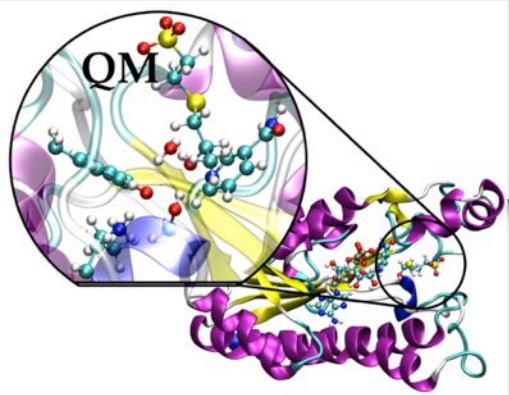
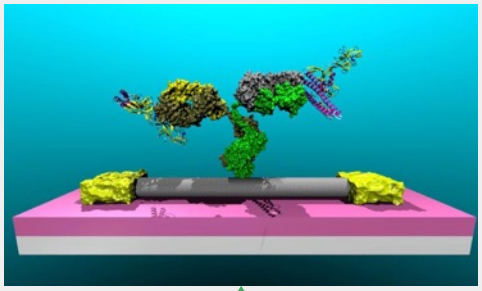
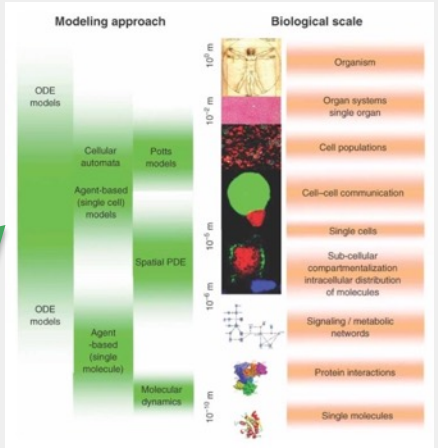
Electronic structure



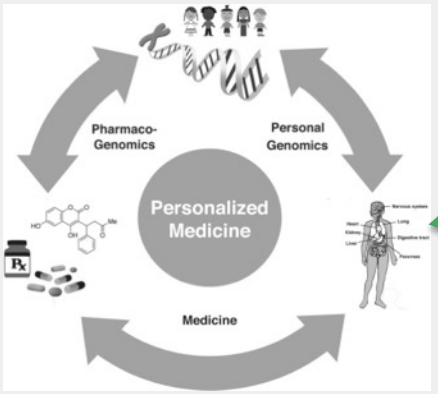
Biomarkers design



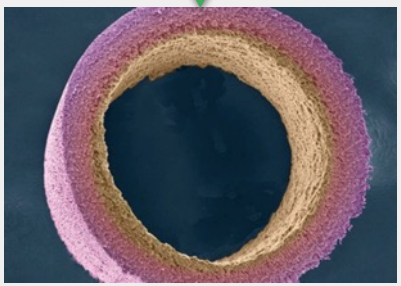
Physiology



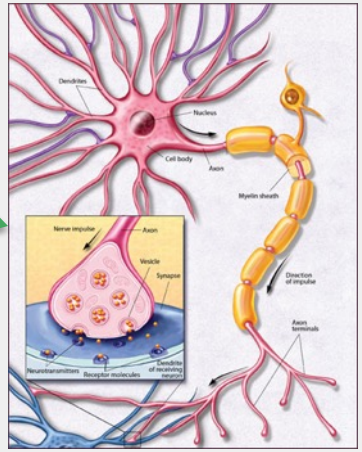
Biomolecular Modeling and Simulations



Personalized medicine



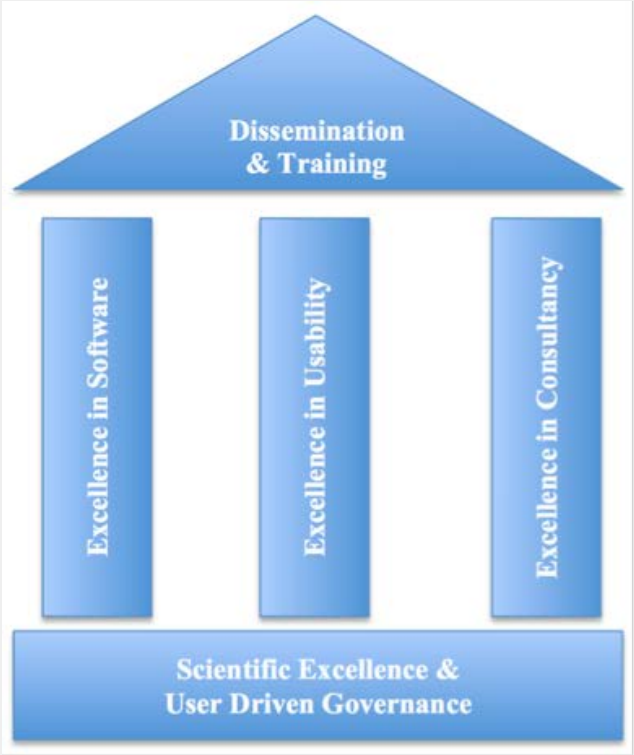
Biomaterials science and nanotechnology



Neuroinformatics

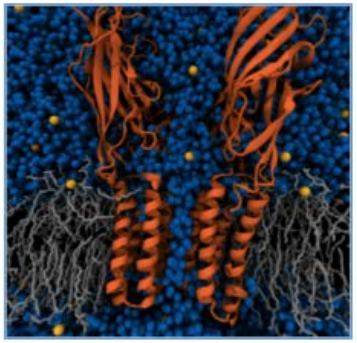
A central hub for biomolecular modeling and simulations

Enabling better science by **improving** the most popular biomolecular **software** and spreading best practices and expertise among the communities through **consultancy** and **training**

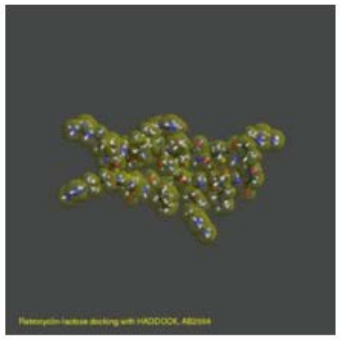


BioExcel supports world-leading European Software

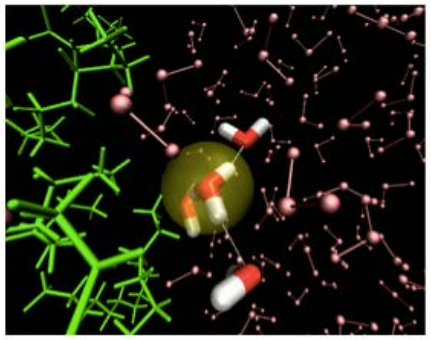
- GROMACS (Molecular Dynamics Simulations) (Strong and weak scaling)
- HADDOCK (Integrative modeling of macro-assemblies) (High throughput scaling to millions of runs)
- CPMD (hybrid QM/MM code) (Multiscale and interoperability of codes)



MD simulations
/GROMACS/



Docking
/HADDOCK/



QM/MM
/CPMD/