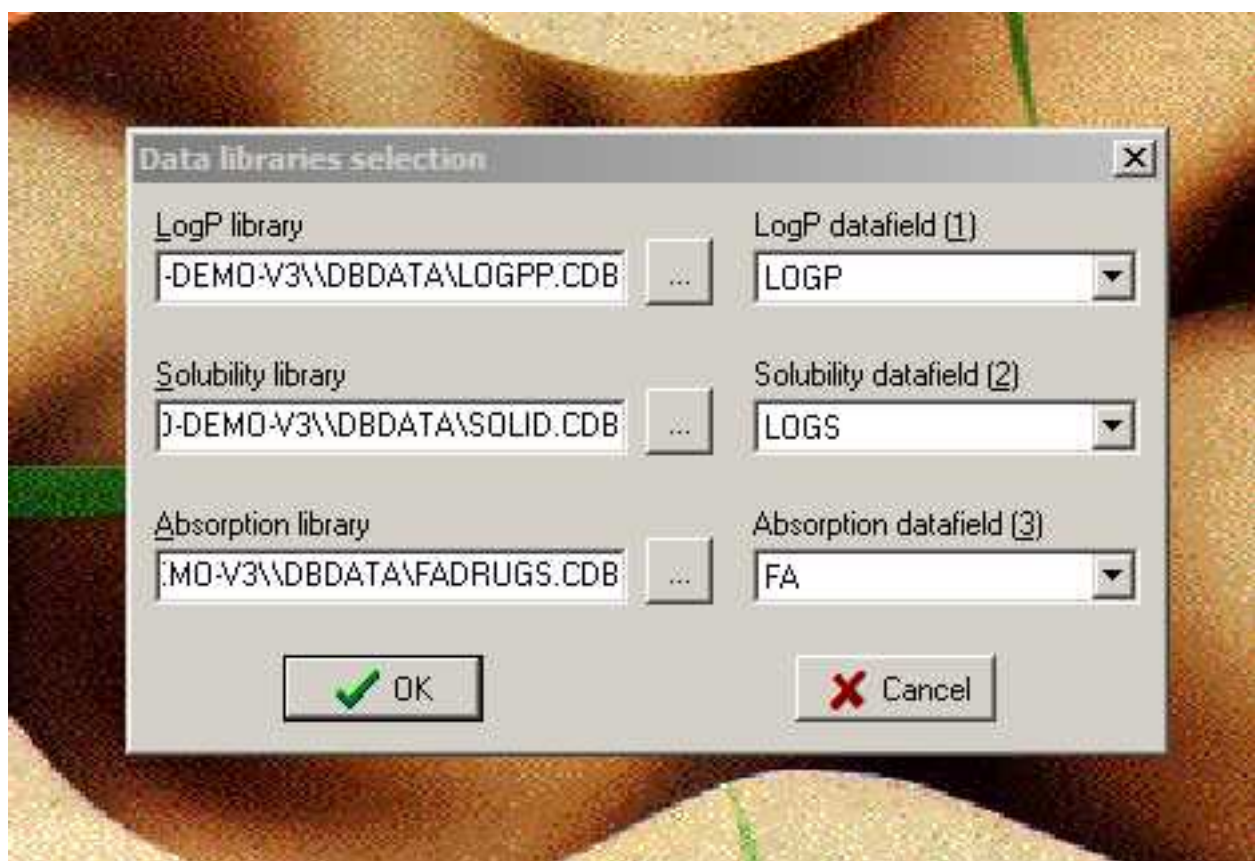


Note: Before this operation you should convert your database written in SDF format in format *.cdb by means of CheD (see Help or Manual of CheD). When you form it don't forget to insert fields for data of values you are interested in (for example, logP, logSw and FA).

Make sure data libraries are selected correctly

In the top Menu - Tools - Slipper - Databases selection. Make sure that LogP, Solubility and Absorption libraries and corresponding fields are selected correctly.



To start prediction

Predict and save results in database - Fadrugs.CDB

Field to save <u>LogP</u>	Field to save <u>solubility</u>	Field to save <u>absorption</u>
<not calculate>	<not calculate>	<not calculate>
Number of neighbours [1]	Number of neighbours [2]	Number of neighbours [3]
5	3	2

pH to predict:

☐ Predict for a structure from database - no pH dependence
☒ Predict to pH: 7.4

Solubility units:

☒ LogSw ☐ mol/l ☐ g/l

Start

File Edit View Options Database Help
 File: Open (Ctrl+O) Save (Ctrl+S) Save as (Ctrl+Shift+S) Print (Ctrl+P) Exit (Ctrl+Q)
 Edit: Undo (Ctrl+Z) Redo (Ctrl+Y) Copy (Ctrl+C) Paste (Ctrl+V) Find (Ctrl+F) Replace (Ctrl+H)
 View: Main window (Ctrl+W) Structure window (Ctrl+S) Solubility window (Ctrl+L) Absorption window (Ctrl+A)
 Database: Connect (Ctrl+D) Disconnect (Ctrl+Shift+D) Refresh (Ctrl+R) Export (Ctrl+E) Import (Ctrl+I)
 Help: About (Ctrl+H) Fadrugs.CDB manual (Ctrl+F1) Fadrugs.CDB online help (Ctrl+F2)