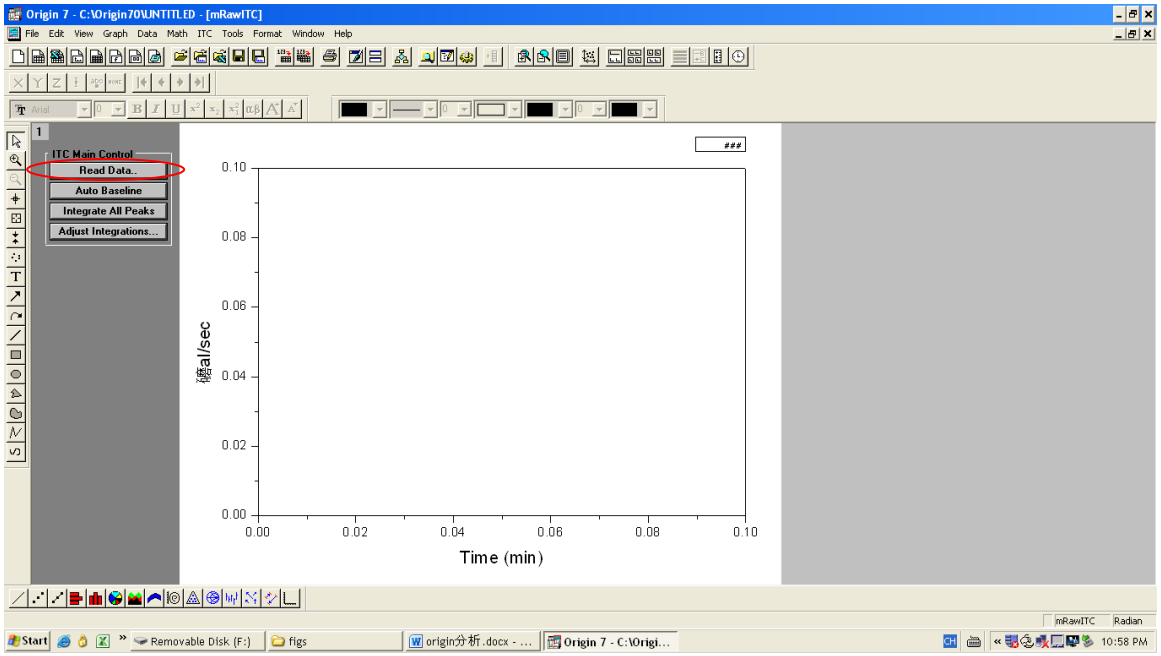
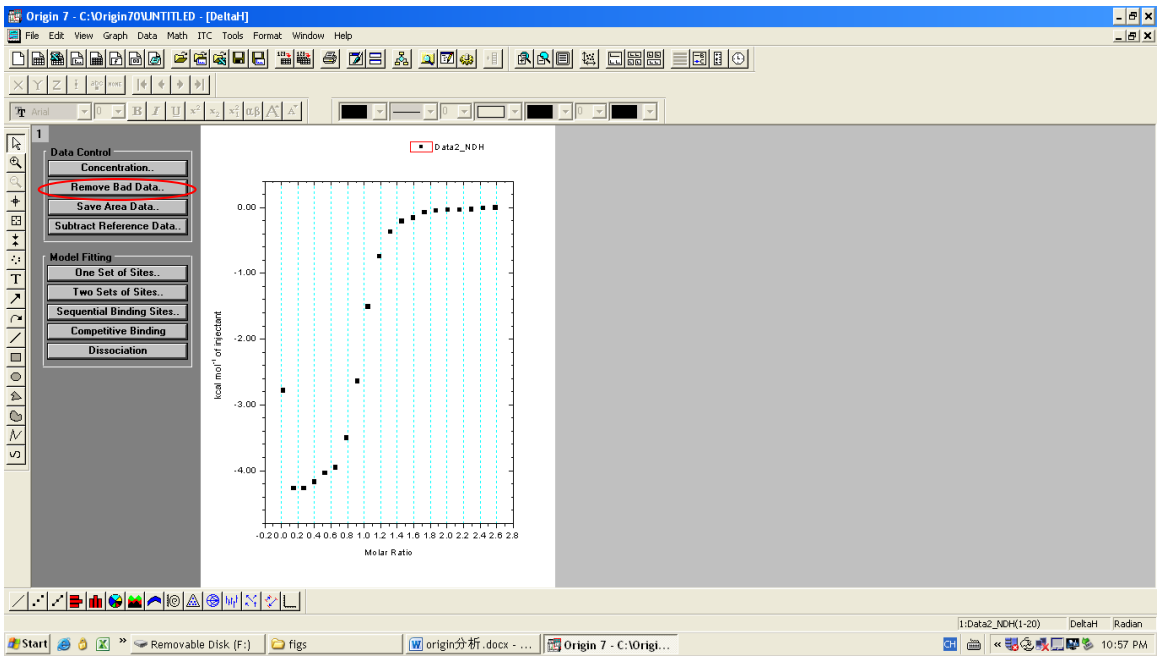
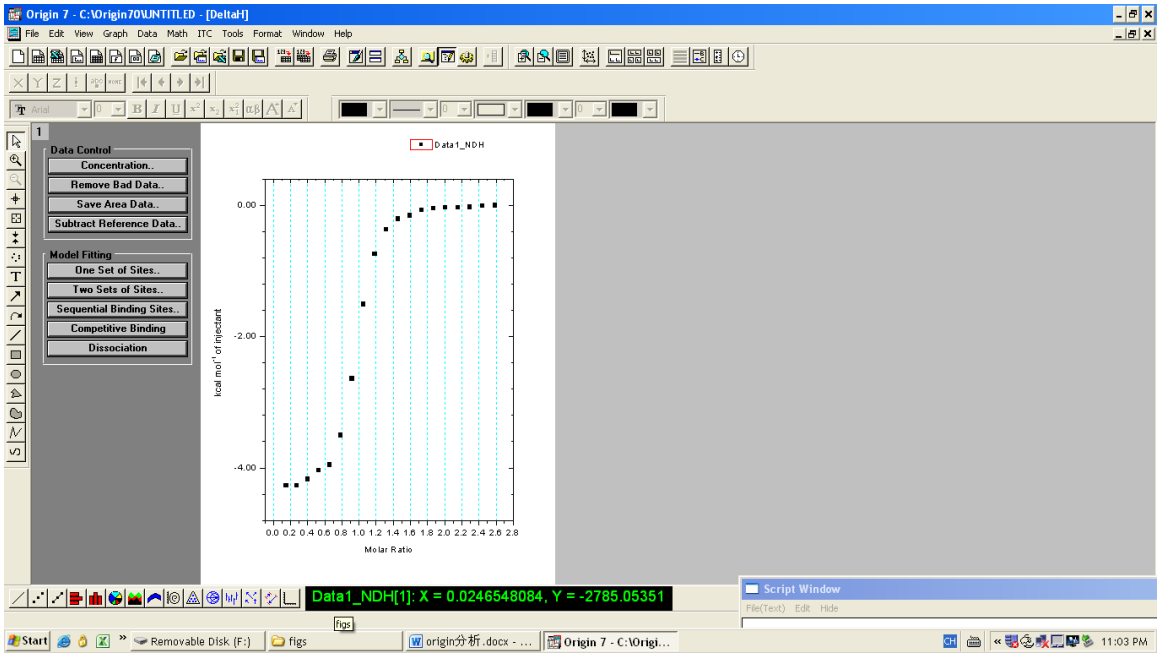


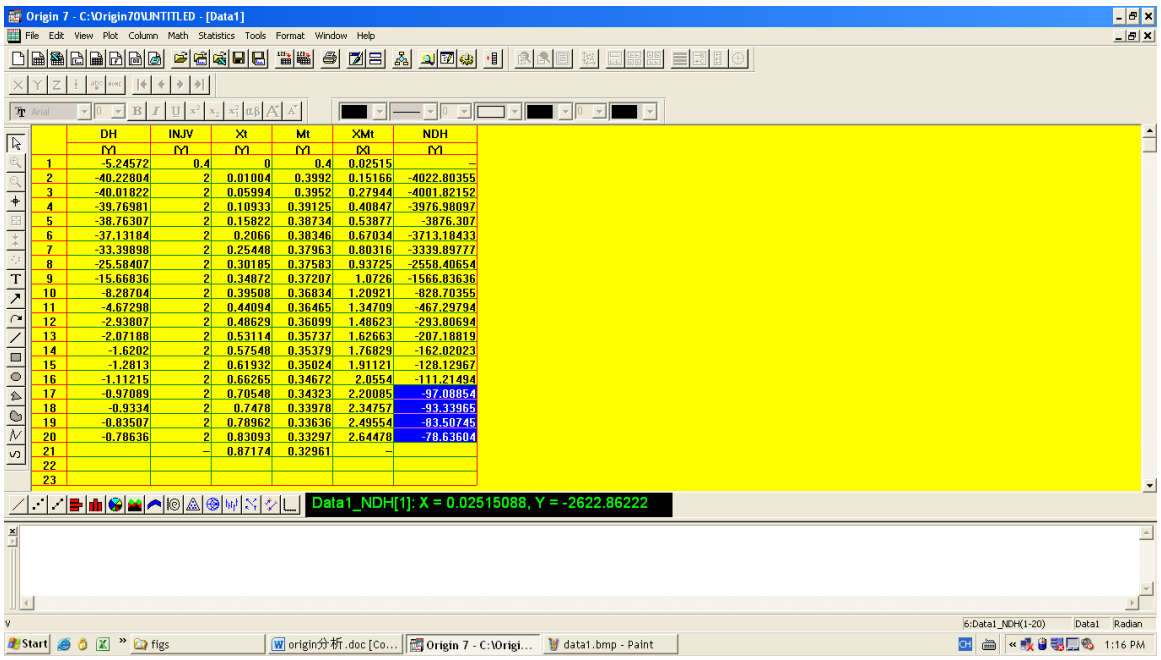
1. 打开 Origin 软件（MicroCal，LLC ITC200），点击“Read data”，在相应文件夹中找到 iTC 实验结果文件，导入软件，如下图所示；



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；

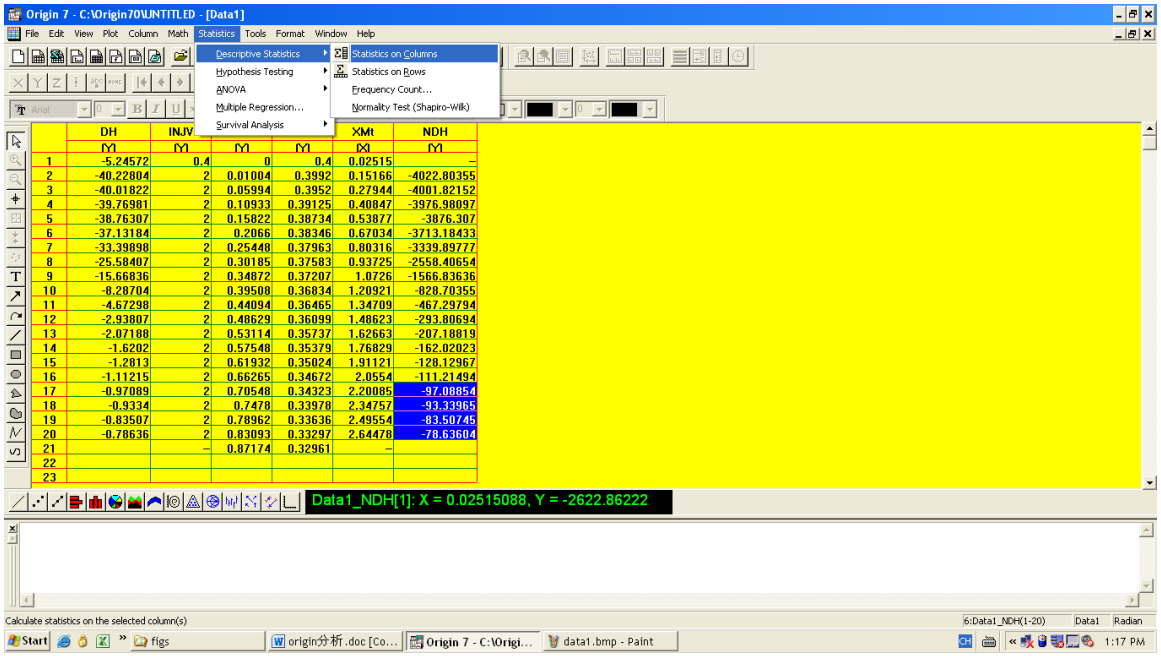


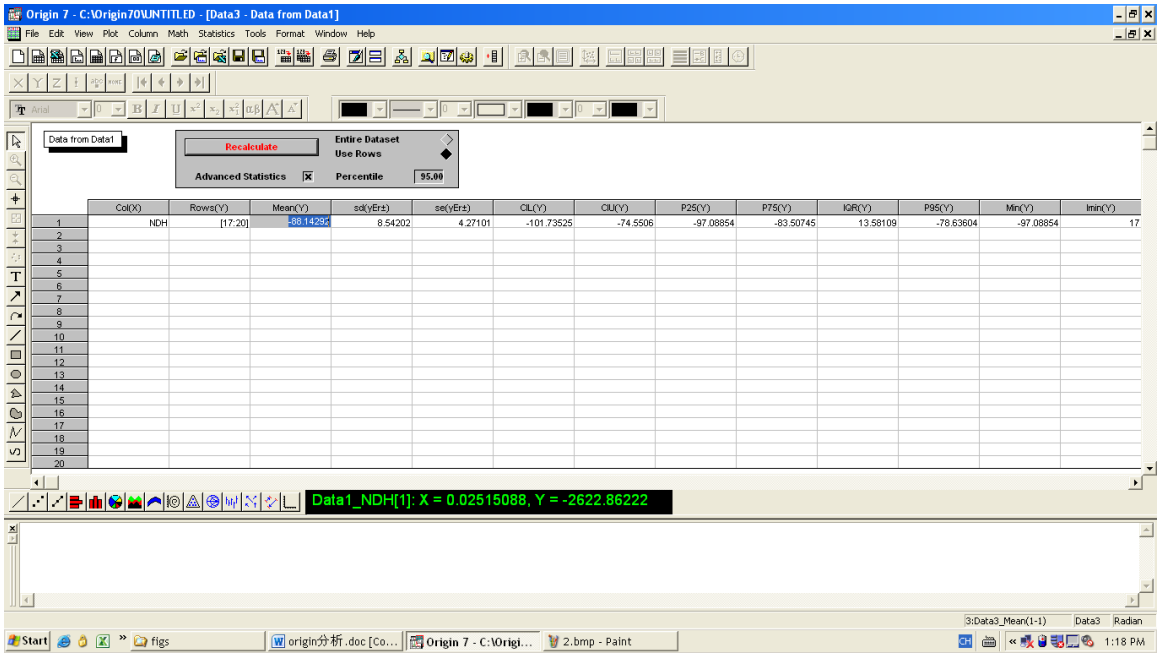
3. 如希望利用点对点扣除背景，请转至步骤 7；如希望用最后几个点进行背景扣除，请按照以下步骤操作；



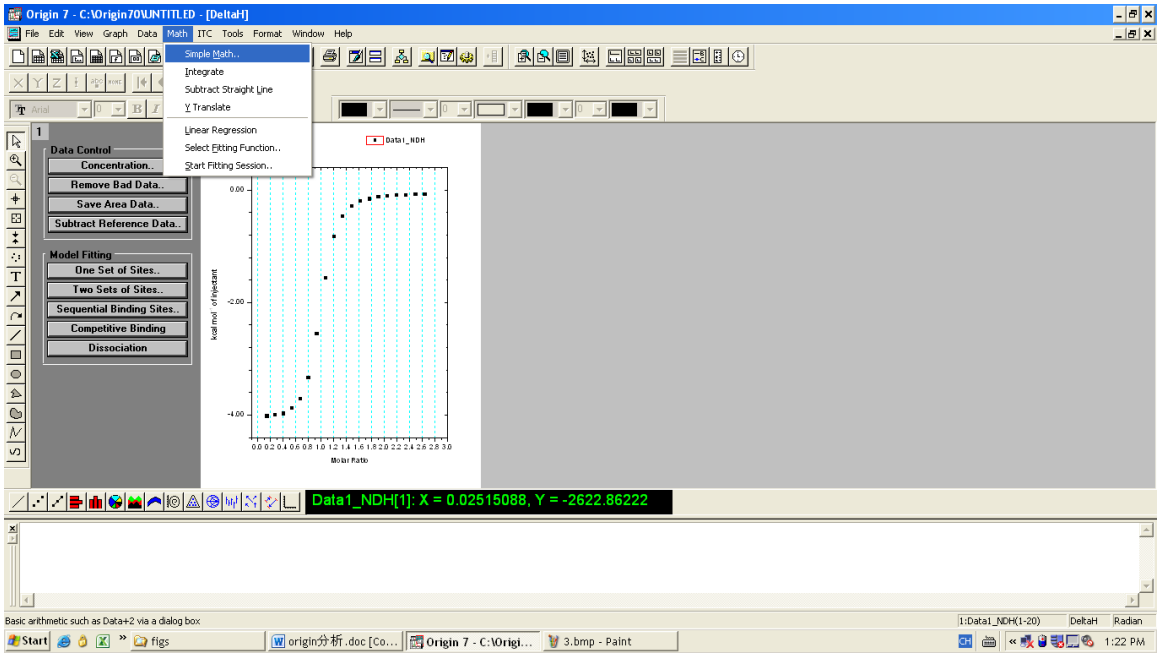
	DH	INJV	Xt	Mt	XMt	NDH
	[Y]	[Y]	[Y]	[Y]	[X]	[Y]
1	-5.24572	0.4	0	0.4	0.02515	–
2	-40.22804	2	0.01004	0.3992	0.15166	-4022.80355
3	-40.01822	2	0.05994	0.3952	0.27944	-4001.82152
4	-39.76981	2	0.10933	0.39125	0.40847	-3976.98097
5	-38.76307	2	0.15822	0.38734	0.53877	-3876.307
6	-37.13184	2	0.2066	0.38346	0.67034	-3713.18433
7	-33.39898	2	0.25448	0.37963	0.80316	-3339.89777
8	-25.58407	2	0.30185	0.37583	0.93725	-2558.40654
9	-15.66836	2	0.34872	0.37207	1.0726	-1566.83636
10	-8.28704	2	0.39508	0.36834	1.20921	-828.70355
11	-4.67298	2	0.44094	0.36465	1.34709	-467.29794
12	-2.93807	2	0.48629	0.36099	1.48623	-293.80694
13	-2.07188	2	0.53114	0.35737	1.62663	-207.18819
14	-1.6202	2	0.57548	0.35379	1.76829	-162.02023
15	-1.2813	2	0.61932	0.35024	1.91121	-128.12967
16	-1.11215	2	0.66265	0.34672	2.0554	-111.21494
17	-0.97089	2	0.70548	0.34323	2.20085	-97.08854
18	-0.9334	2	0.7478	0.33978	2.34757	-93.33965
19	-0.83507	2	0.78962	0.33636	2.49554	-83.50745
20	-0.78636	2	0.83093	0.33297	2.64478	-78.63604
21		–	0.87174	0.32961	–	
22						
23						

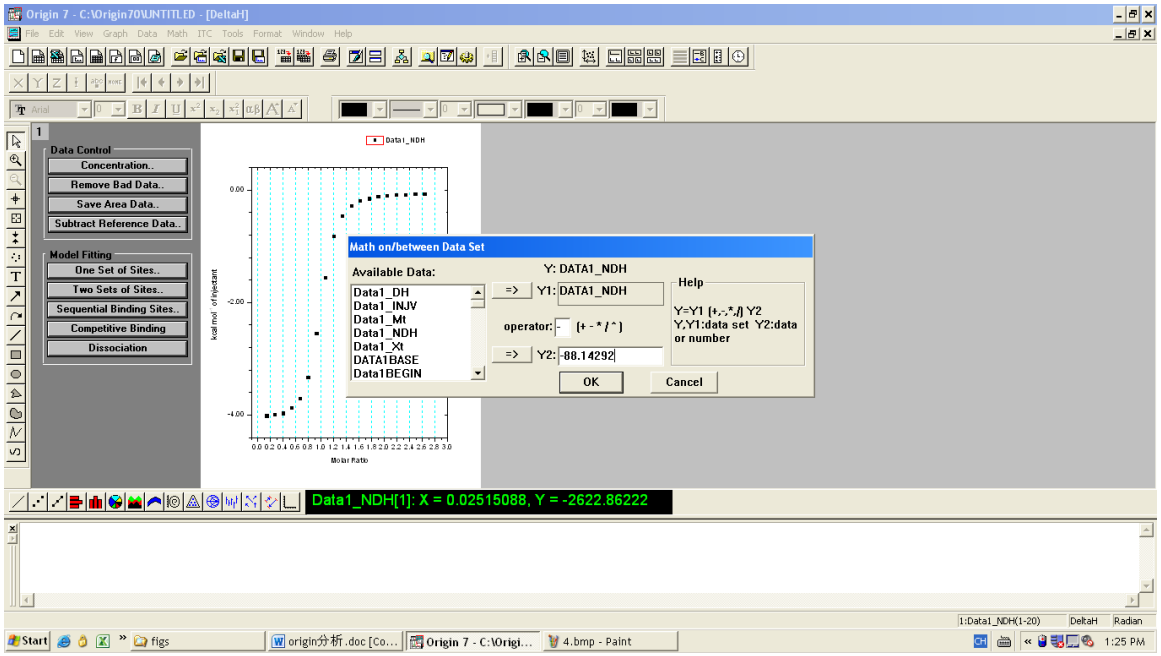
4. 在工具栏“Window”中选择“Data1”，如上图所示。观察 NDH 的最后 4-5 滴的结果，如果与之前对照实验的结果类似，且数值稳定，可以将这几滴对应的数值选中（如图中所示）；



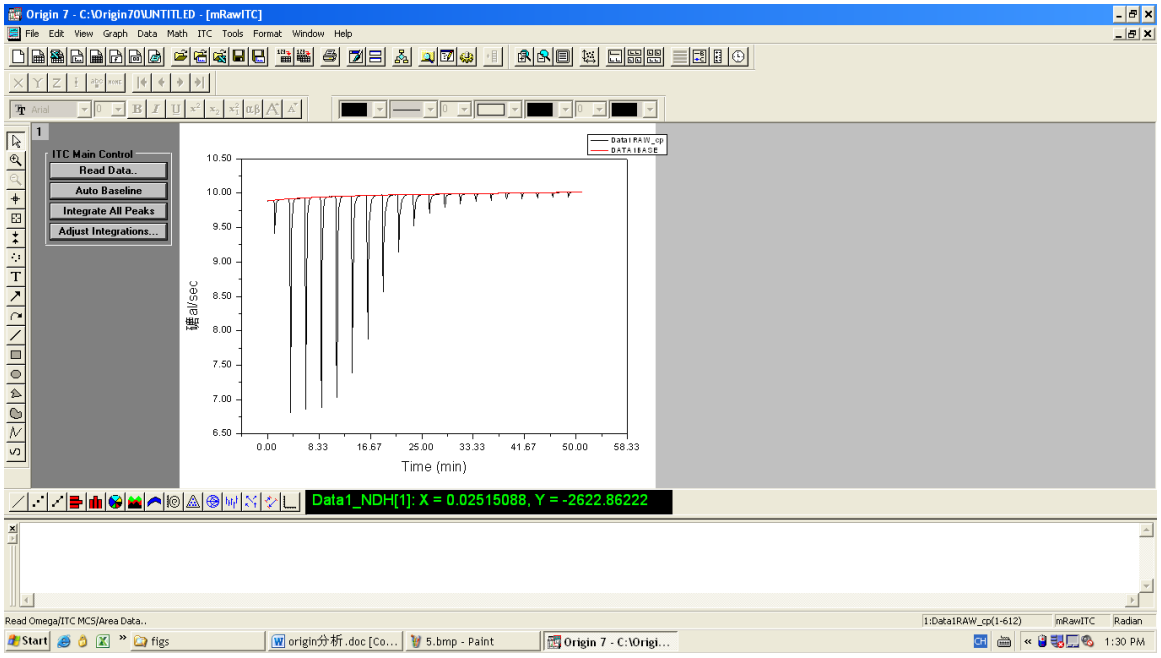


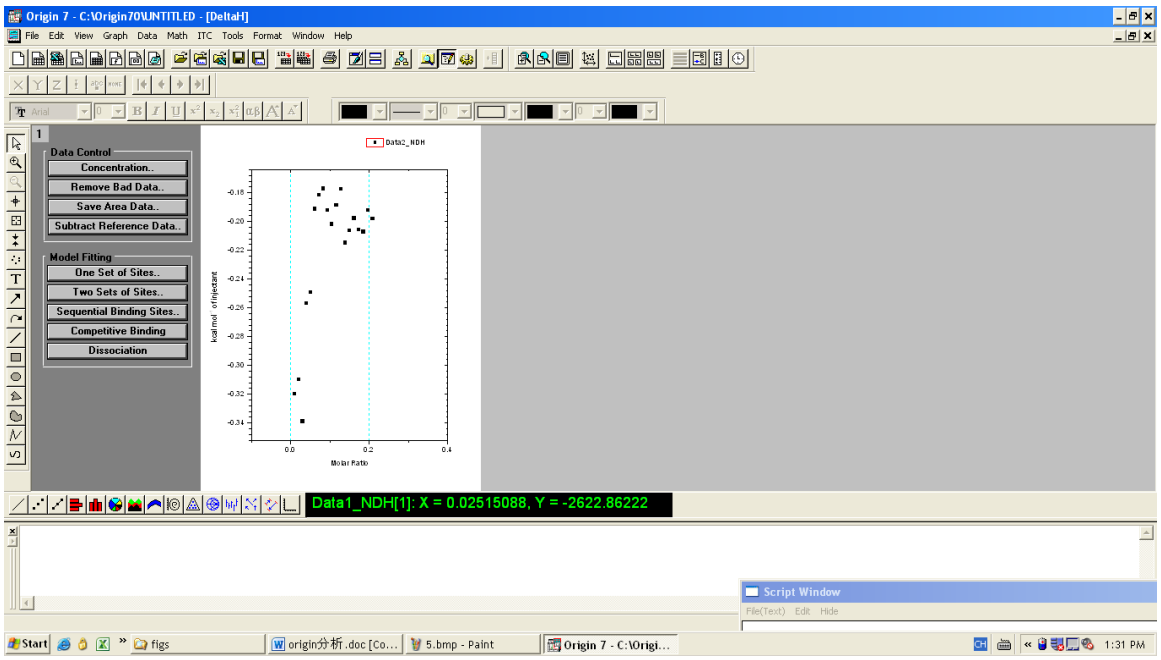
5. 点击工具栏“Statistics”→“Descriptive statistics”→“Statistics on columns”，在弹出的页面中选择“Mean（Y）”对应的数值，copy 该数值；



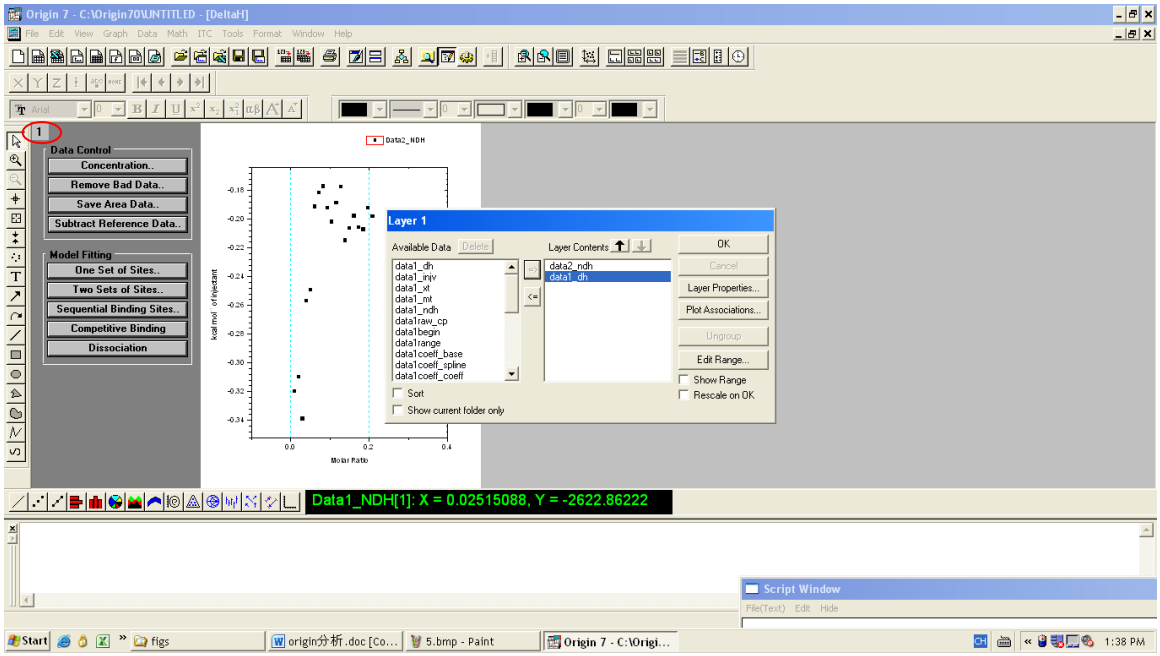


6. 在工具栏“Window”中选择“DeltaH”；在工具栏“Math”中选择“Simple math”，在弹出的对话框中“operator”填“-”号，“Y2”中 paste 上述数值（Mean（Y）），点击 OK 即完成背景扣除。下转步骤 12；

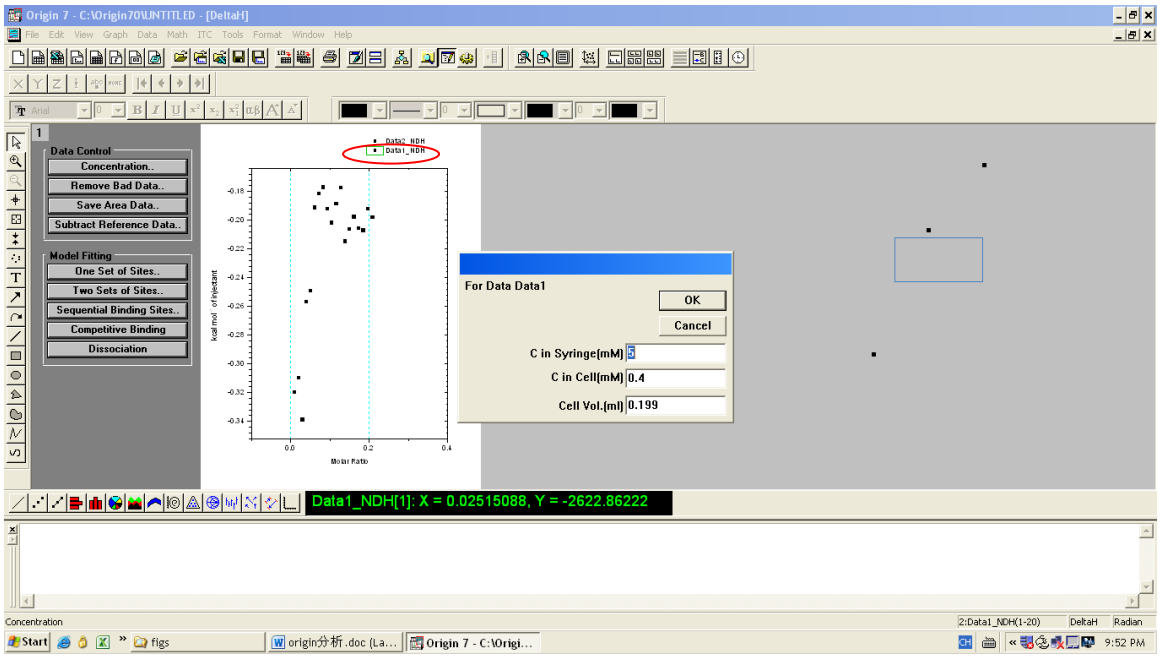




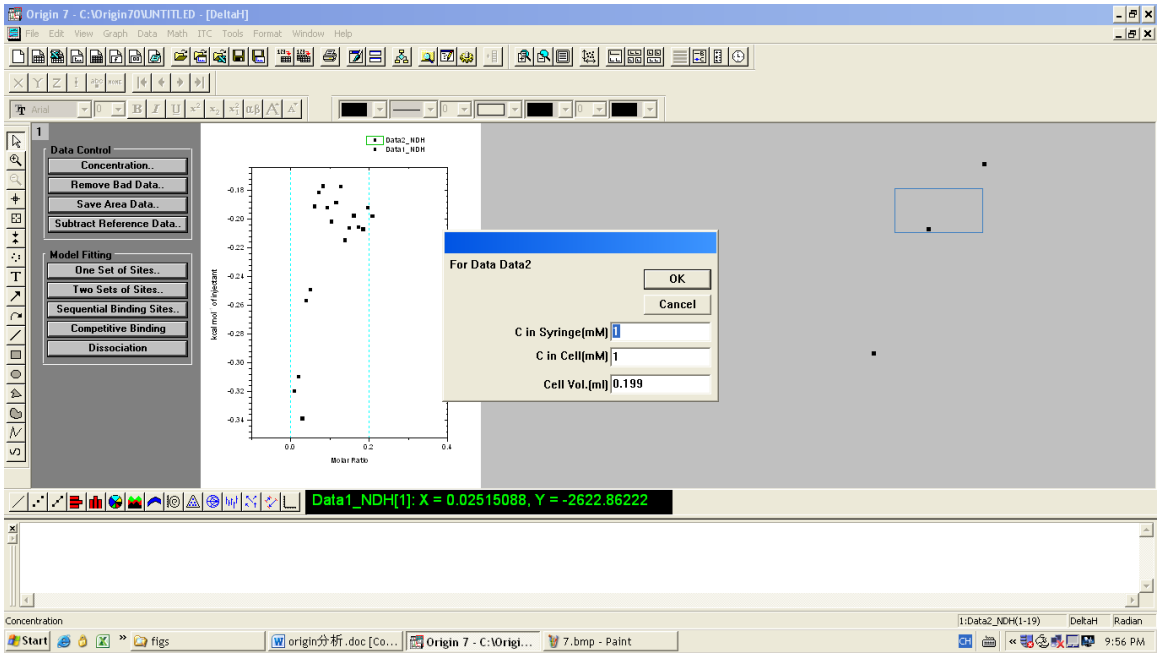
7. 如希望利用点对点扣除背景，请按照以下操作步骤进行。在工具栏“Window”中选择“mRawITC”，点击“Read data”，在相应文件夹中找到对照实验的结果文件，导入软件，此时软件中只会显示第二次导入的数据；

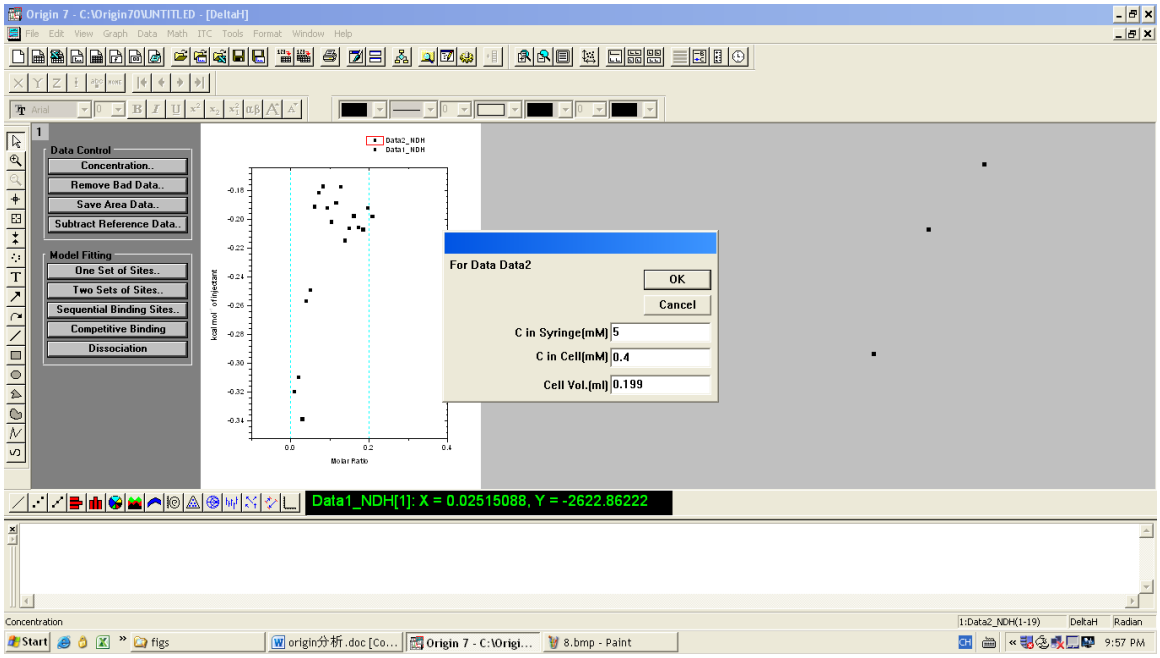


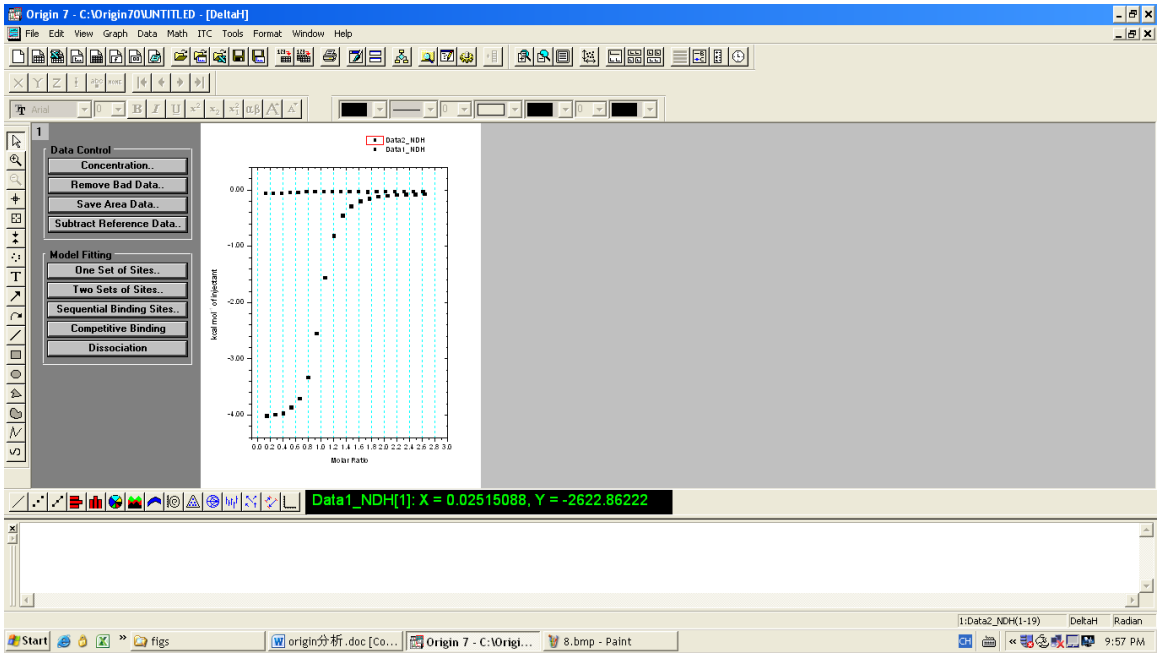
8. 双击左上角数字 1 的灰色方框，出现窗口“Layer1”；选中“data1_NDH”再点击符号“=>”将 data1 的数据导入右侧区域（此时方框内共有 data2_NDH 和 data1_NDH 两组值），点击“OK”，此时“Data1_NDH”、“Data2_NDH”都会显示在窗口中；



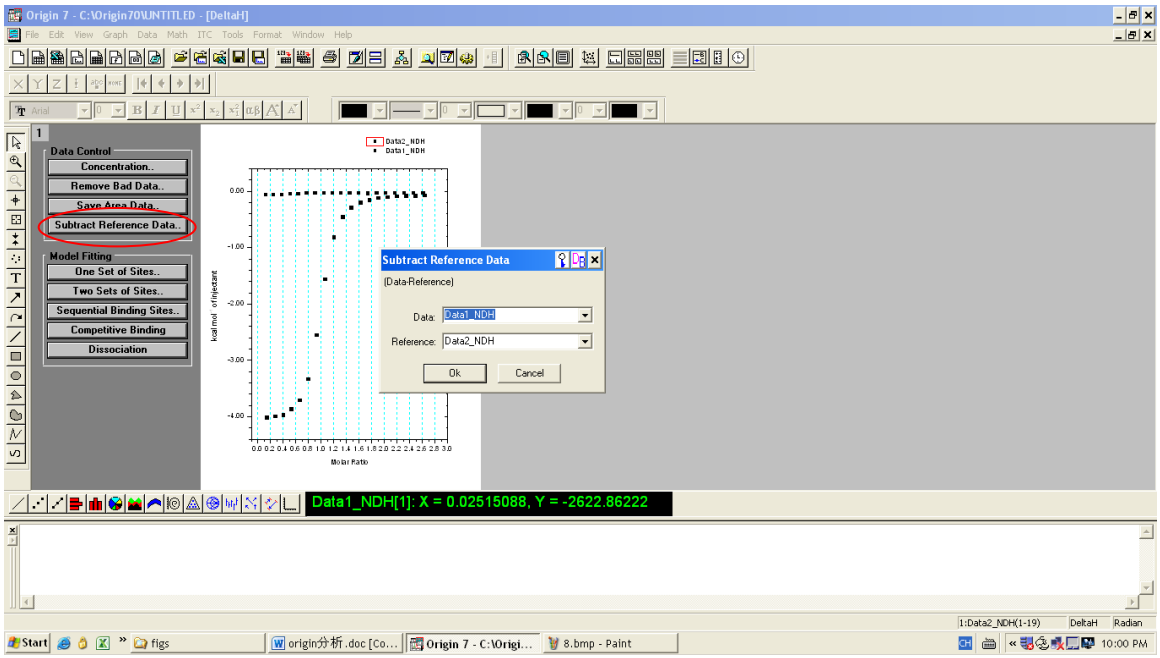
9. 单击“Data1_NDH”左侧黑色小方块，再点击“Concentration”，在弹出的窗口中会显示“C in Syringe”（Syringe 中样品的浓度），“C in cell”（样品池中的浓度），“Cell Vol”（样品池体积，不要更改这个数值！），记录 Syringe 和样品池中样品的浓度, 点击“OK”；

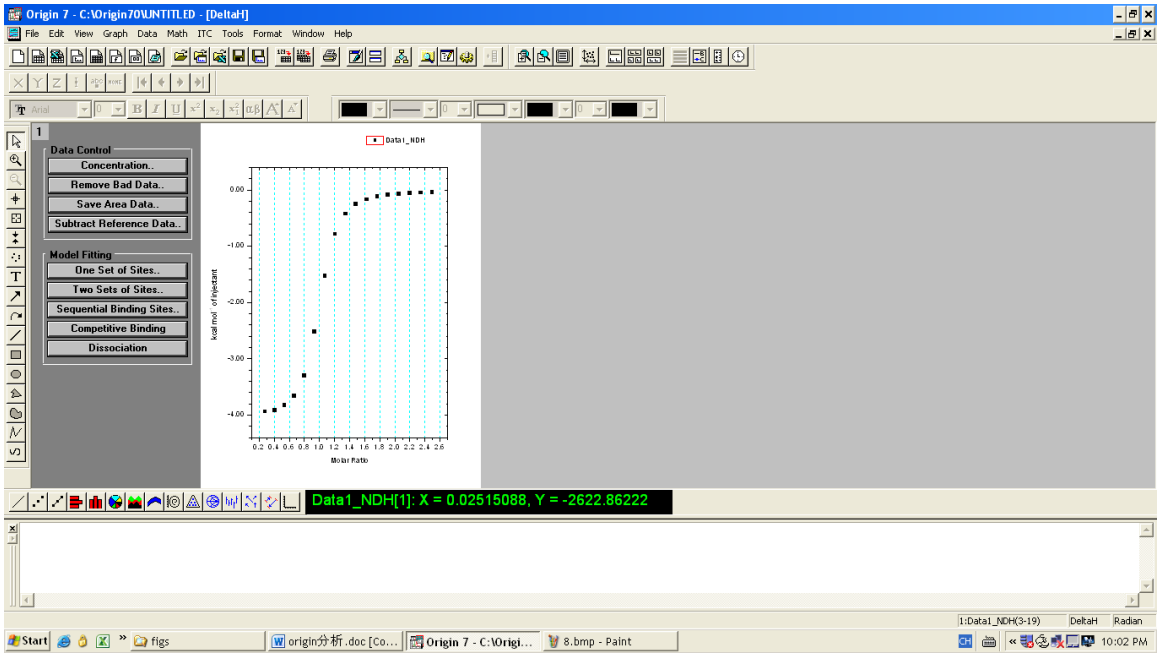

Origin 7 - C:\Origin70\UNTITLED - [DeltaH]
Data Control
Concentration..
Remove Bad Data..
Save Area Data..
Subtract Reference Data..
Model Fitting
One Set of Sites..
Two Sets of Sites..
Sequential Binding Sites..
Competitive Binding
Dissociation
Data2_NDH
Data1_NDH
kcal/mol of Injectant
Molar Ratio
For Data Data2
OK
Cancel
C in Syringe[mM] 1
C in Cell[mM] 1
Cell Vol.[ml] 0.199
Data1_NDH[1]: X = 0.02515088, Y = -2622.86222
Concentration
1:Data2_NDH(1-19)
DeltaH
Radian
Start
figs
origin分析.doc [Co...
Origin 7 - C:\Origi...
7.bmp - Paint
9:56 PM


Origin 7 - C:\Origin70\UNTITLED - [DeltaH]
Data Control
Concentration..
Remove Bad Data..
Save Area Data..
Subtract Reference Data..
Model Fitting
One Set of Sites..
Two Sets of Sites..
Sequential Binding Sites..
Competitive Binding
Dissociation
Data2_NDH
Data1_NDH
kcal/mol of Injectant
Molar Ratio
For Data Data2
OK
Cancel
C in Syringe[mM] 5
C in Cell[mM] 0.4
Cell Vol.[ml] 0.199
Data1_NDH[1]: X = 0.02515088, Y = -2622.86222
Concentration
1:Data2_NDH(1-19)
DeltaH
Radian
Start
figs
origin分析.doc [Co...
Origin 7 - C:\Origi...
8.bmp - Paint
9:57 PM

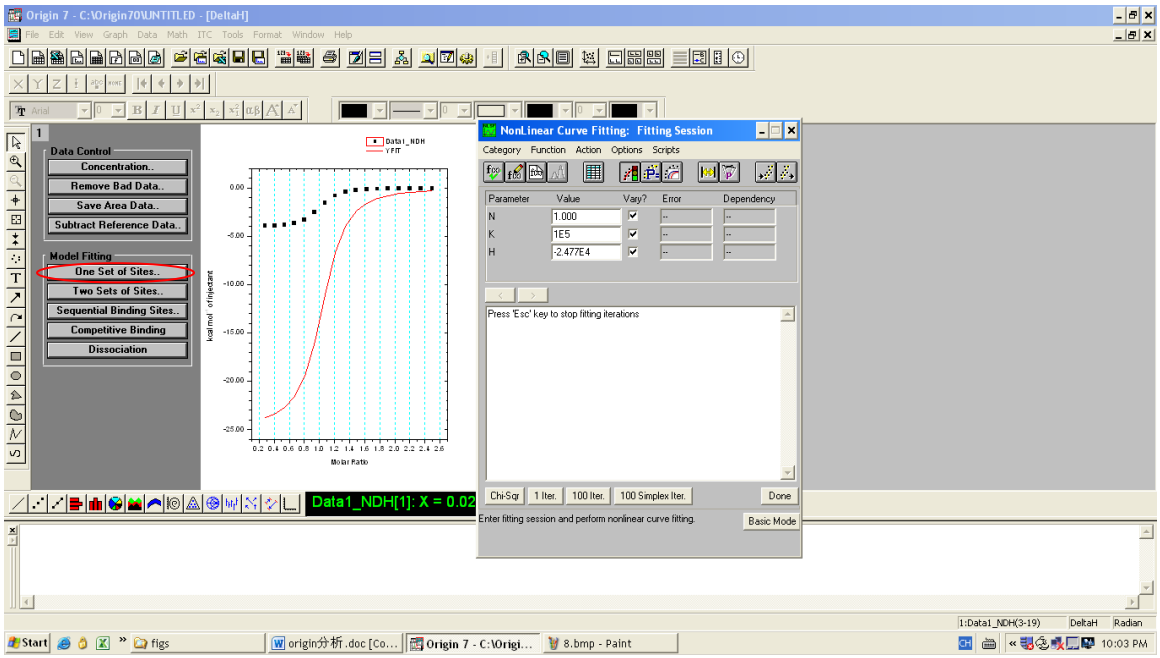


10. 单击“Data2_NDH”左侧黑色小方块，再点击“Concentration”，在弹出的窗口中将“C in Syringe”和“C in cell”分别改成与“Data1_NDH”相同的 Syringe 和样品池浓度，“Cell Vol”不要更改，点击“OK”；

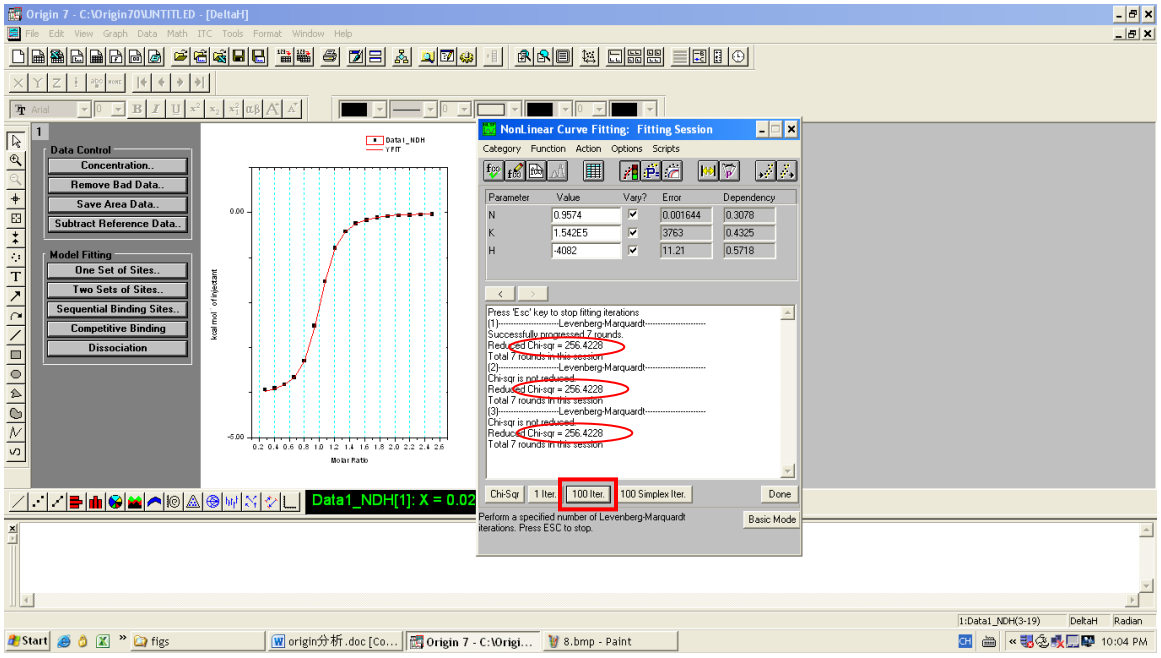


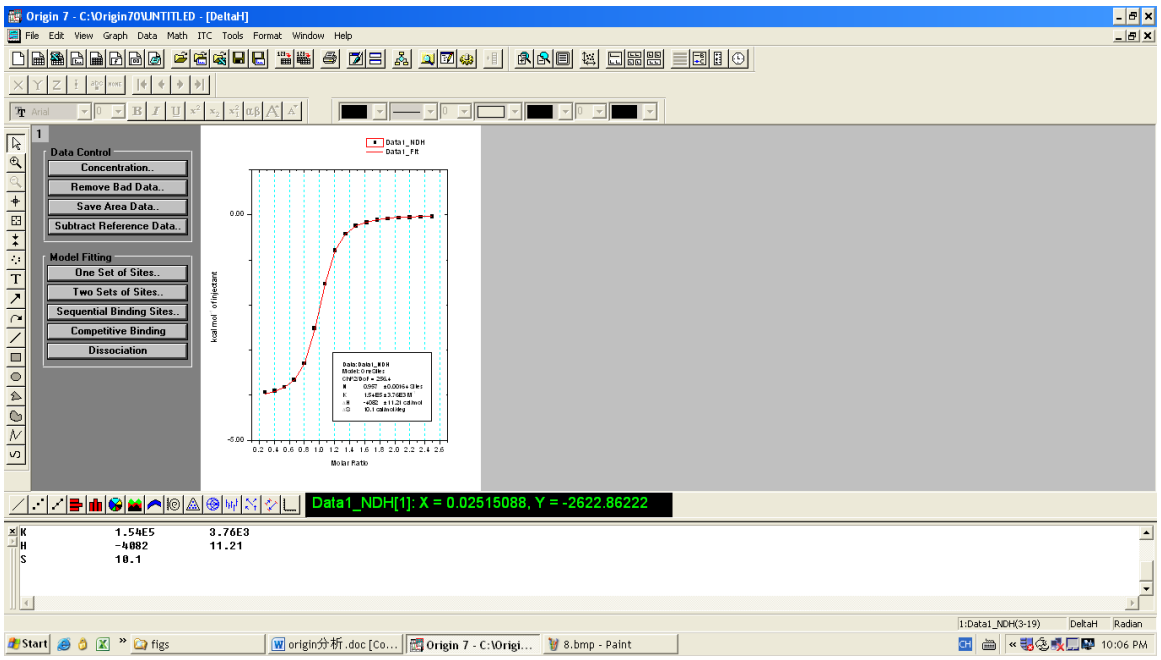


11. 点击“Subtract Reference Data”，在弹出的窗口中将“Data”选为“Data1_NDH”，Reference 选为“Data2_NDH”（Data1 和 Data2 分别为测试样品数据和对照组数据），点击“OK”，软件会完成扣除背景操作；

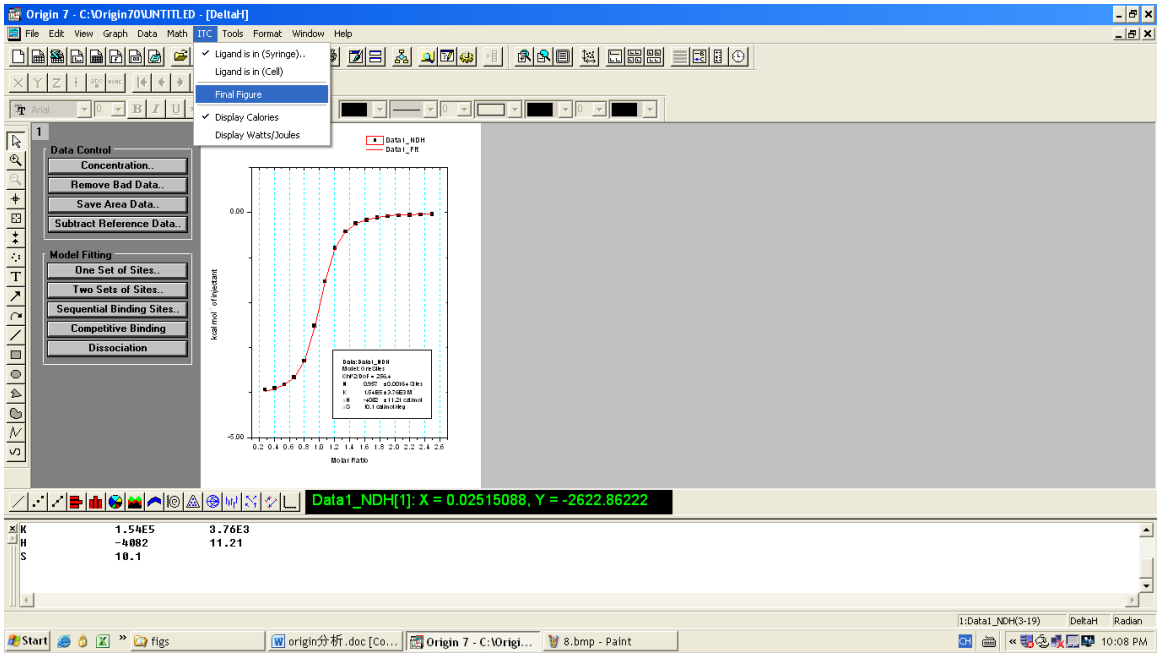


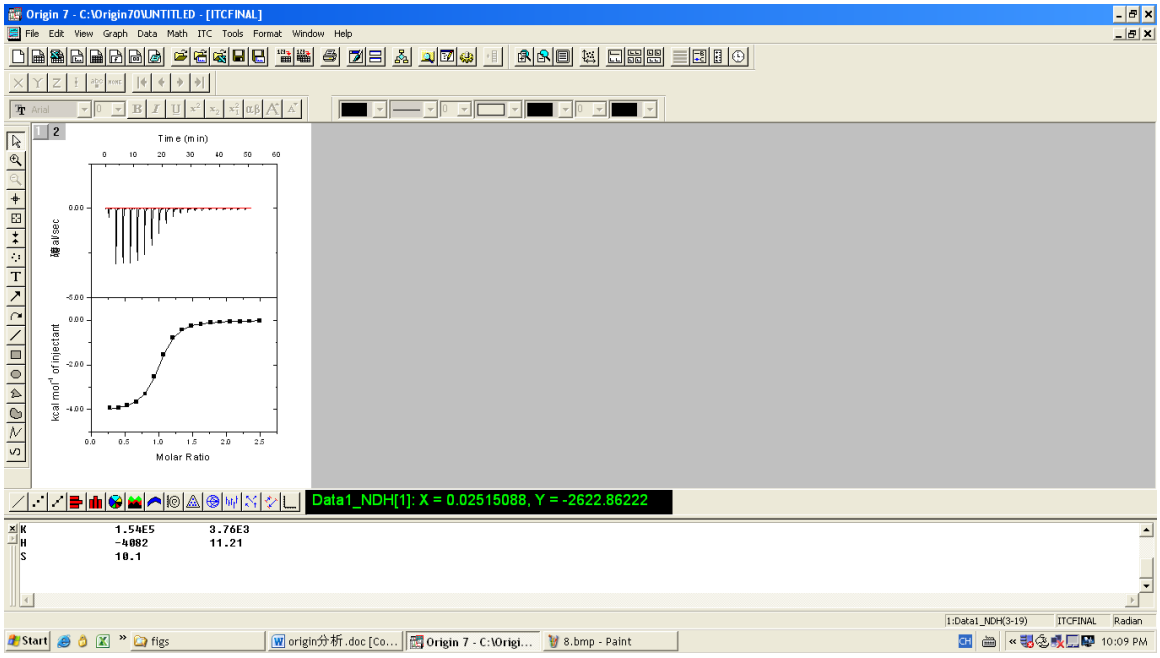
12. 点击“One Set of Sites”，弹出窗口如上图所示；

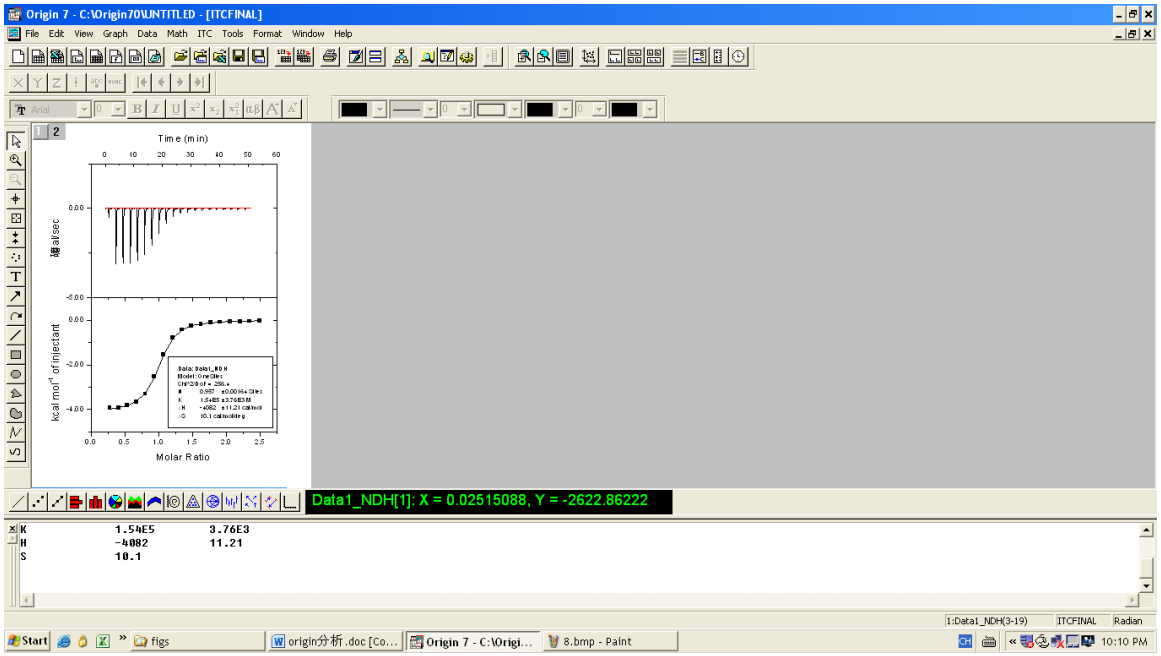




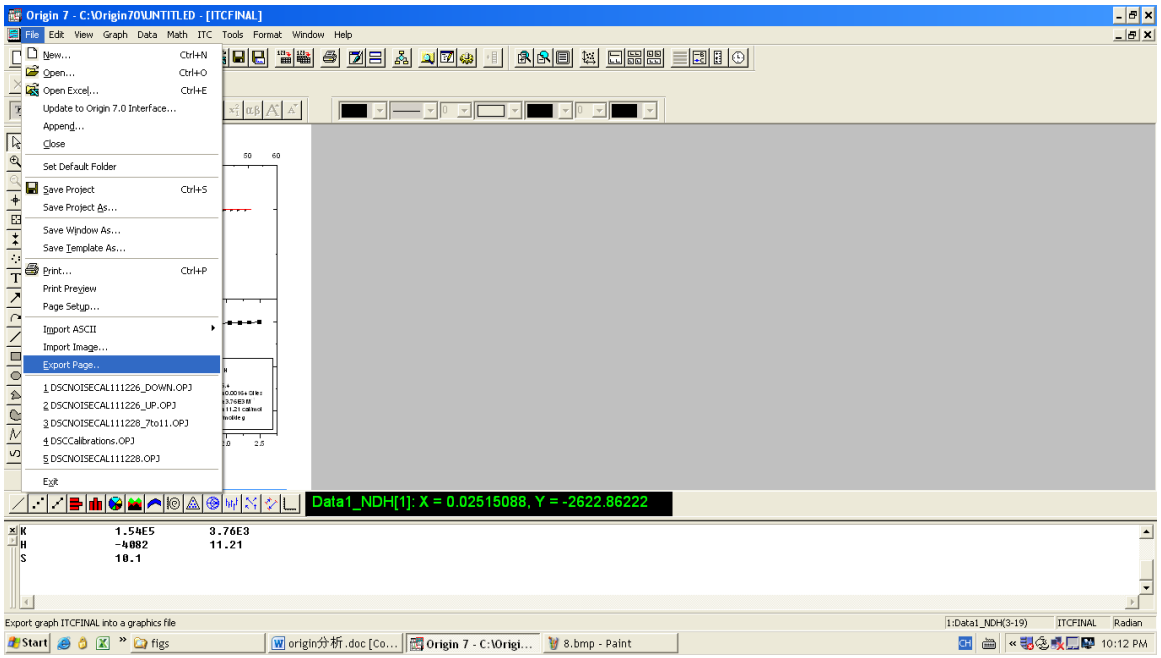
13. 点击 1 liter/100 liter 进行模型拟合运算（推荐使用 100 liter），反复点击直至 Chi-Sqr 值不再减小为止，此时观察拟合曲线（红色），如果拟合效果好，则认为可以接受，点击“Done”，软件计算得出 N、K、ΔH、ΔS；

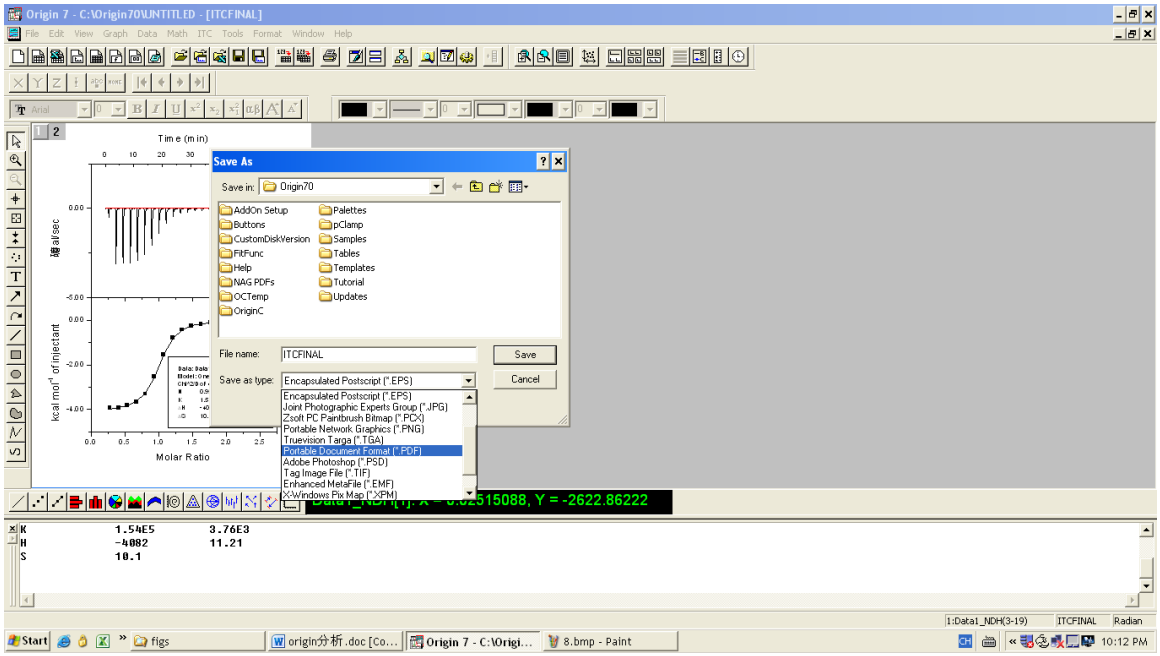

Origin 7 - C:\Origin70\UNTITLED - [DeltaH]
File Edit View Graph Data Math ITC Tools Format Window Help
Ligand is in (Syringe)..
Ligand is in (Cell)
Final Figure
Display Calories
Display Watts/Joules
Data Control
Concentration..
Remove Bad Data..
Save Area Data..
Subtract Reference Data..
Model Fitting
One Set of Sites..
Two Sets of Sites..
Sequential Binding Sites..
Competitive Binding
Dissociation
Data1_NDH
Data1_Fit
kcal/mol of injectant
Molar Ratio
Data1_NDH[1]: X = 0.02515088, Y = -2622.86222
K 1.54E5 3.76E3
H -4082 11.21
S 10.1
1:Data1_NDH(3-19) DeltaH Radian
Start figs origin分析.doc [Co... Origin 7 - C:\Origi... 8.bmp - Paint
10:08 PM


Origin 7 - C:\Origin70\UNTITLED - [ITCFINAL]
File Edit View Graph Data Math ITC Tools Format Window Help
Time (min)
μcal/sec
kcal mol-1 of injectant
Molar Ratio
Data1_NDH[1]: X = 0.02515088, Y = -2622.86222
K 1.54E5 3.76E3
H -4082 11.21
S 10.1
1:Data1_NDH(3-19) ITCFINAL Radian
Start figs origin分析.doc [Co... Origin 7 - C:\Origi... 8.bmp - Paint
10:09 PM



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；





15. 将文件导出：“File”→“Export Page” →通过修改格式可以将图片导出为图片或 pdf 等多种格式；“File”→“Save Project as”→可以将数据保存为 Origin 格式。