A first inter-laboratory review exercise on the acceptance of QSAR results

You can view the results and a report of this exercise **here**

The purpose of the review exercise

We invite you to participate in the first inter-laboratory and cross-institutional review exercise on the acceptance of QSAR results in the evaluation of toxicity.

The purpose is to get feedback from regulators, industry, consultants, researchers and other experts within academia on the possible use of results from QSAR models, by considering practical case studies. (Note that this exercise does NOT address the validation of the models; only their acceptance by the range of stakeholders.)

We are focussing specifically on models to assess bioconcentration factor (BCF). Three chemicals have been evaluated as examples, using the models.

This exercise is part of the activities of the EC projects **ORCHESTRA** and **ANTARES**, and of the Italian Group on QSAR promoted by the Italian Health Ministry. The results of the exercise will be made available at the ANTARES and ORCHESTRA web sites.

What we provide

1. Firstly, we provide some guidance on the information that is produced by three QSAR models: **VEGA**, **EPISuite** and **T.E.S.T.** As you will see, each model provides not only a predicted toxicity value, but several other pieces of information. It is this information which we would like you to review, for each of the three example chemicals.

Guidance: Reports_explanations

2. Secondly, we provide the results for BCF obtained from the three models, for each of the three chemicals. (The three chemicals have been selected because their results have different levels of reliability.)

VEGA **EPISuite** **T.E.S.T.**

What we would like you to do

For each model, we would like you to review all the information it provides, and assess whether you would accept the result.

We ask you to evaluate each model separately, NOT combined.

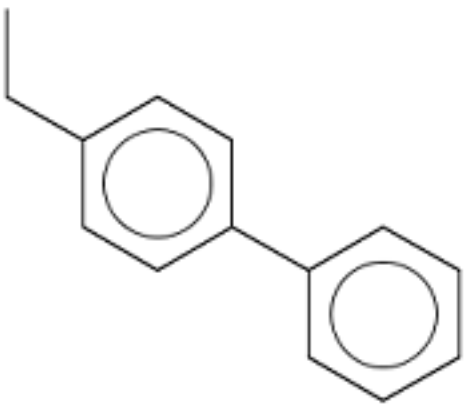
To help your review, please note that the experimental uncertainty/variability for *in vivo* results for this endpoint has been reported to be between 0.4 and 0.75 log units.

How to send your feedback

Please simply fill in the form below. Your input will be anonymous.

Chemical 1

c1ccc(cc1)c2ccc(cc2)CC



On the basis of all the pieces of information provided, do you consider the BCF value obtained from the VEGA model to be sufficiently reliable?: *

Chemical 1 - c1ccc(cc1)c2ccc(cc2)CC

○ Yes ○ No

Comment (Optional):

On the basis of all the pieces of information provided, do you consider the BCF value obtained from the EPISuite model to be sufficiently reliable?: *

Chemical 1 - c1ccc(cc1)c2ccc(cc2)CC

○ Yes ○ No

Comment (Optional):

On the basis of all the pieces of information provided, do you consider the BCF value obtained from the T.E.S.T model to be sufficiently reliable?: *

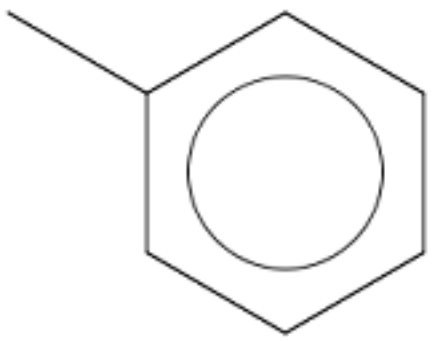
Chemical 1 - c1ccc(cc1)c2ccc(cc2)CC

○ Yes ○ No

Comment (Optional):

Chemical 2

c1ccc(cc1)C



On the basis of all the pieces of information provided, do you consider the BCF value obtained from the VEGA model to be sufficiently reliable?: *

Chemical 2 - c1ccc(cc1)C

○ Yes ○ No

Comment (Optional):

On the basis of all the pieces of information provided, do you consider the BCF value obtained from the EPISuite model to be sufficiently reliable?: *

Chemical 2 - c1ccc(cc1)C

○ Yes ○ No

Comment (Optional):

On the basis of all the pieces of information provided, do you consider the BCF value obtained from the T.E.S.T model to be sufficiently reliable?: *

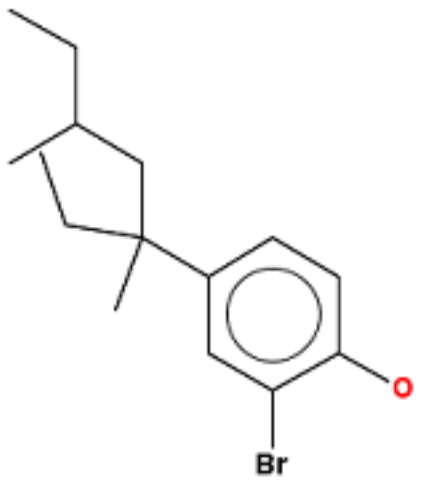
Chemical 2 - c1ccc(cc1)C

○ Yes ○ No

Comment (Optional):

Chemical 3

CCC(C)CC(C)(CC)C1=CC(Br)=C(O)C=C1



On the basis of all the pieces of information provided, do you consider the BCF value obtained from the VEGA model to be sufficiently reliable?: *

Chemical 3 - CCC(C)CC(C)(CC)C1=CC(Br)=C(O)C=C1

○ Yes ○ No

Comment (Optional):

On the basis of all the pieces of information provided, do you consider the BCF value obtained from the EPISuite model to be sufficiently reliable?: *

Chemical 3 - CCC(C)CC(C)(CC)C1=CC(Br)=C(O)C=C1

○ Yes ○ No

Comment (Optional):

On the basis of all the pieces of information provided, do you consider the BCF value obtained from the T.E.S.T model to be sufficiently reliable?: *

Chemical 3 - CCC(C)CC(C)(CC)C1=CC(Br)=C(O)C=C1

○ Yes ○ No

Comment (Optional):

Is your work within: *

- Select -

Do you have experience of QSAR models?: *

○ Yes, as a user ○ Yes, as a reviewer / regulator ○ Yes, as a developer ○ No

Do you have experience of the evaluation of BCF for regulatory purposes?: *

○ Yes ○ No