

Numerical study of laser induced ionized species in breast cancer tumor

MUHAMMAD SHAHID*, NORIAH BIDIN, YACOOB MAT DAUD, GUL BHAR ASHIQ

Department of Physics, Universti Teknologi Malaysia

Laser induced thermotherapy (LITT) of cancer tumors has been taken under serious consideration as being one of several techniques for local treatment of malignancies. In Laser induced plasma produced in the tumors plays a key role to destroy tumors. Plasma contains ions and electrons like species. The exact information about these species inside tumor is essential. We have instigated a Quantum pharmacokinetic model to study the demeanor of these species inside the breast tumor of any dimension. Our simulations have probed the different quantum mechanical parameters associated with the motion of these particles inside tumor.

(Received May 31, 2011; accepted June 30, 2011)

Keywords: LITT, Plasma, Quantum Mechanics, Breast cancer, Tumor

1. Introduction

Breast cancer is the 2nd most common cancer all over the world after lung cancer is the 5th most common cause of cancer death. Recent statistics points up, breast cancer approximately cause 519 000 deaths worldwide every year (7% of cancer death; almost 1% of all deaths). In America, it is ballpark figured that 12.5% women built up breast cancer in their lifetime [1-3].

Minimally invasive laser-induced thermotherapy (LITT) presents an alternative scheme to conventional tumor therapeutically interventions, such as surgery, chemotherapy, radiotherapy or nuclear medicine. Optical tissue features of tumor cells and their heat-induced changes are essential subjects for controlling LITT progressions [4]. Under expedient conditions LITT as a minimally invasive method provides in situ coagulation of tumors using fiber coupled Nd:YAG lasers (1064 nm) without affecting surrounding normal configurations [5,6] like in laser engineering applications. Since applications of optical methods are often favored in medical diagnosis and therapy in order to spare patients invasive intrusions the tissue optics of target tissues bring along some specific circumstances that need to bring about [7].

Laser induced therapy is a tumor treatment modality utilizing light to induce chemical reactions, the products of which are cytotoxic. By the absorption of light two kinds of reactions occur: type I reaction, which engross electron transfer to a target molecule, and type II reaction, which go ahead to energy transfer mainly to oxygen. The type I reaction produces diverse radicals, most often involving oxygen, such as hydrogen peroxide, superoxide anion and hydroxyl radicals.[8] The most important type II reaction is the conversion of ground state oxygen to excited singlet state. Singlet oxygen reacts with amino acids, unsaturated fatty acids and nucleic acids, causing damage to these macromolecules, with resulting damage to cell function

and structure [9]. Oxygen thus plays a significant role in the generation of tissue damage.

We have simulated a new quantum pharmacokinetic model for the motion of ionized particles inside the tumor. Our computational model revealed some important parameters which can play a critical role for LITT treatment of cancer tumor. First parameter is that up till now all the work has been done by classical theory; while we have made a quantum mechanical pharmacokinetic model because quantum mechanical results are very close to experimental results. The second parameter is that most of the work has been focused over the heat caused by the ionized particles; while we focused our attention over the kinetics of these particles. We have studied the wave nature of the ionizing particles. The activities of the particles and their energies profile along with tumor parameters have been provoked efficiently.

2. Theory

2.1 Breast cancer cell

Breast cancer is the abnormalities which most likely occur at ducts (ductal carcinoma in-situ) and lobules (lobular carcinoma in-situ). Almost 90% breast cancer starts from duct and 10% initiate from lobule. Like other cancers, breast cancer also sets up from a sole cell. The conversion from a normal cell to a tumor cell is typically a headway from a pre-cancerous lesion to malignant tumors [10-15]. These changes may be the result of interactions between a genetic factor and the following three external carcinogens:

- a. Physical carcinogens(Ultraviolet and ionizing radiation etc)
- b. Chemical carcinogens(Tobacco smoke and arsenic)

c. Biological carcinogens(infections of viruses, bacteria or parasites)

Aging is another very important factor for cancer maturity because the overall cancer menace is combined with the propensity for cellular repair mechanisms to be less effective as a person grows older. The breast cancer is diagnostically classified by cancer stages primary on the basis of tumor size, invasiveness or non-invasiveness, whether lymph nodes are involved, and whether the cancer has spread beyond the breast. The commonly used staging system is the 4-stage system.

Stage 0 -This breast cancer is non-invasive. Like DCIS and LCIS, there is no evidence of cancer cells or non-cancerous abnormal cells breaking out of the part of the breast where they started, or invading neighboring normal tissue. The tumor size is take away 1 cm.

Stage I - This breast cancer normally becomes invasive. The cancer cells breaks though and invades neighboring normal tissue. The tumor size is less than 2 centimeters, and no lymph nodes are involved.

Stage II - This breast cancer at stage II when the tumor size is more than 2 cm, but less than 5 cm across and/or the lymph nodes in the axillary are affected.

Stage III - This breast cancer at stage III when the tumor size is more than 5 cm across and the lymph nodes in the axillary are affected without further spreading.

Stage IV – This breast cancer has spread to other organs of the body - usually the lungs, liver, bone, or brain. The tumor size is larger than 5 cm and can be any size.

Clinically, breast cancer at stage 0, I, II, and some stage III are gazed at as early stage, while other stage III and stage IV are regarded as advanced stage.

2.2 Schrödinger's wave equation

The Schrodinger equation is the name of the basic non-relativistic wave equation used in one version of quantum mechanics to describe the behavior of a moving particle. The Schrodinger equation gives the quantized energies of the system and gives the form of the wave function so that other properties may be calculated. This equation predicts the future behavior of a dynamic system. It is a wave equation in terms of the wave function which forecasts analytically and precisely the probability of events or outcome.

The steady state Schrodinger's wave equation for a moving particle is given as

$$\nabla^2 \Psi + \frac{2m}{\hbar^2} (E - U) \Psi = 0 \quad (1)$$

Where Ψ is a wave function of moving particle, ∇ is differential operator, where

$$\nabla^2 = \frac{\partial}{\partial x^2} + \frac{\partial}{\partial y^2} + \frac{\partial}{\partial z^2} \quad (2)$$

Where as m is the mass of the particle, E is its kinetic energy and U is potential energy.

The probability density P of particle is

$$P = \int_{-\infty}^{\infty} |\Psi|^2 dv \quad (3)$$

And the normalized condition is

$$\int_{-\infty}^{\infty} |\Psi|^2 dv = 1 \quad (4)$$

3. Results and discussion

In order to investigate the behavior of ionized particles inside the tumor, some important parameter has been simulated. The detail of these parameters is described here under this section.

3.1 Wave Functions profile

To inspect the wave profile, the ionized particles were considered to be trapped inside the tumor. It was due to the fact that if particles did not trap inside the tumor then normal tissue can be damaged. The wave function of these ionized particles at different states inside tumor are shown in Figure 2 and 3. The normalized wave function was of the form

$$\Psi_n = \sqrt{\frac{2}{d}} \sin n \frac{\pi r}{d} \quad (5)$$

Where d is the size of tumor, r is the instantaneous position inside the tumor and n is the quantum number.

Where $n = \pm 1, \pm 2, \pm 3, \pm 4$, $\sqrt{\frac{2}{d}}$ is the amplitude of the

waves. Ψ_1 , Ψ_2 and Ψ_3 are the normalized wave functions at a distance $r/2, 3r/2$ and $5r/2$ respectively. Where as $\Psi_n = 0$ at the boundaries of the tissue i.e. at $r=0$ and $r=d$. Where d is the size of the tumor. $\Psi_n \neq 0$ for the interval $0 < r < d$. The wave function will penetrate the neighboring tissues for the condition $0 > r > d$ and the normal tissue will be damaged. The result indicated that the form of the wave function remained the same although it acquired more and more nodes as n quantum number stepped up. This lead to a shorter and shorter wavelength, which in turn indicates increasing kinetic energy of the corresponding particle. So at distance $5r/2$ particle will dissipate more energy to tumor as compared to $3r/2$ and $r/2$ positions. So higher quantum number wave functions have more capability to dent the tumor.

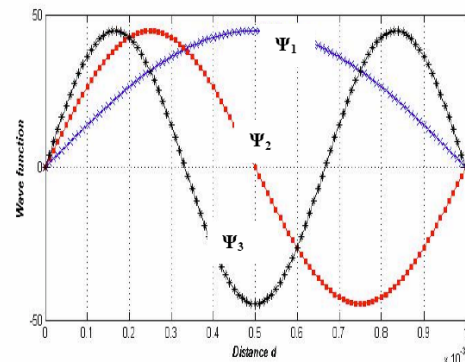


Fig. 2. One dimensional wave functions of trapped ionized particles inside tumor.

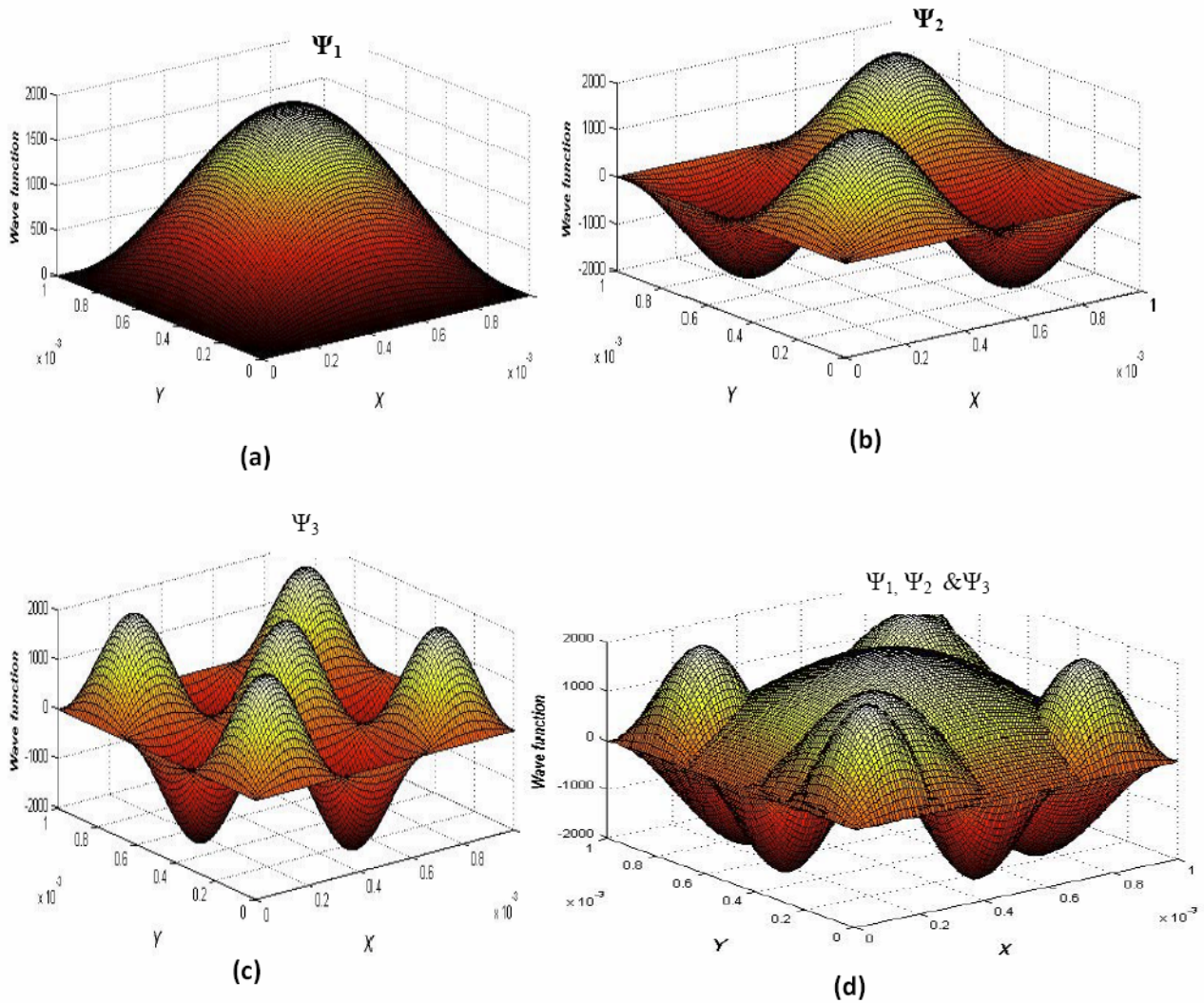


Fig. 3. Two dimensional wave functions of trapped ionized particles (a) At position $r/2$. (b) At position $3r/2$. (c) At position $5r/2$ (d) combined wave functions Ψ_1 , Ψ_2 & Ψ_3

3.2 Probability density functions

The probability densities as a function of tumor size are plotted in Figure 4 and 5. Result envisaged that probability density varies with the size of the tumor. The probability distributions were categorically non uniform at low quantum numbers, but as quantum number n increased, the probability distributions became more uniform. The distribution at high quantum numbers was consistent with the classical results. The highest probability to find the particle in the tumor was where the antinodes of the function appear. It is zero at those locations where the nodes appear. The wave functions were real i.e. those could be positive as well as negative,

while probability density functions were found to be positive. The maximum probability of the particle was at $2/d$ position inside the tumor. While minimum probability was at $r=0$ and $r=d$.

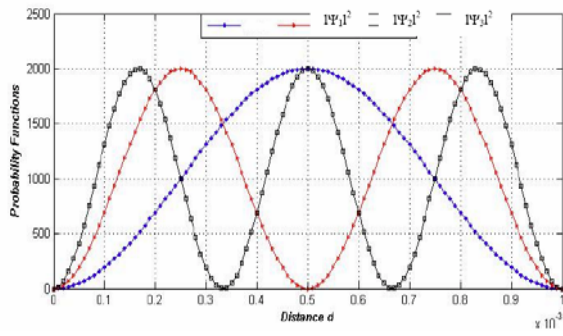
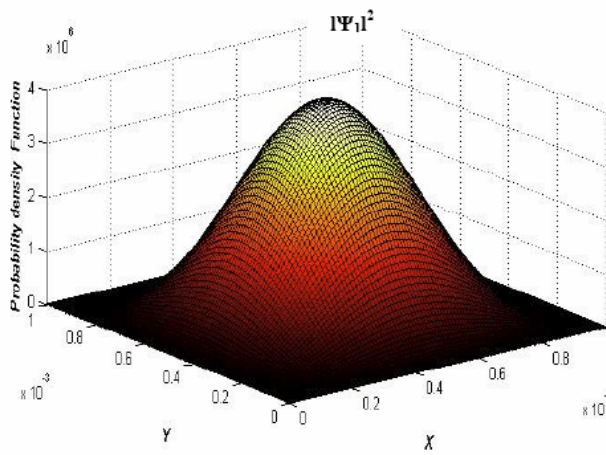
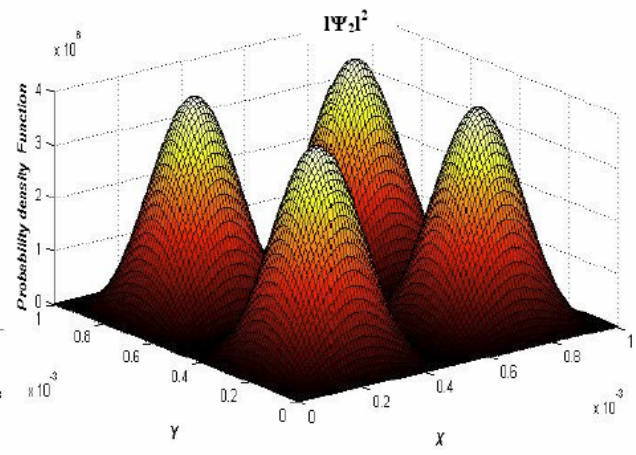


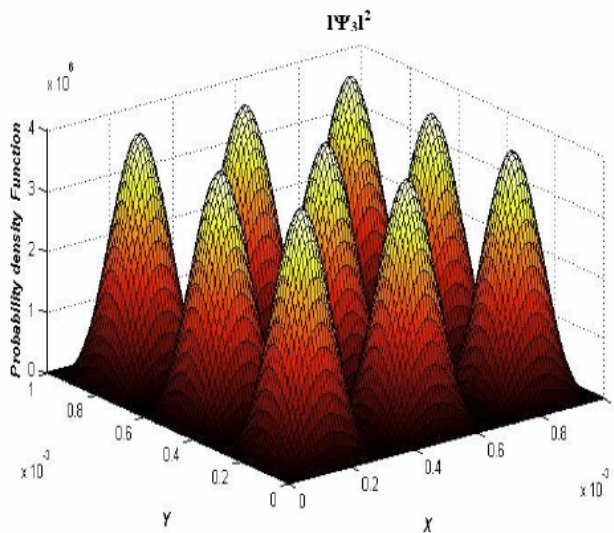
Fig. 4. One dimensional probability density functions of ionized particles inside tumor.



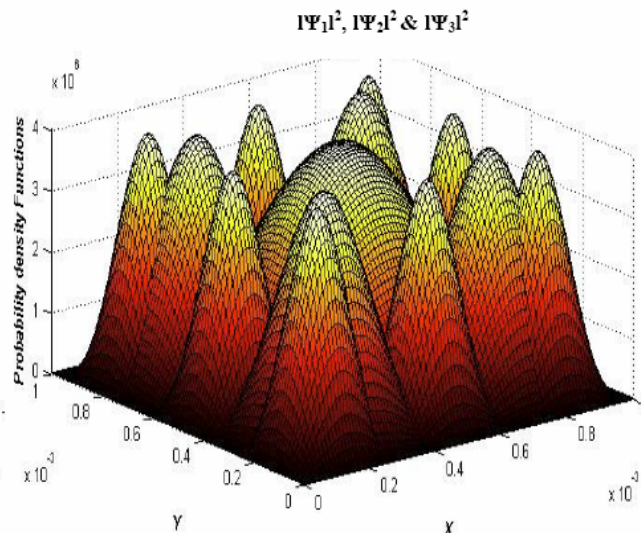
(a)



(b)



(c)



(d)

Fig. 5. Two dimensional probability density functions of ionized particles inside tumor (a)At position $r/2$. (b)At position $3r/2$. (c)At position $5r/2$ (d) combined wave functions $|\Psi_1|^2$, $|\Psi_2|^2$ & $|\Psi_3|^2$

3.3 Energy Eigenvalues

The Energy Eigen values E_n as a function of tumor size are plotted in Figure 11 and 12.

The energy Eigen values of the particles inside the tumor were of the form

$$E_n = \frac{h^2 n^2 \pi^2}{2m a^2} \tag{6}$$

The E_1, E_2 and E_3 are the energy Eigen values related to the Eigen functions Ψ_1, Ψ_2 and Ψ_3 respectively. The simulation results predicted that the energy $E_3 > E_2 > E_1$. Where E_1, E_2 and E_3 were the energies at distance $r/2, 3r/2$ and $5r/2$, respectively.

Results from Figure 6(a) show that the energy of each state decreased as size of the tumor stepped up. It was worth to note that, as tumor size changed the energies changes found to be proportional to $1/d^2$. As the tumor size shrieked, the possible energies of the particles found to be increased. For large quantum numbers, the spacing between nodes in the wave functions became too small to measure. This presages that the particles have an equal probability of being anywhere in the tumor. Similarly, difference in energy between higher levels became too small to measure, so the energy of the particle appeared continuous rather than quantized, when n became large. The key aspects of this result was that the energy increased quadratically with the number of loops in the wave function; it decreased quadratically with the width of the confinement and it decreases in proportion to the mass of the particle. So the hydrogen ions and electron should have greater energy than oxygen and other heavy mass particles.. Similarly it was observed that the energy of the particles increased with increased in the value of propagation vector K . Where $K=2\pi/\lambda$

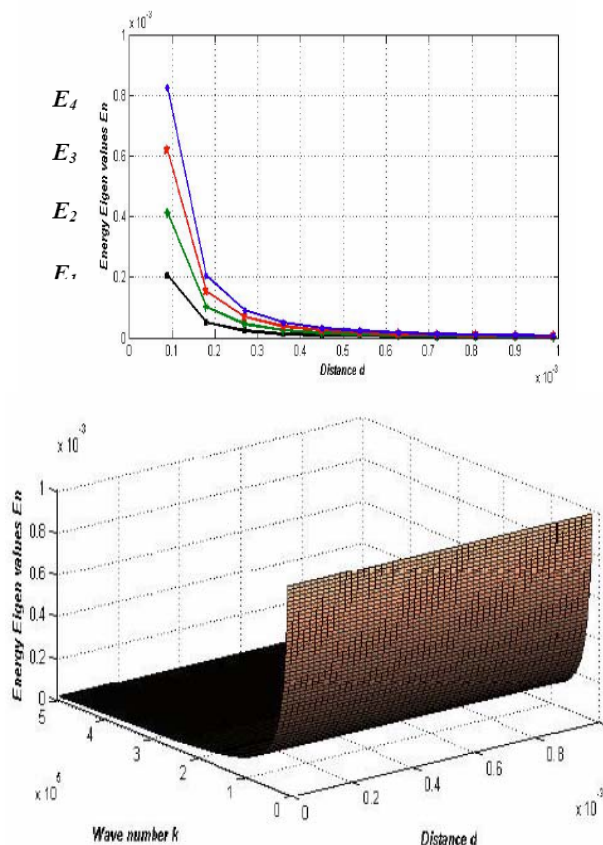


Fig. 6. Two dimensional probability density functions of ionized particles inside tumor (a)At position $r/2$. (b)At position $3r/2$. (c)At position $5r/2$ (d) combined wave functions Ψ_1, Ψ_2 & Ψ_3

4. Conclusions

Our quantum pharmokinetic model has successfully described the motion of ionized particles during LITT treatment of the breast tumor. The wave behavior of these particles gave full detail about the probability, energy and other factors which have key impact during treatment. Simulation predicted that electron, hydrogen and other lighter particles has greater energy inside the tumor, while oxygen and other heavier mass species will have less energy during LITT. The simulations also gave a point by point facet about the species inside the tumor. The quantum mechanical knowledge about the Collision, scattering and diffusion of these ionized species inside the tumor is our future goal.

References

- [1] Nico Schaefer, M.D,1 Hartmut Schafer, M.D. David Maintz, M.D *et al.* Journal of Surgical Research **146**, 230 (2008).
- [2] Tsongalis, Gregory J., Coleman, William L.. Molecular Pathology: The Molecular Basis of Human Disease. Amsterdam: Elsevier Academic

- Press. pp. 66. ISBN 0-12-374419-9.(2009).
- [3] Jemal, A; Bray, F, Center, MM, Ferlay, J, Ward, E, Forman, journal for clinicians **61**(2), 69 (2011).
- [4] C. Dressler, D. Schwandt, et al. : Thermally induced changes of optical and vital parameters. *Laser Phys. Lett.* **7**, No. 11 (2010)
- [5] J.-P. Ritz, K.S. Lehmann, U. Zurbuchen, V. Knappe, T.Schumann, H.J. Buhr, and C. Holmer, *Lasers Surg. Med.* **41**, 479 (2009).
- [6] E. Sobol, O. Zakharkina, A. Baskov, A. Shekhter, I.Borschenko, A. Guller, V. Baskov, A. Omelchenko, and A. Sviridov, *Laser Phys.* **19**, 825 (2009).
- [7] H.L. Ao, D. Xing, H.J. Wei, H.M. Gu, G.Y. Wu, and J.J. Lu, *Phys. Med. Biol.* **53**, 2197 (2008).
- [8] D.L. Liu, S. Andersson-Engels, C. Stureson, K. Svanberg, C.H. Håkansson and S. Svanberg, *Cancer Lett.* **111**, 157 (1997).
- [9] IX. C. Stureson, S. Andersson-Engels, *Phys. Med. Biol.* **41** 445 (1996)..
- [10] Eva Nilsson a, Henrik von Euler b, Jaak Berendson a, Anders Thörne. Electrochemical treatment of tumours. *Bioelectrochemistry* **51**, 1–11 (2000).
- [11] E.D.Kirson et al.Electric field potential as a cancer treatment.*Proc national academy of USA*104(2007).
- [12] E.D.Kirson et al.*Jornal of cancer research.*64(2004).
- [13] L.Cueullo et al.*Glia* **51**,65(2005).
- [14] Turler A, Schaefer H, Schaefer N, *et al.* Experimental low-level direct current therapy in liver metastases: Influence of polarity and current dose. *Bioelectromagnetics*;**21**, 395 (2000).
- [15] N. Olaiza, C. Suáreza, M. Riska, F. Molinab G. Marshall. Tracking protein electrodenaturation fronts in the electrochemical treatment of tumors. *Electrochemistry Communications* **12**(1), 94 (2010).

*Corresponding author: bluefiber08@gmail.com