Smart Compound Library Based on Machine Learning, Sensing Technology, and Programmable Logic Control

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Poster#: P13

Abstract

Compound management is a critical task in pharmaceutical research laboratories, as compounds are an indispensable part of the experiments. The quality of compound management directly affects the safety and efficient operation of the laboratory. Aspects such as the dispatch, reception, storage, and use of compounds all need to be carefully considered[1]. Traditional compound storage systems face challenges such as risks of manual operation, insufficient space utilization, and material inventory issues. By implementing a smart compound library based on automation, these problems can be solved, improving the safety and accuracy of laboratory compound management.

Objectives

To showcase the development and effectiveness of a smart compound library system, which incorporates machine learning, sensing technology, and programmable logic control, in order to enhance the safety, accuracy, and efficiency of compound management in pharmaceutical research laboratories, and to provide new insights and solutions for intelligent compound management.

Methods

In a smart compound library, several major functional modules are typically involved, including compound storage and retrieval port, internal transfer and storage modules. Infrared sensing and intelligent scanning technologies are used for rapid identification, providing accurate information basis for subsequent processes. When the infrared sensor detects an obstacle in the target area, a signal will be sent to the scanning device to start scanning. The system records and verifies all information of compounds entering and exiting the warehouse to ensure the accuracy of each storage and retrieval operation.

There are various types of compound containers. In order to accommodate more types of containers, image recognition and machine learning are employed to achieve precise positioning and adaptive grasping, while pressure sensing technology ensures the safety of grasped compounds. When a new storage plate enters, a high-definition camera will take a photo for storage. Then, through machine learning, it can accurately determine whether there are compounds in each well. Visual recognition technology is used to calculate specific parameters for each well, including coordinates and similarity. The coordinate parameters are used to locate the information of each well to be determined. For each specific well, the presence of compounds is determined by calculating the similarity parameters with the template.

Figure 1. The equipment used in the system, from left to right, are infrared transceiver sensor, smart camera, and claw.

After accurately identifying the information of the compounds, for quick storage and efficient use of space, the three-axis gantry and movable double-sided storage cabinets can effectively address these two issues.

The design of movable dense cabinets allows for the creation of work passages when in operation, enabling the transport robot to retrieve and place compounds within the passage. This design maximizes the number of cabinets, thereby increasing storage capacity. Finally, scheduling algorithms are applied to optimize the overall workflow, and a management system is established to enable human-machine interaction.

Results

As shown in Figure 2, the identification is performed for 1.5mL storage tubes. The specific identification situation of the experimental group can be seen in the box on the left. The program will locate and number each tube, and display its similarity value.

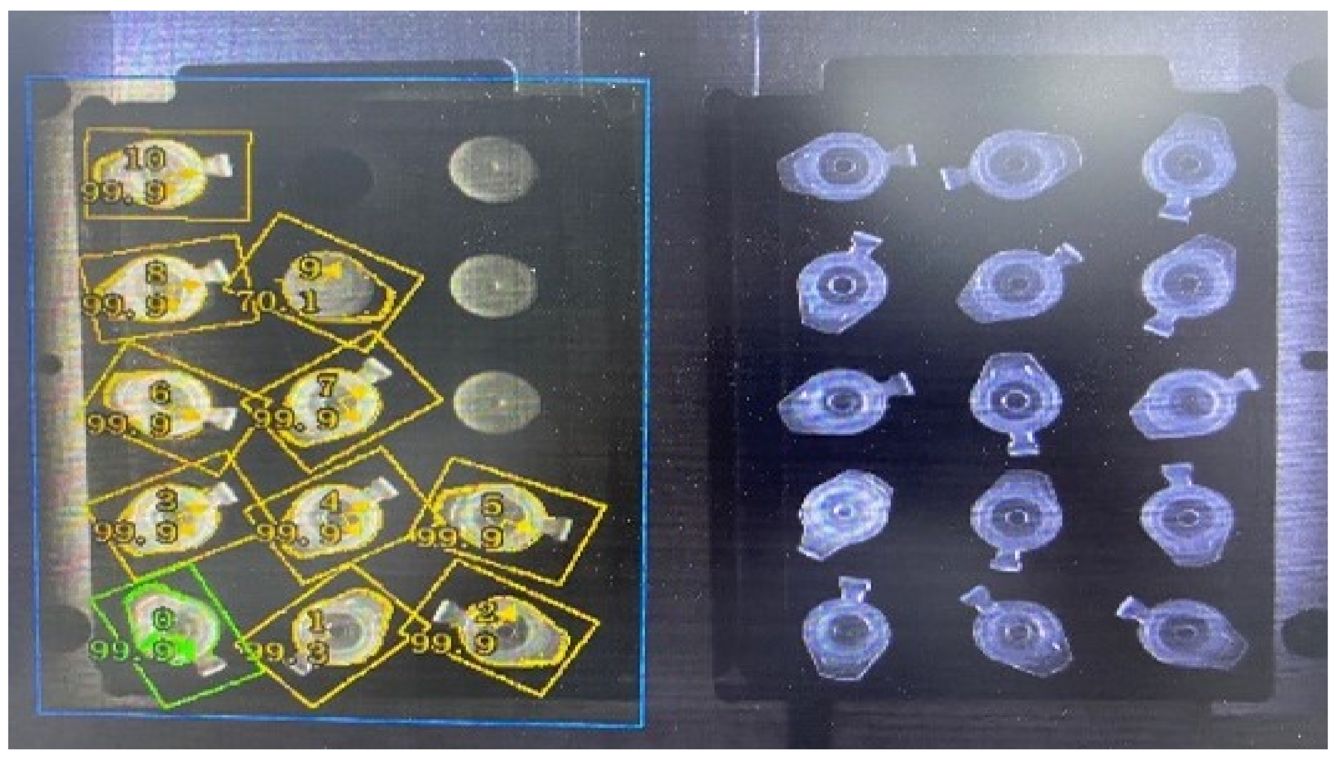

Figure 2. Identification results for 1.5mL storage tubes.

Through a large amount of training on the experimental group, a set of standard parameters for actual judgment is obtained, as shown in Table 1. If the calculated parameters are within the standard parameter range, it can be considered that the well has a storage tube. Similarly, for containers of different specifications, multiple sets of identification and standard parameters are established for judgment.

Table 1. Standard parameters for 1.5mL storage tubes.

Well ID	X axis	Y axis	Lower Limit of Similarity
1	916	1025	70
2	654	1029	76
3	397	1037	82
4	921	1273	65
5	661	1269	74
6	411	1268	83
7	922	1492	77
8	659	1485	86
9	409	1501	99
10	895	558	76
11	645	57	76
12	390	565	82
13	652	791	76
14	392	804	77
15	916	1025	70

Through the integration of technologies such as machine learning, sensing, programmable control, and intelligent scheduling, fully automated warehousing operations and round-the-clock inventory checks have been achieved, which has tripled the storage capacity in the same space. For instance, in a 30 cubic meter space, up to 200k units can be stored using 4mL containers. The system is currently capable of handling 9 types of containers and 5 types of racks, with a positioning accuracy within 0.03mm, and the range of recognizable items will continue to expand.

Conclusion

In this study, the efficient integration of business modules and automation technologies has enhanced the level of intelligence in compound warehousing operations, significantly improving compound management. This study provides new ideas and solutions for intelligent compound management.

References

[1] Yasgar A, Shinn P, Jadhav A, et al. Compound Management for Quantitative High-Throughput Screening. JALA: Journal of the Association for Laboratory Automation. 2008;13(2):79-89. doi:10.1016/j.jala.2007.12.004

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