

Oral presentation

An overview of large chemical structure databases

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from 3rd German Conference on Chemoinformatics
Goslar, Germany. 11-13 November 2007

Published: 26 March 2008

Chemistry Central Journal 2008, 2(Suppl 1):S9 doi:10.1186/1752-153X-2-S1-S9

This abstract is available from: <http://www.journal.chemistrycentral.com/content/2/S1/S9>

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This presentation covers a number of large (arbitrarily defined as greater than 1 million structures) chemical structure databases currently available, or soon to be available, on the Internet. Just a few years ago there were only two large, but rather different databases of organic chemicals available - Beilstein and Chemical Abstracts. For the most part, the former contained data while the latter contained abstracts. Within the past 1-2 years the situation has dramatically changed with well over a dozen large structure databases of all sorts becoming available, some commercial and some no-fee. One example is *Chemisches Zentralblatt*, the German chemical abstracting service from 1830-1969 is the oldest database in terms of content, but is one of the newest as it is just being digitized.

In this presentation the emphasis will be on the content, or lack of content, of these databases including the chemical structures and related/linked information. The one central theme for most all these projects and databases is that they are aimed at scientists in the pharmaceutical/drug/biotechnology communities.