

DSSTox Log File:

EPA Estrogen Receptor Ki Binding Study (*Laws et al.*) (KIERBL)

Database File

(last updated 17 February 2009)

Description: Information in this file documents the creation, review, and update process for the DSSTox KIERBL SDF file, and provides summary information on database content. The first section summarizes the process used for creating the initial DSSTox SDF files and the quality assurance checks and procedures employed, and then provides version history notes. A table providing field and data counts offers summary overview of KIERBL file content. The Log Table documents modifications and revisions to the database content or format in version updates. To obtain the most current version of this Log File and a record of any new modifications, or to report errors in this file, a user should consult the DSSTox KIERBL database page: http://www.epa.gov/ncct/dsstox/sdf_kierbl.html

QA and Development Notes for v1:

The KIERBL SDF file underwent an extensive series of quality review checks prior to publication of initial launch version. The original chemical inventory (CAS and chemical name listing) was obtained from the main study author (S. Laws) in association with the Main Citation (Laws et al., 2006, see http://www.epa.gov/ncct/dsstox/sdf_kierbl.html). We particularly thank Susan Laws (EPA Source Collaborator) for invaluable assistance in various stages of development and quality review, clarifying issues pertaining to the chemical inventory contents, activity assignments and representation, and documentation. The initial CAS and chemical name inventory were imported into Excel and cross-referenced to the existing DSSTox Master File chemical inventory, and DSSTox Standard Chemical Fields (including structures) were assigned when matches to existing DSSTox Master File inventory were found. For those chemical substances not in the existing DSSTox Master File inventory, we employed a number of commercial and public Internet resources for converting name to structure ((ACD/Name, version 10) or assigning chemical structures based on CAS, and populating DSSTox Standard Chemical Fields (for details of general QA review procedures, see <http://www.epa.gov/ncct/dsstox/ChemicalInfQAProcedures.html>). IUPAC systematic chemical names, **STRUCTURE_ChemicalName_IUPAC**, were computed using the ACD/Labs IUPAC Name-Generation software (ACD/Name, version 12); SMILES were generated using ChemOffice Ultra, 2004. **Structure_InChI** and **Structure_InChIKey** codes were automatically generated from the final DSSTox structures using the NIST recommended standard InChI options (see <http://www.epa.gov/ncct/dsstox/MoreonInChI.html#InChIDSSSTox>). All KIERBL Source Toxicity fields were created from Main Citation published content in collaboration with the main EPA Source Collaborator (S. Laws).

Log of SDF Modifications and Version/revision updates:

Date	DSSTox SDF File Name	Modifications from previous version	Additional Notes
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17Feb2009	KIERBL_v1a_228_17Feb2009	Initial launch publication; no previous published versions.	KIERBL is considered a "static" historical database meaning that further expansion of the database to include additional test data is unlikely. Future updates will correct reported errors provided by users or incorporate DSSTox format changes.

KIERBL SDF Content Summary: 17 February 2009

KIERBL SDF Content	Totals_v1a
# Records	278
DSSTox Standard Chemical Fields	20
DSSTox Standard Toxicity Fields	4
KIERBL Source Fields	10
Total # Fields	34
Chemical Content	Counts_v1a
STRUCTURE_ChemicalType:	
defined organic	258
inorganic	0
organometallic	20
no structure	0
STRUCTURE_TestForm_ DefinedOrganic:	
parent	238
complex	3
salt	17

salt complex	0
TestSubstance_Description:	
single chemical compound	270
macromolecule	0
mixture or formulation	8