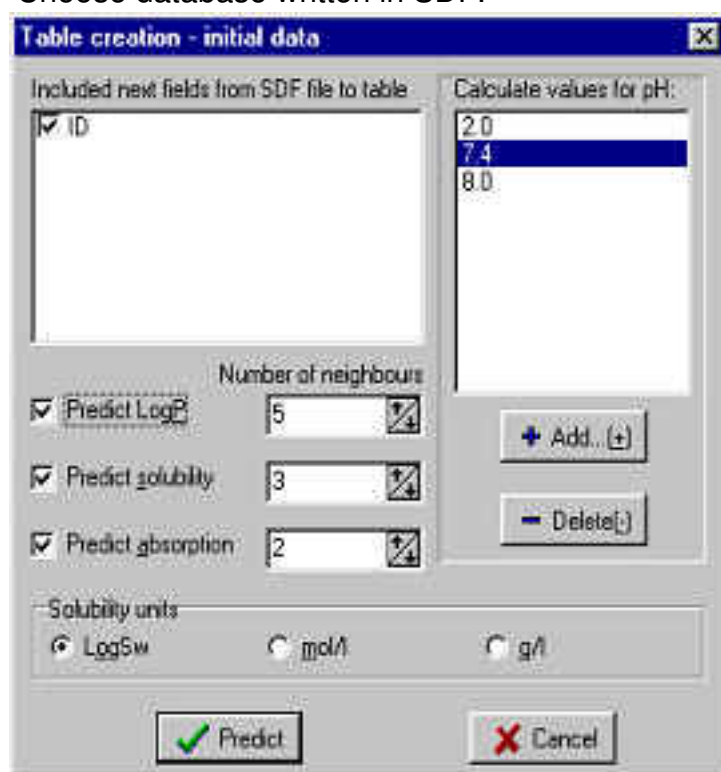


This option allows you to get data on lipophilicity, solubility and absorption for a database written as *.sdf -file.

To get prediction

1. Choose database written in SDF.



2. As you will get data in this option in a table form, in left box you should mark fields existing in your file if you need to have them in a result file.

3. Introduce pH values, that you need.

4. Use check boxes Predict logP, solubility, and absorption to mark characteristics of compound you want to get and choose numbers of nearest neighbors in each case of prediction.

5. If you want to know solubility in mg/l or mol/l mark corresponding radioitems.

6. Press Predict or Cancel.

The table with calculation values will begin to appear in a new window. You may interrupt calculation pressing the Cancel button.

ID	FA	logP at pH=2.0	logSw at pH=2.0	logP at pH=7.4	logSw at pH=7.4	logP at pH=8.0	logSw at pH=
SpecGood-0012	0.58	-2.43	-6.4923	0.22	-6.5958	0.60	-6.7491
SpecGood-0013	0.55	0.52	-3.5125	3.92	-4.3708	3.88	-4.0066
SpecGood-0025	0.86	1.62	-9.3755	3.49	-10.0767	3.49	-10.0669
SpecGood-0029	0.99	-0.14	-3.8022	1.75	-5.1441	1.75	-5.1304
SpecGood-0031	0.12	3.13	-4.7013	3.12	-4.4457	3.08	-4.0815
SpecGood-0045	0.46	-2.62	-3.6214	0.04	-3.5923	0.03	-3.3859
SpecGood-0107	0.85	-1.89	-5.633	-0.07	-5.8312	-0.07	-5.8312
SpecGood-0111	0.89	0.34	-5.4698	2.21	-6.151	2.21	-6.1451
SpecGood-0113	0.99	-1.53	-5.4377	0.34	-6.1369	0.34	-6.129
SpecGood-0121	0.86	1.62	-9.3755	3.49	-10.0767	3.49	-10.0669

You may save the information as *.xls or *.txt file (button Save to file).

The screenshot shows a Microsoft Excel spreadsheet with the following data:

ID	FA	logP at pH	logSw at p	logP at pH	logSw at p	logP at pH	logSw at pH=6.0
2	SpecGood	0.68	-2.43	-6.4923	0.22	-6.6868	0.6 -6.7491
3	SpecGood	0.55	0.52	-3.5125	3.92	-4.3708	3.66 -4.0066
4	SpecGood	0.66	1.62	-9.3755	3.49	-10.0767	3.49 -10.0669
5	SpecGood	0.99	-0.14	-3.8022	1.75	-5.1441	1.75 -5.1304
6	SpecGood	0.12	3.13	-4.7013	3.12	-4.4457	3.08 -4.0615
7	SpecGood	0.46	-2.62	-3.6214	0.04	-3.5923	0.03 -3.3659
8	SpecGood	0.65	-1.89	-5.633	-0.07	-5.8312	-0.07 -5.8312
9	SpecGood	0.89	0.34	-5.4698	2.21	-6.151	2.21 -6.1451
10	SpecGood	0.99	-1.53	-5.4377	0.34	-6.1369	0.34 -6.129
11	SpecGood	0.66	1.62	-9.3755	3.49	-10.0767	3.49 -10.0669

the data to get full profiles of logP at pH, logSw at p, logP at pH, logSw at pH=6.0 for a compound of your interest in

The screenshot displays a software interface for chemical data analysis. It features a table of predicted data for various compounds, a detailed view for a specific compound (FA) with its chemical structure and a titration curve, and a list of chemical identifiers.

ID	FA	logP at pH=2.0	logSw at pH=2.0	logP at pH=7.4	logSw at pH=7.4	logP at pH=8.0	logSw at pH=8.0
SpecGood-0012	0.58	-2.43	-6.4323	0.22	-6.5656	0.00	-6.7491
SpecGood-0013	0.55						
SpecGood-0025	0.86						
SpecGood-0028	0.93						
SpecGood-0031	0.12						
SpecGood-0045	0.48						
SpecGood-0107	0.95						
SpecGood-0111	0.89						
SpecGood-0113	0.93						
SpecGood-0121	0.86						

Predicted data for compound

Case#	pH	logP	logSw	FA	Compound ID
1	4.33	3.833	-4.351	0.954	
	2	0.5209	3.5129		
	7.4	3.9563	-4.3708		
	8	3.8793	-4.0584		

The interface also shows a chemical structure of a complex organic molecule and a titration curve plot with pH on the x-axis and logP/logSw on the y-axis.

Structure of the compound is shown in the image. The predicted data for the compound is shown in the table below.