## **Curriculum Vitae (October 2021) for**

## Paul R. Carlier

Professor

Department of Chemistry

Virginia Tech

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#### **EMPLOYMENT & RESEARCH HISTORY:**

5/07 to present Virginia Tech

Professor, Department of Chemistry

Research Interests: Chemical Biology & Medicinal Chemistry.

8/00 to 4/07 Virginia Tech

Associate Professor, Department of Chemistry

9/91 to 7/00 Hong Kong University of Science and Technology

Assistant to Associate Professor, Department of Chemistry

3/88 to 7/91 Polaroid Corporation (Cambridge, MA)

Scientist, Chemical Research, Organic Chemistry

**EDUCATION:** 

9/83 to 2/88 Massachusetts Institute of Technology (Cambridge, MA)

Research under Professor K. Barry Sharpless, Ph. D., Organic Chemistry, February 1988.

Thesis Title: "Studies of Titanium-Mediated Transformations of Allylic and 2,3-Epoxy

Alcohols."

9/79 to 5/83 Hamilton College (Clinton, NY)

Summa Cum Laude, Honors Thesis, B.A. in Chemistry, Minor in Math.

#### **PROFESSIONAL ACTIVITIES:**

Virginia Tech, Virginia, National and International

2021-present, Chair, Executive Committee, Virginia Drug Discovery Consortium.

2020-present, Co-chair, Antimicrobial Countermeasures (vaccine/drug) thematic focus, Center for Emerging,

Zoonotic, and Anthropod-borne Pathogens, Virginia Tech

2019-present, Director, Virginia Tech Center for Drug Discovery

2018-2019, Associate Director, Virginia Tech Center for Drug Discovery

2015-present, Member, International Advisory Board, International Symposium on Cholinergic Mechanisms

2014-present, North American Regional Editor, Current Topics in Medicinal Chemistry NIH Service

2021 Ad Hoc Reviewer, NIH CSR, ZRG1 AIDC-Q (83) S Drug Discovery and Mechanisms of Resistance in Eukaryotic Pathogenic Organisms

2021 Ad Hoc Reviewer, NIH CSR, Vector Biology

2021 Ad Hoc Reviewer, NIH CSR, ZRG1 AIDC-Y (83) S Eukaryotic Pathogen Drug Discovery and Resistance

2019 Ad Hoc Reviewer, NIH CSR, VB Vector Biology

2018 Ad Hoc Reviewer, NIH CSR, ZRG1 IDM-X (10) Non-HIV Anti-infective Therapeutics

2016 Chair, NIH-CSR, ZAI1-RRS-M-J1 Special Emphasis Panel, "Rapid Assessment of Zika Virus (ZIKV) Complications"

2012-2015 Member, NIH CSR, Drug Discovery for the Nervous System (DDNS) Study Section

2010 Chair, NIH-CSR, COUNTERACT Study Section

2009-2012 Ad Hoc Reviewer, NIH-CSR, Drug Discovery for the Nervous System Special Emphasis Panel

2009 Ad Hoc Reviewer, NIH CSR, Molecular Neuropharmacology and Signaling Study Section

2009 CNS Drug Discovery BRDG-SPAN & Catalyst ARRA Review Panel

#### **DIVERSITY AND INCLUSION:**

I am committed to building a diverse and inclusive group and Department. Among the 22 PhD and Master's students that have graduated from my lab at Virginia Tech, 8 have been women. When in early 2017 the former Presidential administration began to scrutinize Muslim communities and prevent Muslim immigration, I reached out to my Muslim students and participated in two rallies at Virginia Tech. In response to the 2017 white supremacist rally in Charlottesville, I led or participated in numerous community and campus efforts to address both personal and systemic racism against Black Americans: I attended conferences, workshops and NAACP meetings; forged partnerships with Black community leaders, led book groups, and in November 2020 organized a Black history tour of Roanoke Virginia for Virginia Tech students and community members. Lastly, beginning in the Summer of 2020, and intensifying after the March 2021 murders in Atlanta, I have used my voice to speak out against anti-Asian hate. As the husband of a Chinese-American woman, and as someone who lived in Hong Kong for 9 years, I know something of what it feels like to be a "perpetual foreigner." I know all too well that my Asian colleagues and graduate students can feel like non-entities in the Diversity conversation, and for me inclusion means that all voices must be heard.

#### **HONORS AND AWARDS:**

Jimmy Viers Teaching Award, Virginia Tech Department of Chemistry, 2017

North America Regional Editor, Current Topics in Medicinal Chemistry 2015-present

Scholar of the Week, June 2013, Office of the Vice President for Research, Virginia Tech.

Member, International Advisory Board, Cholinergic Mechanisms Meeting 2013-present

Member, NIH Study Section, Drug Discovery for the Nervous System (DDNS-C), 2012-2015

PRC200 selected as AstraZeneca development candidate AZD1858, 2008

Cook Research Award (Virginia Tech Department of Chemistry), 2006

Hamilton College Alumni Achievement Medal, 2005

School of Science Teaching Award, 1997

Outstanding Departmental Safety Officer, 1996

NIH Postdoctoral Fellowship, 1987 (awarded, but declined to take industrial research position at Polaroid

Corporation)
Summa Cum Laude, 1983
Oren Root Fellowship, 1983
Sigma Xi, 1983
Norton Prize in Chemistry, 1983
Underwood Prize in Chemistry, 1983
Phi Beta Kappa, 1982
Outstanding Freshman Chemist Award, 1980

#### **REFEREED JOURNAL PUBLICATIONS:**

#### \* designates corresponding author

- 1. "Enhanced Kinetic Resolution and Enzyme–Like Shape Selectivity" Paul R. Carlier, William S. Mungall, Georg Schröder and K. Barry Sharpless\* *Journal of the American Chemical Society* **1988**, *110*, 2978-2979. DOI: 10.1021/ja00217a052
- 2. "Regioselective Opening of 2,3-Epoxy Alcohols by [Ti(O*i*-Pr)<sub>2</sub>(N<sub>3</sub>)<sub>2</sub>]: Synthesis of ℚ-Amino Acids" Maurice Caron, Paul R. Carlier, and K. Barry Sharpless\* *Journal of Organic Chemistry* **1988**, *53*, 5185-5187. DOI: 10.1021/jo00256a063.
- 3. "Asymmetric Hydrogenation of  $\alpha$ -keto carboxylic esters. A practical, purely chemical access to  $\alpha$ -hydroxy esters in high enantiomeric purity" Paul R. Carlier, K. Barry Sharpless\* *Chemtracts: Organic Chemistry* **1988**, *1*, 16-17 (invited review).
- 4. "Studies on the Mechanism of the Asymmetric Epoxidation: A Ligand Variation Approach" Paul R. Carlier and K. Barry Sharpless\* *Journal of Organic Chemistry* **1989**, *54*, 4016-4018. DOI: 10.1021/jo00278a004.
- 5. "Unexpected Regioselectivity in the Sulfonation of a Leuco Xanthene Dye" Paul R. Carlier,\* Mary P. Lockshin, and Michael P. Filosa *Journal of Organic Chemistry* **1994**, *59*, 3232-3236. DOI: 10.1021/jo00090a050.
- 6. "2,3-Anti-Selective Aldol Reaction of Phenylacetonitrile" Paul R. Carlier,\* Kam Moon Lo Journal of Organic Chemistry **1994**, *59*, 4053-4055. DOI: <a href="https://doi.org/10.1021/j000094a011">10.1021/j000094a011</a>.
- 7. "<sup>6</sup>Li/<sup>15</sup>N NMR-Based Solution Structural Determination of Et<sub>2</sub>O— and TMEDA-Solvated Lithio-Phenylacetonitrile and a LiHMDS Mixed Aggregate" Paul R. Carlier,\* Brett L. Lucht, David B. Collum *Journal of the American Chemical Society* **1994**, *116*, 11602-11603. DOI: <u>10.1021/ja00104a064</u>.
- 8. "Anti-Selective Aldol of Benzylic Nitriles and Synthesis of ②-Aminoalcohols" Paul R. Carlier,\* Kam Moon Lo, Michael M-C. Lo, and Ian D. Williams Journal of Organic Chemistry 1995, 60, 7511-7517. DOI: 10.1021/jo00128a025.
- 9. "Formation of a Novel Sulfonated Enedione" Mary P. Lockshin,\* Michael P. Filosa, Michael J. Zuraw, Paul R. Carlier\* *Journal of Organic Chemistry* **1996**, *61*, 2556-2558. DOI: <u>10.1021/jo9520856</u>.
- 10. "Computer Handling of Chemical and Biological Data of Traditional Chinese Medicines" Chun-Tao Che,\* Paul R. Carlier, Ophelia C. W. Lee *Chemical Research in Chinese Universities* **1996**, *13*, 169-173 (invited article).

- 11. "Development and Application of the Nitrile Aldol Reaction" Paul R. Carlier,\* Kam Moon Lo, Michael M-C. Lo, Weldon W-F. Lam *Youji Huaxue* ("Organic Chemistry," China), **1997**, 17, 57-61 (invited review article).
- 12. "Synthetic Optimization and Structural Limitations of the Nitrile Aldol Reaction" Paul R. Carlier,\* Kam Moon Lo, Michael M-C. Lo, Priscilla C-K. Lo, Cedric W-S. Lo *Journal of Organic Chemistry* **1997**, *62*, 6316-6321. DOI: 10.1021/jo9702148.
- 13. "Diastereoselective Oxidation of 2,3-Epoxy Alcohol-Derived Thiiranes, and <sup>1</sup>H NMR Analysis of the Corresponding Thiirane *S*-Oxides" Paul R. Carlier,\* Guilan Liu, and H. Y. Peter Lam *Phosphorus, Sulfur, and Silicon and the Related Elements*, **1997**, *126*, 223-234. DOI: 10.1080/10426509708043562.
- 14. "Synthesis of a Potent Wide-Spectrum Serotonin-, Norepinephrine-, Dopamine-Reuptake Inhibitor (SNDRI) and a Species-Selective Dopamine-Reuptake Inhibitor Based on the Gamma-Amino Alcohol Functional Group," Paul R. Carlier,\* Michael M-C. Lo, Priscilla C-K. Lo, Elliott Richelson\*, Masahiko Tatsumi, Ian J. Reynolds, Terre A. Sharma *Bioorganic & Medicinal Chemistry Letters* **1998**, *8*, 487-492. PubMed PMID: 9871604. DOI: 10.1016/SO960-894X(98)00062-6
- 15. "Lithium Ephedrinate-Mediated Aldol Reaction of Arylacetonitriles: Thermodynamic Control of Enantioselectivity" Paul R. Carlier,\* Weldon W.-F. Lam, Nan Chi Wan, Ian D. Williams *Angewandte Chemie, International Edition in English* 1998, 37, 2252-2254. DOI: 10.1002/(SICI)1521-3773(19980904)37:16<2252::AID-ANIE2252>3.0.CO;2-Z
- 16. "Evaluation of Short-Tether Bis-THA AChE Inhibitors. A Further Test of the Dual Binding Site Hypothesis" Paul R. Carlier,\* Yifan Han,\* Ella S.-H. Chow, Crystal P.-L. Li, Hong Wang, Thuy Xuan Lieu, Hau Sum Wong, Yuan-Ping Pang *Bioorganic & Medicinal Chemistry* **1999**, *7*, 351-357. PubMed PMID: 10218828. DOI: 10.1016/S0968-0896(98)00213-2
- 17. Attenuation of scopolamine-induced deficits in navigation memory performance in rats by bis(7)-tacrine: a novel dimeric AChE inhibitor. Hong Wang, Paul R. Carlier, Wing Lok Ho, Nelson Tze Kin Lee, Yuan-Ping Pang, Yi-Fan Han\* *Acta Pharmacologica Sinica* **1999**, *20*, 211-217. PubMed PMID: 10452094.
- 18. "Effects of Bis(7)-tacrine, a novel anti-Alzheimer's agent, on Rat Brain AChE" Hong Wang, Paul R. Carlier, Wing Lok Ho, Nelson Tze Kin Lee, Crystal P.-L. Li, Yuan-Ping Pang, and Yi Fan Han\* *Neuroreport* **1999**, *10*, 789-793. PubMed PMID: 10208549.
- 19. "Bis(7)-tacrine, a novel dimeric AChE inhibitor, is a potent GABA<sub>A</sub> receptor antagonist" Chao-Ying Li, Hong Wang, Hong Xue, Paul R. Carlier, Kow Min Hui, Yuan-Ping Pang, Zhi Wang Li, Yifan Han\* *Neuroreport* **1999**, *10*, 795-800. PubMed PMID: 10208550.
- 20. "Dual-Site Binding of Bivalent 4-Aminopyridine- and 4-Aminoquinoline-based AChE Inhibitors: Contribution of the Hydrophobic Alkylene Tether to Monomer and Dimer Affinities" Yi Fan Han, Crystal P.-L. Li, Ella Chow, Hong Wang, Yuan-Ping Pang, Paul R. Carlier\* *Bioorganic & Medicinal Chemistry* 1999, 7, 2569-2575. PubMed PMID: 10632067. DOI: 10.1016/S0968-0896(99)00178-9
- 21. "Potent, Easily Synthesized Huperzine A-Tacrine Hybrid Acetylcholinesterase Inhibitors" Paul R. Carlier,\* Da-Ming Du, Yi Fan Han, Jing Liu, Yuan-Ping Pang *Bioorganic and Medicinal Chemistry Letters* **1999**, *9*, 2335-2338. PubMed PMID: 10476864. DOI: 10.1016/S0960-894X(99)00396-0
- 22. "Heterodimeric Tacrine-Based AChE Inhibitors: Investigating Ligand-Peripheral Site Interactions" Paul R. Carlier,\* Ella S.-H. Chow, Yifan Han, Jing Liu, Jamal El Yazal, Yuan-Ping Pang *Journal of Medicinal Chemistry*, **1999**, *42*, 4225-4231. PubMed PMID: 10514292. DOI: 10.1021/jm990224w

- 23. "Dimerization of an Inactive Fragment of Huperzine A Produces a Drug with Twice the Potency of the Natural Product" Paul R. Carlier,\*, Da-Ming Du, Yi-Fan Han,\* Jing Liu, Emanuele Perola, Ian D. Williams, and Yuan-Ping Pang Angewandte Chemie, International Edition 2000, 39, 1775-1777. PubMed PMID: 10934357. DOI: 10.1002/(SICI)1521-3773(20000515)39:10<1775::AID-ANIE1775>3.0.CO;2-Q.
- 24. "Bis(7)-tacrine, a novel AChE-inhibitor, reverses AF64A-induced deficits in navigational memory in rats" J. Liu, W.-L. Ho, N. T. Lee, P. R. Carlier, Y.-P. Pang, Y.-F. Han\* *Neuroscience Letters* **2000**, *282*, 165-168. PubMed PMID: 10717417.
- 25. "Protection against ischemic injury in primary cultured mouse astrocytes by *bis*(7)-tacrine, a novel anti-Alzheimer's agent," Dong-Cheng Wu, Xiao-Qiu Xiao, Alberto K. Y. Ng, Priscilla M. Y. Chen, Wilson Chung, Nelson T. K. Lee, Paul R. Carlier, Yuan-Ping Pang, Albert C. H. Yu,\* Yi-Fan Han\* *Neuroscience Letters* **2000**, *288*, 95-98. (corrigendum in issue 290, p. 84). PMID: 10876069.
- 26. "HMPA Promotes Retro-Aldol Reaction, Resulting in Syn-Selective Addition of Lithiated 1-Naphthylacetonitrile to Aromatic Aldehydes" Paul R. Carlier,\* Cedric W.-S. Lo, Michael M.-C. Lo, Nan Chi Wan, Ian D. Williams *Organic Letters* **2000**, *2*, 2443-2445. PubMed PMID: 10956517. DOI: 10.1021/ol006099w
- 27. "Bis(7)-tacrine, a promising anti-Alzheimer's agent, reduces hydrogen peroxide-induced injury in rat pheochromocytoma cells: comparison with tacrine," Xiao-Qiu Xiao, Nelson T.-K. Lee, Paul R. Carlier, Yuan-Ping Pang, Yifan Han\* *Neuroscience Letters* **2000**, *290*, 197-200. PubMed PMID: 10963897.
- 28. "Enzyme biosensor for studying therapeutics of Alzheimer's disease" Ralf Lenigk,\* Edmund Lam, Ada Lai, Hong Wang, Yifan Han, Paul Carlier, Reinhard Renneberg *Biosensors & Bioelectronics* **2000**, *15*, 541-547. PMID: 11419651. DOI: 10.1016/S0956-5363(00)00078-6.
- 29. "<sup>7</sup>L/<sup>31</sup>P NMR Studies of Lithiated Arylacetonitriles in THF-HMPA Solution: Characterization of HMPA-Solvated Monomers, Dimers, and Separated Ion Pairs," Paul R. Carlier\* and Cedric W.-S. Lo *Journal of the American Chemical Society.* **2000**, *122*, 12819-12823. DOI: <u>10.1021/ja002318x</u>.
- 30. "'Click Chemistry' in situ: Acetylcholinesterase as a Molecular-Scale Reaction Vessel for the Selective Assembly of a Femtomolar Inhibitor," Warren G. Lewis, Luke G. Green, Flavio Grynszpan, Zoran Radic, Paul R. Carlier, Palmer Taylor, M.G. Finn,\* K. Barry Sharpless\* *Angewandte Chemie, International Edition,* 2002, 41, 1053-1057. PubMed PMID: 12491310. DOI: 10.1002/1521-3773(20020315)41:6<1053::AID-ANIE1053>3.0.CO;2-4.
- 31. "Schisandrin B protects against tacrine- and bis(7)-tacrine-induced hepatotoxicity and enhances cognitive function in mice." S. Y. Pan, Y. F. Han, P. R. Carlier, Y. P. Pang, D, H. F. Mak, B. Y. H. Lam, and K. M. Ko\* *Planta Medica* **2002** *68*, 217-220. PubMed PMID: 11914957.
- 32. Discovery of Non-Zwitterionic GABA<sub>A</sub> Receptor Full Agonists and a Superagonist," Paul R. Carlier,\* Ella S.-H. Chow, Rebecca L. Barlow, Jeffrey R. Bloomquist *Bioorganic & Medicinal Chemistry Letters* **2002**, *12*, 1985-1988. PubMed PMID: 12113824. DOI: 10.1016/S0960-894X(02)00299-8
- 33. "Effective Computational Modeling of Constitutional Isomerism and Aggregation States of Explicit Solvates of Lithiated Phenylacetonitrile," Paul R. Carlier,\* Jeffrey D. Madura *Journal of Organic Chemistry* **2002**, *67*, 3832-3840. PubMed PMID: 12027700. DOI: 10.1021/ja002318x.
- 34. "Catalytic Asymmetric Synthesis of Protected Tryptophan Regioisomers" Paul R. Carlier,\* Polo C.-H. Lam, Dawn M. Wong *Journal of Organic Chemistry* **2002**, *67*, 6256-6259. PubMed PMID: 12182675. DOI: 10.1021/jo025964i.

- 35. "Immobilized Enzymes as Catalytically Active Tools for Nanofabrication" Chang-Hyun Jang, Benjamin D. Stevens, Paul R. Carlier, Michael A. Calter, and William A. Ducker\* *Journal of the American Chemical Society*, **2002**, *124*, 12114-12115. PubMed PMID: 12371849. DOI: 10.1021/ja017686v.
- 36. "Acetylcholinesterase Complexed with Bivalent Ligands Related to Huperzine A: Experimental Evidence for Species-Dependent Protein-Ligand Complementarity" Dawn M. Wong, Harry M. Greenblatt, Hay Dvir, Paul R. Carlier, Yifan Han, Yuan-Ping Pang, Israel Silman, Joel Sussman\* *Journal of the American Chemical Society*, **2003**, *125*, 363-373. PubMed PMID: 12517147. DOI: 10.1021/ja021111w.
- 37. "Configurational Stability of Lithiated Cyclopropylnitriles: A Density Functional Study." Paul R. Carlier\* *Chirality* **2003**, *15*, 340-347. PubMed PMID: 12666242. DOI: 10.1002/chir.10222.
- 38. "Enantioselective Synthesis of "Quaternary" 1,4-Benzodiazepin-2-one Scaffolds via Memory of Chirality," Paul R. Carlier\*, Hongwu Zhao, Joe DeGuzman, Polo C.-H. Lam *Journal of the American Chemical Society* **2003**, *125*, 11482-11483. PMID: 13129335. DOI: 10.1021/ja0365781.
- 39. "Threading the Needle: Mimicking Nature's Toroidal Catalysts" Paul R. Carlier\*, *Angewandte Chemie, International Edition* **2004**, *43*, 2602-2605 (invited review article ("Highlight")). PMID: 18629975. DOI: 10.1002/anie.200301731.
- 40. "Development of Bivalent Acetycholinesterase Inhibitors as Potential Therapeutic Drugs for Alzheimer's Disease," Da-Ming Du, Paul R. Carlier\* *Current Pharmaceutical Design* **2004**, *10*, 3141-3156. PMID: 15544504. DOI: 10.2174/1381612043383412.
- 41. "Memory of Chirality: an Emerging Strategy for Asymmetric Synthesis" Hongwu Zhao, Danny Hsu, Paul R. Carlier\*, invited review, *Synthesis* **2005**, 1-16. DOI: 10.1055/s-2004-834931.
- 42. "Experimental and Computational Studies of Ring Inversion of 1,4-Benzodiazepin-2-ones: Implications for Memory of Chirality Transformations" Polo C.-H. Lam, Paul R. Carlier\* *Journal of Organic Chemistry* **2005**, *70*, 1530-1538. PubMed PMID: 15730270. DOI: 10.1021/jo048450n.
- 43. "A simple route to tetrahydro-1,4-benzodiazepin-3-ones bearing diverse N1, N4, and C10 functionalization" Ella C. Clement, Paul R. Carlier\* *Tetrahedron Letters* **2005**, *46*, 3633-3635. DOI: 10.1016/i.tetlet.2005.03.171.
- 44. "Novel dimeric acetylcholinesterase inhibitor bis(7)-tacrine, but not donepezil, prevents glutamate-induced neuronal apoptosis by blocking N-methyl-D-aspartate receptors" W. Li, R. B. Pi, H. H. N Chan, H. J Fu, N. T. K. Lee, H. W. Tsang, Y. M. Pu, D. C. Chang, C. Y. Li, J. L. Luo, K. M. Xiong, Z. W. Li, H. Xue, P. R. Carlier, Y. P. Pang, K. W. K. Tsim, M. T. Li, Y. F. Han\* *Journal of Biological Chemistry*, 2005, 280, 18179-18188. PubMed PMID:15710623. DOI: 10.1074/jbc.M411085200.
- "Crystal Packing Mediates Enantioselective Ligand Recognition at the Peripheral Site of Acetylcholinesterase" Haim Haviv, Dawn M. Wong, Harry M. Greenblatt, Paul R. Carlier, Yuan-Ping Pang, Israel Silman, Joel L. Sussman\* *Journal of the American Chemical Society* 2005, 127, 11029-11036. PubMed PMID: 16076210. DOI: 10.1021/ja051765f.
- 46. "Memory of Chirality Trapping of Low Inversion Barrier 1,4-Benzodiazepin-2-one Enolates," Paul R. Carlier\*, Polo C.-H. Lam, Joseph C. DeGuzman, and Hongwu Zhao *Tetrahedron: Asymmetry* **2005**, *16*, 2998-3002. DOI: 10.1016/j.tetasy.2005.08.017.
- 47. "Highly enantioselective synthesis of rigid, quaternary 1,4-benzodiazepin-2,5-diones derived from proline" Stephanie MacQuarrie-Hunter, Paul R. Carlier\* *Organic Letters*, **2005**, *7*, 5305-5308. PubMed PMID: 16268564. DOI: 10.1021/ol052182d.

48. "Protonated 2-methyl-1,2-epoxypropane: a challenging problem for density functional theory" Paul R. Carlier\*, Nipa Deora, T. Daniel Crawford *Journal of Organic Chemistry* **2006**, *71*, 1592-1597. PubMed PMID: 16468811. DOI: 10.1021/jo052303n.

- 49. "Complexes of Alkylene-Linked Tacrine Dimers with Torpedo californica Acetylcholinesterase: Binding of bis(5)-Tacrine Produces a Dramatic Rearrangement in the Active-Site Gorge" Edwin H. Rydberg, Boris Brumshtein, Harry M. Greenblatt, Dawn M. Wong, David Shaya, Larry D. Williams, Paul R. Carlier, Yuan-Ping Pang, Israel Silman and Joel L. Sussman\* Journal of Medicinal Chemistry 2006, 49, 5491-5500. PubMed PMID: 16942022. DOI: 10.1021/jm060164b.
- 50. "The effect of 2,6-disubstituted-aryl groups on acyclic conformation: preference for an antiperiplanar orientation of the geminal and vicinal hydrogens" Paul R. Carlier\*, Yiqun Zhang, Carla Slebodnick, Michael M. C. Lo, Ian D. Williams *Journal of Organic Chemistry* **2006**, *71*, 8835-8841. PubMed PMID: 17081013. DOI: 10.1021/jo061495z.
- 51. "Enantioselective Synthesis of Diversely Substituted Quaternary 1,4-Benzodiazepine-2-ones and 1,4-Benzodiazepin-2-,5-diones" Paul R. Carlier\*, Hongwu Zhao, Stephanie L. MacQuarrie, Joseph C. DeGuzman, Danny C. Hsu *Journal of the American Chemical Society* **2006**, *128*, 15215-15220. PubMed PMID: 17117873. DOI: 10.1021/ja0640142.
- 52. "Antidepressant-like effects of novel triple reuptake inhibitors, (2SR, 3RS)-N,N- dimethyl-3-cyclohexyl-3-hydroxy-2-(2'-naphthyl)propylamine (PRC025) and (2RS,3RS)-N-methyl-3-hydroxy-2-(2'-naphthyl)-3-phenylpropylamine (PRC050)." Amanda M. Shaw, Mona Boules, Yiqun Zhang, Katrina Williams, Jessica Robinson, Paul R. Carlier, Elliott Richelson\* *European Journal of Pharmacology* **2007**, *555*, 30-36. PubMed PMID: 17109850. DOI: 10.1016/j.ejphar.2006.10.004.
- 53. "The first enantioenriched, metalated nitrile possessing macroscopic configurational stability" Paul R. Carlier\*, Yiqun Zhang *Organic Letters* **2007**, *9*, 1319-1322. PubMed PMID: 17348666. DOI: 10.1021/ol070149g.
- 54. "Alkylene Tether-Length Dependent GABA<sub>A</sub> Receptor Competitive Antagonism by Tacrine Dimers: Bis(2)-Tacrine Is Ten Times More Potent than (+)-Bicuculline" Chaoying Li, Paul R. Carlier, Hong Ren, Kelvin K.W. Kan, Kwokmin Hui, Hong Wang, Wenming Li, Zhiwang Li, Keming Xiong, Ella Chow Clement, Hong Xue, Xiangou Liu, Mingtao Li, Yuan-Ping Pang, and Yi-Fan Han\* *Neuropharmacology* **2007**, *52*, 436-443. PubMed PMID: 17056074.
- 55. "East Meets West in the Search for Alzheimer's Therapeutics-Novel Dimeric Inhibitors from Tacrine and Huperzine A" W. M. Li, K. K. W. Kan, P. R. Carlier, Y. P. Pang, Y.F. Han\* *Current Alzheimer Research* **2007**, *4*, 386-396. PubMed PMID: 17908041. DOI: 10.2174/156720507781788918.
- 56. "The physicochemical properties and the in vivo AChE inhibition of two potential anti-Alzheimer agents, bis(12)-hupyridone and bis(7)-tacrine," Hua Yu, Wen-Ming Li, Jason M. K. Ho, Paul R. Carlier, Yuan-Ping Pang,, Zhe-Ming Gu, Zuo Zhong, Kelvin Chan, Yi-Tao Wang\*, Yi-Fan Han\* Journal of Pharmaceutical and Biomedical Analysis **2008**, *46*, 75-81. PubMed PMID: 17931815. DOI: 10.1016/j.jpba.2007.08.027.
- 57. Mode of action of the plant-derived silphinenes on insect and mammalian GABA<sub>A</sub> receptor/chloride channel complex. Jeffrey R. Bloomquist\*, Dhana Raj Boina, Ella Chow, Paul R. Carlier, Matías Reina and Azucena Gonzalez-Coloma, *Pesticide Biochemistry and Physiology* **2008**, *91*, 17-23. DOI: 10.1016/j.pestbp.2007.12.002.

- 58. "Towards a Species-Selective Acetylcholinesterase Inhibitor to Control the Mosquito Vector of Malaria, *Anopheles gambiae*" Paul R. Carlier\*, Troy D. Anderson, Dawn M. Wong, Danny C. Hsu, Joshua Hartsel, Ming Ma, Eric A. Wong, Ranginee Choudhury, Polo C-H. Lam, Maxim M. Totrov, Jeffrey R. Bloomquist, *Chemico-Biological Interactions* **2008**, *175*, 368-375. PMID: 18554580. DOI: 10.1016/j.cbi.2008.04.037.
- 59. "Antidepressant-like pharmacological profile of a novel triple re-uptake inhibitor, PRC200" Yanqi Liang, Amanda M. Shaw, Mona Boules, Siobhan Briody, Jessica Robinson, Alfredo Oliveros, Eric Blazar, Katrina Williams, Yiqun Zhang, Paul R. Carlier, Elliott Richelson\*, *Journal of Pharmacology and Experimental Therapeutics* **2008**, *327*, 573-583. PubMed PMID:18689611. DOI: 10.1124/jpet.108.143610.
- 60. "Development and validation of an HPLC-DAD method for *bis*(12)-*hupyridone* and its application to a pharmacokinetic study" Hua Yu, Wen Ming Li, Man Chun Cheung, Zhong Zuo, Paul R. Carlier, Ze Ming Gu, Kelvin Chan, Min Huang, Yi Tao Wang, Yi-Fan Han\*, *Journal of Pharmaceutical and Biomedical Analysis* **2009**, 49, 410-414. PubMed PMID: 19124214. DOI: 10.1016/j.jpba.2008.11.013.
- 61. "Complete mapping of the stereochemical course of retentive deprotonation/alkylation of 1*H*-benzo[e][1,4]diazepin-2(3*H*)-ones" Danny C. Hsu, Polo C.-H. Lam, Carla Slebodnick, Paul R. Carlier\*, *Journal of the American Chemical Society* **2009**, *131*, 18168–18176. PubMed PMID: 19921816. DOI: 10.1021/ja907507j.
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- 27. "Synthesis and Evaluation of Homodimeric and Heterodimeric AChE Inhibitors based on Tacrine" Paul R. Carlier,\* Yifan Han, Ella S.-H. Chow, Crystal P.-L. Li, Hong Wang, Jing Liu, Thuy Xuan Lieu, Hau Sum Wong, Yuan-Ping Pang Book of Abstracts, Sixth Chemistry Postgraduate Research Symposium in Hong Kong, Hong Kong, April 24, 1999, Abstract O-46.
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- 30. "HMPA-Mediated, Syn-Selective Aldol Reaction of Arylacetonitriles with Aromatic Aldehydes," Paul R. Carlier,\* <u>Cedric W.-S. Lo</u>, Michael M.-C. Lo, Nan Chi Wan *Book of Abstracts, Seventh Chemistry Postgraduate Research Symposium in Hong Kong*, Hong Kong, April 29, 2000, Abstract O-40.
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- 41. "Persistence Of Chiral Memory In Enantioselective Alkylation of 1,4-Benzodiazepin-2-ones" Polo C.-H. Lam, Paul R. Carlier\*, Book of Abstracts, 55th Southeast Regional Meeting of the American Chemical Society, Atlanta, GA, November 16-19, 2003; American Chemical Society: Washington, D. C., Abstract 605.
- 42. "Enantioselective Synthesis of Quaternary Proline-derived 1,4-Benzodiazepin-2,5-diones" <a href="Stephanie L. MacQuarrie">Stephanie L. MacQuarrie</a>, Paul R. Carlier\*, Book of Abstracts, 55th Southeast Regional Meeting of the American Chemical Society, Atlanta, GA, November 16-19, 2003; American Chemical Society: Washington, D. C., Abstract 601.
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- 44. "Enantioselective Synthesis Of "Quaternary" 1,4-Benzodiazepin-2-One Scaffolds Via Memory Of Chirality" <u>Joseph C. DeGuzman</u>, Paul R. Carlier\*, <u>Book of Abstracts</u>, 55th Southeast Regional Meeting of the American Chemical Society, Atlanta, GA, November 16-19, 2003; American Chemical Society: Washington, D. C., Abstract 600.
- 45. "A Memory of Chirality Route to Enantioenriched Quaternary 1,4-benzodiazepin-2,5-diones" Paul R. Carlier\*, Stephanie MacQuarrie, Book of Abstracts, 228<sup>th</sup> ACS National Meeting, Philadelphia, PA, August 22-26, 2004; American Chemical Society: Washington, D.C., ORGN 0257.
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  <a href="MacQuarrie">MacQuarrie</a>, Paul R. Carlier\*, Book of Abstracts, 230th National Meeting of the American Chemical Society, Washington D.C., August 28-September 1, 2005; American Chemical Society: Washington, D.C., ORGN0771.
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- 53. "IR, NMR, and computational studies of lithiated phenylacetonitrile in THF/HMPA" H. <u>Jason Harmon</u>, Paul R. Carlier\*,Book of Abstracts, 230<sup>th</sup> National Meeting of the American Chemical Society, Washington D.C, August 28-September 1, 2005; American Chemical Society: Washington, D.C., ORGN0341.
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- 63. "Computational and experimental studies of free and enzyme-bound N-alkyltacrine derivatives" Paul R. Carlier\* and <u>Larry D. Williams</u>, 233<sup>rd</sup> National Meeting of the American Chemical Society, Chicago, IL, March 25-29, 2007; American Chemical Society: Washington D.C. MEDI-010.
- 64. "Biochemical and molecular characterization of bivalent anticholinesterases to the malarial mosquito" <u>Troy D. Anderson</u>, David C. Klorig, Dawn Wong, Paul R. Carlier, and Jeffrey R. Bloomquist\* 233<sup>rd</sup> National Meeting of the American Chemical Society, Chicago, IL, March 25-29, 2007; American Chemical Society: Washington D.C. AGRO-0093.
- 65. "Crystal Structures of Complexes with AChE of Novel Lead Compounds for Treatment of Alzheimer's Disease: Structural Comparison with Aricept" Harry M. Greenblatt, Haim Haviv, Boris Brumstein, Dawn M. Wong, Paul R. Carlier, Yi-Fan Han, Yuan-Ping Pang, Hua-Liang Jiang, Dong-Lu Bai, Israel Silman and Joel L. Sussman\*, Book of Abstracts, IXth International Conference on Cholinesterases, Suzhou, China, May 6-10, 2007, p. 49.
- 66. Invited: "Development of a Mosquito-Selective AChE Inhibitor to Control the Malaria Vector, Anopheles Gambiae" Paul R. Carlier\*, Jeffrey R. Bloomquist, Dawn M. Wong, Larry D. Williams, Nipa Deora, Troy Anderson, Sally Paulson, Ania Wysinski, Eric Wong, Ranginee Choudhury, Maxim Totrov, Polo C.-H. Lam, .Book of Abstracts, IXth International Conference on Cholinesterases, Suzhou, China, May 6-10, 2007, p. 77.
- 67. "Bis(7)-Tacrine, A Potential AChE Inhibitor, Displaces [3H]Dizocilpine Binding to N-Methyl-D-Aspartate Receptors" Zhi-Ling Yu\*, Paul R. Carlier, Yi-Fan Han, Book of Abstracts, IXth International Conference on Cholinesterases, Suzhou, China, May 6-10, 2007, p. 118
- 68. Computational and experimental studies of free and enzyme-bound N-alkyltacrine derivatives" <u>Larry D. Williams</u> and Paul R. Carlier\*, Book of Abstracts, 2007 Meeting of the Southeastern Theoretical Chemistry Association, Blacksburg, VA, May 18-19, 2007.
- 69. Computational Studies on the Mechanism of Memory of Chirality Deprotonation/Alkylation of 1,4-Benzodiazepin-2-ones," <u>Danny C. Hsu</u> and Paul R. Carlier\*, Book of Abstracts, 2007 Meeting of the Southeastern Theoretical Chemistry Association, Blacksburg, VA, May 18-19, 2007.

- 70. "Macroscopic Configurational Stability in a Metalated Nitrile: A Tale of Two Metals" <u>Paul R. Carlier\*</u>, Yiqun Zhang, 8<sup>th</sup> International Symposium on Carbanion Chemistry (ISCC-8), Madison, WI, June 6-10, 2007, Abstract P-05.
- 71. **Invited:** "Freeze frame observation of stereochemical information transfer to and from transiently non-racemic enolates" <u>Paul R. Carlier</u>\*, Danny C. Hsu, 8<sup>th</sup> International Symposium on Carbanion Chemistry (ISCC-8), Madison, WI, June 6-10, 2007, Book of Abstracts, Abstract OP-2.
- 72. "Biochemical analysis of the AChE catalytic gorge in green peach aphid, Myzus persicae (Sulzer) (Hemiptera: Aphididae): Cys286 as a putative target site for insecticide design" T. D. Anderson, D. Hsu, M. Totrov, P. R. Carlier, and J. R. Bloomquist\*. Poster D0283, Annual Entomological Society of America Conference, San Diego, California, December 12, 2007.
- 73. "Bump-hole reoptimization of the tacrine pharmacophore achieves selective inhibition of *Anopheles gambiae* acetylcholinesterase" Paul R. Carlier\*, <u>Larry D. Williams</u>, Jeffrey R. Bloomquist, Troy D. Anderson, Sally Paulson, Ania Wysinski, Book of Abstracts, 235<sup>th</sup> National Meeting of the American Chemical Society, New Orleans, LA, April 6-10, 2008; American Chemical Society: Washington D. C. MEDI-0331.
- 74. "Capture of a transiently non-racemic potassium enolate: Insight into memory of chirality" Paul R. <u>Carlier\*</u>, Danny C. Hsu, Carla Slebodnick, Book of Abstracts, 236<sup>th</sup> National Meeting of the American Chemical Society, Philadelphia, PA, August 17-21, 2008; American Chemical Society: Washington D.C. ORGN-039.
- 75. "Highly species-selective acetylcholinesterase inhibitors for control of Anopheles gambiae, the mosquito vector of malaria" Paul R. Carlier\*, <u>Joshua Hartsel</u>, Ming Ma, Dawn Wong, Jeffrey R. Bloomquist, Troy D. Anderson, Sally Paulson, Ania Wysinski, Eric Wong, Ranginee Choudhury, Book of Abstracts, 236<sup>th</sup> National Meeting of the American Chemical Society, Philadelphia, PA, August 17-21, 2008; American Chemical Society: Washington D.C. MEDI-465.
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- 77. "Computational studies of ion pair separation of organolithium compounds" <u>Nipa Deora</u>, Paul R. Carlier\*, Book of Abstracts, 236<sup>th</sup> National Meeting of the American Chemical Society, Philadelphia, PA, August 17-21, 2008; American Chemical Society: Washington D.C. COMP-131.
- 78. "Differential potency of bivalent anticholinesterases as a model for the molecular design of selective insecticides" <u>James M. Mutunga</u>, Troy D. Anderson, Paul R. Carlier, Jeffrey R. Bloomquist\*, Book of Abstracts, 236<sup>th</sup> National Meeting of the American Chemical Society, Philadelphia, PA, August 17-21, 2008; American Chemical Society: Washington D.C. AGRO-062.
- 79. "Biochemical characterization of a putative insecticide target site in the acetylcholinesterase catalytic gorge of green peach aphid." <u>Troy D. Anderson</u>, Danny C. Hsu, Paul R. Carlier, Polo C.-H. Lam, Maxim M. Totov, Jeffrey R. Bloomquist\*, Book of Abstracts, 236<sup>th</sup> National Meeting of the American Chemical Society, Philadelphia, PA, August 17-21, 2008; American Chemical Society: Washington D.C. AGRO-080.

- 80. "Biochemical and toxicological characterization of highly-selective anticholinesterases developed for malarial mosquito control," <u>Troy. D. Anderson</u>, Joshua Hartsel, Ming Ma, James M. Mutunga, Ania Wysinski, Brian T. Jackson, Dawn Wong, Sally Paulson, Paul R. Carlier, and Jeffrey R. Bloomquist\*, Book of Abstracts, 236<sup>th</sup> National Meeting of the American Chemical Society, Philadelphia, PA, August 17-21, 2008; American Chemical Society: Washington D.C. AGRO-079.
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- 82. "Bump-hole reoptimization of the tacrine pharmacophore achieves selective inhibition of *Anopheles gambiae* acetylcholinesterase Paul R. Carlier,\* <u>Larry D. Williams</u>, Ming Ma, Jeffrey R. Bloomquist, Troy D. Anderson, Lakshmipathi Srigiriraju, Sally Paulson, Ania Wysinski, Eric A. Wong, and Ranginee Choudhury, p. 84, Book of Abstracts, Deans' Forum on Infectious Disease, September 29, 2008, Virginia Tech, Blacksburg, VA.
- 83. "Towards a Species-Selective Acetylcholinesterase Inhibitor to Control the Mosquito Vector of Malaria, *Anopheles gambiae*" Paul R. Carlier\*, Troy D. Anderson, <u>Dawn M. Wong</u>, Danny C. Hsu, Joshua Hartsel, Ming Ma, Eric A. Wong, Ranginee Choudhury, Polo C-H. Lam, Maxim M. Totrov, Jeffrey R. Bloomquist, p.59, Book of Abstracts, Deans' Forum on Infectious Disease, September 29, 2008, Virginia Tech, Blacksburg, VA.
- 84. "Novel carbamates for malaria vector control: impact of recent developments and the future of insecticide use in malaria mosquito control" <u>James M. Mutunga</u>, Troy D. Anderson, Joshua A. Hartsel, Sally L. Paulson, Dawn M. Wong, Paul R. Carlier, Jeffrey R. Bloomquist\*, Book of Abstracts, 2009 Annual Meeting, Kenyan Students and Scholars Association, July 31 August 1, 2009, Bowling Green State University, Bowling Green, OH.
- 85. "DFT studies of ion pair separation of benzylic organolithiums: Importance of both explicit and implicit solvation" Nipa Deora, Paul R. Carlier\*, Book of Abstracts, 238th National Meeting of the American Chemical Society, Washington, D.C, August 16-20, 2009; American Chemical Society: Washington D.C. ORGN-561.
- 86. "Regioselective access to 1,3- and 1,4-diols by opening of *trans*-1,2,4,5-diepoxycyclohexane with anilines" Christopher J. Monceaux, Paul R. Carlier\* Book of Abstracts, 238th National Meeting of the American Chemical Society, Washington, D.C, August 16-20, 2009; American Chemical Society: Washington D.C. ORGN-282.
- 87. "Molecular design and semi-field performance of highly selective carbamates for control of the malaria mosquito, Anopheles gambiae" <a href="Jeffrey R Bloomquist">Jeffrey R Bloomquist</a>\*, Troy D. Anderson, Paul R. Carlier, John Githure, Joshua Hartsel, Polo C-H. Lam, Ming Ma, Hortance Manda, James M Mutunga, Sally L. Paulson, Maxim M. Totrov, Dawn M. Wong, and Eric Wong, Book of Abstracts, 238th National Meeting of the American Chemical Society, Washington, D.C, August 16-20, 2009; American Chemical Society: Washington D.C. AGRO-050.
- 88. "Safety evaluation of newly developed carbamate insecticides" Ying Jiang, Fredrik Ekström, Paul R Carlier, Josh Hartsell, Ming Ma, and Jeffrey R Bloomquist\*, Book of Abstracts, 238th National Meeting of the American Chemical Society, Washington, D.C, August 16-20, 2009; American Chemical Society: Washington D.C. AGRO-053

- 89. "Highly selective carbamates for Anopheles gambiae acetylcholinesterase: Effects of pharmacokinetics on toxicity to mosquitoes" <u>James M. Mutunga</u>, Joshua Hartsel, Ming Ma, Lakshmipathi Srigiriraju, Dawn M. Wong, Bryan T. Jackson, Troy D. Anderson, Sally L. Paulson, Paul R Carlier, and Jeffrey R Bloomquist\*Book of Abstracts, 238th National Meeting of the American Chemical Society, Washington, D.C, August 16-20, 2009; American Chemical Society: Washington D.C. AGRO-086.
- 90. "Development of mosquito-selective acetylcholinesterase inhibitors to control the malaria vector, Anopheles gambiae: Comparative sequence and structure approach" <a href="Dawn M. Wong">Dawn M. Wong</a>, Paul R Carlier, Polo C-H. Lam, Maxim M. Totrov, and Jeffrey R. Bloomquist\*Book of Abstracts, 238th National Meeting of the American Chemical Society, Washington, D.C, August 16-20, 2009; American Chemical Society: Washington D.C. AGRO-093.
- 91. "Biochemical and toxicological assessment of newly designed insect acetylcholinesterase inhibitors against mosquito vectors and agricultural pests" Daniel R. Swale, Paul R Carlier, Josh Hartsel, Ming Ma, and Jeffrey R. Bloomquist\* Book of Abstracts, 238th National Meeting of the American Chemical Society, Washington, D.C, August 16-20, 2009; American Chemical Society: Washington D.C. AGRO-078.
- 92. **Invited:** "Redesign of tacrine to achieve potent and selective inhibition of *Anopheles gambiae* acetylcholinesterase" <u>Paul R. Carlier</u>\*, Larry D. Williams, Ming Ma, Jeffrey R. Bloomquist, Troy D. Anderson, Eric A. Wong, Ranginee Choudhury, Max Totrov, Polo Lam, Invited Lecture, Book of Abstracts, 10<sup>th</sup> International Meeting on Cholinesterases, 20-25 September 2009, Šibenik, Croatia.
- 93. "Discovery of highly species-selective, contact toxic aryl carbamates to control *Anopheles gambiae*, the mosquito vector of malaria" Paul R. Carlier\*, <u>Joshua A. Hartsel</u>, Ming Ma, Dawn M. Wong, Jeffrey R. Bloomquist, Troy D. Anderson, Sally L. Paulson, Ania Wysinski, Eric A. Wong, Ranginee Choudhury, Max Totrov, Polo Lam, Book of Abstracts, 10<sup>th</sup> International Meeting on Cholinesterases, 20-25 September 2009, Šibenik, Croatia.
- 94. "Mosquito-selective acetylcholinesterase inhibitors to control the malaria vector, *Anophles gambiae*: experimental evidence for allosteric solvent effects and antagonism of inhibition" <u>Dawn M. Wong</u>, Daniel Swale, Joshua A. Hartsel, Ming Ma, Paul R. Carlier, Polo C.-H. Lam, Maxim M. Totrov, Jeffrey R. Bloomquist\*, Book of Abstracts, 10<sup>th</sup> International Meeting on Cholinesterases, 20-25 September 2009, Šibenik, Croatia.
- 95. "Molecular interactions of highly selective carbamates with acetylcholinesterase of the malaria mosquito, *Anopheles gambiae*" Jeffrey R. Bloomquist\*, Troy Anderson, Paul Carlier, Joshua Hartsell, Ying Jiang, Polo Lam, Ming Ma, James Mutunga, Daniel Swale, Maxim Totrov, Dawn Wong, Book of Abstracts, 239th National Meeting of the American Chemical Society, San Francisco, CA, March 21-25, 2010; American Chemical Society: Washington D.C. AGRO-167.
- 96. "Evaluation of new carbamate insecticides for neurotoxicity to non-target species" Ying Jiang, Fredrik Ekstrom, Paul Carlier, Josh Hartsel, Ming Ma, Jeffrey R. Bloomquist\* Book of Abstracts, 239th National Meeting of the American Chemical Society, San Francisco, CA, March 21-25, 2010; American Chemical Society: Washington D.C. AGRO-177.
- 97. "Comparison of Pd-catalyzed amination and nucleophilic aromatic substitution routes to *N*-alkyltacrines and analogs" <u>Ming Ma</u>, Jimit Mehta, Larry D. Williams, and Paul R. Carlier\* Book of Abstracts, 239th National Meeting of the American Chemical Society, San Francisco, CA, March 21-25, 2010; American Chemical Society: Washington D.C. ORGN-882.

- 98. "Anopheles gambiae-selective, meta-substituted aryl carbamates for control of malaria" Ming Ma, Joshua A. Hartsel, Troy D. Anderson, James Mutunga, Dawn M. Wong, Polo C.-H. Lam, Max M. Totrov, Jeffery R. Bloomquist, Paul R. Carlier\* Book of Abstracts, 239th National Meeting of the American Chemical Society, San Francisco, CA, March 21-25, 2010; American Chemical Society: Washington D.C. AGRO-269.
- 99. "Kinetic studies of enantiomerization of a highly enantioenriched Grignard reagent" Neeraj Patwardhan, Ming Gao, Paul R. Carlier\* Book of Abstracts, 241st National Meeting of the American Chemical Society, Anaheim, CA, March 27-31, 2011; American Chemical Society: Washington D.C. ORGN-604.
- 100. "Isoxazol-3-yl and pyrazol-5-yl-based AChE inhibitors to combat insecticide resistance in Anopheles gambiae" <u>Astha</u>, Qiao-hong chen, Dawn M. Wong, James Mutunga, Jianyong Li, Polo C.-H. Lam, Max Totrov, Jeffrey R. Bloomquist and Paul R. Carlier\*, Poster -00, *Vector-borne Disease Mini-symposium*, April 22, 2011, Virginia Tech, Blacksburg, VA.
- 101. "Resistance-breaking pyrazol-4-yl acetylcholinesterase inhibitors for the malaria mosquito, *Anopheles gambiae*" Qiao-Hong Chen, Dawn M. Wong, James Mutunga, Jianyong Li, Polo C.-H. Lam, Max M. Totrov, Jeffrey R. Bloomquist, and Paul R. Carlier\*, Poster -00, *Vector-borne Disease Mini-symposium*, April 22, 2011, Virginia Tech, Blacksburg, VA.
- 102. "Kinetic evaluation of *Anopheles gambiae*-selective 2-alkoxyaryl and 2-thioalkylaryl methylcarbamate acetylcholinesterase inhibitors" <u>Dawn Wong</u>, Joshua A. Hartsel, Troy D. Anderson, James Mutunga, Jianyong Li, Jeffrey R. Bloomquist, Paul R. Carlier\* Poster -00, *Vector-borne Disease Mini-symposium*, April 22, 2011, Virginia Tech, Blacksburg, VA.
- 103. "Resistance-breaking acetylcholinesterase inhibitors for the malaria mosquito, Anopheles gambiae" Qiao-Hong Chen, Dawn M. Wong, James Mutunga, FNU Astha, Jianyong Li, Polo C.-H. Lam, Max M. Totrov, Jeffrey R. Bloomquist, and <a href="Paul R. Carlier">Paul R. Carlier</a>\*, Book of Abstracts, 24nd National Meeting of the American Chemical Society, Denver, CO, August 28-September 1, 2011; American Chemical Society: Washington D.C., AGRO-165.
- 104. "Differential Potency and Substrate Kinetics of Acetylcholinesterase Peripheral Site Ligands: The Molecular Basis of Selectivity for Anopheles gambiae." <u>James M. Mutunga</u>, Dawn M. Wong, Ming Ma, Max Totrov, Jianyong Li, Paul R. Carlier and Jeffrey R. Bloomquist\*, Book of Abstracts, 24nd National Meeting of the American Chemical Society, Denver, CO, August 28-September 1, 2011; American Chemical Society: Washington D.C., AGRO-068.
- 105. "Enzyme Kinetic Analysis of Allosteric Solvent Effects When Screening Mosquito-Selective Carbamates Against Anopheles gambiae" <u>Daniel Swale</u>, Paul Carlier, Ming Ma, Dawn Wong, Maxim Totrov, and Jeffrey R. Bloomquist\*, Book of Abstracts, 24nd National Meeting of the American Chemical Society, Denver, CO, August 28-September 1, 2011; American Chemical Society: Washington D.C., AGRO-065.
- 106. J. R. Bloomquist, F. Tong, P. R. Carlier, T. D. Anderson, J. A. Hartsel, M. Ma, D. M. Wong, S. L. Paulson, J. Li, M. Totrov, and P. Lam. Molecular pharmacology of new anticholinesterases for control of the malaria mosquito, *Anopheles gambiae*. National Meeting of the Entomological Society of America, Reno, Nevada, 2011.
- 107. "Anopheles gambiae-selective and resistance-breaking acetylcholinesterase inhibitors for malaria control" <a href="Paul R. Carlier">Paul R. Carlier</a>, Joshua A. Hartsel, Qiao-Hong Chen, Dawn M. Wong, James Mutunga, FNU Astha, Jianyong Li, Jeffrey R. Bloomquist, Polo C.-H. Lam, Max M. Totrov, Book of Abstracts, 60th Annual Meeting of the American Society of Tropical Medicine and Health, Philadelphia, PA, December 4-8, 2011, Philadelphia, PA, Abstract 431.

- 108. "Small ring heterocycle carbamates and carboxamides: the search for resistance-breaking, species-selective acetylcholinesterase inhibitors against the malaria mosquito" <u>Astha</u>, Qiao-hong Chen, Dawn M. Wong, James M. Mutunga, Carla Slebodnick, Polo C-H. Lam, Maxim M. Totrov, Jeffrey R. Bloomquist, Paul R. Carlier\*, p. 23, Book of Abstracts, 2<sup>nd</sup> Virginia Tech Symposium on Vector-Borne Disease Research "Parisitology, Vector Biology, Vaccine, and Drug Discovery," March 9-10, 2012
- 109. "Trifluoromethylketones: Potential new toxicophores towards Anopheles gambiae" <u>Eugene Camerino</u>, Dawn M. Wong, James M. Mutunga, Ming Ma, Jeffrey R. Bloomquist, Paul R. Carlier\*, p. 24, Book of Abstracts, 2<sup>nd</sup> Virginia Tech Symposium on Vector-Borne Disease Research "Parisitology, Vector Biology, Vaccine, and Drug Discovery," March 9-10, 2012.
- 110. "Small ring heterocyclic carbamates and carboxamides: The search for species-selective acetylcholinesterase inhibitors against the malaria mosquito" Fnu Astha, Qiao-Hong Chen, Dawn M Wong, James M Mutunga, Jianyong Li, Polo C.-H. Lam, Maxim M. Totrov, Jeffrey R. Bloomquist, Paul R. Carlier\* 243rd National Meeting of the American Chemical Society, March 25-29 2012, San Diego, California 'American Chemical Society, Washington D. C., ORGN-334.
- 111. **Invited:** "Designing inhibitors for potency against the G119S resistant mutant of *Anopheles gambiae* acetylcholinesterase" <u>Paul R. Carlier\*</u>, Qiao-Hong Chen, Astha, Dawn M. Wong, Jianyong Li, James Mutunga, Polo C.-H. Lam, Maxim M. Totrov, and Jeffrey R. Bloomquist, Invited Lecture, Eleventh International Conference on Cholinesterases, Kazan, Russia, June 4-9, 2012, Abstract L2-6.
- 112. Kinetic, pharmacological, and toxicological consequences of the G119S resistance mutation in acetylcholinesterase-1 of *Anopheles gambiae* (Akron) <u>Dawn M. Wong</u>, Jiangyong Li, Qian Han, James M. Mutunga, Ania Wysinski, Troy D. Anderson, Haizhen Ding, Tiffany L. Carpenetti, Sally L. Paulson, Polo C.-H. Lam, Maxim M. Totrov, Jeffrey R. Bloomquist, and Paul R. Carlier\* Eleventh International Conference on Cholinesterases, Kazan, Russia, June 4-9, 2012, Abstract P2-25.
- 113. Bis(12)-hupyridone protects glutamate-induced neuronal loss via inhibiting GSK3β <u>W. Cui</u>, H.H.N. Chan, J. Luo, S. Hu, W. Li, Y. Zhao, S. Mak, J. Rong, P.R. Carlier, Y. Han\*, Eleventh International Conference on Cholinesterases, Kazan, Russia, June 4-9, 2012, Abstract P7-2.
- 114. "Designing anticholinesterase insecticides to achieve high selectivity for the malaria mosquito, Anopheles gambiae, and potency against known resistance mutations" <u>Paul R. Carlier</u>\*, Jeffrey R. Bloomquist, Jianyong Li, Maxim Totrov, Book of Abstracts, 244th National Meeting of the American Chemical Society, Philadelphia, PA, August 19-23, 2012; American Chemical Society, Washington, D. C., AGRO-125.
- "Five-membered ring heterocyclic carbamates and carboxamides: the quest for resistance-breaking, species-selective acetylcholinesterase inhibitors against the malaria mosquito" <u>Astha</u>, Qiao-Hong Chen, Dawn M. Wong, James Mutunga, Jianyong Li, Carla Slebodnick, Polo C.-H. Lam, Maxim M. Totrov, Jeffrey R. Bloomquist, and Paul R. Carlier\*, Book of Abstracts, 244th National Meeting of the American Chemical Society, Philadelphia, PA, August 19-23, 2012; American Chemical Society, Washington, D. C., AGRO-097.
- 116. "Evaluation of Novel Insecticidal Compounds as New Mosquitocides for Control of Aedes aegypti and Anopheles gambiae" Nicholas R. Larson, Rafique Islam, Paul R. Carlier, Ming Ma, and Jeffrey R. Bloomquist\* Book of Abstracts, 244th National Meeting of the American Chemical Society, Philadelphia, PA, August 19-23, 2012; American Chemical Society, Washington, D. C., AGRO-098.

- 117. "A Novel Carbamate Insecticide with Superior Selectivity for Cattle Tick (Boophilus microplus) and the Sand Fly (Phlebotomus papatasi) Control" <u>Daniel R. Swale</u>, Paul R. Carlier, Joshua A. Hartsel, Maxim M. Totrov, Kevin B. Temeyer, Jeffrey R. Bloomquist\* Book of Abstracts, 244th National Meeting of the American Chemical Society, Philadelphia, PA, August 19-23, 2012; American Chemical Society, Washington, D. C., AGRO-102.
- 118. "Fluorescent assay of acetylcholinesterase ligand interactions for design of insecticides targeting the mosquito vector of malaria, *Anopheles gambiae*" Fan Tong, Paul R. Carlier, Jianyong Li, Max Totrov, Jeffrey R. Bloomquist\* Book of Abstracts, 244th National Meeting of the American Chemical Society, Philadelphia, PA, August 19-23, 2012; American Chemical Society, Washington, D. C., AGRO-209.
- 119. "Structural determinants of Anopheles gambiae-selectivity for acetylcholinesterase inhibitor mosquitocides" Paul R. Carlier\*, Joshua A. Hartsel, Qiao-Hong Chen, Ming Ma, Dawn M. Wong, Jianyong Li, Jeffrey R. Bloomquist, Polo C.-H. Lam, Max M. Totrov, 61st Annual Meeting of the American Society of Tropical Medicine and Health, Nov. 11-15, 2012, Atlanta, GA, paper #24.
- 120. "Evaluation of Novel Synthetic Mosquitocides for Control of Aedes aegypti and Anopheles gambiae" <u>Jeff Bloomquist\*</u>, Nick Larson, Rafique Islam, Ming Ma, Paul Carlier, 61<sup>st</sup> Annual Meeting of the American Society of Tropical Medicine and Health, Nov. 11-15, 2012, Atlanta, GA.
- 121. "Novel mode of action of synthetic mosquitocides for control of disease vector mosquitoes, *Aedes aegypti* and *Anopheles gambiae*" N. Larson, R. Islam, P. Carlier, M. Ma, and J. R. Bloomquist. Annual Research Day, Emerging Pathogens Institute, University of Florida, Gainesville, Florida. February 14, 2013.
- 122. "Kinetic Characterization of the G119S Resistant Mutant of Anopheles gambiae Acetylcholinesterase."

  <u>Dawn M.Wong</u>, Jianyong Li, Qian Han, Haizhen Ding, Polo C.-H. Lam, Max Totrov, Jeffrey R.

  Bloomquist, Paul R. Carlier\*, 3<sup>rd</sup> Virginia Tech Symposium on Vector-Borne Disease Research, March 8-9, 2013, Book of Abstracts, p. 15.
- 123. Trifluoromethylketone prodrugs: potential insecticides against Anopheles gambiae. <u>Eugene Camerino</u>, Dawn M. Wong, Rafique Islam, Jianyong Li, Jeffrey R. Bloomquist, Paul R. Carlier\*, 3<sup>rd</sup> Virginia Tech Symposium on Vector-Borne Disease Research, March 8-9, 2013, Book of Abstracts, p. 21.
- 124. "Kinetic Characterization of the G119S Resistant Mutant of *Anopheles gambiae* AChE," <u>D.M. Wong</u>, J. Li, Q. Han, H. Ding, P.C.-H. Lam, M.M. Totrov, J.R. Bloomquist, and P.R. Carlier\*, XIVth International Symposium on Cholinergic Mechanisms, Hangzhou, China, May 5-9<sup>th</sup>, 2013.
- 125. "C-chiral Grignard Reagents: How do they racemize?" Paul R. Carlier\*, Ming Gao, Neeraj J. Patwardhan, Book of Abstracts, 246th National Meeting of the American Chemical Society, Indianapolis, IN, September 8-13, 2013; American Chemical Society, Washington, D. C., ORGN-160.
- 126. "Enantioselective ring contraction of benzodiazepin-2,5-dione enolates" Paul R. Carlier\*, Stephanie A. Antolak, Zhongke Yao, Carla Slebodnick, Book of Abstracts, 246th National Meeting of the American Chemical Society, Indianapolis, IN, September 8-13, 2013; American Chemical Society, Washington, D. C., ORGN-179.
- 127. "Voltage-sensitive potassium channels as new target sites for biorational insecticide design" J. R. Bloomquist, M. M. Totrov, P. R. Carlier. Book of Abstracts, 246th National Meeting of the American Chemical Society, Indianapolis, IN, September 8-13, 2013; American Chemical Society, Washington, D. C., AGRO-133

- 128. "Inhibitors targeting acetylcholinesterase with high selectivity for arthropod disease vectors" J. R. Bloomquist, J. Li, M. M. Totrov, P. R. Carlier. Book of Abstracts, 246th National Meeting of the American Chemical Society, Indianapolis, IN, September 8-13, 2013; American Chemical Society, Washington, D. C., AGRO-94
- "Evaluation of synthetic compounds as novel mosquitocides targeting potassium channels for control of Aedes aegypti and Anopheles gambiae" N. R. Larson, B. Sun, P. Carlier, M. Ma, and J. R. Bloomquist. 2013. Book of Abstracts, 246th National Meeting of the American Chemical Society, Indianapolis, IN, September 8-13, 2013; American Chemical Society, Washington, D. C., AGRO-131
- 130. "Nitriles as acetylcholinesterase inhibitors? Application of a serine protease strategy to develop new chemical interventions for the malaria mosquito" <u>Maryam Ghavami</u>, Dawn M. Wong, Fan Tong, Jeffrey R. Bloomquist, Paul R. Carlier\*, Virginia Tech Center for Drug Discovery, Drug Discovery Day 2013, Student Poster Session, Abstract A7, September 20, 2013, Blacksburg VA.
- 131. "Enantioselective Synthesis of the Potentially Useful 3-Aminoquinoline-2,4-dione Drug Scaffold" Stephanie Antolak, <u>Zhong-Ke Yao</u>, Gary Richoux, and Paul R. Carlier\*, Virginia Tech Center for Drug Discovery, Drug Discovery Day 2013, Student Poster Session, Abstract A8, September 20, 2013, Blacksburg VA.
- 132. "Isoxazol-3-yl carbamates and carboxamides: resistance-breaking acetylcholinesterase inhibitors against the malaria mosquito, Anopheles gambiae" <a href="Dawn M. Wong">Dawn M. Wong</a>, Astha Verma, James M. Mutunga, Rafique Islam, Fan Tong, Elisabet Viayna, Carla Slebodnick, Polo C.-H. Lam, Jianyong Li, Maxim M. Totrov, Jeffrey R. Bloomquist and Paul R. Carlier\*, Virginia Tech Center for Drug Discovery, Drug Discovery Day 2013, Student Poster Session, Abstract A9, September 20, 2013, Blacksburg VA.
- 133. **Invited:** "Resistance-breaking and species-selective anticholinesterase insecticides for *Anopheles gambiae*" Paul R. Carlier\*, Jeffrey R. Bloomquist, Jianyong Li, Max M. Totrov, 62<sup>nd</sup> Annual Meeting of the American Society of Tropical Medicine and Health, Nov. 13-17, 2013, Washington DC.
- 134. "Fluorinated methylketone produgs: Potential new insecticides against Anophele gambiae" <u>Eugene Camerino</u>, Dawn M. Wong, Rafique Islam, Jianyong Li, Jeffrey R. Bloomquist, Paul R. Carlier\* 2014. Book of Abstracts, 248th National Meeting of the American Chemical Society, San Francisco, CA, August 10-14; American Chemical Society, Washington, D. C., AGRO-678
- 135. "Resistance mechanisms in the Akron strain of west African *Anopheles gambiae* and their impact on new insecticidal chemistries." <u>JR Bloomquist</u>\*, A Verma, Q-H Chen, R Islam, P Lam, M Ma, F Tong, M Totrov, DM Wong, and PR Carlier. 2014. Book of Abstracts, 248th National Meeting of the American Chemical Society, San Francisco, CA, August 10-14; American Chemical Society, Washington, D. C., AGRO-842
- 136. "Serendipity and rational design in the development of resistance-breaking anticholinesterase insecticides for the malaria mosquito, Anopheles gambiae <a href="Paul R. Carlier">Paul R. Carlier</a>\*, Dawn M. Wong, Qiao-Hong Chen, Astha Verma, Rafique Islam, Fan Tong, Jianyong Li, Polo C.-H. Lam, Max Totrov, Jeffrey R. Bloomquist. 2014. Book of Abstracts, 248th National Meeting of the American Chemical Society, San Francisco, CA, August 10-14; American Chemical Society, Washington, D. C., AGRO-343.
- 137. "Effective difluoromethylketone inhibitors of the resistant G119S mutant of *Anopheles gambiae* acetylcholinesterase" Eugene Camerino, <u>Dawn M. Wong</u>, Florian Körber, Rafique Islam, Jianyong Li, Max Totrov, Jeffrey R. Bloomquist, and Paul R. Carlier, Drug Discovery Day 2014 Student Poster Session, Virginia Tech Center for Drug Discovery, Blacksburg, VA, September 26, 2014, Poster A3.

- 138. "Fluorinated methylketone prodrugs: potential new insecticides against *An. gambiae*" Eugene <u>Camerino</u>, Dawn M. Wong, Rafique Islam, Jianyong Li, Jeffrey R. Bloomquist, Paul R. Carlier\*, Drug Discovery Day 2014 Student Poster Session, Virginia Tech Center for Drug Discovery, Blacksburg, VA, September 26, 2014, Poster A4.
- 139. "Preliminary studies to determine the molecular target of the antimalarial drug mefloquine" Maryam Ghavami, Seema Dalal, Kristina Holzschneider, Tina Keller, Priscilla Krai, Michael Klemba, Paul R. Carlier\*, Drug Discovery Day 2014 Student Poster Session, Virginia Tech Center for Drug Discovery, Blacksburg, VA, September 26, 2014, Poster A10.
- 140. "An NMR Investigation of atropisomerism in ortho-substituted 1,1-dibromo-2,2-diphenylcyclopropane" <u>Narasimhamurthy Shanaiah</u>, Amanda Nelson, Neeraj Patwardhan, Carla Slebodnick, Paul R. Carlier, Webster L. Santos\* 56<sup>th</sup> Experimental Nuclear Magnetic Resonance Conference, Poster 502, April 19-24, 2015, Pacific Grove, CA.
- 141. "Acetylcholinesterase mutations and organophosphate resistance in sand flies and mosquitoes" <a href="Mexim"><u>Kevin B. Temeyer</u>\*</a>, Fan Tong, Qiao-hong Chen, Jeffrey Bloomquist, Paul R. Carlier, Maxim Totrov, Andrew Y. Li, and Adalberto A. Pérez de León, Book of Abstracts, American Association of Veterinary Pathologists, 60<sup>th</sup> Annual Meeting, July 11-14, 2015, Boston MA. Abstract 0000
- 142. "Amino acid efflux as a surrogate measure of the inhibition of plasmodial hemoglobin endocytosis by mefloquine and related antimalarials" Maryam Ghavami, Christie Dapper, Seema Dalal, Priscilla Krai, Michael Klemba, and Paul R. Carlier\*, Book of Abstracts, 250th National Meeting of the American Chemical Society, Boston, MA, August 16-20, 2015; American Chemical Society, Washington, D. C., MEDI-407
- 143. "Potassium Channels as Under-Exploited Targets for Insecticide Design." J. R. Bloomquist\*, M. M. Totrov, and P. R. Carlier. Book of Abstracts, 250th National Meeting of the American Chemical Society, Boston, MA, August 16-20, 2015; American Chemical Society, Washington, D. C., AGRO-007
- 144. "Activity of voltage-gated potassium channel blockers and their potential as new type of insecticide to control disease vector mosquitoes." F. Tong, B. Sun, A. Gross, P. Lam, M. Totrov, P. Carlier, and J. R. Bloomquist\* Book of Abstracts, 250th National Meeting of the American Chemical Society, Boston, MA, August 16-20, 2015; American Chemical Society, Washington, D. C., AGRO-246.
- 145. "Di- (not Tri!)fluoromethylketones as potent inhibitors of resistant mutant G119S *Anopheles gambiae* AChE" Invited Lecture, 12<sup>th</sup> International Conference on Cholinesterases and 6<sup>th</sup> International Conference on Paroxonases (12ChEPON6), Elche, Alicante, Spain, September 27-October 2, 2015.
- 146. "Hit to Lead Optimization of the Apicoplast-targeting Antimalarial Agent MMV008138" Zhong-Ke Yao, Priscilla M. Krai, Emilio F. Merino, Morgan E. Simpson, Carla Slebodnick, Maria B. Cassera, Paul R. Carlier\* Book of Abstracts, American Society of Tropical Medicine and Hygiene, Philadelphia, PA, October 25-29, 2015. Abstract 245.
- 147. "Monitoring Leucine Efflux As a Measure of Inhibition of Plasmodial Hemoglobin Endocytosis by Mefloquine and Its Derivatives: A Step Towards Developing Their Mode of Action" Maryam Ghavami, Michael Klemba, Paul R. Carlier\*, Virginia Tech Center for Drug Discovery, Drug Discovery Day 2015, Student Poster Session, Abstract C6, November 6, 2015, Blacksburg VA.
- 148. "Structure-Activity Relationship and Lead Profiling Studies of IspD-targeting Antimalarial Drug Candidates" Zhong-Ke Yao, Priscilla M. Krai, Emilio F. Merino, Rubayet Elahi, Morgan E. Simpson, Maryam Ghavami, Maria B. Cassera, and Paul R. Carlier\*, Virginia Tech Center for Drug Discovery, Drug Discovery Day 2015, Student Poster Session, Abstract A17, November 6, 2015, Blacksburg VA.

- 149. "Synthesis and Conformational Analysis of Mono- and Diacylhydrazine Mosquitocides for the Malaria Vector *Anopheles gambiae*" <u>Joseph C. Clements</u>, Zhong-ke Yao, Fan Tong, Rafique Islam, Jeffrey R. Bloomquist, and Paul R. Carlier\* Virginia Tech Center for Drug Discovery, Drug Discovery Day 2015, Student Poster Session, Abstract A2, November 6, 2015, Blacksburg VA.
- 150. "Triple Reuptake Inhibitor Antidepressant Candidates: Variation on the PRC200 Scaffold" Christopher J. Monceaux, Abdul Fauq, Elliott Richelson, Paul R. Carlier\*, Book of Abstracts, VirginiaBrainRx, May 23-24, 2016, Richmond, VA, Abstract M22.
- 151. "Parallel inhibition of amino acid efflux and parasite growth of erythrocytic *Plasmodium falciparum* by mefloquine and open-ring analogs: implications for the mechanism of antimalarial action" <u>Maryam Ghavami</u>, Christine Dapper, Kristina Holzschneider, Michael Klemba, and Paul R. Carlier\*, Book of Abstracts, 252th National Meeting of the American Chemical Society, Philadelphia, PA, August 21-25, 2016; American Chemical Society, Washington, D. C., MEDI-358
- 152. "Structure-activity studies of IspD-targeting antimalarials related to MMV008138" Zhong-Ke Yao, Maryam Ghavami, Rubayet Elahi, Morgan E. Simpson, Emilio F. Merino, Maxim M. Totrov, Maria B. Cassera, Paul R. Carlier\*, Book of Abstracts, 252th National Meeting of the American Chemical Society, Philadelphia, PA, August 21-25, 2016; American Chemical Society, Washington, D. C., MEDI-006
- 153. "Are muscarinic receptors the target of a new pyrazole oxime insecticide?" <u>Aaron D. Gross</u>, Paul R. Carlier, Shiyao Jiang, Baonan Sun, Fan Tong, Max Totrov, Jeffrey R. Bloomquist\*, Book of Abstracts, 252th National Meeting of the American Chemical Society, Philadelphia, PA, August 21-25, 2016; American Chemical Society, Washington, D. C., AGRO-205.
- 154. "Acetylcholinesterases of Arthropod Ectoparasites: Roles in Organophosphate Resistance and Host-Parasite Interaction" <u>Kevin B. Temeyer</u>\*, Fan Tong, Jeffrey Bloomquist, Paul Carlier, Maxim Totrov, Andrew Y. Li, Adalberto A. Pérez de León and Alexander P. Tuckow, Book of Abstracts, 2016 XXV International Congress of Entomology, September 25-30, 2016, Orlando FL.
- 155. "C- and D-ring SAR exploration of the IspD-targetting antimalarial agent MMV008138," <u>Maryam Ghavami</u>, Zhong-Ke Yao, Lixuan Liu, Emilio F. Merino, Joshua H. Butler, Michael A. Casasanta, Daniel J. Slade, Max Totrov, Maria B. Cassera, Paul R. Carlier\*, Abstract P28, VirginiaCancerRx, May 30-31, 2017, Charlottesville, VA.
- 156. **Invited:** "Lessons learned in the search for mosquitocidal AChE inhibitors having both target selectivity and resistance-breaking properties" Paul R. Carlier\*, Jeffrey R. Bloomquist, Jianyong Li, Max Totrov, Book of Abstracts, 2017, 254<sup>th</sup> National Meeting of the American Chemical Society, Washington, DC, August 20-24, 2017; American Chemical Society, Washington, D. C., AGRO-111.
- "Exploration of A, C, and D-ring SAR or the IspD-targeting Antimalarial Agent MMV008138" Maryam Ghavami, Zhong-ke Yao, Lixuan Liu, Emilio F. Ferino, Joshua H. Butler, Michael A. Cassanta, Daniel J. Slade, Max Totrov, Maria B. Cassera, Paul R. Carlier\*, Book of Abstracts, 2017, 254<sup>th</sup> National Meeting of the American Chemical Society, Washington, DC, August 20-24, 2017; American Chemical Society, Washington, D. C., MEDI-275.
- 158. "Muscarinic acetylcholine receptors as a target for insecticide development." <u>Aaron Gross</u>, Paul R. Carlier, Jeffrey R. Bloomquist\*, Book of Abstracts, 2017, 254<sup>th</sup> National Meeting of the American Chemical Society, Washington, DC, August 20-24, 2017; American Chemical Society, Washington, D. C., AGRO-138.

- 159. "Ni-catalyzed synthesis of enantiomerically-enriched tryptophans and their use to make analogs of the antimalarial compound MMV008138" <u>Lixuan Liu</u>, Paul R. Carlier\*, 5<sup>th</sup> Annual Drug Discovery Day, Virginia Tech Center for Drug Discovery, Abstract A7, November 2, 2017, Blacksburg, VA.
- 160. "Synthesis of analogs of a hit from the Malaria Box," <u>Sha Ding</u>, Michael Klemba, Paul R. Carlier\*, 5<sup>th</sup> Annual Drug Discovery Day, Virginia Tech Center for Drug Discovery, Abstract A3, November 2, 2017, Blacksburg, VA.
- 161. "Toxicity and mode of action of flonicamid and its metabolite against mosquitoes." A. D. Gross, J. Taylor-Wells, S. Jiang, F. Demares, J. Clements, P. R. Carlier, and J. R. Bloomquist, Eastern branch meeting of the Entomological Society of America, March 17-18, 2018, Annapolis, Maryland.
- 162. "C1-Methyl, spiro- and ring-expanded analogs of the antimalarial lead compound MMV008138," Sha Ding, Maryam Ghavami, Joshua H. Butler, Emilio F. Merino, Carla Slebodnick, Maria B. Cassera, and Paul R. Carlier\* Abstract P29, VirginiaDrugDiscoveryRx, Arlington, VA, June 25-26, 2018.
- 163. "A new method for stereochemical assignment of 1,3-disubstituted tetrahydro-β-carbolines," <u>Kristýna Cagasŏvá</u>, Maryam Ghavami, Zhongke Yao and Paul R. Carlier\*, Abstract P29, VirginiaDrugDiscoveryRx, Arlington, VA, June 25-26, 2018.
- 164. **Invited:** "The search for resistance-breaking and species-selective mosquitocidal inhibitors of *Anopheles gambiae* AChE," <u>Paul R. Carlier</u>\*, Jeffrey R. Bloomquist, Jonah Cheung, Jianyong Li, Max Totrov, Abstract S03-5, 13<sup>th</sup> International Meeting on Cholinesterases, and 7<sup>th</sup> International Meeting on Paraoxonases, University of Hradec Králové, Czech Republic, September 9-14, 2018.
- 165. **Invited:** "New method for stereochemical assignment of Pictet-Spengler reaction products," Kristýna Cagasŏvá, Maryam Ghavami, Zhongke Yao and <u>Paul R. Carlier</u>\* Abstract 577, Southeastern Regional Meeting of the American Chemical Society, Augusta, GA, October 31-November 3, 2018.
- 166. "A new method for stereochemical assignment of 1,3-Disubstituted tetrahydro-β-carbolines," <u>Kristýna Cagasŏvá</u>, Maryam Ghavami, Zhongke Yao and Paul R. Carlier\*, 6<sup>th</sup> Annual Drug Discovery Day, Virginia Tech Center for Drug Discovery, Abstract A12, November 8, 2018, Blacksburg, VA.
- "C1-Methyl, spiro-, and ring-expanded analogs of the antimalarial lead compound MMV008138," <a href="Shape: Ding">Shape: Ding</a>, Maryam Ghavami, Joshua H. Butler, Emilio F. Merino, Carla Slebodnick, Maria B. Cassera, and Paul R. Carlier\*, 6th Annual Drug Discovery Day, Virginia Tech Center for Drug Discovery, Abstract A10, November 8, 2018, Blacksburg, VA.
- 168. "Heterocyclic D-Ring analogs of the antimalarial lead compound MMV008138", <u>Haibo Li</u>, Maryam Ghavami, Emilio F. Merino, Zhongke Yao, Daniel J. Slade, Joshua H. Butler, Maria B. Cassera, and Paul R. Carlier\* 6<sup>th</sup> Annual Drug Discovery Day, Virginia Tech Center for Drug Discovery, Abstract A11, November 8, 2018, Blacksburg, VA.
- 169. "Revisiting the gamma-gauche effect: a ¹H NMR method for stereochemical assignment of 1,3-disubstituted-1,2,3,4-tetrahydro-β-carbolines," <u>Kristýna Cagasŏvá</u>, Maryam Ghavami, Zhongke Yao and Paul R. Carlier\* 257th National Meeting of the American Chemical Society, Orlando, FL March 31 April 4, 2019; American Chemical Society, Washington, D. C., ORGN-294.
- 170. Ketone Pictet-Spengler routes to spiro-, C1-methyl, and azepane analogs of an antimalarial tetrahydro-β-carboline, Sha Ding, Maryam Ghavami, Joshua H. Butler, Emilio F. Merino, Carla Slebodnick, Maria Cassera, Paul R. Carlier\*, 257th National Meeting of the American Chemical Society, Orlando, FL March 31 April 4, 2019; American Chemical Society, Washington, D. C., ORGN-289.

- 171. "Synthesis of Azepanes from Pictet-Spengler Reaction of Arylmethyl Ketones: Scope and Mechanism" Sha Ding, Maryam Ghavami, and Paul R. Carlier\* DrugDiscoveryRx: Emerging Targets, Technologies, and Therapeutics for Cancer and Neuroscience, Virginia Drug Discovery Consortium, May 21-22, 2019, Hotel Roanoke, Roanoke Virginia, Poster P-41.
- 172. "Synthesis and Evaluation of 1-Thienyl Pictet-Spengler Adducts as Antimalarials" Haibo Li, Maryam Ghavami, Emilio F. Merino, Zhongke Yao, Rubayet Eli, Maria B. Cassera, and Paul R. Carlier\*, VirginiaDrugDiscoveryRx: Emerging Targets, Technologies, and Therapeutics for Cancer and Neuroscience, Virginia Drug Discovery Consortium, May 21-22, 2019, Hotel Roanoke, Roanoke Virginia, Poster P-44.
- 173. "Synthesis of azepinoindoles via ring expansion of 1-methyl-tetrahydro-β-carbolines" <u>Sha Ding</u>, Maryam Ghavami, Paul R. Carlier\*, Abstract 1136, Southeastern Regional Meeting of the American Chemical Society, Savannah, GA, October 20-23, 2019.
- 174. "Development of a Synthetic Route to the Malaria Box Compound MMV668531 and Analogs," <u>Sha Ding</u>, Michael Klemba, Paul R. Carlier\*, 7<sup>th</sup> Annual Drug Discovery Day, Virginia Tech Center for Drug Discovery, Abstract P1, November 7, 2019, Blacksburg, VA.
- 175. "Potent Beta-carboline Amide Antimalarials Do Not Target the MEP Pathway. <u>Jopaul Matthew</u>, Sha Ding, Kevin Künz, Joshua H. Butler, Emilio F. Merino, Maxim M. Totrov, Maria B. Cassera and Paul R. Carlier\*, 7<sup>th</sup> Annual Drug Discovery Day, Virginia Tech Center for Drug Discovery, Abstract P4, November 7, 2019, Blacksburg, VA.
- 176. "Synthesis of a phosphonic acid isostere of the antimalarial compound MMV008138," <u>Kristýna Cagašová</u>, Joshua H. Butler, Maria B. Cassera and Paul R. Carlier\*, 7<sup>th</sup> Annual Drug Discovery Day, Virginia Tech Center for Drug Discovery, Abstract P18, November 7, 2019, Blacksburg, VA.
- 177. "The Solid State and Solution Structures of the Antimalarial Compound MMV008138," <u>Haibo Li, Kristýna Cagašová</u>, Carla Slebodnick, Paul R. Carlier\*,7<sup>th</sup> Annual Drug Discovery Day, Virginia Tech Center for Drug Discovery, Abstract P3, November 7, 2019, Blacksburg, VA.
- 178. **Invited:** Fluorinated methyl ketone oximes: evaluation of cholinergic and non-cholinergic mechanisms of mosquitocidal action, Eugene Camerino, Dawn M. Wong, Jeffrey R. Bloomquist, Aaron D. Gross, and <u>Paul R. Carlier</u>,\* Abstract XX, 16<sup>th</sup> International Symposium on Cholinergic Mechanisms & 2<sup>nd</sup> Misrahi Symposium on Neurobiology, December 8-13, 2019, Weizmann Institute of Science, Rehovot, Israel
- 179. Synthesis of Enantiopure Antimalarial N2-Acyl Tetrahydro-β-Carbolines, <u>Hanan Almolhim</u>, Joshua H. Butler, Sha Ding, Carla Slebodnick, Maxim M. Totrov, Maria B. Cassera and Paul R. Carlier\*, VirginiaDrugDiscoveryRx Annual Symposium, May 26-27, 2021 (Zoom), Virtual Reality Poster Session, Poster B08, Book of Abstracts, Abstract B08.
- 180. The Unexpected Discovery of Orally Efficacious Betacarboline Antimalarials. <u>Jopaul Mathew</u>, Sha Ding, Kevin Kunz, Joshua H. Butler, Emilio F. Merino, Maxim M. Totrov, Maria B. Cassera and Paul R. Carlier\*, VirginiaDrugDiscoveryRx Annual Symposium, May 26-27, 2021 (Zoom), Virtual Reality Poster Session, Poster B09, Book of Abstracts, Abstract B09.

#### **OTHER ACADEMIC PUBLICATIONS:**

1. "A Specialty Database on Medicinal Plant Information," C. T. Che\*, P. R. Carlier, O. C. W. Lee, Letter to the Editor, *Asia Pacific Journal of Pharmacology*, **1993**, *8*, 171-172.

#### **PATENTS AND DISCLOSURES:**

1. "Sulfonated Xanthene Dyes, and Photographic Products and Processes Employing These Dyes" P. R. Carlier, M. P. Filosa, M. P. Lockshin *U. S. Patent 5,187,282*, February 16, 1993

- 2. "Sulfonated Xanthene Dyes, and Photographic Products and Processes Employing These Dyes" P. R. Carlier, M. P. Filosa, M. P. Lockshin *U. S. Patent 5,264,322*, November 23, 1993.
- 3. "3-Hydroxy-propanamine derived neuronal reuptake inhibitors," Paul R. Carlier, Michael M.-C. Lo, Priscilla C.-K. Lo, Elliott Richelson, U. S. Patent 6,069,177, filed July 8, 1997, issued May 30, 2000.
- 4. "Dimeric Compounds" (Dimeric 5-amino-5,6,7,8-tetrahydroquinolinones and their pharmaceutical use), Paul R. Carlier, Yi-Fan Han, Yuan-Ping Pang, Da-Ming Du, US Patent 6,472,408, issued October 29, 2002.
- 5. "Amine Compounds and Inhibiting Neurotransmitter Uptake," U. S. Patent 6,700,018. Elliott Richelson (Mayo Clinic), Paul R. Carlier, issued March 2, 2004.
- 6. "Amine compounds and inhibiting neurotransmitter reuptake," U.S. Patent 6,914,080. Elliott Richelson (Mayo Clinic), Paul R. Carlier, issued July 5, 2005. This patent is a division of 6,700,018.
- 7. "Amine compounds and inhibiting neurotransmitter reuptake," U.S. Patent 7,214,826. Elliott Richelson (Mayo Clinic), Paul R. Carlier, issued May 8, 2007. This patent is a division of 6,914,080
- 8. "Species-Selective Insecticidal Carbamates for Mosquito Control" U.S. Patent 8,129,428, Paul R. Carlier, Jeffrey R. Bloomquist, Sally L. Paulson, Eric A. Wong, issued March 6, 2012.
- 9. "Insecticidal Carbamates Exhibiting Species-Selective Inhibition of Acetylcholinesterase (AChE)" Paul R. Carlier, Jeffrey R. Bloomquist, Sally L. Paulson, Eric A. Wong, U. S. Patent 8,618,162, issued 12/31/2013.
- 10. "Inhibiting Neurotransmitter Reuptake" Elliott Richelson, Abdul Fauq, Paul R. Carlier, Christopher J. Monceau, U.S. Patent 9,944,618, Issued April 17, 2018.
- 11. "Resistance-breaking insecticides for the malaria mosquito" Paul R. Carlier, Astha Verma, Dawn M. Wong, Jeffrey R. Bloomquist VTIP 14-153, U.S. Patent Application No: 62/033,296 (Provisional), filed 8/5/14.
- 12. "Structurally novel insecticides for the malaria mosquito" Paul R. Carlier, Eugene Camerino, Dawn M. Wong, Jeffrey R. Bloomquist, VTIP 15-003, U.S. Patent Application No: 62/033,341 (Provisional), filed 8/5/14.
- 13. "Novel methylerythritol phosphate pathway inhibitors" Paul R. Carlier, Maria Belen Cassera, Emilio Fernando Merino, Zhong-Ke Yao, Maryam Ghavami, VTIP 15-044, PCT/US2015/058157, filed 10/29/15.
- 14. "Optimized MEP Pathway Inhibitors for Malaria Control" Maria Belen Cassera; Lixuan Liu; Maryam Ghavami; Paul Carlier, VTIP 18-136, filed 6/12/18.
- 15. "Antimalarial Compounds and Uses Thereof", Paul Carlier; Max Totrov; Maria Cassera; Kevin Kunz; Mathew Jopaul; Sha Ding, Disclosure, VTIP, 20-048, filed 12/5/2019. U.S. Provisional Application No. 63/000,691, filed 3/27/2020, combined with U.S. Provisional Application 63/018,430 and converted to utility application PCT/US2021/024542 on March 27, 2021.

16. "Antimalarial compounds and uses thereof," Paul Carlier; Maria Cassera; Max Totrov, Disclosure, VTIP 20-063, 2/19/2020. U.S. Provisional Application 63/018,430, "Antimalarial compounds and uses thereof," filed 4/30/2020, combined with U.S. Provisional Application 63/000,691 and converted to utility application PCT/US2021/024542 on March 27, 2021.

#### THESES SUPERVISED:

Note: The MPhil (Master of Philosophy) is a research master's degree that is offered in some former Commonwealth countries.

- 1. "Novel Reactions of Metallocene and Phosphorus Isocyanates and Isothiocyanates" W. K. Leung, Hong Kong University of Science and Technology, January 31, 1994 (MPhil Thesis).
- 2. "2,3-Anti-Selective Aldol of Benzylic Nitriles" Kam Moon Lo, Hong Kong University of Science and Technology, August 1995 (Ph. D. Thesis).
- 3. "Synthesis of  $\gamma$ -Amino Alcohol Derivatives and Study of the Mechanism of Cp-Ti Protonolysis" Michael M-C. Lo, Hong Kong University of Science and Technology, July 1996 (MPhil Thesis).
- 4. "Progress Towards Asymmetric Aldol Reaction of Arylacetonitriles" Weldon W-F. Lam, Hong Kong University of Science and Technology, August 1996 (MPhil Thesis).
- 5. "Synthesis of Novel Dimeric Acetylcholinesterase Inhibitors" Crystal P.-L. Li, Hong Kong University of Science and Technology, August 1998 (MPhil Thesis).
- 6. "Synthesis and Evaluation of Dimeric and Heterodimeric Tacrine-based Acetylcholinesterase Inhibitors" Ella S.-H. Chow, June 1999 (MPhil Thesis).
- 7. "Effects of HMPA on the Structure and Aldol Stereoselectivity of Lithiated Arylacetonitriles" Cedric W. S. Lo, Hong Kong University of Science and Technology, November 2000 (MPhil Thesis).
- 8. "Experimental and Computational Studies in Bioorganic and Synthetic Organic Chemistry" Polo C.-H. Lam, Virginia Tech, October 2004 (Ph. D. Thesis).
- 9. "Design and Syntheses of Potential Drugs Based on GABA(A) Receptor Pharmacophores" Ella Clement, Virginia Tech, June 2005 (Ph. D. Thesis).
- 10. "Design and Synthesis of Novel 1,4-Benzodiazepines" Stephanie MacQuarrie-Hunter, Virginia Tech, November 2005 (Ph. D. Thesis).
- 11. "Memory of Chirality in 1,4-Benzodiazepin-2-ones" Joseph C. DeGuzman, Virginia Tech, May 2006 (Ph. D. Thesis).
- 12. "Stereochemistry of small molecules: configurational and conformational control" Yiqun Zhang, Virginia Tech, March 2007 (Ph. D. Thesis).
- 13. "Mechanistic Studies on Memory of Chirality Alkylations of 1,4-Benzodiazepin-2-ones & Structure-based Design of Insecticidal AChE Inhibitors for the Malaria Mosquito, *Anopheles gambiae*" Danny C. Hsu, Virginia Tech, September 2007 (Ph.D. Thesis).
- 14. "Computational and Spectroscopic Structural Determination of Lithiated Benzylic Nitriles in THF/HMPA Solution" H. Jason Harmon, Virginia Tech, September 2008 (Ph.D. Thesis).

- 15. "Experimental and Computational Investigation of Tacrine-based Inhibitors of Acetylcholinesterase" Larry D. Williams, Virginia Tech, October 2008 (Ph.D. Thesis).
- 16. "Mild and Convenient Methods to Prepare N-Alkyltacrines" Jimit Mehta, December 2009 (M.S. Thesis)
- 17. "Computational Studies of Protonated Cyclic Ethers and Organolithium Compounds" Nipa Deora, Virginia Tech, May 2010 (Ph.D. Thesis)
- 18. "Triazole-linked reduced amide isosteres: An approach for the fragment-based drug discovery of anti-Alzheimer's BACE1 inhibitors and NH-assisted Fürst-Plattner opening of cyclohexene oxides" Christopher J. Monceaux, Virginia Tech, December 2010 (Ph.D. Thesis)
- 19. "Revisiting aryl *N*-methylcarbamate acetylcholinesterase inhibitors as potential insecticides to combat the malaria-transmitting mosquito, *Anopheles gambiae*," Joshua A. Hartsel, Virginia Tech, March 2011 (Ph.D. Thesis)
- 20. "Study of synthesis, reactions and enantiomerization of  $C_{\alpha}$ -chiral Grignard reagents," Neeraj N. Patwardhan, Virginia Tech, May 2012 (Ph.D. Thesis).
- 21. "Trifluoromethylketones, potential insecticides towards *Anopheles gambiae*," Eugene Camerino, Virginia Tech, December 2012 (M.S. Thesis).
- 22. "Small Core Heterocyclic Carbamates and Carboxamides: Resistance-breaking Acetylcholinesterase Inhibitors Targeting the Malaria Mosquito, *Anopheles gambiae*" Astha Verma, Virginia Tech, April 2014 (Ph.D. Thesis)
- 23. "Fluoromethylketone prodrugs: Potential new insecticides towards Anopheles gambiae" Eugene Camerino, Virginia Tech, May 2015 (Ph.D. Thesis)
- 24. "Enantioselective Synthesis of Drug-like Molecules via Axially-Chiral Intermediates" Gary M. Richoux, Virginia Tech, June 2016 (Ph.D. Thesis).
- 25. "Synthesis of Insecticidal Mono- and Diacylhydrazines for Disruption of K+ Voltage-Gated Channels, Elucidation of Regiochemistry, and Description of Conformational Isomerism by NMR Spectroscopy and Computation" Joseph S. Clements, II, Virginia Tech, May 2017 (Ph.D. Thesis).
- 26. "MMV008138 and analogs: potential novel antimalarial agents for *P. falciparum*" Lixuan (Alexx) Liu, Virginia Tech, March 2018 (M.S. Thesis).
- 27. "Antimalarial agents: new mechanisms of action for old and new drugs" Maryam Ghavami, June 2018 (Ph.D. Thesis).
- 28. "Novel Antimalarial Compounds from the Optimization of the Malaria Box" Sha Ding, August 2020 (Ph.D. Thesis)
- 29. "1,3-disubstituted-tetrahydro-β-carbolines: A New Method for Stereochemical Assignment and Synthesis of Potential Antimalarial Agents" Kristýna Cagašová, May 2021 (Ph.D. Thesis).

#### INVITED SEMINARS (INVITED CONFERENCE LECTURES LISTED ABOVE IN ABSTRACTS)

- 1. "Anti-selective Aldol and <sup>6</sup>Li/<sup>15</sup>N NMR of Lithiated Nitriles", 8 December 1994, Hong Kong University of Science and Technology, Chemistry Department Seminar.
- 2. "Anti-selective Aldol and  $^6\text{Li}/^{15}\text{N}$  NMR of Lithiated Nitriles", 26 April 1995, Hong Kong Baptist University, Chemistry Department Seminar.

- 3. "Development and Application of the Nitrile Aldol Reaction" Fourth International Symposium for Chinese Organic Chemists (ISCOC 96), The Chinese University of Hong Kong, Shatin, New Territories, Hong Kong, April 5-8, 1996.
- 4. "Lithiated Nitriles: Structure and Synthesis of Gamma-Amino Alcohol Antidepressant Candidates", Research Department, Mayo Clinic, Jacksonville, Florida, U. S. A., April 30, 1996.
- 5. "Lithiated Nitriles: Structure and Use in Synthesis of CNS Drug Candidates," HKUST-Bayer Corporation Information Interchange Day, Hong Kong University of Science and Technology, May 31, 1996.
- 6. "The Search for Safe and Effective Alzheimer's Therapeutics: From Huperzine A to Novel Dimeric AChE Inhibitors," Special Session on Traditional Chinese Medicine, Workshop on Molecular Biology & Biotechnology, Association of East Asian Research Universities, Hong Kong University of Science and Technology, April 29, 1997.
- 7. "Development of a Chiral Alkoxide-Mediated Asymmetric Nitrile Aldol Reaction" Shanghai Institute of Organic Chemistry, June 25, 1997.
- 8. "From Nitrile Aldol Reaction to the Discovery of Wide-Spectrum Antidepressant Drug Candidates" Department of Chemistry, University of Hong Kong, February 19, 1998.
- 9. "Dimeric Inhibitors: Structural Probes of Acetylcholinesterase and Potential Therapeutic Agents for Alzheimer's Disease" Department of Chemistry, State University of New York at Binghamton, December 6, 1999.
- 10. "Dimeric Inhibitors: Structural Probes of Acetylcholinesterase and Potential Therapeutic Agents for Alzheimer's Disease" Department of Chemistry, University of Houston, December 8, 1999.
- 11. "Dimeric Inhibitors: Structural Probes of Acetylcholinesterase and Potential Therapeutic Agents for Alzheimer's Disease" Department of Chemistry, San Diego State University, December 10, 1999.
- 12. "Dimeric Inhibitors: Structural Probes of Acetylcholinesterase and Potential Therapeutic Agents for Alzheimer's Disease" Department of Chemistry, Virginia Tech, January 17, 2000.
- 13. "A New Tactic in Bivalent Drug Design: Dimerization of Natural Product Fragments" Research Department, Mayo Clinic Jacksonville, January 20, 2000.
- 14. "Bivalent Ligands for Acetylcholinesterase and the GABA(A) Receptor: Structure-based Design and Serendipity," Departments of Structural Biology and Neurobiology, Weizmann Institute of Science, Rehovot Israel, July 13, 2000.
- 15. "Huperzine A Fragment Dimers: Chinese Natural Product-based Memory Enhancers for Alzheimer's Disease," Department of Chemistry, Chinese University of Hong Kong, Shatin, Hong Kong, November 15, 2000
- 16. "Huperzine A Fragment Dimers: Chinese Natural Product-based Memory Enhancers for Alzheimer's Disease," Department of Chemistry, Duquesne University, Pittsburgh, PA, February 9, 2001.
- 17. "Potent & Selective Acetylcholinesterase Inhibition Through the Use of Dimeric Ligands, FMC Corporation, Princeton, N. J., March 15, 2001.

- 18. "Natural Product Fragment Dimers: A Strategy to Attain High Selectivity for Ligand-Receptor Binding" Invited lecture in the "Selectivity in Organic Chemistry and Catalysis" Symposium at the 221st National Meeting of the American Chemical Society, San Diego, CA, April 1 5, 2001.
- 19. "Buy One, Get One Free! The Chelate Effect in Drug Design," Keynote Speaker, Organic Division Summer Postdoctoral Lecture Series, August 22, 2001, Department of Chemistry, Virginia Tech.
- 20. "Huperzine Fragment Dimers: A Strategy to Obtain Potent and Selective Memory Enhancers for Alzheimer's Disease," Department of Chemistry, Wake Forest University, January 30, 2002.
- 21. "Buy One, Get One Free! The Chelate Effect in Drug Design," Department of Chemistry, Washington & Lee University, February 7, 2002.
- 22. "Planar Chiral Enolates for the Asymmetric Synthesis of 2,2-Dialkylamino Acids" Department of Chemistry, Hong Kong University of Science and Technology, December 23, 2002.
- 22. "Planar Chiral Enolates for the Asymmetric Synthesis of 2,2-Dialkylamino Acids" Department of Chemistry, North Carolina State University, January 13, 2003.
- 23. "Dimeric Drugs and Quaternary Benzodiazepines" Laboratory of Bioorganic Chemistry, NIDDK, National Institutes of Health, Bethesda, MD, October 10, 2003.
- 24. "Dimerization of Natural Product Fragments: A Strategy for Generating Drug Leads" Eleventh Asian Symposium on Medicinal Plants, Spices, and Other Natural Products (ASOMPS-XI), Kunming Institute of Botany, Kunming, China, October 26-30, 2003.
- 25. "Enantioselective Synthesis of Quaternary Benzodiazepine Scaffolds via Memory of Chirality," Department of Chemistry, Chinese University of Hong Kong, Shatin, New Territories, Hong Kong, October 31, 2003.
- 26. "Enantioselective Synthesis of Quaternary Benzodiazepine Scaffolds via Memory of Chirality," Department of Chemistry, Duquesne University, November 14, 2003.
- 27. "Dimeric Drugs and Quaternary Benzodiazepines: New Opportunities in Medicinal Chemistry." Department of Medicinal Chemistry, Research Triangle Institute, March 8, 2004.
- 28. "Memory of Chirality in the Synthesis of Quaternary Benzodiazepine Scaffolds," Department of Chemistry, University College Cork, June 28, 2004.
- 29. "Memory of Chirality in the Enantioselective Construction of Quaternary Centers" Department of Applied Biology and Chemical Technology, Hong Kong Polytechnic University, Hong Kong, October 5, 2004.
- 30. "Enantioselective Synthesis of Quaternary Benzodiazepine Scaffolds via Memory of Chirality," Department of Chemistry, University of Hong Kong, October 6, 2004.
- 31. "Enantioselective Synthesis of Quaternary Benzodiazepine Scaffolds via Memory of Chirality," Department of Chemistry, University of Maryland, October 21, 2004.
- 32. "Enantioselective Synthesis of Quaternary Benzodiazepines via Memory of Chirality" Department of Chemistry, Virginia Tech, November 5, 2004.
- 33. "Drug Discovery Research in the Carlier Group at Virginia Tech," Georgetown University/Virginia Tech Drug Discovery Meeting, Organized by the Dean of Science, Virginia Tech, November 15, 2004.

- 34. "Dimeric Huperzine A-Derived AChE Inhibitors, Dimeric GABAAR Agonists, and Novel Benzodiazepines" Department of Biochemistry & Molecular Biology, Georgetown University Medical School, January 4, 2005.
- 35. "Memory, Mosquitoes, and Malaria" Symposium of Alumni Achievement Medal Award Winners, Hamilton College, Clinton, NY, September 29 October 1, 2005.
- 36. "Dimeric Inhibitors of Mammalian and Mosquito Acetylcholinesterase" Department of Chemistry, Hong Kong University of Science and Technology, December 20, 2005.
- 37. "Asymmetric Synthesis of Quaternary Benzodiazepines" Department of Chemistry, Hong Kong University of Science and Technology, January 4, 2006.
- 38. "X-ray crystallography of acetylcholinesterase/inhibitor complexes: a critical tool for the development of effective memory enhancers for early-stage Alzheimer's disease" invited lecture for Virginia Tech Structural Biology Symposium, March 31, 2006.
- 39. "Transiently non-racemic enolates: synthesis of enantiopure 'quaternary' benzodiazepines" Gordon Conference on Organic Reactions & Processes, Bryant College, Smithfield, RI, July 16-21 2006.
- 40. "Transiently non-racemic enolates: synthesis of enantiopure 'quaternary' benzodiazepines" Bio21 Institute and the Department of Chemistry, University of Melbourne, July 26, 2006
- 41. "Transiently non-racemic enolates: synthesis of enantiopure 'quaternary' benzodiazepines" Department of Chemistry, University of North Carolina, Chapel Hill, September 14, 2006
- 42. "Memory of chirality for the asymmetric synthesis of benzodiazepines," Department of Chemistry, East Carolina University, Greenville, NC, September 15, 2006.
- 43. "Memory of chirality for the asymmetric synthesis of benzodiazepines" Symposium on Advances in Organic Synthesis, SERMACS Augusta, GA, November 1-4, 2006.
- 44. "Transiently non-racemic enolates: synthesis of enantiopure 'quaternary' benzodiazepines" Department of Chemistry, University of Alabama, Birmingham. AL March 1, 2007.
- 45. "Towards an Insect-selective Acetylcholinesterase Inhibitor" IXth International Meeting on Cholinesterases, Suzhou, China, May 6-10, 2007
- 46. "Memory of chirality for the asymmetric synthesis of benzodiazepines," Shanghai ChemExplorer, Shanghai, China, May 11, 2007.
- 47. "Transiently non-racemic enolates: synthesis of enantiopure 'quaternary' benzodiazepines" Institute of Chemistry, Peking University, Beijing, China, May 14, 2007.
- 48. "Transiently non-racemic enolates: synthesis of enantiopure 'quaternary' benzodiazepines" Shanghai Institute of Organic Chemistry, Shanghai, China, May 16, 2007.
- 49. "Freeze frame observation of stereochemical information transfer to and from a transiently non-racemic enolate" Eighth International Conference on Carbanion Chemistry, Madison Wisconsin, 6 -10 June 2007.
- 50. "Molecular design of AChE inhibitors to target Anopheles Gambiae, the mosquito vector of Malaria, " Faculty of Pharmacy, University of Barcelona, Barcelona, Spain, September 13, 2007.

- 51. "Molecular design of selective anticholinesterases for mosquito control" Grand Challenges in Global Health Principal Investigator Meeting, Cape Town, South Africa, October 7, 2007.
- 52. "Enantioselective synthesis of quaternary benzodiazepines via memory of chirality" Department of Chemistry, University of North Carolina, Charlotte, October 29, 2007.
- 53. "Transiently non-racemic enolates: synthesis of enantiopure 'quaternary' benzodiazepines" Department of Chemistry, University of California, Los Angeles, January 17, 2008.
- 54. "Enantioselective synthesis of quaternary benzodiazepines via memory of chirality" Department of Chemistry, University of South Florida, February 21, 2008.
- 55. "Molecular design of selective anticholinesterases for mosquito control" Grand Challenge 8 PI Meeting, Wageningen University, Wageningen, Netherlands, March 9-10, 2008.
- 56. "Discovery of Acetylcholinesterase Inhibitors with High Selectivity for Anopheles Gambiae, the Mosquito Vector of Malaria" Department of Pharmacology, University of California, San Diego, April 29, 2008.
- 57. "Development of Anopheles gambiae-selective Acetylcholinesterase Inhibitors for Deployment on Insecticide Treated Nets" Deans' Forum on Infectious Disease, Virginia Tech, Blacksburg, VA, September 29, 2008.
- 58. "Development of Species-Selective Acetylcholinesterase Inhibitors to Control the Mosquito Vector of Malaria" Department of Chemistry, Hong Kong University of Science and Technology, Hong Kong SAR, China, October 16, 2008.
- 59. "Development of Species-Selective Acetylcholinesterase Inhibitors to Control the Mosquito Vector of Malaria" Department of Chemistry, East Tennesee State University, Johnson City, TN, November 7, 2008.
- 60. "Development of Species-Selective Acetylcholinesterase Inhibitors to Control the Mosquito Vector of Malaria" Department of Chemistry, Michigan State University, East Lansing, MI, January 28, 2009
- 61. "Stopping the Clock; Capturing a Dynamically Chiral Potassium Enolate," Department of Chemistry, Georgetown University, Washington D.C., February 19, 2009.
- 62. "Synthesis of Enantiomerically Pure Quaternary Benzodiazepines and Mosquito-specific Acetylcholinesterase Inhibitors, Chemistry Department, AstraZeneca, Wilmington, DE, May 5, 2009.
- 63. "Development of Species-Selective Acetylcholinesterase Inhibitors to Control the Mosquito Vector of Malaria" Emerging Pathogens Institute, University of Florida, Gainesville, July 15, 2009.
- 64. "Asymmetric synthesis via dynamically chiral enolates and metalated nitriles" Department of Chemistry, University of Florida, Gainesville, July 16, 2009.
- 65. "Redesign of tacrine to achieve potent and selective inhibition of *Anopheles gambiae* acetylcholinesterase" 10<sup>th</sup> International Meeting on Cholinesterases, 20-25 September 2009, Šibenik, Croatia.
- 66. "Vector-specific acetylcholinesterase inhibitors for deployment on insecticide treated nets" Grand Challenges in Global Health Principal Investigator Meeting, Arusha, Tanzania, October 19-21, 2009.

- 67. "Development of new chemical agents to control the malaria mosquito" Department of Chemistry, Appalachian State University, October 30, 2009.
- 68. "Chemistry & Biology: Partners in Reducing Malaria Transmission in SubSaharan Africa" Café Scientifique, Blacksburg, VA, April 20, 2010.
- 69. "Development of species-selective insecticides to reduce malaria transmission" Department of Chemistry and Biochemistry, Hampden-Sydney College, September 17, 2010.
- 70. "Chemistry and Biology: Inseparable Partners for Meeting Challenges in Medicine and Public Health", Plenary Lecture, ACC Forum, October 5, 2010
- 71. "Resistance-breaking and species-selective acetylcholinesterase inhibitors as potential human-safe insecticides against the malaria mosquito" Grand Challenges in Global Health, Principal Investigator Meeting, Seattle, WA, October 25-27, 2010.
- 72. "New approaches towards human-safe insecticides to reduce malaria transmission" Department of Chemistry, Roanoke College, November 19, 2010.
- 73. "New approaches towards human-safe insecticides to reduce malaria transmission" Department of Chemistry, St. John's University, Queens, NY, February 16, 2011.
- 74. "Dynamic stereochemistry of conformationally chiral enolates and enantioenriched grignard reagents" Department of Chemistry, Texas Tech University, April 13, 2011.
- 75. "Designing human-safe insecticides against the malaria mosquito" Department of Chemistry, Winthrop University, November 17, 2011.
- 76. "Chemistry for Global Health: designing new interventions against *Anopheles gambiae*, the malaria mosquito" Department of Chemistry, West Virginia University, September 12, 2012.
- 77. "Resistance-breaking and species-selective acetylcholinesterase inhibitors as potential human-safe insecticides against the malaria mosquito" Department of Entomology, Virginia Tech, October 25, 2012.
- 78. Development of species-selective and resistance-breaking insecticides against *Anopheles gambiae*, Department of Entomology, University of California, Riverside, CA, November 2, 2012.
- 79. "Chemistry for Global Health: designing new interventions against *Anopheles gambiae*, the malaria mosquito" Department of Chemistry, University of Virginia, Charlottesville, VA, September 27, 2013.
- 80. "Design of selective and resistance-breaking acetylcholinesterase inhibitors for *Anopheles gambiae*, the malaria mosquito" Department of Medicinal Chemistry and Pharmacognosy, University of Illinois at Chicago, Chicago, IL, September 5, 2014.
- 81. "Chemistry in Service of Global Health: New Small Molecule Interventions for Malaria," Department of Chemistry, Université Laval, Quebec City, Québec, Canada, April 8, 2015.
- 82. "Chemistry in Service of Global Health: New Small Molecule Interventions for Malaria," Department of Chemistry, Brock University, St. Catherine's, Ontario, Canada, September 11, 2015.
- 83. "Chemistry in Service of Global Health: New Small Molecule Interventions for Malaria," Department of Medicinal Chemistry, Virginia Commonwealth University, Richmond, VA, November 20, 2015.

- 84. "Chemistry in Service of Global Health: New Small Molecule Interventions for Malaria," Department of Medicinal Chemistry, University of North Carolina, Asheville, NC, November 4, 2016.
- 85. "How Organic Chemists Can Contribute to Global Health and the Fight Against Malaria," Department of Chemistry, West Virginia State University, Institute, WV, November 15, 2016.
- 86. "Discovery and optimization of IspD-targeting antimalarial agents" Lecture for the German Pharmaceutical Society, Department of Chemistry, Martin Luther University Halle-Wittenberg, Halle Germany, June 14, 2017.
- 87. "New Strategies to Develop Small Molecule Interventions for Malaria" Medicines For All Global Summit, Virginia Commonwealth University, Richmond, Virginia, November 8-9, 2017.
- 88. "Target Validation for Malaria" Department of Pharmacology, University of Virginia, Charlottesville, VA, March 14, 2019.
- 89. "Serendipity and persistence: discovery of an orally-active antimalarial by optimization of the tetrahydro-beta-carboline scaffold" Department of Chemistry, George Washington University, September 11, 2020 (via Zoom).

# COMPLETED GRANT SUPPORT (U.S. Only, 2000-present; Hong Kong Grant Support 1991-2000 available upon request).

- 1. "Laboratory for the Asymmetric Synthesis of Drug Precursors and Drug Candidates" Paul R. Carlier, (P. I.) Virginia Tech ASPIRES Grant, US\$40,000, 7/1/01-12/31/01.
- 2. "Enantioselective Alkylation of Nonracemic α-Chiral Nitriles Without Using External Chiral Control Elements" Paul R. Carlier, (P.I.), Jeffress Memorial Trust, Total direct funds \$39,600, 7/1/01 11/30/03.
- 3. "Structure-based Design of Dimeric Memory-Enhancing Drugs," Paul R. Carlier (P.I.), Commonwealth of Virginia Alzheimer's and Related Diseases Research Award Fund, \$25,000, 7/01/02 6/30/03.
- 4. "Lithiated Nitriles: Solution Structures and Reaction Stereochemistry," Paul R. Carlier (P.I.), National Science Foundation Grant 0213525. Total funds \$240,000, 8/1/02 7/31/05.
- 5. "Multinuclear NMR Investigations of Lithiated Nitrile Structure," Paul R. Carlier (P.I.), Type AC Grant from Petroleum Research Fund (ACS). 38914-AC4, Total direct funds \$80,000, 7/1/2003 to 8/31/2005.
- 6. "Novel Triple Reuptake Inhibitors" \$50,000, Paul Carlier, P.I. Fund Code MCJPRC. 2005. Internal Funds from Virginia Tech Research Division for collaborative research with the Mayo Clinic to get additional safety and efficacy data for antidepressant candidates covered by U.S. Patent 6,700,018 (VTIP and the Mayo Foundation, Assignees).
- 7. "Molecular Design of Selective Anticholinesterases for Mosquito Control," Jeffrey R. Bloomquist (Lead PI), Paul R. Carlier (Co-PI), Sally L. Paulson (Co-PI), Eric Wong (Co-PI), John Githure (ICIPE, Kenya, Co-PI) Grand Challenge in Global Health Initiative, Foundation for the National Institutes of Health (FNIH)/Bill & Melinda Gates Foundation, GCGH-1497, Total funds \$2,689,726, 9/1/05-8/31/08, Carlier portion \$1,350,000.
- 8. "Development of BACE1 inhibitors for Alzheimer's disease" Yasuji Matsuoka, Paul Aisen, Paul R. Carlier, Georgetown University Virginia Tech Joint Center for Drug Discovery and Development. \$100,000 total direct costs, 5/15/07 5/14/08. Carlier portion \$50,000.

- 9. "Configurationally stable carbanionic reagents for enantioselective synthesis," Paul R. Carlier (PI), Unsolicited NSF Proposal CHE-0750006, total costs \$365,000, 2/15/08 2/14/12.
- 10. "Hydroxyethylamine isostere triazole-linked BACE1 Inhibitors for Alzheimer's disease" Paul R. Carlier (PI), Alzheimer's and Related Diseases Research Award Fund (Commonwealth of Virginia), Grant 09-1, total costs \$40,000, 7/1/08-6/30/09.
- 11. Funded supplement for "Molecular Design of Selective Anticholinesterases for Mosquito Control," Jeffrey R. Bloomquist (Lead PI), Paul R. Carlier (Co-PI), Sally L. Paulson (Co-PI), Eric Wong (Co-PI), Grand Challenge in Global Health Initiative, Foundation for the National Institutes of Health (FNIH), Total costs \$580,933, 9/1/08-6/30/09, Carlier portion \$290,000.
- 12. "Synthesis of structural analogues of PRC200" Paul R. Carlier (PI), Sponsored research agreement from AstraZeneca, Virginia Tech Proposal No. 09-1128-11, Total Costs \$122,000, 12/19/08 4/30/10.
- 13. "Development of vector-specific, resistance-breaking insecticides to reduce malaria transmission," Paul R. Carlier (PD/PI), Jeffrey R. Bloomquist (Co-I, Univ. Florida), Jianyong Li (Co-I), Max Totrov (Co-I, Molsoft LLC), 1R01 Al082581-01, funded by NIH/NIAID, Total award \$3,577,000. 4/1/09-9/30/15, Carlier portion \$2,146,000.
- 14. "Identification of contact-toxic bivalent carbamates" Paul R. Carlier (Co-PI), Jeffrey R. Bloomquist (Co-PI). proposal submitted to the Innovative Vector Control Consortium (IVCC), Liverpool, England, UK, 6/8/09. Total award \$99,500. 3/1/10-1/31/11. Carlier portion \$49,750.
- 15. "Voltage-Sensitive Potassium Channel as a New Target for Mosquitocides" Jeffrey Bloomquist (PI, Univ. Florida), Paul R. Carlier (Co-I), Max Totrov (Co-I, Molsoft), FNIH BLOO11VCTR, Foundation for the NIH New Insecticides for Discovery Research Solicitation, 9/1/11 10/31/15, Total award \$1,469,594; Carlier portion \$468,655.
- 16. "Positioning a class of potent, benzothiophene-core anti-malarial compounds for pre-clinical development" Paul R. Carlier, Mike Klemba, Virginia Tech Center for Drug Discovery, 12/1/15-5/30/16, Total award \$5,000.
- 17. "Synthesis of Potential Mosquito Deterrents," Paul R. Carlier (PI), University of North Texas Health Science Center (UNTHSC), 6/1/16-12/15/17, Total award \$25,680.
- 18. "Structure- and ligand-based optimization of new IspD-targeting antimalarials" Paul R. Carlier (PD/PI), Maria Belen Cassera (Co-I, BICH), Daniel J. Slade (Co-I, BICH), Maxim Totrov (Molsoft LLC consortium PI), 1R21 Al128362-01, National Institutes of Health, 12/16/16-11/30/19, total funds requested \$431,126, Virginia Tech portion \$295,552.
- 19. MRR: A major new chiral analysis technique for new drug discovery, development, and process control B. Frank Gupton (Virginia Commonwealth University, PI), Paul Carlier (Co-I), Robert Lloyd, (BrightSpec LLC), Brooks Pate (University of Virginia, Co-I) Project dates 6/1/18-5/30/19, total funds \$400,000, Carlier portion \$67,000.
- 20. Rapid Drug Development Using Molecular Rotational Resonance (MRR) for Structure Analysis B. Frank Gupton (Virginia Commonwealth University, PI), Paul Carlier (Co-I), Robert Lloyd, (BrightSpec LLC), Brooks Pate (University of Virginia, Co-I) VBHRC Catalyst Award PFHYPGTM, Project dates 6/1/19-11/30/20, total funds \$400,000, Carlier portion \$100,000.

- 21. "Optimization of salicylamide analogs for combating multidrug-resistant Neisseria Gonorrhoeae" Mohamed Seleem, PI (VT VetMed), Paul R. Carlier (Co-I). CeZAP 2020 Interdisciplinary Team-building Pilot Grant Program, Fralin Life Sciences Institute, Virginia Tech. 11/2/20-6/30/21, Total award \$20,000; Chemistry portion \$10,000.
- 22. "Prevention of Zika transmission with novel Aedes personal protective measures" Seongchool Kim (Loyola Chicago, Contact PD/PI), Paul R. Carlier (MPI), John Grieco (Notre Dame, MPI), 1R21 Al130521-01, National Institutes of Health, Project dates 9/10/17-8/31/21, total funds \$427,720, VT Chemistry portion \$147,096.
- 23. "Toxicity Screening of Novel Compounds," Aaron D. Gross (PI, Entomology), Paul R. Carlier (Co-I), USDA, PN2WXO4U, 3/1/19-9/30/21, \$25,000.

#### **CURRENT GRANT SUPPORT**

- 1. "Optimization of antimalarials targeting multiple life stages of the parasite" Paul R. Carlier (PD/PI), Maria B. Cassera (MPI, Univ. of Georgia), Max Totrov (Co-I, Molsoft LLC), 1 R01 Al157445-A1, National Institutes of Health, Project Dates 8/4/21-6/30/26, total funds \$3,721,434, VT portion \$1,825,778
- 2. "Interrogating plasmodial endocytosis with mefloquine-based affinity probes" Michael Klemba (PD/PI), Paul R. Carlier (MPI), Richard Helm (Co-I), Total costs \$428,541, NIH/NIAID R21 Al149190-01 VT Chemistry portion \$298,077. Project dates 2/1/20- 11/30/21; No cost extension to 11/30/22 is planned (>50% of funds remain at present).
- 3. "New Therapeutics to Prevent Malaria Resurgence" VTIP Proof of Concept Proposal, Paul R. Carlier (PI), Jopaul Mathew, Maria B. Cassera, \$50,000, Project dates 3/1/21-2/28/22. Carlier portion \$45,000.

#### PENDING GRANT SUPPORT

None at present

### **TEACHING EXPERIENCE (Virginia Tech)**

CHEM 2535: Organic Chemistry I

 $\mathbf{1}^{\text{st}}$  semester course in Organic Chemistry for non-majors, using Vollhardt & Schore "Organic Chemistry."

CHEM 2536: Organic Chemistry II

2<sup>nd</sup> semester course in Organic Chemistry for non-majors, using Bruice "Organic Chemistry" 7th Ed.

CHEM 2565: Principles of Organic Chemistry

1st semester course in Organic Chemistry for majors, using Bruice "Organic Chemistry" 7th Ed.

CHEM 2566: Principles of Organic Chemistry

2<sup>nd</sup> semester course in Organic Chemistry for majors, using Bruice "Organic Chemistry" 7th Ed.

CHEM 4584: Bioorganic Chemistry

3<sup>rd</sup> semester course in Organic Chemistry focusing on the bridge from organic chemistry to biochemistry, using Bruice "Organic Chemistry" 8<sup>th</sup> Ed and Van Vranken and Weiss "Introduction to Bioorganic Chemistry and Chemical Biology."

CHEM 5505: Advanced Organic Chemistry I

Graduate course on organic structure, reactivity, and mechanism, using Carey & Sundberg "Advanced Organic Chemistry, Part A".

# CHEM 5535: Synthetic Organic Chemistry

Graduate course in organic synthesis, using Carey & Sundberg "Advanced Organic Chemistry, Part B".

## CHEM6564: Bioorganic Principles of Medicinal Chemistry

Graduate course in medicinal chemistry, using Silverman "The Organic Chemistry of Drug Design and Drug Action" 3rd edition.