



University of Milan
Department of Pharmaceutical Sciences



Chemical Laboratory Simulator of
Qualitative Inorganic Analysis

Alessandro Pedretti



What is LabSim¹

LabSim is a laboratory simulator of qualitative inorganic analysis which was mainly developed with the aim to teach the students in laboratory during the COVID pandemic emergency. Its main features are:

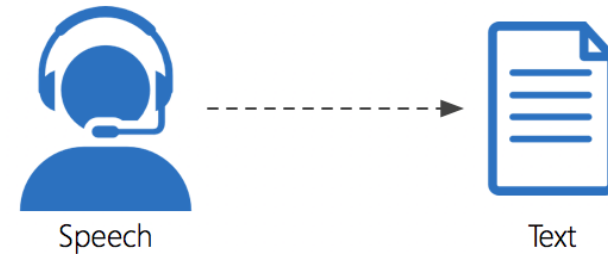
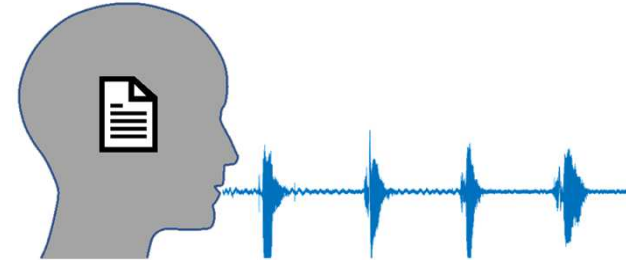
- Complete 3D environment (based on A-Frame/WebGL technology).
- Web-based application:
 - Compatibility with widest range of devices as: VR systems (HTC and Oculus), PCs (Linux, MacOS, and Windows), tablets (Android, iOS and Windows) and smartphones (Android and iOS).
 - Runs inside the web browser (Chromium-based), so no software installation is required.





What is LabSim²

- Support multiple languages (actually *English* and *Italian*).
- Speech synthesis (based on different technologies according to the device).
- Speech recognition for disabled persons.
- Based on a database of more than 3500 reactions that can be used in recognizing 60 analytes.



- 70 video virtual and real tutorials watchable through a TV included in the 3D environment.
- Totally free.



What you can do

With *LabSim*, you can practice as in a real laboratory of qualitative inorganic analysis and the main activities are:

- Solubility test in water of a substance even in the presence of reactants such as strong / weak acids / bases;
- pH measurement of a solution with universal indicator paper;
- Phase separation by centrifugation;
- Heating by plate or water bath;
- Tests for the recognition of anions by wet method;
- Tests for the recognition of cations by wet method;
- Recognition tests by dry method (non water-soluble substances);
- Flame test;
- Complete analysis of an unknown substance (both water-soluble and non-water-soluble);
- Watching video tutorials on both virtual and real laboratory activities.



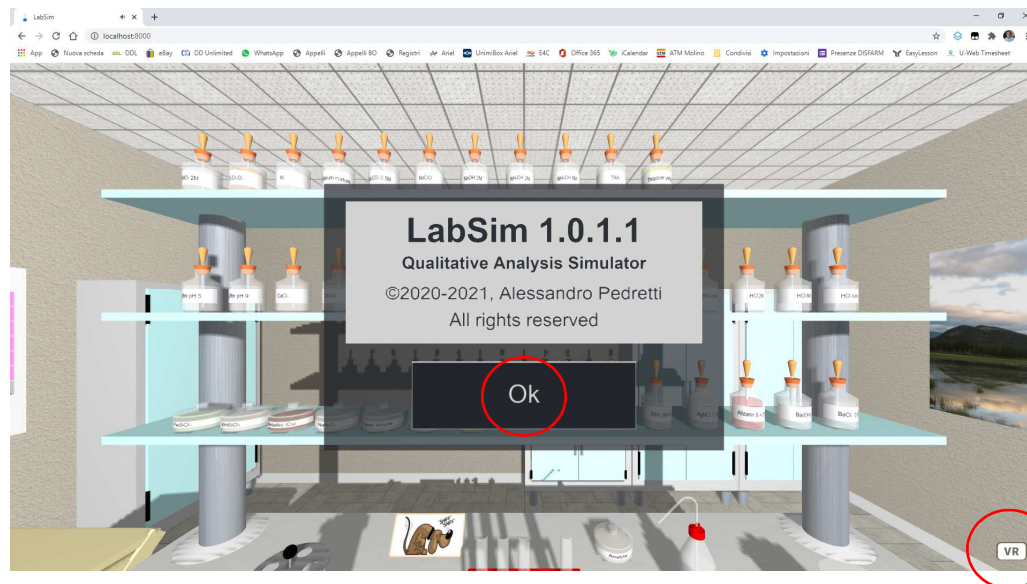


How to try it

In the address bar of the browser (Chrome or Edge), type:

<https://nova.disfarm.unimi.it/labsim>

After the loading screen, it will shown the copyright message:

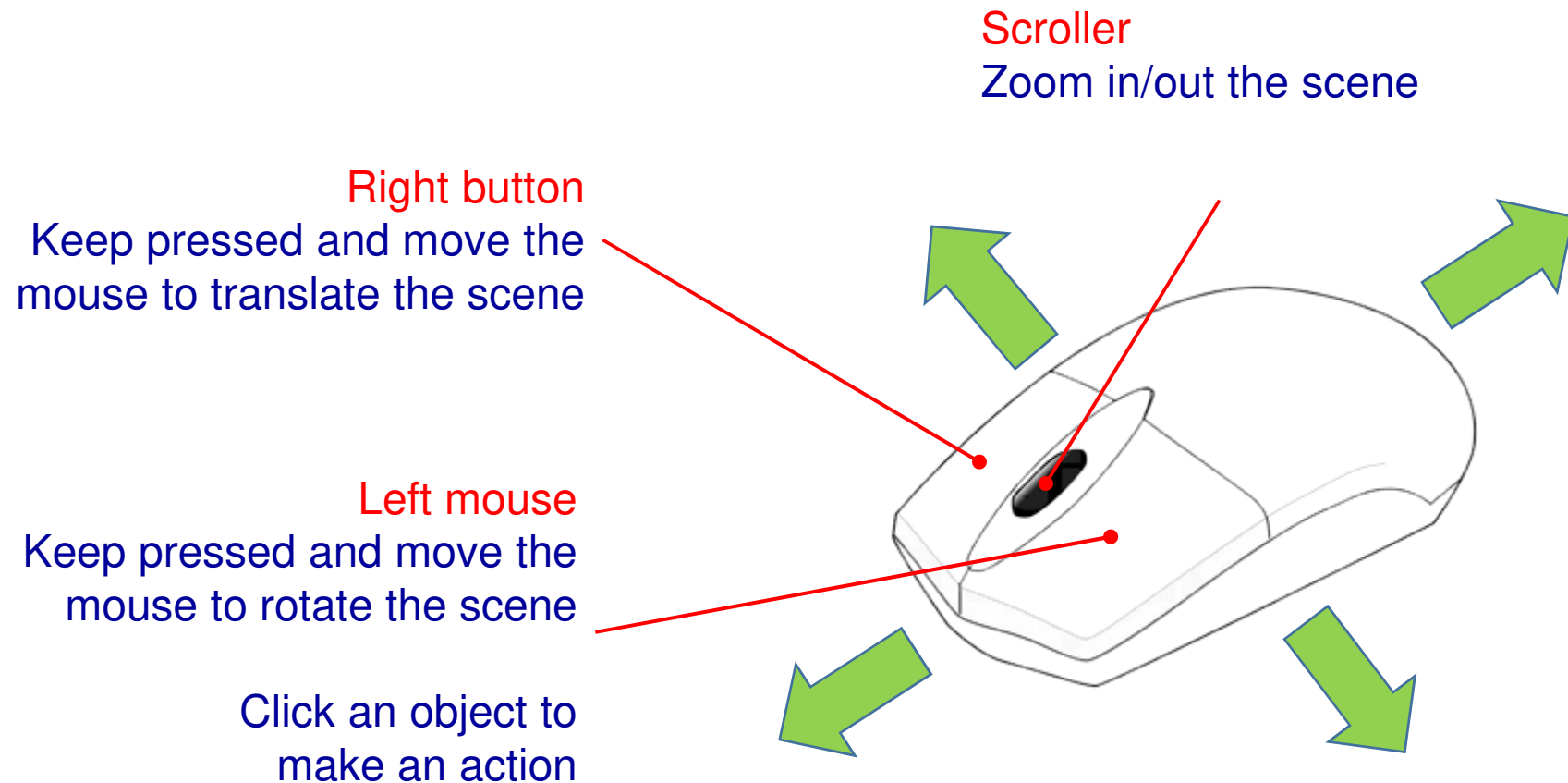


Click the **Ok** button to start the simulation. Clicking the **VR** button, you switch from widowed mode to full-screen or VR mode. Press **Esc** key to return to the standard display mode.



The mouse

The mouse is the preferred input device for non-VR hardware systems:





Other input devices

Some functions are available through the **keyboard**:

- The **cursor key** translate the scene.
- The **space bar** and **m** key show the main menu.
- The **Esc** key closes the menu.

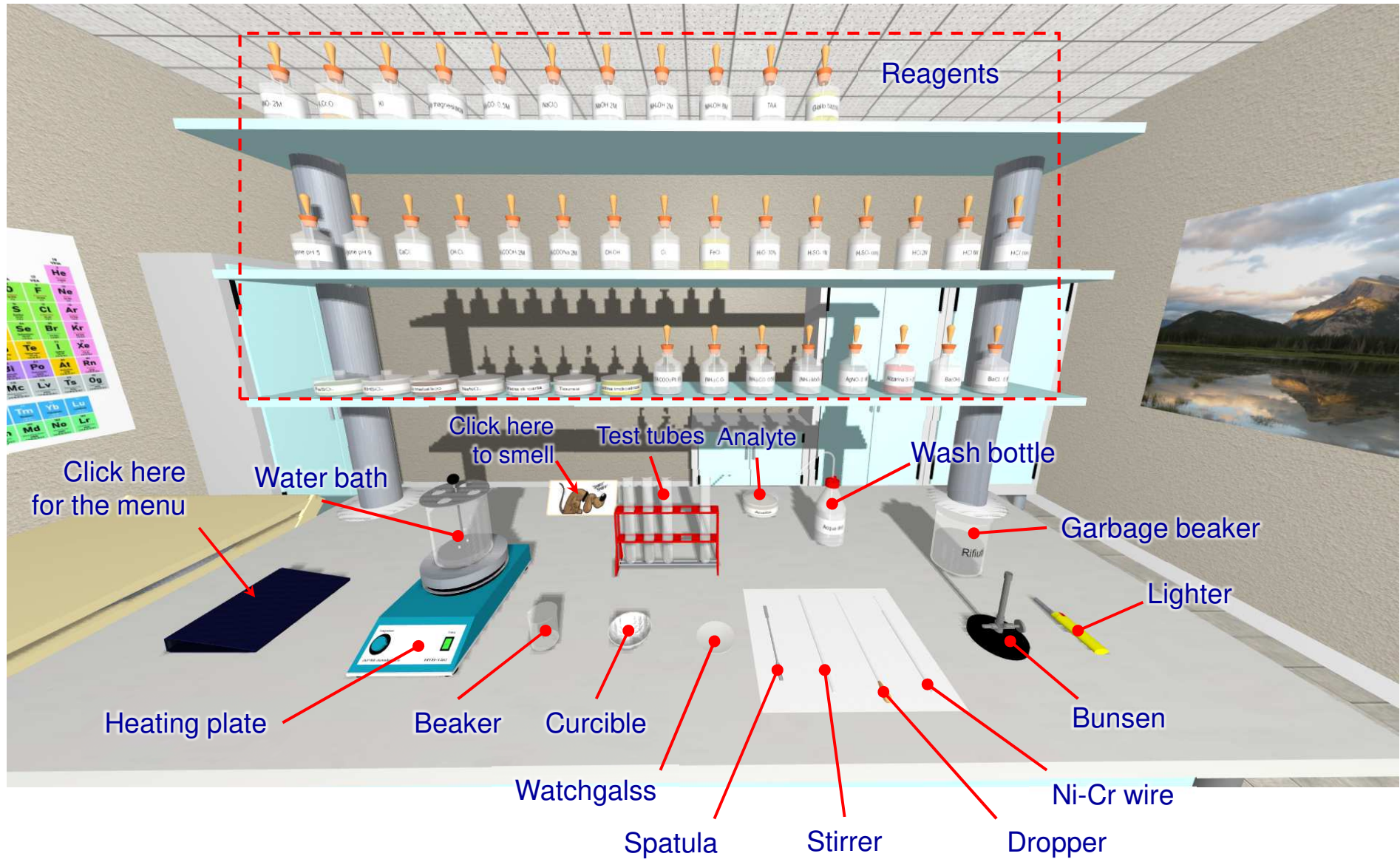


Input devices available only with **tablets** and **smartphones**:

- The **screen touch** (tap) is equivalent to a mouse click.
- The **accelerometer** rotates the scene.

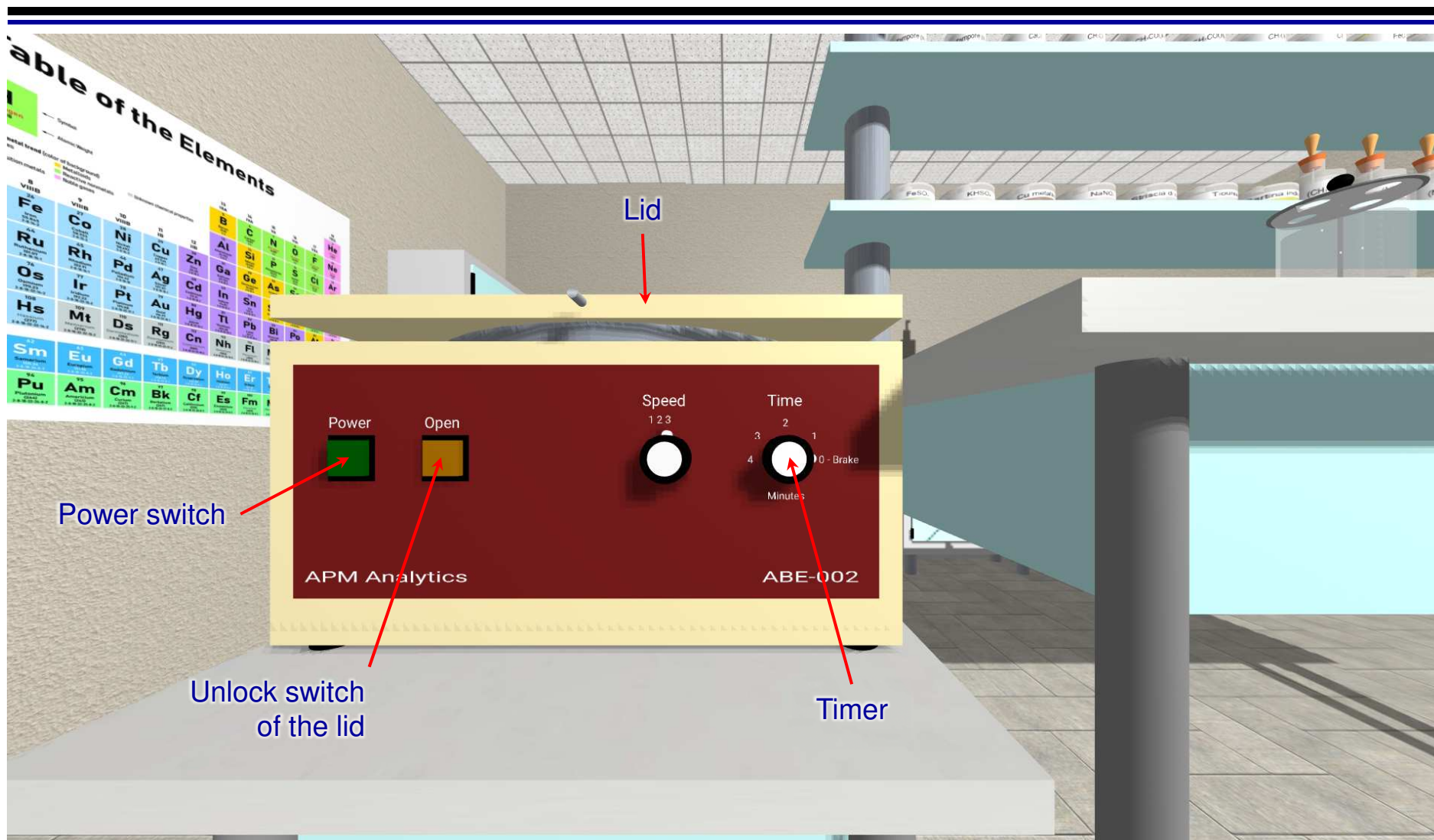


The workbench





The centrifuge



To perform a complete phase separation, at least 3 minutes are needed. Watch the video-tutorial for the right use.



How to watch the video tutorials

When you click the TV, the video *playlist* is shown:

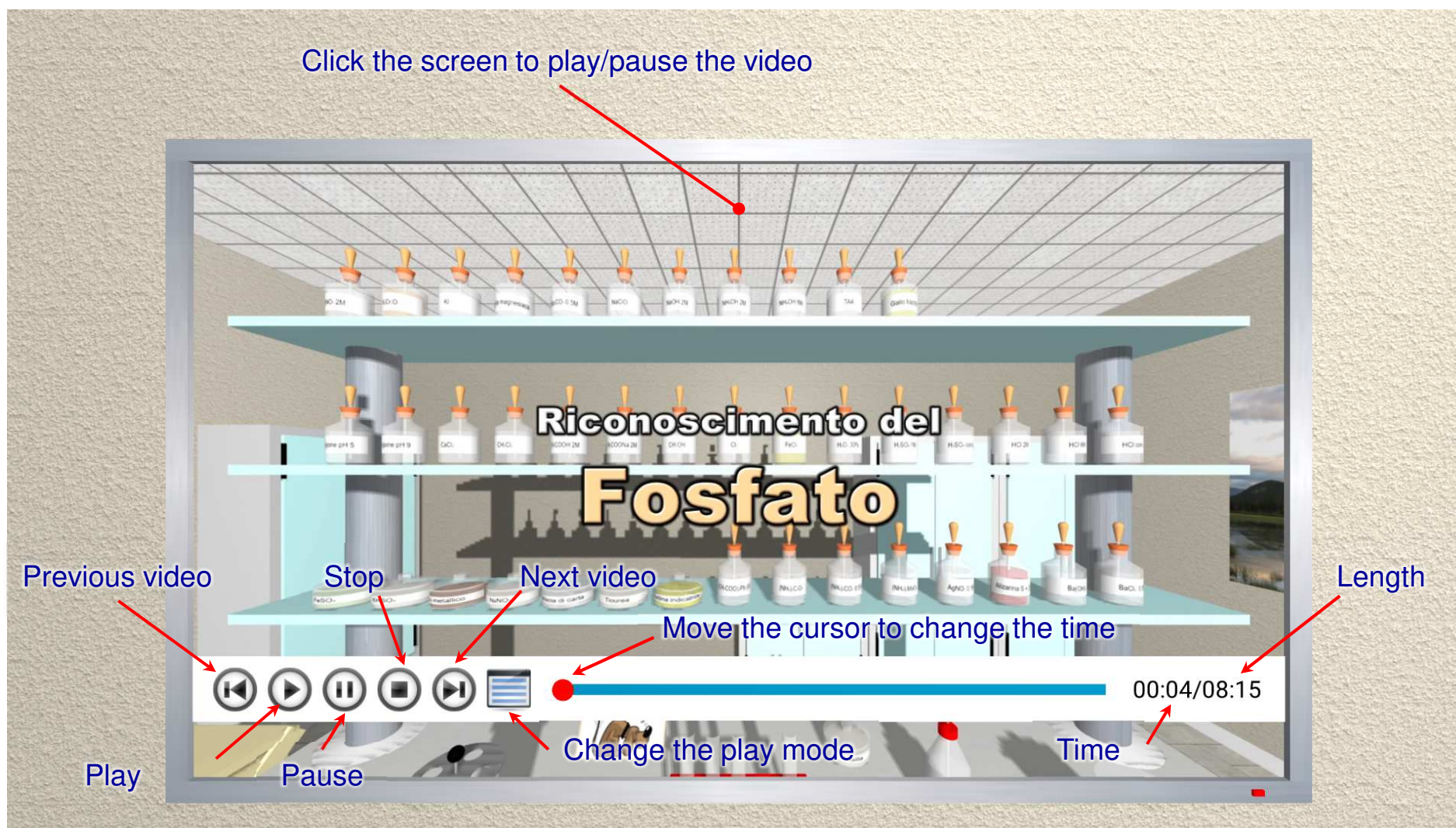
The screenshot shows a video playlist interface with the following elements and annotations:

- Annotations:**
 - "Click one of these buttons to play" points to the first video button.
 - "Click here to turn off the TV" points to the power button in the top right corner.
 - "Previous page" points to the left navigation arrow.
 - "Next page" points to the right navigation arrow.
- Playlist Title:** "List of the videos"
- Power Button:** A red power button icon in the top right corner.
- Video List:**

15. LS Riconoscimento PO_4^{3-}	16. LS Riconoscimento CH_3COO^-
17. LS Riconoscimento F^-	18. LS Riconoscimento BO_3^{3-}
19. LS Riconoscimento I gruppo (Ag^+)	20. LS Riconoscimento II gruppo (Hg^{2+})
21. LS Riconoscimento III gruppo (Al^{3+})	22. LS Riconoscimento IV gruppo (Zn^{2+})
23. LS Riconoscimento V gruppo (Ca^{2+})	24. LS Riconoscimento VI gruppo (NH_4^+)
25. LS Riconoscimento VI gruppo (Mg^{2+})	26. LS Riconoscimento VI gruppo (Li^+)
27. LS Riconoscimento VI gruppo (K^+)	28. LS Riconoscimento VI gruppo (Na^+)
- Navigation:** Left and right arrow buttons at the bottom of the playlist area.



How to control the player



Clicking **Stop**, you return to the video playlist.



Direct access to the videos

You can play the video tutorials outside *LabSim* just with this link:

<https://nova.disfarm.unimi.it/labsim/video.htm>

After the loading screen, the following menu is shown:

The screenshot shows a web browser window with the address bar displaying 'localhost:8000/video.htm'. The page content includes the title 'List of the videos' and the 'LABSIM' logo. Below the title is a grid of 14 blue buttons, each containing a number and a video topic. At the bottom of the page, there is a copyright notice: '© 2020-2021, Alessandro Pedretti - Università degli Studi di Milano'.

List of the videos	
1. LS Solubilità	2. LS Misura pH
3. LS Uso della centrifuga	4. LS Riconoscimento Cl^-
5. LS Riconoscimento Br^-	6. LS Riconoscimento I^-
7. LS Riconoscimento IO_3^-	8. LS Riconoscimento SO_3^{2-}
9. LS Riconoscimento $\text{S}_2\text{O}_3^{2-}$	10. LS Riconoscimento $\text{S}_2\text{O}_8^{2-}$
11. LS Riconoscimento SO_4^{2-}	12. LS Riconoscimento NO_2^-
13. LS Riconoscimento NO_3^-	14. LS Riconoscimento CO_3^{2-} e HCO_3^-

© 2020-2021, Alessandro Pedretti - Università degli Studi di Milano

This playlist works exactly as in *LabSim*.



What you can watch

Tutorials on the virtual lab (LS prefix):

- Base techniques (solubility, pH measurement, centrifuge use).
- Tests for the identifications of the anions.
- Tests for the identifications of the cations.
- Flame test.
- Analysis of water-insoluble molecules.
- Two examples of analysis of unknown molecules.

Tutorials on the real lab:

- Tests for the identifications of the anions.
- Tests for the identifications of the cations.
- Flame test.
- Analysis of some water-insoluble molecules.



How to change the position



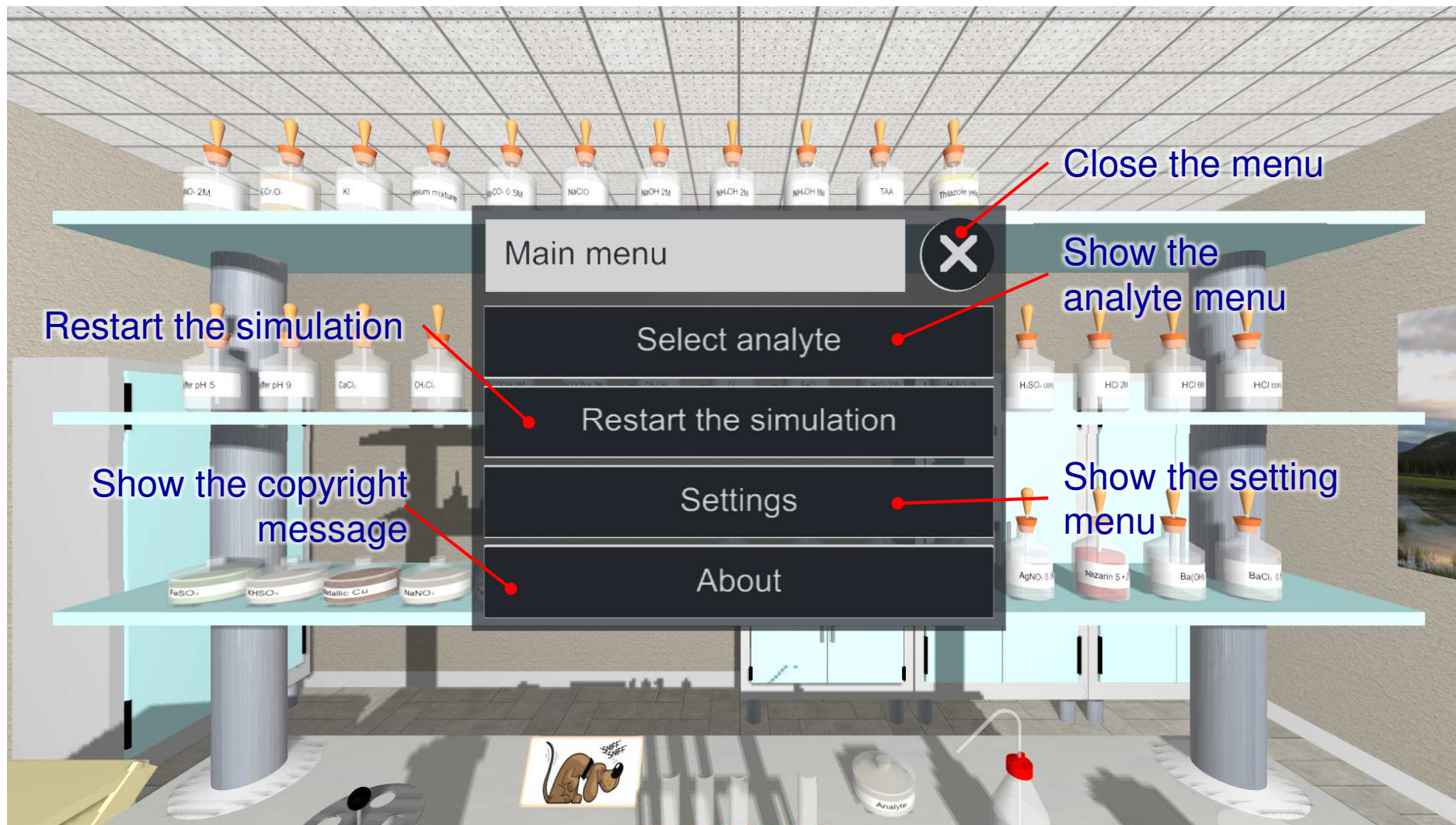
Clicking the footprints, you can change the work position.





Main menu

To open it, you must click the book or press *m* key.





Analyte menu

In this menu, you can choose the analyte.

Back to the previous menu Random selection of the analyte Close the menu

Code for the unknown analysis

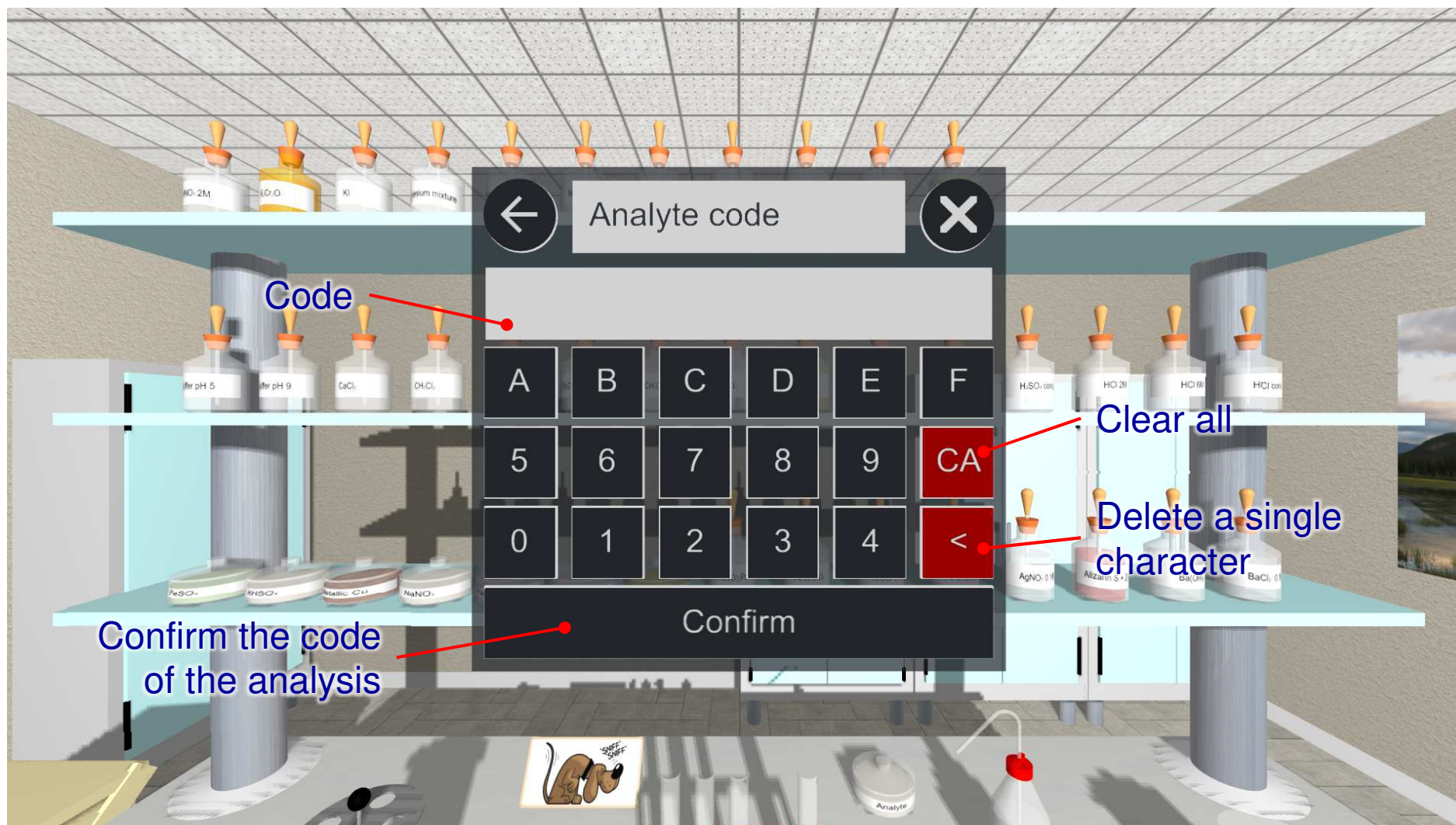
Code	Random	Random soluble	Random insoluble	(CH ₃ COO) ₂ Ca	(CH ₃ COO) ₂ Mg
AgNO ₃	Al ₂ (SO ₄) ₃	AlCl ₃	CaCl ₂	CH ₃ COOK	CH ₃ COONa
H ₃ BO ₃	HgCl ₂	K ₂ CO ₃	K ₂ HPO ₄	K ₂ S ₂ O ₃	K ₂ S ₂ O ₅
K ₂ SO ₃	K ₂ SO ₄	KAlSO ₄	KBr	KCl	KH ₂ PO ₄
KHCO ₃	KI	KIO ₃	KNO ₃	Li ₂ CO ₃	MgCl ₂
MgSO ₄	Na ₂ B ₄ O ₇	Na ₂ CO ₃	Na ₂ HPO ₄	Na ₂ S ₂ O ₃	Na ₂ S ₂ O ₅
Na ₂ SO ₃	Na ₂ SO ₄	NaBr	NaCl	NaF	NaH ₂ PO ₄
NaHCO ₃	NaI	NaNO ₂	NH ₄ Br	NH ₄ Cl	NH ₄ HCO ₃
ZnCl ₂	ZnSO ₄	(BiO) ₂ CO ₃	Al(OH) ₃	AlPO ₄	BaSO ₄
Ca(OH) ₂	Ca ₃ (PO ₄) ₂	CaCO ₃	CaSO ₄	Mg(OH) ₂	MgCO ₃
TiO ₂	ZnO				

Water soluble Water insoluble



Code for the unknown analysis

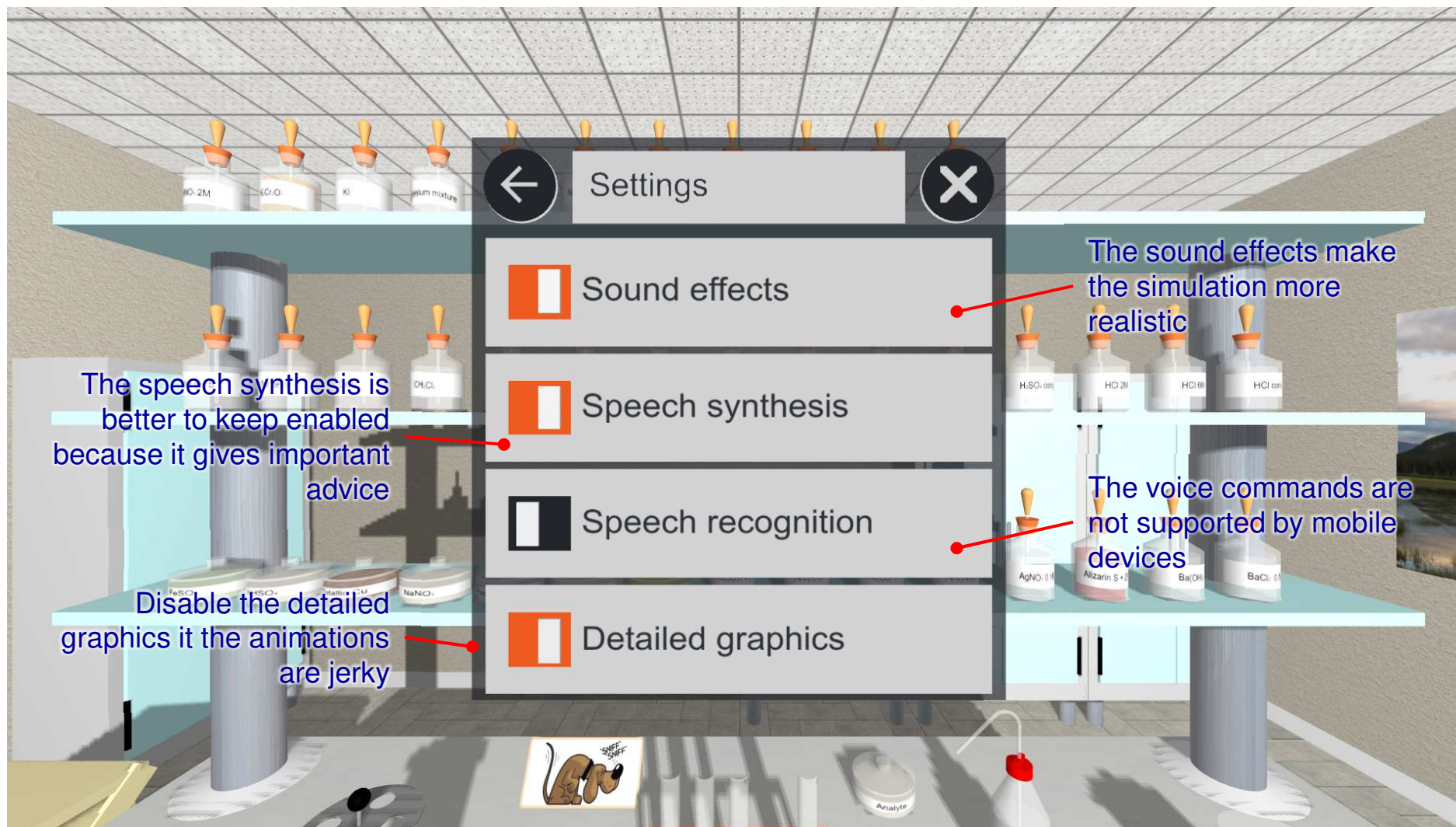
Clicking the keys, you can type the six-character code of the analysis.





Settings menu

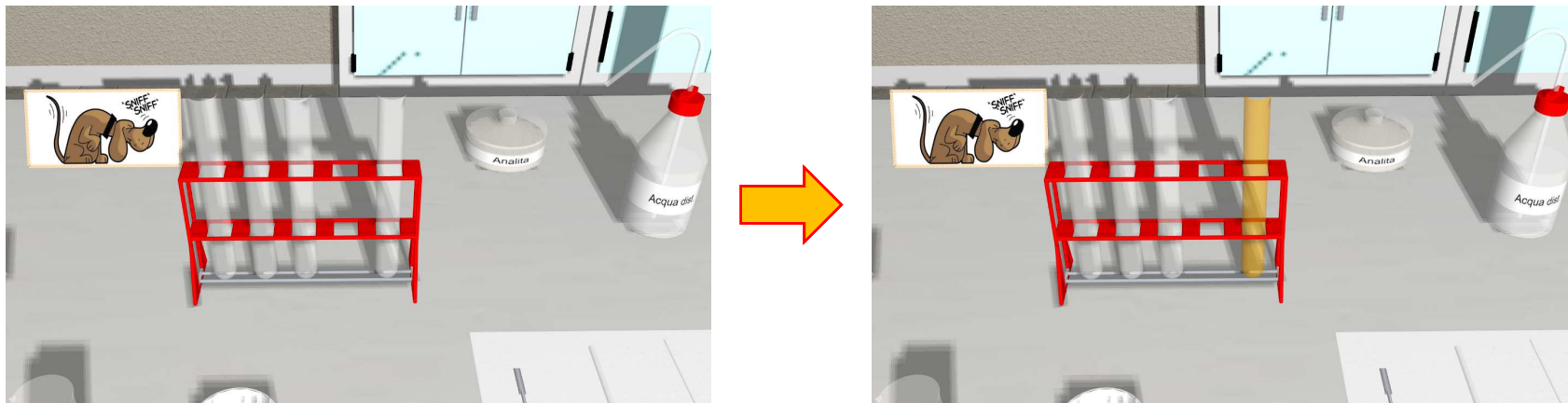
Here you can change some settings of the simulator.





Interaction with the objects¹

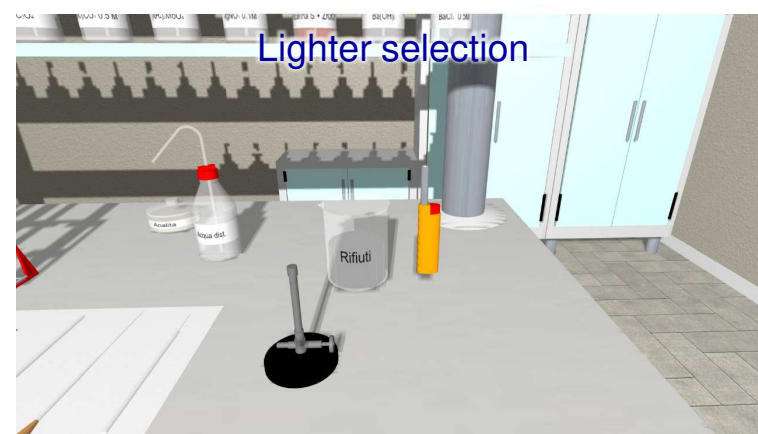
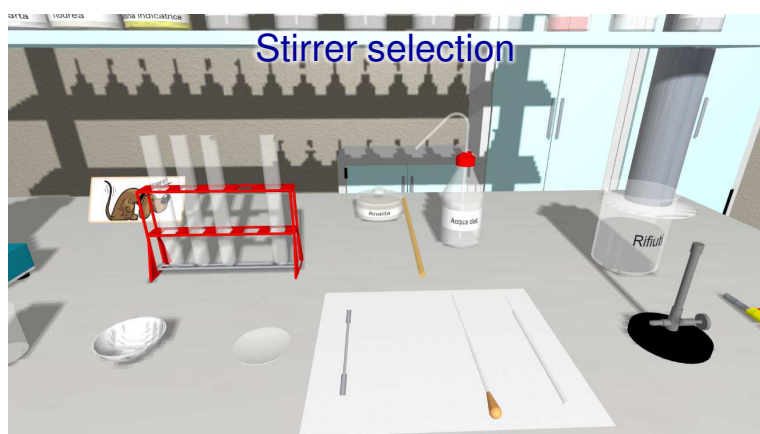
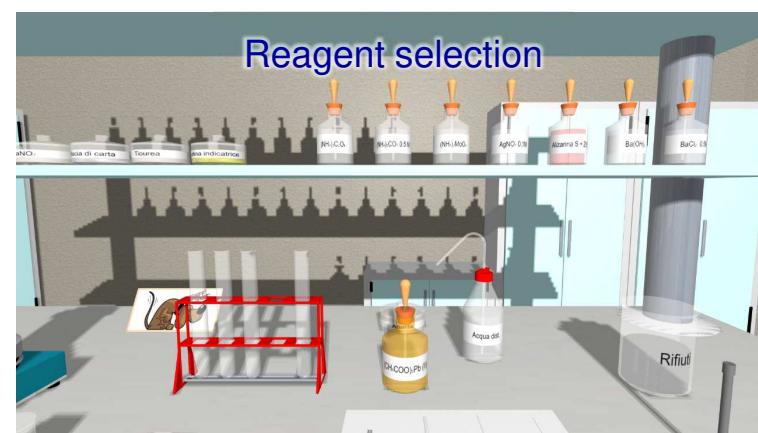
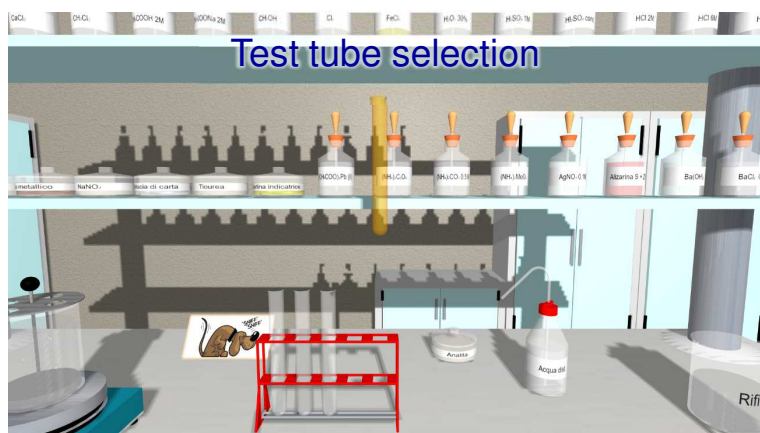
- The objects with which you can interact are highlighted on hover changing their color (orange or red) or size (like the book and the TV).



- You can interact with the objects only by clicking with the mouse or touching the screen (tap).
- The single click (tap) selects the object or starts an action.
- In the case of the trash beaker, double click (double tap) empties automatically all glassware containing something. Several video tutorials show this useful action.

Interaction with the objects²

- To use an object, it must be selected by a mouse click (tap). The selection is highlighted by lifting or moving of the object in the foreground (see reagents and analyte).





Interaction with the objects³

The objects can interact each other through actions given by:

- Selecting the object 1 and clicking the object 2 (e.g. selection of the stirrer and click the test tube to stir the content).
- Selecting the object, selecting the liquid reagent and clicking the reagent dropper (e.g. Selection of the test tube, selection of HCl 2M and click the reagent dropper).
- Selecting the object, selecting the solid reagent or the analyte and clicking the spatula (e.g. selection of the test tube, selection of NaNO_2 and click the spatula).



WARNING:

When an action is not permitted, the speech synthesis warn you and, if it is disabled, the action is just not completed without notice.



The glassware¹

The **glassware is always dirty** and needs to be rinsed with deionized water before the use. The simulator prevents the use of dirty glassware, avoiding the student from making mistakes in the analysis.

Generic cleaning procedure:

- Click the **glassware to clean** (e.g. a test tube) which will be then selected.
- Click the **wash bottle**. Some water will be transferred to the glassware.
- Click the **trash beaker**. The glassware content will be emptied.

Dropper cleaning procedure:

- Click an **empty test tube**. If you are not sure on its content, empty and wash it. The tube will be selected.
- Click the **wash bottle**. About 1 mL of water will be transferred to the tube.
- Click the **dropper** to select it.
- Click the **test tube with the water**. The dropper will suck up the tube content.





The glassware²

- Click the [trash beaker](#). The content will be released.

Ni-Cr wire cleaning procedure:

1. Turn on the [bunsen](#) setting the flame as oxidizing.
2. Put some [concentrated hydrochloric acid](#) in a test tube.
3. Click the [Ni-Cr wire](#) selecting it.
4. Click the [test tube with HCl](#). The wire will be soaked in HCl.
5. Click the [bunsen](#). The wire will be placed into the flame.
6. Repeat the steps from 3 to 5 until the flame does not change more the color (usually this operation must be repeated 3 times).





Transfer of substances

The simulator approximates the liquid and solid quantities according to the action and the size of the glassware on which you act:

Glassware	Liquid	Solid
Test tube	1 mL	One spatula tip
Beaker	5 mL	One spatula tip
Watch glass	1 mL	One spatula
Curcible	5 mL	One spatula
Paper	One drop	-

Therefore, if you want to add 2 mL of water to a test tube, you need to repeat the action twice because 1 mL is transferred at time.

There are some reactions in which the quantities play an important role for their occurrence as:

- **Borate test** (you must add methanol at least twice so that is more than sulfuric acid and can ignite).
- **Nitrate test** (you must add FeSO_4 at least twice so that the solution is enough concentrated to permit the formation of the brown ring).



Chemical reactions

LabSim is based on a database of about 3700 reactions that can occur between:

- Analyte + one reagent
- Analyte + two reagents
- Two reagents
- Reaction product + one reagent
- Reagent product + two reagents



The physical aspects influencing the result of a reaction are:

- Heat given by:
 - water bath (e.g. phosphate test, tests with TAA, dichromate paper, etc.);
 - electric heater (e.g. calcination with con KHSO_4).
- Time.



WARNING:

In order to occur correctly a reaction, the solution must be homogeneous after the addition of each reagent stirring the mixture.



is a web application developed in 2020-2021
by Alessandro Pedretti
All rights reserved

Alessandro Pedretti
Dipartimento di Scienze Farmaceutiche
Facoltà di Scienze del Farmaco
Università degli Studi di Milano
Via Luigi Mangiagalli, 25
I-20133 Milano - Italy
Tel. +39 02 503 19332
E-Mail: info@vegazz.net
WWW: <https://www.ddl.unimi.it/labsim>