Question 2

2.1

The law of mass action can present interactions between molecules. The reaction rate is determined by number of collisions between reactants, together with the probability of any collision can result in molecular combinations.

Based on the law of mass action, four equations for the rate of changes of the four species, E, S, ES, and P can be expressed as the following:

$$\frac{dS}{dt} = k_2 * [ES] - k_1 * [S] * [E]$$

$$\frac{dE}{dt} = (k_2 + k_3) * [ES] - k_1 * [S] * [E]$$

$$\frac{dES}{dt} = k_1 * [S] * [E] - (k_3 + k_2) * [ES]$$

$$\frac{dP}{dt} = k_3 * [ES]$$

2.2

Note: the answer for this question is based on python.

```
### import all utilized packages
>>> from cmepy import model
>>> from cmepy.util import non_neg
>>> from cmepy import solver
>>> import numpy

### set the initial values for 4 variables
>>> s = 10
>>> e = 1
>>> es = 0
>>> p = 0
```

define the enzymatic reaction model with the given reaction rate *k1*=100/μM/min, *k2*=600/min, *k3*=150/min

```
m = model.create(
    name = 'enzyme kinetics',
    species = ('S', 'E', 'ES', 'P', ),
    species_counts = (s, e, es, p, ),
    reactions = ('E+S->ES', 'ES->E+S', 'ES->E+P', ),
    propensities = (
        lambda *x : 100*s(*x)*e(*x),
```

```
        lambda *x : 600*es(*x),
        lambda *x : 150*es(*x),
    ),
    transitions = (
        (-1, 1),
        (1, -1),
        (0, -1)
    ),
    shape = (s_0 + 1, min(s_0, e_0) + 1),
    initial_state = (s_0, 0)
)

### solve the defined model
enzyme_solver = solver.create(
    model = m,
    sink = False
)

### record the solutions
>>> species = ['S', 'E', 'ES', 'P']

r = recorder.create(
    (species, m.species_counts)
)

time_steps = numpy.linspace(0.0, 30.0, 101)

for t in time_steps:
    enzyme_solver.step(t)
    r.write(t, enzyme_solver.y)

### present the calculated results
>>> recorder.display_plots(r)
```

2.3

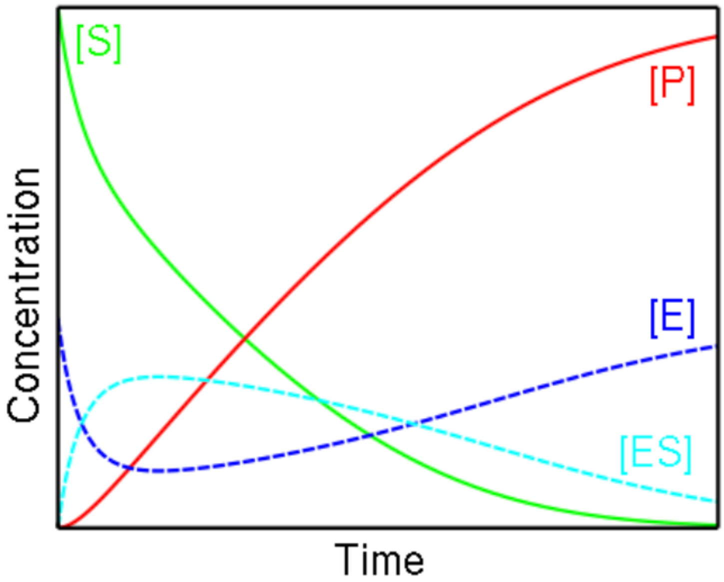
Based on the Michaelis-Menten equation:

$v = V_{max} / (1+(Km/[S]))$

The Lineweaver-Burk double reciprocal plot can rearrange the equation as:

$1/v = 1/V_{max} + Km/V_{max} * 1/[S]$

Therefore, the velocity plot can give the following conclusions.



Vmax = 1/y intercept = Km/gradient = -1/x intercept

Km can be calculated using the speed of reactions.

Km = (k2 + k3)/k1 = (600/μM/min + 150/μM/min) / 100/μM/min = 7.5

Then, V_{max} can be calculated using the following equation.

Km = (Vmax[S] - V[S])/ V

V_{max} = (Km * V + V * [S]) / [S]

= (7.5 * 150/μM/min + 150/μM/min * 10μM) / 10μM = 262.5/μM/min