

Instructions on how to use the EURL ECVAM Genotoxicity & Carcinogenicity Consolidated Database of Ames Positive Chemicals

The **ECVAM Genotoxicity & Carcinogenicity DB** is presented as an Excel table. Users are able to browse through the data with basic Excel functionality, but can also use it for further calculations, if necessary. Detailed information on the criteria adopted for the construction and analysis of the DB can be found in the manuscript: <http://dx.doi.org/10.1016/j.mrgentox.2014.10.006>

Download of the ECVAM Genotoxicity & Carcinogenicity DB

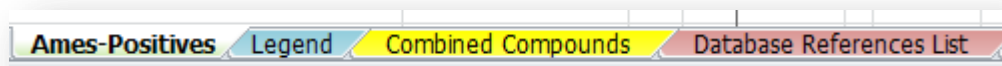
To download the ECVAM Genotoxicity & Carcinogenicity DB, use this link from the European Commission JRC Open Data Catalogue:

ftp://cidportal.jrc.ec.europa.eu/jrc-opendata/EURL-ECVAM/datasets/genotox/ECVAM_Ames_positives_DB.xls

Open the file in your local MS Excel © installation.

Overall structure of the ECVAM Genotoxicity & Carcinogenicity DB

The ECVAM Genotoxicity & Carcinogenicity DB Excel workbook consists of four tabs (see bottom of the Excel screen):



- Tab **Ames-Positives** contains all data.
- Tab **Legend** contains explanations and indications.
- Tab **Combined Compounds** contains the list of combined free bases and respective simple acid salts or R- and S- isomers for those chemicals where, a similar behavior is expected and/or proven in the aqueous environment of the in vitro and in vivo studies under consideration.
- Tab **Database Reference List** contains the information from peer-reviewed literature or expert publications used to fill in missing test data or resolve apparent discrepancies in results among the different sources reporting on the same chemical.

The guidance in this document covers the features of the tab "Ames-Positives".

Chemicals

The ECVAM Genotoxicity & Carcinogenicity DB contains 726 chemicals. Each row in the table reports on one chemical:

| | A | B | F | G |
|----|----------------------------------|----------------|-----------------------|---------------------|
| 1 | | | | |
| 2 | <i>Chemical</i> | <i>CAS No.</i> | <i>Chem Agora</i> | <i>Che LIST</i> |
| 3 | | | | |
| 4 | Acetochlor | 34256-82-1 | » | » |
| 5 | 4-Acetylamino fluorene | 28322-02-3 | » | » |
| 6 | N-Acetoxy-2-acetylamino fluorene | 6098-44-8 | » | » |
| 7 | 1'-Acetoxysafrole | 34627-78-6 | » | » |
| 8 | 2-Acetylamino fluorene | 53-96-3 | » | » |
| 9 | 1-Acetyl-2-phenylhydrazine | 114-83-0 | » | » |
| 10 | Acid blue 9 | 2650-18-2 | » | » |
| 11 | Acranyl dihydrochloride | 1684-42-0 | » | » |
| 12 | Acrolein | 107-02-8 | » | » |
| 13 | Acrylonitrile | 107-13-1 | » | » |
| 14 | Adriamycin [AKA doxorubicin] | 23214-92-8 | » | » |
| 15 | Aflatoxicol | 29611-03-8 | » | » |
| 16 | Aflatoxin B1 | 1162-65-8 | » | » |
| 17 | Agaritin | 2757-90-6 | » | » |

Chemicals are identified by:

- **Name** (column A)
- **CAS** Registration Number (column B), where possible

The table is sorted by Name.

In case more background information is needed for a chemical, columns F and G feature clickable links to two public JRC databases:

- **ChemAgora** (column F), a website that provides direct links to information about the chemical in question in numerous third party DBs;
- **CheLIST** (column G), a website that provides a means of identifying whether a chemical has been used in a research or validation project (including EU-funded, international and JRC projects), and also whether the chemical of interest is regulated and listed under a specific regulatory inventory.

Clicking on the "[>>](#)" symbol leads directly to the external website.

The link to the two websites works via the CAS Registration number. If for a chemical the CAS Registration Number is not known, the link is not provided. If there are two or more CAS Registration numbers in column B, the link uses the first one.

Test results reported in the ECVAM Genotoxicity & Carcinogenicity DB

The ECVAM Genotoxicity & Carcinogenicity DB shows, for each chemical, the available results from different sources for the following *in vitro* and *in vivo* tests:

- AMES test
- In vitro mammalian cell tests

- **MLA:** in vitro MLA Tk^{+/-} gene mutation (Hprt) assay
- **MN:** in vitro Micronucleus test
- **CA:** in vitro Chromosomal Aberrations test
- In vivo tests
 - **MN:** in vivo MN genotoxicity test
 - **CA:** in vivo Chromosomal Aberrations test
 - **UDS:** in vivo Unscheduled DNA Synthesis
 - **transgenic:** in vivo transgenic gene mutation assay
 - **DNA Damage:** in vivo DNA damage (COMET or alkaline elution assay)
- Carcinogenicity studies

| U | V | AH | AT | BH | BI | BJ | BK | BW | CI | CU | DB | DJ | DK | DL | DM | EA |
|--------------|---|----------------------|---------------------|---------------------|----|----|----|--------------------|--------------------|---------------------|--------------------|----------------------------|----|----|----|--------------|
| | | in vitro overall | | | | | | | in vivo overall | | | | | | | |
| Ames Overall | | in vitro MLA Overall | in vitro MN Overall | in vitro CA Overall | + | - | | in vivo MN Overall | in vivo CA Overall | in vivo UDS Overall | transgenic Overall | in vivo DNA damage Overall | + | - | | CARC Overall |

In its

default collapsed view (see chapter "Collapsed vs. expanded view" below), the DB shows the **Overall Call** (final conclusion) made for each test as the result of an expert evaluation of all the single entries (which are visible in the expanded view).

Color coding

Overall calls for each test are limited to the following 4 categories, which are based on defined criteria described in the manuscript, <http://dx.doi.org/10.1016/j.mrgentox.2014.10.006>:

- "+" = positive
- "-" = negative
- "E" = equivocal
- "I" = inconclusive

In order to quickly identify chemicals with a high or low number of "+" or "-" genotoxicity results *in vitro* and *in vivo*, the DB features color-coded indicator columns:

- The more intensive the **red** color shading, the more "+" were reported in the overall summaries.
- The more intensive the **green** color shading, the more "-" were reported in the overall summaries.

| | Chemical | CAS No. | Chem Agora | ChE LIST | Ames Overall | in vitro MLA Overall | in vitro MN Overall | in vitro CA Overall | + - | in vivo MN Overall | in vivo CA Overall | in vivo UDS Overall | transge nic Overall | in vivo DNA damage Overall | + - |
|----|--|--------------------|---------------|-------------|-----------------|----------------------------|---------------------------|---------------------------|-----|--------------------------|--------------------------|---------------------------|---------------------------|-------------------------------------|-----|
| 24 | 2-Aminoanthraquinone | 117-79-3 | Ⓜ | Ⓜ | + | + | + | + | 3 0 | | | | | | 0 0 |
| 25 | 4-Aminozobenzene | 60-09-3 | Ⓜ | Ⓜ | + | E | | | 0 0 | + | | | | + | 2 0 |
| 26 | 4-Aminobiphenyl (free base + HCL salt) | 92-67-1/ 2113-61-3 | Ⓜ | Ⓜ | + | + | | | 2 0 | + | + | + | + | | 4 0 |
| 27 | 4-Amino-4'-chlorobiphenyl | 135-68-2 | Ⓜ | Ⓜ | + | + | | | 0 0 | | + | | | | 1 0 |
| 28 | 5-Amino-4-chloro-o-cresol-HCl-COLPA A117 | 110102-85-7 | Ⓜ | Ⓜ | + | - | + | | 1 1 | - | | | | | 0 1 |
| 29 | 2-Amino-4-chlorophenol | 95-85-2 | Ⓜ | Ⓜ | + | | | + | 1 0 | | | | | | 0 0 |

Please

note that this feature is not intended to express any scientific assessment or classification whatsoever; it is merely indicative and color-codes the numbers of "+" and/or "-" genotoxicity results *in vitro* and *in vivo*.

Collapsed vs. expanded view

The default view when opening the ECVAM Genotoxicity & Carcinogenicity DB is "collapsed", i.e. an overview is shown on the '**Overall Calls**' for each endpoint, with details hidden:

| 1 Collapse everything | | 2 Expand everything | | Expand single test | | | | | | | | | | | | | | | | | | | |
|-----------------------|-----------------------------------|---------------------|-------------|--------------------|----------------------------|---------------------------|---------------------------|-----|--------------------------|--------------------------|---------------------------|---------------------------|-------------------------------------|-----|----------------|----|----|----|----|----|----|----|--|
| A | B | F | G | U | V | AH | AT | BH | BI | BJ | BK | BW | CI | CU | DB | DJ | DK | DL | DN | EA | EB | EC | |
| Chemical | CAS No. | Chem Agora | ChE LIST | Ames Overall | in vitro overall | | | | in vivo overall | | | | CARC Overall | (a) | Other Tests | | | | | | | | |
| | | | | | in vitro MLA Overall | in vitro MN Overall | in vitro CA Overall | + - | in vivo MN Overall | in vivo CA Overall | in vivo UDS Overall | transge nic Overall | in vivo DNA damage Overall | + - | | | | | | | | | |
| 4 | Acetochlor | 34256-82-1 | Ⓜ | Ⓜ | + | + | + | 2 0 | | | | | | | | | | | | | | | |
| 5 | 4-Acetylamino fluorene | 28322-02-3 | Ⓜ | Ⓜ | + | E | - | 0 2 | | | | | | | | | | | | | | | |
| 6 | N-(Acetoxy-2-acetylamino fluorene | 6098-44-8 | Ⓜ | Ⓜ | + | + | + | 2 0 | | | | | | | | | | | | | | | |
| 7 | 1-Acetoxy safrole | 34627-78-6 | Ⓜ | Ⓜ | + | + | + | 0 0 | | | | | | | | | | | | | | | |
| 8 | 2-Acetylamino fluorene | 53-96-3 | Ⓜ | Ⓜ | + | + | + | 3 0 | | | | | | | | | | | | | | | |
| 9 | 1-Acetyl-2-phenylhydrazine | 114-83-0 | Ⓜ | Ⓜ | + | + | + | 0 0 | | | | | | | | | | | | | | | |
| 10 | Acid blue 9 | 2650-18-2 | Ⓜ | Ⓜ | + | - | + | 1 1 | | | | weak + | | | | | | | | | | | |
| 11 | Acranyl dihydrochloride | 1684-42-0 | Ⓜ | Ⓜ | + | | | 0 0 | | | | | | | | | | | | | | | |
| 12 | Acrolein | 107-02-8 | Ⓜ | Ⓜ | + | | | 0 1 | | | | | | | | | | | | | | | |

In this

view, all

details concerning the individual test types are **hidden**.

- Clicking the **2** symbol in the upper left hand corner expands **all** test results;
- Clicking the **1** symbol in the upper left hand corner collapses all test results (= original view is restored);
- Clicking any of the **+** symbols above any test type expands only this one test.

For example, when the **+** symbol in column BH (= in vitro CA overall) is clicked, the detailed results for this test type (in vitro Chromosomal Aberrations test) are shown:

| 1 | | 2 | | | | | | | | | | | | | | | | | | | | |
|---------------------------------------|--------------------------------|---------------|-------------|----------------------------|---------------------------|-----------|----|----|----|--|--------|------|------|------|------|-----|------|--------|-----------------------|---------------------------|-----|-----|
| A | B | F | G | AH | AT | AU | AV | AW | AX | AY | AZ | BA | BB | BC | BD | BE | BF | BG | BH | BI | BJ | |
| in vitro Chromosomal Aberrations test | | | | | | | | | | | | | | | | | | | | | | |
| Chemical | CAS No. | Chem Agora | ChE LIST | in vitro MLA Overall | in vitro MN Overall | CSCL-ISHL | | | | Kirkland et al 2005 & 2011 [1, 2] | US NTP | EFSA | SCCS | CosE | BASF | GSK | ECHA | ISSTex | Literature & Notes | in vitro CA Overall | + - | |
| 12 | Acrolein | 107-02-8 | Ⓜ | Ⓜ | | | | | | | | | | | | | | | | | | 0 1 |
| 13 | Acrylonitrile | 107-13-1 | Ⓜ | Ⓜ | + | | | | | | | | | | | | | | | | | 2 0 |
| 14 | Adriamycin [AKA doxorubicin] | 23214-80-8 | Ⓜ | Ⓜ | + | | | | | | | | | | | | | | | | | 2 0 |
| 15 | Abiraterone | 29911-03-8 | Ⓜ | Ⓜ | + | | | | | | | | | | | | | | | | | 0 0 |
| 16 | Aflatoxin B1 | 1162-65-8 | Ⓜ | Ⓜ | + | | | | | | | | | | | | | | | | | 2 0 |
| 17 | Agariline | 2757-90-6 | Ⓜ | Ⓜ | - | | | | | | | | | | | | | | | | | 0 2 |
| 18 | Aloe emodin | n.a. | Ⓜ | Ⓜ | + | | | | | | | | | | | | | | | | | 2 0 |
| 19 | Allyl chloride (Chloropropene) | 107-05-1 | Ⓜ | Ⓜ | | + | + | + | | | | | | | | | | | | | | 1 0 |
| 20 | Allyl glycidyl ether | 106-90-3 | Ⓜ | Ⓜ | | | | | + | + | | | | | | | | | | | | 1 0 |
| 21 | Allyl isothiocyanate | 57-06-7 | Ⓜ | Ⓜ | 1 | | | | + | + | | | | | | | | | | | | 1 0 |
| 22 | 2-Aminoanthracene | 613-13-6 | Ⓜ | Ⓜ | + | | | | + | + | | | | | | | | | | | | 2 0 |
| 23 | 1-Aminoanthraquinone | 82-45-1 | Ⓜ | Ⓜ | | | | | E | E | | | | | | | | | | | | 0 1 |
| 24 | 2-Aminoanthraquinone | 117-79-3 | Ⓜ | Ⓜ | + | | | | | | | | | | | | | | | | | 1 0 |

Note: The overall result (column BH) is derived from the assessment of the columns AU -> BG (= the individual test results that were taken into account).