QE equations summary

Equations originally derived by Schropp and colleagues.
Additional information provided in supplementary file S3 from Van De Vyver, Eigenmann and colleagues.

User input:

- C:	*the drug concentration of interest*	*nanomole/L*
- KD_1:	*the binding affinity to the tumor target*	*nanomole/L*
- KD_2:	*the binding affinity to CD3*	*nanomole/L*
- $Density_{receptors}$:	*the expression level of target per tumor cell*	*#/cell*
- $Density_{CD3}$:	*the expression level of CD3 per T cell*	*#/cell*
- $Concentration_{Tumor\_cells}$:	*the concentration of tumor cells*	*cells/uL*
- $Concentration_{T\text{-}cells}$:	*the concentration of T cells*	*cells/uL*

Calculating quasi-equilibrium trimer concentration

R^0_{tot} and $CD3^0_{tot}$ are the total tumor target and CD3 concentration at time 0, respectively. Receptor concentrations are calculated by multiplying the expression density with the total concentration of receptor expressing cells. These concentrations are converted into nmol/L through dividing by the Avogadro constant (N_a; $6.022*10^{23}$ molecules/mole):

$$Concentration_{Receptors} = \frac{Density_{Receptors} * Concentration_{cells}}{N_a} * 10^9$$

Quasi-Equilibrium calculations (Eq. S1-S7):

$$aa = (1 + \frac{C}{KD_1}) * \frac{C}{KD_1 * KD_2} \quad \text{(Eq. S1)}$$

$$bb = C * \frac{(R_0^{tot} - CD3_0^{tot})}{KD_1 * KD_2} + (1 + \frac{C}{KD_1}) * (1 + \frac{C}{KD_2}) \quad \text{(Eq. S2)}$$

$$dd = -CD3_0^{tot} * (1 + \frac{C}{KD_1}) \quad \text{(Eq. S3)}$$

Equations S1-S3 are required to calculate the concentration of free R and CD3 (Eq. S4-S6):

$$R = \frac{R_{tot}^0}{1 + \frac{C}{KD_1} + \frac{CD3 * C}{KD_1 * KD_2}} \quad \text{(Eq. S4)}$$

$$CD3 = \frac{(-bb + \sqrt{(bb^2 - 4 * aa * dd)})}{2 * aa} \quad \text{(for C > 0)} \quad \text{(Eq. S5)}$$

$$CD3 = CD3_{tot}^0 \quad \text{(for C = 0)} \quad \text{(Eq. S6)}$$

$$Trimer = \frac{C * R * CD3}{KD_1 * KD_2} \quad \text{(Eq. S7)}$$