



# **ToxML Standards Organisation General Meeting**

1st November 2011

- The ToxML specification is a means for representing and communicating/transferring toxicology data, tests, studies, and compound information between individual and groups creating and/or using such information.
- It is an open standard that is extensible to new types of toxicological data.
- It consists of an XSD defining the toxicology schema and lists of controlled vocabulary that help to ensure consistency of usage when entering data into the ToxML format.

**ToxML Schema Editor**

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**Compound** Studies Primitive Types Find History Export User: Anonymous

- Compound
  - Comments
  - Datasets
  - Descriptors
  - Formulae
  - Ids
  - InChI
  - KnownDrugInformation
  - Manufacturers
  - ModelApplications
  - Names
  - OtherIds
  - OtherProperties
  - OtherRtecsInformation
  - PhysicalProperties
  - Structure
  - TextDatasets
  - ToxicityStudies

**Tag**  
Compound

**Path**

**Type**  
Composite

**Members**

- Comments - Set
- Datasets - List
- Descriptors - Composite
- Formulae - Set
- Ids - Set
- InChI - Set
- KnownDrugInformation - Composite
- Manufacturers - Set
- ModelApplications - List
- Names - Set
- OtherIds - Set
- OtherProperties - List
- OtherRtecsInformation - Composite
- PhysicalProperties - List
- Structure - Composite
- TextDatasets - List
- ToxicityStudies - Composite

**Description**  
A record regarding a single compound

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  - ModelApplications
  - Names
  - OtherIds
  - OtherProperties
  - OtherRtcsInformation
  - PhysicalProperties
  - Structure**
    - Image
    - MolecularFormula
    - Molfile
    - Smiles
      - Smiles
        - Value
  - TextDatasets
  - ToxicityStudies

**Tag**  
Structure

**Path**  
/Compound

**Type**  
Composite

**Members**  
Image - Composite  
MolecularFormula - Composite  
Molfile - Composite  
Smiles - Set

**Description**  
A collection of named property elements

**History**  
Removed LeadscopeFeatures from Structure - by Contributor - 2011-09-20 15:48:09.0  
Removed NewMember from Structure - by Contributor - 2011-09-20 15:47:59.0  
Restored NewMember to Structure - by Contributor - 2011-09-20 09:43:32.0  
Removed NewMember from Structure - by Contributor - 2011-09-20 09:43:23.0  
Added NewMember to Structure - by Contributor - 2011-09-20 09:42:12.0  
Renamed Structure-2 to Structure - by Contributor - 2011-09-20 09:38:42.0  
Renamed Structure to Structure-2 - by Contributor - 2011-09-20

**ToxML Schema Editor**

Compound **Studies** Primitive Types Find History Export User: Anonymous

**Study Types**

- Acute Toxicity Studies
- Aquatic Toxicity Studies
- Bacterial Mutagenesis Studies
- Carcinogenicity Studies
- Chronic Studies
- Developmental Neurotox Studies
- Developmental Studies
- DNA Repair Studies
- Forward Mutation Reciprocal Translocation Studies
- Forward Mutation Sex Linked Recessive Lethal Studies
- In Vitro Chromosome Aberration Studies
- In Vitro Micronucleus Studies
- In Vitro Sister Chromatid Exchange Studies
- In Vivo Chromosome Aberration Studies
- In Vivo Micronucleus Studies
- In Vivo Sister Chromatid Exchange Studies
- Irritation Studies
- LLNA Studies
- Mammalian Mutagenesis Studies
- Multiple Dose Studies
- My New Study Type Studies
- Reproductive Developmental Studies
- Reproductive Studies
- RTECS Mutation Studies
- Skin Penetration Studies
- Subchronic Studies
- Tumorigenic Studies
- Unscheduled Dna Synthesis Studies

**Study Prototypes**

- Generic Studies

- Specification editor currently undergoing internal beta testing
- Available for external testing next week