ISSSTY database on Salmonella typhimurium (Ames test) bacterial mutagenicity

Definition of the fields in files ISSSTY vvv nnn ddddddd.xls and ISSSTY vvv nnn ddddddd.xls

Substance ID: Identification Code of the chemical;

Name: Chemical Name:

CAS: Registry Number of the Chemical Abstract Service;

Formula: Chemical Formula;

FW: Molecular Weight;

Overall: overall outcome of the Ames test. The following codes are used: 1= negative; 2=

equivocal; 3= positive; Inc= inconclusive; ND= no data.

The overall outcome is determined as follows:

Positive: at least one strain is positive (with or without Metabolic activation);

Equivocal: no strain is positive, and at least one equivocal result is present in one of the following strains (with or without Metabolic activation): TA1535, TA100, TA98,

TA1538, TA1535, TA97;

Negative: no positive or equivocal results are present in any strain, and negative outcomes exist for: a) at least one strain from among TA1535 or TA100 or TA97 (with and without Metabolic activation); and b) at least one strain from among TA1538 or

TA98 or TA1537 (with and without Metabolic activation); Inconclusive: If none of the above criteria is fulfilled.

TA100, TA100_S9, etc...: test results for the individual *Salmonella typhimurium* strains, without (e.g., TA100) and with (e.g., TA100_S9) metabolic activation (S9). The following metabolic activation system were considered: rat/mouse/hamster – liver – S9/ microsomes/cytosol.

Results in 31 strains were included.

When more than one experiment in one strain was available, the number of reported positive and negative studies was counted, and the strain overall outcome was determined as follows:

If the percentage of Positive studies is lower than 40 %, then outcome = Negative;

If the percentage of Positive studies is between 40 - 60 %, then outcome = Equivocal;

If the percentage of Positive studies is higher than 60 %, then outcome = Positive.

The experimental results were retrieved from the **Chemical Carcinogenesis Research Information System (CCRIS)** database, in the **Toxnet** databases cluster (http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?CCRIS);