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| **Learning Outcomes** | **Schedule** |
| Use Jupyter notebook to run test Python code, to calculate molecular weight and extract data from known database. | DAY 1: Open Jupyter Notebook using ondemand at UNC;  Mention functions  Introduction to Python in notebook; Load packages;  Enter Python code to run calculation of molecular  weight of ibuprofen and favorite molecule  Use DataMol(?) and/or RDKit to extract data from DB and pull molecular weight and number of atoms. |
| Use Jupyter notebook to analyze reaction kinetics from NMR data (photoNMR) | DAY 2: Given photoNMR data, use of functions, calc rxn rate and quantum yield  HOMEWORK: report rates & yield for unknown data set |
| Learn techniques for processing NMR data using Mnova. | DAY 3. Processing 1D & 2D NMR data using Mnova |
| Extract integrals and intensities for a relaxation experiment; Python for fitting data | DAY 4: process NMR data & extract data  exponential fit to data (sciPy and curvefit), includes data visualization  HOMEWORK: report T1 values for unknown data set |
| Navigate between code, files (local and remote) and output in Jupyter Notebook | DAY 5: data management and chemical shift predictors  HOMEWORK: report chemical shifts from predictors |
|  | DAY 6: Group Projects: Proposal ideas |
|  | DAY 7: Group Projects: Protocol for using Python to analyze data including NMR results |
|  | Day 8: Presentations |