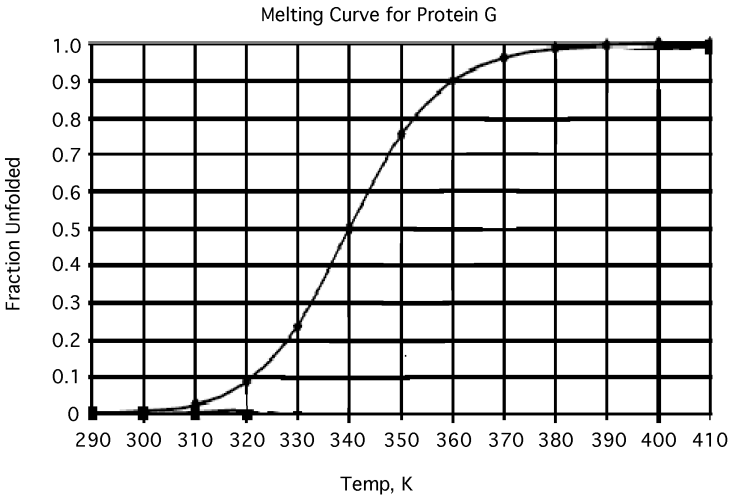
Problem in Protein Thermodynamics:

Sample Question: Determine ΔH and ΔS for the unfolding of Protein G from the melting data.



$$\Delta G = \Delta H - T\Delta S$$

$$\Delta G = -RT\ln\frac{[U]}{[N]} = -RT\ln K_{EQ}$$

$$f_N = \frac{[N]}{[N]+[U]} = \frac{1}{1+K_{EQ}}$$

$$f_U = \frac{[U]}{[N]+[U]} = \frac{K_{EQ}}{1+K_{EQ}}$$

Steps:

1. Vary temperature, record temperature and fraction folded (f_N).
2. Convert temperature from C to K if necessary (K=C+273).
3. Calculate fraction unfolded, f_U. ($f_U=1-f_N$).
4. Calculate K_{EQ} ($K_{EQ}=f_U/f_N$).
5. Plot ln K_{EQ} versus 1/T (K).
6. Use the graphing wizard in Excel (scatter plot).
7. Select plotted data with mouse.
8. Under chart options, select “Add Trendline”.
9. Use linear, under “Options”, select “Display linear equation on chart”.

Slope = -ΔH/R or
ΔH = -slope x 8.3 J/mol-K

The slope of the line is –12,685.
Therefore ΔH=-(-12,685) x 8.3 J/mol-degK=**105 kJ/mol**.

ΔS=ΔH/TM.
Obtain T_M from melting curve at f_U=0.5.

T_M is 340 K.

Thus ΔS=105,000 J/mol / 340 degK = **308 J/mol-degK**.

T (K)	fU/ fN	KEQ	1/T	ln KEQ
330	0.25/0.75	0.33	0.0030303	-1.09861229
340	0.5/ 0.5	1	0.0029411	0
350	0.75/0.25	3	0.0028571	1.09861229