1-204 Computation for Potentials Produced by Interacting Channel Polypeptide on the Excitable Membrane

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To evaluate the inter molecular interaction of cylindrical polypeptides that are composing the ion channel subunit, we computed the distance dependent molecular interaction potential including Coulombic and Van der Waals potentials. We considered two patterns of geometric configuration between two cylindrical polypeptides. One case is that two ones are situated parallelly and another one is crossed. We assumed that two cylinders have different radius, different pitch for the α helix. Six charges for one cylinder and Nine charges for another cylinder. The inter point charge distance differs between two cylinders. By the complex stereo geometric analysis, we could express the distances of two point charges on the surfaces of helicies of two different cylinders. By these geometric consideration, we could calculate the interaction potential when two cylindrical polpeptides are in parallel position and crossed position.

Key Words: Excitable Membrane, Molecular Interaction, Van der Waals Force, Gemoetry

1. Introduction

Ion selective channels on excitable membranes are composed of finite number of cylindrical polypeptides (Fig. 1 from reference (2)). These molecules change their conformations (Fig. 2 from reference (1)) so as to open and close the channel molecules. In the present investigation, we propose a geometric method to compute interacting potentials among these deformable polypeptides to analyze electrodynamical mechanism for ion selective channel opening.

2. Geometric Consideration

The electrical charge distribution of amino acids on the surfaces of channel polypeptides are arranged helically. We represented these charges by point charges (Fig. 3). They are denoted by y'_n for the first cylinder and x'_n for the second cylinder. The pitch of each helix are given by L_a and L_b respectively for the cylinders (Fig. 4). Hence the rise angles of these two helixes are expressed by ϕ_a and ϕ_b. The horizontal displacement between these two cylinders are set by a constant c.

The point charges on one helix are projected on the horizontal cross sectional plane of one cylinder which are denoted by A_n (Fig. 5). These projected pint charges distribute by θ_b on the second cylinder (Fig. 5) and θ_a on the first cylinder. The nearest distance between two cylinders was denoted as R.

The distance between two point charges each of them belong to the first and the second cylinders can be calculated by the trigonometric measure (Fig. 6).

The interaction between one pint charge on the first helix to all the point charges on the second helix are described by Fig. 7 for the case of (y'_2, x'_n), $n = 1$ to 9.

By these geometric consideration, we can calculate the distances, r_n, among all the point charges on the two helixes of two cylinders.

We compute the Van der Waals force $1/r^6$ for one helical turn of two cylinders. For simplicity, all the charges on the helixes are assumed to be unity and we analyzed only the influence of the geometric properties of the helical distribution of the point charges.

3. Computed Results

Figure 8 shows the computed factor $1/r^6$ when L_a and the radius of the first cyinder a, were changed. With an increase of L_a, the $1/r^6$ increased gradually.

Figure 9 shows the $1/r^6$ when L_a and the radius of the second cyinder b, were changed. With an increase of b, the $1/r^6$ decreased rapidly.

4. Discussion

The present work only showed a geometric method to compute the characteristic distance $1/r^6$ for interacting two cylinder polypeptides constituting the channel on excitable cellular systems. The computed results have to be compared with measured Van der Waals potentials in future to examine the validity of the present geometric approach. The defect of the present approach may be the simplification of the charges carried by different type of amino acids that are constituting the channel polypeptides. Since each amino acids has different number of atoms, the magnitude of the point charges are far from the unity and the factor $1/r^6$ have to be weighted by the characteristic amount of the charges carried by the amino acids.

5. Conclusion

The geometric analysis was introduced point charges on interacting two polypeptides that constitute ion selective channel pore on the excitable membrane. The Van der Waals factor $1/r^6$ was influenced strongly by the pitch and the radius of interacting cylinders. The present study may be useful when precise charge on the amino acids are weighted on the factor $1/r^6$.

References

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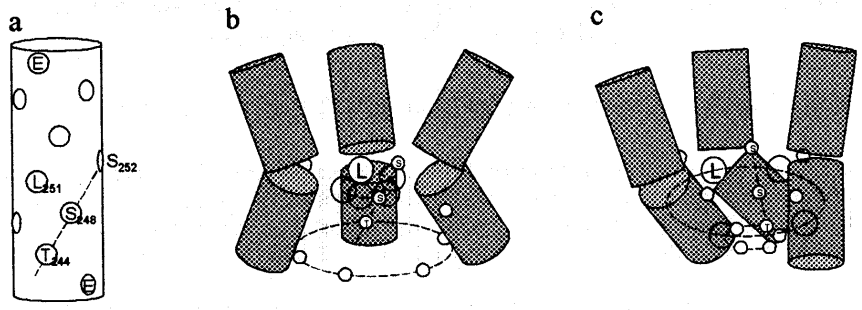


Fig. 2 a: distribution of amino acids residues on the surface of one cylinder of the subunit; b and c: the open and closed conformations of cylindrical peptides constituting the channel pore

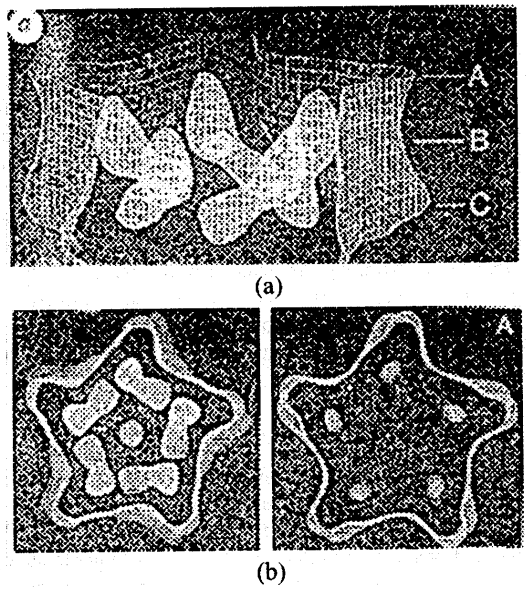


Fig. 1 a: three-dimensional molecular structure of Calcium channel with four subunits surrounded by envelope; b: top view of the channel with different depth from the entrance

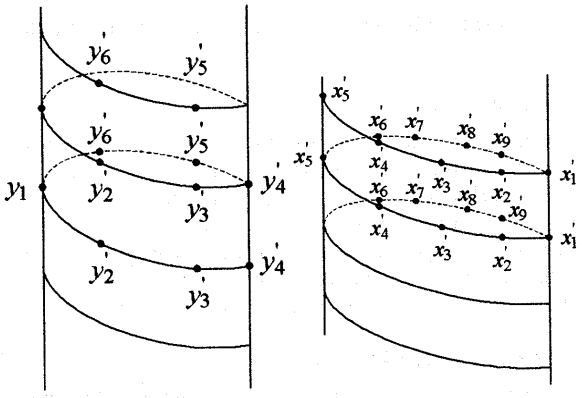


Fig. 3 Distribution of point charges on the cylindrical polypeptides, where the helical distributions of point charges on the first cylinder are denoted by y_n' and those on the second one are by x_n'; for general case, we set that there are six point charges on the first helix and nine point charges on the second one

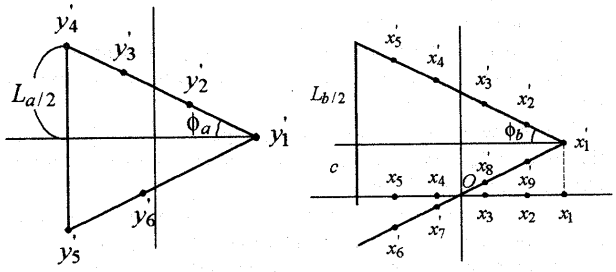


Fig. 4 The side views of the helical distributions of the point charges of Fig. 3, in which for the general case, the horizontal plane of the two cylinder are not coincided but displaced by the constant distance c and x_n denotes the point charge positions that are projected on the cross sectional plane of the cylinder

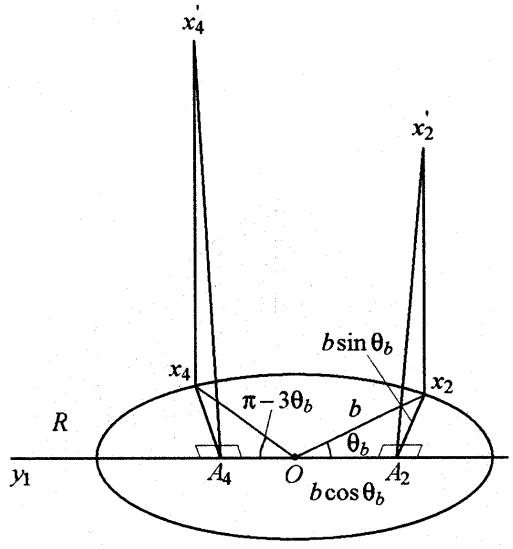


Fig. 5 Spatial positions of two point charges on one helical turn; this shows the geometric of projected point charges on the second cylinder having radius b and the division angle θ_b

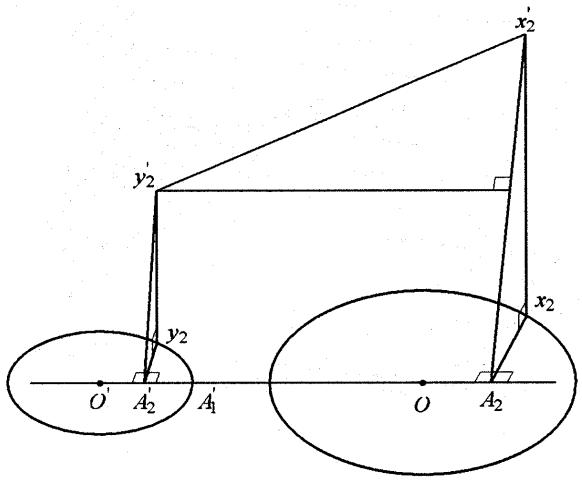


Fig. 6 The distance between two point charges on the helical turn on two cylindrical polypeptides; this shows the distance between two representative point charges on two helixes (x_2', y_2')

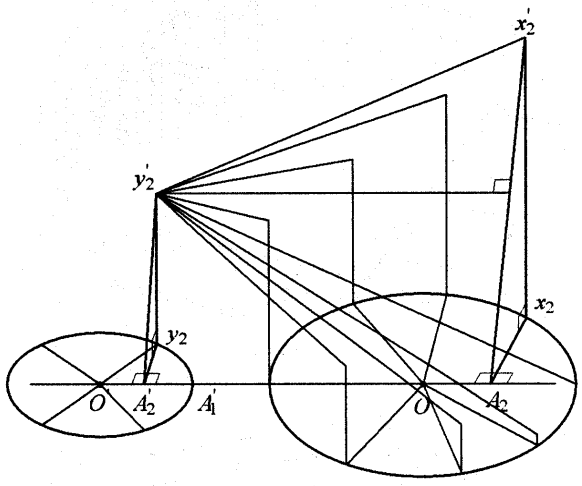
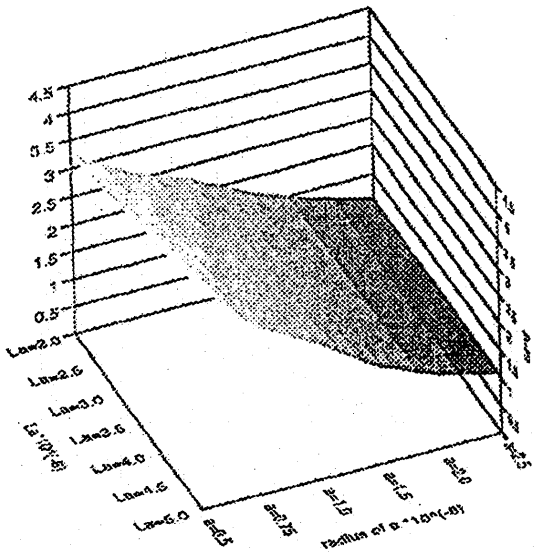
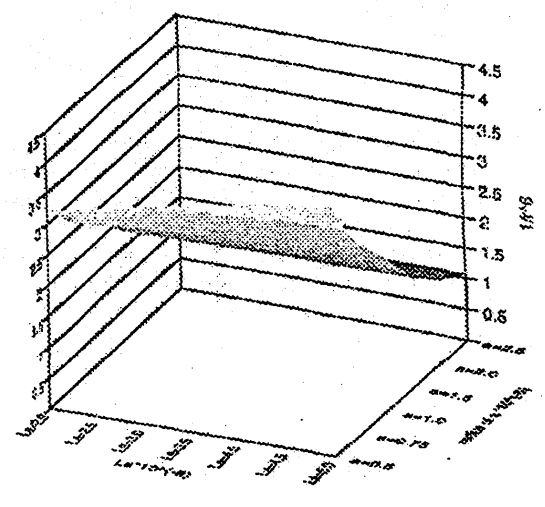


Fig. 7 Relation of multiple interactions for one point charge on the first cylinder to point charges on one helical turn on the second cylinder; this shows distances from y_2 point on the first cylinder to x_2' to x_9' points on the second cylinder, and y_2 and x_2 are the points that are projected on the cross sectional plane of the cylinders

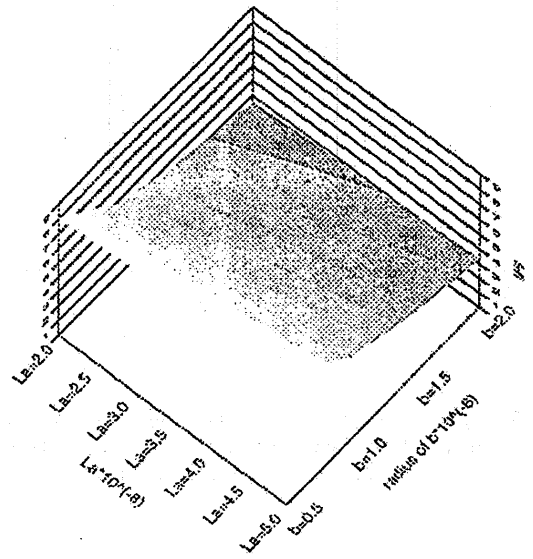


(a)



(b)

Fig. 8 Computed factor $1/r^6$ when L_a and the radius of the first cyinder a, were changed



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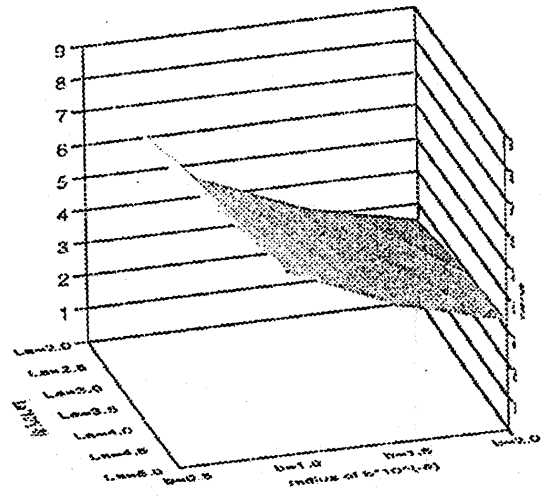

(b)

Fig. 9 Computed factor $1/r^6$ when L_a and the radius of the second cyinder b, were changed