Adrián Gallardo Loya

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Education

UNIVERSIDAD NACIONAL AUTÓNOMA DE MÉXICO CU, CDMX, México
FACULTAD DE QUÍMICA (FQ-UNAM)
Bachelor of Science in Chemistry *Expected Mar 2026*

Relevant coursework: Chemoinformatics for Drug Development (graduate program, 9/10), Solid State Chemistry (10/10), Organic Chemistry V (10/10), Research Work I (10/10), Seminar I (9/10), Optimization and Synthesis Processes (10/10), Experimental Analytical Chemistry III (10/10), Biochemistry (9/10), Instrumental Analytical Chemistry II (9/10), Organometallic Chemistry (8/10), Unified Physical Chemistry Lab (10/10), Coordination Chemistry (9/10), Scientific Communication (10/10).

Publications

[1] G. S. Anaya González, **A. Gallardo Loya**, E. Vázquez Aguilar, M. Flores Álamo, L. Martínez-dlCruz, M. Romero Ávila, D. Solis-Ibarra, N. E. Magaña-Vergara, N. Farfán, and J. Rodríguez-Romero, "Synthesis, phase transition, and band gap analysis of $MorpH_3PbI_5$ perovskite", *Journal of Solid State Chemistry*, vol. 350, 125521, 2025, DOI: 10.1016/j.jssc.2025.125521.

[2] Work in progress: **A. Gallardo Loya**, E. Mayoral-Villa, and A. R. García Márquez, "High-throughput virtual screening of primary ammonium iodide compounds with potential liquid crystalline properties using density functional theory"

Main Research Experience

García Márquez Group | FQ-UNAM Dpt. of Inorganic and Nuclear Chem. CU, CDMX, México
Computational Modeling of Materials (Research Work II and Seminar II) *Aug 2025 – Present*

- Identifying structure-activity relationships that enable the **rational design of liquid crystal ammonium salts as perovskite components**.
- Performing electronic structure calculations of molecular and material systems using Density Functional Theory (DFT) to predict optoelectronic properties and stability.
- Designing computational workflows to extract and analyze physicochemical information from modeling pipelines, enabling reproducible and **data-driven materials discovery**.

Rodríguez Romero Group | FQ-UNAM Department of Organic Chemistry CU, CDMX, México
Energy Materials Chemistry (Main Research Group) ***Mar 2021 – Jul 2025***

- **Co-authored a publication in Journal of Solid State Chemistry** by developing mechanochemical protocols to selectively synthesize and characterize different hybrid perovskite phases.
- Conducted comprehensive instrumental characterization using NMR, single-crystal X-ray diffraction, FTIR, elemental analysis, UV-vis spectroscopy, fluorescence spectroscopy, thermogravimetric analysis, four-point probe conductivity, and contact-angle goniometry.
- Built an internal 1D–2D perovskite database to identify structural trends and enable materials informatics approaches for the rational design of future hybrid materials.
- Fabricated perovskite thin films via spin-coating on indium–tin oxide (ITO) substrates, optimizing film morphology for optoelectronic device integration.
- Synthesized and purified organic and inorganic precursors, including amines and high-purity halide salts.
- Studied crystal structures using Mercury (CSD) and VESTA, generating publication-quality crystallographic figures and analyzing intermolecular-force interactions.
- Designed and 3D-printed custom spectroscopic adapters and chemically-resistant substrate holders to enable precise thin-film characterization and optimize device fabrication workflows.

Additional Research and Research Internships

Group for Molecular Chemistry and Precursors Research | UNAH Tegucigalpa, FM, Honduras
Rational Pesticide Design (Junior Researcher, Remote Collaboration) *Oct 2025 – Present*

- Classifying molecules which inhibit a certain target enzyme in order to write a **review paper for publication**.
- Creating a database of this target's inhibitors, for use in **rational pesticide design**.
- Enumerating compounds for high throughput virtual screening to identify pesticide candidates with desirable ADME-Tox properties.

Martínez Mayorga Group | UNAM Institute of Chemistry at Merida Mérida, Yucatán, México
Chemoinformatic Database Exploration (Research Work I and Seminar I) *Feb 2025 – Jul 2025*

- Engineered automated curation pipelines using Python and RDKit to audit and standardize structural data for over 600 natural products, **establishing quality control protocols for the DiaNat-DB project**.
- Developed high-throughput algorithms to homologate molecular identifiers (SMILES to InChI) and integrate internal datasets with public repositories (ChEMBL, PubChem) via API querying, significantly improving data interoperability.
- Deployed a Python-based pipeline to query the ChEMBL API, systematically retrieving and standardizing inhibition data for over 600 substances across 30+ Type II diabetes-related targets.
- Performed chemoinformatic analyses, utilizing molecular fingerprints, similarity metrics, and Principal Component Analysis (PCA) to map the chemical space and identify structure-activity relationships for Type II diabetes targets.

Juaristi Group | Cinvestav-IPN Department of Chemistry Zacatenco, CDMX, México
Asymmetric Organocatalysis and Biocatalysis (Introductory Internship) *Jan 2024 – Feb 2024*

- Conducted asymmetric syntheses of steroidal intermediates, exploring organocatalytic and biocatalytic strategies for stereoselective transformations.
- Applied radial chromatography and spectroscopic methods to purify and characterize reaction products.
- Gained foundational insight into reaction mechanisms, stereochemical control, and the physicochemical principles underlying catalytic systems.
- Investigated mechanochemical approaches such as high-speed ball milling as green alternatives to conventional solution-phase reactions.

Romero Avila Group | FQ-UNAM Department of Organic Chemistry CU, CDMX, México
Synthetic Organic Chemistry (As International Chemistry Olympiad Training) *Jan 2020 – Mar 2020*

- Performed palladium-catalyzed C–C coupling reactions to synthesize organic dyes tailored for dye-sensitized solar cell (DSSC) applications.
- Gained experience in 2D NMR interpretation, structural elucidation, and chromatographic purification of reaction products.
- Explored the design of aromatic heterocycles and computational modeling of π-π stacking interactions to understand optoelectronic behavior.
- Utilized chemical databases (Reaxys, SciFinder, PubChem) for reaction planning and literature-based experiment design.

Ariza Castolo Group | Cinvestav Department of Chemistry Zacatenco, CDMX, México
Synthetic Organic Chemistry (Introductory Internship) *Oct 2019 – Nov 2019*

- Researched reaction conditions for imine synthesis and reduction to secondary amines, emphasizing selectivity and yield optimization.
- Gained practical experience with nuclear magnetic resonance (NMR) for structural verification and reaction monitoring.
- Explored dry and wet mechanochemical pathways as green alternatives for organic synthesis, establishing early interest in sustainable reaction methodologies.

Presentations

[1] **A. Gallardo Loya**, "Classification Models for Anti-Diabetic Agents of Natural Origin". Seminar presented for the First Seminar Course (1804); February-May 2025; UNAM, Mexico City, Mexico.

[2] R. Téllez Saucedo, A. R. Santiago Jiménez, and **A. Gallardo Loya**, "Foamy & Fizzy Delight: Evaluating Beer Heads by Measuring Foam Stability and Bubble Size". Poster presented during the Unified Physical Chemistry Laboratory Course (1703); December 2024; UNAM, Mexico City, Mexico.

[3] **A. Gallardo Loya**, "Synthesis and Characterization of Mono-Dimensional Hybrid Perovskites". Poster presented at the UNAM's Short Research Internships Program Exposition; October 2023; Coyoacán, Mexico City, Mexico.

[4] M. Aguilera and **A. Gallardo Loya**, "Lecture on Inter-Molecular Forces". Lecture presented at the Honduran Chemistry Olympiad; October 2022; Departmental Institute Alvaro Contreras, Santa Rosa de Copán, Honduras.

[5] J. García Ponce, **A. Gallardo Loya**, H. Tovar Salazar, R. Espadas and R. Herrera, "Obtaining Adhesives from Natural Precursors". Oral presentation delivered during the National Chemistry Week's event organized by the American Chemical Society's International Student Chapter at UNAM; November 2020; Mexico City, Mexico.

Teaching Experience

Honduran Chemistry Olympiad | Honduran Secretary of Education Tegucigalpa, FM, Honduras
Secretary, Director of Training, and Organic Chemistry Tutor *Jul 2021 – Present*

- Mentor students who achieved **Gold medals** and **best theoretical exams** at the Central American and Caribbean Chemistry Olympiad (OCACQ), and **Silver medals** at the Ibero American Chemistry Olympiad (OIAQ).
- Designed and **authored over 30 selection exams** tailored to regional educational contexts, ensuring accessibility while maintaining rigorous academic standards.
- Lead and coordinate a team of subject-area tutors to prepare the national delegation for international competitions, including the International Chemistry Olympiad (IChO), Mendeleev Olympiad, OIAQ, and OCACQ.
- Design and supervise comprehensive training curricula covering physical, inorganic, organic, analytical, and biochemistry, as well as advanced modules in organometallic chemistry, solid-state chemistry, catalysis, and related topics.
- Deliver weekly lectures and problem-solving sessions in organic chemistry, emphasizing molecular orbital theory, stereochemistry, conformational and mechanistic approaches.
- Mentor high-performing students through individualized instruction and advanced topic tutorials, fostering independent research skills and conceptual depth.
- Coordinate the annual national and regional chemistry competitions, overseeing logistics, test design, and the training camp for students representing Honduras at international Olympiads.
- Develop and maintain the official Olympiad website, improving communication, transparency, and outreach for students and educators nationwide.

National Program of Science Olympiads | Senado de la República Tabacalera, CDMX, México
Chemistry Olympiad Tutor *Mar 2025 – Jun 2025*

- Selected to join a Senate-sponsored national program supporting Mexico's Science Olympiad initiatives across chemistry, physics, biology, mathematics, and informatics.
- Taught weekly introductory chemistry workshops for middle and high-school students nationwide, focusing on stoichiometry, molecular structure, and physical chemistry.
- Fostered analytical reasoning and problem-solving skills, contributing to the academic preparation of Mexico's future Olympiad representatives.

Extracurricular and Leadership Activities

Virtual Chemistry Contest | Ntnl. Association of Faculties and Schools of Chem. Online
Founder and Vice-president *Mar 2020 – Jan 2022*

- Founded and co-directed an international virtual chemistry competition **connecting over 7000 students across 20 Spanish-speaking countries**, with academic endorsement from Mexico's National Association of Faculties and Schools of Chemistry.
- Promoted critical thinking and scientific writing through thematic essay challenges evaluated by nationally recognized researchers.
- Launched the Wöhler Challenge of Organic Chemistry, a specialized event exploring modern organic reactions and spectroscopic phenomena, inspiring advanced learning beyond traditional curricula.

Awards and Honors

Short Research Internships Program - UNAM Facultad de Química 2023
Third place in the Chemistry and Materials Engineering category

Mexico's XXIII Ntnl. Mathematics Contest A. N. Kolmogórov - Universidad Anáhuac 2020
Finalist

Mexico's XXIX National Chemistry Olympiad - Academia Mexicana de Ciencias 2019-2020
National Selection Member (2020) Silver Medal (2019)

Skills

Computational Modeling and Software: Gaussian, ORCA, AlphaFold, use of bioinformatic modeling servers, density functional theory, molecular docking, VESTA, Mercury, QSAR model use and development, DataWarrior, RDKit, chemoinformatic database curation, Python, NumPy, pandas, matplotlib, Open Babel, BASH, HTML, CSS, and Linux server management.
Laboratory Techniques: Solution-phase synthesis and reaction setup, mechanochemical techniques, chromatographic purification, instrumental elucidation, Schlenk line techniques, thin-film fabrication, materials property measurements and crystallization techniques.
Instrumental Analysis: NMR, PXRD, UV-Vis, Fluorescence Spectroscopy, Contact Angle Drop Goniometry, Four-Point Probe Conductivity, HPLC, and Atomic Absorption Spectroscopy.
Writing: Academic paper writing, chemistry Olympiad problem writing.
Social Media Content Creation: Short and long format science video production for TikTok, Youtube, and other social media, on-camera presenter, and simple 3D animation.

References

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