**Computational Enviromental Sciences and Toxicology, BIO 592 - 079**

**Spring 2019**

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**Course description**: This 3-credit course will provide an introduction to computational toxicology and informatics methods in environmental sciences, designed for students interested in a survey of related topics. Statistical and computational methods will be introduced at an introductory graduate level. Topics to be covered include: dose-response analysis, physiologically-based pharmacokinetics, methods for exposomics and other 'omics, visualization and summary of high-dimensional data, QSAR, molecular descriptors, docking models, epidemiological designs, spatial analysis, and risk analysis/translation.

**Textbook** (none required)

**Prerequisites**: Some light computer programming is expected. Students with no exposure to programming will need to spend extra time learning introductory *R*.

**Class Hours**: Mondays & Wednesdays, 1:30PM – 2:45PM in Ricks Hall 336

**Office Hours:** Mondays and Wednesdays, directly after class. Other office hours by appointment with relevant instructor.

**Grading**: Based on an overall average of

- attendance (10%)
- homework (60%) – six homeworks will be given (10% each)
- final presentation and short paper (30%) – each student will present their work on a relevant computational env sci or toxicological project. Further details given about midway through the semester.

**Expectations**

-Class attendance is expected. On some days, we will use class time to explore data and discuss problems. Reading assignments in the form of current publications may be given in advance of class.

- Homework is due in class on the due date. Students are encouraged to work together to *understand* problems, but each student *must* complete his/her own work. Direct copying is not acceptable and is strictly prohibited. See https://studentconduct.dasa.ncsu.edu/code/

-Audit credit requires a score of at least 50% on the homework

**Schedule and topics (may be modified)**

| Day | Topic |
|---|---|
| 1/7/2019 | Intro - the evolution of computational environmental sciences |
| 1/9/2019 | current work in computational environmental sciences |
| 1/14/2019 | A basic introduction to toxicological principles |
| 1/16/2019 | Dose response designs: terminology,  time, dose |
| 1/23/2019 | Dose response analysis, points of departure and benchmark dose |
| 1/28/2019 | Physiologically-based pharmacokinetics 1 |
| 1/30/2019 | Physiologically-based pharmacokinetics 2 |
| 2/4/2019 | Exposure science, models and systems, analytical techniques |
| 2/6/2019 | Exposomics |
| 2/11/2019 | High-throughput screening: databases and data structures |
| 2/13/2019 | High-dimensional analysis methods 1: exploratory methods and dat |
| 2/18/2019 | High-dimensional analysis methods 2: multiple testing |
| 2/20/2019 | High-dimensional analysis methods 3: penalized methods and stati |
| 2/25/2019 | Omics methods for environmental sciences 1 |
| 2/27/2019 | Omics methods for environmental sciences 2 |
| 3/4/2019 | Visualization (including ggplot?) |
| 3/6/2019 | Adverse Outcome Pathways |
| 3/18/2019 | Comptox 1: molecular representation, drawing tools |
| 3/20/2019 | Comptox 2: database searching, chemical descriptors |
| 3/25/2019 | Comptox 3: ligand-based comp tox (read-across, QSAR, 2D similari |
| 3/27/2019 | Comptox 4: structure-based comp tox (molecular docking, molecula |
| 4/1/2019 | Epidemiology 1: observational studies and study design |
| 4/3/2019 | Epidemiology 2: measures of risk association and analysis methods |
| 4/8/2019 | Spatial analysis 1: basic principles and point processes |
| 4/10/2019 | Spatial analysis 2: smoothing, kriging, and inference |
| 4/15/2019 | Risk analysis |
| 4/17/2019 | Risk translation |
| 4/22/2019 | Misc/ Student presentations 1 |
| 4/24/2019 | Student presentations 2 |