JCP422H/CHM1455H An introduction to NMR spectroscopy for biological chemists (Theory & applications)

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Philosophy of the course – The goal in this course is to provide a foundation for understanding and implementing NMR experiments with an eye towards biomolecules large and small, drug discovery, and biochemistry. There will be a number of tutorials and exercises devoted to analyzing data and a significant fraction of time will be spent utilizing software and analyzing data. Many of the assignments will involve current papers of interest for which you will be expected to answer general review questions. Each week we will spend 2 hours covering theory (Mondays) and one hour covering modern methods (Wednesdays). The theory sections will make use of Quantum mechanics although the course textbook (Understanding NMR Spectroscopy, 2nd Edition by James Keeler) does a good job explaining NMR phenomena without vigorous quantum.

Assignments will consist of:
-4 tutorials using MestReNova software
1) NMR processing (1D)
2) NMR processing 2D
3) Analysis of mixtures
4) Relaxation data analysis
-Theory and application questions based on assigned papers (Wednesday lectures) & Keeler Ch 1-10 but excluding Ch 6

Graduate students will be responsible for a 10 page research proposal based on any application of NMR or MRI to their own research.

Evaluation:
Undergraduate JCP422H
Assignments (4) each 10% = 40%
Mid Term Exam 20%
Final Exam 40%

Graduate students CHM1455
Problem Sets (5) each 10% = 40% (see above for dates)
Final Research proposal 20%
Final Exam 40%

Schedule:
Theory lectures (2 hours)
Sept 9 Introduction to NMR and Ch 2 & 3
Sept 16 Ch 4 Vector picture of NMR
Sept 23 Ch 5 Processing NMR spectra
Sept 30 Ch 7 Product operator Notation
Oct 7th Ch 8 2D NMR
Oct 14-18 Study Break
Oct 21 Midterm
Oct 28 Relaxation and Dynamics (I)
Nov 4 Relaxation and Dynamics (II)
Nov 11 ^{19}F NMR
Nov 18 Advanced topics (Ch 10)
Nov 25 Advanced Topics (Ch 10)
Dec 2 Review

Special topics lectures (NMR course)

Sept 11 1. Phase equilibria, 2. Pressure experiments, 3. Supercritical fluids & supercooled water
Sept 18 Enhancing NMR sensitivity
Sept 25 Ligand binding by NMR
Oct 2 Drug discovery
Oct 9 Metabolomics
Oct 14-18 Study Break
Oct 23 Tricks: Parallel Detection, projection reconstruction & sparse sampling, SO-FAST HMQC
Oct 30 Paramagnetic shift reagents/relaxation agents as tools in NMR
Nov 6 NMR-based structure determination (Assignment, NOEs, RDCs)
Nov 13 NMR based structure determination (chemical shifts)
Nov 20 Dynamics (1D methods: magnetization exchange, CEST, CPMG)
Nov 27 Dynamics (2D methods: T1, T2, NOE, chemical exchange)
Dec 4 TROSY applications

Policy on lateness
20% per day late

Students may submit a request for special consideration within one week of the assignment due date or date of the missed test, quiz, or discussion period, by noon of that day. Requests for special consideration may be made by e-mail to the Course Instructor, from a valid University of Toronto e-mail account, with additional documentation to be submitted in person, as follows. Valid documents include the University of Toronto (UofT) Verification of Student Illness or Injury form and death certificates, such as a Medical Certificate of Death or Proof of Death Certificate (signed by a licensed funeral director), where special consideration is being requested for bereavement. Medical certificates other than an original, valid UofT Verification of Student Illness or Injury form will not be considered. Students must

also successfully complete an online absence declaration via ROSI/ACORN and provide the Course Instructor with a confirmation of this declaration in hardcopy along with the other documents included in their petition for special consideration. The Course Instructor will inform the student by e-mail (as per the communication policy above) whether special consideration is granted following due diligence on the documentation provided.

ACADEMIC INTEGRITY

It is your responsibility as a student at the University of Toronto to familiarize yourself with, and adhere to, both the Code of Student Conduct and the Code of Behaviour on Academic Matters. Please review the materials available at https://www.academicintegrity.utoronto.ca for more information.