NMRbox Summer Workshop

June 20 – 24, 2016
UConn Health, Farmington, CT

NMRbox
.org

What is NMRbox?

NMRbox is a shared computational platform for NMR developed by the National Center for Biomolecular NMR Data Processing and Analysis, a collaboration among UConn Health, University of Wisconsin, and University of Illinois. The Center is a Biomedical Technology Research Resource (BTRR), supported by the National Institutes of Health (NIH) / National Institute of General Medical Sciences (NIGMS).

Syllabus

Day 1: Introduction and Background [Mon, 6/20]

Introduction to NMRbox Workshop	Jeff Hoch, UCH
NMR data processing workflows using NMRPipe	Frank Delaglio, NIST
Introduction to NMRbox	Mark Maciejewski, UCH
Introduction to CONNJUR-WB	Michael Gryk, UIUC

Day 2: Applications [Tue, 6/21]

Fundamentals of sampling: linear and nonuniform	Adam Schuyler, UCH
Non-Fourier methods overview	Jeffrey Hoch, UCH
Sensitivity	David Rovnyak, Bucknell (invited)
NESTA-NMR	Michelle Gill, NCI (invited)
MaxEnt	Mark Maciejewski, UCH

Day 3: Applications [Wed, 6/22]

Relaxation: DASHA	Dmitry Korzhnev, UCH
Assignment: ABACUS	Irina Bezsonova, UCH
Metabolomics	Bruce Johnson, CUNY
Chemical shift mapping	TBD

Day 4: Applications [Thu, 6/23]

ENSEMBLE	Mickael Krzeminski, U of Toronto
NMRFAM suite of tools	Woonghee Lee, NMRFAM

Day 5: Meta-packages [Fri, 6/24]

ASDP	Janet Huang, Rutgers (invited)
COMPASS	Joseph Courtney, UIUC (invited)
Software development in NMRbox	NMRbox staff

Registration

Contact Jeff Hoch [hoch@uchc.edu]
Visit our website [nmrbox.org]

Think inside the box.