Large scale simulation of transferrin-Aluminium complex

Collaborators:

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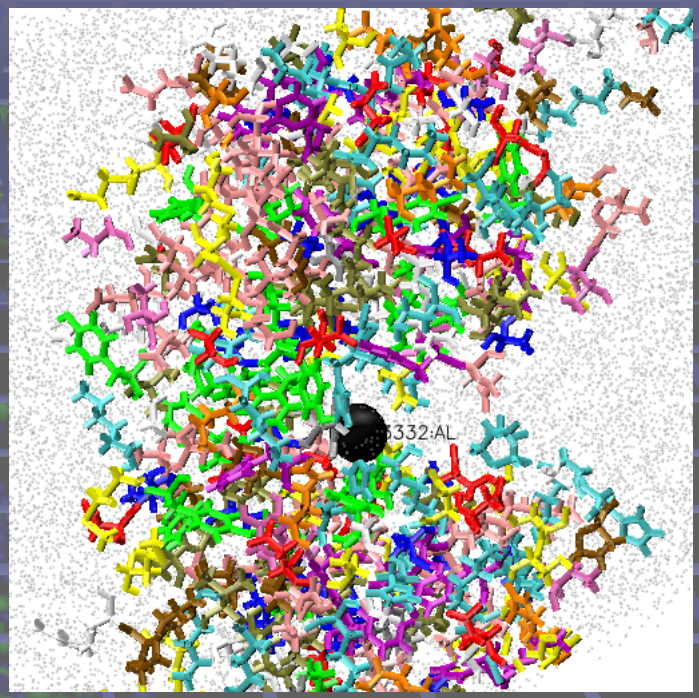

Objective: to study the bioavailability of Aluminium within the living cell

- Serum transferring (sTf): a predominant Aluminium (Al) carrier in serum; controls the levels of free metals in physiological fluids
- Binding and release mechanisms of Al with sTf are studied by atomistic simulation
- Both mechanisms are very slow processes and such calculations are not feasible without enhanced sampling techniques and HPC.