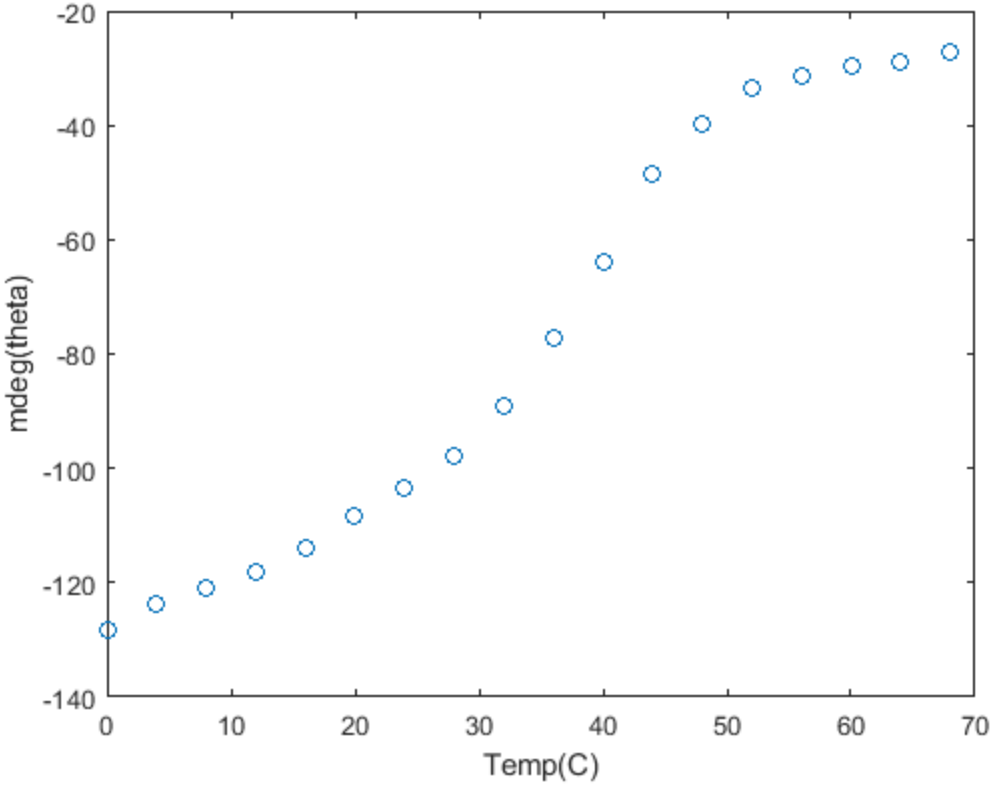
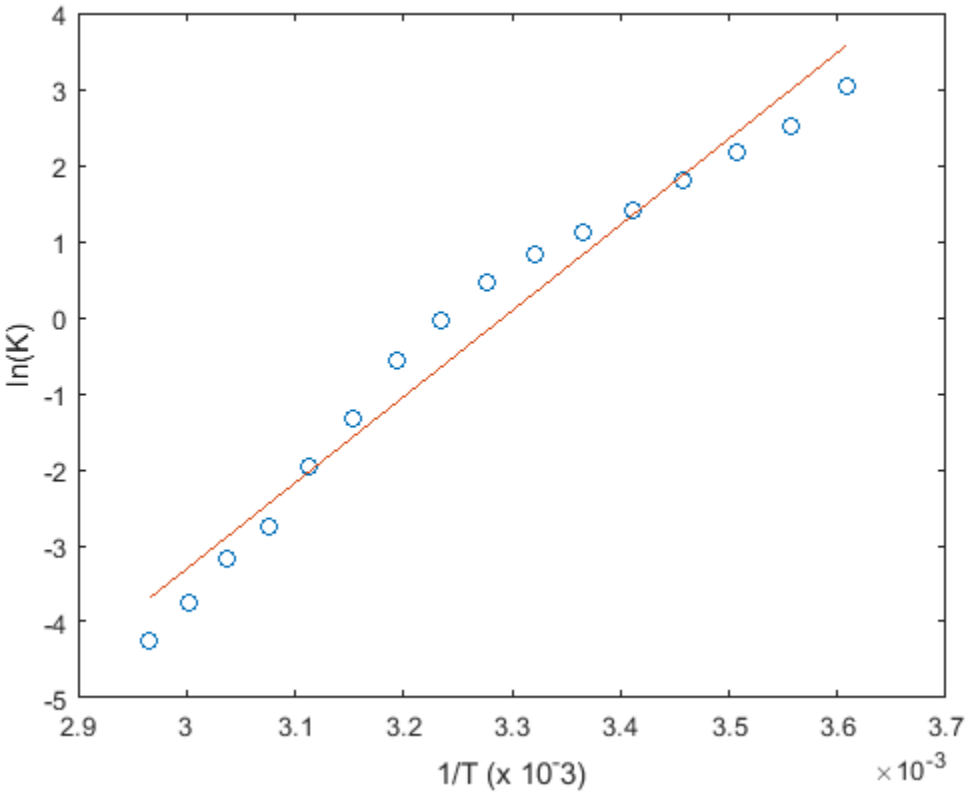
```
cddata     = xlsread('unfolding_data1.xlsx');
tCELS      = cddata(:,1); % temperature in celsius
cdmdeg     = cddata(:,2); % cd signal in millideg

figure(1) % temperature in celsius VS cd signal in millideg
plot(tCELS, cdmdeg,'o')
xlabel('Temp(C)')
ylabel('mdeg(theta)')

inv_tKELV  = 1./(tCELS + 273.15); % inverse temperature in Kelvin
FF         = -(cdmdeg-max(cdmdeg))/(max(cdmdeg)-min(cdmdeg)); %
 fraction folded
Kapp       = FF./(1-FF); % folding constant
lnKapp     = log(Kapp);  % natural log of folding constant

% CRITICAL STEPS
lnK        = lnKapp(2:end-1);     % remove INFINITY values
invT       = inv_tKELV(2:end-1);  % remove INFINITY values
vh         = polyfit(invT,lnK,1); % polyfit, degree 1
vh2        = polyval(vh,invT);    % generate new Y

figure(2) % vant hoff plot
plot(invT, lnK, 'O', invT, vh2)
xlabel('1/T (x 10^-3)')
ylabel('ln(K)')

% folding parameters
fprintf('tCELS  cdmdeg  inv_tKELV   FF  Kapp    lnKapp')
PARAM = [tCELS cdmdeg inv_tKELV FF Kapp lnKapp]
Hvh        = -vh(1)*(1.987/1000)   % vant hoff enthalpy in kcal/mol
Svh        =  vh(2)*(1.987/1000)   % vant hoff entropy in kcal/mol
tm         = (Hvh/Svh)-273.15      % temperature in Celsius
dG         = (1.987*(tCELS+273.15)).*lnKapp % dG = 0 kcal/mol at tm
%
%
```

```
tCELS  cdmdeg  inv_tKELV   FF  Kapp    lnKapp
PARAM =

         0 -128.3453    0.0037    1.0000       Inf       Inf
    4.0000 -123.7410    0.0036    0.9544   20.9375    3.0415
    8.0000 -120.8633    0.0036    0.9259   12.5000    2.5257
   12.0000 -117.9856    0.0035    0.8974    8.7500    2.1691
   16.0000 -113.9568    0.0035    0.8575    6.0200    1.7951
   20.0000 -108.4892    0.0034    0.8034    4.0870    1.4078
   24.0000 -103.3094    0.0034    0.7521    3.0345    1.1100
   28.0000  -97.8417    0.0033    0.6980    2.3113    0.8378
   32.0000  -89.2086    0.0033    0.6125    1.5809    0.4580
   36.0000  -77.1223    0.0032    0.4929    0.9719   -0.0285
   40.0000  -63.8849    0.0032    0.3618    0.5670   -0.5675
   44.0000  -48.3453    0.0032    0.2080    0.2626   -1.3372
   48.0000  -39.7122    0.0031    0.1225    0.1396   -1.9689
   52.0000  -33.3813    0.0031    0.0598    0.0636   -2.7546
```

```
   56.0000  -31.3669    0.0030    0.0399    0.0415   -3.1810
   60.0000  -29.6403    0.0030    0.0228    0.0233   -3.7583
   64.0000  -28.7770    0.0030    0.0142    0.0145   -4.2370
   68.0000  -27.3381    0.0029         0         0      -Inf


Hvh =

  -22.4705


Svh =

   -0.0740


tm =

   30.5843


dG =

   1.0e+03 *

       Inf
    1.6750
    1.4110
    1.2290
    1.0314
    0.8200
    0.6554
    0.5013
    0.2777
   -0.0175
   -0.3531
   -0.8426
   -1.2564
   -1.7797
   -2.0805
   -2.4879
   -2.8384
      -Inf
```


-20
-40
-60
-80
-100
-120
-140
mdeg(theta)
0
10
20
30
40
50
60
70
Temp(C)


4
3
2
1
0
-1
-2
-3
-4
-5
ln(K)
2.9
3
3.1
3.2
3.3
3.4
3.5
3.6
3.7
1/T (x 10^-3)
×10^-3

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