

Short Talking Points on PubChem/CAS Issue

PubChem Background

- PubChem is a free, publicly available database created by NIH in 2004 to provide information about small molecules for use as research tools and as potential starting points that may lead to the development of new medications. The database connects chemical information with biomedical research and clinical information in a connect-the-dots fashion, organizing facts in numerous public databases into a unified whole.
- PubChem is a critical part of the Molecular Libraries initiative of the NIH Roadmap for Medical Research. It will combine new data generated by this initiative with data available from other public sources to create a powerful new research tool.
- PubChem is the latest member of the powerful family of integrated databases operated by the National Library of Medicine, including GenBank, PubMed, GEO, OMIM, and a host of other resources that are utilized millions of times a day by scientists all over the world. The integration of these databases makes the whole much greater than the sum of its parts.

ACS/CAS Background

- NIH met with ACS officials to seek a solution that would resolve the society's concern. Since the initial meeting, there have been multiple communications between NIH and ACS leadership.
- ACS has effectively broken off discussions, leaving the issues unresolved.
- Opposition to PubChem is from the ACS leadership—it is not clear if ACS members are aware of the issue and if they would agree with the ACS leadership's position.
- NIH staff analysis shows that PubChem and CAS overlap relatively little in terms of content. PubChem and CAS differ widely in scope and resources.
 - **Budget:** CAS budget is reported to be \$260 million; PubChem budget is \$3 million.
 - **Staffing:** CAS staff is reported to be 1,300; PubChem staff is 13.
 - **Chemicals:** CAS has information on 25 million unique chemicals; PubChem has information on 850,000 unique chemicals (though this number is expected to grow).

- **Purpose:** CAS provides chemical, commercial and patent information to chemists; PubChem integrates medical information for medical researchers.
 - **PubChem and CAS content are complementary resources tailored to the needs of different segments of the scientific community.**
- PubChem management is willing to link to the CAS database, essentially bringing CAS a new, untapped market of customers. Medical researchers infrequently use CAS at this time.

NIH Position

- PubChem is a critical new tool that will speed the development of new treatments for America's most important health problems.
- PubChem brings information about the biological activities of chemical substances to biomedical researchers on a large scale.
- A bedrock NIH principle is that medical research information developed with public funds must be made freely and publicly available for the good of advancing medical research to cure disease.
- PubChem and CAS are largely complementary, not duplicative.
- NIH is willing to continue discussions with ACS/CAS to benefit the scientific community and biomedical research.