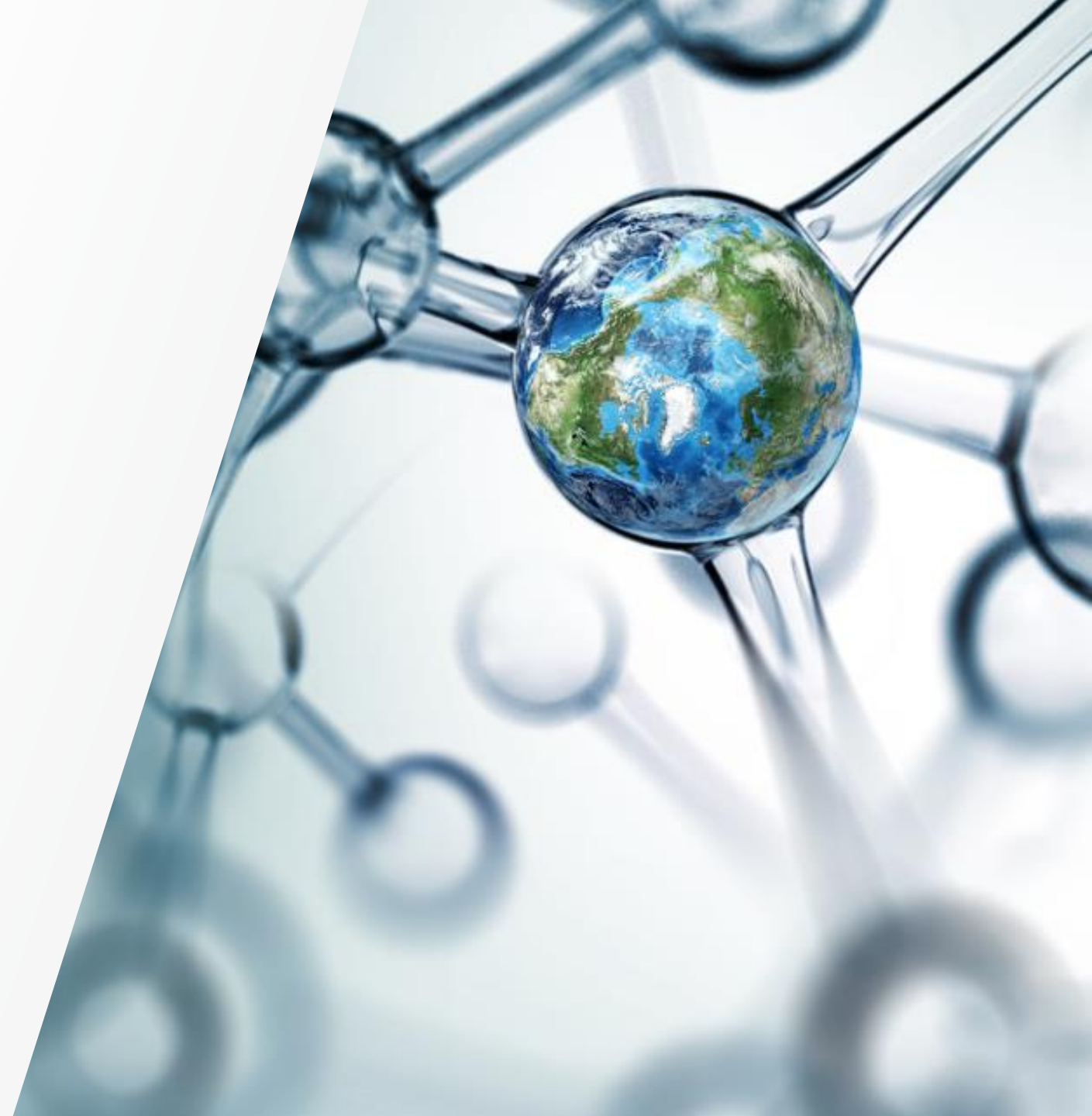


Mask Map By Molecule

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Installation of Xtra „Mask Map By Molecule“

- Unzip archive MaskMapByMolecule.zip
- Copy the contents of folder *local* into the folder specified by AMIRA_LOCAL
- Copy folder *data* to a convenient place in your file system
- Restart Amira
- Find module *Mask Map by Molecule* in category *Xtra > Compute*

[How to register an AMIRA LOCAL directory:](#)

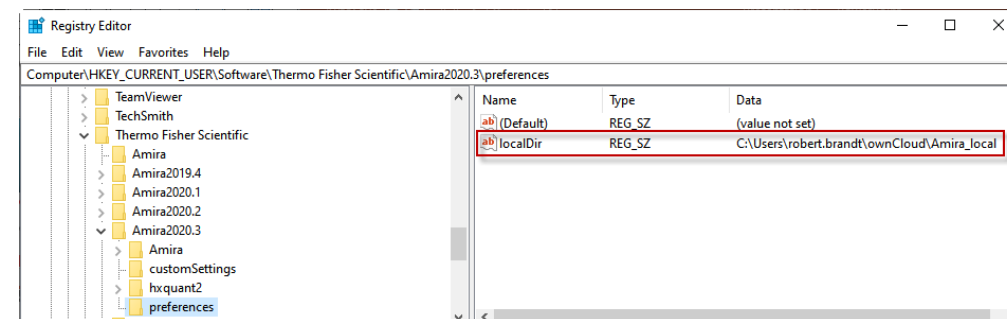
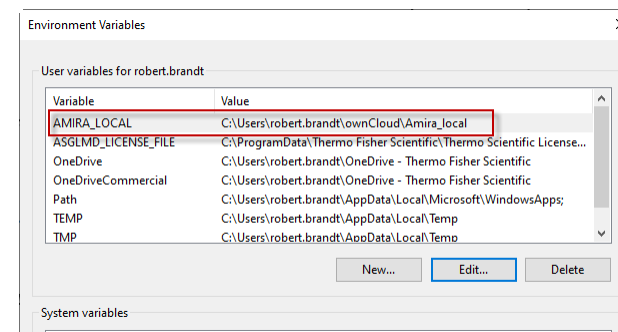
Set environment variable AMIRA_LOCAL:

Go To *Control Panel > Advanced System Settings > Environment variables*, create a new variable „AMIRA_LOCAL“ and set its value to a directory in your home directory.

OR

(Requires Administrator privileges)

Open the Registry Editor (run -> regedit.exe), navigate to *Computer\HKEY_CURRENT_USER\Software\Thermo Fisher Scientific\Amira2020.3\preferences* and set the *localDir* key in the registry to point to Amira_local.



Masking Map – Set-up

Apoferitin is a globular protein involved in storage and transport of iron. Its quaternary structure is composed of 24 identical chains of the same protein.

Because of its octahedral symmetry it is a popular preparation for Single Particle Analysis where it is reconstructed in its 24-meric assembly.

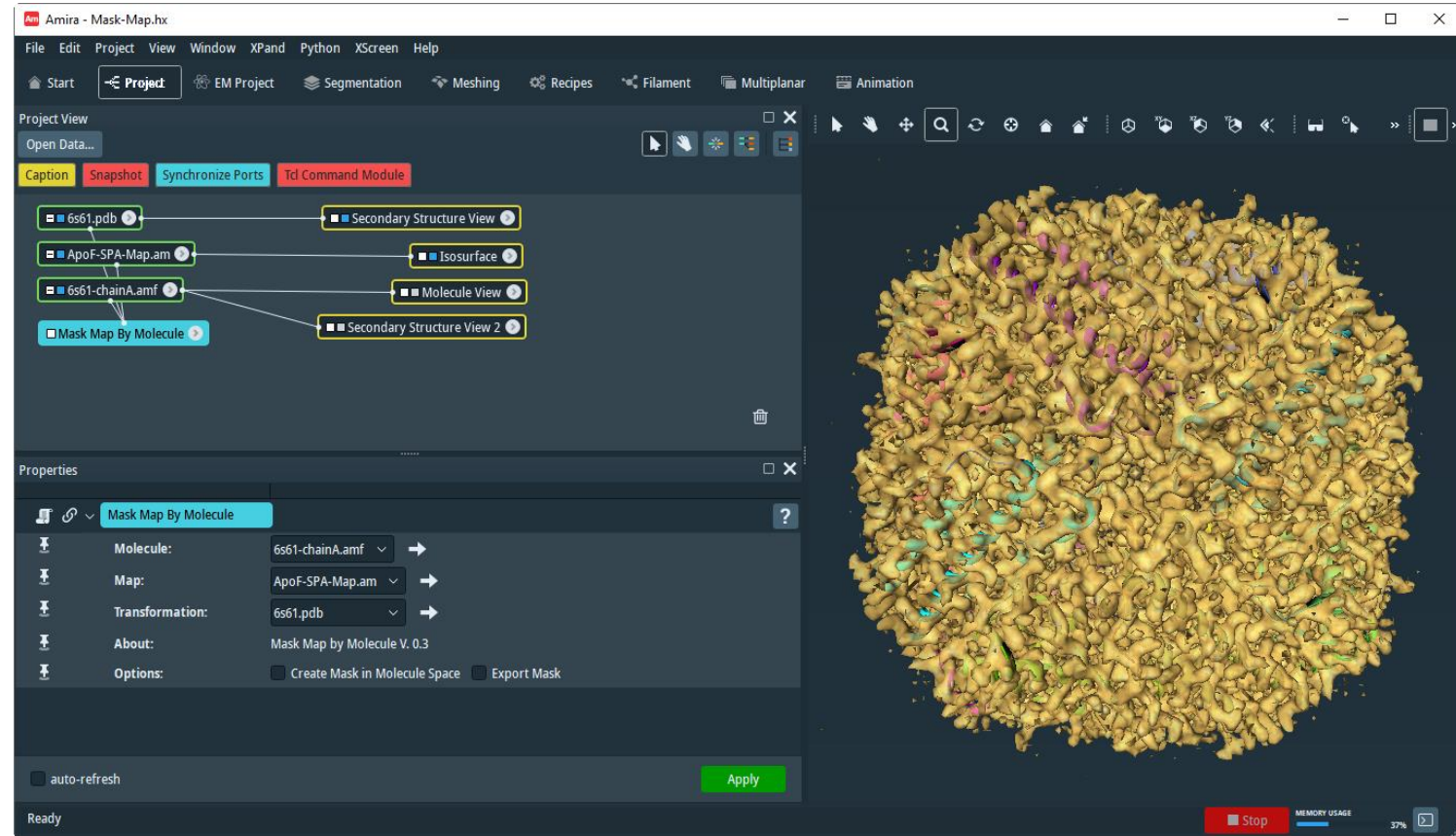
For visualization purposes, however, it is sometimes desirable to get a monomeric representation of the map.

The script-module Mask Map By Molecule can be used to isolate the parts of an Apoferitin map corresponding to a single chain (= Apo Ferritin monomer).

Note: Make sure Units Management is either disabled or set to *Nanometer (nm)*.

- Open project /data/Mask-Map.hx

This loads the PDB model of mouse Apoferitin (6s61) together with a map that has been created using Single Particle Analysis. The map is displayed with a semi-transparent isosurface, through which a secondary structure model of the PDB data shines through.



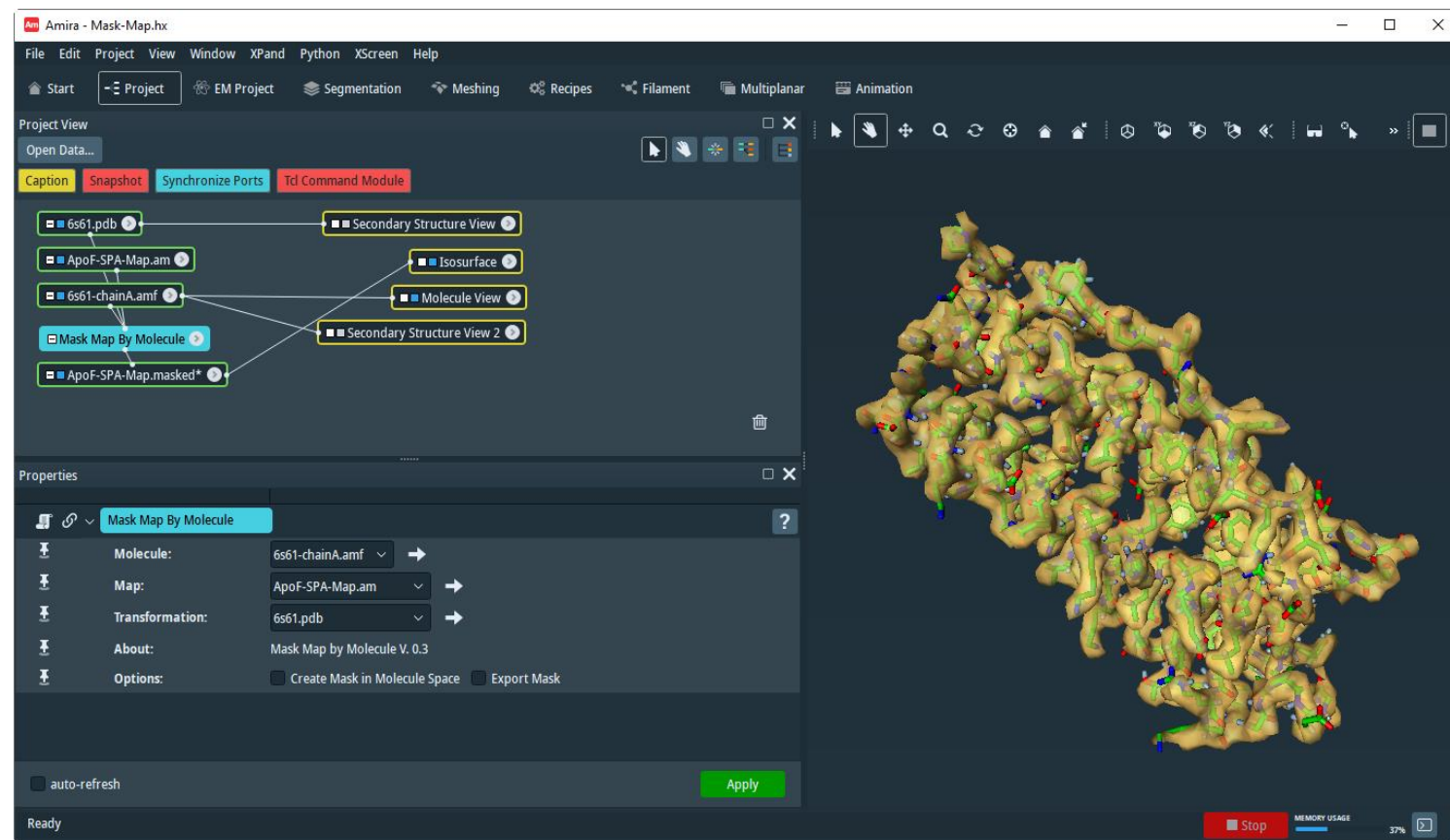
Data source: 6s61.pdb from the Protein Data Bank (<https://www.rcsb.org/>), ApoF-SPA-Map from Thermo Fisher Scientific MSD

Masking Map – Apply and Visualize

- Right-click *6s61-chainA.amf*, connect > *Xtras > Compute > Mask Map By Molecule*
- Connect port *Map* with *ApoF-SPA-Map.am* and port *Transformation* with *6s61.pdb*
- Click *Apply* of module *Mask Map By Molecule*
- Reconnect *Isosurface* with *ApoF-SPA-Map.masked*
- Disable *Secondary Structure View* and *Secondary Structure View 2*
- Enable *Molecule View*

In this way the single chain representation of the map can be easily compared with an atomic model view of the chain.

In this example, model and map are perfectly aligned. In general however, this is not to be expected. Use *Xtra Fit Molecule To Map* to „dock“ the chain or the assembly into the map. In this case you may need to decide whether the masked map has the transformation of the map or that of model. For the latter, check option *Create Mask in Molecule Space*.



Data source: *6s61.pdb* from the Protein Data Bank (<https://www.rcsb.org/>), *ApoF-SPA-Map* from Thermo Fisher Scientific MSD