S-IN BPR services

Biocidal Products Regulation

The Biocidal Products Regulation (BPR, Regulation (EU) 528/2012) concerns the placing on the market and use of biocidal products, which are used to protect humans, animals, materials or articles against harmful organisms like pests or bacteria, by the action of the active substances contained in the biocidal product. This regulation aims to improve the functioning of the biocidal products market in the EU, while ensuring a high level of protection for humans and the environment. Additionally, it aims to harmonise the market at Union level, simplify the approval of active substances and authorisation of biocidal products, and introduce timelines for Member State evaluations, opinion-forming and decision-making. Although the new Regulation will not ban animal testing completely, it attempts to minimise it as much as possible. It introduces an obligation to share data on vertebrate animal tests in exchange for fair compensation, and a prohibition to duplicate such tests. This is expected to save both costs and animal lives. The Regulation introduces specific and general rules for the adaptation of data requirements. Testing may be waived if it is not deemed necessary, and the required information may be provided using: existing *in vivo* data, weight of evidence, (Q)SAR (including grouping and read-across), and *in-vitro* methods.

S-IN computational toxicology expertise

S-IN Soluzioni Informatiche offers complete molecular informatics and QSAR services in compliance with BPR regulation. S-IN provides predictions for (eco)toxicological and physico-chemical properties generated by *in silico* (non-testing) methods, that are used in accordance with the current legislation. S-IN can also support customers with consulting and training services on how non-testing methods can be best applied within BPR. Industry can take advantage on S-IN's expertise in the different *in silico* methods accepted in the regulatory context, i.e. analogue approaches, statistical-based (quantitative) structure-activity relationships (Q)SARs and expert-rule based systems. S-IN always selects and exploits the most suitable methodology in accordance with the specific requirements of each case.

S-IN advantage

Services provided by S-IN are based on two solid pillars:

- The solid scientific background on the methods and approaches used to generate physico-chemical and ADMET (adsorption, distribution, metabolism, excretion and toxicity) properties. S-IN increased its competences by actively participating in a number of projects related to computational toxicology, ADME and toxicity prediction.

- S-IN's team has a long-term experience of more than 10 years on the use of *in silico* methods in the regulatory context and thus in compliance with available regulations and guidelines.

S-IN
soluzioni informatiche

S-IN in silico services for BPR regulation

S-IN's offers the following *in silico* services:

■ **Read-across and grouping analysis:**

a) Structural analogue search and identification of potential candidates for the read-across

b) Checking the availability of toxicological and eco-toxicological experimental data for the candidate substance in the read-across workflow

c) Read-across prediction for the target chemical (weighing the experimental data according to their relevance/reliability)

d) Detailed documentation of the read-across study in line with the corresponding guidelines published by ECHA

■ **Statistical-based QSAR and expert rule-based system predictions:**

a) Predictions generated by existing QSARs and expert rule-based systems implemented in different software, both commercial and freeware

b) Use of different tools to apply a consensus approach and thus enhance the reliability of the predictions

c) Assessment of each prediction reliability, as required by OECD principles for the validation, for regulatory purposes, of QSARs

d) Detailed report compiled according to the information required by the OECD

■ **Documentation:**

a) QSAR Model Reporting Format (QMRF)

b) QSAR Prediction Reporting Format (QPRF)

c) Standardized reporting format for read-across analysis

BPR endpoints covered by S-IN:

▼ **PHYSICO-CHEMICAL PROPERTIES**
- ► 3.2 MELTING/FREEZING POINT
- ► 3.4 BOILING POINT
- ► 3.5 RELATIVE DENSITY
- ► 3.7 VAPOUR PRESSURE
- ► 3.8 SURFACE TENSION
- ► 3.9 WATER SOLUBILITY
- ► 3.10 PARTITION COEFFICIENT n-Octanol/Water
- ► 3.13 DISSOCIATION CONSTANT

▼ **ECOTOXICOLOGICAL PROPERTIES**
- ▼ 9.1 AQUATIC TOXICITY
  - ► 9.1.1 SHORT-TERM TOXICITY TESTING ON FISH
  - ► 9.1.2 SHORT-TERM TOXICITY TESTING ON INVERTEBRATES (DAPHNIA)
  - ► 9.1.3 GROWTH INHIBITION STUDY ON AQUATIC PLANT (ALGAE)
  - ► 9.1.4 BIOCONCENTRATION
  - ▼ 9.1.6 FURTHER TOXICITY STUDIES ON AQUATIC ORGANISMS
    - ► 9.1.6.1 LONG-TERM TOXICITY TESTING ON FISH
    - ► 9.1.6.2 LONG-TERM TOXICITY TESTING ON INVERTEBRATES (DAPHNIA)
  - ► 9.1.7 BIOACCUMULATION

▼ **TOXICOLOGICAL PROPERTIES**
- ► 8.1 SKIN IRRITATION or SKIN CORROSION
- ► 8.2 EYE-IRRITATION
- ► 8.3 SKIN SENSITIZATION
- ▼ 8.5 MUTAGENICITY
  - ► 8.5.1 *IN-VITRO* GENE MUTATION STUDY IN BACTERIA
  - ► 8.5.2 *IN-VITRO* CITOGENICITY STUDY IN MAMMALIAN CELLS
  - ► 8.5.3 *IN-VITRO* GENE MUTATION STUDY IN MAMMALIAN CELLS
- ▼ 8.7 ACUTE TOXICITY
  - ► 8.7.1 ACUTE TOXICITY (by oral route)
- ▼ 8.10 REPRODUCTIVE TOXICITY
  - ► 8.10.1 PRE-NATAL DEVELOPMENTAL TOXICITY STUDY
- ► 8.11 CARCINOGENICITY

▼ **ENVIRONMENTAL PROPERTIES**
- ▼ 10.1.1 DEGRADATION
  - 10.1.1.1 HYDROLYSIS AS A FUNCTION OF pH
  - 10.1.1.2 READY BIODEGRADABILITY
- ► 10.1.2 ABSORPTION/DESORPTION