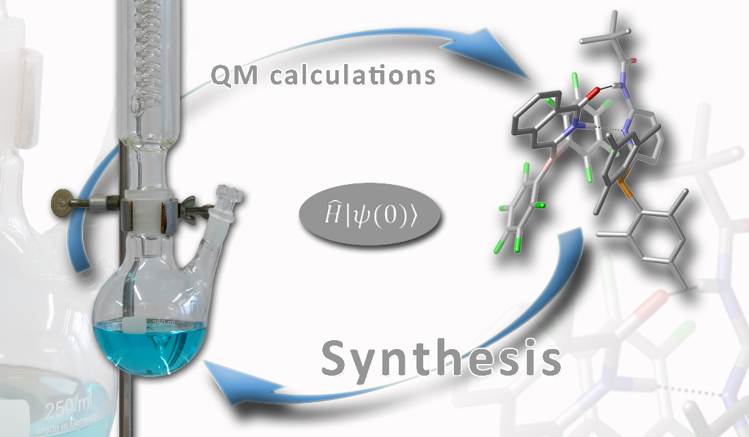
**Welcome to the Research Group of Dr. Urs Gellrich**

**at the Justus-Liebig-University of Gießen**



This guide will show you how to get our scripts to work on the different clusters

(**Fuchs**, **Loewe**, **Skylla** and **Halo**)

Our scripts provide useful help for otherwise time expensive routine work like gathering different parameters from output files or converting output files to xyz files.

Another helpful script allows you to submit different calculations in different folders automatically with just one command

**General Informations on submitting calculations:**

Use **Fuchs**, **Loewe** and **Skylla** to submit your **Gaussian16** calculations

Use **Halo** to submit your **ORCA** calculations

To be able to submit calculations we rely on the excellent scripts from Prof. Schreiner’s group which save a lot of time themselves (e.g. by automatically creating the command files or reading dispersion parameters).

With these scripts you can manually submit your calculations to **ORCA** or **Gaussian16** with the commands „*gaussian16 hh:mm:ss*“ and „*orca input hh:mm:ss*“

To get these scripts to work read and follow the instruction on this website

https://www.uni-giessen.de/fbz/fb08/Inst/organische-chemie/agschreiner/computchem\_jlu\_intern

We use **git/github** for a central version control of our scripts. This will provide you with new scripts and updates everytime you login on a cluster via a ssh-client.

Use the command „*git clone* [*https://github.com/baaam24/gellrich\_scripts.git*](https://github.com/baaam24/gellrich_scripts.git)*“* for downloading the scripts the first time (you have to do this once for every cluster)

Now you should have a new folder called **„gellrich\_scripts“** in your home directory. There you will find all scripts, helpfiles, a readme file and this introduction guide.

Next open your **.bashrc** and add the following line:

**On Skylla:** export PATH=/home/YOUR\_S\_OR\_G\_NUMBER/gellrich\_scripts:$PATH

**On Loewe:** export PATH=/home/chemcalc/YOUR\_ACCOUNT\_NAME/gellrich\_scripts:$PATH

**On Fuchs:** PLACEHOLDER

**On Halo:** export PATH=/home/YOUR\_ACCOUNT\_NAME/gellrich\_scripts:$PATH

Now source your **.bashrc** by switching in your home directory and typing the command

„*source .bashrc*“

You will now be able to execute your scripts indepent from the current directory you are in .

To have the newest updates everytime you login you now just have to add the line **„***cd gellrich\_scripts; git pull; cd“* to your **.bashprofile** (on Skylla, Fuchs and Loewe) or **.profile** (on Halo)

(WARNING: DO NOT WRITE THIS COMMAND INTO YOUR .BASHRC OR YOU WILL NOT BE ABLE TO LOGIN VIA YOUR FTP-CLIENT)

Now you should be able to execute the scripts on all clusters. For a short overview of what every script does read the README.md file.