CATALOGIC BIODEGRADATION MODEL RESULTS

1. Biodegradation

The CATALOGIC biodegradation models provide results for:

- **Percentage of biodegradation** expressed as biological oxygen demand (BOD) or CO_2 released.
- **Primary half-life** defined as the time for a 50% decrease of parent quantity.
- **Ultimate half-life** defined as the time for achieving 50% biodegradation.

The results are included in standard report formats (Fig.1).

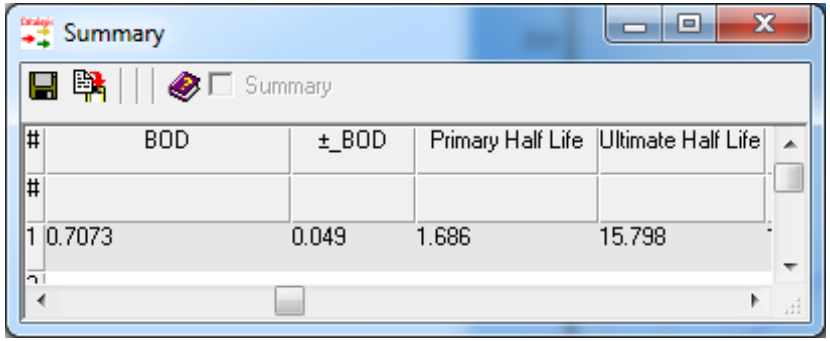

Fig.1. Selected columns of **CATALOGIC summary report** showing predicted BOD, primary and ultimate half-lives

2. Biodegradation map

The CATALOGIC biodegradation models provide a map of the simulated transformations and biodegradation products (Fig.2).

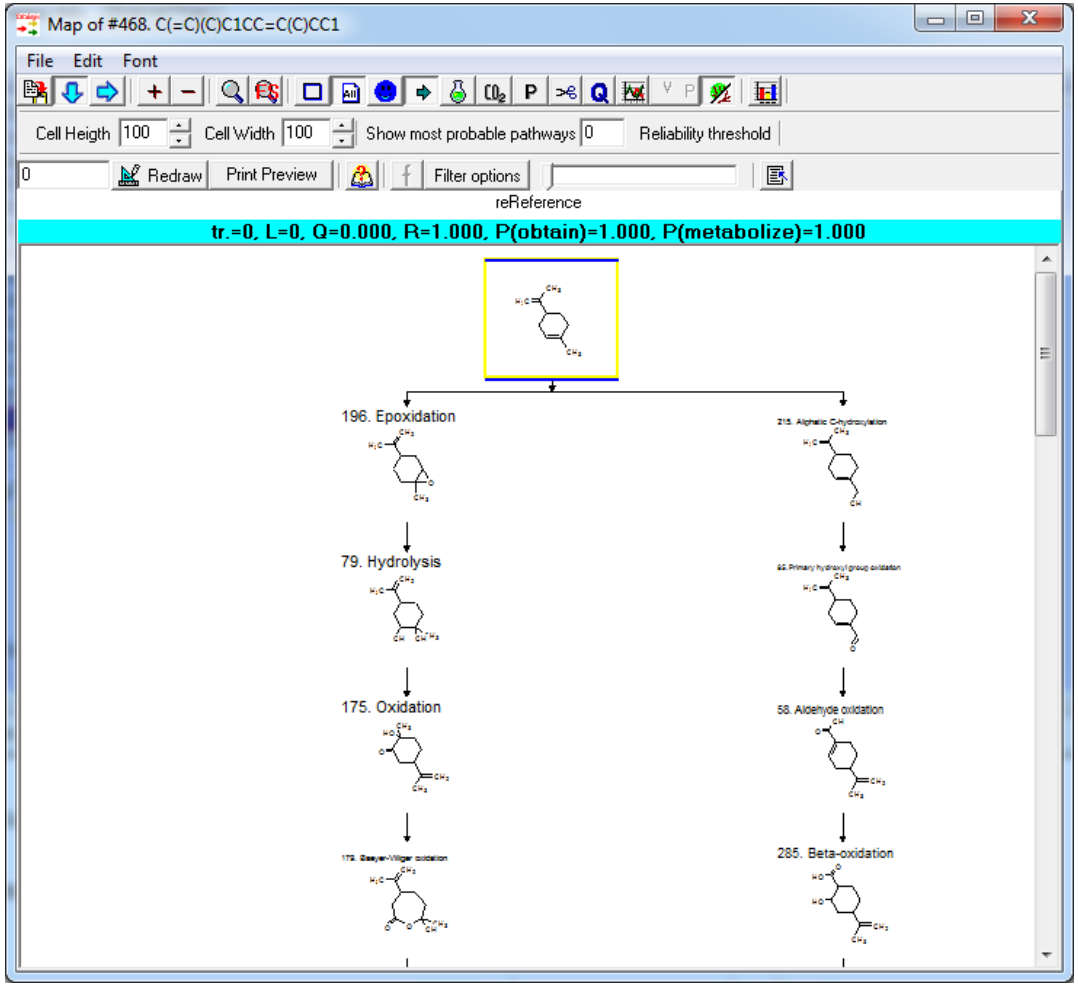

Fig.2. Bidegradation map – two parallel biodegradation pathways and names of transformations are shown

3. Metabolites distribution

Based on the simulated microbial biodegradation and fitted transformation probabilities, the CATALOGIC biodegradation models allow calculation of metabolite characteristics, such as quantity and probability to be obtained. Calculated metabolite parameters are displayed by the **Metabolite distribution** functionality of CATALOGIC. The examples below show its use for analyzing environmental fate of parent chemical and degradants.

- **Identification of stable degradants**

Stable degradants can be identified based on their calculated quantity (mol/mol parent.) In the example below BOD calculated for the parent chemical (Fig.3) is 95%. Fig. 4 shows the distribution of formed metabolites, among them a stable degradant (Quantity=0.854 mol/mol parent).

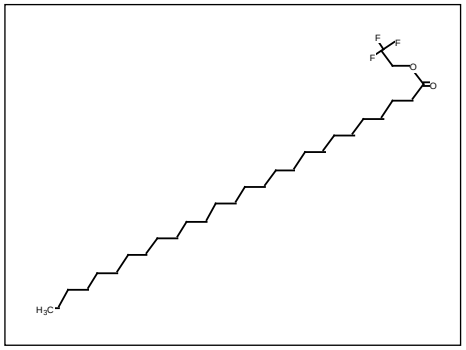

Fig.3 Parent chemical

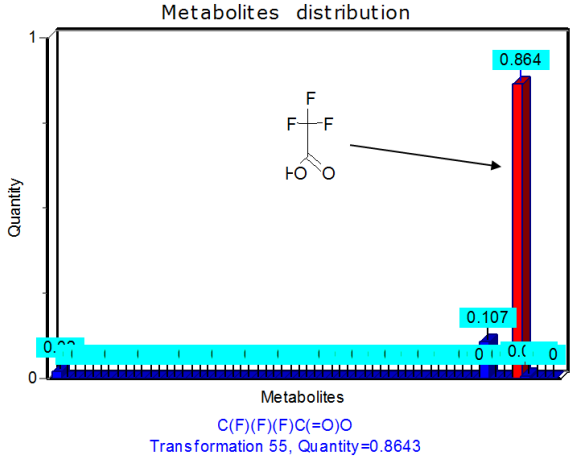

Fig.4. Metabolite distribution

- **Lipophilicity of parent chemicals and degradants**

Based on the analysis of quantity and lipophilicity of limonene and its metabolites performed by CATALOGIC (Fig. 5), the following conclusions can be made:

- Limonene has logKow = 4.83
- Limonene is fully degraded within 28 days
- All degradants have logKow <3.6
- Two metabolites have quantity larger than 0.1 mol/mol parent, but they are also highly hydrophilic (logKow<0).

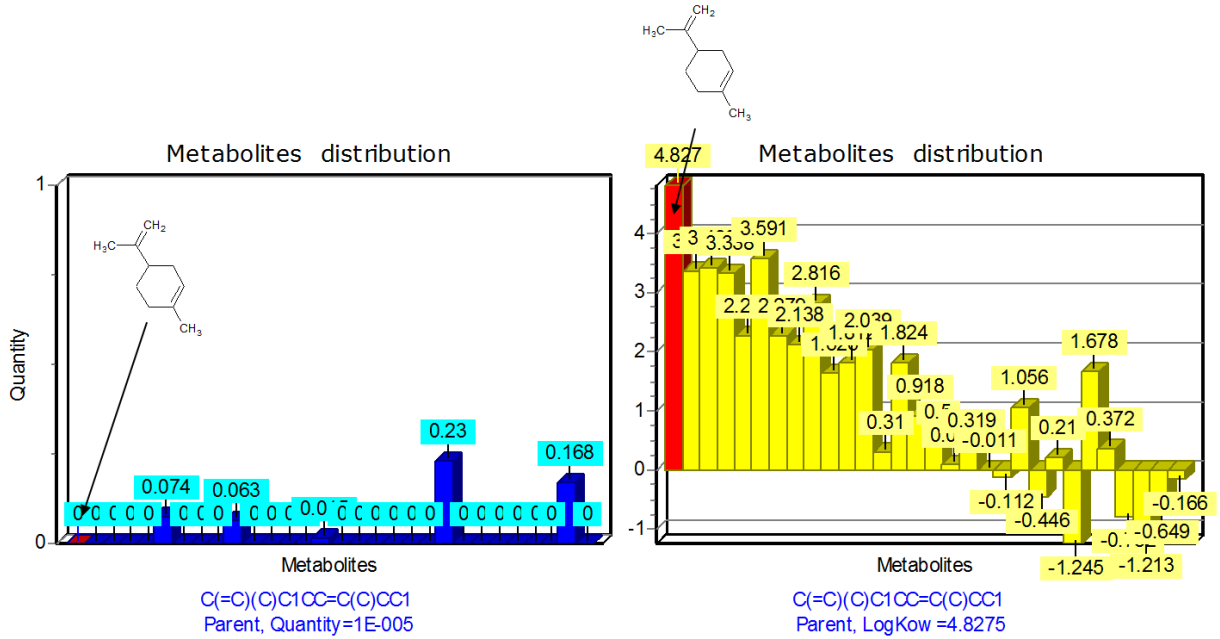

Fig.5. Quantity and logKow distribution of limonene and its degradants

4. Biodegradation kinetics

In addition to the standard CATALOGIC functionalities, the biodegradation kinetic models (OECD 301F and 301B) include predicted biodegradation kinetics – biodegradation curve and quantity of parents and metabolites over time.

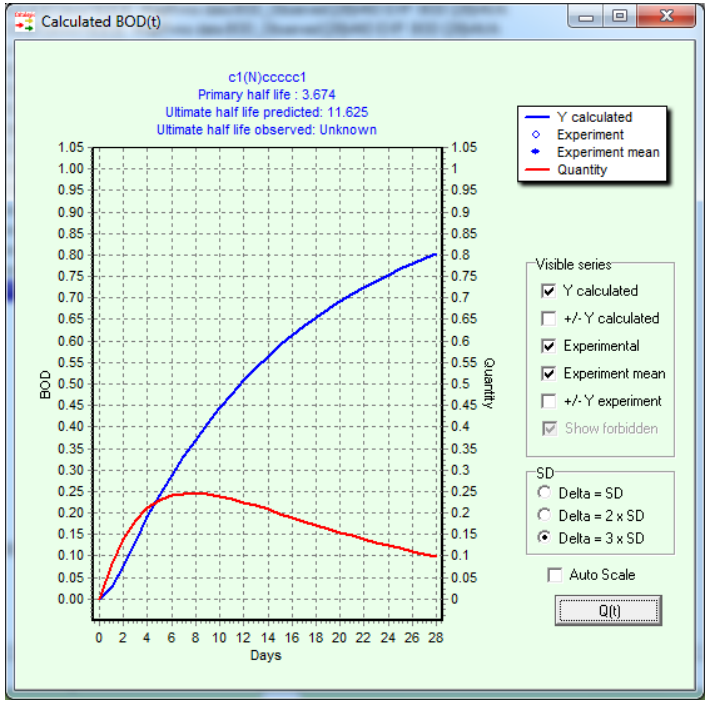

Fig.5. CATALOGIC Kinetic 301F model – Predicted biodegradation curve (−) and quantity of a selected metabolite (−)