

Recent Advances in NMR Techniques in Chemistry

69th Southwest Regional meeting of the American Chemical Society (November 16-19, 2013)
Waco Convention Center (Session Hall: Texas 116) Waco, Texas

November 17 (Sunday), 2013

Starts at 8:00 AM; each presentation is for 25 minutes with 5 minutes for discussion.

Session 1: Macromolecular Assembly and Function

Chair: Sung Joon Kim.

- 8:00 **Chuck Rice**
Department of Chemistry, University of Oklahoma
“H/D Exchange Behavior in Bacterial Spores Resistant to Hydrogen Peroxide Sterilization”
- 8:30 **Moriah Beck**
Department of Chemistry, Wichita State University
“Structural mechanism for control of actin polymerization and organization by paladin”
- 9:00 **Andrew Hinck**
Department of Biochemistry, UT Health Science Center San Antonio School of Medicine
“Ha-detection, methyl labeling, and other NMR methods for studying the assembly of ligand-receptor complexes in the TGF-beta superfamily”
- 9:30 **Tatyana Igumenova**
Department of Biochemistry and Biophysics, Texas A&M
“Protein Kinase C: structure, dynamics, and function of regulatory domains”

10:00 – 10:20 Intermission.

Session 2: Structure, Dynamics, and Function

Chair: Tatyana Igumenova.

- 10:20 **Junji Iwahara**
Department of Biochemistry & Molecular Biology, University of Texas Medical Branch
“NMR study of ion-pair dynamics at protein-DNA interfaces”
- 10:50 **Josep Rizo**
Department of Biophysics, University of Texas Southwestern Medical Center
“Using NMR to Study the Mechanism of Neurotransmitter Release”
- 11:20 **Fernando Correa**
Department of Biophysics, University of Texas Southwestern Medical Center
“Mechanisms of activation in protein switches: Understanding allosteric propagation in multidomain bacterial response regulators”

11:50 – 1:20 LUNCH BREAK.

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Session 3: Structure, Dynamics, and Function

Chair: Moriah Beck.

- 1:30 **Megan Macnaughtan**
Department of Chemistry, Louisiana State University
“NMR and Glycoproteins”
- 2:00 **Om Prakash**
Department of Biochemistry and Molecular Biophysics, Kansas State University
“Structure informs on function: A Tale of a Norovirus Protease”
- 2:30 **Christian Hilty**
Department of Chemistry, Texas A&M
“Dissolution Dynamic Nuclear Polarization of Large Molecules”

3:00 – 3:20 Intermission.

Session 4: Dynamic Nuclear Polarization (DNP)

Chair: Christian Hilty.

- 3:20 **Matthew Merritt**
Advanced Imaging Research Center, University of Texas Southwestern Medical Center
“DNP technology development and applications to intermediary metabolism”
- 3:50 **Lloyd Lumata**
Advanced Imaging Research Center, University of Texas Southwestern Medical Center
“DNP: How to produce a Texas-size nuclear polarization”
- 4:20 **Alexander Barnes**
Department of Chemistry, Washington University in St. Louis
“Dynamic Nuclear Polarization with Frequency Tunable Gyrotrons”

5:10 – 7:00 DINNER.

Speakers and poster presenters are invited to Dinner at Hilton (Brazos Ballroom A).

5:45 – 7:00 Gooch-Stephens Lecture (McLennan)

7:00 – 9:00 OPEN RECEPTION & POSTER SESSION (Brazos Ballroom).

FOOD, CASH BAR, AND POSTER SESSION 1.

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November 18 (Monday), 2013

Starts at 8:30 AM; each presentation is for 25 minutes with 5 minutes for discussion.

Session 1: Three Bs (Biofuel, Biochars, and Bodies?)

Chairs: Alexander Barnes.

- 8:30 **Sung Joon Kim**
Department of Chemistry and Biochemistry, Baylor University
“How *Chlamydomonas* dismantles itself: A story of algal biofuel”
- 9:00 **William C. Hockaday**
Department Geology, Baylor University
“NMR-based estimates of the molecular dimensions in biochars: Implications for their environmental stability”
- 9:30 **Natalie Adolphi**
Cancer Center, University of New Mexico Health Sciences Center
“Post-mortem Magnetic Resonance in the Autopsy Suite: What’s a nice Solid-State NMR Spectroscopist doing in a place like this?”

10:00 – 10:20 Intermission.

Session 2: Catalysts and Surfaces

Chairs: Gary Patti.

- 10:20 **Janet Bluemel**
Department of Chemistry, Texas A&M
“HRMAS solid-state NMR: A powerful method for investigating immobilized linkers and catalysts”
- 10:50 **Terry Gullion**
Department Chemistry, West Virginia University
“Structure of Peptides on Gold Nanoparticles by Solid-State NMR and the Development of ¹H-²H Dipolar Recoupling Experiments”
- 11:20 **Donghua Zhou**
Department of Physics, Oklahoma State University
“NMR measurement of porosity, chemical composition, and mineral surface area of intact bone”

11:50 – 1:20 LUNCH BREAK.

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Session 3: Biological Solids

Chair: William Hockaday.

- 1:30 **Gary Patti**
Department of Chemistry, Washington University in St. Louis
“Whole-Cell Metabolomics: Integrating NMR and Mass Spectrometry to Explore Unknown Biochemical Pathways”
- 2:00 **David Weliky**
Department Chemistry, Michigan State University
“Solid-state NMR of viral fusion proteins and of proteins in cells and cell extracts”
- 2:30 **Lynette Cegelski**
Department of Chemistry, Stanford University
“Structure, Function, and Inhibition of Bacterial Biofilms”

3:00 – 3:20 Intermission.

Session 4: Polymers

Chair: Lynette Cegelski.

- 3:20 **Frank Blum**
Department of Chemistry, Oklahoma State University
“Deuterium NMR of surface-attached copolymers”
- 3:50 **Jacob Schaefer ****Closing Keynote Speaker******
Department of Chemistry, Washington University in St. Louis
“Vol’kenshtein Bundles: Understanding the connection between mechanical properties and molecular structure in polycarbonate-like glasses”

5:10 – 7:00 DINNER.

Speakers and poster presenters are invited to Dinner at Bangkok Royal. We will meet in front of the session room (Texas 116) at 5:10 PM to walk over to the restaurant (across the street).

5:45 – 7:00 Dial-Black Lecture (McLennan)

**7:00 – 9:00 EXPO RECEPTION & POSTER SESSION 2 (Brazos Ballroom).
FOOD, CASH BAR, AND POSTER SESSION 2.**

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Closing Keynote Speaker

November 18th 3:50 PM, Room: Texas 116

Jacob Schaefer

Charles Allen Thomas Professor of Chemistry
WASHINGTON UNIVERSITY IN ST. LOUIS



Vol'kenshtein Bundles: Understanding the connection between mechanical properties and molecular structure in polycarbonate-like glasses

Chain packing of nine structurally different polycarbonate glasses (including the commercially important trimethylcyclohexyl polycarbonates produced by Bayer) have been measured by natural-abundance ^{13}C - ^{13}C spin diffusion using two-dimensional centerband-only detection of exchange (2D CODEX). Some mechanical properties of these polymers include the intensity of the low-temperature shear relaxation, and the ratio of the shear-transition temperature (T) to the glass-transition temperature (T_g). These parameters are related to ^{13}C NMR relaxation sensitive to room-temperature motions in the 20-kHz regime (from dipolar rotational spin-echo experiments), and in the 10-Hz regime (from conventional one-dimensional CODEX) using Eyring rate-law assumptions. The resulting connection leads to a molecular interpretation of macroscopic stress-strain behavior and a molecular description of the requirements for toughness in a polycarbonate-like glass.

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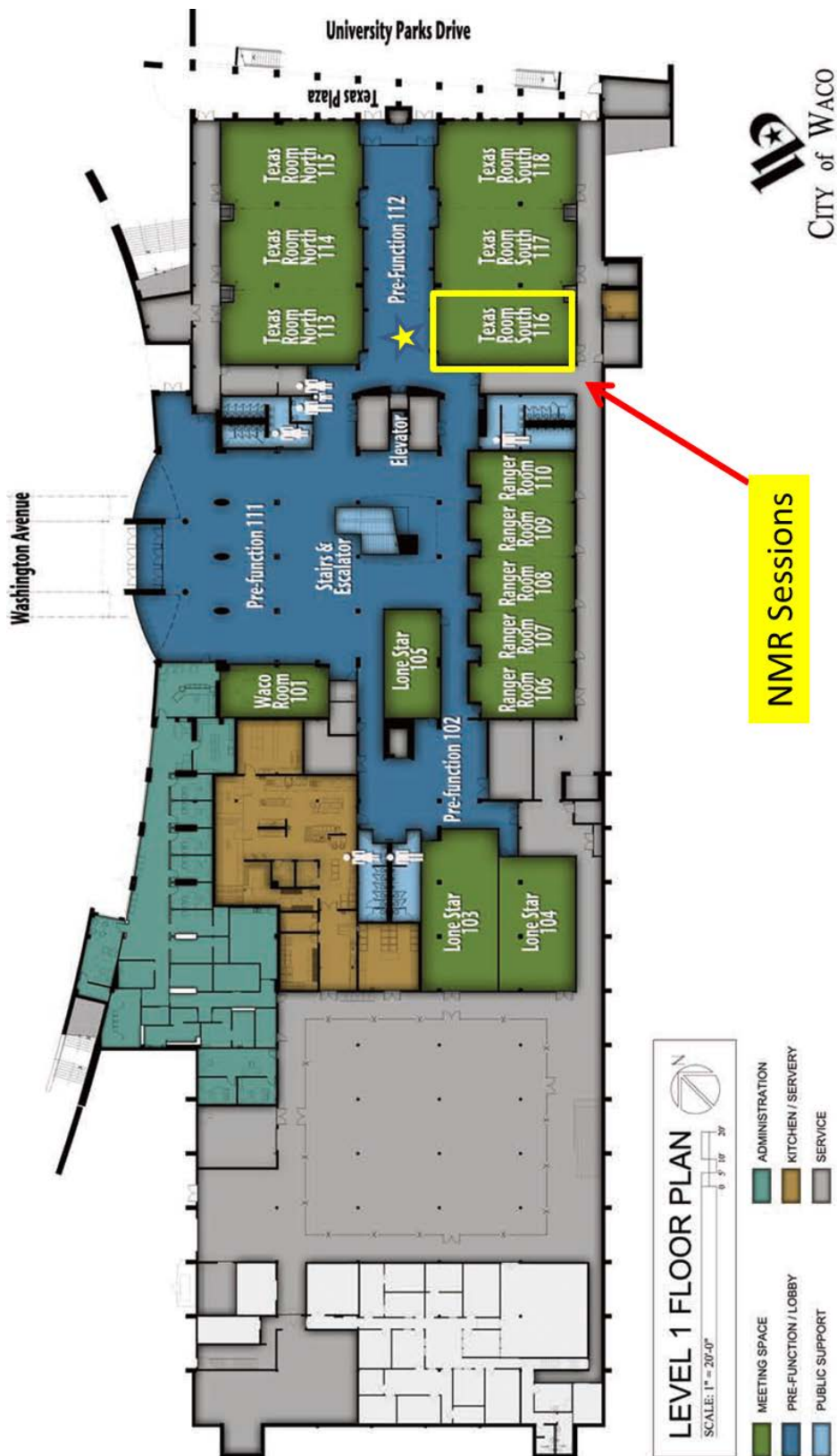
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Posters (Sunday 7-9 PM)

- 253.** Facile lipid formation quantification studies of algae *Chlamydomonas reinhardtii* using ¹³C NMR. **J. D. Chang**, N. A. van der Velde, A. Nguyen, M. Singh, C. Goodson, U. Goodenough, S. J. Kim
- 254.** Reversible CO₂ capture mechanism of a humidity-swing polymeric sorbent. **H. Yang**, M. Singh, R. D. O'Connor, J. Schaefer
- 255.** *Staphylococcus aureus* Peptidoglycan Tertiary Structure by Rotational-Echo Double Resonance NMR Spectroscopy. **M. Singh**, S. J. Kim, M. Preobrazhenskaya, J. Schaefer
- 256.** C-terminal V5 domain of Protein Kinase C α as a membrane anchor and protein interaction module. **Y. Yang**, T. I. Igumenova
- 257.** Metal-dependent function of C2 α : A conditional membrane binding domain. **K. A. Morales**, T. I. Igumenova
- 258.** Cell Wall Composition Analysis of Vancomycin-Resistant *Staphylococcus aureus*. **J. Chang**, E. Luper, A. Abdolvahabi, J. Schaefer, S. Kim

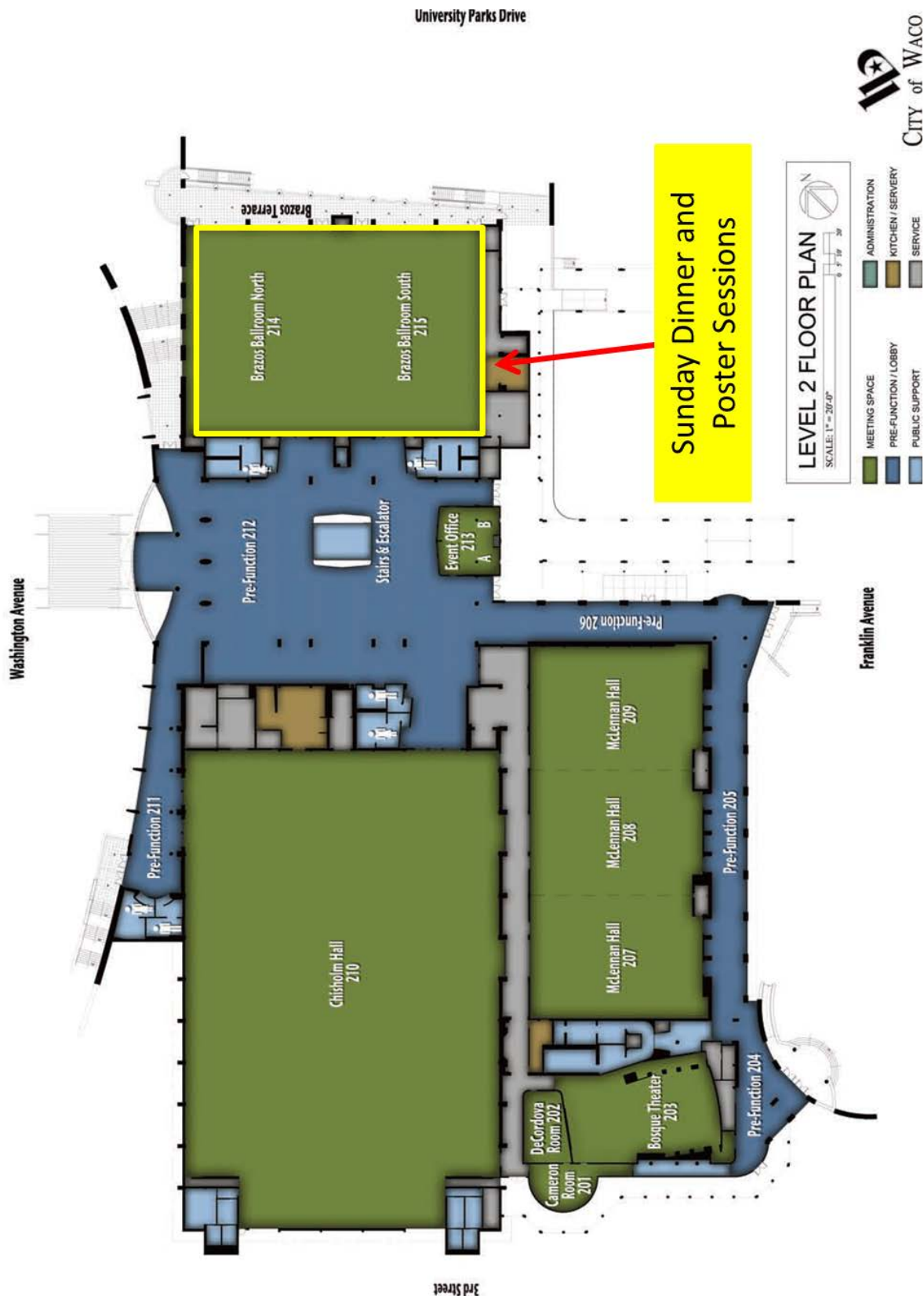
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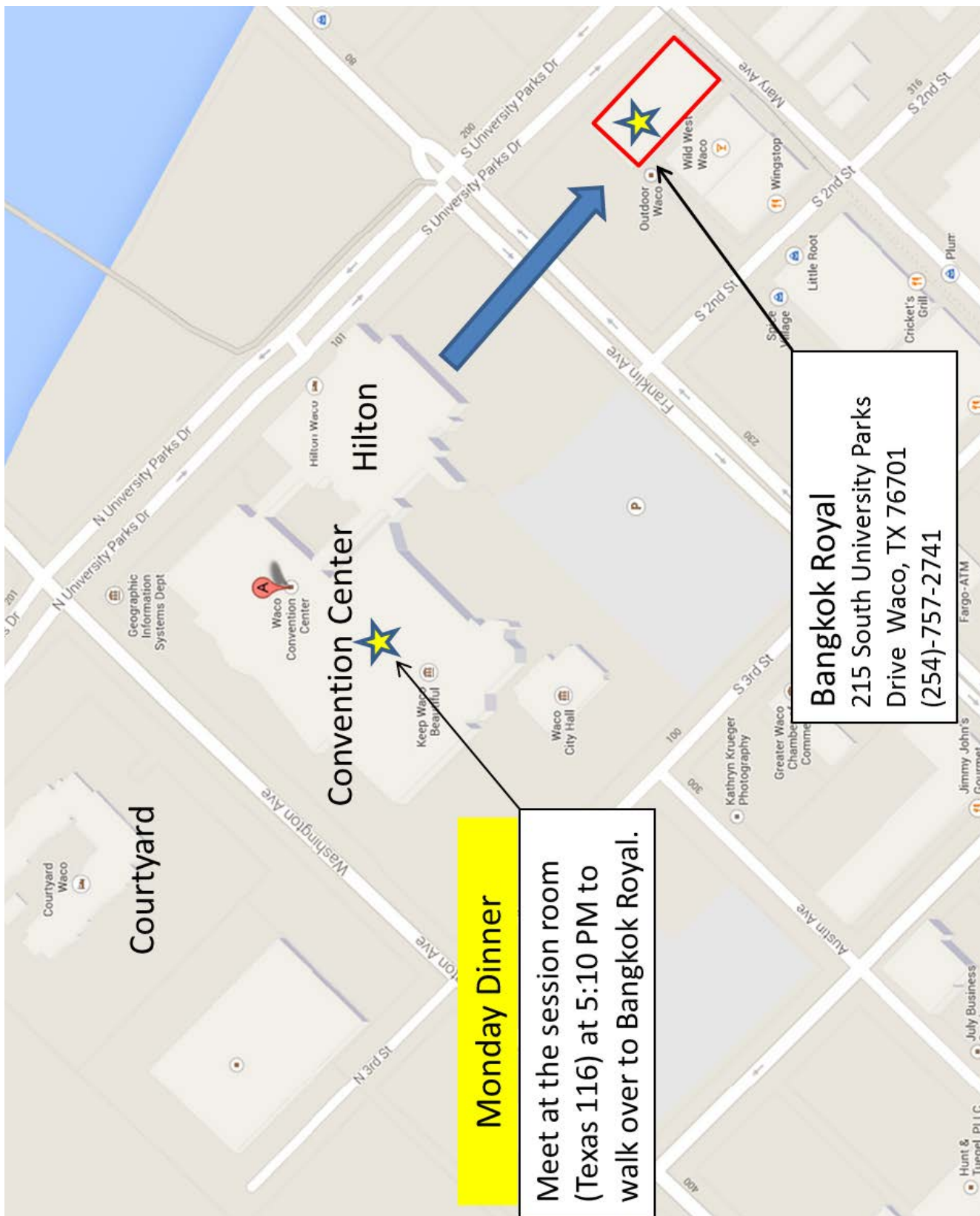
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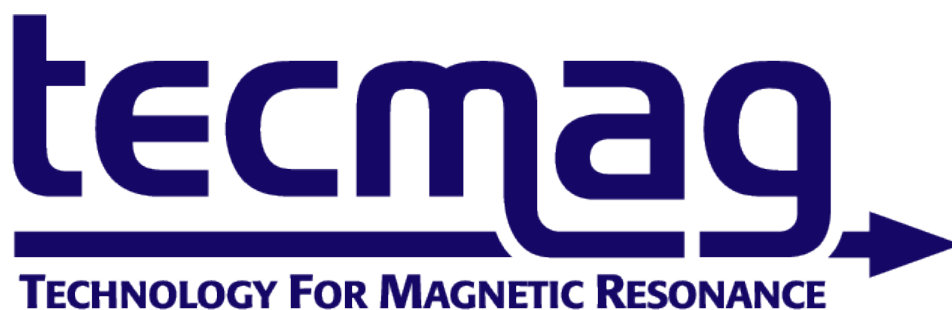
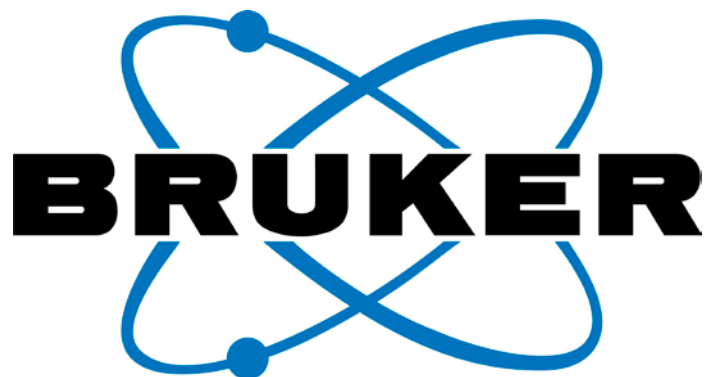
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