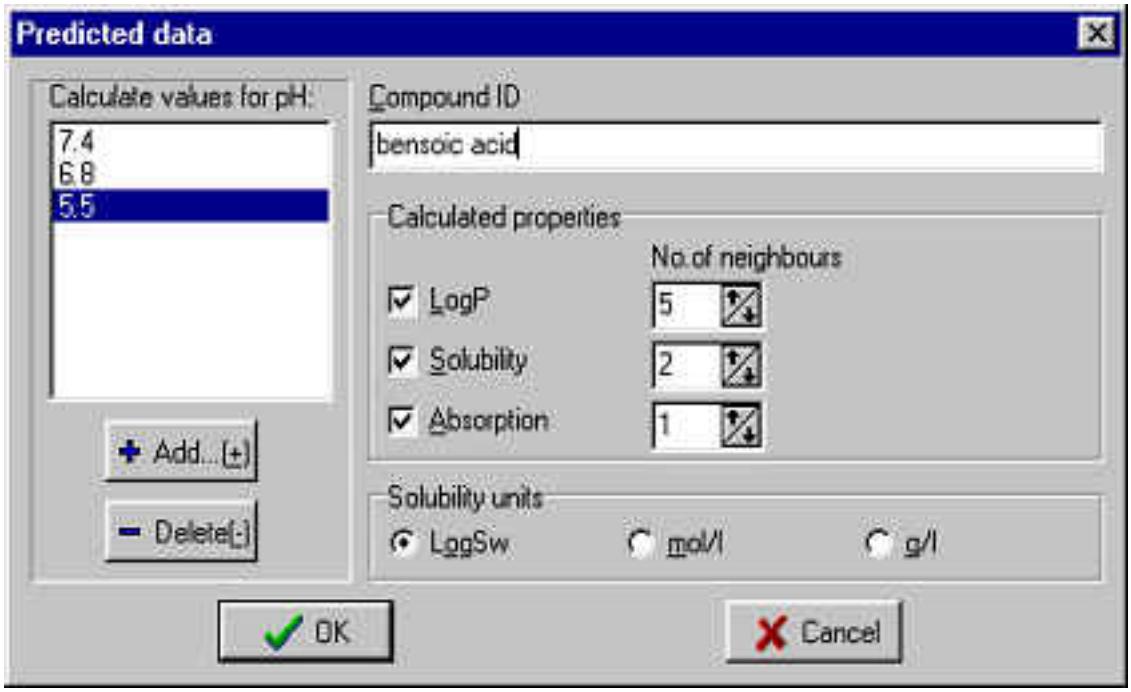
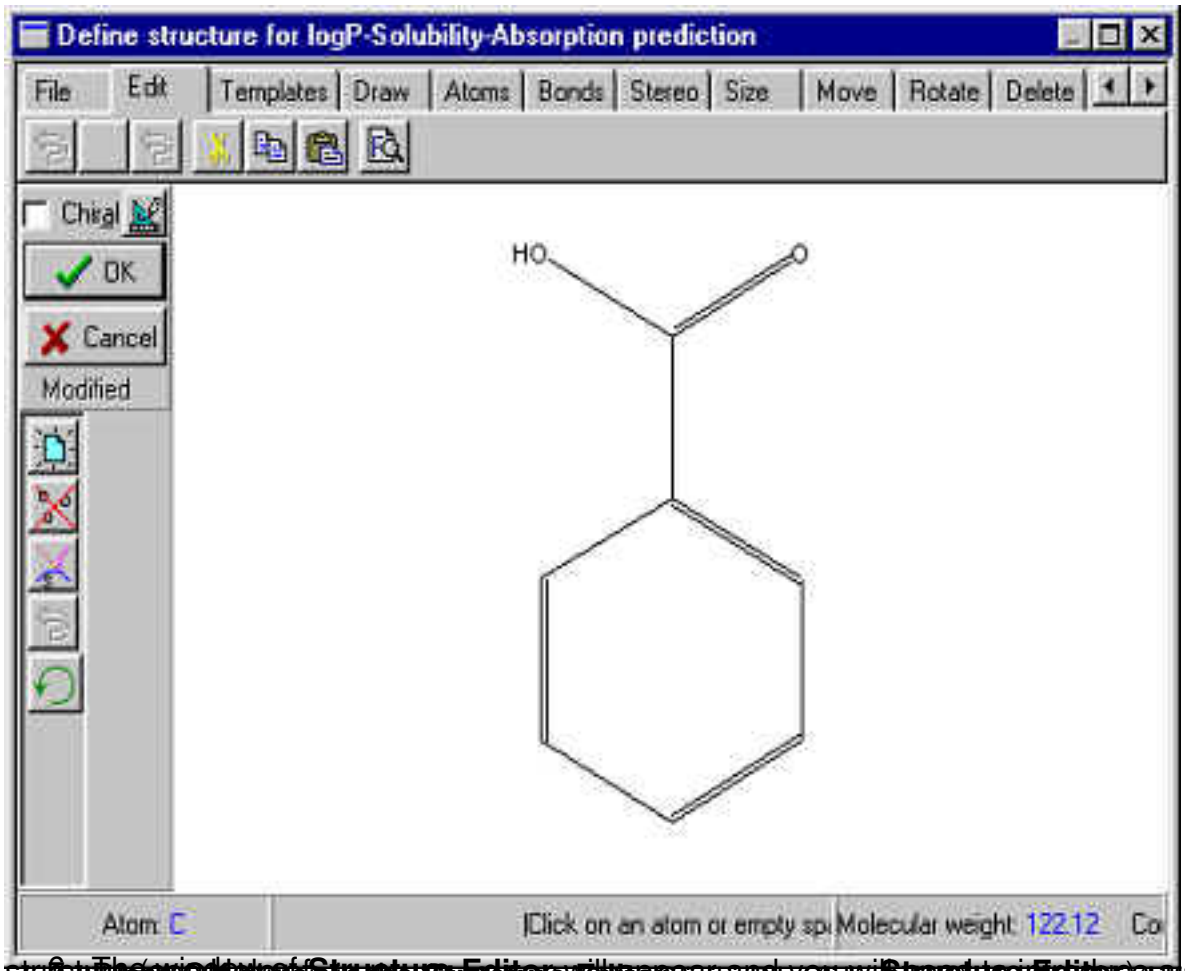
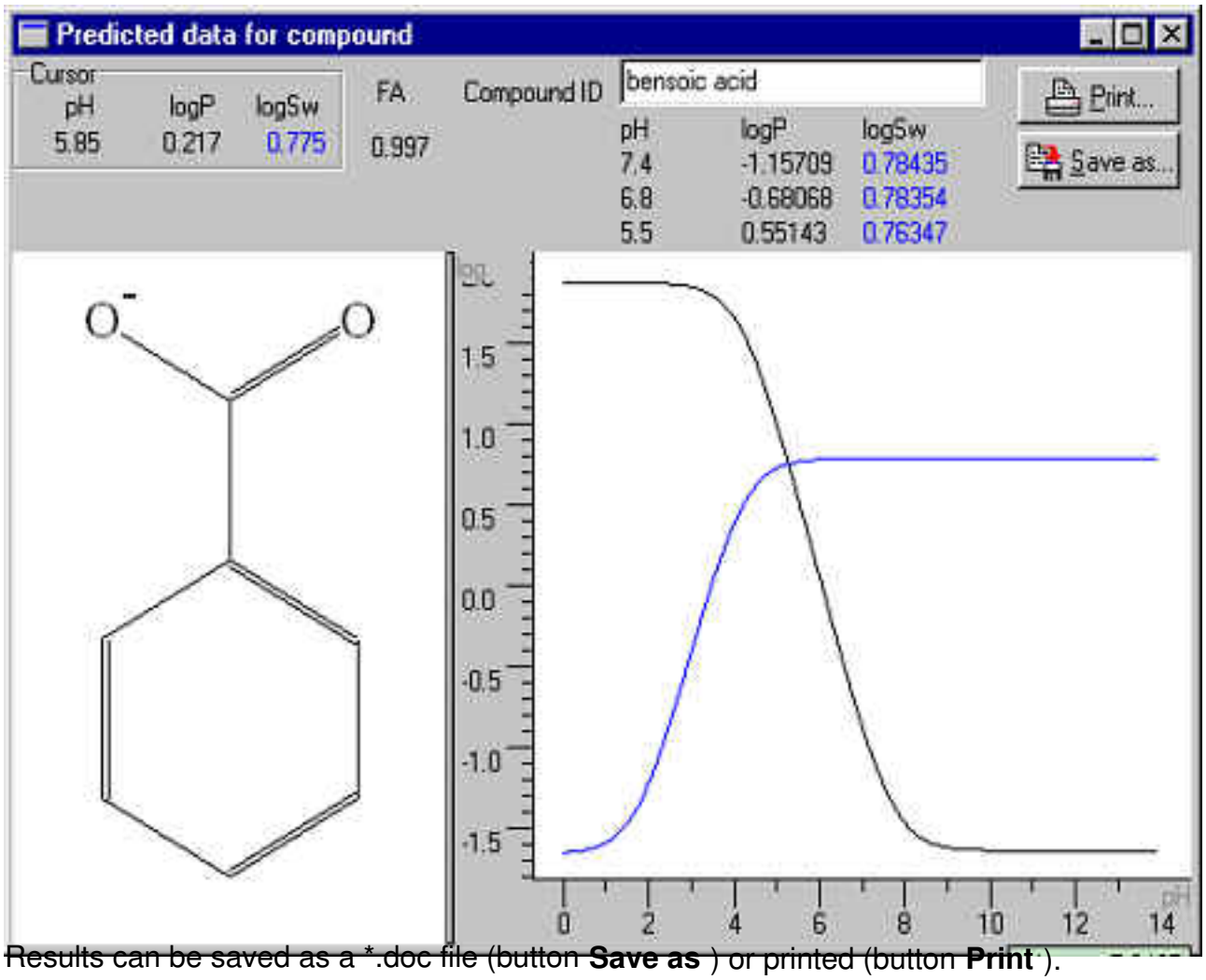
This option allows you to get data on lipophilicity, solubility and adsorption for a single compound.

To get the prediction

1. enter the name of a compound or its ID
2. Enter pH values
3. Use check boxes logP, Solubility and Absorption to mark characteristics of compound you want to calculate and number of nearest neighbors for these calculations.
4. If you need to know solubility in mg/l or mol/l mark corresponding items.
5. Press OK or Cancel.




Define structure for logP-Solubility-Absorption prediction
File
Edit
Templates
Draw
Atoms
Bonds
Stereo
Size
Move
Rotate
Delete
Chiral
OK
Cancel
Modified
HO
O
Atom: C
Click on an atom or empty sp
Molecular weight: 122.12
Co



Results can be saved as a *.doc file (button **Save as**) or printed (button **Print**).