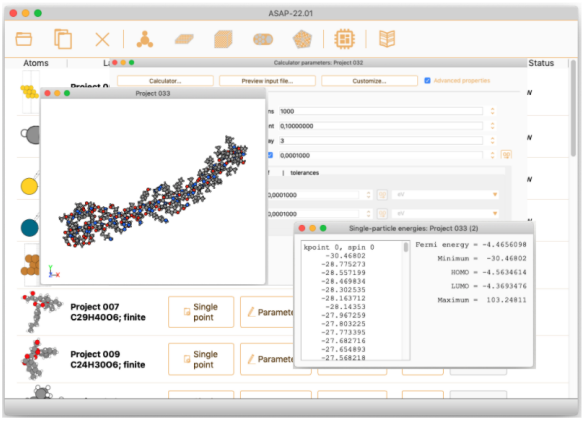
Modelling bio-applications with ASAP

Biological systems represent nested hierarchies of complex patterns and processes. The application of **atomistic and quantum mechanical simulations** to biological systems is challenging. It involves efficient computer algorithms, extensive data analysis and advanced visualization tools

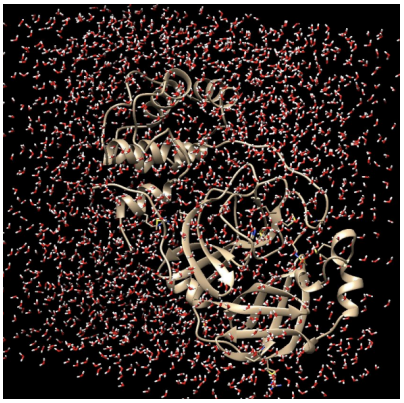
Advanced Simulation Atomistic Platform (**ASAP**) provides a powerful environment for advanced atomistic simulations of bio-matter. **ASAP** allows users to construct and visualise complex bio-models due to flexible structure builder and molecular editor widget.



ASAP employs the **SIESTA** code – well known for its excellent performance for computationally demanding systems over 10000 atoms.

ASAP brings efficient post-production tools to analyse structural, chemical, electronic and dynamic properties of simulated systems. This makes ASAP a very convenient and powerful code for simulating biological systems at an atomic scale.

Rapid development of advanced algorithms and affordability of high performance computational facilities made possible simulations of complex biological systems, acquiring their properties from models, thus developing new medicine, virtually. Quantum mechanical simulations open pathways for **molecular nano-medicine.**



ASAP and **SIESTA** solver provides an optimal approach to model dynamic behaviour of complex systems combining powerful analysis tools and efficiency of quantum mechanical solver.

⇦ *Large-scale (12000 atoms) quantum mechanical modelling of* ***SARS CoV-2 M^{pro}*** *monomers assemble with SIESTA.*

SIMUNE is an expert in atomistic and quantum mechanical simulation for BioTech. You can find a SIESTA case study for modelling biological systems with respect to various solvent models at the SIMUNE web-page.

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