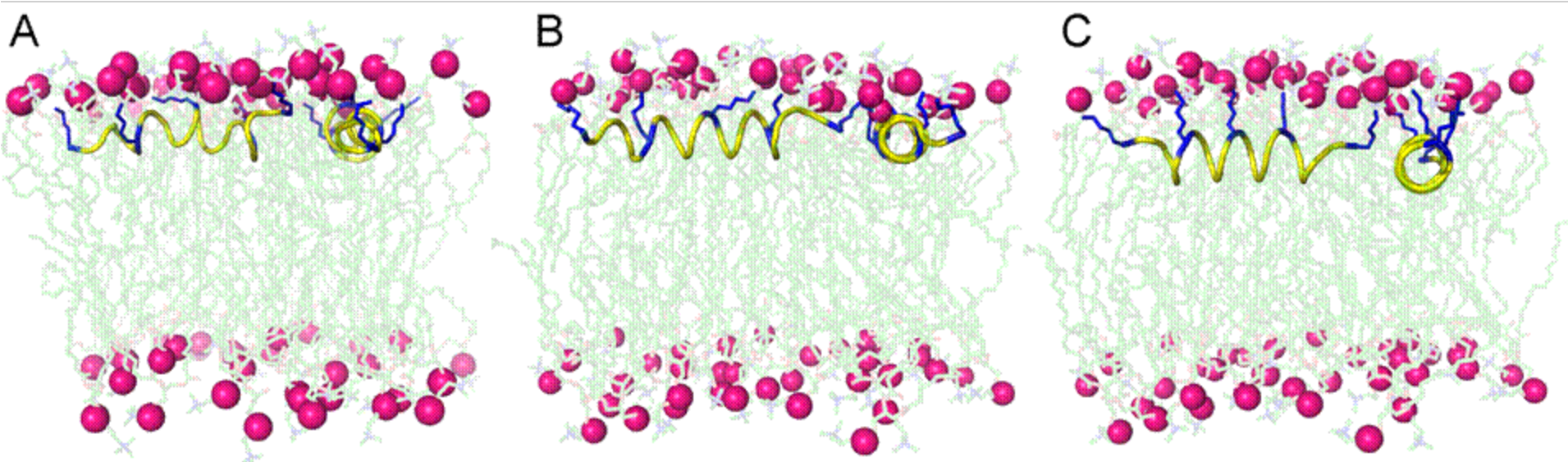
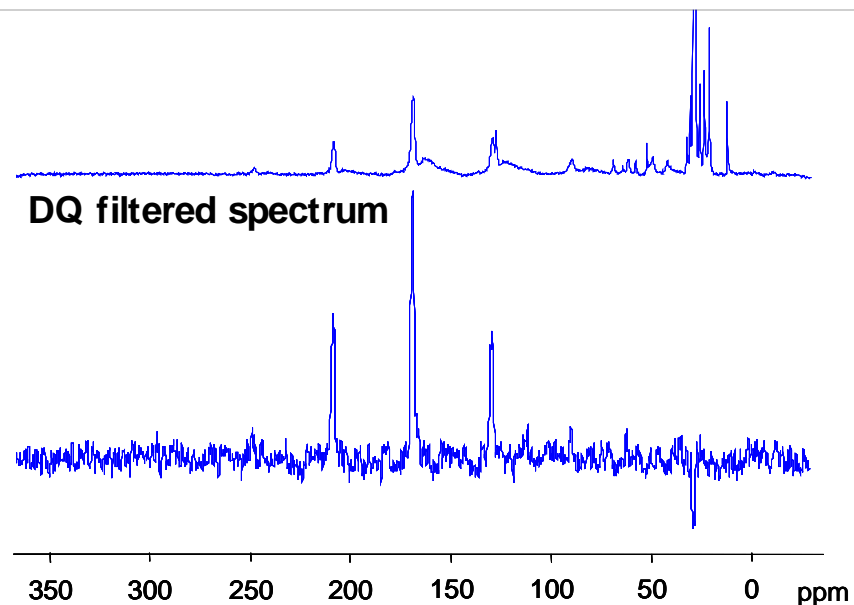


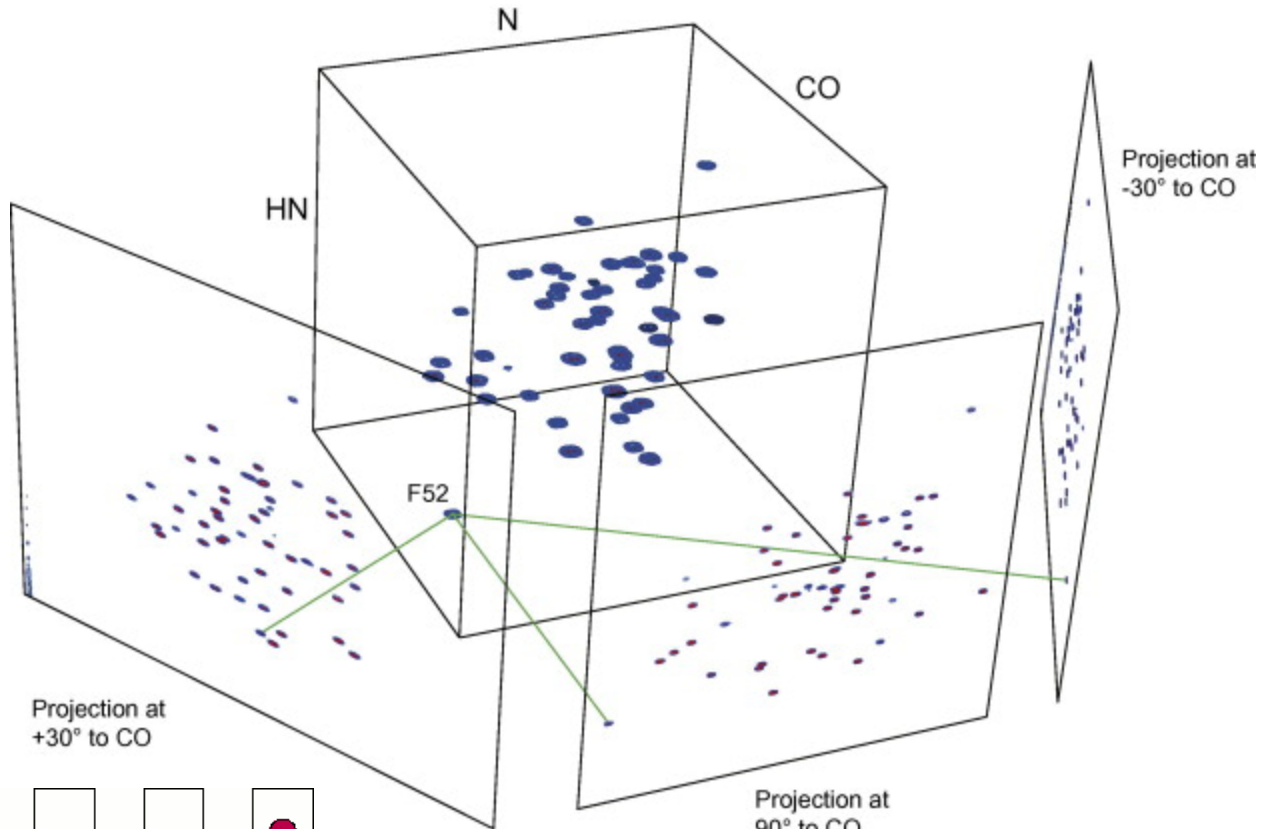
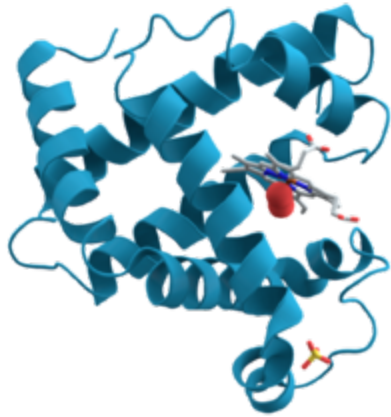
# Big data, big noise, and big simulations



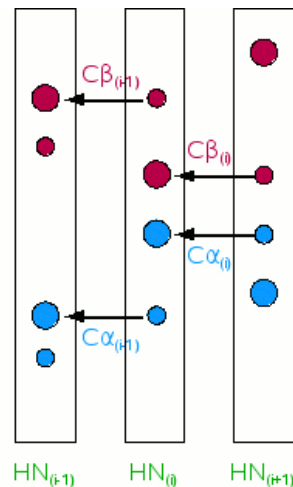
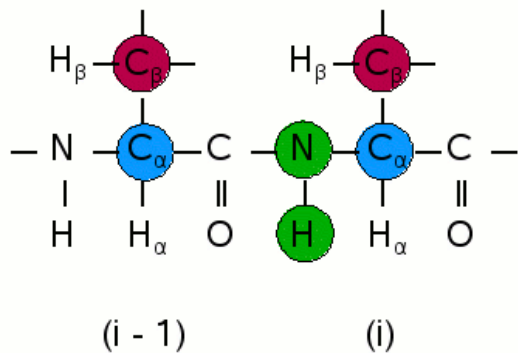
**Joanna R. Long**  
**Department of Biochemistry & Molecular**  
**Biology**  
**McKnight Brain Institute**  
**National High Magnetic Field Laboratory**



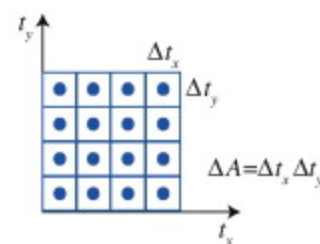
# Protein NMR: measurements of structure and dynamics



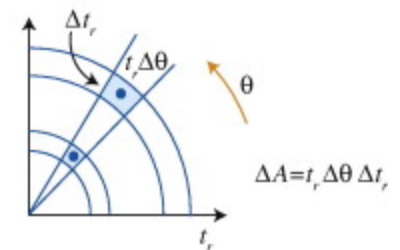
**HNCACB**



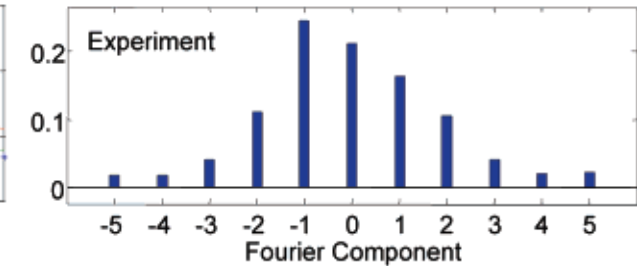
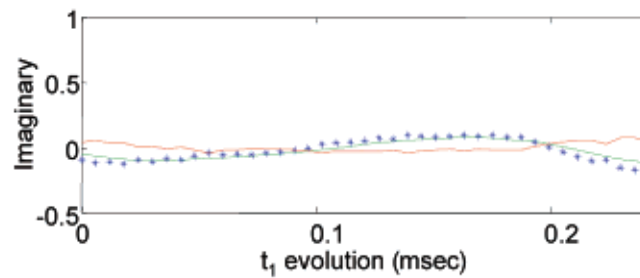
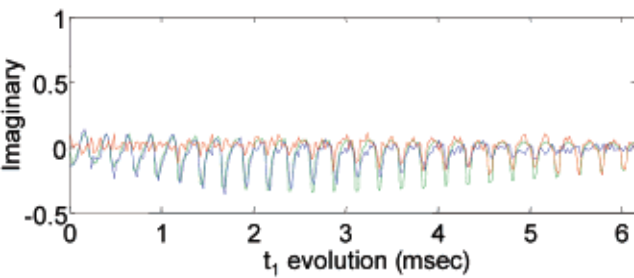
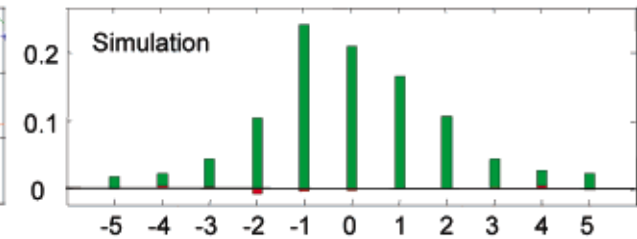
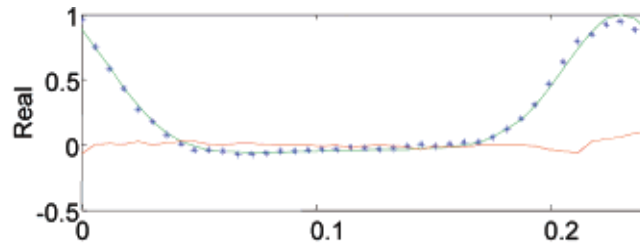
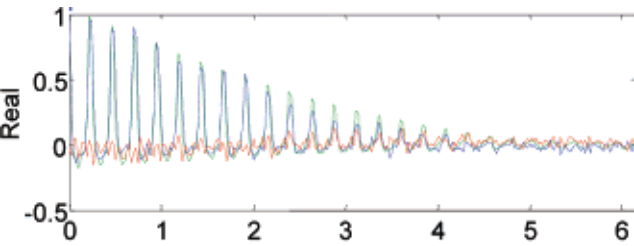
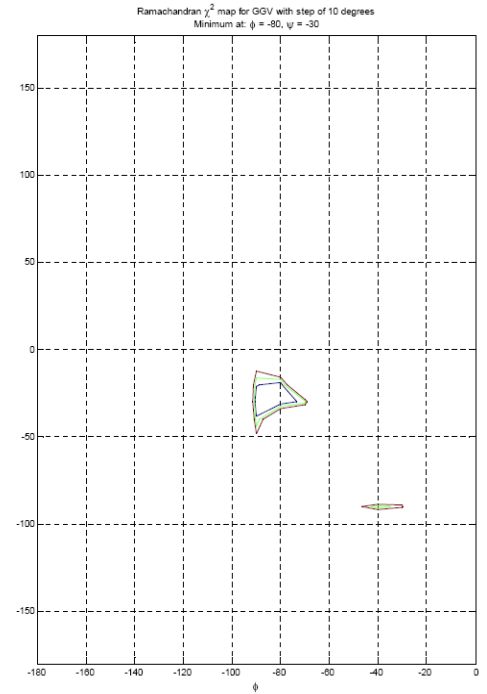
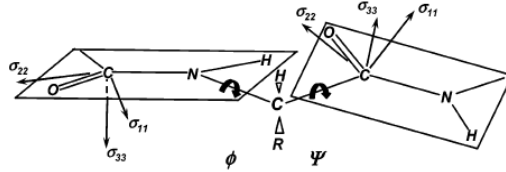
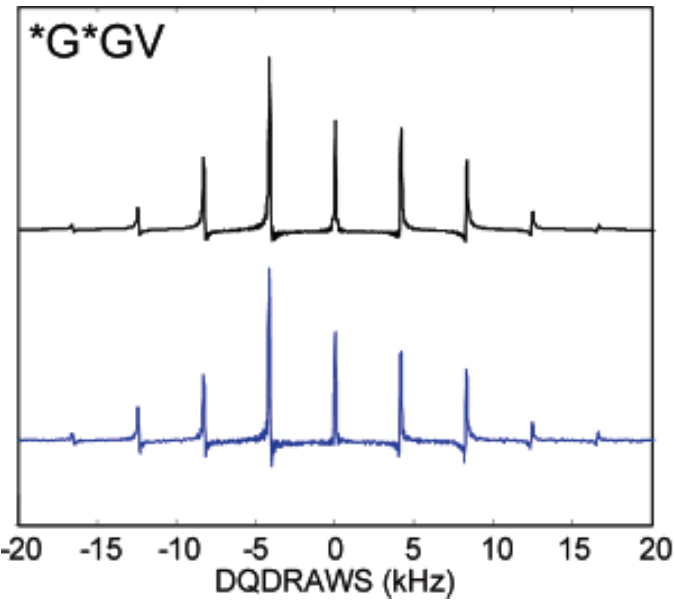
(a) Cartesian



(b) Polar

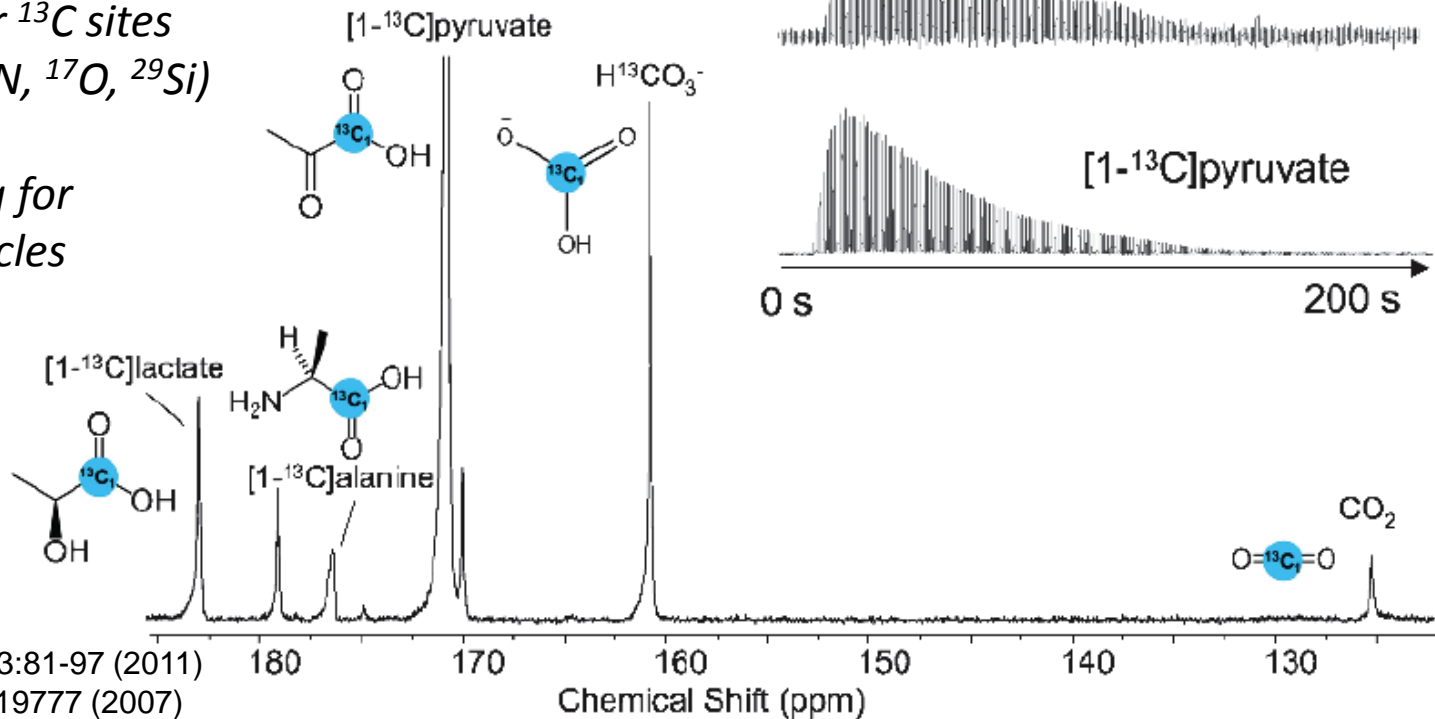
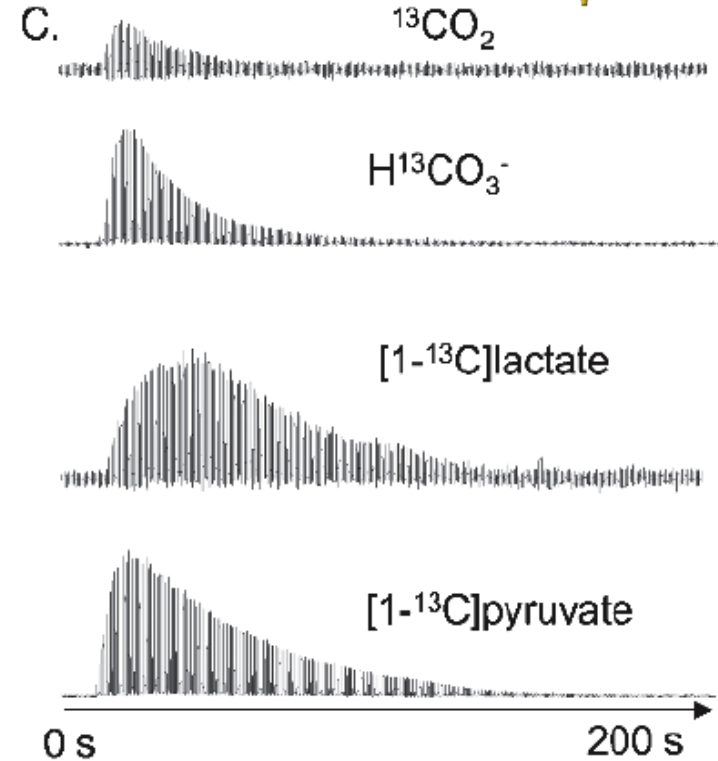
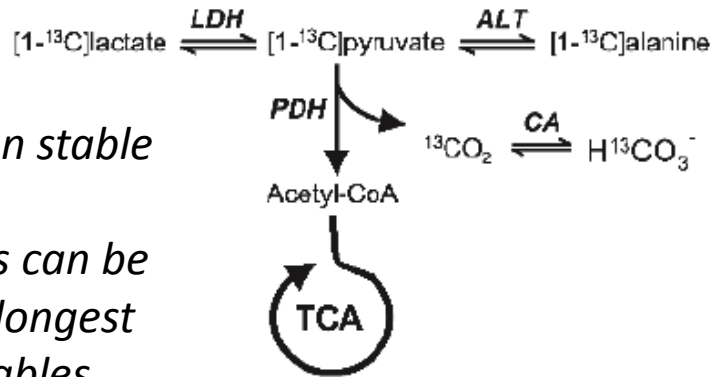


# Protein NMR: measurements of structure and dynamics



# In vivo metabolism via DNP

- $^{13}\text{C}$  is most common stable isotope utilized
- Unprotonated sites can be monitored for the longest
- Perdeuteration enables monitoring of other  $^{13}\text{C}$  sites
- Other nuclei ( $^7\text{Li}$ ,  $^{15}\text{N}$ ,  $^{17}\text{O}$ ,  $^{29}\text{Si}$ ) are feasible
- $^{29}\text{Si}$  looks promising for targeted nanoparticles

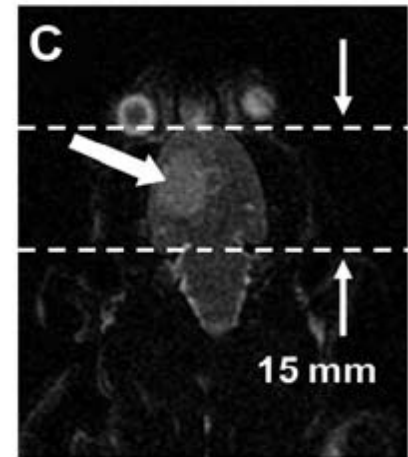
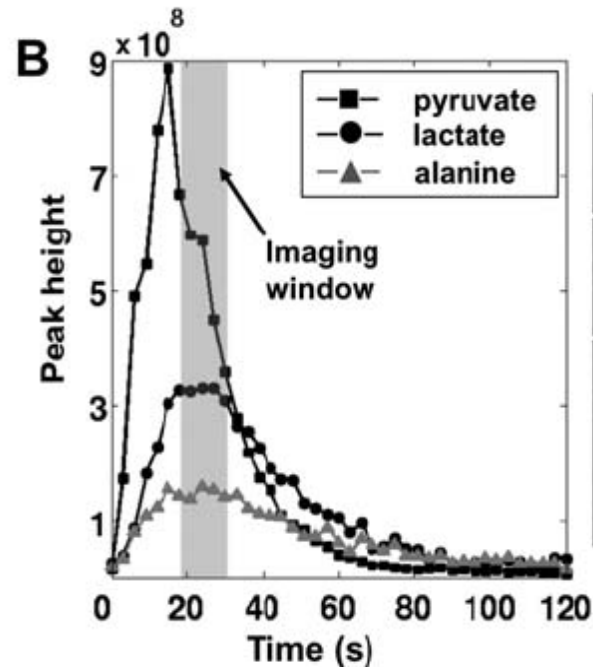
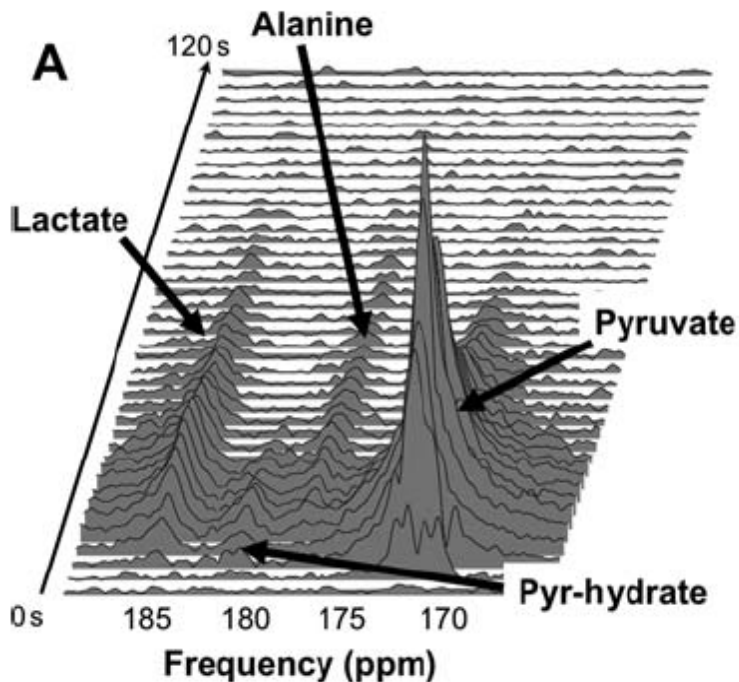


# *In vivo* rat brain measurements

## Hyperpolarized $^{13}\text{C}$ magnetic resonance metabolic imaging: application to brain tumors

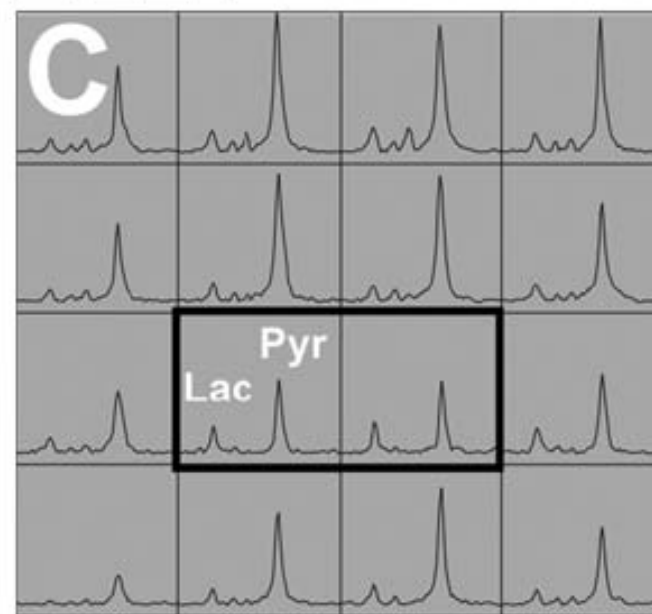
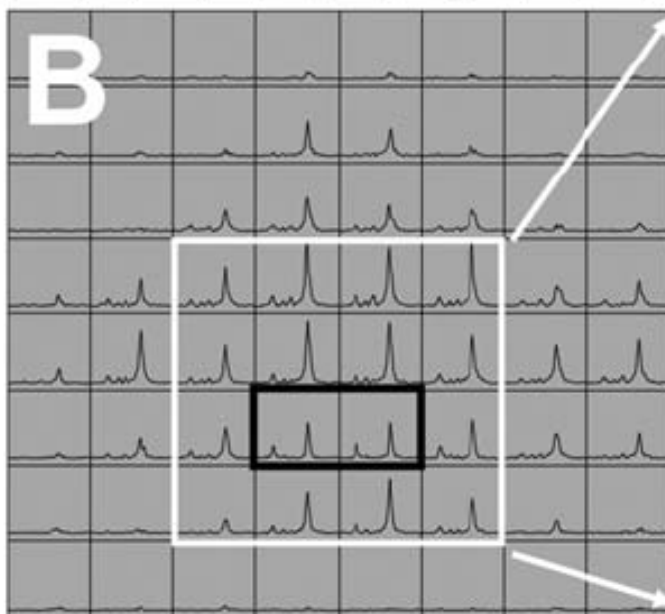
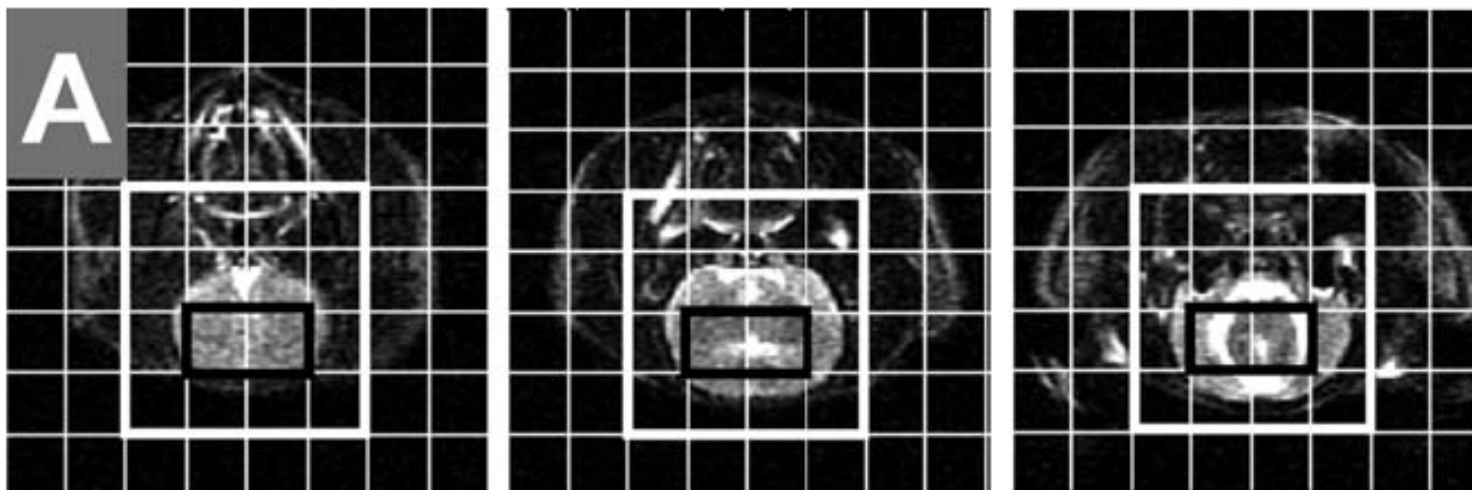
*Neuro-Oncology* 12(2):133–144, 2010.  
doi:10.1093/neuonc/nop043

Ilwoo Park, Peder E. Z. Larson, Matthew L. Zierhut, Simon Hu, Robert Bok, Tomoko Ozawa, John Kurhanewicz, Daniel B. Vigneron, Scott R. VandenBerg, C. David James, and Sarah J. Nelson

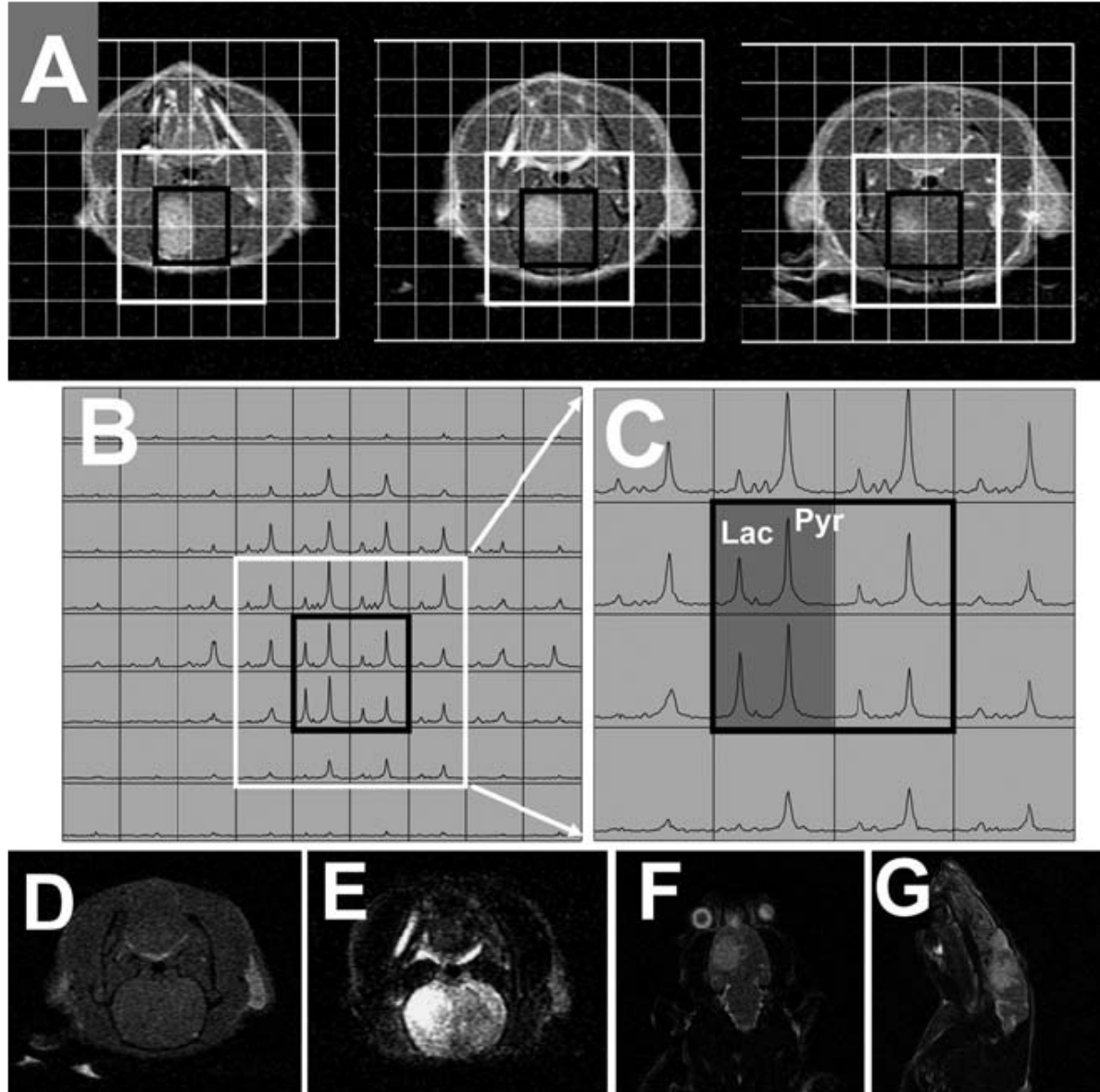


100 mM pyruvate in 2.3 mL buffer tail vein injection over 12 seconds

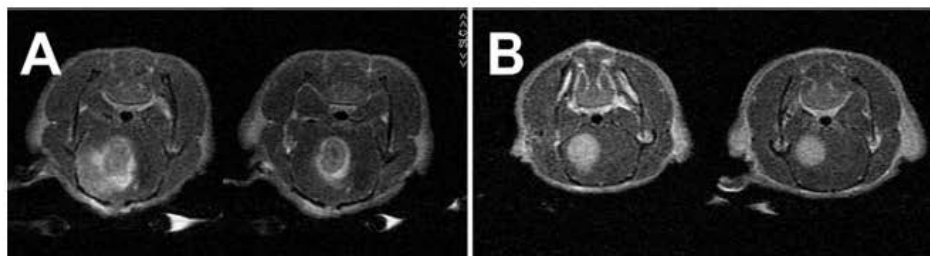
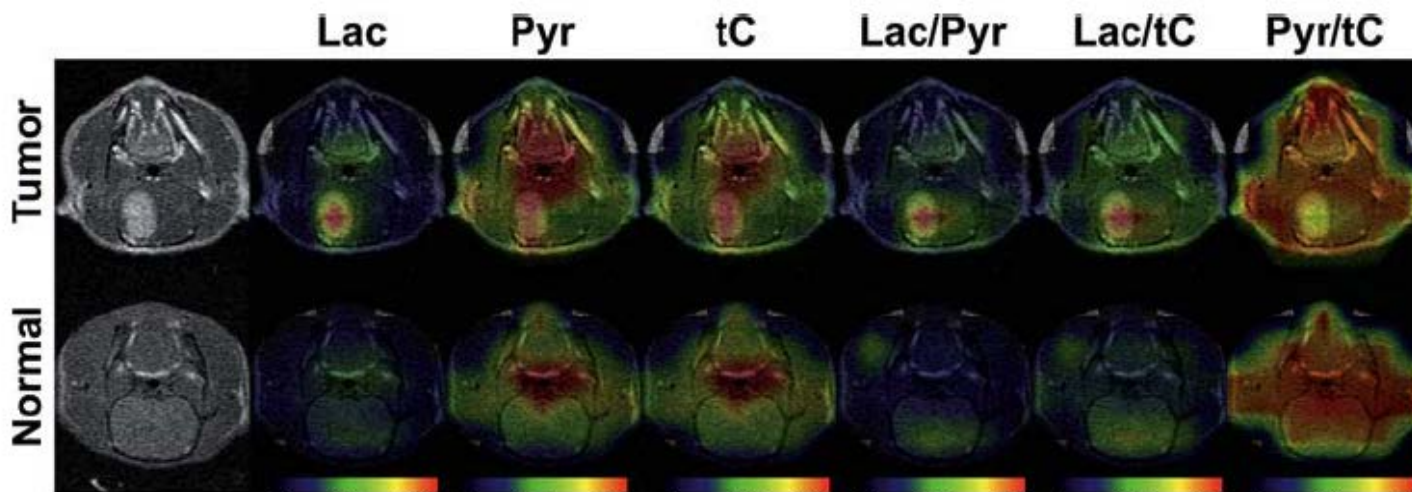
# Normal rat brain measurements



# Tumor measurements



# Comparison



Type of feature	U-251 MG	U-87 MG
Biological	A mixture of malignant spindle and epithelioid cells with irregular borders	Malignant cells in compact fascicles, with well-circumscribed borders
Histological and immunohistochemical	Larger area of necrosis and hypoxia	Little or no necrosis and hypoxia
MRI	Varying levels of contrast enhancement with an irregular tumor margin	Homogeneous levels of contrast enhancement with a well-delineated tumor margin
$^{13}\text{C}$ MRSI	Relatively high SNR of lactate, pyruvate, and total carbon	Relatively low SNR of lactate, pyruvate, and total carbon