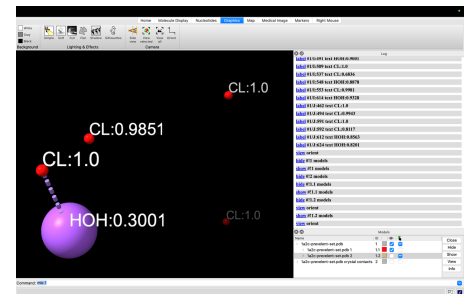
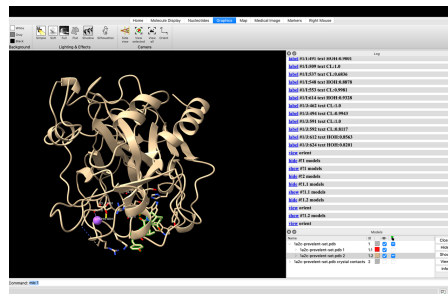


- Run MIC on all ions in Chain A:
 - mic #1/A
- Run MIC on all ions in Chain A and solvents:
 - mic #1/A,solvent

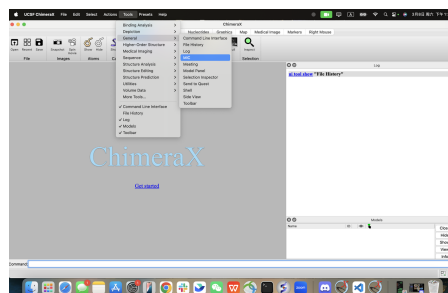
3. MIC Result Displayed

- ions/solvents are moved into model ID.1
- Classified results with confidence are shown in the format 'ion class: probability'

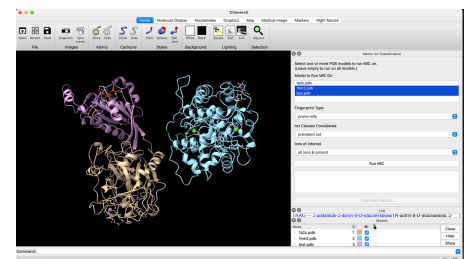


MIC Tool Test Usage

- Open MIC Tool in Tools/Bind Analysis/MIC or Tools/Structure Analysis/MIC



- Select opened PDB model(s) to run MIC

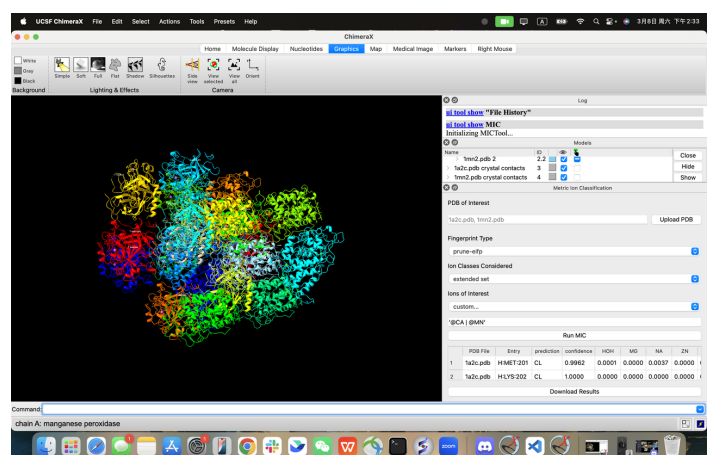


- Specify preferences:

- Fingerprint Type:
- Ion Classes Considered:
 - Prevalent Ion Set: H2O, Mg, Na, Zn, Ca, Cl
 - Extended Ion Set: prevalent set & K, Fe, Mn, Br, I

- Ions of Interest

- Customize ion(s) of interest
 - E.g '@CA | @MN | @CL'

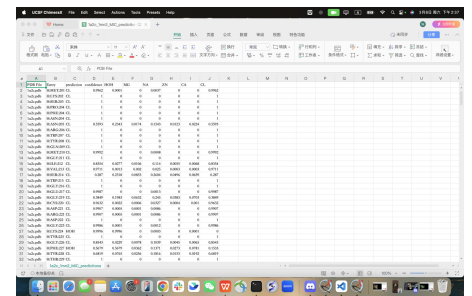
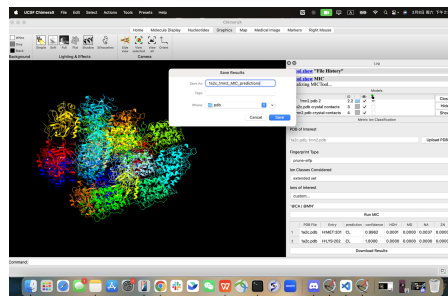


4. Run MIC

- Click the 'Run MIC' button

5. Export Results

- Click 'Download Results' button, name the result file & specify the path to save



- After uploading the PDB file via the 'Upload PDB' button, select 'Custom' under the 'Ion of Interest' dropdown. In the pop-up line box, type the ion class (e.g., @CL or @CL | @MN), then click 'Run MIC'. The results will be displayed and available for download.
- Upload multiple PDB files using the 'Upload' button and specify the ions of interest.
 - If the ions exist in all PDB files, the model will run for all of them.
 - If none of the PDB files contain the specified ions, an error message will appear stating "No Ions Selected."
 - If some PDB files contain the ions and others do not, an error message will indicate which PDB files lack the ions, and results for the valid PDB files will still be downloadable.

Notes for Using MIC in ChimeraX

Re-Open PDB model if reused:

If you've already run the MIC tool on a file (e.g. test.pdb), re-running it may cause errors. Close the model and re-open it to reset.

No spaces in selection syntax:

Use `mic #1/A:MG,CA` (✓)

Do **not** use `mic #1/A:MG, CA` (✗)

Extended set not supported yet:

Set `extended` to false.