Computational Drug Design in Problem-Based Learning: A Pedagogical Experience in Pre-Service Chemistry Teachers

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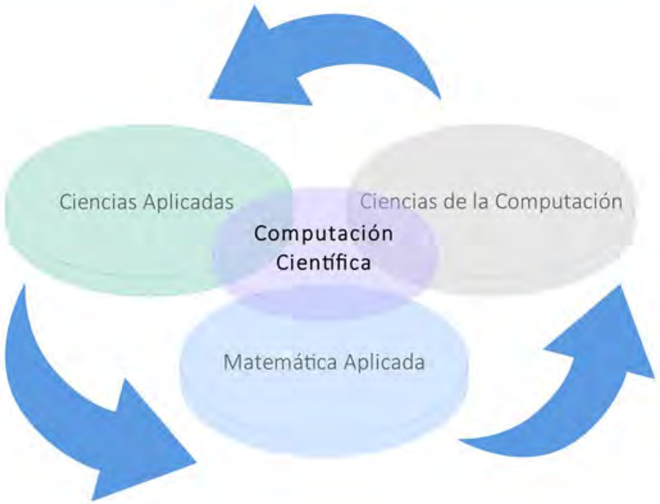
PachemLaB

PENSAMIENTO COMPUTACIONAL

3A-*GT*

Abstracción	Representar datos por medio de MODELOS y SIMULACIONES
Analisis	Implementar posibles soluciones para alcanzar una combinación eficiente y efectiva de pasos y recursos.
Automatización	Soluciones, a través del pensamiento algorítmico.
Generalización y Transferencia	Transferir el proceso de resolución a problemas distintos.

Discriminate
Classify
Decide
Solve problems
Reason
Generalise
Transfer
Understand ideas
Create
Emotion
Conversation
Common sense
Practical sense
Automation
Initiative
Learn
Analysis
Adapt
Abstraction



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NUEVOS CAMPOS

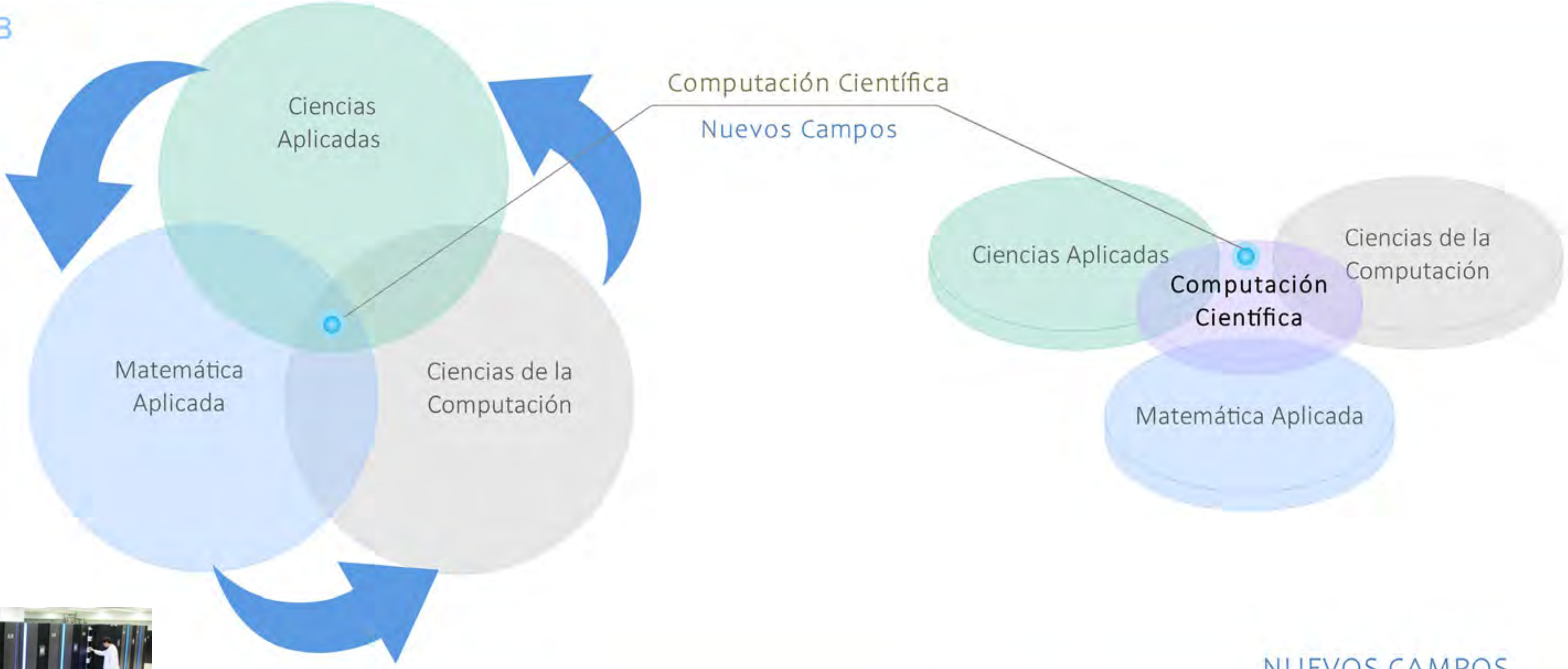
1. Química Computacional
2. Quimioinformatica
3. Biología Computacional
4. Bioinformática

MODELAMIENTO Y SIMULACIÓN COMPUTACIONAL

01 Modelamiento estocastico

02 Simulaciones Monte Carlo

03 Modelamiento de Sistemas dinámicos



NUEVOS CAMPOS

1 Química Computacional | 2 Químioinformatica | 3 Biología Computacional | 4 Bioinformática

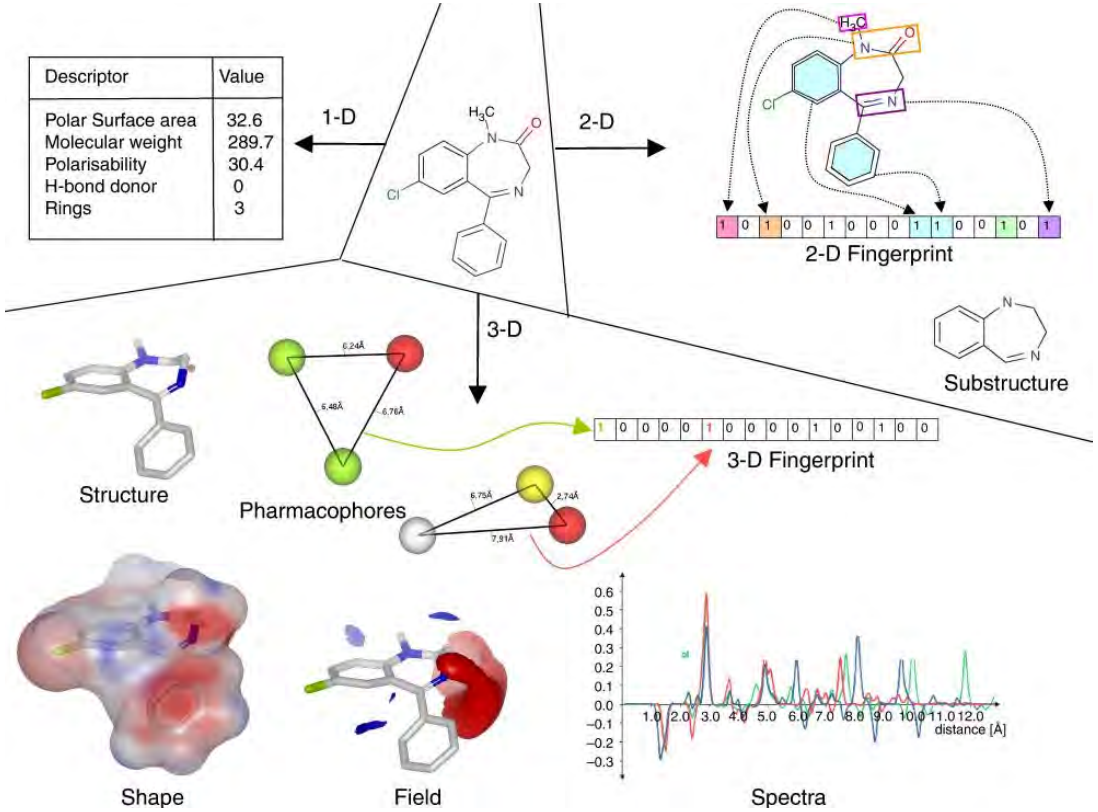
MODELAMIENTO Y SIMULACIÓN COMPUTACIONAL

01 Modelamiento estocastico | 02 Simulaciones Monte Carlo | 03 Modelamiento de Sistemas dinámicos

Computational Science

Computational Science serves as a learning tool or becomes a subject of learning. However, computational science in science classes requires not only devices and software in institutions and schools but also a good selection of concepts contextualized to authentic problems.

Molecular descriptors



Zero - dimensions (0D)

One - dimensional (1D)

Two - dimensional (2D)

Three - dimensional (3D)

Four - dimensions (4D)

"The final result of a logical and mathematical procedure, which transforms chemical information encoded within a symbolic representation of a molecule into a useful number or the result of some standardized experiment."

Todeschini R, Consonni V (2009) Molecular descriptors for chemoinformatics. Wiley-VCH, Weinheim

Rognan D. (2007). Chemogenomic approaches to rational drug design. *British journal of pharmacology*, *152*(1), 38–52. https://doi.org/10.1038/sj.bjp.0707307

TPASK Framework

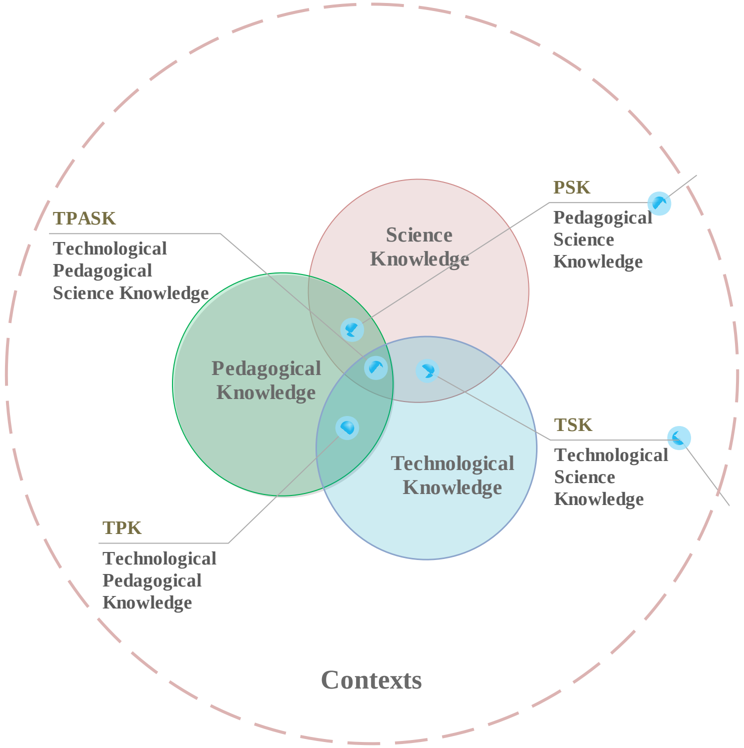


Figure. Venn diagrams representation for TPASK as an interdisciplinary endeavour connecting TK with PK and SK. ECC within technological pedagogical chemistry knowledge (TPAChK) adapted from the TPASK framework.

Chemistry Education
Research and Practice

ROYAL SOCIETY OF CHEMISTRY

PAPER

Developing technological pedagogical science knowledge through educational computational chemistry: a case study of pre-service chemistry teachers' perceptions†

Jorge Rodríguez-Becerra, Lizethly Cáceres-Jensen, Tatiana Díaz, Sofía Druker, Víctor Bahamonde Padilla, Johannes Pernaa and Maija Aksela

Rodríguez-Becerra, J., Cáceres-Jensen, L., Díaz, T., Druker, S., Bahamonde Padilla, V., Pernaa, J., & Aksela, M. **(2020).** Developing technological pedagogical science knowledge through educational computational chemistry: a case study of pre-service chemistry teachers' perceptions. *Chemistry Education Research and Practice, 21*(2), 638-654.

TPASK Framework

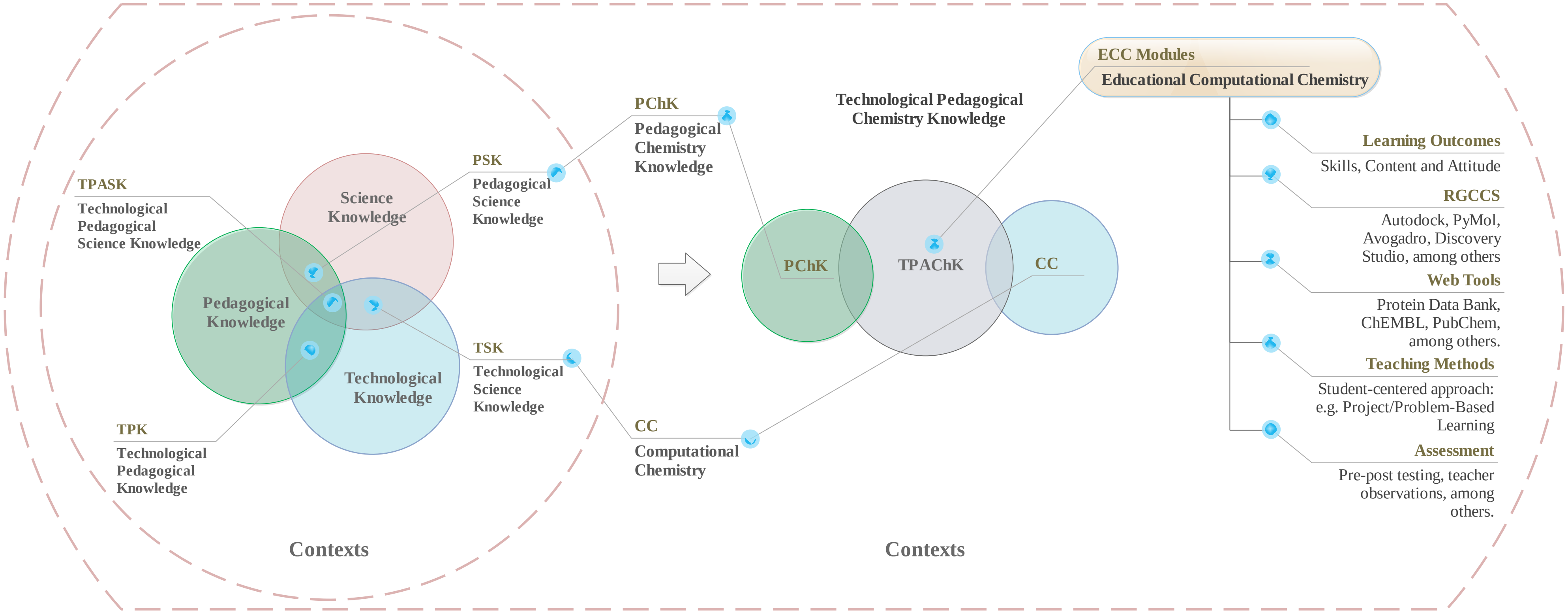


Figure. Venn diagrams representation for TPASK as an interdisciplinary endeavour connecting TK with PK and SK. ECC within technological pedagogical chemistry knowledge (TPAChK) adapted from the TPASK framework.

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TPASK: seven constructs of knowledge

- TK is how to use emerging technologies in a specific scientific domain.
- SK represents understanding the scientific community's models, protocols, practices, and products in science (Cáceres-Jensen et al., 2021).
- PK is the general knowledge about learning and teaching.
- PSK represents the understanding of models, protocols, practices and products of the science fields included in science education and how they can be used to implement learning environments that promote student learning. In addition, it consists of an understanding of students' construction of scientific knowledge in teaching contexts (Cáceres-Jensen et al., 2021).
- TSK represents the knowledge of how to use models and simulations to illustrate and apply scientific concepts using emerging technology, e.g., that linked to scientific computing (Rodríguez-Becerra et al., 2020).
- TPK is the knowledge about the possibilities and challenges involved in different ways of teaching and learning.
- TPASK understands how to use emerging science technology to implement learning environments that promote science learning in students (Rodríguez-Becerra et al., 2020).

Cáceres-Jensen, L., Rodríguez-Becerra, J., Jorquera-Moreno, B., Escudey, M., Druker-Ibañez, S., Hernández-Ramos, J., et al. (2021). Learning Reaction Kinetics through Sustainable Chemistry of Herbicides: A Case Study of Preservice Chemistry Teachers' Perceptions of Problem-Based Technology Enhanced Learning. *Journal of Chemical Education* 98(5), 1571-1582. doi: 10.1021/acs.jchemed.0c00557.

Rodríguez-Becerra, J., Cáceres-Jensen, L., Díaz, T., Druker, S., Bahamonde Padilla, V., Pernaa, J., et al. (2020). Developing technological pedagogical science knowledge through educational computational chemistry: a case study of pre-service chemistry teachers' perceptions. *Chemistry Education Research and Practice* 21(2), 638-654. doi: 10.1039/c9rp00273a.

Computational Chemistry: Teaching Challenges

Figure 1. Five main aspects of problem solving with CC tools construct the CC literacy.

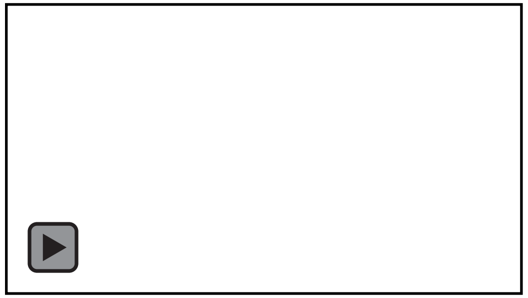

Figure 2. Teaching and learning challenges in implementing CC modules.

Tuvi-Arad, I. (2022). Computational Chemistry in the Undergraduate Classroom – Pedagogical Considerations and Teaching Challenges. *Israel Journal of Chemistry* 62(1-2), e202100042. doi: https://doi.org/10.1002/ijch.202100042.

Aim & Objectives

This High-performance computing is transforming both scientific discovery and science education. To explore its pedagogical potential, we embedded an Educational Computational Chemistry module—focused on computer-aided drug design for SARS-CoV-2—into a first-semester Physical Chemistry course for 20 pre-service chemistry teachers.

METHODOLOGY

Methodology

- This study employed a quantitative, cross-sectional design to examine the integrated technological, pedagogical, and scientific knowledge (TPASK) of pre-service chemistry teachers. Participants were enrolled in a physicochemistry course that integrated computational chemistry tools at a Chilean university, in a program that prepares secondary science teachers (chemistry, biology, physics, mathematics).

- A total of 20 participants from various semesters (4th to 8th) completed the study. The survey was administered digitally during class time with informed consent, adhering to ethical research protocols.

Methodology

- The instrument was designed based on the TPASK theoretical framework and consisted of 56 Likert-scale items. Each item was reviewed by field experts for content validity and piloted with a small sample (n = 5) for clarity and reliability prior to full deployment.

- Data analysis was performed using SPSS and Python. Reliability was evaluated using Cronbach’s alpha for each domain. Descriptive statistics (means, standard deviations) were calculated for all constructs. Exploratory Factor Analysis (EFA) was conducted to assess construct validity. Regression analysis identified predictors of TPASK, while Baron and Kenny’s mediation framework and Sobel tests were applied to test indirect effects. Interaction terms were examined to explore potential moderating relationships. Finally, cluster analysis using K-means and Principal Component Analysis (PCA) was used to identify learner profiles based on knowledge scores across constructs.

The UMCE pre-service Chemistry Teacher

- During this course, students will learn to apply physicochemical knowledge (thermodynamic) and some of the tools of computational chemistry and chemoinformatics to understand current research topics in medical and environmental chemistry.
- After this course, students will gain experience in authentic practical research micro-projects in socio-scientific problems from a perspective that integrates chemical and computational knowledge. Their proposals can be used as opportunities for developing chemical knowledge and scientific skills in the school context.

<table>
<tr><th></th><th colspan="2">PHYSICAL CHEMISTRY QUI6048</th></tr>
<tr><td>Lectures</td><td colspan="2">Mondays 16:15 – 17:45 and 18:00 -19:30.</td></tr>
<tr><td>Periodic Labs</td><td colspan="2">Tuesday and Thursday 9:45 - 11:15 AM and 11:30 - 13:00 AM.</td></tr>
<tr><td rowspan="2">Learning core</td><td colspan="2">Modelling drug-type compounds of interest to human health: introduction to Computational Methods in the discovery of compounds for treating diseases.</td></tr>
<tr><td colspan="2">Introduction to QSAR Modeling: chemical compounds of interest to human health and the environment.</td></tr>
<tr><td>Pedagogical Strategy</td><td colspan="2">Direct Instruction; Hands-On Computational Learning; Problem-based Learning</td></tr>
<tr><td>Instruction Model</td><td colspan="2">Blended learning</td></tr>
<tr><td rowspan="4">Module resources</td><td>Digital Resources</td><td>Websites of interest</td></tr>
<tr><td>- WHO. Coronavirus disease outbreak 2019.
- Center for Systems Science and Engineering (CSSE) at Johns Hopkins University. COVID-19 Dashboard.
- Novel Coronavirus Resource Directory.</td><td>https://www.who.int/es/emergencies/diseases/novel-coronavirus-2019
https://bit.ly/2PMY0eN
https://www.elsevier.com/novel-coronavirus-covid-19</td></tr>
<tr><td>Databases
- DrugBank
- Pubchem
- ChEBML
- Protein Data Bank</td><td>https://go.drugbank.com
https://pubchem.ncbi.nlm.nih.gov
https://www.ebi.ac.uk/chembl
https://www.rcsb.org</td></tr>
<tr><td>Research Grade Scientific Software
- Avogadro
- AutoDock
- MglTools
- Discovery Studio Visualizer</td><td>https://avogadro.cc
http://autodock.scripps.edu/downloads/autodock-registration/autodock-4-2-download-page
http://mgltools.scripps.edu
https://discover.3ds.com/discovery-studio-visualizer-download</td></tr>
</table>

Subject matter courses

- Pedagogical training
  - Pedagogy and teacher professional identity
  - Communicative skills
  - Sociocultural contexts of educational processes
  - Critical and philosophical reflection of educational processes
  - Psychology of learning and educational transformation
  - Public education policies
  - Paradigms, theories and contemporary approaches in education
  - Educational curriculum
  - Educational evaluation
  - Curriculum management and innovation
  - Didactic project
  - Orientation and educational coexistence
  - Learning communities
- Pedagogical Practice training
  - Practice I
  - Practice II
  - Practice III
  - Professional Practice

- Chemistry training
  - General Chemistry I and II
  - Inorganic Chemistry I and II
  - Organic Chemistry I and II
  - Analytical Chemistry I and II
  - Physical chemistry I and II
  - Chemical bond theory I and II
  - Biochemistry
  - Instrumental methods of analysis
  - Education and energy

Didactics of science
Epistemological foundations of science
Fundamentals of learning science
Introduction to learning science
Strengthening scientific skills
Psychological Foundation of Science Learning
Math I, II and III
Physical I and II
Biology
Second language I and II
Specialty I, II, III and IV
Elective course I and II
Applied computing
Investigation methodology I and II
Didactics of chemistry
Strengthening graduation skills I and II

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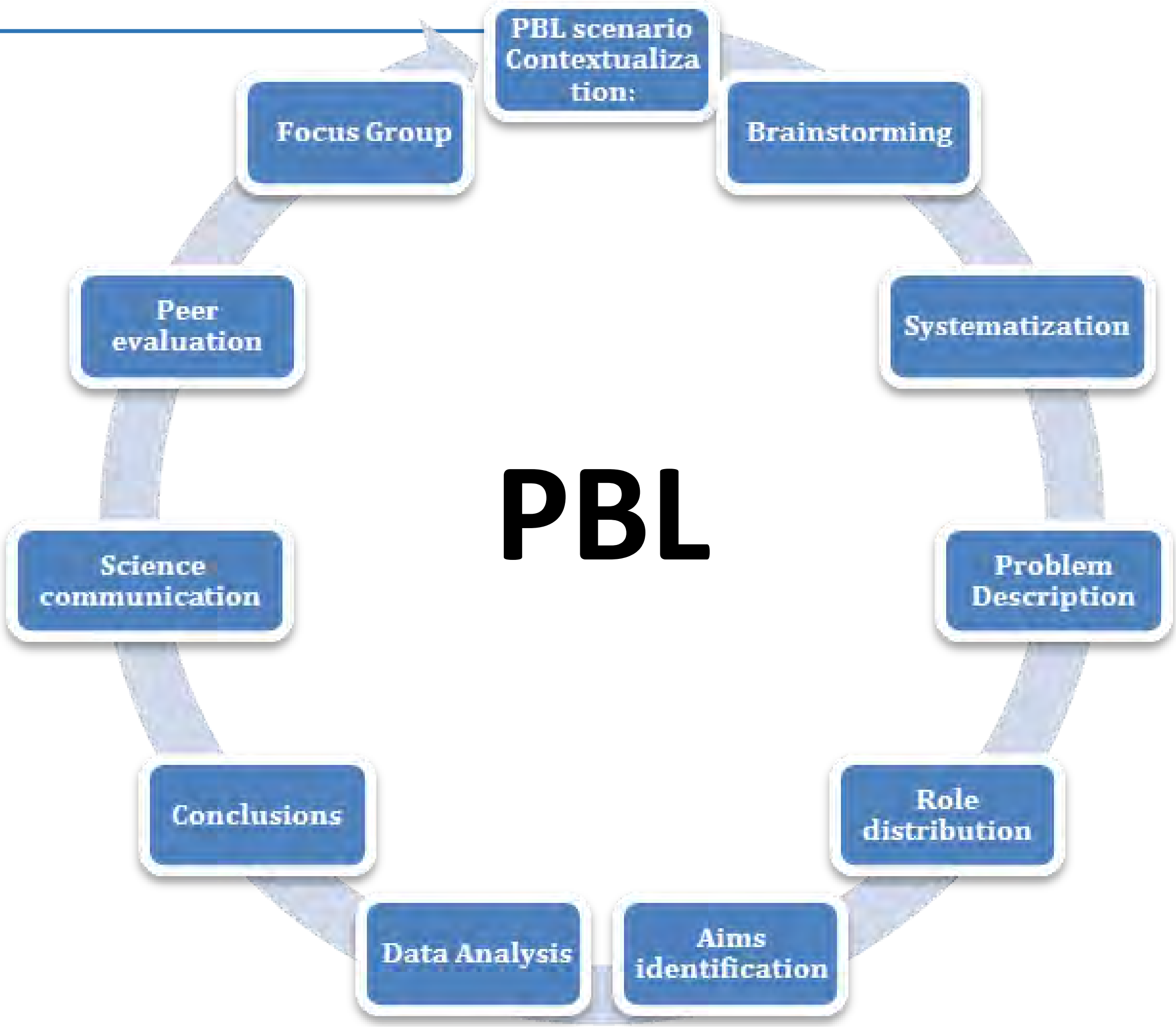
RESULTS AND DISCUSSION

Module implementation



Module implementation

The PBL scenario propose to the students the challenge of:

"Can one or more of the FDA-approved compounds proposed by Singh and Florez (2020) be identified as plausible inhibitors of the SARS-CoV-2 main protease (PDB ID: 6LZE), and how can computational evidence support this hypothesis?"

Module implementation

SCENARIO: REQUIREMENT OF THE WORLD HEALTH ORGANIZATION ON COVID-19

The COVID-19 pandemic, caused by the novel coronavirus SARS-CoV-2, emerged in Wuhan, China in late 2019 and quickly became a global health crisis. Declared a pandemic by the World Health Organization (WHO) on March 11, 2020, this disease has highlighted the urgent need for effective therapeutic solutions. The virus gains entry into human cells via the ACE2 receptor, which is expressed in several organs, including the lungs and gastrointestinal tract. A key viral enzyme, the main protease (Mpro)—specifically identified as PDB ID: 6LZE—has been recognized as a promising drug target due to its central role in viral replication and transcription. In this problem-based learning (PBL) scenario, pre-service chemistry teachers will take on the role of computational drug designers. Drawing on research by Dai et al. (2020), who identified potent Mpro inhibitors, and Singh and Florez (2020), who proposed 20 FDA-approved drugs as potential antivirals using PDB ID: 6M03, students are tasked with evaluating whether these same 20 compounds (see Table 1) might inhibit 6LZE. Students will access the PubChem database to retrieve compound data, apply Lipinski's Rule of Five (RO5) to filter for drug-likeness, and use molecular docking tools (e.g., AutoDock Vina) to simulate interactions between each compound and the Mpro active site. Students will then analyse docking scores, binding affinities, and key interactions, integrating this with existing literature to construct a scientifically grounded argument.

DRIVING QUESTION:

Can one or more of the FDA-approved compounds proposed by Singh and Florez (2020) be identified as plausible inhibitors of the SARS-CoV-2 main protease (PDB ID: 6LZE), and how can computational evidence support this hypothesis?

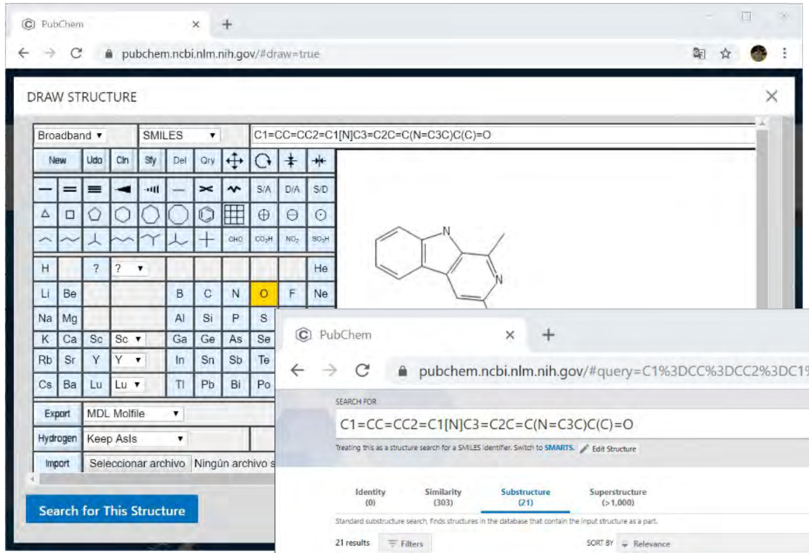
LEARNING OBJECTIVES:

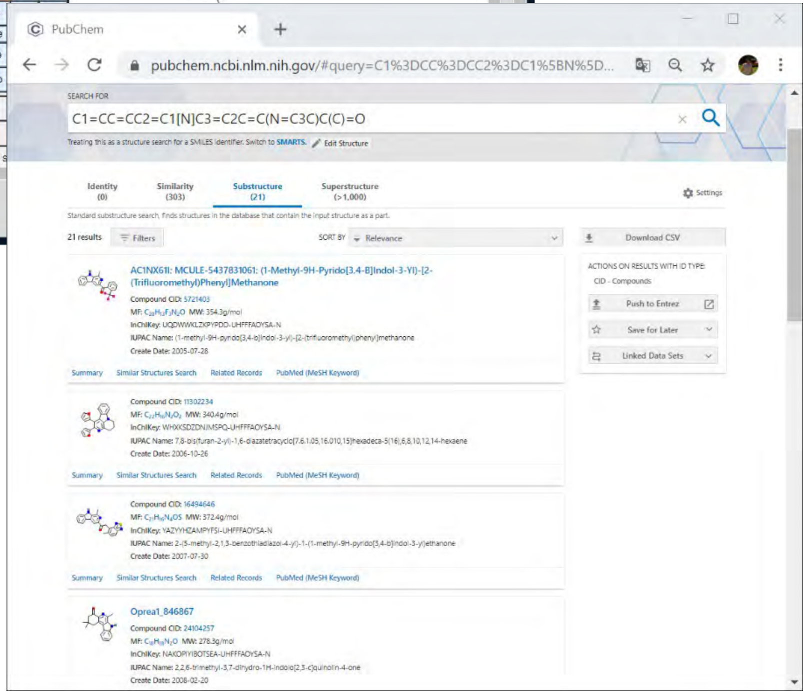
- Develop inquiry and problem-solving skills using real-world, interdisciplinary contexts.
- Apply computational tools to evaluate molecular interactions in drug discovery.
- Interpret and critique docking simulations within the framework of medicinal chemistry.
- Reflect on the role of chemoinformatics in addressing global health challenges.

STEM INTEGRATION:

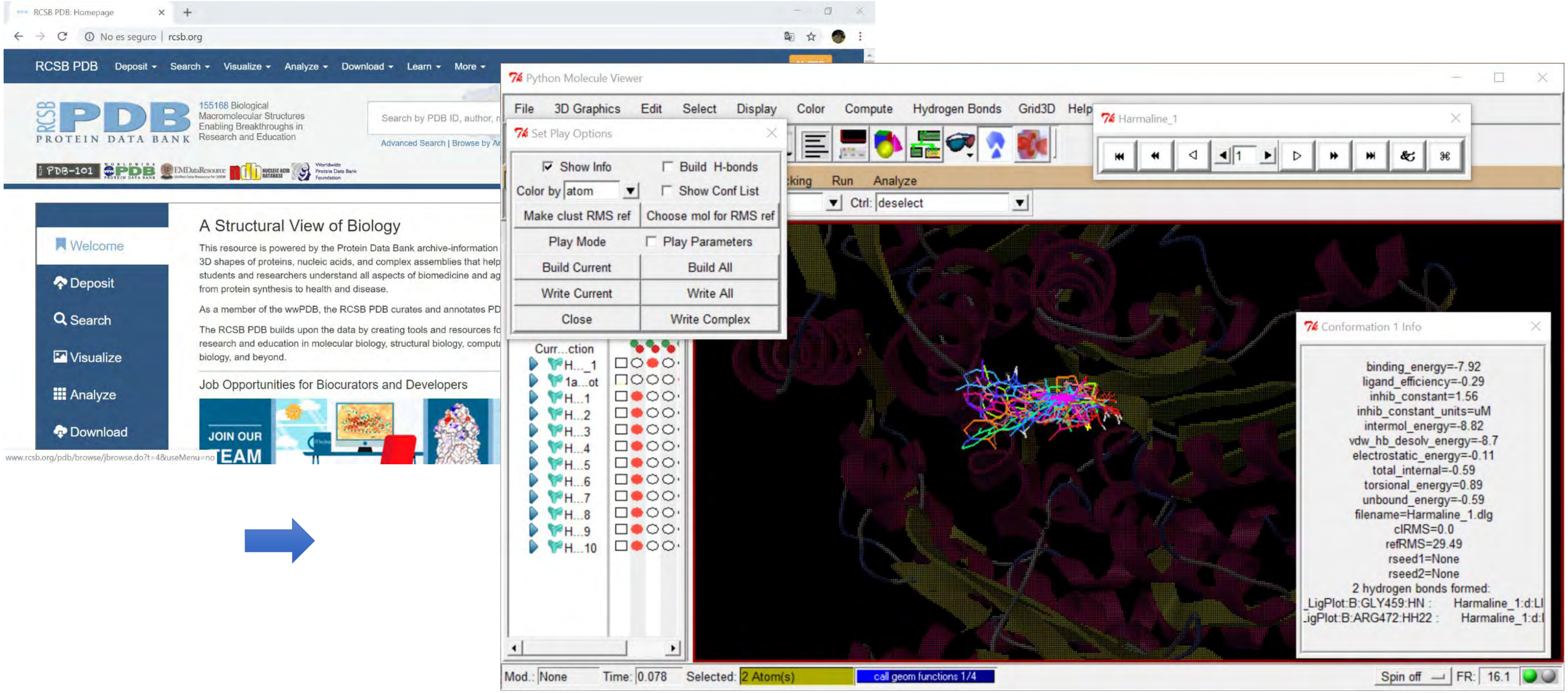
This scenario merges core principles from chemistry, biology, informatics, and technology, reinforcing TPASK competencies through authentic scientific practice. The project culminates in the design of a digital scientific poster or video presentation summarizing each team's findings, supported by PubChem identifiers, 3D visualisations, and structure-activity arguments.

Figure 1. The crystal structure of COVID-19 main protease in complex with an inhibitor.





Module implementation



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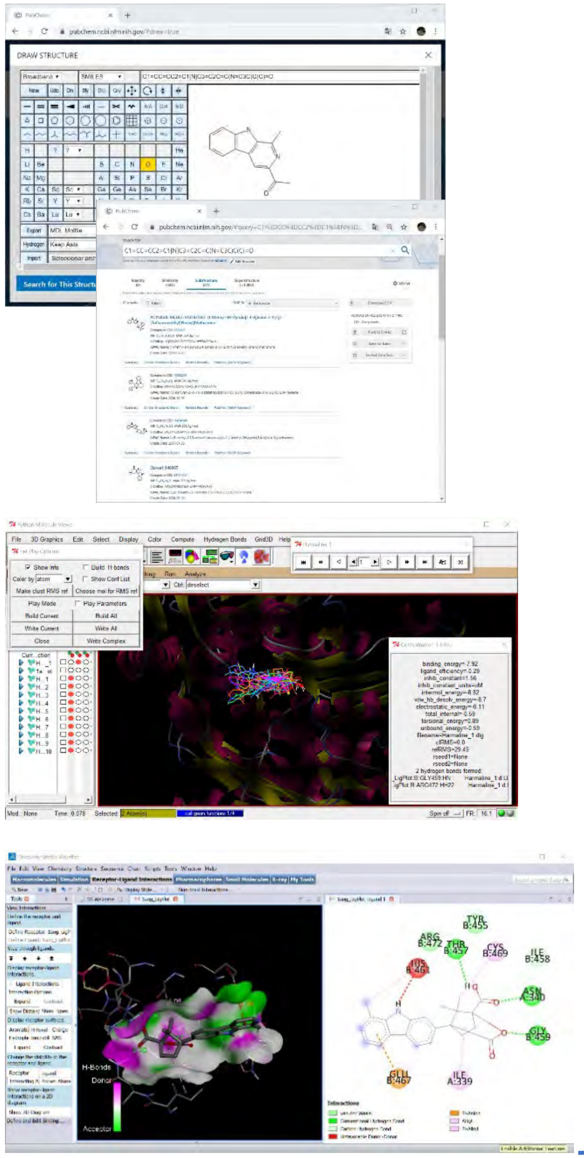

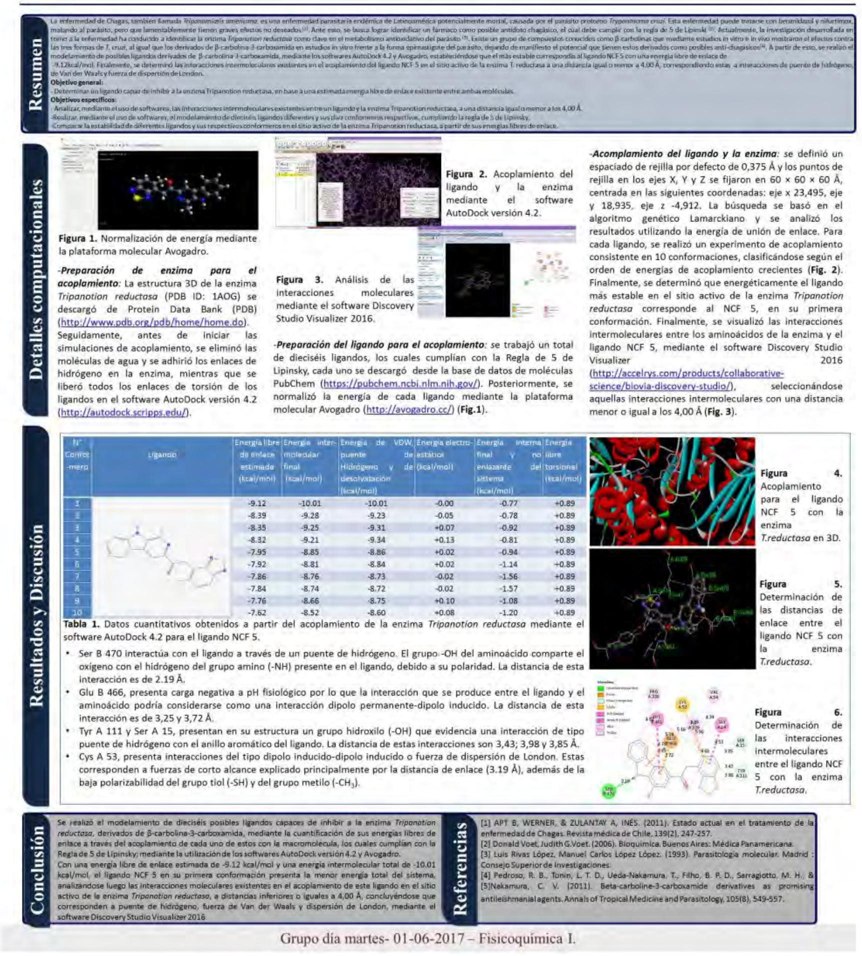

Resumen

La enfermedad de Chagas, también llamada *Tripanomiasis americana*, es una enfermedad parasitaria endémica de Latinoamérica potencialmente mortal, causada por el parásito protozoo *Trypanosoma cruzi*. Esta enfermedad puede tratarse con benznidazol y nifurtimox, matando al parásito, pero que lamentablemente tienen graves efectos no deseados[1]. Ante esto, se busca lograr identificar un fármaco como posible antídoto chagásico, el cual debe cumplir con la regla de 5 de Lipinski [2]. Actualmente, la investigación desarrollada en torno a la enfermedad ha conducido a identificar la enzima *Tripanotion reductasa* como clave en el metabolismo antioxidativo del parásito [3]. Existe un grupo de compuestos conocidos como β-carbolinas que mediante estudios in vitro e in vivo mostraron el efectos contra las tres formas de *T. cruzi*, al igual que los derivados de β-carbolina-3-carboxamida en estudios in vitro frente a la forma epimastigote del parásito, dejando de manifiesto el potencial que tienen estos derivados como posibles anti-chagásicos[4]. A partir de esto, se realizó el modelamiento de posibles ligandos derivados de β-carbolina-3-carboxamida, mediante los softwares AutoDock 4.2 y Avogadro, estableciéndose que el más estable correspondía al ligando NCF 5 con una energía libre de enlace de -9,12kcal/mol. Finalmente, se determinó las interacciones intermoleculares existentes en el acoplamiento del ligando NCF 5 en el sitio activo de la enzima T. reductasa a una distancia igual o menor a 4,00 Å, correspondiendo estas a interacciones de puente de hidrógeno, de Van der Waals y fuerza de dispersión de London.

Objetivo general:
- Determinar un ligando capaz de inhibir a la enzima Tripanotion reductasa, en base a una estimada energía libre de enlace existente entre ambas moléculas.

Objetivos específicos:
- Analizar, mediante el uso de softwares, las intreracciones intermoleculares existentes entre un ligando y la enzima Tripanotion reductasa, a una distancia igual o menor a los 4,00 Å.
-Realizar, mediante el uso de softwares, el modelamiento de dieciséis ligandos diferentes y sus diez conformeros respectivos, cumpliendo la regla de 5 de Lipinsky.
-Comparar la estabilidad de diferentes ligandos y sus respectivos conformeros en el sitio activo de la enzima Tripanotion reductasa, a partir de sus energías libres de enlace.

Detalles computacionales

Figura 1. Normalización de energía mediante la plataforma molecular Avogadro.

-***Preparación de enzima para el acoplamiento***: La estructura 3D de la enzima *Tripanotion reductasa* (PDB ID: 1AOG) se descargó de Protein Data Bank (PDB) (http://www.pdb.org/pdb/home/home.do). Seguidamente, antes de iniciar las simulaciones de acoplamiento, se eliminó las moléculas de agua y se adhirió los enlaces de hidrógeno en la enzima, mientras que se liberó todos los enlaces de torsión de los ligandos en el software AutoDock versión 4.2 (http://autodock.scripps.edu/).

Figura 2. Acoplamiento del ligando y la enzima mediante el software AutoDock versión 4.2.

Figura 3. Análisis de las interacciones moleculares mediante el software Discovery Studio Visualizer 2016.

-***Preparación del ligando para el acoplamiento***: se trabajó un total de dieciséis ligandos, los cuales cumplían con la Regla de 5 de Lipinsky, cada uno se descargó desde la base de datos de moléculas PubChem (https://pubchem.ncbi.nlm.nih.gov/). Posteriormente, se normalizó la energía de cada ligando mediante la plataforma molecular Avogadro (http://avogadro.cc/) (**Fig.1**).

-***Acomplamiento del ligando y la enzima***: se definió un espaciado de rejilla por defecto de 0,375 Å y los puntos de rejilla en los ejes X, Y y Z se fijaron en 60 × 60 × 60 Å, centrada en las siguientes coordenadas: eje x 23,495, eje y 18,935, eje z -4,912. La búsqueda se basó en el algoritmo genético Lamarckiano y se analizó los resultados utilizando la energía de unión de enlace. Para cada ligando, se realizó un experimento de acoplamiento consistente en 10 conformaciones, clasificándose según el orden de energías de acoplamiento crecientes (**Fig. 2**). Finalmente, se determinó que energéticamente el ligando más estable en el sitio activo de la enzima *Tripanotion reductasa* corresponde al NCF 5, en su primera conformación. Finalmente, se visualizó las interacciones intermoleculares entre los aminoácidos de la enzima y el ligando NCF 5, mediante el software Discovery Studio Visualizer 2016 (http://accelrys.com/products/collaborative-science/biovia-discovery-studio/), seleccionándose aquellas interacciones intermoleculares con una distancia menor o igual a los 4,00 Å (**Fig. 3**).

Resultados y Discusión

N° Confor-mero	Ligando	Energía libre de enlace estimada (kcal/mol)	Energía inter-molecular final (kcal/mol)	Energía de VDW, puente de Hidrógeno y de desolvatación (kcal/mol)	Energía electro-estáticos (kcal/mol)	Energía interna final y no enlazante del sistema (kcal/mol)	Energía libre torsional (kcal/mol)
1		-9.12	-10.01	-10.01	-0.00	-0.77	+0.89
2		-8.39	-9.28	-9.23	-0.05	-0.78	+0.89
3		-8.35	-9.25	-9.31	+0.07	-0.92	+0.89
4		-8.32	-9.21	-9.34	+0.13	-0.81	+0.89
5		-7.95	-8.85	-8.86	+0.02	-0.94	+0.89
6		-7.92	-8.81	-8.84	+0.02	-1.14	+0.89
7		-7.86	-8.76	-8.73	-0.02	-1.56	+0.89
8		-7.84	-8.74	-8.72	-0.02	-1.57	+0.89
9		-7.76	-8.66	-8.75	+0.10	-1.08	+0.89
10		-7.62	-8.52	-8.60	+0.08	-1.20	+0.89

Tabla 1. Datos cuantitativos obtenidos a partir del acoplamiento de la enzima *Tripanotion reductasa* mediante el software AutoDock 4.2 para el ligando NCF 5.

- Ser B 470 interactúa con el ligando a través de un puente de hidrógeno. El grupo -OH del aminoácido comparte el oxígeno con el hidrógeno del grupo amino (-NH) presente en el ligando, debido a su polaridad. La distancia de esta interacción es de 2.19 Å.
- Glu B 466, presenta carga negativa a pH fisiológico por lo que la interacción que se produce entre el ligando y el aminoácido podría considerarse como una interacción dipolo permanente-dipolo inducido. La distancia de esta interacción es de 3,25 y 3,72 Å.
- Tyr A 111 y Ser A 15, presentan en su estructura un grupo hidroxilo (-OH) que evidencia una interacción de tipo puente de hidrógeno con el anillo aromático del ligando. La distancia de estas interacciones son 3,43; 3,98 y 3,85 Å.
- Cys A 53, presenta interacciones del tipo dipolo inducido-dipolo inducido o fuerza de dispersión de London. Estas corresponden a fuerzas de corto alcance explicado principalmente por la distancia de enlace (3.19 Å), además de la baja polarizabilidad del grupo tiol (-SH) y del grupo metilo ($-CH_3$).

Figura 4. Acoplamiento para el ligando NCF 5 con la enzima *T.reductasa* en 3D.

Figura 5. Determinación de las distancias de enlace entre el ligando NCF 5 con la enzima *T.reductasa*.

Figura 6. Determinación de las interacciones intermoleculares entre el ligando NCF 5 con la enzima *T.reductasa*.

Conclusión

Se realizó el modelamiento de dieciséis posibles ligandos capaces de inhibir a la enzima *Tripanotion reductasa*, derivados de β-carbolina-3-carboxamida, mediante la cuantificación de sus energías libres de enlace a través del acoplamiento de cada uno de estos con la macromolécula, los cuales cumplían con la Regla de 5 de Lipinsky; mediante la utilización de los softwares AutoDock versión 4.2 y Avogadro.
Con una energía libre de enlace estimada de -9.12 kcal/mol y una energía intermolecular total de -10.01 kcal/mol, el ligando NCF 5 en su primera conformación presenta la menor energía total del sistema, analizándose luego las interacciones moleculares existentes en el acoplamiento de este ligando en el sitio activo de la enzima *Tripanotion reductasa*, a distancias inferiores o iguales a 4,00 Å, concluyéndose que corresponden a puente de hidrógeno, fuerza de Van der Waals y dispersión de London, mediante el software Discovery Studio Visualizer 2016.

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Descriptive Statistics and Reliability

- *Descriptive statistics revealed moderately high self-perceptions across all TPASK domains.*
- *Technological Knowledge (TK) exhibited the highest mean (M = 3.97, SD = 0.30), followed by Scientific Knowledge (SK) and Technological Pedagogical Knowledge (TPK). This trend suggests a student cohort that feels confident with digital tools and scientific content knowledge, though slightly less confident in integrating these into pedagogical strategies.*
- *Reliability analysis using Cronbach's alpha indicated excellent internal consistency across constructs, with all values exceeding α = 0.82, supporting the reliability of the instrument.*

Descriptive Statistics and Reliability

- *A multiple regression model predicting TPASK from PK, SK, TK, PSK, TSK, and TPK showed excellent model fit ($R^2 = 0.934$, $p < .001$).*
- *Significant predictors included:*
  - *TPK ($\beta = 0.645$, $p < .001$): the strongest predictor.*
  - *TK ($\beta = 0.254$, $p = .003$): a meaningful but smaller contributor.*
  - *PK ($\beta = -0.156$, $p = .049$): a small but negative association.*

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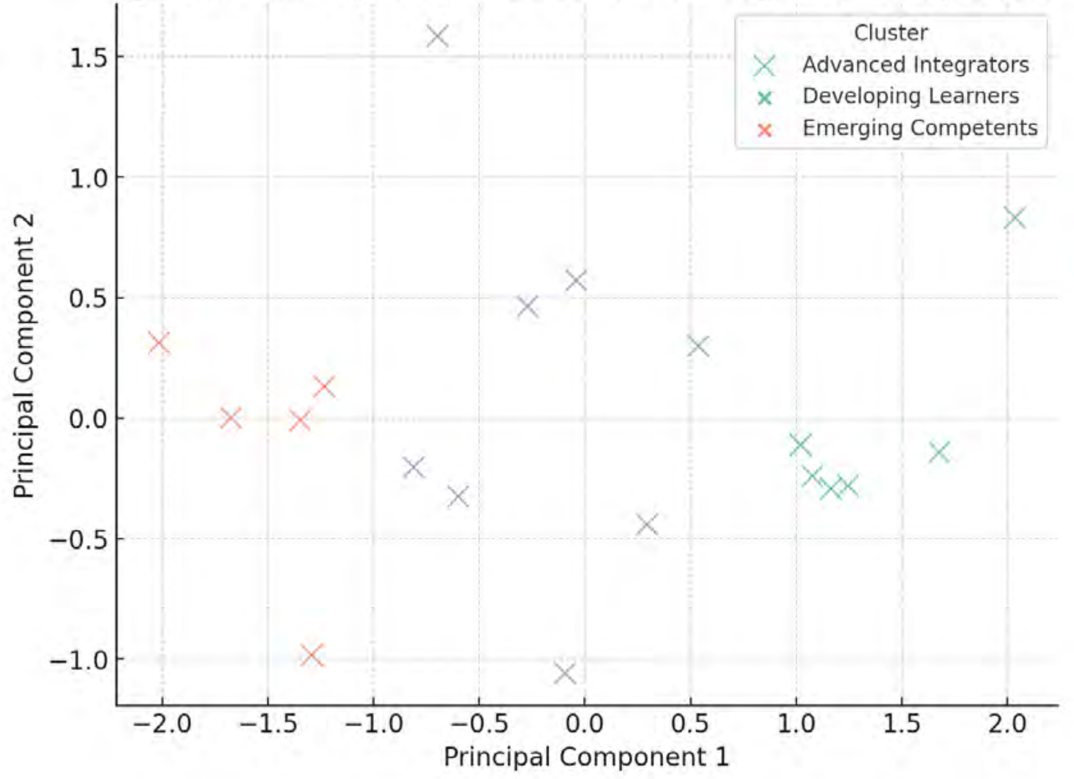
Cluster Analysis

K-means clustering and PCA dimensionality reduction revealed three distinct knowledge profiles among students:

- *Profile 0: Advanced Integrators – high across all domains (e.g., TK = 4.69, TPASK = 4.08).*
- *Profile 1: Developing Learners – lowest in all domains (e.g., SK = 3.16, TPASK = 2.97).*
- *Profile 2: Emerging Competents – moderate levels (e.g., TK = 3.75, TPASK = 3.63).*

Figure 1. PCA Projection of Student Knowledge Profiles by Cluster



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CONCLUSION

Conclusion

- *The Central Role of TPK*
  - *The finding that **TPK is both the strongest predictor and a significant mediator** in TPASK development reinforces the idea that pre-service teachers must go beyond acquiring tools or content knowledge. They must be explicitly taught how to **design, adapt, and evaluate pedagogical strategies** that leverage technology to teach science meaningfully.*

Conclusion

- *Limited Influence of PK and SK*
  - *The weak or negative role of general **Pedagogical Knowledge (PK),** and the nonsignificant role of **Scientific Knowledge (SK),** suggest that competence in TPASK cannot be inferred from strength in these domains alone. Instead, what appears to matter most **is the degree to which pedagogical and technological skills** are blended—a call to restructure how we think about and design teacher preparation curricula.*

Conclusion

- *Implications for Chemistry Teacher Education*

  These findings suggest that teacher education programs should:

  - *Explicitly teach* ***TPK and TPASK*** *through* ***scenario-based learning, interdisciplinary problem-solving, and computational tool immersion****.*
  - *Assess students not only on disciplinary understanding but on their ability to* ***design and justify technology-enhanced learning experiences****.*
  - *Use cluster-based profiling to adapt instruction in real time, ensuring* ***equity in readiness and opportunities for growth.***

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