Dr. Evangelia Kotsikorou

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EDUCATION

- **Ph.D.** Chemistry, May 2006, University of Illinois at Urbana-Champaign, Urbana IL
- **B.S.** General Science (Chemistry concentration)**,** *magna cum laude*, May 2000, Montana State University-Northern, Havre MT
- **B.A.** English, *magna cum laude***,** May 2000, Montana State University-Northern, Havre MT

EMPLOYMENT

2018-Present, Associate Professor, The University of Texas Rio Grande Valley, Edinburg, TX

2015-2018, Assistant Professor, The University of Texas Rio Grande Valley, Edinburg, TX

2012-2015, Assistant Professor, The University of Texas – Pan American, Edinburg, TX

2006-2012, Post-doctoral Research Scientist, University of North Carolina at Greensboro, Greensboro, NC

RESEARCH EXPERIENCE

- Constructed and refined the homology model of the G protein-coupled receptors (GPR119, Cannabinoid 1 and Cannabinoid 2 receptors)
- Docked small molecule and peptide ligands in the active site of G protein-coupled receptors and nuclear receptors
- Developed CHARMM force field parameters for small ligands
- Performed molecular dynamics simulations of G protein-coupled receptors, nuclear receptors, and small molecules in lipid and aqueous environment
- Designed new ligands based on docking results and structure-activity relationships
- Used computer aided ligand-based drug design approaches to deduce quantitative structure-activity relationships for a series of enzyme
- Developed pharmacophore models and used them for database searching

PUBLICATIONS

1. Hamilton, J; **Kotsikorou, E**. Parameterization of the GPR119 Receptor Agonist AR231453. J. Comput. Chem. 2018, 39, 35-41.

2. Meza-Aviña, M. E.; Lingerfelt, M. A.; Console-Bram, L. M.; Gamage, T. F.; Sharir, H.; Gettys, K. E.; Hurst, D. P.; **Kotsikorou, E.**; Shore, D. M.; Caron, M. G.; Rao, N.; Barak, L. S.; Abood, M. E.; Reggio, P. H.; Croatt, M. P. Design, synthesis, and analysis of antagonists of GPR55: Piperidine-substituted 1,3,4-oxadiazol-2-ones. Bioorg. Med. Chem. Lett. 2016, 26, 1827-30.
3. Zhao, P.; Lane, T.; Gao, H. G.; Hurst, D.; **Kotsikorou, E.**; Le, L.; Brailoiu, E.; Reggio, P. H.; Abood, M. E. Crucial Positively Charged Residues For Ligand Activation Of The GPR35 Receptor. J Biol Chem. 2014, 289, 3625-38.
4. **Kotsikorou, E.**; Sharir, H.; Shore, D. M.; Hurst, D. P.; Lynch, D. L.; Madrigal, K. E.; Heynen-Genel, S.; Milan, L. B.; Chung, T. D.; Seltzman, H. H.; Bai, Y.; Caron, M. G.; Barak, L. S.; Croatt, M. P.; Abood, M. E.; Reggio, P. H. Identification of the GPR55 Antagonist Binding Site Using a Novel Set of High-Potency GPR55 Selective Ligands. Biochemistry 2013, 52, 9456-969.
5. **Kotsikorou, E.**; Navas, F. 3rd; Roche, M. J.; Gilliam, A. F.; Thomas, B.; Seltzman, H. H.; Kumar, P.; Song, Z. H.; Hurst, D. P.; Lynch, D. L.; Reggio, P. H. The Importance of Hydrogen Bonding and Aromatic Stacking to the Affinity and Efficacy of Cannabinoid Receptor CB2 Antagonist, 5-(4-chloro-3-methylphenyl)-1-[(4-methylphenyl)methyl]-N-[(1S,2S,4R)-1,3,3-trimethylbicyclo[2.2.1]hept-2-yl]-1H-pyrazole-3-carboxamide (SR144528). J. Med. Chem. 2013, 56, 6593-6612.
6. **Kotsikorou, E.** and Reggio, P. H. Overview of Non-Cannabinoid Receptors: Chemistry and Modeling. In Abood, M.; Sorensen, R.; and Stella, N [eds.], CANNABINOIDS: Actions at Non-CB1/CB2 Cannabinoid Receptors. New York, NY: Springer Publishing Company, 2012. (Book Chapter)
7. **Kotsikorou, E.**; Madrigal, K. E.; Hurst, D. P.; Sharir, H.; Lynch, D. L.; Heynen-Genel, S.; Milan, L. B.; Chung, T. D.; Seltzman, H. H.; Bai, Y.; Caron, M. G.; Barak, L.; Abood, M. E.; Reggio, P. H. Identification of the GPR55 Agonist Binding Site Using a Novel Set of High-potency GPR55 Selective Ligands. Biochemistry. 2011, 50, 5633-5647.
8. Iliff, H. A.; Lynch, D. L.; **Kotsikorou, E.**; Reggio, P. H. Parameterization of Org27569: An Allosteric Modulator of the Cannabinoid CB1 G Protein-coupled Receptor. J. Comp. Chem. 2011, 32, 2119-2126.
9. **Kotsikorou, E.**; Lynch, D. L.; Abood, M. E.; Reggio, P. H. Lipid Molecular Dynamics Simulations Reveal Unique Conformations Associated with Lipid-derived Agonists of the Putative Cannabinoid Receptor GPR55. Chem. Phys. Lipids 2011, 164, 131-143.
10. Chen, Y.; Chen, C.; **Kotsikorou, E.**; Lynch, D. L.; Reggio, P. H.; Liu-Chen, P. Y. GEC1-{kappa} Opioid Receptor Binding Involves Hydrophobic Interactions: GEC1 has chaperone-like effect. J. Biol. Chem. 2009, 284, 1673-1685.
11. Fan, H.; **Kotsikorou, E.**; Hoffman, A. F.; Ravert, H. T.; Holt, D.; Hurst, D. P.; Lupica, C. R.; Reggio, P. H.; Dannals, R. F.; Horti, A. G. Analogs of JHU75528, a PET Ligand for Imaging of Cerebral Cannabinoid Receptors (CB1): Development of Ligands with Optimized Lipophilicity and Binding Affinity. Eur. J. Med. Chem. 2009, 44, 593-608.

12. **Kotsikorou, E.**; Sahota, G.; Oldfield, E. Bisphosphonate Inhibition of Phosphoglycerate Kinase: A Quantitative Structure Activity Relationship and Pharmacophore Modeling Investigation. J. Med. Chem. 2006, 49, 6692-6703.
13. **Kotsikorou, E.**; Song, Y.; Chan, J.; Faelens, S.; Tovian, Z.; Broderic, E.; Bakalara, N.; Docampo, R.; Oldfield, E. Bisphosphonate inhibition of the Exopolyphosphatase Activity of the *Trypanosoma brucei* Soluble Vacuolar Pyrophosphatase. J. Med. Chem. 2005, 48, 6128-6139.
14. Sanders, J. M.; Song, Y.; Chan, J. M. W.; Zhang, Y.; Jennings, S.; Kosztowski, T.; Odeh, S.; Flessner, R.; Schwerdtfeger, C.; **Kotsikorou, E**.; Meints, G. A.; Gomez, A. O.; Gonzalez-Pacanowska, D.; Raker, A. M.; Wang, H.; van Beek, E. R.; Papapoulos, S. E.; Morita, G. T.; Oldfield, E. Pyridinium-1-yl Bisphosphonates are Potent Inhibitors of Farnesyl Diphosphate Synthase and Bone Resorption. J. Med. Chem. 2005, 48, 2957-2963.
15. **Kotsikorou, E**.; Oldfield, E. "A Quantitative Structure Activity Relationship and Pharmacophore Modeling Investigation of Aryl-X and Heterocyclic Bisphosphonates as Bone Resorption Agents." J. Med. Chem. 2003, 46, 2932-2944.

PRESENTATIONS (* undergraduate student, ** graduate student)

1. **Kotsikorou, E.,** (May 23, 2020) Computational Study of the Allosteric Effects of the Androgen Receptor BF3 Site Mutations on Steroid Unbinding, ECE 2020, 22nd European Congress of Endocrinology, Prague, Czech Republic. (Presentation accepted – conference cancelled due to Covid-19)
2. Rosales, M.**, **Kotsikorou, E**., (March 30, 2020) Mutational Study of the GPR119 Receptor Binding Site, ENDO 2020, Endocrine Society Annual Meeting, San Francisco, CA. (Oral presentation accepted – conference cancelled due to Covid-19)
3. Chowdhury, M.**, Dean. F., **Kotsikorou, E.,** (March 28, 2020) Computational Study of the Effect of Androgen Receptor BF 3 Site Mutations on DDE Binding, ENDO 2020, Endocrine Society Annual Meeting, San Francisco, CA. (Poster presentation accepted – conference cancelled due to Covid-19)
4. Chowdhury, M.**, **Kotsikorou, E**., (April 29, 2019). Unbinding Pathways of Testosterone From the Androgen Receptor in the Presence of Endocrine Disrupting Chemicals, College of Sciences Annual Conference University of Texas Rio Grande Valley in Edinburg, TX.
5. **Kotsikorou, E**., (October 20, 2018). Exploring the Reliability of a Homology Model of GPR119 Receptor to Predict the EC50s of a Set of Agonist Compounds, Southwest Theoretical and Computational Chemistry Meeting 2018 The University of Texas Rio Grande Valley in Edinburg, TX.
6. Rosales, M.**, Cruz, A.*, **Kotsikorou, E**., (April 13, 2018). Docking Study of DDT and Analogues on Surface Binding Sites of the Estrogen and Androgen Receptors, College of Sciences Annual Conference University of Texas Rio Grande Valley in Edinburg, TX.

7. Cruz, A. R.*, Rosales, M. D.**, Dean, F., **Kotsikorou, E.,** (March 18, 2018). Docking Study of DDT and Analogues on Surface Binding Sites of the Estrogen and Androgen Receptors., 255th American Chemical Society National Meeting American Chemical Society in New Orleans, LA.
8. **Kotsikorou, E.,** Ortiz, B.*, Dean, F., (October 29, 2017). Molecular Modeling of the Estrogen Receptor Binding Function 3 Interactions with Diethyl Stilbestrol, Tamoxifen, and Its Analogues, 2017 ACS Southwest Regional Meeting American Chemical Society in Lubbock, TX.
9. Cruz, A.*, Rosales, M.**, **Kotsikorou, E.,** (October 6, 2017). Docking Study of DDT and Analogues in the Androgen Receptor BF-3 Surface Binding Site, 2017 UTSA College of Sciences Research Conference University of Texas San Antonio in San Antonio, TX.
10. Kowalski, S.* and **Kotsikorou, E**. Docking Study of Select GPR119 Receptor Inverse Agonists. 2017, 253rd American Chemical Society National Meeting and Exposition, San Francisco, CA.
11. Rosales, M. D.* and **Kotsikorou, E**. Docking Study of an Agonist and an Inverse Agonist in the GPR119 Receptor. 2017, College of Sciences Annual conference, UTRGV, Edinburg, TX.
12. Ortiz, B.* and **Kotsikorou, E**. Effects of Diethylstilbestrol on the Estrogen Receptor. 2017, College of Sciences Annual conference, UTRGV, Edinburg, TX.
13. Cruz, A.* and **Kotsikorou, E**. Endocrine Disrupting Chemicals and their Effects on Androgen Receptors. 2017, College of Sciences Annual conference, UTRGV, Edinburg, TX.
14. Kowalski, S.* and **Kotsikorou, E**. Conformational Study of Select GPR119 Receptor Ligands. 2017, College of Sciences Research Conference, UTSA, San Antonio, TX.
15. Luna, T.* and **Kotsikorou, E**. Leoidin: A Potential New Antibiotic against *P. Aeruginosa.* 2017, College of Sciences Research Conference, UTSA, San Antonio, TX.
16. Hamilton, J.* and **Kotsikorou E**. Parameterization of AR231453: A Potent Agonist for the Potential Treatment of Diabetes. 2016, 7th Annual PACE Bioethics Conference, UTRGV, Edinburg, TX.
17. Kowalski, S.* and **Kotsikorou, E.** Conformational Study of Select GPR119 Receptor Ligands. 2016, 7th Annual PACE Bioethics Conference, UTRGV, Edinburg, TX. (**won PACE Bioethics Student Research Award for undergraduates**)
18. Luna, T.* and **Kotsikorou, E.** Leoidin: A Potential New Antibiotic against *P. Aeruginosa.* 2016, 7th Annual PACE Bioethics Conference, UTRGV, Edinburg, TX.
19. Tamez, A.*; Askar, S.* and **Kotsikorou, E**. GPR119 Receptor: New Frontiers in Type 2 Diabetes Therapy, 2014, Undergraduate Research Conference, UT- Pan American, Edinburg, TX

20. Askar, S.* and **Kotsikorou, E**. Exploring the Binding Site of the G-Protein Coupled Receptor GPR119 Using a Pair of Diastereomers with Opposing Action, 2014, Biophysical Society Annual Meeting, San Francisco, CA.
21. **Kotsikorou, E.** Molecular Dynamics Simulations Applications in Biological and Material Sciences, 2013, UTPA Mechanical Engineering Department Seminar Series, Edinburg, TX (invited presentation).
22. **Kotsikorou, E.**; Hurst, D. P.; Reggio, P. H. The Importance of Hydrogen Bonding to the Binding Affinity of SR144528 at the CB2 Receptor, 2011, Carolina Cannabinoid Collaborative Conference, Durham, NC (Oral presentation).
23. **Kotsikorou, E.**; Hurst, D. P.; Sharir, H.; Rao, N.; Barak, L.; Caron, M.; Seltzman, H. H.; Heynen-Genel, S.; Milan, L. B.; Chung, T. D. Y.; Abood, M. E.; Reggio, P. H. Novel Agonists and Antagonists of the GPR55 Receptor, 2011, International Cannabinoid Research Society Annual Meeting, St. Charles, IL (Oral presentation).
24. **Kotsikorou, E.**; Madrigal, K. E.; Hurst, D. P.; Lynch, D. L.; Abood, M. E.; Reggio, P. H. Probing the binding site of GPR55 with LPI, 2-AGPI and AM251, 2010, International Cannabinoid Research Society Annual Meeting, Lund, Sweden, (**Michael J. Walker Award**).
25. **Kotsikorou, E.**; Lynch, D. L.; Hurst, D. P.; Abood, M. E.; Reggio, P. H. Conformational Analysis and Molecular Dynamics Study of 2-Arachidonoyl-sn-glycero-3-phosphoinositol (2-AGPI) and 1-Stearoyl-sn-glycero-3-phosphoinositol (LPI) in a POPC Bilayer, 2009, International Cannabinoid Research Society Annual Meeting, St. Charles, IL.
26. **Kotsikorou, E.**; Lynch, D. L.; Reggio, P. H. Conformational Analysis and Molecular Dynamics Study: 2-Arachidonoyl-sn-glycero-3-phosphoinositol (2-AGPI) in a POPC Bilayer, 2009, Biophysical Society Annual Meeting, Boston, MA.
27. **Kotsikorou, E.**; Norris, J. B.; Lynch, D. L.; Hurst, D. P.; Reggio, P. H. Identification of the Hemopressin Binding Site at CB1 Receptor, 2008, International Cannabinoid Research Society Annual Meeting, Aviemore, Scotland.

GRANT FUNDING

External Funding

NSF REU Discovery by Computation, Theory and Experiment — May 2017-Apr 2020
Position: Senior personnel
Grant amount: $303,768

Pramana Pharmaceuticals Project Collaboration — Aug. 2016-Dec. 2016
Position: PI
Grant amount: $8,000

Internal Funding

HHMI Undergraduate Support — Spring 2017

STEM ADVANCE Graduate Assistant Support Program — Spring and Summer 2015

Undergraduate Research Initiative Spring 2014
STEM ADVANCE Graduate Assistant Support Program Spring and Summer 2013

TEACHING EXPERIENCE

The University of Texas Rio Grande Valley, Edinburg TX and The University of Texas – Pan American, Edinburg TX

- CHEM 1111, General Chemistry I Lab, 14 courses.
- CHEM 3104, Physical Chemistry I Lab, 22 courses.
- CHEM 3105, Physical Chemistry II Lab, 9 courses.
- CHEM 3304, Physical Chemistry I, 12 courses.
- CHEM 4201, Chemistry Problems I, 7 courses.
- CHEM 4202, Chemistry Problems II, 6 courses.
- CHEM 4378, SpecTp-Computational Chemistry, 1 course.
- CHEM 6325, Physical Chemistry, 6 courses.
- CHEM 6360, Sp Top in Physical Chem, 6 courses.
- CHEM 7101, Seminar I, 4 courses.
- CHEM 7102, Seminar II, 5 courses.
- CHEM 7103, Seminar III, 4 courses.
- CHEM 7300, Thesis I, 2 courses.
- CHEM 7301, Thesis II, 3 courses.

STUDENT MENTORING

Master thesis supervision

- 4 graduated students
- 2 students in progress

Undergraduate research

- 17 students graduated
- 2 students in progress

Highschool student supervision

- 1 student

TECHNICAL SKILLS

Proficient with Unix/Linux. Proficient with Schrödinger (Maestro, Macromodel, Jaguar, Glide), MODELLER, Accelrys (Cerius^2, Insight II, Catalyst), and Tripos (Sybyl) modeling software. Experienced with NAMD and CHARMM molecular dynamics software and Tcl scripting.

AWARDS AND AFFILIATIONS

- Nominated for the Outstanding Mentor Award, University of Texas Rio Grande Valley, 2016.
- College of Science and Math Recognition for Student Mentoring, University of Texas – Pan American, 2015.
- American Institute of Chemists Award for Outstanding Postdoctoral Researcher, University of North Carolina at Greensboro, 2012
- Michael J. Walker Award for the Outstanding Postdoctoral Presentation, ICRS, 2010
- UIUC List of Teachers Ranked as Excellent by Students, University of Illinois at Urbana-Champaign, 2000
- International Cannabinoid Research Society member, 2008 – 2012
- Biophysical Society member, 2009 - 2013
- American Chemical Society member, 2013-present

SERVICE / COMMUNITY INVOLVEMENT

Service to the Academia

- Guest Editor for Special Issues:
    - One of six Guest Editors for the Special Issue in Physics International titled "Studies in History and Philosophy of Physics and Other Sciences"
    - One of three Guest Editors for the Special Issue in BioMed Research International titled "Computational Modeling of Large Neuronal Protein Structures and their Pharmacophores"
- Reviewed 7 manuscripts for the MDPI journals Journal of Molecular Sciences, Molecules, non-Coding RNA, and Polymers.

Service to the Department, College, and University

- University Committees
    - Faculty Reviewer for the Engaged Scholar Award (Fall 2016, Fall 2017)
    - Academic Information Technology Council (member, Fall 2013-Summer 2016)
    - **Women Faculty Network Achievement and Advancement Committee**
        - **Secretary, Fall 2015-Spring 2016**
        - **Chair, Fall 2017-Spring 2018**
- College Committees
    - Faculty Evaluation Criteria Document Committee (August 2016-Fall 2016)
    - STEM Mentor for the Chemistry Department at the Center for Excellence in STEM Sciences (Fall 2012-present)

- Departmental Committees
    - **Department Chair Search Committee (chair Fall 2019-Spring 2020)**
    - **Visioning Committee (co-chair Fall 2019-Spring 2020)**
    - **Graduate Program Coordinator (July 2017-December 2018)**
    - Curriculum Committee (Fall 2012-Summer 2015, Fall 2017-present)
    - Graduate Curriculum Committee (Fall 2015-present)
    - **Space Committee (Fall 2013-present, chair for Fall 2013-Summer 2015)**
    - Departmental Scholarship Committee (Fall 2015-present)
    - Peer Review of Teaching for one or two faculty per year (Fall 2014- present)
    - Graduate Program Committee (Fall 2012-Summer 2015)
    - **Annual Merit Evaluation Committee (Fall 2012-Summer 2015, co-chair Fall 2015-Summer 2017)**
    - **Physical Chemistry Search Committee (co-chair Fall 2012-Summer 2014, chair Fall 2014-Summer 205)**
    - Lecturer Search Committee (Fall 2012 – Summer 2015)
    - Library Committee (Fall 2012 – Summer 2015)
    - Strategic Planning/Program Review Committee (Fall 2012 – Summer 2015)
    - **Biochemistry Major Proposal Committee (Spring 2014)**
    - External Review Response Committee (Spring 2014)
    - Graduate Program Review Committee (Spring 2014)
    - **General Chemistry Committee (Spring 2013)**
    - HESTEC Poster Evaluation Committee (Fall 2012)

Service to the Students

- Graduate Thesis Committee chair for three students (Shane Askar (M.Sc. Chemistry, December 2015), Everado Villarreal II (M.Sc. Chemistry, May 2016), and John Hamilton (M.Sc. Chemistry, May 2017), Matthew Rosales (M.Sc. Chemistry May 2020))
- Graduate Committee member for 15 students (Maria Salinas, Carlos Tamez, Samuel Pina, Iram Lopez, Mariana Ocampo, Sean Pelfrey, Maria Pacheco, Jacob Sollner, Stephanie Palmer, Daniel Cantu, Tahyra Resto, Carolina Valdes, Jesus Cantu, Kenneth Flores, and Javier Perez)
- Advised over 110 Chemistry major students and over five graduate students.
- Wrote over 100 recommendation letters for graduate and undergraduate students. The letters were for medical schools, graduate programs, summer internship programs, school teaching positions, etc.

Service to the Community

- Judge for two science and engineering fairs:
    - Weslaco Independent School District Science and Engineering Fair for middle school and high school students (2013-present)

    - Annual RGV Regional Science and Engineering Fair for the Senior Division (2014-present)
- Guest Speaker at Edinburg North High School for the Science National honor Society Induction Ceremony (Oct 12, 2015)
- Hosted the ACS South Texas Chapter Meeting, guest speaker: Dr. Paul Alivisatos (December 7, 2012)
- Mentored a high school student for 7 weeks during the summer 2014 through the HHMI program. The student conducted research and prepared a poster that was presented the last day of the internship. The student won 3rd place (out of 12 posters) in the poster competition.
- Judged posters for the HESTEC week sponsored by UTPA, both for the High School, Undergraduate and Graduate level competitions, Edinburg, TX 2012.
- Organized and moderated the panel "Graduate Student to Postdoc: Negotiating the Transition" for the Early Careers Committee of the Biophysical Society 55th Annual Meeting, Baltimore, ME 2011.
- Judged posters for the 10th Annual Poster and Vendor Night sponsored by Syngenta and the Central North Carolina section of ACS, Greensboro, NC 2010.