

**U.S. Environmental Protection Agency****Distributed Structure-Searchable Toxicity  
(DSSTox) Public Database Network**[Recent Additions](#) | [Contact Us](#) | [Print Version](#) Search:  **GO**[EPA Home](#) > [Research & Development](#) > [Computational Toxicology Research](#) > [DSSTox](#) > [StructureDataFiles](#) > SDF  
Download Page: NTPBSI

[Home](#)  
[About DSSTox](#)  
[Work in Progress](#)  
[Frequent Questions](#)  
[Structure Data Files](#)  
[Central Field Definition Table](#)  
[Apps, Tools & More](#)  
[DSSTox Community](#)  
[Site Map](#)  
[Glossary of Terms](#)  
[Help](#)

**SDF Download Page:****NTPBSI: National Toxicology Program Bioassay On-line Database*****Structure-Index Locator File*****\*\* New DSSTox [Structure-Index Locator File](#) 10Apr2006****Quick & Easy File Downloads:** [FTP Download Instructions](#)

- [Description](#)
- [Source Website](#)
- [Source Contacts](#)
- [SDF Fields](#)
- [SDF Content Summary](#)
- [SDF Version History](#)
- [SDF Download Table](#) **Download**
- [DSSTox Citation](#)
- [Disclaimer](#)

**Description:** The National Toxicology Program makes available data from more than 500 two-year, two species, toxicology and carcinogenesis studies collected by the NTP and its predecessor, the National Cancer Institute's Carcinogenesis Testing Program. The NTP database also contains the results collected on approximately 300 toxicity studies from shorter duration tests and from genetic toxicity studies, which include both in vitro and in vivo tests. In addition, test data from the immunotoxicity, developmental toxicity and reproductive toxicity studies are continually being added to this database. Data from these various studies are indexed by Chemical Name and CASRN and organized into 5 Study Areas. These data are publicly viewable and accessible from the [NTP Website](#) [EXIT Disclaimer](#), hosted at the National Institute of Environmental Health Sciences (NIEHS); choose the [Study Data Search](#) [EXIT Disclaimer](#) option.

The DSSTox NTPBSI [Structure-Index Locator File](#) offers the full complement of [DSSTox Standard Chemical Fields](#) for the NTP Bioassay On-line Database, and additionally provides indicator fields for each of the 5 study areas represented in the database (a value of "1" indicates study data availability for the chemical record, whereas a value of "0" indicates no study data). Maintenance of this DSSTox NTPBSI file will be coordinated with the NTP database program. In addition, inclusion of the DSSTox NTPBSI structure-index content in the [DSSTox Master Structure-Index File](#) will expand the reach of users to this NTP Bioassay On-line database content. Deposition of the DSSTox NTPBSI 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](#). Deeper content DSSTox databases, with overlapping structure-index content to NTPBSI, are being constructed in the areas of genetox ([NTPGTZ](#)) and immunotox ([IMMTOX](#)). Collaborations with the [NTP High-Throughput Screening](#) [EXIT Disclaimer](#) program are also currently underway, involving publication of a structure-index file ([NTPHTS](#)) for a chemical data set (content largely overlapping with NTPBSI) submitted for bioassay screening at the NIH Molecular Libraries Roadmap - Chemical Genomics Center (NCGC). See [Coordinating Public Efforts](#) and [Work in Progress](#) for additional information on DSSTox NTP collaborations.

**Source Website:** [NIEHS's National Toxicology Program, http://ntp-apps.niehs.nih.gov/ntp\\_tox/index.cfm](http://ntp-apps.niehs.nih.gov/ntp_tox/index.cfm) [EXIT Disclaimer](#)

**Source Contacts:** Beth Bowden, email: [bowden1@niehs.nih.gov](mailto:bowden1@niehs.nih.gov); Ray Tice, email: [tice@niehs.nih.gov](mailto:tice@niehs.nih.gov)

## NTPBSI SDF Fields (24 total)

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

### Website URL

e.g. [\(Diethylamino\)ethanol](#) [EXIT Disclaimer](#)

[NTP\\_StudyArea\\_ImmunoTox](#)  
[NTP\\_StudyArea\\_ReproTox](#)  
[NTP\\_StudyArea\\_GeneTox](#)  
[NTP\\_StudyArea\\_CancerChronicTox](#)  
[NTP\\_StudyArea\\_DevelopTox](#)

NTP\_StudyArea field entries = 1 or 0, indicating presence or absence of data in on-line database for each of 5 NTP study areas

## NTPBSI SDF Content Summary - 10 April 2006

NTPBSI SDF Content	Totals_v1a
# Records	2415
DSSTox Standard Chemical Fields	18
NTPBSI Source Fields	6
Total # Fields	24
Chemical Content	Counts_v1a
<a href="#">STRUCTURE_ChemicalType:</a>	
defined organic	2096
inorganic	84
organometallic	78
no structure	157
<a href="#">STRUCTURE_TestForm_DefinedOrganic:</a>	
parent	2096
complex	139
salt	94
salt complex	4
<a href="#">TestSubstance_Description:</a>	
single chemical compound	2081
defined mixture or formulation	155
undefined mixture	146
macromolecule	27

unspecified or multiple forms

6

[Return to Top](#)




**SDF Version History:** An initial list of NTPBSI chemical names and CASRN was extracted from the [NTP Source Website](#) with assistance from NTP Sources, William (Skip) Eastin and Beth Bowden. Based initially on CASRN matching, [DSSTox Standard Chemical Fields](#) were populated first from the existing [DSSTox Master File](#) content, with remaining chemical information populated from a variety of commercial and public resources (see [Chemical Information Quality Review Procedures](#)) and all CASRN and chemical names reconciled. In addition, NTP Sources provided assistance with collation of chemical-specific URL addresses and provided summary listings allowing population of the Study Area Indicator fields in NTPBSI.

**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: <i>NTPBSI</i>			
<b>SDF Structure Data File</b>	<a href="#">NTPBSI_v1a_2415_10Apr2006.sdf</a>		
• Data Table (no structures)	<a href="#">NTPBSI_v1a_2415_10Apr2006_nostructures.xls</a>	*.zip 2.6MB	
• Structures Table	<a href="#">NTPBSI_v1a_2415_10Apr2006_structures.pdf</a> (PDF, 49pp., 5.7MB)		
<a href="#">File Error Report</a>			

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**DSSTox Citation:** Burch, J., W.C. Eastin, B. Bowden, M.A. Wolf, and A.M. Richard (2006) DSSTox National Toxicology Program Bioassay On-line Database Structure-Index Locator File: SDF File and Documentation, Launch version NTPBSI\_v1a\_2415\_10Apr2006, [www.epa.gov/nheerl/dsstox/](http://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

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*Return to Top*

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Last updated on Thursday, August 24th, 2006  
URL: [http://www.epa.gov/ncct/dsstox/sdf\\_ntpbsi.html](http://www.epa.gov/ncct/dsstox/sdf_ntpbsi.html)