How to run a conformation search run on Murska

Outline: Prepare the calculation on your computer using Maestro Gui. Move the files to Murska and run them from the command line. Copy the result files back to your computer.

1) Draw some molecule with rotatable bonds (~10-15 heavy atoms)
2) Choose: Applications -> Macromodel -> Conformational search
3) Edit options or accept defaults and choose the "write" button, next to the "start" button on the first sheet
4) Choose a name (no spaces) e.g. "haku" and press "write"
    This will write two files in your working directory (where you started Maestro) named "haku.mae" and "haku.com".
5) Log in Murska from another terminal (if you don't have an account, ask for a training account from the lecturer)

```
ssh murska.csc.fi -l your-user-account
```

5.1) Enable passwordless ssh from compute nodes to the login nodes

```
cd
mkdir .ssh
cd ~/.ssh
rm -f authorized_keys
cat $WRKDIR/.ssh/id_rsa.pub > authorized_keys
chmod og-rxw *
```

    * note that it is strictly forbidden to enable passwordless ssh access to any CSC's servers from outside CSC

6) Create a new directory for your job (e.g. hakudir) in your $WRKDIR

```
cd $WRKDIR
mkdir hakudir
cd hakudir
```

7) Transfer the input files to Murska
    Give this command on your own local machine
    Substitute “your-user-account” below with your actual user account in Murska

```
scp haku* your-user-account@murska.csc.fi:/wrk/your-user-account/hakudir
```

8) Initialize the Maestro environment

```
module load maestro
```

9) Submit the conformation search as a serial job:

```
bmin -HOST murska-serial-2days haku
```

    For other queues available give `bmin -HOSTS`

10) Monitor your job if all went well (you can ignore the "ulimit: data seg size:..." complaint)

```
bjobs
```

`bjobs -l JOBID` (replace JOBID with the first column of the previous command output)

```
tail -f haku.log
```

11) When the job has finished copy the files back to the original directory in your local machine.
    First make one tar file of all output. In the "hakudir" directory in Murska give:

```
tar cf valmis.tar *
```

In the *original* directory (on your local machine) where you have only the two haku-files, give:

```
scp your-user-account@murska.csc.fi:/wrk/your-user-account/hakudir/valmis.tar .
```

12) Untar the package

```
tar xvf valmis.tar
```

If you have a Windows machine, you can use “zip” or some other similar functionality.

13) Refresh the view in Maestro and see what you have obtained. Choose "Import structures from file" icon and select haku-out.maegz

Additional notes:

* A parallel MacroModel job (using 4 cores) in Murska would be run with:

```
$SCHRODINGER/utilities/para_bmin -NJOBS 4 -HOST murska-serial-2days:4 haku
```

More information on running jobs in Murska:
http://www.csc.fi/english/research/sciences/chemistry/maestro_files/maestro-standalone