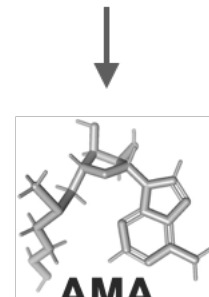
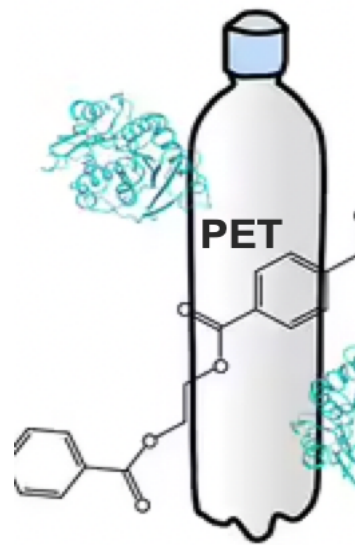
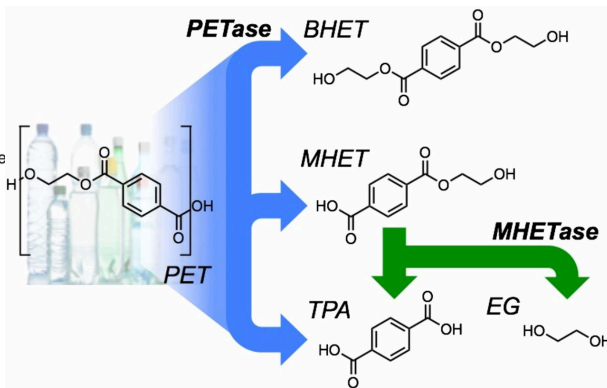
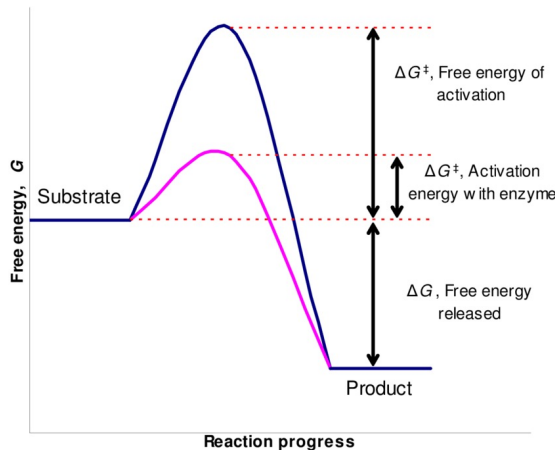


Background: Enzyme Engineering

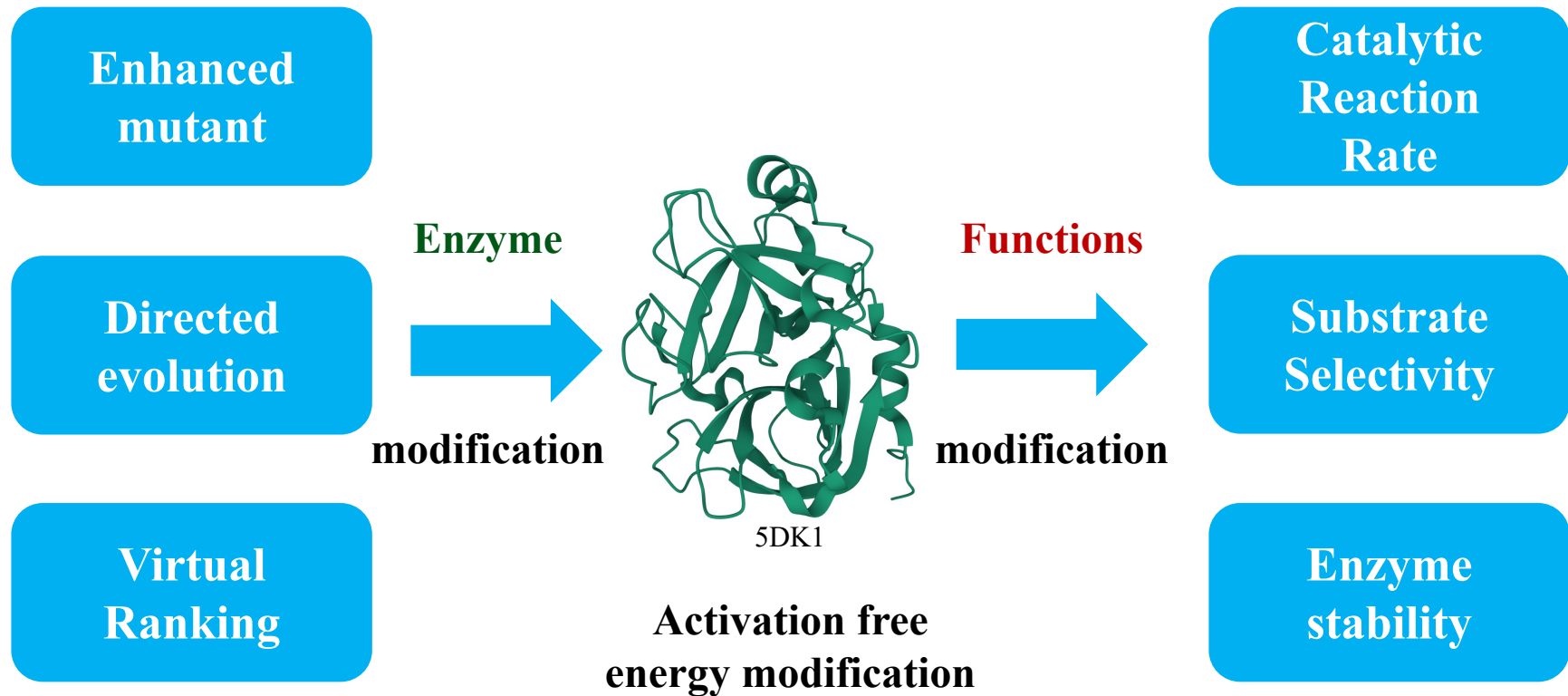
Enzymes are curial in Pharmaceutical and Envi
ronment Engineering such as **PET degradation**
and **anti-biotics syntheses**

Enzymes can make the biocatalytic reaction easier
by reducing the **reaction activation free energy**



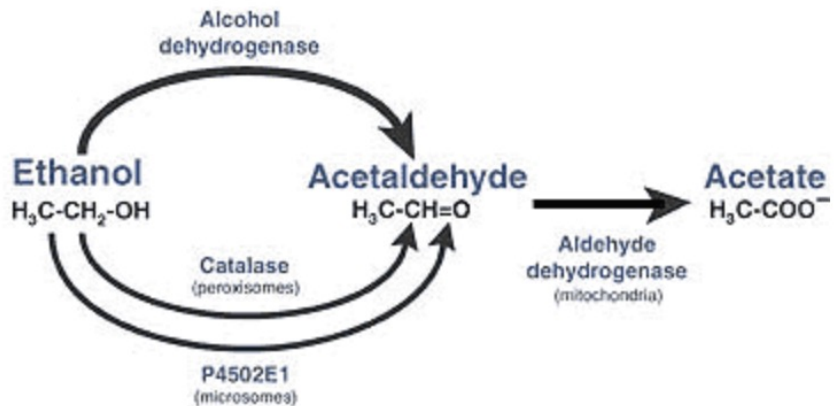
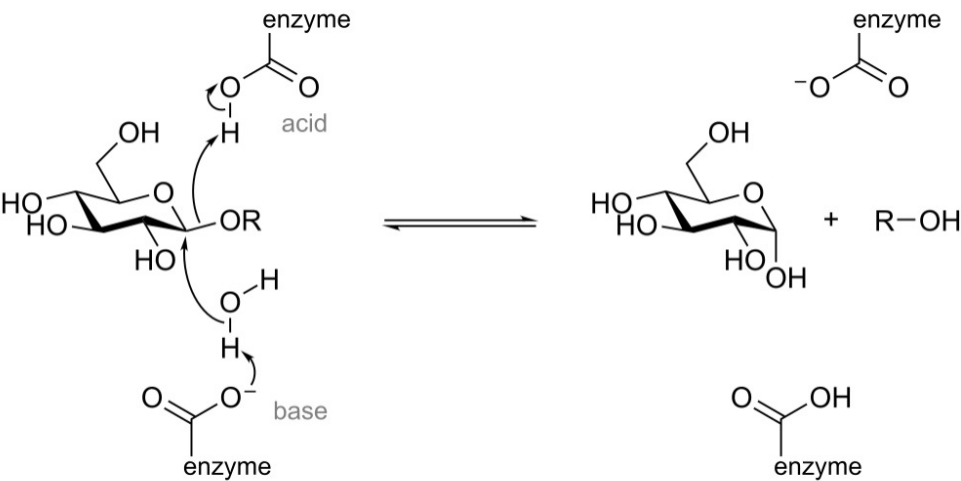
6ANE

Motivation: Activation free energy prediction



How can we **predict** the activation free energy in **high throughput manner**?

Catalytic reaction

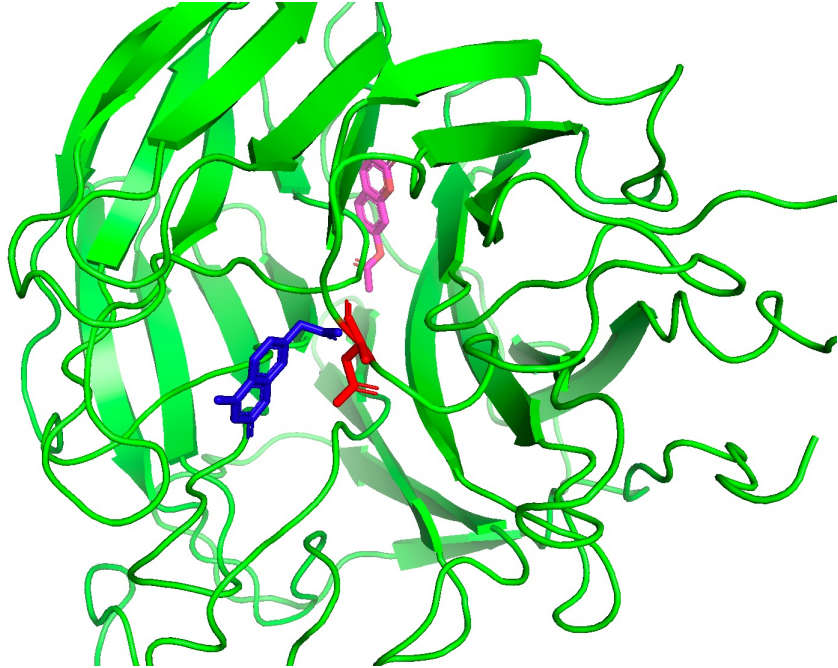


Questions

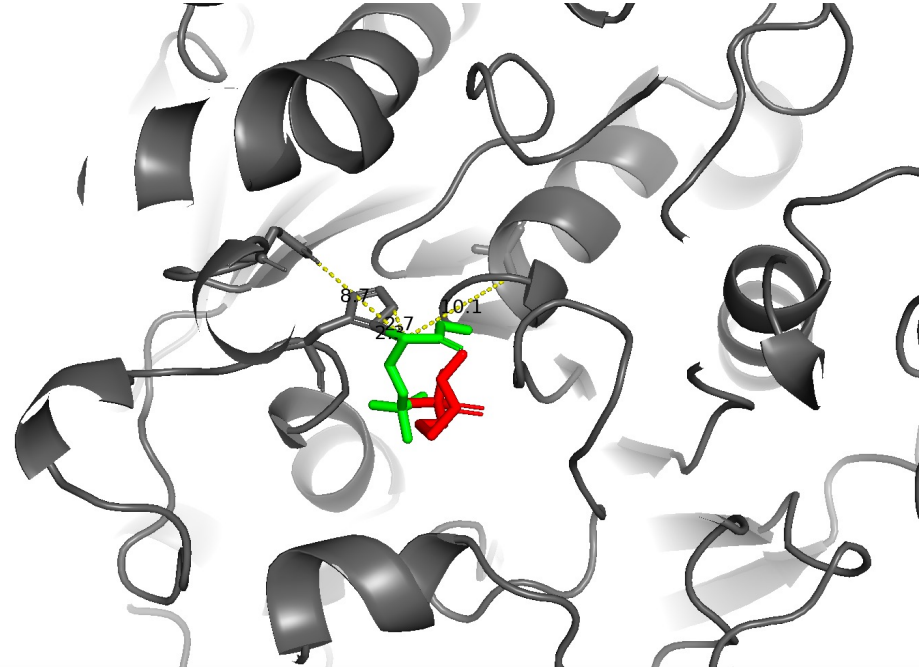


- 1. Can you explain two major enzyme parameters which can affect the catalytic reactions (Hint K_m K_{cat})**
- 2. What does EC number mean?**

Reaction center representations



1B9V reactive Docking



3LII reactive Docking