Binding of doxorubicin to DNA

The free energy of binding of the anti-cancer drug doxorubicin to DNA is ΔG^{o} = -8.6 kcal/mol. Doxorubicin is administered at doses of 10^{-6} M and the effective DNA concentration in the nucleus 10^{-6} M. Calculate the concentration of bound doxorubicin-DNA complex at equilibrium. The binding reaction can be written as

Doxobucin + DNA → Doxorubicin-DNA

(Assume that T = 310 K and that 1 cal = 4.184 Joules)

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Solution: Use 310 K to calculate the equilibrium constant

$$\Delta G^o = 8600 \frac{cal}{mol} \times 4.184 \frac{Joules}{cal} = 36{,}000 \frac{J}{mol}$$

$$K = exp\left\{-\frac{\Delta G^o}{RT}\right\} = exp\left\{-\frac{-36000\ J/mol}{\left(8.31 \frac{J}{molK}\right)(310\ K)}\right\} = 1.17\ x10^6$$

Binding of doxorubicin to DNA

[Doxorubicin] = 10^{-6} M and [DNA] = 10^{-6} M. Calculate the concentration of bound doxorubicin-DNA complex at equilibrium. The binding reaction can be written as

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At equilibrium [Dox] = 10^{-6} –x, [DNA] = 10^{-6} –x and [Dox-DNA] = x

$$K = \frac{[\mathrm{Dox} - \mathrm{DNA}]}{[\mathrm{Dox}][\mathrm{DNA}]}$$

$$1.17\ x10^{6} = \frac{x}{[10^{-6} - x][10^{-6} - x]}$$

$$x = \frac{1.1 \pm \sqrt{1.1^{2} - 4(1.17 \times 10^{-7})(1.17\ x10^{6})}}{2(1.17\ x10^{6})} = 1.2\ x\ 10^{-7}\ M$$