
SCOTT GRONERT

Department of Chemistry,
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Education

- 1983-1987 University of California, Berkeley
Ph.D. in Chemistry
- 1979-1983 California State University at Long Beach
B.S. in Chemistry, Minor in Mathematics
Graduated with Highest Honors

Professional Positions

- 2007-present Virginia Commonwealth University
Professor
- 2016-present Virginia Commonwealth University
Associate Dean, College of Humanities and Sciences
- 2009-2015 Virginia Commonwealth University
Chair, Department of Chemistry
- 1997-2006 San Francisco State University
Professor
- 1994-1997 San Francisco State University
Associate Professor
- 1990-1994 San Francisco State University
Assistant Professor
- 1987-1990 University of Colorado, Boulder
Post-Doctoral Research Associate

Leadership Roles

- Associate Dean of Research, College of Humanities and Sciences, Virginia Commonwealth University
 - College includes 18 departments and schools with over 14,000 majors
 - Over \$17 million in research expenditures in 2015-16.
- Chair, Department of Chemistry, Virginia Commonwealth University.
 - Department is in the top 15 in US in BS Chemistry Degrees (IPEDS data 2013), with over 500 majors and > 35,000 credit hours of instruction.
 - Department is #6 in US for BS Chemistry Degrees for women (IPEDS data 2013).

Highlights

- BS Chemistry degrees increased from 59 (2008/9) to 134 (2014/5).
 - Secured funding for and recruited 14 new faculty positions.
 - Secured over \$700,000 in industrial funds to support program.
 - Realigned staff and created first multi-department fiscal service center.
 - Fully renovated 5 teaching laboratories and three research laboratories.
 - Developed new departmental P&T and workload guidelines.
- Chair, Virginia Section of the American Chemical Society (2014)
 - Chair, Dean Search Committee, School of Science and Engineering, San Francisco State University.
 - Program Director of VCU's institutional effort to secure a Howard Hughes Medical Institute grant as a part of their "Inclusive Excellence: Engaging All Students in Science" program.

Honors and Awards

2016	Fulbright Scholar
2015	Associate Member of Massey Cancer Center
2002	Northern California Phi Beta Kappa Teaching Excellence Award
2000	Wilsmore Fellow, University of Melbourne
1986-1987	W. R. Grace Fellowship
1983-1984	University Fellowship
1983	Outstanding Graduate in School of Natural Sciences

Research

Publications (since 2011)

Career Hirsch Index (h-index) = 35; Citations > 3500; 9 papers with 100+ citations.

96. Gronert, S.; Keeffe, J. R.; O'Ferrall, R. A. M., Stabilities of Carbenes: Independent Measures for Singlets and Triplets *J. Am. Chem. Soc.* **2011**, *133*, 3381-3389.
97. Clodfelter, W. C.; Wong, E. H.; Hay, K. A.; Gronert, S. Gas-Phase Ligand Binding to Jacobsen's Manganese Salen Catalyst: Functional Group and Steric Effects, *Int. J. Mass Spectrom.*, **2011**, *305*, 40-44.
98. Garver, J. M.; Gronert, S. Bierbaum, V. M. Experimental validation of the α -effect in the gas phase, *J. Am. Chem. Soc.* **2011**, *133*, 13894-13897.
99. Liu, Q.; Simpson, D. C.; Gronert, S. The Reactivity of Human Serum Albumin towards trans-4-Hydroxy-2-nonenal *J. Mass. Spectrom.* **2012**, *47*, 411-424.
100. Nettey, S., Swift, C. A.; Joviliano, R., Noin, D. O.; Gronert, S. The Impact of Substituents on the Transition States of S_N2 and $E2$ reactions in Aliphatic and Vinylic Systems: Remarkably Facile Vinylic Eliminations *J. Am. Chem. Soc.*, **2012**, *134*, 9103-9110.
101. Aldajaei, J. T.; Gronert, S. The Gas-Phase Reactions of Metal Porphyrins with Diazoacetate Esters *Int. J. Mass Spectrom.* **2012**, *316-318*, 68-75.
102. Huang, S.; Gronert, S.; Wu, W. Polarization in the structures of uracil and thiouracils: Implication for binding with orotidine 50-monophosphate decarboxylase *Bioorg. Med. Chem. Lett.* **2011**, *21*, 6341-6342.
103. Garver, J. M.; Yang, Z.; Nichols, C. M.; Worker, B. B.; Gronert, S. Bierbaum, V. M. Resolving the α -effect in gas phase S_N2 reactions: A Marcus theory approach. *Int. J. Mass Spectrom.*, **2012**, *316-318*, 244-250.
104. Senger, N. A.; Bo, B.; Cheng, Q.; Keeffe, J. R.; Gronert, S.; Wu, W. M., The Element Effect Revisited: Factors Determining Leaving Group Ability in Activated Nucleophilic Aromatic Substitution Reactions. *J. Org. Chem.* **2012**, *77*, 9535-9540.
105. Ugur, Z.; Coffey, C. M.; Gronert, S., Comparing the efficiencies of hydrazide labels in the study of protein carbonylation in human serum albumin. *Anal. Bioanal. Chem.* **2012**, *404*, 1399-1411.
106. Kudavalli, J. S.; Rao, S. N.; Bean, D. E.; Sharma, N. D.; Boyd, D. R.; Fowler, P. W.; Gronert, S.; Kamerlin, S. C. L.; Keeffe, J. R.; O'Ferrall, R. A. M., Base-Catalyzed Dehydration of 3-Substituted Benzene cis-1,2-Dihydrodiols: Stabilization of a Cyclohexadienide Anion Intermediate by Negative Aromatic Hyperconjugation, *J. Am. Chem. Soc.* **2012**, *134*, 14056
107. Senger, N. A.; Bliss, C. E.; Keeffe, J. R.; Gronert, S.; Wu, W. Stabilities of uracil and pyridone-based carbanions: a systematic study in the gas phase and solution and implications for the mechanism of orotidine-50-monophosphate decarboxylase. *Tetrahedron* **2013**, *69*, 5287-5292.
108. Gronert, S., "Electron Delocalization is not a Satisfactory Explanation for the Preference

- for Branching in the Alkanes", *Chem. Eur. J.* **2013**, *19*, 11090-11092.
109. Erden, I.; Maa, J.; Gartner, C.; Azimi, S.; Gronert, S. Temperature-dependent, competitive 1,3-acyl shift versus decarbonylation of a cyclopropanone intermediate. *Tetrahedron* **2013**, *69*, 5044-5047.
110. Liu, Q.; Simpson, D. C.; Gronert, S., Carbonylation of mitochondrial aconitase with 4-hydroxy-2-(*E*)-nonenal: Localization and relative reactivity of addition sites. *Biochim. Biophys. Acta, Proteins Proteomics* **2013**, *1834*, 1134-1144.
111. Gronert, S.; Keeffe, J. R. "Calculated stabilities and structures for carbocations and singlet carbenes bearing electron-withdrawing groups", *J. Phys. Org. Chem.* **2013**, *26*, 1023-1031.
112. Eanes, A. D.; Noin, D. O.; Kebede, M. K.; Gronert, S. "Nucleophilic Aromatic Substitution with Dianions: Reactions Driven by the Release of Coulomb Repulsion", *J. Am. Soc. Mass Spectrom.*, **2013**, *25*, 10-17.
113. Duarte, F.; Gronert, S.; Kamerlin, S. C. L. "Concerted or Stepwise: How Much Do Free-Energy Landscapes Tell Us about the Mechanisms of Elimination Reactions?" *J. Org. Chem.* **2014** *79*, 1280-1288.
114. Child, B. Z.; Giri, S.; Gronert, S.; Jena, P. "Aromatic Superhalogens" *Chem.- Eur. J.* **2014** *20*, 4736-4745.
115. Soukup, L. L.; Gronert, S. "The Gas-Phase Reactions of Localized and Delocalized Carbanions with Aryl Halides: Competition between Attack on the π -System and the Periphery", *Int. J. Mass Spectrom.*, **2015**, *378*, 31-37.
116. Erden, I.; Gronert, S.; Keeffe, J. R.; Ma, J.; Ocal, N.; Gartner, C.; Soukup, L. L. "Effect of Allylic Groups on S_N2 Reactivity" *J. Org. Chem.*, **2014**, *79*, 6410-6418.
117. Bowler, J. T.; Wong, F. M.; Gronert, S. Keeffe, J. R.; Wu, W. "Reactivity in the Nucleophilic Aromatic Substitution Reactions of Pyridinium Ions", *Org. Biomol. Chem.*, **2014**, *12*, 6175-6180.
118. Narayanasamy, S.; Simpson, D. C.; Martin, I.; Grotewiel, M. S.; Gronert, S. "Paraquat Exposure and sod-2 Knockdown have Dissimilar Impacts on the Drosophila Melanogaster Carbonylated Protein Proteome", *Proteomics*, **2014**, *14*, 2566-2577.
119. Gronert, S.; Garver, J. M.; Nichols, C. M.; Worker, B. B.; Bierbaum, V. M. "Dehalogenation of Arenes via S_N2 Reactions at Bromine: Competition with Nucleophilic Aromatic Substitution", *J. Org. Chem.*, **2014**, *79*, 11020-11028.
120. Bowler, J. T.; Wong, F. M.; Gronert, S.; Keeffe, J. R.; Wu, W. M. "Reactivity in the nucleophilic aromatic substitution reactions of pyridinium ions", *Org. & Biomol. Chem.*, **2014**, *12*, 6175-6180.
121. Aluri, H. S.; Simpson, D. C.; Allegood, J. C.; Szczepanel, K.; Gronert, S.; Chen, Q.; Lesnefsky, E. J. "Electron flow into cytochrome c coupled with reactive oxygen species from the electron transport chain converts cytochrome c to a cardiolipin peroxidase: role during ischemia-reperfusion:", *Biochim. Biophys. ACTA Gen. Sub.* **2014**, *1840*, 3199-3207.
122. Swift, C A.; Gronert, S. "Formation and Reactivity of Gold Carbene Complexes in the Gas Phase", *Organometallics*, **2014**, *33*, 7135-7140.
123. Maclagan, R. G. A. R.; Gronert, S.; Meot-Ner (Mautner), M. "Protonated Polycyclic Aromatic Nitrogen Heterocyclics: Proton Affinities, Polarizabilities, and Atomic and Ring Charges of 1-5-Ring Ions", *J. Phys. Chem. A* **2015**, *119*, 127-139.
124. Wiseman, A.; Sims, L. A.; Snead, R.; Gronert, S.; Maclagan, R. G. A. R.; Meot-Ner (Mautner), M. "Protonation Energies of 1-5-Ring Polycyclic Aromatic Nitrogen Heterocyclics: Comparing Experiment and Theory", *J. Phys. Chem. A*, **2015**, *119*, 118-126.

125. Coskun, N; Cetin, M.; Gronert, S.; Ma, J. X.; Erden, I. "Pyrrolidine catalyzed reactions of cyclopentadiene with alpha,beta-unsaturated carbonyl compounds.: 1,2-versus 1,4-additions", *Tetrahedron*, **2015**, *71*, 2636-2642.
126. Swift, C. A.; Gronert, S. "Intermolecular C-H Bond Activation by a Cationic Iridium(III) Dichloride Phenanthroline Complex", *Angew. Chem. Int. Ed.*, **2015**, *54*, 6475-6478.
127. Aldajaei, J. T. Keeffe, J. R.; Swift, C. A.; Gronert, S. "Are Copper(I) Carbenes Capable Intermediates for Cyclopropanations? The Case for Ylide Intermediates", *Chem Eur. J* **2015** *21*, 12702-12708.
128. Saunders, W. H.; Gronert, S. "The Competition Between Pathways in the Reactions of a Wide Variety of Bases with 2-Fluoro and 2-Chlorobutane in the Gas Phase", *J. Org. Chem.*, **2015**, *80*, 10787-10793.
129. Davis, M. C.; Gronert, S. "A Mass Spectrometric Method for Rapidly Assaying the Chiral Selectivities of the Copper(I) Complexes of C₂-Symmetric Ligands", *J. Mass Spectrom.*, **2015**, *50*, 1279-1287.
130. Coffey, C. M.; Gronert, S. "A Cleavable Biotin Tagging Reagent that Enables the Enrichment and Identification of Carbonylation Sites in Proteins", *Anal. Bioanal. Chem.* **2016**, *408*, 865-874
131. Derkits, D.; Wiseman, A.; Snead, R. F.; Dows, M.; Harge, J.; Lamp, J. A.; Gronert, S. "Development and Evaluation of a Variable-Temperature Ion Trap Mass Spectrometer", *J. Am. Soc. Mass Spectrom.* **2016**, *27*, 339-343.
132. Erden, I.; Basada, J.; Poli, D.; Cabrera, G.; Xu, F.; Gronert, S. "Unusual Hydroxyl Effect on Fulvene Endoperoxide Decompositions", *Tetrahedron Lett.*, **2016**, *57*, 2190-2193.
133. Ugur, Z.; Gronert, S. "A Robust Analytical Approach for the Identification of Specific Protein Carbonylation Sites: Metal-Catalyzed Oxidations of Human Serum Albumin", *Anal. Lett.* **2016**, in press.

Book Chapters

1. Gronert, S., "Carbanions" in *Reactive Intermediate Chemistry*, Moss, R. A.; Platz, M. S.; Jones, M. J., Ed. Wiley Interscience: Hoboken, NJ, 2004; 69-120.
2. Lambert, J. ;Gronert, S.; Survell, H; Lightner, D. *Organic Structural Spectroscopy*, Pearson, New York, 2010, Chapters 7-10.
3. Gronert, S.; Keeffe, J. R.; More O'Farrell, R. A. in *Contemporary Carbene Chemistry*, Moss R. A.; Doyle M. S., Eds. Wiley, New York, NY, 2013, Chapter 1.

External Grant Support (since 2010)

Career Funding > \$4,500,000.

1. ACS-PRF, "Models for Heterogeneous Single Atom and Small Cluster Catalysts on Graphene: A Novel Gas Phase Approach", \$110,000 (total), July 2016 (2 year funding)
2. NSF, "Gas-Phase Studies of Organic Reaction Mechanisms", \$380,000 (total), May 2016, (3 year funding)
3. NSF, "Gas-Phase Studies of Organic Reaction Mechanisms", \$250,000 (total), November 2013 (2.5 year funding).
4. NSF, "Gas-Phase Studies of Organic Reaction Mechanisms", \$408,000 (total) November 2010 (3 year funding).
5. NIH-R01, "Mass Spectrometric Studies of Protein Oxidation: Aging and Environmental Factors", Funded, PI. \$980,000 (total), April 2010, (4 year funding).

Invited Presentations (since 2010)

1. When Radicals And Proteins Meet - A Tangled Path To Aging And Organ Failure, Pittcon Lecture, Duquesne University, October 2016.
2. Ion Trap Reactors to the Rescue: A Tool to Solve Problems in Organic and Organometallic Chemistry, Duquesne University, October 2016.
3. Ion Trap Reactors to the Rescue: A Tool to Solve Problems in Organic and Organometallic Chemistry, University of Oslo, June 2016.
4. Ion Trap Reactors to the Rescue: A Tool to Solve Problems in Organic and Organometallic Chemistry, Pierre and Marie Curie Institute, University of Paris, June 2016.
5. When Radicals And Proteins Meet - A Tangled Path To Aging And Organ Failure, University of Lille 1, PRISM Laboratory Colloquium, January 2016.
6. Ion Trap Reactors to the Rescue: A Tool to Solve Problems in Organic and Organometallic Chemistry, VCU Chemistry, October 2015.
7. When Radicals And Proteins Meet - A Tangled Path To Aging And Organ Failure, VCU College of Humanities and Sciences Faculty Recognition Day, October 2015.
8. Computers in Scientific Discovery 7, June 2015, "Experimental and Computational Studies of C-H Bond Activation and Aromatization of Hydrocarbons by an Iridium (III) Complex"
9. University of Sao Paulo, November 2013, "Mass Spectrometry of Protein Oxidations: The Aging of the Proteome."
10. Virginia Tech University, February 2013, "Mass Spectrometry: A Powerful Tool for Studying Reaction Mechanisms."
11. Old Dominion University, April 2012, "Mass Spectrometry: A Powerful Tool for Studying Reaction Mechanisms."
12. San Francisco State University, April 2012, "Mass Spectrometry: A Powerful Tool for Studying Reaction Mechanisms."
13. University of Colorado, April 2011, "Aldehydes in Your Proteins: The Tree-Rings of Human Aging? A Proteomics Study"
14. Pacifichem 2010, Honolulu, HI, December 2010, "Tactics for the Analysis Of Protein Carbonyl Modifications From In Vitro And In Vivo Oxidative Stress"
15. VCU (Institute for Structural Biology), November 2010, Mass Spectrometry of Protein Oxidations: The Aging of the Proteome."
16. FACSS National Meeting, October 2010, Mass Spectrometry of Protein Oxidations: The Aging of the Proteome."
17. Howard University, March 2010, "Mass Spectrometry: A Powerful Tool for Studying Reaction Mechanisms."
18. Grinnell College, March 2010, "Mass Spectrometry: A Powerful Tool for Studying Reaction Mechanisms."