Daniel P. Flaherty

Ph.D. in pharmaceutical science with expertise in medicinal chemistry

575 Stadium Mall Dr. Heine Pharmacy Building West Lafayette, IN 47907
Phone: (913) 944-1845
Email: dflaher@purdue.edu
Flahertylab.purdue@gmail.com
Website: Flahertylab.com
Twitter: @FlahertyLab

Education

2005 - 2010 **University of Nebraska Medical Center**
Ph.D. in Pharmaceutical Science

2001 - 2005 **Central College, Pella, IA**
B.A. in Chemistry, Summa Cum Laude

Appointments

January 2024 – Present Chip and Jane Rutledge Early Career Associate Professor, **Purdue University**
Borch Department of Medicinal Chemistry and Molecular Pharmacology

August 2022 – Dec 2023 Associate Professor with Tenure, **Purdue University**
Department of Medicinal Chemistry and Molecular Pharmacology

July 2015 – July 2022 Assistant Professor, **Purdue University**
Department of Medicinal Chemistry and Molecular Pharmacology

2014 – 2015 Assistant Research Professor, **University of Kansas**
Higuchi BioSciences Center.
Mentor: Jeffrey Aubé, Ph.D.

2010 – 2014 Postdoctoral Research Associate, **University of Kansas**
Specialized Chemistry Center, NIH Medicinal Chemistry Center for Molecular Libraries Probe Production Network.
Mentor: Jeffrey Aubé, Ph.D.

2005 - 2010 Graduate Research Associate, **University of Nebraska Medical Center**
Department of Pharmaceutical Sciences
Mentor: Jonathan L. Vennerstrom, Ph.D.

2003 – 2005 Undergraduate researcher, **Central College**
Department of Chemistry
Mentor: James A. Shriver, Ph.D.

Affiliations

- Senior Visiting Fellow, School of Chemistry, Faculty of Science, University of New South Wales, Sydney Australia, 1/2025 – 5/2025.
- Adjunct Associate Professor of Pharmacology & Toxicology; Indiana University School of Medicine – West Lafayette
- Purdue Institute for Inflammation, Immunology, and Infectious Disease; Control and Intervention Division
- Purdue Institute for Integrative Neuroscience
- Purdue University Center for Cancer Research; Medicinal Chemistry Division

- Purdue Institute for Drug Discovery
- American Chemical Society; Medicinal Chemistry Division; 2005 - present

Funding

Current:

6. Purdue Office of Research
"Development of adenylyl cyclase 2 inhibitors for neurological disorders"
Flaherty/Watts, Co-PI
Direct Costs: $60,000
The goal of this project is to carry out early hit optimization of a new selective inhibitor for AC2.

5. Purdue Institute for Cancer Research
"Development of covalent inhibitors of UCHL3 for cancer target validation"
Flaherty, PI
Direct Costs: $50,000
The goal of the project is to carry out early hit optimization of covalent UCHL3 inhibitors.

4. NIAID 1R01AI175024 "Inhibitors of adaptive efflux mediated resistance in *Acinetobacter baumannii*"
Flaherty/Dunman, MPI
Period: 3/7/2023 – 3/6/2028
Total Costs: $2,912,287 over entire project
Identification and development of novel small molecules that inhibit the adaptive efflux resistance phenomenon in the *Acinetobacter baumannii*

3. NIAID 1R01AI153264 "Development of novel anti-*Neisseria gonorrhoeae* therapeutic agents"
Flaherty/Seleem, MPI
Period: 8/12/2022 – 7/31/2026
Total Costs: $3,055,792 over entire project
Development of anti-gonococcal agents targeting bacterial carbonic anhydrases.

2. NINDS 1R01NS119917 "Pharmacological validation of adenylyl cyclase 1 as a drug target for chronic pain"
Flaherty/Watts MPI
Period: 12/01/2020 – 11/30/2025
Direct Costs: $250,000/yr
The goal of this project is to develop potent and selective inhibitors of adenylyl cyclase type 1 with physical chemical properties to access the target within the central nervous system to validate AC1 as a viable therapeutic option to treat chronic pain.

1. NIAID 1R01AI148523 "Repurposing novel selective drugs for treatment and decolonization of vancomycin-resistant enterococcus"
Seleem, PI; Flaherty Co-I,
Period: 10/01/19 – 8/31/2024
Direct costs to Flaherty Lab: $224,800/yr
The goal of the project is to optimize FDA-approved molecules with activity against VRE for the treatment of systemic VRE infection and VRE gut decolonization.

Completed:

19. Purdue Institute for Drug Discovery High-Throughput Screening Grant "Identification of covalent inhibitors for the deubiquitinating enzyme UCHL3"
Flaherty, PI

Direct Costs: $16,000
The goal of this project is to conduct a high-throughput screen for irreversible inhibitors of the deubiquitinating enzyme UCHL3.

18. NIAID 1R01AI134685 "Antibacterial inhibitors of RnpA"
Dunman, PI; Flaherty Co-I
Period: 9/01/18 – 4/30/2023: NCE through 3/31/2024
Direct costs to Flaherty Lab: $238,000/yr
The goal of the project is to use a targeted ligand and structure-based design approach to develop novel inhibitors of *Staphylococcus aureus* RnpA.

17. Purdue Institute for Drug Discovery External Advisory Board Program
Flaherty, PI
"Preclinical and IND Enabling Studies for Anti-VRE Therapeutic Agents"
7/1/2022 – 12/31/2023
Direct Costs: $30,000
For *in vivo* PK and efficacy in a Rat endocarditis model for VRE infection for two lead molecules.

16. NINDS 1R61NS111070 "Non-opioids for inflammatory pain: adenylyl cyclase 1 as a novel target"
Roman, PI (U of Iowa)/Watts Co-PI (Purdue University); Flaherty Co-I
Period: 5/1/2021 – 4/30/2023
Hit-to-probe optimization of AC1-CaM PPI inhibitors as probes for target validation to treat chronic pain.

15. Purdue Institute for Drug Discovery Programmatic Grant
Flaherty/Das/Wendt/Hu, Co-PIs
"Development of covalent inhibitors of UCHL1 and UCHL3 for cancer drug discovery"
Period: 12/01/2021 – 11/30/2023
Direct Costs: $50,000/yr
The goal of this project is to perform hit-to-lead optimization of novel covalent inhibitors for the deubiquitinating enzymes UCHL1 and UCHL3. We will use these inhibitors to establish efficacy in models for neuroendocrine prostate cancer, breast cancer, and pancreatic cancer.

14. EVPRP Research Instrument Grant Program
Flaherty, PI; Trader, Altman, Davisson, Co-Is
"Acquisition of multi-column HPLC for separation and purification of chiral molecules"
Period: 1/21/2022 – 5/31/2022
Direct Costs: $98,565
For the purchase of an Agilent 12600 HPLC with 8-column switch valve and fraction collector for the scouting of chromatographic separation conditions and purification of chiral molecules.

13. Purdue Institute for Drug Discovery Programmatic Grant "Drug-repurposing to combat resistant pathogens"
Flaherty, Seleem, Hazbun (Co-I's)
Period: 7/1/18 – 6/30/20
Direct costs to Flaherty Lab: $33,333/yr
The goal of this project is to perform hit-to-lead optimization on FDA approved drugs that inhibit problematic resistant pathogens such as vancomycin-resistant enterococcus, *Neisseria gonorrhoeae*, and *Candida albicans*

12. Purdue Institute for Drug Discovery Hit-to-lead grant "Optimization of inhibitors for AC8"
Flaherty, Watts (Co-I's)
Period: 7/1/19 – 6/30/20
Direct costs to Flaherty Lab: $50,000/yr
The goal of this project is to perform hit-to-lead optimization on two new scaffolds that show inhibitory activity against adenylyl cyclase type 8.

11. Provost's Instructional Equipment Grant "Adding high-performance liquid chromatography experience to undergraduate laboratories"
    Flaherty, PI; 0% Salary support
    Period: 01/01/2020 – 12/31/2020 $61,318 total costs
    This proposal is funded to purchase a U-HPLC system to interface with the existing Advion mass spectrometer that was purchased with the previous Provost's instructional equipment award (2018). This will increase the capabilities of the instrument and allow it to be used for both undergraduate organic labs and BSPS laboratory modules.

10. EVPRP Lab and Core Equipment Grant "Acquisition of a Biacore X-100 Surface Plasmon Resonance Instrument"
    Flaherty, PI
    Period 1/1/2019 – 12/31/2019
    Direct costs: $99,720
    This proposal was for the purchase of a Biacore X-100 surface plasmon resonance instrument to be housed in the Hall for Discovery and Learning Research to be used for walk-up analysis of small molecule binding affinities.

9. Purdue Center for Cancer Research Phase 1 Concept Award "Structure-based design of selective Ubiquitin C-terminal Hydrolase L1 probe"
    Flaherty, PI; 0% salary support
    Period: 02/01/2019 – 1/31/2020 $15,000 total costs
    The goal of this proposal is to use rational design to develop the best-in-class UCHL1 inhibitor as a probe for the UCHL1 biology.

8. Purdue University Discovery Park Big Idea Challenge "Revolutionizing control of vector-borne infectious disease"
    Hill, PI; Flaherty, Watts, Raymond, Co-PI; 5% effort
    Period: 04/2017 – 03/2019
    The goal of this project is to identify novel chemical space for development of new insecticides. We will focus high-throughput screening efforts against mosquito larvae that provide non-lethal phenotypes. This hit criteria is different than decades of previous HTS campaigns in search of novel insecticides that are also safe for the environment. My labs role will be hit identification and preliminary SAR optimization.

7. Purdue Center for Cancer Research Phase 1 Concept Award "Development of novel cell-based ALPHA deubiquitinase inhibition assay"
    Flaherty, PI; 0% salary support
    Period: 01/01/2018 – 06/2018 $15,000 total costs
    The goal of this proposal is to develop a cell-based deubiquitinase (DUB) assay to screen for inhibitors in disease relevant cell lines. Current DUB biochemical assays have little biological relevance contributing to the severe lack of potent and selective DUB inhibitors. To address this drawback we propose to develop an assay using AlphaLISA technology to identify small molecules that perturb the interactions of ubiquitin activity-based probes with the DUBs, in this case applied to UCHL1. This assay is being developed to be applied to cells and recognize endogenous levels of UCHL1 and in theory could be applied to other cells lines or DUBs.

6. MCMP Research Enhancement Award "Development of highly selective inhibitors of AC1 for the evaluation in a mouse model of chronic pain"
    Watts, PI; Flaherty, Co-I – No salary support
    Period: 04/01/2017 – 03/31/2018 $12,000 for Flaherty Lab
    This project seeks to develop novel potent inhibitors for adenylyl cyclase 1 (AC1) with selectivity over the other eight closely related isoforms. Two novel AC1 inhibitor scaffolds have been identified via high-throughput screening and early stage hit-to-lead optimization is underway to optimize for potency and selectivity.

5. Provost's Instructional Equipment Grant "Adding Mass Spectrometry Capabilities to Enhance Pharmacy Education"
    Flaherty, PI; 0% Salary support
    Period: 01/01/2018 – 12/31/2018 $68,000 total costs

This proposal is funded to purchase a user-friendly mass spectrometer to be housed in the undergraduate organic laboratory. This MS will be incorporated into laboratory modules to provide students hands-on experience collecting and analyzing MS data. This will reinforce topics students learn during lecture and provide an instrument to design new, innovative laboratory modules around.

4. Purdue Institute for Drug Discovery "Lead Generation from DNA-encoded Fragment Libraries Enabled by Covalent Crosslinking"
   Flaherty, Co-PI; Krusemark, Co-PI; 0% effort
   Period: 11/01/16 – 10/31/17 $5,000 total costs
   This project will explore the utility of combining the power of DNA-encoded libraries with fragment-based drug discovery to provide a novel method for hit identification.

3. Purdue Institute for Drug Discovery "Discovery of novel UCHL1 small molecule inhibitors"
   Flaherty, PI; 0% effort
   $15,000 credit for high-throughput screening
   Credit to the Purdue Chemical Genomics Facility to perform a high-throughput screen for inhibitors of UCHL1.

2. Purdue University Showalter Trust Award "Discovery of novel and selective inhibitors for UCHL1"
   Flaherty, PI; 10% effort
   Period: 07/01/16 – 06/30/18 $75,000 total costs
   This project seeks to utilize fragment-based hit identification techniques to develop novel, best-in-class inhibitors versus ubiquitin C-terminal hydrolase L1 (UCHL1). These inhibitors will serve as valuable probes to study the diverse role UCHL1 serves in neurodegenerative disease and cancer. Ultimately, high priority inhibitors will be utilized to determine the efficacy of UCHL1 inhibition in the treatment of breast cancer metastasis.

1. NIAID 1R21AI115251 "Ribonuclease E: a novel new Gram-negative antimicrobial target"
   Flaherty, Co-PI; 15% effort
   Period: 04/01/2016 – 03/31/2018 $193,196 total direct costs
   Utilize a bi-lateral fragment-based and traditional high-throughput screening-based approach to identify first-in-class inhibitors of RNase E from multiple Gram-negative pathogens. These inhibitors will serve initially as probes to validate RNase E as a viable antimicrobial therapeutic target with the highest priority analogs progressing to more exhaustive structure-based optimization and biological studies.

Honors/Awards

- Seed for Success Acorn Award – Purdue Office of Research – 2019, 2020, 2024
- Fulbright U.S. Scholar – Australia-United States Fulbright Commission, Sydney, Australia – 2024/2025
- Chaney Family Early Faculty Scholar Award – Purdue College of Pharmacy – 2023
- Best Oral Presentation – 4th International Symposium on Frontiers in Molecular Science – Florence, Italy – 2022
- Chemistry Europe Poster Prize – 37th ACS National Medicinal Chemistry Symposium – New York, NY – 2022
- Purdue Favorite Faculty Nominee - 2022
- Purdue Favorite Faculty Nominee - 2017
- University of Nebraska Medical Center (UNMC) Presidential Graduate Fellow, 2009 – 2010
- American Foundation for Pharmaceutical Education Pre-Doctoral Fellow, 2007 – 2010
- UNMC Berndt Travelship, 2009
- UNMC Graduate Fellow, 2008 – 2009
- Peter Gwilt Pharmaceutical Sciences Travelship, 2008
- Harris Award Recipient for Alzheimer's Disease Research (UNMC), 2008
- Nancy and Ronald Reagan Alzheimer's Scholarship Winner, 2008
- Josiah Kirby Lilly, Sr. Memorial AFPE Pre-Doctoral Fellow, 2007 – 2008
- Bukey Fellow, Pharmaceutical Sciences Graduate Program (UNMC), 2007 – 2008
- UNMC Pharmaceutical Sciences Teaching Assistantship, 2005 – 2006

Professional Service

Editorial Board

Journal of Enzyme Inhibition and Medicinal Chemistry

Review Editor for *Frontiers in Molecular Biosciences*

Peer Reviewer for Scientific Journals

- Cell Chemical Biology
- Chemical Biology & Drug Design
- mSphere
- Journal of Medicinal Chemistry
- ChemMedChem
- ACS Medicinal Chemistry Letters

Study Section Appointments:

- NIH Drug Discovery and Molecular Pharmacology A (DMPA) *Standing Member* – 2024 – 2028
- NIH Special Emphasis Panel ZAI1 RK-M (C4) (*ad hoc*) – 2023
- DoD PRMRP Review Panel (*ad hoc*) – 2023
- NIH Special Emphasis Panel ZRG1 DCAI-M(02) (*ad hoc*) – 2023
- NIH Anti-Infective Resistance and Targets Study Section - AIRT (*ad hoc*), 2023
- NIH Drug Discovery and Mechanisms of Antimicrobial Resistance study section (*ad hoc*), 2022
- NIH HEAL Initiative U19 Study Section, 2021
- DoD MIDRP Panel, 2020
- NIH CARBIRU Special Emphasis Panel (*ad hoc*), 2020
- NIH Drug Discovery for the Nervous System Study Section (*ad hoc*), 2020
- Indiana CTSI, 2019
- DoD CDMRP, 2019
- DoD PRMRP, 2019
- Florida Department of Health, 2018 - 2019

University Service

- Department Level
  - Cume Assessment Committee (2015 – 2018)
  - Cume Task Force (2018)
  - Journal Club Task Force (2018)
  - MCMP Faculty Search Committee (2017)
  - MCMP representative of joint MCMP and Chemistry faculty search committee (2018)
  - Adjunct Faculty Task Force (2020)
  - MCMP Graduate Program Admissions Committee (2020 – 2024)
  - MCMP Graduate Curriculum Evaluation Working Group (2022-23)
  - Mark Cushman Lectureship Planning Group (2023)
  - MCMP Strategic Planning Committee Working Group (2023)
  - MCMP Department Retreat Organizer (2023)
  - MCMP Graduate Curriculum Committee (2023-present)

- College Level
  - BSPS Oversight Committee Member (2016 – 2021)
  - Strategic Planning Task Force – Faculty Recruitment and Retention
  - Evaluator for PharmD Annual Performance Evaluation (APE) – 2019, 2021, 2022
  - Grade Appeals Committee – 2020, 2022, 2023
  - Evaluator for PharmD Annual Performance Evaluation (APE) – 2021, 2022
  - Interviewer for PharmD admissions applications (2016 – 2019, and 2021, 2023)
  - Scholarship and Awards Committee (2021 – 2024)
  - Professional Program Curriculum Committee (2023 – 2026)
  - Graduate Fellowship Committee (2024)

- University Level
  - Member of PULSe admissions committee for chemical biology training group (2017 – 2019)
  - PIDD Chemical Genomics Facility advisory committee
    - Chair of committee 2022 – Present
  - Grant Peer Reviewer for PCCR Phase 1 grants – 2022
  - Training Program Internal Committee Member – May 2022 – present.
  - ADVANCE Purdue FAST panelist – April 2023

Publications

53. Shrinidhi, A.; Dywer, T.S.; Scott, J.A.; Watts, V.J.; **Flaherty, D.P.*** Pyrazolo-Pyrimidinones with Improved Solubility and Selective Inhibition of Adenylyl Cyclase Type 1 Activity for Treatment of Inflammatory Pain. *Journal of Medicinal Chemistry*, **2024**, *67*, 18290 – 18316. https://doi.org/10.1021/acs.jmedchem.4c01645.

52. Youse, M. Y.; Abutaleb, N.S.; Nocentini, A.; Abdelsattar, A. S.; Ali, F.; Supuran, C. T.; Seleem, M. N.; **Flaherty, D. P**.* Optimization of Ethoxzolamide Analogs with Improved Pharmacokinetic Properties for *In Vivo* Efficacy against *Neisseria gonorrhoeae*. *Journal of Medicinal Chemistry*, **2024**, *67,* 15537 – 15556. https://doi.org/10.1021/acs.jmedchem.4c01187.

51. Bonardi, A.; Nocentini, A.; Giovannuzzi, S.; Paoletti, N.; Ammara, A.; Bua, S.; Abutaleb, N. S.; Abdelsattar, A. S.; Capasso, C.; Gratteri, P.; **Flaherty, D. P.**; Seleem, M. N.; Supuran, C. T. Development of Penicillin-Based Carbonic Anhydrase Inhibitors Targeting Multidrug-Resistance *Neisseria gonorrhoeae. Journal of Medicinal Chemistry*, **2024**, *just accepted.* doi: https://doi.org/10/1021/acs.jmedchem.4c00740.

50. Holly, K. J.; Kataria, A.; **Flaherty, D. P.***; Groshong, A.* Unguarded liabilities: Borrelia burgdorferi's complex amino acid dependence presents a unique target for inhibition. *Frontiers in Antibiotics,* **2024**, *3*, 1395425. doi: https://doi.org/10.3389/frabi.2024.1395425.

49. Camara, A.; Chugh, H.; George, A.; Dolidze, L.; Ryu, K.; Holly, K. J.; **Flaherty, D. P.**; Mattoo, S. Discovery and Validation of a Novel Inhibitor of HYPE-mediated AMPylation. *Cell Stress and Chaperones*. **2024**, *29*, 404 – 424. doi: https://doi.org/10.1016/j.cstres.2024.04.001.

48. Jena, B. C.; **Flaherty, D. P.**; O'Brien, V. P.; Watts, V. J. Biochemical Pharmacology of Adenylyl Cyclases in Cancer. *Biochemical Pharmacology*, **2024**, *in press.* doi: https://doi.org/10.1016/j.bcp.2024.116160

47. Imhoff, R.; Patel, R.; Safdar, M. H.; Jones, H.; Pinto-Fernandez, A.; Vendrell, I.; Chen, H.; Muli, C.; Krabill, A.; Kessler, B.; Wendt, M. Das, C.; **Flaherty, D. P.*** Covalent Fragment Screening and Optimization Identifies Chloroacetohydrazide Scaffold as Inhibitors of Ubiquitin C-Terminal Hydrolase L1. *Journal of Medicinal Chemistry*, **2024**, *67*, 4496 - 4524. doi: https://doi.org/10.1021/acs.jmedchem.3c01661

46. Tang, H.; Gupta, A.; Morrisroe, S.; Bao, C.; Schwantes-An, T.-H.; Gupta, G.; Liang, S.; Sun, Y.; Chu, A.; Luo, A.; Elangovan, V.R.; Sangam, S.; Shi, Y.; Naidu, S.; Jheng, J.-R.; Ciftci-Yilmaz, S.; Warfel, N.; Hecker, L.; Mitra, S.;

Coleman, A.; Lutz, K.; Pauciulo, M.; Lai, Y.-C.; Javaheri, A.; Dharmakumar, R.; Wu, W.-H.; **Flaherty, D. P.**; Karnes, J.; Breuils-Bonnet, S.; Boucherat, O.; Bonnet, S.; Yuan, J.; Jacobson, J.; Duarte, J.; Nichols, W.; Garcia, J.; Desai, A. Deficiency of the Deubiquitinase UCHL1 Attenuates Pulmonary Hypertension. *Circulation*, **2024**, *150*, 302 – 316. Doi: doi.org/CIRCULATIONAHA.123.065304

45. Kenny, S.; Lai, C-H.; Chiang, T-S.; Brown, K.; Hewitt, C. S.; Krabill, A. D.; Chang, H-T.; Wang, Y-S.; **Flaherty**, **D. P.**; Hsu, S-T.; Das, C. Altered protein dynamics and a more reactive catalytic cysteine in a neurodegeneration-associated UCHL1 mutant. *Journal of Molecular Biology*, **2024**, *436*, 168438. doi: https://doi.org/10.1016/j.jmb.2024.168438

44. Giovannuzzi, S.; Marakpaka, A. K.; Abutaleb, N. S.; Carta, F.; Liang, H-W.; Nocentini, A.; Pisano, L.; Seleem, M. N.; **Flaherty, D. P.**; Supuran, C. T. Inhibition of pathogenic bacterial carbonic anhydrases by monothiocarbamates. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2023**, *38*, 2284119. doi: https://doi.org/10.1080/14756366.2023.2284119

43. Imhoff, R. D.; Rosenthal, M. R.; Ashraf, K.; Bhanot, P.; Ng, C. L.; **Flaherty, D. P.*** Identification of covalent fragment inhibitors for *Plasmodium falciparum* UCHL3 with anti-malarial efficacy. *Bioorganic and Medicinal Chemistry Letters*, **2023**, *94*, 129458*,* doi: https://doi.org/10.1016/j.bmcl.2023.129458.

42. Graboski, A. L.; Kowalewski, M. E.; Simpson, J. B.; Cao, X.; Ha, M.; Zhang, J.; Walton, W. G.; **Flaherty, D. P.**, Redinbo, M. R. Mechanism-based inhibition of gut microbial tryptophanases reduces serum indoxyl sulfate. *Cell Chemical Biology*, **2023**, *30*, 1402 – 1413. doi: https://doi.org/10.1016/j.chembiol.2023.07.015

41. Young, M.; Chojnacki, M.; Blanchard, C.; Cao, X.; Johnson, W. L.; **Flaherty**, **D. P.***; Dunman, P. D.* Genetic Determinants of *Acinetobacter baumannii* serum-associated adaptive efflux-mediated antibiotic resistance. *Antibiotics*. **2023**, *12*, 1173 – 1195.

40. Chilambi, G. S.; Wang, Y-H.; Wallace, N.; Obiwuma, C.; Evans, K.; Li, Y. Shalaby, M-A.; **Flaherty, D. P.**; Shields, R.; Doi, Y.; Van Tyne, D. Carbonic anhydrase inhibition as a target for antibiotic synergy in enterococci. *Microbiology Spectrum*, **2023**, *published online, e03963-22.*

39. Abutaleb, N. S.; Shrinidhi, A.; Bandara, A. B.; Seleem, M. N.; **Flaherty, D. P.*** Evaluation of 1,3,4-thiadiazole carbonic anhydrase inhibitors for gut decolonization of vancomycin-resistant enterococci. *ACS Medicinal Chemistry Letters*, **2023**, *14*, 487 – 492.

38. Marapaka, A. K.; Nocentini, A; Youse, M. S.; An, W.; Holly, K. J.; Das, C.; Yadav, R.; Seleem, M. N.; Supuran, C. T.; **Flaherty, D. P.*** Structural characterization of thiadiazolesulfonamide inhibitors bound to *Neisseria gonorrhoeae* α-carbonic anhydrase. *ACS Medicinal Chemistry Letters*, **2023**, *14*, 103 - 109.

37. Dwyer, T.; O'Brien, J. B.; Ptak, C.; LaVigne, J. E.; **Flaherty, D. P.**; Watts, V. J.; Roman, D. L. Protein-protein interaction-based high throughput screening for adenylyl cyclase 1 inhibitors: design, implementation, and discovery of a novel chemotype. *Frontiers Pharmacology*, **2022**, *13*, 977742.

36. An, W.; Holly, K. J.; Nocentini, A.; Imhoff, R. D.; Hewitt, C. S.; Abutaleb, N. S.; Cao, X.; Seleem, M. N.; Supuran, C. T.; **Flaherty, D. P.*** Structure-activity relationship studies for inhibitors for vancomycin-resistant *Enterococcus* and human carbonic anhydrases. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2022**, *37*, 1838-1844, DOI: 10.1080/14756366.2022.2092729

35. Scott, J. A.; Soto-Velasquez, M.; Hayes, M. P.; LaVigne, J. E.; Miller, H. R.; Kaur, J.; Ejendal, K. F. K.; Watts, V. J.*; **Flaherty, D. P.*** Optimization of a pyrimidinone series for selective inhibition of Ca^{2+}/calmodulin-stimulated adenylyl cyclase 1 activity for treatment of chronic pain. *Journal of Medicinal Chemistry*, **2022**, *65*, 4667 - 4686. https://doi.org/10.1021/acs.jmedchem.1c01759

34. Giovannuzzi, S.; Hewitt, C. S.; Nocentini, A.; Capasso, C.; Costantino, G.; **Flaherty, D. P.***; Supuran, C. T.* Inhibition studies of bacterial α-carbonic anhydrases with phenols. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2022**, *37*, 666-671. https://doi.org/10.1080/14756366.2022.2038592

33. Murgia, M.V.; Sharan, S.; Kaur, J.; Austin, W.; Hagen, L.; Wu, L.; Chen, L.; Scott, J. A.; **Flaherty, D. P.**; Scharf, M. E.; Watts, V. J.; Hill, C. A. High-content phenotypic screening identifies novel chemistries that disrupt mosquito activity and development. *Pesticide Biochemistry and Physiology*, **2022**, *182*, 105037. https://doi.org/10.1016/j.pestbp.2022.105037

32. Hewitt, C. S.; Das, C.; **Flaherty, D. P.*** Rational development and characterization of a ubiquitin variant with selectivity for ubiquitin C-terminal hydrolase L3. *Biomolecules*, **2022**, *12*, 62. https://doi.org/10.3390/biom12010062

31. Giovannuzzi, S.; Hewitt, C. S.; Nocentini, A.; Capasso, C.; **Flaherty, D. P.***; Supuran, C. T.* Coumarins effectively inhibit bacterial α-carbonic ahydrases. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2022**, *37*, 333-338. https://doi.org/10.1080/14756366.2021.2012174

30. Abutaleb, N. S.; Elhassanny, A. E. M.; Nocentini, A.; Hewitt, C. S.; Elkashif, A.; Cooper, B. R.; Supuran, C. T.; Seleem, M. N.* **Flaherty, D. P.*** Repurposing FDA-approved sulphonamide carbonic anhydrase inhibitors for treatment of *Neisseria gonorrhoeae*. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2022**, *37*, 51-61. DOI: 10.1080/14756366.2021.1991336.

29. Giovannuzzi, S.; Abutaleb, N. S.; Hewitt, C. S.; Carta, F.; Nocentini, A.; Seleem, M. N.; **Flaherty, D. P.***, Supuran, C. T.* Dithiocarbamates effectively inhibit the α-carbonic anhydrase from *Neisseria gonorrhoeae*. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2022**, *37,* 1-8. DOI:10.1080/14756366.2021.1988945.

28. **Flaherty, D. P.**; Seleem, M. N.; Supuran, C.T. Bacterial Carbonic Anhydrases: Underexploited Antibacterial Therapeutic Targets. *Future Medicinal Chemistry*, **2021**, *13*, 1619-1622. DOI: 10.4155/fmc-2021-0207.

27. Nocentini, A.; Hewitt, C. S.; Mastrolorenzo, M.; **Flaherty, D. P.***; Supuran, C. T.* Anion inhibition studies of the α-carbonic anhydrase from *Neisseria gonorrhoeae*. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2021**, *36*, 1061 - 1066. DOI: 10.1080/14756366.2021.1929202.

26. Hewitt, C. S.; Abutaleb, N. S.; Elhassanny, A. E. M.; Nocentini, A.; Cao, X.; Amos, D. P.; Youse, M. S.; Holly, K. J.; Marapaka, A.; An, W.; Kaur, J.; Krabill, A. D.; Elkashif, A.; Elgammal, Y.; Graboski, A. L.; Supuran, C. T.; Seleem, M. N.; **Flaherty, D. P.*** Structure-Activity Relationship Studies of Acetazolamide-Based Carbonic Anhydrase Inhibitors with Activity against *Neisseria gonorrhoeae*. *ACS Infectious Diseases*, **2021**, *7*, 1969 – 1984. DOI: 10.1021/acsinfecdis.1c00055.

25. Chojnacki, M.; Cao, X.; **Flaherty, D. P.***; Dunman, P. D.* Optimization of 2-acylaminocycloalkythiophene derivatives for activity against *Staphylococcus aureus* RnpA. *Antibiotics*, **2021**, *10*, 369 - 386.

24. Krabill, A.D.; Chen, H.; Hussain, S.; Hewitt, C.S.; Imhoff, R.D.; Muli, C.S.; Das, C.; Galardy, P.J.; Wendt, M.K.; **Flaherty, D.P.*** Optimization and Anti-Cancer Properties of Fluoromethylketones as Covalent Inhibitors for Ubiquitin C-Terminal Hydrolase L1. *Molecules*, **2021**, *26*(5), p.1227. https://doi.org/10.3390/molecules26051227. ** Invited Manuscript for special issue on covalent inhibitors **

23. Sheedlo, M. J.; Kenny, S.; Podkoytov, I. S.; Brown, K.; Ma, J.; Iyer, S.; Hewitt, C. S.; Arbough, T.; Mikhailovskii, O.; **Flaherty D. P.**; Wilson, M. A.; Skrynnikov, N. R.; Das, C. Insights into Ubiquitin Product Release in Hydrolysis Catalyzed by the Bacterial Deubiquitinase SdeA. *Biochemistry*, **2021**, *60*, 584 – 596. DOI:10.1021/acs.biochem.0c00760.

22. Abutaleb, N. S.; Elhassanny, A. E. M.; **Flaherty, D. P.**; Seleem, M. N. *In vitro* and *in vivo* activities of carbonic anhydrase inhibitor, dorzolamide, against vancomycin-resistant enterococci. *PeerJ*, **2021**, *9*:e110059.

21. Abutaleb, N. S.; Elkashif, A.; **Flaherty, D. P.**; Seleem, M. N. *In vivo* antibacterial activity of acetazolamide. *Antimicrobial Agents and Chemotherapy*, **2021**, *65*, e01715 – 01720. DOI: 10.1128/AAC.01715-20.

20. Hewitt, C. S.; Krabill, A. D.; Das, C.; **Flaherty, D. P.** Development of Ubiquitin Variants with Selectivity for Ubiquitin C-Terminal Hydrolase Deubiquitinase. *Biochemistry*, **2020**, *59* (37), 3447 – 3462. DOI: 10.1021/acs.biochem.9b01076.

19. Kaur, J.; Cao, X.; Abutaleb, N. S.; Elkashif, A.; Graboski, A. L.; Krabill, A. D.; AbdelKhalek, A. H.; An, W.; Bhardwaj, A.; Seleem, M. N.; **Flaherty, D. P.** Optimization of Acetazolamide-Based Scaffold as Potent Inhibitors of Vancomycin-Resistant Enterococcus. *Journal of Medicinal Chemistry*, **2020**, *63*(17), 9540-9562. DOI:10.1021/acs.jmedchem.0c00734.

18. Chojnacki, M.; Cao, X.; Young, M.; Fritz, R.; Dunman, P. M.; **Flaherty, D. P.** Optimization of 4-substituted Benzenesulfonamide Scaffold to Reverse *Acinetobacter baumannii* Serum-Adaptive Efflux Associated Antibiotic Tolerance. *ChemMedChem*, **2020**, *15* (18), 1731-1740. DOI: 10.1002/cmdc/202000328.

17. Saboo S.; Kestur, U.S.; **Flaherty, D.P.**, Taylor, L.S. Congruent Release of Drug and Polymer from Amorphous Solid Dispersions: Insights into the Role of Drug-Polymer Hydrogen Bonding, Surface Crystallization, and Glass Transition. *Molecular Pharmaceutics*, **2020**, *17*(4), 1261-1275.

16. Krabill, A.D., Chen, H., Hussain, S., Feng, C., Abdullah, A., Hewitt, C.S., Das, C., Aryal, U.K., Post, C.B., Wendt, M.K., Galardy, P.J. and **Flaherty, D.P.** Ubiquitin C-terminal hydrolase L1: Biochemical and Cellular Characterization of a Covalent Cyanopyrrolidine-Based. Inhibitor. *ChemBioChem,* **2020**, *21*, 712-722.

15. Colquhoun, J. M.; Ha, L.; Beckley, A.; Meyers, B.; **Flaherty, D. P.**; Dunman, P. M.; Identification of Small Molecule Inhibitors of *Staphylococcus aureus* RnpA. *Antibiotics*, **2019**, *8* (48).

14. Kaur, J.; Soto-Velasquez, M.; Ding, Z.; Ghanbarpour, A.; Lill, M. A.; van Rijn, R. M.; Watts, V. J.; **Flaherty, D. P.** Optimization of a 1,3,4-oxadiazole series for inhibition of Ca^{2+}/calmodulin-stimulated activity of adenylyl cyclases 1 and 8 for the treatment of chronic pain. *European Journal of Medicinal Chemistry*, **2018**, *162*, 568 – 585.

13. Ha, L; Colquhoun, J.; Noinaj, N.; Das, C.; Dunman, P. M.; **Flaherty, D. P.** Crystal Structure of the ribonuclease P protein subunit from *Staphylococcus aureus*. *Acta Crystallographica Section F.* **2018***, 74,* 632 - 637.

12. **Flaherty, D. P.**; Harris, M. T.; Schroeder, C. E.; Khan, H.; Kahney, E. W.; Hackler, A. L.; Patrick, S. L.; Weiner, W. S.; Aubé, J.; Sharlow, E. R.; Morris, J. C.; Golden, J. E. Optimization and Evaluation of Antiparasitic Benzamidobenzoic Acids as Inhibitors of Kinetoplastid Hexokinase 1. *ChemMedChem,* **2017**, *12*, 1994 – 2005.

11. Hackler, A.; Patrick, S. L.; Kahney, E. W.; **Flaherty, D. P.**; Sharlow, E. R.; Morris, J. C.; Golden, J. E. Antiparasitic lethality of sulfonamidebenzamides in kinetoplastids. *Bioorg. Med. Chem. Lett.* **2017**, *27*, 755 – 758.

10. Lopez-Sambrooks, C.; Shrimal, S.; Khodier, C.; **Flaherty, D. P.**; Charest, J.; Gao, N.; Lewis, T. A.; Lehrman, M. A.; Gilmore, R.; Golden, J.; Contessa, J. N. Oligosaccharyltransferase inhibition induces senescence in RTK-driven tumor cells. *Nat. Chem. Biol.* **2016**, *12*, 1023 – 1030.

9. Matharu, D. S.; **Flaherty, D. P.**; Simpson, D. S; Chung, D.; Yan, D.; Noah, J. W.; Jonsson, C. B.; White, E. L.; Aubé, J.; Plemper, R. K.; Severson, W. E.; Golden, J. E. Optimization of potent and selective quinazolinediones: inhibitors of respiratory syncytial virus that block RNA-dependent-RNA-polymerase complex activity. *J. Med. Chem.* **2014**, *57*, 10314 – 10328.

8. **Flaherty, D. P**; Miller, J. R.; Garshott, D. M.; Hedrock, M.; Gosalia, P.; Li, Y.; Milewski, M.; Sugarman, E.; Suyama, E.; Nguyen, K.; Vasile, S.; Salaniwal, S.; Stonich, D.; Su, Y.; Vicchiarelli, M.; Chung, T. D. Y.; Pinkerton, A. B.; Aubé, J.; Callaghan, M. U.; Golden, J. E.; Fribley, A. M.; Kaufman, R. J. Discovery and development of selective

activators targeting the apoptotic CHOP pathway of the unfolded protein response. *ACS Med. Chem. Lett.* **2014**, *5*, 1278 – 1283.

7. Perlmutter J. I.; Forbes, L. T.; Krysan, D. J.; Ebsworth-Mojica, E.; Dunman, P. M.; **Flaherty, D. P.*** Repurposing the antihistamine terfenadine for antimicrobial activity against *Staphylococcus aureus*. *J. Med. Chem.* **2014**, *57*, 8540 – 8562.
**corresponding author as postdoctoral research associate

6. **Flaherty, D. P.**; Simpson, D. S.; Miller, M.; Maki, B. E.; Zou, B.; Shi, J.; Wu, M.; McManus, O. B.; Aubé, J.; Li, M.; Golden, J. E. Potent and Selective Inhibitors of the TASK-1 Potassium Channel through Chemical Optimization of a Bis-Amide Scaffold. *Bioorganic and Medicinal Chemistry Letters*, **2014**, *24*, 3968 – 3973.

5. Harris, M. T.; Walker, D. M.; Drew, M. E.; Mitchell, W. G.; Dao, K.; Schroeder, C. E.; **Flaherty, D. P.**; Weiner, W. S.; Golden, J. E.; Morris, J. C. Interrogating a Hexokinase-Selected Small Molecule Library for Inhibitors of *Plasmodium falciparum* Hexokinase. *Antimicrobial Agents and Chemotherapy*, **2013**, *57*(8), 3731 – 3737.

4. **Flaherty, D. P.**; Kiyota, T.; Ikezu, I.; Dong, Y.; Vennerstrom, J. L. Phenolic Bis-Styrylbenzenes as *β*-Amyloid Binding Ligands and Free Radical Scavengers. *J. Med. Chem.*, **2010**, *53*, 7992 – 7999.

3. **Flaherty, D. P.**; Dong, Y.; Vennerstrom, J. L. A one-pot synthesis for unsymmetrical bis-styrylbenzenes. *Tetrahedron Lett.*, **2009**, 50, 6228 – 6230.

2. Shriver, J. A.; **Flaherty, D. P.**; Herr, C, C. Aryl Ethers from Arenediazonium Tetrafluoroborate Salts: From Neat Reactions for Solvent Mediated Effects. *J. Iowa. Acad. Sci.* **2009**, *116*, 27 – 35.

1. **Flaherty, D. P.**; Walsh, S. M.; Kiyota, T.; Dong, Y.; Ikezu, T.; Vennerstrom, J. L. Polyfluorinated Bis-styrylbenzene *β*-Amyloid Plaque Binding Ligands. *J. Med. Chem.*, **2007**, *50*, 4986-4992.

Patents

Issued

7. **Flaherty, D. P.**; van Rijn, R. M.; Watts, V. J.; Scott, J. A. Pyrazolyl pyrimidinone compounds and the uses thereof. US Patent 11,690,844. July 4th, 2023.

6. Contessa, Joseph N.; Golden, Jennifer E.; **Flaherty, Daniel P.** Inhibitors of *N*-linked glycosylation and methods of using same. US Patent 11,219,625. January 11, 2022.

5. Watts, Val J.; van Rijn, Richard M.; **Flaherty, Daniel P**; Kaur, Jatinder. Novel scaffold of adenylyl cyclase inhibitors for chronic pain and opioid dependence. U.S. Patent 10,662,176, May 26, 2020.

4. Watts, Val J.; van Rijn, Richard M.; **Flaherty, Daniel P**; Kaur, Jatinder. Adenylyl cyclase inhibitors for the treatment of chronic pain and opioid dependence. U.S. Patent 10,457,653, October 29, 2019.

3. Dunman, Paul M.; Krysan, Damian J.; **Flaherty, Daniel P.** Substituted Piperidine Derivatives and their Preparation, Methods and Compositions for Treating Infection. U.S. Patent 10,004,701, June 26, 2018.

2. Golden, Jennifer E.; Aubé, Jeffrey; **Flaherty, Daniel P.**; Fribley, Andrew M.; Kaufman, Randal J.; Thomas, Chung, D. Y.; Pinkerton, Anthony B.; Hendrick, Michael Pablo. Compounds and Methods for Activating the Apoptotic Arm of the Unfolded Protein Response. U.S. Patent 9,732,067, August 15, 2017.

1. Golden, Jennifer E.; Aubé, Jeffrey; Simpson, Denise S; **Flaherty, Daniel P.**; Matharu, Daljit S.; Severson, William E; Lynn, Rasmussen. Inhibitor of Respiratory Syncytial Virus. U.S. Patent 9,499,496, November 22, 2016.

Pending

4. **Flaherty, Daniel P.**; Watts, V. J.; Dwyer, T. S.; Annadka, S. Pyrazolyl pyrimidine compounds and the uses thereof. U.S. Patent 20230250084A1. 8/10/2023.

3. Graboski, Amanda L.; Redinbo, Matthew R.; **Flaherty, Daniel P.** Characterization of gut microbial tryptophanase and the development of a transition state analog to mitigate indoxyl sulfate-induced toxicity. US Provisional 63/465670.

2. **Flaherty, Daniel P.**; Seleem, Mohamed; Cao, Xufeng, Kaur, Jatinder. Carbonic anhydrase inhibitors for the treatment of *Neisseria gonorrhoeae* infection. US 2022/0213047 A1, July 7th, 2022.

1. **Flaherty, Daniel P.**; Seleem, Mohamed; Kaur, Jatinder; Cao, Xufeng. Carbonic anhydrase inhibitors and antibiotics against multidrug resistant bacteria. US 2022/0056001 A1, February 24, 2022.

Book Chapters

3. Holly, K. J.; Youse, M. S.; **Flaherty, D. P.** (**2024**). Carbonic anhydrases in *Enterococci*. In *The Enzymes*. Academic Press. Doi: 10.1016/bs.enz.2024.05.011

2. Youse, M. S.; Holly, K. J.; **Flaherty, D. P.** (**2024**). *Neisseria gonorrhoeae* carbonic anhydrase inhibition. In *The Enzymes*. Academic Press. Doi: 10/1016/bs.enz.2024.05.008.

1. Wang, K., **Flaherty, D. P.**, Chen, L., & Yang, D. (**2019**). High-Throughput Screening of G-Quadruplex Ligands by FRET Assay. In *G-Quadruplex Nucleic Acids* (pp. 323-331). Humana, New York, NY.

NIH Probe Reports

5. Zou B.; **Flaherty, D. P**; Simpson, D. S.; Maki, B. E.; Miller, M. R.; Shi, J.; Wu, M.; McManus, O. B.; Golden, J. E.; Aubé, J.; Li, M. Development of Bis-Amides as Selective Inhibitors of the KCNK3/TASK1 Two Pore Potassium Channel. Probe Reports from the NIH Molecular Libraries Program [http://mli.nih.gov/mli]. Bethesda, MD: National Center for Biotechnology Information (US), **2013**, Probe ML365.

4. Miller, M. R.; Zou, B.; Shi, J.; **Flaherty, D. P.**; Simpson, D. S.; Yao, T.; Maki, B. E.; Day, V. W.; Douglas, J. T.; Wu, M.; McManus, O. B.; Golden, J. E.; Aubé, J.; Li, M. Development of a Selective Chemical Inhibitor for the Two-Pore Potassium Channel, KCNK9. Probe Reports from the NIH Molecular Libraries Program [http://mli.nih.gov/mli]. Bethesda, MD: National Center for Biotechnology Information (US), **2012**, Probe ML308.

3. **Flaherty, D. P.**; Golden, J. E.; Liu, C.; Hedrick, M.; Gosalia, P.; Li, Y.; Milewski, M.; Sugarman, E.; Suyama, E.; Nguyen, K.; Vasile, S.; Salaniwal, S.; Stonich, D.; Su, Y.; Mangravita-Novo, A.; Vicchiarelli, M.; Smith, L. H.; Diwan, J.; Chung, T. D. Y.; Pinkerton, A. B.; Aubé, J.; Miller, J. R.; Garshott, D. M.; Callaghan, M. U.; Fribley, A. M.; Kaufman, R. J. Selective Small Molecule Activator of the Apoptotic Arm of the UPR. Probe Reports from the NIH Molecular Libraries Program [http://mli.nih.gov/mli]. Bethesda, MD: National Center for Biotechnology Information (US), **2012**, Probe ML291.

2. Noah, J. W.; Severson, W. E.; Chung, D. H.; Moore, B. P.; Jia, F.; Xu, X.; Maddox, C.; Rasmussen, L.; Sosa, M. I; Tower, N. A.; Ananthan, S.; White, E. L.; Jonsson, C. B.; Matharu, D. S.; **Flaherty, D. P.**; Simpson, D. S.; Golden, J. E.; Aubé, J. Identification of a Series of Quinazolinediones as Potent, Selective, Post-Entry Inhibitors of Human Respiratory Syncytial Virus (hRSV) via a Cell-Based High Throughput Screen and Chemical Optimization. Probe Report for the NIH Molecular Libraries Program [http://mli.nih.gov/mli]. Bethesda, MD: National Center for Biotechnology Information (US), **2011**, Probe ML275.

1. Sharlow, E. R.; Golden, J. E.; Dodson, H.; Morris, M.; Hesser, M.; Lyda, T.; Leimgruber, S.; Schreoder, C. E.; **Flaherty, D. P.**; Weiner, W. S.; Simpson, D. S.; Lazo, J. S.; Aubé, J.; Morris, J. C. Identification of Inhibitors of *Trypanosoma brucei* Hexokinases. Probe Reports from the NIH Molecular Libraries Program [https://www.ncbi.nlm.nih.gov/books/NBK47352/]. Bethesda, MD: National Center for Biotechnology Information (US), **2011**, Probe ML205.

Invited Seminars/Lectures

32. **Flaherty, D. P.** Bacterial carbonic anhydrase inhibitors: repurposing a classic enzyme for antibiotic drug discovery. Pharmaceutical Sciences Seminar Series, University of Wisconsin, Madison, WI. November 4th, 2024.

31. **Flaherty, D. P.** Validation of new therapeutic targets for antibiotic and inflammatory pain drug discovery. Center for Natural Products, Drug Discovery and Development Seminar Series, University of Florida, Gainesville, FL. September 25th, 2024. (postponed due to Hurricane Helene)

30. **Flaherty, D. P.** Hit-to-lead optimization of carbonic anhydrase inhibitors for the treatment of VRE and *Neisseria gonorrhoeae*. 2nd Annual Antimicrobial Resistance Conference, Purdue University, West Lafayette, IN. February 27th, 2024.

29. **Flaherty, D. P.** Targeting adenylyl cyclase type 1 for the treatment of chronic pain. 7th International Conference on Drug Discovery and Lead Optimization, San Francisco, CA, November 2nd, 2023.

28. **Flaherty, D. P.** Repositioning of human carbonic anhydrase inhibitor scaffolds for antimicrobial therapeutic applications. Antimicrobial Resistance Seminar Series, West Lafayette, IN, October 25th, 2023.

27. **Flaherty, D. P.** Repositioning of human carbonic anhydrase inhibitor scaffolds for antimicrobial therapeutic applications. Medicinal Chemistry and Molecular Pharmacology Department Retreat, West Lafayette, IN, October 9th, 2023.

26. **Flaherty, D. P.** Development of bacterial carbonic anhydrase inhibitors as anti-*gonorrhoeae* agents. Purdue Institute for Drug Discovery Annual Symposium, West Lafayette, IN, October 6th, 2023.

25. **Flaherty, D. P.** Data Management and Record Keeping in the Flaherty Lab. Data Management and Record Keeping in Research Course, GRAD590, Sept. 22, 2023.

24. **Flaherty, D. P.** Drug discovery against new targets for antibiotics and cancer. University of Illinois at Chicago, Department of Pharmaceutical Sciences Seminar Series, Chicago, IL, January 12th, 2023

23. **Flaherty, D. P.** Bacterial carbonic anhydrase inhibitors for the treatment of drug resistant bacteria. Purdue Institute for Drug Discovery Programmatic Area Talk. West Lafayette, IN, September 30th, 2022

22. **Flaherty, D. P.** Bacterial carbonic anhydrase inhibitors for the treatment of drug resistant bacteria. 4th International Symposium on Frontiers in Molecular Science. Florence, Italy, September 9th, 2022. ***Invited Keynote Address*** - Recipient of Best Oral Presentation

21. **Flaherty, D. P.** Validation of therapeutic targets and drug discovery for antibiotics. Trudeau Institute, Lake Saranac, NY, February 17th, 2022

20. **Flaherty, D. P.** Validation of therapeutic targets and drug discovery for antibiotics and chronic pain. University of Iowa, Department of Pharmaceutical Sciences and Experimental Therapeutics Seminar Series, Iowa City, IA, November 30th, 2021

19. **Flaherty, D. P.** Validation of therapeutic targets and drug discovery for antibiotics and chronic pain. University of Minnesota, Department of Medicinal Chemistry Seminar Series, Minneapolis, MN, October 26th, 2021

18. **Flaherty, D. P.** Validation of therapeutic targets and drug discovery for antibiotics and chronic pain. University of Illinois at Chicago, Department of Pharmaceutical Sciences Seminar Series, Chicago, IL, September 8th, 2021

17. **Flaherty, D. P.** Validation of therapeutic targets and drug discovery for antibiotics and chronic pain. University of Nebraska Medical Center, Department of Pharmaceutical Sciences Seminar Series, Omaha, NE, September 3rd, 2021

16. **Flaherty, D. P.** Optimization and structural studies of inhibitors for bacterial carbonic anhydrases. Hitchhiker's Guide to the Biomolecular Galaxy Symposium, Purdue University, West Lafayette, IN, May 13th, 2021.

15. **Flaherty, D. P**. Targeting bacterial carbonic anhydrases for the treatment of drug-resistant pathogens. Academic Drug Discovery Session, National ACS Meeting, April 7th, 2021. *Invited Lecture as part of special symposium*

14. **Flaherty, D. P.** Medicinal chemistry strategies for combating drug-resistant bacteria. University of Rochester Medical Center, Department of Microbiology and Immunology, Rochester, NY, February 26th, 2021

13. **Flaherty, D. P.** Drug discovery efforts to combat vancomycin-resistant enterococcus and chronic pain. Department of Medicinal Chemistry and Molecular Pharmacology, Purdue University, West Lafayette, IN, December 10th, 2020.

12. **Flaherty, D. P.** Drug discovery efforts to combat vancomycin-resistant enterococcus and chronic pain. Chemistry-Biochemistry-Biology Interface Program, University of Notre Dame, November 19th, 2020.

11. **Flaherty, D. P**. Novel Therapeutic Agents for the Treatment of Drug-Resistant Enterococcus. ACS Fall National Virtual Meeting 2020, August, 18th, 2020.

10. **Flaherty, D. P.** Pharmacologic validation of new targets to treat vancomycin-resistant enterococcus and chronic pain. Department of BioMolecular Sciences, University of Mississippi, April 7th, 2020 (postponed due to COVID-19).

9. **Flaherty, D. P**. Novel therapeutic agents for the treatment vancomycin-resistant enterococcus and chronic pain. Academic Drug Discovery Session, National ACS Meeting, Philadelphia, PA. March 25th, 2020 (postponed due to COVID-19).

8. **Flaherty, D. P.** Pharmacologic validation of new targets to treat vancomycin-resistant enterococcus and chronic pain. Department of Medicinal Chemistry and Pharmacognosy, The Ohio State University, January 21, 2020.

7. **Flaherty, D.** P. Repurposing carbonic anhydrase inhibitors to combat drug-resistant bacteria. Purdue University Drug Discovery Training Program Symposium, November 20th, 2019.

6. **Flaherty, D. P.** Antibiotic drug discovery: inhibiting old targets and validating new ones. Purdue University, Department of Biochemistry, West Lafayette, IN, November, 21, 2016

5. **Flaherty, D. P.** Antibiotic drug discovery: inhibiting old targets and validating new ones. University of Toledo, Department of Medicinal and Biological Chemistry; Toledo, OH, November, 17, 2016

4. **Flaherty, D. P**. Antibiotic drug discovery: inhibiting old targets and validating new ones. Purdue University, Department of Biological Sciences, West Lafayette, IN, April, 20, 2016

3. **Flaherty, D. P.** Fragment-based drug discovery theory and techniques. University of Rochester Medical Center, Department of Microbiology and Immunology, Rochester, NY, April, 15, 2016

2. **Flaherty, D. P.** Small Molecule Probes for Interrogating Biological Pathways. Purdue University, Department of Medicinal Chemistry and Molecular Pharmacology, West Lafayette, IN, January 29, 2015

1. **Flaherty, D. P.** Small Molecule Probes for Interrogating Biological Pathways. University of Nebraska-Lincoln Chemistry Department. Lincoln, NE, October 28, 2013

Scientific Meeting Posters

*Presenters underlined if not presented by Dr. Flaherty

24. Shrinidhi, A.; Dwyer, T. S.; Watts, V. J.; **Flaherty, D. P.** Lead Optimization of adenylyl cyclase type 1 inhibitors for the treatment of chronic pain. ACS-EFMC Frontiers in Medicinal Chemistry, Boston, MA, June 10, 2023.

23. Imhoff, R. D.; Patel, R.; Safdar, M.; Chen, H.; Muli, C.; Krabill, A.; Das, C.; Wendt, M.; **Flaherty, D. P.** Discovery and development of novel covalent inhibitors toward ubiquitin C-terminal hydrolase L1. American Chemical Society National Meeting, Chicago, IL, August 24th, 2022.

22. Kaur, J.; Abutaleb, N.; Cao, X.; Hewitt, C. S.; Marapaka, A. K.; An, W.; Youse, M. S.; Holly, K. J.; Nocentini, A.; Supuran, C. T.; Seleem, M. N.; **Flaherty, D. P.** Targeting Carbonic Anhydrases for Enterococcus and *Neisseria gonorrhoeae* Drug Discovery. American Chemical Society National Meeting, Chicago, IL, August 24th, 2022.

21. Kaur, J.; Abutaleb, N.; Cao, X.; Hewitt, C. S.; Marapaka, A. K.; An, W.; Youse, M. S.; Holly, K. J.; Nocentini, A.; Supuran, C. T.; Seleem, M. N.; **Flaherty, D. P.** Targeting Carbonic Anhydrases for Enterococcus and *Neisseria gonorrhoeae* Drug Discovery. New Antibacterial Discovery and Development Gordon Research Conference, Lucca, Italy, July 27th, 2022.

20. Scott, J. A.; Soto-Velasquez, M.; Hayes, M. P.; LaVigne, J. E.; Miller, H. R.; Kaur, J.; Ejendal, K. F. K.; Watts, V. J.; **Flaherty., D. P.** Inhibition of Ca^{2+}/calmodulin mediated cAMP production via adenylyl cyclase type 1 for the treatment of chronic pain. American Chemical Society National Medicinal Chemistry Symposium, New York, NY, June 27th, 2022.* Chemistry Europe Poster Prize recipient

19. An, W., Holly, K.; **Flaherty, D. P.** Structure-Activity Relationship Studies for Inhibitors of Vancomycin-Resistant Enterococcus Carbonic Anhydrases. Medicinal Chemistry and Molecular Pharmacology Departmental Retreat, October 12th, 2021.

18. Marapaka, A. K.; Hewitt, C. S.; Abutaleb, N. S.; Cao, X.; Nocentini, A.; Supuran, C. T.; Seleem, M. N.; **Flaherty, D. P.** Design, Synthesis and Structural Evaluation of Acetazolamide-based Carbonic Anhydrase Inhibitors Against *Neisseria gonorrhoeae*. Medicinal Chemistry and Molecular Pharmacology Departmental Retreat, October 12th, 2021.

17. Hewitt, C. S.; Das, C.; **Flaherty, D. P.** Development of First-in-Class Ubiquitin Variants for Ubiquitin C-terminal. Hydrolase L1. Bioorganic Gordon Conference, Andover, NH, June 12, **2019**.

16. Yao, T.; **Flaherty, D. P.**; Simpson, D. S.; Maki, B. E.; Miller, M. R.; Zou, B., Shi, J. Wu, M.; McManus, O. B.; Aubé, J.; Li, M.; Golden, J. E. Development of selective inhibitors for the two-pore domain potassium channel KCNK9. Poster Presentation, 248th American Chemical Society National Meeting, San Francisco, CA, August 13, **2014**

15. **Flaherty, D. P.**, Perlmutter, J. I.; Forbes, L. T.; Krysan, D. J.; Ebsworth-Mojica, E.; Dunman, P. M. Repurposing the antihistamine terfenadine for antimicrobial use. Poster Presentation, 248th American Chemical Society National Meeting, San Francisco, CA, August 13, **2014**

14. **Flaherty, D. P.**; Schroeder, C. E.; Sharlow, E. R.; Golden, J. E.; Dodson, H.; Morris, M.; Hesser, M.; Lyda, T.; Leimgruber, S.; Weiner, W. S.; Simpson, D. S.; Lazo, J. S.; Aubé, J.; Morris, J. C. Small Molecule Inhibitors of *Trypanosoma brucei* Hexokinase 1. Poster Presentation, 2011 International Chemical Biology Society Meeting, Kansas City, MO, October 11, **2011**

13. **Flaherty, D. P.**; Dong, Y.; Vennerstrom, J. L. Unsymmetrical Bis-styrylbenzene Structure-Activity Relationship Studies in β-Amyloid Plaque Binding Affinity and Specificity. Poster Presentation, 2010 Spring ACS National Meeting. San Francisco, CA. March 21, **2010**

12. **Flaherty, D. P.**; Dong, Y.; Vennerstrom, J. L. New Method for the Synthesis of Unsymmetrical Bis-styrylbenzenes. Poster Presentation, 2009 Fall ACS National Meeting, Washington, D.C., August 18, **2009**

11. **Flaherty, D. P.**; Dong, Y.; Vennerstrom, J. L. Bis-styrylbenzenes Bind Selectively to *β*-Amyloid Plaques and Alter the Aggregation Process. Podia Presentation, 2009 Midwest Student Biomedical Research Forum, Omaha, NE, February 28, **2009**

10. **Flaherty, D. P.**; Dong, Y.; Vennerstrom, J. L. Bis-styrylbenzenes Bind Selectively to *β*-Amyloid Plaques and Alter the Aggregation Process. Poster Presentation, 2008 American Chemical Society Midwest Regional Meeting, Kearney, NE, October 9, **2008**

9. **Flaherty, D. P.** Bis-styrylbenzenes Bind Selectively to *β*-Amyloid Plaques and Alter the Aggregation Process. Podia Presentation, 2008 Globalization of Pharmaceutical Education Network, Leuven, Belgium, September 12, **2008**

8. **Flaherty, D. P.** Bis-styrylbenzenes as therapeutics in Alzheimer's disease. Podia Presentation, 2008 International Student Research Forum, Omaha, NE, June **2008**

7. **Flaherty, D. P.** The Potential of Bis-styrylbenzenes in Alzheimer's Disease. Podia Presentation, 2008 Midwest Student Biomedical Research Forum, Omaha, NE, March 1, **2008**

6. **Flaherty, D. P.** The Potential of Bis-styrylbenzenes in Alzheimer's Disease. Podia Presentation, 2007 International Student Forum, University of Tokyo, Tokyo, Japan, June 26-27th, **2007**

5. **Flaherty, D. P.**; Walsh, S.; Kiyota, T.; Dong, Y.; Ikezu, T.; Vennerstrom, J. L. Polyfluorinated Amyloid Plaque-Binding Ligands for Early Detection of Alzheimer's Disease with ^{19}F MRI. 38th Annual Midwest Student Biomedical Research Forum, Omaha, NE; February **2007**

4. **Flaherty, D. P.** The Potential of *Bis*-stilbenes in Alzheimer's Disease. Seminar, Omaha, NE, University of Nebraska Medical Center, Pharmaceutical Sciences Graduate Program, November 10th, **2006**

3. **Flaherty, D. P.**; Vennerstrom, J. L.; Dong, Y.; Ikezu, T.; Walsh, S. Polyfluorinated Amyloid Plaque Binding Ligands for Early Detection of Alzheimer's Disease with ^{19}F MRI. 41st Annual Midwest Regional Meeting of the American Chemical Society, Quincy, Illinois; October 25-27, **2006**

2. **Flaherty, D. P.**; Vennerstrom, J. L. Polyfluorinated amyloid plaque binding ligands for early detection of Alzheimer's Disease with ^{19}F MRI. 38th Annual PGSRM Conference, Minneapolis; Minnesota, June **2006**

1. **Flaherty, D. P.**; Marky, L. A. Thermodynamics of Paperclip DNA Triplexes. 19th Annual Gibb's Conference on Biothermodynamics; Carbondale, Illinois, hosted by Southern Illinois University; October **2005**

Advising and Mentoring

Undergraduate

17. Isabella Arauz (major: biology) 3/2024 - present
16. Olivia Snell (major: Biochemistry) 8/2023 - present
15. Zane Lark (major: Pharmaceutical Sciences) 5/2023 - present
14. Faith Drummond (major: Pre-pharmacy) 3/2023 - present
13. Kara LeGoy (major: Pre-pharmacy) 8/2021 – 12/2022.
12. Megan Jurek (major: Chemistry) 8/2020 – 5/2022. Present: Graduate Student in Pharmaceutical Sciences Graduate Program at University of Illinois at Chicago.

11. German Camacho (major: Chemistry) 2/2021 – 12/2021. Colombia-Purdue Partnership Program, Student from National University of Colombia. Current: Medicinal Chemistry Graduate Program at The Ohio State University.
10. Margot Cruz-Portillo (major: Biology) 5/2021 – 7/2021. Purdue University Louis Stokes Alliance for Minority Participation Fellow
9. Devon Amos (major: Biology), 8/2019 – 5/2021, present: University of Indiana Medical School.
8. Amanda Waldbeiser (major: Pre-pharmacy), 8/2019 – 5/2020, present: Pharmacy Program at Purdue University.
7. Margaret Tharp (major: Pharmaceutical Sciences), 1/2019 – 12/2019, present: Indiana University Medical School
6. Collin Sroge (major: Pharmaceutical Sciences), 1/2017 – 5/2019, present: Graduate Student at UC-Irvine
5. Amanda Graboski (major: Pharmaceutical Sciences), 1/2017 – 5/2019, present: graduate student, Biological and Biomedical Sciences Program, University of North Carolina at Chapel Hill.
4. Hyesoo Chae (major: Pre-pharmacy), 8/2016 – 5/2017, present: Manager of Pharmacy Perioperative Services UCSF.
3. Rebecca Fritz (major: Pre-pharmacy), 8/2016 – 5/2017, present: Clinical Scientist at Bristol Myers Squibb.
2. Brittany Griggs (major: Pre-pharmacy), 8/2015 – 5/2016, present: Senior Consulting Analyst at The Dedham Group.
1. Claire Corvari (major: Pre-pharmacy), 8/2015 – 5/2016, present: Pharmacy Program at Purdue University.

Graduate (Students who have graduated)

7. Molly Youse, Ph.D. 2024 – Senior Scientist at IQVIA in Indianapolis, IN

6. Ryan Imhoff, Ph.D. 2024 – Post-doctoral Research Associate, West Lafayette, IN

5. Alexa Clark, M.S., 2023 – Analytical Chemist at Evonik in Lafayette, IN.

4. Jason A. Scott, Ph.D. 2022, Thesis Title "Selective Inhibition of Adenylyl Cyclase Type 1 for the Treatment of Chronic Pain". Present Position – Chemistry and Pharmacology Research Scientist, Atteboro, MA

3. Chad S. Hewitt, Ph.D. 2021, Thesis Title "Development of Ubiquitin Variants with Selectivity for the Ubiquitin C-Terminal Hydrolase Subfamily of Deubiquitinases". Present Position: Scientist at Nurix Therapeutics, San Francisco, CA.

2. Aaron Krabill, Ph.D. 2020, Thesis Title "Development and Characterization of Novel Probes to Elucidate the Role of Ubiquitin C-terminal Hydrolase L1 in Cancer Biology". Present Position: Senior Scientist at Valo Therapeutics in Cambridge, MA.

1. Lisha Ha, M.S. 2019, Thesis Title "Evaluation of *Staphylococcus aureus* RnpA Protein as an Antibacterial Target". Present Position: Research Scientist II, Department of Chromatography and Drug Performance, SSCI (a division of Albany Molecular Research, Inc.)

Post-doctoral (Post-docs who have moved on)

5. Dr. Krishan Yadavalli, 8/2022 – 7/2023. Present: Scientist in India

4. Dr. Weiwei An, 11/2019 – 5/2022. Present Position: Scientist, Chemist, Promega, Inc

3. Dr. Xufeng Cao, 10/2018 – 11/2020. Present Position: Scientist III, Medicinal Chemistry, Hexagon Bio, San Francisco, CA.

2. Dr. Jatinder Kaur, 9/2016 – 5/2018. Present Position: Radiochemist, Nuclear Medicine and Molecular Facility, Memorial University of Newfoundland, Canada

1. Dr. Amer Tarawneh, 11/2015 – 7/2016. Present Position: Assistant Professor of Medicinal Chemistry, Tafila Technical University, Tafila, Jordan.