

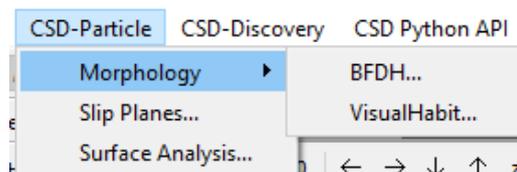
Mercury Tips & Tricks from attendees at the Virtual Workshop of 30/04/2024

Thank you all for sharing your tips and tricks on using Mercury!

We have collected all of them and divided by topic. Similar tips have been merged.

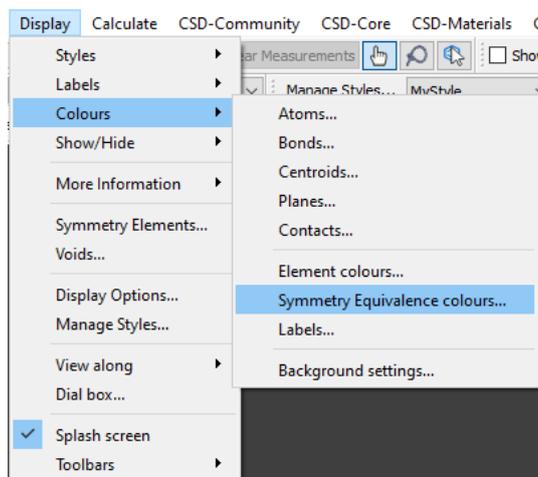
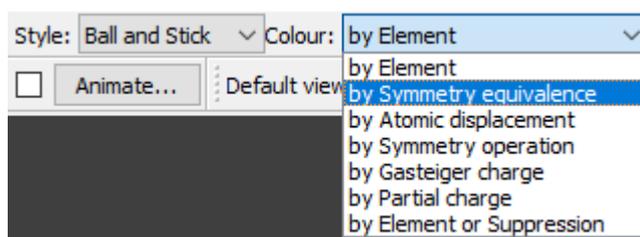
BFDH Morphology

- Accessed from: CSD-Particle > Morphology > BFDH
- Tip: Using BFDH morphology to compare the experimental indexing.



Symmetry Functionality

- Colour molecules by symmetry equivalence.
- Tip: When colouring molecules according to symmetry equivalence (eg for $Z'=2$) DO NOT use red and green since they will both appear to be the same to a colour blind reader. Black and orange are two good contrasting colours.
- Extra Tip: To change the default colours for symmetry equivalence, go to Display > Colours > Symmetry Equivalence colours

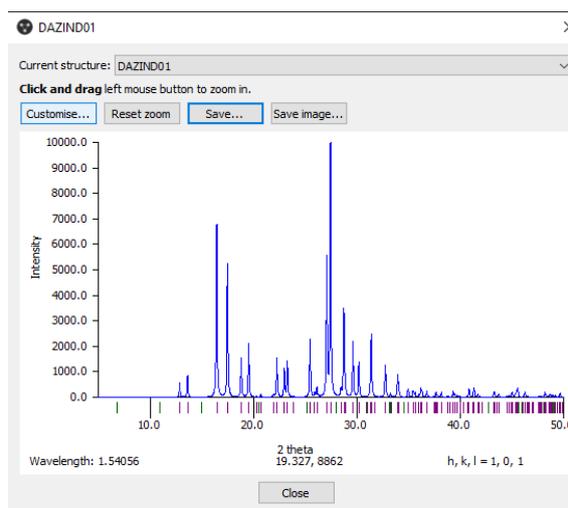


Calculate Menu

- Tips: Calculate planes – see how to on the slides!

PXRD

- Accessed from: Click on the Powder button below the 3D visualiser in Mercury.
- Tip: Calculating PXRD from cif files and customising the output pattern
- Tip: Preparing theoretical PXRD patterns which can be read in Excel or diffrac.eva

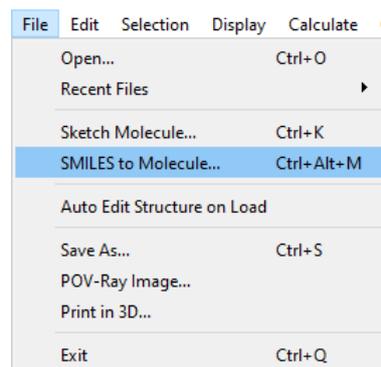


Other uses of Mercury

- I like to use Mercury to analyze my DFT structures.

Input molecules and files

- Tip: You could use the SMILES to Molecule feature (accessed from the File menu) to specify the stereochemistry of the initial structure to use in Conformer Generator.
- Tip: You can drag any file that Mercury can read either into an open Mercury window or onto the Mercury icon on your desktop and it will open it.



Create animations

- Tip: Tick Generate Animation Frames in the POV-Ray window to create frames for an animation showing the structure rotating. Use a gif creator software to collate the frames into a gif / movie.

