

INFORMATION SOCIETY TECHNOLOGIES
(IST)
PROGRAMME



OpenMolGRID

ECOTOX-TERRETOX DATA SPECIFICATION

Contract Reference:	IST-2001-37238
Document identifier:	OpenMolGRID-1-D1.1b-0102-2-1- TerretoxDatSpec
Date:	07/01/2004
Work package:	WP1: Grid Data Warehousing of Molecular Structure – Property (Activity) Information
Partner:	UU, Negri
Lead Partner:	UU
Document status:	DRAFT
Classification:	PUBLIC
Deliverable identifier:	D1.1b

Abstract: This document is to specify what transformations must take place to data before it is placed into the OpenMolGRID data warehouse MOLDW.

Delivery Slip

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Document Log

Issue	Date	Comment	Author
0-0	29/08/03	First Version	Damian McCourt Jean Jing Werner Dubitzky
1-0	09/08/03	First Stable Version	Damian McCourt Jean Jing Werner Dubitzky
2-0	15/09/03	Submitted for Authorisation	Damian McCourt Jean Jing Werner Dubitzky
2-0	14/11/03	Accepted for Authorisation by WPMs, TC and QE, but status will remain as draft	Damian McCourt
2-1	07/01/04	Updated due to the change of the document template (version 1.3)	Jean Jing

Document Change Record

Issue	Item	Reason for Change
1-0	Changes to template	First Stable Version
2-0	Document Status	Submitted and accepted for Authorisation, but status is to remain as draft
2-1	Changes to document template	The standard template of the document is changed

Files

Files in this section relate to actual storage locations on the BSCW server located at <https://hermes.chem.ut.ee/bscw/bscw.cgi>. The URL below describes the location on BSCW from the root OpenMolGRID directory

Software Products	User files / URL
Word 2000/XP	OpenMolGRID/Workpackage 1/Deliverables/ OpenMolGRID-1-D1.1b-0102-2-1-TerretoxDatSpec

Project information

Project acronym:	OpenMolGRID
Project full title:	Open Computing GRID for Molecular Science and Engineering
Proposal/Contract no.:	IST-2001-37238
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1. Introduction

1.1. Purpose and Scope

The purpose of this document is to specify what transformations must take place to data before it is placed into the OpenMolGRID data warehouse MOLDW. This document is intended to accompany deliverable D1.1a [1]. The information to be integrated into MOLDW is based on the information presented in deliverable D1.3 [2].

1.2. Overview

Currently specifications for data transformations have not yet taken place. This document intends to initiate this process by providing a mapping of the data required as stated in deliverable D1.3 [2] to what is available in the Terretox data source available from Exotox. A description of Terretox is provided in document D1.4a [3]. Where possible data transformations have been stated, but other areas require further specification by other partners in the consortium.

1.3. Document Structure

In addition to this section the document contains the following sections:

- Section 2 – identification of chemicals
- Section 3 – Toxicity
- Section 4 – Carcinogenicity
- Section 5 – Physico-Chemical Properties(PCP)
- Section 6 – ADME Related Properties and Descriptors

2. Identification of Chemicals

Name	Type	Description	Present In Source	Format	Conversion Details
CAS (unique identifier)	Integer	The Chemical Abstract Service (CAS) number. This is an integer without hyphens or spaces	Present 'Test CAS' in test.txt	As number without hyphens	No change
Molecular Weight	Float	The Atomic Mass Unit (amu) associated with the CAS.	Not Present		
Chemical Formula	String	The chemical formula associated with the CAS	Not Present		
Chemical Names	List of Strings	The names by which the chemical is known	Referenced from chemicals.txt in common_validation directory	Only as one name	Store as found

3. Toxicity

Name	Type	Description	Present In Source	Format	Conversion Details
CAS (unique identifier)	Integer	The Chemical Abstract Service (CAS) number. This is an integer without hyphens or spaces	Present 'Test CAS' in test.txt	As number without hyphens	No change
Target Species Names	List of Strings	A list of names associated with the target species	Present in test.txt as 'Species Number'	reference to species_common_names.txt and species_latin_names.txt files	Merge target species common names and Latin name from species_common_names.txt and species_latin_names.txt files
End Point Type	String	The type of toxicity measure used in this protocol e.g. LC ₅₀ , LD ₅₀ .	Present 'Endpoint' in result.txt	e.g. BAF/ EC10 EC50 LC50 LD50 LOEC NOEC T1/2 NR	No change Need spec of endpoints to be considered

Doc. Identifier:

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TerretoxDataSpec

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Dose Metric	Float	The dose of chemical studied (for aquatic toxicity the compound is in the tank, and the fish exposed)measured in milligrams per kilogram (mg/kg) or milligrams per litre (mg/l).	Present as 'Dose Mean' in exposure.txt	String e.g. 125 NR	Float
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Dose Units	Metric	String	The units associated with the Metric dose	Present as 'Dose Units' in exposure.txt	Unit standardisation
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e.g.
 ai g/ac, Al
 g/m2,g/ha,g/kg,
 granules,
 kg/ha, lb, lb/ac
 lb/acre
 meq/100g soil

 mg/eu, mg/kg, mg/kg
 bdwt, mg/kg/d, mg/kg
 org, mg/kg org/d, mg/kg
 p/d, mg/kg soil, mg/10g,
 mg/L, mg/l, mg/ml,
 mg/wk

 ml, ml/m2
 mm

 oz/bu
 ppm
 ppt
 uCi
 ug, ug/g, ug/g soil, ug/ml
 , ug/org
 ul
 uM
 1e-4M
 1e-5M
 1e-6M

Dose Mol	Float	The dose of chemical studied measured in millimols per kilogram (mmol/kg) or millimols per litre (mmol/l).	As before	Mmol/L mmol/kg	
Dose Mol Units	String	The units associated with the Mol dose	As before		
Exposure Time	Float	The amount of time the target species was exposed to the chemical. This is measured in hours.	Present as 'Observation Duration Mean' in result.txt	String e.g. 6 NR	Change to Float in accordance with unit standardisation
Protocol Details	Text	General information associated with the protocol. There is no particular format associated with this.			

Mode of Action USA	String	<p>The Mode of Action of the chemical. These are classes based on the EPA (Duluth, USA) standard. These are as follows:</p> <ul style="list-style-type: none"> • Non Polar Narcosis (Base Line Narcosis) • Polar Narcosis (Narcosis II) • Narcosis III (Ester/ Acrylate compounds) • Oxidative Phosphorilation uncoupling • Respiratory inhibition • Electrophile and proelectrophile reactivity • Acetilcholinesterase inhibition • Central nervous system seizure responses 	Present as 'Effect' as result.txt, not USA or EU	<p>e.g. MOR REP</p> <p>The full list presents in effect.txt</p>	
Mode of Action EU	String	<p>The mechanism of action of the chemical. These are classes based on the EU (Netherlands) standard. These classes are as follows:</p> <ul style="list-style-type: none"> • Non Polar Narcosis • Polar Narcosis • Reactive • Receptor Mediated 	Present as 'Effect' as result.txt, not USA or EU	<p>e.g. MOR REP</p> <p>The full list presents in effect.txt</p>	

Author(s)	List of Strings	The author who reported the toxicity measure.	Present as 'Reference Number' in result.txt, reference to 'Author' in reference.txt	e.g. Veldhuizen-Tsoerkan, M.B., D.A. Holwerda, and D.I. Zandee	Multiple authors
Year	Integer	The year in which the author reported the toxicity measure.	Present as 'Reference Number' in result.txt, reference to 'PublicationYear' in reference.txt	String	Change to Integer
Database	String	The database from which the toxicity measure was obtained.		String	TERRETOX(ECOTOX)

4. Carcinogenicity

Name	Type	Description	Present In Source	Format	Conversion Details
CAS (unique identifier)	Integer	The Chemical Abstract Service (CAS) number. This is an integer without hyphens or spaces	Present 'Test CAS' in test.txt	As number without hyphens	No change
Carcinogenicity	String	Classification of carcinogenicity according to classes proposed by the World Health Organisation (International Agency for Research on Cancer- IARC). These classes are as follows: 1 – Carcinogenic to human 2a – Probably Carcinogenic to human 2b – Possibly Carcinogenic to human 3 – Unknown 4 – Non-carcinogenic to human	Not Present		

5. Physico-Chemical Properties(PCP)

Not present in data Source

6. ADME Related Properties and Descriptors

Not present in data source

7. References

Some references in this section relate to documents stored on the BSCW server. These references all start with a location of “/OpenMolGRID”. The BSCW server is located at <https://hermes.chem.ut.ee/bscw/bscw.cgi>.

[1] D. McCourt, "Data Warehouse software Specification," /OpenMolGRID/Workpackage 1/ Deliverables/OpenMolGRID-1-D1.1a-0101-2-0-MOLDW, 15/09/03.

[2] E. Benfenati and A. Papp, "Properties and priorities of the data for pharmaceutical and phytopharmaceutical compounds," /OpenMolGRID/Workpackage 1/ Deliverables/OpenMolGRID-12-D1.3a-0108-1-0, 15/09/03.

[3] D. McCourt, J. Jing and W. Dubitzky, "Description of Ecotox," /OpenMolGRID/Workpackage 1/ Deliverables/OpenMolGRID-1-D1.4a-0109-1-0, 15/09/03.