

**Table S1.** Characterization's survey computational chemistry elements

| Have you used any specific software, like this type?    | Examples                                                                            |
|---------------------------------------------------------|-------------------------------------------------------------------------------------|
| 1. Molecule editor and viewer                           | PyMol<br>Avogadro<br>Chemsketch<br>Other software or applications<br>I don't use it |
| 2. Quantum mechanics                                    | Spartan<br>GAMESS<br>Gaussian 98/03/09<br>I don't use it                            |
| 3. Mathematical modelling and symbolic algebra software | R<br>Geogebra<br>Maple<br>Mathematica<br>I don't use it                             |
| 4. Chemical spreadsheets                                | Seurat<br>Bioclipse<br>Instant JChem<br>I don't use it                              |
| 5. Spreadsheets                                         | Excel<br>Origin<br>Sigmaplot<br>I don't use it                                      |
| 6. QSAR/ADMET modelling                                 | Datawarrior<br>DecoyFinder<br>PaDEL-descriptor<br>I don't use it                    |
| 7. Virtual screening and ligand design                  | PyRx<br>AutoDock<br>MGLTools<br>I don't use it                                      |
| 8. Molecular dynamics                                   | NAMD<br>CHARM<br>GROMACS<br>I don't use it                                          |
| 9. Computational suites                                 | MOE<br>Schrodinger<br>Discovery Studio<br>I don't use it                            |
| 10. Scientific web resources                            | PhET Simulator<br>Protein Data Bank<br>Chemical Databases<br>I don't use it         |

\* Based on the proposal by Rodríguez-Becerra, *et al.* [1] of Computational chemistry resources in educational contexts.

**Table S2.** Focus group script.

| N | Question                                                                                                                                                                                                                                                      |
|---|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 1 | How was your experience with the virtual environment of the e-learning module? In this sense, now thinking as a teacher, what aspects of the e-learning environment would you maintain or modify for this type of educational computational chemistry course? |
| 2 | What aspects of the course do you think act as facilitators for learning chemistry and science in general?                                                                                                                                                    |
| 3 | What computational chemistry or computational skills, in general, do you think you developed or strengthened with the course?                                                                                                                                 |
| 4 | Did you acquire or develop scientific skills during the module? which is it?                                                                                                                                                                                  |
| 5 | What knowledge of computational chemistry or cheminformatics did you acquire during the course?                                                                                                                                                               |
| 6 | How do you project this knowledge, computer skills and learning, in general, to what will be your professional work as a chemistry teacher?                                                                                                                   |
| 7 | Do you think that you managed to appropriate any computational chemistry or cheminformatics tool? In this sense, how did you use these tools to resolve the closing evaluation of the course?                                                                 |
| 8 | What made the planning you did in the closure evaluation easier/difficult?                                                                                                                                                                                    |

**Table S3.** Main ID models reported in the literature.

| <b>ID Model</b>                           | <b>Levels and/or stages of development</b>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
|-------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Gagné and Briggs model [2].               | This model is developed from 4 levels: i) System level, which accounts for the needs and initial arrangements in terms of objectives, resources and scope of the course; ii) Course level, which accounts for the objective of the course, content structure and didactic sequences; iii) Lesson level, at this level the necessary inputs that support the course are developed; iv) Final system level, which incorporates course evaluations, installation and diffusion.                                                                                                                                                                                                                                                                       |
| ASSURE model [3].                         | This model is developed from six levels: i) Analyze social, physical, cognitive and attitudinal characteristics of the student, ii) Establish learning objectives, iii) Selection of strategies, technologies, means and materials for the achievement of learning objectives, iv) Develop the course by creating a learning environment based on previously selected resources and strategies, v) Implementation of the course, and vi) Evaluation and implementation of potential improvements to the course.                                                                                                                                                                                                                                    |
| Dick and Carey model [4].                 | This model is organized into: i) Identification of the objective of the course, ii) Analysis of the theme and the context of the students, iii) Development of evaluation instruments, iv) Development of instructional strategy and generation of resources, v) Design of summative and formative evaluation, and vi) Review of the instruction.                                                                                                                                                                                                                                                                                                                                                                                                  |
| Jonassen model [5].                       | This model is organized from an initial problem or question and is then followed by the following design stages: i) Connect the problem with related experiences and relevant information, ii) Development of cognitive and collaboration tools, and iii) Adapt context factors to promote learning.                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| ADDIE model [6]                           | This model is organized based on five stages: I) Analysis of students and their training needs, ii) Design of the pedagogical approach and sequencing of the content, iii) Development of resources based on the pedagogical design, iv) Implementation of the course, and v) Evaluation of the formative action.                                                                                                                                                                                                                                                                                                                                                                                                                                  |
| Web-based e-learning education model [7]. | This model is organized based on the ADDIE model's five stages and incorporates two new stages: i) Execution of the course by the students and ii) Review of all stages to optimize the course.                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| IDOL model [8].                           | This model is presented as a complement to the Dick and Carey model or the ADDIE model. It is developed from three levels. i) General analysis, which incorporates students, context, objectives, the role of the teacher and pedagogical aspects, ii) Strategy, which accounts for the resources to be used, organizational content and instruction system, and iii) Evaluation, which incorporates the design of formative evaluations and a review of the instruction.                                                                                                                                                                                                                                                                          |
| ICCEE model [9].                          | This model is organized based on five stages: i) Identification, the designer must account for the needs of the course to be built, incorporating the type of course, objective, student needs, and technologies to be used, ii) Planning and organization of content and technological uses, iii) Creation of material and resources to be used, incorporates the inputs linked to the content and the support of the site where it will be hosted, iv) Engage, accounts for the selection of technology means that avoid student desertion during the course, and v) Evaluation, proposes the realization of different evaluations throughout the process and incorporates the perception of the students towards the development of the course. |

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▼ Module I: Introduction to computational chemistry for science education.

### Learning Goal

Analyze the potential of computational chemistry and how it supports the design of new drugs through publicly available chemical databases.

[Mark as done](#)

### Contents

 PAGE

Computational chemistry tools for teaching Sciences

[Mark as done](#)

 PAGE

Avogadro Software - Molecular Editing and Visualization

[Mark as done](#)

 ACTIVITY

Draw a structure with Avogadro

[Mark as done](#)

 PAGE

Discovery and design of new drugs

[Mark as done](#)

 H5P ACTIVITY

Hydrogen bond acceptors

[Mark as done](#)

 H5P ACTIVITY

Hydrogen bond donors

[Mark as done](#)

 QUIZ

Lipinski's Rule

[Mark as done](#)

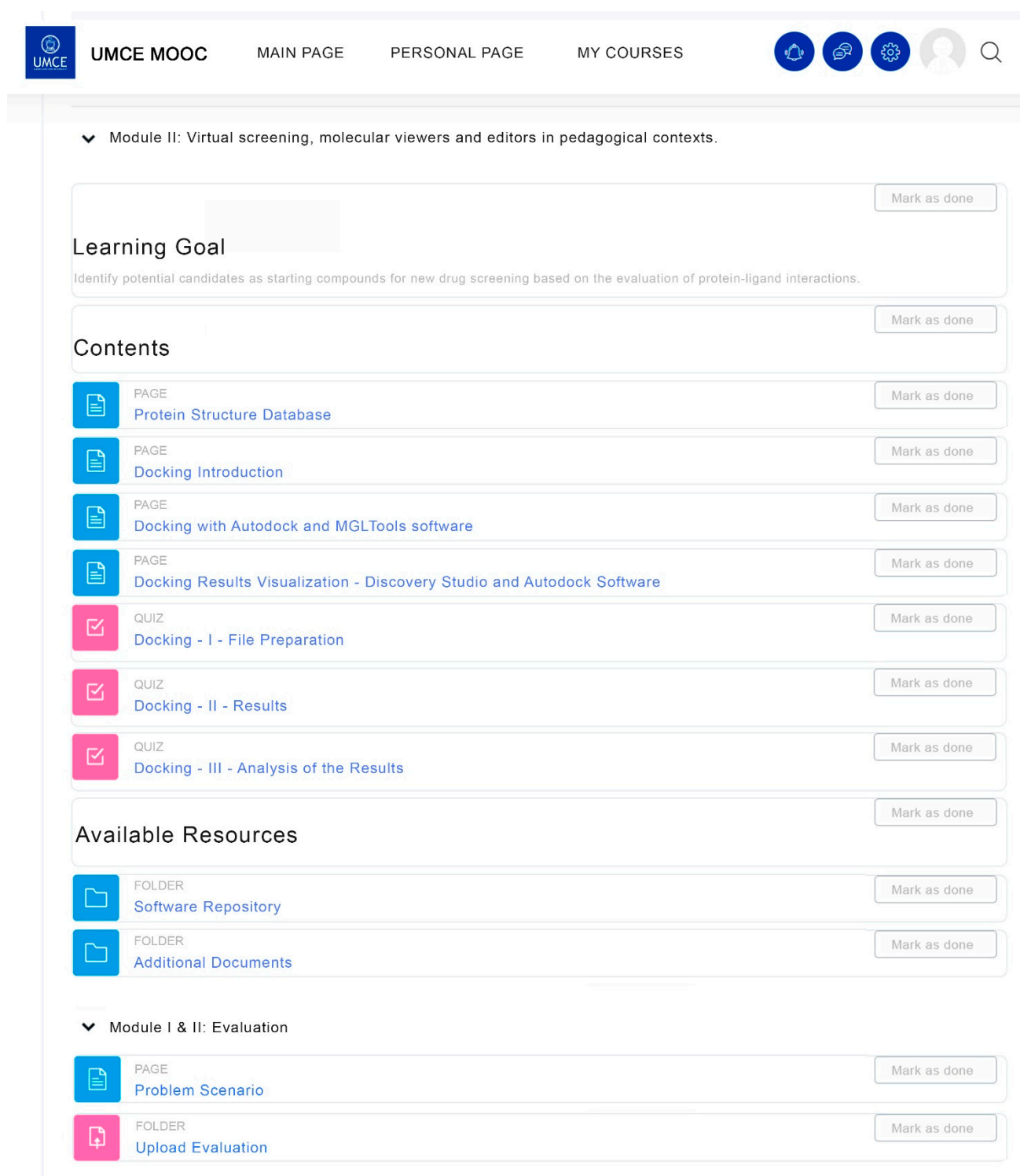
### Available Resources

 FOLDER

Software Repository

[Mark as done](#)

**Figure S1.** Mock-up ECC Course - Module I: Introduction to Computational Chemistry for science teaching, mounted on the Moodle 4.1 system. (Own elaboration)



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Module II: Virtual screening, molecular viewers and editors in pedagogical contexts.

**Learning Goal** Mark as done

Identify potential candidates as starting compounds for new drug screening based on the evaluation of protein-ligand interactions.

**Contents** Mark as done

PAGE Protein Structure Database Mark as done

PAGE Docking Introduction Mark as done

PAGE Docking with Autodock and MGLTools software Mark as done

PAGE Docking Results Visualization - Discovery Studio and Autodock Software Mark as done

QUIZ Docking - I - File Preparation Mark as done

QUIZ Docking - II - Results Mark as done

QUIZ Docking - III - Analysis of the Results Mark as done

**Available Resources** Mark as done

FOLDER Software Repository Mark as done

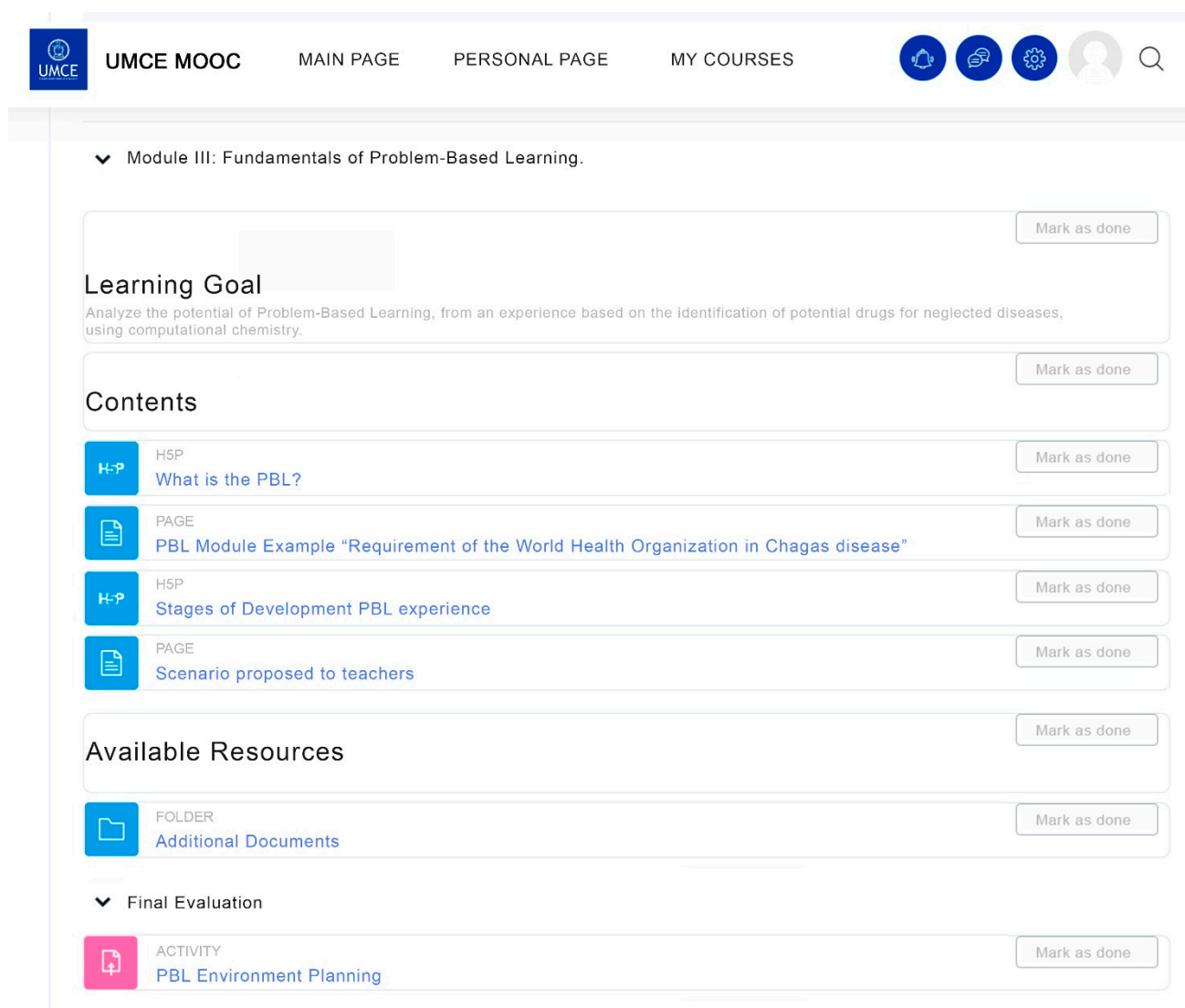
FOLDER Additional Documents Mark as done

Module I & II: Evaluation

PAGE Problem Scenario Mark as done

FOLDER Upload Evaluation Mark as done

**Figure S2.** Mock-up ECC Course - Module II: Virtual screening, molecular viewers and editors in pedagogical contexts, mounted on the Moodle 4.1 system. (Own elaboration)



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Module III: Fundamentals of Problem-Based Learning.

Learning Goal

Analyze the potential of Problem-Based Learning, from an experience based on the identification of potential drugs for neglected diseases, using computational chemistry.

Contents

What is the PBL?

PBL Module Example "Requirement of the World Health Organization in Chagas disease"

Stages of Development PBL experience

Scenario proposed to teachers

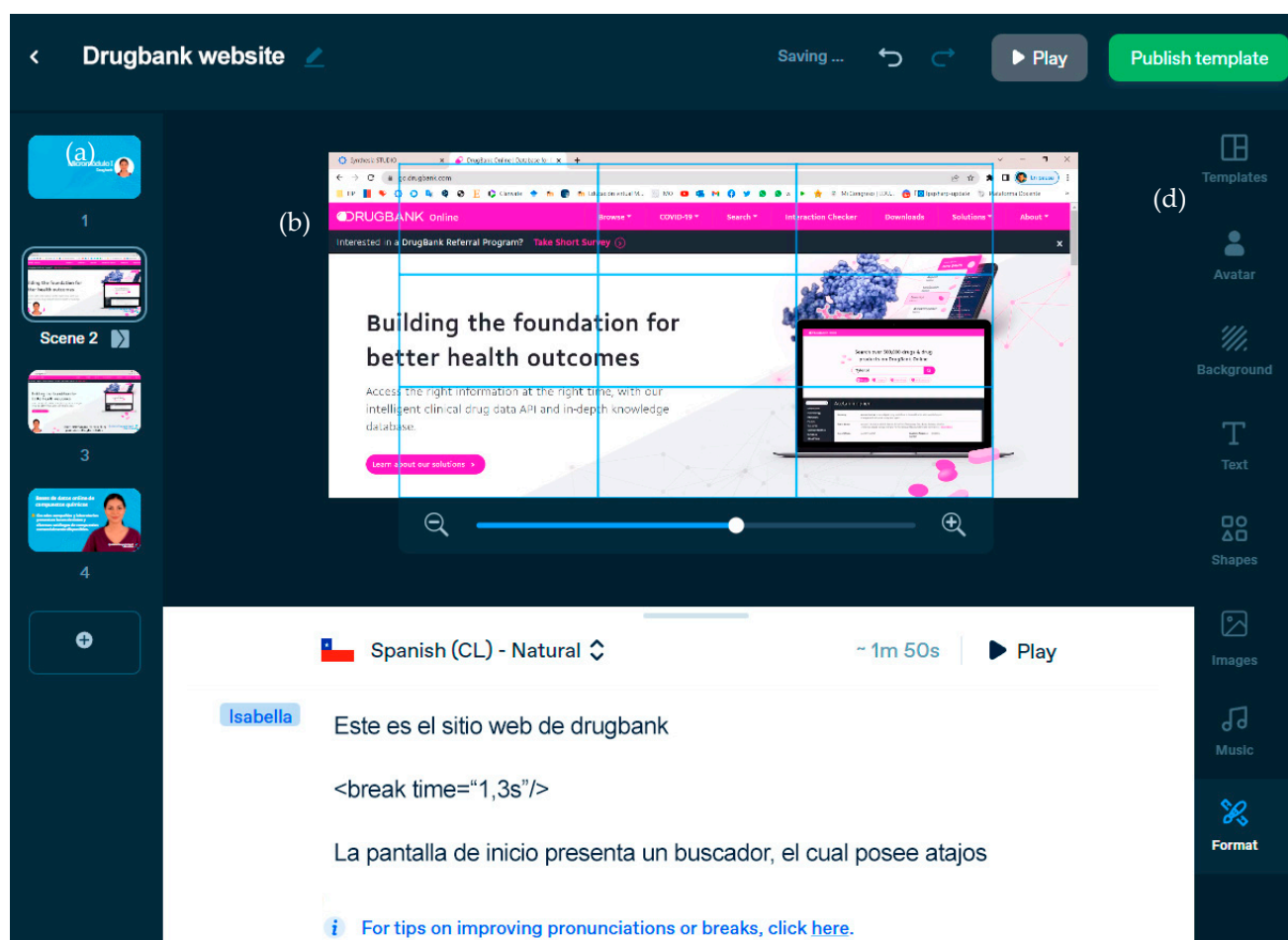
Available Resources

Additional Documents

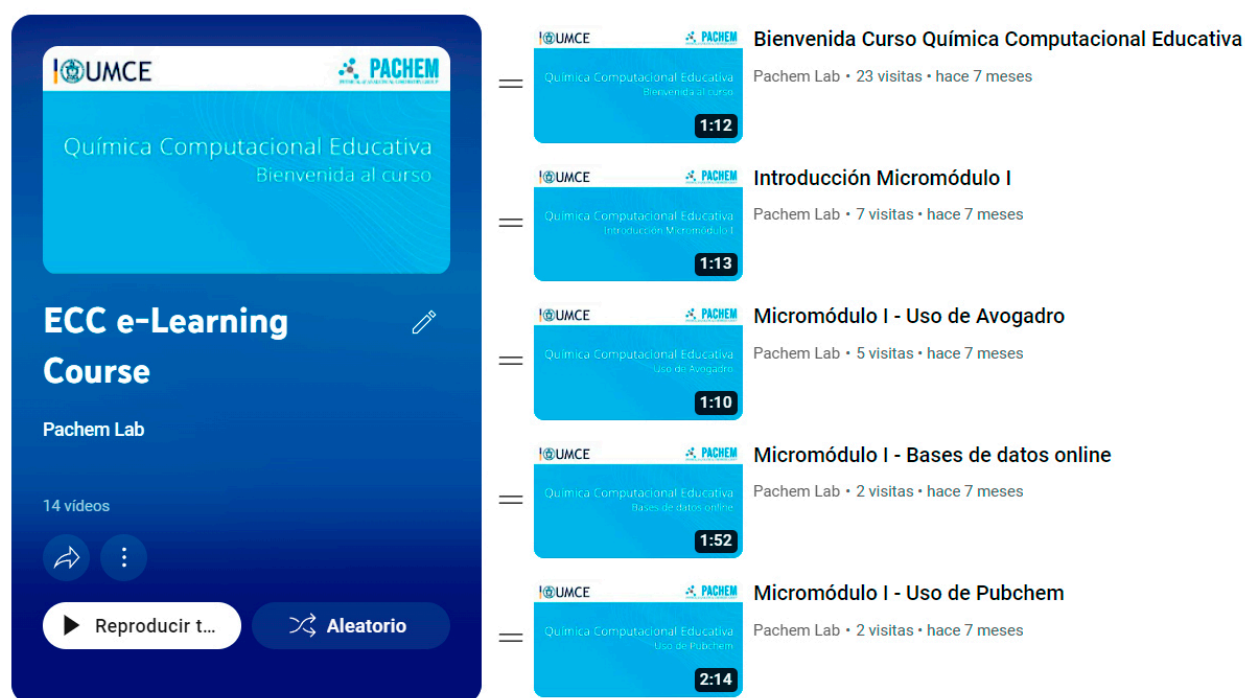
Final Evaluation

PBL Environment Planning

**Figure S3.** Mock-up ECC Course - Module III: Fundamentals of Problem-Based Learning, mounted on the Moodle 4.1 system. (Own elaboration)



**Figure S4.** Synthesia STUDIO Dashboard. (a) slides that make up the video, (b) video preview, (c) script and text/audio/video synchronization elements and (d) other editing elements.



**Figure S5.** Youtube ECC e-Learning course playlist, is possible to access all the training videos in chronological order. [https://youtube.com/playlist?list=PLozAiXUC8e7VOTwU7JoSep-bUPqBnOTA\\_R](https://youtube.com/playlist?list=PLozAiXUC8e7VOTwU7JoSep-bUPqBnOTA_R)

### Participation in the course

Activity Module: Evaluation - Draw a structure with Avogadro. Period: 3 months show only: Student show actions: all actions Go

groups: All participants Task Views Task Messages

| Name / Surname(s) | all actions | Select                              |
|-------------------|-------------|-------------------------------------|
| Student 1         | Yes (8)     | <input type="checkbox"/>            |
| Student 2         | Yes (4)     | <input type="checkbox"/>            |
| Student 3         | No          | <input checked="" type="checkbox"/> |
| Student 4         | No          | <input checked="" type="checkbox"/> |
| Student 5         | No          | <input checked="" type="checkbox"/> |

With selected users: Choose...  
Choose...  
Send a message

**Figure S6.** Control panel to monitor participation in the ECC e-learning course. It is possible to specify the time range and the type of activity, among other parameters.

| Hour                          | Full name of the user | Event context                                                 | Component | event name                              | Description                                                                                                      | Origin |
|-------------------------------|-----------------------|---------------------------------------------------------------|-----------|-----------------------------------------|------------------------------------------------------------------------------------------------------------------|--------|
| January 16, 2023, 11:52:35 PM | Student 1             | Task: Evaluation - Draw a structure with Avogadro.            | Task      | The delivery status has been displayed. | The user with id '85' has viewed the submission status page for the assignment with course module id '13'.       | web    |
| January 16, 2023, 11:52:35 PM | Student 1             | Task: Evaluation - Draw a structure with Avogadro.            | Task      | Seen course module                      | The user with id '85' viewed the 'assign' activity with course module id '13'.                                   | web    |
| January 16, 2023, 11:52:31 PM | Student 1             | Page: Avogadro Software - Molecular editing and visualization | System    | Updated Course Activity Completion      | The user with id '85' updated the completion state for the course module with id '12' for the user with id '85'. | web    |
| January 16, 2023, 11:52:19 PM | Student 1             | Task: Evaluation - Draw a structure with Avogadro.            | Task      | The delivery status has been displayed. | The user with id '85' has viewed the submission status page for the assignment with course module id '13'.       | web    |

**Figure S7.** Tracking log of all ECC e-Learning course events.

## References

1. Rodríguez-Becerra, J.; Cáceres-Jensen, L.; Díaz, T.; Druker, S.; Bahamonde, V.; Perna, J.; Aksela, M. Developing technological pedagogical science knowledge through educational computational chemistry: a case study of pre-service chemistry teachers' perceptions. *Chemistry Education Research and Practice* **2020**, *21*, 638–654, doi:10.1039/c9rp00273a.
2. Gagne, R.M.; Briggs, L.J. *Principles of instructional design*; Holt, Rinehart & Winston: 1974.
3. Heinich, R.; Molenda, M.; Russell, J.; Smaldino, S. The ASSURE model. *Instructional Media and Technologies for Learning, 7th edition*. Upper Saddle River, NJ: Merrill/Prentice Hall **2002**.
4. Dick, W. The Dick and Carey model: Will it survive the decade? *Educational technology research and development* **1996**, *44*, 55–63, doi:10.1007/BF02300425.
5. Jonassen, D.H. Thinking technology: Toward a constructivist design model. *Educational technology* **1994**, *34*, 34–37.
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7. Alonso, F.; López, G.; Manrique, D.; Viñes, J.M. An instructional model for web-based e-learning education with a blended learning process approach. *Br J Educ Technol* **2005**, *36*, 217–235, doi:10.1111/j.1467-8535.2005.00454.x.
8. Siragusa, L.; Dixon, K.C.; Dixon, R. Designing quality e-learning environments in higher education. *Proceedings ascilite Singapore* **2007**, 923–935.
9. Chen, L.-L. A model for effective online instructional design. *Literacy Information and Computer Education Journal* **2016**, *6*, 2303–2308, doi:10.20533/licej.2040.2589.2016.0304.