# MODELING

Our model is based on absorption based on a biological connection

**Affinity absorption**

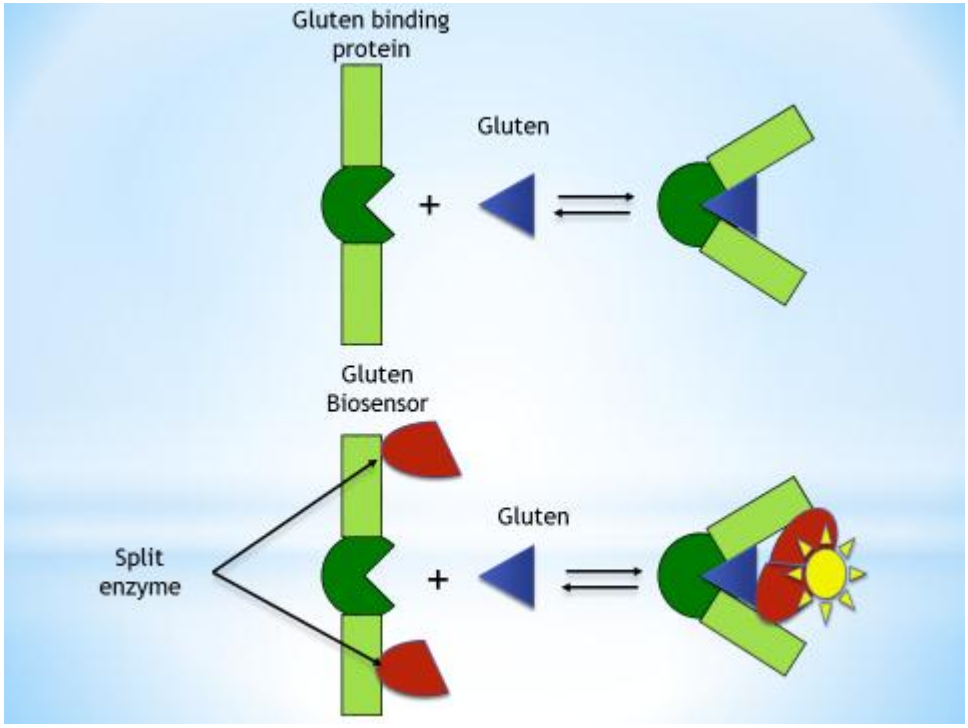



Figure 1: reactionary ligand-protein link (Gln_h- glutamine)

**Based on the enzyme-substrate link reactions the model was constructed based on langmuir isotherm**

The absorption of langmuir describes a model of complex interactions between the absorber and the absorbed. The absorption model of langmuir is valid in systems that can assume the following assumptions:

1. Number of absorption sites on the absorbent bed is final.
2. All absorption sites are homogenic.
3. The absorption is single-layered.

# Development of langmuir isotherm equation

In the case of chemical absorption chemical bonds are formed and absorption energy organizes the size of chemical bond, ie: from 10 to 100 kilocalories compared to absorber material.

In the case of an existing simple open single-layer langmuir equation. To describe isotherms absorption according to this theory, we assume that:

1. A balance between two phases exists.
2. In the solid area there are a few end sites which are equal to each other.

In a dynamic process, and when you get to a balance, the pace of absorption is equal to the pace of separation from the area. We will mark with θ the fractured area covered by molecules in a single layer and with (1−θ) the free space, we will get a langmuir equation.

1. $k_2 \theta = k_1 (1- \theta ) C$

when

θ - degree of coverage area (from 0 to 1),

C - material concentration in the solution, at M,

k2, k1 - constant speed to direction of absorption, and adjust separations respectively (both are dependent on the temperature).

2. θ equals:

$$\theta = \frac{\Gamma}{\Gamma_{max}}$$

When: Γ- represents the number of moles absorbed on the solid adsorbent in a balanced state.

$\Gamma_{max}$ – Represent the no of mols when all the cites are on the solid gram absorber are caught($\theta = 1$).

We will put 2 to 1 and get:

$$\Gamma = \Gamma_{max} \frac{K \cdot C}{K \cdot C + 1} \quad (3)$$

When K=K1\K2 – the constant balance of the absorbing process. Expression 3 known as lagmuir isotherm. Another use for equation No. 3 is:

$$\frac{C}{\Gamma} = \frac{1}{\Gamma_{max} K} + \frac{C}{\Gamma_{max}} \quad (4)$$

From the graph diagram C/Γ against C we will get a staright line cut in axis Y is

.1/$\Gamma_{max}$ gradient 1/$\Gamma_{max}$K

It is easy to see that in low concentrations K·C<<1 we will get from equation No. 3:

$$\Gamma = \Gamma_{max} K \cdot C \quad (5)$$

The dependence on starting the absorption measurement will be linear. On the other hand in high concentration K·C >>1 we will get a border value of$\Gamma=\Gamma_{max}$: equation No.3 ensures that this condition when the entire area is completely covered (0-1) in a monomolecular layer. Isothermic graph is shown in figure No. 2.

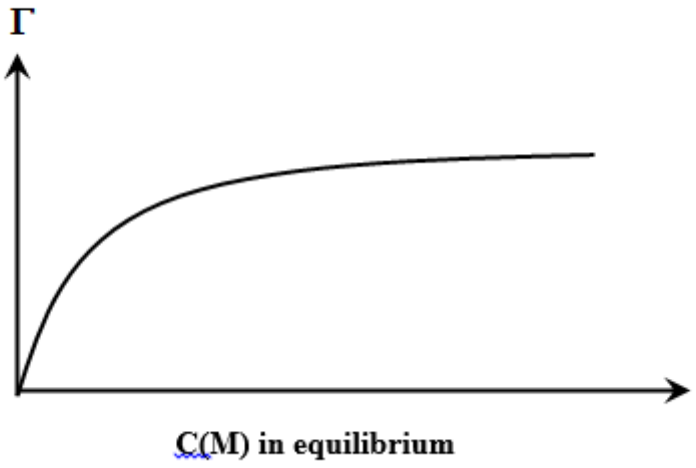



figure No. 2: Isothermic graph

According to the Langmuir model, as long as you keep filling more sites with absorber, it becomes more difficult for the melted molecule to find a free absorbent, and so, isothermic absorber will suit best to this described behavior in absorbing type Langmuir:

q= q max*k2*ce\1+kI*ce

q – the concentrated absorbent of the absorbtion compound

q max – the capacity of the absorbent platform to the absorption of that compound

kI – the constant energy related to the interaction strength between absorbent and the absorption (refined, affinity)

Ce – the concentration of the melted compound in balanced solution

## The sensitivity of our Kit can by calculated from the affinity of the biosensor to gluten by fitting binding data to the Langmuir isotherm equation

Langmuir isotherm equation:

**B=1/(1+(Kd/[L]))**

**B –** the part of all the protein to ligand, fraction bound

KD – constant connection, describes the affinity of the protein connection to ligand

L – the concentration of the ligand

### Equation expalnantion

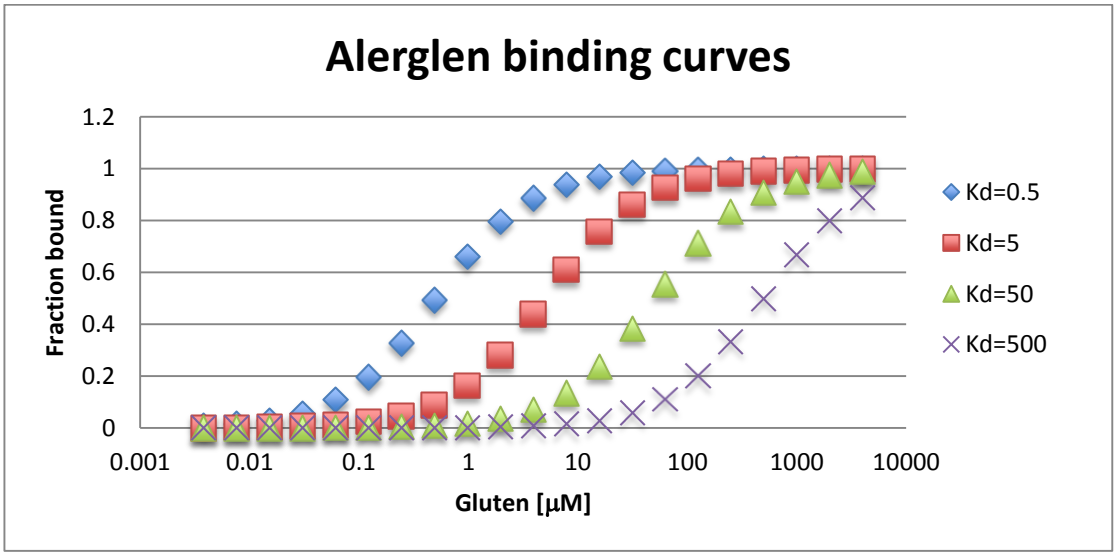
Langmuir isotherm equation represents the dependency of the constancy of the link, protein with high kd will indicate a weak link to the ligand. There will be a need of a high concentrate ligand in order to assist it to link to the protein. The fixed link indicates ligand concentrate in the compound in order for 50% of the protein to be linked.

Using the model in our experimental system:

We would like to determine the kd value of the Gln-H protein, therefore we will use this model and as a result we shall stick to reactionary behavior of the link and find its kd value.

**Hypothetical determination of the fixed link values to test reactionary behavior of the link and building a link curve based on Langmuir isotherm equation**

| Kd |
|---|
| 0.5 |
| 5 |
| 50 |
| 500 |




Graph 1: link curve. Describes 20 theoretical reactions relying on four hypothetical tested link fixes. The purpose of the curve is to examine our reaction behavior and build a model where we will put our link values.