Executive Summary of Activities Conducted During the Implementation Period

Project Name*:* *Adaptive Design and Assembly of Polymer-based nanoplaTforms for smart gene and drug delivery* (**ADAPT4dlvrY**)

The project implementation period was characterized by the execution of five main activities aimed at achieving the central objective: developing a smart design of PBNs (Polymer-Based Nanoplatforms) using structural variety and a multi-stage protocol for Engineering PBNs. During this period, advanced design models based on artificial intelligence algorithms and molecular simulations were developed and validated, utilizing high-performance computing equipment. All activities were successfully completed, demonstrating significant progress in the project.

Activity 1.1 involved the precise construction of pdb and psf structures for synthetic and natural polymers. In Activity 1.2, a polymer design process was developed using machine learning techniques, accelerating the identification of optimal components for high-performance nanoplatforms. Activity 1.3 focused on designing diverse architectures of nanocomposites in various shapes, sizes, and materials, resulting in customized and efficient structures. In Activity 1.4, the self-assembly method of nanoplatforms based on molecular dynamics simulations was validated, demonstrating control over nanoparticle size and properties. Finally, Activity 1.5 explored interactions between lignin derivatives and membrane models using simulations and quantum chemistry calculations, molecular dynamics, and free energy analyses. This activity highlighted the influence of molecular size and concentration on insertion and aggregation behaviors, which are significant in the cosmetic industry.

The obtained results were actively disseminated through four publications in ISI-indexed journals, reflecting the scientific value of the research. Additionally, findings were presented at 30 international conferences and workshops, ensuring global visibility for the research group and the institution. Dissemination was also facilitated by regularly updating the project's website (https://www.itim-cj.ro/PNCDI/adapt4dlvry/), promoting transparency and public awareness.

Technical activities included intensive calculations on graphics processing units for molecular dynamics and interaction analysis, enabling relevant results for the development of effective nanoplatforms for drug and gene delivery. The progress report summarizes key conclusions, highlighting significant advancements in delivery vectors and dissemination efforts. All result indicators were fully achieved, including the creation of structural files for polymers and nanocomposites, scientific reports, and the project website. Participation in over 30 national and international conferences and workshops strengthened the leadership position of the research team and contributed to establishing collaborative networks.

In conclusion, the activities carried out ensured the achievement of the project's objectives, promoted innovation in nanomaterials for personalized medicine, and generated impactful scientific results with international visibility. These outcomes will support further development of technologies in this field.

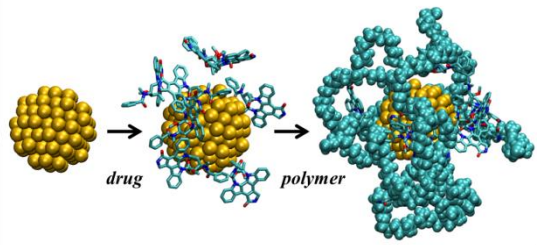

Figure 1. Polymer-based nanoplaTforms for smart gene and drug delivery