VEGA: a new generation of QSAR models for regulatory toxicology and pharmaceuticals development

VEGA is part of a new generation of QSAR model platforms which provide detailed information and analysis to support a toxicity prediction. It enables toxicologists and pharmaceuticals developers to evaluate the reliability of each prediction, and so judge whether it is sufficiently robust to replace or reduce animal experiments. The outputs are also designed specifically to meet the current EU REACH regulatory demands for chemical registration. The models have been developed and tested by an international consortium which combines expertise in QSAR model development and chemical regulation. VEGA can be freely downloaded or used online.

What can your solution be used for?

The VEGA platform provides predictive QSAR models to evaluate chemical properties and predict biological activity. VEGA includes models for hydrophobicity (LogP), bio-concentration factor, aquatic toxicity, mutagenicity, carcinogenicity, developmental toxicity and skin sensitisation.

There are four key areas of use:

- Screening of chemicals for toxicity within toxicological and pharmaceutical research;
- Prioritisation of chemicals which may require *in vivo* and/or *in vitro* testing ;
- Evaluation of physico-chemical properties, environmental fate parameters and toxicological profiles for EU REACH regulatory submissions;
- Analysis of impurities and degradation products.

Need for collaboration

We are looking for toxicologists and pharmaceutical developers interested in:

(i) using VEGA to review its reliability and supporting information across chemical groupings and endpoints (listed above) especially within REACH and within pharmaceutical development;
(ii) providing data to review current predictions and further improve the existing models within VEGA, and to develop new models applicable to further series of chemicals and/or other further endpoints;
(iii) contributing expert understanding of mechanisms of action to help us to improve the prediction capabilities and the applicability domain determination.

3Rs impact assessment

In drug development, QSAR models are used to screen large numbers of chemicals for toxicity and to prioritise only those chemicals of high concern for further preclinical animal testing, potentially reducing the number of compounds entering in vivo studies. VEGA can be used for this purpose for the endpoints described above.

The EU REACH legislation creates an urgent need for QSAR models. To address REACH requirements by traditional *in vivo* testing would take decades, cost billions and involve the use of many additional millions of animals. QSAR models connect, use and extend existing experimental data, potentially enabling industy to assess thousands of chemicals quickly and economically by reducing or replacing the need for costly *in vivo* testing.

To find out more or to connect with the technology developer contact: crackitenquiries@nc3rs.org.uk