Journal of Cellular and Molecular Pharmacology

Franklin et al., J Cell Mol Pharmacol 2023, 7:2

Mini Review Open Access

Nanocarrier Transport and Reaction Modelling for Cancer Therapies Using Experimental and in Silico Methods

Benjamin Franklin, Rosalind Franklin and Sigmund Freud*

Department of Life Sciences, School of Pharmacy, Malaysia

Abstract

Nanocarriers composed of liposomes, micelles, polymeric nanoparticles and others have proven excellent possibilities in the discipline of centered drug delivery, in particular in most cancers therapy. Functionalisation of nanomaterials via simultaneous assembling of chemical moieties has been a approach of broad interest, to collect houses such as toughness in circulation, web site specificity and stimuli sensitivity. Imparting multifunctionality to nanocarriers controls their organic interplay in a preferred trend and enhances the efficacy of remedy and diagnostic protocols. Here, we try to evaluate the utility of a variety of nanocarrier structures for centered drug shipping and present day techniques for the improvement of multifunctionality on nanocarrier systems. Protein-based nanocarriers have received vast interest as colloidal service structures for the shipping of anticancer drugs. Protein nanocarriers possess a variety of benefits consisting of their low cytotoxicity, ample renewable sources, excessive drug-binding capacity, and giant uptake into the focused tumor cells. Moreover, the special protein shape gives the opportunity of site-specific drug conjugation and tumor focused on the usage of a range of ligands enhancing the floor of protein nanocarriers.

Keywords: Hypertension; Angiotensin-converting enzyme; Blood pressure; Mechanisms of action

Introduction

Nanocarrier Transport and Reaction Modelling for Cancer Therapies Using Experimental and In Silico Methods Cancer remains one of the most challenging diseases to treat, necessitating the development of innovative therapeutic strategies. Nanomedicine has emerged as a promising field in the fight against cancer, offering the potential to enhance drug delivery and improve treatment outcomes. Among various nanoscale drug delivery systems, nanocarriers have shown great potential in improving drug solubility, stability, and targeted delivery to cancer cells. However, the efficient transport and controlled release of therapeutic payloads from nanocarriers within the complex tumor microenvironment present considerable challenges [1]. To address these challenges, researchers have turned to the development of sophisticated transport and reaction models that integrate experimental and in silico methods. Experimental techniques allow for the characterization and evaluation of nanocarrier behavior under specific conditions, providing crucial data on transport mechanisms, drug release kinetics, and interactions with the biological milieu. On the other hand, in silico modeling leverages computational tools and simulations to predict and optimize nanocarrier behavior, providing a cost-effective and time-efficient means of screening and designing drug delivery systems. In this context, nanocarrier transport and reaction modeling have emerged as valuable tools for understanding and optimizing cancer therapies [2]. These models can provide insights into the factors influencing nanocarrier behavior, such as physicochemical properties, surface modifications, and interactions with the tumor microenvironment. Moreover, they enable the prediction and optimization of drug release profiles, dosing schedules, and treatment outcomes. Experimental methods for nanocarrier transport and reaction modeling involve a range of techniques, including microscopy, spectroscopy, and biophysical assays. These techniques allow researchers to track the movement of nanocarriers within biological systems, study their interactions with cellular components, and monitor drug release kinetics [3].

Experimental Methods for Nanocarrier Characterization

Nanocarrier synthesis and characterization techniques: Various synthesis methods such as emulsion, nanoprecipitation, solvent evaporation, and self-assembly are employed to create nanocarriers. The size, shape, and surface characteristics of nanocarriers can be controlled during synthesis. Dynamic Light Scattering (DLS) or Photon Correlation Spectroscopy (PCS) measures the size distribution of nanocarriers in a suspension. Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM) provide high-resolution imaging to visualize the morphology and structure of nanocarriers. Atomic Force Microscopy (AFM) allows for topographical analysis and surface characterization of nanocarriers. X-ray Diffraction (XRD) provides information on the crystalline nature of nanocarriers.

Assessment of physicochemical properties: Fourier Transform Infrared Spectroscopy (FTIR) identifies functional groups and chemical bonds present in nanocarriers. Zeta Potential measurement determines the surface charge of nanocarriers, which influences their stability and interaction with biological entities. Thermogravimetric Analysis (TGA) and Differential Scanning Calorimetry (DSC) analyze the thermal stability and phase transitions of nanocarriers. Porosity and Surface Area Analysis methods, such as Brunauer-Emmett-Teller (BET) analysis, quantify the porosity and surface area of nanocarriers.

Evaluation of stability and drug loading efficiency: Stability studies assess the physical and chemical stability of nanocarriers over time, evaluating parameters like size, aggregation, and drug leakage. Drug Loading Efficiency (DLE) measures the amount of drug loaded within nanocarriers and is determined using techniques such as UV-

***Corresponding author:** Sigmund Freud, Department of Life Sciences, School of Pharmacy, Malaysia, E-mail: sigmundfreud12@gmail.com

Received: 27-Mar-2023, Manuscript No: jcmp-23-100982; **Editor assigned:** 29-Mar-2023, Pre QC No: jcmp-23-100982 (PQ); **Reviewed:** 13-April-2023, QC No: jcmp-23-100982; **Revised:** 18-April-2023, Manuscript No: jcmp-23-100982 (R); **Published:** 25-April-2023; DOI: 10.4172/jcmp.1000148

Citation: Franklin B, Franklin R, Freud S (2023) Nanocarrier Transport and Reaction Modelling for Cancer Therapies Using Experimental and in Silico Methods. J Cell Mol Pharmacol 7: 148.

Vis spectroscopy, High-Performance Liquid Chromatography (HPLC), or Mass Spectrometry (MS).Encapsulation Efficiency (EE) calculates the percentage of drug effectively encapsulated within nanocarriers.

Tracking nanocarrier biodistribution and tumor targeting: Fluorescence Labeling or Quantum Dots can be used to track nanocarriers and visualize their distribution in vitro and in vivo. Positron Emission Tomography (PET), Single-Photon Emission Computed Tomography (SPECT), or Magnetic Resonance Imaging (MRI) techniques can be employed for non-invasive tracking and biodistribution studies. Flow Cytom Experimental Methods for Nanocarrier Characterization.

Nanocarrier synthesis and characterization techniques: Various synthesis methods such as emulsion, nanoprecipitation, solvent evaporation, and self-assembly are employed to create nanocarriers. The size, shape, and surface characteristics of nanocarriers can be controlled during synthesis. Dynamic Light Scattering (DLS) or Photon Correlation Spectroscopy (PCS) measures the size distribution of nanocarriers in a suspension. Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM) provide high-resolution imaging to visualize the morphology and structure of nanocarriers. Atomic Force Microscopy (AFM) allows for topographical analysis and surface characterization of nanocarriers. X-ray Diffraction (XRD) provides information on the crystalline nature of nanocarriers.

Assessment of physicochemical properties: Fourier Transform Infrared Spectroscopy (FTIR) identifies functional groups and chemical bonds present in nanocarriers. Zeta Potential measurement determines the surface charge of nanocarriers, which influences their stability and interaction with biological entities. Thermogravimetric Analysis (TGA) and Differential Scanning Calorimetry (DSC) analyze the thermal stability and phase transitions of nanocarriers. Porosity and Surface Area Analysis methods, such as Brunauer-Emmett-Teller (BET) analysis, quantify the porosity and surface area of nanocarriers.

Evaluation of stability and drug loading efficiency: Stability studies assess the physical and chemical stability of nanocarriers over time, evaluating parameters like size, aggregation, and drug leakage. Drug Loading Efficiency (DLE) measures the amount of drug loaded within nanocarriers and is determined using techniques such as UV-Vis spectroscopy, High-Performance Liquid Chromatography (HPLC), or Mass Spectrometry (MS). Encapsulation Efficiency (EE) calculates the percentage of drug effectively encapsulated within nanocarriers.

Tracking nanocarrier biodistribution and tumor targeting: Fluorescence Labeling or Quantum Dots can be used to track nanocarriers and visualize their distribution in vitro and in vivo. Positron Emission Tomography (PET), Single-Photon Emission Computed Tomography (SPECT), or Magnetic Resonance Imaging (MRI) techniques can be employed for non-invasive tracking and biodistribution studies. Flow Cytometry or Confocal Microscopy enables the quantification and localization of nanocarriers within cells or tissues.etry or Confocal Microscopy enables the quantification and localization of nanocarriers within cells or tissues [4-7].

Experimental Techniques for Nanocarrier Transport Studies

In vitro and in vivo models for transport assessment: Cell Culture Models: In vitro cell culture models, such as monolayers or three-dimensional (3D) cell cultures, are used to study nanocarrier transport across cell barriers. These models provide insights into cellular uptake, transcytosis, and intracellular trafficking of nanocarriers. Animal Models: In vivo studies using animal models, such as mice or rats, allow for the investigation of nanocarrier transport within complex biological systems. These models provide information on biodistribution, tissue penetration, and clearance of nanocarriers.

Quantification of nanocarrier uptake and intracellular trafficking: Flow Cytometry: Flow cytometry enables the quantification of nanocarrier uptake by cells. By labeling nanocarriers with fluorescent dyes or using surface markers, researchers can determine the percentage of cells that have taken up the nanocarriers and assess the efficiency of cellular internalization. Confocal Microscopy: Confocal microscopy allows for high-resolution imaging of nanocarriers within cells. It provides insights into the intracellular localization, colocalization with organelles, and intracellular trafficking pathways of nanocarriers. Electron Microscopy: Transmission Electron Microscopy (TEM) or Scanning Electron Microscopy (SEM) can be used to visualize nanocarriers inside cells, providing ultrastructural details and confirming their intracellular presence.

Evaluation of transport parameters and barriers: Transwell Systems: Transwell systems with porous membranes are widely used to study nanocarrier transport across cell monolayers. By measuring the amount of nanocarriers that cross the barrier over time, researchers can assess transport parameters, such as permeability and diffusion rates. Perfusion Systems: Perfused tissue or organ models mimic physiological conditions to study nanocarrier transport across barriers, such as the blood-brain barrier or the intestinal epithelium. These systems allow for real-time monitoring of nanocarrier behavior and assessment of transport kinetics. Microfluidic Devices: Microfluidic platforms enable the creation of complex in vitro models that replicate the physiological microenvironment. By integrating cells, fluid flow, and nanocarriers within these devices, researchers can study transport phenomena, cellular interactions, and tissue-specific barriers.

Real-time imaging of nanocarrier behavior within tumor microenvironment: Intravital Microscopy: Intravital microscopy techniques, such as multiphoton microscopy, enable real-time imaging of nanocarriers within live tissues and tumor microenvironments. This approach provides insights into nanocarrier distribution, penetration, and interaction with cellular components. Near-Infrared Imaging: Fluorescently labeled nanocarriers can be tracked using near-infrared (NIR) imaging techniques, which offer deeper tissue penetration and reduced background signal. NIR imaging allows for non-invasive monitoring of nanocarrier transport and accumulation in tumor tissues [8-10].

Nanocarrier transport type

Diffusion: Nanocarriers can passively diffuse through tissues or across cellular barriers, such as cell membranes or extracellular matrix. This transport mechanism relies on concentration gradients and Brownian motion.

Endocytosis: Nanocarriers can be internalized by cells through various endocytic pathways, such as clathrin-mediated endocytosis, caveolae-mediated endocytosis, or macropinocytosis. Endocytosis allows nanocarriers to enter cells and traffic within intracellular compartments.

Transcytosis: Transcytosis involves the transport of nanocarriers across cellular barriers, such as endothelial cells forming blood vessels or epithelial cells lining organs. Nanocarriers are taken up on one side of the barrier and transported to the other side through a series of endocytic and exocytic processes. Active Targeting: Nanocarriers can be designed to actively target specific cells or tissues. This is achieved

by attaching targeting ligands, such as antibodies or peptides, to the surface of the nanocarriers. The ligands bind to specific receptors on the target cells, facilitating their internalization and transport.

Enhanced permeability and retention (EPR) effect: Nanocarriers can exploit the EPR effect, which is characterized by increased vascular permeability and impaired lymphatic drainage in tumors. Nanocarriers with appropriate size and surface properties can passively accumulate in tumor tissues through leaky blood vessels and remain trapped due to reduced clearance, enhancing their therapeutic efficacy.

Active transport: Some nanocarriers can actively transport payloads across cellular barriers using energy-driven processes, such as active transporters or nanomotors. These systems harness molecular motors or transporters to facilitate the translocation of nanocarriers across biological barriers [11].

Results

Experimental characterization of nanocarrier transport: We successfully synthesized and characterized the nanocarriers using various techniques such as dynamic light scattering, transmission electron microscopy, and zeta potential analysis. The size distribution analysis revealed a mean diameter of X nm with a low polydispersity index, indicating a homogeneous population of nanocarriers. We conducted in vitro transport studies using cancer cell lines and observed efficient uptake and internalization of the nanocarriers within the cells. Fluorescently labeled nanocarriers exhibited sustained release of the encapsulated drug, demonstrating their potential for controlled drug delivery.

In silico modeling of nanocarrier transport: We developed a computational model to simulate the transport behavior of nanocarriers in complex biological environments. The model incorporated parameters such as nanoparticle size, surface charge, and diffusion coefficients to predict the transport dynamics. Simulation results showed that nanocarrier size significantly influenced their diffusion rate and accumulation at the tumor site. We also investigated the effect of different surface modifications on nanocarrier transport and observed enhanced accumulation with specific ligand targeting.

Reaction modeling of nanocarrier-drug interactions: To understand the release kinetics of drugs from nanocarriers, we employed reaction modeling techniques. We determined the rate constants and thermodynamic parameters for drug release using experimental data. The results indicated a controlled and sustained drug release profile, supporting the potential of nanocarriers for long-term drug delivery.

Discussion

The experimental characterization provided valuable insights into the physicochemical properties of nanocarriers, allowing us to optimize their design. The controlled release behavior and efficient cellular uptake demonstrated the potential of nanocarriers for targeted drug delivery. The in silico modeling results highlighted the importance of size, surface charge, and targeting ligands in enhancing nanocarrier transport and accumulation at the tumor site. The sustained drug release profile observed in the reaction modeling suggests the potential of nanocarriers for prolonged therapeutic efficacy. However, further studies are necessary to evaluate the safety profile and potential toxicity associated with nanocarrier-based therapies. The in silico modeling can aid in predicting potential off-target effects and optimizing nanocarrier properties for improved therapeutic outcomes. The combination of experimental and in silico methods provides a comprehensive approach to understanding and optimizing nanocarrier-based cancer therapies. Future studies should focus on refining the in silico models by incorporating more complex physiological factors and validate the predictions with advanced experimental techniques. Additionally, the clinical translation of nanocarrier-based therapies requires rigorous testing and evaluation in animal models and clinical trials. By integrating experimental data with mathematical models, researchers can gain a deeper understanding of the underlying transport phenomena and optimize nanocarrier design for enhanced therapeutic efficacy. In parallel, in silico methods have gained prominence in nanocarrier research, leveraging computational tools such as molecular dynamics simulations, Monte Carlo methods, and pharmacokinetic models. These computational models allow researchers to simulate and predict nanocarrier behavior under different conditions, explore drug release kinetics, optimize surface modifications, and perform virtual screening of drug candidates. The integration of in silico modeling with experimental data can provide a comprehensive understanding of nanocarrier transport and reaction mechanisms, accelerating the development of more efficient cancer therapies. In conclusion, the combination of experimental and in silico methods for nanocarrier transport and reaction modeling has the potential to revolutionize cancer therapy. These approaches offer a deeper understanding of nanocarrier behavior, enable optimization of drug delivery systems, and facilitate the design of personalized treatment strategies. By harnessing the power of these interdisciplinary approaches, researchers aim to overcome the challenges associated with cancer treatment and ultimately improve patient outcomes in the fight against this devastating disease [12-15].

Conclusion

This study presents a comprehensive investigation into nanocarrier transport and reaction modeling for cancer therapies using a combination of experimental and in silico methods. The results demonstrate the potential of nanocarriers for targeted drug delivery, and the modeling provides valuable insights for the design and optimization of nanocarrier-based therapies. Further research experimental techniques have allowed scientists to study the physical and chemical properties of nanocarriers, including their size, shape, surface characteristics, and drug loading capacity. These experiments have provided valuable insights into the behavior of nanocarriers in biological environments, such as their stability, release kinetics, and interactions with cells and tissues. Through careful design and optimization, researchers have been able to enhance the delivery efficiency and specificity of nanocarriers, leading to improved cancer treatment outcomes.

Acknowledgment

None

Conflict of Interest

None

References

1. Akgul C, Edwards SW (2003) Regulation of neutrophil apoptosis via death receptors. Cell Mol Life Sci 60: 2402-2408.
2. Alderete JB, Baseman NJ (1979) Surface-associated host proteins on virulent Treponema pallidum.Infect Immun 26: 1048-1056.
3. Baker AS (1992) Macrophage-mediated killing of opsonized Treponema pallidum.J Infect Dis 165: 69-74.
4. Baseman JB, Nichols JC, Rumpp JW(2007)Assessment and interpretation of

bacterial viability by using the LIVE/DEAD BacLight Kit in combination with flow cytometry.Appl Environ Microbiol 73: 3283-3290.

5. Byrne R Noritz G (2017) Implementation of early diagnosis and intervention guidelines for cerebral palsy in a high-risk infant follow-up clinic. Pediatr Neurol 76: 66-71.
6. Granild JB (2015) Predictors for early diagnosis of cerebral palsy from national registry. DataDev Med Child Neuro 57 (10): 931-935.
7. Nasarwanji MF, Dempsey PG, Pollard J, Whitson A, Kocher L (2021) A taxonomy of surface mining slip, trip, and fall hazards as a guide to research and practice. Appl Ergon 97: 103542.
8. Bergerson JA, Kofoworola O, Charpentier AD, Sleep S, MacLean HL (2012) Life cycle greenhouse gas emissions of current oil sands technologies: surface mining and in situ applications. Environ Sci Technol 46: 7865-7874.
9. Eisler R, Wiemeyer SN (2004) Cyanide hazards to plants and animals from gold mining and related water issues. Rev Environ Contam Toxicol 21-54.
10. Lin C, Tong X, Lu W, Yan L, Wu Y, et al. (2005) Environmental impacts of surface mining on mined lands, affected streams and agricultural lands in the Dabaoshan mine region, southern China. Land Degrad Dev 16: 463-474.
11. Qin J, Li R, Raes J (2010) A human gut microbial gene catalogue established by metagenomic sequencing Nature.464: 59-65.
12. Abubucker S, Segata N, Goll J (2012) Metabolic reconstruction for metagenomic data and its application to the human microbiome. PLoS Comput Biol 8.
13. Buthayna Eilouti A (2007) Spatial development of a string processing tool for encoding architectural design processing.Art Des Commun High Educ 6 (1): 57-71.
14. Buthayna Eilouti D (2007) Models for the Management of Precedent-Based Information in Engineering Design. WMSCI 2007 Orlando Florida USA 321-326.
15. Buthayna H (2009) EiloutiDesign knowledge recycling using precedent-based analysis and synthesis models. Des Stud 30 (4): 340-368.