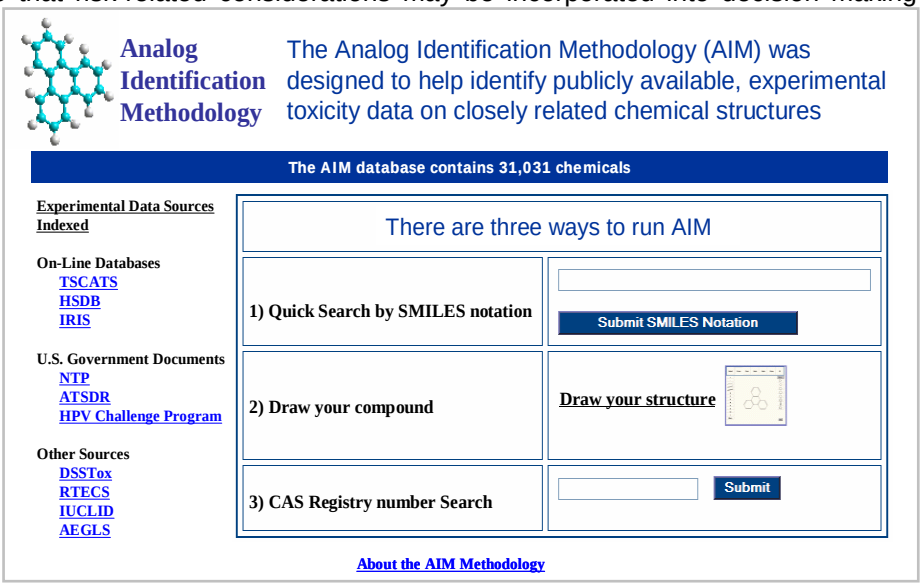
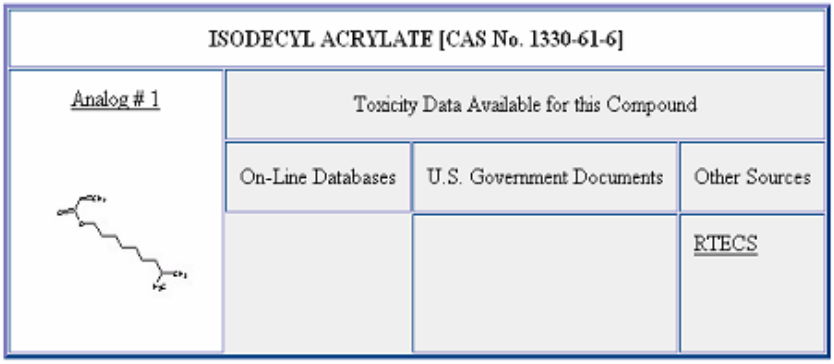
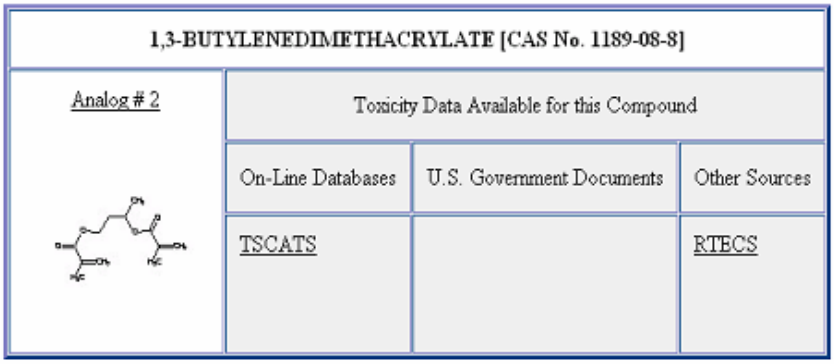
~ The Analog Identification Methodology ~

EPA's Sustainable Futures Initiative http://www.epa.gov/oppt/sf encourages companies to screen chemicals at R&D for potential hazards and risks so that risk-related considerations may be incorporated into decision making processes. Through Sustainable Futures, EPA hopes to encourage the design of safer chemicals and the use of safer chemical alternatives by encouraging the integration of hazard and risk screening into the earliest stages of chemical development. Under Sustainable Futures chemicals are screened for aquatic hazard and human health hazards including cancer and non-cancer health effects such as neurotoxicity, reproductive and developmental toxicity, systemic effects, etc. EPA currently has no computerized methods to predict non-cancer health effects. EPA relies on Structure Activity Relationships (SARs) and nearest analog analysis to predict these non-cancer health effects. Data on a close chemical analog can be used to estimate potential human health hazard(s) of a chemical lacking test data.



Analog Identification Methodology Identifying an appropriate analog can be a very challenging task. To help with this process, EPA developed the Analog Identification Methodology (AIM). AIM is a web-based, computerized tool that identifies analogs based on structure using a chemical fragment-based approach, and points the user to publicly available databases or other sources of information where experimental data on the analog can be obtained. The opening screen of AIM, shown above, indicates that AIM currently contains more than 30,000 potential analogs with publicly available toxicity data. Experimental data sources indexed include: TSCATS, HSDB, IRIS, U.S. Government Documents, NTP, ATSDR, HPV Challenge Program, DSSTox, RTECS, IUCLID, and AEGLS. Sample results, shown on the left, show the first two analogs found after searching for analogs to CAS 1330-61-6. The first analog found is the chemical being searched. This example shows how AIM can be used to identify and locate data on a specific chemical (in this case CAS 1330-61-6), and how it can identify close analogs having data for a chemical that may lack data.





EPA developed a preliminary prototype of AIM which was the subject of a rigorous beta test. The beta test has concluded and comments and suggestions received during the beta test will be used to help in the development of the next version of AIM. EPA plans to make AIM publicly available on the Internet for use at no cost in the future. For any questions regarding the AIM tool, please contact:

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