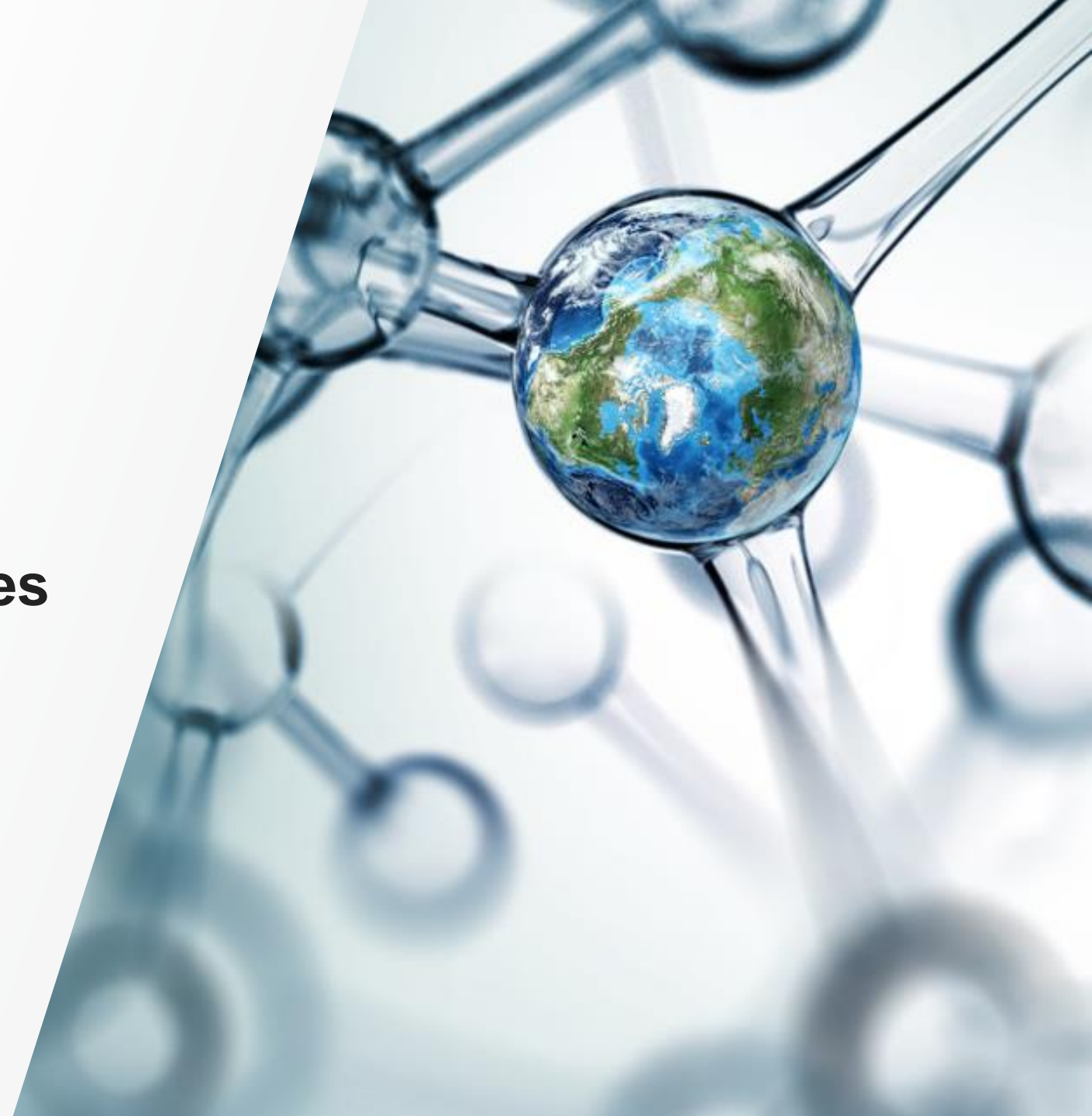


# Fit Molecule To Map A Module for Docking Molecules

Robert Brandt

Send feedback to: [Robert.Brandt@thermofisher.com](mailto:Robert.Brandt@thermofisher.com)

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# Installation of Xtra „Fit Molecule To Map“

- Unzip archive FitMoleculeToMap.zip
- Copy the contents of folder *local* into the folder specified by AMIRA\_LOCAL
- Copy folder *SampleData* to a convenient place in your file system
- Restart Amira
- Find module *Fit Molecule To Map* in category *Xtra > Geometry Transforms*

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

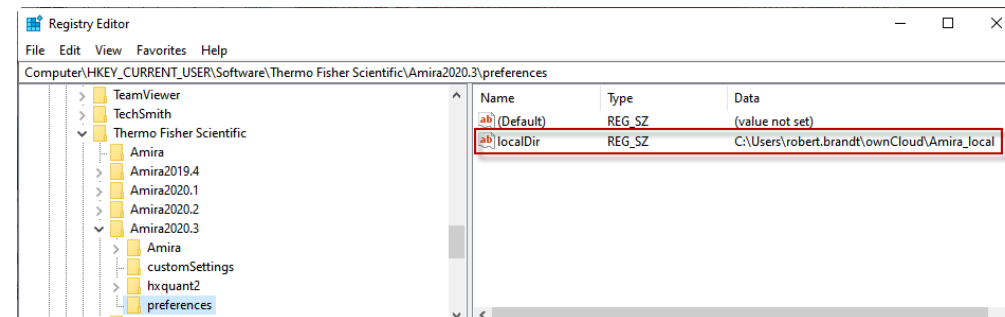
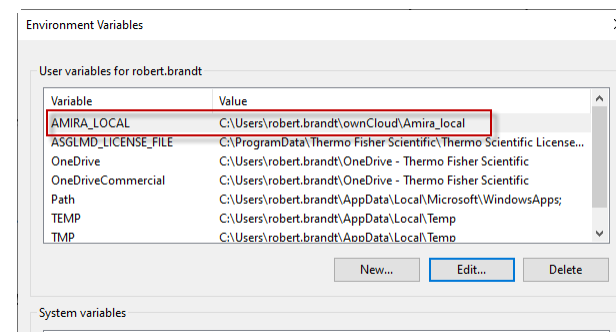
Set environment variable AMIRA\_LOCAL:

Go To *Control > Panel > System Properties > Environment variables* and 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



# Fitting Molecule to Map – Set-up

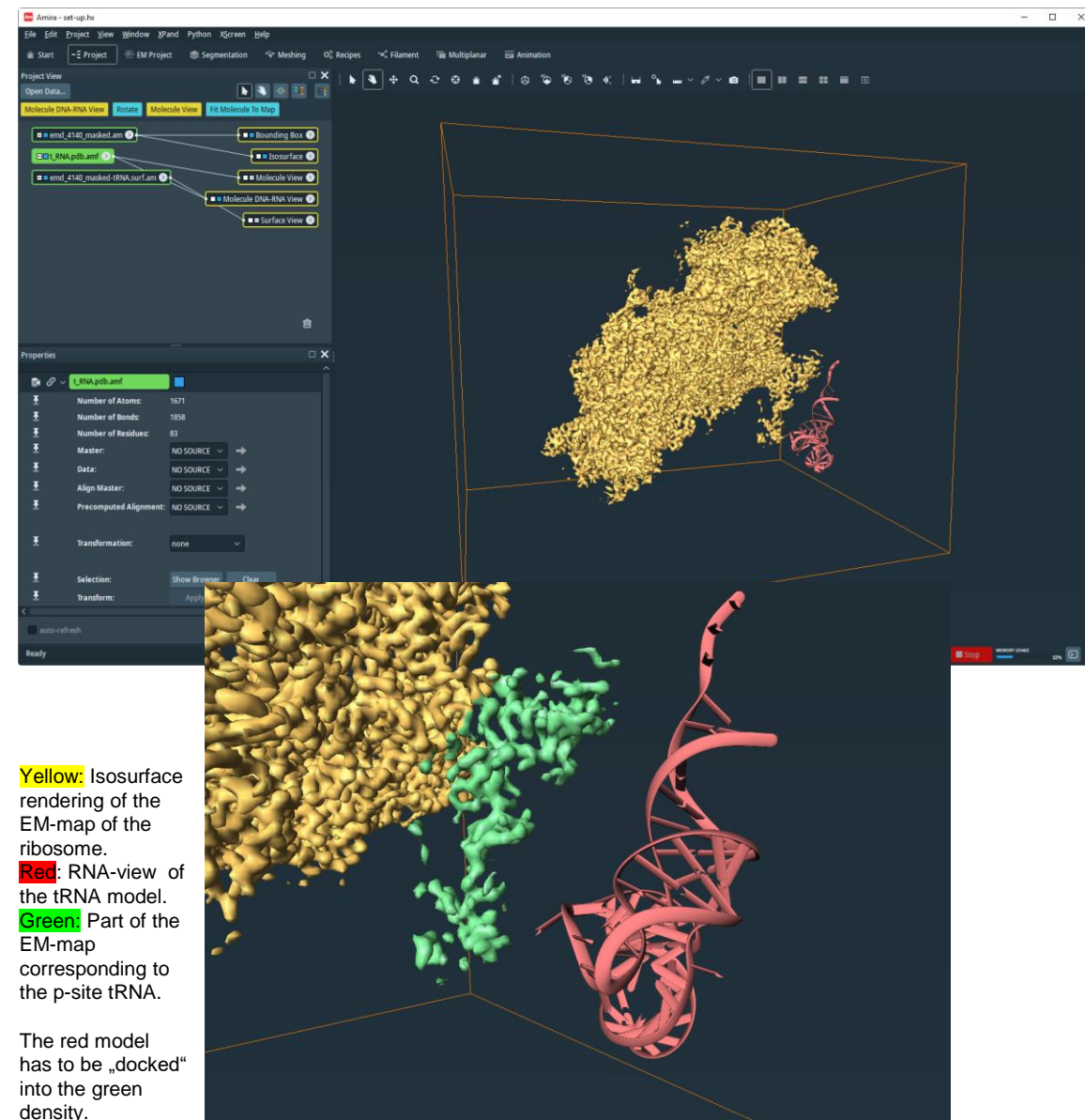
- Open *Sample Data\set-up.hx*

The viewer shows an isosurface of the map of an 80S ribosome (EMD-4140) from which the larger sub-unit has been masked off. Also seen is a model of the p-site tRNA as a secondary structure model.

The goal is to fit the tRNA model into the density representation of the 40S sub-unit.

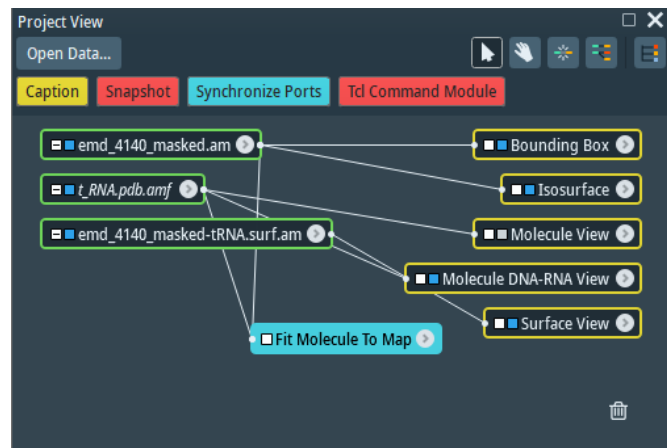
In general, fitting requires the model be sufficiently close to the correct transformation. This means that we have to perform a proper pre-alignment. We will do this interactively using the Transform Editor of the molecule.

- In order to see where the tRNA is located within the map enable the *Surface View* module in the Project Area.





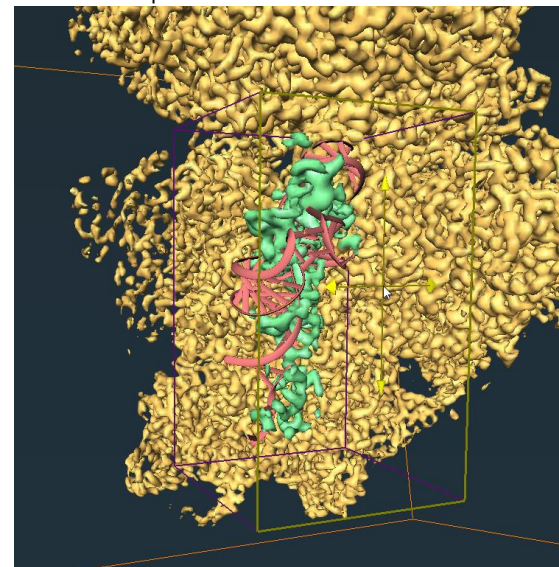
# Fitting Molecule to Map – Interactive Pre-alignment



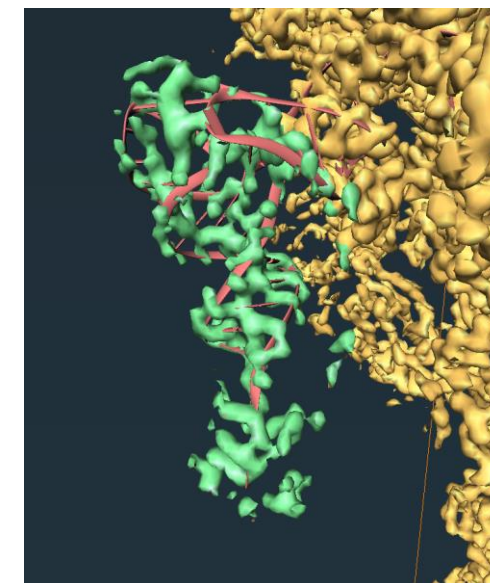
- Connect > *Xtra* > *Geometry Transforms* > *Fit Molecule To Map* to `t_RNA.pdb.amf`
- Connect port *Map* with `emd_4140_masked.am`
- Open the Transform Editor of `t_RNA.pdb.amf`
- In interactive mode (arrow cursor) click onto one of the green handles and drag the mouse upwards (or downwards) to initiate a rotation. Keep on moving until the model has rotated about 180 degrees.
- Then adjust your view on the model and translate it so that it overlaps with the corresponding part of the map (green part in the screenshots)
- Close the Transform Editor
- Click *Apply* of *Fit Molecule To Map*.



To rotate the model, left click a green handle and drag the mouse up or down.



To translate the model, left click into the box and drag the mouse. The translation is restricted to the plane of the box wall you clicked.



After clicking *Apply* the model is fitted to the map.