

Manual for SSETracer_v4

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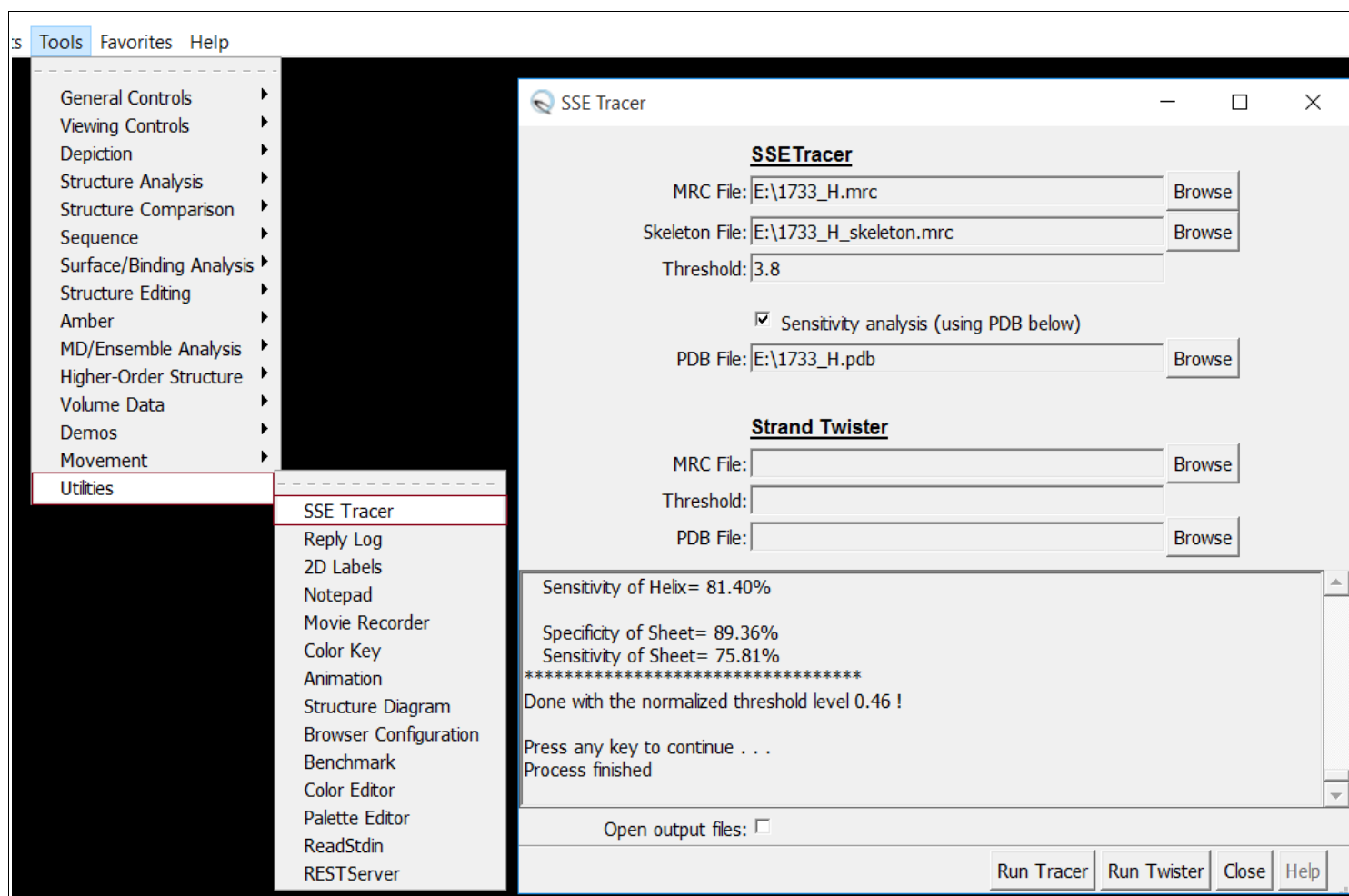
Usage within USCF Chimera

Setup:

To use SSETracer in Chimera, copy the folder “SSETracer” from “SSETracer_Chimera” into Chimera's “share” folder.

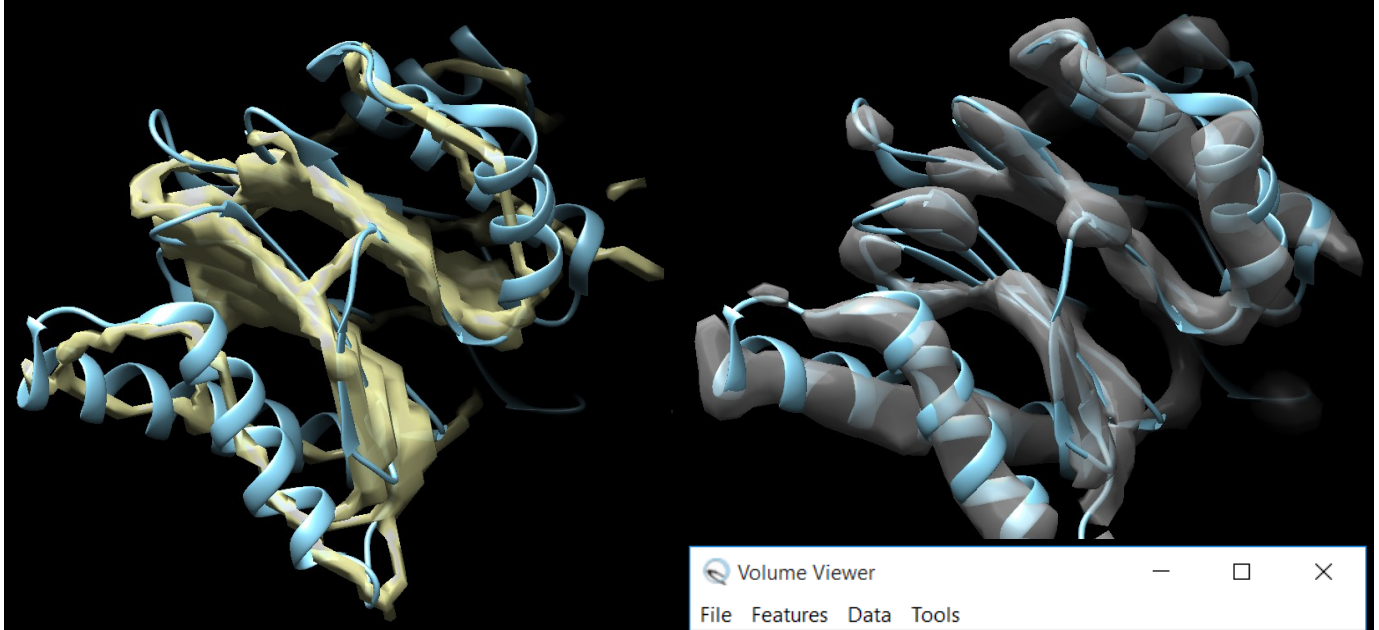
SSETracer will be available for use under Tools → Utilities → SSE Tracer.

SSETracer will automatically populate the input fields based on the files open in Chimera. Alternate files can be selected by hitting each field's corresponding “Browse” button.



Required input:

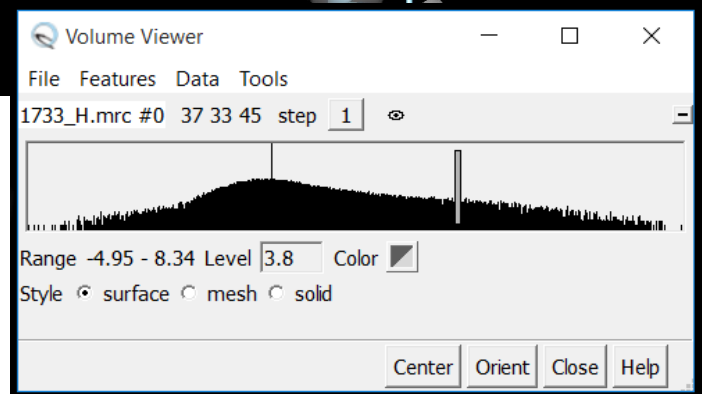
- Density mrc file
- Skeleton mrc file
- Threshold



Example skeleton mrc (top left), and density mrc at appropriate threshold for helix detection (right) are shown.

An ideal skeleton shows the sheets as surfaces and helix/loop sections as curves without having extra connections.

An ideal threshold shows the sheets as thin layers of density and helices as cylinders.



Input skeleton mrc files can be generated using software such as [Gorgon](#). Make sure the “origin index” and “voxel size” of the skeleton and density files are aligned before running SSETracer. (USCF Chimera → Tools → Volume data → Volume Viewer → Features → Coordinates). Save the maps after alignment.

Optional input:

- PDB model file

The accuracy of results can be calculated by checking the box labeled “Sensitivity analysis” and providing a corresponding PDB model file.

To run:

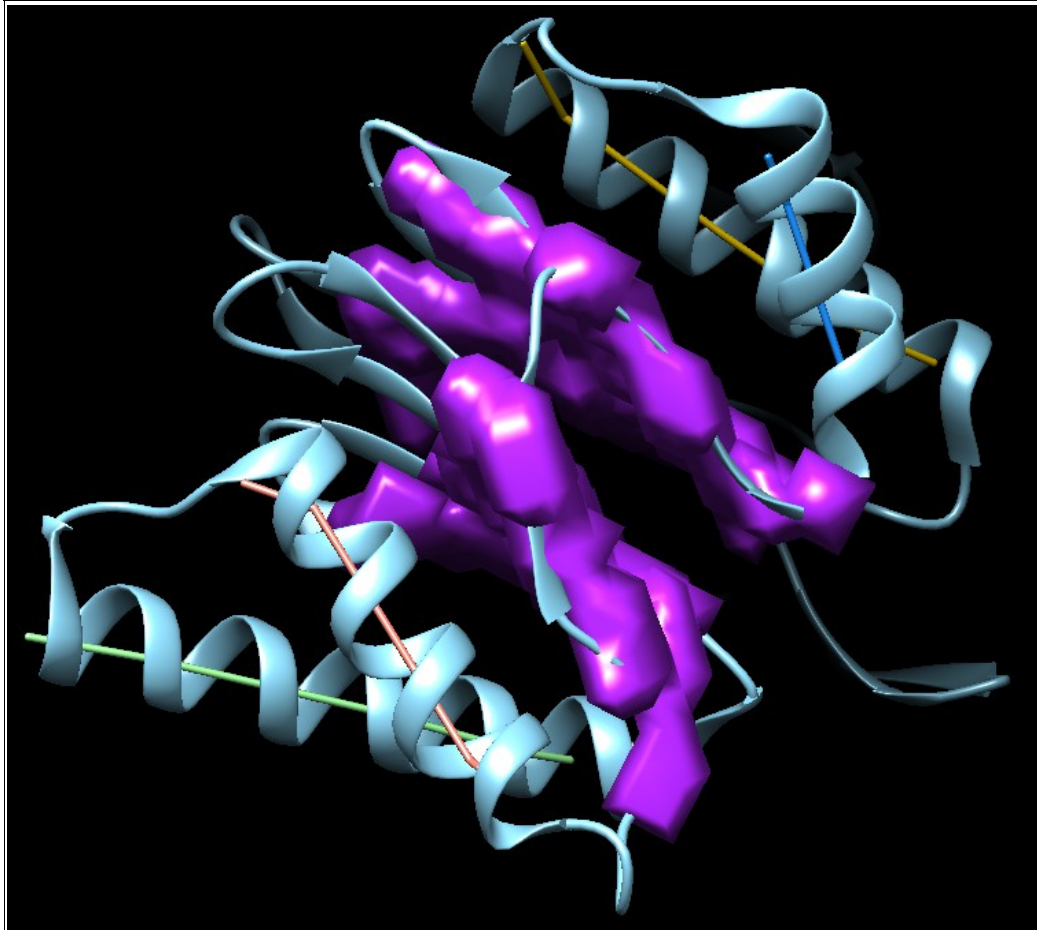
After providing the necessary files and threshold value, hit the button “Run Tracer”.

Output:

Output will be located in the same directory as the density mrc file, in the subdirectory `pdbID_thr_*_outFiles`

Detected helices will be outputted as files labeled “`pdbID_HLX#.pdb`”

Detected sheets will be outputted as a file labeled “`pdbID_SHTestimate_final.mrc`”



Example output with detected helices displayed as sticks and beta sheets displayed as purple density.

Usage with Command Line

To use SSETracer in command line, run with “`tracer_v4_command 1 <mrc> <skeleton> <threshold> 1 <pdb>`” for accuracy analysis or “`tracer_v4_command 1 <mrc> <skeleton> <threshold> 0`” to run without accuracy analysis. Note that the input files must include the path but not the file extension. Required inputs and provided output files are the same as in the GUI version.