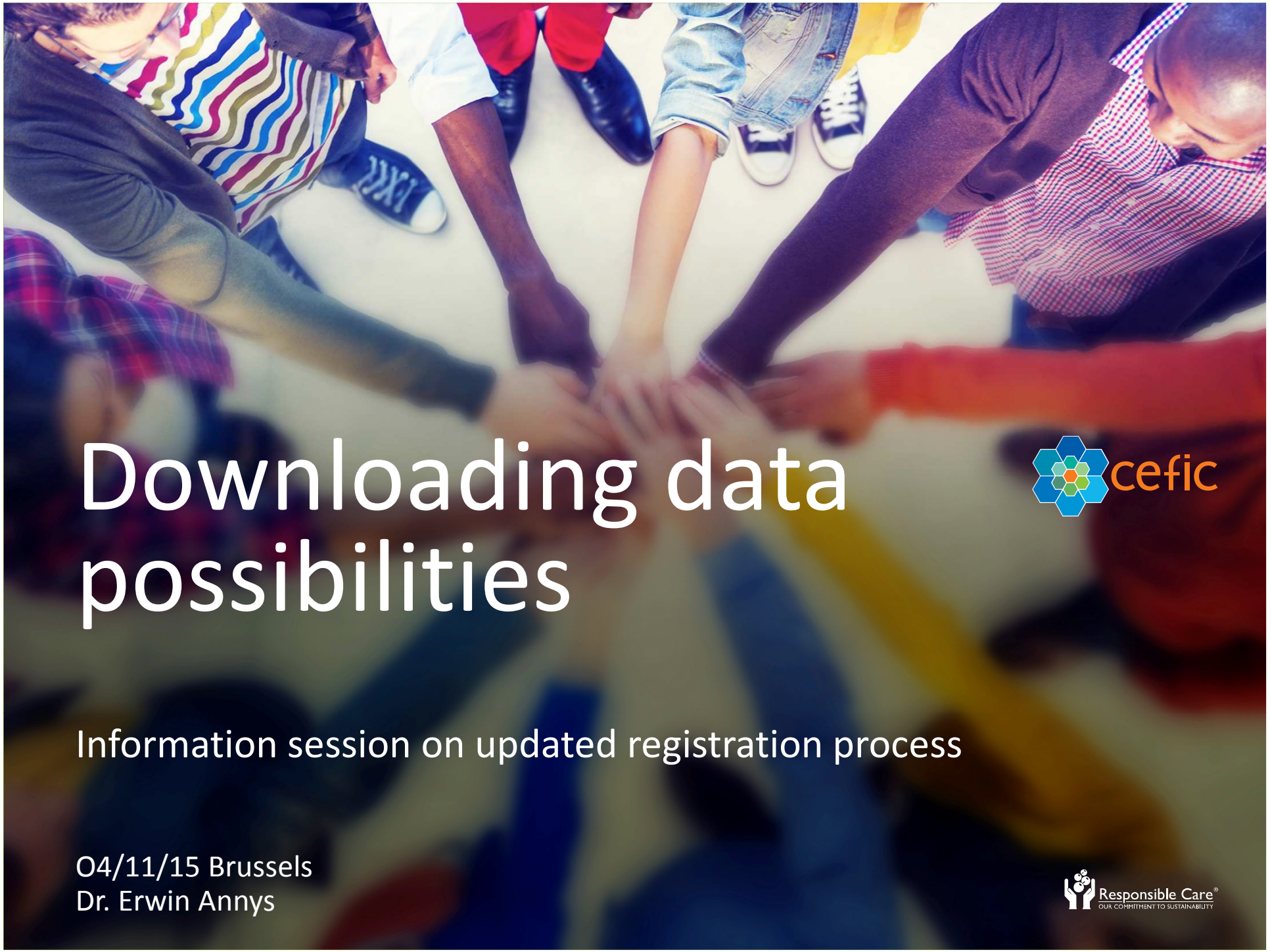


Downloading data possibilities

cefic

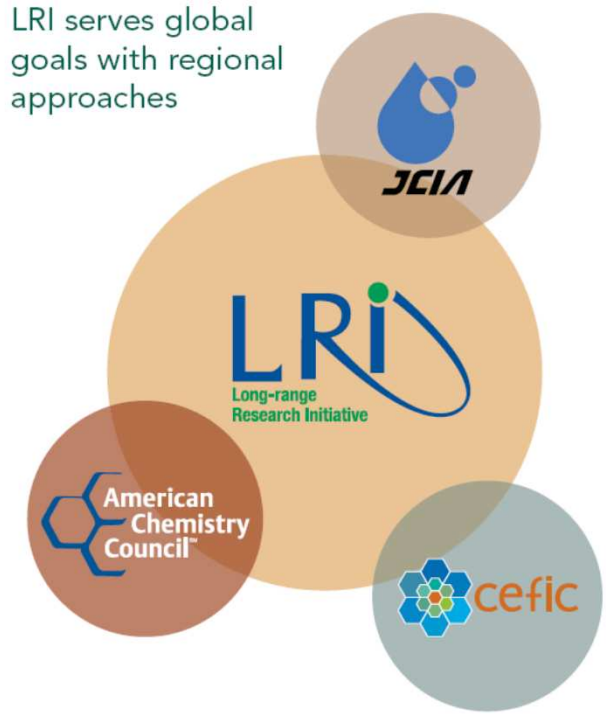
Information session on updated registration process

O4/11/15 Brussels
Dr. Erwin Annys

Responsible Care®
OUR COMMITMENT TO SUSTAINABILITY

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 – interpretation 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 concern

- Eco-systems approach:
  New concept for Ecosystems approach with population relevance

- « Real life Exposure » :
  Predictive, validated exposure scenarios for environmental stressors

- Comparative assessment:
  impact of health and environmental stressors

- Benefit – risks approaches:
  societal drivers for public acceptance for innovation

The Long-range Research Initiative

CEFIC LRI PROJECT EEM9.3-IC
A. THE TOOL: AMBIT-IUCLID

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

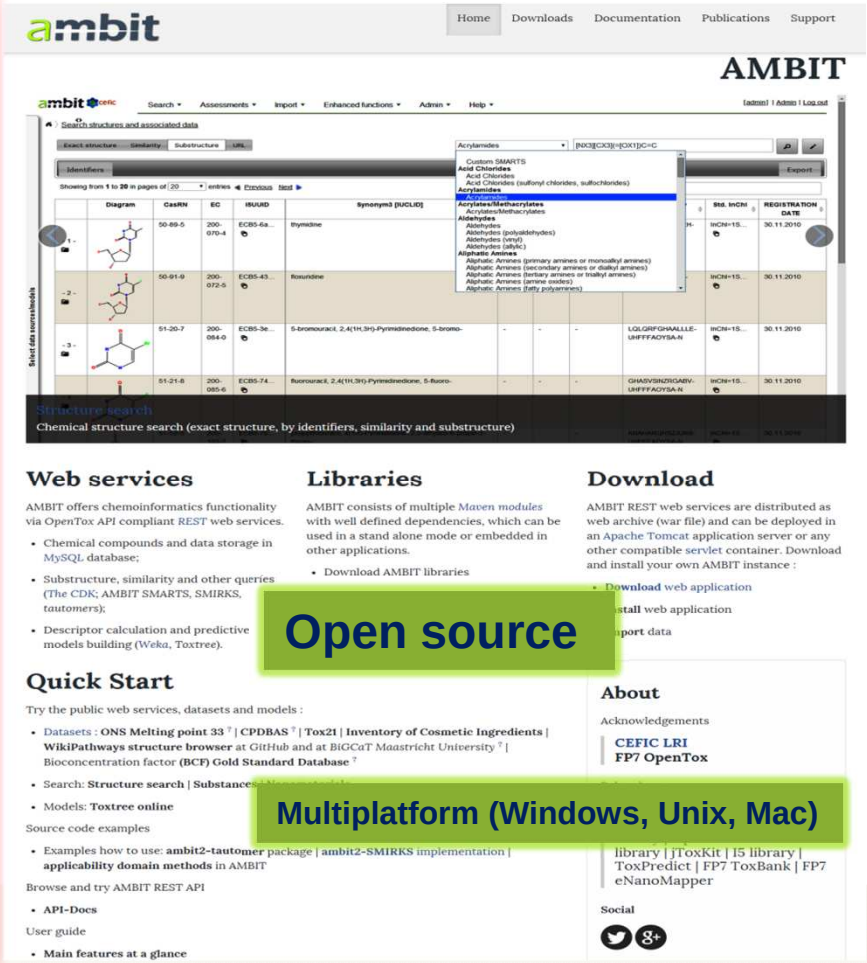
Sep 2013 – Sep 2015

NINA JELIAZKOVA
IdeaConsult Ltd.
Sofia, Bulgaria
www.ideaconsult.net

ambit

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/lri-toolbox/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)



Software

Highly accessed | Open Access

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

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

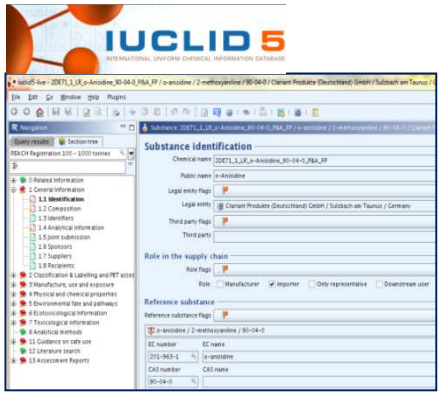
Support read across and category formation workflows

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

Minimize overall testing and resource costs

- Using available studies for other substances as well + WoE

PROJECT OVERVIEW



Data transfer

Company IUCLID DB
ECHA IUCLID DB
As
Major Data Source

Search for data possible but not for structures

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.

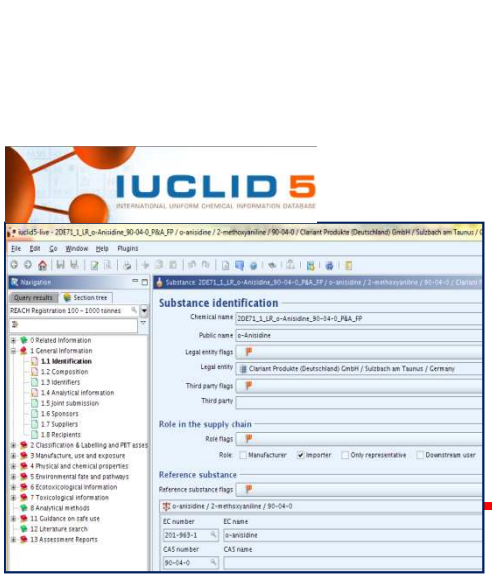
- ***Data management***

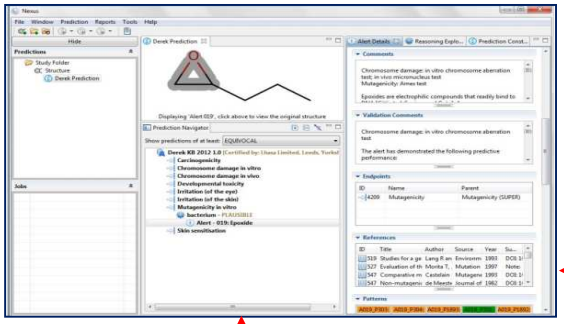
-flexible import/export of data

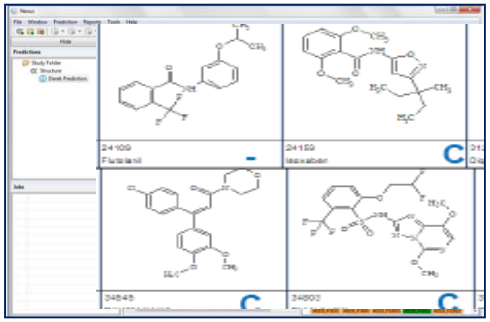
- ***Data exchange***

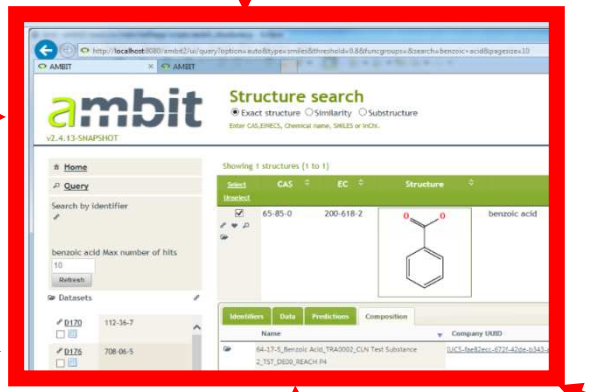
- manual or automated via webservices

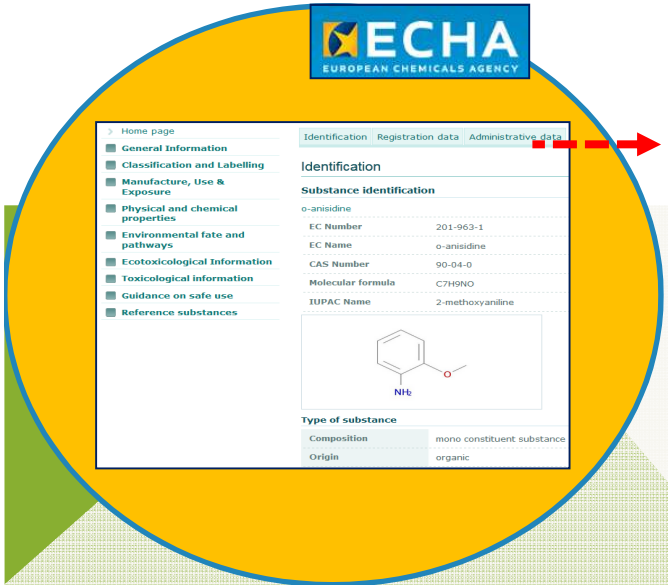
AMBIT COMMUNICATION







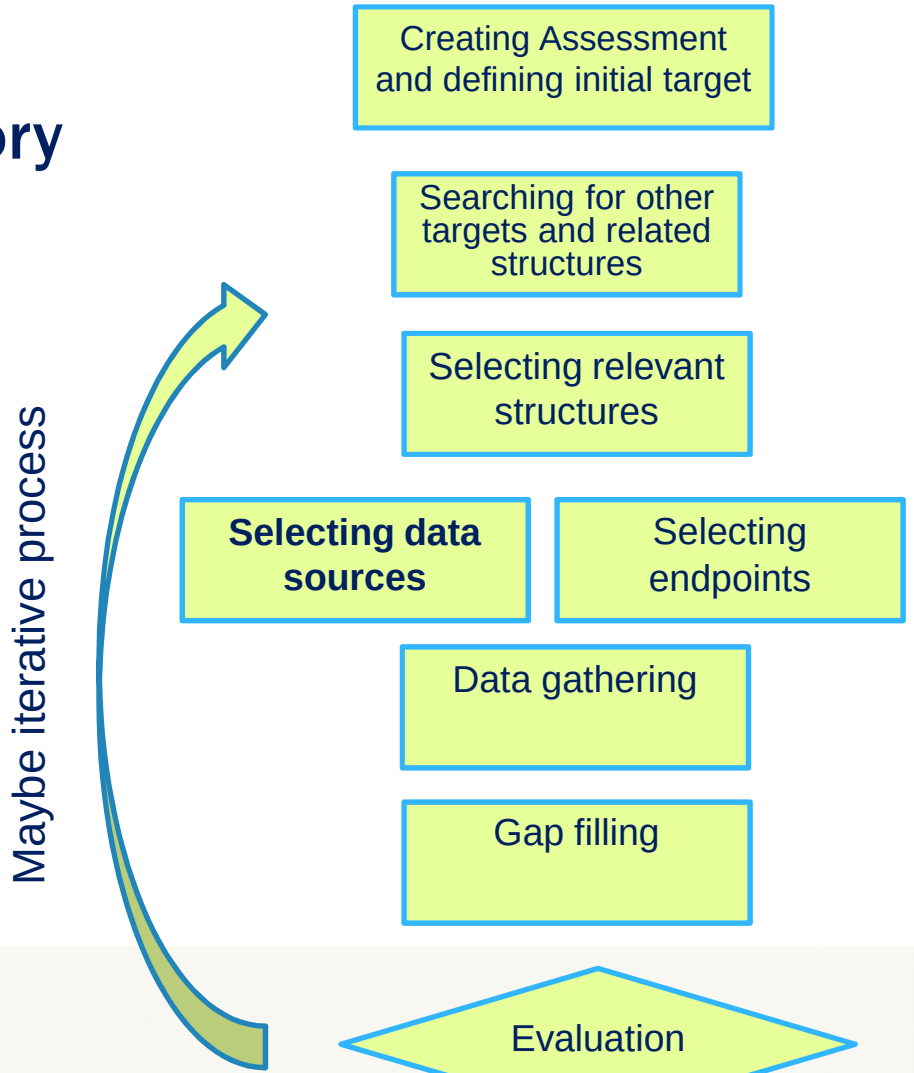




Other Databases & Tools

AMBIT Workflows on Read across & Category formation

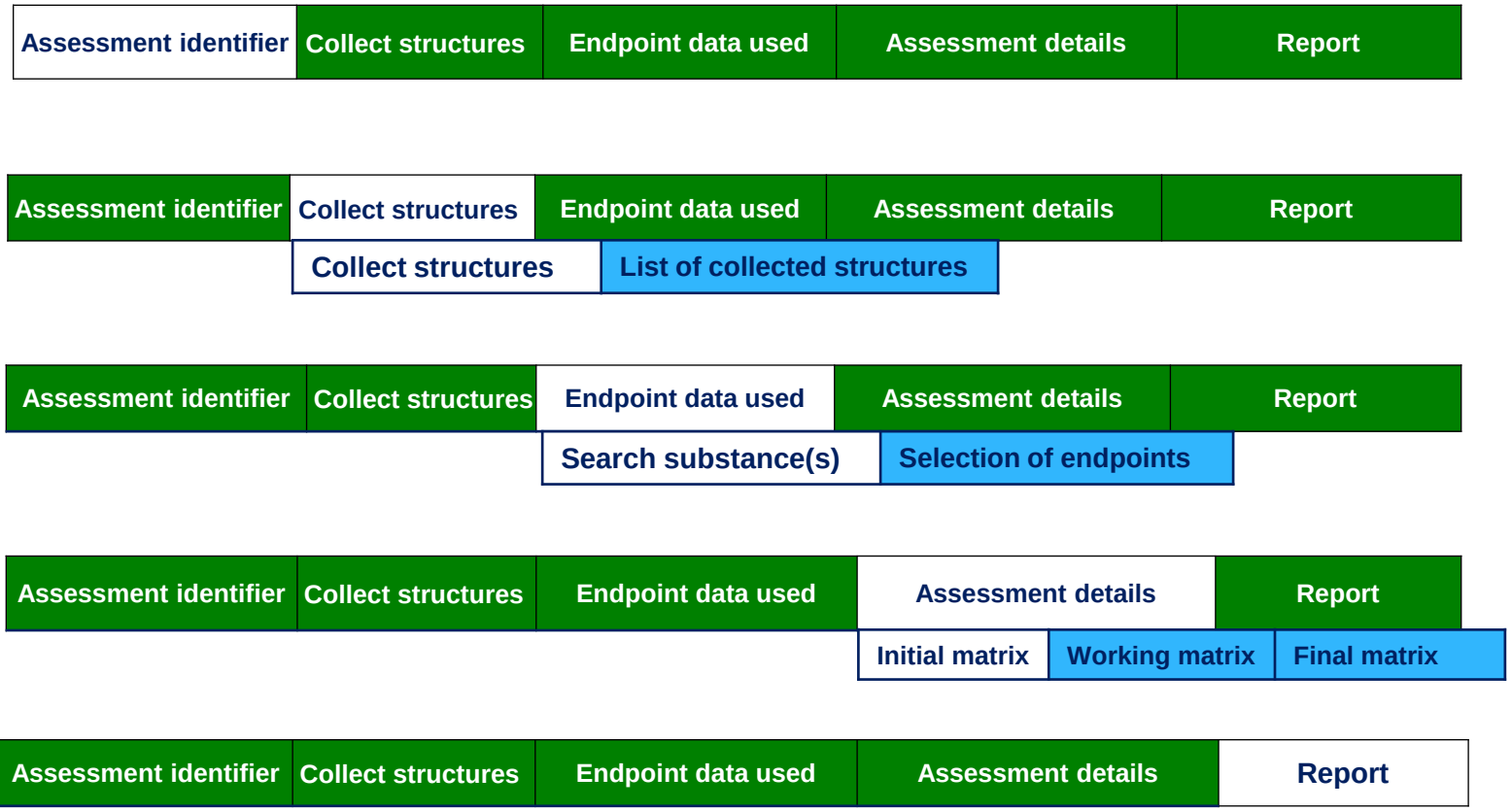
Proposed by Clariant CompTox team



READ ACROSS AND CATEGORY WORKFLOW

5 MAIN STEPS

7 SUB STEPS



- The assessment workflow is organized in five main tabs. Some of the main tabs contain sub-tabs.
- The workflow goes from left to right in the main tabs as well as the sub-tabs.
- In principle, it should be not allowed to leave out any of the steps.

thank you
danke
謝謝
ngiyabonga
teşekkür ederim
gracias
merci
obrigado
dziękuję
bedankt
спасибо
go raibh maith agat
mochchakkeram
sukriya
kop khun krap
terima kasih
감사합니다
ありがとう
grazie
arigatô
takk
dakujem
мерси
tapadh leat
dank je
mauruuru
hvala
sagolun
taiku
ευχαριστώ
рахмат
Баярлалаа
mersi
barka
welalin
tack
spas
kia ora
vinaka
спасибі
blagodaram
misaotra
matondo
paldies
grazzi
mahalo
хвала
asante
manana
obrigada
tenki
murakoze
chokrane
mamnun
дякую
djiere dieuf
tau
akun
dankon
ačiū
köszönöm
gràçie
bayarlalaa
enkosi
nanni
nandri
kiitos
dankie
dhanyavad
chnorakaloutioun
gratias ago
gràcies
sulpáy
sobodi
dèkuji
mèsi
didi madloba
najis tuke
kam sah hamnida
rahmat
tanemirt
rahmet
diolch
dhanyavadagalu
shukriya
merce
trugarez
xièxie
তোমাকে ধন্যবাদ