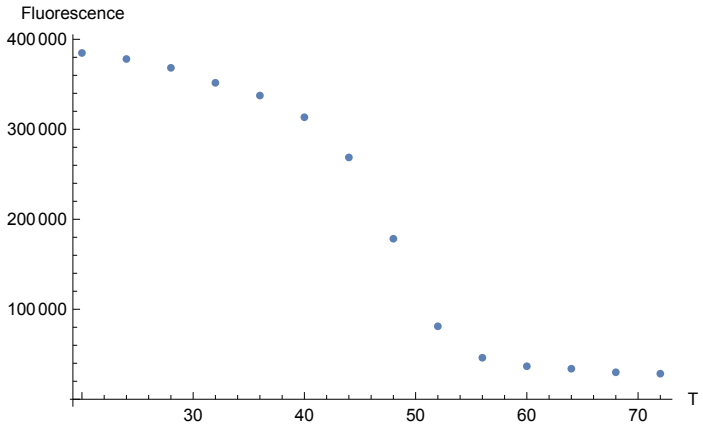
Pchem Assignment 5 – 7 November 2016

Question 1

In[3]:=
```
tdnatall = Transpose[
   Import[ "/Users/Research/JHU_Class_Material/pchem/assignment_5/TDenat.xlsx",
    "Data"]];
tdnat = Transpose[tdnatall[[2 ;;]]][[1]];
```

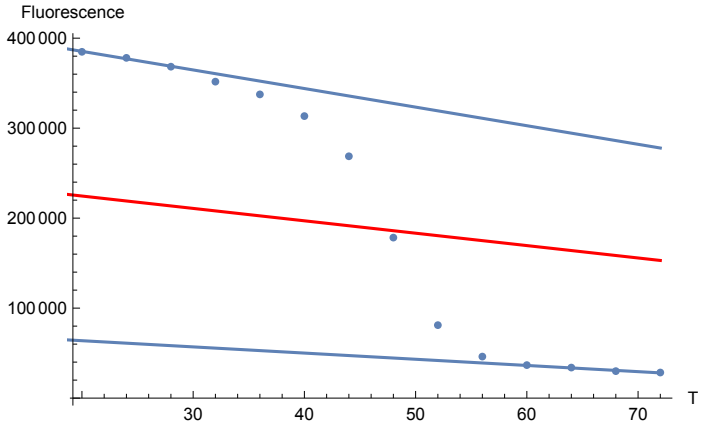
In[5]:=
```
(*Plot the denaturation data*)
tdnatplot = ListPlot[tdnat, PlotRange → All, AxesLabel → {"T", "Fluorescence"}]
```

Out[5]=



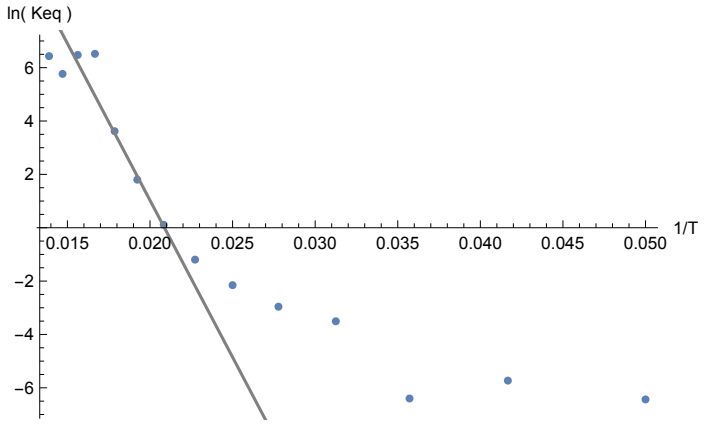
In[6]:=
```
(*Fit the denaturation data to two baselines. Pick
  the first and last few points that would make linear baselines
  we want the baselines so we can calculate a and b
  b/a = fu/fn = Keq
   b is the distance between fn and fm. proporional to U
   a is the distance between fu and fm. proportional to N*)
(*So Tm is around 48*)
(*native baseline uses the first few points*)
ln = LinearModelFit[tdnat[[1 ;; 3]], x, x];
fn[x_] := ln["BestFitParameters"][[1]] + (ln["BestFitParameters"][[2]] * x);
(*unfolded baseline uses the last few points*)
lu = LinearModelFit[tdnat[[-3 ;;]], x, x];
fu[x_] := lu["BestFitParameters"][[1]] + (lu["BestFitParameters"][[2]] * x);
(*The midpoint line is halfway between
 the equations that describe the fn and fu lines*)
lm = Table[{x, ((ln[x] - lu[x]) / 2) + lu[x]}, {x, 0, Max[tdnat[[All, 1]]]}];
Show[tdnatplot, Plot[ln[x], {x, 0, Max[tdnat[[All, 1]]]}],
 Plot[lu[x], {x, 0, Max[tdnat[[All, 1]]]}], ListLinePlot[lm, PlotStyle → Red]]
```

Out[11]=



In[12]:=
```
(*The x-intercept is the Tm. dG = 0 at Keq = 1 at Tm
    dG = -RTln(Keq)
     ln(Keq) = ( -dG/R )(1/T)
      y = mx + b
            but this doesn't actually make sense so never mind...
*)
(*b is the fraction native fit minus the y data*)
b = fn[tdnat[[All, 1]]] - tdnat[[All, 2]];
(*a is the y data minus the fraction unfolded fit*)
a = tdnat[[All, 2]] - fu[tdnat[[All, 1]]];
(*x1 y1 where x is 1/T and y is ln(b/a) (which is fu/fn = Keq)*)
lnkvsinvtdata = Transpose[{(1 / tdnat[[All, 1]]), Re[Log[b / a]]}];
lnkvsinvt = ListPlot[lnkvsinvtdata];
(*get the best fit line of where the data is linear. This
 is where unfolding is happening and you're getting b/a*)
lm2 = LinearModelFit[lnkvsinvtdata[[-7 ;; -5]], x, x];
Show[lnkvsinvt, Plot[lm2[x], {x, Min[lnkvsinvtdata], Max[lnkvsinvtdata]},
  PlotStyle → Gray], AxesLabel → {"1/T", "ln( Keq )"}]
(*y=mx+b --> ((y-b)/m)=x --> 1/((y-b)/m)=Tm*)
Print["inverse of x-intercept = Tm = ",
 tm = 1 / (( 0 - lm2["BestFitParameters"][[1]]) / lm2["BestFitParameters"][[2]])]
```

Out[17]=




```
inverse of x-intercept = Tm = 47.9064
```

Question 2

In[19]:=
```
(*part b of this question needs the b/a thing that
   gets Keq and then you get dG from that. Do dG vs x where the y-
  int is dgh20. Get dG by doing the dG = -RTln(k) equation*)
chemdenat1 = Transpose[Transpose[Import[
       "/Users/Research/JHU_Class_Material/pchem/assignment_5/chemdenatdata1",
       "Data"]][[3 ;;]]][[1]];
```

In[20]:=
```
(*store the raw data plot*)
chemdenat1plot =
  ListPlot[chemdenat1, PlotRange → All, AxesLabel → {"[GdnHCl]", "fluorescence"}];
```

In[21]:=
```
(*values and functions needed to get best fit curve*)
R = 0.0019872041;
T = 288.15;
dg = dgh2o + m * denat;
k = Exp[-dg / (R * T)];
fn = k / (1 + k);
fd = 1 / (1 + k);
yn = an + bn * denat;
yd = ad + bd * denat;
yobs = fn * yn + fd * yd;
```

In[30]:=
```
(*get the best fit line using some guesses from
 the raw data graph and copying what Doug did in class*)
nlmchemdenat1 = NonlinearModelFit[chemdenat1, yobs,
   {
    {an, 8},
    {bn, -0.25},
    {ad, 1},
    {bd, -0.02},
    {dgh2o, 0},
    {m, 0}
   },
   denat];
```

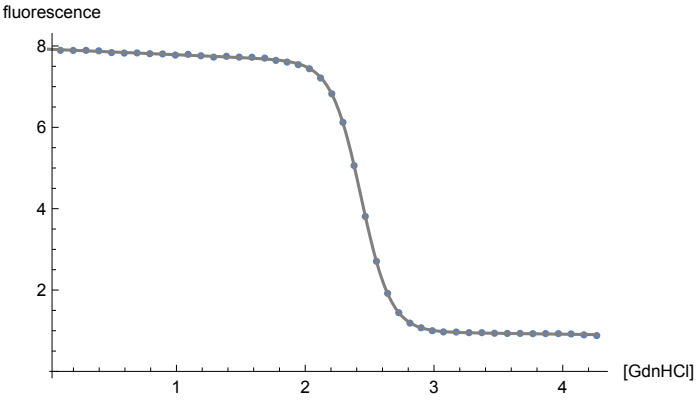
In[31]:=
```
(*check the parameters*)
nlmchemdenat1["ParameterTable"]
```

Out[31]=

	Estimate	Standard Error	t-Statistic	P-Value
an	7.9214	0.00590286	1341.96	1.40399×10^{-92}
bn	−0.13738	0.00496016	−27.6966	2.91735×10^{-27}
ad	1.08241	0.0277132	39.0577	6.98662×10^{-33}
bd	−0.0418501	0.00770027	−5.43488	3.15101×10^{-6}
dgh2o	−12.1427	0.0599425	−202.572	1.46199×10^{-60}
m	4.9885	0.0247218	201.786	1.70121×10^{-60}

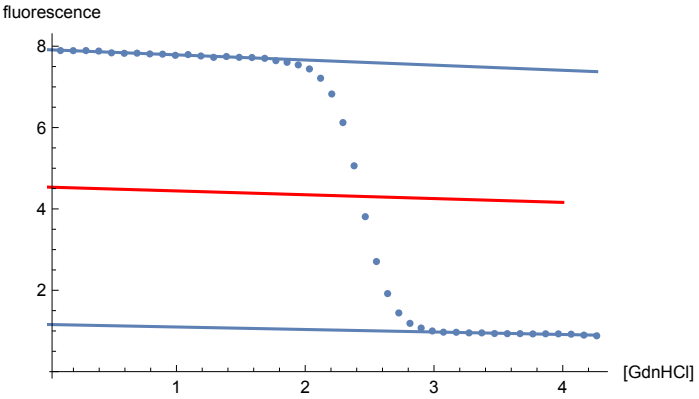
In[32]:=
```
(*graph the best fit line over the raw data*)
Show[chemdenat1plot,
 Plot[nlmchemdenat1[denat], {denat, 0, Max[chemdenat1[[All, 1]]]}, PlotStyle → Gray]]
```

Out[32]=



In[33]:=
```
(*native baseline uses the first few points*)
lnchemdenat1 = LinearModelFit[chemdenat1[[1 ;; 17]], x, x];
fnchemdenat1[x_] := lnchemdenat1["BestFitParameters"][[1]] +
    (lnchemdenat1["BestFitParameters"][[2]] * x);
(*unfolded baseline uses the last few points*)
luchemdenat1 = LinearModelFit[chemdenat1[[-13 ;;]], x, x];
fuchemdenat1[x_] := luchemdenat1["BestFitParameters"][[1]] +
    (luchemdenat1["BestFitParameters"][[2]] * x);
(*The midpoint line is halfway between the equations
 that describe the fn and fu lines*)
lmchemdenat1 = Table[{x, ((lnchemdenat1[x] - luchemdenat1[x]) / 2) + luchemdenat1[x]},
    {x, 0, Max[chemdenat1[[All, 1]]]}];
Show[chemdenat1plot, Plot[lnchemdenat1[x], {x, 0, Max[chemdenat1[[All, 1]]]}],
 Plot[luchemdenat1[x], {x, 0, Max[chemdenat1[[All, 1]]]}],
 ListLinePlot[lmchemdenat1, PlotStyle → Red]]
```

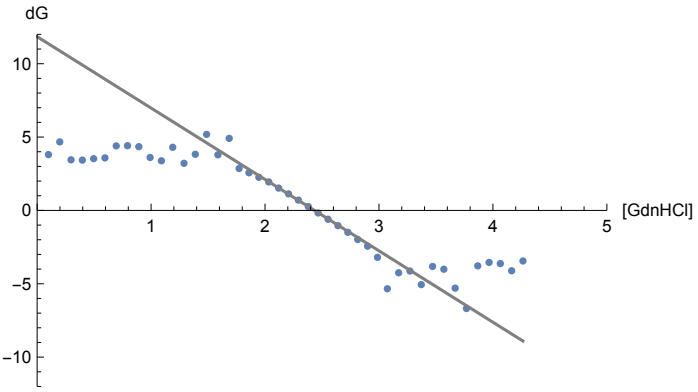
Out[38]=



In[39]:=
```
(*b is the fraction native fit minus the y data*)
bchemdenat1 = fnchemdenat1[chemdenat1[[All, 1]]] - chemdenat1[[All, 2]];
(*a is the y data minus the fraction unfolded fit*)
achemdenat1 = chemdenat1[[All, 2]] - fuchemdenat1[chemdenat1[[All, 1]]];
(*get x1 y1 where x is [GdnHCl] and y is -RTln(b/a)  (b/a = fu/fn = Keq)*)
dgvschemdenat1 =
  Transpose[{chemdenat1[[All, 1]], -R * T * Re[Log[bchemdenat1 / achemdenat1]]}];
(*we know dGh2o is around -12*)
dgvschemdenat1p = ListPlot[dgvschemdenat1,
   AxesLabel → {"[GdnHCl]", "dG"}, PlotRange → {{0, 5}, {-12, 12}}];
```

In[43]:=
```
(*get the best fit line of the dG vs [GdnHCl] plot where it is most linear
 (where it is unfolding and you're getting the actual b/a values)*)
dgvschemdenat1fit = LinearModelFit[dgvschemdenat1[[21 ;; 26]], x, x];
Show[dgvschemdenat1p,
 Plot[dgvschemdenat1fit[denat], {denat, 0, Max[chemdenat1[[All, 1]]]},
  PlotStyle → Gray, PlotRange → {{0, 5}, {-12, 12}}]]
Print["dG is about ", dgvschemdenat1fit[0]]
```

Out[44]=




```
dG is about 11.8424
```

Question 5

In[46]:=
```
(*normalized the chemdenat1 data from Q2*)
min = Min[chemdenat1[[All, 2]]];
max = Max[chemdenat1[[All, 2]]];
fluornorm = Table[ (y - min) / (max - min), {y, chemdenat1[[All, 2]]}];
chemdenat1norm = Transpose[{chemdenat1[[All, 1]], fluornorm}];
chemdenat1normp =
  ListPlot[chemdenat1norm, AxesLabel → {"[GdnHCl]", "Fluorescence normed"}];
```

In[51]:=
```
(*fit the data again*)
(*get the best fit line using some guesses from
 the raw data graph and copying what Doug did in class*)
nlmchemdenat1normfit = NonlinearModelFit[chemdenat1norm, yobs,
   {
    {an, 1},
    {bn, -0.25},
    {ad, 0.1},
    {bd, -0.02},
    {dgh2o, 0},
    {m, 0}
   },
   denat];
nlmchemdenat1normfit["ParameterTable"]
Print["dGh2o and m did not change with normalizing the data"]
```

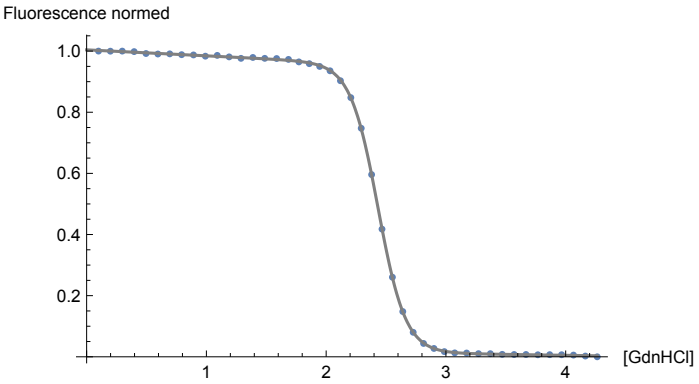
Out[52]=

	Estimate	Standard Error	t-Statistic	P-Value
an	0.0287102	0.00395245	7.2639	9.33021×10^{-9}
bn	−0.00596866	0.00109821	−5.43488	3.15101×10^{-6}
ad	1.00409	0.000841865	1192.69	1.39492×10^{-90}
bd	−0.0195931	0.000707418	−27.6966	2.91735×10^{-27}
dgh2o	12.1427	0.0599425	202.572	1.46199×10^{-60}
m	−4.9885	0.0247218	−201.786	1.70121×10^{-60}

```
dGh2o and m did not change with normalizing the data
```

In[54]:=
```
(*plot the fit data along the normalized data*)
Show[chemdenat1normp, Plot[nlmchemdenat1normfit[denat],
  {denat, 0, Max[chemdenat1norm[[All, 1]]]}, PlotStyle → Gray]]
```

Out[54]=

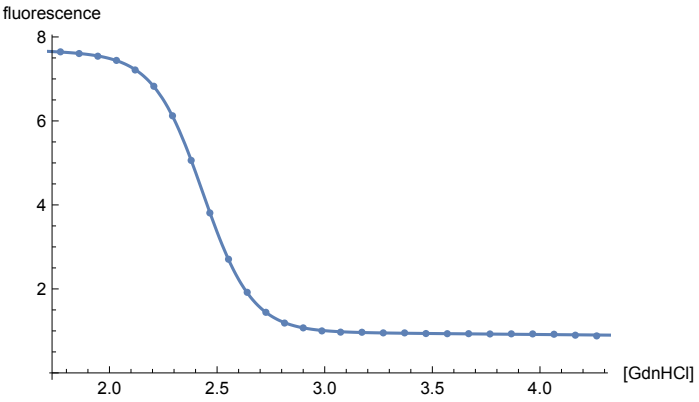


Question 6

In[342]:=
```
(*
(*remove points on the native side*)
*)
chemdenat1removen = chemdenat1[[18 ;;]];
(*native baseline uses the first few points*)
lnchemdenat1rn = LinearModelFit[chemdenat1removen[[1 ;; 5]], x, x];
fnchemdenat1rn[x_] := lnchemdenat1rn["BestFitParameters"][[1]] +
   (lnchemdenat1rn["BestFitParameters"][[2]] * x);
(*The midpoint line is halfway between the equations
 that describe the fn and fu lines*)
lmchemdenat1nend =
  Table[ {x, ((lnchemdenat1rn[x] - luchemdenat1[x]) / 2) + luchemdenat1[x]},
   {x, 0, Max[chemdenat1removen[[All, 1]]]}];
Print["Removing data from the N end. I thought it was supposed
   to have a large effect on dG, but it doesn't seem to"]
Show[ListPlot[chemdenat1removen], Plot[lnchemdenat1rn[x],
   {x, 0, Max[chemdenat1removen[[All, 1]]]}, PlotStyle → Gray],
  Plot[luchemdenat1[x], {x, 0, Max[chemdenat1removen[[All, 1]]]}],
  ListLinePlot[lmchemdenat1nend, PlotStyle → Red],
  AxesLabel → {"[GdnHCl]", "Fluorescence"}];
(*get the best fit line using some guesses from the raw
 data graph and copying what Doug did in class*)
nlmchemdenat1nend = NonlinearModelFit[chemdenat1removen, yobs,
   {
    {an, 8},
    {bn, -0.25},
    {ad, 1},
    {bd, -0.02},
    {dgh2o, 0},
    {m, 0}
   },
   denat];
(*show the fit*)
Show[ListPlot[chemdenat1removen, AxesLabel → {"[GdnHCl]", "fluorescence"}],
 Plot[nlmchemdenat1nend[x], {x, 0, 5}]]
nlmchemdenat1nend["ParameterTable"]
```

```
Removing data from the N end. I thought it was
  supposed to have a large effect on dG, but it doesn't seem to
```

Out[349]=



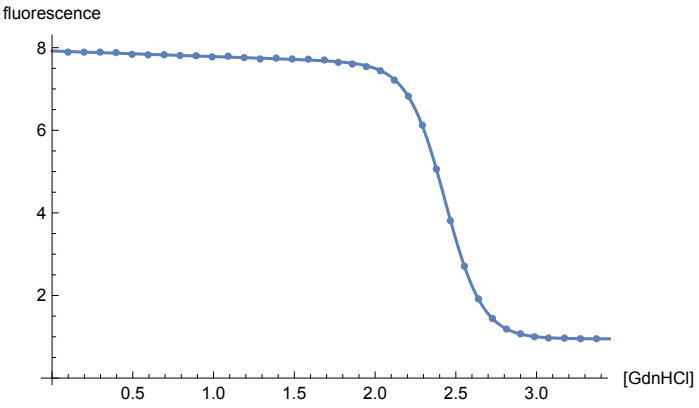
Out[350]=

	Estimate	Standard Error	t-Statistic	P-Value
an	7.8968	0.0913564	86.4395	2.35136×10^{-29}
bn	−0.133463	0.0486392	−2.74395	0.0118472
ad	1.09535	0.0216658	50.5564	2.95206×10^{-24}
bd	−0.045235	0.00598201	−7.56184	1.48439×10^{-7}
dgh2o	−12.2268	0.0711495	−171.847	6.54492×10^{-36}
m	5.02191	0.0277267	181.122	2.0607×10^{-36}

```
(*
(*repeating the same exact thing but from the U side...*)
*)
chemdenat1removeu = chemdenat1[[ ;; -10]];
(*native baseline uses the first few points*)
luchemdenat1ru = LinearModelFit[chemdenat1removeu[[-5 ;;]], x, x];
fuchemdenat1ru[x_] := luchemdenat1ru["BestFitParameters"][[1]] +
   (luchemdenat1ru["BestFitParameters"][[2]] * x);
(*The midpoint line is halfway between the equations
 that describe the fn and fu lines*)
lmchemdenat1uend =
  Table[{x, ((lnchemdenat1[x] - luchemdenat1ru[x]) / 2) + luchemdenat1ru[x]},
   {x, 0, Max[chemdenat1removeu[[All, 1]]]}];
Print["Removing data from the U end. I thought it was supposed
   to have a large effect on dG, but it doesn't seem to"]
Show[ListPlot[chemdenat1removeu], Plot[lnchemdenat1[x],
   {x, 0, Max[chemdenat1removeu[[All, 1]]]}], Plot[luchemdenat1ru[x],
   {x, 0, Max[chemdenat1removeu[[All, 1]]]}, PlotStyle → Gray],
  ListLinePlot[lmchemdenat1uend, PlotStyle → Red],
  AxesLabel → {"[GdnHCl]", "Fluorescence"}];
(*get the best fit line using some guesses from the raw
 data graph and copying what Doug did in class*)
nlmchemdenat1uend = NonlinearModelFit[chemdenat1removeu, yobs,
   {
    {an, 8},
    {bn, -0.25},
    {ad, 1},
    {bd, -0.02},
    {dgh2o, 0},
    {m, 0}
   },
   denat];
(*plot the fit*)
Show[ListPlot[chemdenat1removeu, AxesLabel → {"[GdnHCl]", "fluorescence"}],
 Plot[nlmchemdenat1uend[x], {x, 0, 5}]]
nlmchemdenat1uend["ParameterTable"]
```

```
Removing data from the U end. I thought it was
  supposed to have a large effect on dG, but it doesn't seem to
```

Out[366]=



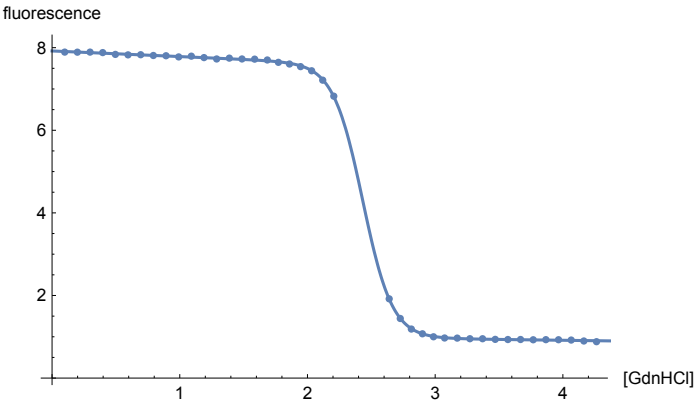
Out[367]=

	Estimate	Standard Error	t-Statistic	P-Value
an	7.92035	0.00608208	1302.24	7.51123×10^{-73}
bn	−0.135894	0.00517608	−26.2541	2.96334×10^{-22}
ad	0.963787	0.0955203	10.0899	3.71315×10^{-11}
bd	−0.00418396	0.0304828	−0.137257	0.891745
dgh2o	−12.0849	0.0718168	−168.274	3.38373×10^{-46}
m	4.96262	0.030426	163.105	8.61926×10^{-46}

In[377]:=

```
(*
(*and again, we do this exact same thing but now in the middle*)
*)
(*native baseline uses the first few points*)
chemdenat1removemid = Drop[chemdenat1, {24, 27}];
lnchemdenat1rmid = LinearModelFit[chemdenat1removemid[[1 ;; 17]], x, x];
fnchemdenat1rmid[x_] := lnchemdenat1rmid["BestFitParameters"][[1]] +
   (lnchemdenat1rmid["BestFitParameters"][[2]] * x);
(*unfolded baseline uses the last few points*)
luchemdenat1rmid = LinearModelFit[chemdenat1removemid[[-13 ;;]], x, x];
fuchemdenat1rmid[x_] := luchemdenat1rmid["BestFitParameters"][[1]] +
   (luchemdenat1rmid["BestFitParameters"][[2]] * x);
(*The midpoint line is halfway between the equations
 that describe the fn and fu lines*)
lmchemdenat1rmid =
  Table[{x, ((lnchemdenat1rmid[x] - luchemdenat1rmid[x]) / 2) + luchemdenat1rmid[x]},
   {x, 0, Max[chemdenat1removemid[[All, 1]]]}];
Show[ListPlot[chemdenat1removemid], Plot[lnchemdenat1rmid[x],
   {x, 0, Max[chemdenat1removemid[[All, 1]]]}],
  Plot[luchemdenat1rmid[x], {x, 0, Max[chemdenat1removemid[[All, 1]]]}],
  ListLinePlot[lmchemdenat1rmid, PlotStyle → Red],
  AxesLabel → {"[GdnHCl]", "Fluorescence"}];
nlmchemdenat1mid = NonlinearModelFit[chemdenat1removemid, yobs,
   {
    {an, 8},
    {bn, -0.25},
    {ad, 1},
    {bd, -0.02},
    {dgh2o, 0},
    {m, 0}
   },
   denat];
(*plot the fit*)
Show[ListPlot[chemdenat1removemid, AxesLabel → {"[GdnHCl]", "fluorescence"}],
 Plot[nlmchemdenat1mid[x], {x, 0, 5}]]
nlmchemdenat1mid["ParameterTable"]
```

Out[385]=



Out[386]=

	Estimate	Standard Error	t-Statistic	P-Value
an	7.92076	0.00617385	1282.95	2.29331×10^{-83}
bn	−0.136425	0.0053781	−25.3668	4.04598×10^{-24}
ad	1.07714	0.0305373	35.2729	6.05902×10^{-29}
bd	−0.0404775	0.008419	−4.80787	0.0000286252
dgh2o	−12.0978	0.079042	−153.055	4.64814×10^{-51}
m	4.97077	0.0322851	153.965	3.77885×10^{-51}

Question 8

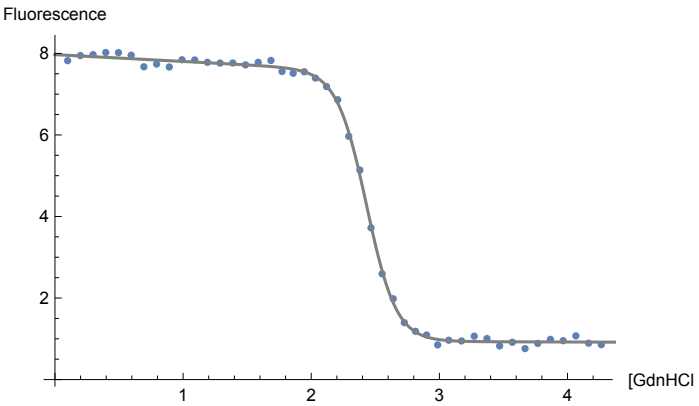
In[222]:=

```
(*introduce random error into the y-values of chemdenat1*)
chemdenat1error = Transpose[{chemdenat1[[All, 1]], chemdenat1[[All, 2]] +
     RandomVariate[NormalDistribution[0, 0.08], Length[chemdenat1]]}];
chemdenat1errorp = ListPlot[chemdenat1error,
   AxesLabel → {"[GdnHCl", "Fluorescence"}];
```

In[224]:=
```
(*get all the baseline and midpoint line data things*)
(*native baseline uses the first few points*)
lnchemdenat1error = LinearModelFit[chemdenat1error[[1 ;; 17]], x, x];
fnchemdenat1error[x_] := lnchemdenat1error["BestFitParameters"][[1]] +
   (lnchemdenat1error["BestFitParameters"][[2]] * x);
(*unfolded baseline uses the last few points*)
luchemdenat1error = LinearModelFit[chemdenat1error[[-13 ;;]], x, x];
fuchemdenat1error[x_] := luchemdenat1error["BestFitParameters"][[1]] +
   (luchemdenat1error["BestFitParameters"][[2]] * x);
(*The midpoint line is halfway between the equations
 that describe the fn and fu lines*)
lmchemdenat1error = Table[
   {x, ((lnchemdenat1error[x] - luchemdenat1error[x]) / 2) + luchemdenat1error[x]},
   {x, 0, Max[chemdenat1error[[All, 1]]]}];
Show[chemdenat1errorp, Plot[lnchemdenat1error[x],
   {x, 0, Max[chemdenat1error[[All, 1]]]}],
  Plot[luchemdenat1error[x], {x, 0, Max[chemdenat1error[[All, 1]]]}],
  ListLinePlot[lmchemdenat1error, PlotStyle → Red]];
```

In[234]:=
```
nlmchemdenat1errorfit = NonlinearModelFit[chemdenat1error, yobs,
   {
    {an, 8},
    {bn, -0.25},
    {ad, 1},
    {bd, -0.02},
    {dgh2o, 0},
    {m, 0}
   },
   denat];
Show[chemdenat1errorp, Plot[nlmchemdenat1errorfit[x], {x, 0, 5}, PlotStyle → Gray]]
```

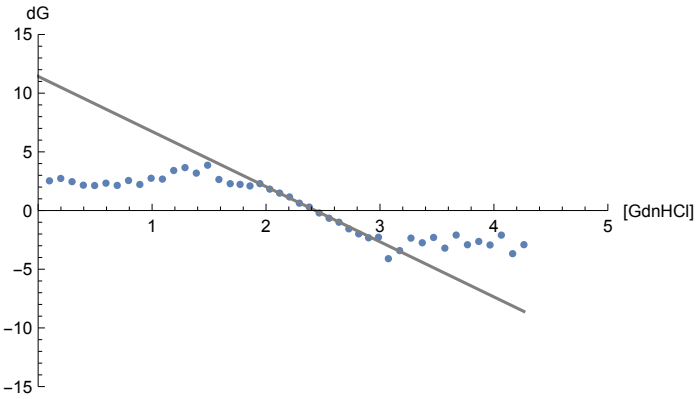
Out[235]=



In[240]:=
```
(*b is the fraction native fit minus the y data*)
bchemdenat1error =
  fnchemdenat1[chemdenat1error[[All, 1]]] - chemdenat1error[[All, 2]];
(*a is the y data minus the fraction unfolded fit*)
achemdenat1error =
  chemdenat1error[[All, 2]] - fuchemdenat1[chemdenat1error[[All, 1]]];
(*get x1 y1 where x is [GdnHCl] and y is -RTln(b/a)  (b/a = fu/fn = Keq)*)
dgvschemdenat1error = Transpose[{chemdenat1error[[All, 1]],
    -R * T * Re[Log[bchemdenat1error / achemdenat1error]]}];
(*we know dGh2o is around -12*)
dgvschemdenat1errorp = ListPlot[dgvschemdenat1error,
   AxesLabel → {"[GdnHCl]", "dG"}, PlotRange → {{0, 5}, {-15, 15}}];
```

In[244]:=
```
(*get the best fit line of the dG vs [GdnHCl] plot where it is most linear
 (where it is unfolding and you're getting the actual b/a values)*)
dgvschemdenat1errorfit = LinearModelFit[dgvschemdenat1error[[20 ;; 26]], x, x];
Show[dgvschemdenat1errorp,
 Plot[dgvschemdenat1errorfit[denat], {denat, 0, Max[chemdenat1error[[All, 1]]]},
  PlotStyle → Gray, PlotRange → {{0, 5}, {-15, 15}}]]
dgvschemdenat1errorfit["ParameterTable"]
Print["dG is about ", dgvschemdenat1errorfit[0]]
```

Out[245]=



Out[246]=

	Estimate	Standard Error	t-Statistic	P-Value
1	11.4314	0.279818	40.8528	1.65733×10^{-7}
x	−4.69774	0.126449	−37.1514	2.66112×10^{-7}

```
dG is about 11.4314
```

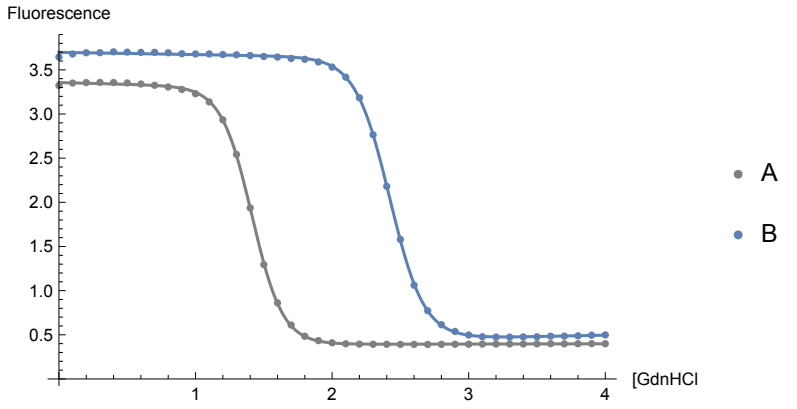
Question 9

In[96]:=
```
(*import and split apart the data*)
chemdenat2 = Transpose[Transpose[Import[
        "/Users/Research/JHU_Class_Material/pchem/assignment_5/chemdenatdata2",
        "Data"]][[3 ;;]]][[1]];
chemdenat2A = Transpose[{chemdenat2[[All, 1]], chemdenat2[[All, 2]]}][[1 ;; 41]];
chemdenat2Ap =
  ListPlot[chemdenat2A, PlotRange → All, PlotStyle → Gray, PlotLegends → {"A"}];
chemdenat2B = Transpose[{chemdenat2[[All, 1]], chemdenat2[[All, 3]]}][[1 ;; 41]];
chemdenat2Bp = ListPlot[chemdenat2B, PlotRange → All, PlotLegends → {"B"}];
```

In[101]:=
```
(*get the best fit line for A using some guesses from
 the raw data graph and copying what Doug did in class*)
nlmchemdenat2A = NonlinearModelFit[chemdenat2A, yobs,
   {
    {an, 3.6},
    {bn, -0.25},
    {ad, 0.5},
    {bd, -0.02},
    {dgh2o, 0},
    {m, 0}
   },
   denat];
nlmchemdenat2Ap =
  Plot[nlmchemdenat2A[denat], {denat, 0, 4}, PlotRange → All, PlotStyle → Gray];
(*get the best fit line for B using some guesses from the
 raw data graph and copying what Doug did in class*)
nlmchemdenat2B = NonlinearModelFit[chemdenat2B, yobs,
   {
    {an, 3.3},
    {bn, -0.25},
    {ad, 0.5},
    {bd, -0.02},
    {dgh2o, 0},
    {m, 0}
   },
   denat];
nlmchemdenat2Bp = Plot[nlmchemdenat2B[denat], {denat, 0, 4}, PlotRange → All];
```

In[105]:=
```
(*
(*overlay the raw data and the best fit lines*)
*)
Show[chemdenat2Ap, chemdenat2Bp, nlmchemdenat2Ap, nlmchemdenat2Bp,
 PlotRange → All, AxesLabel → {"[GdnHCl", "Fluorescence"}]
```

Out[105]=



In[106]:=
```
(* for A
(*native baseline uses the first few points*)
*)
lnchemdenat2A = LinearModelFit[chemdenat2A[[3 ;; 6]], x, x];
fnchemdenat2A[x_] := lnchemdenat2A["BestFitParameters"][[1]] +
    (lnchemdenat2A["BestFitParameters"][[2]] * x);
(*unfolded baseline uses the last few points*)
luchemdenat2A = LinearModelFit[chemdenat2A[[-5 ;;]], x, x];
fuchemdenat2A[x_] := luchemdenat2A["BestFitParameters"][[1]] +
    (luchemdenat2A["BestFitParameters"][[2]] * x);
(*The midpoint line is halfway between the equations
 that describe the fn and fu lines*)
lmchemdenat2A =
  Table[ {x, ((lnchemdenat2A[x] - luchemdenat2A[x]) / 2) + luchemdenat2A[x]},
   {x, 0, Max[chemdenat2A[[All, 1]]]}];
Show[chemdenat2Ap, Plot[lnchemdenat2A[x], {x, 0, Max[chemdenat2A[[All, 1]]]}],
  Plot[luchemdenat2A[x], {x, 0, Max[chemdenat2A[[All, 1]]]}],
  ListLinePlot[lmchemdenat2A, PlotStyle → Red]];
```

In[112]:=
```
(* for B
(*native baseline uses the first few points*)
*)
lnchemdenat2B = LinearModelFit[chemdenat2B[[6 ;; 8]], x, x];
fnchemdenat2B[x_] := lnchemdenat2B["BestFitParameters"][[1]] +
    (lnchemdenat2B["BestFitParameters"][[2]] * x);
(*unfolded baseline uses the last few points*)
luchemdenat2B = LinearModelFit[chemdenat2B[[-4 ;;]], x, x];
fuchemdenat2B[x_] := luchemdenat2B["BestFitParameters"][[1]] +
    (luchemdenat2B["BestFitParameters"][[2]] * x);
(*The midpoint line is halfway between the equations
 that describe the fn and fu lines*)
lmchemdenat2B =
  Table[ {x, ((lnchemdenat2B[x] - luchemdenat2B[x]) / 2) + luchemdenat2B[x]},
    {x, 0, Max[chemdenat2B[[All, 1]]]}];
Show[chemdenat2Bp, Plot[lnchemdenat2B[x], {x, 0, Max[chemdenat2B[[All, 1]]]}],
  Plot[luchemdenat2B[x], {x, 0, Max[chemdenat2B[[All, 1]]]}],
  ListLinePlot[lmchemdenat2B, PlotStyle → Red]];
```

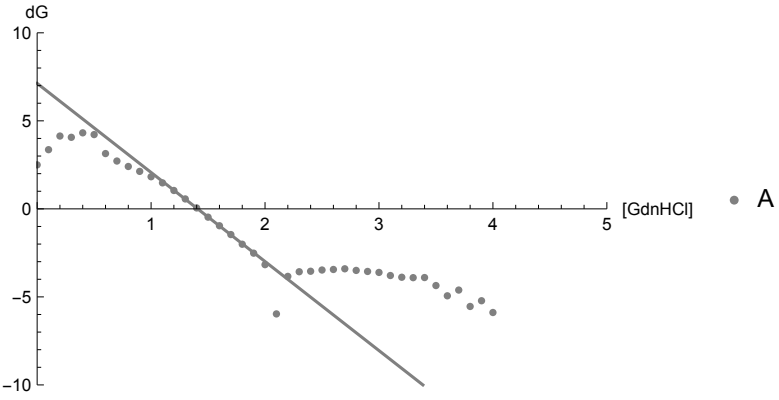
In[286]:=
```
(* for A
(*b is the fraction native fit minus the y data*)
*)
bchemdenat2A = fnchemdenat2A[chemdenat2A[[All, 1]]] - chemdenat2A[[All, 2]];
(*a is the y data minus the fraction unfolded fit*)
achemdenat2A = chemdenat2A[[All, 2]] - fuchemdenat2A[chemdenat2A[[All, 1]]];
(*get x1 y1 where x is [GdnHCl] and y is -RTln(b/a)  (b/a = fu/fn = Keq)*)
dgvschemdenat2A =
  Transpose[{chemdenat2A[[All, 1]], -R * T * Re[Log[bchemdenat2A / achemdenat2A]]}];
dgvschemdenat2Ap = ListPlot[dgvschemdenat2A, AxesLabel → {"[GdnHCl]", "dG"},
    PlotRange → {{0, 5}, {-10, 10}}, PlotStyle → Gray, PlotLegends → {"A"}];
```

In[290]:=
```
(* for B
(*b is the fraction native fit minus the y data*)
*)
bchemdenat2B = fnchemdenat2B[chemdenat2B[[All, 1]]] - chemdenat2B[[All, 2]];
(*a is the y data minus the fraction unfolded fit*)
achemdenat2B = chemdenat2B[[All, 2]] - fuchemdenat2B[chemdenat2B[[All, 1]]];
(*get x1 y1 where x is [GdnHCl] and y is -RTln(b/a)  (b/a = fu/fn = Keq)*)
dgvschemdenat2B =
  Transpose[{chemdenat2B[[All, 1]], -R * T * Re[Log[bchemdenat2B / achemdenat2B]]}];
dgvschemdenat2Bp = ListPlot[dgvschemdenat2B, AxesLabel → {"[GdnHCl]", "dG"},
    PlotRange → {{0, 5}, {-10, 10}}, PlotLegends → {"B"}];
```

In[294]:=

```
(* for A
(*get the best fit line of the dG vs [GdnHCl] plot where it is most linear
 (where it is unfolding and you're getting the actual b/a values)*)
*)
dgvschemdenat2Afit = LinearModelFit[dgvschemdenat2A[[13 ;; 16]], x, x];
Show[dgvschemdenat2Ap,
 Plot[dgvschemdenat2Afit[denat], {denat, 0, Max[chemdenat2A[[All, 1]]]},
  PlotRange → {{0, 5}, {-10, 10}}, PlotStyle → Gray]]
Print["dG for A is about ", dgvschemdenat2Afit[0]]
```

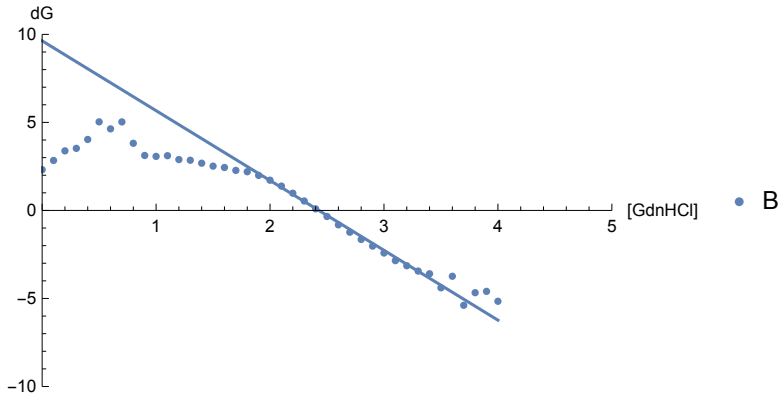
Out[295]=




```
dG for A is about 7.12687
```

In[280]:=
```
(* for B
(*get the best fit line of the dG vs [GdnHCl] plot where it is most linear
 (where it is unfolding and you're getting the actual b/a values)*)
*)
dgvschemdenat2Bfit = LinearModelFit[dgvschemdenat2B[[20 ;; 26]], x, x];
Show[dgvschemdenat2Bp, Plot[dgvschemdenat2Bfit[denat],
  {denat, 0, Max[chemdenat2B[[All, 1]]]}, PlotRange → Full]]
Print["dG for B is about ", dgvschemdenat2Bfit[0]]
```

Out[281]=




```
dG for B is about 9.63316
```