Dear Colleagues,

We are pleased to invite you and your collaborators to join **PRACE Autumn School 2021: „Fundamentals of Biomolecular Modeling and Simulations for Applied Research and Virtual Drug Development",** 20-24 September 2021.

The school will be carried out online using Zoom and is organised jointly by BioExcel Centre of Excellence, STFC Daresbury Laboratory, NCSA Bulgaria, Sofia University within PRACE (Partnership for Advanced Computing in Europe).

The week-long training event will introduce the fundamentals of modern methods for biomolecular simulations - molecular dynamics (MD), 3D QSAR (Quantitative structure-activity relationship models), integrative modelling, free energy and hybrid-QM/MM calculations (quantum mechanics/molecular mechanics). Widely used application codes GROMACS, HADDOCK, PMX, and ChemShell, will be presented, and their execution on High-Performance Computing (HPC) facilities demonstrated.

All lectures and demonstrations will be prepared in a way accessible to applied scientists with little experience with computational methodologies and HPC.

It will be suitable for junior researchers (post-graduates and post-docs) with a background in natural sciences and, in particular, pharmacy, biochemistry and biophysics, but also for scientists interested in the opportunities provided by the HPC in these areas.

Key takeaways from the training:
- What is HPC? How is it different, and why is it useful? Experience running simulations on a supercomputer.
- How do we model proteins, DNA, lipids, cells and biomolecular systems? What methods and techniques are used for simulations, and how do we interpret the results?
- What are the popular software applications in the field and how can we use them?
- **Success stories:** How do we screen for drugs? How do we study biomolecular phenomena? How do we do all that in days instead of months? Learn from leading scientists from academia and pharma companies.

For more information and registration, please visit our event page on the PRACE website.
More details can be found here.

Participation is free

Registration deadline: **July 31, 2021**

Kind regards,

Prof. Stoyan Markov, D.Sc.
Chairman
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