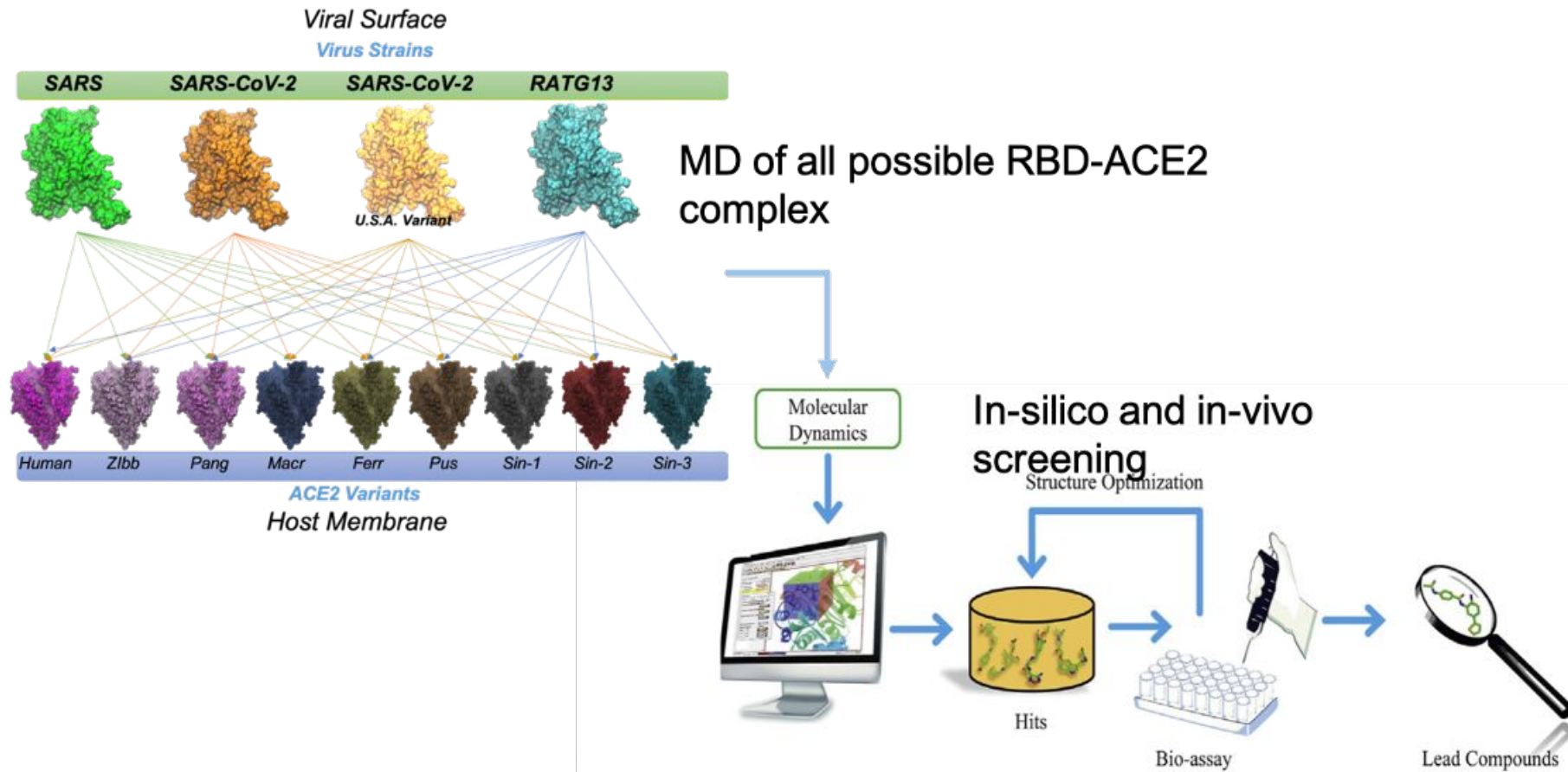


BioExcel Centre of Excellence

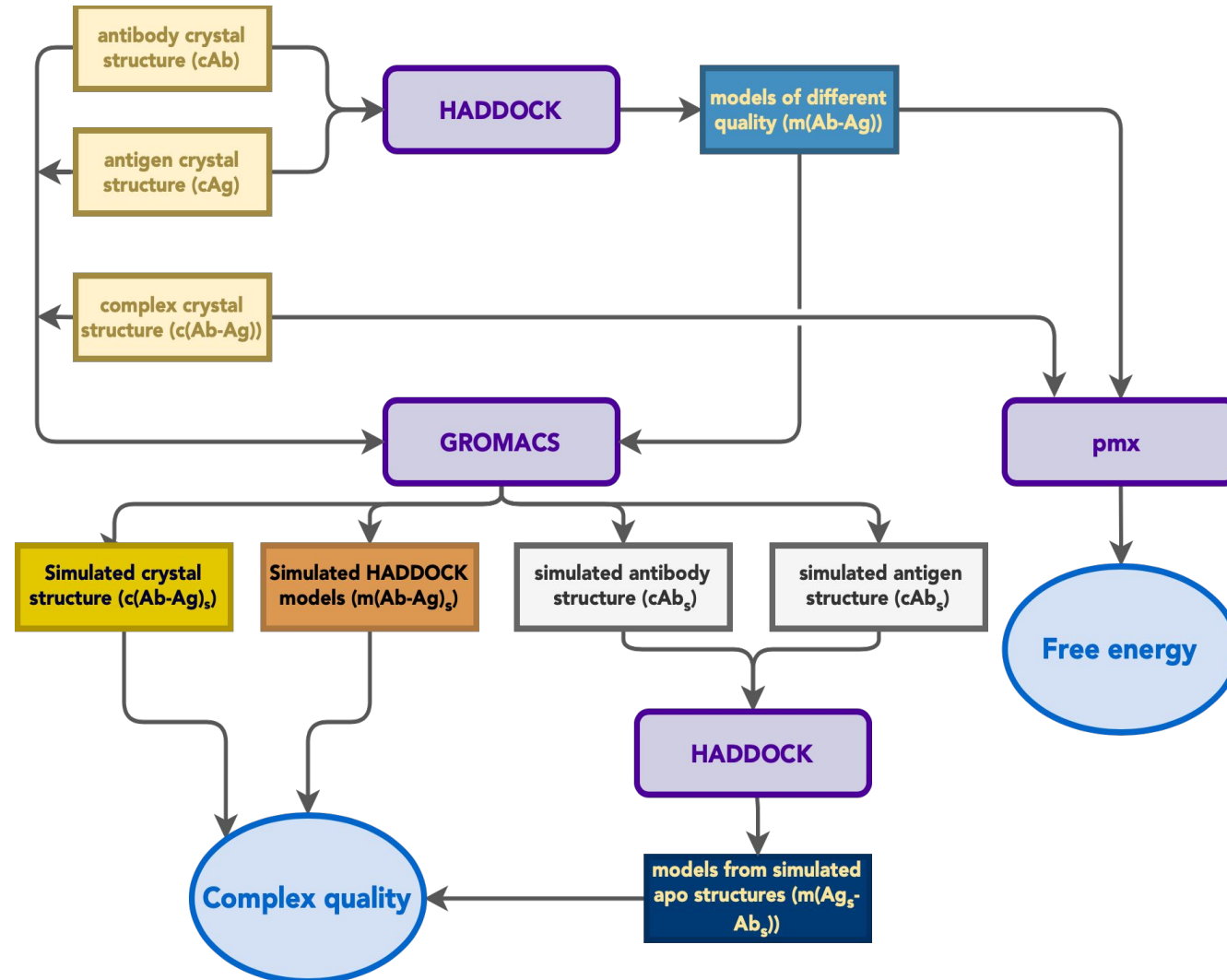
Driving Computational Biomolecular Research in Europe

Rossen Apostolov
rossen@bioexcel.eu

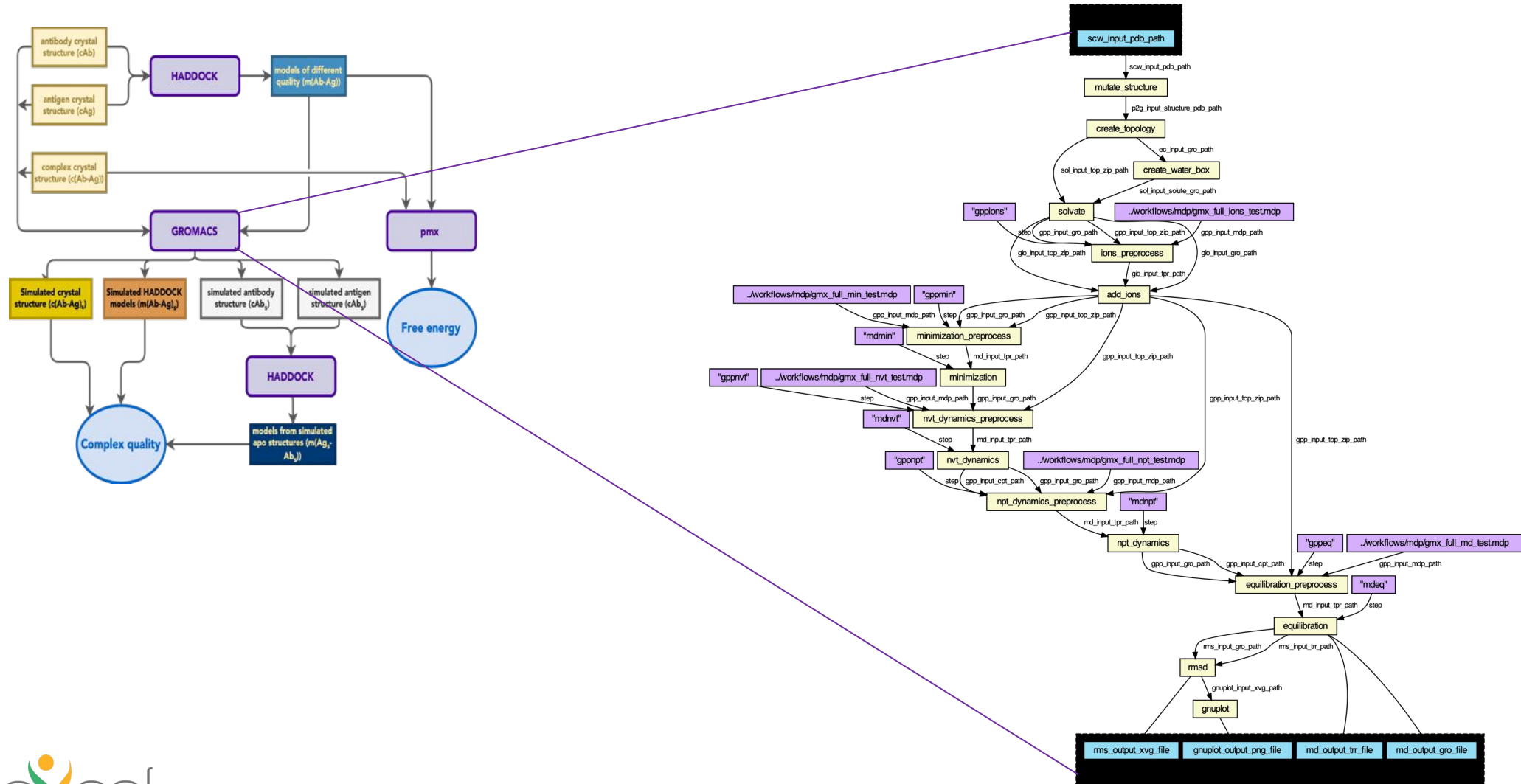
COVID-19 drug screening



Antibody Design



Antibody Design





Summit: 2,400,000 cores



Piz Daint: 387,000 cores



Beskow: 67,000 cores



Sunway: 10,700,000 cores



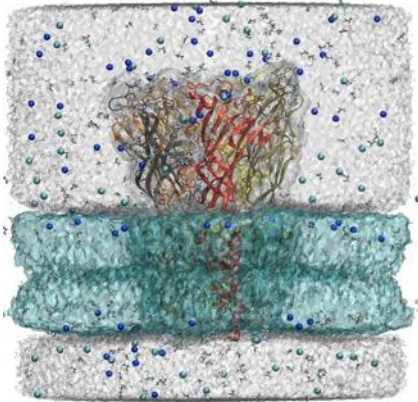
BioExcel Partners



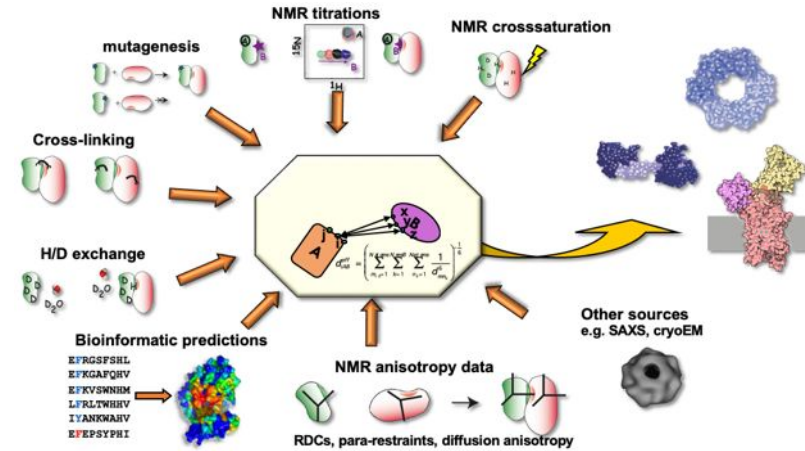
Horizon 2020
European Union Funding
for Research & Innovation

BioExcel is funded by the European Union Horizon 2020 program under grant agreements 675728 and 823830.

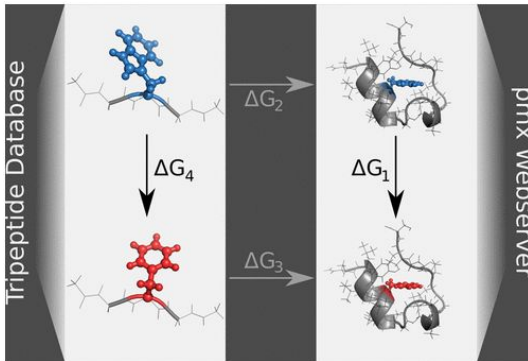
Core Applications



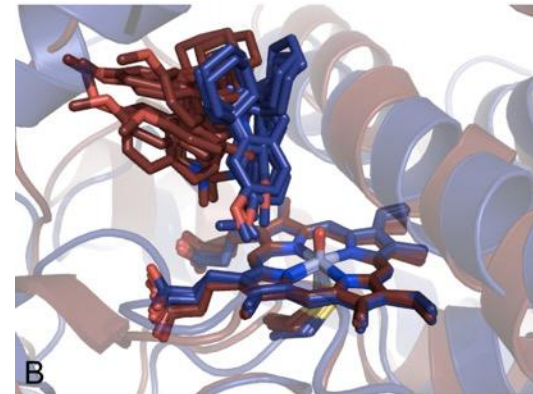
MD with GROMACS



Integrative modelling with HADDOCK



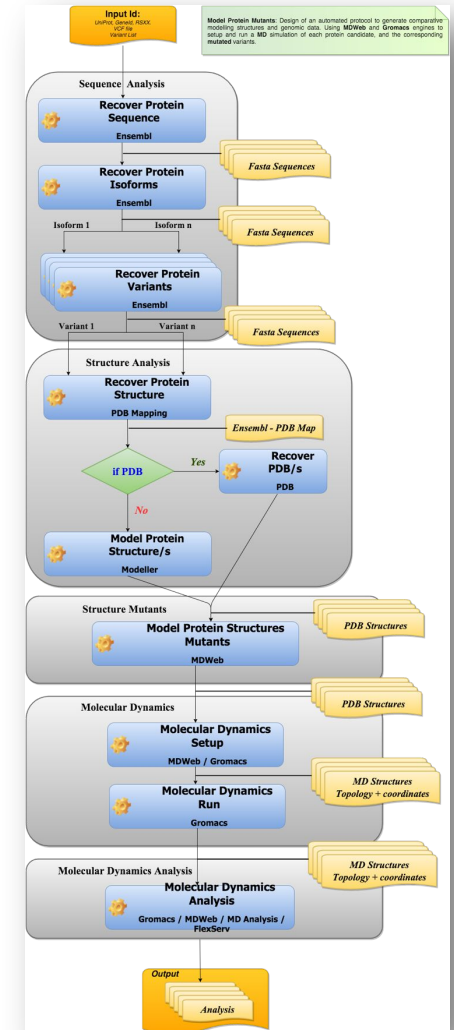
FE with PMX



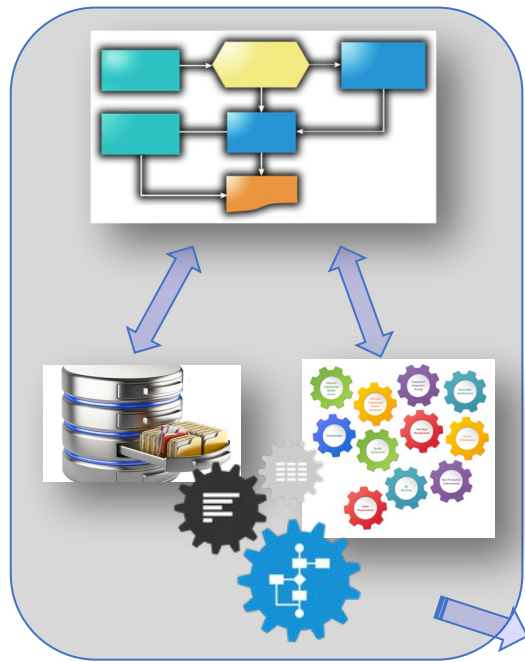
Hybrid QM/MM with CP2K

Workflows - Usability and Automation

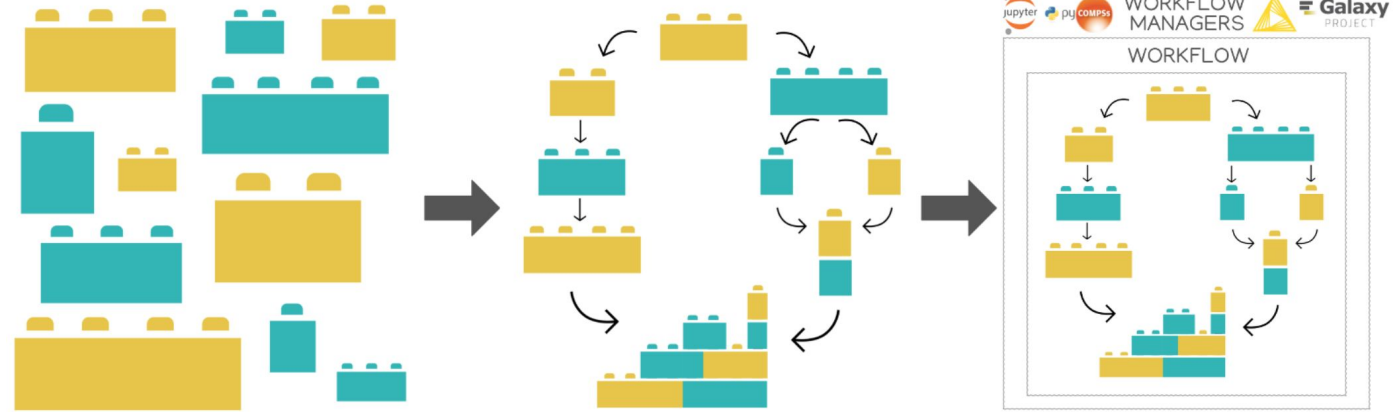
- Make research computing easier to use by biomolecular researchers, both in academia and industry
- Devise efficient workflow environments with associated data integration



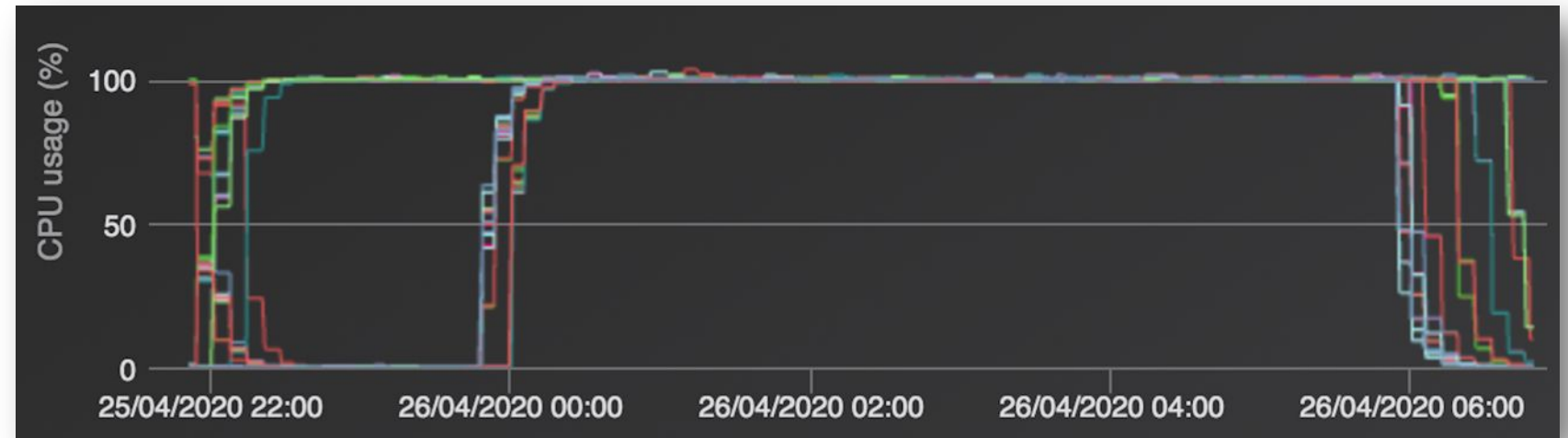
Exascale ready workflows



Workflows Optimization for exascale



✓ Used in COVID-19 studies



Supporting Academia and Industry



Janssen

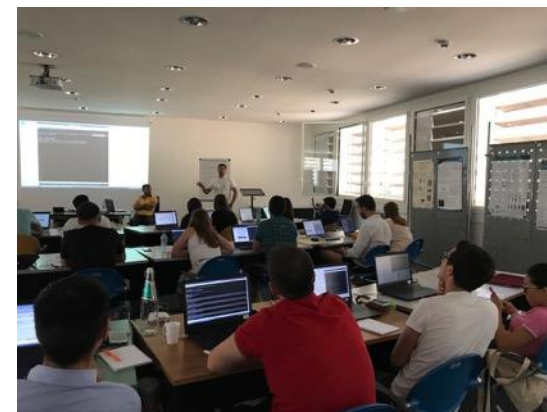
Supporting the Pharmaceutical Industry: BioExcel experts visit Janssen's R&D site in Belgium

27 Apr 2018 in Features / Latest News / Business stories by Ian Harrow

BioExcel continues its direct support to industry through site visits. In early March we were pleased to participate in an exciting day of collaborative talks hosted by Janssen at their research site in Beerse, Belgium.



The morning comprised of presentations by Janssen's Computational Chemistry group, led by Herman van Vlijmen who emphasized that now is an exciting time for computational drug design. Principal scientist, Dr Gary Treasaden covered their interests and needs for molecular dynamics (MD) and free energy (FE) calculations applied to molecular design and virtual screening for drug discovery projects. Important challenges are keeping abreast of the latest methodologies and validation of molecular dynamic predictions in a timely manner. Post-doctoral scientist, Dr Laura Perez presented her recent work on free energy perturbations (FEP) applied to the public 3D structure phosphodiesterase 2 (PDE2) published recently. Predicting Binding Free Energies of PDE2 Inhibitors. The Diffraction of Protein Conformation. Pérez-Bentío L, Karimian H, van Vlijmen H, Treasaden G. Sci Rep. 2018 Mar 20;8(1):4883. DOI: 10.1038/s41598-018-23039-5. Recent collaboration with BioExcel partner, Dr Yuhanna Gaspary on GROMACS3 (gromacs3.sourceforge.net) and PMCE (bioexcel.eu/software/pmce) applied to PDE2 has demonstrated encouraging results.



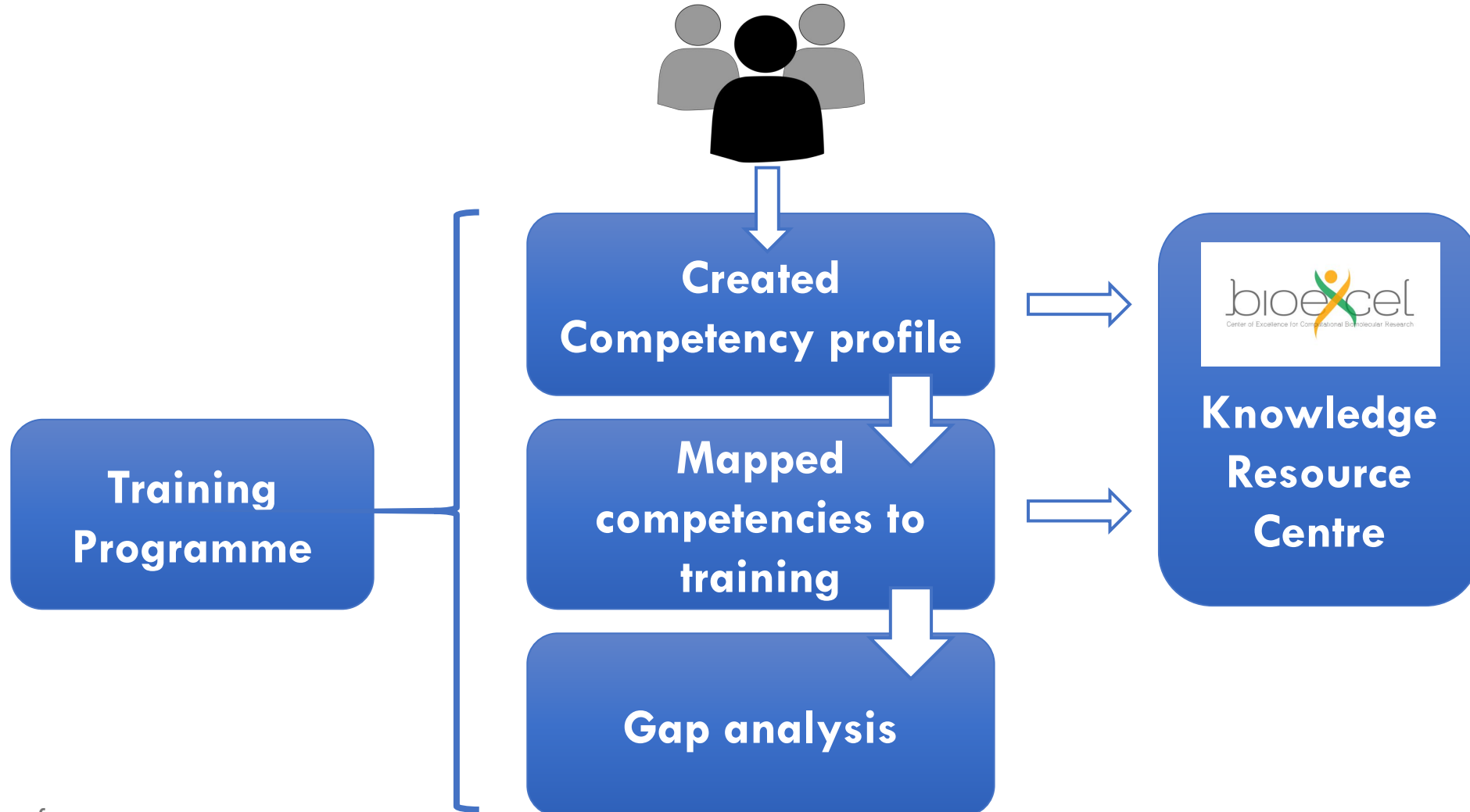
Supporting the Pharmaceutical Industry: BioExcel experts visit UCB's R&D site in Belgium

October 6, 2018 by Ian Harrow



BioExcel continues its direct support to industry through site visits. In late May we were pleased to visit UCB's research site in Braine D'Alleud, Belgium for an exciting day of in depth discussions.

Training Program based on needs analysis



Training events and courses



Reproducible analyses with Common Workflow Language

29 Apr, 2020 @ 13:00 – 15:30 –
Online [\[...\]](#)



Preparing to run biomolecular QM/MM simulations with CP2K using AmberTools Online

09 Jun, 2020 @ 13:00 – 16:00 –
Online [\[...\]](#)



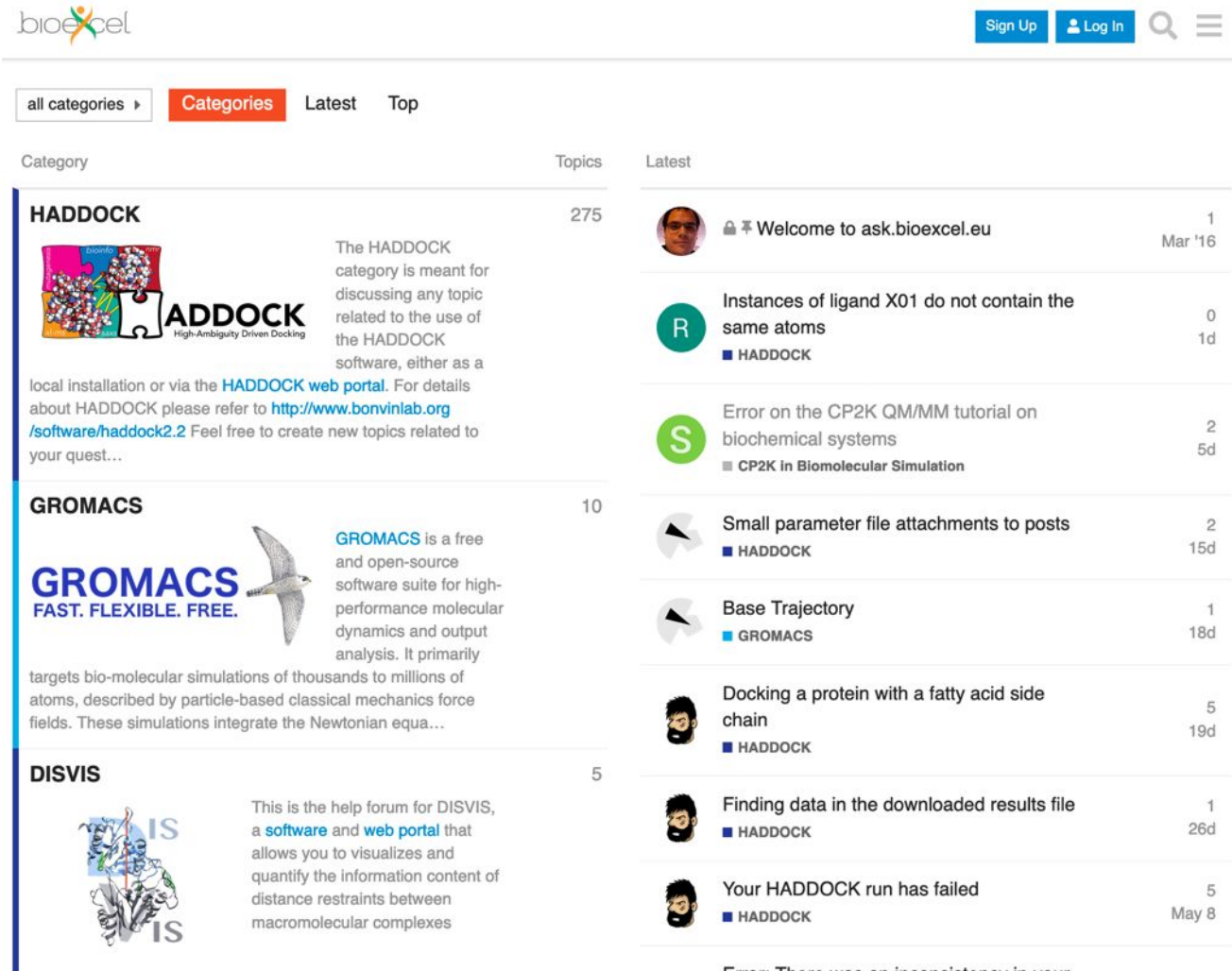
Remote BioExcel Summer School on Biomolecular Simulations

22 Jun, 2020 – 26 Jun, 2020 @ All
Day – Online [\[...\]](#)

Webinar Series <http://bioexcel.eu/webinars>




 <p>BioExcel Webinar #25: Finding a trade off...</p> <p>48 views • 2 weeks ago</p>	 <p>BioExcel Webinar #24: Perspective on the Martini</p> <p>174 views • 3 weeks ago</p>	 <p>BioExcel Webinar Series #23: MC_DNA</p> <p>98 views • 1 month ago</p>	 <p>BioExcel Webinar #22: GROMACS 2018 – overview</p> <p>188 views • 1 month ago</p>	 <p>BioExcel Webinar #21: CWLEXEC: A new open</p> <p>139 views • 2 months ago</p>
 <p>BioExcel Webinar #20: Adaptive resolution methods</p> <p>28 views • 2 months ago</p>	 <p>BioExcel Webinar #19: Hybrid Molecular</p> <p>49 views • 4 months ago</p>	 <p>BioExcel Webinar #18: Multiple timescales in</p> <p>69 views • 6 months ago</p>	 <p>BioExcel Webinar #17: MDStudio, microservice</p> <p>53 views • 6 months ago</p>	 <p>BioExcel Webinar #15: BioExcel and OpenPHACTS:</p> <p>45 views • 9 months ago</p>
 <p>BioExcel Webinar #16: NAFlex, a web server for the study of</p> <p>102 views • 9 months ago</p>	 <p>BioExcel Webinar #14: Introduction to the Common</p> <p>190 views • 10 months ago</p>	 <p>CWLViewer: The Common Workflow Language Viewer</p> <p>886 views • 10 months ago</p>	 <p>Presenting BioExcel: A central hub for biomolecular</p> <p>290 views • 11 months ago</p>	 <p>BioExcel Intro Clip with Music</p> <p>11 views • 11 months ago</p>
 <p>BioExcel Webinar #11: Robust solutions for cryoEM</p> <p>249 views • 1 year ago</p>	 <p>BioExcel Webinar #12: "How to choose compute</p> <p>66 views • 1 year ago</p>	 <p>BioExcel Webinar #10: Assessing structure quality in</p> <p>97 views • 1 year ago</p>	 <p>BioExcel Webinar #9: Defining training</p> <p>62 views • 1 year ago</p>	 <p>BioExcel Webinar #8: Large-scale analytical workflows on</p> <p>50 views • 1 year ago</p>

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











The screenshot shows the bioexcel support forum interface. At the top, there is a navigation bar with the bioexcel logo, a search icon, and buttons for 'Sign Up' and 'Log In'. Below the navigation bar, there are filters for 'all categories', 'Categories', 'Latest', and 'Top'. The main content area is divided into two columns: 'Category' and 'Latest'.

Category

Category	Topics
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
GROMACS  GROMACS FAST. FLEXIBLE. FREE. 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 visualize and quantify the information content of distance restraints between macromolecular complexes	5

Latest

Topic	Replies	Time
 Welcome to ask.bioexcel.eu	1	Mar '16
 Instances of ligand X01 do not contain the same atoms ■ HADDOCK	0	1d
 Error on the CP2K QM/MM tutorial on biochemical systems ■ CP2K in Biomolecular Simulation	2	5d
 Small parameter file attachments to posts ■ HADDOCK	2	15d
 Base Trajectory ■ GROMACS	1	18d
 Docking a protein with a fatty acid side chain ■ HADDOCK	5	19d
 Finding data in the downloaded results file ■ HADDOCK	1	26d
 Your HADDOCK run has failed ■ HADDOCK	5	May 8

Error: There was an inconsistency in your

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