# How To Upload calc’s to ioCHem-bd database

I assume you already have an account at the data base.

<https://iochem-bd.bsc.es/browse/>

## Preparations

The automated shell upload only works on a UNIX machine (Linux, Ubuntu, …). This can be *Photons* or the Ubuntu subsystem available for Windows 10.

Normally, you want to upload only input and output files. For ORCA that’s name.inp and name.out. For Gaussian that’s name.gjf and name.log. These files need to be on the UNIX system.

If you are using your Ubuntu subsystem you can move files from Windows to the current folder of that subsystem with:

cp /mnt/c/.../file.end file.end for a single file

cp -r /mnt/c/.../folder folder for a folder (and all subfolders)

Note, that c is the drive (so might be d). But it always has to start with /mnt/

Install the ioChem shell on your UNIX system as described here:

<https://docs.iochem-bd.org/en/latest/guides/usage/uploading-content-to-create/using-shell-client.html>

## Uploading files

Once logged into your repository via > source start-rep-shell, you can move around in your repository via > cdpro, create projects, etc. You also can still move around your UNIX machine using normal commands. For all repository commands, see:

<https://docs.iochem-bd.org/en/latest/guides/usage/uploading-content-to-create/shell-commands.html>

Move to the project of your repository where you want to upload files to. Also move to the folder on your UNIX machine, where these files are at.

### Uploading a single file:

For ORCA:

loadorca -i name.inp -o name.out -n “name” -d “description”

For Gaussian (note, Gaussian calc’s only work when the #p flag was set during the calculation!)

loadgauss -i name.gjf -o name.log -n “name” -d “description”

“name” and “description” can be any string. They will be displayed in the repository so I usually go with the name of the molecule (“Aniline”) and the job type (“OptFreq”) or something.

### Uploading all files of the current folder

To upload all files (and by that I always mean the pair of input and output files), create the following bash script (you could name it something like autoUpOrca.sh or autoUpGauss.sh)

For ORCA:

#!/bin/bash

#` -pe smp\* 12

#$ -N test

#$ -cwd

for s in "$@"

do

basename=${s%'.inp'}

input=$s

output="$basename.out"

bbase=${basename%'\_OptFreq'}

echo $bbase

loadorca -i $input -o $output -n $bbase -d “OptFreq”

echo ' '

done

And then execute it as > ./autoUpOrca.sh \*.inp

Technically you could use that script also for only a subset of your files (even a single file). It uploads all files given after the execution command (here, all files in the folder). Note, always refer to the .inp files!

For Gaussian we do the same and just switch some file endings:

#!/bin/bash

#` -pe smp\* 12

#$ -N test

#$ -cwd

for s in "$@"

do

basename=${s%'.gjf'}

input=$s

output="$basename.log"

bbase=${basename%'\_OptFreq'}

echo $bbase

loadgauss -i $input -o $output -n $bbase -d “OptFreq”

echo ' '

done

And then execute it as > ./autoUpGauss.sh \*.gjf

Note that in both script, the -d “description” was just set to “OptFreq” (assuming you are uploading a geometry optimization + frequency calculation). This can be set to whatever you want.

Also note that the -n “name” is set to the respective filename minus a \_OptFreq suffix (if there is one). Again, you could make up your own name but normally it’s reasonable to use the name of the file. Do as you like :)

Also also: Uploading might take a while, so be patient and don’t assume that it’s stuck.

More on automated upload scripts: <https://docs.iochem-bd.org/en/latest/guides/usage/uploading-content-to-create/using-shell-client/shell-automated-scripts.html>