Problem 1. Consider a hypothetic reaction A $\rightleftarrows$ B that takes place at 25°C. The reaction started with 180 mM of compound A and no B. The reaction reached the equilibrium when the molar concentration of A dropped to one-sixth of the initial concentration.

(A) (4 points) Determine the equilibrium constant for the forward reaction.
Using the mass conservation law, at the equilibrium point:

$[A]_{eq}$ = 30 mM, $[B]_{eq}$ = 180 mM – 30 mM = 150 mM. This gives $K_{eq} = [B]_{eq} /[A]_{eq} = 5$.

(B) (4 points) Determine the value of ΔG^0 for the forward reaction.

$\Delta G^0 = - RT\times\ln([B]_{eq}/[A]_{eq}) = -RT\times\ln 5 = -3.987\times10^3$ J/mol $\approx$ - 4kJ/mol

(C) (6 points) Calculate the molar concentrations of A and B at the time point in the reaction when the ΔG for the forward reaction was -3 kJ/mol.

From the equation $\Delta G= \Delta G^0 + RT*\ln([B]/[A])$ we get $[B]/[A]=\exp((\Delta G - \Delta G^0)/RT) = 1.489$. Combining this result with the mass conservation law, [A]+[B]=180 mM, we have the following equation: [B]/(180 mM - [B]) = 1.489. Solving it for [B] gives

[B]= 1.489/(1+1.489) × 180 mM = 107.68 ≈107.7; and [A]= 72.3 mM.

Problem 2. (6 points) You need to prepare 100 mL of 50 mM acetate buffer with pH 5.2. You do this by mixing pre-calculated amounts/volumes of acetic acid and sodium acetate with pure water. Calculate how many milliliters of 1M acetic acid and 1M sodium acetate you need for this.

The final concentrations of CH_3COOH and CH_3COO^- are related through the Henderson-Hasselbalch equation: $[CH_3COO^-]/[CH_3COOH] = 10^{pH-pKa} = 10^{5.2-4.76} \approx 2.75$. This gives

$[CH_3COO^-] = 2.75 \times [CH_3COOH]$, and because $[CH_3COO^-] + [CH_3COOH] =(1+2.75) \times [CH_3COOH]= 50$ mM, we obtain $[CH_3COOH]$=50 mM /3.75 = 13.3 mM and $[CH_3COO^-]$ = 36.7 mM.

Now let's determine the volumes of the initial 1000 mM stock solutions needed to have 100 mL of the final mixture with these concentrations.

$\text{Volume}_{[CH3COOH]} \times 1000$ mmol/L = 100 mL × 13.3 mmol/L ➔ $\text{Volume}_{[CH3COOH]}$ = (13.3/1000) ×100 mL = 1.33 mL

$\text{Volume}_{[CH3COO^-]} \times 1000$ mmol/L = 100 mL × 37.6 mmol/L ➔ $\text{Volume}_{[CH3COO^-]}$ = (36.7/1000) ×100 mL = 3.67 mL