DNA fragments, which is ideal for rapid detection using the MAMEF (Microwave-Accelerated Metal-Enhanced Fluorescence) platform[3], as well as diminishing the effects of DNases due to the elevated lysing temperatures.

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1576-Pos Board B527

Rapid Microbial Lysing and DNA Fragmentation by Microwave Focusing

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Bacterial infections are a major health problem worldwide. Identification of disease-causing organisms by culture-based approaches is time-consuming and often lacks sensitivity. Molecular approaches such as PCR and microwave-accelerated metal-enhanced fluorescence (MAMEF) assays1, are more sensitive and faster than traditional culture-based approaches, but require isolation of the target DNA. In order to determine the effect of both boiling and microwave irradiation on microbial lysing and DNA fragmentation, cultures of Neisseria gonorrhoeae and Listeria monocytogenes (108 CFU /mL) were either boiled (range 40° - 70°C) or lysed in a 900-watt microwave on isolator-mounted microscope slides, both with and without the assistance of disjointed antenna gold bow-tie structures. The temperatures of cultures were obtained prior to and after lysing and the resulting lysate cultured on selective agar plates. DNA isolation and fragmentation efficiency were determined by gel electrophoresis and PCR. N. gonorrhoeae lysed at a lower temperature (°C) than L. monocytogenes. Microbial lysing and DNA fragmentation was more effectively carried out in the presence disjointed gold triangle structures, but only when small sample volume were used. Standard boiling was successful for bacterial lysing and DNA fragmentation, but required higher temperatures and longer times than microwave focusing. PCR results suggest that low power microwave irradiation is ideal for PCR methods while higher microwave powers are required to generate DNA fragments ideal for MAMEF analysis. Microbial lysing and DNA fragmentation can be achieved by either boiling or microwave, but microwave lysing is more efficient for DNA fragmentation and is significantly faster. Microwave lysing is the recommended method when rapid isolation and DNA fragmentation is required.

1Melendez, et at. (2013). Blind Evaluation of the Microwave-Accelerated Metal-Enhanced Fluorescence Ultrarapid and Sensitive Chlamydia Trachomatis test by use of Clinical Samples, Journal of Clinical Microbiology, 51(9), 2913-2920.

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Palmitate Re-Directs Glucose Utilization in Type 2 Diabetic Hearts, Improving Function: A Metabolomic-Fluxomic Study

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Hyperglycemia and hyperlipidemia are two main traits of type-2 diabetes (T2DM). T2DM patients may develop a cardiomyopathy, and the excess in nutrients greatly contributes to systolic and diastolic dysfunction. The Randle cycle postulates that fatty acid (FA) utilization further impairs glucose utilization, impeding its oxidation. Yet recent evidence suggests that, when acutely infused, FAs such as palmitate (Palm) actually help in maintaining function in T2DM hearts stressed with high glucose and catecholamines. Thus, under conditions of sustained stress, lipids may be necessary to maintain function in stressed T2DM hearts. Using a novel procedure for translating metabolomics into metabolic fluxes, here we tested whether Palm is able to redirect the glucose fluxome in T2DM hearts, contributing to a better utilization/oxidation of glucose. We found that Palm, without inhibiting glycolysis, led to a 50% increase in glucose oxidation via the pentose phosphate [PP] pathway. Palm presence shifted the control of the glycolytic flux from phosphofructokinase to glucose uptake, glucose 6-phosphate dehydrogenase and glycogenolysis. Palm-induced remodeling of the glucose fluxome decreased the intracellular levels of glucose by 17-fold, owing to reduced uptake at maintained utilization. Moreover, it augmented the content of reduced GSH, via higher NADPH generation through the PP pathway. Our study provides a mechanistic explanation to the in vitro observation that FAs such as Palm are necessary for the T2DM hearts to maintain function when in presence of hyperglycemia and/or increased workload, by remodeling glucose utilization leading to a higher supply of reducing equivalents to the heart. Present findings suggest that in T2DM subjects the Randle cycle may apply to some but not all pathophysiological contexts.

1578-Pos Board B529

Modeling Host - Bacterial Biofilm Interactions in Lower Leg Chronic Wounds

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Chronic wounds are caused by a healing process often stalled at the inflammation, proliferation stages of repair. Each chronic wound displays its own dynamics in a complex 3-dimensional interplay of repair against a range of obstructing factors. These may include host and bacterial genetic makeup, medical and environmental conditions, counter-productive habits and the presence of an opportunistic poly-bacterial biofilm. Currently there is a rapidly growing need to create a treatment plan upon assessment of a wound followed by regular quantitative monitoring. Understanding the spatial and temporal variations in biochemical and biophysical wound parameters will aid a timely healing process. In-silico simulations can support these efforts by modeling the influence of the various factors. Examples are: proper use of smart wound dressings and prevention of the build-up of antibiotic tolerance and resistance.
We present results based on expansions of published models to simulate the destruction of wound bed collagen, the dynamic interplay of host neutrophils, macrophages, fibroblasts and keratinocytes against the detrimental effects of bacterial metalloproteinases (MMPs) under normal, low-oxygen or anaerobic conditions. These simulations also allow to assess the influence of a biofilm even though most of its interactions with host chronic wound-tissue are barely known or understood With growing knowledge computer modeling will aid in management of individual chronic wounds.

1579-Pos Board B530

Model for Aging and Cognitive Decline

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A population of neurons in the cerebral cortex of humans and other mammals organize themselves into vertical microcolumns perpendicular to the pial surface. Anatomical changes to these microcolumns have been correlated with neurological diseases and normal aging, and in particular in area 46 of the rhesus monkey brain the strength of microcolumns was shown to decrease with age. We have previously developed a model to simulate aging brains by constructing a microcolumnar network of neurons and allowing the neurons to undergo Brownian motion while being constrained by a harmonic force that weakens as a function of age. Now, we expand on this model by constructing and simulating the generated neural networks. By generating a young neural network from strong restorative forces, one can create an initial distant dependent connectivity. Then, we age these networks and presume that connectivity between neurons either weakens or severs as a function of neural displacement from initial neuronal positions. We aim to show that older networks are unable to efficiently shift between different firing regimes, providing a potential mechanism for loss of information processing in relation to microcolumnar structure.

Molecular Dynamics II

1580-Pos Board B531

Comparison of Activation Energy and Pore Dynamics in Liquid and Gel Phases of Electroporated Lipid Bilayers using Temperature Dependent MD Simulations

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The molecular level understanding of electroporation has been studied by few research groups [1, 2, 3] over the last decade. We have performed molecular dynamics simulation(MDS) of electroporation at different temperatures to find activation energy as well as pore dynamics in the gel and liquid phases of POPC and DPPC lipid bilayers.
The MDS of bilayers were performed using NAMD, the Particle mesh Ewald(PME) method, the all-atom CHARMM force field and an integrated time-step of 2 fs.
The bilayers were composed of 256 lipids which were solvated with TIP3 water molecules with a low KCl concentration. The MD simulations were performed in temperature range from 250 K to 350 K with varying electric fields (0.02 to 1 V/nm).
A plot of pore initiation rate as a function of inverse temperature showed Arrhenius type behaviour. The activation energy was determined to be 25.5 and