AI Meets Quantum Mechanics:

Unravelling the Molecular Fingerprints of Brain Function and Diseases

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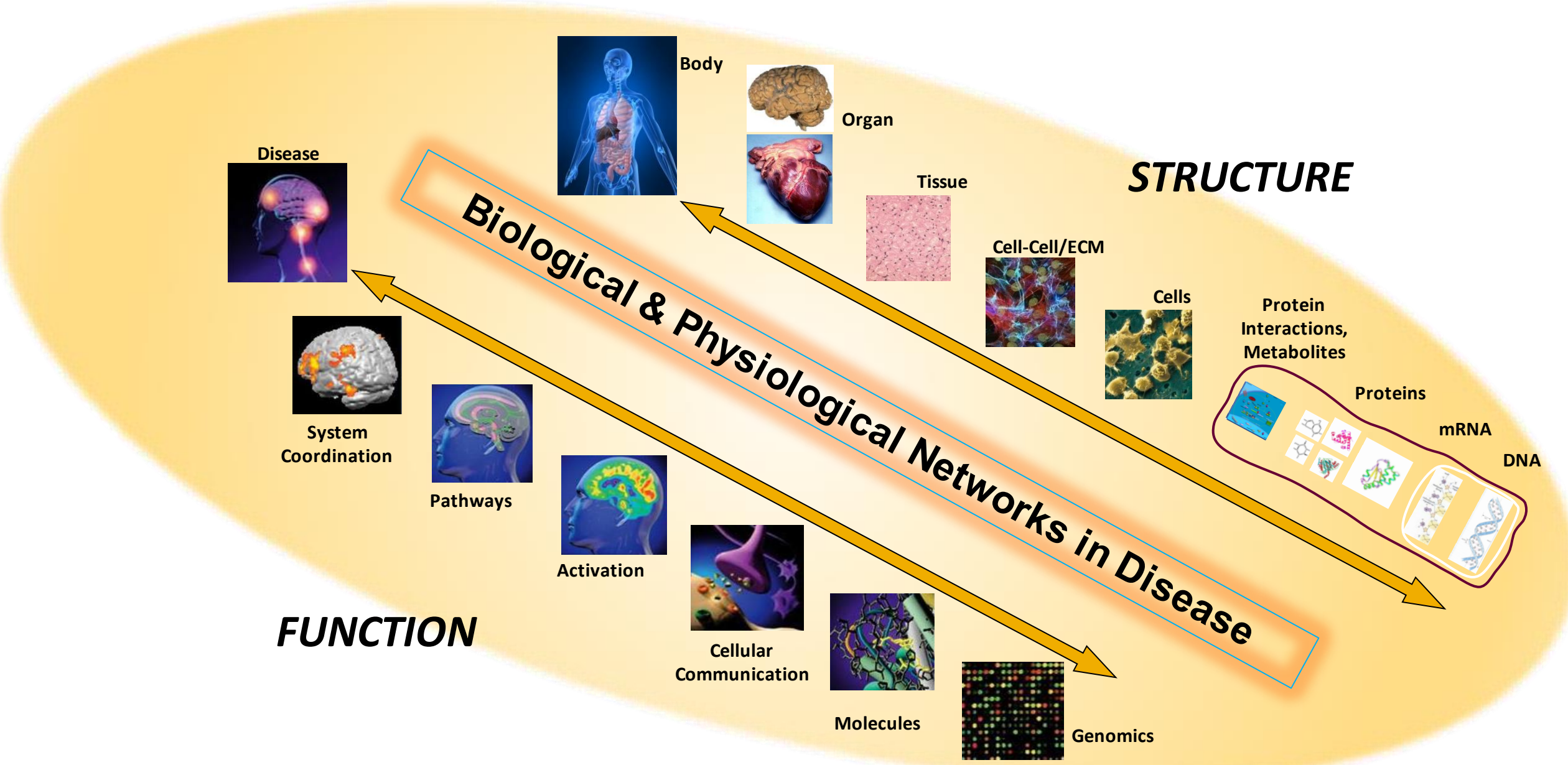
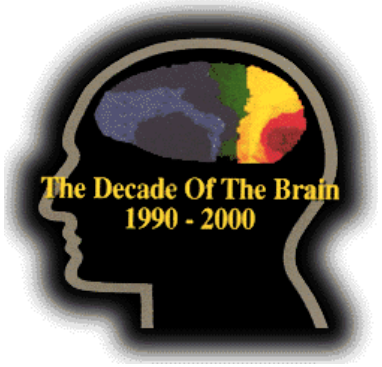
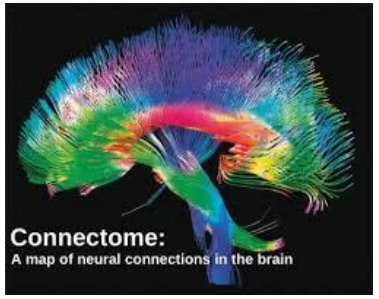
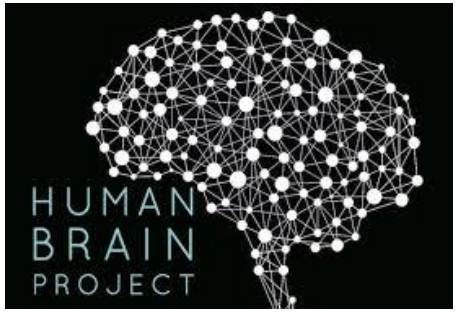
Complexity of the Brain



Brain Mapping: Global Efforts







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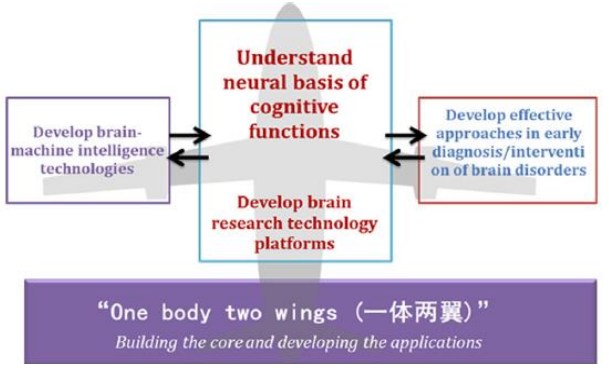
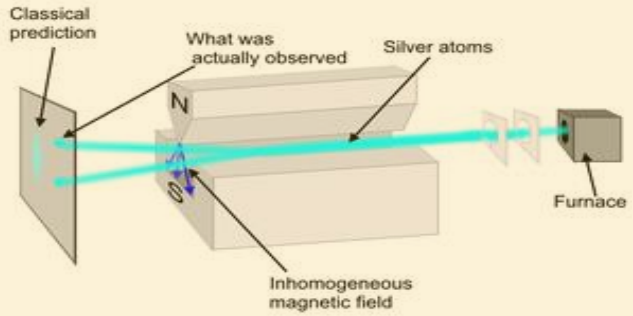


China Brain Project

Magic of Spins

- **Stern–Gerlach experiment (1922)**



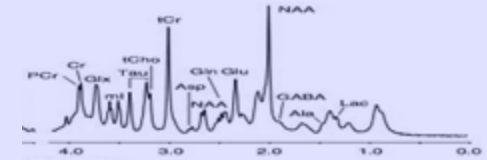
- **Relativistic Schrodinger equation (Paul Dirac, 1928):**

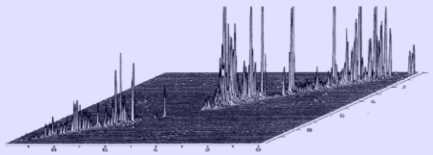
$$ih\frac{\partial\psi}{\partial t} = -\frac{h^2}{2m}\nabla^2\psi + V\psi \longrightarrow ih\frac{\partial\psi}{\partial t} = H\psi$$

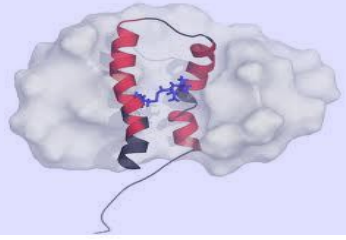
- **"There is nothing nuclear spins will not do for you as long as you treat them as human beings",**

Erwin Hahn

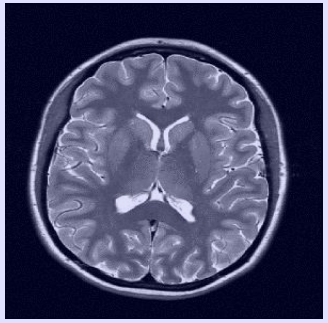
- **Spectroscopy**

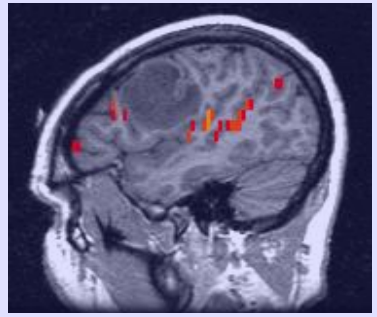


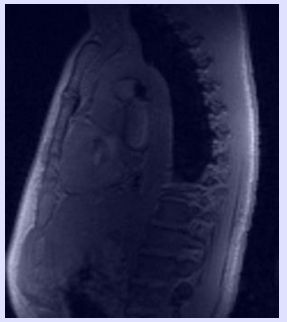


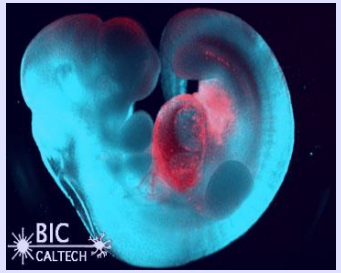


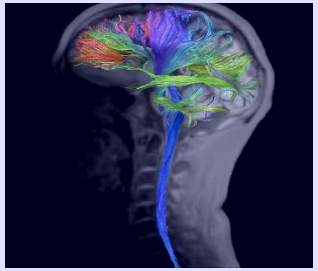
- **Imaging**











Conventional MRI

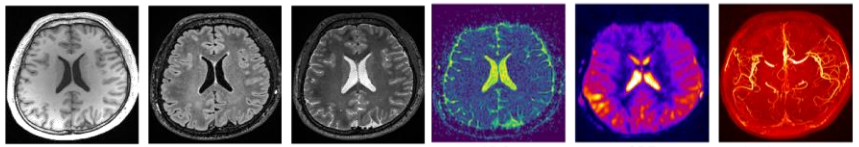
Data Acquisition:

$$s(\mathbf{k},t) = \iint \rho(\mathbf{x}, f) E(\mathbf{x}, f; \mathbf{k}, t) d\mathbf{x} df$$

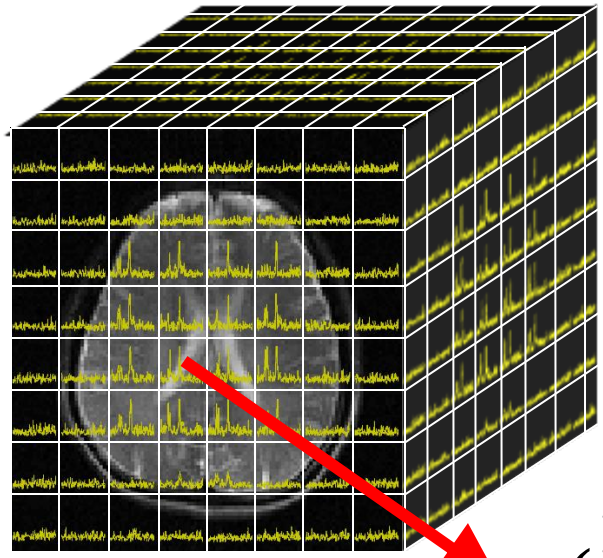
← Fourier encodings at the Nyquist rate

Image Reconstruction:

← Fourier representation of image functions

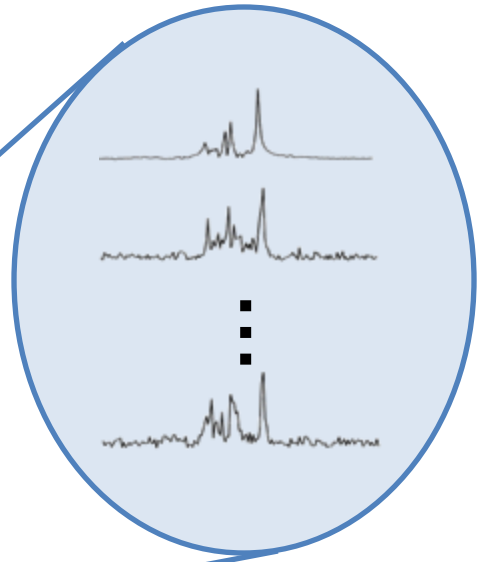


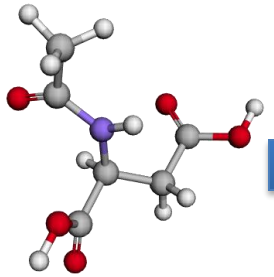
AI-Powered MRI



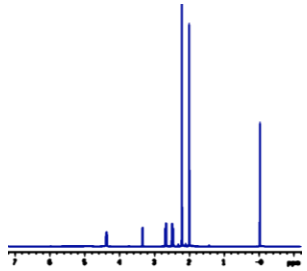
# of molecules

$$\rho(\vec{x}, f) = \sum_{m=1}^{M} \sum_{l=1}^{L} c_{ml}(\vec{x}) \varphi_{ml}(f)$$



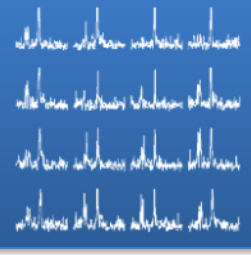


Quantum Mechanics Simulation

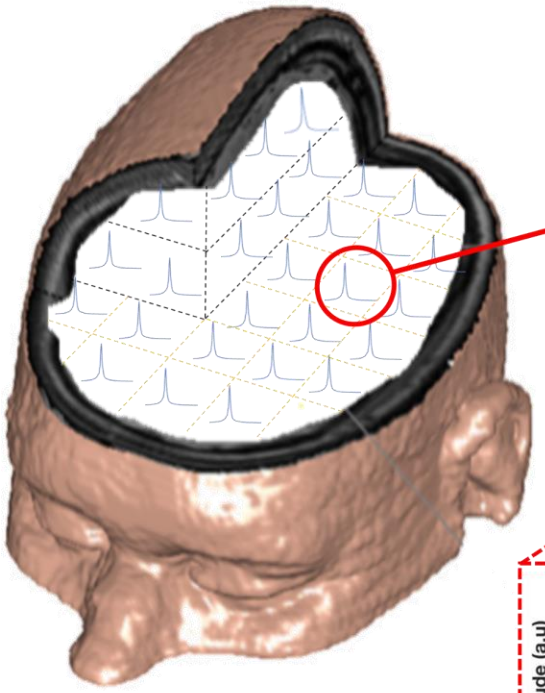


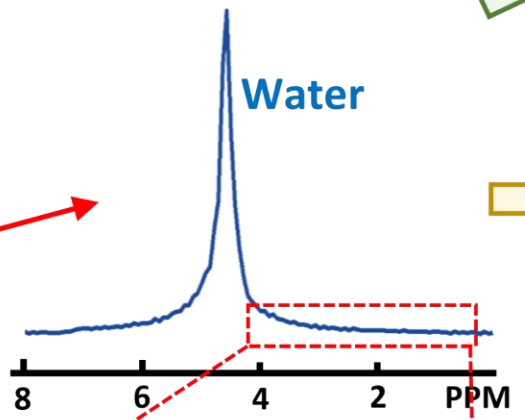
$$\psi(\boldsymbol{x}, t) = \sum_{l=1}^{L} c_l(t) e^{-\frac{iE_l t}{\hbar}} \phi_l(\boldsymbol{x})$$

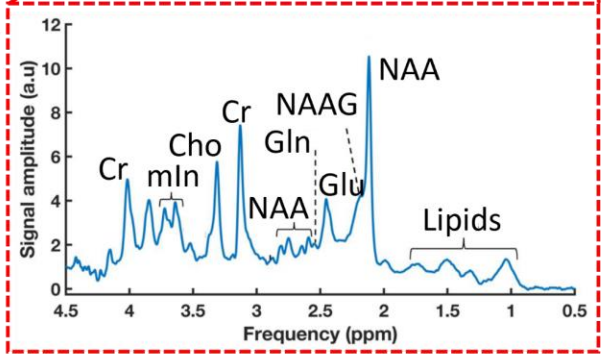
Training Data

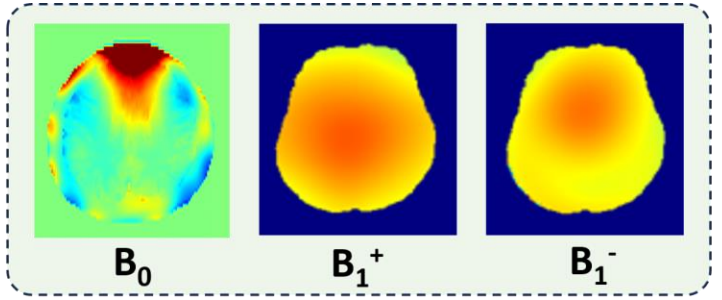


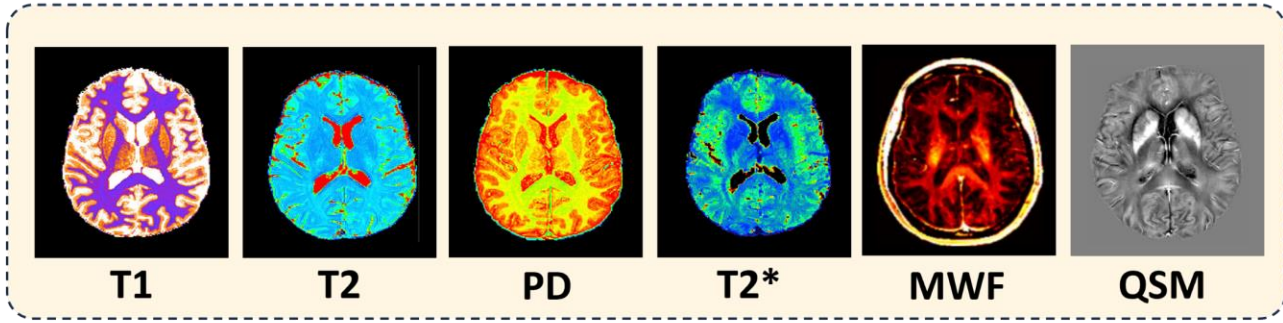
“SPICY” AI-Powered MRI

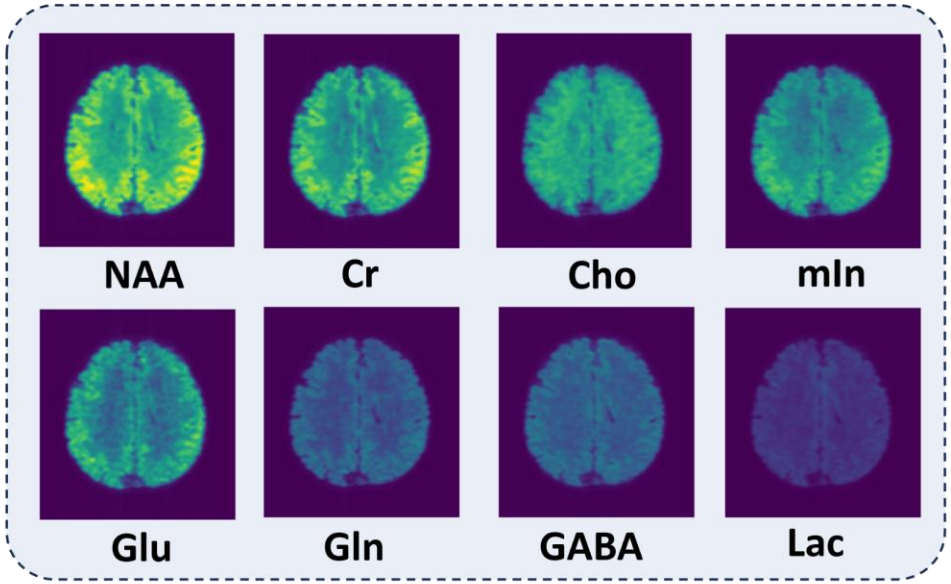










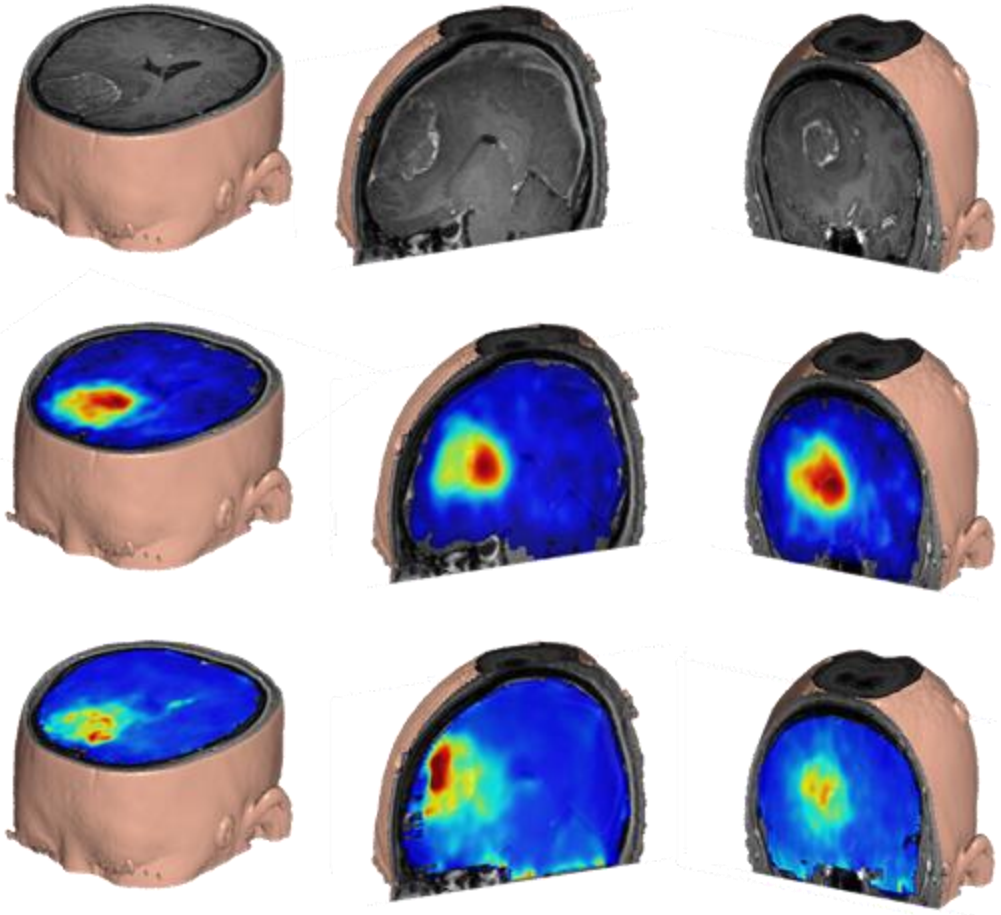


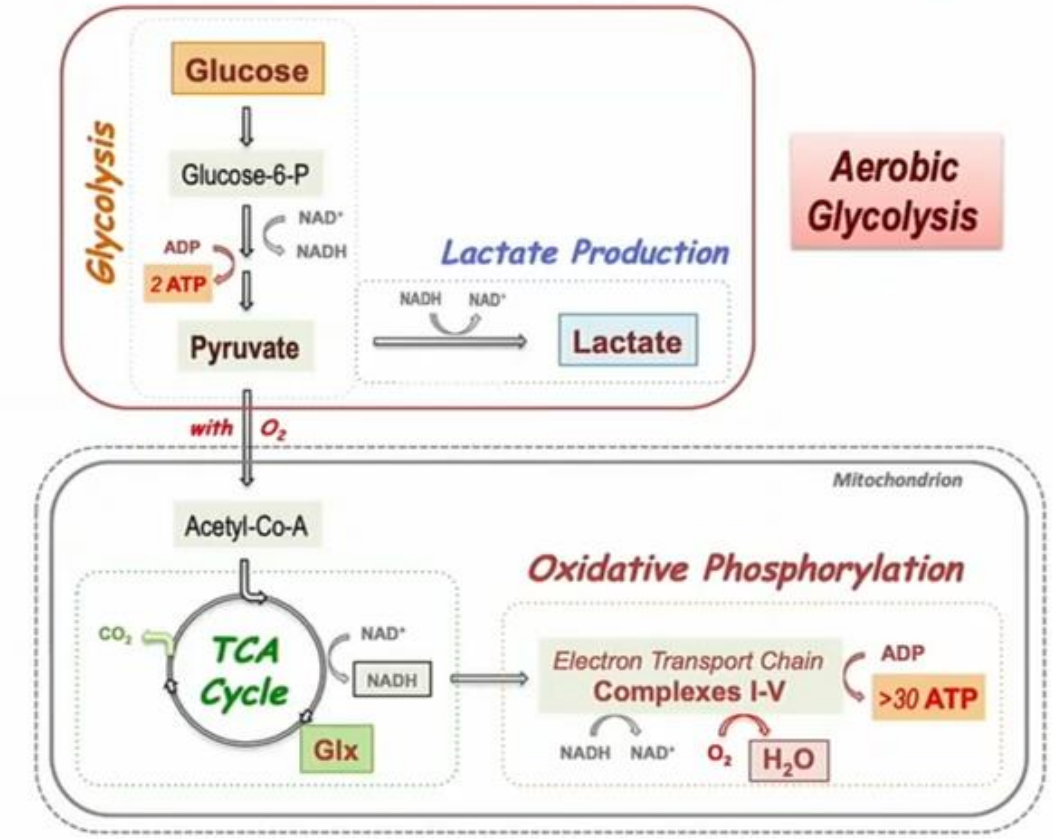
Metabolic Imaging of Brain Tumor

MPRAGE

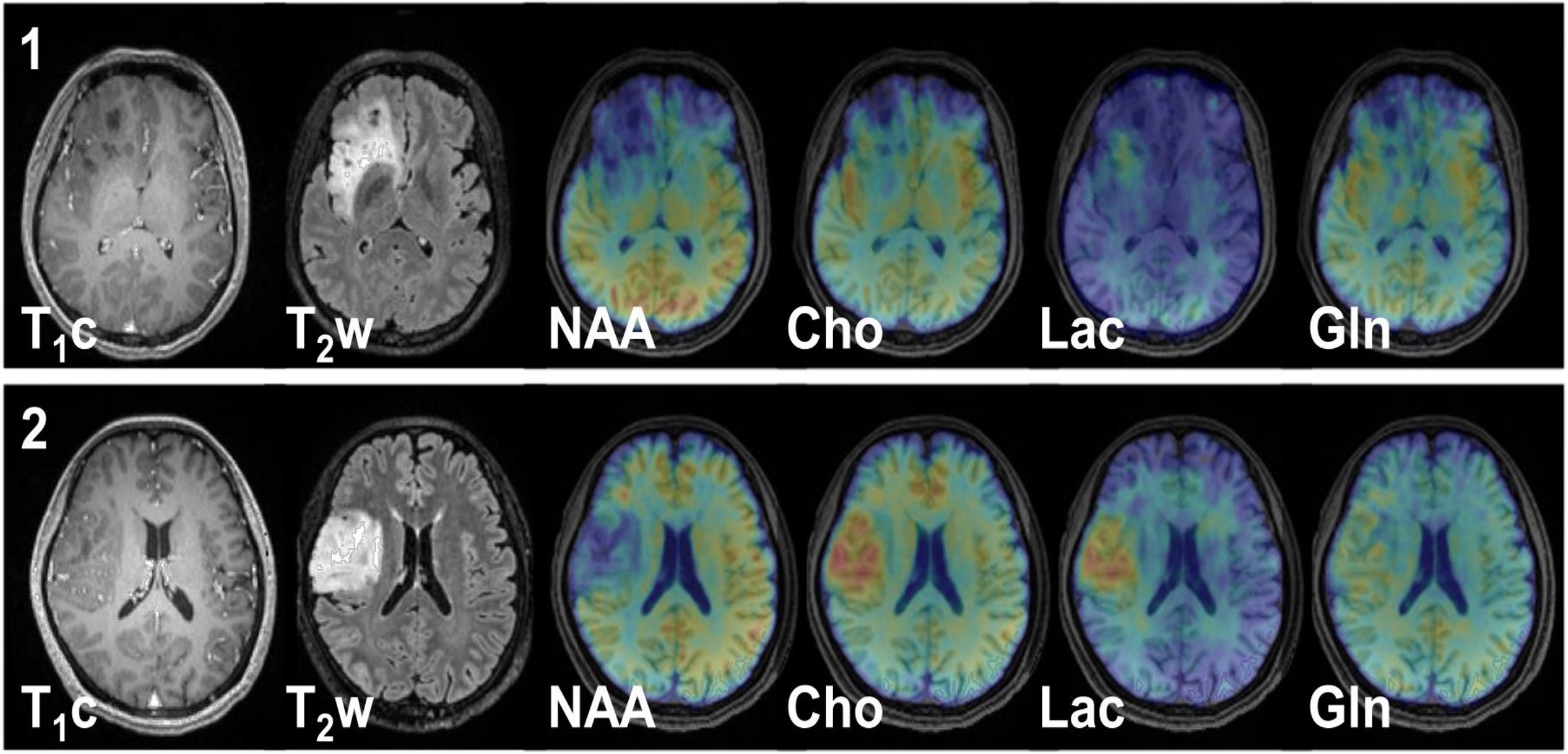
Lac

Cho/NAA

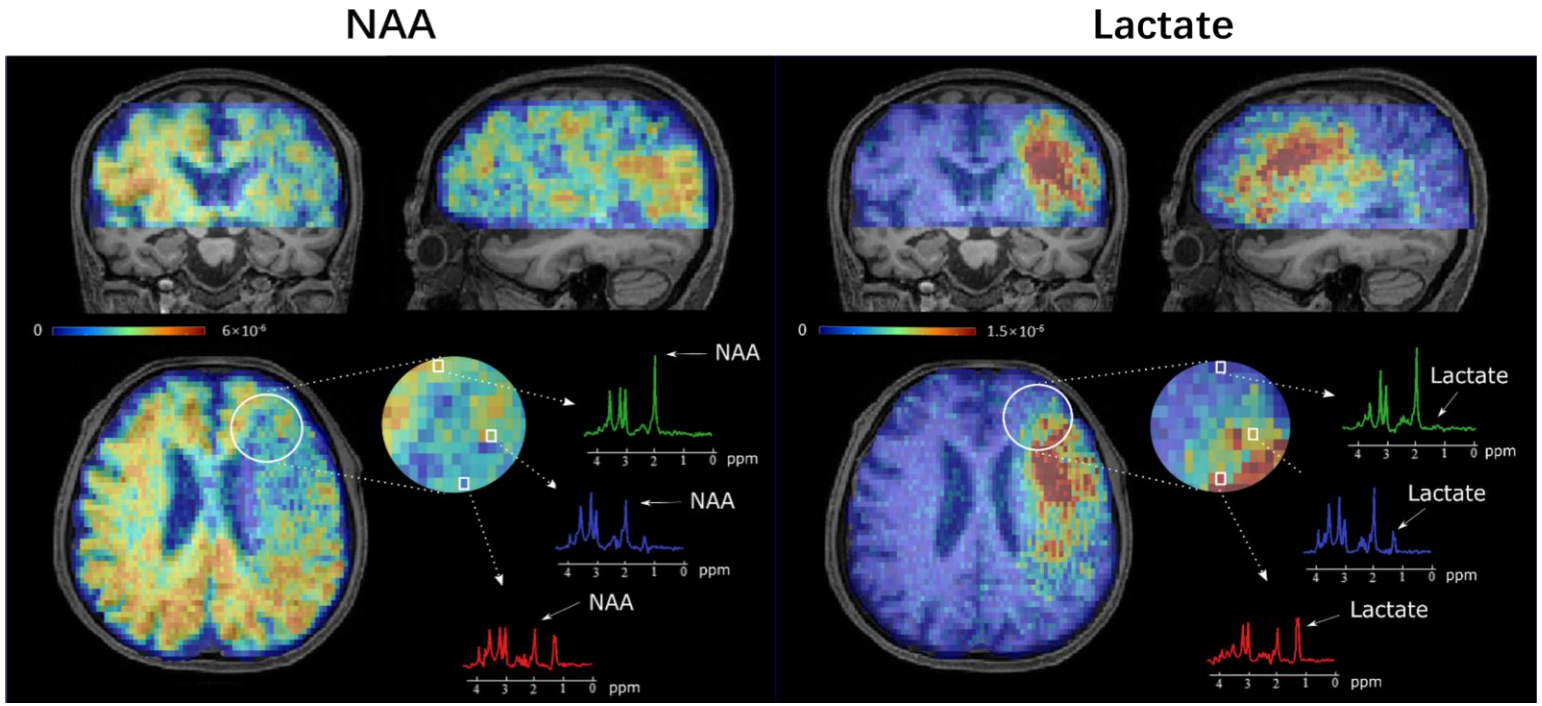


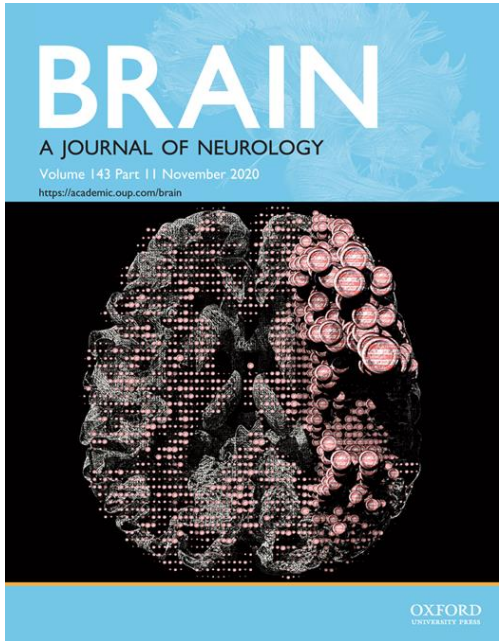


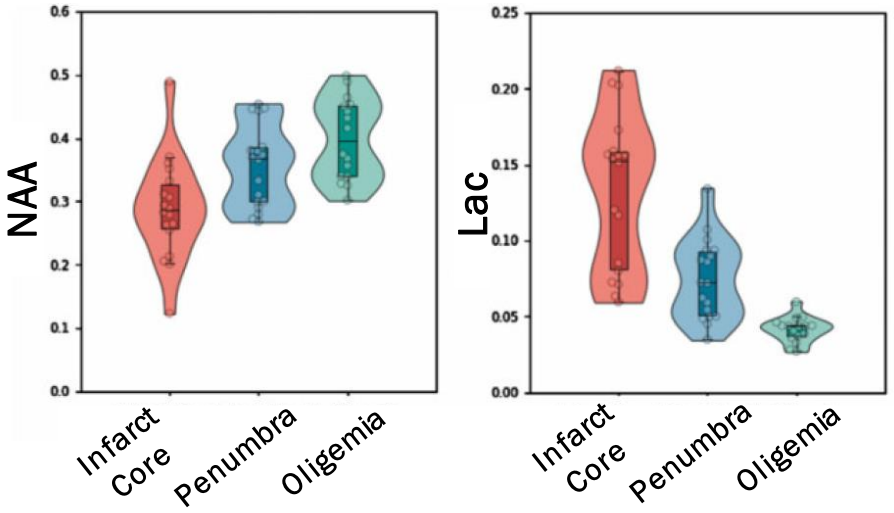
Differentiation of Different Tumors



Imaging Ischemia Stroke: Penumbra Characterization





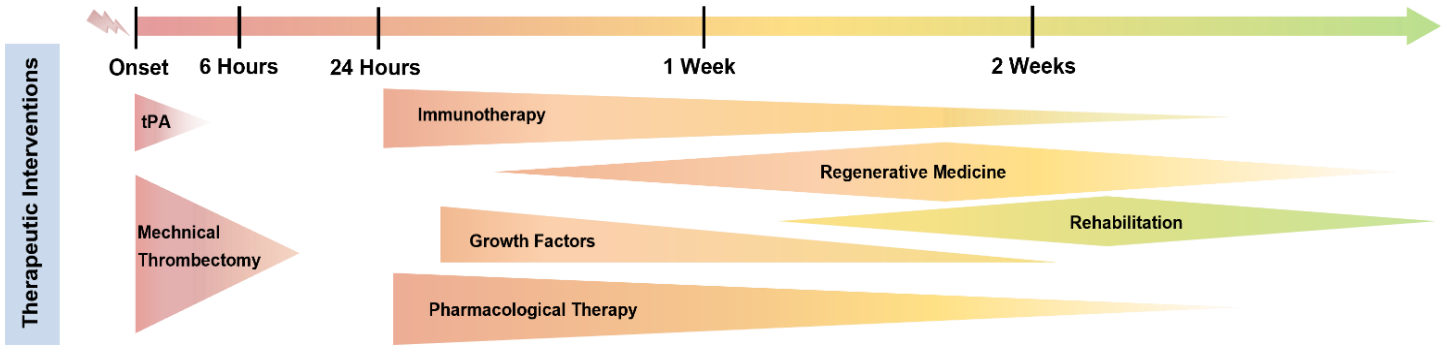


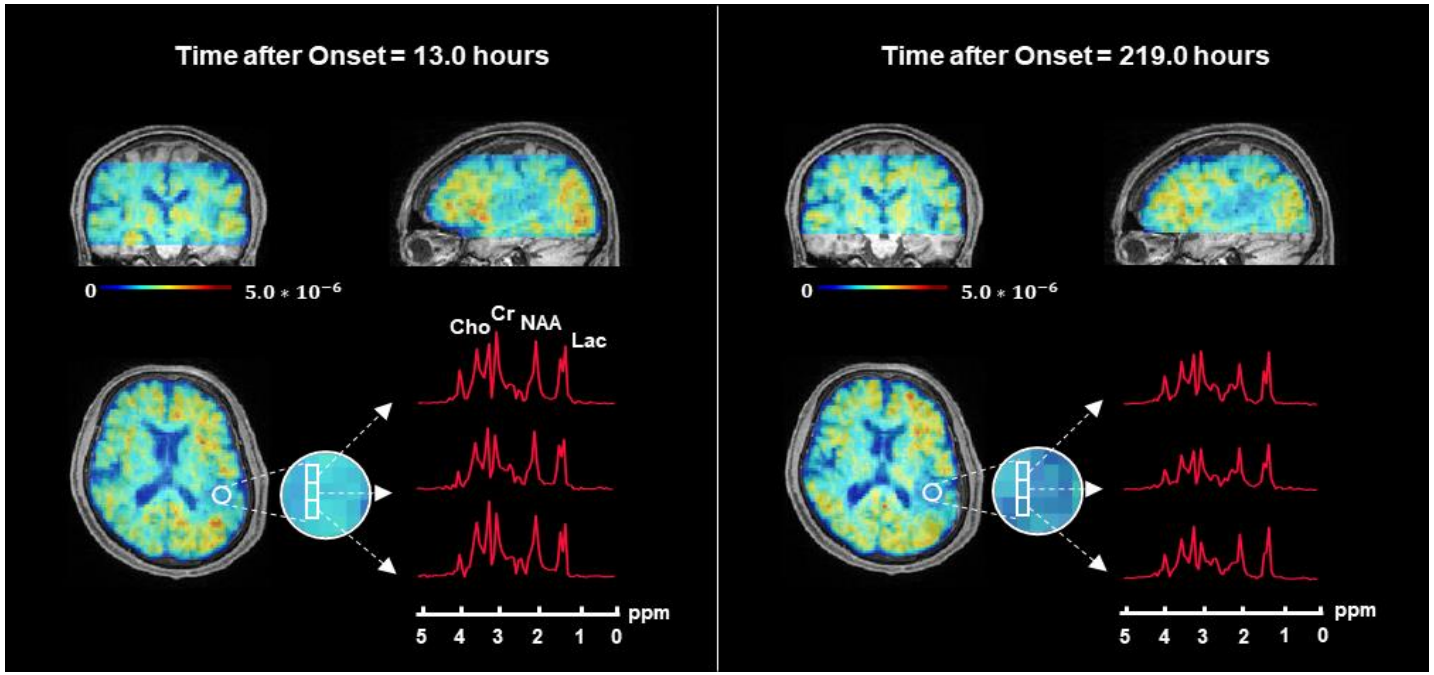
Acquisition Time: 8 minutes

Spatial Resolution: 2.0 x 3.0 x 3.0 mm^3

Li, et al., Brain, Nov. 2020 (Cover Feature Article)*

Imaging Ischemia Stroke: Onset Time Prediction



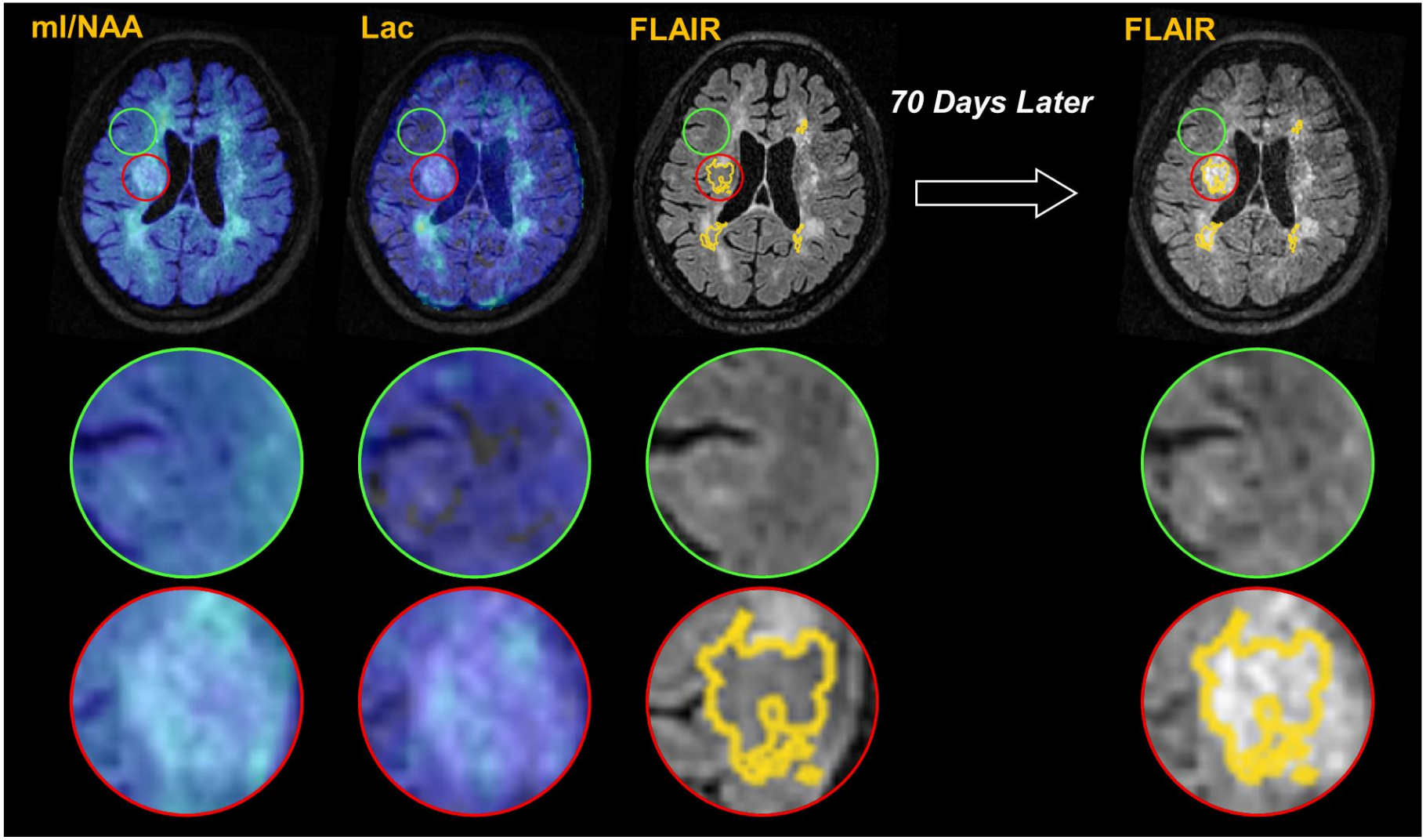


Lin, et al., JMRI, Sep. 2023 (Cover Feature Article)

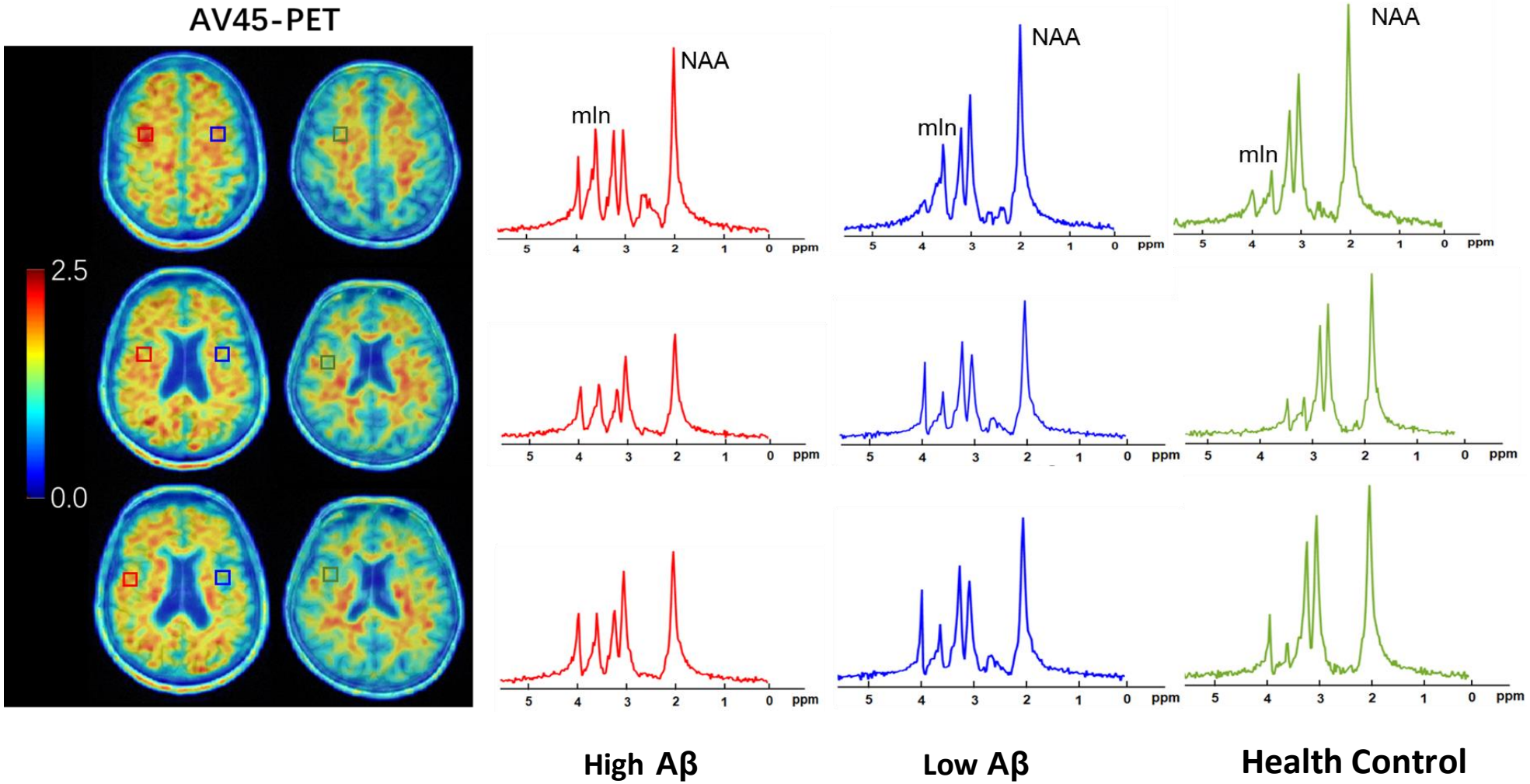
ISMRM W. S. Moore Award, 2023

Metabolic Imaging of Multiple Sclerosis

Detection of MRI-invisible pre-lesion



Metabolic Imaging of Alzheimer's Disease



- **NAA** reduction

  ⬇

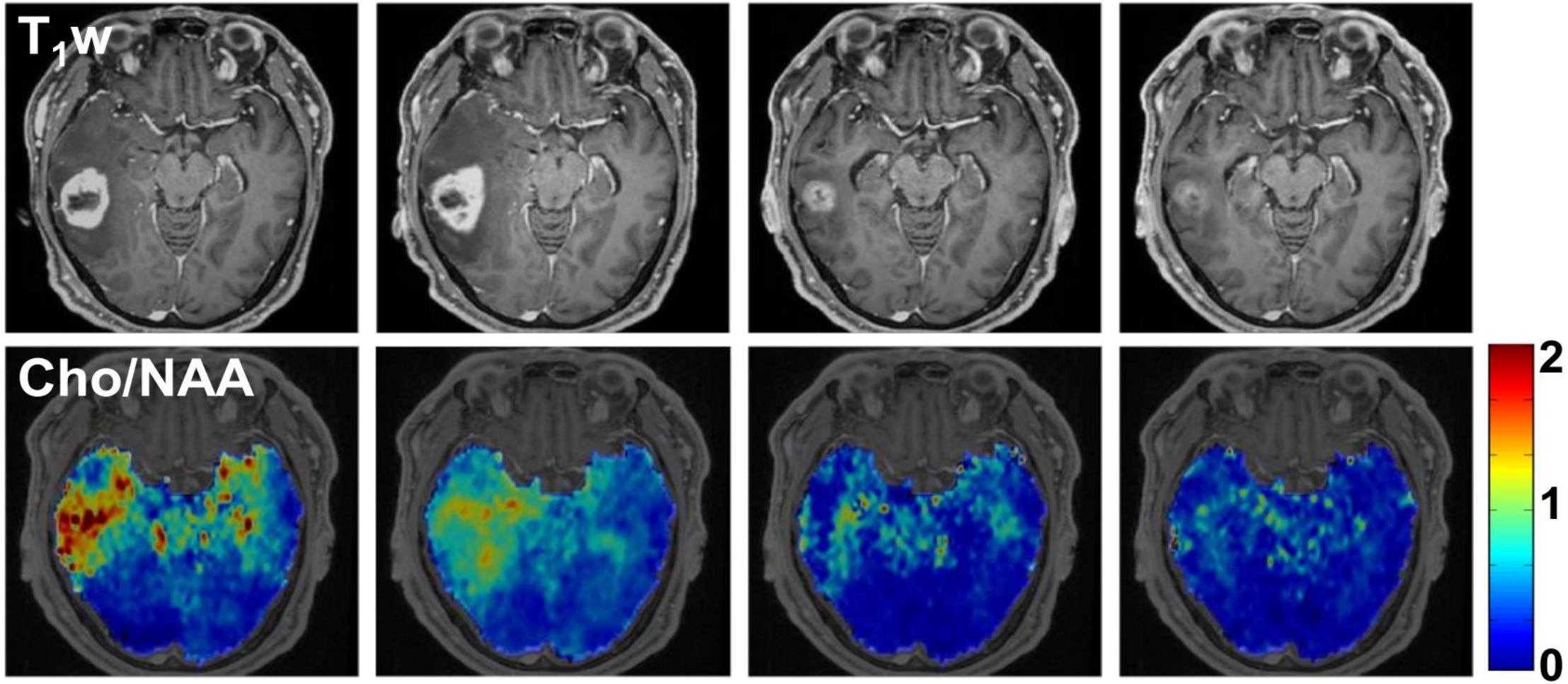
  Neuron/synaptic dysfunction or Neuron loss

- **mI** elevation

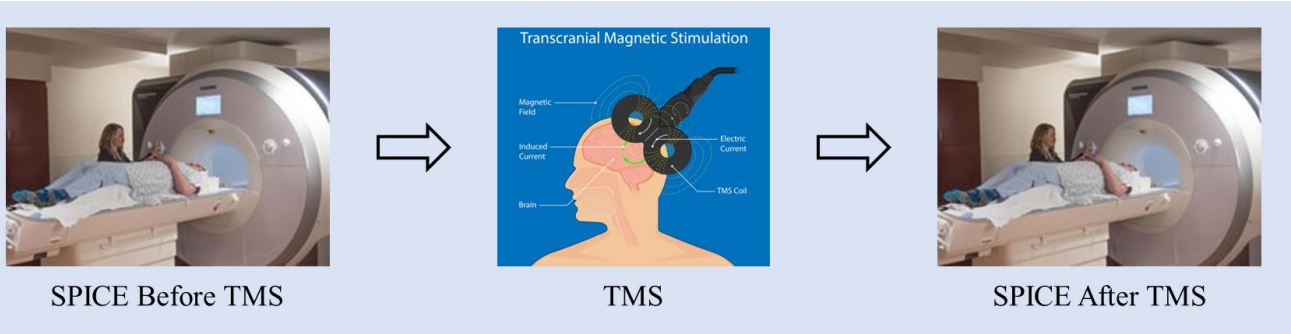
  ⬇

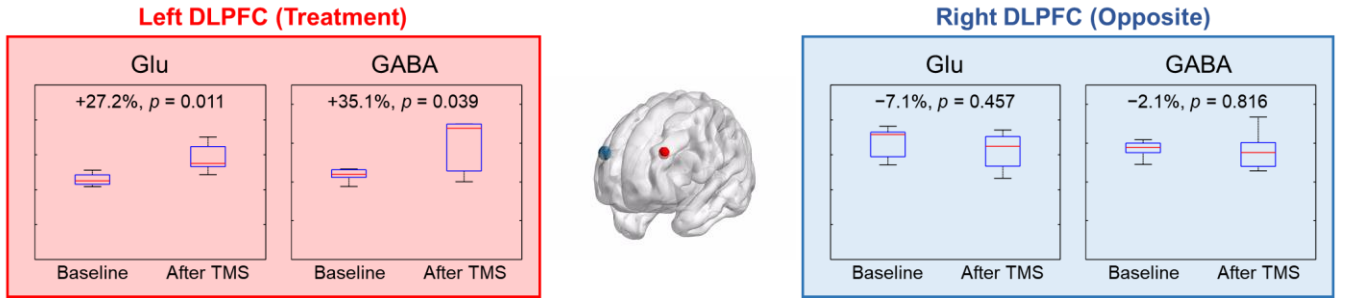
  Microglia and astrocyte activation

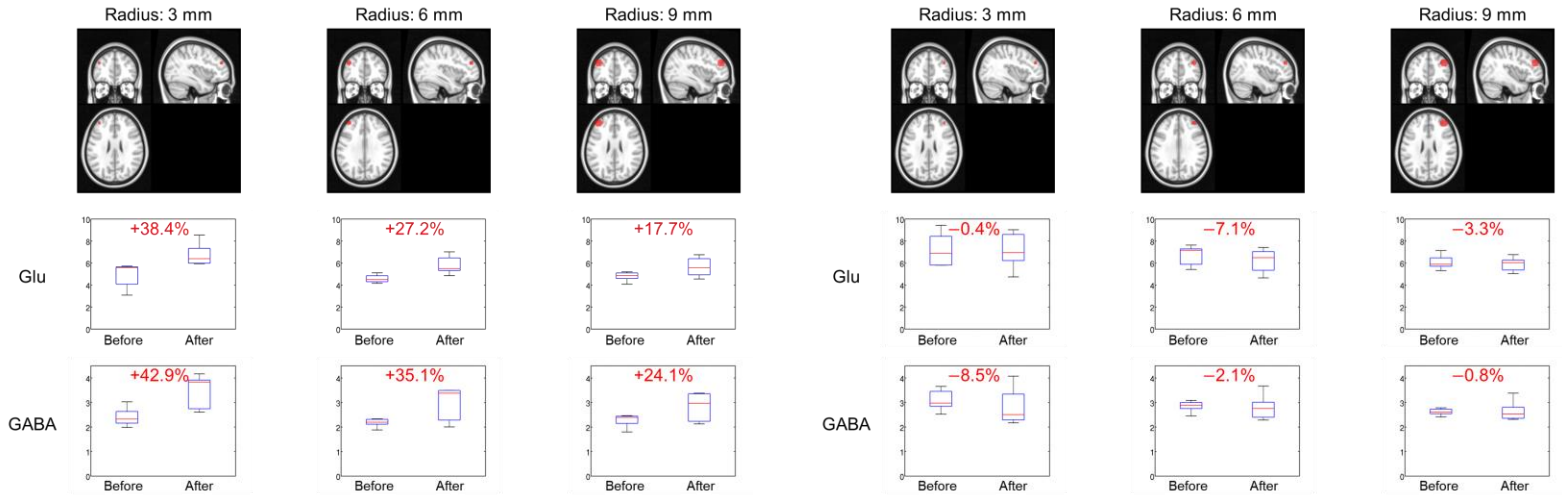
Monitoring Treatment Response: Radiation Therapy



Monitoring Treatment Response: Transcranial Magnetic Stimulation





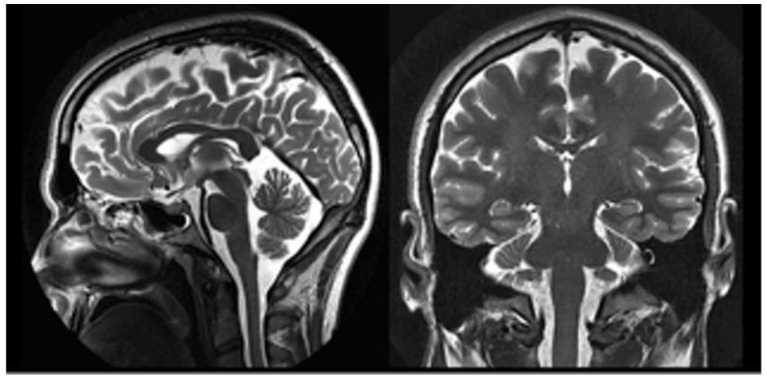


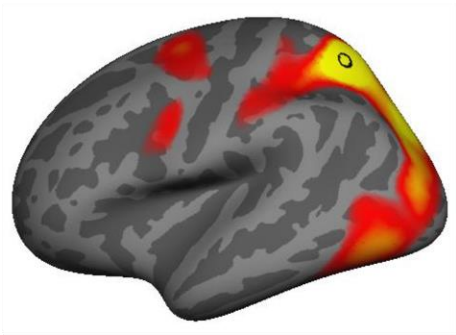
Towards Unraveling Structural, Functional, Molecular Fingerprints of Brain Function and Neurodegenerative Disorders

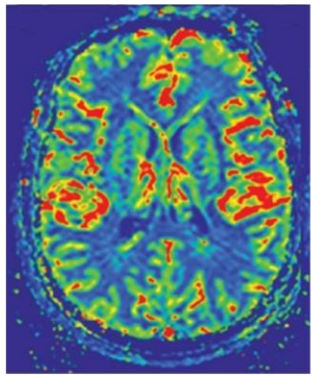
Structure

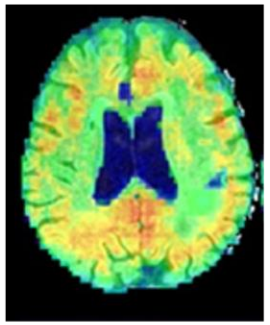
Function

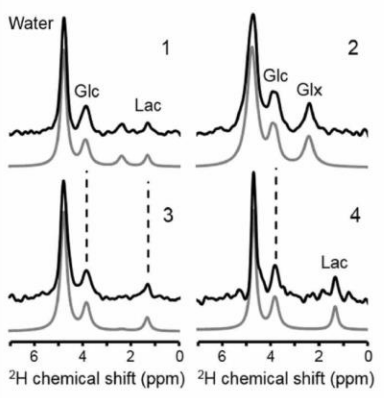
Metabolism

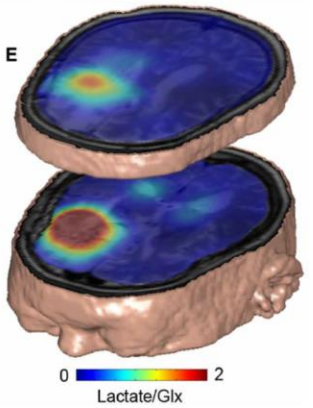












Acknowledgements