

Curriculum vitae

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Personal information

First / Last Name	Alejandro Martínez León
Date of birth	September 12, 1994
Gender	Male
Nationality	Cuban
Actual position	PhD student at Jochen S. Hub's lab in Universität des Saarlandes, Saarbrücken, Germany
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Education

Doctoral Degree in Biophysics (2020-ongoing). Universität des Saarlandes, Saarbrücken, Germany; Jochen S. Hub's Biophysics lab. **Supervisors:** Prof. Dr. Jochen S. Hub and Dr. Peter Pool.

Master's degree in Radiochemistry Sciences (2018-2020) with a qualification of **Excellent**. Higher Institute of Technologies and Applied Sciences (InSTEC), University of Havana, Cuba. **Thesis:** "Evaluación *in silico* de nuevos derivados de antagonistas del

AT₁R: candidatos a radiofármacos para Tomografía por Emisión de Positrones”.

Supervisors: Prof. Dr. Zalua Rodríguez Riera, Prof. Dr. Ulises J. Jáuregui Haza.

Degree in Radiochemistry (2013-2018) (BAC+5) with an average mark of **4.94** (of 5) and a bonus of **0.08**. First of his class. Higher Institute of Technologies and Applied Sciences (InSTEC), University of Havana, Cuba. **Thesis:** “Evaluación *in silico* de la familia Fluoroalquil-Losartán, candidatos a radiofármacos para Tomografía por Emisión de Positrones”. **Supervisors:** Prof. Dr. Zalua Rodríguez Riera, Prof. Dr. Ulises J. Jáuregui Haza.

Training

1. **August 18th – August 28th, 2023.** Visit at Georgia Institute of Technology, Atlanta, United States. School of Physics; group of Prof. James C. Gumbart.
2. **March 1st – Mai 31st, 2023.** Secondment at Institute of Chemistry of the Hebrew University of Jerusalem. Fritz Haber Center for Molecular Dynamics; group of Prof. Noam Agmon. QM/MM methods for proton transport simulations.
3. **May 1st – October 31st, 2022.** Secondment at Boehringer Ingelheim Pharma GmbH & Co. KG. Automated enumeration of a ligand molecule in the protein binding pocket with a feedback loop to prioritize hits.
4. **November 2020-today.** Research Project of Horizon2020, Early-Stage Research 11 from the ITN PROTON under the supervision of Prof. Dr. Jochen S. Hub. Study of the inhibition and permeation processes of *Plasmodium falciparum* Formate Nitrite Transporters.
5. **September 9th – 29th, 2018.** International Student Practice (3rd Stage) held at Joint Institute for Nuclear Research (JINR), Dubna, Moscow region, Russia. Dzelopv Laboratory of Nuclear Problems. Application of Positron Annihilation Spectroscopy for Structural Defect Studies.
6. **September 2018-2020.** Research Project of the National Program of Basics Sciences (PNCB) under supervision of Professor Ulises J. Jáuregui-Haza and Zalua Rodríguez Riera. Molecular modeling of potential radiopharmaceuticals for the development of nuclear medicine.
7. **September 2015-January 2017.** Research Project under supervision of Professor Ulises J. Jáuregui-Haza and Zalua Rodríguez Riera at InSTEC, University of Havana, Havana, Cuba. Theoretical and experimental chemical studies of compounds of interest to Radiopharmacy.
8. **September 2014-January 2016.** Research Project under the supervision of Germán Rojas Lorenzo. Physical-Chemical, theoretical and experimental study of atomic, molecular, and aggregated systems with interest in the production of energy, health care and the environment.

Courses

1. **Workshop: Applying for Research Positions.** Nature Research Academies. Online. Facilitator: Dr. Jeffrey Robens. 30.06-01.07.2022.
2. **2022 BioExcel Summer School on Biomolecular Simulations.** Sicilia, Italy. 12-17.06.2022.
3. **GWDG Course:** Parallel Programming with MPI. (2-3.11.2021). (On-line).
4. **GWDG Course:** Using the GWDG Scientific Compute Cluster –An Introduction. (1.11.2021). (On-line).
5. Course of German language level A1.1 (26.04-23.07.2021).
6. **Workshop: Scientific Writing.** On-line. Facilitator: Justin Mullins (01/072021-02/07/2021).
7. **Workshop: Protein Dynamics,** Les Houches-TSRC. (18/05/2021-19/05/2021), on-line, Les Houches, France.
8. **Workshop on Computer Simulation and Theory of Macromolecules,** Hünfeld 2021. (23/04/2020-24/04/2020), on-line, Hünfeld, Germany.
9. **Workshop: Team Building and Team Dynamics using Team Management Systems as applied to the ITN-PROTON Team.** (12/09/2020-13/09/2020), on-line. Johannes Kepler University of Linz, Facilitator: Betty Boden.
10. **Workshop: News Leaders of Latin America and Caribbean in fields related to nuclear technologies.** (14/10/2019-18/10/2019), Havana Cuba.
11. **Positron Emission Tomography (PET) technology and application.** (5/10/2018-8/10/2018), taught by Professor Antony Gee from King's College of London, at CIMEQ hospital, Havana Cuba.
12. **Workshop: Molecular Dynamics.** (3/7/2018-6/7/2018) Courses taught by Professor Fabrice Lecrec, associated researcher of CNRS-Univ. Paris Sud, in the Faculty of Chemistry, University of Havana, Cuba.
13. **Virtual screening on the design of new pharmaceuticals.** (4/2/2016-22/4/2016) Certificate issued in Havana on May 30, 2016, Faculty of Chemistry, University of Havana, Cuba.
14. **III School of Medical Physics.** (23/10/2017-27/10/2017), taught by Professor Rodolfo Alonso, president of Latin American Association of Medical Physics at Havana, Cuba.
15. **Workshop: News technologies for health.** (12/3/2018-14/3/2018) at CIMEQ hospital, Havana, Cuba.

Programming Projects

1. <https://github.com/ale94mleon/MolDrug>
2. <https://github.com/ale94mleon/Palmiche>
3. <https://github.com/ale94mleon/TOFF>

Publications

4. None yet

International events

1. **Workshop on Computer Simulation and Theory of Macromolecules**, Hünfeld 2023. (28/04/2020-29/04/2020), Hünfeld, Germany.
 - **A. Martínez León**, J. S. Hub. “Overcoming hysteresis in ligand binding free energy calculations.”
2. 11th RDKit User Group Meeting, Berlin, Germany. 12-14.10.2022.
3. German Biophysical Society Meeting, Konstanz, Germany. 25-28.09.2022
 - **A. Martínez León**, J. S. Hub. “Overcoming hysteresis in ligand binding free energy calculations.”
4. Molecular Simulation 2022: Past, present, and future, Erice, Italy. 25-29.06.2022
 - **A. Martínez León**, J. S. Hub. “Binding mode characterization of PffNT inhibitors through Docking and Molecular Dynamic simulations.”
5. Workshop on Computer Simulation and Theory of Macromolecules, Hünfeld 2022. (23/04/2020-24/04/2020), on-line, Hünfeld,
 - **A. Martínez León**, J. S. Hub. “Binding mode characterization of PffNT inhibitors through Docking and Molecular Dynamic simulations.”
6. eSRS Latin America, (Virtual), September 2021.
 - A. Artímez Peña, **A. Martínez León**, Z. Rodríguez Riera, U. Jáuregui Haza. “*In silico* Evaluation of Fluorinated Derivatives of Telmisartan as Potential PET Radiopharmaceuticals”
7. Cell Physics 2021. Saarbrücken, Germany, September 2021.
 - **A. Martínez León**, J. S. Hub. “Binding mode characterization of PffNT inhibitors through Docking and MD simulations.”
8. EBSA2021. Vienna, Austria, July 2021.
 - **A. Martínez León**, J. S. Hub. “Binding mode characterization of PffNT inhibitors through Docking and MD simulations.”
9. EBSA2021, Satellite meeting: Proton and proton coupled transport. Vienna, Austria, July 2021.

- **A. Martínez León**, J. S. Hub. “Binding mode characterization of PffNT inhibitors through Docking and MD simulations.”
10. 7th European Joint Theoretical/Experimental Meeting on Membranes (EJTEMM 2021). On-line, Graz, Austria, April 2021.
 11. 23^{ra} Conferencia de Química. Santiago de Cuba, Cuba, November 2020.
 - A. Artímiez Peña, **A. Martínez León**, Z. Rodríguez Riera, U. Jáuregui Haza. “Synthesis of fluorinated derivatives of Telmisartan. *In silico* evaluation of potential use of PET radiopharmaceuticals.”
 12. Fourth Iberoamerican Symposium on Organic Chemistry (SIBEAQO-IV). Santa María Key, Cuba, December 2019.
 - A. M. Abreu Díaz, J. N. Da Silva, L. M. Esteves Morais, A. García Fleitas, **A. Martínez León**, U. Jáuregui Haza. “Synthesis of Radiopharmaceutical by click chemistry”
 13. 12th Seminars of Advanced Studies on Molecular design and Bioinformatics (SEADIM-2019). Santa María Key, Cuba, June 2019.
 - **A. Martínez León**, A. Artímiez Peña, Z. Rodríguez Riera, Y. M. Álvarez Ginarte, U. Jáuregui Haza. “*In silico* evaluation of two new derivatives of losartan obtained by click chemistry. DFT and Molecular Dynamics approach.”
 14. VII Simposio Internacional de Ciencias Químicas 2019. Santa María Key, Cuba, June 2019.
 - **A. Martínez León**, A. Artímiez Peña, Z. Rodríguez Riera, Y. M. Álvarez Ginarte, U. Jáuregui Haza. “Fluoroalkyl-Losartan family as candidates for Positron Emission Tomography radiopharmaceuticals. *In silico* study.”
 15. Congreso Internacional de Investigación Científica, 2019”, Santo Domingo, República Dominicana June 2019.
 - **A. Martínez León**, A. Artímiez Peña, Z. Rodríguez Riera, Y. M. Álvarez Ginarte, U. Jáuregui Haza. “*In silico* evaluation of two new derivatives of losartan obtained by click chemistry. DFT and Molecular Dynamics approach.”
 16. 5^{to} Encuentro Internacional de Ciencias Farmacéuticas y Alimentarias (ECFA 2019). Habana, Cuba. Mayo 2019
 - **A. Martínez León**, A. Artímiez Peña, Z. Rodríguez Riera, Y. M. Álvarez Ginarte, U. Jáuregui Haza. “*In silico* evaluation of two new derivatives of losartan obtained by click chemistry. DFT and Molecular Dynamics approach.”

17. XVII Workshop on Nuclear Physic and X International Symposium on Nuclear and Related Techniques (WONP-NURT 2019). Havana, Cuba. April 2019.
- **A. Martínez León**, A. Artímez Peña, Z. Rodríguez Riera, Y. M. Álvarez Ginarte, U. Jáuregui Haza. “In silico evaluation of two new derivatives of losartan obtained by click chemistry. DFT and Docking simulation approach.”
18. III Simposio Internacional de Imágenes Moleculares. Havana, Cuba, January 2019
19. IV Congreso Internacional de Investigación-Desarrollo e Innovación Tecnológica en la Industria Biofarmacéutica (IDIFARMA 2018). Havana, Cuba, December 2018.
- **A. Martínez León**, A. García Fleitas, Z. Rodríguez Riera, U. Jáuregui Haza, García A., Álvarez Y.M., Rodríguez Z., Jáuregui U., M.S. Ortega Pijeira, E. Soares. “*In silico* evaluation of the FluoroAlkyl-Losartan family, candidates for positron emission tomography radiopharmaceuticals.”
 - A. García Fleitas, **A. Martínez León**, Z. Rodríguez Riera, U. Jáuregui Haza, García A., Álvarez Y.M., Rodríguez Z., Jáuregui U., M.S. Ortega Pijeira, E. Soares. “Losartan derivatives F-labeled as candidates of radiopharmaceutical. Theoretical studies.”
20. 33^{er} Congreso Latinoamericano de Química (33-CLAQ) and X Congreso de Ciencias Químicas, Tecnología e Innovación (QUIMICUBA'2018). Havana, Cuba, October 2018.
- **A. Martínez León**, A. García Fleitas, Z. Rodríguez Riera, U. Jáuregui Haza, García A., Álvarez Y.M., Rodríguez Z., Jáuregui U., M.S. Ortega Pijeira, E. Soares. “*In silico* evaluation of the FluoroAlkyl-Losartan family, candidates for positron emission tomography radiopharmaceuticals.”
 - A. García Fleitas, **A. Martínez León**, Z. Rodríguez Riera, U. Jáuregui Haza, García A., Álvarez Y.M., Rodríguez Z., Jáuregui U., M.S. Ortega Pijeira, E. Soares. “Losartan derivatives as ¹⁸F-labeled radiopharmaceutical candidates for cancer diagnosis. Theoretical Studies.”
21. Congreso Internacional de Investigación Científica, 2018”, Santo Domingo, República Dominicana June 2018.
- **A. Martínez León**, A. García Fleitas, Z. Rodríguez Riera, U. Jáuregui Haza. “Evaluación *in silico* de la familia FAL, candidatos a radiofármacos derivados del losartán marcados con ¹⁸F”.

22. International Convention of Science, Technology, and Innovation 2018. I International Conference “Nuclear Technology for the life” (TECNUC 2018). Havana, Cuba, March 2018.
- **A. Martínez León**, A. García Fleitas, Z. Rodríguez Riera, U. Jáuregui Haza, García A., Álvarez Y.M., Rodríguez Z., Jáuregui U., M.S. Ortega Pijeira, E. Soares. “Evaluation of Fluoro Alkil losartan derivatives as ¹⁸F-labeled radiopharmaceutical candidates for cancer diagnosis. Theoretical Study.”
 - A. García Fleitas, **A. Martínez León**, Z. Rodríguez Riera, U. Jáuregui Haza, García A., Álvarez Y.M., Rodríguez Z., Jáuregui U. “Losartan derivatives as ¹⁸F-labeled radiopharmaceutical candidates for cancer diagnosis. Theoretical Studies.”
23. 22^{da} Conferencia de Química. Santiago de Cuba, Cuba, November 2017.
- **A. Martínez León**, A. García Fleitas, Y. M. Álvarez Ginarte, Z. Rodríguez Riera, U. Jáuregui Haza. “Evaluation of the fluoro alkil Losartan-derivative as ¹⁸F-labeled radiopharmaceutical candidates for cancer diagnosis. Theoretical study.”
24. XVII Workshop on Nuclear Physic and X International Symposium on Nuclear and Related Techniques (WONP-NURT 2017). Havana, Cuba. April 2017
- **A. Martínez León**, A. García Fleitas, Z. Rodríguez Riera, U. Jáuregui Haza. “Theoretical evaluation of losartan derivatives as ¹⁸F-labeled radiopharmaceutical candidates for cancer diagnosis”.
 - A. García Fleitas, **A. Martínez León**, Z. Rodríguez Riera, U. Jáuregui Haza, García A., Álvarez Y.M., Rodríguez Z., Jáuregui U. “Theoretical evaluation of fluoro n-ethoxy-methyl-triazole losartan-derivatives as ¹⁸f-labeled radiopharmaceutical candidates for cancer diagnosis”.
25. XIII Congreso Internacional de Investigación Científica, XIII CIC. Santo Domingo, Dominican Republic, July 2017.
- **A. Martínez León**, A. García Fleitas, Z. Rodríguez Riera, U. Jáuregui Haza. “Evaluación de tres candidatos a radiofármacos derivados del losartan marcados con ¹⁸F. Estudio teórico.”
26. 11th Seminars of Advanced Studies on Molecular design and Bioinformatics (SEADIM-2017). Varadero, Cuba, July 2017.

- A. García Fleitas, **A. Martínez León**, Z. Rodríguez Riera, U. Jáuregui Haza. “Evaluation of the fluoro alkyl losartan-derivative as ^{18}F -labeled radiopharmaceutical candidates for cancer diagnosis. Theoretical study.”
27. Second International Convention IMMUNOPHARMACOLOGY (VACCIPHARMA 2017), Varadero, Cuba. Junio 2017.
- A. García Fleitas, **A. Martínez León**, Z. Rodríguez Riera, U. Jáuregui Haza. “Theoretical evaluation of ^{18}F -labeled losartan-derivatives as radiopharmaceutical candidates for cancer diagnosis”.

National events

1. Student Scientific Forum “InSTEC 2018-2019”, University of Havana, Cuba, May 2018.
 - **A. Martínez-León**. “Evaluación *in silico* de la familia FAL, candidatos a radiofármacos derivados del losartán marcados con ^{18}F ”.
2. Student Scientific Forum “Faculty of Chemistry 2018-2019”, University of Havana, Cuba, April 2018.
 - **A. Martínez-León**. “Evaluación *in silico* de la familia FAL, candidatos a radiofármacos derivados del losartán marcados con ^{18}F ”.
3. Student Scientific Forum of University of Havana, Cuba, April 2018
 - **A. Martínez-León**. “Evaluación *in silico* de la familia FAL, candidatos a radiofármacos derivados del losartán marcados con ^{18}F ”.
4. Student History Forum “InSTEC 2017-2018”, University of Havana, Cuba, November 2018.
 - **A. Martínez-León**, I. B. Dellundé-García. “¿De niña a hombre?... Solo cuestión de traje”.
5. Student Scientific Forum “InSTEC 2017-2018”, University of Havana, Cuba, March 2018.
 - **A. Martínez-León**, A. García-Fleitas. “Evaluación *in silico* de la familia FAL, candidatos a radiofármacos derivados del losartán marcados con ^{18}F ”.

- A. García-Fleitas, **A. Martínez-León**. “Evaluación teórica de candidatos a radiofármacos derivados del losartán de la familia 18 fluoro n-etoxi metil triazol losartán”.
6. Student Scientific Forum “InSTEC 2016-2017”. InSTEC, University of Havana, Havana, Cuba, March 2017
 - **A. Martínez-León**. “Simulación del proceso de crecimiento de cristales de gases nobles dopados con Cd y Zn”.
 7. State History Forum. Havana, Cuba, May 2015.
 - **A. Martínez-León**, E. Cuba-Rodríguez, A. González-Rivero. “Aproximación a la labor de Rafael Morales y González”.
 8. Student History Forum “InSTEC 2014-2015”, University of Havana, Cuba, November 2014.
 - **A. Martínez-León**, E. Cuba-Rodríguez, A. González-Rivero. “Aproximación a la labor de Rafael Morales y González”.

Awards and distinctions

1. **2018. Mention. National Award to the Most Prominent Junior Research in the category of Natural and Exact Sciences** of the year 2018.
2. **2018. Distinction as Most Prominent Graduate in the Research Sphere of InSTEC.**
3. **2018. Distinction as Most Prominent Graduate in the History Sphere of InSTEC.**
4. **2018. Distinction as Integral Graduate of the Faculty of Nuclear Sciences and Technology, InSTEC.**
5. **2018. Distinction as Integral Graduate of InSTEC.**
6. **2018. Special Award of the Nuclear Energy and Advances Technologies Agency for the Diploma work with the most relevant nuclear research.**
7. **2018. Award for the Scientific Commendation.**
8. **2018. Distinction as Golden Diploma** for academic results
9. **2018. Special Award “Grand Prize InSTEC”** for best work of the Student Scientific Forum InSTEC 2017-2018.
10. **2018. Special Award “Major Scientific Contribution”** in the Student Scientific Forum InSTEC 2017-2018.

11. **2018. 2nd Prize** in Radiochemistry Section of the Student Scientific Forum InSTEC 2017-2018.
12. **2018. 1st Prize** in Computational and Theoretical Chemistry Section of the Student Scientific Forum at Chemical Faculty of University of Havana. 2017-2018.
13. **2018. 1st Prize** in Biotechnology and Biomedicine Section of the Student Scientific Forum at University of Havana. 2017-2018.
14. **2018.** Distinction for exalt the InSTEC in the Research field.
15. **2017. Acknowledgment** for the work as **Tutor Student** in the disciplines: General Chemistry and Inorganic Chemistry.
16. **2017. 1st Prize** in History and Personalities Section of the Student History Forum InSTEC. 2017-2018.
17. **2017. 1st and 3rd Prize** in Radiochemistry Section of the Student Scientific Forum InSTEC 2016-2017.
18. **2016. Mention** in Theoretical Physics Section of the Student Scientific Forum InSTEC. 2015-2016.
19. **2015. Mention** in the Student History Forum at State level. 2014-2015.
20. **2014. Acknowledgment** for the work as **Tutor Student** in the disciplines: General Chemistry and Inorganic Chemistry.
21. **2014. 1st Prize** in History and Personalities Section of the Student History Forum InSTEC. 2014-2015.
22. **2014. 2nd Prize** in English I premium test, InSTEC. 2014-2015.
23. **2014. 2nd Prize** in Mathematic I premium test, InSTEC. 2014-2015.

I declare that the content of this curriculum is strictly adjusted to the truth.

PhD. Student. Alejandro Martínez-León