Curriculum Vitae

Webster L. Santos, Ph.D.

Department of Chemistry
Virginia Tech
Blacksburg, Virginia 24061-0344
Phone: (540) 231-5742 Fax: 540-231-3255
E-mail: santosw@vt.edu
website: http://santosgroup.chem.vt.edu

- **Education**

2002-2006	Harvard University, Cambridge, Massachusetts Postdoctoral Fellow (Advisor: Prof. Gregory Verdine)
1997-2002	University of Virginia, Charlottesville, Virginia Ph.D. (Advisor: Timothy Macdonald)
1993-1997	University of Virginia, Charlottesville, Virginia B.S. (Advisor: Timothy Macdonald)

- **Positions and Employment**

2018-current	Professor, Department of Chemistry, VA Tech, Blacksburg, VA
2013-2018	Associate Professor, Department of Chemistry, VA Tech, Blacksburg, VA
2006-2013	Assistant Professor, Department of Chemistry, VA Tech, Blacksburg, VA
2004-2005	Teaching Fellow, Harvard University, Department of Chemistry, Cambridge, MA.
2002-2006	NIH Postdoctoral Fellow, Harvard University, Cambridge, MA.

- **Honors and Awards**

2022	Director, Virginia Tech Center for Drug Discovery
2021	Outstanding Faculty Mentor, College of Science, Virginia Tech
2019	Fellow of the Royal Society of Chemistry
2018-	Flux Therapeutics, Inc., Co-founder, VP and Head of Medicinal Chemistry
2017-	Continuum Biosciences, Inc., Co-founder, VP and Head of Medicinal Chemistry
2015	ICAT Catalyst Faculty Fellow, Virginia Tech
2014	FLSI-ICTAS Innovators Award, Virginia Tech
2014	Cliff and Agnes Lilly Faculty Fellow of Drug Discovery, Virginia Tech
2014	John C. Schug Research Award, Dept. of Chemistry, Virginia Tech
2012	American Chemical Society Young Academic Investigator
2012-	Core Faculty Member, Virginia Tech Center for Drug Discovery
2011	Chemical Communications Emerging Investigator
2010-2014	Blackwood Junior Faculty Fellow of Life Sciences
2010-2016	SphynKx Therapeutics, LLC, co-Founder and Vice-president of Medicinal Chemistry
2009	Molecular Biosystems Emerging Investigator
2002-2006	Ruth L. Kirschtein Postdoctoral Fellow (NRSA), Harvard University
2002	Third Prize Winner, Robert J. Huskey Graduate Research Symposium, University of Virginia
2000-2002	NIH NRSA Pre-doctoral Traineeship, University of Virginia

1998-1999	Outstanding Graduate Teaching Assistant Award, University of Virginia
1996-1997	Semi-finalist for Seven Society Teaching Fellowship, Secret Seven Society, University of Virginia

Service

2022	Chair of the Organizing Committee, Boron in the Americas XVII International Conference in Blacksburg, VA
2021-present	Steering Committee, Virginia Tech Center for Drug Discovery
2021-present	Executive Committee, Virginia Drug Discovery Consortium
2021-2025	NIH Synthetic and Biological Chemistry B Panel Standing member
2019- present	Editorial Board, *Molecules, Medicinal Chemistry Section*
2017-present	Editorial Board, *Medicinal Research Reviews*
2015-present	Editorial Advisory Board, *Current Topics in Medicinal Chemistry*
2015-2018	Associate Committee on Science, American Chemical Society
2014-present	Editorial Board, *Journal of Biochemistry and Molecular Biology Research*
2014-15	Associate Editor, *Diversity Oriented Synthesis*
2014-present	Advisory board member for the Boron in the Americas Organization
2013-16	Alternate Councilor, Division of Biological Chemistry, American Chemical Society

- **Patents**

1. Lynch, K.R.; Macdonald, T. L.; Heise, C.H.; Santos, W. L . and Okusa, M.D. Novel Lysophosphatidic Acid Receptor Agonists and Antagonists. PCT Int. Appl. 2002 (US 7,169,818 B2 Issued January 30, 2007).

2. Santos, W.L. and Verdine, G.L. Oligonucleotide microarrays comprising nucleic acid analogs for hybridization with target RNA, including RNA in nucleoprotein complexes. PCT Int. Appl. 2005, 60 pp.

3. Santos, W.L. and Gao, M. Synthesis and uses of mixed diboron reagents. US Patent Appl. 61/225,032 July 2009.

4. Santos, W.L. Inhibition of proteases using N-terminal peptidic boronic acids. US Patent Appl. 61/234,399 August 2009.

5. Santos, W.L. Branched peptides as therapeutics for structured RNA targets. US Patent Appl. 61/269,571, June 2009

6. Santos, W.L. and Lynch K.R. Sphingosine kinase inhibitors and therapeutic use thereof. US Patent Appl. 61/375,478, Aug. 2010.

7. Santos, W.L.; Raje, M.R.; Lynch, K.R.; Macdonald, T.L.; Kennedy, A. and Kharel, Y. “Long Chain Base Sphingosine Kinase Inhibitors”, US9,688,688 issued on June 27, 2017.

8. Santos, W.L.; Lynch, K.R. “Sphingosine Kinase Inhibitors”, US Patent Appl. 62/058294, Priority filing date: October 1, 2014.

9. Santos, W.L.; Lynch, K.R.; Childress, E.; Kharel, Y. "Guanidine-Based Aminothiazole Inhibitors of Sphingosine Kinase", U.S. Patent Application No: 62/205,196, Priority filing date: August 14, 2015.

10. Santos, W.L.; Lynch, K.R. “Oxadiazoles as sphingosine kinase inhibitors and their preparation”, PCT Int. Appl. (2016), WO 2016054261 A1 20160407.

11. Santos, W.L.; Childress, E.; Hoehn, K. “Compositions and Methods for Preparing and Using Mitochondrial Uncouplers”, May 2017, U.S. Provisional Patent Application Serial No. 62/509,249. PCT/US2018/033901

12. Thorpe, B. T.; Santos, W.L.; Lynch, K.R. “Sphingosine Kinase Inhibitor Prodrugs”, March 2017, PCT/US2017/024852.

13. Santos, W.L.; Fritzemeier, R. “A process for making 3-substituted-1,2-oxaborol-2(5H)-ol”, July 8, 2019, U.S. Patent Application Serial No.: 62/871,564

14. Santos, W.L.; Murray, J.; Dai, Y.; Santiago-Rivera, J. “Imidazopyridines Useful as Mitochondrial Uncouplers”, April 22, 2019, PCT International Application No.: PCT/US2019/028555.

15. Santos, W.L.; Salamoun, J.; Murray, J.; Garcia, J. “Oxadiazolopyrazines and Oxadiazolopyridines useful as Mitochondrial Uncouplers”, April 22, 2019, PCT International Application No.: PCT/US2019/028544.

16. Santos, W.L; Murray, J.; Nekvinda, J.; Burgio, A. “Aminopyrazines and Related Compounds Useful as Mitochondrial Uncouplers”, April 22, 2019, PCT International Application No.: PCT/US2019/028560.

17. Santos, W.L.; Lynch, K.R., Kharel, Y.; Peralta, A.; Fritzemeier, R.; Foster, D. “Inhibitors of Spinster Homology 2 for Use in Therapy”, January 22, 2020, PCT/US2020/014651.

18. Santos, W.L.; Lynch, K.R., Kharel, Y.; Peralta, A.; Fritzemeier, R.; Foster, D. “Inhibitors of Spinster Homology 2 for Use in Therapy”, PCT Application No. PCT/US2021/049531, September 8, 2021.

19. Lynch, K.R.; Kharel, Y.; Santos, W.L.; Fritzemeier, R.; Burgio, A. L.; Shrader, C.; Foster, D. “Inhibitors of Spinster Homology 2 (SPNS2) for Use in Therapy” PCT/US2021/049534, September 8, 2021.

20. Santos, W.L.; Gaultier, A.; Bowen, J. Compositions and Methods for Treating Multiple Sclerosis. United States Provisional Patent Application Serial No. 63/071,667, filed August 2020.

- **Publications**

1. Santos, W. L.; Rossi, J. R.; Boggs, S. D. and Macdonald, T. L. The molecular pharmacology of lysophosphatidate signaling. *Ann. N. Y. Acad. Sci*. **2000**, *905*, 232-242. DOI: 10.1111/j.1749-6632.2000.tb06553 PMID: 10818457

2. Heise, C. E.; Santos, W. L.; Schreihofer, A. M.; Heasley, B. H.; Mukhin, Y. V.; Macdonald, T. L. and Lynch, K. R. Activity of 2-substituted lysophosphatidic acid (LPA) analogs at LPA receptors: discovery of a LPA_1/LPA_3 receptor antagonist. *Mol. Pharm*. **2001**, *60*, 1173-1180. DOI: 10.1124/mol.60.6.1173 PMID: 11723223

3. Hooks, S. B.; Santos, W. L. ; Im, D-S., Heise, C. H.; Macdonald, T. L. and Lynch, K. R. Lysophosphatidic acid induced mitogenesis is regulated by lipid phosphate phosphatases and is Edg-receptor independent. *J. Biol. Chem.* **2001,** 276**,** 4611-4621. DOI: 10.1074/jbc.M007782200 PMID: 11042183

4. Dieckhaus, C. M.; Santos, W. L. and Macdonald, T. L. The chemistry, toxicology, and identification in rat and human urine of 4-hydroxy-5-phenyl-1,3-oxazaperhydroin-2-one: a reactive metabolite in felbamate bioactivation. *Chem. Res. Toxicol.* **2001**, *14*, 958-964. DOI: 10.1021/tx000139n PMID: 11511169

5. Dieckhaus, C. M.; Roller, S.; Santos, W. L. and Macdonald, T. L. The role of glutathione s-transferases a1-1, p1-1 and m1-1 in the detoxification of 2-phenylpropenal, a reactive felbamate metabolite. *Chem. Res. Toxicol.* **2001**, *14*, 511-516. DOI: 10.1021/tx000141e PMID: 11368548

6. Roller, S. G.; Dieckhaus, C. M.; Santos, W. L.; Duane Sofia, R. and Macdonald, T. L. Interaction between human serum albumin and the felbamate metabolites 4-Hydroxy-5-phenyl-[1,3]oxazinan-2-one and 2-Phenylpropenal. *Chem. Res. Toxicol.* **2002**, *15*, 815-24. DOI: 10.1021/tx025509h PMID: 12067249

7. Kapetanovic, I.M.; Torchin, C.D.; Strong, J.M.; Yonekawa, W.D.; Lu, C.; Li, A.P.; Dieckhaus, C.M.; Santos, W.L.; Macdonald, T.L.; Sofia, R.D. and Kupferberg, H.J. Reactivity of atropaldehyde, a felbamate metabolite in human liver tissue in vitro. *Chem. Biol. Interact.* **2002**, *142*, 119-34. DOI: 10.1016/S0009-2797(02)00058-3 PMID: 12399159

8. Okusa, M.D., Ye, H., Huang, L.P., Heise, C.E., Santos, W.L., Macdonald, T.L., Lynch, K.R.A dual lysophosphatidic acid (LPA) antagonist (LPA(1)/LPA(3)), VPC 12249, reduces renal ischemia-reperfusion injury (IRI). *J. Am. Soc. Neph*. **2002**, *13*, 140A.

9. Santos, W.L.; Heasley, B.H.; Jarosz, R.; Carter, K.M.; Lynch, K.R. and Macdonald, T.L. Synthesis and biological evaluation of phosphonic and thiophosphoric acid derivatives of lysophosphatidic acid. *Bioorg. Med. Chem. Lett.* **2004**, *14*, 3473. DOI: 10.1016/j.bmcl.2004.04.061 PMID: 15177455

10. Paz, Y.E.; Santos, W.L. and Verdine, G.L. Toward determination of the structural basis for HIV-1 integrase substrate recognition. *Nucleus* **2005**, *83*, 12-14.

11. Johnson, A.A.; Santos, W.L.; Pais, G. C.; Marchand, C.; Amin, R.; Burke, T.R. Jr.; Verdine, G.L. and Pommier, Y. Integration requires a specific interaction of the donor DNA terminal 5'-cytosine with glutamine 148 of the HIV-1 integrase flexible loop. *J. Biol. Chem*. **2006**, *281*, 461. DOI: 10.1074/jbc.M511348200 PMID: 16257967

12. Banerjee, A.; Santos, W.L. and Verdine, G.L. Structure of a DNA Glycosylase Searching for Lesions. *Science*, **2006**, *311*, 1153. DOI: 10.1126/science.1120288 PMID: 16497933

13. Zhao, Z.; McKee, C.J.; Kessl, J.J.; Santos, W.L.; Daigle, J.E.; Engelman, A.; Verdine, G. and Kvaratshelia, M. Subunit specific protein footprinting reveals significant structural rearrangements and a role for N-terminal LYS-14 of HIV-1 integrase during viral DNA binding. *J. Biol. Chem.* **2008**, *283*, 5632. DOI: 10.1074/jbc.M705241200 PMID: 18093980

14. Komazin-Meredith, G.; Santos, W.L., Filman, D.J.; Hogle, J.M.; Verdine, G.L. and Coen, D.M. The positively charged surface of herpes simplex virus UL42 mediates DNA binding. *J. Biol. Chem*. **2008**, *283,* 6154. DOI: 10.1074/jbc.M708691200 PMID: 18178550

15. Komazin-Meredith, G.; Petrella, R.J.; Santos, W. L.; Filman, D. J.; Hogle, J. M.; Verdine, G. L.; Karplus, M. and Coen, D. M. The Human Cytomegalovirus UL44 C Clamp Wraps Around DNA. *Structure* **2008**, *16*, 1214. DOI: 10.1016/j.str.2008.05.008 PMID: 18682223

16. Gao, M.; Thorpe, S.B. and Santos, W.L. sp^2-sp^3 Hybridized Mixed Diboron: Synthesis, Characterization, and Copper-Catalyzed β Boration of α,β -Unsaturated Conjugated Compounds. *Org. Lett.* **2009**, *11*, 3478. DOI: 10.1021/ol901359n PMID: 19594167

17. Bryson, D.I.; Zhang, W.; Ray, W.K. and Santos, W. L. Screening of a branched peptide library with HIV-1 TAR RNA. *Mol. BioSyst*. **2009**, *5*, 1070. (*Emerging investigator issue*) DOI: 10.1039/b904304g PMID: 19668873

18. Knott, K.; Fishovitz, J.; Thorpe, S.B.; Lee, I. and Santos, W.L. N-terminal Peptidic Boronic Acids Selectively Inhibit ClpXP. *Org. Biomol. Chem*. **2010**, *8*, 3451. (*Highlighted in an OBC Chemical Biology Issue*). DOI: 10.1039/c004247a PMID: 20523950

19. Thorpe, S.B. and Santos, W.L. Regio- and stereoselective copper-catalyzed β-borylation of allenoates by a preactivated diboron. *Chem. Commun*. **2011**, *47*, 424. (*Emerging investigator issue*) DOI: 10.1039/c0cc02270e PMID: 20852792

20. Gao, M.; Thorpe, S.B.; Kleeberg, C.; Slebodnick, C.; Marder, T.B. and Santos, W.L. Structure and Reactivity of a Preactivated Unsymmetrical Diboron: Catalytic Regioselective Boration of α, β-Unsaturated Conjugated Compounds. *J. Org. Chem*. **2011**, *76*, 3997–4007. DOI: 10.1021/jo2003488 PMID: 21491953
    - Highlighted in (1) *Synfacts*, **2011**, *9*, 995. (2) *ChemInform*, **2011**, *42*, no. doi: 10.1002/chin.201133182

21. Sun, J.; Perfetti, M.T. and Santos, W.L. A method for the deprotection of alkylpinacolyl boronate esters. *J. Org. Chem*., **2011**, *76*, 3571–3575. DOI: 10.1021/jo200250y PMID: 21449603

22. Crumpton, J.B.; Zhang, W. and Santos, W.L. Facile Analysis and Sequencing of Linear and Branched Peptide Boronic Acids by MALDI Mass Spectrometry. *Anal. Chem*. **2011**, *83*, 3548–3554. DOI: 10.1021/ac2002565 PMID: 21449540

23. Raje, M.; Knott, K.; Kharel, Y.; Bissel, P.; Lynch, K.R. and Santos, W.L. Design, synthesis and biological activity of sphingosine kinase 2 selective inhibitors. *Bioorg. Med. Chem.* **2012**, *20*, 183-194. DOI: 10.1016/j.bmc.2011.11.011 PMID: 22137932

24. Knott, K.; Kharel, Y.; Raje, M.R.; Lynch, K.R. and Santos, W.L. Effect of alkyl chain length on sphingosine kinase 2 selectivity. *Bioorg. Med. Chem. Lett.* **2012**, 22, 6817-6820. DOI: 10.1016/j.bmcl.2012.01.050. PMID: 22321213

25. Crumpton, J.B. and Santos, W.L. Site-specific incorporation of diamondoids on DNA using click chemistry. *Chem. Commun*. **2012**, *48*, 2018 - 2020. DOI: 10.1039/c2cc16860j PMID: 22237385

26. Bryson, D.R.; Zhang, W.; McLendon, P.M.; Reineke, T.M. and Santos, W.L. Toward Targeting RNA Structure: Branched Peptides as Cell-Permeable Ligands to TAR RNA. *ACS Chem. Biol.* **2012**, *7*, 210–217. DOI: 10.1021/cb200181v PMID: 22003984
    - Highlighted by the editors as a podcast interview: http://pubs.acs.org/page/acbcct/audio/index.html

27. Thorpe, S. B., Calderone, J. A., and Santos, W. L. Unexpected Copper(II) Catalysis: Catalytic Amine Base Promoted beta-Borylation of alpha, beta-Unsaturated Carbonyl Compounds in Water, *Org. Lett.* **2012**, *14*, 1918-1921. DOI: 10.1021/ol300575d PMID: 22428578
    - Highlighted in *ChemInform*, **2012**, *43*, no. doi: 10.1002/chin.201231192

28. Calderone, J. and Santos, W.L. Copper(II)-Catalyzed Silyl Conjugate Addition to α,β-Unsaturated Conjugated Compounds: Brønsted Base-Assisted Activation of Si—B bond in Water, *Org. Lett*. **2012**, 14, 2090-2093. DOI: 10.1021/ol300618j PMID: 22494333
    - Highlighted in (1) *Synfacts*, **2012***,* 8, 781. (2) *ChemInform*, **2012**, *43*, no. doi: 10.1002/chin.201231192

29. Gude, L., Berkovitch, S. S., Santos, W. L., Kutchukian, P. S., Pawloski, A. R., Kuimelis, R., McGall, G., and Verdine, G. L. Mapping targetable sites on the human telomerase RNA pseudoknot/template domain using 2'-OMe RIPtide microarrays, *J. Biol. Chem.*, **2012**, 287, 18843-18853. DOI: 10.1074/jbc.M111.316596 PMID: 22451672

30. Thorpe, S.B. and Santos, W.L. 4,8-Dimethyl-2-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3,6,2-dioxazaborocane, Encyclopedia of Reagents for Organic Synthesis, **2012**, John Wiley & Sons, Ltd. DOI: 10.1002/047084289X.rn01517.

31. Kharel, Y., Raje, M., Gao, M., Gellett, A.M., Tomsig, J.L., Lynch, K.R. and Santos, W.L. Sphingosine Kinase Type 2 Inhibition Elevates Circulating Sphingosine 1-Phosphate, *Biochem. J*. **2012**, *447,* 149-157. DOI: 10.1042/BJ20120609 PMID: 22747486

32. Zhang, W.; Bryson, D.I.; Crumpton, J.B.; Wynn, J. and Santos, W. L. Branched Peptide Boronic Acids (BPBAs): A Novel Mode of Binding Towards RNA. *Chem. Commun*. **2013**, *49,* 2436-*2438.* DOI: 10.1039/c3cc00243h PMID: 23412370

33. Daengngam, C.; Thorpe, S.; Guo, X.; Stoianov, S.; Santos, W. L.; Morris, J.; Robinson, H. High Photoreactivity of O-Nitrobenzyl Ligands on Gold. *J. Phys. Chem.* **2013**, *117,* 14165–14175. DOI: 10.1021/jp4019102

34. Zhang, W.; Bryson, D.I.; Crumpton, J.B.; Wynn, J.; Santos, W. L. Targeting folded RNA: a branched peptide boronic acid that binds to a large surface area of HIV-1 RRE RNA. *Org. Biomol. Chem.*, **2013**, *11*, 6263-6271. DOI: 10.1039/c3ob41053f PMID: 23925474
    - This work was featured on the journal's front cover.

35. Carreon, A.; Santos, W.L.; Matson, J.B. and So, R. Cationic Polythiophenes as Responsive DNA-Binding Polymers. *Polym. Chem.*, **2014**, *5*, 314-317. DOI: 10.1039/C3PY01069D

36. Kenwood, B.M.; Weaver, J.L.; Bajwa, A.; Byrne, F.L.; Poon, I.V.; Murrow, B.A.; Calderone, J.A.; Huang, L.; Divakaruni, A.S.; Okabe, K.; Columbus, L.; Yan, Z.; Saucerman, J.J.; Smith, J.S.; Holmes, J.W.; Lynch, K.R.; Ravichandran, K.S.; Uchiyama, S.; Santos, W.L.; Rogers, G.W.; Okusa, M.D.; Bayliss, D.A. and Hoehn, K.L. Identification of a novel mitochondrial uncoupler that does not depolarize the plasma membrane. *Mol. Metab*. **2014**, *3*, 114-123. DOI: 10.1016/j.molmet.2013.11.005 PMID: 24634817 PMCID: PMC3953706
    - Highlighted in *Mol. Met*. **2014**, *3*, 86-87.

37. Calderone, J.A. and Santos, W.L. Copper(II)-Catalyzed Silylation of Activated Alkynes in Water: Diastereodivergent Access to (*E*)- or (*Z*)-β-Silyl-α,β-Unsaturated Carbonyl and Carboxyl Compounds. *Angew. Chem. Int. Ed.* **2014**, *53*, 4154 –4158. DOI: 10.1002/anie.201310695 PMID: 24532188
    - Highlighted in *Synfacts*, **2014**, *10*, 731.

38. Ashry, A.; Kandas, I.; Wei, X.; Calderone, J.A.; Zhang, B.; Robinson, H.; Heflin, J.R.; Santos, W.L. and Xu, Y. T. Impact of Lithography on the Fluorescence Dynamics of Self-Assembled Fluorophores, *Optics Express*, **2014**, *22,* 12935-12943. DOI: 10.1364/OE.22.012935 PMID: 24921491

39. Islam, A. Zhang, B.; Khalifa, M.B.; Calderone, J.A.; Santos, W.L.; Heflin, J.R.; Robinson, H. and Xu, Y. Fluorescence Lifetime Based Characterization of Active and Tunable Plasmonic Nanostructures, *Optics Express.* **2014**, 22, 20720-20726. DOI: 10.1364/OE.22.020720 PMID: 25321275

40. Tang, X.; Benesch, M.G.K.; Dewald, J.; Zhao, Y.Y.; Patwardhan, N.; Santos, W.L.; Curtis, J.M.; McMullen, T.P.W. and Brindley, D.N. Lipid phosphate phosphatase-1 expression in cancer cells attenuates tumor growth and metastasis in mice, *J. Lipid Res.*, **2014**, 55, 2389-2400. DOI: 10.1194/jlr.M053462 PMID: 25210149

41. Santos, W.L. and Lynch, K.R. Drugging Sphingosine Kinases. *ACS Chem. Biol*. **2015**, *10*, 225-223. DOI: 10.1021/cb5008426 PMID: 25384187

42. Patwardhan, N.N.; Morris, E.A.; Kharel, Y.; Raje, M.R.; Gao, M.; Tomsig, J.L.; Lynch, K.R. and Santos, W.L. Structure-Activity Relationship Studies and In Vivo Activity of Guanidine-based Sphingosine Kinase Inhibitors: Discovery of SphK1- and SphK2-Selective Inhibitors, *J. Med. Chem*., **2015**, *58,* 1879-1899. DOI: 10.1021/jm501760d. PMID: 25643074

43. Xi, G.; Nelson, A. and Santos, W.L. Regio- and Chemoselective Diboration of Allenes with Unsymmetrical Diboron: Formation of Vinyl and Allyl Boronic Acid Derivatives, *ACS Catal*., **2015**, *5*, 2172−2176. DOI: 10.1021/acscatal.5b00387.

44. Congdon, M.D.; Childress, E.S.; Patwardhan, N.N.; Gumkowski, J.; Morris, E.A.; Kharel, Y.; Lynch, K.R. and Santos, W.L. Structure-activity relationship studies of the lipophilic tail region of sphingosine kinase 2 inhibitors, *Bioorg. Med. Chem. Lett*., **2015**, *25*, 4858-4861. (Invited 25th anniversary symposium-in-print, Prof. Dale Boger)

45. Wynn, J. and Santos, W.L. HIV-1 Drug Discovery: Targeting Folded RNA Structures With Branched Peptides. *Perspective*, *Org. Biomol. Chem*., **2015**, *13*, 5848-5858.

46. Kharel, Y.; Morris, E.A.; Thorpe, S.B.; Tomsig, J.L.; Santos, W.L. and Lynch, K.R. Sphingosine Kinase Type 2 and Blood S1P. *J. Pharm. Exp. Ther*. **2015**, *355*, 23–31. DOI: 10.1124/jpet.115.225862
    - This article was recently highlighted in J. Pharm. Exp. Ther. 2015, 355, 1.

47. Peck, C.L.; Calderone, J.A. and Santos, W.L. Copper(II)-catalyzed Regio-, Stereo-, and Chemoselective β-Borylation of Acetylenic Esters in Water. *Synthesis* **2015**, 47, 2242-2248. DOI: 10.1055/s-0034-1380524. Invited contribution on conjugate addition themed edition by Prof. Erick Carreira.
    - Highlighted in organic chemistry portal.

48. Kenwood, B.M.; Calderone, J.A.; Hoehn, K.L. and Santos, W.L. Structure-activity relationship studies of the mitochondrial protonophore uncoupler BAM15, *Bioorg. Med. Chem. Lett.*, **2015**, 25, 4858-4861. DOI: 10.1016/j.bmcl.2015.06.040.

49. Babahosseini, H.; Srinivasarahavan, V.; Zhao, Z.; Gillam, F.; Childress, E.; Strobl, J.; Santos, W.L.; Zhang, C.; Agah, M. The Impact of Sphingosine Kinase Inhibitor-Loaded Nanoparticles on Bioelectrical and Biomechanical Properties of Cancer Cells, *Lab on a Chip*, **2016**, *16*, 23-31. doi: 10.1039/c5lc01201e

50. Congdon, M.; Kharel, Y.; Lynch, K.R. and Santos, W.L. Design, synthesis and biological evaluation of naphthalene-containing sphingosine kinase 2 inhibitors. *ACS Med. Chem. Lett*., **2016**, *7*, 229-234. DOI: 10.1021/acsmedchemlett.5b00304.
    - This work was featured on the front cover of the journal.

51. Wynn, J.E.; Zhang, W.; Tebit, D.M.; Gray, L.R.; Hammarskjold, M-L.; Rekosh, D.R. and Santos, W.L. Characterization and *in vitro* activity of a branched peptide boronic acid that interacts with HIV-1 RRE RNA. *Bioorg. Med. Chem.* **2016**, *24*, 3947-3952. http://dx.doi.org/10.1016/j.bmc.2016.04.009. Symposium-in-print in honor of Prof. Matthew Disney.
    - This work was highlighted in *Bioorg. Med. Chem*. **2016**, *24*, 3875.

52. Wynn, J.E.; Zhang, W.; Tebit, D.M.; Gray, L.R.; hammarskjold, M-L.; Rekosh, D.R. and Santos, W.L. Synergistic Effect of Intercalator and Lewis Acid-base Branched Peptide Complexes: Boosting Affinity Towards HIV-1 RRE RNA. *MedChemComm*, **2016**, *7*, 1436-1440. DOI:10.1039/C6MD00171H .

53. Nelson, A.K.; Peck, C.L.; Rafferty, S.M.; Santos, W.L. Chemo-, Regio-, and Stereoselective Copper(II)-Catalyzed Boron Addition to Acetylenic Esters and Amides in Aqueous Medium. *J. Org. Chem*. **2016**, *81*, 4269-4279. **DOI:**10.1021/acs.joc.6b00648.

54. Lynch, K.R.; Thorpe, S.B.; Santos, W.L. Sphingosine kinase inhibitors: a patent review (2005-2015). *Exp. Op. Ther. Pat*. **2016**, *26*, 1409-1416. DOI: dx.doi.org/10.1080/13543776.2016.1226282.

55. Pashikanti, S.; Calderone, J.A.; Nguyen, M.K.; Sibley, C.D.; Santos, W.L. Regio- and Stereoselective Copper(II)-Catalyzed Hydrosilylation of Activated Allenes in Water: A Convenient Access to Vinylsilanes. *Org. Lett.* **2016**, *18*, 2443-2446. DOI:10.1021/acs.orglett.6b00981.
    - This article was highlighted in Synfacts, **2016**, *12*, 836.

56. Verma, A.; Santos, W.L. Copper-Catalyzed Coupling Reactions of Organoboron Compounds. Boron Reagents in Synthesis, **2016**, 313-356. DOI:10.1021/bk-2016-1236.ch010

57. Valenciano, A.; Ramsey, A.C.; Santos, W.L.; Mackey, Z.B. Discovery and antiparasitic activity of AZ960 as a *Trypanosoma brucei* ERK8 inhibitor, *Bioorg. Med. Chem.* **2016**, *24,* 4647-4651. DOI: 10.1016/j.bmc.2016.07.069

58. Verma, A.; Snead, R.F.; Dai, Y.; Slebodnick, C.; Yang, Y.; Yu, H.; Yao, F.; Santos, W.L. Substrate-assisted, Transition Metal-free Diboration of Alkynamides with Mixed Diboron: Regio- and Stereoselective Access to *trans* 1,2-Vinyldiboronates. *Angew. Chem. Int. Ed*. **2017**, 56, 5111-5115. DOI: 10.1002/anie.201700946
- This article was recently highlighted in Synfacts, **2017**, *13*, 0644.

59. See, E.; Peck, C.; Guo, X.; Santos, W.L.; Robinson, H. Plasmon-Induced Photoreaction of *ortho*-Nitrobenzyl Based Ligands Under 550 nm Light. *J. Phys. Chem.* ***2017****, 121,* 13114-13124. ***DOI:****10.1021/acs.jpcc.7b00707*.

60. Childress, E.; Kharel, Y.; Lynch, K.R.; Santos, W.L. Transforming Sphingosine Kinase 1 Inhibitors into Dual and Sphingosine Kinase 2 Selective Inhibitors: Design, Synthesis, and In Vivo Activity. *J. Med. Chem.* **2017**, *60*, 3933-3957. DOI: 10.1021/acs.jmedchem.7b00233.
- This article was F1000 prime recommended.

61. Wynn, J.E.; Zhang, W.; Falkinham, J.; Santos, W.L. Branched peptides: acridine and boronic acid derivatives as antimicrobial agents. *ACS Med. Chem. Lett.* **2017***, 8,* 820–823. DOI: http://dx.doi.org/10.1021/acsmedchemlett.7b00119 .

62. Adamiak, M; Chelvarajan, L.; Lynch, K.R.; Santos, W.L.; Abdel-Latif, A. and Ratajczak, M. Mobilization studies in mice deficient in sphingosine kinase 2 support a crucial role of the plasma level of sphingosine-1-phosphate in the egress of hematopoietic stem progenitor cells. *Oncogene* **2017**, *8*, 65588-65600. https://doi.org/10.18632/oncotarget.19514

63. See, E.M.; Peck, C.L.; Santos, W.L.; Robinson, H.D. Light-Directed Patchy Particle Fabrication and Assembly from Isotropic Silver Nanoparticles. *Langmuir,* **2017**, *33*, 10927–10935. DOI: 10.1021/acs.langmuir.7b02307

64. Fritzemeier. R.; Santos, W.L. Brønsted Base Catalyzed Regio- and Stereoselective trans Silaboration of Propargylamides: Access to 1,2-Vinylborasilanes. *Chem. Eur. J.* **2017**, *23,* 15534-15537. http://dx.doi.org/10.1002/chem.201703774

65. Childress, E.S.; Alexopoulos, S.; Hoehn, K.L.; Santos, W.L. Small Molecule Mitochondrial Uncouplers and Their Therapeutic Potential. *J. Med. Chem*. **2018**, *61*, 4641-4655. **DOI:** 10.1021/acs.jmedchem.7b01182

66. Kharel, H.; Agah, S.; Mendelson, A.J.; Eletu, O.T.; Gesualdi, J.; Smith, J.S.; Santos, W.L.; Lynch, K.R. *Saccharomyces cerevisiae* as a Platform for Assessing Sphingolipid Lipid Kinase Inhibitors. *PLoS ONE* **2018***, 13,* e0192179. https://doi.org/10.1371/journal.pone.0192179

67. Hemming, D.; Fritzemeier, R.; Wescott, S.A.; Santos, W.L.*; Steel, P.G.* Copper-Boryl Mediated Organic Synthesis. *Chem. Soc. Rev*. **2018**, *47*, 7477. DOI:10.1039/C7CS00816C
    *corresponding authors

68. Fritzemeier, R.; Gates, A.; Guo, X.; Lin, Z.; Santos, W.L. Transition metal-free *trans* hydroboration of alkynoic acid derivatives: Experimental and theoretical studies. *J. Org. Chem.* **2018**, *83*, 10436-10444. DOI: 10.1021/acs.joc.8b01493.

69. Dai, Y.; Peralta, A.N.; Wynn, J.E.; Chringma, S.; Jayaraman, B.; Li, H.; Verma, A.; Frankel, A.D.; Le Grice, S.F.; Santos, W.L. Discovery of a Branched Peptide that Recognizes the Rev Response Element (RRE) RNA and Blocks HIV-1 Replication. *J. Med. Chem.* **2018**, *61,* 9611-9620. DOI: 10.1021/acs.jmedchem.8b01076

70. Cao, R.; Li, J.; Kharel, Y.; Zhang, C.; Santos, W.L.; Lynch, K.R.; Zuo, Z.; Hu, S. Photoacoustic Microscopy Reveals the Hemodynamic Basis of Sphingosine 1-phosphate Neuroprotection against Ischemic Stroke. *Theranostics* **2018**, 8, 6111-6120. doi:10.7150/thno.29435.

71. Magill, B.; Guo, X.; Peck, C.; Reyes, R.; See, E.; Santos, W.L.; Robinson, H. Multi-photon patterning of photoactive o-nitrobenzyl ligands bound to gold surfaces. *Photochem. Photobiol. Sci.,* **2019**,*18*, 30-44. DOI: 10.1039/C8PP00346G

72. Hoagland, D.; Poelzing, S.; Santos, W.L.; Gourdie, R. The role of the gap junction perinexus in cardiac conduction: potential as a novel anti-arrhythmic drug target. *Prog. Biophys. Mol. Biol*. **2019**, *144*, 41-50. DOI: 10.1021/acs.jmedchem.8b01076.

73. Worrell, B.L.; Brown, A.M.; Santos, W.L.; Bevan, D.R. In silico Characterization of Structural Distinctions Between Isoforms of Human and Mouse Sphingosine Kinases for Accelerating Drug Discovery. *ACS J. Chem. Inf. Mod*. **2019**, *59*, 2339-2351. DOI: 10.1021/acs.jcim.8b00931.

74. Dai, Y.; Peralta, A.N.; Wynn, J.E.; Sherpa, C.; Li, H.; Verma, A.; Le Grice, S.F.; Santos, W.L. Molecular Recognition of a Branched Peptide with HIV-1 Rev Response Element (RRE) RNA. *Bioorg. Med. Chem*. **2019**, 27, 1759-1765. https://doi.org/10.1016/j.bmc.2019.03.016

75. Verma, A.; Grams, J.; Rastatter, B.P. Santos, W.L. Transition metal-free α borylation-protodeborylation of alkynoic acids. *Tetrahedron*, **2019**, *75*, 2113-2117. https://doi.org/10.1016/j.tet.2019.02.030.
    - Special issue on Frustrated Lewis Acids and Organoboranes

76. Gates, A.M.; Santos, W.L. Diboron-mediated semireduction of terminal allenes. *Synthesis,* **2019**, *51*, 4619–4624. https://www.thieme-connect.com/products/ejournals/pdf/10.1055/s-0039-1690207.pdf

77. Peralta, N.; Dai, Y.; Sherpa, C.; Le Grice, S.F.; Santos, W.L. Molecular Recognition of HIV-1 RNAs with Branched Peptides. *Methods Enzymol*. **2019**, *623*, 373-400. https://doi.org/10.1016/bs.mie.2019.04.021

78. Grams, R.J.; Fritzemeier, R.G.; Slebodnick, C.; Santos, W.L. Transition Metal-Free trans-Hydroboration of Propiolamides: Access to Primary and Secondary (*E*)-beta-borylacrylamides. *Org. Lett.* **2019**, *21*, 6795-6799. https://pubs.acs.org/doi/full/10.1021/acs.orglett.9b02408

79. Fritzemeier, R.G.; Medici, E.J.; Szwetkowski, C.; Wonilowicz, L.G.; Sibley, C.D.; Slebodnick, C.; Santos, W.L. Facile Route to Air and Moisture Stable β-Difluoroboryl Acrylamides, *Org. Lett.* **2019**, *21,* 8053-8057. https://doi.org/10.1021/acs.orglett.9b03031

80. Blais-Lecours, P.; Laouafa, S.; Arias-Reyes, C.; Santos, W.L.; Joseph, V.; Halayko, A. J.; Soliz, J.; Marsolais, D. A Metabolic adaptation of airway smooth muscle cells to a SPHK2 substrate precedes cytostasis. *Am. J. Respir. Cell. Mol. Biol.* **2020**, *62*, 35-42. https://doi.org/10.1165/rcmb.2018-0397OC

81. Byrne, F.; Olzomer, E.; Marriott, G.; Quek, L.; Katen, A.; Su, J.; Nelson, M.; Hart-Smith, G.; Larance, M.; Sebesfi, V.; Cuff, J.; Martyn, G.; Childress, E.; Alexopoulos, S.P; Poon, I.; Faux, M.; Burgess, A.; Reid, G.; McCarroll, J.; Santos, W.L.; Quinlan, K.; Turner, N.; Fazakerley, D.; Kumar, N.; Hoehn, K. Phenotypic screen for oxygen consumption rate identifies a cancer-selective naphthoquinone that induces mitochondrial oxidative stress, *Redox Biol.* **2020**, 28, 101374, https://doi.org/10.1016/j.redox.2019.101374.

82. Sibley, C.D.; Morris, E.A.; Kharel, Y.; Brown, A.M.; Bevan, D.R.; Lynch, K.R.; Santos, W.L. Discovery of a Small Side Cavity in Sphingosine Kinase 2 that Enhances Inhibitor Potency and Selectivity, *J. Med. Chem.* **2020**, *63, 1178-1198* https://pubs.acs.org/doi/10.1021/acs.jmedchem.9b01508
- Selected as front cover

83. Childress, E.S.; Salamoun, J.M.; Hargett, S.R.; Santiago-Rivera, J.; Garcia, C.J.; Alexopoulos, S.J.; Chen, S-Y; Dai, Y.; Hoehn, K.L. and Santos, W.L. Small Molecule Mitochondrial Uncouplers as Potential Treatment of Nonalcoholic Steatohepatitis, *J. Med. Chem.* **2020**, *63,* 2511-2526. https://doi.org/10.1021/acs.jmedchem.9b01440.

84. Kharel, Y.; Huang, T.; Salamon, A.; Harris, T.E.; **Santos, W.L**.; Lynch, K.R. Clearance of sphingosine 1-phosphate from blood, *Biochem. J*. **2020**, *477*, 925–935. https://doi.org/10.1042/BCJ20190730.

85. Murray, J.; Hargett, S.; Hoehn, K.L.; Santos, W.L. Anilinopyrazines as potential mitochondrial uncouplers, *Bioorg. Med. Chem. Lett.* **2020**, *30,* 127057. https://doi.org/10.1016/j.bmcl.2020.127057.

86. Liu, X.; Ming, W.; Luo, X.; Friedrich, A.; Maier, J.; Radius, U.; Santos, W.L.; Marder, T.B. Regio- and Stereoselective Synthesis of 1,1-Diborylalkenes via Brønsted Base-Catalyzed Mixed Diboration of Alkynes with BpinBdan, *Eur. J. Org. Chem*. **2020**, 1941-1946. http://dx.doi.org/10.1002/ejoc.202000128.

87. Alexopoulos, S.J.; Chen, S.; Brandon, A.E.; Salamoun, J.M.; Byrne, F.L.; Garcia, C.J.; Beretta, M.; Olzomer, E.M.; Shah, D.P.; Philp, A.M.; Hargett, S.R.; Lawrence, R.T.; Lee, B.; Sligar, J.; Carrive, P.; Tucker, S.P.; Philp, A.; Lackner, C.; Turner, N.; Cooney, G.J.; Santos, W.L.; Hoehn, K.L. Mitochondrial uncoupler BAM15 reverses diet-induced obesity and insulin resistance in mice, *Nat. Commun*. **2020**, *11*, 2397. *Santos is corresponding author

- highlighted in Science Daily, VT News, News Break, Medicalxpress

88. Salamoun, J.M.; Garcia, C.J.; Hargett, S.R.; Murray, J.; Chen, S-Y; Beretta, M.; Alexopoulos, S.J.; Shah, D.; Olzomer, E.M.; Tucker, S.P.; Hoehn, K.L. and Santos, W.L. 6-Amino-[1,2,5]oxadiazolo[3,4-*b*]pyrazin-5-ol Derivatives as Efficacious Mitochondrial Uncouplers in STAM Mouse Model of Non-alcoholic Steatohepatitis, *J. Med. Chem.* **2020**, *63*, 6203-6224. https://doi.org/10.1021/acs.jmedchem.0c00542
- Selected as front cover

89. Nekvinda, J.; Santos, W.L. Copper-Catalyzed Cross-Coupling Reactions of Organoboron Compounds in Anilkumar, G. and Saranya, S. (eds) *Copper Catalysis in Organic Synthesis*, Wiley-VCH: Weinheim, 2020, p. 23-50.

90. Fritzemeier, R.G.; Nekvinda, J.; Vogels, C.M.; Rosenblum, C.A.; Slebodnick, C.; Westcott, S.A.; Santos, W.L. Organocatalytic *trans* Phosphinoboration of Internal Alkynes, *Angew. Chem. Int. Ed*. **2020**, *59,* 14358 –14362. https://doi.org/10.1002/anie.202006096

91. Grams, R.J.; Garcia, C.J.; Szwetkowski, C.; Santos, W.L. Catalytic, Transition Metal-Free Semireduction of Propiolamide Derivatives: Scope and Mechanistic Investigation. *Angew. Chem. Int. Ed*. *Org. Lett.* **2020**, *22*, 7013–7018. doi.org/10.1021/acs.orglett.0c02567

92. Peck, C.; Nekvinda, J.; Santos, W.L. Diboration of 3-Substituted Propargylic Alcohols using a Bimetallic Catalyst System: Access to (Z)-Allyl, Vinyldiboronates. *Chem. Commun.* **2020**, *56*, 10313-10316. doi.org/10.1039/D0CC03563G

93. McDaniels, J.M.; Huckaby, A.C.; Carter, S.A.; Lingeman, S.; Francis, A.; Congdon, M.; Santos, W.L.; Phillips, M.A.; Rathod, P.K.; Guler, J. A. The Generation of Extra-chromosomal DNA Amplicons in Antimalarial Resistant *Plasmodium falciparum*, **2021**, *115,* 574–590. https://doi.org/10.1111/mmi.14624

94. Snead, R. J.; Nekvinda, J.; Santos, W.L. Copper(II)-catalyzed Protoboration of Allenes in Aqueous Media and Open Air. *New J. Chem.* **2021***, 45*, 14925-14931. *DOI: 10.1039/D0NJ02010A* .
- *Invited contribution: "Boron & Beyond – Todd B. Marder's Contributions to Chemistry"*
- Selected as front cover

95. Jos, S.; Santos, W.L. Copper-catalyzed Synthesis of α-Trifluoromethylacrylates from Trifluoroborylacrylates via Stereoretentive Radical Trifluoromethylation. *Adv. Syn. Catal.* **2021,** *363*, 425–430. *VIP communication* https://doi.org/10.1002/adsc.202000937
- Selected as front cover

96. Li, H.; Sibley, C.D.; Kharel, Y.; Brown, A.M.; Bevan, D.R.; Lynch, K.R.; Santos, W.L. Lipophilic Tail Modifications of (*R*)-prolinol-based Inhibitors of Sphingosine Kinase 1. *Bioorg. Med. Chem.* **2021**, *30,* 115941. https://doi.org/10.1016/j.bmc.2020.115941

97. Congdon, M.; Fritzemeier, R. F.; Kharel, Y.; Brown, A.M.; Bevan, D.R.; Lynch, K.R.; Santos, W.L. Probing the Substitution Pattern of Indole-Based Scaffold Reveal Potent and Selective

Sphingosine Kinase 2 Inhibitors. *Eur. J. Med. Chem.* **2021**, *30*, 115941. https://doi.org/10.1016/j.ejmech.2020.113121

98. Murray, J.H.; Santos, W.L. Bis(1,1-dimethylethyl)[2',4',6'-tris-(1-methylethyl)[1,1'-biphenyl]-2-yl]-phosphine and Dicyclohexyl[2',4',6'-tris(1-methylethyl)[1,1'-biphenyl]-2-yl]phosphine (XPhos). *e-EROS Encyclopedia of Reagents for Organic Synthesis*, **2021**, https://onlinelibrary.wiley.com/doi/10.1002/047084289X.rn00923.pub4.

99. Chen, S-Y; Beretta, M.; Alexopoulos, S.J.; Shah, D.; Olzomer, E.M.; Hargett, S.R.; Childress, E.S.; Salamoun, J.M.; Roseblade, A.; Cranfield, C.; Rawling, T.; Tucker, S.P.; Santos, W.L.; Hoehn, K.L. Potent mitochondrial uncoupler SHC517 reverses diet-induced obesity in mice. *Metabolism* **2021,** *117***,** 154724**.** https://doi.org/10.1016/j.metabol.2021.154724

100. Bose, S.;* Mao, L.;* Kuehn, L.; Radius, U.;* Nekvinda, J.; Santos, W.L.;* Westcott, S.A.;* Steel, P.G.;* Marder, T.B.* First-Row d-Block Element-Catalyzed Carbon-Boron Bond Formation and Related Processes. *Chem. Rev*. **2021**, *21*, 13238–13341. https://pubs.acs.org/doi/abs/10.1021/acs.chemrev.1c00255.
* indicates corresponding author

101. Grams, R.J.; Lawal, M.M.; Szwetkowski, C.; Foster, D.; Rosenblum, C.A.; Slebodnick, C.; Welborn, V.V.; Santos, W.L. Organocatalytic trans Semireduction of Primary and Secondary Propiolamides: Substrate Scope and Mechanistic Studies. *Adv. Syn. Cat.* **2022,** *364,* 172-178. DOI 10.1002/adsc.202101020

102. Gates, A.M.; Jos, S.; Santos, W.L. Ligand-free copper-catalyzed borylative defluorination: Access to *gem*-difluoroallyl boronic acid derivatives. *Org. Biomol. Chem*. **2022**, *20*, 366-374. DOI: 10.1039/D1OB01533H.
- This article is part of the themed collection: p-Block Lewis Acids in Organic Synthesis

103. Szwetkowski, C.; Slebodnick, C.; Santos, W.L. Regio- and stereoselective copper-catalyzed β, γ-protoboration of allenoates. Org. Biomol. Chem. **2022**, *20*, 3287-3291. DOI: 10.1039/D2OB00423B

104. Bowen, J.; Slebodnick, C.; Santos, W.L. Phosphine-catalyzed Hydroboration of Propiolonitriles: Access to (*E*)-1,2-vinylcyanotrifluoroborate derivatives. *Chem. Commun.* **2022**, *58*, 5984–5987. doi.org/10.1039/D2CC00603K

105. Fritzemeier, R.G.; Foster, D.; Peralta, A.; Payette, M.; Kharel, Y.; Lynch, K.R.; Santos, W.L. Discovery of in vivo active sphingosine-1-phosphate transporter Spns2 inhibitors. *J. Med. Chem.* **2022**, in press. doi.org/10.1021/acs.jmedchem.1c02171

106. Oyewole, O.; Dunnavant, K.; Bhattarai, S.; Kharel, Y.; Lynch, K.L.; Santos, W.L.; Reid, S.P. A Novel Sphingosine Kinase Inhibitor Suppresses Chikungunya Virus Infection. *Viruses*, **2022**, *14*, 1123. doi.org/10.3390/v14061123

107. Jos, S.; Szwetkowski, C.; Slebodnick, C.; Ricker, R.; Chan, K.L.; Chan, W.C.; Radius, U.; Lin, Z.; Marder, T.B.; Santos, W.L. Transition Metal-Free Regio- and Stereo- Selective *trans* Hydroboration of

1,3-Diynes: A Phosphine Catalyzed Access to (*E*)-1-Boryl-1,3-Enynes. *Chem. Eur. J.* **2022**, *in press.* *DOI: 10.1002/chem.202202349*

108. Pashikanti, S.; Foster, D.; Kharel, Y.; Brown, A.M.; Bevan, D.R.; Lynch, K.R.; Santos, W.L. *In Vivo* Active Sphingosine Kinase 2 Inhibitors: Probing Rigid Aliphatic Tail Derivatives Delivers Potent and Selective Analogs. *ACS Bio & Med Chem Au*, **2022**, *in press*. doi.org/10.1021/acsbiomedchemau.2c00017

109. Tanaka, s.; Zheng, S.; Kharel, Y.; Fritzemeier, R.G.; Huang, T.; Foster, D.; Poudel, N.; Goggins, E.; Yamaoka, Y.; Rudnicka, K.P.; Lipsey, J.E.; Radel, H.V.; Ryuh, S.M.; Inoue, T.; Yao, J.; Rosin, D.L.; Schwab, S.R.; Santos, W.L.; Lynch, K.R.; Okusa, M.D. S1P signaling in perivascular cells enhances inflammation and fibrosis in the kidney. *Science Trans. Med*. ***2022***, 14, eabj2681. https://doi.org/10.1126/scitranslmed.abj2681

- highlighted in a commentary: Idowu and Parikh, *Sci. Transl. Med.* **2022**, *14*, eadd2826.

110. Garcia, C.J.; Salamoun, J.M.; Hargett, S.R.; Murray, J.; Chen, S-Y; Beretta, M.; Alexopoulos, S.J.; Shah, D.; Olzomer, E.M.; Tucker, S.P.; Hoehn, K.L. and Santos, W.L. 6-(Biphenylamino)-[1,2,5]oxadiazolo[3,4-b]pyrazin-5-ol Derivatives As Mild Mitochondrial Uncouplers for Treating NASH. **2022**, *Under review.*

111. Dai, Y.; Santiago-Rivera, J.A.; Hargett, S.; Hoehn, K.L.; Santos, W.L. Synthesis of imidazo[4,5-b]pyrazine derivatives from oxadiazolo[3,4-b]pyrazines via a tandem reduction-cyclization sequence and evaluation as mitochondrial uncouplers. *Bioorg. Med. Chem. Lett.* **2022**, *73*, 128912. doi.org/10.1016/j.bmcl.2022.128912

112. Jos, S.; Tan, C.; Thilmany, P.; Saadane, A.; Evano, G.; Santos, W.L. Phosphine-Catalyzed Regio- and Stereo-selective Hydroboration of Ynamides to (*Z*)-*β*-borylenamides. *Chem. Commun.* **2022**, *under review*.

Published conference proceedings and abstracts

1. Santos WL, Hooks SB, Lynch KR, Macdonald TL. Structure-activity relationships in lysophosphatic acid. Abstracts of Papers of the American Chemical Society. Aug 2000, Washington, DC.

2. Santos WL, Heise CE, Lynch KR, Lynch KR, Macdonald TL. Structure-activity relationships of lysophosphatidic acid: Synthesis and analysis of Edg receptor agonists and antagonists. Abstracts of Papers of the American Chemical Society. Aug 2001, Chicago, IL

3. Santos WL, Macdonald TL. Synthesis of a caprolactam inverse gamma turn mimic. Abstracts of Papers of the American Chemical Society. Aug 2002, Boston, MA.

4. Santos WL, Heise CE, Jarosz R, Lynch KR, Macdonald TL. Structure-activity relationships of LPA: Design, synthesis and evaluation of subtype-selective LPA receptor agonists and antagonists. Abstracts of Papers of the American Chemical Society. Aug 2002, Boston, MA.

5. Paz YE, Santos WL, Verdine GL.Toward determination of the structural basis for HIV-1 integrase substrate recognition. Abstracts of Papers of the American Chemical Society, Mar 2005, San Diego, CA.

6. Santos WL, Paz YE, Verdine GL. Toward determination of the structural basis for HIV-1 integrase substrate recognition. Abstracts of Papers of the American Chemical Society. Aug 2005, Washington, D.C.

7. Santos, WL and Verdine, GL. RNA interacting polynucleotides: a novel approach to targeting RNA. Abstracts of Papers of the American Chemical Society. Aug 2005, Washington, DC.

8. Santos, WL. Targeting RNA with small molecules. Book of Abstracts of the 10th Eurasia Conference on Chemical Sciences. Jan 2008, Manila, Philippines.

9. Santos, WL. New RNA Selective Ligands. Abstracts of Papers, 236th ACS National Meeting, Philadelphia, PA, USA, August 2008.

10. Santos, WL; Bryson, DI; Pagano, A. Targeting HIV-1 TAR with Branched Peptides. Abstracts of Papers, 237th ACS National Meeting, Salt Lake City, UT, USA, March 2009.

11. Gao, M; Thorpe, SB; Santos, WL. sp^2-sp^3 Hybridized mixed diboron reagent: Synthesis, characterization, and copper-catalyzed beta-boration of alpha, beta-unsaturated carbonyl compounds. Abstracts of Papers, 238th ACS National Meeting, Washington, DC, United States, August 16-20, 2009.

12. Knott, KM; Fishovitz, JE; Lee, I; Santos, WL. N-Terminal peptidic boronic acid as a selective inhibitor of ClpXP. Abstracts of Papers, 238th ACS National Meeting, Washington, DC, United States, August 16-20, 2009.

13. Bryson, DI; Zhang, W; Ray, WK; Helm, RF; Santos, WL. Branched peptides as ligands for HIV-1 TAR RNA. Abstracts of Papers, 238th ACS National Meeting, Washington, DC, United States, August 16-20, 2009.

14. Crumpton, JB; Bissel, P; Ray, W.; Helm, RF; Santos, WL. Controlling gene expression using clickable oligonucleic acids. Abstracts of Papers, 238th ACS National Meeting, Washington, DC, United States, August 16-20, 2009.

15. Santos, WL; Gao, M; Thorpe, SB. sp^2-sp^3 Mixed diboron reagent: copper-catalyzed beta boration of alpha, beta-unsaturated carbonyl compounds. Abstracts of Papers, 238th ACS National Meeting, Washington, DC, United States, August 16-20, 2009.

16. Santos, WL; Gao, M; Thorpe, SB. Preactivated unsymmetrical diboron: Catalytic regioselective boration of α,β-unsaturated conjugated compounds. Abstracts of Papers, 240th ACS National Meeting, Boston, MA, United States, August 22-26, 2010.

17. Raje, M.; Yugesh, K.; Lynch, K.R.; Santos, W.L. Structure-activity relationship studies of sphingosine kinase inhibitors. Abstracts of Papers, 240th ACS National Meeting, Boston, MA, United States, August 22-26, 2010.

18. Santos, WL; Thorpe, SB; Gao, M. Novel diboron reagent: Regioselective β-boration of activated carbon-carbon bonds. Abstracts of Papers, 241st ACS National Meeting & Exposition, Anaheim, CA, United States, March 27-31, 2011.

19. Thorpe, SB; Guo, X; Santos, WL. Regio- and stereoselective copper-catalyzed β-borylation of allenoates by a preactivated diboron. Abstracts of Papers, 241st ACS National Meeting & Exposition, Anaheim, CA, United States, March 27-31, 2011.

20. Santos, WL.; Bryson, D.; Zhang, W.; Crumpton, JB. Targeting RNA structures with branched peptide libraries. Abstracts of Papers, 241st ACS National Meeting & Exposition, Anaheim, CA, United States, March 27-31, 2011.

21. Crumpton, J.B., Zhang, W., Santos, W.L. Facile analysis and sequencing of linear and branched peptide boronic acids by MALDI mass spectrometry, Abstracts of Papers, 242nd ACS National Meeting & Exposition, Denver, CO, United States, August 28-September 1, 2011.

22. Santos, W.L.; Bryson, D., Zhang, W., Crumpton, J.B., Rekosh, D.R. Inhibiting RNA-Protein Interactions: Cell Permeable Branched Peptide Boronic Acids Inhibit Tat-TAR and Rev-RRE Interactions, Keystone Symposia: Frontiers in HIV Pathogenesis, Therapy and Eradiation, March 26-31, 2012.

23. Santos, W.L. Activation of diboron reagents: Catalytic copper-catalyzed borylation of electrophilic alkenes, Abstracts of Papers, 244th ACS National Meeting & Exposition, Philadelphia, PA, United States, August 19-23, 2012.

24. Santos, W.L. Discovery and in vivo activity of sphingosine kinase 2 selective inhibitors. Abstracts of Papers, 244th ACS National Meeting & Exposition, Philadelphia, PA, United States, August 19-23, 2012.

25. Santos, W.L. Lewis base assisted copper catalyzed borylation and silylation of electrophilic alkenes. 14th Florida Heterocyclic and Synthetic IUPAC Sponsored Conference, University of Florida, Gainesville, FL, March 3-6, 2013.

26. Calderone, J.A.; Santos, W.L. Copper(II)-catalyzed silylation of internal alkynes in water: Highly diastereoselective access to β-silyl-α,β-unsaturated carbonyl compounds. Abstracts of Papers, 246th ACS National Meeting & Exposition, Indianapolis, IN, United States, September 8-12, 2013.

27. Patwardhan, N.N.; Raje, M.R.; Morris, E.A.; Knott, K.; Congdon, M.; Gao, M.; Kharel, Y.; Lynch, K.; Santos, W.L. Structure-activity relationship studies of novel guanidine based inhibitors of Sphingosine kinase-2. Abstracts of Papers, 246th ACS National Meeting & Exposition, Indianapolis, IN, United States, September 8-12, 2013.

28. Santos, W.L.; Zhang, W.; Wynn, J. Drugging RNA: Targeting structured HIV-1 RNA with branched peptide boronic acids. Abstracts, 65th Southeast Regional Meeting of the American Chemical Society, Atlanta, GA, United States, November 13-16 (2013), SERM-348.

29. Santos, W.L.; Calderone, J.; Thorpe, S. B. Copper-catalyzed borylation/silylation of α,β-unsaturated carbonyls. Abstracts of Papers, 247th ACS National Meeting & Exposition, Dallas, TX, United States, March 16-20, 2014 (2014), ORGN-370.

30. Guo, X; Nelson, A; Santos, WL. Chemo- and regioselective diboration of allenes with differentially protected diboron. Abstracts of Papers, 247th ACS National Meeting & Exposition, Dallas, TX, United States, March 16-20, 2014 (2014), ORGN-579.

31. Wynn, J.; Zhang, W.; Santos, W.L. "Boron-Acridine Chimeras: Functionalizing Branched Peptides Toward Targeting Folder RNA Structures", BORAM XIV, Rutgers University, Newark, NJ, June 17, 2014.

32. Santos, W.L. "Pt- and Cu-catalyzed Mono- and Diboration of C=C bonds", BORAM XIV, Rutgers University, Newark, NJ, June 18, 2014.

33. Nelson, A.; Guo, X.; Santos, W.L. "Chemo- and Regioselective Diboration of Allenes with Differentially Protected Diboron", BORAM XIV, Rutgers University, Newark, NJ, June 18, 2014.

34. Peck, C.L.; Calderone, J.A.; Santos, W.L. "Cu(II)-Catalyzed Regio- and Stereoselective Monoboration of Acetylenic Esters", BORAM XIV, Rutgers University, Newark, NJ, June 17, 2014.

35. Patwardhan, N.N.; Santos, W.L. "Design, synthesis, and biological activity of guanidine based inhibitors of sphingosine kinase 2 (SphK2)", Abstracts of Papers, 248th ACS National Meeting & Exposition, San Francisco, CA, United States, Aug. 10-14, 2014 (2014), AEI-45.

36. Santos, W.L. "Metal-catalyzed borylation electrophilic alkenes and allenes", IME Boron XV, Prague, Czech Republic, August 28, 2014.

37. Wynn, Jessica E.; Peralta, Ashley N.; Dai, Yumin; Santos, Webster L. "Rev"olutionary library containing unnatural amino acids: Functionalizing branched peptides toward targeting folded RNA structures. 250th ACS National Meeting & Exposition, Boston, MA, United States, August 16-20, 2015 (2015), BIOL-192.

38. Congdon, Molly; Kharel, Yugesh; Lynch, Kevin R.; Santos, Webster L. Structure-activity-relationship studies investigating the substitution pattern around the indole ring of sphingosine kinase 2 selective inhibitors. 250th ACS National Meeting & Exposition, Boston, MA, United States, August 16-20, 2015 (2015), MEDI-527.

39. Childress, Elizabeth S.; Kharel, Yugesh; Brown, Anne M.; Bevan, D. R.; Lynch, Kevin R.; Santos, Webster L. Structure-activity relationship studies of guanidine-based aminothiazole inhibitors of sphingosine kinase. 250th ACS National Meeting & Exposition, Boston, MA, United States, August 16-20, 2015 (2015), MEDI-528.

40. Peck, Cheryl L.; Calderone, Joseph A.; Santos, Webster L. Cu(II)-Catalyzed Regio-, Stereo-, and Chemoselective β-Borylation of Acetylenic Esters in Water. 250th ACS National Meeting & Exposition, Boston, MA, United States, August 16-20, 2015 (2015), ORGN-382.

41. Childress, Elizabeth S.; Kharel, Yugesh; Brown, Anne; Bevan, David R.; Lynch, Kevin R.; Santos, Webster L. Structure-activity relationship studies of guanidine-based aminothiazole inhibitors of sphingosine kinase. 251st ACS National Meeting & Exposition, San Diego, CA, United States, March 13-17, 2016 (2016), MEDI-182.

42. Dai, Yumin; Peralta, Ashley; Wynn, Jessica; Sherpa, Chringma; Le Grice, Stuart; Santos, Webster. Targeting RRE IIB RNA with functionalizing branched peptides: Unnatural amino acid series. 252nd ACS National Meeting & Exposition, Philadelphia, PA, United States, August 21-25, 2016 (2016), BIOL-260.

43. Congdon, Molly; Kharel, Yugesh; Lynch, Kevin; Santos, Webster. Structure-activity relationship studies of the lipophilic tail region of indole derived sphingosine kinase 2 inhibitors. 252nd ACS National Meeting & Exposition, Philadelphia, PA, United States, August 21-25, 2016 (2016), MEDI-7.

44. Santos, Webster L.; Dai, Yumin; Wynn, Jessica; Peralta, Ashley; Rekosh, David; Hammarskjold, Marie-Louise. Targeting RNA with branched peptide boronic acids: Unnatural amino acids, molecular recognition, and in vitro activity against HIV-1 RRE RNA. 253rd ACS National Meeting & Exposition, San Francisco, CA, United States, April 2-6, 2017 (2017), BIOL-336.

45. Santos, Webster L.; Snead, Russell; Astha, Fnu; Dai, Yumin. Transition metal-free activation and intramolecular trans diboration of propargylamides using unsymmetrical diboron. 253rd ACS National Meeting & Exposition, San Francisco, CA, United States, April 2-6, 2017 (2017), ORGN-438.

46. Peralta, Ashley; Dai, Yumin; Wynn, Jessica; Chringma, Sherpa; Le Grice, Stuart F.; Santos, Webster L. Targeting folded HIV-1 RRE RNA with unnatural branched peptides: Boosting affinity and selectivity. Abstracts of Papers, 254th ACS National Meeting & Exposition, Washington, DC, USA, August 20-24, 2017 (2017), BIOL-48.

47. Li, Hao; Kharel, Yugesh; Lynch, Kevin; Santos, Webster L. Development of prolinol based derivatives targeting sphingosine kinase-1. Abstracts of Papers, 254th ACS National Meeting & Exposition, Washington, DC, USA, August 20-24, 2017 (2017), MEDI-200.

48. Santos, Webster L. Stereoselective borylation reactions. 69th Southeastern Regional Meeting of the American Chemical Society, Charlotte, NC, United States, November 7-11 (2017), SERMACS-138.

49. Santos, Webster L. Targeting HIV-1 Rev response element with branched peptides. Abstracts of Papers, 255th ACS National Meeting & Exposition, New Orleans, LA, USA, March 18-22, 2018 (2018), ORGN 365.

50. Santos, Webster L. In vivo chemical probes of sphingosine kinase function. Abstracts of Papers, 256th ACS National Meeting & Exposition, Boston, MA, USA, August 1-23, 2018 (2018), BIOL 275.

51. Sibley, Christopher; Kharel, Yugesh; Brown, Anne; Bevan, David R.; Lynch, Kevin R.; Santos, Webster L. Aryl ring modifications of sphingosine kinase 2 selective inhibitors. 71st Southeastern

Regional Meeting of the American Chemical Society, Savannah, GA, United States, October 20-23 (2019), SERMACS-783.

52. Afrin, Farjana; Obuch, Katherine; Kharel, Yugesh; Santos, Webster L.; Lynch, Kevin R.; Pashikanti, Srinath. Design, synthesis, and structure-activity relationship studies of phthalimide-based sphingosine kinase inhibitors. 257th ACS National Meeting & Exposition, Orlando, FL, United States, Mar. 31-Apr. 4, 2019 (2019), MEDI-0354.

53. Garcia, Christopher J.; Salamoun, Joseph; Santos, Webster. Mitochondrial uncouplers as disease therapeutics. 71st Southeastern Regional Meeting of the American Chemical Society, Savannah, GA, United States, October 20-23 (2019), SERMACS-61.

54. Grams, Robert J.; Allen, Mitchell; Pennington, Edward; Bandara, Aloka B.; Thomson, Alex; Perry, Justin; Green, Tom; Ryan, Terence; Gates, Ashley; Santos, Webster; Brown, David. Novel peptide protects mitochondrial structure-function: Implications for cationic, lipophilic peptides as endogenous assembly factor mimetics. 71st Southeastern Regional Meeting of the American Chemical Society, Savannah, GA, United States, October 20-23 (2019), SERMACS-36.

55. Fritzemeier, Russell; Grams, Robert J.; Santos, Webster L. Broensted base mediated trans hydroboration of alkynamides. 71st Southeastern Regional Meeting of the American Chemical Society, Savannah, GA, United States, October 20-23 (2019), SERMACS-1350.

56. Grams, Robert Justin; Szwetkowski, Connor; Foster, Daniel; Lawal, Monsurat; Rosenblum, Carol Ann; Welborn, Valerie; Santos, Webster L. Organocatalytic semireduction of primary and secondary propiolamides: Substrate scope and mechanistic studies. 261st ACS National Meeting, April 5-16, 2021.

57. Szwetkowski, Connor; Santos, Webster Regio- and stereoselective copper catalyzed β-borylation of allenoates. 262nd ACS National Meeting, Aug 22-26, 2021.

58. Salamoun, Joseph; Garcia, Christopher; Hargett, Stefan; Murray, Jacob; Chen, Sing-Young; Beretta, Martina; Alexopoulos, Stephanie; Shah; Divya; Olzomer, Ellen; Hoehn, Kyle; Santos, Webster. 6-Amino[1,2,5]oxadiazolo[3,4-b]pyrazin-5-ol derivatives as novel mitochondrial uncouplers efficacious in mouse models of nonalcoholic steatohepatitis. 262nd ACS National Meeting, Aug 22-26, 2021.

59. Afrin, Farjana; Mateen, Sameena; Kharel, Yugesh; Santos, Webster L.; Lynch, Kevin R.; Pashikanti, Srinath. Strategy towards the design, synthesis & structure: Activity relationship of γ-lactam linker-based sphingosine kinase inhibitors. 262nd ACS National Meeting, Aug 22-26, 2021.

60. Jos, Swetha; Santos, Webster L. Copper-catalyzed synthesis of α–trifluoromethylacrylates from trifluoroborylacrylates via stereoretentive radical trifluoromethylation. 262nd ACS National Meeting, Aug 22-26, 2021.

61. Bowen, Johnathan; Santos, Webster L. Transition metal free *trans* hydroboration of propiolonitriles. 262nd ACS National Meeting, Aug 22-26, 2021.

62. Foster, Daniel; Lynch, Kevin, R.; Fritzemeier, Russell; Kharel, Yugesh; Santos, Webster, L. Targeting the Sphingosine-1-phosphate Transporter SPNS2 for the Treatment of Multiple Sclerosis. Southeastern Regional Meeting of the American Chemical Society (SERMACS) 2021, November 10-13, 2021.

63. Foster, Daniel; Lynch, Kevin, R.; Fritzemeier, Russell; Kharel, Yugesh; Santos, Webster, L. Potent inhibitors of the sphingosine-1-phosphate transporter spns2 as immunosuppressive agents. 263rd ACS National Meeting, March 20-24, 2022.

64. Szwetkoswski, C.; Santos, W.L. Organocatalytic cis phosphinoboration of 1,3-diynes. 263rd ACS National Meeting, March 20-24, 2022.

65. Santos, W.L. Small molecule mitochondrial uncouplers as anti-obesity agents. 263rd ACS National Meeting, March 20-24, 2022.

66. Santos, W.L. *trans* Hydroboration of 3-substituted-propiolonitriles and allenoates. 263rd ACS National Meeting, March 20-24, 2022.

- **Active Research Support**

Takeda Pharmaceuticals Santos (PI) $129,250 02/25/2022-02/24/2023
NMR Reaction Monitoring
The goal of this project is to develop NMR methods to understand reaction mechanisms and catalysis.

R21NS124168 Santos, Gaultier (MPI) $440,030 08/01/2021 - 01/31/2023
NIH/NINDS
Discovering new therapies to promote myelin repair
The goal of this project is to develop compounds that promote myelin repair as therapeutics for MS.

1R01DK128612-01 Santos, Hoehn MPI $2,200,000 04/01/2021 - 04/30/2025
NIH/NIDDK
Therapeutic mitochondrial uncouplers
The goal of this project is to develop mitochondrial uncouplers for the potential treatment of non-alcoholic steatohepatitis (NASH).

R01AI144026 Santos, Lynch MPI $2,800,000 01/01/2019-12/31/2023
NIH/NIAID
Controlling the flux of sphingosine-1-phosphate in vivo
The goal of this project is to develop small molecule inhibitors of sphingosine-1-phosphate transporters and validate them as therapeutics in mouse models of multiple sclerosis. This work is performed in collaboration with Profs. Kevin Lynch (University of Virginia, Pharmacology, Charlottesville, VA) & Alban Gaultier (University of Virginia, Neuroscience, Charlottesville, VA).

DMR 1905527 Robinson PI, Santos co-PI $390,000 09/01/2019-08/31/2022
NSF
Lithography on a nanosphere--an optical approach to arbitrarily patterned patchy particles

The goal of this project is to develop a new paradigm for patchy particle synthesis and perform self-assembly with patchy particles.

1R01HL141855-01 Gourdie, Poelzing MPI 07/01/2018-04/30/2022
NIH/NHLBI ($15k/year is Santos portion)
The role of the sodium channel beta subunit in cardiac conduction
This project will test a new idea for how "ephaptic coupling" electrically triggers the heartbeat and develop new drugs to treat deadly arrhythmias based on this idea.
Role: Co-investigator

- **Pending**

R01HL168537 Santos, Lynch (MPI) $3,895,707
NIH/NHLBI
Controlling red blood cell sphingosine 1-phosphate transport
The goal of this project is to develop inhibitors of S1P transporter mfsd2b from red blood cells and determine their clinical application in wound healing and ischemic insults.

R41AI157678 Santos (PI) $299,067
NIH/NIAID
S1P modulation and multiple sclerosis
This project will validate S1P transporter (spns2) inhibitors as therapeutics for multiple sclerosis.

R01DK128824 Santos, Lynch (MPI) $2,733,271
Sphingosine kinase 2 inhibitors and fibrosis
This project will determine whether sphingosine kinase 2 inhibitors will lead to the development of drugs against liver and kidney fibrosis

- **<u>Completed Research Support</u>**

R01GM121075-04S1 Santos, Lynch MPI $90,940 09/01/2016-08/31/2021
NIH/NIGMS
Controlling sphingosine 1-phosphate synthesis and trafficking
This grant was for acquisition of a helium recovery system for Virginia Tech's NMR facility.

5R01GM121075 Santos, Lynch MPI $2,100,000 09/01/2016-08/31/2021
NIH/NIGMS
Controlling sphingosine 1-phosphate synthesis and trafficking
The goal of this project is to develop inhibitors of sphingosine kinases and S1P transporter SPNS2. Molecular docking as well as X-ray crystal structures of inhibitors bound to sphingosine kinases will be determined. This work is performed in collaboration with Prof. Kevin Lynch (University of Virginia, Pharmacology, Charlottesville, VA).

Continuum Biosciences, Inc. Santos, PI $1,066,312 05/01/2018-08/31/2020
Mitochondrial Uncoupler Drug Discovery
The goal of this project is to develop small molecule mitochondrial uncouplers into preclinical drug candidates for the treatment of diseases associated with mitochondrial dysfunction.

LINK+LAUNCH+LICENSE Santos (PI) $47,000 08/15/2020-08/14/2021
S1P Modulation and Multiple Sclerosis

The goal of this project is to determine whether spns2 inhibition is a therapeutic for multiple sclerosis.

4-VA Santos (PI), Gaultier $25,000 (Santos portion) 03/01/2020-02/27/2021
A novel mechanism of action for treating multiple sclerosis
The goal of this project is to develop novel molecules that will promote the re-myelination for the potential treatment of multiple sclerosis.

Virginia Catalyst Santos, PI $400,000 07/01/2018-12/31/2019
Safe Mitochondrial Uncouplers for the Treatment of Human Disease
The goal of the proposed research is to develop BAM15 derivatives into drug-like leads for testing in non-alcoholic steatohepatitis (NASH) mouse models. This work is performed in collaboration with Prof. Kyle Hoehn (University of Virginia, Pharmacology, Charlottesville, VA).

MPI: Santos, Lynch, Gaultier $75,000 01/01/2017-12/31/2017
UVA-VTC neuroscience seed fund
Sphingosine Kinase Inhibitors and Multiple Sclerosis.
The goal of this project is to determine the efficacy of sphingosine kinase inhibitors in mouse model of multiple sclerosis.

Alzheimer's & Related Diseases Research Award Fund (ARDRAF)
ARDRAF Santos, PI $45,000 07/01/2018-06/31/2019
Safe Mitochondrial Uncouplers for the treatment of Parkinson's Disease
The goal of this project is to determine whether mitochondrial uncouplers decrease reactive oxygen species in neurons and protect neurons against inflammatory insults.

1R01GM093834 Santos (PI) $1,580,000 09/13/2010-01/31/2017
NIGMS
RNA as a therapeutic target
The major goals of this project are to develop cell permeable ligands for target RNA structures associated with HIV.

R01 GM104366-01A1 (Santos PI) $1,150,955 10/01/2013-09/30/2017
NIH/NIGMS
In Vivo Probes of Sphingosine Kinase Function
The goal of the proposed research is to improve, through iterative chemical synthesis and pharmacological testing, lead lipid kinase (e.g. sphingosine kinase-1) inhibitors so as to make them drug-like, i.e. suitable for use in vivo. This project is a collaborative effort with the laboratory of Dr. Kevin R. Lynch as MPI (University of Virginia, Pharmacology, Charlottesville, VA).

CHE-1414458 Santos (PI) $950,000 01/15/2014-12/31/2016
NSF/IUPAC
Earth Abundant Metal Catalyzed Borylations
This international collaboration with Todd Marder (Universitat Wurzburg, Germany, funded by DFG) and Yao Fu (University of Science and Technology, China, funded by NSFC) aims to develop efficient, environmentally friendly, and simple copper-catalyzed transformations for the formation and subsequent reactions of aryl, heteroaryl, vinyl, allyl and alkyl boronates.

Alzheimer's & Related Diseases Research Award Fund (ARDRAF)

16-6 Santos (PI), Valdez $45,000 07/1/2015-6/30/2016
Controlling neuronal sphingosine-1-phosphate as Alzheimer's disease therapy
The goal of this project is to determine whether varying levels of S1P have therapeutic benefit towards AD.

VBHRC Santos (PI) $400,000 04/01/2014-3/31/2015
Virginia Biosciences Health Research Corporation
Lead Optimization of a SphK2 Inhibitor for the Treatment of CKD
The goal of this project is to make drug-like sphingosine kinase 2 inhibitors and subject them to animal models of chronic kidney disease. This work is performed in collaboration between Kevin Lynch (UVA) and Brandon Thorpe (SphynKx Therapeutics).

DMR 1006753 Santos (co-PI) $500,001 08/16/2010-08/15/2013
National Science Foundation
A nonlinear optical approach to patchy particles
The major goals of this project are to develop methods of assembling complex nanostructures using nanoparticles made of silver and gold.

PRF 50806-ND3 Santos (PI) $100,000 01/01/2011-08/13/2013
ACS Petroleum Research Fund
Development of unsymmetrical diboron compounds for regioselective diboration and chemoselective cross-coupling reactions
The major goals of this project are to develop diboron reagents for the mild boration of activated carbon-carbon bonds.
RAP Grant VT-Carillion Institute Santos (co-PI) $25,000 06/01/2010-05/31/2011
Inhibition of miR21 RNA with peptides

ICTAS Santos (PI) $100,000 07/2009-06/2011
Institute for Critical Technology and Applied Science
Inhibiting HIV-1 TAR RNA function using nanoparticle-delivered branched peptides
This study aims to discover and develop strategies for selectively inhibiting highly structured RNA.

J-892 Santos (PI) $40,000 01/01/2008-12/31/2011
Jeffress Memorial Trust
Synthesis of Borinic and N-terminal Boronic Acids as Inhibitors of the Malarial Protease Falcilysin
This study will develop inhibitors for malarial protease, Falcilysin.

"CHE-0722638 Deck (PI) 09/01/2007-08/31/2010
National Science Foundation
"Acquisition of an LC-ESI-MS for Open Access Use in Support of Chemical Synthesis and Education at Virginia Tech"
Role: Co-PI

DGE-0333378 Duncan (PI) ($73,500) 6/01/2008-2/27/2010
NSF
"Macromolecular Interfaces with Life Sciences"

This program is to prepare doctoral-level candidates in chemistry, engineering, and life sciences to work in multidisciplinary research. The program provided salary support, tuition and benefits for David Bryson for two years.

- **Theses Supervised**
    1. "Diastereoselective alpha-Alkylation of Chiral beta-Borylated Esters" Michael T. Perfetti, December 9, 2009 (Master's Thesis).

    2. "Synthesis and Application of Boronic Acid Derivatives" Jing Sun, May 5, 2010 (Master's Thesis).

    3. "Borylations and Silylations of Alkenyl and Alkynyl Carbonyl Compounds Employing a Mild and Environmentally Friendly Cu(II) Catalyst" Joseph A. Calderone, III, April 4, 2014 (Master's Thesis).

    4. "Structure-activity relationship studies and biological evaluation of selective sphingosine kinase inhibitors" Emily A. Morris, April 20, 2015 (Master's Thesis).

    5. "Facile route to air and moisture stable β-difluoroboryl acrylamides" Eric J. Medici, September 18, 2019 (Master's Thesis).

- **Dissertations Supervised**
    1. "Targeting RNA Structures with Multivalent Branched Peptide Libraries" David I. Bryson, Jr. March 19, 2012. (Ph.D. Thesis)

    2. "Activation of Diboron Reagents: The Development of Mild Conditions for the Synthesis of Unique Organoboron Compounds" S. Brandon Thorpe, March 23, 2012. (Ph.D. Thesis)

    3. Design, synthesis and biological evaluation of selective sphingosine kinase inhibitors", Mithun R. Raje, April 13, 2012. (Ph.D. Thesis)

    4. "Click Chemistry on DNA and Targeting RNA structure with Peptide Boronic Acids" Jason B. Crumpton, April 20, 2012. (Ph.D. Thesis)

    5. "Targeting HIV-1 RNAs with Medium Sized Branched Peptides Featuring Boron and Acridine. Branched Peptide Library Design, Synthesis, High-Throughput Screening and Validation", Wenyu Zhang, March 31, 2014. (Ph.D. Thesis)

    6. "Development and Applications of Unsymmetrical Diboron Compounds", Xi Guo, November 6, 2014. (Ph.D. Thesis)

    7. "Functionalizing Branched Peptides with Unnatural Amino Acids Toward Targeting HIV-1 RRE RNA and Microbials", Jessica Wynn, July 14, 2016. (Ph.D. Thesis)

    8. "Structure-Activity Relationship Studies and Molecular Modeling of Sphingosine Kinase 2 Inhibitors", Molly D. Congdon, July 18, 2016. (Ph.D. Thesis)

9. “Metal-Catalyzed Formation and Transformations of Carbon–Boron Bonds”, Amanda K. Nelson, October 27, 2016. (Ph.D. Thesis)

10. “Structure–Activity Relationship Studies of Sphingosine Kinase Inhibitors and Mitochondrial Uncouplers”, Elizabeth S. Childress, June 22, 2017. (Ph.D. Thesis)

11. “Development of Transition Metal-Catalyzed Borylation Protocols using Symmetrical and Unsymmetrical Diboron Reagents”, Cheryl L. Peck, September 7, 2017. (Ph.D. Thesis)

12. “Development of Novel, Regioselective Borylation Protocols”, Russell Snead, July 27, 2018. (Ph.D. Thesis)

13. “Design, Synthesis, and Structure-Activity Relationship Investigation of Selective Sphingosine Kinase Inhibitors”, Hao Li, December 3, 2018. (Ph.D. Thesis)

14. “Development of Methods for Boron Reagents”, Ashley Gates, February 14, 2020. (Ph.D. Thesis)

15. “Trans Addition of B-X Reagents Across Polarized Triple Bonds and Development of Sphingosine-1-Phosphate Transport Inhibitors”, Russell Fritzemeier, March 17, 2020. (Ph.D. Thesis)

16. “Branched Peptides Targeting HIV-1 RRE RNA and Structure-Activity Relationship Studies of a Spinster Homolog 2 Transport Inhibitor”, Ashley Peralta, April 8, 2020. (Ph.D. Thesis)

17. “Design and Synthesis of Orally Bioavailable Sphingosine Kinase 2 Selective Inhibitors”, Christopher Sibley, June 15, 2020. (Ph.D. Thesis)

18. “Complex Heterocycles as Mitochondrial Uncouplers”, Jacob Hadley Murray, March 25, 2021. (Ph.D. Thesis)

19. “Mitochondrial Uncouplers: Development as Therapeutics for Metabolic Diseases”, Christopher James Garcia, April 15, 2021. (Ph.D. Thesis)

20. “Boron-Mediated Semireduction of Alkynoic Acid Derivatives”, Robert Justin Grams, April 13, 2021. (Ph.D. Thesis)

21. “Structure-Activity Relationship Studies of Imidazo[4,5-b]pyrazin-5,6-diamines as Mitochondrial Uncouplers and their Potential in the Treatment of Obesity”, Jose Antonio Santiago-Rivera, October 19, 2021. (Ph.D. Thesis)

22. “Selective Borylations of Carbon-carbon pi-Bonds”, Connor D. Szwetkowski, April 19, 2022. (Ph.D. Thesis)

23. “Development of Potent Inhibitors of the Sphingosine-1-Phosphate Transporter Spns2 for the Treatment of Multiple Sclerosis”, Daniel J. Foster, May 4, 2022. (Ph.D. Thesis)

Postdoctoral Fellows

Student Name	University Affiliation	Duration	Current Position
1. **Dr. Ming Gao**	Chinese Academy of Science, Peking, PRC	2008-09, 2011-2012	Senior Research Chemist, Merieux NutriSciences
2. **Dr. Philippe Bissel**	University Louis Pasteur, Strasbourg, France	2007-08	Instructor, Hollins College
3. **Dr. Neeraj Patwardhan**	Virginia Tech	05/2012-06/2014	Postdoc at Duke University
4. **Dr. Srinath Pashikanti**	University of Kansas	04/01/2014-7/01/2016	Assistant Prof at Idaho State University
5. **Dr. Astha Verma**	Virginia Tech	08/01/2014-06/01/2016	Scientist at KBI Pharma
6. **Dr. Yumin Dai**	Virginia Tech	02/1/2015-02/2019	Takeda Pharmaceuticals
7. **Dr. Daniel Hoagland**	St. Jude's Children's Hospital	07/2016-08/31/2020	Scientist at Alcami Corporation
8. **Dr. Joseph Salamoun**	University of Pittsburg	09/01/2017-10/2019	Techulon
9. **Jan Nekvinda**	Charles University, Prague	10/01/2018-08/31/2020	Czech Academy of Sciences

- **Current Graduate Students**

Student Name	University Affiliation	Year Entered	Graduation
1. **Daniel Foster**	Purdue University	2017	Spring 2022
2. **Johnathan Bowen**	Wake Forest University	2017	Spring 2022
3. **Connor Szwetkowski**	Rider University	2017	Spring 2022
4. **Ariel Burgio**	University of Buffalo	2018	Spring 2023
5. **Swetha Jos**	Indian Institute of Science Education and Research, Pune	2018	Spring 2023
6. **Christopher Shrader**	Virginia Commonwealth University	2019	Spring 2024
7. **Michael Payette**	Old Dominion University	2019	Spring 2024
8. **Kyle Dunnavant**	Northern Ohio University	2019	Spring 2024
9. **Mary Olson**	Old Dominion University	2020	Spring 2025
10. **Joseph Quinlan**	Montclair State University	2020	Spring 2025
11. **Emily Krinos**	Westminster College	2021	Spring 2026
12. **Nicklas Buchbinder**	University of Louisville	2021	Spring 2026

- **Previous Graduate Students**

Student Name	Year Graduated	Degree	Current Position
1. **Daniel Foster**	2022	Ph.D.	Principal Scientist, Johnson Matthey
2. **Connor Szwetkowski**	2022	Ph.D.	Med Chemist, Fischer Scientific
3. **Jose Santiago-Rivera**	2021	Ph.D.	Principal Scientist, Boehringer Ingelheim
4. **Robert Justin Grams**	2021	Ph.D.	Postdoc, UVA Ken Hsu
5. **Jacob Murray**	2021	Ph.D.	Postdoc, Vanderbilt U with Craig Lindsley

6.	**Christopher Garcia**	2021	Ph.D.	Law School, U Colorado (Denver)
7.	**Christopher Sibley**	2020	Ph.D.	Postdoc, NIH w/ Jay Schneekloth
8.	**Ashley Peralta**	2020	Ph.D.	Postdoc, Los Alamos Nat'l Labs
9.	**Russell Fritzemeier**	2020	Ph.D.	Postdoc, Emory University
10.	**Ashley Gates**	2020	Ph.D.	Law Firm
11.	**Eric Medici**	2019	MS	R&D Chemist, Chattem Chemical
12.	**Hao Li**	2018	Ph.D.	Takeda Pharmaceuticals
13.	**Russell Snead**	2018	Ph.D.	Analyst, Geico
14.	**Cheryl Peck**	2017	Ph.D.	Process Scientist II at AMPAC Fine Chemicals
15.	**Elizabeth Childress**	2017	Ph.D.	Drug Discovery Scientist I with Craig Lindsley, Vanderbilt U
16.	**Molly Congdon**	2016	Ph.D.	NIH Postdoc with Jeff Gildersleeve
17.	**Amanda Nelson**	2016	Ph.D.	Lecturer at Stanford Chemistry
18.	**Jessica Wynn**	2016	Ph.D.	Principal Scientist at Merck Inc.
19.	**Kenneth Knott**	2015	MS	Analytical Services, Virginia Tech
20.	**Emily Morris**	2015	MS	Teacher at Manassas High School
21.	**Xi Guo**	2014	Ph.D.	Rutgers University Statistics
22.	**Joseph Calderone**	2014	MS	R&D Engineer at Afton Chemicals
23.	**Wenyu Zhang**	2014	Ph.D.	Postdoc at NIH with Kuan Wang
24.	**Mithun Raje**	2012	Ph.D.	Senior research associate at Rosalind Franklin University
25.	**David Bryson**	2012	Ph.D.	Scientist at Beam Therapeutics
26.	**Jason Crumpton**	2012	Ph.D.	Assistant Professor at Lynchburg College
27.	**Brandon Thorpe**	2012	Ph.D.	Project Manager at Center for Open Science
28.	**Jing Sun**	2010	MS	Scientist at BASF
29.	**Michael Perfetti**	2009	MS	Associate Director, Brand Development

- **Visiting Scholars**

Student Name	Year	University Affiliation	Country
1. **Analyn Carreon**	2013	Ateneo de Manila	Philippines
2. **Antonius Eichhorn**	2015	Wurtzburg University	Germany

- **Current Undergraduate Students**

	Student Name	Degree	Expected Graduation
1.	**Long Nguyen**	Chemistry	2025
2.	**Sarah Seay**	Chemistry	2023
3.	**Christine Tan**	Chemistry	2023
4.	**Taylor Yates**	Chemistry	2023
5.	**Ethan Duerre**	Medicinal Chemistry	2024

- **Previous Undergraduate Students**

	Student Name	Degree	Year	Current Position
6.	**Analize Pham**	Neuroscience	2021	unknown
7.	**Carol Ann Rosenblum**	Chemistry	2021	Grad Student, U Pittsburg

8. Laura Wonilowicz	Biochemistry	2019	Grad Student UCLA
9. Greg Traverse	Chemistry	2019	Grad Student, U Penn
10. Jonathan Roof	Chemistry	2019	unknown
11. Brett Rastatter	Integrated Science Curriculum	2017	unknown
12. Zach Powers	Chemistry	2017	Unknown
13. Sean M. Rafferty	Chemistry	2015	Grad Student Ohio State
14. Christopher Sibley	Biochemistry	2015	Grad Student VT
15. Michael Lazear	Biochemistry	2015	Grad Student Scripps, CA
16. Matthew Nguyen	BS, Biochemistry 2nd Place Winner, Undergrad Research Poster Arthur Meakin Scholar, 2013 McKnight Prize in Chemistry, James Lewis Howe Award	2014	VCU School of Medicine
17. Joseph Hirst	Biochemistry	2014	1 yr break before Med School
18. Kris Manino	BS, ChemEng	2013	Unknown
19. Julie Ta	BS, Biochemistry 1st Place Winner, Undergrad Research Poster	2011-12	Medical School
20. Valerie Rojas	BS, Chemistry NIH PREP Scholar	2012	Grad student at Duke University, Cancer Center
21. Joseph Calderone	BS, Chemistry	2011	Grad Student at VA Tech
	Academic Excellence Awardee, Outstanding Undergrad Research Award, 1st Place Winner: Undergrad Poster Session		
22. Leah Heist	BS, Chemistry	2011	Grad Student at UNC, Chapel Hill
	Arthur Meakin Scholar, Academic Excellence Awardee		
23. Marietou Paye	BS, Biochemistry	2010	Grad Student at Georgia Tech
	NIH PREP Scholar		
24. Evan Gilius	BS, Biochemistry	2009	Unknown
25. Allison Pagano	BS, Biochemistry	2009	Medical School
26. Ryan Stephens	BS, Biochemistry	2009	UNC Medical School
	Arthur Meakin Scholar		
27. Wes Morris	BS, Chemistry	2009	Grad Student at Cornell University
	James L. Howe Awardee, HyperCube Scholar		
28. Brandon Thorpe	BS, Biochemistry	2009	Senior Research Scientist, Sphynknx Therapeutics, LLC
29. Caitlyn Criss	BS, Biochemistry	2008	WVU School of Osteopathic Medicine
30. Daniel Shook	BS, Chemistry	2007	US Patent & Trademark Office

- **Invited Lectures/Seminars**

1. "RNA Interacting Polynucleotides (RIPtides): Targeting Hepatitis C Virus RNA with Small Molecules and Proteins," Edward Via Virginia College of Ostheopathic Medicine, February 20, 2007, Blacksburg, VA.

2. "Chemical Biology Approaches to Disease States," College of William and Mary, October 5, 2007, Williamsburg, VA.

3. "Chemical Biology Approaches to Disease States," University of Mary Washington, November 30, 2007, Fredericksburg, VA.

4. "Targeting RNA with Small Molecules," The 10th Eurasia Conference on Chemical Sciences (EuAs C_2S-10), January 9, 2008, Manila, Philippines.

5. "Developing Small Molecule RNA Ligands," 1st Frontier Seminar in Materials Science Creation of Function by Molecular Design, Nagoya University, January 12, 2008, Nagoya, Japan

6. "RNA: A Drug Discovery Challenge," Eisai Co. Ltd., January 15, 2008, Tsukuba, Japan.

7. "RNA as a Therapeutic Target," NIH Workshop, May 4, 2008, Dallas, Texas, Organizers: Dr. John Schwab and Prof. Michael Doyle.

8. "Development of Catalytic Stereoselective Synthesis of α-substituted, β-boronic Esters,"NSF Workshop on Physical Organic Chemistry, Lake Tahoe, CA, September 16, 2008.

9. "Boron and Branched-Peptides in the Chemical Biology Approach of Targeting Diseases," University of Texas, Arlington, Texas, March 27, 2009.

10. "Thinking Outside the Box: Targeting RNA Structures with Branched Peptides," State University of New York, Binghamton, NY, October 23, 2009.

11. "Boron at the Interface of Chemistry and Biology," Virginia Commonwealth University, Richmond, VA, November 6, 2009.

12. "Mixed diboron as boration reagent and borono-branched peptides as HIV-1 RNA ligands," Lafayette College, Easton, PA, November 13, 2009.

13. "Mixed diboron as boration reagent and borono-branched peptides as HIV-1 RNA ligands," Muhlenberg College, Allentown, PA, November 13, 2009.

14. "Targeting HIV-1 RNA with branched peptides and new tricks,"James Madison University, Harrisonburg, VA, February 19, 2010.

15. "N-terminal peptidic boronic acids selectively inhibit ClpXP," Virginia Tech, Blacksburg, VA, April 7, 2010, Protein Structure and Function Symposium.

16. "Selective targeting of RNA structures,"Federation of American Societies for Experimental Biology (FASEB), Nucleic Acids, Saxtons River, VT, June 11, 2010.

17. "Boron chemistry: addition to activated C-C bonds and applications in chemical biology**,"** University of North Carolina, Charlotte, NC, September 27, 2010.

18. “Organoboron chemistry: synthesis and applications in infectious diseases**,”** University of Richmond, Richmond, VA, October 29, 2010.

19. “Drugging the undruggable: Targeting RNA structures**,”** Virginia Tech, Department of Chemistry Alumni Council (DCAC), November 6, 2010.

20. “Organoboron chemistry: synthesis and applications in infectious diseases, and Structure-activity relationships of sphingosine kinase inhibitors,” Case Western Reserve University, Cleveland, OH, November 18, 2010.

21. “Molecular pharmacology of sphingosine kinase inhibitors and branched peptide libraries to disrupt Tat/TAR RNA interactions,” European Molecular Biology Laboratory (EMBL), Heidelberg, Germany, January 11, 2011.

22. “Branched peptide libraries to disrupt Tat/TAR RNA interactions, and Chemical genetic approach to understanding sphingosine kinase function,” University of Southampton, United Kingdom, January 15, 2011.

23. “Organoboron: Synthesis and Application in Disrupting RNA/Protein Interactions in HIV-1,” Dartmouth College, February 23, 2011.

24. “Organoboron: Synthesis and Application in Disrupting RNA/Protein Interactions in HIV-1,” University of Vermont, February 25, 2011.

25. “Disrupting RNA-protein interactions with branched peptides, and Chemical genetic approach to understanding sphingosine kinase function,” Michigan State University, East Lansing, MI, March 11, 2011.

26. “Disrupting RNA-protein interactions with branched peptides, and Chemical genetic approach to understanding sphingosine kinase function,” Virginia Tech, Blacksburg, VA, March 25, 2011.

27. “Targeting RNA structures with branched peptides,” Molecular BioSystems Award Symposium: Emerging Investigators, ACS National Meeting, Anaheim, CA, March 29, 2011.

28. “Disrupting RNA-protein interactions with branched peptides, and Chemical genetic approach to understanding sphingosine kinase function,” Georgia State University, April 15, 2011.

29. “Disrupting RNA-protein interactions with branched peptides,” Bioorganic Gordon Research Conference, June 16, 2011, Proctor Academy, Andover, New Hampshire.

30. “Copper-catalyzed regioselective boration of α,β-unsaturated carbonyl compounds with unsymmetrical, preactivated diboron reagent,” CNRS, Laboratoire de Chimie de Coordination, Toulouse, France, July 12, 2011.

31. “The old problem of targeting RNA: Are peptide boronic acids the solution?” Universidad de Alcala de Henares, Madrid, Spain, July 18, 2011.

32. “Multivalent branched peptide boronic acids inhibit RNA-protein interactions” University of Nottingham, Nottingham, United Kingdom, July 20, 2011.

33. “Copper-catalyzed regioselective boration of α,β-unsaturated carbonyl compounds with unsymmetrical, preactivated diboron reagent,” Durham University, Durham, United Kingdom, July 21, 2011.

34. “Disrupting RNA-protein interactions with branched peptide boronic acids,” University of Cambridge, Cambridge, United Kingdom, July 27, 2011.

35. “Copper-catalyzed regioselective boration of α, β-unsaturated carbonyl compounds with unsymmetrical, preactivated diboron reagent,” IME Boron XIV, Niagara Falls, Canada, September 11-15, 2011.

36. “Disrupting RNA-protein interactions with branched peptide boronic acids,” Clemson University, Clemson, South Carolina, September 22, 2011.

37. “Copper-catalyzed borylation and inhibition of protein-RNA interactions” University of Virginia, Charlottesville, VA, September 30, 2011.

38. “Copper-catalyzed borylation and inhibition of protein-RNA interactions” Wayne State University, Detroit, MI, October 5, 2011.

39. “Copper-catalyzed borylation and inhibition of protein-RNA interactions” University of North Carolina, Chapel Hill, NC, October 13, 2011.

40. “Copper-catalyzed borylation and inhibition of protein-RNA interactions” North Carolina State University, Raleigh, NC, October 14, 2011.

41. “Copper-catalyzed borylation and inhibition of protein-RNA interactions” University of Pennsylvania, Philadelphia, PA, October 17, 2011.

42. “Copper-catalyzed borylation and inhibition of protein-RNA interactions” New York University, NY, October 25, 2011.

43. “Copper-catalyzed borylation and inhibition of protein-RNA interactions” Hunter College, New York, October 26, 2011.

44. “Copper-catalyzed borylation and inhibition of protein-RNA interactions” State University of New York, Stony Brook, October 28, 2011.

45. “The chemical biology of targeting sphingosine kinase and HIV-1 RNAs” Virginia Tech, Life Science Seminar, Blacksburg, VA January 20, 2012.

46. “The chemical biology of targeting sphingosine kinase and HIV-1 RNAs” University of Kansas, Medicinal Chemistry Department, Lawrence, Kansas, February 9, 2012.

47. “The chemical biology of targeting sphingosine kinase and HIV-1 RNAs” Virginia Tech, GBCB Seminar, February 23, 2012.

48. “Copper-catalyzed borylation and chemical biology of targeting HIV-1 RNA”, University of British Columbia, Vancouver, Canada, March, 30, 2012.

49. “Lewis Base-Assisted Nucleophilic Boron: Borylation of Electrophilic Alkenes”, University of Virginia, Symposium in honor of Prof. Timothy Macdonald, Charlottesville, VA, April 28, 2012.

50. “Lewis base activation of boron: Catalytic copper-catalyzed borylation and silylation of electrophilic alkenes”, Ateneo de Manila, Manila, Philippines, June 21, 2012.

51. “Branched peptide boronic acids: Novel RNA ligands as anti-HIV therapy” University of the Philippines, Diliman, Philippines, June 22, 2012.

52. “Boronic acids: Synthetic methods and application towards RNA structures”, University of California, San Diego, La Jolla, CA, October 22, 2012.

53. “Boronic acids: Synthetic methods and application towards RNA structures”, Scripps Research Institute, La Jolla, CA, October 23, 2012.

54. “Sphingosine Kinase Drug Discovery: The Search for Disease Targets”, Virginia Tech Center for Drug Discovery, Blacksburg, VA, January 21, 2013.

55. “Lewis base assisted copper catalyzed borylation and silylation of electrophilic alkenes”, 14th Florida Heterocyclic and Synthetic Chemistry IUPAC Sponsored Conference, University of Florida, Gainesville, FL, March 3-6, 2013.

56. “Boron vs Silicon: Addition to Carbon-Carbon Multiple Bonds”, College of William and Mary, Williamsburg, VA, October 4, 2013.

57. “Copper Catalysis: B/Si Addition to C-C Bonds & Chemical Biology of Targeting RNA Structures”, University of Virginia, Charlottesville, VA, November 4, 2013.

58. “Modulating In Vivo Sphingosine-1-phosphate Levels with Sphingosine Kinase Inhibitors”, University of Virginia, Charlottesville, VA, November 5, 2013.

59. “Drugging RNA: Targeting Structured HIV-1 RNA with Branched Peptide Boronic Acids”, Frontiers in Nucleic Acids, 2013 Southeastern Regional Meeting, Atlanta, GA, November 13-14, 2013.

60. “Combating Human Immunodeficiency Virus: Inhibiting RNA Function Using Chemistry”, Virginia State University, Petersburg, VA, January 24, 2014.

61. “Chemical Tools to Study RNA In Vitro and Sphingosine Kinase In Vivo”, The University of Mississippi, Oxford, MS, April 17, 2014.

62. “Pt- and Cu-catalyzed Mono- and Diboration of C=C bonds”, BORAM XIV, Rutgers University, Newark, NJ, June 18, 2014.

63. “Metal-catalyzed borylation electrophilic alkenes and allenes”, IME Boron XV, Prague, Czech Republic, August 28, 2014.

64. “*In vivo* Probes of Sphingosine Kinase Function”, Kings College, London, England UK, November 18, 2014.

65. “Borylation and Silylation of Activated C-C Bonds”, University of Manchester, England UK, November 25, 2014.

66. “Drugging Sphingosine Kinases and Environmentally Friendly Borylation/Silylation Reactions”, Alcala de Henares, Madrid, Spain, December 3, 2014.

67. “Nanoassembly of Nanoparticles”, Alcala de Henares, Madrid, Spain, December 3, 2014.

68. “Transition Metal-Catalyzed Borylation and Silylation of C-C Bonds”, Universitat Rovira i Virgili, Tarragona, Spain, December 5, 2014.

69. “Sphingosine Kinase as a Drug Target”, Virginia Tech Center for Drug Discovery, Blacksburg, Virginia, January 14, 2015.

70. “A Step Closer to Green Reactions: Copper-catalyzed Borylation/silylation Reactions in Water”, Saint Louis University, St. Louis, MO, April 10, 2015.

71. “The Complexity of Controlling Sphingosine-1-phosphate Levels via Sphingosine Kinases”, Dongguk University, Seoul, South Korea, August 10, 2015.

72. “The Complexity of Controlling Sphingosine-1-phosphate Levels via Sphingosine Kinases”, Pusan National University, Busan, South Korea, August 11, 2015.

73. “Sphingosine Kinase Drug Discovery: Treatment Towards Kidney Injury”, University of the Philippines, Laguna, Philippines, August 17, 2015.

74. “B-X bond: Chemoselective Transfer of Boron or Silicon into C-C Bonds”, Shanghai Institute of Organic Chemistry, Shanghai, China, October 19, 2015.

75. “B-X bond: Chemoselective Transfer of Boron or Silicon into C-C Bonds”, University of Science and Technology, Hefei, China, October 21, 2015.

76. “B-X bond: Chemoselective Transfer of Boron or Silicon into C-C Bonds”, Peking University, Beijing, China, October 23, 2015.

77. “Copper-Catalyzed Borylation: Towards Sustainable Chemistry”, Universitat Wurzburg, Wurzburg, Germany, Nov. 16, 2015.

78. “Drugging Sphingosine Kinase: Medicinal Chemistry and Animal Studies”, North Carolina A&T, Greensboro, North Carolina. February 23, 2017.

79. “The Sphingosine-1-phosphate pathway: Sphingosine kinase as a drug target”, George Mason University, Manassas, Virginia, September 15, 2017.

80. “Faculty Entrepreneurship in Drug Discovery: Challenges and Opportunities”, Virginia Tech Center for Drug Discovery, Virginia Tech, Blacksburg, Virginia, January 11, 2018.

81. “Stereoselective Borylation Reactions & Sphingosine Kinase Medicinal Chemistry”, West Virginia University, Morgantown, West Virginia, February 28, 2018.

82. “Controlling sphingosine-1-phosphate levels as a therapeutic strategy”, Virginia Drug DiscoveryRx Symposium, George Mason University, Arlington, VA, June 26, 2018.

83. “Towards Sustainable Stereoselective Borylation Chemistry”, University of Edinburgh, Edinburgh, Scotland, September 10, 2018.

84. “Towards Sustainable Stereoselective Borylation Chemistry”, University of St. Andrews, St. Andrews, Scotland, September 12, 2018.

85. “Controlling Sphingosine-1-Phosphate Levels as a Therapeutic Strategy”, Durham University, Durham, England, September 15, 2018.

86. “Inhibiting Sphingosine Kinases as a Therapeutic Strategy”, George Washington University, Washington, D.C., October 1, 2018.

87. “Treating Fatty Liver Disease”, Virginia Tech, Celebration of Chemistry, Blacksburg, VA, October 20, 2018.

88. “Academic Drug Discovery: MedChem Strategies Toward Treating Fatty Liver Disease and Multiple Sclerosis”, Rensselaer Polytechnic Institute, Troy, New York, February 5, 2019.

89. “Academic Drug Discovery: MedChem Strategies Toward Treating Fatty Liver Disease and Multiple Sclerosis”, Monash University, Victoria, Australia, February 12, 2019.

90. “Academic Drug Discovery: MedChem Strategies Toward Treating Fatty Liver Disease and Multiple Sclerosis”, Wake Forrest University, Winston-Salem, North Carolina, February 20, 2019.

91. “Addition of B-X reagents across C-C multiple bonds & Mitochondrial uncouplers for the treatment of fatty liver disease”, University of California, Los Angeles, November 6, 2019.

92. “Addition of B-X reagents across C-C multiple bonds & Mitochondrial uncouplers for the treatment of fatty liver disease”, University of California, Riverside, November 8, 2019.

93. “Academic Drug Discovery: Toward Treating Fatty Liver Disease and Multiple Sclerosis”, University of the Philippines, Diliman, Quezon City, Philippines, November 11, 2019.

94. “Academic Drug Discovery: Toward Treating Fatty Liver Disease and Multiple Sclerosis”, Ateneo de Manila University, Quezon City, Philippines, November 12, 2019.

95. “S1P transport inhibitors: the new frontier in sphingolipid biology”, Virginia Tech, VT Center for Drug Discovery, Blacksburg, Virginia, January 10, 2020.

96. “trans Selective Borylation Reactions & Drug Discovery Strategies”, University of Rochester, Rochester, New York, January 15, 2020.

97. “trans Selective Borylation Reactions & Exercise Pill—a Chemist Approach”, University of Alberta, Edmonton, Canada, January 29, 2020.

98. “Stereoselective Borylation Reactions”, Wurzburg University, Wurzburg, Germany, February 19, 2020.

99. “*trans* Selective Borylation Reactions & Drug Discovery Strategies”, University of Freiburg, Freiburg, Germany, February 21, 2020.

100. “Stereoselective Borylation Reactions & Exercise Pill—a Chemist Approach”, University of New England, Biddeford, Maine, September 15, 2021.

101. “Transition Metal-Free Stereoselective Borylation Reactions”, Old Dominion University, Norfolk, Virginia, March 4, 2022.

102. “Drugging the Sphingosine-1-Phosphate Pathway and others”, Virginia Commonwealth University, Richmond, Virginia, April 8, 2022.

103. “Exercise Pill—a Chemist Approach”, University of Virginia, Charlottesville, Virginia, April 29, 2022.

104. “Small molecule mitochondrial uncouplers as anti-obesity agents”, Virginia Drug DiscoveryRx 2022, Richmond, Virginia, May 25, 2022.

Professional/Scientific Presentations

1. Santos, Webster, L. Stereoselective addition of B-X reagents to activated carbon-carbon bonds. 102nd Canadian Chemistry Conference and Exhibition, Quebec, Canada, June 7, 2019. (Invited oral)

2. Santos, Webster, L. Small molecule mitochondrial uncouplers for the treatment of NASH, Integrated Pathways of Disease in NASH and NAFLD, Keystone Conference, Santa Fe, New Mexico, January 20-25, 2019.

3. Santos, Webster L. Controlling Sphingosine-1-Phosphate Levels as a Therapeutic Strategy. XXV EFMC International Symposium on Medicinal Chemistry, Ljubljana, Slovenia, September 5, 2018. (Invited oral)

4. Santos, Webster L. In vivo chemical probes of sphingosine kinase function. Abstracts of Papers, 256th ACS National Meeting & Exposition, Boston, MA, USA, August 1-23, 2018 (2018), BIOL 275. (Invited oral)

5. Santos, Webster L. Molecular Recognition and in vitro Activity of Branched Peptide Boronic Acids against HIV-1 Rev Response Element RNA, BORAM XVI, Boston College, Boston, MA, June 27, 2018. (Invited oral)

6. Santos, Webster L. Controlling sphingosine-1-phosphate levels as a therapeutic strategy, Virginia Drug DiscoveryRx Symposium, George Mason University, Arlington, VA, June 26, 2018. (Invited oral)

7. Santos, Webster L. Targeting HIV-1 Rev response element with branched peptides. Abstracts of Papers, 255th ACS National Meeting & Exposition, New Orleans, LA, USA, March 18-22, 2018 (2018), ORGN 365. (Invited oral)

8. Santos, Webster L. Stereoselective borylation reactions. 69th Southeastern Regional Meeting of the American Chemical Society, Charlotte, NC, United States, November 7-11 (2017), SERMACS-138. (Invited oral)

9. Santos, Webster L.; Snead, Russell; Astha, Fnu; Dai, Yumin. "Transition metal-free activation and intramolecular trans diboration of propargylamides using unsymmetrical diboron" 253rd ACS National Meeting & Exposition, San Francisco, CA, United States, April 2-6, 2017 (2017), ORGN-438. (oral)

10. Santos, Webster L.; Dai, Yumin; Wynn, Jessica; Peralta, Ashley; Rekosh, David; Hammarskjold, Marie-Louise. "Targeting RNA with branched peptide boronic acids: Unnatural amino acids, molecular recognition, and in vitro activity against HIV-1 RRE RNA" 253rd ACS National Meeting & Exposition, San Francisco, CA, United States, April 2-6, 2017 (2017), BIOL-336. (oral)

11. Santos, W. L. "*trans* Diboration/Silaboration Reaction and Branched Peptide Boronic Acids as HIV-1 RNA Inhibitors", IME Boron XVI. Hongkong, China. July 15, 2017. (Invited oral)

12. Santos, W.L. "Transition Metal-free trans Diboration of Alkynamides", FACS XVI, University of California, Santa Barbara, Santa Barbara, CA July 29, 2016. (Invited oral)

13. Santos, W.L. "Boron Activation in B-(B/Si) Bonds: Addition to C-C Multiple Bonds", BORAM XV, Queens University, Kingston, Ontario, Canada, June 26, 2016. (Invited oral)

14. Santos, W.L. "Toward Borylation Reactions in Aqueous Medium", Dalton 2016, University of Warwick, Coventry, UK, March 29, 2016. (Invited oral)

15. Santos, W.L. "Branched peptide boronic acids: molecular recognition of folded HIV-1 RNA structures", Pacifichem, Honolulu, Hawaii, December 17, 2015 (invited oral)

16. Santos, W.L. "Copper-catalyzed Borylation and Silylation Reactions in Water", Pacifichem, Honolulu, Hawaii, December 18, 2015. (invited oral)

17. Santos, W.L. "Copper-Catalyzed Borylation: Towards Sustainable Chemistry", Todd Marder Symposium, Wurzburg, Germany, Nov. 16, 2015. (invited oral)

18. Santos, W.L. "Progress Toward Borylation Reactions in Water", IUPAC Sustainable Catalysis, Busan, South Korea, August 13, 2015 (invited oral)

19. Santos, W.L., Patwardhan, N.; Morris, E.; Congdon, M.; Kharel, Y.; Lynch, K.R. "Structure-Activity Relationship Studies and In Vivo Activity of Guanidine-Based Sphingosine Kinase Inhibitors", Medicinal Chemistry Gordon Research Conference, Colby-Sawyer College, New London, NH. (Poster Contribution)

20. Santos, W.L., Calderone, J.A.; Guo, X.; Nelson, A.; Peck, C.; Thorpe, S.B. "Metal-catalyzed Borylation/Silylation Reactions", Organic Reactions and Processes Gordon Research Conference, July 19-24, 2015, Bates College, Lewiston, ME. (Poster Contribution)

21. Santos, W.L., Patwardhan, N.; Congdon, M.; Morris, E.; Kharel, Y.; Lynch, K.R. "In Vivo Chemical Probes to Understand Sphingosine Kinase Function", Bioorganic Chemistry Gordon Research Conference, June 8-13, 2014, Proctor Academy, Andover, NH. (Poster Contribution)

22. Santos, W.L., Patwardhan, N.; Congdon, M.; Morris, E.; Kharel, Y.; Lynch, K.R. "Modulating In Vivo Sphingosine-1-Phosphate Levels with Sphingosine Kinase Inhibitors", Bioorganic Chemistry Gordon Research Conference, June 9-14, 2013, Proctor Academy, Andover, NH. (Poster Contribution)

23. Santos, W.L. "Lewis base assisted copper catalyzed borylation and silylation of electrophilic alkenes", 14th Florida Heterocyclic and Synthetic IUPAC Sponsored Conference, University of Florida, Gainesville, FL, March 3-6, 2013. (Oral Contribution, Invited)

24. Santos, W.L. "Activation of diboron reagents: Catalytic copper-catalyzed borylation of electrophilic alkenes", 244th ACS National Meeting, Philadelphia, PA, Aug. 21, 2012. Young Academic Investigator Symposium, Organic Division. (Oral Contribution, Invited).

25. Santos, W.L.; Bryson, D.I.; Zhang, W.; Crumpton, J.B.; and Rekosh, D.R. "Inhibiting RNA-Protein Interactions: Cell Permeable Branched Peptide Boronic Acids Inhibit Tat-TAR and Rev-RRE Interactions," Keystone Symposia: Frontiers in HIV Pathogenesis, Therapy and Eradication, Whistler, British Columbia, Canada, March 28, 2012. (Oral Contribution, Invited)

26. Santos, W.L.; Thorpe, S.B.; Gao, M. and Guo, X. "Copper-catalyzed regioselective boration of α,β-unsaturated carbonyl compounds with unsymmetrical, preactivated diboron reagent," IME Boron XIV, Niagara Falls, Canada, September 12, 2011. (Oral Contribution, Invited)

27. Santos, W.L. "Disrupting RNA-protein interactions with branched peptides," Bioorganic Gordon Research Conference, June 16, 2011, Proctor Academy, Andover, NH. (Oral Contribution, Invited)

28. Santos, WL; Thorpe, SB; Gao, M. Novel diboron reagent: Regioselective β-boration of activated carbon-carbon bonds. 241st ACS National Meeting, Anaheim, CA, March 27-31, 2011. (Oral Contribution)

29. Santos, WL.; Bryson, D.; Zhang, W.; Crumpton, JB. Targeting RNA structures with branched peptide libraries. 241st ACS National Meeting, Anaheim, CA, March 27-31, 2011. (Oral Contribution, Invited)

30. Santos, WL; Gao, M; Thorpe, SB. Preactivated unsymmetrical diboron: Catalytic regioselective boration of α,β-unsaturated conjugated compounds. 240th ACS National Meeting, Boston, MA, August 22-26, 2010. (Oral Contribution)

31. Santos, W.L. "Inhibiting TAR RNA with Branched Peptides," Chemistry and Biology of Peptides Gordon Conference, Ventura, CA, February 2010. (Poster Contribution)

32. Santos, W.L. "Targeting RNA Structures with Branched Peptides," 2nd Biennial Chemical Insights into Biological Processes, NIH/NCI, Hood College, Frederick, MD, August 9-10, 2010. (Poster Contribution)

33. Santos, WL; Gao, M; Thorpe, SB. sp^2-sp^3 Mixed diboron reagent: copper-catalyzed beta boration of alpha, beta-unsaturated carbonyl compounds. 238th ACS National Meeting, Washington, DC, August 16-20, 2009. (Oral Contribution)

34. Santos, W.L. "Targeting RNA with Branched Peptide Libraries," Bioorganic Chemistry Gordon Conference, Proctor Academy, Andover, NH, June 2010. (Poster Contribution)

35. Santos, W.L. Targeting HIV-1 TAR with Branched Peptides. Nucleosides, Nucleotides and Oligonucleotides Gordon Research Conference, Salve Regina University, Newport, RI, June 2009. (Poster Contribution)

36. Santos, W.L. sp^2-sp^3 hybridized mixed diboron reagent: synthesis, characterization and copper-catalyzed β-boration of α,β-unsaturated carbonyl compounds. Organic Reactions and Processes Gordon Research Conference, Bryant University, Smithfield, RI, July 2009. (Poster Contribution)

37. Santos, WL; Bryson, DI; Pagano, A. Targeting HIV-1 TAR with Branched Peptides. 237th ACS National Meeting, Salt Lake City, UT, March 2009. (Oral Contribution)

38. Santos, W.L. "Developing New RNA Ligands," Bioorganic Chemistry Gordon Conference, Procter Academy, Andover, NH, June 15-20, 2008. (Poster Contribution)

39. Santos, WL. Targeting RNA with small molecules. 10th Eurasia Conference on Chemical Sciences. Jan 2008, Manila, Philippines. (Oral Contribution)

40. Santos, WL. New RNA Selective Ligands. 236th ACS National Meeting, Philadelphia, PA, USA, August 2008. (Poster Contribution)

41. Santos, W.L. "RNA as a Therapeutic Target," Bioorganic Gordon Conference, June 10-15, 2007, Procter Academy, Andover, NH. (Poster Contribution)

Courses Taught

Year	Session	Course	Course Title	# of Students	SPOT
2006*	Fall	Chem 5505	Advanced Organic Chemistry	24	n/a
2007	Spring	Chem 2566	Principles of Organic Chemistry	50	2.9
		Chem 2566H	Principles of Organic Chemistry	10	3
2008	Spring	Chem 2566	Principles of Organic Chemistry	67	3.3
		Chem 2566H	Principles of Organic Chemistry	7	3.3
	Fall	Chem 5505	Advanced Organic Chemistry	23	3.6
2009	Spring	Chem 2566	Principles of Organic Chemistry	75	3.1
		Chem 2566H	Principles of Organic Chemistry	2	3.5
	Fall	Chem 5505	Advanced Organic Chemistry	19	3.6
2010	Spring	Chem 5535	Synthetic Organic Chemistry	8	3.6
	Summer	Chem 2536	Organic Chemistry	113	3.3
	Fall	Chem 2535	Organic Chemistry	131	3.0
2011	Spring	Chem 5535	Synthetic Organic Chemistry	13	3.4
Starting 2012 SPOT scores are out of 6.0 instead of 4.0 scale					
2012	Spring	Chem 5535	Synthetic Organic Chemistry	9	4.5
	Spring**	Chem 2984	Drugs, Bugs and Entrepreneurship	18	5.0
	Fall	Chem 5505	Advanced Organic Chemistry	20	5.67
2013	Spring	Chem 5535	Synthetic Organic Chemistry	8	5.57
	Fall	Chem 2984	Drugs, Bugs and Entrepreneurship	8	6.0
2014	Spring	Chem 6564	Special Topics: Chemical Biology	4	6.0
	Fall	--	On sabbatical		
2015	Spring	Chem 5506	Advanced Organic Chemistry II	12	5.67
	Fall	Chem 2535	Organic Chemistry	140	3.49
2016	Spring	Chem 6564	Chemical Biology	3	5.67
	Fall	Chem 2565	Organic Chemistry	60	3.87
2017	Spring		Teaching buy-out	--	--
	Fall		Teaching buy-out		
2018	Spring		Teaching buy-out		
	Fall		Teaching buy-out		
2019	Spring		Teaching buy-out		
	Fall		Teaching buy-out		
2020	Spring		Teaching buy-out		
	Fall	Chem 6564	Bioorganic Principles of MedChem	11	5.3
2021	Spring	Chem 2565	Organic Chemistry	44	4.78

	Fall		Teaching buy-out		
2022	Spring	Chem 2565	Organic Chemistry	40	5.5

**Co-taught with Prof. David Kingston; **Co-taught with Prof. Joseph Falkinham and Tim Howland*
CHEM 2566: Principles of Organic Chemistry: 2nd semester course in organic chemistry for majors, using Bruice "Organic Chemistry" 5thEd.
CHEM 2535: Organic Chemistry: 1st semester course in organic chemistry for non-majors, using Bruice "Organic Chemistry" 6th Ed.
CHEM 5505: Advanced Organic Chemistry: Graduate course in organic chemistry, using Carey & Sundberg "Advanced Organic Chemistry, Part A" 4th/5th Ed.
CHEM 5535: Synthetic Organic Chemistry: Graduate course in synthetic organic chemistry using Carey & Sundberg's "Advanced Organic Chemistry, Part B" 5th Ed and "Strategic Applications of Named Reactions in Organic Synthesis" by Kurti and Czako.

- **Departmental Service**

Organic Chemistry Faculty Search Chair, **2021**
Analytical Services and Facilities Advisory Group, **2019-present**
Organic Chemistry Faculty Search Chair, **2017**
Personnel Committee, **2015-2016, 2018-2020, 2021-2024**
Executive Committee, **2014-2015, 2017-2019**
Graduate Education Committee Chair, **2013-present**
Colloquium Committee Chair, **2016-**
Biochemistry Faculty Search Committee, **2015**
Drug Discovery Faculty Search Committee, **2012**
Bioanalytical Chemistry Faculty Search Committee, **2011**
Organic Chemistry Division Coordinator, **2011-2014**
Chemistry Department Executive Committee, **2008**, **2012, 2014-2015**
Chemistry Department Graduate Recruiting Committee, **2006-2010**
Organic Chemistry Division Representative for the Davidson Renovation, **2010**
Chemistry Graduate Advising (1st week of class), **2009**, **2010**
Hokie Focus, research presentation to incoming first year undergraduates majoring in chemistry; ~50 attendees, **April 17, 2010**
Chemistry Faculty Search Committee, **2010-2011**
"Chemistry Magic Show", yearly AXE fundraising chemistry demo, **2006-present**
Hosted Jennifer Rodriguez (high school, minority) in the "Agricultural Scholars Program", **Summer 2009**
"Chemistry Magic Show", Tall Oaks Elementary, **March 16, 2011**
Thesis/Dissertation Graduate Advisory Committee, 30 students for AY**2011**

- **University Service**

Search Committee: Conflict of Interest Director, **Spring 2019**
SGA: Innovation and Entrepreneurship, **Dec 2016-present**
Faculty Advisory Board, Apex Systems Center for Innovation and Entrepreneurship, **2015-present**
Virginia Tech Center for Drug Discovery Member, **2012-present**
Mass Spectrometry Incubator Advisory Committee, **2008**
Macromolecular Interfaces with Life Science, NSF-IGERT, Core faculty member, **2007-2010**
Filipino Student Association, Advisor, **2007-present**
Initiative for Maximizing Student Development (VT-IMSD), Faculty Mentor, **2010-present**

Post Baccalaureate Research & Education Program (VT-PREP), Faculty Mentor, **2010-present**
Bringing Science to Market (BS2M) committee, **2010-15**
ICTAS Proposal Review Panel, **2012-present**
ICTAS Doctoral Scholar Review Panel, **Spring 2011, Spring 2012, Spring 2016**
1st Cancer Research Symposium at Virginia Tech, Poster Session Judge, **March 29, 2011**
Session chair, ACC Interdisciplinary Forum for Discovery in Life Science at VT, **Oct. 6, 2010**

- **Professional Activities**
  - Referee for the *Proceedings of the National Academy of Sciences, Journal of the American Chemical Society, Accounts of Chemical Research, ACS Chemical Biology, Bioorganic and Medicinal Chemistry Letters, Bioorganic and Medicinal Chemistry, Journal of Organic Chemistry, Chemical Communications, Angewandte Chemie International Edition, European Journal of Organic Chemistry, Molecular Biosystems, Analytical Chemistry, Organic and Biomolecular Chemistry, Chemical Reviews, ACS Medicinal Chemistry Letters, ACS Chemical Neuroscience, Tetrahedron Letters, Organometallics, Synthesis, Current Organic Chemistry, Mini-reviews in Medicinal Chemistry, Monatschefte fur Chemie, Organic Letters, Advanced Synthesis and Catalysis, ACS Catalysis, Synthesis, ChemBioChem, ChemMedChem, and Amino Acids.*

  - Proposal Reviewer:
    (1) *Jeffress Memorial Trust*
    (2) ACS Petroleum Research Fund
    (3) *National Institutes of Health Study Sections:* (i) ZRG1 MDCN-C 58, Drug discovery for the nervous system (DDNS), (ii) ZRG1 OTC-X(80) Oncological Sciences AREA Grant Applications), (iii) F04A-W(20)L fellowship panel, Synthetic and biological chemistry, (iv) Synthetic and Biological Chemistry B (SBCB), Synthetic and Biological Chemistry A (SBCA)
    (4) *Netherlands Organisation for Scientific Research*
    (5) *Cottrell Scholar Awards*
    (6) *National Science Foundation*
    (7) Engineering and Physical Sciences Research Council (EPSRC)
    (8) NIH SBCB study section standing member

  - Served as a panel speaker at VirginiaDrugDiscoveryRx: Emerging Targets, Technologies, and Therapeutics for Cancer and Neuroscience. The topic was “Key Success Factors for Early Stage Companies” held at Hotel Roanoke on May 2019.

  - Organized a symposium (April 28, 2012) with Prof. Jetze Tepe in honor of Prof. Timothy Macdonald that involved invitation of speakers, solicitation of funds and coordination of manuscript submissions to Bioorg. Med. Chem. Lett. The number of attendees from academia and industry was approximately 60.

  - Alternate Councilor for the Division of Biological Chemistry of the American Chemical Society (2013-2016)

  - Member of the American Chemical Society, Biological and Organic Chemistry Divisions

  - Member of International Union of Applied Chemists (IUPAC)

- Discussion Leader at the IME Boron XIV Conference, Niagara Falls, Canada, Sept. 13, 2011

- Discussion Leader at the Bioorganic Chemistry Gordon Research Conference (Frontiers in Bioorganic and Medicinal Chemistry), Proctor Academy, Andover, NH, June 2010.

- Discussion Leader at the Nucleosides, Nucleotides, and Oligonucleotides GRC Conference, Salve Regina, June 23-28, 2019.

- Host and Chair of the Boron in the Americas XVIII Conference at Virginia Tech Inn & Conference Center, June 20-24, 2022. This is an international meeting of boron chemists that meets every two years. The week-long meeting brings together world leaders to discuss and disseminate the forefront of science dealing with boron.