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

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PURPOSE

In pharmaceutical research laboratories, compound handling is a key process as compounds are the fundamental elements of experiments. The handling quality of these compounds directly influences the lab's safety and operational efficiency. Detailed consideration is needed for aspects such as the dispatch, receipt, storage, and use of compounds[1]. Traditional compound storage systems face challenges such as risks associated with manual operations, inefficient space utilization, and material inventory problems. By implementing an automated intelligent compound library, these issues can be resolved, thus improving the safety and accuracy of compound management in the laboratory.

OBJECTIVE(S)

This study aims to create a smart compound library for enhancing compound management in pharmaceutical research labs. The library integrates key functional modules and applies advanced technologies such as infrared sensing, intelligent scanning, image recognition, and machine learning for fast and accurate compound identification and positioning. Additionally, a three-axis gantry and movable double-sided storage cabinets are employed for optimal space utilization, ensuring safety and precision in compound management.

METHOD(S)

The study utilizes a smart compound library which integrates several key functional modules, including compound storage retrieval port, and internal transfer and storage modules. Technologies like infrared sensing and intelligent scanning are employed for rapid identification, providing accurate information for subsequent processes. The system logs and verifies all compound information during each storage and retrieval operation to ensure accuracy.

The system accommodates various types of compound containers, utilizing image recognition and machine learning for precise positioning and adaptive grasping. A smart camera captures images of new storage racks, which are analyzed to determine the presence of compounds in each well.

The system incorporates a three-axis gantry and movable double-sided storage cabinets for optimal storage and space efficiency. Scheduling algorithms streamline the overall workflow, and a system is established to facilitate human-machine interaction.

RESULT(S)

As shown in Figure 1, we use a smart-camera to perform image recognition on 8 mL storage tubes. The specific identification situation of the experimental group can be seen in the left panel. The program will locate and mark each tube, and calculate its similarity. The similarity is calculated by comparing the corresponding holes of the left side with the actual storage tube and the right side with the blank rack. As can be seen in Figure 2, the program will calculate several parameter results corresponding to the storage tubes.

By conducting a large amount of image recognition training on the experimental group containing the same specification containers, a set of standard parameters for judgment is obtained. If the calculated parameters are within the standard parameter range, it can be considered that the well has a storage tube. Some key parameters are displayed, such as coordinate information and similarity. Since factors like lighting and angle can affect the identification of storage tubes at different positions, each well will have corresponding standard parameter. Similarly, for containers of different specifications, multiple sets of recognition and standard parameters are established for judgment. As shown in Table 1, it is a standard parameter example of 8 mL storage tubes.

Through the integration of technologies such as machine learning, sensing, PLC (programmable logical controller), 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 4 mL containers. The system is currently capable of handling 9 types of containers and 5 types of racks, with a positioning accuracy within 0.03 mm, and the range of recognizable items will continue to expand.

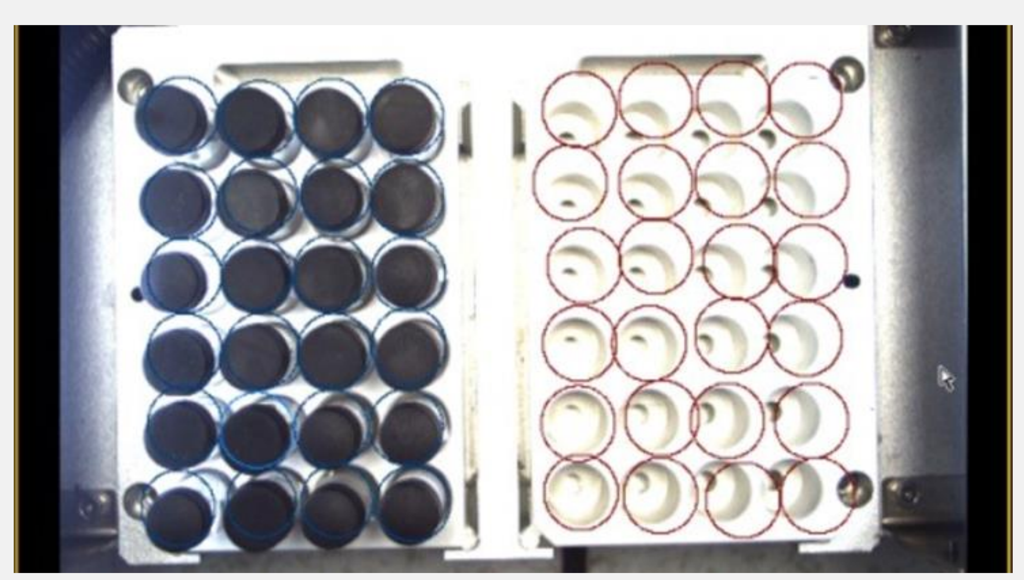

Figure 1. Identification results for 8 mL storage tubes.

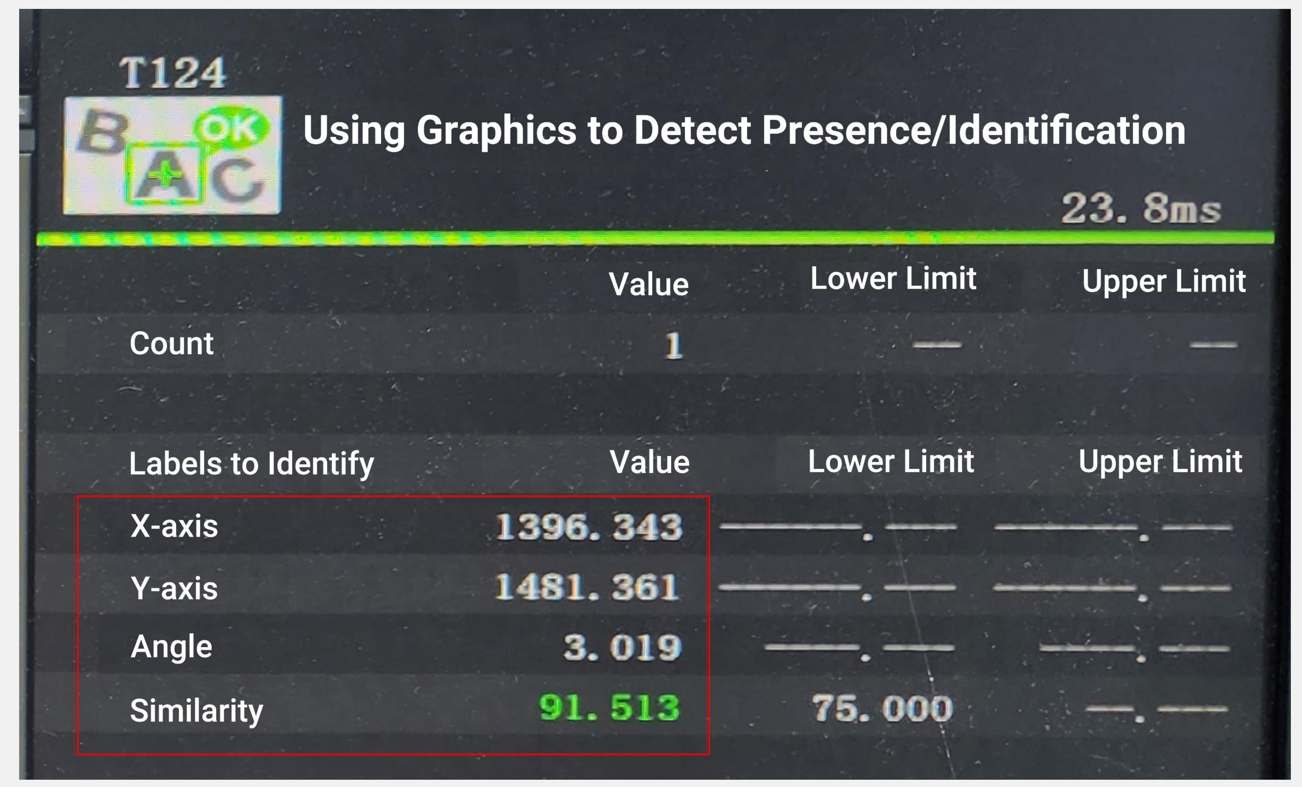

Figure 2. The schematic diagram of the parameter calculation results for storage tube in a certain well position.

Table 1. Standard parameters for 8 mL storage tubes.

Well ID	X axis	Y axis	Lower Limit of Similarity
1	412	1518.5	85
2	606	1518	90
3	791.5	1512	82
4	983	1529	85
5	405	1343	82
6	585	1319	82
7	803	1302	70
8	985	1287	70
9	394	1150.5	80
10	588.5	1148	85
11	799	1113	80
12	983	1102	70
13	407	945	80
14	581.5	935.5	80
15	800	927	80
16	981	923	80
17	409.5	757	80
18	538	739.5	90
19	791	750	82
20	948	741	85
21	408.5	573	80
22	573	569.5	80
23	793	573	90
24	975	562	90

CONCLUSION(S)

This research demonstrates the effective integration of business modules and automation technologies, which enhances the sophistication of compound warehousing operations and leads to significant improvements in compound management. The study presents innovative approaches and strategies for the enhancement of intelligent compound management.

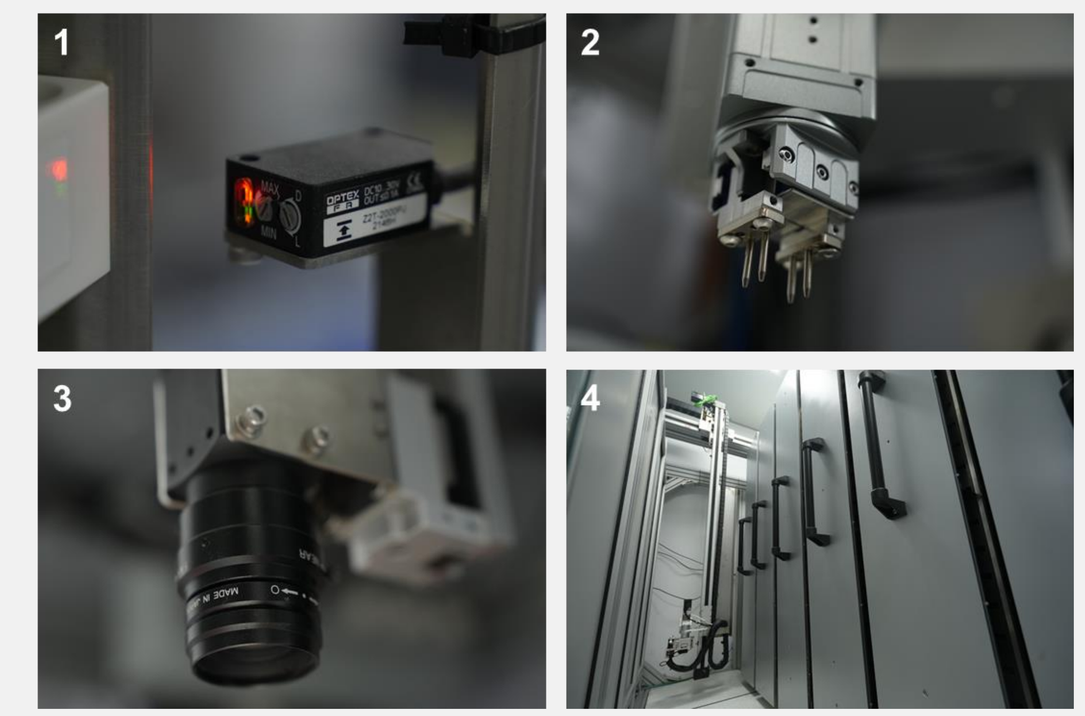

Figure 3. The equipment used in the system, in order, are the infrared sensor, gripper, smart camera and double-sided storage cabinet.

REFERENCE

[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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