

Curriculum Vitae

VELUPILLAI, SANTHANA M

University of Iowa
W184 Chemistry Building
Iowa City, IA 52242
319-335-1336, 319-353-2291
santhana-velupillai@uiowa.edu

EDUCATION

- Indian Institute of Technology, Madras, India
Ph.D. in Chemistry 1990
Dissertation: "NMR Relaxation and Nuclear Overhauser Effect: Theory and Applications to Chemical and Biological Systems"
- The American College, Madurai, Tamil Nadu, India
M. Sc. in Chemistry 1983
Thesis: "Studies on the Kinetics of Iodination of N, N-Dimethyl Aniline by Iodine Mono-chloride in Aqueous Sulfuric Acid"
- The M.D.T. Hindu College
B.Sc. in Chemistry 1981
Areas of Concentration: Physical Chemistry
Minor: Mathematics and Physics

POSITIONS AND HONORS

EMPLOYMENT

- University of Iowa, Iowa City, Iowa
Director, University of Iowa Central NMR Facility, Department of Chemistry 2011
- University of Iowa, Iowa City, Iowa
Associate Research Scientist, Department of Chemistry 2005
Director, NMR Facilities, OVPR and Department of Chemistry
- University of Iowa, Iowa City, Iowa
Associate Research Scientist, Department of Chemistry 2004
Director, NMR Facility, Department of Chemistry
Co-Director, High-Field NMR Research Facility, OVPR
- University of Illinois, Chicago, Illinois
Research Assistant Professor, College of Pharmacy 2001
Director, NMR Facility, College of Pharmacy

University of Texas, San Antonio, Texas
Research Associate IV, Department of Chemistry **2000**
Teaching Faculty, Department of Chemistry

Los Alamos National Laboratory, Los Alamos, New Mexico
Technical Staff Member, Theoretical Biology and Biophysics Group **1997**
Technical Staff Member, Life Science Division

PROFESSIONAL TRAINING

Postdoctoral Fellowship, *Los Alamos National Laboratory, Los Alamos, New Mexico* **1994**
Postdoctoral Fellowship, *University of California, Riverside, California* **1991**
Graduate Research Fellow, *Indian Institute of Technology, Madras, India* **1983**

RESEARCH INTERESTS

Solution- and Solid-State NMR spectroscopy of Chemical and Biological Materials, Structural biology, Bimolecular Structure and Dynamics, Structure and function of nucleic acids and proteins, Medicinal chemistry, Metabolomics, NMR education

HONORS, GRANTS AND AWARDS

CLAS Student Technology Fee Off-Cycle Award "Acquisition of Refurbished Base Control Unit for SampleXpress-60 Autosampler", \$12,335 **2022-2023**

CLAS Student Technology Fee off-cycle Award (Chemistry-23101) "Acquisition of 400-MHz Radio-Frequency Console and Autosampler", \$171,335 **2022-2023**

Co-PI (PI, James B. Gloer), *NSF/Major Research Instrumentation (MRI) (NSF ID: 2017828) "Acquisition of a 400-MHz NMR Spectrometer with Nitrogen-Cooled Probe"*, \$431,230 **2020-2023**

Review Panelist, NSF, Major Research Instrumentation Grant Program, NMR/EPR Section **2021-2022**

Review Panelist, NSF, Major Research Instrumentation Grant Program, NMR/EPR Section **2016-2017**

CLAS Student Technology Fee off-cycle Award "Upgrade of Instructional NMR Computer and Software", \$6,600 **2014-2015**

Co-PI (PI, James B. Gloer), *NIH Shared Instrumentation Grant Award (NIH ID: 1 S10 RR025500-01) "Acquisition of a 600-MHz Nuclear Magnetic Resonance Spectrometer"*, \$500,000 **2009-2012**

Co-PI (PI, David E. Wiemer), <i>NSF Shared Instrumentation Grant Award (NSF ID: 0840371) "Acquisition of a Cyber Enabled 500-MHz Solid State NMR Spectrometer"</i> , \$512,460	2009-2012
Co-PI, <i>University of Iowa Matching Funds Award</i> , Office of the Vice President for Research, University of Iowa, Iowa City, Iowa, \$74,000	2008-2009
Co-PI, <i>University of Iowa Matching Funds Award</i> , Office of the Vice President for Research, University of Iowa, Iowa City, Iowa, \$89,000	2008-2009
PI, <i>Campus Research Board Award</i> , University of Illinois at Chicago, Chicago, Illinois, "DNA Triplexes in Friedreich's Ataxia: Biophysical and Structural Studies", \$12243	2002-2003
PI, <i>Integrative Structural Biology Research Award</i> , Los Alamos National Laboratory, Los Alamos, New Mexico, \$5,000	1991-1994
Council of Scientific and Industrial Research Fellow, <i>India</i>	1987-1991
Department of Science and Technology Fellow, <i>India</i>	1983-1987

RECENT PUBLICATIONS

S. L. Tun, S. V. *Santhana Mariappan* and F. C. Pigge, "Imidazolidine hydride donors in palladium-catalyzed alkyne hydroarylation", *J. Org. Chem.* **2022**, 87, 8059-8070.

C. E. Peroza, F. Chen, D.E. Wurster and S. V. *Santhana Mariappan**, "Solubilization of Organics I: ¹H NMR chemical shift perturbations, diffusometry, and NOESY indicate biphenyls internalize in micelles formed by cetyltrimethylammonium bromide", *Magn. Reson. Chem.* **2019**, 57, 1097-1106.

G. Campillo-Alvarado, K. P. D'mello, D. C. Swenson, S. V. *Santhana Mariappan*, H. Höpfl, H. Morales-Rojas and L. R. MacGillivray, "Exploiting Boron Coordination: B←N Bond Supports a [2+2] Photodimerization in the Solid State and Generation of a Diboron Bis-Tweezer for Benzene/Thiophene Separation", *Angew. Chem. Int. Ed.* **2019**, 58, 1-5.

G. Campillo-Alvarado, K. Aslan, M. A. Sinnwell, E. W. Reinheimer, S. V. *Santhana Mariappan*, L. R. MacGillivray, R. H. Gronenman, "A solid-state [2+2] photodimerization involving coordination of Ag(I) ions to 2-pyridyl groups", *J. Coord. Chem.* **2018**, 71, 2875-2883.

Q. Chu, A. J. E. Duncan, G. S. Papaefstathiou, T. D. Hamilton, M. B. J. Atkinson, S. V. *Santhana Mariappan* and L. R. MacGillivray, "Putting cocrystal stoichiometry to work: A reactive hydrogen bonded Superassembly enables nanoscale enlargement of a metal-organic rhomboid via a solid state photocycloaddition", *J. Am. Chem. Soc.* **2018**, 140, 4940-4944.

RECENT PRESENTATIONS

C.A. Peroza, F. Chen, S. V. *Santhana Mariappan* and D.E. Wurster, "Solubilization of Biphenyl Analogs in Cationic, Neutral and Anionic Surfactants", From Abstracts, American Association of Pharmaceutical Scientists Annual Meeting and Exposition, San Diego, United States, November 2-6 (2014), W-5129.

R.C. Laird, N.P. Nguyen, S.F. Rusch, D.C. Swenson, S.V. *Santhana Mariappan*, J. Baltrusaitis, and L.R. MacGillivray, "Towards modularity in engineering reactivity in the crystalline state", From Abstracts, 48th Midwest Regional Meeting of the American Chemical Society, Springfield, MO, United States, October 16-19 (2013), NWRM-143.

R.A. Friedman, F. Chen, S. V. *Santhana Mariappan* and D.E. Wurster, "Dehydration of Theophyllin Monohdrate under Mechanical Load as a Function of Molecular Mobility", From Abstracts, American Association of Pharmaceutical Scientists Annual Meeting And Exposition, San Antonio, TX, United States, November 10-14 (2013), W-5129.

E. P. Azevedo, S.V. *Santhana Mariappan*, Vijay Kumar, "Preparation and Characterization of Oxidized Chitosans ", From Abstracts, 44th Midwest Regional Meeting of the American Chemical Society, Iowa City, IA, United States, October 21-24 (2009), NWRM-374.

OTHER PROFESSIONAL INTERESTS

Alternative Energy, Photovoltaics, Sociology, School education

Full list of publications

51. S. L. Tun, S. V. *Santhana Mariappan* and F. C. Pigge, "Imidazolidine hydride donors in palladium-catalyzed alkyne hydroarylation", *J. Org. Chem.* **2022**, 87, 8059-8070.
50. C. E. Peroza, F. Chen, D.E. Wurster and S. V. *Santhana Mariappan**, "Solubilization of Organics I: ¹H NMR chemical shift perturbations, diffusometry, and NOESY indicate biphenyls internalize in micelles formed by cetyltrimethylammonium bromide", *Magn. Reson. Chem.* **2019**, 57, 1097-1106.
49. G. Campillo-Alvarado, K. P. D'mello, D. C. Swenson, S. V. *Santhana Mariappan*, H. Höpfl, H. Morales-Rojas and L. R. MacGillivray, "Exploiting Boron Coordination: B← N Bond Supports a [2+2] Photodimerization in the Solid State and Generation of a Diboron Bis-Tweezer for Benzene/Thiophene Separation", *Angew. Chem. Int. Ed.* **2019**, 58, 1-5.
48. G. Campillo-Alvarado, K. Aslan, M. A. Sinnwell, E. W. Reinheimer, S. V. *Santhana Mariappan*, L. R. MacGillivray, R. H. Gronenman, "A solid-state [2+2] photodimerization involving coordination of Ag(I) ions to 2-pyridyl groups", *J. Coord. Chem.* **2018**, 71, 2875-2883.

47. Q. Chu, A. J. E. Duncan, G. S. Papaefstathiou, T. D. Hamilton, M. B. J. Atkinson, S. V. *Santhana Mariappan* and L. R. MacGillivray, "Putting cocrystal stoichiometry to work: A reactive hydrogen bonded Superassembly enables nanoscale enlargement of a metal-organic rhomboid via a solid state photocycloaddition", *J. Am. Chem. Soc.* **2018**, 140, 4940-4944.
46. S. M. Oburn, D. C. Swenson, S. V. *Santhana Mariappan* and L. R. MacGillivray, "Supramolecular construction of an aldehyde-cyclobutane via the solid state: Combining reversible imine formation and metal-organic self-assembly", *J. Am. Chem. Soc.* **2017**, 139, 8452-8454.
45. A. J. E. Duncan, R. L. Dudovitz, S. J. Dudovitz, J. Stojakovic, S. V. *Santhana Mariappan* and L. R. MacGillivray, "Quantitative and Regiocontrolled Cross-photocycloaddition of the Anticancer Drug 5-fluorouracil Achieved in a Cocrystal", *Chem. Comm.* **2016**, 52, 13109-13111.
44. A. I. Lansakara, S. V. *Santhana Mariappan* and F. C. Pigge, "Alkylidene dihydropyridines as synthetic intermediates: Model Studies toward the Synthesis of the Bis(piperidine) Alkaloid Xestoproxamine C", *J. Org. Chem.* **2016**, 81, 10266-10278.
43. O. Wangpradit, A. Rahaman, S. V. *Santhana Mariappan*, G. R. Buettner, L. W. Robertson and G. Luthe, "Breaking the dogma: PCB-derived semi-quinone free radicals do not form covalent adducts with DNA, GSH, and amino acids", *Environ. Sci. Pollut. Res.* **2016**, 23, 2138-2147.
42. R. C. Laird, M. A. Sinnwell, N. P. Nguyen, D. C. Swenson, S. V. *Santhana Mariappan* and L. R. MacGillivray, "Intramolecular [2+2] Photodimerization Achieved in the Solid State via Coordination-driven Self-assembly", *Org. Lett.* **2015**, 17, 3233-3235.
41. S. E. Lehman, Y. Tataurova, P. S. Mueller, S. V. *Santhana Mariappan* and S. C. Larsen, "Ligand Characterization of Covalently-functionalized Mesoporous Silica Nanoparticles: An NMR Toolbox Approach", *J. Phys. Chem. C* **2014**, 118, 29943-29951.
40. E. P. Azevedo, S.V. *Santhana Mariappan**, and Vijay Kumar, "Preparation and Characterization of Chitosans Carrying Aldehyde functions Generated by Nitrogen Oxides", *Carbohydrate Polymers* **2012**, 87, 1925-1932.
39. D-K Bucar, A. Sen, S.V. *Santhana Mariappan*, and L.R. MacGillivray, "A [2+2]" Cross-photodimerization of Photostable Olefins via a Three-component Cocrystal Solid Solution", *Chem. Commun.* **2012**, 48, 1790-1792.
38. D.G. Anderson, S.V. *Santhana Mariappan*, G. R. Buettner, and J. A. Doorn, "Oxidation of 3,4-Dihydroxyphenylacetaldehyde, a Toxic Dopaminergic Metabolite, to a Semiquinone Radical and an *ortho*-Quinone *J. Biol. Chem.* **2011**, 286, 26978-26986.
37. M. B. J. Atkinson, S.V. *Santhana Mariappan*, D-K Bucar, J. Baltrusaitis, T. Friscic, N.G. Sinada, and L.R. MacGillivray, "Crystal Engineering Rescues a Solution Organic Synthesis in a

- Cocrystallization that Confirms the Configuration of a Molecular ladder”, *PNAS* **2011**, 108, 10974-10979.
36. M. B. J. Atkinson, A. N. Sokolov, D-K. Bucar, S.V. *Santhana Mariappan*, M. T. Mwangi, M. C. Tiedman, and L.R. MacGillivray, “Applications of hydrogen-bond-acceptor templates to direct in-phase reactivity of a diene diacid in the solid state”, *Photochem. Photobiol. Sci.* **2011**, 10, 1384-1386.
 35. M. B. J. Atkinson, I. Halasz, D-K. Bucar, R. E. Dinnebier, S.V. *Santhana Mariappan*, A. N. Sokolov, and L.R. MacGillivray, “A solid state trimerization of a diene diacid affords a bicyclobutyl:reactant structure from x-ray powder data and product separation and structure determination via cocrystallisation”, *Chem. Comm.* **2011**, 47, 236-238.
 34. X. Wei, Q. Wu, K-K Izabela, J. C. Tharappel, S. Telu, M. C. Coleman, H. P. Glauert, K. Kuranthachalam, S. V. *Santhana Mariappan*, D. R. Spitz, J. Weydert and H-J. Lehmler, “Subacute exposure to N-ethyl perfluorooctaneamidoethanol results in the formation of perfluorooctane sulfonate and alters superoxide dismutase activity in female rats”, *Arch. of Toxicol.* **2009**, 17, 909-924.
 33. Aleksej Kronic, Dahua Pan, William J. Dunn III, and S. V. *Santhana Mariappan**, “The stereochemistry of N-methyl and aryl substituents determine the biological activities of 3-aryl-8-azabicyclo[3.2.1]oct-2,3-enes”, *Bioorg. Med. Chem.* **2009**, 17, 811-819.
 32. Orarat Wangpradit, S. V. *Santhana Mariappan*, Lynn M. Teesch, Michael W. Duffel, Karin Norstrom, Larry W. Robertson, and Gregor Luthe, “Oxidation of 4-chlorobiphenyl metabolites to electrophilic species by Prostaglandin H Synthase”, *Chem. Res. Toxicol.* **2009**, 22, 64-71.
 31. Aleksej Kronic, S. V. *Santhana Mariappan**, M. E. A. Reith and W. J. Dunn III, “Synthesis and monoamine transporter affinity of 3-aryl substituted trop-2-enes”, *Bioorg. Med. Chem. Letters* **2005**, 15, 5488-5493.
 30. S. V. *Santhana Mariappan**, X. Cheng, R. B. van Breemen, L. A. Silks, and G. Gupta, “Analysis of GAA/TTC DNA triplexes using Nuclear Magnetic Resonance and Electrospray Ionization Mass Spectrometry”, *Analytical Biochem.* **2004**, 334, 216-226.
 29. M. Appell, A. Kronic, T. J. Choi, S. V. *Santhana Mariappan*, W. J. Dunn III, M. E. A. Reith, “NMR study of conformational preferences of inhibitors of monoamine uptake”, *QSAR* **2002** 21, 38-40.
 28. J. R. Cort, S. V. *Santhana Mariappan*, C. Y. Kim, M. S. Park, T. S. Peat, G. S. Waldo, T. C. Terwilliger, and M. A. Kennedy, “Solution structure of Pyrobaculum Aerophilum DsrC, An Archaeal Homologue of the Gamma Subunit of Dissimilatory Sulfite Reductase”, *Eur. J. Biochem.* **2001**, 268, 5842-5850.
 27. R. Wu, C. C. Orji, M. Ryszard, J. G. Schmidt, Z. Li, E. M. Stocking, D. A. Ashburn, J. A. Kelly, O. Khalsa, R. A. Martinez, S. V. *Santhana Mariappan*, and L. A. Silks, “Synthesis and application

- of labeled nucleic acids, amino acids and carbohydrates", *Rec. Res. Develop. Org. & Bioinorg. Chem.* **1999**, *3*, 1-27.
26. S.V. Santhana Mariappan, P.Catasti, L.A. Silks, E.M. Bradbury and G.Gupta,"The High-resolution Structure of the Triplex Formed by the GAA/TTC Triplet Repeat Associated with Friedreich's Ataxia", *J. Mol. Biol.* **1999**, *285*, 2035-2052.
25. P.Catasti, X. Chen, S.V. Santhana Mariappan, E.M. Bradbury and G.Gupta, "DNA Repeats in Human Genome", *NATO Sci. Ser. 3: High technol. Struct. Biol. Functional Genom.* **1999**, *71*, 19-51.
24. P.Catasti, X. Chen, S.V. Santhana Mariappan, E.M. Bradbury and G.Gupta, "DNA Repeats in Human Genome", *Genetica* **1999**, *106*, 15-36.
23. C. Spiro, R. Pelletier, M. L. Rolfsmeier, M. J. Dixon, R. S. Lahue, G. Gupta, M. S. Park, X. Chen, S.V. Santhana Mariappan and C. T. McMurray, "Inhibition of FEN-1 processing by DNA secondary structure at trinucleotide repeats", *Mol. Cell* **1999**, *4*, 1079-1085.
22. S.V. Santhana Mariappan, X. Chen, P.Catasti, E.M. Bradbury and G.Gupta, "Structural studies on the unstable triplet repeats", In *Genetic Instabilities and Hereditary Neurological Diseases* (Editors, R. D. Wells and S. T. Warren) **1998**, 647-676.
21. S.V. Santhana Mariappan, L.A. Silks, E.M. Bradbury and G.Gupta, "Fragile X DNA Triplet Repeats, (GCC)_n, form Hairpins with Single Hydrogen-bonded C.C Mispairs at the CpG Sites: Isotope-edited NMR Spectroscopy on (GCC)_n with Selective ¹⁵N4-labeled Cytosine Bases", *J. Mol. Biol.* **1998**, *283*, 111-120.
20. X. Chen, S.V. Santhana Mariappan, J. J. Kelley III, J. H. Bushweller, E.M. Bradbury and G.Gupta, "A PCR-based method for uniform ¹³C/¹⁵N labeling of long DNA oligomers", *FEBS Lett.* **1998**, *436*, 372-376.
19. R. Laflamme, E. Knill, W. H. Zurek, P.Catasti and S.V. Santhana Mariappan, "NMR Greenberger-Horne-Zeilinger states", *Phil. Trans. Roy. Soc.London Ser. A: Math. Phys. Eng. Sci* **1998**, *356*, 1941-1948.
18. S.V. Santhana Mariappan, L. A. Silks, X. Chen, P. A. Springer, R. Wu, R. K. Moyzis, E. M. Bradbury, A. E. Garcia and G. Gupta, "Solution structures of the Huntington's disease DNA triplets, (CAG)_n", *J. Biomol. Struct. Dyn.* **1998**, *15*, 723-744.
17. X. Chen, S.V. Santhana Mariappan, R. K. Moyzis, E. M. Bradbury and G. Gupta, "Hairpin induced slippage and hyper-methylation of the fragile X DNA triplets", *J. Biomol. Struct. Dyn.* **1998**, *15*, 745-756.
16. C.E. Edwards, C.S. Tung, L.A. Silks, J.M. Gatewood, J.A. Fee and S.V. Santhana Mariappan*, "Probing Site-specific Interactions in Protein-DNA Complexes using Hetero-nuclear NMR

Spectroscopy and Molecular Modeling: Binding of Cro Repressor to OR3", *J. Biomol. Str. Dyn.* **1998**, *16*, 1-8.

15. S.V. Santhana Mariappan, A. E. Garcia and G. Gupta. "Structure and Dynamics of the DNA Hairpins formed by Tandemly Repeated CTG Triplets Associated with Myotonic Dystrophy", *Nucleic Acids Res.* **1996**, *24*, 775-783.
14. S.V. Santhana Mariappan, X. Chen, R. Ratliff, R. K. Moyzis, E. M. Bradbury and G. Gupta, "Solution structures of the individual single strands of the fragile X DNA triplets, (GCC)_n(GGC)_n", *Nucleic Acids Res.* **1996**, *24*, 784-792.
13. S.V. Santhana Mariappan, X. Chen, R. Ratliff, R. K. Moyzis, A. Laayoun, S. S. Smith, E. M. Bradbury and G. Gupta, "Hairpin and junction structures of fragile X triplet", *Biomol. Struct. Dyn. Proc. Conv. Discipline Biomol. Stereodyn.* **1996**, *2*, 105-119.
12. X. Chen, S.V. Santhana Mariappan, P. Catasti, R. Ratliff, R. K. Moyzis, E. M. Bradbury and G. Gupta, "Hairpins are formed by the Single DNA Strands of the Fragile X Repeats: Structure and Biological Implications", *PNAS USA* **1995**, *92*, 5199-5203.
11. J. D. Fontenot, J. M. Gatewood, S.V. Santhana Mariappan, C-P. Pau, B. S. Parekh, J. R. George and G. Gupta, "Human immunodeficiency virus (HIV) antigens: structure and serology of multivalent human mucin MUC1-HIV V3 chimeric proteins", *PNAS USA* **1995**, *92*, 315-319.
10. J. D. Fontenot, S.V. Santhana Mariappan, P. Catasti, N. Domenech, O. J. Finn and G. Gupta, "Structure of a tumor associated antigen containing a tandemly repeated immunodominant epitope", *J. Biomol. Str. Dyn.* **1995**, *13*, 245-260.
9. D. A. Keire, S. V. Santhana Mariappan, J. Peng, and D. L. Rabenstein, "Nuclear magnetic resonance studies of the binding of captopril and penicillamine by serum albumin", *Biochem. Pharmacol.* **1993**, *46*, 1059-1069.
8. S. V. Santhana Mariappan and D. L. Rabenstein, "Determination of ¹⁵N isotope effects on the acid-base equilibria of amino groups in amino acids by carbon-13 NMR", *J. Org. Chem.* **1992**, *58*, 4487-4489.
7. S. V. Santhana Mariappan and D. L. Rabenstein, "Kinetics and thermodynamics of cis-trans isomerization of captopril and related compounds", *J. Org. Chem.* **1992**, *57*, 6675-6678.
6. S. V. Santhana Mariappan and D. L. Rabenstein, "Analysis of inversion magnetization transfer experiments", *J. Magn. Reson.* **1992**, *100*, 183-188.
5. S. V. Santhana Mariappan and S. Subramanian, "Simultaneous suppression of water and broad resonances in proton NMR and its relevance to biofluids", *Magn. Reson.* **1991**, 136-149.

4. S. V. Santhana Mariappan and S. Subramanian, "Structural changes in the complexation of benzo-crown ethers – NOESY and variable temperature carbon-13 NMR study", *Magn. Reson. Chem.* **1991**, *29*, 656-666.
3. S. V. Santhana Mariappan and S. Subramanian, "Ring puckering in crown ether complexation studied by 2D NOESY", *Bull. Magn. Reson.* **1989**, *11*, 254-257.
2. S. V. Santhana Mariappan and S. Subramanian, "Optimization of NOESY and ROESY through computer simulation", *Bull. Magn. Reson.* **1989**, *11*, 258-261.
1. S. V. Santhana Mariappan, S. Subramanian, N. Chandrakumar, K. R. Rajalakshmi and S. S. Sukumaran, "Proton relaxation times in cancer diagnosis", *Magn. Reson. Med.* **1988**, *8*, 119-128.