2022 Spring Science Research Symposium
Gustavus Adolphus College, May 6th, 2022

Session A: Oral Presentations, Beck Hall 101	
4:00 pm	**A Strategy for Assessing Peak Purity of Pharmaceutical Peptides in Reversed-Phase Chromatography Methods Using 2D-LC-MS** This contribution describes the development of a 2D-LC-MS-based strategy for assessing main peak purity in the analysis of pharmaceutical peptides. Our focus is on 2D-LC separations using reversed-phase (RP) separations in both dimensions, and particularly isomer selectivity, since isobaric compounds are not readily distinguished (or differentiated) by mass spectrometry (MS) and therefore must be separated chromatographically. In a first step of the study several mobile/stationary phase combinations were evaluated for both general separation performance (i.e., peak shape, selectivity) and isomer selectivity using forcibly degraded peptide samples. A ranking of the hundreds of chromatograms resulting from this step suggests that when developing a new method, screening a set of four columns and four volatile mobile phases should be adequate to both cover the selectivity space, and yield good separation performance as measured by the metrics mentioned above. When 2D-LC- MS is to be used to check peak purity for a new method, our results show that a second dimension based involving a C8/C18 column with neutral phase chemistry and an acetic acid / ammonium acetate mobile phase buffered at pH 5 provides good selectivity for peptide isomers. Finding the conditions needed for resolution of these isomers (i.e., gradient elution with shallow slopes (<< 1% ACN/min)) can be time- consuming. In this work we have developed a workflow that utilizes retention information obtained from the second dimension of carefully designed 2D-LC experiments to train a retention model that enables prediction of the desired conditions. We will demonstrate the performance of such models for multiple peptides, and the implementation of the approach in multiple laboratories. **Maria Sylvester** and Dwight Stoll Advisor: Dwight Stoll, Chemistry
4:15 pm	**Development and Application of a Web-Based Simulator for Multi-Dimensional Liquid Chromatography** Currently there are a variety of high-performance liquid chromatography simulators available in a variety of formats, and with varying levels of sophistication. However, to the best of our knowledge all existing simulators support one-dimensional separations only. In this work we have developed a web-based application and application programming interface for interacting with two core simulation components previously described in the literature, with options for both one-dimensional and two-dimensional separations in heartcutting or comprehensive modes. The first core component is based on calculation of the widths and retention times of injected analyte pulses, and is computationally inexpensive, allowing fast simulations. The second core component, based on the Craig countercurrent distribution model, is computationally expensive but more accurate under a wider range of conditions. Simulation conditions can be rapidly prototyped using the faster approach, and then fine-tuned using the slower but more accurate approach. Both approaches support the use of Linear Solvent Strength and Neue-Kuss retention models. The interface displays chromatograms with realistic peak shapes, which can be helpful to guide 2D-LC method development in cases where mobile phase mismatch is significant. Each separation dimension or individual heartcut can use different separation conditions, including column dimensions, stationary phase type, particle size, mobile phase type and strength (isocratic or gradient mode), and interface conditions such as dilution via active solvent modulation. The interface is available free on the web with no download required, and is licensed under CC BY-NC-SA 4.0 for Educational and Research purposes. **Thomas Lauer,** Caden Gunnarson, Tyler Brau, and Dwight Stoll Advisor: Dwight Stoll, Chemistry

4:30 pm	**Characterization of proteases involved in neurodegeneration** In every eukaryotic cell, there are vacuoles and/or lysosomes that are responsible for the degradation of waste that the cell produces. If all goes according to plan, this should be a continuous process. However, sometimes a process goes wrong and waste cannot be delivered properly to the vacuole. When this happens in neurons, it can lead to neurodegeneration due to the death of neuron cells. The process with how proteases in vacuoles and lysosomes degrade waste is still widely unknown, and this project searches to find how these proteases interact with other proteins to degrade them. The main questions we are trying to answer with this research are how proteins are degraded in the vacuole and how neurological diseases may develop due to misfolded proteins and inactive proteases. To do this, we intend to express PEP4 and PRB1 in E. coli cells in order to create large scale protein purification. We then intend to extract and purify the protein, and observe their biochemical properties. **Kimberly Hareland** and **Tessa Bierbaum** Advisor: Brooke Shields, Biology
4:45 pm (30 minutes)	**The Effect of Wet and Dry Cycles on the Export of Dissolved Organic Carbon from an Ombrotrophic Peatland** Peatland systems cover over 400 million hectares of the Earth's surface and store one-third of the world's soil carbon pool. The cycling and sequestration of carbon has long been studied in peatland systems in Northern Europe and North America. One long-term research site is the S2 ombrotrophic peatland bog at the Marcell Experimental Forest (MEF), a research facility located in Northern Minnesota. Previous literature has shown that the important role peatland systems play in the global carbon cycle is predominantly facilitated through the export of dissolved organic carbon (DOC). DOC in peatlands is highly regulated and controlled by hydrological conditions, including water-table depth. The goal of this study was to compare the concentrations of DOC overtime within peat cores from S2 to the annual system-wide trends in S2. Initial experimental data, collected over a six-month period, showed concentration levels of DOC in leachate samples remaining consistent with an unchanging water table level. However, after these cores dried for three months, DOC concentrations dramatically increased for a short period of time. The environmental phenomena captured within the experimental peat cores is supported by field data collected. These results support the theory that consistent water-table depth creates steady, moderate exports of DOC, while large fluctuations generate more variable, high DOC concentrations. Ultimately, the shifts in precipitation events resulting from climate change will cause a disturbance within peatland biogeochemical processes. We speculate that changes in the water regime in peatlands will cause a net loss of carbon from the system. **Collin Carlson** Advisor: Jeff Jeremiason, Chemistry and Environmental Studies
5:15 pm (30 minutes)	**Effect of American Bison Grazing on Species Richness, Above ground Biomass, and Plant Community Composition of a Native Oak Savanna Ecosystem** American bison (Bison bison) were once keystone species in the Great Plains region of the United States, altering the landscape through their grazing, wallowing, and movements. Bison primarily graze on C4 grasses, many of which are found in oak savanna ecosystems. Oak savannas are declining throughout Minnesota. In the summer of 2018, a group of bison were re-introduced onto a 200-acre enclosure at Cedar Creek Ecosystem Science Reserve in East Bethel, MN. Groups of bison have been present in the enclosure from late May through September for 2018, 2019, 2020, and 2021. Pairs of plots were set up across the enclosure. Plot pairs consist of one 49 m2 fenced plot to exclude bison grazing and an unfenced 49 m^2 plot open to bison grazing. We harvested a 2 m^2 area of aboveground biomass approximately every 3 weeks during the field season (June-August). Biomass was sorted by species, dried, and then weighed. The objective was to determine if bison grazing had a significant effect on species richness, aboveground biomass, and plant community composition. While bison grazing had no significant effect on species

	richness or aboveground biomass, trends in the data suggest that with more time the grazed plots may have a higher species richness and lower biomass than ungrazed plots and that grazing had some influence on plant composition of the grazed compared to the ungrazed plots. **Lila Beck** Advisor: Jon Grinnell, Biology

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Session B: Oral Presentations, Beck Hall 111	
4:00 pm	**Investigating Student Participation and Performance in Calculus I Courses that Utilize Standards-Based Grading** Standards-based grading does not rely on traditional methods of grading, but rather focuses on complete understanding of concepts deemed essential by the instructor. A student's grade depends on the number of standards the student meets where standards are graded pass/fail without partial credit. However, each student is given multiple chances to meet every standard. In this study, we analyzed student participation and success in a college-level calculus I course that utilized standards-based grading. By defining student "buy-in" as the level to which students participate in this class structure, we were able to use a clustering algorithm that revealed multiple groupings of students that were distinct based on activity throughout the semester. Additionally, we analyzed student progress, defined as the number of graded activities completed each week. We found that students who progressed steadily throughout the semester, and thus had lower variability in the number of completed activities per week, tended to receive a higher overall grade. Students whose progress was less consistent, and thus exhibited higher variability in weekly activities completed, tended to receive a lower grade. Overall, this shows implications for the pay-off of buying into the method of standards-based grading and succeeding in a course. **Rachel Erickson,** Ha Le, Kaylee Vick, and Jillian Downey Advisor: Jillian Downey, Mathematics, Computer Science, and Statistics
4:15 pm	**Utilizing Pattern Mining and Classification Algorithms to Identify Risk for Anxiety and Depression in the LGBTQ+ Community During the COVID-19 Pandemic** We examined the results of pattern mining and decision trees applied to a dataset of survey responses about life for individuals in the LGBTQ+ community during COVID, which have the potential to be used as a tool to identify those at risk for anxiety and depression. The world was immensely affected by the pandemic in 2020 through 2022, and our study attempts to use the data from this period to analyze the impact on anxiety and depression. First, we used the FP-growth algorithm for frequent pattern mining, which finds groups of items that frequently occur together, and utilized the resulting patterns and measures to determine which features were significant when inspecting anxiety and depression. Then, we trained a decision tree with the selected features to classify if a person has anxiety or depression. The resulting decision trees can be used to identify individuals at risk for these conditions. From our results, we also identified specific risk factors that helped predict whether an individual was likely to experience anxiety and/or depression, such as satisfaction with their sex life, cutting meals, and worries of healthcare discrimination due to their gender identity or sexual orientation. **Josephine Bierbaum**, Melissa Lynn, and Louis Yu Advisor: Melissa Lynn, Mathematics, Computer Science, and Statistics
4:30 pm	**Modeling Drought Response in St. Croix State Forest** The climate and regular weather patterns of Minnesota are forecasted to change corresponding to global climate change. With warmer summers and wetter winters Minnesota will continue to experience more frequent, widespread, and intense meteorological drought conditions than previously recorded. Groundwater resources are negatively impacted during drought conditions because of limited recharge and increased extraction due to dry weather. Groundwater is irreplaceable for residents as well as for industry, agriculture, and ecosystem health. The ability to predict the changes and the recovery time following intense drought conditions can influence policy and decision making at a state, local, and

	personal level regarding water consumption. The high-resolution historical records of water table elevation at the S3 fen within the Marcel Experimental Forest showed evidence of 1-5 year recovery to pre-drought water table levels. Prediction methods using ¼ year water table elevation trends resulted in an accuracy window of 14 months on average linear recovery. Due to the similar geological and hydrological conditions shared by the Marcel Experimental Forest and Pine County study area, the water table elevation recovery time in the Pine County study area, following the end of 2021 drought conditions, can be predicted to occur within 0-6 years. **Andrew Dooley** Advisor: Laura Triplett, Geology
4:45 pm	**Characterization of Prenatal Zika Virus Exposure in Rhesus Macaques Via Ultrasonography** Exposure to Zika virus (ZIKV) in utero negatively impacts fetal development, resulting in a spectrum of outcomes that range from asymptomatic, birth defects, developmental deficits, to fetal demise. Studies involving the use of obstetric ultrasonography to detect early signs of damage from ZIKV exposure have focused on the presence or absence of severe deficits, but no studies to date have broadly characterized the effects of prenatal ZIKV exposure by comparing all exposed fetuses (potentially symptomatic and asymptomatic) to non-exposed controls. As detailed, weekly examinations of human pregnancies with known gestational ages of inoculation and known virus isolates cannot be performed, we utilized a rhesus macaque model of prenatal ZIKV exposure by inoculating dams in their first trimester of pregnancy with either 10^4 PFU of a contemporary strain of ZIKV (n=31) or saline (n=15). Of the infected animals, 8 dams had previously been exposed to dengue virus and cleared the infection before becoming pregnant. No differences were detected in general fetal growth between ZIKV-exposed groups and controls. The pulsatility index of the middle cerebral artery, a calculated parameter that is used to examine blood flow to the brain, was found to be consistent across all groups. No difference was found between groups in umbilical artery systolic-diastolic ratio, which is a measure of resistance that is used to assess blood flow to the placenta. Ultrasonography remains a useful tool in screening for severe ZIKV-related defects but may not be clinically useful in looking for early signs of ZIKV exposure in utero. **Jessica Schwartz**, Rachel Spanton, Elaina Razo, Ann Mitzey, Chelsea Crooks, Dawn Dudley, Jens Eickhoff, Kathleen Antony, Saverio Capuano III, Karla Auderau, Matthew Aliota, Thomas Friedrich, David H. O'Connor, Thaddeus Golos, and Emma L. Mohr Advisor: Amanda Nienow, Chemistry
5:00 pm	**Comparison of leucosome networks in migmatitic orthogneiss and paragneiss from the Pioneer Mountains, Idaho** We are investigating the effect of preexisting layering on the formation and organization of leucosome networks in migmatites from the Pioneer Mountains, Idaho. Migmatites form where melt is created and transferred as it moves from the deep to the upper crust. Large magnitude extension in the Pioneer Mountains exposed two distinct migmatitic gneiss: orthogneiss and paragneiss. Both kinds of migmatites have lighter areas referred to as leucosomes, which are networks of former partial melt. By studying the leucosome we can determine whether the networks are a self-organized system based on if the thickness and spacing are scale invariant. Knowing if migmatites have self-sustaining leucosome networks explains what is happening in other parts of the crust, since a self-sustaining system illustrates what criteria is needed for melt to move freely towards the surface, leading to crustal differentiation, potentially feeding plutons. In this study, we are investigating the effect preexisting layering from migmatitic paragneiss has on the formation and organization of leucosome networks, since paragneiss come from a sedimentary parent rock. Given the orthogneiss and paragneiss of the Pioneer Mountains have the same deformation history, we can determine how preexisting layering affects leucosome development. To determine the scale-dependency of leucosome networks we created cumulative thickness and cumulative frequency

	plots using methodology demonstrated in other studies. These plots suggest the leucosome networks are not a self-organized critical system, meaning melt did not flow freely through a fully interconnected network of melt pathways. **Hannah Schroeder**, Rory McFadden, and Cora Hentges Advisor: Rory McFadden, Geology
5:15 pm	**Effects of Viscoelasticity on the Oscillatory Behavior of a Two-link Filament Model** A subgroup of microscopic organisms, known as swimmers, use thin rod-like structures called cilia and flagella to propel themselves in various fluid environments. This locomotion is driven by both the dynamics of intracellular molecular motors within the flagella/cilia and the hydrostatic elastic forces exerted on the swimmer. Both swimmer gait and the stability of the swimmers' motion are subject to changes in both external and internal environments. In this work, we are interested in the 2D planar motion of a flagellum driven by a follower force applied tangentially at the tail and pinned at the head. To characterize this phenomenon, we consider a discretized, two-link filament model that exhibits oscillatory behavior. We explore this motion in three different fluid models: a viscous model, a Maxwell elastic model, and an Oldroyd-B viscoelastic model. Changes in the frequency, amplitude, and stability of the emergent oscillations were observed as a result of variations in fluid properties. This result highlights the adaptive nature of swimmers in viscoelastic environments. **Sophia Nelson** Advisor: Jeff Ford, Mathematics, Computer Science, and Statistics

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Session C: Oral Presentations, Beck Hall 119	
4:00 pm	**Analyzing Carbonate Associate Sulfates in Ancient Carbonates** This study is investigating levels of carbonate-associated sulfate (CAS) in a suite of Proterozoic (1.0-1.4-billion-year-old) carbonate rocks. CAS is sulfate bound within the calcium carbonate mineral structure. CAS concentration indicates the concentration of sulfate in the waters from which the carbonate precipitated, which can be linked to marine oxygenation or hypersalinity of the depositional environment. Conventional techniques require a large sample size and thus provide only average, whole-rock values. By modifying the method to use smaller sample sizes and analyzing CAS using ion chromatography (IC) on homogeneous samples of individual carbonate phases (carbonate rock layers), a more detailed understanding of CAS levels can be obtained. An IC technique developed by Present et al. (2015) established the technique for high-CAS carbonate samples; our study aims to test this technique in a suite of Proterozoic-aged (~1.4-billion-year-old) samples with high whole-rock CAS concentration, but unknown distribution of CAS among phases. Preliminary analyses indicate that CAS can be detected using this technique in our laboratory, and ongoing work is investigating the phase-specific distribution of CAS in these samples. **Erin Fisher** Advisor: Julie Bartley, Geology
4:15 pm	**Long-term Water Quality Monitoring in Seven Mile Creek Watershed** Agricultural runoff is one of the leading contributors to nutrient pollution in waterways around Minnesota and this pollution can have lasting consequences on the quality of the downstream ecosystems and communities' water supplies. Therefore it is critical to study these systems and see how different farming practices are affecting water quality. Over the last 5 years a team of students and professors at Gustavus Adolphus College, alongside the Minnesota Pollution Control Agency, Great River Greening and Nicollet Soil and Water Conservation District, have been monitoring the Seven Mile Creek watershed. The watershed is 23,551 acres with 79% of acres being intensively managed for corn and soybean production and 14% being in forests, wetlands, and grasslands. The two largest sub-watersheds were monitored separately to better isolate the farming practices that could contribute to helping improve water quality. From these sections, measurements of nitrate, E. coli, phosphate and total suspended solids were taken. It was found that the watershed regularly contains nitrate levels well over the state standard of 10 mg/L, sometimes reaching as high as 42.8 mg/L. E Coli levels were also seen to be quite high, and strain analysis suggests the possibility of high human waste contamination. Finally TSS samples showed that 60% of the time TSS concentration was well over the cold water stream state standard. The Seven Mile Creek watershed has indeed proven to be an area of concern, but further analysis may shed light on ways the quality of water can be improved by better farming practices. **Luke Dragseth,** Elizabeth Lawrence, CJ Miller, and Laura Triplett Advisor: Laura Triplett, Geology and Environmental Studies
4:30 pm	**Effect of Buffer pH and Aging on Retention in High Performance Liquid Chromatography** The effect of pH on retention in high performance liquid chromatography (HPLC) has been well documented in the literature. The pH of the mobile phase affects compounds differently, but affects things including retention, peak shape, and selectivity. For example, nucleotides have been shown to have an inverse relationship between retention and pH. As pH decreases, retention increases for nucleotides, which is a trend consistent with most molecules. Because even small pH changes can affect retention, buffers are often used to maintain a consistent pH in the mobile phase. If buffers aren't at a consistent pH then it's likely there will be differences in retention when new buffers are used.

	In this study, we aimed to see how differences in the pH of different batches of buffer prepared on the same day would affect retention. Four mixtures of compounds were tested to determine how pH differences in buffers affect a variety of compounds. Significant differences across five buffer batches were observed for 6-n-heptylaniline while the other compound's retention times remained relatively unchanged. The retention times of nortriptyline and amitriptyline followed a downward trend as the buffers aged, especially apparent for amitriptyline. **Carter Henning,** Trevor Kempen, Tina Dahlseid, and Dwight Stoll Advisor: Dwight Stoll, Chemistry
4:45 pm	**Pressure Induced Retention Changes Affect the Accuracy of Retention Models in HPLC** The effect of pressure on retention in liquid chromatography (LC) has been well documented in the literature. Multiple findings have demonstrated that a compound's behavior as pressure increases is explained by a complex relationship between the mobile phase composition, the properties of the stationary phase, and the properties of the compound. For example, it has been shown that the effect of pressure on a compound varies depending on the percent organic solvent in the mobile phase. This has implications when retention models are used to predict retention at a given mobile phase composition. As the percent organic solvent is varied in the mobile phase, the viscosity of the mobile phase changes, resulting in pressure changes. All existing retention models for reversed-phase LC ignore the changes in pressure as the mobile phase composition changes, which means the applicability and usefulness of the model decreases with compounds that are sensitive to pressure changes. In this study, the effect of pressure on specific retention models was isolated. When pressure is accounted for, there is a significant difference in the fitting parameters of the model. Understanding the effect of pressure and its influence on retention models may improve the utility of retention parameters obtained from the models, and their usefulness in HPLC method development. **Trevor Kempen,** Dwight Stoll, Tina Dahlseid, and Bob Pirok Advisor: Dwight Stoll, Chemistry
5:00 pm	**Effect of Analyte Mixture Composition on Observed Retention Factors in Reversed-Phase Liquid Chromatography** Current resources used by chromatographers to predict analyte retention time, such as hplccolumns.org and MultiSimLC, are valuable in many aspects. However, as a result of their design, each harbors certain limitations. In the case of hplccolumns.org, mixtures of compounds are injected to determine the retention characteristics of each column. For MultiSimLC, individual compounds are injected to obtain experimental retention data, but when these data are used to predict separations, an assumption is made that each compound behaves independently of others in a mixture. Little is known about how exactly analytes interact inside of these columns, thus the assumption about the independent behavior of analytes is questionable. In this study, we aimed to examine this assumption by monitoring shifts in retention time as a function of the composition of the injected sample (i.e., analyte mixtures, or individual compounds). Mixtures were designed to identify whether attributes such as charge, acidity, or polarity impact the retention of other compounds. It was determined that for specific pairings of compounds, a shift in retention is observed. One example of this was the combination of amitriptyline and 4-n-heptylaniline, in which an increase in 4-n-heptylaniline concentration correlated with a decrease in retention of amitriptyline. However, this effect was only observed at relatively high sample concentrations of analyte, thus we find that the effect will be insignificant for most practical applications of reversed-phase LC. **Haley Jostes,** Ryan Schimek, Tina Dahlseid, Bob Pirok, and Dwight Stoll Advisor: Dwight Stoll, Chemistry