Presentation Abstracts

CHEM 23201 - Thursday

Fall 2018
Updated: 6 Dec @ 9:14 AM
1. Lewisite is a vesicant used in chemical warfare in WWI and the Sino-Russian war that irreversibly binds to enzymes involved in cellular respiration. Many countries still have stockpiles of this agent, and the health and environmental impact of this is still a serious concern.

2. The goal of this research is to understand how Lewisite acts as a suicide inhibitor and how British Anti-Lewisite (BAL) deactivates Lewisite.

3. Literature was reviewed to determine the mechanisms or if the mechanisms have been elucidated.

4. BAL is a chelator and binds the arsine, preventing lewisite from binding to pyruvate dehydrogenase in the cell.

5. Moving forward, it should be investigated if there is a better antidote to lewisite and other heavy metal toxins than BAL.

Once promoted as being a cure for cancer, amygdalin was discovered to cause cyanide poisoning to some patients that the drug was supposed to cure. The source of the cyanide poisoning and how different administration techniques of the drug impacted the hydrolysis of amygdalin were researched using the literature. It was determined that there was a substantial increase in cyanide levels in the body when it was taken orally versus parenterally, because the hydrolysis is done by bacteria in human feces. However, there have been tests done which demonstrate that treating the patient with antibiotics prior to the ingestion of amygdalin will suppress the bacteria. This information prompts the discussion of the potential health effects of amygdalin if the cyanide poisoning could be avoided.

An issue during warfare is promoting wounds to blood clot, as bleeding out can be fatal. Chitosan is a polysaccharide derived from chitin that has medical capabilities, such as promoting blood clotting and helping with weight loss. In my research, I address the properties of chitosan that allow it to clot blood and promote weight loss. Scholarly research provides insight on chitosan’s properties, current medicinal uses, and claimed effects with weight loss. Literature indicates that chitosan’s NH3+ groups’ positive charges interact with red blood cells’ negative charges, leading to clotting. For weight loss chitosan binds with fat, preventing its absorption. The FDA considers it safe, but people allergic to shellfish will react. A question raised from this is what could be chitosan’s future medical uses?
Date-rape is an extensive problem in the United States today, with 1 in 6 women experiencing it within her lifetime. One of the most common mediators for this crime is rohypnol, which is also known as flunitrazepam. Increasing knowledge and awareness of the chemistry behind this central nervous system depressant could help decrease the rate of date-rape in the US as well as develop new methods of discovery or even counteraction. From this approach, new detection methods and antidotes, as well as much general information, can be learned about rohypnol. Understanding the original purpose and synthesis is also important to perceiving the impact, intentional or otherwise, that it had on society. Since antidotes and detection methods have been identified, what are the next steps to make them readily available and to reduce this sort of crime in the United States and beyond?

Essential oils are one type of natural product that are frequently utilized for their potential benefits. As an essential oil, thujone may have an incredibly beneficial physiological effect that could be of use to humanity. However, thujone is most frequently associated with psychoactive effects which lead people to believe it may be harmful. This research focused on finding information on physiological effects of thujone—a chemical compound commonly found in essential oils—and understanding how they develop. This was accomplished by reviewing literature from a variety of databases, narrowing searches via key concepts and synonyms associated with thujone, such as “essential oils” and “physiological effects”. Research showed that high levels of thujone have been shown to impair sensory and neural function. Several other studies have shown that thujone may exhibit beneficial antimicrobial activity. The results of this research led to an interest in determining if there a particular method of consuming thujone or dosage level that allows a person to reap the anti-microbial benefits of thujone without suffering the impairments.

Insects are vectors for many harmful pathogens. Recent efforts have been made to find novel vector controls that eliminate these insects, yet do not harm humans. The invertebrate neurotransmitter octopamine shows potential for developing better commercial insecticides and bug sprays. After reviewing the literature, it was found that octopamine, with one hydroxyl side group, does not bind to adrenergic, G-protein coupled, receptors in
humans, which bind to catecholamines, benzenes with two hydroxyl groups and a side chain amine. The structure of octopamine indicates that it does have potential in more effective commercial insect repellents that do not harm the human nervous system. Other neurotransmitters which do not have the catecholamine structure, such as FMRFamide neuropeptides, may be other potential targets for developing safer insecticides.

1:09 – 1:21 Morgan McCabe The Biochemistry Behind the Meth Epidemic

A societal problem that America faces is addiction. Many relationships are strained because of the consequences of highly addictive drugs. Methamphetamine’s attack on the central nervous system is what makes it so addictive. After searching through various pieces of literature, it was found that the positive side effects that methamphetamine causes are due to its interaction with norepinephrine and dopamine receptors. These interactions prove to be negative once there is no methamphetamine within one’s system because their affinity decreases, and users experience extreme withdrawal effects and potentially overdose. Because this high is based on the affinity of the receptors, further research is being conducted to investigate whether a vaccine could decrease the effects of methamphetamine to make it less desirable and decrease the number overdoses.

1:22 – 1:33 Andrew Smith An Investigation into the Chemical Character of Theophyllin

Pulmonary diseases are treatable with the advent of corticosteroids and PDE4 inhibitors. However, individuals who cannot tolerate either drug must instead use an alternative theophylline-based treatment. Chronic treatment with theophylline, however, can be toxic for the body. Therefore, an understanding of theophylline’s chemistry may help to limit the disadvantages in theophylline treatment. A literature review of theophylline’s experimental physical and spectral data was conducted to elucidate its character. Theophylline was revealed to be a methylxanthine, a class of compounds is known to be a natural stimulant. As such, significant doses would lead to the observed deleterious effects. Despite this characterization of theophylline, the drug’s mechanism of treatment is not understood. Further work should be directed towards cellular metabolism to reveal how theophylline inhibits pulmonary inflammation.

15 November 2018

Section 03 – Does not meet today
Levofloxacin, a type of fluoroquinolone, is one type of antibiotic that is used to treat bacterial infections, such as urinary tract infections and pneumonia. This presentation seeks to understand how the antibiotic levofloxacin works to treat common infections by looking into its structure and chemical characteristics. This was accomplished by checking the literature and reading scientific journals and articles, where key concepts searched included the synthesis and structure of levofloxacin. The results showed that levofloxacin is the S-enantiomer of the compound ofloxacin and works by sufficiently attaching and binding to the DNA gyrase enzyme to combat infection. Future research should address how resistance to the drug levofloxacin occurs and builds up in the human body over time.

The food packaging industry was lacking a sturdy, moldable, and clear plastic for containers until Bisphenol-A was synthesized. Bisphenol-A, or BPA, is a pluripotent polymer used in everything from lining cans to water bottles. BPA is found in most every drink that is packaged with it, and can also be absorbed through the skin. It or its metabolites can be detected in nearly every person tested. It is not a direct estrogen mimetic, but one possible metabolite of the compound is calculated to have a poor binding affinity for estradiol receptors. This is not a concern as of now due to the low calculated binding affinity, but should a replacement be found, it would decrease the health risks associated with potential hormone mimetics.
As the world continues to develop a growing need for alternate fuel sources, hydrogen fuel cells exhibit a great potential to alleviate the growing energy demand. By researching the literature, I have found that riboflavin, a molecule most commonly known as vitamin B, may play a significant role in a developing energy crisis. Riboflavin and its derivatives may display great synthetic utility as organocatalysts by mechanically splitting hydrogen to power fuel cells. If possible in the future, this process would greatly reduce the cost barrier to using fuel cells as well as provide a more environmentally friendly alternative to other forms of energy generation.

Sunburn is a threat to everyone who spends time outdoors. To counter this, many people use titanium dioxide in the form of sunscreen. TiO₂ has a wide range of other uses, including nanoscience. What are the TiO₂ nanoparticles primarily used for? Are they hazardous to human health? After consulting various articles from the scientific literature, it was determined that TiO₂ nanoparticles are toxic, as well as a carcinogen. However, they are still used as a substrate and photocatalyst, and the powder is used regularly in sunscreens. Based on these results, it is possible that the toxicity of the nanoparticles translates to the properties of the powder. Since it is used so frequently in sunscreens and cosmetics, this may be a significant area of research.

Heart disease leads to myocardial infarctions and strokes by causing arrhythmia and hypertension. Various factors impact cardiovascular health such as age, weight, sex, and the use of certain medications. Pseudoephedrine, a commonly used decongestant, exacerbates these symptoms, but what chemical properties of pseudoephedrine adversely affect the cardiovascular system? After researching the literature, it was discovered that pseudoephedrine interferes with normal functions of the nervous system by displacing norepinephrine from storage vesicles in presynaptic neurons, thereby releasing norepinephrine into neural synapses and stimulating alpha-adrenergic receptors. The arteries vasoconstrict, increasing both blood pressure and heart rate. This raises the issue of whether or not alternative forms of decongestants exist that do not adversely affect the cardiovascular system. If so, how do they differ chemically from pseudoephedrine?
Toxins are harmful products in nature, but understanding their effects and reactivity may be beneficial. Tetrodotoxin is produced by marine species (e.g. pufferfish) and is known for causing paralysis in neuromuscular tissue, but perhaps it has clinical uses in pain management. The mechanism of how tetrodotoxin’s chemical structure affects sodium channels, along with its potential benefits to humans were investigated. By reviewing the literature, it was found that tetrodotoxin halts action potentials by binding to sodium channel receptor sites, reacting with its glutamic acid components, and blocking the passage of sodium ions. While recent studies are still in progress, tetrodotoxin was found effective in treating neuropathic pain as an analgesic. Perhaps other therapeutic uses can be found in pathological nervous signaling such as seizures.

The metabolism provides energy through a collection of chemical reactions within the body's cells. In humans, biotin functions as a cofactor of enzymes involved in metabolic pathways such as gluconeogenesis, fatty acid synthesis, and amino acid catabolism. Thus, the regulation of biotin is important in the maintenance of metabolic homeostasis. To learn more about the sources of biotin deficiency, databases such as SciFinder and Web of Science were screened for journal articles and scientific papers that examine biotin's in carboxylation reactions. The literature reveals biotin availability is indirectly influenced by the availability of two compounds: biotinidase and holocarboxylase. Future research can explore how early biotin deficiency can be detected and whether its importance extends to all organisms.

Drug delivery is important in many aspects of medical and research industries. ZIF-8, a compound in the Zeolitic Imidazolate Framework, is porous and a metal organic framework (MOF). It can be used in gas delivery and drug delivery. The topic of how zeolitic imidazolate frameworks, especially ZIF-8, can be used for drug delivery was explored. After searching the literature, it was found that the compound ZIF-8 is relatively stable, and since it is stable in water and sensitive to changes in pH around it, it may be able to be utilized for drug delivery. Looking forward, is it possible to have ZIF-8 end up at selective locations in the body, and if so, how may this further the future of drug delivery?
Cancer kills millions of people each year. Topoisomerase, an enzyme that unwinds DNA and can potentially upset the integrity of the genome, is a common source of cancer growth. Thus, the inhibition of topoisomerase is a form of anti-cancer therapy, and there are many drugs that do this. However, Topotecan inhibits both topoisomerase I and topoisomerase II, which makes it more effective in preventing cancer growth than many other drugs that can only inhibit one type of topoisomerase. How is topotecan synthesized and what are the chemical features of this compound? In order to find this information, multiple databases such as Reaxys and SciFinder were utilized in order to consult the literature published about the compound. It was found that Topotecan is synthesized by first carrying out an aminoalkylation and amidoalkylation of an aromatic compound, which then underwent a hydroxylation at an aromatic carbon. This consistently gave a product with approximately 72% yield. Furthermore, topotecan is a chiral compound and is exclusively synthesized for the use of medical purposes into the (S) conformer, which allows it to be used to inhibit both Topoisomerase I and Topoisomerase II. It is a solid at standard temperature and pressure as it has high melting and boiling points, and it has an alcohol group that is the major reactor in almost all reactions involving this compound. The alcohol is deprotonated and the oxygen attacks various other molecules, creating a reaction. These results raise questions about the potential use of topotecan in other reactions that do not strictly include inhibiting topoisomerase and various proteins? Does topotecan have other uses?

Opioids are controlled substance used for pain-relief but can be harmful if consumed abusively. Researchers are seeking a new type of drug that creates the same pain-relieving effect but minimizes the resulting addiction. Epibatidine has been identified as a compound that could replace opioids since it can attach to the same neurotransmitters yet not cause a drastic level of addiction. Looking into different literatures, not enough research has been performed to determine how safe it is for human consumption. Future research should look into the viability of human research to see if epibatidine could be a new opioid.

Skin cancer is a common and potentially deadly form of cancer. Some compounds, such as octyl methoxycinnamate (OCM), can help absorb harmful UVB radiation that causes these skin cancers. However, this paper examined how OCM blocks UVB radiation. To answer this, a literature review
was conducted to find out the properties of OCM. It was found that OCM is an organic chemical absorber that absorbs UVB radiation specifically, with its maximum absorption around 290 nm. However, when exposed to light, OCM undergoes a configuration change, which alters the molecules ability to absorb light. Since this conformational change hinders the ability of OCM to absorb UVB radiation, it would be important to see in what ways sunscreen formulas seek to limit this conformational change.

1:22 – 1:33  Rhea Desouza  The Hidden Potential of Cinnamaldehyde

Pest infestation is a major problem for agriculture across the world. Every year 40% of global food production ($500 billion) is lost to crop diseases. Several efforts have been made to develop pesticides to battle this problem but now, natural compounds like cinnamaldehyde are being investigated. Until now, Cinnamaldehyde has only been known for its aromatic and flavorful cinnamon characteristic. This investigation was conducted to determine what anti-pathogenic properties cinnamaldehyde possessed and how these could be harnessed to be utilized to combat pests that affect crops. Literature was reviewed to find that cinnamaldehyde has a tremendous antimicrobial property but this power is limited by its volatility and rapid degradation due to its low melting point. To overcome this, labs are looking into methods to synthesize cinnamaldehyde accessibly. The investigation revealed that the essential oils of cinnamaldehyde can be captured in mesoporous silica nanoparticles (MSNPs), which are smart nanodevices that can be used to deliver drugs through targeted stimuli. This was tested on Pseudomonas syringae, the causative agent of pea bacterial blight, and demonstrated to increase the number of symptomless plants. These answers give rise to new questions regarding harnessing anti-pathogenic properties of several other volatile compounds like pyridines and purines through nanoparticles. Could cinnamaldehyde in the oxidized form of trans-cinnamic acid be better harnessed?
An Overview of the Chemical Effects of Tyramine on the body

Antidepressants are some of the most used drugs in America. One molecule that frequently causes dangerous side effects from antidepressants is tyramine. This presentation will examine the effects of tyramine, discussing the mechanisms of tyramine and how diet plays a critical role. I read biological and chemical journal articles to determine the effects of tyramine when it encounters antidepressants. When antidepressant inhibitors are in the block enzymes molecules like tyramine are not degraded. Tyramine then can cause high levels of adrenaline and raise blood pressure. The results of this study are very concerning for companies that produce MAOI antidepressants and the consumers who take them. These enzymes can cause a significant build-up of tyramine, which can be exasperated by a tyramine based diet.

Weighing the Positive and Negative Effects of Digitoxin

Heart disease is the leading cause of death in the United States, but drugs like digitoxin can help treat it. Digitoxin is a drug that specifically treats heart failure and rhythm problems. Some side effects may be dangerous for patients due to digitoxin’s physical and chemical properties. Several studies have shown how the structure and function of digitoxin can have both beneficial and negative side effects. Experiments show that digitoxin reduces cardiac impairment, but also reduces sodium and potassium sensibility. In addition to treating heart failure, digitoxin has been shown to induce apoptosis in cancer cells, an interesting medical implication for the future. With this in mind, there may be more diseases that digitoxin could have effects on for humans in the future.

Combatting Hydrocodone Overdose with Naloxone

Many drugs exist that relieve pain or suppress coughing, but hydrocodone is one medicine that can do both. As an opioid, however, hydrocodone is addictive, so the risks may outweigh those benefits. Naloxone, an opioid antagonist, can reverse hydrocodone overdoses. Is it effective enough to provide a solution to the opioid epidemic? This investigation analyzes recent scholarly articles involving naloxone and hydrocodone overdoses to determine their correlation and naloxone’s effectiveness. If administered swiftly, naloxone displaces hydrocodone from opioid receptors and takes its place, reversing the overdose effects. Naloxone is the best-in terms of effectiveness and usefulness-opioid antagonist available. Despite this fact,
naloxone has its flaws. Can this mechanism assist in creating a drug with a longer time period for administration after an overdose?

11:39 – 11:51 Alejandro Clare  Medicinal Properties of Lawson and its Derivatives

The Henna tattoo, composed of Lawson, is an art form that has roots reaching as far as 3400 BC, having wide usage in the Egyptian, Hindu, Muslim, and Moroccan cultures, which also has a well-documented folklore history for treating maladies. Through this research paper the medical implications of lawson and its synthetic derivatives, naphthoquinone analogues, are explored. Scientific literature will be consulted order to answer the inquiry. Pharmaceuticals synthesized from Lawson and its synthetic derivatives, such as the amino-naphthoquinone and Alkyl derivatives, have pharmacological implications, including antioxidant, anti-cancer, antibiotic and antiparasitic activity, as well as wound healing of numerous skin disorders. Naphthoquinones can act as electrophiles to form covalent bonds with nucleophilic groups, as well as undergo reversible oxidation-reduction reactions in order to interact with biological targets by forming highly reactive anions. One can add substituents to the compounds to modify their capability to accept electrons, as well as modify the chemical environment to control their reactivity. The incorporation of amino groups results in stronger activity against cancer and microorganisms. Despite the evident medicinal advantages of Lawson, and its derivatives, it poses a health risk if exposed to the compound in a large dosage, as found by a toxicity study of Henna. The question now is, what would be proper dosage of Lawson based medicine to both treat the sicknesses and avoid its toxic properties?

6 December 2018

12:30 – 12:42 Joseph Mullen  Understanding Ferrocene’s Method of Chemotherapy Drug Delivery

While surgery and radiation are viable cancer therapies, chemotherapy is an increasingly important option. In particular, ferrocene is an organometallic molecule that effectively delivers drugs to cancer cells. This research focuses on Ferrocene’s drug delivery method to cancer cells and its alternative medical applications. This presentation’s resources were obtained through a comprehensive review of the literature on Ferrocene’s medical uses to date, especially drug delivery. Ferrocene is an electronically stable molecule with filled s-, p- and d-orbitals and surprisingly minor steric issues. This electron-rich molecule has the versatility and resonance to stabilize while attaching to many different sites, supporting drug delivery by assisting the approach to cancer cells. However, this research raises questions about how ferrocene avoids steric issues at small, specific cellular delivery sites.
Deficiencies of vitamins, or vital molecules which are not synthesized in the body, can be very harmful. Thiamin, or vitamin B1, plays many vital roles in the body, one important of which is aiding lipid and carbohydrate metabolism. This research focuses on the chemical properties that allow thiamin to fulfill this role. Information about thiamin and its biochemical properties were collected from the extensive literature on the topic. The research showed that thiamin plays an important role in the body’s metabolism, through production of Acetyl-CoA from pyruvate. The research also raises further questions about other functions of the versatile molecule.

Saccharin’s ability to be 300 times sweeter than sucrose has made it a popular choice for food companies. I will investigate the history of the formation of saccharin and the chemical reason why it is so much sweeter than sucrose. I can use scientific articles to determine what makes certain molecules sweet, and what makes saccharin especially so sweet. The reason why saccharin is so much sweeter than sucrose is because it follows the AH-B-X rule of sweetness, while sucrose only satisfies the AH-B rule. A further question is if it is possible to take saccharin and make it sweeter instead of using other molecules with it for increased sweetness.

In the agricultural industry synthetic herbicides are often used with great success; however, they come with certain drawbacks, such as causing herbicide resistant weeds. Juglone is a natural herbicide found in the black walnut tree that could potentially solve the issues of synthetic herbicides. This investigation sought to discover how juglone acts like a natural herbicide, and its consequences. By searching the literature, it was found that juglone inhibits plant growth by impairing root and leaf respiration of other plants through inhibiting RNA polymerase II. However, it is not commonly used because it fails against certain weed species. Future research could determine why juglone only works as an herbicide on some plant species.