraw Plugin Success

At that time I thought, "Why not look at CambridgeSoft's site?" We used ChemDraw to draw the structures of known chemicals and CambridgeSoft's site could help us pinpoint the needed information. In that way, I encountered the ChemFinder WebServer. I was truly astonished with the information that ChemFinder came up with! Not only did I find the wanted information on the chemical, but with the ChemDraw Plugin installed in Netscape Navigator, I also found the structure, as well as links to information about the biochemical pathways involved, toxicological data, bioaccumulation and biomagnification data, metabolites, the no-observed-adverse-effect level (NOAEL), commercial information, and much more! With the ChemDraw Plugin I didn't even need to draw the structures myself, I could easily copy them from the Internet.

Using the ChemFinder Web-Server, we were able to find all the so-needed information on the hundreds of different compounds our laboratory had found. Then, using ChemDraw along with MS Word, we were able to present the information on our company-wide intranet so that all of my colleagues could easily retrieve the information that they needed to do their job.

Now, whenever we find a chemical of unknown origin, my colleagues immediately ask me to find information about the compound, and present it using our intranet. I am back in business again!

Footnote: This article was first published in the CS Catalyst. Check it out at: www.camsoft.com

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Comments

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