Setting up MQ on BMC cluster from windows client

- 1. Download and install gitbash from https://gitforwindows.org/
- 2. Launch gitbash on your local windows pc and connect to cluster using ssh
- -t <username>@<cluster-ip-address/name> 'cd
- </work/project/project-dir>; bash'
- *stuffs inside angle brackets are variable for other systems/based on your choice and when ever I write local pc it means local windows pc
- 3. Then update gcc on the Linux cluster/machine using the script from https://github.com/darrenjs/howto/blob/master/build_scripts/build_gcc_9.sh
 Run the script in the terminal as: ./build_gcc_9.sh
- 4. Download MONO from https://download.mono-project.com/sources/mono/
- 5. Install on Linux cluster using instructions from https://www.mono-project.com/docs/compiling-mono/linux/ and add to path variable.
- 6. Copy MQ folder from local pc to cluster using rsync -avP <username>@<cluster-ip-address/name>:</work/project/project-dir>.
 This is the entire MQ folder after you downloaded from here.
- 7. Create MQ alias in the .bashrc file on the cluster

Example:

<MQ_1_6_15_0>=<path-to-MQ-dir/MaxQuant_1.6.15.0/bin/MaxQuantCmd. exe>

- 8. Copy raw data from local pc to cluster
- 9. Copy mqpar from local pc to cluster. Here the assumption is that you created the mqpar on windows by setting parameters in the MQ gui and killing it shortly after it passes "Testing raw files" step. Then you copy the latest mqpar.xml generated in local pc to the cluster.
- 10. Then modify the mapar file for correct raw, fasta filepaths based on the directory paths on the cluster .
- 11. Now you have two choices to run MQ on Linux:
 - I. Interactive mode: Run MQ on the linux terminal using the command "srun -p <name-of-the-partition> -I -c <#-of-cpus> --mem

- <memory-in-MB> --time <days-hr:min:sec> mono \$<MQ_1_6_15_0> <mqpar.xml>" or
- II. Submit the job: you can create a slurm script and submit the job by running "sbatch <slurm-script>.sh" in the linux/cluster machine terminal. You can find an example slurm script file here.
- 12. In case you are not using slurm manager and/or decide to run MQ on a linux workstation rather than on a cluster then perform the steps 1-11, then simply run MQ on a Linux terminal as "mono \$<MQ_1_6_15_0> <mqpar.xml>"

Important Note: from 1.6.15.0 version onwards MQ uses dot net core. So download .NET core 2.1 SDK from here