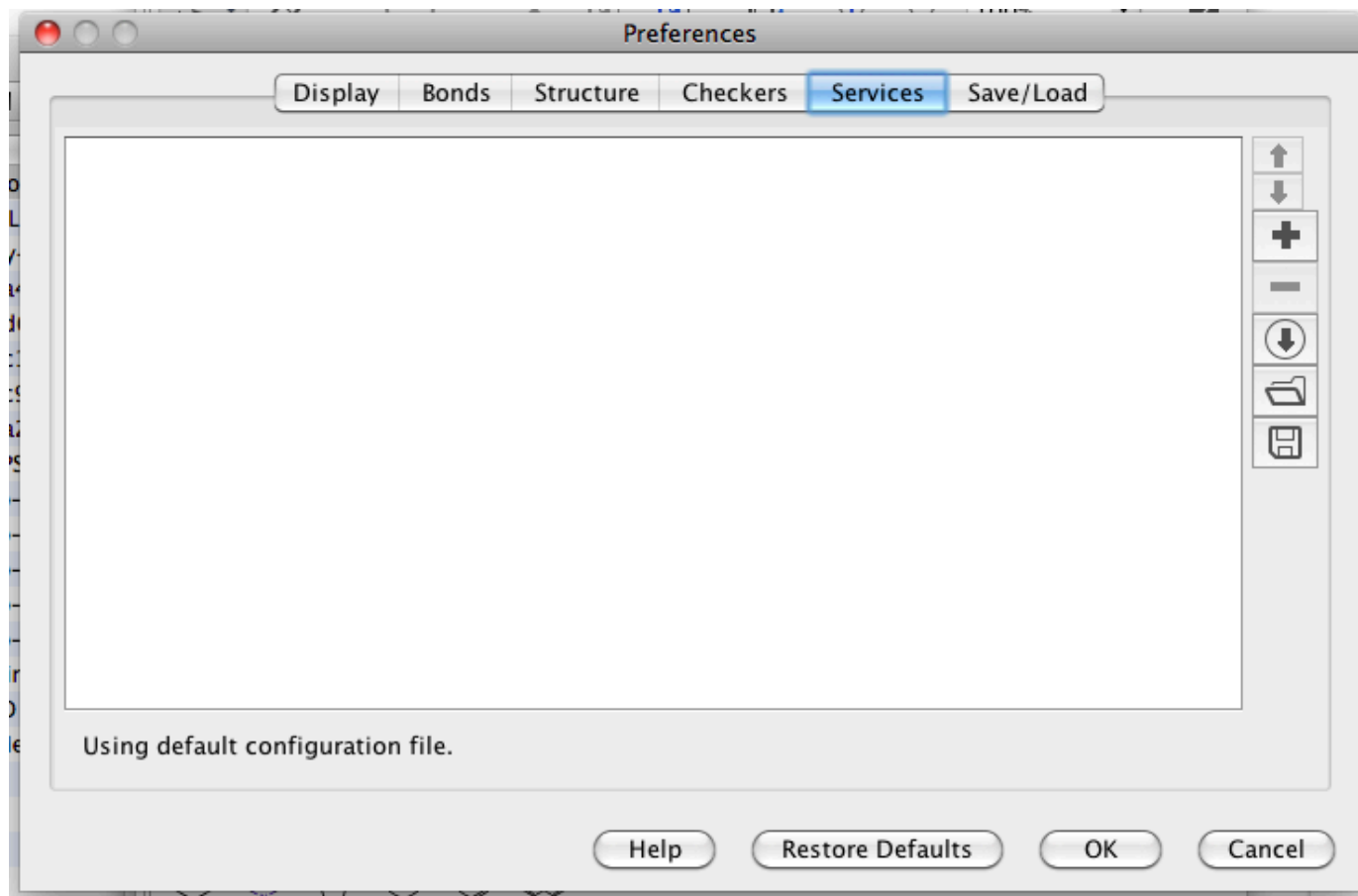


Integration with MarvinSketcher

Predictions by the models developed using OCHEM can be accessed from MarvinSketch. To add an OCHEM model into MarvinSketch, you can add it as an HTTP service.

Go to Edit > Preferences menu and open the "Services" tab:



Add a new service and configure it as show in the dialog below:

Preferences

Display Bonds Structure Checkers **Services** Save/Load

Service name:

Service description:

Service type:

Service URL:

Call Method:

Type	Name	Evaluation	Value
String	mol	Molecule format	smiles
<Select Type>			

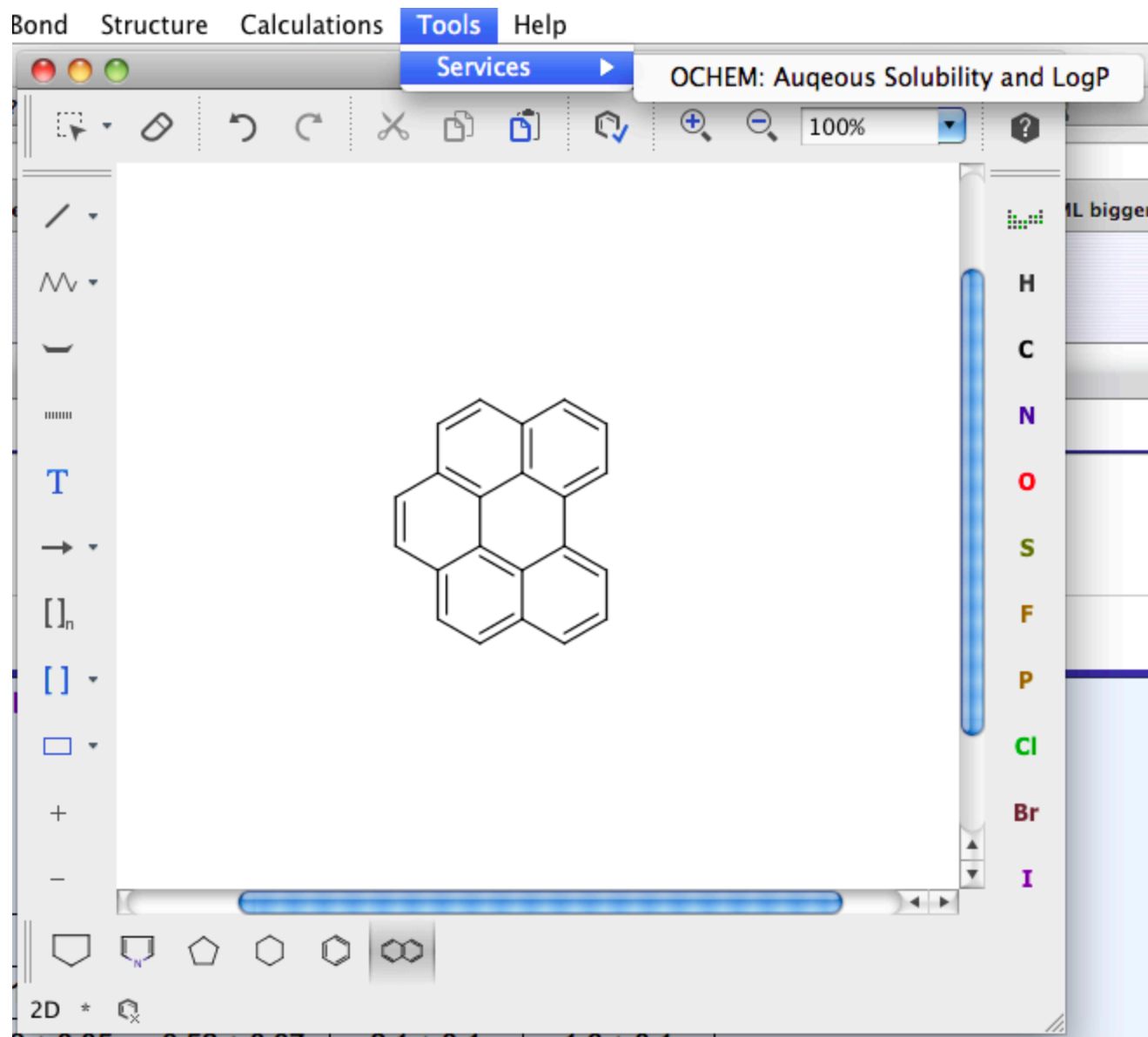
Accept Cancel

Help Restore Defaults OK Cancel

where the URL will look `https://ochem.eu/marvinintegration/<YOUR_MODEL_ID>.do`

In the example above, "4" stands for the public ID of aqueous solubility model.


Once the service is configured, you can run predictions via the "Services" menu:



The calculation can take some time (from several seconds to minutes).
After the calculation is completed, the prediction results will be displayed in a separate dialog:

OCHEM: Aqueous Solubility and LogP

► Structure



Update

► Arguments

mol	smiles
-----	--------

► Results

OCHEM prediction results

logPow is 7.01 Log unit (RMSE is 0.391)
Aqueous Solubility is 8.88 -log(mol/L) (RMSE is 0.721)

☐ Calculate automatically

Calculate