MICROELECTRONIC NETWORKS ANALOGOUS TO PROTEIN HYDROGEN BONDED NETWORKS MADE FROM BACKBONE PEPTIDES AND WATER MOLECULES

Rostislav Pavlov Rusev[1], Boris Petkov Atanasov[2], Tihomir Borisov Takov[1], Marin Hristov Hristov[1]

(1) ECAD Laboratory, FETT, Technical University of Sofia, 8 Kliment Ohridski Str., 1797 Sofia, Bulgaria, rusev@ecad.tu-sofia.bg, mhristov@ecad.tu-sofia.bg, takov@ecad.tu-sofia.bg
(2) Biophys. Chem. Proteins Lab, Institute of Organic Chemistry, Bulgarian Academy of Science, Acad. G,Bonchev Str., Bl.9, rm 405, BG-1113-SOFIA, Bulgaria, Tel:(+359) 2 9606123, boris@orgchm.bas.bg

For microelectronic purposes, signal transfer (proton transfer) in a hydrogen bonding network is studied. The network is extracted from β-lactamase and it includes atoms from protein backbone and water molecules. The model of proton transfer in hydrogen bonds is developed on the basis of Marcus theory and the protein electrostatic theory. The investigations show that the characteristics of hydrogen bonds are similar to V-A characteristics of single-electron transistor, semiconductor diode and current generator. The entire network is similar to a microelectronic circuit with two inputs and two outputs. In addition, it can be used for a signal transfer.

Keywords: microelectronics, proton transfer, hydrogen bond, single-electron transistor

1. INTRODUCTION

Bioelectronics/Biomimetics is a new direction that in the last few years it has a rapid development. It explores the potential of bio-materials for making of microelectronics devices. The scientists successfully integrated various organic and bio-organic components in the structure of the field effect transistors. For example, Lee and co-authors [1] integrated proteins in the field effect transistor. Subsequently, this element can be used as a sensor for detection of acetylcholine. Other authors [2] use DNA as a gate dielectric for the correction of threshold voltage in the field effect transistors. They believe that on this basis can be manufactured microelectronic memories.

The proteins and DNA contain huge quantity of hydrogen bonds. They are of great interest for the microelectronics because many their characteristics are similar to the characteristics of the microelectronics devices. For instance, the hydrogen bonds have both the proton (charge) donor and proton acceptor, respectively and the field effect transistors possess source and drain. The drain-source current depends on the potentials of the source and drain. The proton transfer also depends on the potential of the donor and acceptor. In field effect transistor, the current is determined by the gate potential. On another hand, in hydrogen bonds the proton transfer depends on their surrounding potentials. Some authors predicted that the hydrogen bond can

be used as electronic switches and logical elements [3]. Because of the above mentioned facts, the biomimetic exploration of the hydrogen bonding network will be studied. The aim is to investigate the hydrogen bond characteristics and to compare them with V-A characteristics of the known microelectronic devices.

2. MATERIALS AND METHODS

A network of hydrogen bonds is extracted from β-lactamase protein through WHAT_IF server [4]. The β-lactamase (1btl) is taken from the Protein Data Bank [5]. The electrostatic potentials of all atoms in bio-molecule are calculated by PHEPS [6]. In particular, the donor and acceptor potentials and pKa's of all participants in the hydrogen bonding network are evaluated by this server. The program allows variation of pH, as a result of which the potential-values and pKa-values are varied.

For quantity estimation of proton current, the parameter of proton transfer (K, [J/mol]) is introduced. This parameter is proportional of proton current. For calculation of this parameter, the software based on Markus A. Lill and Volkhard Helms parameterization [7] is written. The equations used in the program are:

$$K = \frac{k_B T}{2\pi} \exp\left(-\frac{Eb - h\omega/2}{k_B T}\right) \quad (1)$$

where: K [kcal/mol] – proton transfer parameter, kB – Boltzmann constant, Eb – energy barrier, h – Planck constant, ω – frequency, T – temperature [K].

The energy barrier is calculated by:

$$Eb = (s_A(R(DA) - t_A)^2 + v_A) + s_B E_{12} + (s_C \exp(-t_C(R(DA) - 2)) + v_C)(E_{12})^2 \quad (2)$$

where: R(DA) – donor-acceptor distance, E12 – energy difference between the bottoms of the potential wells. The values of the remaining parameters are taken from [7].

3. RESULTS AND DISCUSSION

The subject of this work is the hydrogen bonding network formed between the protein's main chain and water molecules. It is shown in Fig.1.

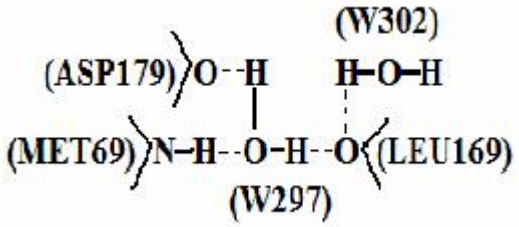

Fig. 1 Hydrogen bonding network, where N is nitrogen atom of methionine residue (MET69), O is oxygen atom of water molecules W (297, 302), leucine residue (LEU169) and aspartic acid residue (ASP179).

In this system the water molecule (W297) forms branches. Also, it appears as donor of two oxygen atoms from the main chain (ASP179 (O), LEU169 (O)) and as acceptor of MET69 (N). On the other hand, LEU169 (O) forms two hydrogen bonds with water molecules W297, and W302.

The proton current which goes through the different hydrogen bonds is examined by pH-varying. Under its change, the polarization and ionization of groups is

occurred. As a result, the charges in protein-water system are redistributed and the examined donor/acceptor electrostatic potentials are changed. The proton transfer parameter (respectively proton current) between them is also changed. The K-dependencies from acceptor electrostatic potentials are shown on Figures 2-5.

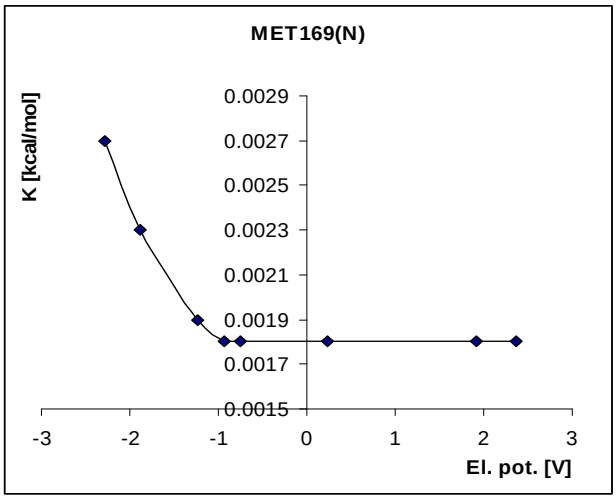

Fig. 2. K-values versus electrostatic potentials (El. Pot) of MET169N donor atom

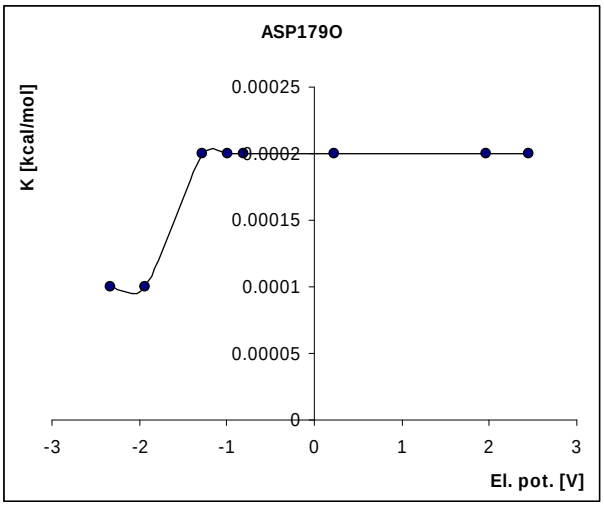

Fig. 3. K-values versus electrostatic potentials (El. pot) of ASP179O acceptor atom

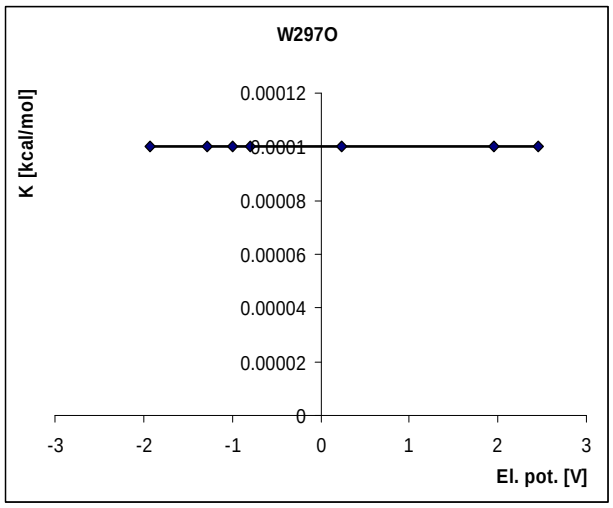

Fig. 4. K-values versus electrostatic potentials (El. pot) of W297O donor atom

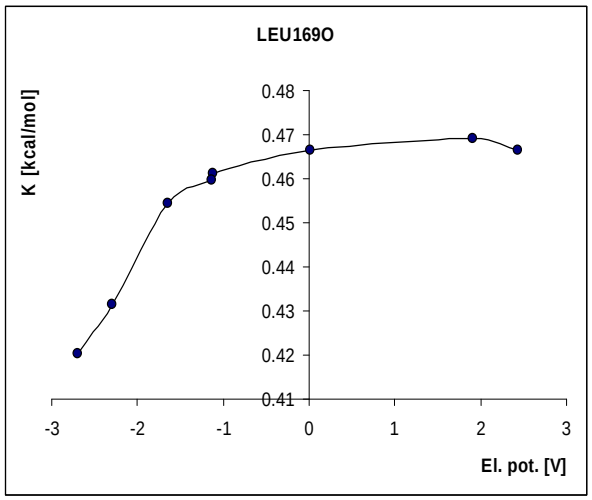

Fig. 5. K-values versus electrostatic potentials (El. pot) of LEU169O acceptor atom

The curves of Figures 3 and 5 have S-form. These are the characteristics of the hydrogen bonds formed from identical donors and acceptors (water molecules and oxygen atoms from protein backbone). They are similar to the curves obtained by other authors who used different computational formalism and other model systems [8]. On the other hand, those curves resemble V-A characteristics of a single-electron transistor. Comparing both figures, the acceptor potentials are changed in range of -2.6 to +2.6 [V], while the levels of the proton current (proton transfer parameter) are quite different. Therefore, the levels can be set by altering the distances between the donor and acceptor which are: 2.89 Å between ASP179 (O) and W297 (O); 2.76 Å between LEU169 (O) and W302 (O). The curve on Fig. 2 is similar to V-A characteristic of the Si-diode, while the current through W297 (O)…(O) LEU169

does not depend on the voltage (Fig. 4). This hydrogen bond has functions similar to the current generator.

In the contrary of the previous beliefs, these studies indicate that proton transfer can be accomplished in hydrogen bonding networks composed by protein backbone. They are in agreement with the newer spectroscopic investigation of J. Tomkinson and F. Fillaux [9]. Their investigations showed that the proton between such chains is highly delocalized. Since such bonds are formed (and stabilize) in all proteins, it may be considered that the proteins are similar to VLSI, which is able to process the information. The herein analyzed network of hydrogen bonds is a subsystem of the protein, which has two inputs and two outputs. Therefore, it may be used as a microelectronic circuit for signals transmission.

4. CONCLUSION

The current investigations of the proton transfer in the hydrogen bonding network show that the parameters of the proton transfer (respectively proton current) depend on donor and acceptor electrostatic potentials. These relationships are similar to V-A characteristics of the single-electron transistor, semiconductor diode and current generator. However, the proton transfers in hydrogen bonding networks formed between the protein main chain and the water molecules indicate that the proteins can be used to process information. In particular, the investigated hydrogen bonding network has two inputs and two outputs and it is similar to microelectronic signal transfer circuit.

5. ACKNOWLEDGMENTS

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6. REFERENCES

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