

**Universidad de Puerto Rico
Recinto Universitario de Mayagüez
Decanato: Artes y Ciencias
Departamento de Química**

Informe Anual 2017– 2018

Sometido por:

Dr. Enrique Meléndez

16 de octubre de 2019

Informe de iniciativas, actividades y logros de acuerdo al Plan Estratégico

A. Resumen Ejecutivo

A través de las iniciativas y actividades llevadas a cabo durante el año académico 2017-18 y los logros alcanzados, el Departamento de Química cumple con los aspectos descritos en su misión y visión.

Misión: Preparar profesionales en la disciplina de la química ofreciendo programas de excelencia tanto a nivel graduado como subgraduado, y programas de investigación de alta calidad. Generar conocimiento que contribuya al desarrollo de la sociedad y a la solución de los problemas que aquejan. Contribuir a la cultura de la comunidad académica y de la sociedad en general.

Visión: Ser un Departamento de Química líder en el Siglo XXI, a nivel nacional e internacional, en la preparación de profesionales en la disciplina de la química y áreas afines. Aportar al desarrollo y la diseminación del conocimiento en las áreas fundamentales, aplicadas e interdisciplinarias de las ciencias químicas.

B. Institucionalizar una cultura de Planificación Estratégica y Avalúo

Actividades Completadas:

- Sometió reporte anual requerido por la Sociedad Americana de Química (ACS) del Bachillerato en Química.
- Avalúo periódico del Programa Doctoral en Química Aplicada mediante el Comité Graduado de Química.
Revisión de la Guía de Programa Doctoral en Química Aplicada.
- Evaluación de las mejoras y necesidades del edificio de Química con énfasis en el sistema de aire acondicionado, la humedad y filtraciones. Coordinación con la Oficina de Mejoras Permanentes.
- Evaluación de los espacios del edificio, incluyendo laboratorios, salones y oficinas.
Evaluación de los equipos dañados por causa del Huracán María.

Actividades en progreso:

- Continuar con el avalúo de los Programas de Bachillerato y Doctoral en Química.
- Continuar con la evaluación continua de los espacios físicos del Edificio de Química
- Continuar solicitando apoyo administrativo para las mejoras permanentes de nuestro departamento: planta física, aire acondicionado.

C. Estar a la vanguardia de la educación superior en Puerto Rico garantizando que nuestros alumnos reciben la mejor educación

Actividades:

1. Se está trabajando el Programa Ciencia Forense UPRM y una Certificación en Química Forense (en Progreso) 2017-2018.
 2. Elmer Ortiz, Angel Rodriguez, J. Lopez-Garriga. Myoglobin's Hydrogen sulfide pathways to produce the sulfheme derivatives. STEP-UP program NIH, Maryland, U.S. **Aug 2017**
 3. Saraswati Sridhar, J. Lopez-Garriga Formation of Sulfmyoglobin as function of the pH. **SESO– Puerto Rico Science Fair**. Selected as a top 300 Broadcom nominees **September 2017**
 4. Co-Chairman Fourteenth Annual IFPAC®/QbD/PAT Summit with INDUNIV, June 19-20, 2018, Rodolfo Roma164ach. A meeting that included over 60 of the top technical leaders of Puerto Rico's pharmaceutical industry.
- Support of Student Activities**
Mentor Future Pharmacists Association
Mentor Graduate Students Association
5. **Sigma Xi Poster Day**, Coordinadores *Drs. Alberto Santana, Emilio Díaz y Carmen Vega*.
 6. Participation in the ASCB NSF Faculty Research and Education Development (FRED) Program, Dra. Celine Casse.
 7. Talleres de Enseñanza para Química General, Dra. Ivelisse Padilla y Prof. Verónica Sánchez.

D. Aumentar y Diversificar las Fuentes de Ingreso de la Institución

Propuestas Sometidas:

1. UPRM-Student Development Center for Food, Agriculture, Natural and Human Resources (UPRM-SDC-FANHR). USDA - -PI: Dr. Félix Román, Co-PI: Dr. E. Meléndez.
2. UPRM Center for Training Opportunities for Underrepresented Food, Agriculture and Natural Resource Students (UPRM-CTOU-FANRS) – USDA, -PI: Dr. Félix Román, Co-PI: Dr. E. Meléndez.
3. REU Site: Center in Chemical Structure, NSF. PI: Dr. Dr. E. Meléndez.
4. PR _INBRE, NIH: PI: Dr. Elsie Parés.
5. Approval of “URPM Ph.D. Enrichment Program” by Alfred P. Sloan for \$498,065, August 2018- Dec. 2022. Professor Romañach

6. UPRM Emergency Aid, Obtained \$76,000 from Sloan Foundation to aid 19 PhD students following Hurricane María, October 13, 2017. Professor Romañach
7. Student Internship and Visiting Faculty at Rutgers to Reduce Effect of Hurricane María on UPR-Mayagüez Students \$65,000, Janssen Ortho LLC & Rutgers University, April 2018. Professor Romañach.
8. Avara Pharmaceutical Services approved: "A Proposal for Increased Process Understanding through NIR Spectroscopy and Chemometrics", \$38, 200, June 2018-December 2019. Professor Romañach
9. HSI Conference, Grant No. 1802252: Accelerating the Impact of HSI STEM Education and Research on Innovation Ecosystems. Professor Romañach
10. Recipient of the 2017-18 UPRM seed-fund money: \$4,870.19. Prof. Celine Casse.

E. Implementar Procesos Administrativos Ágiles y Eficientes

1. Comité Distribución de Espacios (laboratorios y oficinas). Se generó un mapa del edificio con los encargados de las áreas y se redistribuyó nuevos espacios.
2. Comité de Infraestructura. Análisis de las condiciones físicas del edificio.
3. Estableció Comité de salud y Seguridad donde se planificó un simulacro y un shake out..
4. Monitoreo del Programa Graduado y progreso académico de los estudiantes.

F. Fortalecer la Investigación y Labor Creativa Competitiva

Publicaciones:

1. "In silico Virtual Screening on Estrogen Receptor Alpha Protein Ligand Binding Domain for the Development of New Selective Estrogen Receptor Modulators" José A. Carmona-Negón and Enrique Meléndez. J. Drug Des. Res. **2018**, 5(1): 1064.
2. "Para-Substituted Functionalized Ferrocene Esters with Novel Antibacterial Properties" Kevin Muñoz Forti, Faviola Bernard, Gustavo Santiago, Waldemar Garcia, José L. Vera, Enrique Meléndez and Edu B. Suarez-Martinez. J. Clin. Diag. Res. **2018**, Vol-12(2): DC01-DC04.
3. "Biological Interaction of Molybdenocene Dichloride with Bovine Serum Albumin Using Fluorescence Spectroscopy" Moralba Domínguez, José E. Cortés-Figueroa, Enrique Meléndez. J. Chem. Ed. **2018**, 95(1), 152-157.
4. "A molecular docking study of the interactions between human transferrin and seven metallocene dichloride" Jorge R. Güette-Fernández, Enrique Meléndez, Wilson Maldonado-Rojas, Carlos Ortega-Zúñiga, Jesus Olivero-Verbel, Elsie I. Parés-Matos. J. Mol. Graph. Model. **2017**, 75, 250-265.
5. "Ferrocene-steroid conjugates: Synthesis, structure and biological activity" Xiomara Narváez-Pita, Arnold L. Rheingold, Enrique Meléndez. J. Organometal. Chem. **2017**, 846, 113-120.

6. Quiñones-Ruiz, Tatiana; Rosario-Alomar, Manuel; Ruiz-Esteves, Karina; Shanmugasundaram, Maruda; Grigoryants, Vladimir; Scholes, Charles; Lopez-Garriga, Juan; Lednev, Igo. Purple fibrils: a new type of protein chromophore. **Journal of the American Chemical Society (2017)** 139:9755-9758. doi: 10.1021, PMID:28689402
7. I. M. Montes-Rodríguez, C. L. Cadilla R. González-Méndez, J. López-Garriga and A. Ropelewski. 2017. De Novo Assembly of *Lucina pectinata* Genome using Ion Torrent Reads. **Practice and Experience in Advanced Research Computing 2017 Proceedings, (2017)** New Orleans, LA, USA, July 09-13, 2017 (PEARC17), 7 pages. DOI: 10.1145/3093338.3093362
8. Dorottya Garai; Bessie B Ríos-González; Paul G Furtmüller, PhD; Jon M Fukuto, PhD; Ming Xian, PhD; Juan López Garriga, PhD; Christian C Obinger, PhD; Peter Nagy. Mechanisms of myeloperoxidase catalyzed oxidation of H₂S by H₂O₂ or O₂ to produce potent protein Cys-polysulfide-inducing species. **Free Radical Biology & Medicine. 2017.** 113:551-563. doi: 10.1016/
9. Gonzalez-Ramirez, Luis Antonio; Ruiz-Martínez, Carlos; Estremera-Andújar, Rafael; Nieves-Marrero, Carlos; Garcia Caballero, Alfonso; Gavira, Jose; López-Garriga, Juan; García-Ruiz, Juan Manuel. An efficient screening methodology for protein crystallization based on the Counter-diffusion technique. **Crystal Growth & Design. (2017),** 17 (12), pp 6780–6786 DOI: 10.1021/acs.cgd.7b01353
10. Díaz-Ayala R, Torres-González L, Pietri R, Cabrera CR, López-Garriga J. Engineered (Lys)₆-Tagged Recombinant Sulfide-Reactive Hemoglobin I for Covalent Immobilization at Multiwalled Carbon Nanotubes. **ACS Omega. (2017)** Dec 31;2(12):9021-9032. doi: 10.1021/acsomega.7b01500. Epub 2017 Dec 15. PMID:29302632
11. Hector D. Arbelo-Lopez, Angel D. Rodriguez-Mackenzie, Eddie M. Roman-Morales, Troy Wymore, and Juan Lopez-Garriga. Sulfheme π to d_{π} Charge Transfer and π to π^* Transitions Leads to Its Like Deoxy and Met Isomeric Structures Visible Spectra. **J. Chem. Phys. B. (2018),** 122, 4947–4955. doi:10.1021/acs.jpcc.7b12393.
12. Esbensen, K. H.; **Romañach, R. J.**; Román-Ospino, A. D., Chapter 4 - Theory of Sampling (TOS): A Necessary and Sufficient Guarantee for Reliable Multivariate Data Analysis in Pharmaceutical Manufacturing A2 - Ferreira, Ana Patricia. In *Multivariate Analysis in the Pharmaceutical Industry*, Menezes, J. C.; Toby, M., Eds. Academic Press: **2018**; pp 53-91.
13. Sierra-Vega, N. O.; Sánchez-Paternina, A.; Maldonado, N.; Cárdenas, V.; Romañach, R. J.; Méndez, R., In line monitoring of the powder flow behavior and drug content in a Fette 3090 feed frame at different operating conditions using Near Infrared spectroscopy. *J. Pharm. Biomed. Anal.* **2018**, 154, 384-396.
14. Romañach, R. J.; Sanchez-Paternina, A.; Esbensen, K. H., Variographic Analysis of 1-D lots in Pharmaceutical Manufacturing (Powder Mixing). *American Pharmaceutical Review* **2018**, 21 (1), 22-26.
15. Vargas, J. M.; Nielsen, S.; Cárdenas, V.; Gonzalez, A.; Aymat, E. Y.; Almodovar, E.; Classe, G.; Colón, Y.; Sanchez, E.; Romañach, R. J., Process analytical technology in continuous manufacturing of a commercial pharmaceutical product. *Int. J. Pharm.* **2018**, 538 (1–2), 167-178.
16. Hausner, D. B.; Romañach, R. J., Progress Towards Advanced Pharmaceutical Manufacturing. *American Pharmaceutical Review* **2017**, 20 (July-August), 54-57.

17. Synthesis, characterization, and electrocatalytic ability of γ -Fe₂O₃ nanoparticles for sensing acetaminophen Beer Pal Singh, Arun Kumar, Hector I Areizaga-Martinez, Carmen A Vega-Olivencia & M S Tomar, Indian Journal of Pure & Applied Physics , OCTOBER 2017,55(10), 722.
18. Submission of the following scientific article: *Molecular mechanisms of Annona muricata anti-proliferative/anti-cancer properties* to the Journal of Oncological Sciences (JOS). Celine Casse.

Presentaciones

1. Metallocene Steroid Conjugates as Potential Target Specific Drugs, Ponce School of Medicine, January 26, 2018. E. Meléndez.
2. Application of Metallocenes as Anti-Cancer Drugs, Mini symposium on Metals in Medicine, University of Puerto Rico-Rio Piedras, April 12, 2018. E. Meléndez.
3. R.J. Romañach, Visualization is Essential for Obtaining Information from Outlier Diagnostics, 15th Annual IFPAC & Induniv Summer Summit on Quality by Design and Process Analytical Technology, June 21, 2018.
4. R.J. Romañach, Accelerating the Impact of HSI STEM Education and Research on Innovation Ecosystems, 5th National Forum on Entrepreneurial Education in Puerto Rico, June 8, 2018.
5. R.J. Romañach, Forum: Challenges in the chemical sciences and engineering; where the innovation is going?, American Chemical Society Entrepreneurial and Innovation for Scientists in Puerto Rico, Molecular Sciences Research Center, May 26, 2018, Río Piedras, PR.
6. R.J. Romañach, Panel Discussion: Opportunities: I-Corps, SBIR, STTRs, etc. American Chemical Society Entrepreneurial and Innovation for Scientists in Puerto Rico, Molecular Sciences Research Center, May 26, 2018, Río Piedras, PR.
7. R.J. Romañach, Accelerating the Impact of HSI STEM Education and Research on Innovation Ecosystems, Inter-American University, San Germán, April 11, 2018.
8. A. Sánchez, K.H. Esbensen, R.J. Romañach, What would be the Composition of a Flowing Powder if it is Analyzed Again?, International Foundation for Process analytical Chemistry (IFPAC), North Bethesda, MD, February 12, 2018.
9. J. Aldama Guardia, S. Lysenko, L. Chevres, V. Cárdenas, Z. Shi, R.J. Romañach, Light Scattering by Pharmaceutical Tablets: Fractal and Polarization Properties, International Foundation for Process analytical Chemistry (IFPAC), North Bethesda, MD, February 12, 2018.
10. R.J. Romañach, Economic Development Opportunities in Continuous Manufacturing, Presented to EDA, FEMA, and DOE Task Force, in activity organized by Dr. José I. Vega and Dr. Ubaldo Córdova-Figueroa, March 9, 2018.
11. R.J. Romañach, Lessons from the Road Less Traveled: I-Corps & SBIR programs, Chemistry Department Seminar, March 9, 2018.
12. R.J. Romañach, "From Knowledge to Commercial Economies – The Need for Education", guest lecture in Business Models & Commercialization Strategies for Technology Ventures", ADMI 6835, Graduate Level Course in the UPRM School of Business Administration, September 13, 2017.

Graduate Students National/International Presentations in Technical Meetings

1. Marchany-Rivera, Darya and Lopez-Garriga, Juan. *Oxy-hemoglobin III crystal quality optimization*. 4th BioXFEL Conference, Las Vegas, Nevada. **Jan 2017**.
2. Josiris Rodriguez-Perez and Juan López-Garriga. Gel-mix as a recipe for fast crystal growing. BioXFEL STC 4th Annual International Conference, Las Vegas, Nevada **January, 2017**
- 3, Marchayny-Rivera, Darya and Lopez-Garriga, Juan. Effect of pH on Fe-O₂ bond in the oxygen reactive hemoglobins of *L. pectinata* by X-ray Crystallography. 5th International BioXFEL Conference, New Orleans, Louisiana, USA. **February 2018**.

Graduate Students Presentations in Technical Meetings in Puerto Rico

1. Josiris Rodriguez-Perez, Juan López-Garriga, Structure of the α Hbl dimer-Protein rich cysteine complex from *L. pectinata*. PR-INBRE & COBRE Symposium, San Juan P.R. **May 2017**
2. Marchany-Rivera, Darya and Lopez-Garriga, Juan Crystal structures of Mb SH2 complex. PR-INBRE & COBRE Symposium, San Juan P.R. **May 2017**

Undergraduate Students Presentations National and International

1. Fabiola M. Moreno Echevarria, Darya Marchany-Rivera and Juan Lopez-Garriga. Sulfmyoglobin and Hydrogen Sulfide in Metmyoglobin Crystals. 4th International BioXFEL Conference, Las Vegas, Nevada, USA. **January 2017**.
2. Hernán E. Machado-Hernandez, Darya Marchany-Rivera and Juan Lopez-Garriga. Formation of sulfmyoglobin upon addition of H₂S to crystallized oxymyoglobin. 4th International BioXFEL Conference, Las Vegas, Nevada, USA. **January 2017**.
3. Borges, H. , Reyes, A. , Lopez-Garriga, J., Hemoglobin I from *Lucina pectinata* as a novel protein donor of Hydrogen Sulfide, BioXFEL, Las Vegas, NV, **January 2017**
4. Aldarondo Torres, Álani; Colón Ríos, Daniel; Soto Ocaña, Joshua; López Garriga, Juan; Hydrogen Sulfide: An Inhibitor of Insulin Amyloid Fibrils, 4th Annual BioXFEL Conference, Las Vegas, NV **January 2017**
5. Alfredo Reyes-Oliveras, Hazel M. Borges-Arias, Juan López-Garriga, Hemoglobin I from *Lucina pectinata* as a Novel Protein Donor of Hydrogen Sulfide, BioXFEL 4th International Conference, Las Vegas, NV, U.S. **January 2017**.
6. Indra M. Gonzalez, Juan Lopez-Garriga, Sulfhydic Acid (H₂S) Limits Lysozyme Amyloid Development and Enhances Soft Matter Assembly, BioXFEL Annual Scientific Conference, Las Vegas, NV, **Jan 2017**
7. Indra M. González, Tatiana Quiñones, Manuel Rosario, Igor K. Lednev, Juan López-Garriga, Towards the Inhibition Mechanism of Lysozyme Fibrillation by Hydrogen Sulfide, University at Buffalo McNair Conference, **Jul 2017**
8. Indra M. González, Tatiana Quiñones, Manuel Rosario, Igor K. Lednev, Juan López-Garriga, Towards the Inhibition Mechanism of Lysozyme Fibrillation by Hydrogen Sulfide, University at Albany Summer Research Program Research Symposium, **Aug 2017**
9. Aldarondo Torres, Álani; Colón Ríos, Daniel; Soto Ocaña, Joshua; López Garriga, Juan; Hydrogen Sulfide: An Inhibitor of Insulin Amyloid Fibrils, ABRCMS, Phoenix, Arizona, **November 2017**

10. Alfredo Reyes-Oliveras, Hazel M. Borges-Arias, Juan López-Garriga, rHbl-S₂H as a potential Hydrogen Sulfide Donor 5th BioXFEL International Conference Symposium – New Orleans, LA, **US February 15, 2018**

11. Reyes-Oliveras, A.; Borges-Arias, H. and López-Garriga, J. Studies of rHbl-SH₂ at Physiological Conditions for Potential Use as a Novel Hydrogen Sulfide Donor. Awarded "People's Choice for Overall Best Poster"AMSA Convention and Exposition – Washington, DC, US **March 9, 2018**

12. Fabiola M. Moreno Echevarria, Hernan Machado, Darya Marchany-Rivera and JuanLopez-Garriga. Metmyoglobin Crystals Soaking with Hydrogen Sulfide: Sulfmyoglobin and Metmyoglobin-SH₂ derivatives. INBRE External Advisory Committee Meeting.Dorado, P.R. **March, 2017**

13. Sánchez-Ortiz K, Morales-Lopez C, Durán D, Oliver V, López-Garriga J. Photolytic Studies of the Carbon Monoxide Complex with Deoxy-myoglobin. **BioXFEL International Conference. January 2018.**

14. Indra M. González, Tatiana Quiñones, Manuel Rosario, Igor K. Lednev, Juan López-Garriga, Hydrogen Sulfide (H₂S) Disrupts Lysozyme Aggregation in Lag Phase of Amyloid Formation, BioXFEL International Conference, **Feb 2018**

Undergraduate Students Presentations in Local Technical Meetings

1. Daniel Colon, Aldarondo Torres, Álani; Juan Lopez-Garriga Hydrogen Sulfide (H₂S): An Inhibitor of Insulin (IBP) Amyloid FibrilsSixth Lilly Academy Technical Forum Puerto Rico Convention Center, San Juan, PR **March, 2017**

2. Fabiola M. Moreno Echevarria, Hernan Machado, Darya Marchany-Rivera and Juan Lopez-Garriga. Metmyoglobin Crystals Soaking with Hydrogen Sulfide: Sulfmyoglobin and Metmyoglobin-SH₂ derivatives. INBRE External Advisory Committee Meeting.Dorado, P.R. **March 2017**

3. Aldarondo Torres, Álani; Daniel Colon, Juan Lopez-GarrigaHydrogen Sulfide (H₂S): An Inhibitor of Insulin (IBP) Amyloid Fibrils 1st Puerto Rico INBRE and COBRE Symposium , Caribe Hilton Hotel, San Juan, PR, **May 19th, 2017**

4. Daniel Colon, Aldarondo Torres, Álani; Juan Lopez-Garriga Hydrogen Sulfide (H₂S): An Inhibitor of Insulin (IBP) Amyloid Fibrils 7th AEMPR Annual Research Symposium, Los Paseos Convention Center, San Juan, PR **May 27th, 2017**

5. Aldarondo Torres, Álani; Colón Ríos, Daniel; Soto Ocaña, Joshua; López Garriga, Juan; Hydrogen Sulfide: An Inhibitor of Isulin Amyloid Fibrils, PR-INBRE & COBRE Symposium, San Juan P.R. **May 2017**

High School Students Presentations in National and Local Technical Meetings

1. Elmer Ortiz, Angel Rodriguez, J. Lopez-Garriga. Myoglobin's Hydrogen sulfide pathways to produce the sulfheme derivatives. STEP-UP program NIH, Maryland, U.S. **Aug 2017**

2. Saraswati Sridhar, J. Lopez-Garriga Formation of Sulfmyoglobin as function of the pH. SESO– Puerto Rico Science Fair. Selected as a top 300 Broadcom nominees **September 201**

H. Fortalecer el Sentido de Pertenencia y “Orgullo Colegial”

1. Demostraciones y orientación a estudiantes de escuela superior.
2. Organizar y obtener materiales para las demostraciones.
3. Obtener y crear material de promoción.