

Two-step techniques for accurate selection of small elements in VR environments

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ABSTRACT

One of the key interactions in 3D environments is target acquisition, which can be challenging when targets are small or in cluttered scenes. Here, incorrect elements may be selected, leading to frustration and wasted time. The accuracy is further hindered by the physical act of selection itself, typically involving pressing a button. This action reduces stability, increasing the likelihood of erroneous target acquisition. We focused on molecular visualization and on the challenge of selecting atoms, rendered as small spheres. We present two techniques that improve upon previous progressive selection techniques. They facilitate the acquisition of neighbors after an initial selection, providing a more comfortable experience compared to using classical ray-based selection, particularly with occluded elements. We conducted a pilot study followed by two formal user studies. The results indicated that our approaches were highly appreciated by the participants. These techniques could be suitable for other crowded environments as well.

1. Introduction

Immersive analytics is an emerging field that explores the utilization of Virtual Reality (VR) and 3D interaction to facilitate the visual analysis of complex data [1]. This approach has gained significant popularity across various domains, including biology, particularly in the analysis of molecular models. While Virtual Environments (VE) offer several advantages over desktop-based systems, such as enhanced spatial understanding of 3D structures and natural interaction gestures, there remain limitations in molecular visualization VR systems compared to desktop systems (e.g., [2–7]), particularly in terms of interaction, collaboration, and data visualization [7]. In this paper, our focus is on addressing interaction challenges, specifically the accurate selection of small objects. Molecular models often consist of minute elements, such as atoms, which are also prevalent in other visualization techniques like scatterplots and dot plots. The selection of these small elements becomes challenging in highly cluttered scenes, a common occurrence in molecular datasets.

Raycasting is the prevalent selection technique employed in VE due to its versatility, requiring only two degrees of freedom and working effectively at any distance. However, raycasting is not free of limitations. It becomes slow and prone to errors when the target's visual size is small or when the scene is cluttered [8,9]. Molecular visualization poses specific challenges for accurate selection, including occlusion (partial or complete hiding of elements), small target size (atom selection difficulty), ambiguity (multiple feasible candidates for a ray direction),

and neighbor navigation (selection of multiple atoms, e.g., for torsion angle query). Despite these challenges, raycasting remains the common selection system in molecular visualization packages, possibly due to its simplicity.

To address these issues, we propose and evaluate two different progressive methods. Both methods involve a two-step selection process: an initial ray-based selection, that may target an atom in proximity to the final goal, followed by navigation through neighboring atoms using visual cues that do not require precise pointing. The two proposals differ in the visual feedback used to indicate selectable neighboring atoms through the touchpad, such as arrows on the spheres or colored circles around the atoms (as depicted in Fig. 1). Our techniques offer several advantages:

- Use as a basis a familiar method.
- Preserve the 3D structure of the scene.
- Enable neighbor navigation, which is useful for other high-level tasks that may imply the selection of several atoms, such as for measure queries.

In addition, our research revealed that the recently developed methods were deemed more comfortable and desirable than the conventional use of Raycasting alone.

We implemented these techniques over UnityMol, a molecular viewer and prototyping platform [3] coded in C# with Unity3D game

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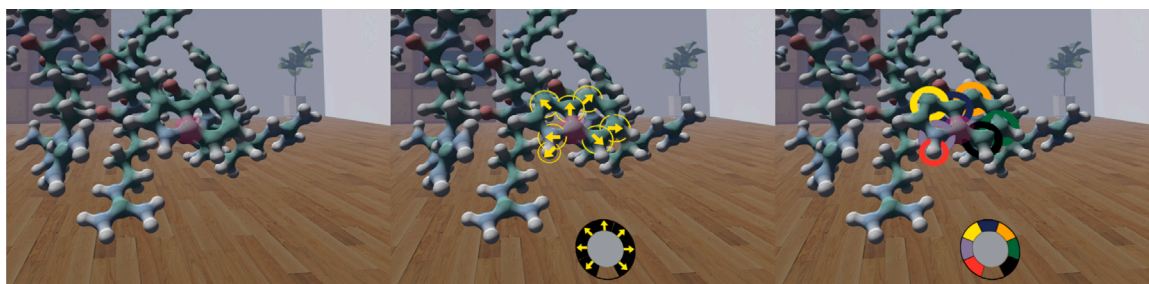


Fig. 1. Our new selection methods (center and right) as compared to classical ray selection (left). To facilitate atom picking in crowded scenes, we have created two new world-space visual feedback elements. From left to right: Raycasting, *Ray + arrows* and *Ray + colors*. Visual feedback is coupled with a technique to select the desired neighbors through the use of the touchpad, which requires no pointing precision.

engine, which is actively developed by Marc Baaden's team at the LBT laboratory (IBPC institute of CNRS in Paris) and with an HTC Vive.

This paper is an extension of our previous publication [10]. In this version, we extended the former in the following ways: (a) we added new participants to the user experiment that compares the different interaction techniques and performed a new statistics analysis, (b) we designed and carried out a new experiment focusing on the acquisition of occluded targets, (c) we validated the color palette selection with three colorblind users, and finally (d) on top of the more typical statistical analysis of the results for the new experiment, we also added an interval analysis to provide further insights of the user performance.

The rest of the paper is organized as follows. Section 2 deals with the related work. Then, Section 3 states our objectives and the research questions we want to solve. In Section 4 we propose the new techniques, that are initially evaluated in Section 5 in a pilot study. In Section 6 we present the improvements and the study that compares the techniques. Then, 7 presents a user study focused on highly occluded targets. Finally, Section 8 discusses the results, and Section 9 concludes our work.

2. Related work

Although ray-casting techniques for target acquisition have great popularity, they encounter challenges, particularly in densely populated scenes with small objects. Consequently, several techniques have been proposed to facilitate pointing. Some strategies involve various approaches, such as considering a group of potential candidates and implementing disambiguation strategies, or making the initial selection easier or faster. Regrettably, not all of these techniques are applicable to molecular models.

2.1. Pointing facilitation

The main purpose of these strategies is to simplify or accelerate the initial selection process. For instance, we have sticky targets from Arge-laguet and Andujar [11]. Motivated by a 2D technique, this approach is based on targets *attracting* the pointer when the ray/pointer is close, facilitating the selection of small objects. However, when there are many, close objects, such as touching atoms, like in molecular models, it is still difficult to select the proper one. Another approach is proposed by Lu et al. [12], an extension of the bubble technique to select small objects without requiring precision. But also has problems with scenes with many candidates. Elmqvist and Fekete [13] propose the use of semantic information to accelerate target acquisition. It is based on the idea that selectable targets are known by the application, and it is rarely used. As before, this is less useful with highly cluttered scenes.

2.2. Target disambiguation

Accurate selection can also be addressed through multiple-step selection [9]. Such techniques typically consist of an initial selection, that can be done in several ways. This step generates a group of potential candidates. Then, a different mechanism facilitates the disambiguation of the desired target. The initial selection does not need to be precise and may consider a volume of selection, which can be, for instance, a sphere or a cylinder around the pointing ray.

For example, in [14] they use 3D boxes that can be combined to select fibers. As another example, Grosman and Balakrishnan use the *Lock Ray* strategy [15]: the initial selection locks a ray, and all the objects intersecting the ray are selected as candidates. Then, a depth marker is used to disambiguate the interesting element. Similarly, Baloup et al. [16] implement a ray cursor in 3D. After an initial selection, several candidates are identified along the ray direction, and the user can use the touchpad to move among those.

These techniques are most useful when lower levels of occlusion are present, such as when scenes are composed of small, but sparse objects. However, when many candidate points are in the same line, some disambiguation techniques may be required. For example, Monclús et al. [17] also use a ray-cursor for medical models in the context of volume rendering. To facilitate the disambiguation in largely occluded scenes, two helper views are shown, with a custom transfer function, and projected onto two different planes. These helper views provide contextual information on the surfaces where the candidate points are located. In the case of Maslych et al. [18] they use a projection of the region of interest on a disc or a cylinder where the user can select one of the elements. Although this is useful to select occluded elements, with molecular models where there are many similar elements the use of these techniques would be challenging.

Instead of adding extra helper views, other systems focus on the disambiguation by a progressive refinement that uses secondary views, different from the original. After an initial selection, candidate objects may be presented in the form of pies or menus [15,19]. Kopper et al. [20] address this problem by another progressive approach: an initial selection gathers objects in a region, and then iteratively reduces the set of selectable objects by placing groups of objects in quadrants of a 2D plane the user can further click on. In the end, a single object will appear in each region. This facilitates the selection since each subset of objects is separated from the other. Thus, the user only needs to select one quadrant. Similarly, Yu et al. [21] proposed several techniques to select occluded elements with a disambiguation process. Some of them are based on an additional view of the elements on a grid. However, for scenarios such as molecular models, where the positions of the atoms may be relevant for the selection, displacing the atoms would remove important structural information. Furthermore, these techniques also show a degradation in time for scenes with large densities of objects, due to the increased number of steps required to select the target.

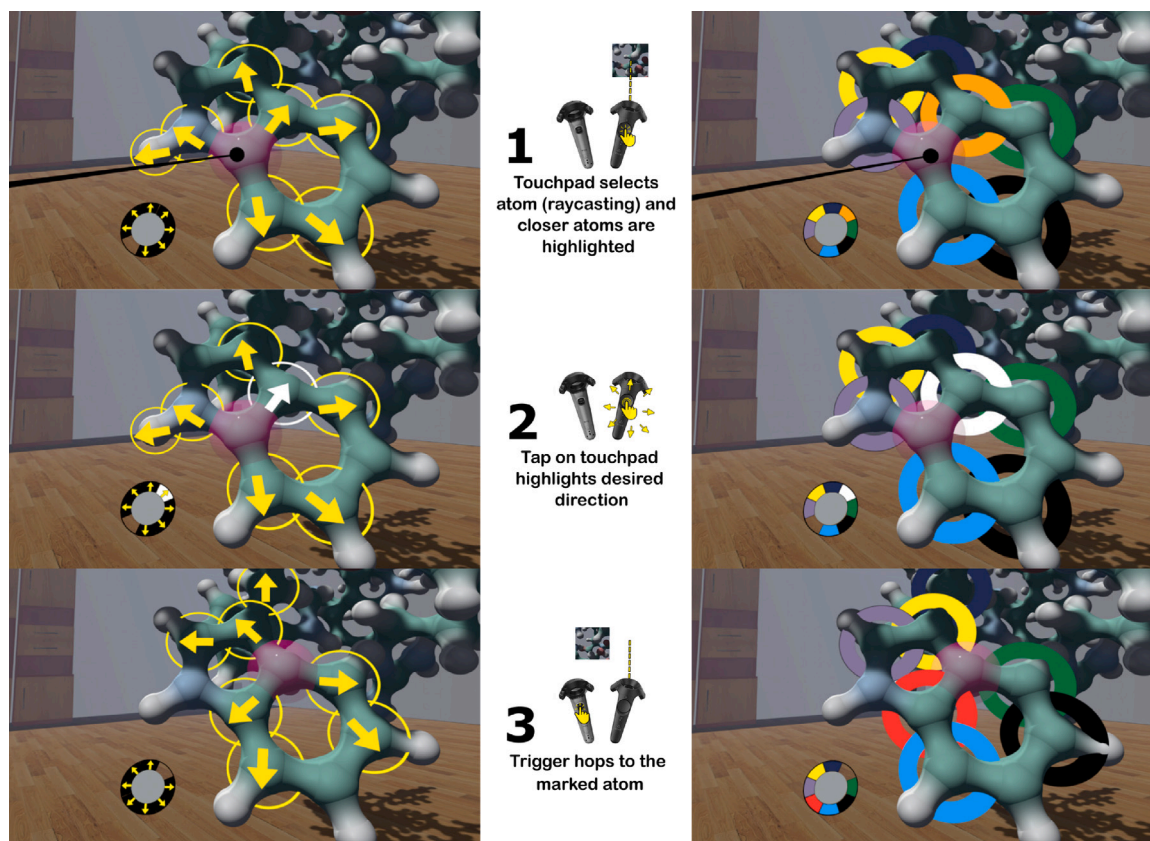


Fig. 2. Process to select an atom and choose and navigate to the available neighbors. **Left:** Ray + arrows technique. **Right:** Ray + colors technique. Initially, the user selects an atom by clicking the touchpad (top). Then, candidates are highlighted, and the user can navigate to them using the touchpad (center). When the user is satisfied with the desired candidate, the trigger can be used to select the atom (bottom). Upon this selection, neighbors are recalculated and highlighted, and the user can repeat the neighbor navigation as many times as needed.

3. Objectives

In our case, our goal was to develop and evaluate new techniques for the accurate selection of small elements that were able to reduce errors and frustration. More concretely, we defined the following requirements:

- Create an approach that preserves the original scene's 3D structure, unlike previous approaches, since the shape of the protein is key to understanding it.
- Facilitate a comfortable, easy-to-learn technique that is preferred by the participants to select little accessible elements. It would also enable the navigation of neighbors, an action useful for common tasks such as exploring the distance between atoms or angles between bonds.
- Reduce the frustration in the user, making selections easier.

With all this in mind, we carry out the user studies that we explain in the following sections.

4. Two-step ray-based selection

We propose two new progressive target acquisition techniques based on Raycasting intended to facilitate the precise selection of atoms. The core idea is to facilitate quick access among neighboring atoms in a region of interest, without requiring precision. We call these techniques: *Ray + arrows* and *Ray + colors*. Both techniques work with the same two-step process, illustrated in Fig. 2. It works as follows:

1. An initial selection is made using the Raycasting method (step 1 at the top).

2. The user can hop to any of the (up to) eight neighbors of the selected atom using the touchpad.

- The candidate is then highlighted in white (step 2).
- When the user has defined the desired atom, it can be selected with the trigger (step 3).

The novelty of our approach is the way we select the candidate neighbors, the visual feedback provided, and the technique to select the neighboring atom, which relies on the use of the touchpad and the trigger, without further need of pointing at the screen. In both cases, upon the initial atom selection, the atom is marked, and then, the system automatically highlights a set of up to 8 neighbors the user can travel to.

The difference between both techniques consists in providing different visual feedback on the neighbors. In one case, the candidate directions of the touchpad, which represent the neighboring atoms where the user can move, are indicated by arrows over the atoms. On the other, these are indicated by colors that are painted as discs around the atoms. Both have their particularities: arrows might seem more intuitive, and circles may be less prone to occlusion by other atoms. In both cases, we further reinforce the set of valid directions with an informative widget that displays the valid directions in front of the user (on top of their nose). Each candidate's destinations are in one of the main directions: up, down, left, right, and the corresponding diagonals. And these directions map to eight regions of the controller's touchpad. And these directions map to eight regions of the controller's touchpad. Initially, we designed the version with feedback consisting of colors. However, we had the impression that associating the color of the atoms with the position of the touchpad would require a steep learning curve. Therefore, we designed the second alternative, with the arrows, so that we could compare the performance.

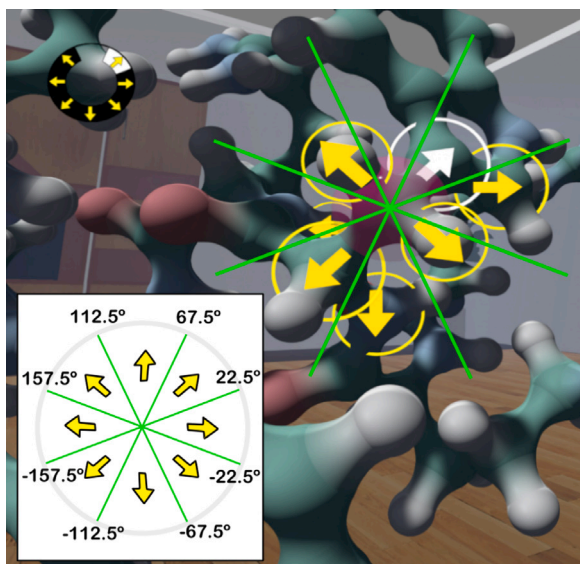


Fig. 3. Available neighbors and their corresponding directions based on the angle in Ray + arrows.

The candidate neighbors are defined in object space. Both techniques generate the candidate set using the same algorithm. The region in which neighbors are searched for is defined by a radius that could be easily configured by the user. For the experiments, though, we do not let the user change this parameter so that they do not change it during the tasks, and therefore we fix it. Since UnityMol is built over Unity, the elements of the scene (atoms in the examples shown) are represented as spheres, that are stored in a spatial structure, to accelerate operations such as collision detection. This is calculated with the Unity function *OverlapSphere*.

The candidates' selection follows this scheme:

- Upon atom selection, the algorithm searches for the eight atoms closer to the selected one inside the defined radius.
- To create the visual feedback, those candidate atoms are projected onto a virtual plane perpendicular to the axis that goes from the viewer to the center of the selected atom.
- The virtual plane is subdivided into sectors (see Fig. 3), and the atoms are assigned to the sector they fall into. If more than one atom projects into the same sector, we keep the one that is closer to the camera.

This means that atoms that are completely overlapped will not be displayed as available candidates, only the one closer to the user position. When we recalculate the neighbors, for example when traveling to a candidate, the list of possibilities is modified and the atoms discarded before could now be available.

The resulting valid directions are encoded in the accompanying widget as colors or arrows. Directions without candidates are left empty. We now proceed to describe both techniques in detail.

Method 1: Ray + arrows. The available neighbors are shown by a yellow arrow and a yellow ring around the corresponding atom. Both elements are oriented so that their planes are perpendicular to the user's vision. A guide appears over the user's nose, showing the user which directions are available. The user can select the desired direction, resulting in the arrow and the ring turning white as feedback. In the same way, the direction indicated in the guide turns white. The rationale behind that is that we believe that showing arrows naturally leads the user to decide which touchpad direction is the desired one.

Method 2: Ray + colors. Following the same model as in the previous method, we show the possible neighbors employing a colored ring that surrounds the corresponding atom, oriented perpendicular to the user's vision. These rings are of different colors, identifying the different directions they represent. In the same way, a guide is displayed over the users' nose that will show the available directions utilizing the corresponding colors. Likewise, the ring and the color in the guide of the selected direction turn white when their direction is selected. In contrast to the previous method, although here the directions need to be learned, the visual cues (rings around atoms) are seemingly more visible in cluttered scenes.

Our initial implementation, the one tested in our pilot study, placed the guide widget top left, in the peripheral view of the user. As described later, the change of position was a result of the analysis of the pilot study and the interviews with participants.

Neighbors calculation. In both cases, the available neighbors are obtained with the selection sphere centered on the currently selected atom, and the directions are calculated by a transformation to a new coordinate system. Given A as the current atom position, and C as the camera position, the new reference system is calculated as:

$$\text{Origin} = A,$$

$$\vec{Y} = \text{Cameraup},$$

$$\vec{Z} = A - C,$$

$$\vec{X} = \vec{Z} \times \vec{Y}$$

With these new coordinates, we will know the corresponding direction, obtaining the angle defined with $\arctan(\frac{y}{x})$. See Fig. 3.

The initial implementation was analyzed by the authors and tested informally with a naive user with more than 20 years of experience in VR environments. She gave us numerous suggestions that we included in the implementation. With those modifications, we performed a pilot study to evaluate how the users interacted with the newly developed techniques and to get more insights on the possible problems (see Section 5). After analyzing in depth the initial results, as well as the comments of the users during the discussion sessions, we decided to introduce several changes to the interaction metaphors and perform the final study, described in Section 6.

5. Pilot study

This initial implementation was refined with help from expert colleagues and evaluated through a pilot user study.

5.1. Experiment design

The pilot study consisted of the selection of 6 atoms with a protein of less than 200 atoms, 2M7D from the PDB database [22], and 6 selections with a protein of about 17K atoms, 6EZD [23]. Before starting the tasks, the users were introduced to the experiment with a briefing session and a video that showed the different interactions and visual feedback. Furthermore, they had to fill out a consent questionnaire with some demographic information. After the video was reproduced, participants practiced with a test molecule, 6RQS [24] of 195 atoms, to become familiar with the techniques. They could perform as many search tasks as necessary until they felt comfortable with the method. Initially, the participant saw the protein and the menu. The user could always move freely around the room or interact with the molecule to move or rotate it. To accomplish this, while aiming at the molecule and holding down the trigger, moving the arm would move the model, and rotating the wrist would rotate it. When the user was ready, the selection task started. A task is defined as:

1. The participant clicks a button on the virtual menu to activate the target.

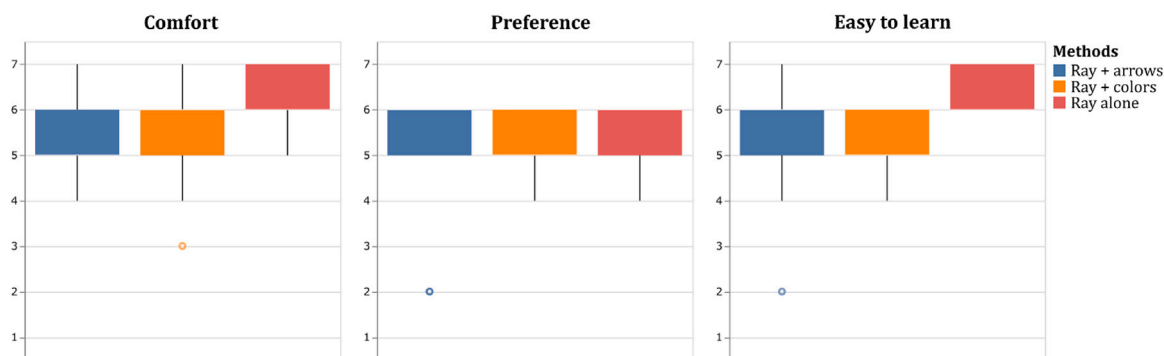


Fig. 4. Perceived comfort (left), preference (center), and ease of use (right) of our first implementation of the two-step selection techniques against simple ray selection (red) in our Pilot study. In this case, ray-based selection is the technique preferred. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

2. The target is shown in cyan as a sphere larger than the atom it indicates. Then, it reduces its size after 2 s and adjusts to a size similar to that of the target atom.
3. The user selects the atom with the current method.
4. Upon objective selection, the task ends. If there are still pending tasks, a new task can be started by going to step 1.

The user always knew how many selections were still unfinished, since the interface updated a message upon each selection. After the user had finished with one protein, the other one was loaded, and the remaining tasks could be performed.

The target marker was a sphere of size equal to the atom's size, multiplied by 0.1. To indicate the participant where it was, we scaled its size and then reduced it. The upscaled size was calculated by multiplying it with $a = \frac{0.1}{s}$, where s means the global scale of the molecule (*lossyScale* in Unity).

The experiments were performed using Latin squares to sort participants, to avoid learning and fatigue effects. Therefore, we were changing the order of the molecules and, inside each molecule, the order of the techniques. However, the order of selection of atoms in each molecule was always the same. Users could take a break between each method and molecule if needed. After the tests, participants were asked to complete a questionnaire with 19 questions to be answered on a 1–7 Likert scale (7 meaning “Completely agree”). Finally, they also assigned a global score of 1 to 10 to each technique (10 meaning best). The questions asked whether:

- One of the techniques makes the selection easier than the others.
- The technique is comfortable to use
- The technique is easy to learn.
- Most people would quickly understand the technique.
- The way of showing the colors/arrows and the atom that is selected with the touchpad is understandable.
- Overall score.

5.2. Participants

Nine participants between the ages of 18 and 36 carried out the experiment, one of them being female. Only 3 of them had medium or high experience in VR. All had studies related to computer science or bioinformatics.

5.3. Results

We can see in Fig. 4 the results of the questionnaire with a Likert scale of 1–7 in terms of perceived comfort with the technique, preference (as the ease of achieving the objective), and ease of learning. The first two cases, comfort, and learning, suggest that users preferred the Raycasting technique. However, when evaluating its performance,

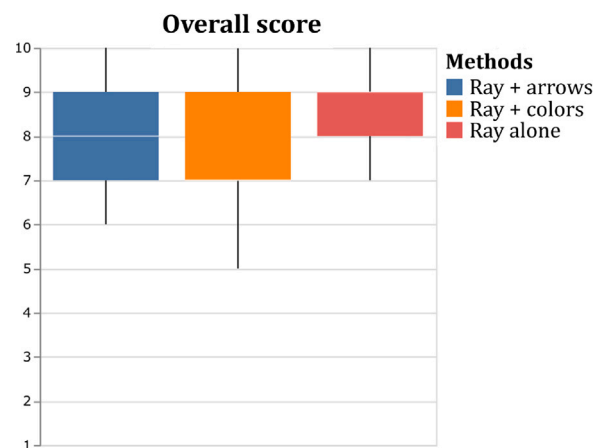


Fig. 5. Overall score in our first implementation of the two-step selection techniques, *Ray + arrows* (blue) and *Ray + colors* (yellow), against simple ray selection (red) in our Pilot study. In this case, Raycasting (8.625) was the preferred one over *Ray + arrows* (8). *Ray + colors* was the least valued technique (7.375). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

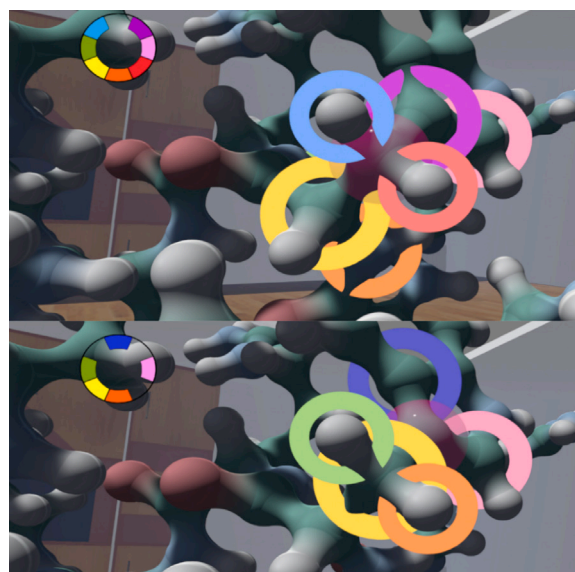


Fig. 6. Two examples of the colors used for the *Ray + colors* technique in the Pilot study and how they are seen on screen. The initial palette was a rainbow one and was changed to a colorblind safe one in the final implementation.



Fig. 7. The menu options the user sees and needs to click on to perform the tasks. The top view shows the menu before starting the task, the center image shows the status in the middle of the training (we offered many selections, but users could stop as they were ready), and the bottom one shows the task finished. The upper part indicates the method being tested, and the lower part allows you to start and end searches, and indicates the number of remaining targets.

users assigned the same value to Raycasting (5.25) than to the *Ray + arrows* (5.25) technique, and *Ray + colors* is barely behind (5.125).

When the users gave a grade between 1 and 10 to the techniques (see Fig. 5), all techniques achieved a high value, which indicates that users recognized the potential of the new techniques proposed. More concretely, the grades were, on average, 8.625 for Raycasting, 8 for *Ray + arrows*, and 7.375 for *Ray + colors* (7.375). Thus, Raycasting was ranked slightly higher. We believe, though, that the wording of the questions might have been slightly misleading (implying that the Raycasting was not part of the other two selection techniques). Additionally, users themselves commented on this fact, indicating that the ray alone was more complicated when they worked with the larger molecule. Since we believed our techniques would be suitable for this scenario, we tested larger molecules and explored scenes with greater occlusion in our following studies.

After analyzing the results of the pilot study, we implemented several changes. The most relevant ones were: First, the informative widget, which in the pilot study was located in the upper left region of the vision, was moved to its final position on the nose. Second, the colors of the *Ray + colors* technique were modified. Initially, we were using a rainbow palette (see Fig. 6), and we changed it to a categorical palette that is color-blind safe. The new colors were the ones in Fig. 2. Third, the color of the target was also changed into a more salient one, which can be seen in Fig. 8.

6. First study: Techniques evaluation

6.1. Experiment design

The procedure was the same as in the previous study: consent and tutorial, experiment, and questionnaire. The tutorial part was the

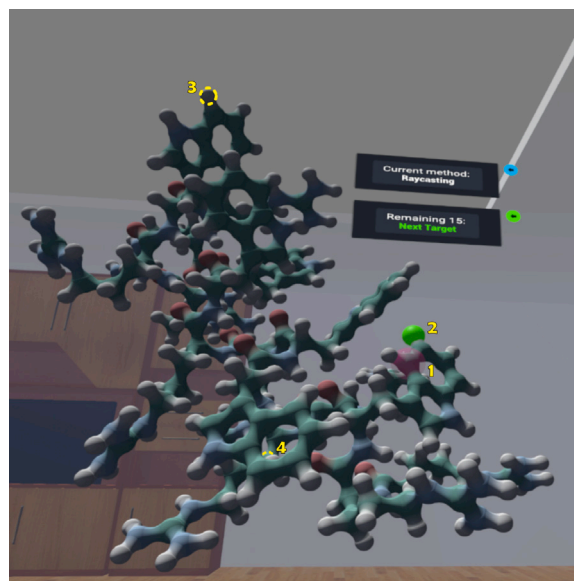


Fig. 8. The aspect of the screen when the user receives the hint on the atom to select (middle right sphere, encoded in green, with its normal size). The elements in yellow do not appear on the screen, we are using them as a guide to show examples of close atoms (1 and 2), a distant atom (3), and an occluded atom (4). The pink sphere around the atom marked as 1 identifies the currently selected atom. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

same as in the pilot study. The questions in the questionnaire were reformulated to be more clarifying. The tasks were designed similarly to the pilot study: First, users clicked to start a task. Second, a marker highlighted the element to select (see Fig. 8). Third, the user used the current metaphor to select the item, and finally, confirmed the selection. Tasks were solved using the same interactions as before. However, in this case, the scenes were closer to a real-world scenario. First, they still had a significant difference in the number of atoms, but proteins were larger. In this experiment, they were: 1QM5 from the PDB database [25], with around 14K atoms, and 1BR1 [26], with around 30K atoms. This size is far from the range of the largest proteins that exist, which is near 540K atoms, but we wanted to keep it manageable. Second, the tasks also included the selection of internal atoms, which is more challenging. We also gave the users feedback upon the completed selection in the form of a soft chime, preventing them from advancing until they achieve this. As previously indicated, the sphere marker was changed to a saturated green, since it seemed more salient than the cyan used in the previous study.

As commented, the tasks had the same structure as the ones defined in the pilot study, as well as similar feedback on their progress. The user could see the current selection method, and also the number of tests remaining. In Fig. 7 we show how these visual feedbacks looked like in the initial training.

In addition, we collected information on the selection actions they performed and on the time it took users to carry out each selection. We timed from the moment they started a new search by pressing a button on the virtual menu, until they selected the correct atom, when they received a success sound as feedback, and pressed again the same button. Each session was also recorded.

In this case, users used each technique to perform 9 searches in both proteins. As in the Pilot study, the configurations, the combination of the two proteins and the three techniques, were sorted using Latin squares, to avoid learning and fatigue effects. For this experiment, a pattern was designed for each molecule's search, thus, the pattern of selection of atoms was kept. For the small molecule, the order was: atoms 1 and 2 were close but distant from the others, atom 3 was

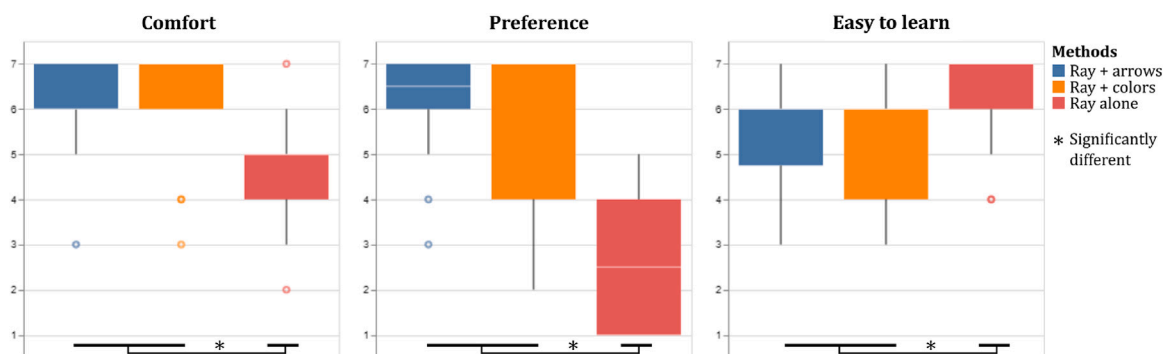


Fig. 9. In the First study, our improved implementation of the techniques exhibit a better-perceived comfort (left), preference (center), and learnability (right) than the first implementations in the Pilot study. Moreover, both helper techniques (blue and orange) are felt more comfortable and useful than simply using the ray. In terms of time, ray alone (red) is usually faster. Significant differences are marked with star glyphs. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

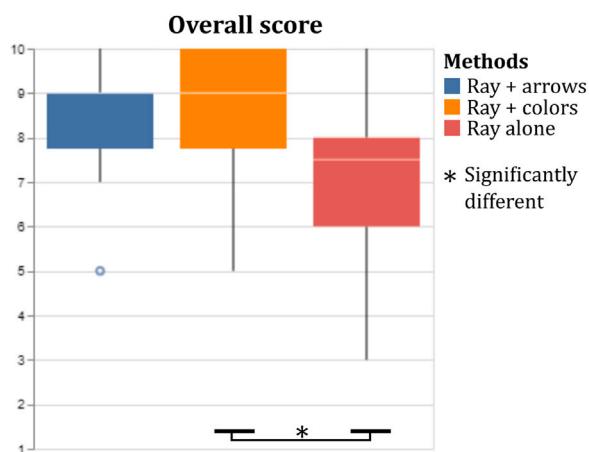


Fig. 10. Overall score in our improved implementation for the First study. In this case, *Ray + colors* (9 median) was the preferred one over *Ray + arrows* (9). Raycasting was the least valued technique (7.5). Significant differences are marked with star glyphs.

distant from the others, then, the other pairs 4–5, 6–7, and 8–9 behaved like the first pair. This last pair was very occluded in an internal part of the molecule. For the large molecule, we used the same scheme, but without occlusion. We consider *close* atoms as those where the user can travel from one to the other by simply employing our complementary techniques in one or two hops. Some examples can be seen in Fig. 8.

6.2. Participants

We recruited 18 participants (9 female), with ages between 18 and 30. None of them had participated in the pilot study. 9 of them had medium or high experience in VR. Only 9 of them had studies related to computer science. One of them was color-blind and confirmed that the colors were distinguishable.

6.3. Results

After discarding one participant who did not follow the instructions and another whose data was incomplete, we ended up with 16 participants.

Besides gathering the opinions of the users regarding the comfort and learnability of the techniques, we additionally tracked the time required to solve each of the tasks, as well as the distances the users moved throughout the experiment. This enables both a qualitative and a quantitative analysis of the results, that are presented next. To analyze qualitative data, we used the Kruskal–Wallis Test followed by

post-hoc Dunn's test, since the data were not normally distributed. To analyze the quantitative data, we used Repeated Measures ANOVA with Bonferroni post-hoc test.

6.3.1. Qualitative analysis

The new versions of the progressive techniques were widely approved by the participants. When asked about comfort and preference (comparing the usefulness of the technique regarding using the ray alone), users graded our new techniques above Raycasting, as can be seen in Fig. 9 (left and center). The comfort of the techniques showed significant differences (p -value = 0.001, H = 14.61), and Dunn's test determined Ray alone was significantly less comfortable than the others. Preference also yielded significant differences (p -value = 0.000, H = 23.04) and Dunn's test showed both Ray+Colors and Ray+Arrows were significantly preferred. Regarding learnability, Raycasting still stayed as the best technique (right), with significant differences (p -value = 0.005, H = 10.57), confirmed by Dunn's test. We somewhat expected ray alone to be ranked higher because the other two techniques also use the ray for selection, and then require an extra step that must be learned. In general, users preferred colors to arrows, partly because of the design. The arrows are located in front of the atom they refer to, and can sometimes be hidden from other atoms by a bond or by transformations applied to the molecule. In addition, we were surprised to see that some users rapidly got used to the color order, and as a consequence, stopped consulting the informative widget. This eliminates the initial advantage of the arrows of having an associated direction.

Users commented that the ray alone fell short on certain occasions, and that they appreciated having the other techniques to refine the search. However, despite the expressed user's preference, our quantitative analysis (see Section 6.3.2) showed that Raycasting usually required shorter times to perform the tasks.

In line with the previous responses, the scoring questionnaire also showed that the new implementations of our progressive selection methods were appreciated by the users (see Fig. 10). There were significant differences (p -value = 0.034, H = 6.73) and Dunn's test showed the difference between Ray alone and Ray+Colors. Raycasting received the lower median grade (7.5), while the others got 9.

6.3.2. Quantitative analysis

In addition to the qualitative analysis, we were also interested in the actual performance of the participants when using the different methods. So, we measured the time required to select each atom for all the tasks. Selection time was measured from the moment the menu button was clicked to start a search, until it was clicked again, after hearing the feedback sound when selecting the right target.

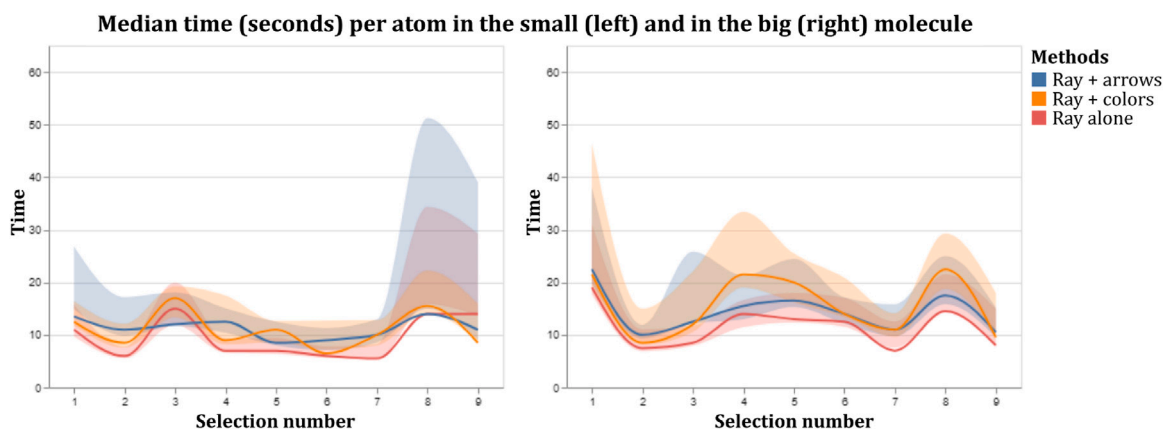


Fig. 11. The lines show the median time (seconds) per atom selection, with monotonic interpolation, and the areas show the variance in the data. On the left we have data regarding the small molecule and on the right about the big molecule. The peaks and descending slopes clearly show that when atoms are far and followed by a closer one, the first selection takes more time, and the second, less. We also see the effect in time of an atom being occluded, as in the eighth atom of the small molecule, which requires significantly larger to be picked.

Time per selection. Calculating rough averages among all tasks would somewhat lose detail because not all atoms were equally accessible. As explained, we purposely selected some close and some distant atoms, even one pair which was especially occluded. Thus, to better understand the user performance, we plot the times per atom in a line chart, that plots every atom selection time in the same order they were performed. In Fig. 11, on the left, we can see the times to select the atoms in the small molecule, while the right chart shows the times required to select the atoms in the larger protein. Fully opaque lines indicate the median of the observations (since it is more robust to outliers), and the background semi-transparent area charts represent the confidence intervals. The first impression, when we see the charts next to each other, is that the selection in the large protein takes slightly higher, which is to be expected. But the time differences are minimal, which is a bit surprising.

We now proceed to dig into the details of the small molecule (Fig. 11-left). The second insight we obtain is that, as expected, when atoms were closer to the previous selection (atoms 2, 5, 7, and 9, in the small molecule, as described earlier), the subsequent selection was faster, as can be seen through the peaks followed by a descending slope. This is especially notable that atom 8, which was purposely selected as an internal atom, quite occluded. In this case, users took quite a long to achieve the selection. We can see more detail on the required times to select each of the atoms for the smaller protein in Fig. 12. Atoms that were closer to the previous selection required less time to acquire with any of the techniques, with no technique clearly superior to the others. Distant object acquisition is slower and also typically presents a larger number of outliers. As an example, atom 8, besides taking more time, also has a larger variance in its results. This suggests that acquiring occluded elements may exhibit different behavior and thus, it is worth examining this scenario deeper. The same behavior occurred with the larger protein, as shown in Figs. 11-right and 13: closer atoms (2, 5, 7, and 9) required less time to be selected than their predecessors. And distant atoms (4, 6, and 8) exhibit larger times, variances, and outliers. The aggregated times per method can be seen in Fig. 14.

We also analyzed the time distributions for significance and found that, indeed, those present some differences. For the small molecule, Repeated Measures ANOVA yielded a p -value of 0.020, $F = 4.45$, with a strong power ≈ 1 , and Bonferroni confirmed that the Ray alone technique was significantly faster than Ray+Arrows. Ray and Ray+Colors showed no differences. In the large molecule, the Ray alone is significantly faster than the other two techniques (p -value = 0.000, $F = 10.31$), with a strong power ≈ 1 .

Occluded vs. non-occluded. To show more insights on the time required to select non-occluded versus occluded atoms, we generated a boxplot of the times, partitioned based on the occlusion condition, as shown in Fig. 15. We can see that the three techniques required larger times, and exhibit larger variances than the same techniques when used for the selection of non-occluded atoms, even if they are distant.

When we compared the three techniques in non-occluded with Repeated Measures ANOVA, there were significant differences (p -value = 0.000, $F = 21.94$), with a strong power ≈ 1 , and Bonferroni showed that Raycasting was faster. On the other hand, in the occluded ones, no differences were found.

Despite not seeing differences in the times among the techniques in the case of the occluded atoms, there were differences in user preference. Many indicated that they appreciated having our complementary techniques in these cases. As a result of this analysis, we considered investigating the case of occlusion more thoroughly, and we decided to design a new study as described in the following section.

7. Second study: Selection of occluded elements

The developed selection techniques were designed to make the acquisition of neighbors easier, and as a consequence, it seems intuitive to think that partially or totally occluded elements could be easier to acquire in a two-step approach if the user succeeds at selecting a close atom in the first step. The previous study was intended to evaluate the performance of those techniques in a general scenario. In that experiment, the increase in times incurred when occluded atoms were present suggests that it is an interesting case to be analyzed in depth. Thus, to get further insights, we designed a second study focused on this scenario: when a significant number of elements are occluded.

7.1. Experiment design

We selected two molecules, with medium and large sizes. The same first molecule from the previous experiment of around 14K atoms, 1QM5 from the PDB database [25] that already presented several possibilities to study occluded atoms, from now on referred to as the small molecule, and a protein of about 34K atoms, 6WUB [27], referred to as the big molecule, selected by its shape that presents more occlusion. Both can be seen in Fig. 16. As before, the possible combinations of the two proteins and the three techniques were sorted using Latin squares, to avoid learning and fatigue effects. Then, we picked 8 atoms to be acquired by the users. Those atoms formed pairs where the first one was distant from the others and the second one was close to the first one. *Close* means that the user can travel from one to

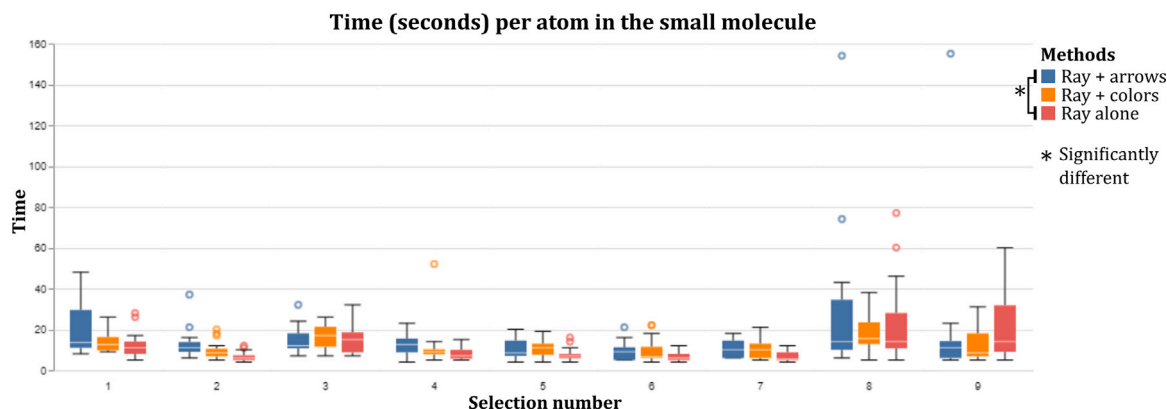


Fig. 12. Time (seconds) required to make the 9 selections for each technique in the **small protein**: Raycasting (red), *Ray + arrows* (blue) and *Ray + colors* (yellow). Note how atoms 2, 5, and 7 require less time to be selected since they were close to the previous one. Atom 8 was highly occluded, which causes higher acquisition times and larger variances, and 9 was close to the previous one, with reduced times again. Significant differences are marked with star glyphs. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

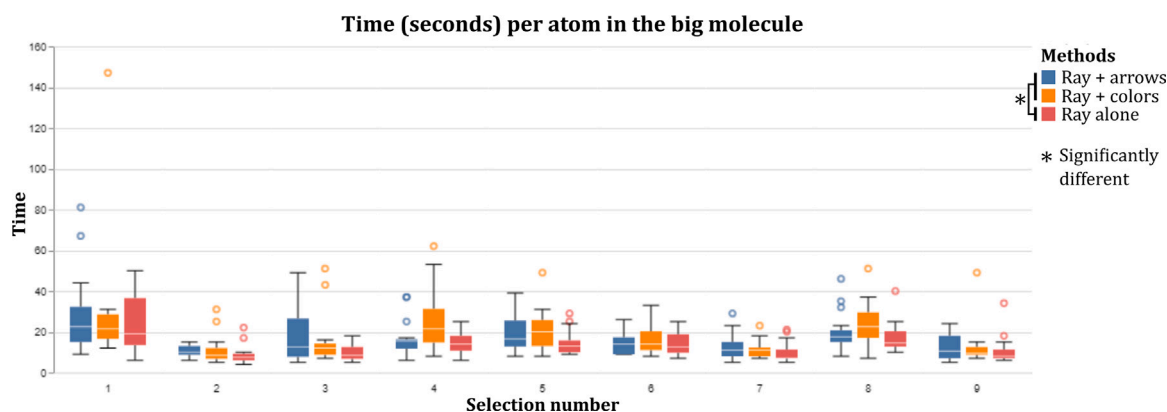


Fig. 13. Time (seconds) required to make each of the 9 selections for each technique in the case of the **large protein**: Raycasting (red), *Ray + arrows* (blue) and *Ray + colors* (yellow). Like in the previous case, distant atoms (e.g. 1, 4, 6, and 8) required larger times than their closer counterparts (e.g., 2, 7, and 9), which were generally acquired in shorter times. Significant differences are marked with star glyphs. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

the other by simply employing the complementary techniques in one or two hops. The first and third pairs of atoms were on the surface of the molecule, and the second and last were occluded, an example of exposed and occluded atoms can be seen in Fig. 17. This way, we ensured that the participants had to perform a more complex search for the selection of each occluded element. Therefore, we did not apply a Latin square order to the atoms. A comparison between the different designs of atom's order among the experiments and its purposes can be seen in Fig. 18.

We also designed new questions intended to get additional information on the users' preferences in this scenario. Furthermore, this questionnaire has been incorporated into the VR experiment so that users can answer the questions immediately after the experiment to keep their experience fresh. Additionally, the first questionnaire with consent and demographic questions was also included in VR. A snapshot can be seen in Fig. 19. Together with the previous questions, that evaluated comfort, preference, learnability, and overall score, the new questions that were added to the final questionnaire were:

- I think that the RAY alone lets me select external atoms (on the surface) in an easier way than with any of the additional techniques (ARROWS or COLORS)
- I think that the combination of RAY + ARROWS lets me select external atoms in an easier way than with the RAY alone
- I think that the combination of RAY + COLORS lets me select external atoms in an easier way than with the RAY alone

- I think that the RAY alone lets me select internal atoms in an easier way than with any of the additional techniques (ARROWS or COLORS)
- I think that the combination of RAY + ARROWS lets me select internal atoms in an easier way than with the RAY alone
- I think that the combination of RAY + COLORS lets me select internal atoms in an easier way than with the RAY alone

This way, we get absolute rankings and pairwise comparisons.

We followed the same procedure and measured the time required to acquire each target and compared the performance among the different techniques.

7.2. Participants

We got 16 users (7 female), ages between 22 and 30. 6 of them had medium or high experience in VR. Only 8 of them with studies related to computer science. On this occasion, two of the participants were color-blind and confirmed that they could distinguish all colors.

7.3. Results

Like in the previous experiment, we conducted a qualitative study of users' responses to the questionnaire and a quantitative study of the times measured by search. For the former, we analyzed the results using the Kruskal–Wallis Test followed by post-hoc Dunn's test, due to

Aggregated time (seconds) per method per molecule

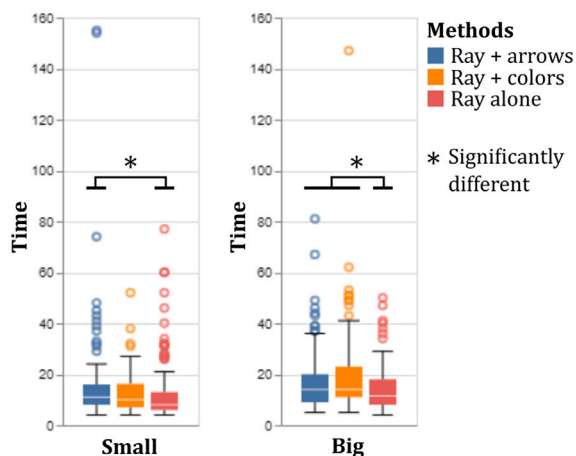


Fig. 14. Aggregated times in seconds per method, Raycasting (red), Ray + arrows (blue) and Ray + colors (yellow), and per molecule, small (left) and big (right). Significant differences are marked with star glyphs. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Time (seconds) per method with or without occlusion

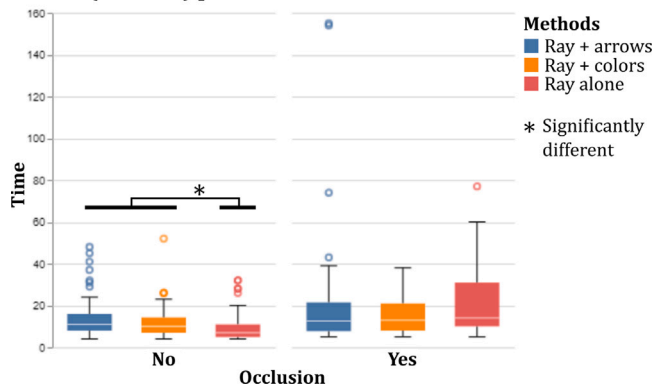


Fig. 15. Selecting visible versus occluded atoms in the small molecule. We can see how non-occluded targets (atoms 1–7) required significantly less time to be selected than occluded ones (atoms 8–9). The use of only the ray (red) would be faster than using the auxiliary methods (blue and yellow) for the exposed atoms. But they seem to help when selecting occluded ones. Note that the sample size of the occluded is smaller. Significant differences are marked with star glyphs. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

the lack of normality. For the last, we analyzed the results using two methods. First, using Repeated Measures ANOVA with Bonferroni post-hoc test. Second, given the problems that appear when using p -values to analyze human interaction data [28,29], we decided to also use the Cousineau–Morey method [30–32] that gives us the Confidence Intervals (CIs), as 95%. In this way, we can compare the results obtained with p -value and intervals.

7.3.1. Qualitative analysis

In the questionnaire, the users had to score on a Likert scale from 1 to 7 their level of preference, if the technique was comfortable to use, if it was easy to learn, if the task with the exposed atoms was simpler than with the other techniques, the same but with the occluded and, finally, give a score of 1 to 10 to each technique. Regarding preference,

there were significant differences (p -value = 0.000, H = 19.15), and Dunn's test determined ray alone was different from the others, which were preferred. The same happened with comfort (p -value = 0.000, H = 32.00). In the case of learnability, there was only a difference between Ray and Ray+Colors (p -value = 0.021, H = 7.71). We did not find differences when we had non-occluded atoms, but when we had occluded atoms users preferred the other techniques available, scoring significantly less the Ray alone technique (p -value = 0.000, H = 31.50). Finally, the Ray alone technique had the lowest score (p -value = 0.000, H = 19.15). In this experiment in which we emphasize the cases with occluded elements, we see how the score of the Raycasting technique falls, as seen in Figs. 20 and 22, except in the case of the exposed atoms, as seen in Fig. 21.

7.3.2. Quantitative analysis

We also analyzed the timings of the users under different conditions. The results are summarized next.

General comparison of techniques. First, we found no evidence of differences among techniques in the time required to select atoms for the small molecule or the large molecules as a whole, neither with Repeated ANOVA nor with the CIs that can be seen in Fig. 23. What we saw is that with the big molecule, more time was needed to perform each search, as expected, considering the dimensions and the need to perform more transformations in the model.

Occluded vs not occluded: comparison of techniques. However, if we compare techniques for the two conditions (non-occluded and occluded atoms), different results were obtained. In the small molecule, when the atom to select was visible, there was a significant difference between the techniques (p -value = 0.0148, F = 4.35), with a power of ≈ 1 . Post hoc analysis with Bonferroni test indicated that the differences were between Raycasting and the other two techniques (p -values of 0.0060 and 0.0124, respectively). Raycasting was faster than the other two techniques. In the top right chart from Fig. 24 we can see the intervals: Raycasting(6.98, 8.43), Arrows (8.43, 10.60) and Colors (8.76, 8.91). These intervals confirm the above, although the first two techniques are on the verge of overlapping. But this result was not visible for the large molecule (p -value = 0.1349), the bottom right chart from Fig. 24. Regarding the occluded atoms, no significant differences appeared between the techniques in both the small and large molecules, left charts from Fig. 24.

Occluded vs. not occluded: Raycasting. The time required to select occluded elements was significantly large for both the small molecule (p -value = 0.0000, F = 30.96) with a strong power = 0.9998 and the large molecule (p -value = 0.0000, F = 37.02) with a strong power = 0.9998. Confirmed by the intervals shown in the charts on the left of Fig. 25.

Occluded vs. not occluded: Arrows. Like in the previous case, time was significantly larger for occluded elements in the small molecule (p -value = 0.0002, F = 16.25) with a power of 0.9998, and the large molecule (p -value = 0.0002, F = 15.95), power = 0.9998. Confirmed by the intervals shown in the charts in the middle of Fig. 25.

Occluded vs. not occluded: Colors. Similarly, time was significantly larger for occluded elements in the small molecule (p -value = 0.0002, F = 16.04) with a power of 0.9998, and the large molecule (p -value = 0.0000, F = 21.56), power = 0.9998. Confirmed by the intervals shown in the charts on the right of Fig. 25.

8. Discussion

We found in both experiments that the enhanced interaction techniques achieved higher appreciation (comfort, preference, and overall grading), although Raycasting remained the most intuitive. The technique that ended up with a higher overall score was Ray + Arrows (9

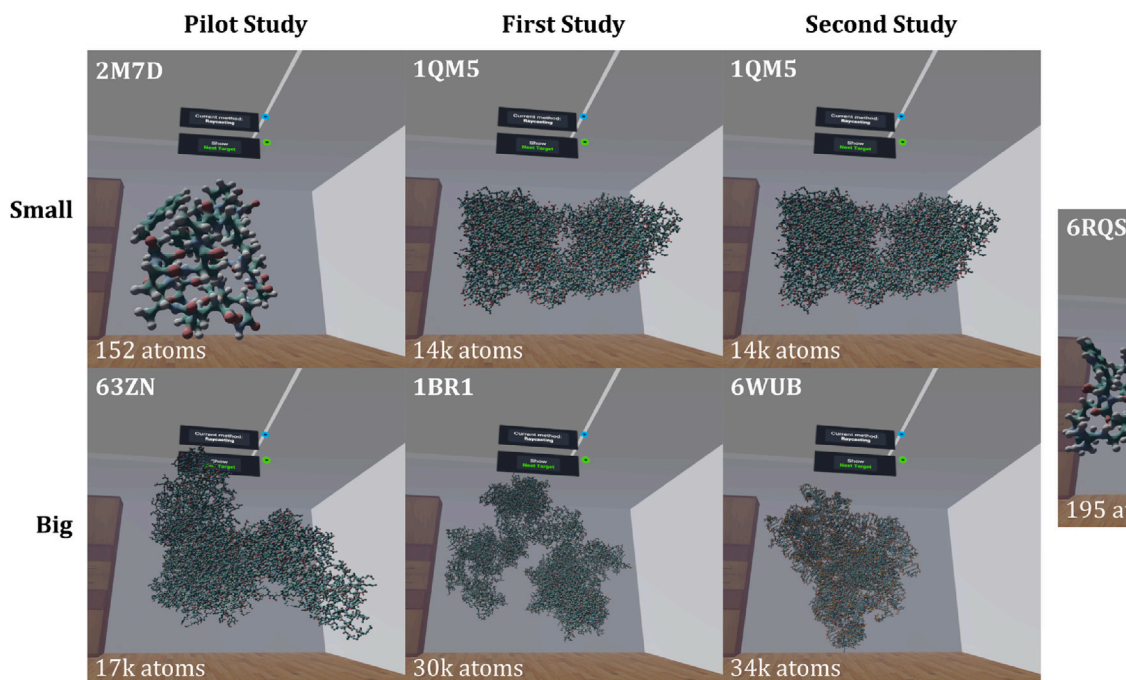


Fig. 16. Comparison of the two selected molecules in each experiment and the molecule used for the training phase. For the Pilot study, we selected two rather small molecules to test our designs and how users welcomed our techniques. For the First Study, we modified the sizes to study more realistic cases while keeping them manageable. In the Second Study, we used molecules with a more globular structure that enabled the study of occlusion.

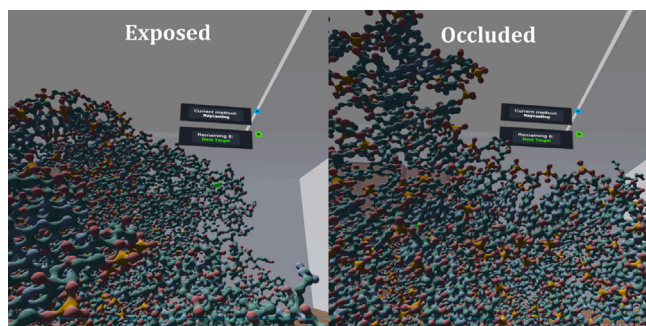


Fig. 17. Snapshot of an exposed atom in the big molecule of the Second study (left) and of an occluded atom in the same molecule (right).

Pilot study	small	●x6 randomly selected the first time	Check design
	big	●x6 randomly selected the first time	
First study	small	● ● ● ● ● ● ● ●	Realistic sizes Detect important cases
	big	● ● ● ● ● ● ● ●	
Second study	small	● ● ● ● ● ● ● ●	Evaluate techniques with occlusion
	big	● ● ● ● ● ● ● ●	

● ● = close atoms ● ● = distant atoms ● = occluded atom

Fig. 18. A comparison between the different designs of atom's order among the experiments. The purpose of each one can be read in the last column: test our initial designs, have more realistic sizes while keeping them manageable, and study the effect of occlusion. The atoms are represented as dots. Yellow dots mean that the atoms are occluded. If two dots are nearby, it means that the atoms are close, that the user can travel from one to the other by employing the complementary techniques in one or two hops. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Fig. 19. Snapshot of some questions of the first questionnaire, done in VR.

out of 10) in both experiments (Sections 6 and 7), while Raycasting achieved the lowest (7.5 out of 10) and (6 out of 10), respectively. The analysis of quantitative data in Section 6 study also showed a difference between atoms with greater occlusion and atoms clearly exposed, with the occluded ones seeming more difficult to achieve with the ray-alone method. This takes us to the final experiment where we deepened the occlusion analysis, and we saw that, in terms of time, the only case in which Raycasting was better was in the small molecule with exposed atoms. In the rest of the cases, it does not present better results than the other techniques and, in addition, users expressed their preference for the latter.

From these studies, we can conclude that the Raycasting technique benefits from some method of refinement for cases in which the occlusion prevents a correct direct selection, or for cluttered scenes where the initial selection may be wrong, but close to the desired target. Although these additions result in a longer training time, the results

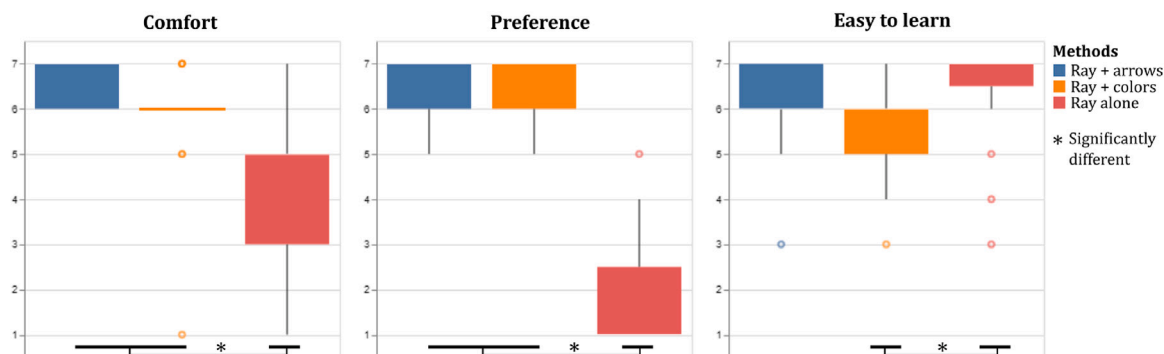


Fig. 20. In the Second study, the complementary techniques maintain a better-perceived comfort (left) and preference (center). As expected, Raycasting scored more regarding learnability (right). Given the exploration of more cases of occlusion, the perceived ease of completing the task (preference) decreases compared to previous studies. Significant differences are marked with star glyphs.

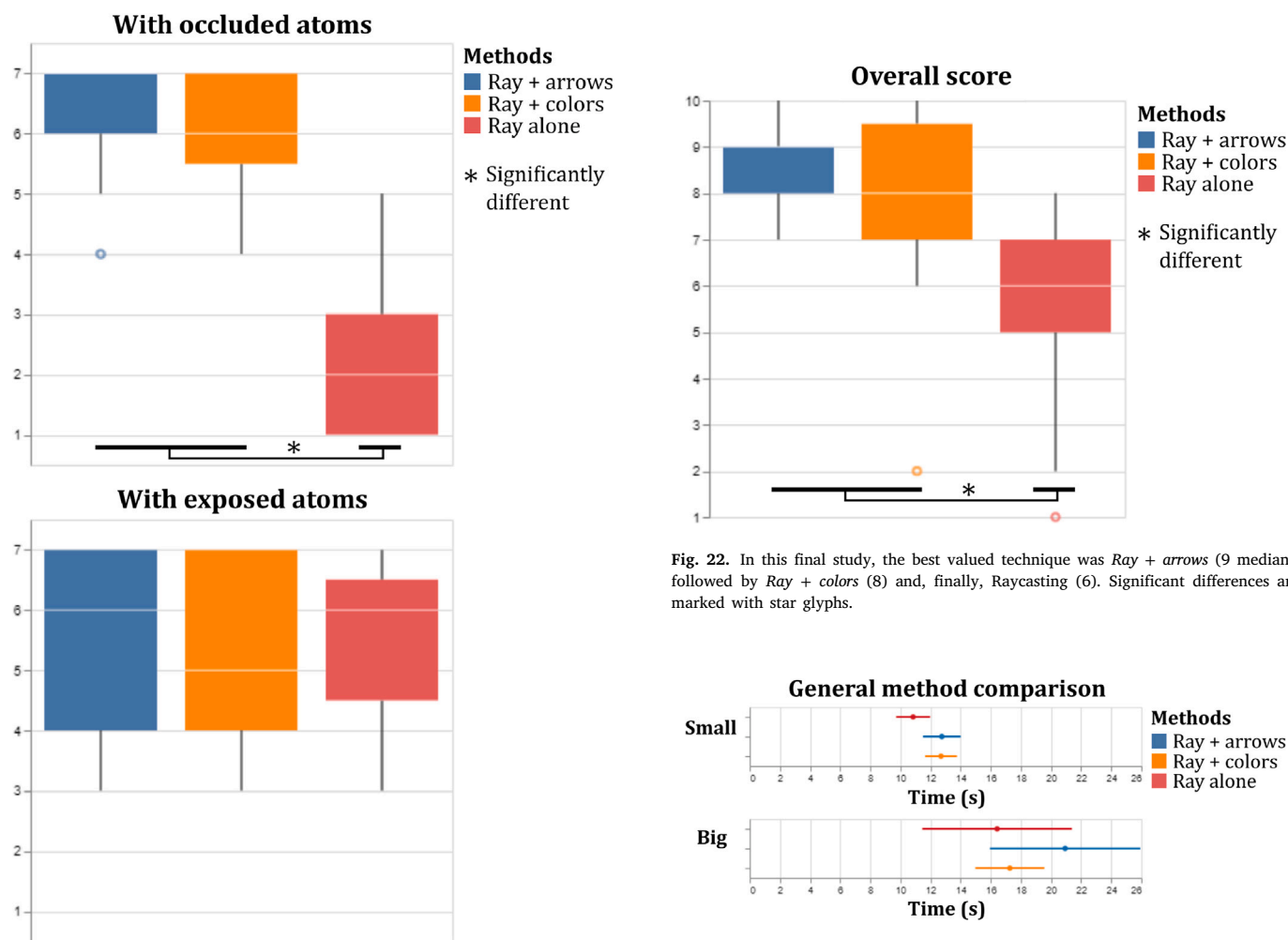


Fig. 22. In this final study, the best valued technique was Ray + arrows (9 median), followed by Ray + colors (8) and, finally, Raycasting (6). Significant differences are marked with star glyphs.

Fig. 21. When comparing techniques in cases of occluded and exposed atoms, users do not show a preference for any of the techniques when the atoms are on the surface. However, when the atoms are inside, users prefer the techniques of Arrows or Colors. Significant differences are marked with star glyphs.

indicate that they are compensated for by the selection time and user appreciation. In addition, users eventually become accustomed to the techniques, and they no longer needed to check the direction widget to match colors and directions. Moreover, in the event of prolonged sessions, the arm could rest since the neighbor navigation does not require pointing at the virtual space. Even though statistical analysis

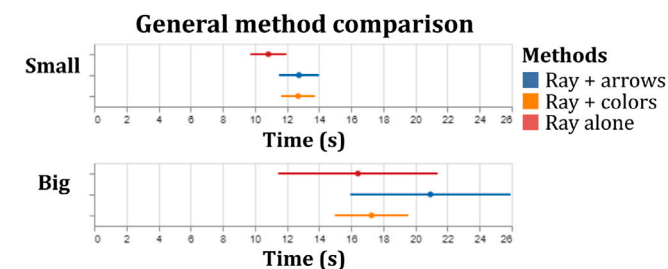


Fig. 23. 95% CI of time needed to complete the different searches in the different molecules with the different methods.

has also shown that using only the ray tends to get better times, the users feel more comfortable with the other techniques. Therefore, we would suggest that users should be allowed to use these techniques and choose between them based on their preferences. Since the arrows can be more easily occluded than the color rings, we personally would use the Colors technique, although it would mean more training. In addition, we would allow the user to adjust the position of the guide on the nose.

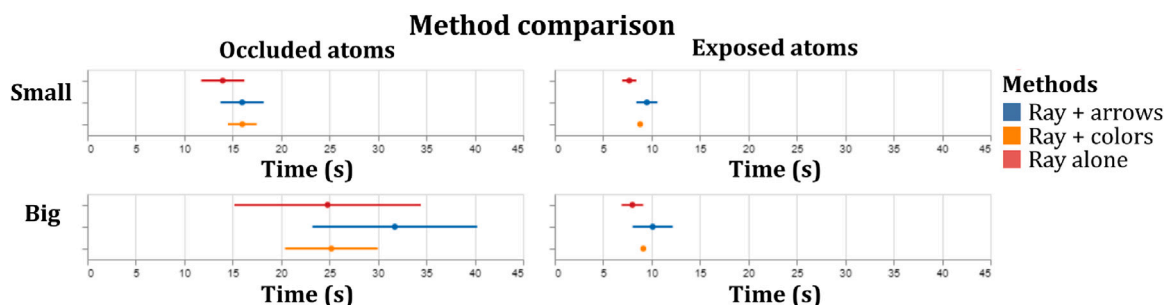


Fig. 24. 95% CI of time needed to complete the different searches in the different molecules with the different methods, differentiating the exposed atoms (first and third pair) and those occluded (second and last pair). Grouped by the occlusion.

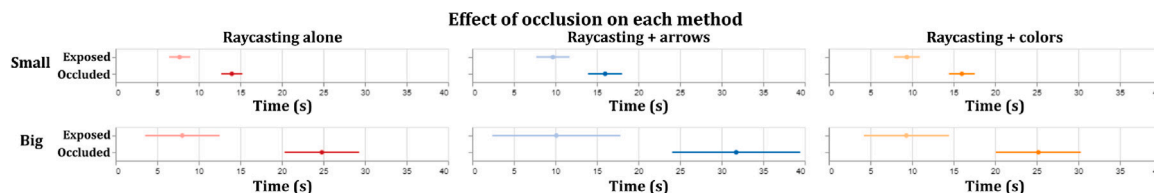


Fig. 25. 95% CI of time needed to complete the different searches in the different molecules with the different methods, differentiating the exposed atoms (first and third pair) and those occluded (second and last pair). Grouped by the method.

9. Conclusions and future work

This paper presents two new target acquisition techniques for accurately selecting small elements in cluttered scenes. A pilot study was initially conducted, which indicated that both techniques were understandable and easy to use. Users still seemed to prefer the ray interaction over the newly developed techniques, despite recognizing that it was difficult to use when molecules were large. Based on the lessons learned from the pilot study, we modified the visual feedback of both techniques in sensitive ways. Furthermore, a formal study was prepared to explore the relevant cases of interest. These include scenes with a more significant number of atoms and, therefore, smaller spheres. After this, the results suggested that these new techniques, although slower than ray alone, were preferred and found to be more comfortable by the participants. Another experiment was conducted in which the difference between occluded and exposed atoms was explored in greater depth. In this case, it was observed that the proposed techniques did not accelerate the acquisition of the objectives but helped reduce the users' frustration. In the questionnaire, participants indicated that they preferred the techniques we propose for selecting the occluded atoms. With these experiments, we can affirm on the one hand that the proposed techniques generally allow equally fast selections as with Raycasting alone. And on the other hand, having them can reduce the frustration of the user, who appreciates being able to use them when occluded elements or when the initial selection is close to the target. Tests with color-blind users showed that colors could be distinguished.

One of the elements that we do not study here, but that intrigues us, is the effect of the movement of the participants. There was a wide variety of behaviors, participants who moved all the time, who were static, or a combination. But to discuss the effect of these movements on time per selection, we would have to do a study that, for now, we do not have. In the future, we want to compare time having users sitting with restricted movement and having users who can move freely. As a first impression, the combination of walking and using the controller would be faster by reducing the number of translations with the controller. But there are movements, such as showing the upper part of the molecule, that must be done with the controller. Nevertheless, there were participants who finally preferred not to move after trying both methods.

We focused on the size of molecules and the presence of clutter, since it was a scenario we clearly envisioned as a limiting factor in ray-based selection. We believe that the techniques developed can be applied to other scenarios with similar characteristics. However, as mentioned previously, whether users can move or have restrictions may also play a role in the time needed to select the molecules. Therefore, our results might not be directly transferred to scenarios where the freedom of movement is clearly different from ours. We have tested proteins with sizes that are common in pharmacological simulations. Though larger molecules can also be considered, this is not common, and massive models exceeding 100K atoms will certainly increase the number of situations where the atoms to select are occluded.

Furthermore, it would be interesting to study the fatigue and frustration of users, for which we could use standardized questionnaires to avoid possible bias with the questions.

In the future, we intend to expand our research and further investigate the number of selections, hops, errors, and fatigue of all the presented methods. And as commented, it would also be interesting to explore the effect of limiting the users' movement in the room and compare the results to a free-motion scenario.

CRediT authorship contribution statement

Elena Molina: Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Visualization, Writing – original draft. **Pere-Pau Vázquez:** Conceptualization, Methodology, Investigation, Writing – review & editing, Supervision, Funding acquisition, Project administration.

Declaration of competing interest

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: Elena Molina reports financial support was provided by Spain Ministry of Science and Innovation.

Data availability

We only have permission to use the data for statistical analysis. The data include some personal information that we cannot share. Anonymized version could be generated upon request.

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