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## **SimCardioTest - Simulation of Cardiac Devices & Drugs for in-silico Testing and Certification**



### **Technical Report D1.5: Cloud-based platform for drugs simulation**

#### **Work Package 1 (WP 1) Model Standardisation & Interoperability**

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## DELIVERABLE INFORMATION

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## Table of Contents

EXECUTIVE SUMMARY	4
1- INTRODUCTION	5
2- OBJECTIVES	5
3- METHODOLOGIES	6
4- RESULTS	6
5- CONCLUSION	6



## EXECUTIVE SUMMARY

A first version of the SimCardioTest cloud-based in-silico trials platform is released as a milestone of the SimCardioTest project. Specifically, the platform has been developed to host the three Use Cases developed within the project, and a user-friendly interface for each Use Case has been created. Users will be able to run simulations on the browser leveraging the models created by the SimCardioTest partners.

This deliverable consists in a recorded demo demonstrating the first version of the cloud-based platform developed for Use Case 3, showing drugs simulation. The video is available on Youtube: [SimcardioTest UC3 demo video showing drugs simulation - YouTube](#) and on SimCardioTest website: [In-silico trials – SimCardioTest](#)

## 1- Introduction

In WP1, a cloud-based in-silico trial platform has been developed to host the three Use Cases developed within the project, and a user-friendly interface for each Use Case has been created. The interface serves as the interconnection layer between the models developed by the SCT partners and the input provided by the user through the web-interface. With this cloud-based platform, users will have the ability to run model simulations by simply accessing the platform via any browser, without the need of computational expertise and solvers/IT infrastructure. Also, users cannot download or modify the original models, thus preserving the intellectual property of the model creators.

In this deliverable, the UC3 cloud-based platform is presented. The workflow has been developed by IST in close collaboration with WP4 partners, who provided support to the integration of the model, as well as suggestions, feedbacks and comments on the user interface throughout the development process.

## 2- Objectives

This deliverable consists on a recorded demo demonstrating the first version of the cloud-based platform for drug effects simulations.

The workflow to perform in-silico clinical trials for drug safety and efficacy consists of 3 parts: 1) drug pharmacokinetics, 2) populations of cellular models (0D), 3) populations of 3D models. The workflow is already described in [D4.1](#).

Drug pharmacokinetics is performed in the ExactCure platform directly, with .json files data exchange between IST and EXC platforms via API.

The objective of the workflow is to perform in-silico clinical trials on drug safety and efficacy. The platform enables the user to select a specific drug with its dose, administered to a certain population, providing as an output the time course of free plasma concentration and the effects of this concentration on a population of cells or 3D cardiac tissues. Simulations provide specific biomarkers, which will assess the safety of this drug and/or its efficacy under a specific diseased situation.

Electrophysiological and mechanical models are programmed in MATLAB and the solver has been integrated into the platform to be used for the numerical computation.

In the workflow, the inputs required by the user are numbers or choices from a drop-down list, which are collected and passed to the back-end infrastructure. When the simulation is finished, results are stored in the database and can be viewed through a specific user interface which has been designed specifically for each Use Case.

Moreover, user access and management have been implemented, as well as the possibility to monitor of the status of an ongoing simulation and to retrieve the results of all simulations previously run, which are securely stored in a private database within the dedicated SimCardioTest environment.

### 3- Methodologies

To develop the platform, the following activities have been performed:

- Demos, meetings and documents exchange with UC3 partners to discuss and agree on a final simulation workflow
- Setup of a dedicated, isolated and white-labeled environment for SimCardioTest
- Creation of Login page and user account management
- Implementation of the standardised workflow for Use Case 3 into cloud-based high-performance computing clusters (making use of Microsoft Azure virtual machines)
- Creation of all required interfaces, from homepage to model results
- Implementation of MATLAB on the virtual machines and model integration in the workflow
- Definition and mapping of input and output parameters in the web-interface and in the model
- Definition of the interchange standard format of input and output files between IST and ExactCure platforms
- Definition of the communication interfaces between IST and ExactCure platforms. Standard REST over HTTPS API with JWT authentication has been used
- Use Case testing and bug fixing

### 4- Results

The result of the activities described is shown in the video recording available on Youtube/SimCardioTest channel [SimcardioTest UC3 demo video showing drugs simulation - YouTube](#) and on SimCardioTest website: [In-silico trials – SimCardioTest](#)

### 5- Conclusion

In this deliverable, we presented the demo of the cloud-based platform for drugs simulation.

The platform has been created by integrating UC3 electrophysiology and mechanical models within a dedicated cloud-based environment, as well as setting up the data exchange with EXC platform. Following steps foreseen until M48 will include the refinement of the platform and running in-silico trials.



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