

Curriculum Vitae

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- **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**

- 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 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
- 2013- Techulon, Inc., Consultant
- 2012 ACS Young Academic Investigator
- 2012- Core Faculty Member, Virginia Tech Center for Drug Discovery
- 2011 Chemical Communications Emerging Investigator (January 2011 issue)
- 2010-2014 Blackwood Junior Faculty Fellow of Life Sciences
- 2010- SphynKx Therapeutics, LLC, co-Founder and Vice-president of Medicinal Chemistry
- 2009 Molecular Biosystems Emerging Investigator (May 2009 issue)
- 2007- Core Faculty Member, Macromolecular Interface with Life Sciences (NSF IGERT)
- 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

2017- Editorial Board, *Medicinal Research Reviews*
2015- Editorial Advisory Board, *Current Topics in Medicinal Chemistry*
2015- Associate Committee on Science, American Chemical Society
2014- Editorial Board, *Journal of Biochemistry and Molecular Biology Research*
2014-15 Associate Editor, *Diversity Oriented Synthesis*
2014- Advisory Committee, Boron in the Americas (BORAM)
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. "Sphingosine Kinase Inhibitors", US Patent Appl. 62/058294, Priority filing date: October 1, 2015.
11. Santos, W.L.; Lynch, K.R. "Oxadiazoles as sphingosine kinase inhibitors and their preparation", PCT Int. Appl. (2016), WO 2016054261 A1 20160407.

12. 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
13. Thorpe, B. T.; Santos, W.L.; Lynch, K.R. "Sphingosine Kinase Inhibitor Prodrugs", March 2017, PCT/US2017/024852.
14. Santos, W.L.; Salamoun, J.; Murray, J. "Novel Small Molecule Heterocycles as Mitochondrial Uncouplers: Composition, Method of Preparation, and Uses Thereof", April 20, 2018, U.S. Provisional Patent Application Serial No. 62/660,880.
15. Santos, W.L.; Fritzemeier, R. "A process for making 3-substituted-1,2-oxaborol-2(5H)-ol", July 10, 2018, U.S. Patent Application No: 62/696,073.
16. Santos, W.L. Lynch, K.R., Kharel, Y.; Peralta, A.; Fritzemeier, R.; Foster, D. "Inhibitors of Spinster Homology 2 for Use in Therapy", January 25, 2019, U.S. Patent Application Serial No.: 62/797,054.

- **Publications**

Papers from graduate and postdoctoral training

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](https://doi.org/10.1111/j.1749-6632.2000.tb06553) PMID: [10818457](https://pubmed.ncbi.nlm.nih.gov/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 LPA₁/LPA₃ receptor antagonist. *Mol. Pharm.* **2001**, *60*, 1173-1180. DOI: [10.1124/mol.60.6.1173](https://doi.org/10.1124/mol.60.6.1173) PMID: [11723223](https://pubmed.ncbi.nlm.nih.gov/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](https://doi.org/10.1074/jbc.M007782200) PMID: [11042183](https://pubmed.ncbi.nlm.nih.gov/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](https://doi.org/10.1021/tx000139n) PMID: [11511169](https://pubmed.ncbi.nlm.nih.gov/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](https://doi.org/10.1021/tx000141e) PMID: [11368548](https://pubmed.ncbi.nlm.nih.gov/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](https://doi.org/10.1021/tx025509h) PMID: [12067249](https://pubmed.ncbi.nlm.nih.gov/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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 Kvaratskhelia, 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](https://doi.org/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](https://doi.org/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](https://doi.org/10.1016/j.str.2008.05.008) PMID: 18682223

Papers as an independent investigator

16. Gao, M.; Thorpe, S.B. and Santos, W.L. sp²-sp³ 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](https://doi.org/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](https://doi.org/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](https://doi.org/10.1039/c004247a) PMID: 20523950
19. Thorpe, S.B. and Santos, W.L. Regio- and stereoselective copper-catalyzed β -borylation of allenates by a preactivated diboron. *Chem. Commun.* **2011**, *47*, 424. (Emerging investigator issue) DOI: [10.1039/c0cc02270e](https://doi.org/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](https://doi.org/10.1021/jo2003488) PMID: 21491953
- Highlighted in (1) *Synfacts*, **2011**, *9*, 995. (2) *ChemInform*, **2011**, *42*, no. doi: [10.1002/chin.201133182](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/10.1021/ol300618j) PMID: 22494333

- Highlighted in (1) *Synfacts*, **2012**, 8, 781. (2) *ChemInform*, **2012**, 43, no. doi: [10.1002/chin.201231192](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/10.1021/jp4019102)
 34. Zhang, W.; Bryson, D.I.; Crumpton, J.B.; Wynn, J. and 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](https://doi.org/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](https://doi.org/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](https://doi.org/10.1016/j.molmet.2013.11.005) PMID: 24634817 PMCID: [PMC3953706](https://pubmed.ncbi.nlm.nih.gov/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](https://doi.org/10.1002/anie.201310695) PMID: [24532188](https://pubmed.ncbi.nlm.nih.gov/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](https://doi.org/10.1364/OE.22.012935) PMID: [24921491](https://pubmed.ncbi.nlm.nih.gov/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](https://doi.org/10.1364/OE.22.020720) PMID: [25321275](https://pubmed.ncbi.nlm.nih.gov/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](https://doi.org/10.1194/jlr.M053462) PMID: [25210149](https://pubmed.ncbi.nlm.nih.gov/25210149/)
41. Santos, W.L. and Lynch, K.R. Drugging Sphingosine Kinases. *ACS Chem. Biol.* **2015**, 10, 225-223. DOI: [10.1021/cb5008426](https://doi.org/10.1021/cb5008426) PMID: [25384187](https://pubmed.ncbi.nlm.nih.gov/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](https://doi.org/10.1021/jm501760d). PMID: [25643074](https://pubmed.ncbi.nlm.nih.gov/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](https://doi.org/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](https://doi.org/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](https://doi.org/10.1055/s-0034-1380524). Invited contribution on conjugate addition themed edition by Prof. Erick Carreira.
- Highlighted in [organic chemistry portal](http://organicchemistryportal.com).
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](https://doi.org/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](https://doi.org/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/acsmchemlett.5b00304](https://doi.org/10.1021/acsmchemlett.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](https://doi.org/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](https://doi.org/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](https://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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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/acsmchemlett.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](https://doi.org/10.1021/acs.langmuir.7b02307)
64. Fritzeimer, 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](https://doi.org/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.; Fritzeimer, 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](https://doi.org/10.1039/C7CS00816C)
*corresponding authors
68. Fritzeimer, 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](https://doi.org/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](https://doi.org/10.1021/acs.jmedchem.8b01076)
70. 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.* **2018**, *in press*. DOI: [10.1021/acs.jmedchem.8b01076](https://doi.org/10.1021/acs.jmedchem.8b01076).

71. 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](https://doi.org/10.7150/thno.29435).
72. 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](https://doi.org/10.1039/C8PP00346G)
73. 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, *Cancer Discov.* **2018**, submitted.
74. 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**, *in press*: [DOI: 10.1021/acs.jcim.8b00931](https://doi.org/10.1021/acs.jcim.8b00931).
75. Li, H.; Wonilowicz, L.; Kharel, Y.; Brown, A.; Bevan, D.; Lynch, K.R.; Santos, W.L. Lipophilic tail modifications of (R)-prolinol-based inhibitors of sphingosine kinase 1. *Eur. J. Med. Chem.* **2018**, submitted.
76. Snead, R.F.; Santos, W.L. Copper(II)-catalyzed protoboration of allenes in aqueous media. *Adv. Synth. Catal.* **2018**, submitted.
77. Gates, A.; Santos, W.L. Diboron-Mediated Regioselective Semi-Reduction of Allenes. *Synthesis* **2018**, invited feature article.
78. Verma, A.; Grams, J.; Rastatter, B.P. Santos, W.L. Transition metal-free α borylation-protodeborylation of alkyanoic acids. *Tetrahedron*, **2019**, <https://doi.org/10.1016/j.tet.2019.02.030>.
79. 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**, under review.
80. 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**, *in press*. <https://doi.org/10.1016/j.bmc.2019.03.016>
81. Blais-Lecours, P.; Laouafa, S.; Arias-Reyes, C.; Santos, W.L.; Joseph, V.; Halayko, A. J.; Soliz, J.; Marsolais, D. A sphingosine kinase 2 substrate impairs the respiratory capacity of airway smooth muscle cells. *International Journal of Radiation Oncology, Biology, Physics* **2019**, minor revision.

- **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. sp²-sp³ 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 allenolates 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 Eradication, 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, W.L. 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.

- **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).

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)

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-present	--
8.	Dr. Joseph Salamoun	University of Pittsburg	09/01/2017-present	
9.	Jan Nekvinda	Charles University, Prague	10/01/2018-present	

- **Current Graduate Students**

	Student Name	University Affiliation	Year Entered	Expected Graduation
1.	Ashley Peralta	Hampton University	2014	Spring 2019
2.	Russell Fritzemeier	Virginia Tech	2016	Spring 2020
3.	Ashely Gates	Penn State University	2016	Spring 2020
4.	Eric Medici	Davidson College	2015	Spring 2020
5.	Christopher Sibley	Virginia Tech	2015	Spring 2020
6.	Jacob Murray	Nazarene College, NY	2016	Spring 2021

7.	Jose Santiago-Rivera	Univ. of Puerto Rico	2016	Spring 2021
8.	Christopher Garcia	Cal State University	2017	Spring 2022
9.	Daniel Foster	Purdue University	2017	Spring 2022
10.	Johnathan Bowen	Wake Forest University	2017	Spring 2022
11.	Connor Szwetkowski	Rider University	2017	Spring 2022

- **Previous Graduate Students**

	Student Name	Year Graduated	Degree	Current Position
1.	Hao Li	2018	Ph.D.	Postdoc with Pablo Sobrado
2.	Russell Snead	2018	Ph.D.	
3.	Cheryl Peck	2017	Ph.D.	Postdoc with Frank Gupton, VCU
4.	Elizabeth Childress	2017	Ph.D.	Postdoc with Craig Lindsley, Vanderbilt U
5.	Molly Congdon	2016	Ph.D.	NIH Postdoc
6.	Amanda Nelson	2016	Ph.D.	Staff scientist at Stanford Chemistry
7.	Jessica Wynn	2016	Ph.D.	Scientist at Merck Inc.
8.	Kenneth Knott	2015	MS	Analytical Services, Virginia Tech
9.	Emily Morris	2015	MS	Teacher at Manassas High School
10.	Xi Guo	2014	Ph.D.	Rutgers University Statistics
11.	Joseph Calderone	2014	MS	R&D Engineer at Afton Chemicals
12.	Wenyu Zhang	2014	Ph.D.	Postdoc at NIH with Kuan Wang
13.	Mithun Raje	2012	Ph.D.	Postdoc at Johns Hopkins with Takashi Tsukamoto
14.	David Bryson	2012	Ph.D.	Postdoc at Harvard University with David Liu
15.	Jason Crumpton	2012	Ph.D.	Assistant Professor at Lynchburg College
16.	Brandon Thorpe	2012	Ph.D.	Project Manager at Center for Open Science
17.	Jing Sun	2010	MS	BASF
18.	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.	Laura Wonilowicz	Biochemistry Fralin Summer Research Fellow	2019
2.	Greg Traverse	Chemistry	2019
3.	Jonathan Roof	Chemistry	2019

- **Previous Undergraduate Students**

	Student Name	Degree	Year	Current Position
4.	Brett Rastatter	Integrated Science Curriculum	2017	unknown

5. Zach Powers	Chemistry	2017	Unknown
6. Sean M. Rafferty	Chemistry	2015	Grad Student Ohio State
7. Christopher Sibley	Biochemistry	2015	Grad Student VT
8. Michael Lazear	Biochemistry	2015	Grad Student Scripps, CA
9. Matthew Nguyen	BS, Biochemistry 2 nd Place Winner, Undergrad Research Poster Arthur Meakin Scholar, 2013 McKnight Prize in Chemistry, James Lewis Howe Award	2014	VCU School of Medicine
10. Joseph Hirst	Biochemistry	2014	1 yr break before Med School
11. Kris Manino	BS, ChemEng	2013	Unknown
12. Julie Ta	BS, Biochemistry 1 st Place Winner, Undergrad Research Poster	2011- 12	Medical School
13. Valerie Rojas	BS, Chemistry NIH PREP Scholar	2012	Grad student at Duke University, Cancer Center
14. Joseph Calderone	BS, Chemistry	2011	Grad Student at VA Tech Academic Excellence Awardee, Outstanding Undergrad Research Award, 1 st Place Winner: Undergrad Poster Session
15. Leah Heist	BS, Chemistry	2011	Grad Student at UNC, Chapel Hill Arthur Meakin Scholar, Academic Excellence Awardee
16. Marietou Paye	BS, Biochemistry NIH PREP Scholar	2010	Grad Student at Georgia Tech
17. Evan Gilius	BS, Biochemistry	2009	Unknown
18. Allison Pagano	BS, Biochemistry	2009	Medical School
19. Ryan Stephens	BS, Biochemistry Arthur Meakin Scholar	2009	UNC Medical School
20. Wes Morris	BS, Chemistry	2009	Grad Student at Cornell University James L. Howe Awardee, HyperCube Scholar
21. Brandon Thorpe	BS, Biochemistry	2009	Senior Research Scientist, Sphynknx Therapeutics, LLC
22. Caitlyn Criss	BS, Biochemistry	2008	WVU School of Osteopathic Medicine
23. 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 Osteopathic 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 C₂S-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 Alcalá 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.

Professional/Scientific Presentations

1. 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)
2. 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)
3. 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)
4. 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)

5. 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)
6. 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)
7. 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)
8. 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)
9. 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)
10. 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)
11. 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)
12. Santos, W.L. "Toward Borylation Reactions in Aqueous Medium", Dalton 2016, University of Warwick, Coventry, UK, March 29, 2016. (Invited oral)
13. Santos, W.L. "Branched peptide boronic acids: molecular recognition of folded HIV-1 RNA structures", Pacificchem, Honolulu, Hawaii, December 17, 2015 (invited oral)
14. Santos, W.L. "Copper-catalyzed Borylation and Silylation Reactions in Water", Pacificchem, Honolulu, Hawaii, December 18, 2015. (invited oral)
15. Santos, W.L. "Copper-Catalyzed Borylation: Towards Sustainable Chemistry", Todd Marder Symposium, Wurzburg, Germany, Nov. 16, 2015. (invited oral)
16. Santos, W.L. "Progress Toward Borylation Reactions in Water", IUPAC Sustainable Catalysis, Busan, South Korea, August 13, 2015 (invited oral)
17. 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)

18. 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)
19. 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)
20. 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)
21. 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)
22. 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).
23. 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)
24. 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)
25. Santos, W.L. "Disrupting RNA-protein interactions with branched peptides," Bioorganic Gordon Research Conference, June 16, 2011, Proctor Academy, Andover, NH. (Oral Contribution, Invited)
26. 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)
27. 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)
28. 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)
29. Santos, W.L. "Inhibiting TAR RNA with Branched Peptides," Chemistry and Biology of Peptides Gordon Conference, Ventura, CA, February 2010. (Poster Contribution)

30. 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)
31. Santos, WL; Gao, M; Thorpe, SB. sp²-sp³ 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)
32. Santos, W.L. "Targeting RNA with Branched Peptide Libraries," Bioorganic Chemistry Gordon Conference, Proctor Academy, Andover, NH, June 2010. (Poster Contribution)
33. 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)
34. Santos, W.L. sp²-sp³ 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)
35. 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)
36. Santos, W.L. "Developing New RNA Ligands," Bioorganic Chemistry Gordon Conference, Procter Academy, Andover, NH, June 15-20, 2008. (Poster Contribution)
37. Santos, WL. Targeting RNA with small molecules. 10th Eurasia Conference on Chemical Sciences. Jan 2008, Manila, Philippines. (Oral Contribution)
38. Santos, WL. New RNA Selective Ligands. 236th ACS National Meeting, Philadelphia, PA, USA, August 2008. (Poster Contribution)
39. Santos, W.L. "RNA as a Therapeutic Target," Bioorganic Gordon Conference, June 10-15, 2007, Procter Academy, Andover, NH. (Poster Contribution)

Active Research Support

R01AI144026	Santos, Lynch MPI		01/15/2019-12/31/2023
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).			
5R01GM121075	Santos, Lynch MPI	\$2,100,000	09/01/2016-08/31/2020
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).

Virginia Catalyst Santos, PI \$400,000 07/01/2018-06/30/2019

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).

Continuum Biosciences, Inc. Santos, PI \$516,312 05/01/2018-08/31/2019

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.

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.

R01AI144026 Santos, Lynch MPI \$2,800,000 04/01/2019-03/31/2024

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).

R01DK122445 Santos, Hoehn MPI \$2,978,893 07/01/2019 - 06/30/2024

NIH/NIDDK

pending, not yet reviewed

Selective mitochondrial uncouplers for the treatment of NASH

The goal of the proposed research is to develop small molecule mitochondrial uncouplers into drug-like leads for testing in non-alcoholic steatohepatitis (NASH) mouse models. This work will be performed in collaboration with Prof. Kyle Hoehn (University of Virginia, Pharmacology, Charlottesville, VA).

- **Completed Research Support**

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.

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.

Teaching Experience

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
2009	Fall	Chem 5505	Advanced Organic Chemistry	23	3.6
	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	3	3.87
2017	Spring		Teaching buy-out	--	--
	Fall		Teaching buy-out		
2018	Spring		Teaching buy-out		
	Fall		Teaching buy-out		

*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, **2017**

Personnel Committee, **2015-2016**

Executive Committee, **2014-2015, 2017-2019**

Graduate Education Committee Chair, **2013-present**

Seminar 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**

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*, *Monatshefte für 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).

(4) *Netherlands Organisation for Scientific Research*

(5) *Cottrell Scholar Awards*

- Editorial Board, *Medicinal Research Reviews*, Associate Editor, *Diversity Oriented Synthesis*; Editorial Advisory Board, *Current Topics in Medicinal Chemistry*; Editorial Board, *Journal of Biochemistry and Molecular Biology Research*
- International meeting organizer and host at Virginia Tech, Blacksburg, VA, Boron in the Americas (BORAM XVII, June 2020). 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 fore-front of science dealing with boron.
- 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.