THE FUTURE OF MEDICAL RESEARCH...
COMPUTATIONAL CHEMISTRY

MBRU

UAEU — جامعة الإمارات العربية المتحدة — United Arab Emirates University

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What is Computational Chemistry?

Using *computer software* to help us solve *complex chemical reactions* by using theoretical chemical models incorporated into computer programs.
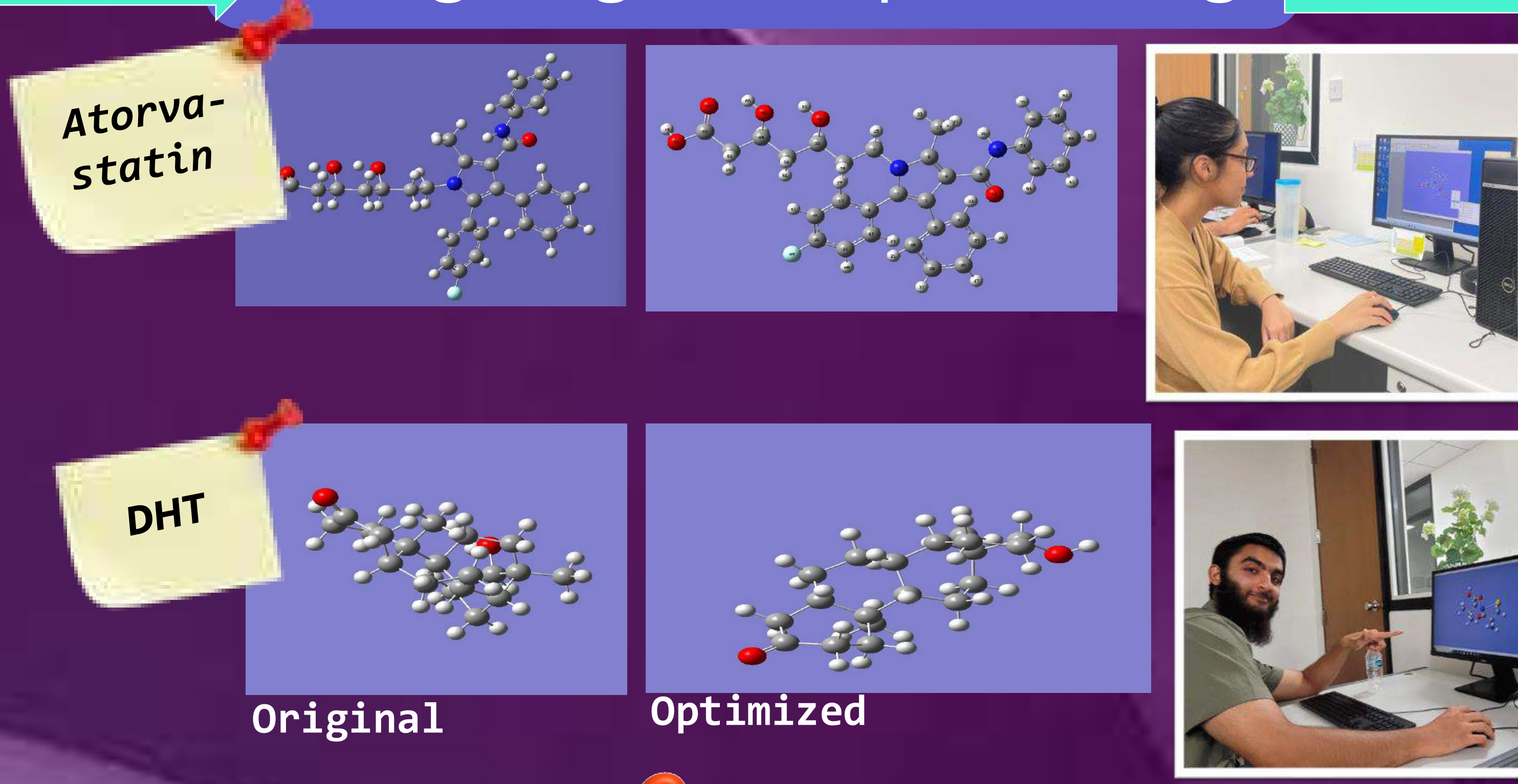
Medical Applications?

➤ Discovering and building novel *drugs*
➤ Studying physiological mechanisms such as enzyme binding
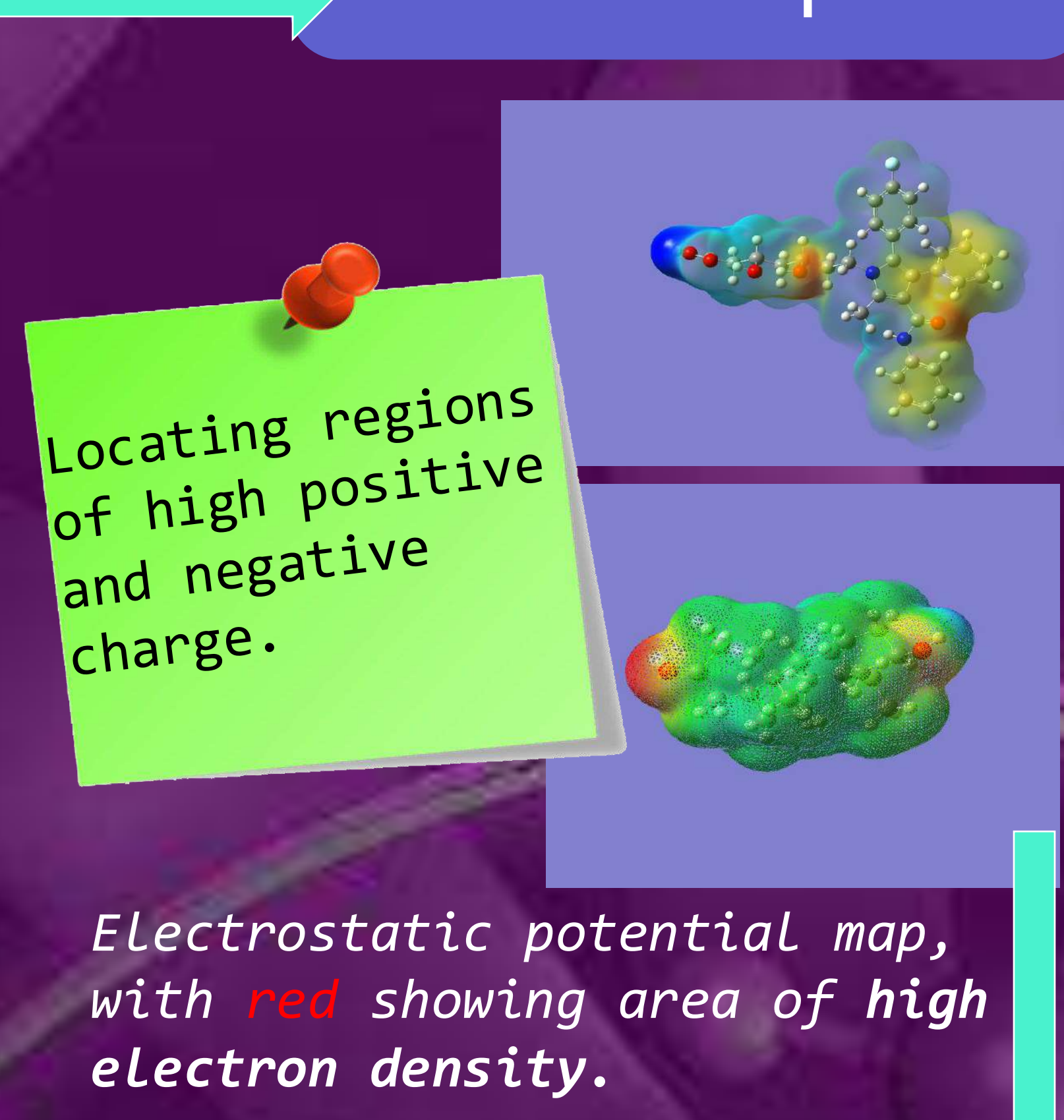➤ Calculating thermodynamics of reactions

Step 1 - Researching
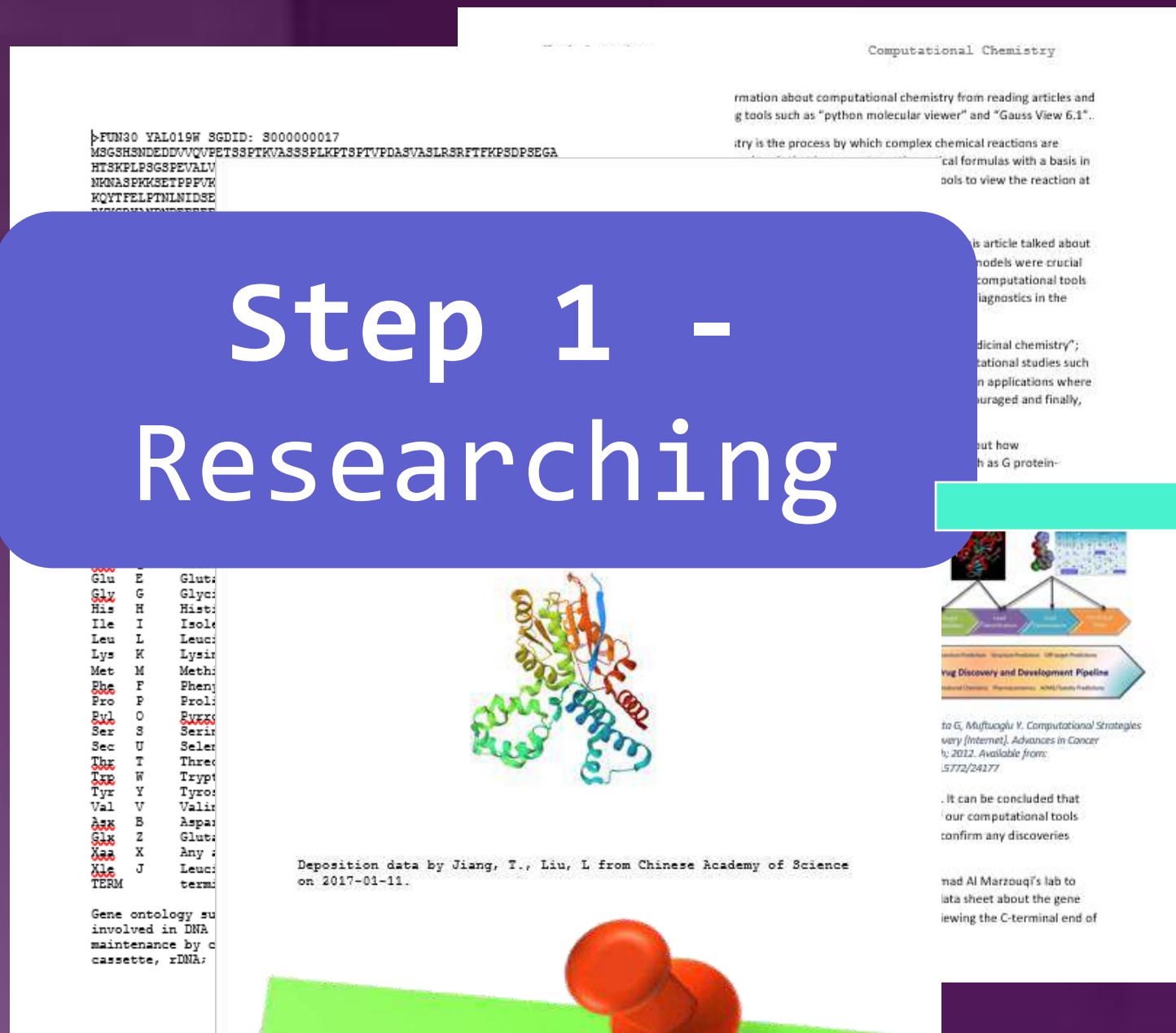
Designing molecules using *Gauss View*. The computer software then calculates a more optimum structure with the *least energy*; this energy value is known as the "Global Minimum".

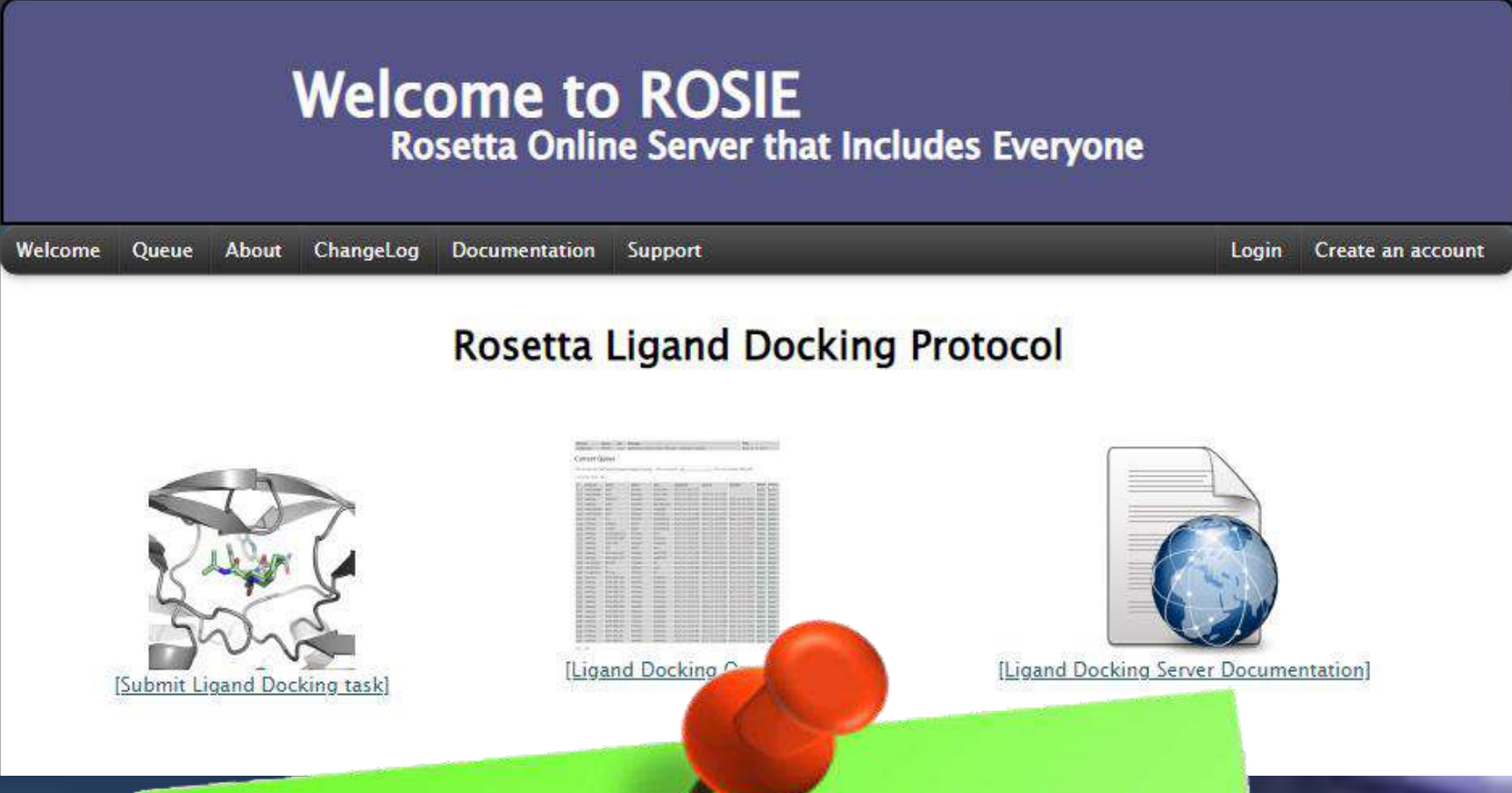### Step 2 - Designing and Optimizing

Atorva-statin

DHT

Original   Optimized

Step 3 - ESP Maps

Locating regions of high positive and negative charge.

Electrostatic potential map, with red showing area of high electron density.

Different reactions can be studied and the **energy values** for each step of the reaction can be measured and plotted.

Step 4 - Understanding Reaction Mechanisms

Si + H2   TS   SiH4

Formaldehyde   TS   CO + H2

Energies for Formaldehyde Dissociation Rxn

IR Spectrum

Step 5 - Molecular Docking

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Rosetta Ligand Docking Protocol

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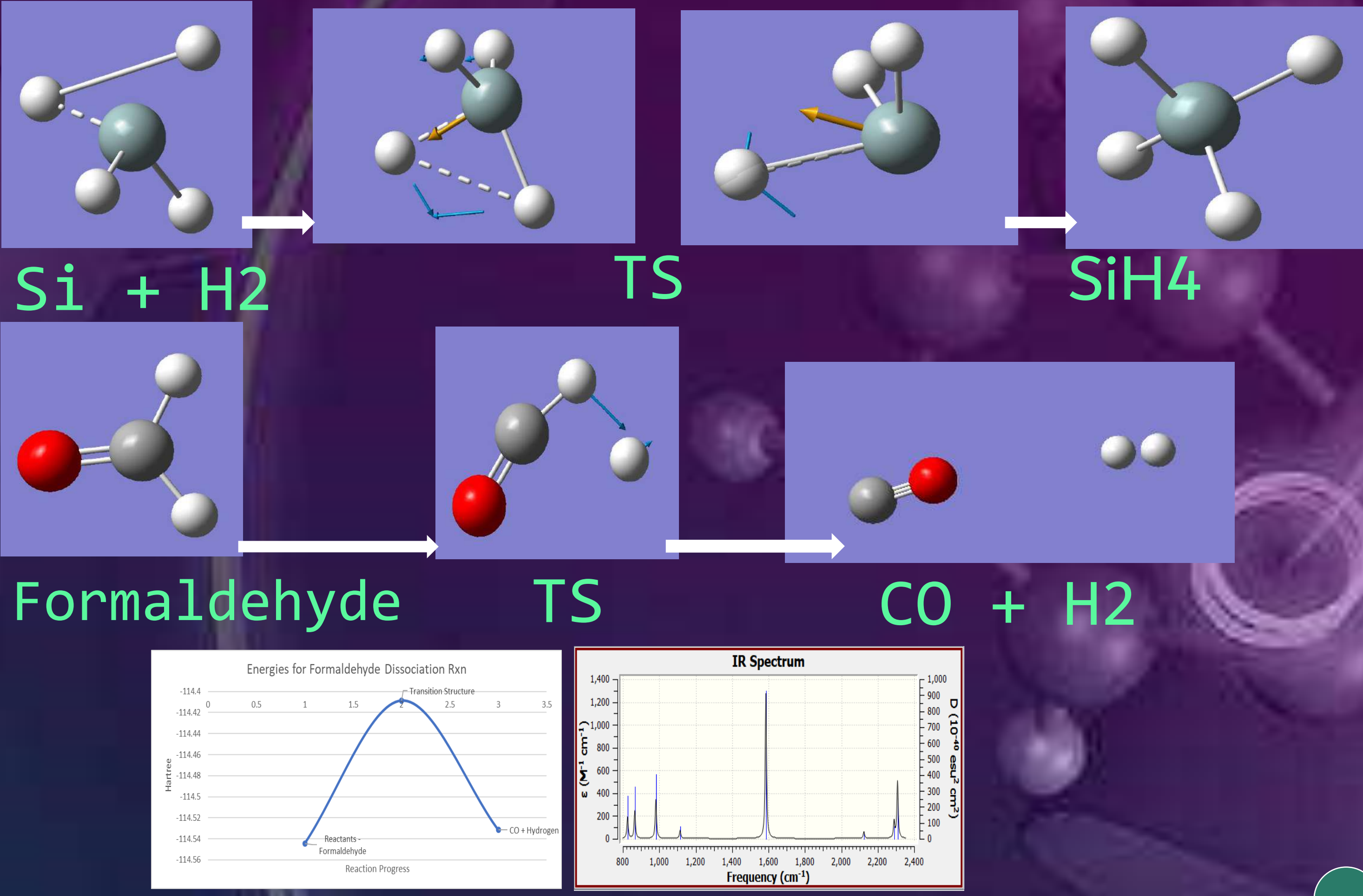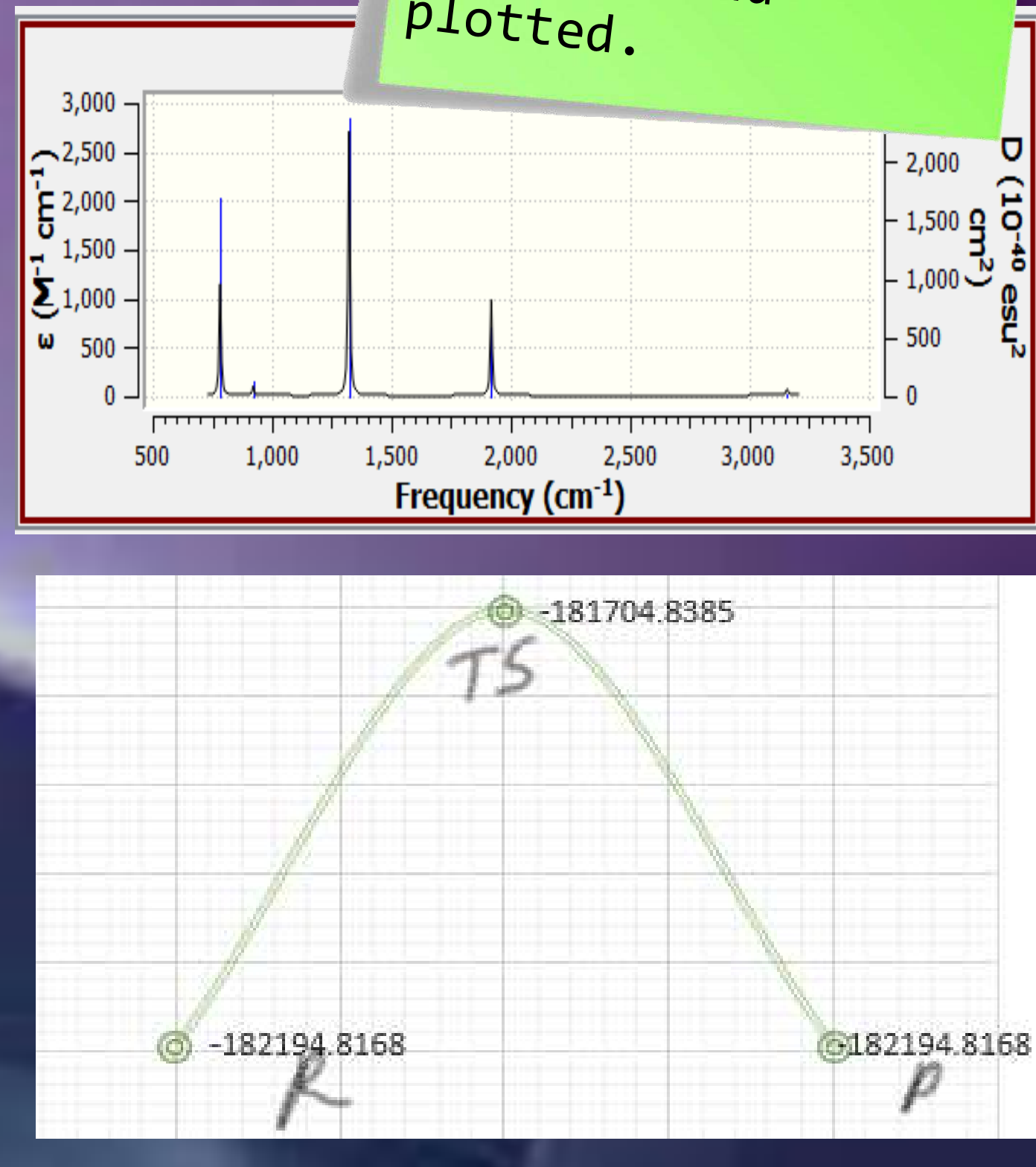
Molecular Docking programs the **interactions** between proteins and their ligands. We used the publicly available **Rosie Rosetta** software online (John Hopkins).

Gallery of Molecules

Glucagon receptor

DHT

Hemoglobin Dimer

Heam group and O2 ligand

Atorvastatin