

# **Using the Go3R search engine to collect toxicological data and 3Rs relevant information for REACH registration dossiers**

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**Neubiberg / Munich - Germany**

# Go3R: 3Rs information & toxicity data for REACH

## 1. Introduction

- How does searching avoid animal testing?
- How can “semantic” tools help searching?

## 2. Go3R

- How is the search engine built →  
to find 3Rs information & toxicity data?

## 3. Search examples

## 4. Outlook

# 1. How does searching help avoid animal testing?

## REACH registration dossiers

### → Information on substance properties

- Collection of all available existing data
- Before compiling new data → info on 3Rs methods  
→ **replacement > reduction / refinement**

→ REACH: Animal testing  
only as a last resort

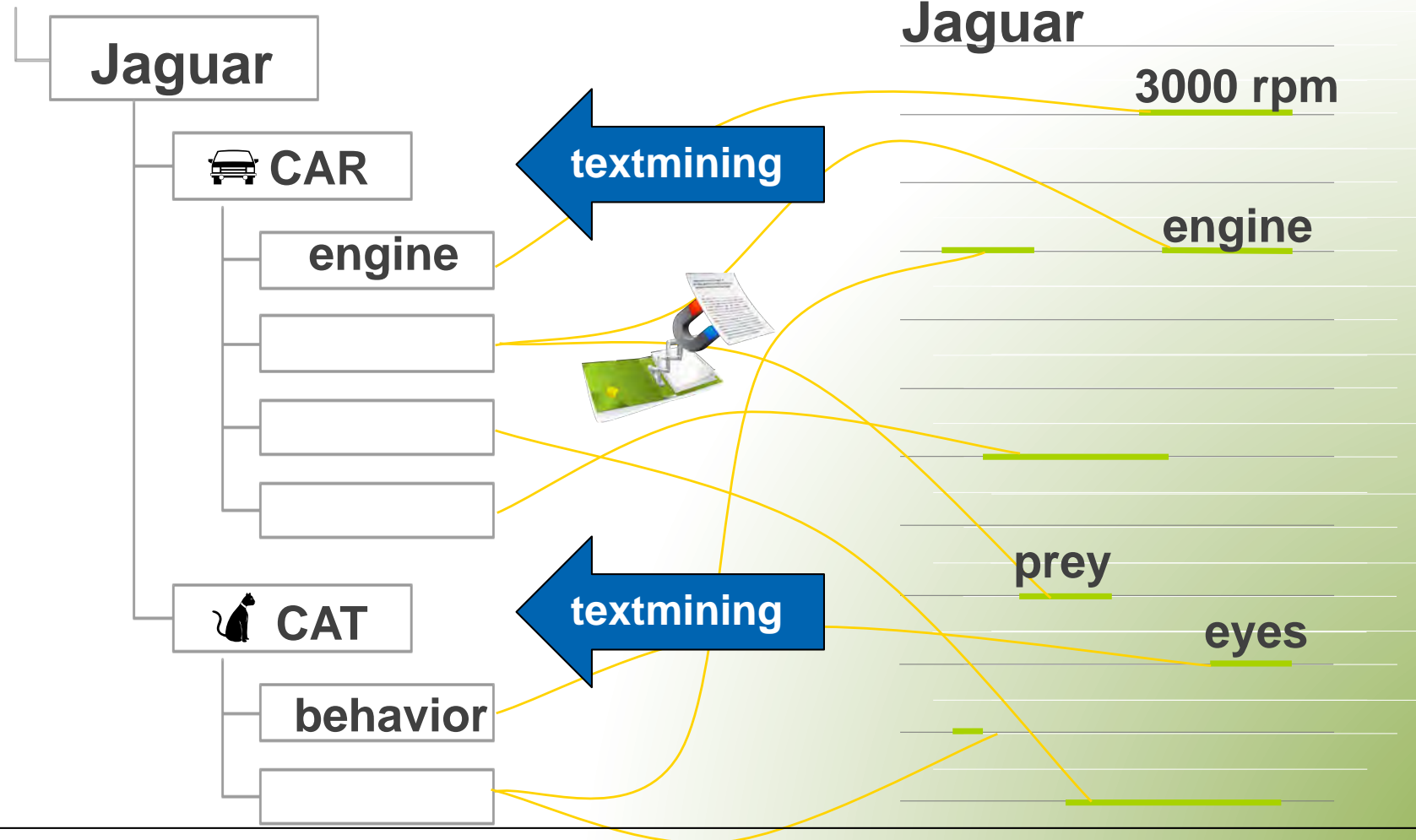
→ Directive 2010/63/EU: 3Rs

# How can semantic tools help searching?

# Semantic tools “understand” and sort information by comparing text to underlying expert knowledge

## Semantic search tool

## Text



**Semantic tools:**

**Underlying expert knowledge:**

**Ontology**

= “Mind map” with concepts, terms and synonyms

### **Go3R**

- **≈ 20,000 3Rs relevant terms**
- **≈ 90,000 synonyms**
- **sorted into 22 branches**
- **up to 11 levels (sub-terms)**

## **...Synonyms:**

Never underestimate the authors' linguistic imagination

### **Example: “eye irritation”**

- eye irritancy
- ocular irritancy
- irritating to the eye, irritant to the eye
- irritant / irritating reactions on [rabbit] eyes
- adverse effects on eyes
- conjunctival reactions
- corneal lesion, corneal opacity
- ocular damage
- ocular safety

**Formulation search query → outcome of search?**

**No: Go3R terms automatically include synonyms**

## 2. How is Go3R built to “understand” & sort information? → [www.Go3R.org](http://www.Go3R.org)

The screenshot shows the Go3R website interface. On the left, there is a sidebar with sections: "my search" (containing Show Clipboard [2], Favorites, Filter Suggestions with filters for Rat, Mouse, Metabolism, Plants, and Gene Expression, and Search in Knowledge Base), "what" (containing 3Rs Searches, Toxicological Information Searches, Nanomaterial-related Searches (BETA), and Knowledge Base), "who" (containing Author list), "where" (containing Pubmed Documents, Toxline Documents, Search the Web for 3Rs Methods, Global, and Find Specific Journal...), and "when" (containing Publication Date with filters for Last Day, Last Week, Last Month, Last Year, and Last 5 Years). The main content area features a search bar with the text "All" and a "find" button. A callout box points to the search bar with the text "box for search queries, searching in PubMed and Toxnet". Above the search bar, there is a navigation bar with links for "Ursula Sauer [Logout]", "Go3R Web", and "Ontology Editor". To the right of the search bar, there is a "Please join and help us helping!" section with a "Donate" button. The footer contains links for "Help", "Contact", "Terms Of Use", "Imprint & Disclaimer", "BMBF Project", and "© 2002-2012 Transinsight GmbH". The right sidebar contains logos for "partners" including BASF, BfR, TECHNISCHE UNIVERSITÄT DRESDEN, and IUCLO 5.



underlying expert knowledge is used to build “table of contents” presented alongside search retrieval

“understand” & sort information?

The screenshot shows the 3R search interface with several filters highlighted by red ovals and callouts:

- my search**: Callout: **personal settings**
- what**: Callout: **topic-related table of contents**
- who**: Callout: **author-related table of contents**
- where**: Callout: **database-, affiliation- and journal-related table of contents**
- when**: Callout: **time-related table of contents**

The interface also includes a search bar, a "find" button, and a "Donate" button. The right sidebar lists partners: BASF, BfR, TECHNISCHE UNIVERSITÄT DRESDEN, and IUCLO 5. The bottom right features a hand holding a white mouse and the text "animal experiments".

## 2. How is Go3R built to “understand” & sort information?

The screenshot displays the Go3R web interface. On the left is a 'Knowledge Base' sidebar with a tree structure of categories and counts. The main content area shows search results for the query '"Eye Irritation"[go3r]'. A search bar at the top right contains the query. Below the search bar, it indicates '7,147 documents found'. The results are listed with titles, authors, and publication details. Several terms in the titles and abstracts are highlighted in green, indicating they are relevant to the search query. A 'Donate' button is visible in the top right corner.

**Knowledge Base**

- 3Rs Institutions [15]
- 3Rs Method Types [1,207]
- 3Rs Methods in the Life Sciences [730]
- 3Rs Principle [75]
- 3Rs Toxicity Testing Strategies [84]
- Animal Care & Handling [109]

**7,147 documents retrieved**

**list of documents, relevant terms highlighted in green**

**box for search queries; using Go3R terms automatically includes synonyms and subordinate terms**

**Search Results:**

**"Eye Irritation"[go3r]**  
7,147 documents found

**statistics**  
**documents**

**Application of the reconstructed rabbit corneal epithelium model to assess the in-vitro eye irritant test of chemicals.**  
Matsuda, Sanae, Hisama, Masayoshi, Shibayama, Hiroharu, Ito, Norihiko, Iwaki, Masahiro  
Yakugaku zasshi : Journal of the Pharmaceutical Society of Japan, Vol. 129 (9): 1113-20, 2009  
The rabbit corneal epithelium model (RCE model) was developed as a three-dimensional in vitro model to replace animal testing for the assessment of eye irritation.

**An alternative test battery in detecting ocular irritancy of agrochemicals.**  
Tavaszi, J, Budai, P, Pálovics, A, Kismányoki, A  
Communications in agricultural and applied biological sciences, Vol. 73 (4): 891-5, 2008  
To get knowledge about eye irritation, recently only the in vivo Draize-test is accepted, which is one of the most criticized methods because of the injuries inflicted on the test animals.

**Acute toxicity testing of chemicals-Opportunities to avoid redundant testing and use alternative approaches.**  
Creton, Stuart, Dewhurst, Ian C, Earl, Lesley K, Gehen, Sean C, Guest, Robert L, Hotchkiss, Jon A, Indans, Ian, Woolhiser, Michael R, Billington, Richard  
Critical reviews in toxicology, Vol. 40 (1): 50-83, 2010  
Assessment of the acute systemic oral, dermal, and inhalation toxicities, skin and eye irritancy, and skin sensitisation potential of chemicals is required under regulatory schemes worldwide.

**Novel cultured porcine corneal irritancy assay with reversibility endpoint.**  
Piehl, Michelle, Gilotti, Albert, Donovan, Alison, DeGeorge, George, Cerven, Daniel

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See also: OECD TG 405



# “table of contents” built to “understand” & sort information?

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  - Animal Care & Handling [109]
  - Animal Conditions, Physiological or Psychological [80]
  - Animal Experiments [1,209]
  - Animal Species [3,141]
  - Body Systems & Structures [6,767]
  - Cell Culture Technology, Etc. [390]
  - Cultured Cells, Tissues, Etc. [1,139]
    - Organisms for Animal Use Alternatives [694]
    - Cells, Cultured [494]
      - Primary Cells [255]
        - Animal Primary Cells [180]
          - Human Primary Cells [84]
        - Cell Lines [239]
          - Cell Lines, Specific Lines [194]
            - Animal Cell Lines [166]
              - Fibroblast Cell Lines [56]
                - V79 Cells [30]
                - 3T3 Cells [22]
                - BHK 21 Cells [3]
                - Mouse Embryonic Fibroblast Cell Line [1]
                - CV-1 Cells [1]
              - CHO Cells [48]
              - Cornea Cell Lines [22]
              - Cancer Cell Lines [18]
              - Lung Cell Lines [17]
              - Epithelial Cell Lines [14]
              - Kidney Cell Lines [10]
              - Neural Cell Lines [3]
              - Endothelial Cell Lines [1]
              - Prostate Cell Lines [1]
            - Human Cell Lines [55]
              - Human Cancer Cell Lines [29]
              - Human Epithelial Cell Lines [20]
                - Human Corneal Epithelial Cell Lines [16]
                - Human Lung Epithelium Cell Lines [3]
                  - Human Alveolar Epithelial Cell Lines [3]
                    - A549 Cells [3]
                - Human Lung Cell Lines [3]

Go3R compares terms in title & abstract to terms in ontology and sorts documents accordingly

Ursula Sauer (Logout)

"Eye Irritation"[go3r]

7,147 documents found

statistics

documents

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ontology branch  
3Rs methods

number of documents  
automatically assigned to  
respective topic

ontology branch  
“animal experiments”

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find

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See also:  
OECD  
TG 405



## agrochemicals.

See also:  
OECD  
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# “table of contents” built to “understand” & sort information?

The screenshot shows the EURL-ECVAM Knowledge Base interface. On the left is a hierarchical tree of categories. A red circle highlights the 'Organisms for Animal Use Alternatives' category, which is expanded to show various cell lines. Three callout boxes provide commentary on the interface:

- “table of contents”** (pointing to the left-hand tree)
- ontology branch *in vitro* test systems** (pointing to the 'Organisms for Animal Use Alternatives' category)
- different levels of terms and subordinate terms** (pointing to the expanded list of cell lines)
- not shown: further ontology branches for *in vitro* endpoints, *in vitro* endpoint detection methods, validation of test methods, etc.** (pointing to the bottom of the tree)

The main content area displays search results. The top result is titled 'model to assess the in-vitro eye' and mentions 'OECD TG 405'. The second result is 'An alternative test battery in detecting ocular irritancy of agrochemicals' by Tavaszi, J., Budai, P., Pálovics, A., and Kismányoki, A. The third result is 'ndant testing and use alternative approaches' by Atchkiss, Jon A., Indans, Ian, Woolhiser, Michael R., and others. The interface includes a search bar, a 'find' button, and a 'Donate' button.

**Finding relevant “topic”  
in table of contents...**

**...too complicated?**

also because relevant information spread out over  
different ontology branches

→ Further processing of underlying expert knowledge

**Goal:**  
for a given test substance, automatically sort all toxicity data into respective IUCLID endpoint categories

- ▼ Toxicological Information Searches
  - ▼ IUCLID 5, Chapter 7
    - ▼ 7.1. Toxicokinetics, metabolism and distribution [3.424 M]
      - 7.1.1. Basic toxicokinetics [3.410 M]
      - 7.1.2. Dermal absorption [14,936]
    - ▼ 7.2. Acute toxicity [353,377]
      - 7.2.1. Acute toxicity: oral [14,174]
      - 7.2.2. Acute toxicity: inhalation [15,851]
      - 7.2.3. Acute toxicity: dermal [3,124]
      - 7.2.4. Acute toxicity: other routes [11,431]
    - ▼ 7.3. Irritation / corrosion [56,775]
      - 7.3.1. Skin irritation / corrosion [11,736]
      - 7.3.2. Eye irritation [9,907]
    - ▼ 7.4. Sensitisation [19,052]
      - 7.4.1. Skin sensitisation [16,308]
      - 7.4.2. Respiratory sensitisation [762]
    - ▼ 7.5. Repeated dose toxicity [64,167]
      - 7.5.1. Repeated dose toxicity: oral [22,786]
      - 7.5.2. Repeated dose toxicity: dermal [1,447]
      - 7.5.3. Repeated dose toxicity: inhalation [8,763]
      - 7.5.4. Repeated dose toxicity: other routes [990]
    - ▼ 7.6. Genetic toxicity [0.923 M]
      - 7.6.1. Genetic toxicity in vitro [26,672]
      - 7.6.2. Genetic toxicity in vivo [533]
    - ▼ 7.7. Carcinogenicity [3.109 M]
    - ▼ 7.8. Toxicity to reproduction [2.864 M]
      - 7.8.1. Toxicity to reproduction [476,148]
      - 7.8.2. Developmental toxicity / teratogenicity [2.504 M]
      - 7.8.3. Toxicity to reproduction: other studies [14,555]
    - ▼ 7.9. Specific investigations [6.112 M]
      - 7.9.1. Neurotoxicity [4.056 M]
      - 7.9.2. Immunotoxicity [1.463 M]
      - 7.9.3. Specific investigations: other studies [2.442 M]
    - ▼ 7.10. Exposure related observations in humans [6.208 M]
      - 7.10.4. Sensitisation data (humans) [79,789]
    - 7.11. Toxic effects on livestock and pets [169,105]
    - 7.12. Additional toxicological information [1.129 M]



## How:

BASF literature for  
registration dossiers as  
“gold standard”

- one-by-one manual  
evaluation of TI / AB
- recognize relevant terms
- process into underlying  
“search term phrase”
- supplementary to  
textmining

The image shows a screenshot of a hierarchical table of contents for 'Toxicological Information Searches'. The structure is as follows:

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**How:**

BASF literature


referred to as  
“go to”

- one manual evaluation of TI / AB
- recognize relevant terms
- process into underlying “search term phrase”
- supplementary to textmining

additional table of contents for IUCILID chapter on toxicological information

|  |  |
|--|--|
| Toxicological Information Searches                         |  |
| IUCILID 5, Chapter 7                                       |  |
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| 7.12. Additional toxicological information [1.129 M]       |  |

## Penetration of benzene, toluene and xylenes contained in gasolines through human abdominal skin in vitro.

 Adami, G, Larèse, F, Venier, M, Barbieri, P, Lo Coco, F, Reisenhofer, E


 Toxicology in vitro ; an international journal published in association with BIBRA, Vol. 20 (8): 1321-30, 2006

We examined three commercial gasolines using the Franz cells and human abdominal full thickness skin.

## IUCLID 7.4.1 – Skin sensitisation

## Spindle disturbances in mammalian cells Toxicity, c-mitosis and aneuploidy with 22 different compounds. Specific and unspecific mechanisms.

 Onfelt, A

 Mutation research, Vol. 182 (3): 135-54, 1987


This points to Ca<sup>2+</sup>-sequestering by mitochondria and/or cellular pH regulation (chlorophenols), Ca<sup>2+</sup> + release and sequestering by the


## IUCLID 7.1.2 - Dermal absorption

## Human potency predictions for aldehydes using the local lymph node assay.

See also:  
OECD  
TG 429 



 Basketter, D A, Wright, Z M, Warbrick, E V, Dearman, R J, Kimber, I, Ryan, C A, Gerberick, G F, White, I R

 Contact dermatitis, Vol. 45 (2): 89-94, 2001

The murine local lymph node assay (LLNA) assesses skin sensitization potential as a function of proliferative responses induced in lymph nodes draining the site of topical exposure to test chemical.

## IUCLID 7.6.1 – (In vitro) genotoxicity



## The joint toxic action of perchloroethylene with benzene or toluene in rats.


 Withey, R J , Hall, J W

 Toxicology, Vol. 4 (1): 5-15, 1975

The joint toxic action of mixtures of perchloroethylene with benzene or toluene was tested at five dose levels for each of six binary combinations with 20 rats per dose.

**IUCLID 7.3.1 –  
Skin irritation;  
(test substance?)**

## Solvent ototoxicity in the rat and guinea pig.

 Lataye, Robert , Campo, Pierre , Pouyatos, Benoît ,  
Cossec, Benoît , Blachère, Véronique , Morel, Georges


 Neurotoxicology and teratology, Vol. 25 (1): 39-50, 2003 Jan-Feb

In the current investigation, the effects of two solvents, toluene (600 ppm) and styrene (1000 ppm), were studied in both Long-Evans rats and pigmented guinea pigs exposed 6 h/day for 5 consecutive days.

**IUCLID 7.2.1 –  
(Acute oral)  
toxicity**

## Evaluation of the cutaneous-irritation potential of 56 compounds.

 Guillot, J P , Gonnet, J F , Clement, C , Caillard, L , Truhaut, R

 Food and chemical toxicology : an international journal published for the  
British Industrial Biological Research Association, Vol. 20 (5): 563-72,  
1982

The primary cutaneous irritation of 56 chemicals was tested in the rabbit using three different procedures.

**IUCLID 7.5.3 –  
Repeated-dose  
inhalation toxicity**

# Examples – just for show!

## 7.3.2. Eye irritation

“In Vivo Test Methods, Eye Irritation”[go3r] OR “3Rs in Eye Irritation Testing”[go3r]

“Eye Irritation”[go3r] OR “Eye Corrosivity”[go3r]

## 7.8.2. Developmental toxicity / teratogenicity

(“Developmental Toxicity”[go3r] OR “Prenatal Developmental Toxicity”[go3r] OR Embryotoxicity[go3r] OR Teratogenicity[go3r] OR “Developmental Neurotoxicity”[go3r] OR “Ovarian Toxicity”[go3r]) NOT fish[go3r] NOT “Daphnia magna”[go3r] NOT Amphibian[go3r]

“Neonatal Exposure”[go3r] OR “Prenatal Exposure”[go3r] OR “Juvenile Exposure”[go3r] OR “Maternal Weight Gain”[go3r] OR “Weaning”[go3r] OR “Gestational Exposure”[go3r]

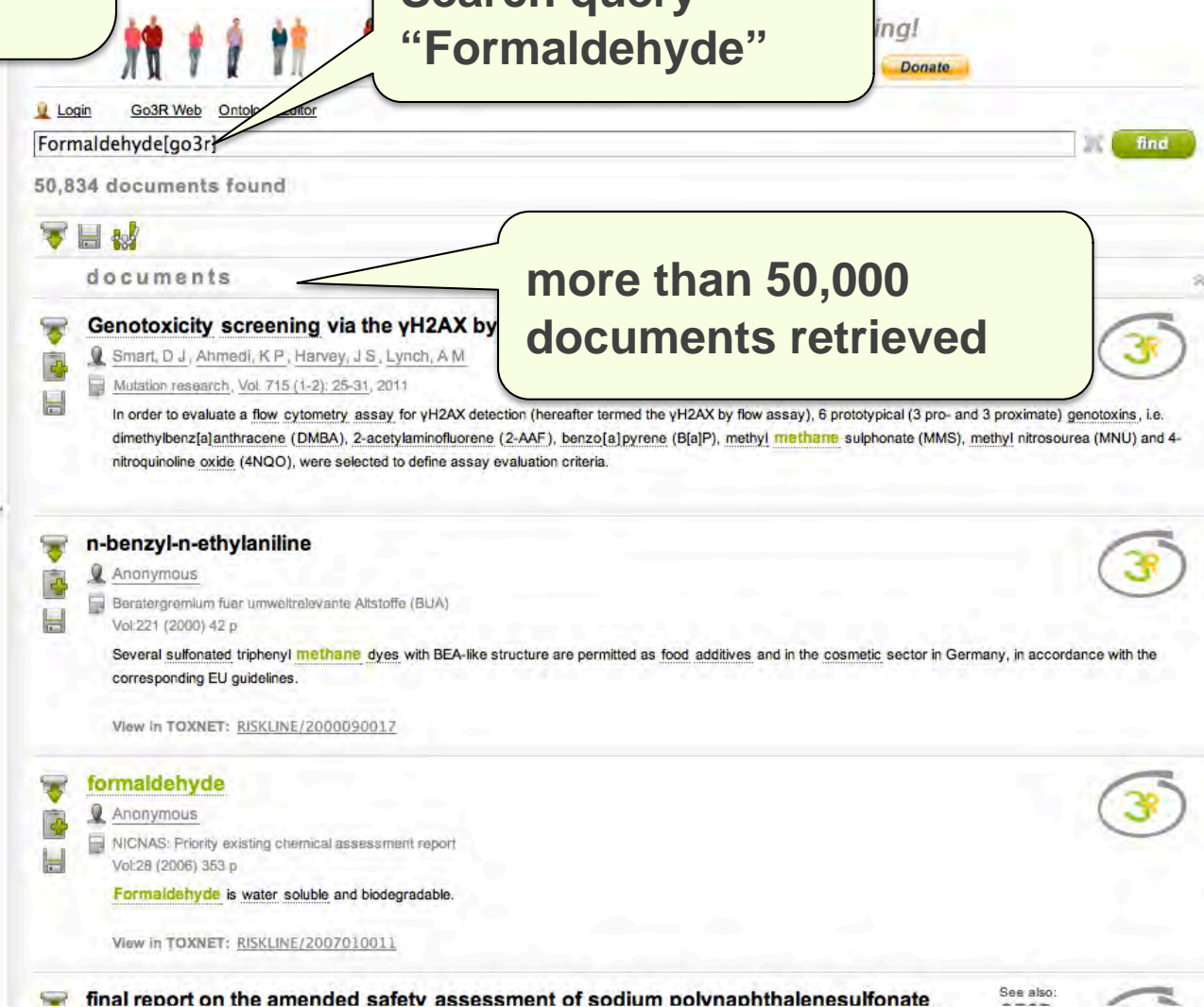
(“Prenatal Developmental Toxicity Study”[go3r] OR “Developmental Neurotoxicity Study”[go3r]) NOT Fish[go3r] NOT “Daphnia Magna”[go3r] NOT Amphibian[go3r]

(“Congenital, Hereditary, and Neonatal Diseases and Abnormalities”[go3r] OR “Pregnancy Complications”[go3r] OR “Embryonic Structures”[go3r] OR “Developmental Biology”[go3r] OR “Embryo-Related Endpoints”[go3r] OR “Embryonic and Fetal Development”[go3r]) NOT “Fetal Blood”[go3r]

### 3. Get relevant documents sorted in accordance to respective IUCLID endpoints



Search query  
"Formaldehyde"





### 3. Go3R: Retrieving toxicological data for a given test substance

The screenshot displays the IUCLID 7.6.1 web interface. On the left, a tree view shows the hierarchy of toxicological endpoints. A yellow callout box highlights 'IUCLID 7.6.1 Genetic toxicity in vitro'. A red circle highlights the '7.6.1. Genetic toxicity in vitro [288]' item in the tree. On the right, the search results page shows '288 of 50,834 documents found (browsed for 7.6.1. Genetic toxicity in vitro)'. A red arrow points to the search bar. The first document is titled 'A metabolomic and multivariate statistical process to assess the effects of genotoxins in Saccharomyces cerevisiae.' and includes a red circle around the text 'Current in vitro strategies for genotoxicity testing suffer from high irrelevant positive rate, requiring the need for the development of new in vitro tools.' The second document is titled 'Genotoxicity screening via the γH2AX by flow assay.' and includes a red circle around the text 'Results were compared with Ames bacterial and in vitro mammalian genotoxicity tests (mouse lymphoma assay and/or chromosome aberration assay). γH2AX by flow assay results were highly predictive of Ames (sensitivity 100%; specificity 67%; concordance 82%) and in vitro mammalian genotoxicity tests (sensitivity 91%; specificity 89%; concordance 91%) and provide additional evidence that γH2AX is a biomarker of potential genotoxic activity, underpinned mechanistically by the cellular response to DSBs.' The third document is titled 'Extended-term cultures of human T-lymphocytes and the comet assay: a useful combination when testing for genotoxicity in vitro?' and includes a red circle around the text 'The use of extended-term cultures of human T-lymphocytes in the alkaline single-cell gel electrophoresis assay (comet assay) was evaluated as a test for the potential genotoxicity of chemicals.'

**IUCLID 7.6.1**  
**Genetic toxicity in vitro**

Please join and help us helping!  
Donate to contribute to further developments and keep this free service alive

288 of 50,834 documents found (browsed for 7.6.1. Genetic toxicity in vitro)

**documents**

**A metabolomic and multivariate statistical process to assess the effects of genotoxins in *Saccharomyces cerevisiae*.**  
Titman, Christopher M., Downs, Susan A., Oliver, Stephen G., Carmichael, Paul L., Scott, Andrew D., Griffin, Julian L.  
Molecular bioSystems, Vol. 5 (12): 1913-24, 2009  
Current in vitro strategies for genotoxicity testing suffer from high irrelevant positive rate, requiring the need for the development of new in vitro tools.

**Genotoxicity screening via the γH2AX by flow assay.**  
Smart, D. J., Ahmed, K. P., Harvey, J. S., Lynch, A. M.  
Mutation research, Vol. 715 (1-2): 25-31, 2011  
Results were compared with Ames bacterial and in vitro mammalian genotoxicity tests (mouse lymphoma assay and/or chromosome aberration assay). γH2AX by flow assay results were highly predictive of Ames (sensitivity 100%; specificity 67%; concordance 82%) and in vitro mammalian genotoxicity tests (sensitivity 91%; specificity 89%; concordance 91%) and provide additional evidence that γH2AX is a biomarker of potential genotoxic activity, underpinned mechanistically by the cellular response to DSBs.

**Extended-term cultures of human T-lymphocytes and the comet assay: a useful combination when testing for genotoxicity in vitro?**  
Andersson, Maria, Agurell, Eva, Vaghef, Hamid, Bolosfoldi, George, Hallman, Björn  
Mutation research, Vol. 540 (1): 43-55, 2003  
The use of extended-term cultures of human T-lymphocytes in the alkaline single-cell gel electrophoresis assay (comet assay) was evaluated as a test for the potential genotoxicity of chemicals.

**4: final report on the amended safety assessment of sodium**  
See also: OECD

# **How well does Go3R address the challenge to collect information under REACH?**

Find the right balance:

Underlying search term phrases too broad:

> too many insignificant documents

Underlying search term phrases too narrow:

> too many significant documents missing



### 3. Go3R: Sorting into IUCLID categories

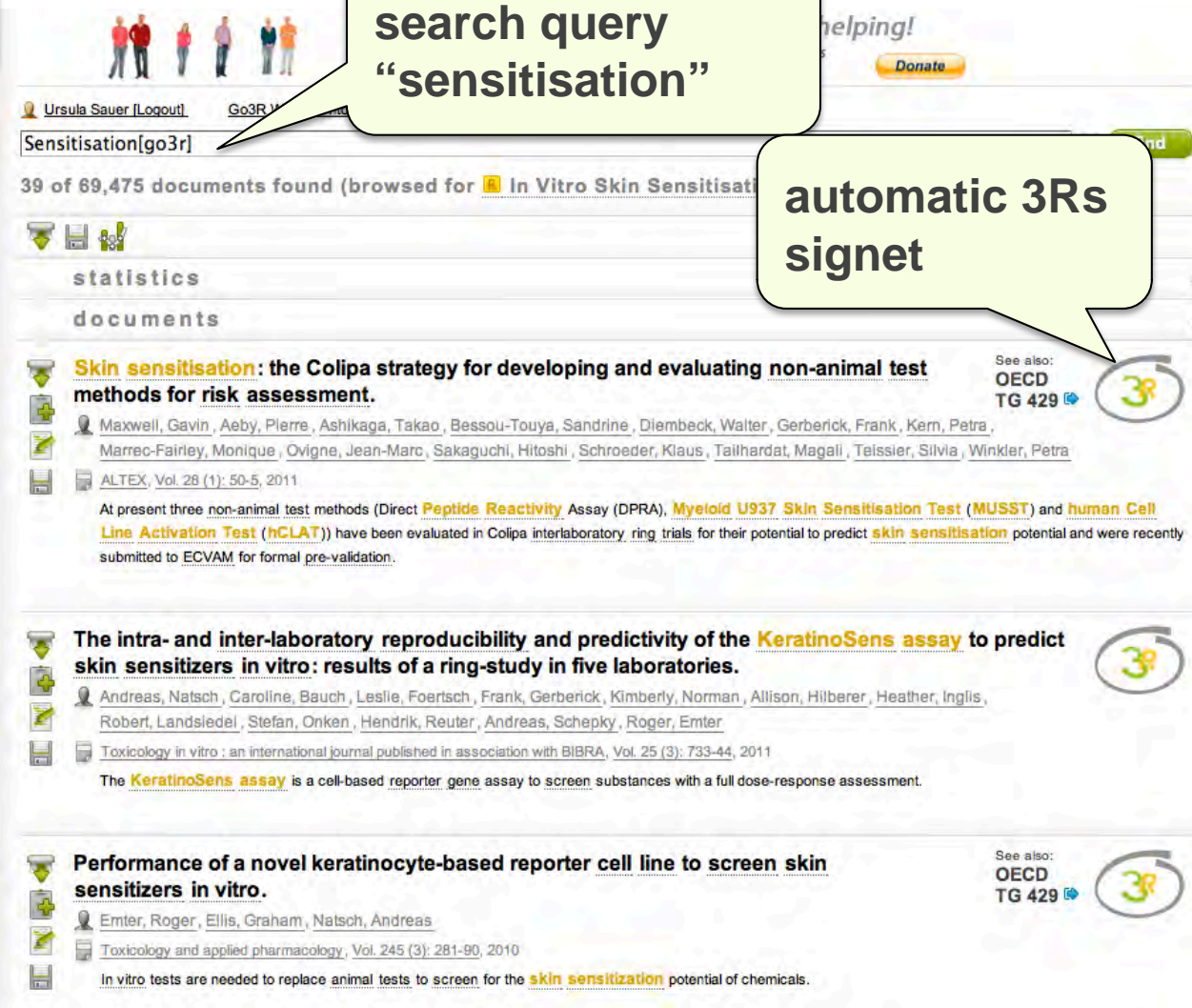
| IUCLID category                 | Substance 1 | Substance 2 | Substance 3 |
|---------------------------------|-------------|-------------|-------------|
| 7.1 toxicokinetics              | 88 %        | 100%        | 100%        |
| 7.2 acute toxicity              | 75 %        | -           | 60%         |
| 7.3 irritation / corrosion      | 75 %        | 88%         | 100%        |
| 7.4 sensitisation               | -           | 71%         | -           |
| 7.5 repeated dose toxicity      | 57%         | 100%        | 33%         |
| 7.6 genetic toxicity            | 100%        | 100%        | 100%        |
| 7.7 carcinogenicity             | 100%        | 100%        | 100%        |
| 7.8 reprodct./develop. toxicity | 67%         | 100%        | 95%         |
| 7.9.1 neurotoxicity             | 100%        | -           | 100%        |
| 7.9.2 immunotoxicity            | -           | -           | 100%        |
| 7.9.3 other investigations      | 79%         | 67%         | 85%         |
| 7.10 human data                 | 44%         | 92%         | 83%         |
| <b>Total</b>                    | <b>71%</b>  | <b>85%</b>  | <b>89%</b>  |

### 3. Go3R: Retrieving information on 3Rs methods

3Rs methods sorted  
by area of use

search query  
“sensitisation”

automatic 3Rs  
signet



### 3. Go3R: Retrieving information on 3Rs methods

Area of use “toxicity testing” > “skin sensitisation” > “reduction / refinement methods”

search query  
“sensitisation”

Area of use “toxicity testing” > “skin sensitisation” > “replacement methods”

my search results

what

3Rs Search

3Rs in Toxicology [39]

3Rs Methods [39]

3Rs in Human [39]

3Rs in Acute [6]

3Rs in Mutagenicity [0]

3Rs in Sensitisation [39]

3Rs in Skin Sensitisation Testing [39]

Local Lymph Node Assay [24]

Non-Radio Isotopic LLNA [0]

Reduced LLNA [0]

Murine Skin Sensitisation Test [0]

Popliteal Lymph Node Assay [0]

Skin Sensitisation Testing, Replacement Methods [39]

In Vitro Skin Sensitisation Testing [39]

Peptide Reactivity Assay [22]

Human Cell Line Activation Test [11]

KeratinoSens Assay [3]

Modular Immune In Vitro Construct [2]

Myeloid U937 Skin Sensitisation Test [2]

Human Skin Chick CAM Model [1]

3Rs in Organ Specific Toxicity Testing [0]

3Rs in Toxicokinetics Testing [0]

3Rs in Carcinogenicity Testing [0]

3Rs in Irritation Testing [2]

3Rs in Repeated-Dose Toxicity Testing [0]

3Rs in Photosensitisation Testing [0]

3Rs in Reproductive and Developmental Toxicity Testing [0]

3Rs in Endocrine Disruptor Testing [0]

QSAR / In Silico Toxicity Testing [1]

3Rs in Ecotoxicity Testing [0]

3Rs in Nanomaterial Testing [0]

3Rs in Biocompatibility Testing [0]

3Rs in Pharmacology [0]

3Rs in Pharmacy [0]

Ursula Sauer (Logout) Go3R V...

Sensitisation[go3r]

39 of 69,475 documents found (browsed for In Vitro Skin Sensitisation Testing)

statistics

documents

**Skin sensitisation: the Colipa strategy for developing and evaluating non-animal test methods for risk assessment.**

See also: OECD TG 429

Maxwell, Gavin, Aeby, Pierre, Ashikaga, Takao, Bessou-Touya, Sandrine, Diembeck, Walter, Gerberick, Frank, Kern, Petra, Marrec-Fairley, Monique, Ovigne, Jean-Marc, Sakaguchi, Hitoshi, Schroeder, Klaus, Tailhardat, Magali, Teissier, Silvia, Winkler, Petra

ALTEX, Vol. 28 (1): 50-5, 2011

At present three non-animal test methods (Direct Peptide Reactivity Assay (DPRA), Myeloid U937 Skin Sensitisation Test (MUSST) and human Cell Line Activation Test (hCLAT)) have been evaluated in Colipa interlaboratory ring trials for their potential to predict skin sensitisation potential and were recently submitted to ECVAM for formal pre-validation.

predictivity of the KeratinoSens assay to predict five laboratories.

See also: OECD TG 429

Gerberick, Kimberly, Norman, Allison, Hilberer, Heather, Inglis, Shepky, Roger, Emter

ALTEX, Vol. 25 (3): 733-44, 2011

open substances with a full dose-response assessment.

cell line to screen skin

See also: OECD TG 429

Emter, Roger, Ellis, Graham, Natsch, Andreas

Toxicology and applied pharmacology, Vol. 245 (3): 281-90, 2010

in vitro tests are needed to replace animal tests to screen for the skin sensitization potential of chemicals.



### 3. Go3R: PubMed & Toxnet not enough? > Go3R-Web

Google search  
> higher ranking for  
170 selected 3Rs websites

e.g. TSAR, ICCVAM,  
ECVAM, AltTox, AltWeb

information on

- test protocols
- validation
- regulatory acceptance

The screenshot shows the Go3R-Web search interface. The search term 'sensitisation' is entered in the search bar. Below the search bar, there are filters for 'Ergebnisse verfeinern' (Refine results) with options: 'Alle Ergebnisse' (All results), 'Reduction', 'In vitro endpoints', 'Animal', 'Replacement', 'Non-animal', 'Refinement', 'Validated test method', 'Human', and 'Toxicology'. The search results show approximately 120,000 results in 0.35 seconds. The first result is 'TSAR (Tracking System for Alternative test methods Review ...)' with a link to 'tsar.jrc.ec.europa.eu/Label Refinement'. The second result is 'OECD GUIDELINE FOR TESTING OF CHEMICALS' with a link to 'iccvam.niehs.nih.gov/SuppDocs/FedDocs/OECD/OECDtg406.pdf'. The third result is 'Skin sensitisation' with a link to 'ecvam.jrc.it/page\_pdf.cfm?voce=ip&idvoce=258'. The fourth result is 'Skin Sensitization: What is it? Why is it important? What are the ...' with a link to 'alttox.org/ttr/toxicity-tests/skin/.../kimber-gerberick/Label Refinement'. The fifth result is 'Skin Sensitisation: The Colipa Strategy for Developing and ...' with a link to 'altweb.jhsph.edu/altex/28\_1/altex\_2011\_1\_maxwell.pdf'.

# Go3R: Semantic search engine to avoid animal testing in regulatory toxicity testing



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# Go3R: Conclusion and outlook

## BMBF Project Go3R

**End 31 May 2012**

- Established to be used in the context of REACH
- Toxicological data and information 3Rs methods
- Currently searching in PubMed and Toxnet
- Can be adapted to search in other databases
- Can be adapted to search in in-house databases
- Ontology and search queries require further processing and continuous updating
- Ontology: unfinished branches for further topics other than regulatory toxicology