Daniel P. Flaherty

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

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Education

2005 - 2010 **University of Nebraska Medical Center**
Ph.D. in Pharmaceutical Science, emphasis on medicinal chemistry

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

Appointments

July 2015 – present Assistant Professor, **Purdue University**
Department of Medicinal Chemistry and Molecular Pharmacology
- Employ fragment-based, covalent and traditional reversible inhibitor design to validate novel therapeutic targets for the treatment of bacterial infections, cancer and chronic pain. We then leverage these new targets for drug discovery to develop first- or best-in-class inhibitors.

2014 – 2015 Assistant Research Professor, **University of Kansas**
Higuchi BioSciences Center
- Design and synthesis of antimicrobial compounds as part of a drug repurposing effort. Also participated in further hit-to-probe optimization of small molecule probes for various biological targets.
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.
- Design and synthesis of analogs for hit-to-probe optimization of small molecules as part of a multi-disciplinary research teams.
Mentor: Jeffrey Aubé, Ph.D.

2005 - 2010 Graduate Research Associate, **University of Nebraska Medical Center**
Department of Pharmaceutical Sciences
- Design, synthesis and biological evaluation of bis-styrylbenzene analogs as amyloid-β plaque binding ligands in Alzheimer's disease.
Mentor: Jonathan L. Vennerstrom, Ph.D.

2003 – 2005 Undergraduate researcher, **Central College**
Department of Chemistry
- Optimization of aryl ether forming reactions coupling alcohols with diazonium tetrafluoroborate salts.
Mentor: James A. Shriver, Ph.D.

Affiliations

- Adjunct Assistant 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:

4. NINDS 1R01NS119917 "Pharmacological validation of adenylyl cyclase 1 as a drug target for chronic pain"
   Flaherty/Watts MPI, van Rijn Co-I
   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.

3. NIAID 1R01AI148523 "Repurposing novel selective drugs for treatment and decolonization of vancomycin-resistant enterococcus"
   Flaherty Co-I, Seleem, PI
   Period: 10/01/19 – 9/31/2024
   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.

2. NIAID 1R01AI134685 "Antibacterial inhibitors of RnpA"
   Flaherty Co-I, Dunman, PI
   Period: 9/01/18 – 8/31/2023
   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.

1. NINDS 1R61NS111070 "Non-opioids for inflammatory pain: adenylyl cyclase 1 as a novel target"
   Flaherty Co-I (5% effort year 1, 10% year 2); Roman, PI (U of Iowa)/Watts Co-PI (Purdue University)
   Period: 5/1/2021 – 4/30/2023
   Direct Costs to Flaherty Lab:
   Hit-to-probe optimization of AC1-CaM PPI inhibitors as probes for target validation to treat chronic pain.

Completed:

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 suppor
    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

- 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

Peer Reviewer for Grants

- NIH HEAL Initiative U19 Study Section, 2021
- DoD MIDRP W-1 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

Publications

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*, **2021**, *just accepted.* 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*, **2021**, *just accepted.* 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**, *just accepted.* 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. ** 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 Benzensulfonamide 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

6. 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.

5. 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.

4. 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.

3. 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.

2. Contessa, Joseph N.; Golden, Jennifer E.; **Flaherty, Daniel P.** Inhibitors of *N*-linked glycosylation and methods of using same. WIPO PCT/US2016/043664. 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.

Book Chapters

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

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, 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, 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, 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, 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

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

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: Pharmacy Program at Purdue University.
3. Rebecca Fritz (major: Pre-pharmacy), 8/2016 – 5/2017, present: Pharmacy Program at Purdue University.
2. Brittany Griggs (major: Pre-pharmacy), 8/2015 – 5/2016, present: Pharmacy Program at Purdue University.
1. Claire Corvari (major: Pre-pharmacy), 8/2015 – 5/2016, present: Pharmacy Program at Purdue University.

Graduate (Students who have graduated)

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: Post-doctoral research associate in the laboratory of Dr. Zhong-Yin C Zhang, Purdue University.
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)

3. Dr. Xufeng Cao, 10/2018 – 11/2020. Present Position: Scientist III, Medicinal Chemistry, Olema Pharmaceuticals, San Francisco, CA.
2. Dr. Jatinder Kaur, 9/2016 – 5/2018. Present Position: Radiochemist, Lawson Health Research Institute, London, Ontario, Canada.
1. Dr. Amer Tarawneh, 11/2015 – 7/2016. Present Position: Assistant Professor of Medicinal Chemistry, Tafila Technical University, Tafila, Jordan.