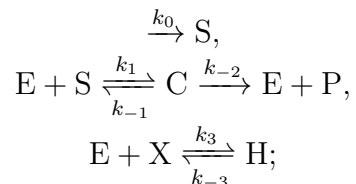# Chemistry 4000/5000/7000 Fall 2010 Assignment 4

Due: Friday, Oct. 8, 4:00 p.m.

Marks: 32

In this assignment, you will study the competitive inhibition system

$$\xrightarrow{k_0} S,$$
$$E + S \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} C \xrightarrow{k_{-2}} E + P,$$
$$E + X \underset{k_{-3}}{\overset{k_3}{\rightleftharpoons}} H;$$

with the following rate constants: $k_0 = 0.05\,\text{M/s}$, $k_1 = 10^7\,\text{M}^{-1}\text{s}^{-1}$, $k_{-1} = 10\,\text{s}^{-1}$, $k_{-2} = 100\,\text{s}^{-1}$, $k_3 = 10^4\,\text{M}^{-1}\text{s}^{-1}$, $k_{-3} = 0.1\,\text{s}^{-1}$, $E_0 = 1\,\text{mM}$, $X_0 = 2\,\text{mM}$. In the numerical work required, integrate your equations for at least $2000\,\text{s}$.

1. Provide your `xppaut` input file (electronic or printed) with your assignment. [2 marks]

2. A good numerical method for a problem would be reasonably fast and would reliably give an accurate numerical solution. Experiment with different numerical methods and step sizes and give a full report on your observations (what you tried, what happened, what works, what doesn't); then, recommend a numerical integration method (including a step size) for this system. [20 marks]

3. Study the effect of varying k_0, the rate at which the substrate is synthesized and report on your observations. [10 marks]