Issue Brief: PubChem and the American Chemical Society
By Prue Adler

Background:
The ACS has asked that the National Institutes of Health (NIH) terminate, or significantly alter, PubChem, a publicly available database that includes information about the biological activities of chemical compounds. Information included in PubChem is available from disparate public sources. PubChem is considered the "informatics backbone" of the NIH Molecular Libraries Initiative http://nihroadmap.nih.gov/molecularlibraries, an effort launched by NIH last fall that focuses on helping scientists use small molecule chemical compounds in their research. The Molecular Libraries Initiative is a part of NIH's Roadmap Initiative http://nihroadmap.nih.gov/index.asp, which seeks to accelerate the development of new research and medical treatments. PubChem is but one of several integrated databases managed by NLM that permit researchers to effectively mine relevant literature and data.

Two users of PubChem, Peter Murray-Rust, Reader in Molecular Informatics, University of Cambridge, UK Henry Rzepa, Professor of Chemistry, Imperial College, UK provide extremely helpful information regarding PubChem's value to science.

"In our laboratories we are using PubChem for systematic research and are enhancing its value by publishing the results to the world. We have systematically computed the properties of over 200,000 molecules and published our peer-reviewed results freely. These properties are typical of those used in computer-aided drug discovery or the prediction of the safety of compounds. We have automated the process so that eventually all molecules in PubChem will have this information. Using InChI we have recently created a web site so that anyone can use search engines (e.g. Google(TM) or MSN(TM)) on this database without prior chemical knowledge. This is typical of the way in which information-driven science builds on, and enhances, existing knowledge.

Finally we re-emphasize the global nature of scientific information. By sharing resources freely we detect and correct errors, and encourage innovation in the way we access information. Many developments in bioscience and healthcare come not from the wet laboratory, but through computational knowledge-driven methods. PubChem represents the start of such a process in chemical bioscience. No one site holds the totally of the world's knowledge and through the Web we create distributed resources from which all of us benefit."

ACS is concerned that PubChem, as a free publicly available database, will cause economic harm to the society's fee-based Chemical Abstracts Service (CAS). ACS has asked that NIH either shut down PubChem or eliminate any overlap with CAS.

ACS is seeking to make these changes via the appropriations process.

6/8/05