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Monitoring Metabolic Changes of Creatinine and in Amino Acid Cycle using BATMAN Software

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Monitoring metabolic changes of Creatinine and in the Amino Acid cycle using BATMAN software

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**Project Summary:**
Mixture analysis is a difficult task. Analyzing body fluids typically leads to mixtures of 300+ components; quantitative analysis, however, is important to monitor metabolic changes and draw conclusions in terms of biological impact.

**Research Plan:**
We have already collected NMR data on 500+ urine samples and developed protocols to identify up to 15 individual components, per sample. Careful application of these protocols based on Bayesian statistics in combination with spiking of the samples, and thus positive identification of those components in the mixture shall lead to a comprehensive list of changes that occur during the life time of our model animals.

**Student Duties:**
Run NMR; identify components and monitor concentration differences between different samples. Improve standard operation procedures. Analyze biological samples.

**Tentative plan for the 10 week schedule:**

- **week 1/3:** familiarization with VNMRJ, MestreNova (NMR), and BATMAN for data analysis.
- **week 4/6:** building of reference data files, establishing position of peaks for the relevant compounds.
- **week 7/8:** analysis of data sets.
- **week 9/10:** refine measurements.

**Manuscript preparation:**
Dr. Vogler encourages all undergraduate student researchers to write up their results in the form of a manuscript for publication. The RCEU participant, under the supervision of Dr. Vogler, will help prepare the manuscript(s), which may include data from other undergraduate or graduate students.

**Expected Student Background:**
Students should have good background in General Chemistry, knowledge of Organic Chemistry is advantageous, so typically students with a major in Biology, Chemistry, and or Chemical Engineering should be ok. However, Dr Vogler will take all applications into account and makes his final decision based on an interview. Previous exposure to analytical instrumentation is a clear benefit. This is an expansion of a RCEU project from 2019.

*Expected results and deliverables:*

The student will be exposed to important instrumental techniques such as NMR spectroscopy, analysis of spectra, in particular mixture analysis, preparation of samples in smallest concentrations, error analysis, literature studies. Exposure to state of the art instrumental techniques will greatly enhance any students’ career chances in chemistry or related disciplines. Instrumental skills are highly regarded.

*Faculty Supervision and Mentoring:*

NMR measurements will be supervised by Dr. Vogler and James Wolfsberger, my graduate student. Manuscript preparation will be supervised by Dr. Vogler. We will hold regular group meetings weekly.

The student will be part of a group of three graduate students, two undergraduate Students, and two high school students and will have access to the instructor at least once a day.