

DSSTox Field Definition File:

Carcinogenic Potency Database Summary Tables – All Species (CPDBAS)

(last updated 20 November 2008)

Description: Information in this file is intended to document the DSSTox SDF (Structure Data Format) file created for the Carcinogenic Potency Database Summary Tables – All Species (CPDBAS), obtained from the CPDB Source website: <http://potency.berkeley.edu/>. CPDBAS_v5 contains consolidated DSSTox CPDB files for rat/mouse, hamster, dog, and non-human primates and includes additional fields, modified fields, and URL links to chemical data pages on the CPDB website (see current CPDBAS SDF Download Page and CPDBAS_LogFile for more details). For further explanation of Source-specific toxicity fields, a user is encouraged to consult the CPDB website, listed references, and documentation. Additional information is provided on the DSSTox CPDBAS SDF Download Page http://www.epa.gov/ncct/dsstox/sdf_cpdbas.html. All modifications to the original fields contained in the CPDB Summary Tables are documented in the **Comments** section of the table below.

Description of **DSSTox Standard Chemical Fields** can be found in the Central Field Definition Table located at: <http://www.epa.gov/ncct/dsstox/CentralFieldDef.html>

The first section of the Table below lists the **DSSTox Standard Toxicity Fields** employed for this database, followed by the **CPDBAS Source-Specific Fields** containing the toxicity information particular to CPDBAS. The **Field Type** indicates the type of the field, such as numeric, integer, defined text, memo, etc. All **Units** and **Descriptions** are extracted from Source reference materials unless otherwise noted. **Allowable Entries** lists allowed field entries occurring in CPDBAS, separated by slashes for exclusive entries (i.e., cannot occur with another entry) and semicolons or spaces for non-exclusive entries (i.e., can occur with other values). These are defined and explained in the **Description** section.

The **Note_CPDBAS** field (previously **ToxicityNote**) is used for several purposes in CPDBAS. This field documents any additions of new chemical record or data modifications from CPDB(RM,HA,DG,PR)_v1 to CPDBAS_v2a and subsequent versions of CPDBAS. In addition, any information specific only to the chemical information in CPDBAS (i.e., not pertaining to any other data file containing this same chemical record) that was previously provided in the **ChemicalNote** field (v3) has been moved to the **Note_CPDBAS** field. New or modified activity summary fields added to CPDBAS_v5b correspond to activities represented in PubChem and include **ActivityOutcome_CPDBAS_...**, fields for Mutagenicity, SingleCellCall, MultiCellCall, Rat, Mouse, Hamster, and Dog_Primates, and **ActivityScore_CPDBAS_...** fields [Log(1/TD50mmol) mapped onto 0-100 integer range] for Rat, Mouse, Hamster, and Dog_Primates. Since two species listed in the Source CPDB Summary Tables (Bush Baby and Tree Shrew) have data for only a single chemical record each, and the chemical record in each case is also listed in the CPDB Rat Mouse table, data for these species are provided only in the **TD50_Dog_Primates_Note** field of the corresponding chemical record.

Source Website: The complete, updated CPDB, from which the Summary Tables and CPDBAS are derived, is available in several formats at: <http://potency.berkeley.edu/>

Source Contact: Please contact Lois Swirsky Gold for questions pertaining to the content of the CPDB Summary Tables; email: cpdb@potency.berkeley.edu
Please contact [DSSTox Support](#) for questions or comments pertaining to the DSSTox CPDBAS SDF file.

Main Citations: Publications reporting use of the DSSTox SDF file for the CPDB Summary Tables are asked to list the full DSSTox file name, including date stamp, and to cite as primary reference the following citations:

Gold, L.S., T.H. Slone, B.N. Ames, N.B. Manley, G.B. Garfinkel, and L. Rohrbach (1997) Chapter 1: Carcinogenic Potency Database. In: Gold, L.S., and E. Zeiger, Eds. Handbook of Carcinogenic Potency and Genotoxicity Databases. Boca Raton, FL: CRC Press, pp. 1-605.
<http://potency.berkeley.edu/text/methods.html>

Gold, L.S., N.B. Manley, T.H. Slone, and J.M. Ward (2001) Compendium of chemical carcinogens by target organ: Results of chronic bioassays in rats, mice, hamsters, dogs and monkeys. Toxicol. Pathol. 29: 639-652. <http://potency.berkeley.edu/text/ToxicolPathol.pdf>

Gold, L. S., Manley, N. B., Slone, T. H., Rohrbach, L., and Garfinkel, G.B. Supplement to the Carcinogenic Potency Database (CPDB): Results of Animal Bioassays Published in the General Literature through 1997 and by the National Toxicology Program in 1997 and 1998. *Toxicol. Sci.* 85: 747-800 (2005). <http://potency.berkeley.edu/pdfs/ToxSciPlot.pdf>

Carcinogenicity Potency Data Base (2008) <http://potency.berkeley.edu/>

Summary Table of Chemicals in the Carcinogenic Potency Database: Results for Positivity, Potency (TD50), and Target Sites: <http://potency.berkeley.edu/chemicalsummary.html>

See also, a full listing of Data Plots (from which the CPDB Summary Table was derived) and CPDB publications at: <http://potency.berkeley.edu/listofpubs.topic.html#plots>
<http://potency.berkeley.edu/listofpubs.topic.html>

SDF Usage Notes:

Each DSSTox SDF file contains a single **STRUCTURE** field. For each chemical record, the **STRUCTURE** field entry directly corresponds to the content of the **STRUCTURE_...** fields. The **STRUCTURE_Shown** field documents the relationship between what is displayed in the **STRUCTURE** field and the actual tested chemical substance, i.e. **TestSubstance_...** fields, with the latter corresponding directly to the toxicity data field entries. Commercial chemical relational database (CRD) applications may automatically insert one or more structure identifier fields upon import or export of an SDF file (e.g., Formula, FW or Mol_ID), fields that may augment or duplicate one or more of the DSSTox Standard Chemical Fields. Users are cautioned that fields containing null values in the first record of the SDF will be reordered upon import into most applications; for this reason, the word "blank" has been inserted into null fields in Record 1 of DSSTox SDF files and can be deleted after SDF import. Users are additionally cautioned that some fields (**STRUCTURE_SMILES** and **STRUCTURE_InChI**, in particular) may exceed the 200 character limit specified in the MDL CTFiles SDF standard (see <http://www.epa.gov/ncct/dsstox/MoreonSDF.html>), and that some CRD applications may insert a line break or truncate these fields upon SDF import or export. Finally, CRD application-specific molecular header information in the SDF file is deleted in the final DSSTox SDF files; users running CRD applications requiring a unique molecule header upon import of the SDF can specify either **DSSTox_RID** or the **DSSTox_FileID** be used. Upon SDF import, **DSSTox_CID** can be used to identify and manage chemical structure duplicates and **DSSTox_Generic_SID** can be used to identify common Test Substances across and within DSSTox files (similar to CASRN-substance, but available for all DSSTox substances and further distinguishes among different purity/grade substances).

As an MS Word document, the following table is best viewed onscreen using either Normal or Web Layout View in Landscape page orientation.

Field Name	Field Type	Units	Allowable Entries	Description	Comments
DSSTox Standard Toxicity Fields					
Study Type <i>(no spaces)</i>	defined text		Carcinogenicity	Field is used to label all records in the database, generally with the same entry, and is designed to facilitate record identification for cross-database structure searching. Field entry refers to the main type of toxicity study for which data is represented in the database.	Field names and content are being coordinated with the public ToxML standardization effort.

Endpoint	defined text		TD50, Tumor Target Sites	Field is used to label all records in the database, generally with the same entry, and is designed to facilitate record identification for cross-database structure searching. Field entry refers to the type of toxicity measure represented within the database.	Field names and content are being coordinated with the public ToxML standardization effort.
Species	defined text		rat, mouse, hamster, dog, rhesus, cynomolgus, tree shrew, bush baby	Field is used to label all records in the database and is designed to facilitate record identification for cross-database structure searching. Field entry refers to the species of animal(s) listed in the data record and used in the toxicity study or studies.	Field names and content are being coordinated with the public ToxML standardization effort.
CPDBAS Source-Specific Fields					
ActivityOutcome_ _CPDBAS_ Mutagenicity	defined text		active/ inactive/ <i>blank</i>	<p>A chemical is classified within the CPDB as mutagenic, i.e. "active", in the <i>Salmonella</i> assay if it was evaluated overall as either "mutagenic" or "weakly mutagenic" by Zeiger [4] or as overall "positive" by the EPA Gene-Tox Program [5,6]. All other chemicals evaluated for mutagenicity by these two sources are reported as "inactive".</p> <p>"<i>blank</i>" or null entry indicates no evaluation of mutagenicity from either source.</p> <p>This is a summary mutagenicity determination in the CPDB Summary Table that is based on overall evaluations (not strain-specific for <i>Salmonella</i>) from two sources of overall evaluations, using the above rule.</p>	<p>This field is titled "Salmonella" in the original CPDB Summary Tables; symbol entries appearing in this field were converted to the following DSSTox text equivalents:</p> <p>"+" = active "- " = inactive "." = <i>blank</i> (no evaluation)</p> <p>Activity field deposited in PubChem.</p> <p><i>Field renamed and modified in v5b; previously Mutagenicity_SAL_CPDB.</i></p>

<p>TD50_Rat_mg</p> <p>TD50_Mouse_mg</p> <p>TD50_Hamster_mg</p> <p>TD50_Dog_mg</p> <p>TD50_Rhesus_mg</p> <p>TD50_Cynomolgus_mg</p> <p><i>(no spaces)</i></p>	<p>numeric</p>	<p>mg/kg-body wt/day</p>	<p>#/ <i>blank</i></p>	<p>TD50 is a standardized quantitative measure of carcinogenic potency (analogous to an LD50) and is computed in the CPDB for each species/sex/tissue/tumor type for each experiment.</p> <p>TD50 is defined as: “that dose-rate in mg/kg body wt/day which, if administered chronically for the standard lifespan of the species, will halve the probability of remaining tumorless throughout that period” [4-6]. In the CPDB Summary Tables, a TD50 (#) is reported for a chemical in each species with a positive evaluation of carcinogenicity in at least one experiment. If there is only one positive test on the chemical in the species, then the most potent TD50 from that test is reported. If more than one experiment is positive, the reported TD50 is the harmonic mean of the most potent TD50 values from each positive experiment in the species and is described at http://potency.berkeley.edu/td50harmonicmean.html [2,3,7-9].</p> <p>Comments pertaining to the TD50 (corresponding to footnote indices in the original CPDB Summary Table) are provided in the TD50_..._Note field entry for the corresponding Species (see below).</p> <p><i>“blank”</i> or null entry indicates no TD50 computed for that chemical and species or species-sex category due to one of two conditions: either no experiment reported in CPDB, or no positive results reported.</p>	<p>These fields appear under the column headings “Harmonic mean of TD50 (mg/kg/day)” in the original CPDB Summary Tables by Species.</p> <p>All footnotes and text entries from the original CPDB Summary Tables have been expanded and moved to the corresponding TD50_..._Note field – see below.</p> <p>In the CPDB Summary Table for Non-Human Primates, TD50 results were reported for only a single chemical in the case of either the Tree Shrew and Bush Baby; in each case, for a chemical already present in another species CPDB Summary Table. The single data result in each case is listed in the TD50_Dog_Primates_Note field with a corresponding species entry in the Species field, i.e. separate TD50_... and TargetSites_... fields are not included for these two species in CPDBAS.</p> <p><i>Converted to pure numeric field in v4a; footnotes moved to TD50_species_Note fields.</i></p>
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<p>TD50_Rat_mmol</p> <p>TD50_Mouse_mmol</p> <p>TD50_Hamster_mmol</p> <p>(no spaces)</p>	<p>numeric</p>	<p>mmol/kg-bodywt/day</p>	<p>#/ <i>blank</i></p>	<p>TD50_Rat_mmol = TD50_Rat_mg / STRUCTURE_MolecularWeight etc.</p> <p>See definition for TD50_Rat_mg etc for details. TD50 columns in mmol/kg/bodyweight/day units provided for 3 species (Rat, Mouse, Hamster).</p> <p>Since mg to mmol conversion requires knowledge of the structure and corresponding molecular weight, mmol values are provided only for cases where a STRUCTURE entry is provided and TestSubstance_Description =</p> <p>“single chemical compound”;</p> <p>“mixture or formulation” and STRUCTURE_Shown = “active ingredient in formulation” , where it is assumed the mg dose reported is the active ingredient dose;</p> <p>“mixture or formulation” and STRUCTURE_Shown = “representative isomer in mixture”, where isomers have the same molecular weight</p> <p>TD50..._mmol fields are offered in pure numeric form for use in SAR modeling.</p> <p>Comments pertaining to the TD50 (corresponding to footnote indices in the original CPDB Summary Table) are provided in the TD50..._Note field entry for the corresponding Species (see below).</p> <p>“<i>blank</i>” or null entry indicates no data available for that chemical and species-sex category due to one of the following conditions: no experiment reported in CPDB; no positive results reported; or no mmol conversion due to substance being a mixture and having different Molecular Weight components.</p>	<p>See comments for TD50..._mg.</p>
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<p>TD50_Rat_Note</p> <p>TD50_Mouse_Note</p> <p>TD50_Hamster_Note</p> <p>TD50_Dog_Primates_Note</p>	<p>memo</p>	<p>positive test results only by intraperitoneal or intravenous injection;</p> <p>TD50 is harmonic mean of more than one positive test;</p> <p>no positive results are statistically significant;</p> <p>greater than ten-fold variation among TD50 values for positive results;</p> <p>TD50 value is overestimated as upper 99% confidence limit from study with 100% tumor incidence but no lifetable;</p> <p>TD50_Rat_mmol was not calculated for this mixture, but Activity Score is assigned value of "50" to indicate active;</p> <p>TD50 not calculated by CPDB Source;</p> <p>TD50 value less than the reported upper confidence limit;</p> <p>harmonic mean of TD50 includes a value for the upper 99% confidence limit/</p> <p>no positive results/</p> <p>NTP bioassay inadequate/</p>	<p>If a numerical value of the TD50 is listed for a given Species, it may be accompanied by one or more of the notes in this field.</p> <p>If there were no positive experiments in a species but the chemical was tested in the species, the field entry will be one of the following:</p> <p>“no positive results” = all experiments in the species group were negative, i.e. not carcinogenic</p> <p>“NTP bioassay inadequate” = NCI/NTP bioassays were the only available experiments in the species, and results for both sexes in the species were evaluated by NCI/NTP as inadequate</p>	<p>These comments replace the following footnote indices annotating the TD50 result in the original Source CPDB Summary Tables:</p> <p>i = Intraperitoneal or intravenous injection are the only routes of administration with positive tests in the CPDB.</p> <p>m = More than one positive test in the species in the CPDB; in this case the reported TD50 is the harmonic mean of those positive results [7].</p> <p>n = “no positive results are statistically significant” corresponding to the CPDB text: “No results that were evaluated as positive for this species in the CPDB are statistically significant (p<0.1).”</p> <p>v = Variation is greater than ten-fold among statistically significant (p<0.1) TD50 values from different positive experiments in the species.</p> <p>Abbreviations from the original CPDB Summary Tables appearing in the TD50 fields were converted to the following DSSTox text equivalents:</p> <p>“-” = “no positive results” (formerly NP);</p> <p>“i” = “NTP bioassay inadequate” (formerly IA) indicates NCI/NTP bioassays were the only available experiments and both sexes in the species were evaluated as inadequate</p> <p>“.” = <i>blank</i> indicates no data are available for that chemical and species or species-sex category</p> <p>P = harmonic mean of TD50 includes a value for upper 99% confidence limit from study with 100% tumor incidence but no lifetable</p> <p>< = TD50 value is overestimated as upper 99% confidence limit from study with 100% tumor incidence but no lifetable</p> <p>In the CPDB Summary Table for Non-Human Primates, TD50 results were reported for only a single chemical in the case of either the Tree Shrew and Bush Baby; in each case, for a chemical already present in another species CPDB Summary Table. The single data result in each case is listed in the TD50_Dog_Primates_Note field with a corresponding species entry in the Species field, i.e. separate TD50_... and TargetSites_... fields are not included for these two species in CPDBAS.</p> <p><i>Modified field entries (January 2008).</i></p>
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<p>TargetSites_Rat_Male/</p> <p>TargetSites_Rat_Female/</p> <p>TargetSites_Rat_BothSexes/</p> <p>TargetSites_Mouse_Male/</p> <p>TargetSites_Mouse_Female/</p> <p>TargetSites_Mouse_BothSexes /</p> <p>TargetSites_Hamster_Male/</p> <p>TargetSites_Hamster_Female/</p> <p>TargetSites_Hamster_BothSexes/</p> <p>TargetSites_Dog/</p> <p>TargetSites_Rhesus/</p> <p>TargetSites_Cynomolgus/</p>	<p>defined text</p>		<p><u>adrenal gland</u>;</p> <p><u>bone</u>;</p> <p><u>clitoral gland</u>;</p> <p><u>esophagus</u>;</p> <p><u>ear Zymbals gland</u>;</p> <p><u>gall bladder</u>;</p> <p><u>harderian gland</u>;</p> <p><u>hematopoietic system</u>;</p> <p><u>kidney</u>;</p> <p><u>large intestine</u>;</p> <p><u>liver</u>;</p> <p><u>lung</u>;</p> <p><u>mesovarium</u>;</p> <p><u>mammary gland</u>;</p> <p><u>mixture</u>;</p> <p><u>myocardium</u>;</p> <p><u>nasal cavity</u>;</p> <p><u>nervous system</u>;</p> <p><u>oral cavity</u>;</p> <p><u>ovary</u>;</p> <p><u>pancreas</u>;</p> <p><u>peritoneal cavity</u>;</p> <p><u>pituitary gland</u>;</p> <p><u>preputial gland</u>;</p> <p><u>prostate</u>;</p> <p><u>skin</u>;</p> <p><u>small intestine</u>;</p> <p><u>spleen</u>;</p> <p><u>stomach</u>;</p> <p><u>subcutaneous tissue</u>;</p> <p>all tumor bearing animals;</p> <p><u>testes</u>;</p> <p><u>thyroid gland</u>;</p> <p><u>urinary bladder</u>;</p>	<p>Target sites are reported for each sex-species group with a positive result in the CPDB. Target sites are identified on the basis of a positive opinion by the published author for the particular site, in any experiment in the species-sex or species, using all results from both the general literature and NCI/NTP bioassays. If a chemical has two or more target sites listed, the results may be from different experiments, and a single site may be a target organ in more than one experiment [2,3]. CPDB data organized by target site have been published by Gold et al. [3] and are updated on the CPDB website to include all results in CPDB to date at: http://potency.berkeley.edu/pathology.table.html.</p> <p>nasal cavity (includes tissues of the nose, nasal turbinates, paranasal sinuses and trachea);</p> <p>oral cavity (includes tissues of the mouth, oropharynx, pharynx, and larynx);</p> <p>Maltoni head cancers = A mix of carcinomas of the ear duct, Zymbal's gland, oral cavity or nasal cavity were combined by single author, Maltoni, in his category "Head cancers", which he reports as induced by the chemical.</p> <p>TargetSites_species_BothSexes is used for experiments where results in the general literature are reported only for males and females combined, with a positive author's opinion for the particular site.</p> <p>If a tumor target site is not reported for the listed chemical and species/sex cell, the field entry will be one of the following:</p> <p>"no positive results" = indicates that all experiments in the sex species group were negative, i.e. not carcinogenic.</p> <p>"no positive results – CPDB evaluation based on NCI Technical Report" = In these few cases an NCI Technical Report prior to 1983 did not evaluate the evidence as "carcinogenic" and, later, NTP reassigned the level of evidence of "positive".</p> <p>"NTP bioassay inadequate" = NCI/NTP bioassays were the only available experiments in the species and results for both sexes in the species were evaluated by NCI/NTP as inadequate.</p> <p>"blank" or null entry indicates no experiment reported in CPDB for that chemical and species-sex category.</p> <p>The 3-letter abbreviation used for tumor sites in the</p>	<p>These fields appear under the column headings "Rat target sites", "Mouse target sites" and "Target sites" in the original CPDB Summary Tables. The field names have been separated and standardized in the DSSTox SDF files.</p> <p>The original CPDB Summary Tables reports tumor target sites as 3 letter mnemonic codes, e.g. adr=adrenal gland. In this and subsequent versions of CPDBAS, the 3 letter codes have been replaced by the corresponding target site.</p> <p>Abbreviations from the original CPDB Summary Tables appearing in the Target site fields were converted to the following DSSTox text equivalents:</p> <p>“.” = “no positive results” (formerly NP)</p> <p>“I” = “NTP bioassay inadequate” (formerly IA) indicates NCI/NTP bioassays were the only available experiments and both sexes in the species were evaluated as inadequate</p> <p>“u” = “no positive results – CBDP evaluation based on NCI Technical Report” where in these few cases an NCI Technical Report prior to 1983 did not evaluate the evidence as "carcinogenic" and, later, NTP reassigned the level of evidence of "positive".</p> <p>“.” = <i>blank</i> (no experiment reported)</p> <p>In the CPDB Summary Table for Non-Human Primates, TargetSites were reported for only a single chemical in the case of both the Tree Shrew and Bush Baby; in each case, for a chemical already present in another species CPDB Summary Table. The single data result in each case is listed in the TD50_Dog_Primates_Note field with a corresponding species entry in the Species field, i.e. separate TD50_... and TargetSites_... fields are not included for these two species in CPDBAS.</p> <p>In the CPDB Summary Tables for Rats, Mice, and Hamsters, the notation (B) is used in conjunction with a species-sex target site, e.g., "adr (B)" to indicate that a study reported tumors at the adrenal gland only for the two sexes combined. This notation would appear for the target site under both Male and Female headings unless one of two conditions held: (1) positive results were available for the target site in the other sex of the species; or (2) negative results were reported for the other sex of the species. A "B-" would be listed alone (i.e., without target site codes) if negative results were only found in a study where the two sexes were combined. Since these results are not</p>
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		<p><u>uterus</u>;</p> <p><u>vagina</u>;</p> <p><u>vascular system</u>;</p> <p>Maltoni <u>head cancers</u>;</p> <p>no positive results;</p> <p>NTP assigned level of evidence positive;</p> <p>NTP bioassay inadequate/ <i>blank</i></p>	<p>original CPDB Summary Tables is underlined in the expanded text of the <i>Allowable Entries</i>.</p>	<p>resolved to species-sex, we have created separate fields to accommodate this information: TargetSites_Rat_BothSexes TargetSites_Mouse_BothSexes TargetSites_Hamster_BothSexes</p> <p>Non-<i>blank</i> entries in these fields only occur under the same conditions reported in the CPDB Summary Tables, i.e. if combined-sex results are available and species-sex results are unavailable for either sex. The TargetSites_... for dogs and non-human primate species (rhesus, cynomolgus, tree shrew, bush baby) are reported without sex specification or with sexes combined.</p> <p>In the CPDB Summary Tables, four chemicals in rats include the footnote "H" to denote a positive opinion for a consolidated site "head tumors", by only a single research group. Maltoni et al. evaluated head as a target site for a combination of carcinomas at various sites in the head (ear duct, Zymbal's gland, nasal cavity, or oral cavity). When this result has confirming results from other studies for either nas or orc target sites in the head, it is reported as nash and orch in the CPDB Summary Table. When no other positive results are reported, the result is designated "+H" in the CPDB Summary Table [4]. Both "H" and "+H" have been replaced with "Maltoni head cancers" in the CPDBAS file. This occurs either alone, or following a target site, such as nasal or oral cavity.</p> <p>In the CPDB Summary Tables, the footnote indicators "L, a, and x" are listed for 3 or fewer compounds. In the DSSTox CPDBAS data files, these footnotes are deleted from the Target Sites field and the corresponding text has been incorporated into either the corresponding TD50_species_Note field or the NTP_TechnicalReport field.</p>
<p>ActivityOutcome_CPDBAS_Rat/ ActivityOutcome_CPDBAS_Mouse/ ActivityOutcome_CPDBAS_Hamster/ ActivityOutcome_CPDBAS_Dog_Primates/ <i>(no spaces)</i></p>	defined text	<p>active/ inactive/ unspecified/ <i>blank</i></p>	<p>An assignment of categorical carcinogenic activity based on evidence for or against activity within a species or species group as provided in the CPDB Summary Table (e.g., Rat, Mouse, etc):</p> <p>"active" = one or more TD50 and tumor site listed for one or more species-specific (e.g., Rat) carcinogenicity sex/species cell (e.g., Rat Male, Rat Female, Rat Both);</p> <p>"inactive" = no TD50 or tumor site is listed AND one or more "no positive results" entry for one or more species specific (e.g., Rat) carcinogenicity sex/species cell (e.g., Rat Male, Rat Female, Rat Both), i.e. one or more experiments are reported in the CPDB for species, but none are positive;</p> <p>"unspecified" = NCI/NTP bioassays were the only available experiments and both sexes in the</p>	<p>Summary activity call for use in PubChem and structure-activity relationship studies.</p> <p><i>New fields added to v5b.</i></p>

				<p>species were evaluated by NCI/NTP as inadequate, corresponds to "NTP bioassay inadequate" entry in TargetSites field</p> <p>"<i>blank</i>" or null entry indicates no experiments reported in CPDB for that chemical and species category.</p> <p>All substance records in CPDBAS having a non-<i>blank</i> entry in the ActivityOutcome_CPDBAS_Rat field will have a corresponding entry in the ActivityScore_CPDBAS_Rat field; likewise for corresponding Mouse and Hamster fields.</p>	
<p>ActivityScore_CPDBAS_Rat/ ActivityScore_CPDBAS_Mouse/ ActivityScore_CPDBAS_Hamster/ <i>(no spaces)</i></p>	integer		<p>INTEGER [0-100] <i>blank</i></p>	<p>Mapping of LOG10 (1/TD50_species_mmol) values spanning range [MIN, MAX] onto Integer 1-100 Activity range (for carcinogenic compounds), where 100 represents the highest potency and 1 the lowest:</p> <p>ActivityScore = 100 * INTEGER[(log10(1/Activity) - MIN)/(MAX - MIN)]</p> <p>ActivityScore (0) is assigned when corresponding ActivityOutcome_CPDBAS_... field entry for species is "inactive" or "unspecified".</p> <p>"<i>blank</i>" or null entry indicates no experiments reported in CPDB for that chemical and species-sex category.</p> <p><i>Note:</i> In a small number of "active" cases where substance is mixture with different Molecular Weight components, such that TD50_Rat_mmol and TD50_Mouse_mmol could not be calculated, the ActivityScore was arbitrarily assigned a value of "50" to indicate activity.</p> <p>All substance records in CPDBAS having a non-<i>blank</i> entry in the ActivityOutcome_CPDBAS_Rat field will have a corresponding entry in the ActivityScore_CPDBAS_Rat field; likewise for corresponding Mouse and Hamster fields.</p>	<p>Summary activity ranking for use in PubChem and structure-activity relationship studies.</p> <p><i>New fields added to v5b.</i></p>
<p>ActivityOutcome_SingleCellCall <i>(no spaces)</i></p>	defined text		<p>active/ inactive/ unspecified/</p>	<p>An assignment of categorical carcinogenic activity based on minimal evidence for or against activity:</p> <p>"active" = one or more TD50 and tumor site listed for one or more carcinogenicity sex/species cell (e.g., Rat Male, Rat Female, etc);</p> <p>"inactive" = no TD50 or tumor site listed AND one or more "no positive results" entry for one or more carcinogenicity sex/species cell (e.g., Rat Male, Rat Female, etc), i.e. one or more experiments are reported in the CPDB, but none are positive;</p> <p>"unspecified" = NCI/NTP bioassays were the only available experiments and both sexes in the species were evaluated by NCI/NTP as inadequate, corresponds to "NTP bioassay inadequate" entry in TargetSites field</p> <p><i>Note:</i> This field contains no "blank" entries, since CPDB</p>	<p>Type of conservative activity call used by the National Toxicology Program, where a statistically significant tumor site finding in a single sex/species of rodent is considered a significant carcinogenic concern.</p> <p>Summary activity call for use in PubChem and structure-activity relationship studies.</p> <p><i>Field entries modified in v5d; 3 records for Rat have "unspecified" entry based on NTP call.</i></p>

				reports results of at least one experiment for each substance in CPDBAS.	
ActivityOutcome_ CPDBAS_ MultiCellCall <i>(no spaces)</i>	defined text		active/ inactive/ <i>blank</i>	<p>An assignment of categorical carcinogenic activity based on multicell evidence for or against activity:</p> <p>“active” = more than one TD50 or tumor site listed for carcinogenicity sex/species cells (e.g., liver, lung, or Rat Male, Rat Female, etc), where tumor sites may be reported from different experiments;</p> <p>“inactive” = no TD50 or tumor site listed AND more than one "no positive results" entry for carcinogenicity sex/species cells (e.g., Rat Male, Rat Female, etc), i.e. one or more experiments are reported in the CPDB, but none are positive;</p> <p>"<i>blank</i>" or null entry indicates neither condition for multicell activity nor condition for inactivity was met.</p>	<p>CPDB Summary Table tumor site codes “mix” or “H” count as a single site or experimental observation for the purposes of this activity assignment.</p> <p>A result reported in the CPDB Summary Table for “Both Sexes”, i.e. the experimental results were reported in the published paper only for both sexes combined for the species, is not considered a separate result for a “multisex” assignment (e.g., a result listed for Male Rat and Rat Both Sexes would not be considered a “multisex” result due to the uncertainties in reporting.</p> <p>Type of activity call used by the Food and Drug Administration (FDA), where greater weight is given to multisite, multisex (usually accompanied by multispecies) or multispecies carcinogens in modeling and in carcinogenicity assessments.</p> <p>Summary activity call for use in PubChem and structure-activity relationship studies</p> <p><i>Field modified in v5b for use in PubChem, with details provided in the text field,</i> ActivityOutcome__CPDBAS_MultiCellCall_Details</p>

<p>ActivityOutcome_CPDBAS_MultiCellCall_Details (no spaces)</p>	<p>defined text</p>		<p>multisite active, multisex active, multispecies active/ multisex inactive, multispecies inactive/ <i>blank</i></p>	<p>Details pertaining to entry in ActivityOutcome_CPDBAS_MultiCellCall:</p> <p>If field entry of ActivityOutcome_CPDBAS_MultiCellCall is "active", one or more of the following are listed:</p> <p>multisite active = multiple tumor sites reported from different experiments;</p> <p>multisex active = male and female sexes (possibly of different species) tested positive for one or more tumor sites, possibly from different experiments;</p> <p>multispecies active = multiple species (e.g., rat, mouse, etc) tested positive at one or more tumor sites, possibly from different experiments.</p> <p>If field entry of ActivityOutcome_CPDBAS_MultiCellCall is "inactive", one or more of the following are listed:</p> <p>multisex inactive = ActivityOutcome_CPDBAS_SingleCellCall is "0" AND more than one "no positive results" entry for male and female sexes (possibly of different species), possibly from different experiments;</p> <p>multispecies inactive = ActivityOutcome_CPDBAS_SingleCellCall is "0" AND more than one "no positive results" entry for multiple species (e.g., rat, mouse, etc), possibly from different experiments.</p> <p>"<i>blank</i>" or null entry indicates neither condition for multicell activity or inactivity was met in ActivityOutcome_CPDBAS_MultiCellCall.</p>	<p><i>Fieldname modified in v5b, previously: ActivityCategory_MultiCellCall.</i></p>
<p>Note_CPDBAS</p>	<p>memo</p>		<p><i>Text</i></p>	<p>Field used to provide supplementary Source-specific information pertaining to the chemical and toxicity fields, with text entries to allow a user to easily locate added or modified records in version.</p>	<p>Single entries for TD50_... and TargetSites_... values for each of two species (bush baby and tree shrew) were moved to the new TD50_Dog_Primates_Note field in v5b.</p> <p>Field is additionally used to document any additions of new chemical record or data modifications in subsequent versions of CPDBAS. Controlled text entries include:</p> <ul style="list-style-type: none"> chemical added v5a Rat added v5a Mouse added v5a TD50_Rat_Note modified v5a Mutagenicity_SAL_CPDB added v5a

					<p>TD50_Rat modified v5a TargetSites_Mouse_Female modified v5a ... etc</p> <p>CPDB-specific information pertaining to the Source-specific toxicity information previously included in ChemicalNote field has been moved to this field.</p> <p><i>Replaces ToxicityNote field (May 2007).</i></p>
<p>NTP_ TechnicalReport (no spaces)</p>	memo		Text	<p>National Toxicology Program Technical Report number of study included in this CPDBAS record.</p> <p>Note is also included in this field if NTP study results differ from CPDB summary call to alert users to this discrepancy. The CPDB summary call can differ from the NTP call when additional literature studies meeting CPDB protocol requirements are factored into the CPDB assessment.</p>	<p>Users wishing to extract only the NTP records from CPDB for modeling purposes are cautioned that in a few cases the NTP study results differ from the CPDB summary call. These cases are flagged in this field.</p>
<p>ChemicalPage_ URL</p>	memo		URL	<p>Internet URL website address for chemical-specific data or content.</p> <p>URL was checked at time of DSSTox data file publication. Please send DSSTox Error Report if website URL address no longer works or is changed.</p>	<p>URLs were previously included in general field Website_URL.</p> <p><i>New field added (October 2007).</i></p>

Additional CPDB references:

A list of citations and text files to 100 papers by the Carcinogenic Potency Project: <http://potency.berkeley.edu/listofpubs.year.html>

1. Gold, L.S. and Zeiger, E., Eds. (1997). Handbook of Carcinogenic Potency and Genotoxicity Databases. Boca Raton, FL: CRC Press. <http://potency.berkeley.edu/CRCbook.html>
2. Gold, L.S., T.H. Slone, and B. Ames (1999) Summary of Carcinogenic Potency Database by Chemical. <http://potency.berkeley.edu/chemicalsummary.html>
3. Gold, L.S., N.B. Manley, T.H. Slone, and J.M. Ward (2001) Compendium of chemical carcinogens by target organ: Results of chronic bioassays in rats, mice, hamsters, dogs and monkeys. *Toxicol. Pathol.* 29: 639-652. <http://potency.berkeley.edu/text/ToxicolPathol.pdf>
4. Zeiger, E. (1997) Genotoxicity Database. In: Gold, L.S., and Zeiger, E., Eds. Handbook of Carcinogenic Potency and Genotoxicity Databases. Boca Raton, FL: CRC Press, pp. 687-729. <http://potency.berkeley.edu/CRCbook.html>
5. Kier, L.E., D.J. Brusick., A.E. Auletta, E.S. Von Halle, M.M. Brown, V.F. Simmon, V. Dunkel, J. McCann, K. Mortelmans, M. Prival, T.K. Rao, and V. Ray (1986) The *Salmonella typhimurium*/mammalian microsomal assay: A report of the U.S. Environmental Protection Agency Gene-Tox Program. *Mutat. Res.* 168: 69-240.
6. Auletta, A.E., Personal communication (with L.S.Gold).
7. Peto, R., M.C. Pike, L. Bernstein, L.S. Gold, and B.N. Ames (1984) The TD₅₀: A proposed general convention for the numerical description of the carcinogenic potency of chemicals in chronic-exposure animal experiments. *Environ. Health Perspect.* 58: 1-8.

8. Sawyer, C., R. Peto, L. Bernstein, and M.C. Pike (1984) Calculation of carcinogenic potency from long-term animal carcinogenesis experiments. *Biometrics* 40: 27-40.
9. Gold, L.S., T.H. Slone, and L. Bernstein (1989) Summary of carcinogenic potency (TD_{50}) and positivity for 492 rodent carcinogens in the Carcinogenic Potency Database. *Environ. Health Perspect.* 79: 259-272.