

# View Abstract

**ABSTRACT SYMPOSIUM NAME:** General Posters

**ABSTRACT SYMPOSIUM PROGRAM AREA NAME:** CHED

**CONTROL ID:** 3986411

**PRESENTATION TYPE:** Poster Only : Do not consider for Sci-Mix

**TITLE:** Improving the ability of biochemistry students to solve problems in the context of drug discovery

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**ABSTRACT BODY:**

**Abstract:**

Drug discovery at early stages provides a good scenario to simulate real world problems that could help to engage science undergraduate students to take more active roles in their learning process. The widespread use of *cookbook* laboratory protocols throughout their studies may lead to certain limitations in some general skills needed for a successful professional development, including autonomous learning, planning of experiments, time and resource management, or the ability to conduct presentations in public or to work as a team. Our Educational Innovation Group *TR4BIOCHEM (PIE22-067)* is involved in the implementation of new Problem Based Learning experiences for chemistry and biochemistry undergraduate students. In the subject "Pharmacological Biochemistry", 4th year-biochemistry undergraduate students are trained in some stages of early drug discovery, including the *in vitro* blind screening assay of enzyme inhibitors and the *in silico* modeling. Based on a high throughput screening (HTS) strategy and guided by a meaningful driving question (i.e. to discover new drugs to treat Alzheimer, bacterial contaminations or cancer) students must search for information and design protocols, putting into practice some concepts that they have learned throughout their studies. In this regard, principles of enzymatic analysis and enzyme inhibition must be adapted to the implementation of a HTS *in vitro* enzymatic assay for the fast screening of low molecular weight inhibitors. This makes students to face, in some cases for the first time, the process of selecting which experimental procedure is more suitable, considering some aspects that include cost, speedness, capability to be automatized, equipment needed, etc. In the Computational Biology part of this experience, students recreate the protein-drug interactions by means of a docking experiment in order to predict the interaction of drugs with the molecular target used in the *in vitro* blind screening. For this purpose, they benchmark the obtained docking solutions with the x-ray-solved structure of the complex. The study of the docking technique is implemented with PyRosetta in Jupyter notebooks. Finally, results are summarized and conclusions presented to a diverse audience. Our results indicate that inquiry-based approaches based on the simulation of a real world problem are very positively perceived by students, who find this type of research experience very rewarding.

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**Presentation Preference:** I will not travel to New Orleans and wish to participate virtually.

# ACS SPRING 2024

## CERTIFICATE OF ATTENDANCE

This certifies that

Ana Rodríguez Quesada

attended the hybrid ACS Spring 2024 Conference  
March 17 - 21, 2024  
New Orleans, LA, USA



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DIRECTOR, MEETINGS AND EVENTS

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# CERTIFICATE OF PRESENTATION

This is to certify that

**Ana Quesada**

presented research titled

**Improving the ability of biochemistry students to solve problems in the context of drug discovery**

at

ACS Spring 2024  
New Orleans, Louisiana & Hybrid  
March 17 - 21, 2024

*Liz Huh*

**Liz Huh**

Sr. Director, Meetings and Events



Program Area: Division of Chemical Education

Session Type: Poster - Virtual

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