Downloading data possibilities

cefic

Information session on updated registration process

O4/11/15 Brussels Dr. Erwin Annys





What is LRI? – A Global Programme

- Commitment demonstration to RC and GPS
- ICCA-LRI: A global effort under ICCA
 - ACC
 - Cefic
 - JCIA



Executing the long-term refocus of the LRI Key questions (< 10y)

• Omics:

21st Century Toxicology; Link information at molecular level to health impact – <u>interpretation</u> of results until we know all; 3Rs for animal testing

- Predictive tools for health impact: pragmatic approaches to reduce complexity, but still robust in predicting health effects
- Combination effects:
 Identify combination effects scenarios of <u>concern</u>
- Eco-systems approach: New concept for Ecosystems approach with <u>population relevance</u>
- « Real life Exposure » : <u>Predictive, validated</u> exposure scenarios for environmental stressors
- Comparative assessment: <u>impact of health</u> and environmental stressors
- Benefit risks approaches: societal drivers for public acceptance for innovation





Linking LRI AMBIT Chemoinformatic System with the IUCLID Substance Database to Support Read across of Substance Endpoint data & Category Formation

Sep 2013 – Sep 2015



mh

http://ambit.sourceforge.net

► AMBIT Cefic LRI-EEM9.3

- "Building blocks for a future (Q)SAR decision support system: databases, applicability domain, similarity assessment and structure conversions" (2004, 2008)
- Part of the LRI Toolbox (http://www.cefic-lri.org/lritoolbox/ambit)

➤AMBIT REST web services

- **OpenTox Application Programming Interface** (API) since 2009
- Dataset web services (import / export)
- Chemical search [exact, similar, substructure] and meta data, data pooling, structure QA, structure optimisation, tautomers generation
- Prediction tools e.g. Cramer rules, Protein binding, pKa etc
- Data analysis tools e.g. regression, classification, clustering, descriptor calculation
- Web Applications using AMBIT REST web services
- New 2014: Embeddable JS widgets

► AMBIT Cefic LRI-EEM9.3-IC (2013)

AMBIT ambit menc Search * Assessments * Import * Enhanced for P 1 autors of Beneficial Mark B. EC. 0.60.5 200-ECB5-6a Ĵ 20.11.2010 30 11 2010 ture search (exact structure, by identifiers, similarity and su

Web services

MySOL database:

ambit

Download

Home Downloads Documentation Publications Support

AMBIT offers chemoinformatics functionality AMBIT consists of multiple Maven modules via OpenTox API compliant REST web services. with well defined dependencies, which can be used in a stand alone mode or embedded in · Chemical compounds and data storage in other applications. Download AMBIT libraries

Libraries

- Substructure, similarity and other queries (The CDK: AMBIT SMARTS, SMIRKS,
- tautomers); **Open source** Descriptor calculation and predictive models building (Weka, Toxtree)

Quick Start

Source code examples

· API-Docs

User guide

Browse and try AMBIT REST AP

Main features at a glance

- Try the public web services, datasets and models
- Datasets : ONS Melting point 33 7 | CPDBAS 7 | Tox21 | Inventory of Cosmetic Ingredients WikiPathways structure browser at GitHub and at BiGCaT Maastricht University? Bioconcentration factor (BCF) Gold Standard Database

Search: Structure search | Subs · Models: Toxtree online

applicability domain methods in AMBIT

other compatible servlet container. Download and install your own AMBIT instance oad web application stall web application oart data

AMBIT REST web services are distributed a

an Apache Tomcat application server or any

web archive (war file) and can be deployed in

About Acknowledgements CEFIC LRI FP7 OpenTox

Social

08



library | jToxKit | 15 library | ToxPredict | FP7 ToxBank | FP7 eNanoMapper

5

Software



· Examples how to use: ambit2-tautomer package | ambit2-SMIRKS

Open Access

AMBIT RESTful web services: an implementation of the OpenTox application programming interface



11/16/2015

Journal of Cheminformatics

2011, 3:18 doi:10.1186/1758-2946-3-18

MAJOR GOALS OF THE CEFIC LRI PROJECT EEM9.3-IC

Enhancing the predictive power of in-silico tools like LRI AMBIT

- Use of Substance data which are already available in a company IUCLID Database.
- In addition Cefic asked ECHA to make the data from the ECHA Dissemination site publically available in a downloadable way
- Other reliable (quality) data will be integrated as well

Support read across and category formation workflows

Avoiding animal tests and enhance the justification for read across and category formation as requested by authorities

Minimize overall testing and resource costs

WoE well the studies for other substances as well the WoE

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PROJECT OVERVIEW

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Company IUCLID DB ECHA IUCLID DB As Major Data Source

> Search for data possible but not for structures

11162015

CEFIC LRI AMBIT Chemoinformatics System

Supporting Read across & Category formation

AMBIT FUNCTIONS Assigning structures -to constituents, impurities ... Search structures & Data - exact, similar, substructure - combined with data search Read across/category formation -Workflows supporting the user Prediction tools -Cramer rules, Protein binding etc > Data analysis tools -Regressions, clustering etc. Data management -flexible import/export of data > Data exchange

- manual or automated via webservices

AMBIT COMMUNICATION





READ ACROSS AND CATEGORY WORKFLOW

	Assessment identifier	Collect structures	Endpoint data used	Assessment details	Report
5 MAIN STEPS					
	Assessment identifier	Collect structures	Endpoint data used	Assessment details	Report
7 SUB STEPS		Collect structures	s List of collected st	tructures	
	Assessment identifier	Collect structures	Endpoint data used	Assessment details	Report
			Search substance(s)	Selection of endpoints	5
	Assessment identifier	Collect structures	Endpoint data used	Assessment details	Report
				Initial matrix Working	matrix Final matrix
	Assessment identifier	Collect structures	Endpoint data used	Assessment details	Report
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