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**1.** 打开 Origin 软件(MicroCal, LLC ITC200),点击"Read data",在相应文件夹中找到 iTC 实验结果文件,导入软件,如下图所示;



2. 点击"Remove Bad Data",光标变为方框,将光标移动至需要删除的点处,单击选中 该点,再按"Enter"键即可消除 bad data,结果如下图所示;



3. 如希望利用点对点扣除背景,请转至步骤7;如希望用最后几个点进行背景扣除,请 按照以下步骤操作;

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4. 在工具栏"Window"中选择"Data1",如上图所示。观察 NDH 的最后 4-5 滴的结果,如果与之前对照实验的结果类似,且数值稳定,可以将这几滴对应的数值选中(如图中所示);

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 点击工具栏 "Statistics" → "Descriptive statistics" → "Statistics on columns", 在弹出 的页面中选择 "Mean (Y)"对应的数值, copy 该数值;



- 在工具栏"Window"中选择"DeltaH";在工具栏"Math"中选择"Simple math", 在弹出的对话框中"operator"填"-"号,"Y2"中 paste 上述数值(Mean(Y)), 点击 OK 即完成背景扣除。下转步骤 12;



 如希望利用点对点扣除背景,请按照以下操作步骤进行。在工具栏"Window"中选择 "mRawITC",点击"Read data",在相应文件夹中找到对照实验的结果文件,导入 软件,此时软件中只会显示第二次导入的数据;

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8. 双击左上角数字1的灰色方框,出现窗口"Layer1";选中"data1\_NDH"再点击符号 "=>"将 data1 的数据导入右侧区域(此时方框内共有 data2\_NDH 和 data1\_NDH 两组 值),点击"OK",此时"Data1\_NDH"、"Data2\_NDH"都会显示在窗口中;



9. 单击 "Data1\_NDH" 左侧黑色小方块,再点击 "Concentration",在弹出的窗口中会显示 "C in Syringe" (Syringe 中样品的浓度), "C in cell" (样品池中的浓度), "Cell Vol" (样品池体积,不要更改这个数值!),记录 Syringe 和样品池中样品的浓度,点击 "OK";



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10. 单击 "Data2\_NDH" 左侧黑色小方块,再点击 "Concentration",在弹出的窗口中将 "C in Syringe"和 "C in cell"分别改成与 "Data1\_NDH"相同的 Syringe 和样品池浓 度, "Cell Vol"不要更改,点击 "OK";

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11. 点击 "Subtract Reference Data",在弹出的窗口中将"Data"选为"Data1\_NDH", Reference 选为"Data2\_NDH"(Data1 和 Data2 分别为测试样品数据和对照组数据),点击"OK",软件会完成扣除背景操作;

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12. 点击"One Set of Sites",弹出窗口如上图所示;



 点击 1 liter/100 liter 进行模型拟合运算(推荐使用 100 liter),反复点击直至 Chi-Sqr 值不再减小为止,此时观察拟合曲线(红色),如果拟合效果好,则认为可以接受, 点击"Done",软件计算得出 N、K、ΔH、ΔS;





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14. 复制含有 N、K、ΔH、ΔS 数值的方框,点击工具栏 "ITC"中 "Final Figure",在得到 的图片中粘贴上述方框;

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等多种格式; "File"→ "Save Project as"→可以将数据保存为 Origin 格式。