

**U.S. Environmental Protection Agency****Distributed Structure-Searchable Toxicity
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SDF Download Page:**NTPHTS: National Toxicology Program High Throughput
Screening Project
Structure-Index File****** New DSSTox [Structure-Index File](#) 10Apr2006****Quick & Easy File Downloads:** [FTP Download Instructions](#)

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Description: The [National Toxicology Program \(NTP\)](#) has initiated a [High Throughput Screening \(HTS\) Project](#) [EXIT Disclaimer](#) to explore new approaches to evaluating chemicals across a spectrum of high-throughput biological assays. Assays are being selected based on their potential be informative of animal bioassay results and relevant to human health risk assessments. As an initial phase of this project, the NTP has provided a set of 1408 chemicals from NTP inventories for HTS in bioassays relevant to toxicology, to the [NIH Chemical Genomics Center \(NCGC\)](#), part of the [NIH Molecular Libraries & Imaging Roadmap \(MLR\) Initiative](#) [EXIT Disclaimer](#). Assays will be described and assay results reported in [PubChem](#) for this NTPHTS chemical data set in the same manner as for compounds from the [Molecular Libraries Small Molecule Repository](#) [EXIT Disclaimer](#). For a recent interview on this NTP HTS project, see: [Newsletter of the Society for Biomolecular Sciences - Chris Portier: HTS Takes US National Toxicology Program to Next Level](#) [EXIT Disclaimer](#).

The DSSTox project is collaborating with the NTP HTS project to provide structure-annotation and chemoinformatics support for this effort. Drawing largely from the contents of the existing [NTPBSI Structure-Index Locator File](#), with many of the 1408 NTP HTS chemicals having been used in historical NTP toxicity studies, the DSSTox NTPHTS [Structure-Index File](#) provides the full complement of [DSSTox Standard Chemical Fields](#) for the NTP HTS chemical set. Additionally, the DSSTox NTPHTS file includes the [PubChem_SID](#) (Substance Identifier) code for each chemical record listed (assigned upon depositing the NTPHTS SDF into PubChem). These [PubChem_SID](#) codes correspond directly to the relevant [PubChem](#) SID record that will contain the corresponding NTP HTS assay results deposited by the NCGC.

Maintenance of this DSSTox NTPHTS file will be coordinated with expansion of the NTP HTS program. Inclusion of the DSSTox NTPHTS structure-index content in the [DSSTox Master Structure-Index File](#) additionally allows linkages to be made to other DSSTox Structure-Data Files, including the [NTPBSI Structure-Index Locator File](#) which links to the chemical-specific content of the [NTP Bioassay On-line Database](#). Deposition of the DSSTox NTPHTS SDF into [PubChem](#)

enables broad structure and analog-searching capabilities both across the entire DSSTox data inventory, and across the very large bioassay data inventory maintained within [PubChem](#). See [Coordinating Public Efforts](#) and [Work in Progress](#) for additional information on DSSTox NTP collaborations.

Source Website: [NIEHS's National Toxicology Program, NTP High Throughput Screening Project](#) [EXIT Disclaimer](#)

Source Contact: Ray Tice, email: tice@niehs.nih.gov; Cynthia Smith, email: smith19@niehs.nih.gov

PubChem Bioassay Data:

HTS bioassay data is to be deposited in [PubChem](#) [EXIT Disclaimer](#) for the NTPHTS substance list under the depositor keywords:

"EPA DSSTox" [sourcename] "ntphts"

and will be additionally searchable by substance keywords **"ntphts"** or **"ntphts_ncgc"**.

HTS bioassays used to screen this NTPHTS set will be further described in PubChem and will be used to screen larger sets of chemicals. These larger chemical sets will be retrievable within PubChem using the appropriate Bioassay search criteria.

For example, HTS data for NTPHTS has been generated by the [NCGC](#) [EXIT Disclaimer](#) for:

Cell viability assay (AID 421):
<http://pubchem.ncbi.nlm.nih.gov/assay/assay.cgi?aid=421>

As data and bioassay information relevant to NTPHTS become available from NCGC and PubChem, more guidance on retrieving these HTS data will be provided here (also see [Searching DSSTox Files in PubChem](#)).

NTPHTS SDF Fields (19 total)

[DSSTox Standard Chemical Fields](#) (18; includes optional [ChemicalReplicateCount](#) field)

[PubChem_SID](#)

NTPHTS SDF Content Summary - 10 April 2006

NTPHTS SDF Content	Totals_v1a
# Records	1408
DSSTox Standard Chemical Fields	18
NTPHTS Source Fields	1
Total # Fields	19
Chemical Content	Counts_v1a
STRUCTURE ChemicalType :	

defined organic	1348
inorganic	27
organometallic	19
no structure	14
STRUCTURE TestedForm DefinedOrganic:	
parent	1279
complex	51
salt	19
salt complex	1
TestSubstance Description:*	
single chemical compound	1343
defined mixture or formulation	47
undefined mixture	5
macromolecule	3
unspecified or multiple forms	0

* **Note:** NTPHTS_v1a contains 55 chemical records with duplicate structures (duplicate [DSSTox_CID](#)); 1 pair of these consists of a monomer and polymer with same [STRUCTURE](#) represented, whereas 54 of these pairs are ostensibly the same Test Substances (same [TestSubstance_CASRN](#) and [TestSubstance_Description](#)), but were obtained from different lots or chemical manufacturers (different Lot and Vial numbers are maintained in internal NTP tracking identification). Because these chemical substances are provided as distinct chemical samples for HTS evaluation, they must be differentiated as separate chemical records in the DSSTox SDF, as well as by distinct [DSSTox_SID](#) and [PubChem_SID](#) assignments. The HTS data for these duplicates will be presented as separate PubChem SID listings, but will be grouped for easy viewing and comparison by common chemical structures and PubChem CID values. For more information on accessing NTP HTS data within PubChem, see [Searching DSSTox Files in PubChem](#).

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SDF Version History: An initial list of NTP HTS chemical names and CASRN was provided to us by NTP Sources Brad Collins and Cynthia Smith. Based initially on CASRN matching, [DSSTox Standard Chemical Fields](#) were populated largely from the existing [DSSTox Master File](#) content (see also [Chemical Information Quality Review Procedures](#)), with approximately 200 substances not contained in [NTPBSI](#). Some corrections were applied to the original NTP HTS Source information (and communicated back to the NTP Source) and information on new substances not already occurring in the [DSSTox Master File](#) were entered into the Master File and NTPHTS after thorough [Chemical Information Quality Review Procedures](#).




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](#).

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Zip files may be decompressed using a utility such as [WinZip](#). [EXIT Disclaimer](#)

File Types	Description	File Size	Format
Data Files: <i>NTPHTS</i>			
SDF Structure Data File	NTPHTS_v1a_1408_10Apr2006.sdf		
• Data Table (no structures)	NTPHTS_v1a_1408_10Apr2006_nostructures.xls	*.zip 1.4MB	
• Structures Table	NTPHTS_v1a_1408_10Apr2006_structures.pdf (PDF, 29pp., 3.2MB)		
File Error Report			

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DSSTox Citation: Smith, C., B. Collins, R. Tice, M.A. Wolf, and A.M. Richard (2006) DSSTox National Toxicology Program High Throughput Screening Structure-Index File: SDF File and Documentation, Launch version NTPHTS_v1a_1408_10Apr2006, www.epa.gov/nheerl/dsstox/

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URL: http://www.epa.gov/ncct/dsstox/sdf_ntphts.html