ADVANCING NANO DRUG DELIVERY SYSTEM DETECTION THROUGH DEEP LEARNING: A MOBILENET MODEL APPROACH

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ABSTRACT
An AI-based approach has the potential to improve treatment outcomes, increase patient satisfaction, and advance the field of pharmaceutical science. This study aims to address the existing limitations in NDDS classification, such as the variability in nanoparticle formulations and the complex nature of their interactions with biological systems by leveraging MobileNet's capabilities. The pre-processing pipeline implemented for this study comprises Gaussian blurring, Contrast Limited Adaptive Histogram Equalization (CLAHE), Otsu's thresholding, and image resizing, alongside conversion to a format suitable for input into the MobileNet architecture. The evaluation of the model on the set aside for testing produced an accuracy of 84.37% and a loss of 0.5543. In conclusion, we have succeeded in combining nanotechnology and pharmaceutical sciences with artificial intelligence to prepare a trained model to recognize the liposomes as Novel Drug Delivery System (NDDS) and to evaluate the nature and concentration of active ingredients carried inside them by utilizing a MobileNet model.

Key word: Liposomes; NDDS; Artificial intelligence; Algorithms; Mobile Net; Computer Vision.

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1. Introduction

Nanotechnology has been identified as one of the most vigorously pursued areas of research [1]. It has garnered increasing attention in scientific and technological circles due to its diverse applications across biomedicine, optics, and electronics [2]. Nanotechnology integrates insights from various disciplines, including chemistry, physics, materials science, engineering, biology, and health sciences [3]. Over the past few years, the use of nanotechnology in medicine has increased rapidly in order to both prevent and treat diseases within the human body [4]. Nanotechnology provides numerous advantages in the treatment of persistent human diseases by delivering medications precisely and targeting specific sites [5]. The evolution of drug formulations based on nanoparticles has gave in the chances to address and treat difficult diseases [6]. A Novel Drug Delivery System (NDDS) is an inventive strategy that uses new technologies, innovative ideas, and methodologies to deliver the active compounds in safe yet effective concentration to make desired pharmacological effect [7]. The active pharmaceutical ingredient can be released to produce the necessary therapeutic response thanks to the drug delivery system [8]. Drug delivery systems based on liposome have played a significant role in the formulation of powerful drugs to enhance therapeutics [9]. Liposomes have been considered promising and versatile drug vesicles. Liposomes exhibit better belongings compared with traditional drug delivery systems, including site-targeting, sustained or controlled release, protection of drugs against degradation and clearance, more effective therapeutic effects, and lower toxic side effects [10]. Liposomes are spherical vesicles formed up of one or more phospholipid bilayers, which are under extensive studies as drug carriers to enhance the delivery of several substances and bioactive agents in medical, pharmacological, nutritional, and biological research [11]. Significant developments in machine learning and artificial intelligence (AI) technology offer a transformative opportunity in the drug discovery, formulation, and testing of pharmaceutical dosage forms [12]. This artificial intelligence (AI)-based approach has the potent to enhance therapy results, improve patient satisfaction, and advance the field of pharmaceutical sciences [13]. Yet, applying advanced AI models like MobileNet for classifying NDDS types still needs to be explored.

This research aims to bridge the gap in the field by employing a MobileNet model renowned for its efficiency and accuracy in image-based classification tasks to the specific challenge of classifying NDDS types. By leveraging MobileNet's capabilities, this study seeks to address the existing limitations in NDDS classification, such as the variability in nanoparticle formulations and the complex nature of their interactions with biological systems. Our approach promises to enhance the accuracy of NDDS classification and contribute to a novel application of MobileNet models within the pharmaceutical sciences.

2. Material and Methods

2.1. Preparation of Aqueous Extract

Ocimum basilicum L. was collected in August 2022 from the El-Oued (Guemar) region, Algeria. The basil leaves were cleaned and dried away from direct sunlight at room temperature. The dry leaves were ground into a fine powder. Plant powder is kept at room temperature in airtight containers until the experiment begins. Pr. Youssef Hallis identified of this plant. The aqueous extract was prepared by boiling 10 g of dried *Ocimum basilicum* L. leaves powder in 100 ml of distilled water for two hours at 50 degrees Celsius. The mixture was allowed to cool and macerate at room temperature for 24 hours, then filtered through Whatman filter paper. Afterward, the extract was evaporated using a rotary evaporator and dried in an oven [14] [15].

2.2. Biosynthesis of MnO NPs

Biosynthesis of MnO nanoparticles (NPs) was carried out according to the method of Boulaares *et al*. Aqueous basil extract was mixed with a manganese (II) chloride solution. Sodium hydroxide solution was added dropwise under constant and gradual stirring until the pH reached 8, forming tiny particles. The mixture was then stirred using a magnetic stirrer at 65°C for 6 hours, during which the solution's color changed from golden yellow to dark brown, indicating the successful biosynthesis of MnO NPs. The mixture was next centrifuged at 5000 rpm for 20 minutes, and the supernatant was discarded. The precipitate was washed three times with distilled water and ethanol before being dried to obtain the final product [16].

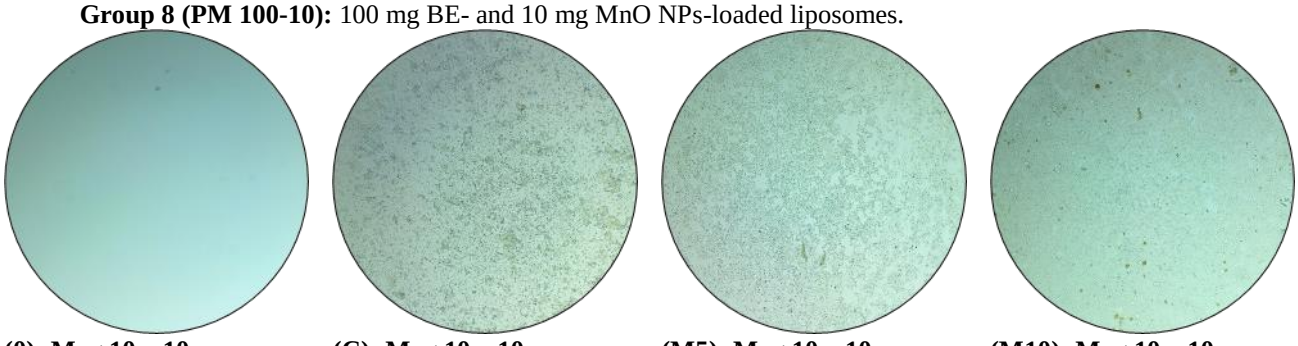
2.3. Preparation of Liposomes

The method used for liposomes preparation is the thin film hydration method (Bangham method). This technique entails dissolving lipids in an organic solvent (ethanol). After that, the solvent is removed by evaporation under vacuum at a 45-60 °C temperature to form a thin lipid film. Then, the lipid film is hydrated in aqueous media through continuous agitation at a temperature of 60-70 °C for up to 2 hours, forming round and closed liposomes [17]. A phosphate buffer solution (50 mM, pH 6.5) was used to dissolve orcinol and glutamine at a concentration of 200 mg/mL. The process involved combining 50 mL of the orcinol and glutamine mixtures with 950 mL of liposomes. This reaction was allowed to proceed overnight at room temperature, ultimately leading to the creation of a bioconjugation [18].

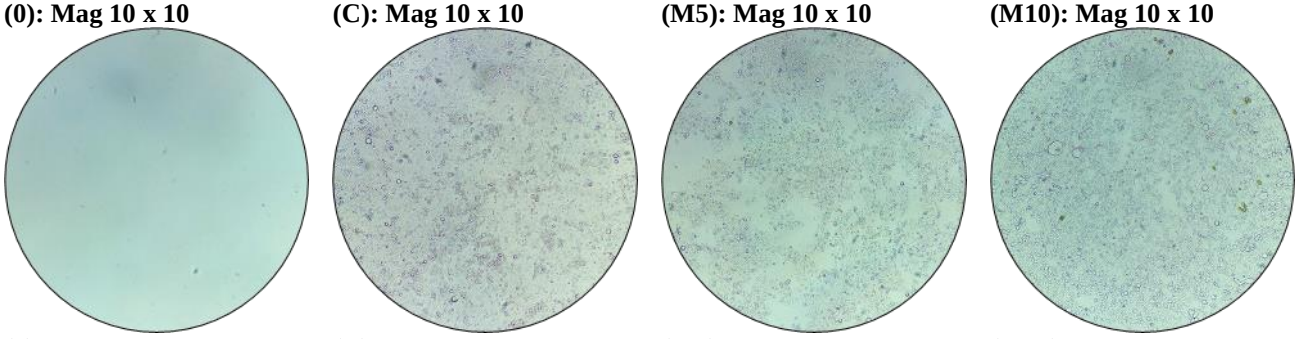
2.4. Data Set Collection

The dataset comprises 960 photos of various liposome samples under different conditions (magnifications of 10x, 40x, 100x, various illuminations, and angles) on microscope slides. Photos were taken with an SM-E22SF/DS camera phone and saved in JPG format at 2250 × 4000 pixels. The dataset is divided into eight groups based on the composition of the liposomes (Fig.1):

Group 1 (0): Physiological water without liposomes.
Group 2 (C): Empty liposomes without BE and MnO NPs.
Group 3 (M5): 05 mg MnO NPs-loaded liposomes.
Group 4 (M10): 10 mg MnO NPs-loaded liposomes.
Group 5 (P50): 50 mg BE-loaded liposomes.
Group 6 (P100): 100 mg BE-loaded liposomes.
Group 7 (PM 50-5): 50 mg BE- and 05 mg MnO NPs-loaded liposomes.
Group 8 (PM 100-10): 100 mg BE- and 10 mg MnO NPs-loaded liposomes.



(0): Mag 10 x 10 **(C): Mag 10 x 10** **(M5): Mag 10 x 10** **(M10): Mag 10 x 10**



(0): Mag 40 x 10 **(C): Mag 40 x 10** **(M5): Mag 40 x 10** **(M10): Mag 40 x 10**

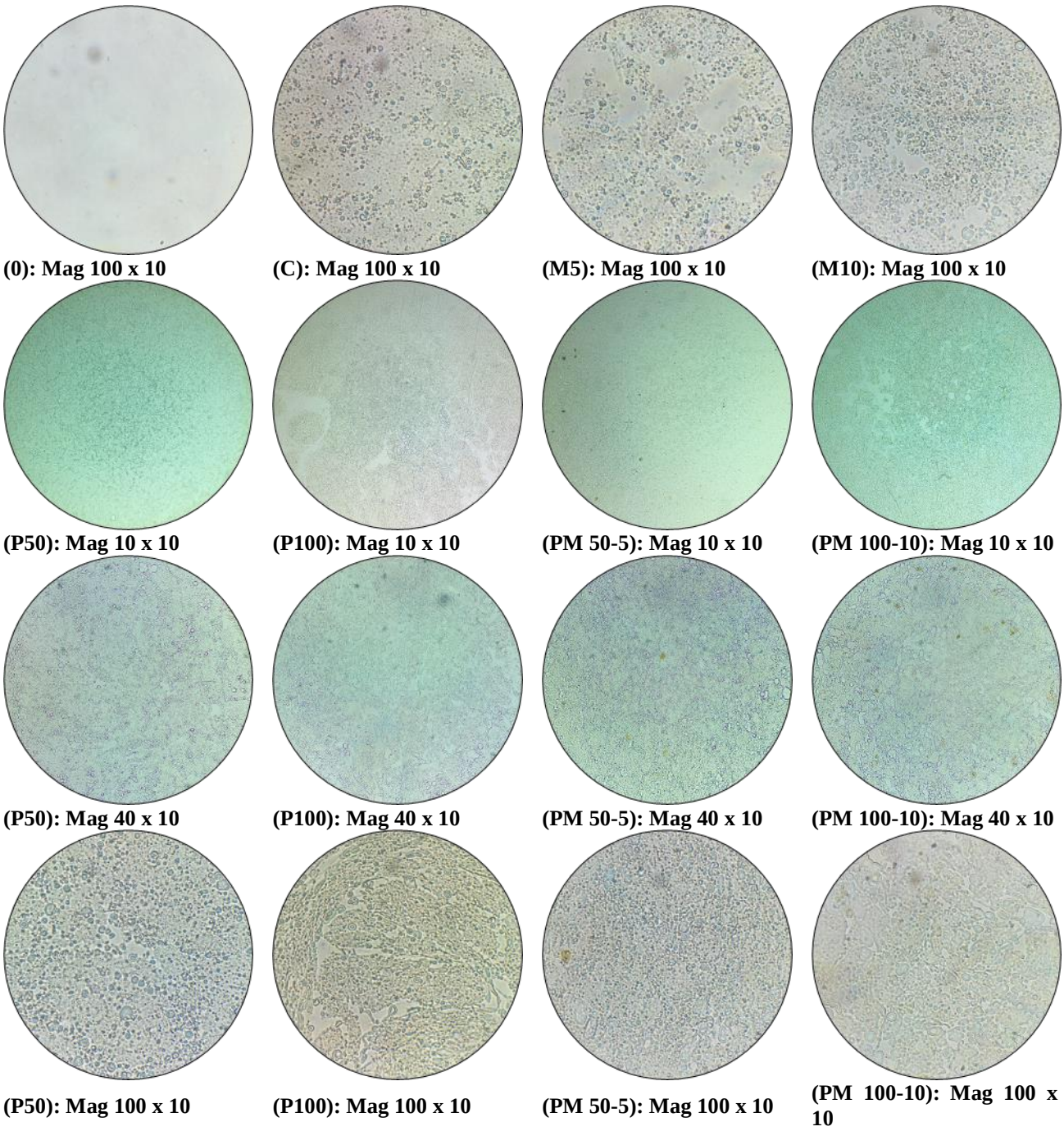


Fig.1. Liposomes as a novel drug delivery system (NDDS) photo in the eight groups.

2.5. Image Pre-Processing

In pursuing accurate classification of NDDS through deep learning models, pre-processing input images constitutes a critical step. This process entails a series of operations to enhance the images' quality and consistency, facilitating more effective model training and prediction. The pre-processing pipeline implemented for this study comprises Gaussian blurring, Contrast Limited Adaptive Histogram Equalization (CLAHE), Otsu's thresholding, and image resizing, alongside conversion to a format suitable for input into the MobileNet architecture.

The initial step involves the application of Gaussian blur to the input images. This technique utilizes a Gaussian kernel to smooth the image, effectively reducing noise and minor details that are not critical for the classification task. By applying this filter with a kernel size of (5, 5), we ensure that the essential structures within the NDDS images are retained while extraneous information is minimized. This operation is crucial for enhancing the robustness of the subsequent image analysis steps, particularly in environments with variable lighting conditions or where the samples may exhibit slight physical variations.

Following noise reduction, the next operation aims to enhance the contrast of the images. CLAHE is employed for this purpose, targeting the grayscale version of the blurred image. Unlike standard histogram equalization, CLAHE limits

contrast amplification to prevent the over-enhancement of noise in relatively homogeneous image regions. This is achieved by dividing the image into contextual regions and applying histogram equalization to each separately, with a clip limit 2.0 and a tile grid size of (8, 8). The result is a balanced enhancement of the visual clarity and definition of the NDDS, facilitating more accurate edge detection and feature extraction in later stages.

After contrast enhancement, Otsu's method converts the image into a binary format, distinguishing the foreground (NDDS particles) from the background. This thresholding technique selects the optimum threshold value by minimizing intra-class variance in the image, thus effectively segmenting the relevant features from the surroundings. This binary representation simplifies the identification and classification of NDDS by focusing on the shape and distribution of the particles.

The final steps in the pre-processing pipeline involve resizing the binary image to a standard dimension of 640x640 pixels, ensuring consistency across the dataset and aligning with the input size requirements of the MobileNet model. To accommodate the model's three-channel input specification, the grayscale image is stacked across three channels, simulating the format of an RGB image without introducing additional color information. This standardized input format is crucial for the efficient and accurate processing of images by the MobileNet architecture. By meticulously executing each of these pre-processing steps, the study ensures that the images of NDDS are optimally prepared for the subsequent application of deep learning models. As shown in Fig.2, this preparation enhances the model's ability to learn meaningful patterns from the data and contributes to the overall reliability and accuracy of the NDDS classification outcomes.

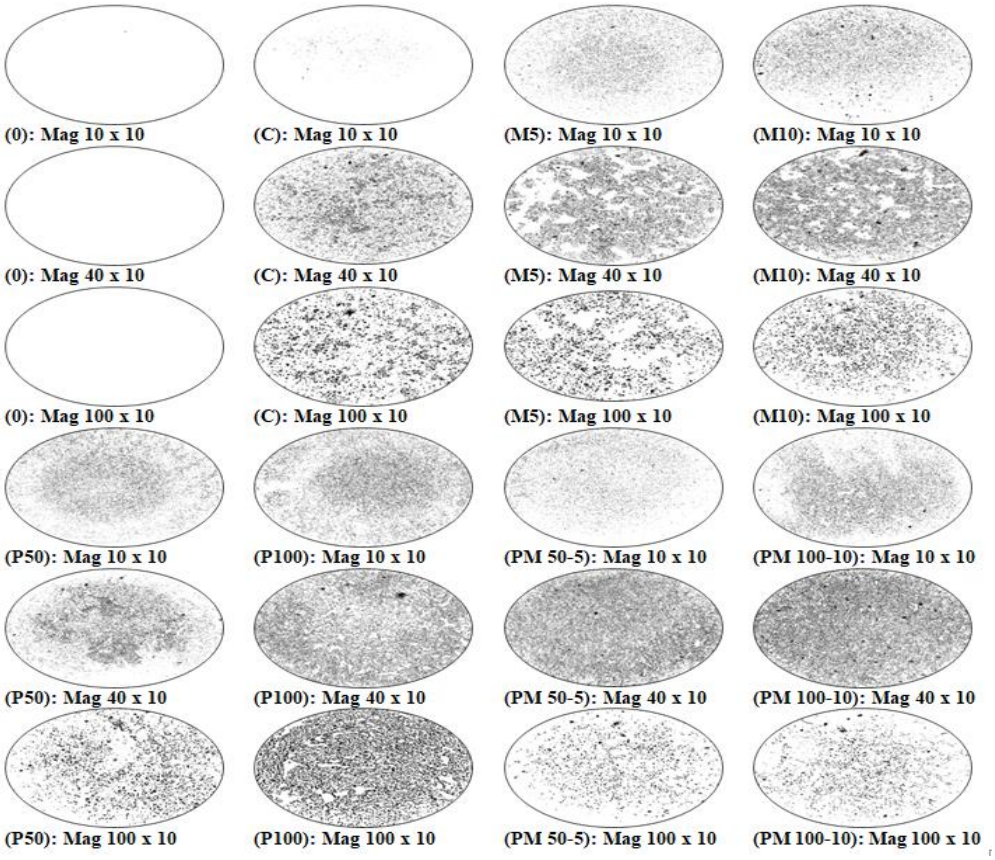


Fig.2. Liposomes as a novel drug delivery system (NDDS) photo in the eight groups after pre-processing

2.6. Training Process and MobileNet Architecture

The foundational dataset was systematically partitioned into three subsets: training, validation, and test. This tripartite division is crucial for assessing the model's learning efficacy, adaptability to novel data, and ultimate performance in a controlled, unbiased evaluation. Table 1 summarizes the dataset distribution, ensuring transparency in the model's experimental environment.

Table 1. Dataset split summary

Dataset	Description	Size
Training Set	Used to train the model, allowing it to learn the distinctions between different categories.	768 Image
Validation Set	Provides a form of early feedback on the model's generalization capability.	96 Image
Test Set	Evaluates the model's final performance on unseen data.	96 Image

To streamline the training process, the data frames were transformed into TensorFlow datasets, leveraging the platform's efficient data handling and processing capabilities. This conversion enables sophisticated batching, shuffling, and prefetching operations, significantly enhancing computational efficiency. The parameters employed in this conversion are detailed in Table 2.

Table 2. TensorFlow dataset conversion parameters

Parameter	Functionality	Specified Value
buffer_size	Determining the dataset's shuffling capacity is crucial for mitigating order-induced bias in the learning process.	Length of Dataset
batch_size	Regulates the quantity of data samples the model processes per iteration, balancing computational load and learning granularity.	32
prefetch_buffer	Pre-fetches data batches to expedite data processing, optimizing pipeline throughput.	AUTOTUNE

The MobileNetV2 architecture, renowned for its computational efficiency and robust feature extraction capabilities, was selected for this study's classification task. This model's integration, configured with a custom top layer tailored for NDDS classification, underscores the study's innovative approach. The configuration specifics are elucidated in Table 3.

Table 3. MobileNetV2 configuration details

Configuration Element	Description
Base Model	MobileNetV2 was initialized with ImageNet weights and adapted to exclude the top layer, which serves as the foundation for feature extraction.
GlobalAveragePooling2D	Condenses the feature maps into a singular vector per image, simplifying the model's interpretative process.
Dense Layer	It comprises 1024 neurons with ReLU activation and is tasked with learning complex associations within the data.
Dropout Layer	Implements a 50% dropout rate to mitigate overfitting by randomly excluding neurons during training.
Output Layer	Culminates in a softmax-activated layer, outputting a probabilistic distribution across the NDDS categories.

The training regime was underpinned by the Adam optimizer, selected for its adaptive learning rate capabilities, facilitating nuanced model adjustments. The incorporation of early stopping, predicated on validation loss performance, exemplifies the methodical approach to preventing overfitting. The training and evaluation metrics, crucial for interpreting the model's efficacy, are summarized in Table 4.

Table 4. Training parameters and evaluation metrics

Training/Evaluation Parameter	Description
Optimizer	Adam was chosen for its effectiveness in handling sparse gradients and adaptive learning rate adjustments.
Learning Rate	Set to 0.0001, ensuring gradual convergence and minimizing the risk of overshooting the loss function's minimum.
Loss Function	Sparse Categorical Crossentropy, aligning with the multi-class nature of the NDDS classification task.
Evaluation Metrics	Model performance is assessed using accuracy, providing a direct measure of classification success rates.

This meticulous approach to model training and architecture design underscores the study's commitment to precision and reproducibility. By adhering to these methodological standards, the research contributes to the burgeoning field of NDDS classification and paves the way for future explorations into AI-driven pharmaceutical innovations.

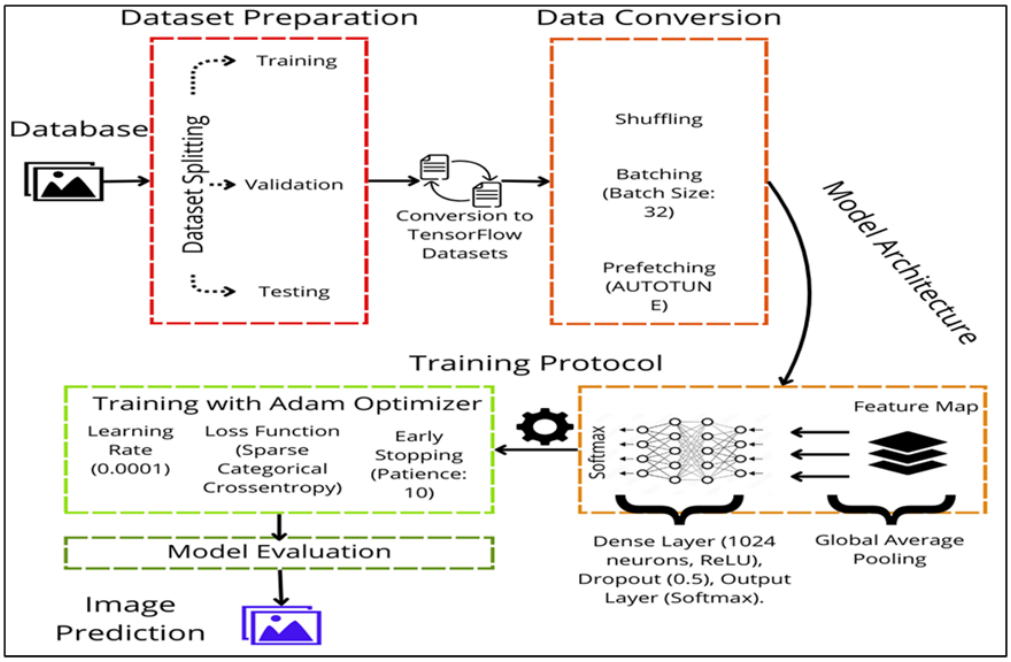


Fig.3. MobileNet model training and architecture for Nano Drug Delivery Systems (NDDS) classification in a graphical format.

3. Results

Our deep learning model, leveraging the MobileNetV2 architecture through transfer learning, underwent a comprehensive training process spanning 50 epochs. The initiation of training was characterized by a loss of 2.1227 and an accuracy of 29.43%, as anticipated due to the initial untrained state of the model. Throughout the training phase, there was a discernible improvement in the model's accuracy, reaching a training accuracy of 81.77% by the final epoch. The validation accuracy commenced at 35.42% and experienced fluctuations, indicative of the model's adaptation to the validation dataset, eventually peaking at 76.04% in the 50th epoch. Correspondingly, the validation loss decreased over time, barring sporadic increases common during the optimization process (Table 5).

Table 5. Model training and validation performance

Epoch	Training Loss	Training Accuracy	Validation Loss	Validation Accuracy
1	2.1227	29.43%	1.5338	35.42%
...	...	...	...	...
50	0.4794	81.77%	0.6688	76.04%

The final evaluation of the model on the test set, which had been held out from the training process, yielded an accuracy of 84.37% and a loss of 0.5543. This performance benchmark reflects the model's capability to generalize well and signifies its robustness when faced with unseen data. The learning curves (Fig.4) provide insight into the model's learning trajectory. Training accuracy shows a consistent increase as the model learns from the data. In contrast, validation accuracy tracks closely behind, suggesting that the model is generalizing effectively rather than memorizing the training data. Similarly, both training and validation loss metrics decrease over time, which is congruent with the increases in accuracy.

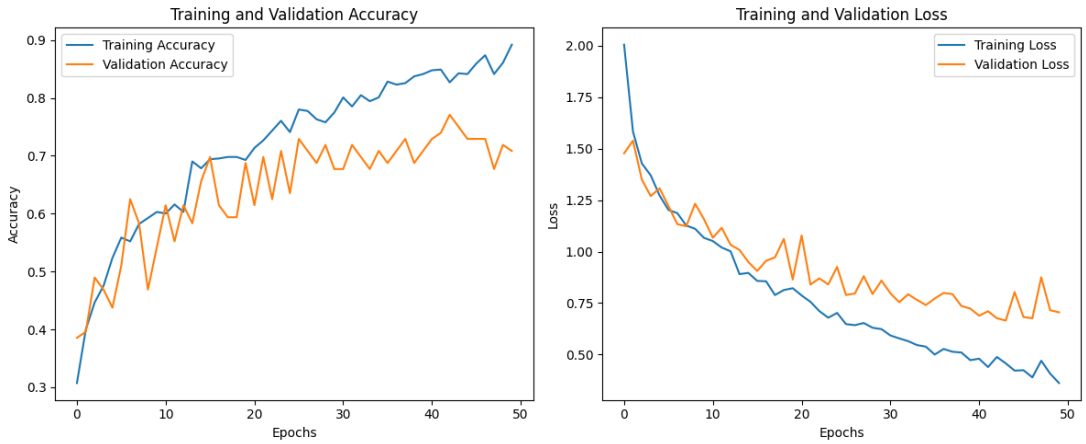


Fig.4. Training and validation accuracy and loss curves

Visual examination of predictions made by the model offers a qualitative perspective on its performance. Fig.5 presents a selection of images from the test set, depicting the model's predicted class labels alongside the actual labels. This visual assessment reveals instances of both correct classifications, such as 'C' being accurately predicted as 'C', and misclassifications, wherein a sample of 'PM 50-5' was incorrectly predicted as 'PM 100-10'. These examples highlight the model's strengths and pinpoint areas where its classification capabilities can be further honed.

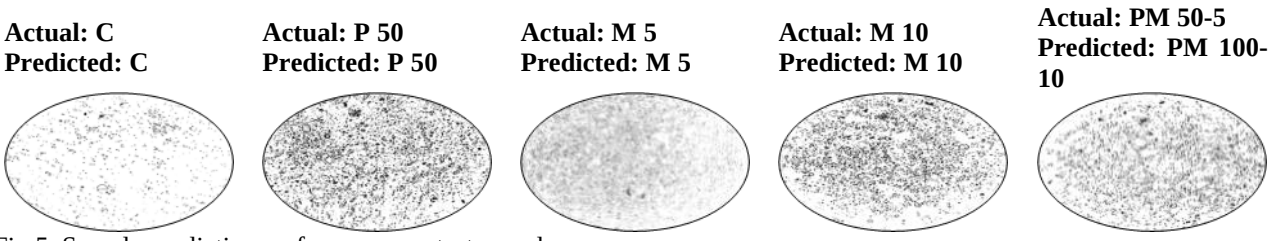


Fig.5. Sample predictive performance on test samples

The instances of accurate predictions affirm the model's effectiveness in classifying NDDS. On the other hand, the misclassifications offer valuable insights into possible confusion between classes and underscore the need for further refinement of the model's training to enhance its discriminative power for closely related classes.

In summary, the trained MobileNetV2 model demonstrates promising performance in classifying Nano Drug Delivery Systems. The results reveal the model's ability to learn and generalize from the provided data, as evidenced by the high accuracy on the test set and the learning curves during training. The visual predictions further validate the model's practical capabilities while guiding future improvements. This study sets a solid foundation for applying deep learning models in nanomedicine, with potential implications for enhancing precision in NDDS characterization.

4. Discussion

The pursuit of integrating automation with artificial intelligence (AI) allows for the optimization of targeted therapeutic nanoparticles to specific cell types and individuals [19]. Computer algorithms and computational models capable of predicting the physico-chemical properties of nanosystems can significantly expedite the development of nanoparticle systems [20]. Convolutional neural networks (CNNs) have become extremely popular in research, especially in the domain of computer vision, where they are frequently employed for tasks like facial recognition, image classification, weather forecasting, and object detection [21]. MobileNet is a type of convolutional neural network (CNN) that boasts a high recognition rate and requires fewer calculations and parameters, making it an ideal choice for use on embedded devices [22]. In the field of image recognition, MobileNet presently is achieving successful outcomes [23]. The intersection of Machine learning (ML) and computer vision continues to be a prolific area of recent research [24]. Computer vision analyzes data from images using machine learning [25]. The study by **Cern *et al.*** has successfully applied Quantitative Structure-Property Relationship (QSPR) models for designing liposomal drugs. This method demonstrated impressive external validation accuracy, with results showing 81.8% accuracy using k-nearest Neighbors (KNN) and 92.3% using Iterative Stochastic Elimination (ISE), underscoring the reliability and effectiveness of these models in predicting drug encapsulation and release behaviors [26]. To the best of our knowledge, this research marks the first exploration of utilizing MobileNet tools to classify liposomes as innovative drug delivery systems. Given the absence of prior studies in this specific application, this pioneering work opens new avenues for research and potential improvements in the efficacy of drug delivery methodologies.

5. Conclusion

In conclusion, we have succeeded in combining nanotechnology and pharmaceutical sciences with artificial intelligence to prepare a trained model to recognize the liposomes as Novel Drug Delivery System (NDDS) and to evaluate the nature and concentration of active ingredients carried inside them by utilizing a MobileNet model, which is well-known for its effectiveness and precision in image-based classification tasks. The evaluation of the model on the test set, which was excluded from the training process, yielded an 84.37% accuracy rate and a loss of 0.5543. In the future, we hope that this study will continue and the trained model will develop to determine which organ or disease the drug will target.

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Author contribution All authors contributed to the study conception and design. Material preparation, data collection, and analysis were performed by, IB, and AMN and SD supervised the experiments. The first draft of the manuscript was written by IB, and all authors commented on previous versions of the manuscript. All authors read and approved the final manuscript.

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Data availability the datasets generated during and/or analyzed during the current study are available from the corresponding author on reasonable request.

Declarations

Ethics approval and consent to participate All institutional and national guidelines for the care and use of laboratory animals were followed. The

Consent for publication All authors give consent for publication. Competing interests the authors declare no competing interests.

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