Please be aware that there is a problem with the "Dissociation ITC" analysis program in earlier (and possibly later) versions of MicroCal Origin for ITC. MicroCal (now GE Healthcare) have not yet (apparently) alerted users or issued a fix so, for the benefit of other users, I am copying below a previous communication on this issue.

The corrected DeltaH.ogs and Dissociation.fdf may be uploaded from our website.

AC – December 2009

From Alan Cooper (Glasgow) - August 2008

Colleagues:

Update on Dissociation ITC (apologies for the blanket email - there are lots of you with this problem!)

After intense discussions at the recent Heidelberg meeting and subsequent exchanges by email, MicroCal have now accepted that there is a fundamental problem with their "Dissociation" model for fitting dilution ITC data. However, working with Mike Rongner at MicroCal, we have now fixed the problem (basically the concentration calculations were wrongly coded - as some of you had spotted). I am hoping that MicroCal will issue an upgrade (or something) soon, but meantime I thought that you might like to try the new version for yourselves.

Attached are the two files needed for the new model. DeltaH.ogs should be copied into C:\Origin70 folder and Dissociation.fdf should be copied into C:\Origin70\FitFunc. You should overwrite (or re-name) the old files.

I have tested this on a range of data, and in all cases the agreement with our own (Glasgow) routines is excellent, and the results are now consistently reasonable. There are some cosmetic changes still to be done, but I am reasonably confident that this now works - just remember, when reading data into Origin for ITC, use the **"Dissociation (*.it?)"** option for file format. This will avoid potential confusion in subsequent analysis.

One nice feature of the new version is the incorporation of an "OFFSET" parameter. This is essentially the estimated baseline. As you will know, it is hard to do the proper baseline controls for dilution/dissociation ITC experiments, so this offset-fitting is one way of getting around this. But it is not a substitute for proper buffer equilibration, and I would caution against its use if the real data do not approach a sensible baseline.

Hope this helps. Let me know how it works out for you.

Alan

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