

After today...

- ARCHER2 accounts under ta025 will keep access until June 1st
 - Download any data *before* June 1st
- 1000 CU compute time available (1000 node hours)
 - ARCHER2 downtime expected in May – use sooner rather than later
- Course feedback survey (registration page on PRACE website)
- Recordings will appear on youtube.com/bioexcelcoe

Best Practices in QM/MM Simulation of Biomolecular Systems

Challenges

research question

the scope of QM/MM simulations

starting structure

x-ray/NMR/Cryo-EM/homology model

tautomers (protons), heterogeneity

Hamiltonian

force field and level of quantum chemistry theory

size of QM and MM regions

QM/MM boundary

sampling

QM/MM interactions

static or dynamics

validation

collective variables / reaction coordinates

soft- and hardware

convergence



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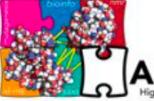
Gerrit Groenhof
(co-organiser)

Support Forums <http://ask.bioexcel.eu>

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Thank you for attending!

