Exercise Sheet 1

1) Enzyme Reaction
Consider the following chemical reaction network (enzyme reaction), where the reaction rate constants are given by the arrow labels $k_1, k_2, k_3$.

\[ E + S \xrightleftharpoons[k_2]{k_1} C \xrightarrow{k_3} E + P. \]  

Derive the system of differential equations for the chemical concentrations of $E$, $S$, $C$ and $P$. Solve the resulting ODE system using Matlab’s `ode23` routine. Plot the solution for initial conditions $E(0) = 80$, $S(0) = 50$, $C(0) = P(0) = 0$ and parameters $t \in [0, 5)$, $k_1 = 0.1$, $k_2 = k_3 = 1$.

2) Conservation Laws
Consider again the enzyme reaction in Eq. (1). Note that the system is closed, i.e. molecules can neither “dissapear” nor “appear from nothing”. Derive algebraic equations (equations that relate the chemical concentrations without any time derivative) that reflect the conservation laws of the system where you assume the following initial concentrations: $E(0) = e_0$, $S(0) = s_0$, $C(0) = P(0) = 0$.

*Hint: Start with a very small example, i.e., $e_0 = 2$, $s_0 = 2$. Which relations between the molecule numbers do you observe. To prove the correctness of the conservation relations you have to sum up some of the rate equations.*

3) Production Rate Approximation  Consider the enzyme reaction in Eq. (1). Assume that the reactions $E + S \xrightleftharpoons[k_2]{k_1} C$ are very fast compared to $C \xrightarrow{k_3} E + P$ (this assumption is called quasi-steady-state assumption). Thus, these two reactions will quickly approach some (intermediate) steady-state value. According to this we assume that $C(t) \approx \text{const}$. Try to derive an approximation for the change of concentration of product $P$ that depends only on $S(t)$ and the total number of enzymes (enzyme molecules are either free or bound as a part of a complex).

*Hint: Exploit the algebraic relations you derived in 2) and set $\frac{d}{dt}C(t) = 0$.*

4) Lung cancer example
Consider the lung cancer example in the lecture notes (section on conditional probabilities). Compute the probability that a person who is not a smoker gets lung cancer. How much lower is it compared to smokers?