

## Your use of QSAR / In Silico methods

### Q1 Have you used or tested QSAR / In Silico methods?

<input type="checkbox"/> Yes <input type="checkbox"/> Yes, with expert support <input type="checkbox"/> No
<p><i>If 'Yes', which In Silico models / methods / software have you used / tested? Please indicate the name of the software, or indicate if the source is internal</i></p>    
<p><i>If no:</i></p> <input type="checkbox"/> We wanted to use <i>In Silico</i> methods, but there was no relevant model available. <input type="checkbox"/> We have tried to use <i>In Silico</i> methods, but it was not successful <input type="checkbox"/> We have not needed (or wanted) to use <i>In Silico</i> methods so far.

### Q2 Domains for using QSAR / In Silico methods *Please tick all which apply to you.*

<p><b>We have used In Silico methods for:</b></p> <p style="text-align: center;">↘</p> <input type="checkbox"/> Physico-chemical properties..... <input type="checkbox"/> Human toxicology..... <input type="checkbox"/> Environmental fate properties..... <input type="checkbox"/> Ecotoxicology..... <input type="checkbox"/> None.....	<p style="text-align: center;">↙</p> <p><b>We want to use In Silico methods for:</b></p> <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/>
<p><i>Please identify some example endpoints:</i></p>   	

### Q3 Functions of QSAR / In Silico methods *Please tick or rank 1, 2... all which apply to you.*

<p><b>We have used In Silico methods for:</b></p> <p style="text-align: center;">↘</p> <input type="checkbox"/> Prioritisation of compounds for further analysis..... <input type="checkbox"/> Fast evaluation of the properties of chemicals of interest..... <input type="checkbox"/> Research and development, for the evaluation of toxicity..... <input type="checkbox"/> Regulatory requirements - as supporting information..... <input type="checkbox"/> Regulatory requirements - as part of a weight-of-evidence approach..... <input type="checkbox"/> Regulatory requirements - as the key study..... <input type="checkbox"/> None / not sure.....	<p style="text-align: center;">↙</p> <p><b>We want to use In Silico methods for:</b></p> <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/> <input type="checkbox"/>
<input type="checkbox"/> Other functions (please explain):   	

## The challenges / barriers to using *In Silico* methods

### Q4 What prevents or limits your use of QSAR / *In Silico* methods?

Please tick or rank 1, 2... all which apply to you. (If a set of issues is not significant, leave it blank.)

↓ You can select just the headings - the detailed responses are optional.

***In Silico* methods are not a priority for us**

- other priorities are more important at this time;
- we want to focus on using traditional methods, where our expertise is strong;
- we want to focus on using traditional methods which we know have been accepted in the past.

Other (please explain):

**We need more information and/or regulatory guidance**

- to know more about when and how QSAR *In Silico* methods can be used;
- to know what QSAR models are available or appropriate for our work;
- to assess whether a model can be viewed as scientifically valid and adequately documented;
- to be able to use the technical software, and understand the outputs from it;
- to know how to integrate different kinds of results from different methods into a submission.

Other (please explain):

**We are concerned about the potential costs or delays if we use *In Silico* methods**

- that the models (or our use of them) may not be accepted by the regulator, and so create additional costs for us in delay and resubmission;
- that we need to invest in technical training and/or consultancy;
- that using QSAR models might commit us to using expensive commercial software in future.

Other (please explain):

**The current QSAR models don't yet provide what we need**

- the range of models is currently too limited for us to start using these methods regularly;
- we fear the models may not be reliable, and require support from other models and/or tests;
- current models often do not provide what the toxicologist needs for making decisions on toxicity;
- models can be a 'black box, lacking the documentation we need to check their quality and their applicability to our work, and/or lacking the transparency that is required in REACH submissions;
- models do not (yet) evaluate chemicals in combination, or adequately evaluate chronic toxicity.

Other (please explain):

**QSAR / *In Silico* methods will not / cannot provide what we need**

Please explain:

## Ways forward

Please tick or rank 1, 2, 3... all which apply to you.

### Q5 What are the *main* reasons to use QSAR / *In Silico* methods, in your view?

<input type="checkbox"/> To assess potentially thousands of chemicals simultaneously <input type="checkbox"/> To identify and prioritise substances of concern. <input type="checkbox"/> To improve the response to regulatory requirements such as risk assessment and classification and labelling. <input type="checkbox"/> To address endpoints for which animal models are not fully accepted. <input type="checkbox"/> To reduce the time and costs of experiments. <input type="checkbox"/> To reduce the use of vertebrates in experiments - to meet regulatory requirements. <input type="checkbox"/> To reduce the use of vertebrates in experiments - to meet our own ethical policies.
<input type="checkbox"/> Other reasons (please explain):

### Q6 What would help you to use QSAR / *In Silico* methods?

<input type="checkbox"/> Lists and reviews of the available models, with information on where to access them. <input type="checkbox"/> Seeing good examples of industry using <i>In Silico</i> methods successfully (in documentary video, industry events, online reports and trade magazines). <input type="checkbox"/> Seeing more peer-reviewed journal articles about the practical applications of <i>In Silico</i> methods, illustrated by case studies. <input type="checkbox"/> Examples from the regulators about acceptance of / enthusiasm for <i>In Silico</i> methods. <input type="checkbox"/> Clear standardisation of the ways in which individual QSAR models and their appropriate uses are described, and their applicability domains are defined. <input type="checkbox"/> Clear guidelines for reporting toxicity results from <i>In Silico</i> methods (maybe as an automatic report generator within the software that matches the submission format). <input type="checkbox"/> Examples of the reasoning and transparent documentation required for submissions. <input type="checkbox"/> Support and guidance from laboratories with expertise in the uses of QSARs.
<input type="checkbox"/> Other (please explain):

### Q7 What will have most impact on the wider acceptance and use of *In Silico* methods?

<input type="checkbox"/> Industry using <i>In Silico</i> methods more, and producing high quality results. <input type="checkbox"/> Use by high-profile companies / organisations, and in cases with high visibility. <input type="checkbox"/> The trademarking of models by trusted software companies or organisations. <input type="checkbox"/> The monitoring, review and updating of models by specialist QSAR laboratories. <input type="checkbox"/> Case study research evidence of the quality and reliability of <i>In Silico</i> methods.
<input type="checkbox"/> Other (please explain):

*Finally...*

**Q8 What are your main sources of information about methods for toxicity assessment for regulatory purposes?**

And where else would you like to see or hear information about QSAR / *In Silico* methods?

**Would you like to be notified of events and information about QSAR / *In Silico* methods?**

- Yes (*Please include some contact details below*)  No

**Can you offer an example or experience of using *In Silico* methods?**

Would you be willing to say more (perhaps by phone) about one experience of using *In Silico* methods? This will help us to ensure the information and guidance we produce is informed by experience and by real examples, and so can inform future use.

- Yes (*If yes, please include your email and phone below*)  No

*Thank you*

**Please indicate your relation to chemical evaluation (*Please tick or rank 1, 2, 3... all which apply to you.*)**

<input type="checkbox"/> Regulator or national competent authority <input type="checkbox"/> Industry user / association / trade union, inc. SMEs <input type="checkbox"/> Distributor / retailer <input type="checkbox"/> Consultant <input type="checkbox"/> Association for alternative methods <input type="checkbox"/> Information technology user or evaluator <input type="checkbox"/> QSAR / <i>In Silico</i> methods developer	<input type="checkbox"/> Scientist or science associations <input type="checkbox"/> University researcher <input type="checkbox"/> Non-university researcher <input type="checkbox"/> Governmental organisation; national or internat. <input type="checkbox"/> Non-governmental organisations (NGO) <input type="checkbox"/> Media, online communicator or journalist <input type="checkbox"/> Citizen, inc. citizen groups and online communities.
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*Allocate a professional association or network according to the member type.*

**Optional personal details:**

Title:	First name:	Last name:
Organisation:		
Position:		Department:
Email:		Website:
Phone:		Country:
Address:		
<input type="checkbox"/> I have given my contact details but I want my responses to be used anonymously.		
<input type="checkbox"/> I would be willing to offer comments or advice to the dissemination project in the future.		