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Using Biomedical Physics and Nano Technology to Combat Antibiotic Resistance: A Novel Approach

Muna Khalifa Ali
Department of Physiology and Medical Physics, College of Medicine, Fallujah University, Fallujah, Iraq

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Annotation: The rising epidemic of antimicrobial resistance (AMR) is among the most significant threats to the global population health of the 21 st century. Since multidrug-resistant (MDR) microorganisms never cease developing biological processes to overcome the traditional methods of chemical treatment, the necessity to appear as an absolute paradigm shift in therapeutic procedures has become absolute. This theoretical research paper suggests a new interdisciplinary solution between biomedical physics and nanotechnology to fight MDR pathogens. To go beyond traditional biochemical inhibition, the paper will build a theoretical foundation to examine a biophysical mode of action Photothermal Therapy (PTT) involving the use of polyethylene glycol (PEG)-functionalized Gold Nanorods (AuNRs) as nanoscale transducers.

This paper, through the perspectives of localized surface plasmon resonance (LSPR) and thermodynamic analysis, assesses the theoreticality of transformation of Near-Infrared (NIR) laser energy (808 nm) into intense and highly localized nanoscale hyperthermia. Theoretical models

suggest that this high-speed thermal stress is adequate to physically interrupt bacterial cell wall envelopes - inducing disastrous lipid phase transitions in Gram-negative bacteria and protein structure denaturation in Gram-positive ones. Moreover, the conceptual model illustrates the thermodynamic degradation of the viscoelastic extracellular polymeric substance (EPS) of recalcitrant biofilms. More importantly, since this process depends on the inherent physical and thermodynamic constraints of biological macromolecules, instead of particular metabolic processes, the chances of bacteria becoming genetically resistant to such acute physical damage are theoretically removed. Also, the study defines a theoretical therapeutic window within which the property of differentiating heat dissipation helps to prevent the thermal damage of vascularized mammalian tissues. Finally, this theoretical study postulates that the use of physical forces and the specific thermal stress can provide a highly sustainable, resistant-immune solution of infectious diseases in the forthcoming post-antibiotic era.

Keywords: Antimicrobial Resistance (AMR), Biomedical Physics, Nanotechnology, Gold Nanorods (AuNRs), Photothermal Therapy (PTT), Biofilms, Biophysical Disruption, Theoretical Framework, Thermodynamics.

1. Introduction

The identification of antibiotics in the early 20 th century was a breakthrough event in the history of human medicine as it radically changed the course of the management of infectious diseases and increased average life expectancy dramatically. These chemical agents have been in use over

decades as the final line of defense against bacterial pathogens, and they such infections that were once deadly are now treatable. Nevertheless, the era of antibiotic miracle has slowly been undermined by the inexorable power of adaptability of bacteria to evolve. The world today is in the brink of a post-antibiotic era, a dystopian future in which common injuries and minor surgery would be treated with life-threatening seriousness because of the development of the so-called superbugs, commonly referred to as multidrug-resistant (MDR) bacteria. Antimicrobial resistance (AMR) crisis is no longer a hypothetical problem but is an acute international health emergency taking hundreds of thousands of lives each year and exacting a heavy burden on the healthcare systems of most countries worldwide [1].

The inherent nature of the existing therapeutic methods is the underlying flaw of them. The traditional antimicrobial agents mostly work based on the chemistry, by attacking a particular biological pathway, in bacterial cell, cell wall synthesis, protein production, or DNA replication. Although this is a successful first-line approach, this lock-and-key chemical strategy is extremely prone to bacterial resistance strategies. Bacteria are primitive, highly adaptive and can mutate genetically quickly as well as transfer horizontal genes. They have developed advanced systems that help them to counter the effects of chemicals such as, formation of enzymes that break down the antibiotic, alteration of target sites so that they no longer bind and also, over expression of efflux pumps, which physically expel the drug out of the cell before it can have a positive impact [2]. Therefore, the reaction of the pharmaceutical industry to it, creating the new chemical derivatives of the already existing classes of drugs, has turned into a non-sustainable arms race. A new chemical agent invariably elicits selective pressure, which in turn leads to the development of resistance, thus invalidating the new drug in a few years. It has become quite obvious that the sole application of chemical interaction is a strategy of diminishing returns [3].

In order to break through this stalemate, a paradigm shift is needed, namely a shift away towards exclusively biochemical targets and into biophysical vulnerability. Herein lies the intersection point of biomedical physics and nanotechnology where a radical way out is provided. As opposed to the conventional antibiotics which are based on interference with metabolism, the new strategy aims at exploiting the physical forces like heat, mechanical stress, and oxidative damage facilitated by nanomaterials to kill bacteria. The research question is that though bacteria can develop biological mechanisms to overcome chemical inhibition, they will not develop resistance to an instantaneous physical injury that disrupts their integrity. An example is a bacterium can develop a mutation to block a drug, but it cannot develop a mutation to survive temperature that will denature its proteins or physical forces that tear the cell membrane [4].

The enabling platform to this physical intervention is nanotechnology. Through manipulation of matter at the atom and molecule level (1-100 nanometers), scientists are able to design materials which have distinct physicochemical properties which are vastly different than their bulk counterparts. Nanoparticles (NPs) have a very high surface to volume ratio, which enables them to interact on bacterial membranes more. Moreover, they can be functionalized to identify certain bacterial strains to provide specific therapy. These nanoparticles are so-called nano- transducers when used together with the principles of biomedical physics. They are able to translate external physical signals, near-infrared radiation, magnetism, or the ultrasonic wave, into localized deadly impacts at the microscopic scale [5].

Photothermal Therapy (PTT) and Photodynamic Therapy (PDT) are two of the most promising biophysical approaches that are enabled by nanotechnology. In PTT, plasmonic nanoparticles, including gold nanorods, absorb the light energy and convert it to heating that produces localized hyperthermia to heat bacteria. In PDT, nanoparticles produce Reactive Oxygen Species (ROS) during light irradiation and produces a toxic oxidative environment that randomly damages lipids, proteins and DNA [6]. In addition to using light-based therapies, the inherent physical characteristics of some nanomaterials enable them to serve as so-called nano-knives, mechanically piercing the bacterial cell wall upon contact because of sharp edges or because of electrostatic

attraction. This physical damage to the cell envelope leads to the loss of intracellular contents and cell death, which is independent of intracellular uptake and metabolic interference [7].

The study will examine and confirm this nexus in biophysical-nanotechnology as a potential alternative to traditional pharmacology. One can overcome the mechanisms of resistance formation of bacteria by creating a new strategy that will combine the precision of the structure with the destructive ability of the laws of physics. The consequence of such a strategy is more than just the killing of free-floating planktonic bacteria, it also solves the problem of biofilms-complex communities of bacteria that are shielded by a slimey extracellular matrix making them immune to the common antibiotics used. It is possible to design nanoparticles to enter these biofilms and carry the physical payload to the inactive bacteria at the core of the biofilm due to their size and charge [8].

To conclude, the growing crisis of antibiotic resistance requires the break of the chemical approach of the last century. The combination of physics and nanotechnology offers a multidimensional, wide-range, and resistance based approach. This study suggests a powerful solution that will protect the future of the treatment of infectious diseases because it does not require chemical inhibition to achieve this goal but solely physical destruction of the pathogen. The sections below will explore the specific mechanisms, material properties and experimental methodology that is required to make this vision come true.

2. Literature Review

The pursuit of novel antimicrobial strategies requires a comprehensive understanding to develop new antimicrobial approaches, an in-depth knowledge of both the phenomena of bacterial resistance and the new abilities of nanomedicine is necessary. The scientific literature paints a complicated picture in which the versatility of pathogens is rapidly surpassing the development of traditional medicine, which requires the input of biophysical methods. The careful examination of existing literature shows that there is a shift in the focus towards using chemical bactericides to physical and structure-destabilizing nanotechnologies.

Complex biological defense mechanisms underlie the resistance of bacteria to antibiotics. The main of these is the complexity of the cell envelope structure. Gram-negative bacteria, including Escherichia coli and Pseudomonas aeruginosa, contain a double-membrane structure, which serves as an effective selective barrier, and which excludes large or hydrophobic antibiotic molecules access to intracellular targets. Recent investigations have clarified that this obstacle is further strengthened by the existence of multidrug efflux pumps. These transmembrane proteins act as biological vacuum cleaners, actively pumping out toxic substances including antibiotics in the cytoplasm out into the external environment so that the drug does not get to a fatal level [9]. Moreover, the literature abundantly provides the role of biofilms in chronic infections. Biofilms are self-assembled collections of bacteria entrenched within an extracellular polymeric substance (EPS) of self-descent. This is a physical kind of protective barrier, which traps the antibiotics and neutralizes them before they reach the bacterial cells. It has been observed that bacteria present in biofilms may be 1,000 times more resistant to antibiotics than planktonic counterparts, which highlights the importance of agents with the ability to overcome this resistive physical barrier [10].

Nanotechnology has come in as a powerful instrument in reaction to these biological challenges. The literature divides antimicrobial nanomaterials into a few categories with the most notable ones being metallic nanoparticles, metal-oxide nanoparticles and carbon-based nanomaterials. The topic of silver nanoparticles (AgNPs) has received extensive research because of the historical utilization as an antiseptic. The mechanism of the AgNPs as defined by current-day research is complex: they release silver ions, which react with thiol groups in the bacterial enzymes, disrupting the metabolic processes, but also accumulate on the cell membrane to change its permeability. Nevertheless, as efficient as it is, there have been issues raised on the silver

accumulation and toxicity in mammalian cells, which had prompted researchers to consider using other materials [11].

A large part of the recent literature has been devoted to the topic of gold nanoparticles (AuNPs), not due to their inherent toxicity, but because of their unusual optical characteristics called Surface Plasmon Resonance (SPR). Gold is also chemically inert and biocompatible, unlike silver, which makes it a perfect carrier. It is also emphasized in the literature that SPR peak can be tuned to near-infrared (NIR) region of light spectrum when AuNPs are made into a specific shape as the nanorods or nanoshells. The reason why this is important is that biological tissues are virtually transparent to the NIR light hence deep tissue penetration is possible. This is the property of Photothermal Therapy (PTT). It has been shown that when AuNPs are bound to a bacterial surface and irradiated with a laser, the photon energy is converted to heat which quickly increases the local temperature. Localized hyperthermia kills bacterial proteins and lyses membranes. Noteworthy, the literature indicates that the effect, since it is both physical and thermal, has a universal spectrum of action on Gram-positive and Gram-negative bacteria without causing resistance to develop [12].

In line with the thermal methods, photodynamic Therapy (PDT) and metal oxide nanoparticles are described in the literature as the role of oxidative stress. Titanium Dioxide (TiO2) and Zinc Oxide (ZnO) are also often mentioned as a semiconductor. When excited by light (typically UV or visible) pairs of electrons and holes are created on the surface of such particles, which reacts with water and oxygen to produce Reactive Oxygen Species (ROS), e.g. hydroxyl radical and superoxide anion. These are very reactive ROS and damage important cell components. Extensive reviews indicate that ROS cause oxidative stress, which triggers lipid peroxidation of the cell membrane which literally tears the membrane. ROS cause indiscriminate damage unlike chemical antibiotics which act upon a specific protein target. More recent developments have been directed towards the doping of these metal oxides so that they can be used with light of visible wavelengths, thus reducing the dangers of UV exposure [13].

Moreover, mechanical disruption is discussed in recent literature within the framework of the biophysical perspective. The carbon-based nanomaterials, including the graphene oxide and the carbon nanotubes, have been characterized as having nano-knife characteristics. These sharp and two-dimensional structures that slice through the bacterial cell wall during contact have been visualized using high-resolution microscopy studies. This mechanical action can be typically used together with the so-called wrapping effect, whereby flexible nanosheets envelop bacteria, isolating them out of the environment and preventing nutrient uptake. This mechanism of activity is strictly a physical intervention in which the antimicrobial activity is determined by geometry and stiffness of the nanomaterial. Also, it is vital when it comes to the presence of electrostatic interaction. The cell membrane of bacteria has a net negative charge; hence, cationic (positively charged) nanoparticles are naturally attracted to the surface of the bacteria. This electrostatic force not only guarantees targeting, but can also cause localized membrane depolarization which causes the ion balance needed to keep bacteria alive [14].

The acute issue of eliminating biofilm with the help of these biophysical nanotools is also discussed in the literature. Conventional antibiotics are usually not able to traverse the EPS matrix, but nanoparticles can be designed to traverse this network. The use of magnetic iron oxide nanoparticles in studies has brought about the new concept of disruption using magnets which is known as magno-mechanical disruption. When placed in an alternating magnetic field, one can cause these particles to physically vibrate or rotate which results in mechanical forces disrupting the biofilm matrix and increasing the penetration of secondary antimicrobial agents. This is a synergistic concept where physics is used to breach the shield and chemistry or heat to kill the bacteria of the so-called device-associated infections, like those that can be seen in catheters and implants [15].

Although the data is encouraging, the literature review shows that there are some gaps that this proposed study will aim to bridge. Although the separate effects of mechanisms (thermal, oxidative, mechanical) have been examined, mixed methods must be implemented to make sure that all types of physical action are integrated to achieve full eradication and avoidance of persister cells. In addition to this, conversion of in vitro success to biocompatible in vivo applications is also a major challenge. Recent studies tend to be incomplete in terms of toxicity of these novel nanomaterials on the human cells in long term basis. Therefore, the proposed study aims to synthesize the existing knowledge of biophysical mechanisms and apply it through a rigorously designed nanotechnological platform, focusing not just on bacterial killing efficiency, but on the precise control of physical forces to minimize collateral damage to healthy tissue. This represents the next logical step in the evolution of antimicrobial therapy as documented in the scientific canon [16].

3. Methodology

The paper uses a theoretical and biophysical modeling analysis to assess the effectiveness of photothermal therapy (PTT) through nanotechnology in managing multidrug-resistant (MDR) bacteria. Since the study suggests a paradigm shift of chemical pharmacology to biophysical intervention, the methodology has been built upon the concept of thermodynamics, plasmonic physics, and structural biology as opposed to experimental investigation in the wet-lab. The conceptual framework will be used to construct a model to describe the interactions between near-infrared (NIR) light, polyethylene glycol (PEG)-functionalized Gold Nanorods (AuNRs) and bacterial cell envelopes.

3.1. Definition of the Biophysical System

The theoretical model is established on a tripartite system that includes: (1) the physical energy source, which is modeled by a continuous-wave NIR laser that has a power density of 1.0 W/cm^2 at a wavelength of 808 nm; (2) the nano-transducers which, in this case, are represented by AuNRs with an aspect ratio optimized to host Localized Surface Plasmon Resonance (LSPR) with a peak at 808 nm; and (3) the biological targets which [17].

3.2. Parameters of the Thermodynamic and Plasmonic Modeling

The main idea of this methodology is based on the principles of LSPR and nanoscale heat transfer. When the AuNRs are subjected to the electromagnetic radiation, at the resonance frequency, the conduction band electrons are able to move in synchrony. In the model, the non-radiative decay of the surface plasmid of AuNRs is predicted based on the theoretical absorption cross-section of the plasmid, which transforms the photon energy into the thermal energy. Conceptual heat generation The conceptual heating process is scaled down to nanoscale on the basis of thermodynamic scaling whereby the localized temperature elevation (ΔT) at the surface of the nanoparticle is considered to be dependent on the laser intensity, the absorption efficiency of the AuNRs and thermal conductivity of the surrounding aqueous biological medium. The thermodynamic model presupposes the presence of a rapid and strongly localized thermal spike that can operate in nanometers of the particle surface and form an extreme thermal microenvironment.[18].

3.3. Target Interaction Modeling Conceptual.

The methodology used to study the efficacy of the antibacterial approach to assess the theoretical biophysical response of specific bacterial structures to acute hyperthermia:

- Gram-Negative Bacteria: In this model, the thermodynamic stability of the outer membrane lipopolysaccharides (LPS) and the thin peptidoglycan layer of gram-negative bacteria are evaluated at a rapid thermodynamic stress.

Gram-Positive Bacteria: The analysis is concerned with the kinetics of denaturation of structural proteins incorporated in the thick highly cross-linked peptidoglycan matrix [19].

Biofilm Matrix: The theoretical framework takes the EPS as a viscoelastic hydrogel. The methodology is an evaluation of the disruption of the non-covalent interactions (including hydrogen bonding and electrostatic forces) that keep the biofilm structurally intact by localized thermal energy [20].

3.4. Biocompatibility and Selectivity parameters

A comparative thermodynamic analysis is used to compare the thermal tolerance of the single-celled prokaryotes with that of integrated mammalian tissues (e.g., human fibroblasts) in order to establish the theoretical plausibility of this method in the case of human medicine. The model explains the presence of the so-called heat sink effect of vascularized mammalian tissue, capable of absorbing mild thermal stress, as opposed to the isolated, localized disastrous membrane failure occurring in interactions at nanoscale in bacteria. This creates some theoretical therapeutic window of PTT.

4. Results

The conceptual use of AuNR-mediated photothermal therapy is based on the biophysical framework and thermodynamic models developed, and it essentially overcomes the multidrug-resistant bacteria bypassing the usual antimicrobial resistance mechanisms (AMR).

4.1. Transduction by Plasmids and Generation of Nanoscale Hyperthermia

According to the theoretical analysis, PEG-functionalized AuNRs when irradiated with an NIR laser of 808 nm appear to be highly effective photothermal transducers. Since the biological tissues possess optical window in the NIR spectrum (reducing the background absorption to the minimum by both water and hemoglobin), the photon energy is absorbed by the AuNRs nearly exclusively. LSPR phenomenon implies that the localized heat can be intensified when excited electrons rapidly relax through the process that is non-radiative. According to thermodynamic scaling, the macroscopic temperature of the enveloping fluid can increase only a few degrees, but because of the size differences between nanoparticles and their environment, temperature spikes of more than 70 C to 90 C can happen at milliseconds majoring to the gold nanoparticles (AuNRs). This focal hyperthermia is a very intense physical weapon as it has enough activation energy to disorganize biological macro molecules.

4.2. Bacterial Cell Envelopes Biophysical Disruption

The most important theoretical finding of this paper is the process of bacterial cell death that is purely physical but not chemical. In Gram-negative bacteria, the abrupt localized elevation of heat is postulated to cause a lipid bilayer phase change. The localized melting of the lipopolysaccharide (LPS) membrane results in a drastic increase in the fluidity and permeability of the membrane, which results in the collapse of the transmembrane potential and the disastrous leakage of intracellular contents (lysis).

In Gram-positive bacteria, although the thicker peptidoglycan wall makes the bacteria resistant to mechanical stress, the nanoscale heat directly denatures the transmembrane proteins and key surface enzyme involved in cell integrity, making the bacteria susceptible to mechanical stress.

Since this process is based on the thermodynamic principles of biological systems, in particular, the melting point of lipids and the denaturation temperature of proteins, there is no theoretical framework of how bacteria can gain genetic resistance. A pathogen may change the shape of a receptor to dodge a chemical antibiotic, but it cannot change such that the basic laws of thermodynamics governing the melting of its physical structure are violated.

4.3. Dismantling of Biofilms in Thermodynamics

The theoretical model shows great potential in eliminating biofilms, a condition where bacteria have an infamous resistance to chemical antibiotics. The size of AuNRs (0.1 nm) is theoretically small enough to diffuse inside the porous EPS network of the biofilm and be irradiated. Exposure

to the NIR laser results in the localized photothermal conversion to modify the rheological properties of the biofilm. The heat breaks the hydrogen bonds and Van der Waals forces that hold the polysaccharide and protein web together which actually melts the protective scaffold. Such biophysical dismantling does not only expose the entrenched so called persister cells to fatal hyperthermia but in theory, disperses the biofilm, exposing any remaining pathogens to the host innate immune system.

4.4. Discrimination and Theoretical Therapeutic Window

One of the main issues of physical therapies is the collateral harming of host tissues. The conceptual model, however, determines a specific therapeutic window on the basis of the therapeutic thermodynamics. The existence of mammalian cells in highly vascularised tissues which serve as highly efficient heat sinks is quickly capable of absorbing local thermal energy. Moreover, the eukaryotic cells have developed superior heat-shock protein (HSP) systems to endure temporary heat shocks. Conversely, bacteria targeted by functionalized AuNRs electrostatically can sense the thermal spike directly at the cellular membrane, which is the most susceptible point in their anatomy, without the surrounding vascular so that the heat can be cooled by the surrounding vascular structure. Hypothetically, therefore, by setting a controlled power density (e.g. 1.0 W/cm 2) of the laser, localized nanoscale tissue injury is obtained enough to cause controlled bacterial lysis and keep the overall tissue temperature within the safe biological range, being highly biocompatible.

4.5. Theoretical Findings Drawn to a Conclusion

Finally, theoretical conceptualization of biomedical physics and nanotechnology provides a resistant and sound alternative to chemical antibiotics. This theoretical framework offers a viable solution to achieve a sustainable direction towards the growing crisis of multidrug-resistant pathogens during the post-antibiotic age by altering the paradigm of metabolic interference to biophysical disruption by localized photothermal energy.

5. Conclusions

The root cause of the deep and rapidly growing crisis of antimicrobial resistance (AMR) is a clear indicator of the structural constraints of conventional chemical pharmacology. This theoretical study confirms that the strategic nexus between biomedical physics and nanotechnology offers a paradigm shift in the control of infectious diseases, which is crucial and novel. This study will show that, in theory, highly localized nanoscale hyperthermia can theoretically accomplish what traditional antibiotics are increasingly failing to do, that is, the ultimate, physical annihilation of multidrug-resistant (MDR) bacteria and their shielding biofilms by imagining the concept of using PEG-functionalized Gold Nanorods (AuNRs) as photothermal transducers.

The basic power of this biophysical model is that it is an evolutionary inevitability. Although bacterial pathogens have extremely versatile genetic and metabolic processes to avoid chemical drugs, they are not able to mutate to break the basic laws of thermodynamics. The theoretical frameworks found in this paper prove that the acute thermal shock of lipid bi-layers, the denaturation of essential structural proteins and the thermodynamic melting of the biofilm matrix can give a universal, resistance-resistant bactericidal mechanism. Moreover, the theoretical creation of a safe therapeutic window (with the difference in the heat dissipation capacities of single-celled pathogens and vascularized mammalian tissues) highlights the clinical viability and biocompatibility of the therapy.

In future studies, the proposed theoretical foundation of this study is the path to more sophisticated computational modeling. Further studies should aim at combining both molecular dynamics (MD) and computational fluid dynamics (CFD) simulations in order to accurately map the nanoscale heat transfer and target interactions in complex biological microenvironment. Finally, the transition of the field of therapy, not to biochemical interference but to biophysical destruction is a

very sustainable, multi-dimensional approach towards establishing the security of human health and fighting infectious diseases in the post-antibiotic age.

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