Robot-friendly Design Guidebook

Deliverable 1.2

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Abstract	Thes guidelines that can be used to design laboratory equipment that is more robot friendly. It describes challenges that are frequently encountered in the automation and suggests solutions to overcome these challenges. The intended audience includes providers of automated solutions, equipment manufacturers and the general laboratory automation community.

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1 Executive Summary

This document contains guidelines that can be used to design laboratory equipment that is more robot friendly. It describes challenges that are frequently encountered in the automation of pharmaceutical laboratory processes and suggests solutions to overcome these challenges. The intended audience includes providers of automated solutions, equipment manufacturers and the general laboratory automation community. Since the guidelines presented in this document are primarily derived from the challenges encountered during the development of TraceBot, it is closely related to the TraceBot use case definition, i.e. D1.6 Use Case Specification.

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2 Introduction

Today's pharmaceutical laboratories are dominated by manual processes and rife with opportunities for automation. Robots offer a promising way to exploit this untapped automation potential by implementing tasks for which no commercial off-the-shelf device exists and aggregating separate process steps into larger, fully automated chains. While most experts agree that the pharmaceutical lab of the future will be significantly more automated than it is today, there is still considerable uncertainty as to when automated solutions are ready to be deployed at scale. It is not clear, for example, whether labs can be fully automated within two, five or even ten years. The challenges prohibiting further automation are manifold: the tasks to be automated are complex and differ greatly from lab to lab (even though the work in a single lab can be quite repetitive), regulations require certainty in the execution of each process step and lab equipment is usually designed with humans instead of robots in mind.

For automated solutions to be deployed, all of the aforementioned challenges have to be addressed. The first challenge, namely the wide variety of tasks to be automated, can be addressed using smart robotics that can be quickly adapted to novel use cases without requiring in-depth engineering knowledge. The second challenge, i.e. the certainty in execution, is an ongoing research topic and directly addressed by the traceability framework that is at the core of TraceBot.

This document addresses the third challenge, i.e. how lab equipment can be designed in such a way that it is more robot friendly or, in other words, more amenable to automation via a robotic system. To this end, both existing and yet to be developed devices and consumables are considered. The goal is to provide a comprehensive set of guidelines, hence the title "Robot-friendly Design Guidebook."

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3 Design Guidelines

The following sections provide guidelines that can be used to design equipment that is more robot friendly. The guidelines are based on feedback from the TraceBot team and either directly derived from challenges encountered during the development of TraceBot or drawn from prior experiences of the team.

3.1 Graspable Surfaces

To interact with its environment, a robot usually has to pick up at least some of the objects in its vicinity. To pick up an object, the object must have surfaces that can be grasped securely. A hard to grasp object can be dealt with in one of two ways: using a special gripper that is more suited to handle the object in question or a custom adapter/holder that provides a surface that can be grasped using a standard gripper. While both approaches do work in practice, they come with drawbacks that need to be considered. If the robot is required to pick up multiple hard to grasp objects using special grippers, it may need to swap grippers in between, which complicates the process and prolongs the execution time. If custom adapters are used, every object must be touched by a human at least once to attach the adapter. This, however, means that the system can no longer handle consumables autonomously.

Figure 1: A parallel gripper (left) and the two yellow caps that need to be attached to the bottom of the canisters of the sterility testing kit used by TraceBot (right).

Parallel grippers like the one shown in **Fehler! Verweisquelle konnte nicht gefunden werden.** (left) are ubiquitous within the robotics industry. Making sure that objects can be grasped using a parallel gripper thus eliminates the need for custom adapters as well as the need to swap grippers in between work steps. Equipment that is intended to be picked up by a robot should therefore contain at least two parallel surfaces. These surfaces should be at most 5 to 10 cm apart so that their distance does not exceed the maximum opening width of most grippers. Furthermore, each surface should ideally be between 1 and 2 cm^2 large to ensure a secure grip. This is particularly important for small objects that cannot be grasped otherwise. In many cases it is possible to adapt the geometry of these objects in such a way that they contain suitable surfaces without negatively affecting their intended functionality. A good example for this are the yellow caps of the sterility testing kit used by TraceBot

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that is shown in Figure 1 (right). The handles of these caps can be easily extended by a few millimetres on each side without affecting their intended function.

3.2 3D Models and Material Properties

There are several ways in which the use of 3D models can benefit a robotic system. In the following, three specific applications are considered: collision avoidance and motion planning, digital twins, and the generation of synthetic training data for computer vision systems.

3D models can be easily integrated into many motion planning and collision avoidance systems. This allows a robot to dynamically plan its next action and makes the overall system much more flexible. If a 3D model contains annotations, i.e. if it comes with a list of spatial locations that a robot can interact with, the 3D model can also be used to define high level operations. As an example, consider the magnetic stirrer with 15 stirring points depicted in Figure 2. If the number and relative location of each stirring point is known, operations such as "placing a flask on stirring point 7" can be implemented without much effort. 3D annotations are particularly useful when combined with a vision system that can compute the position and orientation of a given object. In this case the object can be placed almost arbitrarily within the vicinity of the robot and the robot will still be able to interact with it due to the relative definition of the spatial locations. Note that this naturally leads to equipment that can be replaced in a plug & play manner. In such a system, the stirrer in Figure 2, for example, could be replaced with a stirrer of a different size and with a different number of stirring points. This is especially true if the relative locations are stored in a standardized format such as the one defined by the OPC UA Relative Spatial Location (RSL)[1] standard.

Figure 2: A magnetic stirrer with 15 stirring points.

Besides basic motion planning and collision avoidance, 3D models can also be used to implement more sophisticated digital twins like the one shown in **Fehler! Verweisquelle konnte nicht**

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[1] https://reference.opcfoundation.org/RSL/

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gefunden werden.. Assuming some basic material properties like, for example, friction coefficients are known, the 3D models can be used to physically simulate actions before they are executed. Doing this has two advantages. First, it allows the robot to determine if a dynamically planned action is safe to execute, i.e. if the action is likely to produce the desired outcome. Second, it enables the robot to automatically detect failures by comparing the simulated world state with the perceived real-world state after executing the action. The use of a digital twin can therefore make a system more robust and

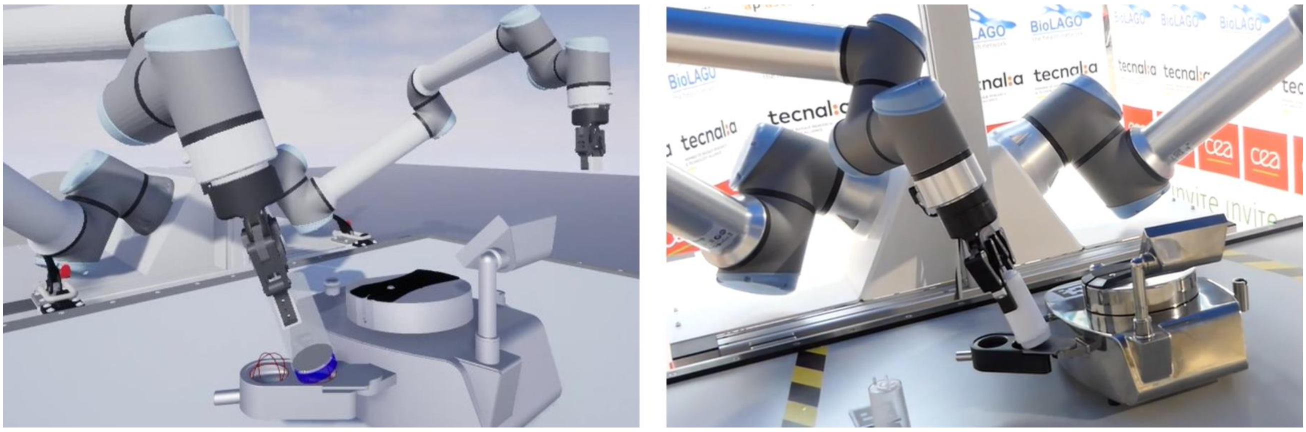

Figure 3 The TraceBot digital twin (left) uses several 3D models to simulate interactions between their real-world counterparts (right). Shown here are two robot arms, the attached grippers, a sterility testing pump and two plastic canisters.

less error prone.

Another application of 3D models is the training of AI-based computer vision systems using synthetically generated images. For this, a 3D model should ideally be textured and/or include a material description that can be used for rendering. As a result such 3D models would more easily allow the simulation based training of AI-based methods increasing flexibility and reliability of the overall system.

Figure 4: Two synthetic images from the dataset that was used to train TraceBot's pose estimation network. Artificial backgrounds were used to make the network more robust

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Fehler! Verweisquelle konnte nicht gefunden werden.4 shows some example images of a dataset that was generated to train the pose estimation network for TraceBot.

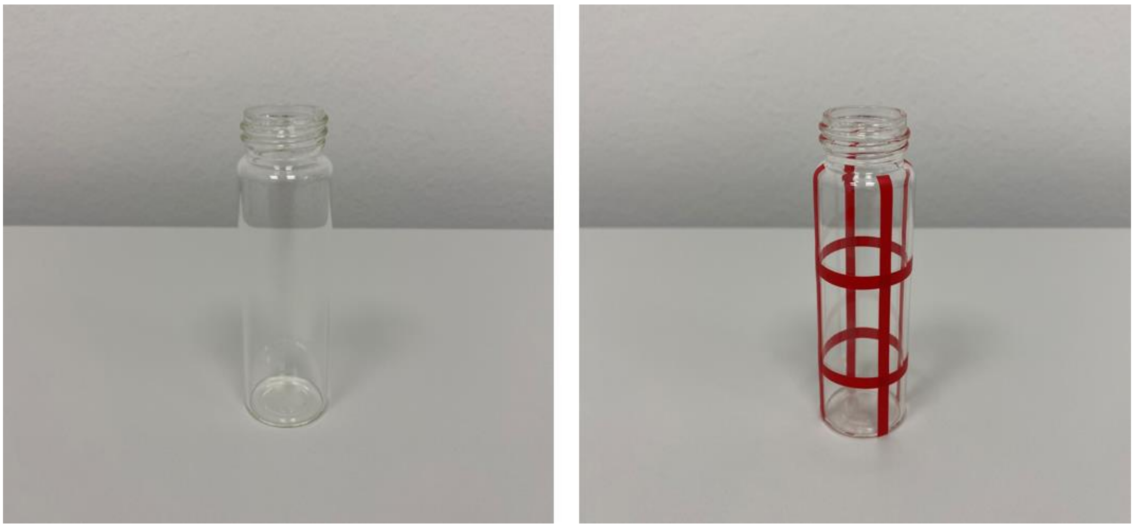

Figure 5: A transparent vile without (left) and with (right) visual guidelines. Note that the vile with guidelines is much easier to recognize.

3.3 Visual Guides

Automatically detecting all objects within the working area of a robot is useful for two reasons. First, it allows objects that should be manipulated by the robot to be placed arbitrarily within the robot's vicinity, leading to a more flexible and adaptive system. Second, it enables the robot to systematically verify that all objects are where they are supposed to be, as, for example, done in TraceBot with the help of the digital twin shown in **Fehler! Verweisquelle konnte nicht gefunden werden.** (left). For both applications to work reliably, computer vision algorithms must be able to detect and estimate the pose of the objects in question. Unfortunately, not all objects can be easily detected. As an example, consider the transparent vile depicted in Figure 5 (left). The vile is barely visible which makes it hard to accurately estimate its pose. A straightforward solution would be to replace the vile with an opaque one. This, however, would mean that lab technicians could no longer inspect the contents of the vile without pouring it into another container. A more practical solution in this case is to print visual guidelines onto the surface of the vile as show in Figure 5 (right). Crucially these guidelines should be visible from all viewing angles.

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Another example where visual guidelines can support pose estimation algorithms is the needle that can be seen in Figure 6. In TraceBot, a robot has to remove the blue lid from the body of the needle and then pierce the exposed needle through a membrane. To ensure the successful execution of this step, the estimated pose of the needle should be as precise as possible. Visual guidelines can help to achieve this goal. Note that the depicted guidelines are intentionally asymmetrical to resolve ambiguities due to rotational symmetries.

3.3.1 Experiments to Evaluate the Usefulness of Visual Guides

To evaluate if these visual guides indeed improve the quality and accuracy of object detection and pose estimation, we carried out an initial experiment. To capture comparable scenes with objects without and with visual guides, we rendered two similar datasets with eight scenes with the only difference being in one canister with the stripes and the other without. For every scene we created one thousand images. Each scene contains the randomly placed canister and several distractor objects. For examples of the dataset, see Figure 7. In a part of the scenes the canister is partially occluded. The occlusion is up to 80% leaving at least 20% of the object visible. The images show the objects in medium size, but there are also images where objects are smaller, see Figure 8. The idea is to check what role object size in the images plays for detecting the candidate canister with and without visual guides.

To test which of the canisters are best suited for the task, i.e., the transparent “Vanilla” canister vs.

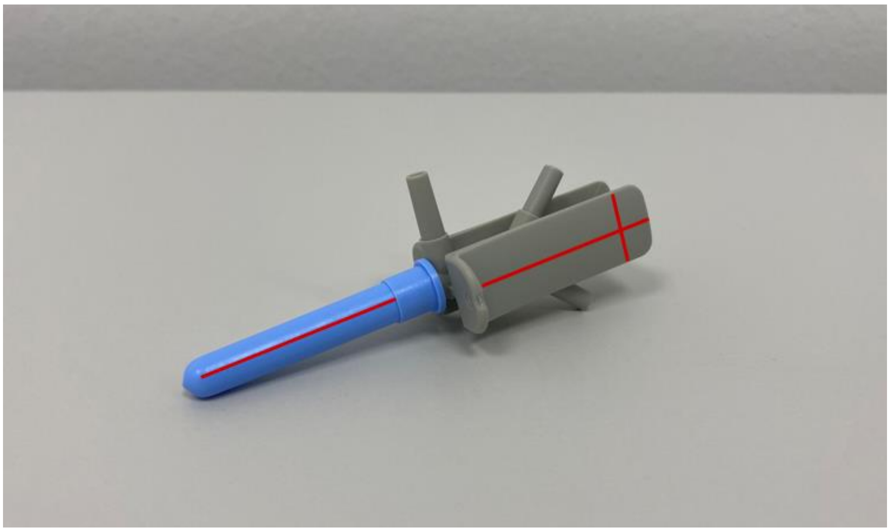

Figure 6: Visual guides like the red lines on this needle can make pose estimation algorithms more robust.

the striped canister with Visual Guides, we resorted to training an object detection model, specifically the Yolox model. The results are two trained models:

1. Model 1 or **Mw/o**, the model with the transparent canisters without visual guides, and
2. Model 2 or **MVG**, the model with Visual Guides.

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For the training of both models, we used the YOLOX [2] object detector implemented in GDRNPP [3], the BOP challenge 2022 winner, and the version of the original GDR-Net [4]. The object detection model is trained for 60 epochs with a batch size of eight for both datasets. For our experiment's purpose, we kept 7 scenes for training and 1 for testing.

Figure 7: Sample images of the created dataset. Left: Images with transparent canister and detection marked. Right: Images with added visual guides and detection boxes in red.

[2] Zheng Ge, Songtao Liu, Feng Wang, Zeming Li, Jian Sun: YOLOX: Exceeding YOLO Series in 2021; arXiv, 2021. DOI: https://doi.org/10.48550/arXiv.2107.08430. Code available from https://github.com/Megvii-BaseDetection/YOLOX?tab=readme-ov-file

[3] Yukang Zhang, Gu Wang, Xiangyang Ji: GDRNPP: Extending Geometry-Guided Direct Regression Network in 2022; *European Conference on Computer Vision WorkShop (ECCVW)*, 2022. Code: https://github.com/shanice-l/gdrnpp_bop2022

[4] Gu Wang, Fabian Manhardt, Federico Tombari, Xiangyang Ji: GDR-Net: Geometry-Guided Direct Regression Network for Monocular 6D Object Pose Estimation; IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR), 2021, pp. 16611-16621.

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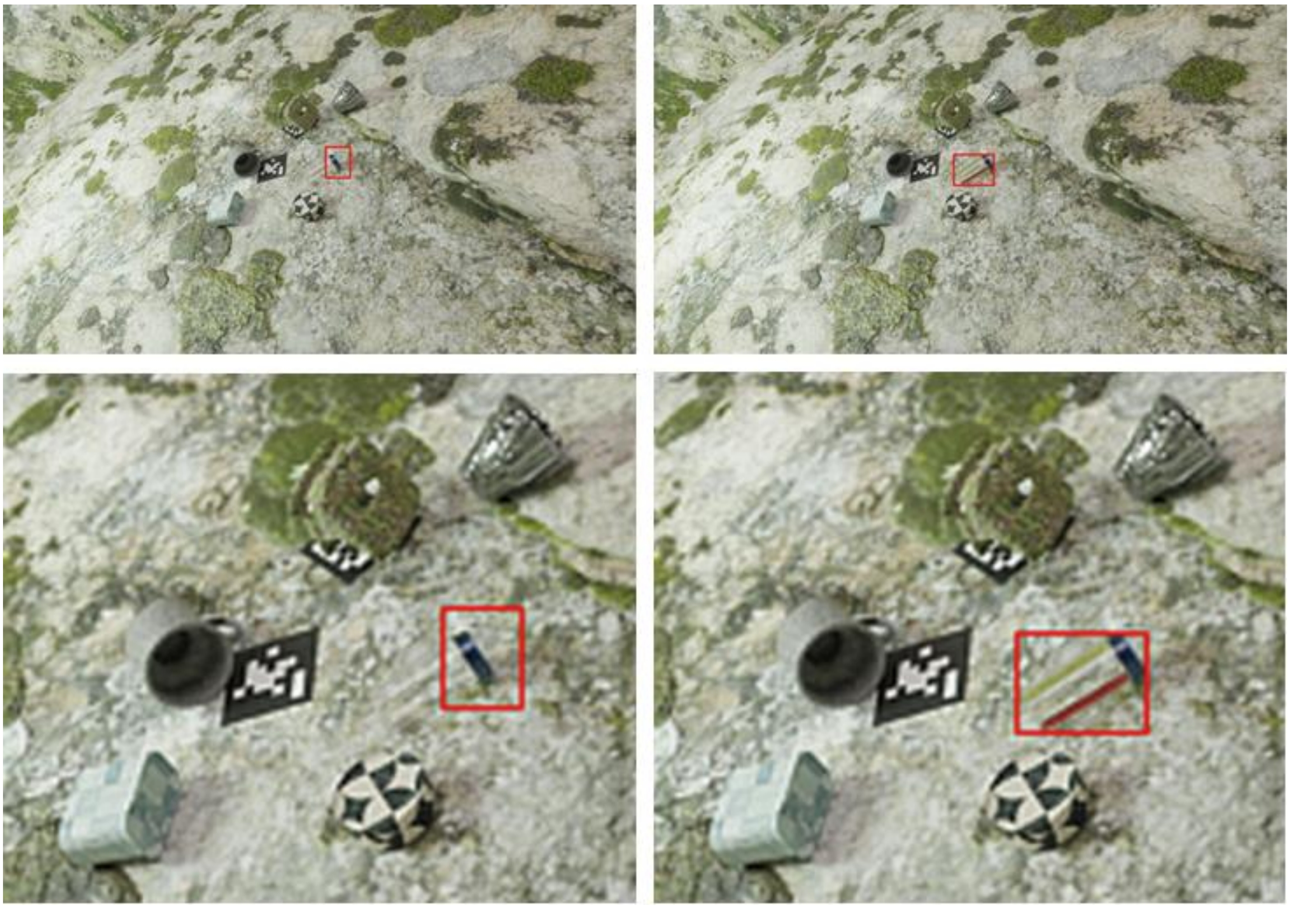

Fig. 8: Sample images of the test of size 728x1280 pixel. Top line: full images with detected canister. Left column: transparent object without visual guides. Right column: canister with added visual guides. Bottom line: Focus on the centre of the scene to highlight the detection. Bottom Left: The transparent canister is detected but mostly with its base plate and part of the top is missing. Bottom Right: With the visual guide, the canister is fully detected.

The results of the experiments are summarised below comparing the two models, **Mw/o** vs. **MVG**. Table 1 presents the quantitative metrics for the experiment. The results clearly show that adding a pattern like the proposed Visual Guides significantly improves the object detection rates.

The overall performance is best seen with metric AP, where MVG significantly outperforms Mw/o, with an AP of 85.512 compared to 37.793. This indicates that MVG is much better at detecting objects across all sizes and IoU thresholds.
The performance at different IoU Thresholds (AP50, AP75) shows that at AP50 MVG has a very high AP50 of 98.576, while Mw/o has a much lower AP50 of 57.455. This suggests that MVG is far more reliable in detecting objects even with a lenient IoU threshold. AP75: The gap remains large at the more stringent IoU threshold. MVG 1 maintains high precision even at higher overlap requirements. As last point we investigate object size in the image. APs for small objects: here MVG scores 47.404, which is double the performance of Mw/o at 23.811. Small objects are challenging for both

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models, but Model 2, MVG, handles them much better. For both, APm (medium) and APl (large object size), MVG clearly outperforms Mw/o.

Table 1: Results of comparing object detections for canisters without visual guides, Model Mw/o, and with added Visual Guides, Model MVG. Bold numbers indicate better values. The metrics are explained below.

Model \ Metric	**AP**	**AP50**	**AP75**	**APs**	**APm**	**APl**
Mw/o: canister **without** visual guides	37.793	57.455	42.568	23.811	39.157	32.515
MVG: canister **with** Visual Guides	**85.512**	**98.576**	**96.088**	**47.404**	**85.793**	**89.204**

AP (Average Precision): AP is the mean of the precision values at different recall levels. It provides a single number that summarizes the precision-recall curve for a particular class. In practice, AP is computed by averaging precision at a set of evenly spaced recall levels, typically from 0 to 1. Higher is better.
AP50/75 refers to the Average Precision when the IoU(Intersection of Union) threshold is set at 50/75%. This means that for a predicted bounding box to be considered a true positive, it must overlap with the ground truth bounding box by at least 50/75%. 50% is considered a relatively lenient threshold, 75% is a more stringent measure, usually indicating better localization precision.
APs/m/l (AP for small/medium/large objects) evaluates the performance specifically on small/medium/large-sized objects. The size categories (small, medium, large) are typically defined based on the area of the ground truth bounding box. This metric helps to understand how well the model performs on objects that appear rather small or large in the image.

In summary, this clearly indicates the significance of adding Visual Guides to assist the visual perception of transparent objects for future industrial usage.

3.4 Packaging of Consumables

Looking at the sterility testing use case targeted by TraceBot, one can observe that the robot primarily interacts with its environment through the manipulation of consumables. More specifically, the robot

Figure 7: The sterility testing kit used by TraceBot.

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performs multiple actions that involve two single-use plastic canisters connected to a needle via a tube. Consider the packaging of these items shown in Figure 7 (left).

While the packaging of the canisters, tube and needle is perfectly fine for human operators, it is somewhat suboptimal for handling via a robot. The foil, for example, that is used to seal the testing kit is difficult for a robot to remove. While a robot can easily grasp the corner of the paper foil that is used to open the package and shown in Figure 7 (middle, right), it cannot securely grasp the body of the package due to the elasticity of the used materials. This, however, is necessary to counteract the force required to rip off the foil. A solution to this problem is to manufacture the package using more rigid materials. Alternatively, the package can also be locally reinforced to allow a robot to grasp it at a designated location (see Section 3.1 Graspable Surfaces).

Once the package has been opened, the robot must unpack the contents of the kit depicted in Figure 8. This presents additional challenges since the tube, needle and clamps are stored in an intertwined manner and only loosely placed inside the body of the kit. Storing the contents of the kit in a disentangled manner would therefore make the unpacking of the kit more robot friendly. Of course, it would be best if all parts of the kit were placed in predefined positions or holders that are built into the package. Apart from this, increasing the space between the canisters and the plastic packaging would make it easier to pick up the canisters without special grippers. The required space depends on the fingers of the grippers, but for most grippers, a 1 cm gap on each side would be sufficient. Furthermore, attaching small handles to the tube would allow a robot to better grasp the tube and, assuming that the handles are placed at predefined positions, provide information about the exact position on the tube that was grasped. A slightly longer tube would simplify the insertion of the tube

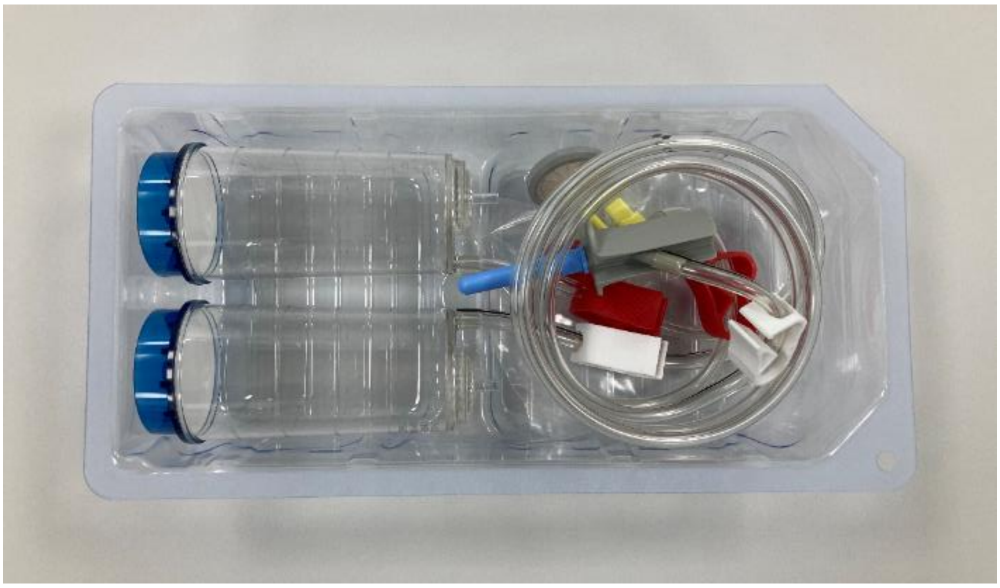

Figure 8: The contents of the sterility testing kit after removing the protective cover.

into the pump by providing the robot with more leeway. Finally, the use of visual guides on the two canisters, tube and needle would make them easier to detect visually (see Section 3.3 Visual Guides).

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3.5 Software Interfaces

Whereas the previous items focus in one way or another on hardware, this item focuses on software or, more specifically, software interfaces. Software interfaces are important because they enable a lab automation system to programmatically control equipment in a way that is both robust and safe. Software interfaces are less error prone than manual interfaces (pressing a button, reading data from a screen, etc.) and therefore generally preferred. As such one of the most important properties of a lab device in an automated system is that it has a software interface at all. Note that this requirement applies to most devices in practice, as every device that needs to be switched on and off should ideally be controlled via software and not the press of a button. Fortunately, many legacy devices offer serial interfaces that make it possible to send commands to these devices and receive sensor values from them. More modern devices sometimes provide higher level interfaces that offer more advanced features such as user authentication. REST APIs[5], for example, are particularly easy to integrate due to their widespread use in the software industry. More recently, specialized standards for the integration of lab equipment into IT systems have been developed. Examples are the OPC UA Laboratory and Analytical Device Standard (OPC UA LADS)[6] and the Standardization in Lab Automation (SiLA)[7] standard. Both aim to enhance interoperability within lab automation and data management systems and offer robust frameworks for the seamless integration of devices and software packages. Equipment developed today should support at least one of the aforementioned communication standards to ensure interoperability with other systems.

[5] https://en.wikipedia.org/wiki/REST
[6] https://opcfoundation.org/markets-collaboration/lads/
[7] https://sila-standard.com/

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4 Adapter Exchange

Most devices and consumables used in today's pharmaceutical labs do not adhere to the guidelines set out in this document. Consumables, for example, usually have no visual markers for pose estimation and offer few graspable surfaces. As a result, integrators frequently have to design custom adapters to allow a robot to first locate and then interact with these objects – a task that is currently carried out separately for every project. An online platform, or exchange, where CAD models of adapters can be freely shared could reduce this effort and promote reuse across labs. Similar exchanges already exist in the hobbyist 3D printing community. A popular example is the Thingiverse[8] platform shown in Figure 9, which is operated by the Dutch 3D printer manufacturer Ultimaker[9].

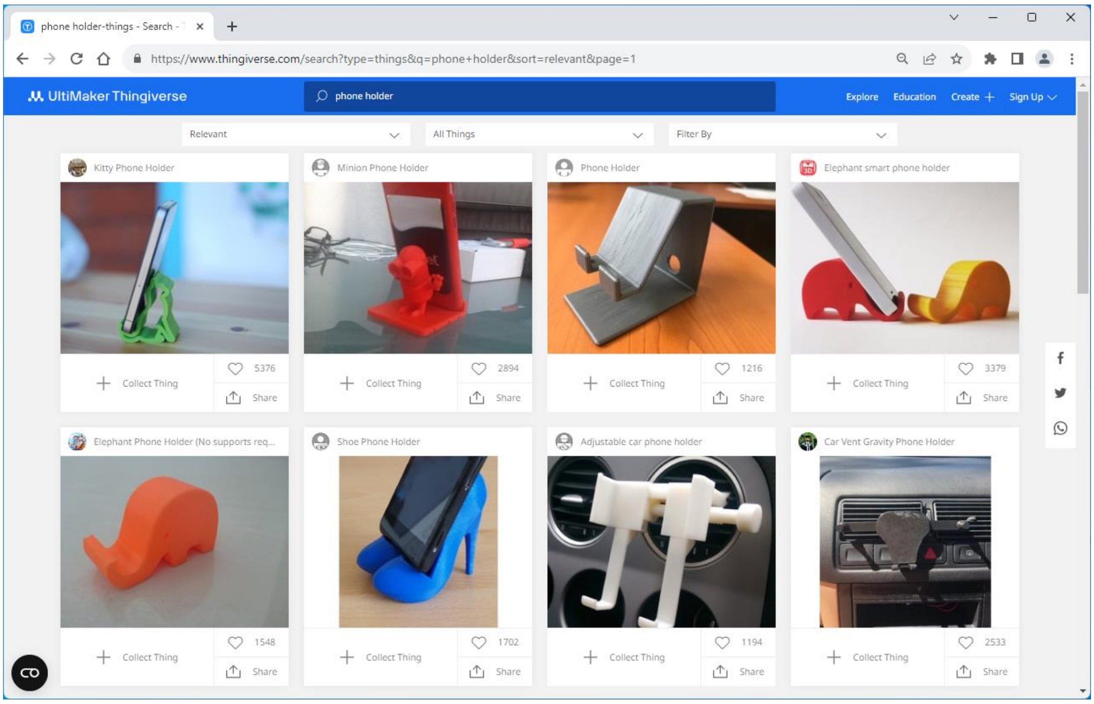

Figure 9: The Thingiverse platform that allows users to share CAD files online.

The creation of such an exchange for pharma applications would enable integrators and lab operators to share their adapters/holders online and allow them to integrate existing equipment into robot workflows more easily. Note however, that there is no need to create a custom platform for the lab automation community. Instead, 3D models could simply be uploaded to one of the existing exchanges and then tagged using a common tag such as "labautomation". Doing so would provide value today and act as an interim solution until more robot friendly devices and consumables are commercially available.

TraceBot focuses on lab automation using (collaborative) robot arms. However, an online exchange such as the one proposed here would not have to be limited to adapters for robot arms. As an example, consider the magnetic stirrer extension depicted in Figure 10. This custom adapter was recently

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[8] https://www.thingiverse.com/
[9] https://ultimaker.com/

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designed at INVITE to retrofit an existing Chemspeed Swing (XL)[10] system with magnetic stirrers. To this end, four 2mag MIXdrive 1 XS[11] stirrers were placed in a custom 3D printed part that is mounted into a standard Chemspeed double-level holder.

Figure 10: A custom holder designed to retrofit a Chemspeed Swing (XL) system with four magnetic stirrers.

Since the stirrers can be controlled via a serial interface (see Section 3.5 Software Interfaces), they can be integrated into the Chemspeed software with just a few clicks. This allows users of the Chemspeed system to easily incorporate the stirrers into their automated workflows. It is reasonable to assume that an extension like this would also be useful for other labs.

[10] https://www.chemspeed.com/example-solutions/swing/
[11] https://2mag.de/en/products/single-point-stirres/single-point-stirrers-with-external-control/mixdrive-1-xs.html/

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5 Deviations from the workplan

None

6 Conclusion

Although automating pharmaceutical processes is a difficult task, it provides significant potential for increased operational efficiency and reliability. To make automation possible, this guidebook considers a variety of ways in which lab equipment can be made more robot friendly. Graspable surfaces enable a robot to pick up objects more securely using standard grippers. Furthermore, the availability of 3D CAD models represents a major advantage since 3D models can be used in collision avoidance and motion planning, the creation of digital twins, and for the generation of synthetic training data. To make pose estimation algorithms more robust, it is crucial that the objects in question can be clearly seen using a camera. By printing visual guidelines onto transparent objects, pose estimation becomes more reliable. The packaging of consumables also plays a key role in robot friendly design. Packaging should be rigid and contain easily graspable surfaces to facilitate robotic manipulation. Organizing objects in a disentangled manner can further help robots to unpack the contents of a container. Finally, robust software interfaces are essential in the context of lab automation. Modern devices should support standardized communication protocols like OPC UA and SiLA to ensure interoperability and ease of integration. In addition to these guidelines, the lab automation community should consider the creation of an online platform to share CAD models of adapters and holders. This could greatly reduce the effort required for custom integrations and promote standardization across laboratories. By leveraging existing exchanges and tagging models appropriately, the lab automation community could share solutions online and accelerate the adoption of robot friendly design principles.

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