

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

QM/MM interactions

validation

soft- and hardware

sampling

static or dynamics

collective variables / reaction coordinates

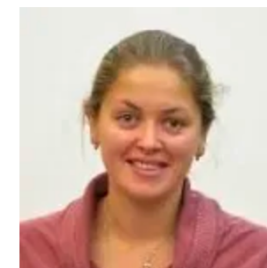
convergence



Maria João Ramos



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

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Category	Topics	Latest
HADDOCK  The HADDOCK category is meant for discussing any topic related to the use of the HADDOCK software, either as a local installation or via the HADDOCK web portal . For details about HADDOCK please refer to http://www.bonvinlab.org/software/haddock2.2 Feel free to create new topics related to your quest...	275	  Welcome to ask.bioexcel.eu 1 Mar '16
		 Instances of ligand X01 do not contain the same atoms 0 1d ■ HADDOCK
		 Error on the CP2K QM/MM tutorial on biochemical systems 2 5d ■ CP2K in Biomolecular Simulation
		 Small parameter file attachments to posts 2 15d ■ HADDOCK
		 Base Trajectory 1 18d ■ GROMACS
		 Docking a protein with a fatty acid side chain 5 19d ■ HADDOCK
		 Finding data in the downloaded results file 1 26d ■ HADDOCK
		 Your HADDOCK run has failed 5 May 8 ■ HADDOCK
		Error: There was an inconsistency in your
GROMACS  GROMACS is a free and open-source software suite for high-performance molecular dynamics and output analysis. It primarily targets bio-molecular simulations of thousands to millions of atoms, described by particle-based classical mechanics force fields. These simulations integrate the Newtonian equa...	10	
DISVIS  This is the help forum for DISVIS, a software and web portal that allows you to visualizes and quantify the information content of distance restraints between macromolecular complexes	5	

Thank you for attending!

