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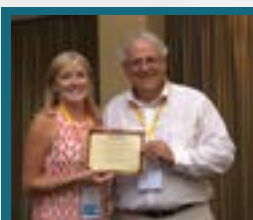
21<sup>st</sup> International Conference and Exhibition on  
**Materials Science and Chemistry**

**33<sup>rd</sup> Annual European Pharma Congress**

5<sup>th</sup> World Summit on  
**Renewable Energy**

March 13-14, 2023

Frankfurt, Germany



## Scientific Tracks & Abstracts

## Immobilizing lipase on hydrophobic wrinkled silica nanoparticles from a water/oil mixture as a strategy to induce hyperactivation

Valeria Califano

Institute of Sciences and Technologies for Sustainable Energy and Mobility (STEMS), Italy

Wrinkled Silica Nanoparticles (WSNs) with central-radial pore structure were hydrophobized by chemical vapor deposition of perfluorodecyltriethoxysilane (PDTES): surface functionalization was used to design a hydrophobic surface to induce interfacial activation of lipase by lid opening. In fact, lipases are unique often require interfacial activation for full catalytic performance. Actually, since lipids are water insoluble, lipases act on emulsified systems. Upon adsorption at a hydrophobic/hydrophilic interface, lipase undergoes a conformational change from the inactive to the active conformation. This change is promoted by the movement of a helical loop from the 'closed' form in which the catalytic site is inaccessible to the 'open' active one. To further modulate the closed/open form equilibrium, n-hexane was added to the water/lipase solution, creating a micro-oily environment [Figure 1].



Figure 1. Hydrophobization of wrinkled silica nanoparticles and lipase immobilization procedure

Three different supports were prepared, varying the degree of hydrophobicity. The effect of the different hydrophobicity and of the addition of n-hexane on the adsorption of lipase was evaluated. The best biocatalyst obtained was tested in the transesterification of sunflower seed oil to produce biodiesel, showing hyperactivation. The reaction yields were 93% for the immobilized enzyme and 56% for the free one. The results suggest that both the hydrophobicity of the support and the addition of n-hexane favor the adsorption of lipase in the active conformation.

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**Methodology:** Physicochemical characterization of supports was carried out by solid state <sup>29</sup>Si Nuclear Magnetic Resonance (NMR), the Brunauer–Emmett–Teller (BET) method, Thermo-Gravimetric (TG) analysis, Contact Angle (CA) measurement, Scanning Electron Microscopy (SEM) and Fourier Transform Infrared (FT-IR) Spectroscopy.

### **Biography**

Valeria Califano Graduated in Industrial Chemistry at the University of Naples Federico II, She obtained her doctorate in 2005 at the Laboratoire de Physico-Chimie des Matériaux Luminescents (LPCML) at Claude Bernard Lyon University, France. The PhD thesis focused on the "Structural study of oxide-based glasses for non-linear optics: growth of nanostructures and the effect of an electric field ('poling')." From 2006 to 2009 she worked as a research fellow in the Applied Optics laboratory of the Ettore Pacini Department of Physics, at the Federico II University of Naples. In 2009 she won a scholarship at the then Istituto Motori (CNR), now STEMS, where she became a researcher in 2011. Her research field ranges from the immobilization of enzymes for the production of liquid biofuels, to CO<sub>2</sub> capture by hybrid materials based on mesoporous silica and amines, laser deposition of thin films and formulation, characterization and analysis of the combustion of water/oil emulsions.

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Christian Schafer, Glob J Res Rev 2023, Volume 11

## **Identifying the sweet spots in milestone decision making–Monte Carlo simulation of net present value for pipeline projects in pharma**

**Christian Schafer**

Baden-Württemberg Cooperative State University Mannheim (DHBW), Germany

Uncertainty is by definition an unpreventable aspect of all projects. In the pharmaceutical industry development projects for a New Chemical/Biological Entity (NCE/NBE) are generally associated with low probabilities of success compared to other industries. Assessing the sweet spots of favourable risk-return-relationship in milestone decision making of pipeline projects–also under a portfolio point of view–is tricky but nicely achievable.

At start of development, a project's rate of success is only 4% to 7%, the time span of a project from start of development to the potential launch of a product being 10 years or even more. Thus, effective management of commercial risk and uncertainty becomes tremendously important.

The Pharmaceutical Benchmark Forum in the United States collected industry-wide historical data on the drug development process. The result of this research shows that the total project development costs for a NCE which reaches the market are in the range of \$1 billion. The actual costs of a successful project are usually significantly lower, but every successful project needs to cover the costs of multiple other projects which did not in the end reach the market.

In addition to the low success rates of pure development, further uncertainties affect the continuation of a project and its final accomplishment. Examples are commercial risks like the potential competitive landscape a product faces at launch, the uncertainty whether a certain Target Product Profile (TPP) can be achieved, pricing, market access risks and others (the TPP defines the potential product characteristics and benefits, like the drug's efficacy, safety and formulation at launch). All these factors are dynamic over time, thus complicating the forecasting of these projects. As the development progresses over the years the potential TPP evolves gradually, resulting in success or failure–and therefore financial gain or loss.

The path to get FDA's and EMA's approval to market a new drug is uncertain and the project must overcome several hurdles. So best informed milestone decisions must be taken. The–at least historical–success rates and time spans for each development step are known and can be used as a proxy for the implied future success rates in a Monte Carlo Simulation Model.

**To summarize:** The mixture of high and early upfront investments and a high uncertainty about a project's development and commercial success puts pressure on forecasting and even more on controlling, which aims to show a balanced picture of the project's opportunities and risks. Here the reliability and transparency of strategic forecasts become key success factors to support senior management in their decision-making process. Often

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risk and uncertainty are (closely) intertwined, leading to misinterpretation of forecasts and erroneous decisions.

Patient-based strategic forecasts, with certain base, best and worst-case scenarios are an important source of information within the process of development. Even though, these types of forecasts all plan for success of the project, which is human nature. But unfortunately, this is the case associated with the lowest likelihood compared to the unfortunate more likely failure of a pharmaceutical pipeline project.

To make this risk of failure transparent, Monte Carlo Simulation is a useful and powerful method to simulate each project's Net Present Value (NPV) distribution at each time, a milestone decision must be taken. When combining these NPV simulation results with the patient-based scenario forecasts, Senior Management can compare different projects more equally and should be able to manage a company's overall portfolio development risk more accurately and take more informed decision. Monte Carlo Models do not need to be over complex and as such are nicely explainable to Management, which generates trust in the results. Without trust in the validity of the method a forecast is worthless. That's a big plus compared to other even more sophisticated forecasting methods.

There is a high degree of competition between the different pipeline projects of a company to get budget for the next phase of development. So the NPV simulation of each project should be standard information included at each milestone decision to be taken. It's not only the commercial attractiveness of a new product, measured in peak sales, which plays a role. It's like in other businesses: Identify the sweet spot of a favourable risk and return relationship to run a company's pipeline development successful and maximize a company's mid to long term wealth.

## **Biography**

Christian Schäfer is a Full-Professor at the Department of Business Administration at Baden-Württemberg Cooperative State University Mannheim (DHBW) Germany. He teaches quantitative Methods, simulation in strategic forecasting and market research in healthcare. His research interests are in the fields of quantification of uncertainty, *Patient-Behaviour-Modelling* and Partial Least Squares Structural Equation Modeling (PLS-SEM). He also runs special forecast-simulation and market research projects for the Pharmaceutical Industry. Prior to taking this role in 2015, he covered different Management and Director Positions in Marketing, Competitive Intelligence, Strategic Forecasting and PM-Strategy within two International Pharmaceutical Company for 8 years. He earned a Diploma (Master) in Economics, a Master of Business Administration (MBA) degree from University of Gavle, Sweden and received his PhD (Dr.) from the Department of Business Administration and Economics at Johannes Gutenberg-University Mainz, Germany, where he worked 4 years as a research assistant. He published more than 25 articles and 4 Books.

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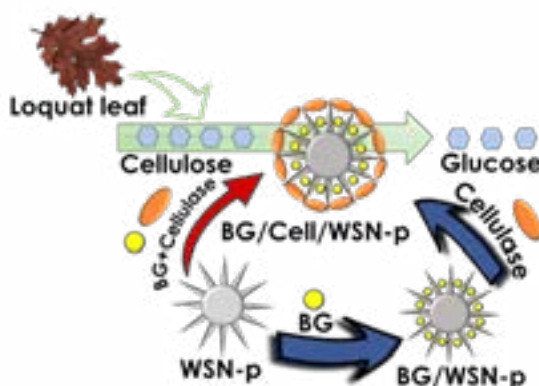
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## Efficient and easy physical co-immobilization procedure of cellulase and $\beta$ -glucosidase into wrinkled silica nanoparticles for the hydrolysis of cellulose extracted from agricultural waste

Aniello Costantini

University of Naples Federico II, Italy

The efficiency of cellulose hydrolysis is negatively affected by the low amount of  $\beta$ -glucosidase (BG) contained in fungal cellulase enzyme cocktail. So, we implemented a strategy to physically co-immobilize  $\beta$ -glucosidase and cellulase on Wrinkled Mesoporous Silica Nanoparticles (WSNs) to enhance glucose production. WSNs are nanoparticles with radial and hierarchical open pore structure, exhibiting smaller (WSN) and larger (WSN-p) inter-wrinkle distance depending on the synthesis strategy. The immobilization was carried out separately on different vectors (WSN for BG and WSN-p for cellulase); simultaneously on the same vector (WSN-p) and sequentially on the same vector (WSN-p) in order to optimize the synergy between cellulase and BG. The obtained results highlighted that simultaneous immobilization of BG and cellulase on the same vector (WSN-p) results in the best biocatalyst. In this case, the adsorption resulted in 20% yield of immobilization, corresponding to an enzyme loading of 100 mg/g of support. 82% yield of reaction and 72  $\mu\text{mol}/\text{min}\cdot\text{g}$  activities were obtained, evaluated for the hydrolysis of cellulose extracted from *Eriobotrya japonica* leaves. All reactions were carried out at a standard temperature of 50°C. The biocatalyst retained 83% of the initial yield of reaction after 9 cycles of reuse. Moreover, it had better stability than the free enzyme mixture in a wide range of temperatures, preserving 72% of the initial yield of reaction up to 90°C [Figure 1].



**Figure 1.** Graphical scheme of the whole process of glucose production from lignocellulosic biomass (*Eriobotrya japonica* leaves), highlighting the different strategies followed for enzyme co-immobilization.

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## **Biography**

Aniello Costantini is Professor of Chemistry since December 2004 in the Department of Chemical Engineering, Materials and Industrial Production at the University of Naples Federico II. He received his Master Science (Laurea) in Engineering with full marks and honours from the University of Naples Federico II. He received his PhD in Materials Engineering from the same University. Until January 2023, he appears as author in more than 111 publications in international high quality peer reviewed journals. His research work has been focused on the synthesis of glasses, ceramics, glass-ceramics and nanostructured hybrids. He is highly skilled in synthesis and functionalization of ceramic nanostructures through sol-gel method. Accurate design of process parameters has been exploited to produce ceramic and hybrid nanostructures, tuning size, shape and surface chemistry to obtain bioactive hybrids and nanocomposites, multifunctional coatings, smart drug delivery carriers, mesoporous silica materials as supports for enzyme immobilization.

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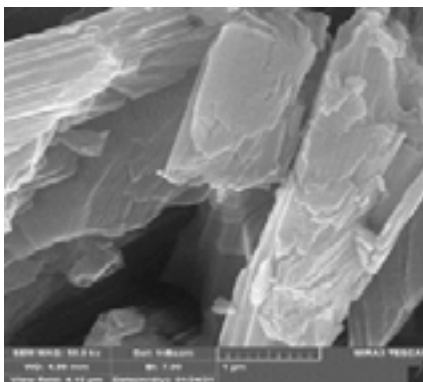
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## Investigation of magnetosome as the magnetic targeting drug delivery system for Sorafenib tosylate anticancer drug

**Gholamhossein Sodeifian**  
University of Kashan, Iran

**H**epato-Cellular Carcinoma (HCC) is the fifth prevalent malignant tumor having the third rank in the global mortality chart. Sorafenib tosylate (SFB) is approved as the first anticancer drug for the treatment of HCC. According to the Biopharmaceutical Classification Scheme (BCS), SFB belongs to class II compounds that indicate a very poor solubility in the aqueous solution at different pH values from pH=1.2 to pH=7.4 (slow dissolution rate within the gastrointestinal tracts) and high permeability from the gastrointestinal lumen. The drug has low oral bioavailability (8.43%); consequently, high dose treatment is necessary which may cause the systemic toxicity. Nanotechnology based novel drug delivery systems are applied to design the systems with improved biocompatibility and biodegradability which can deliver the drug molecule efficiently and safely to the target tissue thus decrease the side effects, especially for drugs with narrow therapeutic index or cytotoxic effects. In this research, for the first time, the magnetosome was developed as the biocompatible nanocarrier with improved drug encapsulation efficiency (up to 77%), extended stability, proper particle size (<150 nm) and industrial upscaling (Mozafari method was applied to prepare the tocosome) for controlled drug delivery of sorafenib tosylate to cancerous tissue. The optimum composition of tocosome was determined based on particle size and drug loading and then it was used to prepare the magnetosome [Figure 1]. In addition, the effect of phosphatidylcholine on the properties of Super Paramagnetic Iron Oxide (SPIO) nanoparticles was examined. The prepared nanocarrier can improve bioavailability of drug and be used in the hyperthermia and controlled and targeted release of drug particles.



**Figure 1.** FE-SEM images of original SFB and Magnetosome suspension.



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## Biography

Gholamhossein Sodeifian (1971) graduated in chemical engineering (M.S) from University of Tehran, in 1997 and received his doctorate (PhD), in polymer engineering from Tarbiat Modares University, Tehran, in 2002. He is currently academic member of Chemical Engineering Department of University of Kashan. His research group focused on extraction of essential and seed oils, solubility measurement of solid medicines and micro and nanoparticle formation of pharmaceutical materials in Supercritical Carbon Dioxide (SCCO<sub>2</sub>) via various methods. He has also developed, for the first time in the world; a new and efficient technique for nanoparticle formation, i.e., Ultrasonic assisted Rapid Expansion of Supercritical Solution into a Liquid Solvent (US-RESOLV). He has published more than 83 ISI scientific papers and several books. Furthermore, he has developed Sodeifian's model for drugs solubility. He has been assigned and included in the worlds' top 2% of scientists list in 2021 and 2022.

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Anahita Rabii, Glob J Res Rev 2023, Volume 11

## **Optimization of anaerobic co-digestion of multiple feedstocks for bioenergy recovery: An empirical model application**

**Anahita Rabii**

Toronto Metropolitan University, Canada

**T**ransition from wastewater treatment facilities as energy consumers to resource recovery facilities with ability to produce energy and value-added products is achievable by optimizing digestion capacity with the existing infrastructure. This study investigated a novel method for optimizing anaerobic digestion of multiple feedstocks for biomethane recovery. A series of experiments were conducted to develop an empirical model for optimizing the mixing ratio based on lipids, proteins and carbohydrates ratios of the feedstocks as compared to carbon to nitrogen (C:N) or COD to nitrogen ratio (COD:N). The selected feedstocks were real municipal wastes including dairy manure; Source Separated Organic (SSO) and Thickened Waste Activated Sludge (TWAS). The experimental data were fitted into the proposed second order polynomial model. The COD:N ratios of TWAS, manure and SSO were 15, 47 and 27 respectively. For the co-digesters, COD:N varied from 19 to 40. The lipids:proteins:carbohydrates ratios were 1:10:4, 1:4:20 and 1:1.6:9 for TWAS, manure and SSO respectively. Among them SSO had the most ultimate methane production and methane yield corresponding to 1373 mL and 332 mL CH<sub>4</sub>/g COD added. The minimum ultimate methane production and the methane yield occurred at TWAS mono digestion corresponding to the COD:N ratio of 15 and lipids:proteins:carbohydrates ratio of 1:10:4. The results indicated that both minimum ultimate methane and minimum methane yield values occurred at TWAS mono digestion corresponding to the COD:N ratio of 15 and lipids:proteins:carbohydrates ratio of 1:10:4. On the other hand, the maximum ultimate methane and methane yields occurred at the mixing ratios of 2:4:4 corresponding to the COD:N ratio of 28 and lipids:proteins:carbohydrates ratio of 1:3:12 in co-digestion of TWAS/manure/SSO.

### **Biography**

Anahita Rabii obtained her PhD in Civil-Environmental Engineering from Toronto Metropolitan University and is focused on waste to energy conversions. Currently her expertise is harnessed with Anaergia Inc. North America, in resource recovery. She and the engineering group at Anaergia Inc. are developing leading industry innovations by taking waste and wastewater treatment technologies to a whole level of energy conversions by anaerobic digestion and co-digestion. She is Chair of Magazine Committee at Water Environment Association of Ontario and is a Sessional Lecturer at George Brown College in Toronto, Ontario, Canada.

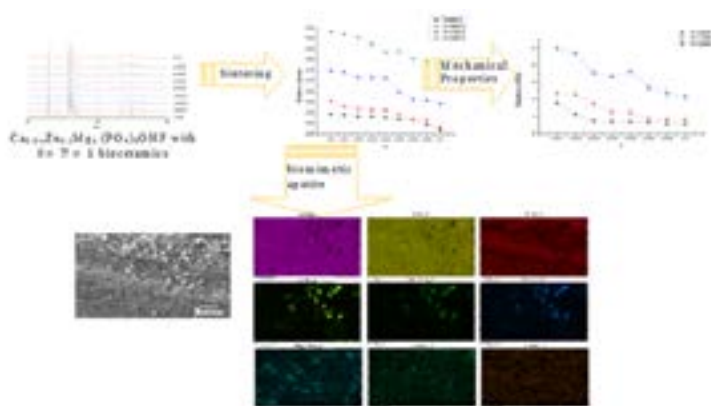
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## Hydroxyapatite bioceramics doped with ions for orthopedic and dentistry surgery

**Mustapha Hidouri**

Gabes University, Tunisia

Bioceramics designed to replace failing bone, teeth and dentins have two important properties: biocompatibility and the ability to absorb at a rate comparable to bone growth. Because of its close similarity to the inorganic mineral components of the bone and teeth, calcium phosphate, and particularly hydroxyapatite (HAp,  $\text{Ca}_{10}(\text{PO}_4)_6\text{OH}_2$ ), is the most widely used bioceramics in a variety of biomedical applications, most notably orthopedics and dental repair. Indeed, due to the complexity of the chemistry of bone and dentine, which contain multiple elements, no identical to natural material has been discovered. All existing research has attempted to obtain the most comparable material. Several attempts have been made to introduce as many ions as possible into the structure of the HAp. As a result, magnesium  $\text{Mg}^{2+}$ , strontium  $\text{Sr}^{2+}$ , zinc  $\text{Zn}^{2+}$ , sodium  $\text{Na}^+$ , potassium  $\text{K}^+$ , carbonates  $\text{CO}_3^{2-}$ , fluorures  $\text{F}^-$ , and chlorine ions  $\text{Cl}^-$  have been incorporated into the apatite structure. Several techniques (DRX, FTIR, chemistry analysis, G-DTA, RMN 31P, Raman, SEM) were used to verify the purity of the materials and confirm the ions' incorporation into the structure. The materials were pressure-less sintered, and the densification conditions were optimized. The densest materials have also been mechanically characterized. The biological properties of dense bodies have been tested in vitro, and the bioactivity and biocompatibility of the materials have been determined. In the final stage, the appropriate materials were tested in vitro for their potential use as implants [Figure 1].



**Figure 1.** Densification, mechanical and biological characterization of multiple substituted hydroxyapatite bioceramics.

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## **Biography**

Mustapha Hidouri is a Teacher-Researcher in the field of materials and environment. He received his PhD in [Materials Chemistry](#) in 2004. Currently he occupied the post of associate professor at Gabes University, Tunisia. His researches deal with biomaterials and environmental studies. He published more than 25 papers and 2 books and presented more than 30 oral and poster presentations in scientific congresses. His is a reviewer in many impacted journals.

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