(Q)SAR APPLICATION TOOLBOX

VERSION 1.1

TIPS AND TRICKS

October 2009

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FOREWORD

This document is one of a series of guidance documents accompanying the OECD (Q)SAR Application Toolbox. The main objective of the Toolbox is to allow the user to use (Q)SAR methodologies to group chemicals into categories and to fill data gaps by read-across, trend analysis and (Q)SARs. For in-depth background information on the concept of chemical categories, the user is invited to consult the guidance document for grouping of chemicals published in the Series on Testing and Assessment of the OECD Environment, Health and Safety Publications [OECD (2007); ENV/JM/MONO(2007)28: http://appli1.oecd.org/olis/2007doc.nsf/linkto/env-jm-mono(2007)28].

The current document is aimed at providing some guidance on some advanced features for using the Toolbox. It will be updated and expanded as further guidance becomes available.

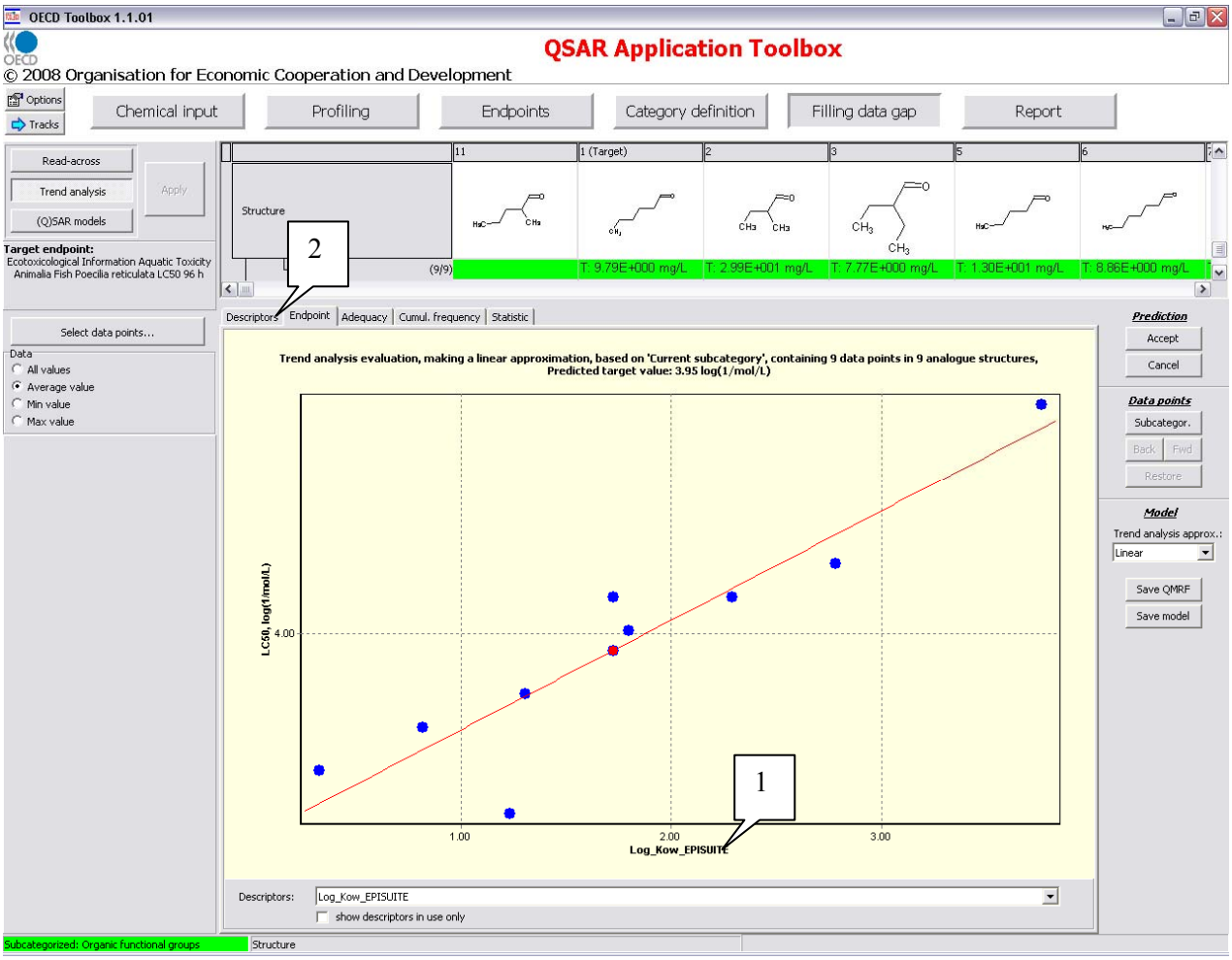
Additional guidance and training material will be made available on the internet site for the OECD (Q)SAR Project [www.oecd.org/env/existingchemicals/qsar] as well as the internet site of the Laboratory of Mathematical Chemistry [http://toolbox.oasis-lmc.org/] and the user is invited to regularly consult these two internet sites.

The OECD (Q)SAR Application Toolbox has been developed with the financial assistance of the European Union.

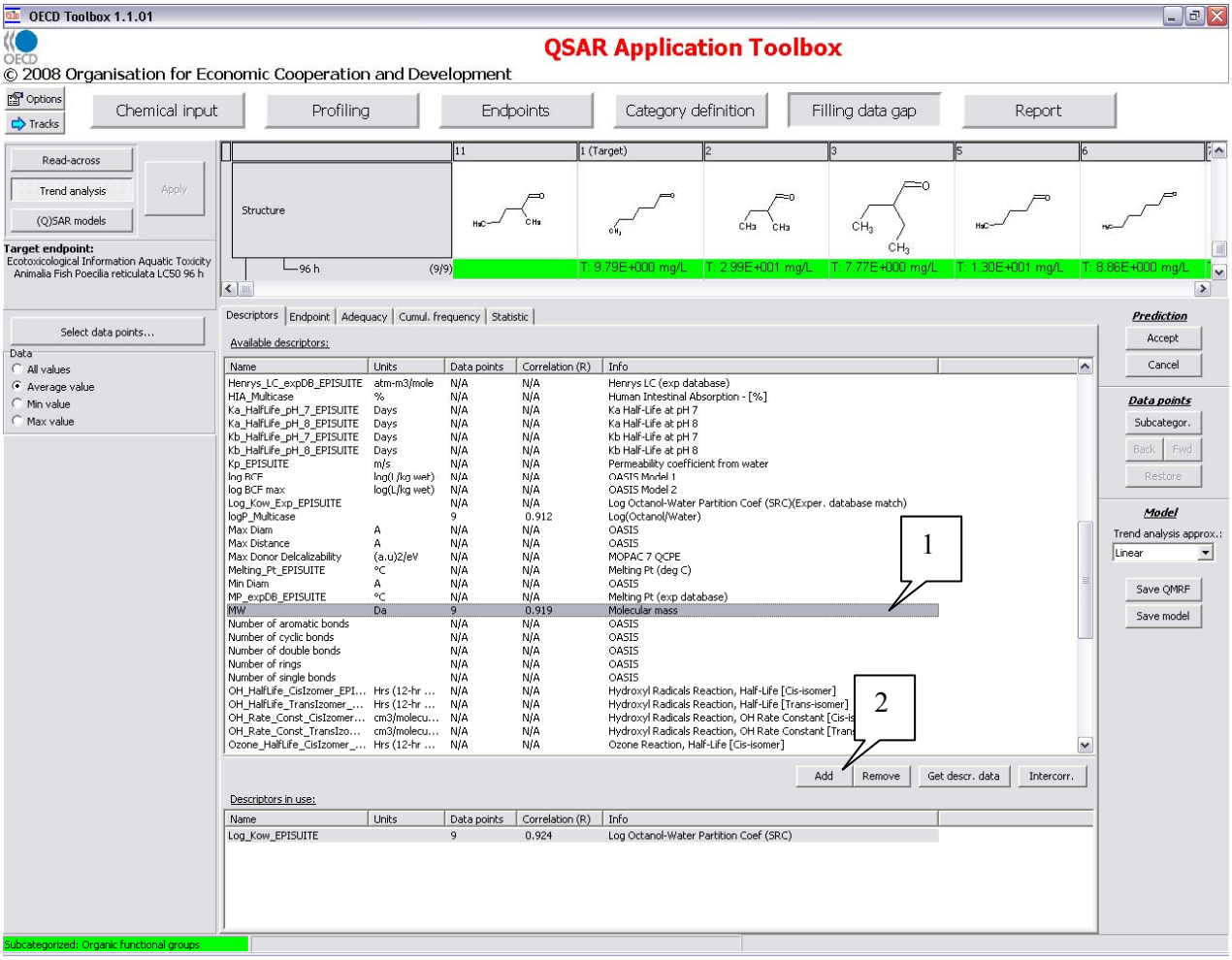
1. CHANGING THE X-AXIS DESCRIPTOR WHEN PERFORMING TREND ANALYSIS WITH THE TOOLBOX.

When performing a trend analysis within a category to estimate missing data with the Toolbox, the default X-axis descriptor is Log_Kow_EPISUITE, i.e the Log Kow estimated with the EPISUITE program (1) [see screenshot below]. While this descriptor may be pertinent for many endpoints, e.g. aquatic toxicity, alternative descriptors may be warranted for other endpoints (e.g. vapour pressure for acute inhalation toxicity).

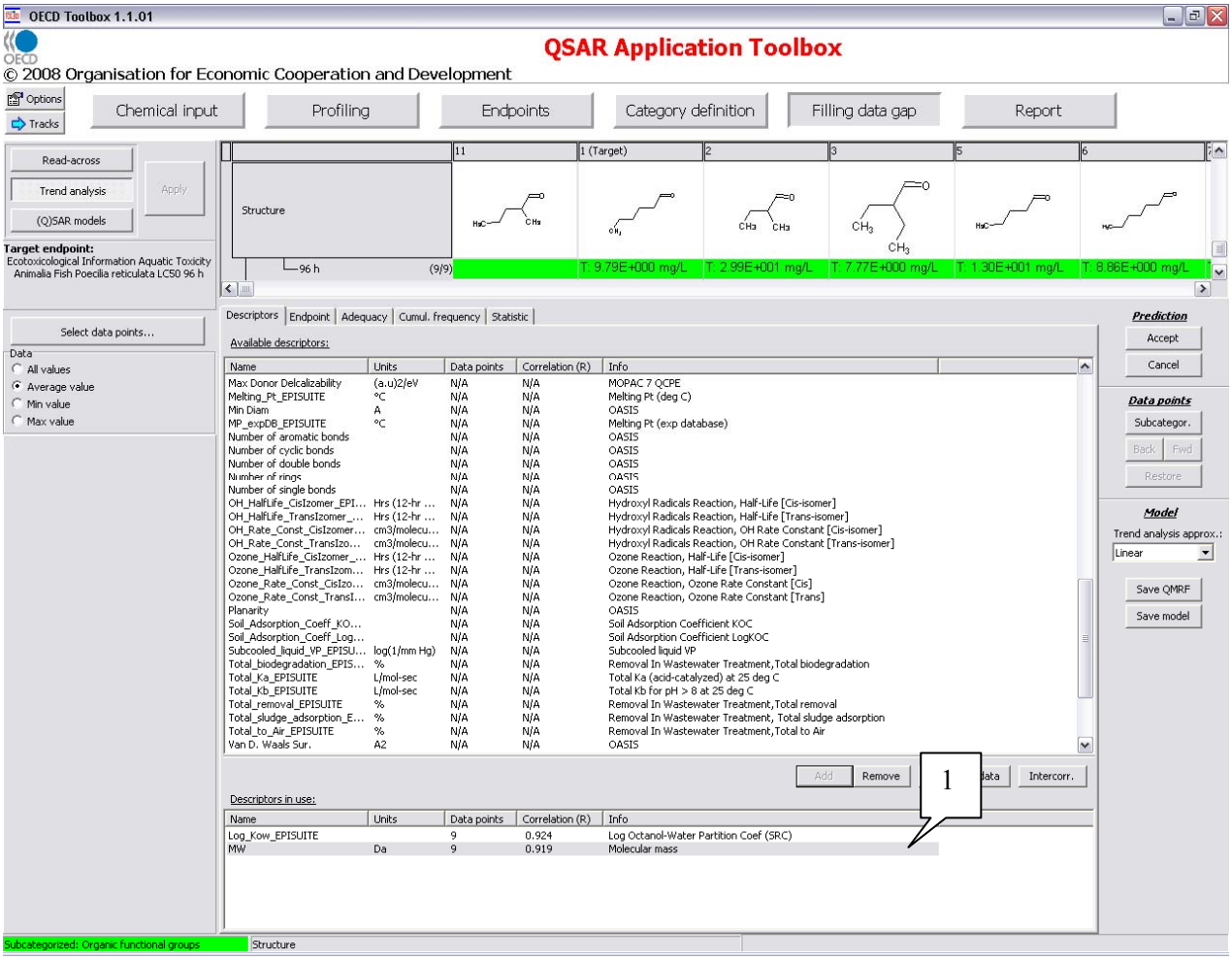
It is possible to change the descriptor and re-estimate the property. For that the user has to select the tab **Descriptor** (2)



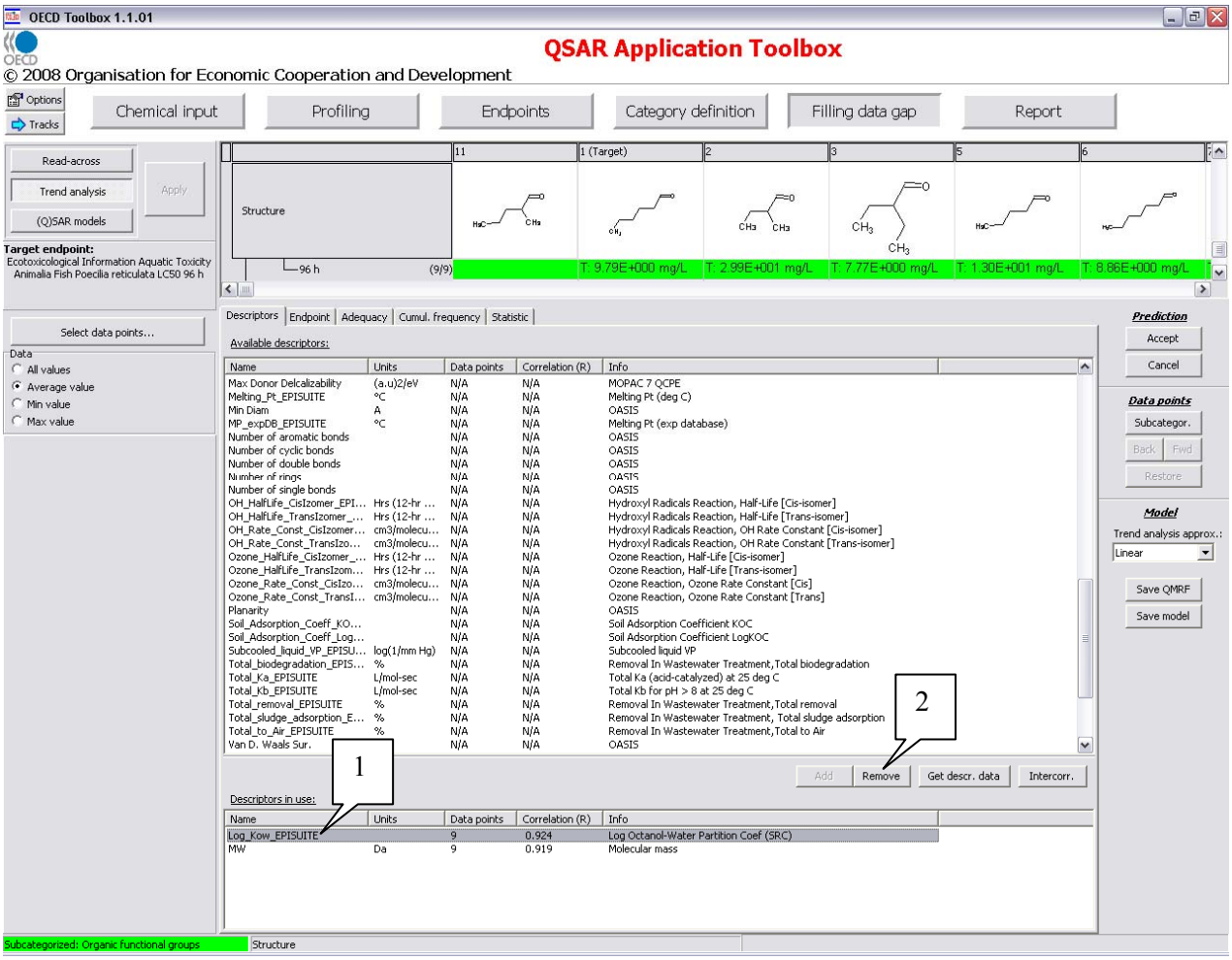
Among the available descriptors the user then has to select the desired descriptor (1) and click the button **Add (2)**.



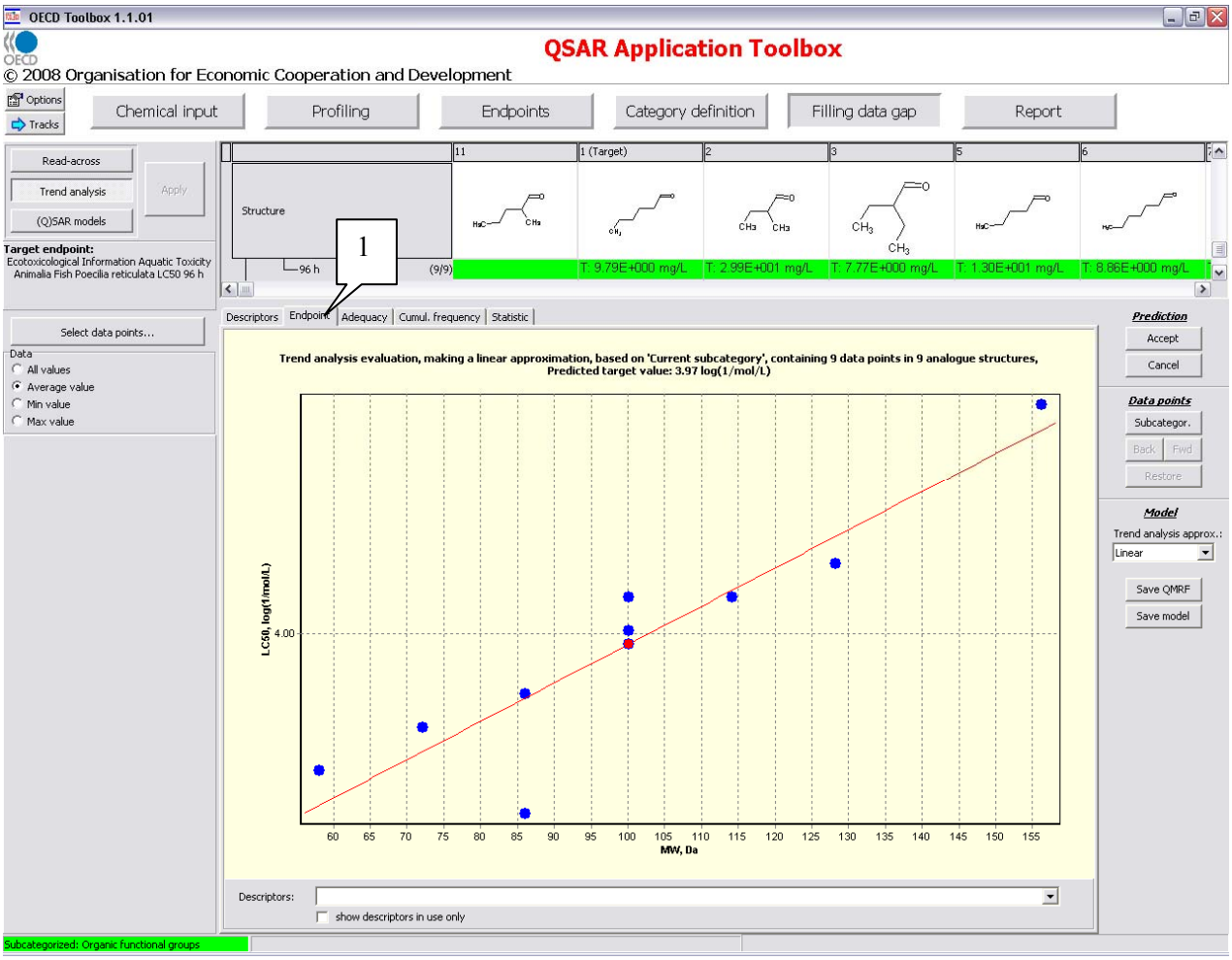
The correlation is then calculated for the new descriptor and added into the window **Descriptors in use** (1)



The user can then simply delete the previous descriptor in use by selecting it (1) and clicking **Remove** (2).



By selecting the tab **Endpoint** (1) the graph with the new interpolation appears.



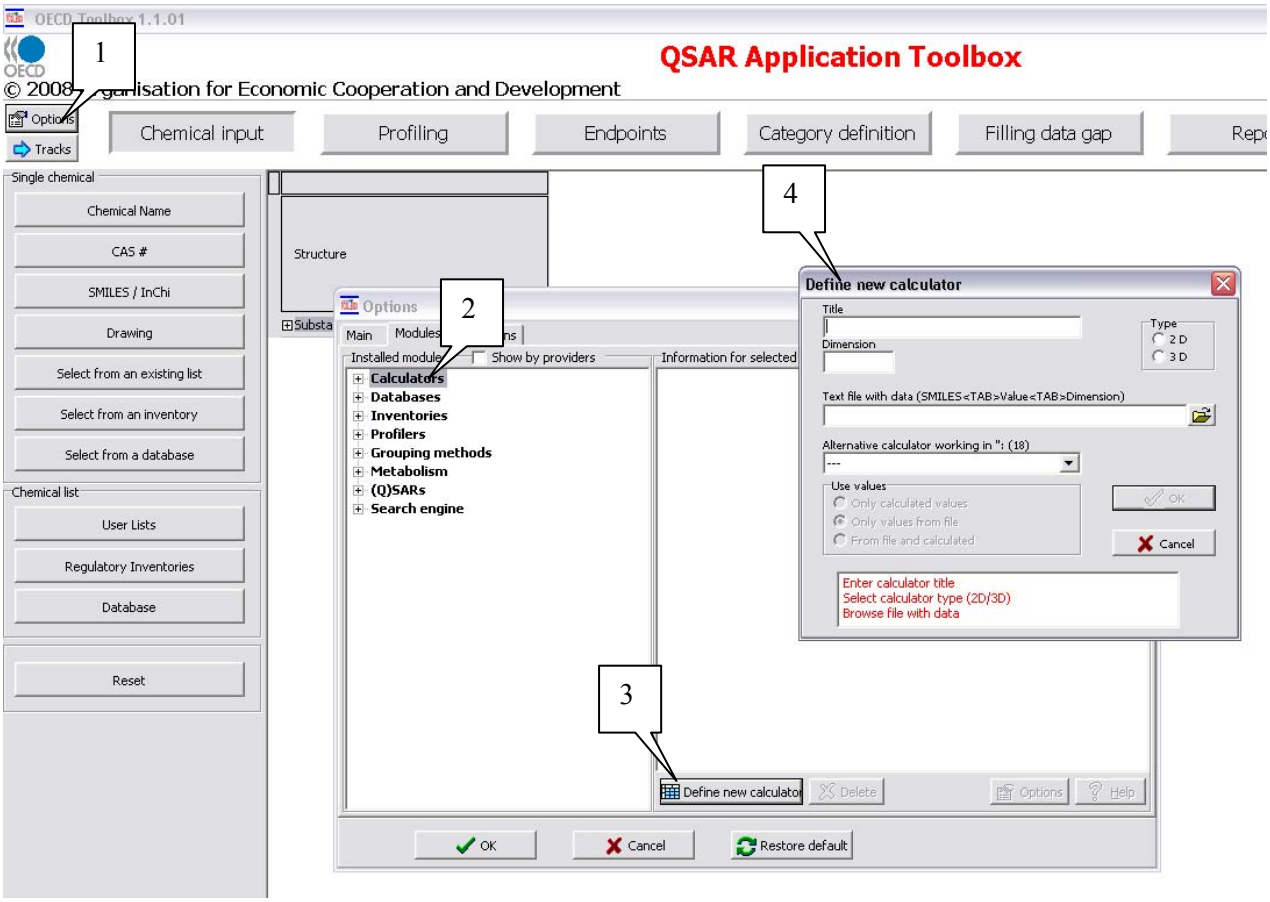
2. USING EXPERIMENTAL RESULTS FOR THE X-AXIS DESCRIPTOR

When performing trend-analysis and read-across, a number of X-axis descriptors can be used (see chapter

1. Changing the X-axis descriptor when performing trend analysis with the Toolbox.). Most of these descriptors are derived by calculation e.g. Log Kow from the KowWin module in EPISUITE.

In addition to using those calculators, the user has the possibility to load datasets with experimental data to be used instead of the estimated descriptors. This is illustrated with an example below of loading a database with experimental Log Kow results.

New X-axis descriptors can be added via the module **Options** (1) [see screenshot below]. In the new window, the user then has to select the item **Calculators** (2) and click the button **Define new calculator** (3). This opens a third window dedicated to providing details of the new descriptor (4).



To define the new descriptor, the following steps should be followed (see also screenshot below):

1. Add a title. In this example “Log Kow internal”

2. Add a dimension or unit. In this example the descriptor is dimensionless and the field is left blank.

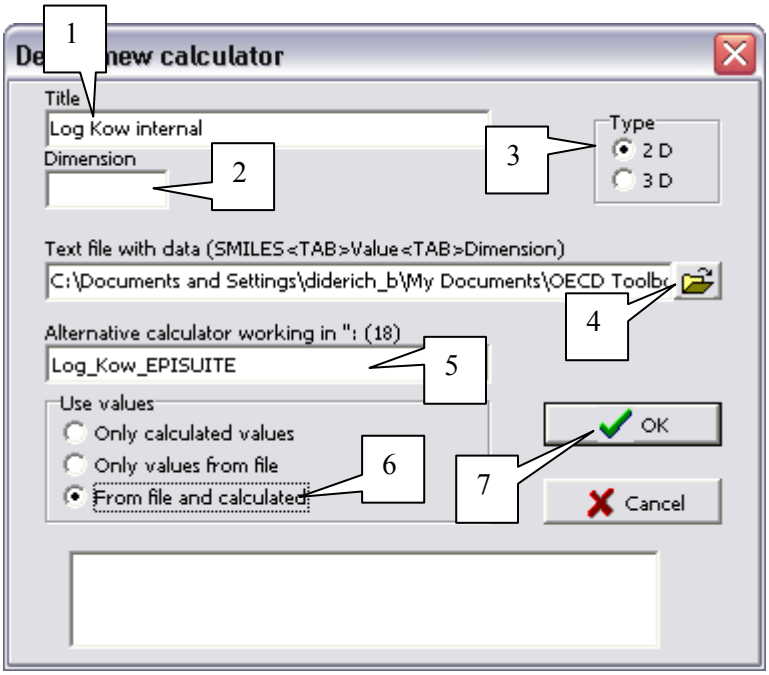
3. Select a type: 2D or 3D. The distinction is made depending on whether the descriptor could be calculated based on a 2D or 3D configuration of the structure. Kow being usually derived from a 2D structure, the 2D button can be selected.

4. Indicate the path of the file containing the Log Kow results. The file should be a normal tab delineated text file, each line having the format: SMILES<TAB>Value<TAB>Dimension. Please note that in case the descriptor is dimensionless, each line should nevertheless contain a <TAB> after the Value an example of a text file is presented in Box 1.

5. The user can choose an existing calculator to estimate the descriptor for chemicals not listed in the file with experimental data. In this example, the EPISUITE model could be chosen to fill data gaps in the experimental file.

6. Please not that if an alternative calculator is chosen, the radio button **From file and calculated** has to be checked.

7. By clicking the **OK** button, the file is imported as a new descriptor. And the user can return to a normal work session.



Box 1. Format of a text file with experimental results

C(C)S <TAB> 1.4 <TAB>

C(S)CCCCC <TAB> 3.3 <TAB>

C(S)CCCCCCC <TAB> 4.3 <TAB>

Notes:

- There should be no title line and no empty line at the bottom of the file (i.e. no “Carriage Return” at the end of the last line).

- The file has to be saved with a TXT extension (e.g. Log_KOW_internal.txt).

When performing a trend analysis or read-across the new descriptor appears in the list (see screenshot below), and can be used as an X-axis descriptor as outlined in chapter 1 of this guidance document.