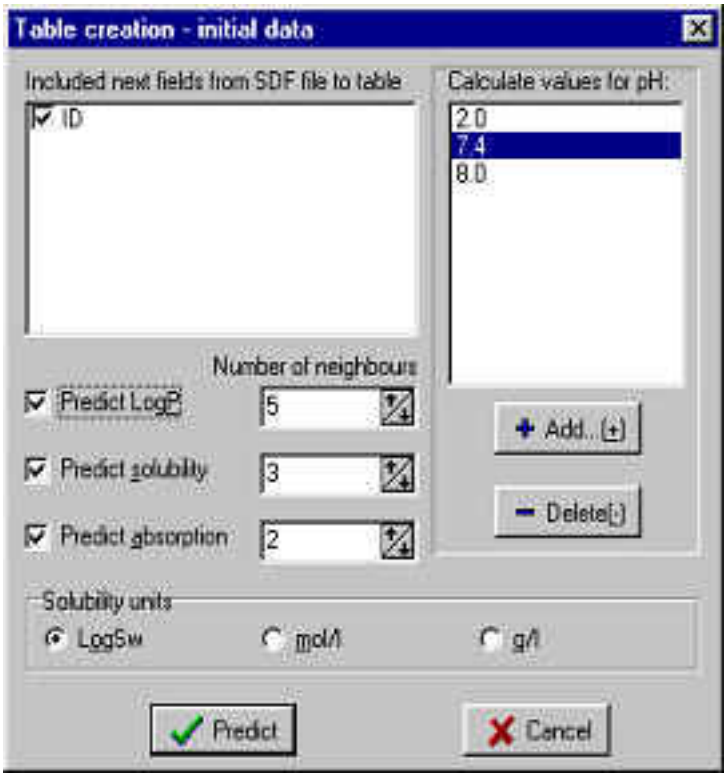
This option allows you to get data on lipophilicity, solubility and absorption for a database written as *.sdf -file.

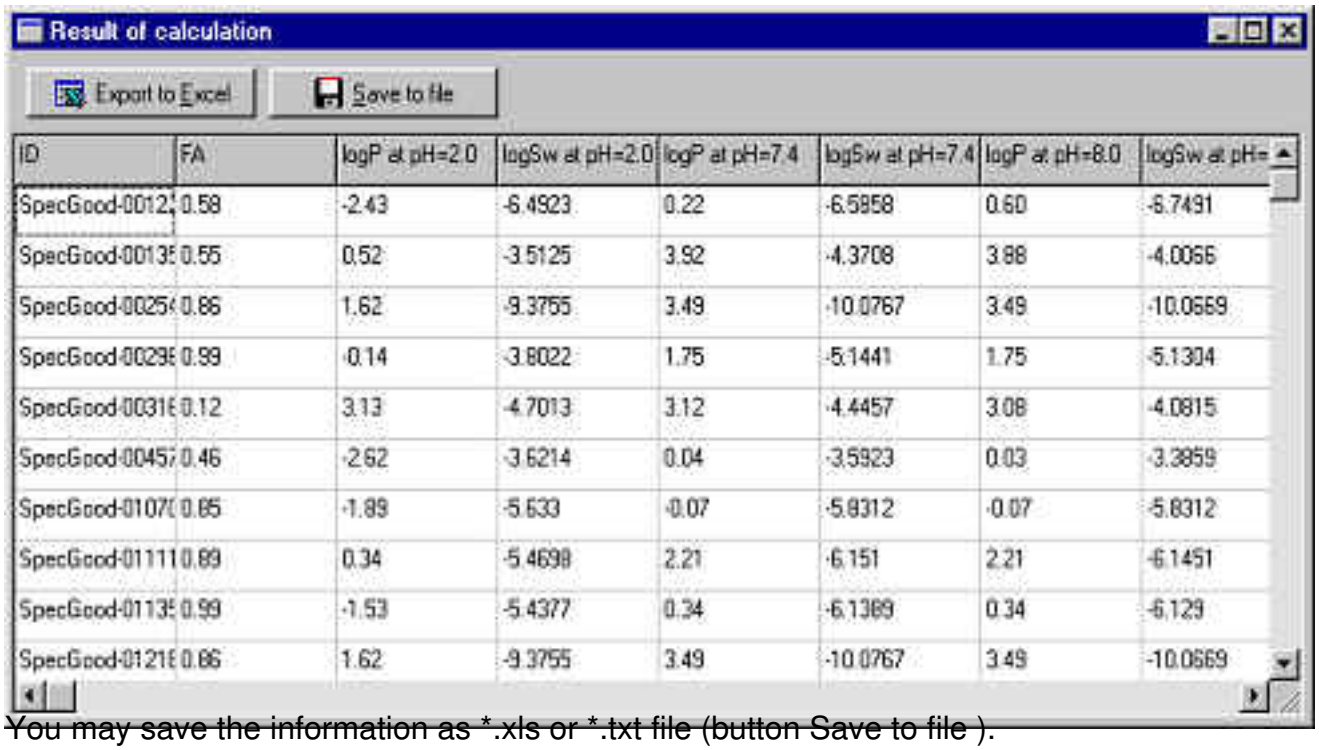
To get prediction

1. Choose database written in SDF.



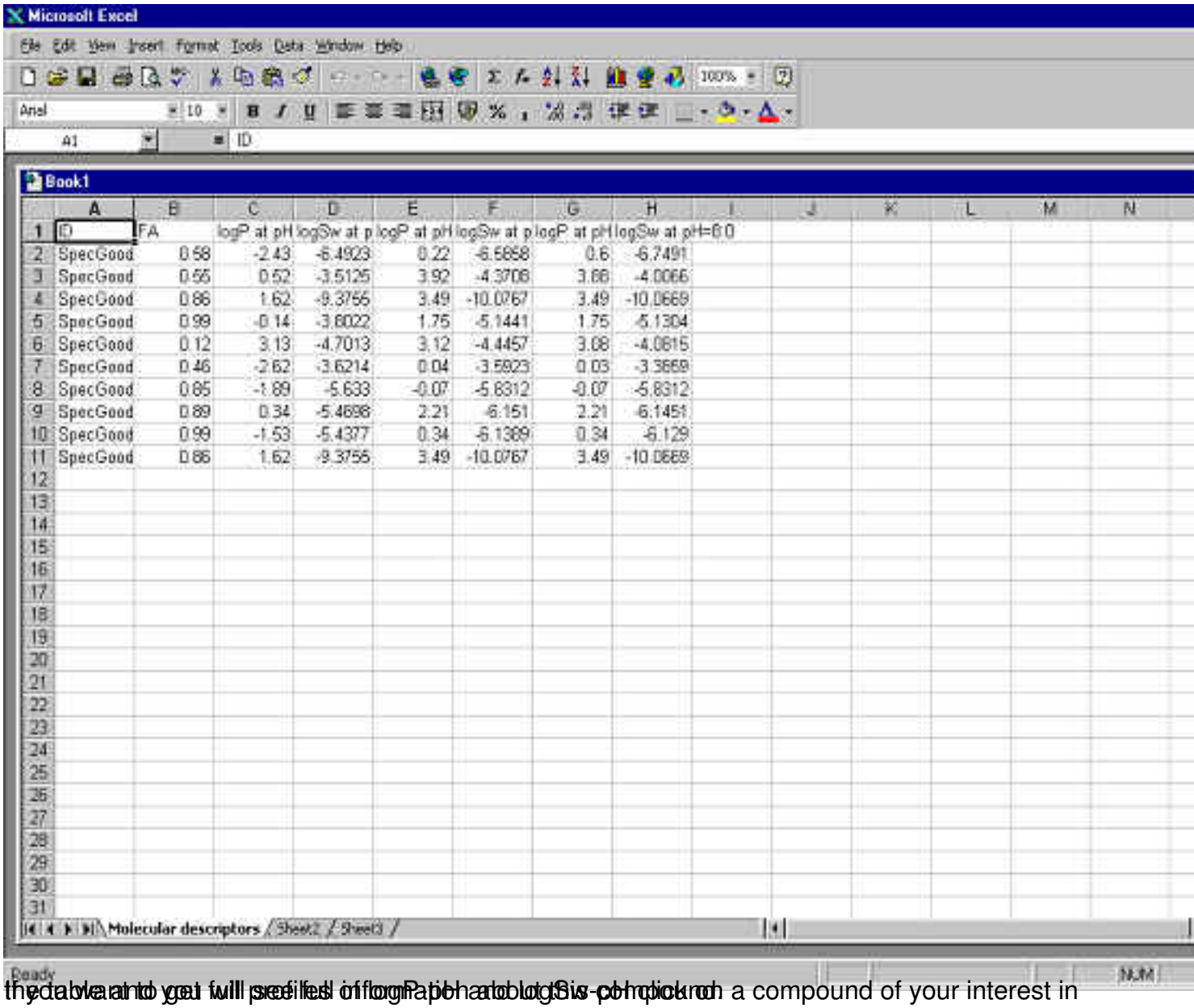
2. As you will get data in this option in a table form, in left box you should mark fields existing in your file if you need to have them in a result file.
3. Introduce pH values, that you need.
4. Use check boxes Predict logP, solubility, and absorption to mark characteristics of compound your want 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.



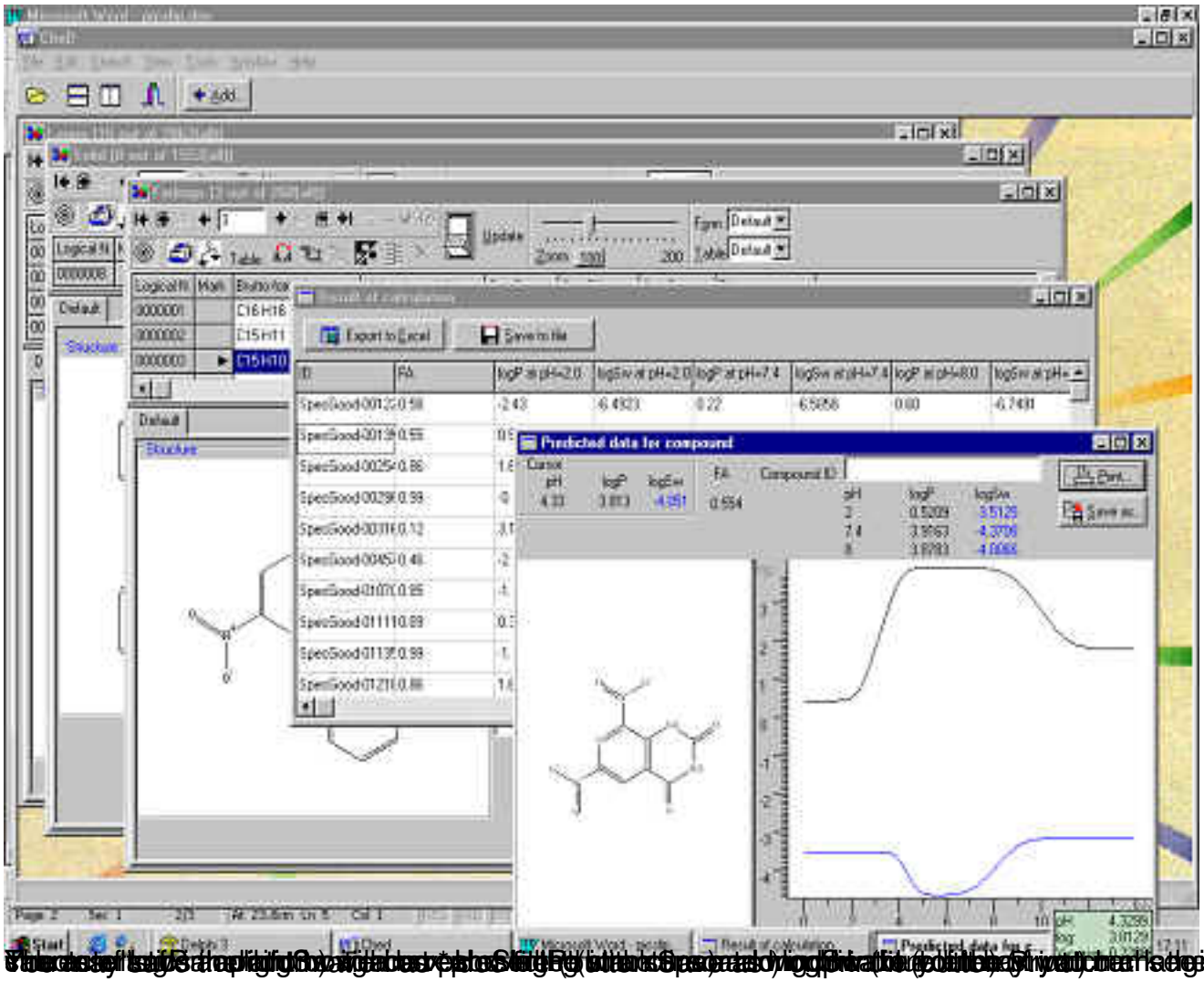
ID	FA	logP at pH=2.0	logSw at pH=2.0	logP at pH=7.4	logSw at pH=7.4	logP at pH=8.0	logSw at pH=
SpecGood-0012	0.58	-2.43	-6.4923	0.22	-6.5958	0.60	-6.7491
SpecGood-0013	0.55	0.52	-3.5125	3.92	-4.3708	3.88	-4.0066
SpecGood-0025	0.86	1.62	-9.3755	3.49	-10.0767	3.49	-10.0669
SpecGood-0029	0.99	-0.14	-3.8022	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-01111	0.89	0.34	-5.4698	2.21	-6.151	2.21	-6.1451
SpecGood-0113	0.99	-1.53	-5.4377	0.34	-6.1389	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).



	A	B	C	D	E	F	G	H
1	ID	FA	logP at pH	logSw at p	logP at pH	logSw at p	logP at pH	logSw at pH=6.0
2	SpecGood	0.58	-2.43	-6.4923	0.22	-6.5858	0.6	-6.7491
3	SpecGood	0.55	0.52	-3.5125	3.92	-4.3708	3.66	-4.0066
4	SpecGood	0.86	1.62	-9.3755	3.49	-10.0767	3.49	-10.0669
5	SpecGood	0.99	-0.14	-3.6022	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	-3.3669
8	SpecGood	0.85	-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	-6.1389	0.34	-6.129
11	SpecGood	0.86	1.62	-9.3755	3.49	-10.0767	3.49	-10.0669

the table and you will see the logP and logSw predicted for a compound of your interest in


Predicted data for compound
Export to Excel
Save to file