U.S. Environmental Protection Agency

Distributed Structure-Searchable Toxicity (DSSTox) Public Database Network

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HPVCSI: EPA High Production Volume (HPV) Challenge Program
Structure-Index File

*** New DSSTox** Structure-Index File *10Apr2006*

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Description: EPA's High Production Volume Challenge Program is supervising the collection and public dissemination of toxicity data on several thousand chemicals. These data are being incorporated into the HPV Information System, a relational, searchable data warehouse soon to be made publicly available on the EPA HPV Information System website (not yet posted). The DSSTox HPVCSI Structure-Index File consolidates three HPV Chemical Lists associated with multiple public notices of the HPV voluntary chemical adoption program. HPVCSI contains the full complement of DSSTox Standard Chemical Fields as well as URL links to the three main chemical listings posted on the EPA HPV Challenge Program Source Website. Note that not all chemicals in these listings have undergone voluntary testing or will have corresponding data in the HPV Information System. For instance, those chemicals identified on the European HPV list or as close analogs of another HPV chemical for which test data will be available may not be included. As further information becomes available from the EPA HPV Information System, the DSSTox HPVCSI SDF file can be specifically associated with toxicity data content provided in the on-line HPV Information System, and can be used to create a structure-searching capability on the EPA HPV Information System website.

Maintenance of this DSSTox HPVCSI file will be coordinated with the EPA HPV Information System program to provide corresponding chemical structure content. Inclusion of the DSSTox HPVCSI structure-index content in the DSSTox Master Structure-Index File will expand the reach of users to this HPV Information System data content. In addition, deposition of the DSSTox HPVCSI SDF into PubChem under the "EPA DSSTox" [sourcename] will enable broad structure and analog-searching capabilities both across the entire DSSTox data inventory, and across the very large bioassay data inventory maintained within PubChem. Future enhancements of HPVCSI could include explicit incorporation of summary data values extracted from the on-line HPV Information System into DSSTox SDF data fields for enhanced relational searching capabilities. See EPA Activities for a more complete listing of DSSTox EPA program activities & collaborations.

Source Website: http://www.epa.gov/chemrtk/

HPVCSI SDF Fields (18 total)

DSSTox Standard Chemical Fields (17)

Website_URL (3 possible URL entries):

http://www.epa.gov/chemrtk/hpv_1990.htm
http://www.epa.gov/chemrtk/hpv_1994.htm
http://www.epa.gov/chemrtk/hpvadds.htm

HPVCSI SDF Content Summary - *10 April 2006*

HPVCSI SDF Content	Totals_v1a
# Records	3548
DSSTox Standard Chemical Fields	17
HPVCSI Source Fields	1
Total # Fields	18
Chemical Content	**Counts_v1a**
STRUCTURE_ChemicalType:	
defined organic	2209
inorganic	73
organometallic	181
no structure	1085
STRUCTURE_TestedForm_DefinedOrganic:	
parent	1911
complex	63
salt	237
salt complex	2
TestSubstance_Description:*	
single chemical compound	2008
defined mixture or formulation	422
undefined mixture	1087
macromolecule	28
unspecified or multiple forms	3

* ***Note:*** HPVCSI contains a relatively large percentage of undefined mixtures compared to other DSSTox Structure Data Files, for which no chemical structure is provided (i.e., 1085 records). Where possible, we provide some description of the substance in the **ChemicalNote** field. In addition, HPVCSI contains a relatively large number of "defined mixture or formulation" and "macromolecule" substances for which a single representative **STRUCTURE** is provided based on expert review. This structure information is provided not as definitive characterization, but to allow the HPVCSI record to be "located" by a structure analog search.

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SDF Version History: An initial SDF for an earlier version of the HPV chemical lists was kindly provided by Jay Tunkel (Syracuse Research Corp) at the start of HPVCSI construction. Each record was subsequently independently reviewed, verified within the existing DSSTox Master

File or by multiple public sources (see Chemical Information Quality Review Procedures), corrected and further annotated within the DSSTox HPVCSI SDF. HPVCSI_v1a includes full structure annotation of all published EPA HPV chemical lists on the HPV Source Website, regardless of which of these chemicals will have data reported.

File Download and View Notes: Provided below, in addition to the main SDF file (see More on SDF), are: a downloadable MS Excel (MS Office 2003) file containing the full SDF data contents in table form, minus the chemical structure field [file created with CambridgeSoft ChemFinder plug-in to MS Excel 2003]; and a PDF tiling view of all chemical structures contained in the SDF, annotated with **TestSubstance_CASRN** and truncated **TestSubstance_ChemicalName** field entries for the tested form of the chemical [file created with ACD ChemFolder, ver. 8.0, ACD Labs].

The files contained in the following download table constitute the main DSSTox products. DSSTox Structure Data Files *and* DSSTox File Names *adhere to strict formatting standards and conventions. For additional information, see* More on DSSTox Standard Chemical Fields, Known Problems & Fixes, Chemical Information Quality Review Procedures, *and* How to Use DSSTox Files.

> You will need Adobe Acrobat Reader, available as a free download, to view the Adobe PDF files on this page. See EPA's PDF page to learn more about PDF, and for a link to the free Acrobat Reader.

> Zip files may be decompressed using a utility such as WinZip. EXIT Disclaimer

File Types	Description	File Size	Format
Data Files: *HPVCSI* **SDF Structure Data File**	HPVCSI_v1a_3548_10Apr2006.sdf		SDF
• Data Table (no structures)	HPVCSI_v1a_3548_10Apr2006_nostructures.xls	*.zip 3.0MB	XLS
• Structures Table	HPVCSI_v1a_3548_10Apr2006_structures.pdf (PDF, 71 pp., 6.8MB)		PDF

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DSSTox Citation:
M.A. Wolf, J. Burch, and A.M. Richard (2006) DSSTox EPA High Production Volume Challenge Program Structure-Index File: SDF File and Documentation, Launch version HPVCSI_v1a_3548_10Apr2006, www.epa.gov/nheerl/dsstox/

Disclaimer: Every effort is made to ensure that DSSTox SDF files and associated documentation are error-free, but neither the DSSTox Source collaborators nor the EPA DSSTox project team make guarantees of accuracy, nor are any of these persons to be held liable for any subsequent use of these public data. The contents of this webpage and supporting documents have been subjected to review by the EPA National Center for Computational Toxicology and approved for publication. Approval does not signify that the contents reflect the views of the Agency, nor does mention of trade names or commercial products constitute endorsement or recommendation for use.

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