maintaining of plasticity of cement paste. This study opens up a possible way to control the sedimentation process while maintaining the required spreading and other physical and mechanical properties of the cement paste.

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Intelligent software for automated TLC image analysis and substance prediction

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Abstract. *This paper presents a software solution for automated analysis of thin-layer chromatography (TLC) images, combining a Python client application with a Microsoft SQL Server database. The system enables management of TLC experiments, automatic segmentation, and qualitative analysis of substances, including prediction of unknown substances based on retention factors, improving accuracy and efficiency in TLC research.*
Keywords: *thin-layer chromatography, image analysis, automated segmentation, retention factor, substance prediction.*

In modern conditions, there is a growing need to create intelligent tools for processing and interpreting the results of thin-layer chromatography, since traditional methods for evaluating TLC images remain predominantly subjective and laborious. Despite significant progress in the field of computer vision and deep learning, including in image segmentation tasks [1-3], the issues of adapting these technologies to the specific tasks of segmentation and recognition of analytes on chromatographic tracks have still not been sufficiently studied. This creates an urgent scientific and practical problem - the development of approaches and software tools capable of providing automated and reproducible analysis of TLC images to increase the accuracy and efficiency of research processes.

To solve the problem of qualitative analysis of TLC images, it is necessary to develop an appropriate software solution that would provide the ability to keep track of various thin-layer chromatography experiments and automatically analyze unknown substances on the experiment tracks based on previously defined known substances of other tracks. Accordingly, it is necessary to create a database that will store information on the experiments of the specified chemical analysis, link experiments with the tracks related to them, and also store information on the substances available in the software solution directory. In addition to the specified tables, the database should also store procedure objects, with the help of which work will be carried out on creating new experiments, obtaining information on the experiments available in the database, etc. On the part of the client application, interaction with the database should be configured to call the developed procedures and present the obtained data in a convenient and user-friendly visual interface. In general, the functions of creating experiments and automatically predicting unknown substances on the experiment tracks should be implemented.

The above-mentioned task was implemented by developing a software solution, which is a system of a client application in Python, as well as an instance of the Microsoft SQL Server database server. These platforms were chosen to solve the task based on the priority of the availability of detailed documentation and the number of supported functions of the software platforms in view of the widest possible further use of the developed software solution.

On the server side, a database called TLC_APP was created. Table objects were created in it: "Experiments" for storing general information on TLC experiments, "Experiment_Images" for storing information on experiment images, and "Substances" for storing a dictionary of substances supported by the application (Fig. 1). Procedures were also created: "Create_Experiment" for creating a new experiment, "Get_Experiment_Info" for obtaining information on the experiment, "Get_Experiments_List" for obtaining a list of experiments available in the database, "Get_Substances_List" for obtaining a list of substances available in the database, and "Change_Experiment_Substance" for changing the correspondence of the experiment track to a specific substance (Fig. 2).

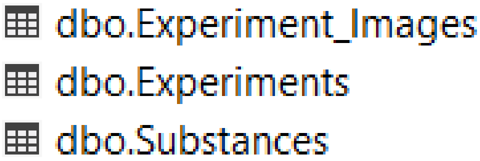

Fig. 1. Database tables

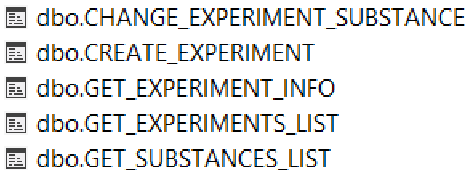

Fig. 2. Database procedures

On the client side, the ability to add a new experiment in a separate window that opens by clicking the "New Experiment" button (Fig. 3), view and open existing experiments in the database in the window that opens by clicking the "Open Experiment" button (Fig. 4), view general experiment information, information on the user's determination of the correspondence of the experiment track to a specific substance (Fig. 5) (respectively, by clicking the "Define substances" button, the user has the opportunity to define the substances of the experiment tracks (Fig. 6)), the results of automatic segmentation of the track image by the segmentation model selected by the user, as well as the results of automatic quantitative and qualitative analysis (Retention factor) of the track substance (Fig. 7).

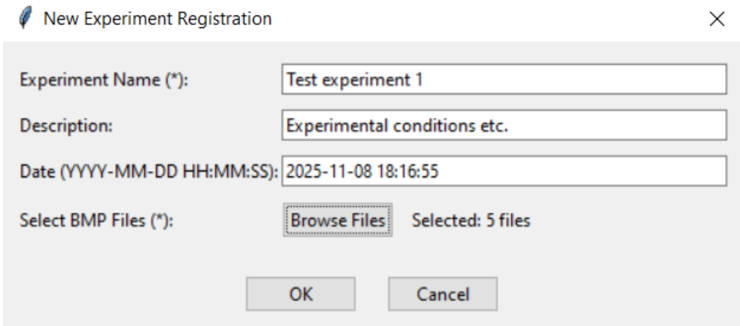

Fig. 3. Adding new experiment window

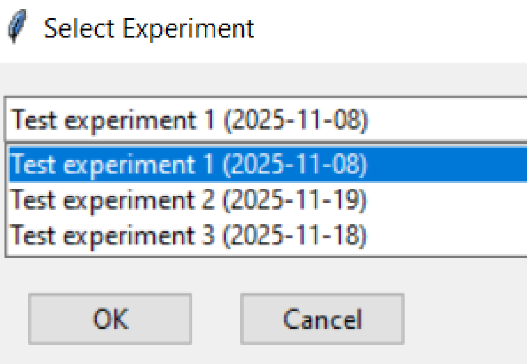

Fig. 4. Experiment selection window

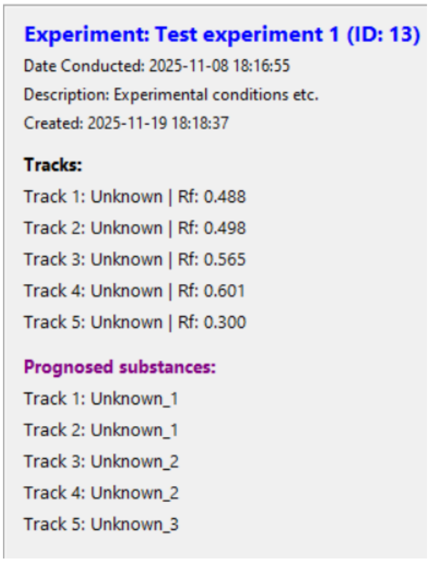

Fig. 5. Section for viewing information about the experiment
(before entering information about known substances)

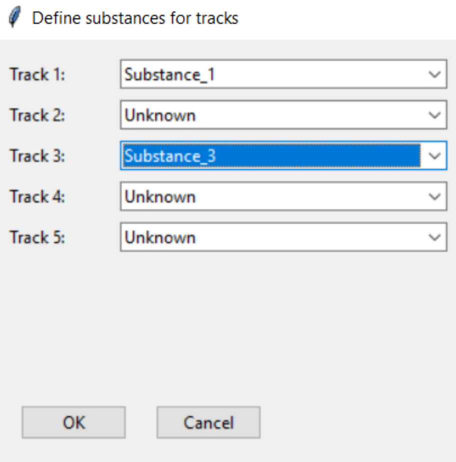

Fig. 6. Window for determining the substances of the experimental tracks

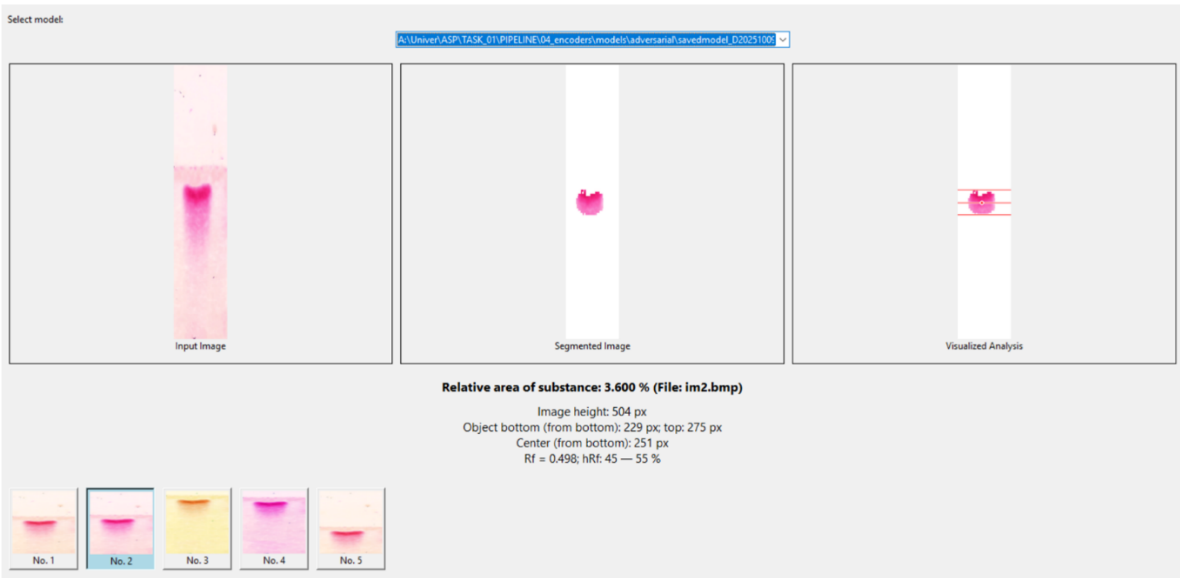

Fig. 7. Section for viewing experiment tracks and their automatic analysis

The application also implements automatic prediction of unknown track substances based on comparison with the Retention factor of other application tracks (Fig. 8).

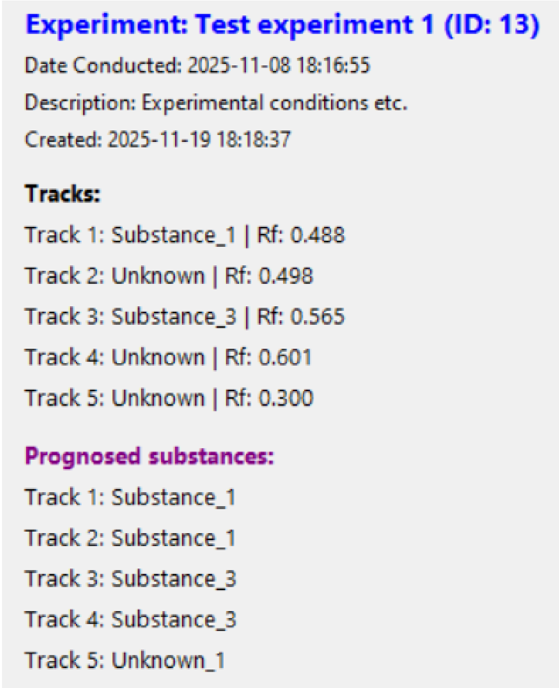

Fig. 8. Section for viewing information about the experiment
(after entering information about known substances)

The developed software solution successfully addresses the challenges of automating thin-layer chromatography image analysis by integrating experiment management, automatic segmentation, and substance prediction based on retention factors. This system enhances the objectivity, reproducibility, and efficiency of TLC research, providing a valuable tool for researchers in various chemical analysis fields. Future work may focus on improving segmentation accuracy and expanding the substance database for broader applicability.

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