**Proposal**

Created: 10/03/2023 by Tom Lever

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I propose to work with Naomi Ohashi to develop a Docking-Score Predictor. A docking score is measure of how well a molecule binds to another molecule. A docking score is a change in the molar Gibbs free energy of a compound. A docking score is measured in kilocalories per mole. According to Dr. Ryan Weil, is amazing and is okay.

Our predictor will receive Simplified Molecular Input Line Entry System (SMILES). A SMILES is a string. There is one SMILES per compound. There is one compound per SMILES.

The enthalpy of a compound is the sum of the compound’s internal energy and the pressure energy of the compound. The pressure energy is the energy required to establish the compound’s physical dimensions. The pressure energy is the product of the pressure on the compound by its surroundings and the volume of the compound.

The molar internal energy of a compound is the internal energy of the compound per mole.

The molar volume is the volume of the compound per mole.

The molar pressure energy of a compound is the pressure energy of the compound per mole.

The molar enthalpy of a compound is the enthalpy of the compound per mole. The molar enthalpy of a compound is the sum of the compound’s molar internal energy and molar pressure energy.

The change in enthalpy of a reaction is the difference between the sum of the enthalpies of the products of the reaction and the sum of the enthalpies of the reactants.

The change in molar enthalpy of a reaction is the difference between the sum of the molar enthalpies of the products and the sum of the molar enthalpies of the reactants.

The entropy of a compound is a measure of uncertainty, disorder, or mixedupness of the compound. The entropy measures the degree to which the probability of the compound being in a particular microstate is spread out over different microstates. A microstate specifies all molecular details about the system including the position and velocity of every molecule. The more such states are available to the compound with appreciable probability, the greater the entropy.

is the probability that the compound is in the th state according to the Boltzmann distribution.

is the number of microstates whose energy equals the compound’s energy.

For an isolated system, .

The entropy of a compound is a quantity that satisfies “an infinitesimal change in entropy is equal to the ratio of an infinitesimal quantity of heat in a reversible reaction and the temperature of the compound”.

The molar entropy of a compound is the entropy of the compound per mole.

The change in entropy of a reaction is the difference between the sum of the entropies of the products of the reaction and the sum of the entropies of the reactants.

The change in molar entropy of a reaction is the difference between the sum of the molar entropies of the products of the reaction and the sum of the molar entropies of the reactants.

The Gibbs free energy of a compound at some time is the difference between the enthalpy of the compound and the product of the temperature and entropy of the compound.

The molar Gibbs free energy is the difference between the molar enthalpy of the compound and the product of the temperature and the molar entropy of the compound.

The change in Gibbs free energy of a reaction is the maximum amount of free and useful energy available to do non-volume-expansion work that can be extracted from the reactants at fixed temperature and pressure, which can be attained only in a completely reversible process. The change in Gibbs free energy of a reaction is the difference between the change in enthalpy of the reaction and the change in the product of the temperature and entropy of the compound.

The change in molar Gibbs free energy of a compound is the difference between the change in molar enthalpy of the compound and the change in the product of the temperature and molar entropy of the compound.