S-IN REACH services

REACH Regulation

REACH (Registration, Evaluation, Authorisation and Restriction of Chemicals) is a European Regulation concerning chemicals and their safe use, entered into force on 1 June 2007. It aims to improve the protection of human health and the environment from the chemical risks while enhancing the competitiveness of the EU chemicals industry. It requires registration over a tiered timescale of all substances; not only those used in industrial processes but also in the day-to-day life produced or imported into the EU at ≥1 tpa. The next major deadline is May 2018 for substances in the 1-100 tpa band. REACH places the burden of proof on companies. To comply with the regulation, companies must identify and manage the risks linked to the substances they manufacture or import and market in the EU. The regulation has important implications for the testing methods used for evaluating the effects of chemical substances. In fact, to minimise the number of animal tests required in implementing the REACH Regulation, provision has been made to provide a number of possibilities for adapting the testing requirements, and to use existing data and alternative assessment approaches instead.

S-IN computational toxicology expertise

S-IN Soluzioni Informatiche offers complete molecular informatics and QSAR services in compliance with REACH 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 REACH. 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 REACH

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 the 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

REACH endpoints covered by S-IN:

- PHYSICO-CHEMICAL PROPERTIES
  - 7.2 MELTING/FREEZING POINT
  - 7.3 BOILING POINT
  - 7.4 RELATIVE DENSITY
  - 7.5 VAPOUR PRESSURE
  - 7.6 SURFACE TENSION
  - 7.7 WATER SOLUBILITY
  - 7.8 PARTITION COEFFICIENT n-Octanol/Water
  - 7.9 FLASH POINT
  - 7.16 DISSOCIATION CONSTANT
- TOXICOLOGICAL PROPERTIES
  - 8.1 SKIN IRRITATION or SKIN CORROSION
  - 8.2 EYE-IRRITATION
  - 8.3 SKIN SENSITIZATION
  - 8.4 MUTAGENICITY
    - 8.4.1 IN-VITRO GENE MUTATION STUDY IN BACTERIA
    - 8.4.2 IN-VITRO CITOGENICITY STUDY IN MAMMALIAN CELLS OR IN-VITRO MICRONUCLEUS STUDY
    - 8.4.4 IN-VIVO MUTAGENICITY STUDY
  - 8.5 ACUTE TOXICITY
    - 8.5.1 ACUTE TOXICITY (by oral route)
  - 8.7 REPRODUCTIVE TOXICITY
    - 8.7.1 SCREENING FOR REPRODUCTIVE/DEVELOPMENTAL TOXICITY
    - 8.7.2 PRE-NATAL DEVELOPMENTAL TOXICITY STUDY
  - 8.9 CARCINOGENICITY
- ECOTOXICOLOGICAL PROPERTIES
  - 9.1 AQUATIC TOXICITY
    - 9.1.1 SHORT-TERM TOXICITY TESTING ON INVERTEBRATES (DAPHNIA)
    - 9.1.2 GROWTH INHIBITION STUDY ON AQUATIC PLANT (ALGAE)
    - 9.1.3 SHORT-TERM TOXICITY TESTING ON FISH
    - 9.1.5 LONG-TERM TOXICITY TESTING ON INVERTEBRATES (DAPHNIA)
    - 9.1.6 LONG-TERM TOXICITY TESTING ON FISH
- ENVIRONMENTAL PROPERTIES
  - 9.2 DEGRADATION
    - 9.2.1 BIOTIC
      - 9.2.1.1 READY BIODEGRADABILITY
      - 9.2.1.3 SOIL SIMULATION TESTING
    - 9.2.2 ABIOTIC
      - 9.2.2.1 HYDROLYSIS AS A FUNCTION OF pH
  - 9.3 FATE AND BEHAVIOUR IN THE ENVIRONMENT
    - 9.3.1 ABSORPTION/DESORPTION SCREENING
    - 9.3.2 BIOACCUMULATION IN AQUATIC SPECIES, PREFERABLE FISH

REACH Ready Approved Supplier

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