Example of current calibration problem: this reference sample peak should be at ~1.64 Å.

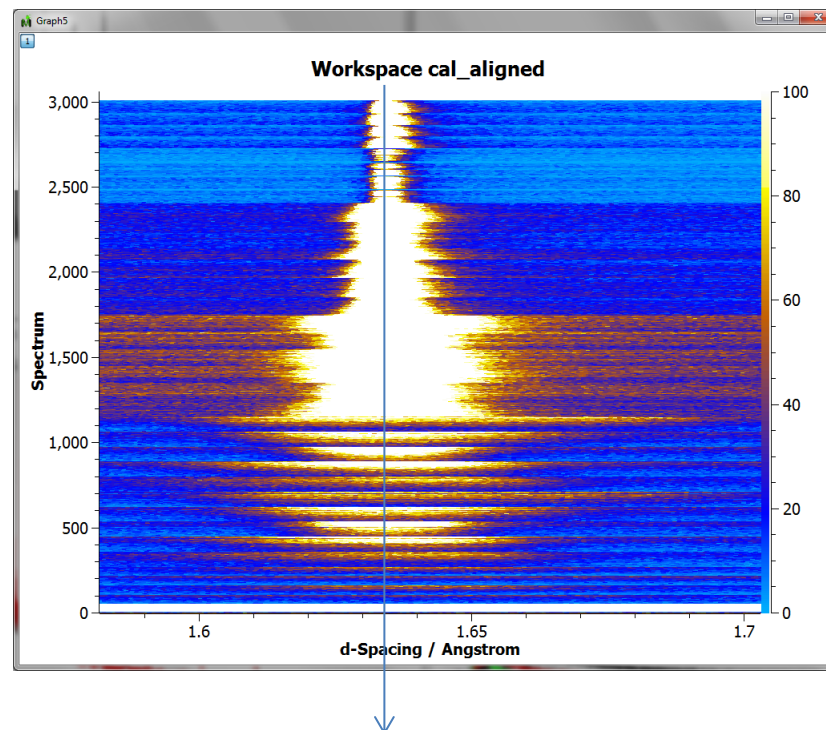

Peak position   Ideal peak position!
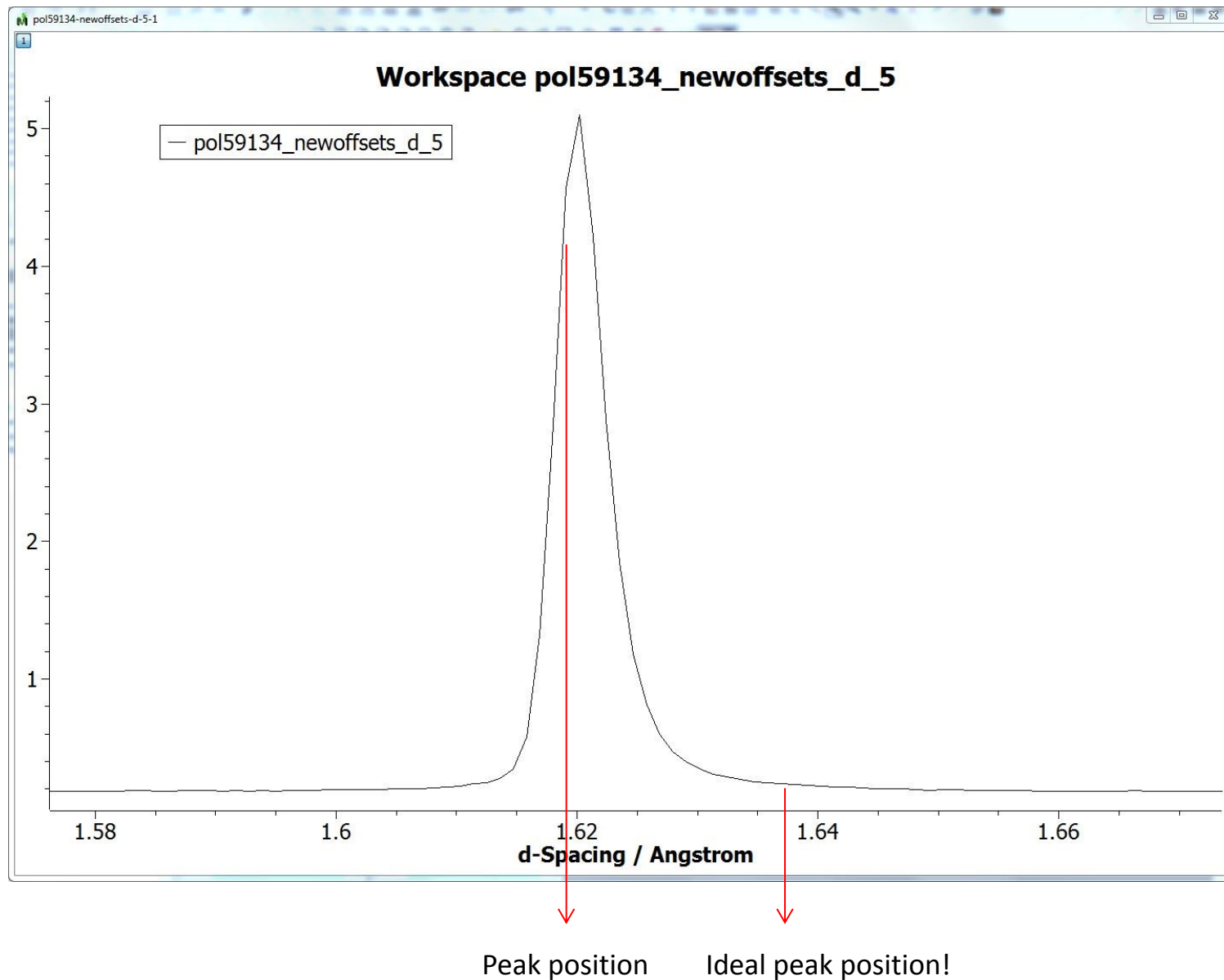
Data from standard reference sample

Possible solution?

Workspace cal_Drebin
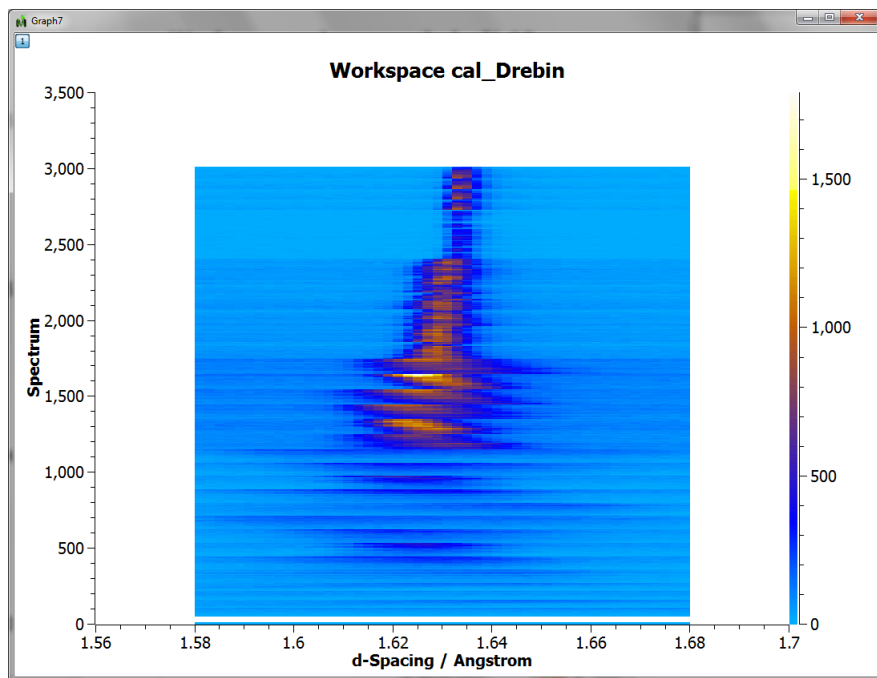
Detectors aligned based on reference spectrum

Workspace cal_aligned

Correct Calfile produced for use with all datasets (that don't have a known peak position.)

Deviation from ideal position ("Dideal") determined and global shift applied to match.